



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 10:56 PM UTC

PDB ID : 9I4T / pdb_00009i4t
EMDB ID : EMD-52620
Title : Photosystem II from Arabidopsis thaliana
Authors : Forsman, J.A.; Graca, A.T.; Hussein, R.; Hall, M.; Messinger, J.; Schroder, W.P.; Aydin, A.O.
Deposited on : 2025-01-26
Resolution : 2.44 Å(reported)
Based on initial model : 3JCU

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:

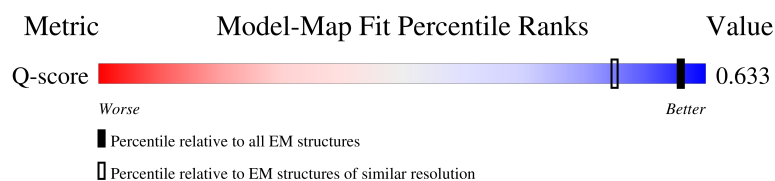
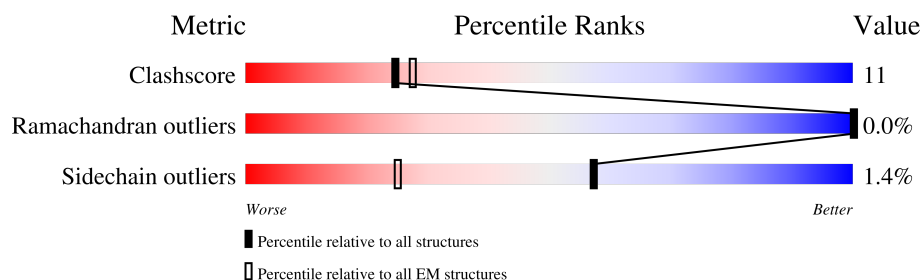
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.44 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.






















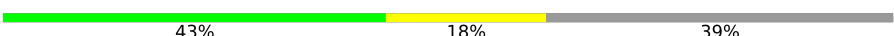





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5856 (1.94 - 2.94)

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

Mol	Chain	Length	Quality of chain
1	A	353	
1	a	353	
2	B	508	
2	b	508	


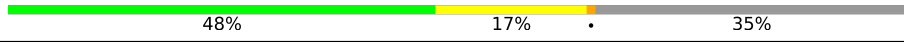
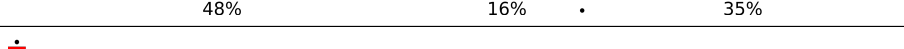




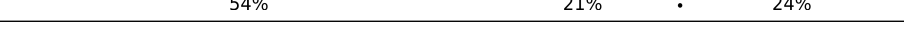








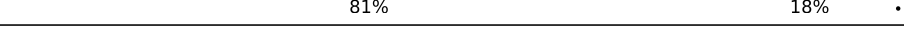
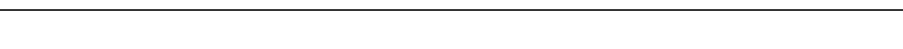
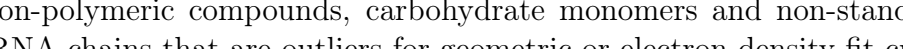

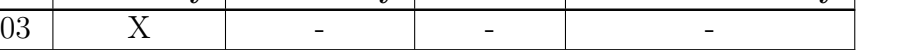
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	473	
3	c	473	
4	D	353	
4	d	353	
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	G	267	
7	N	267	
7	g	267	
7	n	267	
8	H	73	
8	h	73	
9	I	36	
9	i	36	
10	J	40	
10	j	40	
11	K	61	
11	k	61	
12	L	38	
12	l	38	
13	M	34	
13	m	34	
14	O	332	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	o	332	
15	P	263	
15	p	263	
16	Q	224	
16	q	224	
17	R	290	
17	r	290	
18	S	280	
18	s	280	
19	T	33	
19	t	33	
20	U	103	
20	u	103	
21	W	133	
21	w	133	
22	X	116	
22	x	116	
23	Y	265	
23	y	265	
24	Z	62	
24	z	62	

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
26	CLA	A	403	X	-	-	-
26	CLA	A	405	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	B	601	X	-	-	-
26	CLA	B	602	X	-	-	-
26	CLA	B	603	X	-	-	-
26	CLA	B	604	X	-	-	-
26	CLA	B	605	X	-	-	-
26	CLA	B	606	X	-	-	-
26	CLA	B	607	X	-	-	-
26	CLA	B	609	X	-	-	-
26	CLA	B	610	X	-	-	-
26	CLA	B	611	X	-	-	-
26	CLA	B	612	X	-	-	-
26	CLA	B	613	X	-	-	-
26	CLA	B	615	X	-	-	-
26	CLA	B	616	X	-	-	-
26	CLA	B	617	X	-	-	-
26	CLA	B	618	X	-	-	-
26	CLA	C	504	X	-	-	-
26	CLA	C	505	X	-	-	-
26	CLA	C	506	X	-	-	-
26	CLA	C	507	X	-	-	-
26	CLA	C	508	X	-	-	-
26	CLA	C	511	X	-	-	-
26	CLA	C	512	X	-	-	-
26	CLA	C	515	X	-	-	-
26	CLA	C	516	X	-	-	-
26	CLA	C	517	X	-	-	-
26	CLA	C	519	X	-	-	-
26	CLA	C	520	X	-	-	-
26	CLA	C	521	X	-	-	-
26	CLA	D	401	X	-	-	-
26	CLA	D	406	X	-	-	-
26	CLA	D	409	X	-	-	-
26	CLA	D	412	X	-	-	-
26	CLA	G	302	X	-	-	-
26	CLA	G	304	X	-	-	-
26	CLA	G	306	X	-	-	-
26	CLA	G	307	X	-	-	-
26	CLA	G	313	X	-	-	-
26	CLA	G	314	X	-	-	-
26	CLA	G	317	X	-	-	-
26	CLA	G	319	X	-	-	-
26	CLA	N	306	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	N	307	X	-	-	-
26	CLA	N	308	X	-	-	-
26	CLA	N	309	X	-	-	-
26	CLA	N	312	X	-	-	-
26	CLA	N	313	X	-	-	-
26	CLA	N	318	X	-	-	-
26	CLA	N	319	X	-	-	-
26	CLA	R	302	X	-	-	-
26	CLA	R	306	X	-	-	-
26	CLA	R	308	X	-	-	-
26	CLA	R	309	X	-	-	-
26	CLA	R	310	X	-	-	-
26	CLA	R	313	X	-	-	-
26	CLA	R	314	X	-	-	-
26	CLA	R	316	X	-	-	-
26	CLA	R	317	X	-	-	-
26	CLA	S	303	X	-	-	-
26	CLA	S	304	X	-	-	-
26	CLA	S	307	X	-	-	-
26	CLA	S	308	X	-	-	-
26	CLA	S	309	X	-	-	-
26	CLA	S	310	X	-	-	-
26	CLA	S	311	X	-	-	-
26	CLA	S	314	X	-	-	-
26	CLA	S	315	X	-	-	-
26	CLA	Y	301	X	-	-	-
26	CLA	Y	305	X	-	-	-
26	CLA	Y	308	X	-	-	-
26	CLA	Y	310	X	-	-	-
26	CLA	Y	311	X	-	-	-
26	CLA	Y	312	X	-	-	-
26	CLA	Y	313	X	-	-	-
26	CLA	Y	316	X	-	-	-
26	CLA	a	402	X	-	-	-
26	CLA	a	409	X	-	-	-
26	CLA	a	411	X	-	-	-
26	CLA	b	601	X	-	-	-
26	CLA	b	602	X	-	-	-
26	CLA	b	604	X	-	-	-
26	CLA	b	605	X	-	-	-
26	CLA	b	606	X	-	-	-
26	CLA	b	607	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	b	608	X	-	-	-
26	CLA	b	609	X	-	-	-
26	CLA	b	610	X	-	-	-
26	CLA	b	611	X	-	-	-
26	CLA	b	612	X	-	-	-
26	CLA	b	613	X	-	-	-
26	CLA	b	614	X	-	-	-
26	CLA	b	616	X	-	-	-
26	CLA	b	617	X	-	-	-
26	CLA	b	618	X	-	-	-
26	CLA	c	502	X	-	-	-
26	CLA	c	503	X	-	-	-
26	CLA	c	504	X	-	-	-
26	CLA	c	505	X	-	-	-
26	CLA	c	506	X	-	-	-
26	CLA	c	508	X	-	-	-
26	CLA	c	510	X	-	-	-
26	CLA	c	513	X	-	-	-
26	CLA	c	514	X	-	-	-
26	CLA	c	515	X	-	-	-
26	CLA	c	516	X	-	-	-
26	CLA	c	518	X	-	-	-
26	CLA	c	520	X	-	-	-
26	CLA	d	403	X	-	-	-
26	CLA	d	404	X	-	-	-
26	CLA	d	411	X	-	-	-
26	CLA	g	302	X	-	-	-
26	CLA	g	303	X	-	-	-
26	CLA	g	304	X	-	-	-
26	CLA	g	305	X	-	-	-
26	CLA	g	308	X	-	-	-
26	CLA	g	315	X	-	-	-
26	CLA	g	317	X	-	-	-
26	CLA	g	318	X	-	-	-
26	CLA	n	302	X	-	-	-
26	CLA	n	303	X	-	-	-
26	CLA	n	304	X	-	-	-
26	CLA	n	305	X	-	-	-
26	CLA	n	309	X	-	-	-
26	CLA	n	310	X	-	-	-
26	CLA	n	312	X	-	-	-
26	CLA	n	315	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	r	303	X	-	-	-
26	CLA	r	305	X	-	-	-
26	CLA	r	306	X	-	-	-
26	CLA	r	308	X	-	-	-
26	CLA	r	310	X	-	-	-
26	CLA	r	311	X	-	-	-
26	CLA	r	313	X	-	-	-
26	CLA	r	314	X	-	-	-
26	CLA	r	315	X	-	-	-
26	CLA	r	317	X	-	-	-
26	CLA	s	301	X	-	-	-
26	CLA	s	304	X	-	-	-
26	CLA	s	305	X	-	-	-
26	CLA	s	306	X	-	-	-
26	CLA	s	307	X	-	-	-
26	CLA	s	310	X	-	-	-
26	CLA	s	311	X	-	-	-
26	CLA	s	314	X	-	-	-
26	CLA	s	315	X	-	-	-
26	CLA	y	304	X	-	-	-
26	CLA	y	306	X	-	-	-
26	CLA	y	309	X	-	-	-
26	CLA	y	310	X	-	-	-
26	CLA	y	313	X	-	-	-
26	CLA	y	315	X	-	-	-
26	CLA	y	316	X	-	-	-
26	CLA	y	317	X	-	-	-
39	CHL	G	301	X	-	-	-
39	CHL	G	303	X	-	-	-
39	CHL	G	305	X	-	-	-
39	CHL	G	309	X	-	-	-
39	CHL	G	311	X	-	-	-
39	CHL	G	318	X	-	-	-
39	CHL	N	303	X	-	-	-
39	CHL	N	304	X	-	-	-
39	CHL	N	310	X	-	-	-
39	CHL	N	311	X	-	-	-
39	CHL	N	316	X	-	-	-
39	CHL	N	317	X	-	-	-
39	CHL	R	301	X	-	-	-
39	CHL	R	312	X	-	-	-
39	CHL	R	315	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CHL	R	318	X	-	-	-
39	CHL	S	302	X	-	-	-
39	CHL	S	312	X	-	-	-
39	CHL	S	313	X	-	-	-
39	CHL	S	316	X	-	-	-
39	CHL	Y	302	X	-	-	-
39	CHL	Y	307	X	-	-	-
39	CHL	Y	314	X	-	-	-
39	CHL	Y	317	X	-	-	-
39	CHL	Y	318	X	-	-	-
39	CHL	g	307	X	-	-	-
39	CHL	g	311	X	-	-	-
39	CHL	g	312	X	-	-	-
39	CHL	g	313	X	-	-	-
39	CHL	g	314	X	-	-	-
39	CHL	g	319	X	-	-	-
39	CHL	n	306	X	-	-	-
39	CHL	n	307	X	-	-	-
39	CHL	n	308	X	-	-	-
39	CHL	n	311	X	-	-	-
39	CHL	n	318	X	-	-	-
39	CHL	n	319	X	-	-	-
39	CHL	r	301	X	-	-	-
39	CHL	r	309	X	-	-	-
39	CHL	r	316	X	-	-	-
39	CHL	r	318	X	-	-	-
39	CHL	s	303	X	-	-	-
39	CHL	s	313	X	-	-	-
39	CHL	s	316	X	-	-	-
39	CHL	s	317	X	-	-	-
39	CHL	y	302	X	-	-	-
39	CHL	y	303	X	-	-	-
39	CHL	y	305	X	-	-	-
39	CHL	y	312	X	-	-	-
39	CHL	y	314	X	-	-	-

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 76824 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2613	1707	430	463	13		
1	a	334	Total	C	N	O	S	0	0
			2613	1707	430	463	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	485	Total	C	N	O	S	0	0
			3800	2489	642	657	12		
2	b	485	Total	C	N	O	S	0	0
			3800	2489	642	657	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	447	Total	C	N	O	S	0	0
			3468	2279	579	599	11		
3	c	447	Total	C	N	O	S	0	0
			3468	2279	579	599	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2713	1795	444	462	12		
4	d	341	Total	C	N	O	S	0	0
			2713	1795	444	462	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	74	Total	C	N	O	0	0
			604	395	99	110		
5	e	74	Total	C	N	O	0	0
			604	395	99	110		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
6	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	33	PHE	SER	variant	UNP P62095
f	33	PHE	SER	variant	UNP P62095

- Molecule 7 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	211	Total	C	N	O	S	0	0
			1606	1037	264	300	5		
7	N	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		
7	g	211	Total	C	N	O	S	0	0
			1606	1037	264	300	5		
7	n	202	Total	C	N	O	S	0	0
			1536	994	251	286	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total	C	N	O	S	0	0
			438	289	68	79	2		
8	h	59	Total	C	N	O	S	0	0
			438	289	68	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			266	184	39	42	1		
9	i	33	Total	C	N	O	S	0	0
			266	184	39	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	35	Total	C	N	O		0	0
			255	174	39	42			
10	j	35	Total	C	N	O		0	0
			255	174	39	42			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			302	211	44	46	1		
11	k	37	Total	C	N	O	S	0	0
			302	211	44	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	35	Total	C	N	O		0	0
			293	195	45	53			
12	l	35	Total	C	N	O		0	0
			293	195	45	53			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	31	Total	C	N	O		0	0
			242	168	34	40			
13	m	31	Total	C	N	O		0	0
			242	168	34	40			

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	241	Total	C	N	O	S	0	0
			1829	1157	297	371	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	241	Total	C	N	O	S	0	0
			1829	1157	297	371	4		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	171	Total	C	N	O	S	0	0
			1319	836	217	264	2		
15	p	171	Total	C	N	O	S	0	0
			1319	836	217	264	2		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	146	Total	C	N	O	S	0	0
			1139	726	193	220			
16	q	146	Total	C	N	O	S	0	0
			1139	726	193	220			

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	220	Total	C	N	O	S	0	0
			1710	1109	281	317	3		
17	r	220	Total	C	N	O	S	0	0
			1710	1109	281	317	3		

- Molecule 18 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		
18	s	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	32	Total	C	N	O	S	0	0
			261	181	37	42	1		
19	t	32	Total	C	N	O	S	0	0
			261	181	37	42	1		

- Molecule 20 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	28	Total	C	N	O	S	0	0
			219	138	40	38	3		
20	u	28	Total	C	N	O	S	0	0
			219	138	40	38	3		

- Molecule 21 is a protein called Photosystem II reaction center W protein, chloroplastic.

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

- Molecule 22 is a protein called Expressed protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	39	Total	C	N	O	0	0
			279	183	46	50		
22	x	39	Total	C	N	O	0	0
			279	183	46	50		

- Molecule 23 is a protein called Chlorophyll a-b binding protein 2.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	214	Total	C	N	O	S	0	0
			1652	1075	265	307	5		
23	y	214	Total	C	N	O	S	0	0
			1652	1075	265	307	5		

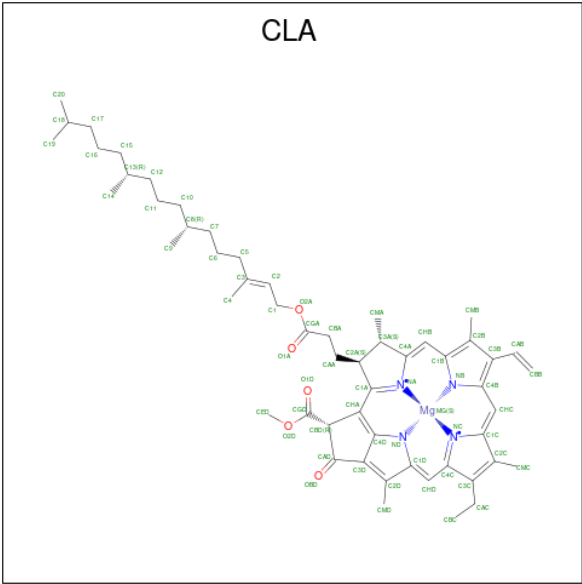
- Molecule 24 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Z	61	Total	C	N	O	0	0
			456	308	68	80		
24	z	61	Total	C	N	O	0	0
			456	308	68	80		

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	C	1	Total 64	C 55	Mg 1	N 3	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
26	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Y	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 64	C 55	Mg 1	N 3	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

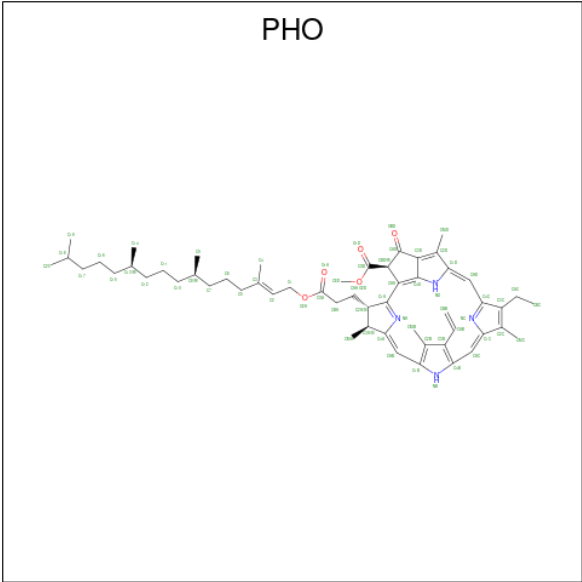
Mol	Chain	Residues	Atoms					AltConf
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	r	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	r	1	Total 49	C 39	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

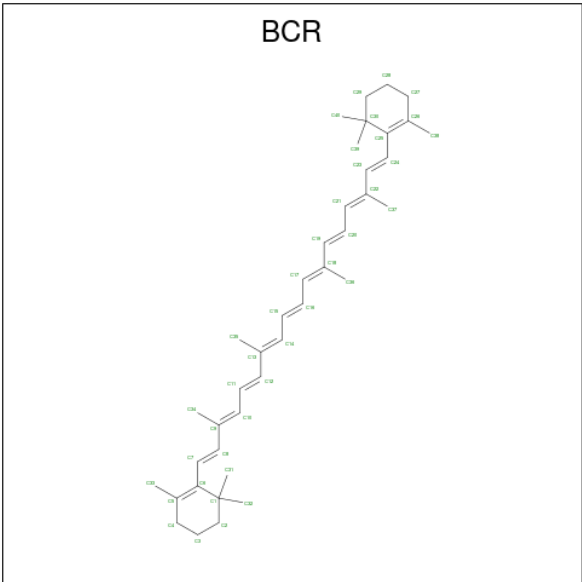
Mol	Chain	Residues	Atoms					AltConf
26	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	y	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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



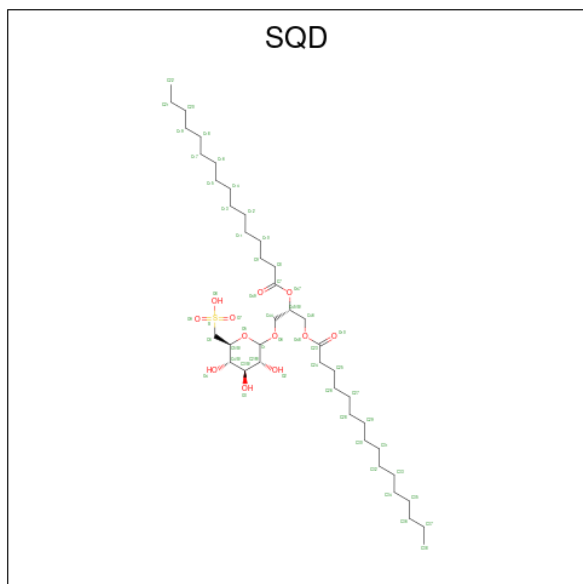
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	D	1	Total	C	N	O	0
			64	55	4	5	
27	a	1	Total	C	N	O	0
			64	55	4	5	
27	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



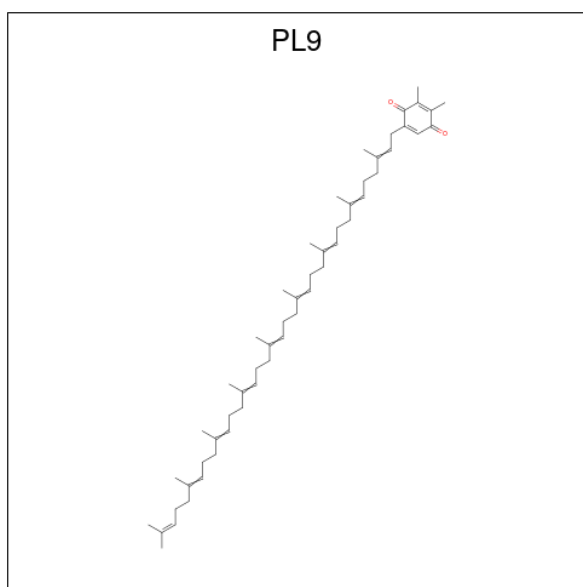
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	C	1	Total C 40 40	0
28	C	1	Total C 40 40	0
28	D	1	Total C 40 40	0
28	H	1	Total C 40 40	0
28	J	1	Total C 40 40	0
28	K	1	Total C 40 40	0
28	T	1	Total C 40 40	0
28	a	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	c	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	j	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	t	1	Total C 40 40	0

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	S	0
			54	41	12	1	
29	A	1	Total	C	O	S	0
			50	37	12	1	
29	B	1	Total	C	O	S	0
			54	41	12	1	
29	W	1	Total	C	O	S	0
			33	20	12	1	
29	a	1	Total	C	O	S	0
			54	41	12	1	
29	a	1	Total	C	O	S	0
			50	37	12	1	
29	b	1	Total	C	O	S	0
			54	41	12	1	
29	w	1	Total	C	O	S	0
			33	20	12	1	

- Molecule 30 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: $C_{53}H_{80}O_2$).

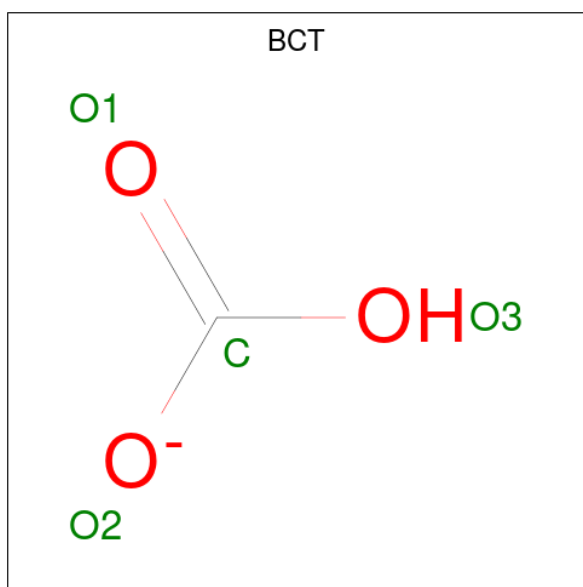


Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			22	20	2	
30	D	1	Total	C	O	0
			55	53	2	
30	a	1	Total	C	O	0
			22	20	2	
30	d	1	Total	C	O	0
			55	53	2	

- Molecule 31 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

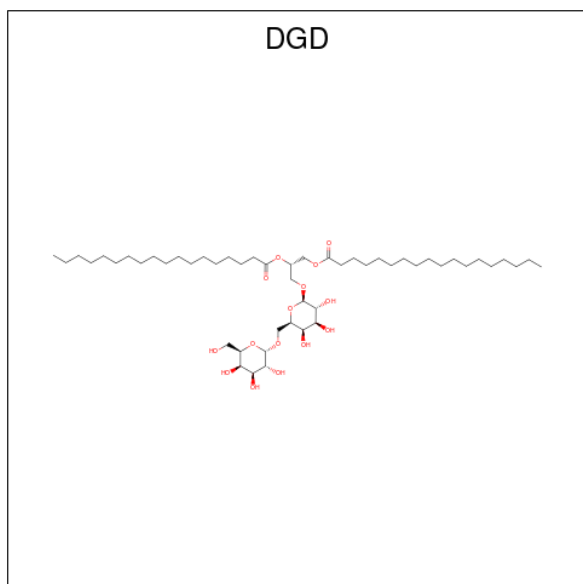
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	Fe	0
			1	1	
31	a	1	Total	Fe	0
			1	1	

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



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

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



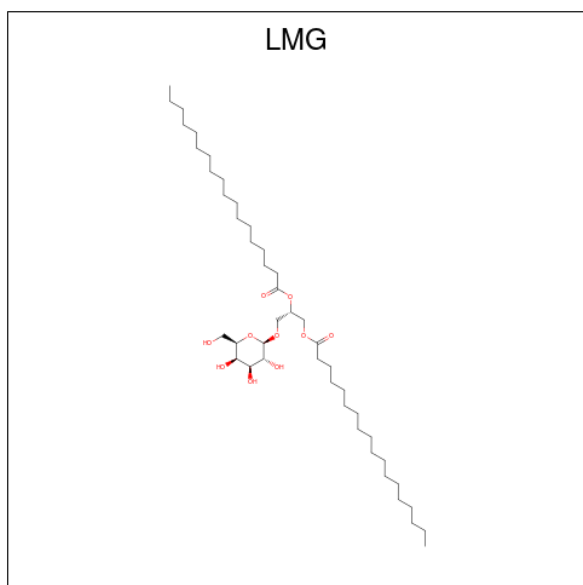
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			62	47	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			55	40	15	
33	C	1	Total	C	O	0
			62	47	15	
33	C	1	Total	C	O	0
			62	47	15	
33	Y	1	Total	C	O	0
			43	28	15	
33	b	1	Total	C	O	0
			62	47	15	
33	c	1	Total	C	O	0
			62	47	15	
33	c	1	Total	C	O	0
			55	40	15	
33	c	1	Total	C	O	0
			62	47	15	
33	y	1	Total	C	O	0
			43	28	15	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



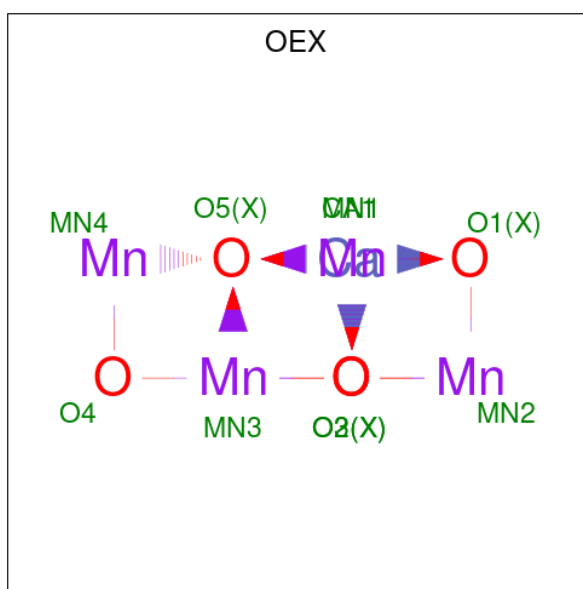
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			51	41	10	
34	C	1	Total	C	O	0
			51	41	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			51	41	10	
34	D	1	Total	C	O	0
			46	36	10	
34	W	1	Total	C	O	0
			48	38	10	
34	b	1	Total	C	O	0
			51	41	10	
34	c	1	Total	C	O	0
			51	41	10	
34	c	1	Total	C	O	0
			51	41	10	
34	d	1	Total	C	O	0
			46	36	10	
34	w	1	Total	C	O	0
			48	38	10	

- Molecule 35 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
35	C	1	Total	Ca	Mn	O	0
			10	1	4	5	
35	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 36 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total 35	C 24	O 11	0
36	d	1	Total 35	C 24	O 11	0

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



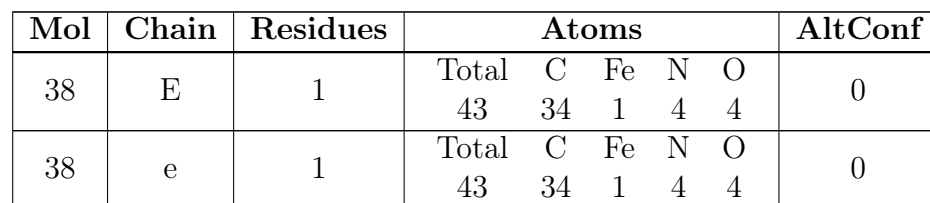
Mol	Chain	Residues	Atoms				AltConf
37	D	1	Total	C	O	P	0
			43	32	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
37	D	1	Total	C	O	P	0
			49	38	10	1	
37	D	1	Total	C	O	P	0
			37	26	10	1	
37	G	1	Total	C	O	P	0
			49	38	10	1	
37	L	1	Total	C	O	P	0
			49	38	10	1	
37	N	1	Total	C	O	P	0
			49	38	10	1	
37	R	1	Total	C	O	P	0
			49	38	10	1	
37	S	1	Total	C	O	P	0
			49	38	10	1	
37	Y	1	Total	C	O	P	0
			49	38	10	1	
37	d	1	Total	C	O	P	0
			43	32	10	1	
37	d	1	Total	C	O	P	0
			49	38	10	1	
37	d	1	Total	C	O	P	0
			37	26	10	1	
37	g	1	Total	C	O	P	0
			49	38	10	1	
37	l	1	Total	C	O	P	0
			49	38	10	1	
37	n	1	Total	C	O	P	0
			49	38	10	1	
37	r	1	Total	C	O	P	0
			49	38	10	1	
37	s	1	Total	C	O	P	0
			49	38	10	1	
37	y	1	Total	C	O	P	0
			49	38	10	1	

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



- # CHL

Mol	Chain	Residues	Atoms						AltConf
39	G	1	Total 50	C 39	Mg 1	N 4	O 6	0	
39	G	1	Total 50	C 39	Mg 1	N 4	O 6	0	



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	G	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	N	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	R	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	S	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
39	S	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	S	1	Total 52	C 41	Mg 1	N 4	O 6	0
39	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

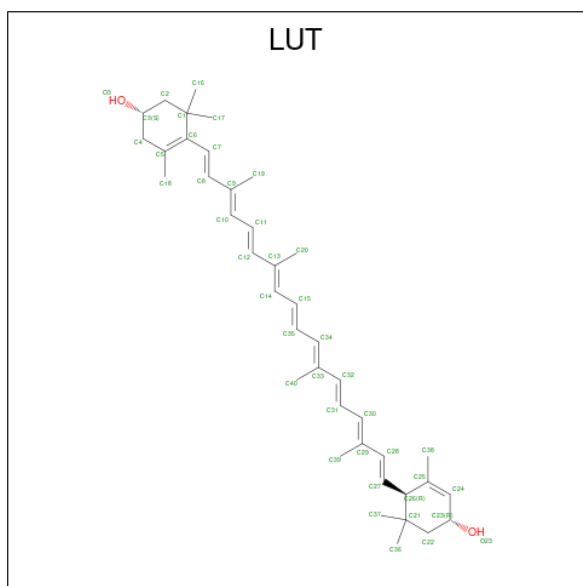
Mol	Chain	Residues	Atoms					AltConf
39	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	n	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
39	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	r	1	Total 48	C 37	Mg 1	N 4	O 6	0
39	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	r	1	Total 50	C 39	Mg 1	N 4	O 6	0
39	s	1	Total 52	C 41	Mg 1	N 4	O 6	0
39	s	1	Total 49	C 38	Mg 1	N 4	O 6	0
39	s	1	Total 50	C 39	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
39	s	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
39	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 40 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



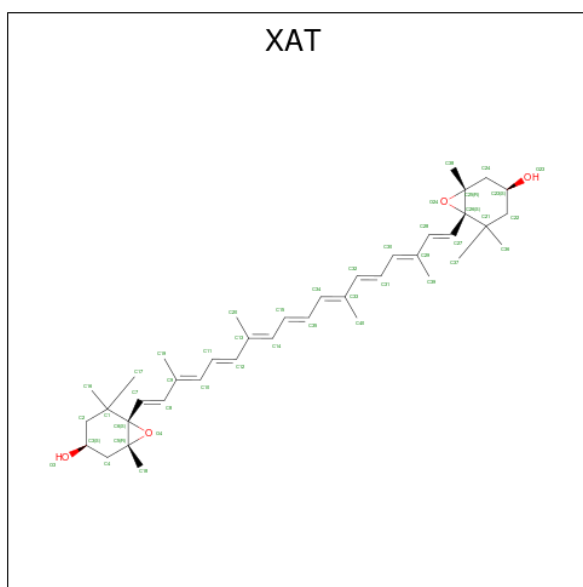
Mol	Chain	Residues	Atoms				AltConf
40	G	1	Total	C	O		0
			42	40	2		
40	G	1	Total	C	O		0
			42	40	2		
40	N	1	Total	C	O		0
			42	40	2		
40	N	1	Total	C	O		0
			42	40	2		
40	R	1	Total	C	O		0
			42	40	2		

Continued on next page...

Continued from previous page...

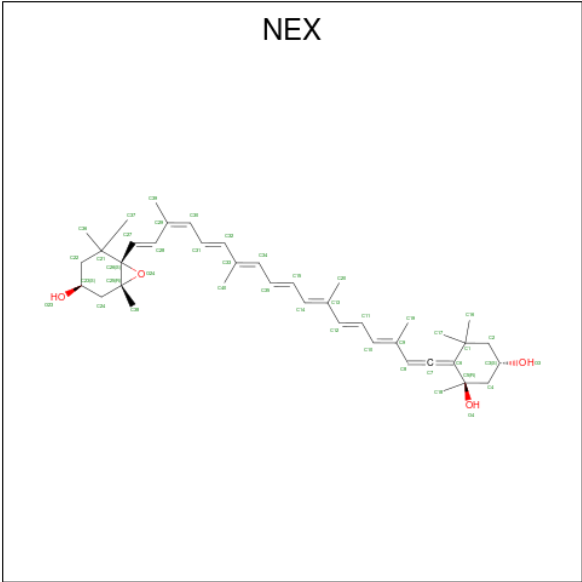
Mol	Chain	Residues	Atoms			AltConf
40	S	1	Total	C	O	0
			42	40	2	
40	S	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
40	Y	1	Total	C	O	0
			42	40	2	
40	g	1	Total	C	O	0
			42	40	2	
40	g	1	Total	C	O	0
			42	40	2	
40	n	1	Total	C	O	0
			42	40	2	
40	n	1	Total	C	O	0
			42	40	2	
40	r	1	Total	C	O	0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

- 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	G	1	Total	C	O	0
			44	40	4	
41	G	1	Total	C	O	0
			44	40	4	
41	N	1	Total	C	O	0
			44	40	4	
41	R	1	Total	C	O	0
			44	40	4	
41	g	1	Total	C	O	0
			44	40	4	
41	g	1	Total	C	O	0
			44	40	4	
41	n	1	Total	C	O	0
			44	40	4	
41	r	1	Total	C	O	0
			44	40	4	

- Molecule 42 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



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

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
43	A	82	Total	O	0
			82	82	
43	B	115	Total	O	0
			115	115	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
43	C	104	Total 104	O 104	0
43	D	78	Total 78	O 78	0
43	E	19	Total 19	O 19	0
43	F	3	Total 3	O 3	0
43	G	5	Total 5	O 5	0
43	H	15	Total 15	O 15	0
43	I	6	Total 6	O 6	0
43	J	4	Total 4	O 4	0
43	K	5	Total 5	O 5	0
43	L	9	Total 9	O 9	0
43	M	3	Total 3	O 3	0
43	N	5	Total 5	O 5	0
43	O	39	Total 39	O 39	0
43	P	17	Total 17	O 17	0
43	Q	1	Total 1	O 1	0
43	R	19	Total 19	O 19	0
43	S	5	Total 5	O 5	0
43	T	7	Total 7	O 7	0
43	U	1	Total 1	O 1	0
43	W	18	Total 18	O 18	0
43	X	5	Total 5	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
43	Y	36	Total 36	O 36	0
43	Z	2	Total 2	O 2	0
43	a	90	Total 90	O 90	0
43	b	114	Total 114	O 114	0
43	c	100	Total 100	O 100	0
43	d	76	Total 76	O 76	0
43	e	19	Total 19	O 19	0
43	f	3	Total 3	O 3	0
43	g	5	Total 5	O 5	0
43	h	15	Total 15	O 15	0
43	i	6	Total 6	O 6	0
43	j	4	Total 4	O 4	0
43	k	5	Total 5	O 5	0
43	l	9	Total 9	O 9	0
43	m	3	Total 3	O 3	0
43	n	5	Total 5	O 5	0
43	o	38	Total 38	O 38	0
43	p	17	Total 17	O 17	0
43	q	1	Total 1	O 1	0
43	r	19	Total 19	O 19	0
43	s	5	Total 5	O 5	0

Continued on next page...

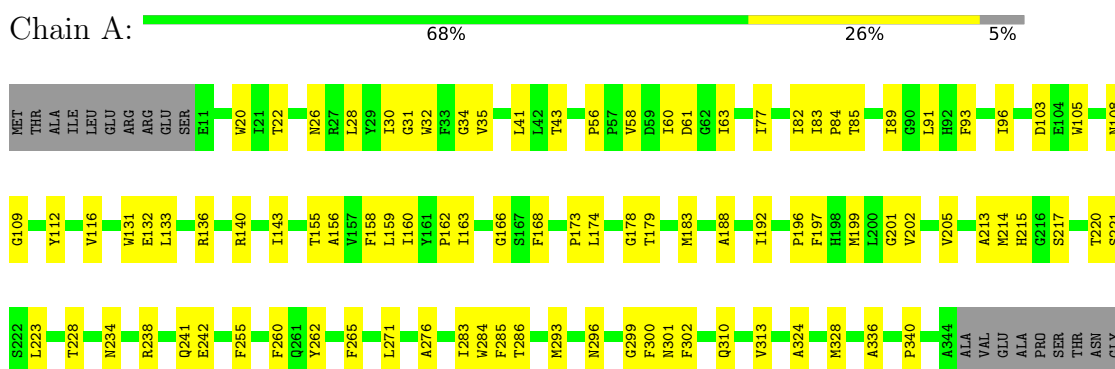
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
43	t	7	Total 7	O 7	0
43	u	1	Total 1	O 1	0
43	w	18	Total 18	O 18	0
43	x	5	Total 5	O 5	0
43	y	36	Total 36	O 36	0
43	z	2	Total 2	O 2	0

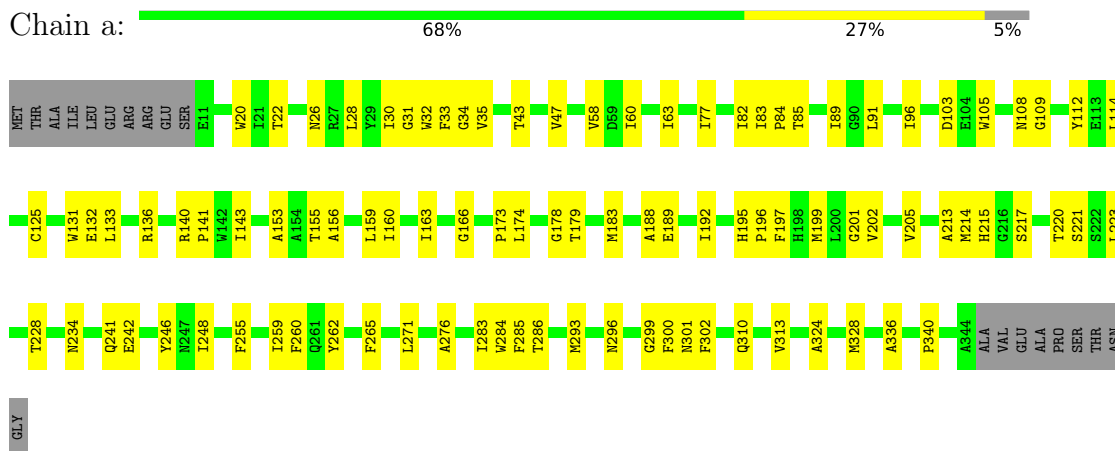
3 Residue-property plots

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

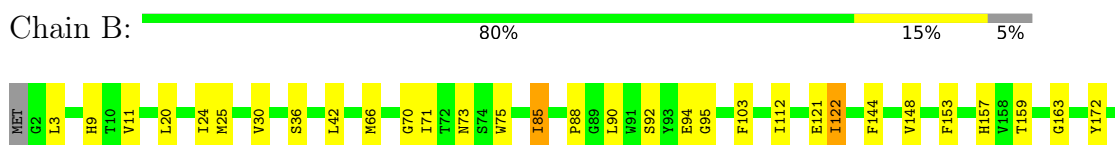
• Molecule 1: Photosystem II protein D1

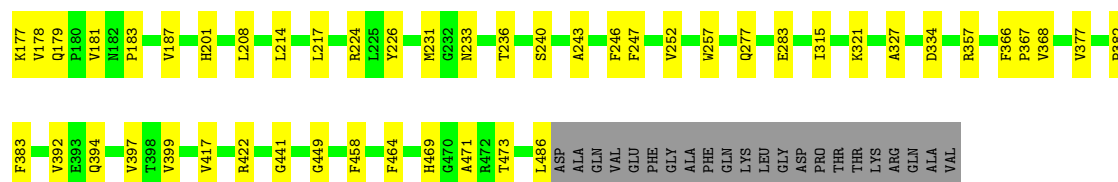


• Molecule 1: Photosystem II protein D1



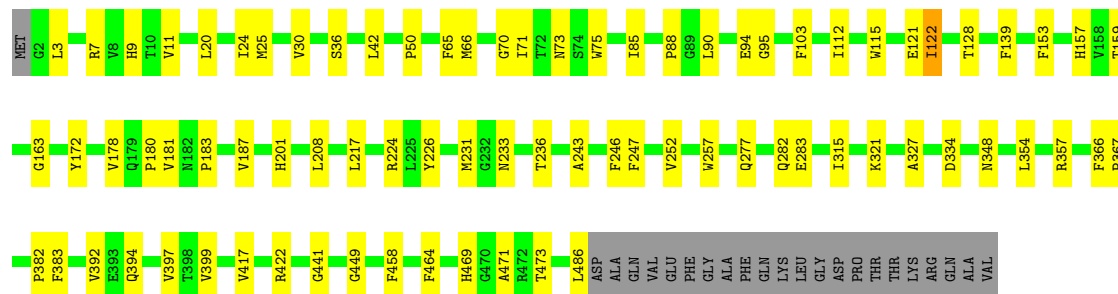
• Molecule 2: Photosystem II CP47 reaction center protein





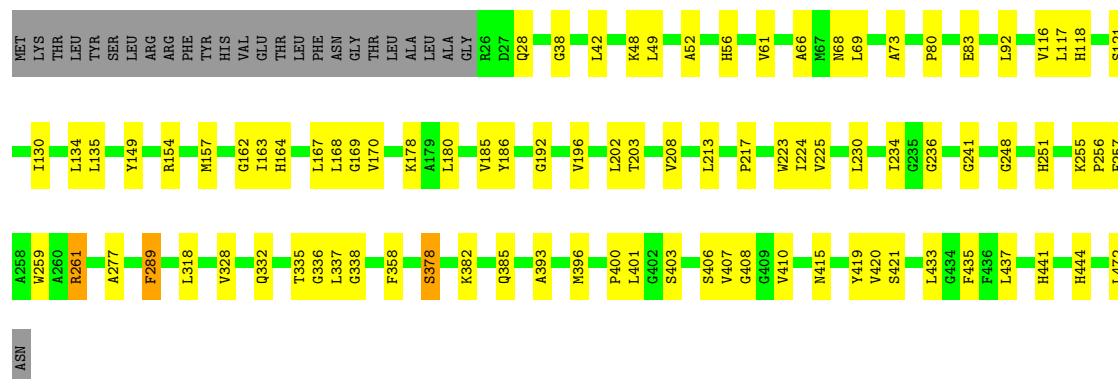
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 80% 16% 5%



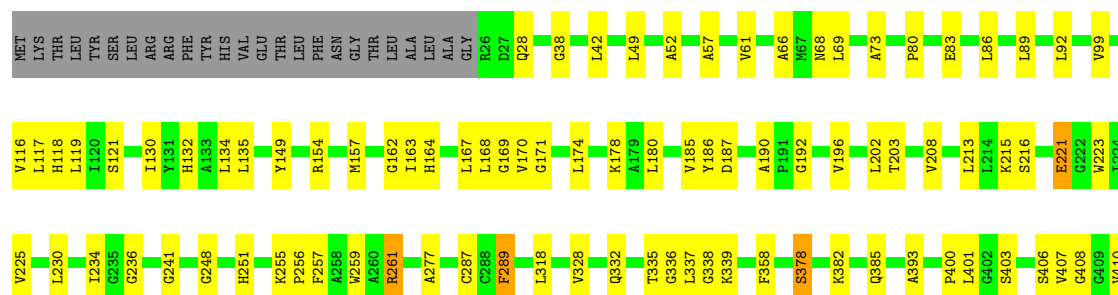
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 76% 18% 5%



• Molecule 3: Photosystem II CP43 reaction center protein

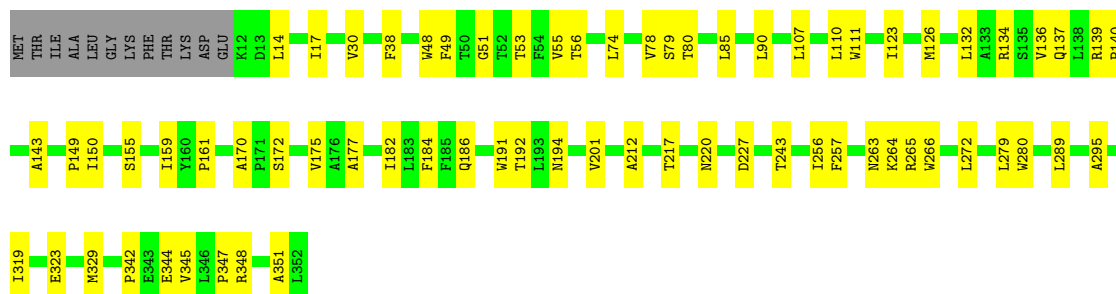
Chain c: 74% 20% 5%





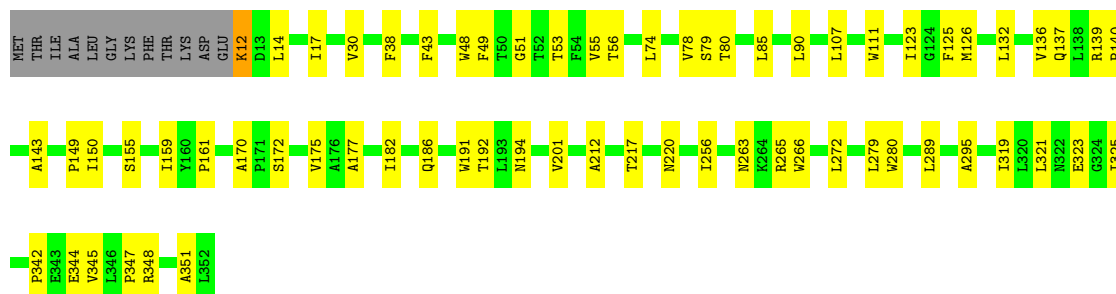
- Molecule 4: Photosystem II D2 protein

Chain D: 77% 20% .



- Molecule 4: Photosystem II D2 protein

Chain d: 78% 18% .



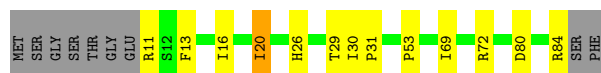
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 72% 17% 11%



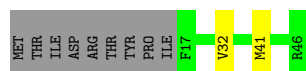
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 73% 14% 11%



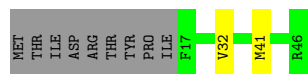
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 72% 5% 23%



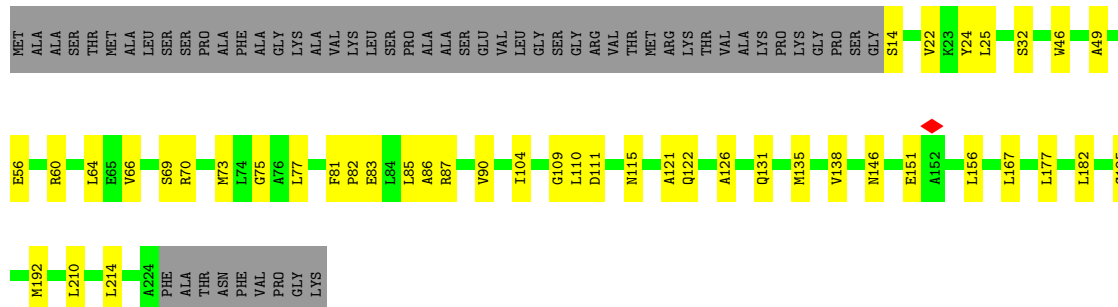
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  72% 5% 23%



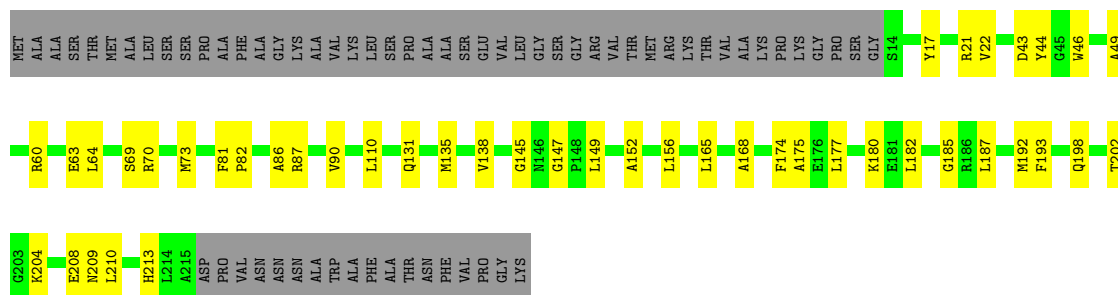
- Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain G:  63% 16% 21%



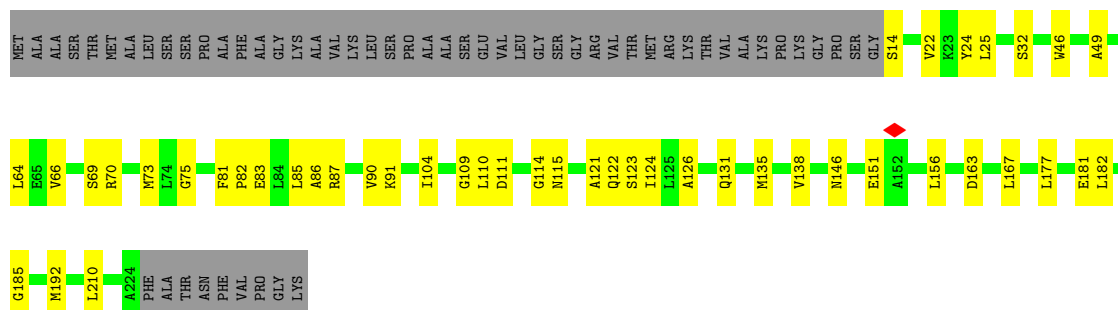
- Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain N:  59% 17% 24%



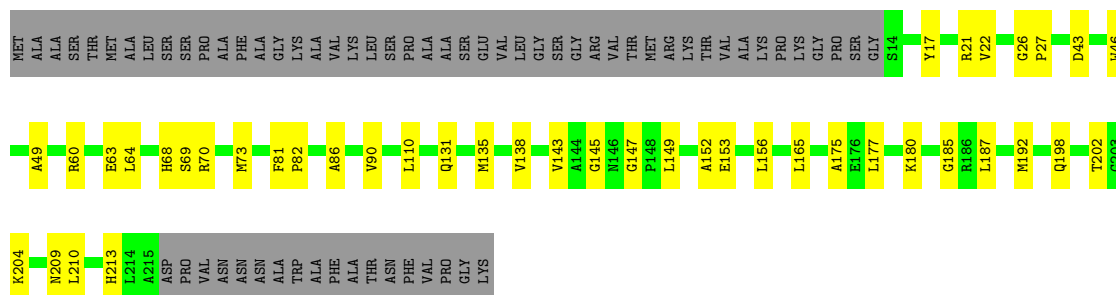
- Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain g:  62% 17% 21%



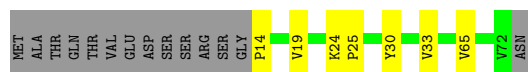
- Molecule 7: Chlorophyll a-b binding protein 1, chloroplastic

Chain n:  60% 16% 24%



• Molecule 8: Photosystem II reaction center protein H

Chain H:  71% 10% 19%




• Molecule 8: Photosystem II reaction center protein H

Chain h:  71% 10% 19%




• Molecule 9: Photosystem II reaction center protein I

Chain I:  86% 6% 8%




• Molecule 9: Photosystem II reaction center protein I

Chain i:  86% 6% 8%




• Molecule 10: Photosystem II reaction center protein J

Chain J:  82% 5% 12%



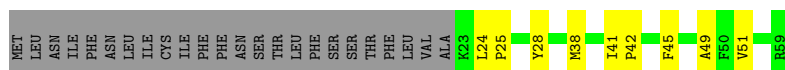
• Molecule 10: Photosystem II reaction center protein J

Chain j:  78% 10% 12%



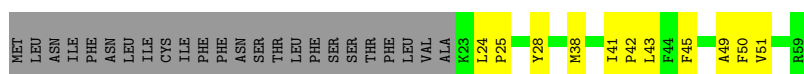
- Molecule 11: Photosystem II reaction center protein K

Chain K: 46% 15% 39%



- Molecule 11: Photosystem II reaction center protein K

Chain k: 43% 18% 39%



- Molecule 12: Photosystem II reaction center protein L

Chain L: 76% 16% 8%



- Molecule 12: Photosystem II reaction center protein L

Chain l: 71% 21% 8%



- Molecule 13: Photosystem II reaction center protein M

Chain M: 68% 24% 9%



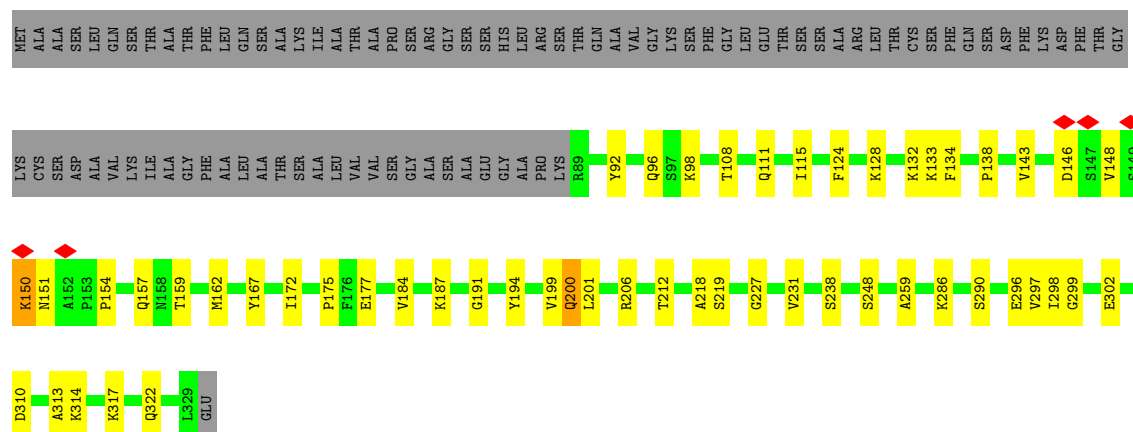
- Molecule 13: Photosystem II reaction center protein M

Chain m: 71% 21% 9%

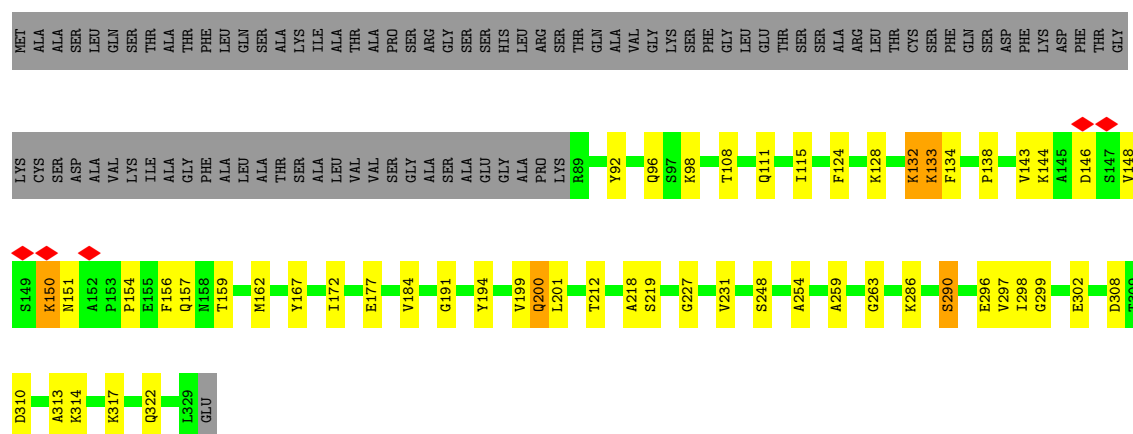


- Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

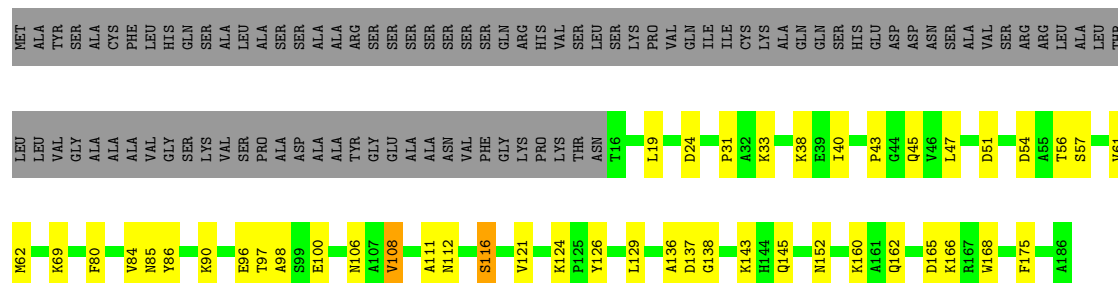
Chain O: 57% 15% 27%



• Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

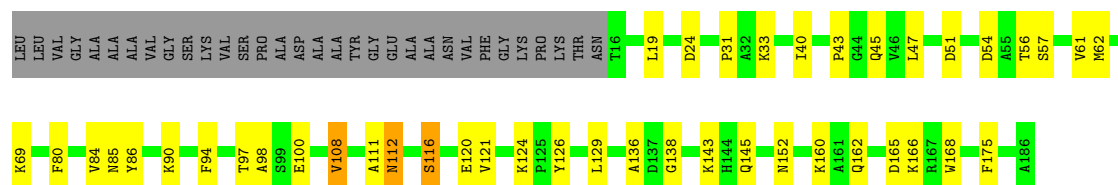


• Molecule 15: Oxygen-evolving enhancer protein 2-1, chloroplastic

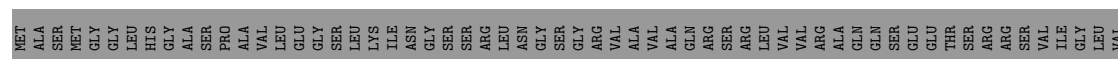


• Molecule 15: Oxygen-evolving enhancer protein 2-1, chloroplastic





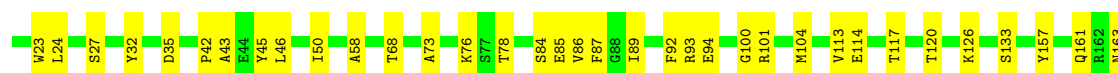
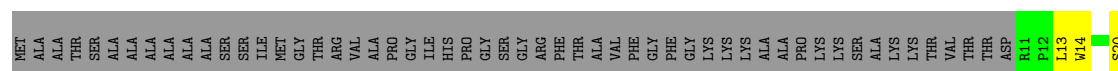
- Molecule 16: Oxygen-evolving enhancer protein 3-1, chloroplastic



- Molecule 16: Oxygen-evolving enhancer protein 3-1, chloroplastic

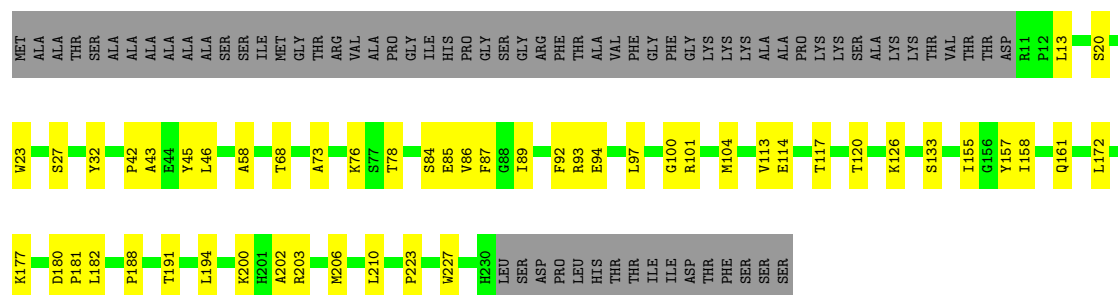


- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic



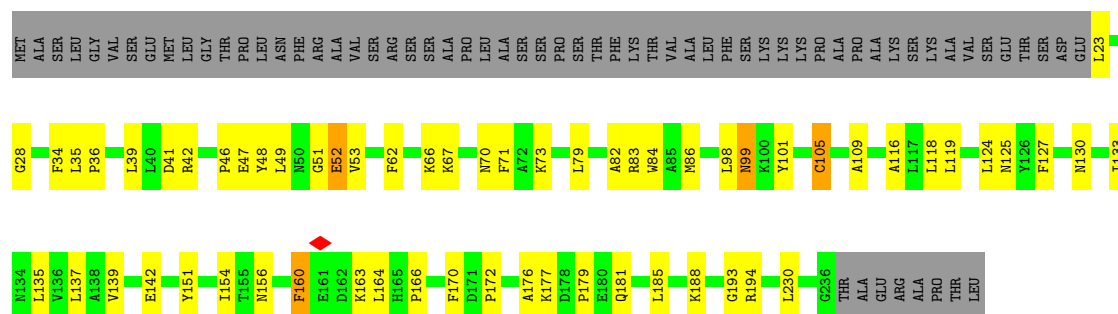
- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic





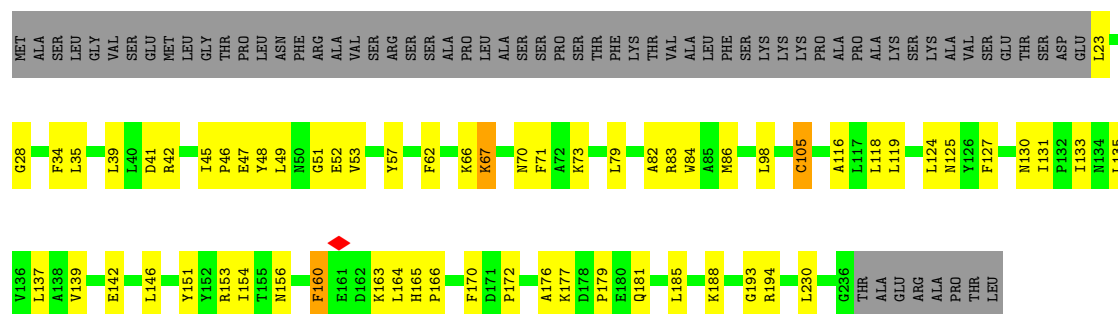
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

Chain S: 55% 20% 24%



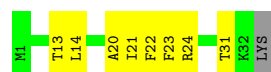
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic

Chain s: 54% 21% 24%



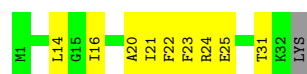
- Molecule 19: Photosystem II reaction center protein T

Chain T: 73% 24% 3%



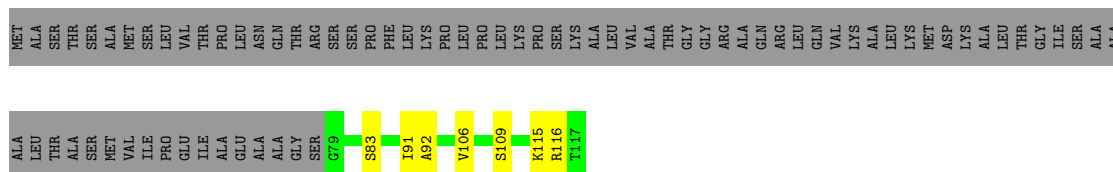
- Molecule 19: Photosystem II reaction center protein T

Chain t: 70% 27% 3%



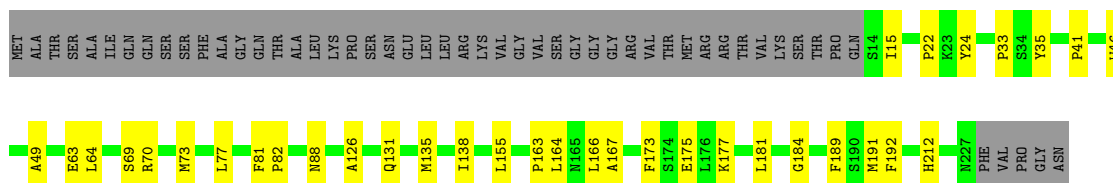
- Molecule 22: Expressed protein

Chain x:  28% 6% 66%



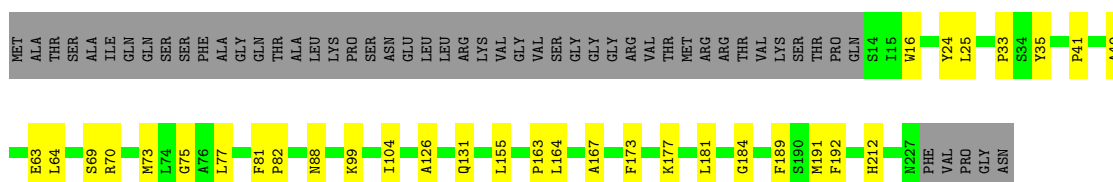
- Molecule 23: Chlorophyll a-b binding protein 2.1, chloroplastic

Chain Y:  68% 13% 19%




- Molecule 23: Chlorophyll a-b binding protein 2.1, chloroplastic

Chain y:  68% 12% 19%




- Molecule 24: Photosystem II reaction center protein Z

Chain Z:  81% 18% .



- Molecule 24: Photosystem II reaction center protein Z

Chain z:  79% 19% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	72301	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.641	Depositor
Minimum map value	-0.646	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.149	Depositor
Map size (Å)	560.952, 560.952, 560.952	wwPDB
Map dimensions	784, 784, 784	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71550006, 0.71550006, 0.71550006	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/2694	0.36	0/3674
1	a	0.26	0/2694	0.36	0/3674
2	B	0.25	0/3930	0.33	0/5354
2	b	0.25	0/3930	0.34	0/5354
3	C	0.24	0/3583	0.33	0/4883
3	c	0.24	0/3583	0.33	0/4883
4	D	0.26	0/2806	0.35	0/3825
4	d	0.26	0/2806	0.35	0/3825
5	E	0.20	0/622	0.29	0/846
5	e	0.19	0/622	0.29	0/846
6	F	0.21	0/248	0.32	0/335
6	f	0.21	0/248	0.33	0/335
7	G	0.16	0/1653	0.29	0/2249
7	N	0.18	0/1580	0.31	0/2146
7	g	0.16	0/1653	0.28	0/2249
7	n	0.18	0/1580	0.31	0/2146
8	H	0.24	0/447	0.33	0/608
8	h	0.24	0/447	0.34	0/608
9	I	0.23	0/274	0.30	0/371
9	i	0.23	0/274	0.30	0/371
10	J	0.14	0/261	0.26	0/354
10	j	0.14	0/261	0.24	0/354
11	K	0.20	0/313	0.33	0/428
11	k	0.20	0/313	0.33	0/428
12	L	0.24	0/301	0.28	0/409
12	l	0.25	0/301	0.27	0/409
13	M	0.21	0/246	0.34	0/337
13	m	0.21	0/246	0.34	0/337
14	O	0.21	0/1867	0.37	0/2525
14	o	0.21	0/1867	0.37	0/2525
15	P	0.19	0/1349	0.34	0/1827

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	p	0.19	0/1349	0.35	0/1827
16	Q	0.18	0/1162	0.35	0/1575
16	q	0.18	0/1162	0.35	0/1575
17	R	0.19	0/1758	0.34	0/2395
17	r	0.19	0/1758	0.34	0/2395
18	S	0.18	0/1698	0.39	0/2305
18	s	0.18	0/1698	0.38	0/2305
19	T	0.20	0/268	0.28	0/362
19	t	0.21	0/268	0.28	0/362
20	U	0.18	0/222	0.37	0/296
20	u	0.17	0/222	0.39	0/296
21	W	0.20	0/438	0.37	0/594
21	w	0.20	0/438	0.36	0/594
22	X	0.19	0/282	0.32	0/383
22	x	0.19	0/282	0.32	0/383
23	Y	0.20	0/1704	0.32	0/2319
23	y	0.20	0/1704	0.32	0/2319
24	Z	0.17	0/466	0.37	0/639
24	z	0.18	0/466	0.33	0/639
All	All	0.22	0/60344	0.34	0/82078

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

Mol	Chain	#Chirality outliers	#Planarity outliers
24	z	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	z	3	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2613	0	2521	78	0
1	a	2613	0	2521	79	0
2	B	3800	0	3681	70	0
2	b	3800	0	3681	72	0
3	C	3468	0	3400	73	0
3	c	3468	0	3400	76	0
4	D	2713	0	2609	59	0
4	d	2713	0	2609	61	0
5	E	604	0	586	10	0
5	e	604	0	586	9	0
6	F	241	0	246	2	0
6	f	241	0	246	2	0
7	G	1606	0	1538	34	0
7	N	1536	0	1480	35	0
7	g	1606	0	1538	35	0
7	n	1536	0	1480	34	0
8	H	438	0	465	7	0
8	h	438	0	465	7	0
9	I	266	0	276	2	0
9	i	266	0	276	2	0
10	J	255	0	269	2	0
10	j	255	0	269	2	0
11	K	302	0	313	8	0
11	k	302	0	313	10	0
12	L	293	0	283	7	0
12	l	293	0	283	8	0
13	M	242	0	267	10	0
13	m	242	0	267	9	0
14	O	1829	0	1792	38	0
14	o	1829	0	1792	37	0
15	P	1319	0	1262	30	0
15	p	1319	0	1262	28	0
16	Q	1139	0	1171	21	0
16	q	1139	0	1171	27	0
17	R	1710	0	1668	41	0
17	r	1710	0	1668	38	0
18	S	1653	0	1639	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	s	1653	0	1639	54	0
19	T	261	0	280	9	0
19	t	261	0	280	9	0
20	U	219	0	235	6	0
20	u	219	0	235	7	0
21	W	427	0	405	5	0
21	w	427	0	405	4	0
22	X	279	0	307	5	0
22	x	279	0	307	7	0
23	Y	1652	0	1581	33	0
23	y	1652	0	1581	34	0
24	Z	456	0	483	8	0
24	z	456	0	483	7	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	125	0	131	3	0
26	B	1040	0	1152	60	0
26	C	828	0	903	42	0
26	D	244	0	255	15	0
26	G	424	0	378	17	0
26	N	424	0	378	15	0
26	R	522	0	456	21	0
26	S	441	0	351	21	0
26	Y	472	0	477	27	0
26	a	190	0	203	5	0
26	b	1040	0	1152	60	0
26	c	828	0	903	47	0
26	d	179	0	183	15	0
26	g	424	0	378	16	0
26	n	424	0	378	13	0
26	r	522	0	456	23	0
26	s	441	0	351	20	0
26	y	472	0	477	27	0
27	A	64	0	74	2	0
27	D	64	0	74	7	0
27	a	64	0	74	1	0
27	d	64	0	74	8	0
28	A	40	0	56	1	0
28	B	120	0	168	11	0
28	C	80	0	112	6	0
28	D	40	0	56	0	0
28	H	40	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	40	0	56	4	0
28	K	40	0	56	5	0
28	T	40	0	56	6	0
28	a	40	0	56	1	0
28	b	120	0	168	13	0
28	c	80	0	112	7	0
28	d	40	0	56	0	0
28	h	40	0	56	3	0
28	j	40	0	56	4	0
28	k	40	0	56	5	0
28	t	40	0	56	6	0
29	A	104	0	145	7	0
29	B	54	0	78	2	0
29	W	33	0	30	0	0
29	a	104	0	145	8	0
29	b	54	0	78	3	0
29	w	33	0	30	0	0
30	A	22	0	25	3	0
30	D	55	0	80	3	0
30	a	22	0	25	4	0
30	d	55	0	80	2	0
31	A	1	0	0	0	0
31	a	1	0	0	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	62	0	82	3	0
33	C	179	0	232	10	0
33	Y	43	0	44	3	0
33	b	62	0	82	3	0
33	c	179	0	232	8	0
33	y	43	0	44	2	0
34	B	51	0	72	2	0
34	C	102	0	144	3	0
34	D	46	0	62	1	0
34	W	48	0	66	3	0
34	b	51	0	72	3	0
34	c	102	0	144	2	0
34	d	46	0	62	2	0
34	w	48	0	66	2	0
35	C	10	0	0	2	0
35	a	10	0	0	3	0
36	D	35	0	46	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	d	35	0	46	0	0
37	D	129	0	177	11	0
37	G	49	0	74	6	0
37	L	49	0	74	2	0
37	N	49	0	74	5	0
37	R	49	0	74	0	0
37	S	49	0	74	2	0
37	Y	49	0	74	4	0
37	d	129	0	177	10	0
37	g	49	0	74	8	0
37	l	49	0	74	3	0
37	n	49	0	74	5	0
37	r	49	0	74	2	0
37	s	49	0	74	2	0
37	y	49	0	74	4	0
38	E	43	0	30	5	0
38	e	43	0	30	4	0
39	G	314	0	251	24	0
39	N	314	0	251	17	0
39	R	198	0	144	7	0
39	S	201	0	147	14	0
39	Y	282	0	251	17	0
39	g	314	0	251	26	0
39	n	314	0	251	19	0
39	r	198	0	144	8	0
39	s	201	0	147	15	0
39	y	282	0	251	16	0
40	G	84	0	112	5	0
40	N	84	0	112	7	0
40	R	42	0	56	5	0
40	S	84	0	112	6	0
40	Y	84	0	112	12	0
40	g	84	0	112	7	0
40	n	84	0	112	7	0
40	r	42	0	56	6	0
40	s	84	0	112	5	0
40	y	84	0	112	11	0
41	G	88	0	112	10	0
41	N	44	0	56	6	0
41	R	44	0	56	1	0
41	g	88	0	112	10	0
41	n	44	0	56	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	r	44	0	56	2	0
42	G	44	0	56	4	0
42	N	44	0	56	2	0
42	R	44	0	56	3	0
42	S	44	0	56	7	0
42	Y	44	0	56	3	0
42	g	44	0	56	4	0
42	n	44	0	56	1	0
42	r	44	0	56	4	0
42	s	44	0	56	6	0
42	y	44	0	56	3	0
43	A	82	0	0	0	0
43	B	115	0	0	0	0
43	C	104	0	0	0	0
43	D	78	0	0	1	0
43	E	19	0	0	1	0
43	F	3	0	0	0	0
43	G	5	0	0	0	0
43	H	15	0	0	1	0
43	I	6	0	0	0	0
43	J	4	0	0	0	0
43	K	5	0	0	0	0
43	L	9	0	0	0	0
43	M	3	0	0	0	0
43	N	5	0	0	0	0
43	O	39	0	0	0	0
43	P	17	0	0	0	0
43	Q	1	0	0	0	0
43	R	19	0	0	1	0
43	S	5	0	0	0	0
43	T	7	0	0	0	0
43	U	1	0	0	0	0
43	W	18	0	0	0	0
43	X	5	0	0	0	0
43	Y	36	0	0	0	0
43	Z	2	0	0	0	0
43	a	90	0	0	1	0
43	b	114	0	0	0	0
43	c	100	0	0	0	0
43	d	76	0	0	1	0
43	e	19	0	0	1	0
43	f	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	g	5	0	0	0	0
43	h	15	0	0	1	0
43	i	6	0	0	0	0
43	j	4	0	0	0	0
43	k	5	0	0	0	0
43	l	9	0	0	0	0
43	m	3	0	0	0	0
43	n	5	0	0	0	0
43	o	38	0	0	0	0
43	p	17	0	0	0	0
43	q	1	0	0	0	0
43	r	19	0	0	1	0
43	s	5	0	0	0	0
43	t	7	0	0	0	0
43	u	1	0	0	0	0
43	w	18	0	0	0	0
43	x	5	0	0	0	0
43	y	36	0	0	0	0
43	z	2	0	0	0	0
All	All	76824	0	75622	1602	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 11.

The worst 5 of 1602 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)
35:a:408:OEX:CA1	35:a:408:OEX:O1	1.31	1.05
35:C:501:OEX:O1	35:C:501:OEX:CA1	1.40	0.96
3:c:68:ASN:HD21	3:c:92:LEU:HD11	1.34	0.92
4:D:175:VAL:HG13	26:D:412:CLA:HED1	1.56	0.87
39:s:316:CHL:HBB2	39:s:317:CHL:HBB1	1.55	0.86

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/353 (94%)	328 (99%)	4 (1%)	0	100	100
1	a	332/353 (94%)	327 (98%)	5 (2%)	0	100	100
2	B	483/508 (95%)	476 (99%)	7 (1%)	0	100	100
2	b	483/508 (95%)	477 (99%)	6 (1%)	0	100	100
3	C	445/473 (94%)	437 (98%)	8 (2%)	0	100	100
3	c	445/473 (94%)	438 (98%)	7 (2%)	0	100	100
4	D	339/353 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	339/353 (96%)	332 (98%)	7 (2%)	0	100	100
5	E	72/83 (87%)	71 (99%)	1 (1%)	0	100	100
5	e	72/83 (87%)	71 (99%)	1 (1%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	0	100	100
6	f	28/39 (72%)	28 (100%)	0	0	100	100
7	G	209/267 (78%)	206 (99%)	3 (1%)	0	100	100
7	N	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
7	g	209/267 (78%)	206 (99%)	3 (1%)	0	100	100
7	n	200/267 (75%)	195 (98%)	5 (2%)	0	100	100
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
9	I	31/36 (86%)	31 (100%)	0	0	100	100
9	i	31/36 (86%)	31 (100%)	0	0	100	100
10	J	33/40 (82%)	33 (100%)	0	0	100	100
10	j	33/40 (82%)	33 (100%)	0	0	100	100
11	K	35/61 (57%)	35 (100%)	0	0	100	100
11	k	35/61 (57%)	35 (100%)	0	0	100	100
12	L	33/38 (87%)	33 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	33/38 (87%)	33 (100%)	0	0	100	100
13	M	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
13	m	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
14	O	239/332 (72%)	228 (95%)	11 (5%)	0	100	100
14	o	239/332 (72%)	228 (95%)	11 (5%)	0	100	100
15	P	169/263 (64%)	161 (95%)	8 (5%)	0	100	100
15	p	169/263 (64%)	162 (96%)	7 (4%)	0	100	100
16	Q	144/224 (64%)	136 (94%)	8 (6%)	0	100	100
16	q	144/224 (64%)	136 (94%)	8 (6%)	0	100	100
17	R	218/290 (75%)	210 (96%)	8 (4%)	0	100	100
17	r	218/290 (75%)	211 (97%)	7 (3%)	0	100	100
18	S	212/280 (76%)	204 (96%)	8 (4%)	0	100	100
18	s	212/280 (76%)	203 (96%)	9 (4%)	0	100	100
19	T	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
19	t	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
20	U	26/103 (25%)	24 (92%)	2 (8%)	0	100	100
20	u	26/103 (25%)	23 (88%)	3 (12%)	0	100	100
21	W	52/133 (39%)	47 (90%)	4 (8%)	1 (2%)	6	4
21	w	52/133 (39%)	47 (90%)	4 (8%)	1 (2%)	6	4
22	X	37/116 (32%)	36 (97%)	1 (3%)	0	100	100
22	x	37/116 (32%)	36 (97%)	1 (3%)	0	100	100
23	Y	212/265 (80%)	206 (97%)	6 (3%)	0	100	100
23	y	212/265 (80%)	206 (97%)	6 (3%)	0	100	100
24	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
24	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	7448/9452 (79%)	7256 (97%)	190 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	W	86	ASP
21	w	86	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/285 (95%)	270 (100%)	0	100	100
1	a	270/285 (95%)	270 (100%)	0	100	100
2	B	384/402 (96%)	381 (99%)	3 (1%)	73	81
2	b	384/402 (96%)	381 (99%)	3 (1%)	73	81
3	C	351/373 (94%)	347 (99%)	4 (1%)	65	75
3	c	351/373 (94%)	344 (98%)	7 (2%)	48	62
4	D	273/283 (96%)	269 (98%)	4 (2%)	57	69
4	d	273/283 (96%)	271 (99%)	2 (1%)	76	83
5	E	66/73 (90%)	66 (100%)	0	100	100
5	e	66/73 (90%)	65 (98%)	1 (2%)	57	69
6	F	25/34 (74%)	25 (100%)	0	100	100
6	f	25/34 (74%)	25 (100%)	0	100	100
7	G	161/201 (80%)	159 (99%)	2 (1%)	63	74
7	N	154/201 (77%)	154 (100%)	0	100	100
7	g	161/201 (80%)	158 (98%)	3 (2%)	50	63
7	n	154/201 (77%)	153 (99%)	1 (1%)	78	85
8	H	49/61 (80%)	49 (100%)	0	100	100
8	h	49/61 (80%)	49 (100%)	0	100	100
9	I	30/33 (91%)	30 (100%)	0	100	100
9	i	30/33 (91%)	30 (100%)	0	100	100
10	J	26/30 (87%)	26 (100%)	0	100	100
10	j	26/30 (87%)	24 (92%)	2 (8%)	12	14
11	K	32/55 (58%)	32 (100%)	0	100	100
11	k	32/55 (58%)	32 (100%)	0	100	100
12	L	33/36 (92%)	33 (100%)	0	100	100
12	l	33/36 (92%)	33 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	27/30 (90%)	27 (100%)	0	100	100
13	m	27/30 (90%)	27 (100%)	0	100	100
14	O	200/268 (75%)	195 (98%)	5 (2%)	42	54
14	o	200/268 (75%)	194 (97%)	6 (3%)	36	48
15	P	139/210 (66%)	135 (97%)	4 (3%)	37	49
15	p	139/210 (66%)	134 (96%)	5 (4%)	31	42
16	Q	124/178 (70%)	121 (98%)	3 (2%)	43	56
16	q	124/178 (70%)	121 (98%)	3 (2%)	43	56
17	R	174/225 (77%)	170 (98%)	4 (2%)	44	57
17	r	174/225 (77%)	170 (98%)	4 (2%)	44	57
18	S	165/219 (75%)	160 (97%)	5 (3%)	36	48
18	s	165/219 (75%)	160 (97%)	5 (3%)	36	48
19	T	29/30 (97%)	29 (100%)	0	100	100
19	t	29/30 (97%)	28 (97%)	1 (3%)	32	45
20	U	23/82 (28%)	23 (100%)	0	100	100
20	u	23/82 (28%)	23 (100%)	0	100	100
21	W	47/102 (46%)	47 (100%)	0	100	100
21	w	47/102 (46%)	47 (100%)	0	100	100
22	X	33/92 (36%)	33 (100%)	0	100	100
22	x	33/92 (36%)	33 (100%)	0	100	100
23	Y	168/209 (80%)	166 (99%)	2 (1%)	63	74
23	y	168/209 (80%)	168 (100%)	0	100	100
24	Z	53/54 (98%)	51 (96%)	2 (4%)	29	41
24	z	53/54 (98%)	51 (96%)	2 (4%)	29	41
All	All	6072/7532 (81%)	5989 (99%)	83 (1%)	57	70

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	o	132	LYS
17	r	27	SER
14	o	150	LYS
15	p	112	ASN
18	s	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	234	ASN
4	d	263	ASN
1	a	304	GLN
3	c	332	GLN
6	f	45	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 332 ligands modelled in this entry, 6 are monoatomic - leaving 326 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	$\# Z > 2$
26	CLA	g	303	7	69,73,73	1.17	9 (13%)	82,113,113	1.21	6 (7%)
26	CLA	Y	310	23	53,57,73	1.29	8 (15%)	61,93,113	1.25	5 (8%)
42	NEX	y	307	-	40,46,46	1.33	7 (17%)	50,70,70	1.95	9 (18%)
26	CLA	C	519	3	53,57,73	1.27	8 (15%)	61,93,113	1.37	6 (9%)
26	CLA	r	314	17	69,73,73	1.11	7 (10%)	82,113,113	1.22	7 (8%)
26	CLA	R	317	17	53,57,73	1.27	7 (13%)	61,93,113	1.40	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	g	307	-	44,58,74	2.14	11 (25%)	37,94,114	3.03	18 (48%)
26	CLA	r	311	43	53,57,73	1.31	9 (16%)	61,93,113	1.39	8 (13%)
26	CLA	s	301	37	53,57,73	1.28	8 (15%)	61,93,113	1.34	5 (8%)
30	PL9	D	411	-	55,55,55	1.34	6 (10%)	68,69,69	1.49	12 (17%)
39	CHL	G	301	-	44,58,74	2.19	11 (25%)	37,94,114	3.11	16 (43%)
26	CLA	N	318	7	53,57,73	1.29	8 (15%)	61,93,113	1.40	5 (8%)
42	NEX	S	305	-	40,46,46	1.31	7 (17%)	50,70,70	2.19	15 (30%)
34	LMG	C	503	-	51,51,55	0.48	0	59,59,63	0.64	0
26	CLA	R	314	37	53,57,73	1.31	8 (15%)	61,93,113	1.37	5 (8%)
39	CHL	S	302	-	44,58,74	2.18	11 (25%)	37,94,114	3.15	17 (45%)
26	CLA	G	302	-	53,57,73	1.32	9 (16%)	61,93,113	1.30	4 (6%)
26	CLA	s	314	18	53,57,73	1.27	7 (13%)	61,93,113	1.32	9 (14%)
39	CHL	Y	317	43	44,58,74	2.11	11 (25%)	37,94,114	3.11	16 (43%)
26	CLA	R	309	17	53,57,73	1.30	7 (13%)	61,93,113	1.29	5 (8%)
40	LUT	N	305	-	42,43,43	0.46	0	51,60,60	0.82	1 (1%)
26	CLA	S	314	18	53,57,73	1.25	6 (11%)	61,93,113	1.13	4 (6%)
30	PL9	a	407	-	22,22,55	1.28	3 (13%)	27,29,69	1.56	8 (29%)
26	CLA	b	601	2	69,73,73	1.11	7 (10%)	82,113,113	1.16	6 (7%)
40	LUT	g	310	-	42,43,43	0.43	0	51,60,60	0.74	1 (1%)
40	LUT	S	306	-	42,43,43	0.47	0	51,60,60	0.87	1 (1%)
26	CLA	b	610	2	69,73,73	1.12	8 (11%)	82,113,113	1.22	7 (8%)
26	CLA	B	602	2	69,73,73	1.11	8 (11%)	82,113,113	1.20	6 (7%)
26	CLA	y	306	23	69,73,73	1.12	7 (10%)	82,113,113	1.27	8 (9%)
28	BCR	c	511	-	41,41,41	0.34	0	56,56,56	0.82	2 (3%)
35	OEX	C	501	1,43,3	0,15,15	-	-	-	-	-
37	LHG	D	407	-	42,42,48	0.56	0	45,48,54	0.51	0
39	CHL	N	303	-	60,74,74	1.84	12 (20%)	58,114,114	2.51	18 (31%)
39	CHL	S	316	18	46,60,74	2.15	12 (26%)	40,97,114	3.07	18 (45%)
39	CHL	N	310	7	42,56,74	2.18	11 (26%)	36,92,114	3.09	17 (47%)
39	CHL	s	316	-	44,58,74	2.20	11 (25%)	37,94,114	3.16	17 (45%)
39	CHL	g	319	-	44,58,74	2.15	12 (27%)	37,94,114	3.07	17 (45%)
28	BCR	b	603	-	41,41,41	0.36	0	56,56,56	0.74	0
26	CLA	R	316	17	53,57,73	1.29	8 (15%)	61,93,113	1.28	4 (6%)
26	CLA	R	310	17	53,57,73	1.24	8 (15%)	61,93,113	1.27	4 (6%)
26	CLA	d	404	4	69,73,73	1.11	7 (10%)	82,113,113	1.13	4 (4%)
28	BCR	b	619	-	41,41,41	0.33	0	56,56,56	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	NEX	R	305	-	40,46,46	1.32	7 (17%)	50,70,70	2.10	14 (28%)
26	CLA	r	310	17	53,57,73	1.24	6 (11%)	61,93,113	1.27	4 (6%)
27	PHO	d	407	-	58,69,69	2.09	10 (17%)	55,99,99	1.51	6 (10%)
42	NEX	N	302	-	40,46,46	1.33	7 (17%)	50,70,70	2.09	10 (20%)
39	CHL	r	309	43	44,58,74	2.12	12 (27%)	37,94,114	3.08	16 (43%)
33	DGD	b	620	-	63,63,67	0.58	0	77,77,81	0.77	1 (1%)
29	SQD	b	621	-	52,54,54	0.77	1 (1%)	62,65,65	0.80	2 (3%)
41	XAT	G	310	-	41,47,47	1.09	4 (9%)	54,74,74	2.12	12 (22%)
26	CLA	S	303	18	53,57,73	1.29	8 (15%)	61,93,113	1.29	5 (8%)
28	BCR	d	401	-	41,41,41	0.33	0	56,56,56	0.73	1 (1%)
26	CLA	n	305	7	69,73,73	1.13	8 (11%)	82,113,113	1.22	7 (8%)
26	CLA	c	508	43	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
26	CLA	B	604	2	69,73,73	1.19	8 (11%)	82,113,113	1.19	9 (10%)
26	CLA	C	507	3	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
37	LHG	g	301	26	48,48,48	0.52	0	51,54,54	0.53	0
39	CHL	n	318	-	60,74,74	1.85	12 (20%)	58,114,114	2.50	18 (31%)
33	DGD	y	308	-	44,44,67	0.70	0	58,58,81	0.87	1 (1%)
42	NEX	G	315	-	40,46,46	1.29	6 (15%)	50,70,70	2.19	12 (24%)
26	CLA	B	615	2	69,73,73	1.23	7 (10%)	82,113,113	1.44	7 (8%)
26	CLA	y	309	23	69,73,73	1.12	7 (10%)	82,113,113	1.11	6 (7%)
26	CLA	b	608	43	69,73,73	1.14	8 (11%)	82,113,113	1.22	4 (4%)
26	CLA	b	607	2	69,73,73	1.13	9 (13%)	82,113,113	1.17	6 (7%)
26	CLA	g	302	-	53,57,73	1.32	8 (15%)	61,93,113	1.29	4 (6%)
26	CLA	c	503	3	69,73,73	1.08	7 (10%)	82,113,113	1.21	6 (7%)
26	CLA	Y	312	23	69,73,73	1.14	8 (11%)	82,113,113	1.24	6 (7%)
26	CLA	B	606	2	69,73,73	1.11	7 (10%)	82,113,113	1.15	5 (6%)
26	CLA	D	412	43	53,57,73	1.30	8 (15%)	61,93,113	1.22	7 (11%)
26	CLA	b	617	2	69,73,73	1.10	8 (11%)	82,113,113	1.23	6 (7%)
39	CHL	Y	302	23	60,74,74	1.86	12 (20%)	58,114,114	2.59	18 (31%)
26	CLA	S	315	18	53,57,73	1.28	8 (15%)	61,93,113	1.28	5 (8%)
26	CLA	N	309	7	53,57,73	1.28	7 (13%)	61,93,113	1.31	4 (6%)
39	CHL	s	313	-	43,57,74	2.20	11 (25%)	37,93,114	3.19	17 (45%)
34	LMG	D	404	-	46,46,55	0.61	0	54,54,63	0.69	1 (1%)
26	CLA	s	307	18	53,57,73	1.29	7 (13%)	61,93,113	1.30	5 (8%)
39	CHL	G	305	-	44,58,74	2.16	11 (25%)	37,94,114	3.05	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	c	506	3	61,70,73	1.24	4 (6%)	73,103,113	1.44	6 (8%)
26	CLA	B	607	43	69,73,73	1.12	7 (10%)	82,113,113	1.22	6 (7%)
32	BCT	a	405	31	3,3,3	0.82	0	2,3,3	3.26	2 (100%)
26	CLA	r	308	17	53,57,73	1.29	8 (15%)	61,93,113	1.28	4 (6%)
39	CHL	G	318	7	60,74,74	1.87	12 (20%)	58,114,114	2.51	18 (31%)
26	CLA	G	317	7	53,57,73	1.29	9 (16%)	61,93,113	1.36	5 (8%)
26	CLA	d	403	4	69,73,73	1.12	7 (10%)	82,113,113	1.22	6 (7%)
26	CLA	G	313	37	53,57,73	1.32	8 (15%)	61,93,113	1.37	6 (9%)
26	CLA	R	302	17	53,57,73	1.27	8 (15%)	61,93,113	1.56	13 (21%)
26	CLA	a	409	43	69,73,73	1.10	8 (11%)	82,113,113	1.17	8 (9%)
26	CLA	c	504	3	69,73,73	1.13	7 (10%)	82,113,113	1.26	7 (8%)
37	LHG	r	312	26	48,48,48	0.51	0	51,54,54	0.52	0
26	CLA	C	520	3	61,70,73	1.24	4 (6%)	73,103,113	1.44	6 (8%)
42	NEX	g	306	-	40,46,46	1.30	7 (17%)	50,70,70	2.19	11 (22%)
26	CLA	C	505	3	69,73,73	1.12	7 (10%)	82,113,113	1.20	8 (9%)
39	CHL	n	306	7	44,58,74	2.16	11 (25%)	37,94,114	3.18	18 (48%)
26	CLA	C	521	43	69,73,73	1.12	8 (11%)	82,113,113	1.21	7 (8%)
28	BCR	D	405	-	41,41,41	0.33	0	56,56,56	0.72	1 (1%)
39	CHL	r	301	23	42,56,74	2.16	11 (26%)	36,92,114	3.15	18 (50%)
39	CHL	g	312	7	44,58,74	2.15	11 (25%)	37,94,114	3.15	18 (48%)
26	CLA	c	520	3	69,73,73	1.12	7 (10%)	82,113,113	1.21	8 (9%)
26	CLA	r	313	17	53,57,73	1.27	7 (13%)	61,93,113	1.55	13 (21%)
37	LHG	D	410	-	36,36,48	0.61	0	39,42,54	0.59	0
41	XAT	n	316	-	41,47,47	1.10	4 (9%)	54,74,74	2.12	13 (24%)
39	CHL	N	304	43	44,58,74	2.12	11 (25%)	37,94,114	3.13	17 (45%)
26	CLA	Y	316	43	53,57,73	1.34	7 (13%)	61,93,113	1.25	5 (8%)
28	BCR	T	101	-	41,41,41	0.31	0	56,56,56	1.48	10 (17%)
26	CLA	b	612	2	69,73,73	1.18	8 (11%)	82,113,113	1.19	10 (12%)
26	CLA	S	311	18	53,57,73	1.26	7 (13%)	61,93,113	1.32	9 (14%)
26	CLA	S	307	18	53,57,73	1.30	8 (15%)	61,93,113	1.22	6 (9%)
37	LHG	G	312	26	48,48,48	0.52	0	51,54,54	0.52	0
36	LMT	D	402	-	36,36,36	0.57	0	47,47,47	0.68	0
26	CLA	c	516	3	69,73,73	1.14	8 (11%)	82,113,113	1.22	7 (8%)
26	CLA	s	310	-	53,57,73	1.33	9 (16%)	61,93,113	1.27	5 (8%)
26	CLA	Y	313	23	69,73,73	1.11	8 (11%)	82,113,113	1.31	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	S	308	37	53,57,73	1.28	8 (15%)	61,93,113	1.33	5 (8%)
26	CLA	N	313	7	53,57,73	1.31	10 (18%)	61,93,113	1.34	6 (9%)
28	BCR	H	101	-	41,41,41	0.33	0	56,56,56	0.69	0
39	CHL	R	312	43	44,58,74	2.12	12 (27%)	37,94,114	3.07	16 (43%)
34	LMG	b	622	-	51,51,55	0.52	0	59,59,63	0.65	0
41	XAT	G	320	-	41,47,47	1.06	3 (7%)	54,74,74	2.29	16 (29%)
40	LUT	R	311	-	42,43,43	0.47	0	51,60,60	1.05	4 (7%)
26	CLA	r	317	37	53,57,73	1.31	8 (15%)	61,93,113	1.37	5 (8%)
26	CLA	c	514	43	69,73,73	1.12	9 (13%)	82,113,113	1.21	7 (8%)
26	CLA	C	517	3	69,73,73	1.13	7 (10%)	82,113,113	1.26	6 (7%)
26	CLA	n	315	7	53,57,73	1.33	9 (16%)	61,93,113	1.37	5 (8%)
39	CHL	N	311	-	44,58,74	2.10	11 (25%)	37,94,114	3.08	16 (43%)
26	CLA	b	618	2	69,73,73	1.14	9 (13%)	82,113,113	1.25	8 (9%)
26	CLA	a	411	1	69,73,73	1.12	8 (11%)	82,113,113	1.16	7 (8%)
39	CHL	y	303	23	60,74,74	1.86	12 (20%)	58,114,114	2.58	18 (31%)
26	CLA	y	310	23	69,73,73	1.15	7 (10%)	82,113,113	1.25	6 (7%)
28	BCR	K	101	-	41,41,41	0.34	0	56,56,56	0.90	3 (5%)
37	LHG	l	101	-	48,48,48	0.52	0	51,54,54	0.54	0
37	LHG	d	410	-	36,36,48	0.61	0	39,42,54	0.59	0
26	CLA	R	306	17	69,73,73	1.12	8 (11%)	82,113,113	1.10	6 (7%)
26	CLA	Y	301	37	69,73,73	1.13	7 (10%)	82,113,113	1.24	5 (6%)
37	LHG	s	309	26	48,48,48	0.52	0	51,54,54	0.52	0
26	CLA	c	502	3	69,73,73	1.12	9 (13%)	82,113,113	1.19	6 (7%)
26	CLA	d	411	43	53,57,73	1.31	8 (15%)	61,93,113	1.22	6 (9%)
35	OEX	a	408	1,43,3	0,15,15	-	-	-	-	-
26	CLA	r	306	17	69,73,73	1.11	8 (11%)	82,113,113	1.09	6 (7%)
39	CHL	y	305	43	44,58,74	2.11	11 (25%)	37,94,114	3.11	16 (43%)
42	NEX	n	313	-	40,46,46	1.31	7 (17%)	50,70,70	2.06	10 (20%)
36	LMT	d	406	-	36,36,36	0.57	0	47,47,47	0.69	0
37	LHG	D	408	-	48,48,48	0.52	0	51,54,54	0.58	1 (1%)
42	NEX	Y	304	-	40,46,46	1.33	7 (17%)	50,70,70	1.95	9 (18%)
27	PHO	a	410	-	58,69,69	2.07	11 (18%)	55,99,99	1.43	7 (12%)
28	BCR	B	614	-	41,41,41	0.33	0	56,56,56	0.55	0
37	LHG	d	409	-	48,48,48	0.52	0	51,54,54	0.58	1 (1%)
26	CLA	B	611	2	69,73,73	1.14	9 (13%)	82,113,113	1.20	6 (7%)
26	CLA	C	512	3	69,73,73	1.09	7 (10%)	82,113,113	1.28	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	y	314	23	60,74,74	1.86	12 (20%)	58,114,114	2.53	18 (31%)
26	CLA	b	613	2	69,73,73	1.13	9 (13%)	82,113,113	1.22	7 (8%)
26	CLA	B	601	2	69,73,73	1.13	9 (13%)	82,113,113	1.16	6 (7%)
26	CLA	D	409	4	69,73,73	1.11	7 (10%)	82,113,113	1.14	4 (4%)
27	PHO	D	403	-	58,69,69	2.08	10 (17%)	55,99,99	1.51	6 (10%)
26	CLA	b	614	43	69,73,73	1.15	8 (11%)	82,113,113	1.26	6 (7%)
26	CLA	y	304	37	69,73,73	1.15	7 (10%)	82,113,113	1.22	5 (6%)
26	CLA	s	304	18	53,57,73	1.28	8 (15%)	61,93,113	1.40	7 (11%)
28	BCR	a	404	-	41,41,41	0.33	0	56,56,56	0.51	0
40	LUT	r	307	-	42,43,43	0.47	0	51,60,60	1.06	4 (7%)
26	CLA	S	304	18	53,57,73	1.27	8 (15%)	61,93,113	1.25	6 (9%)
26	CLA	B	603	2	69,73,73	1.10	7 (10%)	82,113,113	1.22	7 (8%)
33	DGD	Y	303	-	44,44,67	0.68	0	58,58,81	0.85	1 (1%)
39	CHL	n	311	43	44,58,74	2.12	11 (25%)	37,94,114	3.11	17 (45%)
26	CLA	N	306	7	53,57,73	1.33	9 (16%)	61,93,113	1.38	5 (8%)
26	CLA	c	518	3	69,73,73	1.13	8 (11%)	82,113,113	1.35	4 (4%)
41	XAT	g	309	-	41,47,47	1.09	4 (9%)	54,74,74	2.11	12 (22%)
26	CLA	c	513	3	69,73,73	1.12	6 (8%)	82,113,113	1.26	6 (7%)
26	CLA	N	308	43	53,57,73	1.33	10 (18%)	61,93,113	1.23	5 (8%)
26	CLA	g	317	7	69,73,73	1.14	8 (11%)	82,113,113	1.10	7 (8%)
30	PL9	A	408	-	22,22,55	1.26	3 (13%)	27,29,69	1.53	7 (25%)
39	CHL	G	303	-	44,58,74	2.13	11 (25%)	37,94,114	3.04	18 (48%)
26	CLA	C	506	3	69,73,73	1.12	9 (13%)	82,113,113	1.21	6 (7%)
33	DGD	C	513	-	63,63,67	0.63	0	77,77,81	0.69	0
38	HEM	e	101	5,6	50,50,50	1.40	8 (16%)	67,82,82	1.15	5 (7%)
29	SQD	a	413	-	48,50,54	0.78	1 (2%)	58,61,65	0.98	2 (3%)
26	CLA	B	605	43	69,73,73	1.14	7 (10%)	82,113,113	1.24	4 (4%)
26	CLA	G	319	7	53,57,73	1.29	8 (15%)	61,93,113	1.34	5 (8%)
26	CLA	G	306	7	53,57,73	1.32	9 (16%)	61,93,113	1.31	5 (8%)
28	BCR	J	101	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
26	CLA	A	403	1	69,73,73	1.13	8 (11%)	82,113,113	1.15	6 (7%)
41	XAT	g	320	-	41,47,47	1.06	3 (7%)	54,74,74	2.29	17 (31%)
40	LUT	Y	309	-	42,43,43	0.49	0	51,60,60	0.88	1 (1%)
37	LHG	S	317	26	48,48,48	0.52	0	51,54,54	0.52	0
26	CLA	c	515	3	69,73,73	1.09	7 (10%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	c	507	-	41,41,41	0.33	0	56,56,56	0.75	2 (3%)
40	LUT	y	318	-	42,43,43	0.48	0	51,60,60	0.87	1 (1%)
40	LUT	G	308	-	42,43,43	0.44	0	51,60,60	0.73	0
26	CLA	D	406	4	69,73,73	1.11	7 (10%)	82,113,113	1.22	6 (7%)
26	CLA	C	511	3	69,73,73	1.08	7 (10%)	82,113,113	1.21	6 (7%)
26	CLA	Y	305	23	69,73,73	1.12	7 (10%)	82,113,113	1.13	7 (8%)
26	CLA	B	613	-	69,73,73	1.14	8 (11%)	82,113,113	1.21	5 (6%)
26	CLA	g	305	7	53,57,73	1.32	9 (16%)	61,93,113	1.31	5 (8%)
28	BCR	t	101	-	41,41,41	0.32	0	56,56,56	1.42	10 (17%)
33	DGD	B	620	-	63,63,67	0.58	0	77,77,81	0.76	1 (1%)
37	LHG	y	301	26	48,48,48	0.52	0	51,54,54	0.52	0
29	SQD	A	407	-	52,54,54	0.77	1 (1%)	62,65,65	0.92	4 (6%)
26	CLA	g	315	37	53,57,73	1.31	8 (15%)	61,93,113	1.36	6 (9%)
26	CLA	b	602	2	69,73,73	1.11	8 (11%)	82,113,113	1.23	7 (8%)
29	SQD	B	621	-	52,54,54	0.78	1 (1%)	62,65,65	0.80	2 (3%)
40	LUT	n	314	-	42,43,43	0.47	0	51,60,60	0.86	0
26	CLA	s	315	18	53,57,73	1.25	7 (13%)	61,93,113	1.13	4 (6%)
26	CLA	R	313	17	69,73,73	1.12	7 (10%)	82,113,113	1.21	7 (8%)
39	CHL	G	309	7	42,56,74	2.24	11 (26%)	36,92,114	3.08	17 (47%)
41	XAT	N	315	-	41,47,47	1.10	4 (9%)	54,74,74	2.14	15 (27%)
33	DGD	c	519	-	63,63,67	0.62	0	77,77,81	0.69	0
26	CLA	y	316	23	69,73,73	1.14	8 (11%)	82,113,113	1.29	6 (7%)
29	SQD	a	403	-	52,54,54	0.77	1 (1%)	62,65,65	0.91	3 (4%)
28	BCR	j	101	-	41,41,41	0.31	0	56,56,56	0.68	1 (1%)
39	CHL	G	311	7	44,58,74	2.15	11 (25%)	37,94,114	3.15	17 (45%)
26	CLA	n	304	7	53,57,73	1.32	10 (18%)	61,93,113	1.36	6 (9%)
26	CLA	G	314	7	69,73,73	1.17	9 (13%)	82,113,113	1.21	6 (7%)
26	CLA	B	618	2	69,73,73	1.13	9 (13%)	82,113,113	1.20	7 (8%)
34	LMG	B	622	-	51,51,55	0.53	0	59,59,63	0.64	0
28	BCR	B	608	-	41,41,41	0.31	0	56,56,56	0.52	0
26	CLA	n	312	43	53,57,73	1.33	10 (18%)	61,93,113	1.24	5 (8%)
26	CLA	y	317	23	53,57,73	1.30	9 (16%)	61,93,113	1.27	5 (8%)
39	CHL	n	308	7	42,56,74	2.19	11 (26%)	36,92,114	3.08	17 (47%)
26	CLA	R	308	43	53,57,73	1.31	9 (16%)	61,93,113	1.39	7 (11%)
42	NEX	s	302	-	40,46,46	1.31	7 (17%)	50,70,70	2.14	14 (28%)
38	HEM	E	101	5,6	50,50,50	1.39	7 (14%)	67,82,82	1.14	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	G	304	7	53,57,73	1.30	8 (15%)	61,93,113	1.36	5 (8%)
39	CHL	s	303	18	46,60,74	2.16	12 (26%)	40,97,114	3.07	18 (45%)
28	BCR	h	101	-	41,41,41	0.33	0	56,56,56	0.68	0
26	CLA	S	310	-	53,57,73	1.34	9 (16%)	61,93,113	1.27	5 (8%)
42	NEX	r	302	-	40,46,46	1.32	7 (17%)	50,70,70	2.12	14 (28%)
26	CLA	n	303	7	69,73,73	1.10	7 (10%)	82,113,113	1.06	7 (8%)
37	LHG	Y	306	26	48,48,48	0.52	0	51,54,54	0.52	0
37	LHG	d	402	-	42,42,48	0.57	0	45,48,54	0.50	0
39	CHL	r	316	43	44,58,74	2.09	10 (22%)	37,94,114	3.16	19 (51%)
39	CHL	N	316	7	44,58,74	2.16	11 (25%)	37,94,114	3.18	18 (48%)
39	CHL	n	307	-	44,58,74	2.10	11 (25%)	37,94,114	3.11	16 (43%)
39	CHL	n	319	7	44,58,74	2.13	11 (25%)	37,94,114	3.15	17 (45%)
39	CHL	y	312	43	44,58,74	2.10	11 (25%)	37,94,114	3.09	17 (45%)
37	LHG	R	303	26	48,48,48	0.51	0	51,54,54	0.52	0
26	CLA	D	401	43	69,73,73	1.10	8 (11%)	82,113,113	1.18	9 (10%)
26	CLA	B	609	2	69,73,73	1.14	9 (13%)	82,113,113	1.26	8 (9%)
26	CLA	g	318	7	53,57,73	1.29	7 (13%)	61,93,113	1.36	5 (8%)
40	LUT	y	311	-	42,43,43	0.48	0	51,60,60	0.87	1 (1%)
39	CHL	s	317	-	44,58,74	2.14	11 (25%)	37,94,114	3.16	17 (45%)
26	CLA	c	510	3	53,57,73	1.27	8 (15%)	61,93,113	1.37	6 (9%)
33	DGD	c	501	-	63,63,67	0.63	0	77,77,81	0.70	0
26	CLA	r	315	17	53,57,73	1.27	7 (13%)	61,93,113	1.38	8 (13%)
28	BCR	C	514	-	41,41,41	0.33	0	56,56,56	0.74	2 (3%)
39	CHL	Y	307	23	60,74,74	1.86	12 (20%)	58,114,114	2.52	18 (31%)
39	CHL	Y	314	43	44,58,74	2.12	11 (25%)	37,94,114	3.11	17 (45%)
40	LUT	S	301	-	42,43,43	0.45	0	51,60,60	0.73	0
40	LUT	s	308	-	42,43,43	0.45	0	51,60,60	0.72	0
37	LHG	L	101	-	48,48,48	0.52	0	51,54,54	0.56	0
41	XAT	R	304	-	41,47,47	1.13	4 (9%)	54,74,74	2.03	12 (22%)
32	BCT	A	411	31	3,3,3	2.36	1 (33%)	2,3,3	1.87	1 (50%)
39	CHL	g	314	7	42,56,74	2.24	11 (26%)	36,92,114	3.09	17 (47%)
26	CLA	C	515	3	69,73,73	1.12	7 (10%)	82,113,113	1.25	7 (8%)
29	SQD	w	202	-	31,33,54	1.01	2 (6%)	41,44,65	1.06	2 (4%)
39	CHL	g	311	7	60,74,74	1.87	12 (20%)	58,114,114	2.51	18 (31%)
39	CHL	R	301	43	44,58,74	2.09	10 (22%)	37,94,114	3.17	19 (51%)
26	CLA	s	311	18	53,57,73	1.29	8 (15%)	61,93,113	1.23	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	C	502	-	41,41,41	0.35	0	56,56,56	0.86	2 (3%)
26	CLA	b	605	2	69,73,73	1.12	8 (11%)	82,113,113	1.21	6 (7%)
41	XAT	r	304	-	41,47,47	1.12	4 (9%)	54,74,74	2.01	12 (22%)
26	CLA	R	307	17	53,57,73	2.64	11 (20%)	61,93,113	1.41	4 (6%)
39	CHL	R	318	23	42,56,74	2.15	11 (26%)	36,92,114	3.14	18 (50%)
39	CHL	R	315	43	44,58,74	2.12	12 (27%)	37,94,114	3.13	18 (48%)
26	CLA	b	606	2	69,73,73	1.14	9 (13%)	82,113,113	1.21	6 (7%)
26	CLA	C	508	3	69,73,73	1.14	9 (13%)	82,113,113	1.22	7 (8%)
40	LUT	Y	315	-	42,43,43	0.47	0	51,60,60	0.86	1 (1%)
26	CLA	B	610	2	69,73,73	1.10	8 (11%)	82,113,113	1.25	6 (7%)
26	CLA	y	315	23	53,57,73	1.26	7 (13%)	61,93,113	1.42	6 (9%)
26	CLA	b	604	-	69,73,73	1.15	8 (11%)	82,113,113	1.21	5 (6%)
26	CLA	B	617	2	69,73,73	1.11	8 (11%)	82,113,113	1.24	8 (9%)
39	CHL	r	318	43	44,58,74	2.10	12 (27%)	37,94,114	3.13	18 (48%)
26	CLA	n	302	7	53,57,73	1.30	9 (16%)	61,93,113	1.39	4 (6%)
40	LUT	n	317	-	42,43,43	0.47	0	51,60,60	0.85	1 (1%)
40	LUT	s	312	-	42,43,43	0.47	0	51,60,60	0.88	1 (1%)
26	CLA	B	616	2	69,73,73	1.12	5 (7%)	82,113,113	1.29	6 (7%)
28	BCR	A	406	-	41,41,41	0.32	0	56,56,56	0.51	0
26	CLA	A	405	1	64,68,73	1.14	8 (12%)	76,107,113	1.21	6 (7%)
40	LUT	G	316	-	42,43,43	0.47	0	51,60,60	0.96	0
29	SQD	A	410	-	48,50,54	0.79	1 (2%)	58,61,65	0.98	2 (3%)
39	CHL	S	312	-	43,57,74	2.21	12 (27%)	37,93,114	3.18	16 (43%)
39	CHL	S	313	-	44,58,74	2.15	11 (25%)	37,94,114	3.14	17 (45%)
28	BCR	k	101	-	41,41,41	0.35	0	56,56,56	0.89	3 (5%)
26	CLA	N	319	37	53,57,73	1.31	7 (13%)	61,93,113	1.35	6 (9%)
26	CLA	g	308	7	53,57,73	1.30	9 (16%)	61,93,113	1.36	5 (8%)
37	LHG	n	301	26	48,48,48	0.52	0	51,54,54	0.47	0
33	DGD	C	509	-	56,56,67	0.69	0	70,70,81	0.74	0
39	CHL	g	313	-	44,58,74	2.20	11 (25%)	37,94,114	3.10	15 (40%)
34	LMG	c	509	-	51,51,55	0.52	0	59,59,63	0.60	0
28	BCR	b	615	-	41,41,41	0.32	0	56,56,56	0.53	0
39	CHL	Y	318	-	44,58,74	2.13	13 (29%)	37,94,114	3.16	18 (48%)
26	CLA	C	516	43	69,73,73	1.16	7 (10%)	82,113,113	1.30	5 (6%)
26	CLA	N	307	7	69,73,73	1.12	7 (10%)	82,113,113	1.22	7 (8%)
40	LUT	N	314	-	42,43,43	0.47	0	51,60,60	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	Y	308	23	69,73,73	1.11	7 (10%)	82,113,113	1.28	8 (9%)
34	LMG	W	201	-	48,48,55	0.58	0	56,56,63	0.63	1 (1%)
26	CLA	b	616	43	69,73,73	1.12	7 (10%)	82,113,113	1.22	6 (7%)
33	DGD	c	517	-	56,56,67	0.70	0	70,70,81	0.75	0
27	PHO	A	404	-	58,69,69	2.08	11 (18%)	55,99,99	1.44	7 (12%)
26	CLA	B	612	43	69,73,73	1.14	8 (11%)	82,113,113	1.23	6 (7%)
26	CLA	G	307	7	69,73,73	1.13	8 (11%)	82,113,113	1.10	7 (8%)
26	CLA	s	305	18	53,57,73	1.26	7 (13%)	61,93,113	1.25	6 (9%)
26	CLA	r	303	17	53,57,73	1.30	9 (16%)	61,93,113	1.28	4 (6%)
34	LMG	C	518	-	51,51,55	0.52	0	59,59,63	0.58	0
39	CHL	y	302	-	44,58,74	2.13	12 (27%)	37,94,114	3.14	18 (48%)
26	CLA	n	309	7	53,57,73	1.28	7 (13%)	61,93,113	1.31	4 (6%)
26	CLA	S	309	18	53,57,73	1.29	8 (15%)	61,93,113	1.40	7 (11%)
28	BCR	B	619	-	41,41,41	0.37	0	56,56,56	0.73	0
34	LMG	c	512	-	51,51,55	0.48	0	59,59,63	0.64	0
26	CLA	b	609	2	69,73,73	1.11	5 (7%)	82,113,113	1.30	6 (7%)
26	CLA	b	611	2	69,73,73	1.23	8 (11%)	82,113,113	1.44	8 (9%)
33	DGD	C	510	-	63,63,67	0.63	0	77,77,81	0.68	0
26	CLA	a	402	1	64,68,73	1.15	9 (14%)	76,107,113	1.19	6 (7%)
30	PL9	d	408	-	55,55,55	1.36	6 (10%)	68,69,69	1.48	10 (14%)
26	CLA	N	312	7	69,73,73	1.11	7 (10%)	82,113,113	1.06	6 (7%)
26	CLA	y	313	43	53,57,73	1.35	8 (15%)	61,93,113	1.25	6 (9%)
39	CHL	N	317	7	44,58,74	2.14	11 (25%)	37,94,114	3.16	17 (45%)
29	SQD	W	202	-	31,33,54	1.02	2 (6%)	41,44,65	1.06	2 (4%)
37	LHG	N	301	26	48,48,48	0.52	0	51,54,54	0.48	0
40	LUT	g	316	-	42,43,43	0.47	0	51,60,60	0.94	0
26	CLA	Y	311	23	53,57,73	1.26	7 (13%)	61,93,113	1.42	6 (9%)
26	CLA	r	305	17	53,57,73	1.31	7 (13%)	61,93,113	1.29	5 (8%)
26	CLA	n	310	37	53,57,73	1.32	7 (13%)	61,93,113	1.37	6 (9%)
34	LMG	w	201	-	48,48,55	0.59	0	56,56,63	0.65	1 (1%)
26	CLA	s	306	18	53,57,73	1.29	7 (13%)	61,93,113	1.28	5 (8%)
26	CLA	c	505	3	69,73,73	1.15	9 (13%)	82,113,113	1.28	6 (7%)
26	CLA	C	504	3	69,73,73	1.12	8 (11%)	82,113,113	1.30	4 (4%)
26	CLA	g	304	7	53,57,73	1.30	8 (15%)	61,93,113	1.34	5 (8%)
34	LMG	d	405	-	46,46,55	0.60	0	54,54,63	0.68	1 (1%)

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
26	CLA	g	303	7	1/1/15/20	10/39/115/115	-
26	CLA	Y	310	23	1/1/11/20	11/20/96/115	-
42	NEX	y	307	-	-	2/27/83/83	0/3/3/3
26	CLA	C	519	3	1/1/11/20	5/20/96/115	-
26	CLA	r	314	17	1/1/15/20	13/39/115/115	-
26	CLA	R	317	17	1/1/11/20	2/20/96/115	-
39	CHL	g	307	-	3/3/16/26	8/20/118/137	-
26	CLA	r	311	43	1/1/11/20	12/20/96/115	-
26	CLA	s	301	37	1/1/11/20	9/20/96/115	-
39	CHL	G	301	-	3/3/16/26	10/20/118/137	-
30	PL9	D	411	-	-	5/53/73/73	0/1/1/1
26	CLA	N	318	7	1/1/11/20	7/20/96/115	-
42	NEX	S	305	-	-	7/27/83/83	0/3/3/3
34	LMG	C	503	-	-	19/46/66/70	0/1/1/1
26	CLA	R	314	37	1/1/11/20	10/20/96/115	-
39	CHL	S	302	-	3/3/16/26	13/20/118/137	-
26	CLA	G	302	-	1/1/11/20	8/20/96/115	-
26	CLA	s	314	18	1/1/11/20	10/20/96/115	-
39	CHL	Y	317	43	3/3/16/26	5/20/118/137	-
26	CLA	R	309	17	1/1/11/20	11/20/96/115	-
40	LUT	N	305	-	-	3/29/67/67	0/2/2/2
26	CLA	S	314	18	1/1/11/20	5/20/96/115	-
30	PL9	a	407	-	-	5/14/34/73	0/1/1/1
26	CLA	b	601	2	1/1/15/20	12/39/115/115	-
40	LUT	g	310	-	-	1/29/67/67	0/2/2/2
40	LUT	S	306	-	-	2/29/67/67	0/2/2/2
26	CLA	b	610	2	1/1/15/20	7/39/115/115	-
26	CLA	B	602	2	1/1/15/20	14/39/115/115	-
26	CLA	y	306	23	1/1/15/20	12/39/115/115	-
28	BCR	c	511	-	-	2/29/63/63	0/2/2/2
39	CHL	N	303	-	3/3/20/26	12/39/137/137	-
37	LHG	D	407	-	-	15/47/47/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	S	316	18	3/3/17/26	6/23/121/137	-
39	CHL	N	310	7	3/3/16/26	5/18/116/137	-
39	CHL	s	316	-	3/3/16/26	13/20/118/137	-
39	CHL	g	319	-	3/3/16/26	6/20/118/137	-
28	BCR	b	603	-	-	0/29/63/63	0/2/2/2
26	CLA	R	316	17	1/1/11/20	6/20/96/115	-
26	CLA	R	310	17	1/1/11/20	6/20/96/115	-
26	CLA	d	404	4	1/1/15/20	8/39/115/115	-
28	BCR	b	619	-	-	4/29/63/63	0/2/2/2
42	NEX	R	305	-	-	2/27/83/83	0/3/3/3
26	CLA	r	310	17	1/1/11/20	6/20/96/115	-
27	PHO	d	407	-	-	12/37/103/103	0/5/6/6
42	NEX	N	302	-	-	2/27/83/83	0/3/3/3
39	CHL	r	309	43	3/3/16/26	10/20/118/137	-
33	DGD	b	620	-	-	18/51/91/95	0/2/2/2
29	SQD	b	621	-	-	26/49/69/69	0/1/1/1
41	XAT	G	310	-	-	0/31/93/93	0/4/4/4
26	CLA	S	303	18	1/1/11/20	6/20/96/115	-
28	BCR	d	401	-	-	9/29/63/63	0/2/2/2
26	CLA	n	305	7	1/1/15/20	7/39/115/115	-
26	CLA	c	508	43	1/1/15/20	10/39/115/115	-
26	CLA	B	604	2	1/1/15/20	3/39/115/115	-
26	CLA	C	507	3	1/1/15/20	11/39/115/115	-
37	LHG	g	301	26	-	16/53/53/53	-
39	CHL	n	318	-	3/3/20/26	13/39/137/137	-
33	DGD	y	308	-	-	14/32/72/95	0/2/2/2
42	NEX	G	315	-	-	2/27/83/83	0/3/3/3
26	CLA	B	615	2	1/1/15/20	17/39/115/115	-
26	CLA	y	309	23	1/1/15/20	11/39/115/115	-
26	CLA	b	608	43	1/1/15/20	18/39/115/115	-
26	CLA	b	607	2	1/1/15/20	12/39/115/115	-
26	CLA	g	302	-	1/1/11/20	7/20/96/115	-
26	CLA	c	503	3	1/1/15/20	15/39/115/115	-
26	CLA	Y	312	23	1/1/15/20	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	606	2	1/1/15/20	13/39/115/115	-
26	CLA	D	412	43	1/1/11/20	8/20/96/115	-
26	CLA	b	617	2	1/1/15/20	10/39/115/115	-
39	CHL	Y	302	23	3/3/20/26	12/39/137/137	-
26	CLA	S	315	18	1/1/11/20	10/20/96/115	-
26	CLA	N	309	7	1/1/11/20	10/20/96/115	-
39	CHL	s	313	-	3/3/16/26	8/19/117/137	-
34	LMG	D	404	-	-	10/41/61/70	0/1/1/1
26	CLA	s	307	18	1/1/11/20	6/20/96/115	-
39	CHL	G	305	-	3/3/16/26	7/20/118/137	-
26	CLA	c	506	3	1/1/15/20	13/51/101/115	-
26	CLA	B	607	43	1/1/15/20	10/39/115/115	-
26	CLA	r	308	17	1/1/11/20	7/20/96/115	-
39	CHL	G	318	7	3/3/20/26	19/39/137/137	-
26	CLA	G	317	7	1/1/11/20	9/20/96/115	-
26	CLA	d	403	4	1/1/15/20	12/39/115/115	-
26	CLA	G	313	37	1/1/11/20	6/20/96/115	-
26	CLA	R	302	17	1/1/11/20	10/20/96/115	-
26	CLA	a	409	43	1/1/15/20	1/39/115/115	-
26	CLA	c	504	3	1/1/15/20	8/39/115/115	-
37	LHG	r	312	26	-	16/53/53/53	-
26	CLA	C	520	3	1/1/15/20	12/51/101/115	-
42	NEX	g	306	-	-	2/27/83/83	0/3/3/3
26	CLA	C	505	3	1/1/15/20	10/39/115/115	-
39	CHL	n	306	7	3/3/16/26	6/20/118/137	-
26	CLA	C	521	43	1/1/15/20	7/39/115/115	-
28	BCR	D	405	-	-	9/29/63/63	0/2/2/2
39	CHL	r	301	23	3/3/16/26	7/18/116/137	-
39	CHL	g	312	7	3/3/16/26	8/20/118/137	-
26	CLA	c	520	3	1/1/15/20	9/39/115/115	-
26	CLA	r	313	17	1/1/11/20	10/20/96/115	-
37	LHG	D	410	-	-	9/41/41/53	-
41	XAT	n	316	-	-	0/31/93/93	0/4/4/4
39	CHL	N	304	43	3/3/16/26	7/20/118/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	Y	316	43	1/1/11/20	5/20/96/115	-
28	BCR	T	101	-	-	16/29/63/63	0/2/2/2
26	CLA	b	612	2	1/1/15/20	3/39/115/115	-
26	CLA	S	311	18	1/1/11/20	7/20/96/115	-
26	CLA	S	307	18	1/1/11/20	9/20/96/115	-
37	LHG	G	312	26	-	15/53/53/53	-
36	LMT	D	402	-	-	7/21/61/61	0/2/2/2
26	CLA	c	516	3	1/1/15/20	11/39/115/115	-
26	CLA	s	310	-	1/1/11/20	14/20/96/115	-
26	CLA	Y	313	23	1/1/15/20	16/39/115/115	-
26	CLA	S	308	37	1/1/11/20	9/20/96/115	-
26	CLA	N	313	7	1/1/11/20	9/20/96/115	-
28	BCR	H	101	-	-	2/29/63/63	0/2/2/2
39	CHL	R	312	43	3/3/16/26	10/20/118/137	-
34	LMG	b	622	-	-	16/46/66/70	0/1/1/1
41	XAT	G	320	-	-	4/31/93/93	0/4/4/4
40	LUT	R	311	-	-	8/29/67/67	0/2/2/2
26	CLA	r	317	37	1/1/11/20	10/20/96/115	-
26	CLA	c	514	43	1/1/15/20	7/39/115/115	-
26	CLA	C	517	3	1/1/15/20	4/39/115/115	-
26	CLA	n	315	7	1/1/11/20	10/20/96/115	-
39	CHL	N	311	-	3/3/16/26	10/20/118/137	-
26	CLA	b	618	2	1/1/15/20	10/39/115/115	-
26	CLA	a	411	1	1/1/15/20	8/39/115/115	-
39	CHL	y	303	23	3/3/20/26	12/39/137/137	-
26	CLA	y	310	23	1/1/15/20	12/39/115/115	-
28	BCR	K	101	-	-	2/29/63/63	0/2/2/2
37	LHG	l	101	-	-	13/53/53/53	-
37	LHG	d	410	-	-	9/41/41/53	-
26	CLA	R	306	17	1/1/15/20	7/39/115/115	-
26	CLA	Y	301	37	1/1/15/20	11/39/115/115	-
37	LHG	s	309	26	-	22/53/53/53	-
26	CLA	c	502	3	1/1/15/20	10/39/115/115	-
26	CLA	d	411	43	1/1/11/20	8/20/96/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	r	306	17	1/1/15/20	5/39/115/115	-
39	CHL	y	305	43	3/3/16/26	5/20/118/137	-
42	NEX	n	313	-	-	3/27/83/83	0/3/3/3
36	LMT	d	406	-	-	7/21/61/61	0/2/2/2
37	LHG	D	408	-	-	15/53/53/53	-
42	NEX	Y	304	-	-	2/27/83/83	0/3/3/3
27	PHO	a	410	-	-	10/37/103/103	0/5/6/6
28	BCR	B	614	-	-	3/29/63/63	0/2/2/2
37	LHG	d	409	-	-	13/53/53/53	-
26	CLA	B	611	2	1/1/15/20	14/39/115/115	-
26	CLA	C	512	3	1/1/15/20	8/39/115/115	-
39	CHL	y	314	23	3/3/20/26	11/39/137/137	-
26	CLA	b	613	2	1/1/15/20	10/39/115/115	-
26	CLA	B	601	2	1/1/15/20	12/39/115/115	-
26	CLA	D	409	4	1/1/15/20	8/39/115/115	-
27	PHO	D	403	-	-	12/37/103/103	0/5/6/6
26	CLA	b	614	43	1/1/15/20	4/39/115/115	-
26	CLA	y	304	37	1/1/15/20	11/39/115/115	-
26	CLA	s	304	18	1/1/11/20	7/20/96/115	-
28	BCR	a	404	-	-	2/29/63/63	0/2/2/2
40	LUT	r	307	-	-	8/29/67/67	0/2/2/2
26	CLA	S	304	18	1/1/11/20	6/20/96/115	-
26	CLA	B	603	2	1/1/15/20	7/39/115/115	-
39	CHL	n	311	43	3/3/16/26	7/20/118/137	-
33	DGD	Y	303	-	-	13/32/72/95	0/2/2/2
26	CLA	N	306	7	1/1/11/20	10/20/96/115	-
26	CLA	c	518	3	1/1/15/20	6/39/115/115	-
41	XAT	g	309	-	-	0/31/93/93	0/4/4/4
26	CLA	c	513	3	1/1/15/20	4/39/115/115	-
26	CLA	N	308	43	1/1/11/20	7/20/96/115	-
26	CLA	g	317	7	1/1/15/20	10/39/115/115	-
30	PL9	A	408	-	-	4/14/34/73	0/1/1/1
39	CHL	G	303	-	3/3/16/26	9/20/118/137	-
26	CLA	C	506	3	1/1/15/20	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	DGD	C	513	-	-	17/51/91/95	0/2/2/2
38	HEM	e	101	5,6	-	2/14/54/54	-
29	SQD	a	413	-	-	17/45/65/69	0/1/1/1
26	CLA	B	605	43	1/1/15/20	17/39/115/115	-
26	CLA	G	319	7	1/1/11/20	11/20/96/115	-
26	CLA	G	306	7	1/1/11/20	8/20/96/115	-
28	BCR	J	101	-	-	8/29/63/63	0/2/2/2
26	CLA	A	403	1	1/1/15/20	8/39/115/115	-
41	XAT	g	320	-	-	3/31/93/93	0/4/4/4
40	LUT	Y	309	-	-	3/29/67/67	0/2/2/2
37	LHG	S	317	26	-	22/53/53/53	-
26	CLA	c	515	3	1/1/15/20	9/39/115/115	-
28	BCR	c	507	-	-	4/29/63/63	0/2/2/2
40	LUT	y	318	-	-	3/29/67/67	0/2/2/2
40	LUT	G	308	-	-	1/29/67/67	0/2/2/2
26	CLA	D	406	4	1/1/15/20	12/39/115/115	-
26	CLA	C	511	3	1/1/15/20	12/39/115/115	-
26	CLA	Y	305	23	1/1/15/20	12/39/115/115	-
26	CLA	B	613	-	1/1/15/20	9/39/115/115	-
26	CLA	g	305	7	1/1/11/20	9/20/96/115	-
28	BCR	t	101	-	-	15/29/63/63	0/2/2/2
33	DGD	B	620	-	-	16/51/91/95	0/2/2/2
37	LHG	y	301	26	-	28/53/53/53	-
29	SQD	A	407	-	-	23/49/69/69	0/1/1/1
26	CLA	g	315	37	1/1/11/20	6/20/96/115	-
26	CLA	b	602	2	1/1/15/20	7/39/115/115	-
29	SQD	B	621	-	-	25/49/69/69	0/1/1/1
40	LUT	n	314	-	-	1/29/67/67	0/2/2/2
26	CLA	s	315	18	1/1/11/20	5/20/96/115	-
26	CLA	R	313	17	1/1/15/20	11/39/115/115	-
39	CHL	G	309	7	3/3/16/26	12/18/116/137	-
41	XAT	N	315	-	-	0/31/93/93	0/4/4/4
33	DGD	c	519	-	-	17/51/91/95	0/2/2/2
26	CLA	y	316	23	1/1/15/20	14/39/115/115	-
29	SQD	a	403	-	-	22/49/69/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	j	101	-	-	7/29/63/63	0/2/2/2
39	CHL	G	311	7	3/3/16/26	8/20/118/137	-
26	CLA	n	304	7	1/1/11/20	9/20/96/115	-
26	CLA	G	314	7	1/1/15/20	9/39/115/115	-
26	CLA	B	618	2	1/1/15/20	10/39/115/115	-
34	LMG	B	622	-	-	17/46/66/70	0/1/1/1
28	BCR	B	608	-	-	1/29/63/63	0/2/2/2
26	CLA	n	312	43	1/1/11/20	7/20/96/115	-
26	CLA	y	317	23	1/1/11/20	11/20/96/115	-
39	CHL	n	308	7	3/3/16/26	5/18/116/137	-
26	CLA	R	308	43	1/1/11/20	12/20/96/115	-
42	NEX	s	302	-	-	6/27/83/83	0/3/3/3
38	HEM	E	101	5,6	-	2/14/54/54	-
26	CLA	G	304	7	1/1/11/20	8/20/96/115	-
39	CHL	s	303	18	3/3/17/26	6/23/121/137	-
28	BCR	h	101	-	-	2/29/63/63	0/2/2/2
26	CLA	S	310	-	1/1/11/20	14/20/96/115	-
42	NEX	r	302	-	-	2/27/83/83	0/3/3/3
26	CLA	n	303	7	1/1/15/20	9/39/115/115	-
37	LHG	Y	306	26	-	28/53/53/53	-
37	LHG	d	402	-	-	15/47/47/53	-
39	CHL	r	316	43	3/3/16/26	10/20/118/137	-
39	CHL	N	316	7	3/3/16/26	6/20/118/137	-
39	CHL	n	307	-	3/3/16/26	10/20/118/137	-
39	CHL	n	319	7	3/3/16/26	6/20/118/137	-
39	CHL	y	312	43	3/3/16/26	8/20/118/137	-
37	LHG	R	303	26	-	17/53/53/53	-
26	CLA	D	401	43	1/1/15/20	1/39/115/115	-
26	CLA	B	609	2	1/1/15/20	9/39/115/115	-
26	CLA	g	318	7	1/1/11/20	8/20/96/115	-
40	LUT	y	311	-	-	0/29/67/67	0/2/2/2
39	CHL	s	317	-	3/3/16/26	7/20/118/137	-
26	CLA	c	510	3	1/1/11/20	5/20/96/115	-
33	DGD	c	501	-	-	18/51/91/95	0/2/2/2
26	CLA	r	315	17	1/1/11/20	2/20/96/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	C	514	-	-	4/29/63/63	0/2/2/2
39	CHL	Y	307	23	3/3/20/26	12/39/137/137	-
39	CHL	Y	314	43	3/3/16/26	8/20/118/137	-
40	LUT	S	301	-	-	3/29/67/67	0/2/2/2
40	LUT	s	308	-	-	3/29/67/67	0/2/2/2
37	LHG	L	101	-	-	9/53/53/53	-
41	XAT	R	304	-	-	1/31/93/93	0/4/4/4
39	CHL	g	314	7	3/3/16/26	11/18/116/137	-
26	CLA	C	515	3	1/1/15/20	8/39/115/115	-
29	SQD	w	202	-	-	13/28/48/69	0/1/1/1
39	CHL	g	311	7	3/3/20/26	18/39/137/137	-
39	CHL	R	301	43	3/3/16/26	11/20/118/137	-
26	CLA	s	311	18	1/1/11/20	7/20/96/115	-
28	BCR	C	502	-	-	1/29/63/63	0/2/2/2
26	CLA	b	605	2	1/1/15/20	14/39/115/115	-
41	XAT	r	304	-	-	1/31/93/93	0/4/4/4
39	CHL	R	318	23	3/3/16/26	8/18/116/137	-
26	CLA	R	307	17	-	7/20/96/115	-
39	CHL	R	315	43	3/3/16/26	8/20/118/137	-
26	CLA	b	606	2	1/1/15/20	14/39/115/115	-
26	CLA	C	508	3	1/1/15/20	12/39/115/115	-
40	LUT	Y	315	-	-	2/29/67/67	0/2/2/2
26	CLA	B	610	2	1/1/15/20	10/39/115/115	-
26	CLA	y	315	23	1/1/11/20	7/20/96/115	-
26	CLA	b	604	-	1/1/15/20	9/39/115/115	-
26	CLA	B	617	2	1/1/15/20	8/39/115/115	-
39	CHL	r	318	43	3/3/16/26	7/20/118/137	-
26	CLA	n	302	7	1/1/11/20	7/20/96/115	-
40	LUT	n	317	-	-	3/29/67/67	0/2/2/2
40	LUT	s	312	-	-	2/29/67/67	0/2/2/2
26	CLA	B	616	2	1/1/15/20	10/39/115/115	-
28	BCR	A	406	-	-	2/29/63/63	0/2/2/2
26	CLA	A	405	1	1/1/14/20	4/33/109/115	-
40	LUT	G	316	-	-	0/29/67/67	0/2/2/2
29	SQD	A	410	-	-	17/45/65/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	CHL	S	312	-	3/3/16/26	8/19/117/137	-
39	CHL	S	313	-	3/3/16/26	8/20/118/137	-
28	BCR	k	101	-	-	2/29/63/63	0/2/2/2
26	CLA	N	319	37	1/1/11/20	10/20/96/115	-
26	CLA	g	308	7	1/1/11/20	9/20/96/115	-
37	LHG	n	301	26	-	12/53/53/53	-
33	DGD	C	509	-	-	18/44/84/95	0/2/2/2
39	CHL	g	313	-	3/3/16/26	10/20/118/137	-
34	LMG	c	509	-	-	19/46/66/70	0/1/1/1
28	BCR	b	615	-	-	1/29/63/63	0/2/2/2
39	CHL	Y	318	-	3/3/16/26	6/20/118/137	-
26	CLA	C	516	43	1/1/15/20	10/39/115/115	-
26	CLA	N	307	7	1/1/15/20	6/39/115/115	-
40	LUT	N	314	-	-	0/29/67/67	0/2/2/2
26	CLA	Y	308	23	1/1/15/20	12/39/115/115	-
34	LMG	W	201	-	-	14/43/63/70	0/1/1/1
26	CLA	b	616	43	1/1/15/20	10/39/115/115	-
33	DGD	c	517	-	-	18/44/84/95	0/2/2/2
27	PHO	A	404	-	-	10/37/103/103	0/5/6/6
26	CLA	B	612	43	1/1/15/20	4/39/115/115	-
26	CLA	G	307	7	1/1/15/20	11/39/115/115	-
26	CLA	s	305	18	1/1/11/20	5/20/96/115	-
26	CLA	r	303	17	1/1/11/20	6/20/96/115	-
34	LMG	C	518	-	-	19/46/66/70	0/1/1/1
39	CHL	y	302	-	3/3/16/26	6/20/118/137	-
26	CLA	n	309	7	1/1/11/20	9/20/96/115	-
26	CLA	S	309	18	1/1/11/20	7/20/96/115	-
28	BCR	B	619	-	-	0/29/63/63	0/2/2/2
34	LMG	c	512	-	-	19/46/66/70	0/1/1/1
26	CLA	b	609	2	1/1/15/20	10/39/115/115	-
26	CLA	b	611	2	1/1/15/20	17/39/115/115	-
33	DGD	C	510	-	-	15/51/91/95	0/2/2/2
26	CLA	a	402	1	1/1/14/20	4/33/109/115	-
30	PL9	d	408	-	-	4/53/73/73	0/1/1/1
26	CLA	N	312	7	1/1/15/20	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	y	313	43	1/1/11/20	5/20/96/115	-
39	CHL	N	317	7	3/3/16/26	6/20/118/137	-
29	SQD	W	202	-	-	14/28/48/69	0/1/1/1
37	LHG	N	301	26	-	13/53/53/53	-
40	LUT	g	316	-	-	1/29/67/67	0/2/2/2
26	CLA	Y	311	23	1/1/11/20	7/20/96/115	-
26	CLA	r	305	17	1/1/11/20	10/20/96/115	-
26	CLA	n	310	37	1/1/11/20	11/20/96/115	-
34	LMG	w	201	-	-	15/43/63/70	0/1/1/1
26	CLA	s	306	18	1/1/11/20	10/20/96/115	-
26	CLA	c	505	3	1/1/15/20	12/39/115/115	-
26	CLA	C	504	3	1/1/15/20	8/39/115/115	-
26	CLA	g	304	7	1/1/11/20	11/20/96/115	-
34	LMG	d	405	-	-	10/41/61/70	0/1/1/1

The worst 5 of 1969 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	307	CLA	MG-NC	14.46	2.40	2.06
27	d	407	PHO	C1B-C2B	8.98	1.49	1.39
27	A	404	PHO	C1B-C2B	8.95	1.49	1.39
27	D	403	PHO	C1B-C2B	8.95	1.49	1.39
27	a	410	PHO	C1B-C2B	8.89	1.49	1.39

The worst 5 of 2193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	303	CHL	C1B-CHB-C4A	12.88	129.61	121.32
39	Y	302	CHL	C1B-CHB-C4A	12.86	129.59	121.32
39	N	316	CHL	C1B-CHB-C4A	12.83	129.57	121.32
39	n	306	CHL	C1B-CHB-C4A	12.77	129.54	121.32
39	g	311	CHL	C1B-CHB-C4A	12.67	129.47	121.32

5 of 305 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	403	CLA	ND
26	A	405	CLA	ND
26	B	601	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
26	B	602	CLA	ND
26	B	603	CLA	ND

5 of 2875 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	B	601	CLA	CAD-CBD-CGD-O1D
26	B	601	CLA	CAD-CBD-CGD-O2D
26	B	605	CLA	CAD-CBD-CGD-O2D
26	B	606	CLA	C1A-C2A-CAA-CBA
26	B	606	CLA	C4-C3-C5-C6

There are no ring outliers.

304 monomers are involved in 836 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	g	303	CLA	3	0
26	Y	310	CLA	1	0
42	y	307	NEX	3	0
26	C	519	CLA	1	0
26	r	314	CLA	3	0
26	R	317	CLA	2	0
39	g	307	CHL	4	0
26	r	311	CLA	4	0
26	s	301	CLA	3	0
30	D	411	PL9	3	0
39	G	301	CHL	5	0
26	N	318	CLA	3	0
42	S	305	NEX	7	0
34	C	503	LMG	2	0
39	S	302	CHL	6	0
26	G	302	CLA	2	0
26	s	314	CLA	2	0
39	Y	317	CHL	3	0
26	R	309	CLA	2	0
40	N	305	LUT	3	0
26	S	314	CLA	4	0
30	a	407	PL9	4	0
26	b	601	CLA	6	0
40	g	310	LUT	4	0
40	S	306	LUT	3	0
26	b	610	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	602	CLA	7	0
26	y	306	CLA	3	0
28	c	511	BCR	4	0
35	C	501	OEX	2	0
37	D	407	LHG	3	0
39	N	303	CHL	3	0
39	S	316	CHL	1	0
39	N	310	CHL	2	0
39	s	316	CHL	6	0
39	g	319	CHL	3	0
28	b	603	BCR	5	0
26	R	316	CLA	1	0
26	d	404	CLA	9	0
28	b	619	BCR	5	0
42	R	305	NEX	3	0
27	d	407	PHO	8	0
42	N	302	NEX	2	0
39	r	309	CHL	3	0
33	b	620	DGD	3	0
29	b	621	SQD	3	0
41	G	310	XAT	6	0
26	S	303	CLA	2	0
26	n	305	CLA	2	0
26	c	508	CLA	3	0
26	B	604	CLA	2	0
26	C	507	CLA	5	0
37	g	301	LHG	8	0
39	n	318	CHL	5	0
33	y	308	DGD	2	0
42	G	315	NEX	4	0
26	B	615	CLA	4	0
26	y	309	CLA	7	0
26	b	608	CLA	6	0
26	b	607	CLA	5	0
26	g	302	CLA	2	0
26	c	503	CLA	5	0
26	Y	312	CLA	5	0
26	B	606	CLA	6	0
26	D	412	CLA	3	0
26	b	617	CLA	6	0
39	Y	302	CHL	7	0
26	S	315	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	s	313	CHL	6	0
34	D	404	LMG	1	0
26	s	307	CLA	2	0
39	G	305	CHL	3	0
26	c	506	CLA	5	0
26	B	607	CLA	3	0
26	r	308	CLA	1	0
39	G	318	CHL	7	0
26	G	317	CLA	3	0
26	d	403	CLA	4	0
26	G	313	CLA	2	0
26	R	302	CLA	6	0
26	a	409	CLA	2	0
26	c	504	CLA	5	0
37	r	312	LHG	2	0
26	C	520	CLA	5	0
42	g	306	NEX	4	0
26	C	505	CLA	3	0
39	n	306	CHL	6	0
26	C	521	CLA	4	0
39	r	301	CHL	2	0
39	g	312	CHL	4	0
26	c	520	CLA	3	0
26	r	313	CLA	7	0
37	D	410	LHG	2	0
41	n	316	XAT	4	0
39	N	304	CHL	1	0
26	Y	316	CLA	3	0
28	T	101	BCR	6	0
26	b	612	CLA	2	0
26	S	311	CLA	2	0
26	S	307	CLA	3	0
37	G	312	LHG	6	0
26	c	516	CLA	2	0
26	s	310	CLA	4	0
26	Y	313	CLA	3	0
26	S	308	CLA	3	0
26	N	313	CLA	2	0
28	H	101	BCR	2	0
39	R	312	CHL	3	0
34	b	622	LMG	3	0
41	G	320	XAT	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	R	311	LUT	5	0
26	r	317	CLA	1	0
26	c	514	CLA	5	0
26	C	517	CLA	3	0
26	n	315	CLA	2	0
39	N	311	CHL	4	0
26	b	618	CLA	3	0
26	a	411	CLA	3	0
39	y	303	CHL	6	0
26	y	310	CLA	6	0
28	K	101	BCR	5	0
37	l	101	LHG	3	0
37	d	410	LHG	2	0
26	R	306	CLA	4	0
26	Y	301	CLA	3	0
37	s	309	LHG	2	0
26	c	502	CLA	4	0
26	d	411	CLA	3	0
35	a	408	OEX	3	0
26	r	306	CLA	5	0
39	y	305	CHL	3	0
42	n	313	NEX	1	0
37	D	408	LHG	6	0
42	Y	304	NEX	3	0
27	a	410	PHO	1	0
28	B	614	BCR	3	0
37	d	409	LHG	4	0
26	B	611	CLA	3	0
26	C	512	CLA	5	0
39	y	314	CHL	3	0
26	b	613	CLA	7	0
26	B	601	CLA	5	0
26	D	409	CLA	9	0
27	D	403	PHO	7	0
26	b	614	CLA	3	0
26	y	304	CLA	3	0
26	s	304	CLA	2	0
28	a	404	BCR	1	0
40	r	307	LUT	6	0
26	S	304	CLA	1	0
26	B	603	CLA	4	0
33	Y	303	DGD	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	n	311	CHL	1	0
26	N	306	CLA	1	0
26	c	518	CLA	8	0
41	g	309	XAT	4	0
26	c	513	CLA	3	0
26	g	317	CLA	6	0
30	A	408	PL9	3	0
39	G	303	CHL	3	0
26	C	506	CLA	3	0
33	C	513	DGD	3	0
38	e	101	HEM	4	0
29	a	413	SQD	3	0
26	B	605	CLA	7	0
26	G	319	CLA	2	0
28	J	101	BCR	4	0
26	A	403	CLA	1	0
41	g	320	XAT	6	0
40	Y	309	LUT	5	0
37	S	317	LHG	2	0
26	c	515	CLA	4	0
28	c	507	BCR	3	0
40	y	318	LUT	5	0
40	G	308	LUT	4	0
26	D	406	CLA	1	0
26	C	511	CLA	4	0
26	Y	305	CLA	8	0
26	g	305	CLA	1	0
28	t	101	BCR	6	0
33	B	620	DGD	3	0
37	y	301	LHG	4	0
29	A	407	SQD	5	0
26	g	315	CLA	2	0
26	b	602	CLA	4	0
29	B	621	SQD	2	0
40	n	314	LUT	4	0
26	s	315	CLA	2	0
26	R	313	CLA	2	0
39	G	309	CHL	4	0
41	N	315	XAT	6	0
33	c	519	DGD	3	0
26	y	316	CLA	4	0
29	a	403	SQD	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	j	101	BCR	4	0
39	G	311	CHL	3	0
26	n	304	CLA	2	0
26	G	314	CLA	4	0
26	B	618	CLA	7	0
34	B	622	LMG	2	0
28	B	608	BCR	3	0
26	y	317	CLA	1	0
39	n	308	CHL	1	0
26	R	308	CLA	4	0
42	s	302	NEX	6	0
38	E	101	HEM	5	0
26	G	304	CLA	1	0
39	s	303	CHL	1	0
28	h	101	BCR	3	0
26	S	310	CLA	4	0
42	r	302	NEX	4	0
26	n	303	CLA	3	0
37	Y	306	LHG	4	0
37	d	402	LHG	4	0
39	r	316	CHL	1	0
39	N	316	CHL	5	0
39	n	307	CHL	4	0
39	n	319	CHL	2	0
39	y	312	CHL	2	0
26	D	401	CLA	3	0
26	B	609	CLA	4	0
40	y	311	LUT	6	0
39	s	317	CHL	3	0
26	c	510	CLA	2	0
33	c	501	DGD	3	0
26	r	315	CLA	1	0
28	C	514	BCR	2	0
39	Y	307	CHL	3	0
39	Y	314	CHL	1	0
40	S	301	LUT	3	0
40	s	308	LUT	2	0
37	L	101	LHG	2	0
41	R	304	XAT	1	0
39	g	314	CHL	4	0
26	C	515	CLA	5	0
39	g	311	CHL	7	0

Continued on next page...

Continued from previous page...

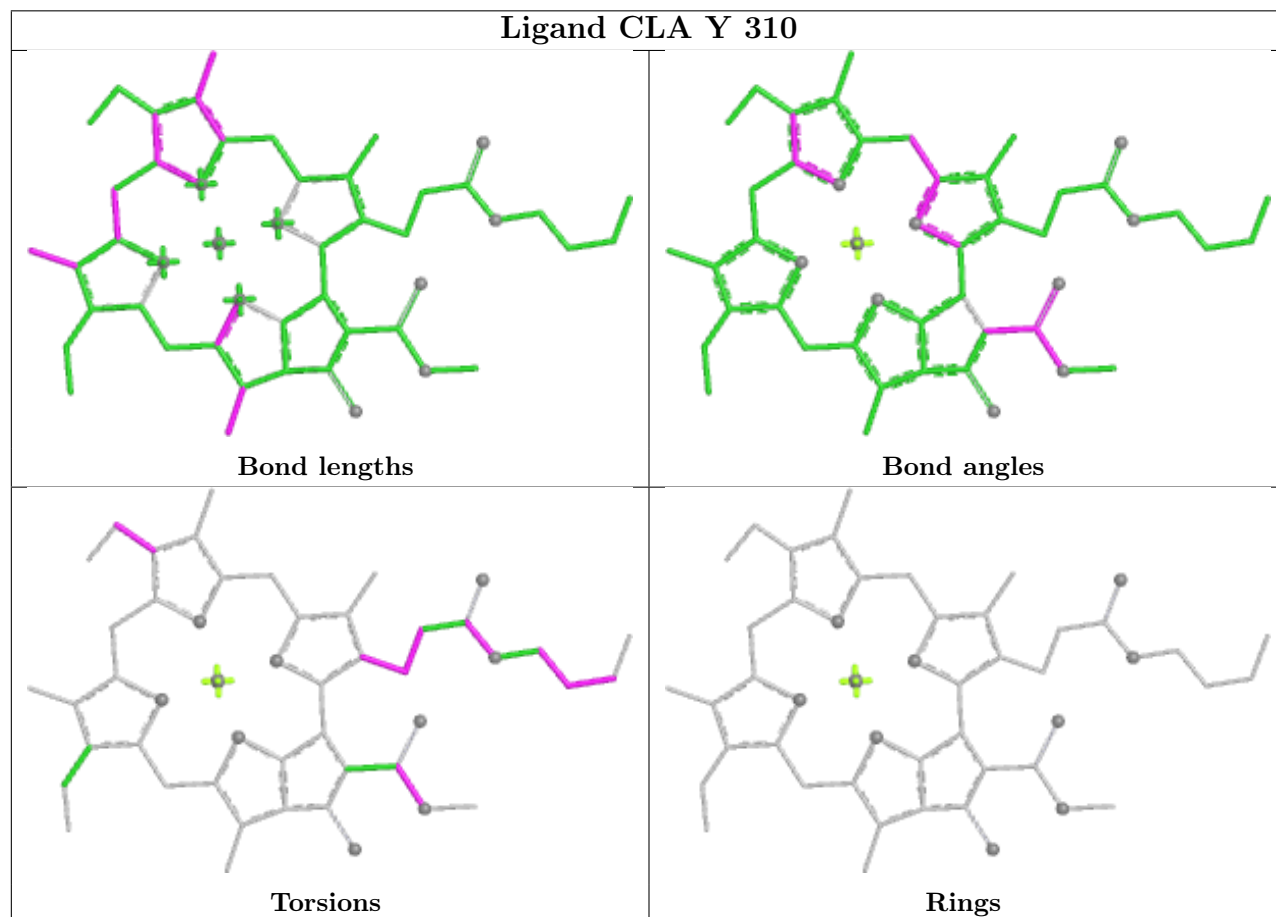
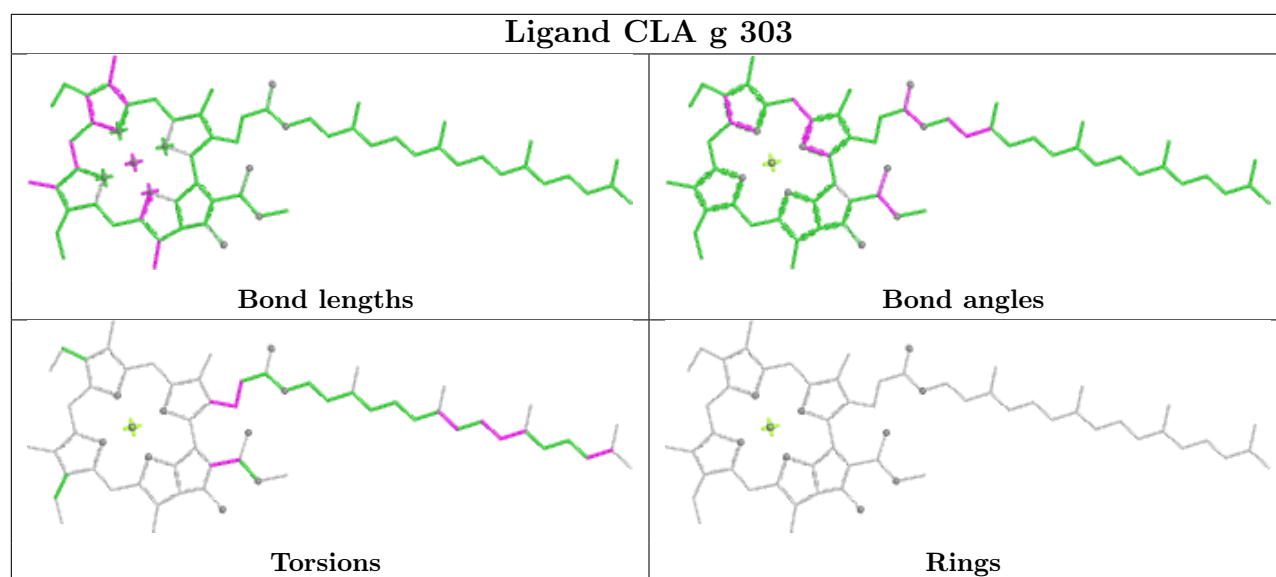
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	R	301	CHL	2	0
26	s	311	CLA	4	0
28	C	502	BCR	4	0
26	b	605	CLA	7	0
41	r	304	XAT	2	0
26	R	307	CLA	1	0
39	R	318	CHL	1	0
39	R	315	CHL	1	0
26	b	606	CLA	3	0
26	C	508	CLA	1	0
40	Y	315	LUT	7	0
26	B	610	CLA	7	0
26	y	315	CLA	2	0
26	B	617	CLA	2	0
39	r	318	CHL	2	0
26	n	302	CLA	2	0
40	n	317	LUT	3	0
40	s	312	LUT	3	0
26	B	616	CLA	6	0
28	A	406	BCR	1	0
26	A	405	CLA	2	0
40	G	316	LUT	1	0
29	A	410	SQD	2	0
39	S	312	CHL	5	0
39	S	313	CHL	3	0
28	k	101	BCR	5	0
26	N	319	CLA	3	0
26	g	308	CLA	3	0
37	n	301	LHG	5	0
33	C	509	DGD	4	0
39	g	313	CHL	5	0
28	b	615	BCR	3	0
39	Y	318	CHL	3	0
26	C	516	CLA	4	0
26	N	307	CLA	4	0
40	N	314	LUT	4	0
26	Y	308	CLA	4	0
34	W	201	LMG	3	0
26	b	616	CLA	1	0
33	c	517	DGD	2	0
27	A	404	PHO	2	0
26	B	612	CLA	2	0

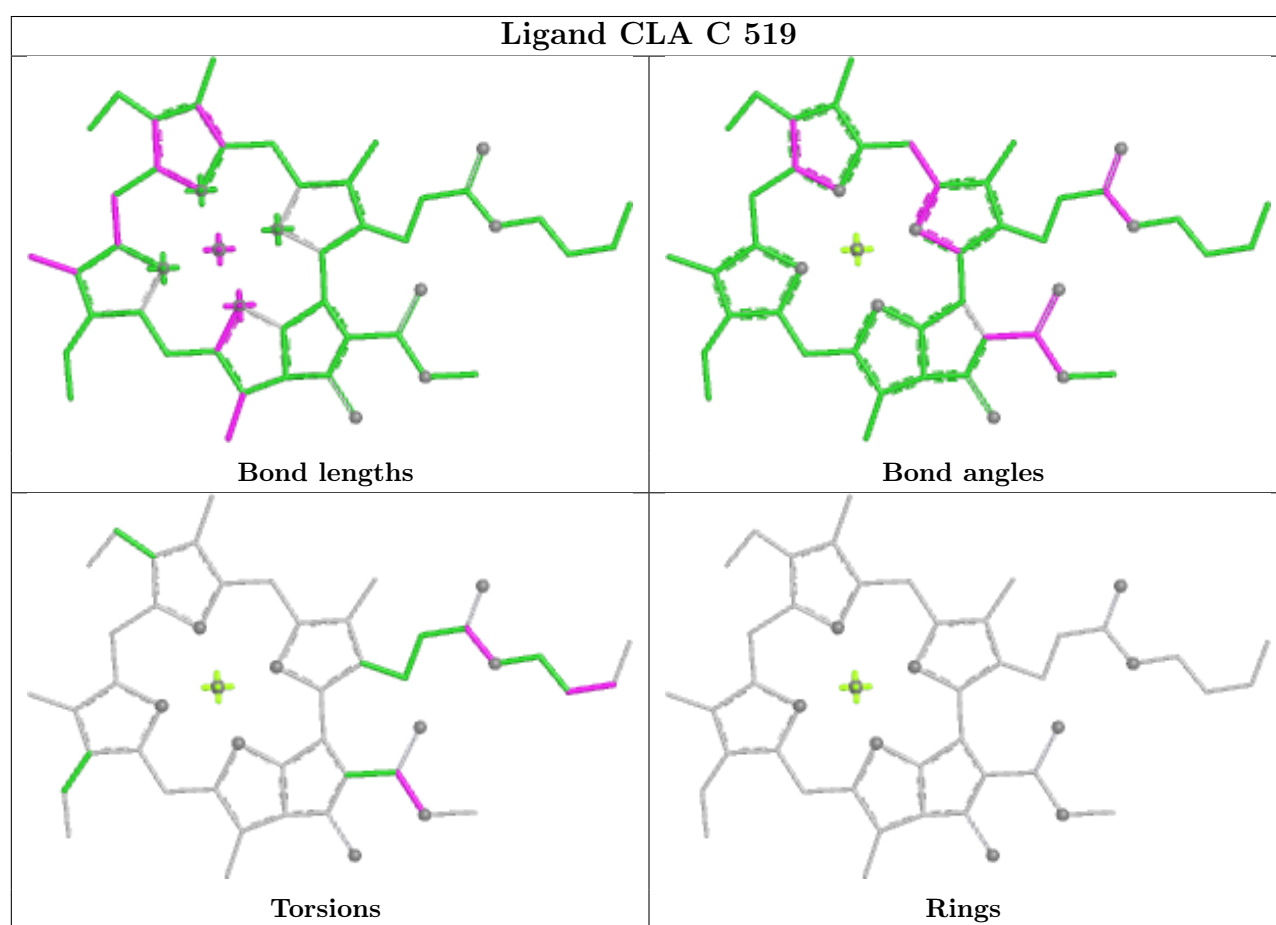
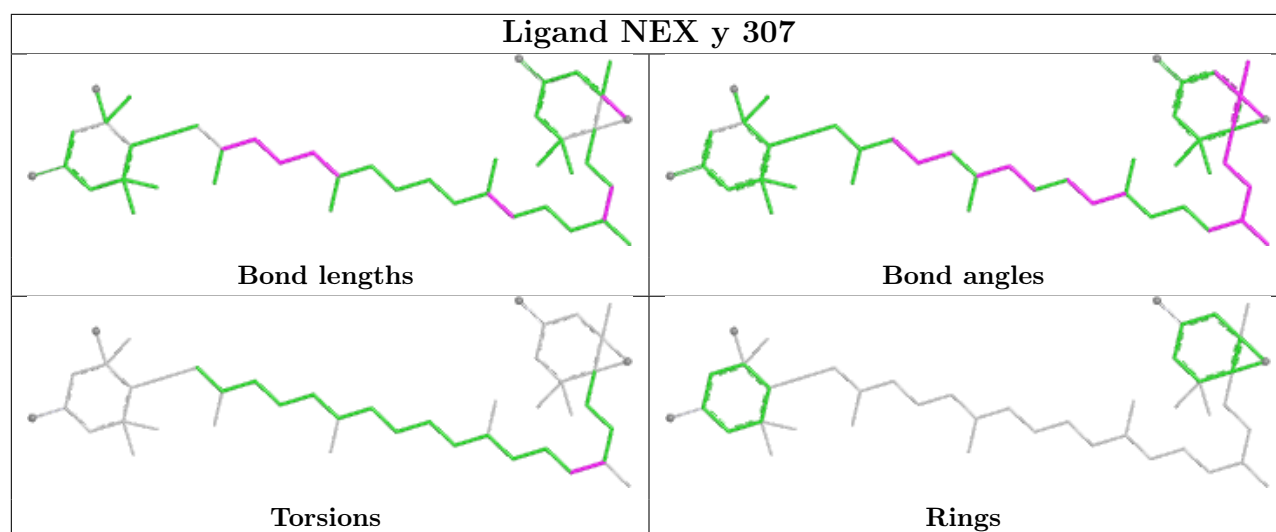
Continued on next page...

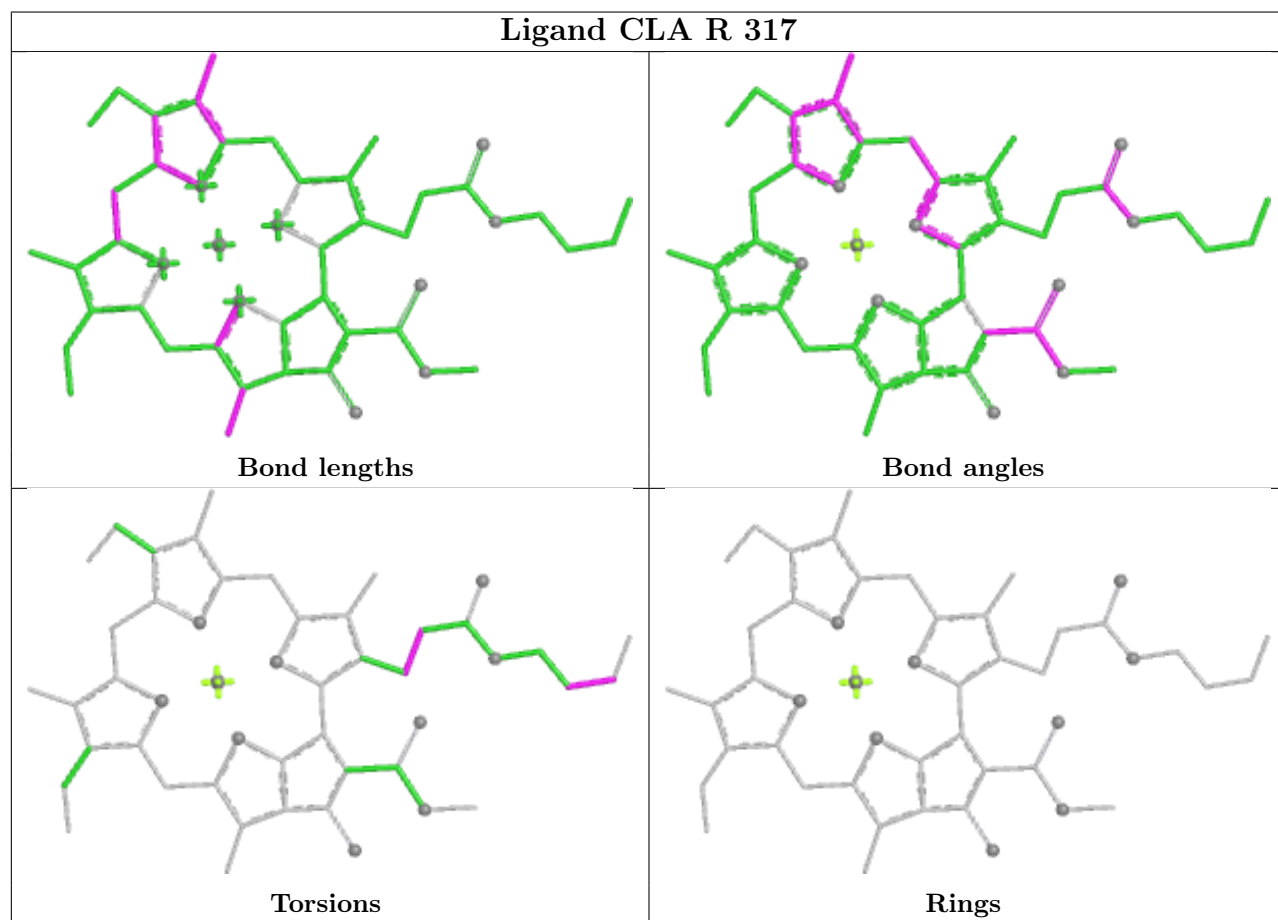
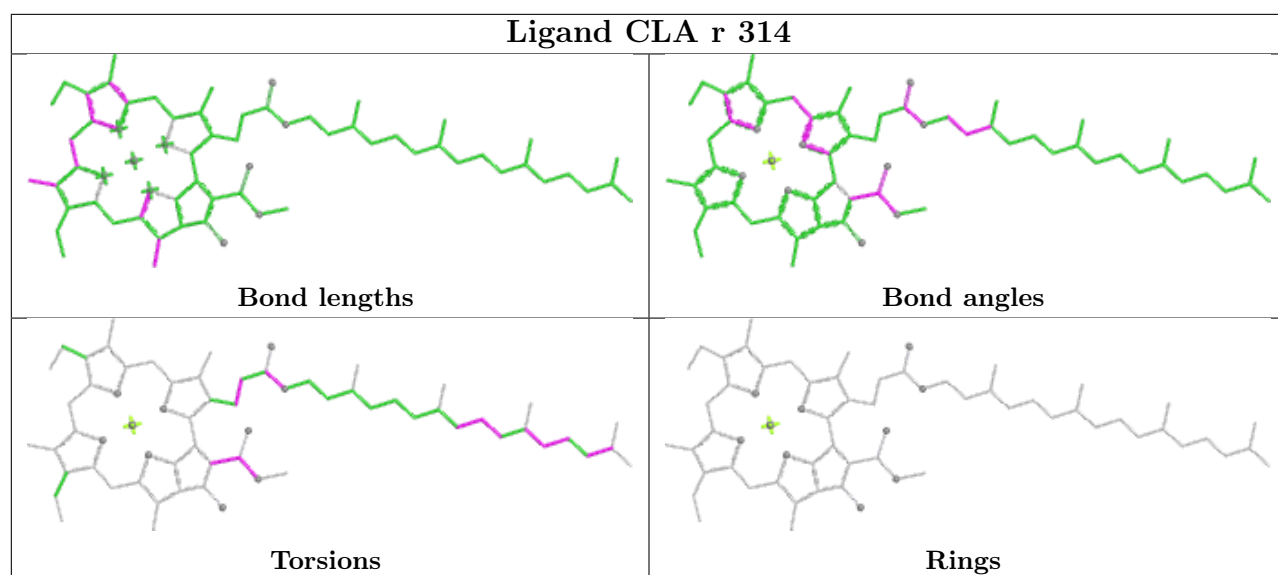
Continued from previous page...

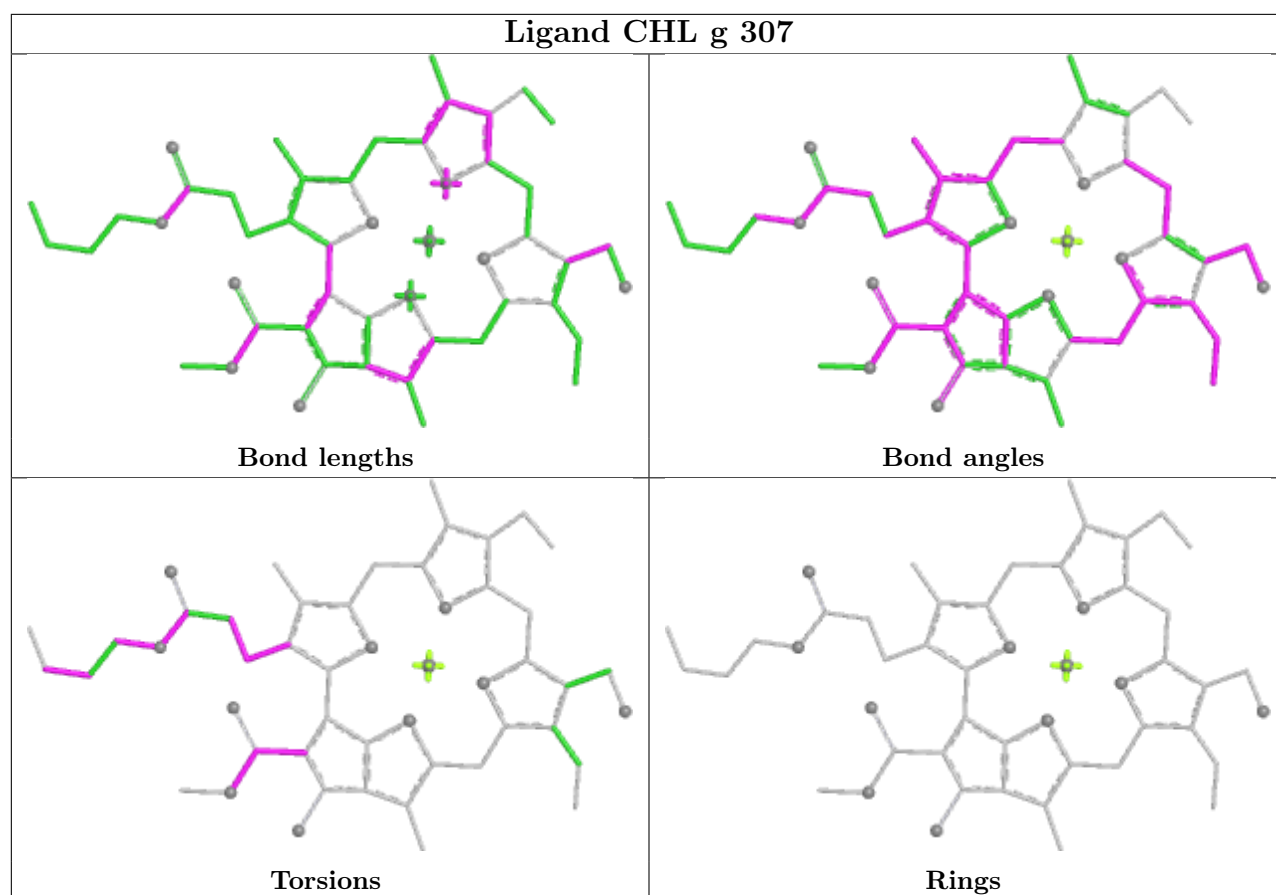
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	G	307	CLA	5	0
26	s	305	CLA	1	0
26	r	303	CLA	1	0
34	C	518	LMG	1	0
39	y	302	CHL	2	0
26	S	309	CLA	2	0
28	B	619	BCR	5	0
34	c	512	LMG	2	0
26	b	609	CLA	7	0
26	b	611	CLA	6	0
33	C	510	DGD	3	0
26	a	402	CLA	1	0
30	d	408	PL9	2	0
26	N	312	CLA	3	0
26	y	313	CLA	2	0
39	N	317	CHL	2	0
37	N	301	LHG	5	0
40	g	316	LUT	3	0
26	Y	311	CLA	1	0
26	r	305	CLA	1	0
26	n	310	CLA	3	0
34	w	201	LMG	2	0
26	c	505	CLA	6	0
26	C	504	CLA	7	0
26	g	304	CLA	1	0
34	d	405	LMG	2	0

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

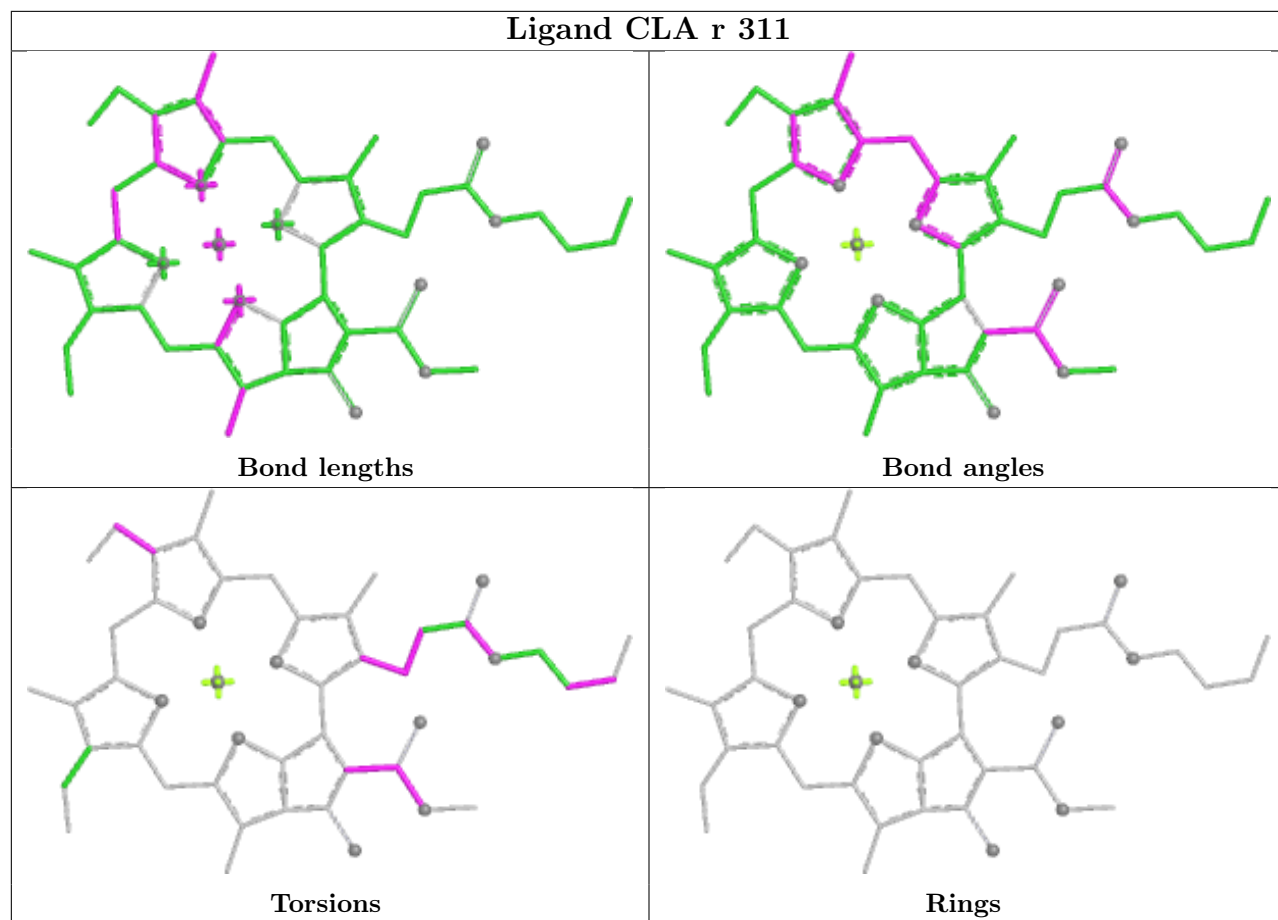


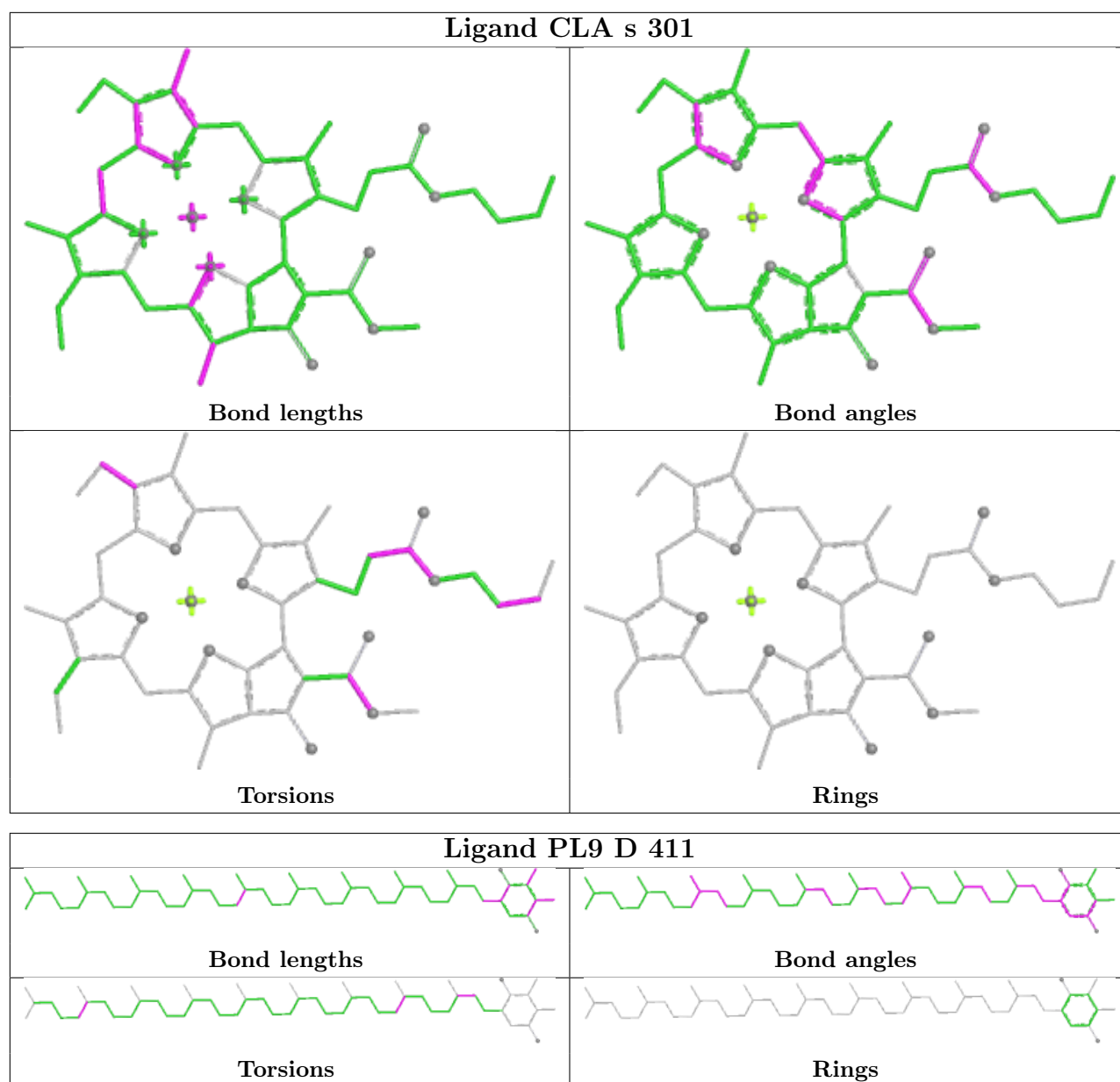


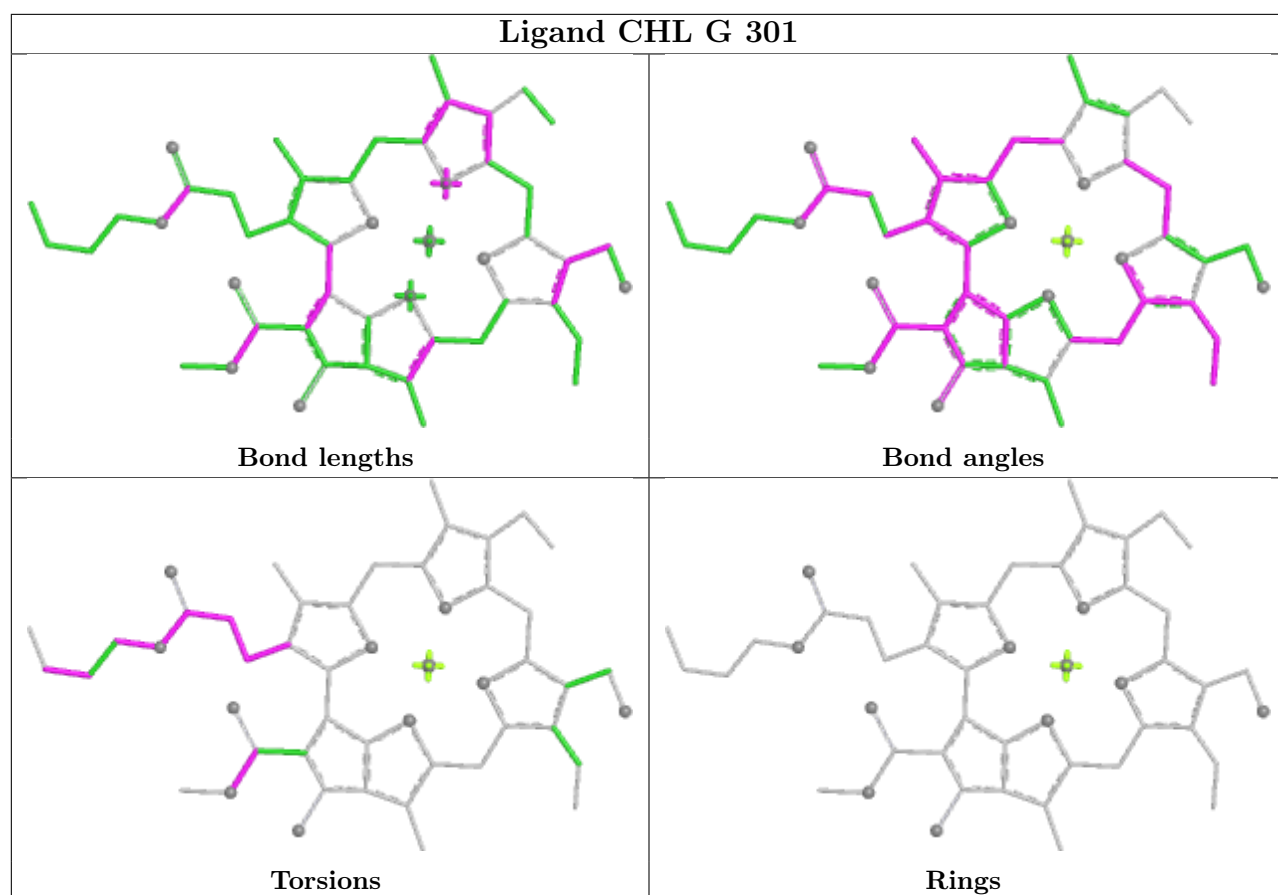




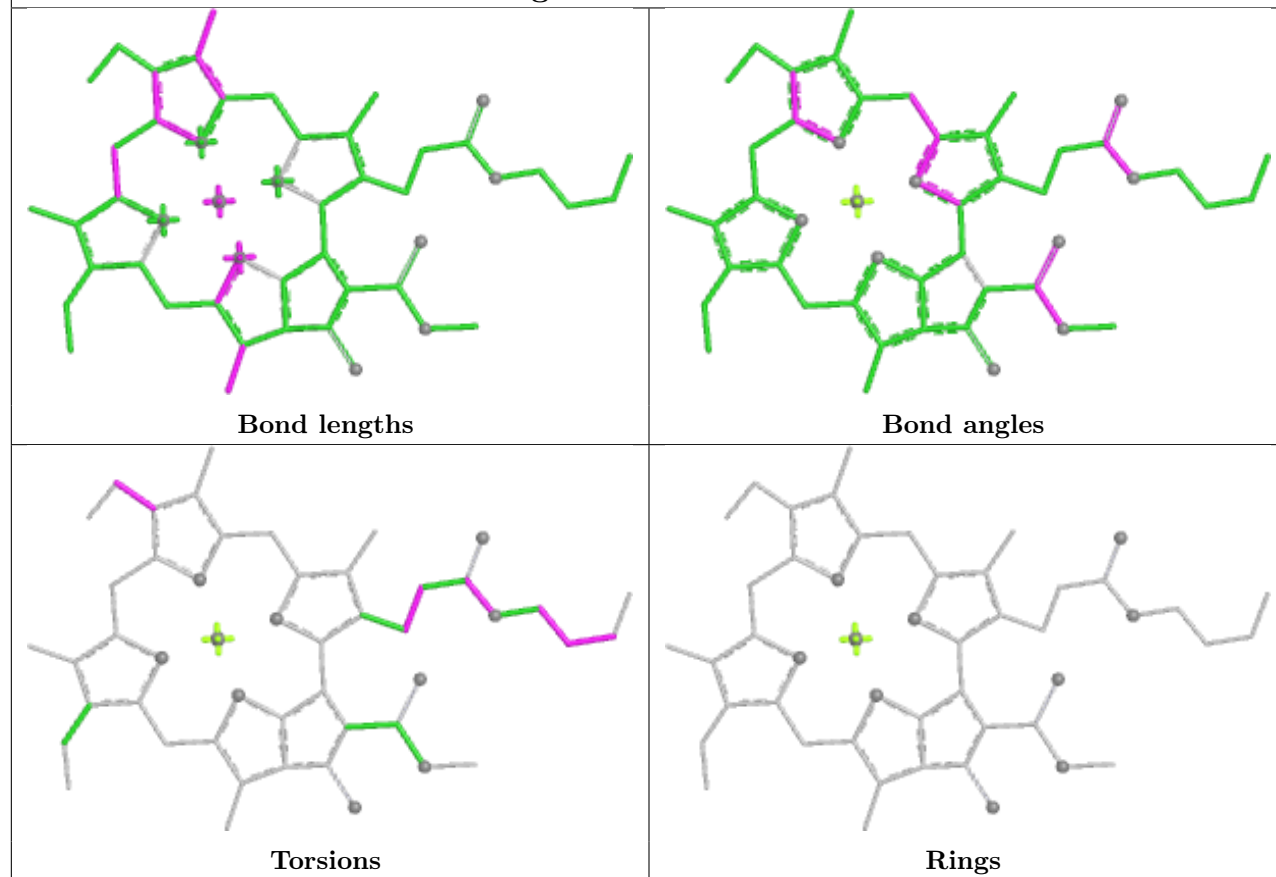
Ligand CLA r 311



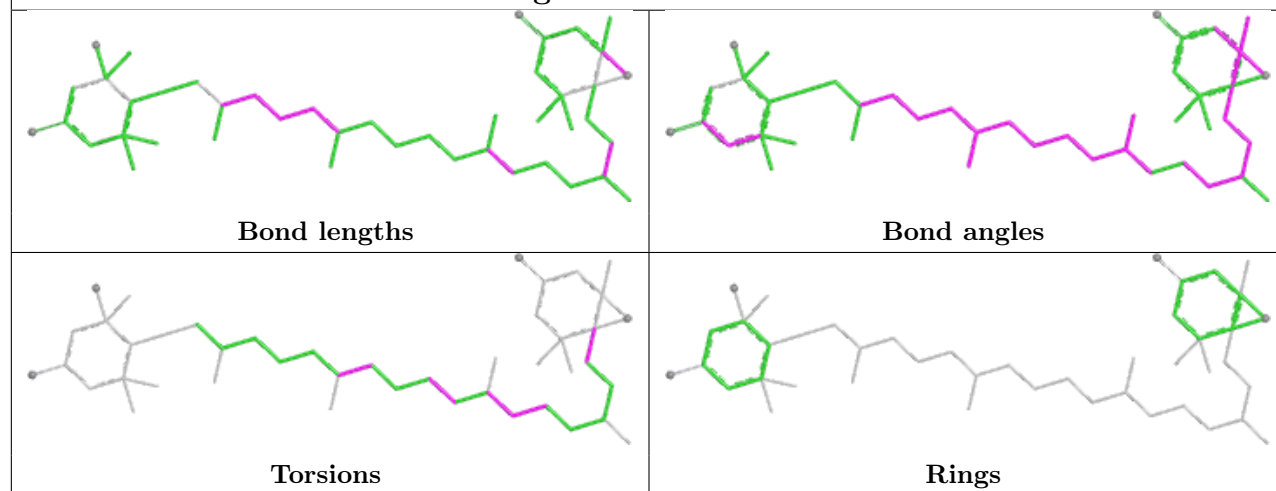


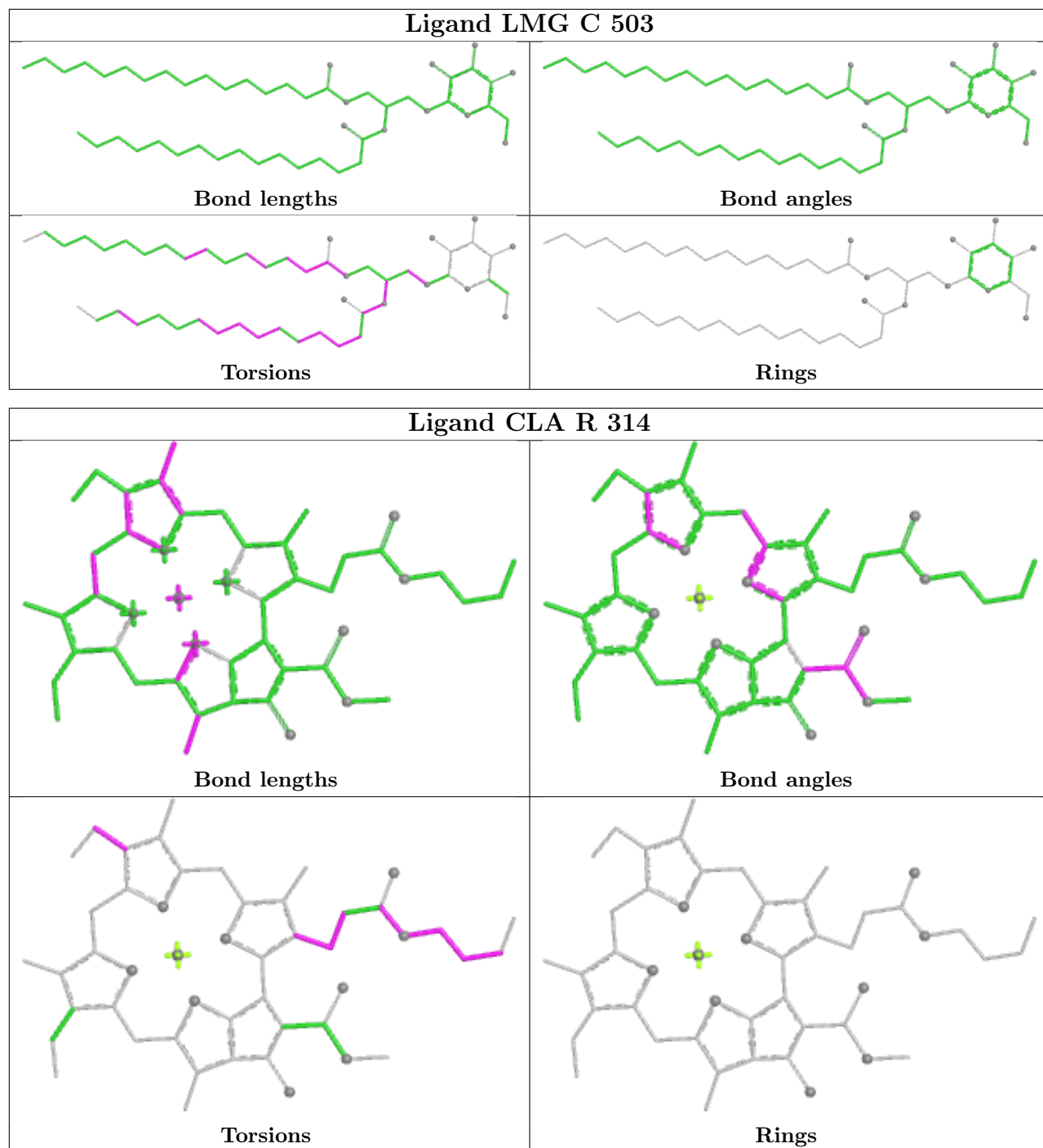


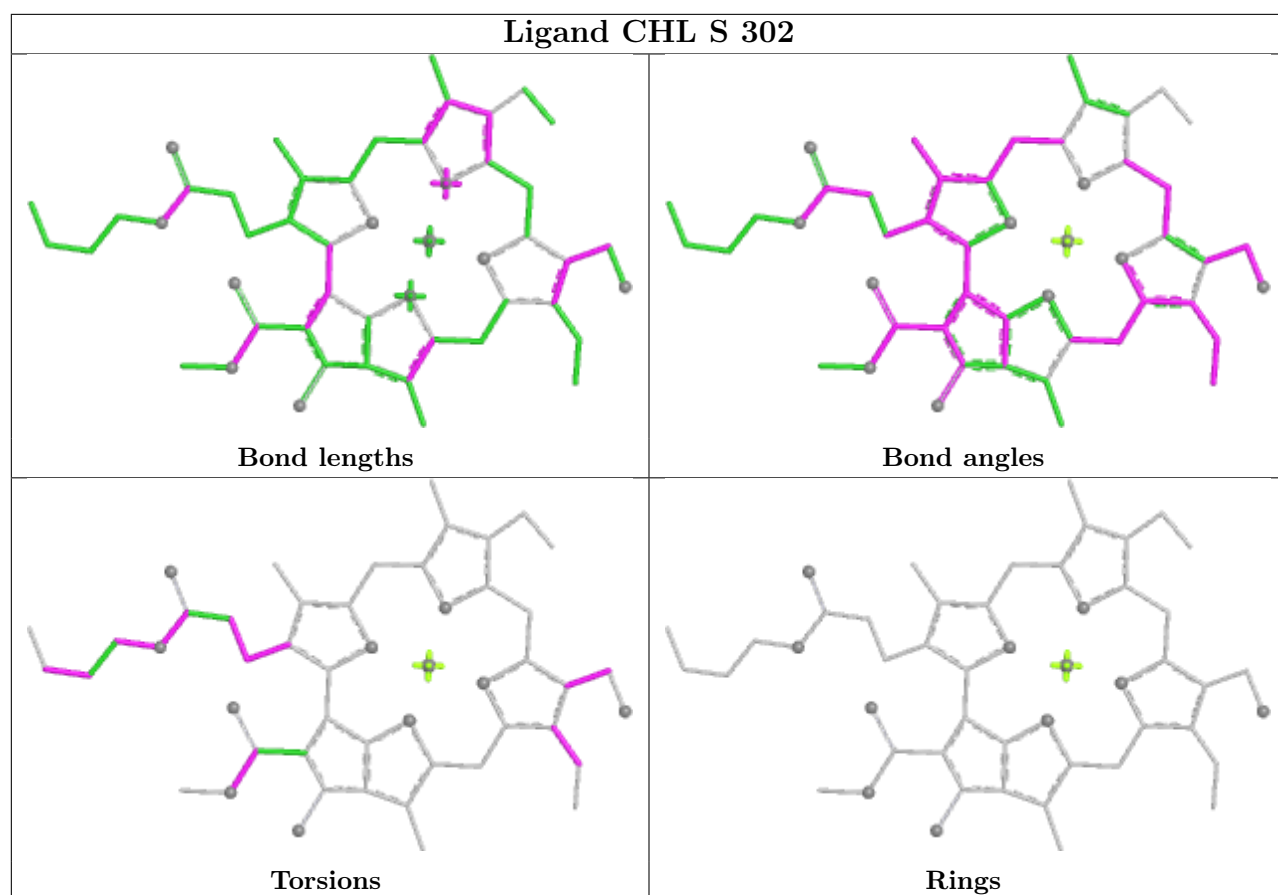
Ligand CLA N 318

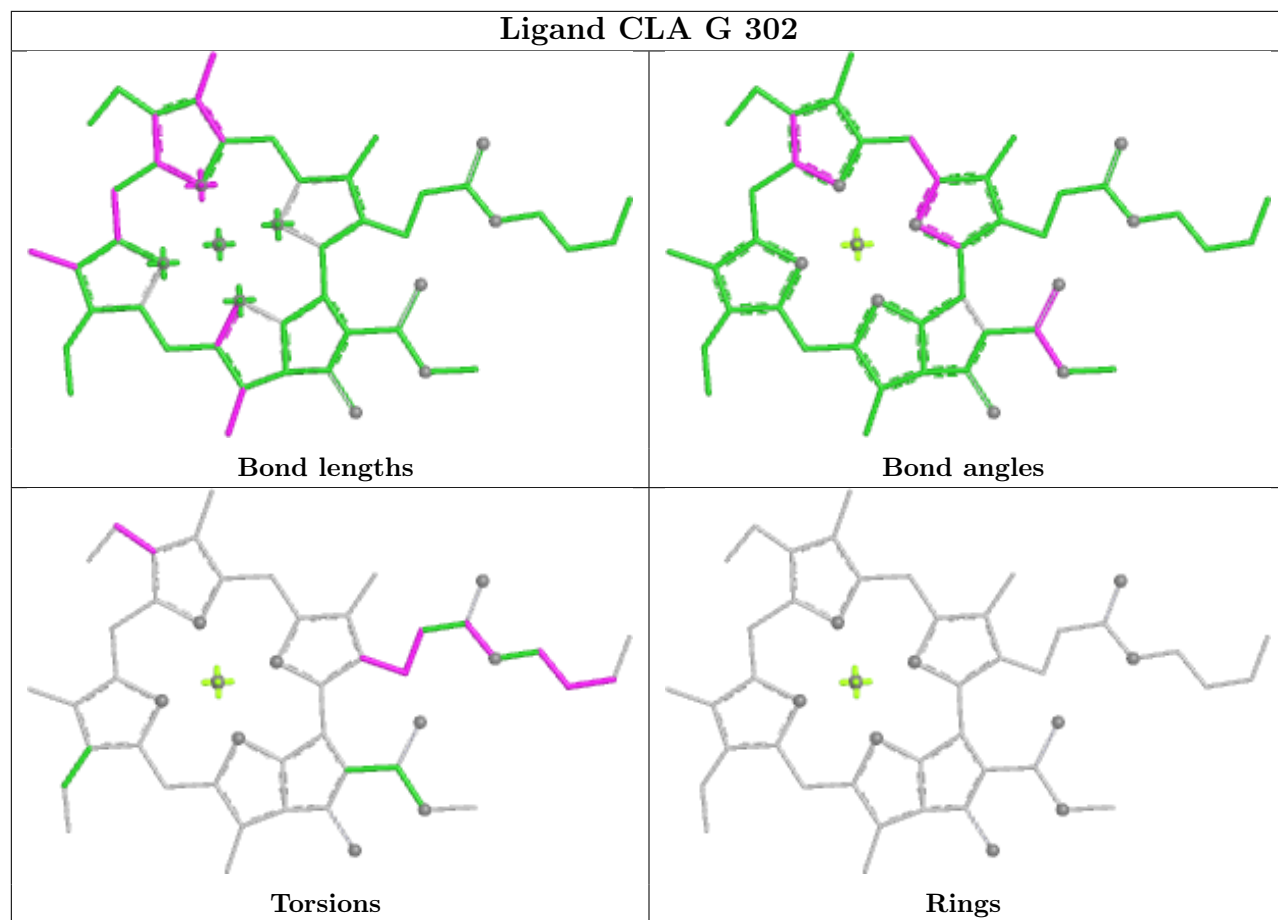


Ligand NEX S 305

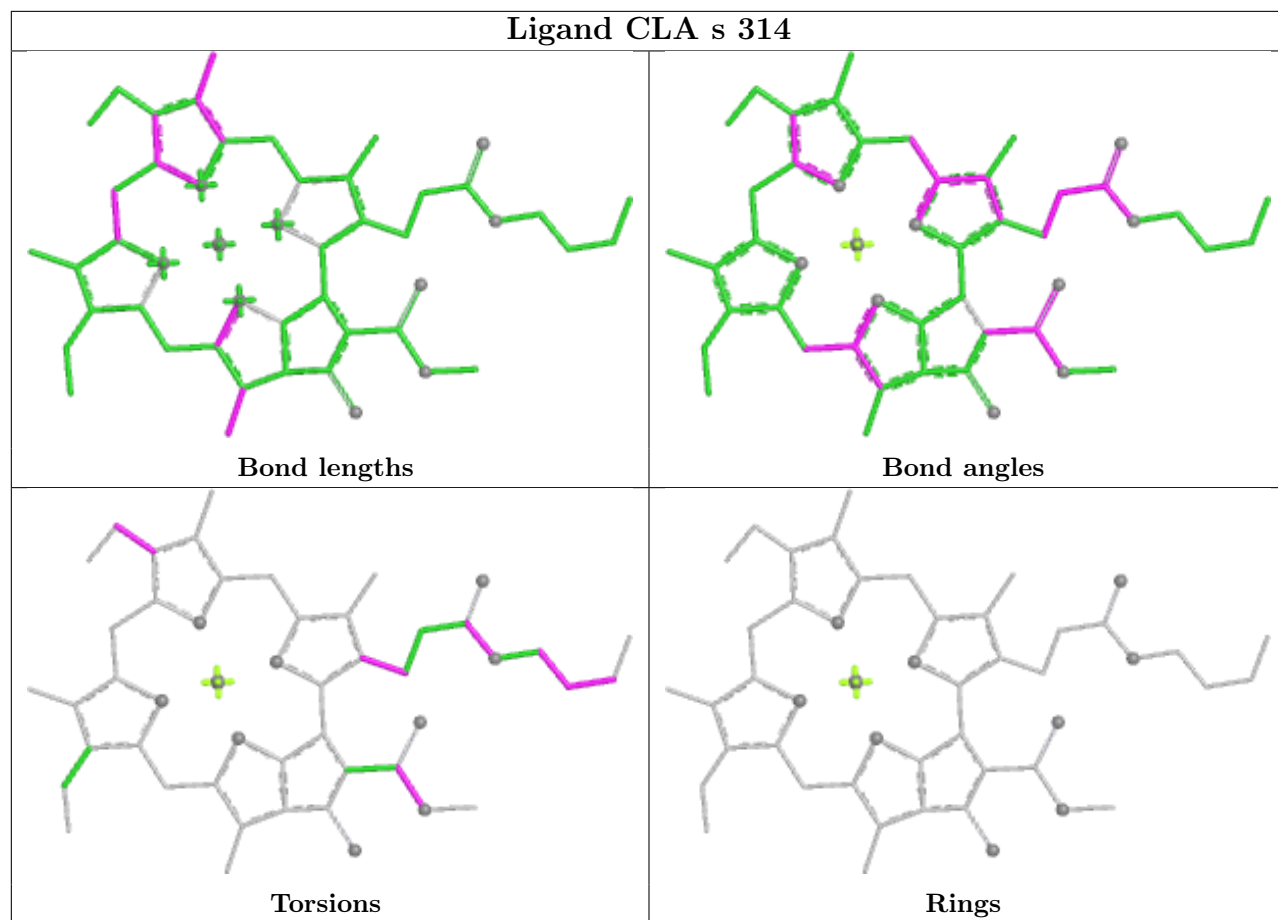


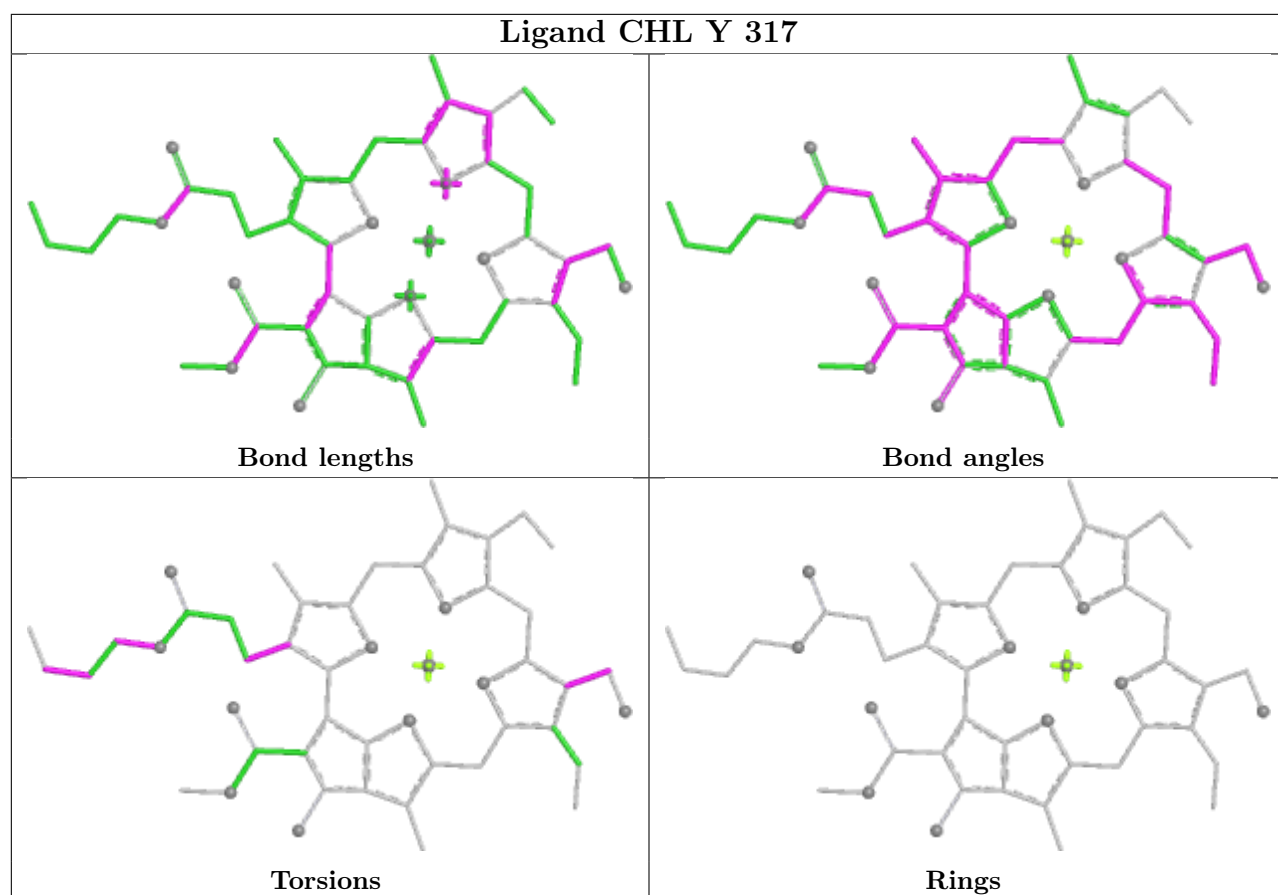




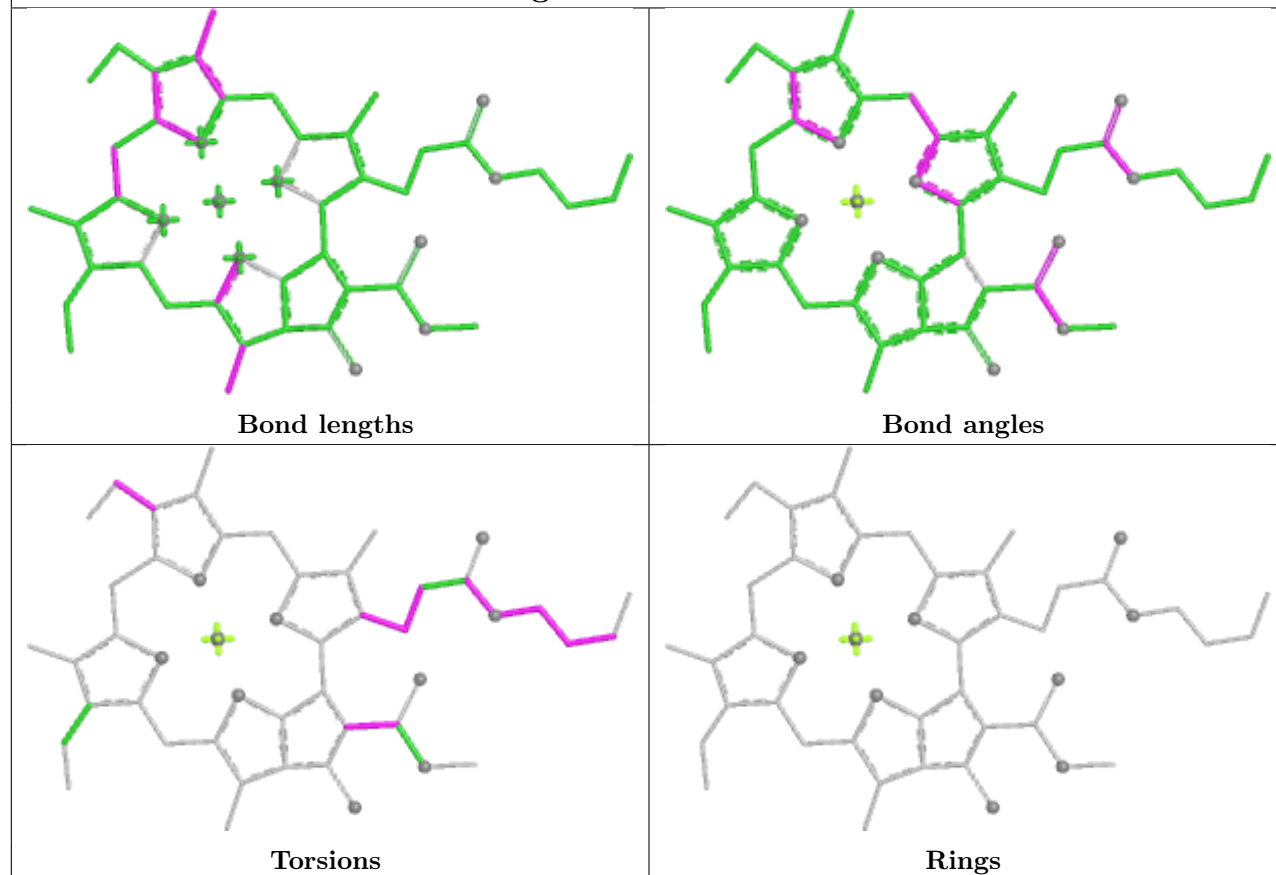


Ligand CLA s 314

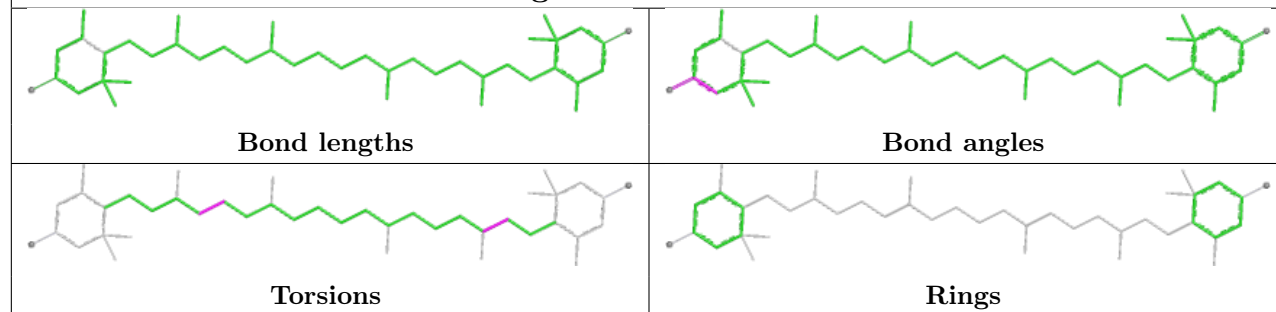




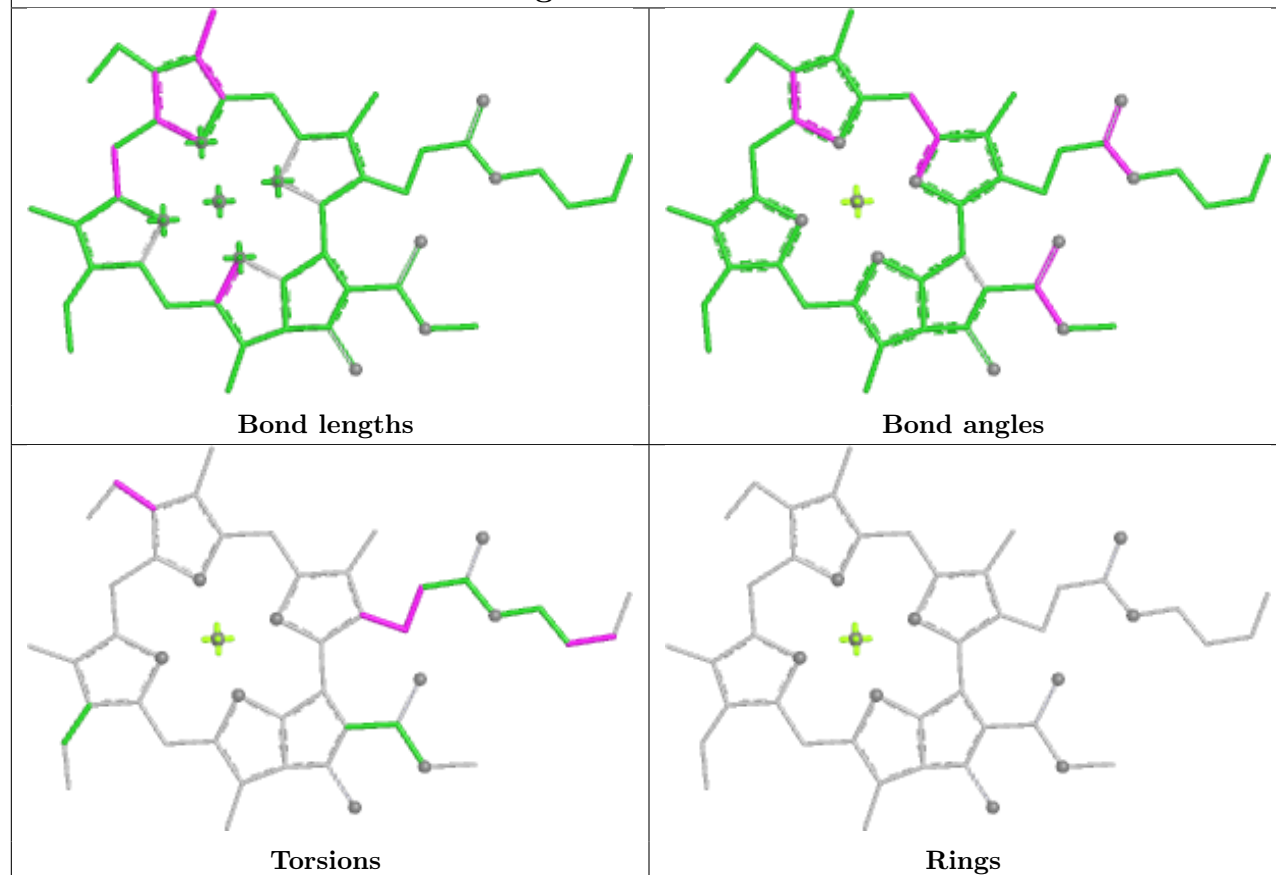
Ligand CLA R 309



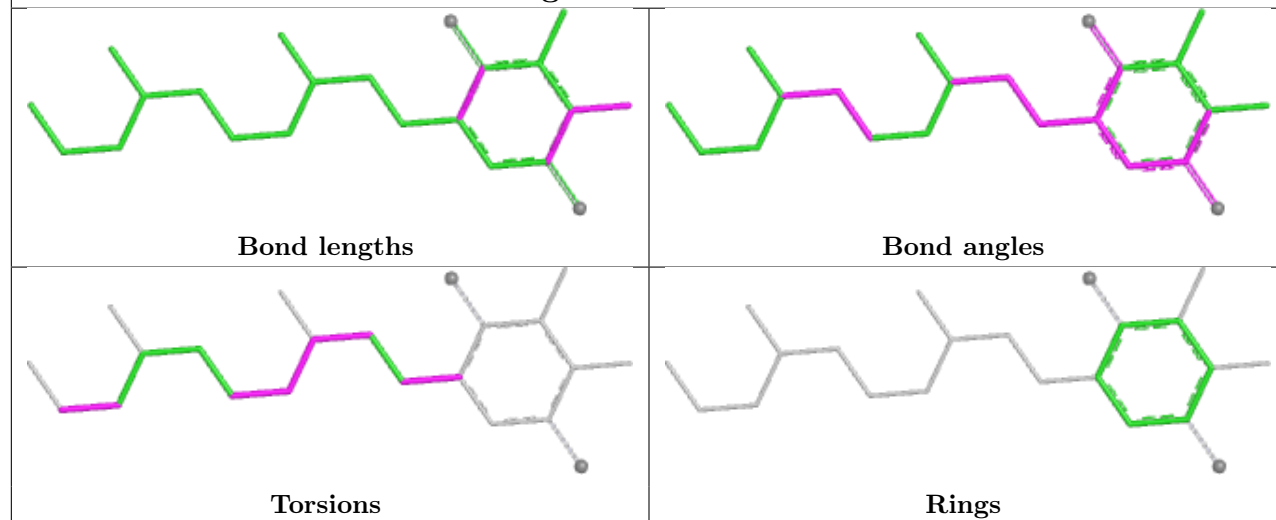
Ligand LUT N 305

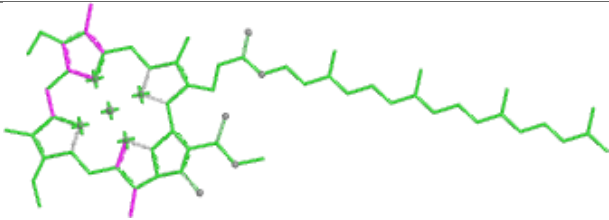
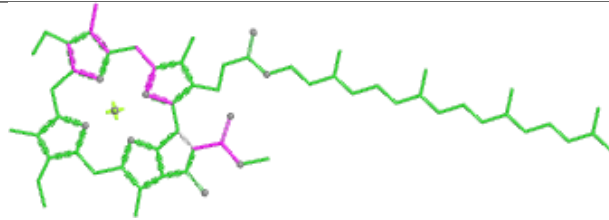
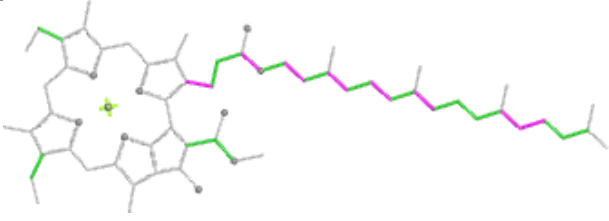
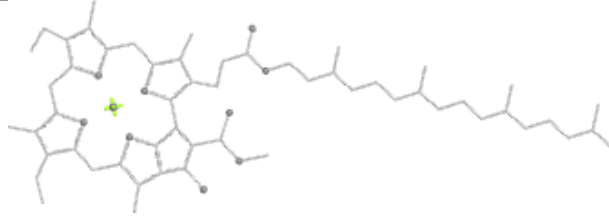




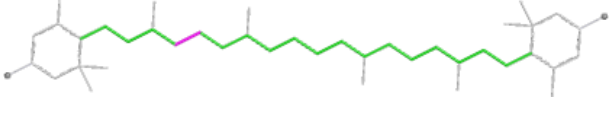
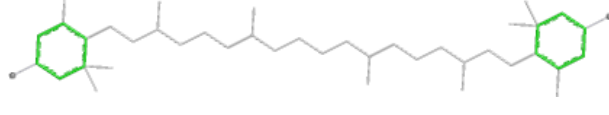
Ligand CLA S 314

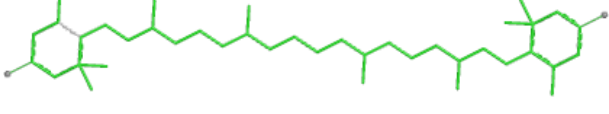
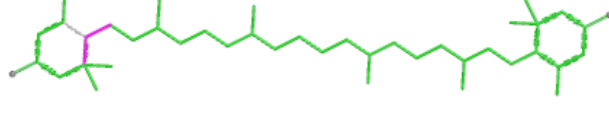
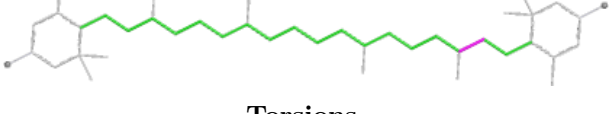
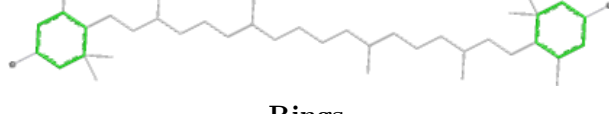


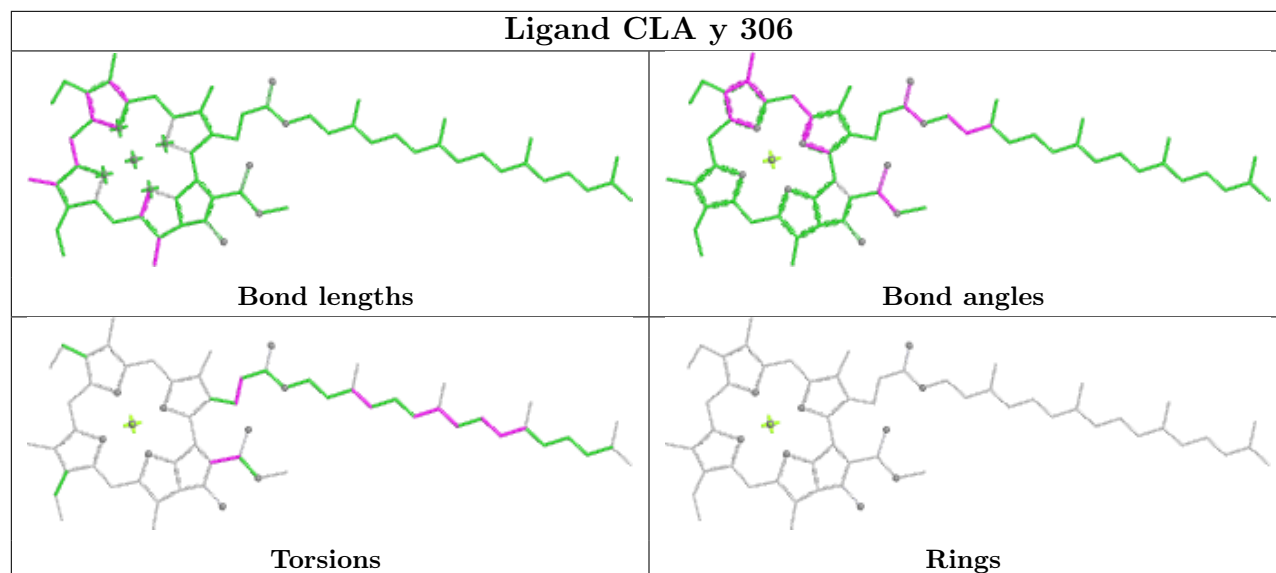
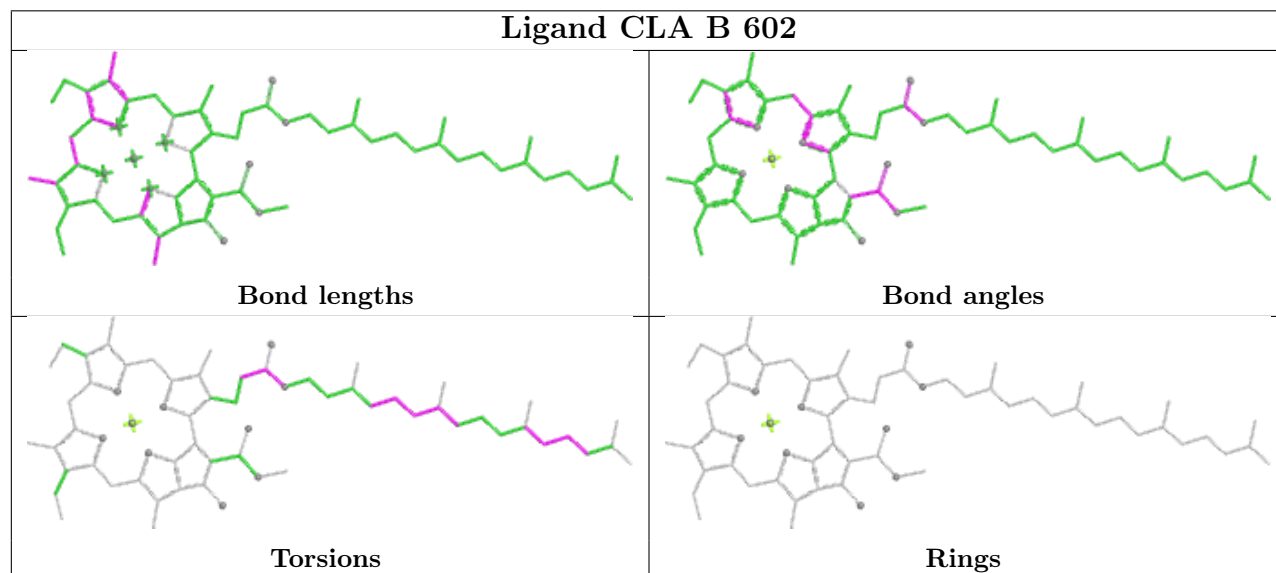
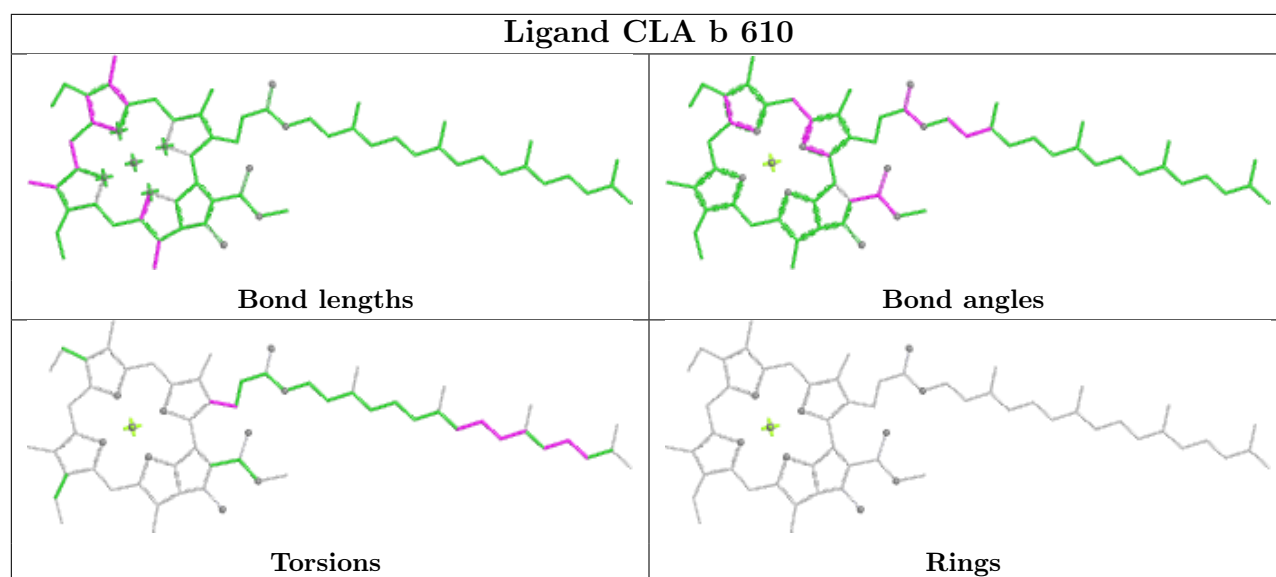
Ligand PL9 a 407

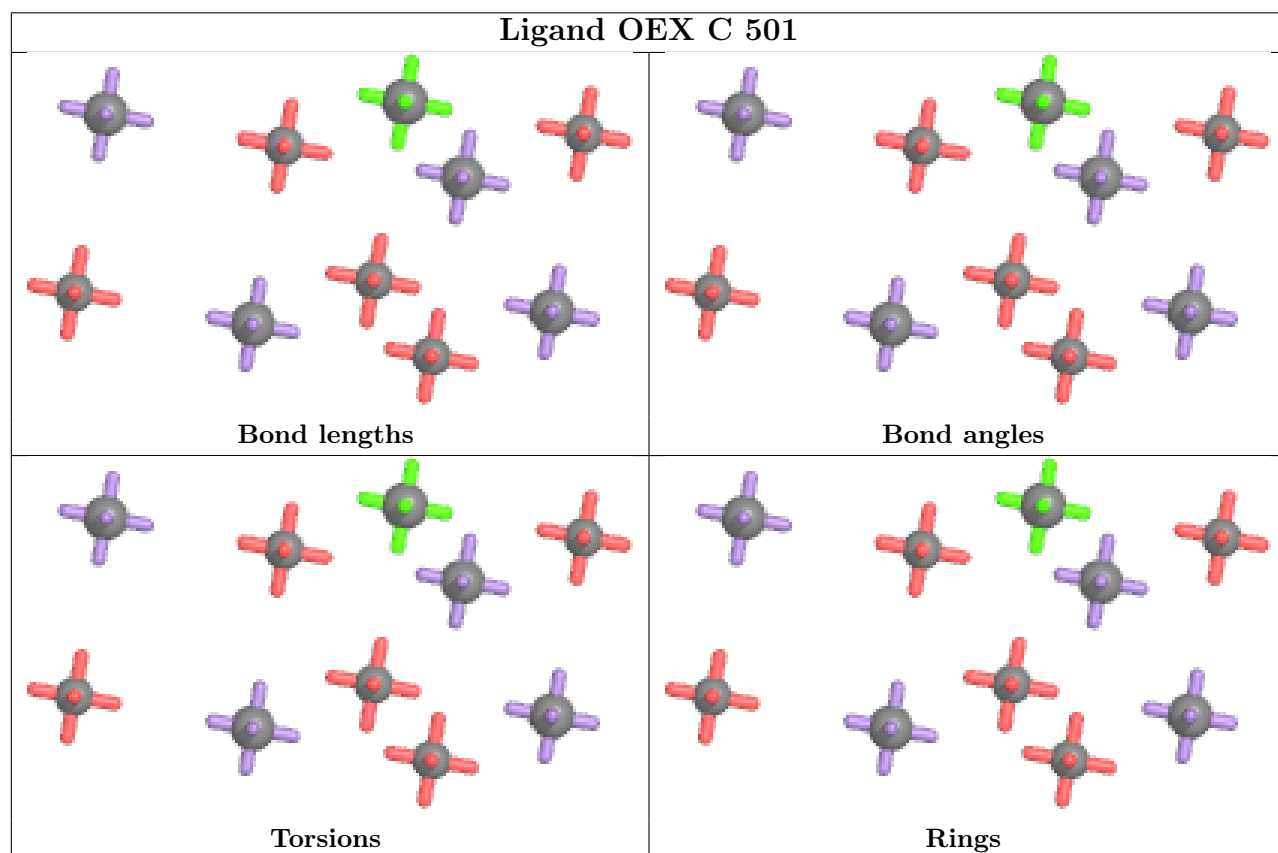
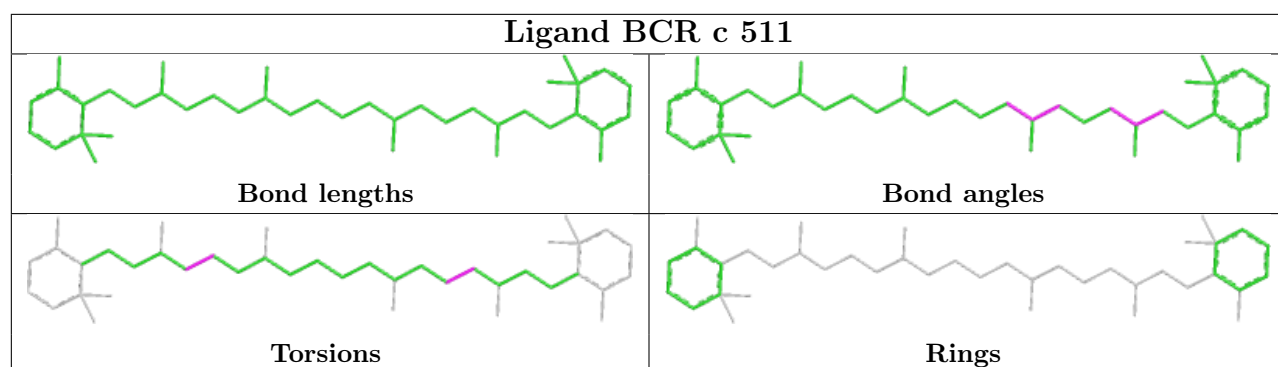


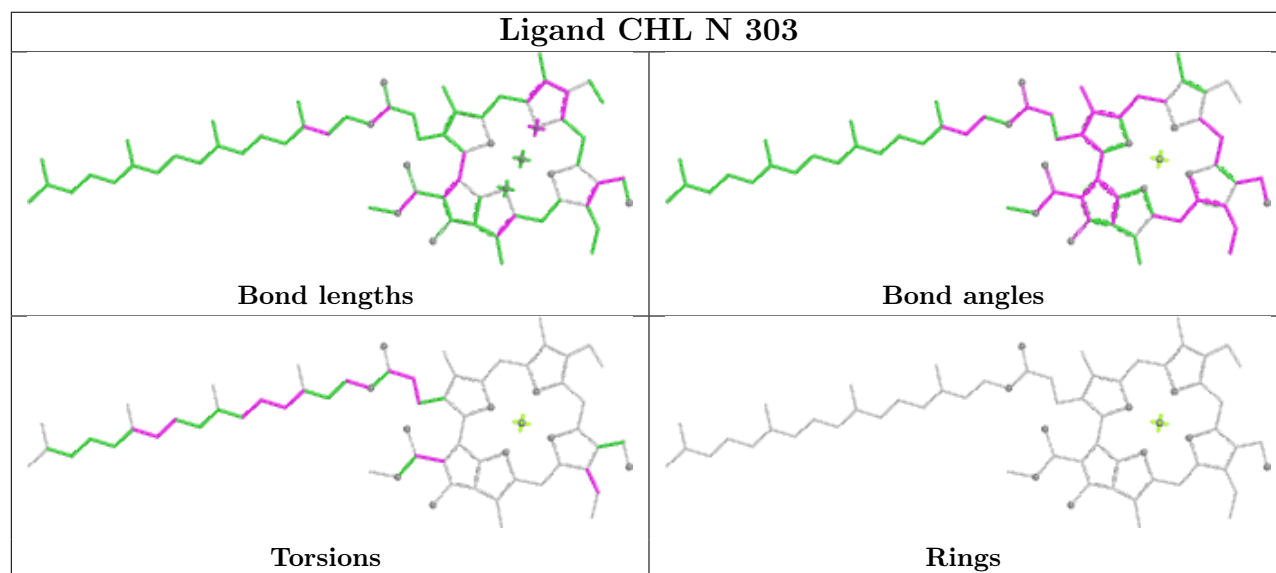
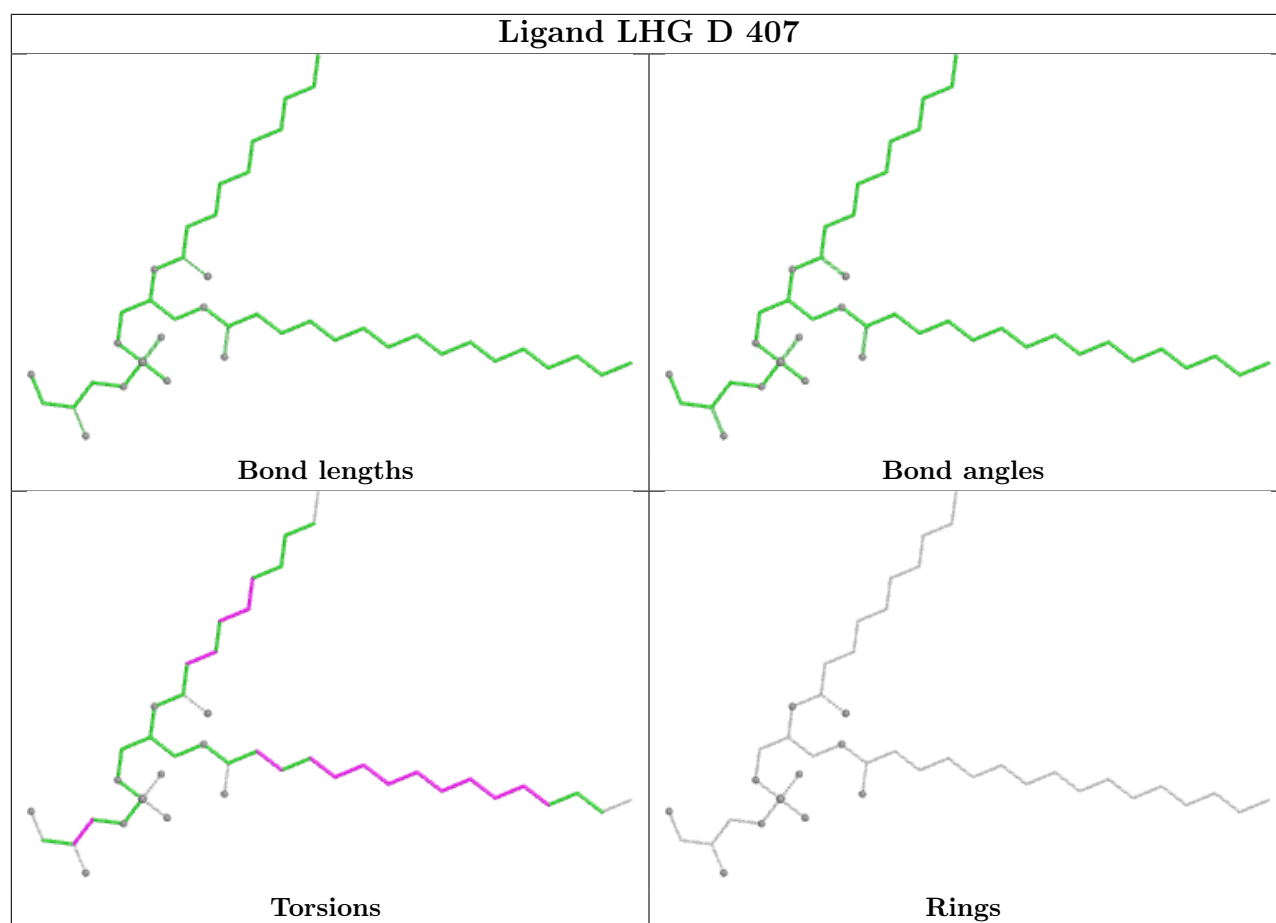
Ligand CLA b 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

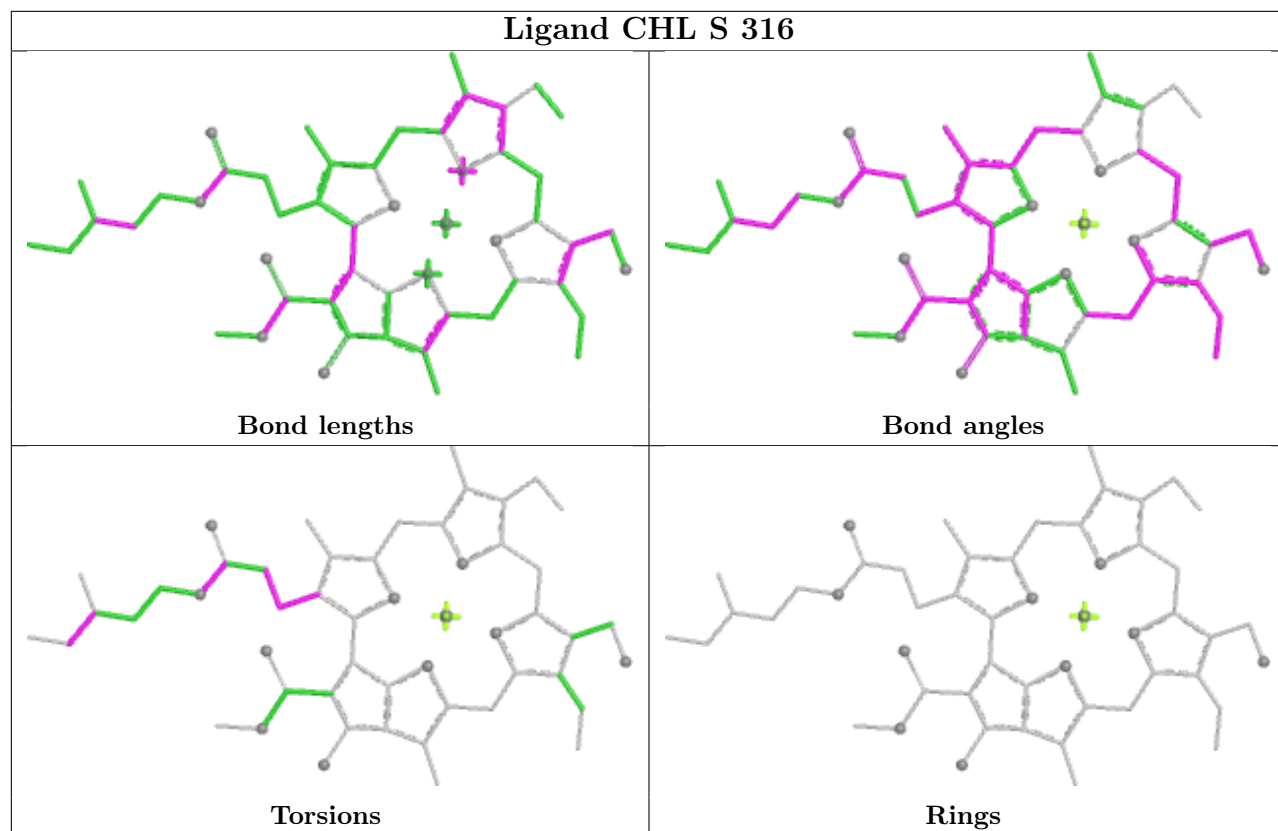
Ligand LUT g 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

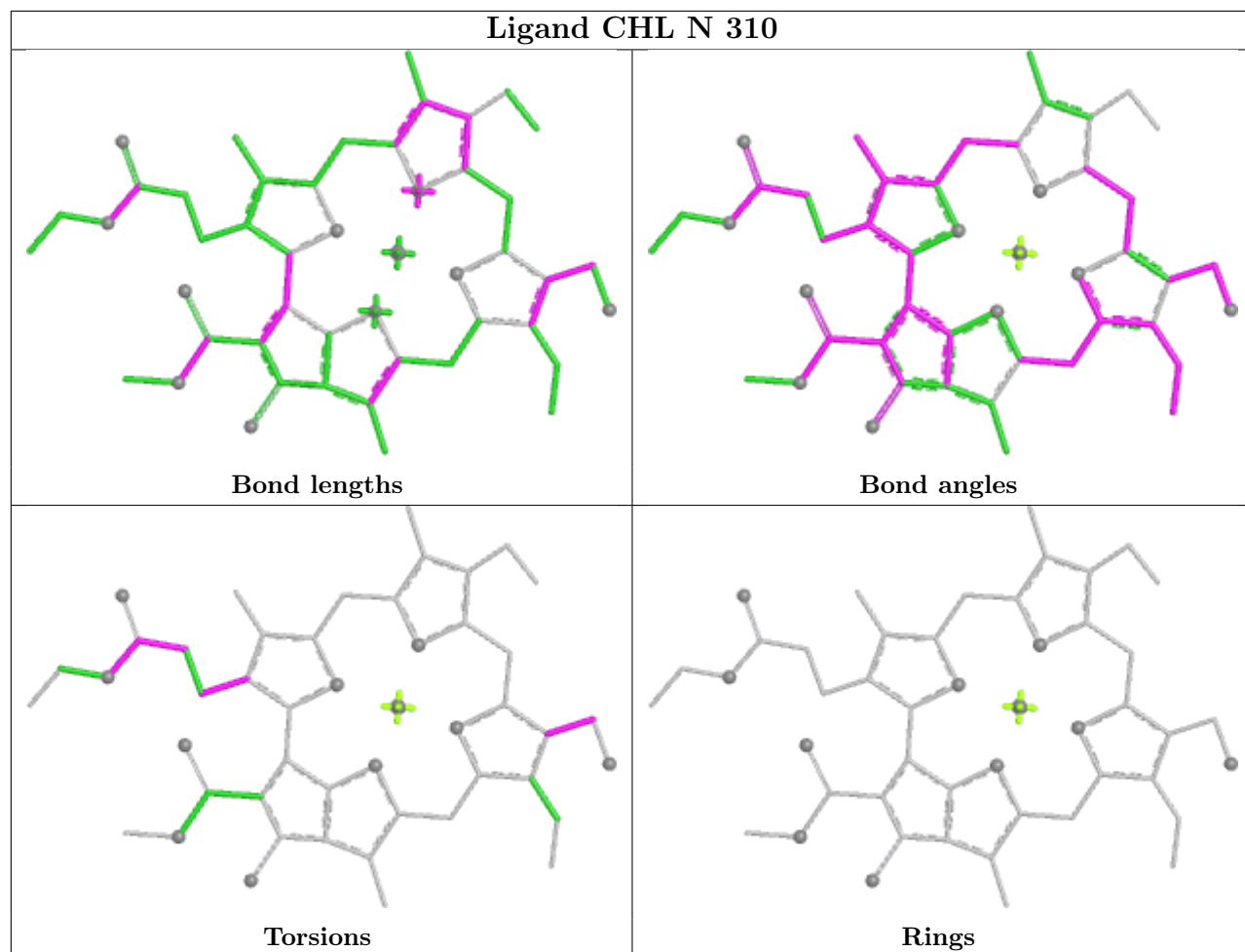
Ligand LUT S 306	
	
Bond lengths	Bond angles
	
Torsions	Rings



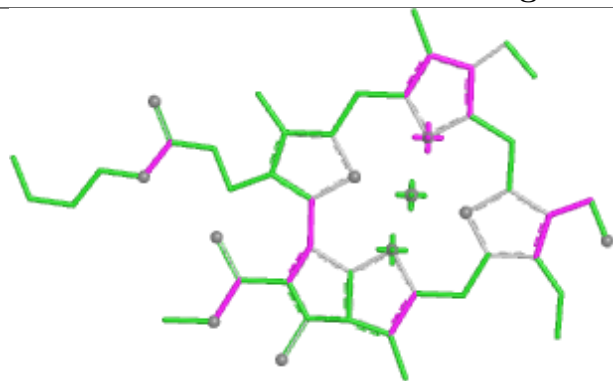




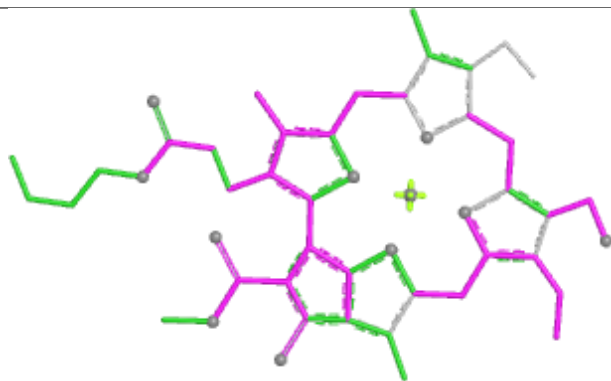




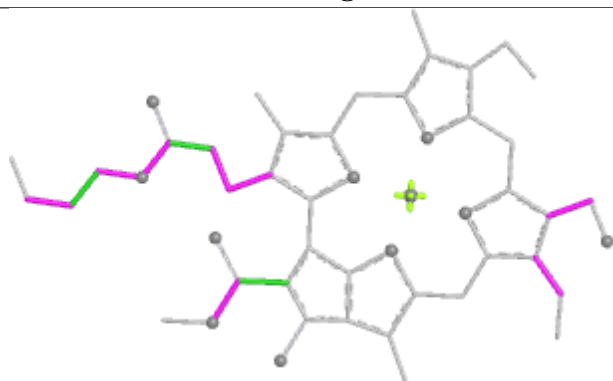
Ligand CHL s 316



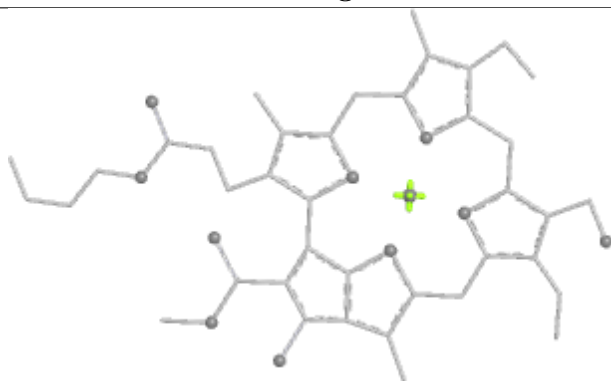
Bond lengths



Bond angles

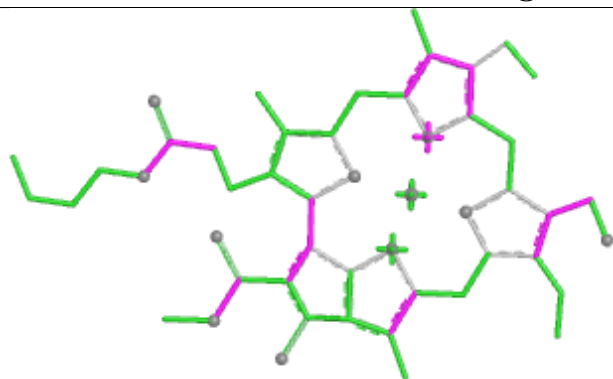


Torsions

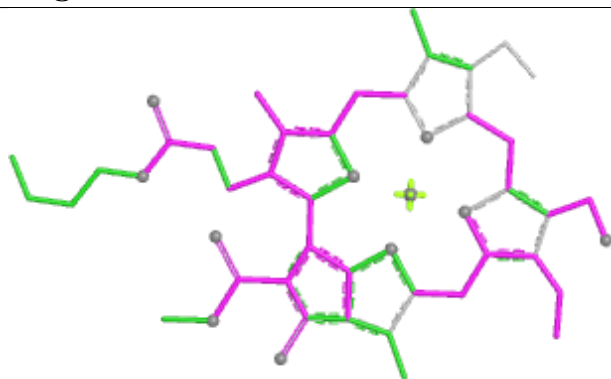


Rings

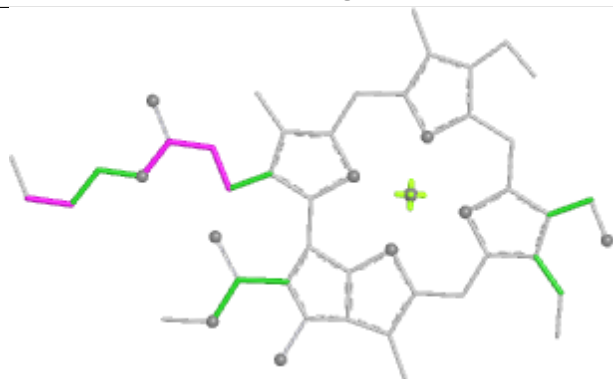
Ligand CHL g 319



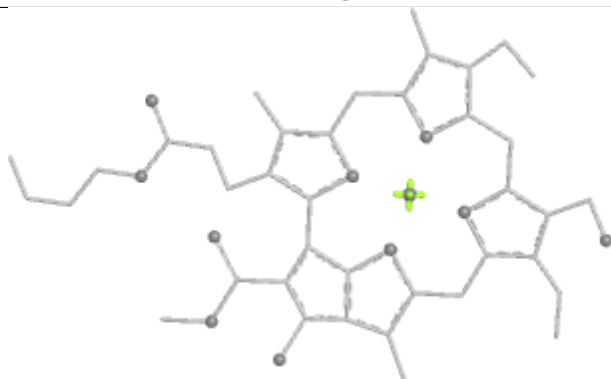
Bond lengths



Bond angles

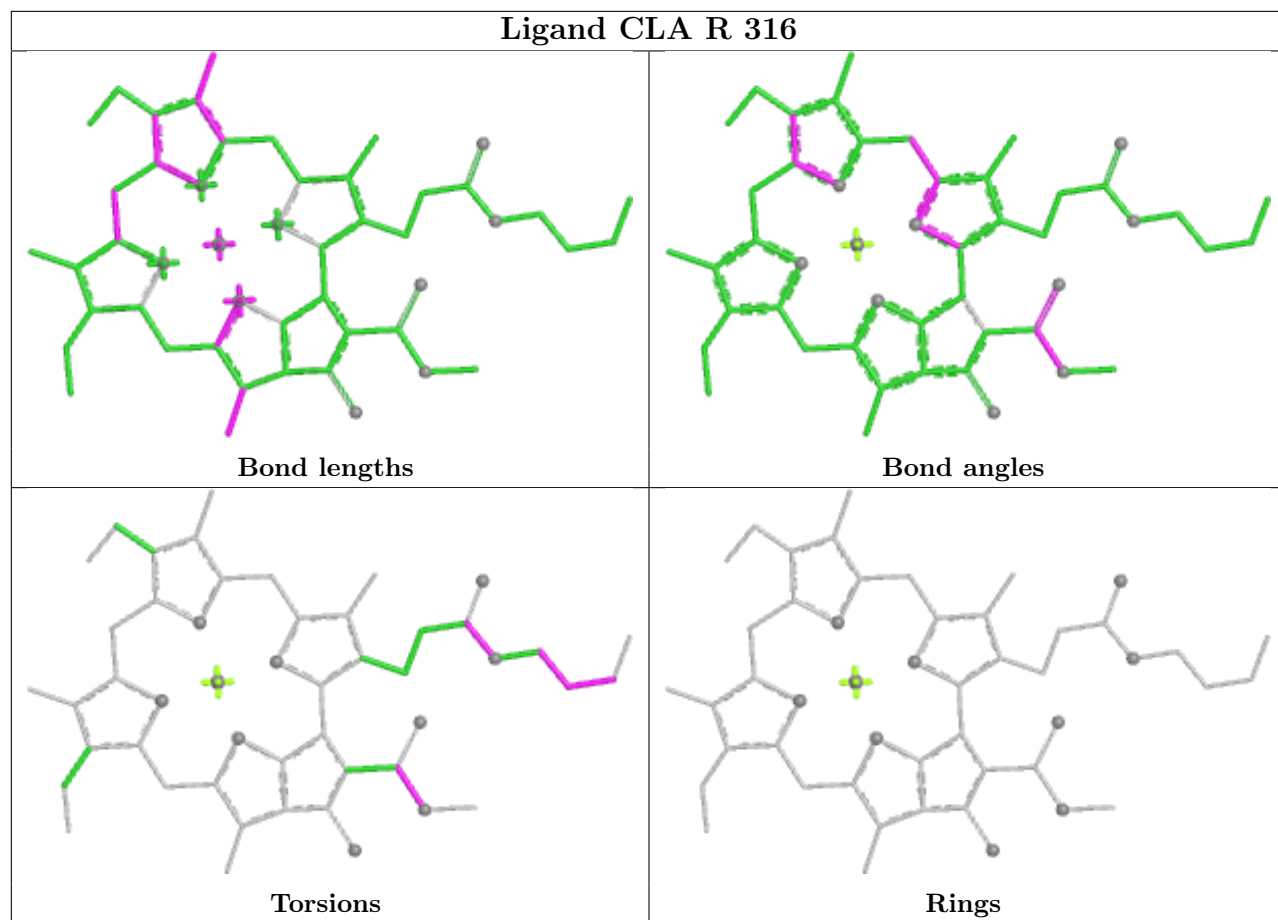


Torsions

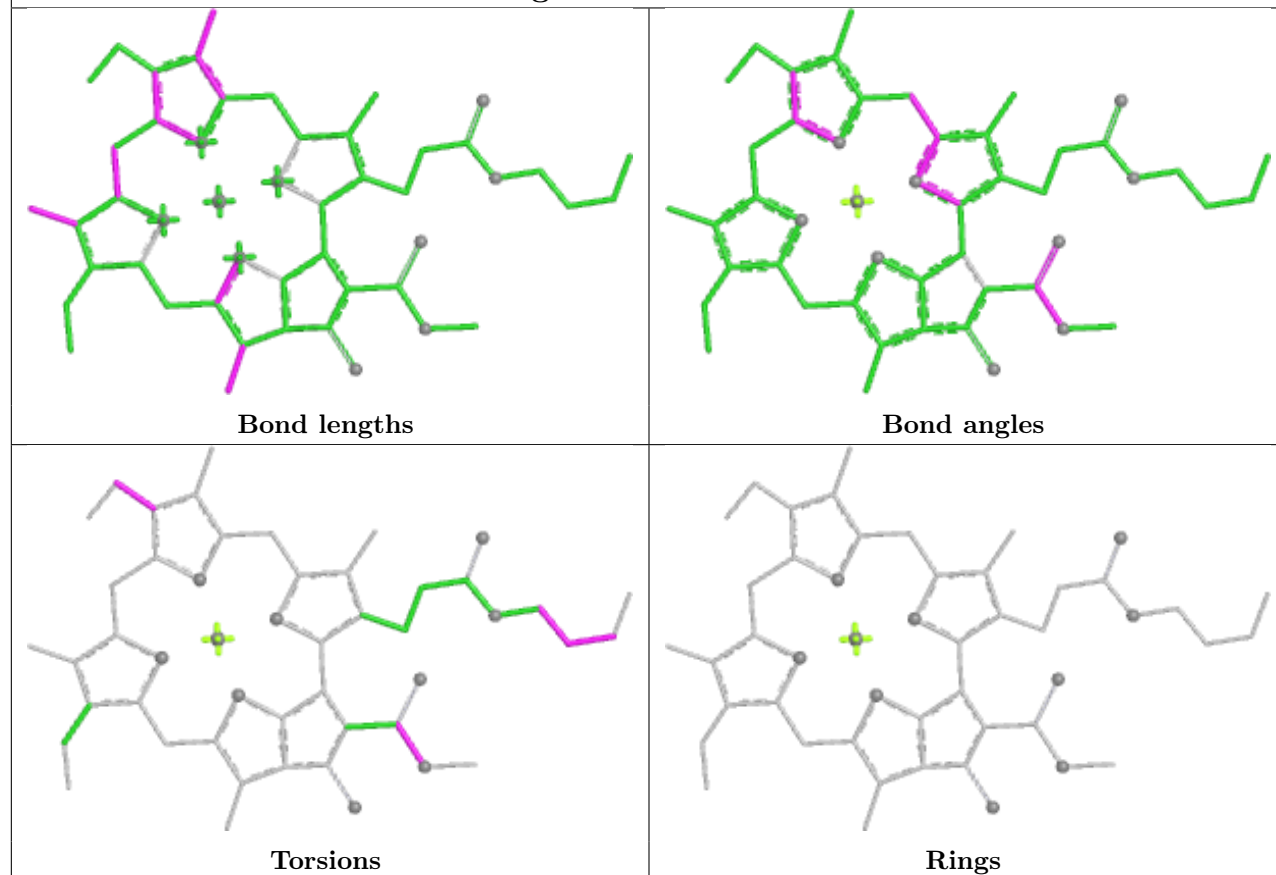


Rings

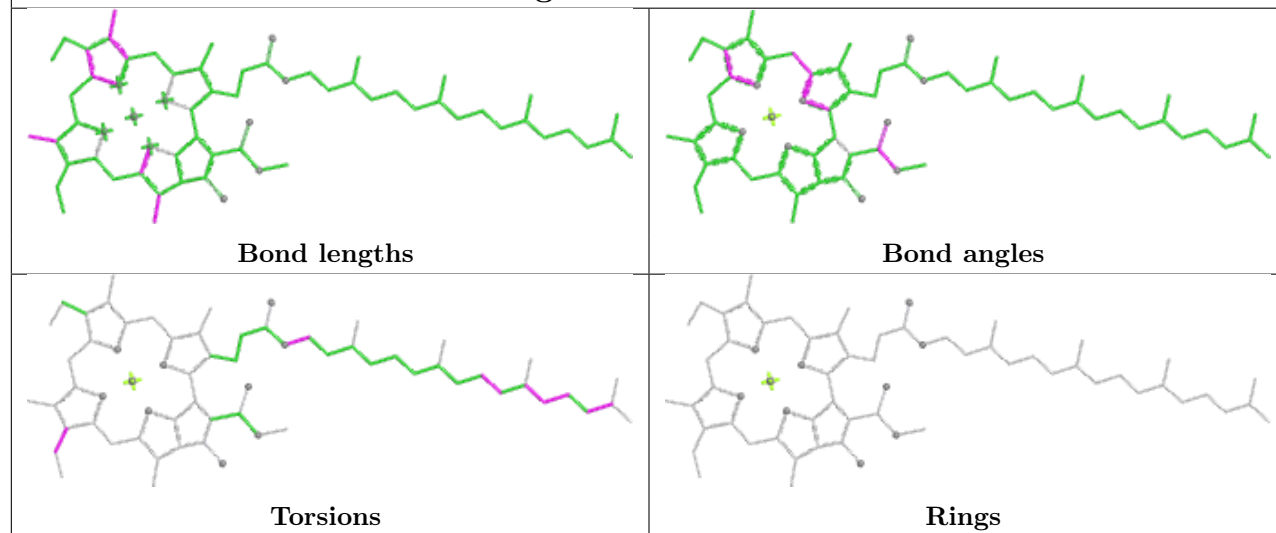
Ligand CLA R 316

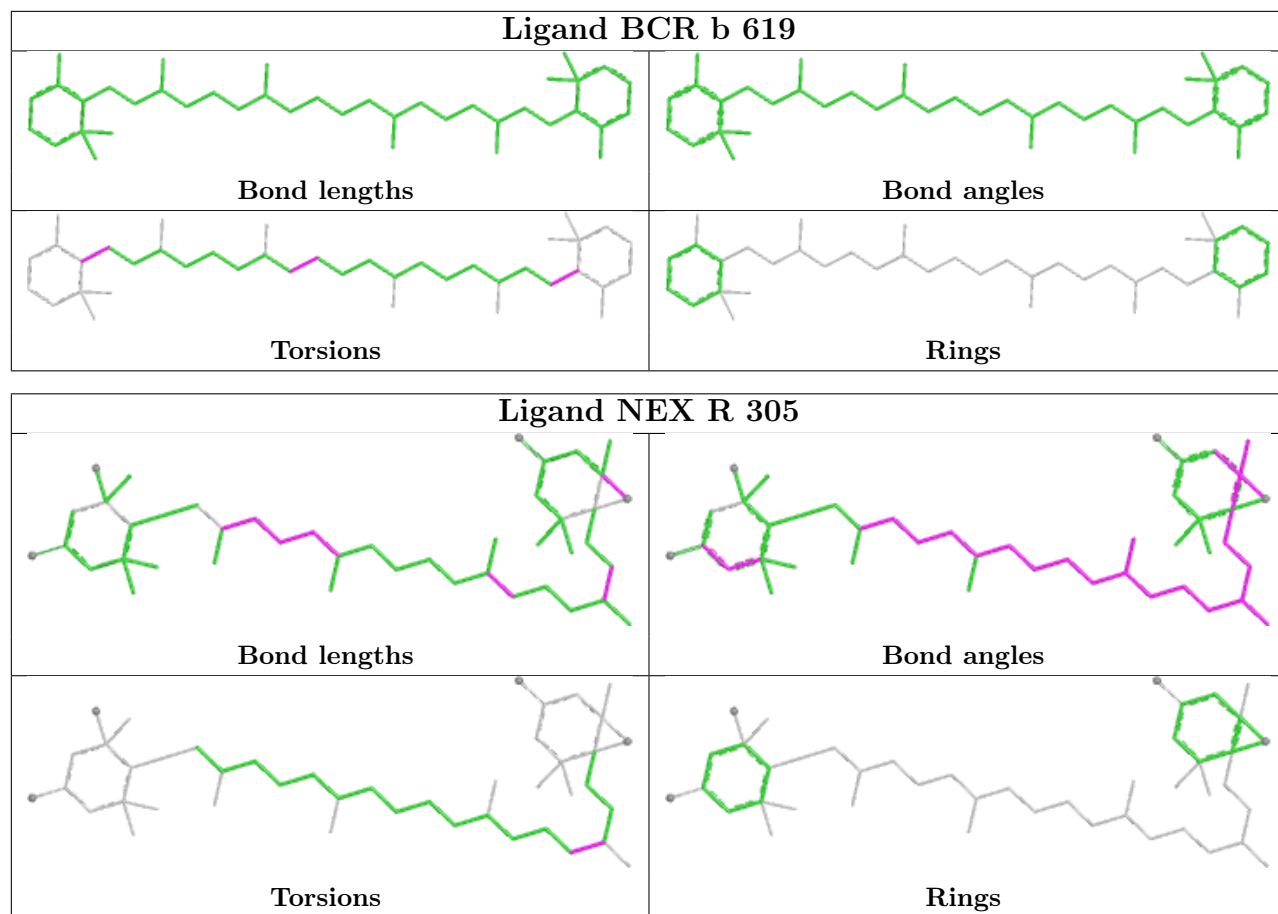


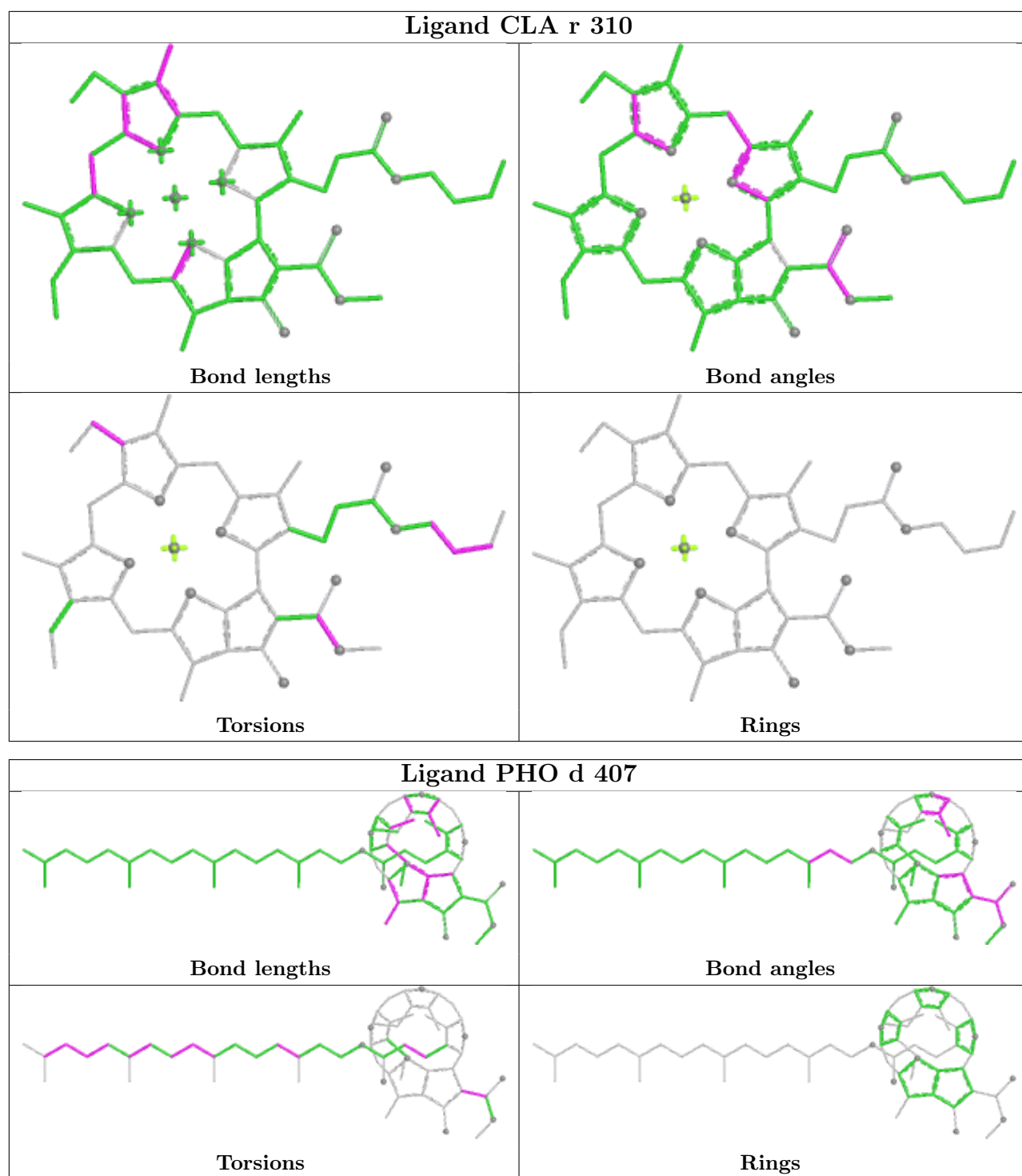
Ligand CLA R 310

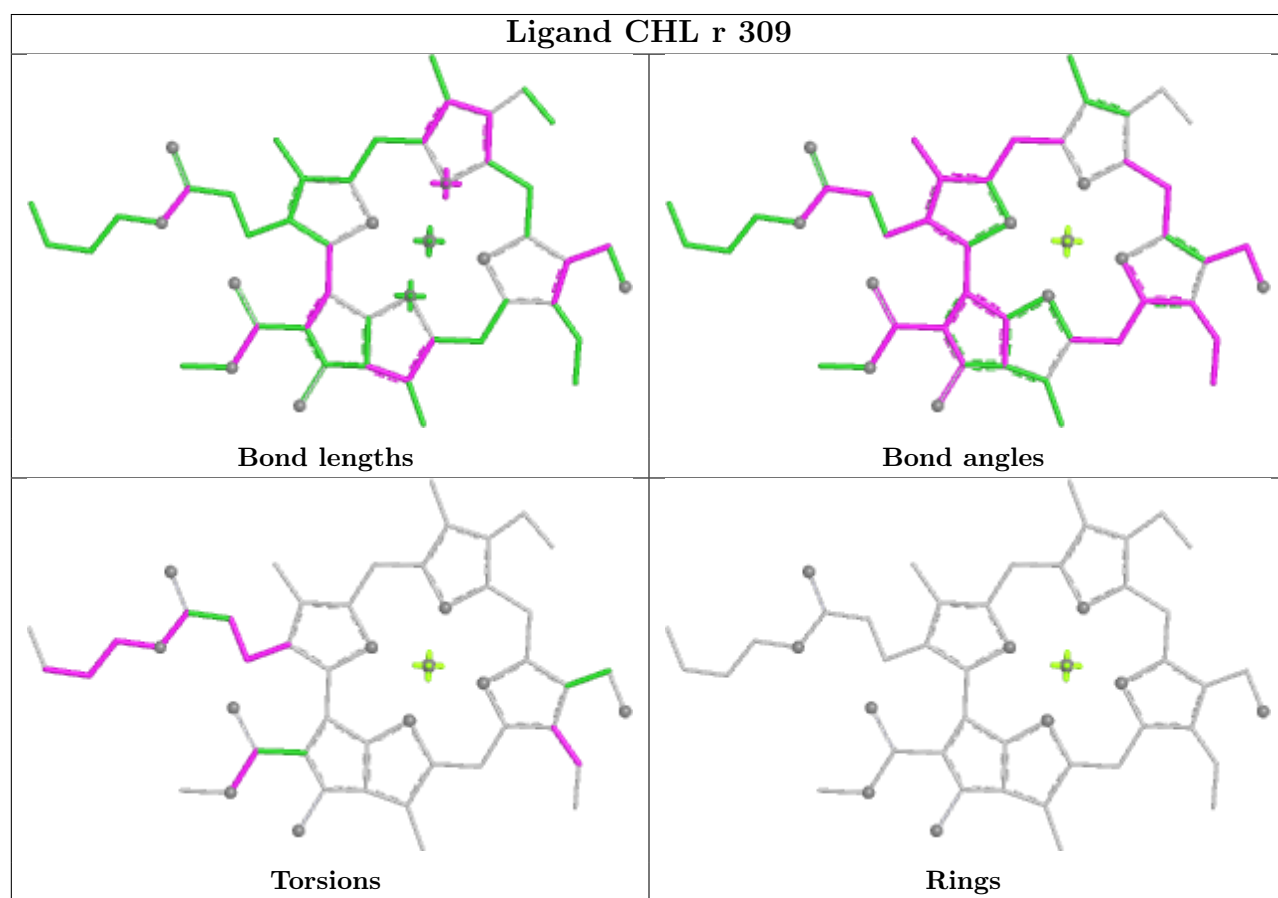
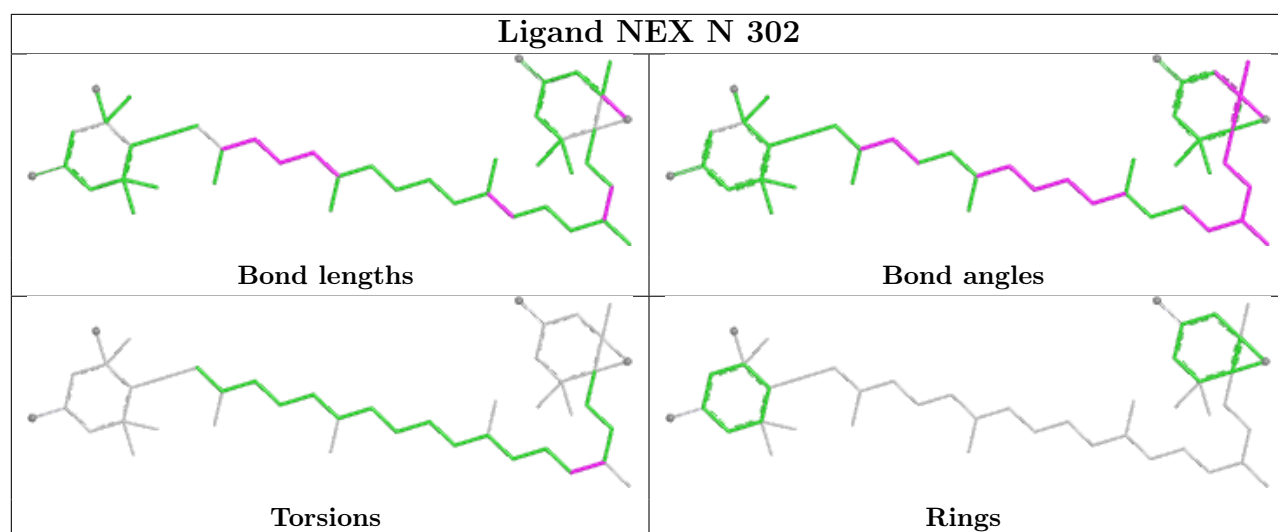


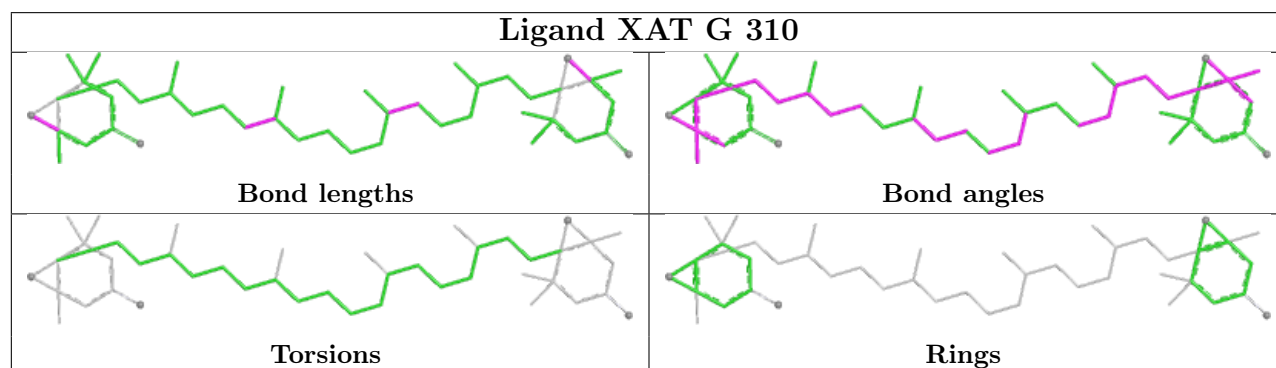
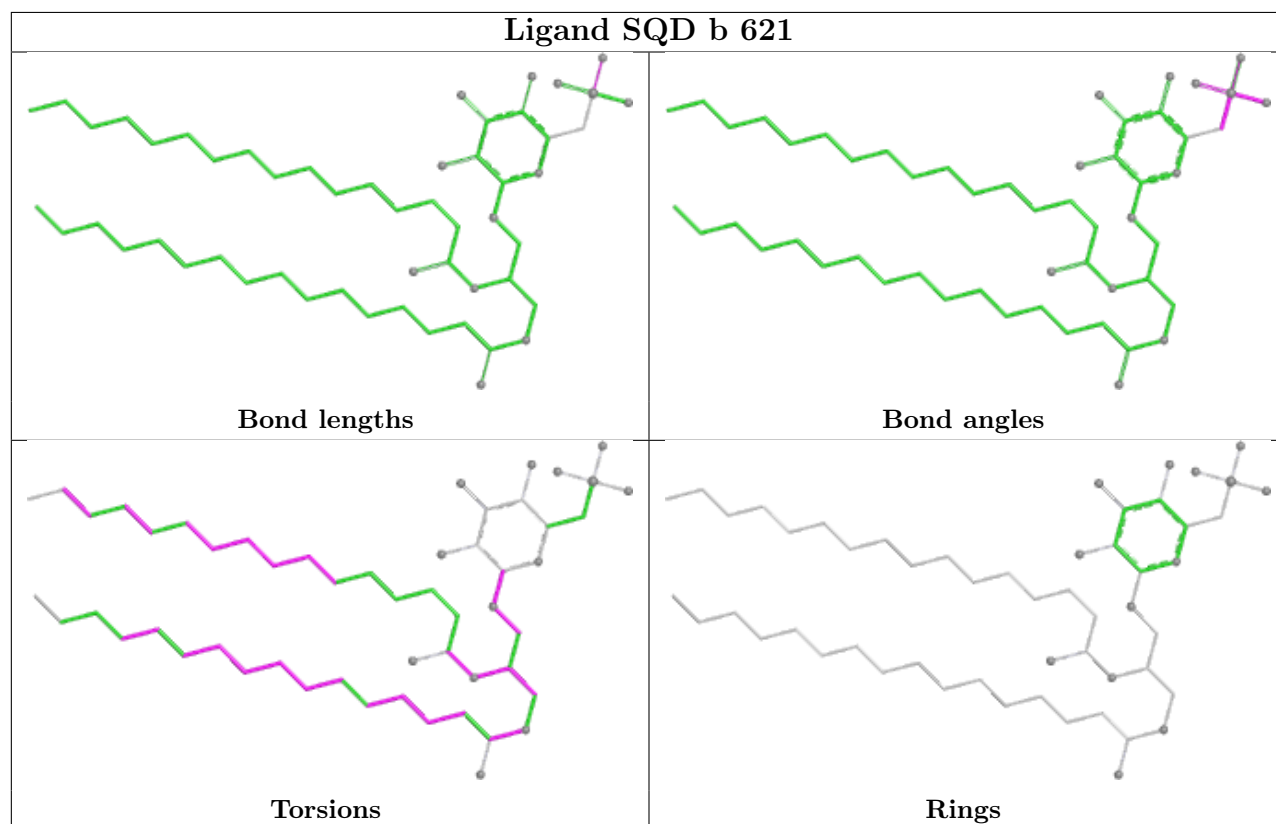
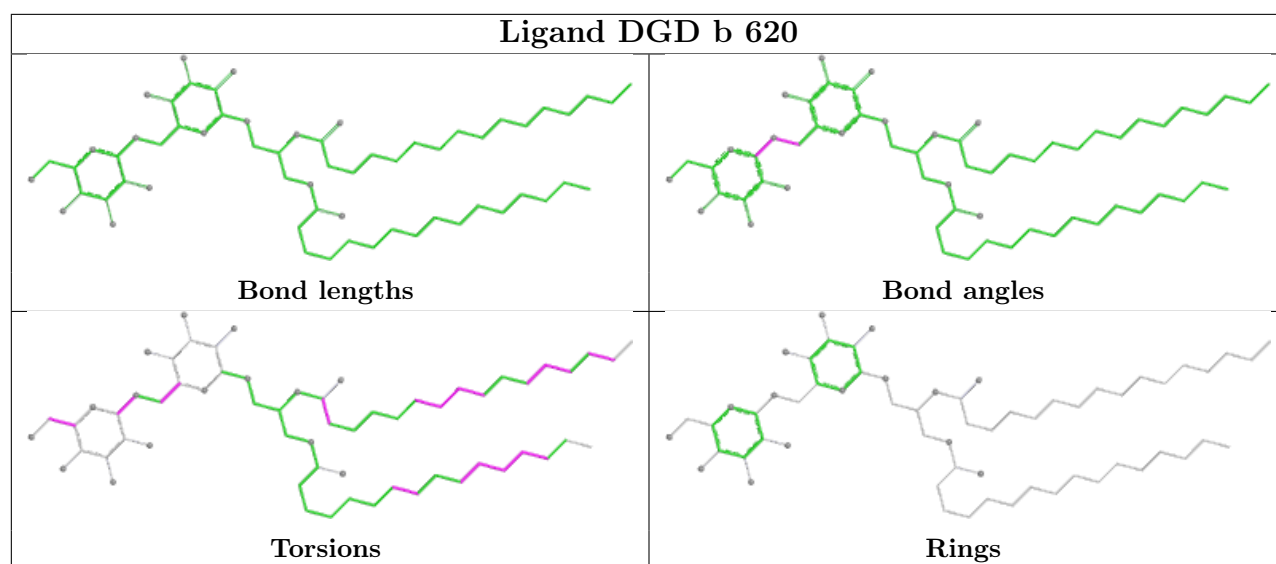
Ligand CLA d 404



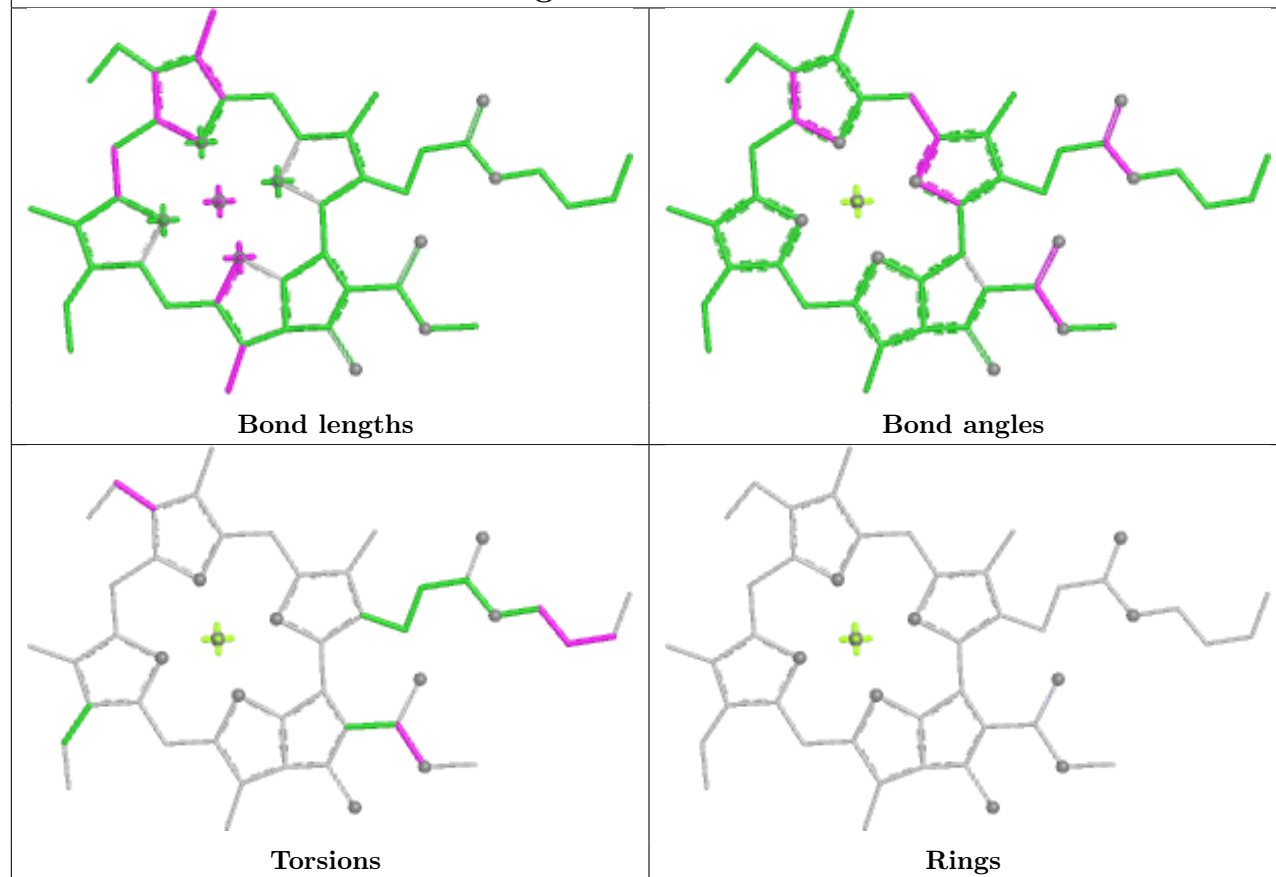




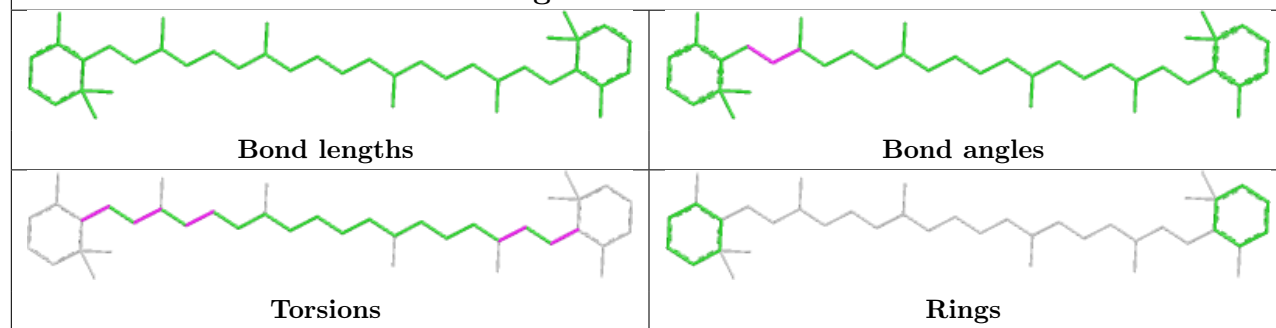


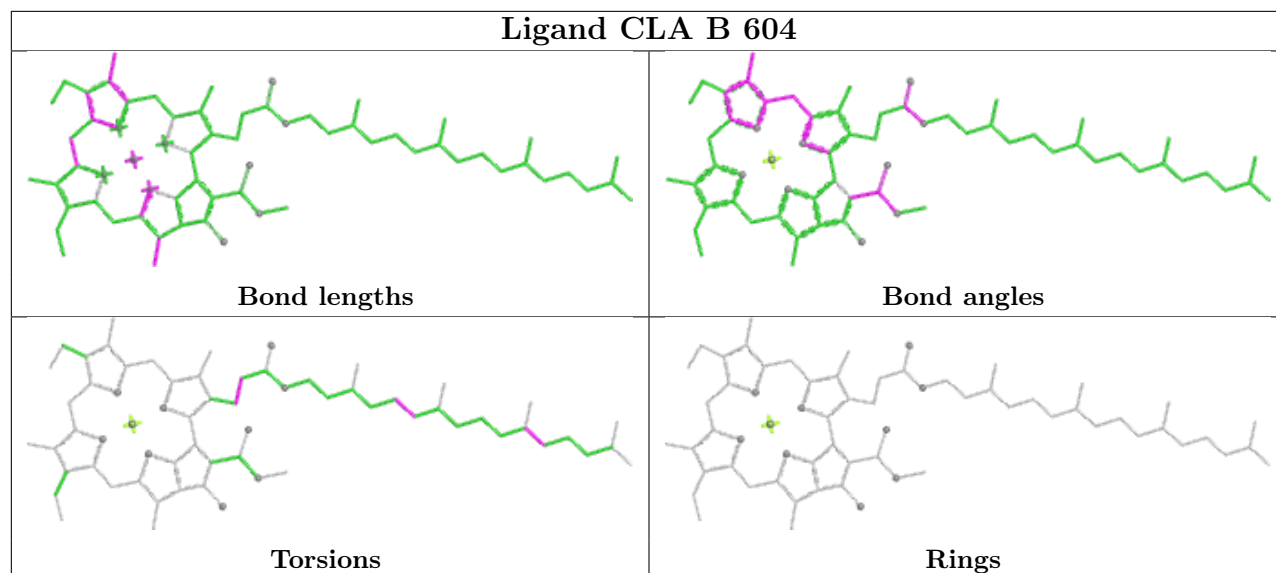
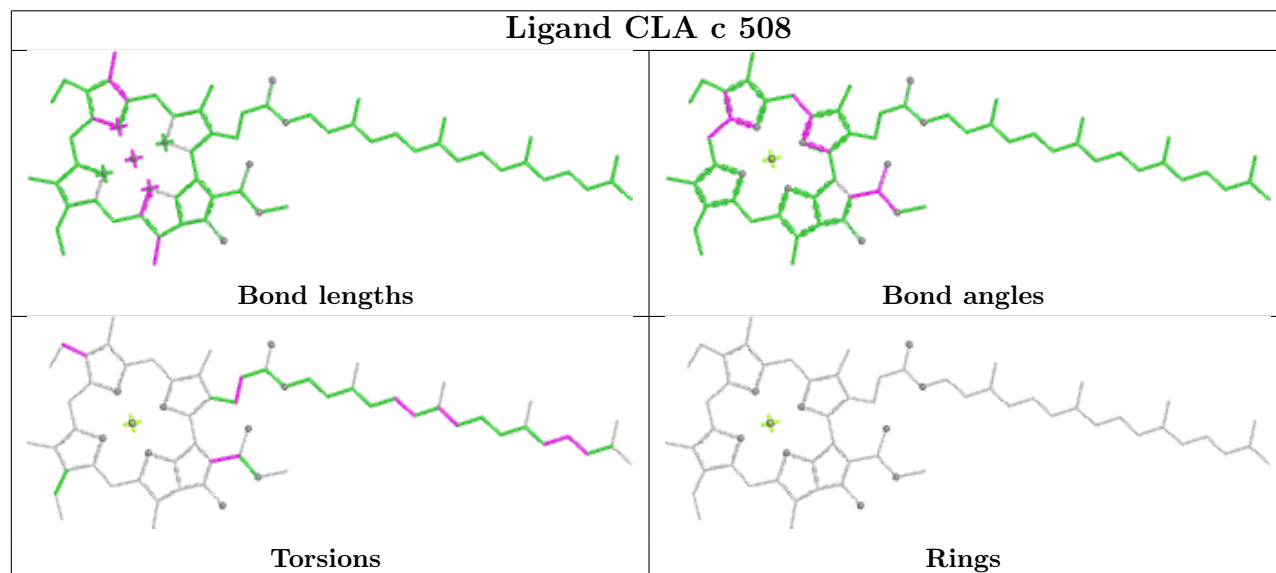
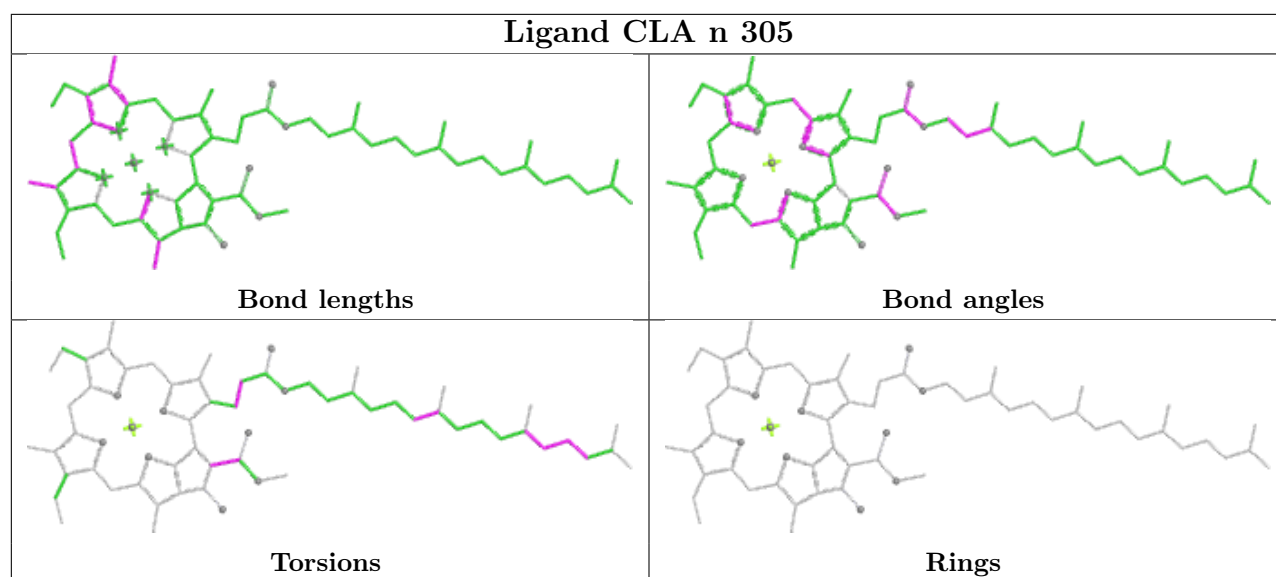


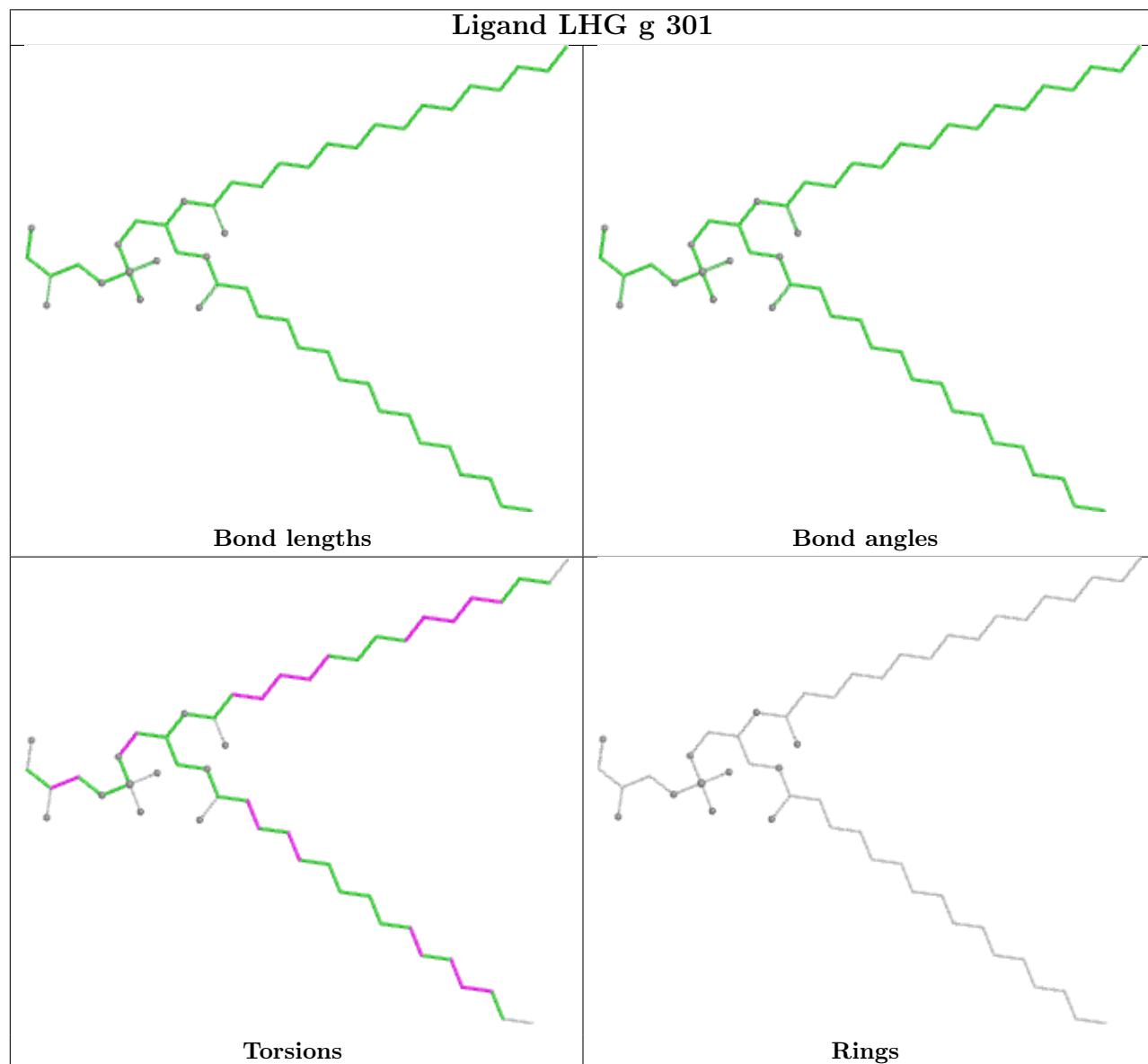
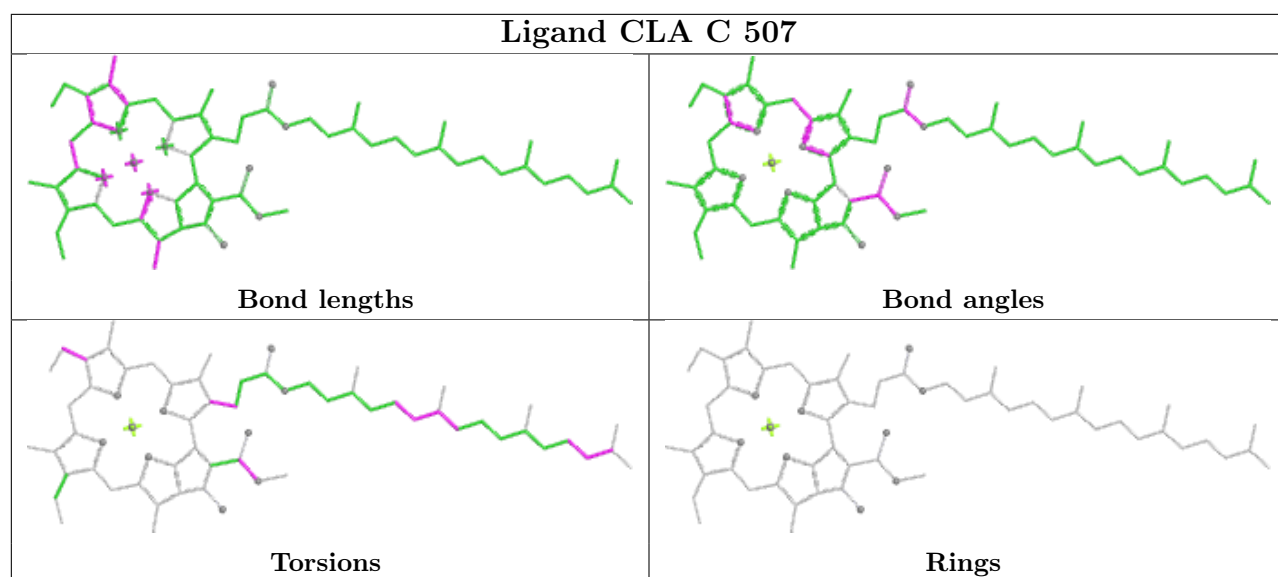
Ligand CLA S 303

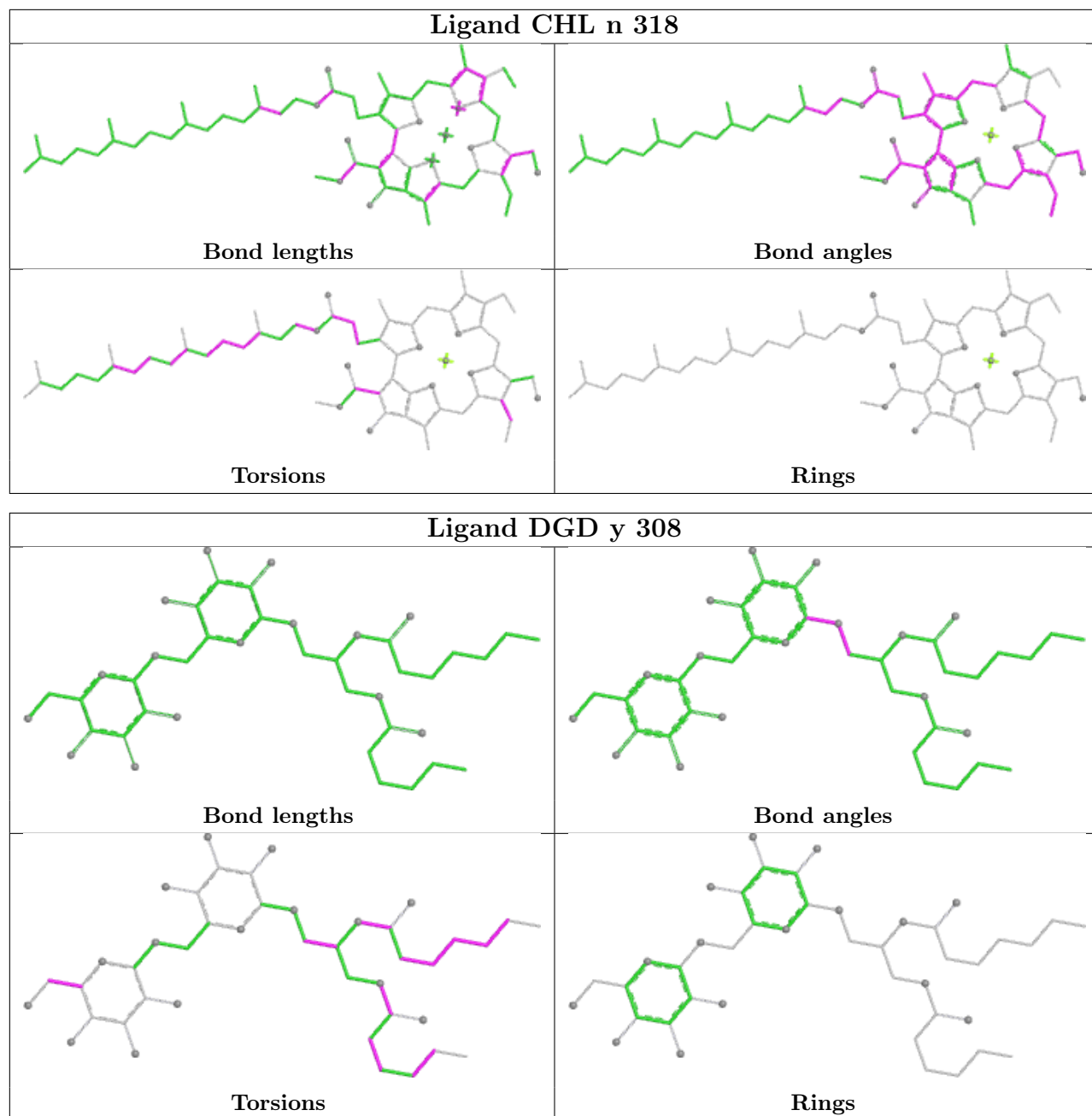


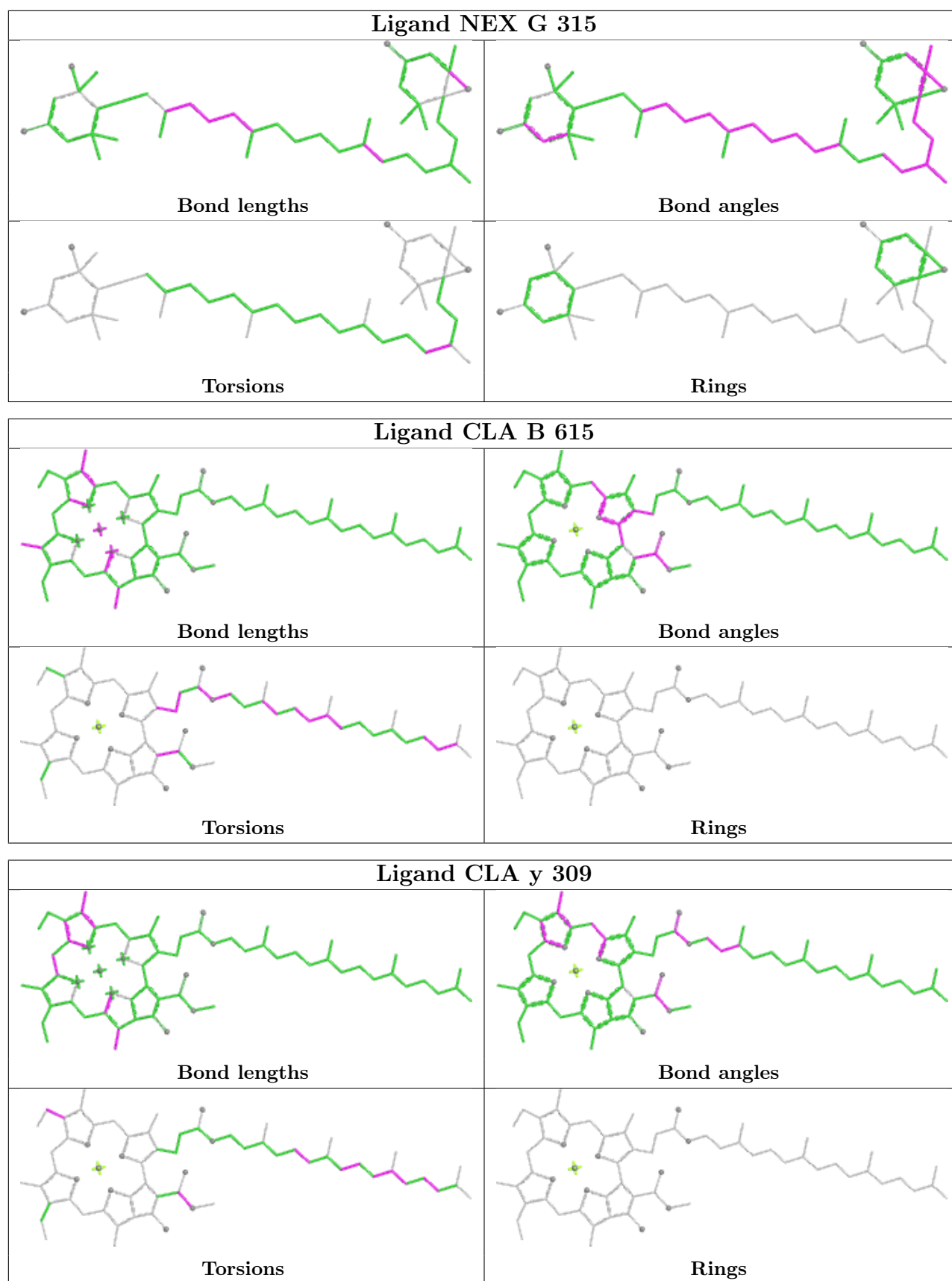
Ligand BCR d 401

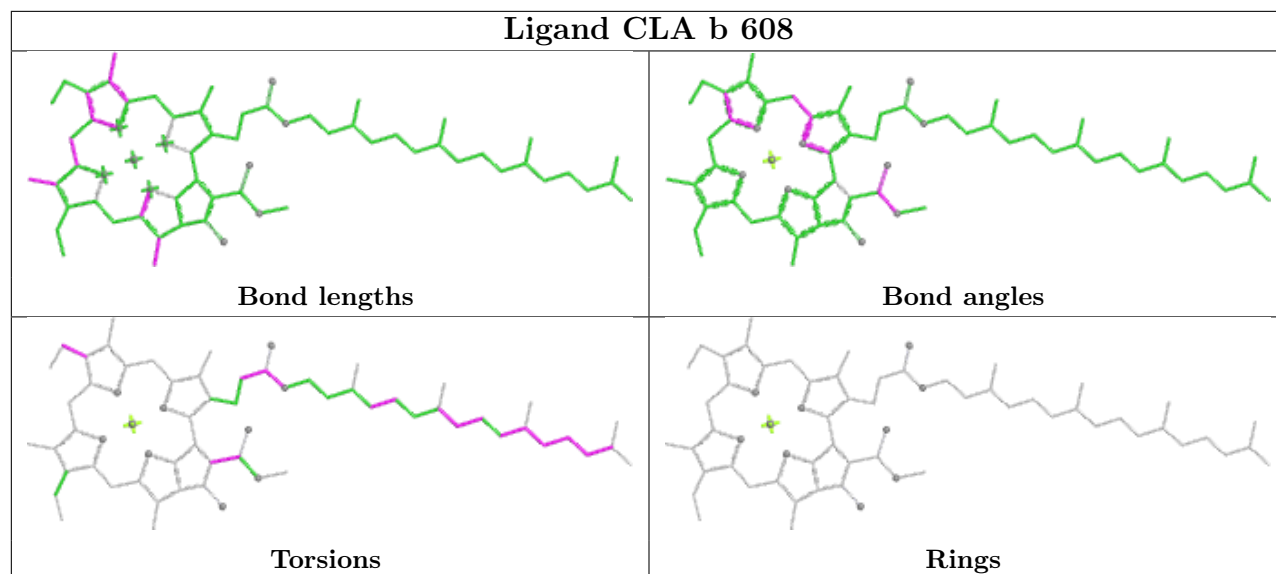
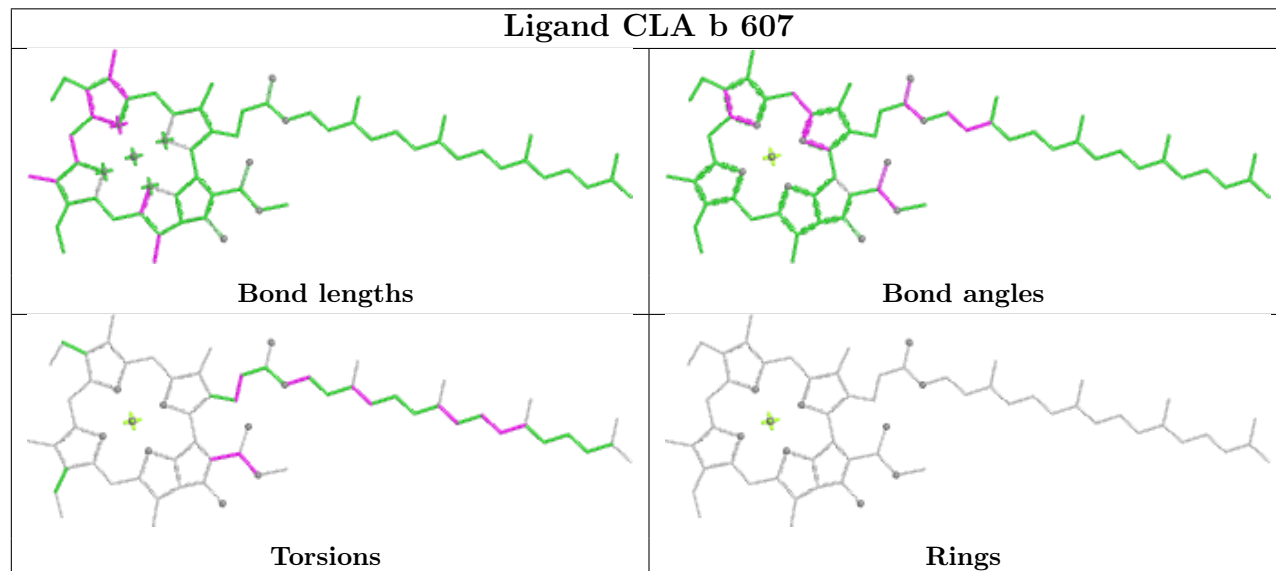




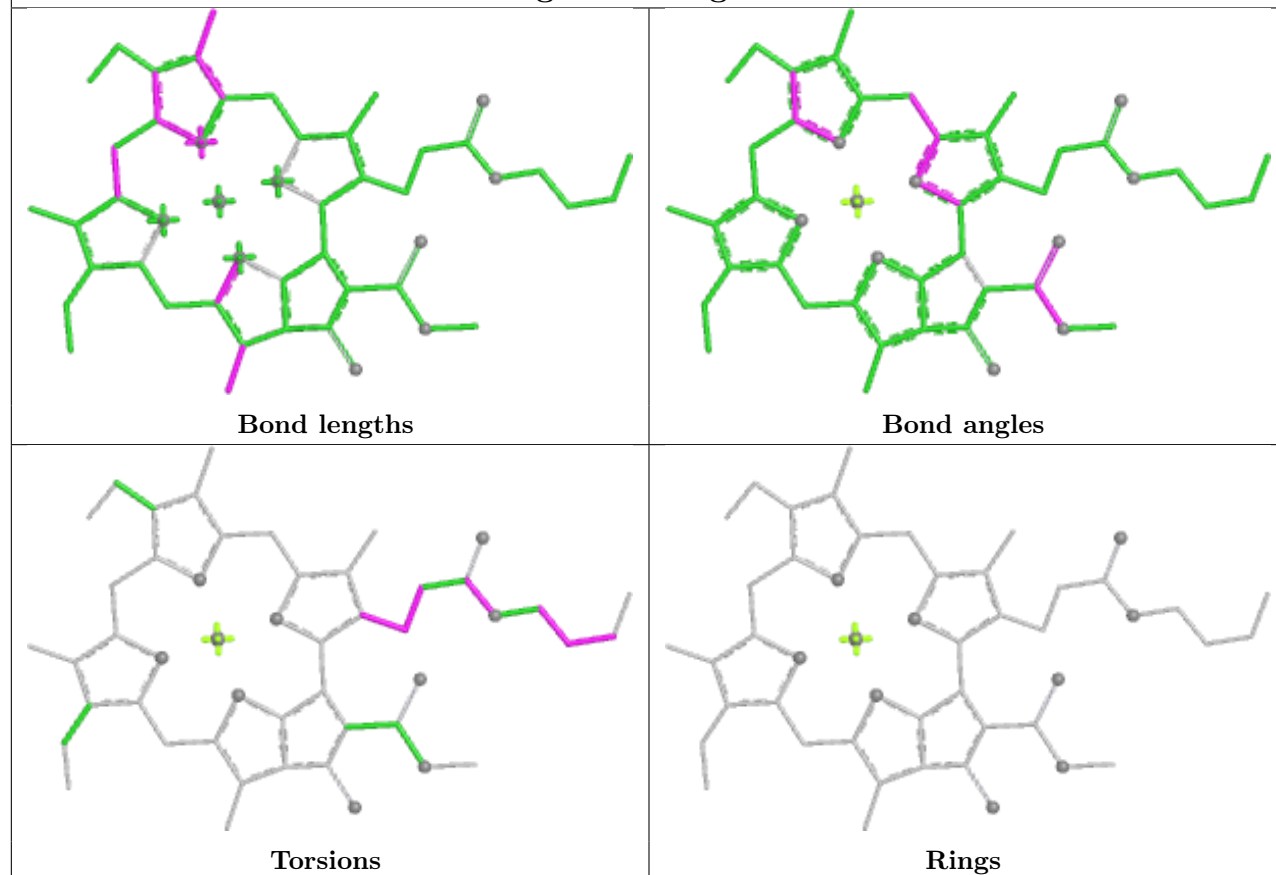




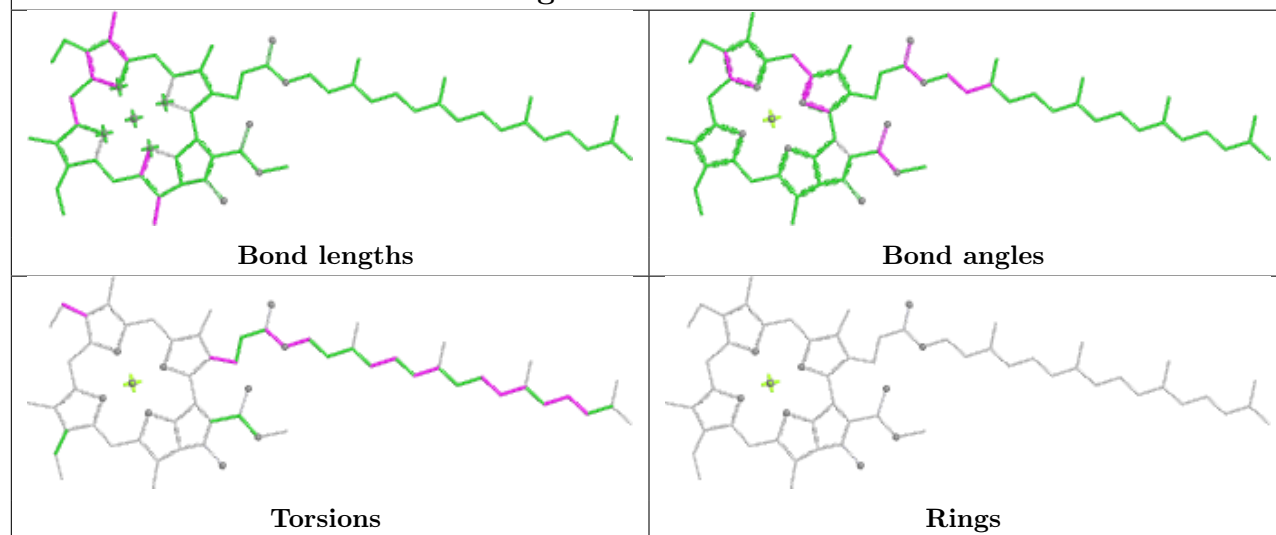


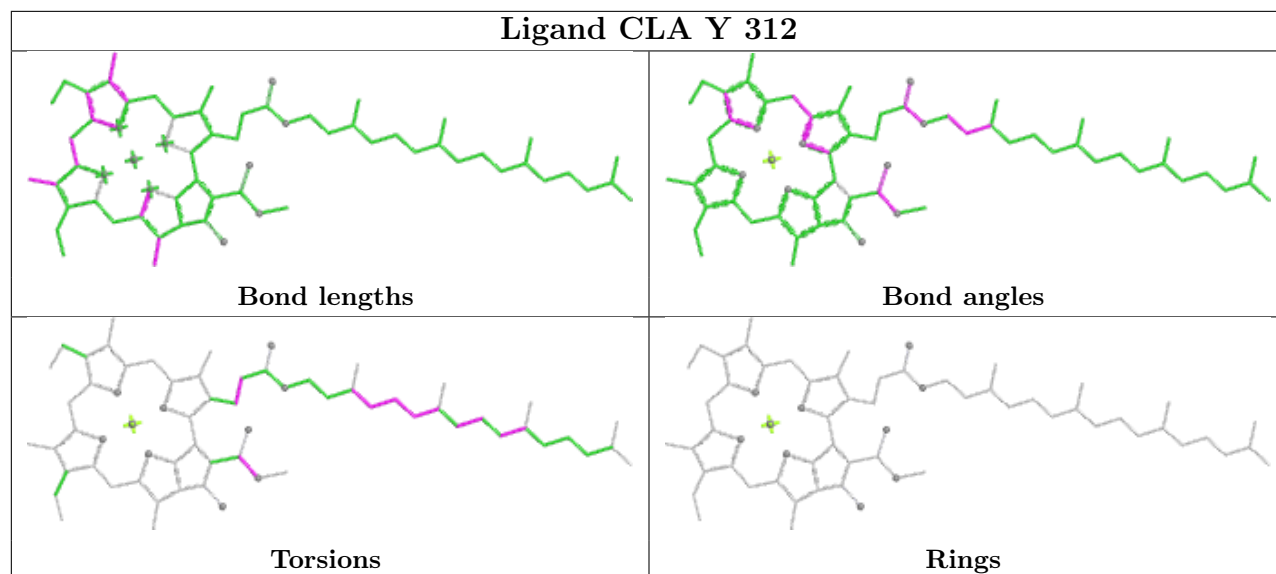
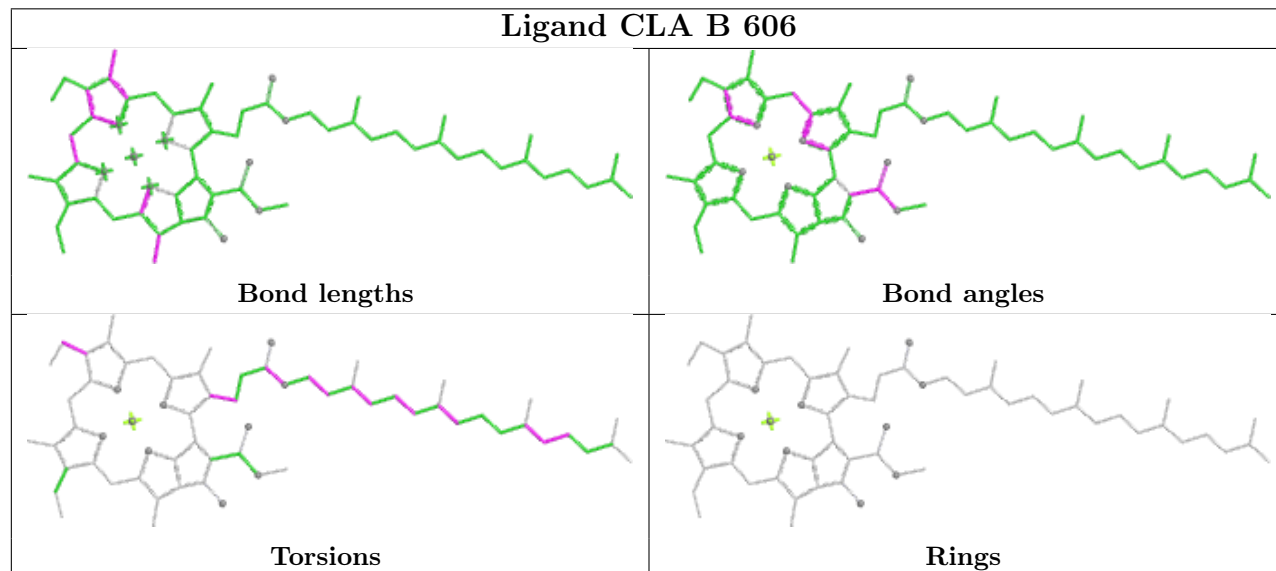
Ligand CLA b 608**Ligand CLA b 607**

Ligand CLA g 302

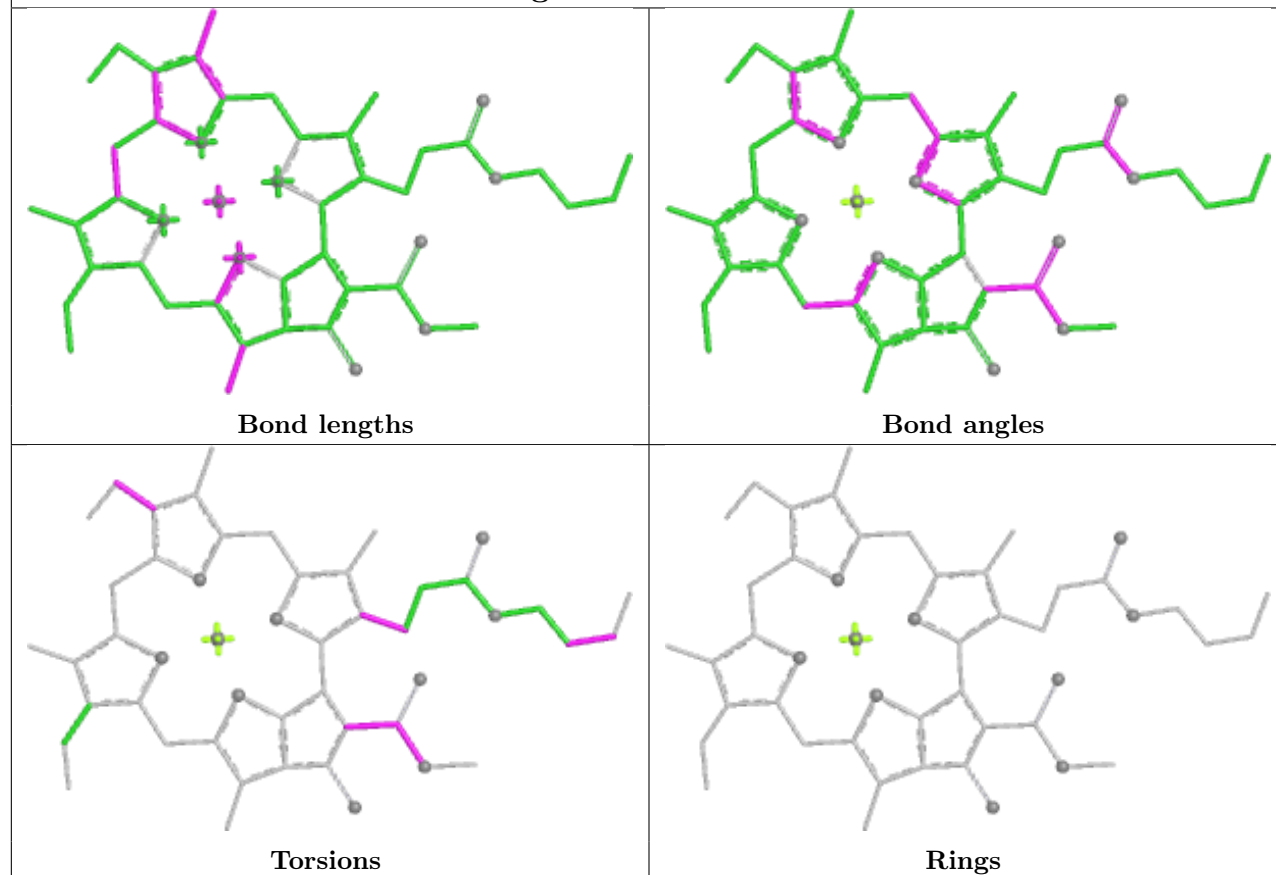


Ligand CLA c 503

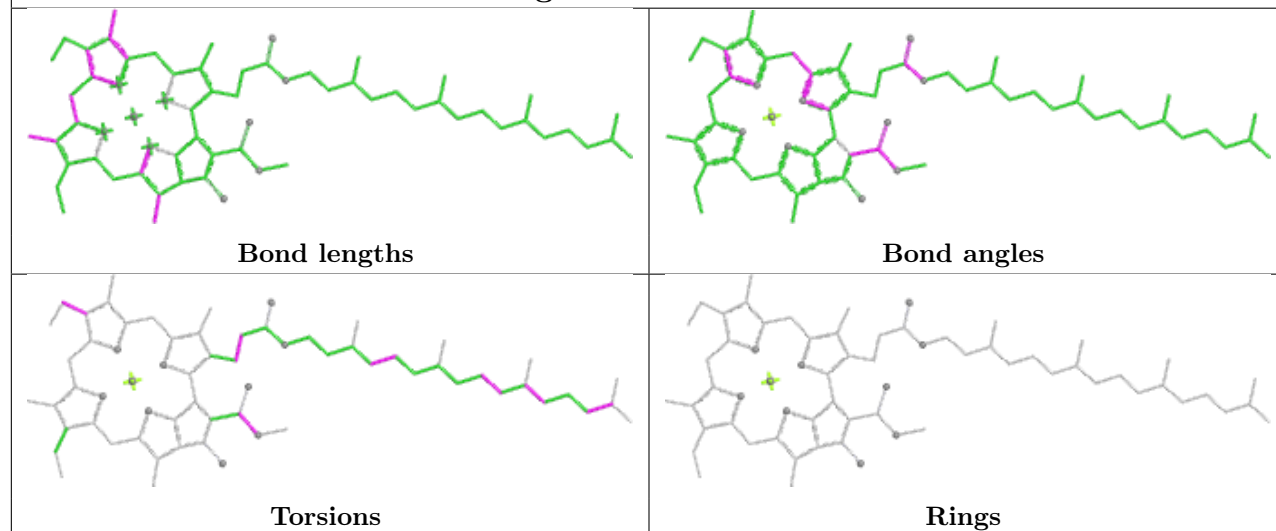


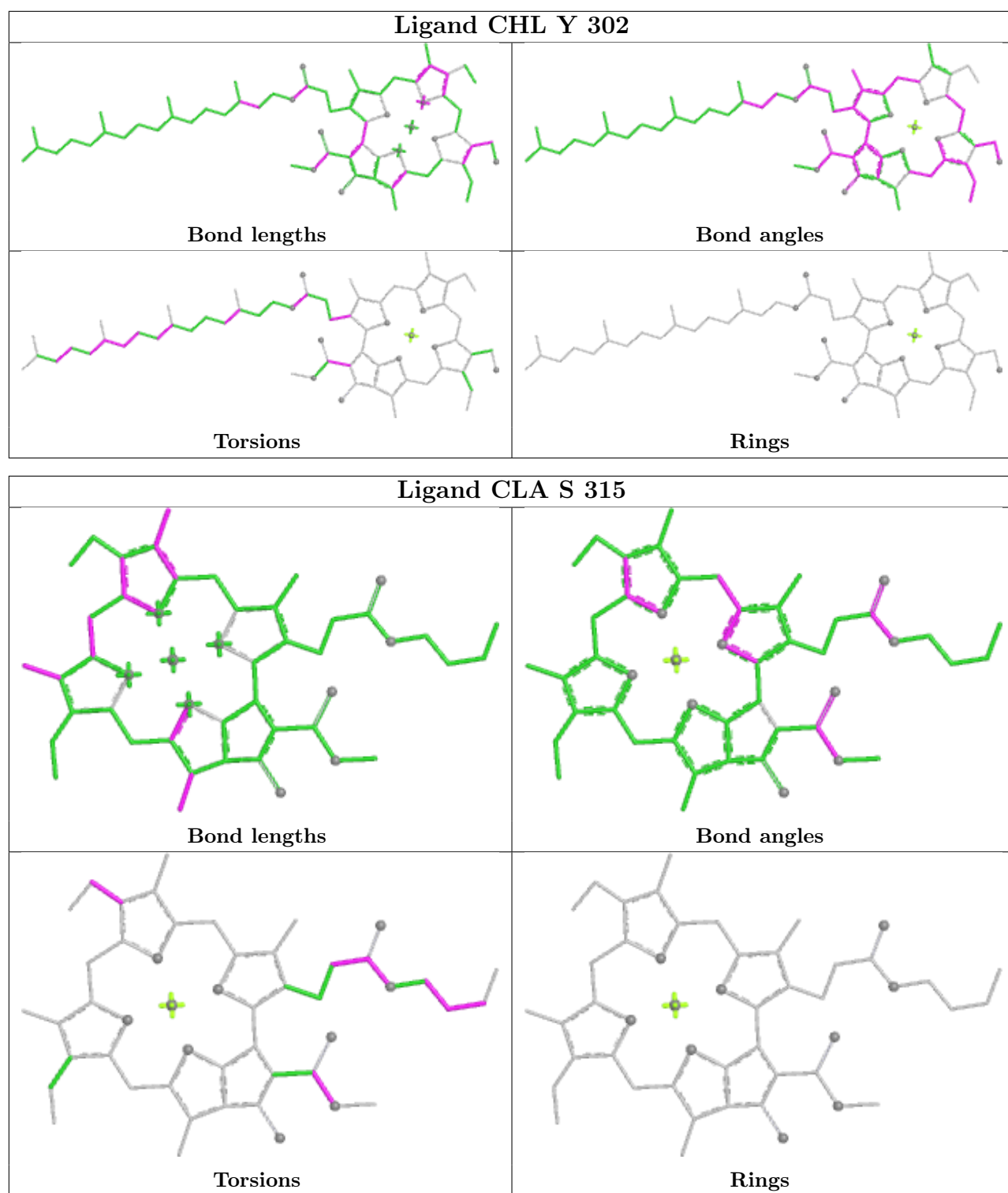
Ligand CLA Y 312**Ligand CLA B 606**

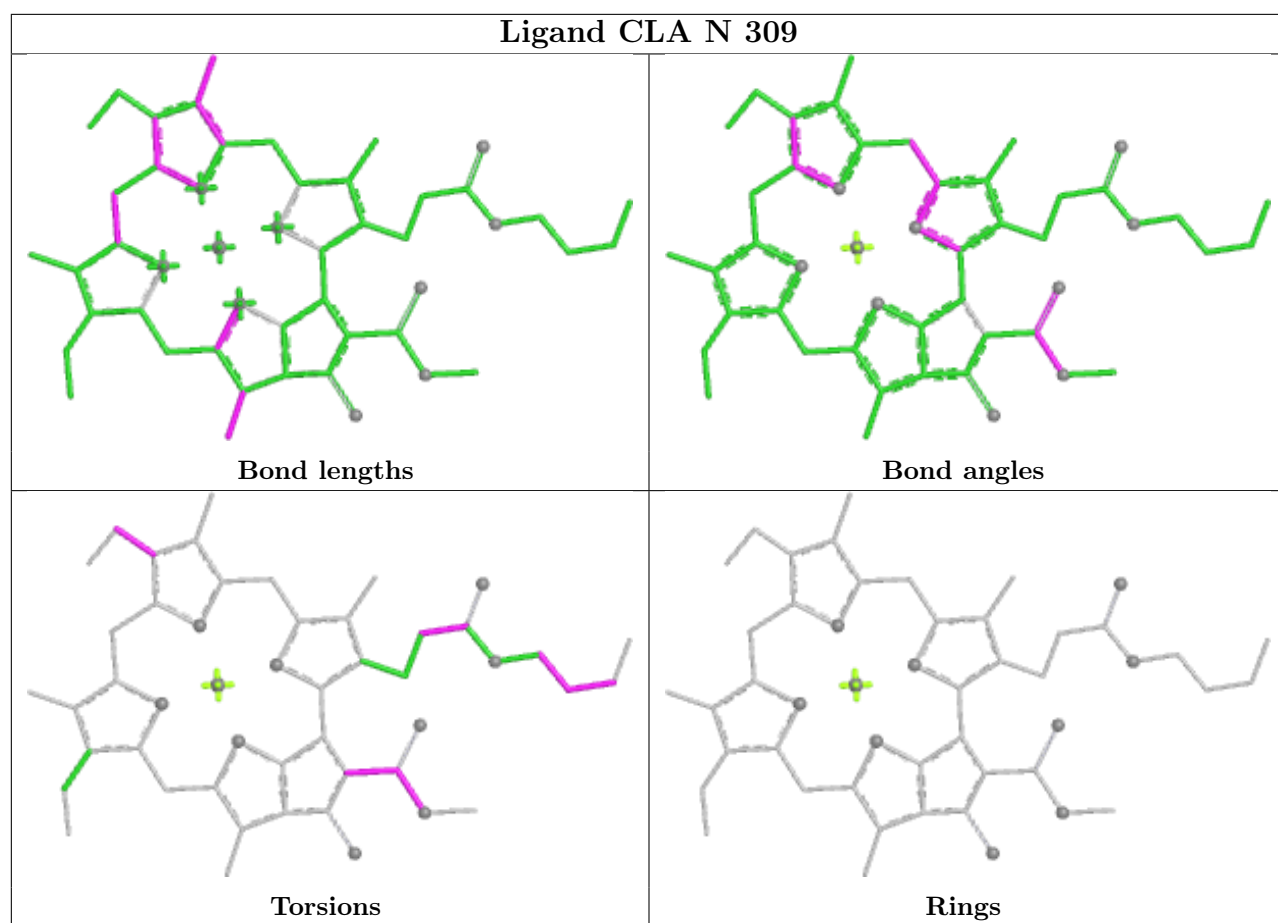
Ligand CLA D 412

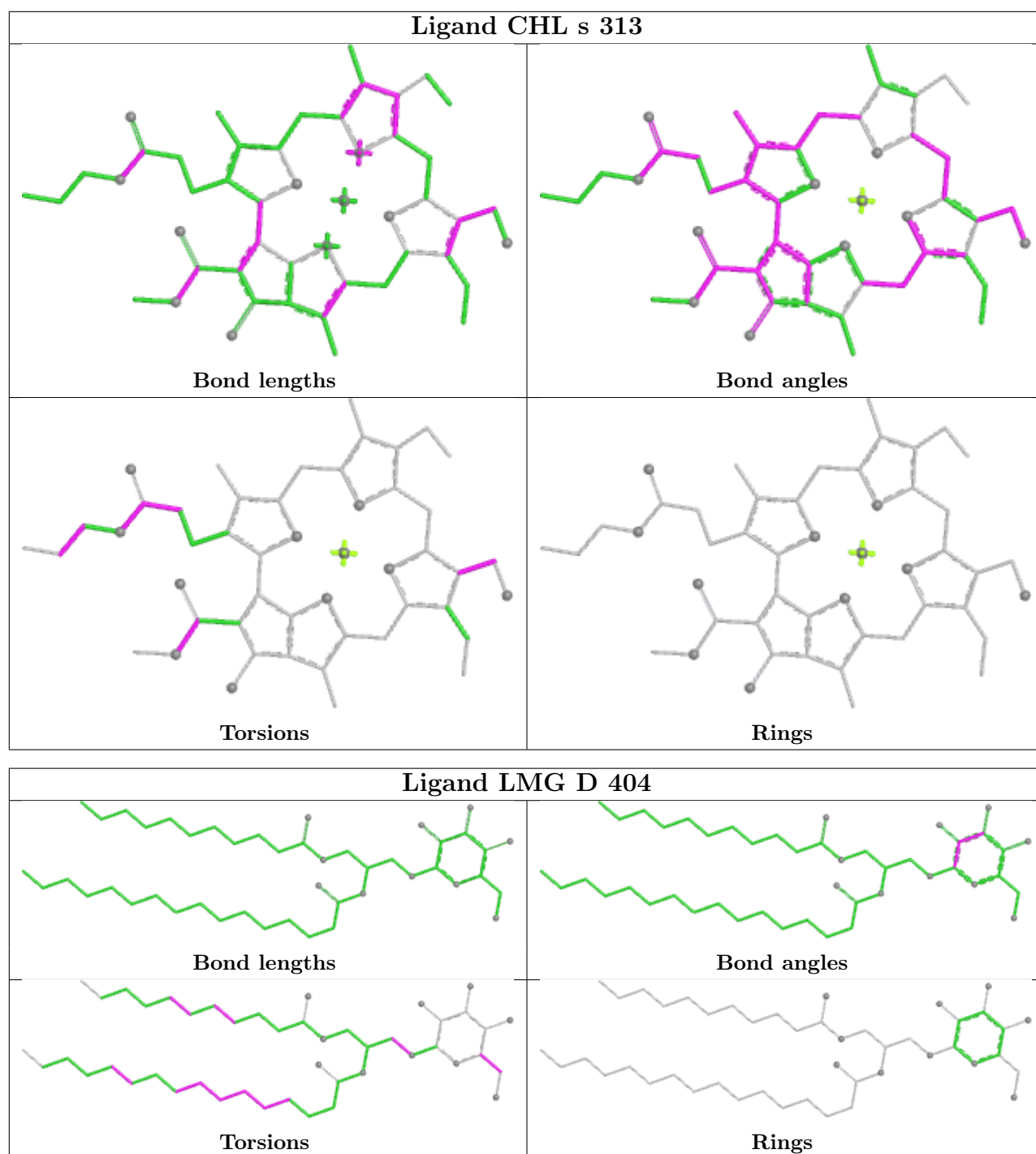


Ligand CLA b 617

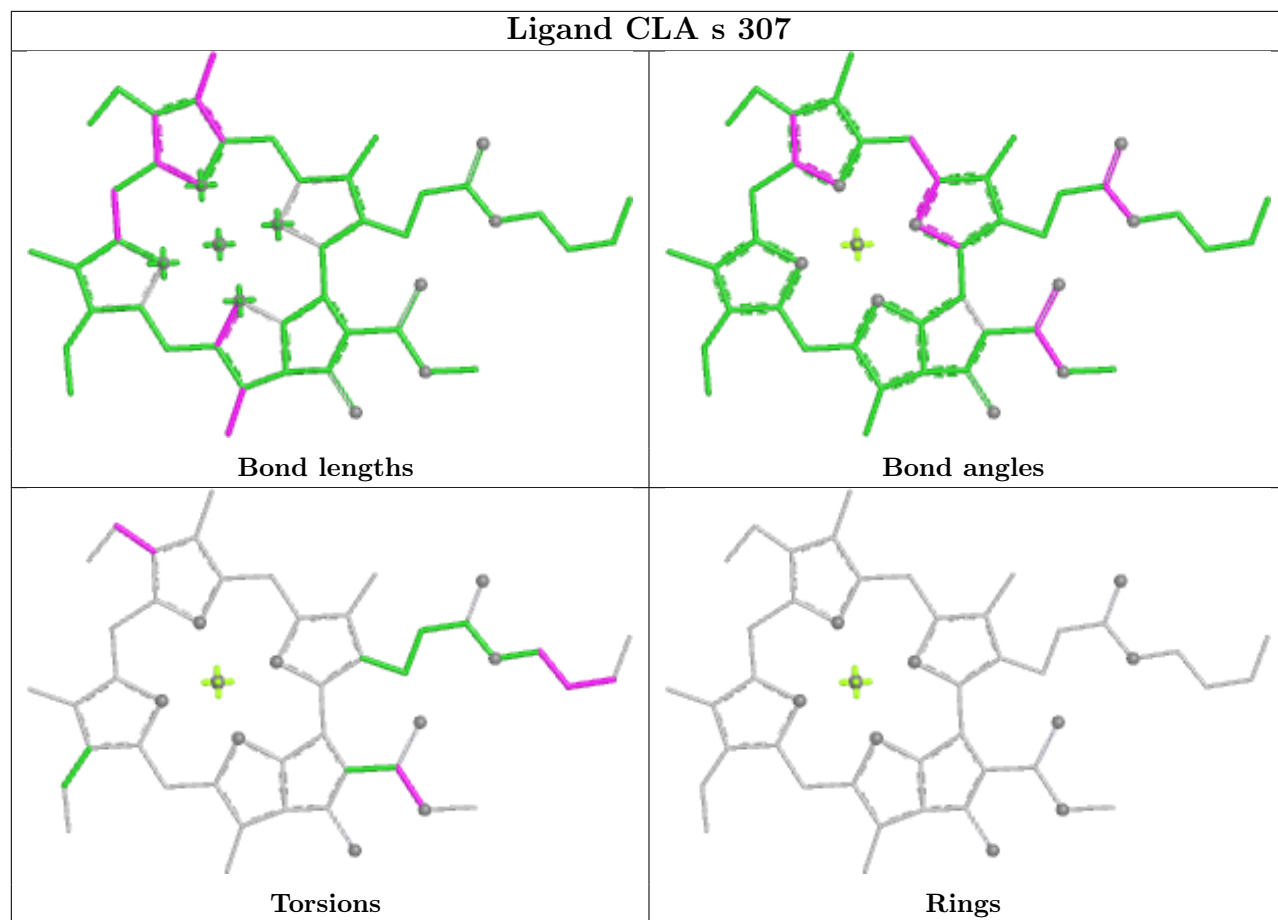


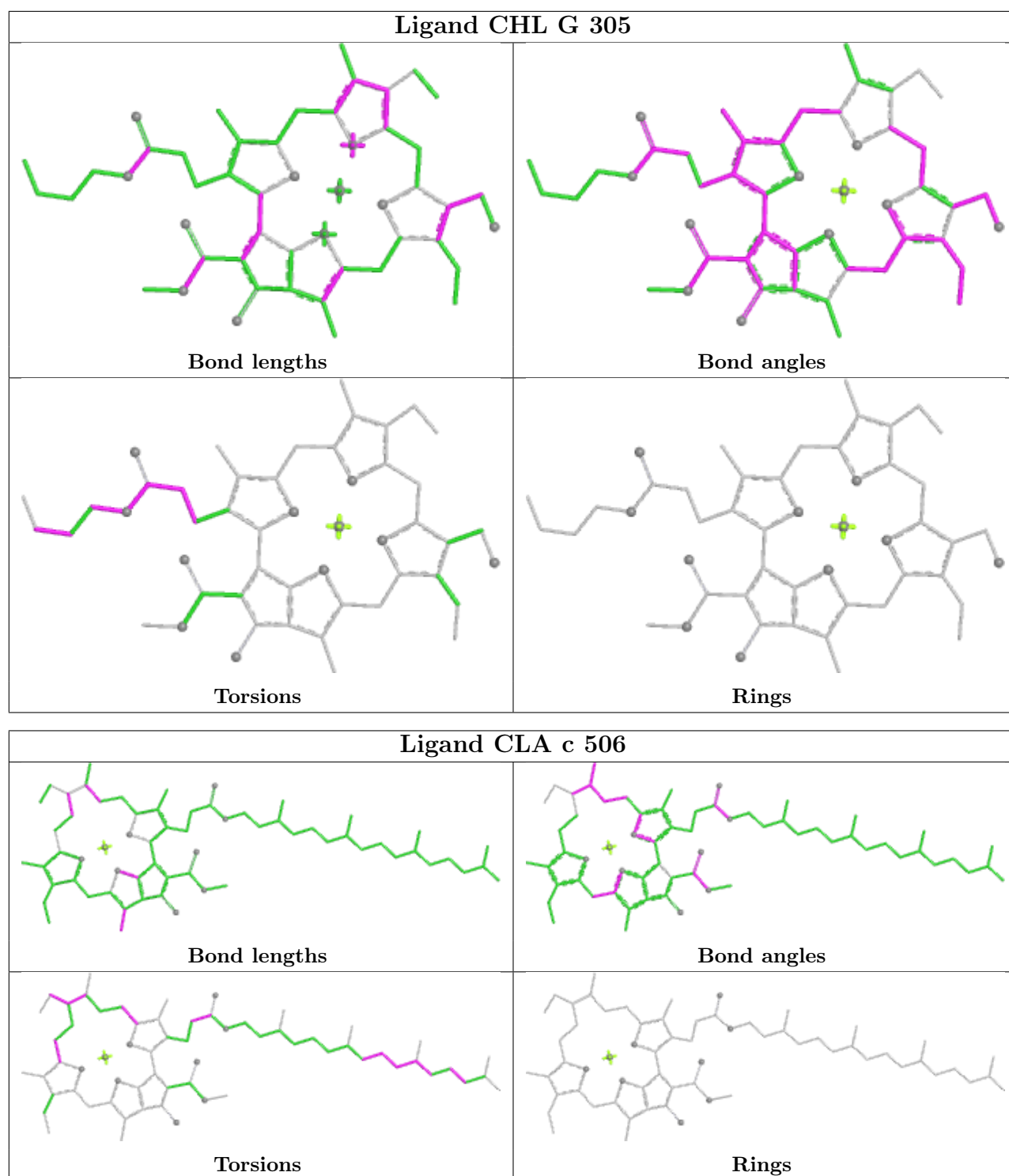




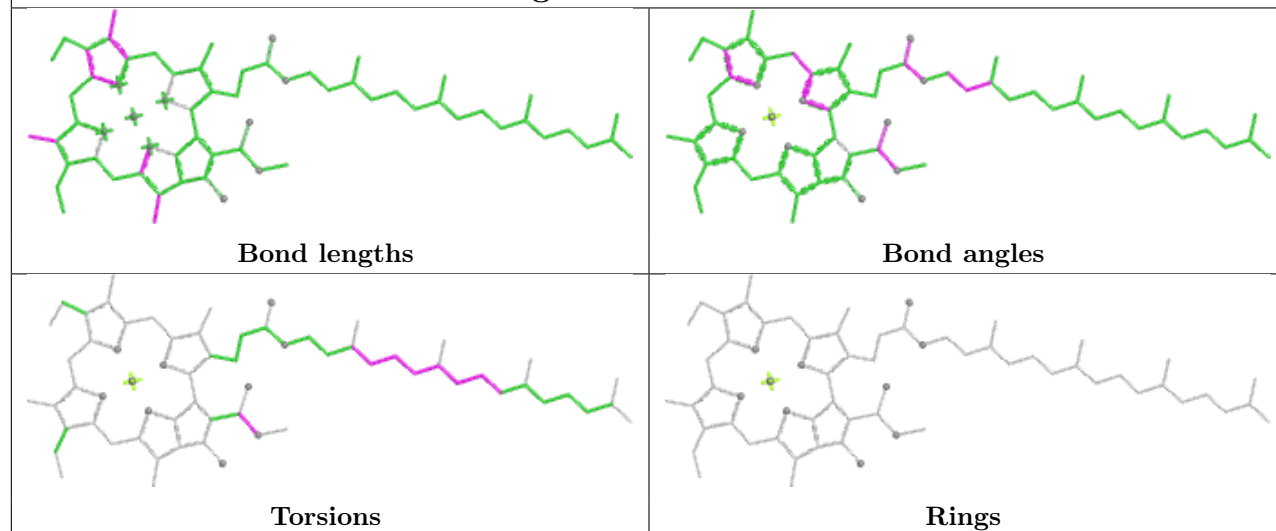


Ligand CLA s 307

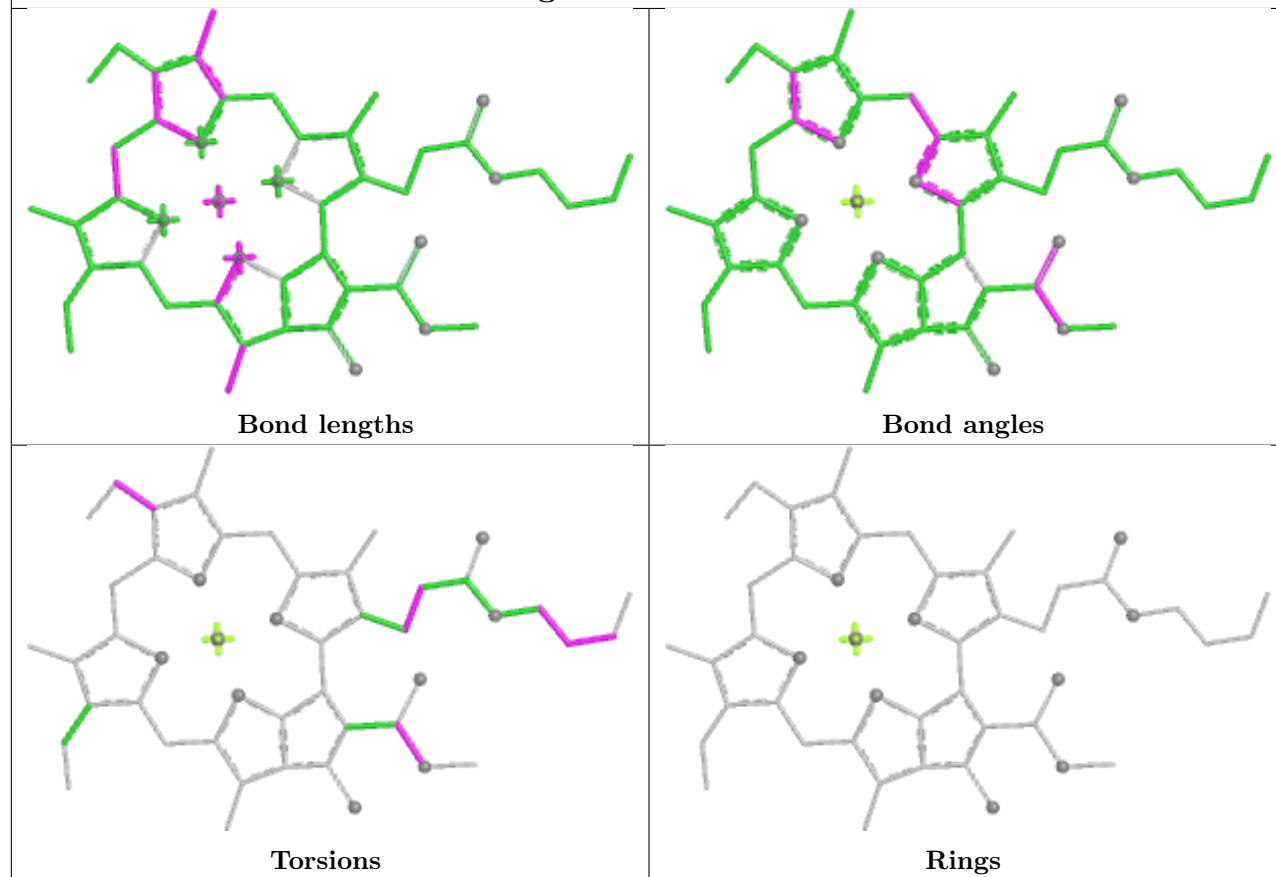


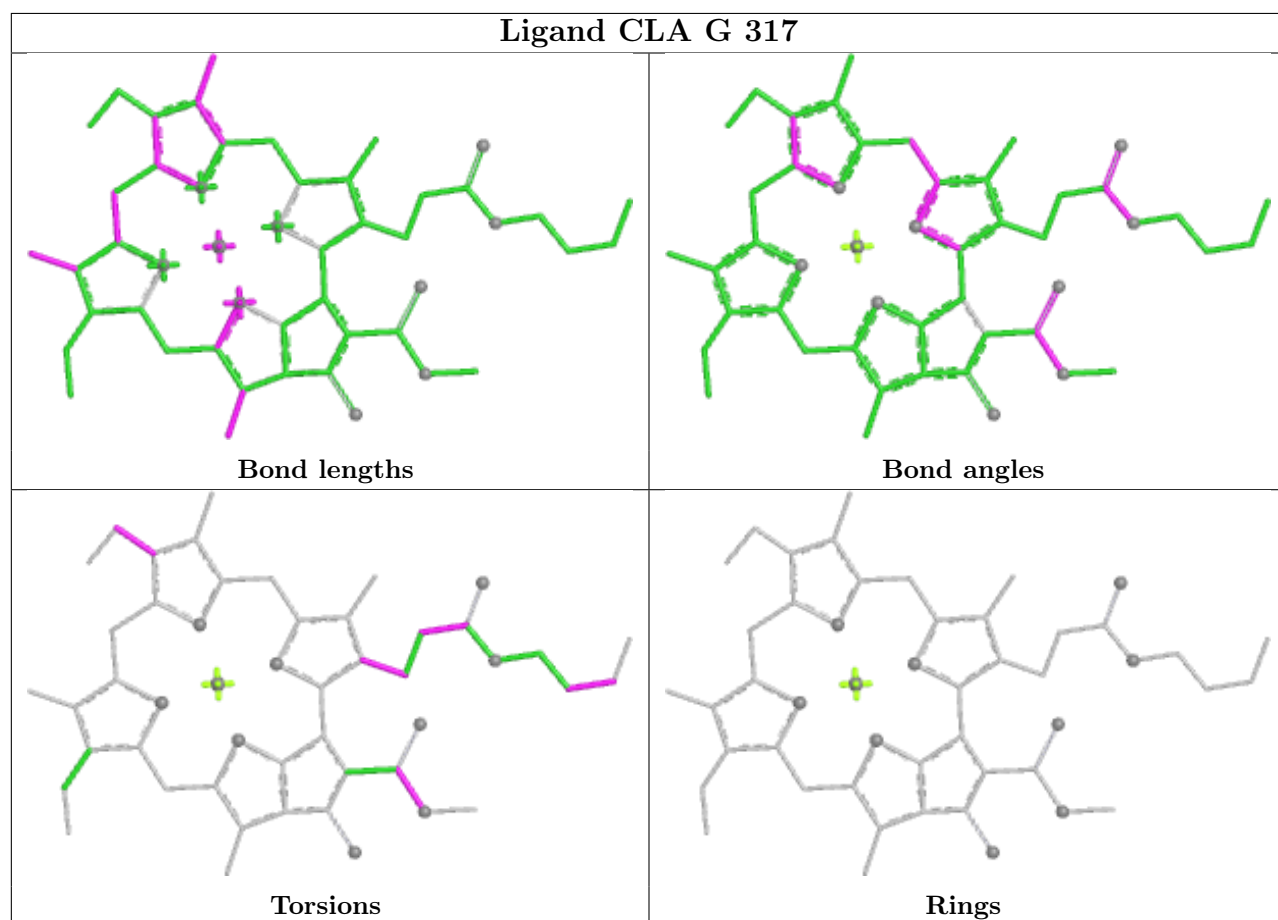
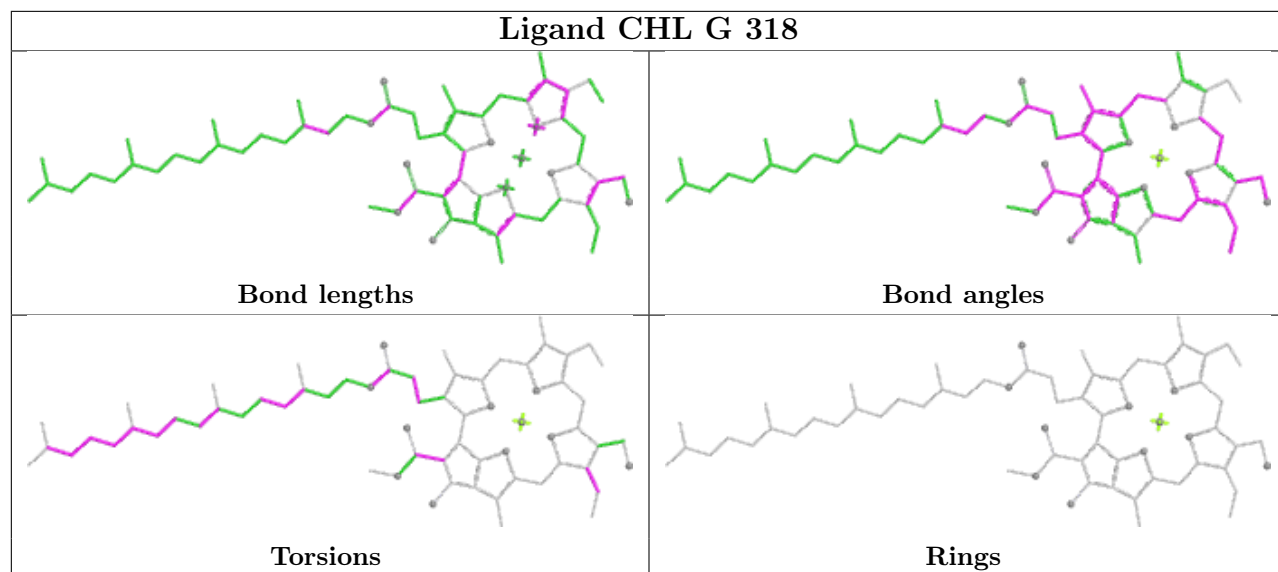


Ligand CLA B 607

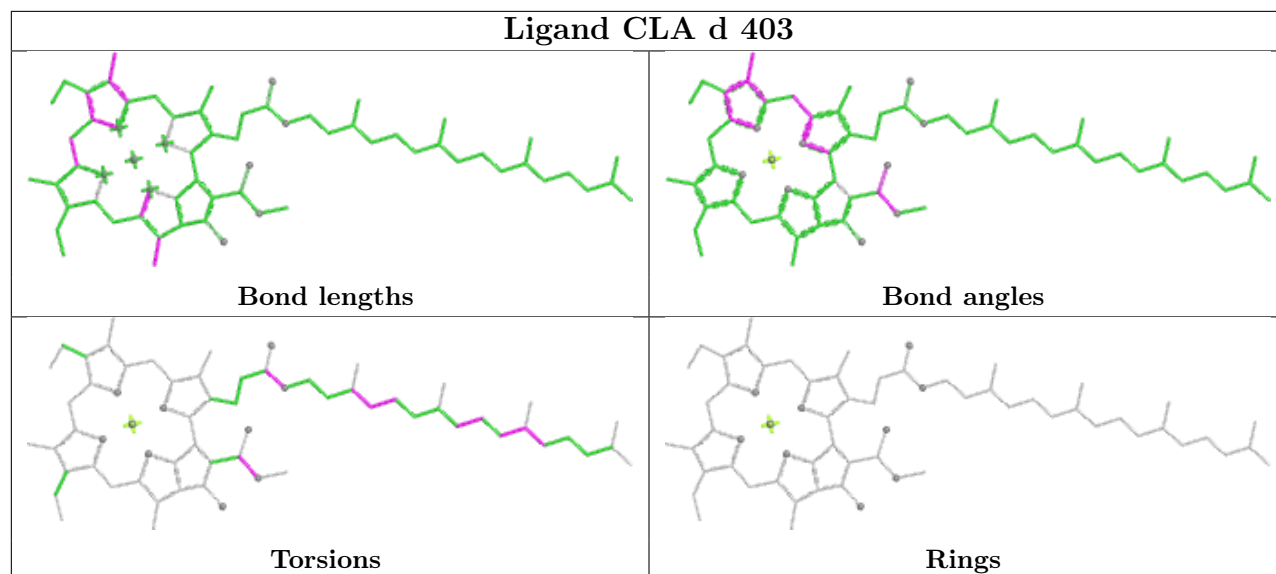


Ligand CLA r 308

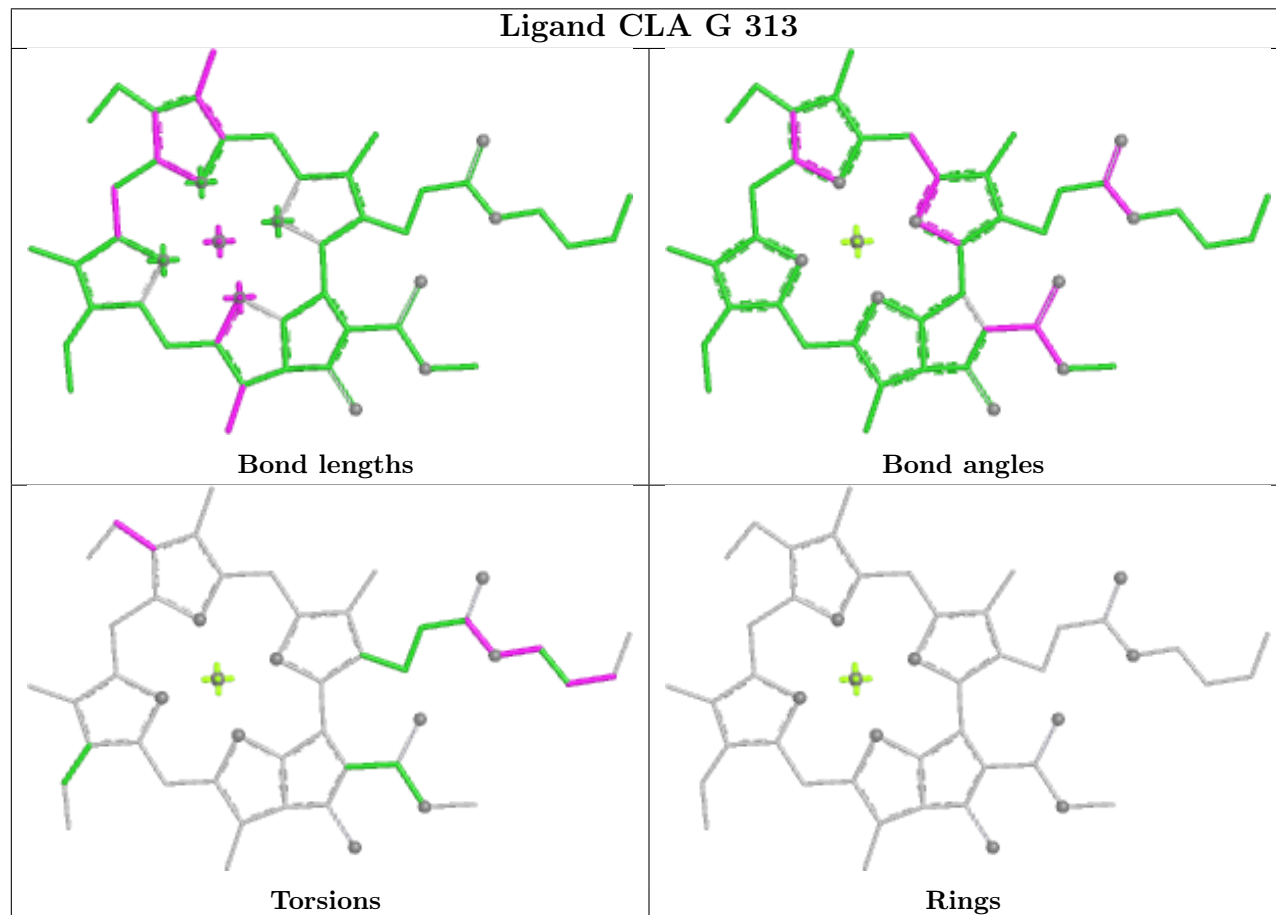




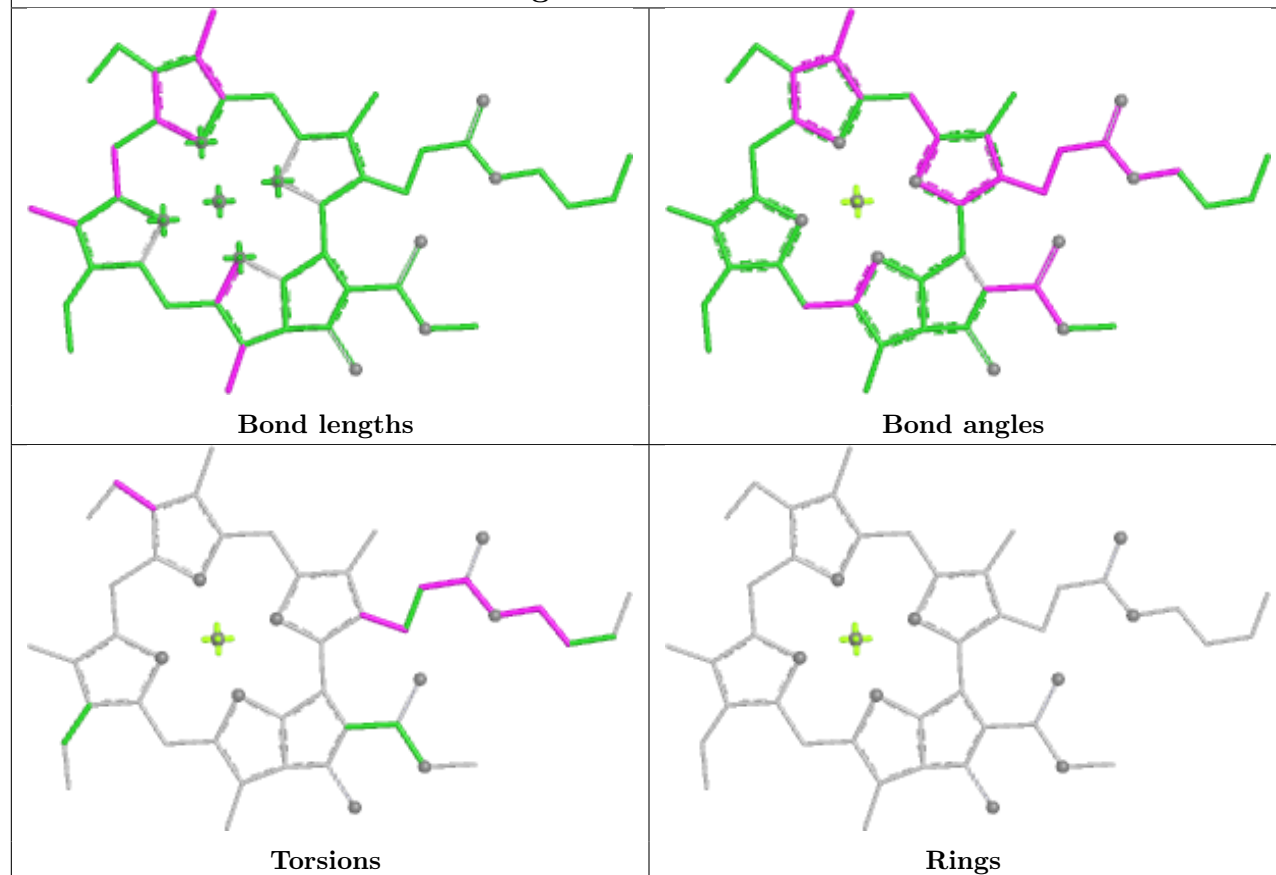
Ligand CLA d 403



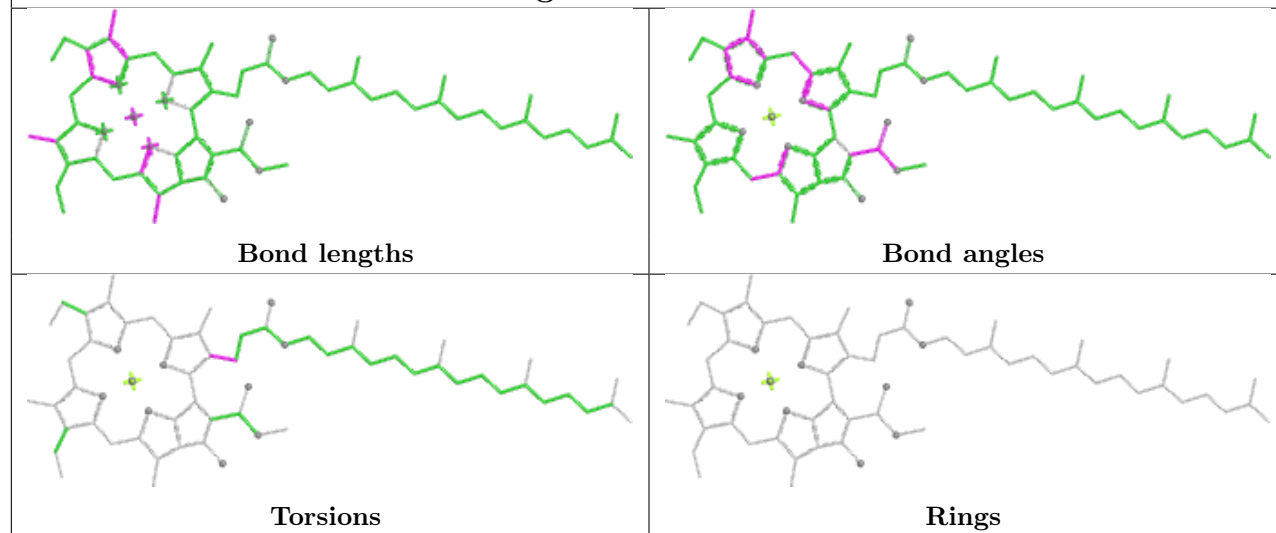
Ligand CLA G 313

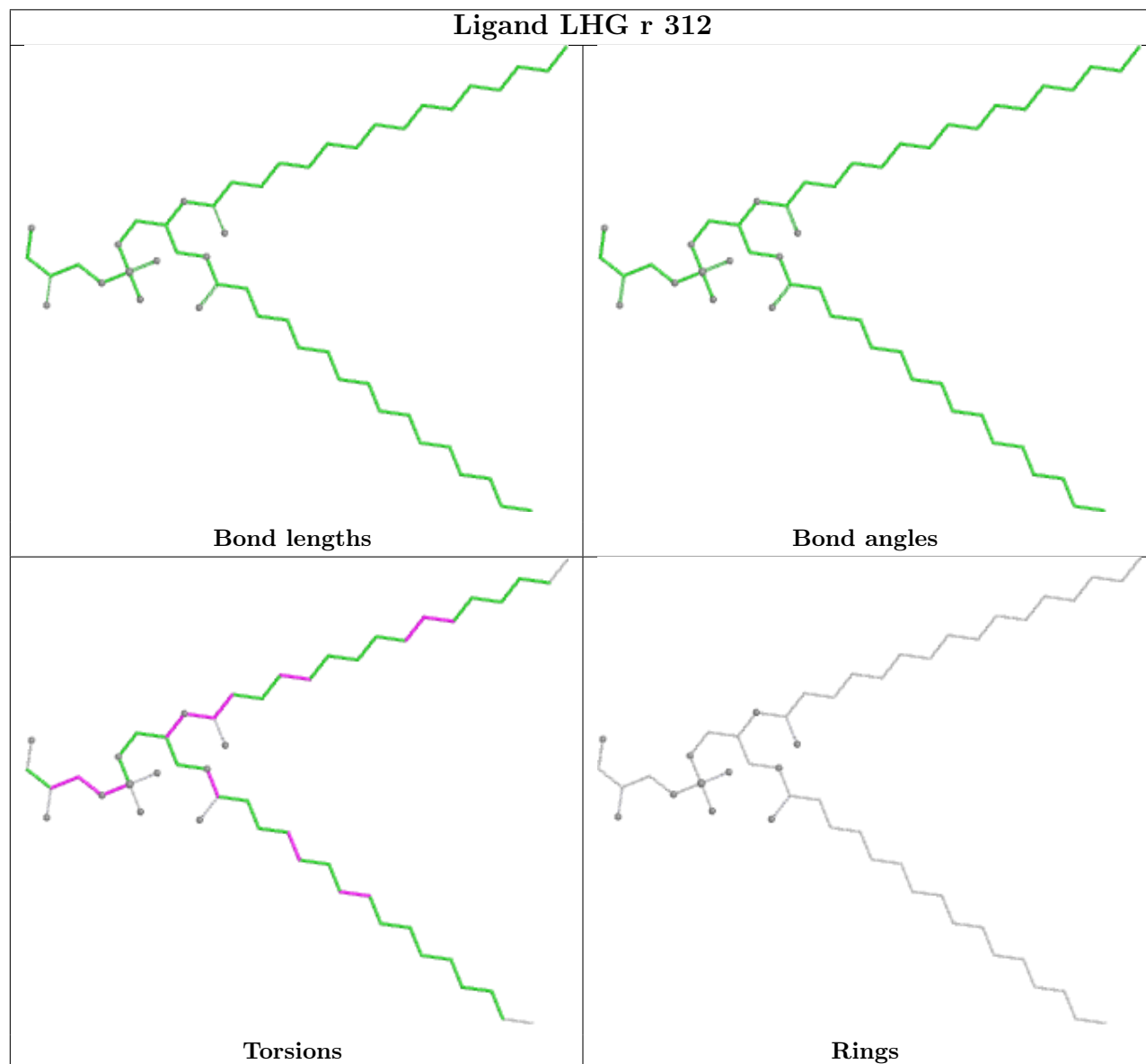
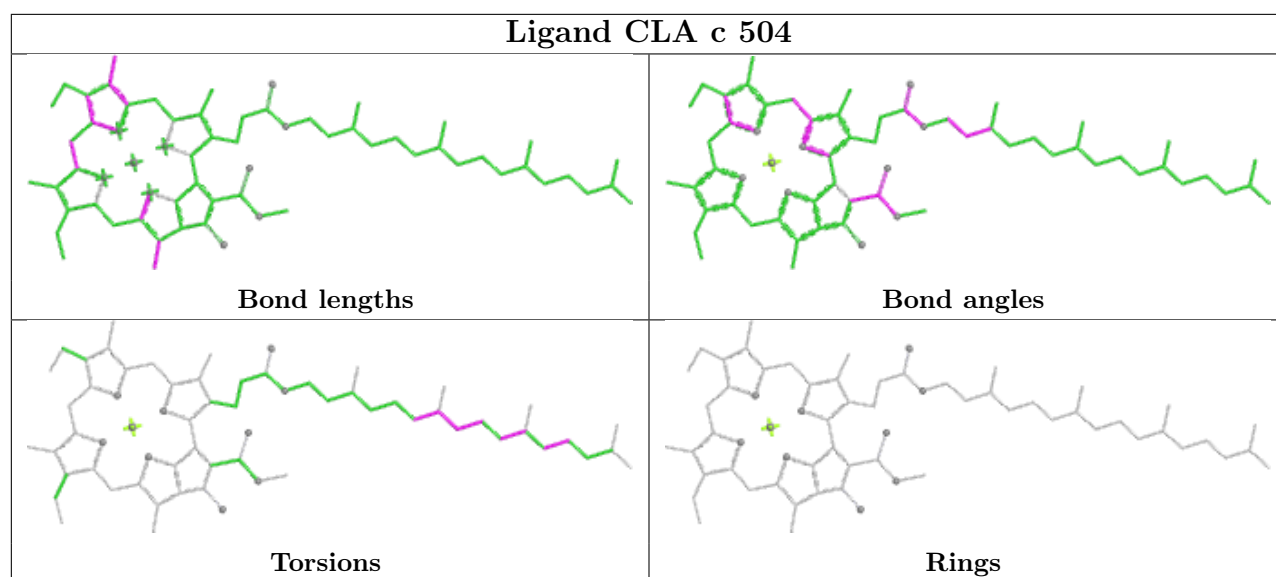


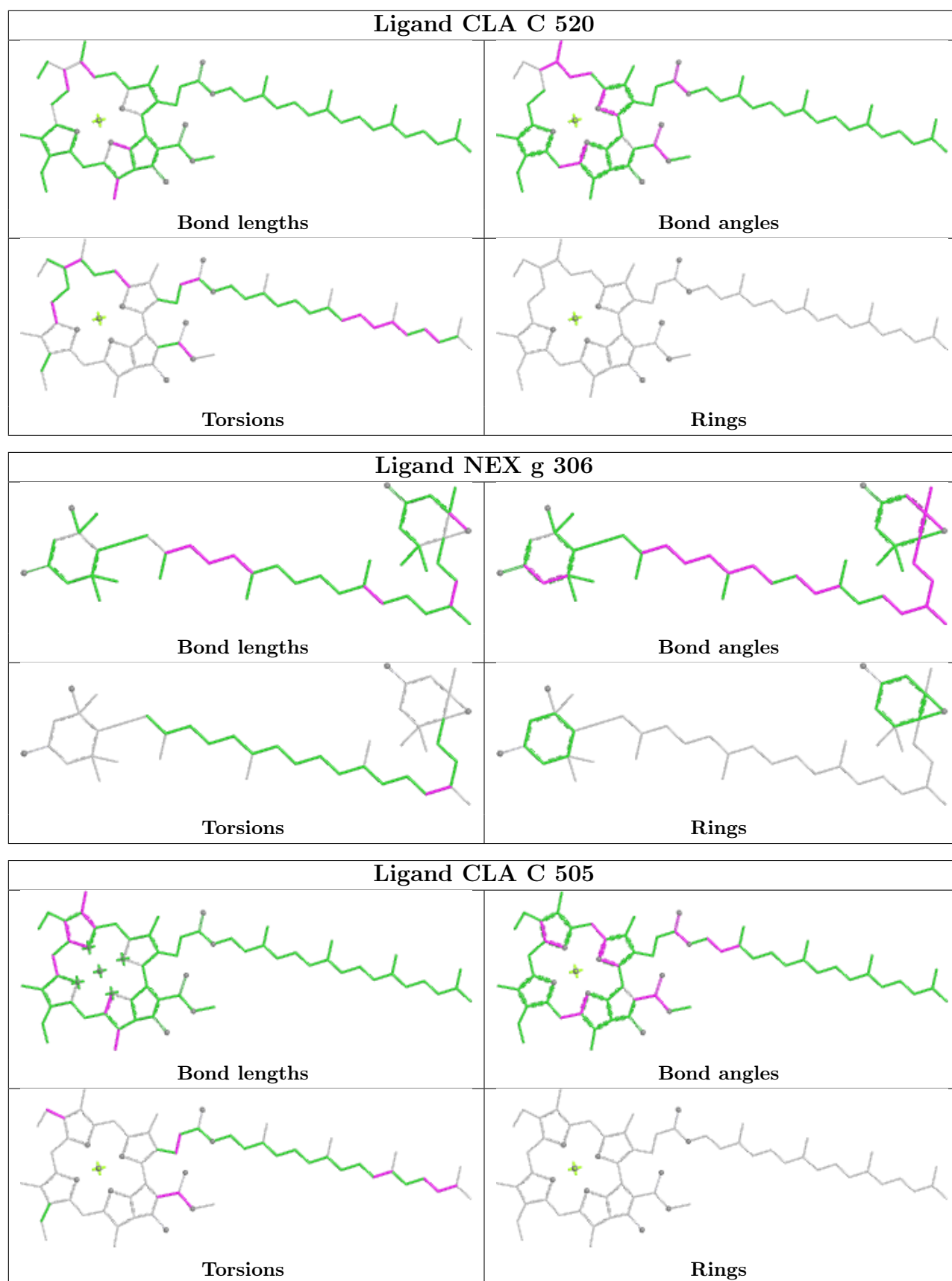
Ligand CLA R 302

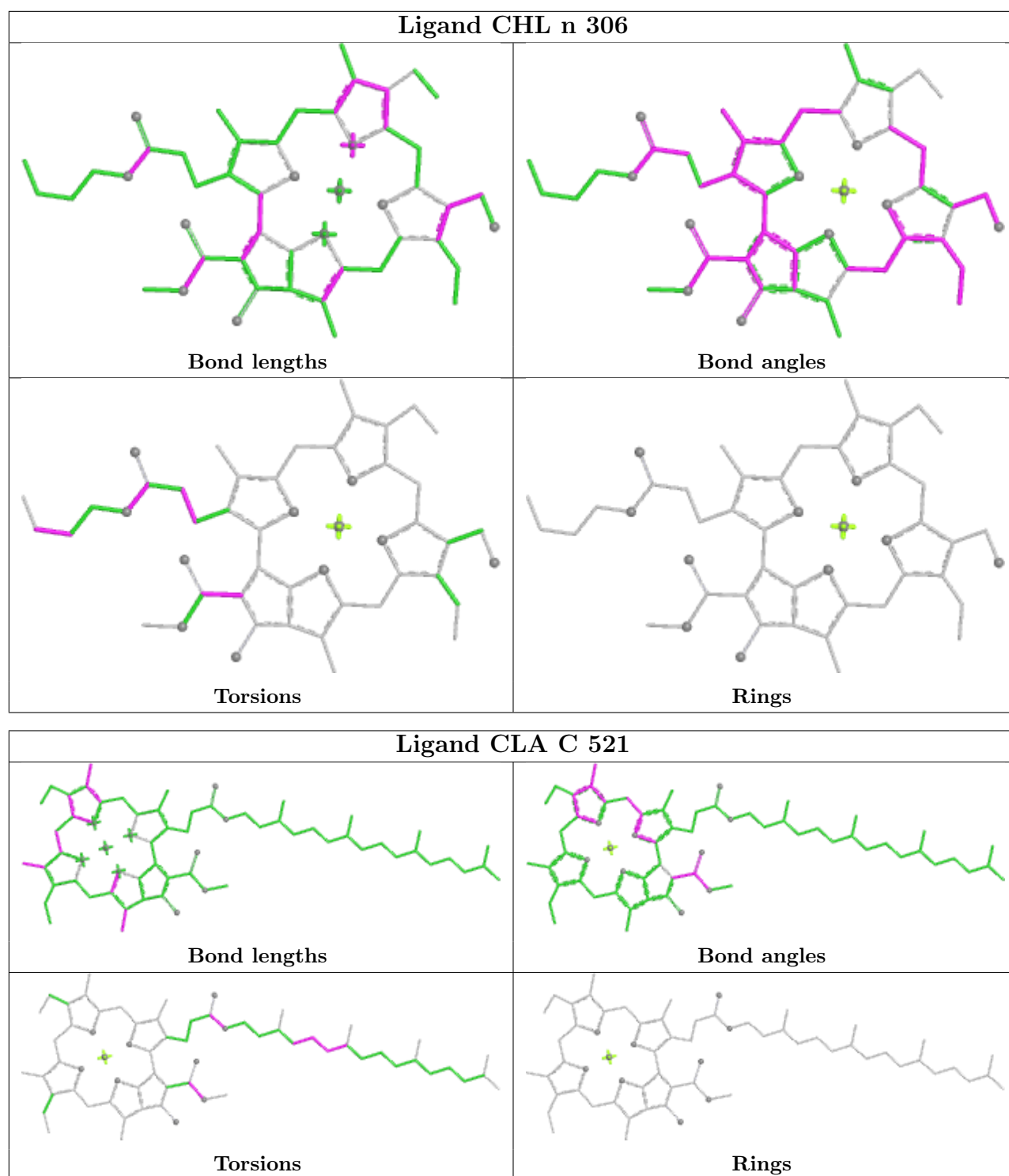


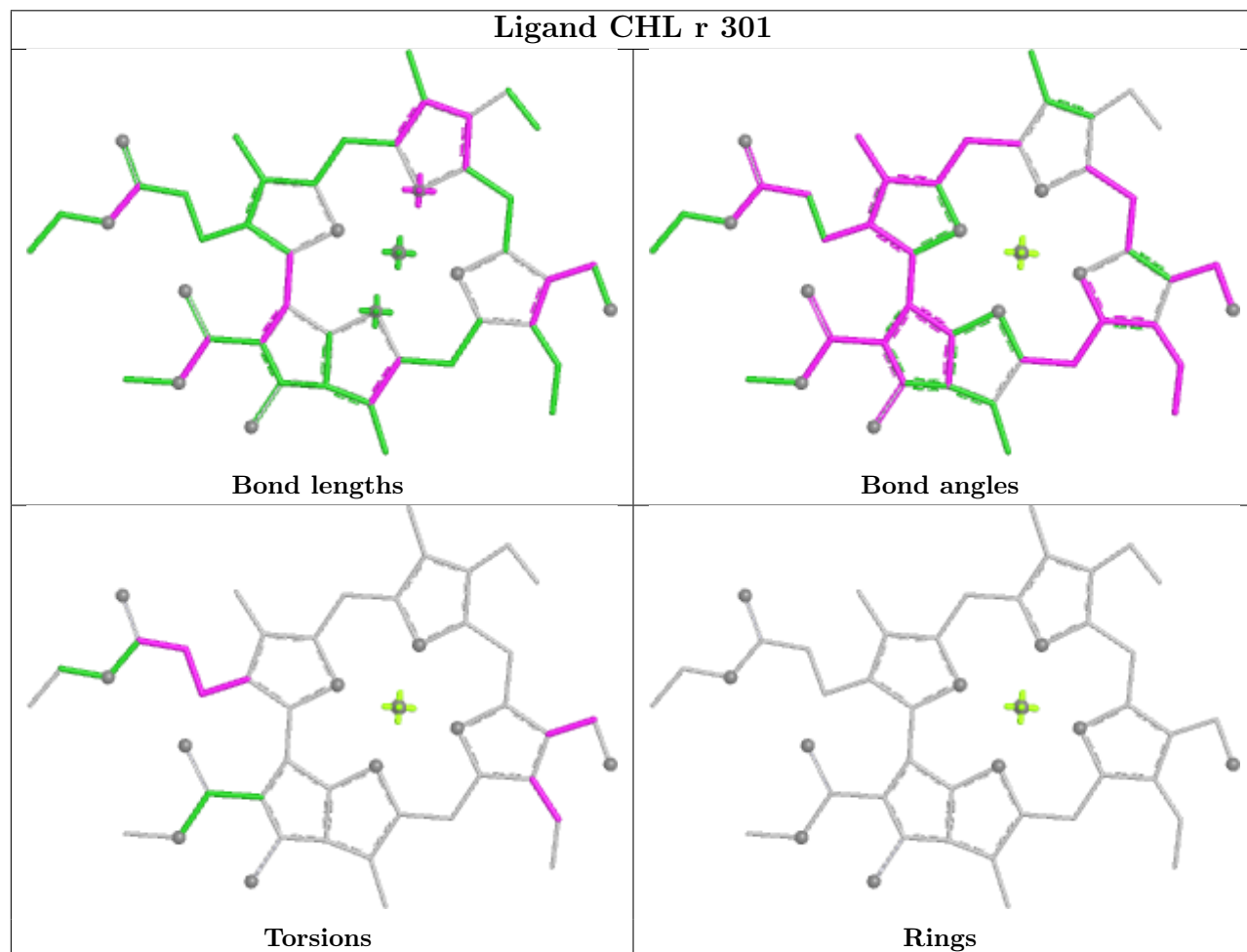
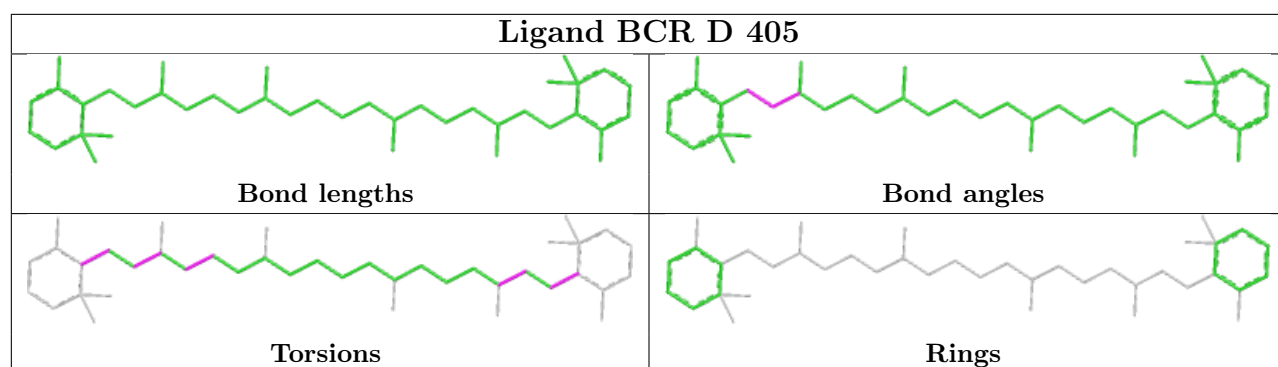
Ligand CLA a 409

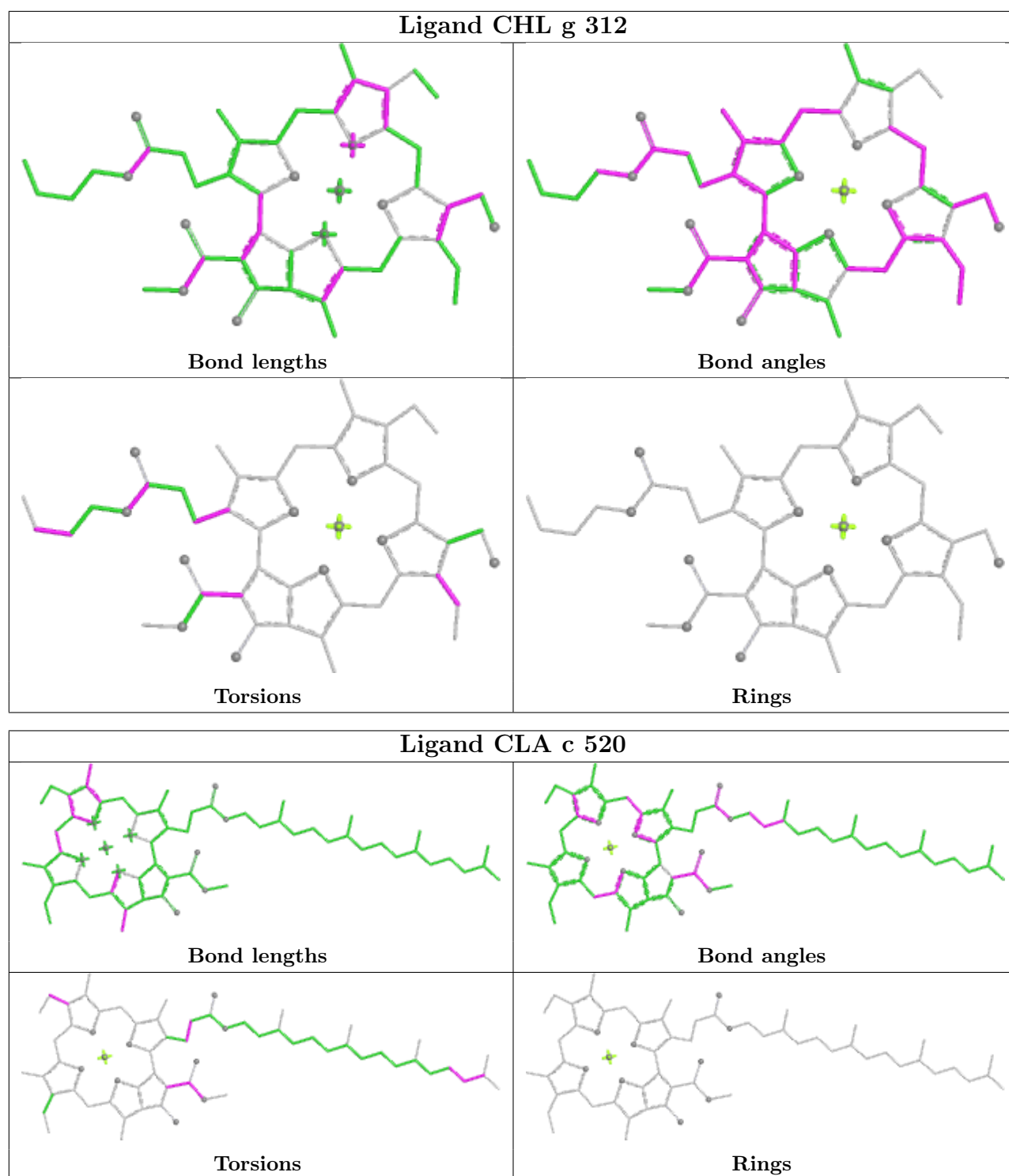




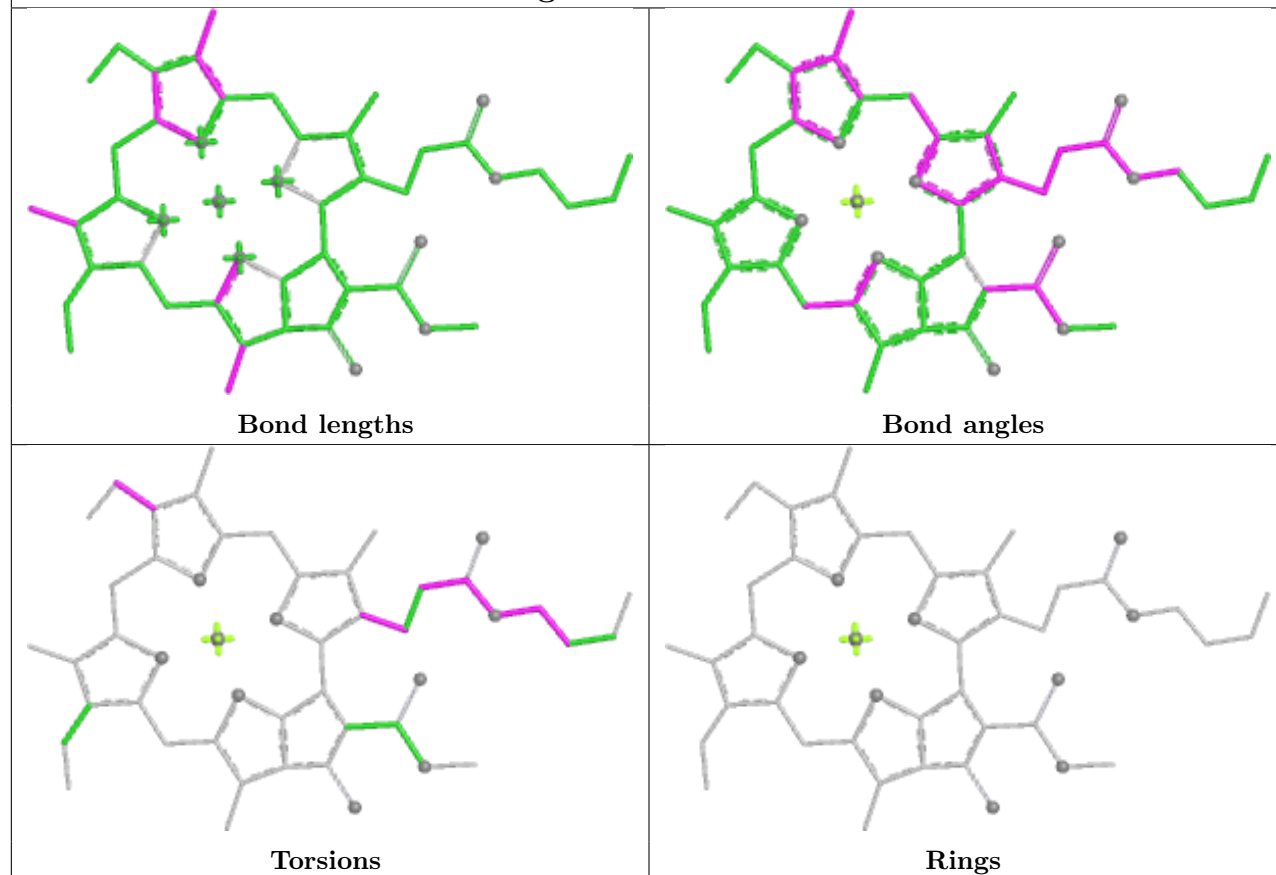




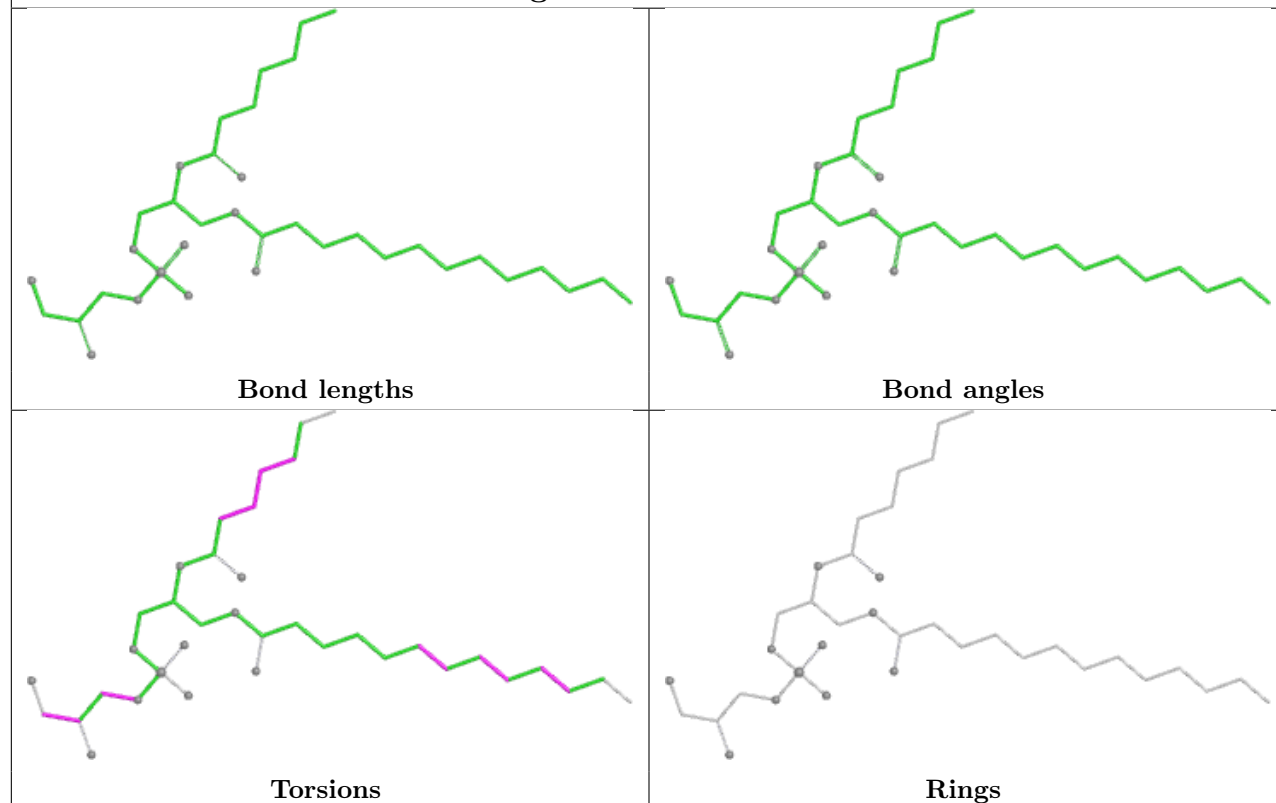


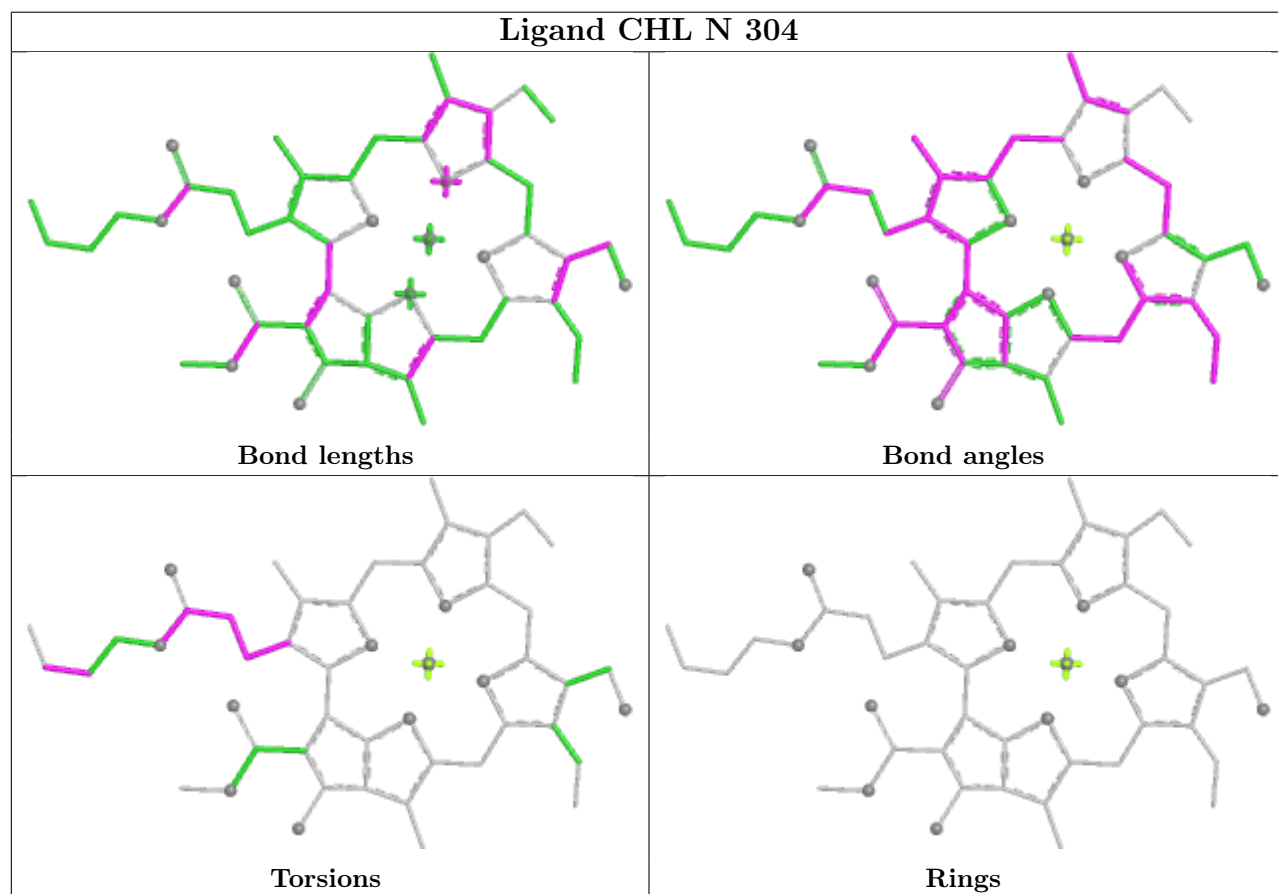
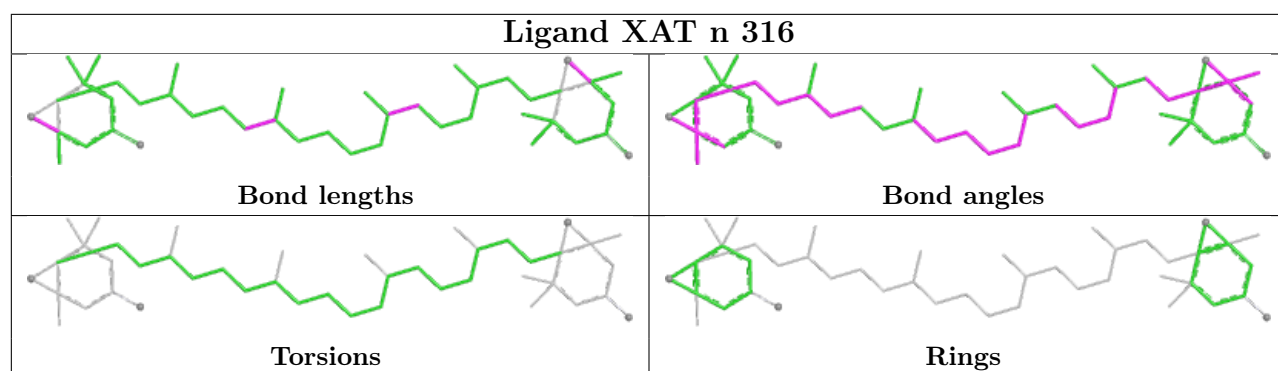


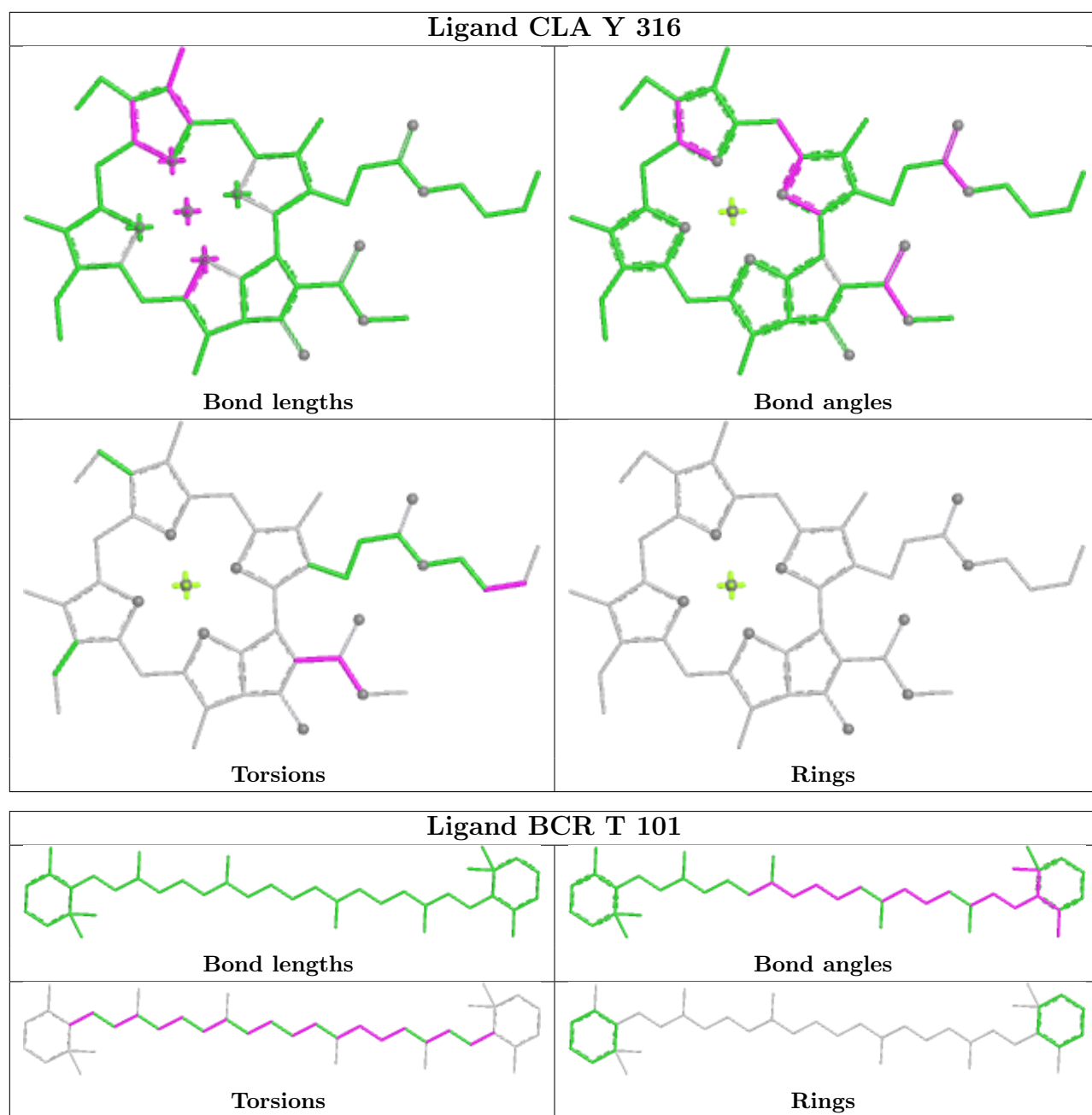
Ligand CLA r 313



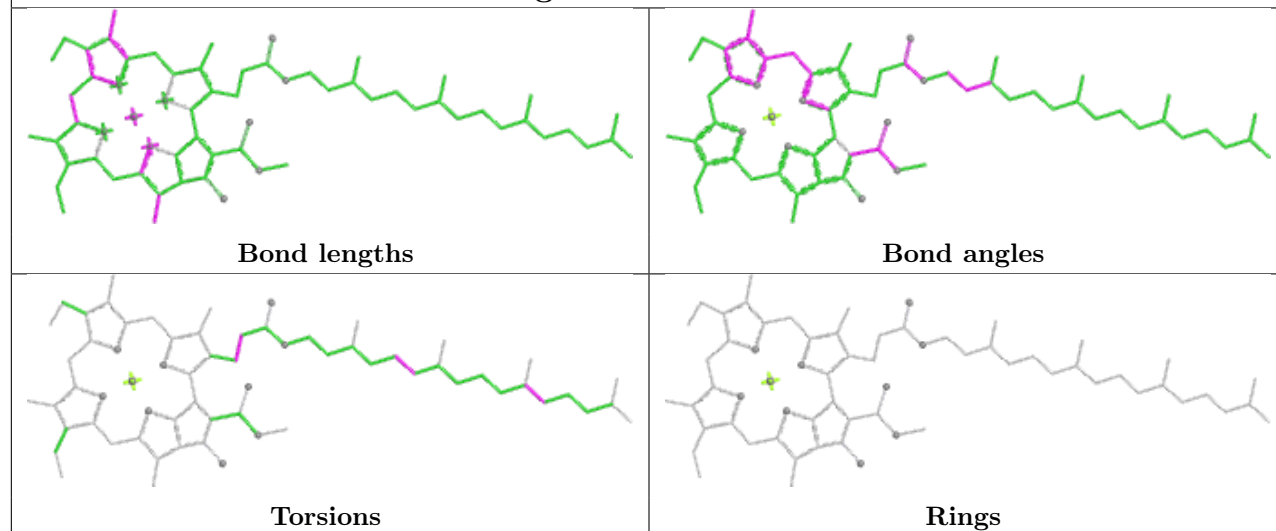
Ligand LHG D 410



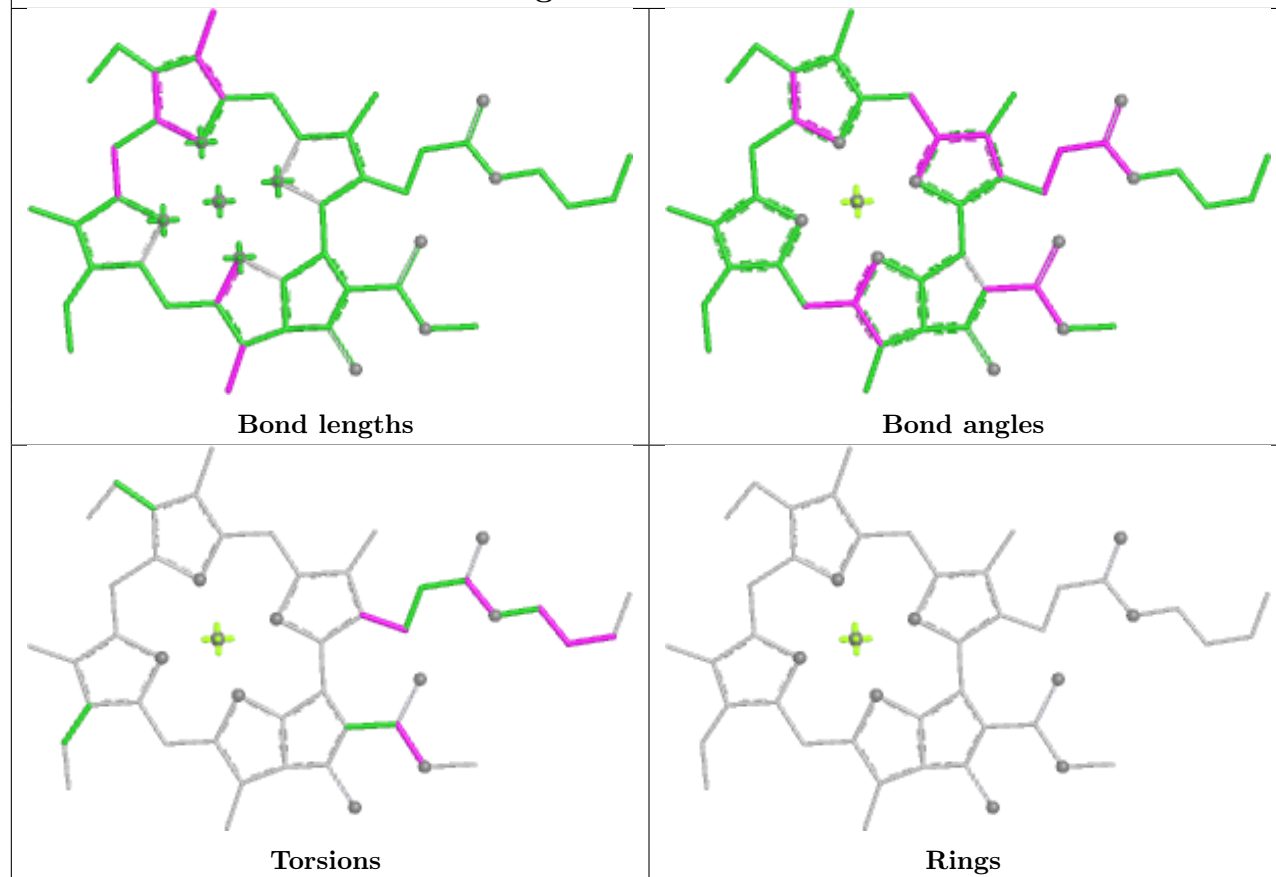




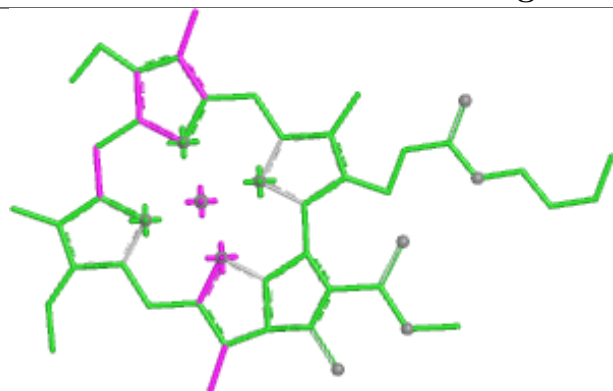
Ligand CLA b 612



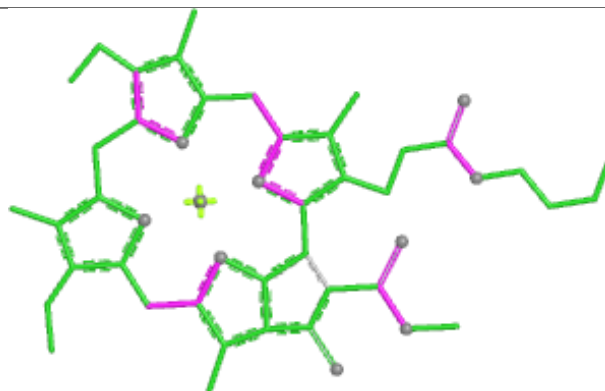
Ligand CLA S 311



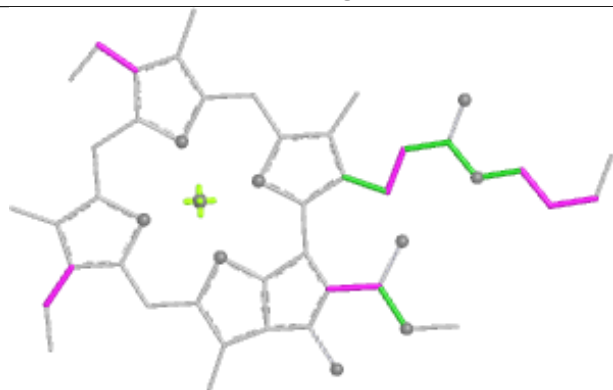
Ligand CLA S 307



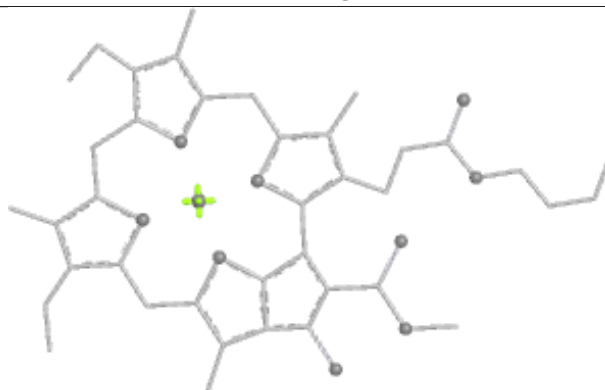
Bond lengths



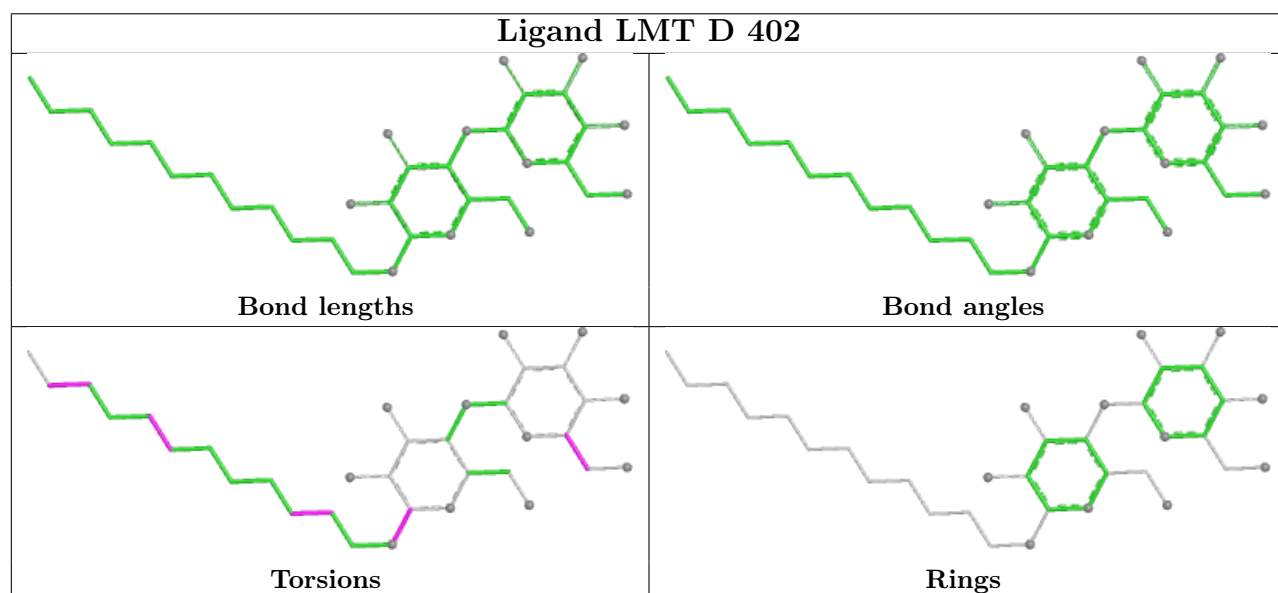
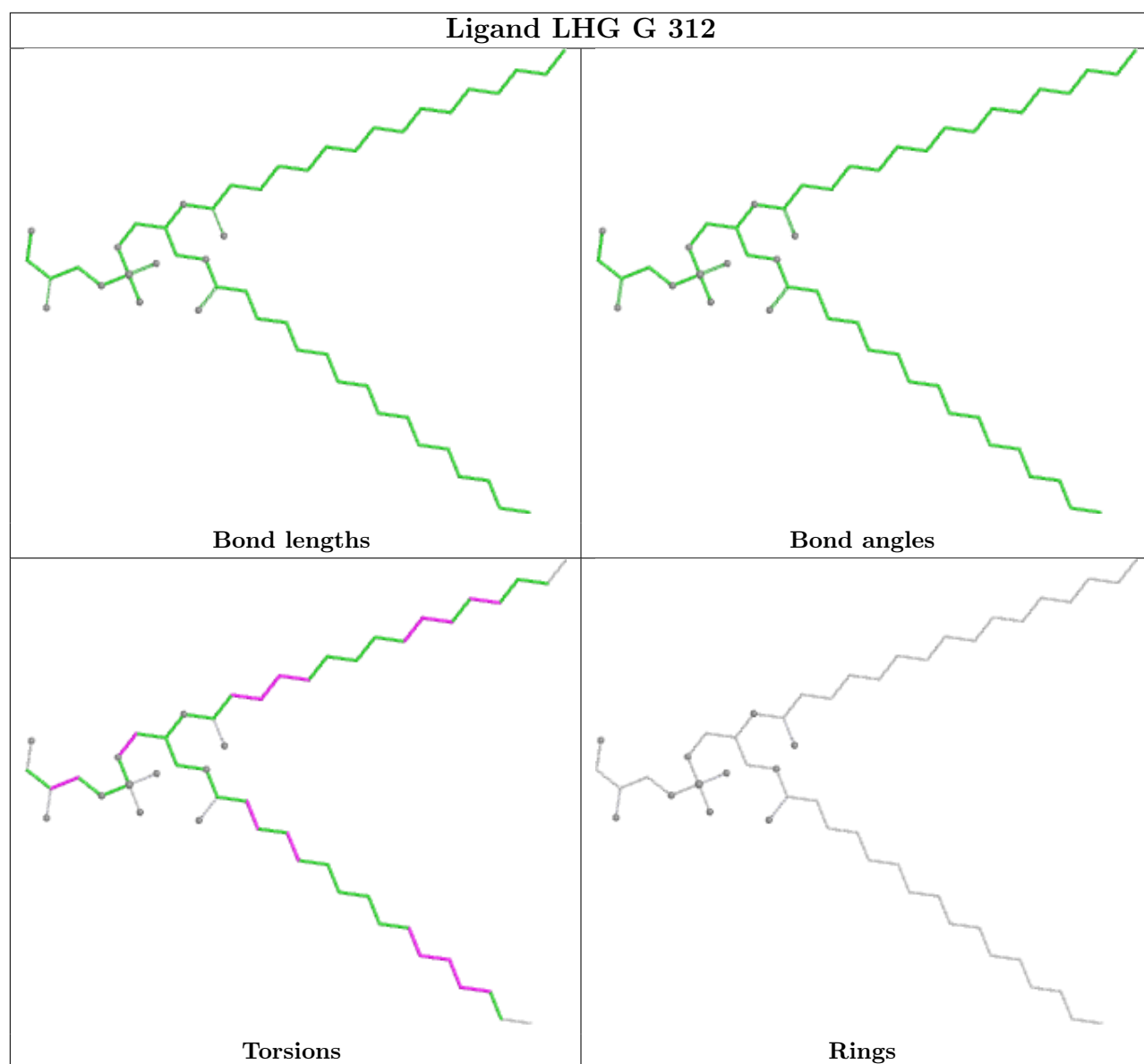
Bond angles

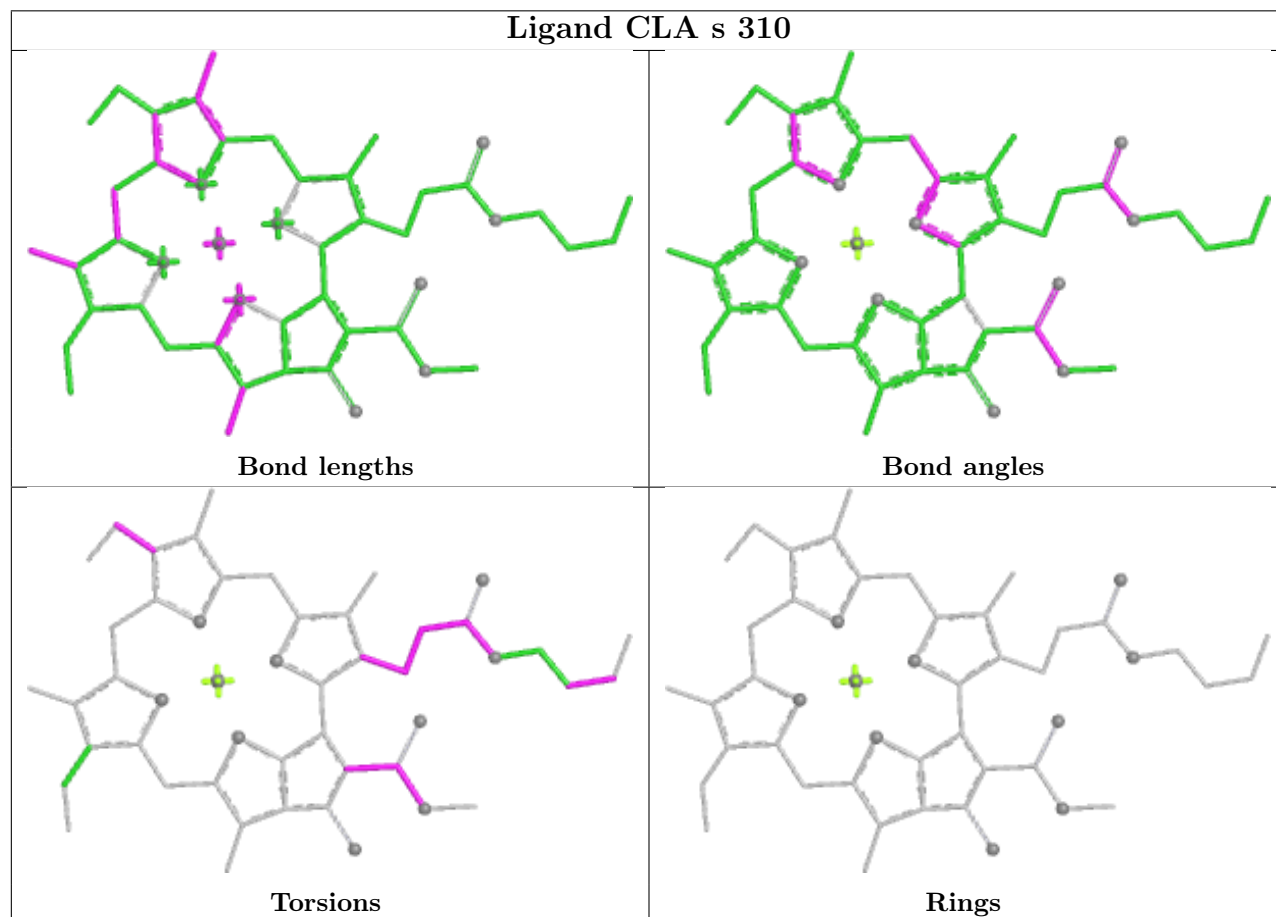
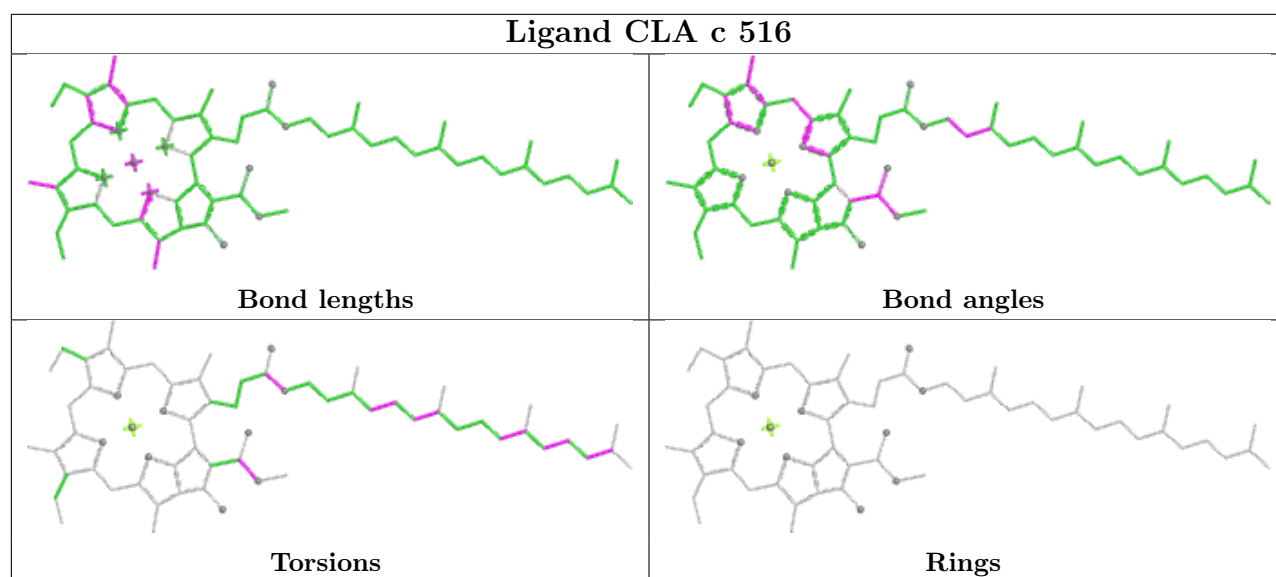


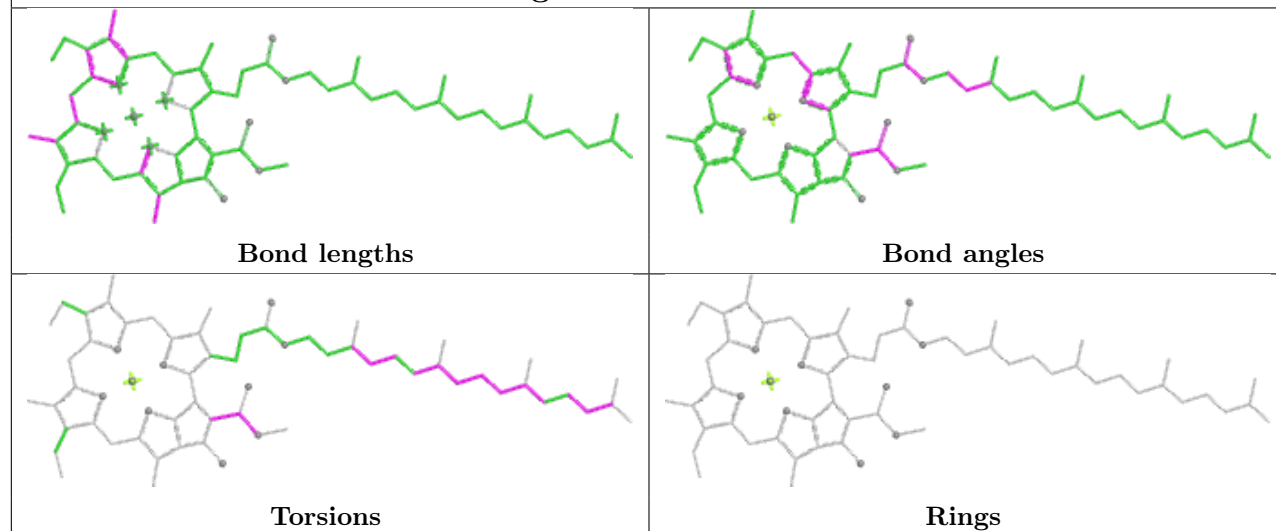
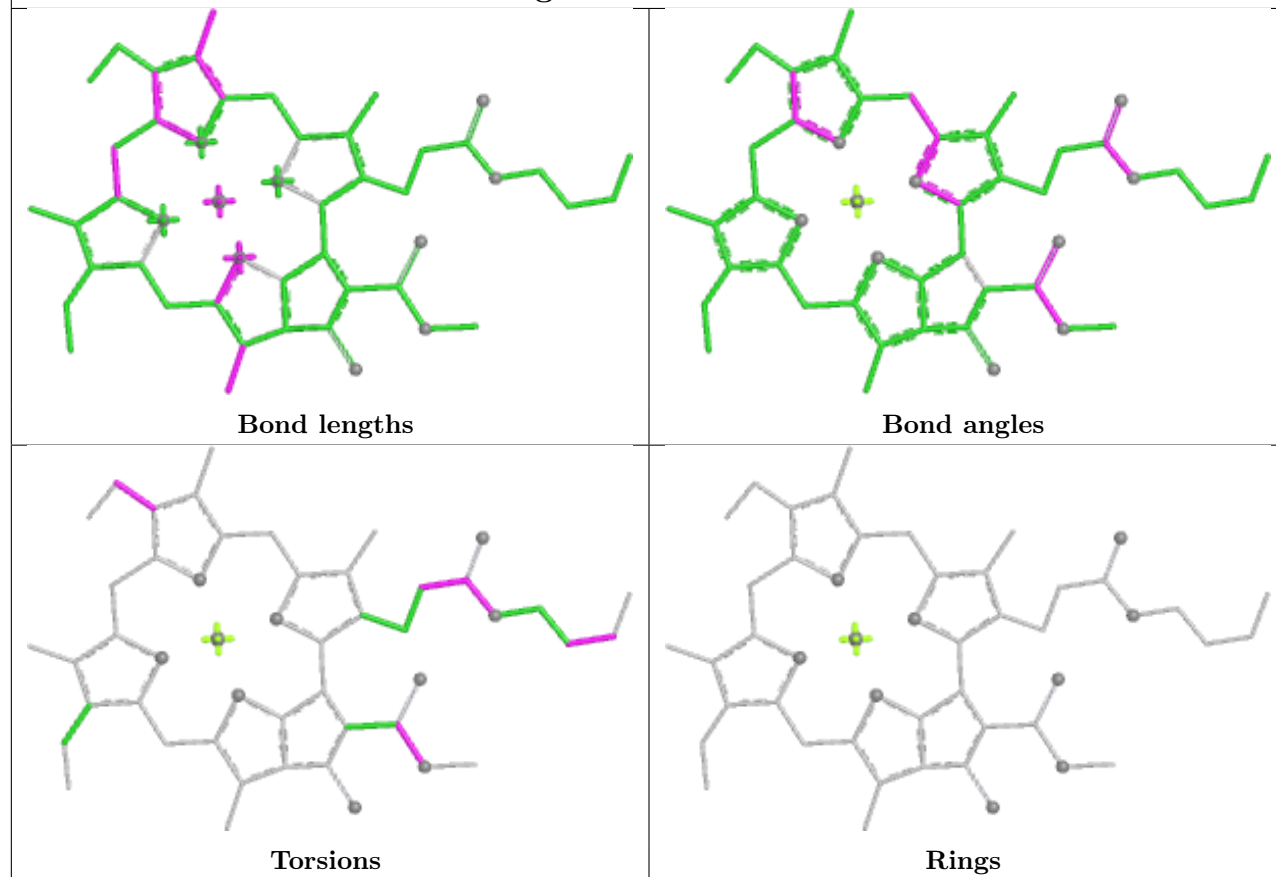
Torsions

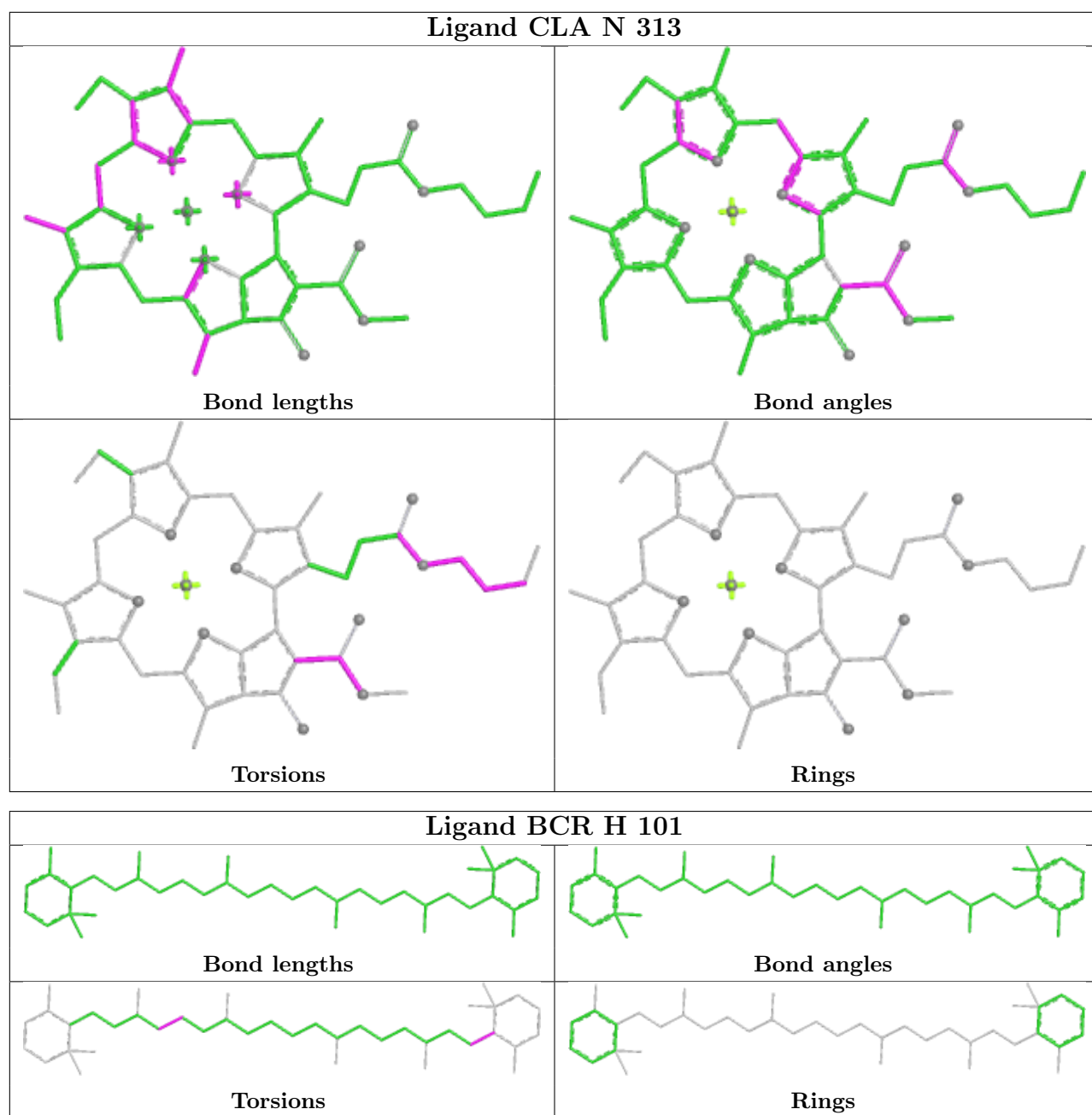


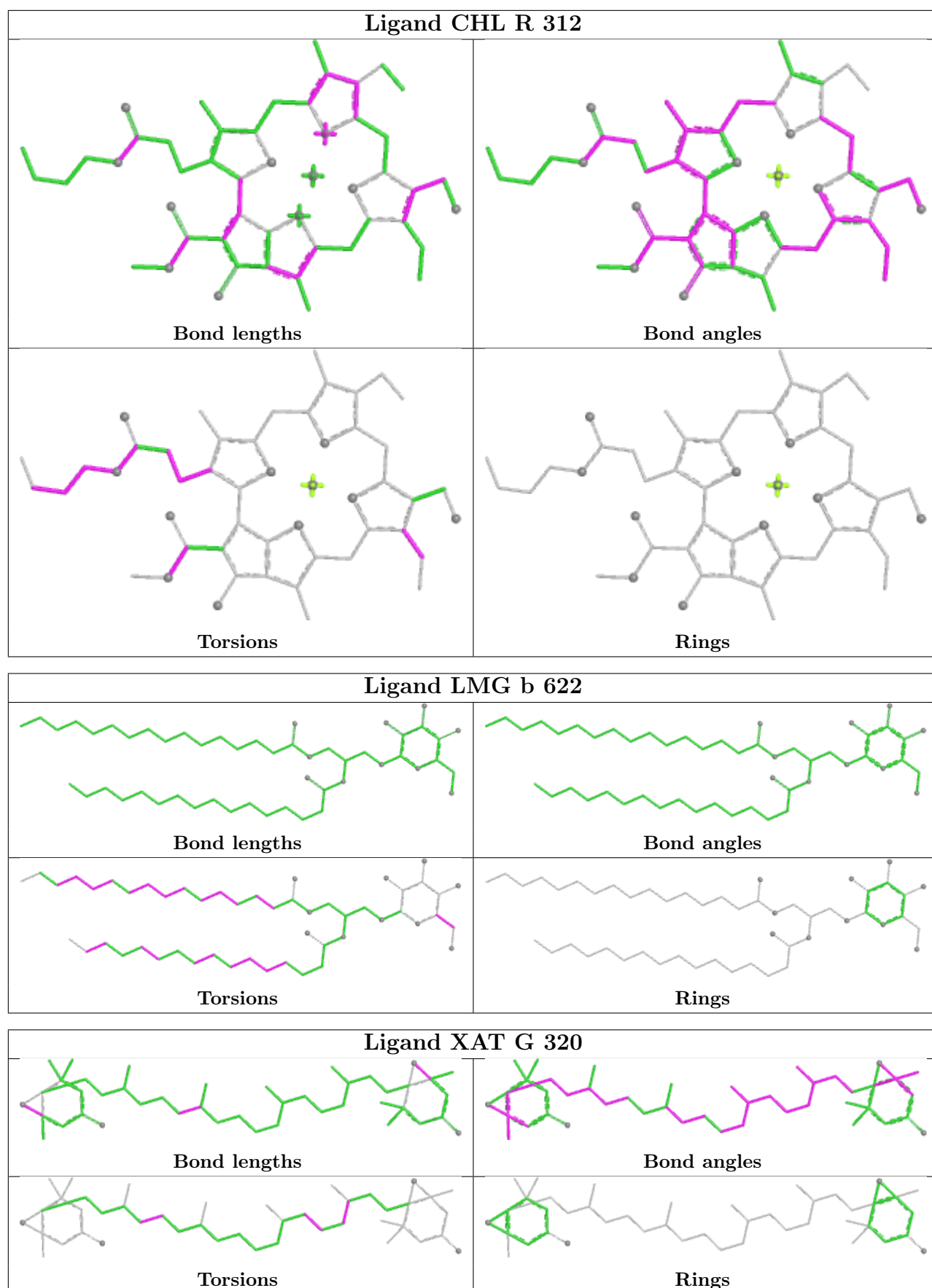
Rings

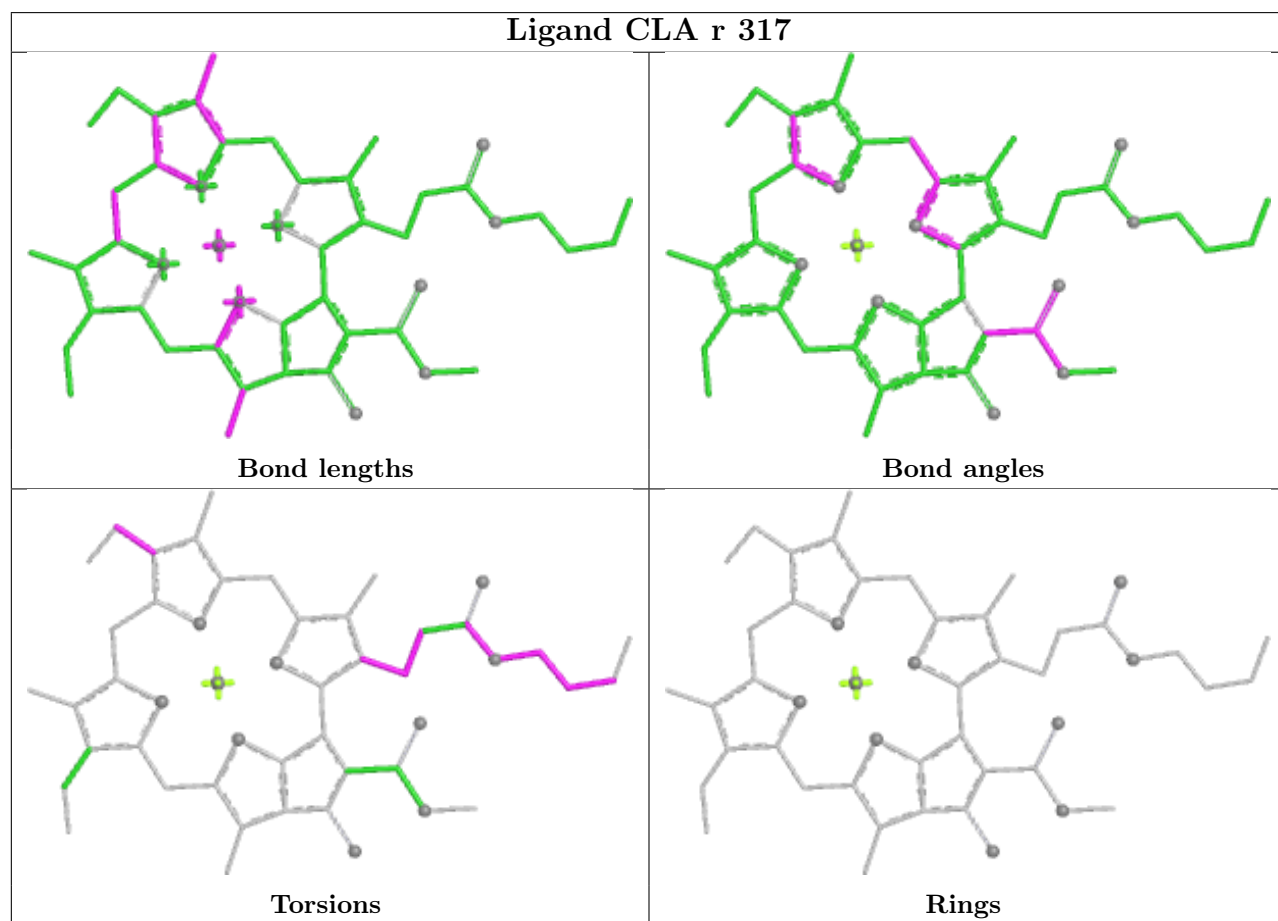
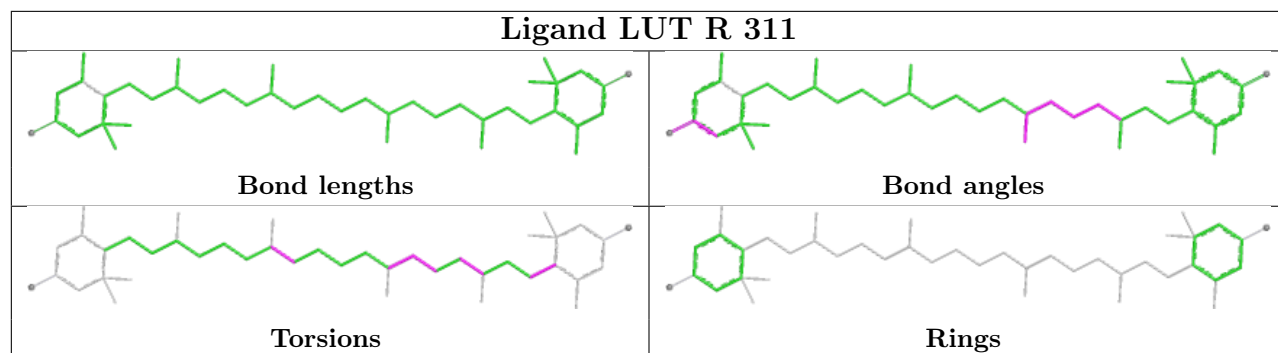


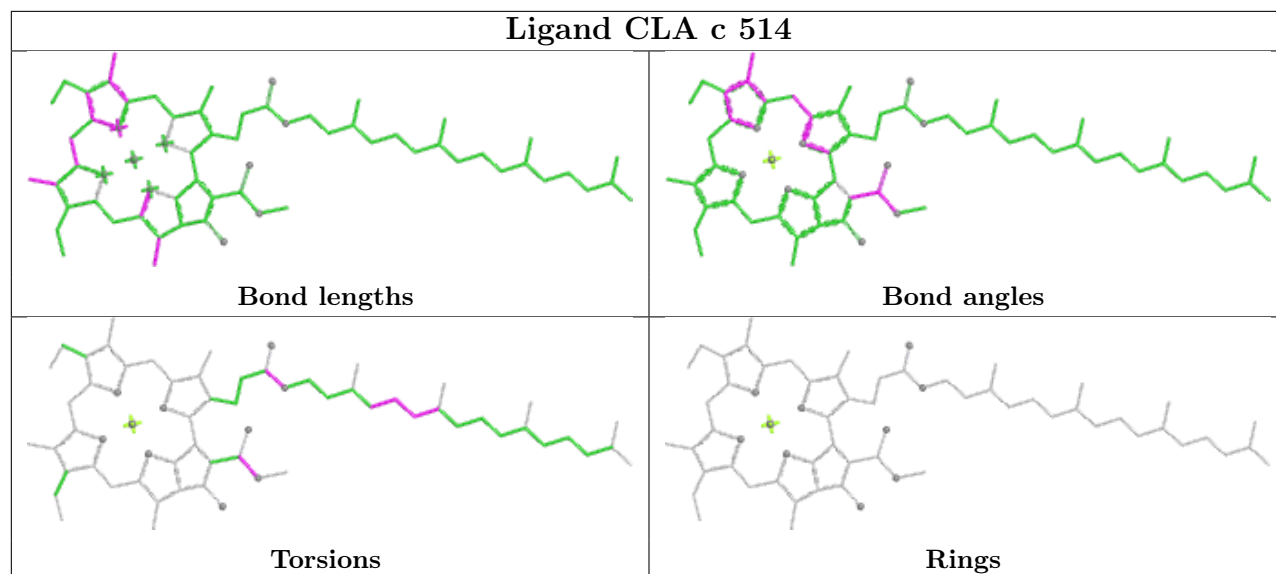
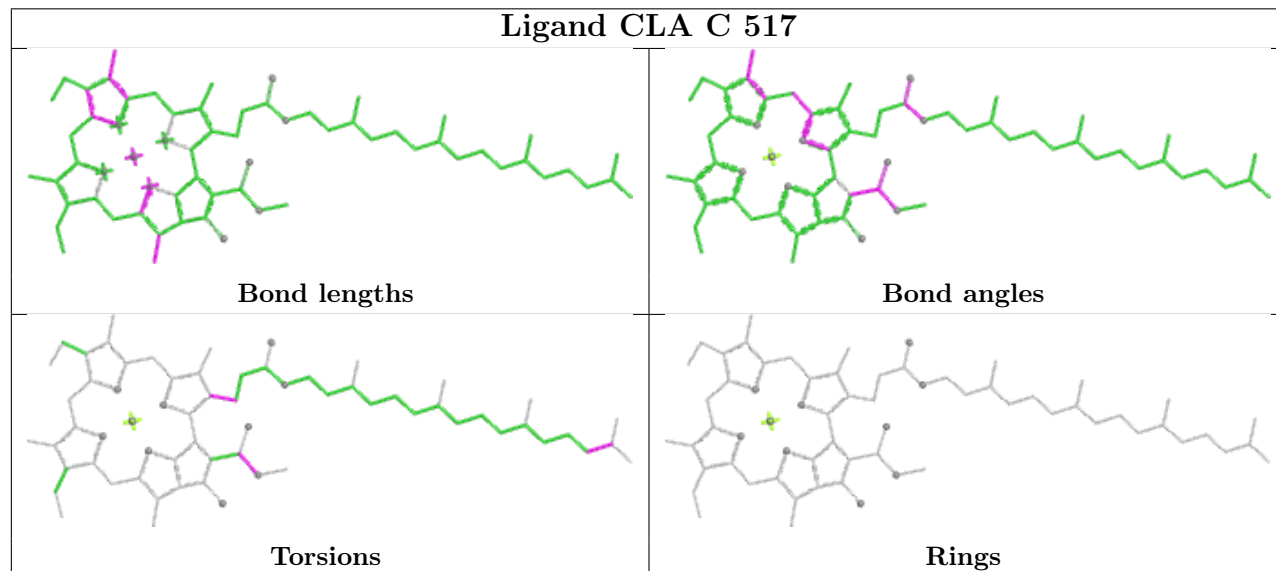


Ligand CLA Y 313**Ligand CLA S 308**

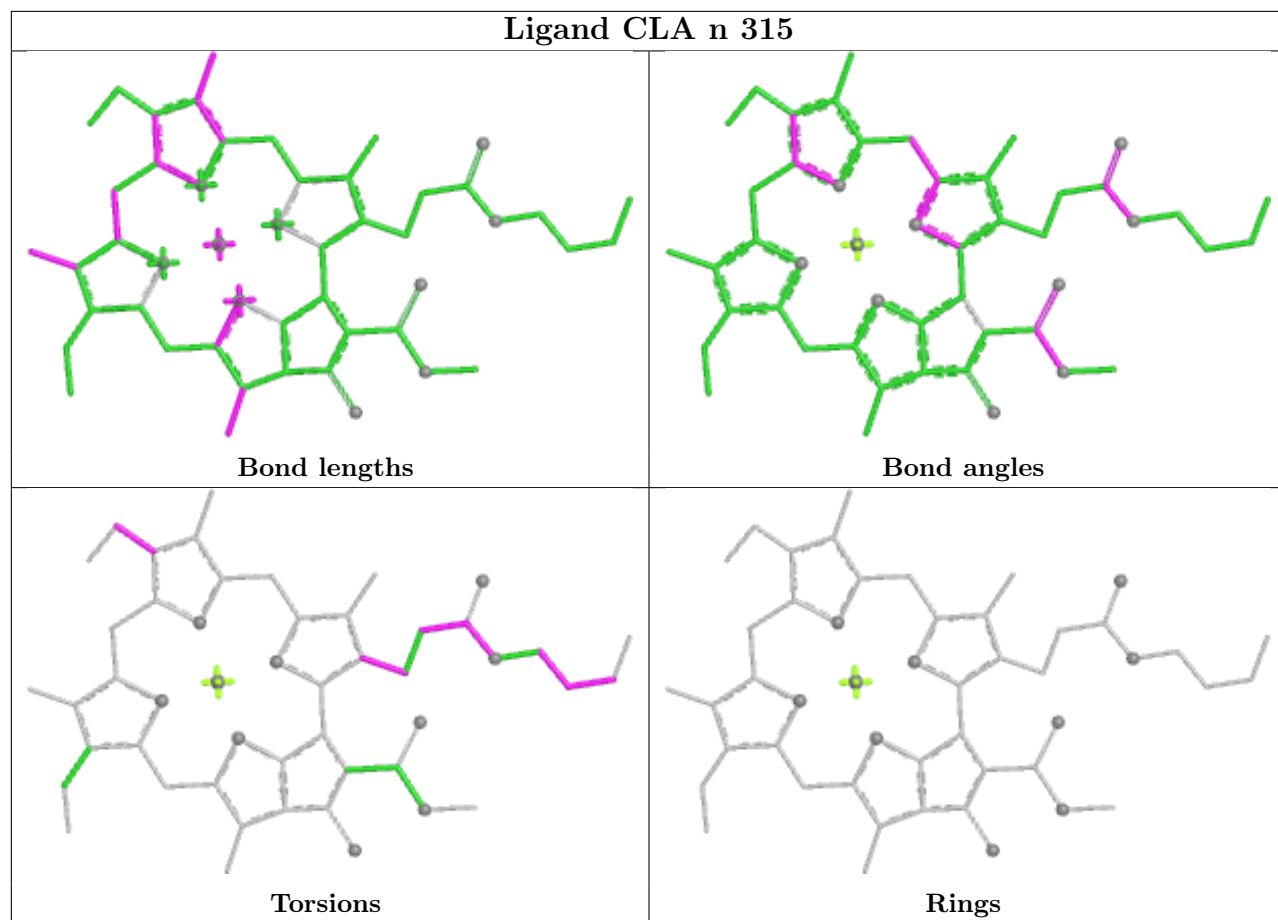


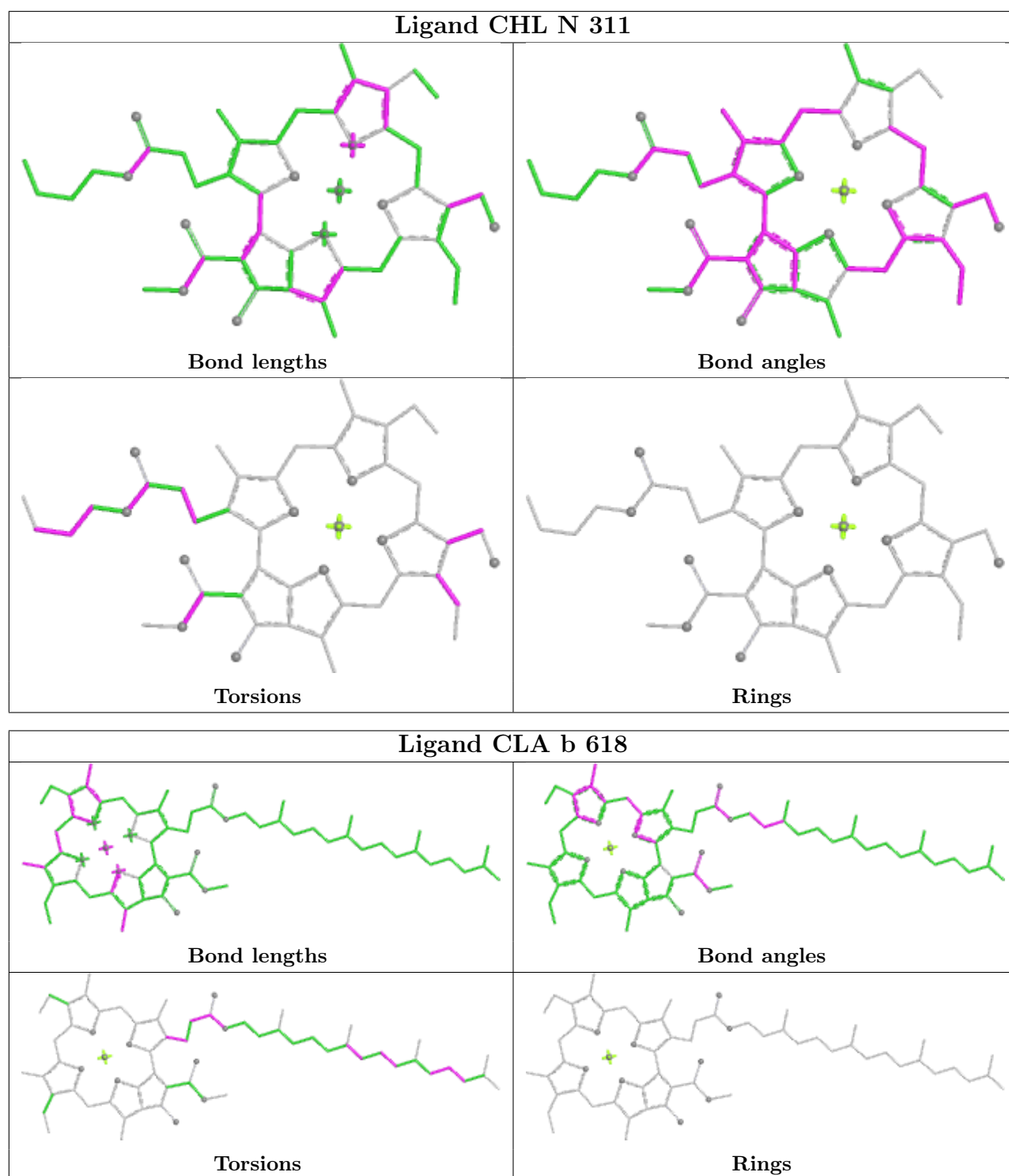


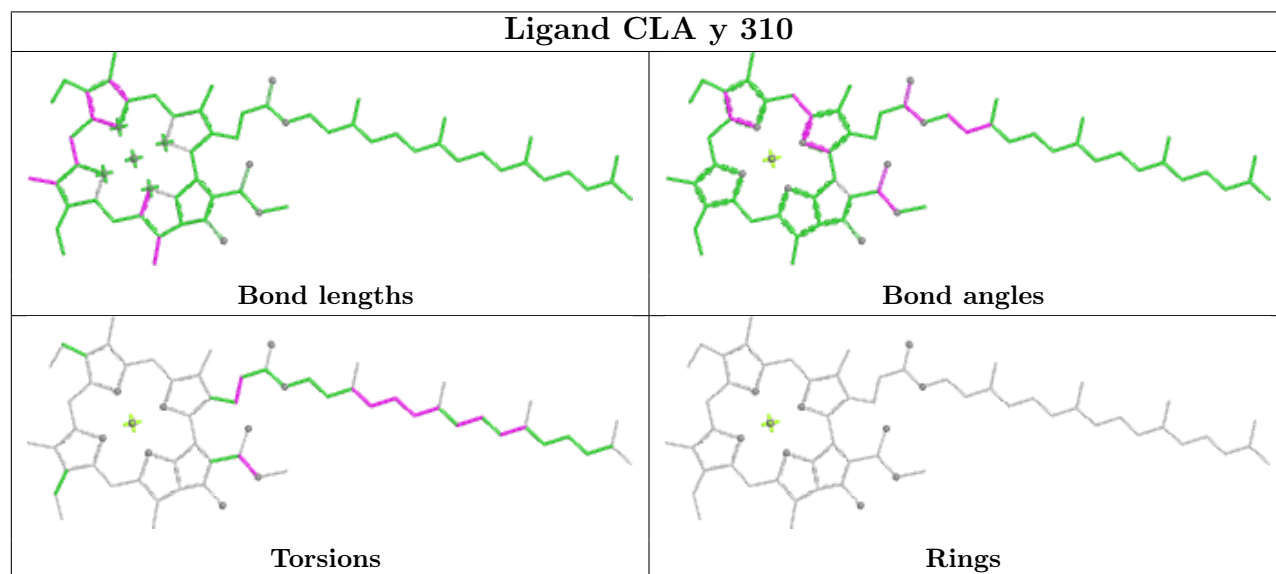
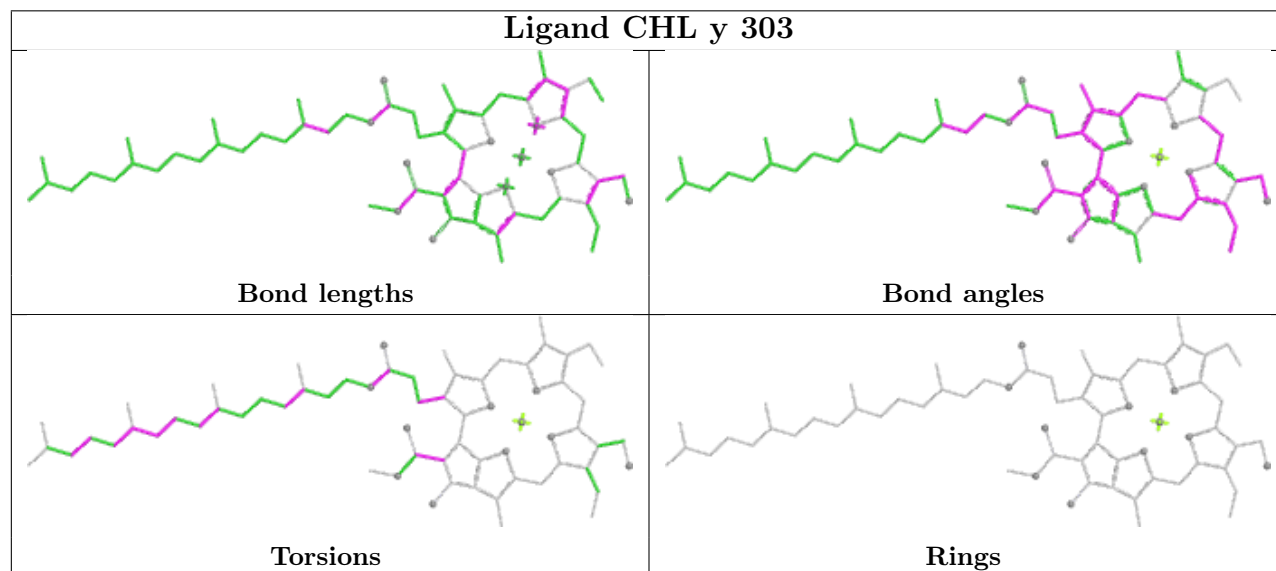
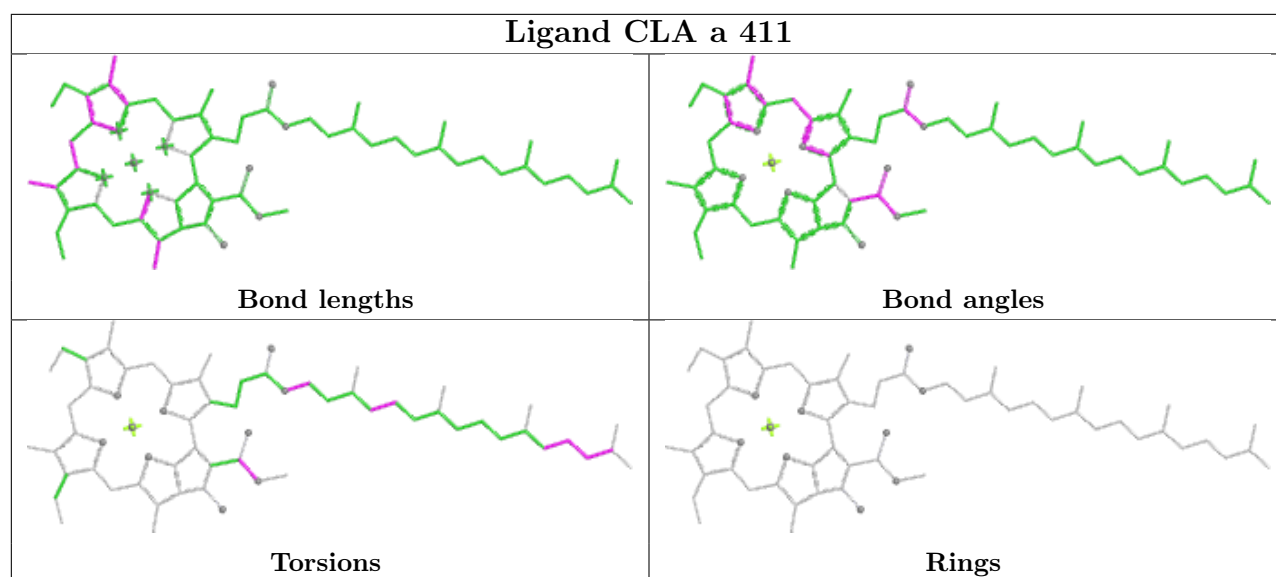


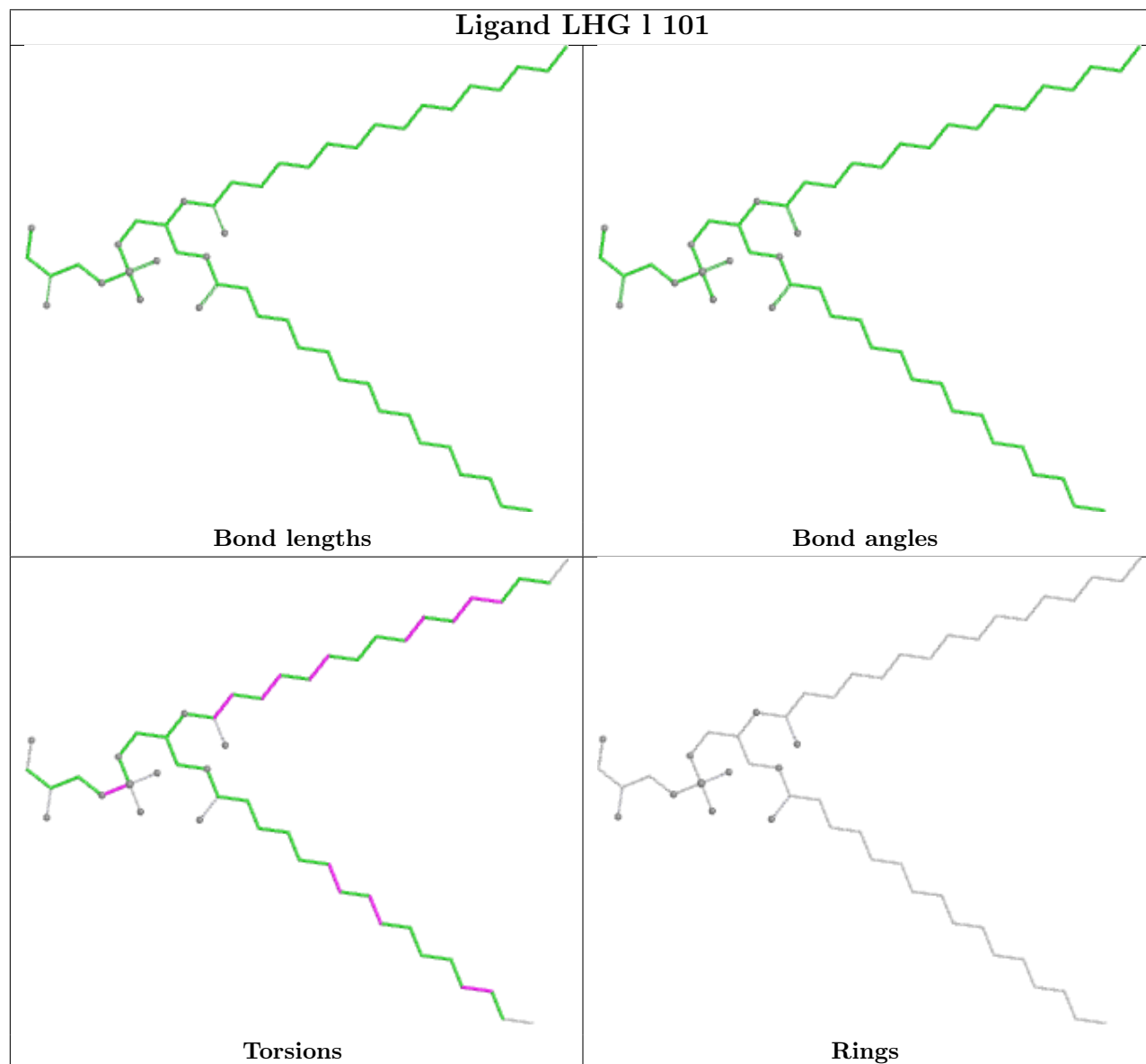
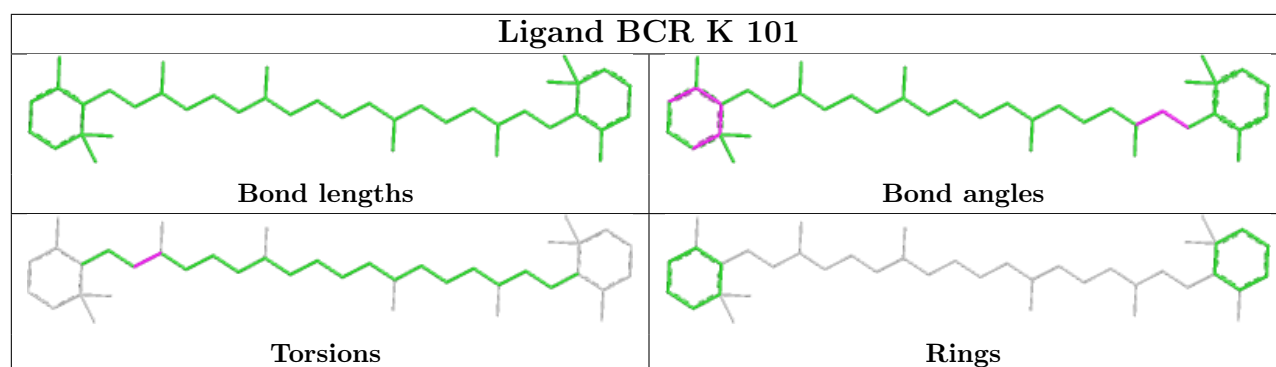
Ligand CLA c 514**Ligand CLA C 517**

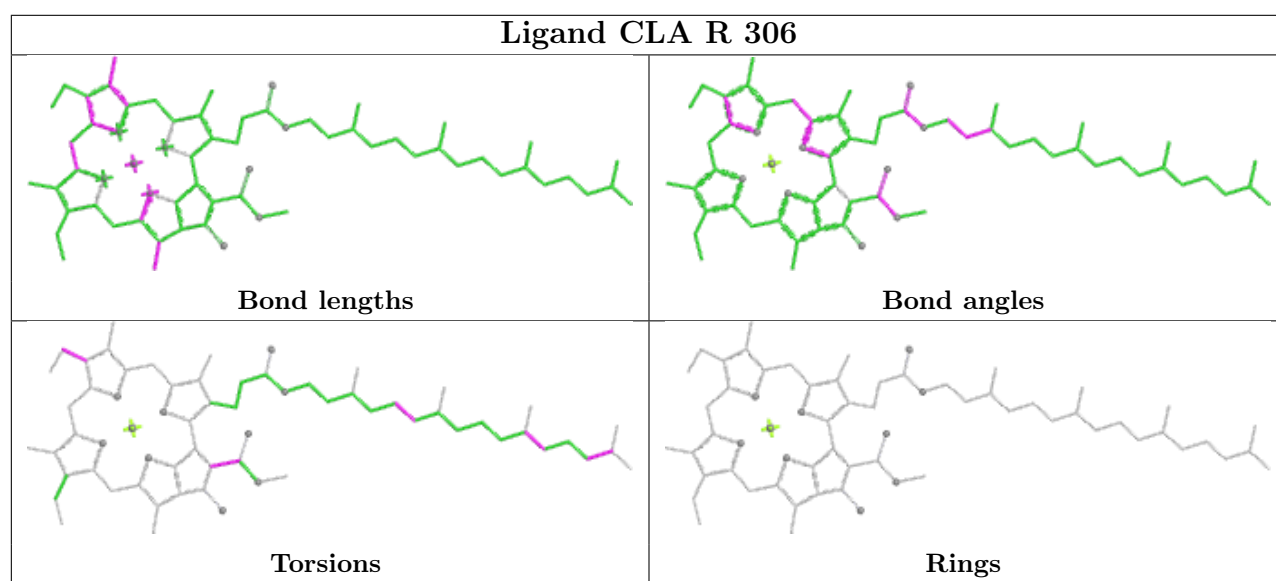
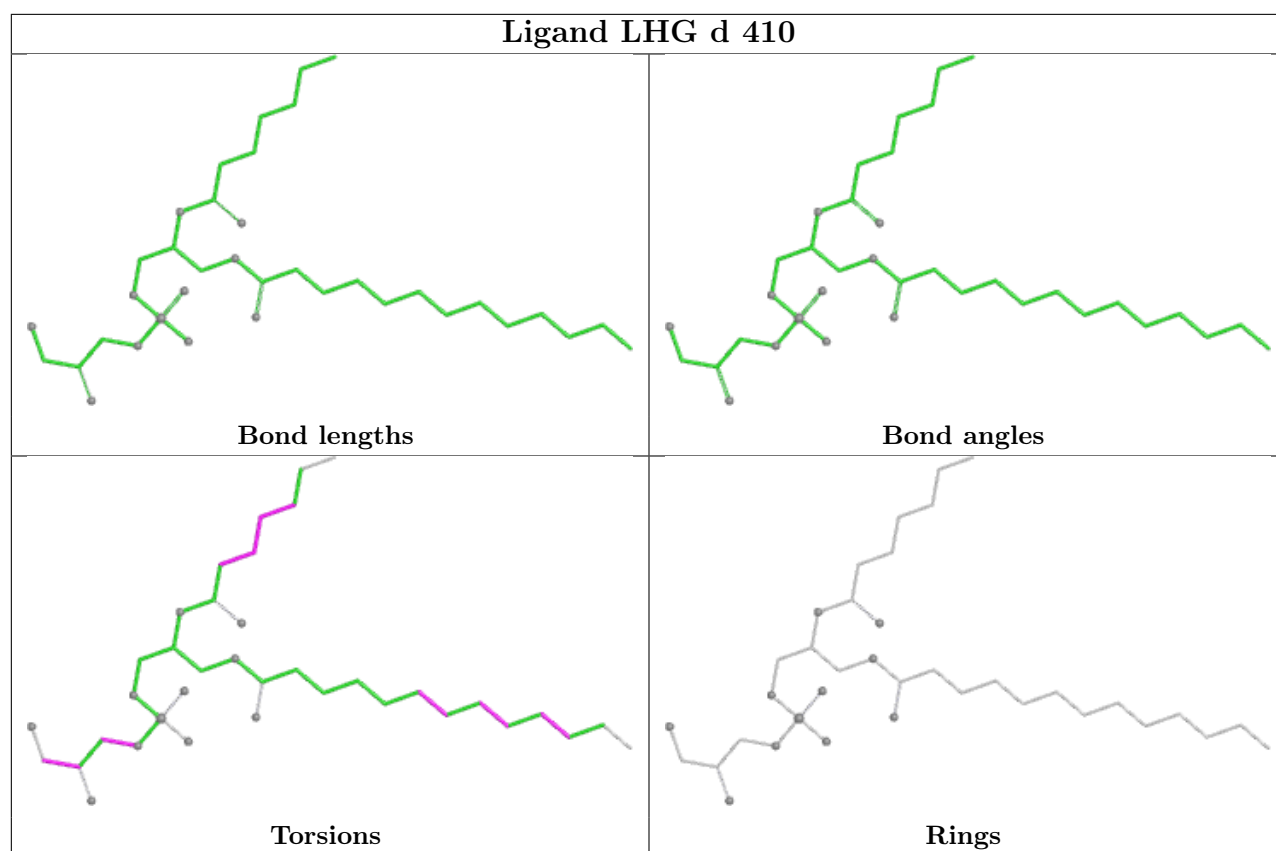
Ligand CLA n 315

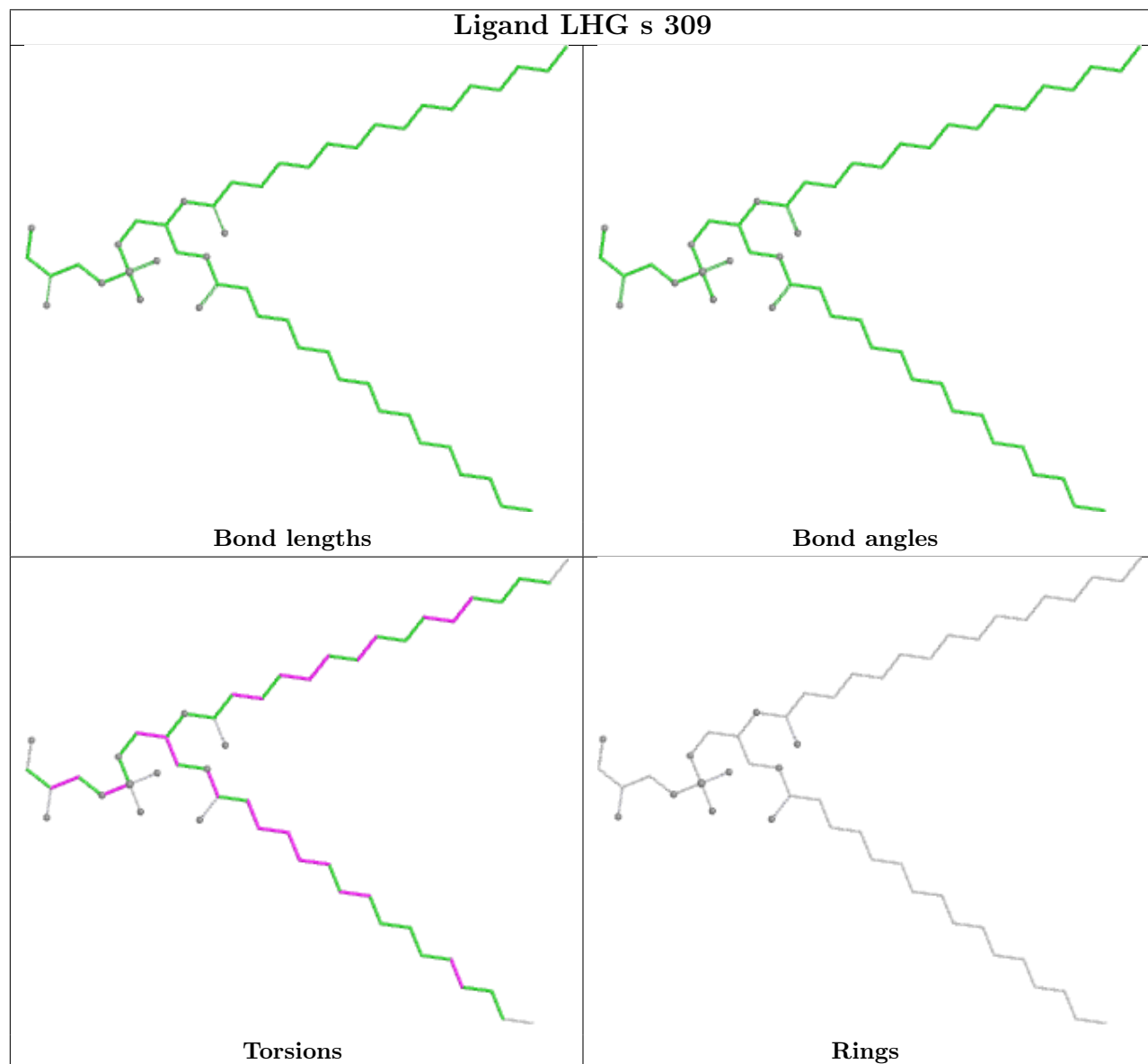
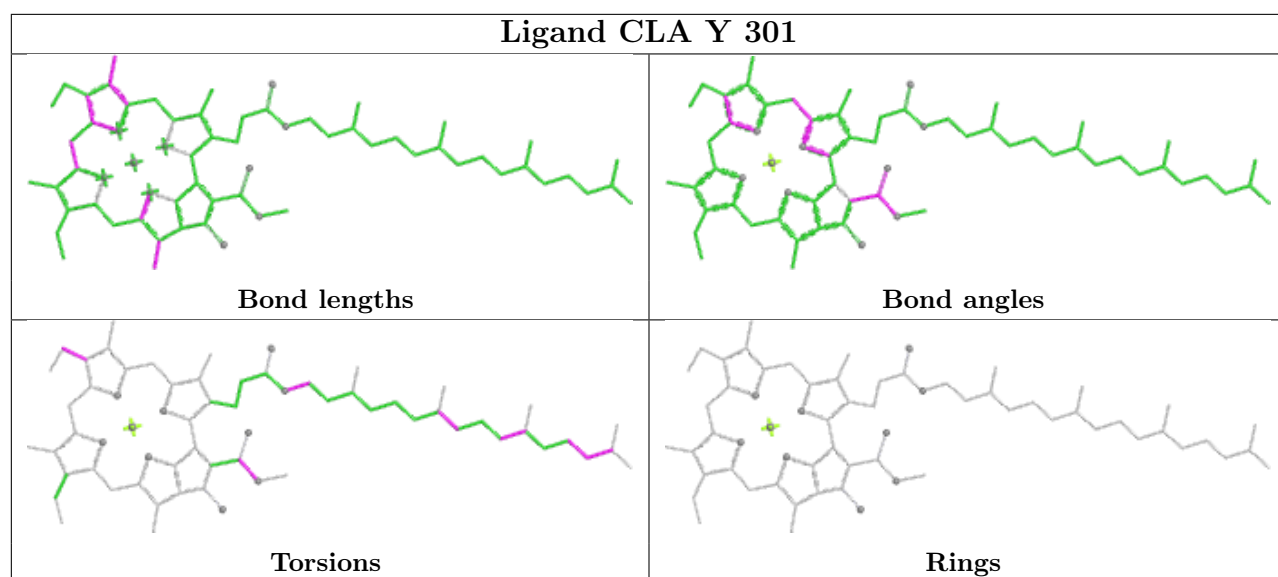




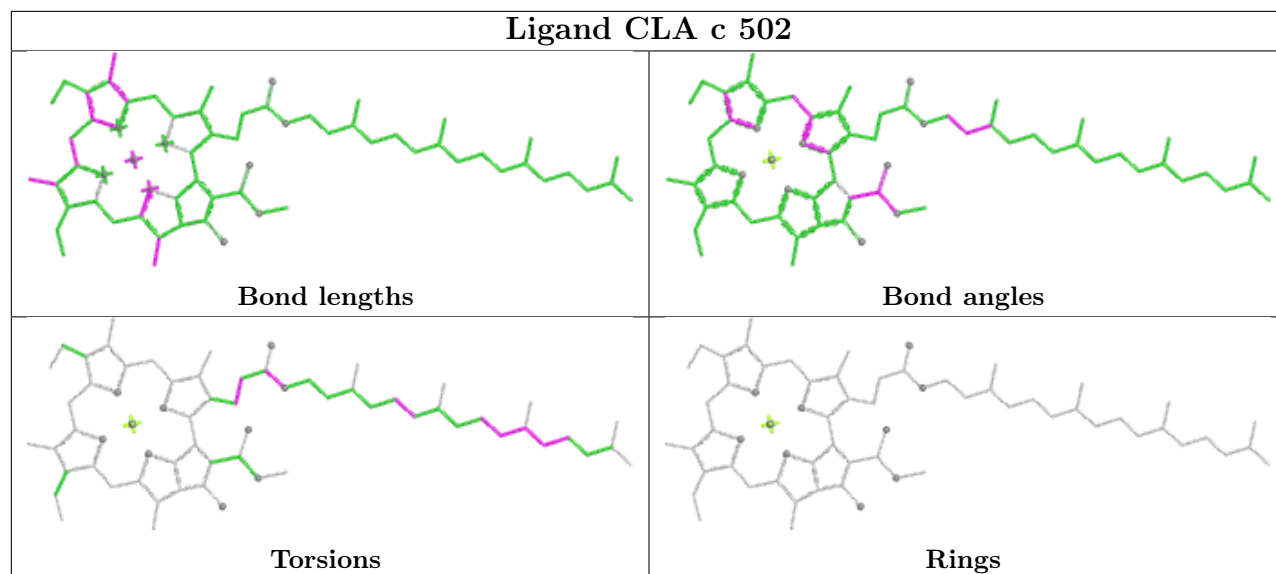




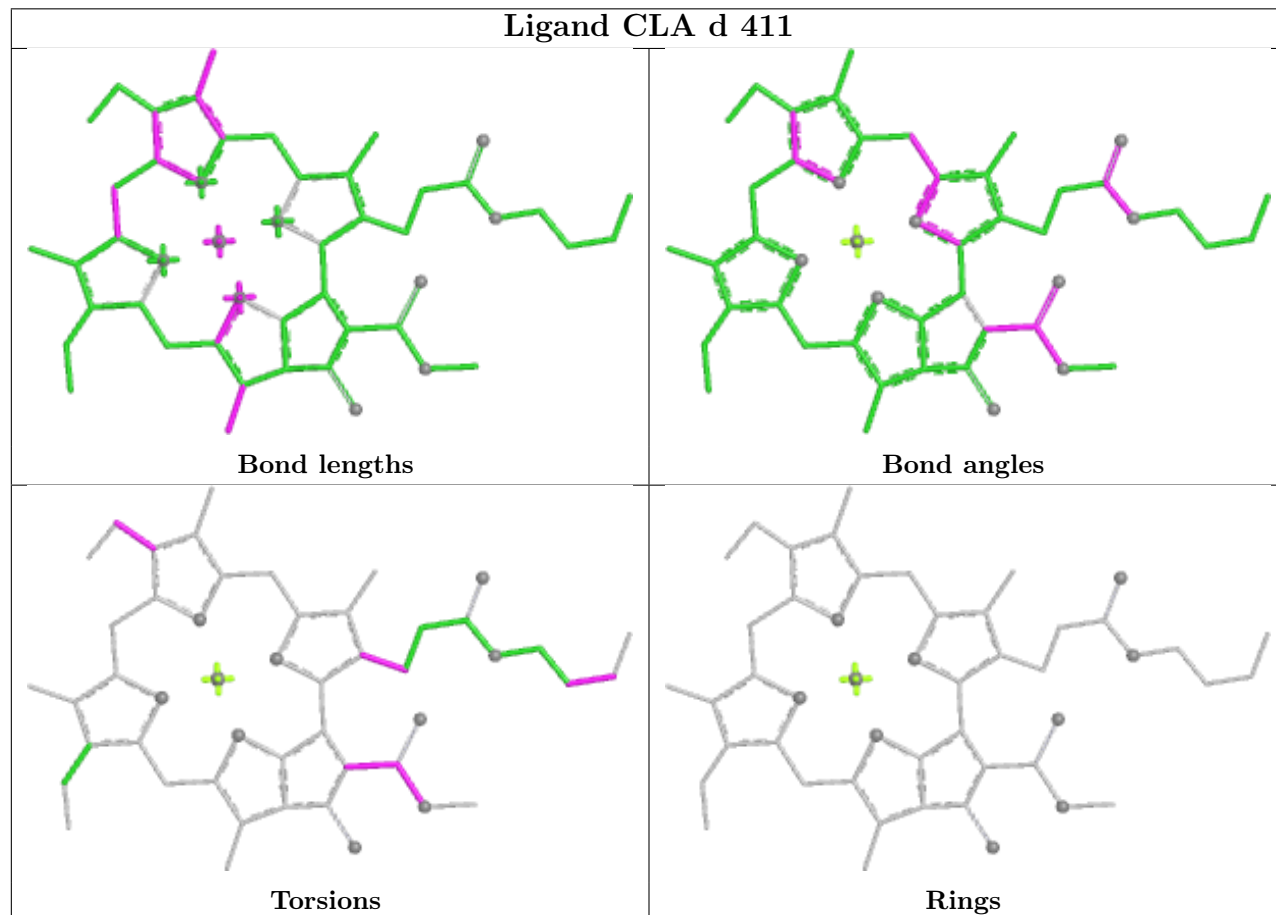


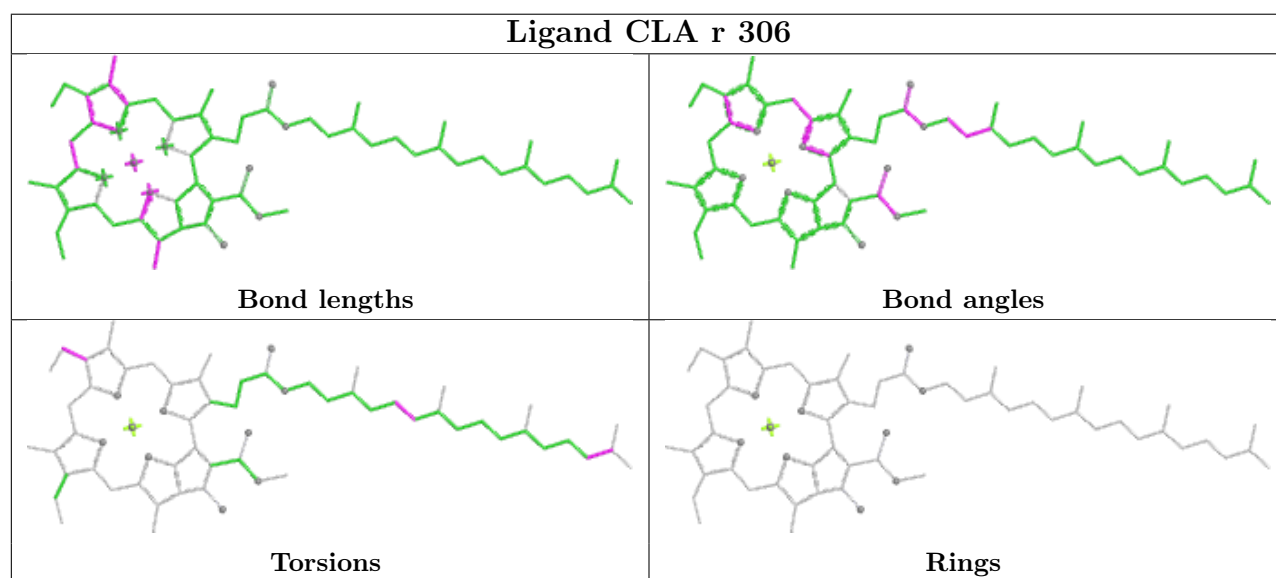
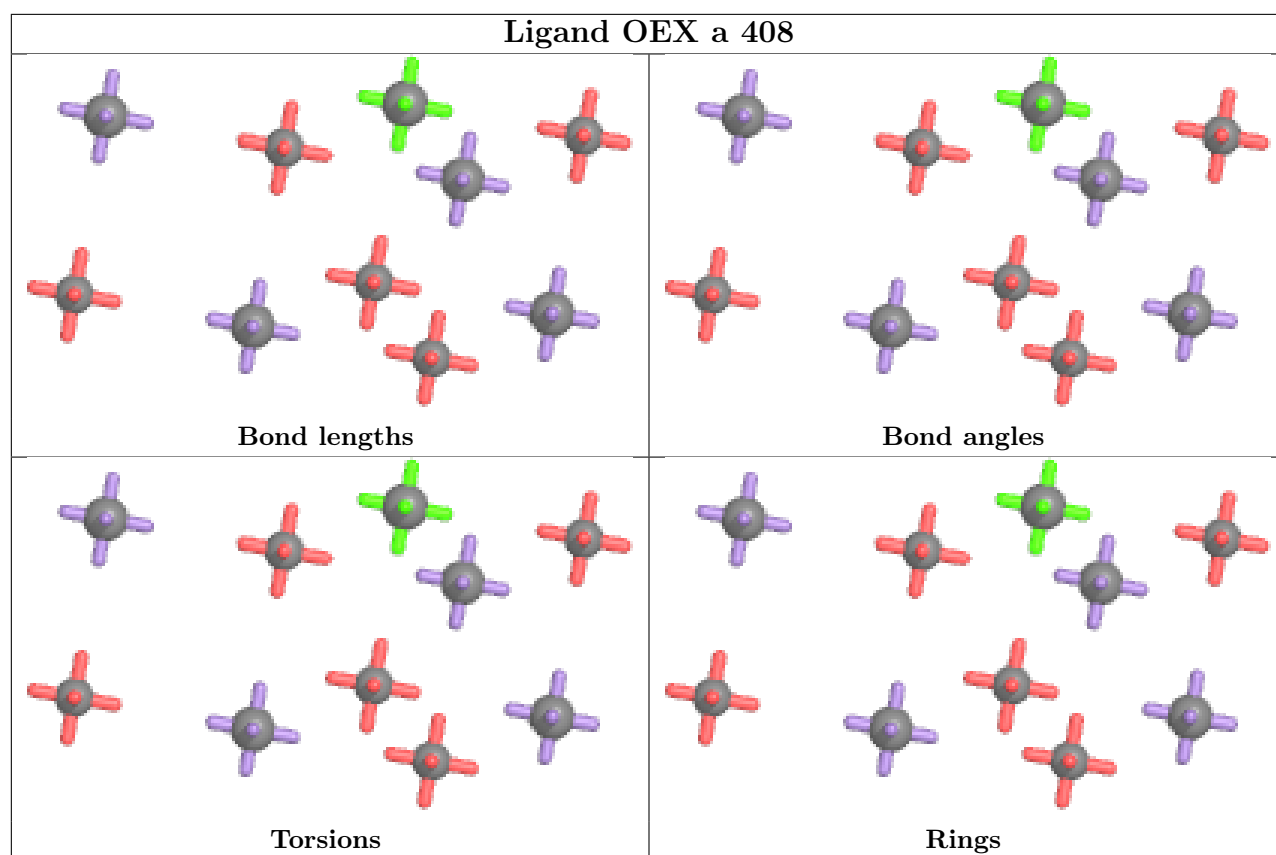


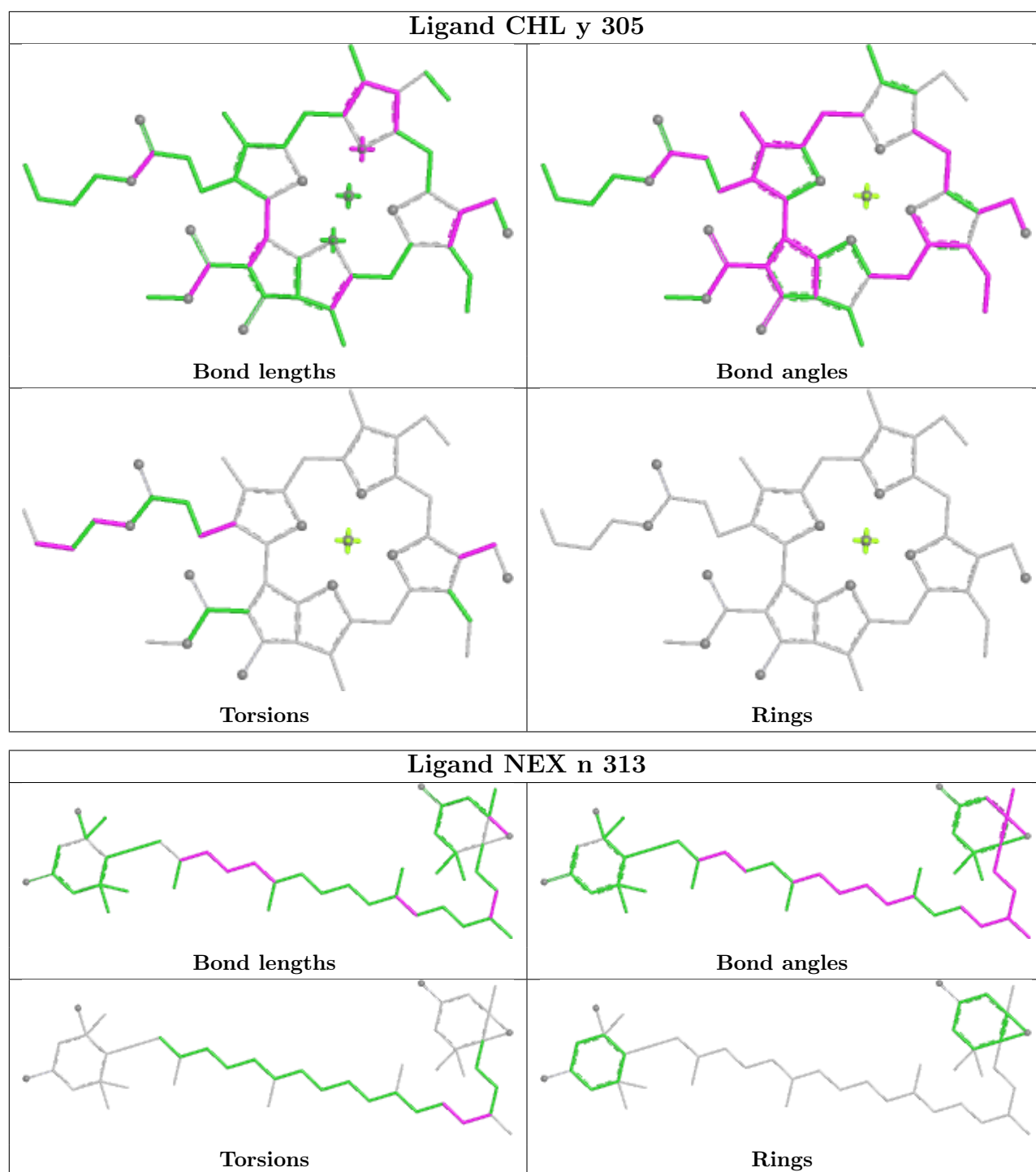
Ligand CLA c 502

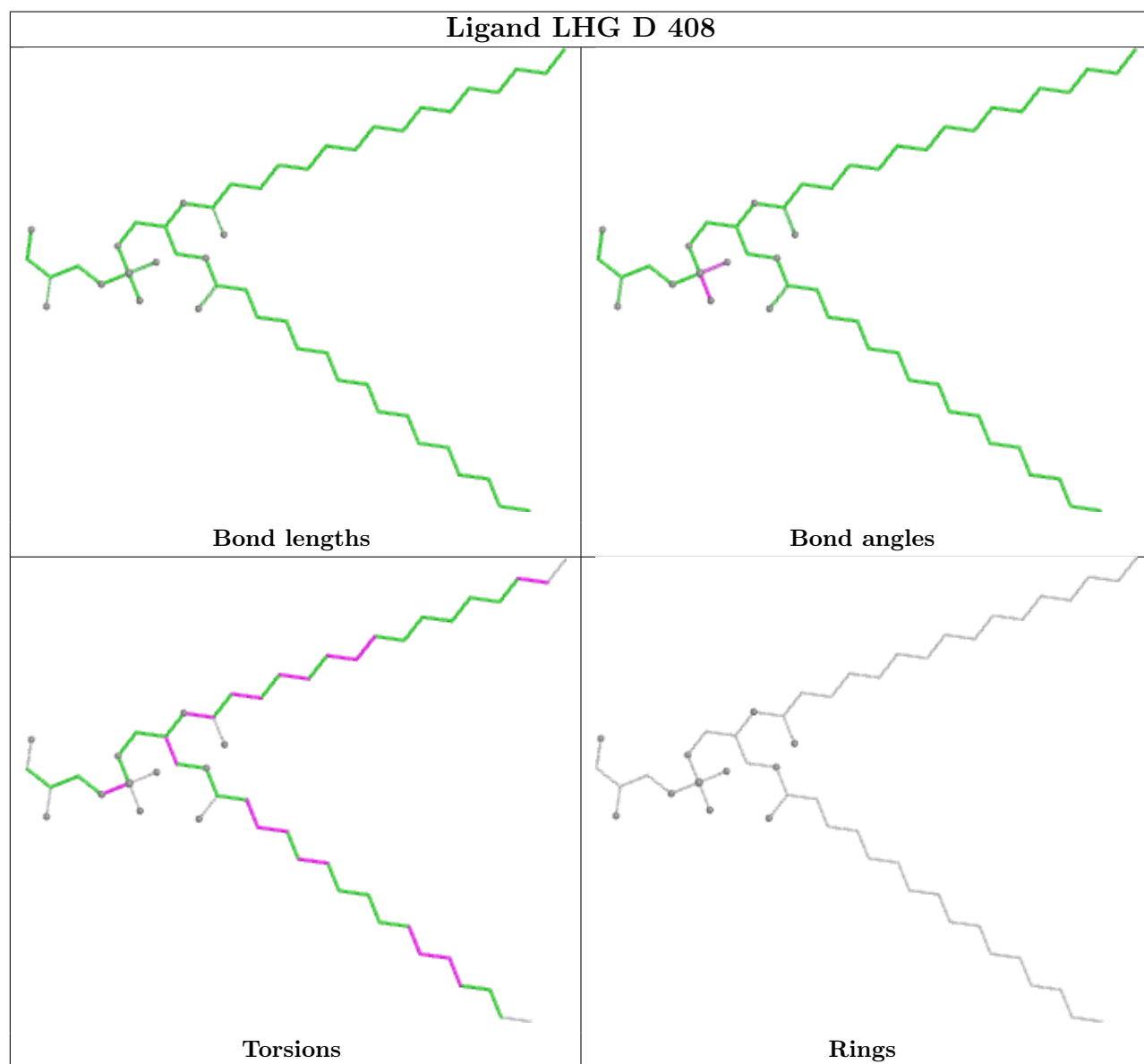
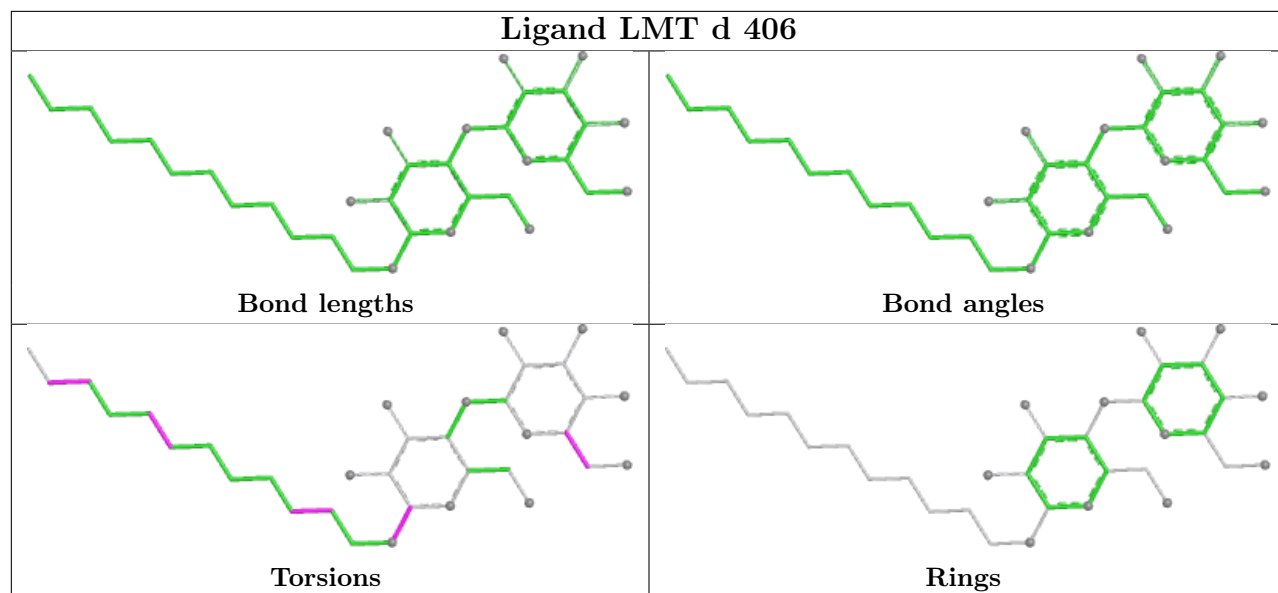


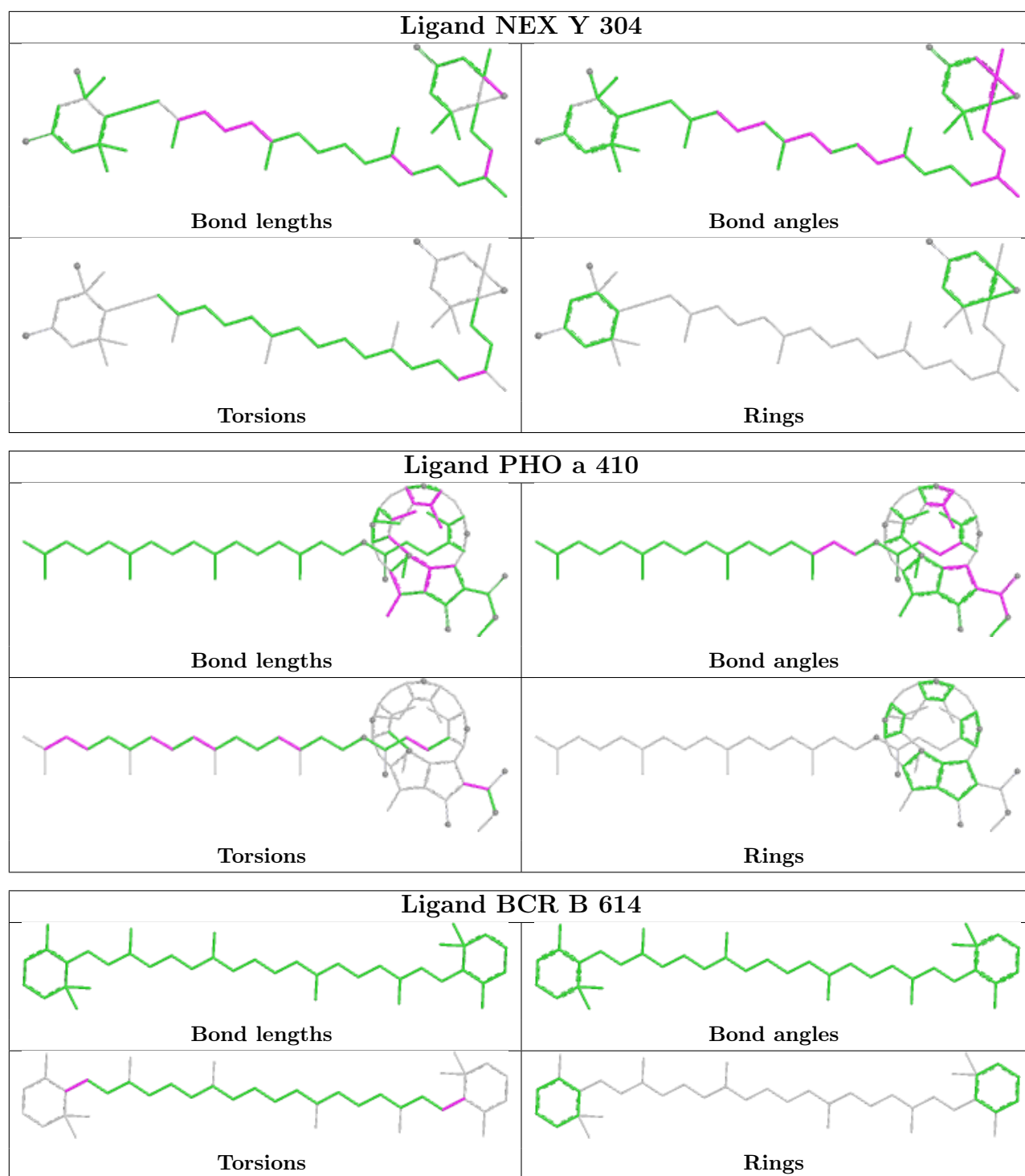
Ligand CLA d 411

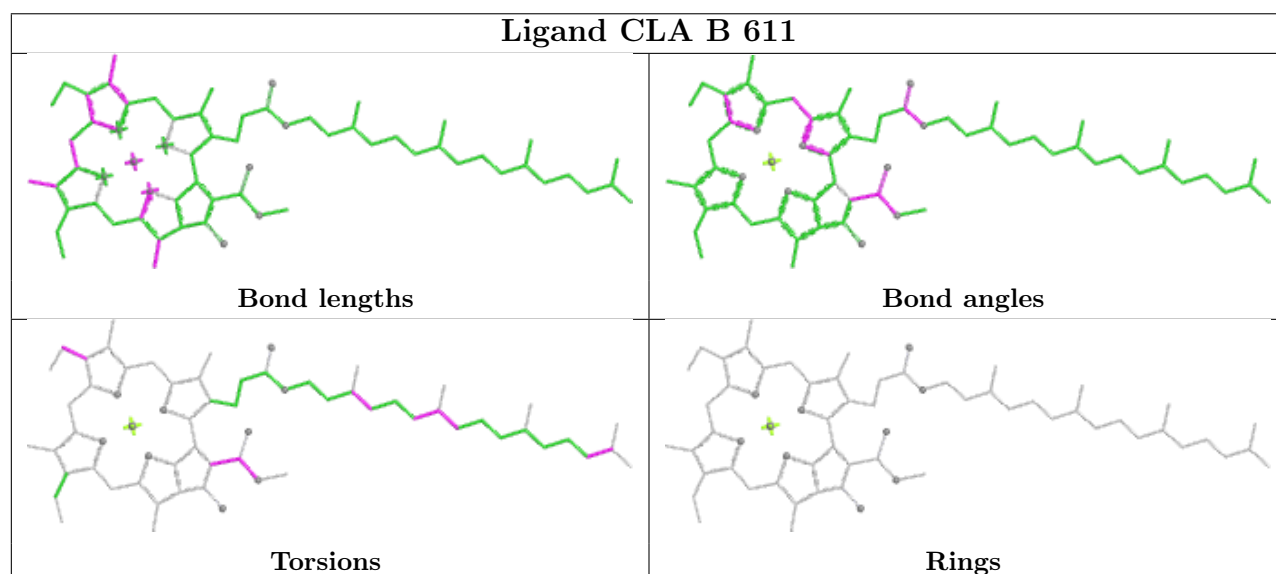
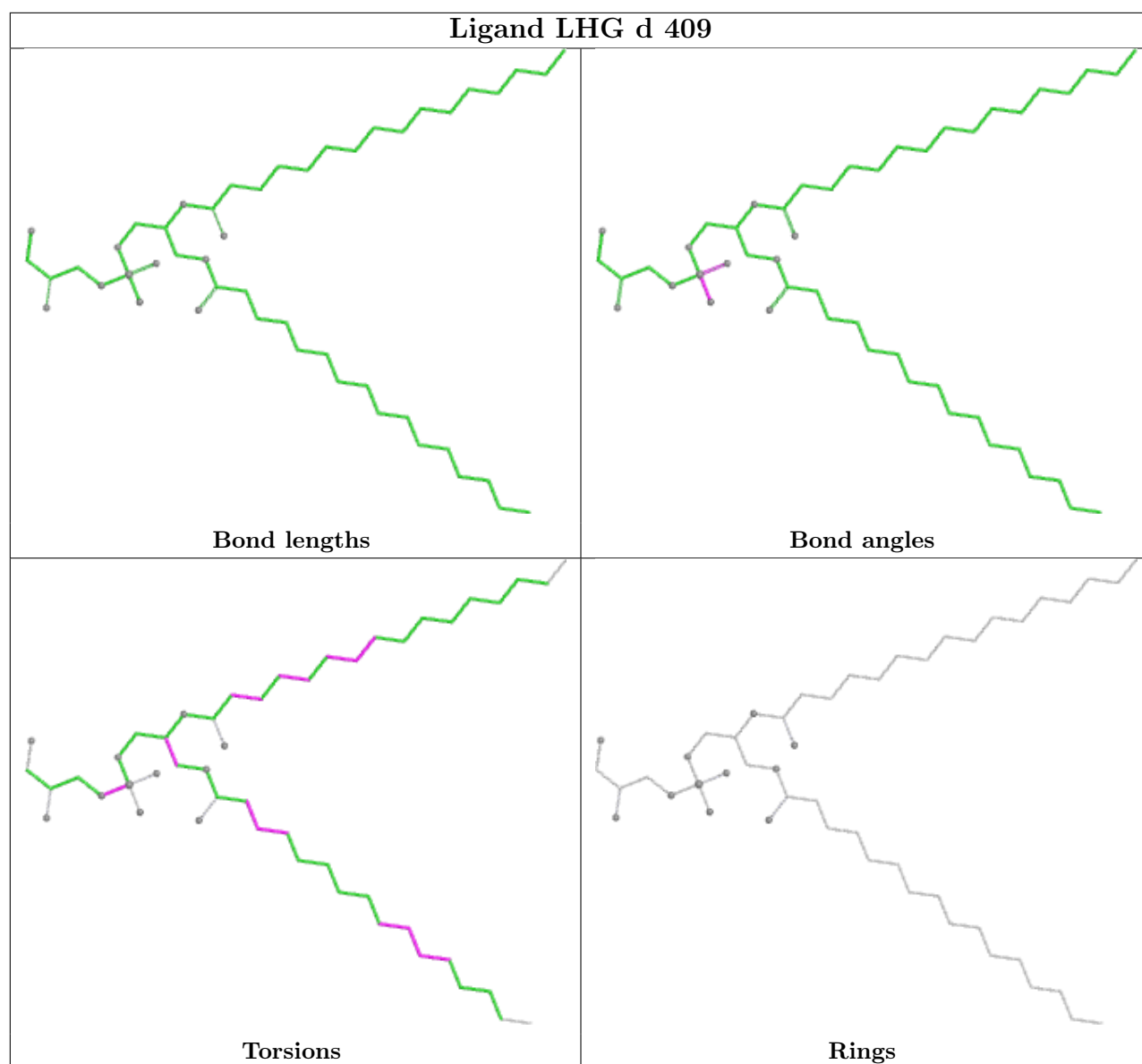


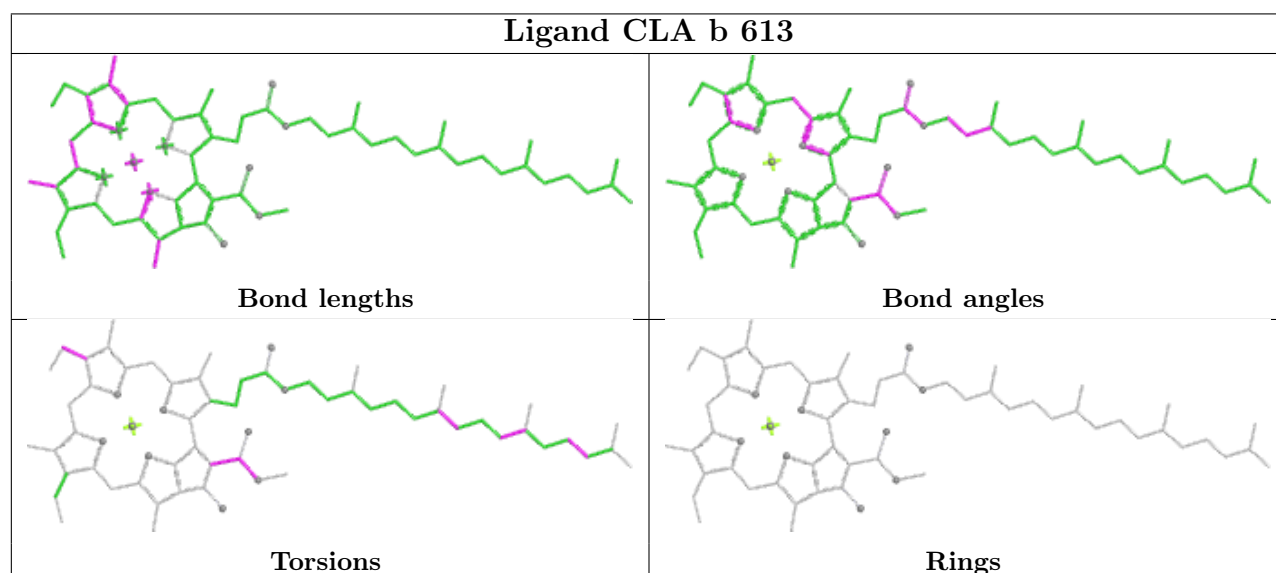
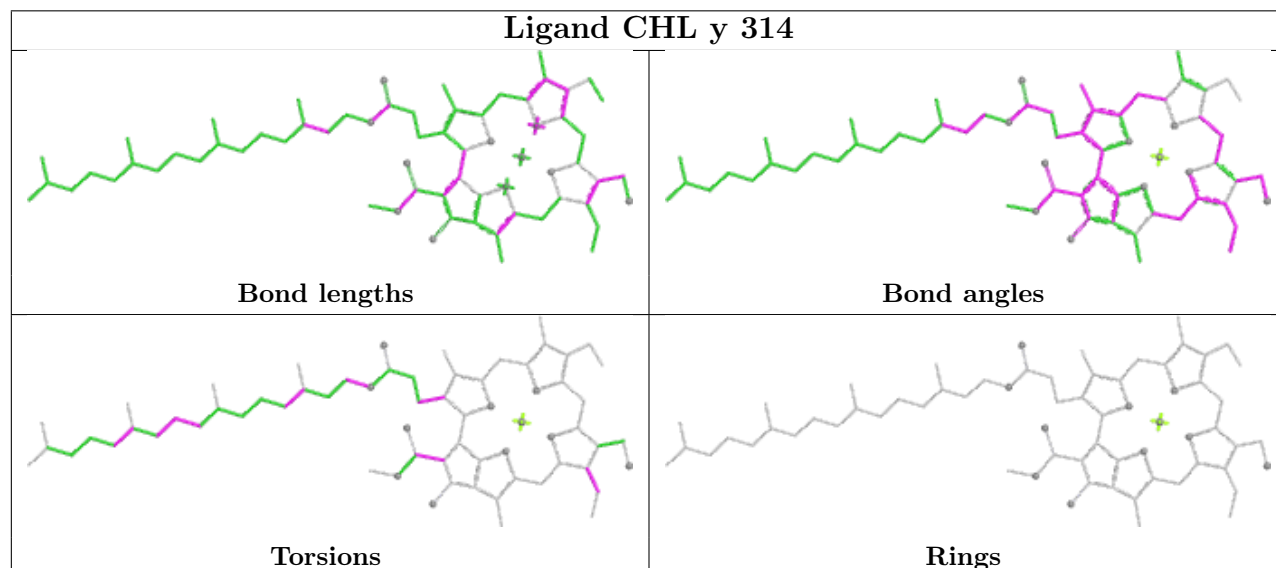
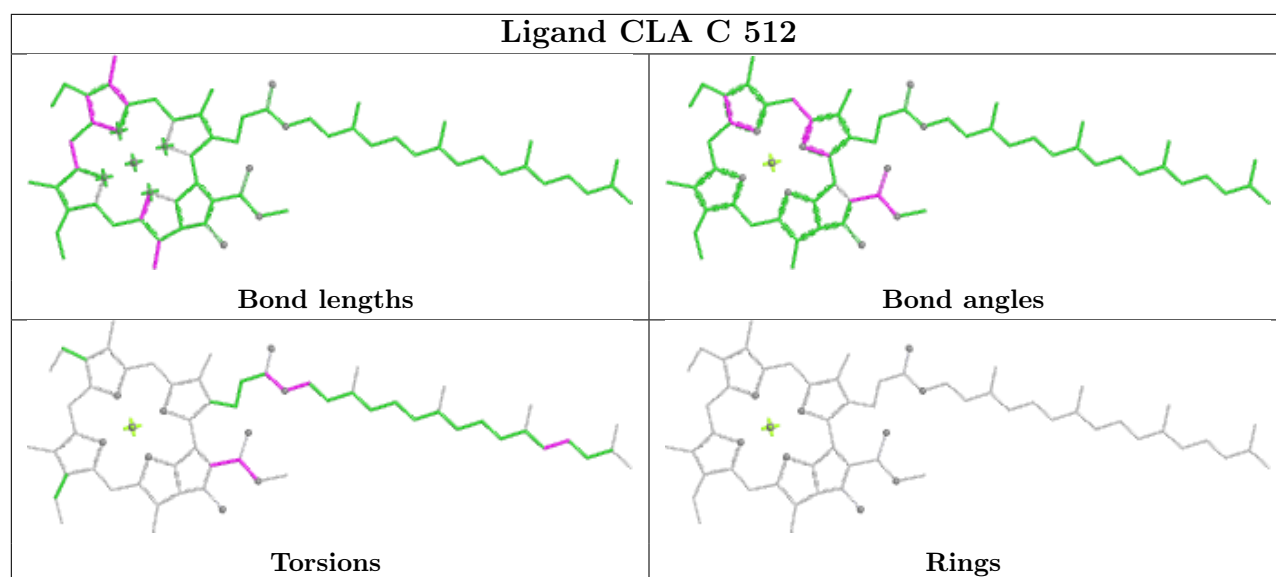


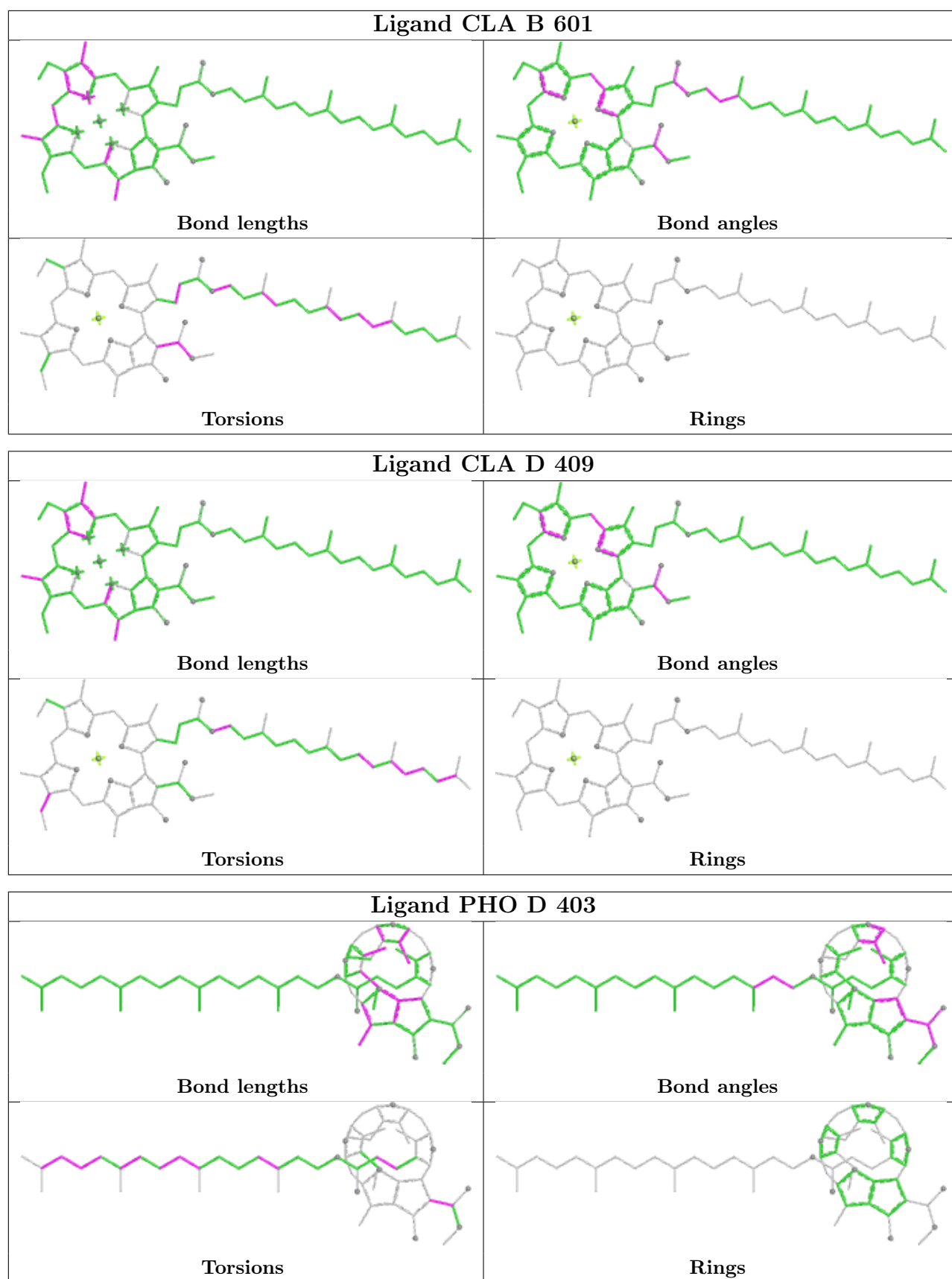


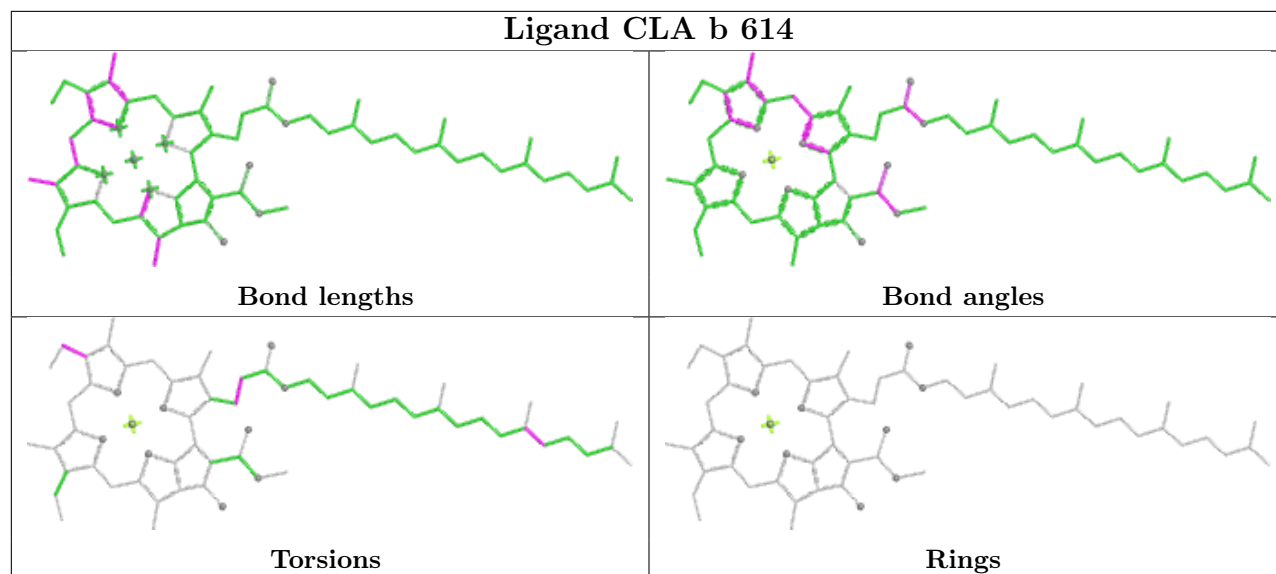
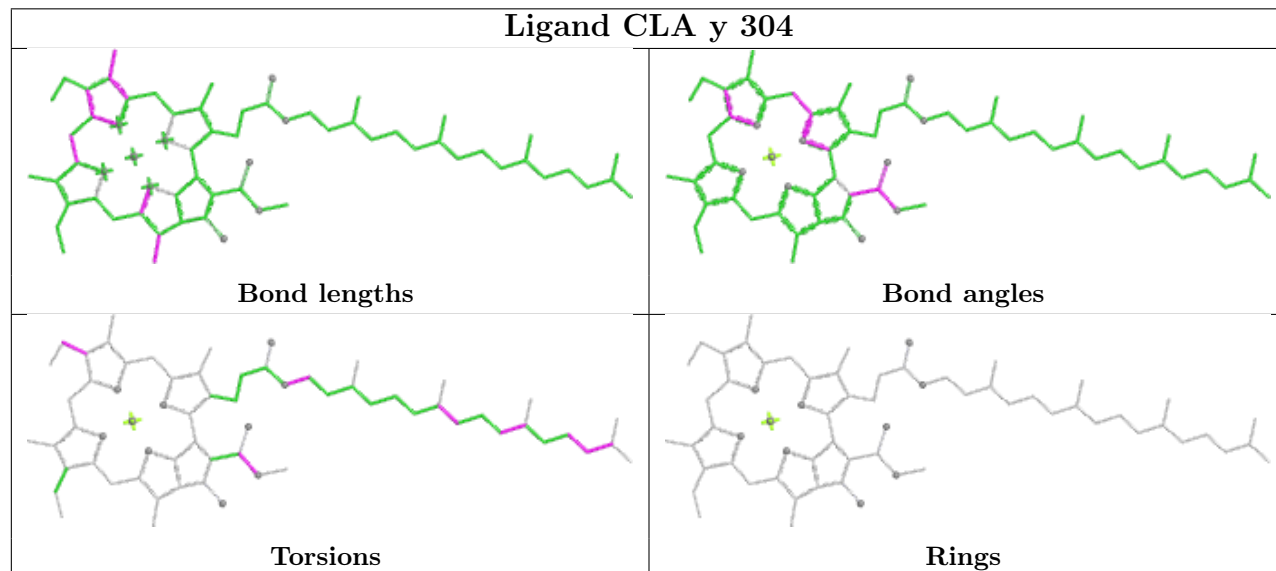


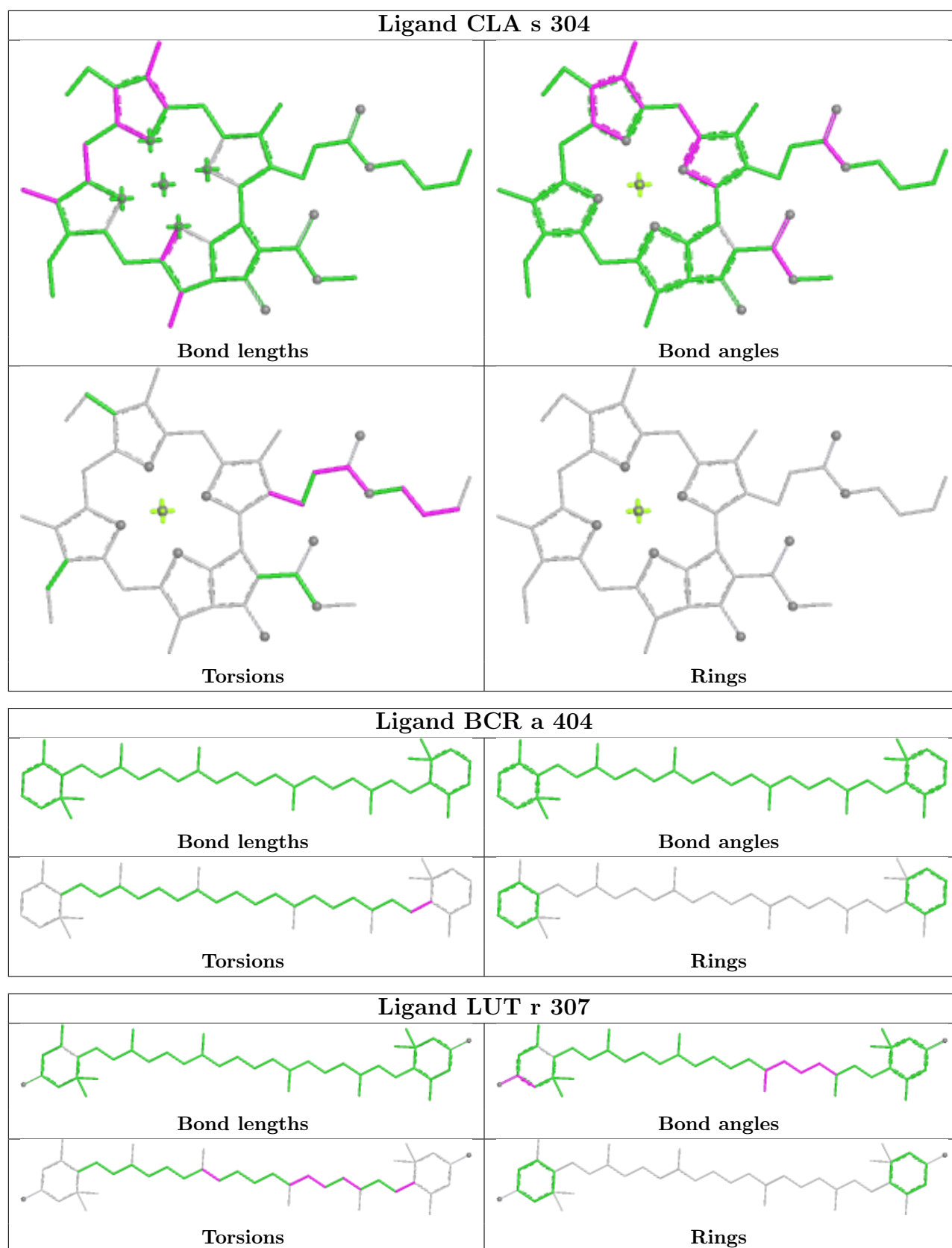




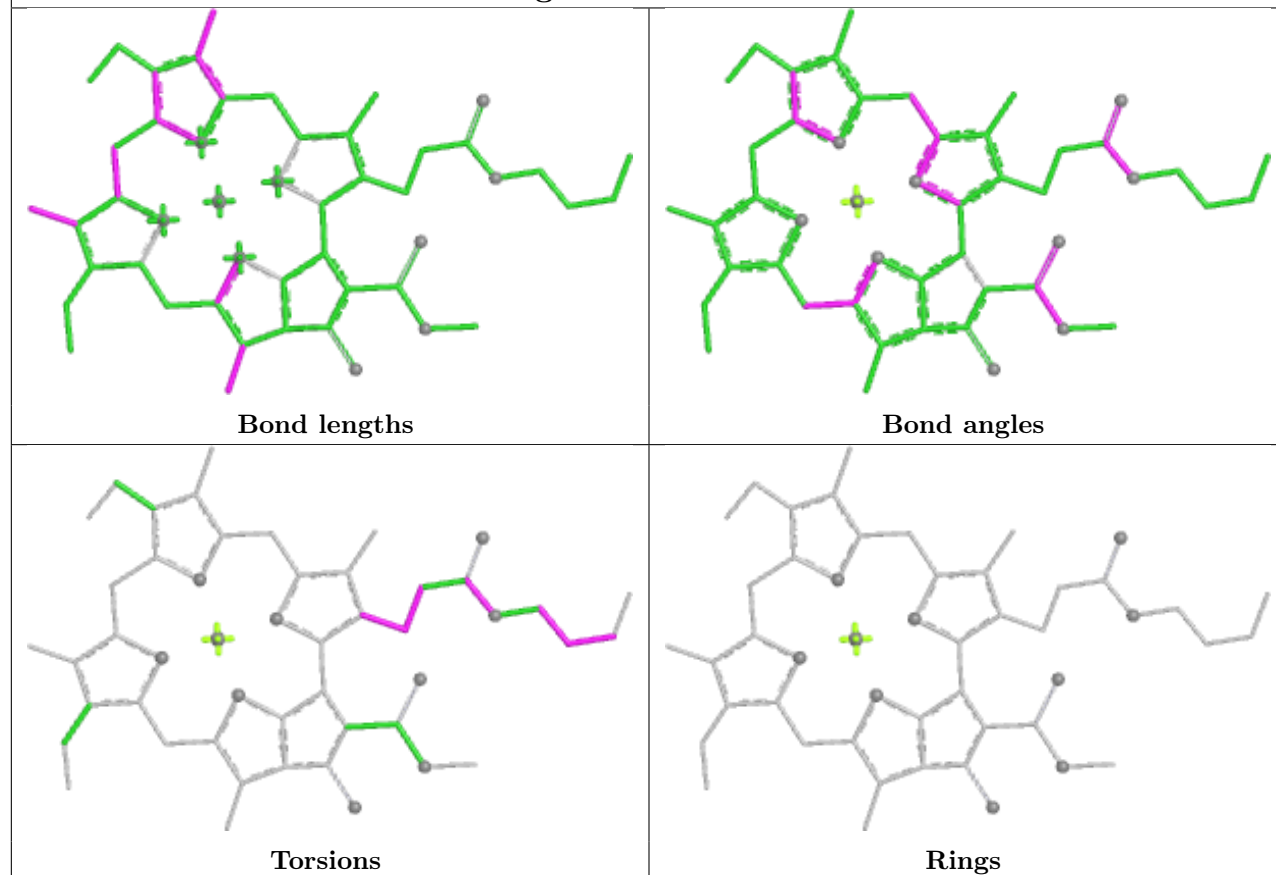




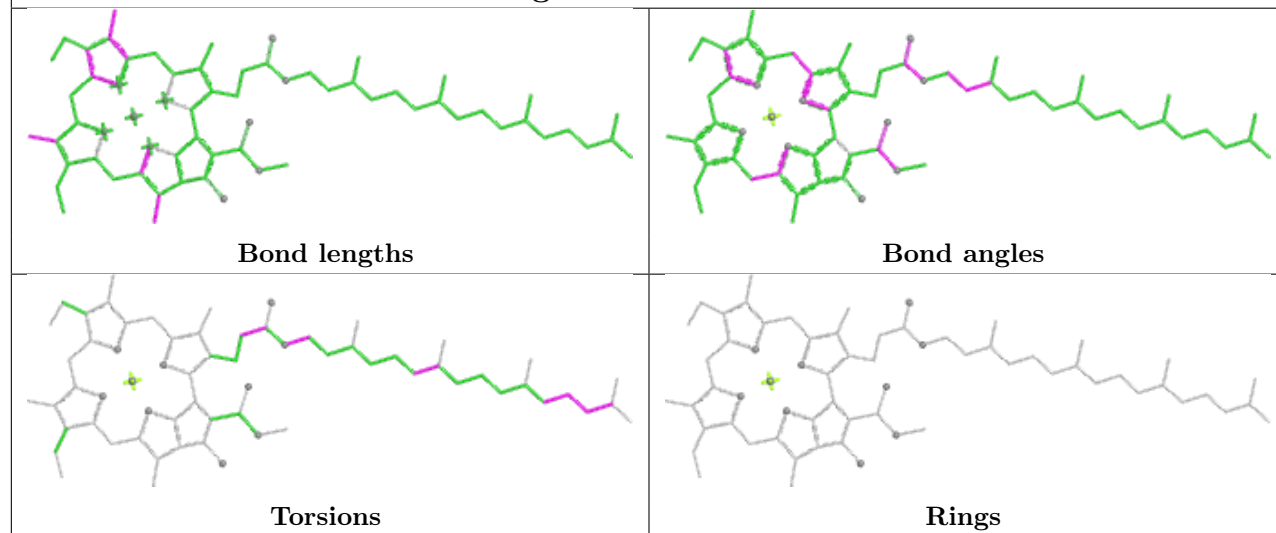
Ligand CLA b 614**Ligand CLA y 304**

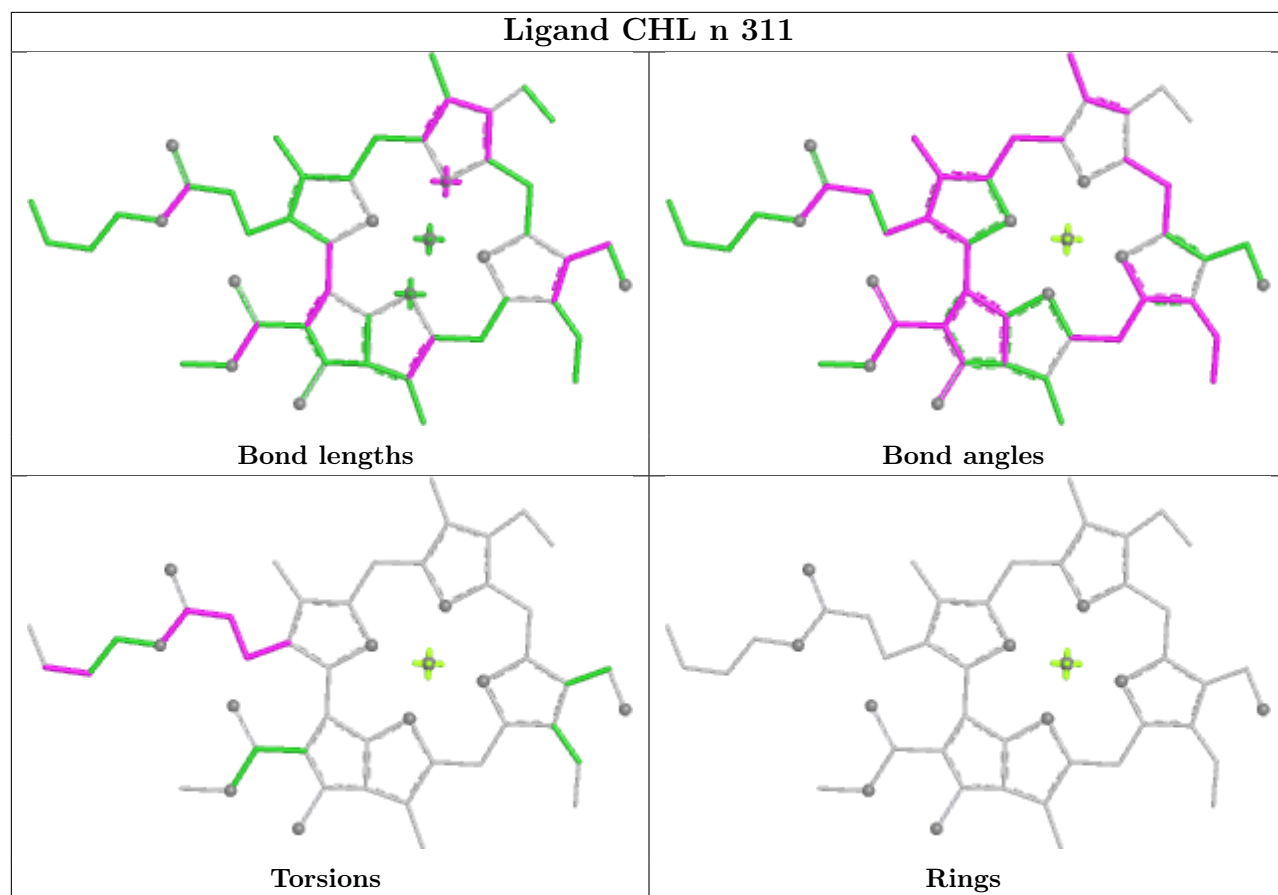
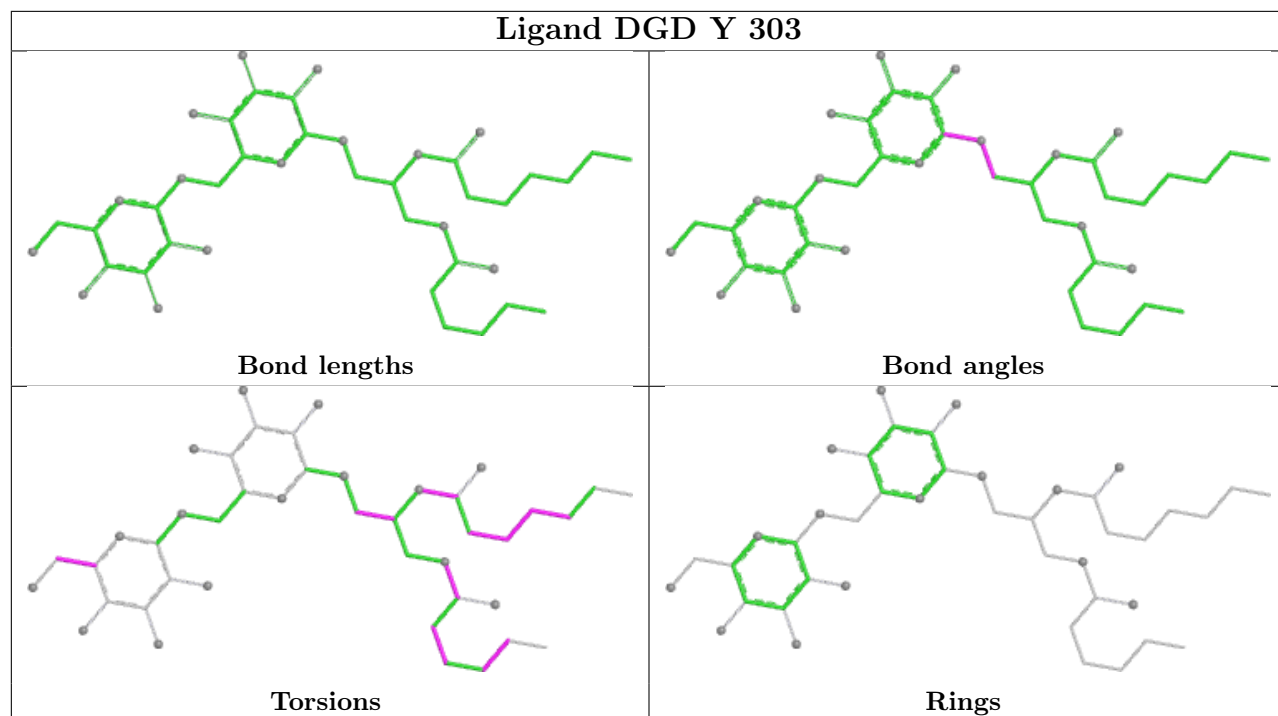


Ligand CLA S 304

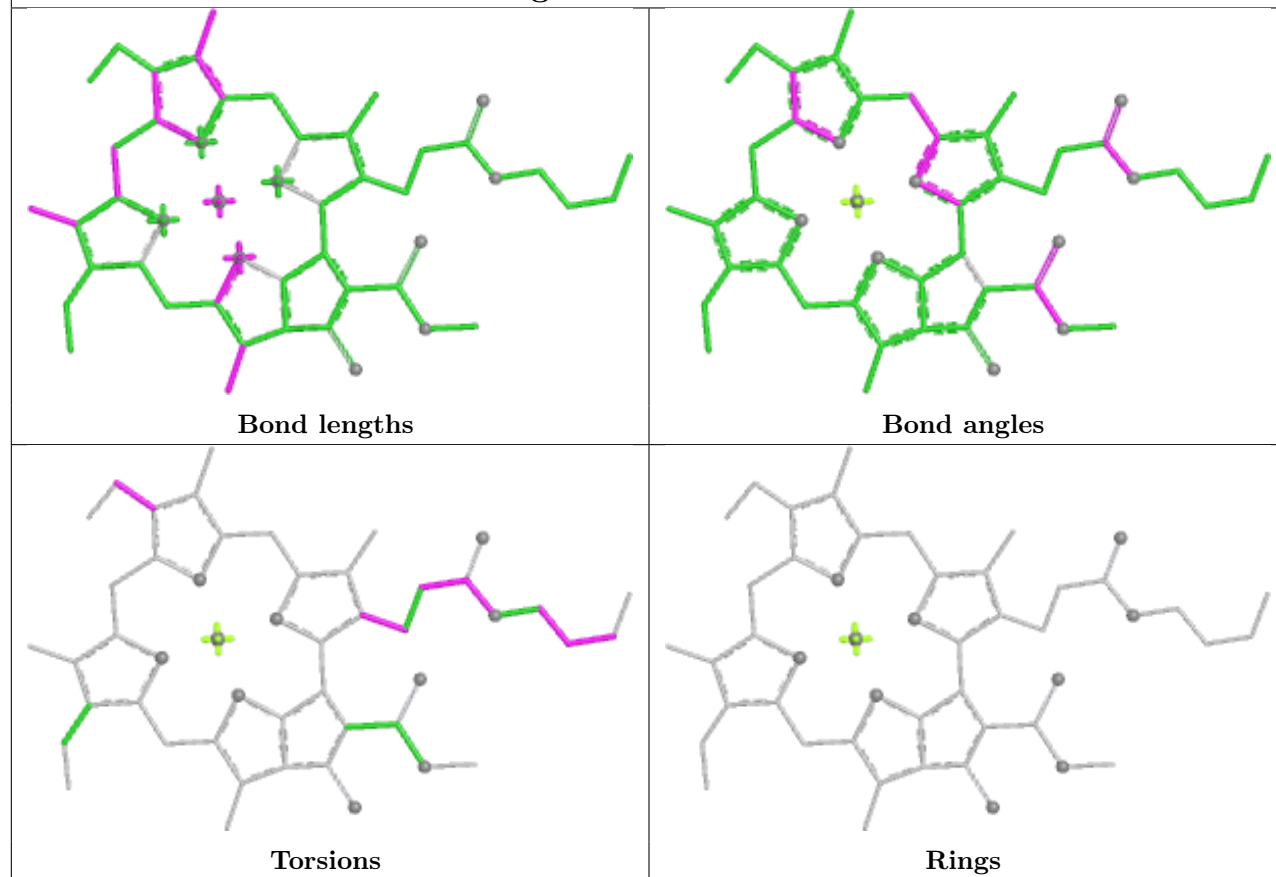


Ligand CLA B 603

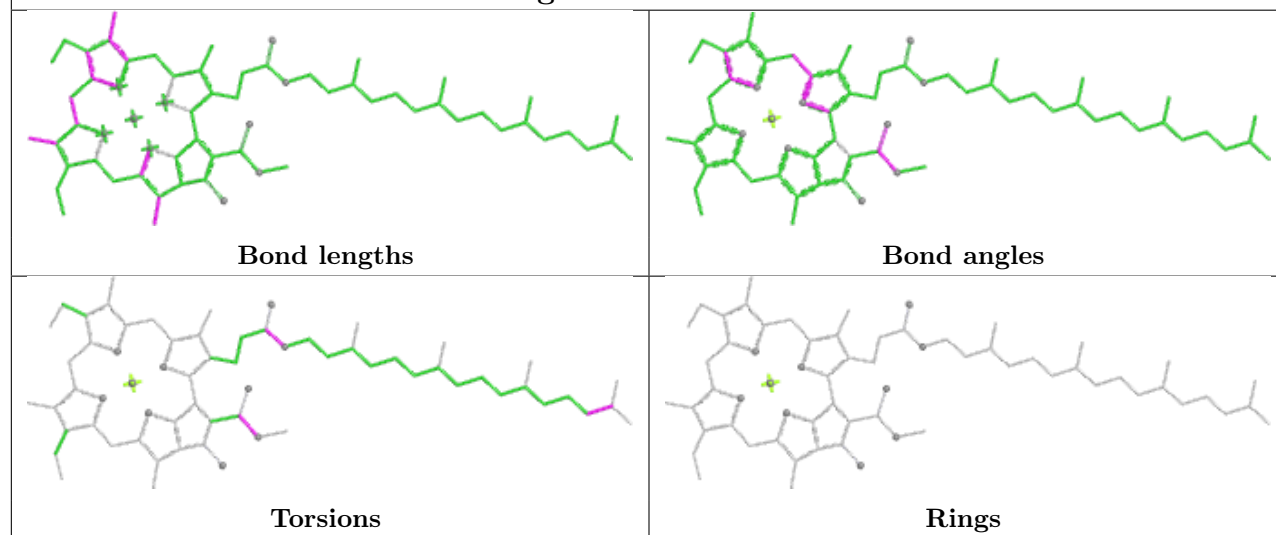


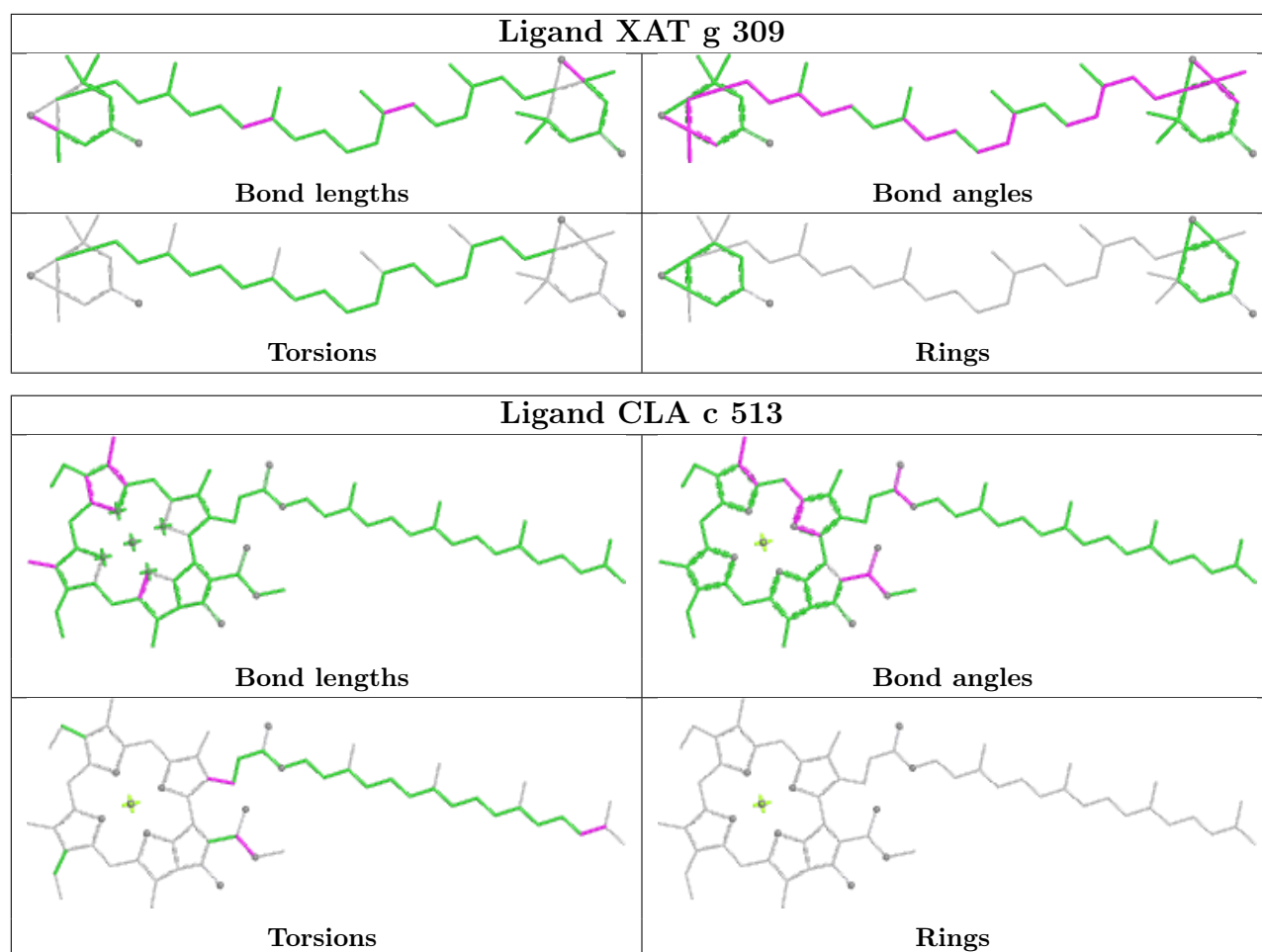


Ligand CLA N 306

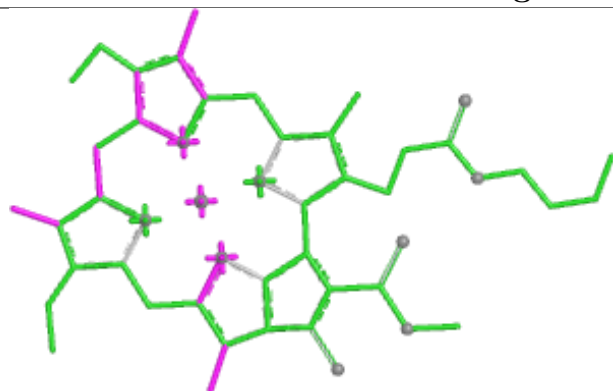


Ligand CLA c 518

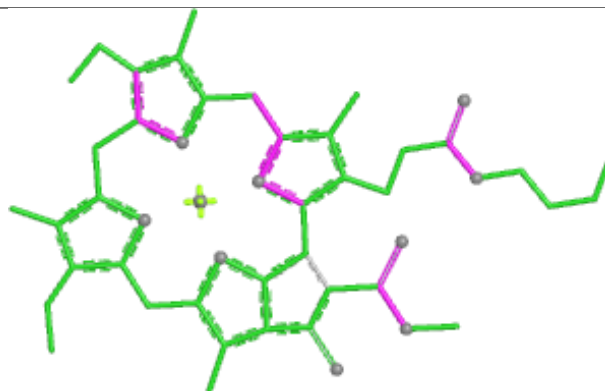




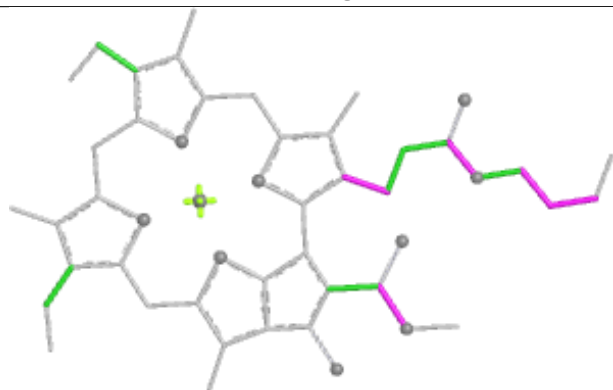
Ligand CLA N 308



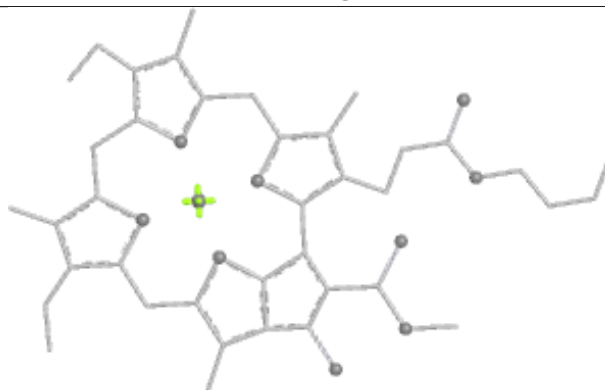
Bond lengths



Bond angles

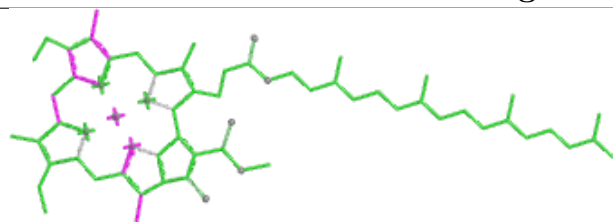


Torsions

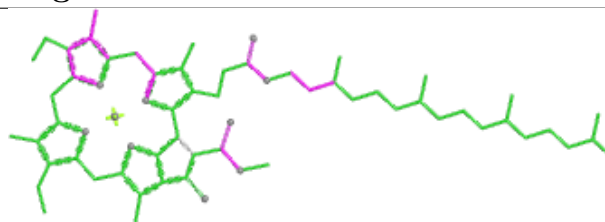


Rings

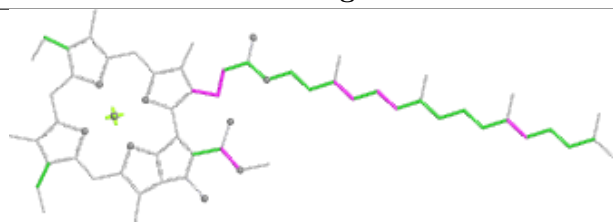
Ligand CLA g 317



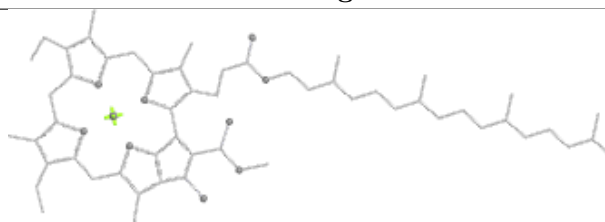
Bond lengths



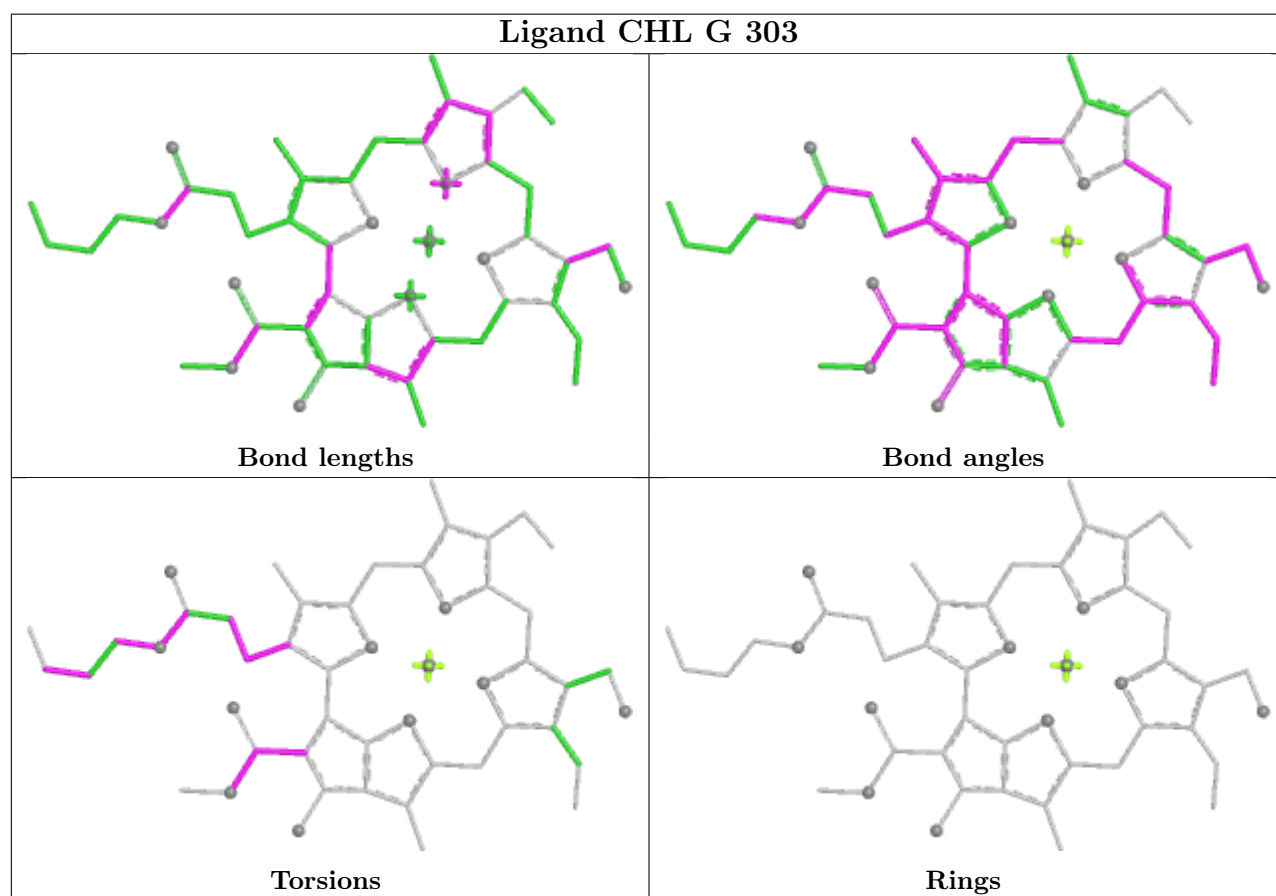
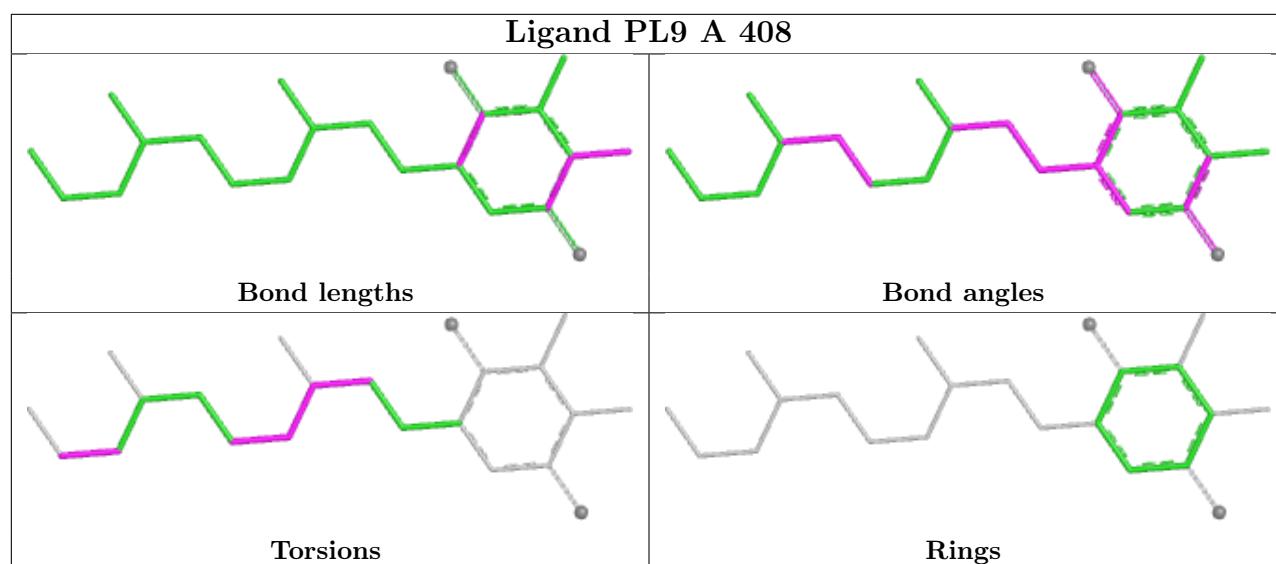
Bond angles

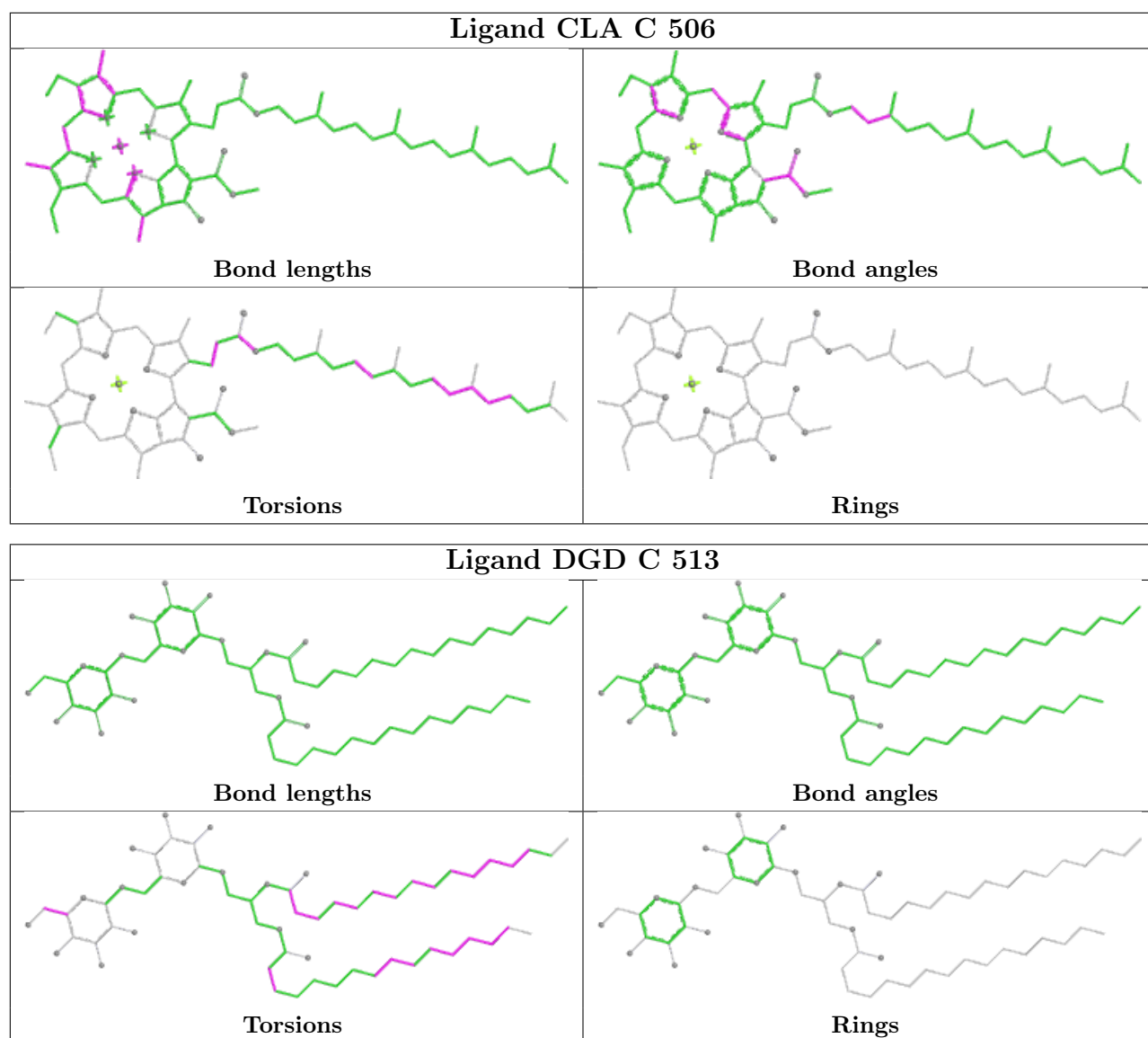


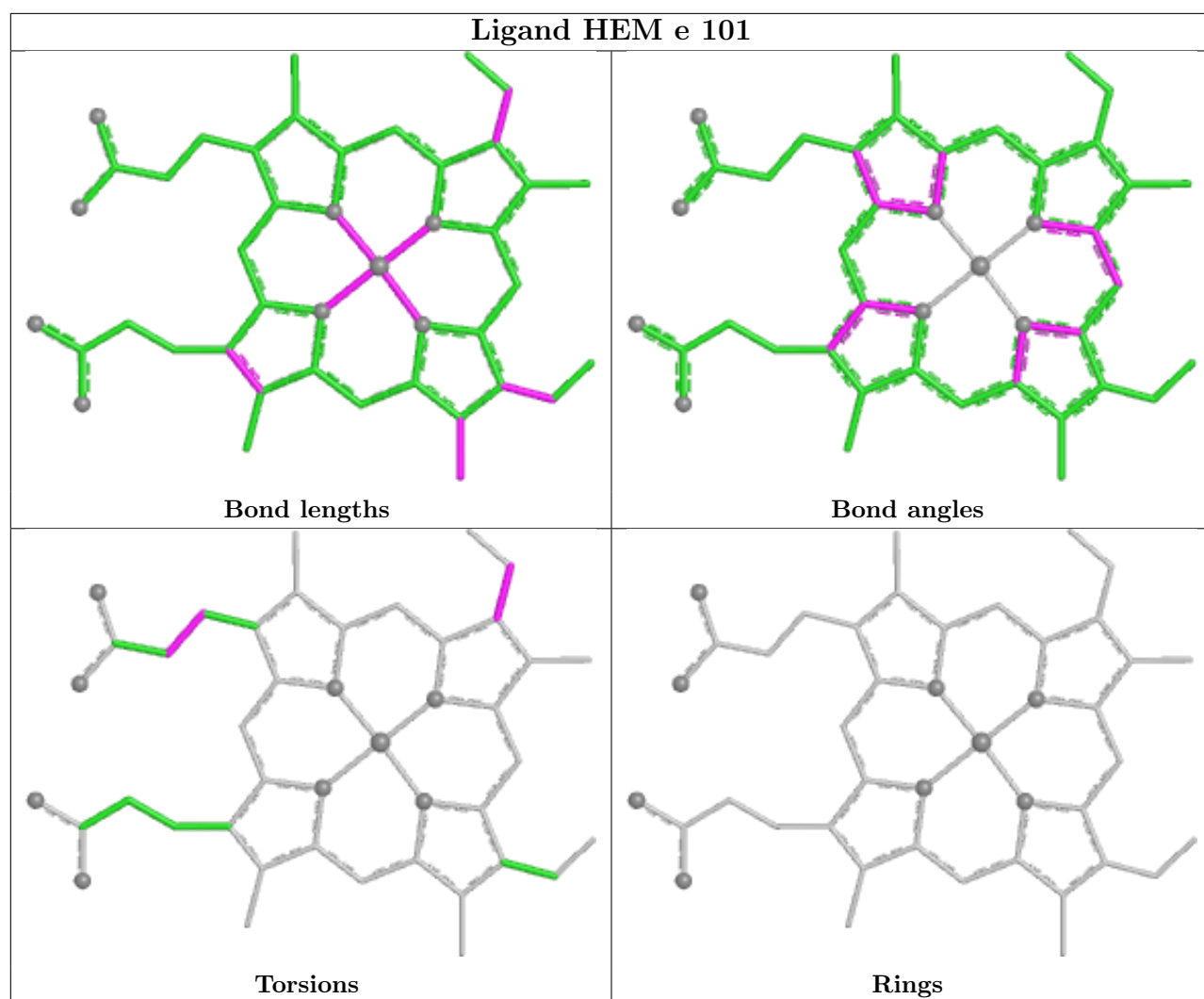
Torsions

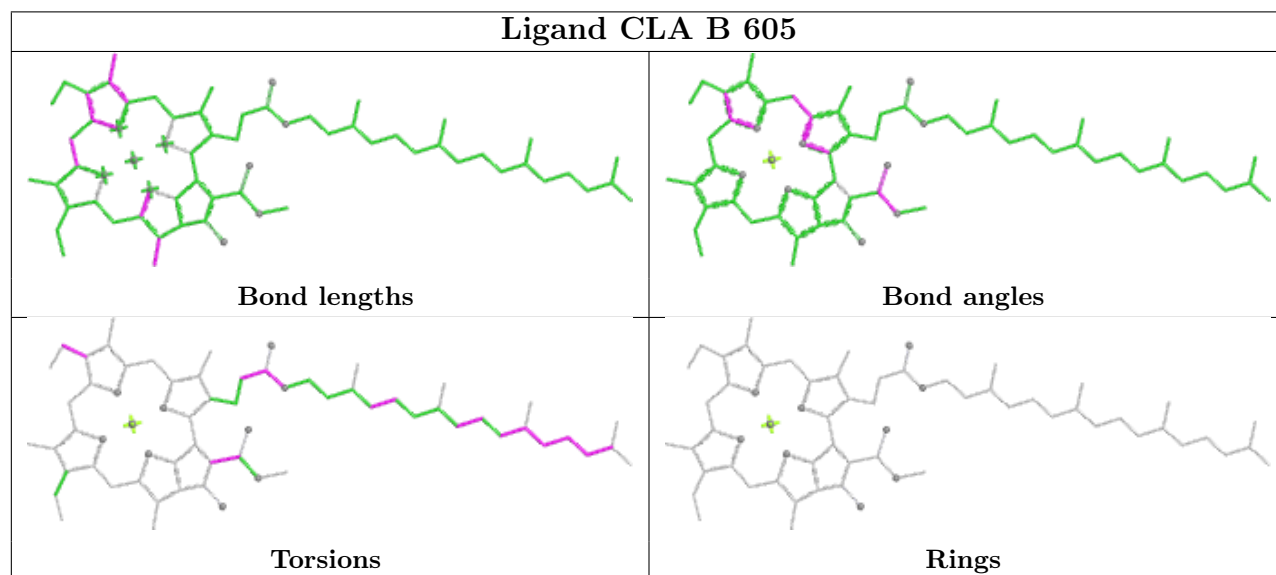
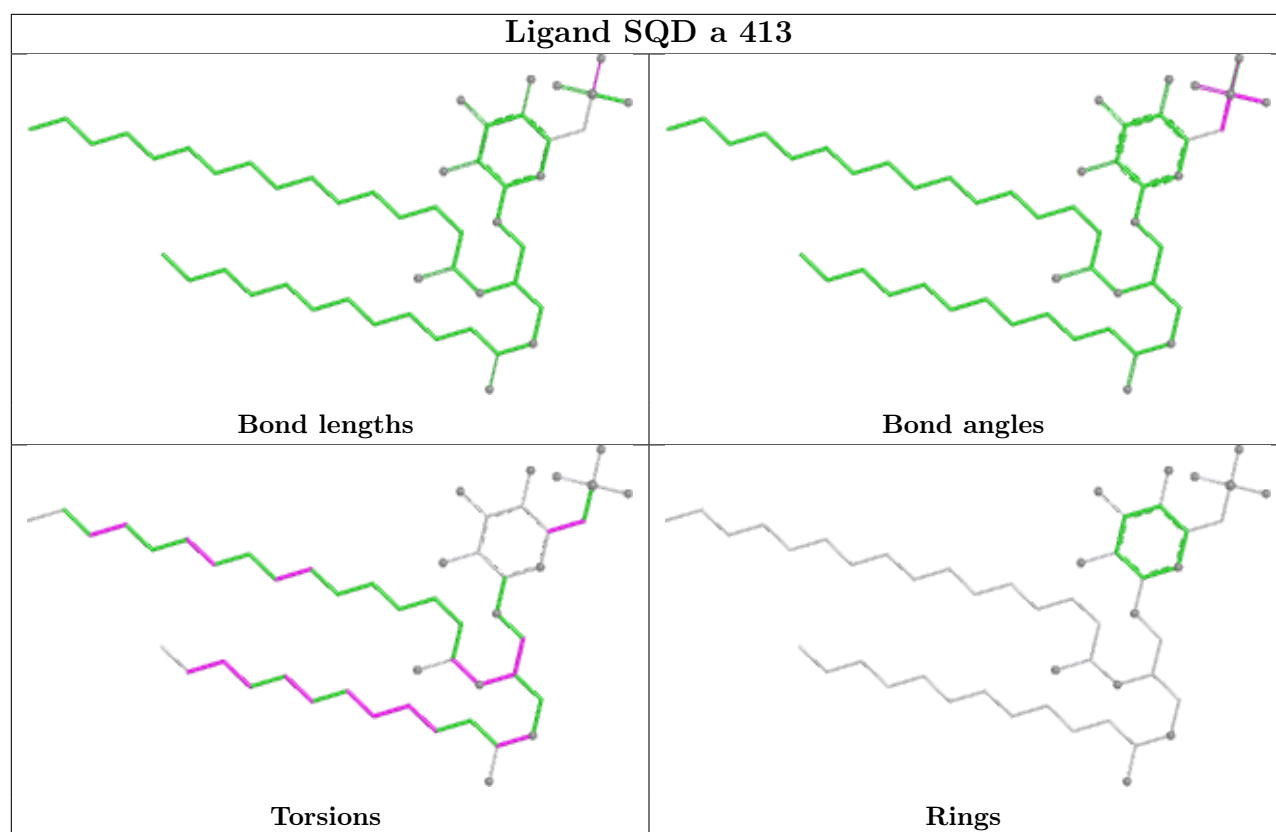


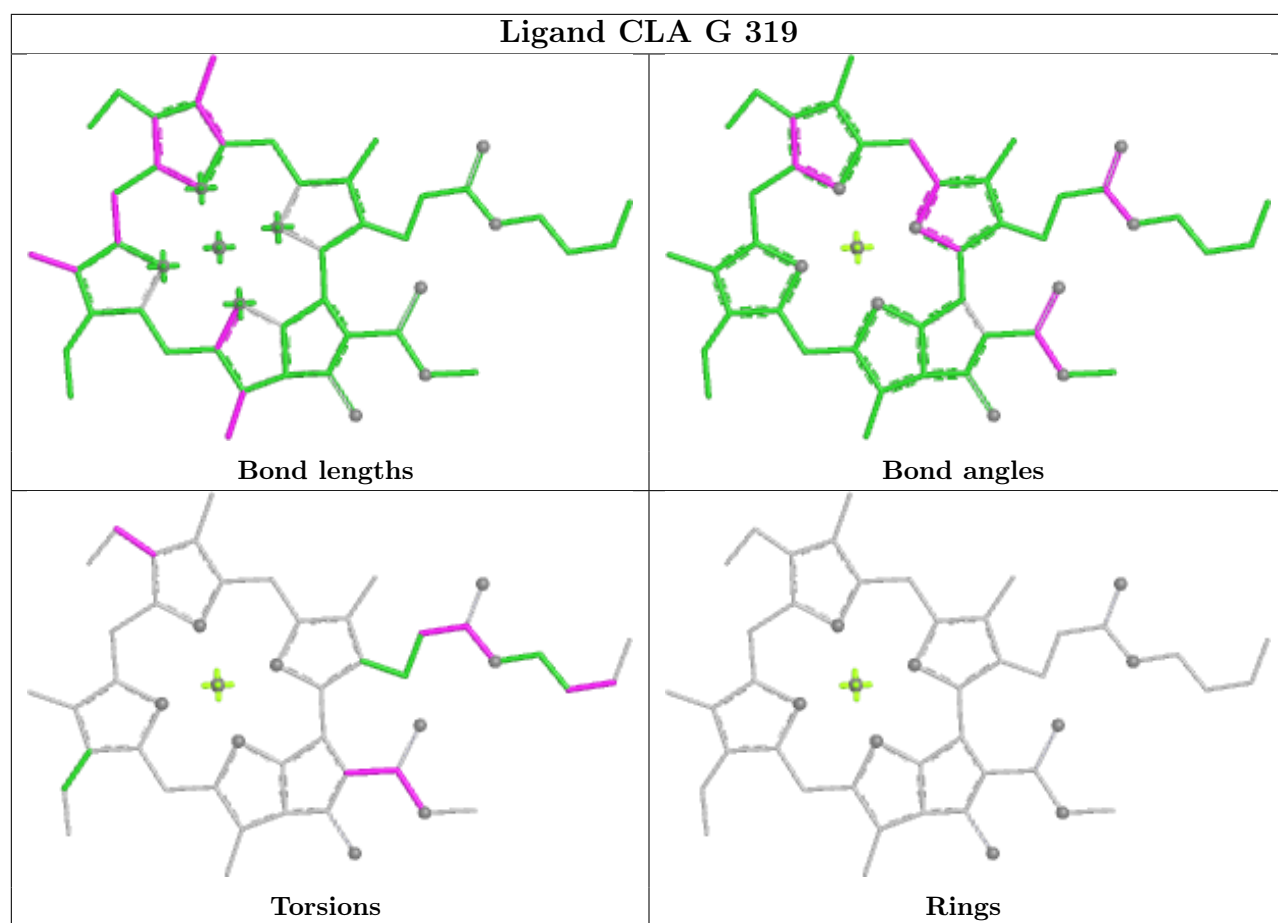
Rings

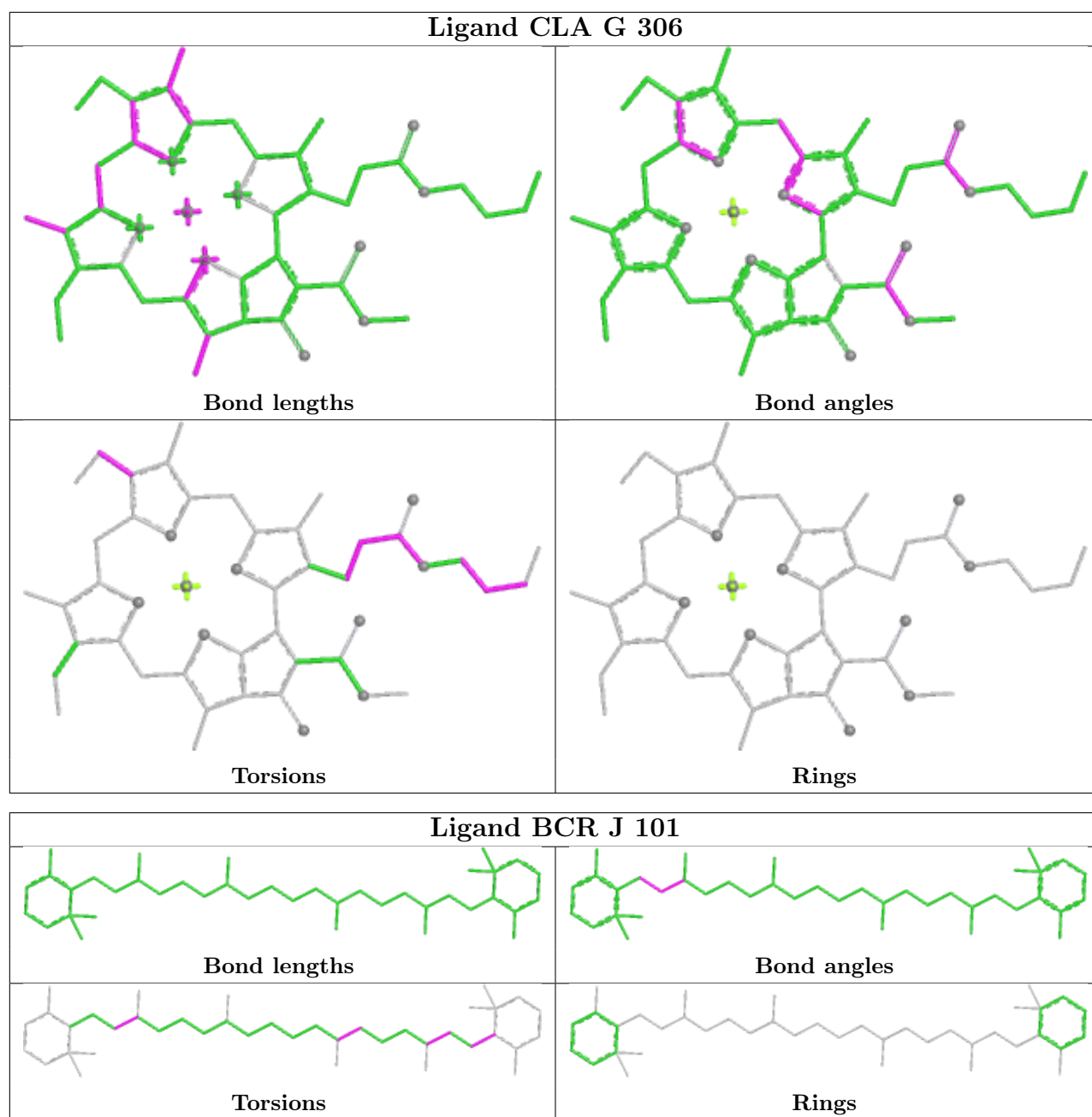


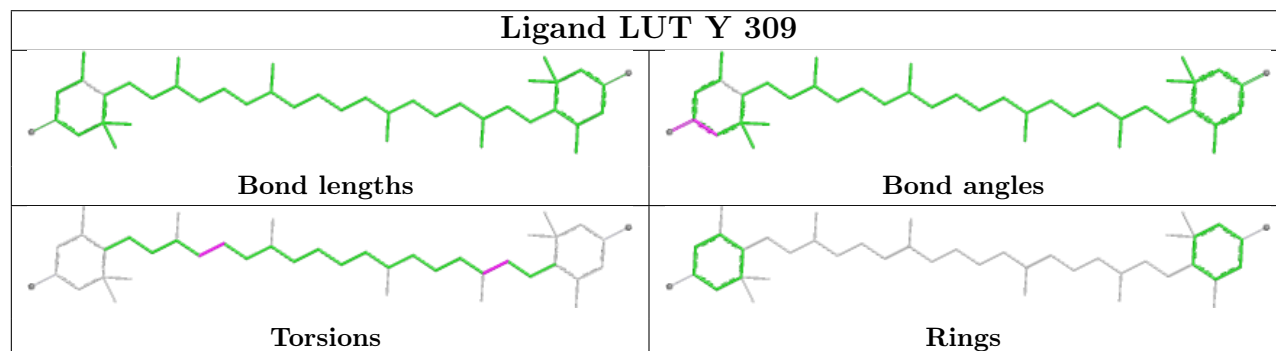
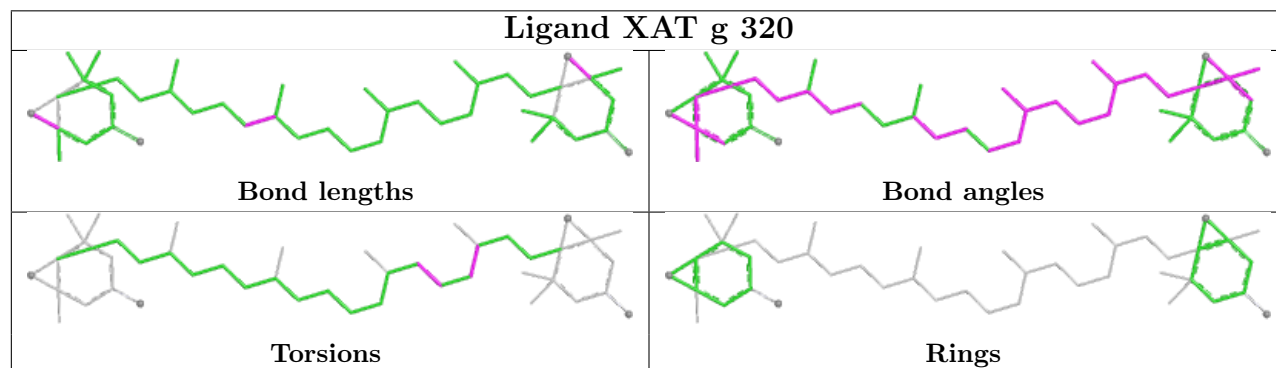
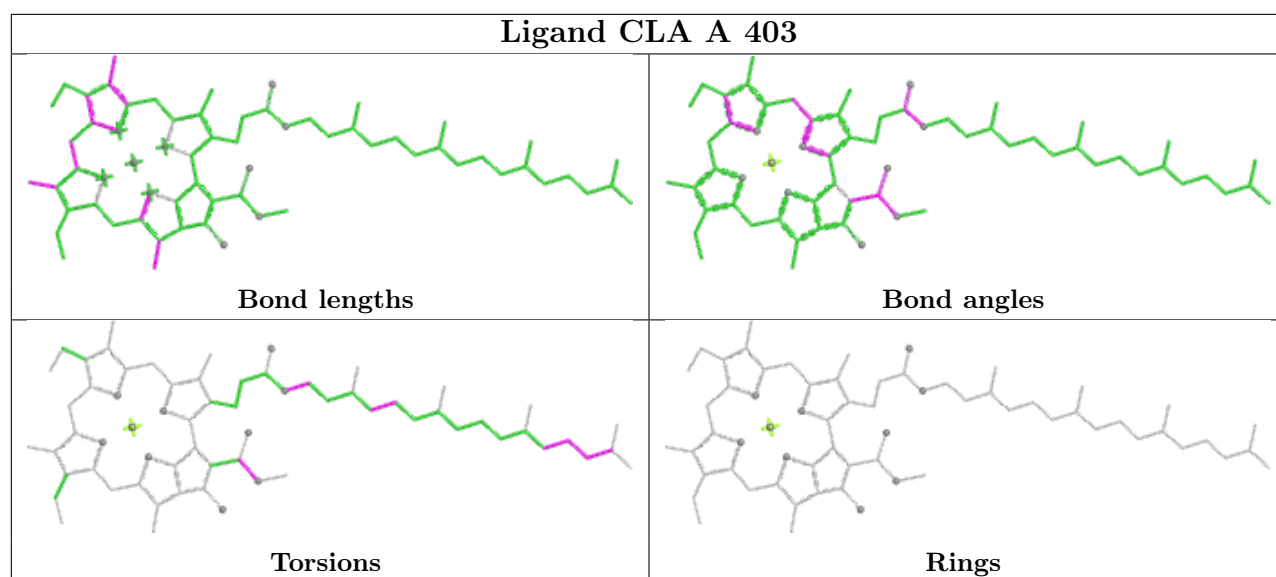


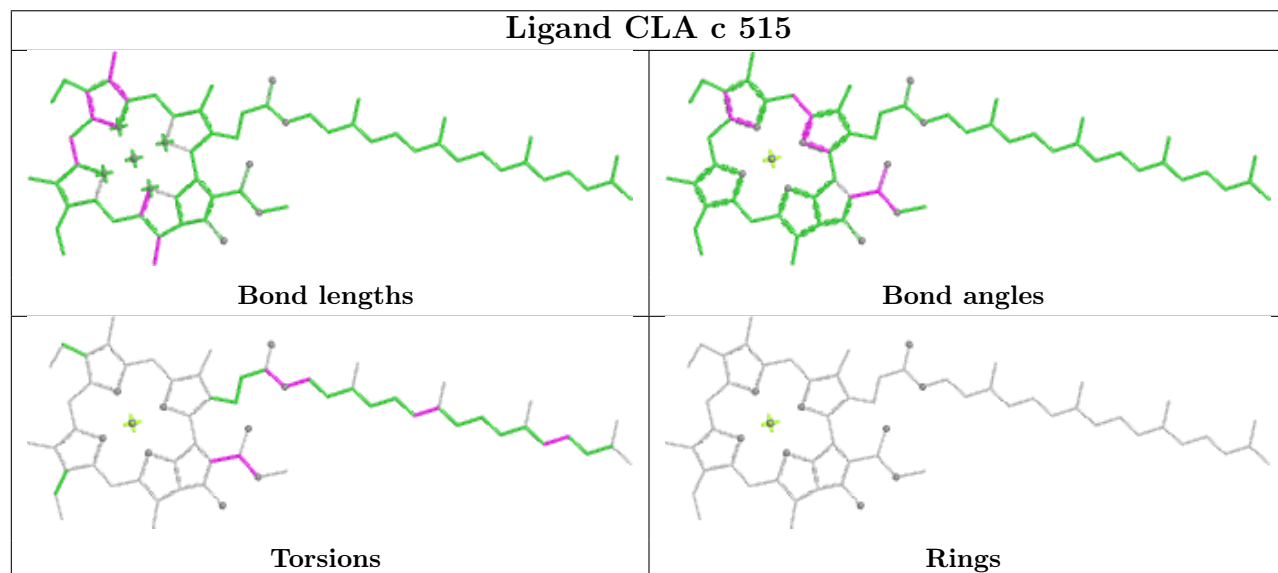
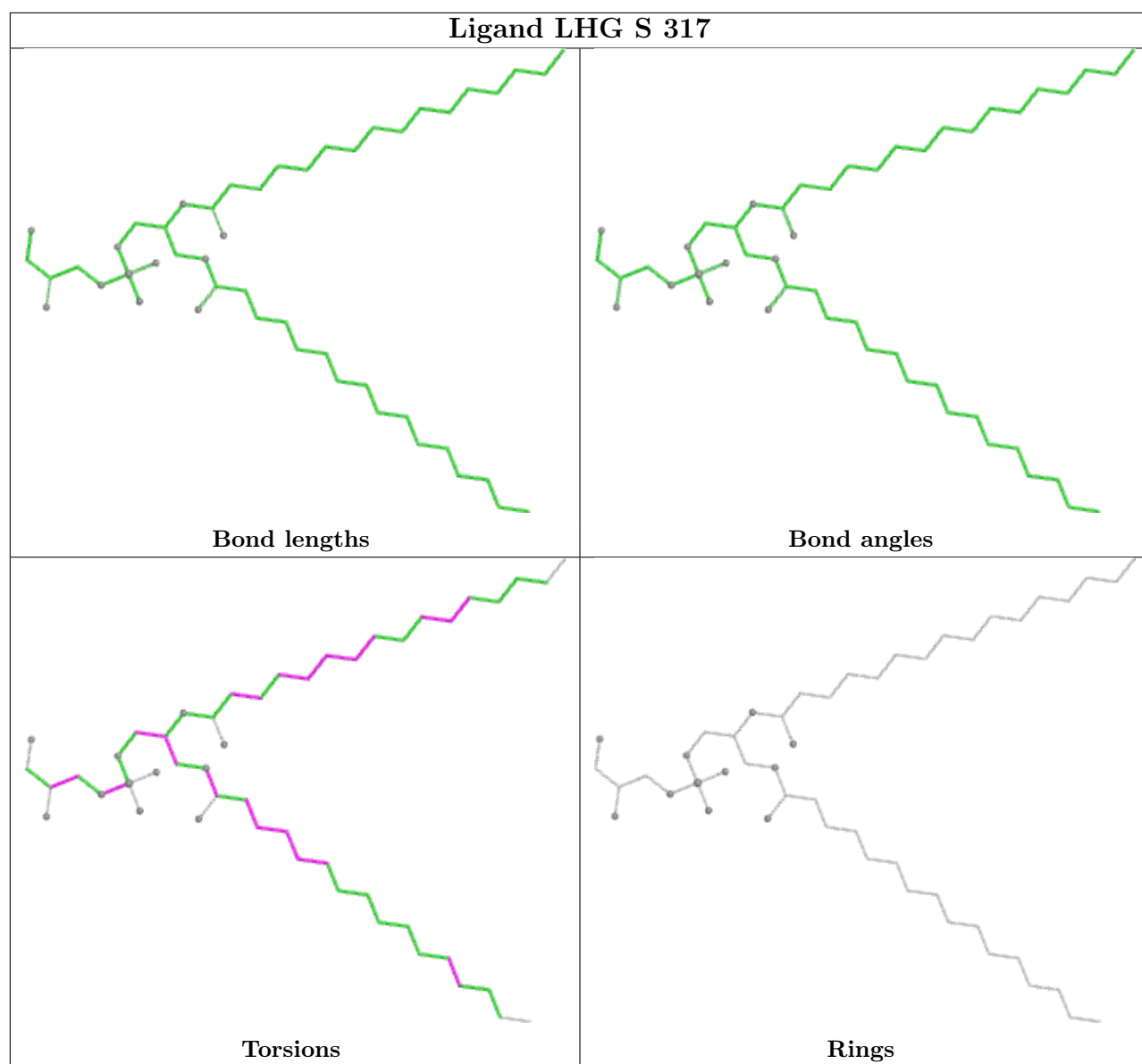


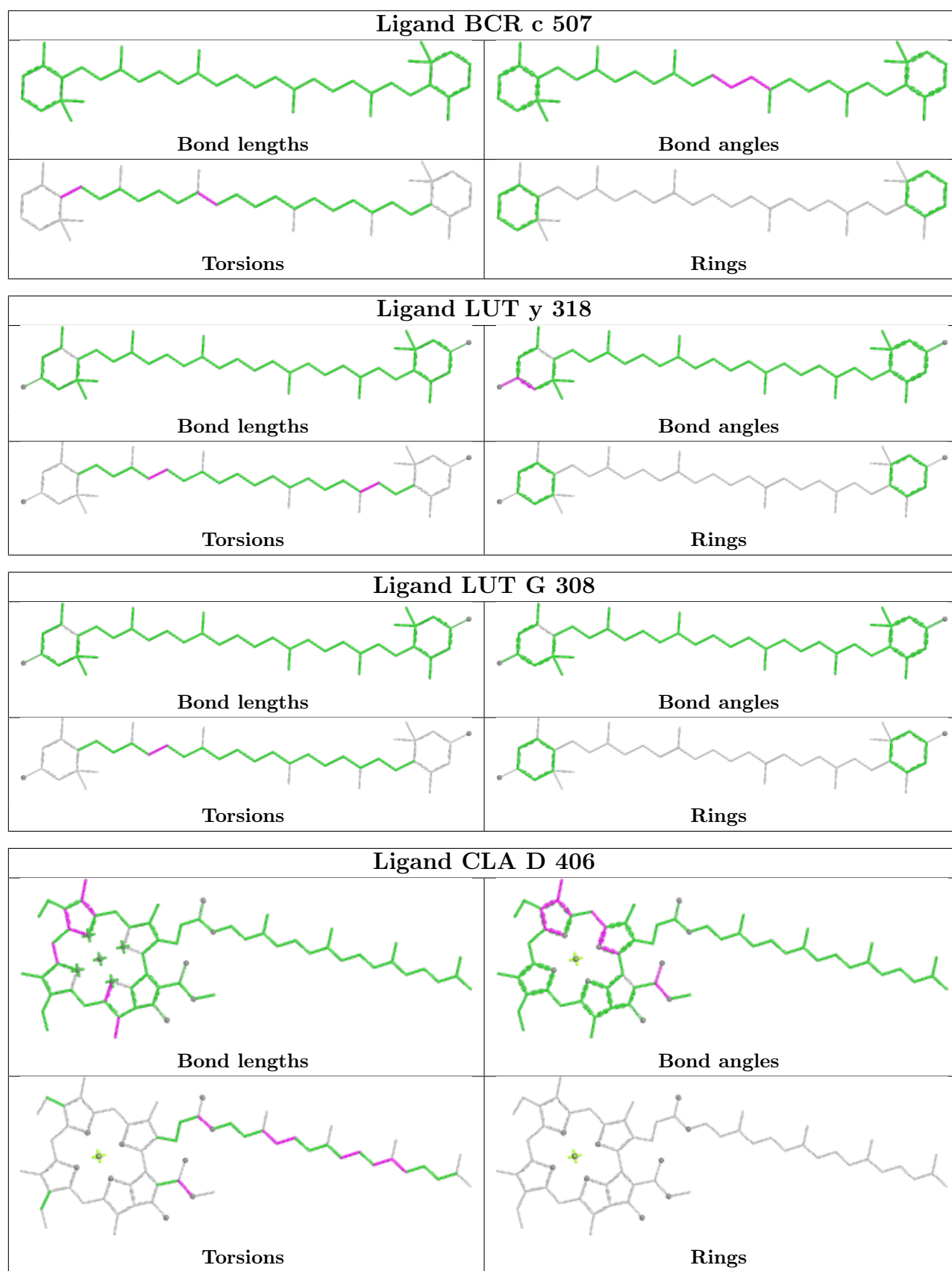


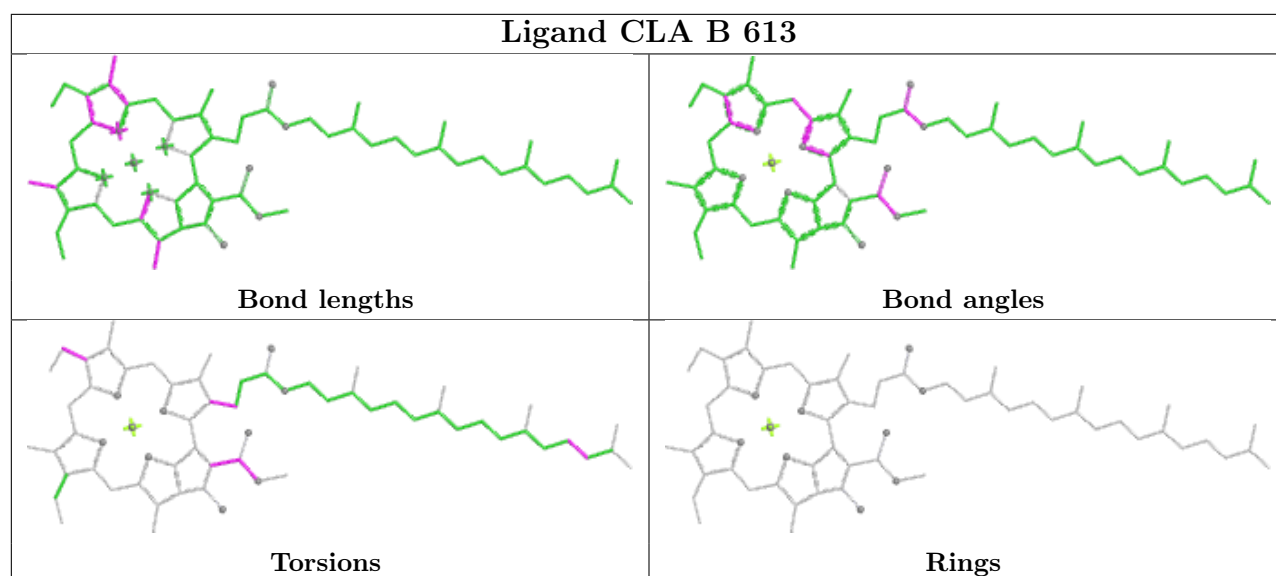
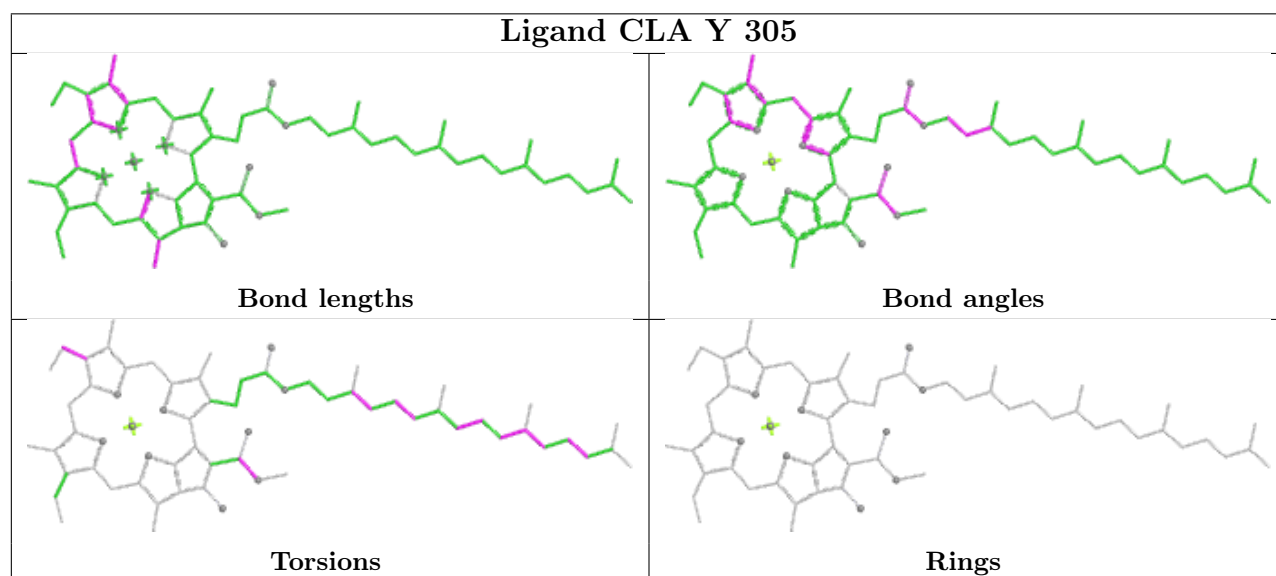
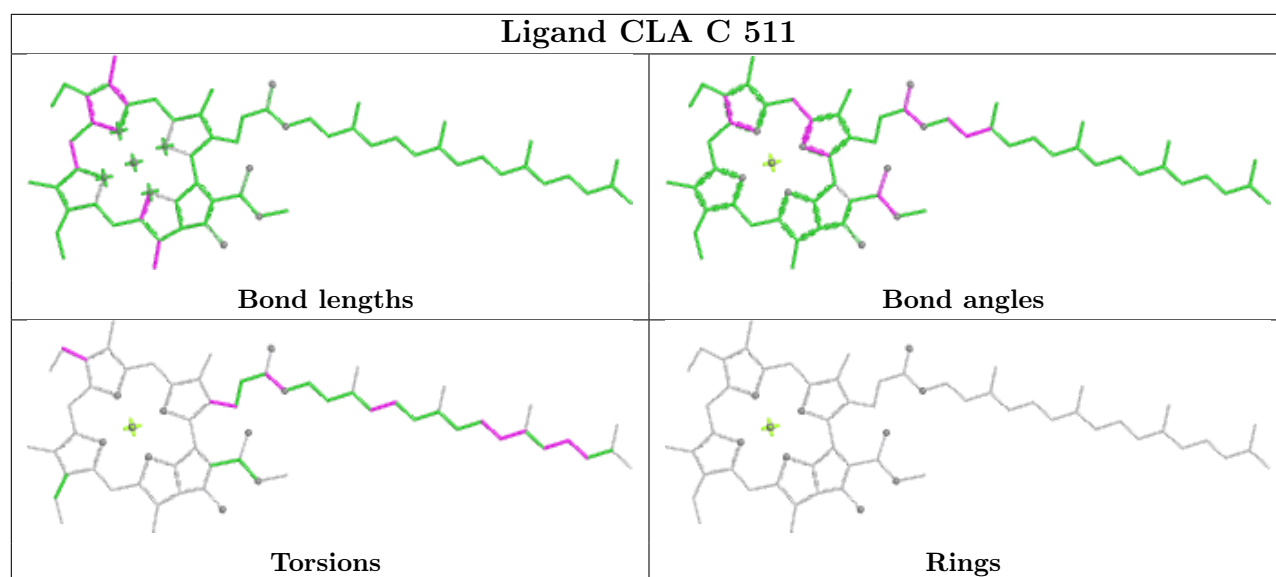


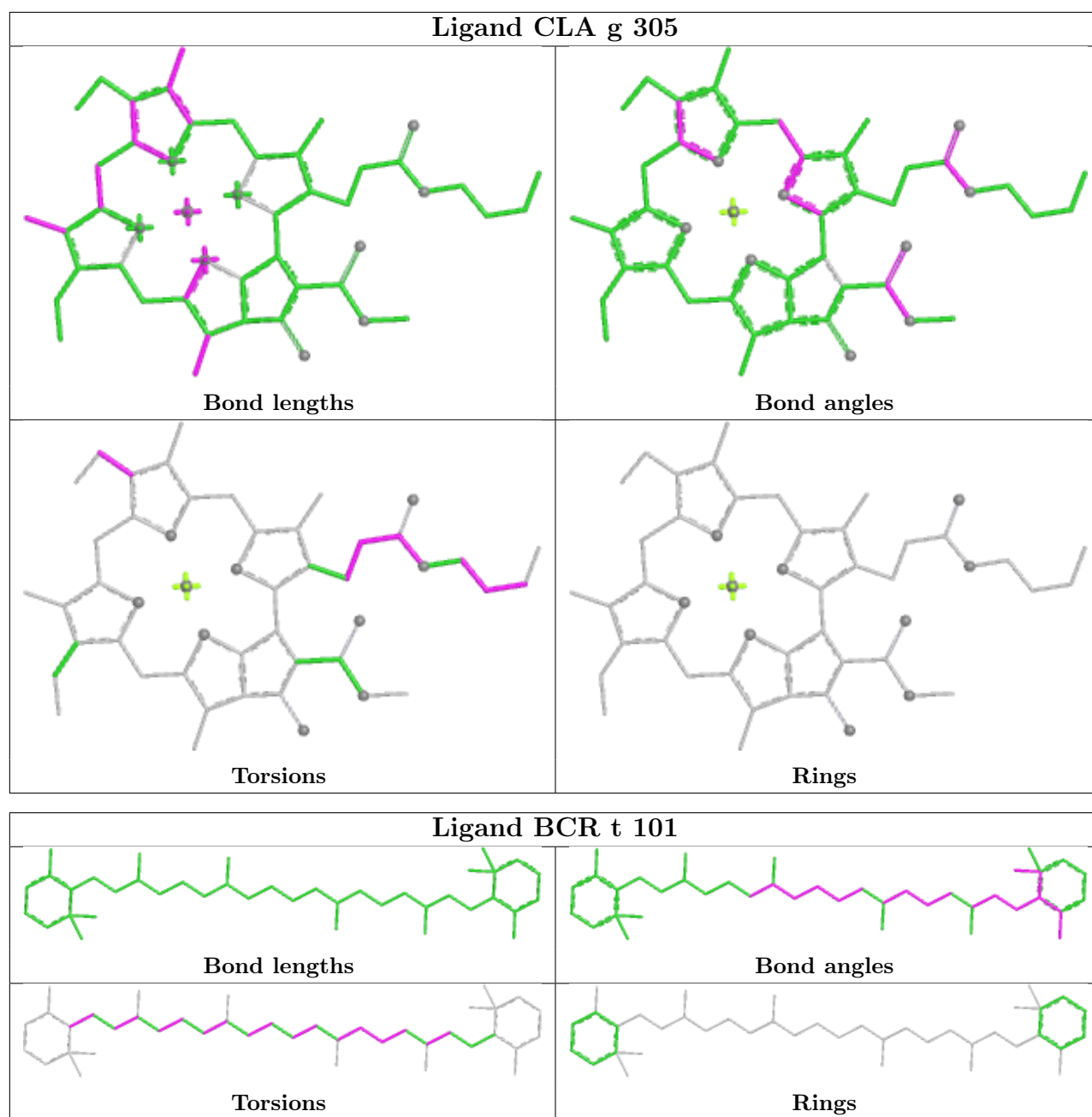


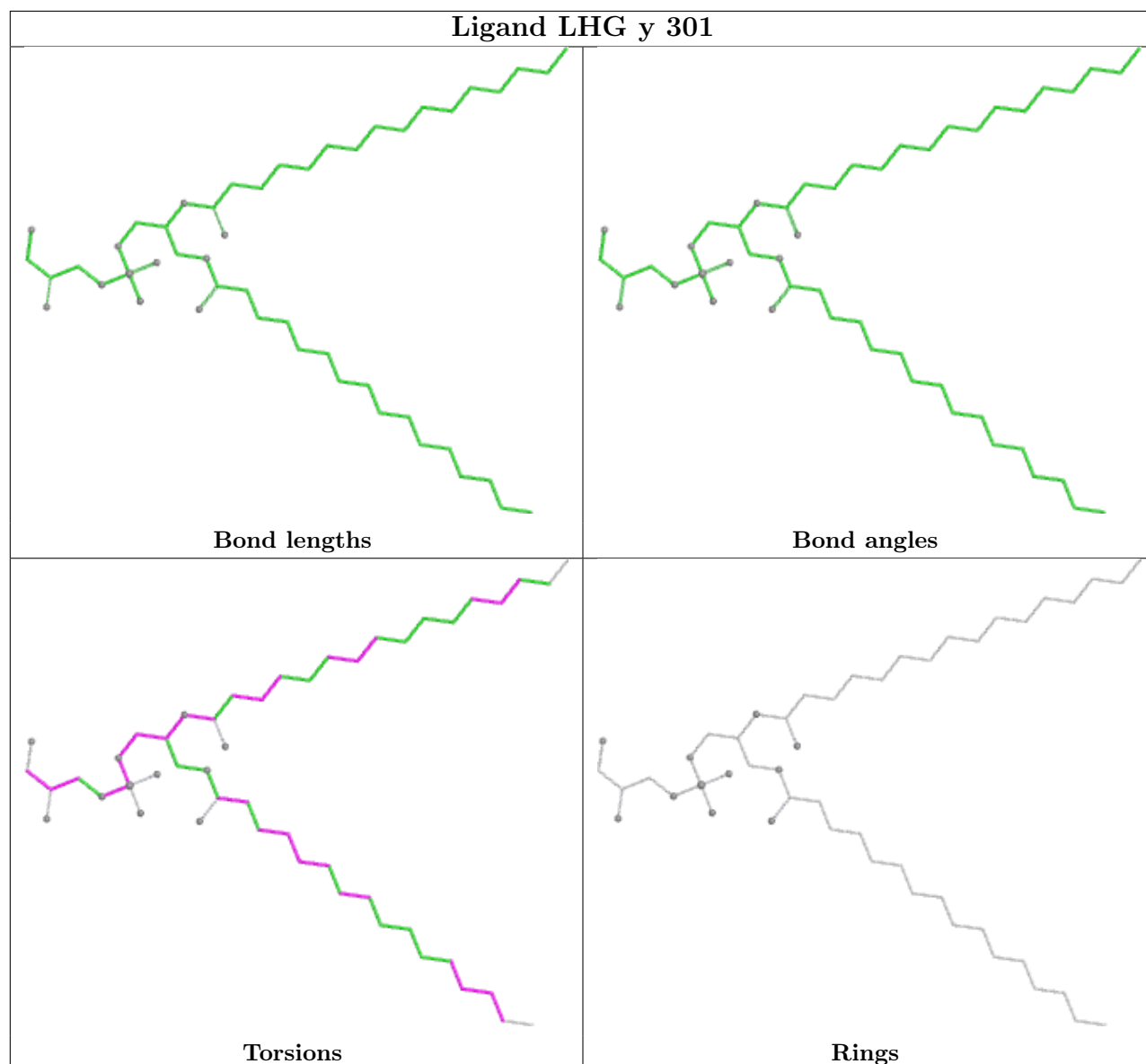
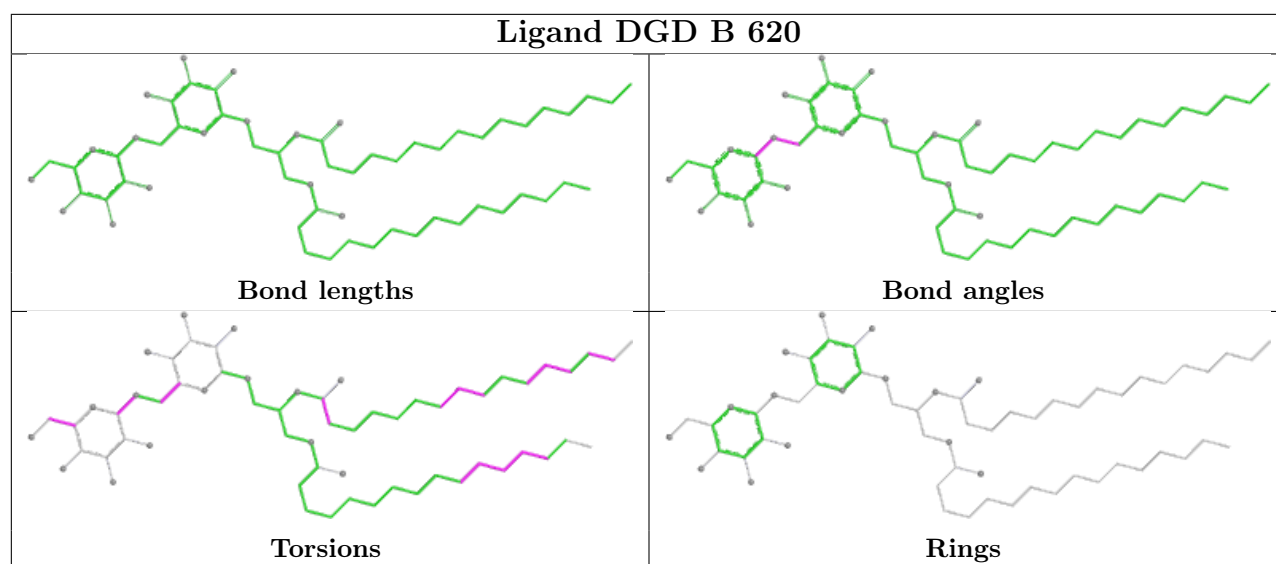


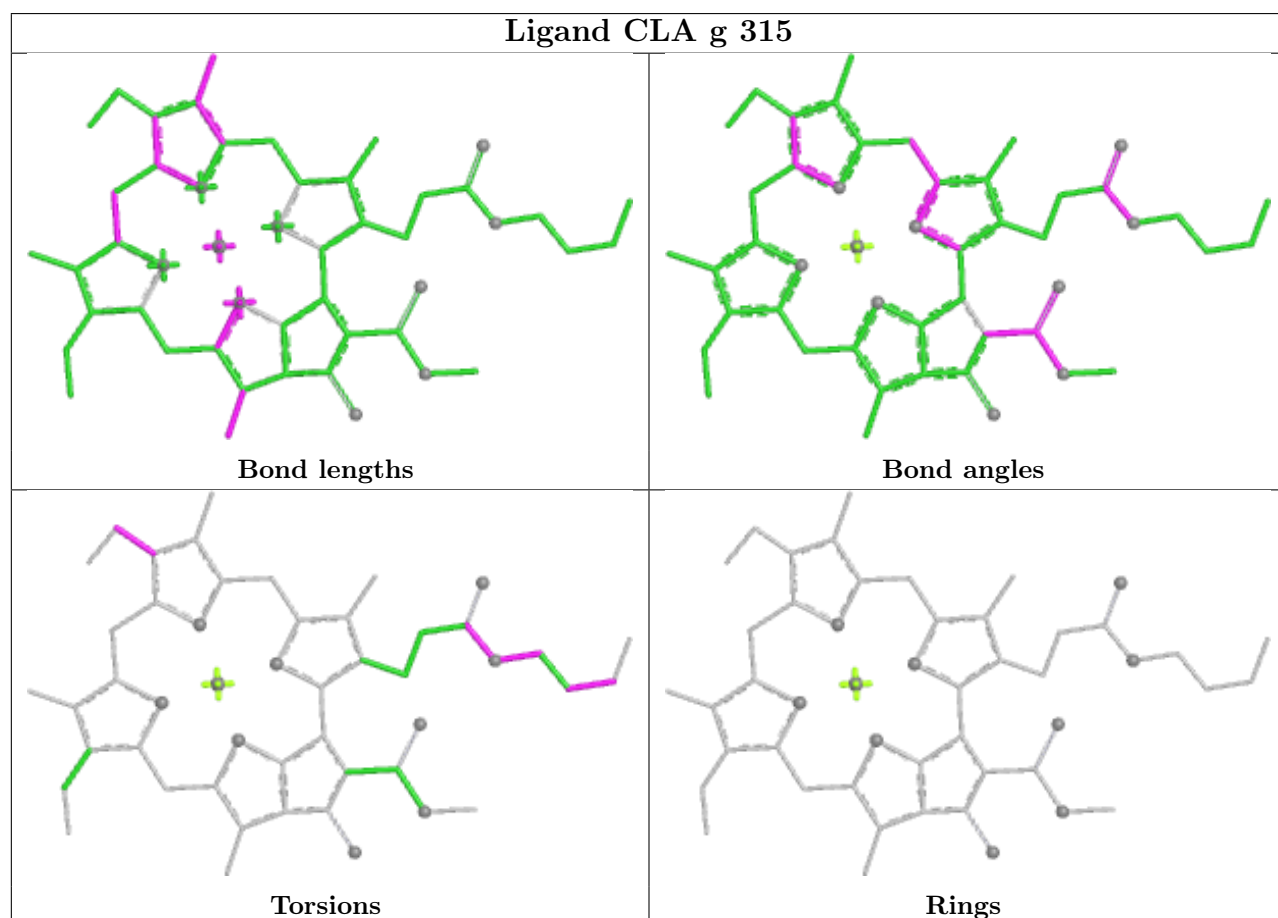
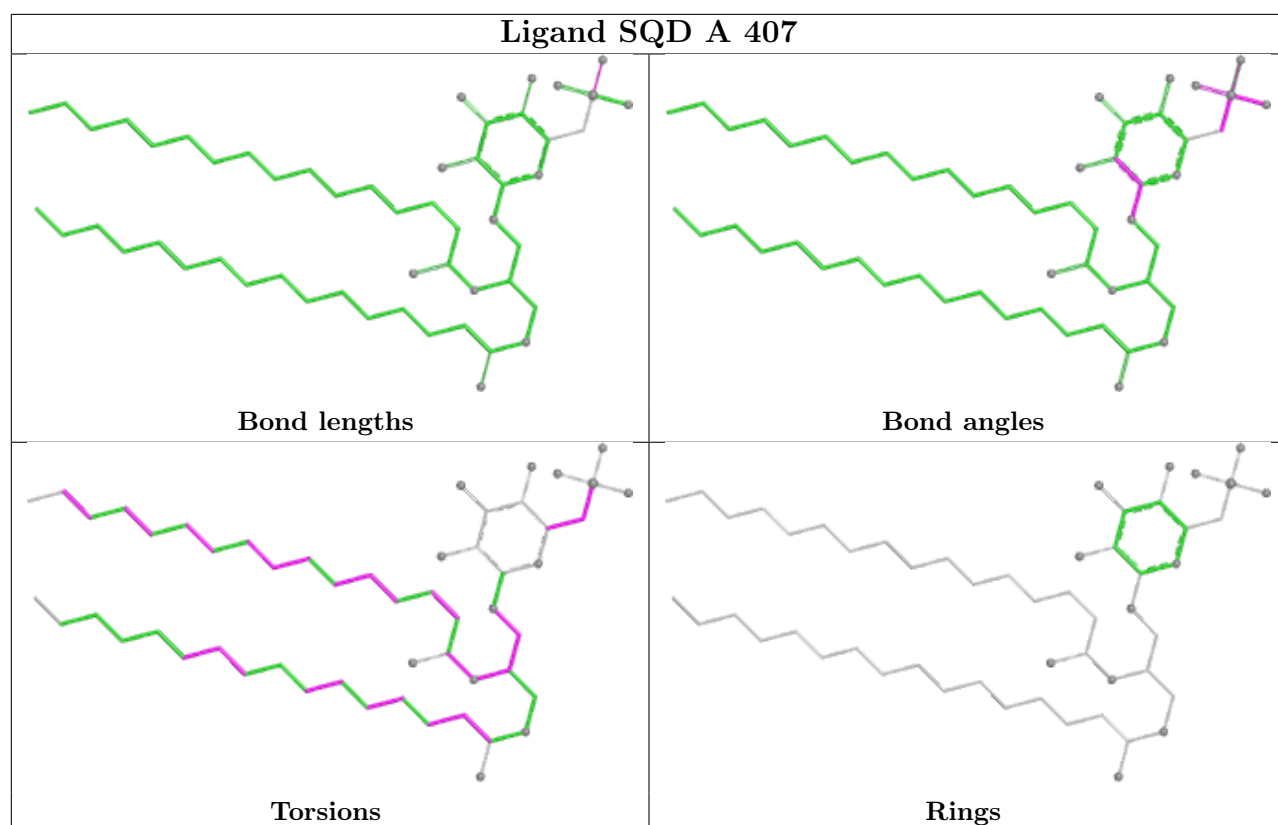


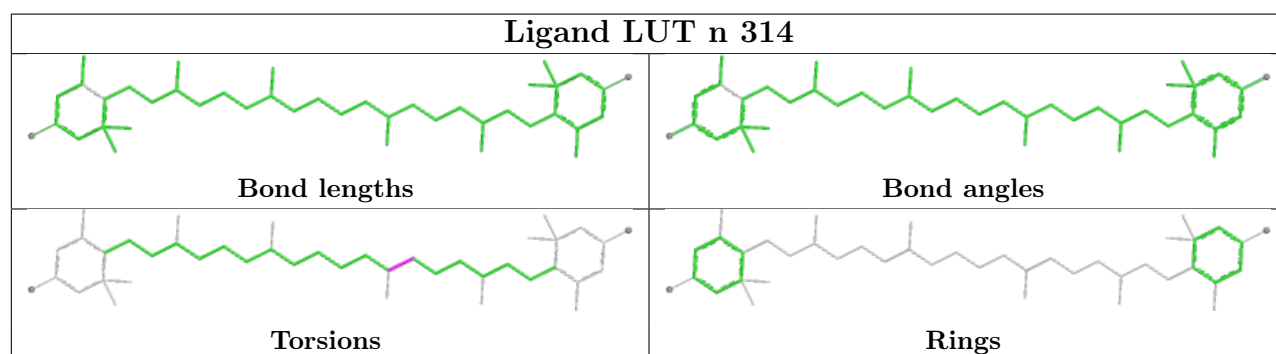
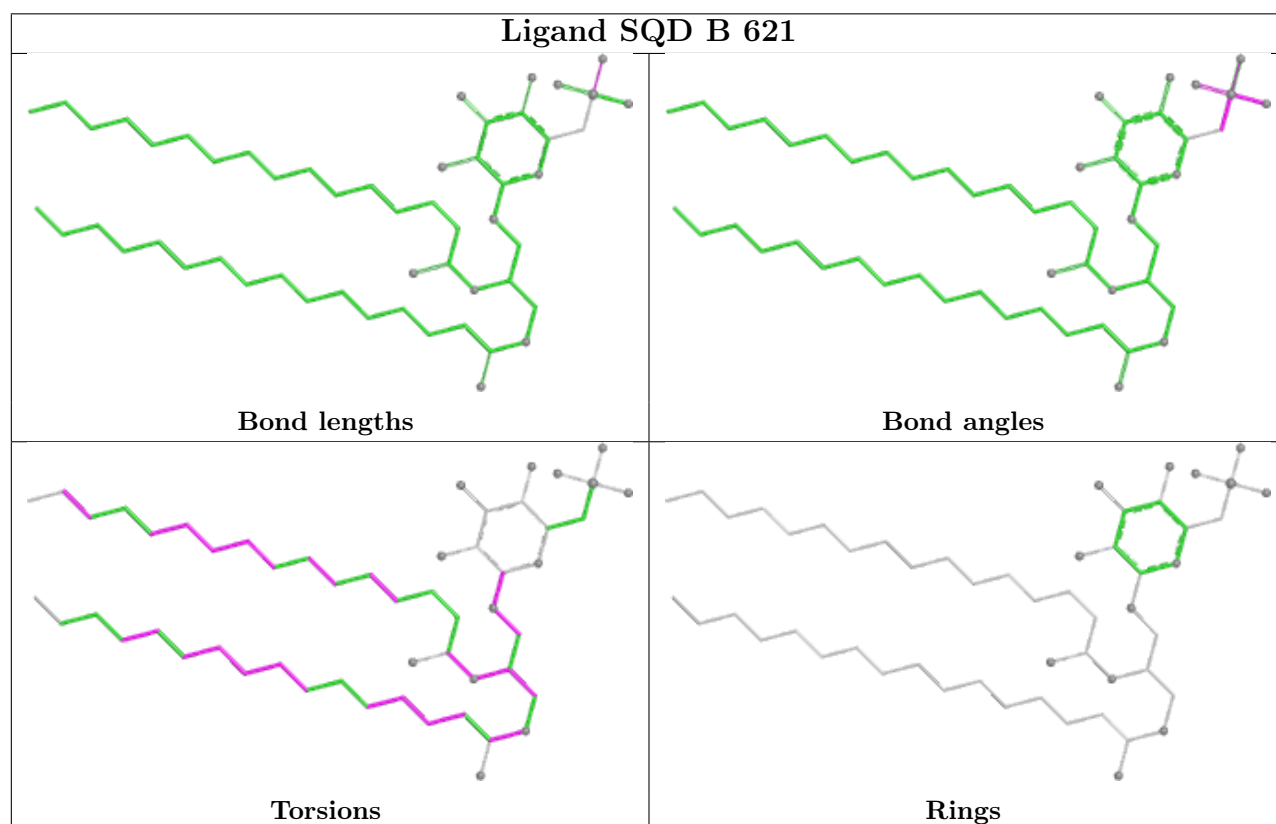
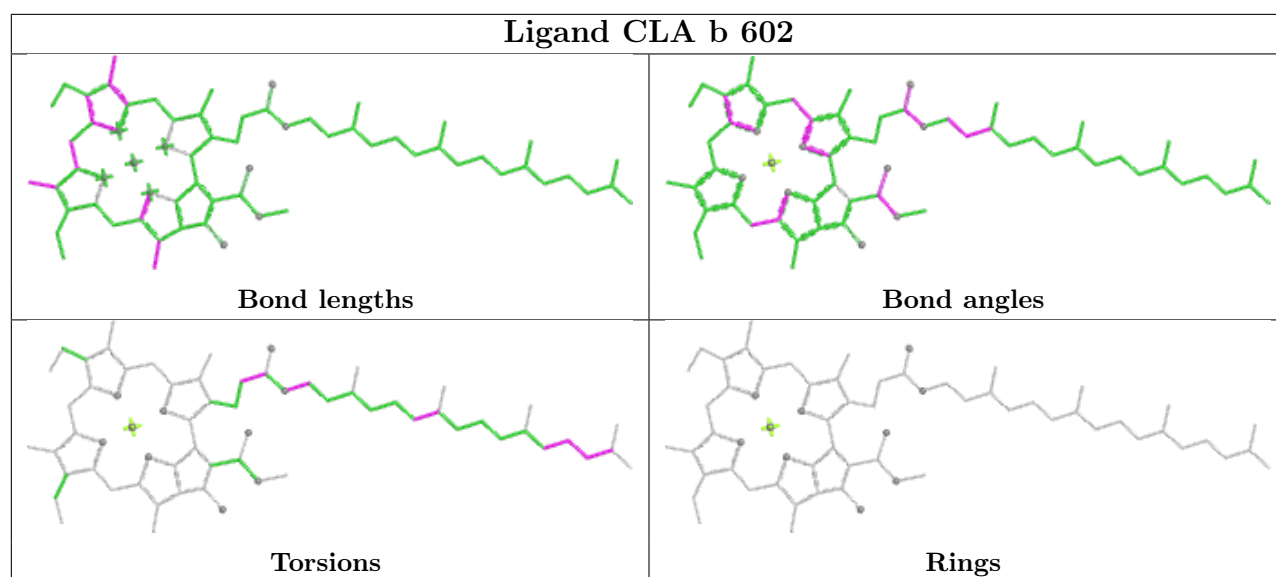




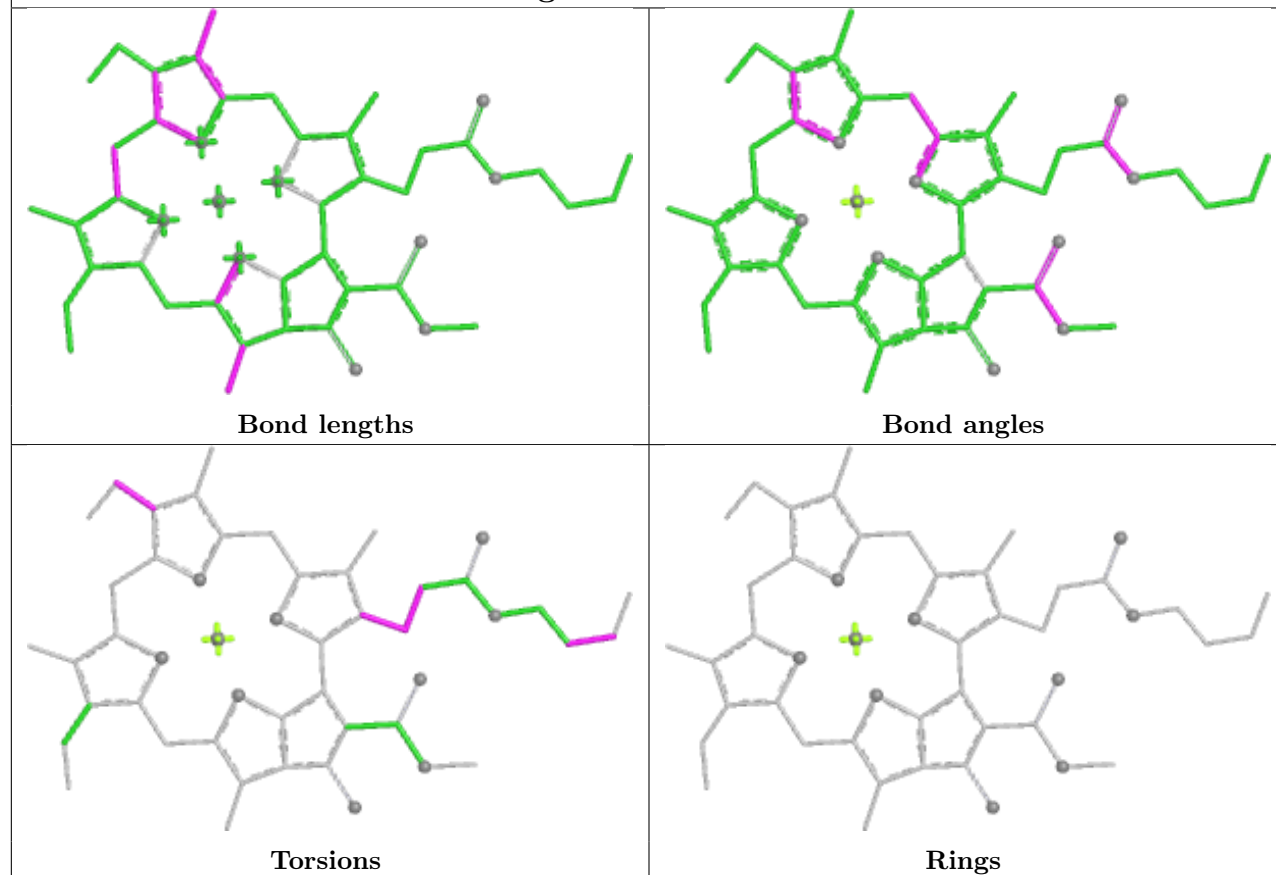




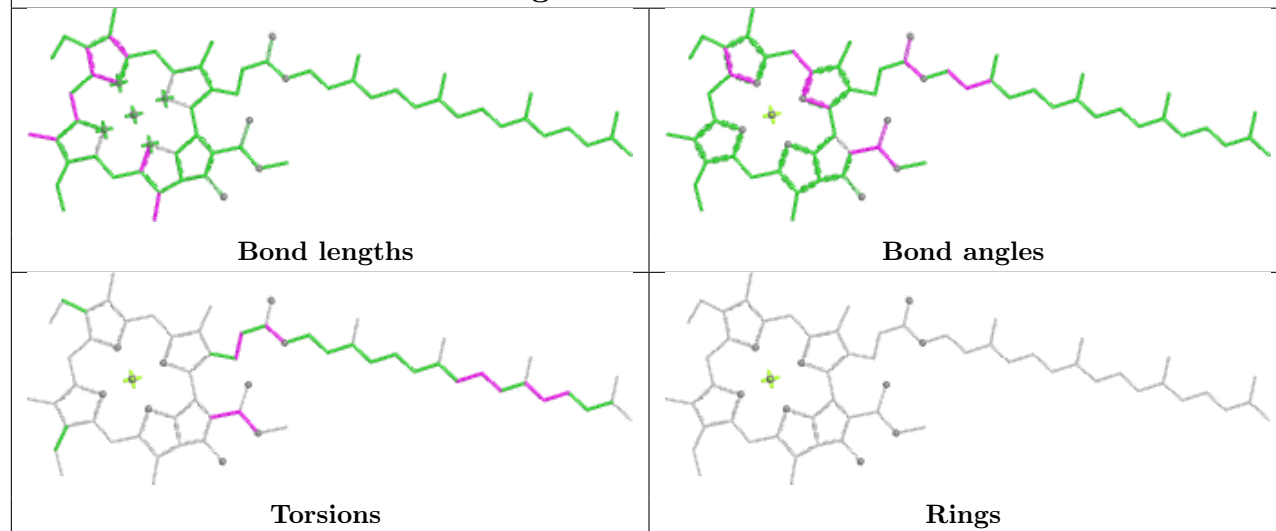


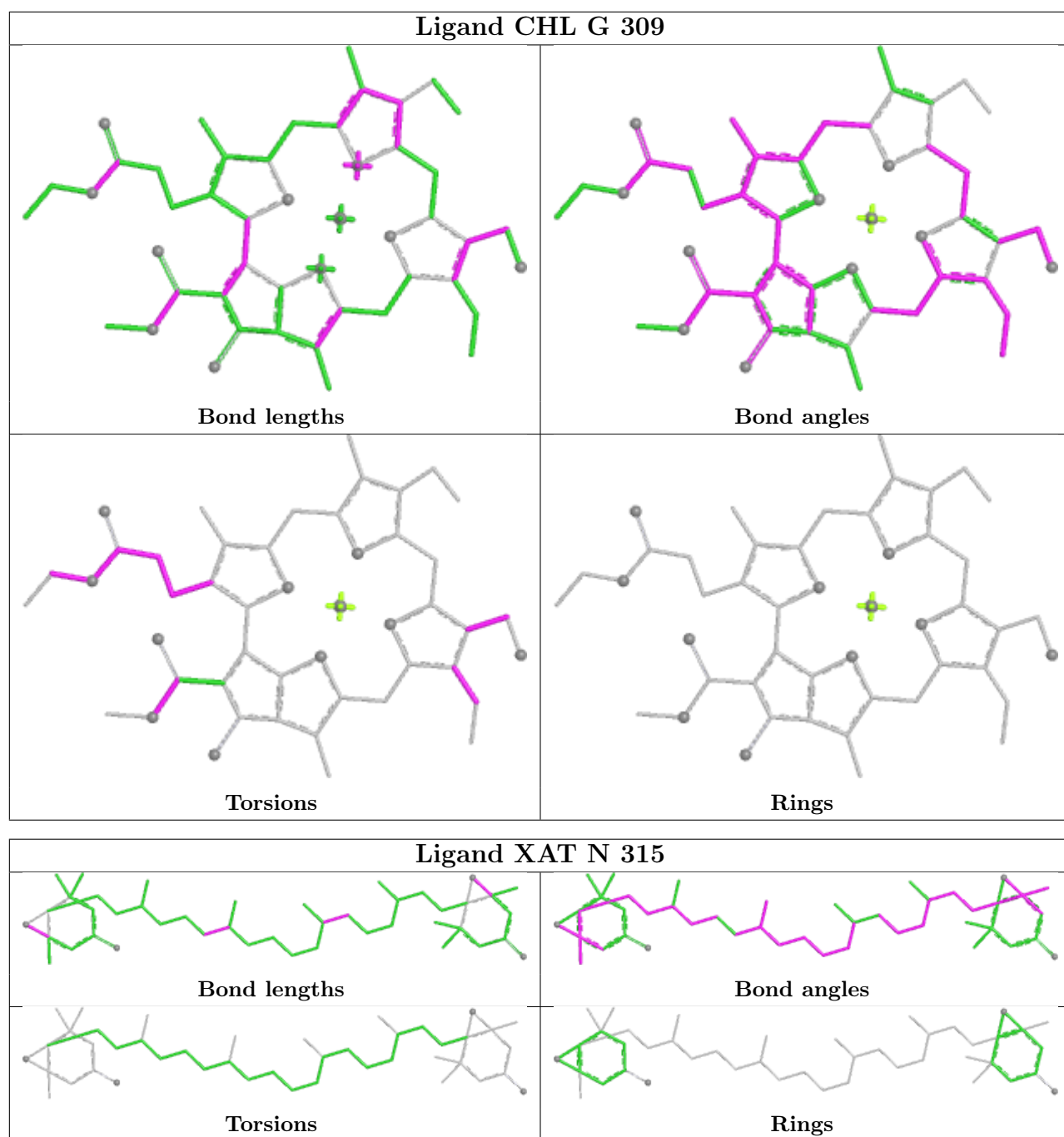


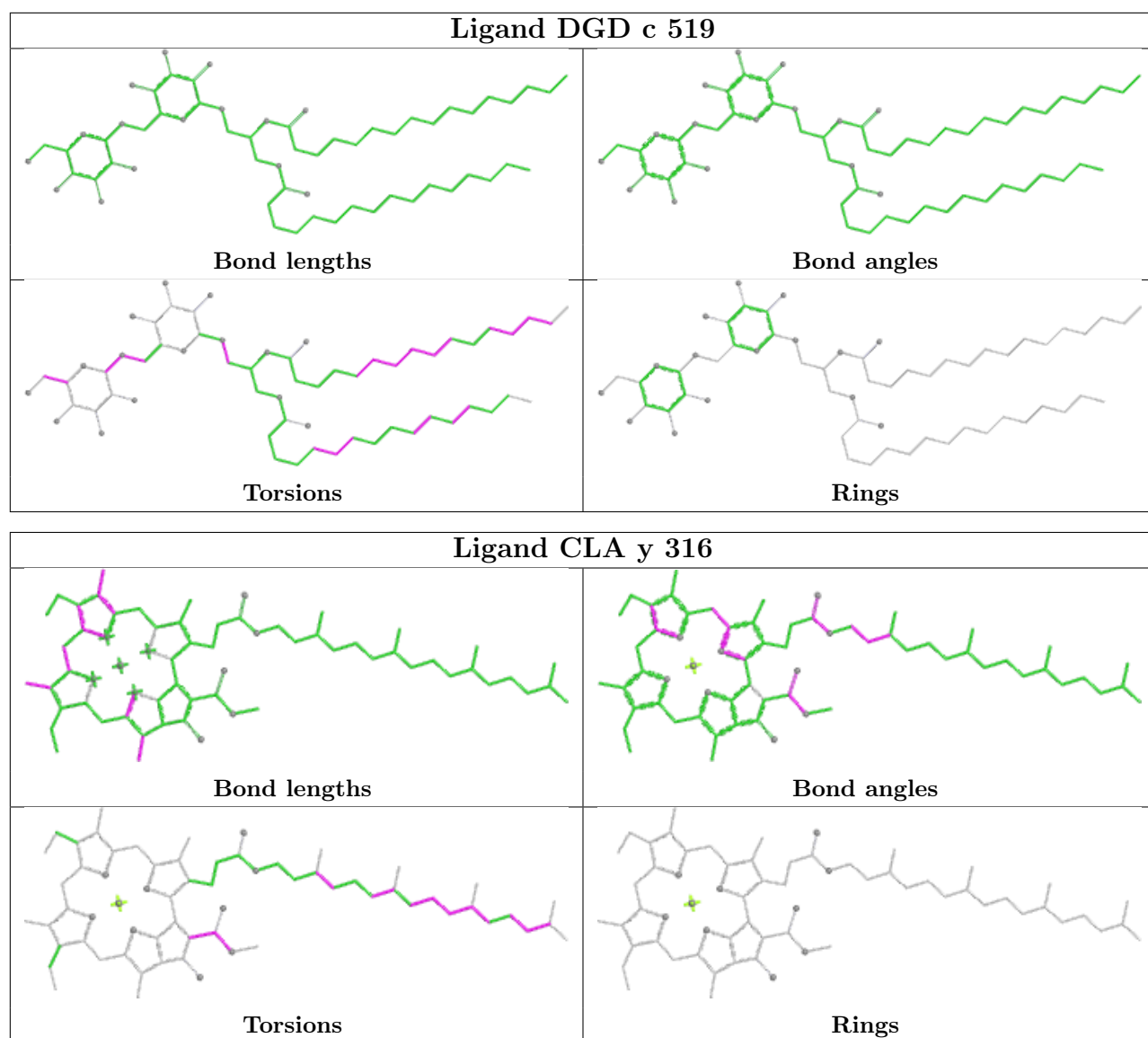
Ligand CLA s 315

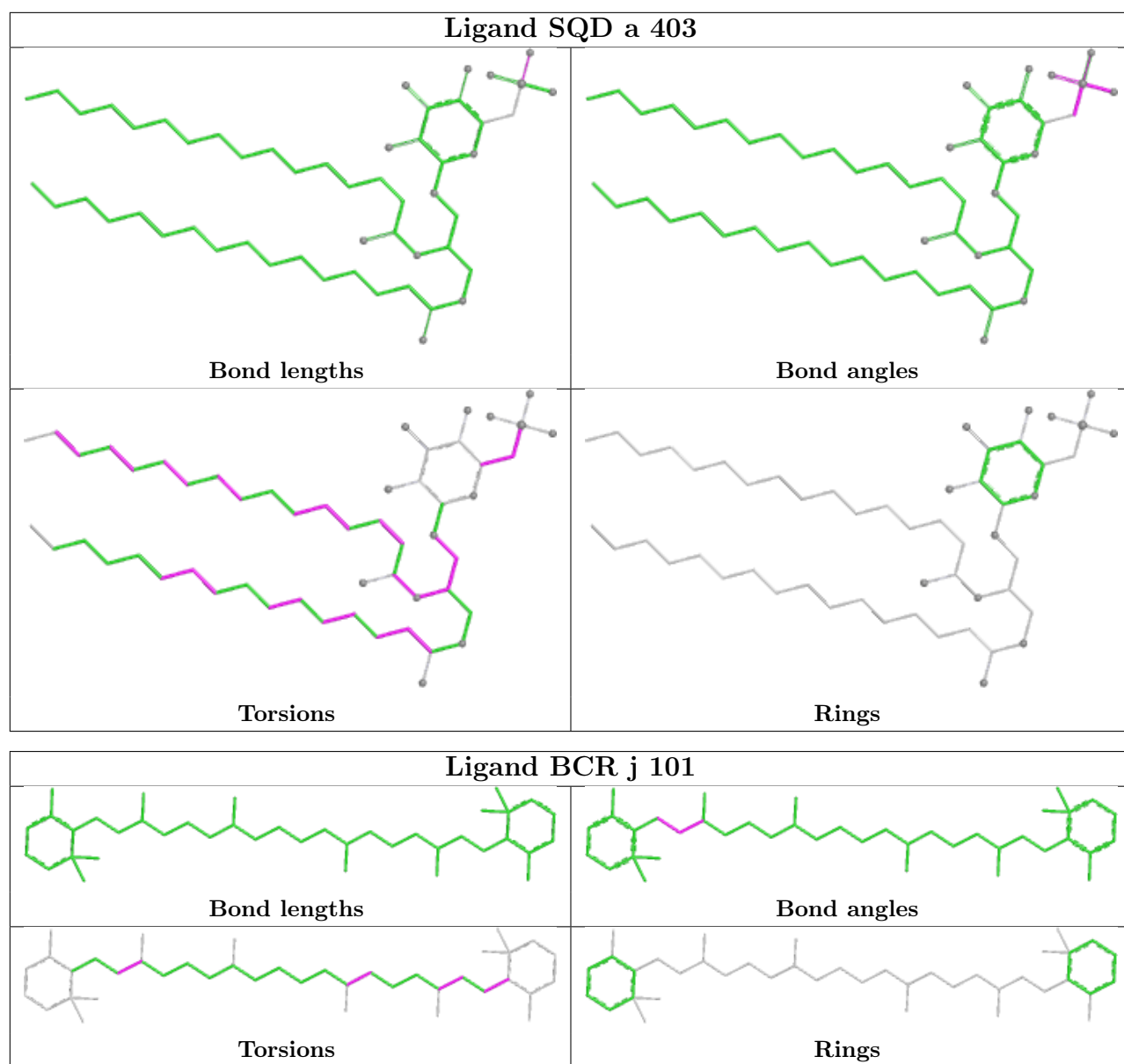


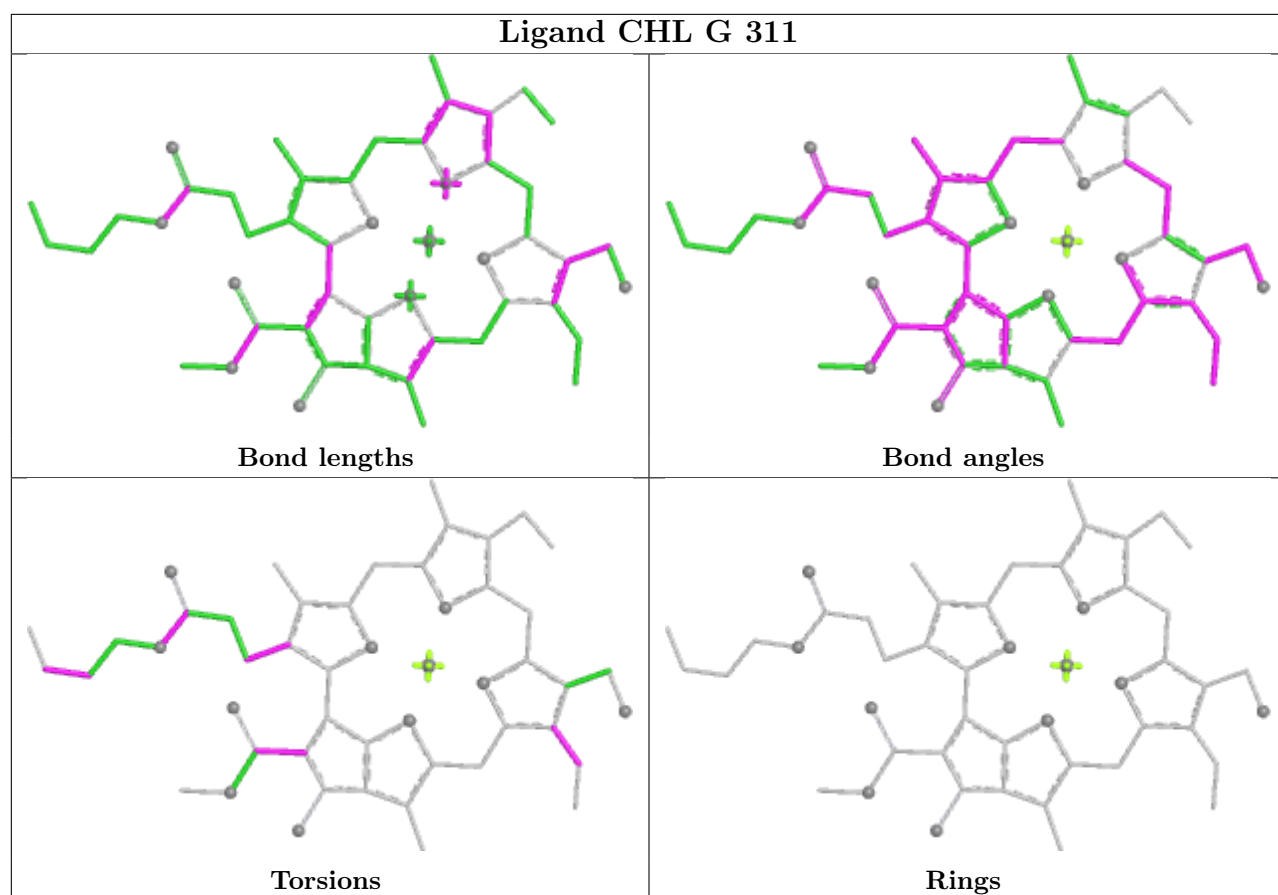
Ligand CLA R 313



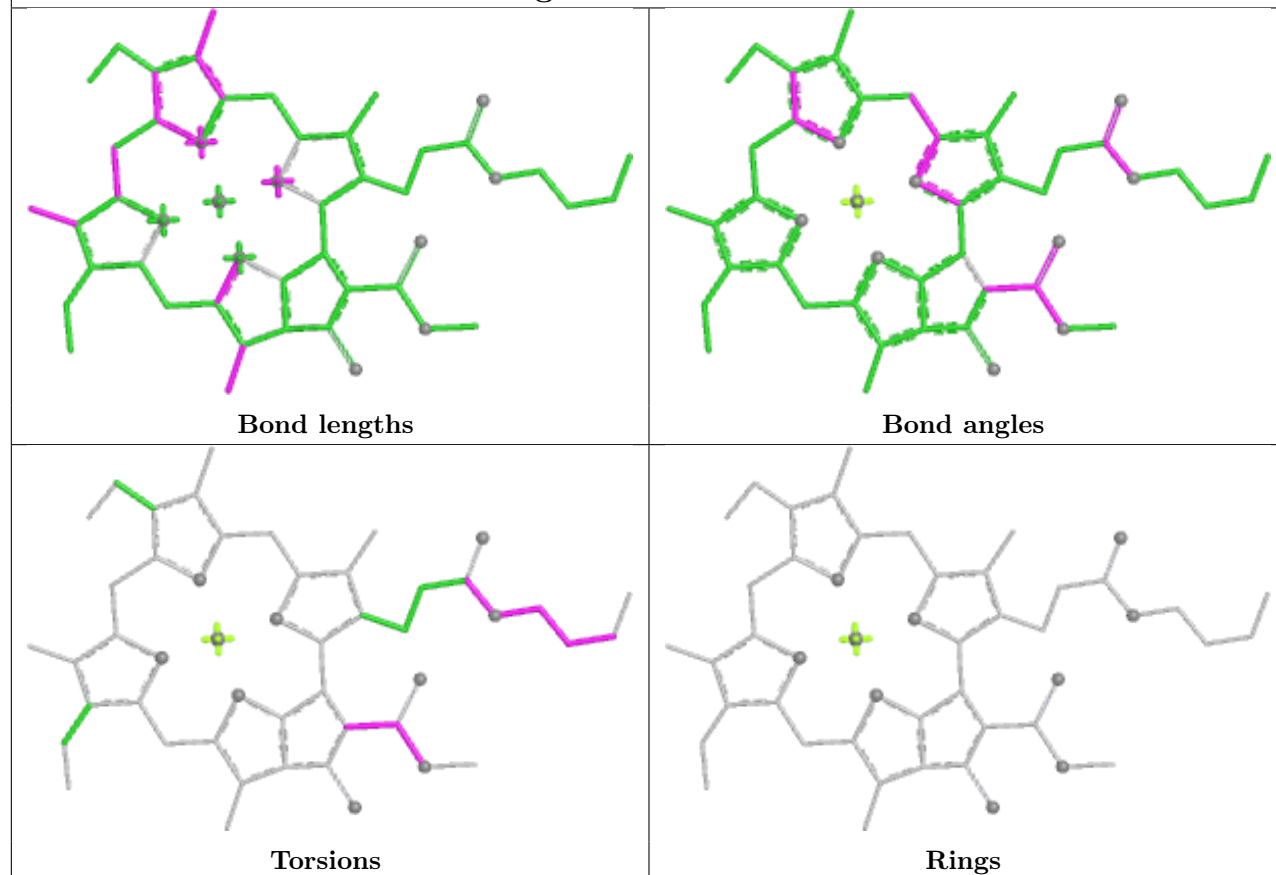




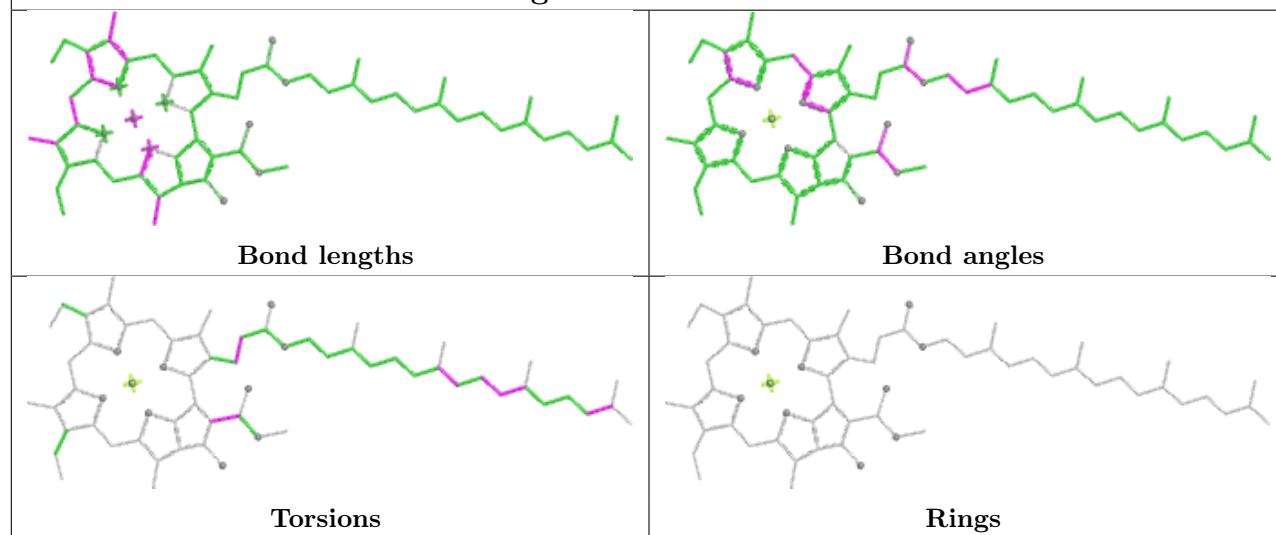


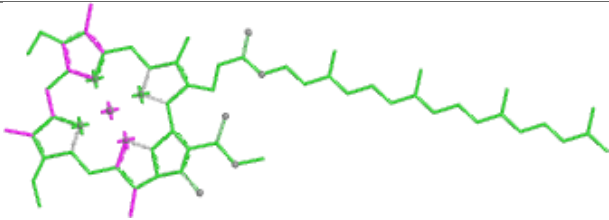
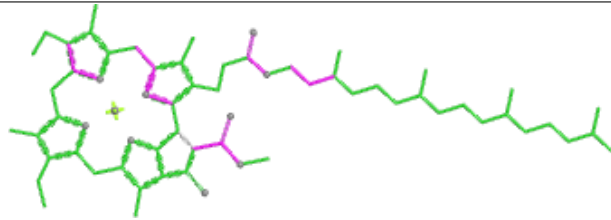
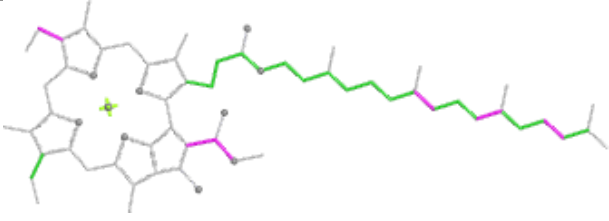
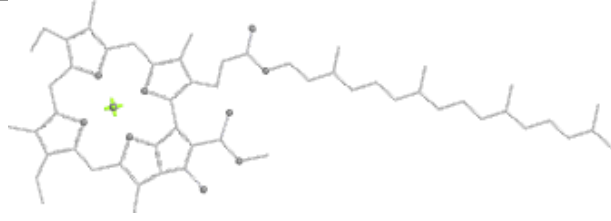


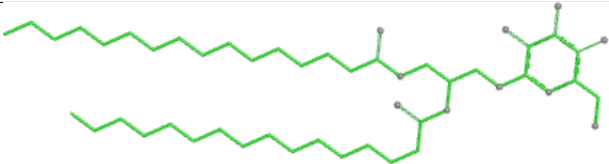
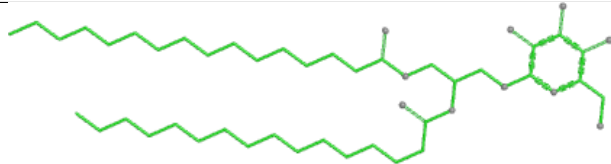
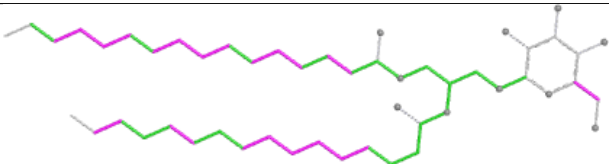
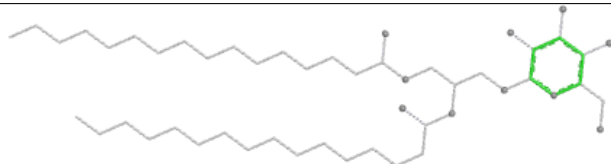
Ligand CLA n 304



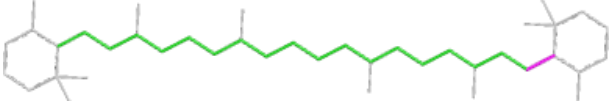
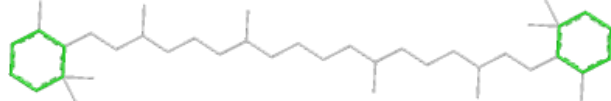


Ligand CLA G 314

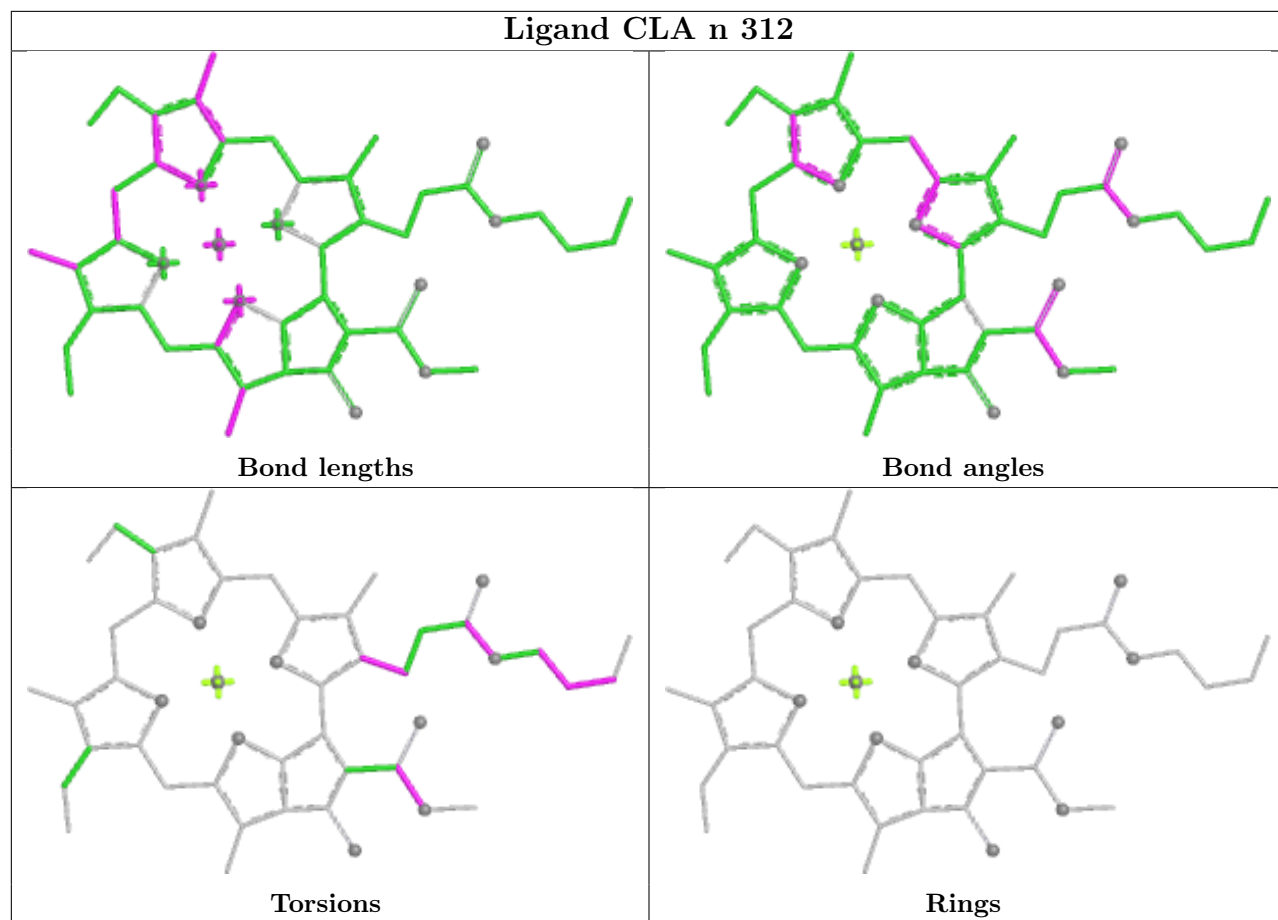


Ligand CLA B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

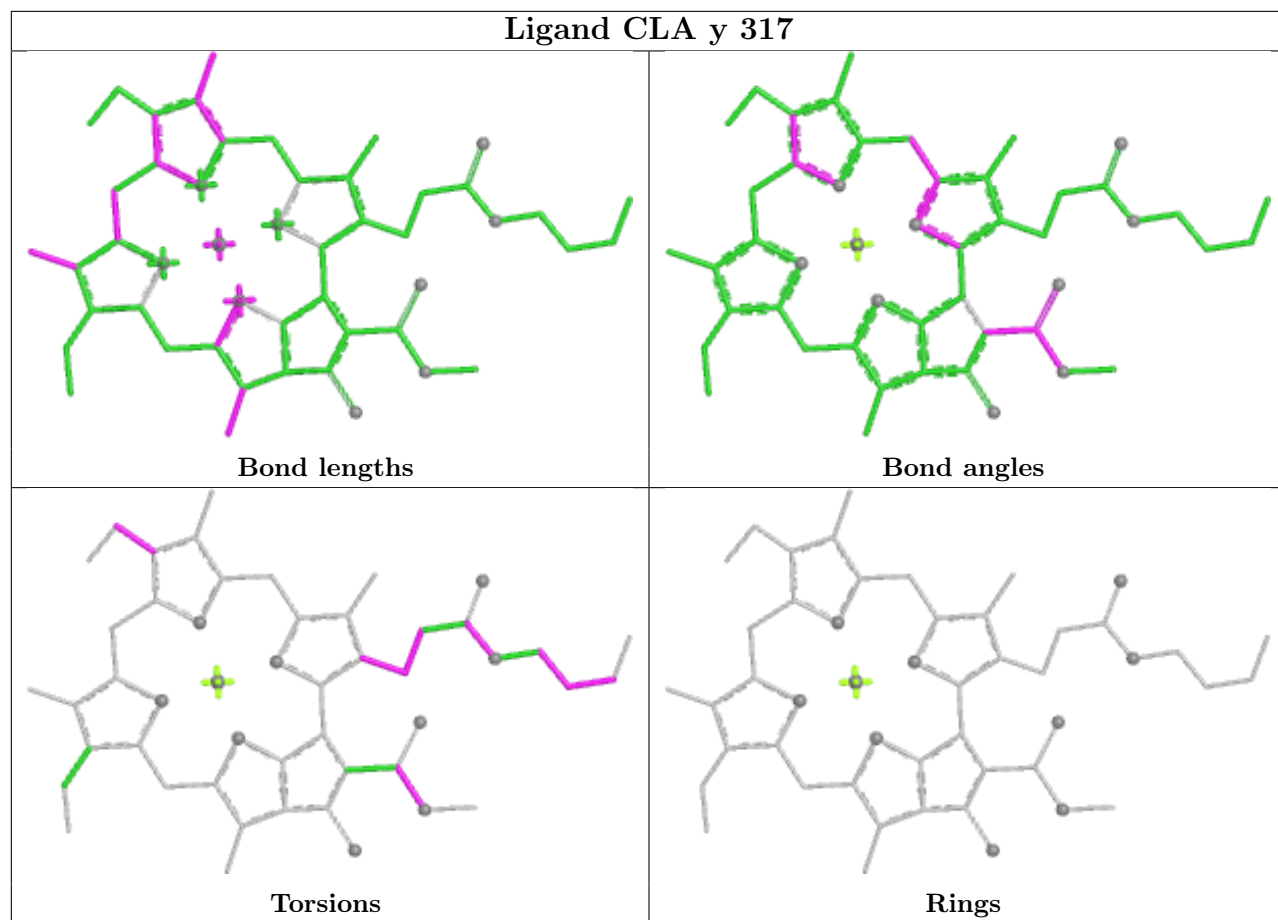
Ligand LMG B 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

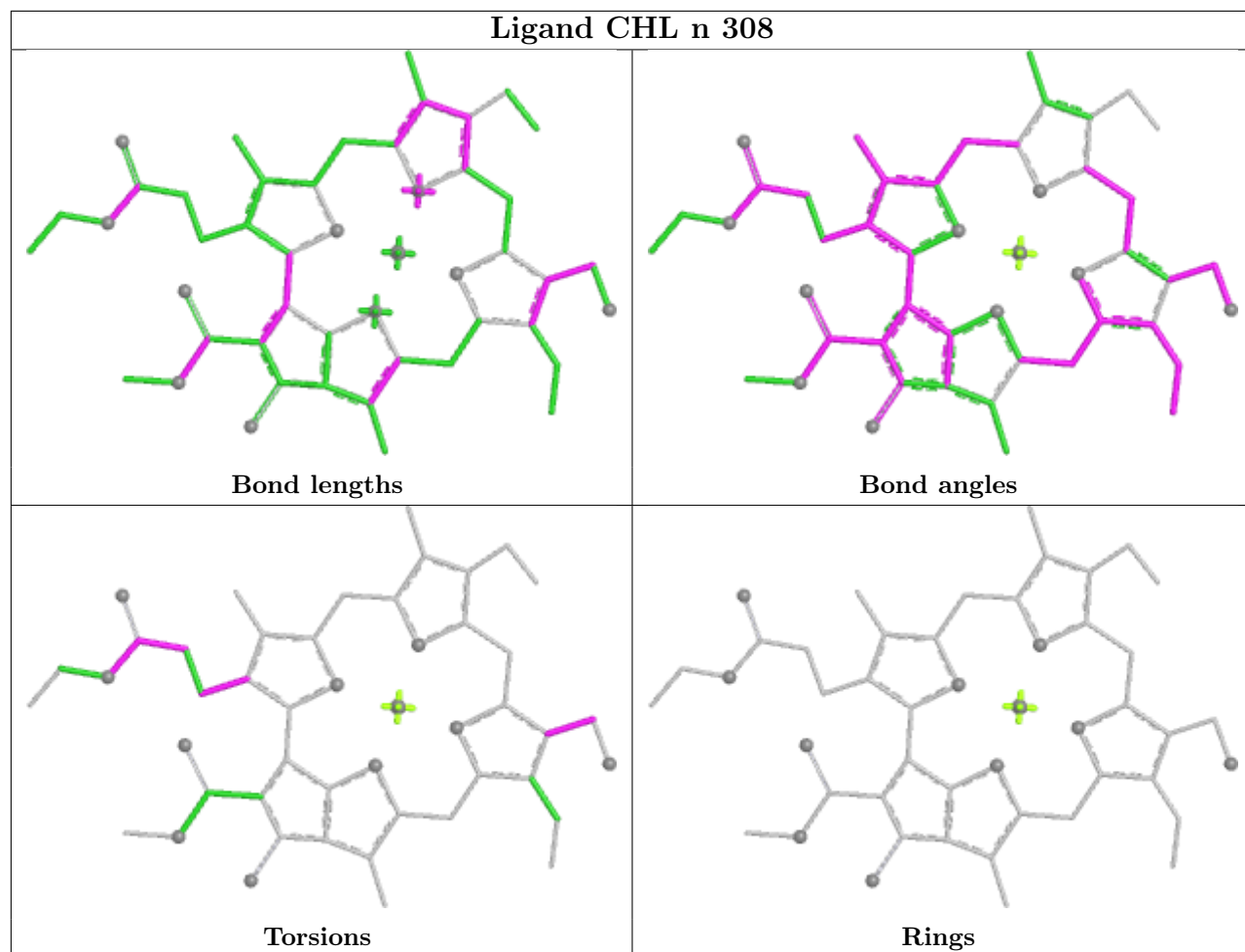
Ligand CLA n 312



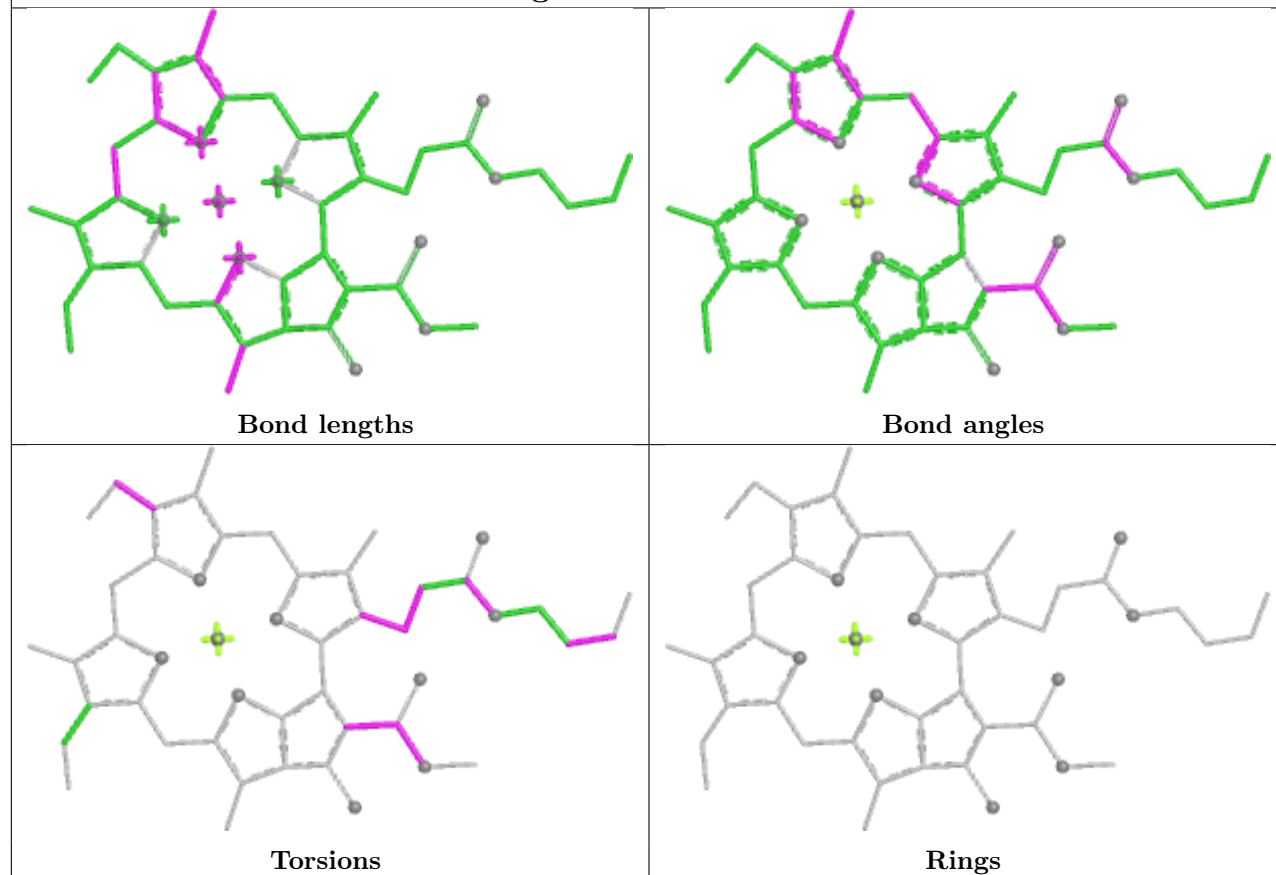
Ligand CLA y 317



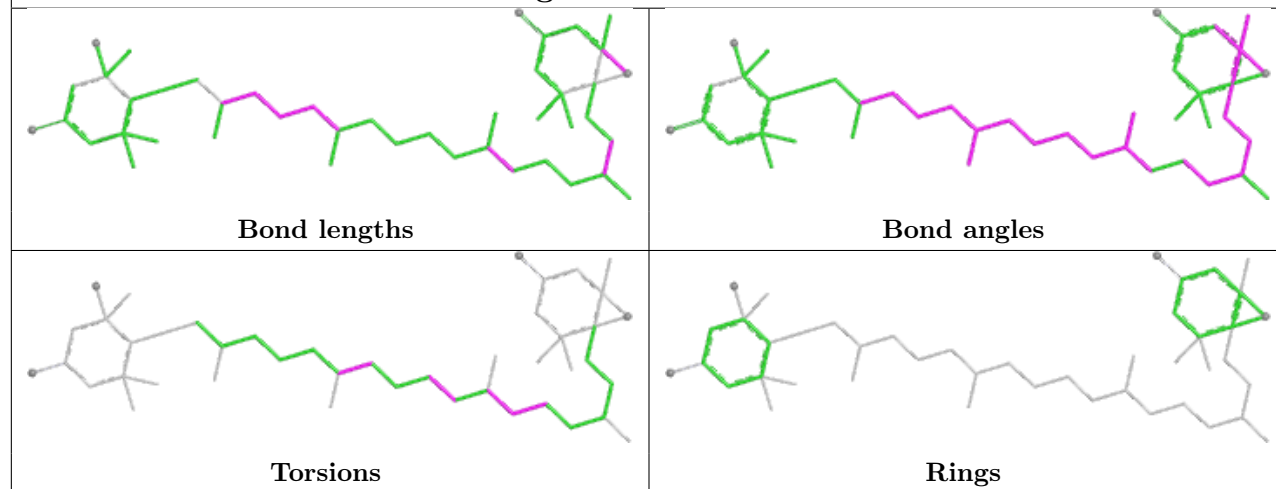
Ligand CHL n 308

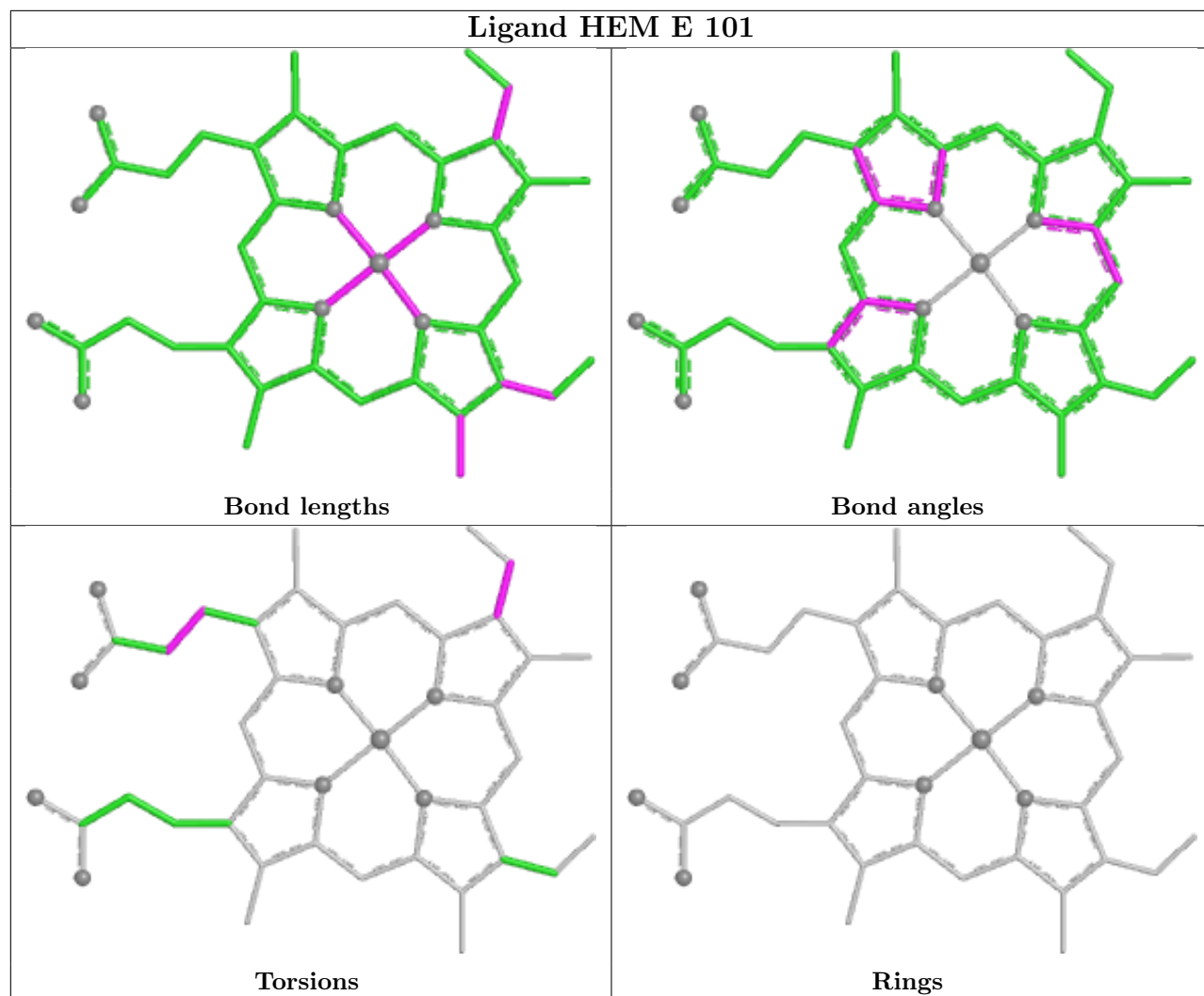


Ligand CLA R 308

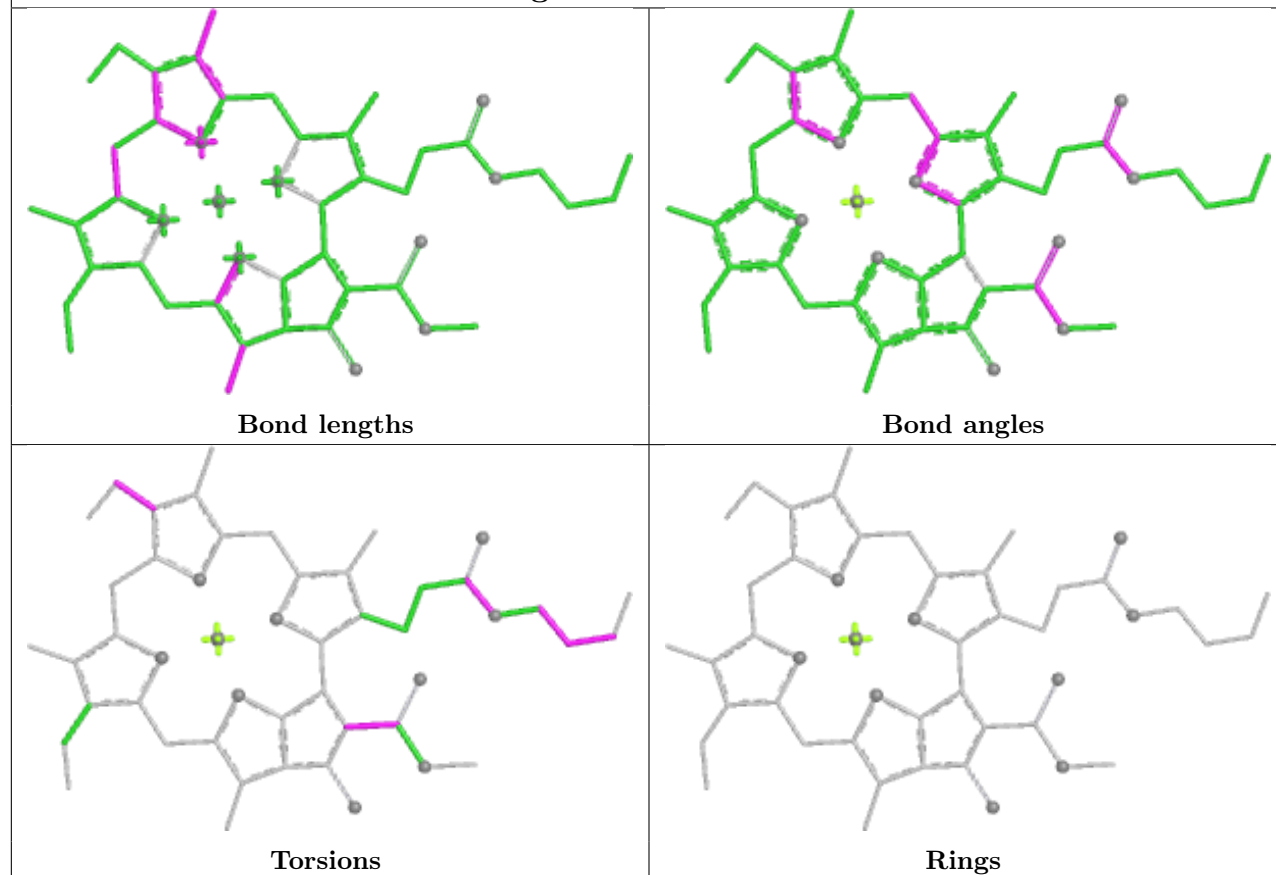


Ligand NEX s 302

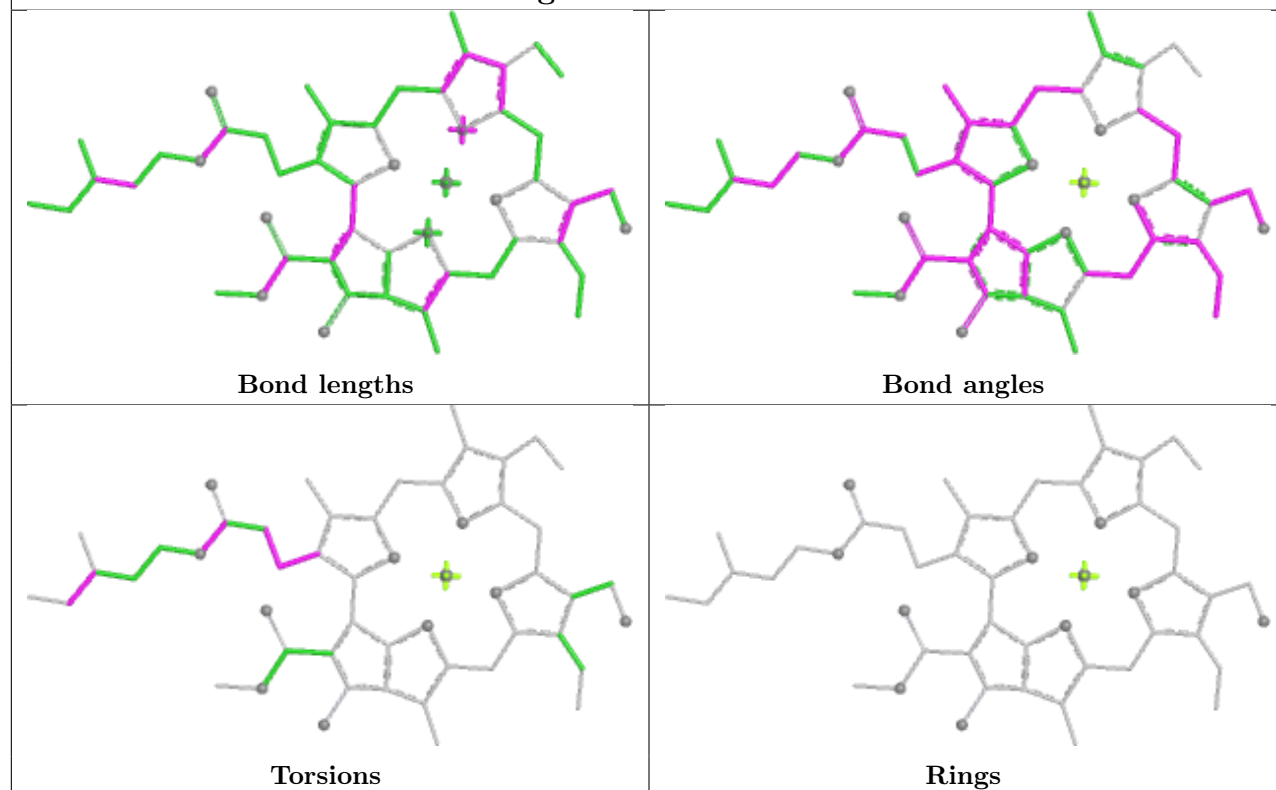


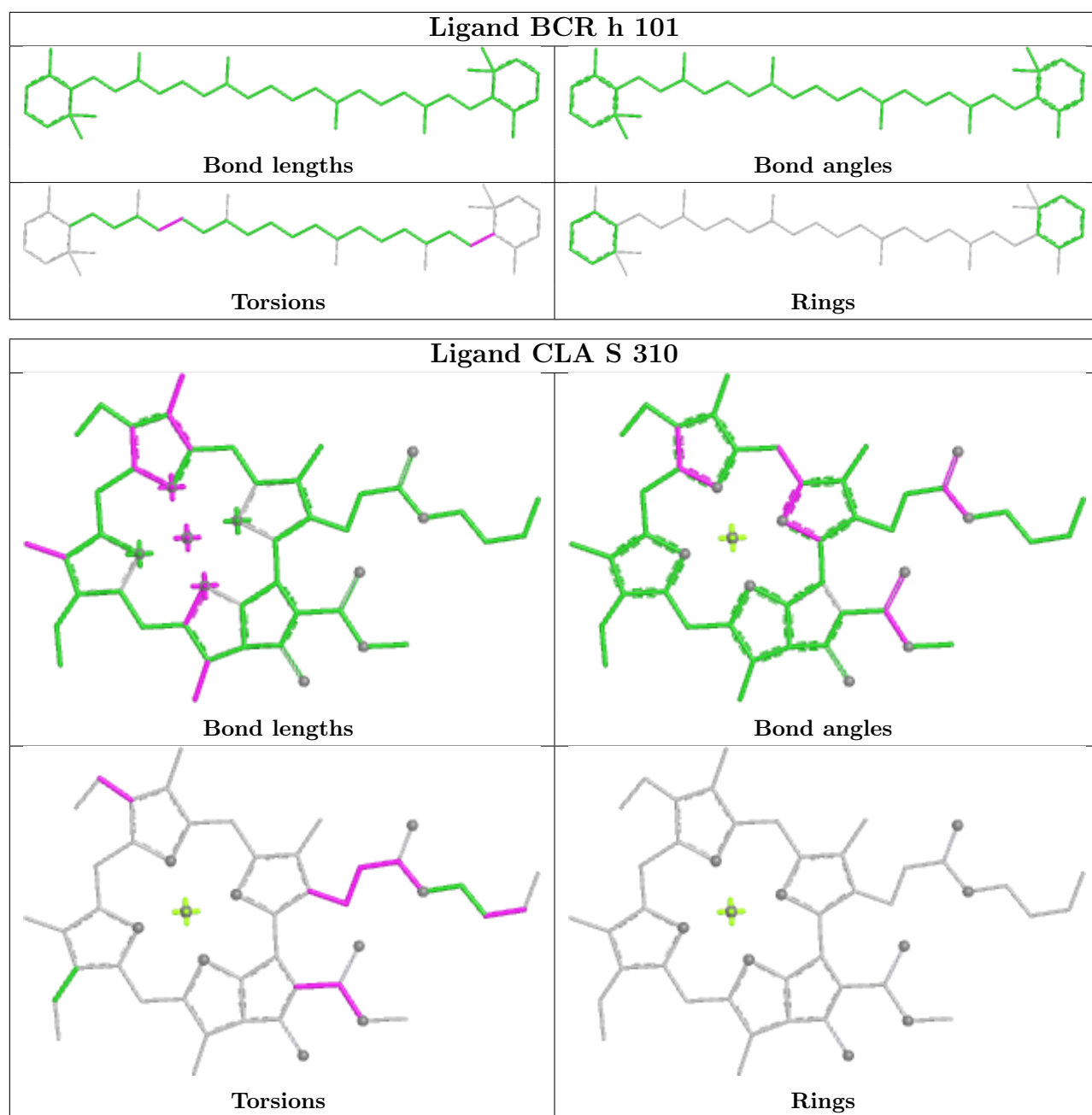


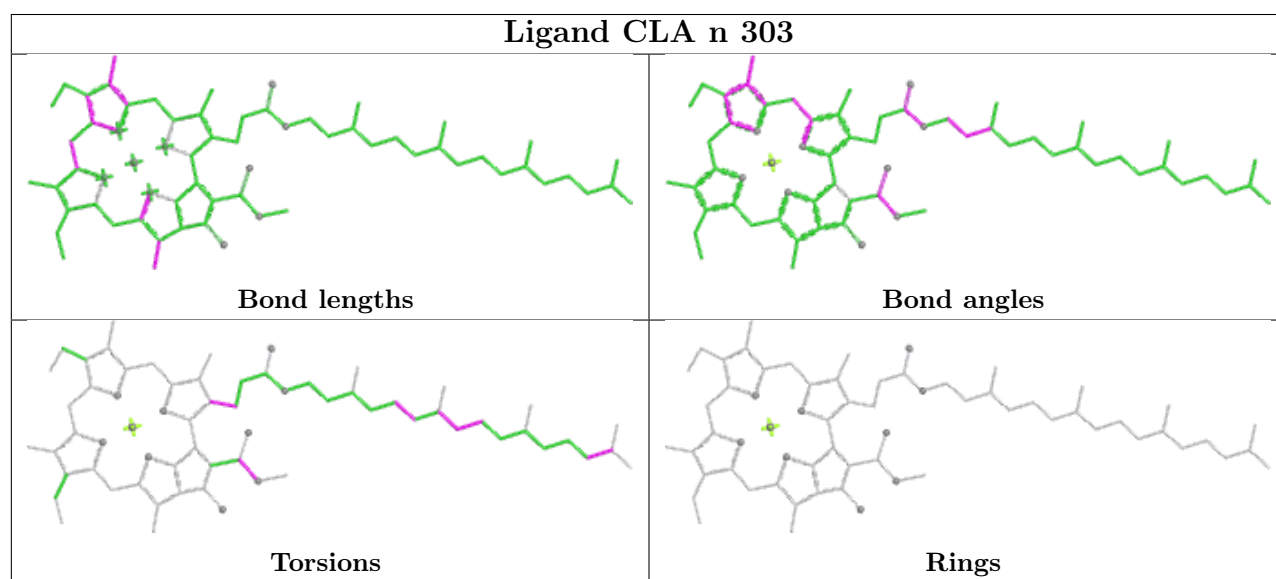
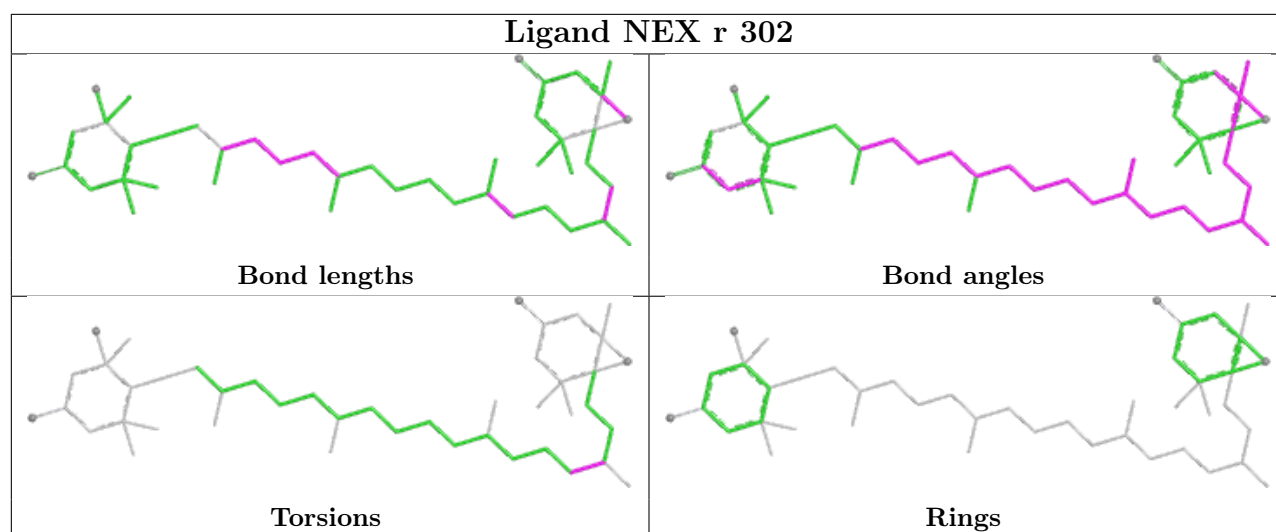
Ligand CLA G 304

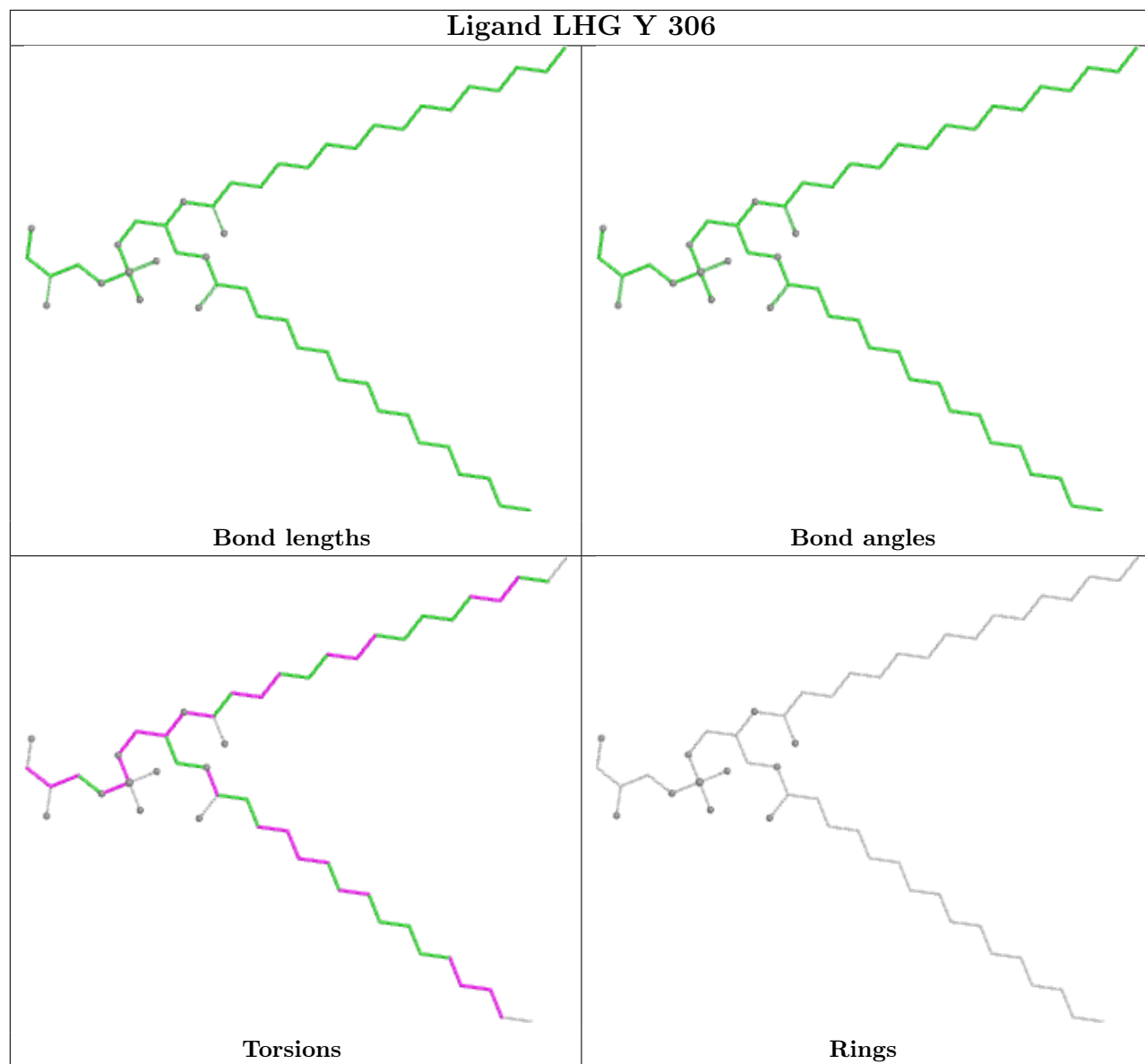


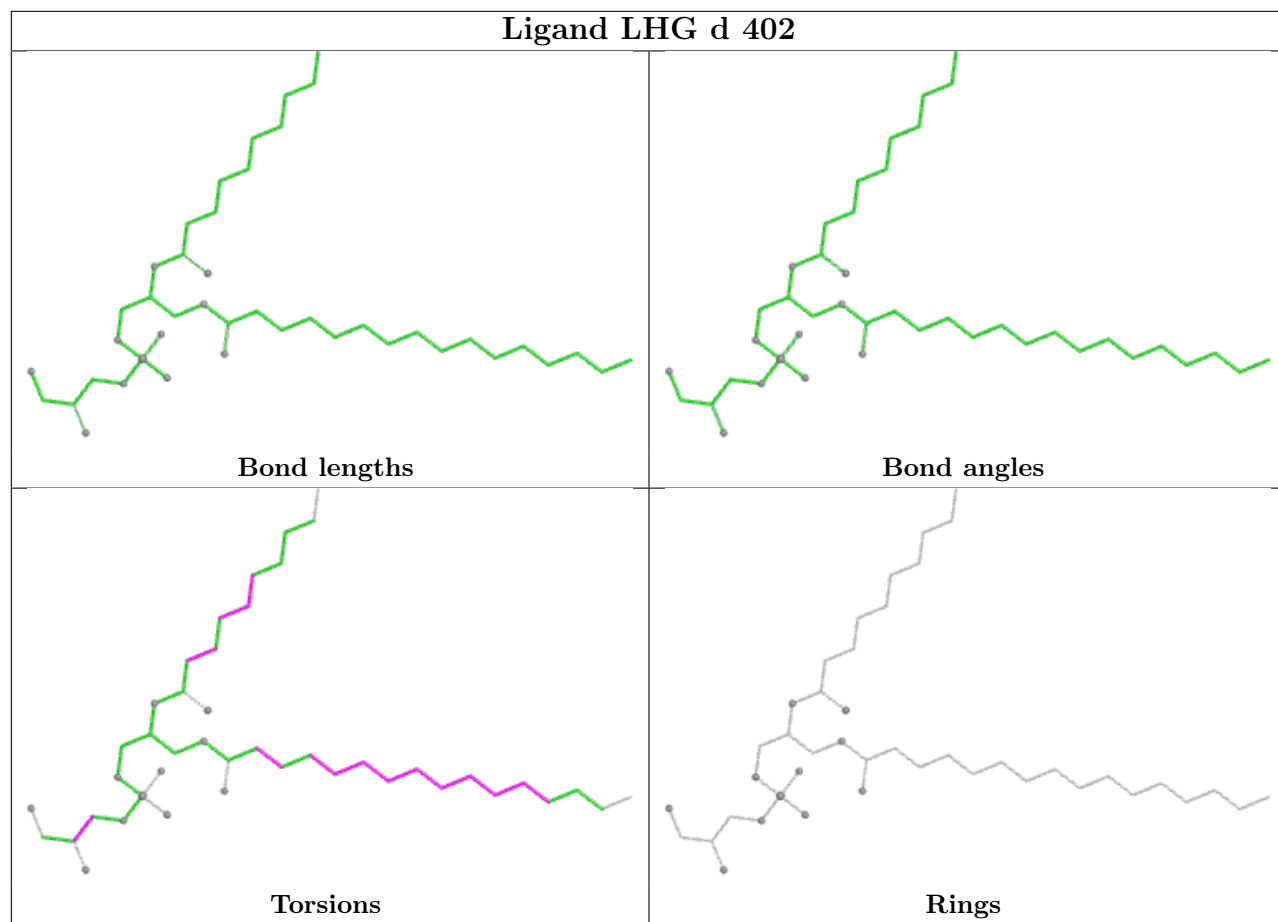
Ligand CHL s 303



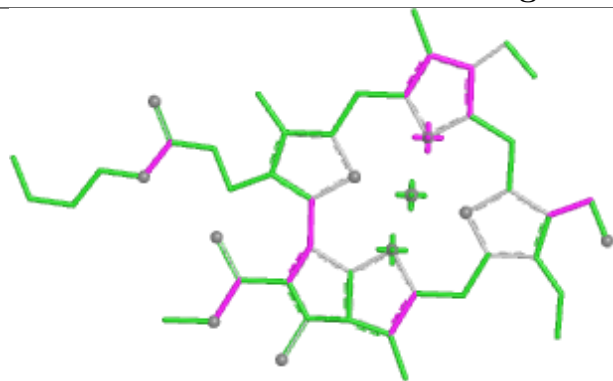




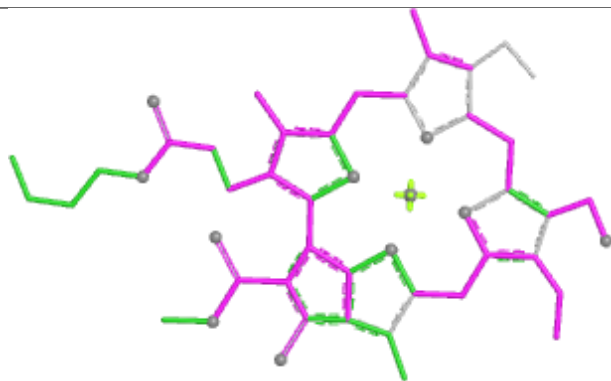




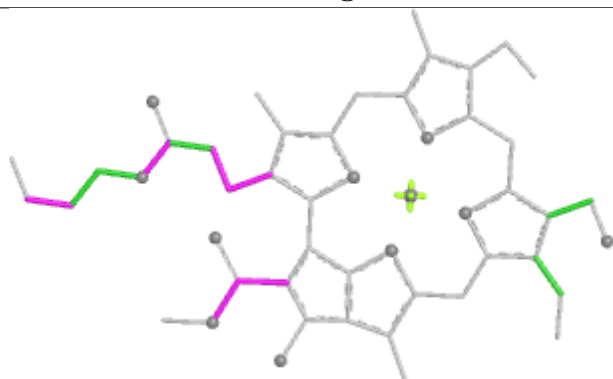
Ligand CHL r 316



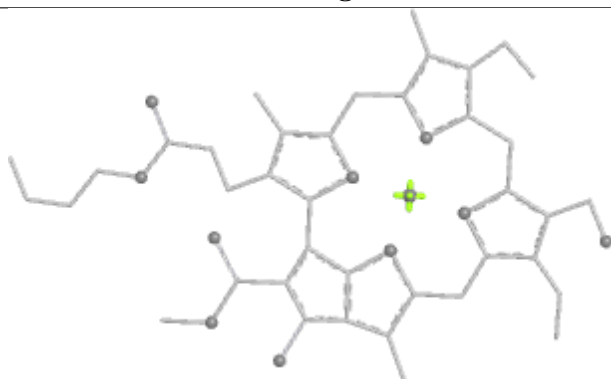
Bond lengths



Bond angles

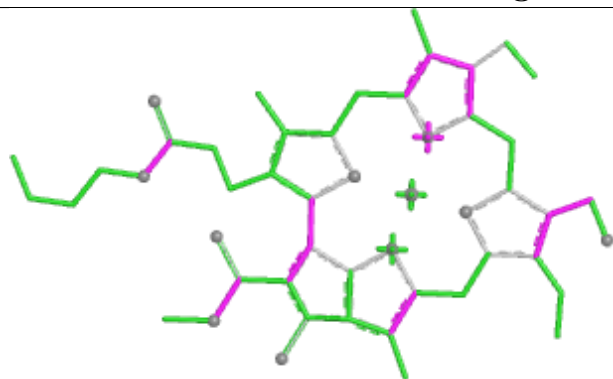


Torsions

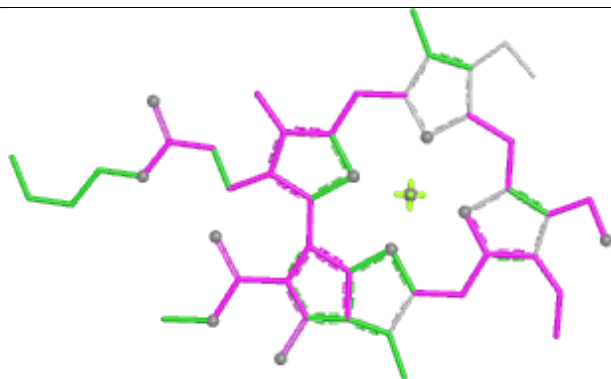


Rings

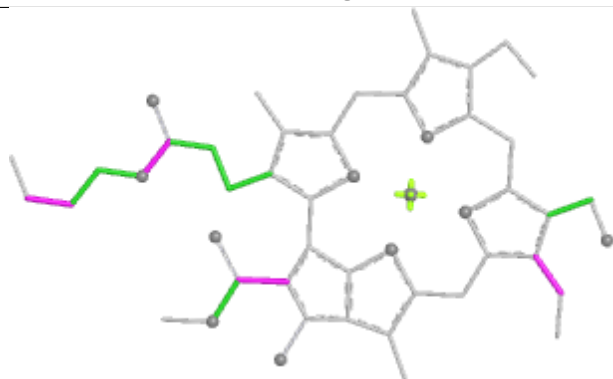
Ligand CHL N 316



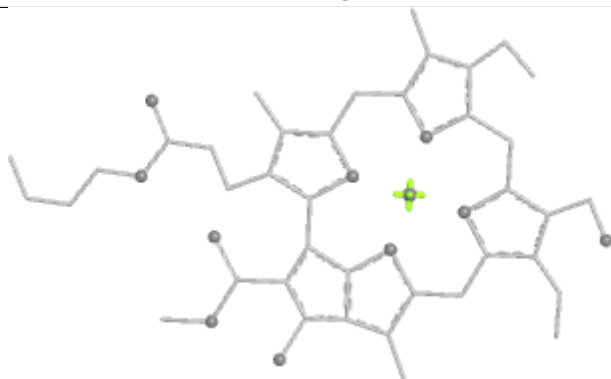
Bond lengths



Bond angles

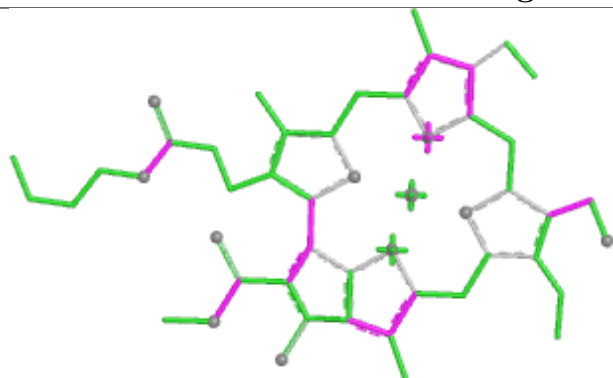


Torsions

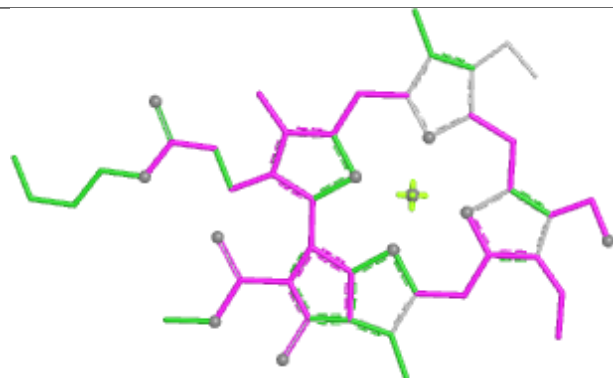


Rings

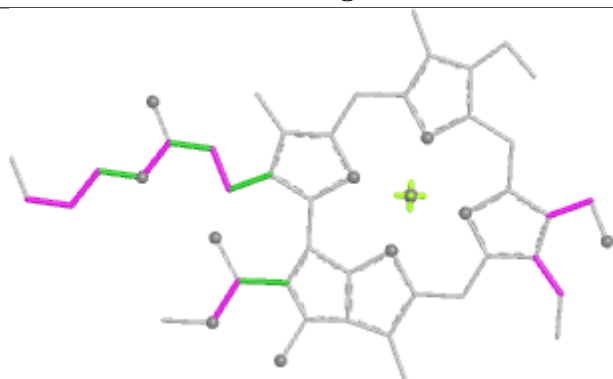
Ligand CHL n 307



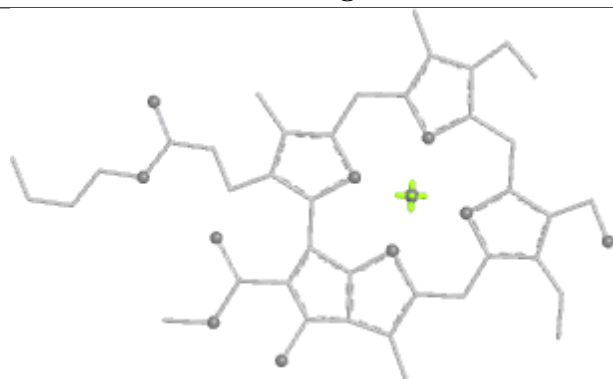
Bond lengths



Bond angles

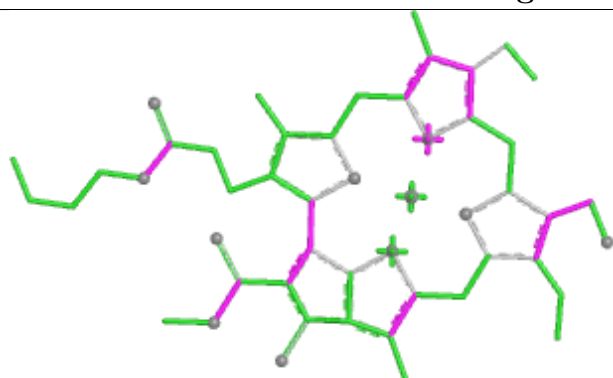


Torsions

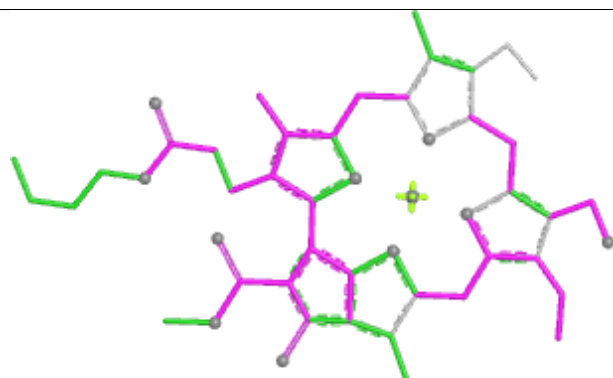


Rings

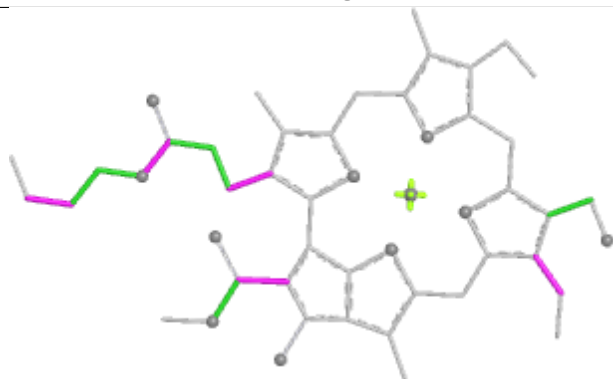
Ligand CHL n 319



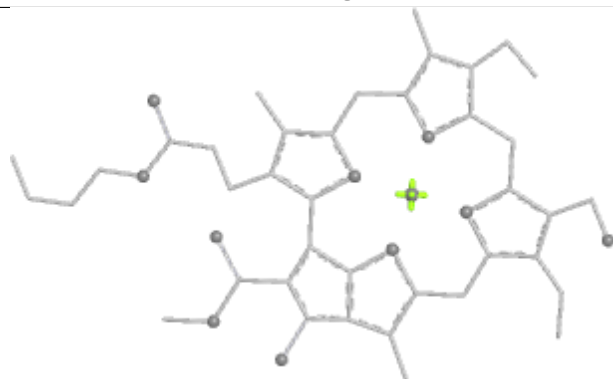
Bond lengths



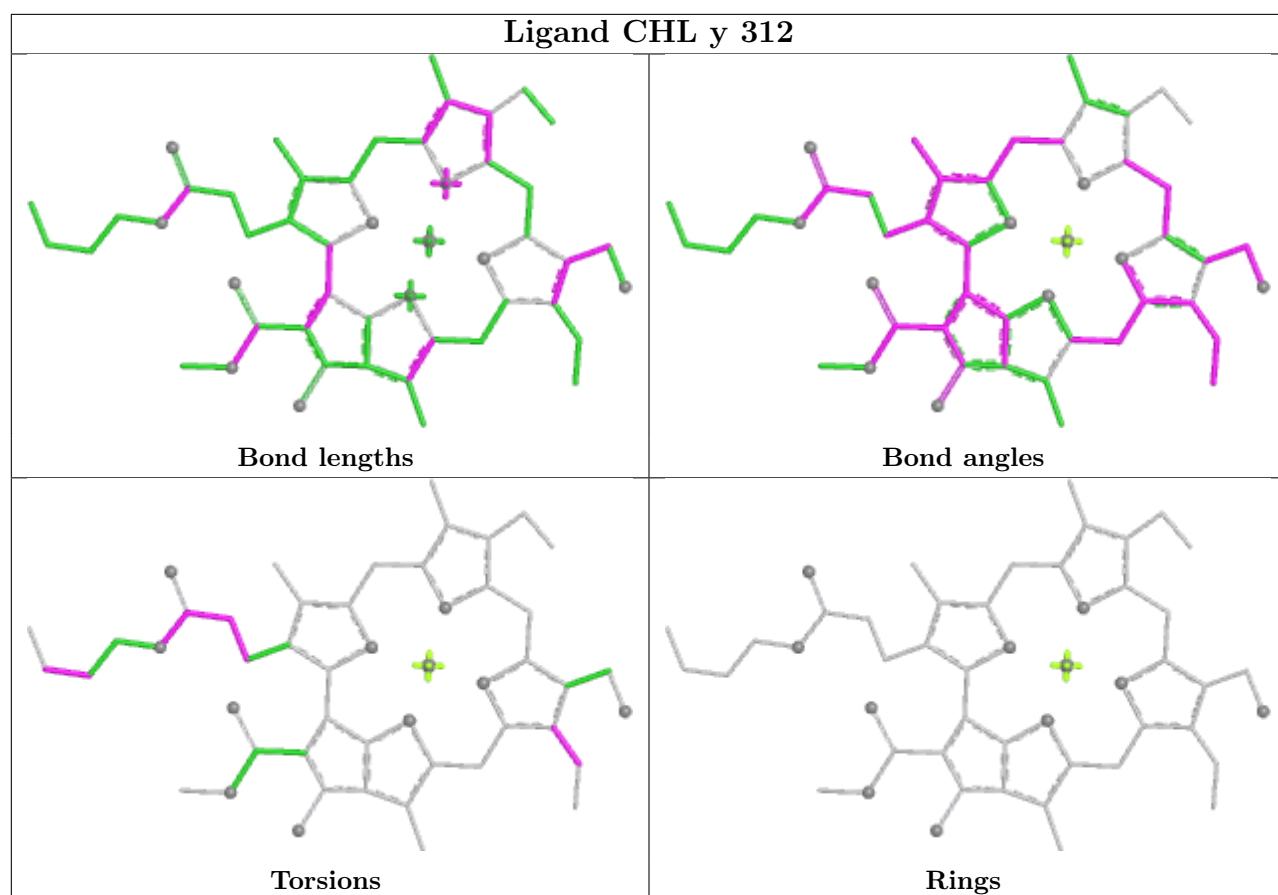
Bond angles

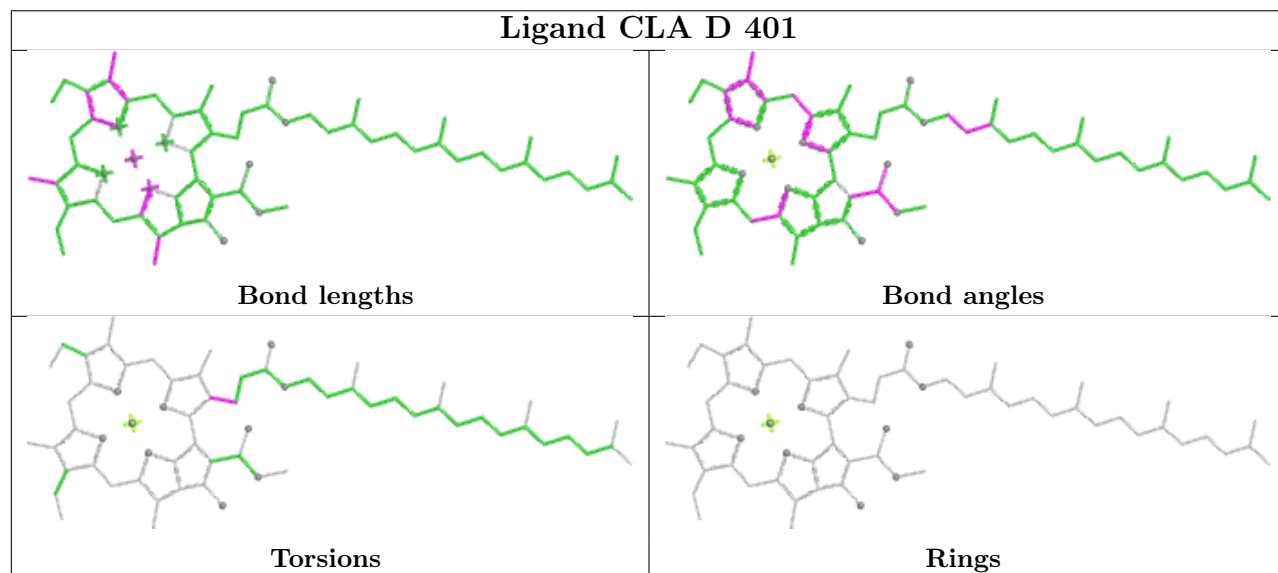
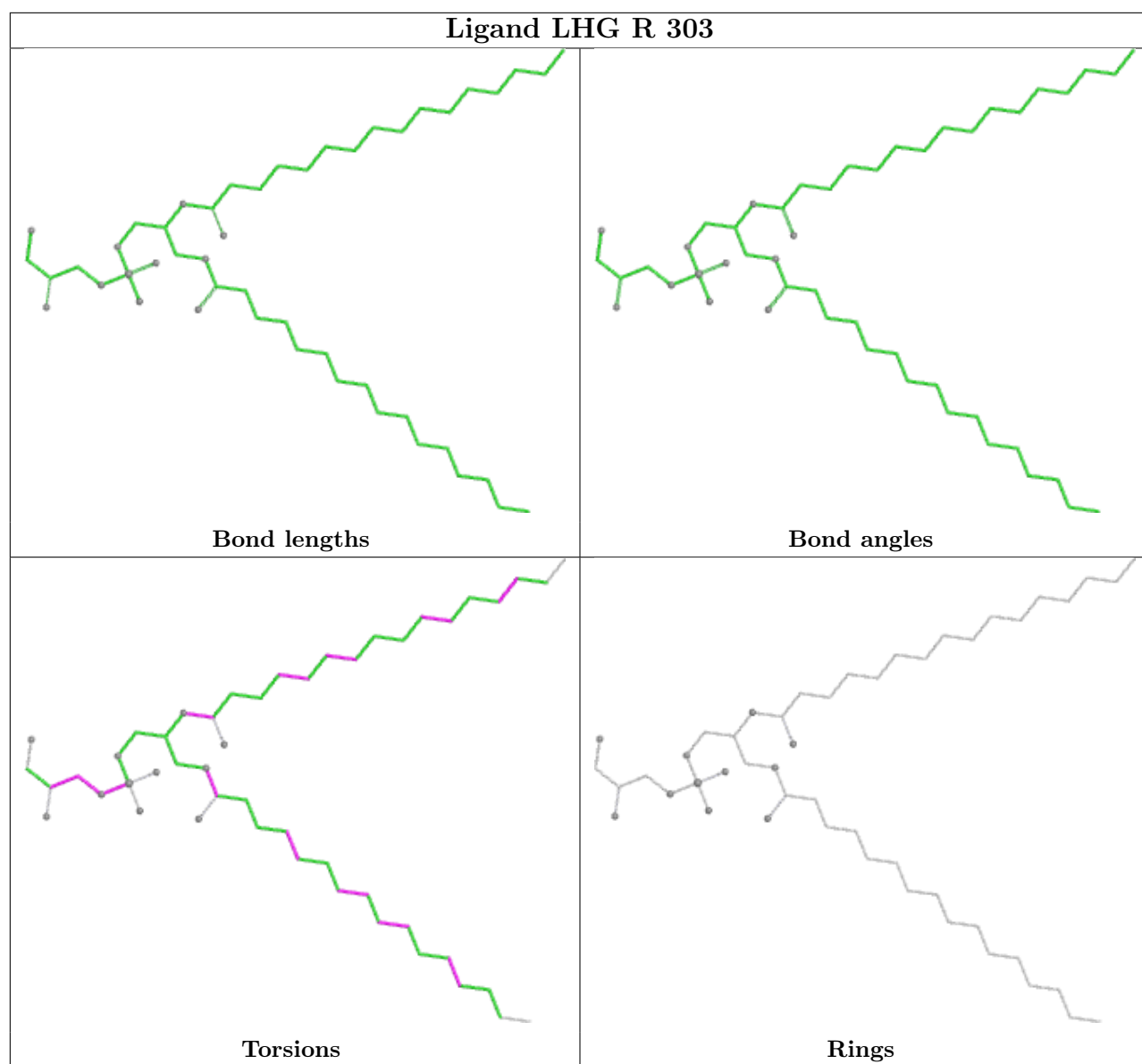


Torsions

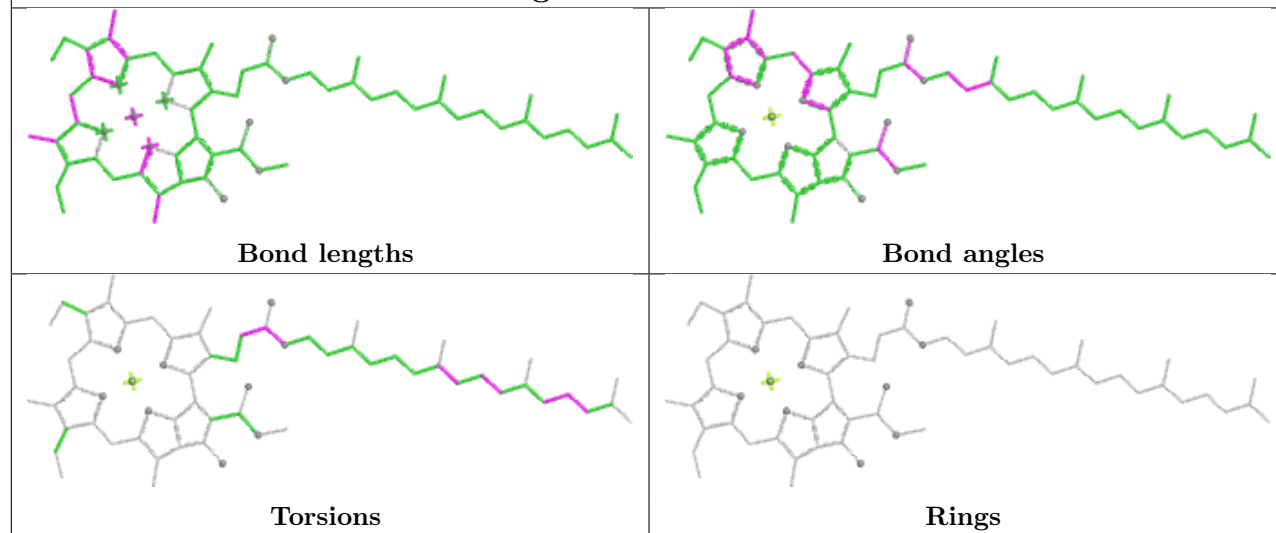


Rings

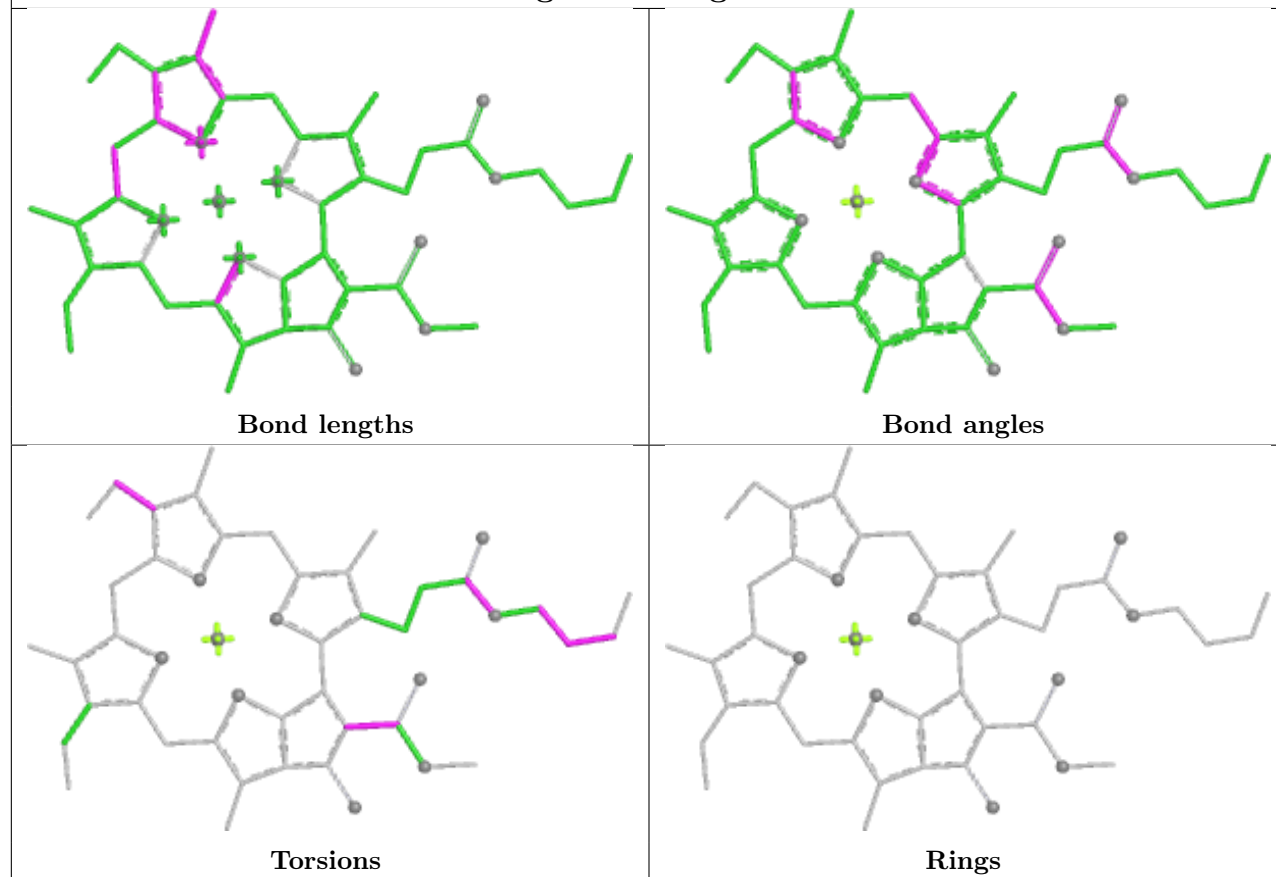


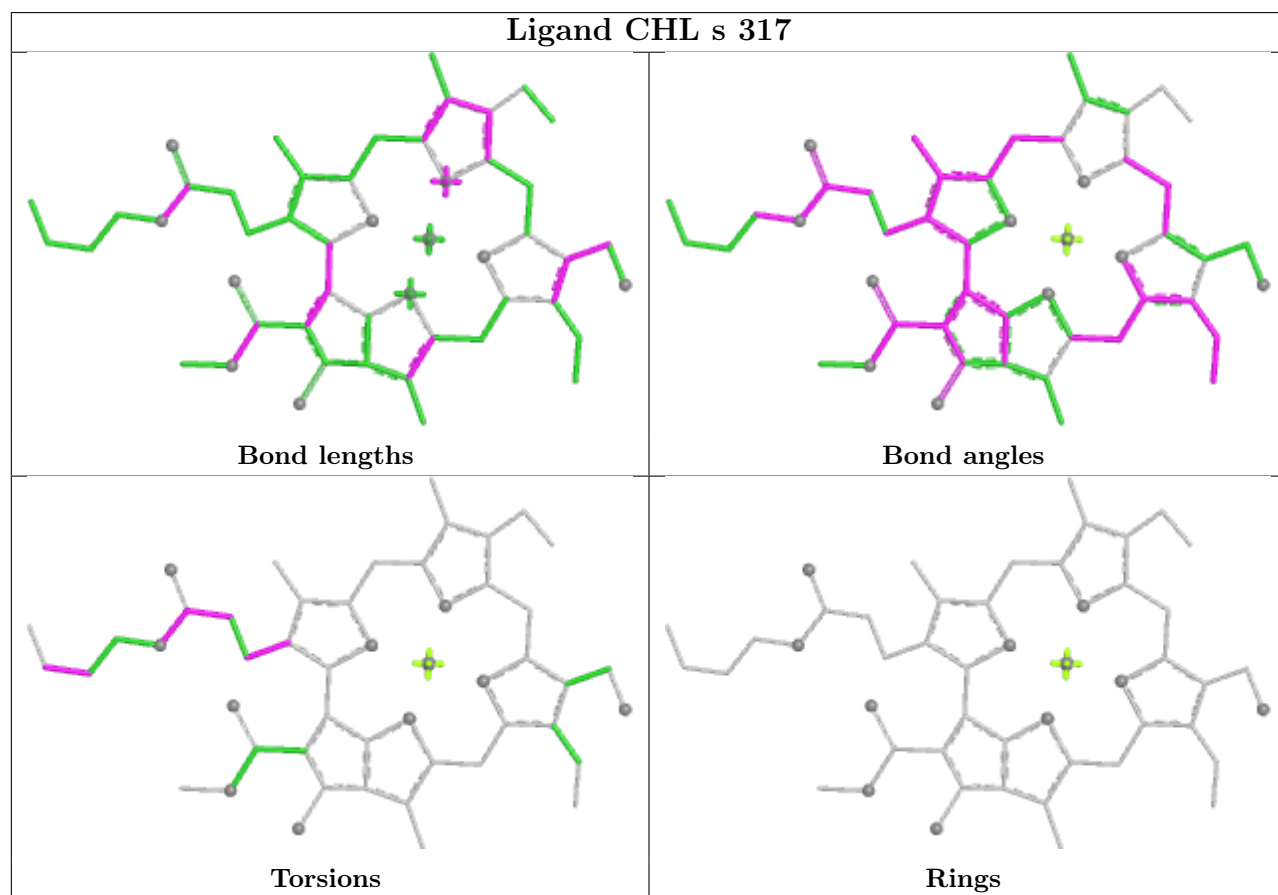
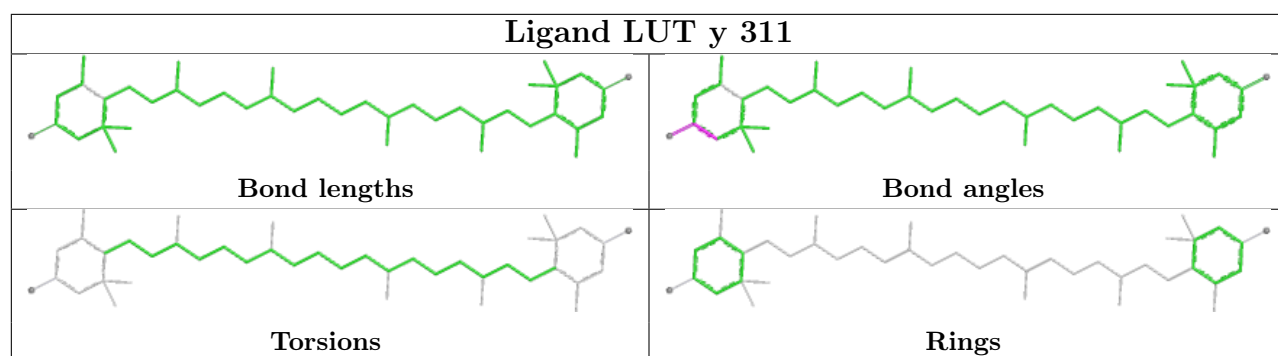


Ligand CLA B 609

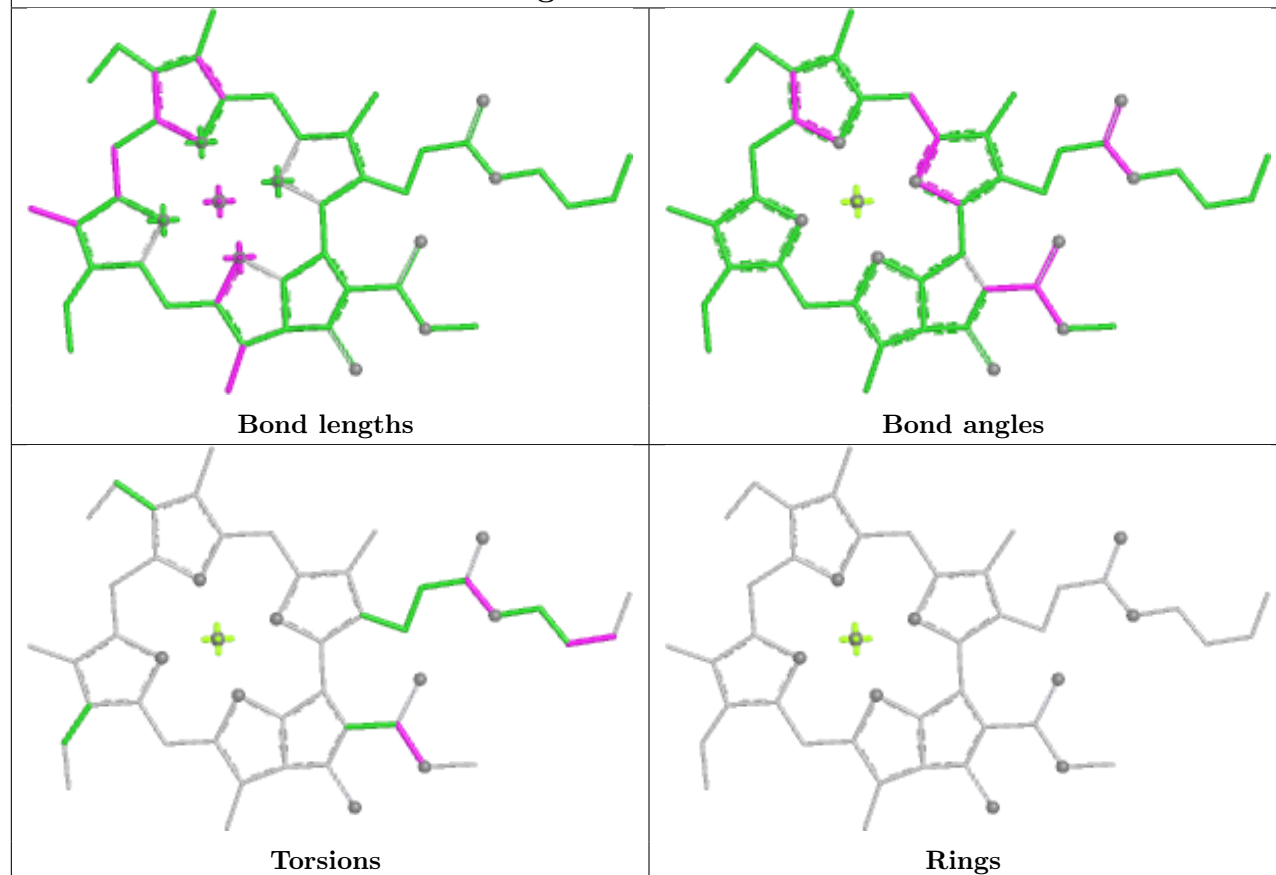


Ligand CLA g 318

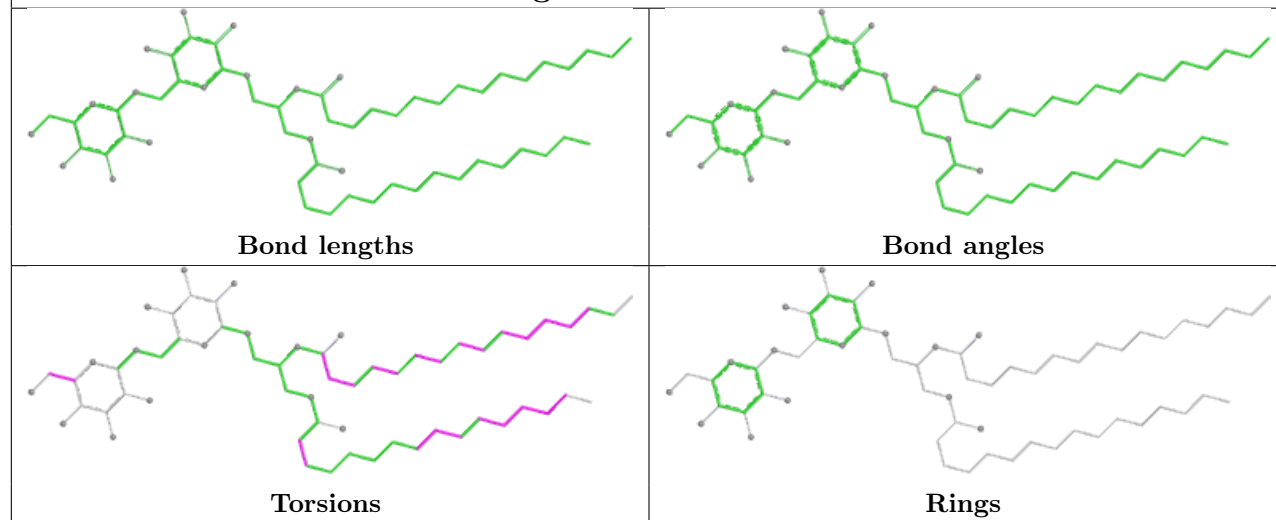


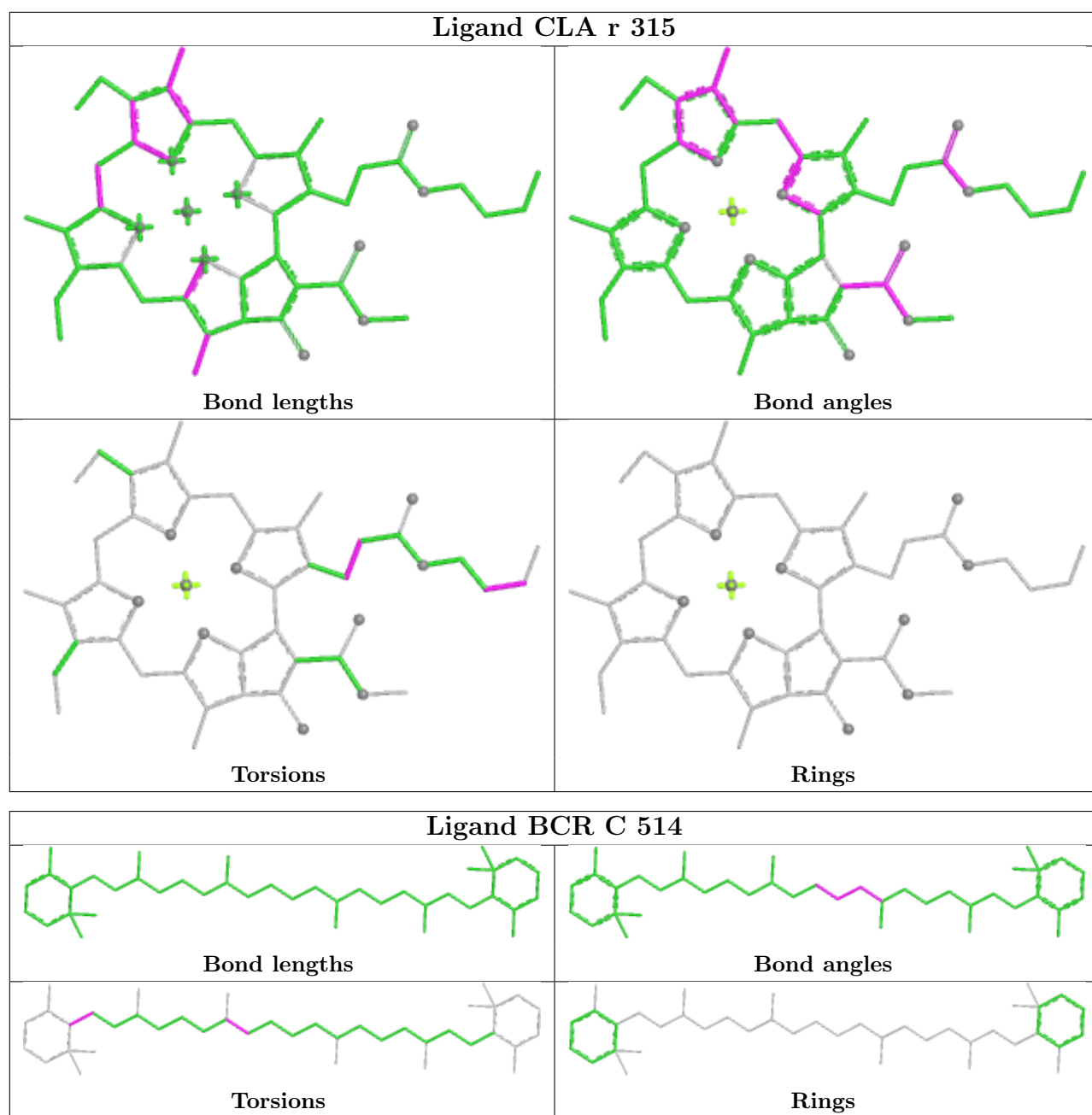


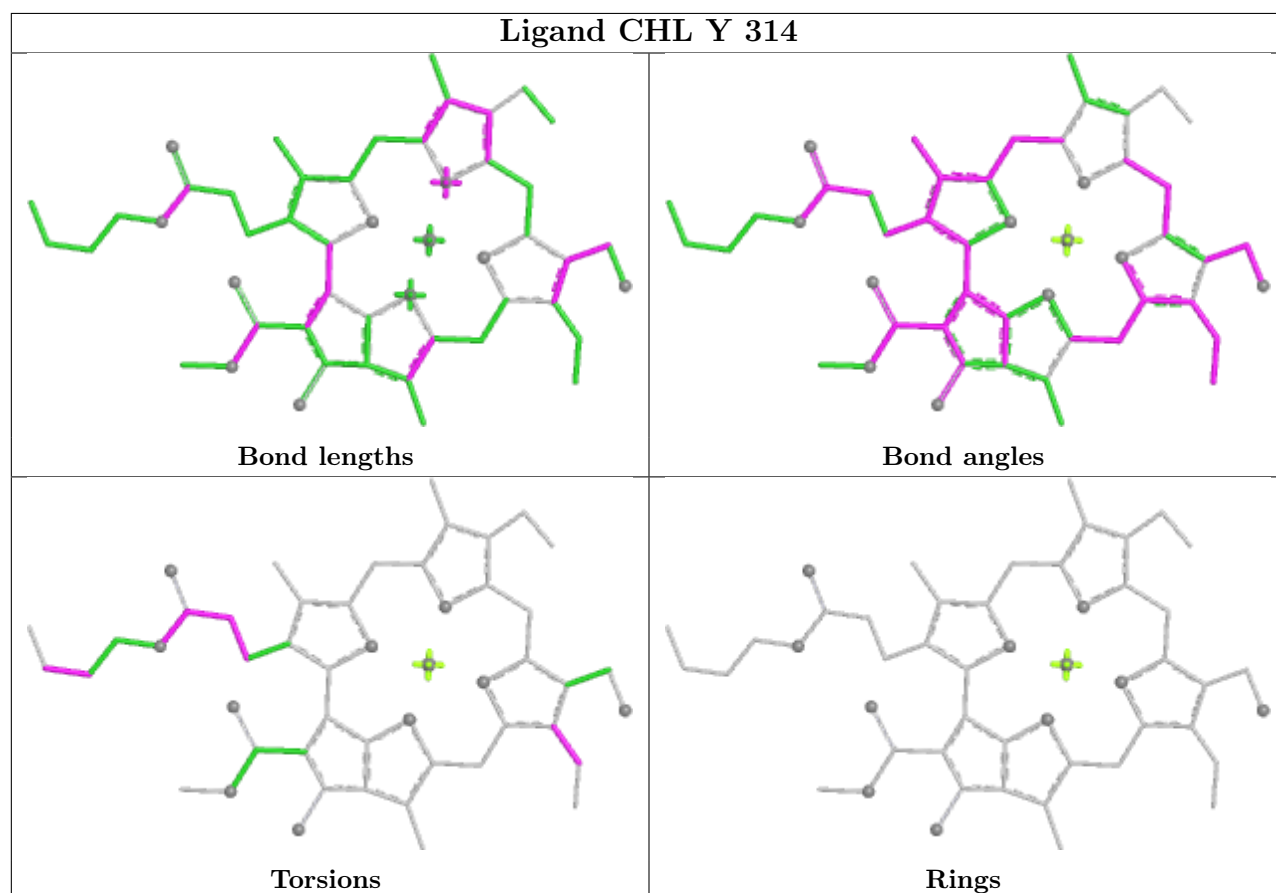
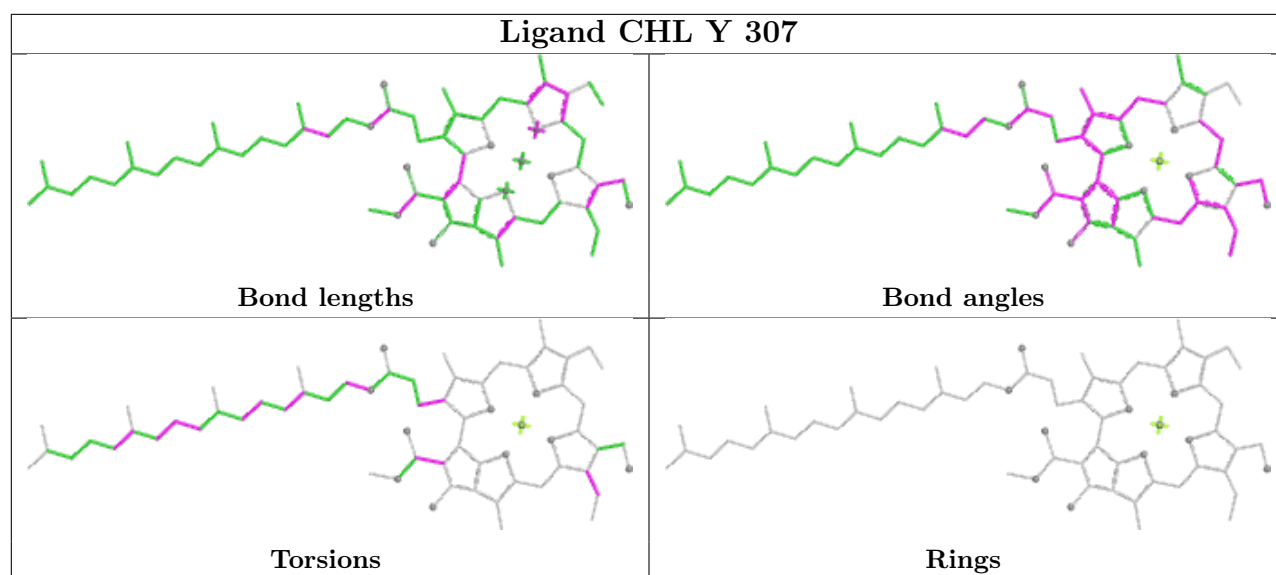
Ligand CLA c 510

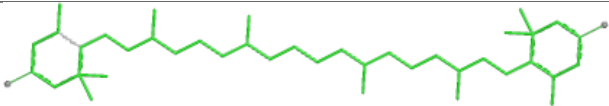
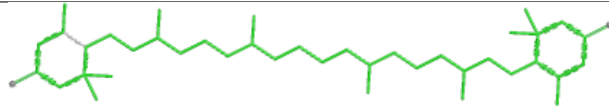

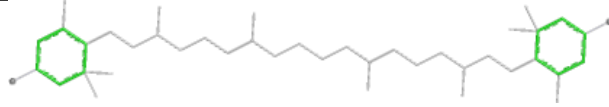


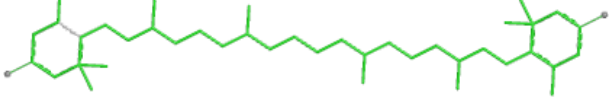
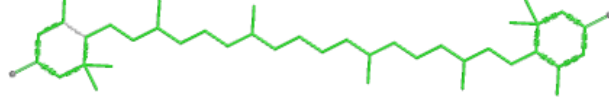
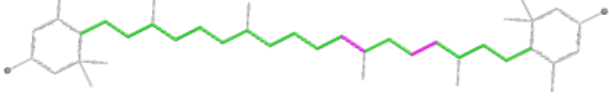
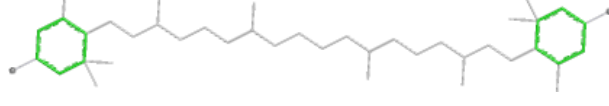
Ligand DGD c 501

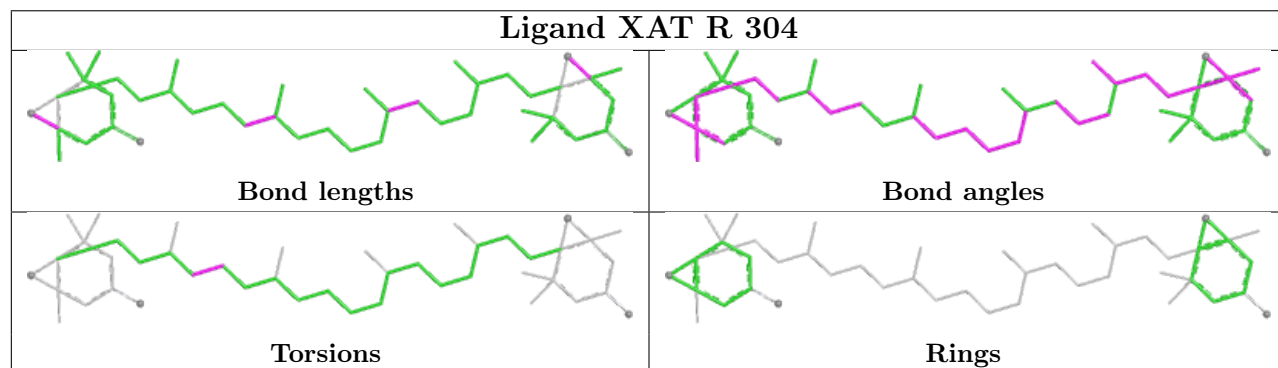
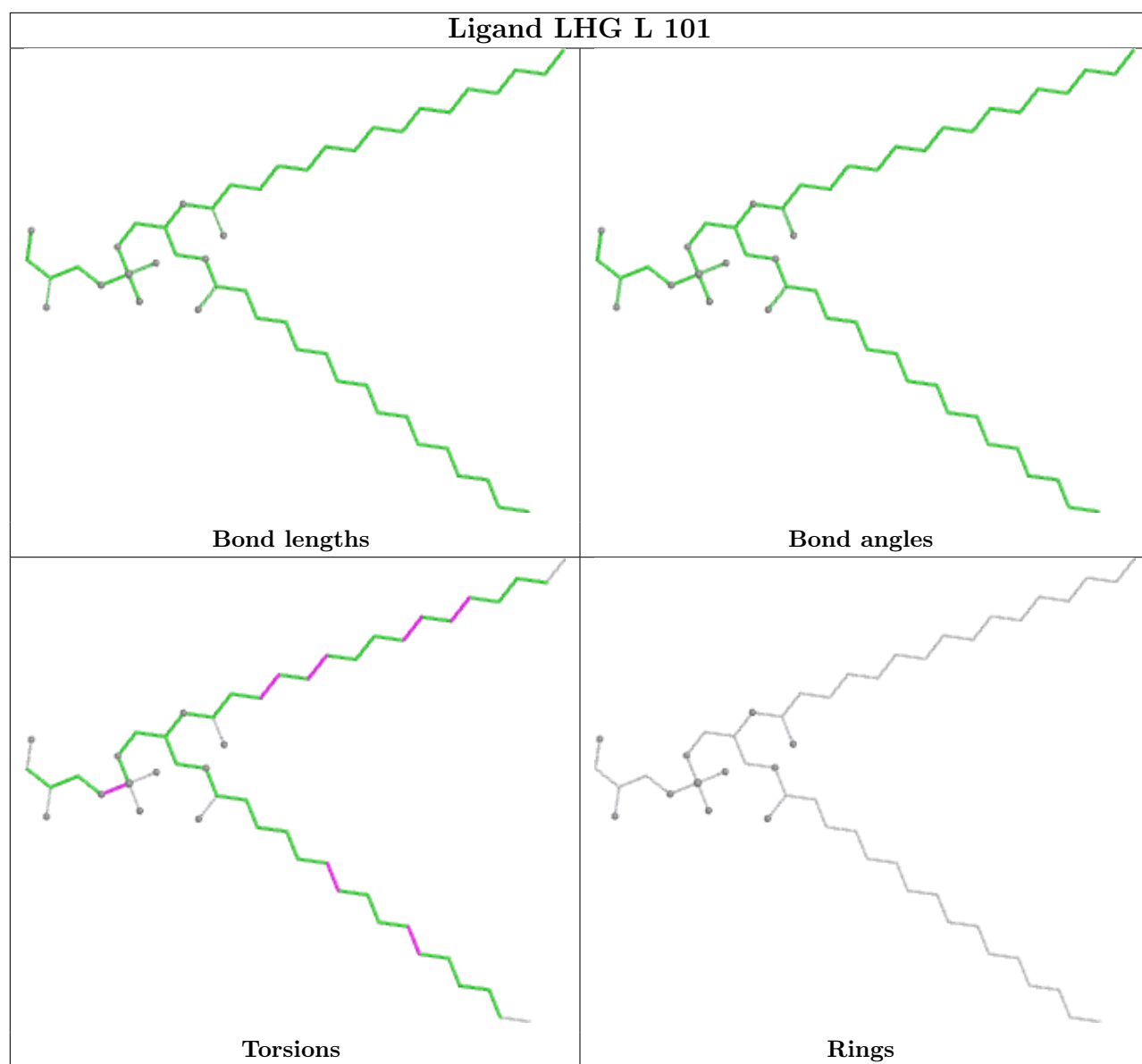


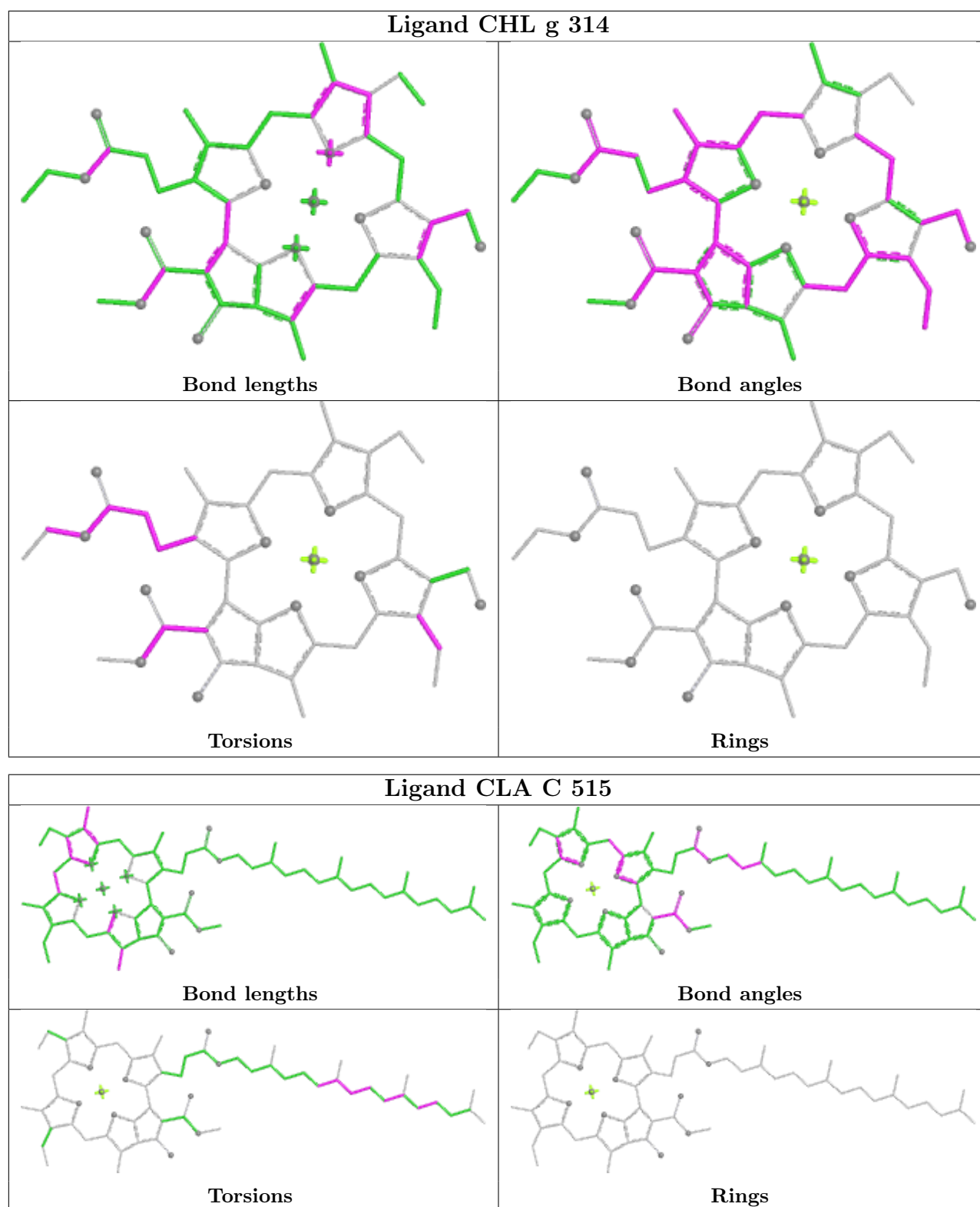


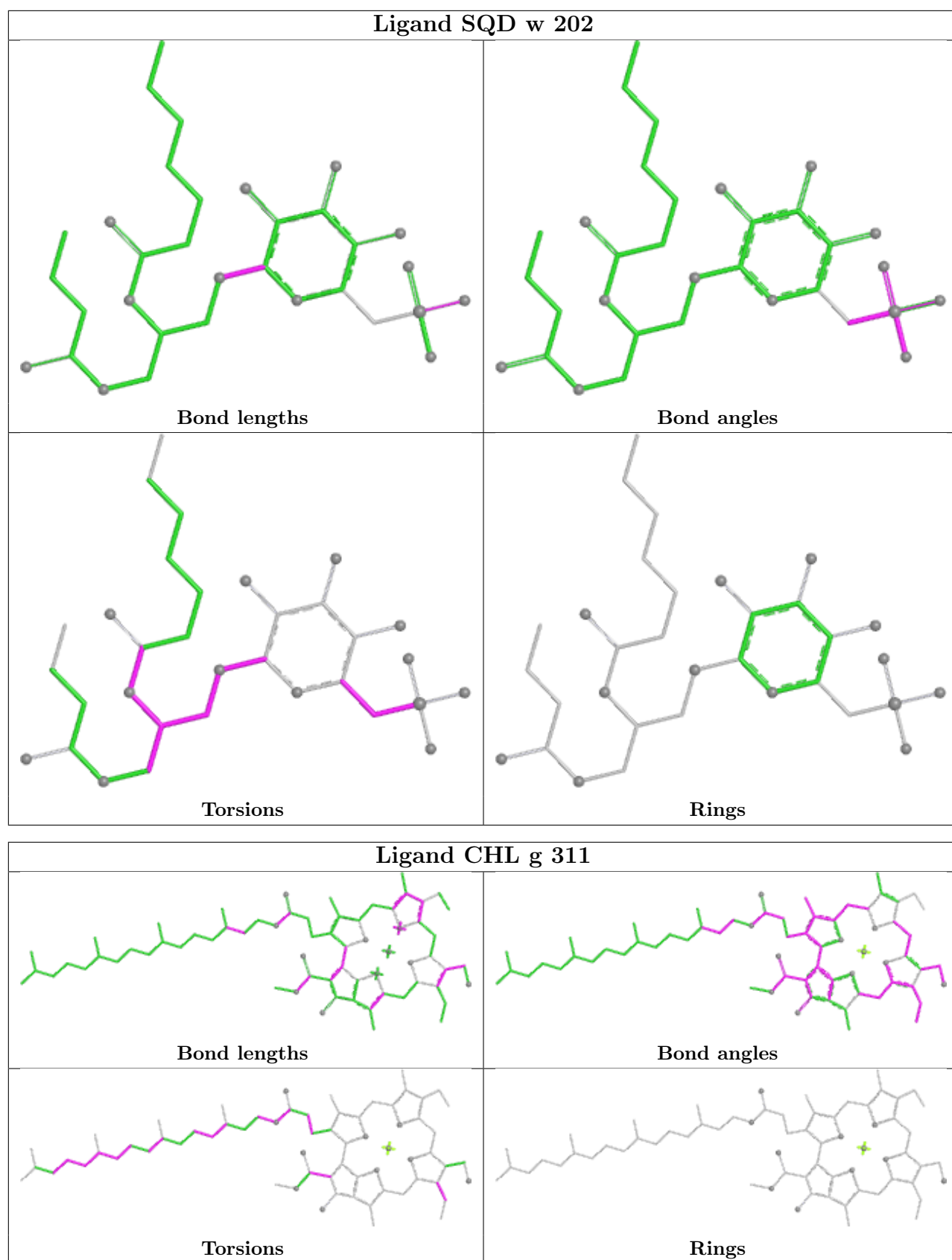


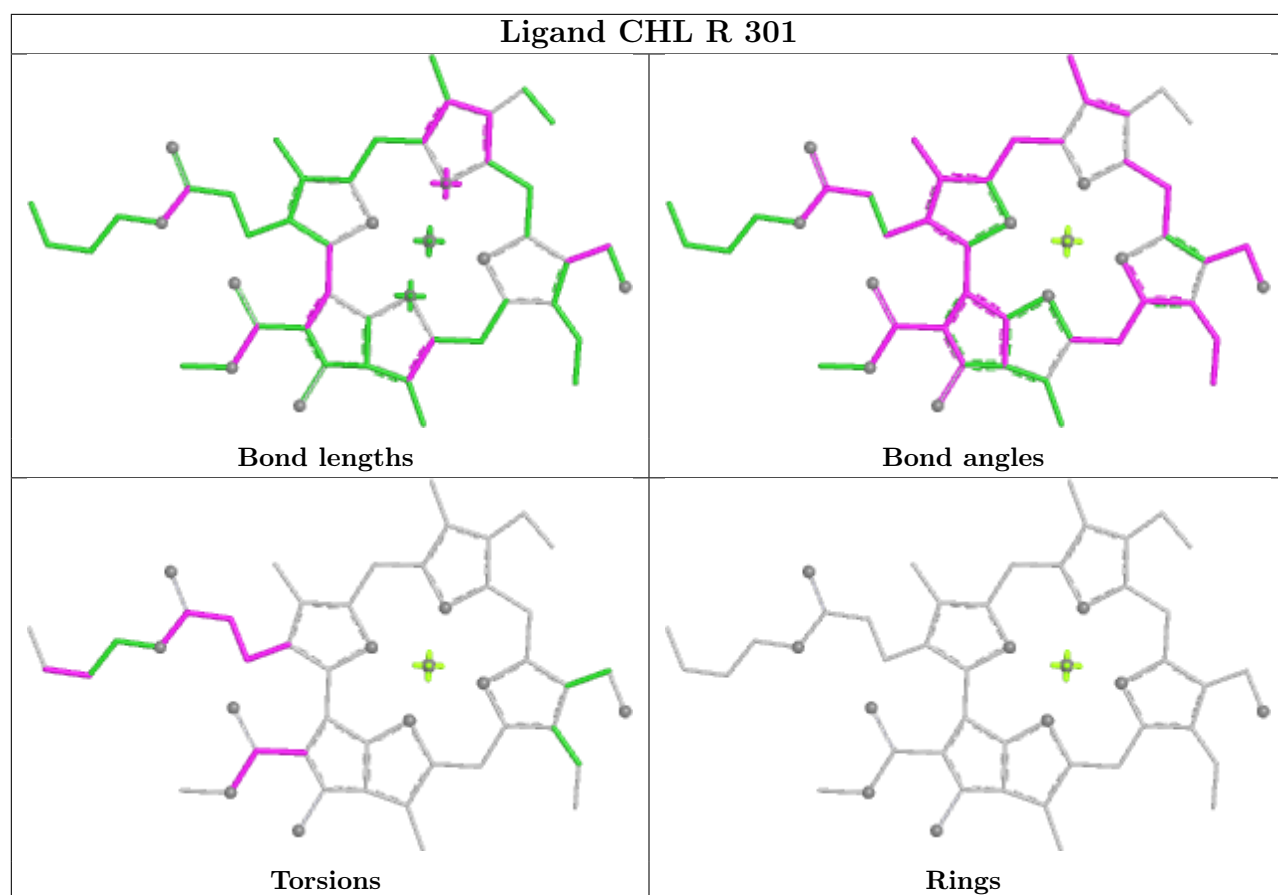
Ligand LUT S 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

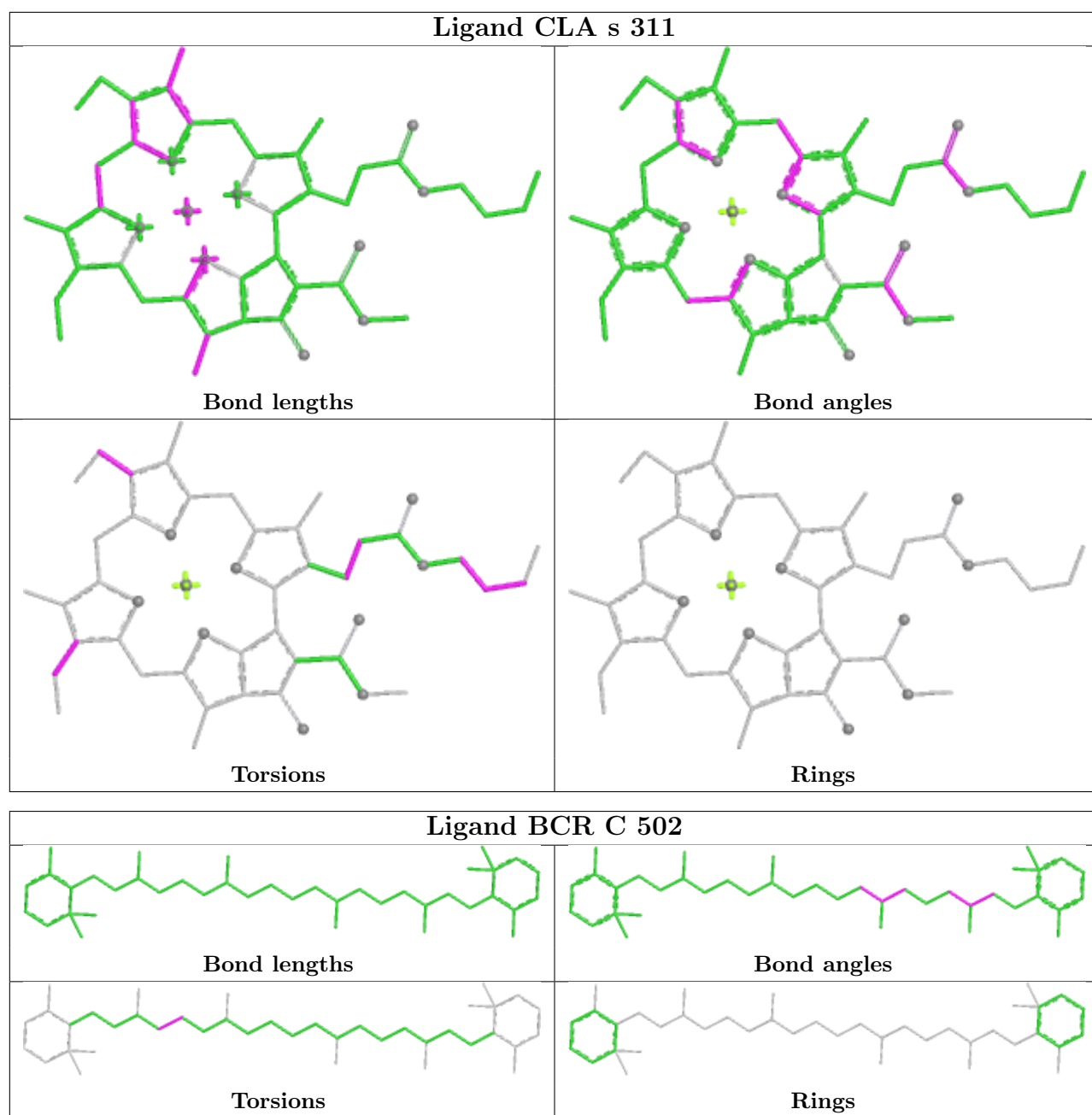
Ligand LUT s 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

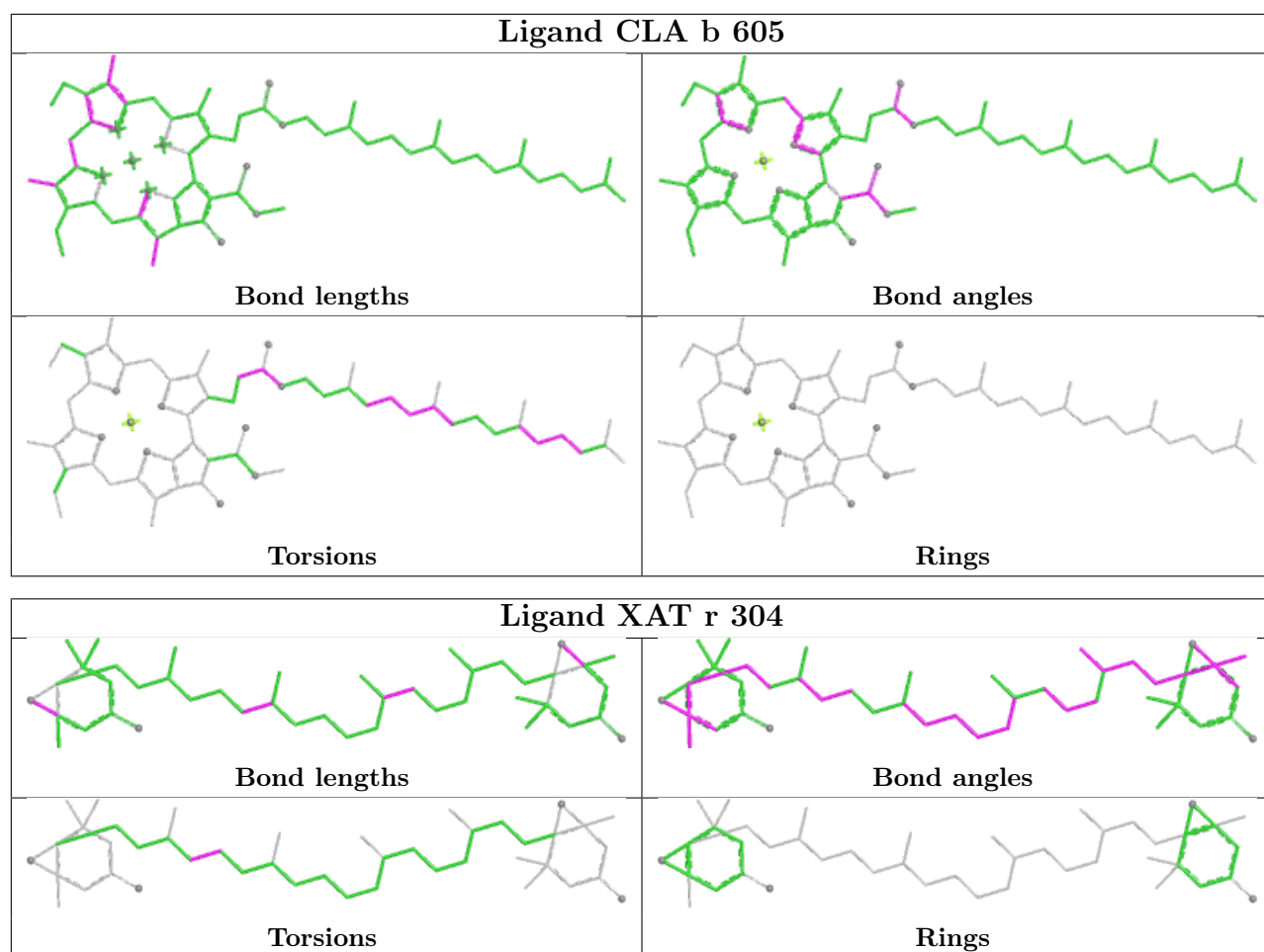


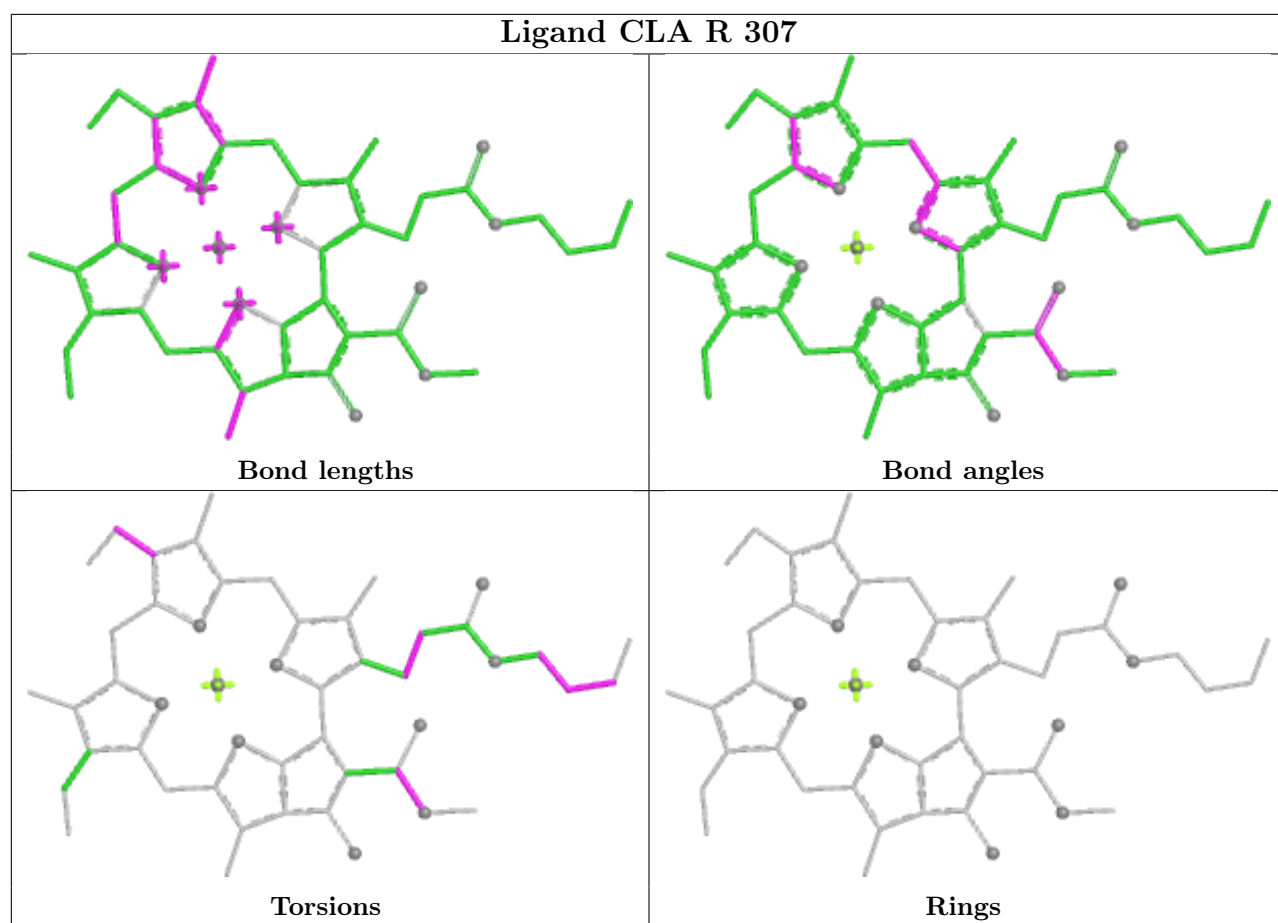


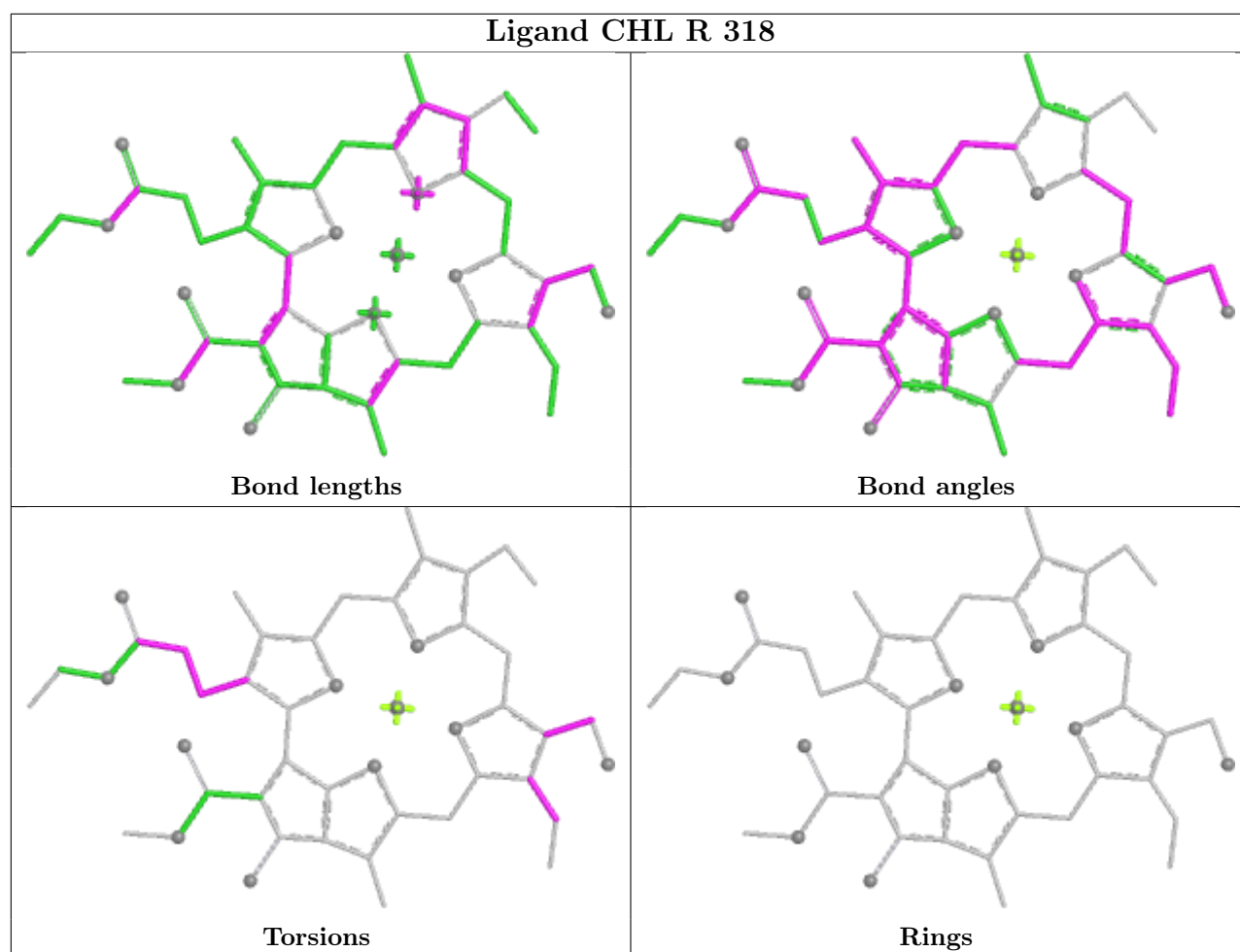


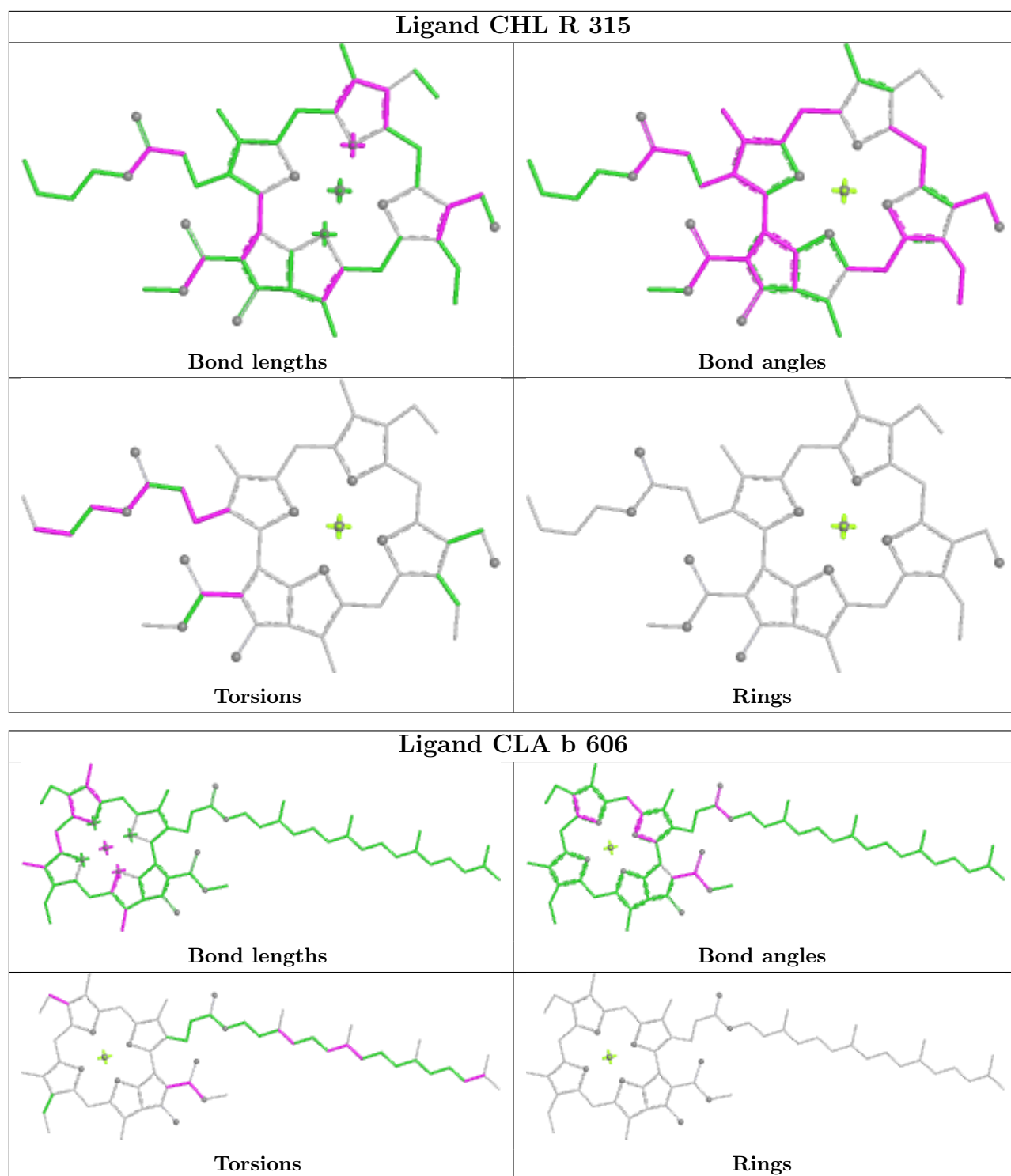


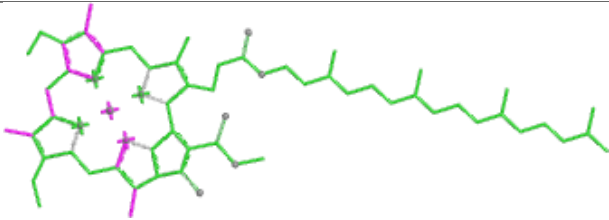
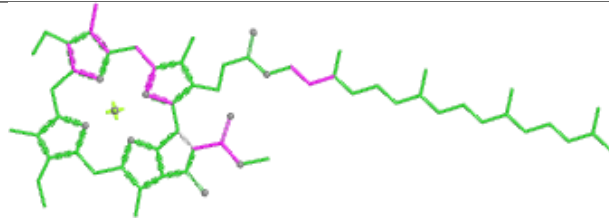
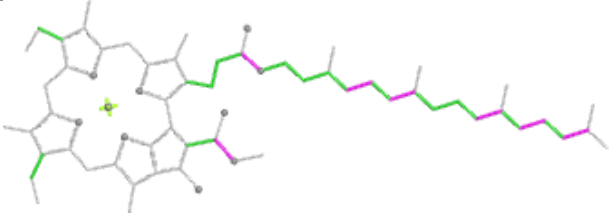
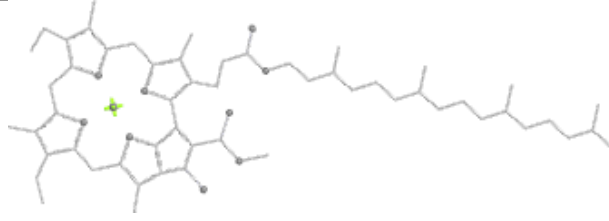




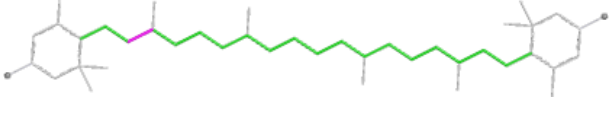
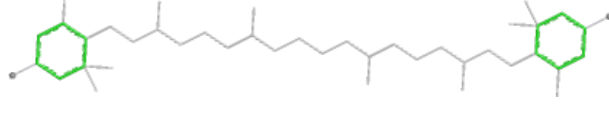


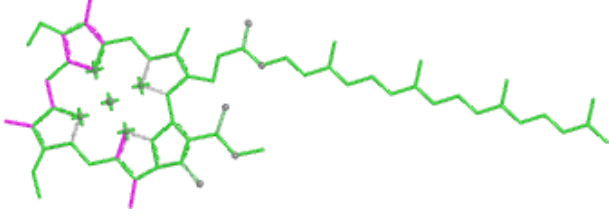
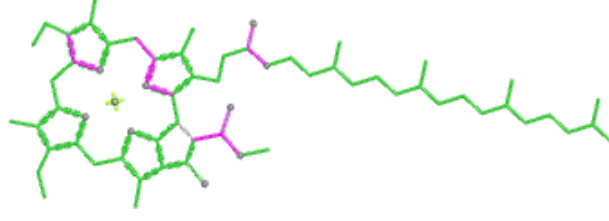
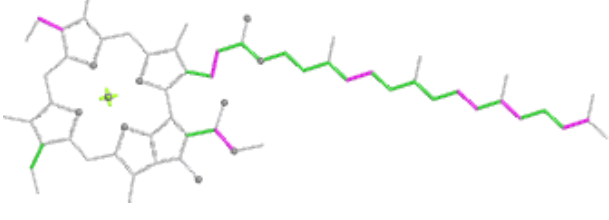
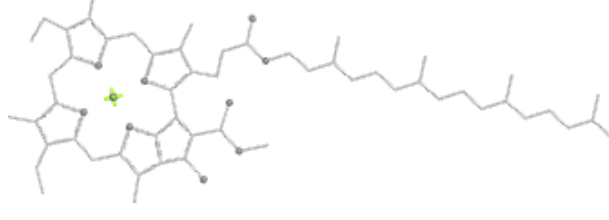




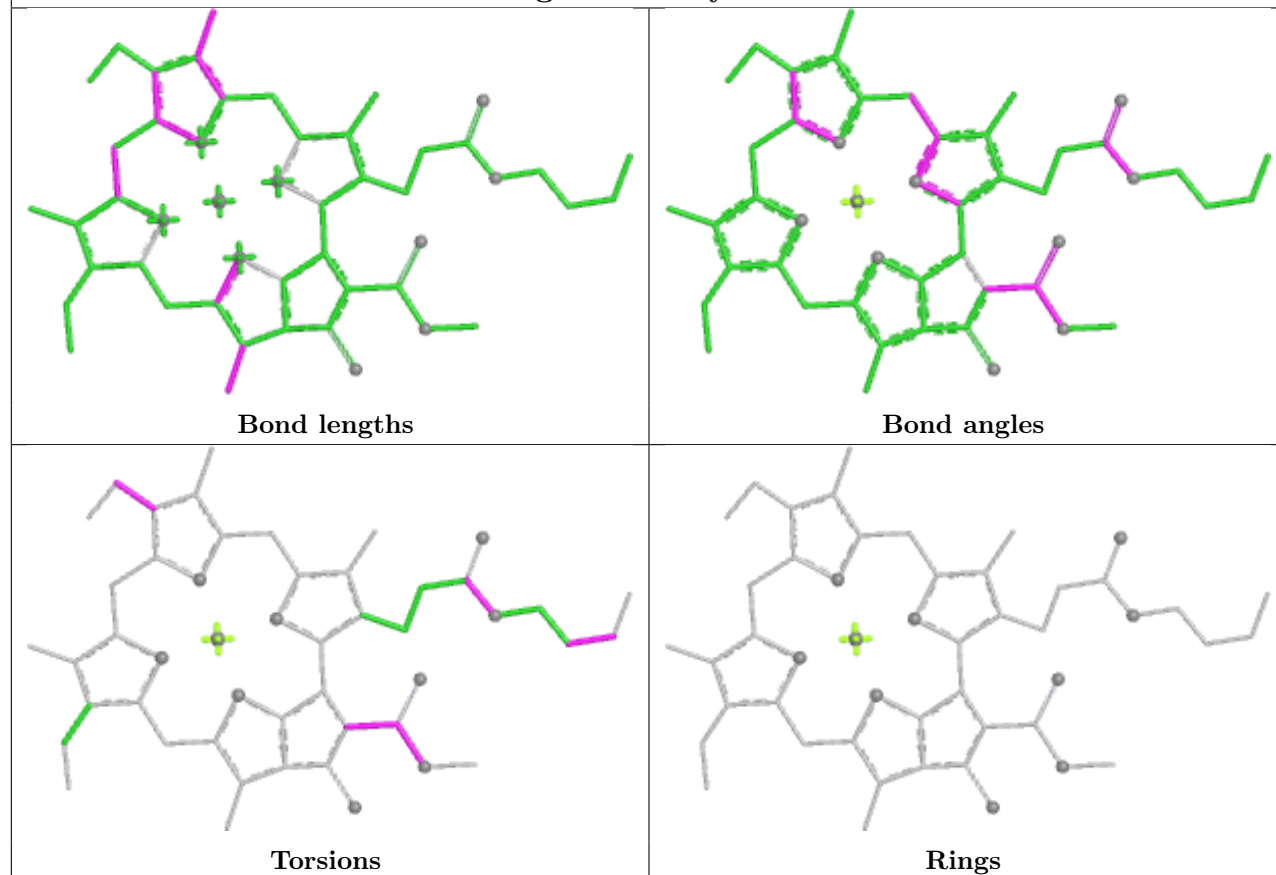


Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

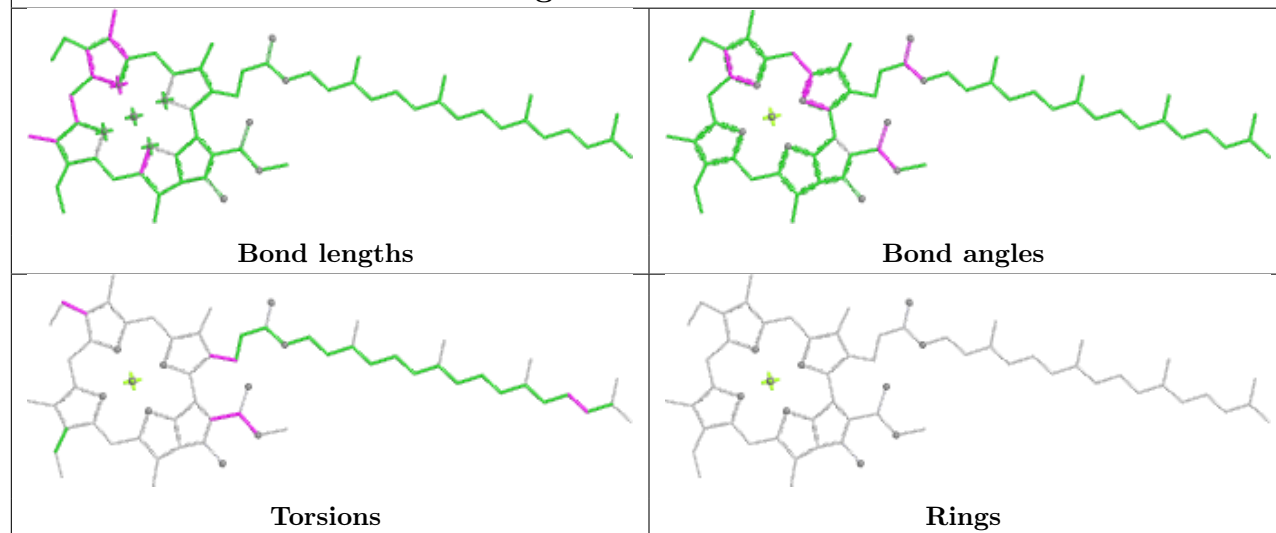
Ligand LUT Y 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

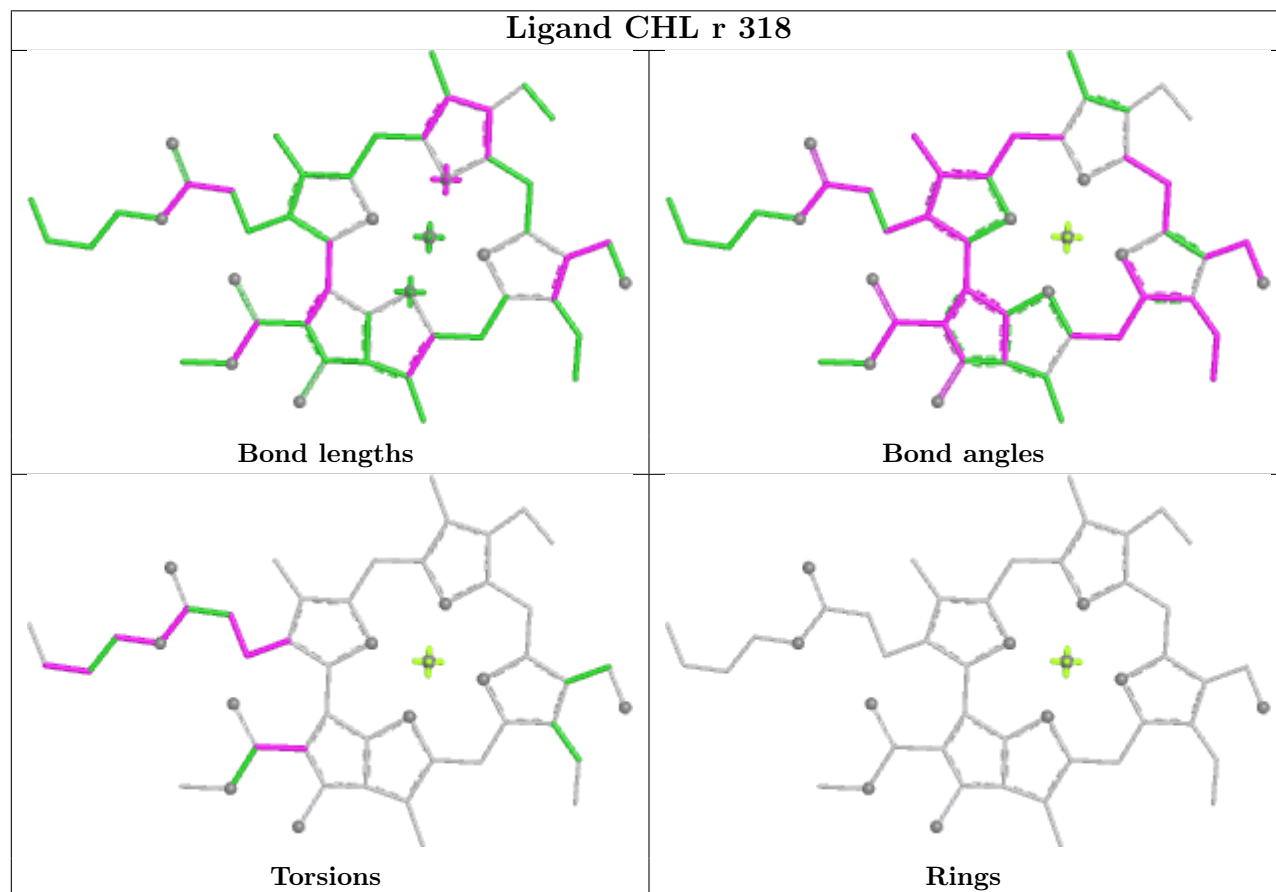
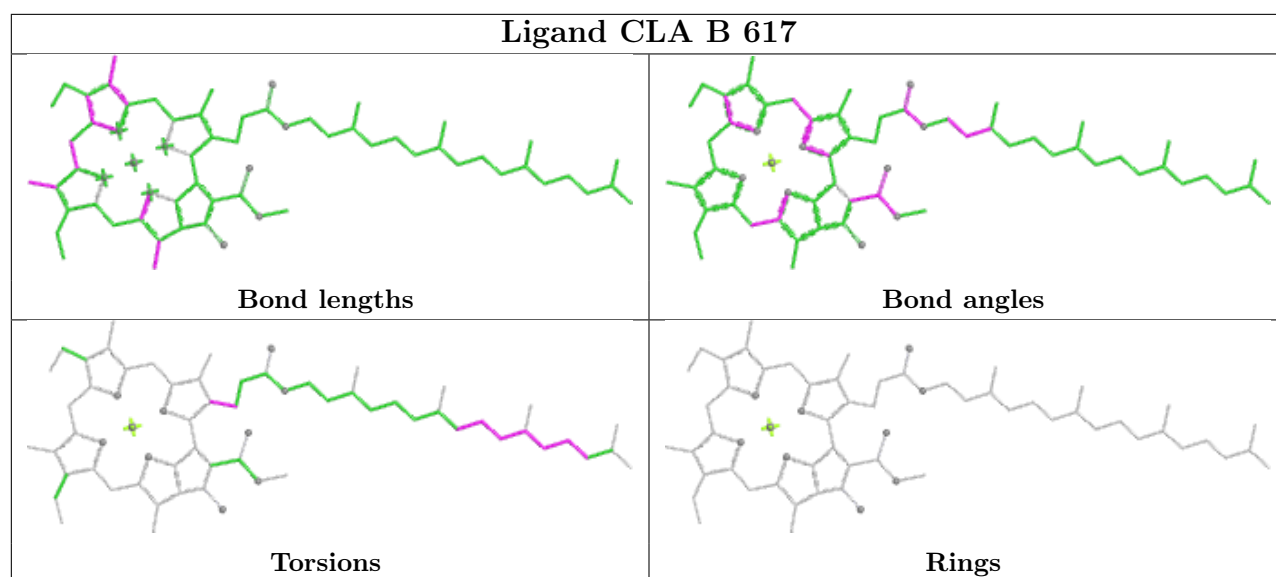
Ligand CLA B 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

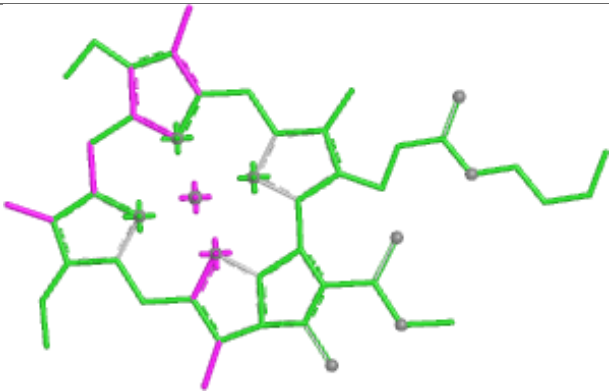
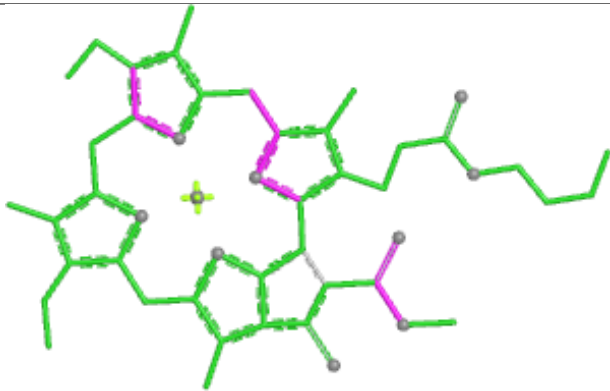
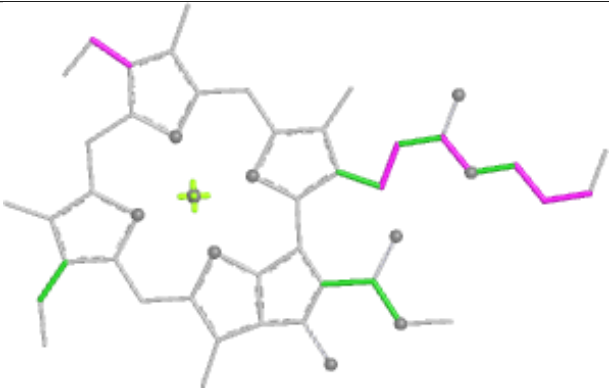
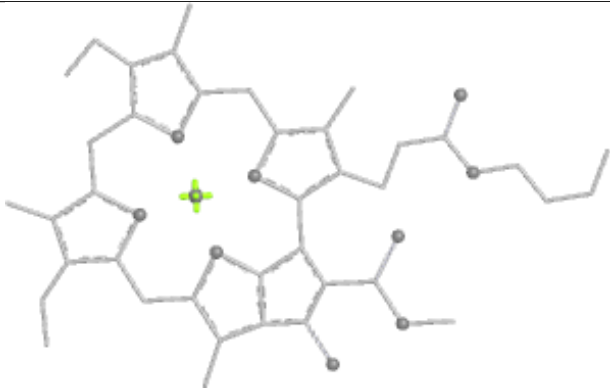
Ligand CLA y 315

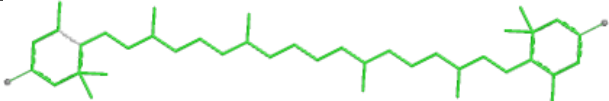
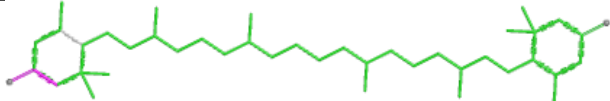
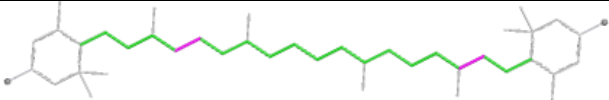
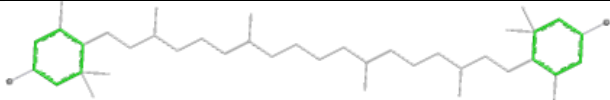




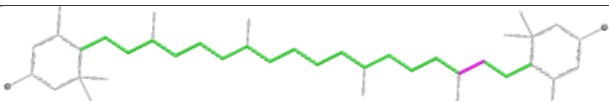
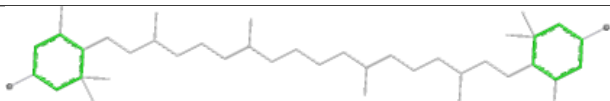
Ligand CLA b 604

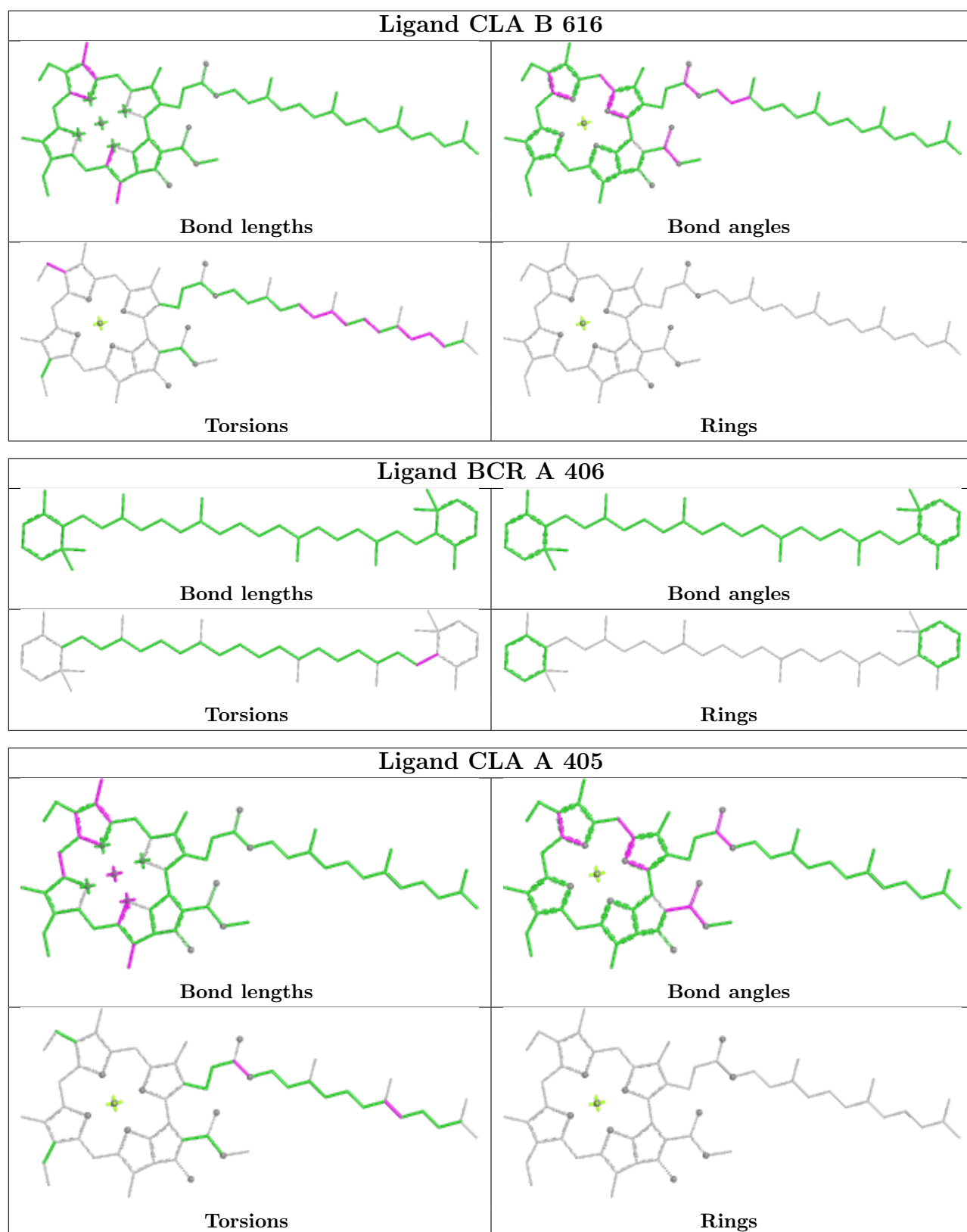


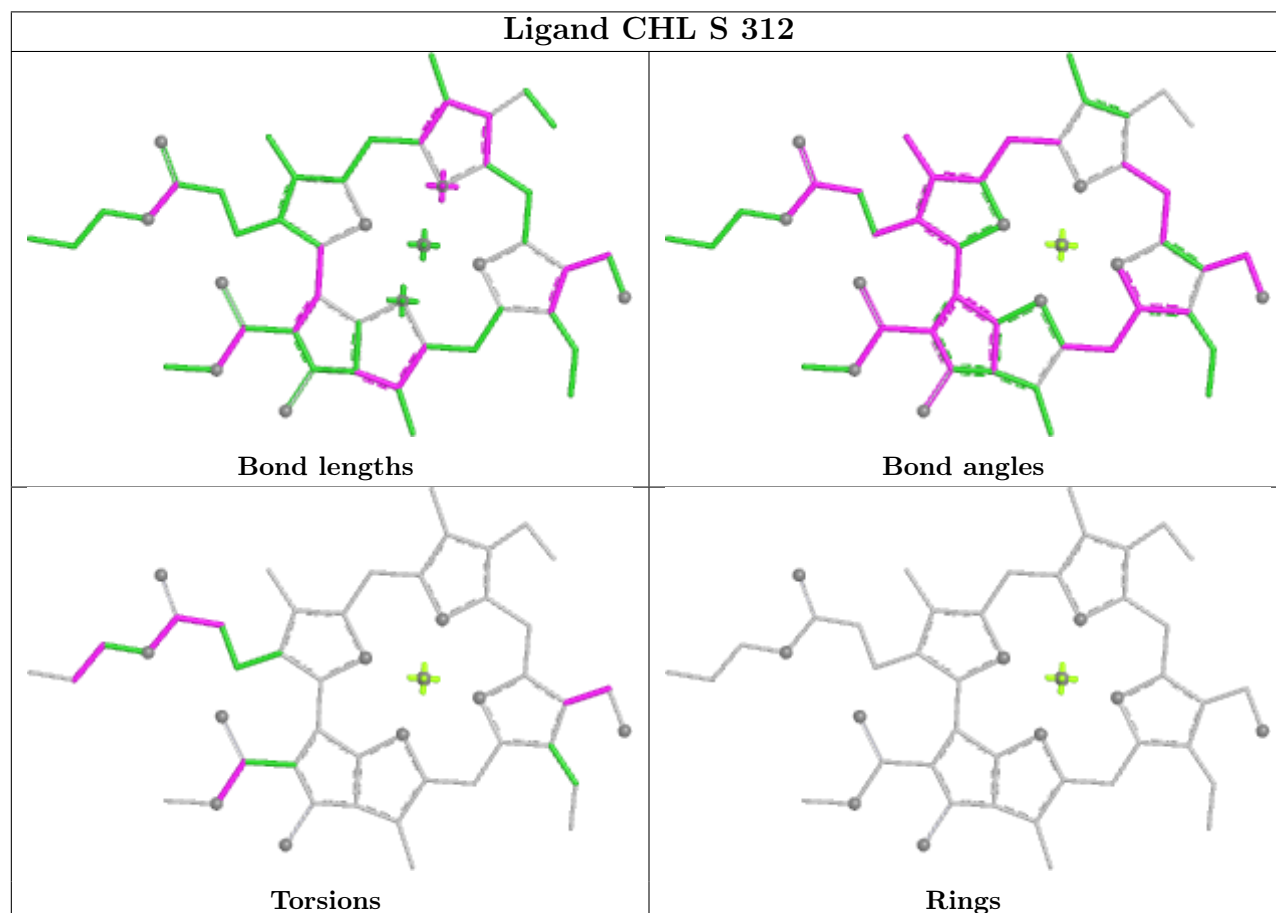
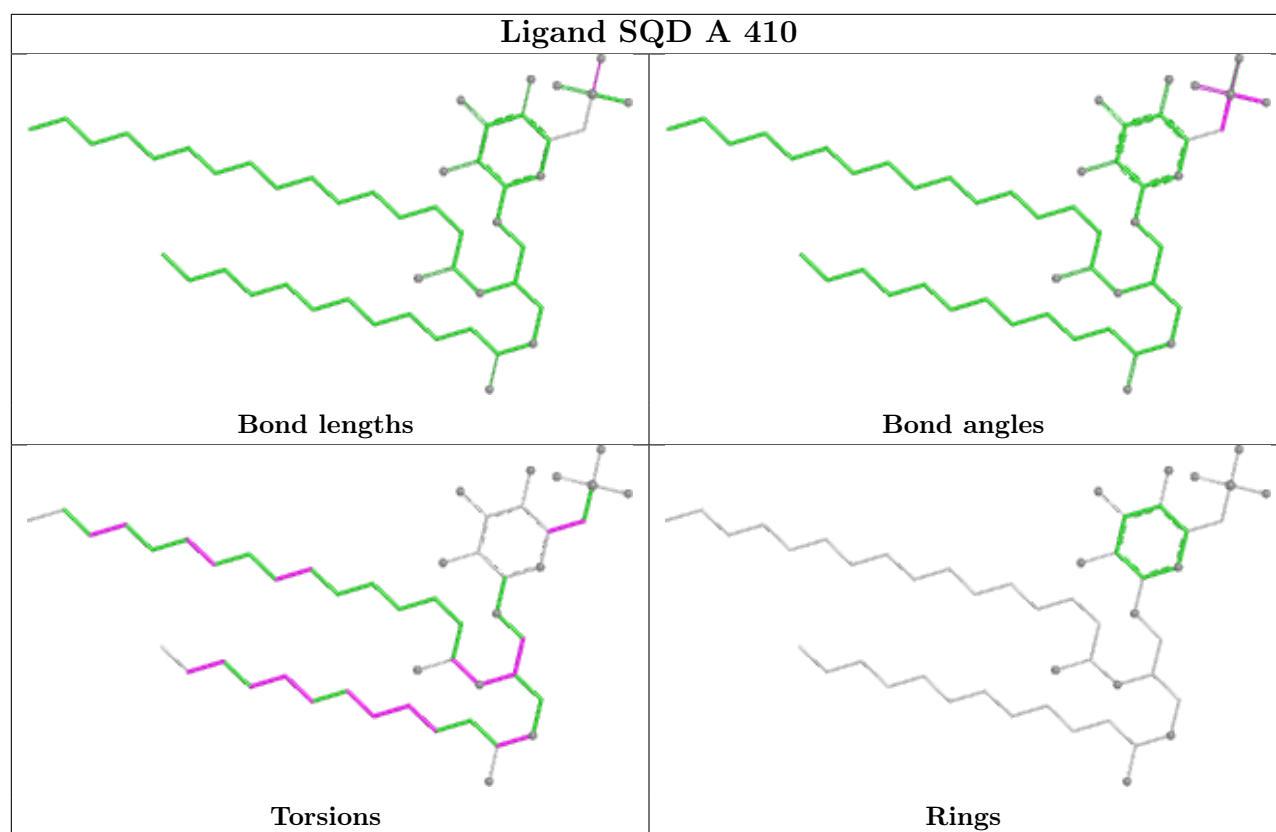


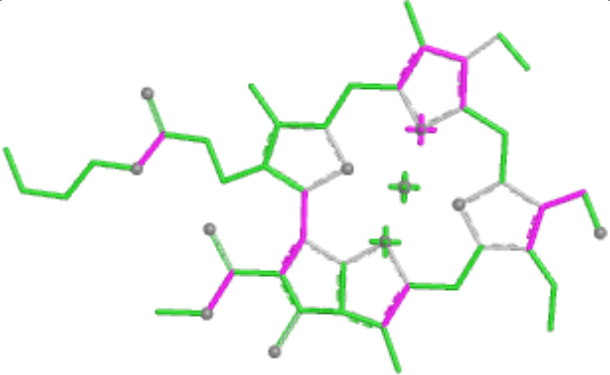
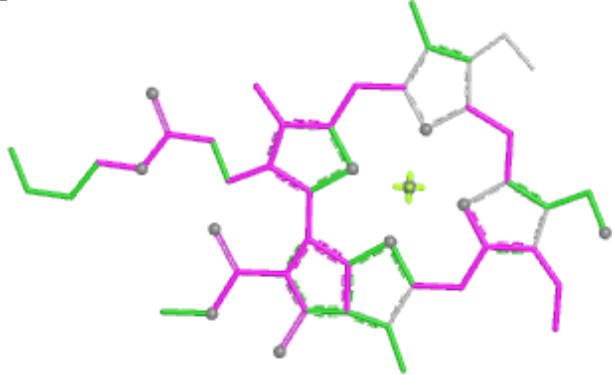
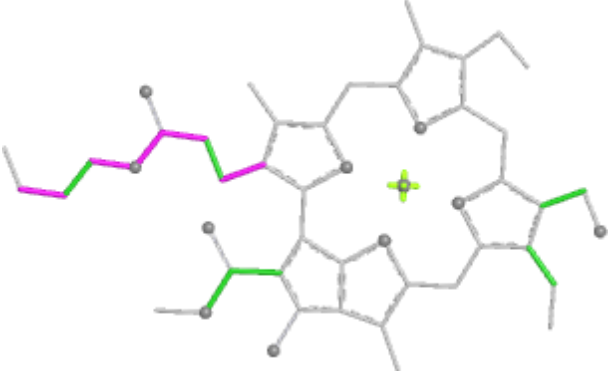
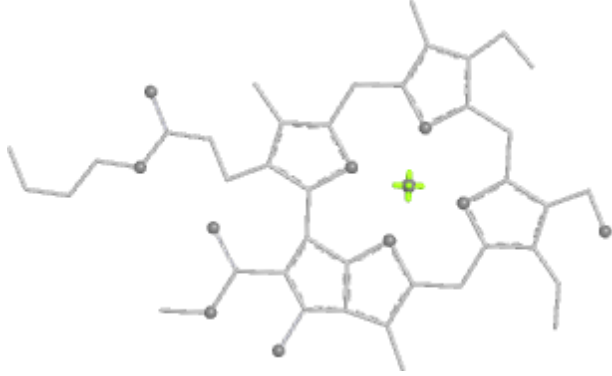

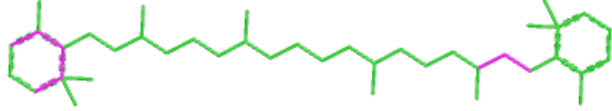
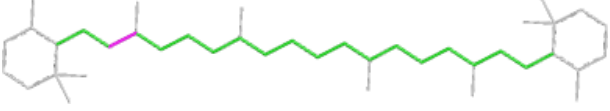
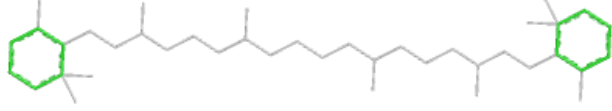
Ligand CLA n 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

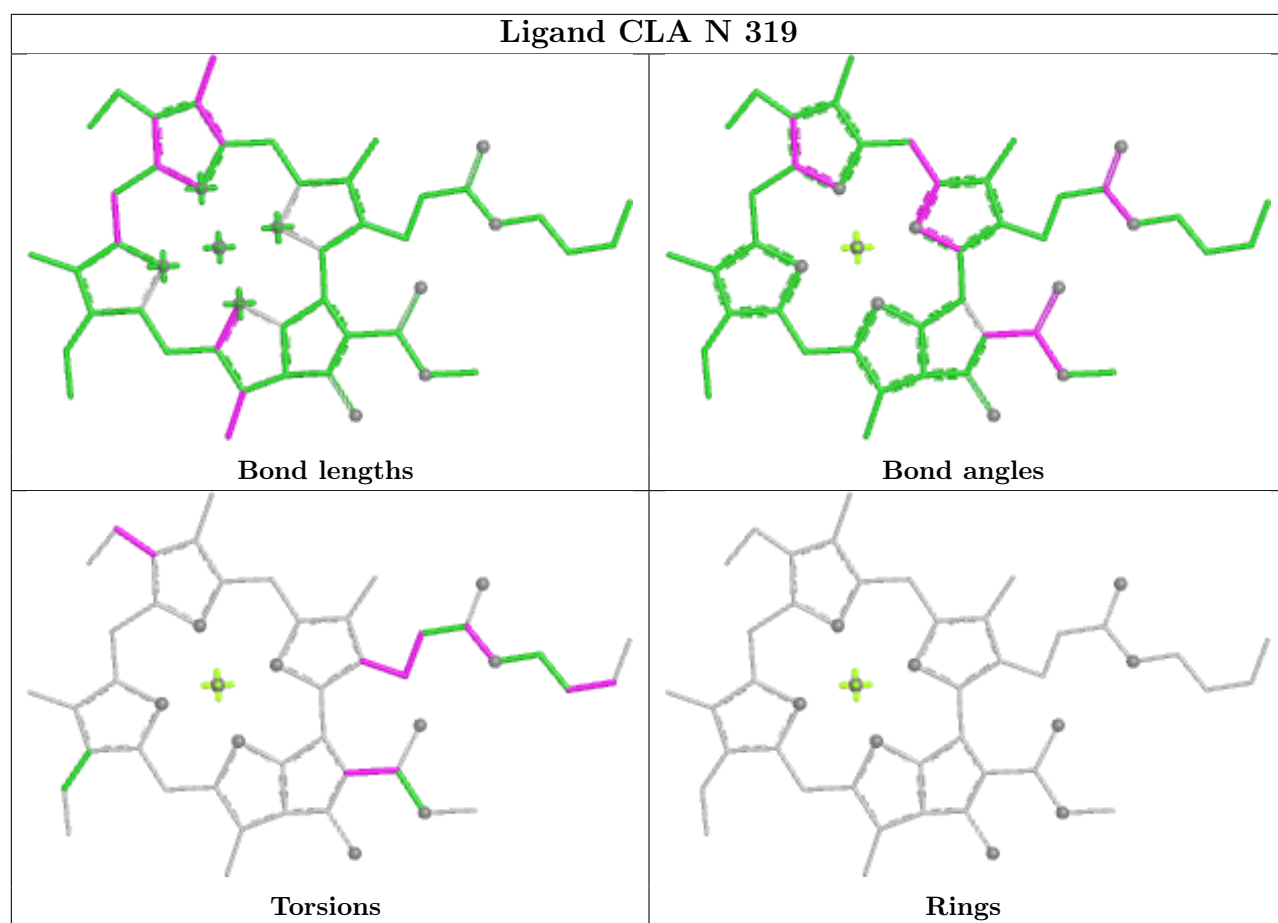
Ligand LUT n 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT s 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

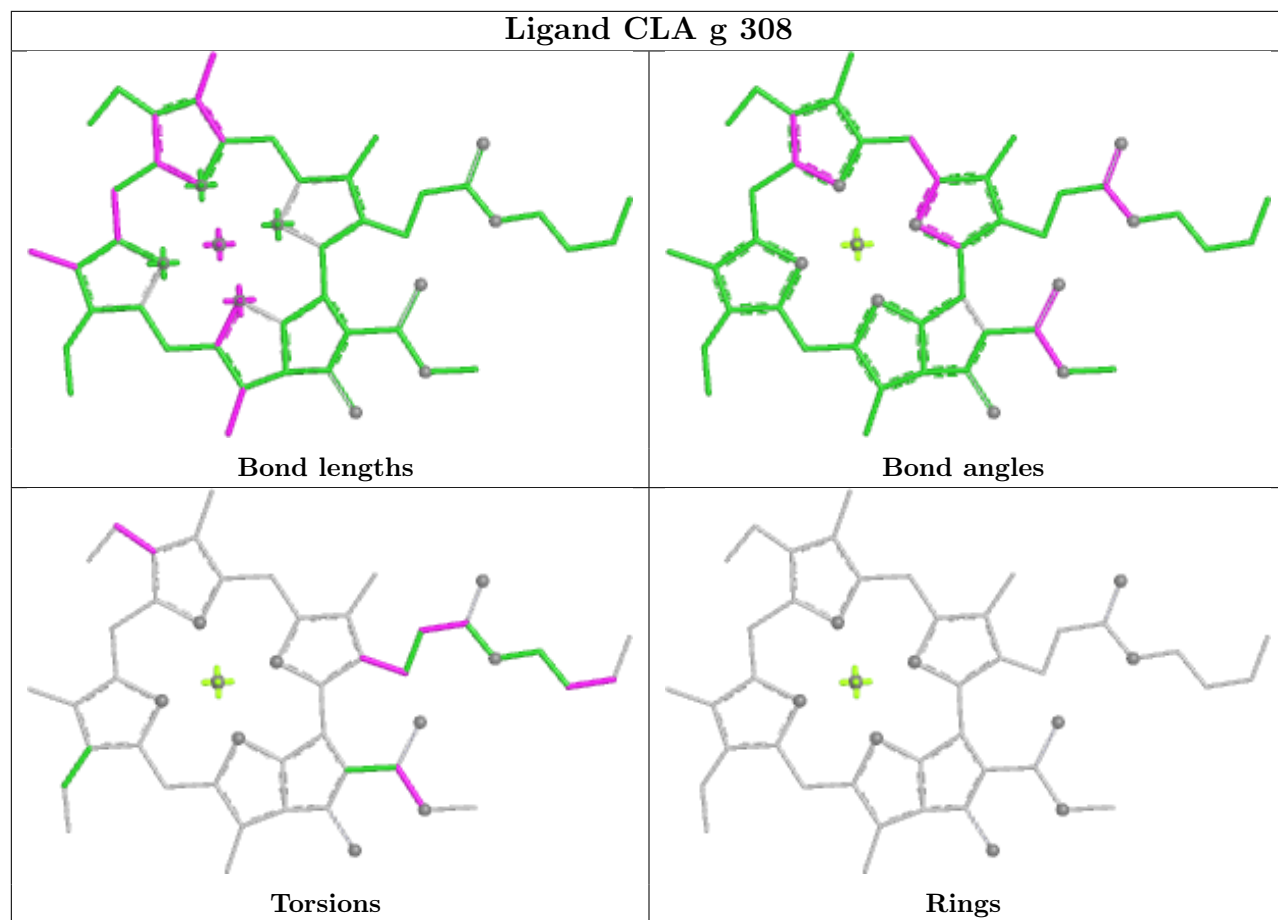


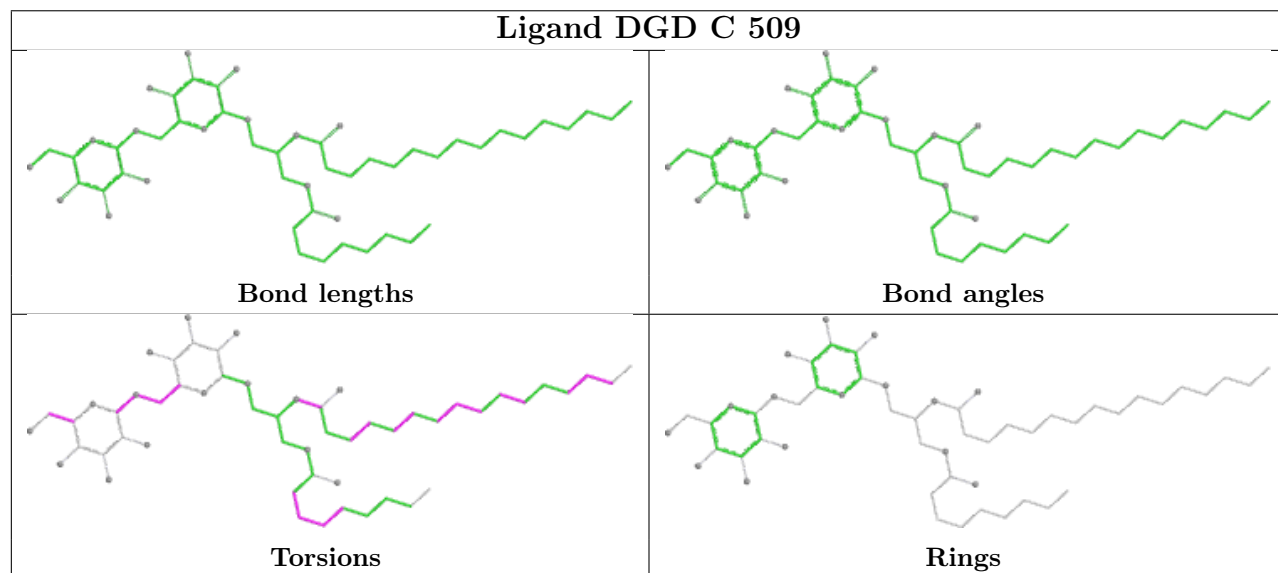
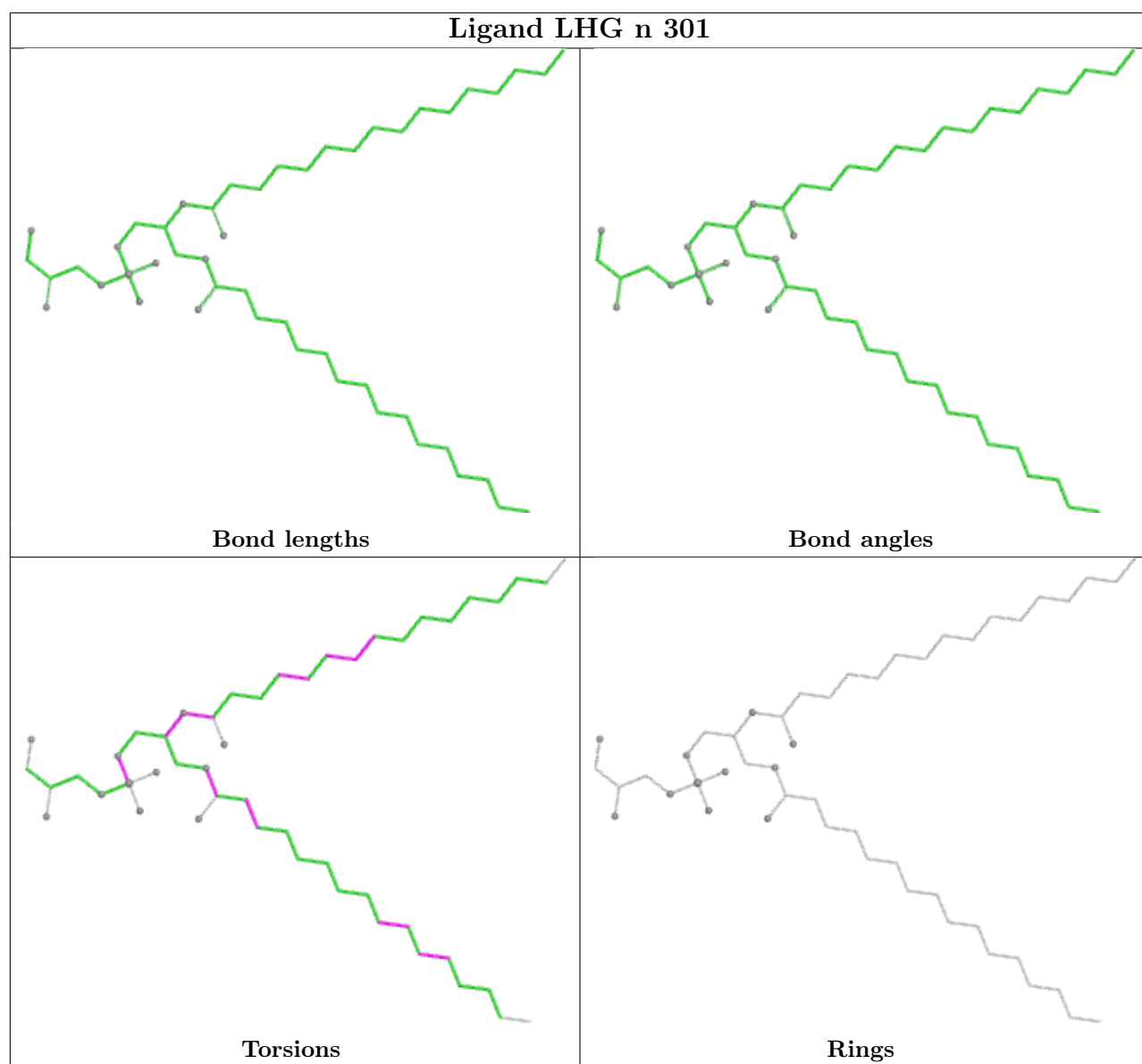


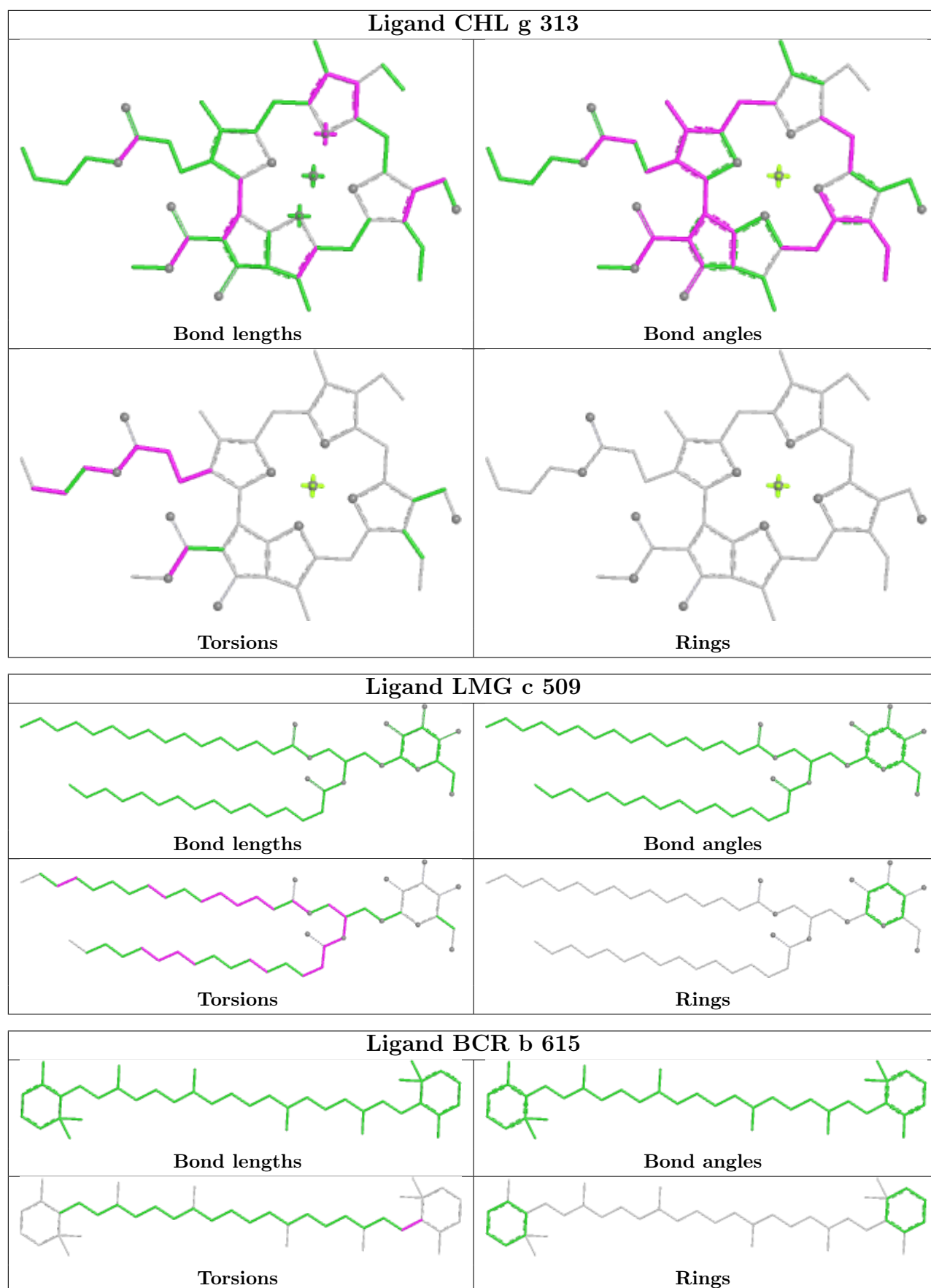
Ligand CHL S 313	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR k 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



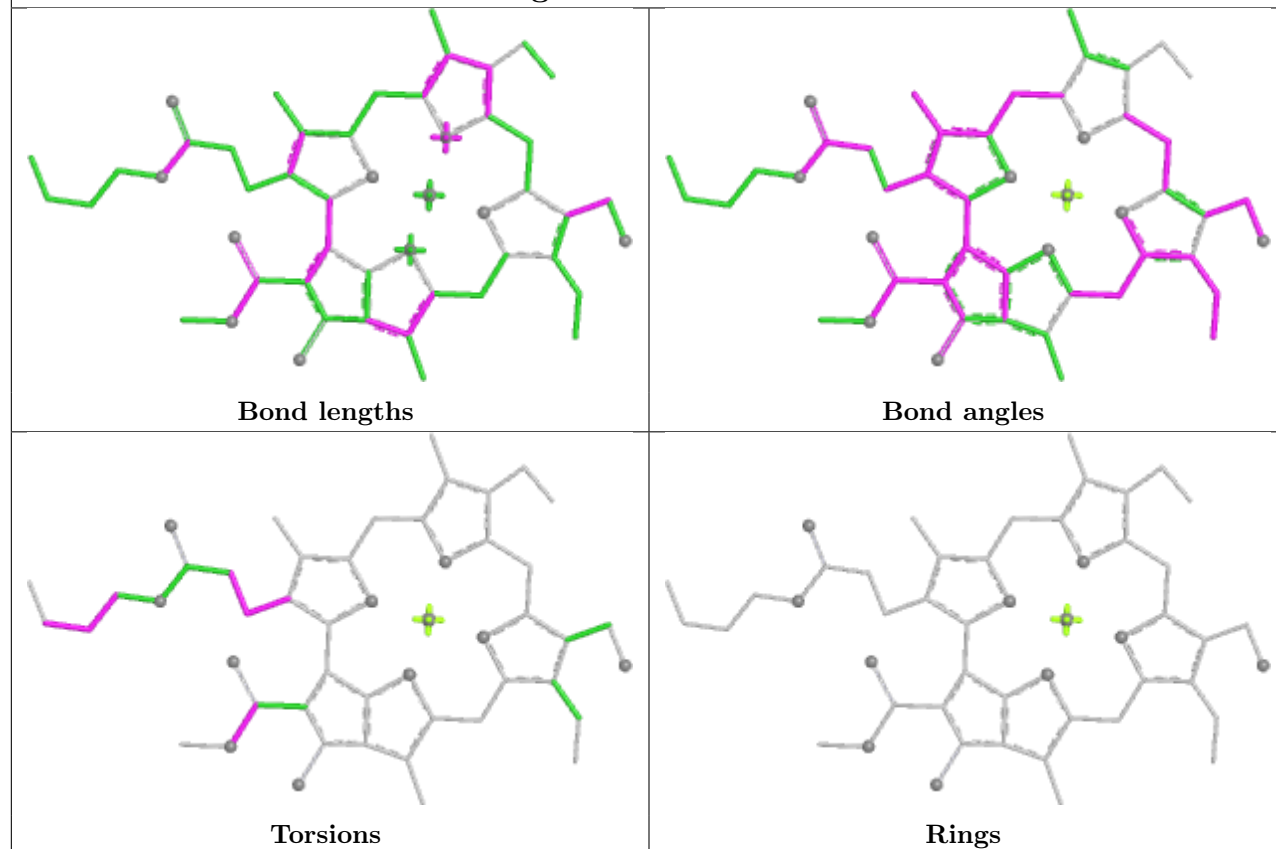
Ligand CLA g 308



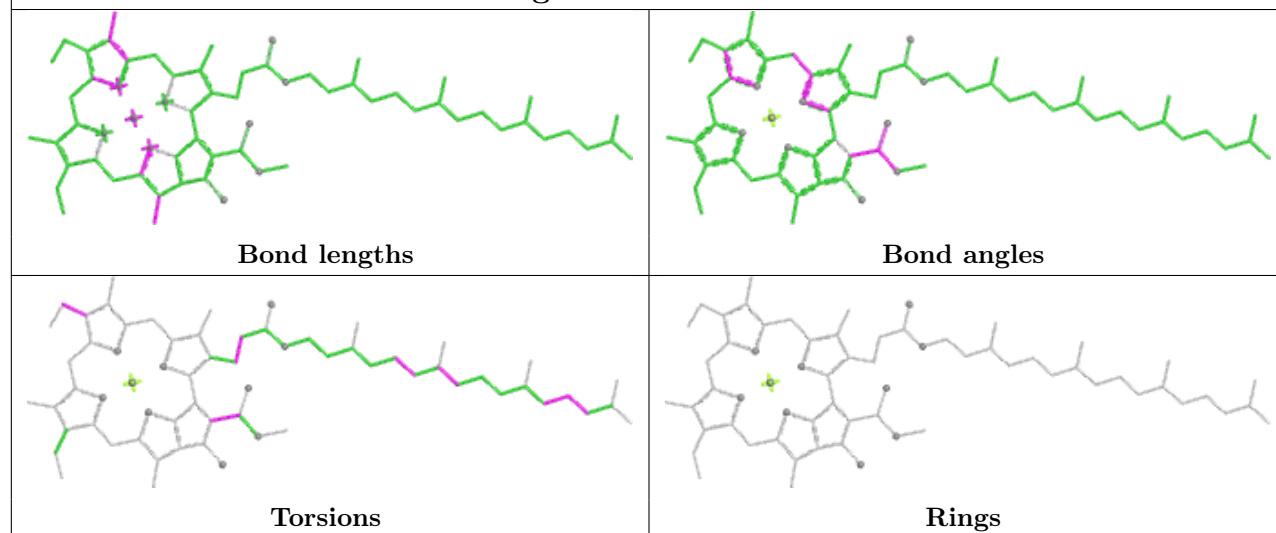


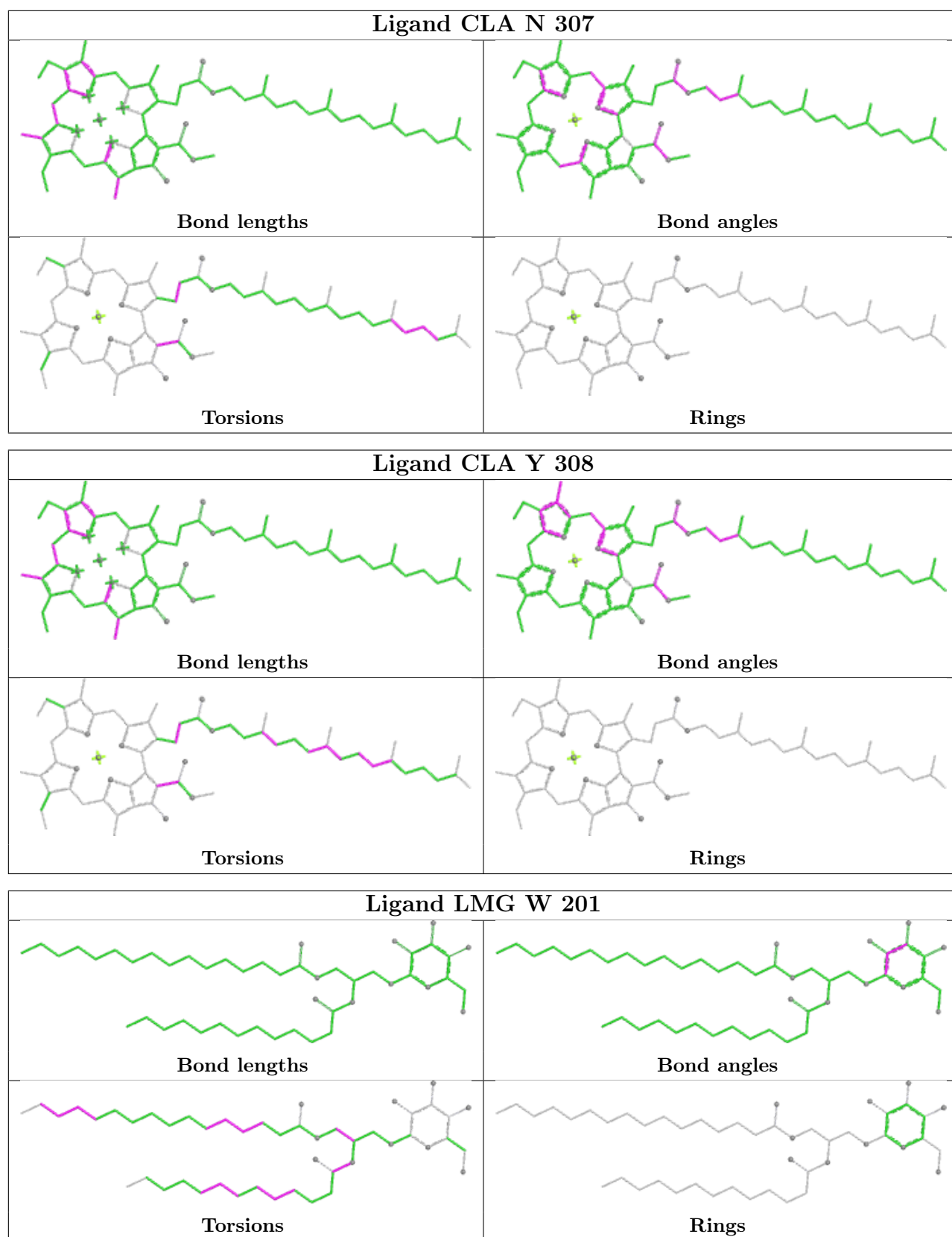


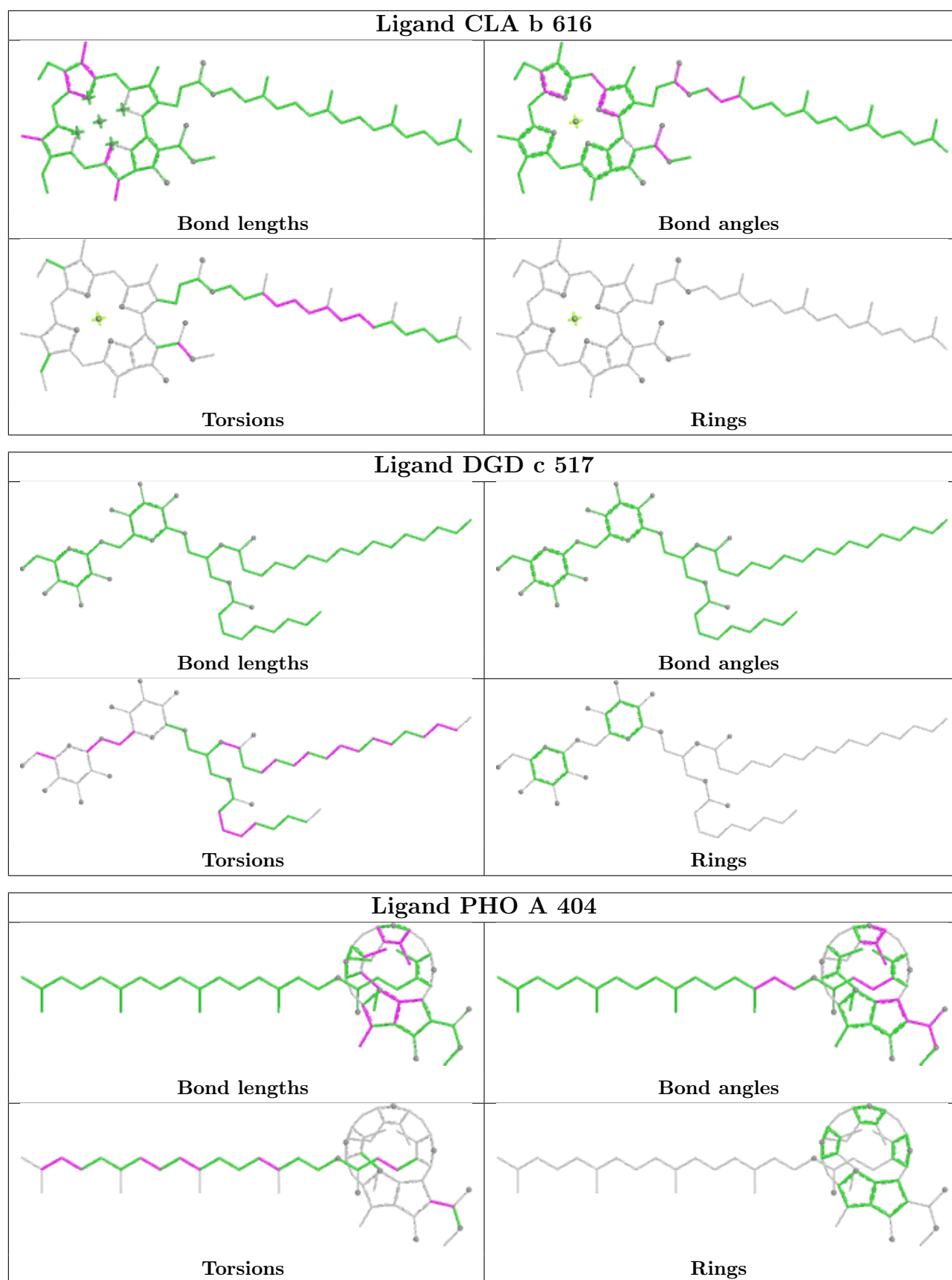
Ligand CHL Y 318

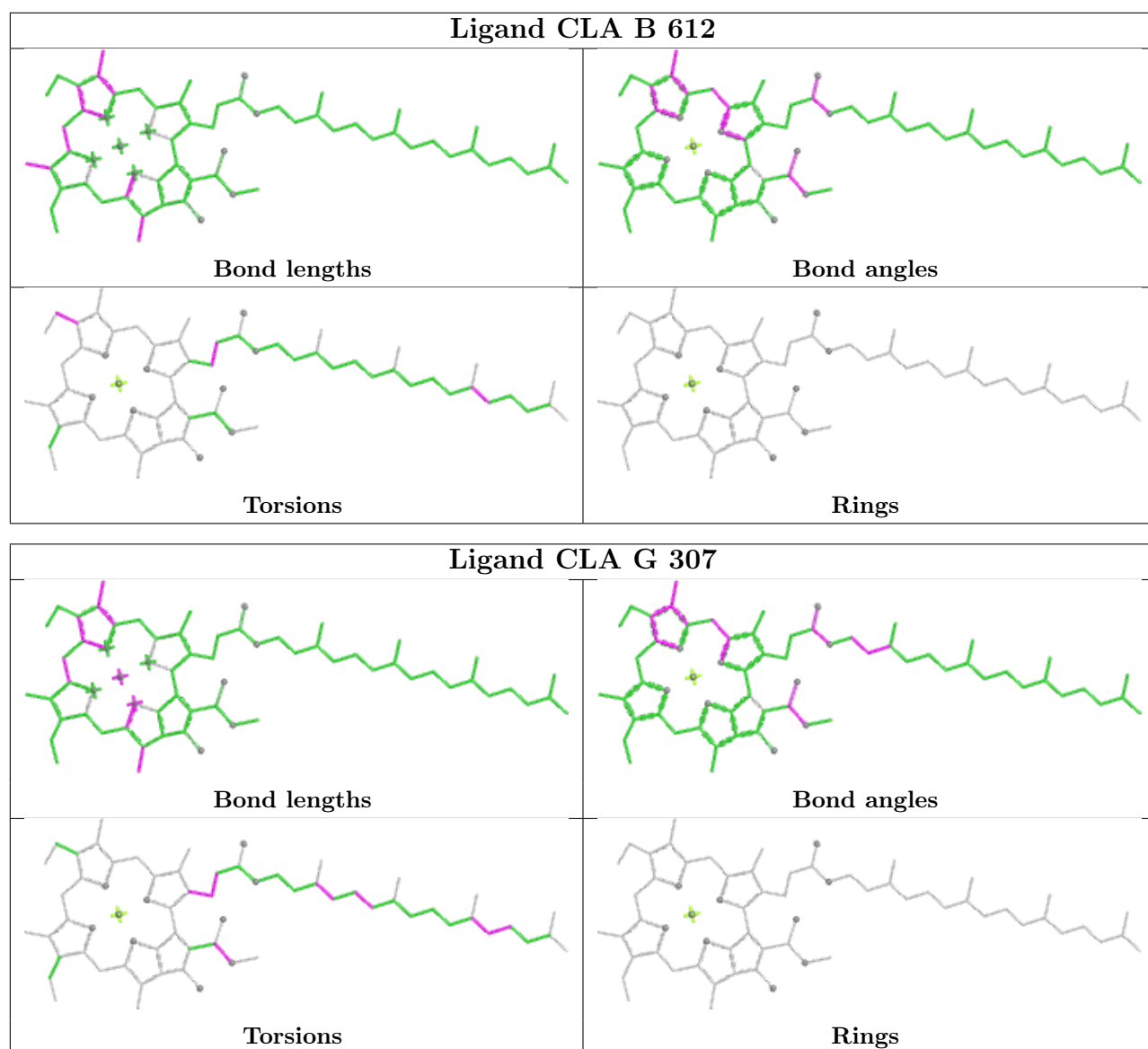


Ligand CLA C 516

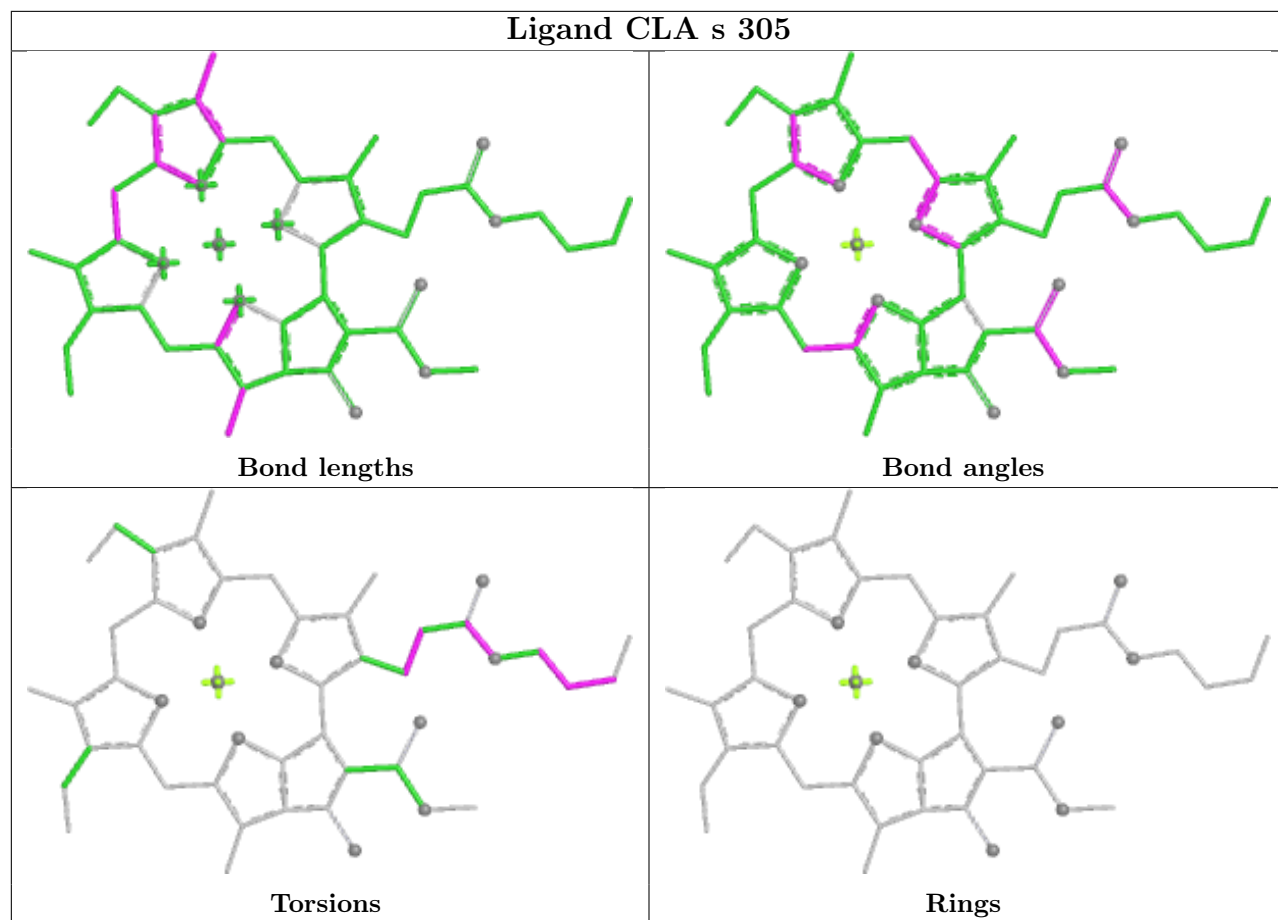


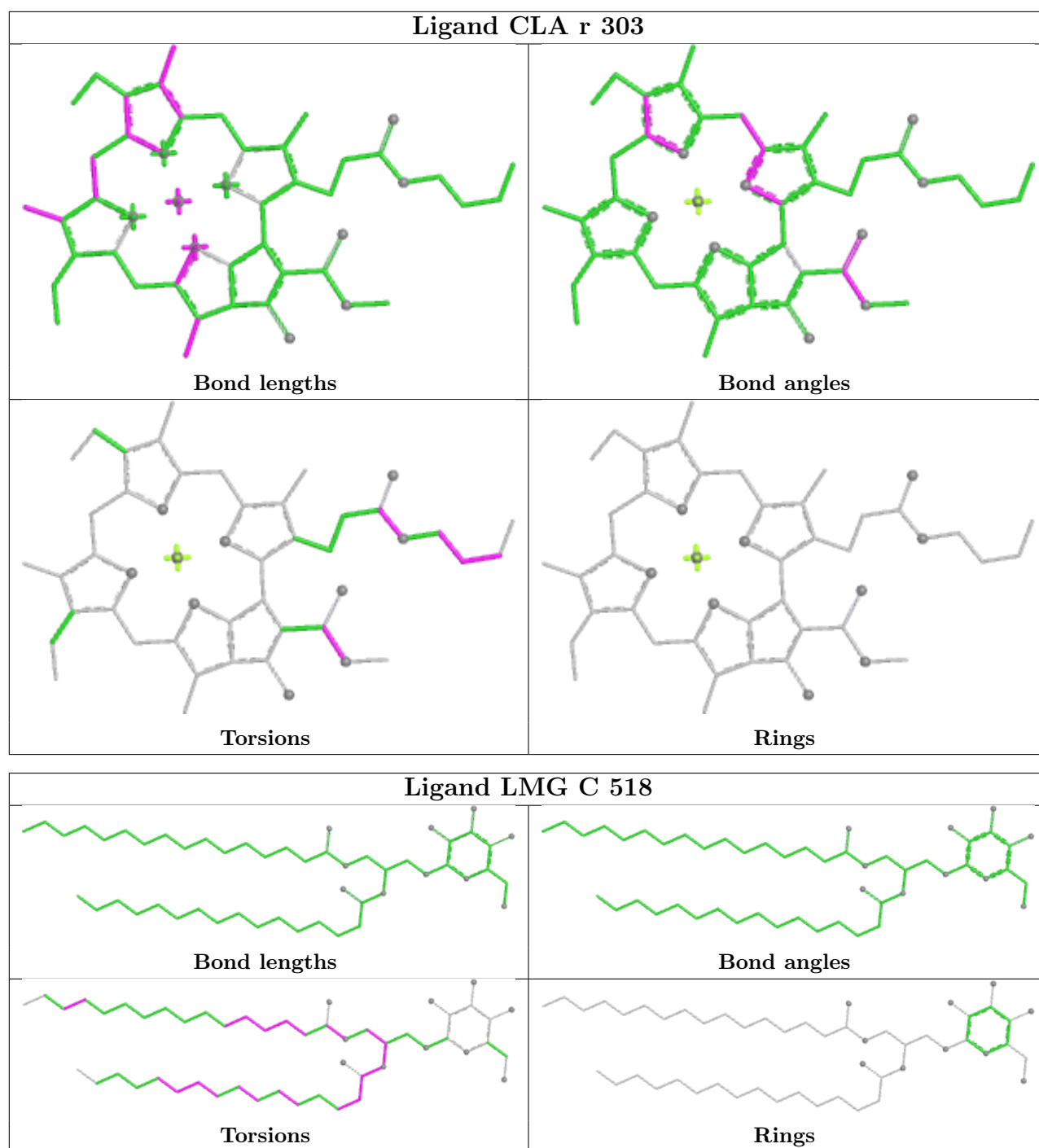


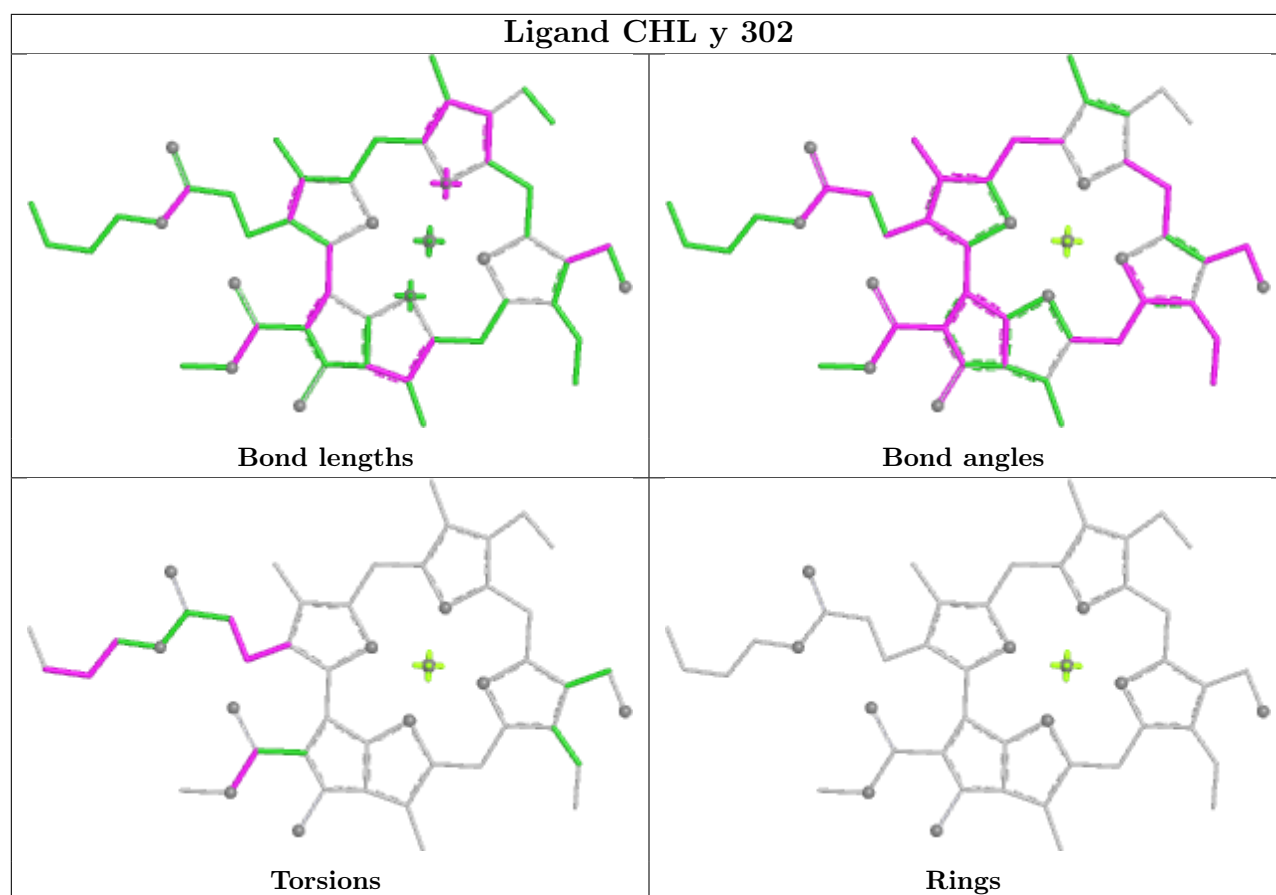




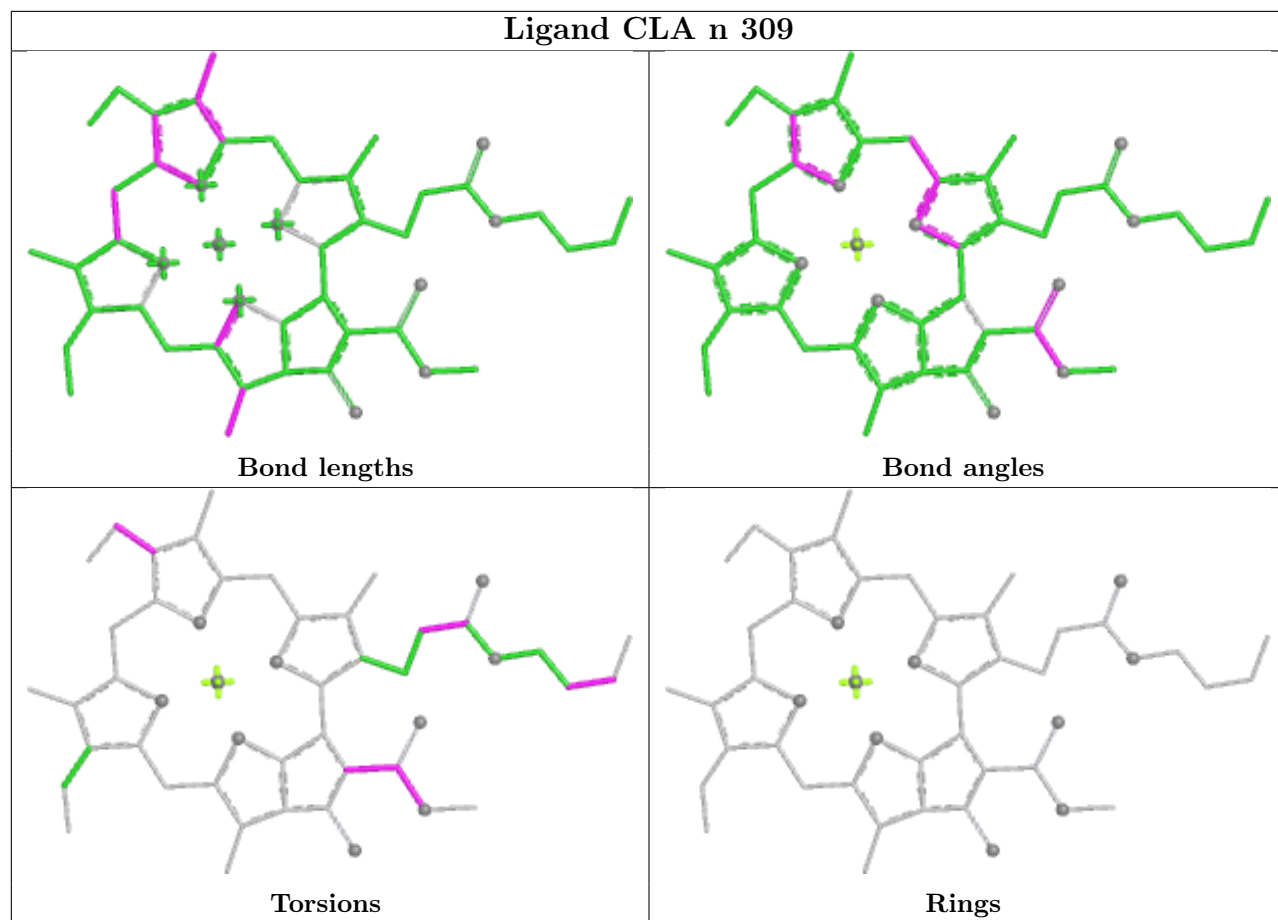
Ligand CLA s 305



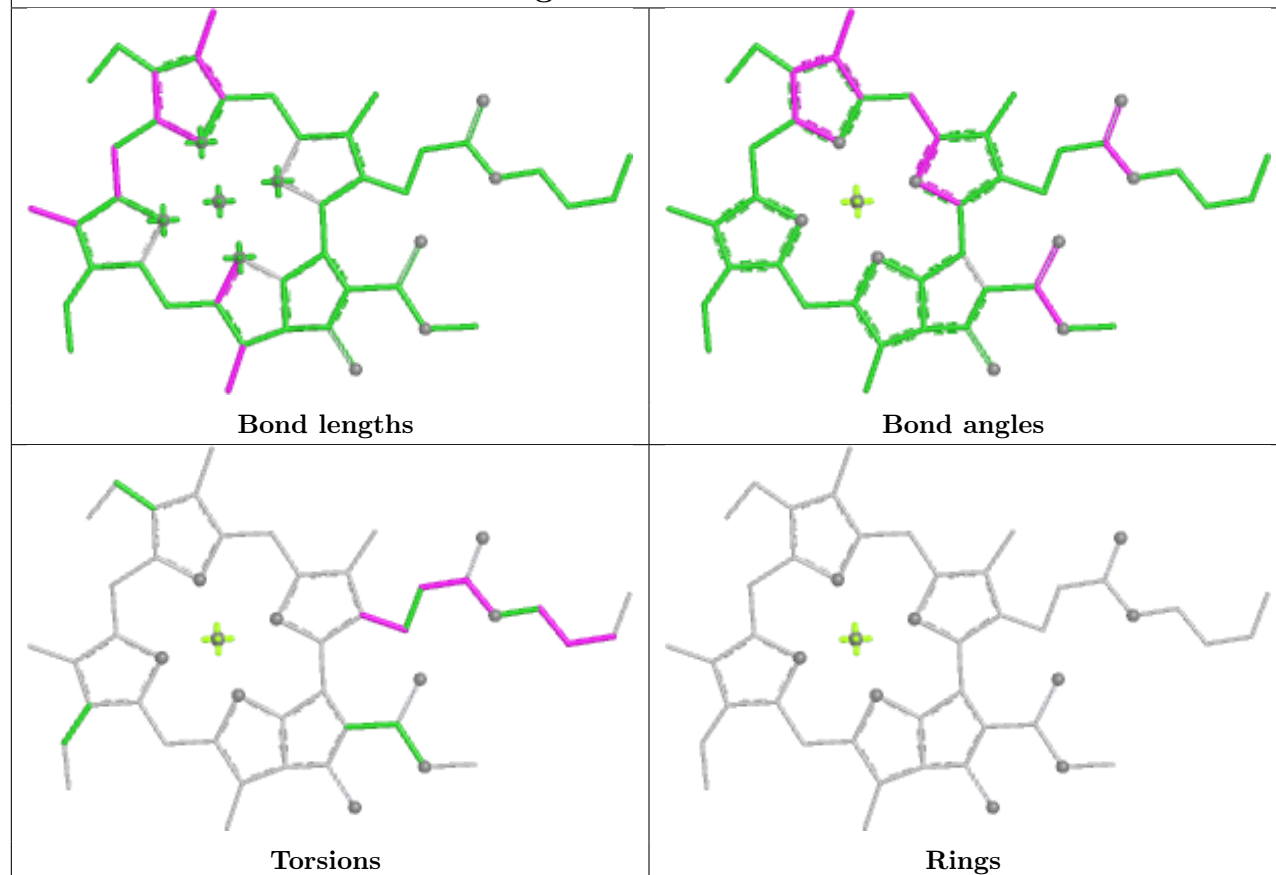




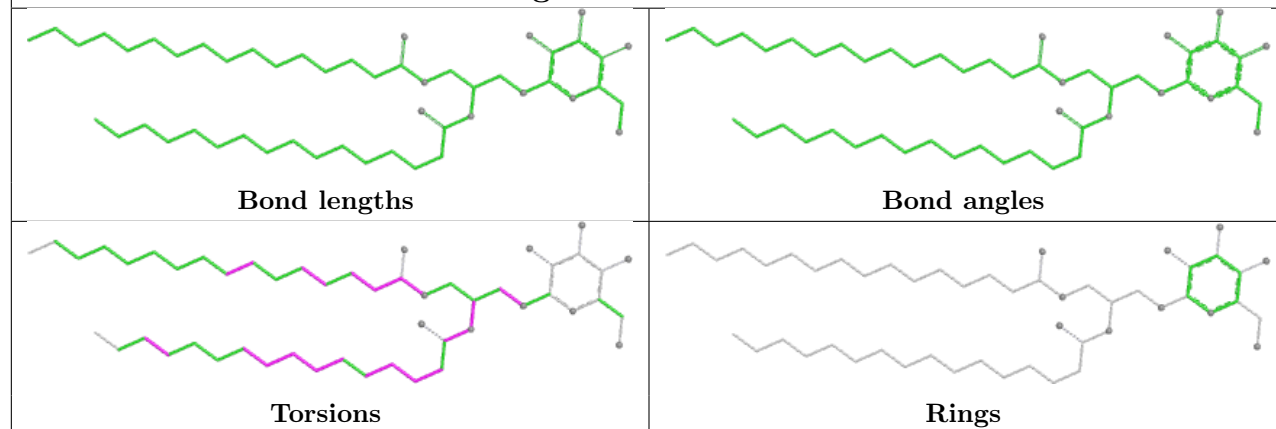
Ligand CLA n 309

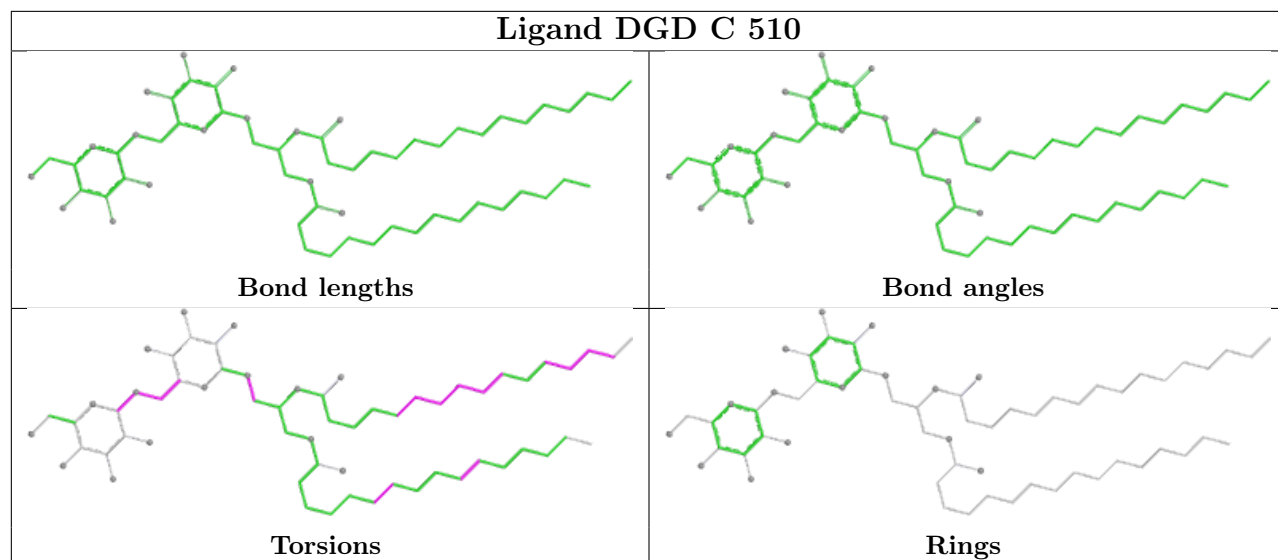
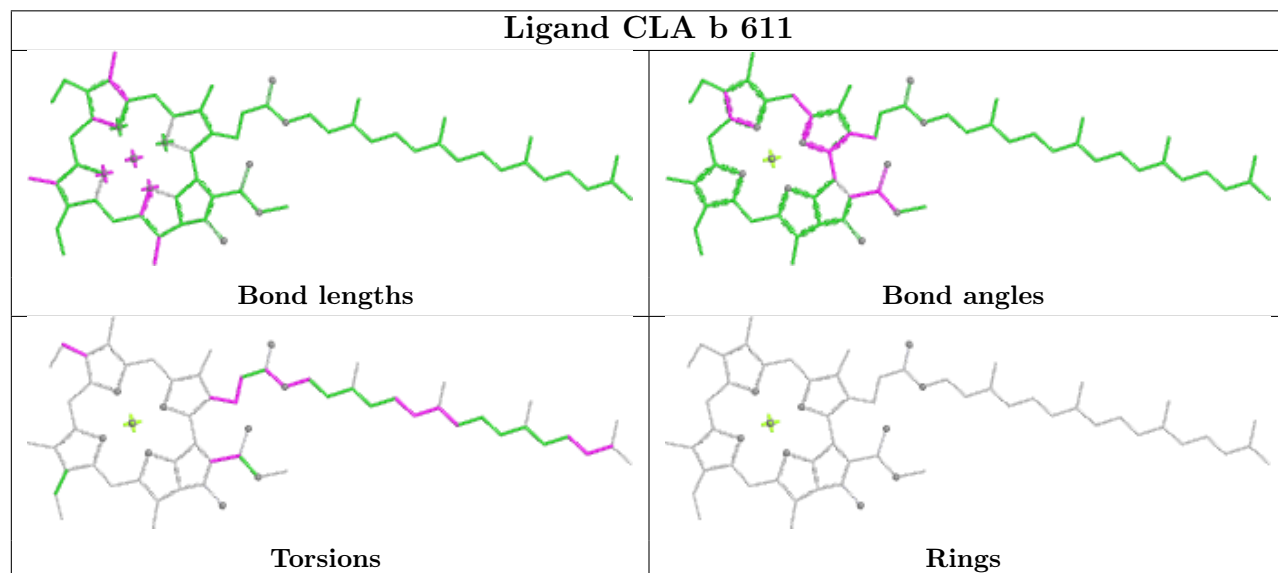
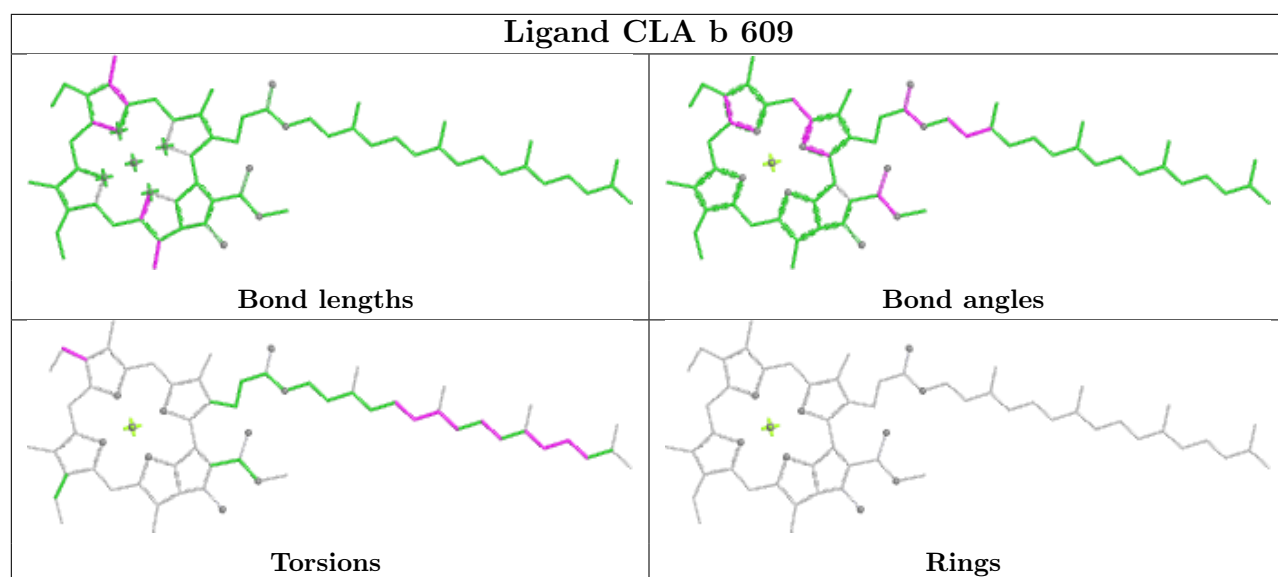


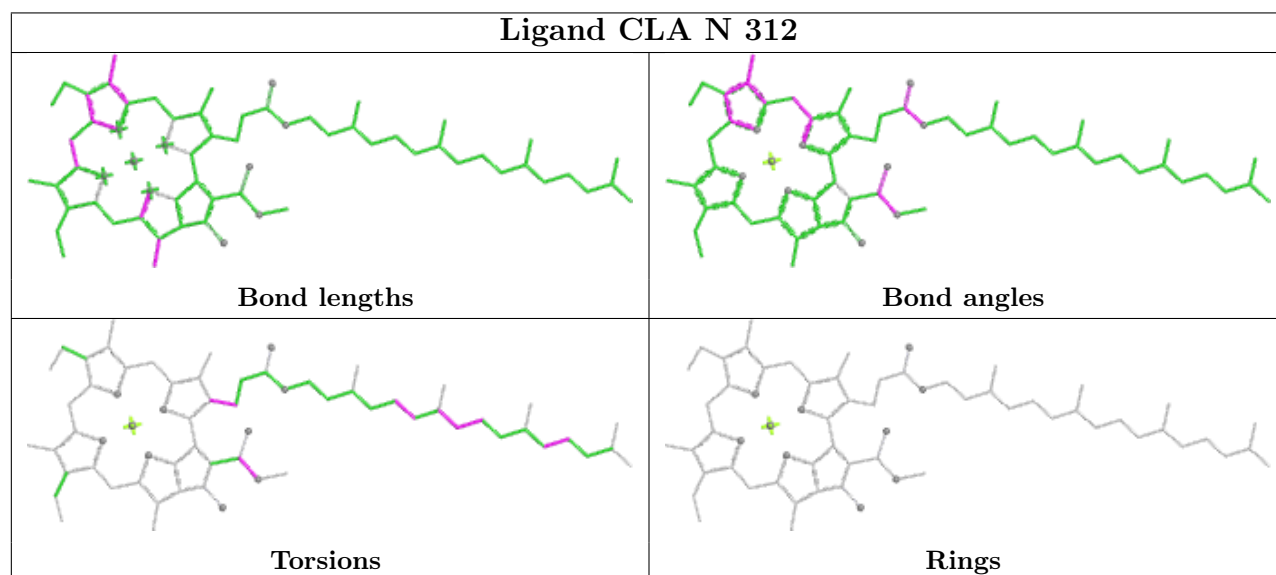
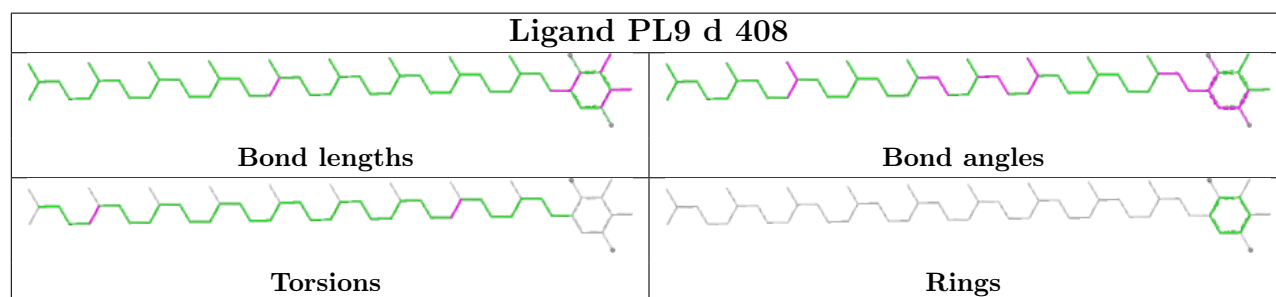
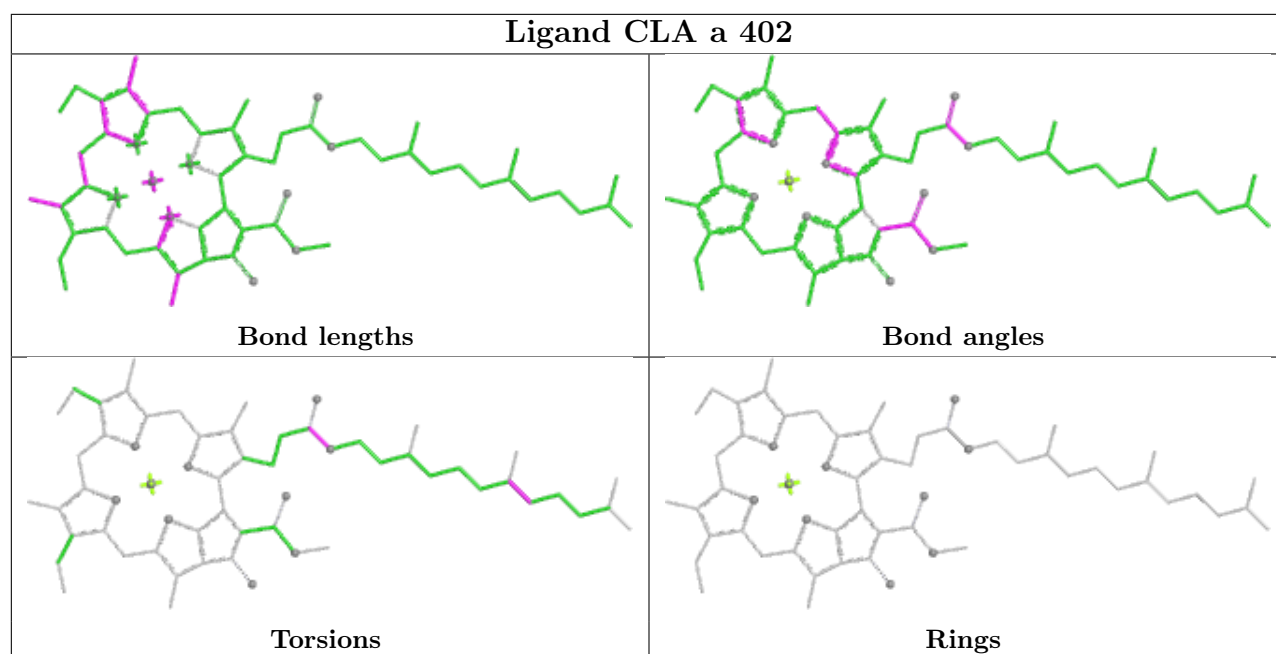
Ligand CLA S 309



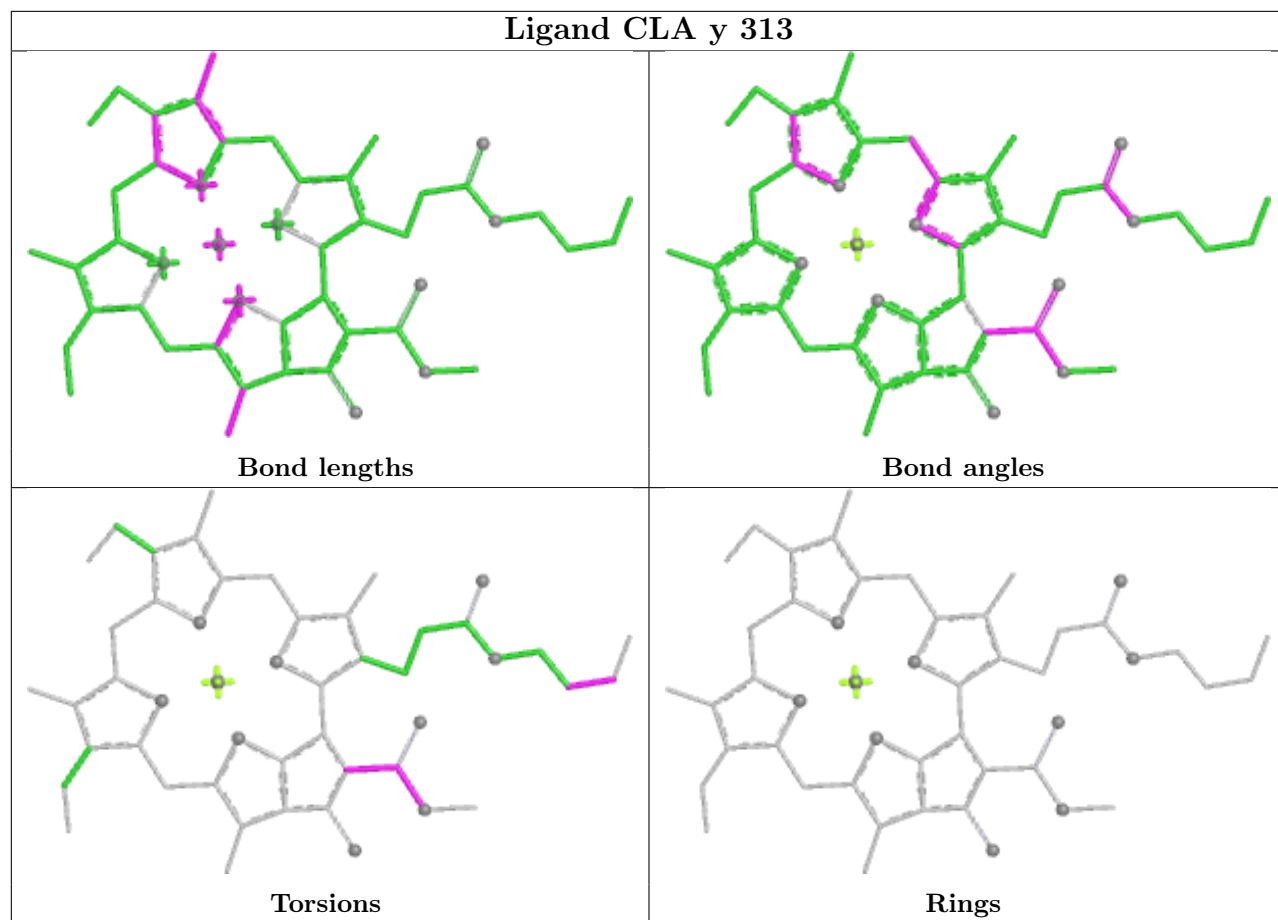
Ligand LMG c 512

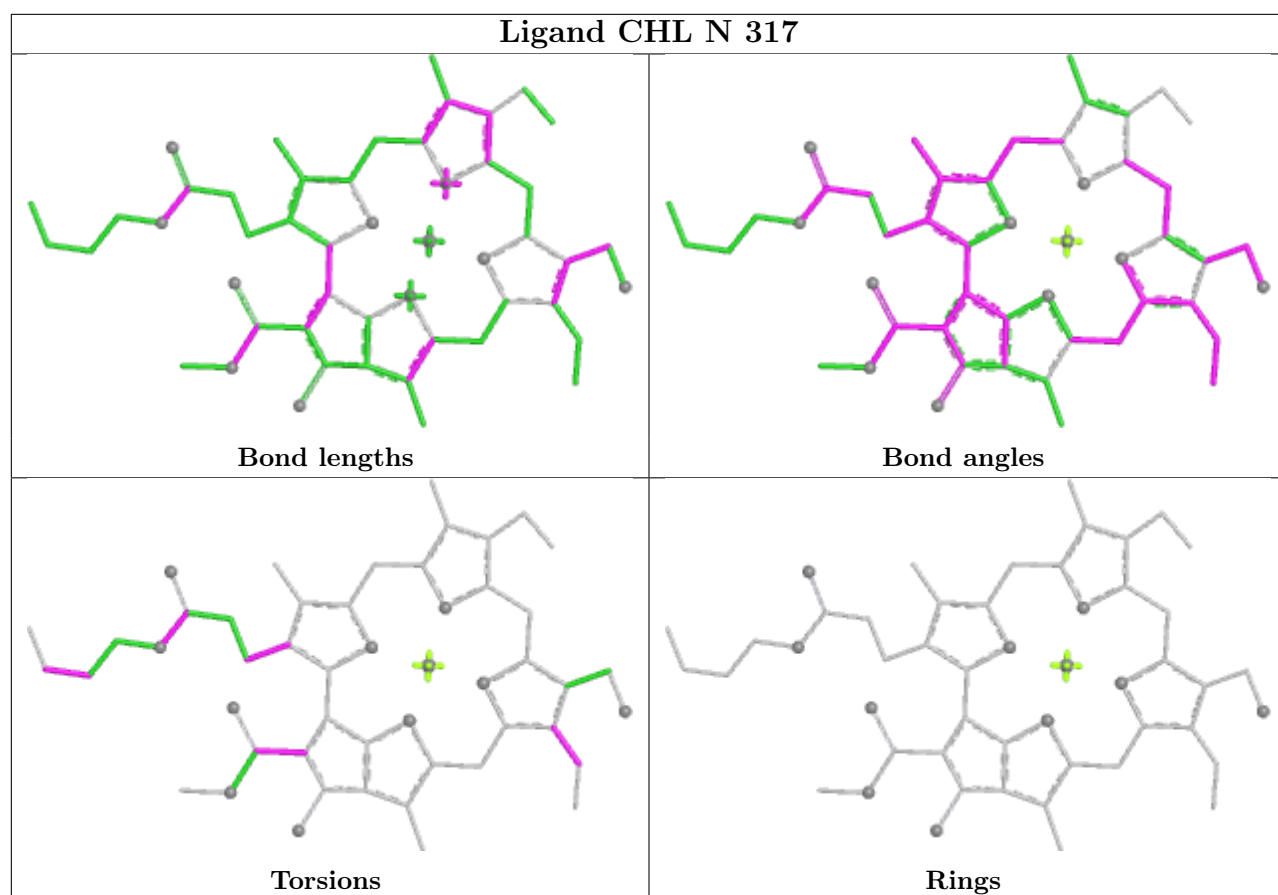


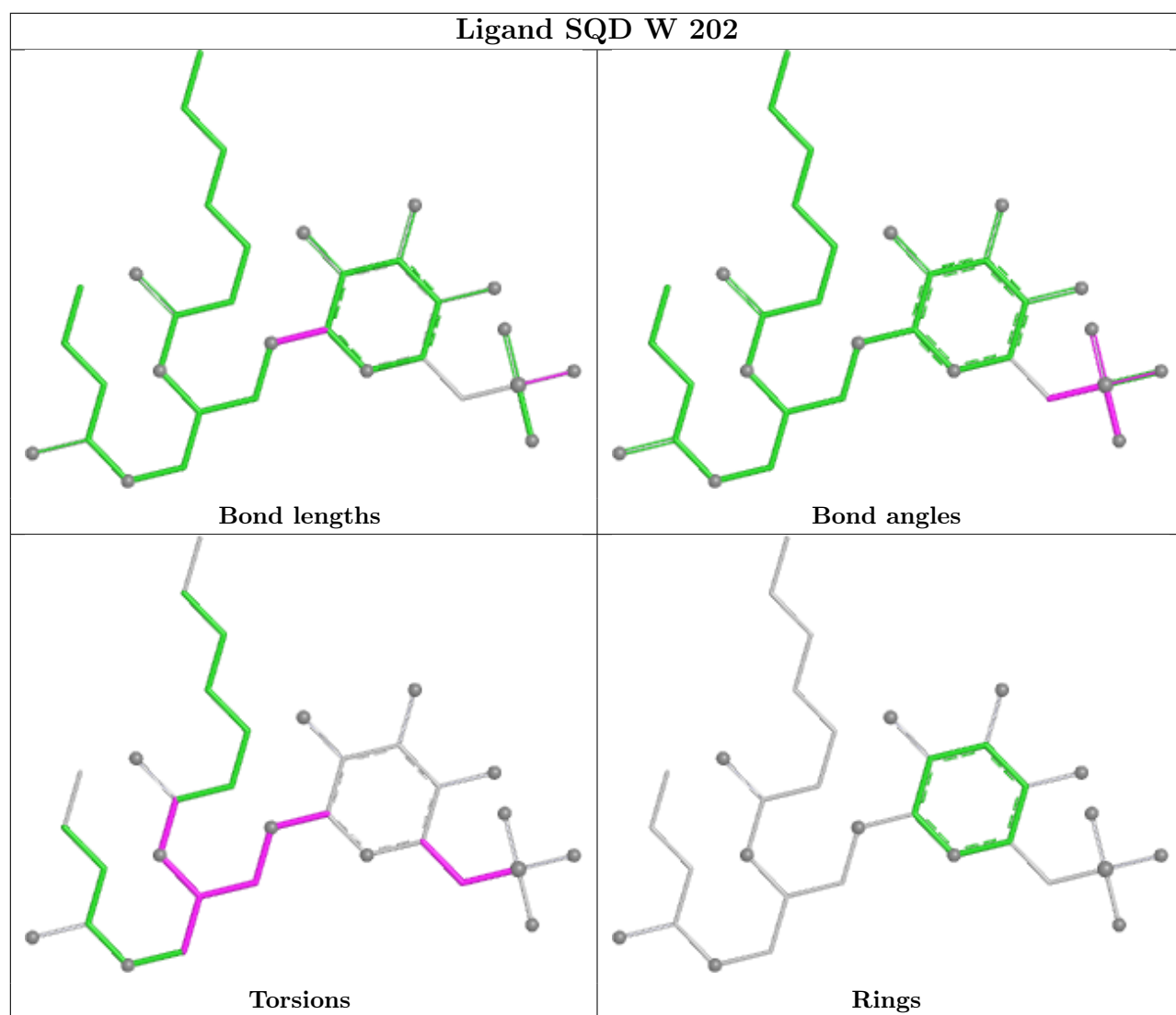


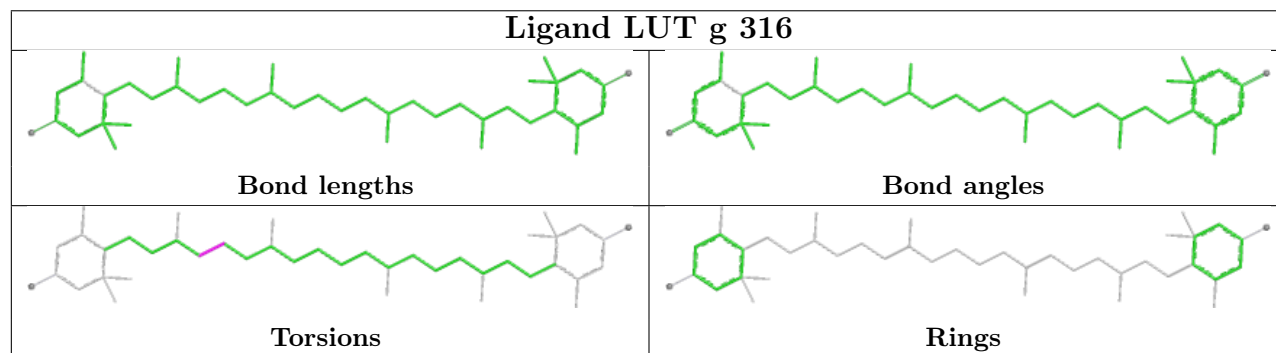
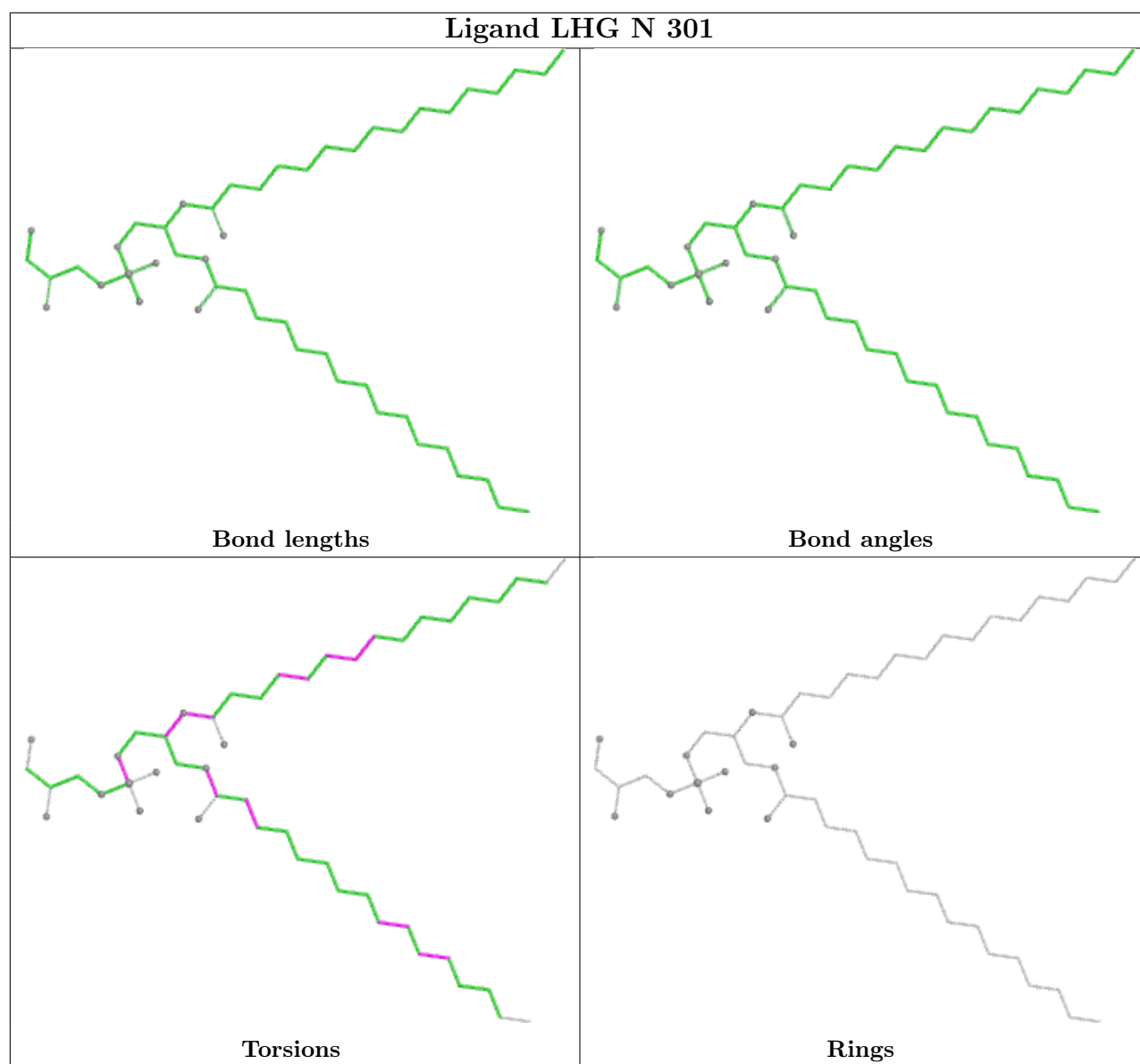


Ligand CLA y 313

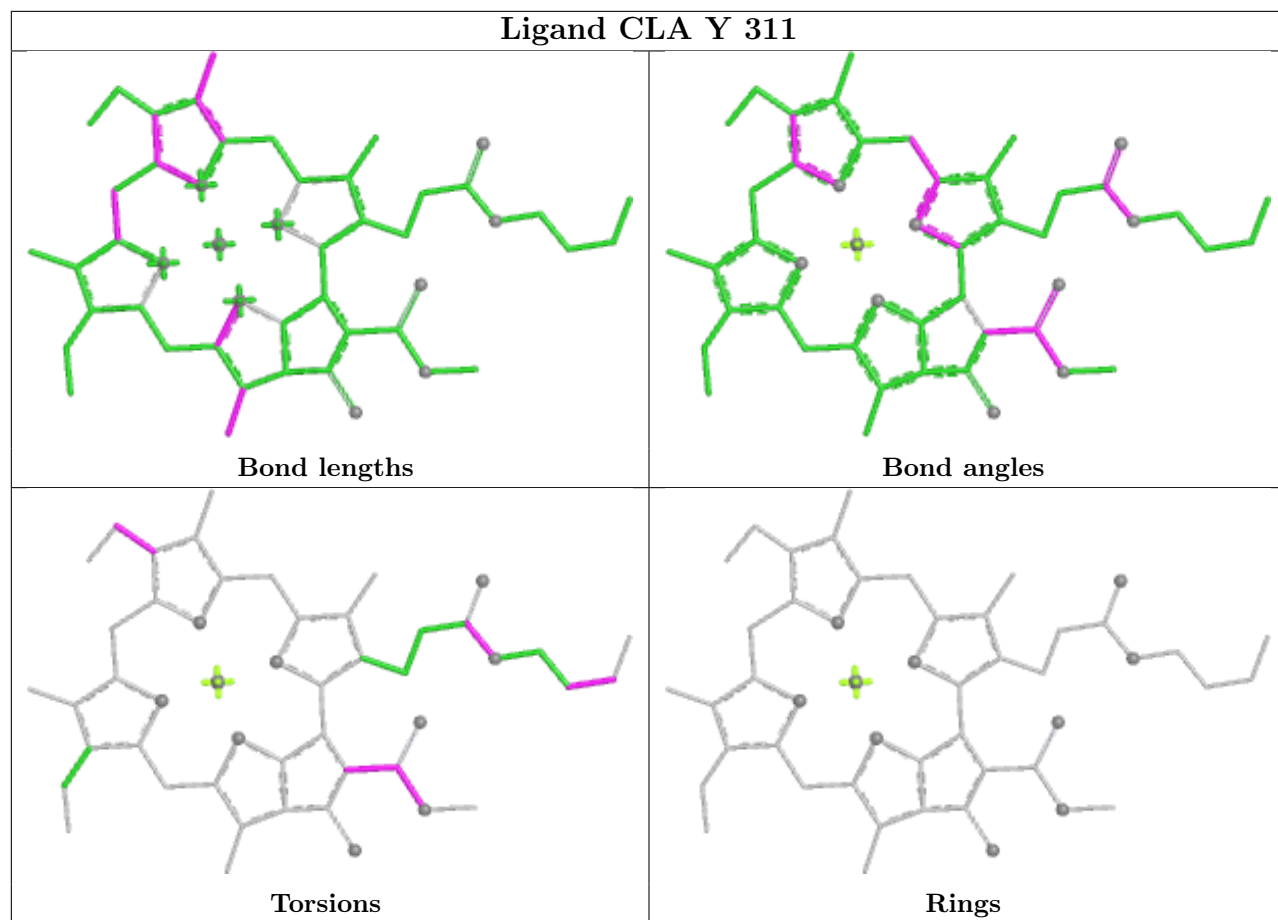




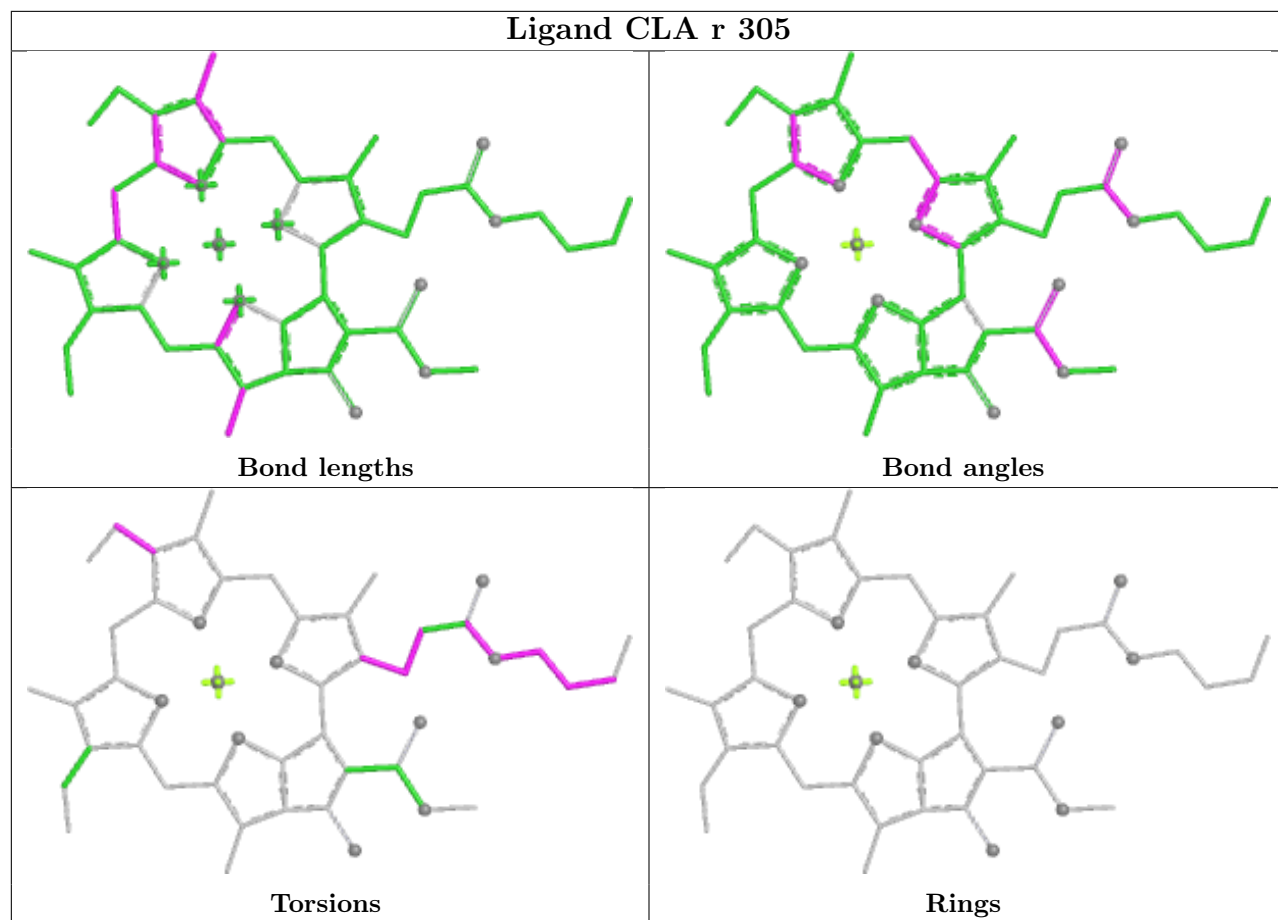


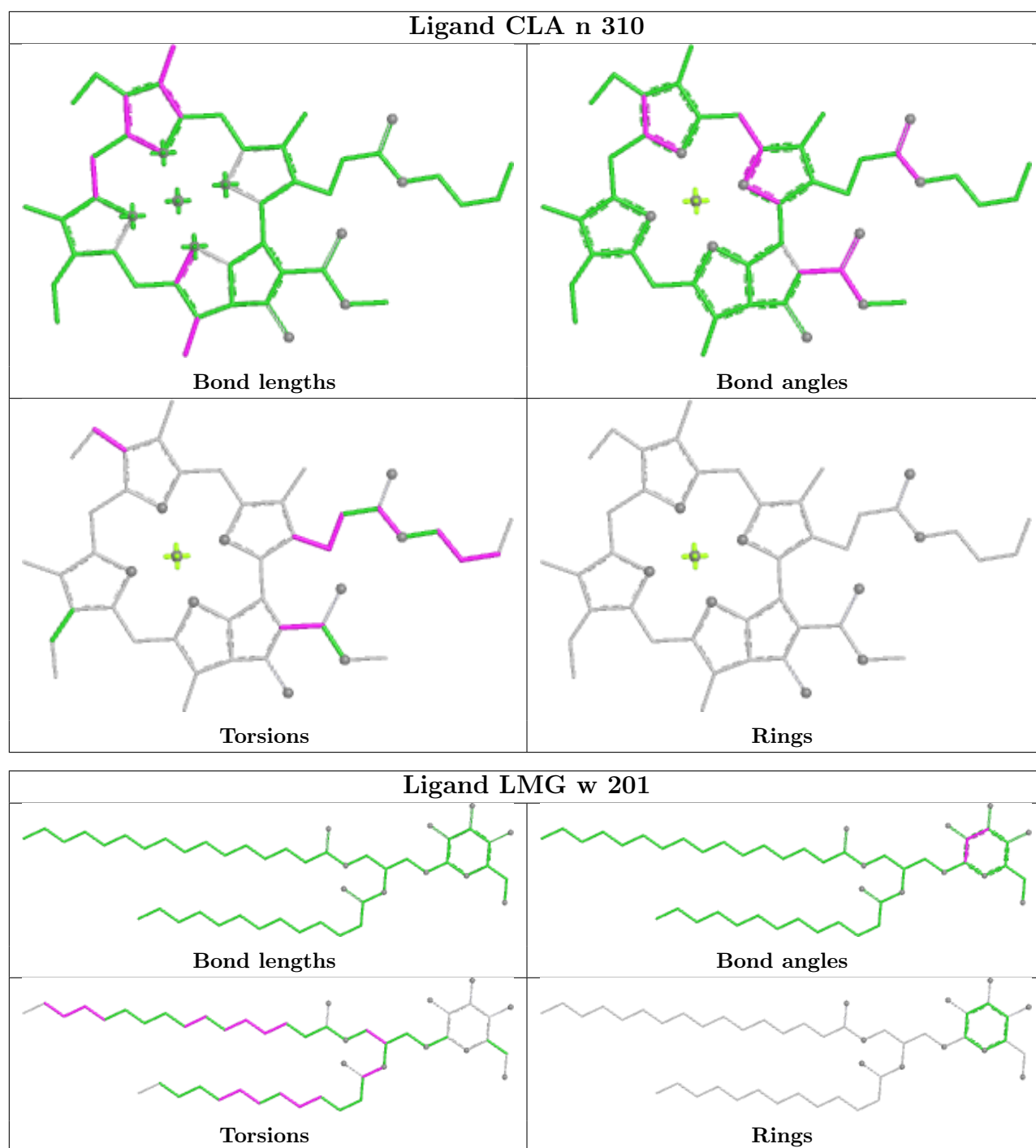


Ligand CLA Y 311

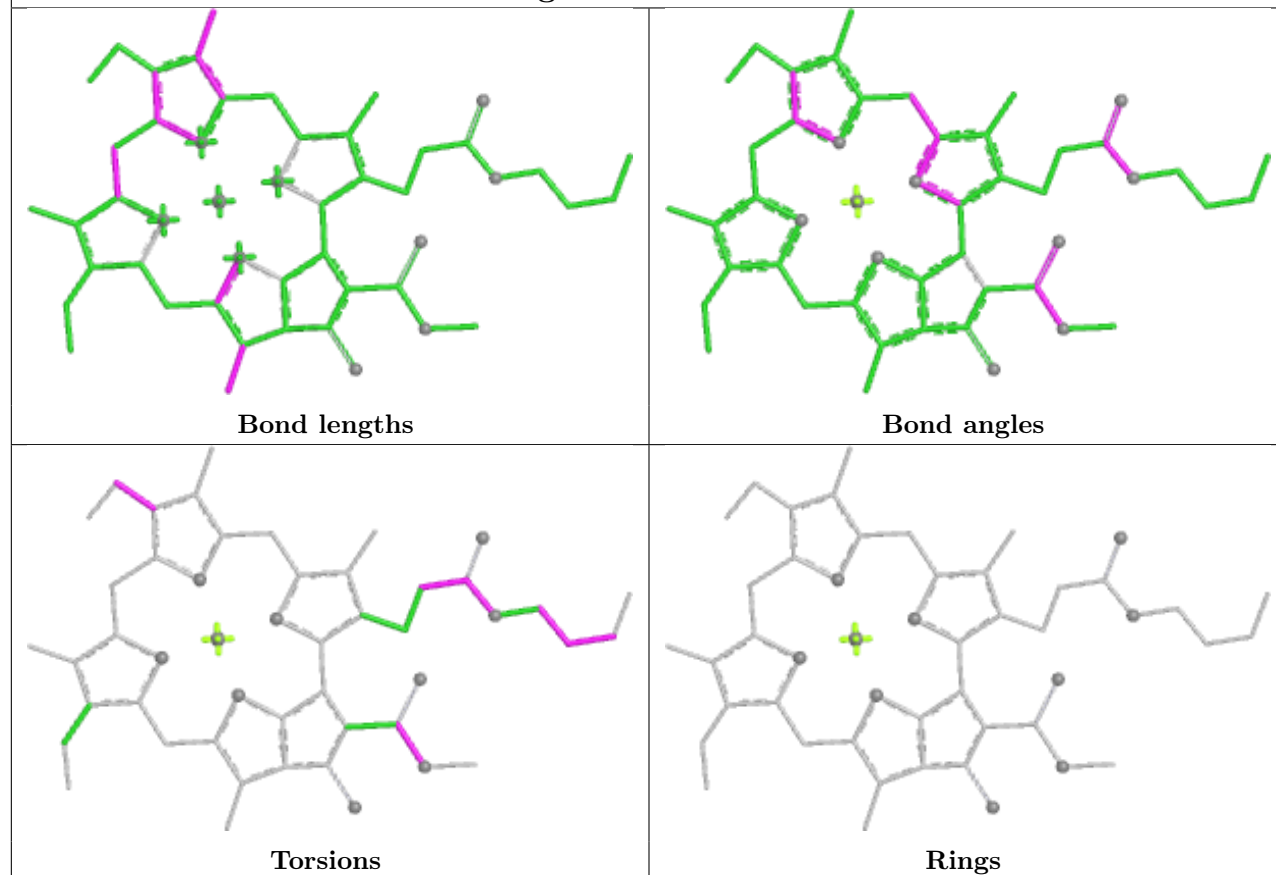


Ligand CLA r 305

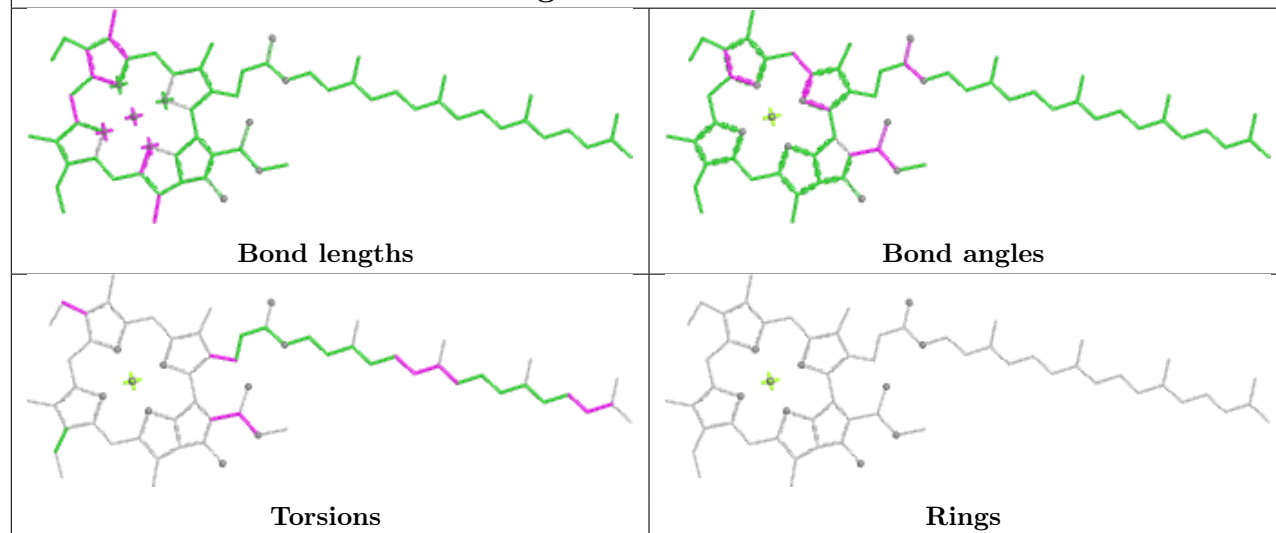


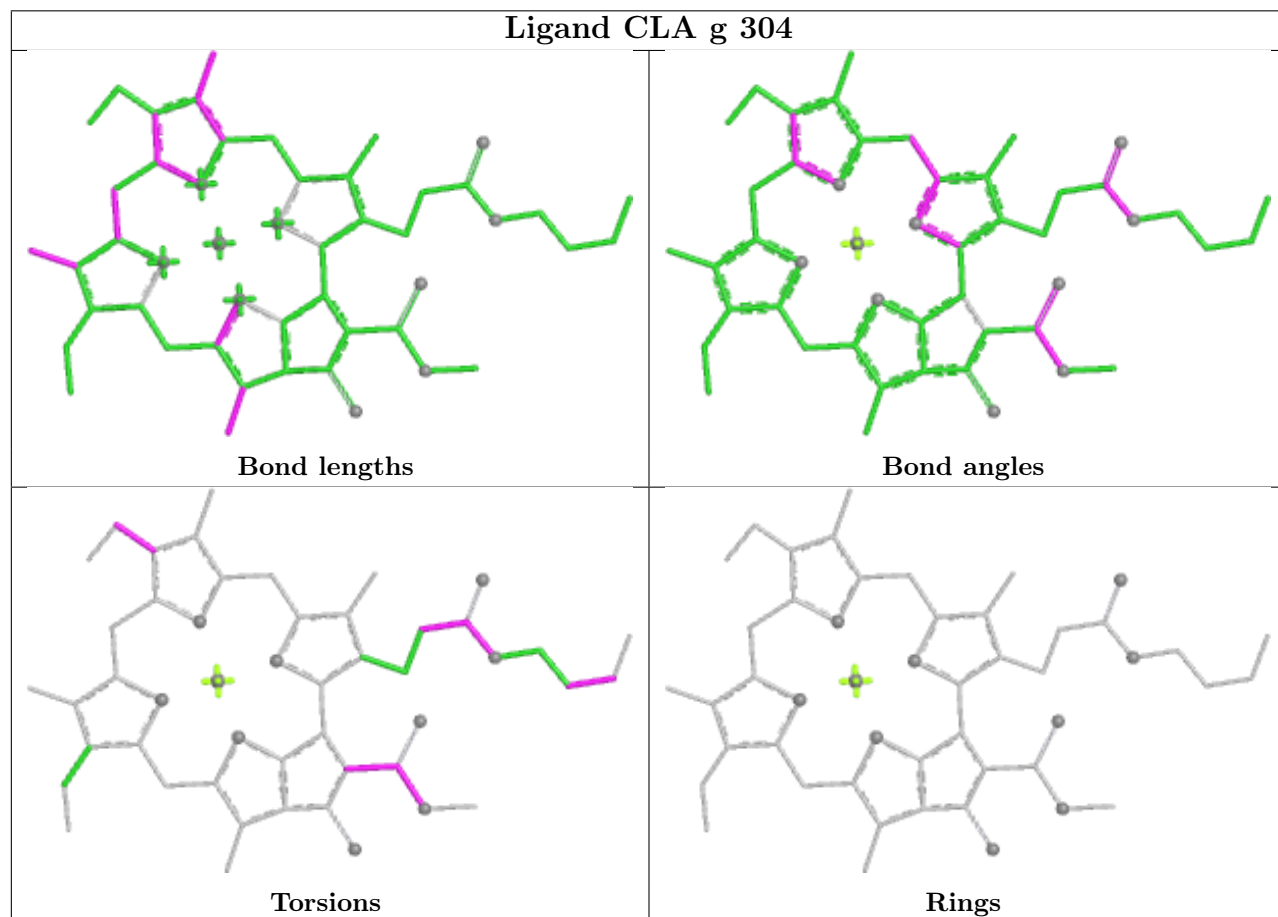
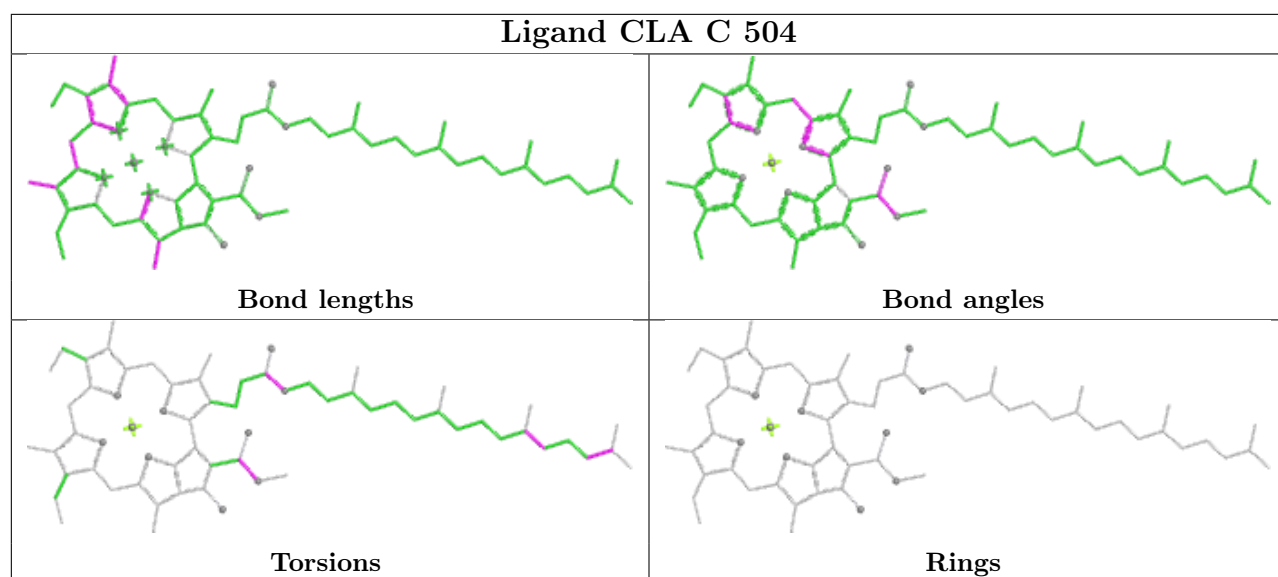


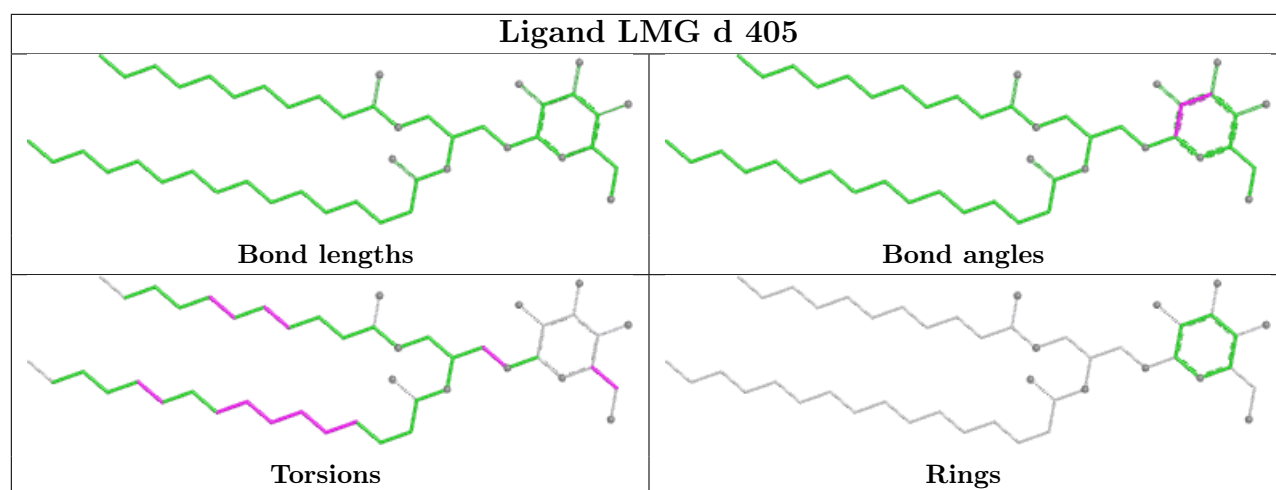
Ligand CLA s 306



Ligand CLA c 505







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.

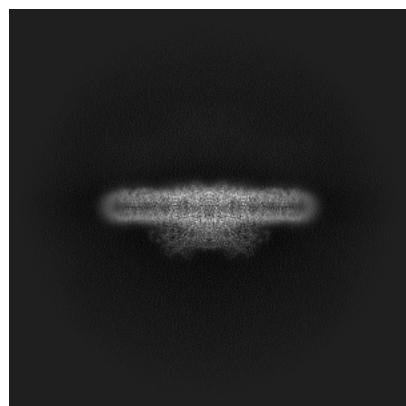
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52620. These allow visual inspection of the internal detail of the map and identification of artifacts.

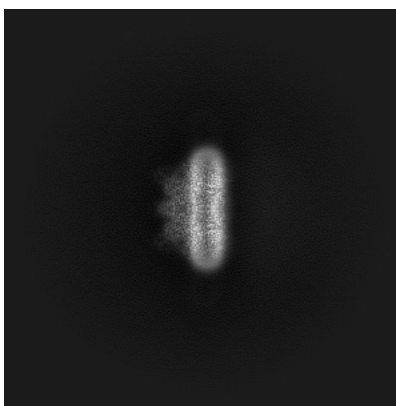
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

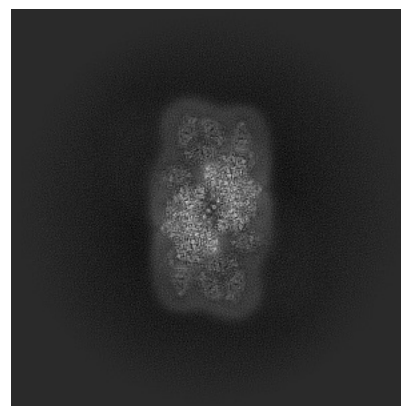
6.1.1 Primary map



X

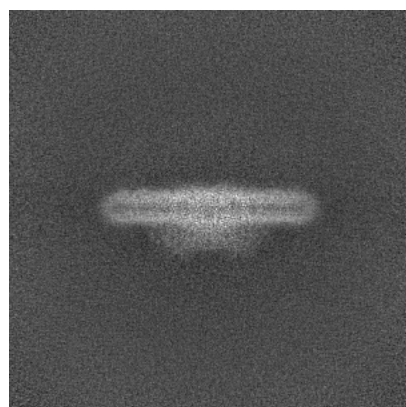


Y

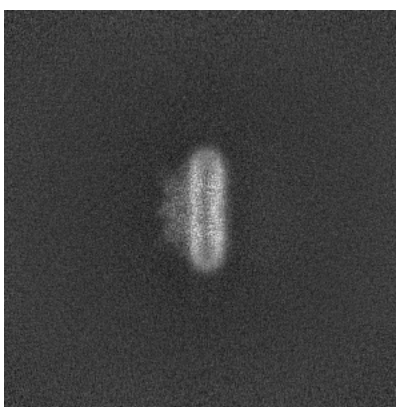


Z

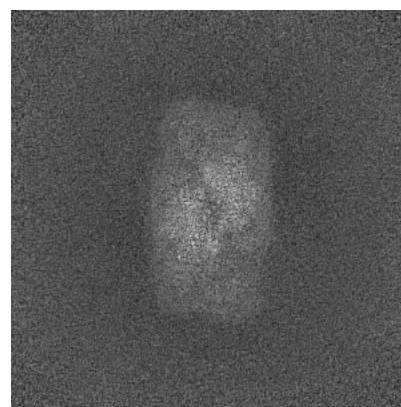
6.1.2 Raw map



X



Y

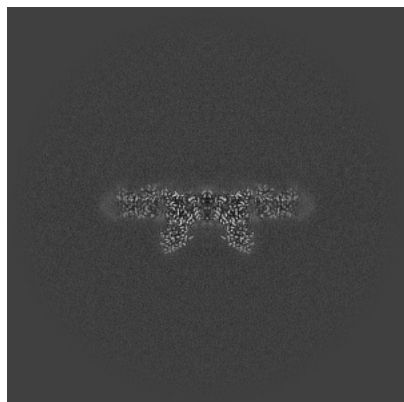


Z

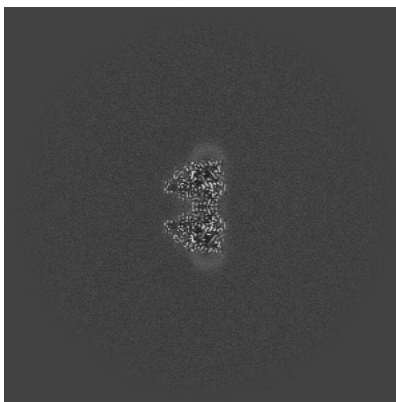
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

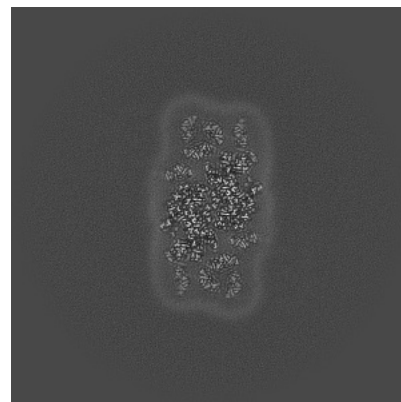
6.2.1 Primary map



X Index: 392

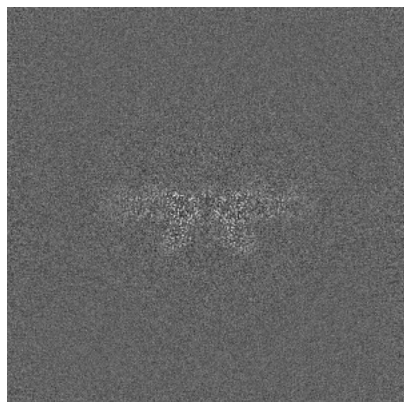


Y Index: 392

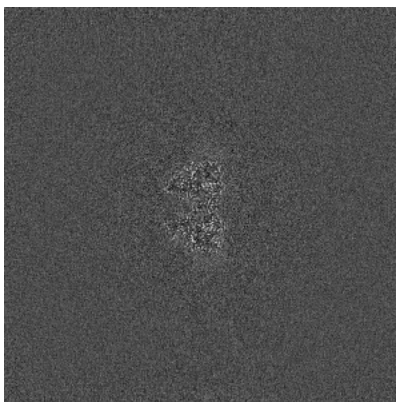


Z Index: 392

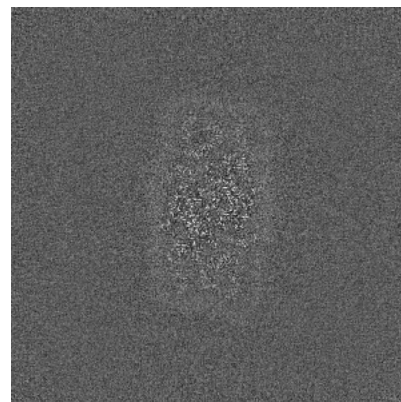
6.2.2 Raw map



X Index: 392



Y Index: 392

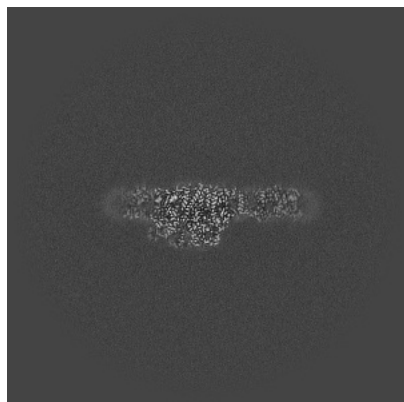


Z Index: 392

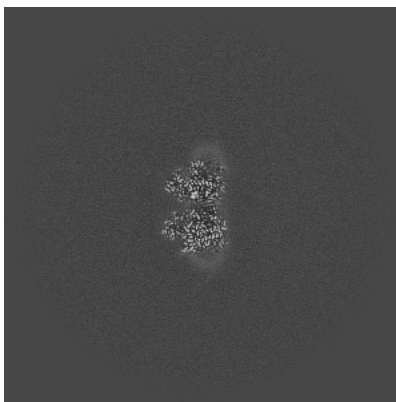
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

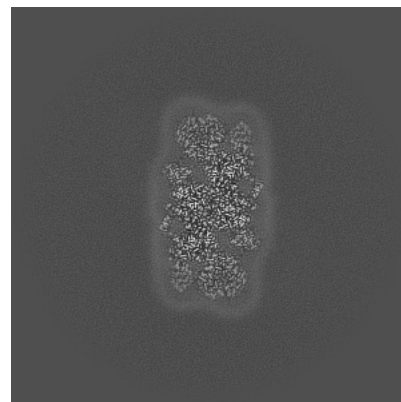
6.3.1 Primary map



X Index: 348

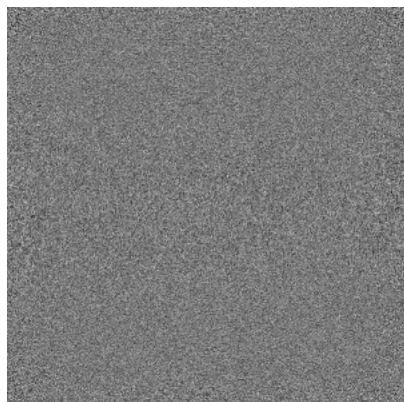


Y Index: 381

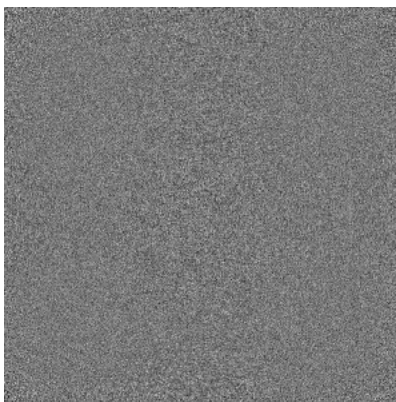


Z Index: 408

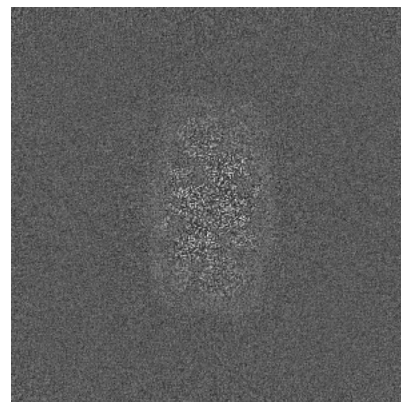
6.3.2 Raw map



X Index: 0



Y Index: 0

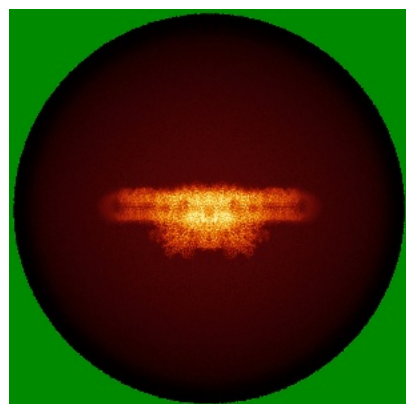


Z Index: 408

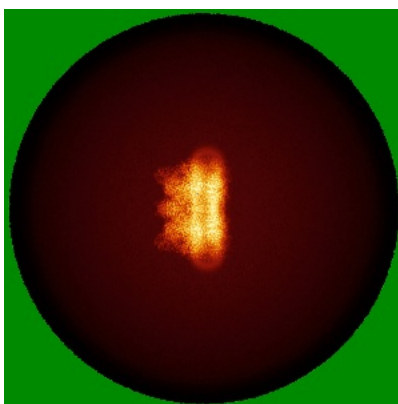
The images above show the largest variance slices of the map in three orthogonal directions.

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

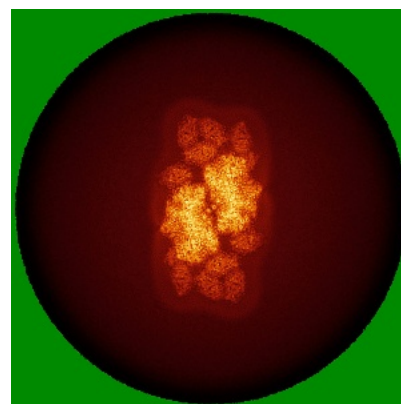
6.4.1 Primary map



X

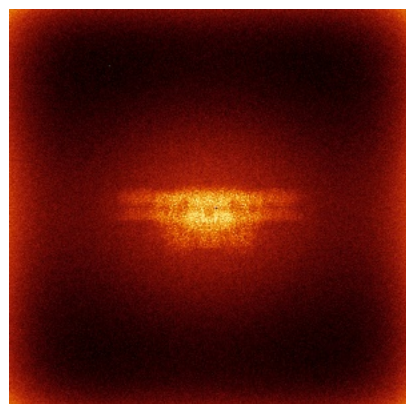


Y

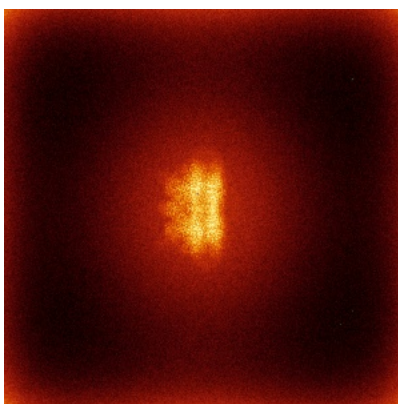


Z

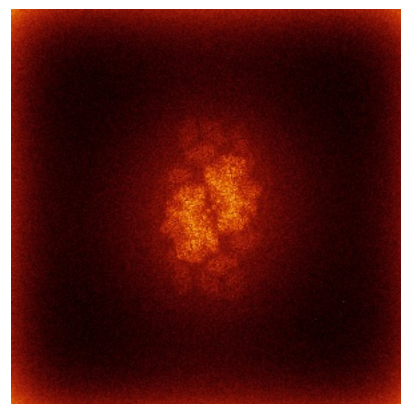
6.4.2 Raw map



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



X



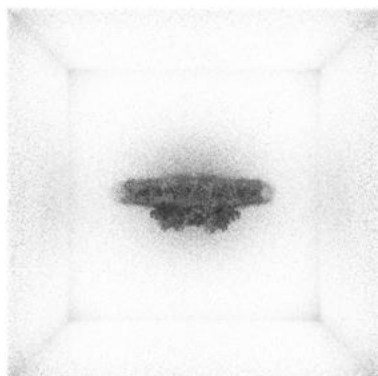
Y



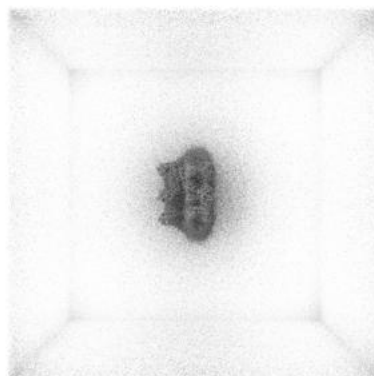
Z

The images above show the 3D surface view of the map at the recommended contour level 0.149. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

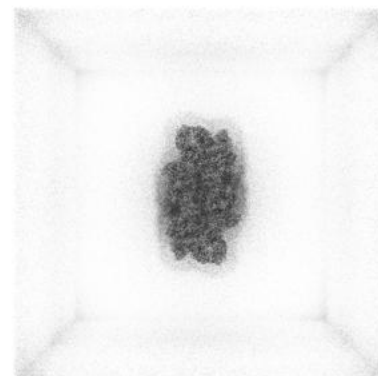
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

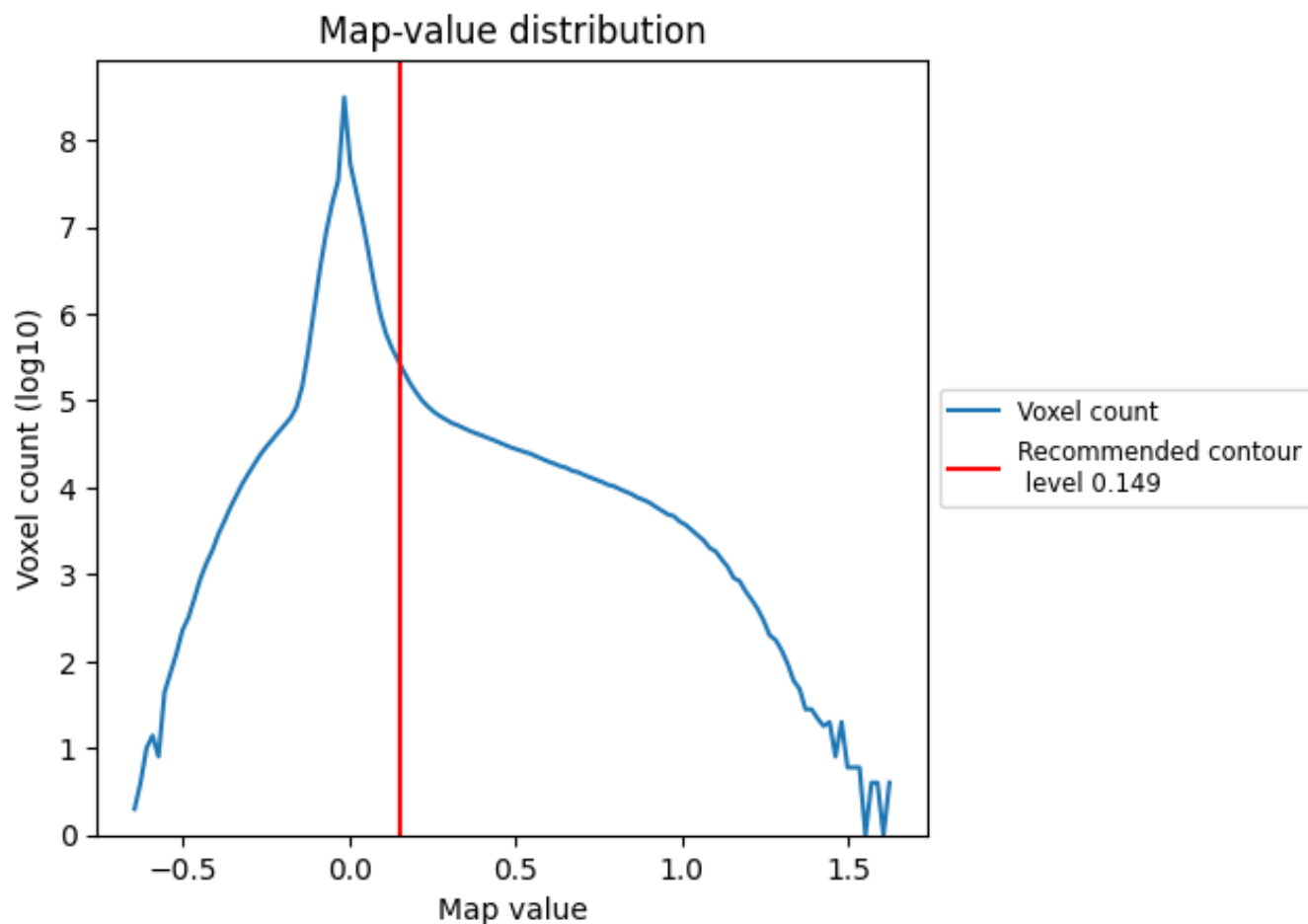
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

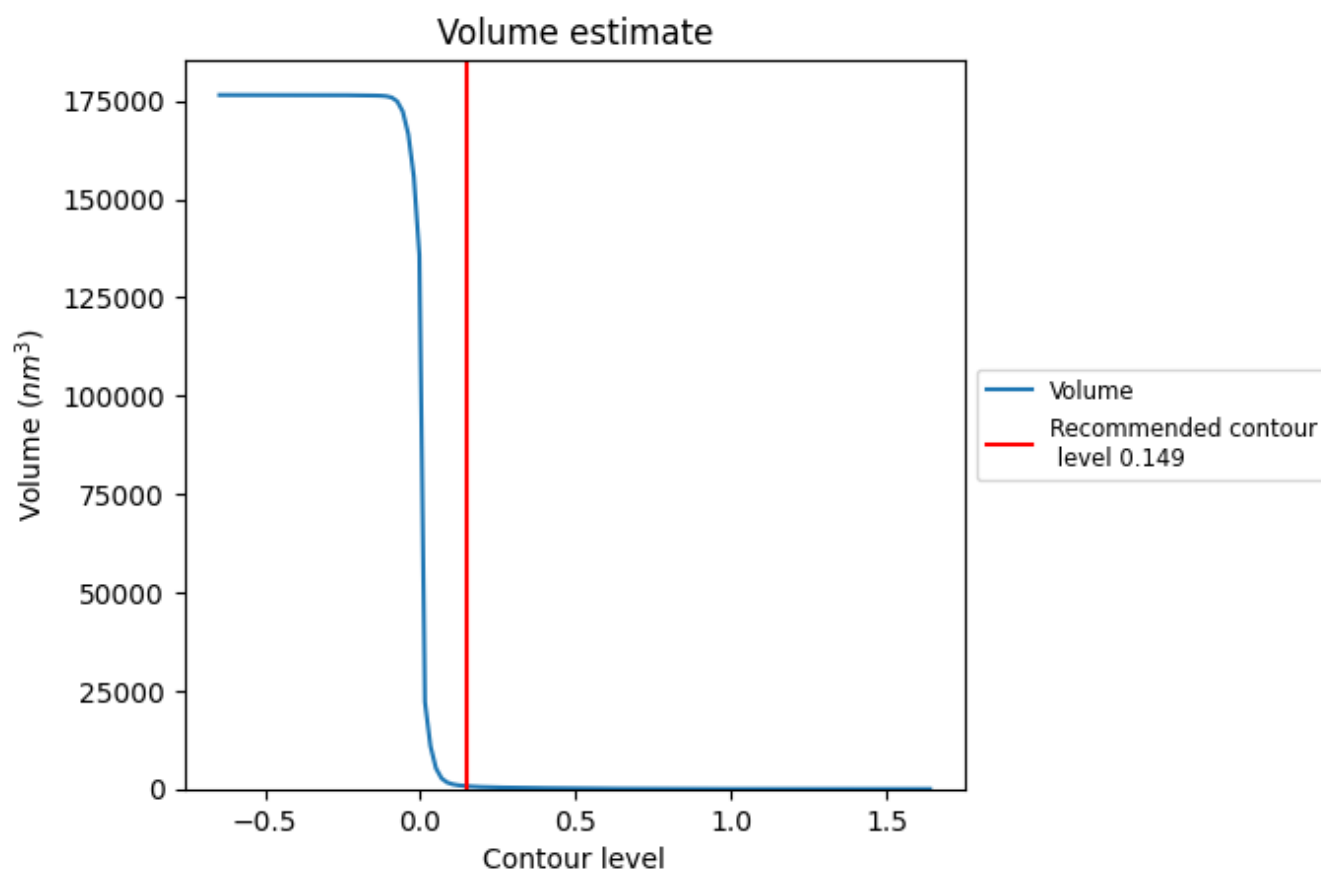
This section contains the results of statistical analysis of the map.

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.

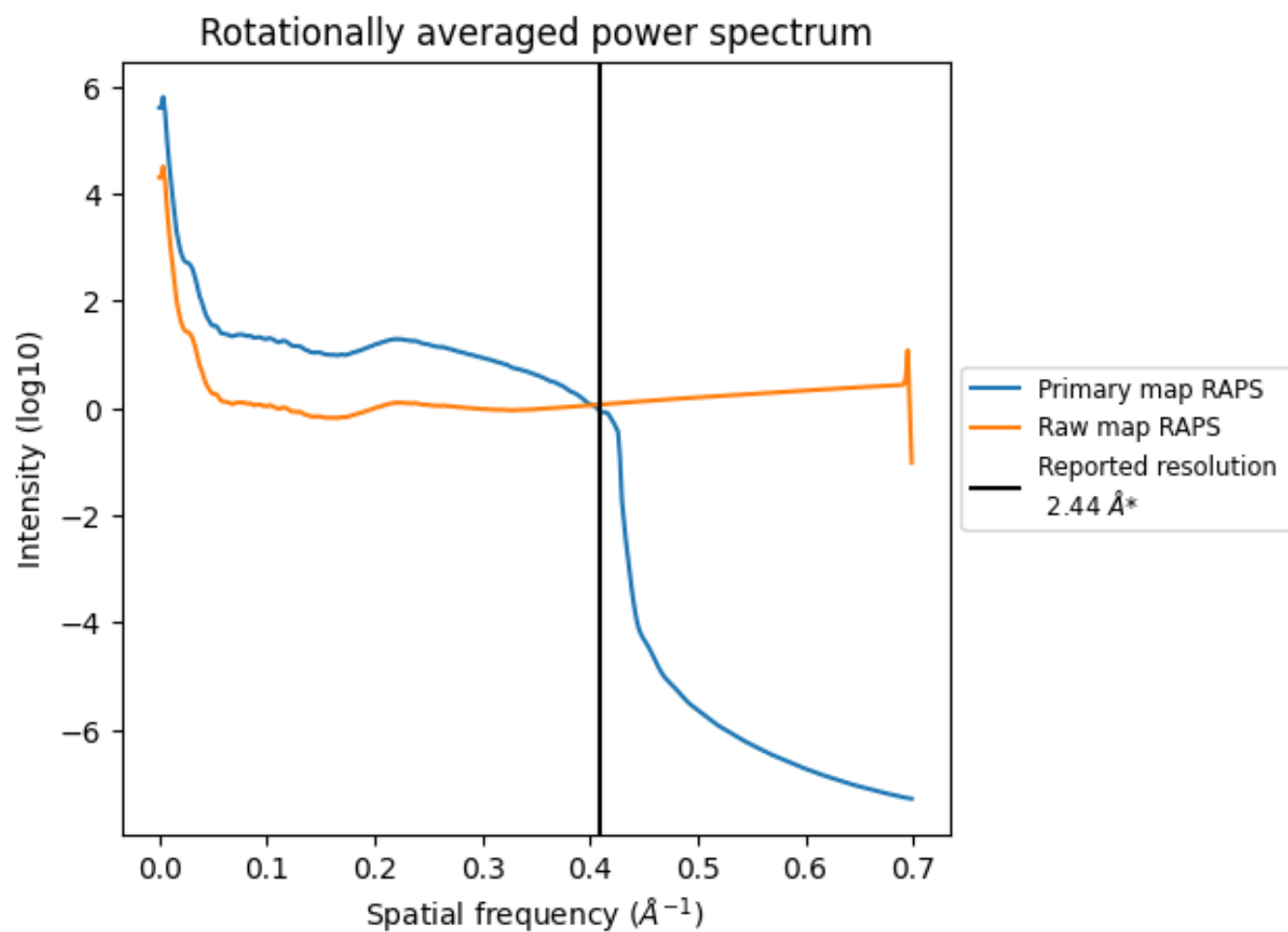
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 724 nm^3 ; this corresponds to an approximate mass of 654 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 ⓘ

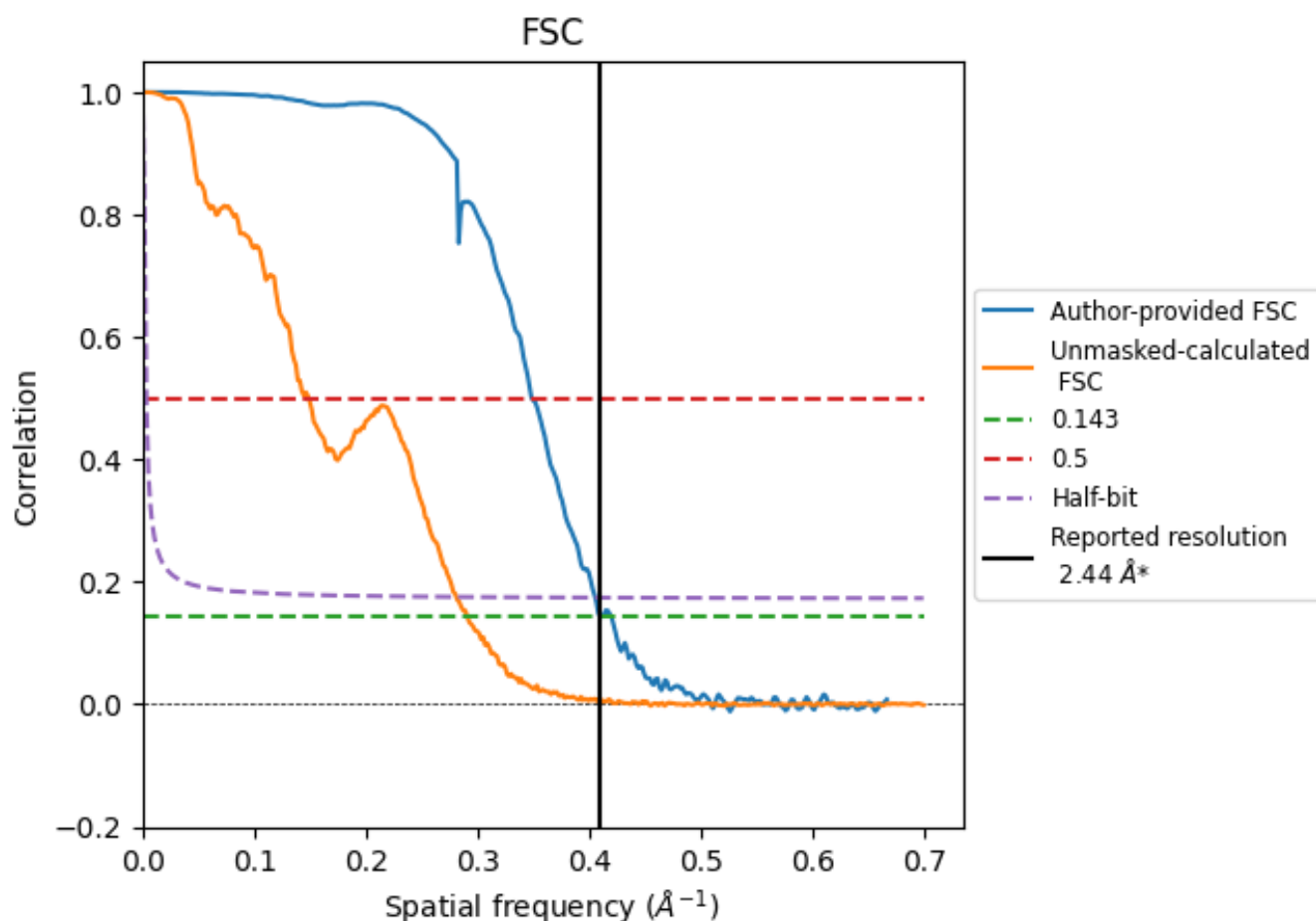


*Reported resolution corresponds to spatial frequency of 0.410 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.410 \AA^{-1}

8.2 Resolution estimates [i](#)

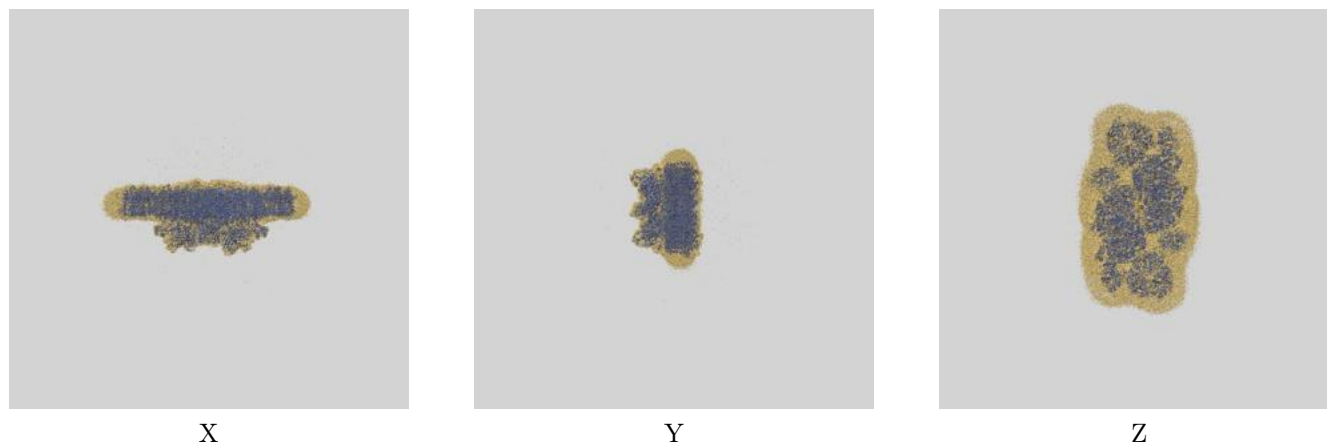
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.44	-	-
Author-provided FSC curve	2.44	2.87	2.47
Unmasked-calculated*	3.44	6.72	3.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.44 by more than 10 %

9 Map-model fit [i](#)

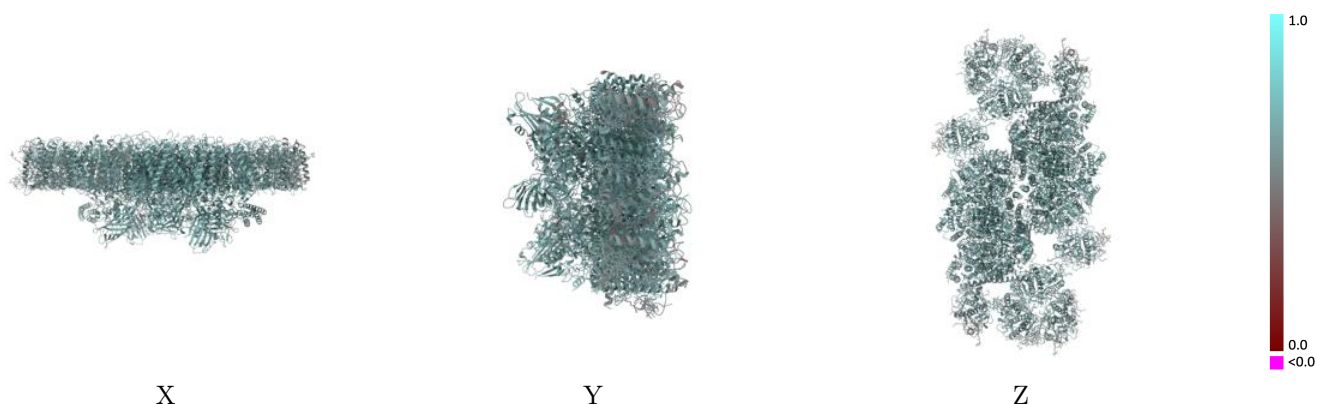
This section contains information regarding the fit between EMDB map EMD-52620 and PDB model 9I4T. Per-residue inclusion information can be found in [section 3](#) on [page 42](#).

9.1 Map-model overlay [i](#)



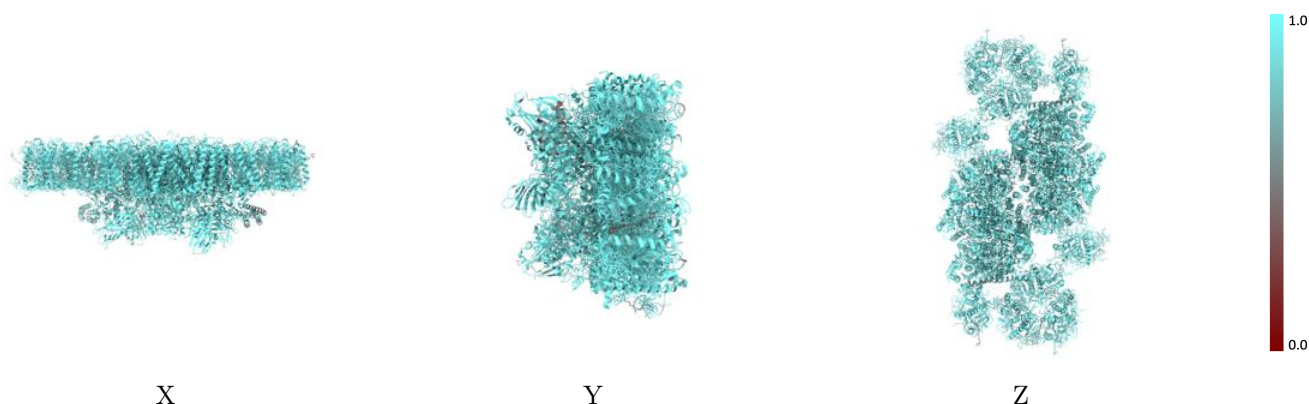
The images above show the 3D surface view of the map at the recommended contour level 0.149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



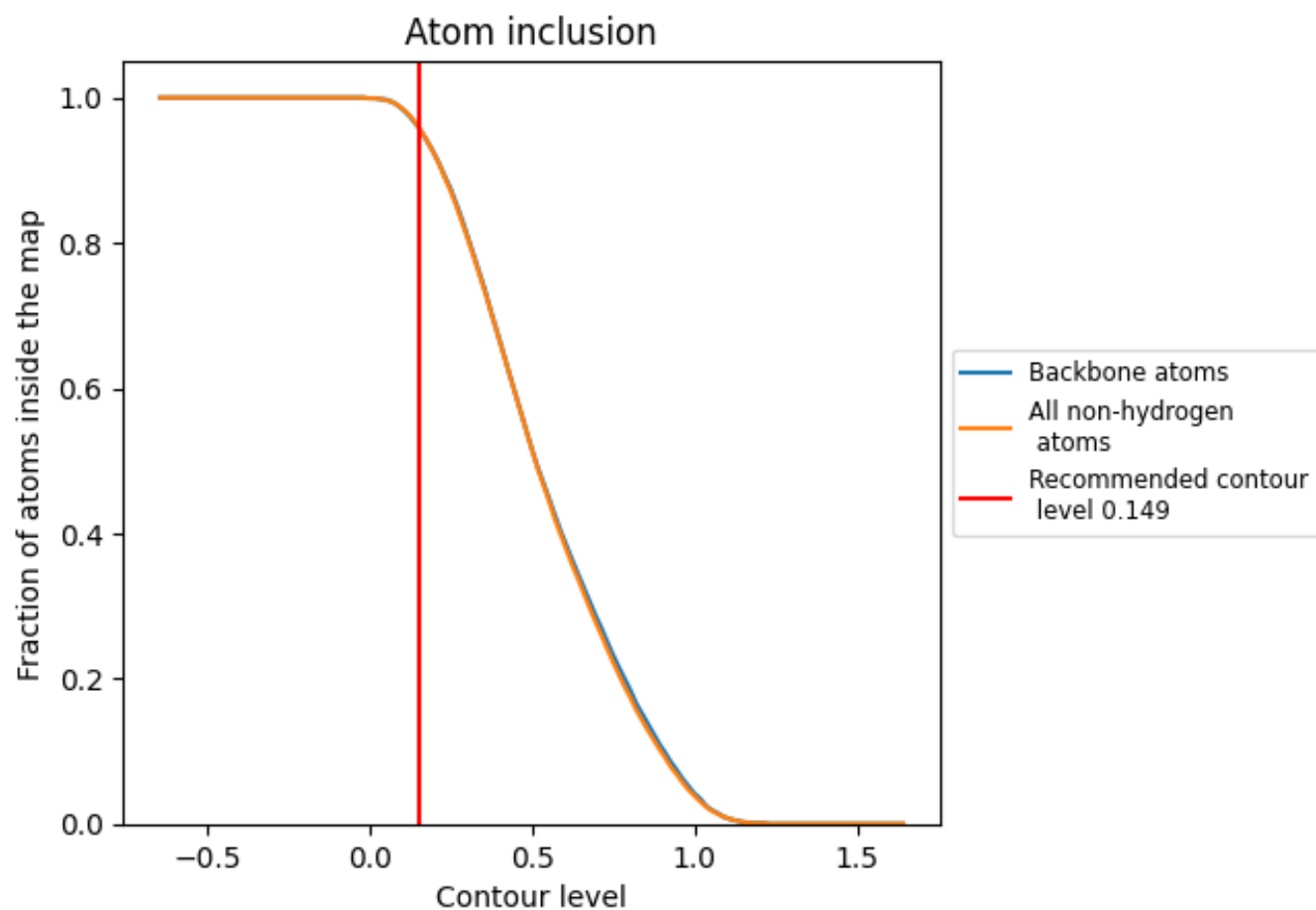
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.149).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.6330
A	 0.9940	 0.6680
B	 0.9920	 0.6650
C	 0.9830	 0.6550
D	 0.9910	 0.6720
E	 0.9900	 0.6360
F	 0.9830	 0.6340
G	 0.8890	 0.5710
H	 0.9960	 0.6570
I	 1.0000	 0.6690
J	 0.9900	 0.6260
K	 0.9820	 0.6380
L	 0.9970	 0.6720
M	 0.9880	 0.6430
N	 0.9390	 0.5990
O	 0.9570	 0.6270
P	 0.9530	 0.6390
Q	 0.7890	 0.5870
R	 0.9490	 0.6090
S	 0.9120	 0.5660
T	 0.9530	 0.6360
U	 0.9480	 0.6290
W	 0.9600	 0.6250
X	 0.9780	 0.6270
Y	 0.9720	 0.6380
Z	 0.9630	 0.5960
a	 0.9940	 0.6680
b	 0.9910	 0.6640
c	 0.9830	 0.6540
d	 0.9910	 0.6710
e	 0.9890	 0.6340
f	 0.9790	 0.6330
g	 0.8900	 0.5700
h	 0.9940	 0.6580
i	 1.0000	 0.6700



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j	 0.9830	 0.6240
k	 0.9820	 0.6360
l	 0.9970	 0.6680
m	 0.9880	 0.6440
n	 0.9400	 0.5990
o	 0.9550	 0.6260
p	 0.9520	 0.6360
q	 0.7920	 0.5870
r	 0.9480	 0.6090
s	 0.9110	 0.5670
t	 0.9560	 0.6300
u	 0.9480	 0.6300
w	 0.9620	 0.6220
x	 0.9780	 0.6220
y	 0.9720	 0.6370
z	 0.9600	 0.5930