



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:12 AM UTC

PDB ID : 7PI0 / pdb_00007pi0
EMDB ID : EMD-13429
Title : Unstacked compact Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-08-19
Resolution : 2.43 Å (reported)
Based on initial model : 6KAC

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

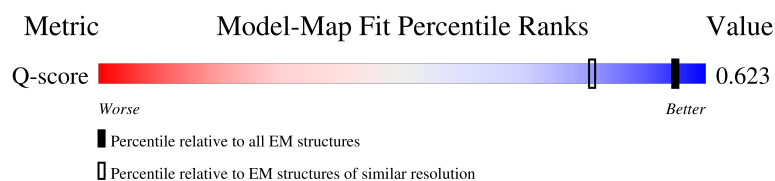
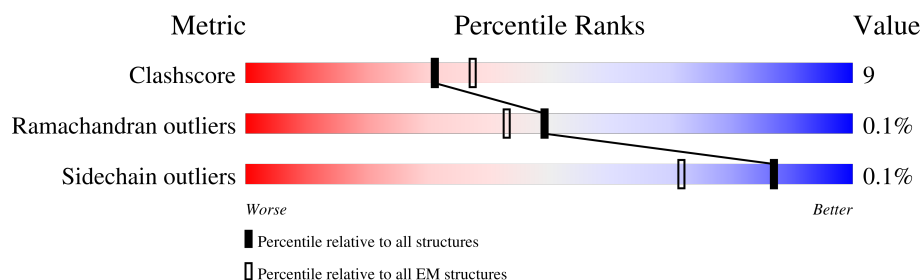
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.43 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.



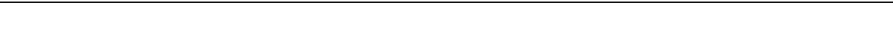
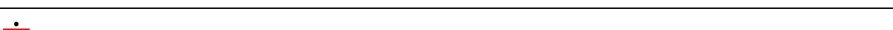
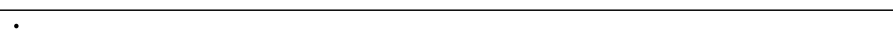
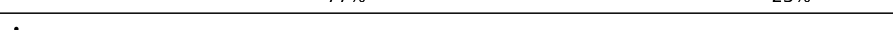
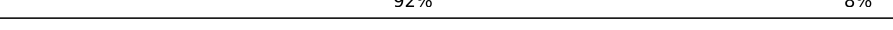
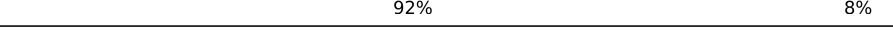
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5787 (1.94 - 2.93)

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

Mol	Chain	Length	Quality of chain
1	A	336	 76% 22% .
1	a	336	 79% 21%
2	B	484	 84% 16%
2	b	484	 80% 20%

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Mol	Chain	Length	Quality of chain
3	V	32	 88% 12%
3	v	32	 88% 12%
4	C	449	 85% 15%
4	c	449	 85% 15%
5	D	348	 82% 17%
5	d	348	 86% 14%
6	E	76	 82% 18%
6	e	76	 83% 17%
7	F	31	 90% 10%
7	f	31	 74% 26%
8	H	67	 90% 10%
8	h	67	 90% 10%
9	I	35	 77% 23%
9	i	35	 77% 23%
10	J	36	 86% 14%
10	j	36	 92% 8%
11	K	37	 86% 14%
11	k	37	 86% 14%
12	L	38	 92% 8%
12	l	38	 87% 13%
13	M	31	 81% 19%
13	m	31	 77% 23%
14	O	238	 81% 19%
14	o	238	 79% 21%
15	P	187	 21% 78% 22%

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Mol	Chain	Length	Quality of chain
15	p	187	 8% 81% 19%
16	T	30	 83% 17%
16	t	30	 80% 20%
17	W	44	 93% 7%
17	w	44	 82% 18%
18	X	30	 83% 17%
18	x	30	 80% 20%
19	Z	61	 93% 7%
19	z	61	 93% 7%
20	N	222	 83% 17%
20	n	222	 84% 16%
21	G	221	 90% 10%
21	g	221	 83% 17%
22	R	196	 85% 15%
22	r	196	 85% 15%
23	S	243	 88% 12%
23	s	243	 85% 15%
24	Y	222	 85% 15%
24	y	222	 86% 14%
25	U	27	 67% 33%
25	u	27	 63% 37%

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	407	X	-	-	-
29	CLA	B	501	X	-	-	-
29	CLA	B	502	X	-	-	-
29	CLA	B	503	X	-	-	-
29	CLA	B	504	X	-	-	-
29	CLA	B	505	X	-	-	-
29	CLA	B	506	X	-	-	-
29	CLA	B	507	X	-	-	-
29	CLA	B	508	X	-	-	-
29	CLA	B	509	X	-	-	-
29	CLA	B	510	X	-	-	-
29	CLA	B	512	X	-	-	-
29	CLA	B	513	X	-	-	-
29	CLA	B	514	X	-	-	-
29	CLA	B	515	X	-	-	-
29	CLA	B	516	X	-	-	-
29	CLA	C	503	X	-	-	-
29	CLA	C	505	X	-	-	-
29	CLA	C	506	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	C	513	X	-	-	-
29	CLA	D	404	X	-	-	-
29	CLA	D	405	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	N	602	X	-	-	-
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	N	614	X	-	-	-
29	CLA	R	301	X	-	-	-
29	CLA	R	303	X	-	-	-
29	CLA	R	306	X	-	-	-
29	CLA	R	307	X	-	-	-
29	CLA	R	308	X	-	-	-
29	CLA	R	309	X	-	-	-
29	CLA	S	303	X	-	-	-
29	CLA	S	304	X	-	-	-
29	CLA	S	305	X	-	-	-
29	CLA	S	306	X	-	-	-
29	CLA	S	310	X	-	-	-
29	CLA	S	311	X	-	-	-
29	CLA	S	312	X	-	-	-
29	CLA	S	313	X	-	-	-
29	CLA	S	314	X	-	-	-
29	CLA	S	315	X	-	-	-
29	CLA	S	316	X	-	-	-
29	CLA	Y	303	X	-	-	-
29	CLA	Y	304	X	-	-	-
29	CLA	Y	305	X	-	-	-
29	CLA	Y	309	X	-	-	-
29	CLA	Y	311	X	-	-	-
29	CLA	Y	312	X	-	-	-
29	CLA	Y	313	X	-	-	-
29	CLA	Y	314	X	-	-	-
29	CLA	Y	315	X	-	-	-
29	CLA	a	404	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	b	501	X	-	-	-
29	CLA	b	502	X	-	-	-
29	CLA	b	503	X	-	-	-
29	CLA	b	504	X	-	-	-
29	CLA	b	505	X	-	-	-
29	CLA	b	506	X	-	-	-
29	CLA	b	507	X	-	-	-
29	CLA	b	509	X	-	-	-
29	CLA	b	510	X	-	-	-
29	CLA	b	512	X	-	-	-
29	CLA	b	513	X	-	-	-
29	CLA	b	514	X	-	-	-
29	CLA	b	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	b	516	X	-	-	-
29	CLA	c	502	X	-	-	-
29	CLA	c	504	X	-	-	-
29	CLA	c	505	X	-	-	-
29	CLA	c	507	X	-	-	-
29	CLA	c	508	X	-	-	-
29	CLA	c	509	X	-	-	-
29	CLA	c	510	X	-	-	-
29	CLA	c	512	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	d	404	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	609	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-
29	CLA	n	613	X	-	-	-
29	CLA	r	302	X	-	-	-
29	CLA	r	304	X	-	-	-
29	CLA	r	307	X	-	-	-
29	CLA	r	308	X	-	-	-
29	CLA	r	309	X	-	-	-
29	CLA	r	310	X	-	-	-
29	CLA	s	303	X	-	-	-
29	CLA	s	305	X	-	-	-
29	CLA	s	310	X	-	-	-
29	CLA	s	311	X	-	-	-
29	CLA	s	312	X	-	-	-
29	CLA	s	313	X	-	-	-
29	CLA	s	314	X	-	-	-
29	CLA	s	315	X	-	-	-
29	CLA	s	316	X	-	-	-
29	CLA	y	304	X	-	-	-
29	CLA	y	305	X	-	-	-
29	CLA	y	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	y	310	X	-	-	-
29	CLA	y	312	X	-	-	-
29	CLA	y	313	X	-	-	-
29	CLA	y	314	X	-	-	-
29	CLA	y	316	X	-	-	-
34	C7Z	B	519	X	-	-	-
34	C7Z	b	519	X	-	-	-
45	RRX	H	101	X	-	-	-
45	RRX	h	101	X	-	-	-
46	CHL	G	601	X	-	-	-
46	CHL	G	605	X	-	-	-
46	CHL	G	606	X	-	-	-
46	CHL	G	607	X	-	-	-
46	CHL	G	608	X	-	-	-
46	CHL	G	609	X	-	-	-
46	CHL	N	601	X	-	-	-
46	CHL	N	605	X	-	-	-
46	CHL	N	606	X	-	-	-
46	CHL	N	607	X	-	-	-
46	CHL	N	608	X	-	-	-
46	CHL	N	609	X	-	-	-
46	CHL	R	304	X	-	-	-
46	CHL	R	305	X	-	-	-
46	CHL	S	302	X	-	-	-
46	CHL	S	307	X	-	-	-
46	CHL	S	308	X	-	-	-
46	CHL	S	309	X	-	-	-
46	CHL	Y	302	X	-	-	-
46	CHL	Y	306	X	-	-	-
46	CHL	Y	307	X	-	-	-
46	CHL	Y	308	X	-	-	-
46	CHL	Y	310	X	-	-	-
46	CHL	g	601	X	-	-	-
46	CHL	g	605	X	-	-	-
46	CHL	g	606	X	-	-	-
46	CHL	g	607	X	-	-	-
46	CHL	g	608	X	-	-	-
46	CHL	g	609	X	-	-	-
46	CHL	n	601	X	-	-	-
46	CHL	n	605	X	-	-	-
46	CHL	n	606	X	-	-	-
46	CHL	n	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	CHL	n	608	X	-	-	-
46	CHL	r	305	X	-	-	-
46	CHL	r	306	X	-	-	-
46	CHL	s	302	X	-	-	-
46	CHL	s	307	X	-	-	-
46	CHL	s	308	X	-	-	-
46	CHL	s	309	X	-	-	-
46	CHL	y	301	X	-	-	-
46	CHL	y	303	X	-	-	-
46	CHL	y	307	X	-	-	-
46	CHL	y	308	X	-	-	-
46	CHL	y	309	X	-	-	-
46	CHL	y	311	X	-	-	-
49	XAT	G	619	X	-	-	-
49	XAT	N	619	X	-	-	-
49	XAT	R	311	X	-	-	-
49	XAT	Y	301	X	-	-	-
49	XAT	g	619	X	-	-	-
49	XAT	n	618	X	-	-	-
49	XAT	r	312	X	-	-	-
49	XAT	y	302	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 77465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		
1	a	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		
2	b	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	76	Total	C	N	O	S	0	0
			621	404	102	115			
6	e	76	Total	C	N	O	S	0	0
			621	404	102	115			

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			266	183	40	43		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called Hypothetical protein.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called Chlorophyll a-b binding protein of LHCII type 3, chloroplastic.

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

- Molecule 21 is a protein called Chlorophyll a-b binding protein of LHCII type 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		
21	g	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	196	Total	C	N	O	P S	0	0
			1490	943	251	292	1 3		
22	r	196	Total	C	N	O	P S	0	0
			1490	943	251	292	1 3		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

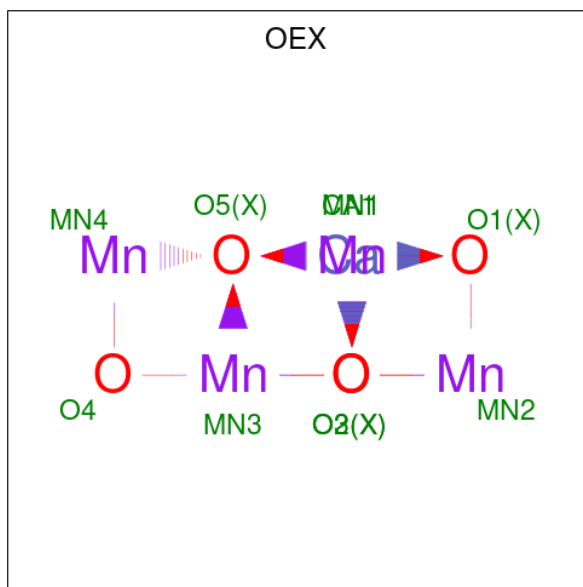
- Molecule 24 is a protein called Chlorophyll a-b binding protein of LHCII type 1, chloroplastic.

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

- Molecule 25 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

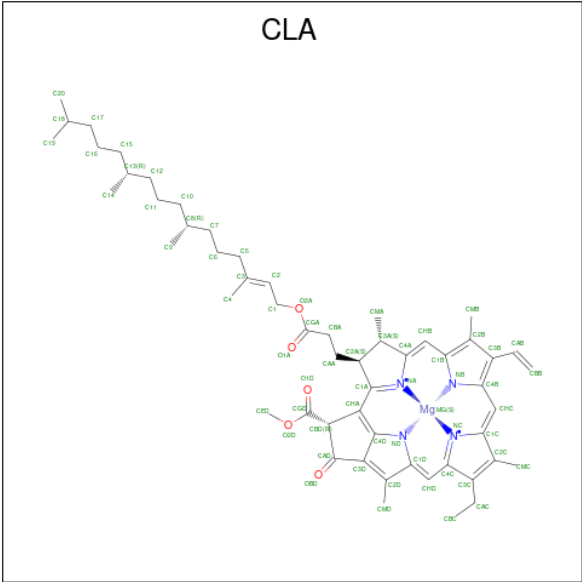
- Molecule 27 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D	1	Total 60	C 50	Mg 1	N 4	O 5	0

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

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

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Mol	Chain	Residues	Atoms					AltConf
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	n	1	Total 45	C 35	Mg 1	N 4	O 5	0

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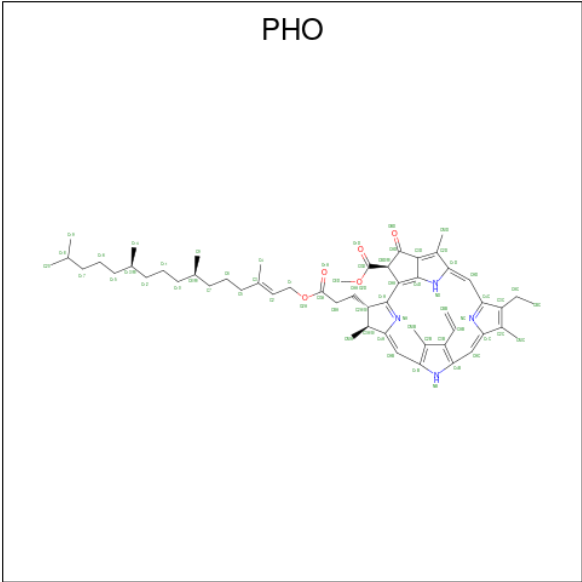
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s	1	Total 50	C 40	Mg 1	N 4	O 5	0

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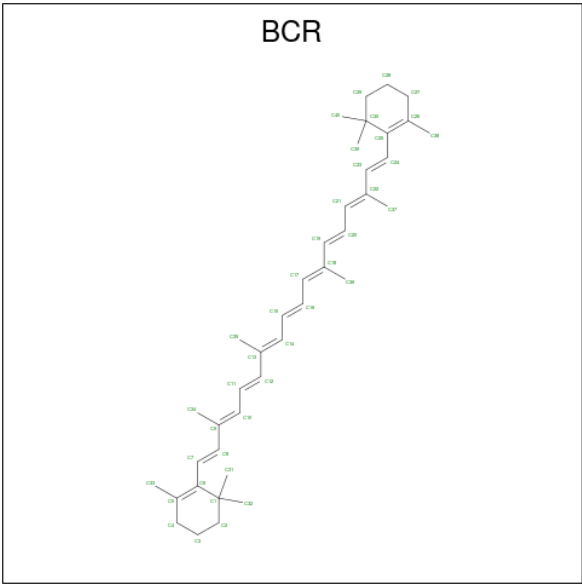
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0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

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).

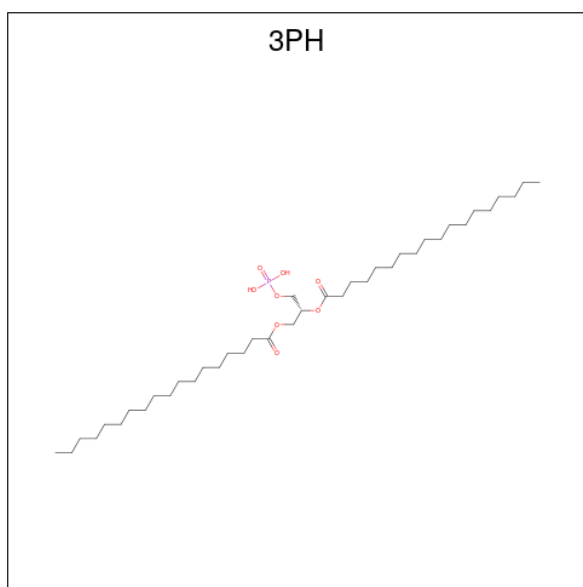


Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	F	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	v	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	f	1	Total C 40 40	0
31	z	1	Total C 40 40	0

- Molecule 32 is SODIUM ION (CCD ID: NA) (formula: Na).

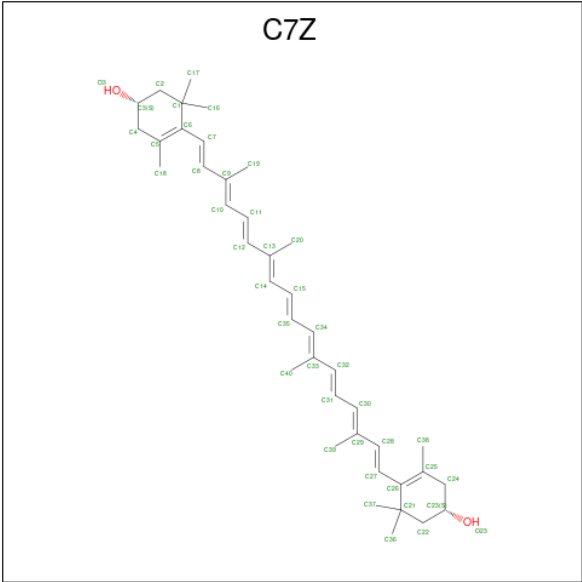
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total Na 1 1	0
32	a	1	Total Na 1 1	0

- Molecule 33 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



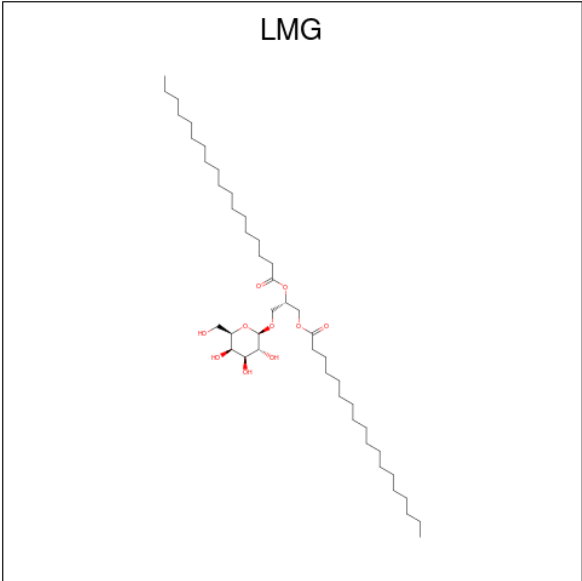
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	P	0
			48	39	8	1	
33	B	1	Total	C	O	P	0
			48	39	8	1	
33	S	1	Total	C	O	P	0
			30	21	8	1	
33	a	1	Total	C	O	P	0
			48	39	8	1	
33	b	1	Total	C	O	P	0
			39	30	8	1	
33	s	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 34 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			42	40	2	
34	b	1	Total	C	O	0
			42	40	2	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



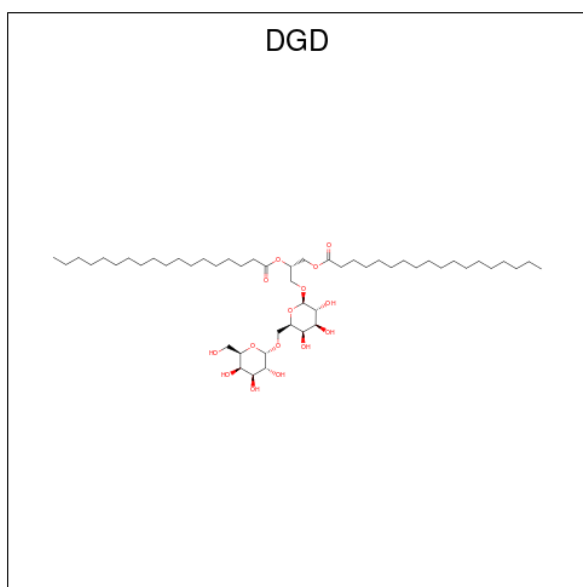
Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			44	34	10	

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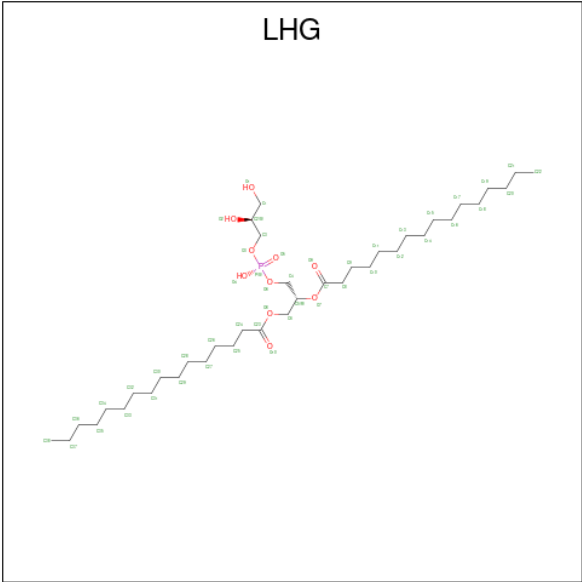
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			47	37	10	
35	C	1	Total	C	O	0
			55	45	10	
35	C	1	Total	C	O	0
			42	32	10	
35	D	1	Total	C	O	0
			42	32	10	
35	D	1	Total	C	O	0
			48	38	10	
35	W	1	Total	C	O	0
			40	30	10	
35	W	1	Total	C	O	0
			39	29	10	
35	b	1	Total	C	O	0
			44	34	10	
35	c	1	Total	C	O	0
			51	41	10	
35	c	1	Total	C	O	0
			55	45	10	
35	d	1	Total	C	O	0
			46	36	10	
35	d	1	Total	C	O	0
			48	38	10	
35	i	1	Total	C	O	0
			48	38	10	
35	w	1	Total	C	O	0
			39	29	10	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			43	28	15	
36	C	1	Total	C	O	0
			51	36	15	
36	C	1	Total	C	O	0
			53	38	15	
36	C	1	Total	C	O	0
			53	38	15	
36	c	1	Total	C	O	0
			55	40	15	
36	c	1	Total	C	O	0
			62	47	15	
36	c	1	Total	C	O	0
			59	44	15	
36	r	1	Total	C	O	0
			43	28	15	

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



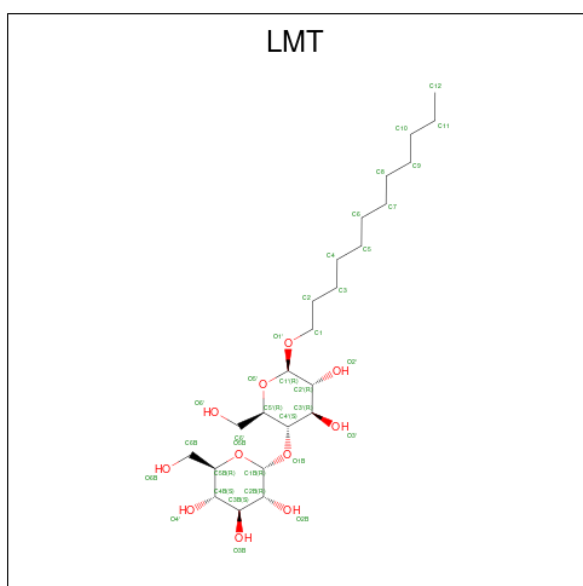
Mol	Chain	Residues	Atoms				AltConf
37	B	1	Total	C	O	P	0
			44	33	10	1	
37	D	1	Total	C	O	P	0
			49	38	10	1	
37	D	1	Total	C	O	P	0
			39	28	10	1	
37	L	1	Total	C	O	P	0
			49	38	10	1	
37	N	1	Total	C	O	P	0
			49	38	10	1	
37	G	1	Total	C	O	P	0
			49	38	10	1	
37	S	1	Total	C	O	P	0
			35	24	10	1	
37	S	1	Total	C	O	P	0
			45	34	10	1	
37	Y	1	Total	C	O	P	0
			49	38	10	1	
37	a	1	Total	C	O	P	0
			44	33	10	1	
37	a	1	Total	C	O	P	0
			39	28	10	1	
37	c	1	Total	C	O	P	0
			47	36	10	1	
37	d	1	Total	C	O	P	0
			49	38	10	1	
37	l	1	Total	C	O	P	0
			49	38	10	1	

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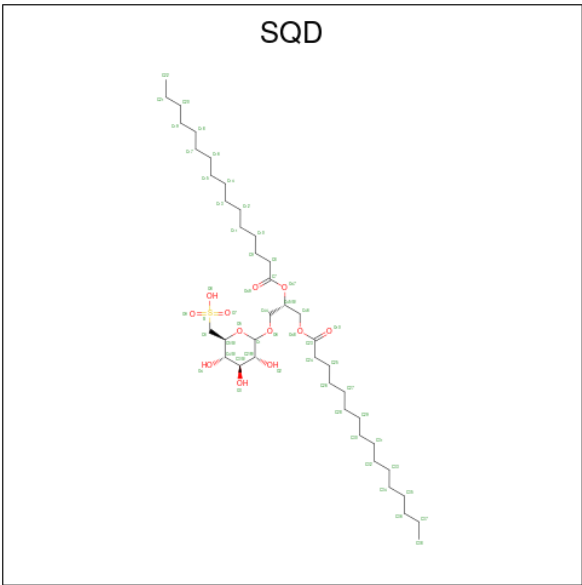
Mol	Chain	Residues	Atoms				AltConf
37	n	1	Total	C	O	P	0
			42	31	10	1	
37	g	1	Total	C	O	P	0
			49	38	10	1	
37	s	1	Total	C	O	P	0
			38	27	10	1	
37	s	1	Total	C	O	P	0
			45	34	10	1	
37	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 38 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			35	24	11	
38	b	1	Total	C	O	0
			35	24	11	

- Molecule 39 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	O	S	0
			42	29	12	1	
39	C	1	Total	C	O	S	0
			36	23	12	1	
39	L	1	Total	C	O	S	0
			42	29	12	1	
39	M	1	Total	C	O	S	0
			42	29	12	1	
39	a	1	Total	C	O	S	0
			51	38	12	1	
39	b	1	Total	C	O	S	0
			54	41	12	1	
39	c	1	Total	C	O	S	0
			54	41	12	1	
39	l	1	Total	C	O	S	0
			42	29	12	1	
39	m	1	Total	C	O	S	0
			42	29	12	1	
39	o	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 40 is SPHINGOSINE (CCD ID: SPH) (formula: C₁₈H₃₇NO₂).



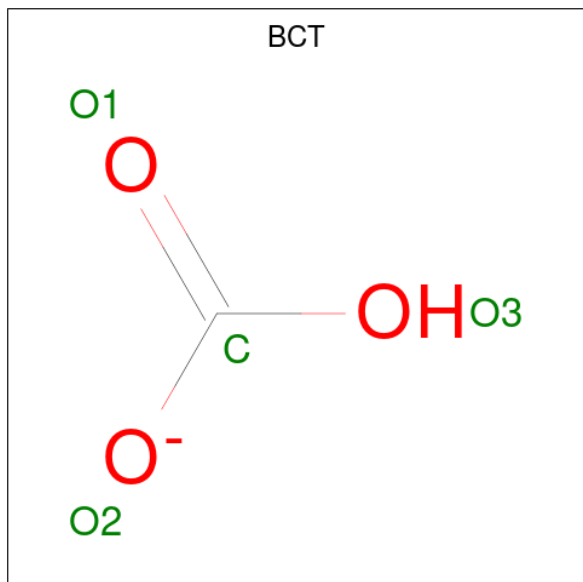
Mol	Chain	Residues	Atoms				AltCon
40	C	1	Total 21	C 18	N 1	O 2	0
40	I	1	Total 21	C 18	N 1	O 2	0
40	c	1	Total 21	C 18	N 1	O 2	0
40	i	1	Total 21	C 18	N 1	O 2	0

- Molecule 41 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $\text{C}_{39}\text{H}_{76}\text{O}_5$).



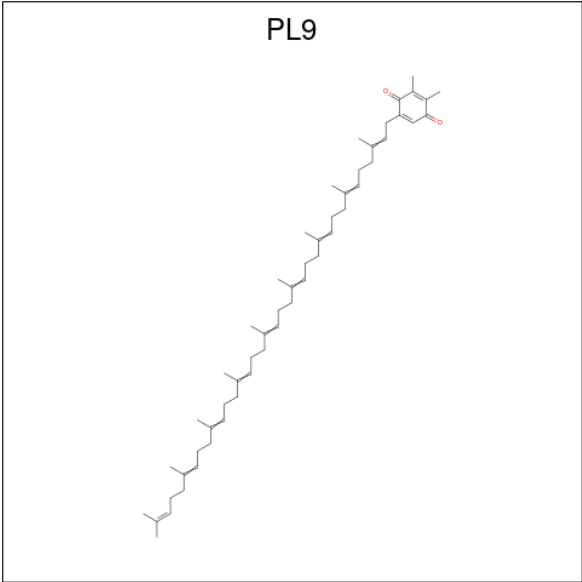
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			37	32	5	
41	J	1	Total	C	O	0
			29	24	5	
41	W	1	Total	C	O	0
			44	39	5	
41	b	1	Total	C	O	0
			44	39	5	
41	j	1	Total	C	O	0
			29	24	5	
41	w	1	Total	C	O	0
			44	39	5	

- Molecule 42 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



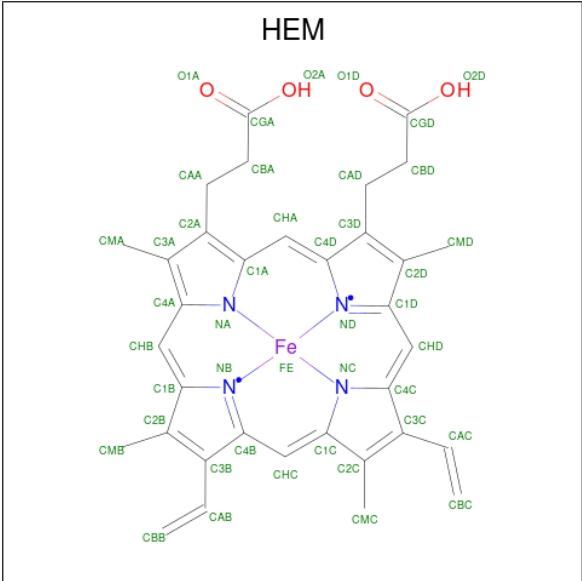
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			4	1	3	
42	a	1	Total	C	O	0
			4	1	3	

- Molecule 43 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



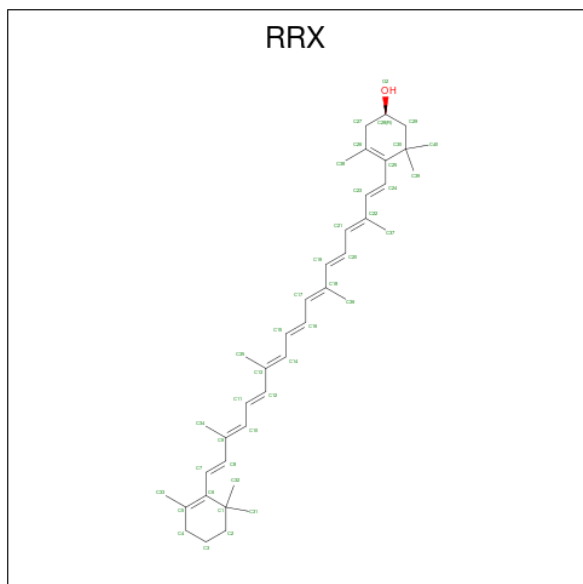
Mol	Chain	Residues	Atoms					AltConf
44	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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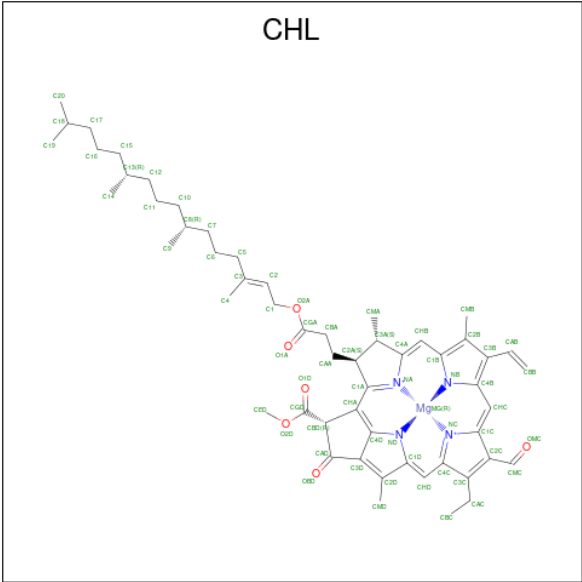
Mol	Chain	Residues	Atoms					AltConf
44	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 45 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



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

- Molecule 46 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



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

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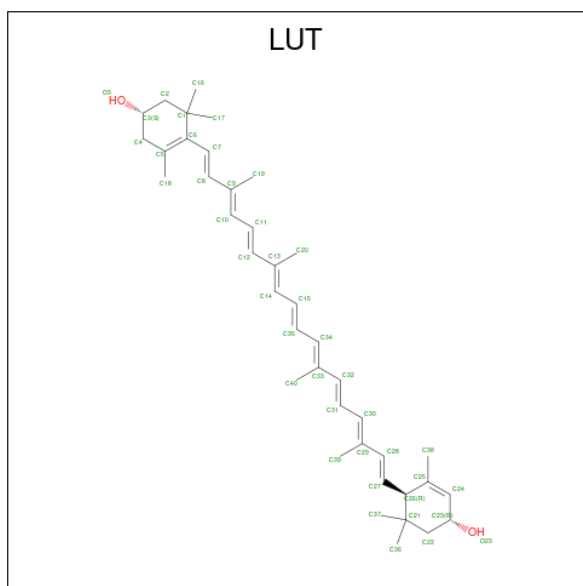
Mol	Chain	Residues	Atoms					AltConf
46	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
46	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
46	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
46	S	1	Total 61	C 50	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total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

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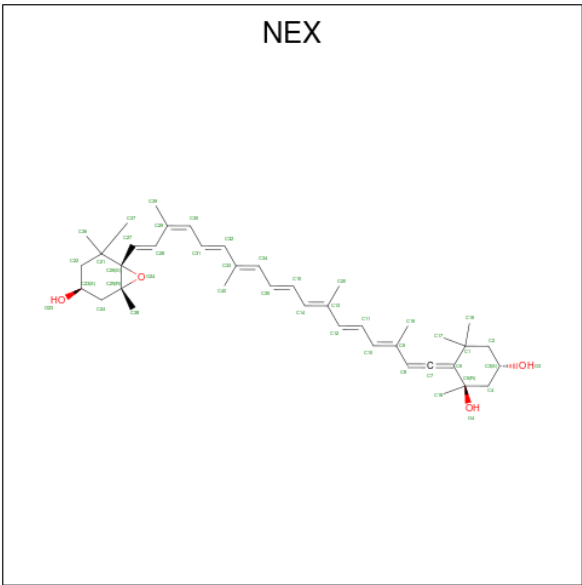
Mol	Chain	Residues	Atoms					AltConf
46	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
46	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
46	s	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 47 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



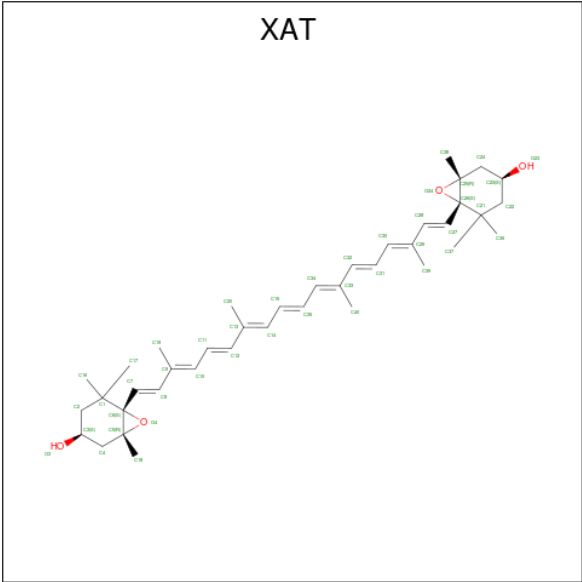
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			42	40	2	
47	N	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	R	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0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

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



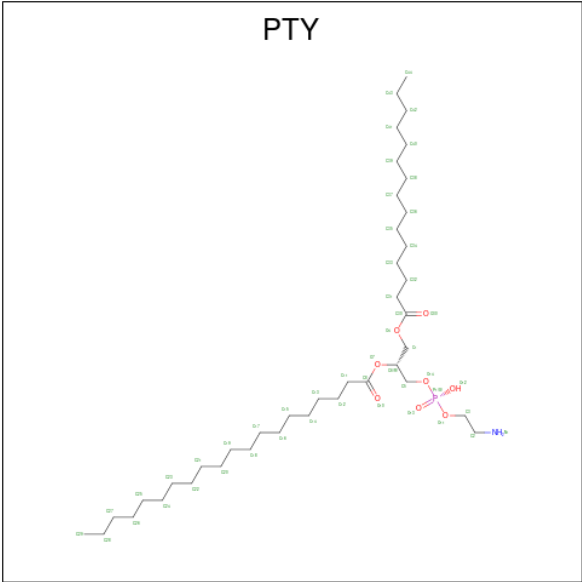
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	R	1	Total	C	O	0
			27	25	2	
48	S	1	Total	C	O	0
			44	40	4	
48	Y	1	Total	C	O	0
			44	40	4	
48	n	1	Total	C	O	0
			44	40	4	
48	g	1	Total	C	O	0
			44	40	4	
48	r	1	Total	C	O	0
			27	25	2	
48	s	1	Total	C	O	0
			44	40	4	
48	y	1	Total	C	O	0
			44	40	4	

- Molecule 49 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).



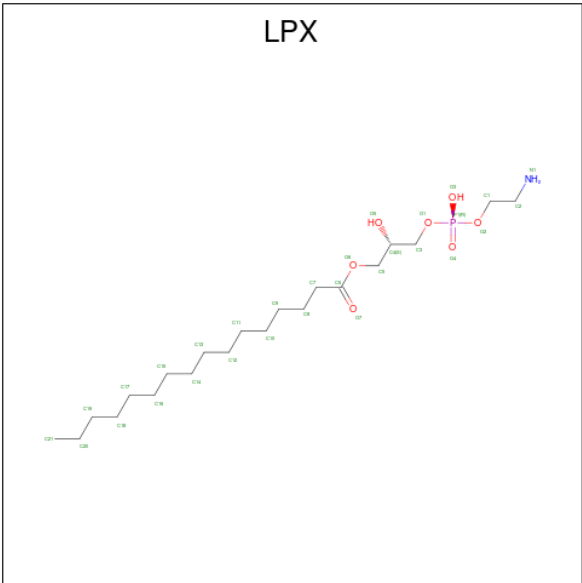
Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	R	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	
49	n	1	Total	C	O	0
			44	40	4	
49	g	1	Total	C	O	0
			44	40	4	
49	r	1	Total	C	O	0
			44	40	4	
49	y	1	Total	C	O	0
			44	40	4	

- Molecule 50 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
50	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
50	Y	1	Total	C	N	O	P	0
			19	9	1	8	1	
50	n	1	Total	C	N	O	P	0
			50	40	1	8	1	
50	y	1	Total	C	N	O	P	0
			19	9	1	8	1	

- Molecule 51 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
51	S	1	Total	C	N	O	P	0
			20	11	1	7	1	
51	s	1	Total	C	N	O	P	0
			19	10	1	7	1	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	A	93	Total	O	0
			93	93	
52	B	144	Total	O	0
			144	144	
52	V	7	Total	O	0
			7	7	
52	C	110	Total	O	0
			110	110	
52	D	74	Total	O	0
			74	74	
52	E	15	Total	O	0
			15	15	
52	F	2	Total	O	0
			2	2	
52	H	13	Total	O	0
			13	13	
52	I	9	Total	O	0
			9	9	
52	J	5	Total	O	0
			5	5	
52	K	9	Total	O	0
			9	9	
52	L	14	Total	O	0
			14	14	
52	M	9	Total	O	0
			9	9	
52	O	75	Total	O	0
			75	75	
52	P	22	Total	O	0
			22	22	
52	T	5	Total	O	0
			5	5	
52	W	9	Total	O	0
			9	9	
52	X	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
52	Z	4	Total 4	O 4	0
52	N	63	Total 63	O 63	0
52	G	60	Total 60	O 60	0
52	R	36	Total 36	O 36	0
52	S	33	Total 33	O 33	0
52	Y	55	Total 55	O 55	0
52	U	8	Total 8	O 8	0
52	a	91	Total 91	O 91	0
52	b	123	Total 123	O 123	0
52	v	3	Total 3	O 3	0
52	c	102	Total 102	O 102	0
52	d	68	Total 68	O 68	0
52	e	23	Total 23	O 23	0
52	f	3	Total 3	O 3	0
52	h	18	Total 18	O 18	0
52	i	11	Total 11	O 11	0
52	j	3	Total 3	O 3	0
52	k	9	Total 9	O 9	0
52	l	8	Total 8	O 8	0
52	m	6	Total 6	O 6	0
52	o	78	Total 78	O 78	0

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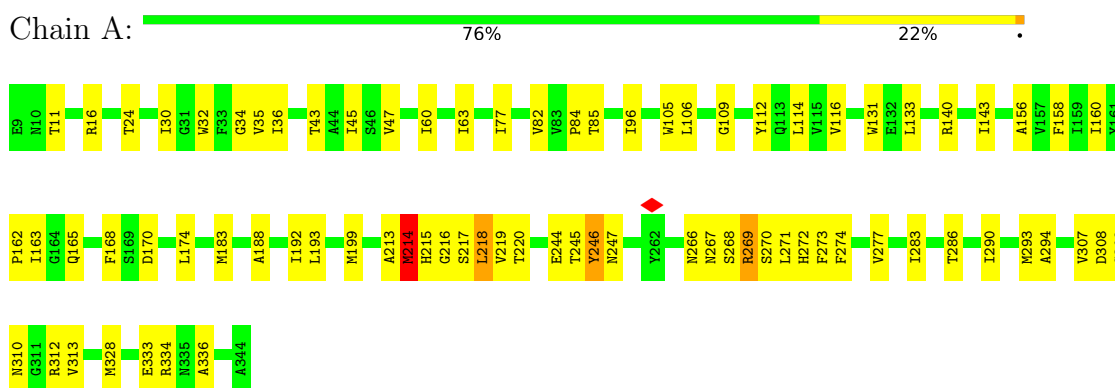
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Mol	Chain	Residues	Atoms		AltConf
52	p	64	Total 64	O 64	0
52	t	2	Total 2	O 2	0
52	w	12	Total 12	O 12	0
52	x	9	Total 9	O 9	0
52	z	6	Total 6	O 6	0
52	n	36	Total 36	O 36	0
52	g	33	Total 33	O 33	0
52	r	33	Total 33	O 33	0
52	s	40	Total 40	O 40	0
52	y	61	Total 61	O 61	0
52	u	5	Total 5	O 5	0

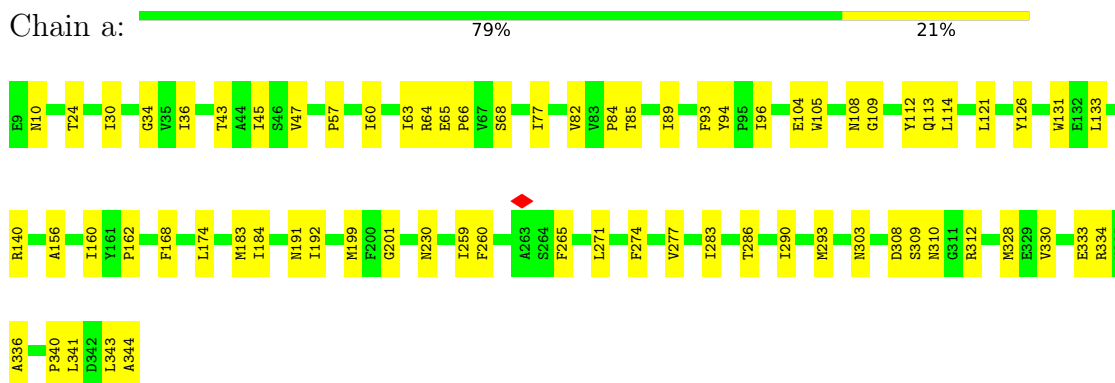
3 Residue-property plots

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.

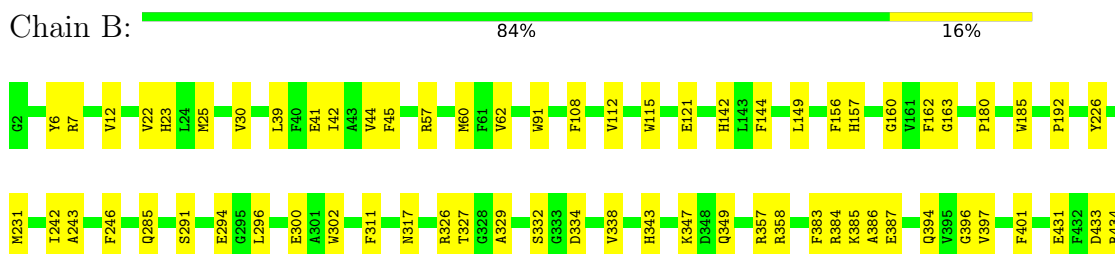
• Molecule 1: Photosystem II protein D1



• Molecule 1: Photosystem II protein D1



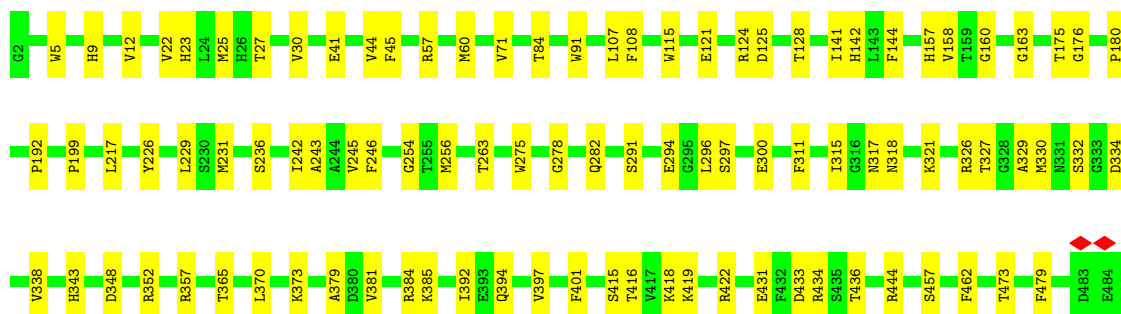
• Molecule 2: Photosystem II CP47 reaction center protein





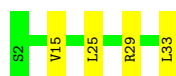
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 80% 20%



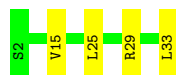
• Molecule 3: Photosystem II reaction center protein Ycf12

Chain V: 88% 12%



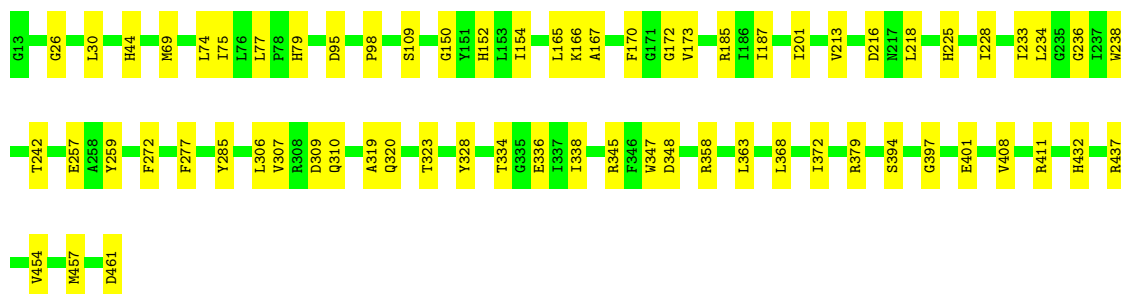
• Molecule 3: Photosystem II reaction center protein Ycf12

Chain v: 88% 12%



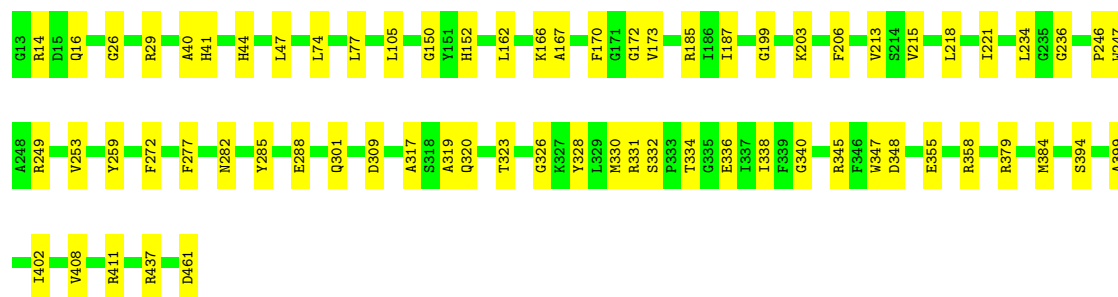
• Molecule 4: Photosystem II CP43 reaction center protein

Chain C: 85% 15%



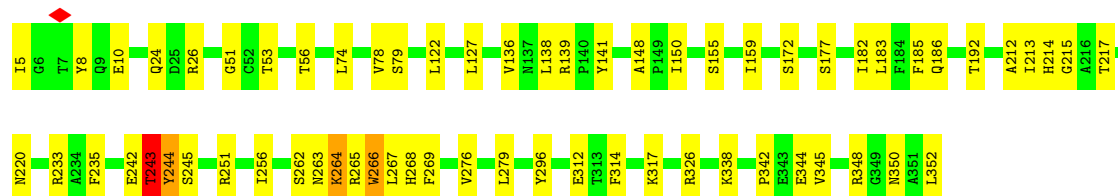
• Molecule 4: Photosystem II CP43 reaction center protein

Chain c: 85% 15%



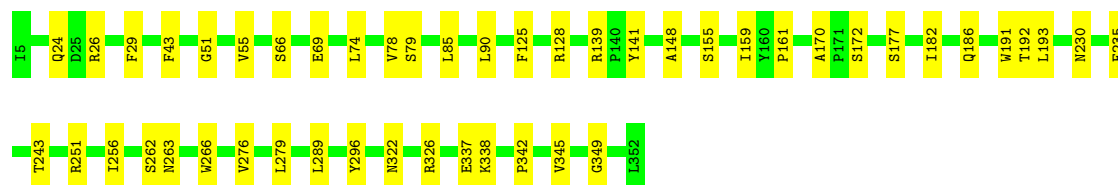
• Molecule 5: Photosystem II D2 protein

Chain D: 82% 17%



• Molecule 5: Photosystem II D2 protein

Chain d: 86% 14%



• Molecule 6: Cytochrome b559 subunit alpha

Chain E: 82% 18%



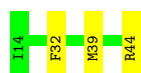
• Molecule 6: Cytochrome b559 subunit alpha

Chain e: 83% 17%



• Molecule 7: Cytochrome b559 subunit beta

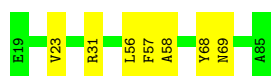
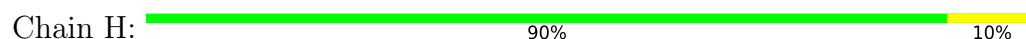
Chain F: 90% 10%



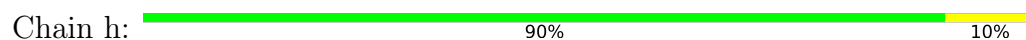
- Molecule 7: Cytochrome b559 subunit beta



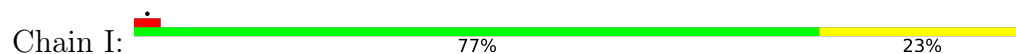
- Molecule 8: Photosystem II reaction center protein H



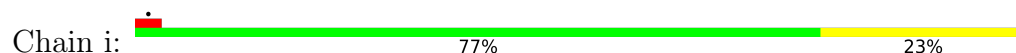
- Molecule 8: Photosystem II reaction center protein H



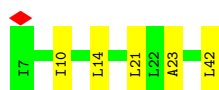
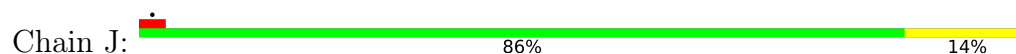
- Molecule 9: Photosystem II reaction center protein I



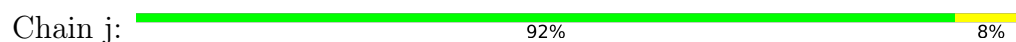
- Molecule 9: Photosystem II reaction center protein I



- Molecule 10: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein J





- Molecule 11: Photosystem II reaction center protein K

Chain K: 86% 14%



- Molecule 11: Photosystem II reaction center protein K

Chain k: 86% 14%



- Molecule 12: Photosystem II reaction center protein L

Chain L: 92% 8%



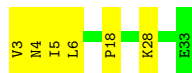
- Molecule 12: Photosystem II reaction center protein L

Chain l: 87% 13%



- Molecule 13: Photosystem II reaction center protein M

Chain M: 81% 19%



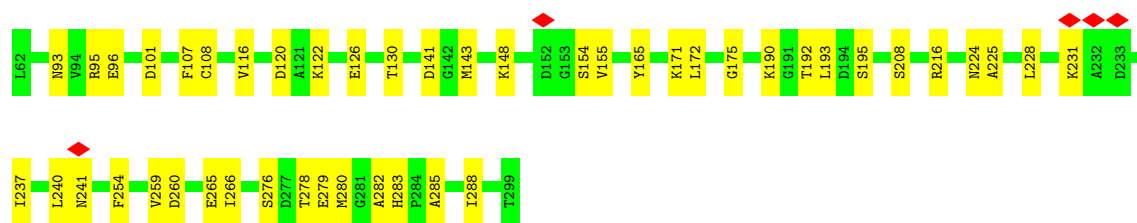
- Molecule 13: Photosystem II reaction center protein M

Chain m: 77% 23%



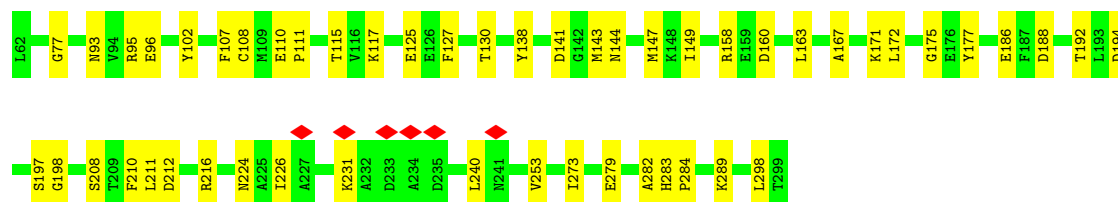
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O: 81% 19%



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

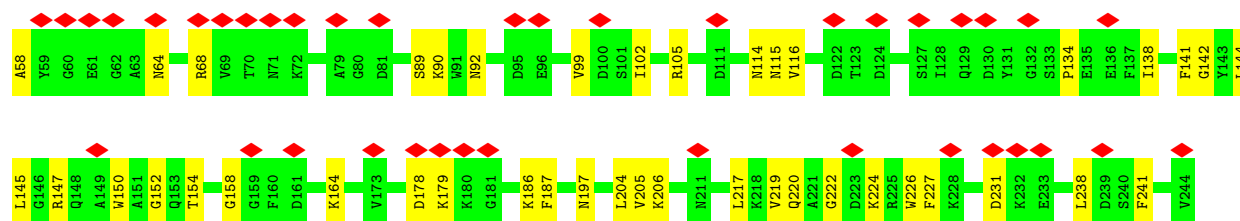
Chain o: 79% 21%



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

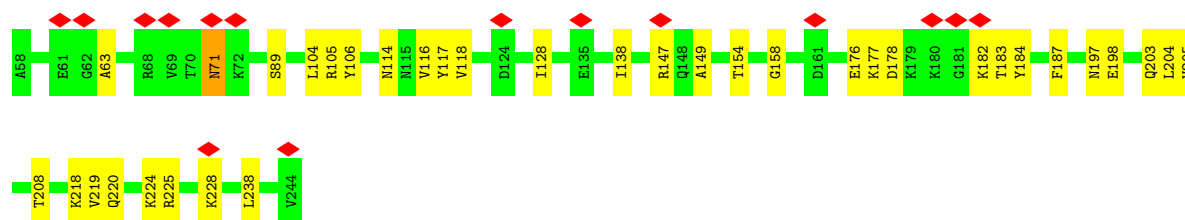
Chain P: 21% 78%

Chain p: 81% 19%



- Molecule 16: Photosystem II reaction center protein T

Chain p: 81% 19%



- Molecule 16: Photosystem II reaction center protein T

Chain T: 83% 17%



- Molecule 16: Photosystem II reaction center protein T

Chain t:  80% 20%



- Molecule 17: PSII 6.1 kDa protein

Chain W:  93% 7%



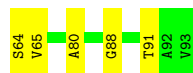
- Molecule 17: PSII 6.1 kDa protein

Chain w:  82% 18%



- Molecule 18: Hypothetical protein

Chain X:  83% 17%



- Molecule 18: Hypothetical protein

Chain x:  80% 20%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  93% 7%



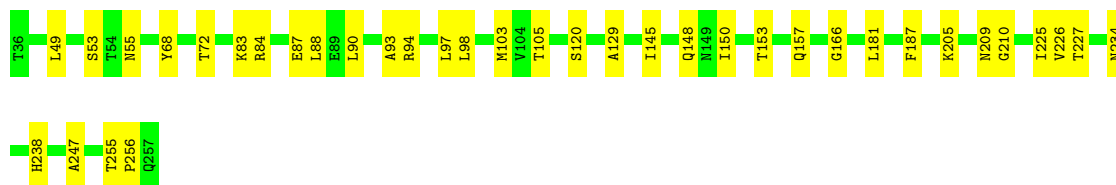
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  93% 7%



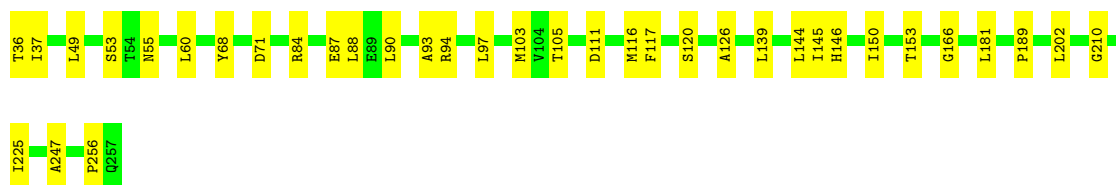
- Molecule 20: Chlorophyll a-b binding protein of LHCII type 3, chloroplastic

Chain N:  83% 17%



- Molecule 20: Chlorophyll a-b binding protein of LHCII type 3, chloroplastic

Chain n:  84% 16%



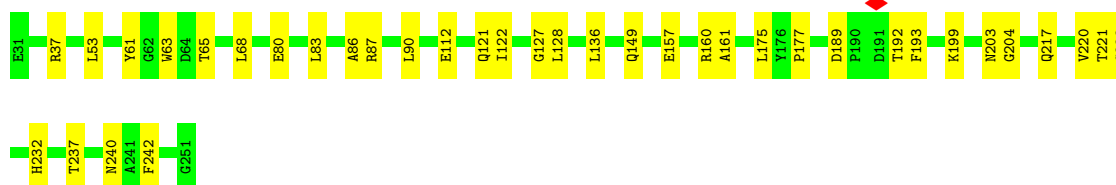
- Molecule 21: Chlorophyll a-b binding protein of LHCII type 2, chloroplastic

Chain G:  90% 10%



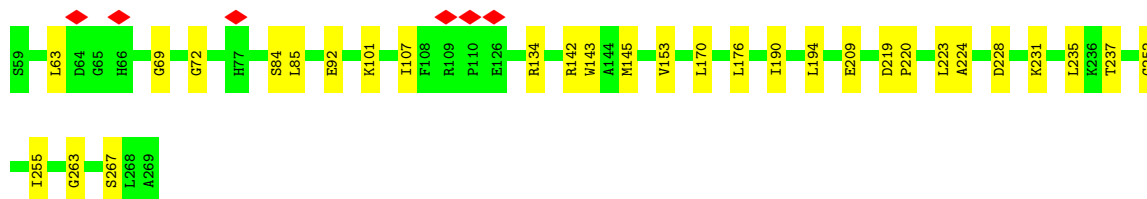
- Molecule 21: Chlorophyll a-b binding protein of LHCII type 2, chloroplastic

Chain g:  83% 17%



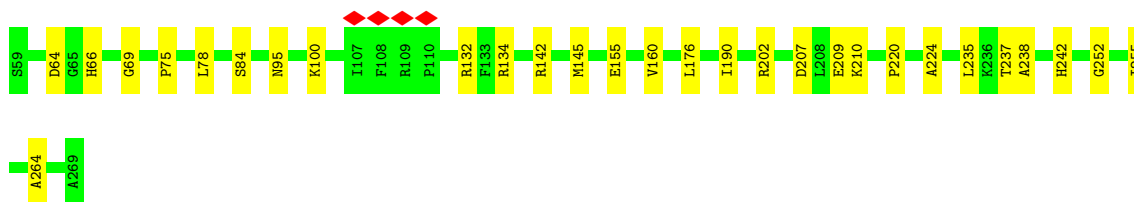
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic, CP29

Chain R:  85% 15%



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

Chain r:  85% 15%



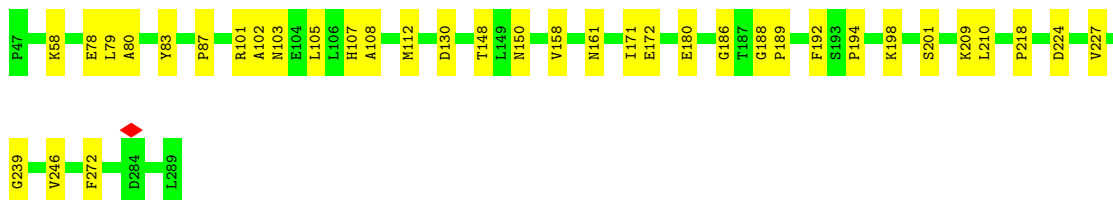
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic, CP26

Chain S: 88% 12%



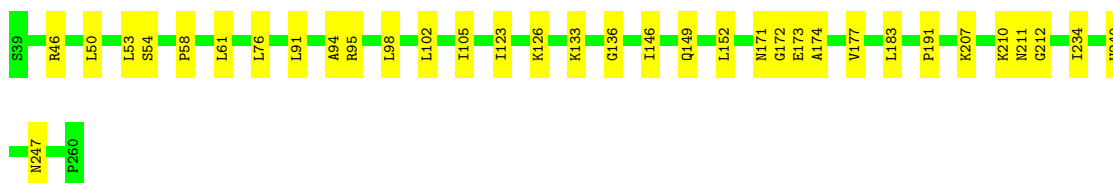
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic, CP26

Chain s: 85% 15%



- Molecule 24: Chlorophyll a-b binding protein of LHCII type 1, chloroplastic

Chain Y: 85% 15%



- Molecule 24: Chlorophyll a-b binding protein of LHCII type 1, chloroplastic

Chain y: 86% 14%



- Molecule 25: Photosystem II extrinsic protein U

Chain U: 67% 33%



- Molecule 25: Photosystem II extrinsic protein U



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39357	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	39.371	Depositor
Minimum map value	-16.255	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	2.5	Depositor
Map size ($\text{\AA}$)	448.0, 448.0, 448.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.896, 0.896, 0.896	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.76	49/2717 (1.8%)	0.97	38/3707 (1.0%)
1	a	0.24	0/2717	0.42	0/3707
2	B	0.21	0/3906	0.37	0/5319
2	b	0.21	0/3906	0.38	0/5319
3	V	0.14	0/228	0.33	0/311
3	v	0.15	0/228	0.33	0/311
4	C	0.18	0/3602	0.37	0/4913
4	c	0.19	0/3602	0.35	0/4913
5	D	1.89	46/2860 (1.6%)	0.92	36/3899 (0.9%)
5	d	0.23	0/2860	0.38	0/3899
6	E	0.19	0/639	0.44	0/870
6	e	0.18	0/639	0.43	0/870
7	F	0.19	0/259	0.38	0/351
7	f	0.16	0/259	0.33	0/351
8	H	0.16	0/513	0.36	0/703
8	h	0.17	0/513	0.34	0/703
9	I	0.24	0/287	0.40	0/386
9	i	0.20	0/287	0.40	0/386
10	J	0.12	0/272	0.26	0/369
10	j	0.14	0/272	0.31	0/369
11	K	0.25	0/308	0.60	2/423 (0.5%)
11	k	0.25	0/308	0.49	0/423
12	L	0.19	0/321	0.33	0/435
12	l	0.21	0/321	0.31	0/435
13	M	0.24	0/237	0.48	0/323
13	m	0.25	0/237	0.51	0/323
14	O	0.16	0/1855	0.40	0/2505
14	o	0.17	0/1855	0.40	0/2505
15	P	0.15	0/1473	0.40	0/1988
15	p	0.15	0/1473	0.42	2/1988 (0.1%)
16	T	0.22	0/254	0.38	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.21	0/254	0.32	0/342
17	W	0.17	0/339	0.38	0/460
17	w	0.21	0/339	0.39	0/460
18	X	0.19	0/202	0.42	0/276
18	x	0.17	0/202	0.38	0/276
19	Z	0.14	0/469	0.30	0/641
19	z	0.14	0/469	0.30	0/641
20	N	0.17	0/1751	0.36	0/2386
20	n	0.18	0/1751	0.36	0/2386
21	G	0.16	0/1725	0.34	0/2348
21	g	0.17	0/1725	0.35	0/2348
22	R	0.15	0/1506	0.33	0/2035
22	r	0.15	0/1506	0.33	0/2035
23	S	0.18	0/1903	0.39	0/2590
23	s	0.18	0/1903	0.38	0/2590
24	Y	0.18	0/1715	0.36	0/2338
24	y	0.19	0/1715	0.33	0/2338
25	U	0.19	0/224	0.41	0/298
25	u	0.30	0/224	0.67	0/298
All	All	0.59	95/59130 (0.2%)	0.46	78/80432 (0.1%)

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
5	D	0	2

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	213	ILE	C-O	-30.87	0.88	1.24
1	A	216	GLY	C-O	-30.70	0.87	1.23
5	D	264	LYS	C-O	-30.20	0.88	1.24
5	D	268	HIS	C-O	-26.99	0.90	1.24
5	D	265	ARG	C-O	-26.81	0.93	1.24

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	MET	CA-C-O	-13.04	106.59	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	263	ASN	CA-CB-CG	11.75	124.35	112.60
1	A	269	ARG	CB-CA-C	11.29	131.37	110.70
5	D	267	LEU	N-CA-C	10.04	123.48	111.33
5	D	265	ARG	CB-CA-C	9.94	126.72	110.92

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	243	THR	Mainchain
5	D	244	TYR	Mainchain

5.2 Too-close contacts [i](#)

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	2635	0	2535	50	0
1	a	2635	0	2536	52	0
2	B	3785	0	3663	64	0
2	b	3785	0	3663	74	0
3	V	227	0	261	3	0
3	v	227	0	261	4	0
4	C	3483	0	3376	49	0
4	c	3483	0	3376	51	0
5	D	2766	0	2654	41	0
5	d	2766	0	2655	36	0
6	E	621	0	605	11	0
6	e	621	0	605	10	0
7	F	252	0	265	5	0
7	f	252	0	265	8	0
8	H	503	0	532	8	0
8	h	503	0	532	8	0
9	I	279	0	288	8	0
9	i	279	0	288	7	0
10	J	266	0	286	4	0
10	j	266	0	286	3	0
11	K	297	0	312	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	k	297	0	312	4	0
12	L	313	0	325	3	0
12	l	313	0	325	5	0
13	M	234	0	258	6	0
13	m	234	0	258	6	0
14	O	1820	0	1776	32	0
14	o	1820	0	1776	35	0
15	P	1444	0	1403	39	0
15	p	1444	0	1403	28	0
16	T	247	0	260	6	0
16	t	247	0	260	6	0
17	W	332	0	323	3	0
17	w	332	0	323	7	0
18	X	201	0	224	4	0
18	x	201	0	224	4	0
19	Z	457	0	478	4	0
19	z	457	0	478	4	0
20	N	1703	0	1641	30	0
20	n	1703	0	1641	28	0
21	G	1680	0	1614	15	0
21	g	1680	0	1614	27	0
22	R	1490	0	1454	24	0
22	r	1490	0	1454	20	0
23	S	1856	0	1816	23	0
23	s	1856	0	1816	26	0
24	Y	1667	0	1624	22	0
24	y	1667	0	1624	21	0
25	U	224	0	226	8	0
25	u	224	0	226	9	0
26	A	10	0	0	1	0
26	a	10	0	0	1	0
27	A	1	0	0	0	0
27	d	1	0	0	0	0
28	A	2	0	0	0	0
28	a	2	0	0	0	0
29	A	240	0	242	19	0
29	B	1030	0	1129	41	0
29	C	830	0	900	27	0
29	D	125	0	131	9	0
29	G	466	0	471	20	0
29	N	468	0	471	17	0
29	R	385	0	347	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	S	620	0	582	29	0
29	Y	570	0	615	24	0
29	a	239	0	242	14	0
29	b	1032	0	1133	41	0
29	c	840	0	923	33	0
29	d	130	0	144	7	0
29	g	466	0	471	16	0
29	n	468	0	471	22	0
29	r	400	0	375	19	0
29	s	625	0	592	23	0
29	y	570	0	615	27	0
30	A	64	0	74	5	0
30	D	64	0	74	3	0
30	a	64	0	74	4	0
30	d	64	0	74	2	0
31	A	40	0	53	3	0
31	B	80	0	105	7	0
31	C	120	0	158	11	0
31	F	40	0	53	2	0
31	K	40	0	53	4	0
31	a	40	0	53	2	0
31	b	80	0	106	10	0
31	c	80	0	105	8	0
31	f	40	0	53	2	0
31	v	40	0	53	3	0
31	z	40	0	53	5	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	A	48	0	75	1	0
33	B	48	0	75	3	0
33	S	30	0	33	2	0
33	a	48	0	75	3	0
33	b	39	0	51	4	0
33	s	48	0	75	3	0
34	B	42	0	0	0	0
34	b	42	0	0	0	0
35	B	44	0	58	3	0
35	C	144	0	204	5	0
35	D	90	0	120	5	0
35	W	79	0	98	4	0
35	b	44	0	58	4	0
35	c	106	0	158	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	d	94	0	128	4	0
35	i	48	0	66	2	0
35	w	39	0	48	2	0
36	B	43	0	44	1	0
36	C	157	0	188	9	0
36	c	176	0	226	11	0
36	r	43	0	44	1	0
37	B	44	0	61	3	0
37	D	88	0	122	9	0
37	G	49	0	74	1	0
37	L	49	0	74	3	0
37	N	49	0	74	4	0
37	S	80	0	103	6	0
37	Y	49	0	74	8	0
37	a	83	0	109	5	0
37	c	47	0	67	7	0
37	d	49	0	74	5	0
37	g	49	0	74	4	0
37	l	49	0	74	3	0
37	n	42	0	57	5	0
37	s	83	0	109	6	0
37	y	49	0	74	3	0
38	B	35	0	44	2	0
38	b	35	0	44	4	0
39	C	78	0	82	2	0
39	L	42	0	47	5	0
39	M	42	0	47	2	0
39	a	51	0	68	1	0
39	b	54	0	77	4	0
39	c	54	0	77	3	0
39	l	42	0	47	3	0
39	m	42	0	47	1	0
39	o	54	0	77	1	0
40	C	21	0	37	1	0
40	I	21	0	37	3	0
40	c	21	0	37	4	0
40	i	21	0	37	1	0
41	D	37	0	56	3	0
41	J	29	0	40	2	0
41	W	44	0	76	4	0
41	b	44	0	76	2	0
41	j	29	0	40	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	w	44	0	76	6	0
42	D	4	0	0	1	0
42	a	4	0	0	0	0
43	D	55	0	80	2	0
43	d	55	0	80	2	0
44	E	43	0	30	1	0
44	e	43	0	30	3	0
45	H	41	0	56	3	0
45	h	41	0	56	2	0
46	G	340	0	305	12	0
46	N	380	0	382	20	0
46	R	94	0	66	3	0
46	S	194	0	144	12	0
46	Y	310	0	308	12	0
46	g	340	0	306	13	0
46	n	314	0	314	15	0
46	r	94	0	66	4	0
46	s	194	0	144	8	0
46	y	361	0	344	16	0
47	G	84	0	110	6	0
47	N	84	0	110	6	0
47	R	42	0	55	4	0
47	S	84	0	110	8	0
47	Y	84	0	110	6	0
47	g	84	0	110	6	0
47	n	84	0	110	7	0
47	r	42	0	55	3	0
47	s	84	0	110	6	0
47	y	84	0	110	4	0
48	G	44	0	54	3	0
48	N	44	0	54	3	0
48	R	27	0	32	3	0
48	S	44	0	54	4	0
48	Y	44	0	54	3	0
48	g	44	0	55	2	0
48	n	44	0	54	1	0
48	r	27	0	32	1	0
48	s	44	0	54	3	0
48	y	44	0	54	3	0
49	G	44	0	56	3	0
49	N	44	0	56	5	0
49	R	44	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	Y	44	0	56	3	0
49	g	44	0	56	2	0
49	n	44	0	56	4	0
49	r	44	0	56	4	0
49	y	44	0	56	4	0
50	N	50	0	79	8	0
50	Y	19	0	11	0	0
50	n	50	0	79	5	0
50	y	19	0	11	0	0
51	S	20	0	20	3	0
51	s	19	0	18	0	0
52	A	93	0	0	0	0
52	B	144	0	0	3	0
52	C	110	0	0	3	0
52	D	74	0	0	0	0
52	E	15	0	0	1	0
52	F	2	0	0	0	0
52	G	60	0	0	0	0
52	H	13	0	0	0	0
52	I	9	0	0	1	0
52	J	5	0	0	0	0
52	K	9	0	0	0	0
52	L	14	0	0	0	0
52	M	9	0	0	1	0
52	N	63	0	0	1	0
52	O	75	0	0	0	0
52	P	22	0	0	1	0
52	R	36	0	0	0	0
52	S	33	0	0	0	0
52	T	5	0	0	0	0
52	U	8	0	0	1	0
52	V	7	0	0	0	0
52	W	9	0	0	0	0
52	X	3	0	0	1	0
52	Y	55	0	0	0	0
52	Z	4	0	0	1	0
52	a	91	0	0	2	0
52	b	123	0	0	1	0
52	c	102	0	0	1	0
52	d	68	0	0	0	0
52	e	23	0	0	0	0
52	f	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	g	33	0	0	0	0
52	h	18	0	0	0	0
52	i	11	0	0	0	0
52	j	3	0	0	0	0
52	k	9	0	0	0	0
52	l	8	0	0	0	0
52	m	6	0	0	0	0
52	n	36	0	0	0	0
52	o	78	0	0	1	0
52	p	64	0	0	1	0
52	r	33	0	0	1	0
52	s	40	0	0	1	0
52	t	2	0	0	0	0
52	u	5	0	0	0	0
52	v	3	0	0	0	0
52	w	12	0	0	0	0
52	x	9	0	0	0	0
52	y	61	0	0	0	0
52	z	6	0	0	1	0
All	All	77465	0	76472	1333	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 9.

The worst 5 of 1333 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)
29:R:306:CLA:HMB2	48:R:312:NEX:H35	1.60	0.83
29:C:507:CLA:H91	31:C:516:BCR:H14C	1.63	0.80
29:r:309:CLA:H2	47:r:311:LUT:H28	1.63	0.80
29:n:603:CLA:H2	29:n:603:CLA:HMA2	1.65	0.77
29:c:503:CLA:H172	29:c:510:CLA:HBB2	1.67	0.76

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	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
1	a	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
2	B	481/484 (99%)	470 (98%)	11 (2%)	0	100	100
2	b	481/484 (99%)	468 (97%)	13 (3%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
4	c	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
5	D	346/348 (99%)	338 (98%)	8 (2%)	0	100	100
5	d	346/348 (99%)	340 (98%)	6 (2%)	0	100	100
6	E	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
6	e	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
8	h	65/67 (97%)	65 (100%)	0	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
14	o	236/238 (99%)	218 (92%)	18 (8%)	0	100	100
15	P	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	0	100	100
16	t	28/30 (93%)	28 (100%)	0	0	100	100
17	W	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	24	29
20	n	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	24	29
21	G	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
21	g	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
22	R	191/196 (97%)	178 (93%)	13 (7%)	0	100	100
22	r	191/196 (97%)	174 (91%)	16 (8%)	1 (0%)	24	29
23	S	241/243 (99%)	228 (95%)	13 (5%)	0	100	100
23	s	241/243 (99%)	220 (91%)	21 (9%)	0	100	100
24	Y	220/222 (99%)	213 (97%)	6 (3%)	1 (0%)	24	29
24	y	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	24	29
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
All	All	7334/7442 (98%)	7065 (96%)	264 (4%)	5 (0%)	49	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	r	176	LEU
24	y	146	ILE
24	Y	146	ILE

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Mol	Chain	Res	Type
20	n	145	ILE
20	N	145	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/275 (100%)	274 (100%)	1 (0%)	84	89
1	a	275/275 (100%)	275 (100%)	0	100	100
2	B	387/387 (100%)	387 (100%)	0	100	100
2	b	387/387 (100%)	387 (100%)	0	100	100
3	V	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	277 (99%)	2 (1%)	76	83
5	d	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	o	195/195 (100%)	195 (100%)	0	100	100
15	P	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
23	S	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
All	All	5934/5934 (100%)	5931 (100%)	3 (0%)	87	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	MET
5	D	243	THR
5	D	264	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
5	d	83	ASN
20	n	39	GLN
5	d	186	GLN
15	p	71	ASN
20	n	241	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
2	CSD	b	218	2	4,7,8	1.05	0	1,8,10	0.57	0
22	SEP	R	84	22	8,9,10	1.56	1 (12%)	7,12,14	1.35	1 (14%)
22	SEP	r	84	22	8,9,10	1.58	1 (12%)	7,12,14	1.41	1 (14%)
2	CSD	B	218	2	4,7,8	0.97	0	1,8,10	0.56	0

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
2	CSD	b	218	2	-	1/2/6/8	-
22	SEP	R	84	22	-	2/6/8/10	-
22	SEP	r	84	22	-	4/6/8/10	-
2	CSD	B	218	2	-	1/2/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.50	1.61	1.50
22	r	84	SEP	P-O1P	3.48	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r	84	SEP	OG-CB-CA	2.94	111.00	108.14
22	R	84	SEP	OG-CB-CA	2.94	111.00	108.14

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	R	84	SEP	C-CA-CB-OG
22	r	84	SEP	N-CA-CB-OG
22	r	84	SEP	CB-OG-P-O1P
22	r	84	SEP	CB-OG-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 8 are monoatomic - leaving 346 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
29	CLA	B	515	-	69,73,73	0.99	4 (5%)	82,113,113	0.94	4 (4%)
39	SQD	l	101	-	40,42,54	0.86	0	50,53,65	0.93	3 (6%)
29	CLA	B	511	-	69,73,73	0.98	5 (7%)	82,113,113	1.06	3 (3%)
29	CLA	y	313	37	69,73,73	0.98	4 (5%)	82,113,113	0.97	5 (6%)
46	CHL	y	307	24	40,54,74	1.73	9 (22%)	34,90,114	2.07	10 (29%)
29	CLA	c	511	4	69,73,73	1.00	4 (5%)	82,113,113	1.10	3 (3%)
51	LPX	S	321	-	19,19,29	1.22	2 (10%)	21,23,33	1.06	1 (4%)
29	CLA	C	508	52	69,73,73	0.98	4 (5%)	82,113,113	1.07	3 (3%)
30	PHO	a	407	-	58,69,69	2.05	10 (17%)	55,99,99	1.47	6 (10%)
41	DGA	D	402	-	36,36,43	1.21	2 (5%)	38,38,45	1.33	3 (7%)
36	DGD	c	516	-	56,56,67	1.05	4 (7%)	70,70,81	0.95	2 (2%)
37	LHG	a	414	-	38,38,48	0.42	0	41,44,54	1.10	2 (4%)
29	CLA	b	503	-	69,73,73	0.98	5 (7%)	82,113,113	1.11	5 (6%)
33	3PH	B	522	-	47,47,47	0.87	4 (8%)	50,52,52	1.13	2 (4%)
29	CLA	s	310	-	64,68,73	1.03	4 (6%)	76,107,113	1.04	3 (3%)
29	CLA	c	510	-	69,73,73	0.97	3 (4%)	82,113,113	0.97	5 (6%)
30	PHO	d	402	-	58,69,69	2.11	10 (17%)	55,99,99	1.61	7 (12%)
29	CLA	R	301	22	64,68,73	1.01	4 (6%)	76,107,113	1.09	5 (6%)
35	LMG	C	521	-	47,47,55	1.08	4 (8%)	55,55,63	1.13	4 (7%)
31	BCR	C	515	-	41,41,41	1.62	4 (9%)	56,56,56	4.37	13 (23%)
29	CLA	s	313	23	49,53,73	1.17	4 (8%)	58,89,113	1.10	4 (6%)
29	CLA	s	305	-	59,63,73	1.05	5 (8%)	70,101,113	1.20	3 (4%)
48	NEX	G	617	-	40,46,46	2.67	11 (27%)	50,70,70	1.77	13 (26%)
29	CLA	a	404	-	69,73,73	0.99	4 (5%)	82,113,113	1.10	3 (3%)
29	CLA	C	512	4	69,73,73	1.00	4 (5%)	82,113,113	1.00	5 (6%)
29	CLA	r	304	-	53,57,73	1.11	4 (7%)	61,93,113	1.02	2 (3%)
39	SQD	c	522	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
29	CLA	S	306	23	54,58,73	1.12	5 (9%)	64,95,113	1.29	5 (7%)
31	BCR	f	101	-	41,41,41	1.60	4 (9%)	56,56,56	4.44	18 (32%)
29	CLA	a	408	-	64,68,73	1.01	6 (9%)	76,107,113	1.11	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	R	303	-	53,57,73	1.11	4 (7%)	61,93,113	0.97	1 (1%)
46	CHL	G	609	21	60,74,74	1.45	9 (15%)	58,114,114	1.62	13 (22%)
29	CLA	b	516	-	69,73,73	1.00	6 (8%)	82,113,113	1.02	5 (6%)
48	NEX	s	319	-	40,46,46	2.70	11 (27%)	50,70,70	1.54	8 (16%)
29	CLA	b	501	-	69,73,73	0.98	4 (5%)	82,113,113	1.00	6 (7%)
29	CLA	b	515	-	69,73,73	0.99	4 (5%)	82,113,113	0.96	4 (4%)
31	BCR	c	514	-	41,41,41	1.62	5 (12%)	56,56,56	4.33	19 (33%)
29	CLA	R	309	-	54,58,73	1.13	5 (9%)	64,95,113	1.14	6 (9%)
31	BCR	K	101	-	41,41,41	1.60	4 (9%)	56,56,56	4.41	14 (25%)
29	CLA	d	403	-	69,73,73	0.97	5 (7%)	82,113,113	1.03	3 (3%)
29	CLA	R	307	22	50,54,73	1.13	4 (8%)	59,90,113	1.13	6 (10%)
47	LUT	n	615	-	42,43,43	2.42	1 (2%)	51,60,60	1.68	10 (19%)
29	CLA	s	304	-	69,73,73	1.05	7 (10%)	82,113,113	1.24	6 (7%)
29	CLA	G	604	-	53,57,73	1.13	4 (7%)	61,93,113	1.05	5 (8%)
46	CHL	S	302	23	40,54,74	1.82	8 (20%)	34,90,114	2.17	11 (32%)
29	CLA	Y	304	-	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
41	DGA	W	202	-	43,43,43	1.15	3 (6%)	45,45,45	1.50	3 (6%)
46	CHL	R	305	-	44,58,74	1.62	9 (20%)	37,94,114	2.12	11 (29%)
29	CLA	Y	315	-	69,73,73	0.97	4 (5%)	82,113,113	1.08	6 (7%)
29	CLA	C	502	-	69,73,73	0.97	4 (5%)	82,113,113	1.01	5 (6%)
29	CLA	G	603	-	69,73,73	0.99	4 (5%)	82,113,113	0.99	5 (6%)
29	CLA	c	501	-	69,73,73	0.97	4 (5%)	82,113,113	1.05	6 (7%)
29	CLA	B	505	-	69,73,73	0.99	4 (5%)	82,113,113	1.15	4 (4%)
29	CLA	G	612	21	47,51,73	1.16	4 (8%)	55,86,113	1.07	3 (5%)
37	LHG	B	523	-	43,43,48	0.41	0	46,49,54	1.04	2 (4%)
47	LUT	g	616	-	42,43,43	2.47	1 (2%)	51,60,60	1.93	12 (23%)
38	LMT	B	524	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	5 (10%)
49	XAT	N	619	-	41,47,47	0.69	1 (2%)	54,74,74	1.98	13 (24%)
29	CLA	b	507	52	69,73,73	0.98	4 (5%)	82,113,113	1.08	2 (2%)
43	PL9	D	406	-	55,55,55	1.31	5 (9%)	68,69,69	1.44	11 (16%)
34	C7Z	b	519	-	43,43,43	5.37	26 (60%)	56,60,60	2.47	23 (41%)
35	LMG	C	522	-	55,55,55	1.27	6 (10%)	63,63,63	1.06	2 (3%)
29	CLA	c	504	-	69,73,73	0.96	5 (7%)	82,113,113	1.04	4 (4%)
49	XAT	y	302	-	41,47,47	0.68	1 (2%)	54,74,74	2.04	13 (24%)
46	CHL	S	308	-	37,51,74	1.65	8 (21%)	30,86,114	2.29	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	C	516	-	41,41,41	1.61	4 (9%)	56,56,56	4.39	14 (25%)
39	SQD	a	410	-	49,51,54	0.79	0	59,62,65	0.87	2 (3%)
37	LHG	D	407	-	48,48,48	0.41	0	51,54,54	1.01	3 (5%)
40	SPH	c	523	-	19,20,20	0.66	0	18,21,21	1.12	1 (5%)
29	CLA	S	313	23	49,53,73	1.17	4 (8%)	58,89,113	1.03	5 (8%)
36	DGD	c	517	-	63,63,67	1.22	7 (11%)	77,77,81	0.95	3 (3%)
29	CLA	g	604	-	53,57,73	1.11	5 (9%)	61,93,113	1.07	3 (4%)
48	NEX	g	617	-	40,46,46	2.65	11 (27%)	50,70,70	1.81	11 (22%)
29	CLA	b	509	-	69,73,73	0.99	5 (7%)	82,113,113	1.07	6 (7%)
46	CHL	Y	302	24	60,74,74	1.17	9 (15%)	58,114,114	1.79	12 (20%)
46	CHL	N	608	-	44,58,74	1.51	7 (15%)	37,94,114	2.04	12 (32%)
29	CLA	N	604	-	69,73,73	0.99	5 (7%)	82,113,113	1.02	5 (6%)
35	LMG	c	520	-	55,55,55	1.28	6 (10%)	63,63,63	1.03	2 (3%)
29	CLA	g	603	-	69,73,73	0.99	5 (7%)	82,113,113	1.04	4 (4%)
29	CLA	c	502	-	69,73,73	0.98	4 (5%)	82,113,113	1.08	5 (6%)
46	CHL	Y	306	24	40,54,74	1.72	9 (22%)	34,90,114	2.06	10 (29%)
29	CLA	y	316	-	69,73,73	0.98	4 (5%)	82,113,113	1.02	5 (6%)
49	XAT	G	619	-	41,47,47	0.67	1 (2%)	54,74,74	3.77	17 (31%)
29	CLA	g	610	21	69,73,73	0.99	6 (8%)	82,113,113	1.25	6 (7%)
29	CLA	N	612	20	49,53,73	1.17	4 (8%)	58,89,113	1.08	4 (6%)
46	CHL	N	601	20	60,74,74	1.28	8 (13%)	58,114,114	1.79	12 (20%)
47	LUT	S	317	-	42,43,43	2.33	1 (2%)	51,60,60	1.79	12 (23%)
29	CLA	c	505	-	69,73,73	1.00	5 (7%)	82,113,113	1.09	5 (6%)
29	CLA	S	315	-	54,58,73	1.11	4 (7%)	64,95,113	1.07	5 (7%)
29	CLA	Y	303	24	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
31	BCR	v	101	-	41,41,41	1.60	4 (9%)	56,56,56	4.45	19 (33%)
29	CLA	R	306	-	64,68,73	1.03	6 (9%)	76,107,113	1.03	2 (2%)
29	CLA	B	512	-	69,73,73	0.98	4 (5%)	82,113,113	1.01	2 (2%)
29	CLA	b	506	-	61,65,73	1.03	5 (8%)	72,103,113	1.11	5 (6%)
29	CLA	y	306	52	69,73,73	0.98	5 (7%)	82,113,113	1.09	5 (6%)
29	CLA	C	504	-	69,73,73	0.99	4 (5%)	82,113,113	0.99	3 (3%)
29	CLA	s	303	23	64,68,73	1.01	4 (6%)	76,107,113	1.13	5 (6%)
29	CLA	G	613	21	69,73,73	0.98	4 (5%)	82,113,113	0.95	2 (2%)
29	CLA	g	613	21	69,73,73	1.00	4 (5%)	82,113,113	0.97	3 (3%)
46	CHL	g	605	21	42,56,74	1.71	9 (21%)	36,92,114	2.15	11 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LHG	y	320	29	48,48,48	0.39	0	51,54,54	1.12	4 (7%)
29	CLA	n	611	20	49,53,73	1.17	4 (8%)	58,89,113	1.14	5 (8%)
46	CHL	s	309	-	55,69,74	1.37	9 (16%)	52,108,114	1.69	9 (17%)
29	CLA	C	513	-	69,73,73	0.99	4 (5%)	82,113,113	0.93	3 (3%)
29	CLA	A	405	-	69,73,73	0.98	4 (5%)	82,113,113	1.00	3 (3%)
29	CLA	b	511	-	69,73,73	0.98	5 (7%)	82,113,113	1.08	5 (6%)
29	CLA	c	512	-	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
46	CHL	n	601	20	60,74,74	1.34	8 (13%)	58,114,114	1.78	12 (20%)
29	CLA	g	602	21	69,73,73	0.97	4 (5%)	82,113,113	1.00	4 (4%)
37	LHG	n	617	-	41,41,48	0.42	0	44,47,54	1.17	4 (9%)
50	PTY	y	321	-	18,18,49	1.33	3 (16%)	21,23,54	1.47	2 (9%)
29	CLA	s	315	-	59,63,73	1.08	5 (8%)	70,101,113	1.05	4 (5%)
29	CLA	a	405	52	69,73,73	0.98	5 (7%)	82,113,113	1.04	6 (7%)
29	CLA	d	404	-	69,73,73	0.99	4 (5%)	82,113,113	1.10	7 (8%)
42	BCT	D	403	27	3,3,3	1.05	0	2,3,3	1.24	0
46	CHL	G	601	21	60,74,74	1.35	9 (15%)	58,114,114	1.71	11 (18%)
29	CLA	N	614	-	53,57,73	1.13	4 (7%)	61,93,113	1.07	6 (9%)
35	LMG	i	101	-	48,48,55	1.11	5 (10%)	56,56,63	1.08	3 (5%)
29	CLA	S	304	-	69,73,73	1.03	6 (8%)	82,113,113	1.21	10 (12%)
37	LHG	Y	319	29	48,48,48	0.40	0	51,54,54	1.00	2 (3%)
31	BCR	B	517	-	41,41,41	1.66	5 (12%)	56,56,56	4.38	19 (33%)
36	DGD	C	519	-	54,54,67	1.07	4 (7%)	68,68,81	0.92	3 (4%)
46	CHL	s	308	-	37,51,74	1.72	9 (24%)	30,86,114	2.34	11 (36%)
48	NEX	r	313	-	25,28,46	2.60	7 (28%)	32,42,70	1.78	6 (18%)
47	LUT	Y	316	-	42,43,43	2.46	1 (2%)	51,60,60	1.77	16 (31%)
37	LHG	D	408	-	38,38,48	0.42	0	41,44,54	1.06	3 (7%)
46	CHL	G	607	-	60,74,74	1.19	7 (11%)	58,114,114	1.77	12 (20%)
46	CHL	g	609	21	60,74,74	1.47	10 (16%)	58,114,114	1.62	12 (20%)
49	XAT	r	312	-	41,47,47	0.65	1 (2%)	54,74,74	1.88	12 (22%)
29	CLA	R	302	-	64,68,73	1.05	6 (9%)	76,107,113	1.12	6 (7%)
50	PTY	Y	320	-	18,18,49	1.33	3 (16%)	21,23,54	1.50	2 (9%)
46	CHL	n	605	20	60,74,74	1.66	9 (15%)	58,114,114	1.66	11 (18%)
46	CHL	g	608	-	38,52,74	1.73	9 (23%)	31,87,114	2.17	10 (32%)
46	CHL	y	303	24	60,74,74	1.38	10 (16%)	58,114,114	1.74	12 (20%)
37	LHG	S	320	29	44,44,48	0.41	0	47,50,54	1.05	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	CHL	y	301	-	60,74,74	1.26	7 (11%)	58,114,114	1.73	12 (20%)
29	CLA	y	304	24	69,73,73	1.00	4 (5%)	82,113,113	1.10	6 (7%)
29	CLA	c	506	-	64,68,73	1.01	3 (4%)	76,107,113	1.10	6 (7%)
30	PHO	A	408	-	58,69,69	2.10	10 (17%)	55,99,99	1.50	7 (12%)
47	LUT	r	311	-	42,43,43	2.54	2 (4%)	51,60,60	1.84	13 (25%)
39	SQD	L	102	-	40,42,54	0.85	0	50,53,65	0.89	2 (4%)
35	LMG	d	407	-	46,46,55	1.03	4 (8%)	54,54,63	1.06	2 (3%)
29	CLA	n	610	-	53,57,73	1.14	5 (9%)	61,93,113	1.04	4 (6%)
29	CLA	G	614	-	53,57,73	1.12	4 (7%)	61,93,113	1.06	3 (4%)
29	CLA	r	309	22	64,68,73	1.02	4 (6%)	76,107,113	1.17	7 (9%)
41	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.26	2 (6%)
29	CLA	A	407	-	54,58,73	1.09	4 (7%)	64,95,113	1.09	6 (9%)
29	CLA	S	312	37	69,73,73	1.00	4 (5%)	82,113,113	1.07	4 (4%)
37	LHG	l	102	-	48,48,48	0.40	0	51,54,54	1.01	2 (3%)
46	CHL	y	309	-	60,74,74	1.10	7 (11%)	58,114,114	1.80	12 (20%)
29	CLA	B	504	-	69,73,73	1.00	3 (4%)	82,113,113	1.24	6 (7%)
29	CLA	B	514	-	69,73,73	0.99	4 (5%)	82,113,113	1.07	5 (6%)
37	LHG	d	406	-	48,48,48	0.40	0	51,54,54	1.02	3 (5%)
29	CLA	y	305	-	69,73,73	0.98	4 (5%)	82,113,113	1.00	4 (4%)
46	CHL	y	308	52	45,59,74	1.61	8 (17%)	40,96,114	1.91	12 (30%)
29	CLA	C	510	-	69,73,73	0.99	4 (5%)	82,113,113	1.02	4 (4%)
47	LUT	S	318	-	42,43,43	2.40	1 (2%)	51,60,60	1.82	13 (25%)
46	CHL	Y	307	-	60,74,74	1.58	10 (16%)	58,114,114	1.63	10 (17%)
42	BCT	a	412	27	3,3,3	0.59	0	2,3,3	5.12	2 (100%)
29	CLA	C	506	-	64,68,73	1.03	6 (9%)	76,107,113	1.06	4 (5%)
29	CLA	r	302	22	64,68,73	1.01	4 (6%)	76,107,113	1.10	5 (6%)
29	CLA	y	312	24	69,73,73	0.99	6 (8%)	82,113,113	1.08	5 (6%)
31	BCR	z	101	-	41,41,41	1.61	4 (9%)	56,56,56	4.45	11 (19%)
29	CLA	g	614	-	53,57,73	1.12	4 (7%)	61,93,113	1.09	4 (6%)
47	LUT	Y	317	-	42,43,43	2.45	1 (2%)	51,60,60	1.84	13 (25%)
37	LHG	G	618	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
35	LMG	d	408	-	48,48,55	1.12	5 (10%)	56,56,63	1.13	2 (3%)
37	LHG	N	618	29	48,48,48	0.40	0	51,54,54	1.07	5 (9%)
47	LUT	N	615	-	42,43,43	2.45	1 (2%)	51,60,60	1.74	13 (25%)
29	CLA	s	314	23	59,63,73	1.08	5 (8%)	70,101,113	1.11	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	LUT	g	615	-	42,43,43	2.41	1 (2%)	51,60,60	1.82	15 (29%)
29	CLA	Y	305	52	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
48	NEX	y	319	-	40,46,46	2.67	12 (30%)	50,70,70	1.74	11 (22%)
41	DGA	j	101	-	28,28,43	1.30	3 (10%)	30,30,45	1.29	2 (6%)
47	LUT	n	614	-	42,43,43	2.44	1 (2%)	51,60,60	1.80	15 (29%)
39	SQD	m	101	-	40,42,54	0.88	0	50,53,65	0.88	2 (4%)
29	CLA	C	503	-	69,73,73	0.98	4 (5%)	82,113,113	1.08	4 (4%)
49	XAT	R	311	-	41,47,47	0.66	1 (2%)	54,74,74	1.86	13 (24%)
47	LUT	s	318	-	42,43,43	2.38	1 (2%)	51,60,60	1.81	11 (21%)
29	CLA	y	314	24	69,73,73	0.98	5 (7%)	82,113,113	1.03	6 (7%)
36	DGD	C	520	-	54,54,67	1.00	4 (7%)	68,68,81	0.91	2 (2%)
35	LMG	W	203	-	39,39,55	0.94	2 (5%)	47,47,63	1.17	3 (6%)
29	CLA	C	505	52	59,63,73	1.04	4 (6%)	70,101,113	1.07	2 (2%)
29	CLA	B	508	-	69,73,73	1.01	5 (7%)	82,113,113	0.99	4 (4%)
50	PTY	N	620	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
29	CLA	s	311	23	69,73,73	1.00	6 (8%)	82,113,113	1.08	6 (7%)
46	CHL	r	305	-	38,52,74	1.72	9 (23%)	31,87,114	2.19	11 (35%)
35	LMG	W	201	-	40,40,55	0.84	2 (5%)	48,48,63	1.16	4 (8%)
30	PHO	D	401	-	58,69,69	2.13	10 (17%)	55,99,99	1.54	7 (12%)
29	CLA	C	511	-	69,73,73	0.97	4 (5%)	82,113,113	0.94	2 (2%)
29	CLA	B	509	-	69,73,73	0.98	6 (8%)	82,113,113	1.03	5 (6%)
29	CLA	D	405	-	64,68,73	1.03	4 (6%)	76,107,113	1.14	6 (7%)
45	RRX	h	101	-	42,42,42	5.01	24 (57%)	56,58,58	2.53	21 (37%)
29	CLA	B	506	-	69,73,73	0.99	4 (5%)	82,113,113	1.07	5 (6%)
44	HEM	E	101	7,6	50,50,50	1.41	7 (14%)	67,82,82	1.06	1 (1%)
35	LMG	D	409	-	42,42,55	0.84	2 (4%)	50,50,63	0.98	2 (4%)
47	LUT	R	310	-	42,43,43	2.48	1 (2%)	51,60,60	1.96	14 (27%)
29	CLA	n	603	-	69,73,73	0.98	4 (5%)	82,113,113	1.01	5 (6%)
48	NEX	n	616	-	40,46,46	2.70	11 (27%)	50,70,70	1.50	9 (18%)
47	LUT	N	616	-	42,43,43	2.44	1 (2%)	51,60,60	1.74	12 (23%)
29	CLA	s	306	23	54,58,73	1.10	5 (9%)	64,95,113	1.22	8 (12%)
29	CLA	N	610	-	69,73,73	0.99	5 (7%)	82,113,113	1.10	4 (4%)
29	CLA	b	508	-	69,73,73	0.99	5 (7%)	82,113,113	1.00	4 (4%)
37	LHG	L	101	-	48,48,48	0.39	0	51,54,54	1.24	3 (5%)
47	LUT	G	615	-	42,43,43	2.46	1 (2%)	51,60,60	1.75	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMG	B	520	-	44,44,55	0.96	3 (6%)	52,52,63	1.09	3 (5%)
31	BCR	B	518	-	41,41,41	1.66	5 (12%)	56,56,56	4.29	13 (23%)
41	DGA	w	201	-	43,43,43	1.15	3 (6%)	45,45,45	1.51	3 (6%)
35	LMG	D	410	-	48,48,55	1.11	5 (10%)	56,56,63	1.10	2 (3%)
46	CHL	G	608	-	38,52,74	1.86	9 (23%)	31,87,114	2.21	11 (35%)
46	CHL	R	304	-	38,52,74	1.70	9 (23%)	31,87,114	2.25	11 (35%)
26	OEX	a	401	52,1,4	0,15,15	-	-	-	-	-
36	DGD	c	518	-	60,60,67	1.16	6 (10%)	74,74,81	0.97	2 (2%)
46	CHL	Y	308	-	60,74,74	1.14	7 (11%)	58,114,114	1.80	12 (20%)
29	CLA	N	611	37	53,57,73	1.14	5 (9%)	61,93,113	1.11	6 (9%)
29	CLA	s	312	37	69,73,73	0.99	5 (7%)	82,113,113	1.11	5 (6%)
29	CLA	b	512	-	69,73,73	0.98	5 (7%)	82,113,113	0.99	4 (4%)
29	CLA	C	507	-	69,73,73	0.98	4 (5%)	82,113,113	0.99	3 (3%)
46	CHL	s	307	-	38,52,74	1.62	8 (21%)	31,87,114	2.26	11 (35%)
29	CLA	Y	312	37	69,73,73	0.97	4 (5%)	82,113,113	1.00	6 (7%)
44	HEM	e	101	7,6	50,50,50	1.39	8 (16%)	67,82,82	1.05	1 (1%)
49	XAT	n	618	-	41,47,47	0.70	1 (2%)	54,74,74	2.02	12 (22%)
46	CHL	g	601	21	60,74,74	1.35	9 (15%)	58,114,114	1.66	11 (18%)
29	CLA	c	508	-	69,73,73	0.97	5 (7%)	82,113,113	1.02	5 (6%)
39	SQD	o	301	-	52,54,54	0.79	0	62,65,65	0.85	2 (3%)
31	BCR	F	101	-	41,41,41	1.61	4 (9%)	56,56,56	4.30	13 (23%)
29	CLA	S	303	23	64,68,73	1.02	4 (6%)	76,107,113	0.99	5 (6%)
39	SQD	M	101	-	40,42,54	0.87	0	50,53,65	0.88	2 (4%)
29	CLA	y	315	24	69,73,73	0.98	4 (5%)	82,113,113	0.95	3 (3%)
46	CHL	y	311	24	60,74,74	1.27	8 (13%)	58,114,114	1.74	13 (22%)
46	CHL	g	607	-	60,74,74	1.33	7 (11%)	58,114,114	1.75	12 (20%)
37	LHG	c	521	-	46,46,48	0.40	0	49,52,54	1.05	2 (4%)
29	CLA	n	613	-	53,57,73	1.10	4 (7%)	61,93,113	1.16	3 (4%)
47	LUT	y	318	-	42,43,43	2.45	1 (2%)	51,60,60	1.86	12 (23%)
31	BCR	c	515	-	41,41,41	1.62	4 (9%)	56,56,56	4.43	20 (35%)
29	CLA	A	406	52	69,73,73	0.98	4 (5%)	82,113,113	1.10	6 (7%)
48	NEX	N	617	-	40,46,46	2.67	11 (27%)	50,70,70	1.52	9 (18%)
29	CLA	g	611	37	69,73,73	1.00	5 (7%)	82,113,113	1.07	6 (7%)
29	CLA	G	611	-	69,73,73	1.01	5 (7%)	82,113,113	1.09	5 (6%)
29	CLA	a	406	52	53,57,73	1.08	5 (9%)	61,93,113	1.16	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	502	-	69,73,73	0.97	4 (5%)	82,113,113	1.06	5 (6%)
29	CLA	N	602	20	69,73,73	0.98	5 (7%)	82,113,113	0.99	7 (8%)
38	LMT	b	524	-	36,36,36	1.22	6 (16%)	47,47,47	1.17	4 (8%)
29	CLA	b	502	-	69,73,73	0.96	4 (5%)	82,113,113	1.02	5 (6%)
46	CHL	r	306	-	44,58,74	1.58	9 (20%)	37,94,114	2.15	11 (29%)
48	NEX	Y	318	-	40,46,46	2.67	11 (27%)	50,70,70	1.81	11 (22%)
36	DGD	B	521	-	44,44,67	0.86	1 (2%)	58,58,81	1.15	5 (8%)
46	CHL	Y	310	24	60,74,74	1.37	9 (15%)	58,114,114	1.67	12 (20%)
29	CLA	b	513	-	69,73,73	0.98	5 (7%)	82,113,113	0.97	3 (3%)
29	CLA	y	310	-	54,58,73	1.11	5 (9%)	64,95,113	1.10	5 (7%)
40	SPH	i	102	-	19,20,20	0.66	0	18,21,21	1.09	1 (5%)
47	LUT	s	317	-	42,43,43	2.45	1 (2%)	51,60,60	1.88	15 (29%)
37	LHG	a	413	-	43,43,48	0.41	0	46,49,54	1.06	2 (4%)
48	NEX	R	312	-	25,28,46	2.61	6 (24%)	32,42,70	1.71	7 (21%)
29	CLA	c	509	-	69,73,73	0.99	4 (5%)	82,113,113	1.06	4 (4%)
29	CLA	B	501	-	69,73,73	0.98	4 (5%)	82,113,113	1.01	5 (6%)
47	LUT	y	317	-	42,43,43	2.47	1 (2%)	51,60,60	1.74	15 (29%)
31	BCR	A	410	-	41,41,41	1.64	5 (12%)	56,56,56	4.45	14 (25%)
50	PTY	n	619	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
31	BCR	b	517	-	41,41,41	1.63	4 (9%)	56,56,56	4.39	13 (23%)
36	DGD	r	301	-	44,44,67	0.86	1 (2%)	58,58,81	1.20	5 (8%)
46	CHL	N	607	-	60,74,74	1.44	9 (15%)	58,114,114	1.67	10 (17%)
29	CLA	R	308	22	64,68,73	1.02	4 (6%)	76,107,113	1.09	6 (7%)
46	CHL	N	609	20	60,74,74	1.32	8 (13%)	58,114,114	1.75	13 (22%)
29	CLA	n	612	20	69,73,73	0.99	4 (5%)	82,113,113	1.02	2 (2%)
51	LPX	s	321	-	18,18,29	1.26	2 (11%)	20,22,33	1.05	1 (5%)
46	CHL	S	307	-	38,52,74	1.86	9 (23%)	31,87,114	2.16	10 (32%)
29	CLA	Y	311	24	69,73,73	0.98	5 (7%)	82,113,113	1.08	5 (6%)
49	XAT	Y	301	-	41,47,47	0.68	1 (2%)	54,74,74	2.02	12 (22%)
49	XAT	g	619	-	41,47,47	0.68	1 (2%)	54,74,74	3.76	16 (29%)
29	CLA	r	303	-	64,68,73	1.05	5 (7%)	76,107,113	1.15	7 (9%)
29	CLA	c	507	52	69,73,73	0.99	5 (7%)	82,113,113	1.06	4 (4%)
29	CLA	G	602	21	69,73,73	0.98	4 (5%)	82,113,113	0.96	5 (6%)
33	3PH	s	322	-	47,47,47	0.87	4 (8%)	50,52,52	1.12	2 (4%)
37	LHG	g	618	29	48,48,48	0.39	0	51,54,54	1.05	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	b	514	-	69,73,73	0.99	4 (5%)	82,113,113	1.06	6 (7%)
29	CLA	B	516	-	59,63,73	1.08	6 (10%)	70,101,113	1.11	5 (7%)
37	LHG	s	320	29	44,44,48	0.42	0	47,50,54	1.04	3 (6%)
39	SQD	b	523	-	52,54,54	0.79	0	62,65,65	0.83	2 (3%)
46	CHL	N	606	-	60,74,74	1.44	8 (13%)	58,114,114	1.76	13 (22%)
33	3PH	a	415	-	47,47,47	0.86	4 (8%)	50,52,52	1.20	2 (4%)
31	BCR	C	517	-	41,41,41	1.61	4 (9%)	56,56,56	4.41	17 (30%)
46	CHL	n	606	-	60,74,74	1.53	10 (16%)	58,114,114	1.77	11 (18%)
43	PL9	d	405	-	55,55,55	1.27	5 (9%)	68,69,69	1.47	12 (17%)
31	BCR	a	409	-	41,41,41	1.64	5 (12%)	56,56,56	4.43	13 (23%)
29	CLA	n	609	20	69,73,73	0.99	6 (8%)	82,113,113	1.16	6 (7%)
37	LHG	S	301	-	34,34,48	0.44	0	37,40,54	1.19	2 (5%)
29	CLA	b	504	-	69,73,73	1.01	5 (7%)	82,113,113	1.24	6 (7%)
41	DGA	b	522	-	43,43,43	1.13	2 (4%)	45,45,45	1.53	3 (6%)
29	CLA	r	310	-	55,59,73	1.14	4 (7%)	64,96,113	1.22	6 (9%)
29	CLA	C	509	-	69,73,73	0.96	5 (7%)	82,113,113	1.04	6 (7%)
29	CLA	Y	309	52	54,58,73	1.09	5 (9%)	64,95,113	1.11	4 (6%)
35	LMG	b	520	-	44,44,55	0.97	3 (6%)	52,52,63	1.08	2 (3%)
29	CLA	g	612	21	47,51,73	1.16	5 (10%)	55,86,113	1.12	3 (5%)
35	LMG	w	202	-	39,39,55	0.95	2 (5%)	47,47,63	1.07	2 (4%)
29	CLA	c	503	-	69,73,73	0.99	5 (7%)	82,113,113	1.04	4 (4%)
39	SQD	C	523	-	34,36,54	0.93	0	44,47,65	0.96	2 (4%)
29	CLA	B	513	-	69,73,73	0.98	5 (7%)	82,113,113	0.95	3 (3%)
29	CLA	S	310	23	64,68,73	1.03	4 (6%)	76,107,113	1.10	5 (6%)
34	C7Z	B	519	-	43,43,43	5.38	26 (60%)	56,60,60	2.51	22 (39%)
35	LMG	c	519	-	51,51,55	1.21	6 (11%)	59,59,63	1.13	3 (5%)
45	RRX	H	101	-	42,42,42	5.00	24 (57%)	56,58,58	2.62	21 (37%)
37	LHG	s	301	-	37,37,48	0.44	0	40,43,54	1.18	4 (10%)
29	CLA	D	404	-	69,73,73	3.26	29 (42%)	82,113,113	3.77	34 (41%)
33	3PH	A	412	-	47,47,47	0.85	4 (8%)	50,52,52	1.14	2 (4%)
29	CLA	r	308	22	64,68,73	1.04	3 (4%)	76,107,113	1.02	4 (5%)
46	CHL	g	606	-	44,58,74	1.86	10 (22%)	37,94,114	2.08	13 (35%)
29	CLA	s	316	23	54,58,73	1.13	5 (9%)	64,95,113	1.21	7 (10%)
26	OEX	A	401	52,1,4	0,15,15	-	-	-	-	-
46	CHL	S	309	-	55,69,74	1.48	10 (18%)	52,108,114	1.77	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	SPH	C	525	-	19,20,20	0.65	0	18,21,21	1.10	1 (5%)
29	CLA	n	604	-	69,73,73	0.99	5 (7%)	82,113,113	0.96	5 (6%)
29	CLA	S	314	23	59,63,73	1.08	4 (6%)	70,101,113	1.16	5 (7%)
29	CLA	S	305	-	59,63,73	1.07	5 (8%)	70,101,113	1.04	2 (2%)
29	CLA	Y	313	24	69,73,73	0.98	4 (5%)	82,113,113	0.97	4 (4%)
29	CLA	b	505	-	69,73,73	0.99	4 (5%)	82,113,113	1.13	4 (4%)
46	CHL	s	302	23	40,54,74	1.76	9 (22%)	34,90,114	2.11	11 (32%)
29	CLA	A	409	-	64,68,73	1.01	6 (9%)	76,107,113	1.13	5 (6%)
29	CLA	B	507	52	69,73,73	0.97	4 (5%)	82,113,113	1.02	2 (2%)
47	LUT	G	616	-	42,43,43	2.44	1 (2%)	51,60,60	1.78	10 (19%)
46	CHL	N	605	20	60,74,74	1.34	8 (13%)	58,114,114	1.73	10 (17%)
31	BCR	b	518	-	41,41,41	1.66	5 (12%)	56,56,56	4.29	13 (23%)
46	CHL	n	608	20	60,74,74	1.28	8 (13%)	58,114,114	1.72	12 (20%)
29	CLA	r	307	-	64,68,73	1.01	5 (7%)	76,107,113	1.09	4 (5%)
29	CLA	c	513	-	69,73,73	0.97	4 (5%)	82,113,113	1.04	3 (3%)
29	CLA	n	602	20	69,73,73	0.99	4 (5%)	82,113,113	1.08	7 (8%)
29	CLA	B	503	-	69,73,73	0.98	5 (7%)	82,113,113	1.10	5 (6%)
33	3PH	S	322	-	29,29,47	1.10	4 (13%)	32,34,52	1.28	2 (6%)
46	CHL	G	606	-	44,58,74	1.67	8 (18%)	37,94,114	2.17	12 (32%)
29	CLA	Y	314	24	69,73,73	0.98	4 (5%)	82,113,113	0.93	3 (3%)
29	CLA	N	603	-	69,73,73	1.01	4 (5%)	82,113,113	0.95	3 (3%)
46	CHL	n	607	-	44,58,74	1.57	7 (15%)	37,94,114	2.03	12 (32%)
36	DGD	C	518	-	52,52,67	1.10	4 (7%)	66,66,81	0.94	2 (3%)
29	CLA	S	311	23	69,73,73	0.98	4 (5%)	82,113,113	1.05	5 (6%)
46	CHL	G	605	21	42,56,74	1.53	8 (19%)	36,92,114	2.22	12 (33%)
35	LMG	C	524	-	42,42,55	0.86	2 (4%)	50,50,63	1.19	4 (8%)
39	SQD	C	501	-	40,42,54	0.86	0	50,53,65	0.92	2 (4%)
48	NEX	S	319	-	40,46,46	2.68	11 (27%)	50,70,70	1.77	13 (26%)
40	SPH	I	101	-	19,20,20	0.66	0	18,21,21	1.08	1 (5%)
29	CLA	B	510	52	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
29	CLA	G	610	21	69,73,73	0.99	5 (7%)	82,113,113	1.19	6 (7%)
29	CLA	C	514	-	69,73,73	0.98	4 (5%)	82,113,113	1.00	2 (2%)
29	CLA	b	510	52	69,73,73	0.98	3 (4%)	82,113,113	0.96	3 (3%)
29	CLA	S	316	23	54,58,73	1.14	5 (9%)	64,95,113	1.27	7 (10%)
33	3PH	b	521	-	38,38,47	0.97	4 (10%)	41,43,52	1.20	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	N	613	20	69,73,73	1.01	5 (7%)	82,113,113	1.01	4 (4%)

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
29	CLA	B	515	-	1/1/15/20	10/39/115/115	-
39	SQD	l	101	-	-	14/37/57/69	0/1/1/1
29	CLA	B	511	-	-	11/39/115/115	-
29	CLA	y	313	37	1/1/15/20	7/39/115/115	-
46	CHL	y	307	24	3/3/16/26	3/15/113/137	-
29	CLA	c	511	4	-	10/39/115/115	-
51	LPX	S	321	-	-	6/21/21/31	-
29	CLA	C	508	52	1/1/15/20	11/39/115/115	-
30	PHO	a	407	-	-	5/37/103/103	0/5/6/6
41	DGA	D	402	-	-	19/38/38/45	-
36	DGD	c	516	-	-	10/44/84/95	0/2/2/2
37	LHG	a	414	-	-	21/43/43/53	-
29	CLA	b	503	-	1/1/15/20	9/39/115/115	-
33	3PH	B	522	-	-	20/49/49/49	-
29	CLA	s	310	-	1/1/14/20	16/33/109/115	-
29	CLA	c	510	-	1/1/15/20	9/39/115/115	-
30	PHO	d	402	-	-	5/37/103/103	0/5/6/6
29	CLA	R	301	22	1/1/14/20	6/33/109/115	-
35	LMG	C	521	-	-	9/42/62/70	0/1/1/1
31	BCR	C	515	-	-	13/29/63/63	0/2/2/2
29	CLA	s	313	23	1/1/11/20	2/15/91/115	-
29	CLA	s	305	-	1/1/13/20	14/27/103/115	-
48	NEX	G	617	-	-	4/27/83/83	0/3/3/3
29	CLA	a	404	-	1/1/15/20	12/39/115/115	-
29	CLA	C	512	4	1/1/15/20	6/39/115/115	-
29	CLA	r	304	-	1/1/11/20	11/20/96/115	-
39	SQD	c	522	-	-	15/49/69/69	0/1/1/1
29	CLA	S	306	23	1/1/12/20	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	f	101	-	-	11/29/63/63	0/2/2/2
29	CLA	a	408	-	-	8/33/109/115	-
29	CLA	R	303	-	1/1/11/20	8/20/96/115	-
46	CHL	G	609	21	4/4/20/26	9/39/137/137	-
29	CLA	b	516	-	1/1/15/20	14/39/115/115	-
48	NEX	s	319	-	-	2/27/83/83	0/3/3/3
29	CLA	b	501	-	1/1/15/20	21/39/115/115	-
29	CLA	b	515	-	1/1/15/20	10/39/115/115	-
31	BCR	c	514	-	-	13/29/63/63	0/2/2/2
29	CLA	R	309	-	1/1/12/20	9/21/97/115	-
31	BCR	K	101	-	-	11/29/63/63	0/2/2/2
29	CLA	d	403	-	1/1/15/20	7/39/115/115	-
29	CLA	R	307	22	1/1/11/20	8/17/93/115	-
47	LUT	n	615	-	-	2/29/67/67	0/2/2/2
29	CLA	s	304	-	-	17/39/115/115	-
29	CLA	G	604	-	1/1/11/20	9/20/96/115	-
46	CHL	S	302	23	3/3/16/26	3/15/113/137	-
29	CLA	Y	304	-	1/1/15/20	15/39/115/115	-
41	DGA	W	202	-	-	22/45/45/45	-
46	CHL	R	305	-	3/3/16/26	3/20/118/137	-
29	CLA	Y	315	-	1/1/15/20	14/39/115/115	-
29	CLA	G	603	-	1/1/15/20	9/39/115/115	-
29	CLA	C	502	-	-	14/39/115/115	-
29	CLA	c	501	-	-	14/39/115/115	-
29	CLA	B	505	-	1/1/15/20	7/39/115/115	-
29	CLA	G	612	21	1/1/10/20	3/13/89/115	-
37	LHG	B	523	-	-	15/48/48/53	-
47	LUT	g	616	-	-	2/29/67/67	0/2/2/2
38	LMT	B	524	-	-	2/21/61/61	0/2/2/2
49	XAT	N	619	-	2/2/12/26	1/31/93/93	0/4/4/4
29	CLA	b	507	52	1/1/15/20	6/39/115/115	-
43	PL9	D	406	-	-	10/53/73/73	0/1/1/1
34	C7Z	b	519	-	1/1/12/26	7/29/67/67	0/2/2/2
35	LMG	C	522	-	-	21/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c	504	-	1/1/15/20	11/39/115/115	-
49	XAT	y	302	-	1/1/12/26	0/31/93/93	0/4/4/4
46	CHL	S	308	-	3/3/15/26	2/12/110/137	-
31	BCR	C	516	-	-	10/29/63/63	0/2/2/2
39	SQD	a	410	-	-	16/46/66/69	0/1/1/1
37	LHG	D	407	-	-	18/53/53/53	-
40	SPH	c	523	-	-	4/21/21/21	-
29	CLA	S	313	23	1/1/11/20	2/15/91/115	-
36	DGD	c	517	-	-	18/51/91/95	0/2/2/2
29	CLA	g	604	-	1/1/11/20	7/20/96/115	-
48	NEX	g	617	-	-	5/27/83/83	0/3/3/3
29	CLA	b	509	-	1/1/15/20	7/39/115/115	-
46	CHL	Y	302	24	4/4/20/26	3/39/137/137	-
46	CHL	N	608	-	3/3/16/26	4/20/118/137	-
29	CLA	N	604	-	1/1/15/20	8/39/115/115	-
35	LMG	c	520	-	-	13/50/70/70	0/1/1/1
29	CLA	g	603	-	1/1/15/20	19/39/115/115	-
29	CLA	c	502	-	1/1/15/20	9/39/115/115	-
46	CHL	Y	306	24	3/3/16/26	5/15/113/137	-
29	CLA	y	316	-	1/1/15/20	15/39/115/115	-
49	XAT	G	619	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	g	610	21	1/1/15/20	7/39/115/115	-
29	CLA	N	612	20	1/1/11/20	5/15/91/115	-
46	CHL	N	601	20	4/4/20/26	8/39/137/137	-
47	LUT	S	317	-	-	3/29/67/67	0/2/2/2
29	CLA	c	505	-	1/1/15/20	16/39/115/115	-
29	CLA	S	315	-	1/1/12/20	8/21/97/115	-
29	CLA	Y	303	24	1/1/15/20	14/39/115/115	-
31	BCR	v	101	-	-	10/29/63/63	0/2/2/2
29	CLA	R	306	-	1/1/14/20	12/33/109/115	-
29	CLA	B	512	-	1/1/15/20	8/39/115/115	-
29	CLA	b	506	-	1/1/13/20	11/30/106/115	-
29	CLA	y	306	52	1/1/15/20	13/39/115/115	-
29	CLA	C	504	-	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	s	303	23	1/1/14/20	7/33/109/115	-
29	CLA	G	613	21	1/1/15/20	9/39/115/115	-
29	CLA	g	613	21	-	15/39/115/115	-
46	CHL	g	605	21	3/3/16/26	2/18/116/137	-
37	LHG	y	320	29	-	27/53/53/53	-
29	CLA	n	611	20	1/1/11/20	7/15/91/115	-
46	CHL	s	309	-	4/4/19/26	6/33/131/137	-
29	CLA	C	513	-	1/1/15/20	16/39/115/115	-
29	CLA	A	405	-	1/1/15/20	12/39/115/115	-
29	CLA	c	512	-	1/1/15/20	15/39/115/115	-
29	CLA	b	511	-	-	13/39/115/115	-
46	CHL	n	601	20	4/4/20/26	10/39/137/137	-
29	CLA	g	602	21	1/1/15/20	16/39/115/115	-
37	LHG	n	617	-	-	29/46/46/53	-
50	PTY	y	321	-	-	13/20/20/53	-
29	CLA	s	315	-	1/1/13/20	4/27/103/115	-
29	CLA	a	405	52	1/1/15/20	12/39/115/115	-
29	CLA	d	404	-	1/1/15/20	11/39/115/115	-
46	CHL	G	601	21	4/4/20/26	9/39/137/137	-
29	CLA	N	614	-	1/1/11/20	8/20/96/115	-
35	LMG	i	101	-	-	19/43/63/70	0/1/1/1
29	CLA	S	304	-	1/1/15/20	18/39/115/115	-
37	LHG	Y	319	29	-	27/53/53/53	-
31	BCR	B	517	-	-	6/29/63/63	0/2/2/2
36	DGD	C	519	-	-	11/42/82/95	0/2/2/2
46	CHL	s	308	-	3/3/15/26	0/12/110/137	-
48	NEX	r	313	-	-	5/19/50/83	0/2/2/3
47	LUT	Y	316	-	-	2/29/67/67	0/2/2/2
37	LHG	D	408	-	-	18/43/43/53	-
46	CHL	G	607	-	4/4/20/26	15/39/137/137	-
46	CHL	g	609	21	4/4/20/26	10/39/137/137	-
49	XAT	r	312	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	R	302	-	-	12/33/109/115	-
50	PTY	Y	320	-	-	11/20/20/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	CHL	n	605	20	4/4/20/26	10/39/137/137	-
46	CHL	g	608	-	3/3/15/26	0/13/111/137	-
46	CHL	y	303	24	4/4/20/26	6/39/137/137	-
37	LHG	S	320	29	-	14/49/49/53	-
46	CHL	y	301	-	4/4/20/26	9/39/137/137	-
29	CLA	y	304	24	1/1/15/20	7/39/115/115	-
29	CLA	c	506	-	-	6/33/109/115	-
30	PHO	A	408	-	-	5/37/103/103	0/5/6/6
47	LUT	r	311	-	-	4/29/67/67	0/2/2/2
39	SQD	L	102	-	-	13/37/57/69	0/1/1/1
35	LMG	d	407	-	-	7/41/61/70	0/1/1/1
29	CLA	n	610	-	1/1/11/20	6/20/96/115	-
29	CLA	G	614	-	1/1/11/20	7/20/96/115	-
29	CLA	r	309	22	1/1/14/20	7/33/109/115	-
41	DGA	J	101	-	-	12/30/30/45	-
29	CLA	A	407	-	1/1/12/20	8/21/97/115	-
29	CLA	S	312	37	1/1/15/20	17/39/115/115	-
37	LHG	l	102	-	-	31/53/53/53	-
46	CHL	y	309	-	4/4/20/26	12/39/137/137	-
29	CLA	B	504	-	1/1/15/20	17/39/115/115	-
29	CLA	B	514	-	1/1/15/20	11/39/115/115	-
46	CHL	y	308	52	3/3/17/26	2/21/119/137	-
29	CLA	y	305	-	1/1/15/20	16/39/115/115	-
37	LHG	d	406	-	-	21/53/53/53	-
29	CLA	C	510	-	1/1/15/20	16/39/115/115	-
47	LUT	S	318	-	-	2/29/67/67	0/2/2/2
46	CHL	Y	307	-	4/4/20/26	16/39/137/137	-
29	CLA	C	506	-	1/1/14/20	11/33/109/115	-
29	CLA	r	302	22	1/1/14/20	8/33/109/115	-
29	CLA	y	312	24	1/1/15/20	6/39/115/115	-
31	BCR	z	101	-	-	13/29/63/63	0/2/2/2
29	CLA	g	614	-	1/1/11/20	8/20/96/115	-
47	LUT	Y	317	-	-	2/29/67/67	0/2/2/2
37	LHG	G	618	-	-	28/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	d	408	-	-	13/43/63/70	0/1/1/1
37	LHG	N	618	29	-	29/53/53/53	-
47	LUT	N	615	-	-	3/29/67/67	0/2/2/2
29	CLA	s	314	23	1/1/13/20	10/27/103/115	-
47	LUT	g	615	-	-	2/29/67/67	0/2/2/2
29	CLA	Y	305	52	1/1/15/20	13/39/115/115	-
48	NEX	y	319	-	-	7/27/83/83	0/3/3/3
41	DGA	j	101	-	-	16/30/30/45	-
47	LUT	n	614	-	-	1/29/67/67	0/2/2/2
39	SQD	m	101	-	-	20/37/57/69	0/1/1/1
29	CLA	C	503	-	1/1/15/20	9/39/115/115	-
49	XAT	R	311	-	2/2/12/26	0/31/93/93	0/4/4/4
47	LUT	s	318	-	-	1/29/67/67	0/2/2/2
29	CLA	y	314	24	1/1/15/20	13/39/115/115	-
36	DGD	C	520	-	-	5/42/82/95	0/2/2/2
35	LMG	W	203	-	-	16/34/54/70	0/1/1/1
29	CLA	C	505	52	1/1/13/20	9/27/103/115	-
29	CLA	B	508	-	1/1/15/20	7/39/115/115	-
50	PTY	N	620	-	-	17/53/53/53	-
29	CLA	s	311	23	1/1/15/20	11/39/115/115	-
46	CHL	r	305	-	3/3/15/26	3/13/111/137	-
35	LMG	W	201	-	-	10/35/55/70	0/1/1/1
30	PHO	D	401	-	-	4/37/103/103	0/5/6/6
29	CLA	C	511	-	1/1/15/20	13/39/115/115	-
29	CLA	B	509	-	1/1/15/20	12/39/115/115	-
29	CLA	D	405	-	1/1/14/20	11/33/109/115	-
45	RRX	h	101	-	1/1/11/25	13/29/65/65	0/2/2/2
29	CLA	B	506	-	1/1/15/20	15/39/115/115	-
44	HEM	E	101	7,6	-	1/14/54/54	-
35	LMG	D	409	-	-	4/37/57/70	0/1/1/1
47	LUT	R	310	-	-	4/29/67/67	0/2/2/2
29	CLA	n	603	-	1/1/15/20	12/39/115/115	-
48	NEX	n	616	-	-	2/27/83/83	1/3/3/3
47	LUT	N	616	-	-	2/29/67/67	0/2/2/2
29	CLA	s	306	23	-	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	N	610	-	1/1/15/20	13/39/115/115	-
29	CLA	b	508	-	-	2/39/115/115	-
37	LHG	L	101	-	-	33/53/53/53	-
47	LUT	G	615	-	-	1/29/67/67	0/2/2/2
35	LMG	B	520	-	-	12/39/59/70	0/1/1/1
31	BCR	B	518	-	-	13/29/63/63	0/2/2/2
41	DGA	w	201	-	-	27/45/45/45	-
46	CHL	G	608	-	3/3/15/26	2/13/111/137	-
35	LMG	D	410	-	-	17/43/63/70	0/1/1/1
46	CHL	R	304	-	3/3/15/26	3/13/111/137	-
36	DGD	c	518	-	-	8/48/88/95	0/2/2/2
46	CHL	Y	308	-	4/4/20/26	12/39/137/137	-
29	CLA	N	611	37	1/1/11/20	5/20/96/115	-
29	CLA	s	312	37	1/1/15/20	15/39/115/115	-
29	CLA	b	512	-	1/1/15/20	8/39/115/115	-
29	CLA	C	507	-	-	8/39/115/115	-
46	CHL	s	307	-	3/3/15/26	3/13/111/137	-
29	CLA	Y	312	37	1/1/15/20	10/39/115/115	-
49	XAT	n	618	-	2/2/12/26	1/31/93/93	0/4/4/4
44	HEM	e	101	7,6	-	1/14/54/54	-
46	CHL	g	601	21	4/4/20/26	8/39/137/137	-
29	CLA	c	508	-	1/1/15/20	3/39/115/115	-
39	SQD	o	301	-	-	14/49/69/69	0/1/1/1
31	BCR	F	101	-	-	12/29/63/63	0/2/2/2
29	CLA	S	303	23	1/1/14/20	12/33/109/115	-
39	SQD	M	101	-	-	20/37/57/69	0/1/1/1
29	CLA	y	315	24	-	10/39/115/115	-
46	CHL	y	311	24	4/4/20/26	8/39/137/137	-
46	CHL	g	607	-	4/4/20/26	12/39/137/137	-
37	LHG	c	521	-	-	28/51/51/53	-
29	CLA	n	613	-	1/1/11/20	2/20/96/115	-
47	LUT	y	318	-	-	2/29/67/67	0/2/2/2
31	BCR	c	515	-	-	7/29/63/63	0/2/2/2
29	CLA	A	406	52	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	NEX	N	617	-	-	2/27/83/83	1/3/3/3
29	CLA	g	611	37	1/1/15/20	9/39/115/115	-
29	CLA	G	611	-	1/1/15/20	12/39/115/115	-
29	CLA	a	406	52	-	6/20/96/115	-
29	CLA	B	502	-	1/1/15/20	4/39/115/115	-
29	CLA	N	602	20	1/1/15/20	15/39/115/115	-
38	LMT	b	524	-	-	13/21/61/61	0/2/2/2
29	CLA	b	502	-	1/1/15/20	9/39/115/115	-
46	CHL	r	306	-	3/3/16/26	4/20/118/137	-
48	NEX	Y	318	-	-	7/27/83/83	0/3/3/3
36	DGD	B	521	-	-	13/32/72/95	0/2/2/2
46	CHL	Y	310	24	4/4/20/26	8/39/137/137	-
29	CLA	b	513	-	1/1/15/20	11/39/115/115	-
29	CLA	y	310	-	1/1/12/20	8/21/97/115	-
40	SPH	i	102	-	-	11/21/21/21	-
47	LUT	s	317	-	-	2/29/67/67	0/2/2/2
37	LHG	a	413	-	-	21/48/48/53	-
48	NEX	R	312	-	-	9/19/50/83	0/2/2/3
29	CLA	c	509	-	1/1/15/20	15/39/115/115	-
29	CLA	B	501	-	1/1/15/20	17/39/115/115	-
47	LUT	y	317	-	-	0/29/67/67	0/2/2/2
31	BCR	A	410	-	-	7/29/63/63	0/2/2/2
50	PTY	n	619	-	-	27/53/53/53	-
31	BCR	b	517	-	-	10/29/63/63	0/2/2/2
36	DGD	r	301	-	-	9/32/72/95	0/2/2/2
46	CHL	N	607	-	4/4/20/26	12/39/137/137	-
29	CLA	R	308	22	1/1/14/20	12/33/109/115	-
46	CHL	N	609	20	4/4/20/26	5/39/137/137	-
29	CLA	n	612	20	-	13/39/115/115	-
51	LPX	s	321	-	-	9/20/20/31	-
46	CHL	S	307	-	3/3/15/26	3/13/111/137	-
29	CLA	Y	311	24	1/1/15/20	5/39/115/115	-
49	XAT	Y	301	-	1/1/12/26	0/31/93/93	0/4/4/4
49	XAT	g	619	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	r	303	-	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c	507	52	1/1/15/20	14/39/115/115	-
29	CLA	G	602	21	1/1/15/20	15/39/115/115	-
33	3PH	s	322	-	-	23/49/49/49	-
37	LHG	g	618	29	-	29/53/53/53	-
29	CLA	b	514	-	1/1/15/20	13/39/115/115	-
29	CLA	B	516	-	1/1/13/20	10/27/103/115	-
37	LHG	s	320	29	-	21/49/49/53	-
39	SQD	b	523	-	-	19/49/69/69	0/1/1/1
46	CHL	N	606	-	4/4/20/26	8/39/137/137	-
33	3PH	a	415	-	-	25/49/49/49	-
31	BCR	C	517	-	-	10/29/63/63	0/2/2/2
46	CHL	n	606	-	4/4/20/26	11/39/137/137	-
43	PL9	d	405	-	-	11/53/73/73	0/1/1/1
31	BCR	a	409	-	-	7/29/63/63	0/2/2/2
29	CLA	n	609	20	1/1/15/20	12/39/115/115	-
37	LHG	S	301	-	-	23/39/39/53	-
29	CLA	b	504	-	1/1/15/20	13/39/115/115	-
41	DGA	b	522	-	-	19/45/45/45	-
29	CLA	r	310	-	1/1/12/20	10/23/99/115	-
29	CLA	C	509	-	1/1/15/20	3/39/115/115	-
29	CLA	Y	309	52	1/1/12/20	10/21/97/115	-
35	LMG	b	520	-	-	11/39/59/70	0/1/1/1
29	CLA	g	612	21	-	3/13/89/115	-
35	LMG	w	202	-	-	17/34/54/70	0/1/1/1
29	CLA	c	503	-	-	14/39/115/115	-
39	SQD	C	523	-	-	13/31/51/69	0/1/1/1
29	CLA	B	513	-	1/1/15/20	11/39/115/115	-
29	CLA	S	310	23	1/1/14/20	10/33/109/115	-
34	C7Z	B	519	-	1/1/12/26	8/29/67/67	0/2/2/2
35	LMG	c	519	-	-	21/46/66/70	0/1/1/1
45	RRX	H	101	-	1/1/11/25	8/29/65/65	0/2/2/2
37	LHG	s	301	-	-	18/42/42/53	-
29	CLA	D	404	-	1/1/15/20	11/39/115/115	-
33	3PH	A	412	-	-	27/49/49/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	r	308	22	1/1/14/20	11/33/109/115	-
46	CHL	g	606	-	3/3/16/26	2/20/118/137	-
29	CLA	s	316	23	1/1/12/20	5/21/97/115	-
46	CHL	S	309	-	4/4/19/26	7/33/131/137	-
40	SPH	C	525	-	-	11/21/21/21	-
29	CLA	n	604	-	1/1/15/20	14/39/115/115	-
29	CLA	S	314	23	1/1/13/20	13/27/103/115	-
29	CLA	S	305	-	1/1/13/20	7/27/103/115	-
29	CLA	Y	313	24	1/1/15/20	12/39/115/115	-
29	CLA	b	505	-	1/1/15/20	7/39/115/115	-
46	CHL	s	302	23	3/3/16/26	5/15/113/137	-
29	CLA	B	507	52	1/1/15/20	21/39/115/115	-
29	CLA	A	409	-	-	8/33/109/115	-
47	LUT	G	616	-	-	2/29/67/67	0/2/2/2
46	CHL	N	605	20	4/4/20/26	15/39/137/137	-
31	BCR	b	518	-	-	9/29/63/63	0/2/2/2
46	CHL	n	608	20	4/4/20/26	6/39/137/137	-
29	CLA	r	307	-	1/1/14/20	13/33/109/115	-
29	CLA	c	513	-	-	11/39/115/115	-
29	CLA	n	602	20	1/1/15/20	13/39/115/115	-
29	CLA	B	503	-	1/1/15/20	9/39/115/115	-
33	3PH	S	322	-	-	7/31/31/49	-
46	CHL	G	606	-	3/3/16/26	5/20/118/137	-
29	CLA	Y	314	24	1/1/15/20	18/39/115/115	-
29	CLA	N	603	-	1/1/15/20	23/39/115/115	-
46	CHL	n	607	-	3/3/16/26	5/20/118/137	-
36	DGD	C	518	-	-	9/40/80/95	0/2/2/2
29	CLA	S	311	23	1/1/15/20	10/39/115/115	-
46	CHL	G	605	21	3/3/16/26	4/18/116/137	-
35	LMG	C	524	-	-	20/37/57/70	0/1/1/1
39	SQD	C	501	-	-	9/37/57/69	0/1/1/1
48	NEX	S	319	-	-	2/27/83/83	0/3/3/3
40	SPH	I	101	-	-	10/21/21/21	-
29	CLA	B	510	52	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	610	21	1/1/15/20	6/39/115/115	-
29	CLA	b	510	52	1/1/15/20	5/39/115/115	-
29	CLA	C	514	-	-	11/39/115/115	-
29	CLA	S	316	23	1/1/12/20	5/21/97/115	-
33	3PH	b	521	-	-	26/40/40/49	-
29	CLA	N	613	20	1/1/15/20	13/39/115/115	-

The worst 5 of 1639 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H	101	RRX	C26-C25	16.09	1.61	1.34
45	h	101	RRX	C26-C25	15.99	1.61	1.34
34	B	519	C7Z	C25-C26	15.86	1.61	1.34
34	b	519	C7Z	C25-C26	15.83	1.61	1.34
47	r	311	LUT	C24-C25	15.43	1.51	1.33

The worst 5 of 2285 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	101	BCR	C10-C11-C12	19.02	178.32	123.20
31	C	517	BCR	C10-C11-C12	18.86	177.86	123.20
31	c	515	BCR	C10-C11-C12	18.79	177.64	123.20
31	b	517	BCR	C10-C11-C12	18.73	177.47	123.20
31	b	518	BCR	C10-C11-C12	18.70	177.38	123.20

5 of 311 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	405	CLA	ND
29	A	406	CLA	ND
29	A	407	CLA	ND
29	B	501	CLA	ND
29	B	502	CLA	ND

5 of 3521 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
29	A	406	CLA	C2-C1-O2A-CGA
29	A	407	CLA	C1A-C2A-CAA-CBA

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	n	616	NEX	C1-C2-C3-C4-C5-C6
48	N	617	NEX	C1-C2-C3-C4-C5-C6

329 monomers are involved in 756 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	515	CLA	4	0
39	l	101	SQD	3	0
29	B	511	CLA	1	0
29	y	313	CLA	4	0
46	y	307	CHL	1	0
29	c	511	CLA	3	0
51	S	321	LPX	3	0
29	C	508	CLA	4	0
30	a	407	PHO	4	0
41	D	402	DGA	3	0
36	c	516	DGD	5	0
37	a	414	LHG	3	0
33	B	522	3PH	3	0
29	s	310	CLA	3	0
29	c	510	CLA	3	0
30	d	402	PHO	2	0
35	C	521	LMG	1	0
31	C	515	BCR	8	0
29	s	313	CLA	2	0
29	s	305	CLA	2	0
48	G	617	NEX	3	0
29	a	404	CLA	5	0
29	C	512	CLA	3	0
29	r	304	CLA	3	0
39	c	522	SQD	3	0
29	S	306	CLA	1	0
31	f	101	BCR	2	0
29	a	408	CLA	5	0
29	R	303	CLA	2	0
46	G	609	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	s	319	NEX	3	0
29	b	501	CLA	2	0
29	b	515	CLA	7	0
31	c	514	BCR	5	0
31	K	101	BCR	4	0
29	d	403	CLA	4	0
29	R	307	CLA	1	0
47	n	615	LUT	4	0
29	s	304	CLA	5	0
29	G	604	CLA	3	0
46	S	302	CHL	1	0
29	Y	304	CLA	3	0
41	W	202	DGA	4	0
46	R	305	CHL	1	0
29	Y	315	CLA	4	0
29	C	502	CLA	2	0
29	G	603	CLA	6	0
29	c	501	CLA	1	0
29	B	505	CLA	4	0
29	G	612	CLA	2	0
37	B	523	LHG	3	0
47	g	616	LUT	4	0
38	B	524	LMT	2	0
49	N	619	XAT	5	0
29	b	507	CLA	4	0
43	D	406	PL9	2	0
35	C	522	LMG	2	0
29	c	504	CLA	2	0
49	y	302	XAT	4	0
46	S	308	CHL	3	0
31	C	516	BCR	1	0
39	a	410	SQD	1	0
37	D	407	LHG	7	0
40	c	523	SPH	4	0
29	S	313	CLA	4	0
36	c	517	DGD	5	0
29	g	604	CLA	2	0
48	g	617	NEX	2	0
29	b	509	CLA	5	0
46	Y	302	CHL	2	0
46	N	608	CHL	1	0
29	N	604	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	c	520	LMG	9	0
29	g	603	CLA	3	0
29	c	502	CLA	2	0
46	Y	306	CHL	1	0
29	y	316	CLA	3	0
49	G	619	XAT	3	0
29	g	610	CLA	2	0
29	N	612	CLA	1	0
46	N	601	CHL	2	0
47	S	317	LUT	5	0
29	c	505	CLA	5	0
29	S	315	CLA	1	0
29	Y	303	CLA	2	0
31	v	101	BCR	3	0
29	R	306	CLA	4	0
29	B	512	CLA	4	0
29	b	506	CLA	3	0
29	y	306	CLA	2	0
29	C	504	CLA	2	0
29	s	303	CLA	3	0
29	G	613	CLA	3	0
29	g	613	CLA	1	0
46	g	605	CHL	1	0
37	y	320	LHG	3	0
29	n	611	CLA	1	0
46	s	309	CHL	4	0
29	C	513	CLA	2	0
29	A	405	CLA	9	0
29	b	511	CLA	1	0
29	c	512	CLA	4	0
46	n	601	CHL	4	0
29	g	602	CLA	4	0
37	n	617	LHG	5	0
29	s	315	CLA	1	0
29	a	405	CLA	4	0
29	d	404	CLA	3	0
42	D	403	BCT	1	0
46	G	601	CHL	2	0
29	N	614	CLA	1	0
35	i	101	LMG	2	0
29	S	304	CLA	4	0
37	Y	319	LHG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	517	BCR	6	0
36	C	519	DGD	2	0
46	s	308	CHL	2	0
48	r	313	NEX	1	0
47	Y	316	LUT	3	0
37	D	408	LHG	2	0
46	G	607	CHL	5	0
46	g	609	CHL	1	0
49	r	312	XAT	4	0
29	R	302	CLA	2	0
46	n	605	CHL	4	0
46	g	608	CHL	2	0
46	y	303	CHL	1	0
37	S	320	LHG	3	0
46	y	301	CHL	5	0
29	y	304	CLA	6	0
29	c	506	CLA	4	0
30	A	408	PHO	5	0
47	r	311	LUT	3	0
39	L	102	SQD	5	0
35	d	407	LMG	2	0
29	n	610	CLA	2	0
29	G	614	CLA	1	0
29	r	309	CLA	5	0
41	J	101	DGA	2	0
29	A	407	CLA	1	0
29	S	312	CLA	7	0
37	l	102	LHG	3	0
46	y	309	CHL	6	0
29	B	504	CLA	4	0
29	B	514	CLA	4	0
37	d	406	LHG	5	0
29	y	305	CLA	5	0
46	y	308	CHL	1	0
29	C	510	CLA	1	0
47	S	318	LUT	3	0
46	Y	307	CHL	3	0
29	C	506	CLA	2	0
31	z	101	BCR	5	0
29	g	614	CLA	1	0
47	Y	317	LUT	3	0
37	G	618	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	d	408	LMG	2	0
37	N	618	LHG	4	0
47	N	615	LUT	2	0
47	g	615	LUT	2	0
29	Y	305	CLA	2	0
48	y	319	NEX	3	0
41	j	101	DGA	3	0
47	n	614	LUT	3	0
39	m	101	SQD	1	0
29	C	503	CLA	1	0
49	R	311	XAT	1	0
47	s	318	LUT	3	0
29	y	314	CLA	4	0
36	C	520	DGD	3	0
35	W	203	LMG	3	0
29	C	505	CLA	3	0
29	B	508	CLA	2	0
50	N	620	PTY	8	0
29	s	311	CLA	3	0
46	r	305	CHL	3	0
35	W	201	LMG	1	0
30	D	401	PHO	3	0
29	C	511	CLA	1	0
29	B	509	CLA	3	0
29	D	405	CLA	3	0
45	h	101	RRX	2	0
29	B	506	CLA	1	0
44	E	101	HEM	1	0
35	D	409	LMG	2	0
47	R	310	LUT	4	0
29	n	603	CLA	6	0
48	n	616	NEX	1	0
47	N	616	LUT	4	0
29	s	306	CLA	2	0
29	N	610	CLA	3	0
29	b	508	CLA	3	0
37	L	101	LHG	3	0
47	G	615	LUT	2	0
35	B	520	LMG	3	0
31	B	518	BCR	1	0
41	w	201	DGA	6	0
35	D	410	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	G	608	CHL	1	0
46	R	304	CHL	2	0
26	a	401	OEX	1	0
36	c	518	DGD	1	0
46	Y	308	CHL	4	0
29	N	611	CLA	2	0
29	s	312	CLA	6	0
29	b	512	CLA	3	0
29	C	507	CLA	4	0
46	s	307	CHL	2	0
29	Y	312	CLA	3	0
44	e	101	HEM	3	0
49	n	618	XAT	4	0
46	g	601	CHL	3	0
29	c	508	CLA	4	0
39	o	301	SQD	1	0
31	F	101	BCR	2	0
29	S	303	CLA	3	0
39	M	101	SQD	2	0
29	y	315	CLA	2	0
46	y	311	CHL	5	0
46	g	607	CHL	3	0
37	c	521	LHG	7	0
29	n	613	CLA	1	0
47	y	318	LUT	3	0
31	c	515	BCR	3	0
29	A	406	CLA	6	0
48	N	617	NEX	3	0
29	g	611	CLA	3	0
29	G	611	CLA	1	0
29	a	406	CLA	1	0
29	B	502	CLA	2	0
29	N	602	CLA	2	0
38	b	524	LMT	4	0
29	b	502	CLA	3	0
46	r	306	CHL	1	0
48	Y	318	NEX	3	0
36	B	521	DGD	1	0
46	Y	310	CHL	4	0
29	b	513	CLA	4	0
29	y	310	CLA	1	0
40	i	102	SPH	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	s	317	LUT	3	0
37	a	413	LHG	2	0
48	R	312	NEX	3	0
29	c	509	CLA	2	0
29	B	501	CLA	2	0
47	y	317	LUT	1	0
31	A	410	BCR	3	0
50	n	619	PTY	5	0
31	b	517	BCR	10	0
36	r	301	DGD	1	0
46	N	607	CHL	4	0
29	R	308	CLA	5	0
46	N	609	CHL	5	0
29	n	612	CLA	2	0
46	S	307	CHL	3	0
29	Y	311	CLA	1	0
49	Y	301	XAT	3	0
49	g	619	XAT	2	0
29	r	303	CLA	5	0
29	c	507	CLA	2	0
29	G	602	CLA	5	0
33	s	322	3PH	3	0
37	g	618	LHG	4	0
29	b	514	CLA	3	0
29	B	516	CLA	4	0
37	s	320	LHG	4	0
39	b	523	SQD	4	0
46	N	606	CHL	2	0
33	a	415	3PH	3	0
31	C	517	BCR	2	0
46	n	606	CHL	5	0
43	d	405	PL9	2	0
31	a	409	BCR	2	0
29	n	609	CLA	6	0
37	S	301	LHG	3	0
29	b	504	CLA	2	0
41	b	522	DGA	2	0
29	r	310	CLA	1	0
29	Y	309	CLA	1	0
35	b	520	LMG	4	0
35	w	202	LMG	2	0
29	c	503	CLA	1	0

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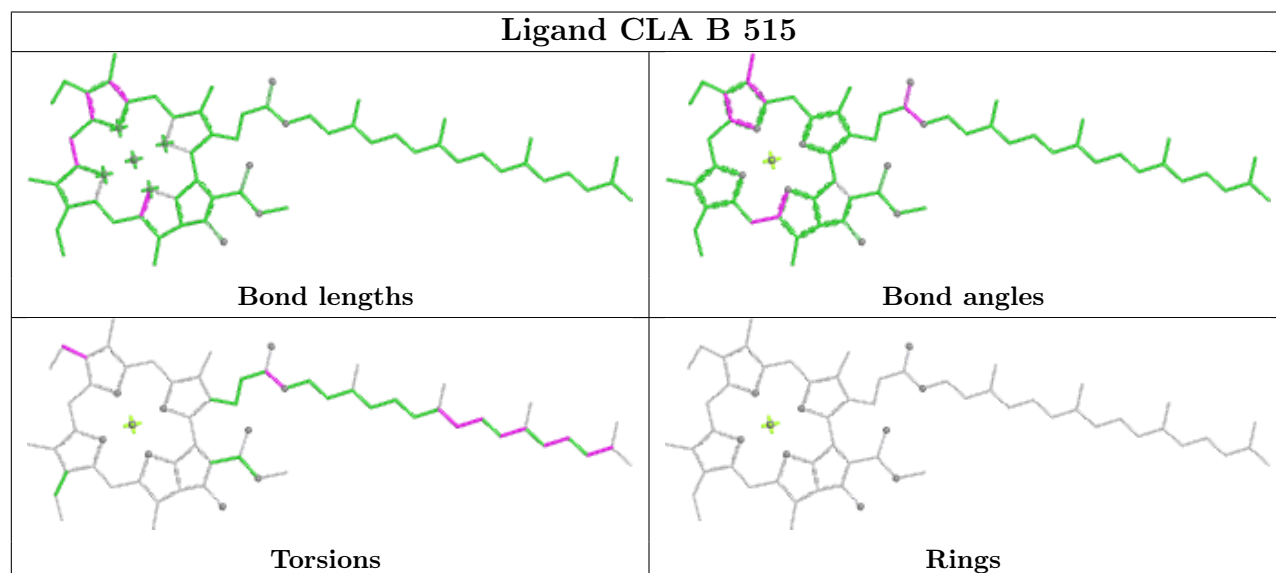
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	513	CLA	3	0
29	S	310	CLA	1	0
35	c	519	LMG	1	0
45	H	101	RRX	3	0
37	s	301	LHG	2	0
29	D	404	CLA	6	0
33	A	412	3PH	1	0
29	r	308	CLA	3	0
46	g	606	CHL	3	0
29	s	316	CLA	1	0
26	A	401	OEX	1	0
46	S	309	CHL	6	0
40	C	525	SPH	1	0
29	n	604	CLA	2	0
29	S	314	CLA	3	0
29	S	305	CLA	1	0
29	Y	313	CLA	2	0
29	b	505	CLA	3	0
46	s	302	CHL	1	0
29	A	409	CLA	5	0
29	B	507	CLA	4	0
47	G	616	LUT	4	0
46	N	605	CHL	7	0
46	n	608	CHL	2	0
29	r	307	CLA	3	0
29	c	513	CLA	6	0
29	n	602	CLA	4	0
29	B	503	CLA	1	0
33	S	322	3PH	2	0
46	G	606	CHL	2	0
29	Y	314	CLA	6	0
29	N	603	CLA	3	0
46	n	607	CHL	1	0
36	C	518	DGD	4	0
29	S	311	CLA	6	0
46	G	605	CHL	1	0
35	C	524	LMG	2	0
39	C	501	SQD	2	0
48	S	319	NEX	4	0
40	I	101	SPH	3	0
29	B	510	CLA	3	0
29	G	610	CLA	2	0

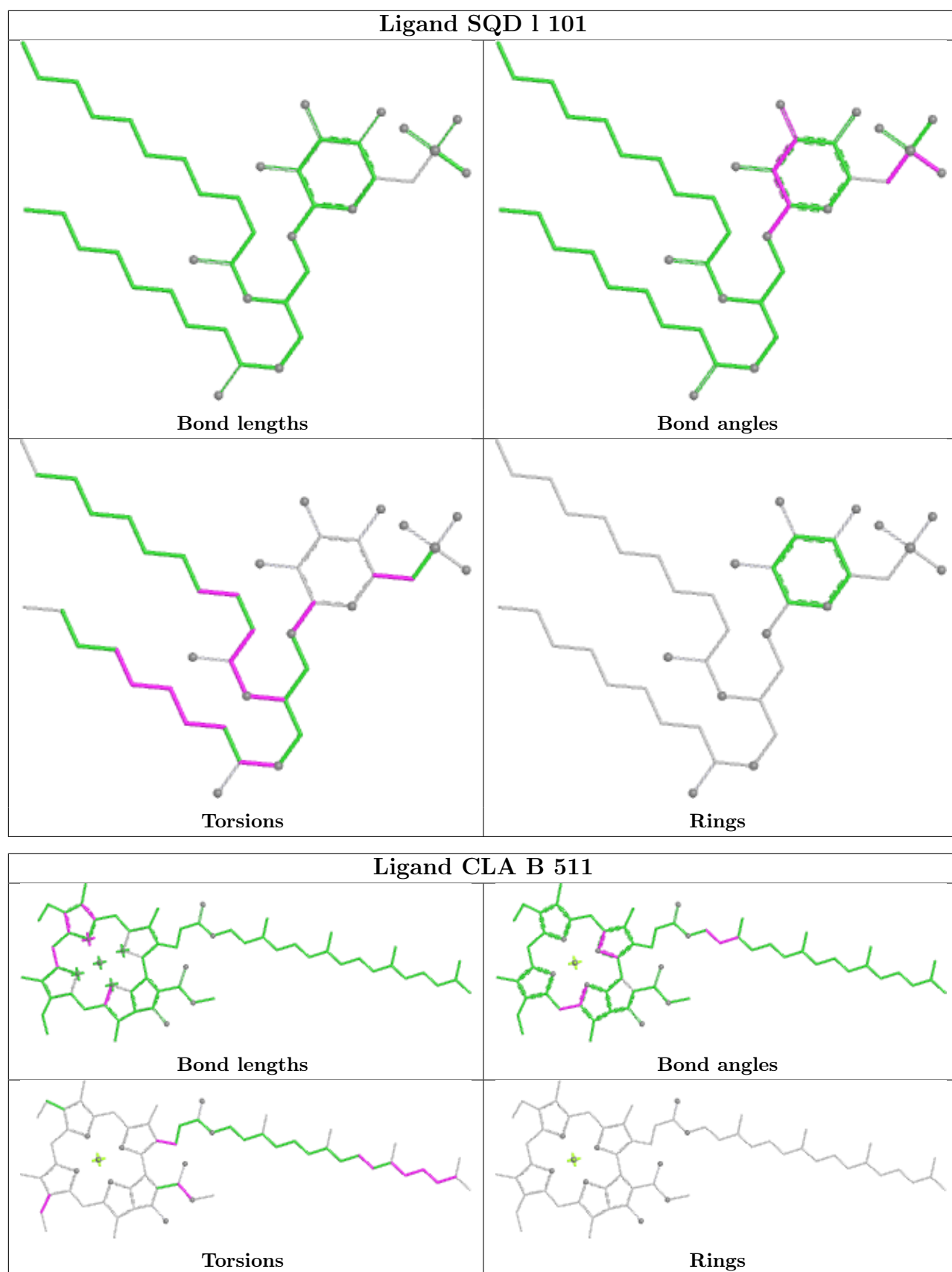
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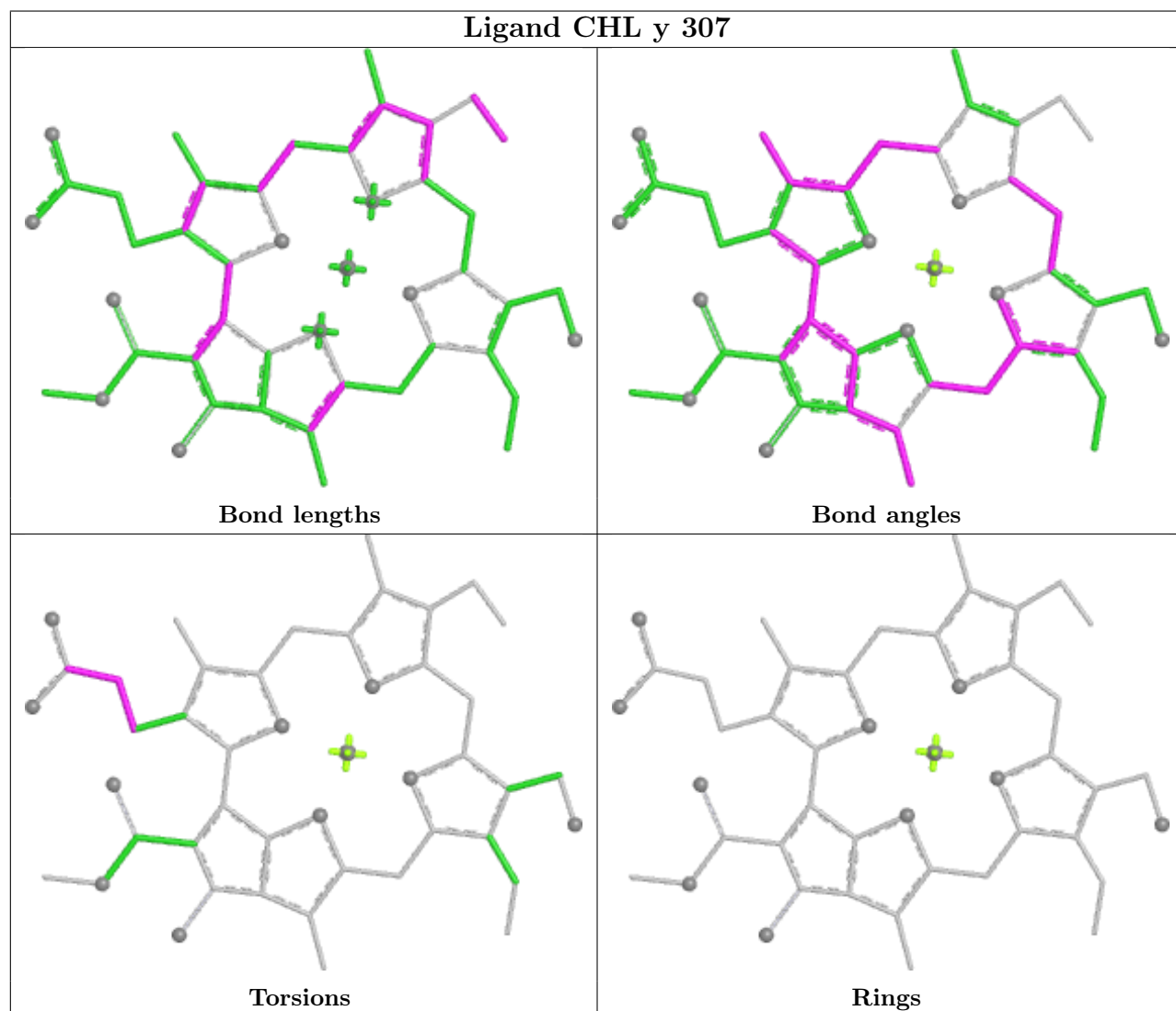
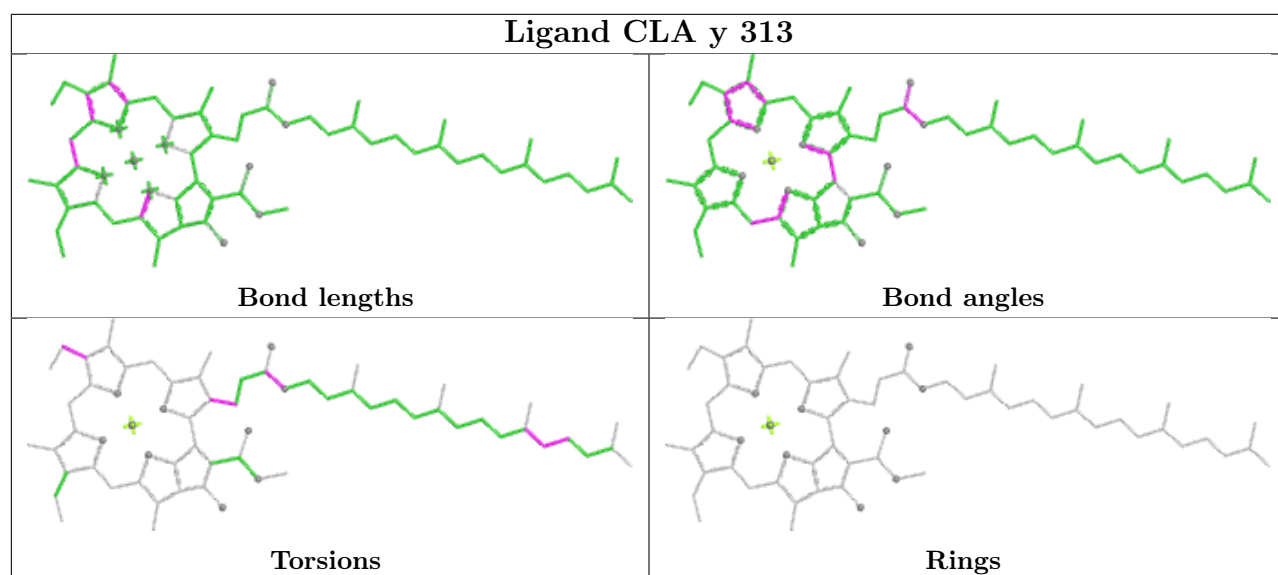
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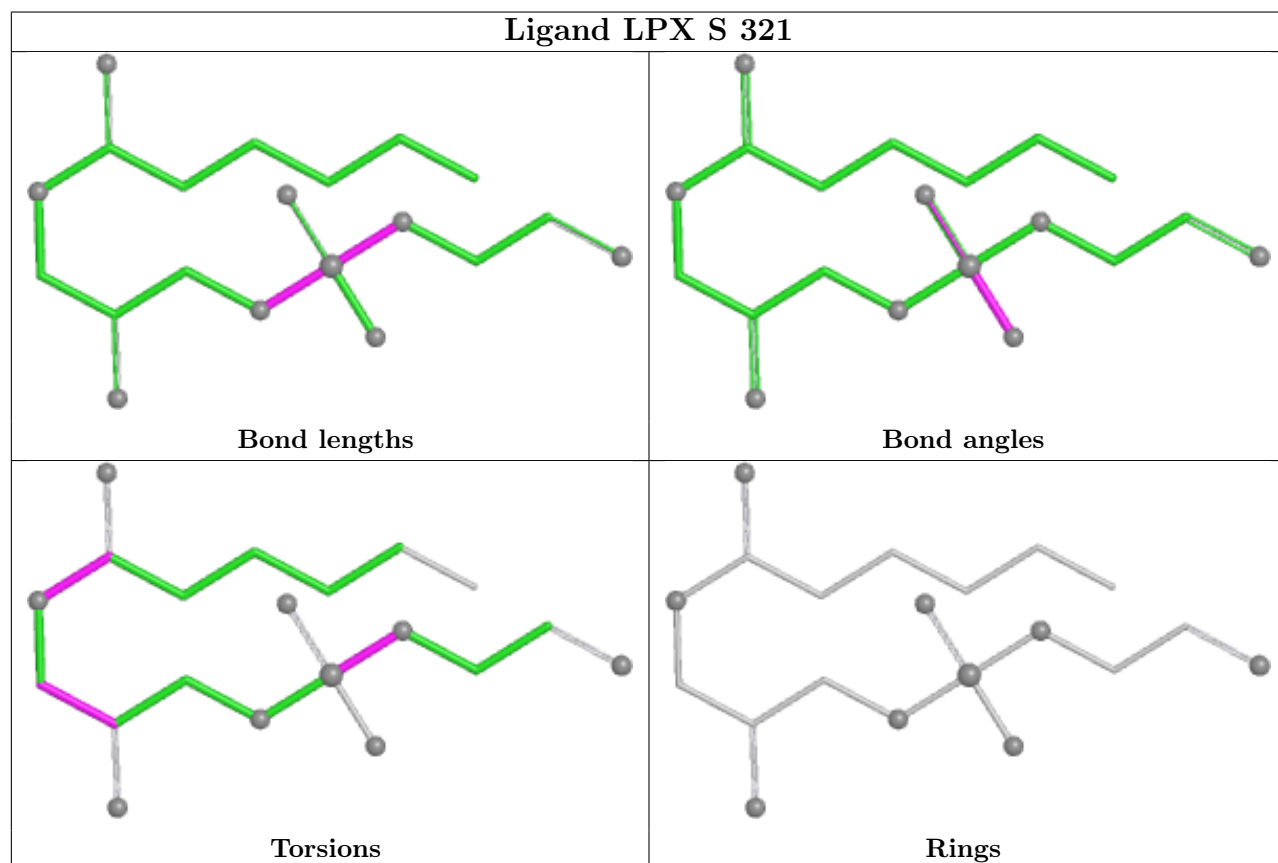
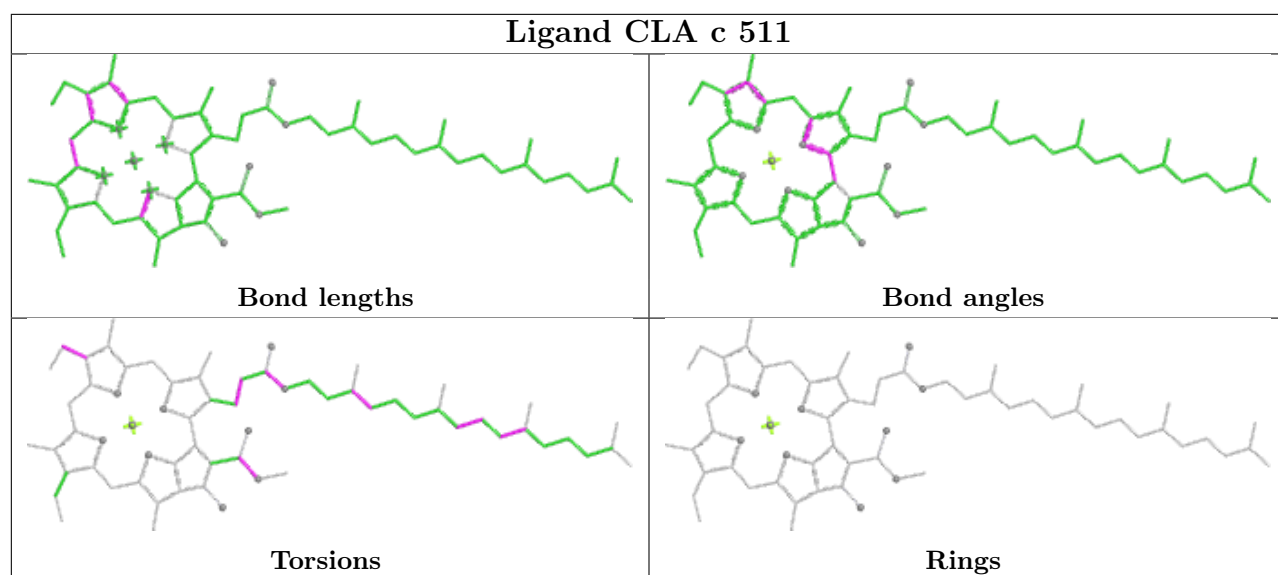
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	C	514	CLA	6	0
29	b	510	CLA	2	0
29	S	316	CLA	3	0
33	b	521	3PH	4	0
29	N	613	CLA	3	0

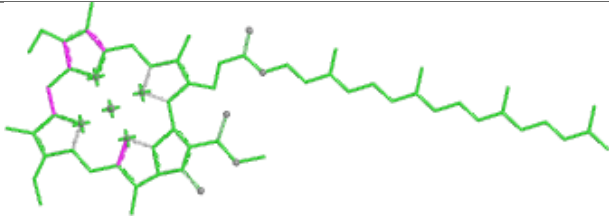
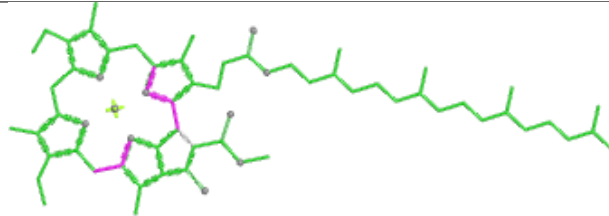
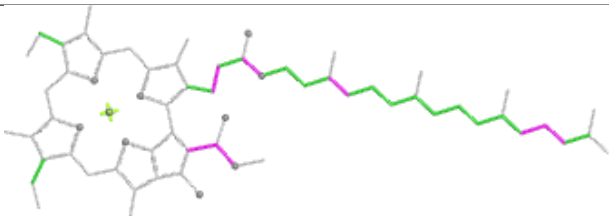
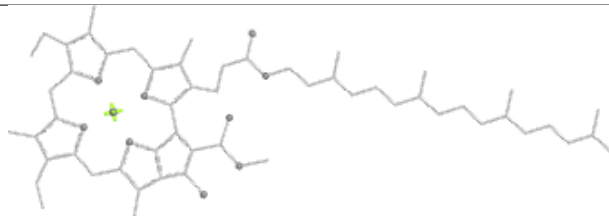
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

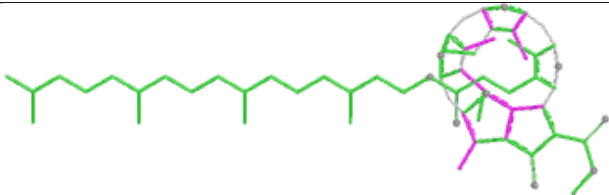
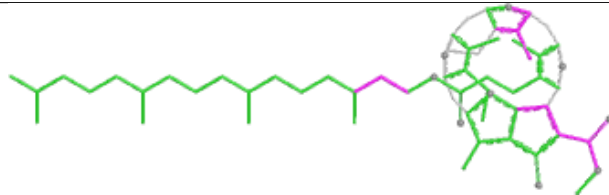
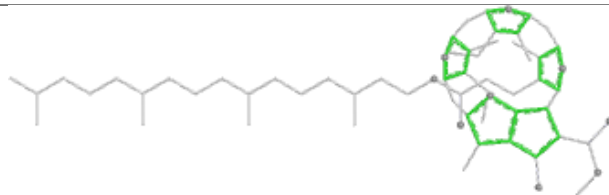


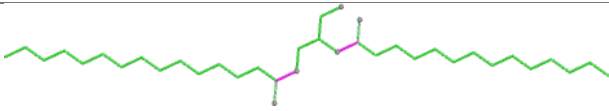
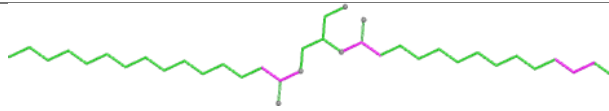
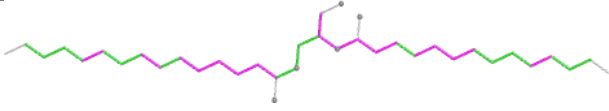
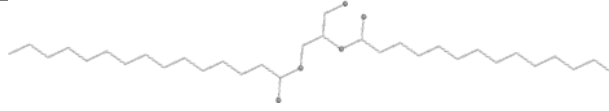


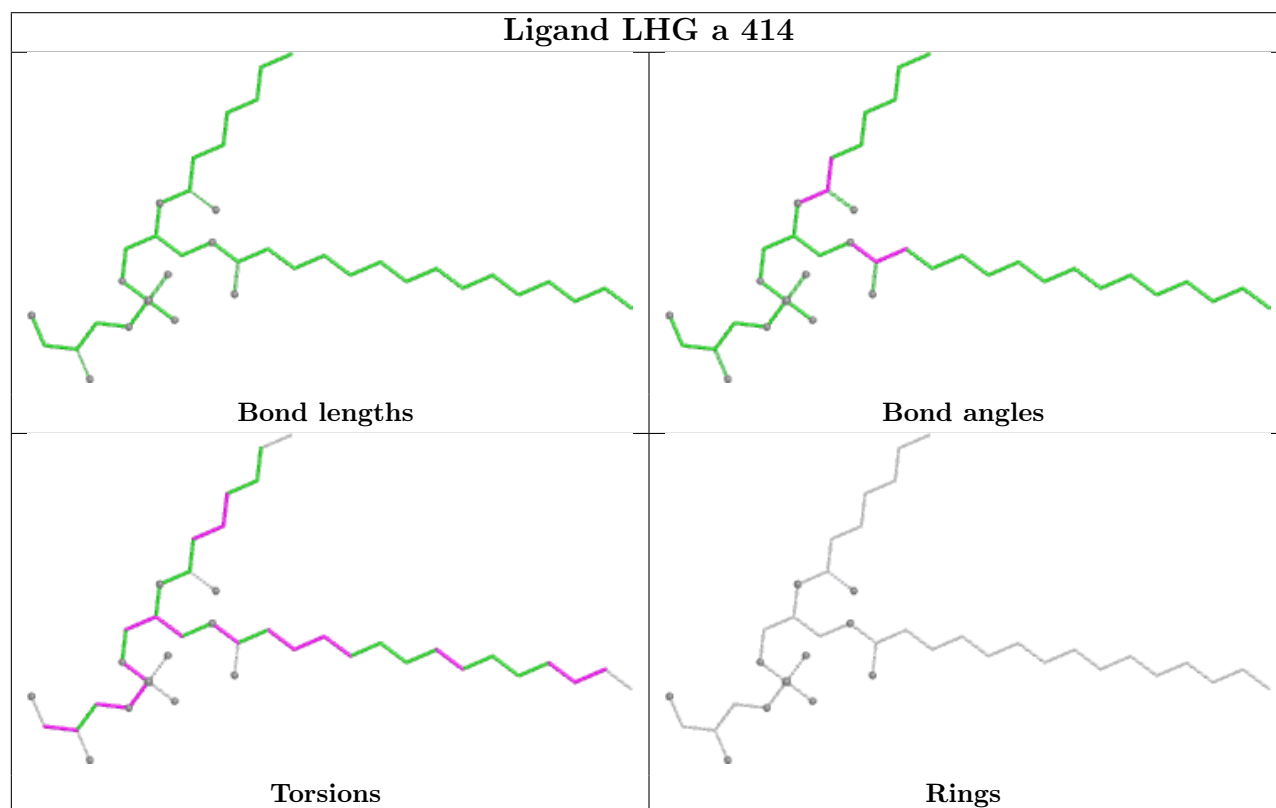
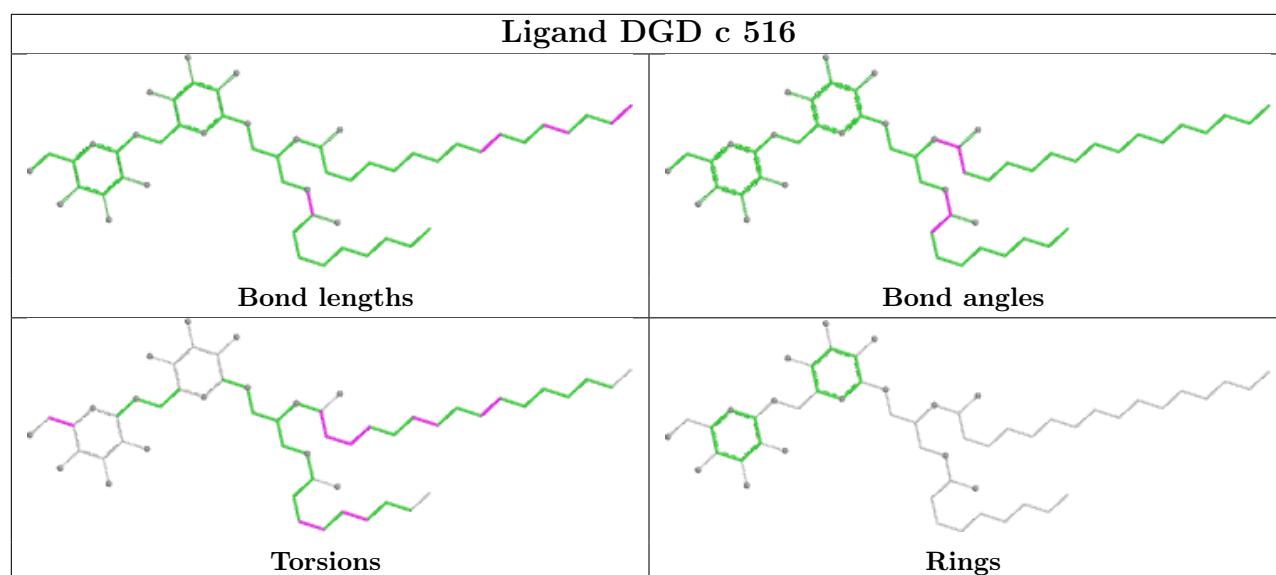


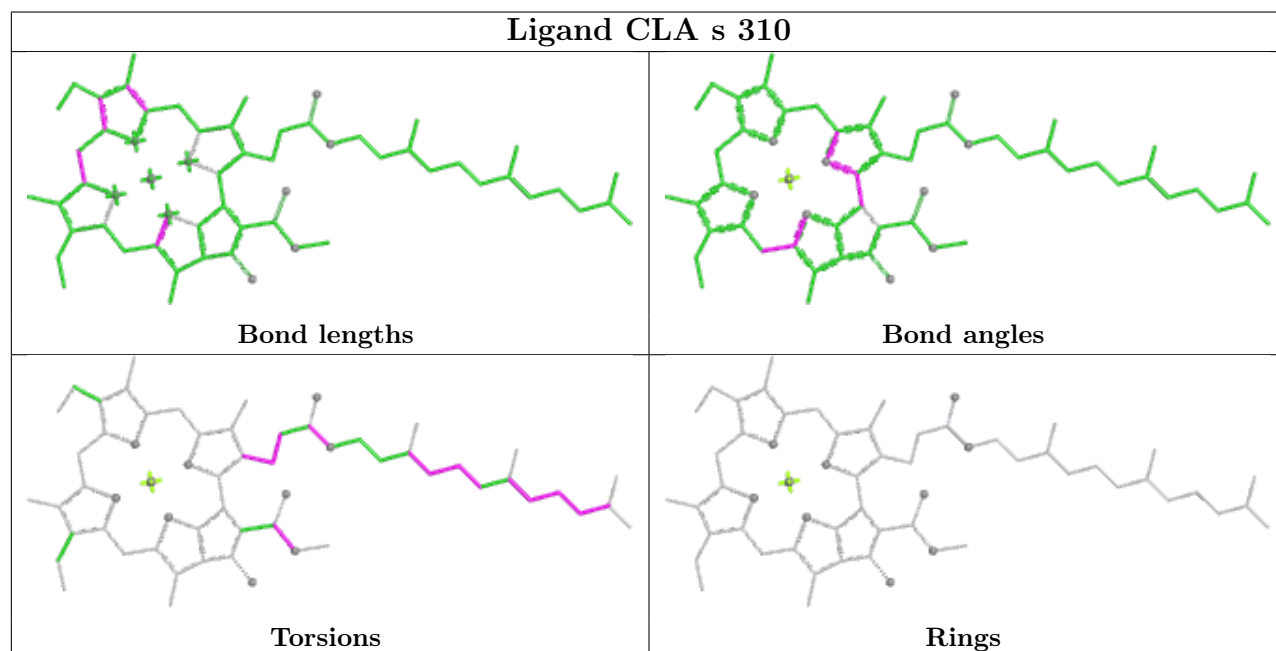
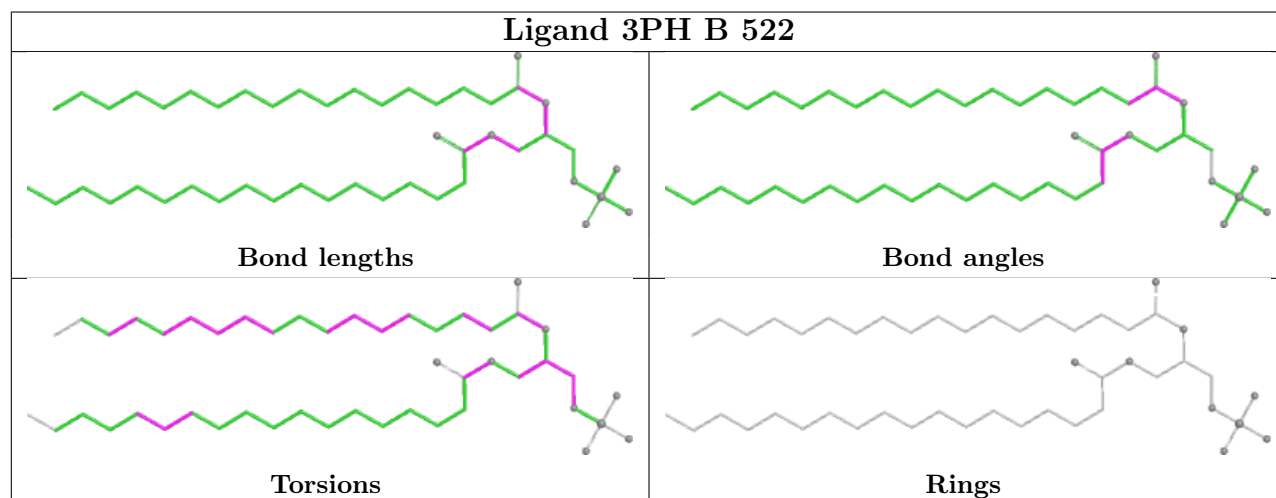
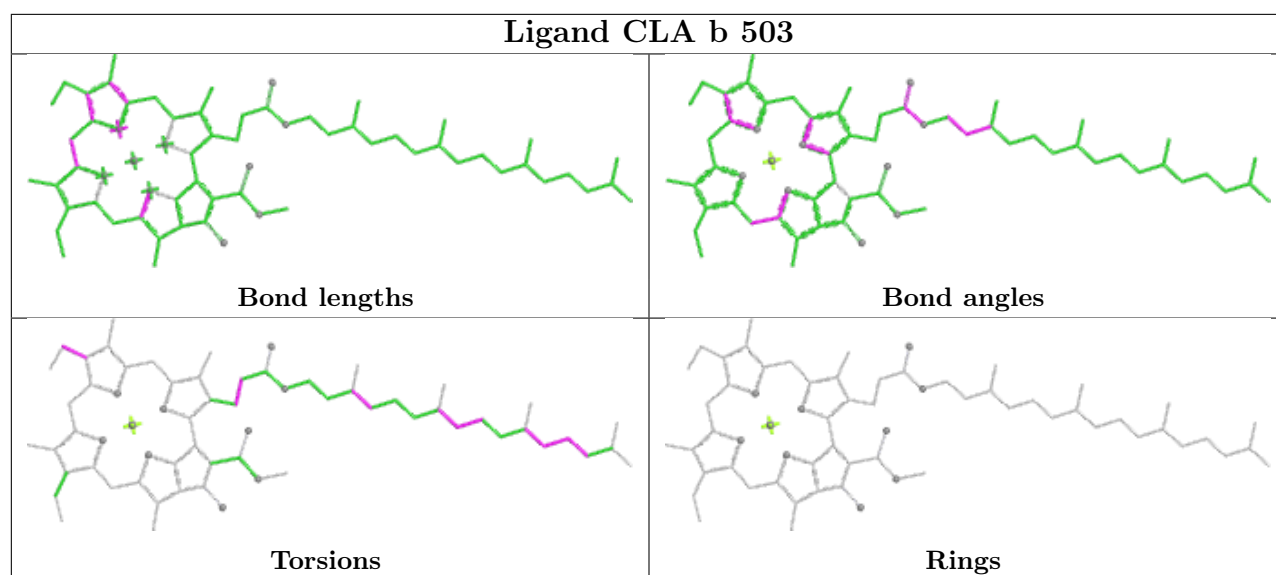


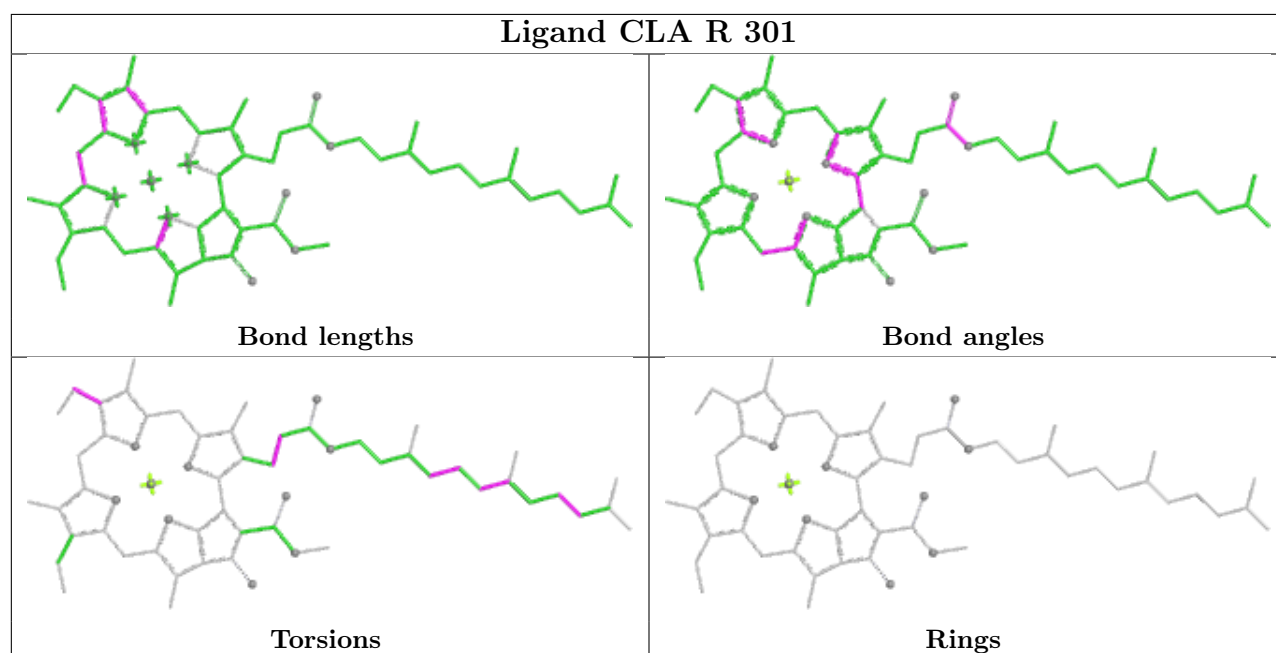
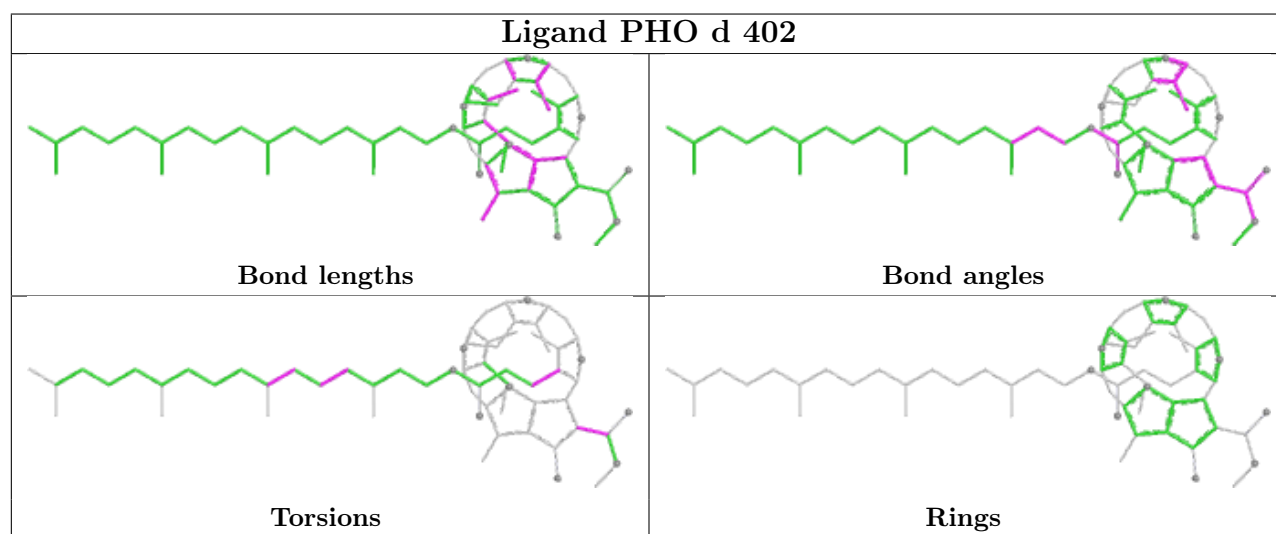
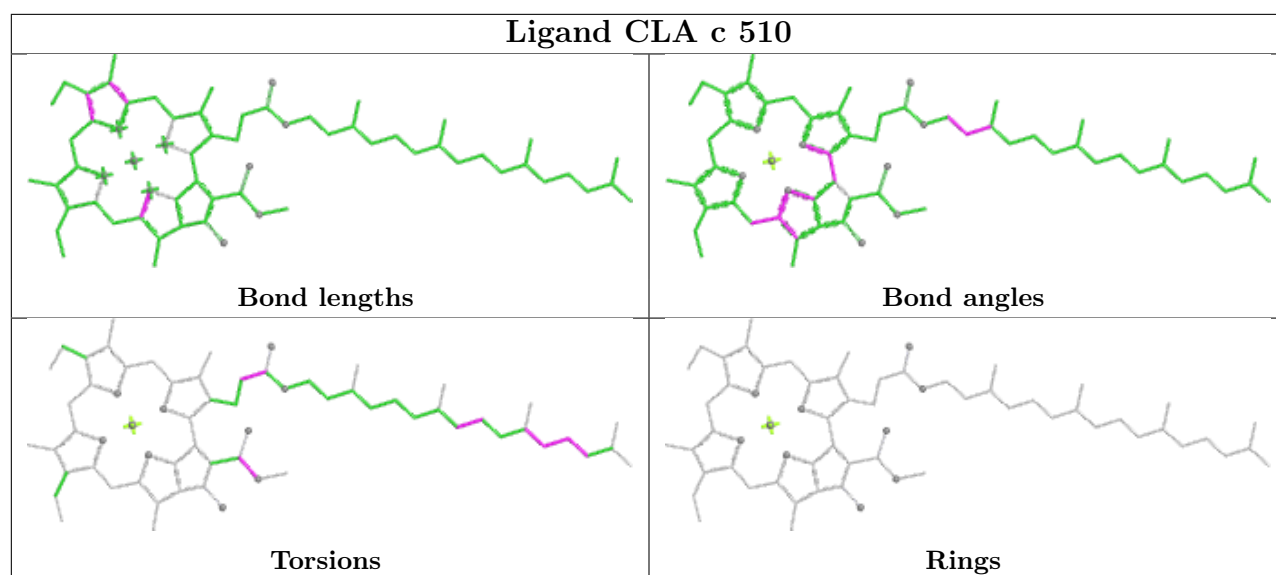
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

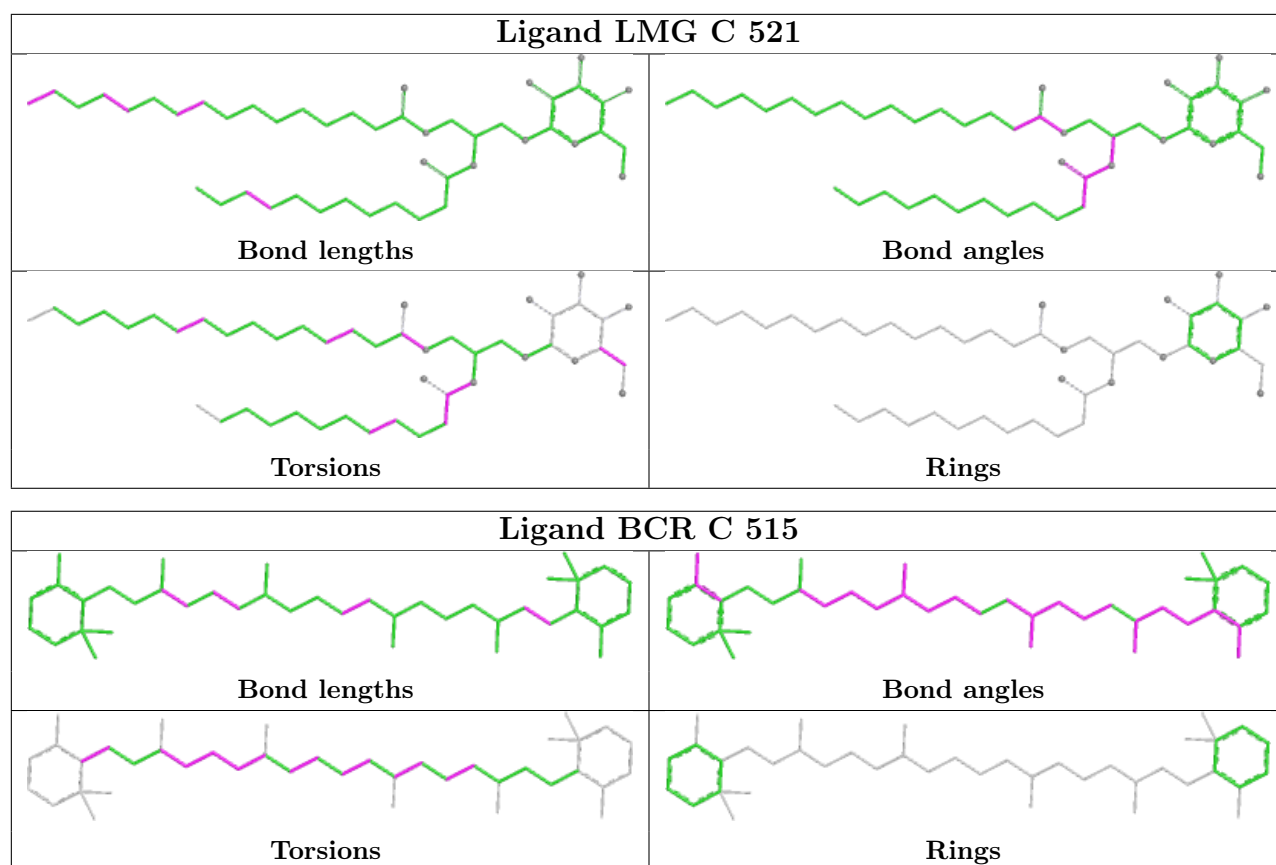
Ligand PHO a 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGA D 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

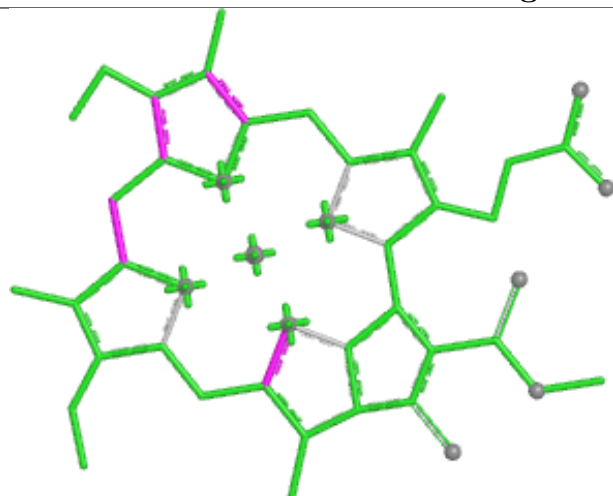




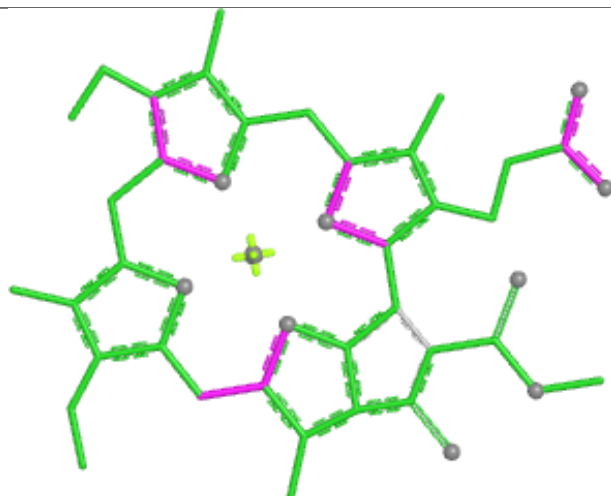




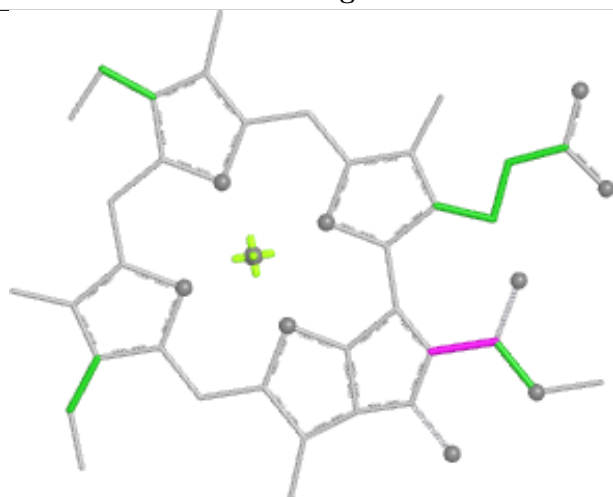
Ligand CLA s 313



Bond lengths



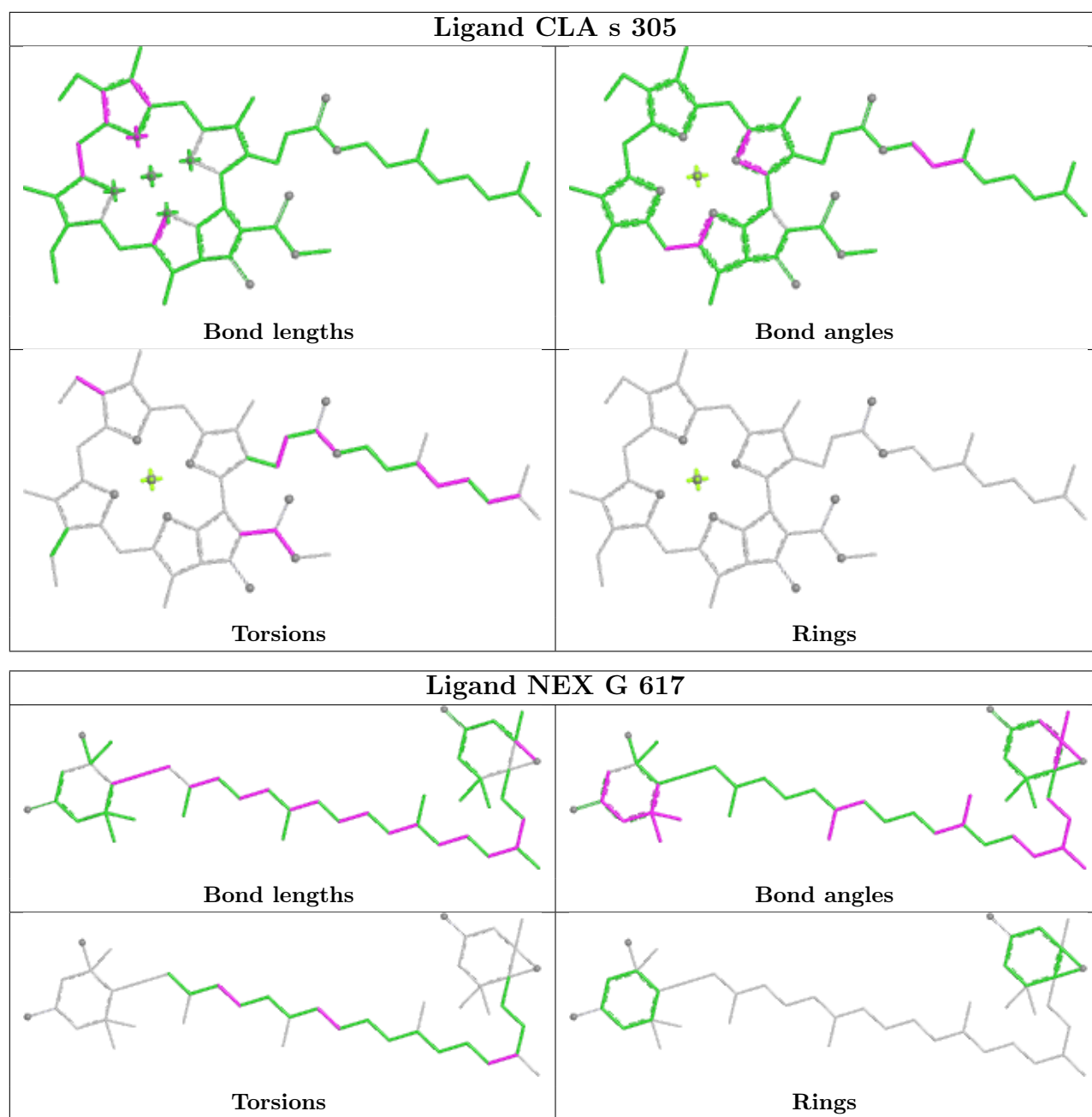
Bond angles

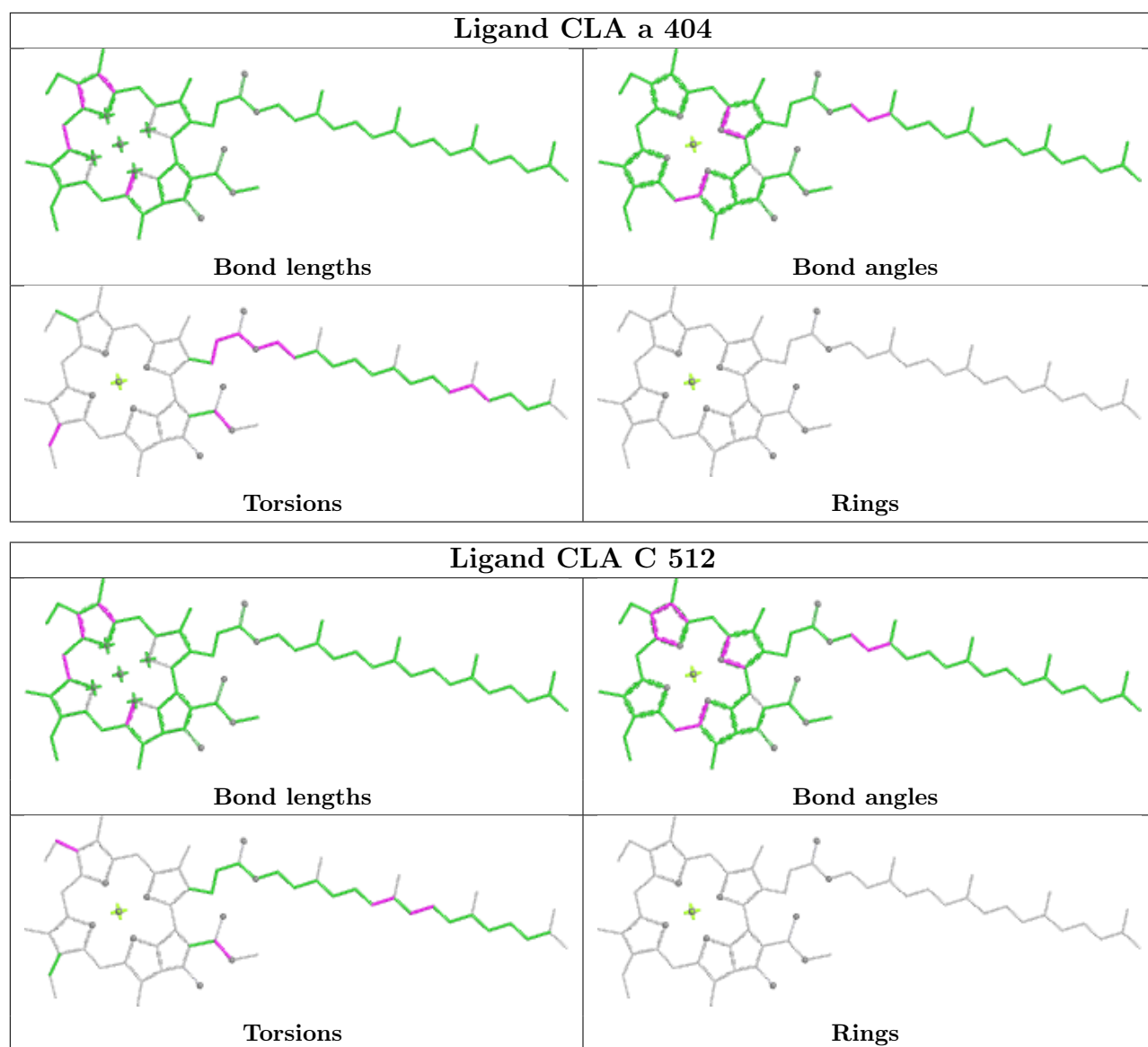


Torsions

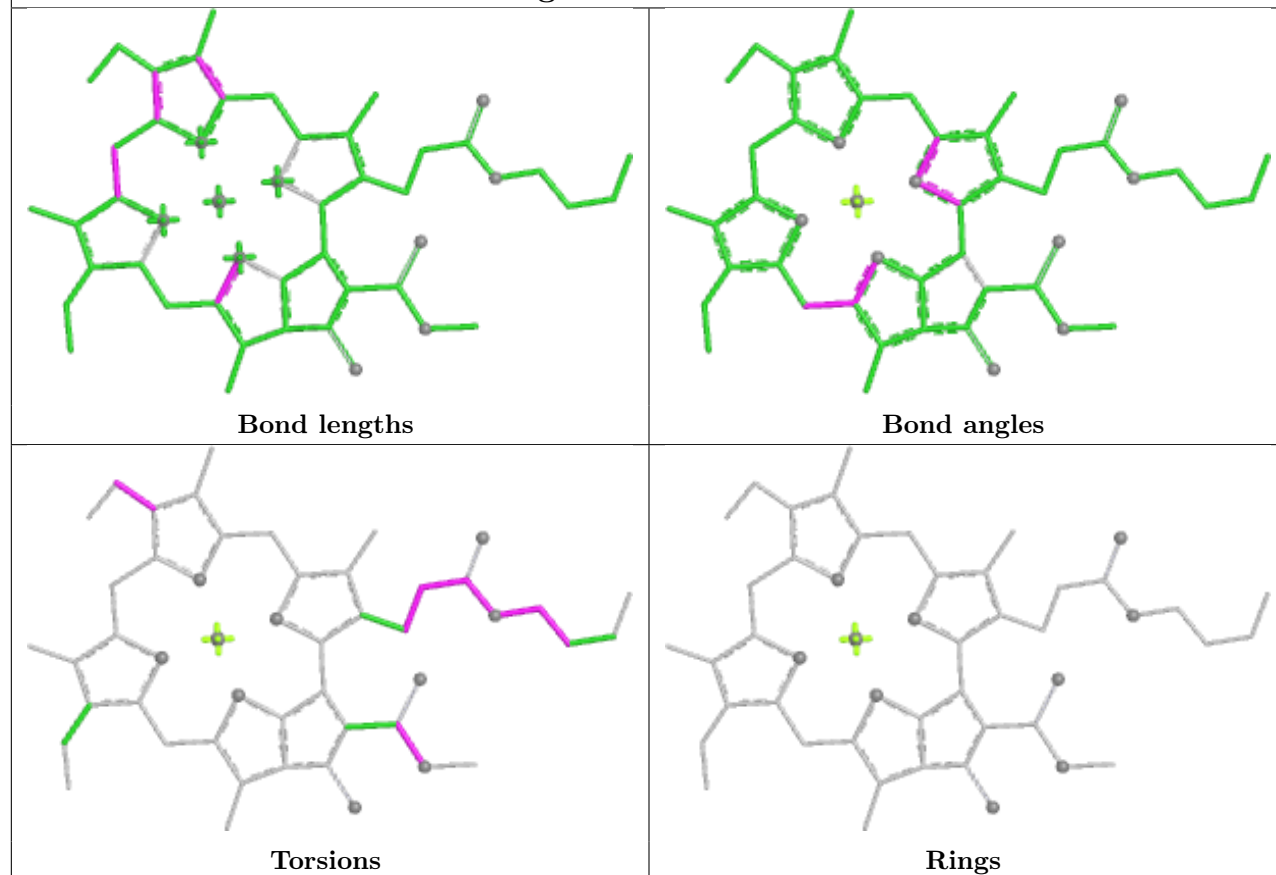


Rings

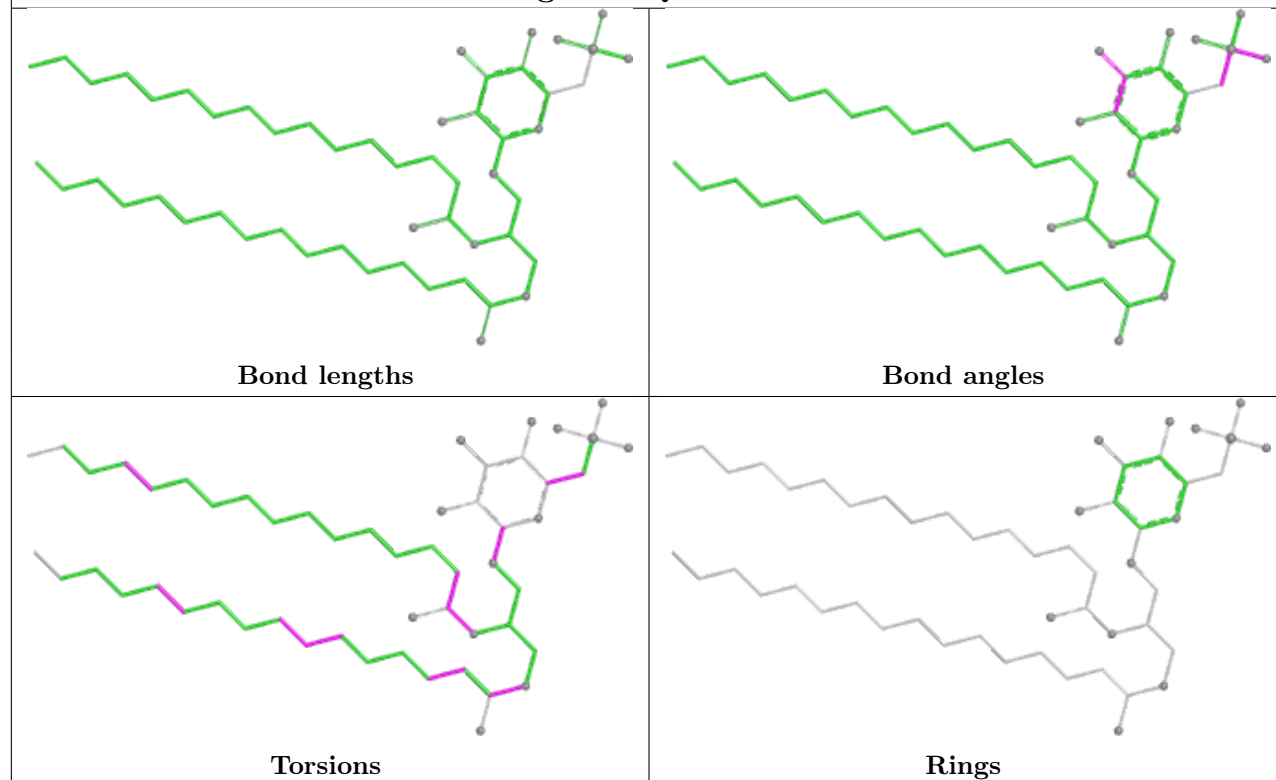




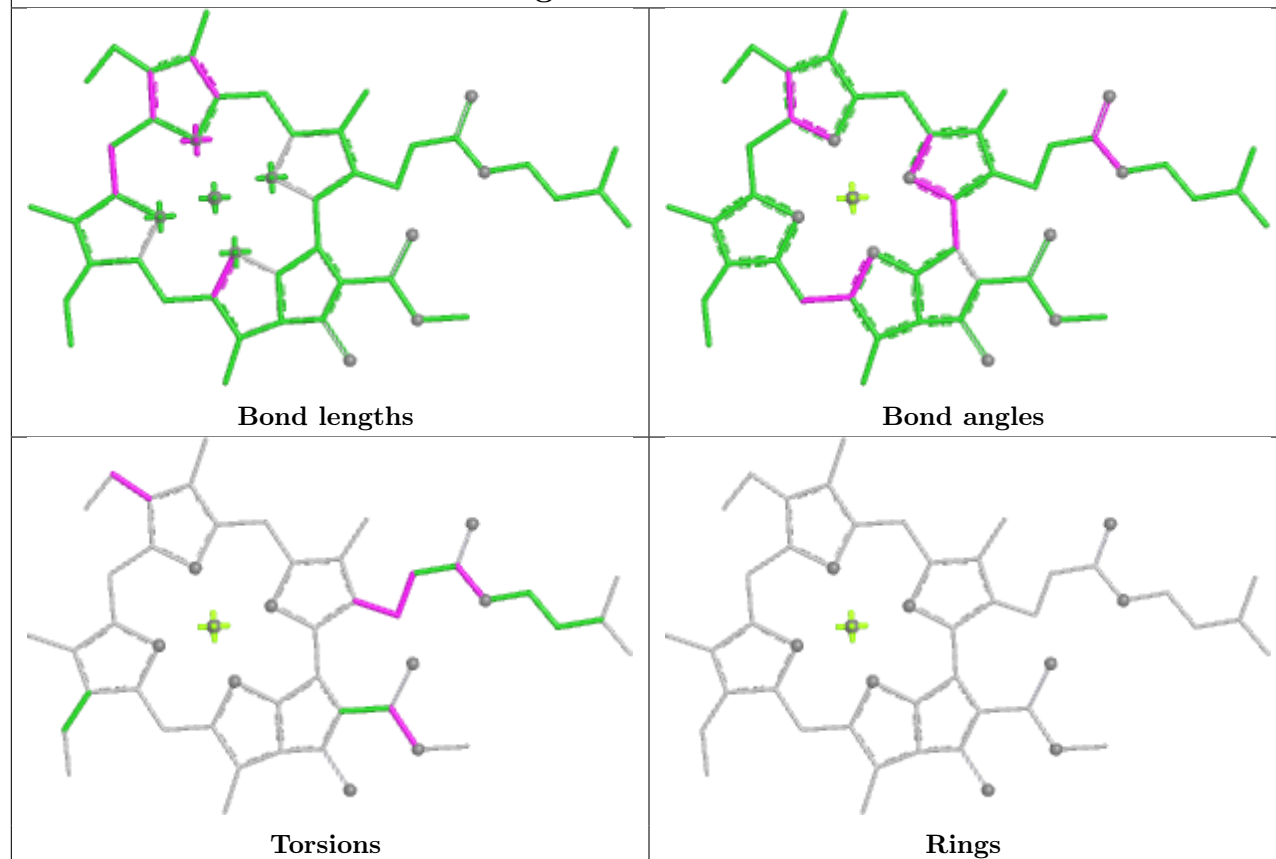
Ligand CLA r 304



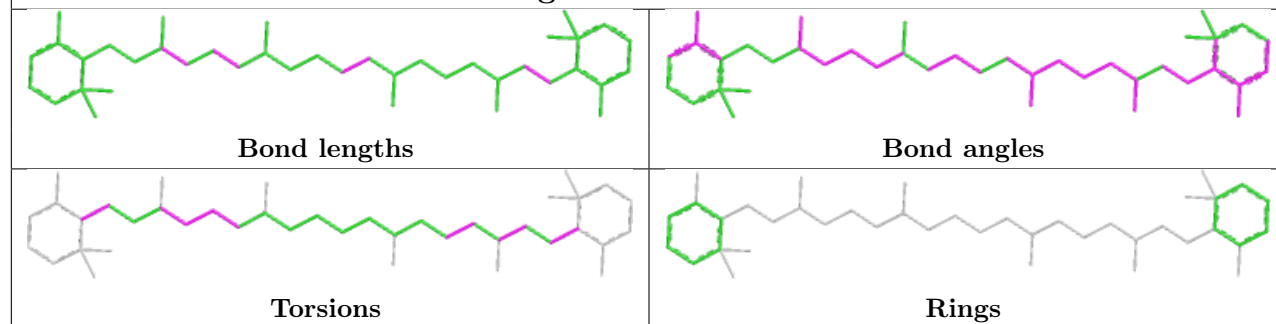
Ligand SQD c 522



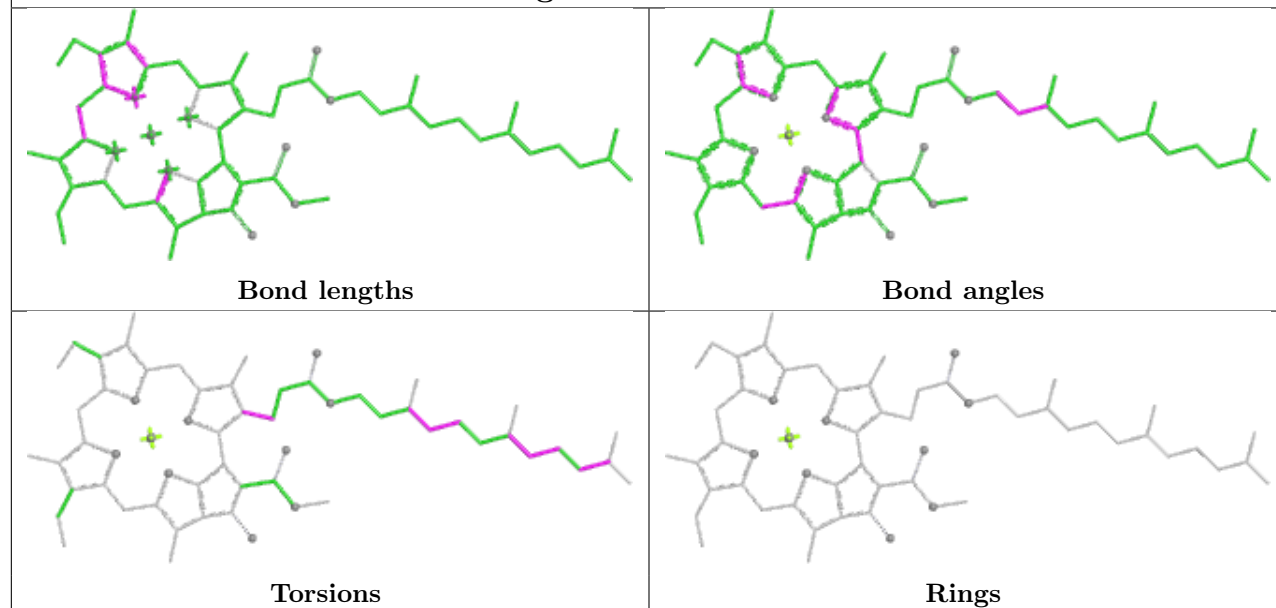
Ligand CLA S 306



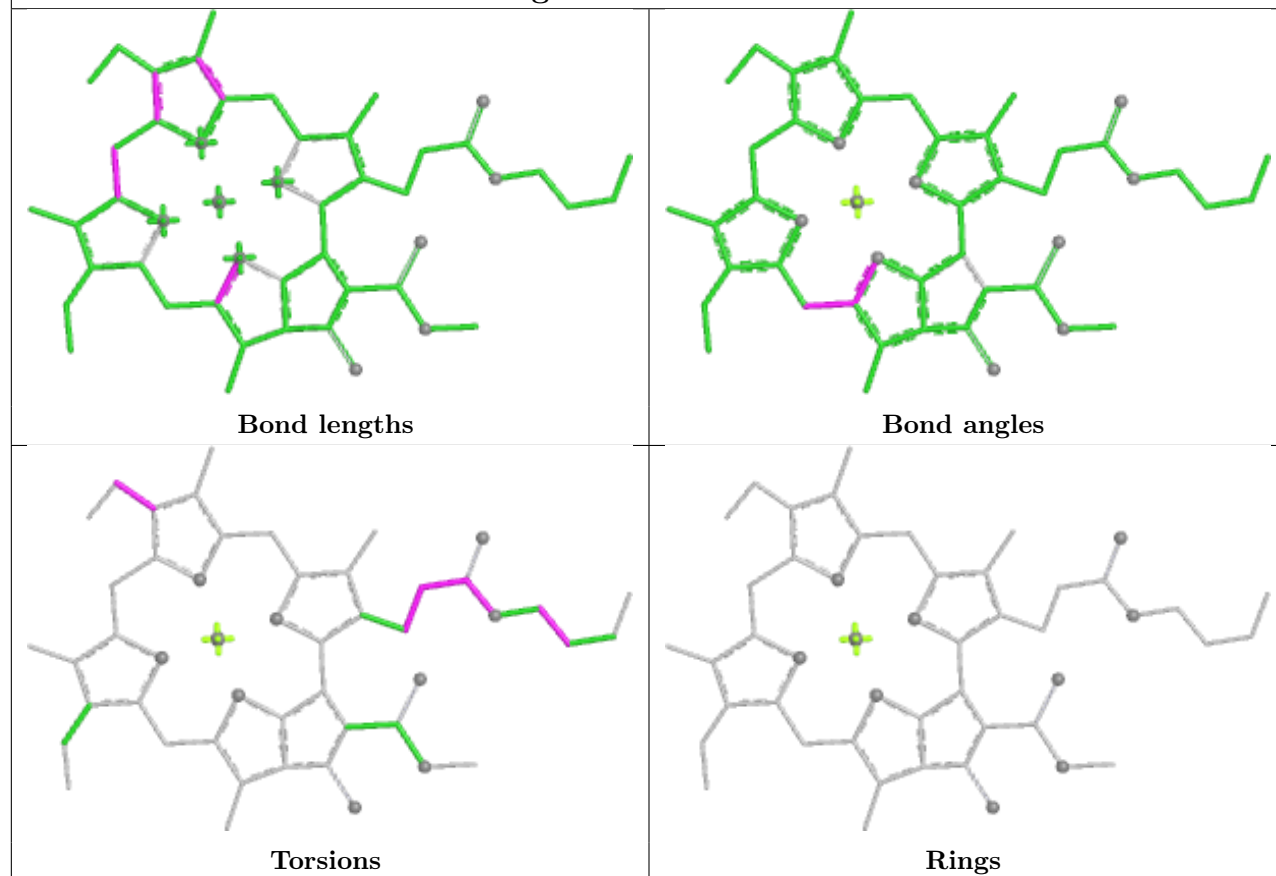
Ligand BCR f 101

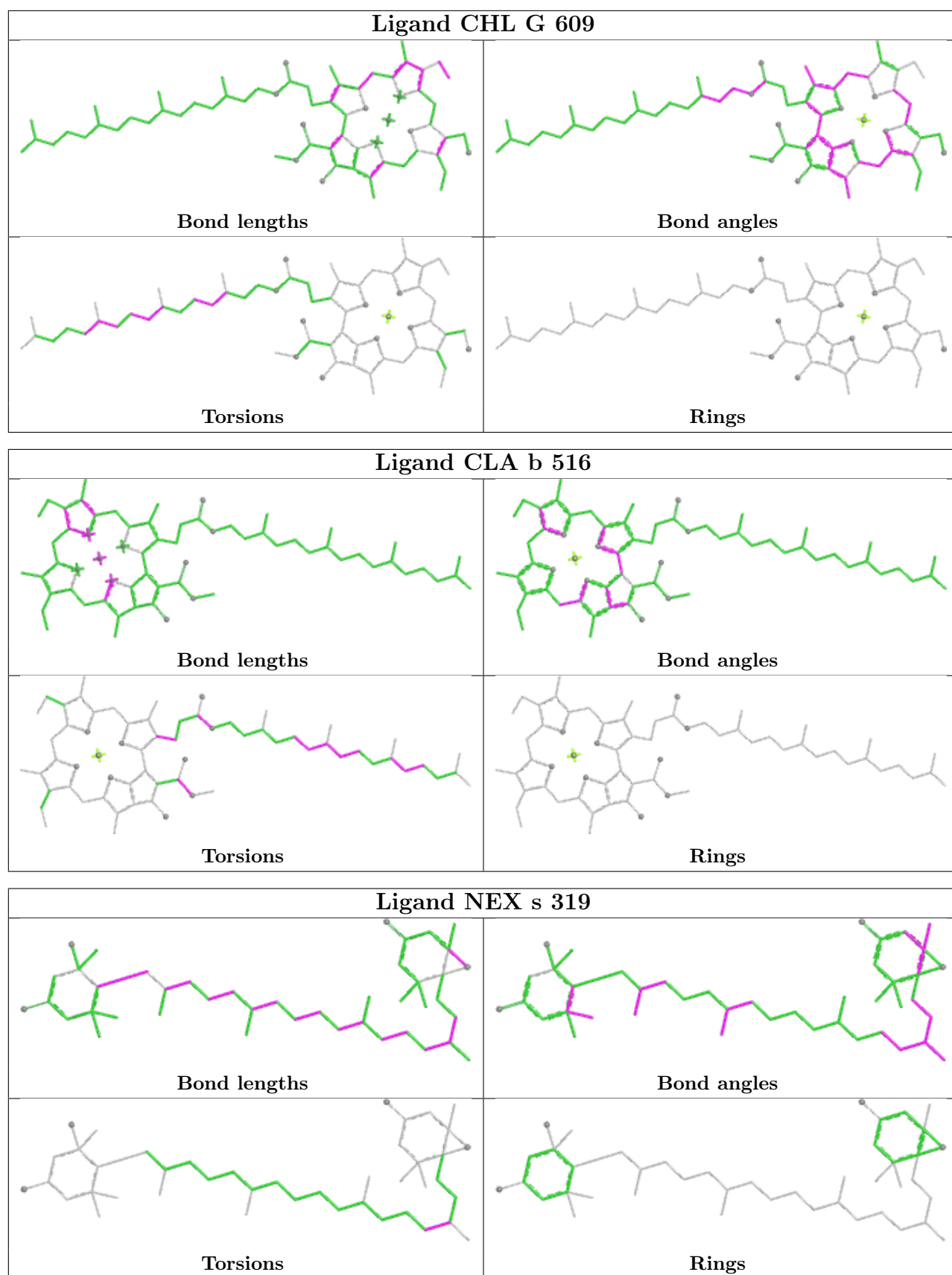


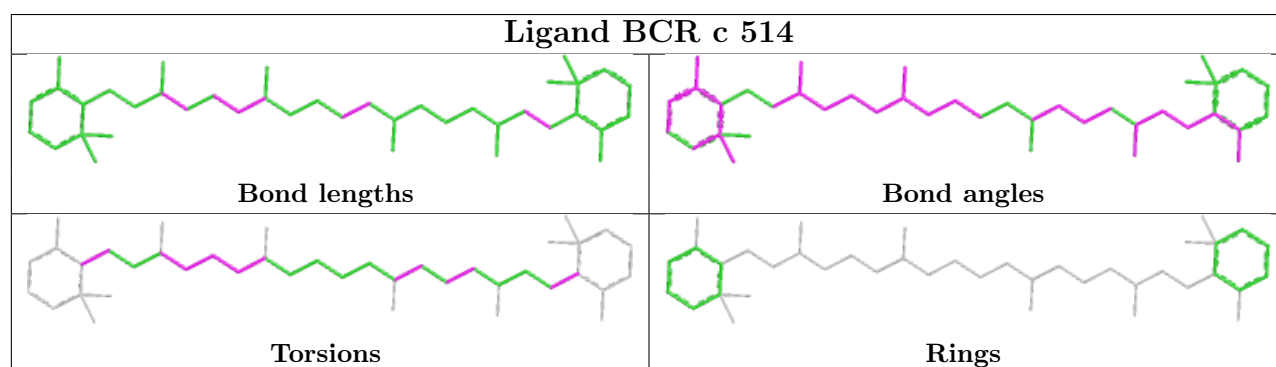
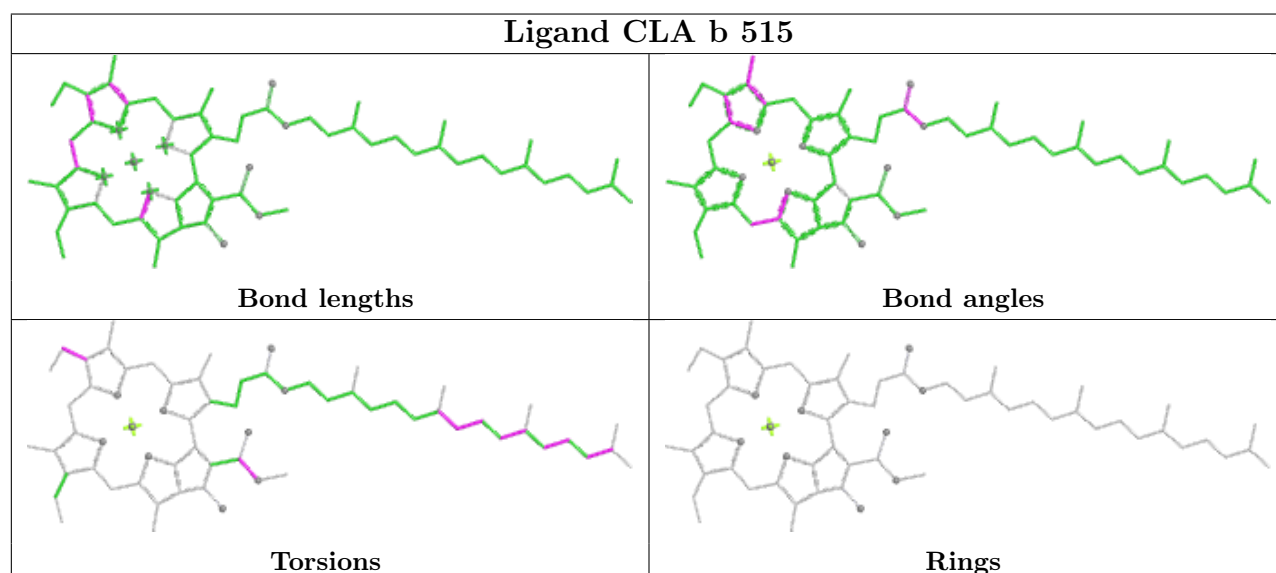
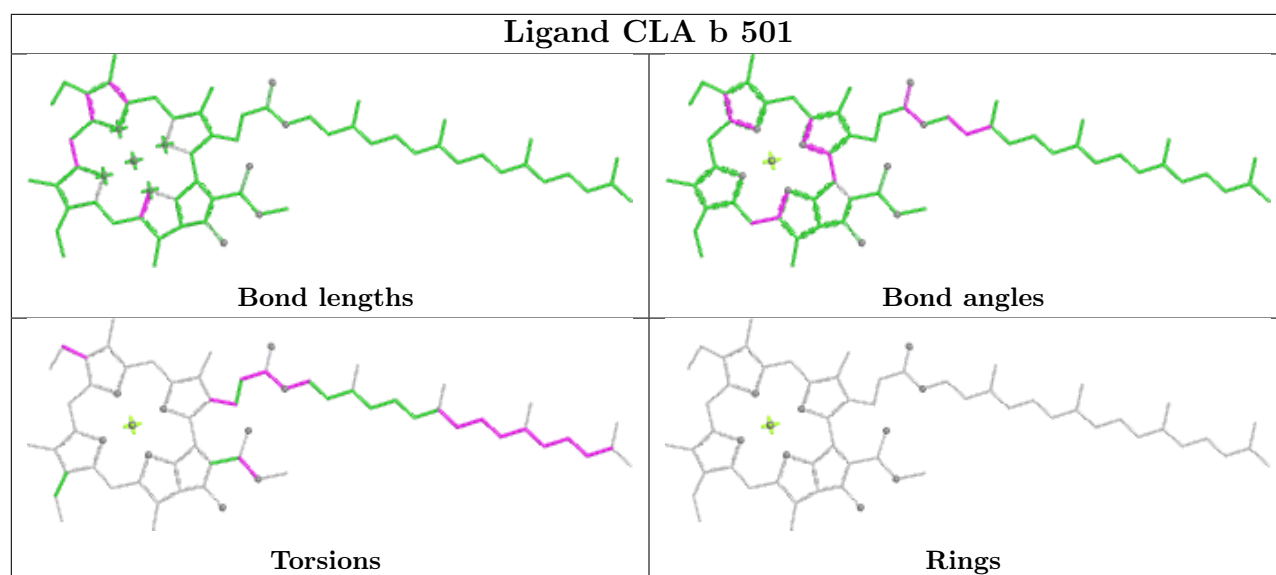
Ligand CLA a 408

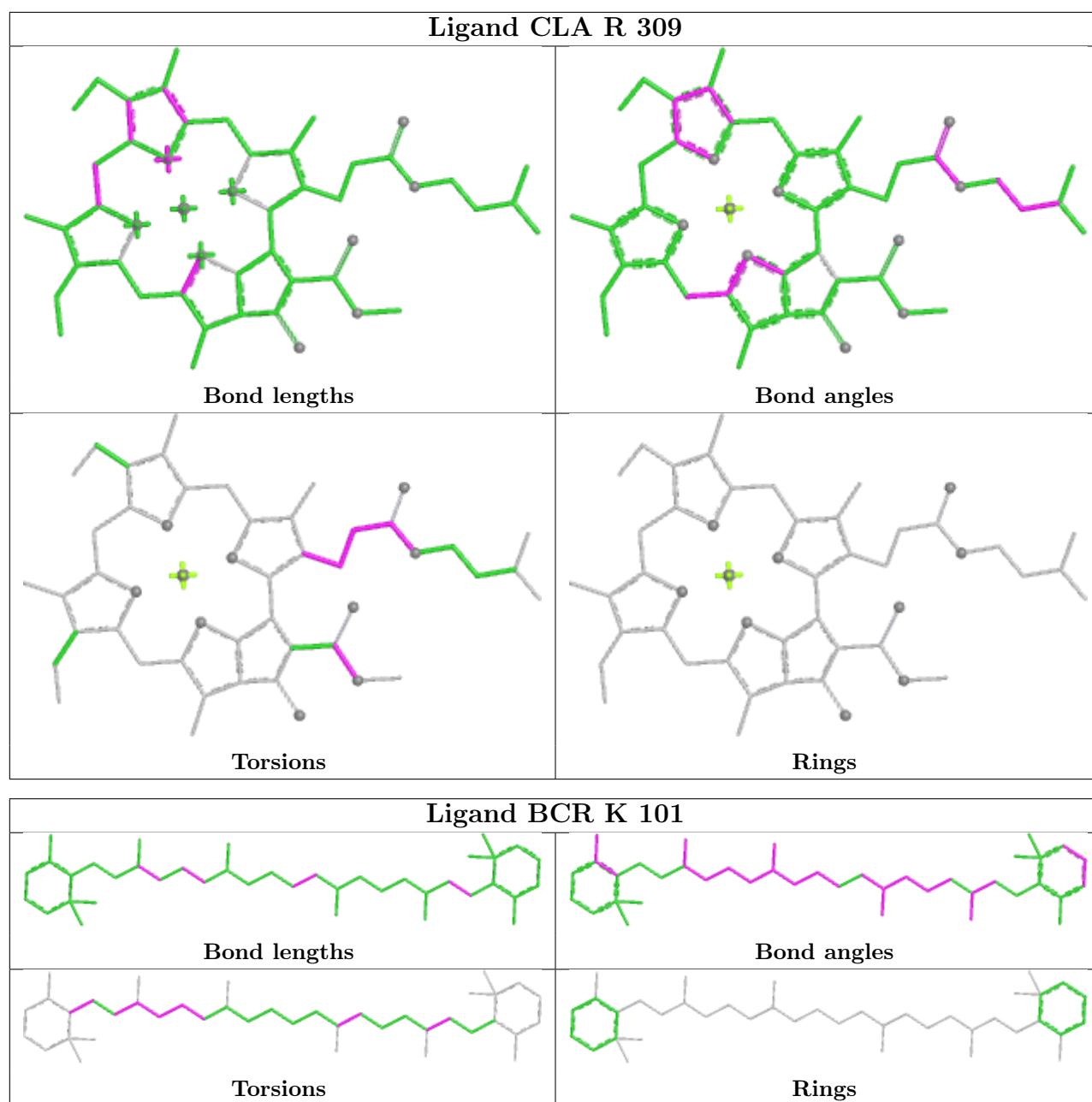


Ligand CLA R 303

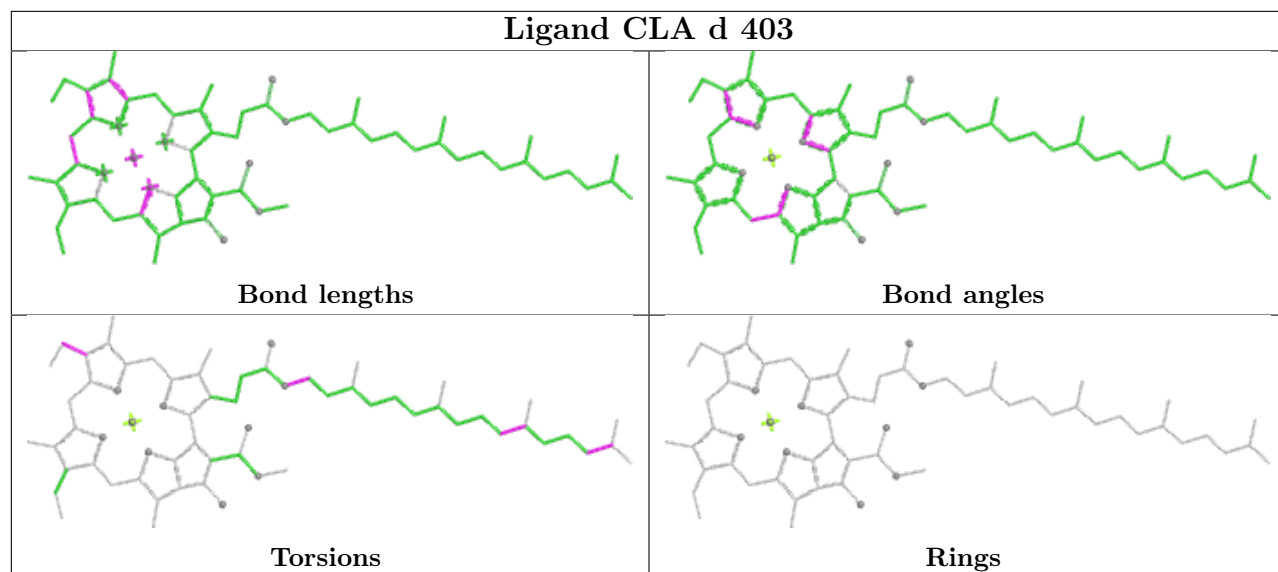




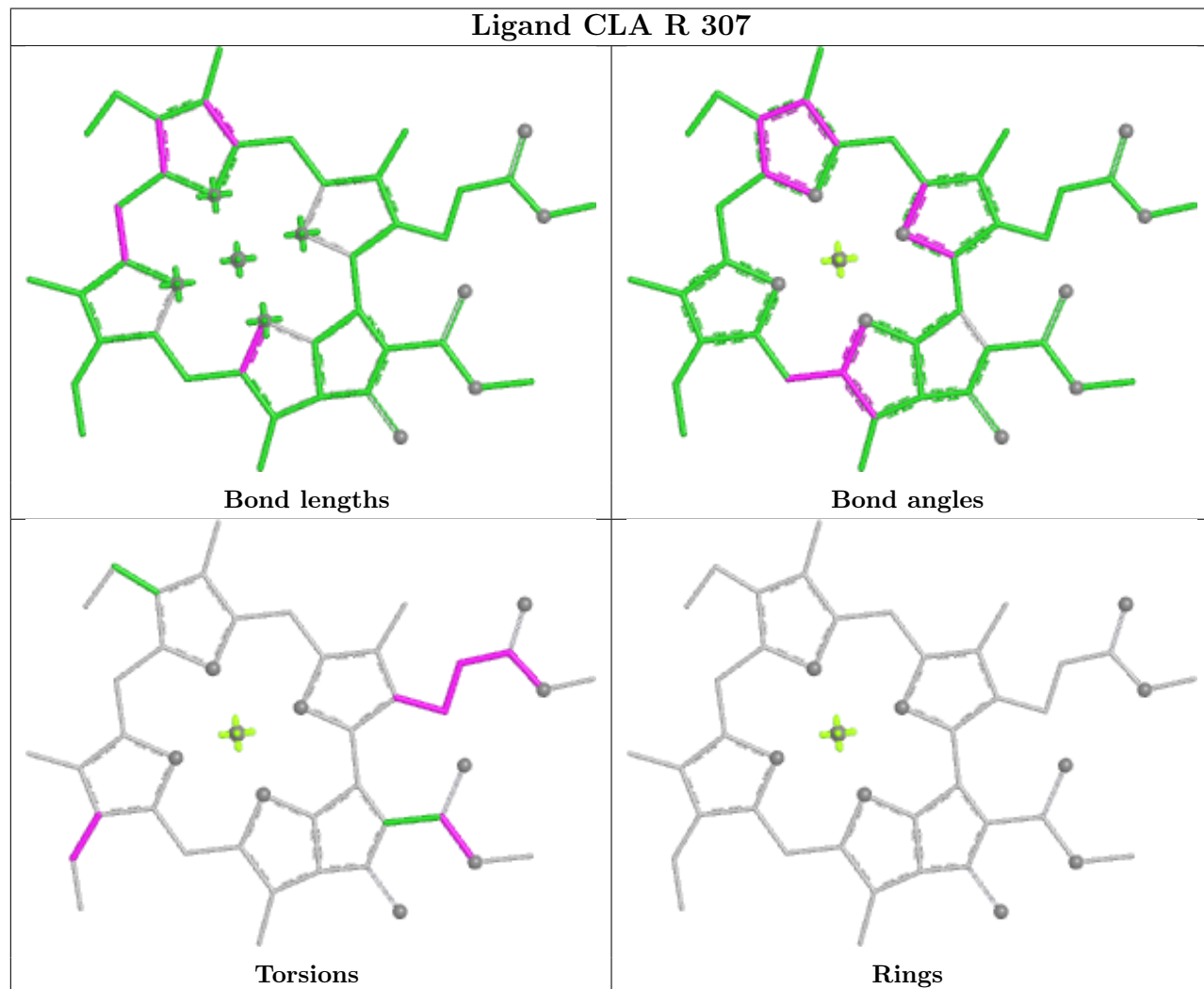


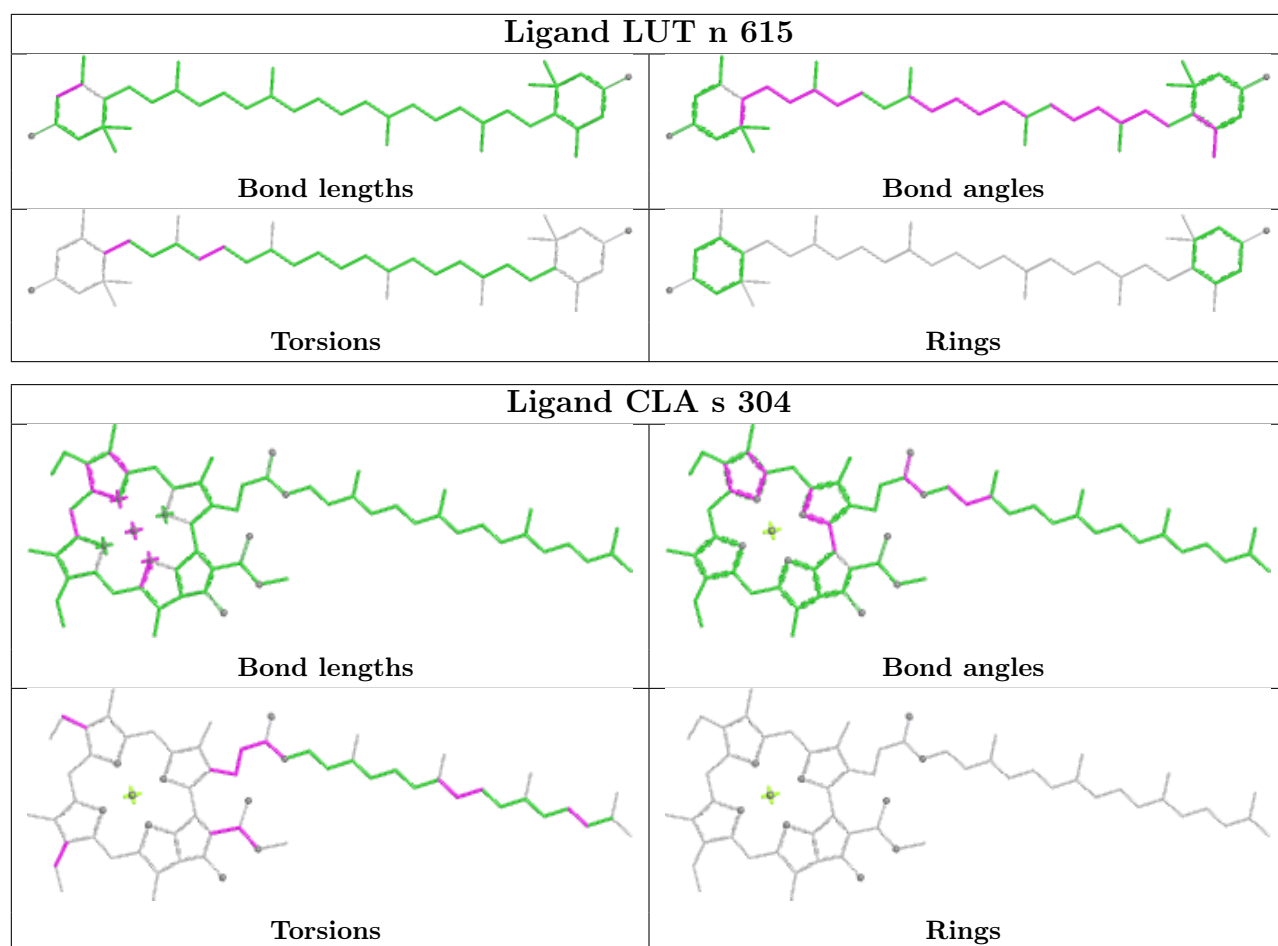


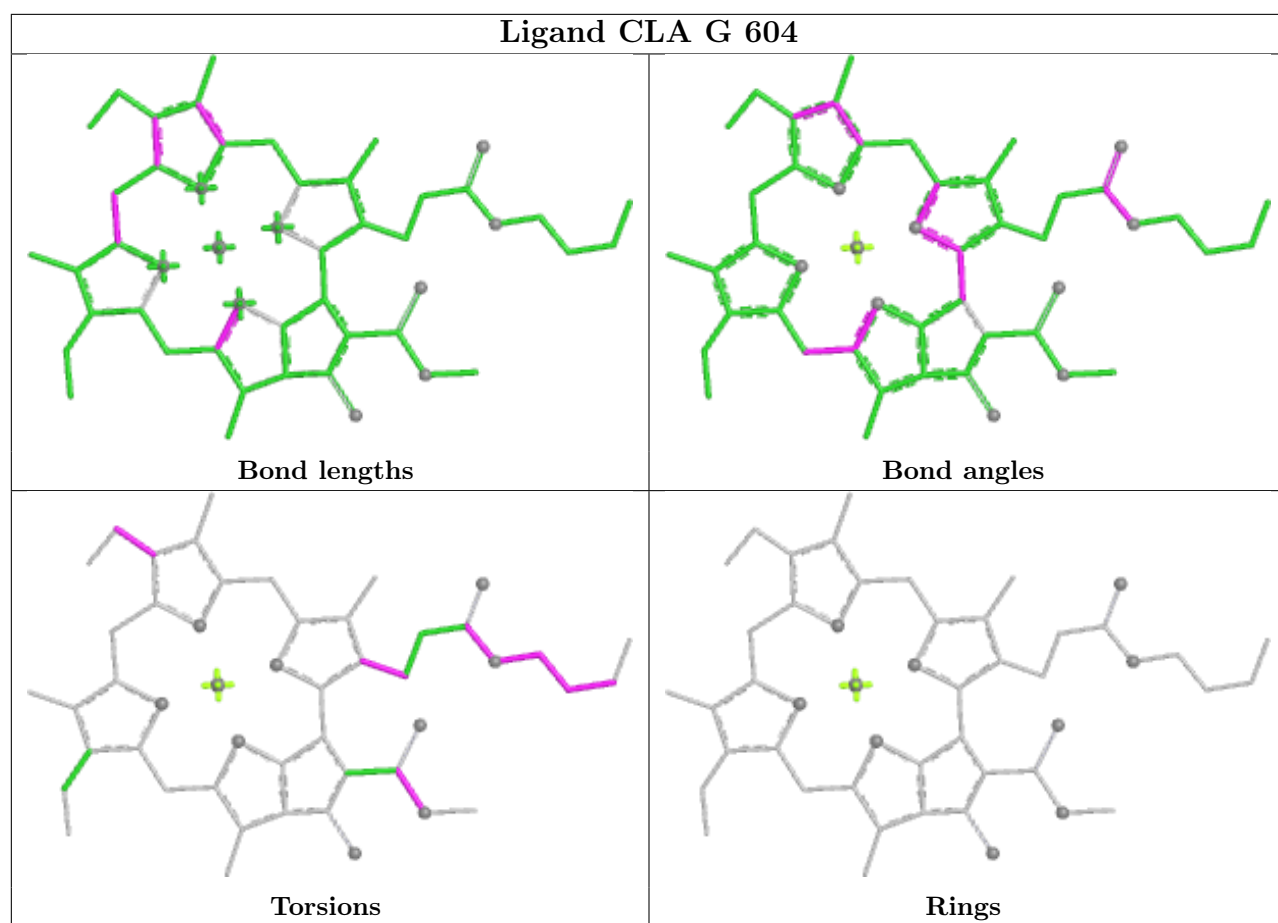
Ligand CLA d 403



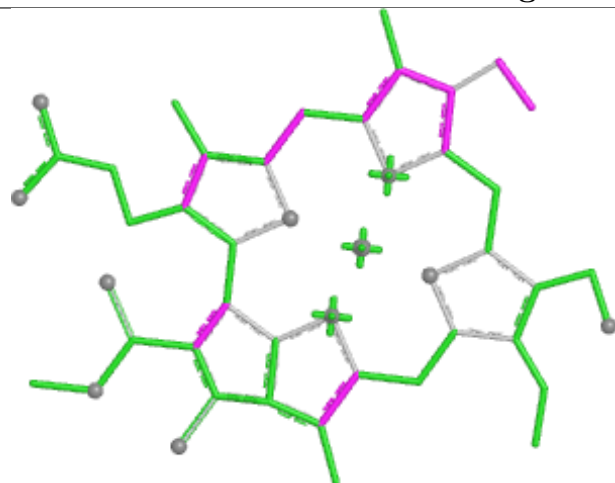
Ligand CLA R 307



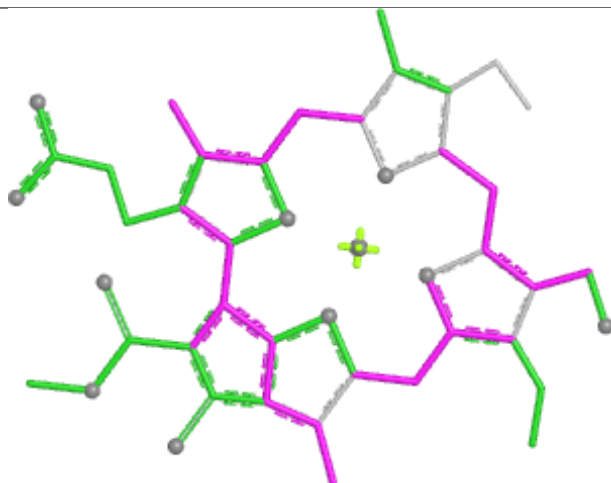




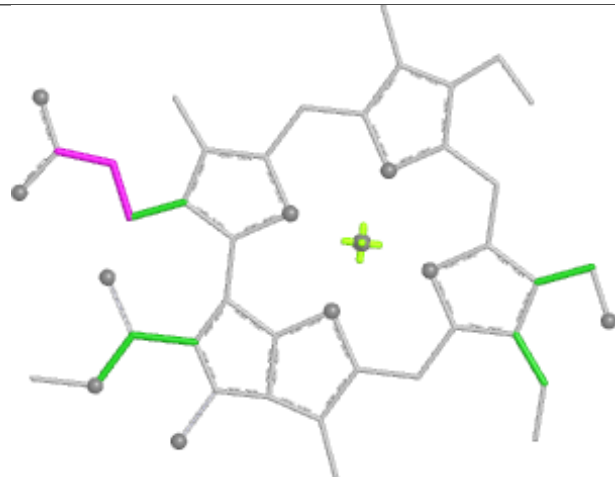
Ligand CHL S 302



Bond lengths



Bond angles

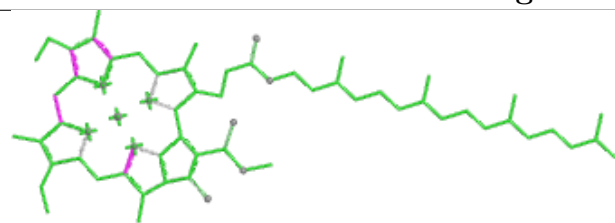


Torsions

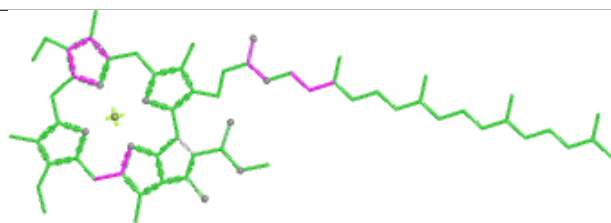


Rings

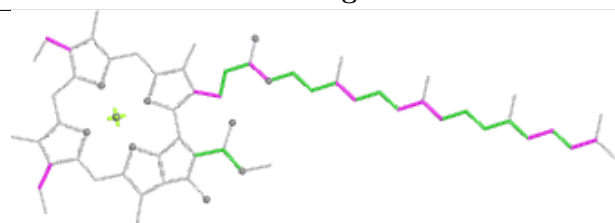
Ligand CLA Y 304



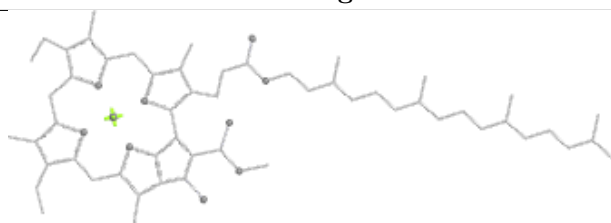
Bond lengths



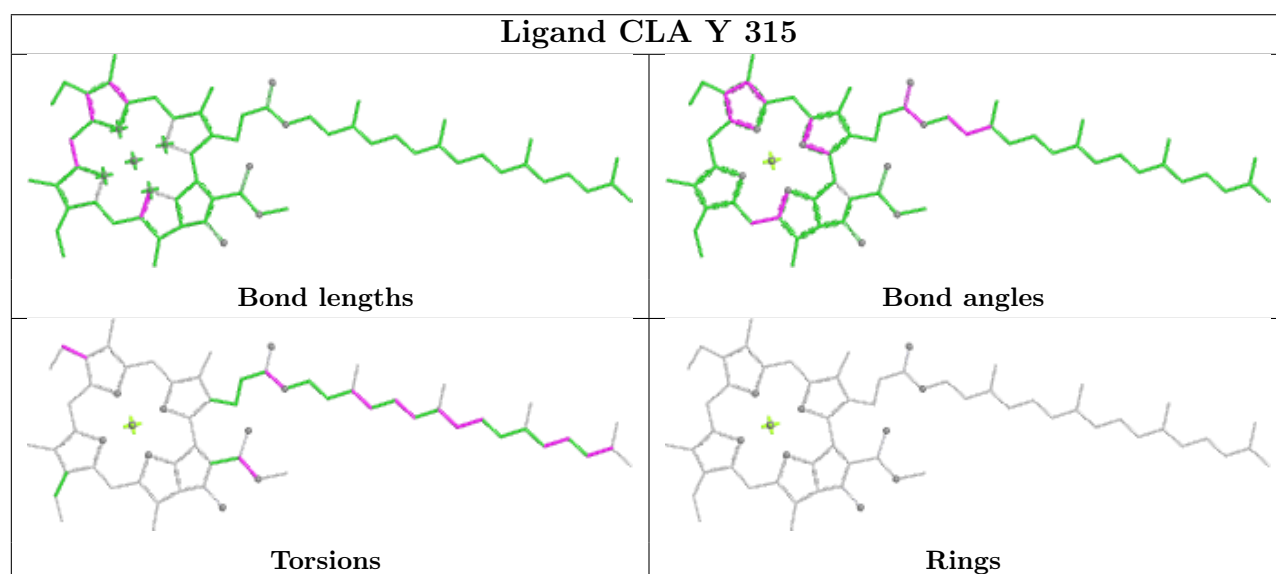
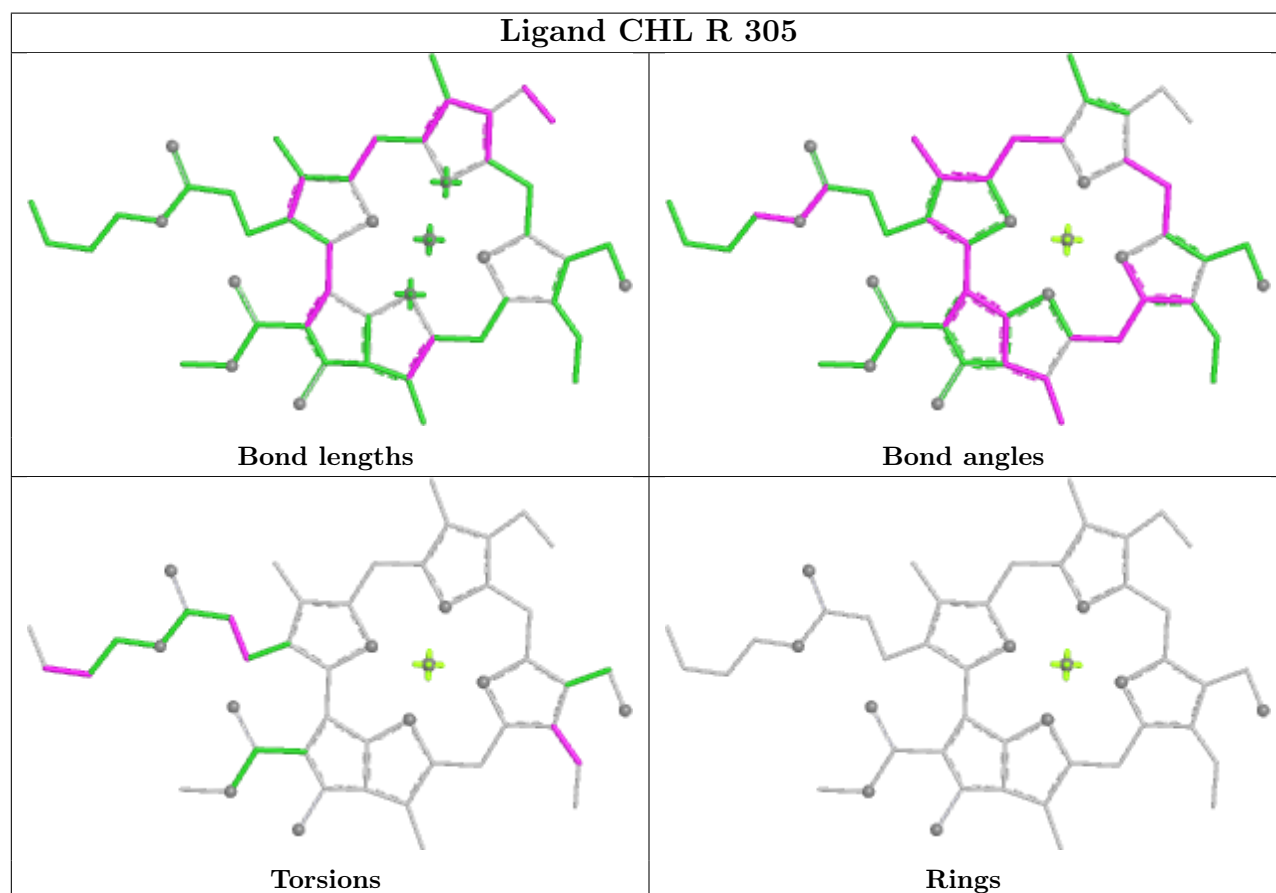
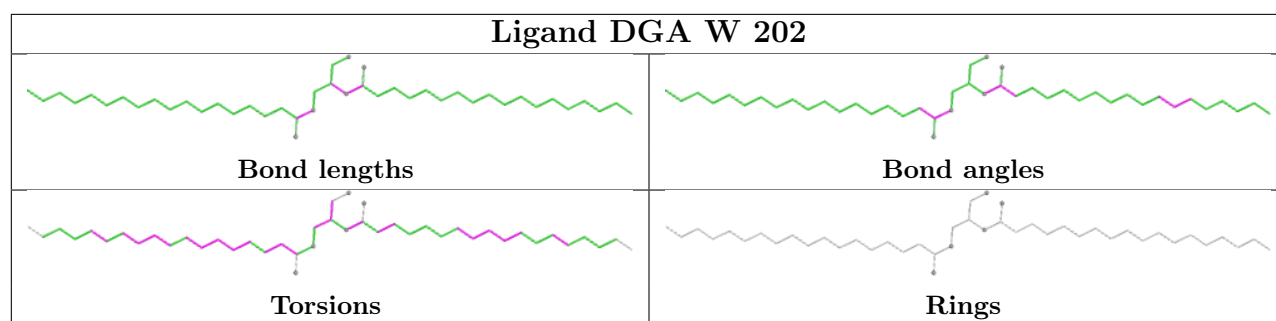
Bond angles

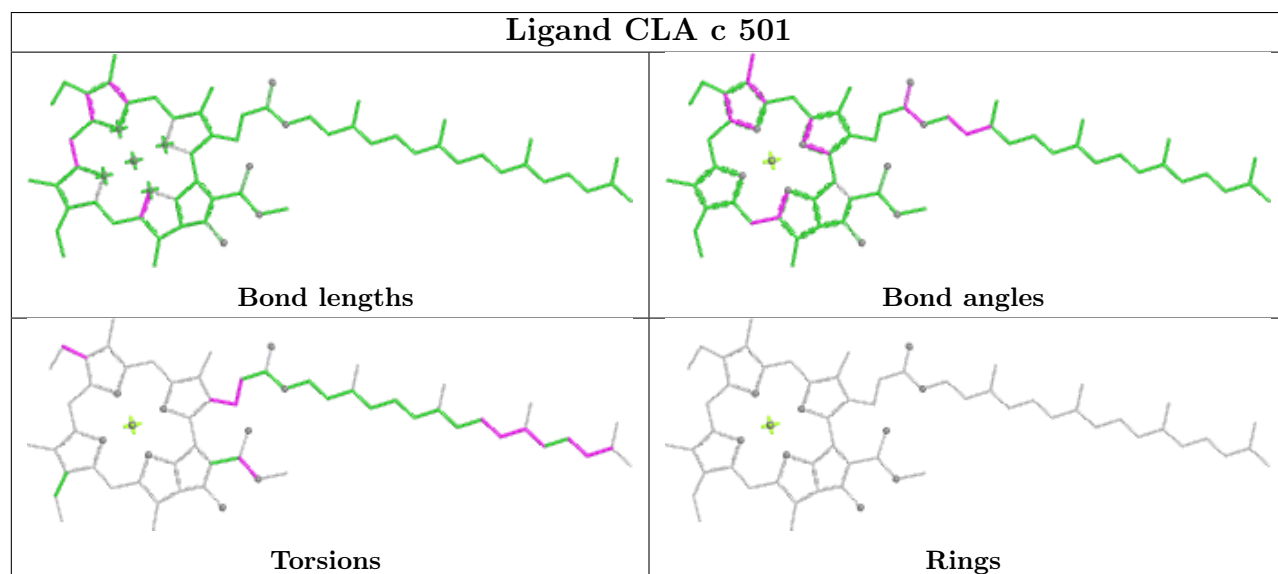
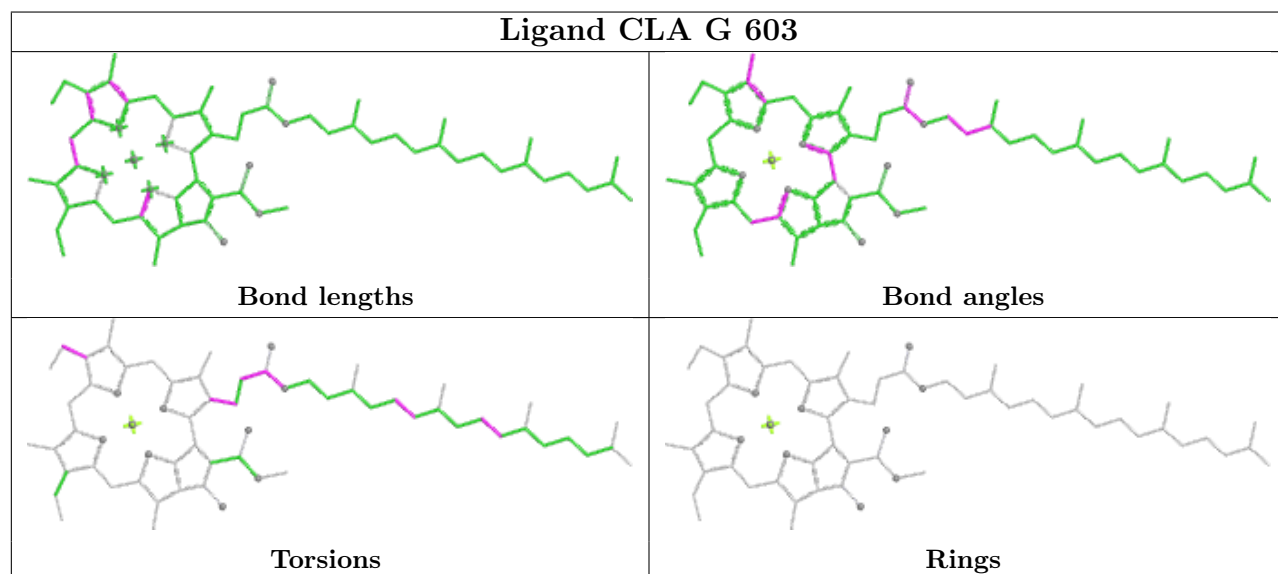
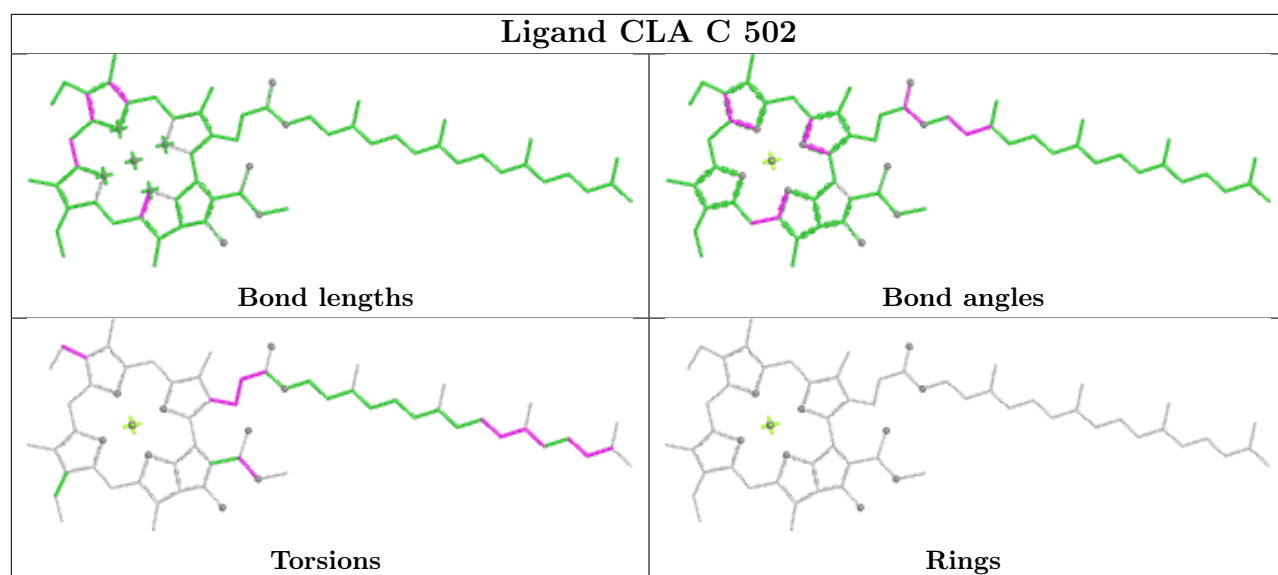


Torsions

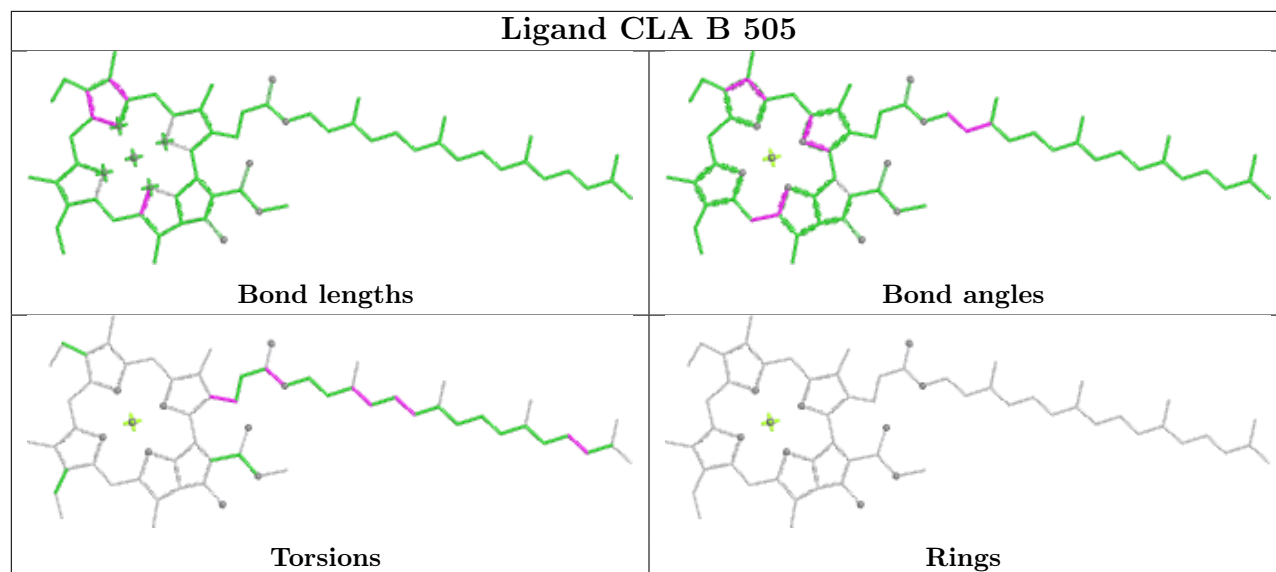


Rings

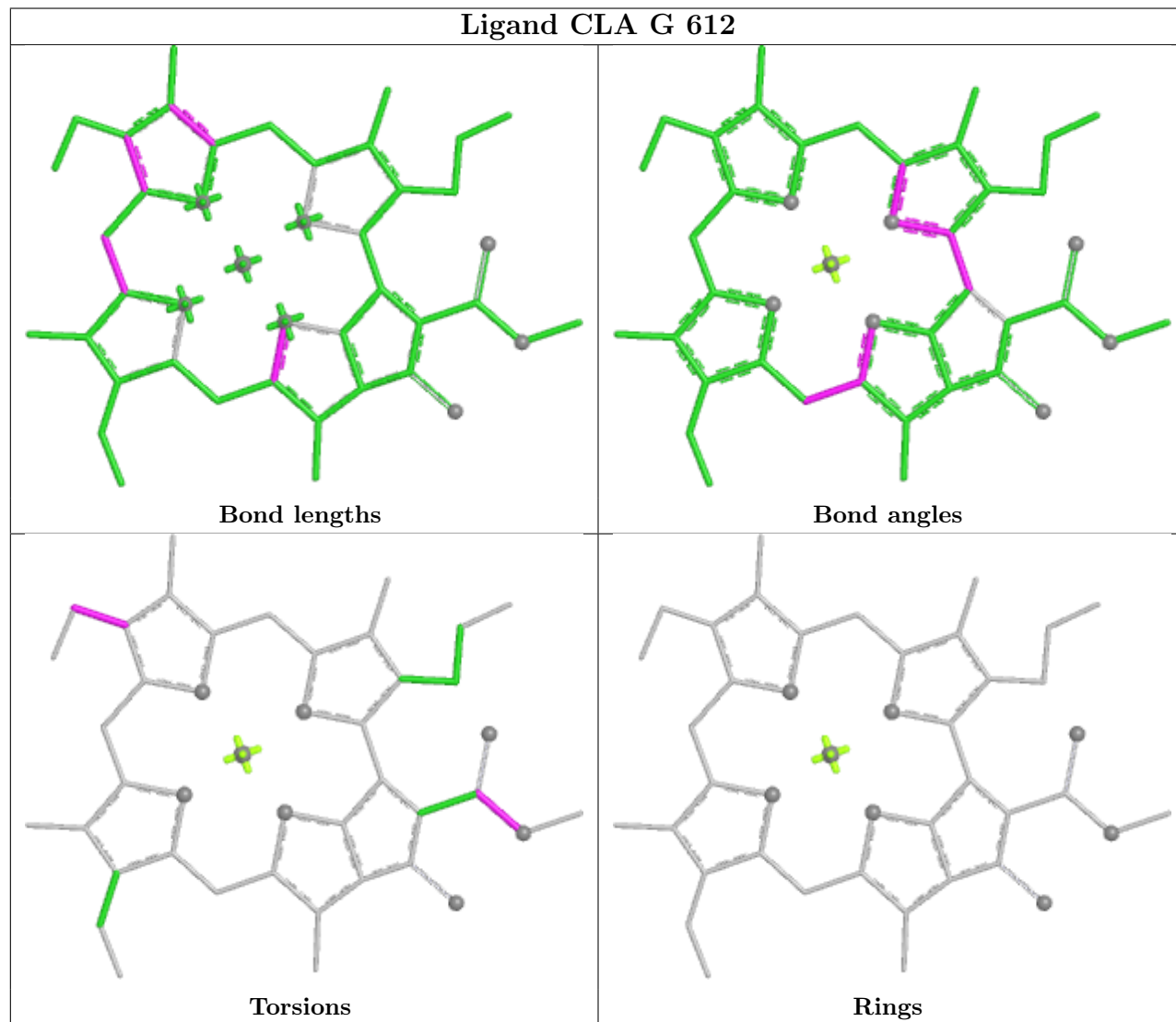


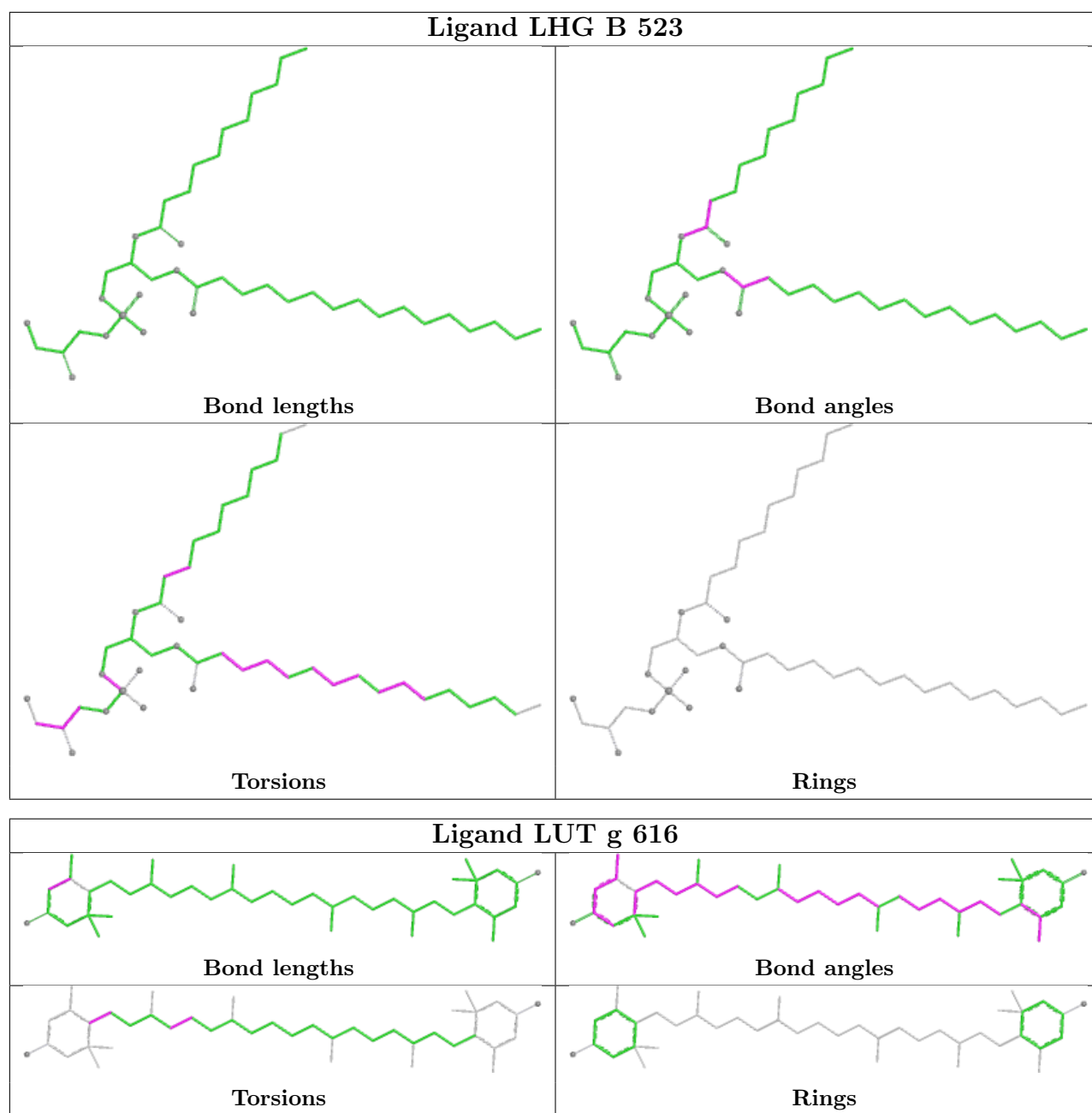


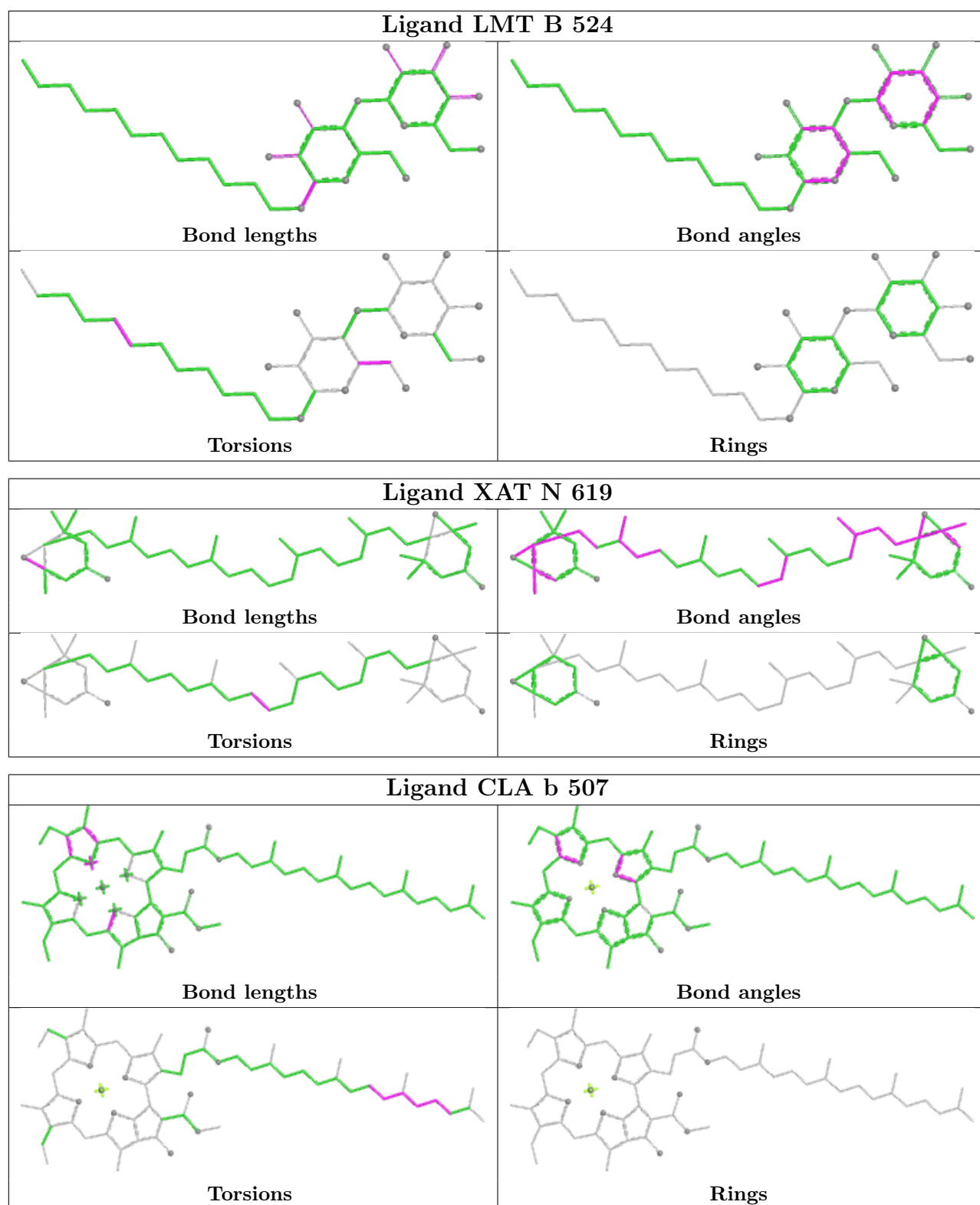
Ligand CLA B 505

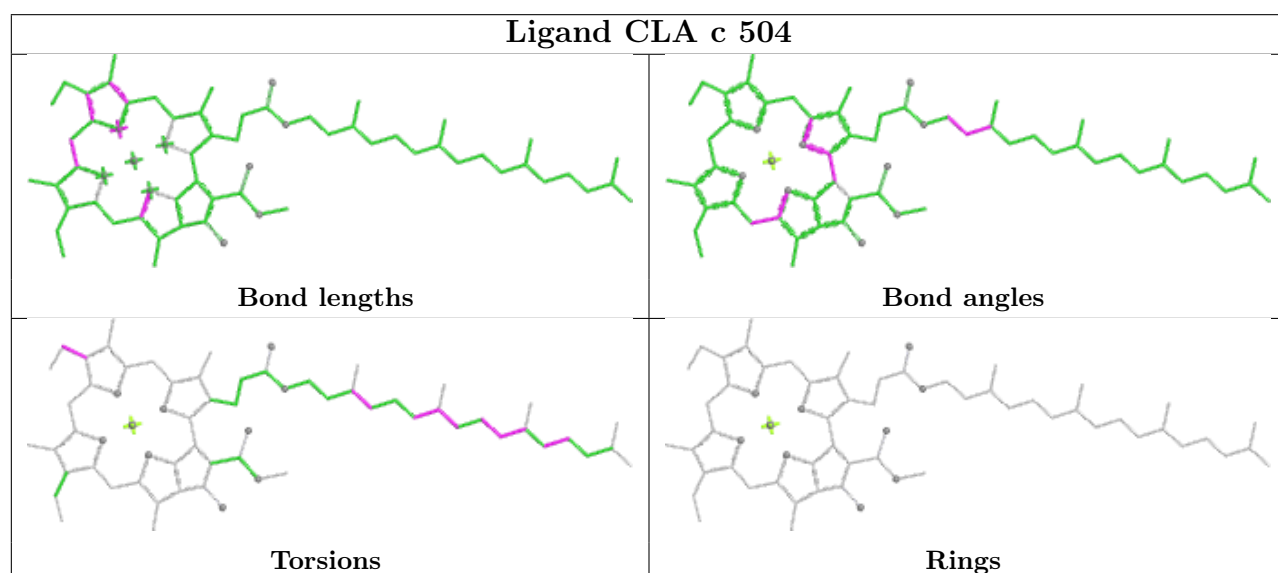
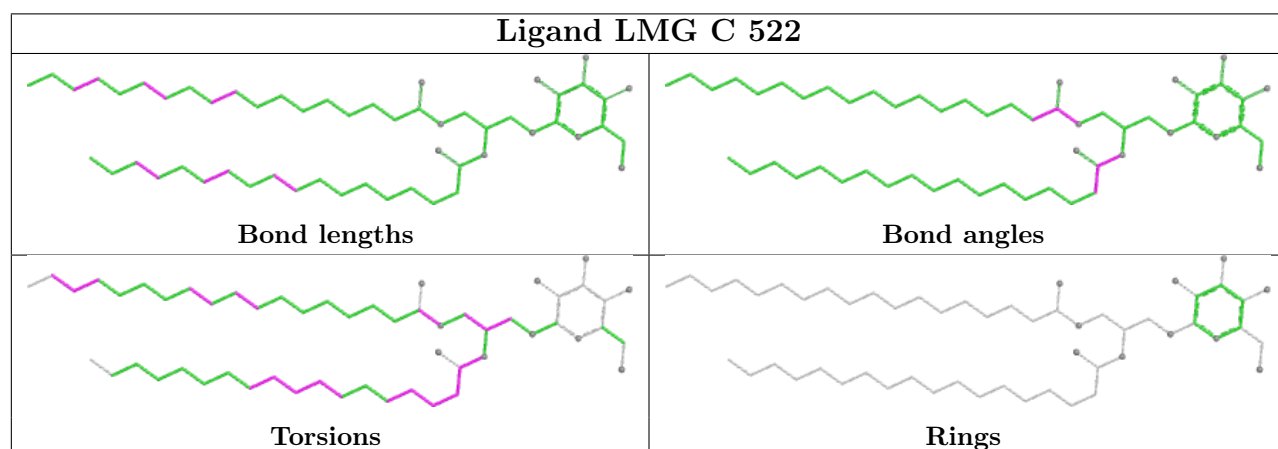
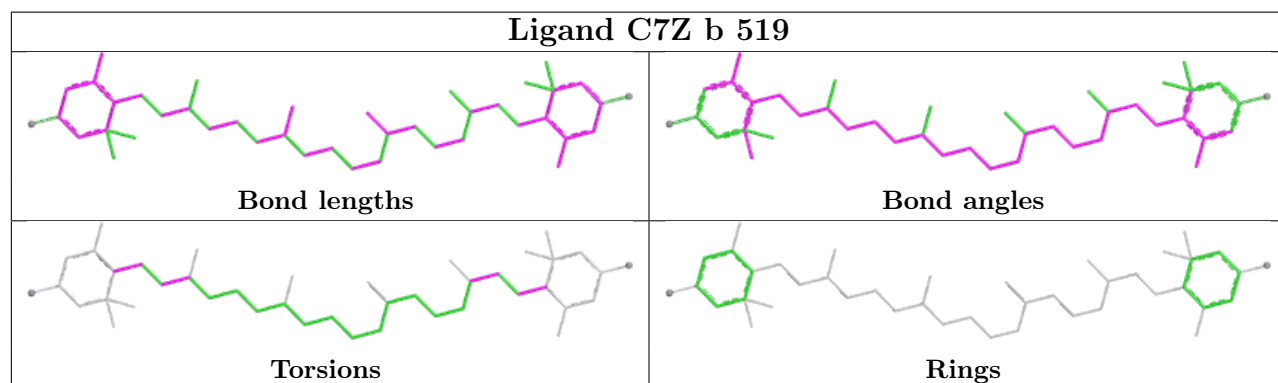
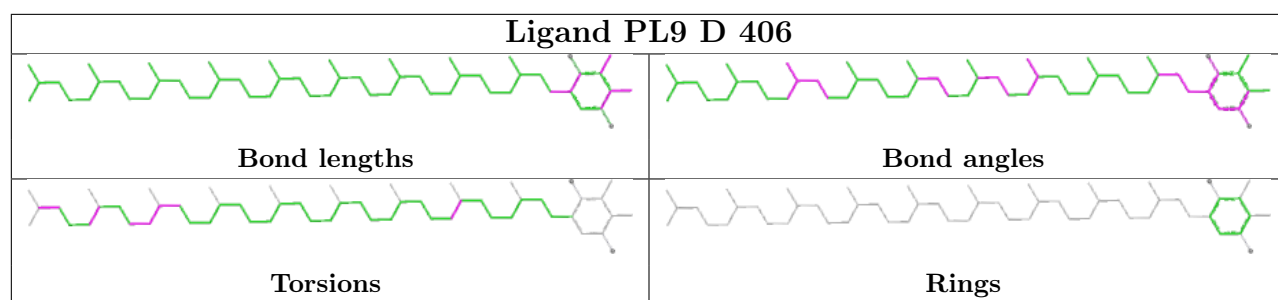


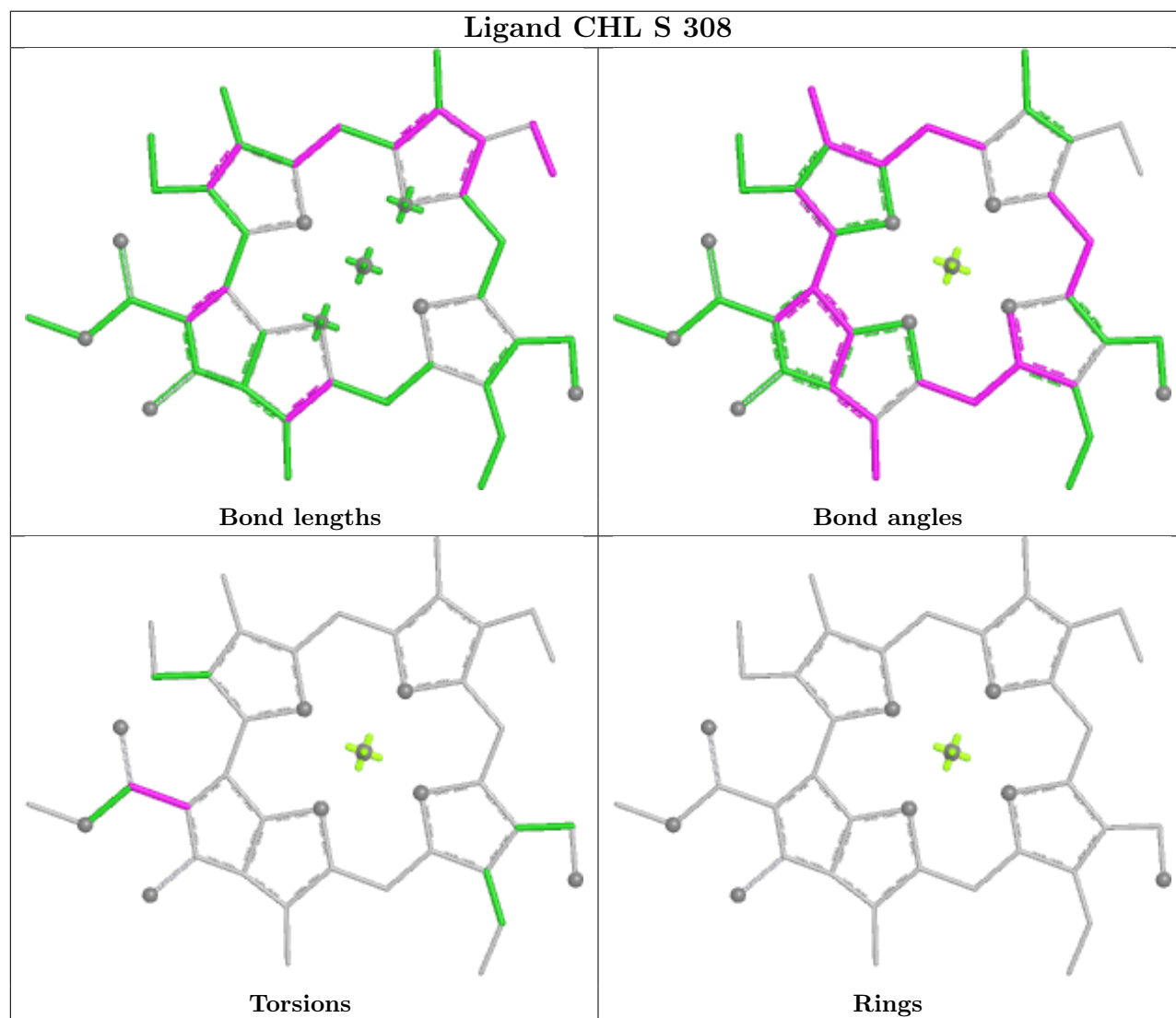
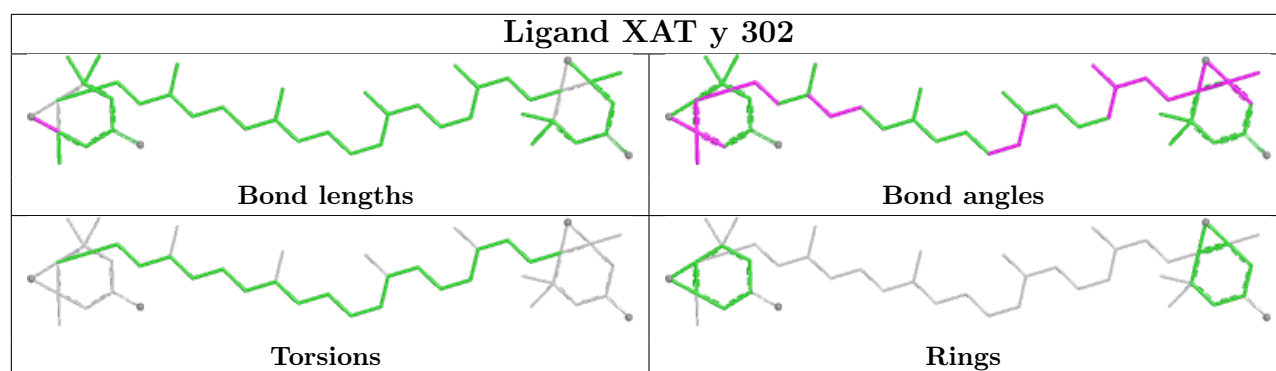
Ligand CLA G 612

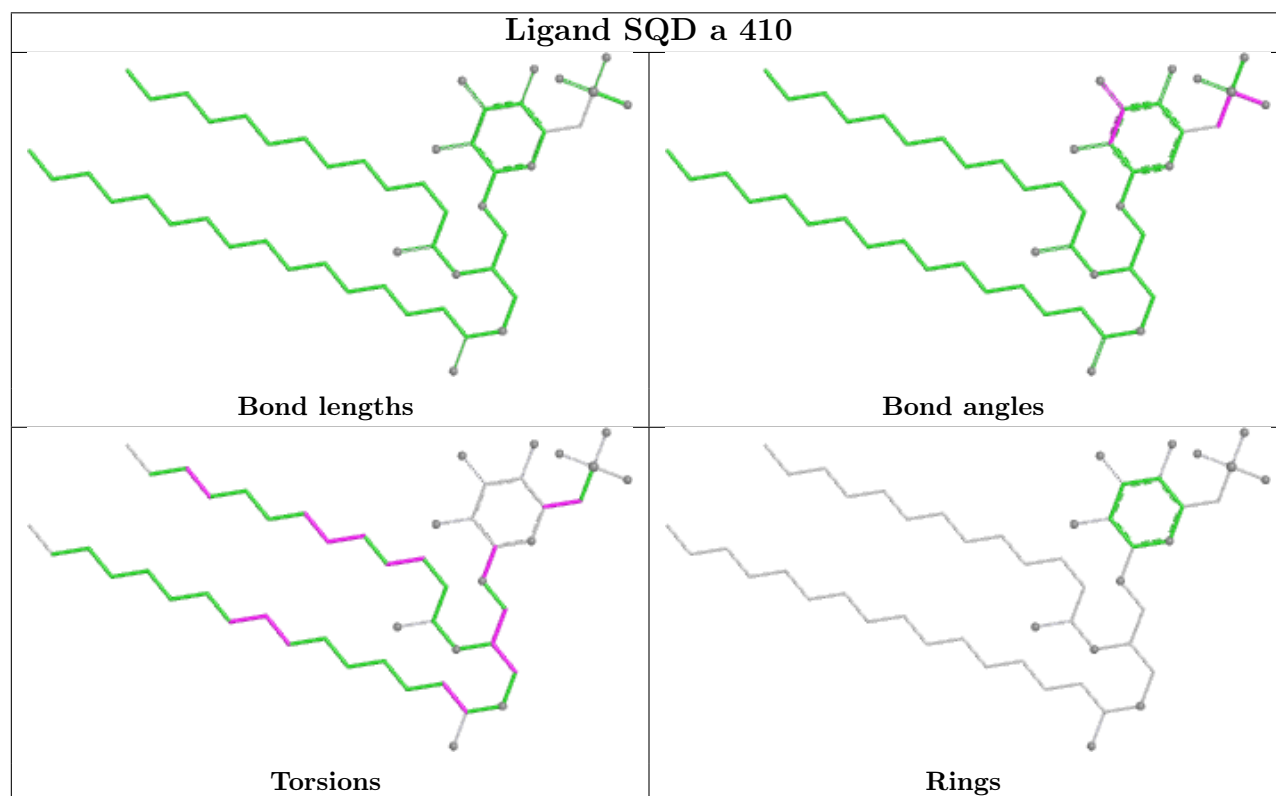
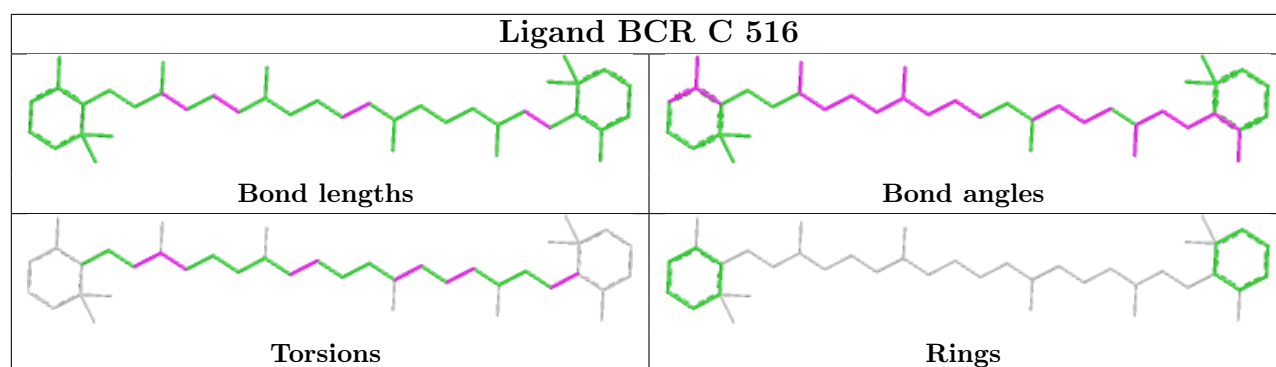


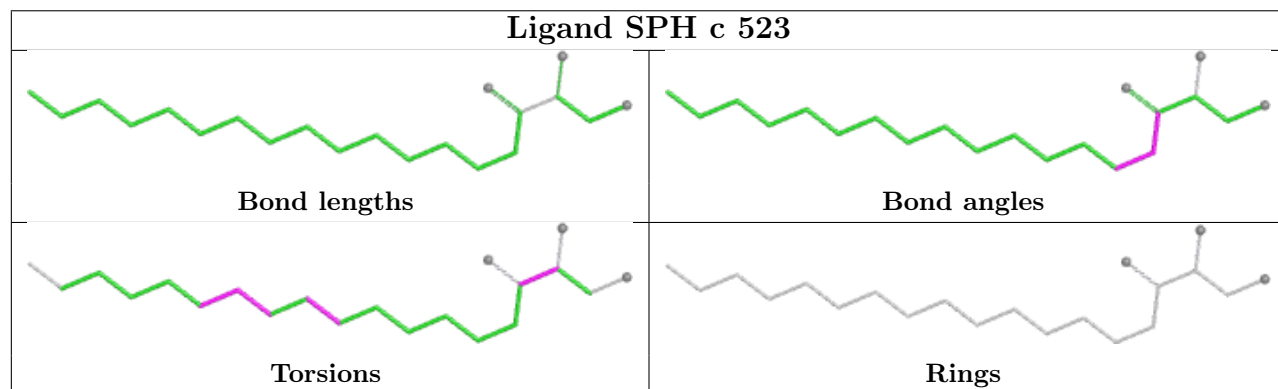
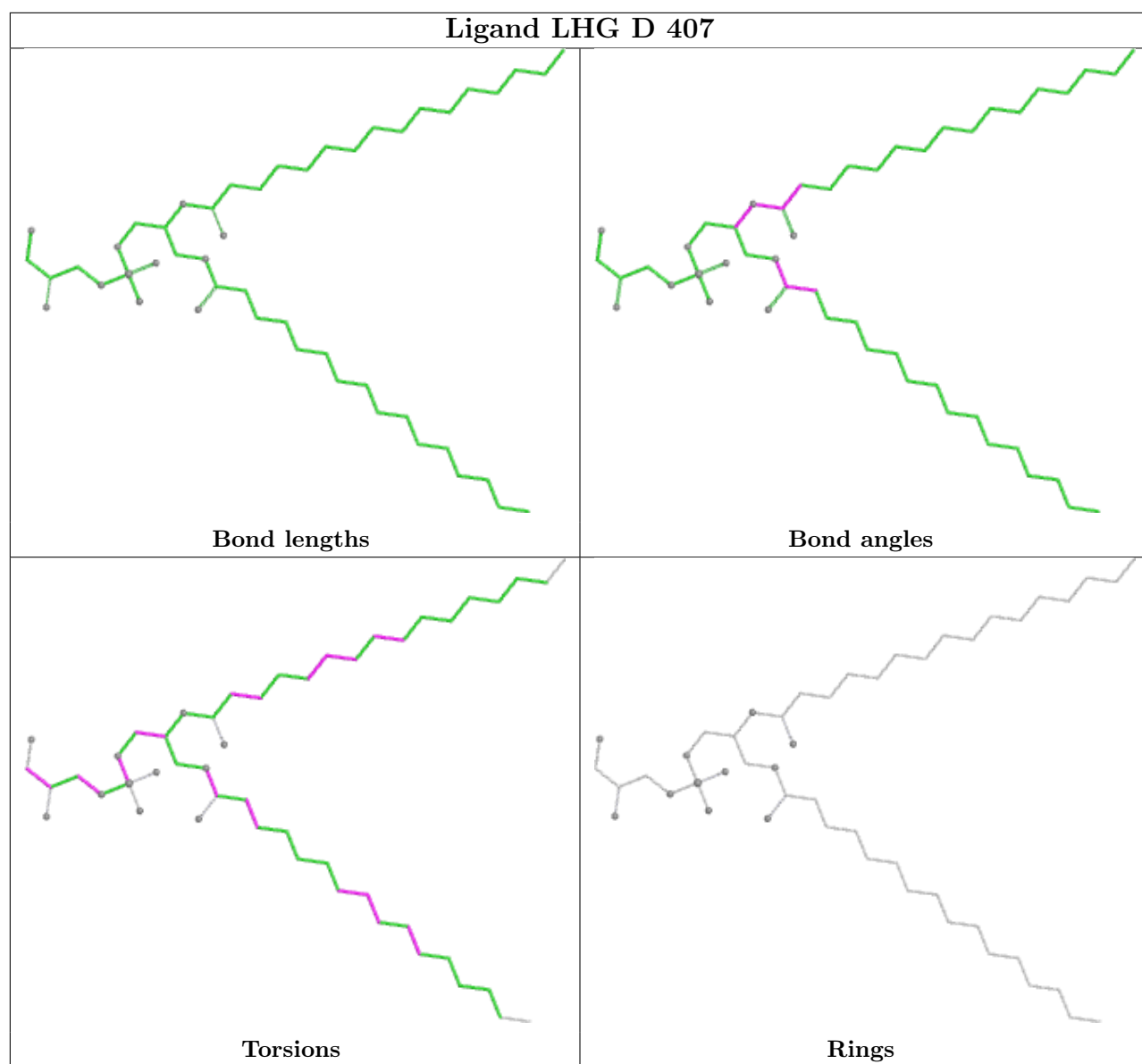




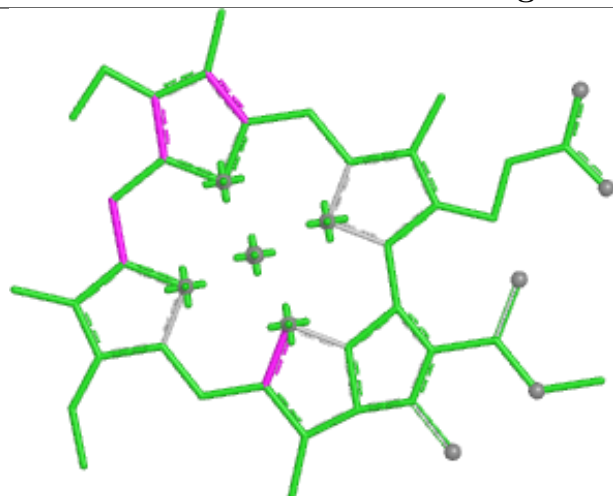




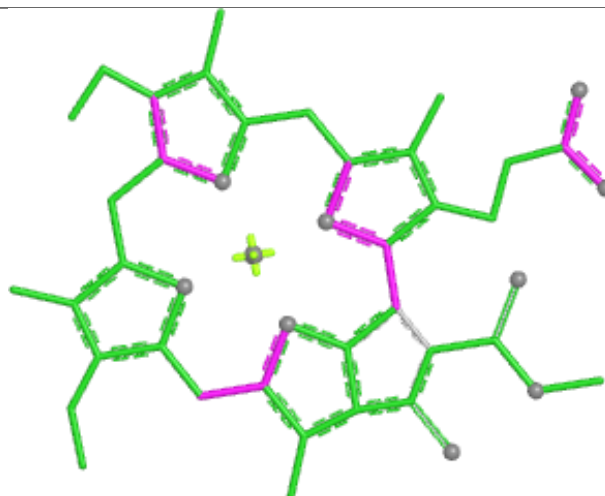




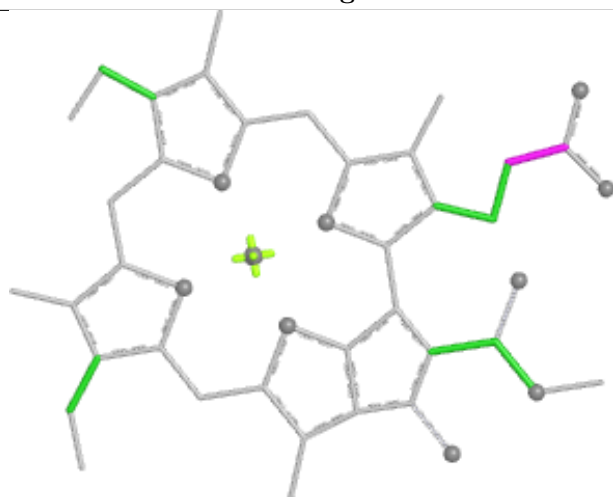
Ligand CLA S 313



Bond lengths



Bond angles

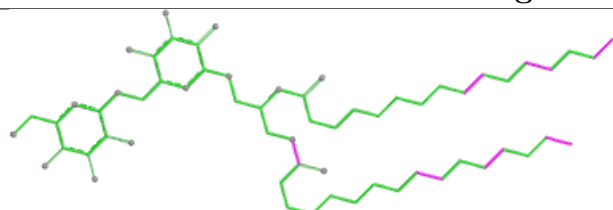


Torsions

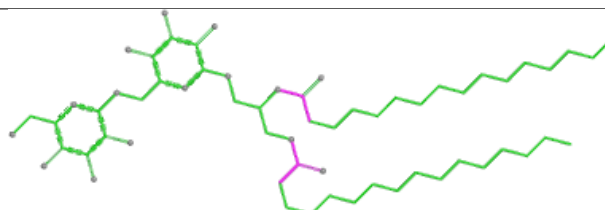


Rings

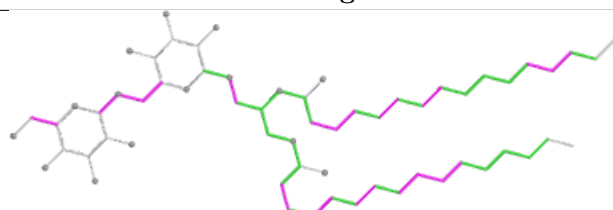
Ligand DGD c 517



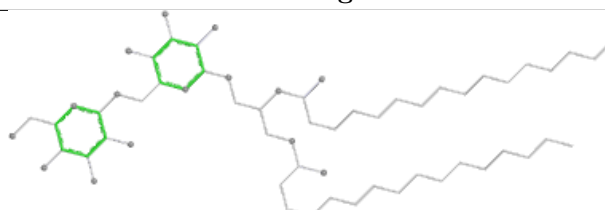
Bond lengths



Bond angles

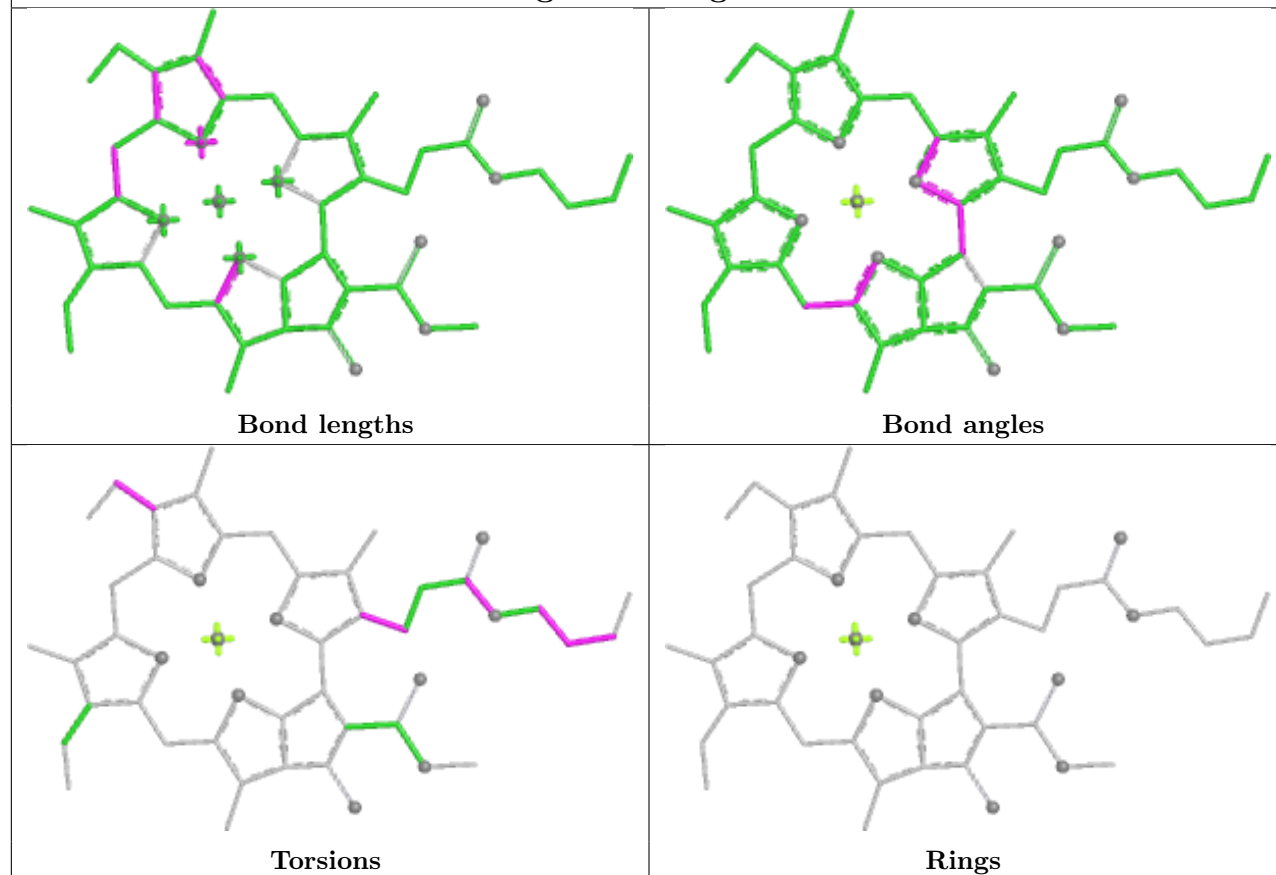


Torsions

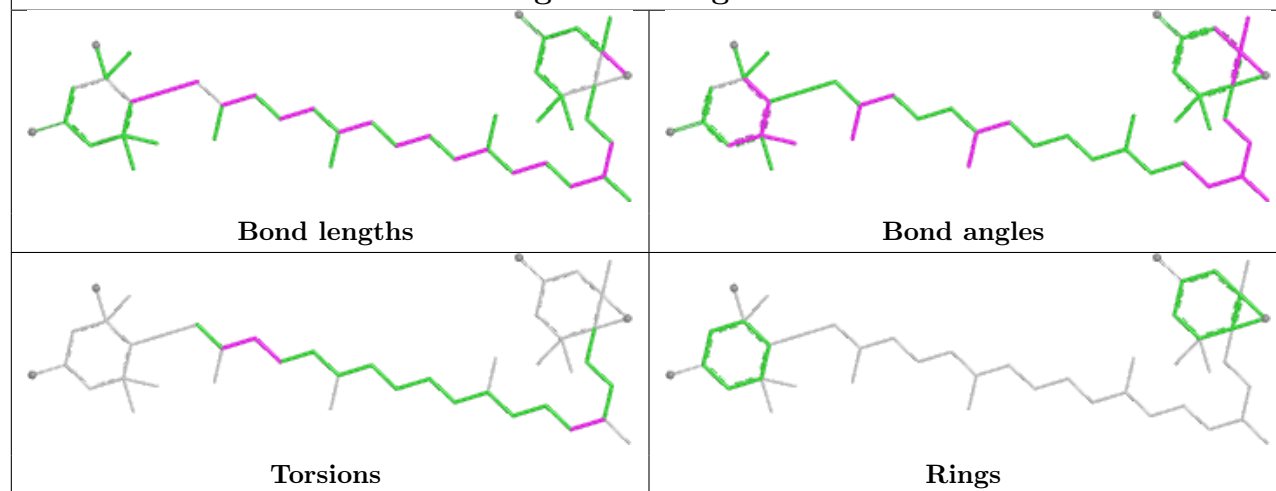


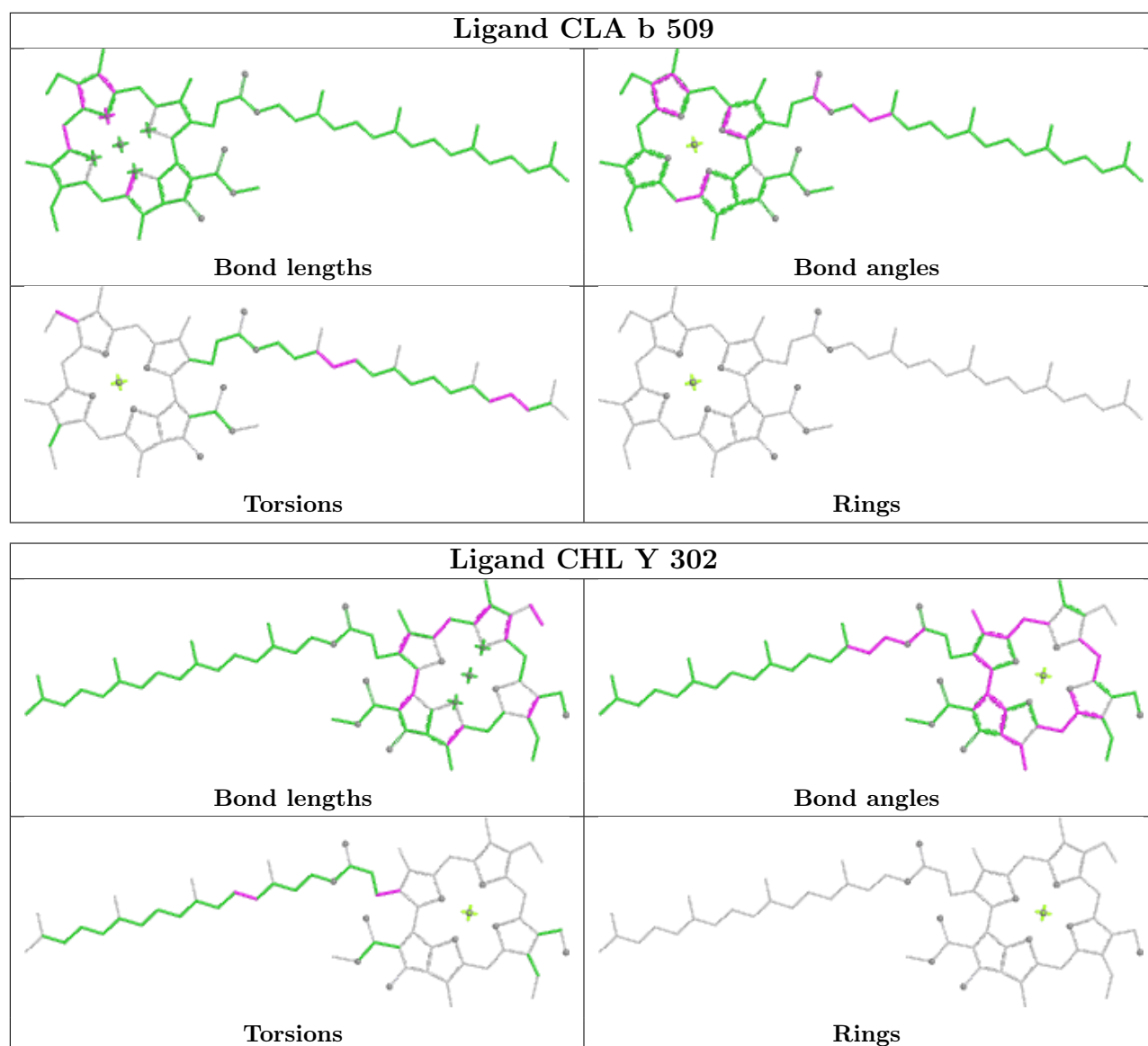
Rings

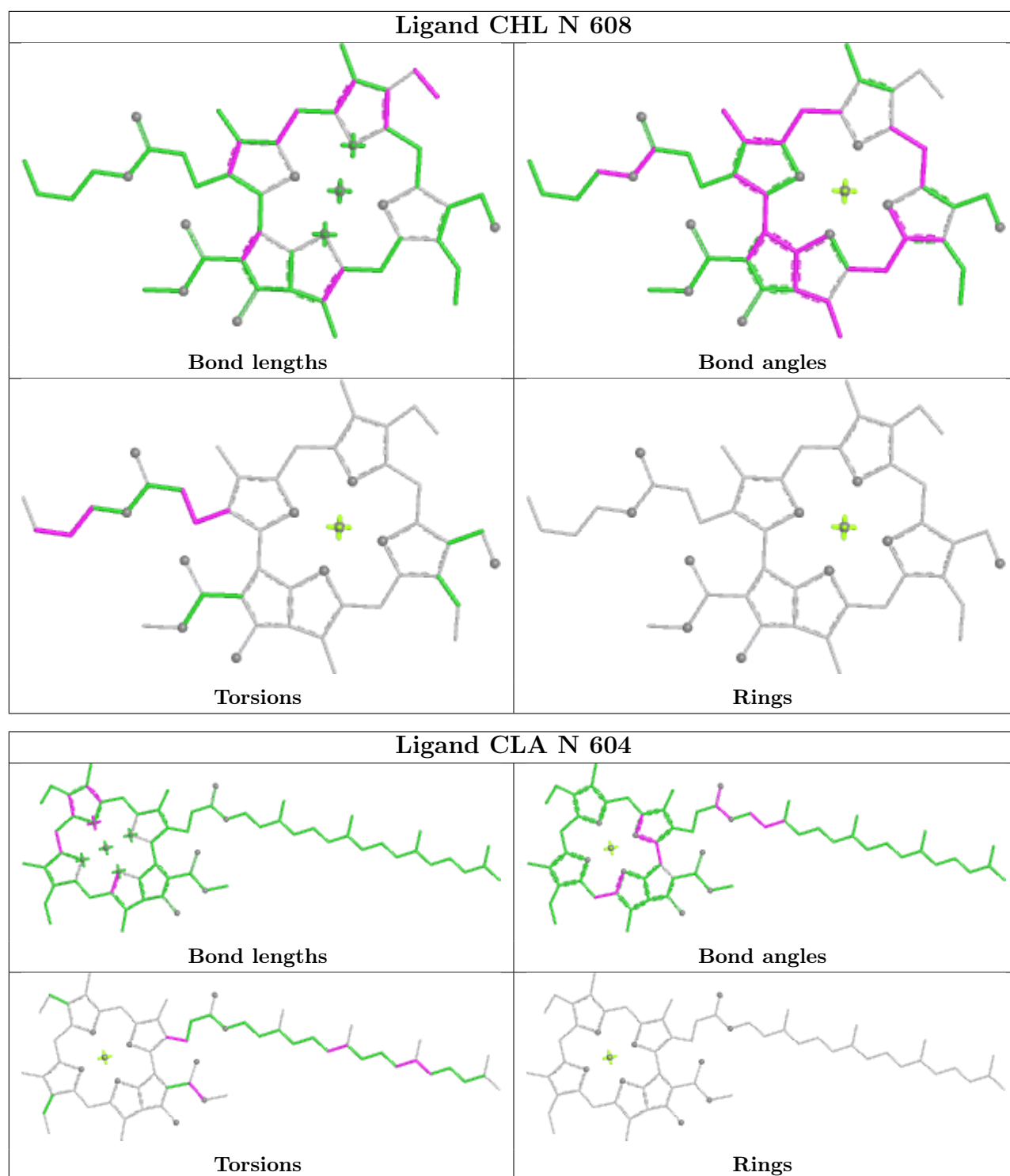
Ligand CLA g 604

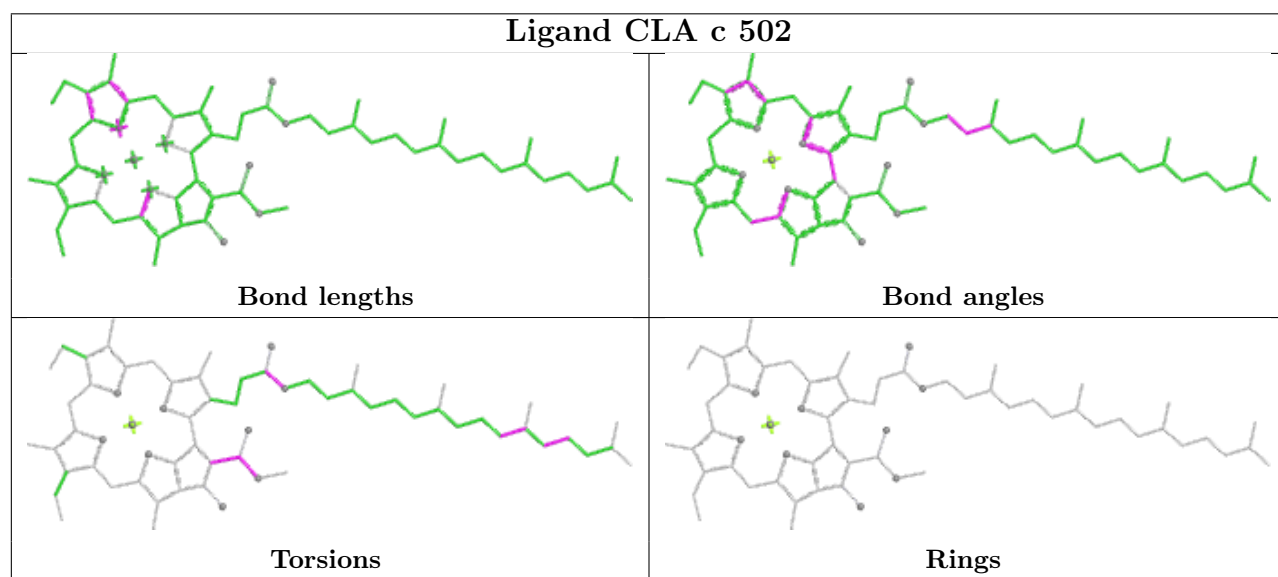
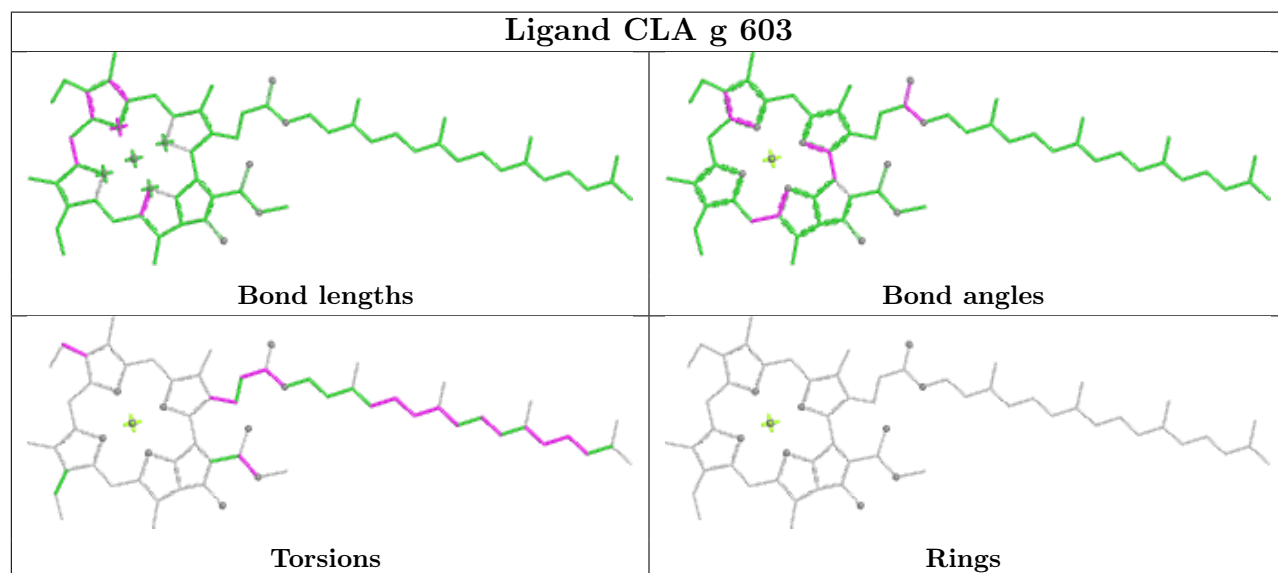
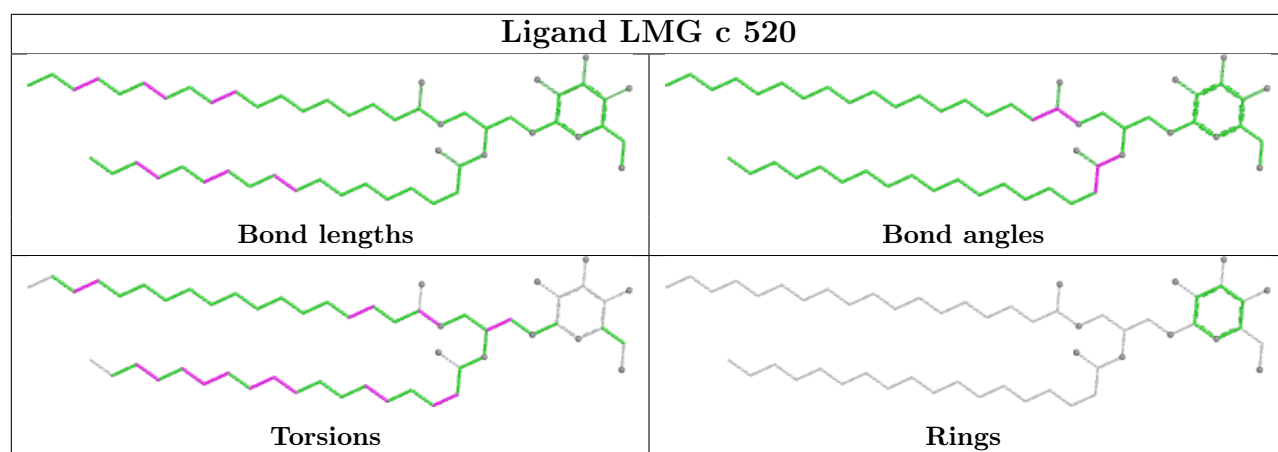


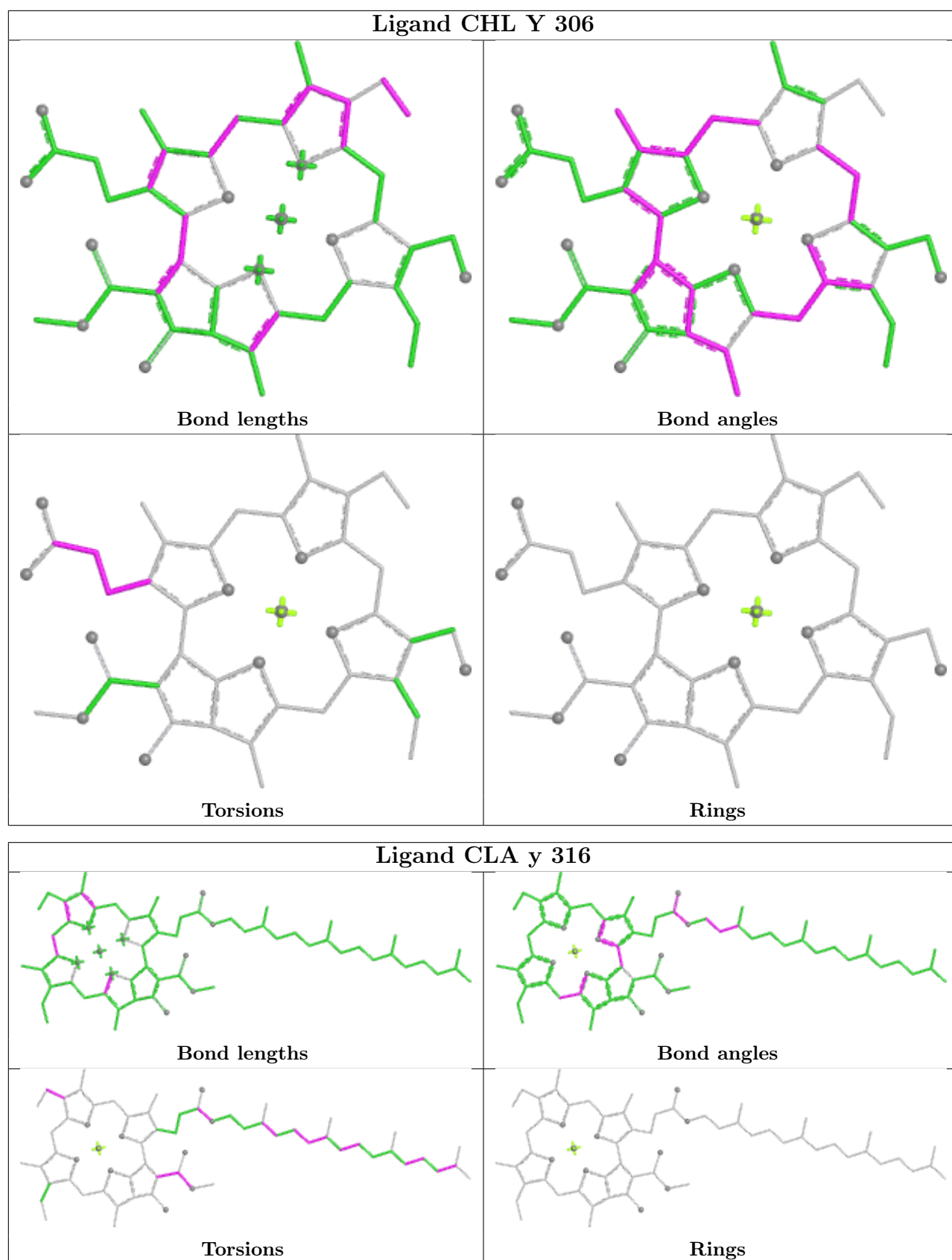
Ligand NEX g 617

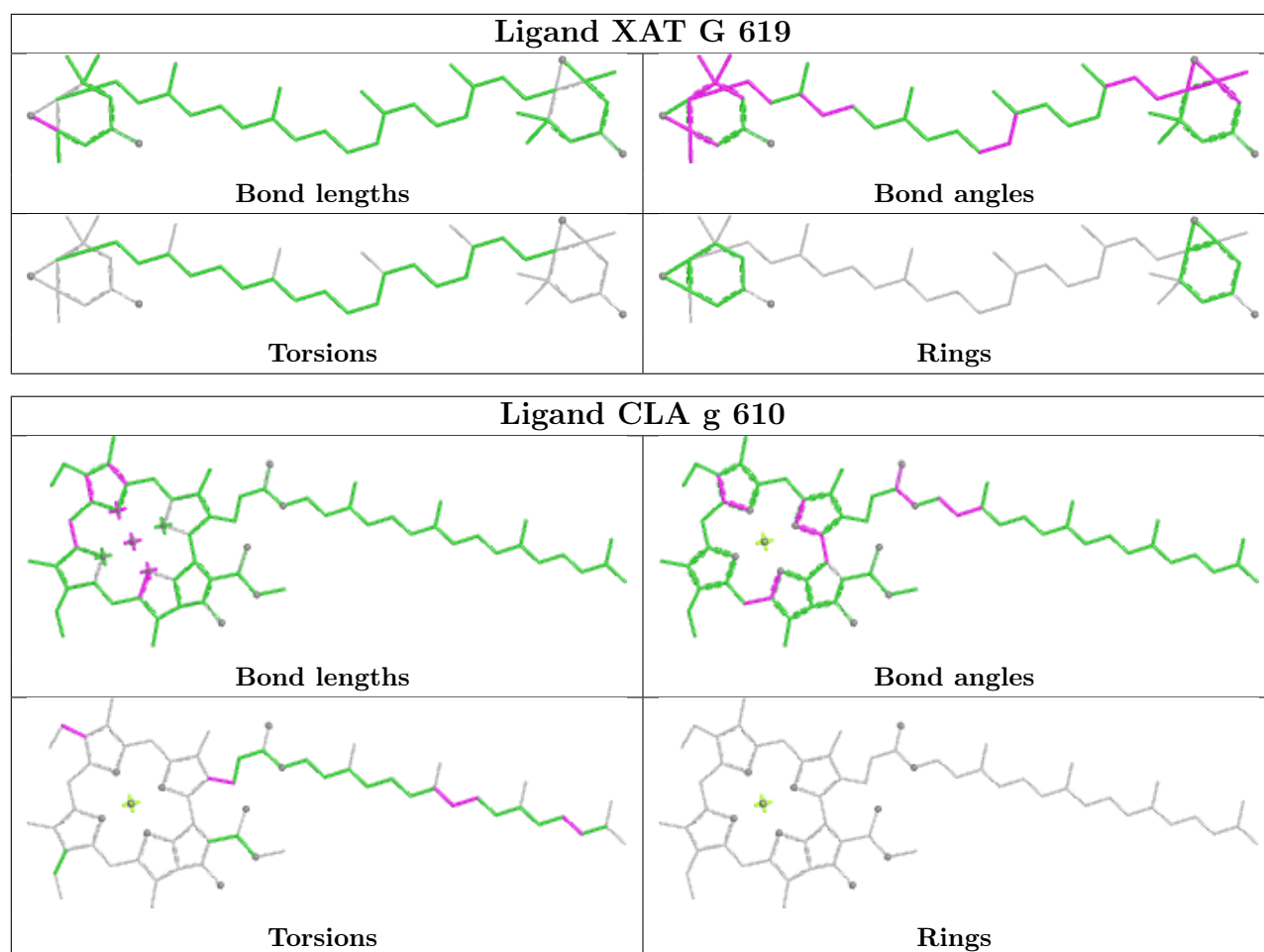


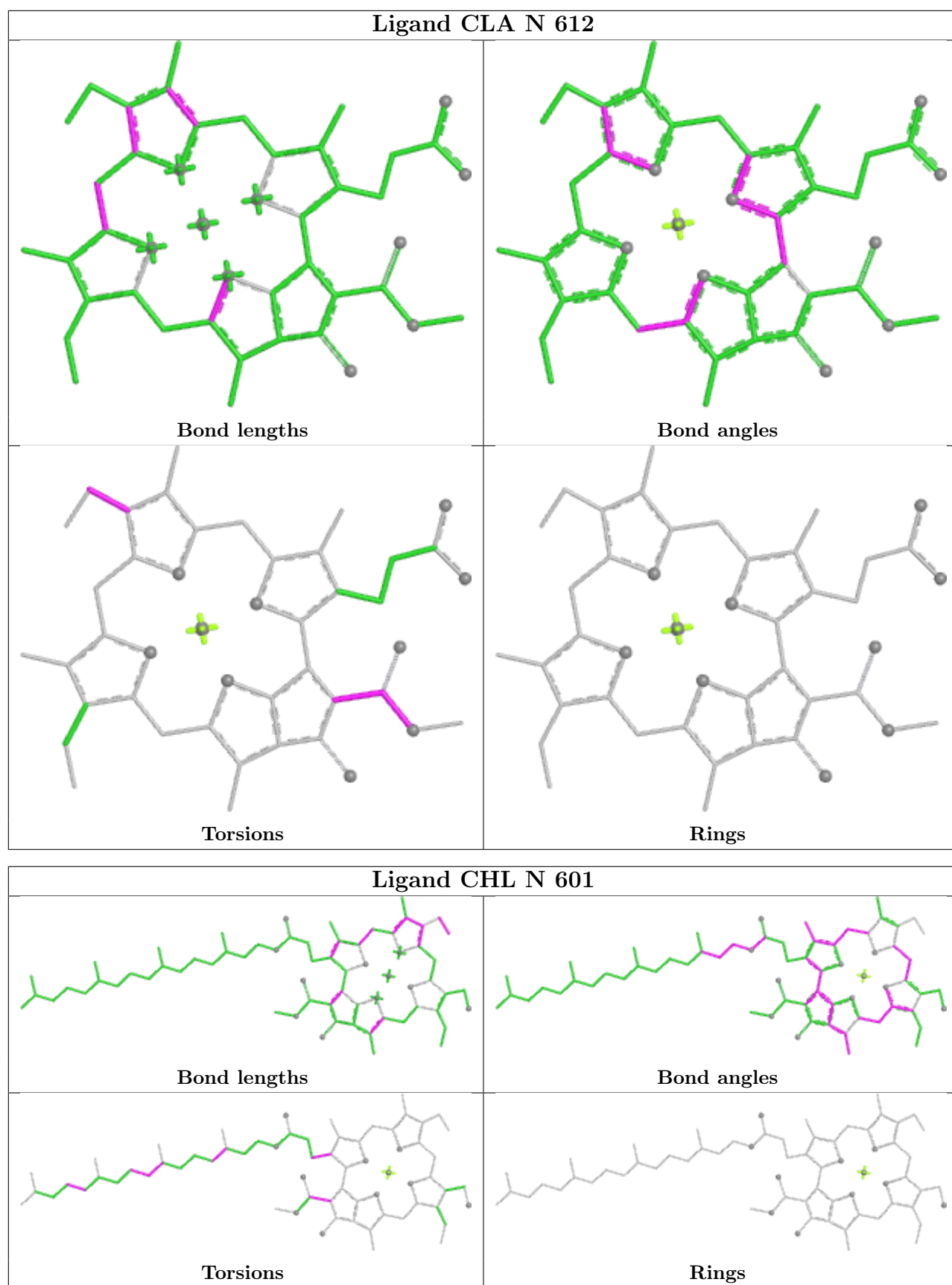


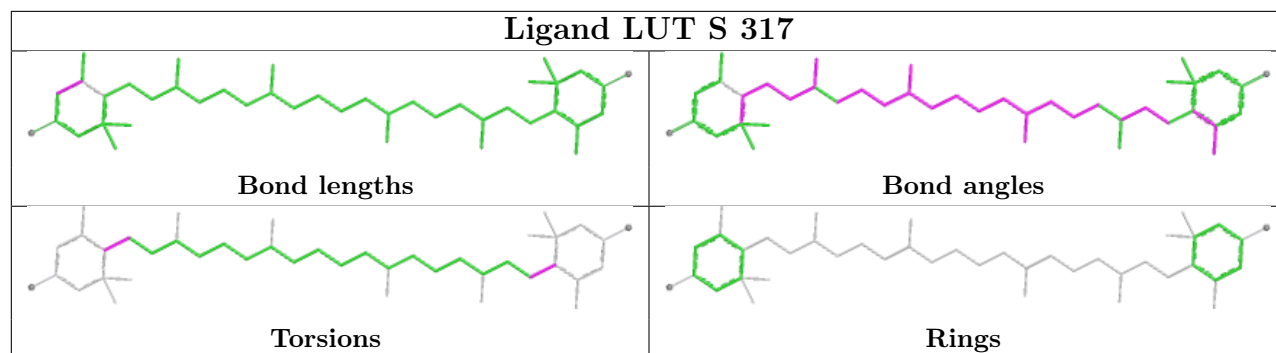
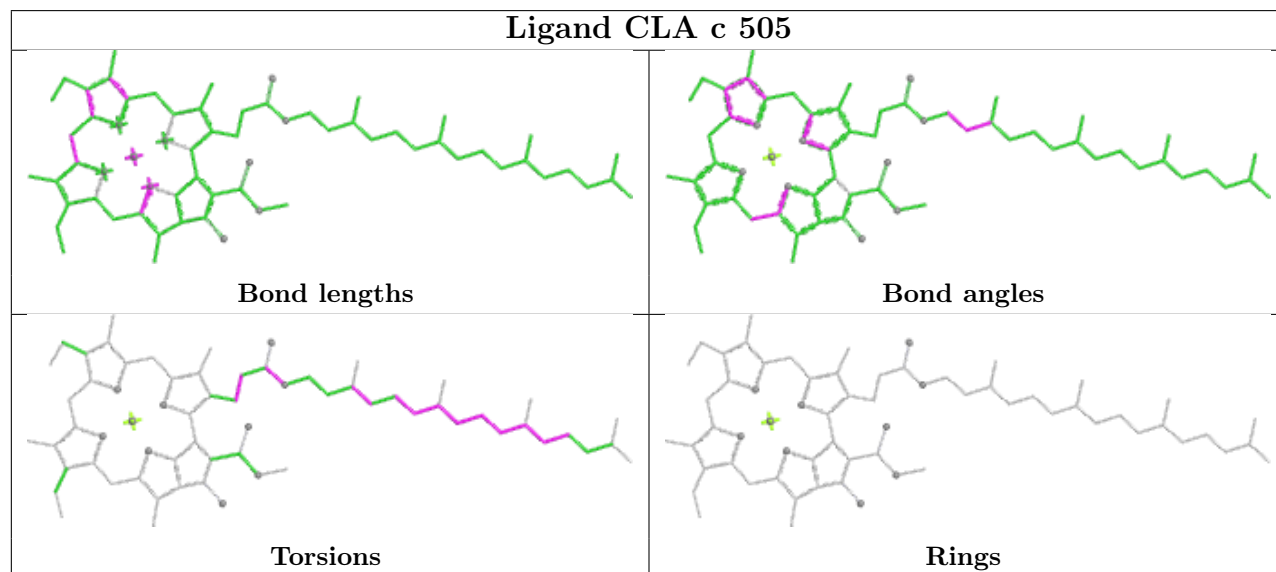




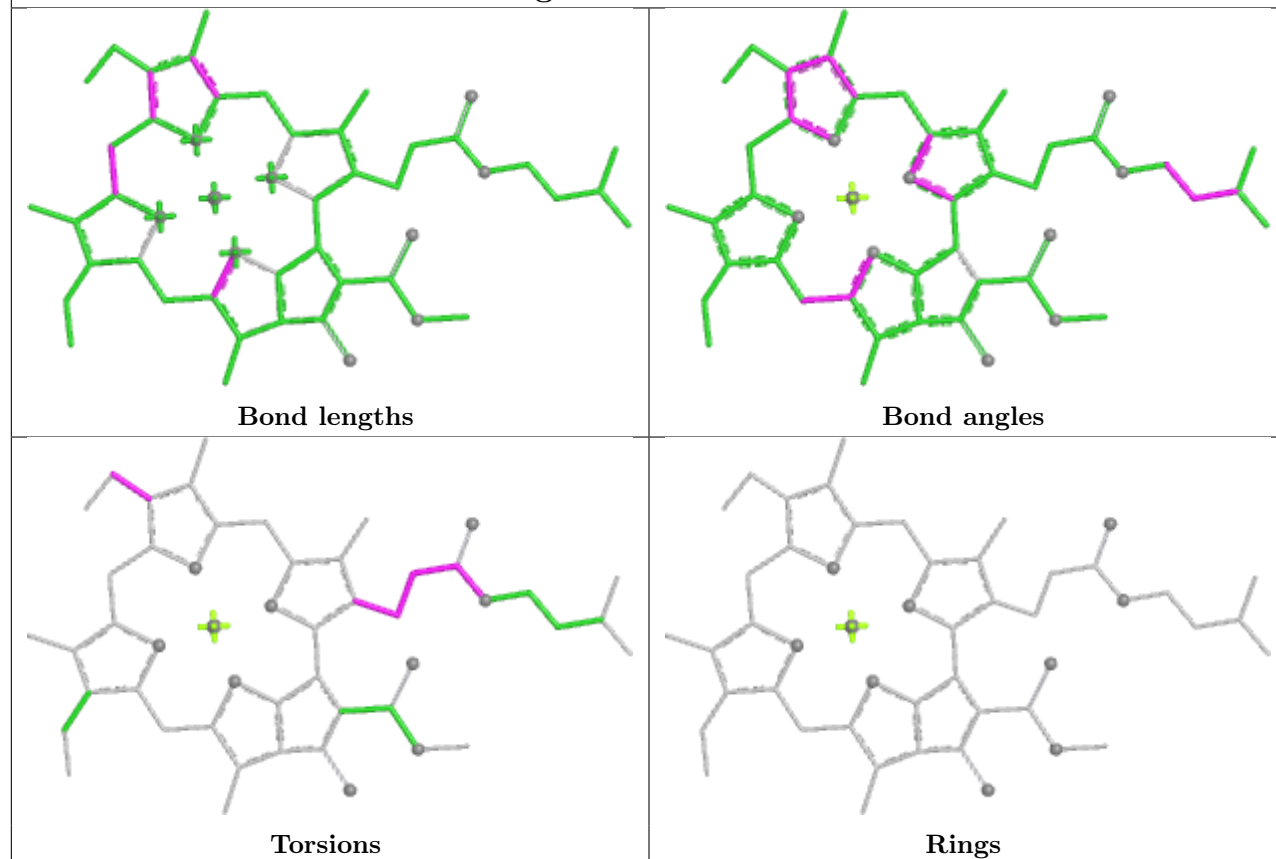




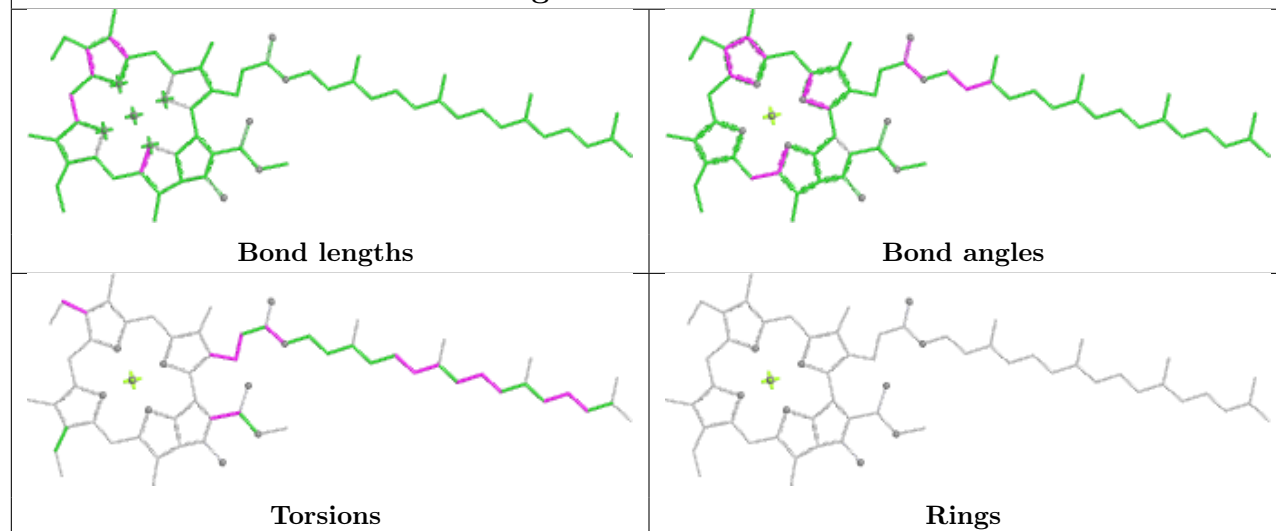


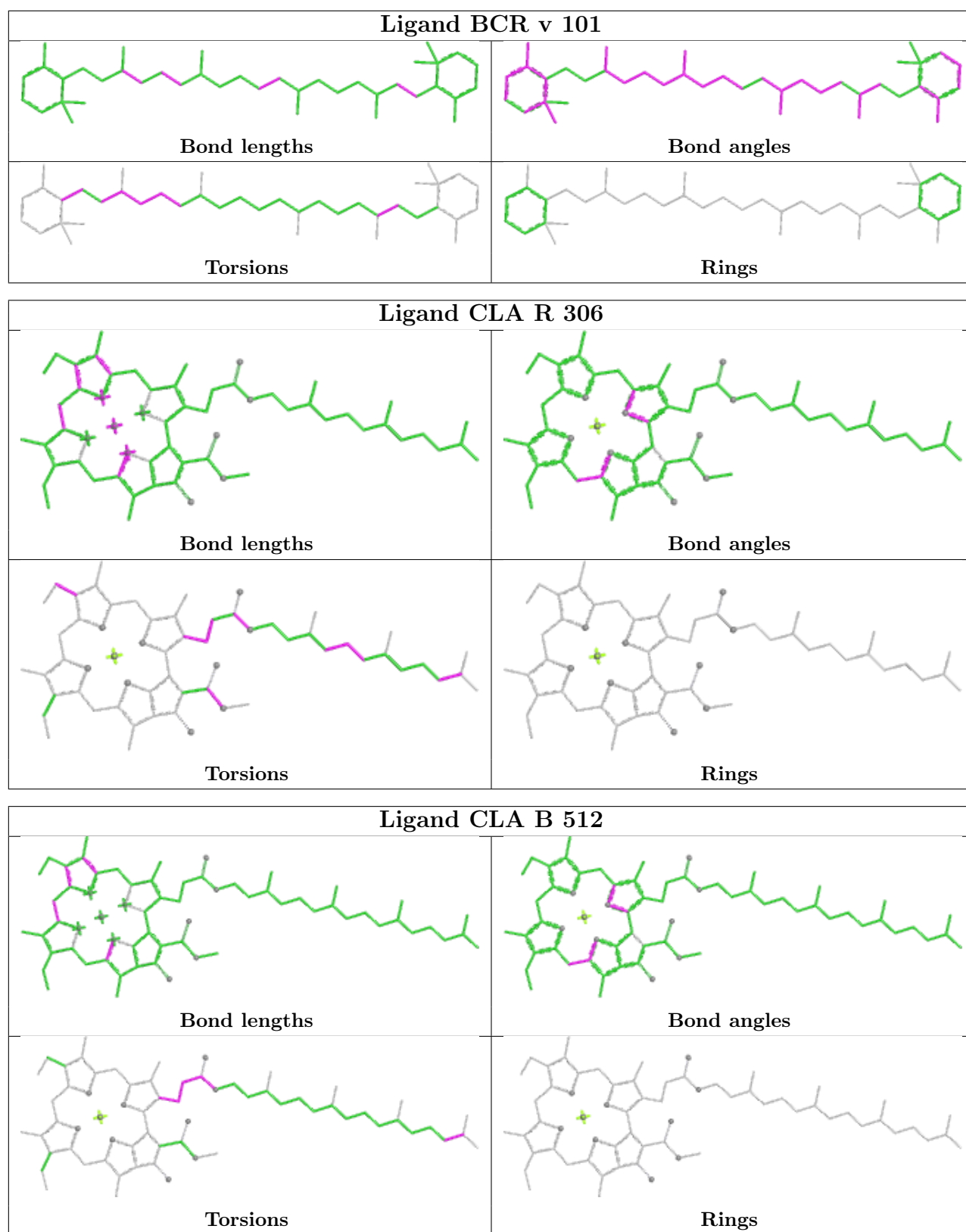
Ligand LUT S 317**Ligand CLA c 505**

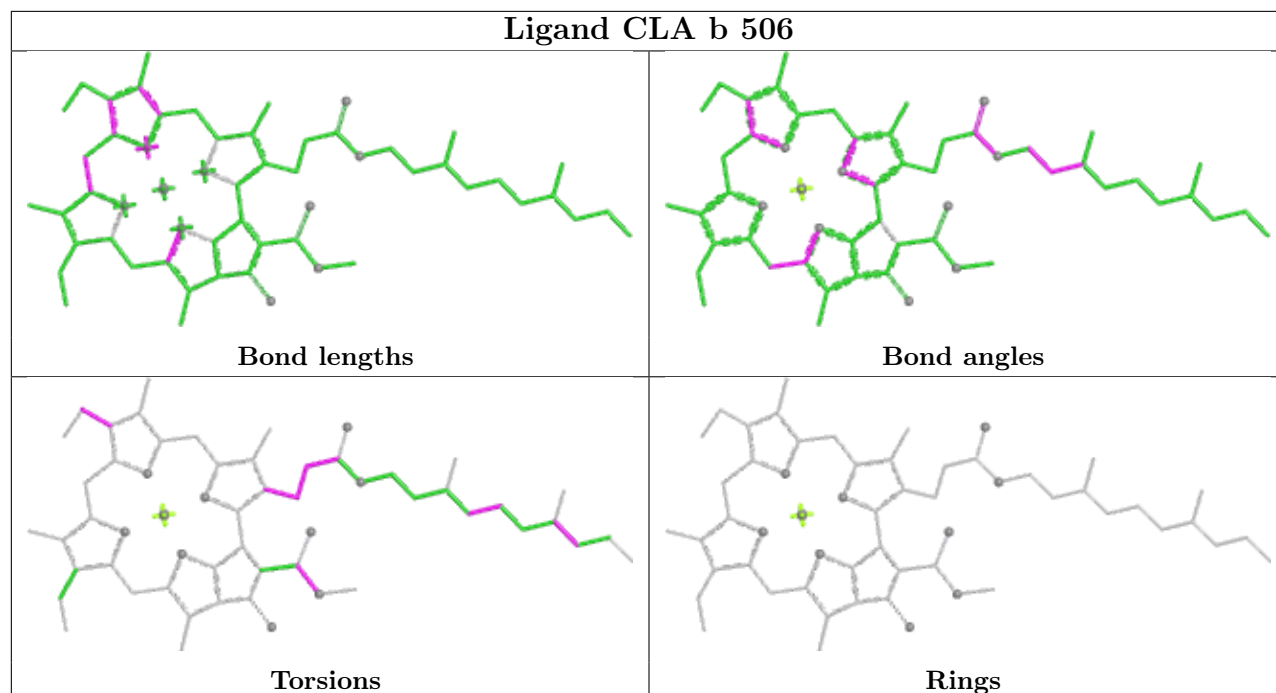
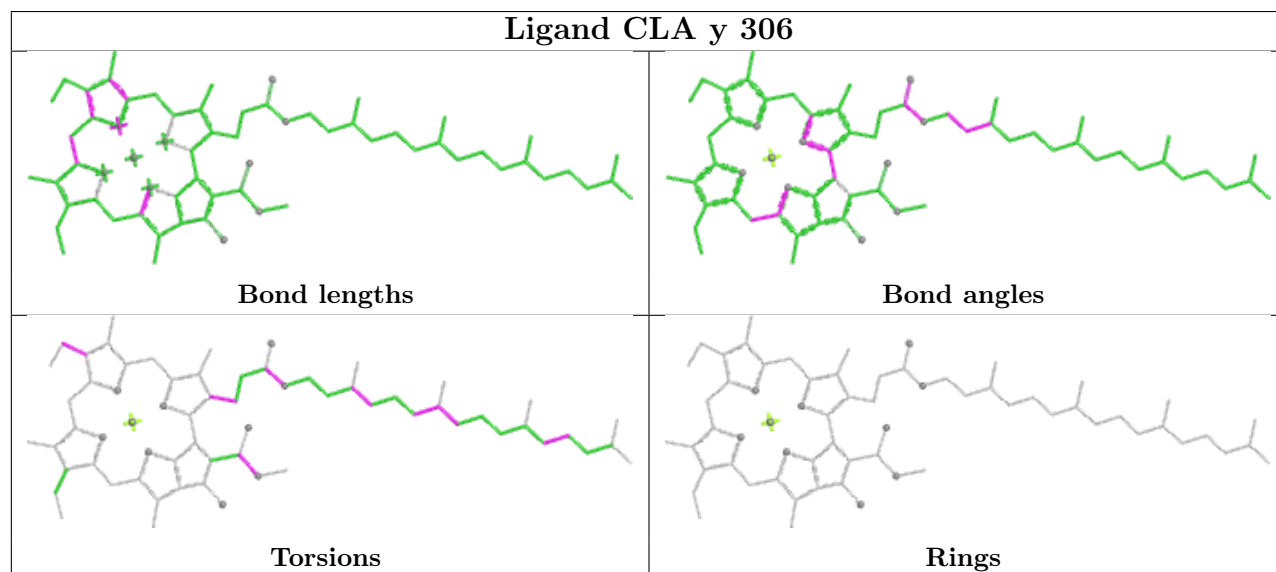
Ligand CLA S 315

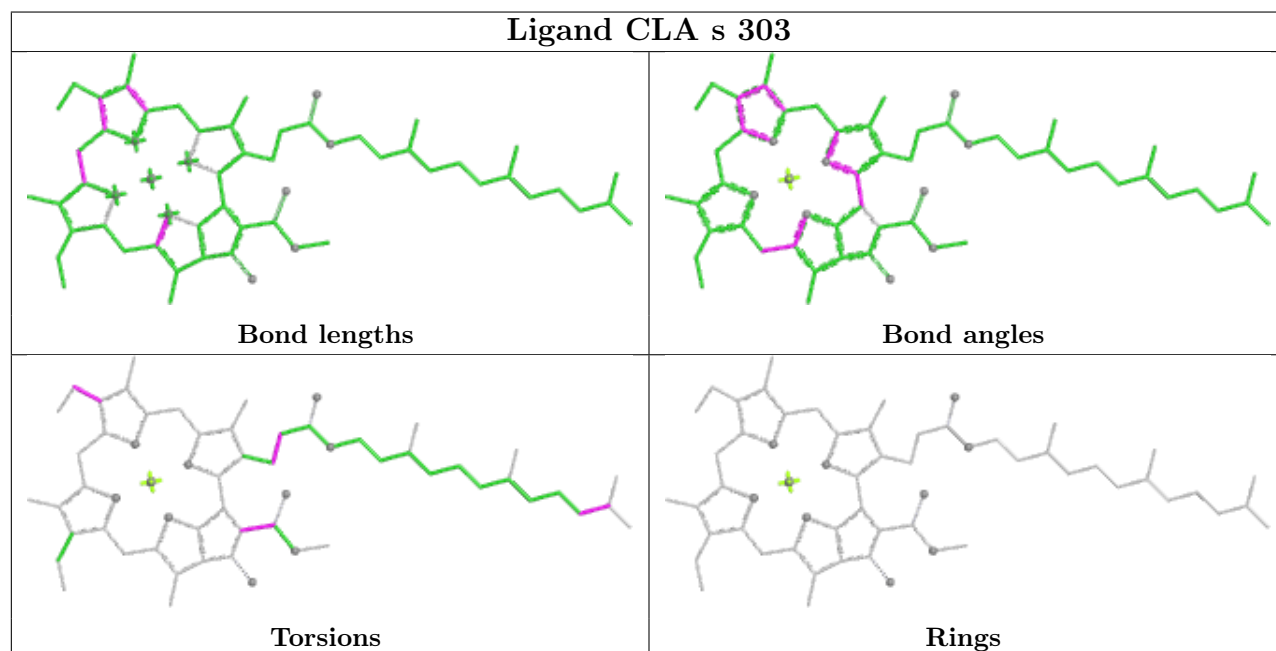
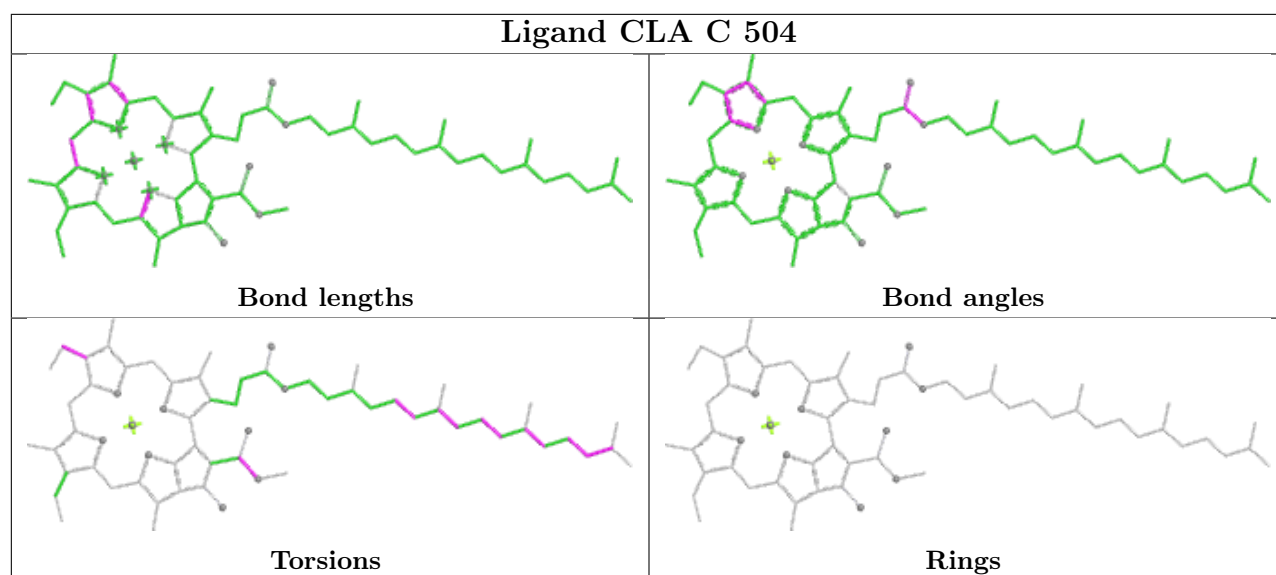


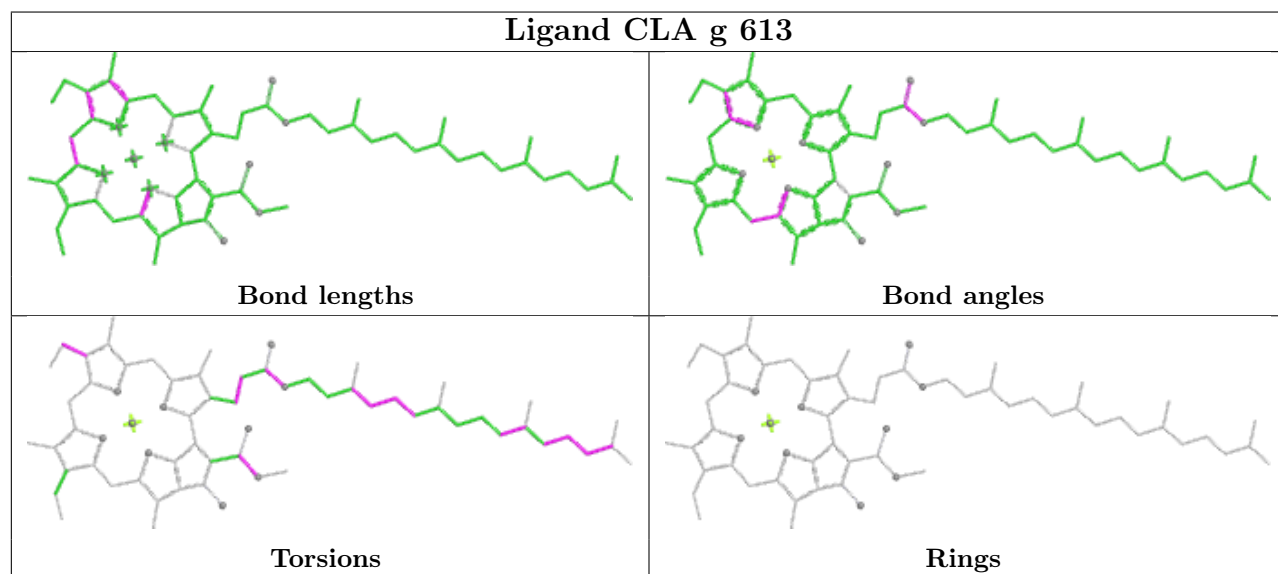
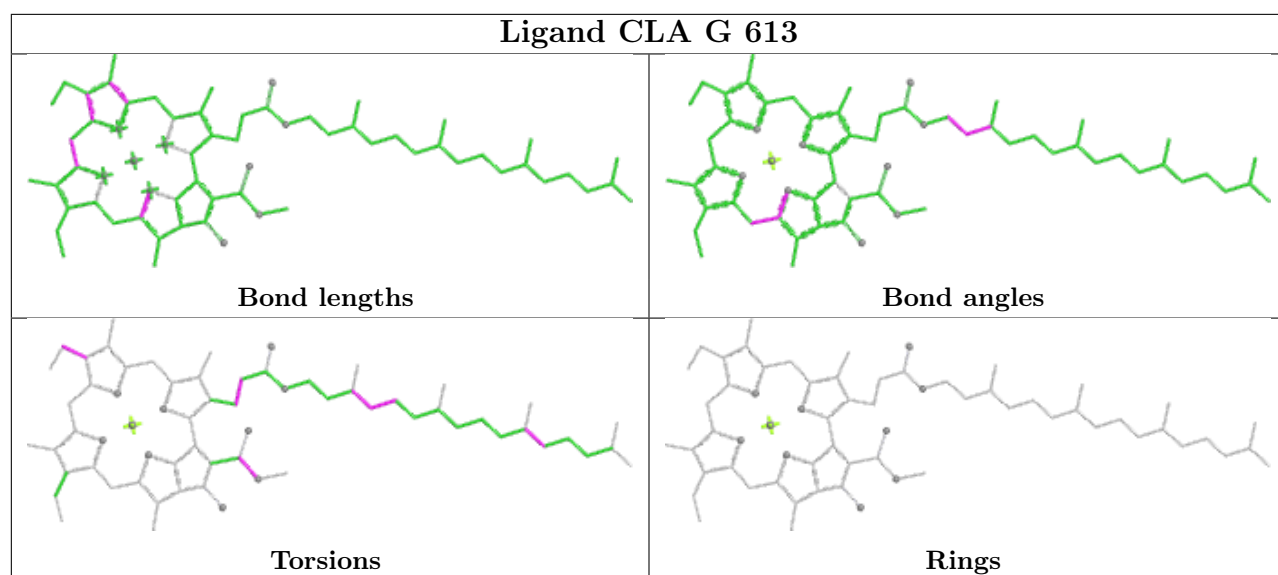
Ligand CLA Y 303



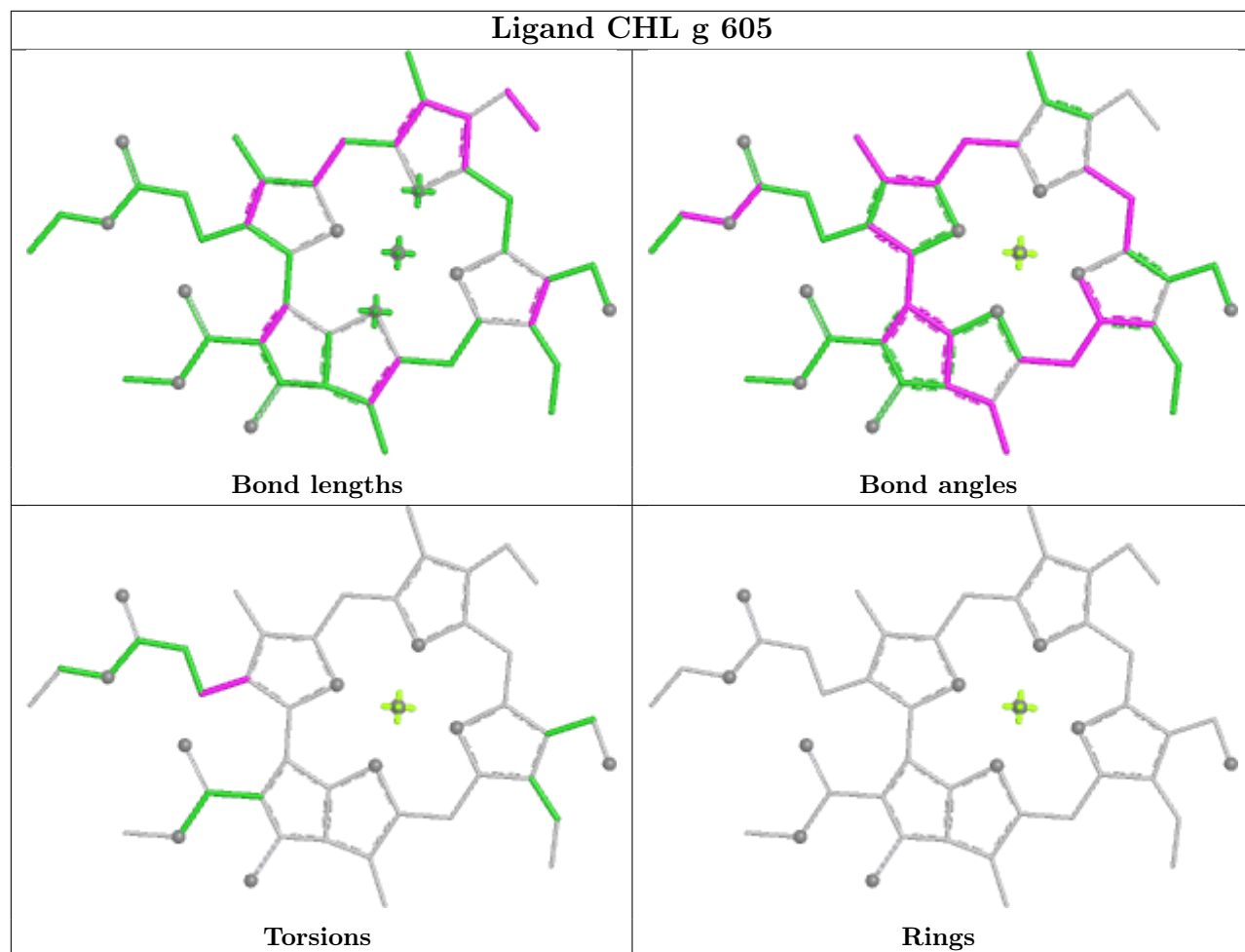


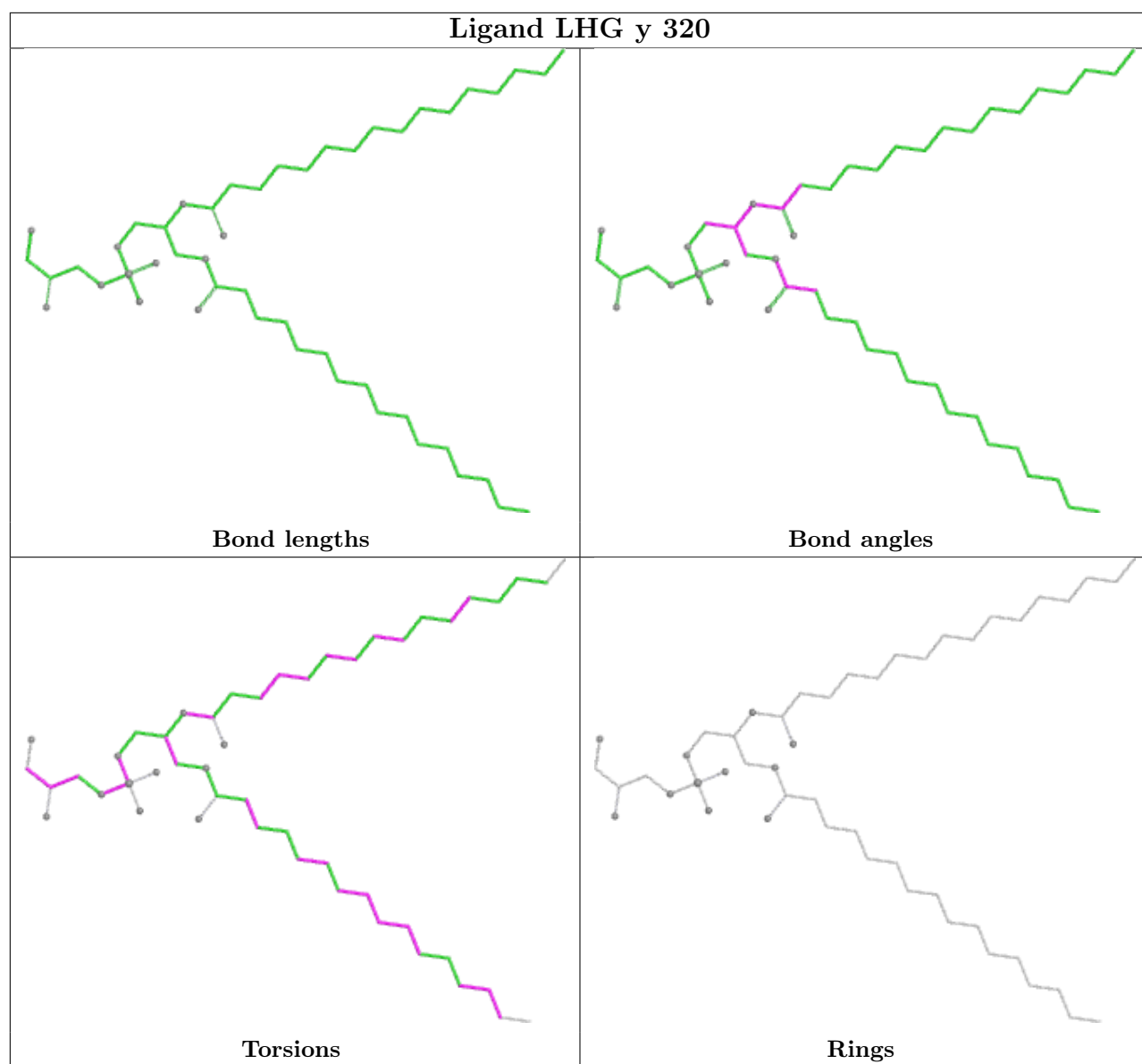
Ligand CLA b 506**Ligand CLA y 306**



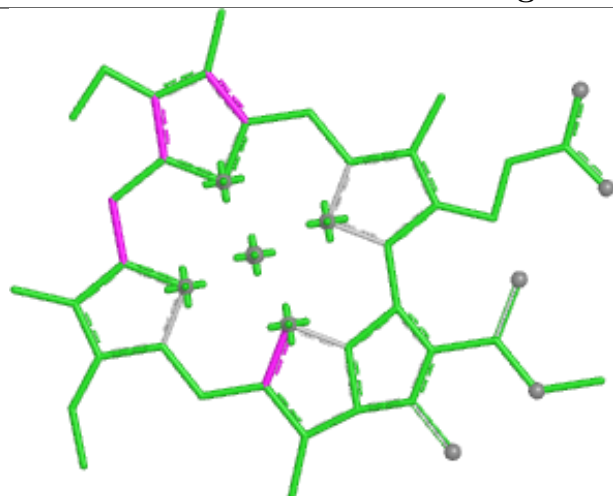


Ligand CHL g 605

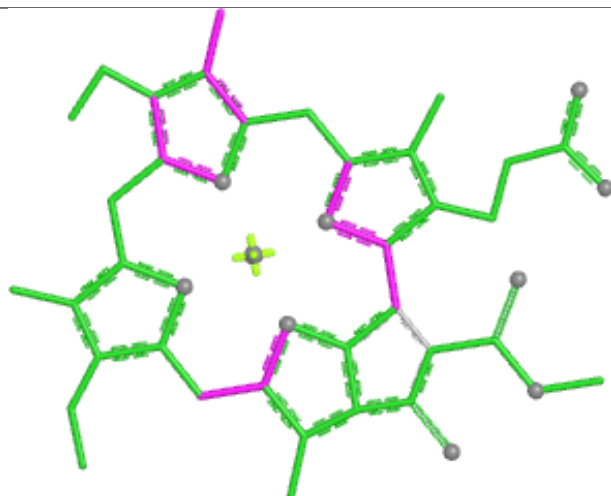




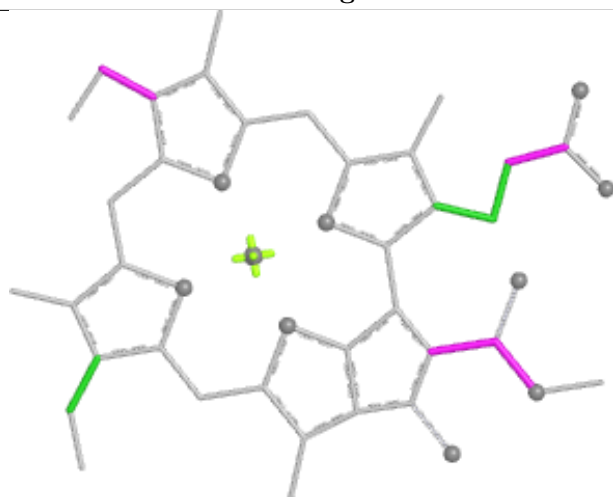
Ligand CLA n 611



Bond lengths



Bond angles

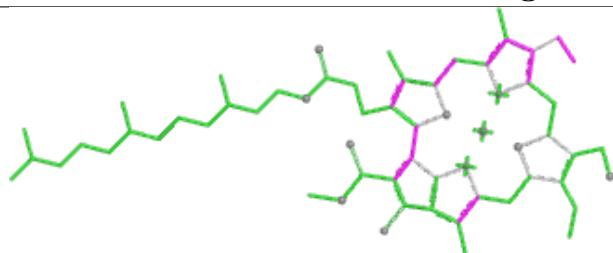


Torsions

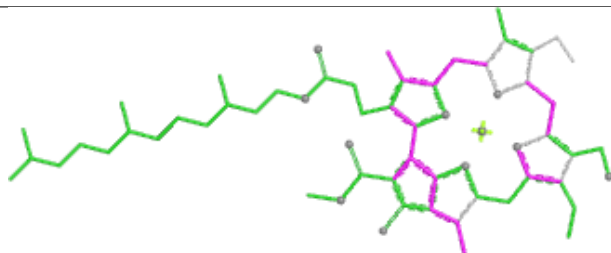


Rings

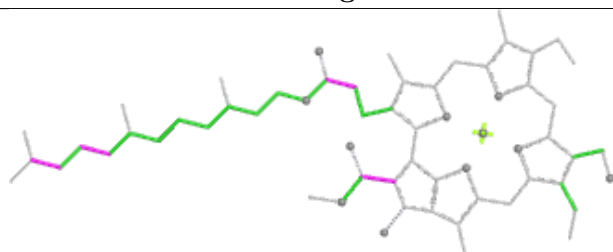
Ligand CHL s 309



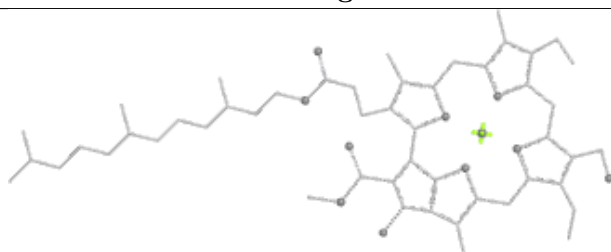
Bond lengths



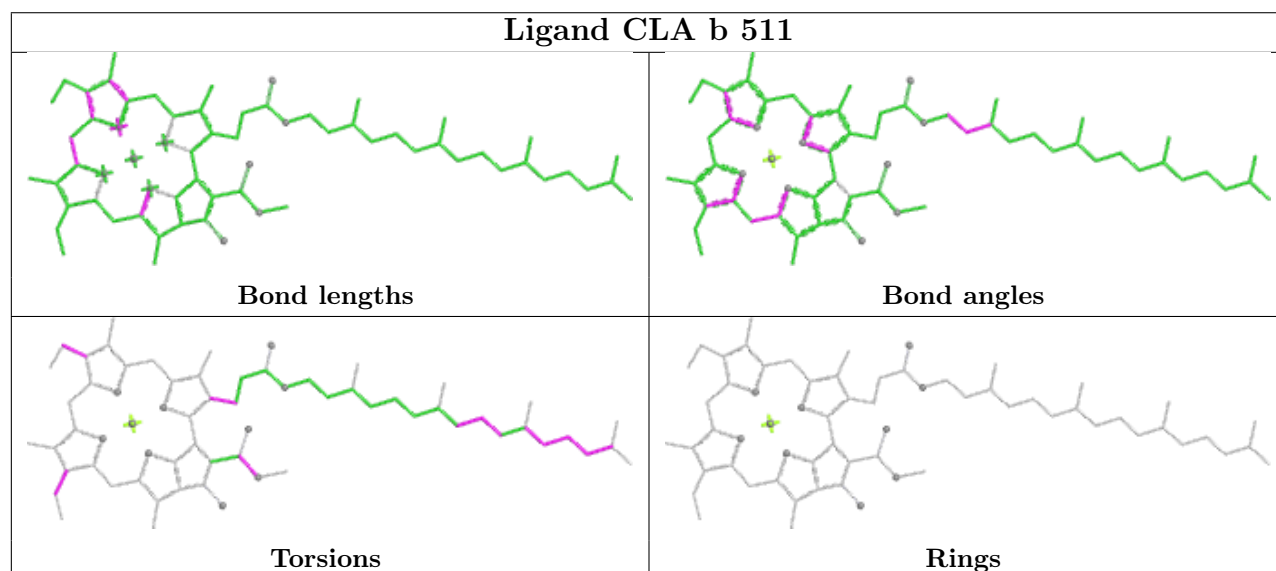
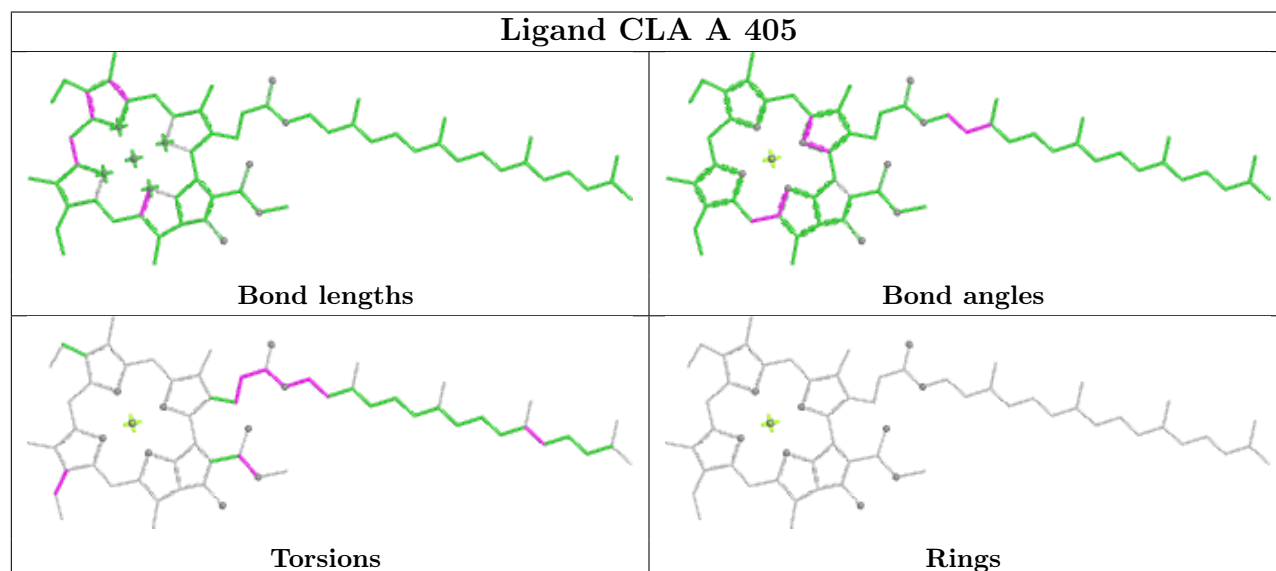
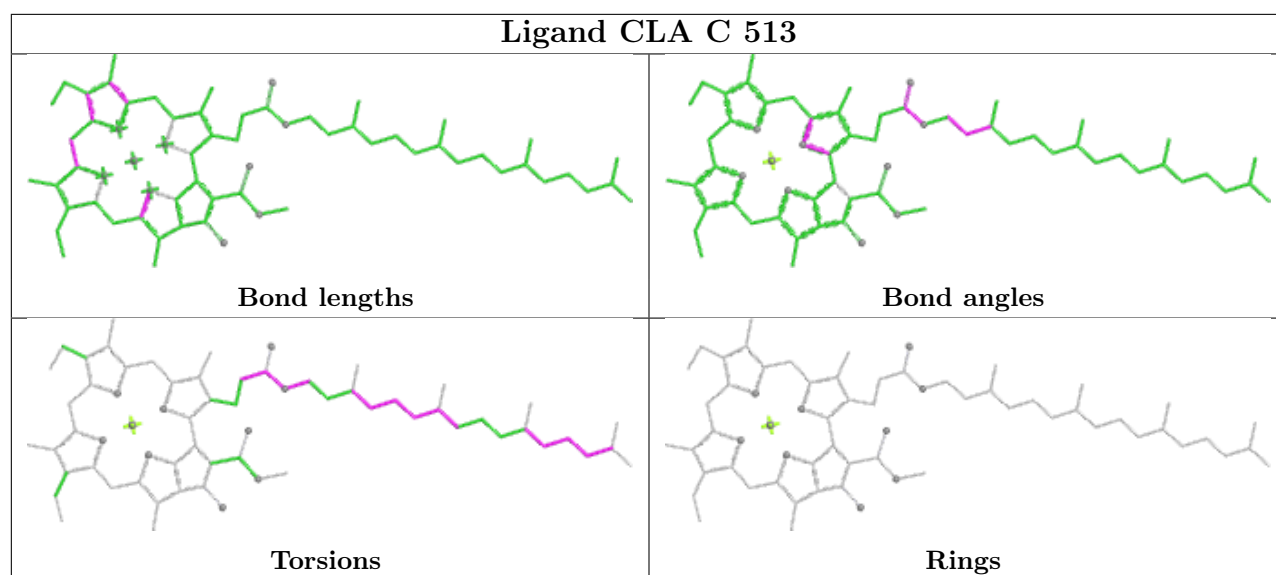
Bond angles

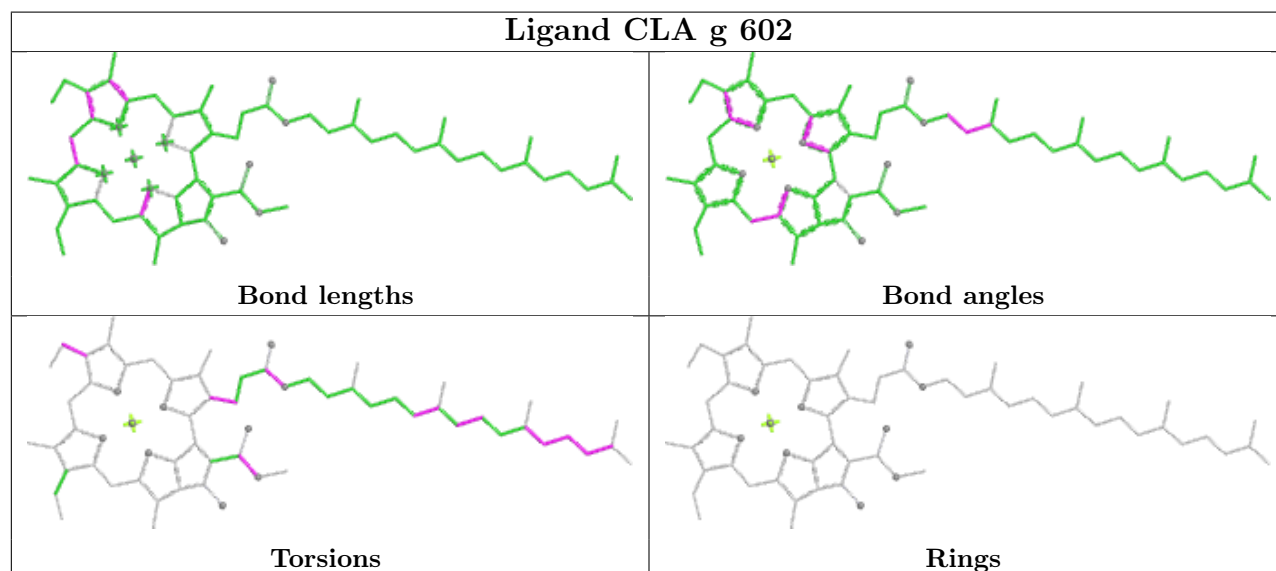
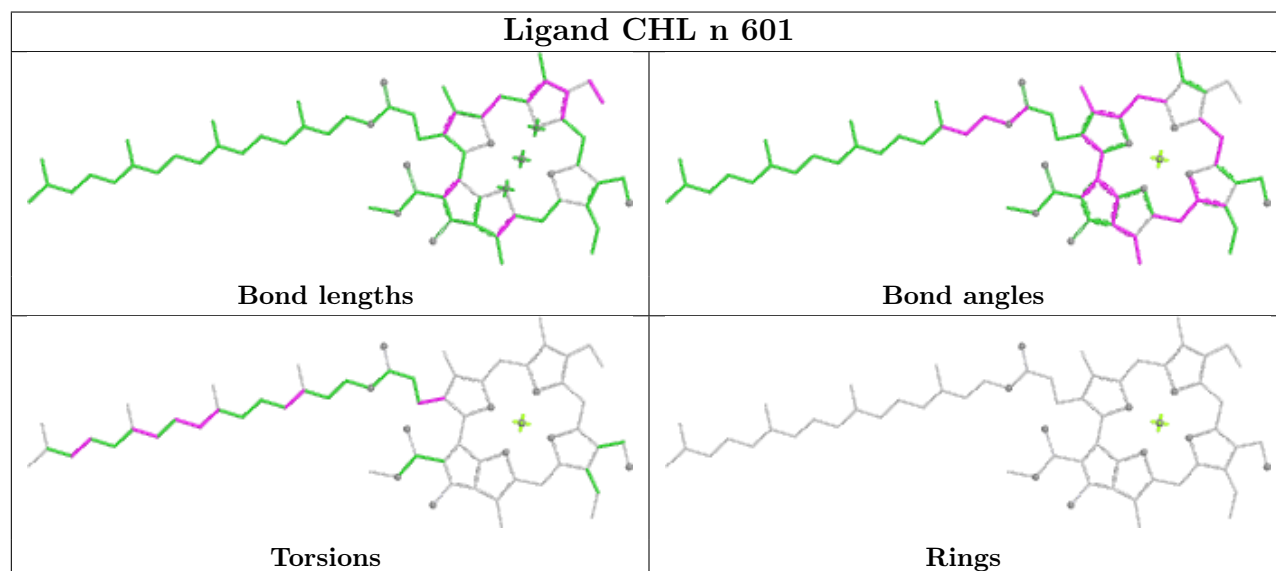
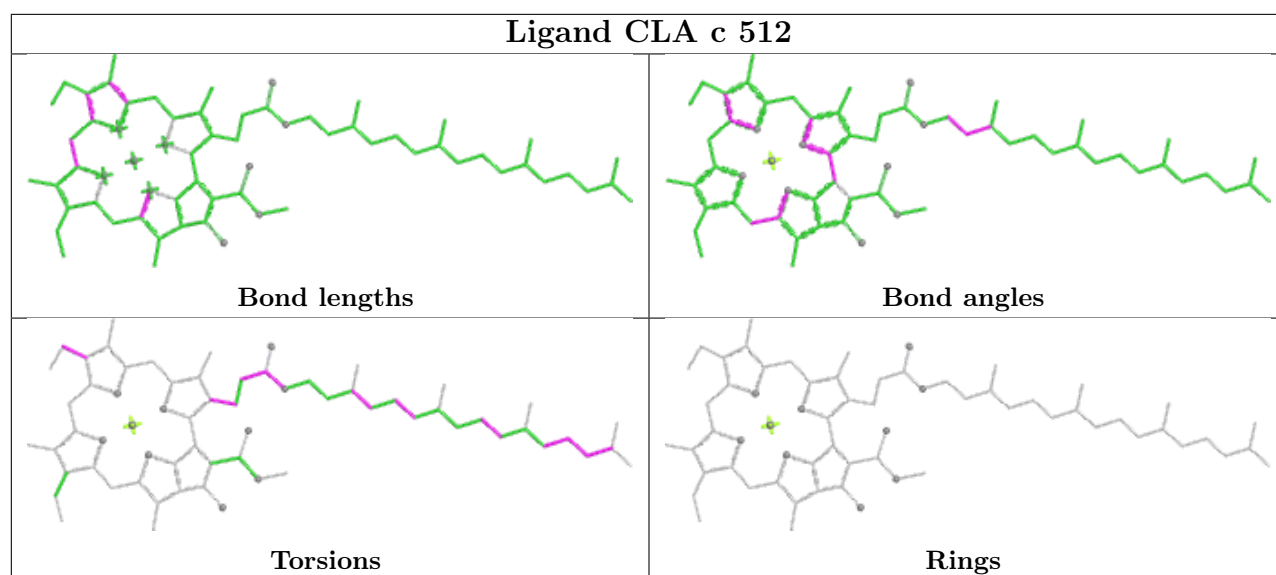


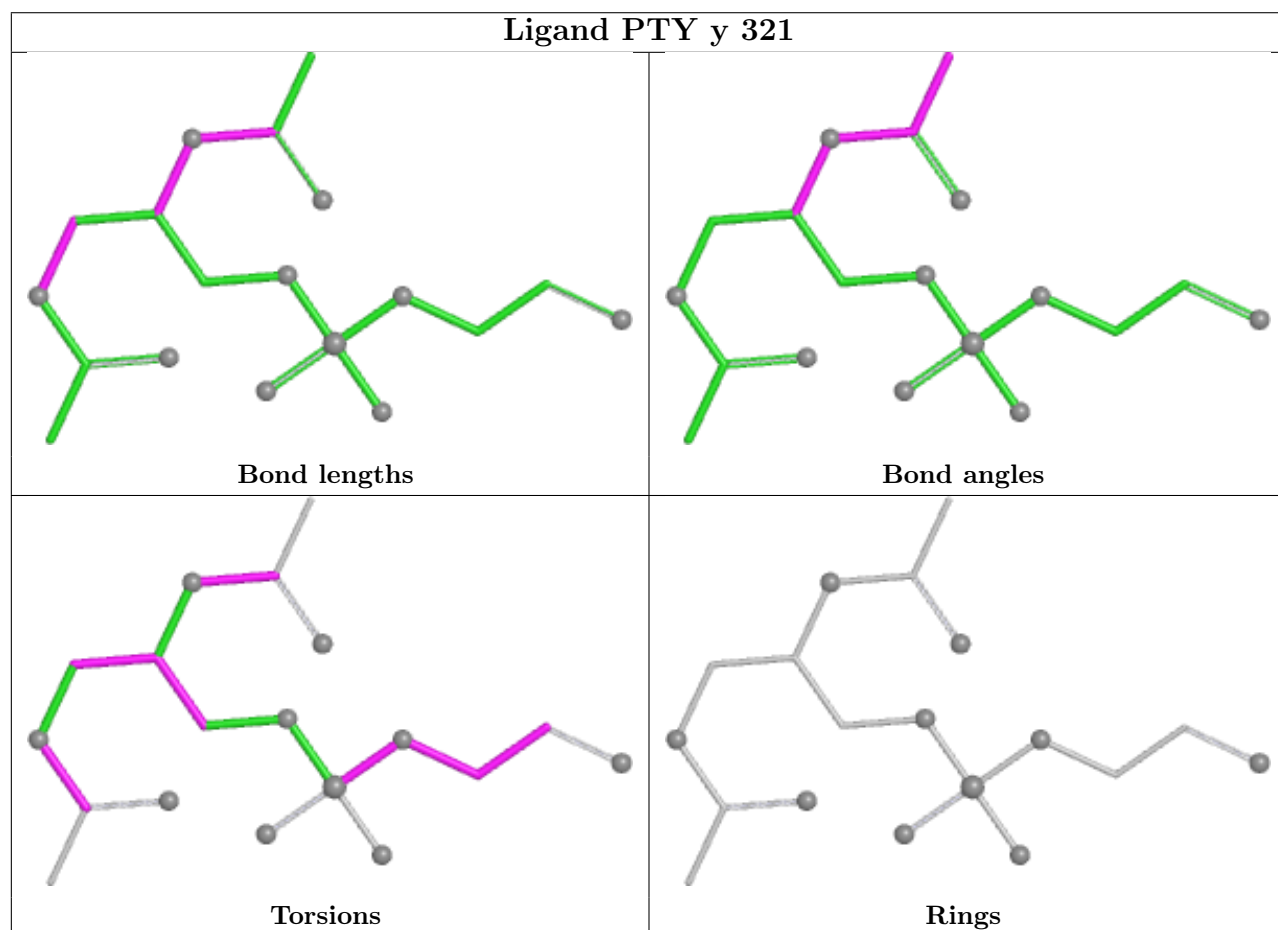
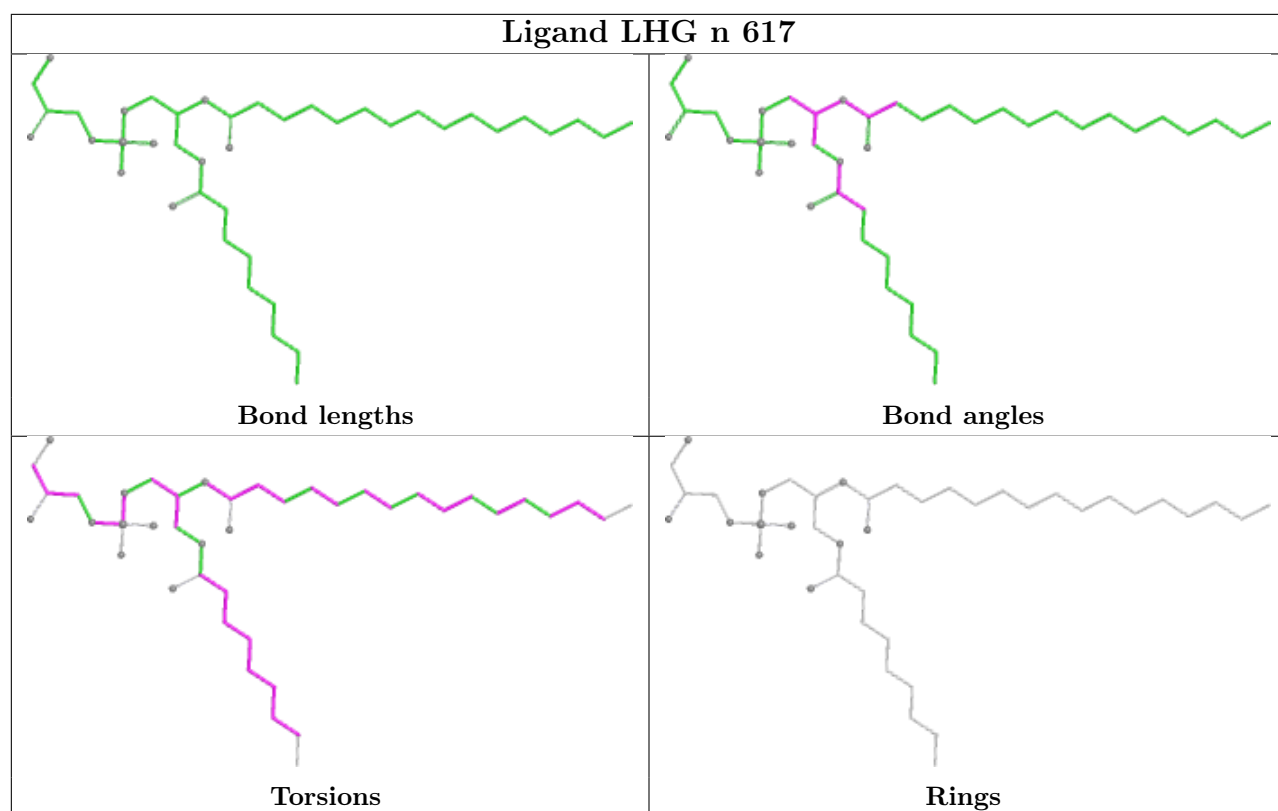
Torsions



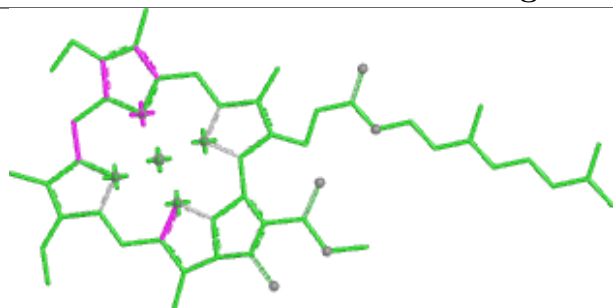
Rings



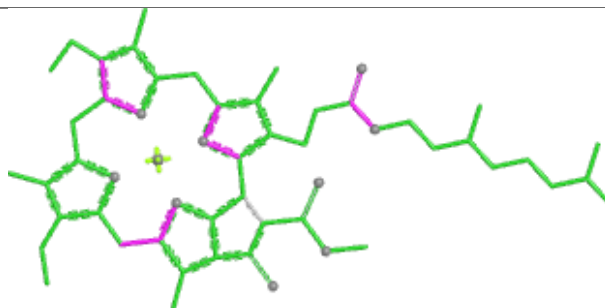




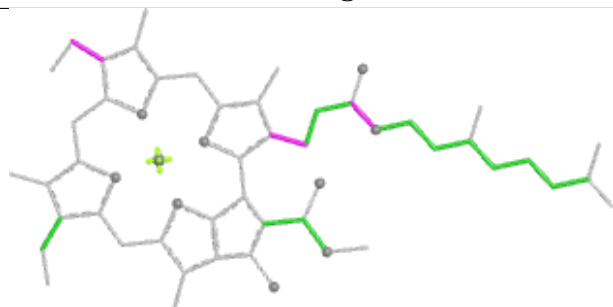
Ligand CLA s 315



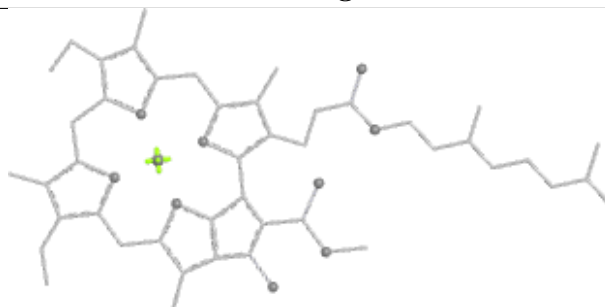
Bond lengths



Bond angles

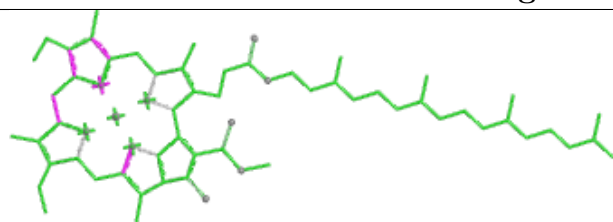


Torsions

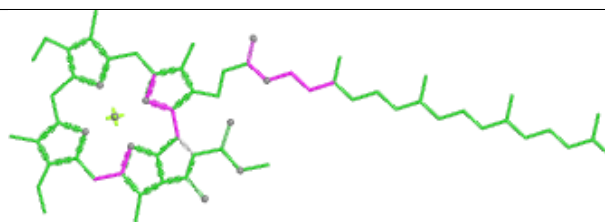


Rings

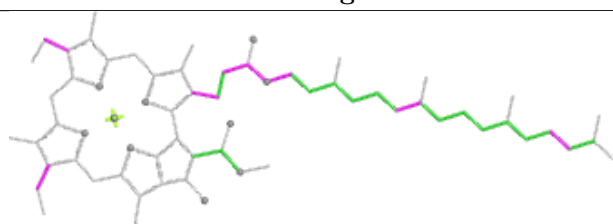
Ligand CLA a 405



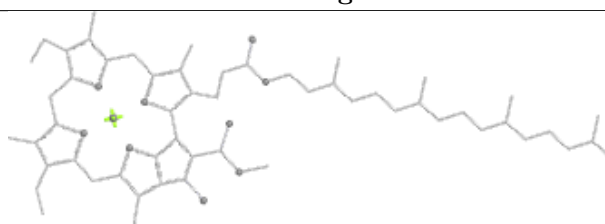
Bond lengths



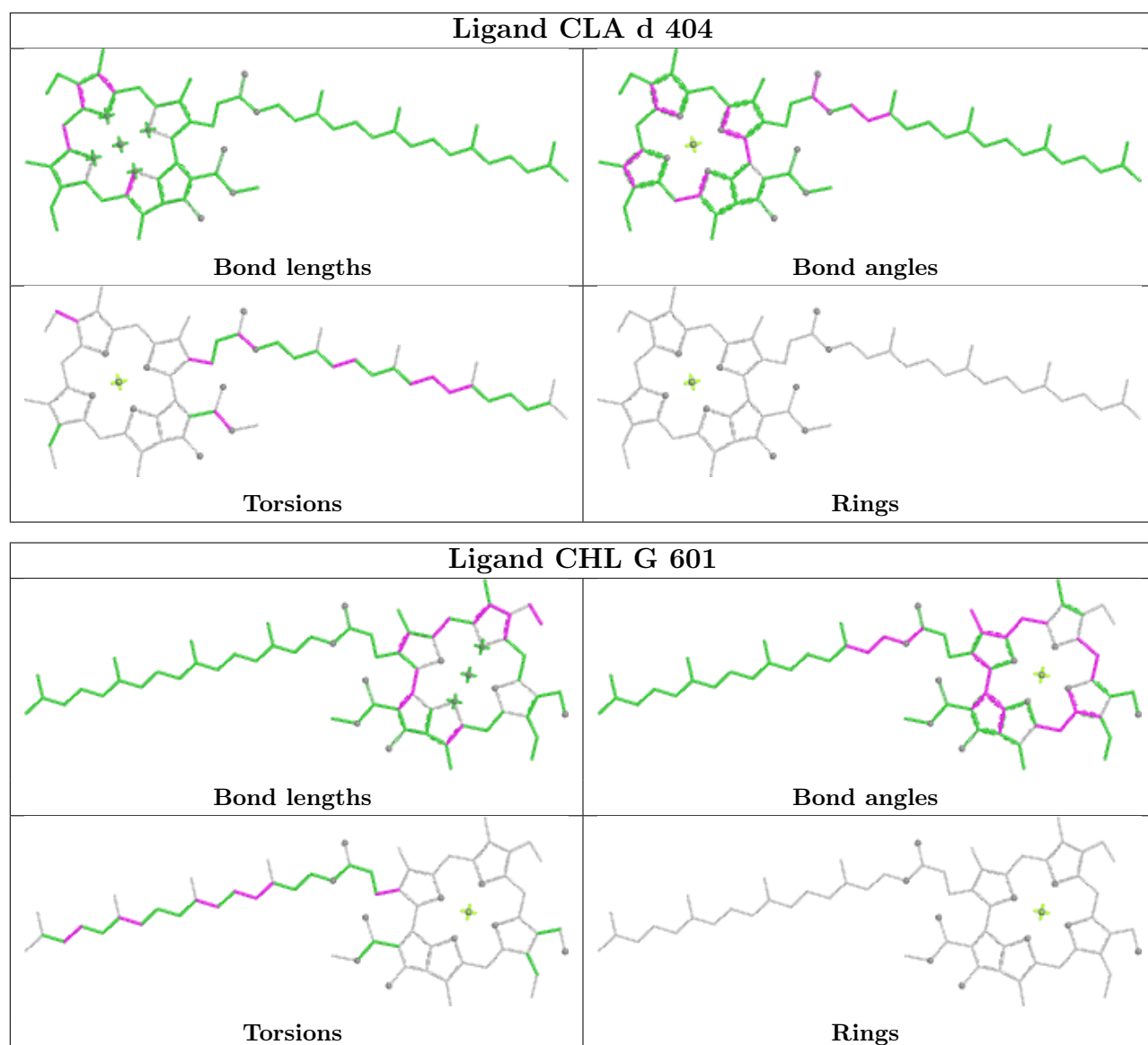
Bond angles



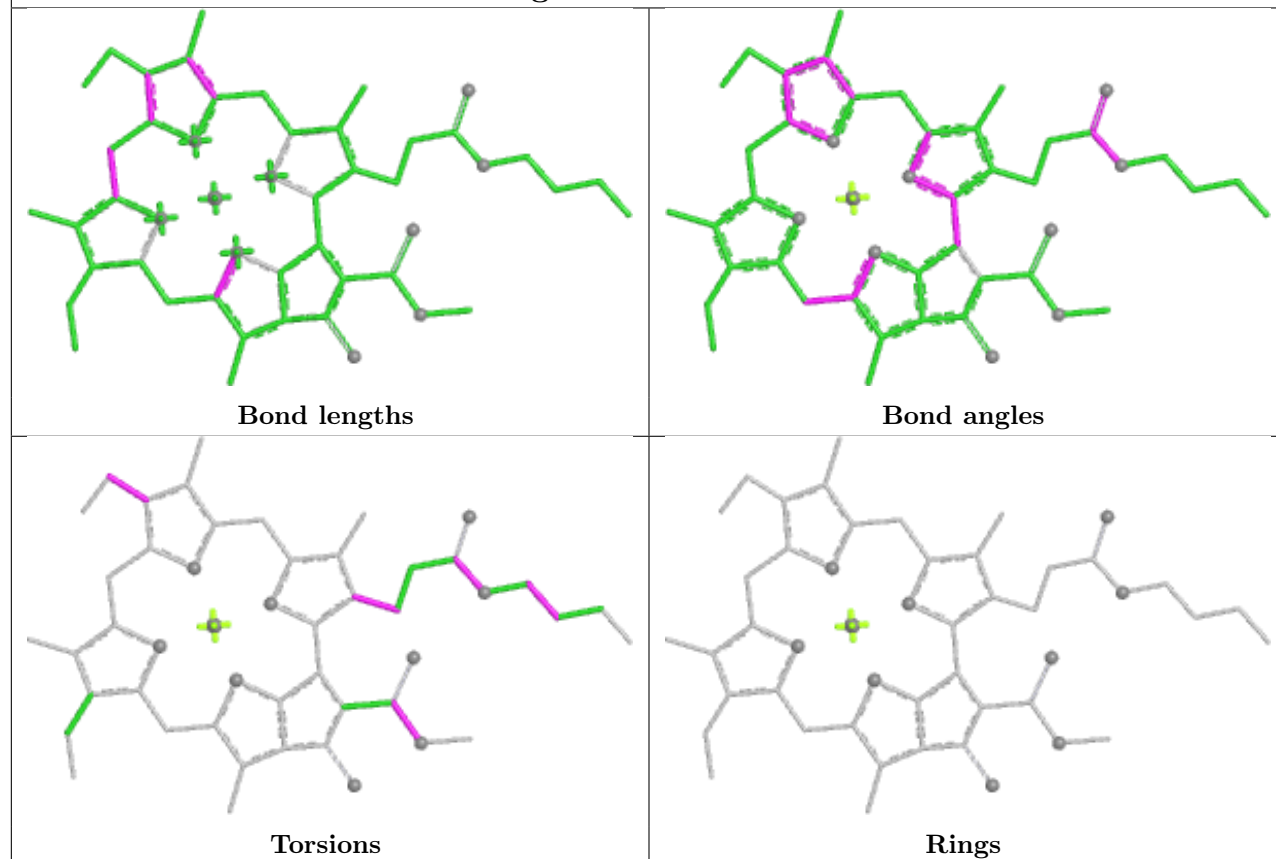
Torsions



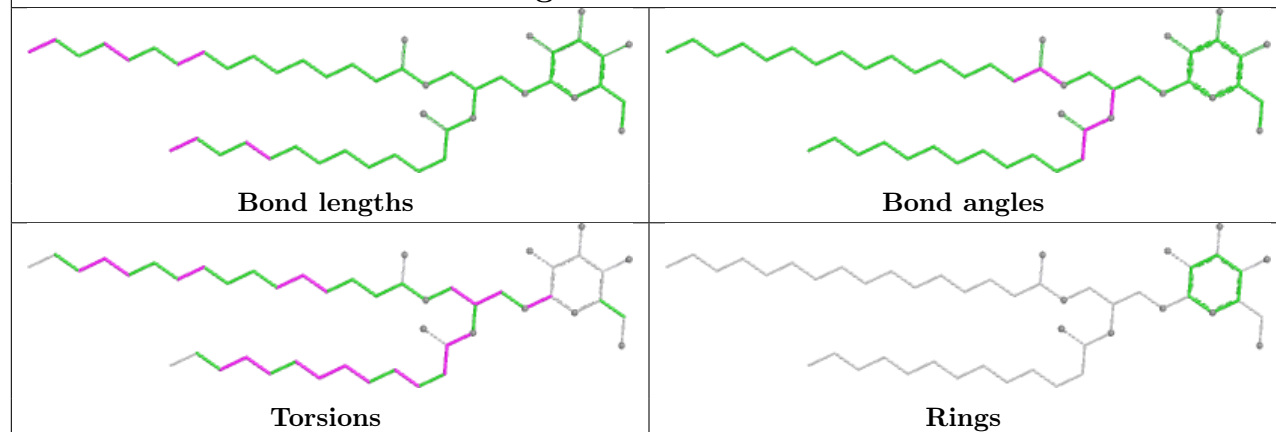
Rings

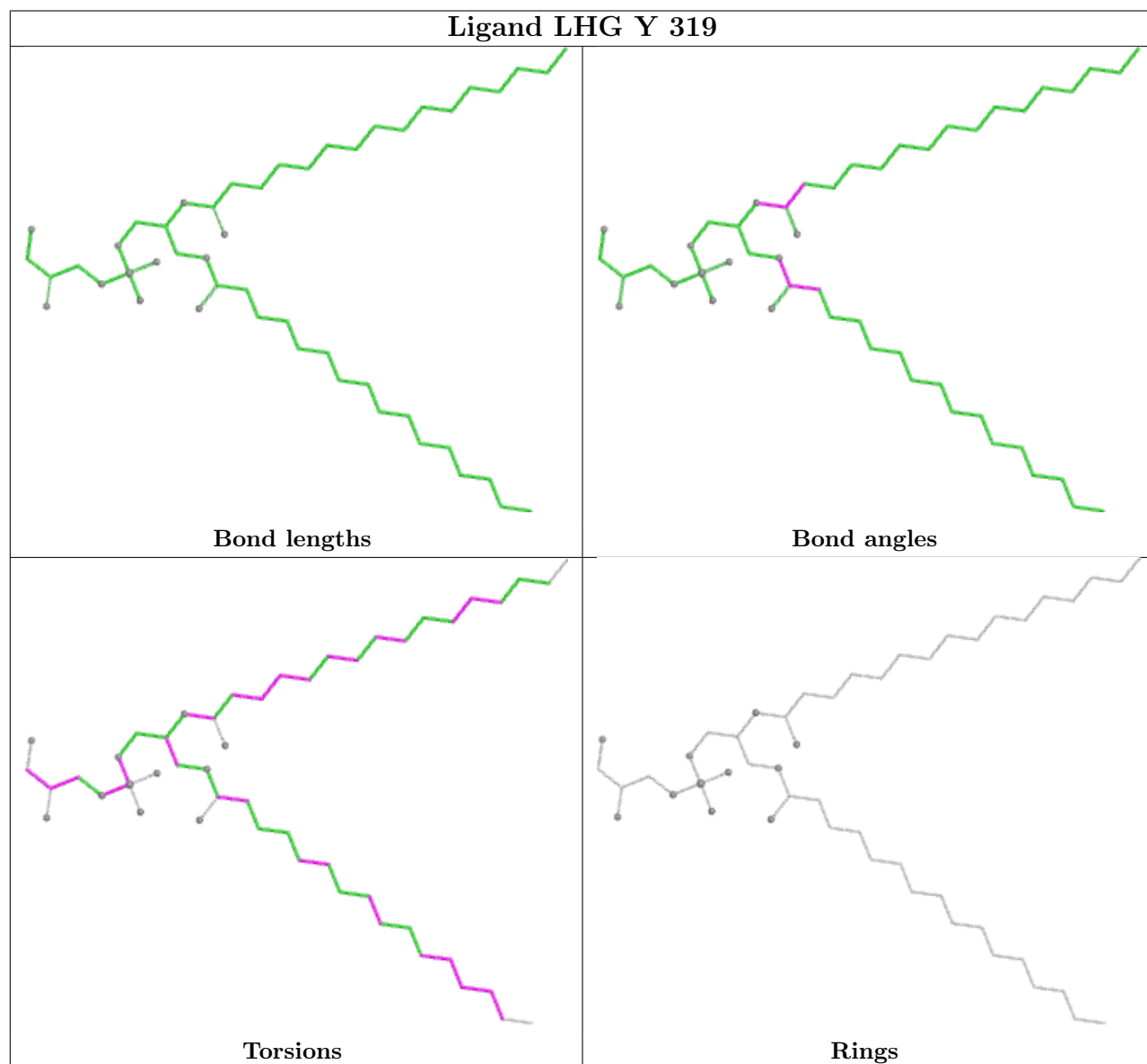
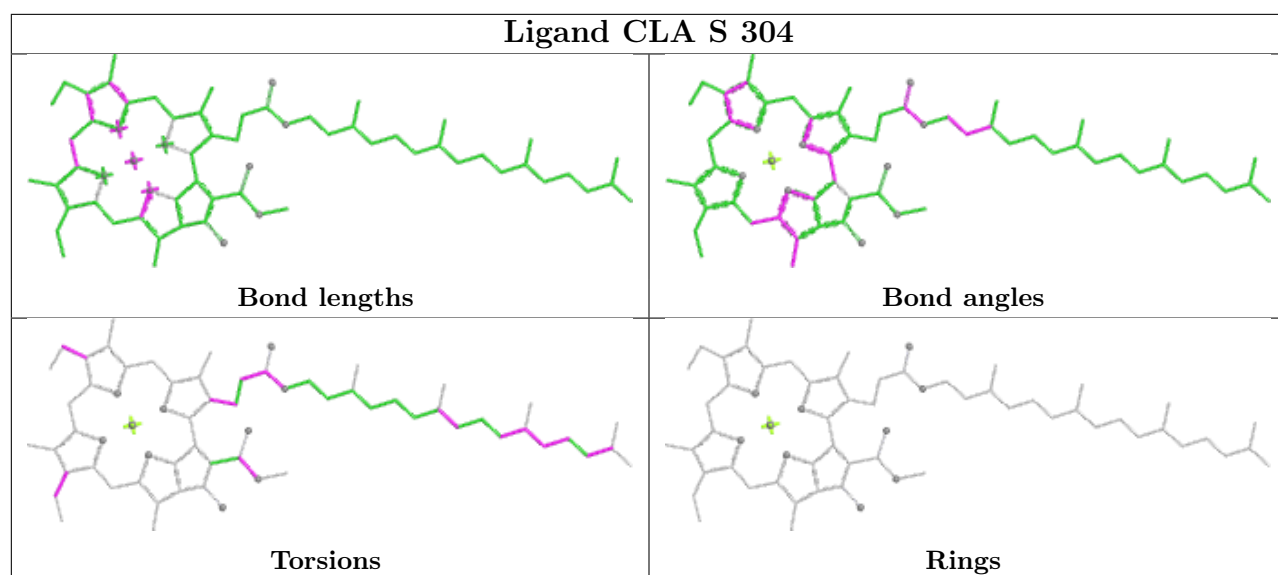


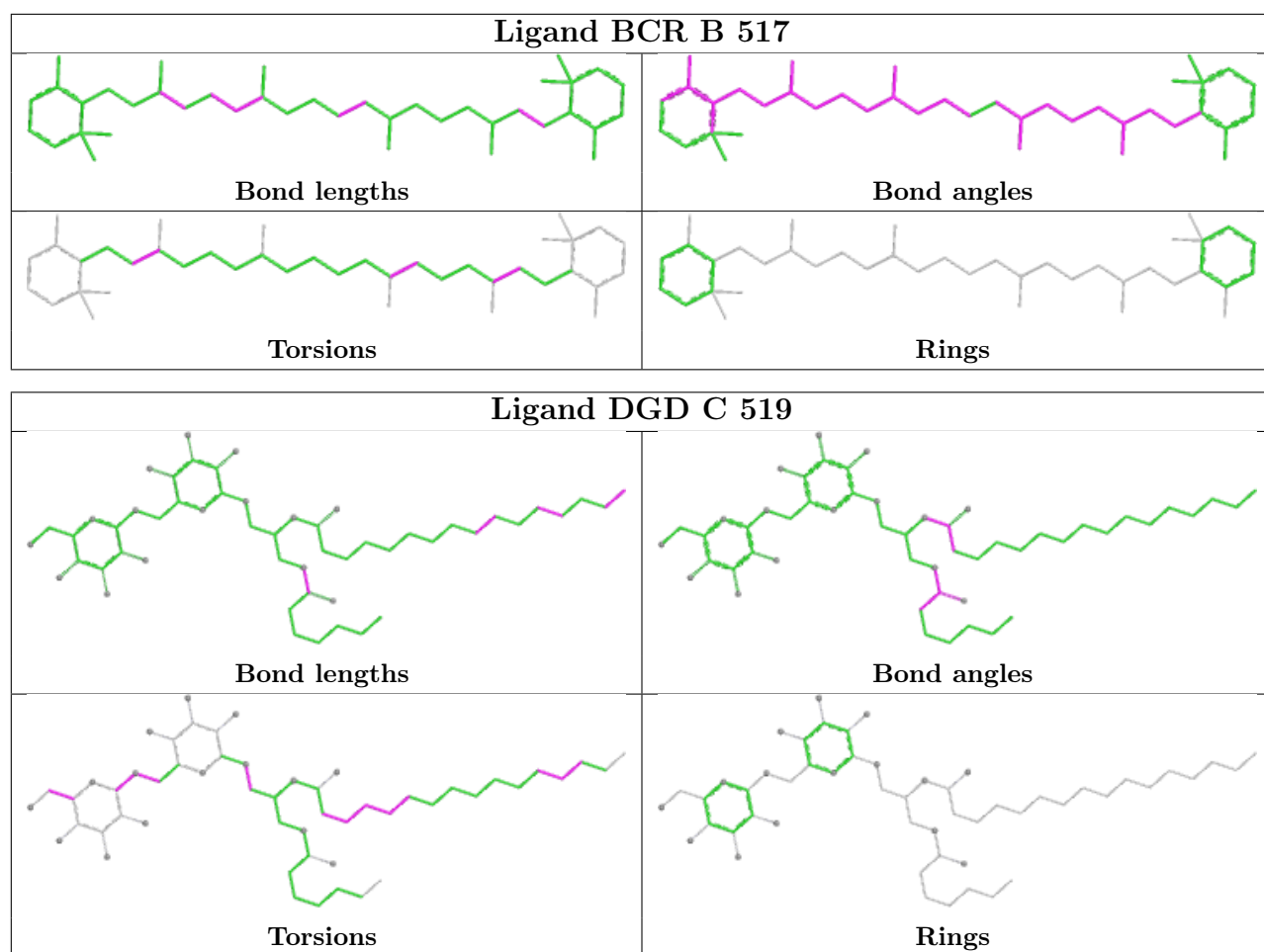
Ligand CLA N 614



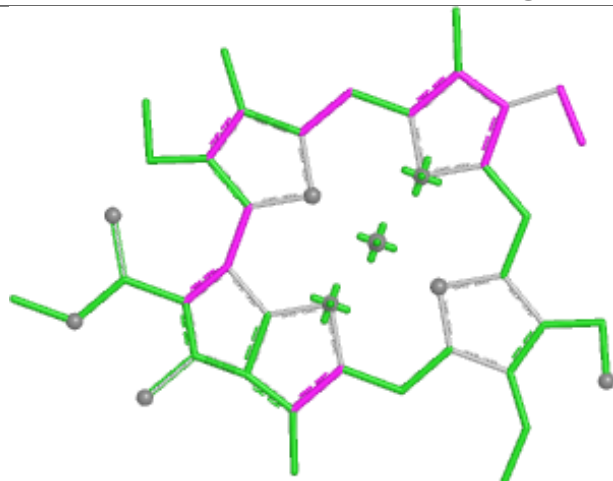
Ligand LMG i 101



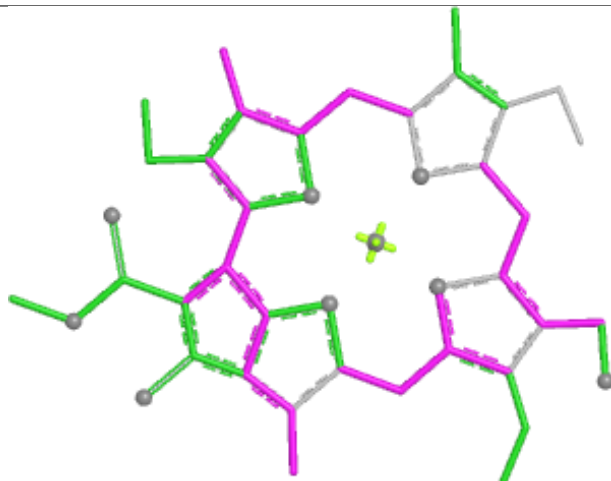




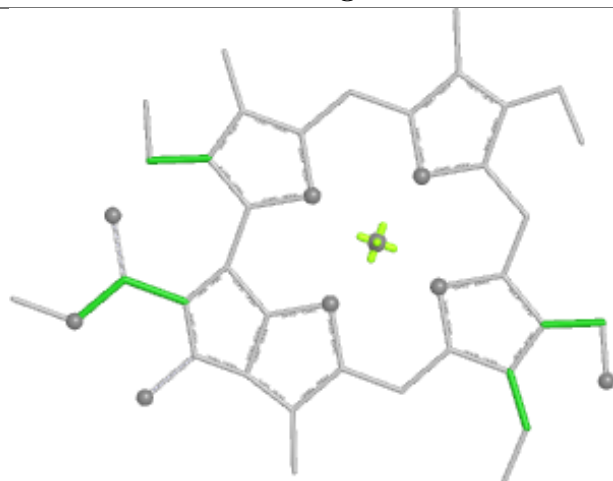
Ligand CHL s 308



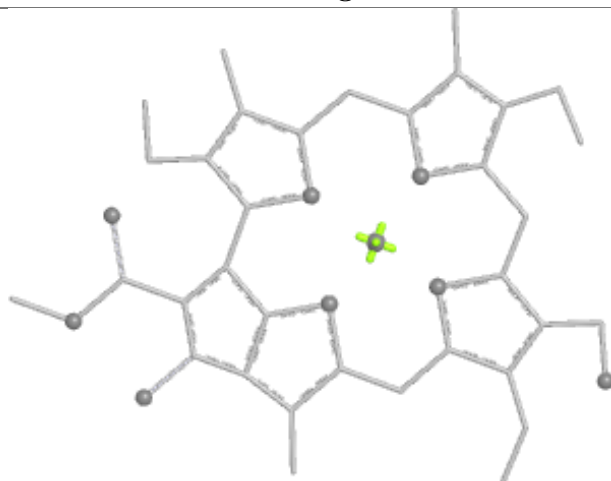
Bond lengths



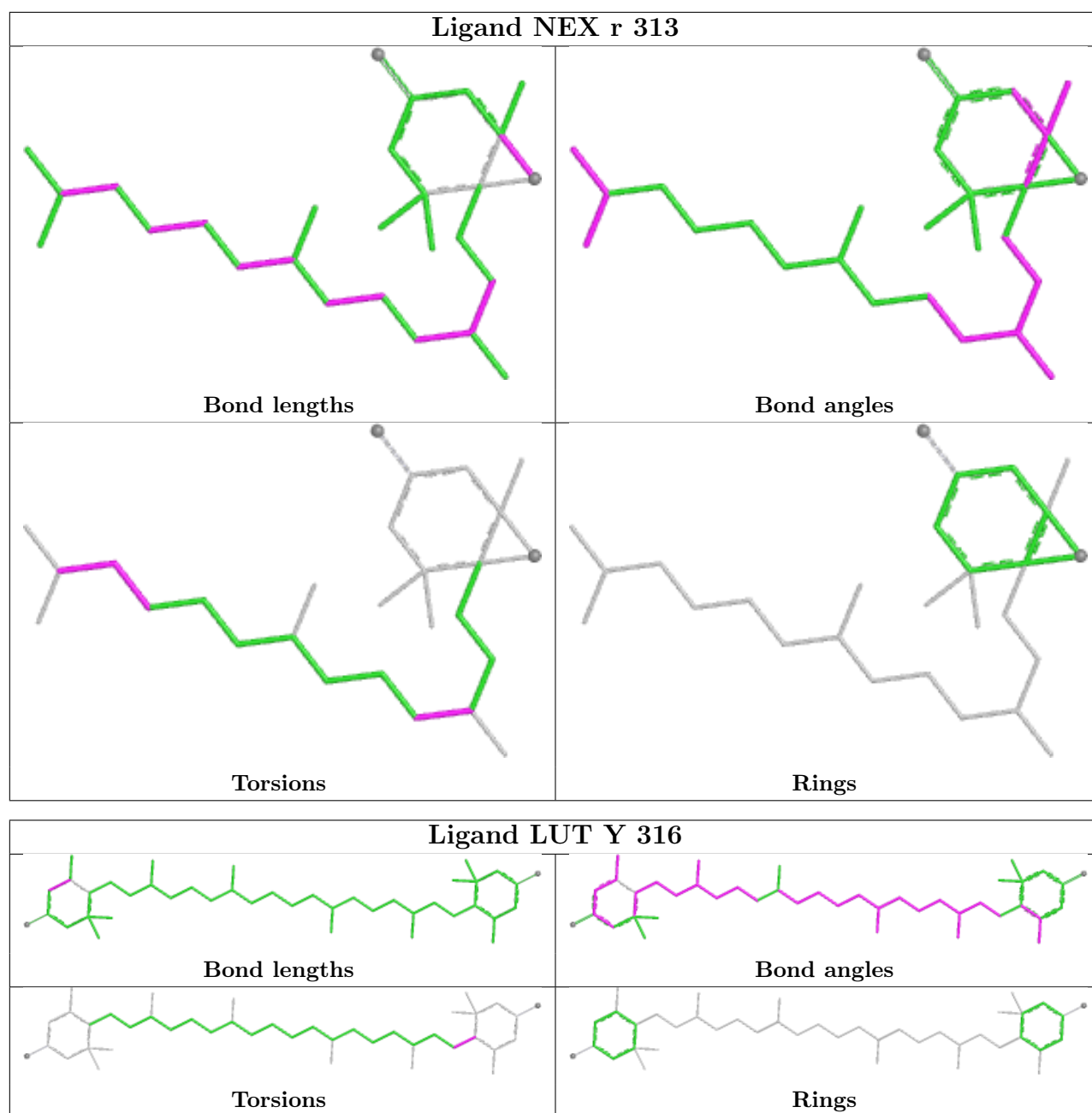
Bond angles

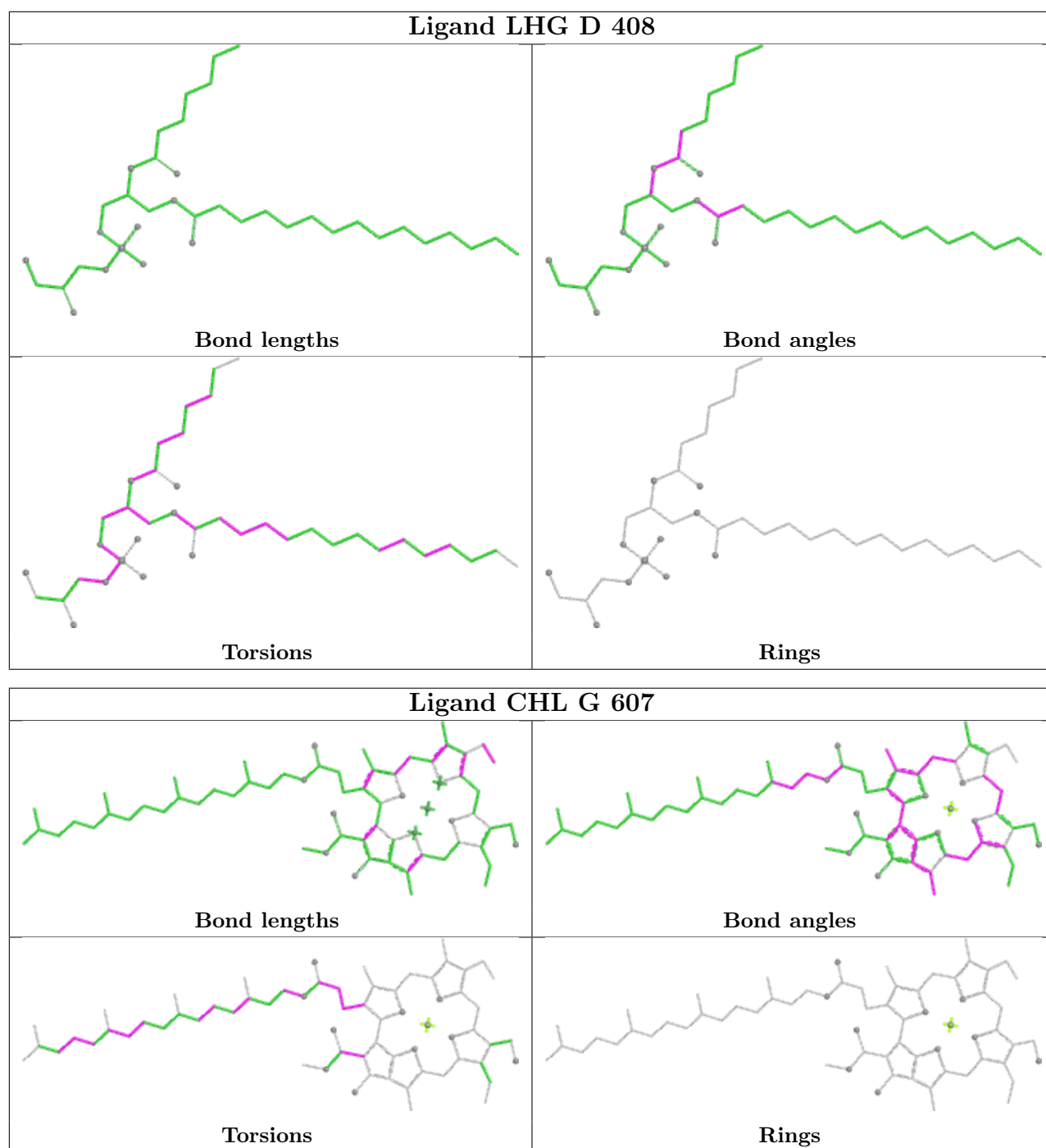


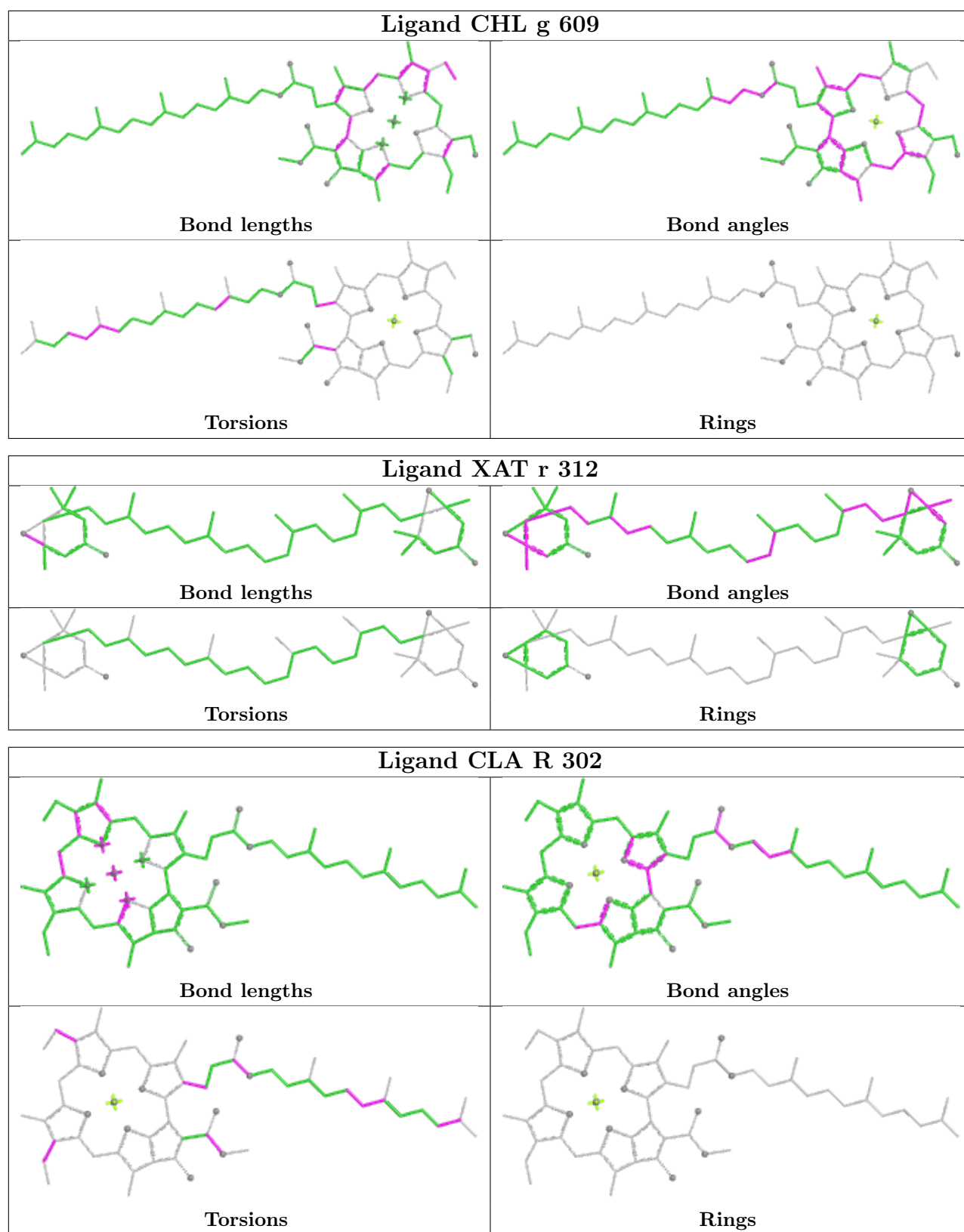
Torsions



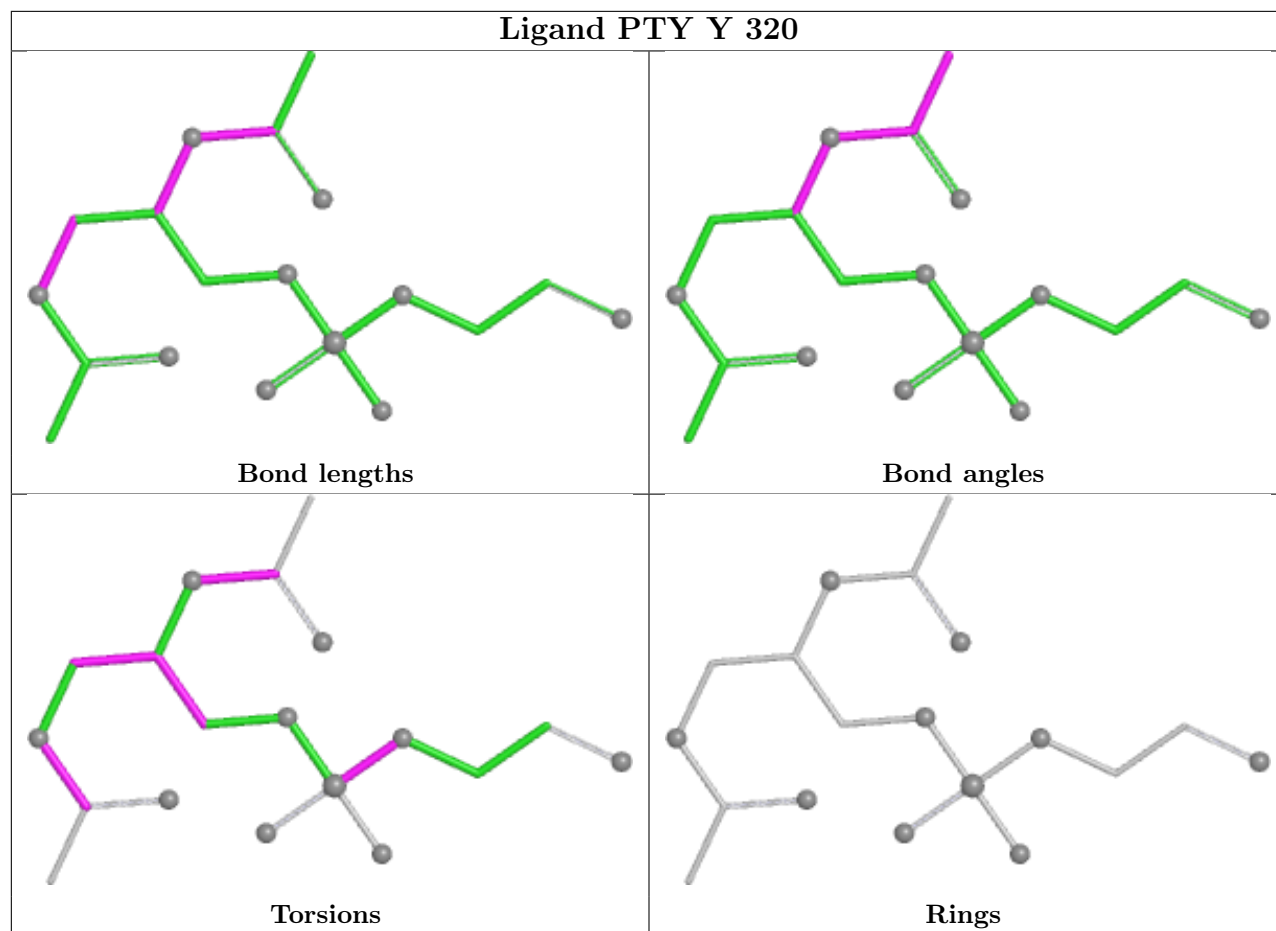
Rings



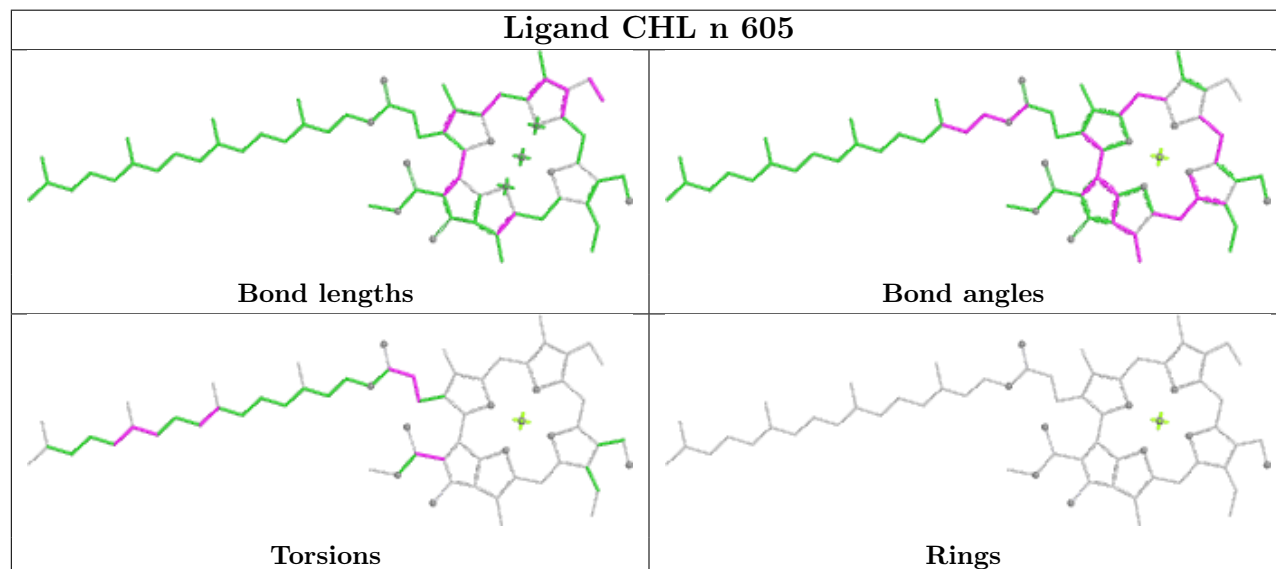


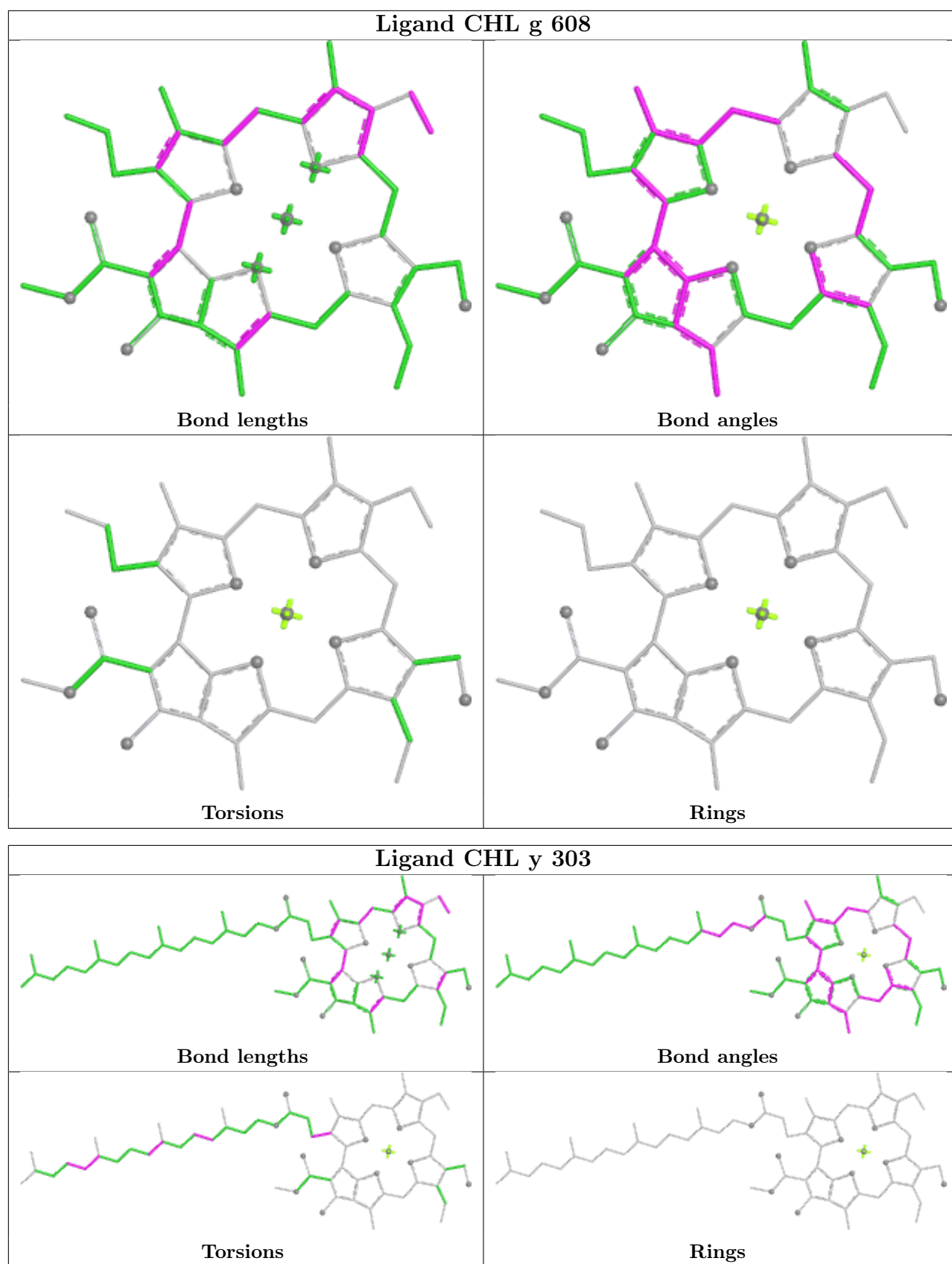


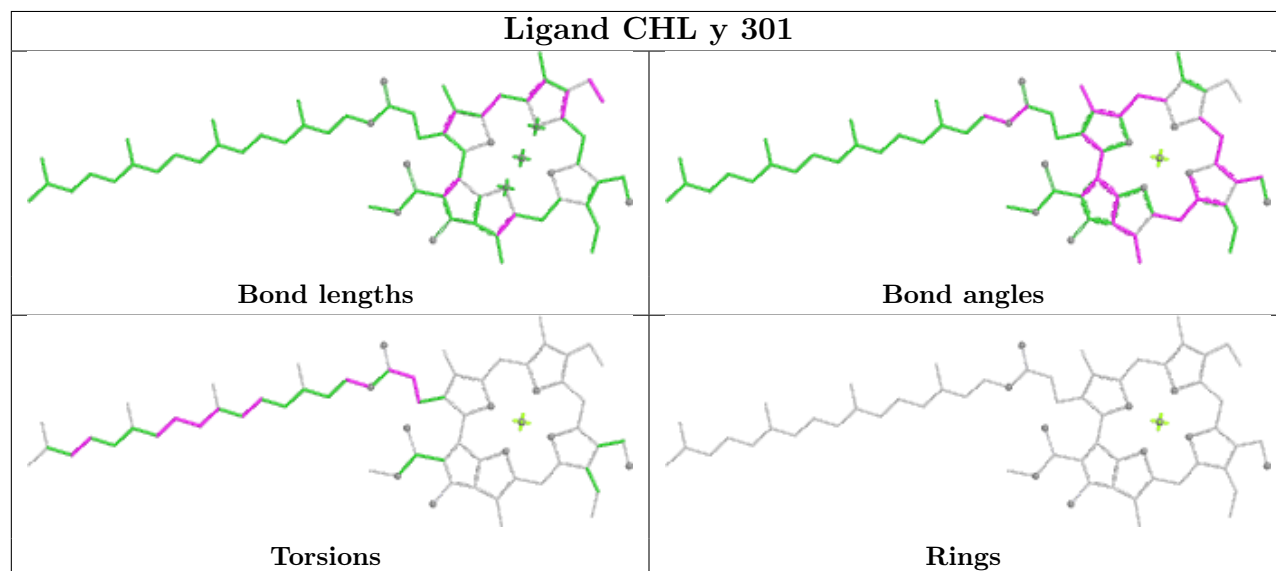
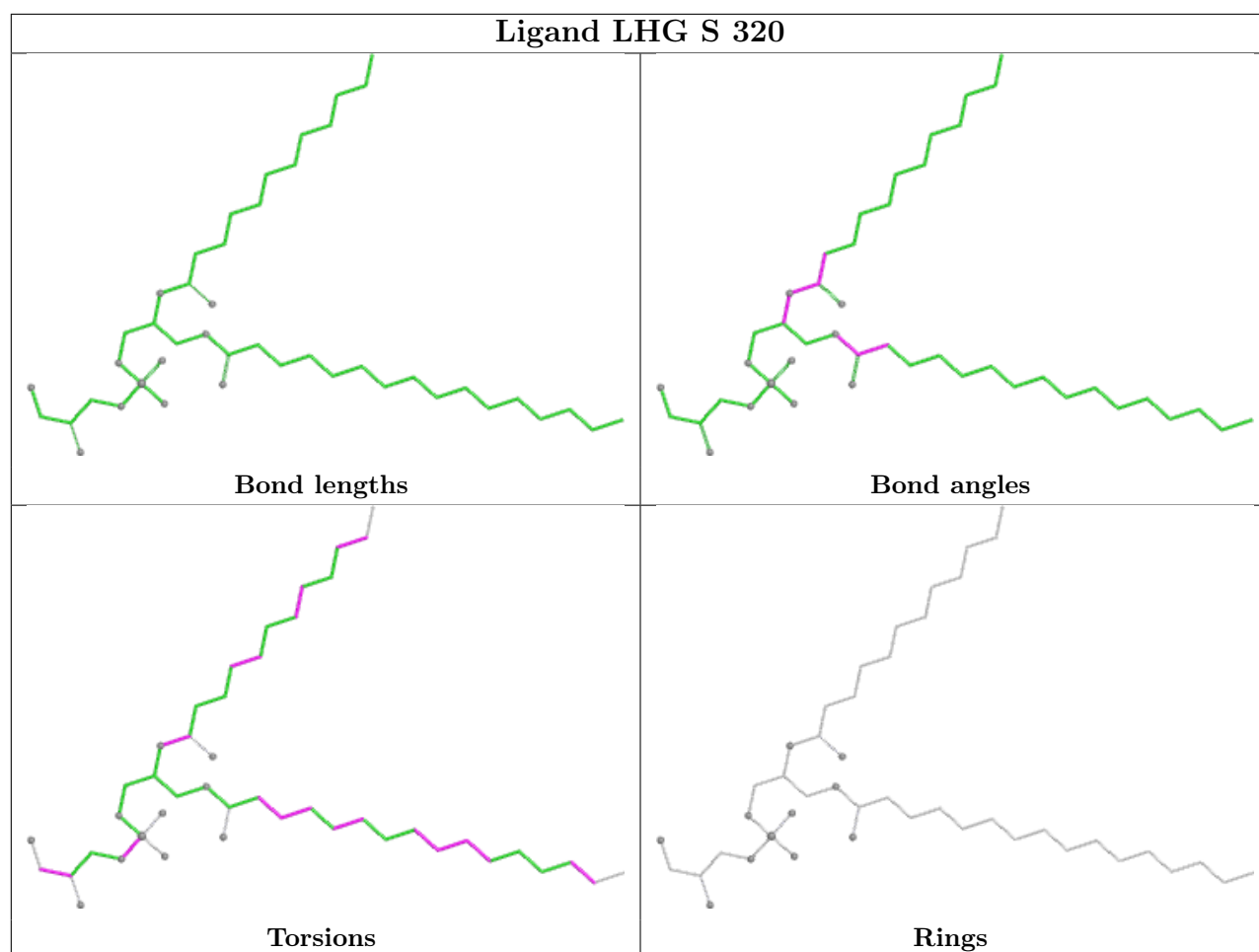
Ligand PTY Y 320

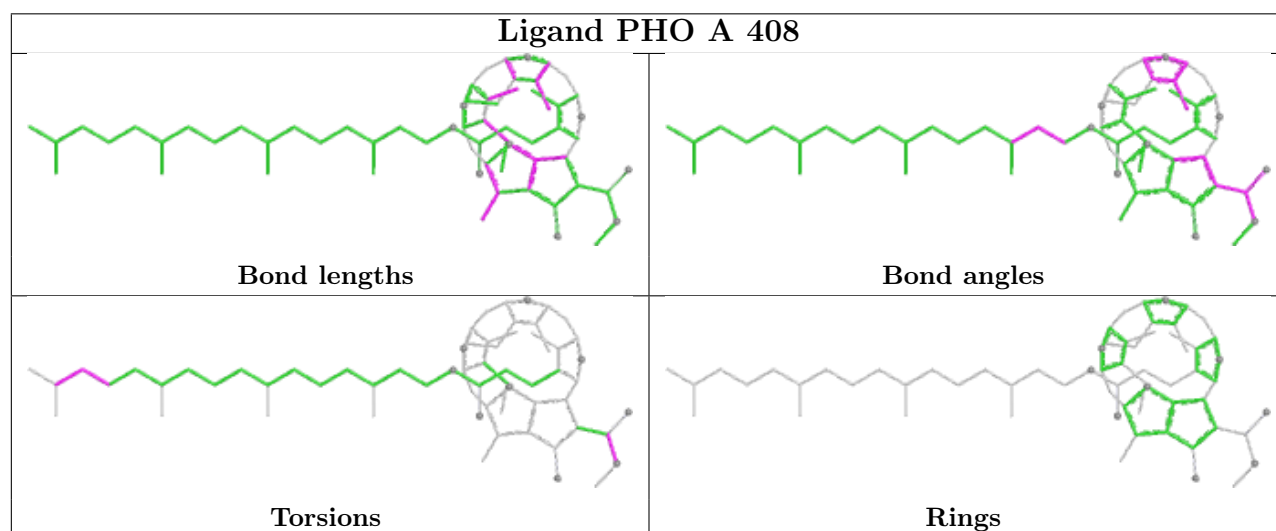
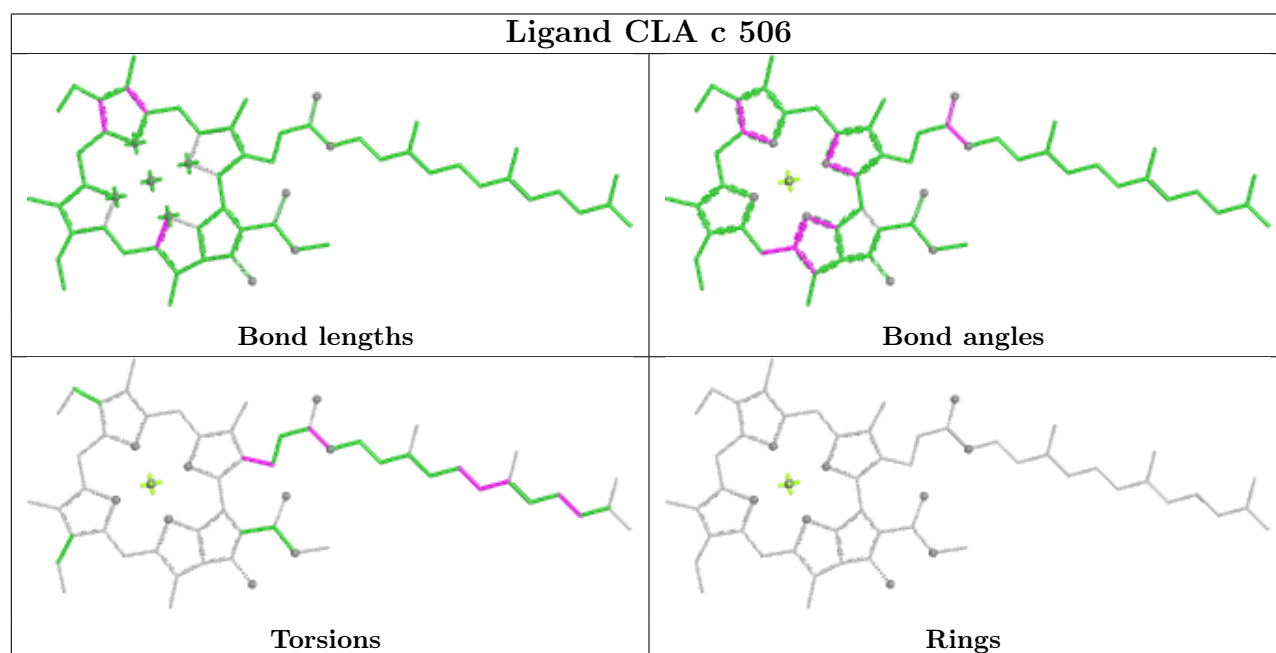
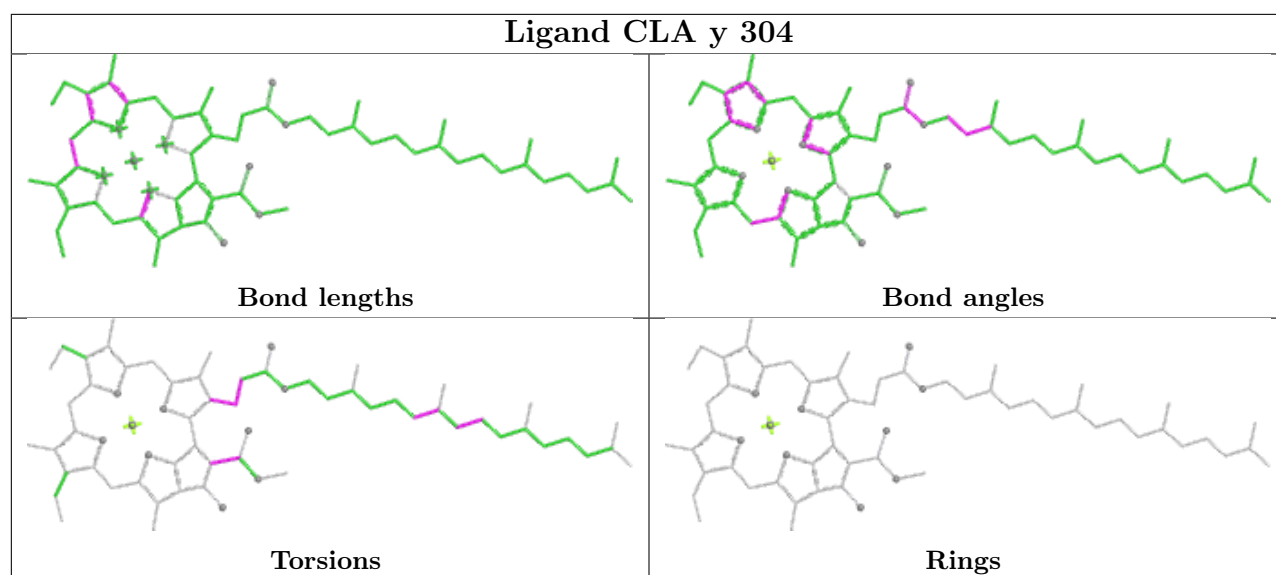


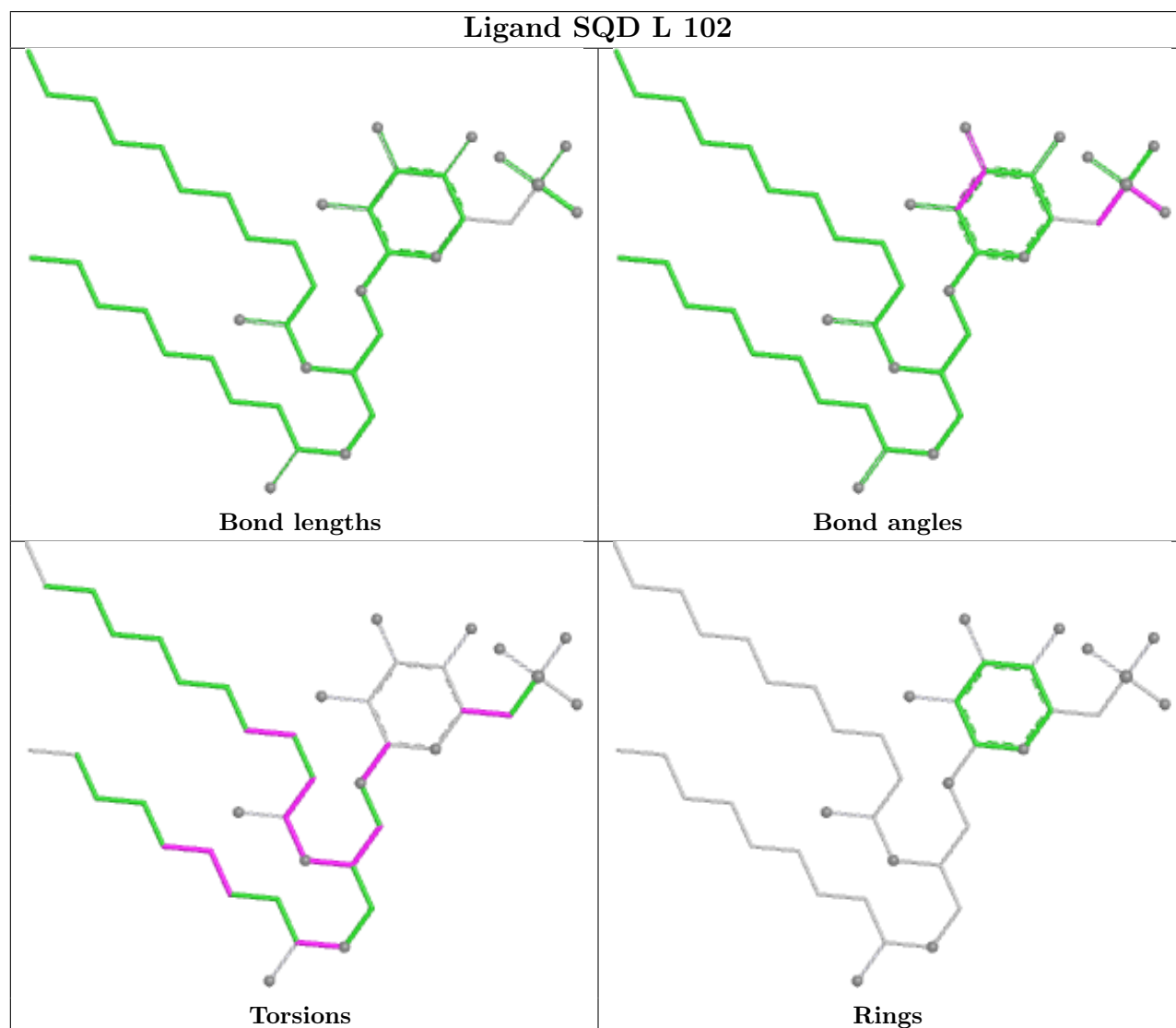
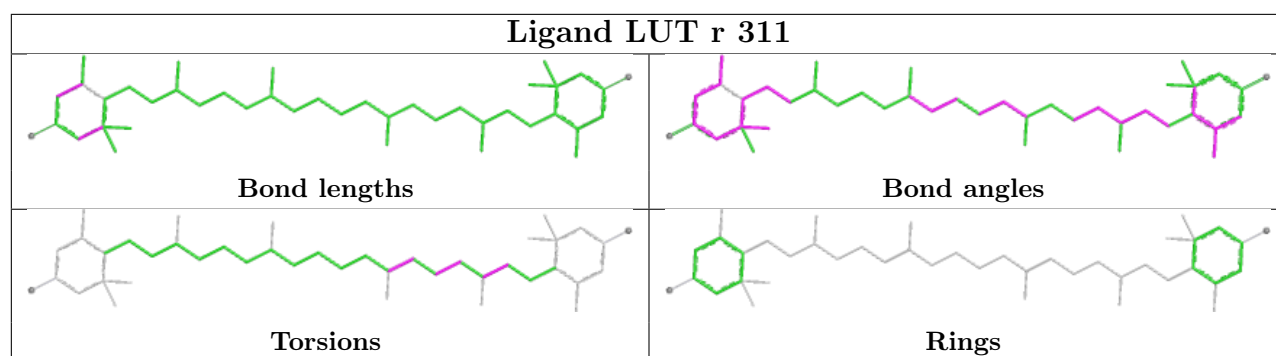
Ligand CHL n 605

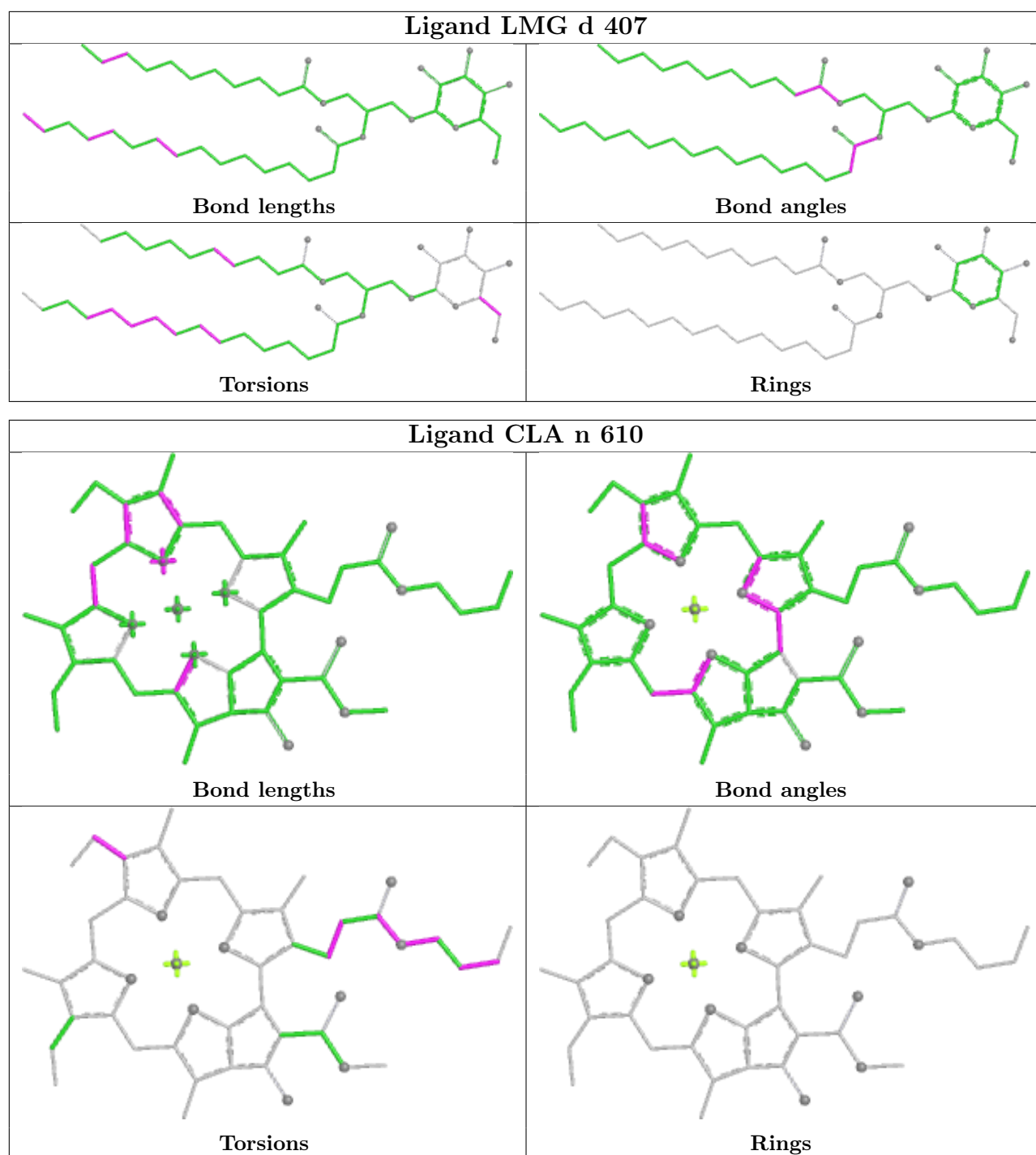




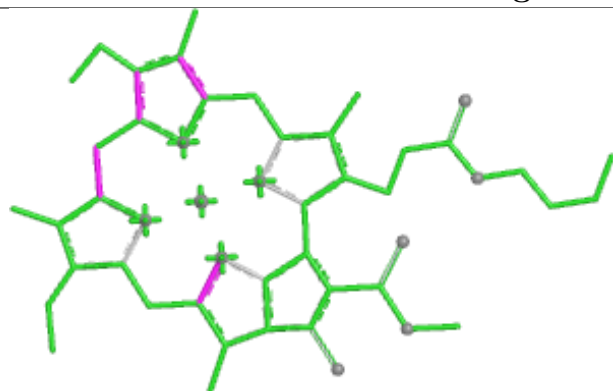




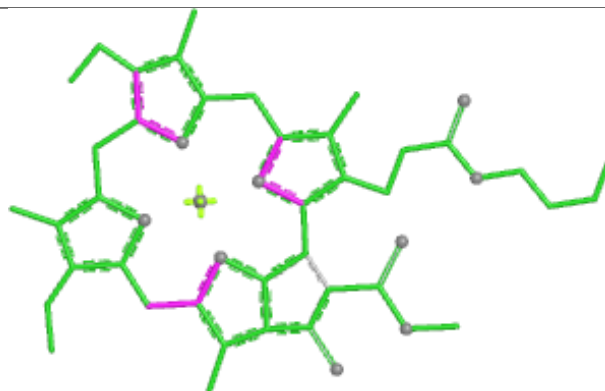




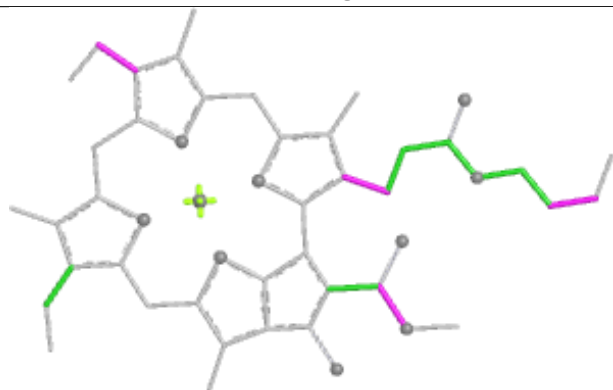
Ligand CLA G 614



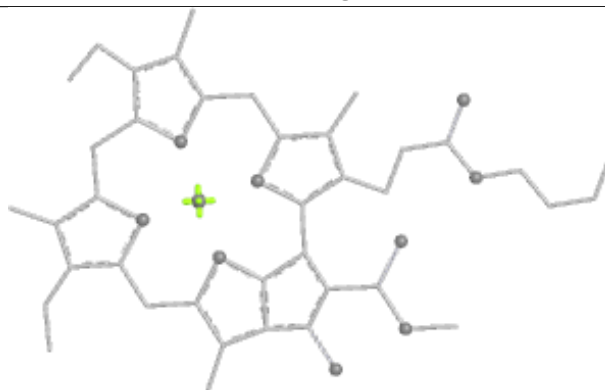
Bond lengths



Bond angles

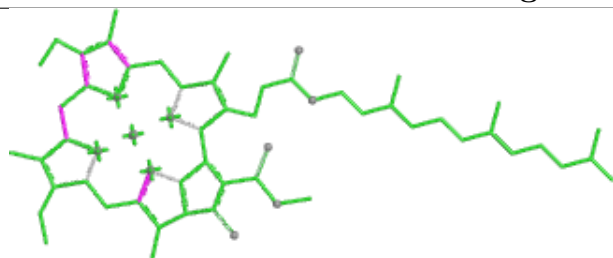


Torsions

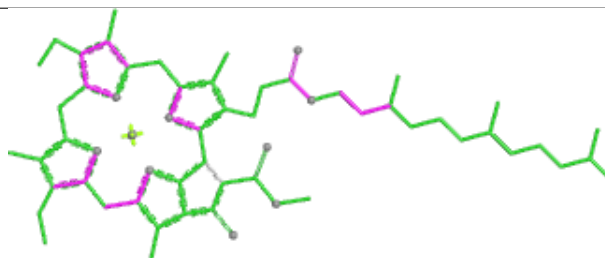


Rings

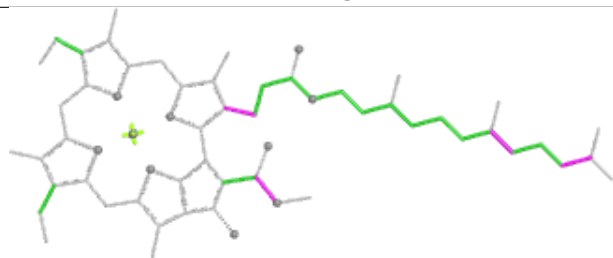
Ligand CLA r 309



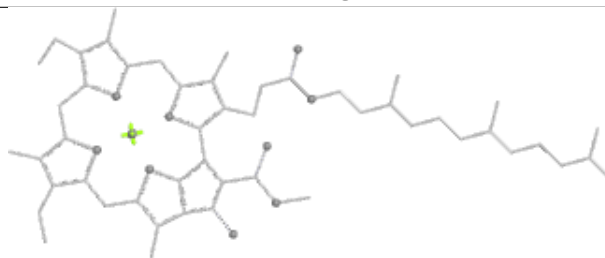
Bond lengths



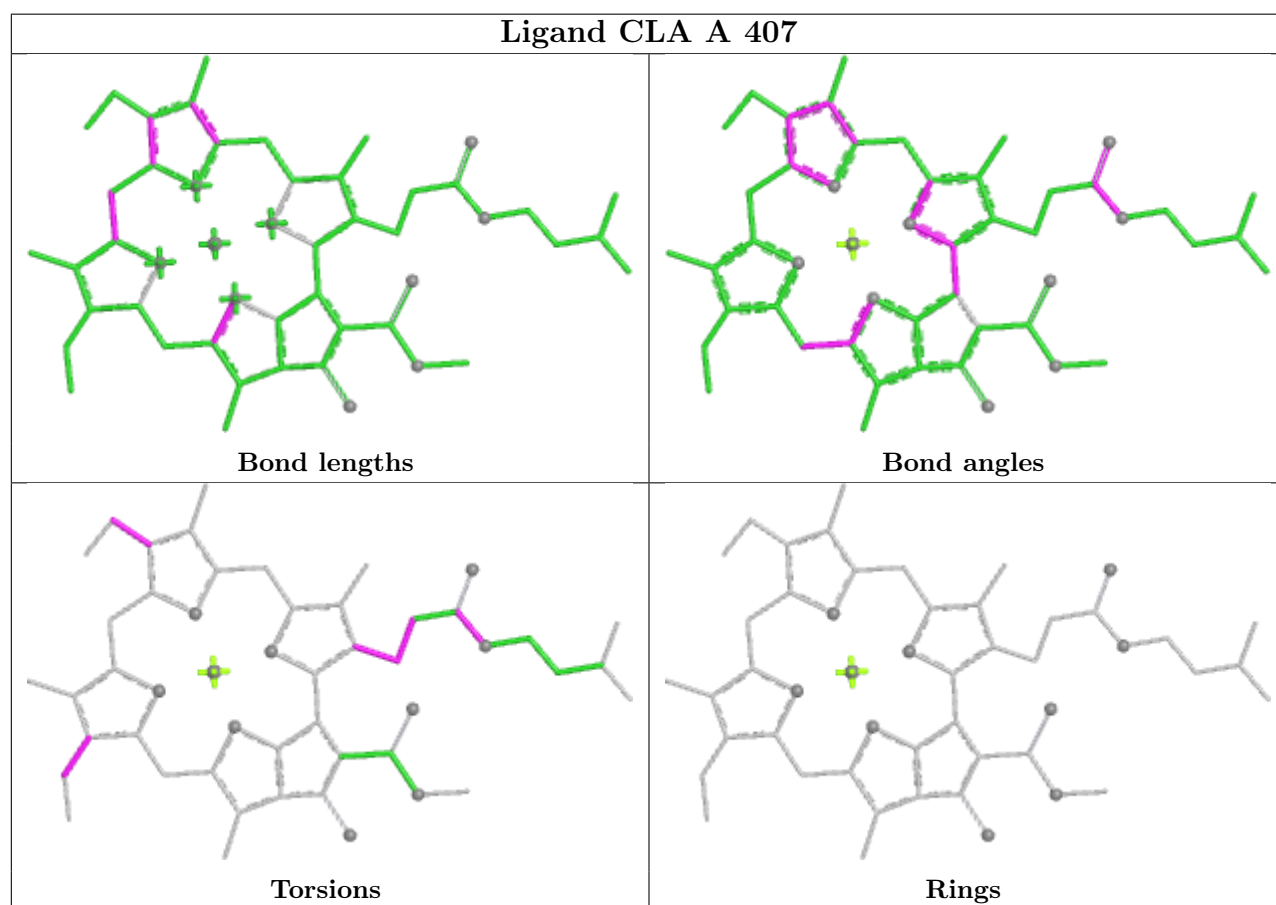
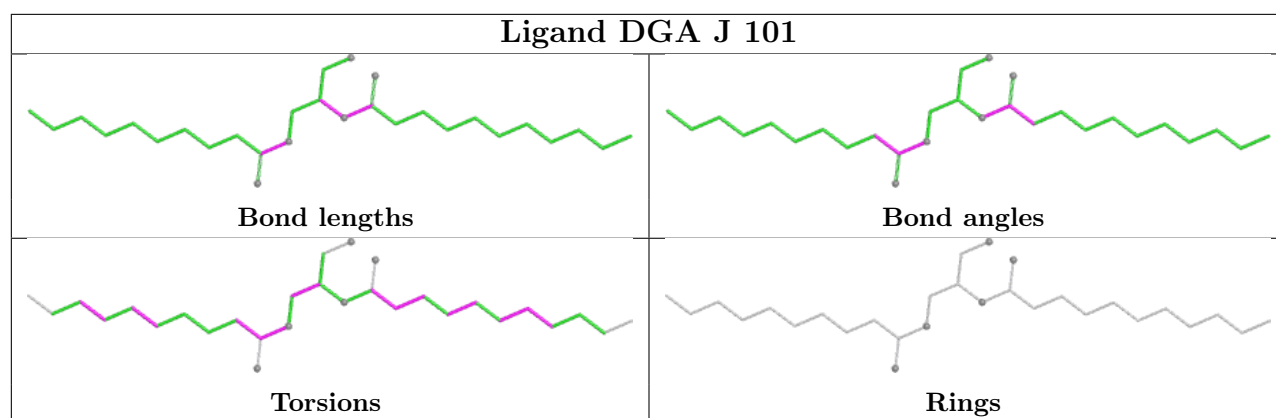
Bond angles

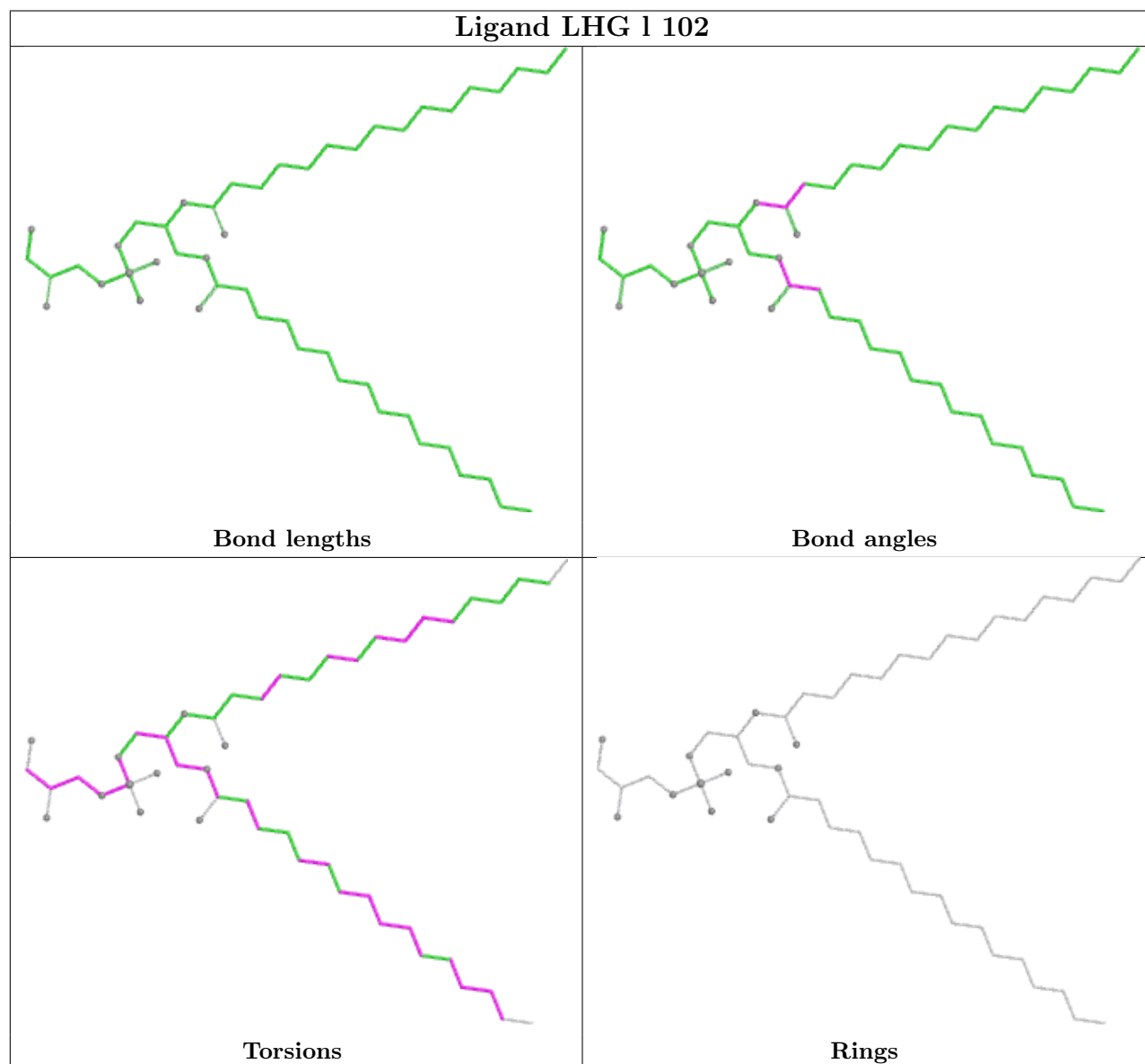
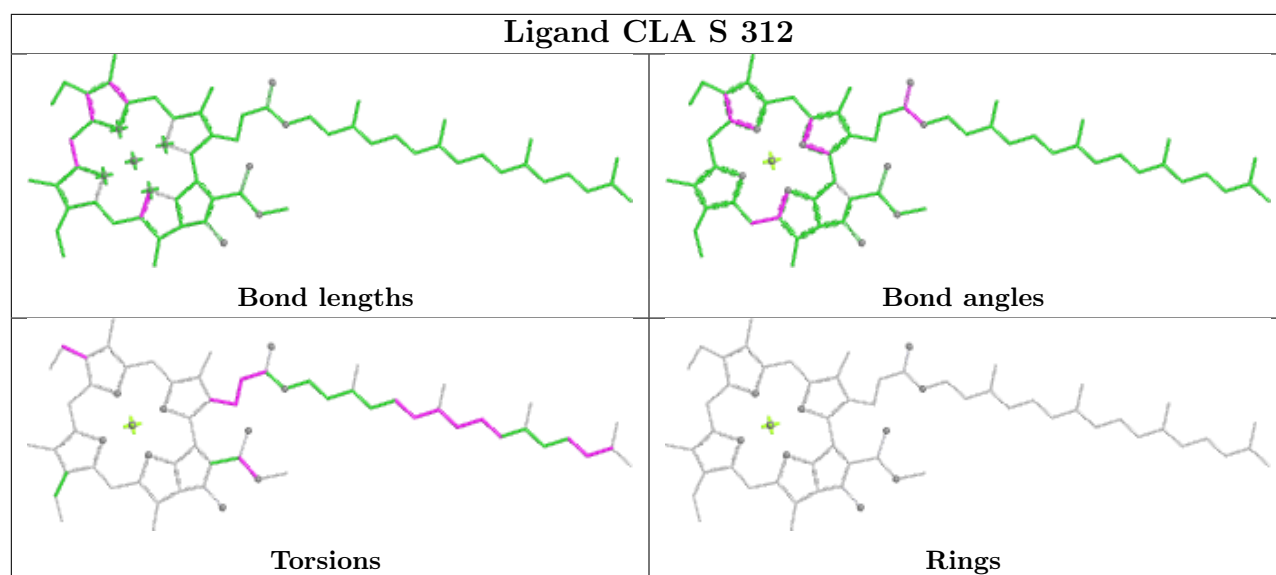


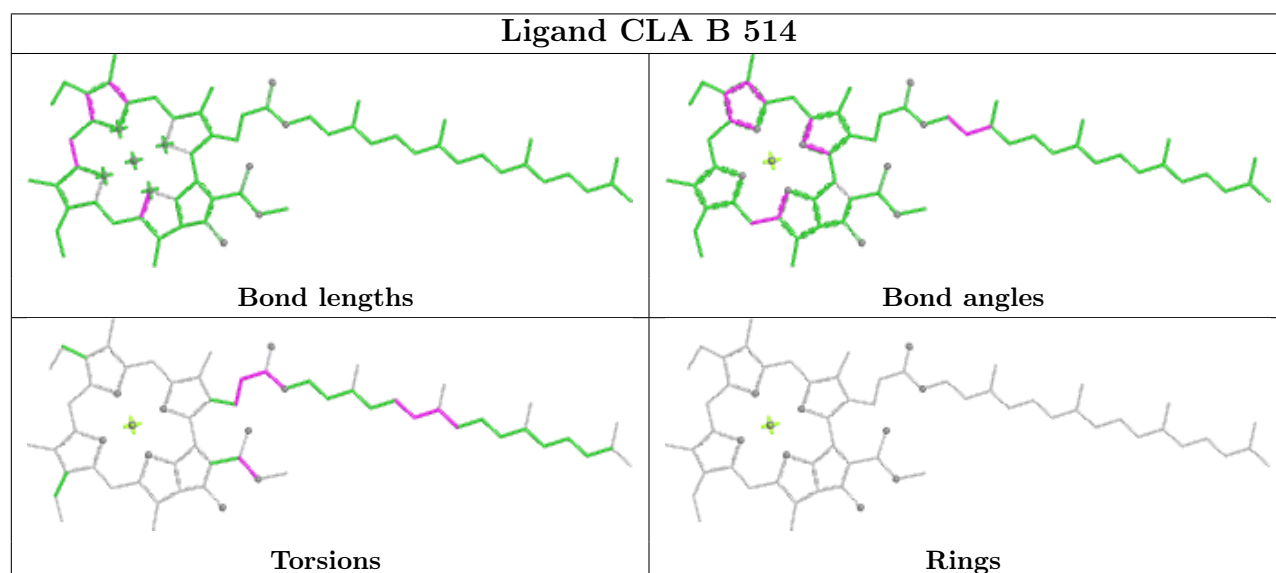
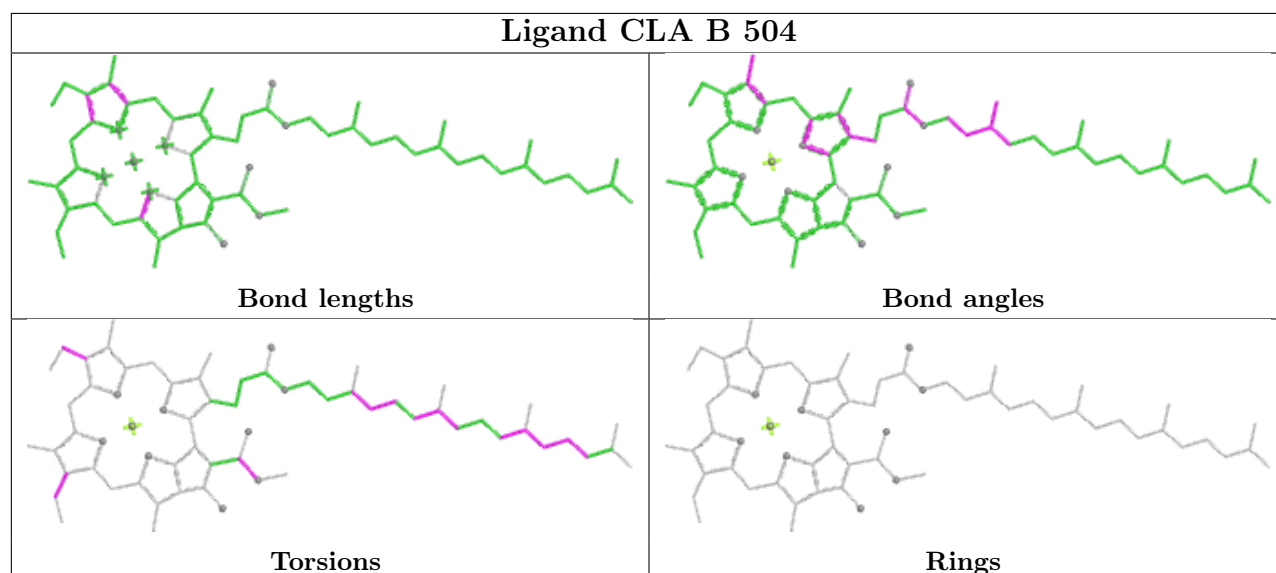
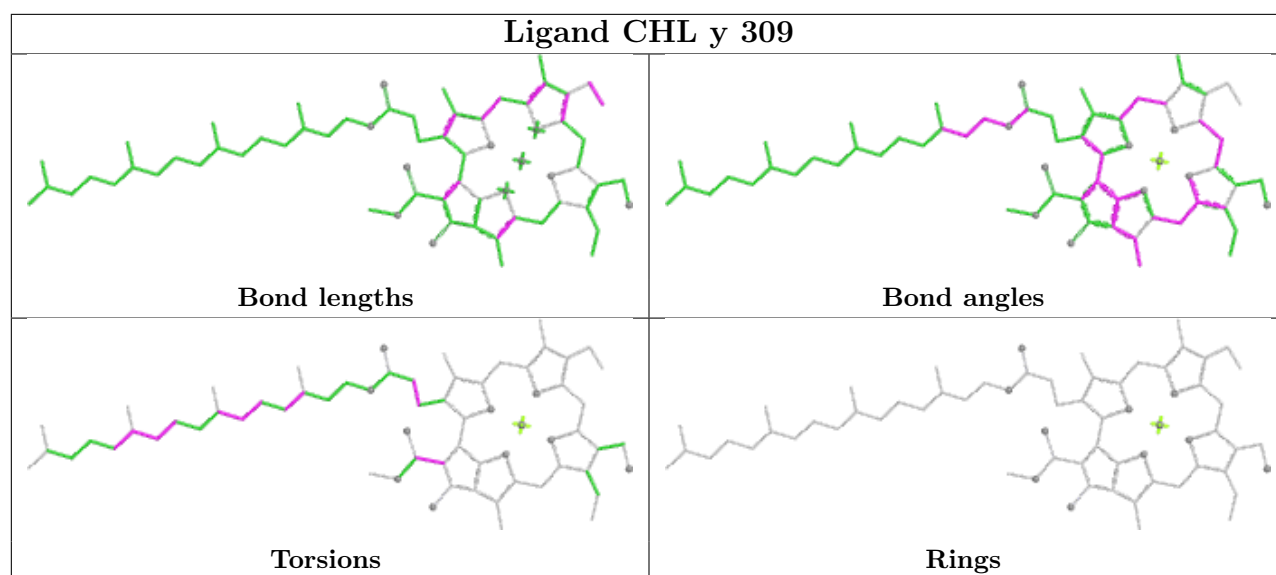
Torsions

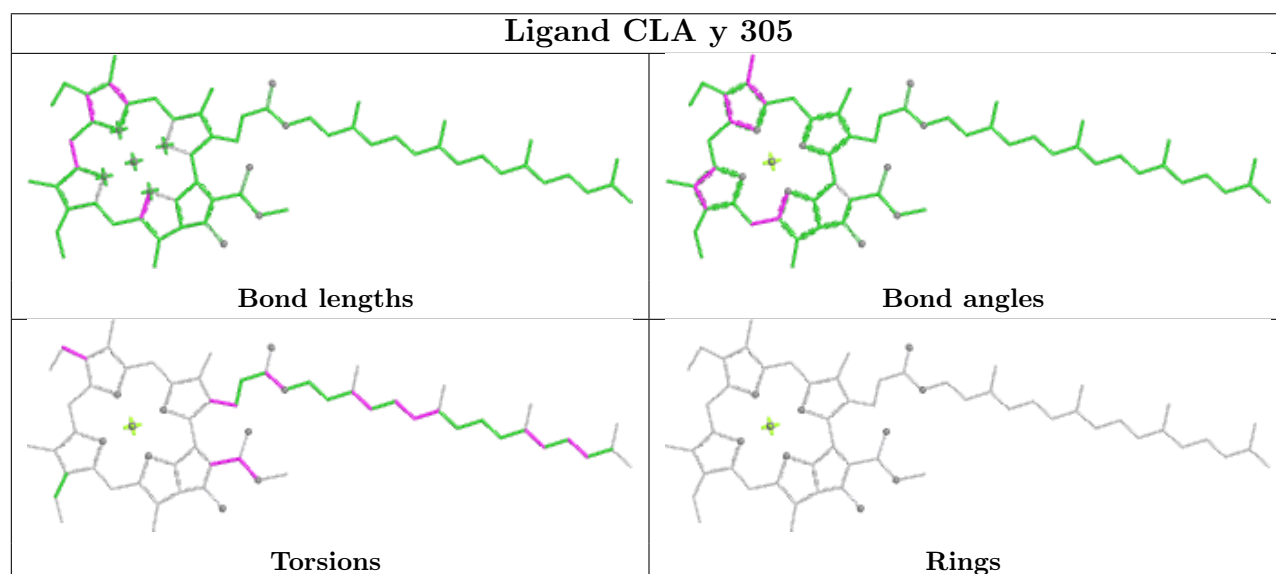
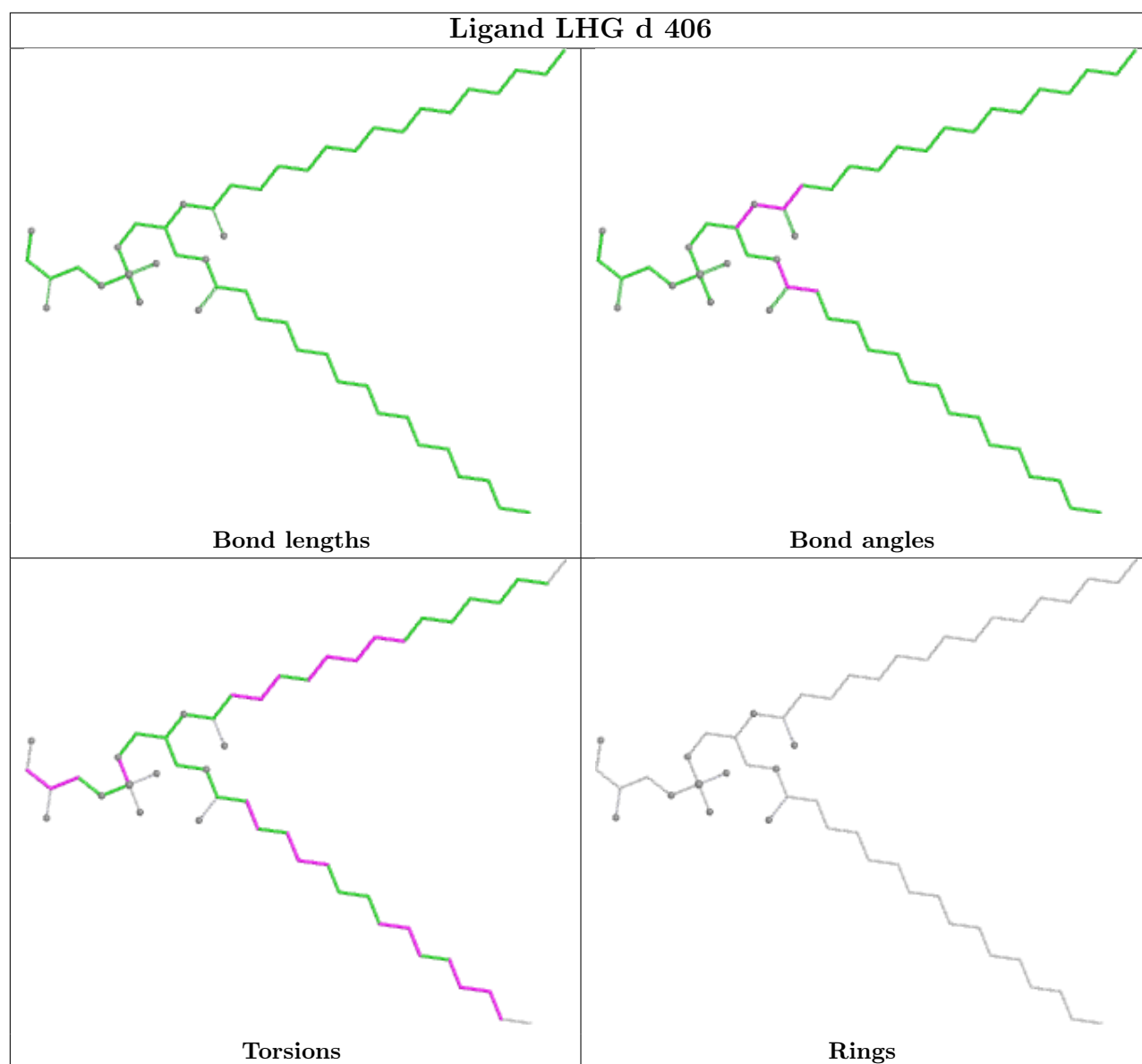


Rings

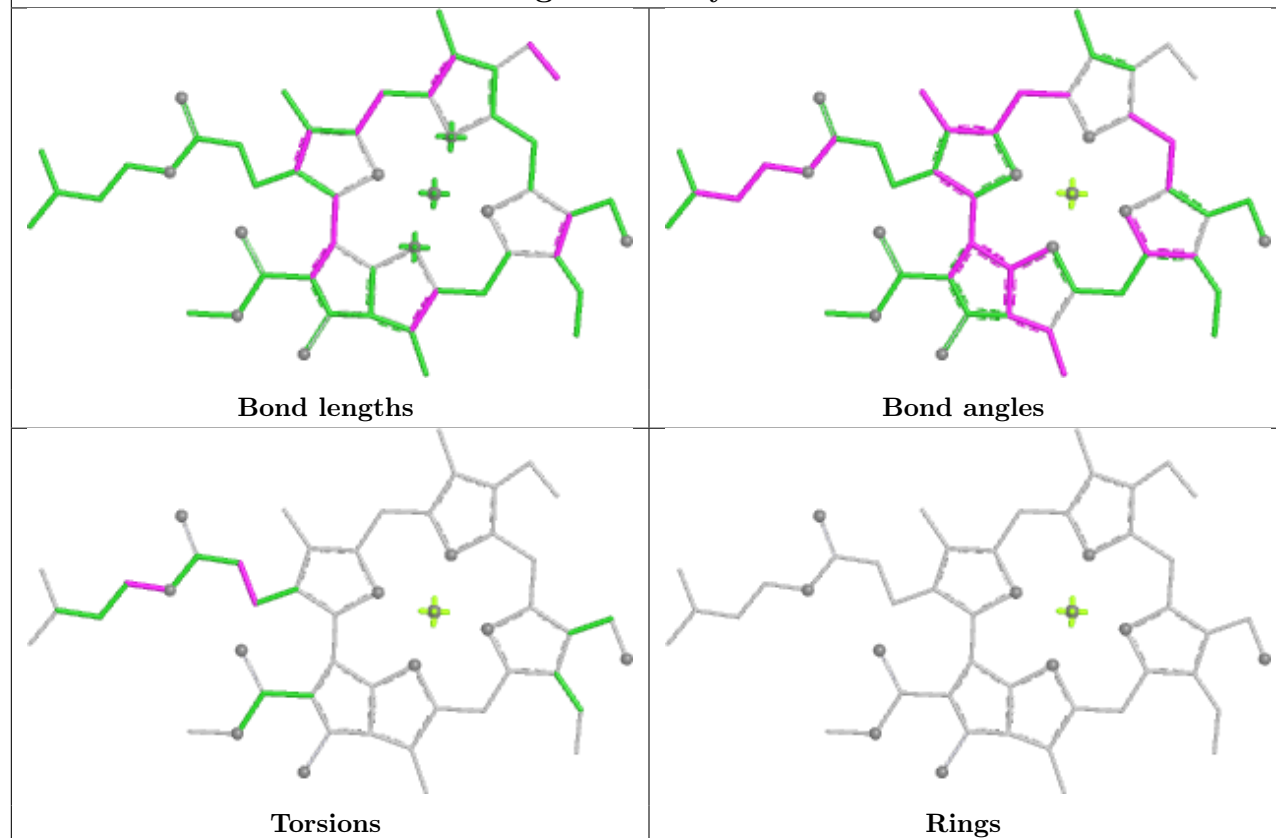




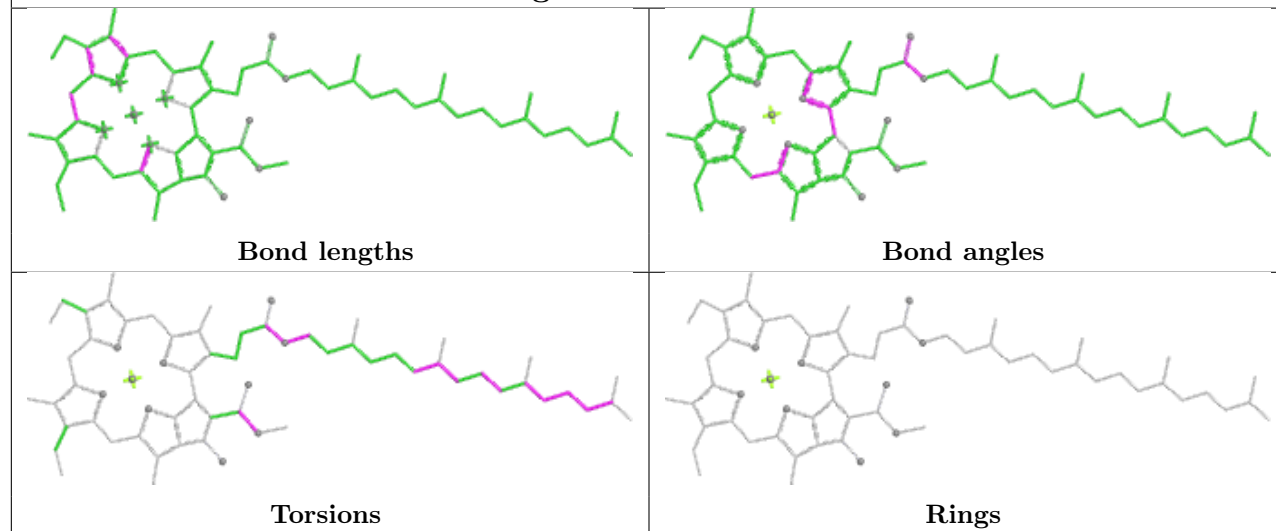


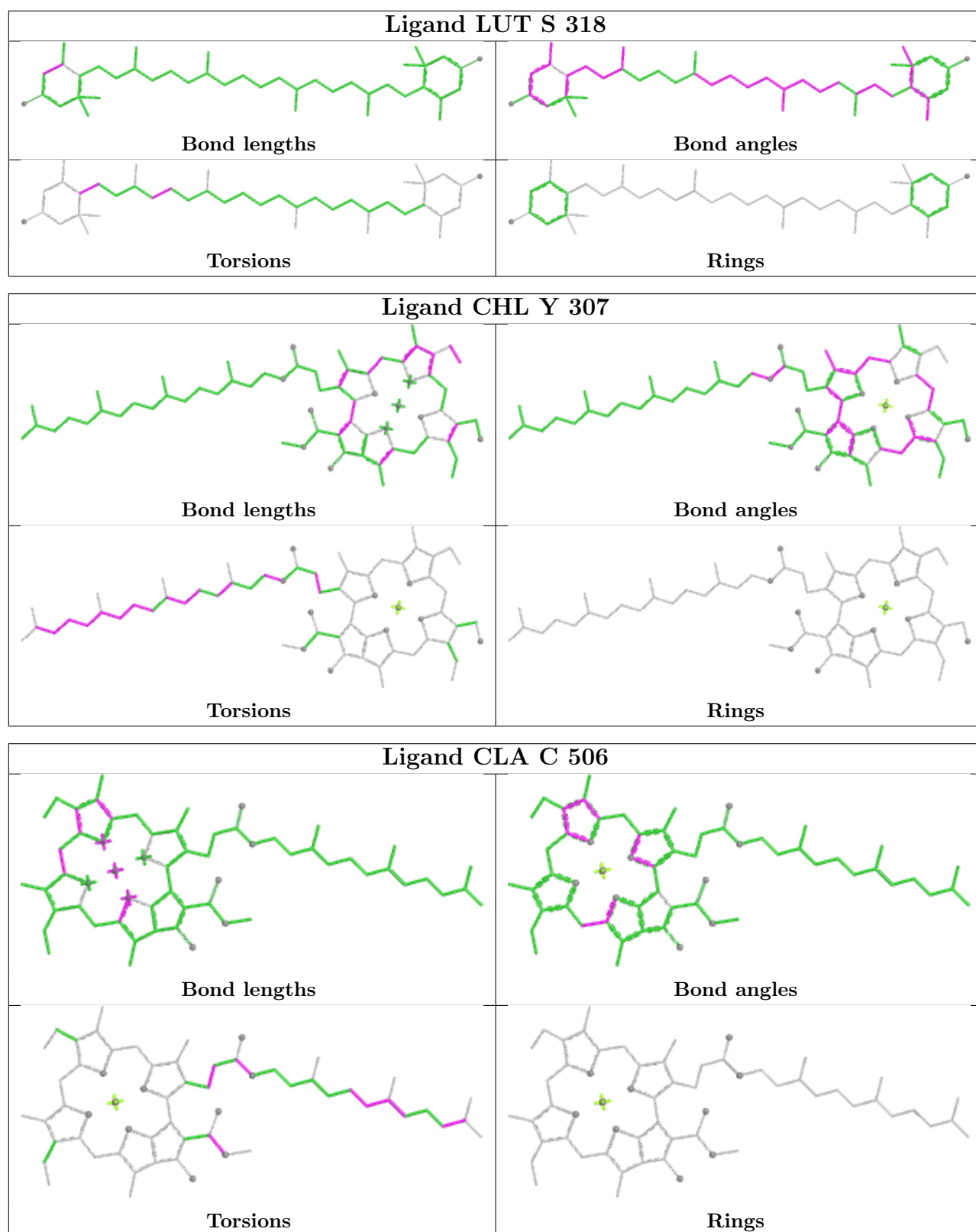


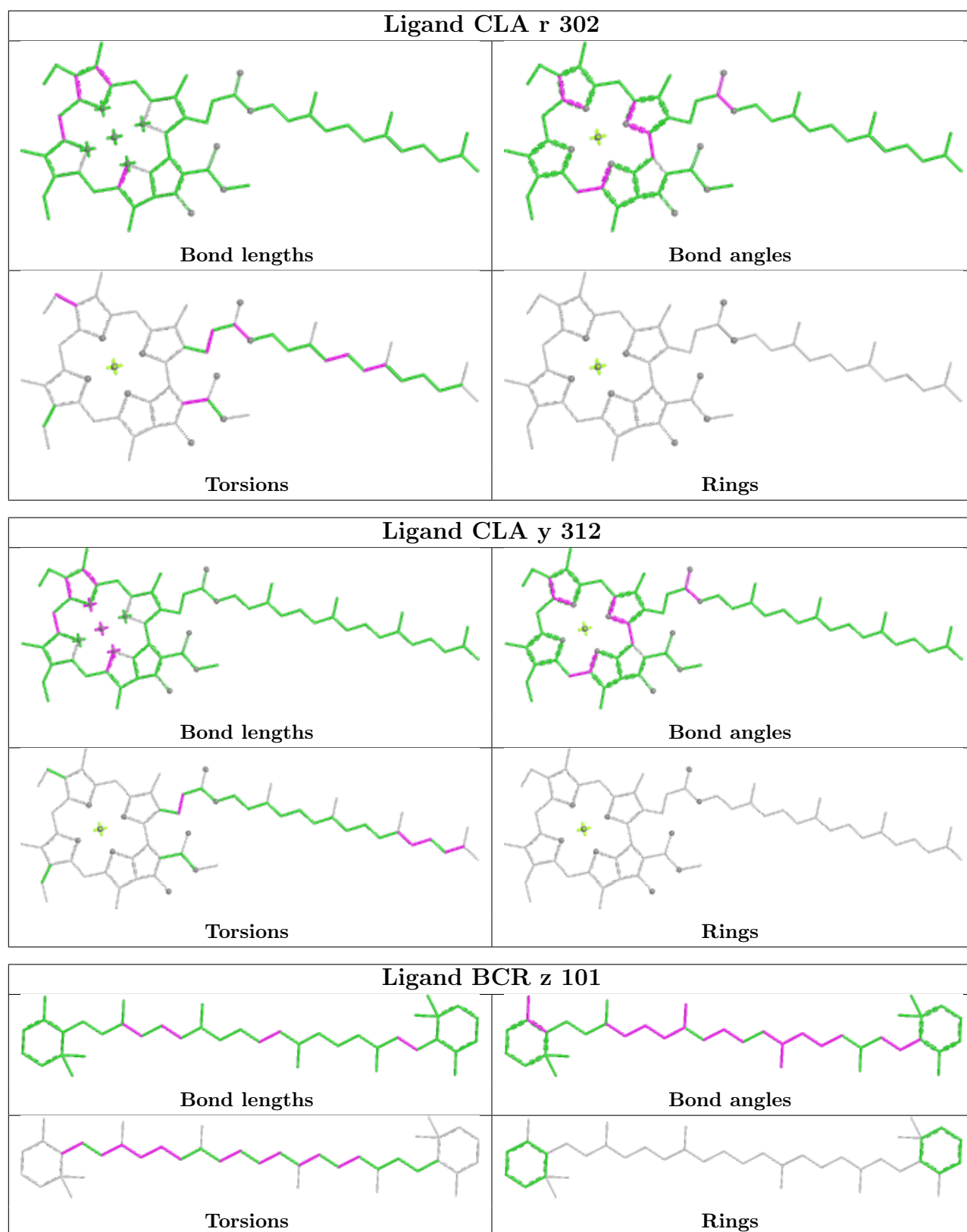
Ligand CHL y 308



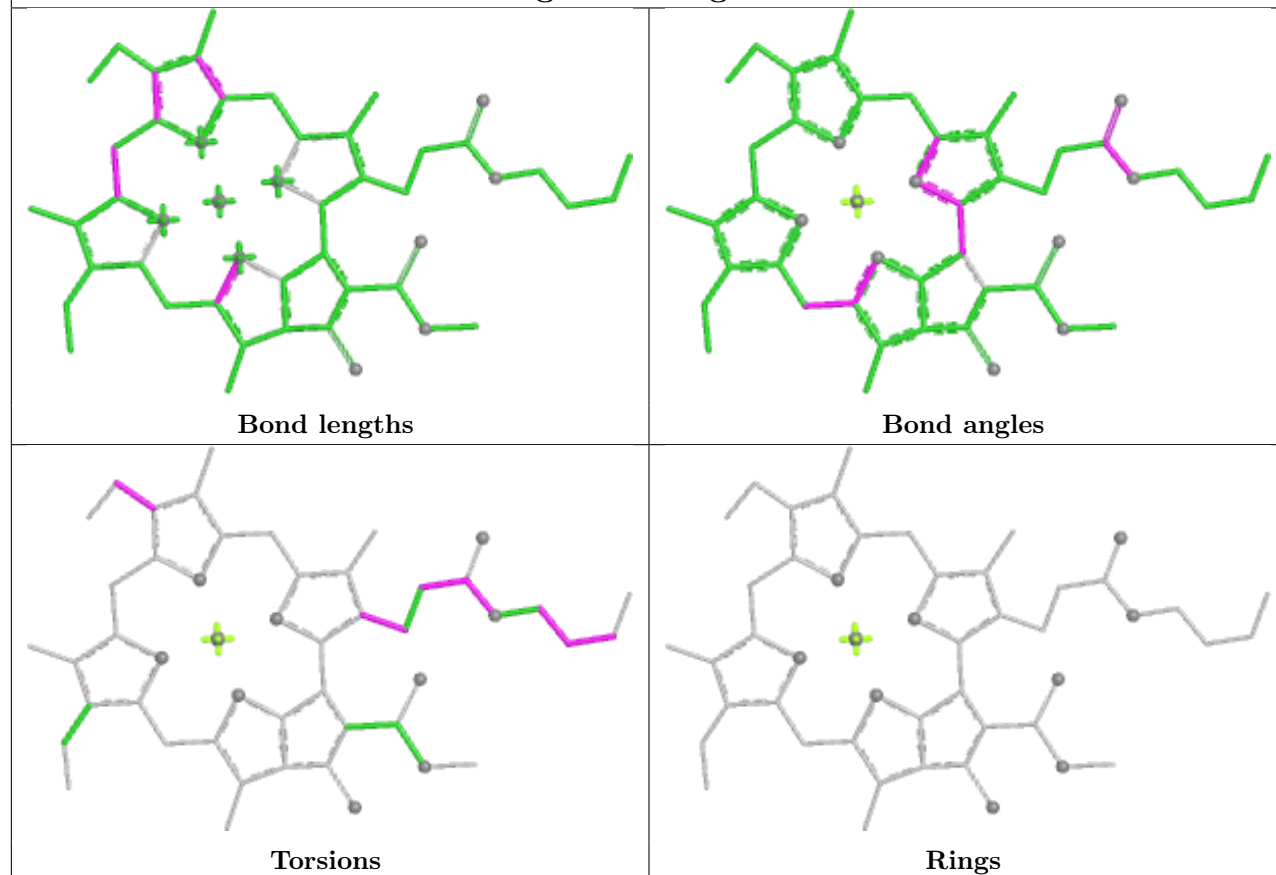
Ligand CLA C 510



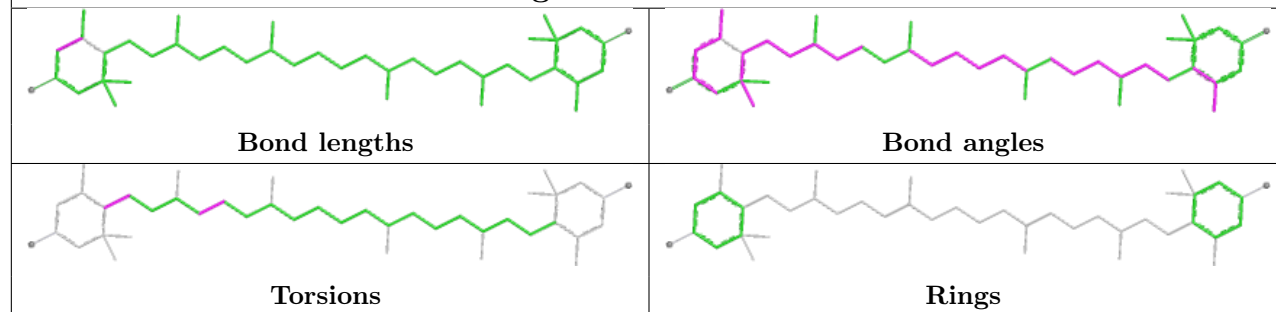


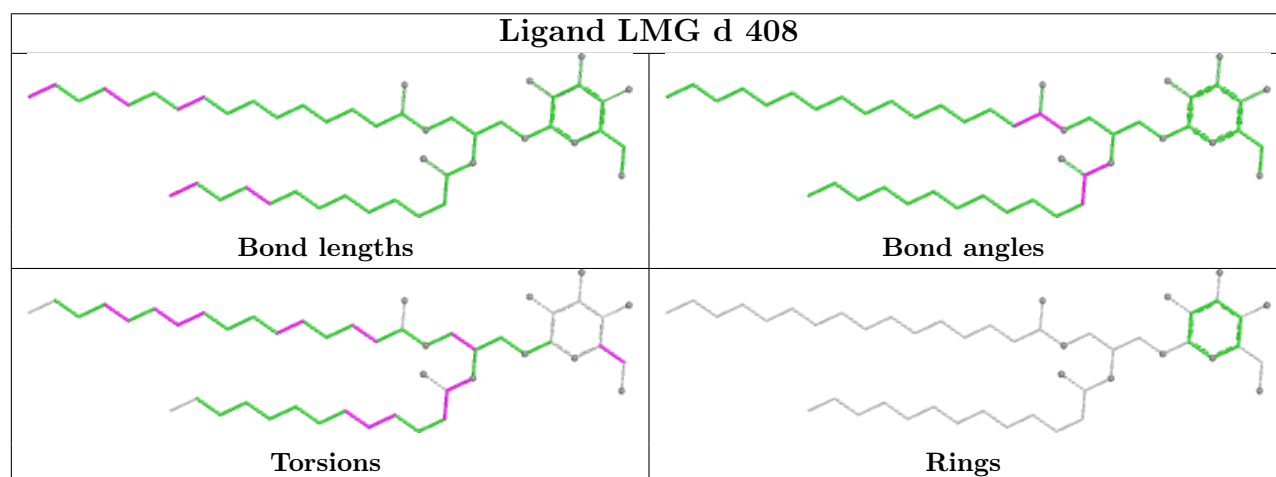
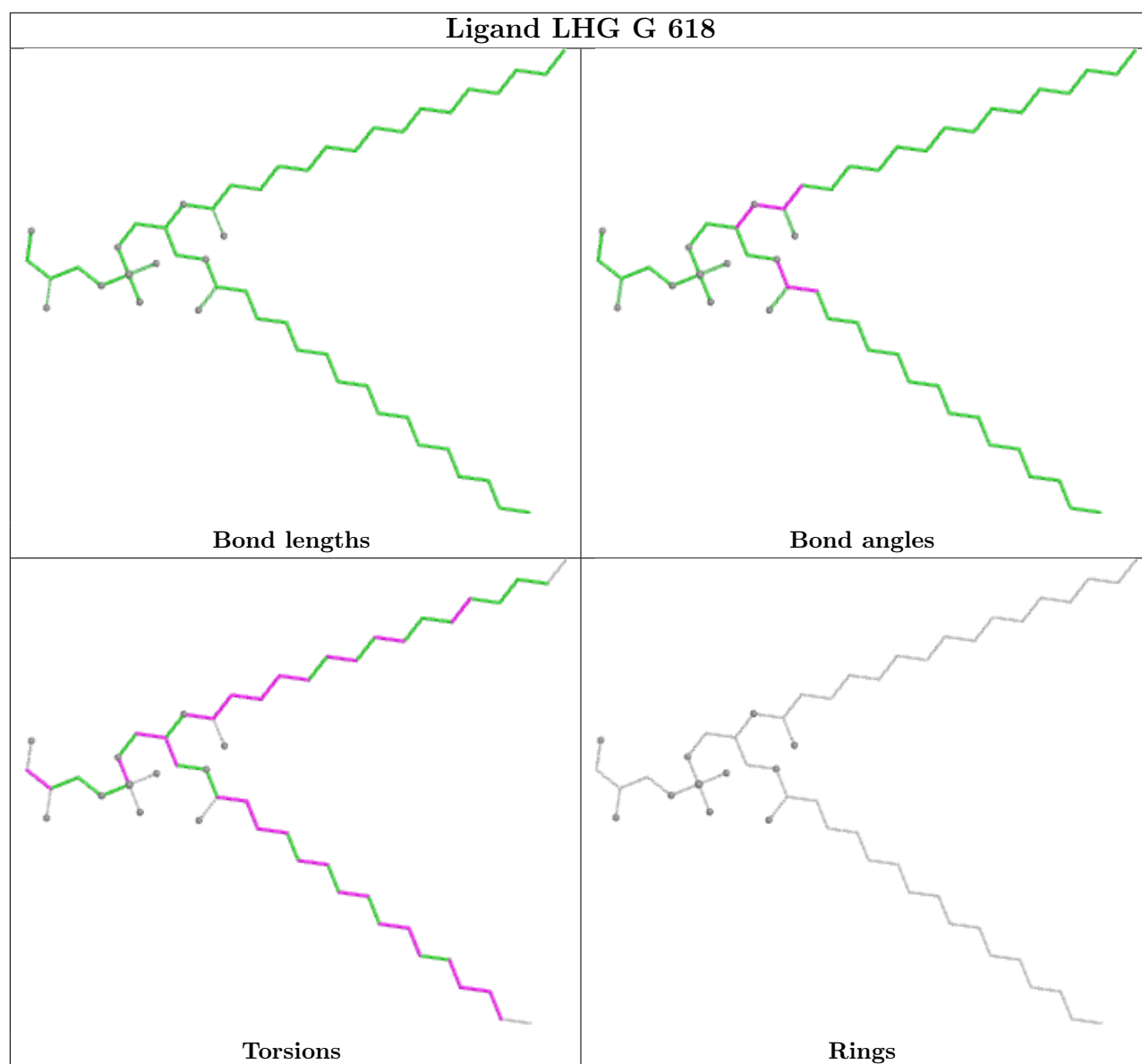


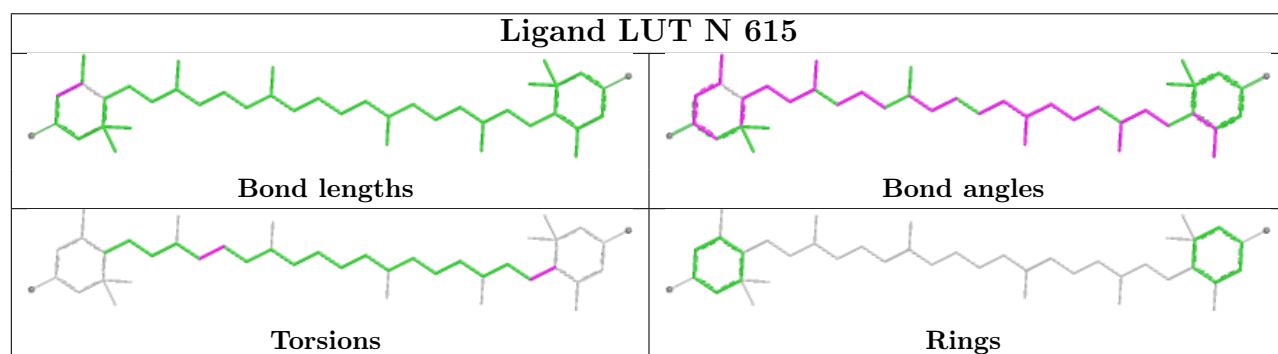
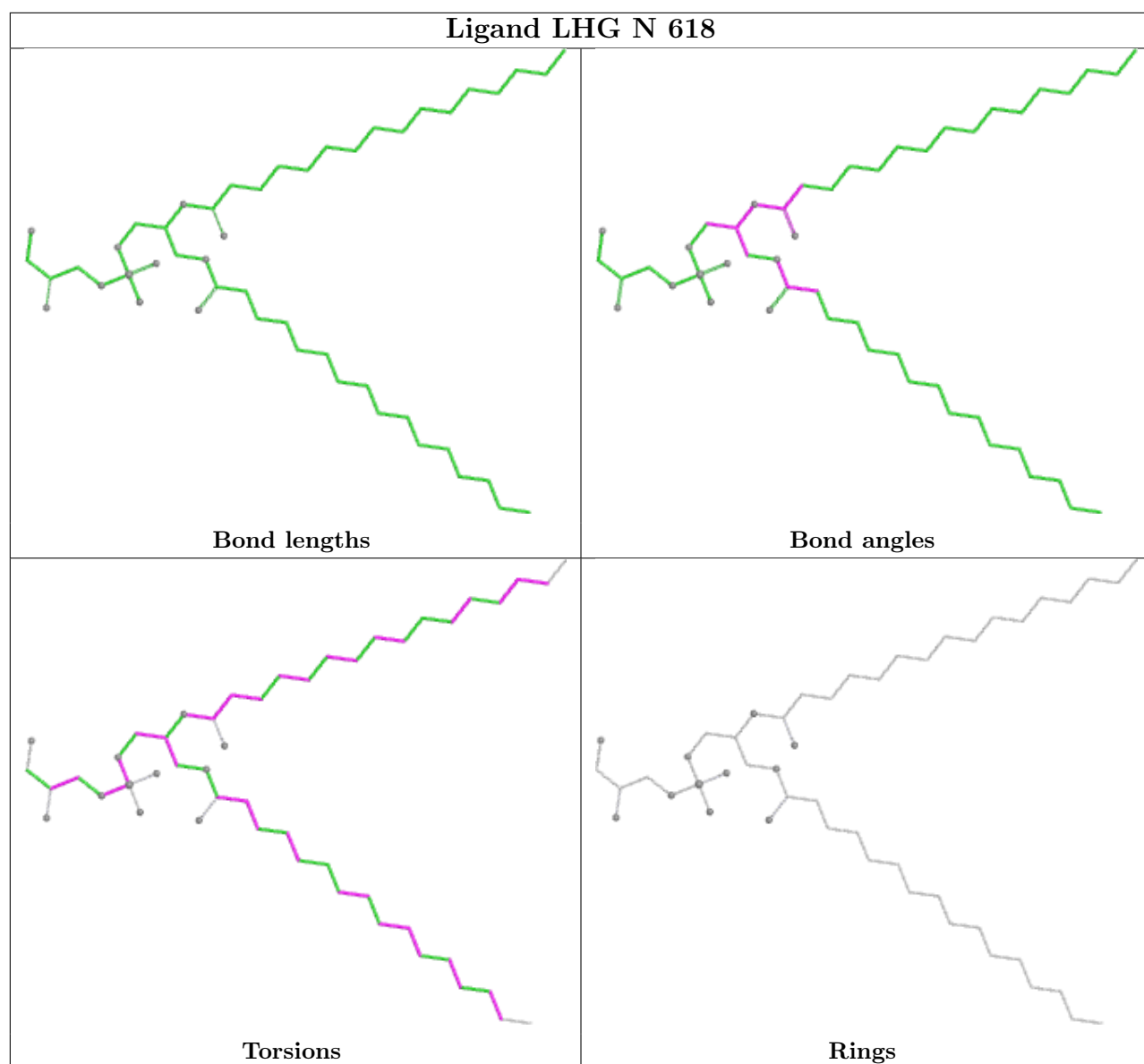
Ligand CLA g 614



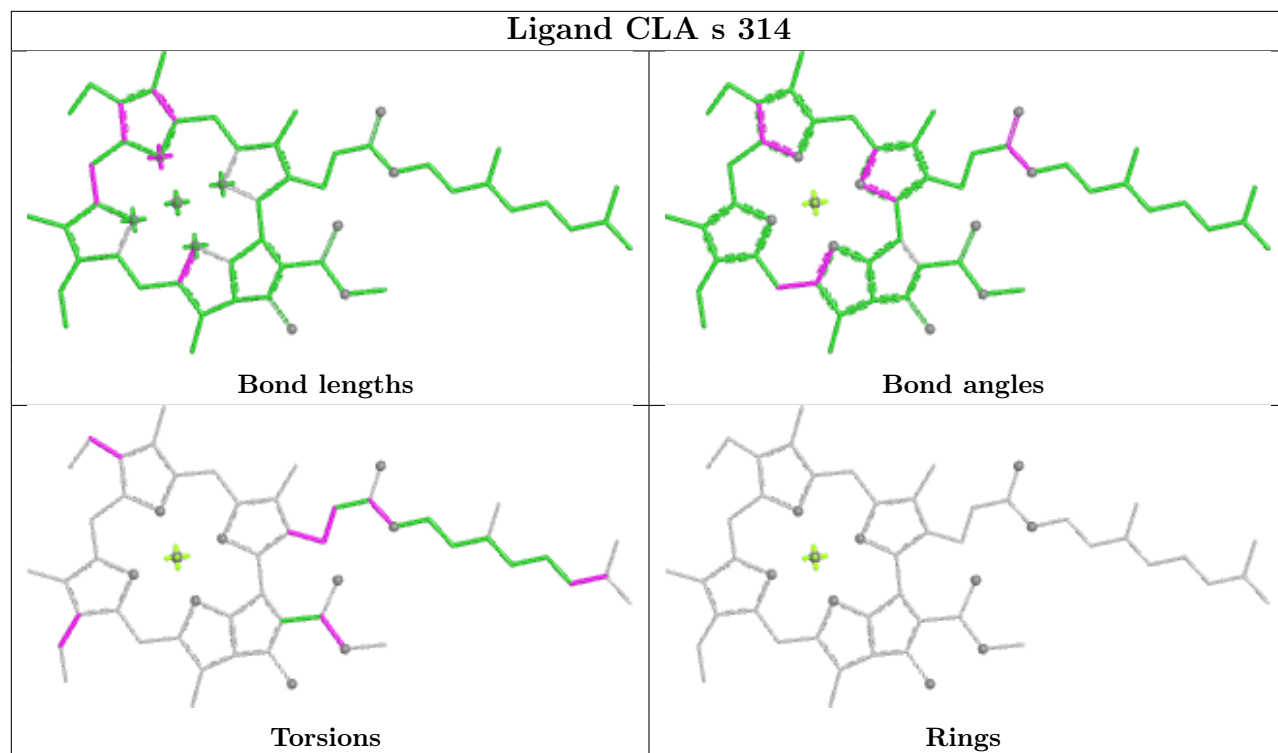
Ligand LUT Y 317



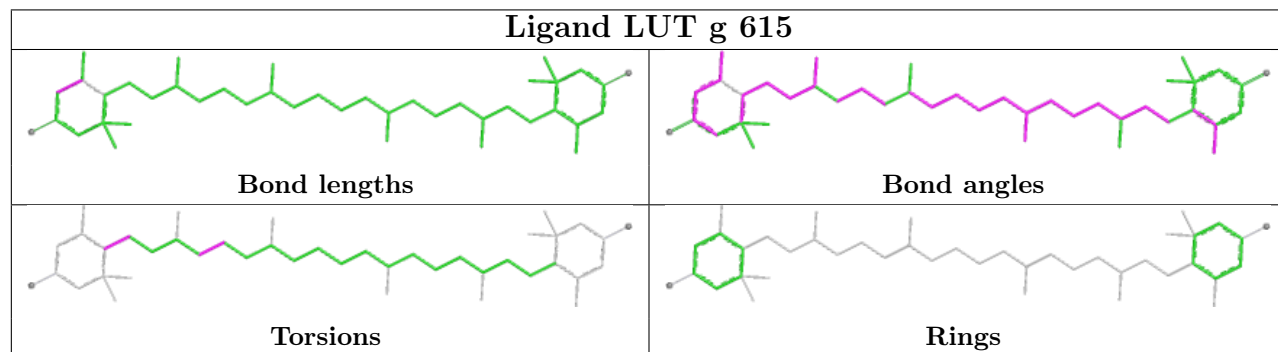




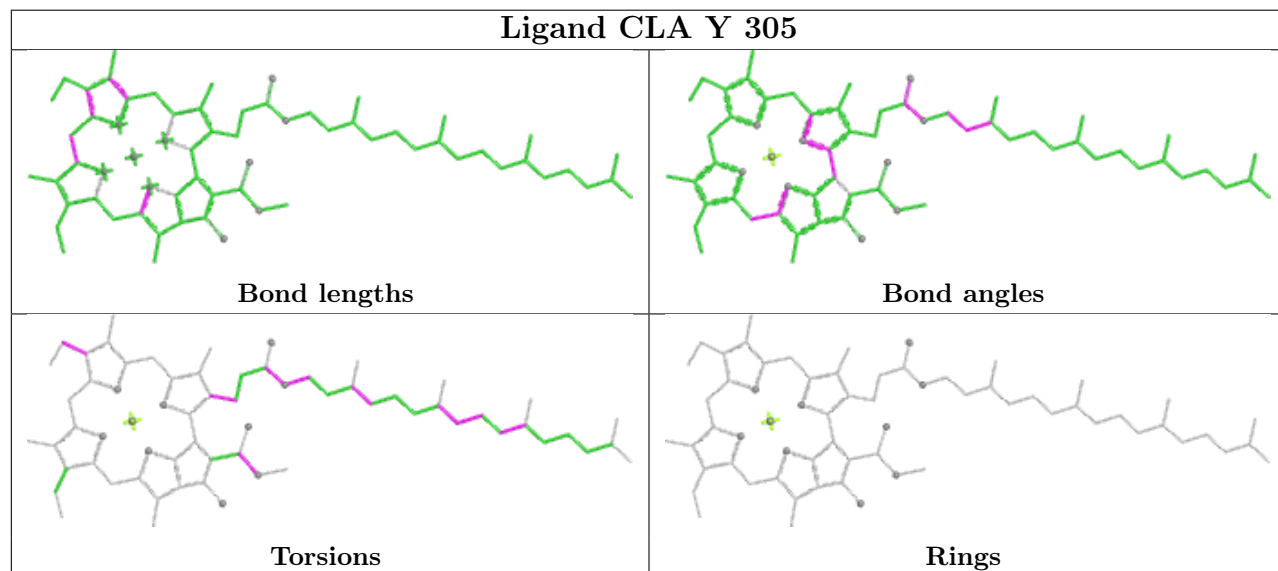
Ligand CLA s 314

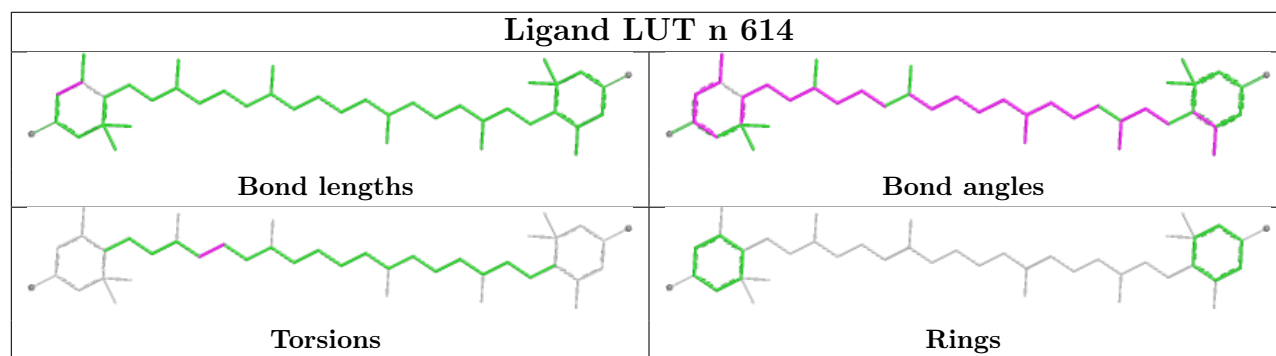
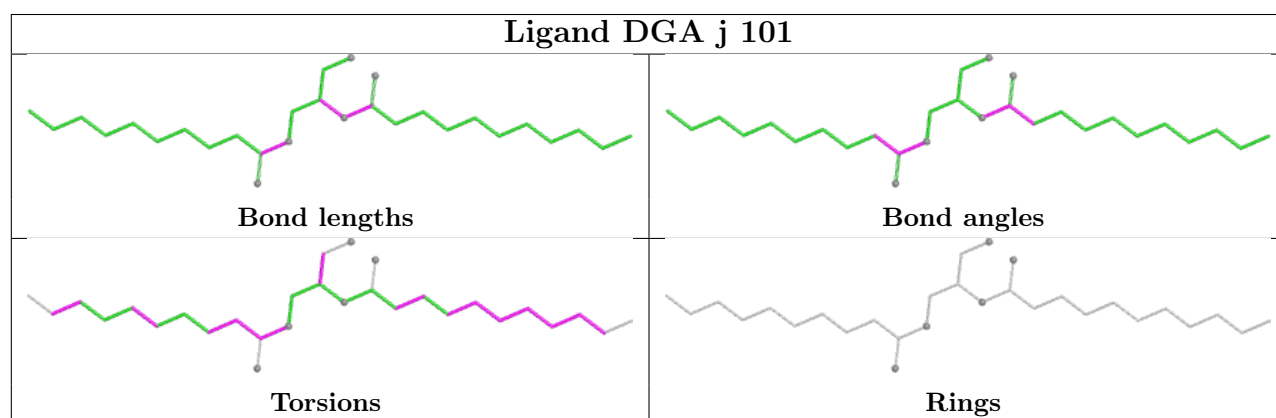
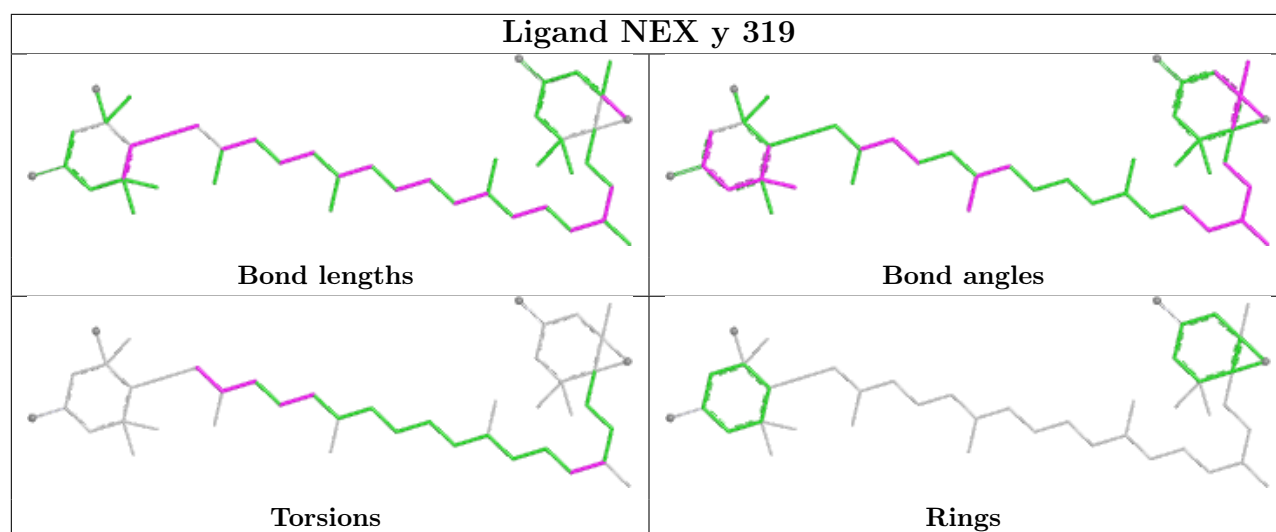


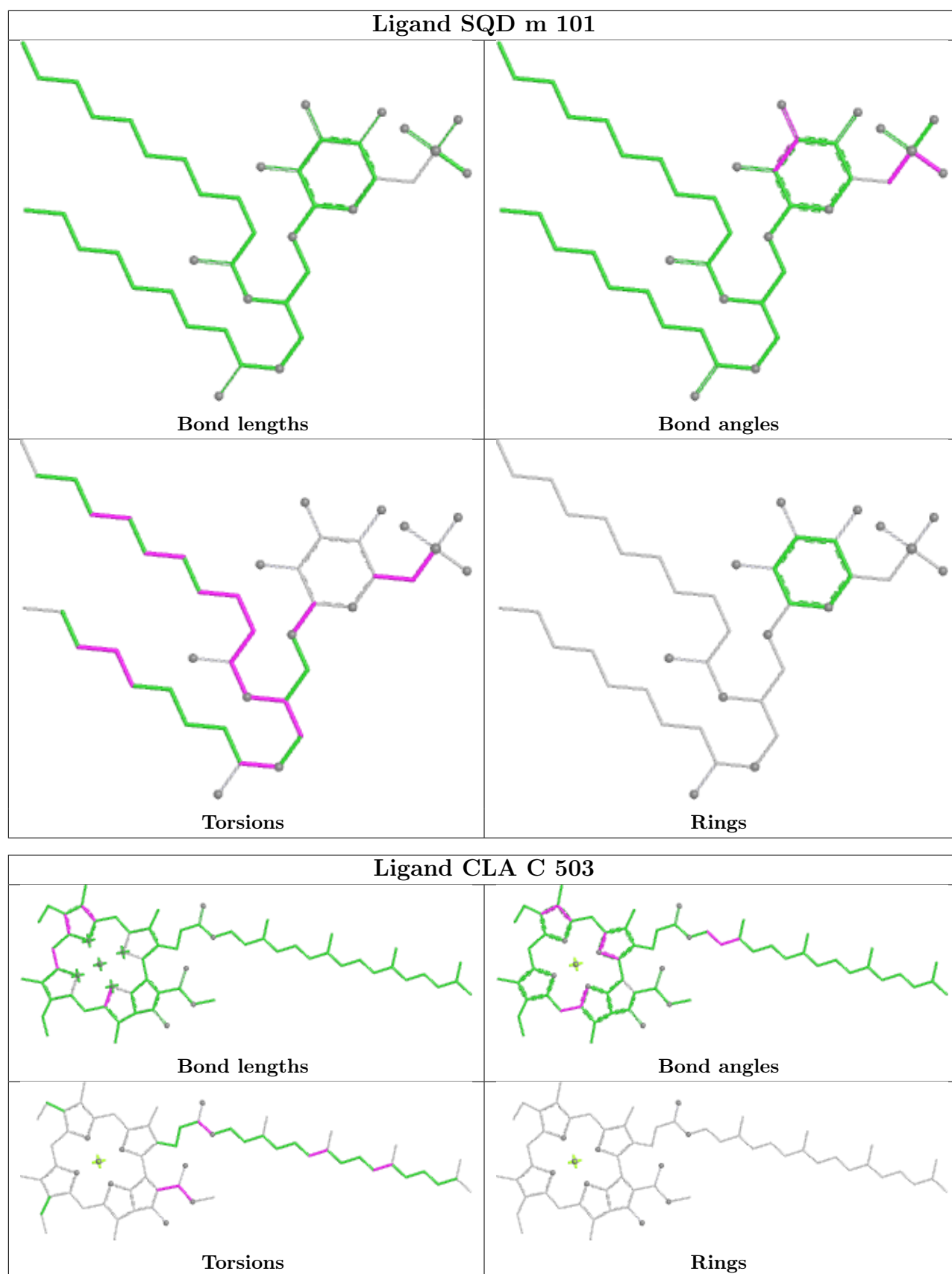
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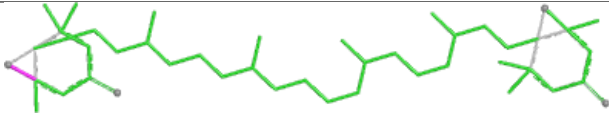
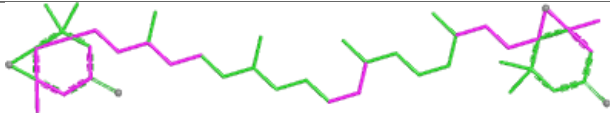
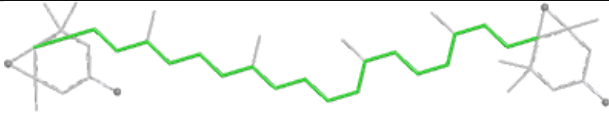
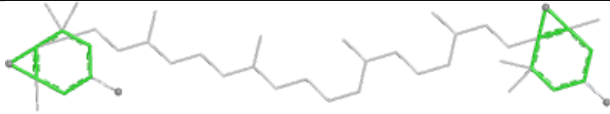


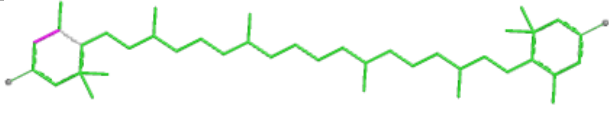
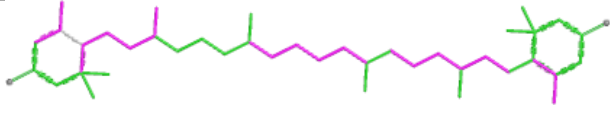
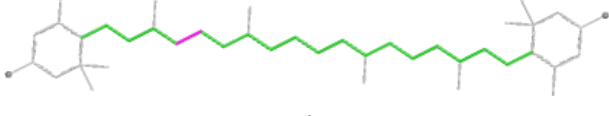
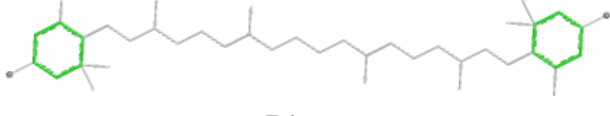
Ligand CLA Y 305

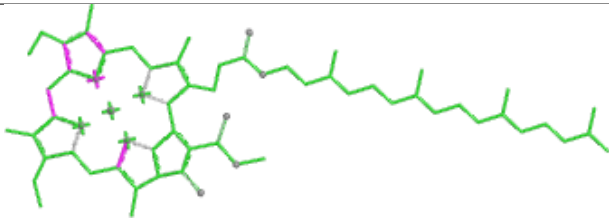
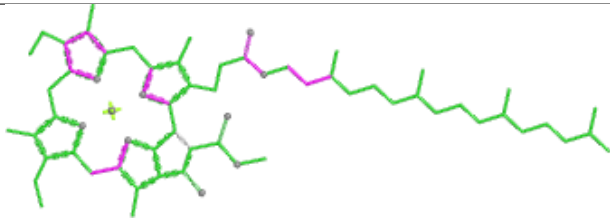
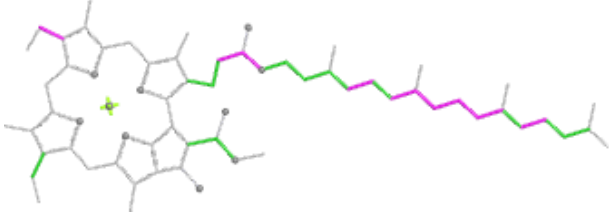
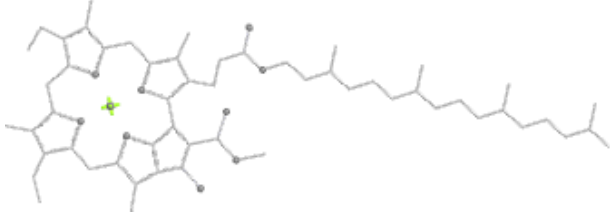


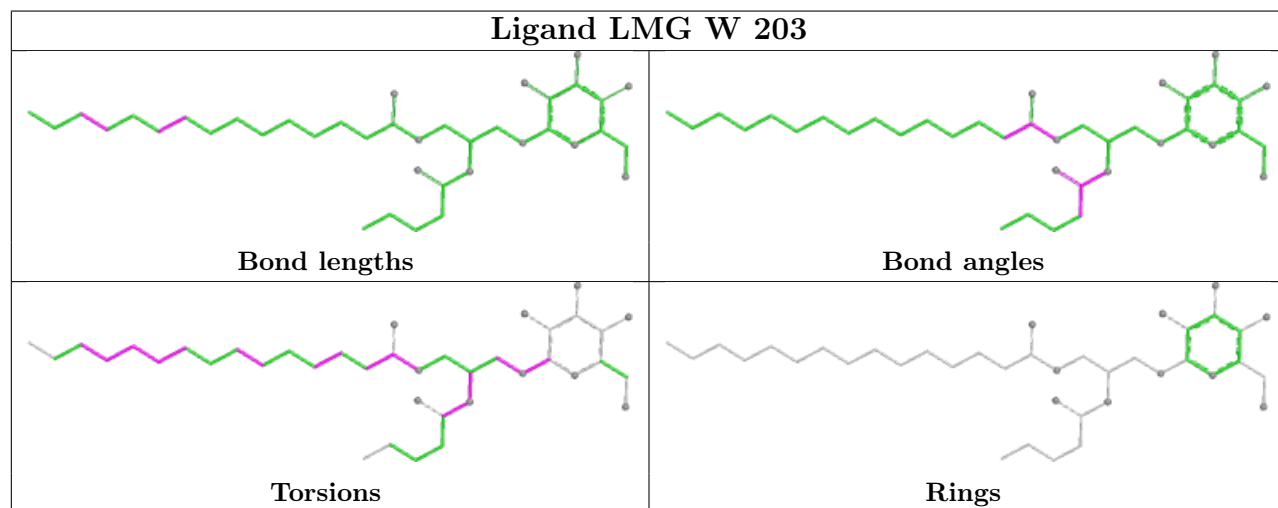
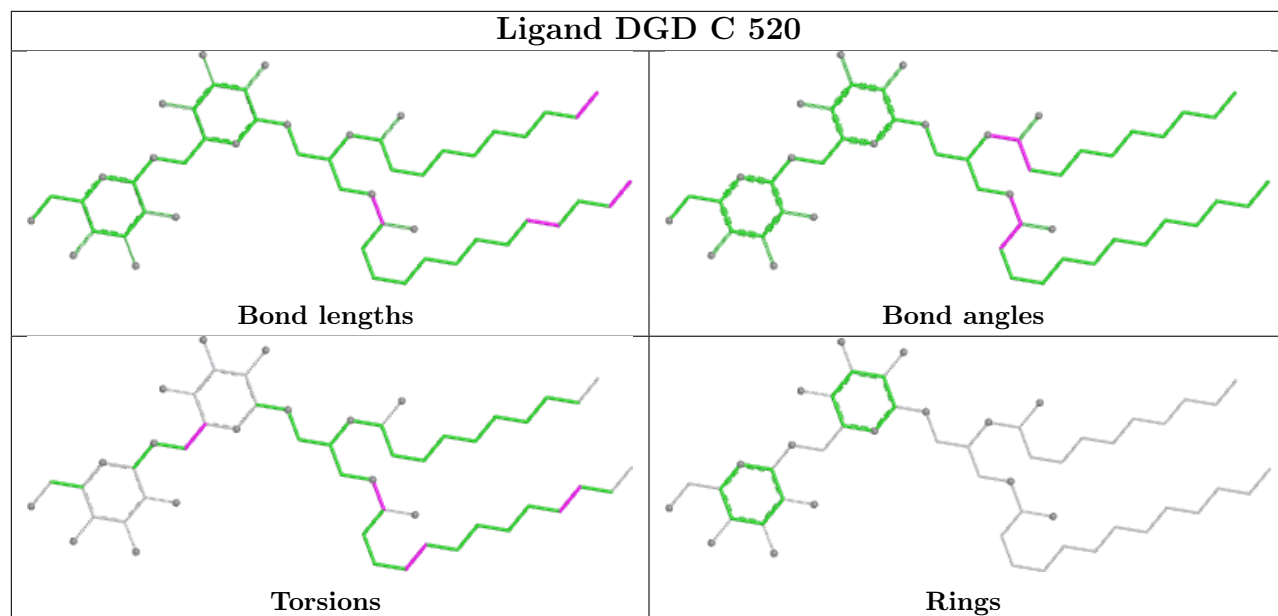


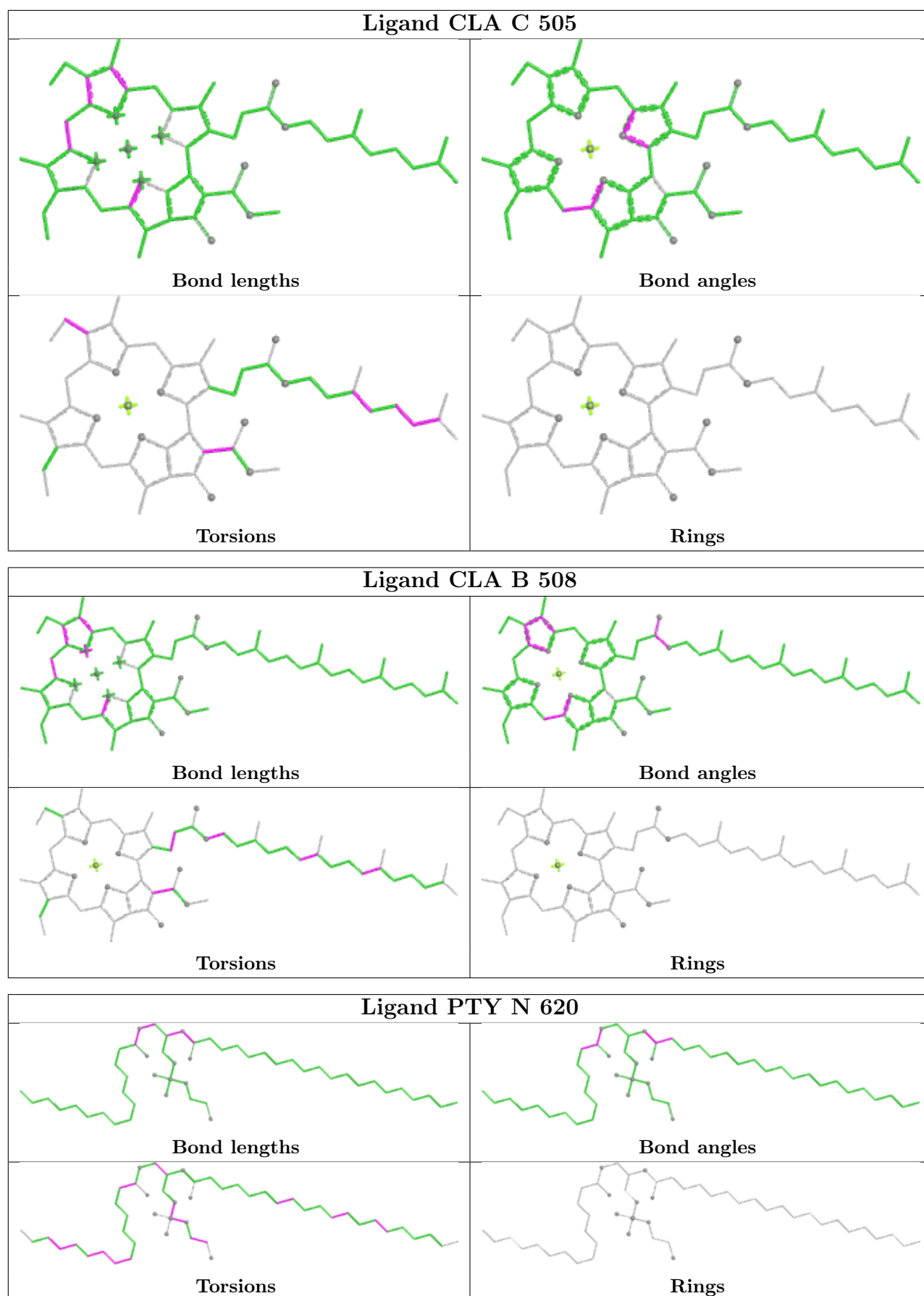


Ligand XAT R 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

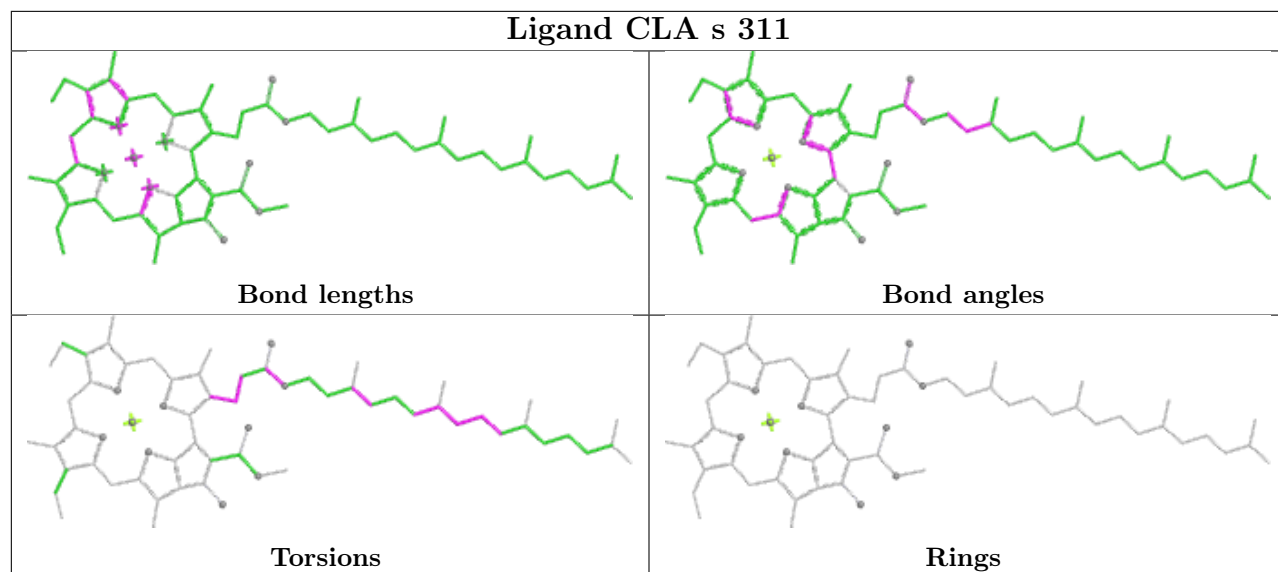
Ligand LUT s 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA y 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

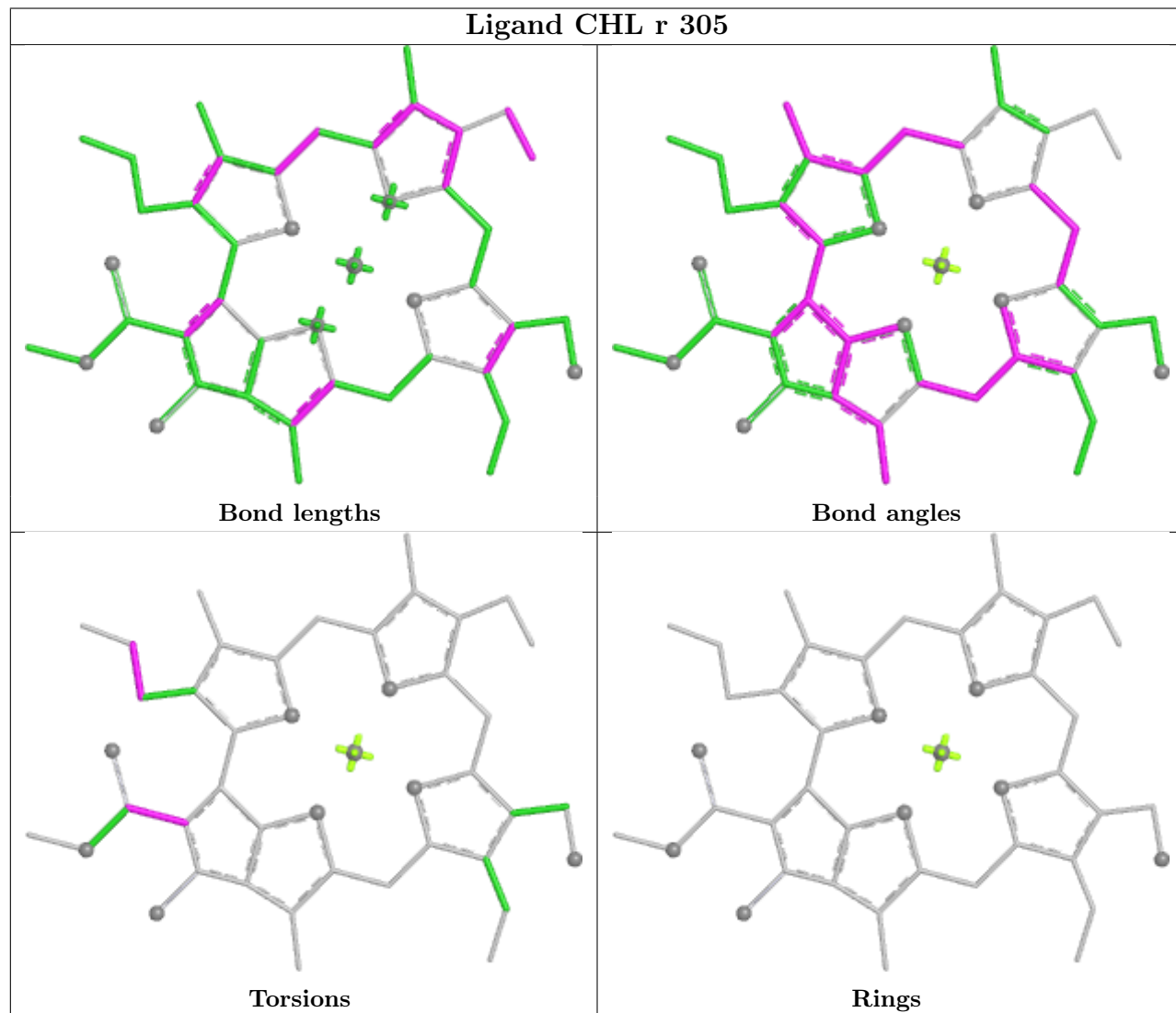


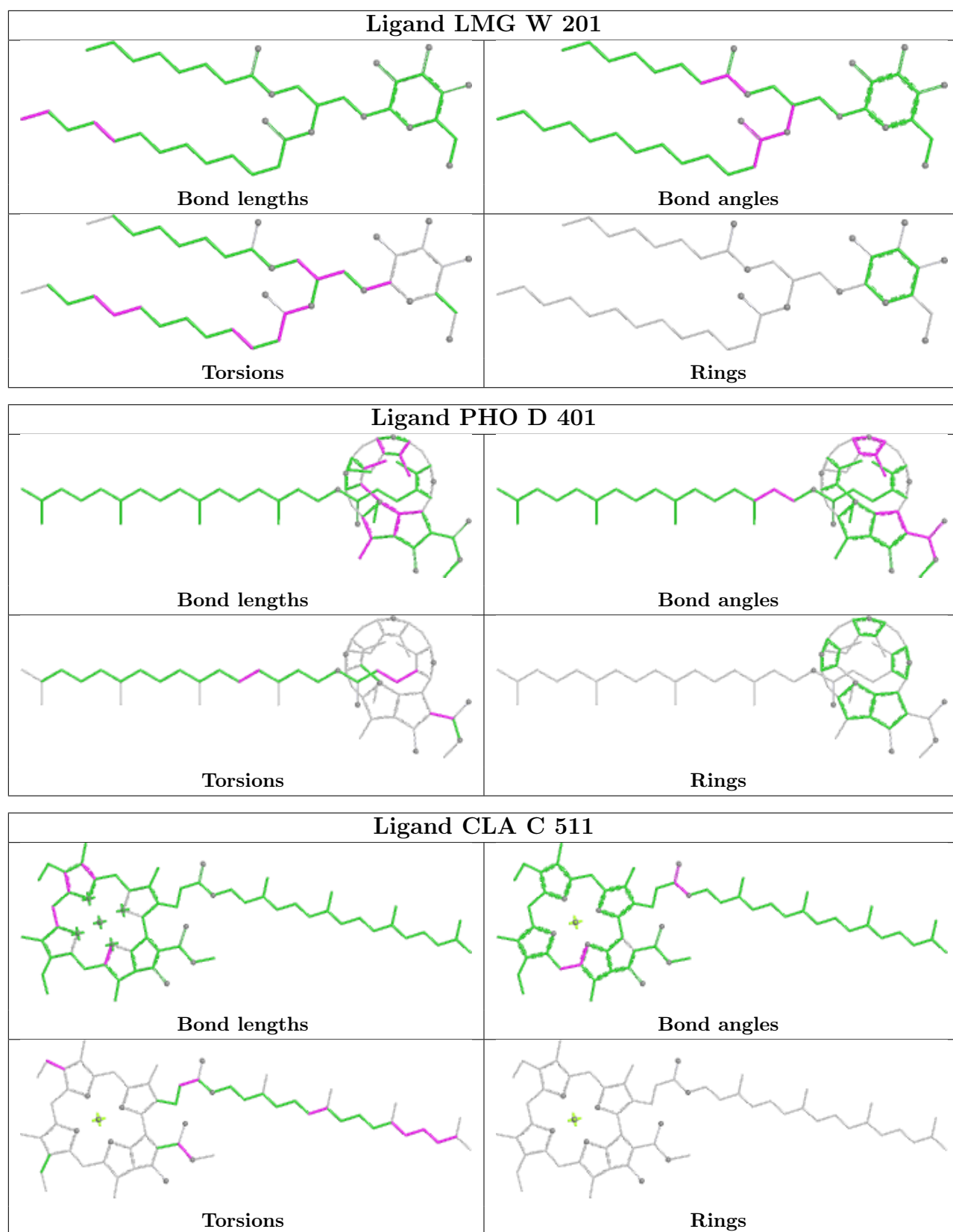


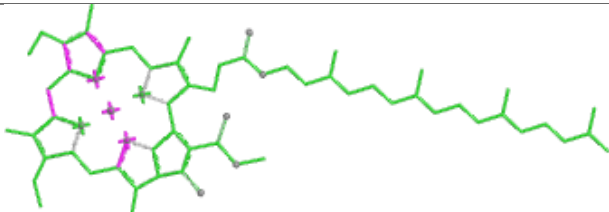
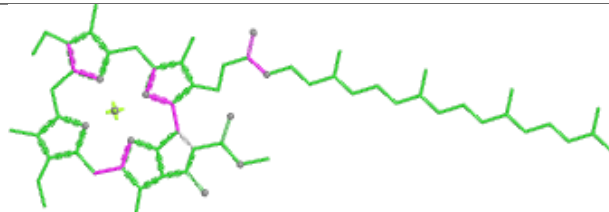
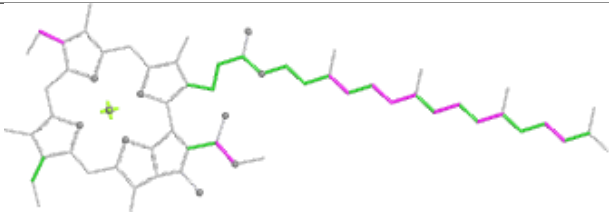
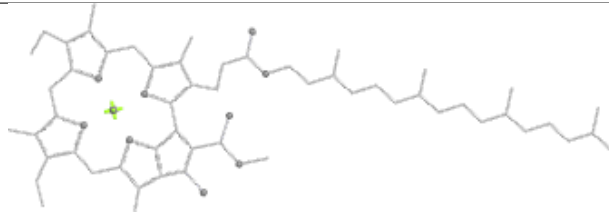
Ligand CLA s 311

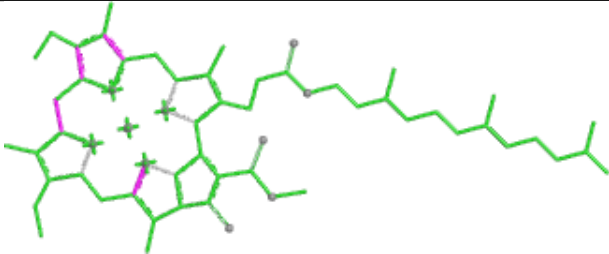
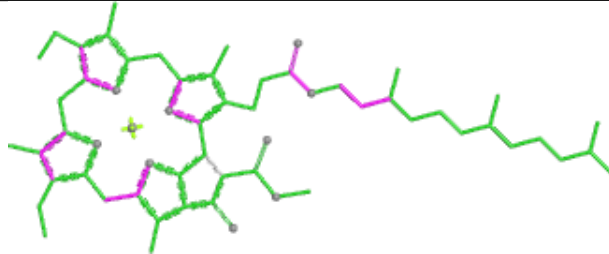
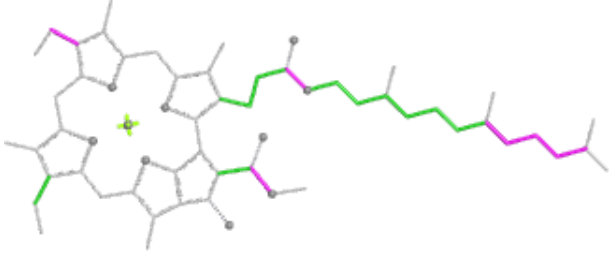
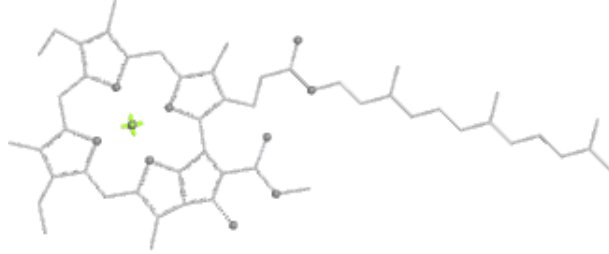


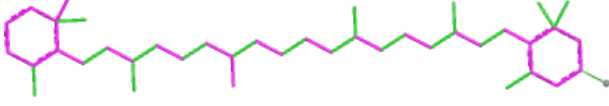
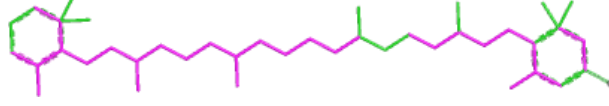
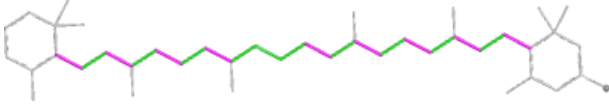
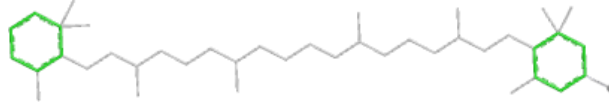
Ligand CHL r 305



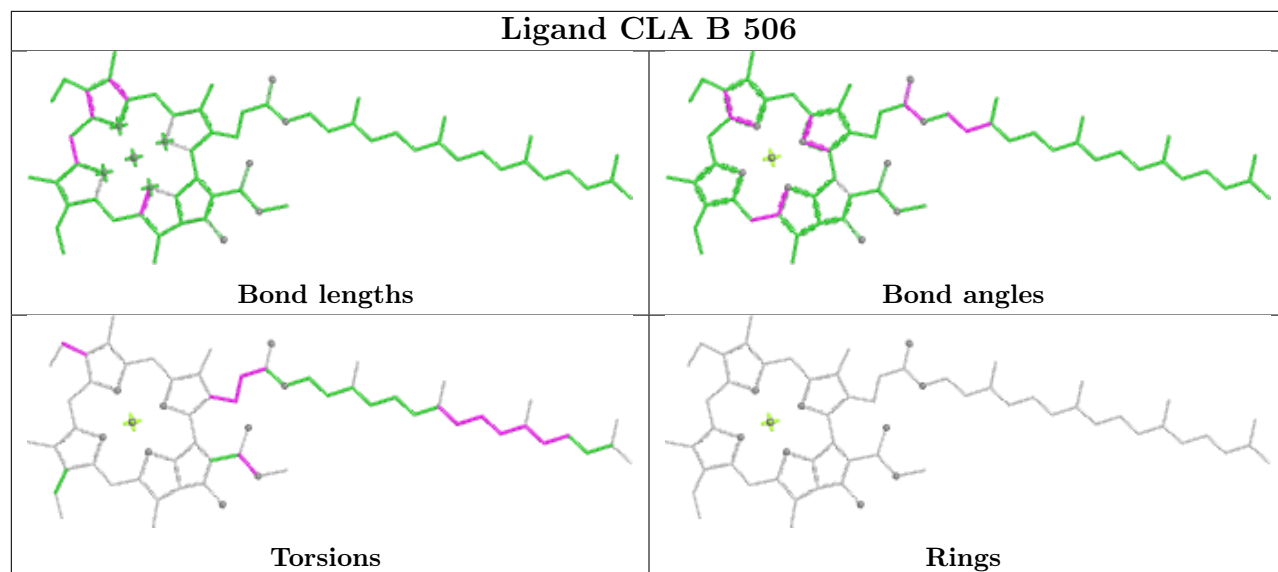


Ligand CLA B 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

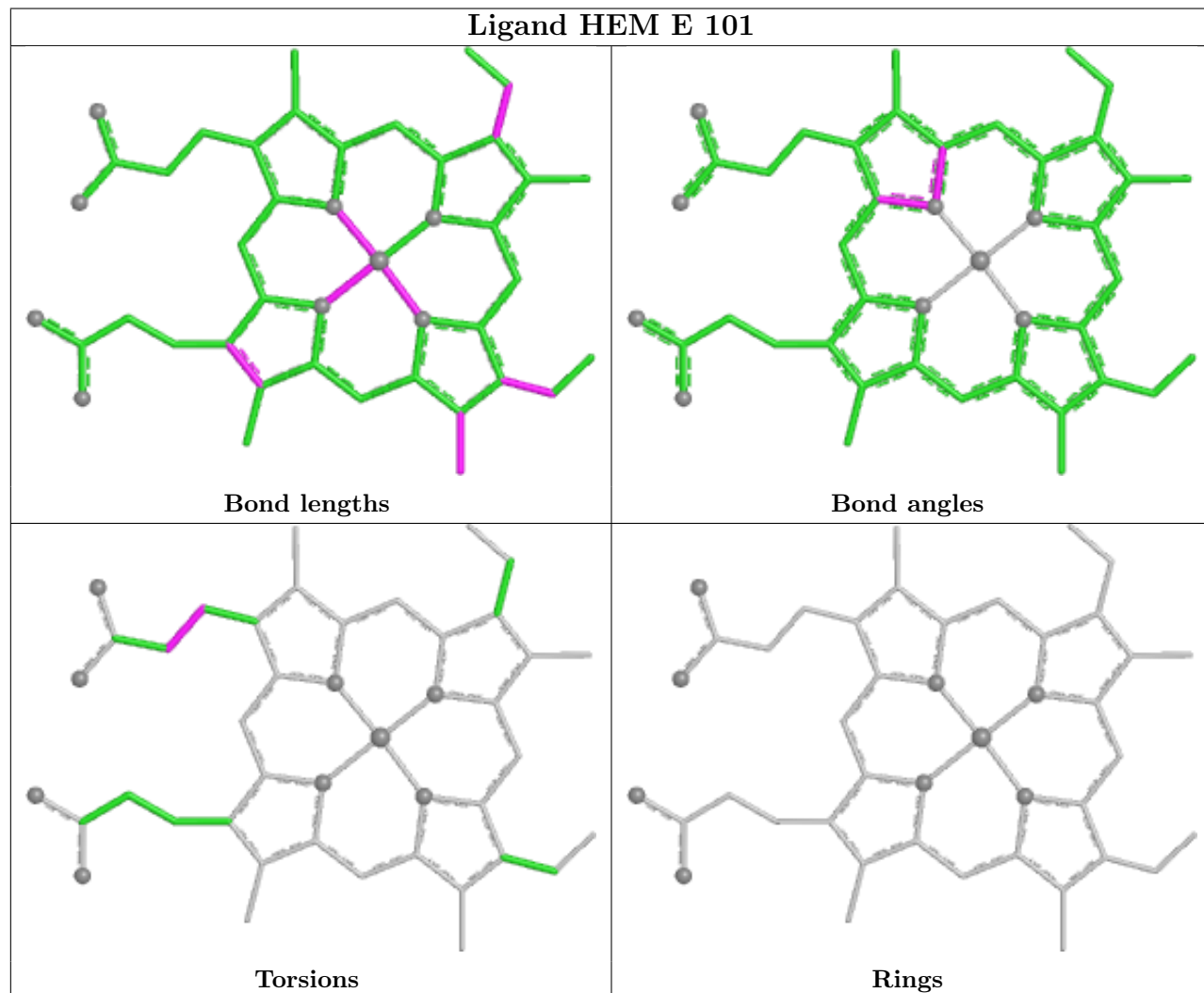
Ligand CLA D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

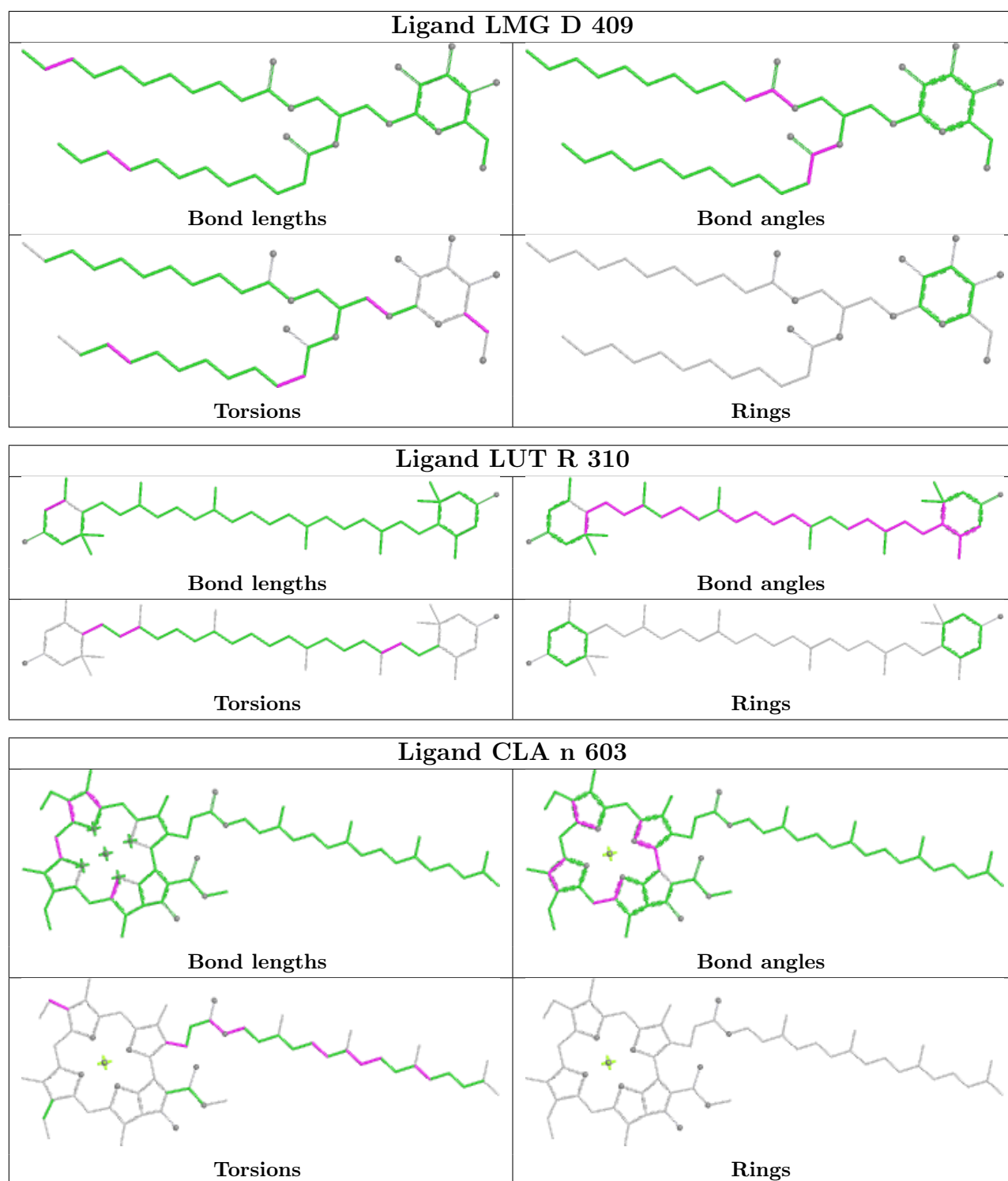
Ligand RRX h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

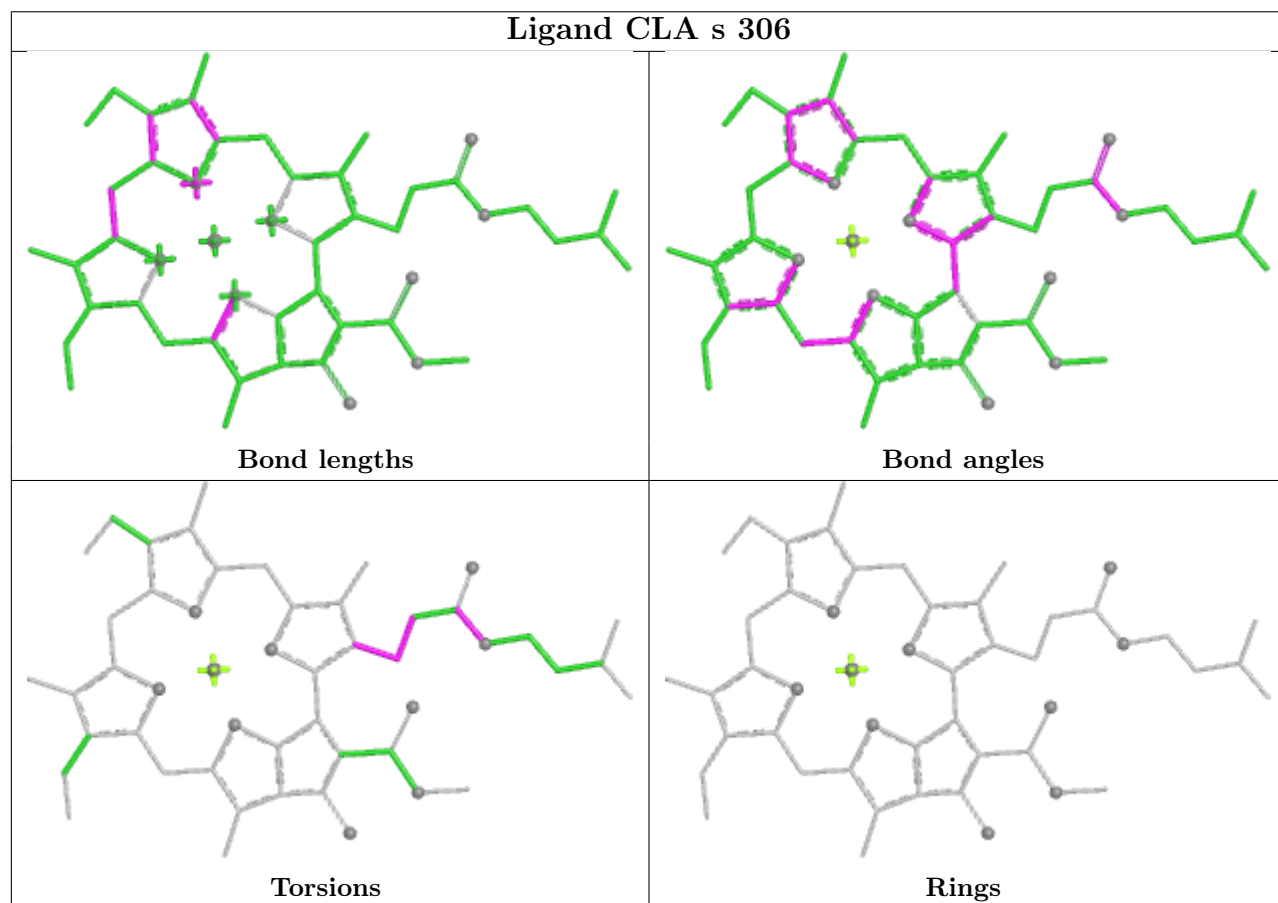
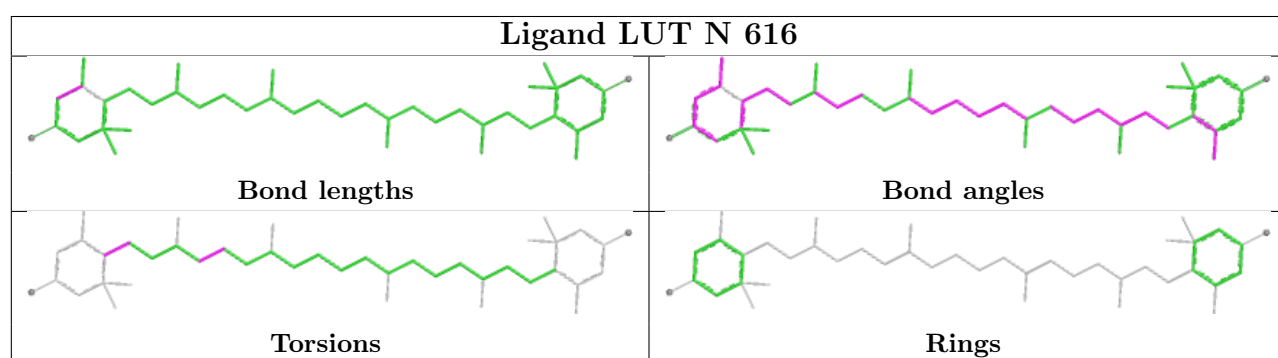
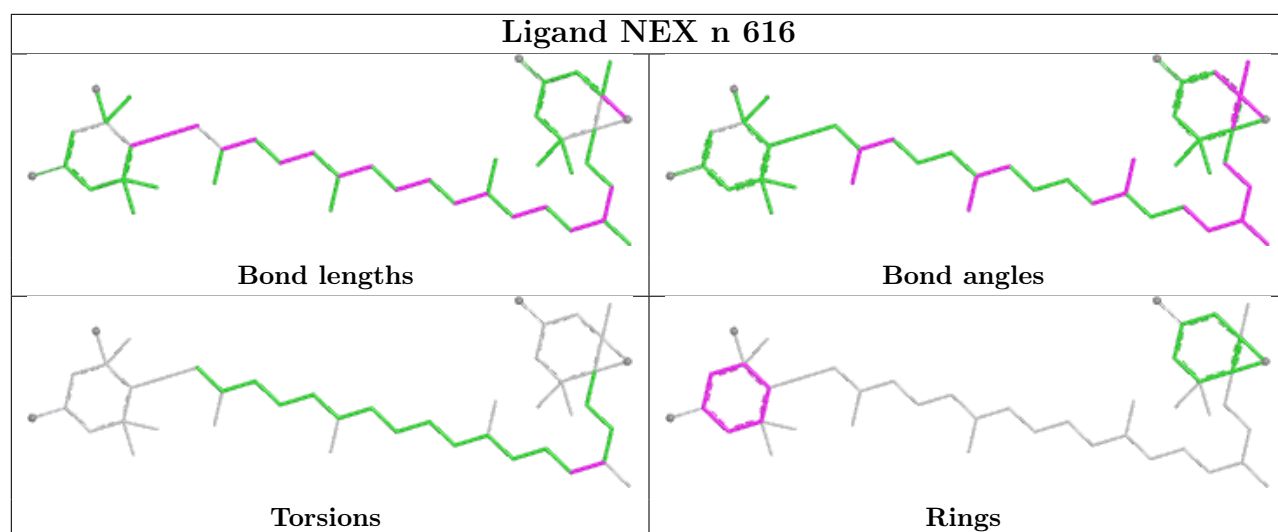
Ligand CLA B 506

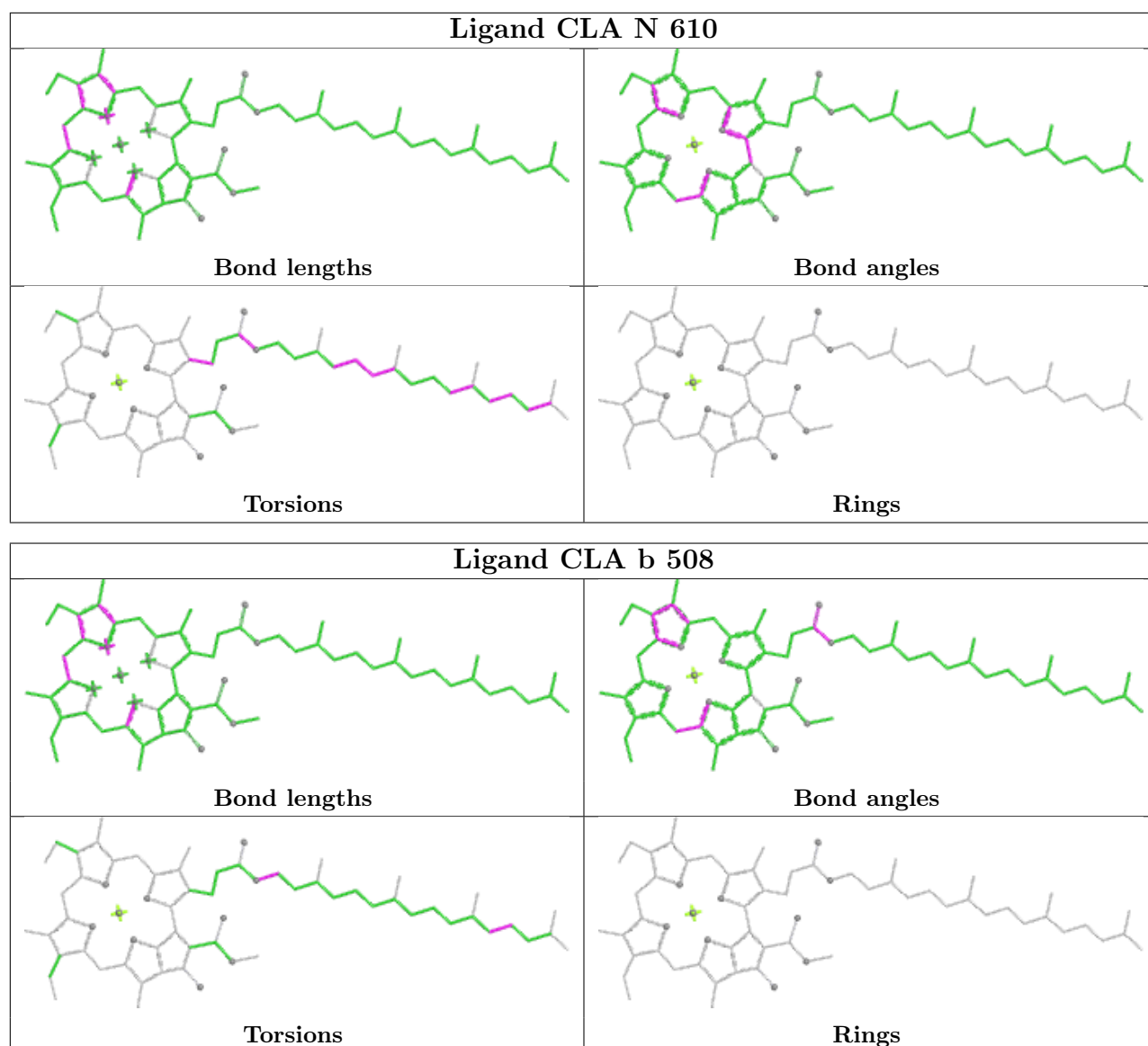


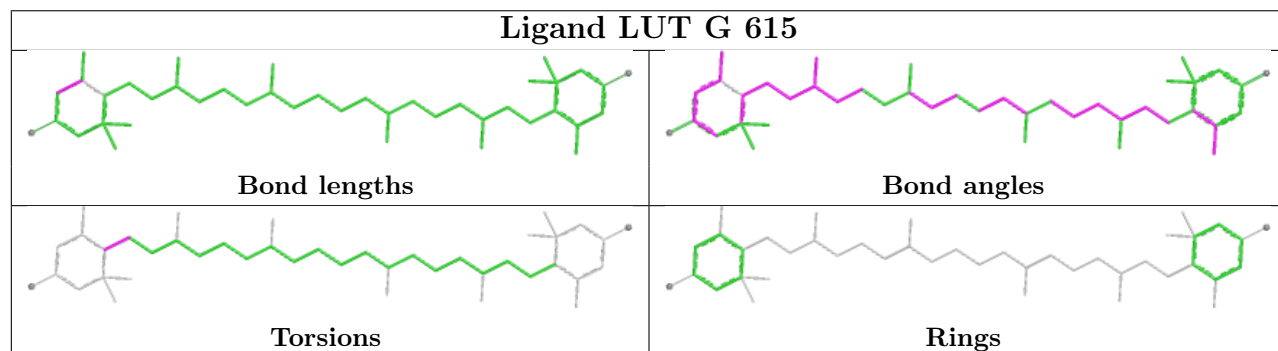
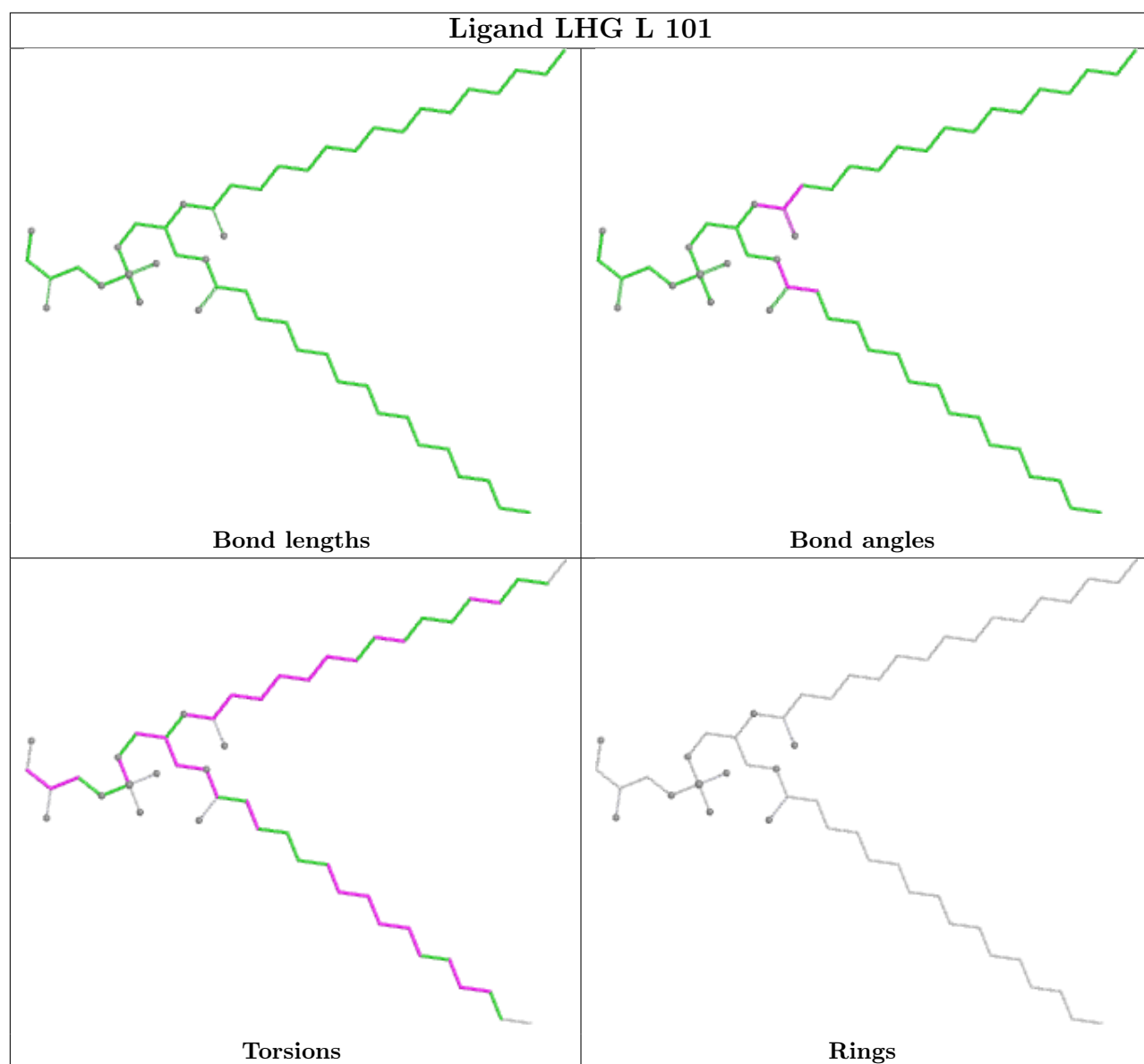
Ligand HEM E 101

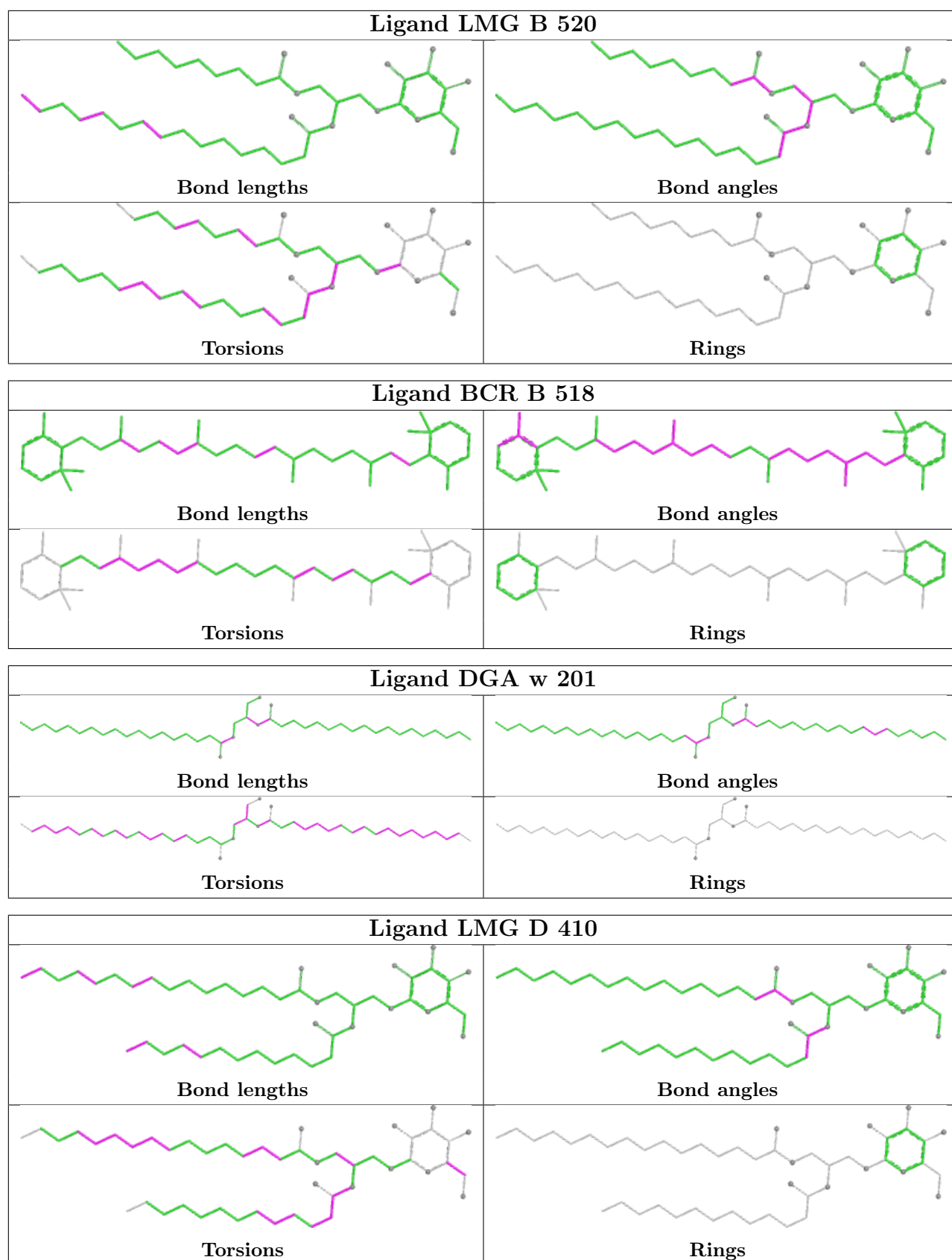




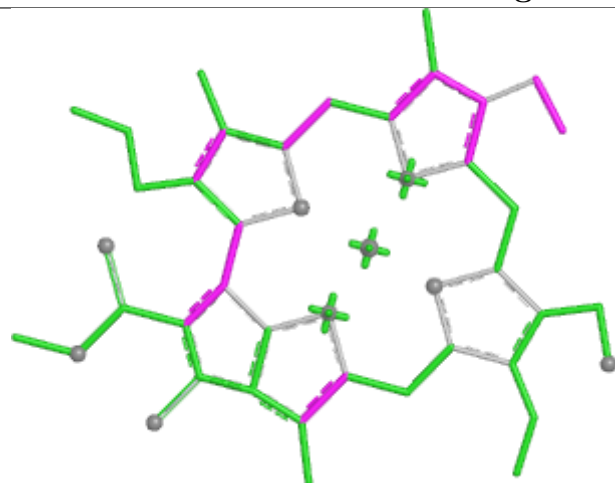




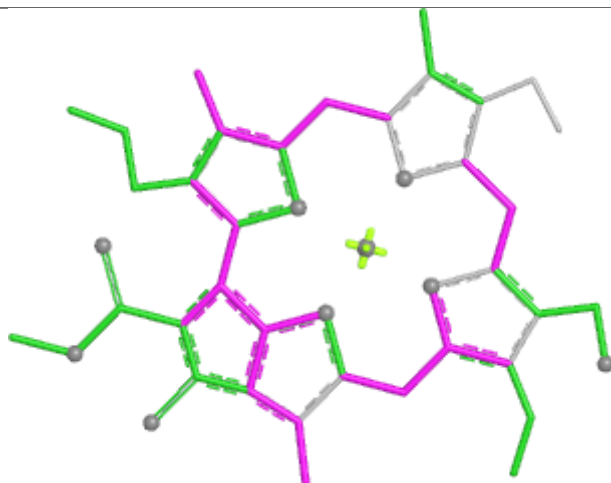




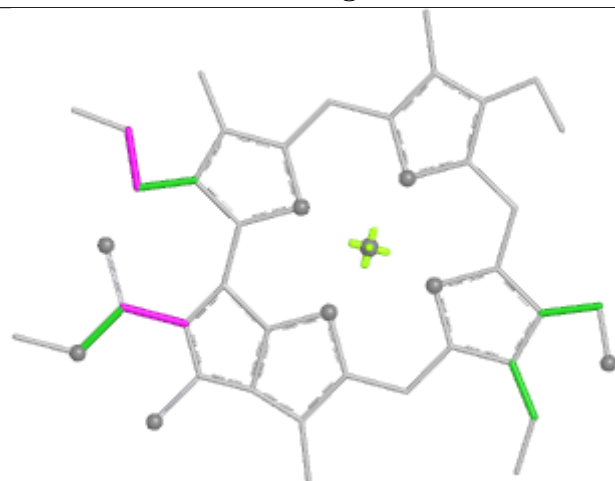
Ligand CHL G 608



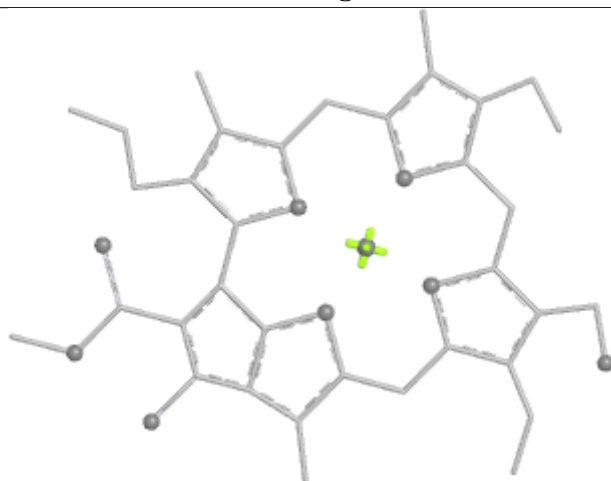
Bond lengths



Bond angles

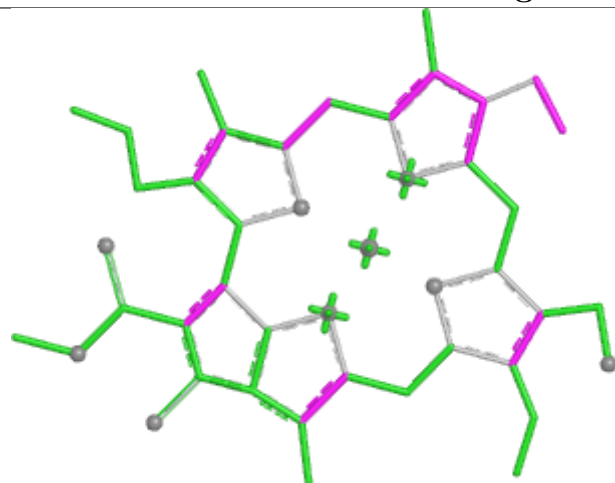


Torsions

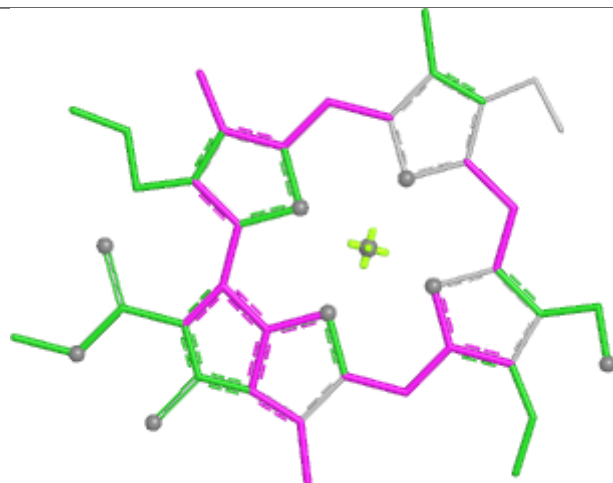


Rings

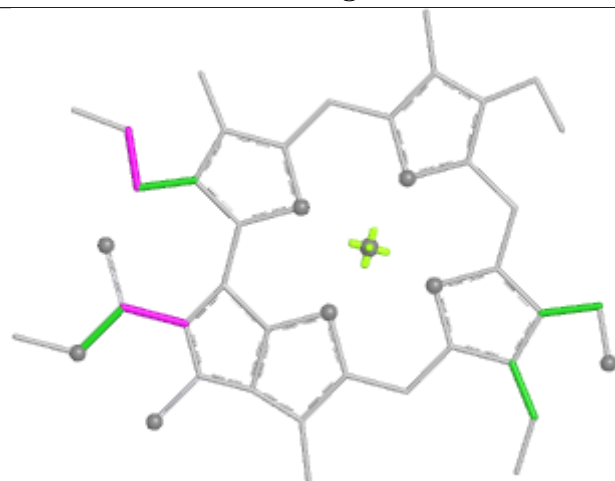
Ligand CHL R 304



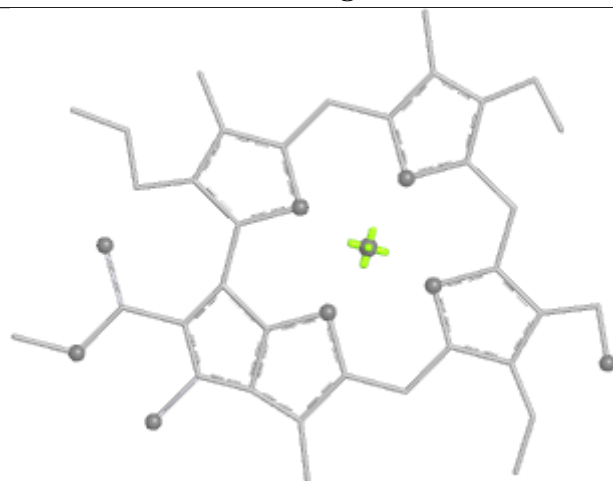
Bond lengths



Bond angles

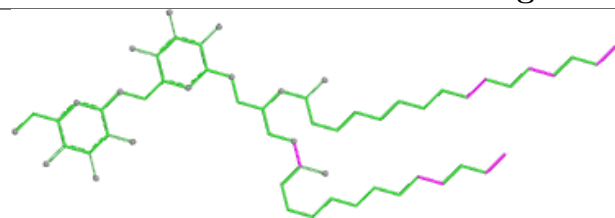


Torsions

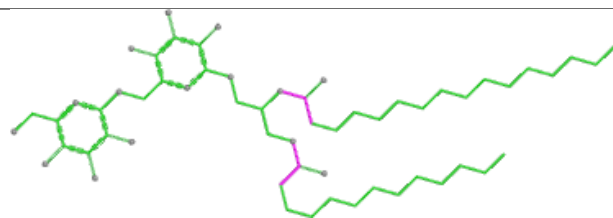


Rings

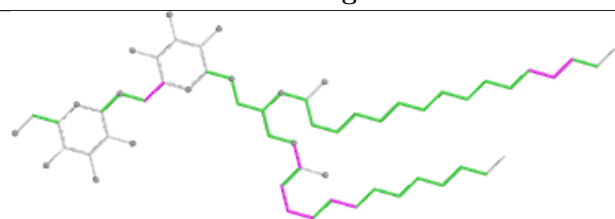
Ligand DGD c 518



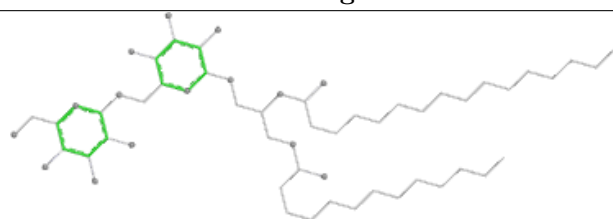
Bond lengths



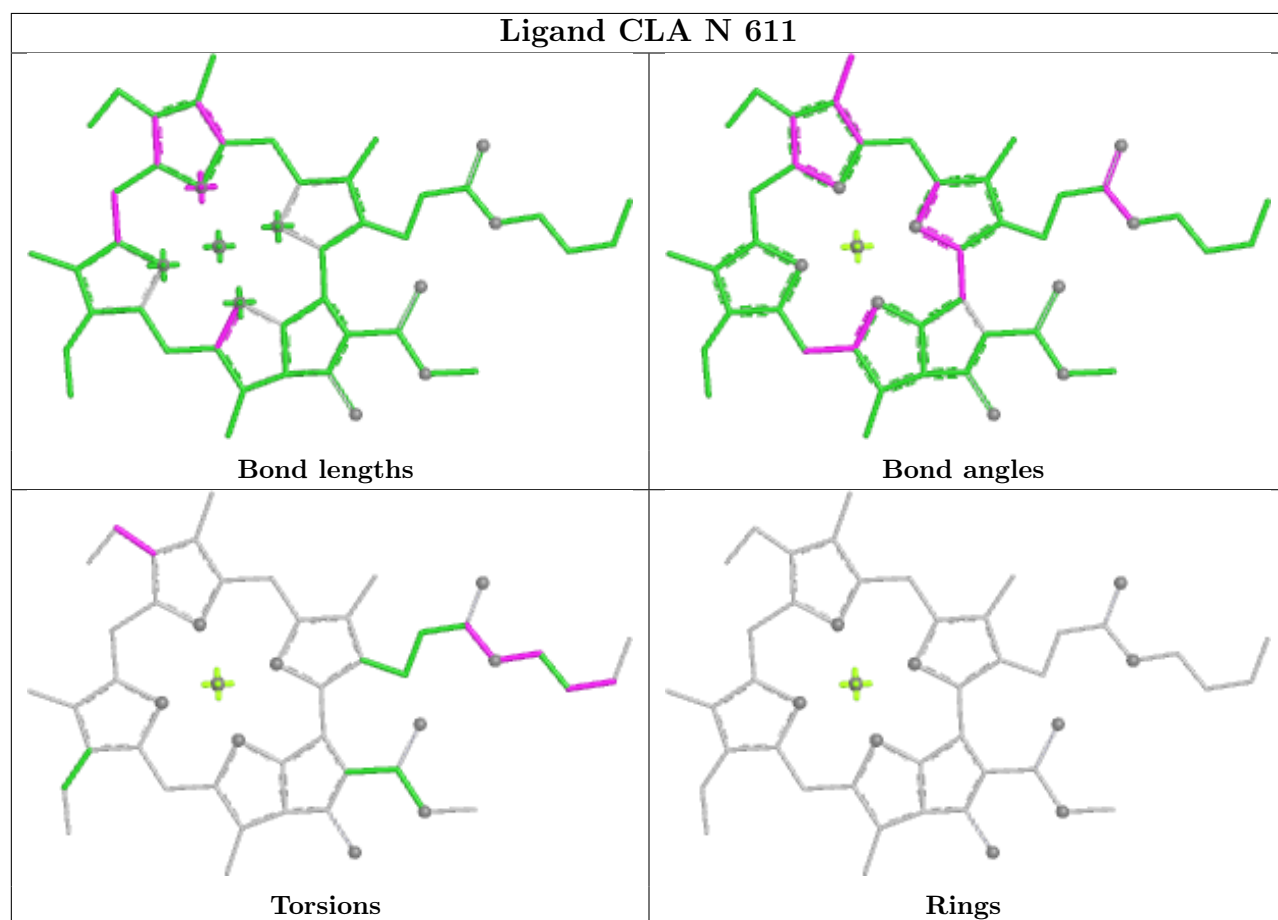
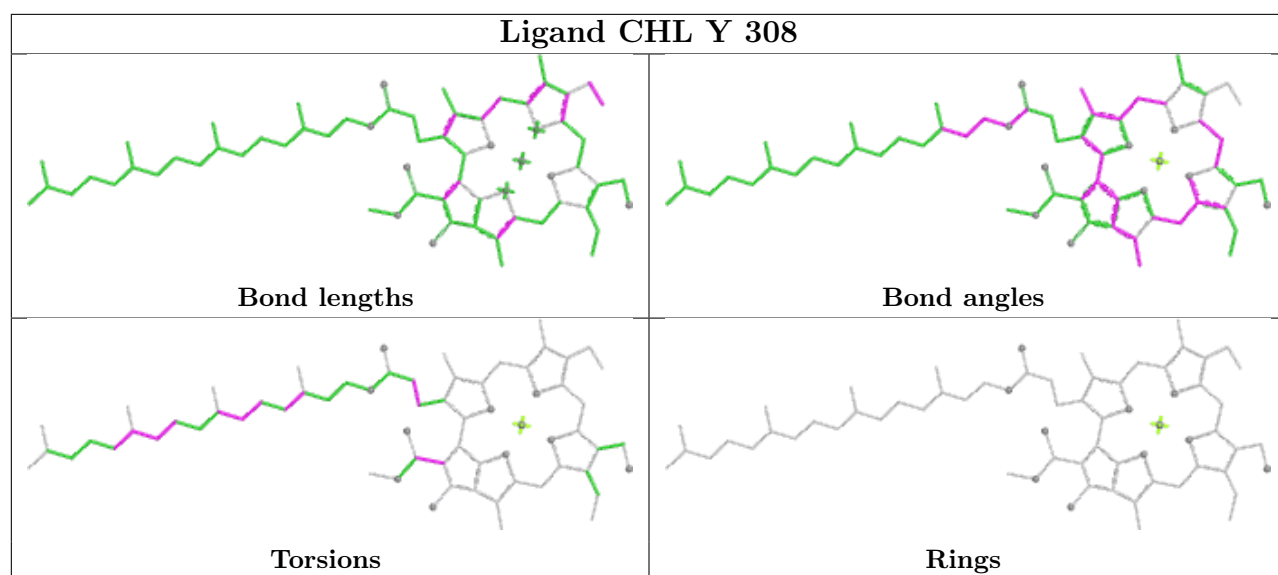
Bond angles

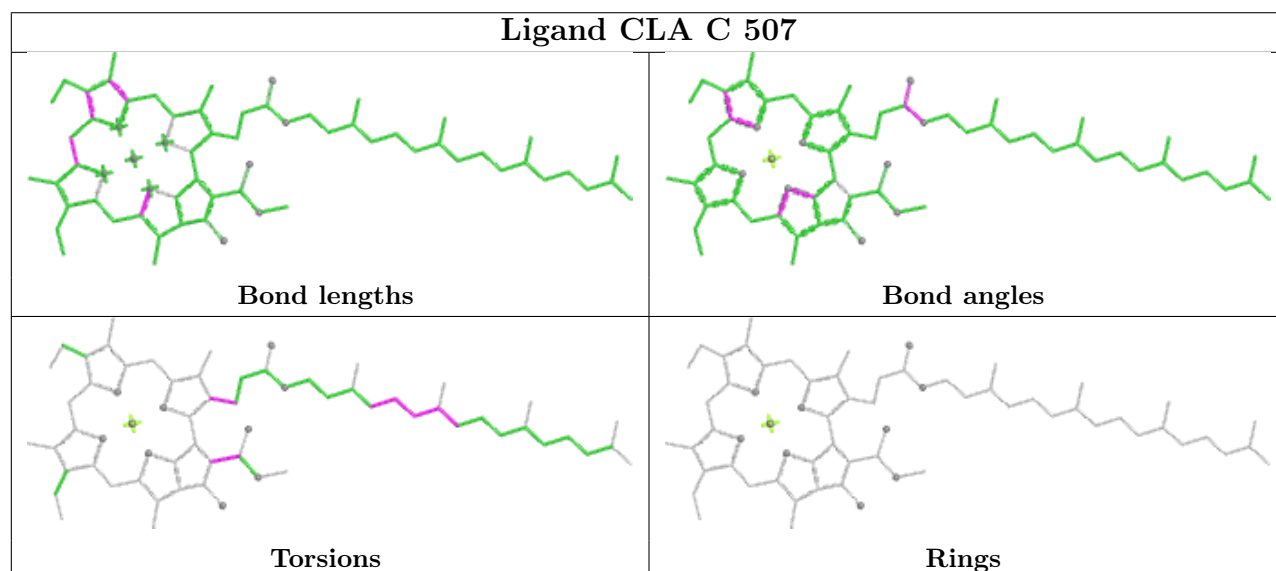
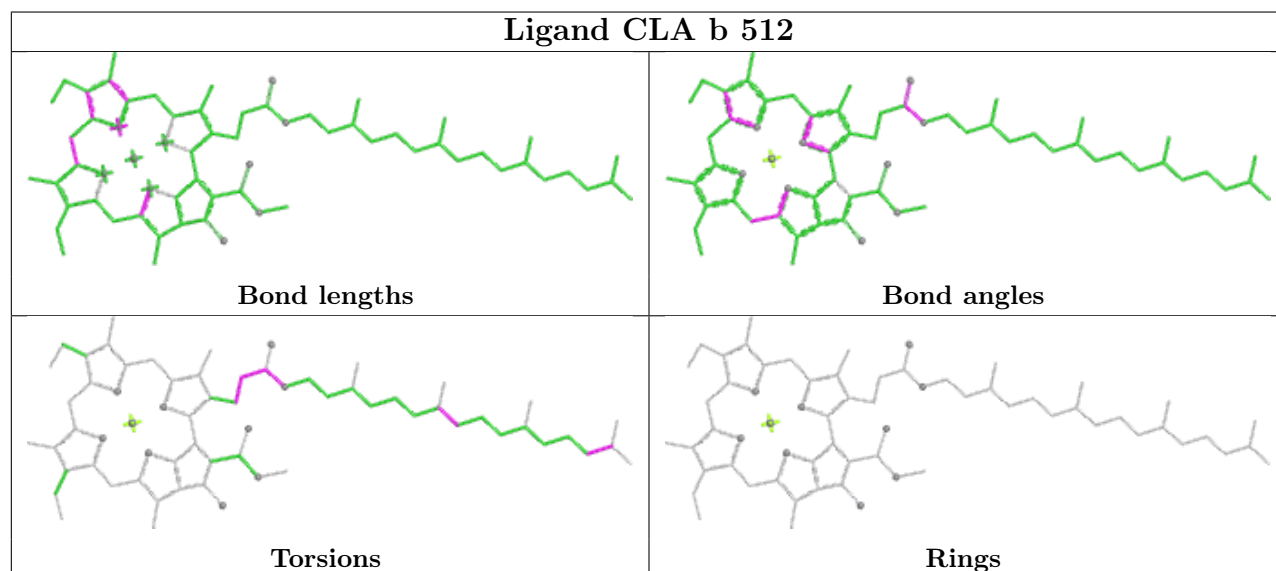
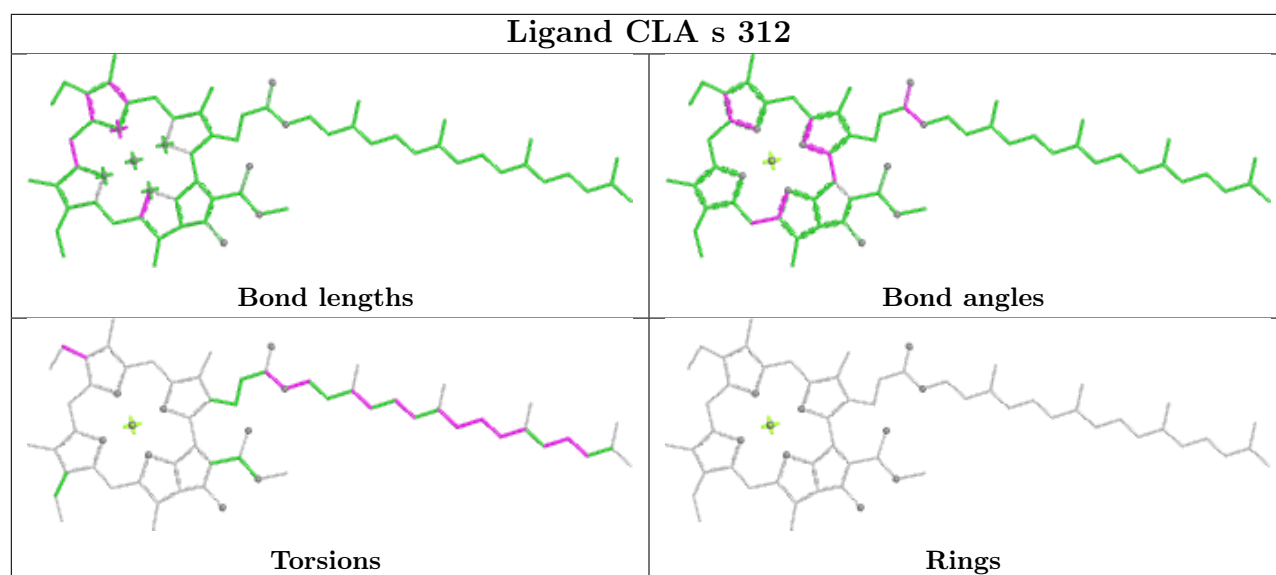


Torsions

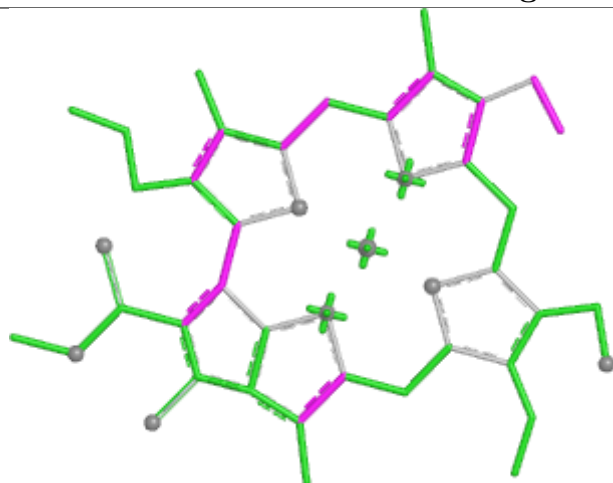


Rings

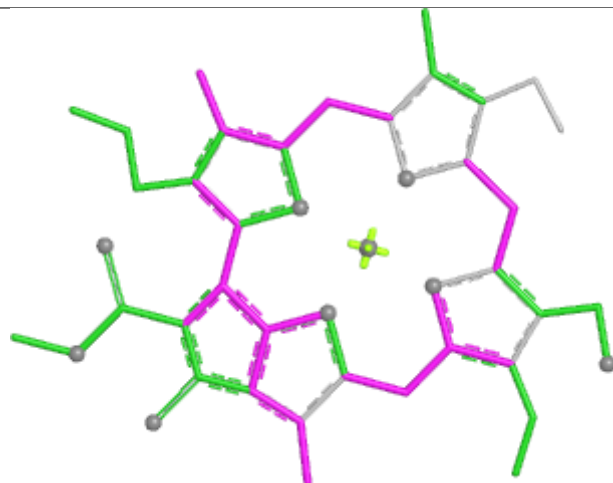




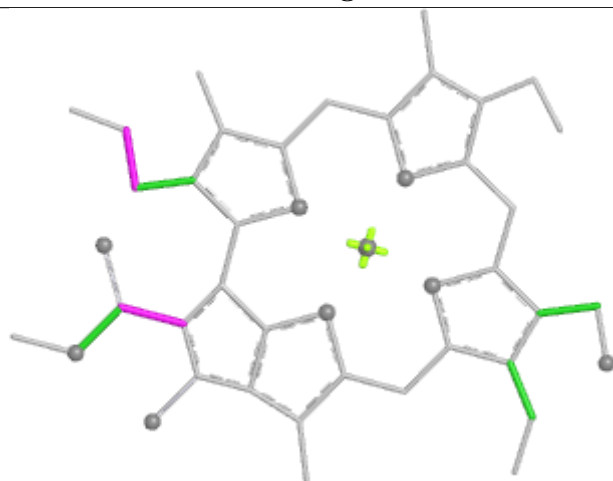
Ligand CHL s 307



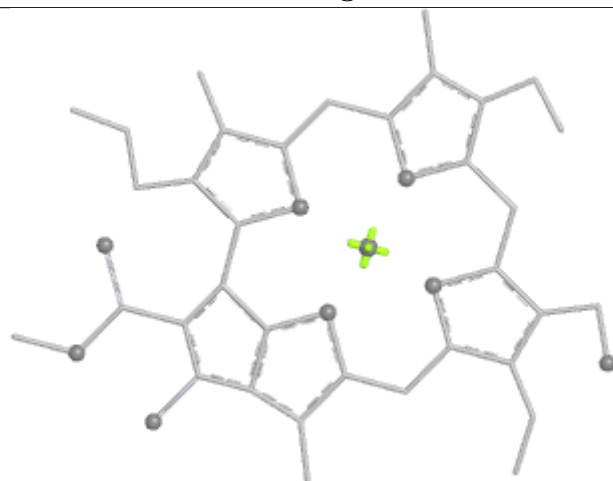
Bond lengths



Bond angles

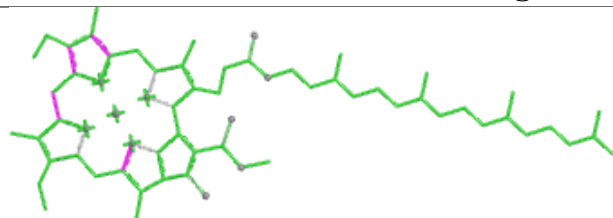


Torsions

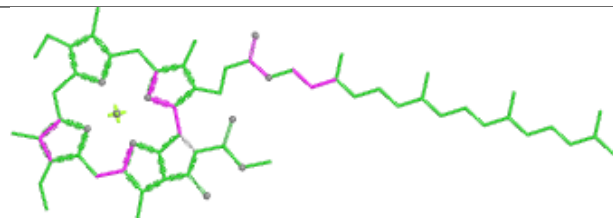


Rings

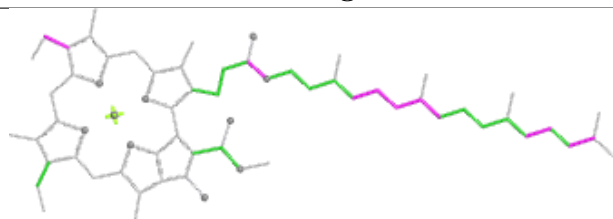
Ligand CLA Y 312



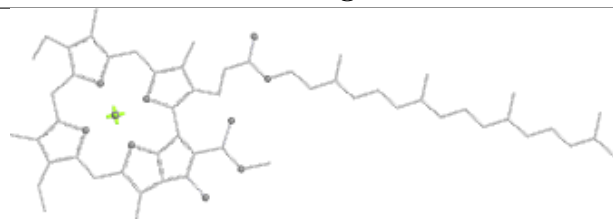
Bond lengths



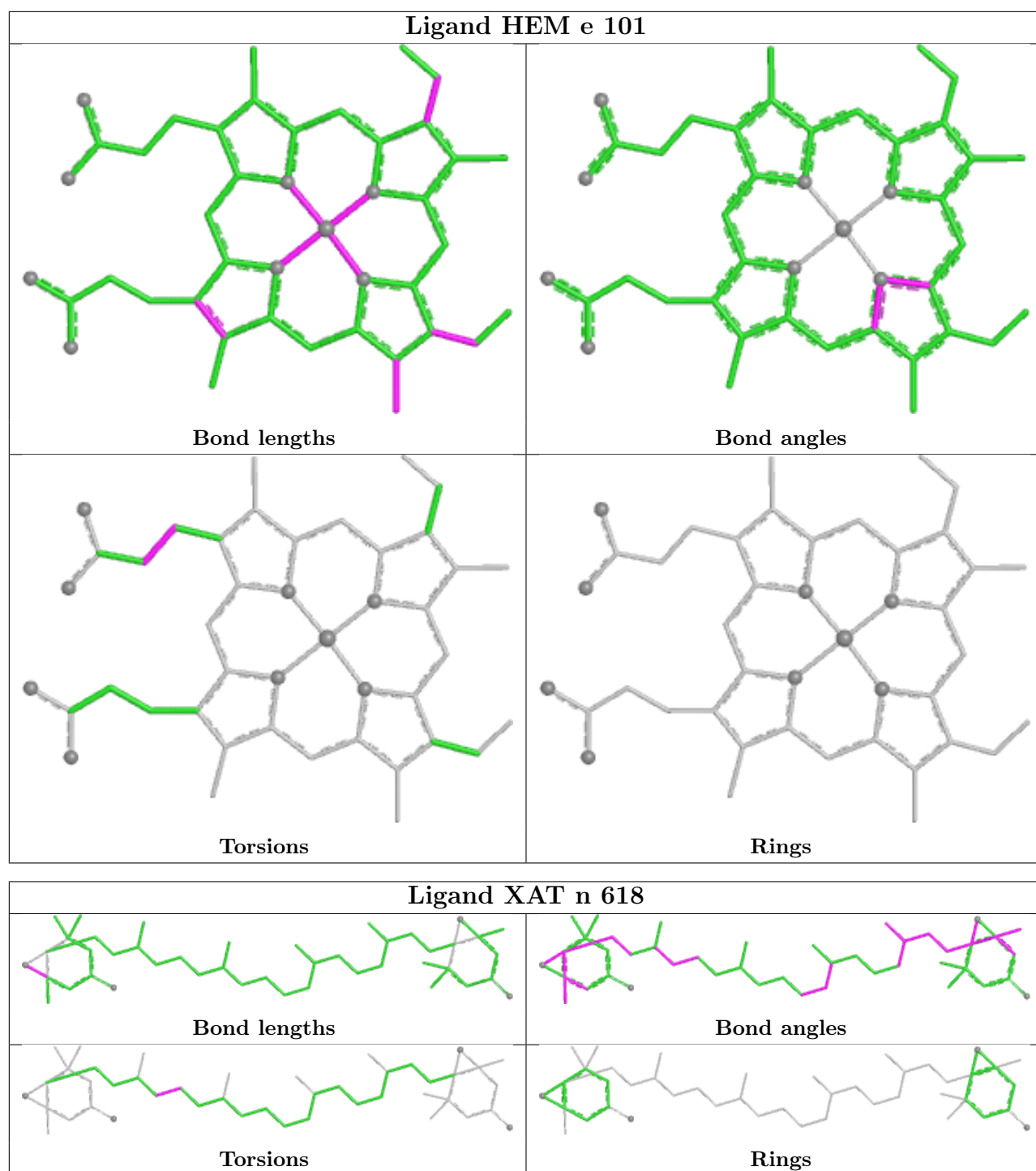
Bond angles

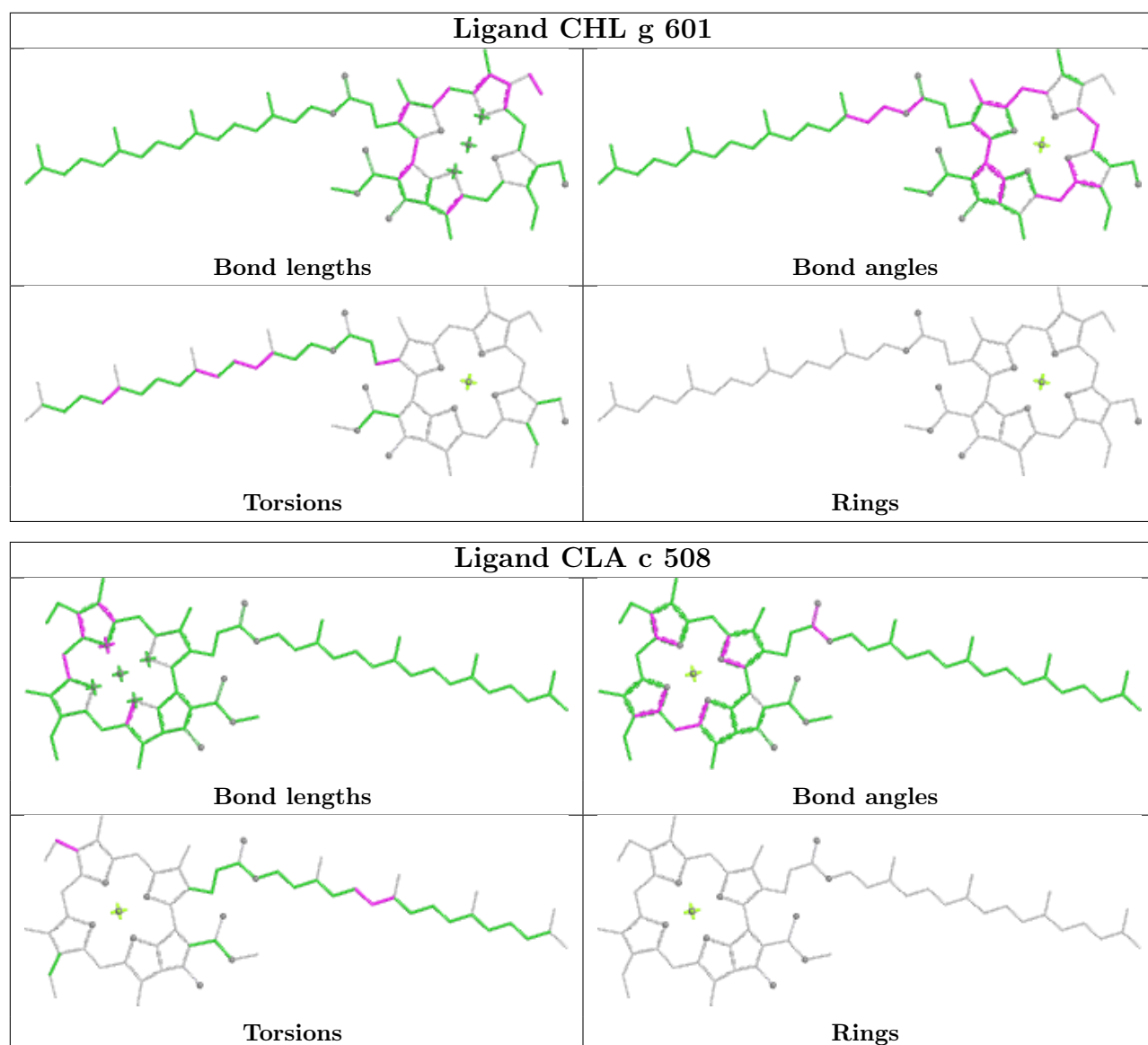


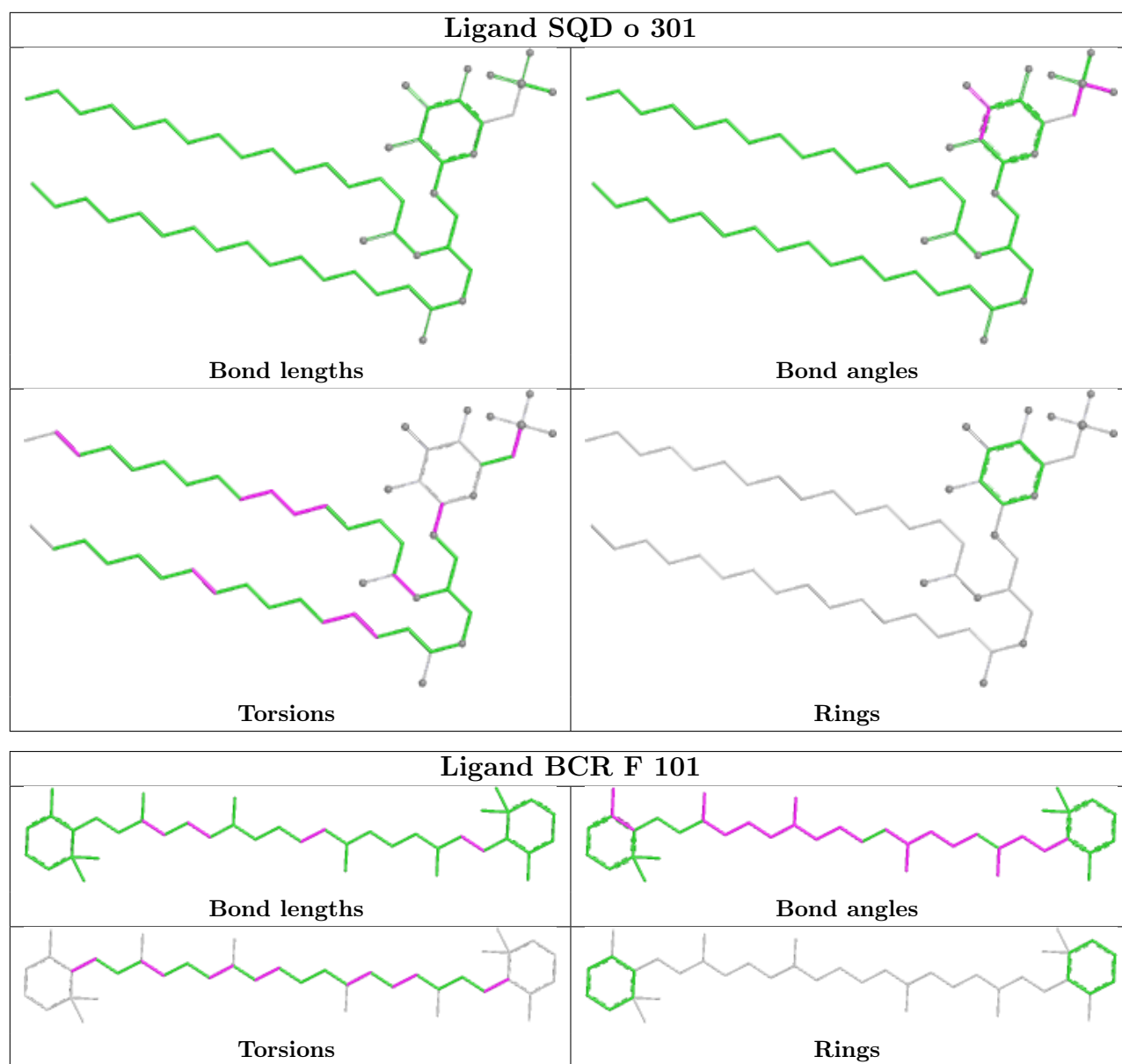
Torsions

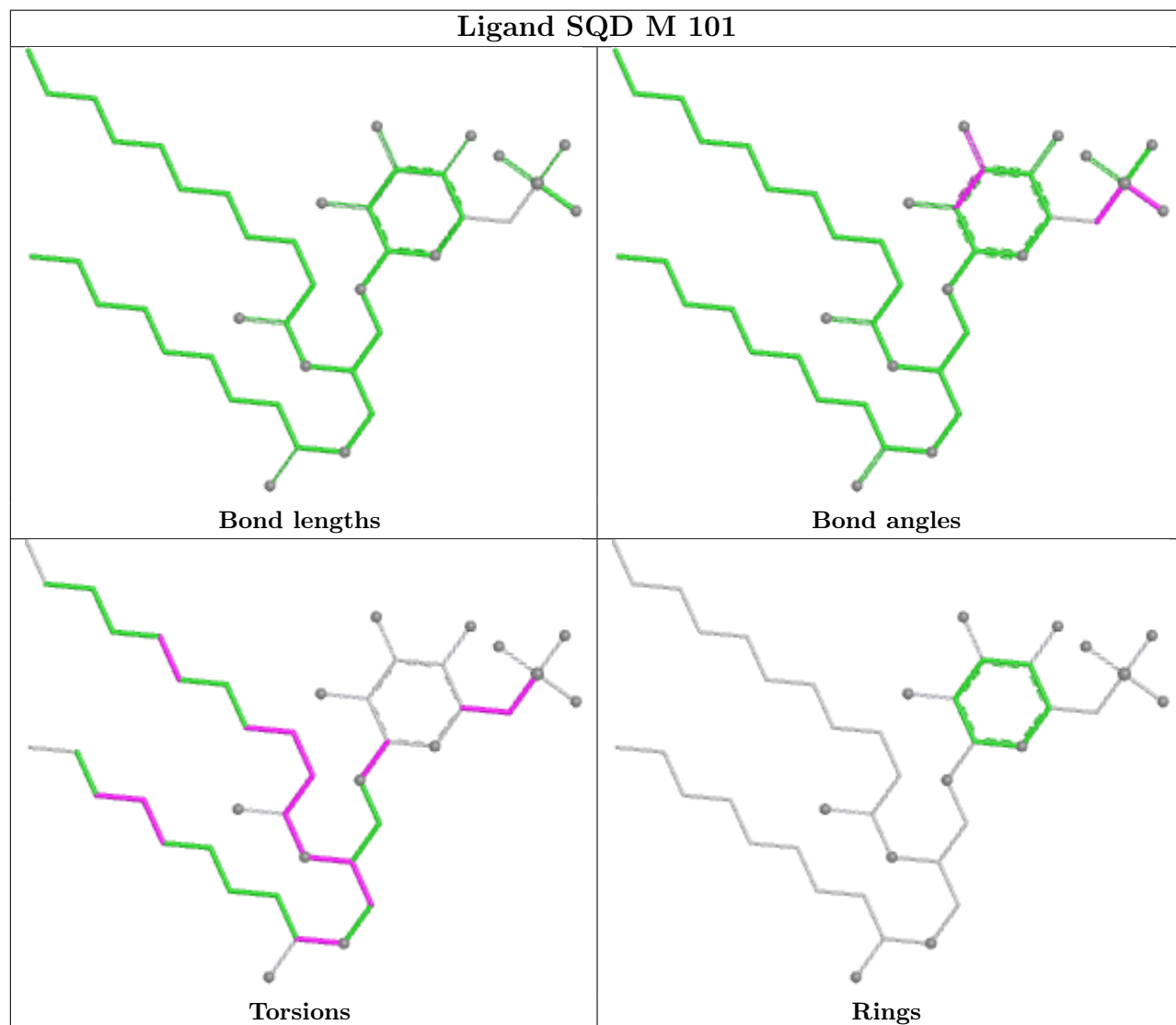
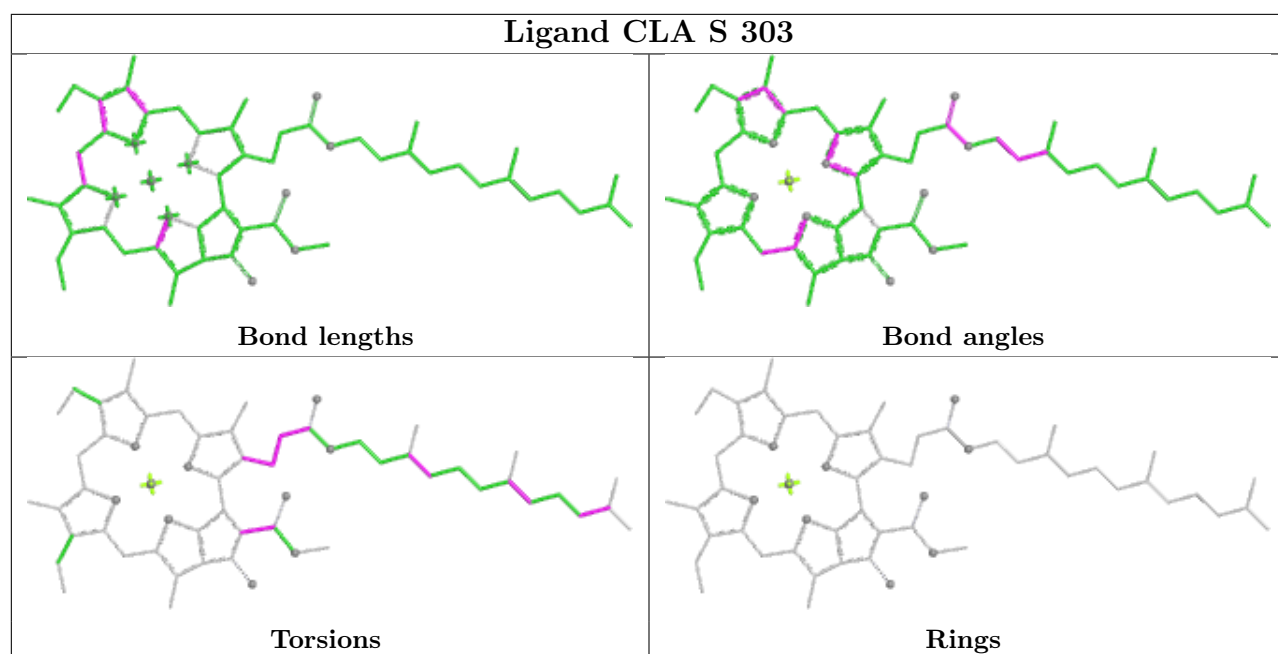


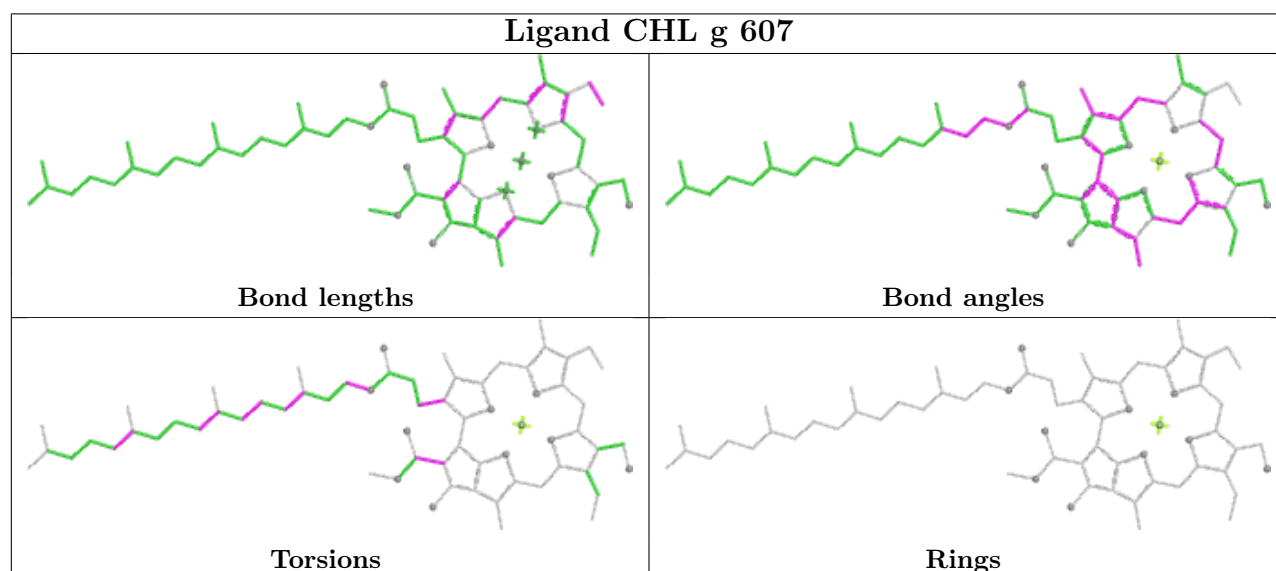
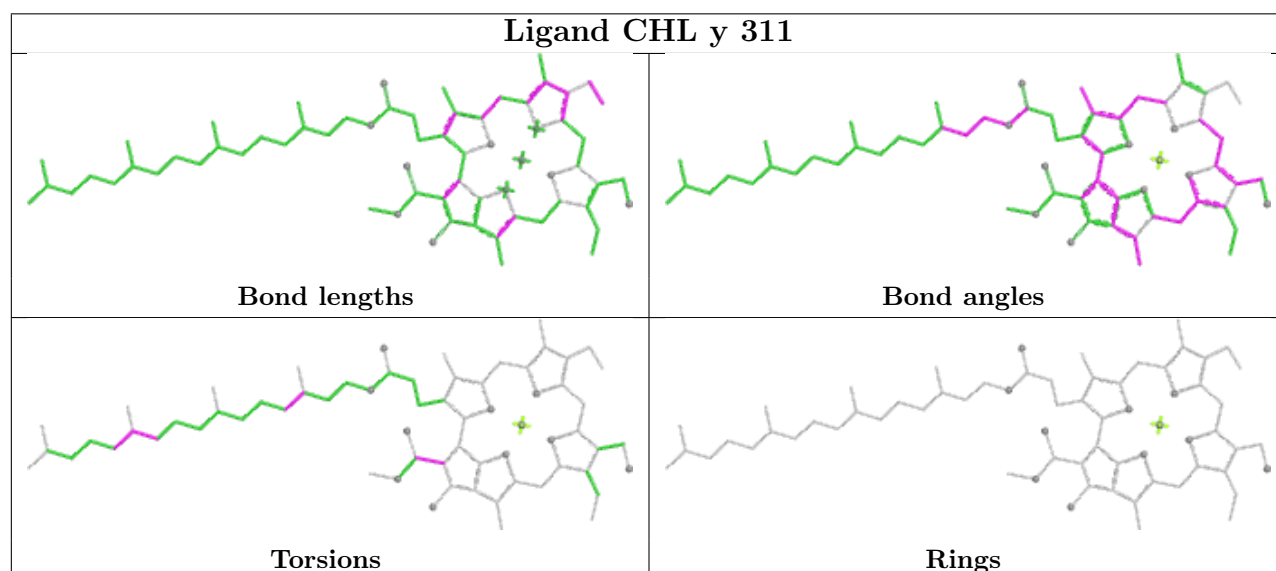
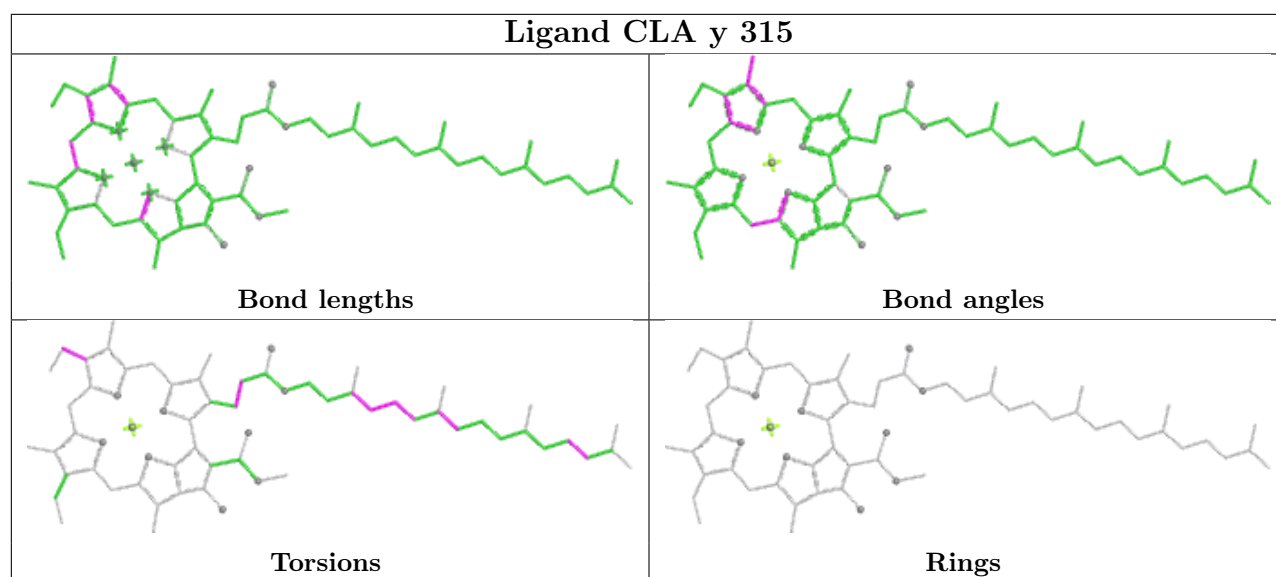
Rings

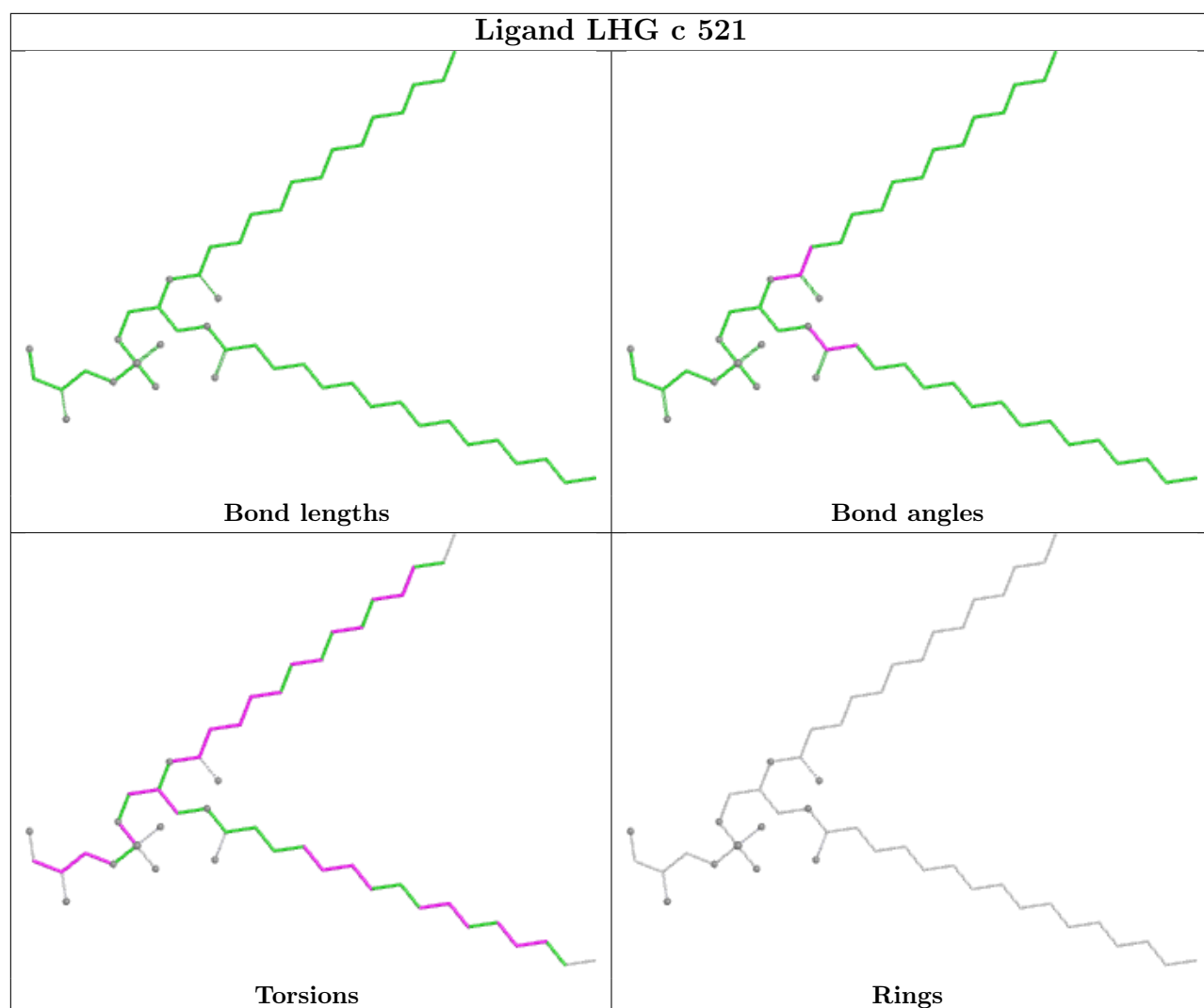


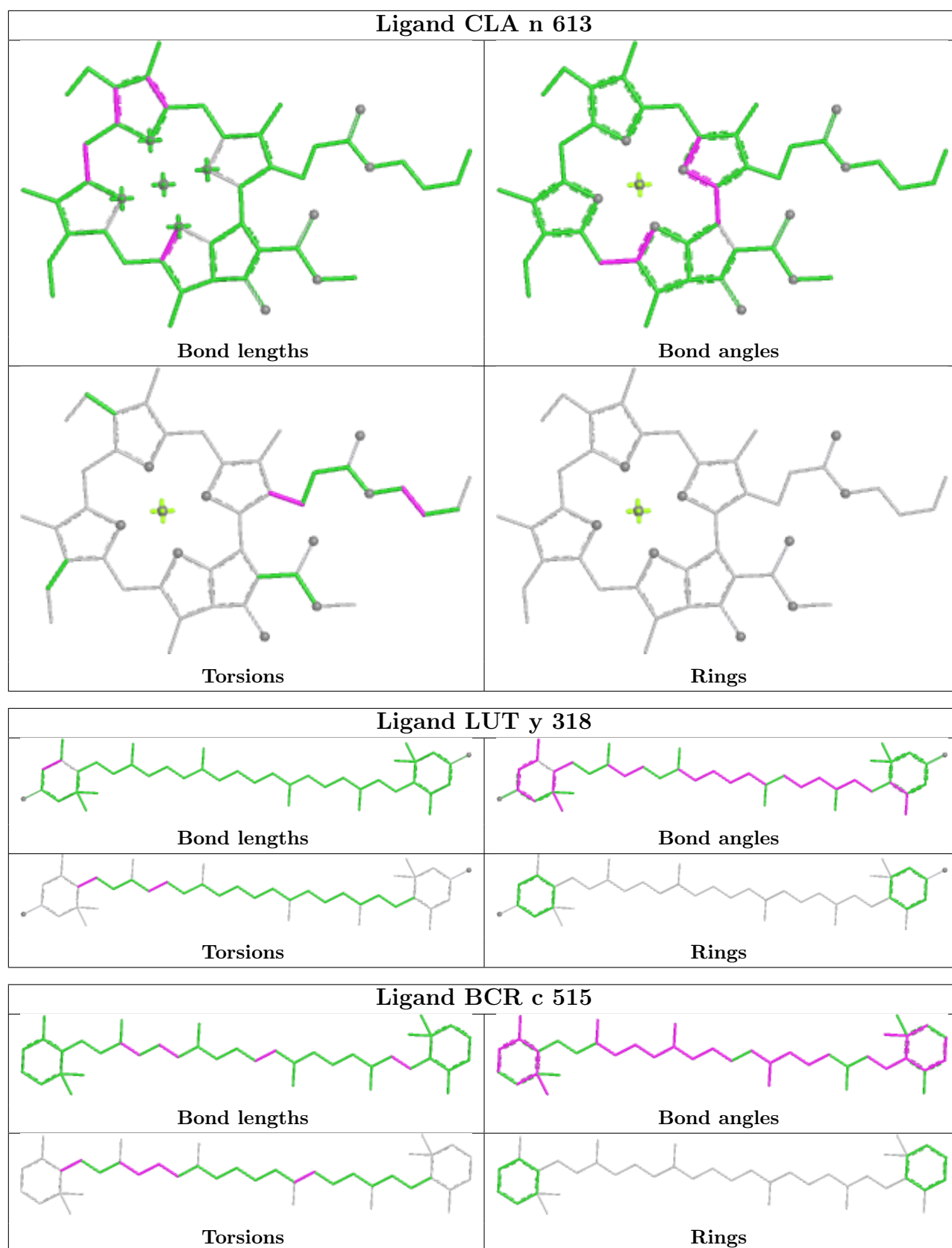


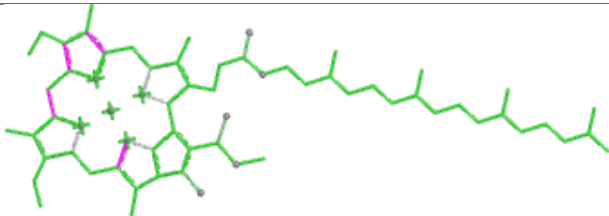
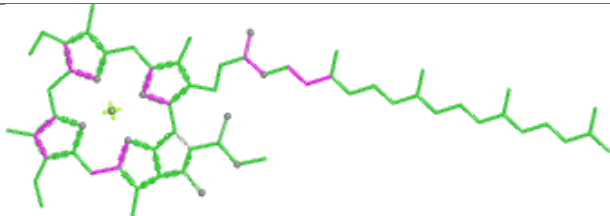
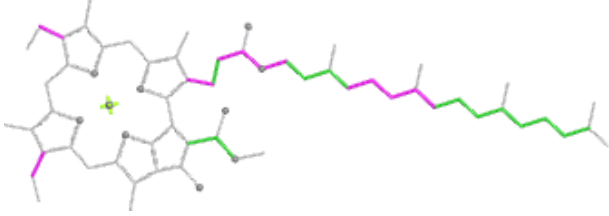
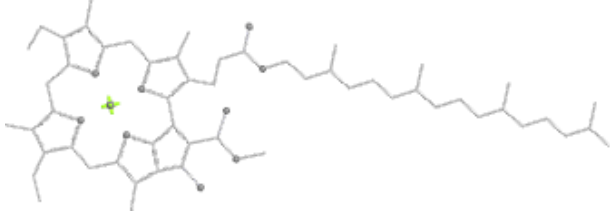


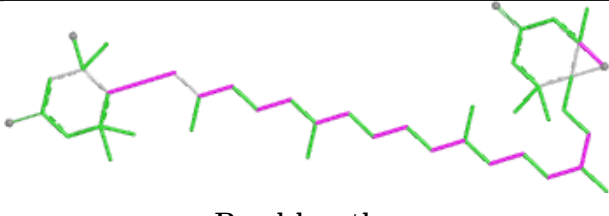
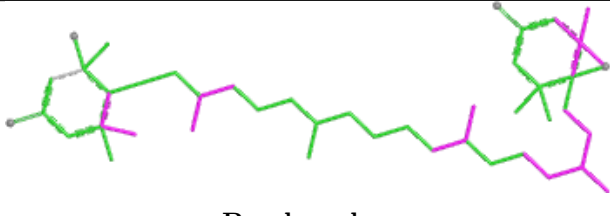
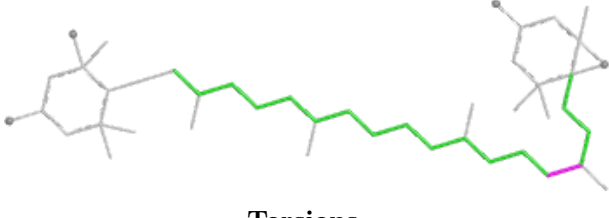
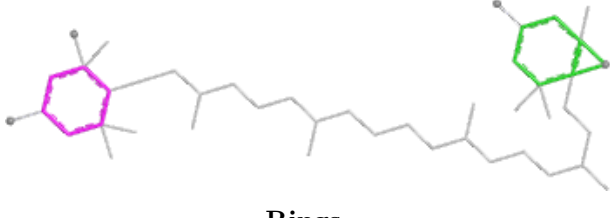


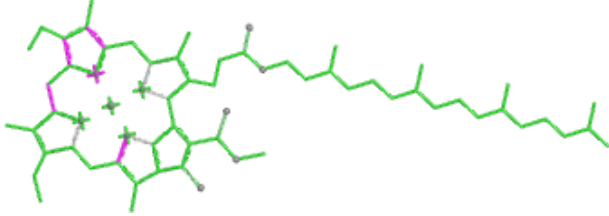
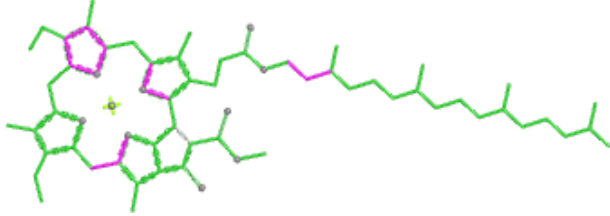
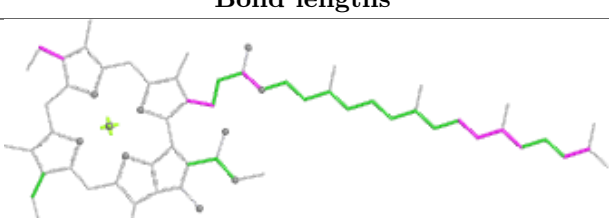
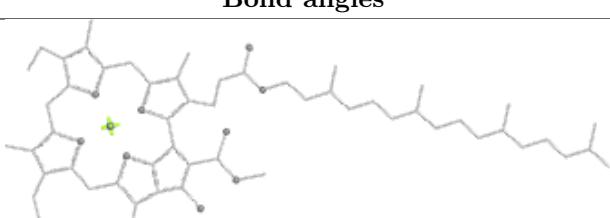


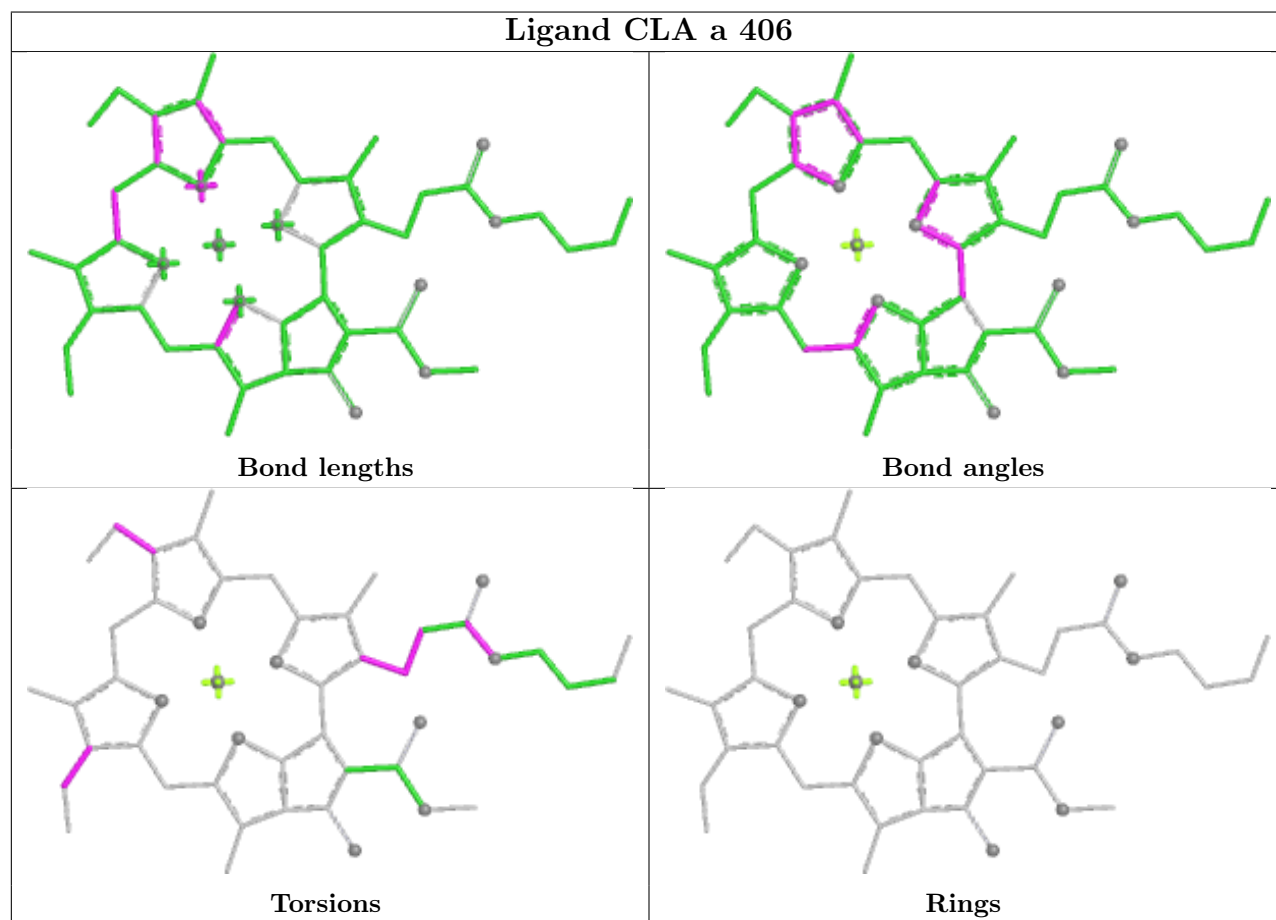
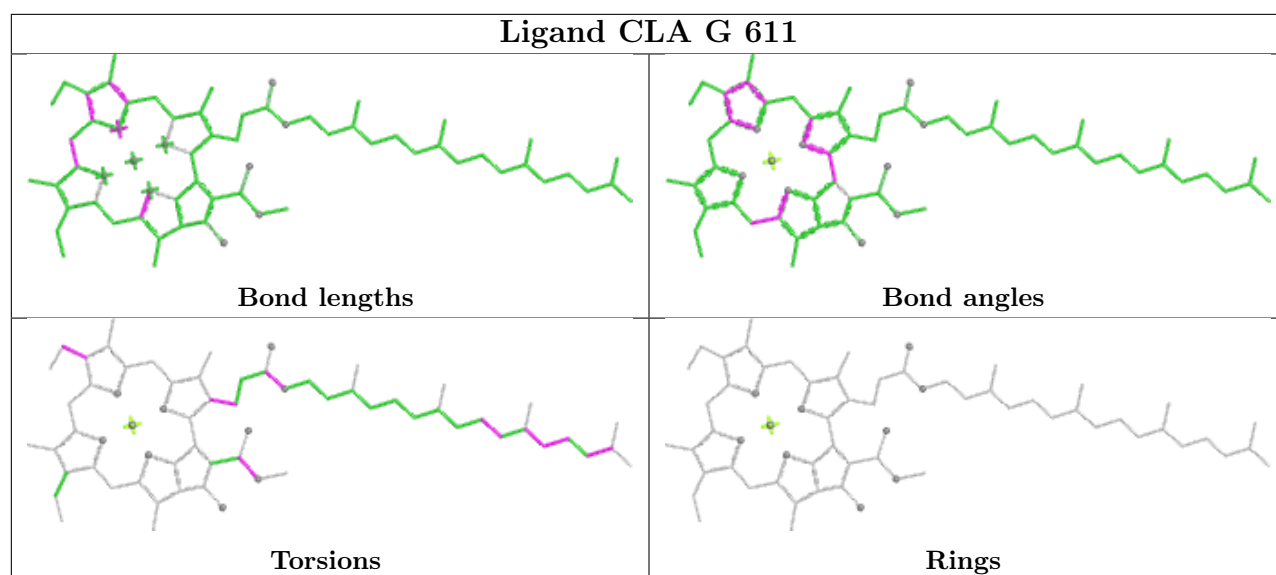


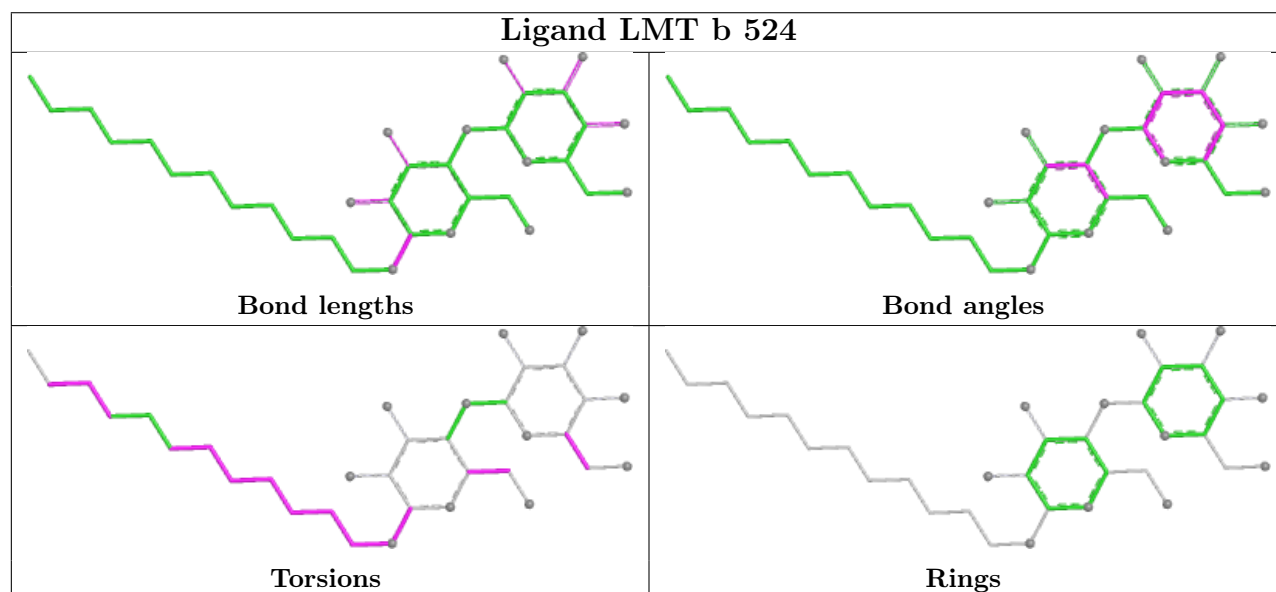
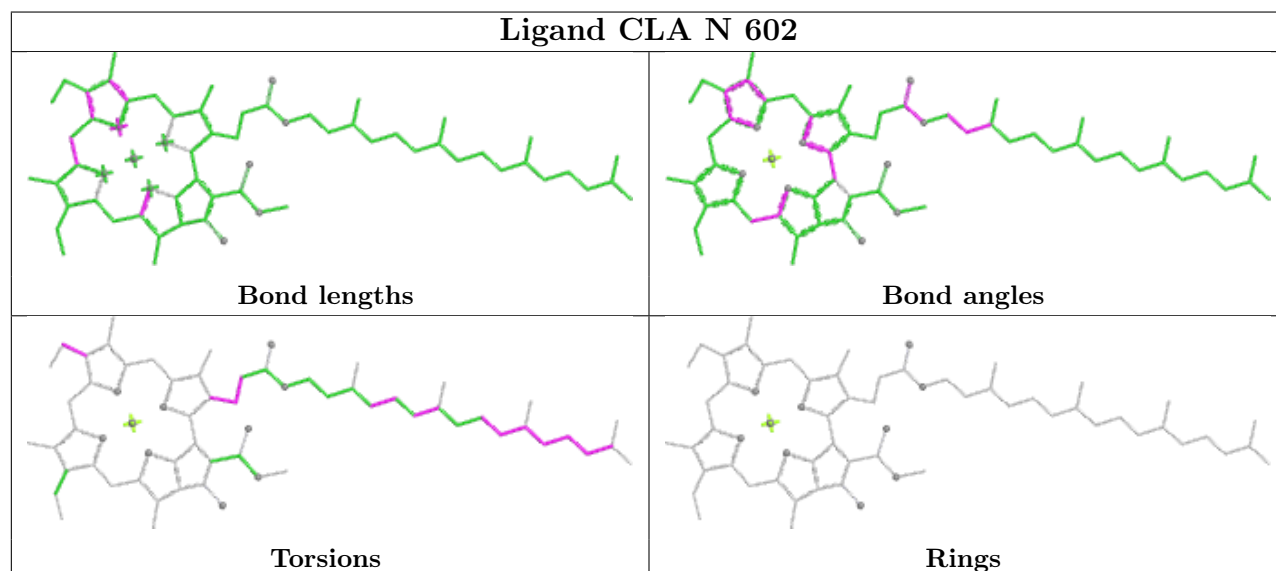
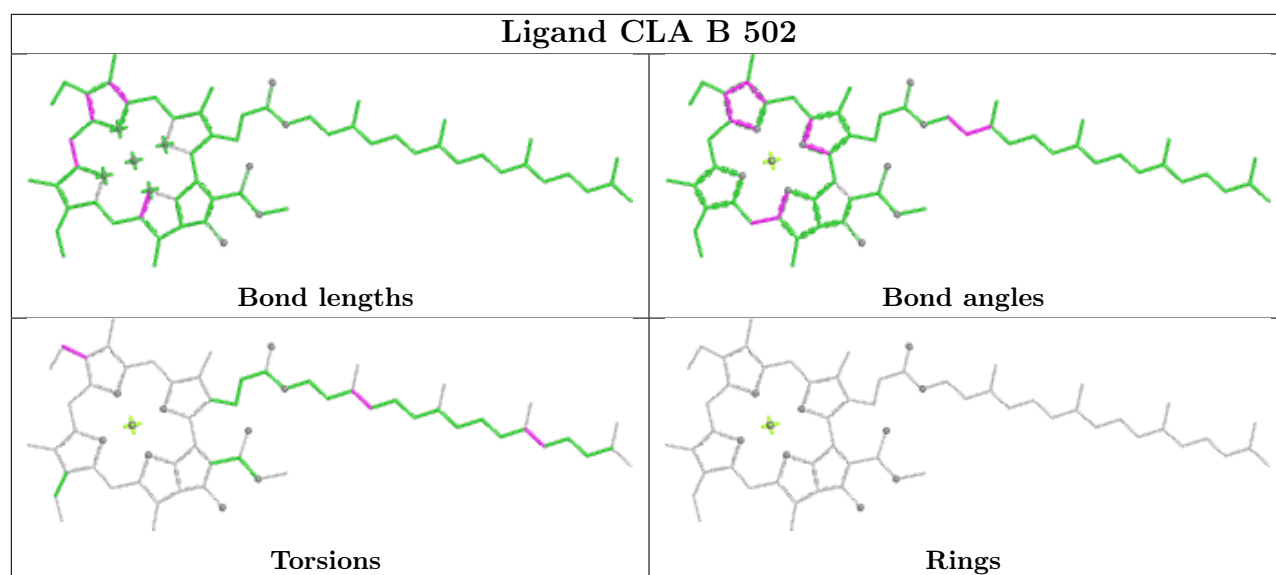


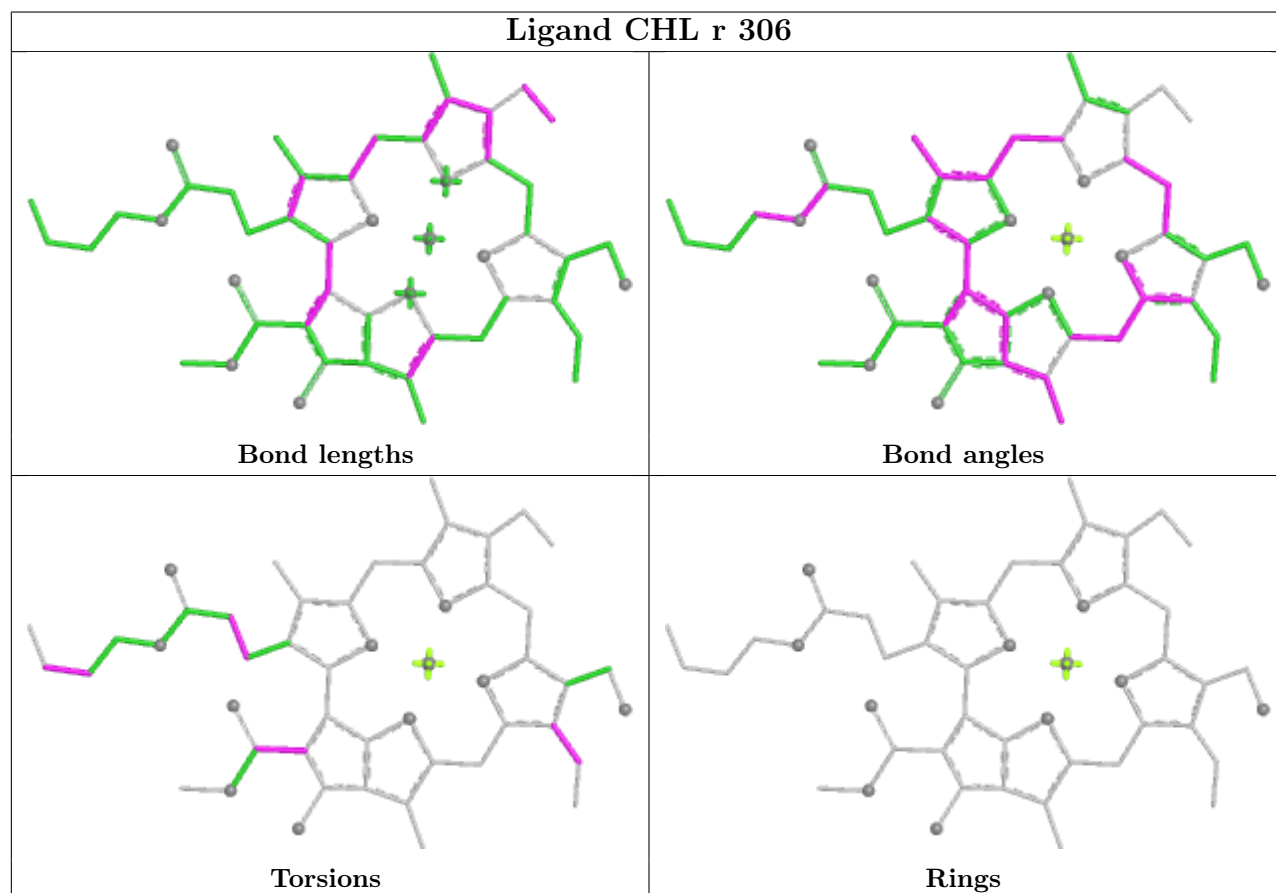
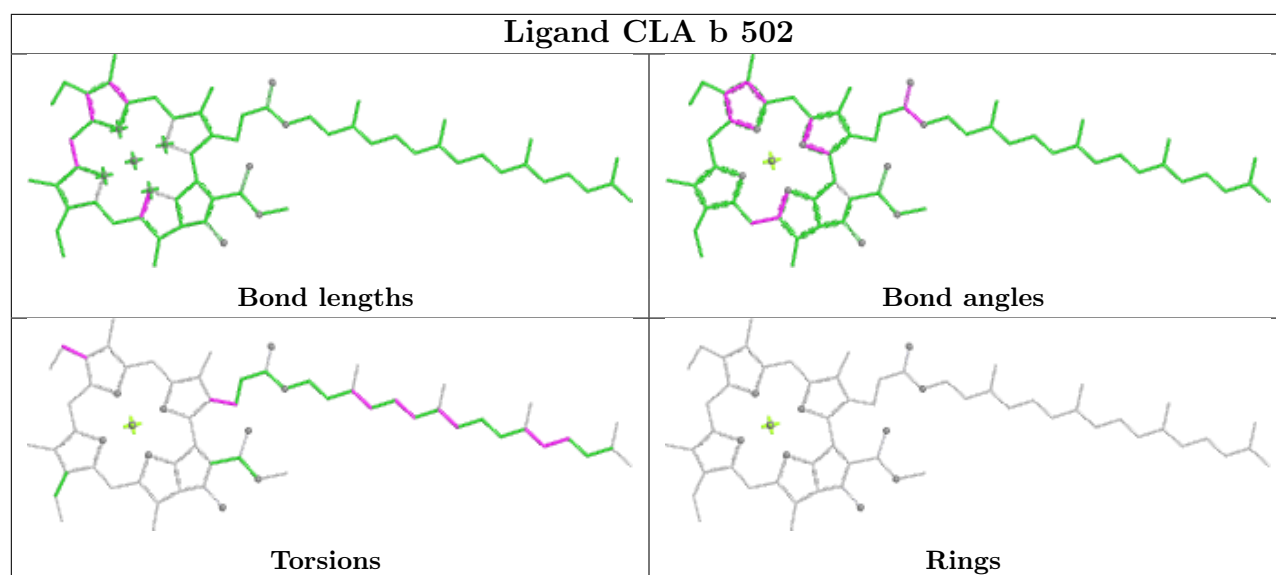
Ligand CLA A 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

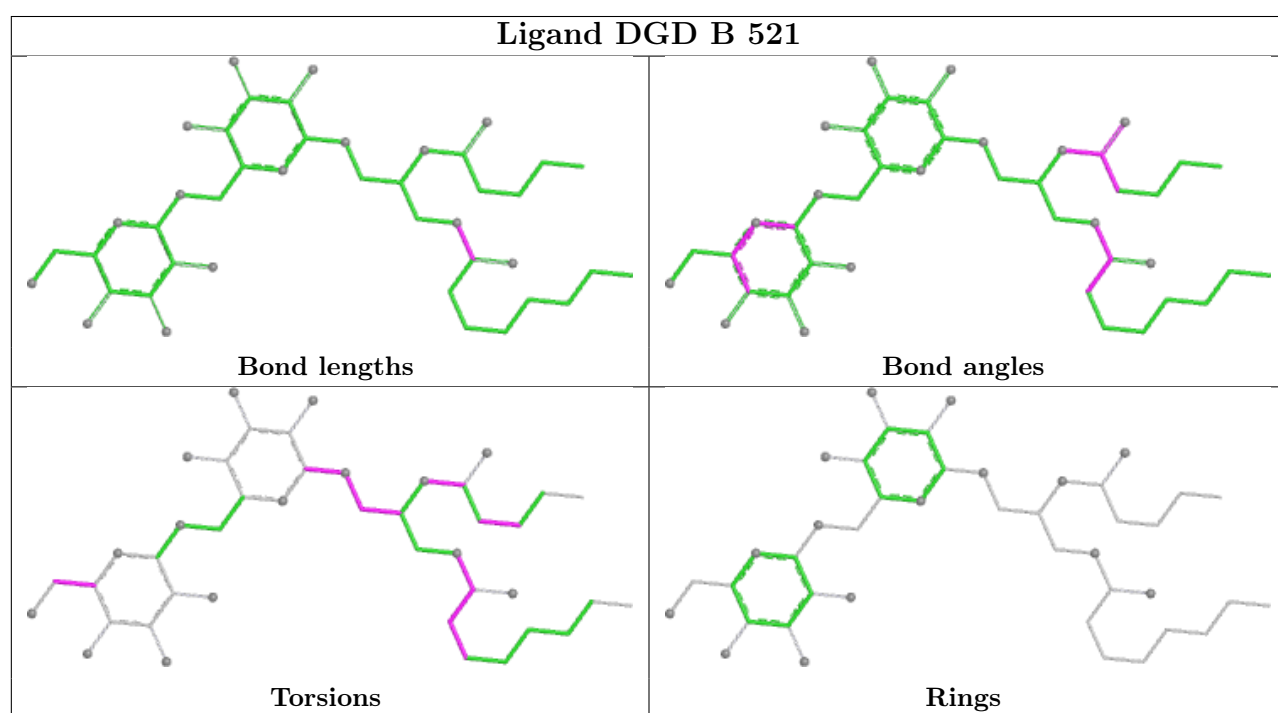
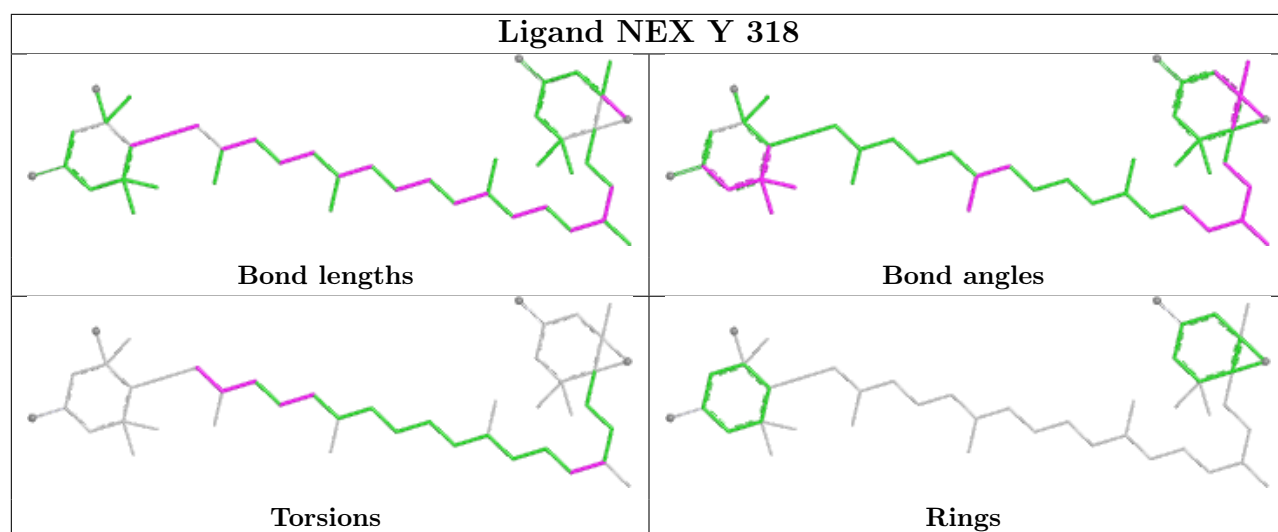
Ligand NEX N 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

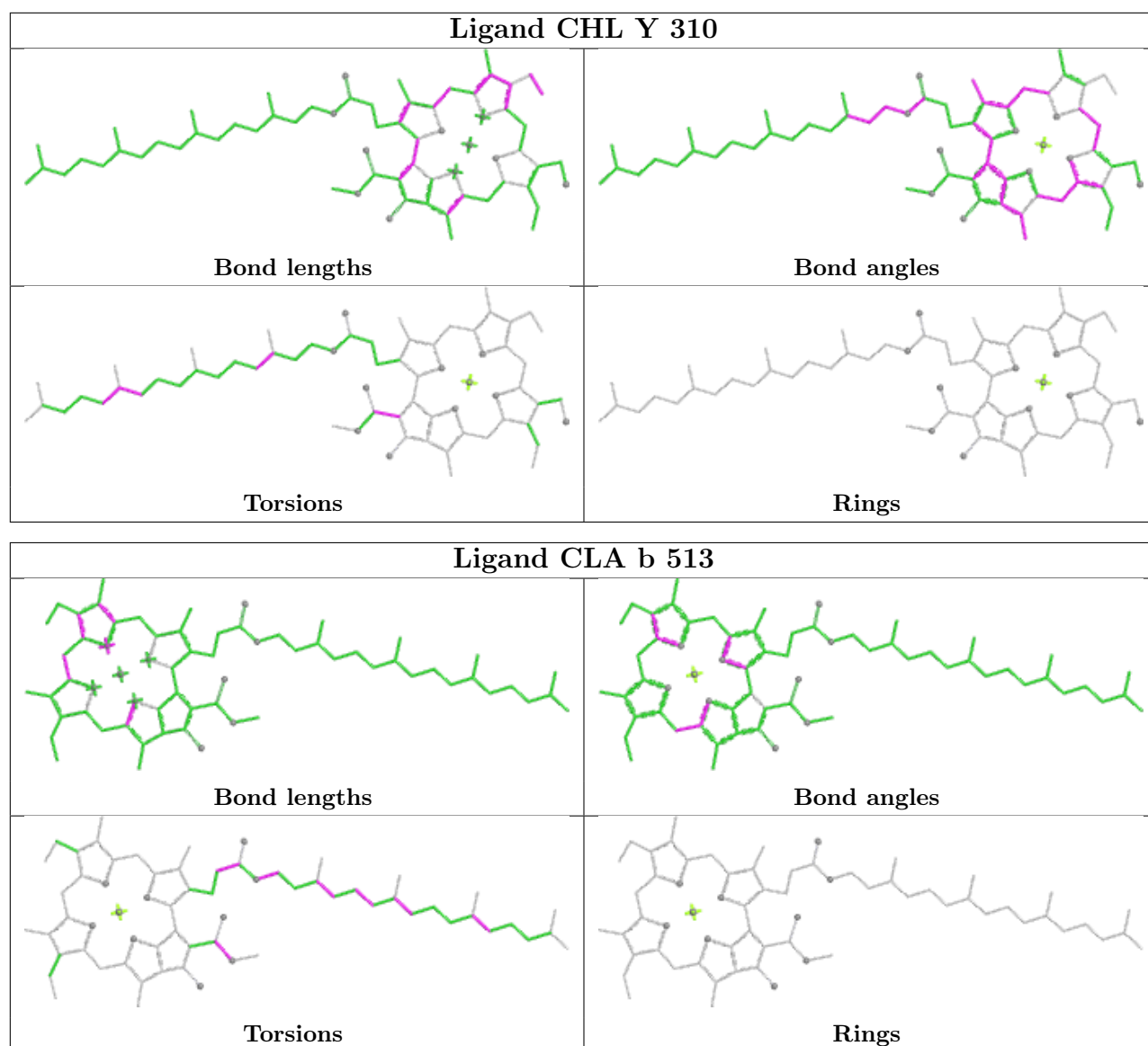
Ligand CLA g 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

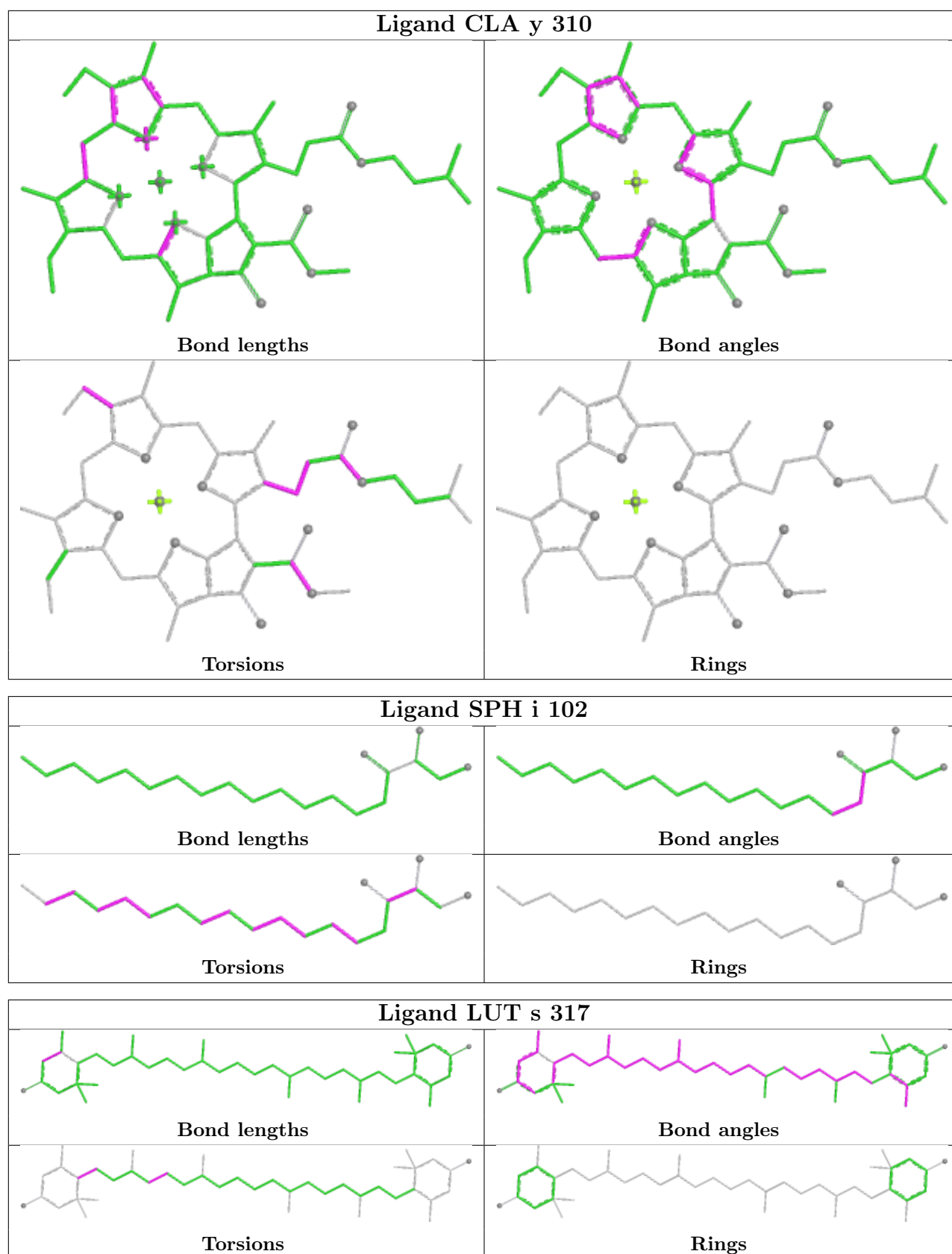


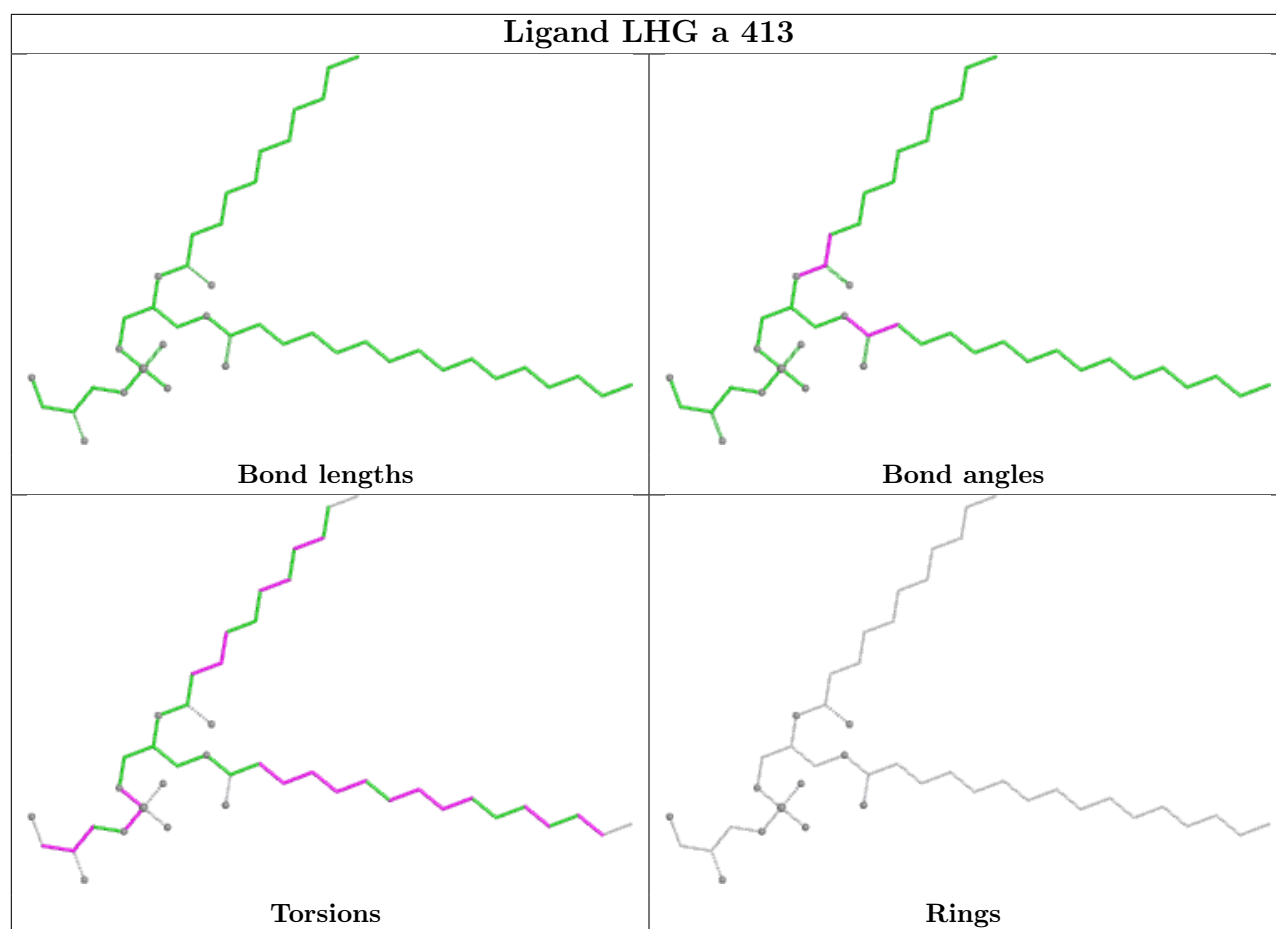


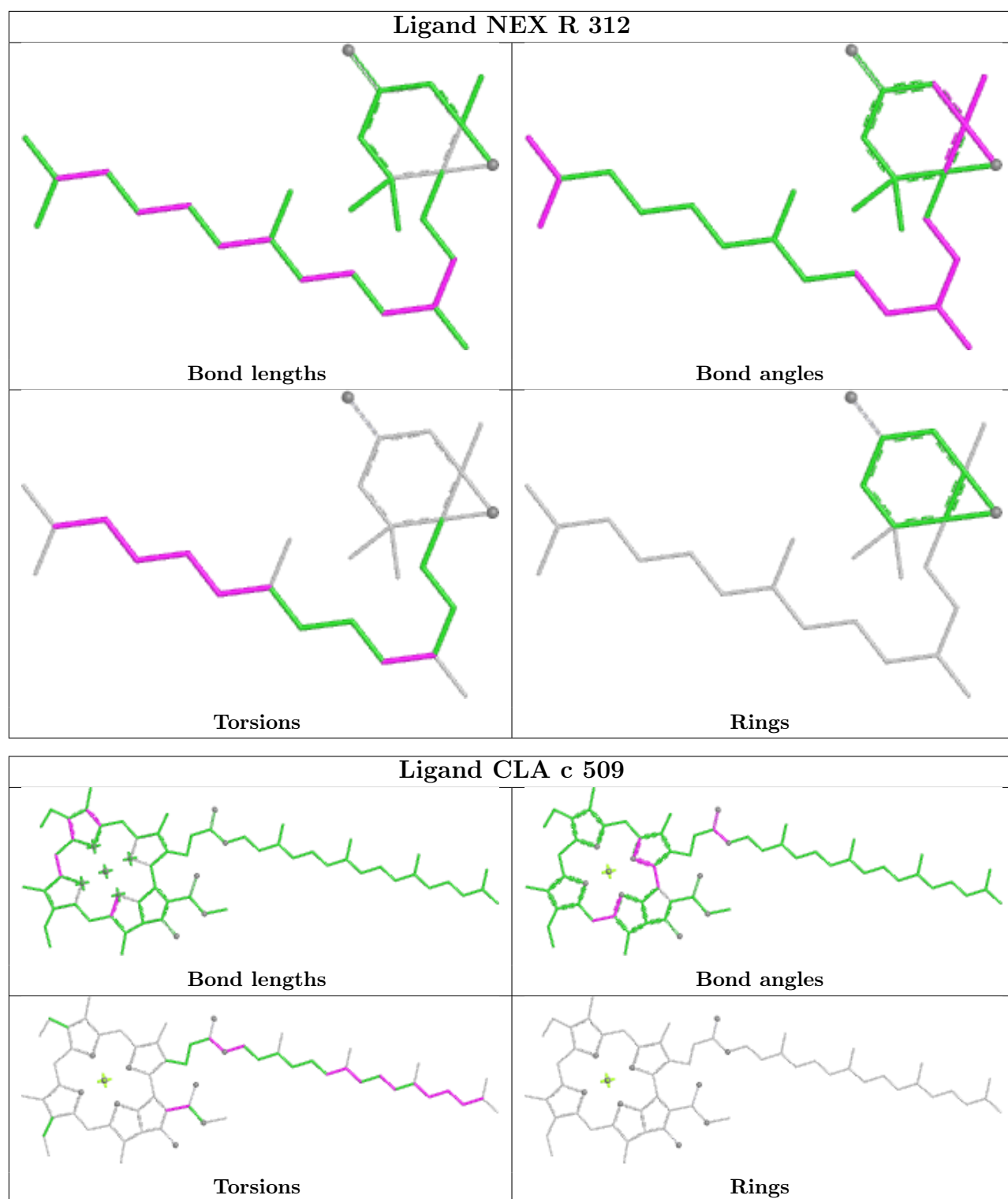


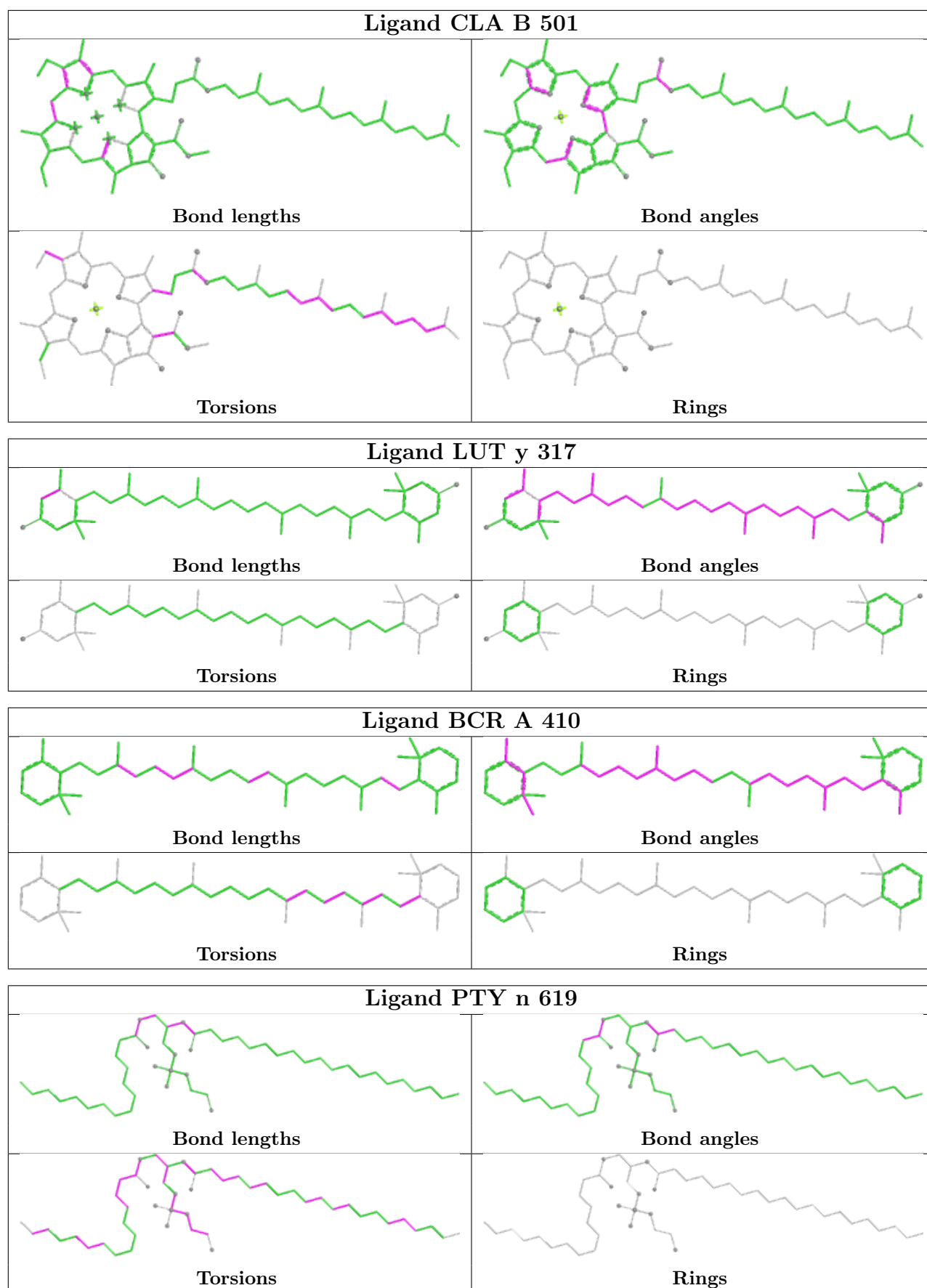


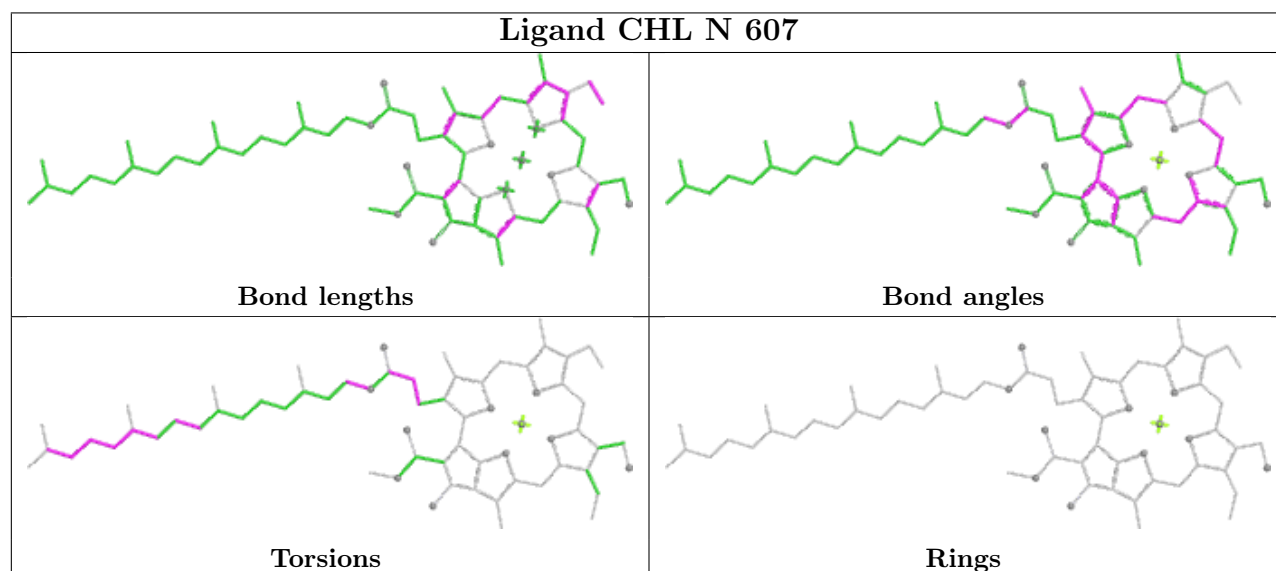
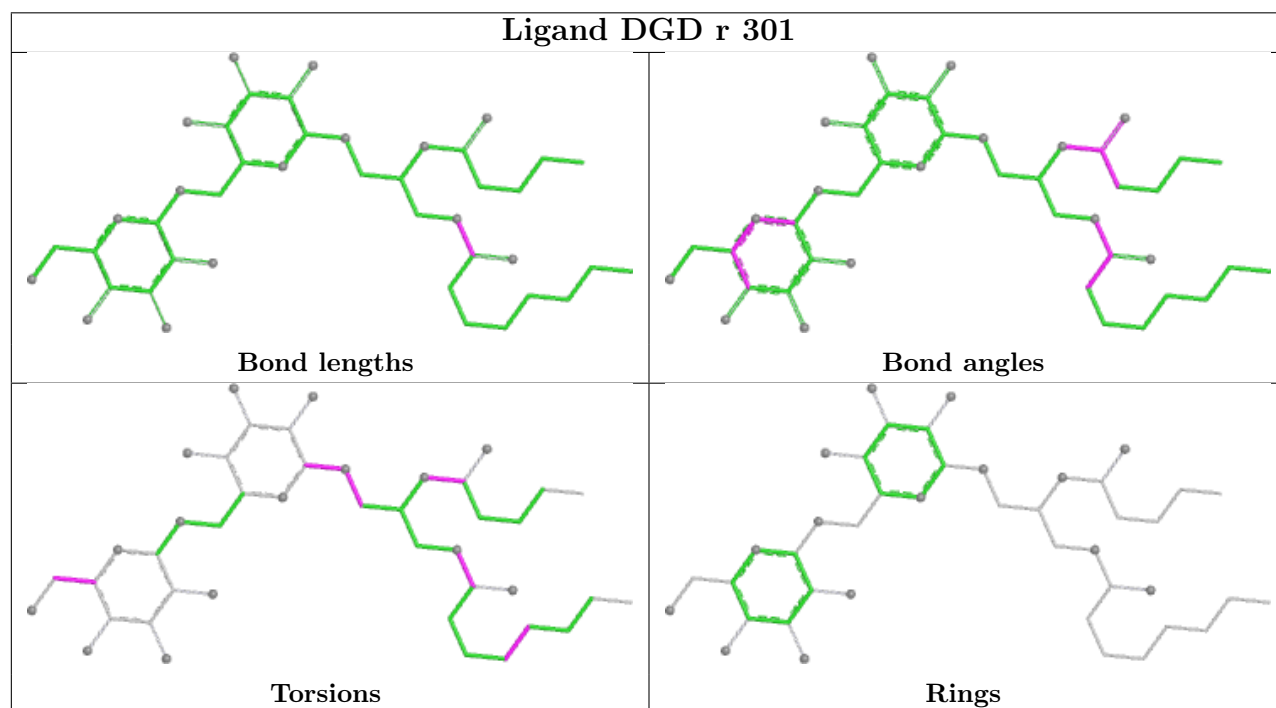
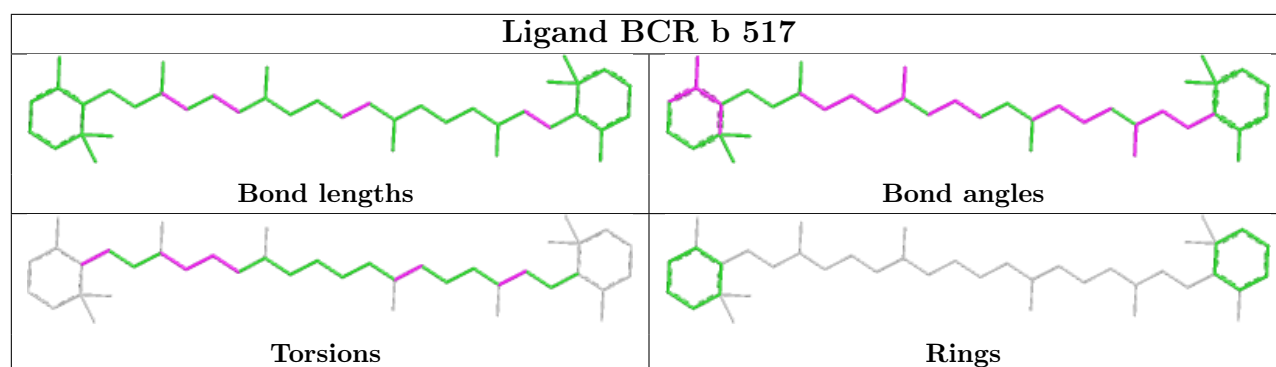


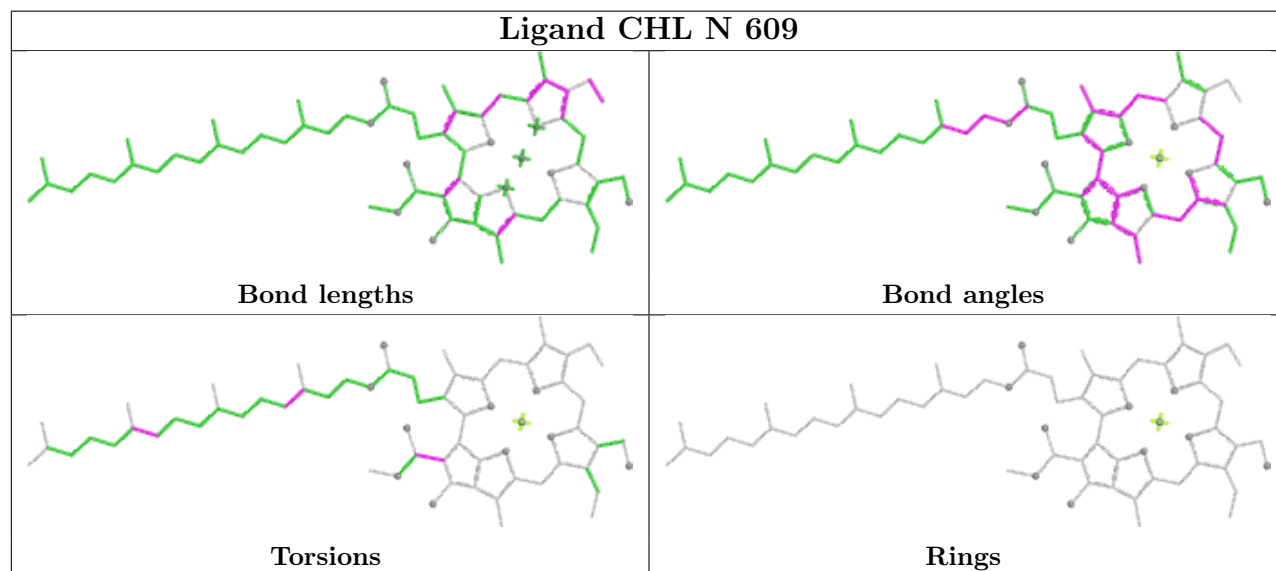
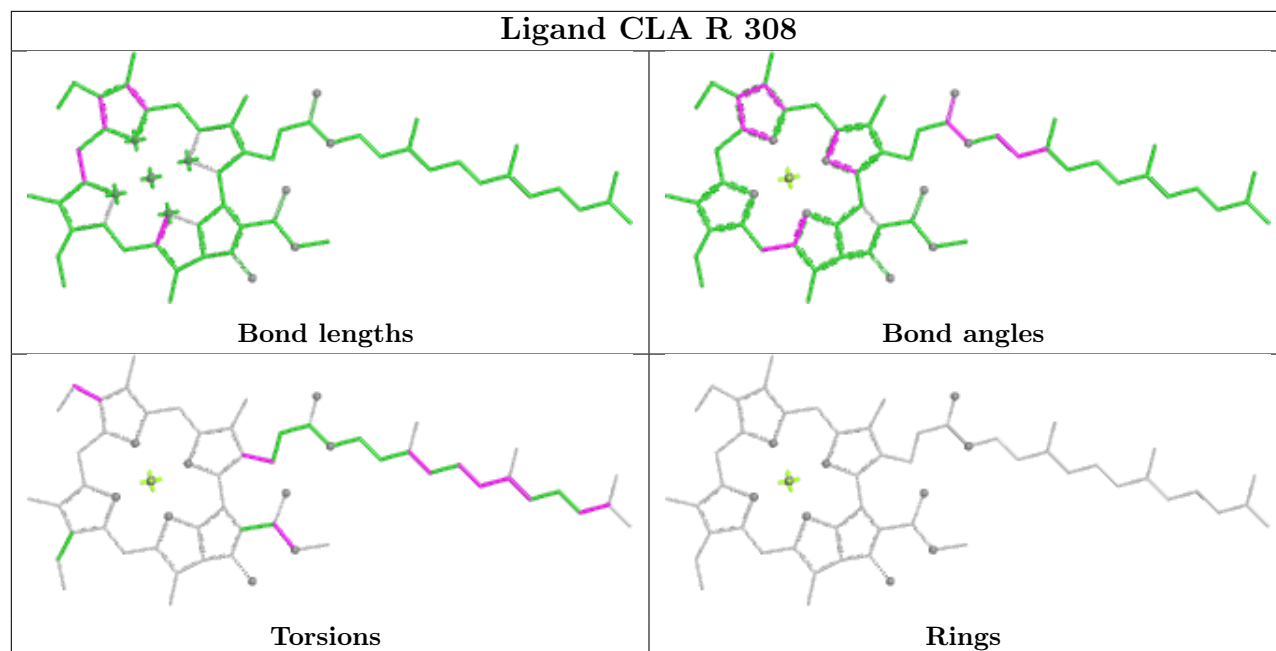


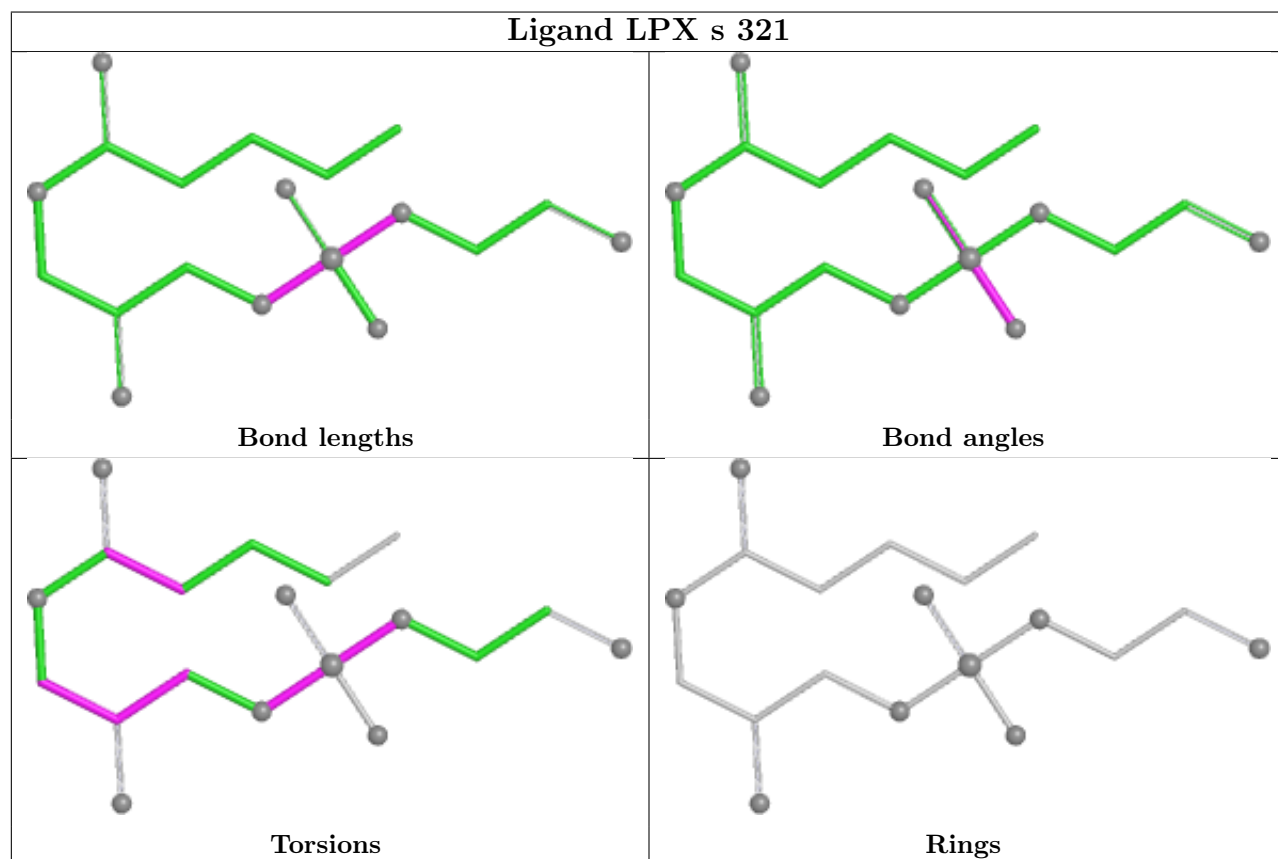
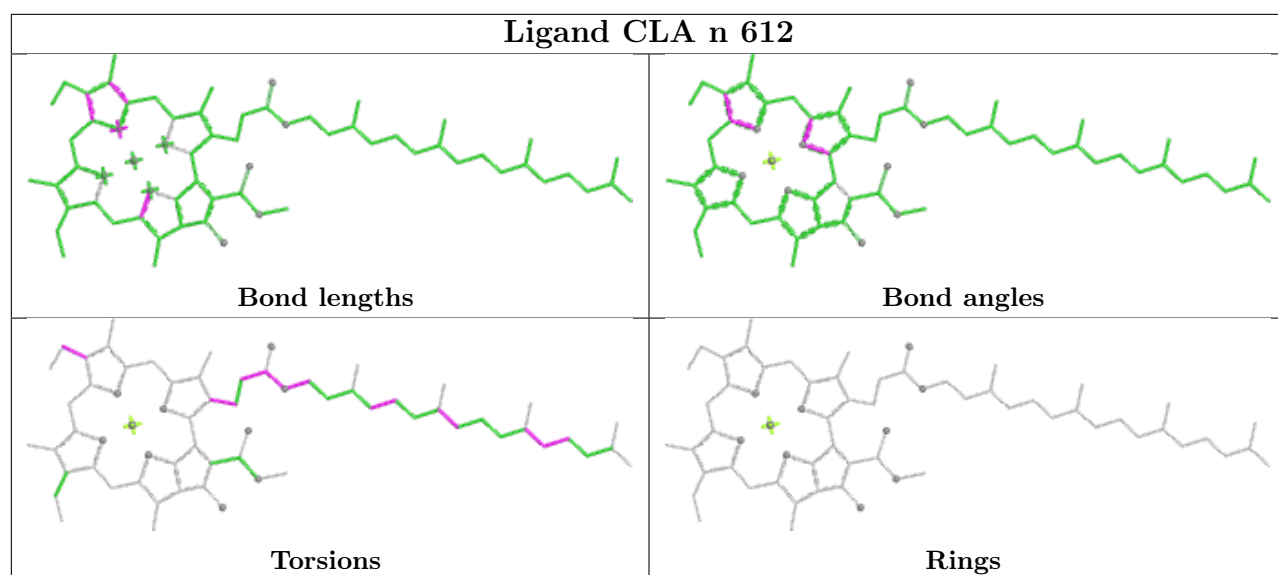




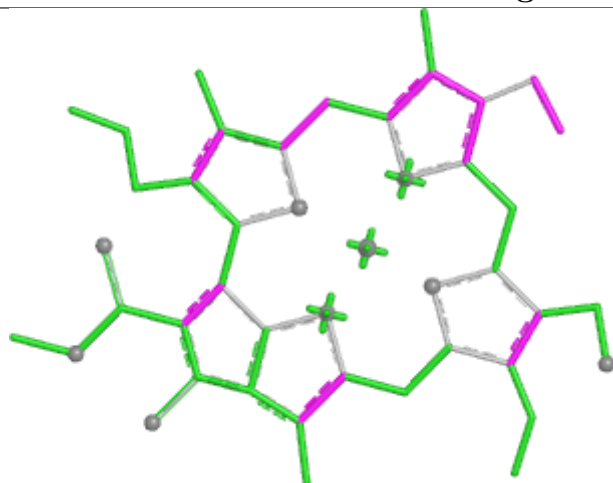




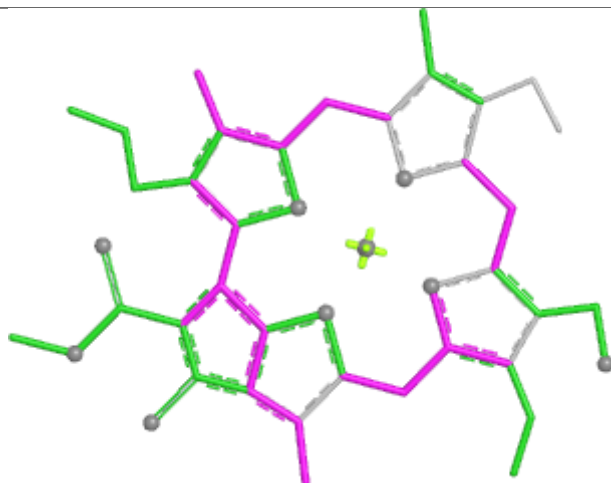




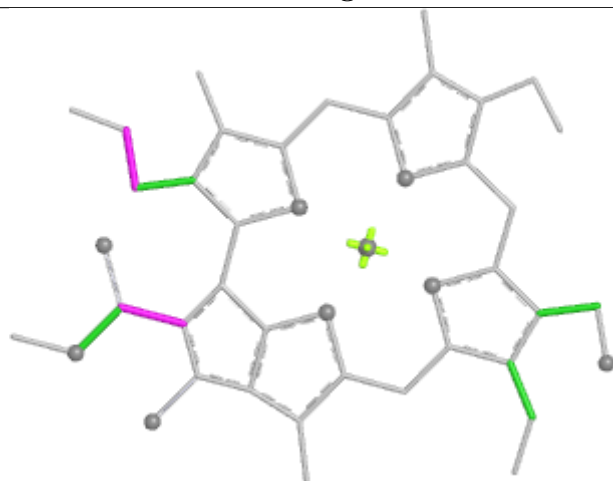
Ligand CHL S 307



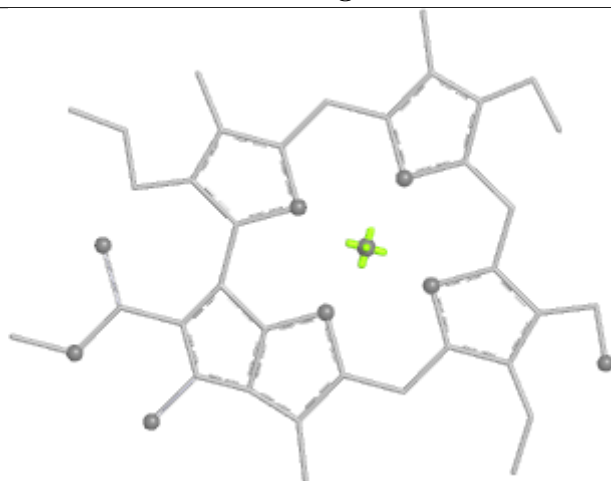
Bond lengths



Bond angles

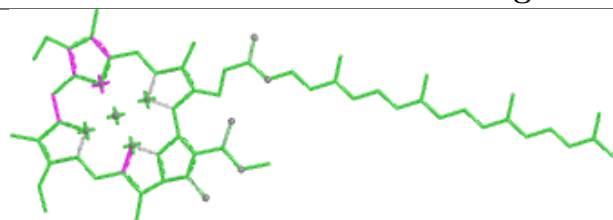


Torsions

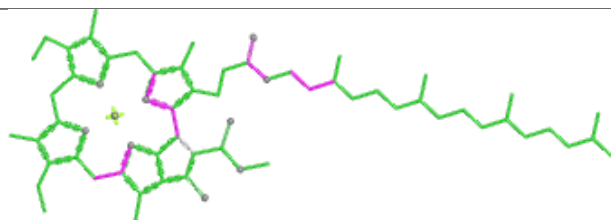


Rings

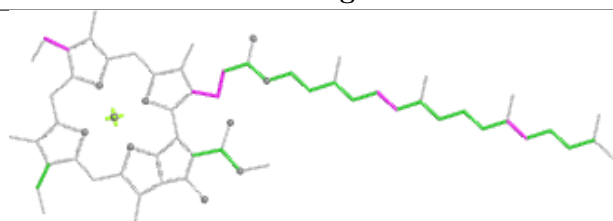
Ligand CLA Y 311



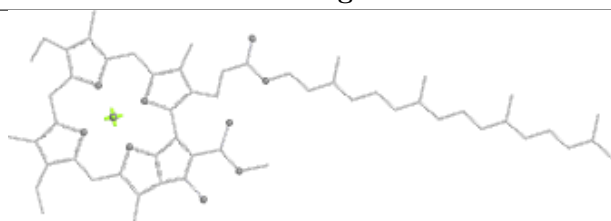
Bond lengths



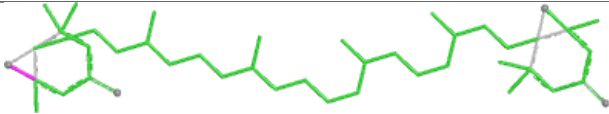
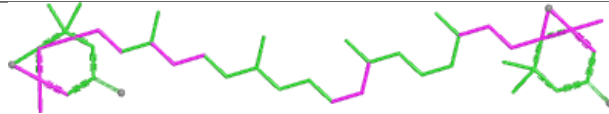
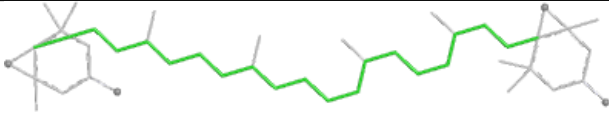
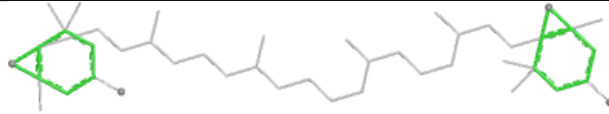
Bond angles

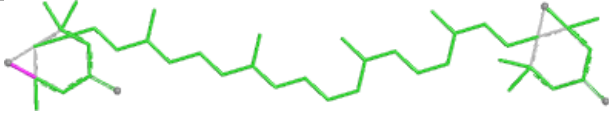
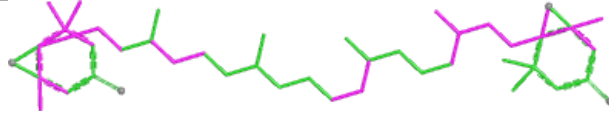
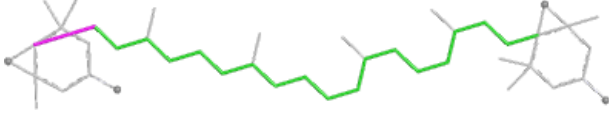
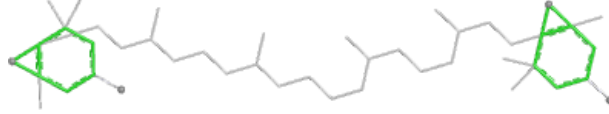


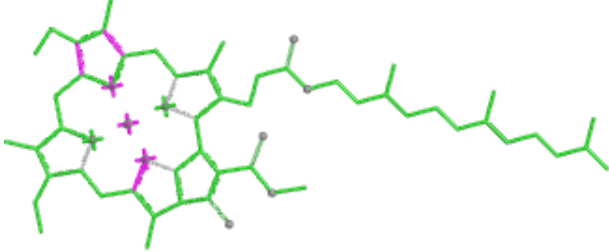
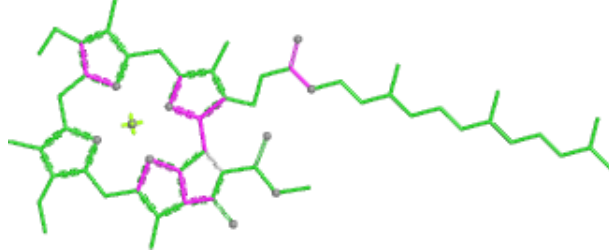
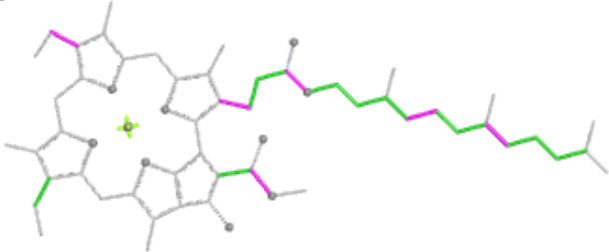
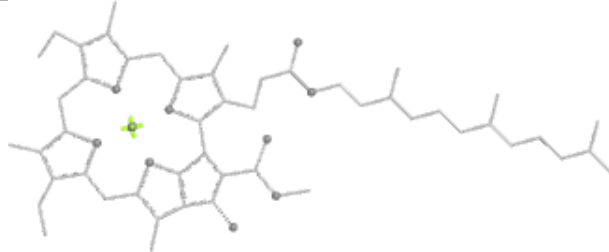
Torsions

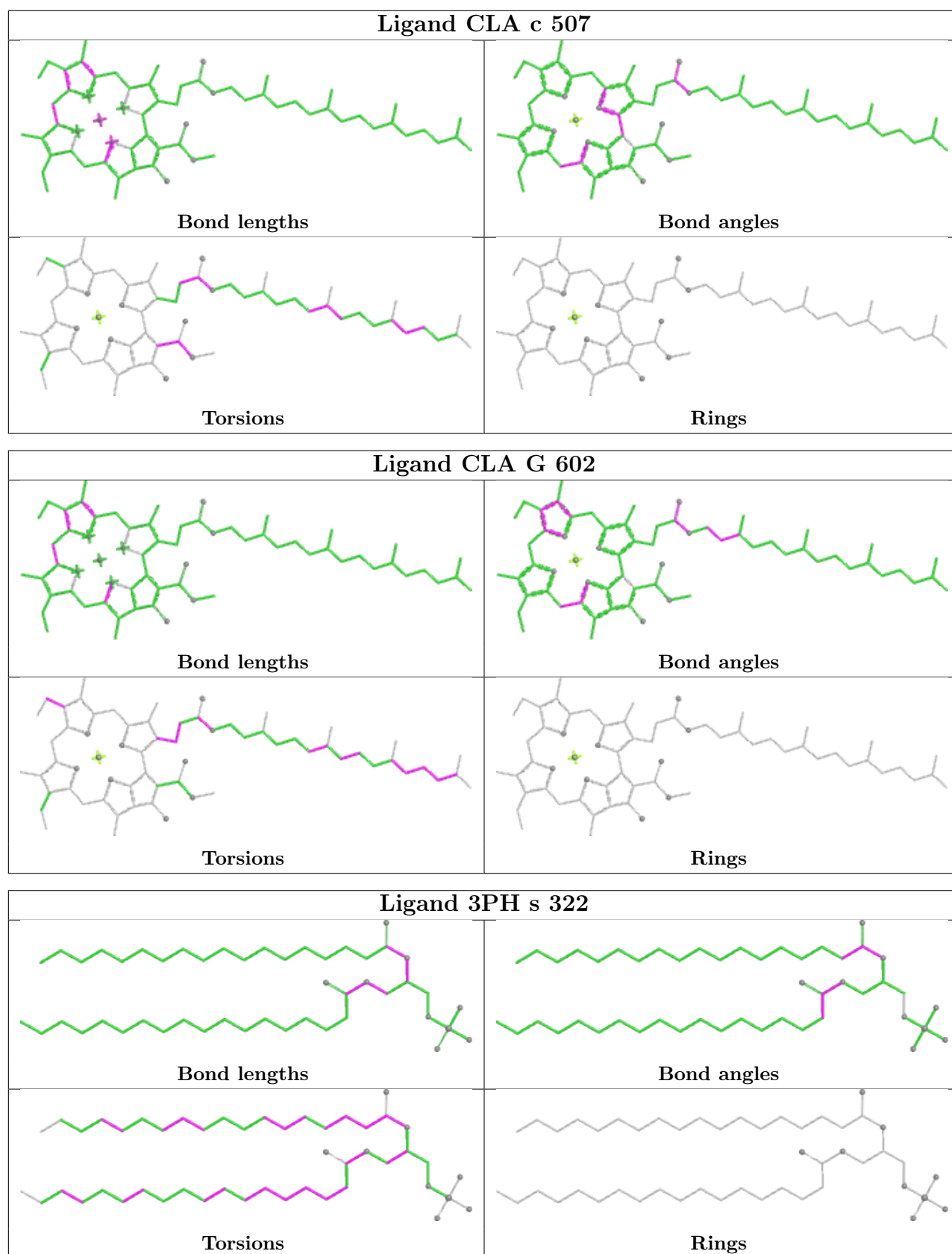


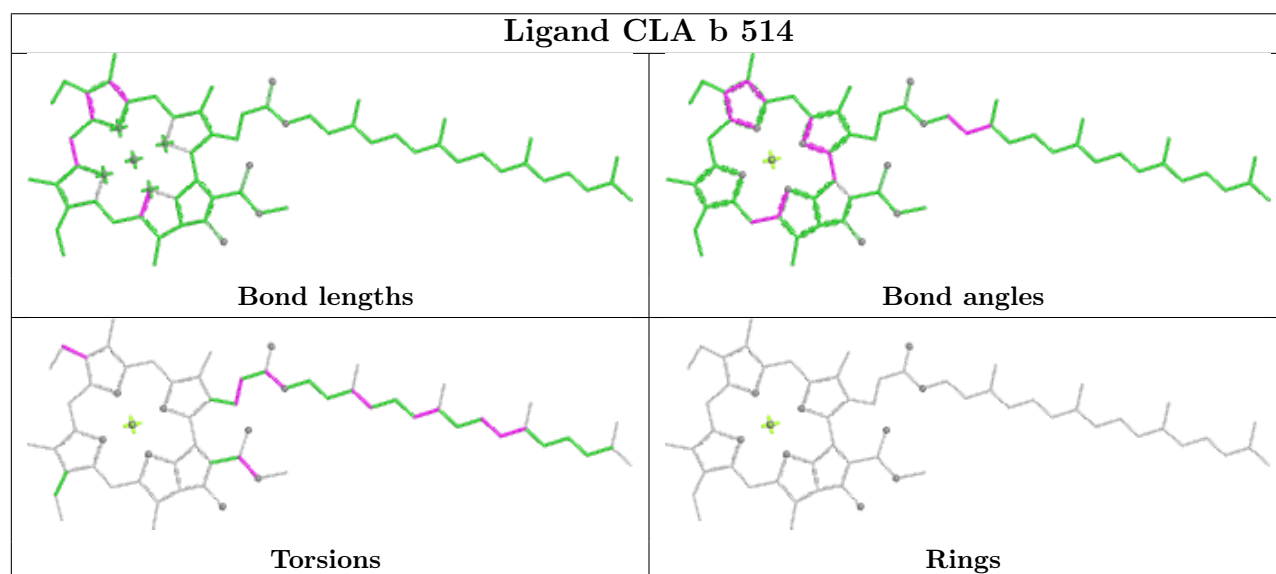
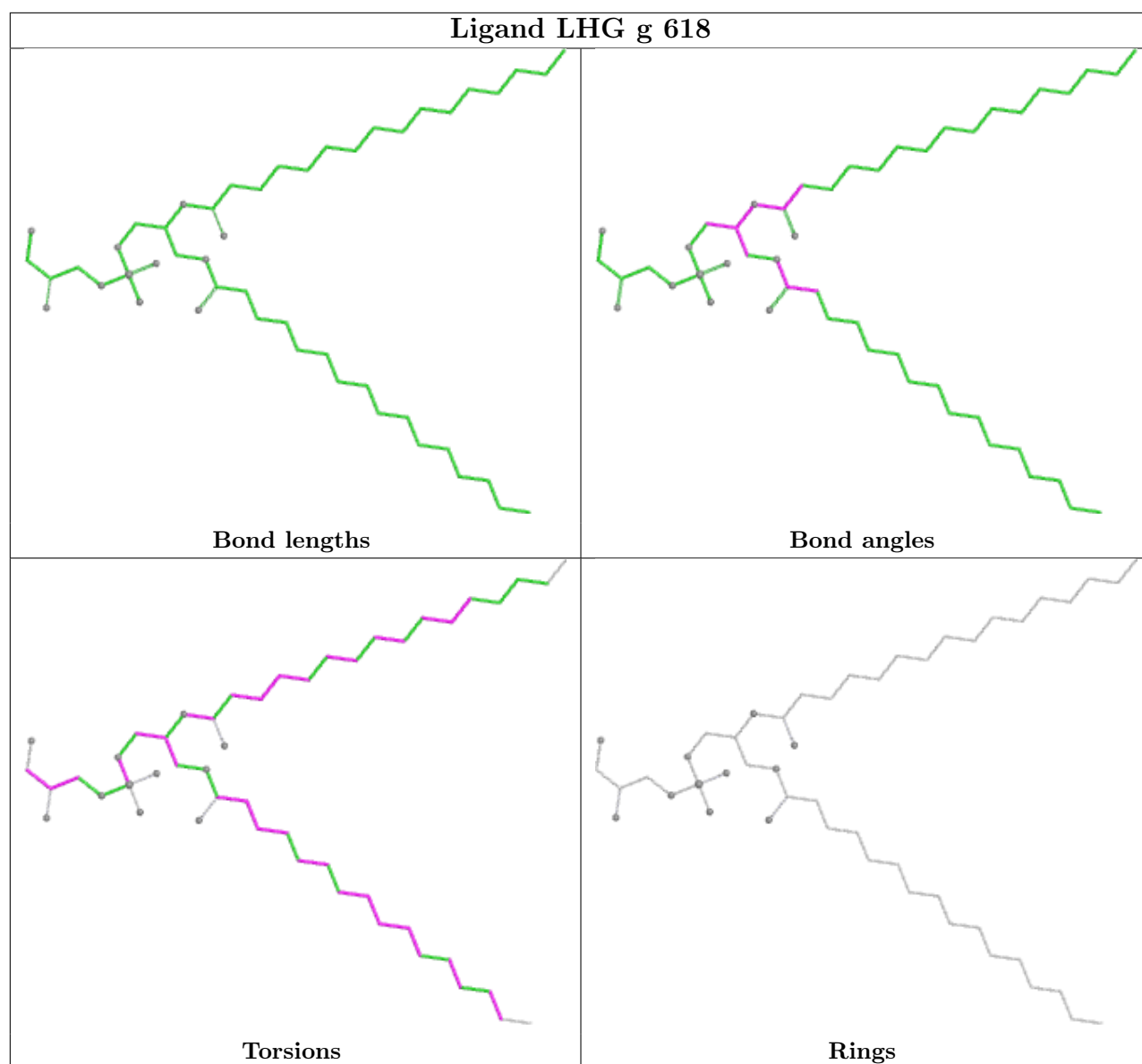
Rings

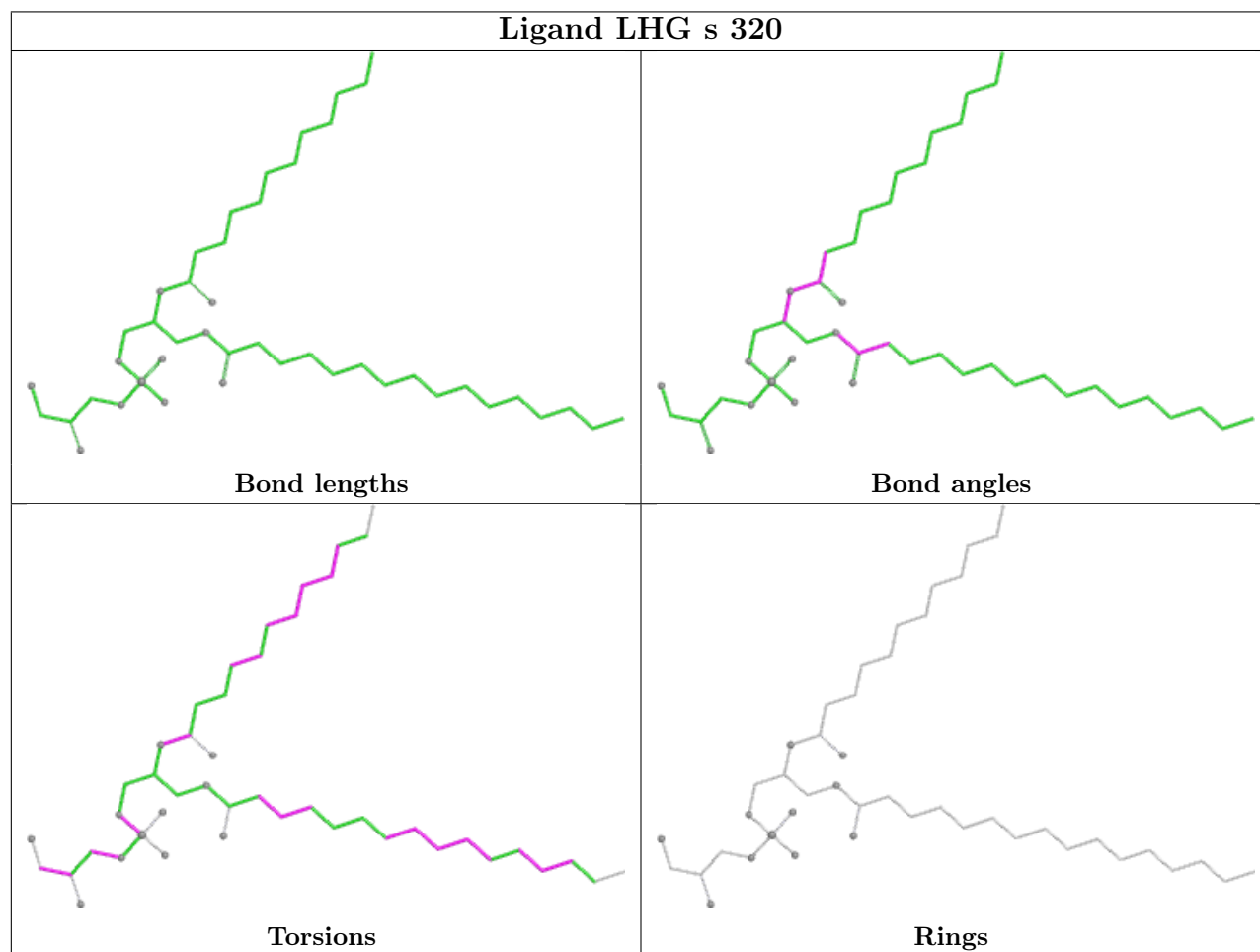
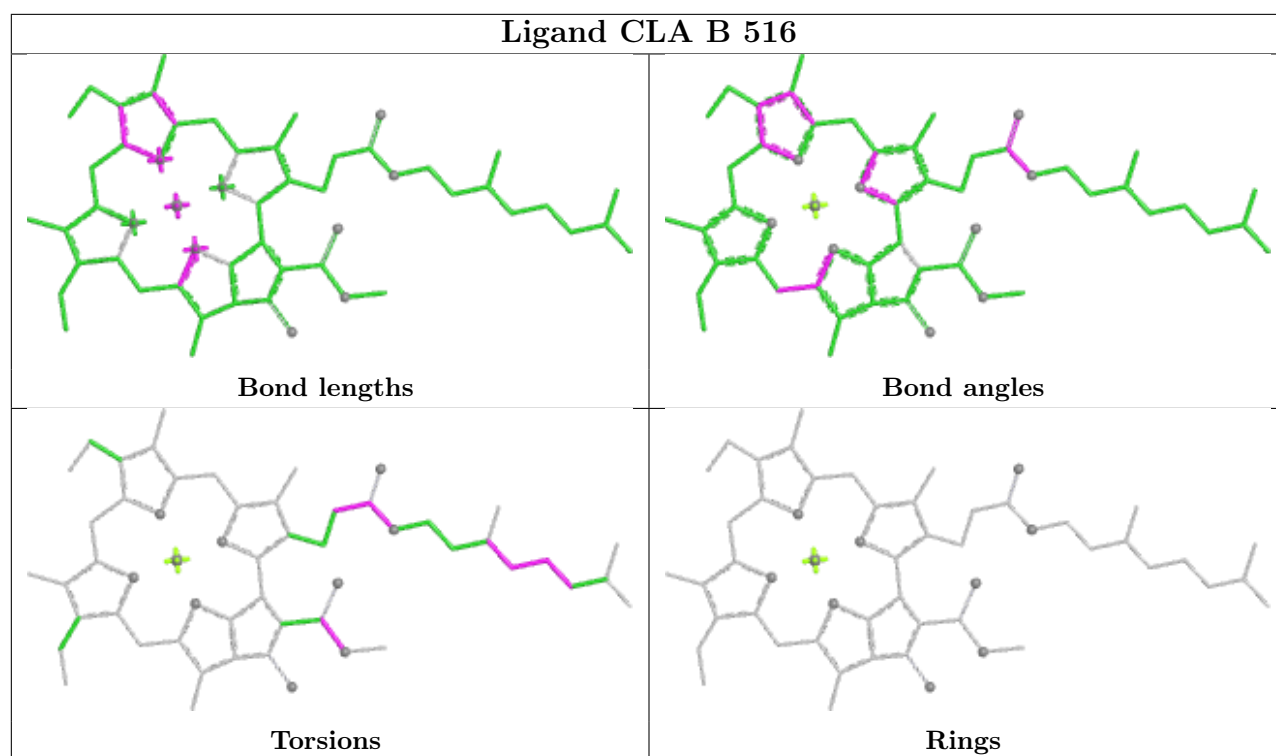
Ligand XAT Y 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

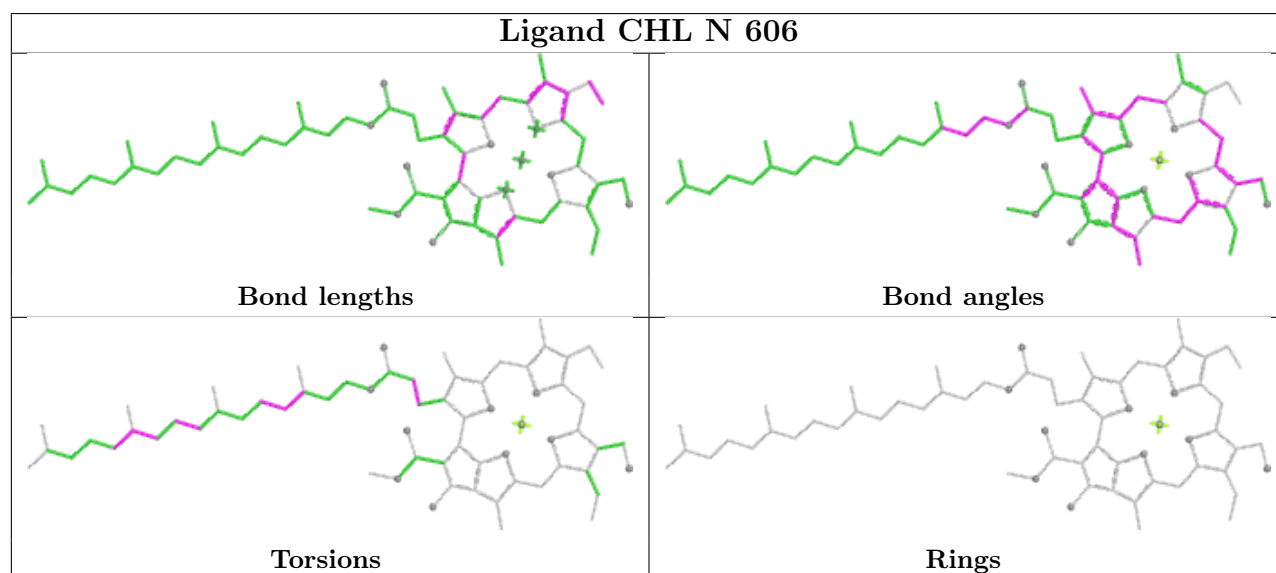
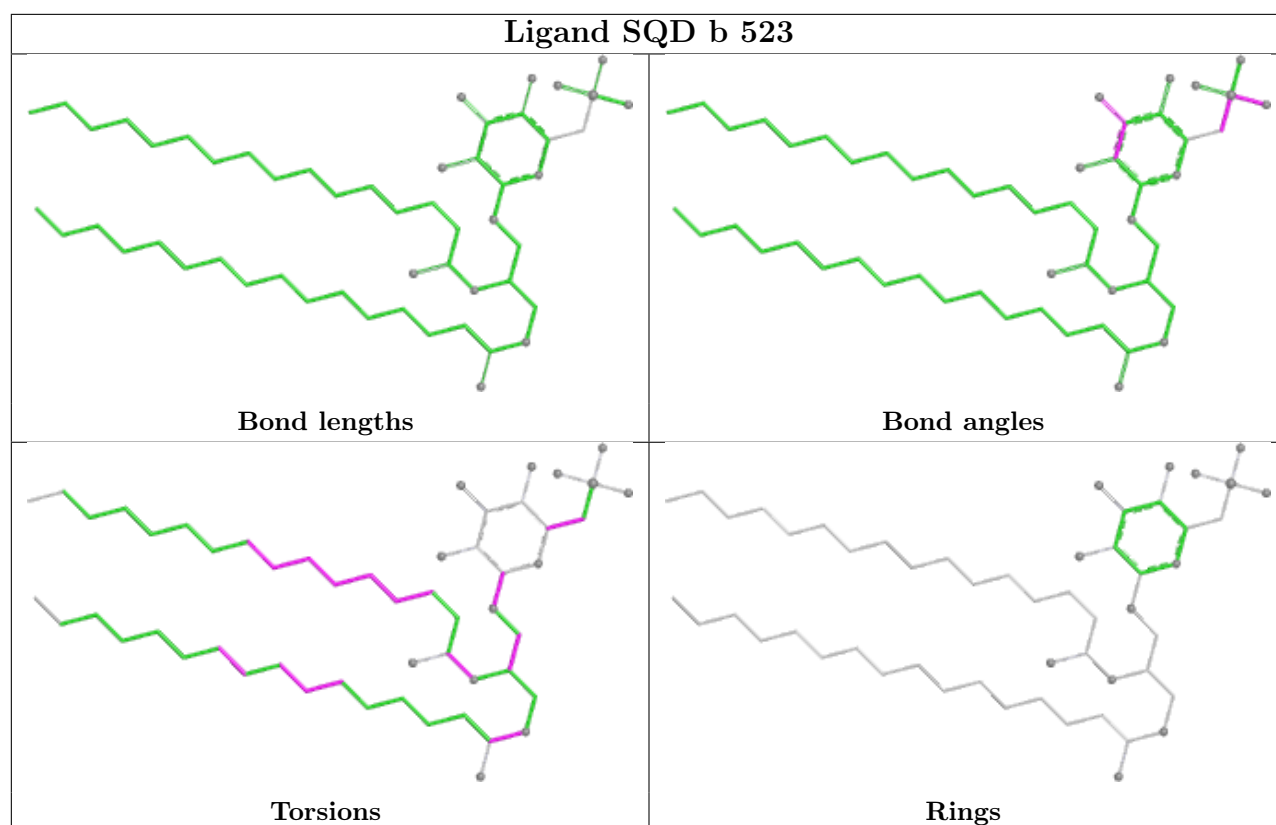
Ligand XAT g 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

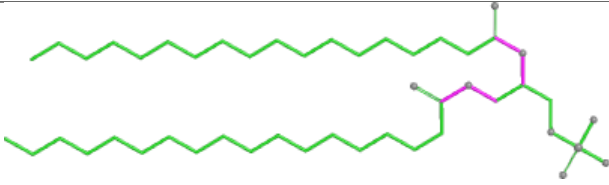
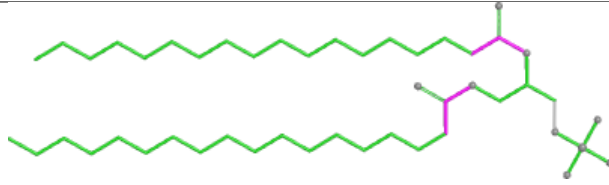
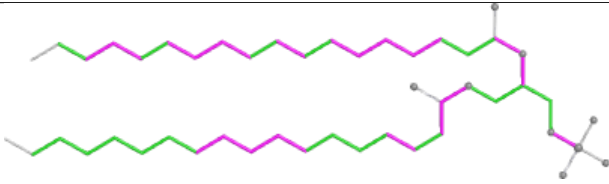
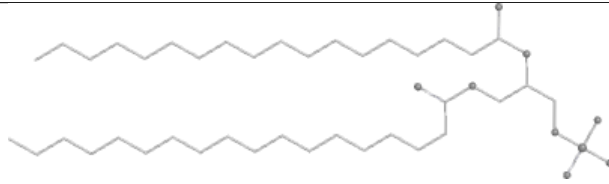
Ligand CLA r 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

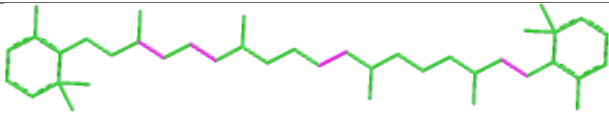
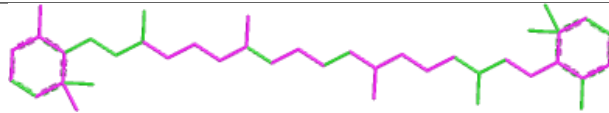
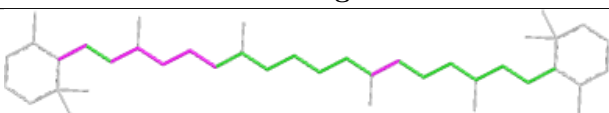
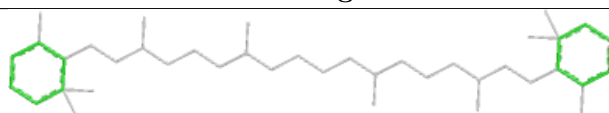


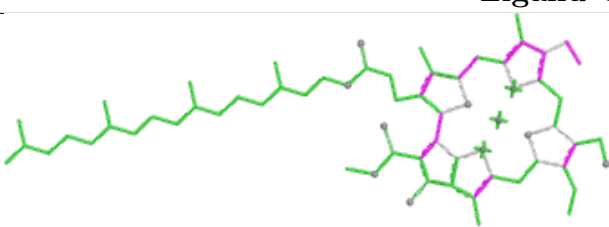
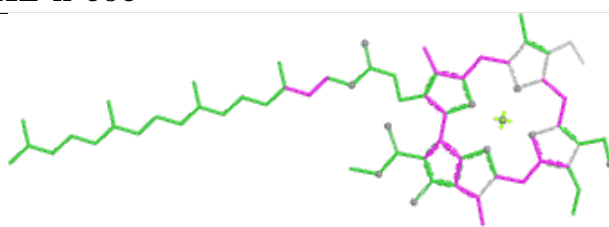
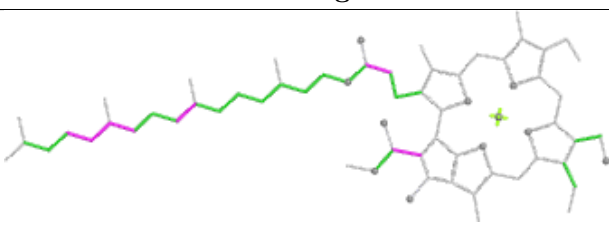
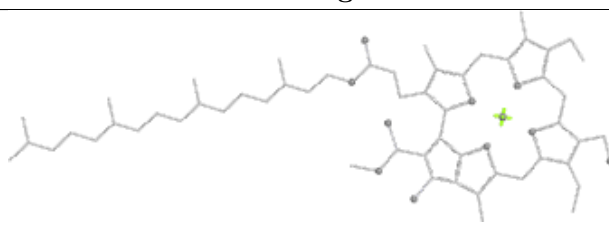


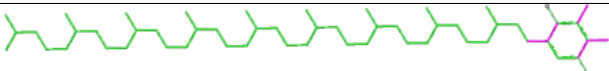
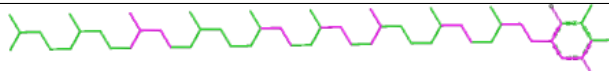
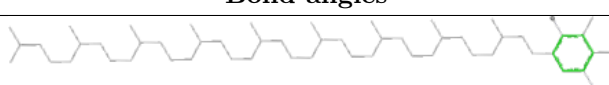


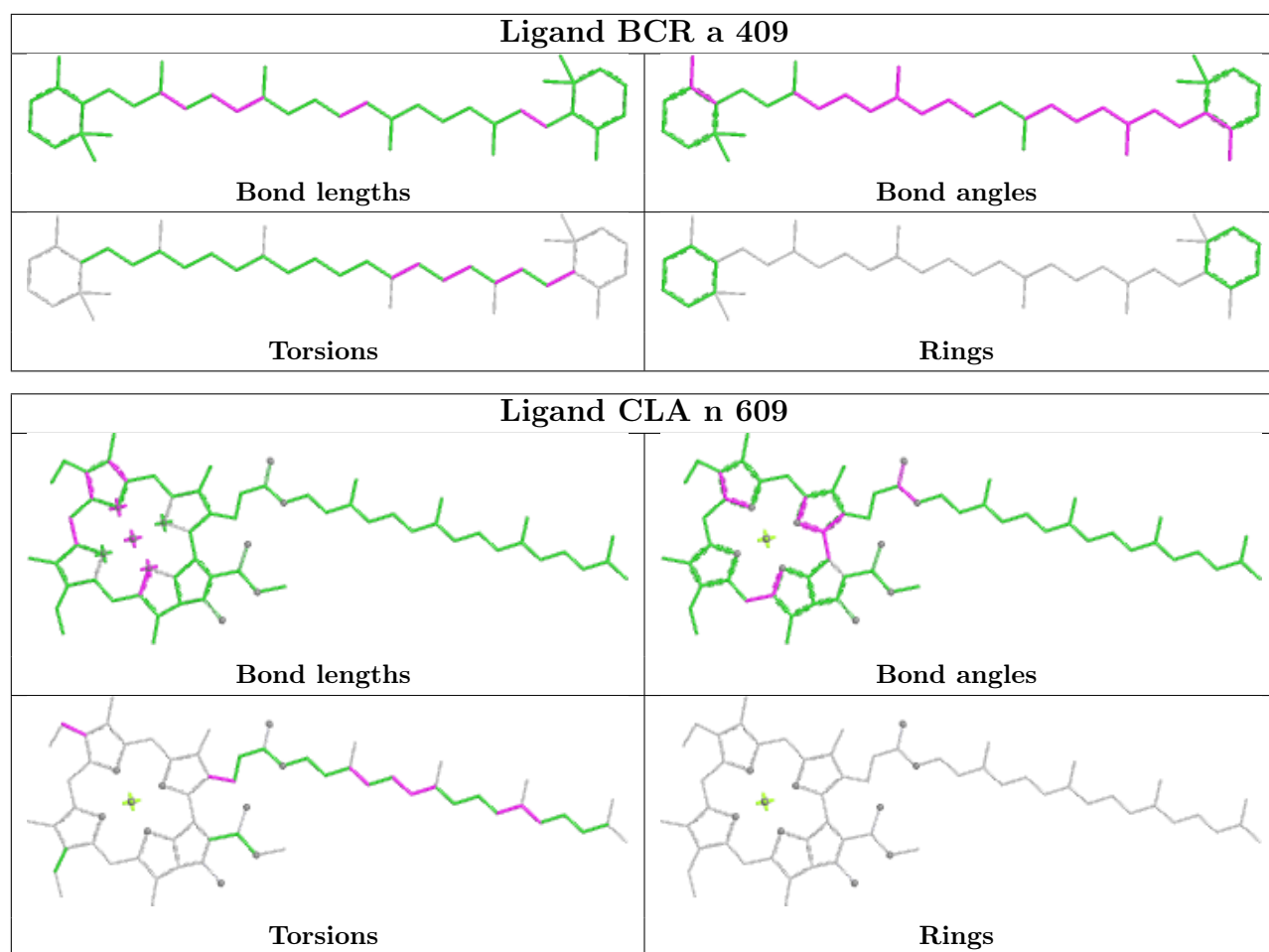


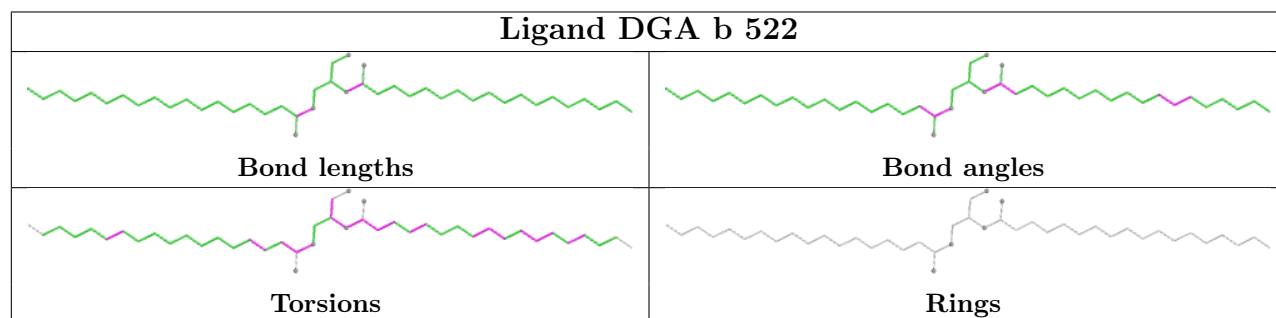
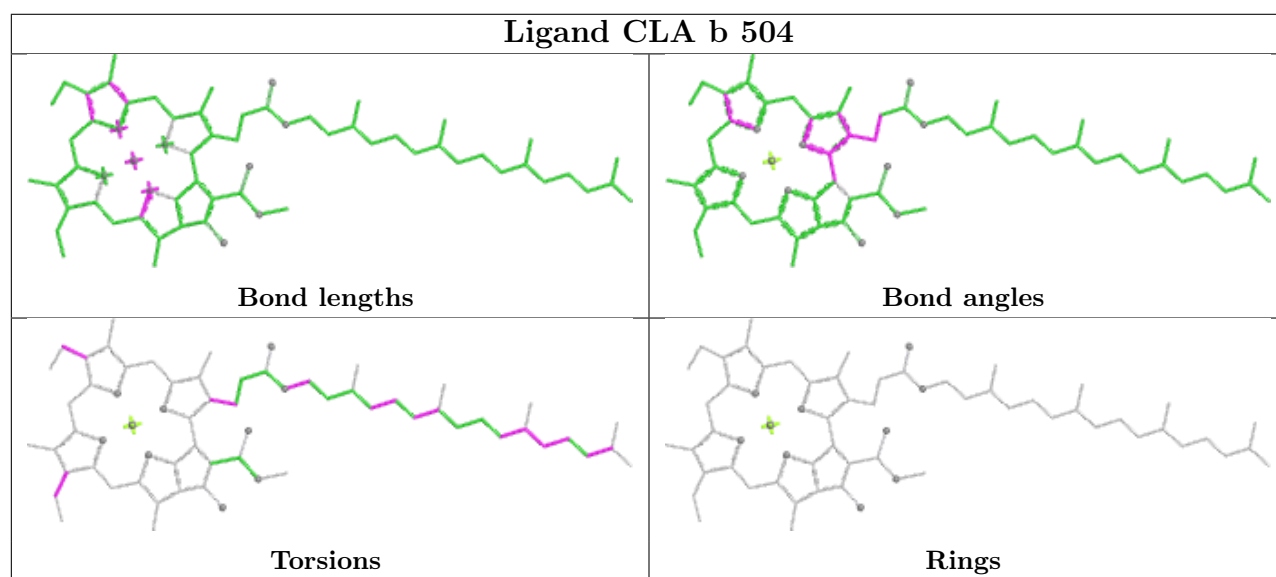
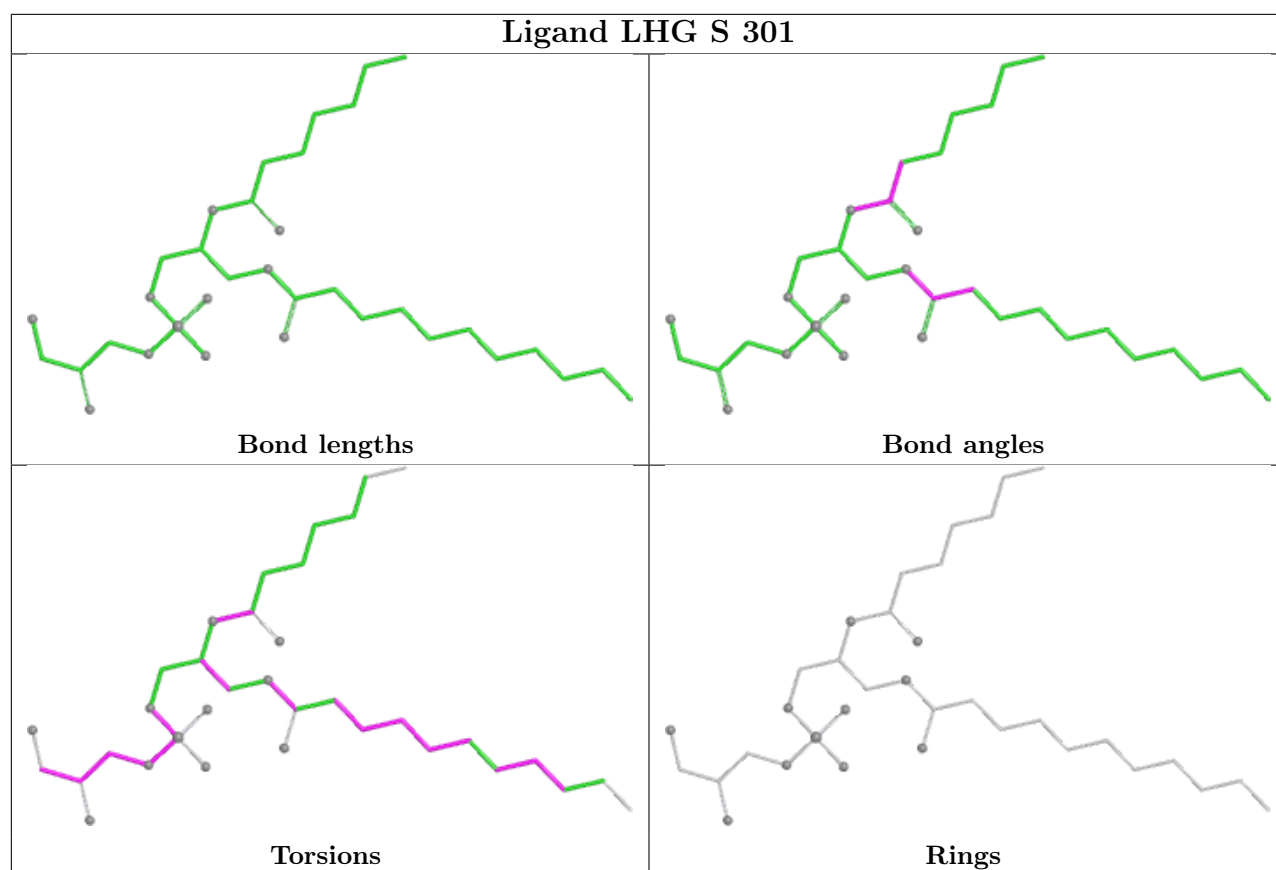
Ligand 3PH a 415	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

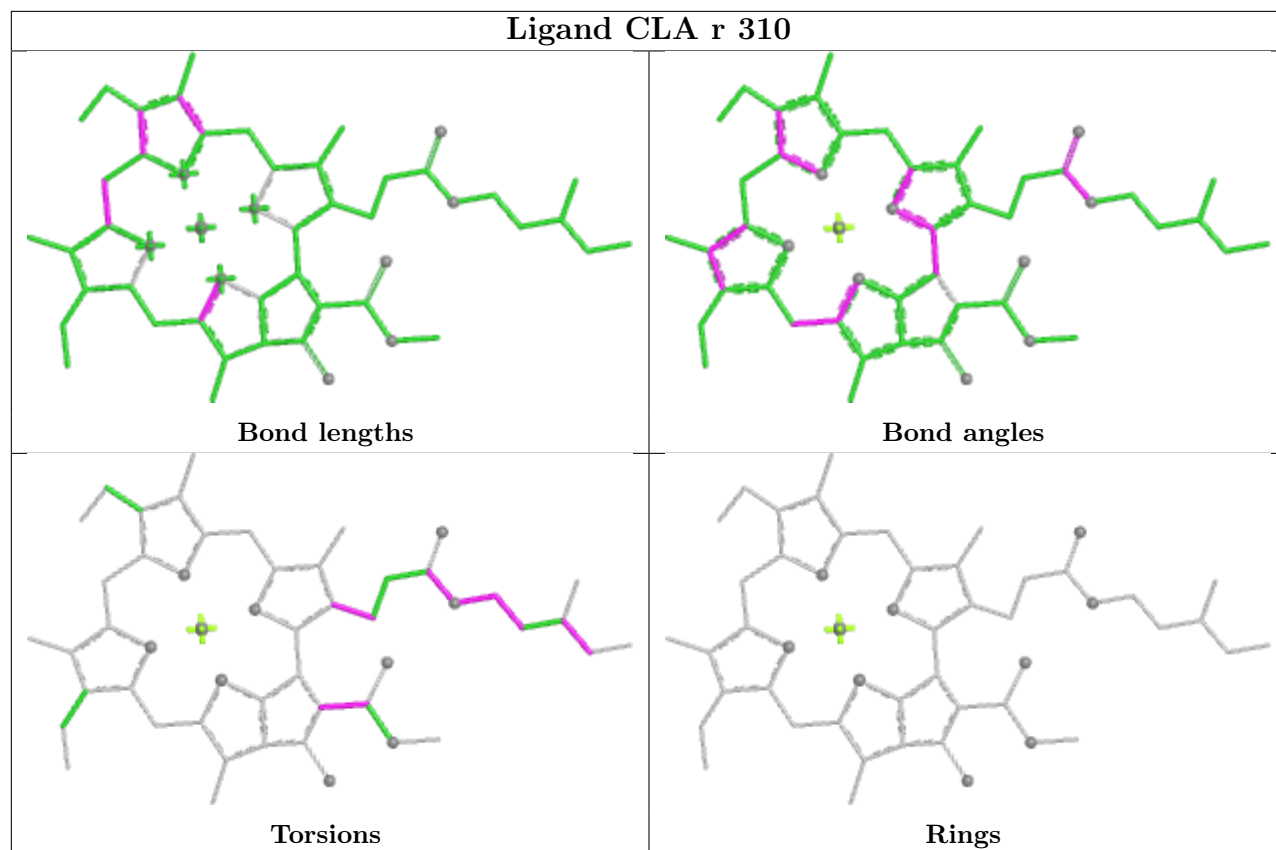
Ligand CHL n 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

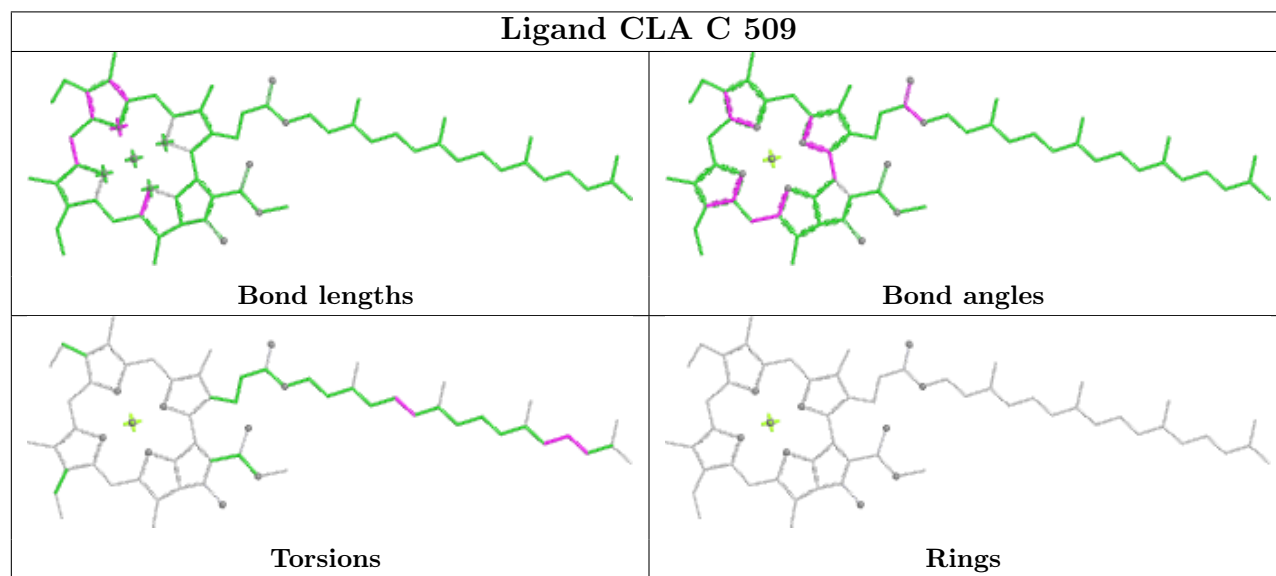




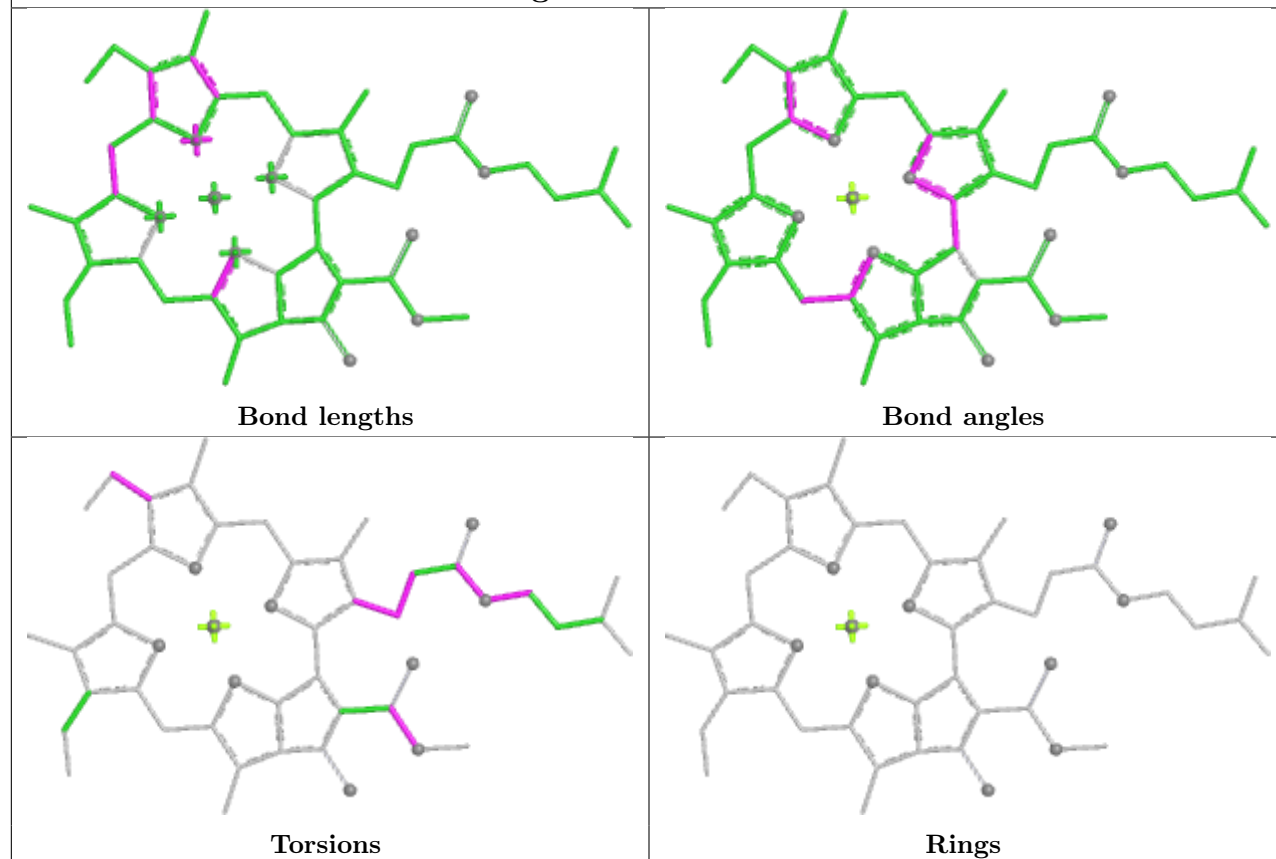
Ligand CLA r 310



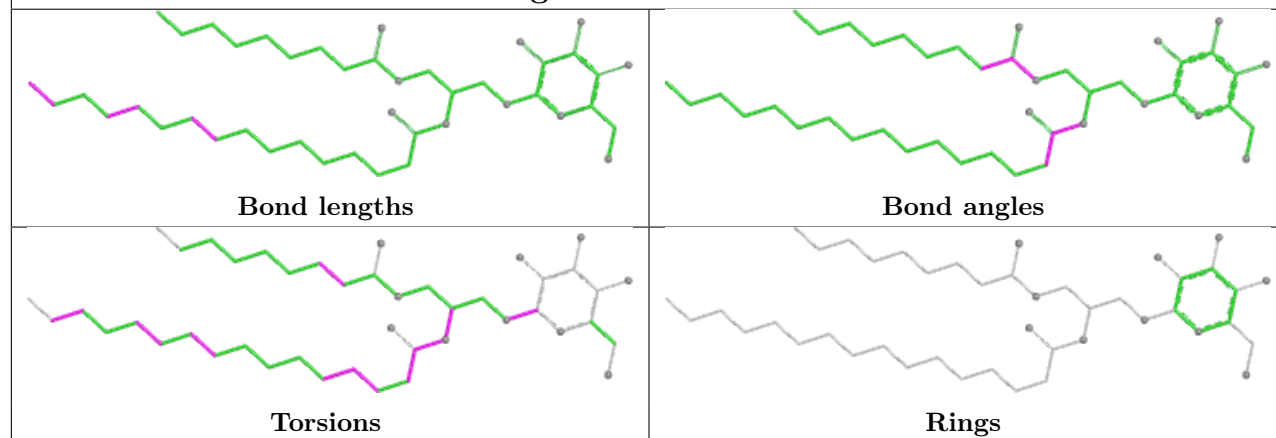
Ligand CLA C 509



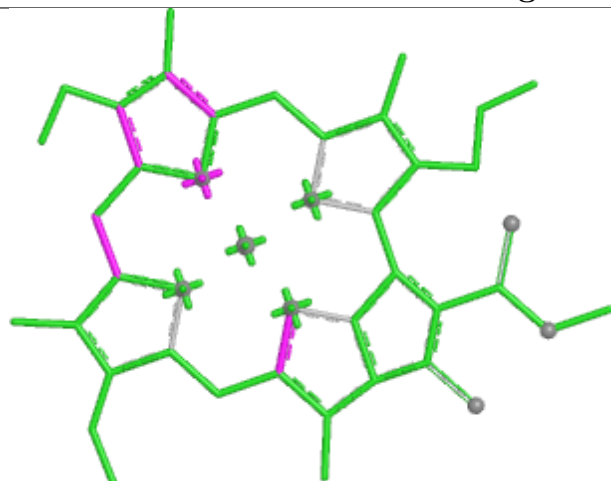
Ligand CLA Y 309



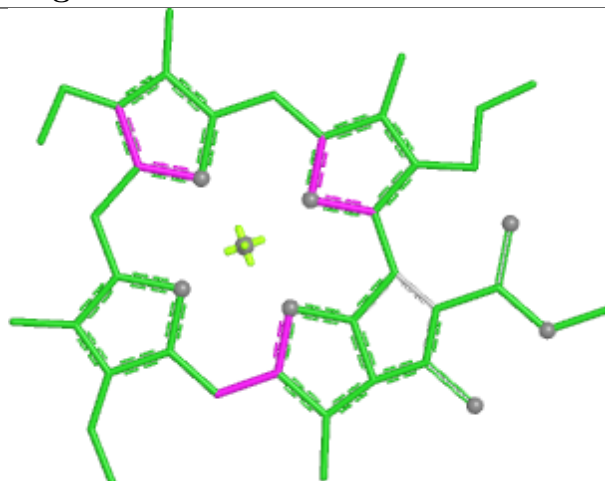
Ligand LMG b 520



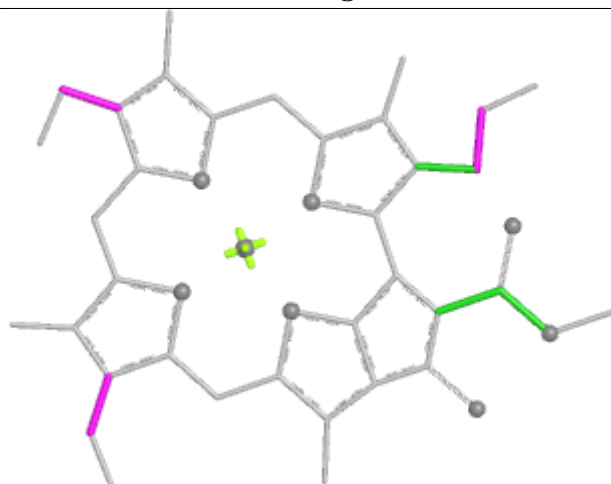
Ligand CLA g 612



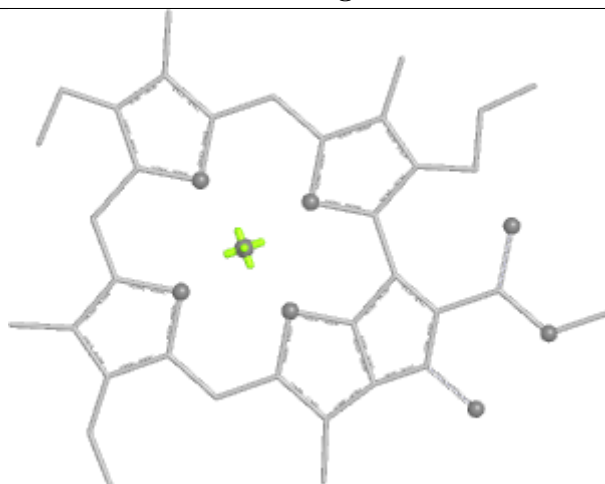
Bond lengths



Bond angles

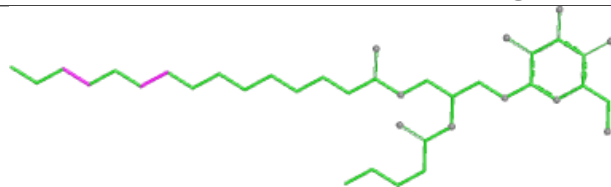


Torsions

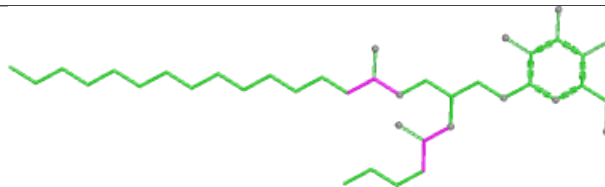


Rings

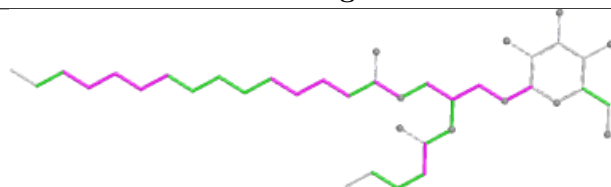
Ligand LMG w 202



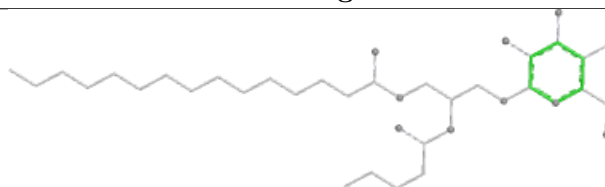
Bond lengths



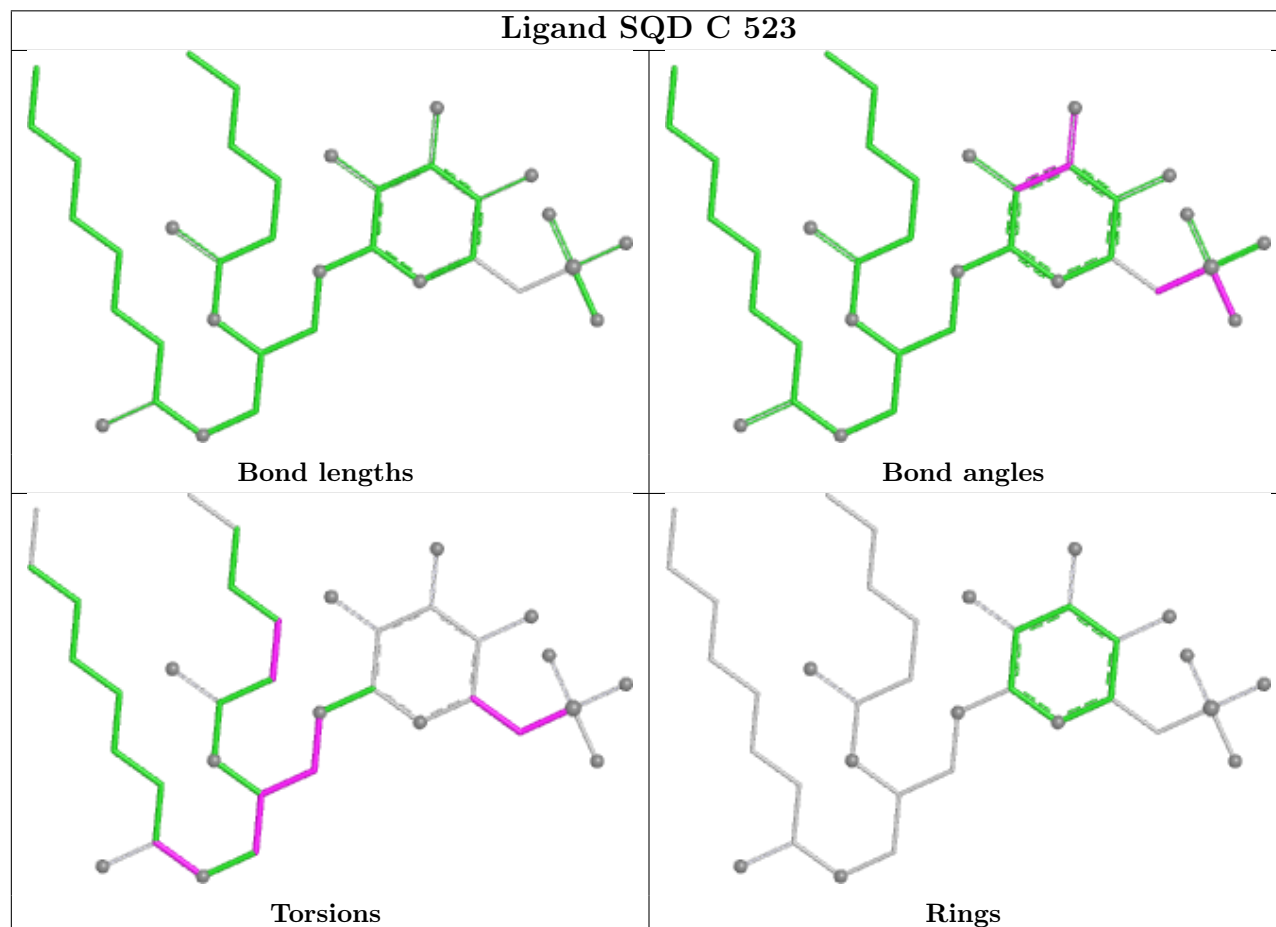
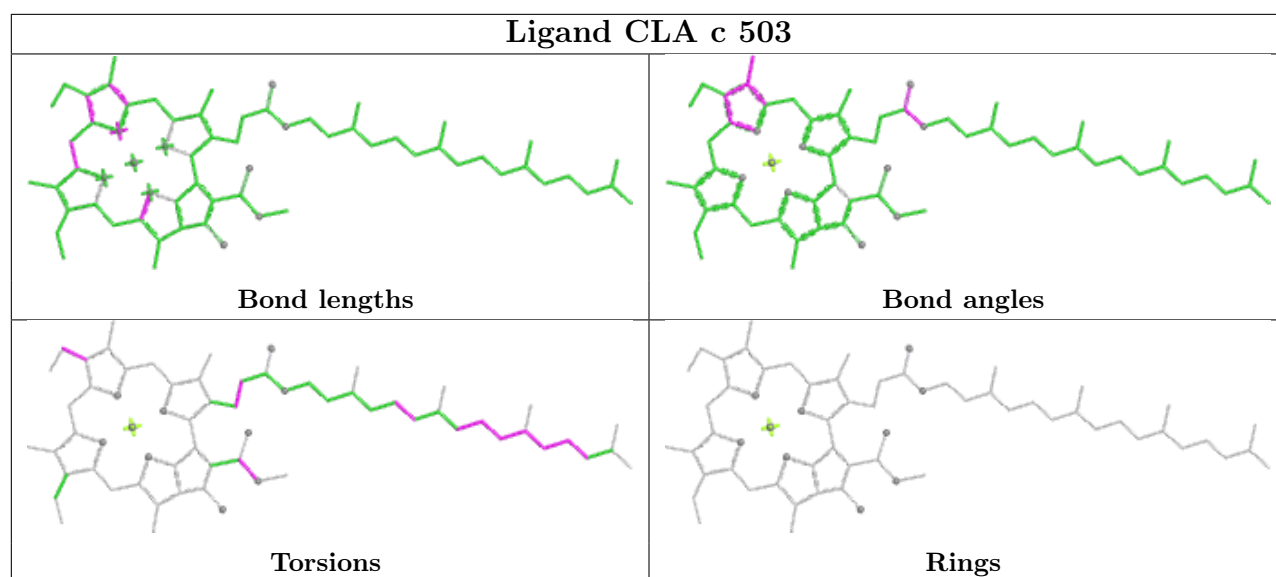
Bond angles

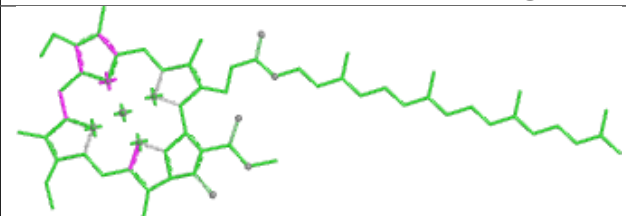
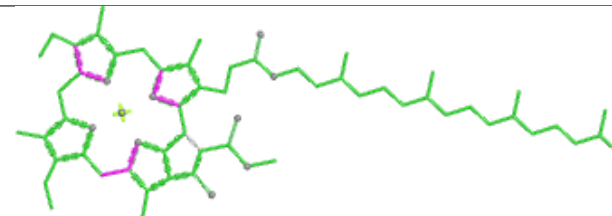
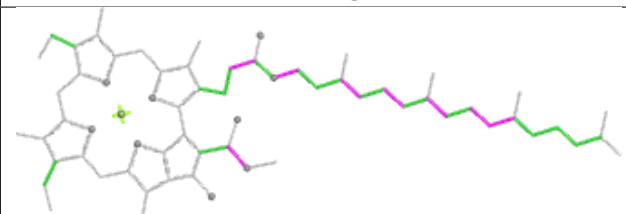
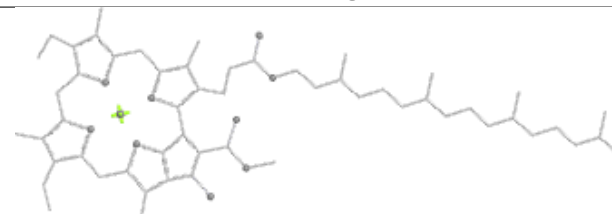


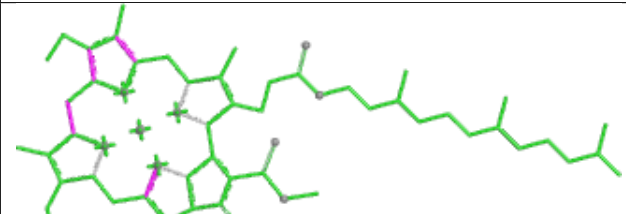
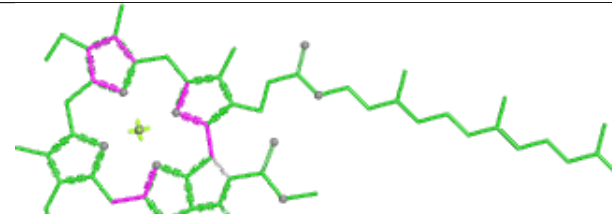
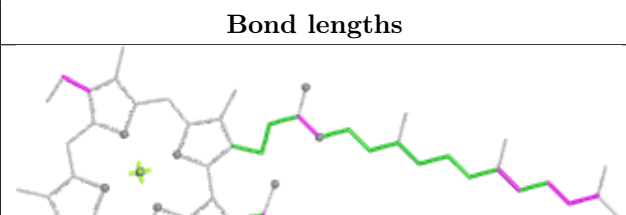
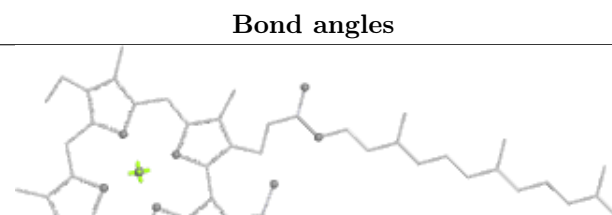
Torsions

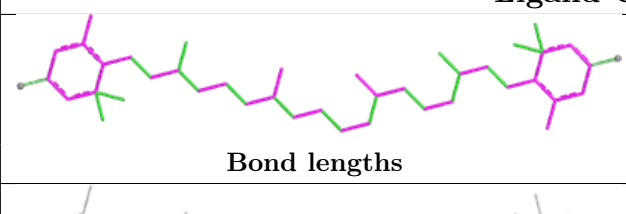
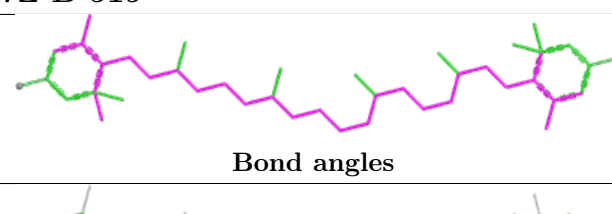
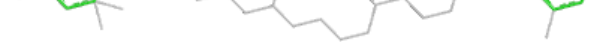


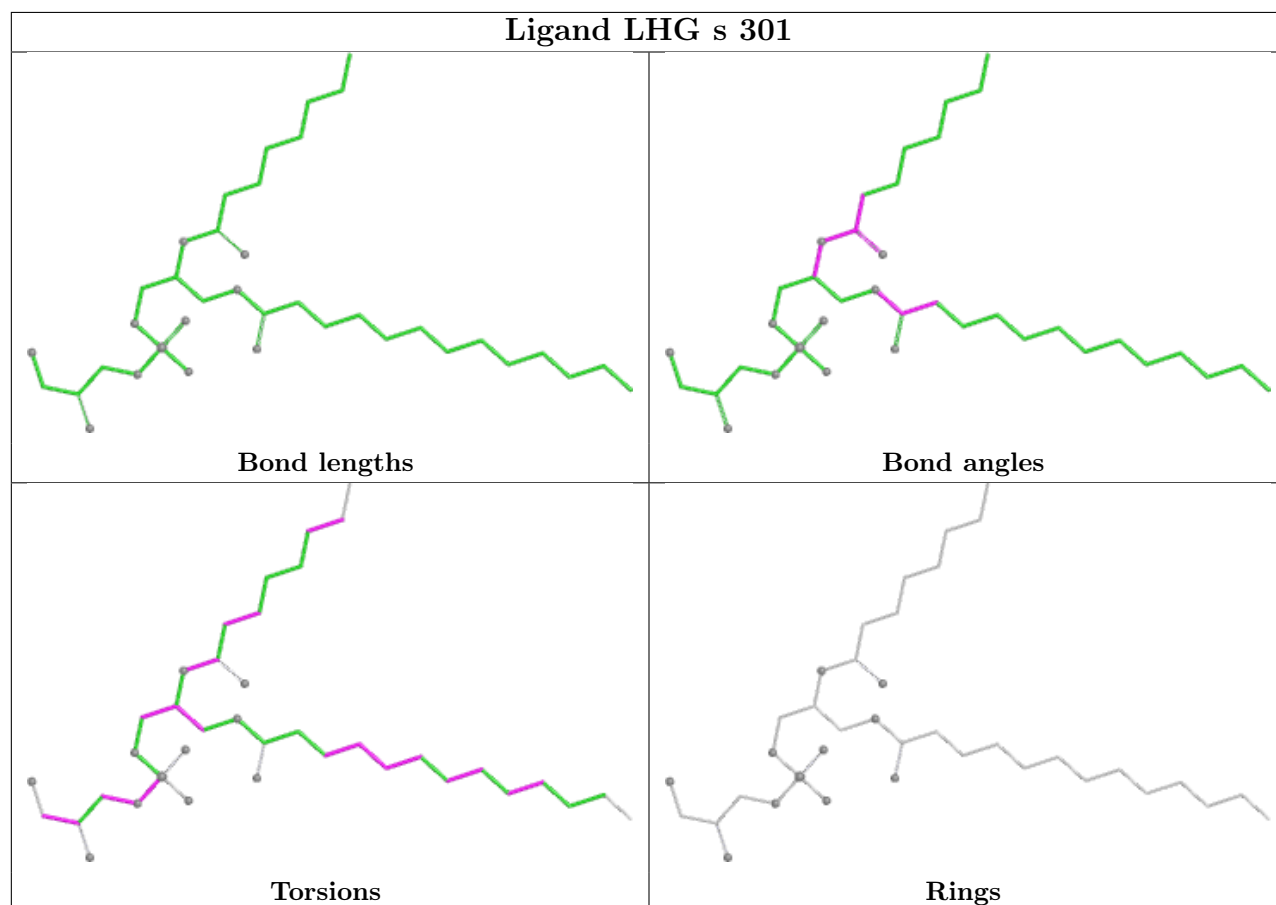
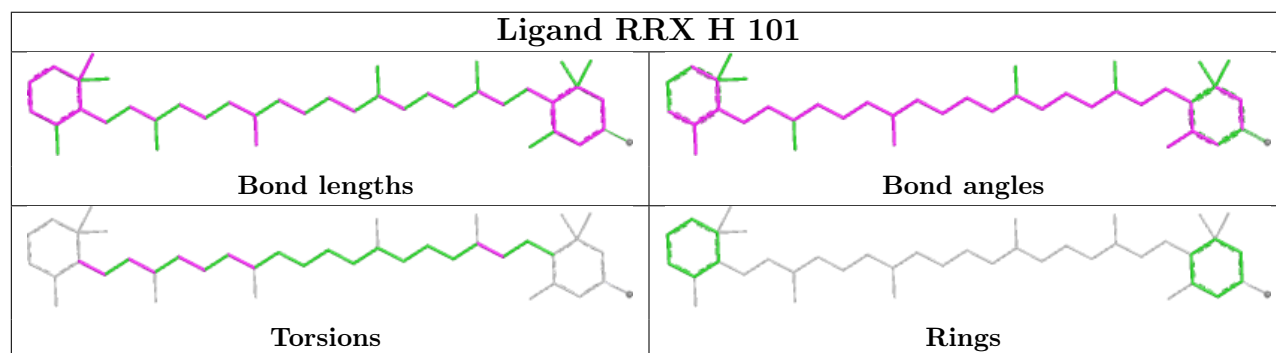
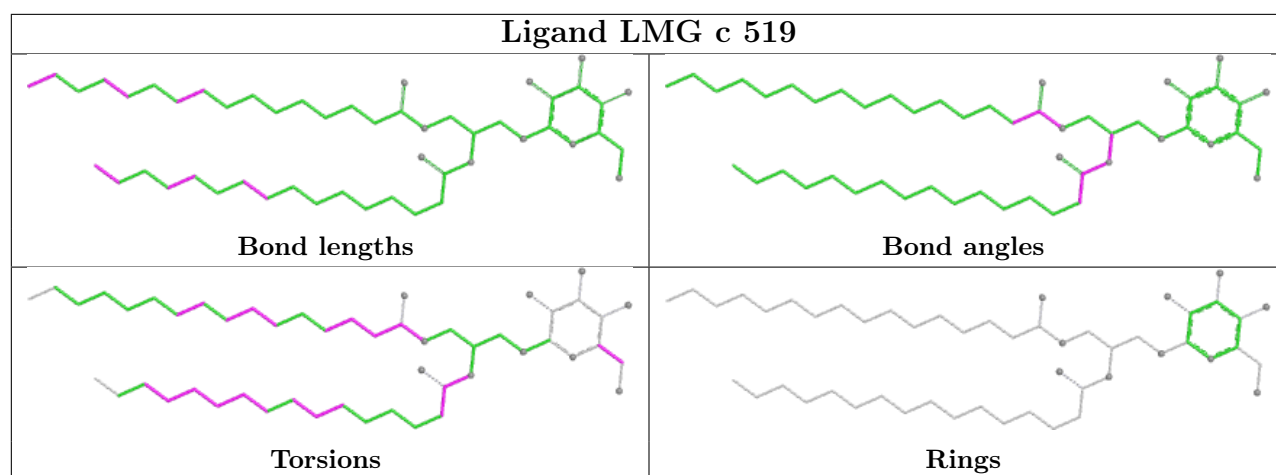
Rings

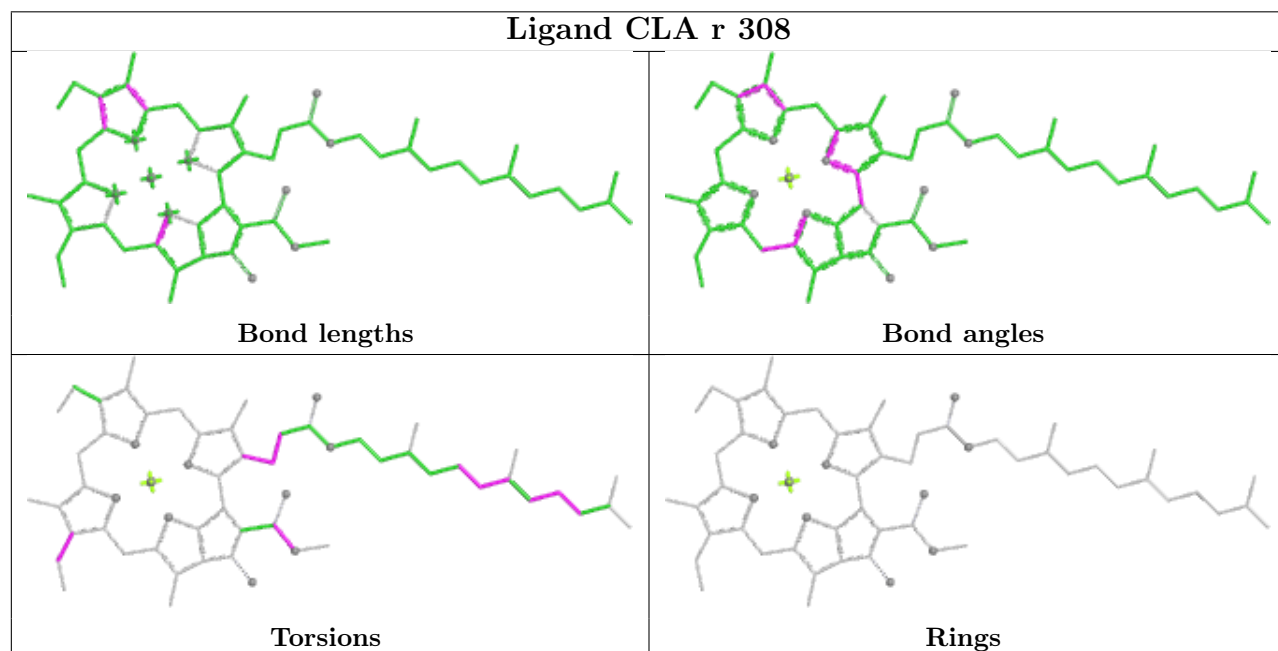
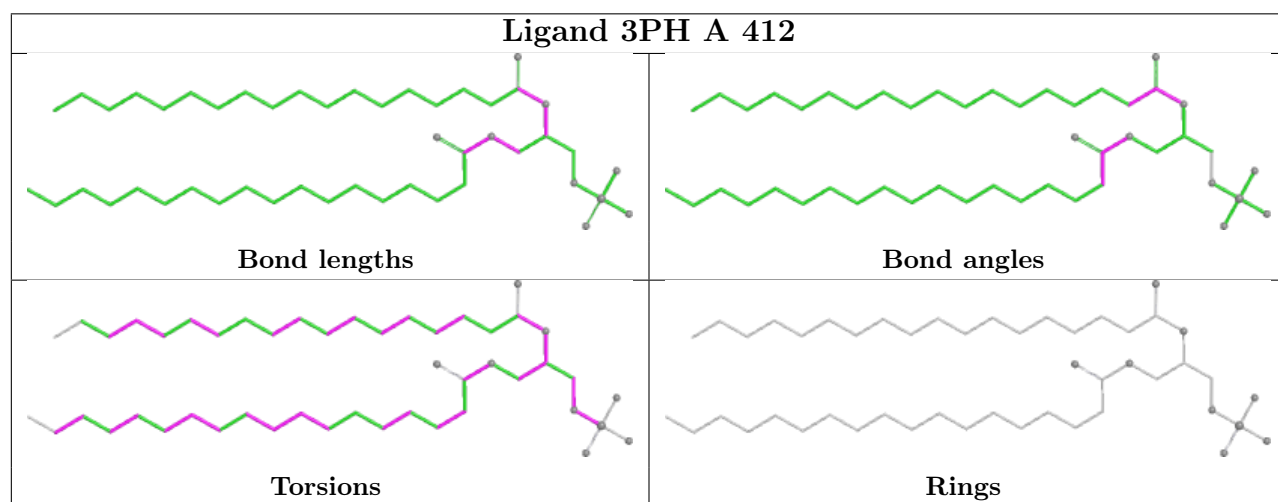
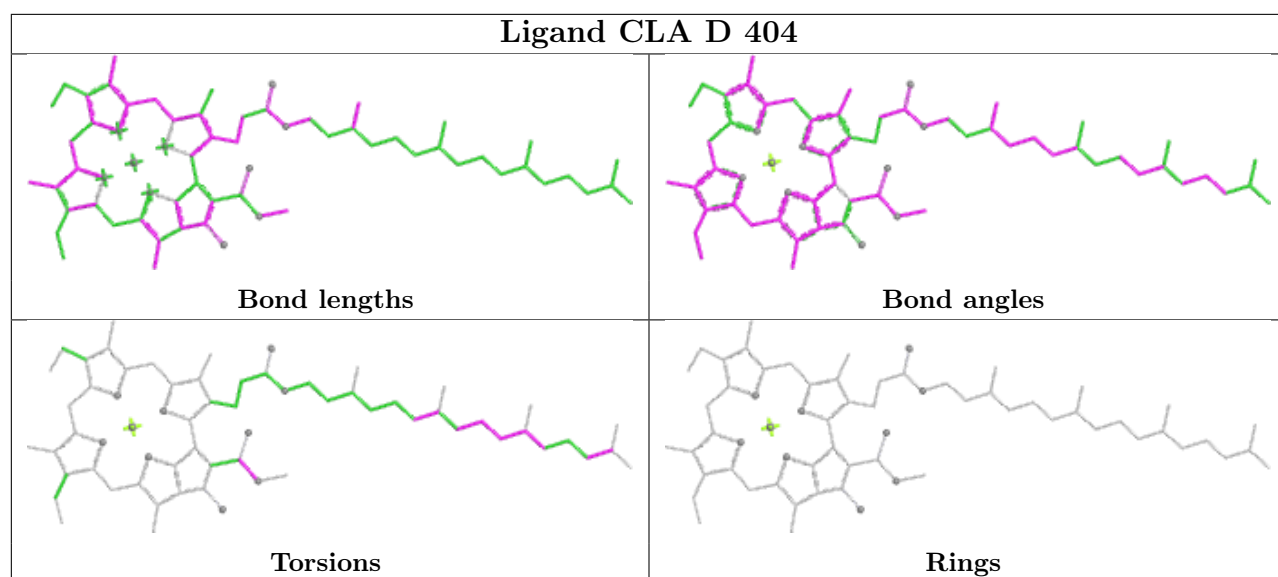


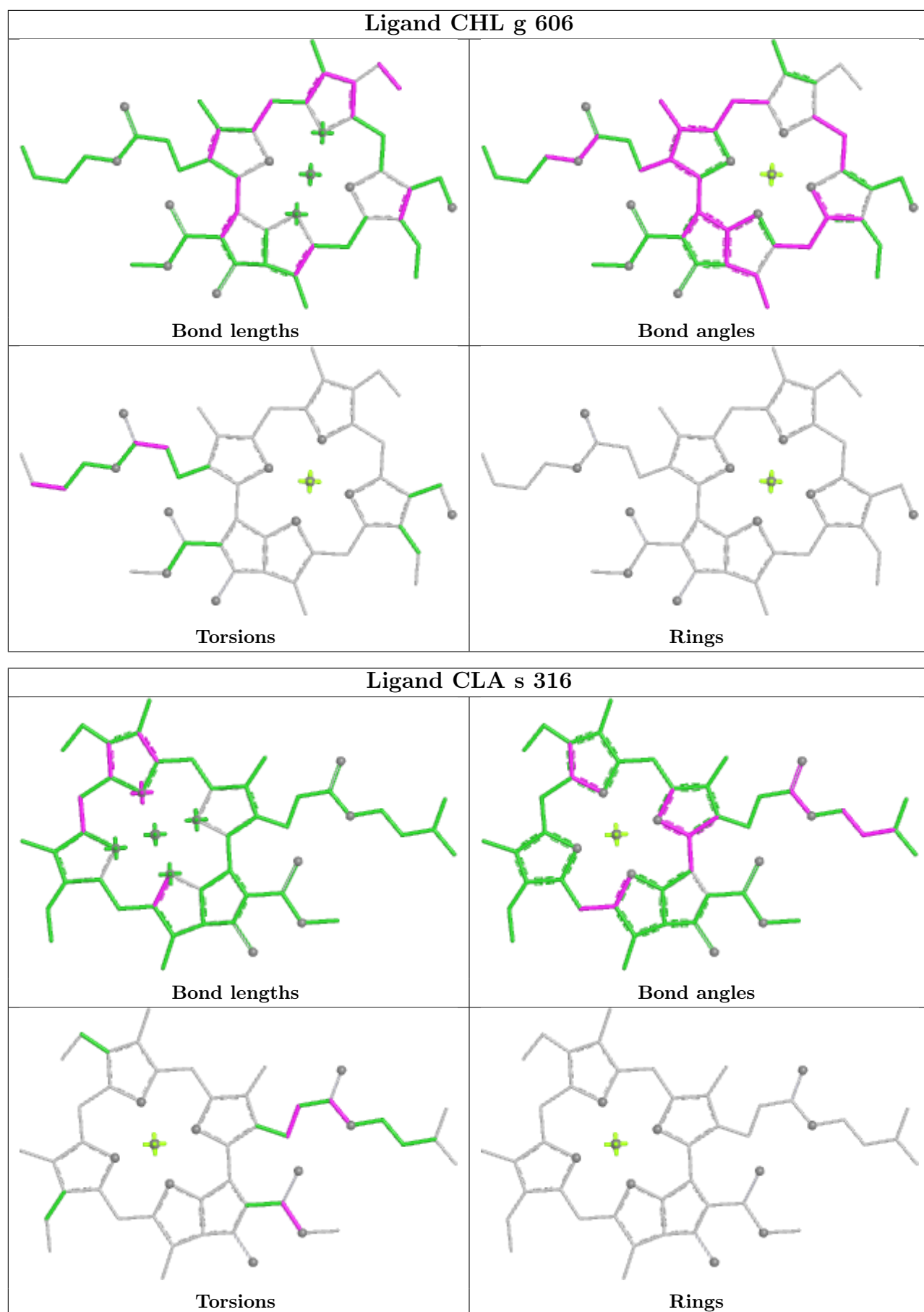
Ligand CLA B 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

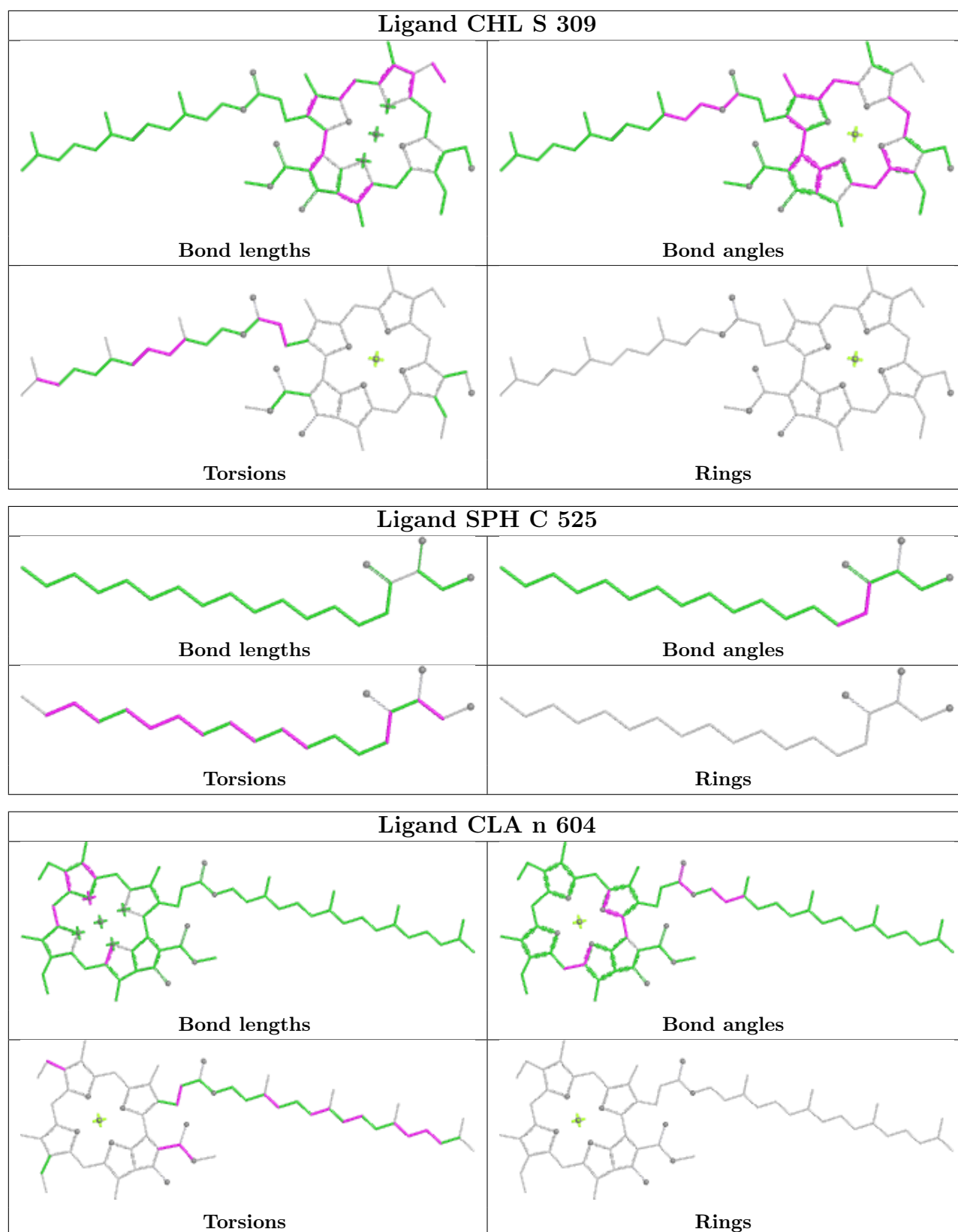
Ligand CLA S 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand C7Z B 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

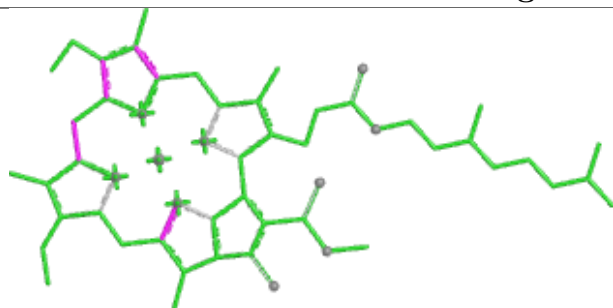




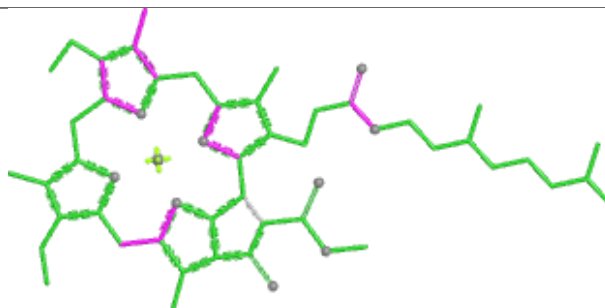




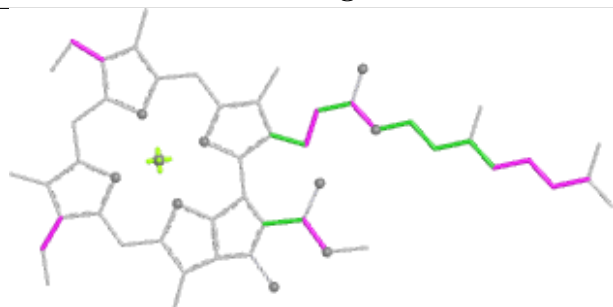
Ligand CLA S 314



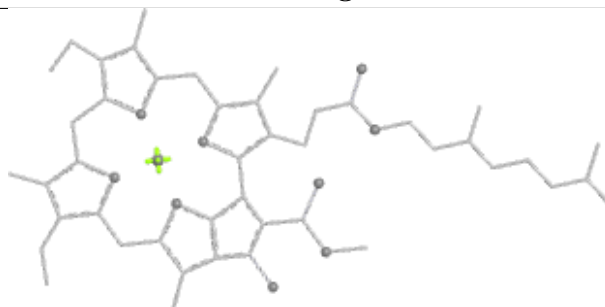
Bond lengths



Bond angles

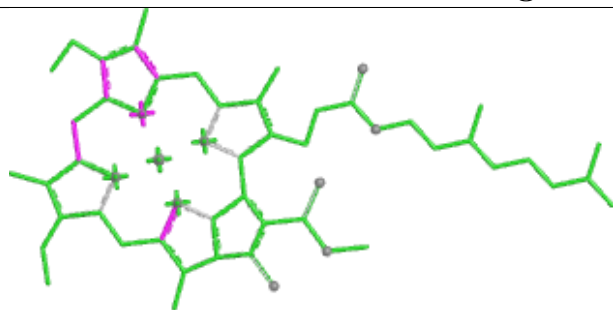


Torsions

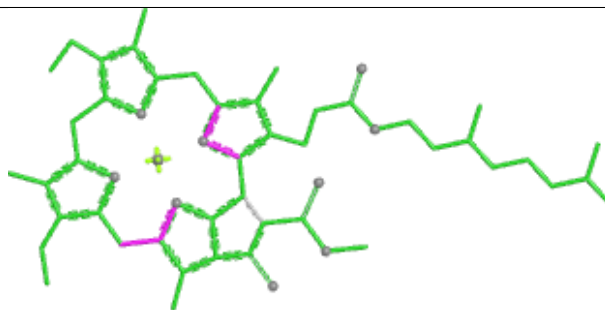


Rings

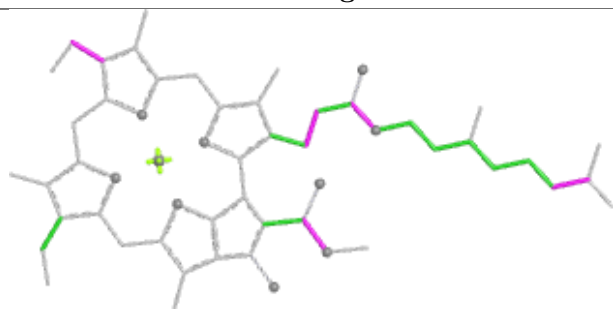
Ligand CLA S 305



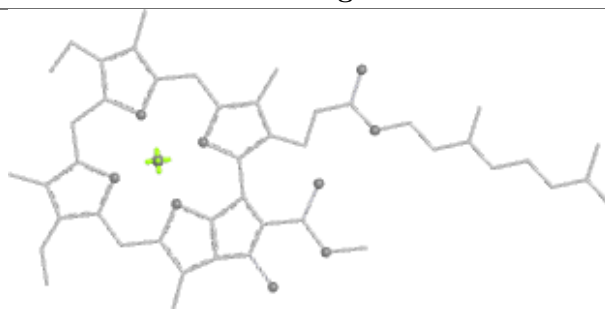
Bond lengths



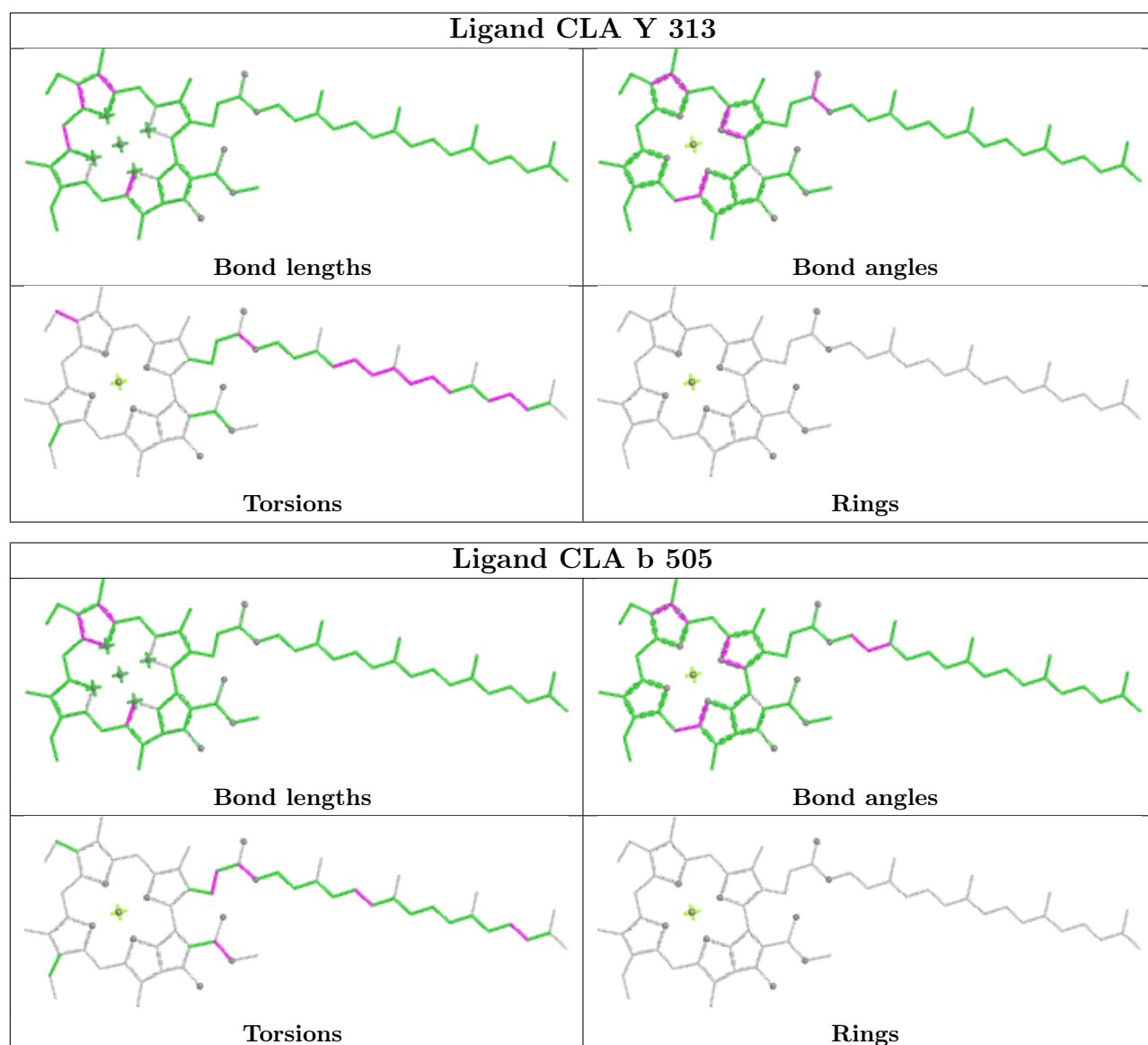
Bond angles



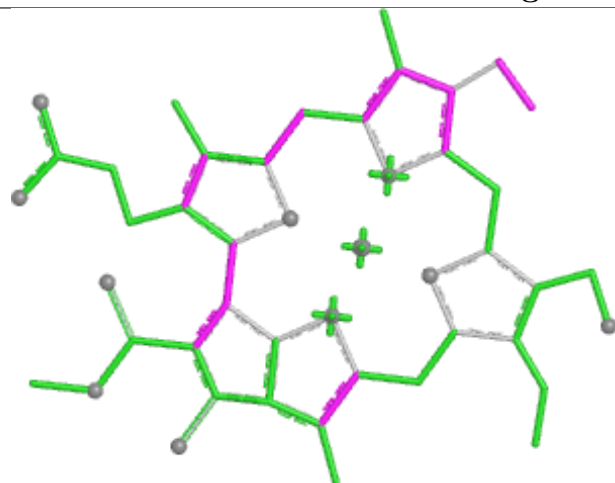
Torsions



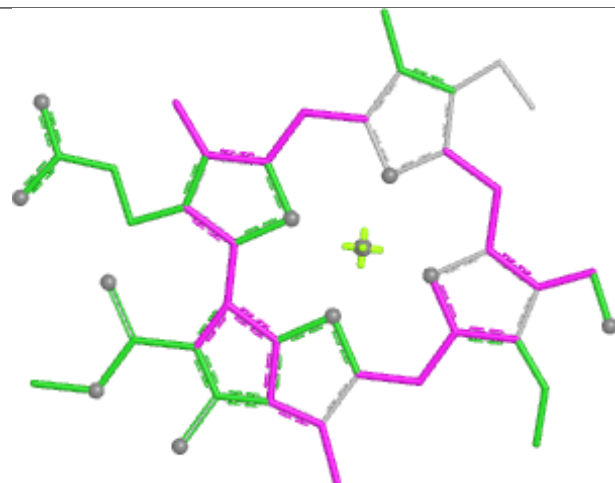
Rings



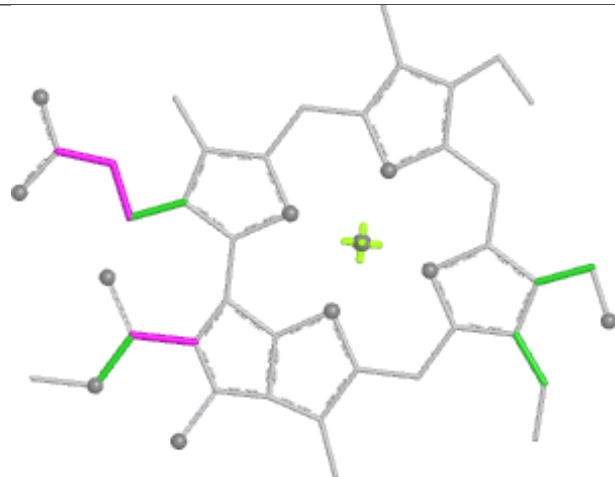
Ligand CHL s 302



Bond lengths



Bond angles

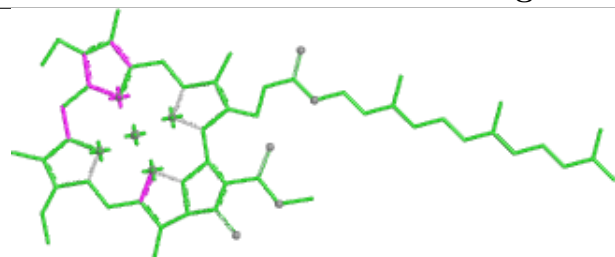


Torsions

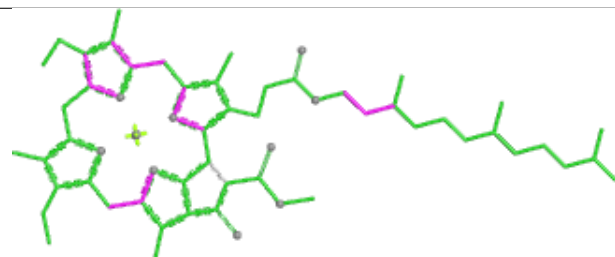


Rings

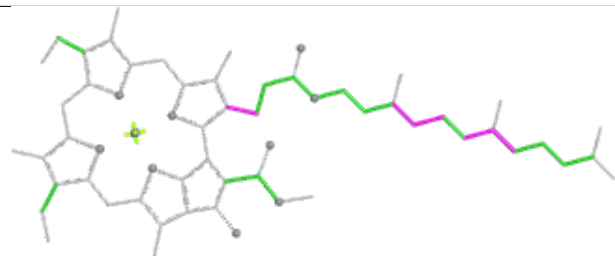
Ligand CLA A 409



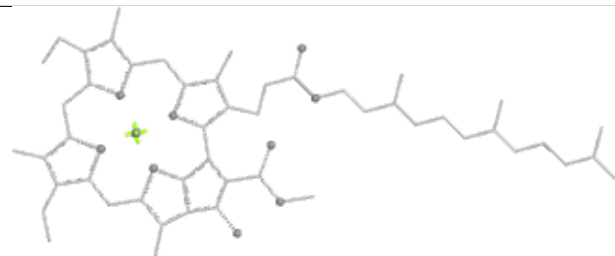
Bond lengths



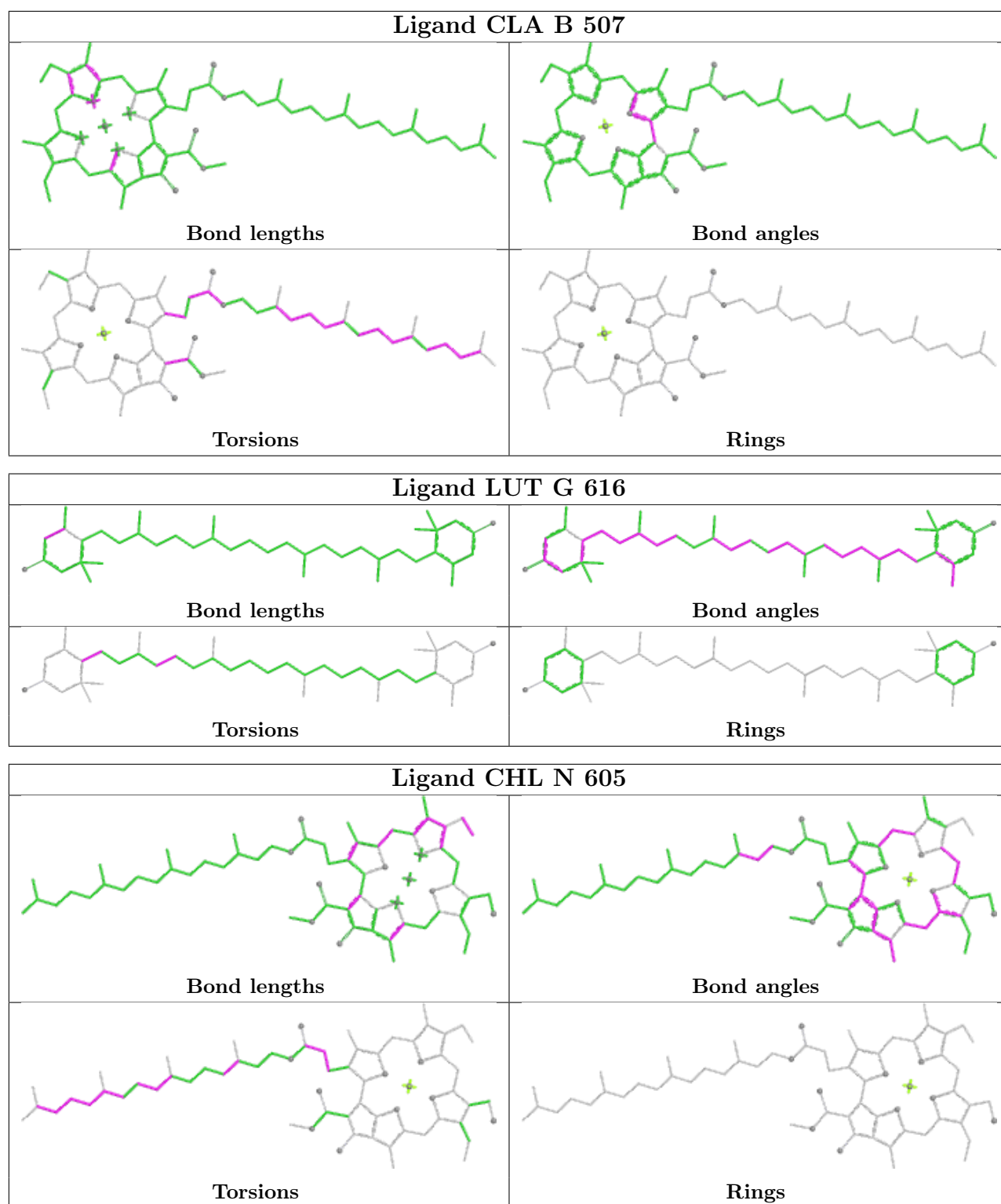
Bond angles

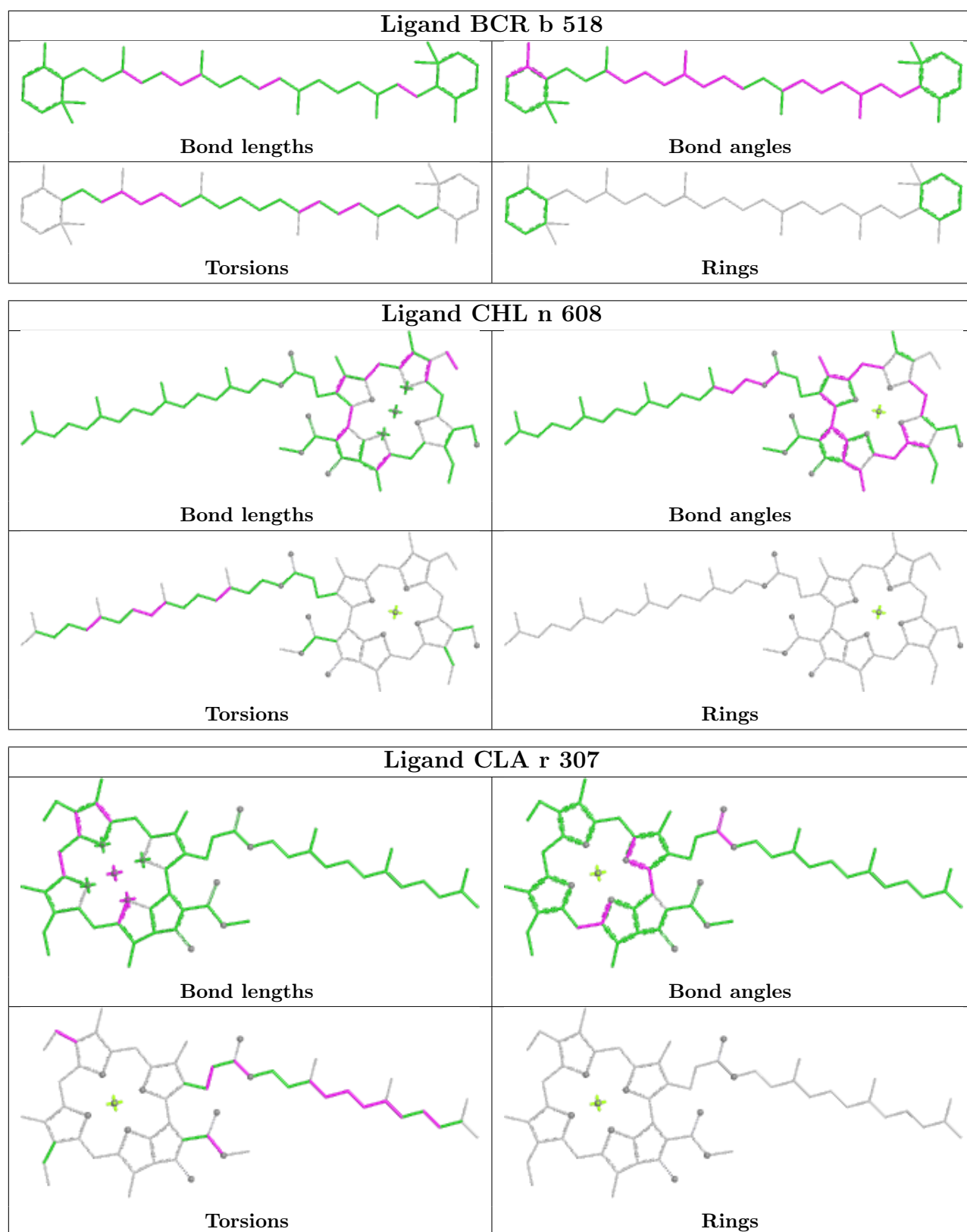


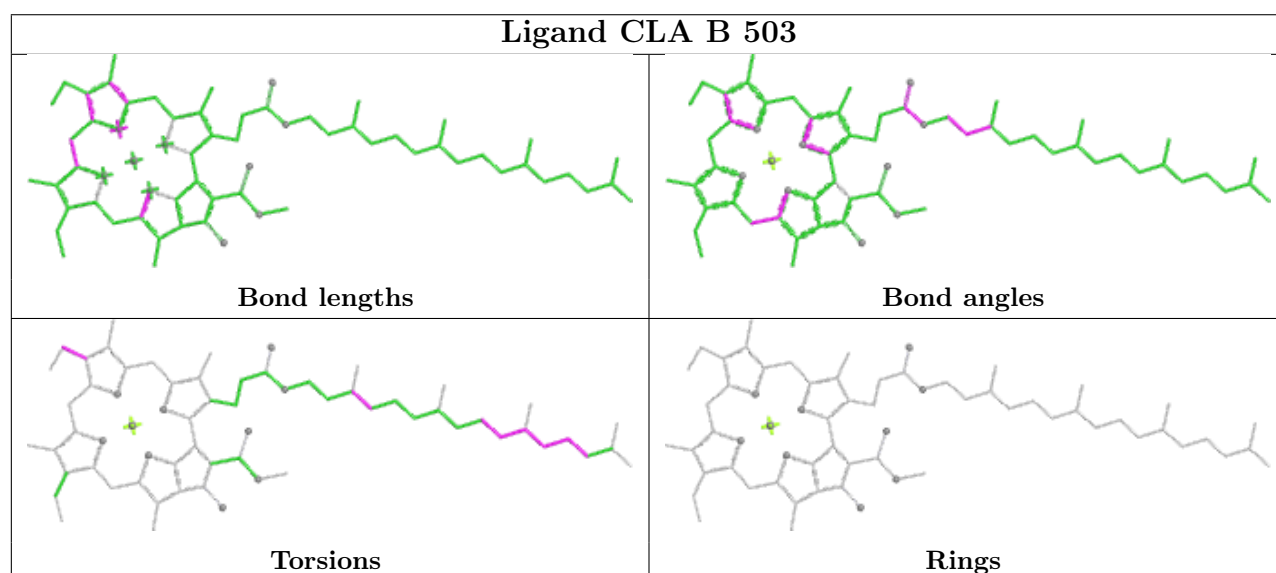
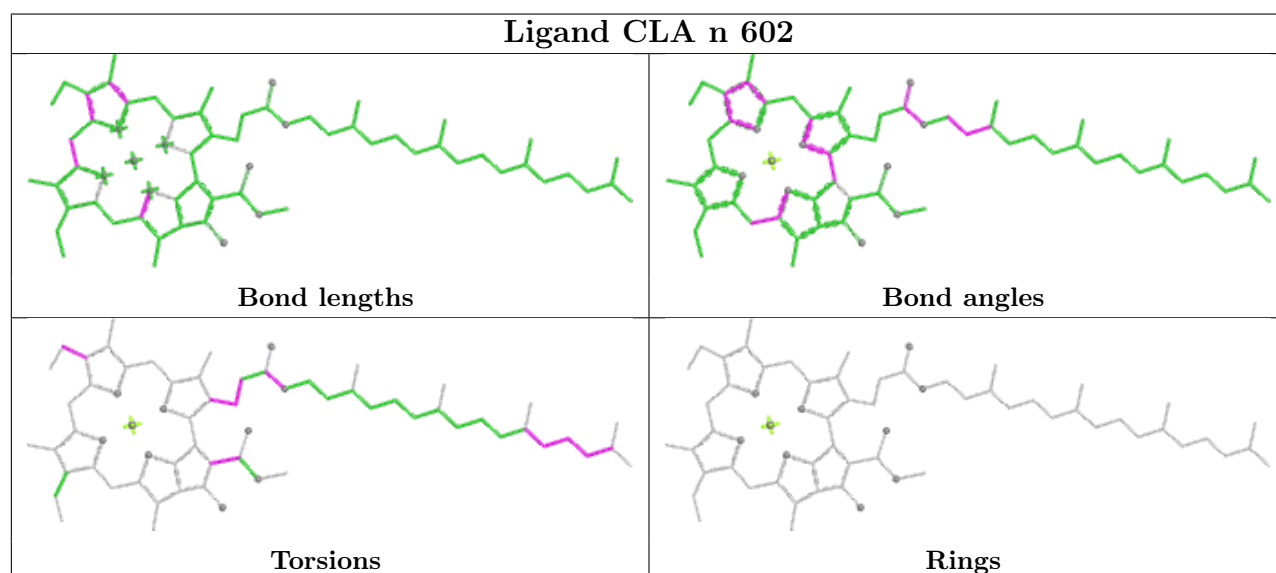
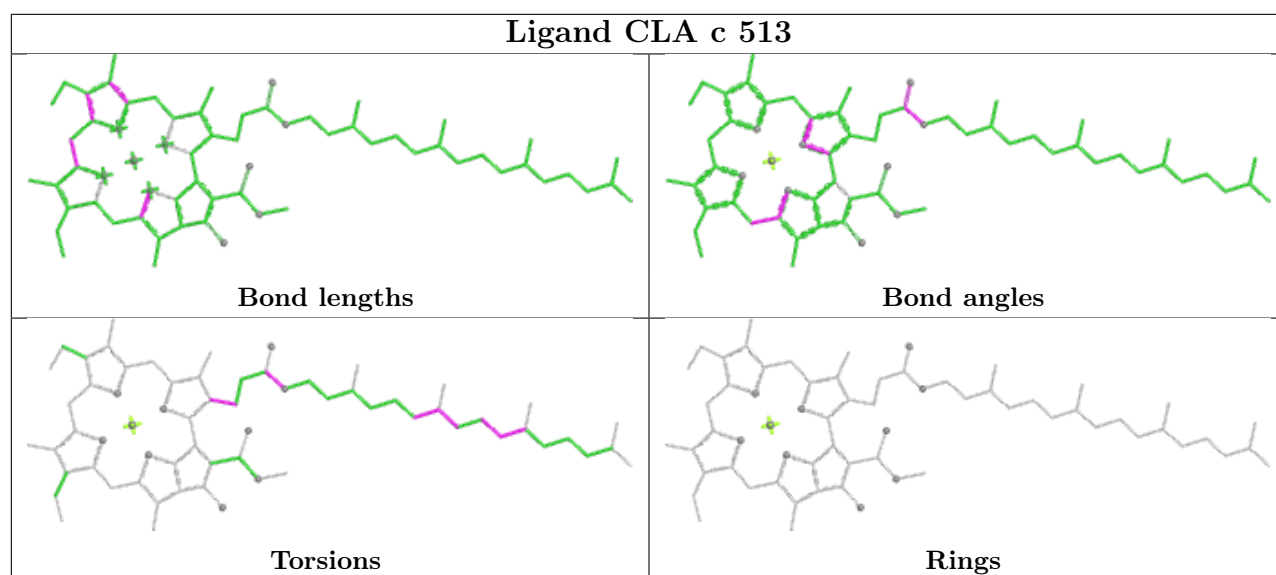
Torsions

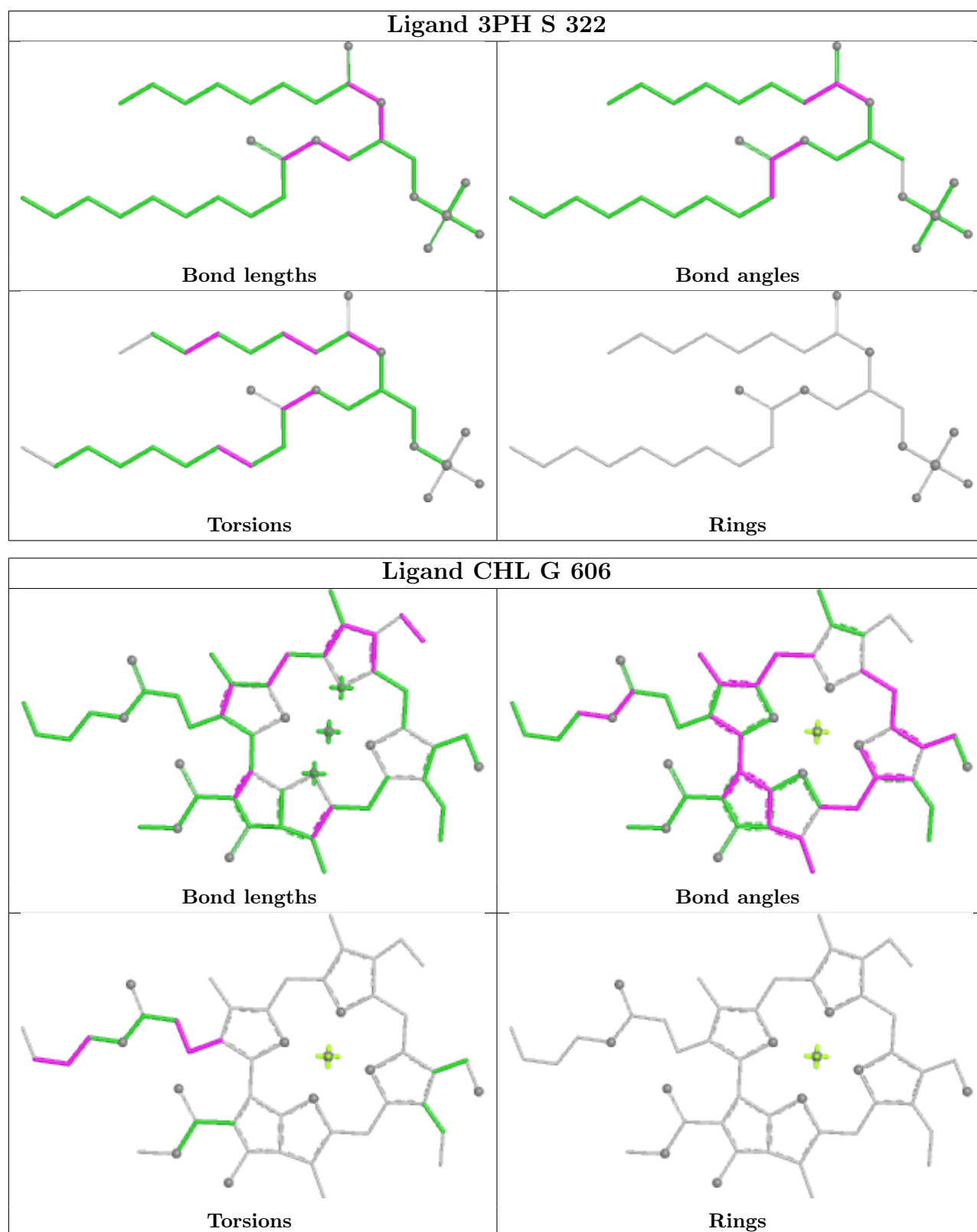


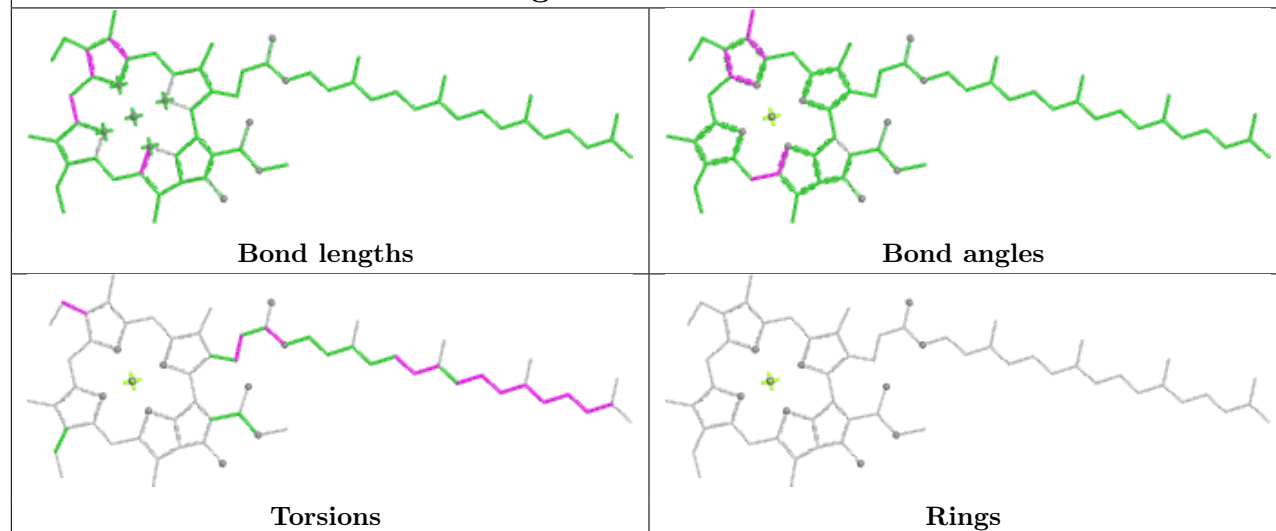
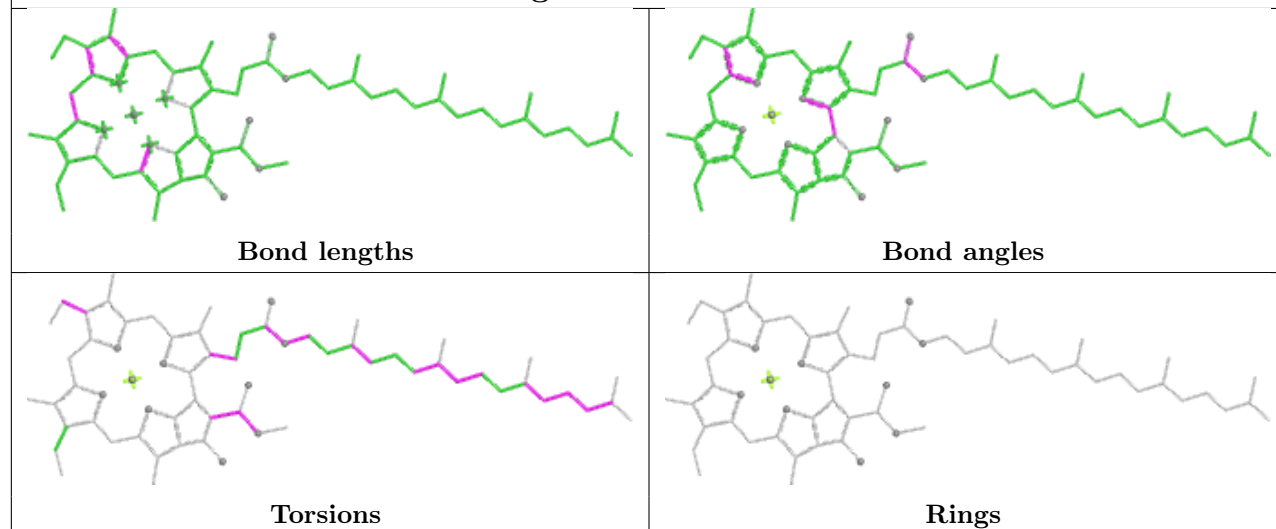
Rings

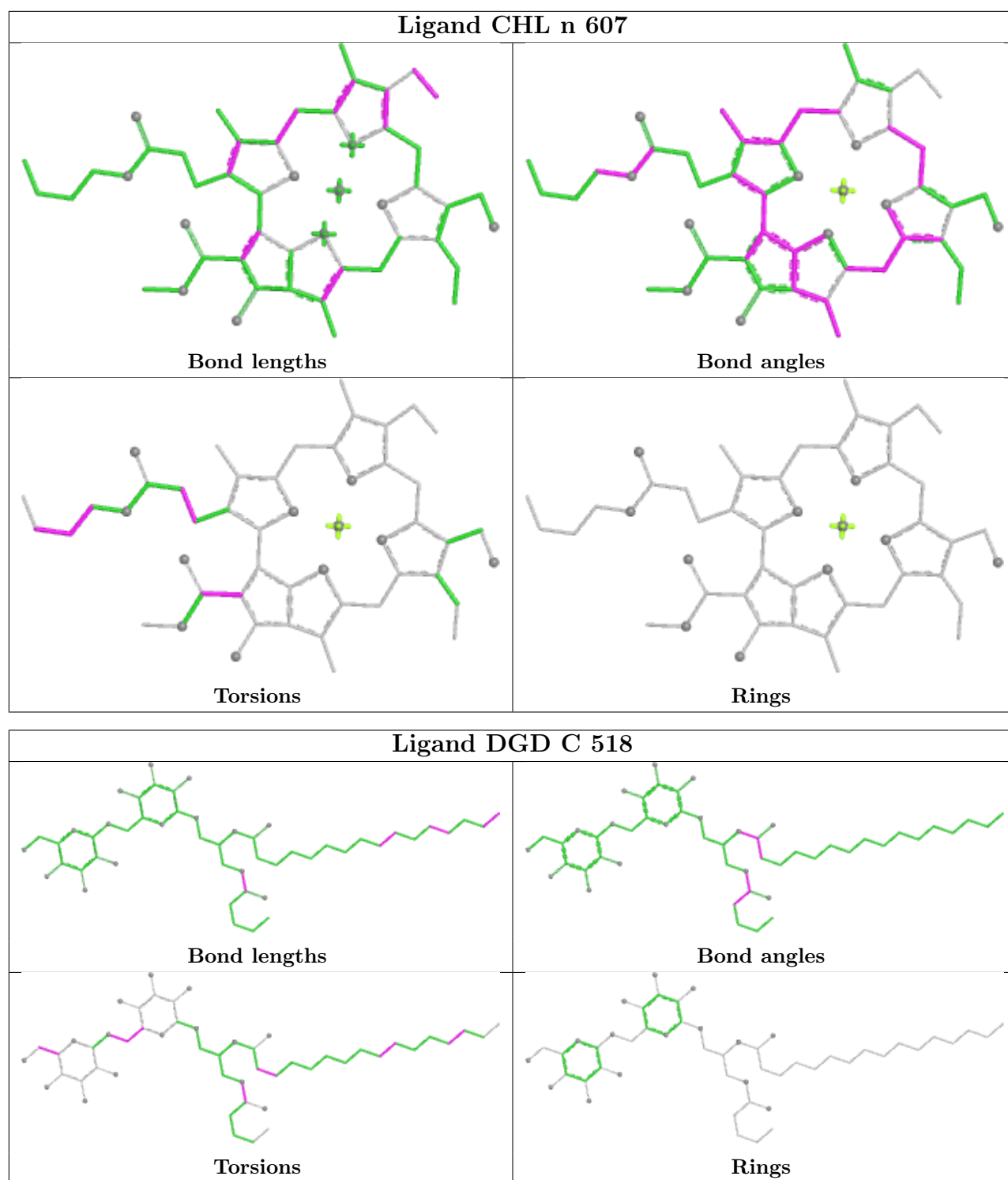


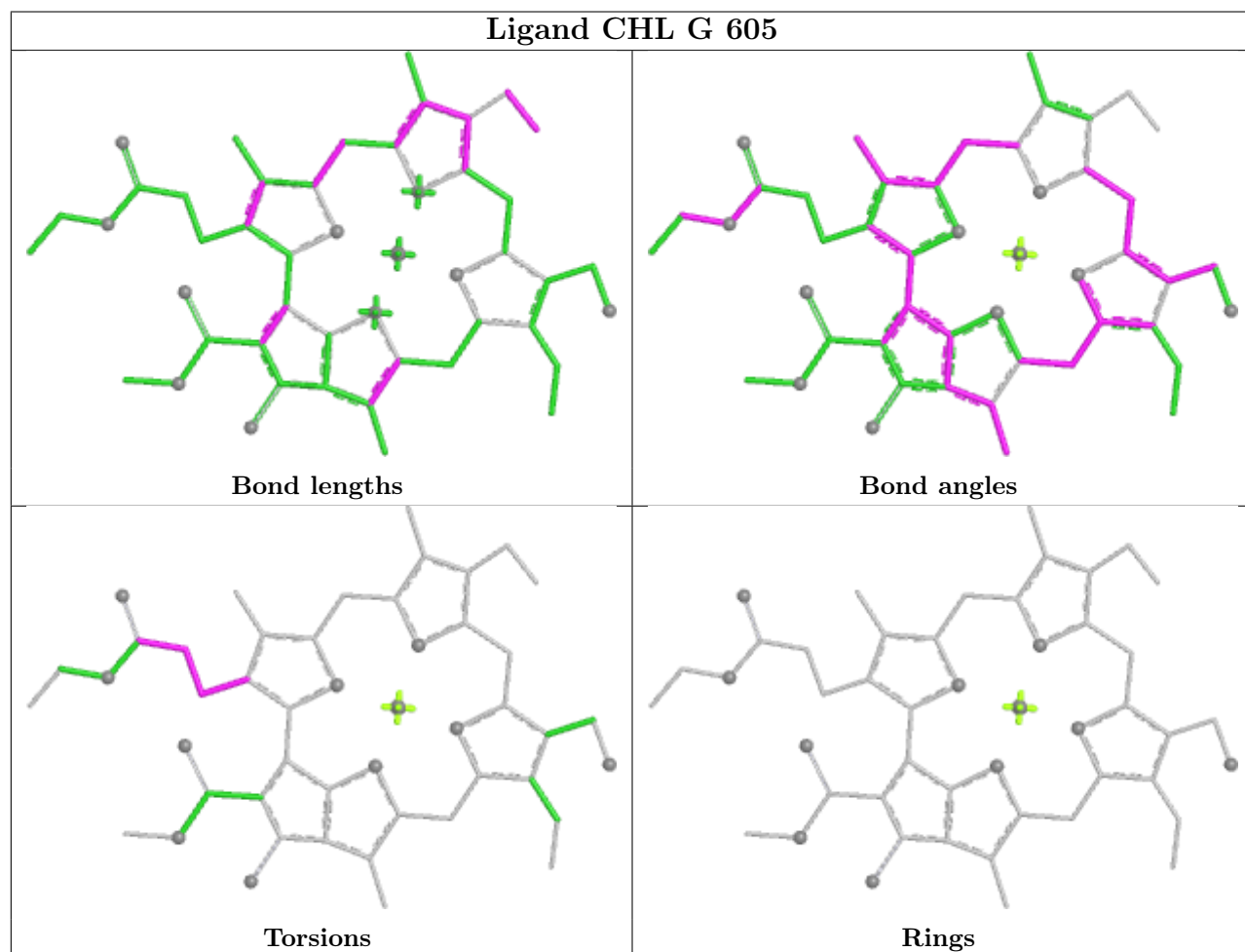
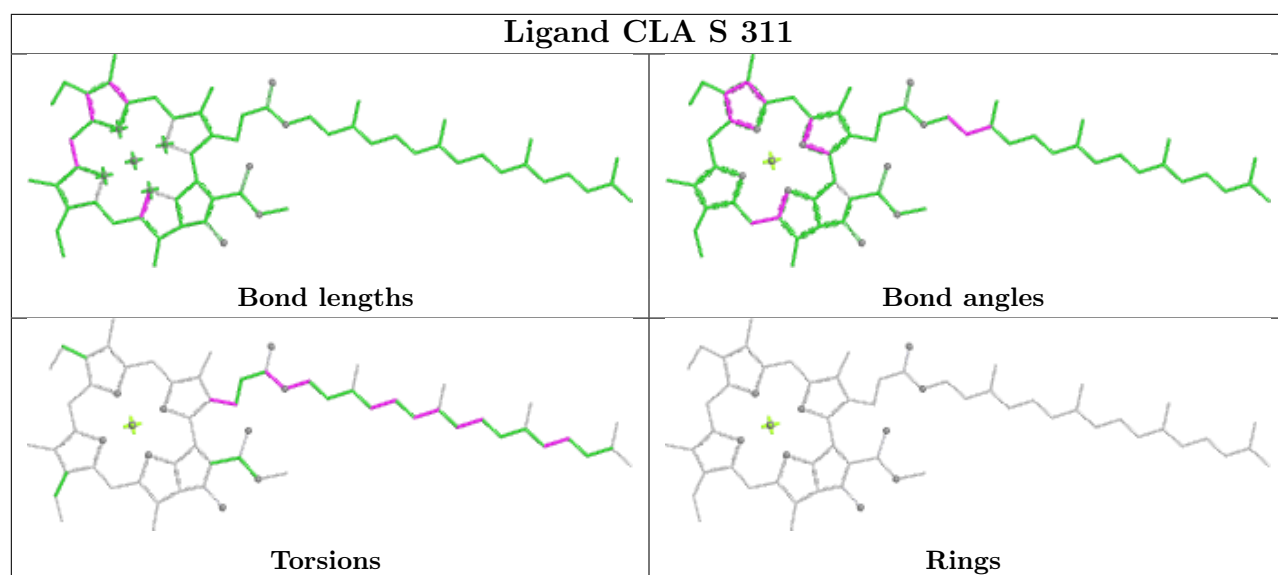


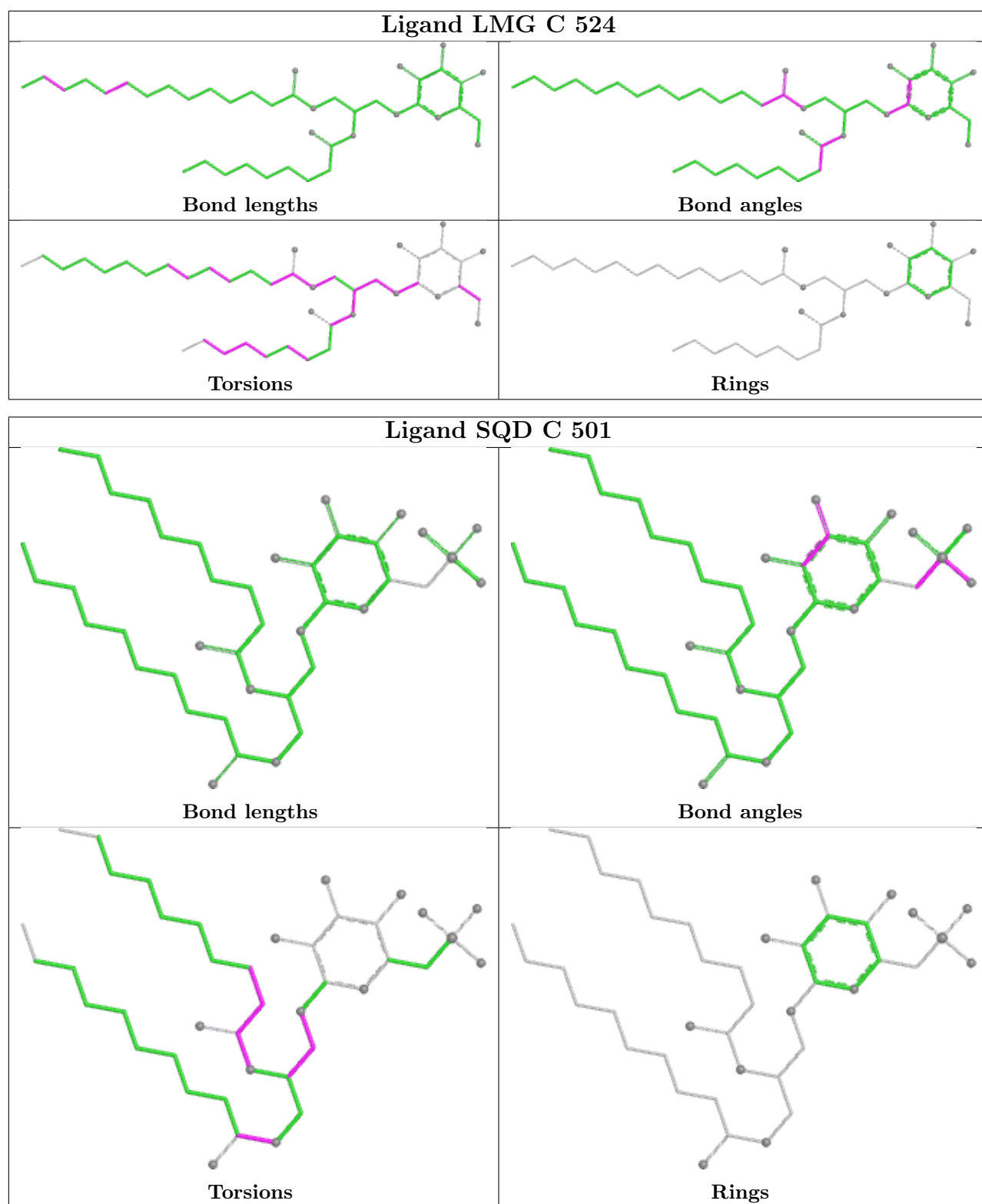


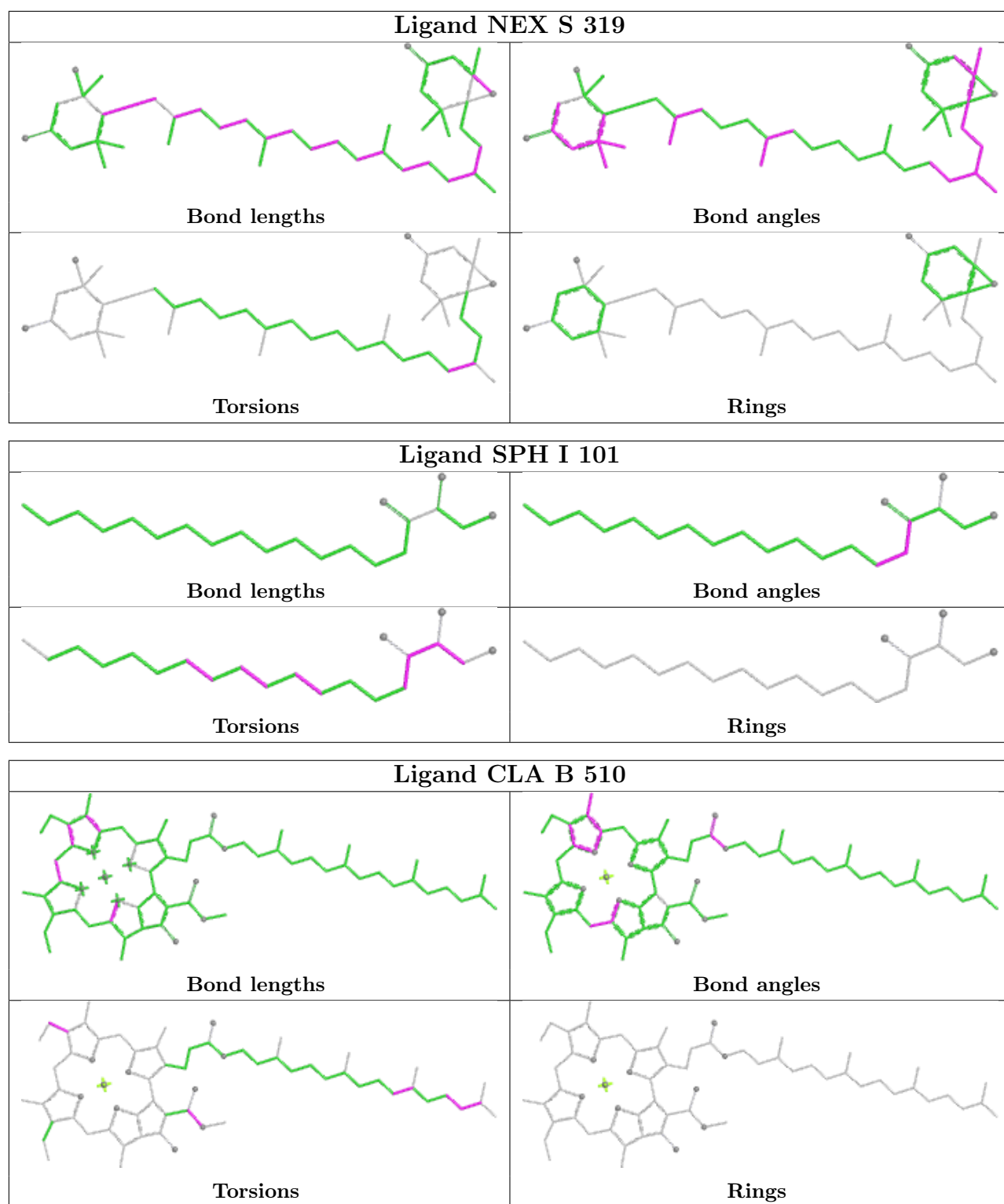


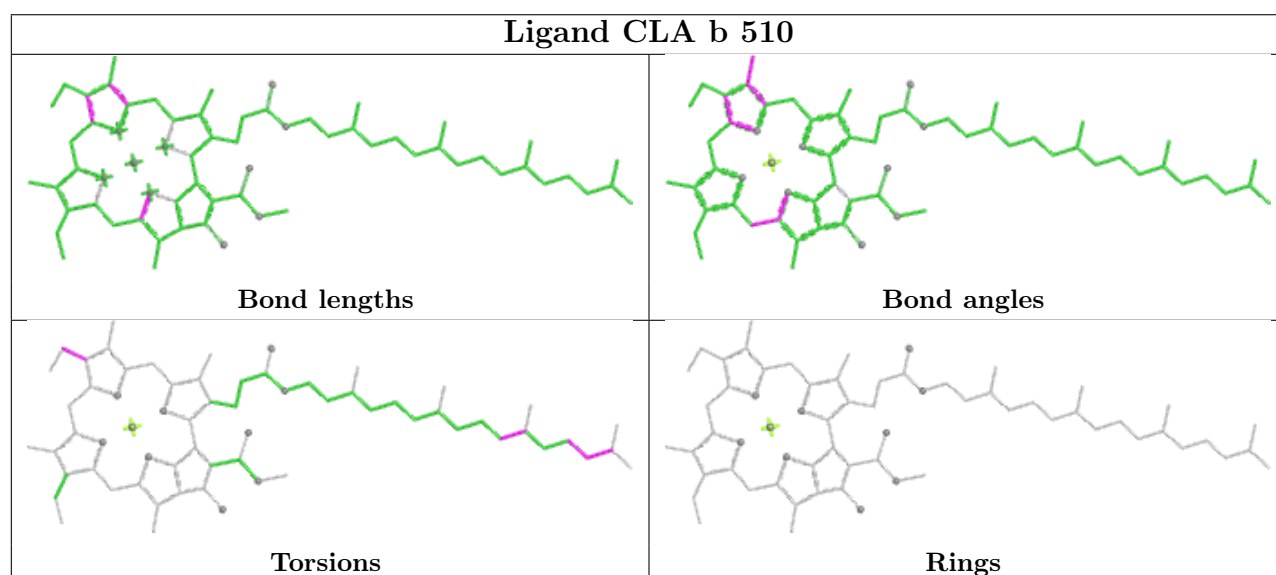
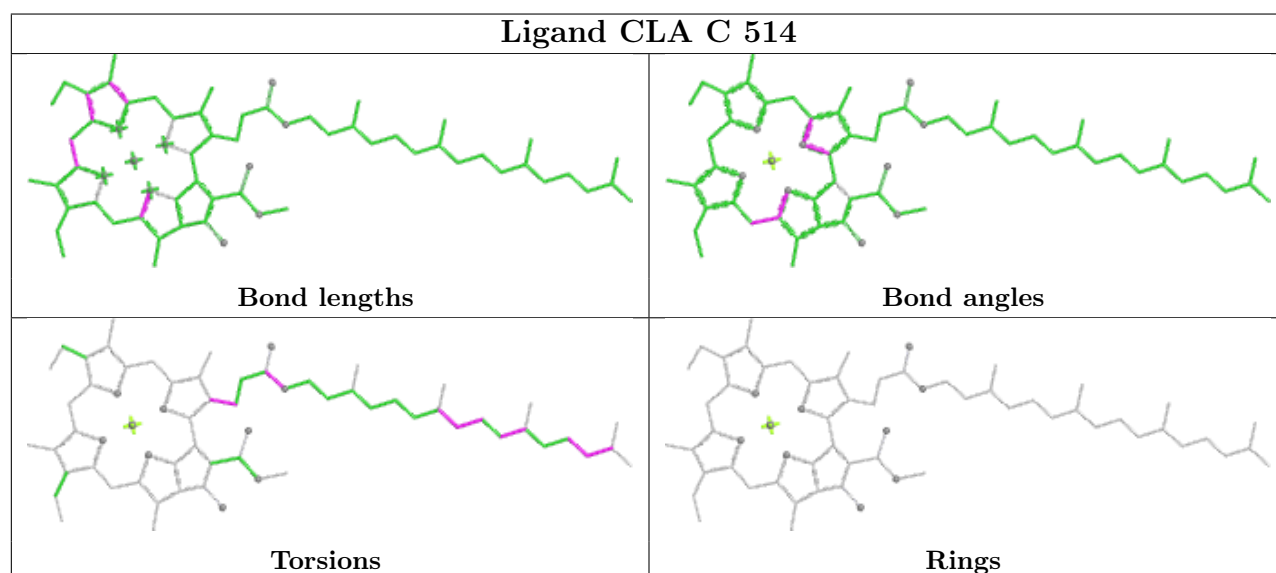
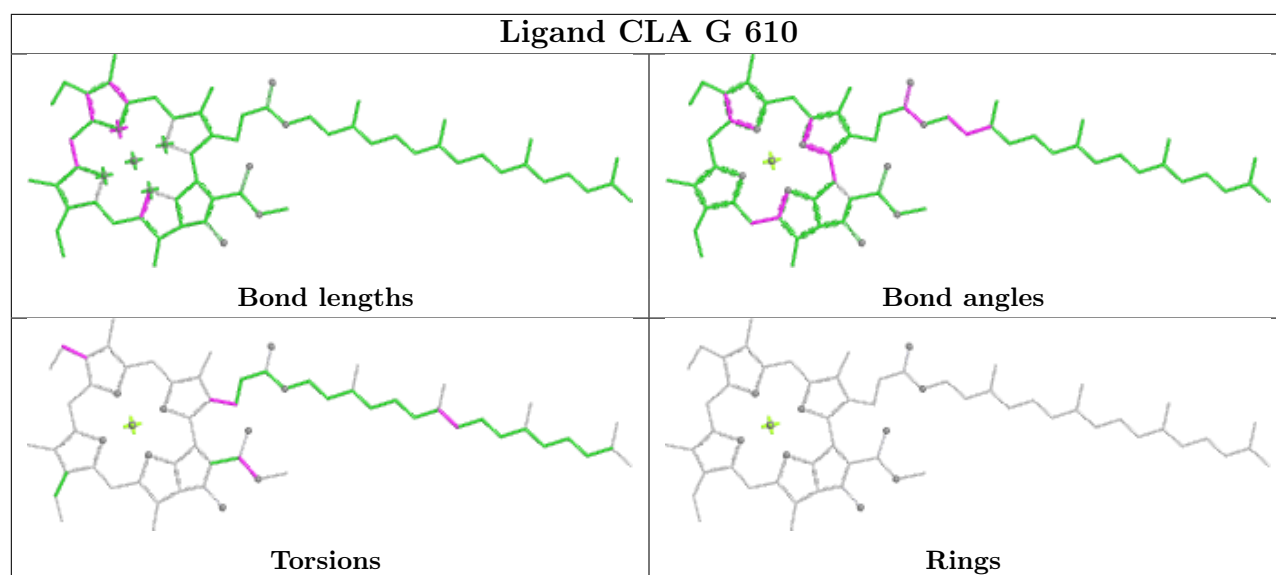
Ligand CLA Y 314**Ligand CLA N 603**



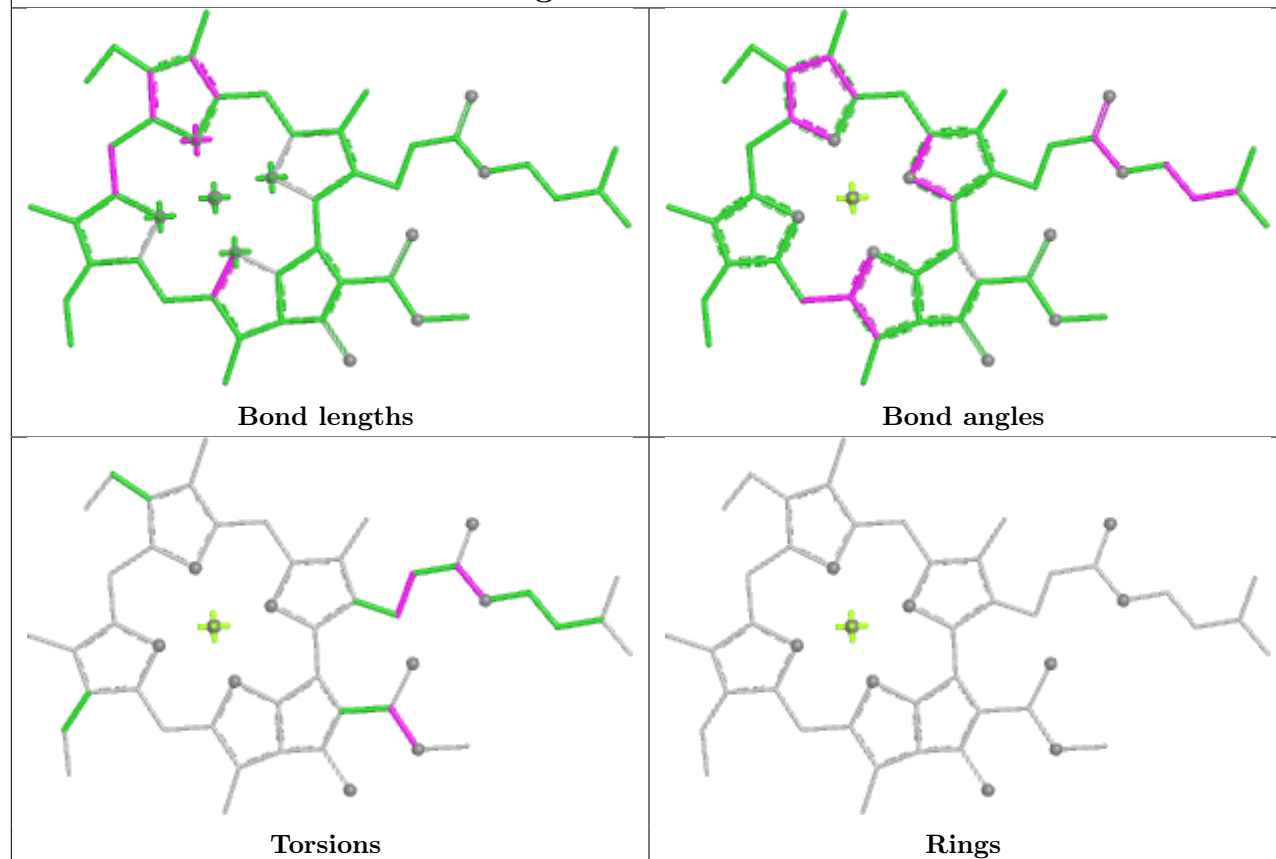




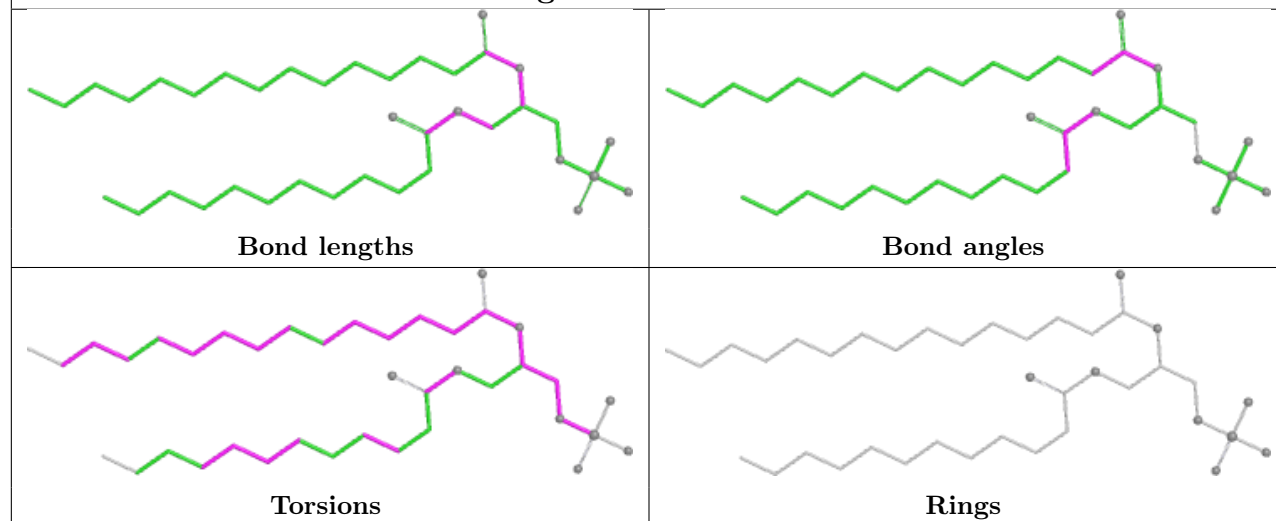


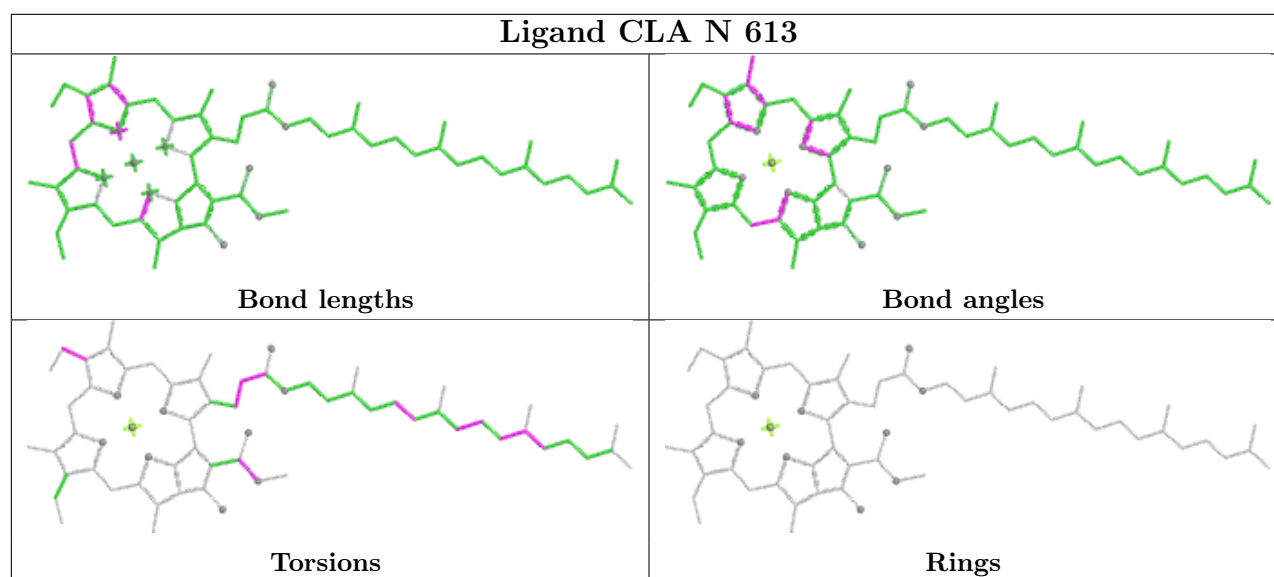


Ligand CLA S 316



Ligand 3PH b 521





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	D	6
1	A	3
22	r	1
22	R	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.60
1	R	110:PRO	C	126:GLU	N	12.92
1	A	269:ARG	C	270:SER	N	1.20
1	D	243:THR	C	244:TYR	N	1.20
1	D	213:ILE	C	214:HIS	N	1.19

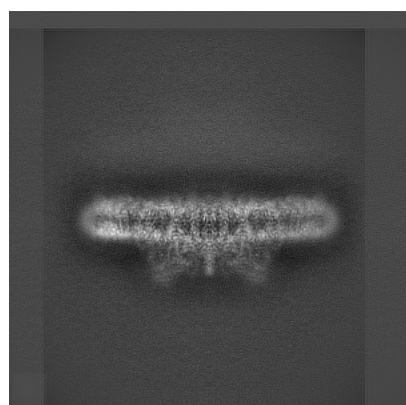
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13429. These allow visual inspection of the internal detail of the map and identification of artifacts.

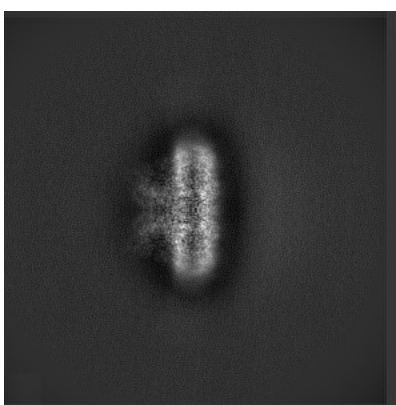
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

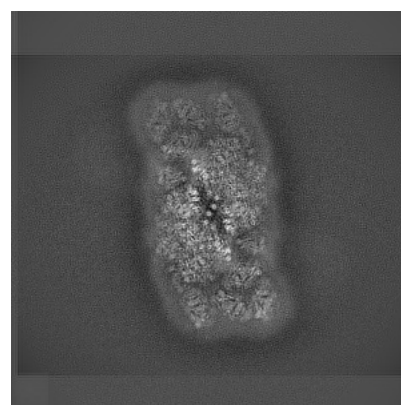
6.1.1 Primary map



X



Y

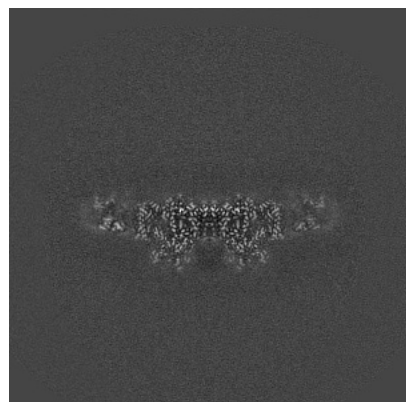


Z

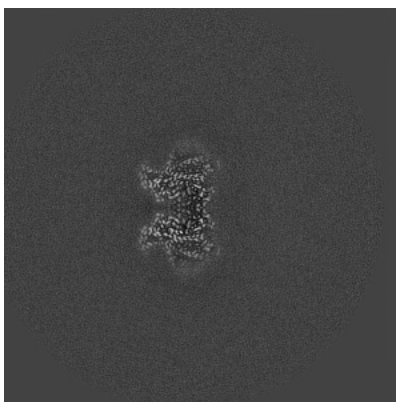
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

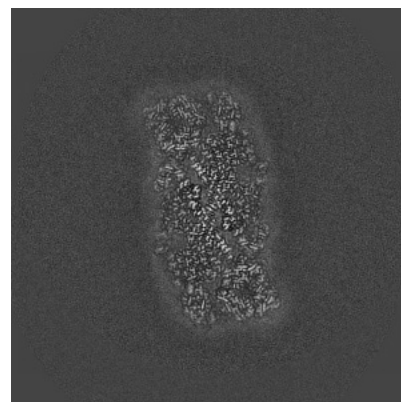
6.2.1 Primary map



X Index: 250



Y Index: 250

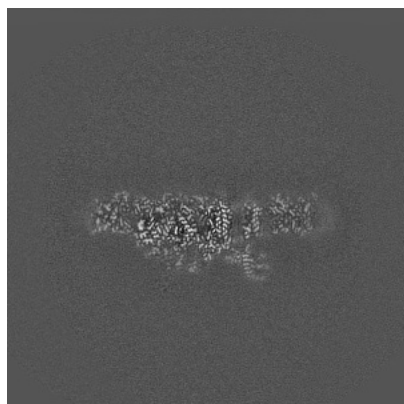


Z Index: 250

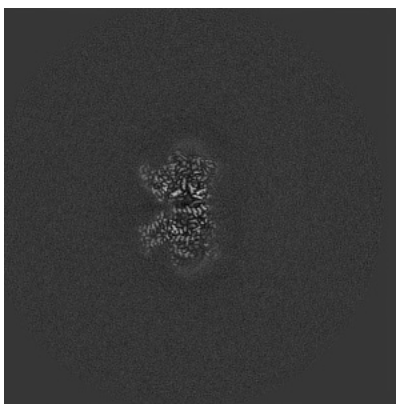
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

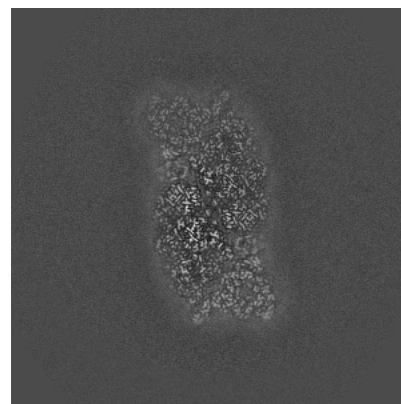
6.3.1 Primary map



X Index: 229



Y Index: 247

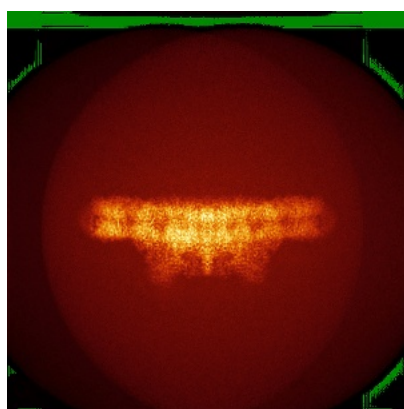


Z Index: 221

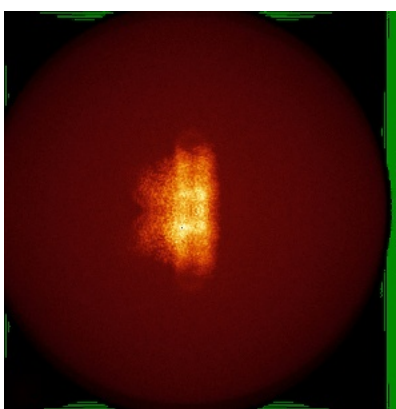
The images above show the largest variance slices of the map in three orthogonal directions.

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

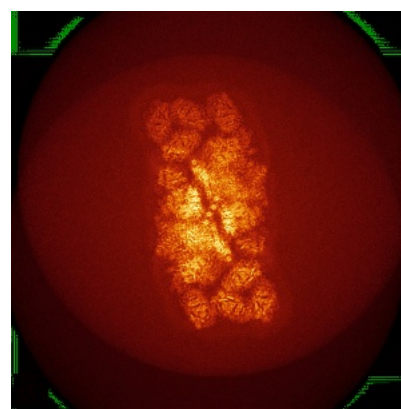
6.4.1 Primary map



X



Y

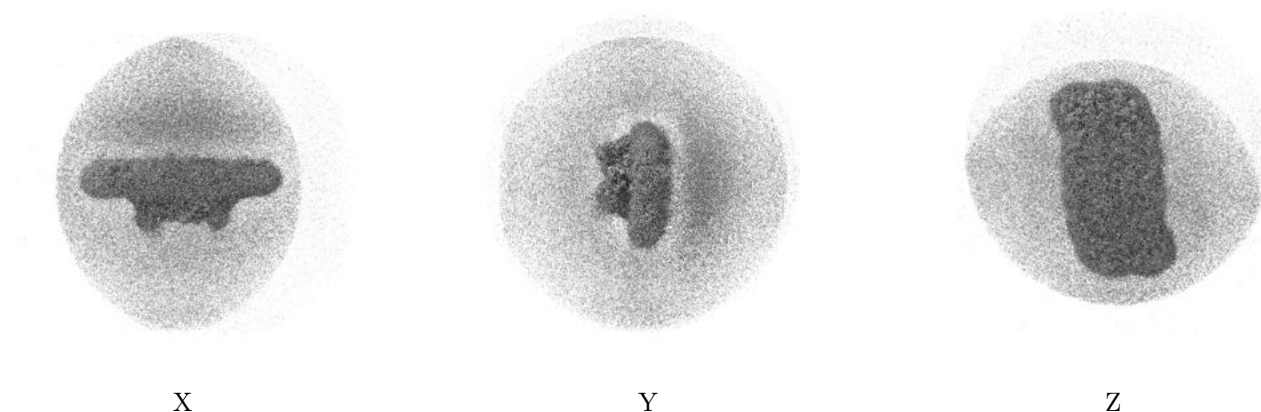


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

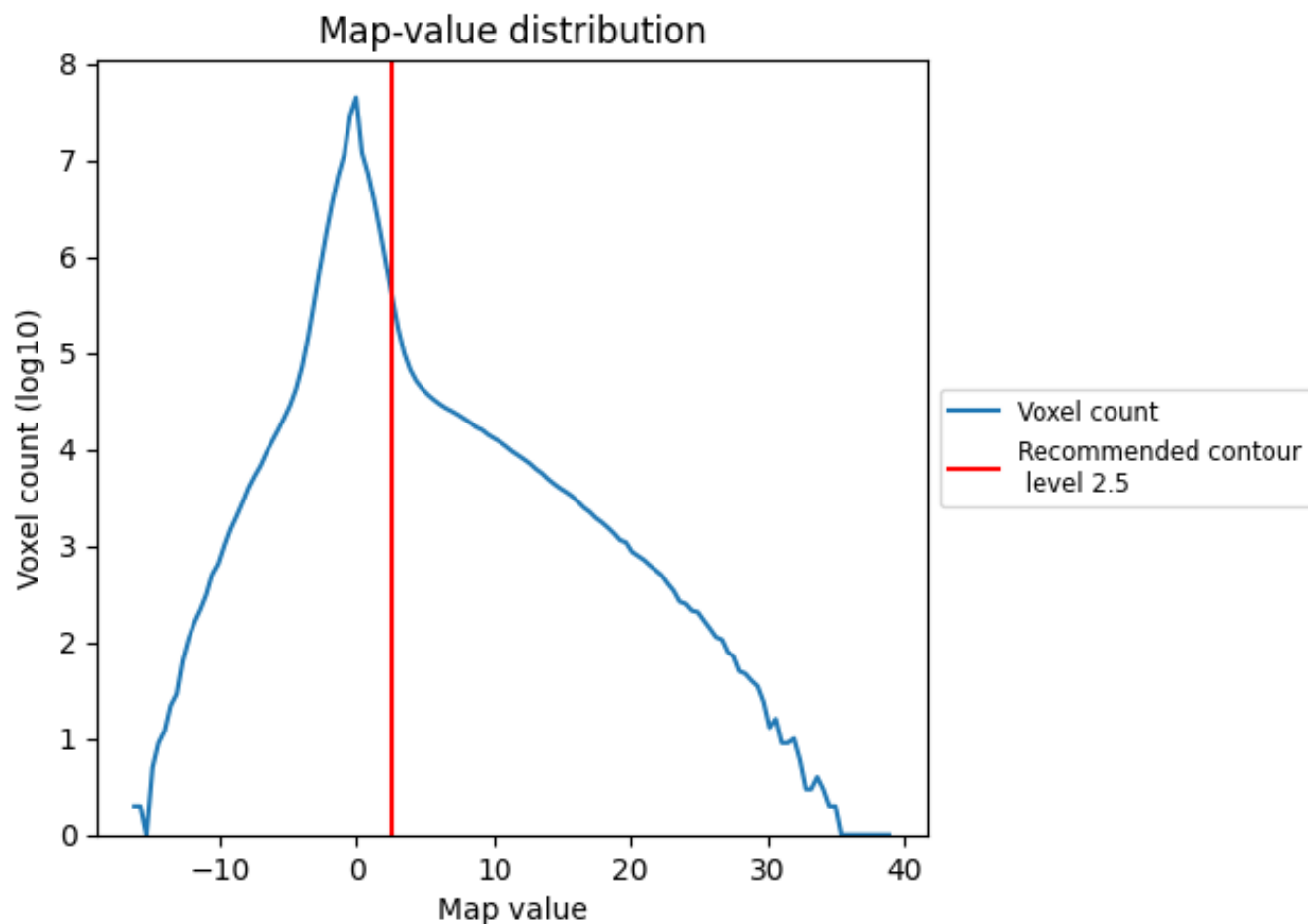
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

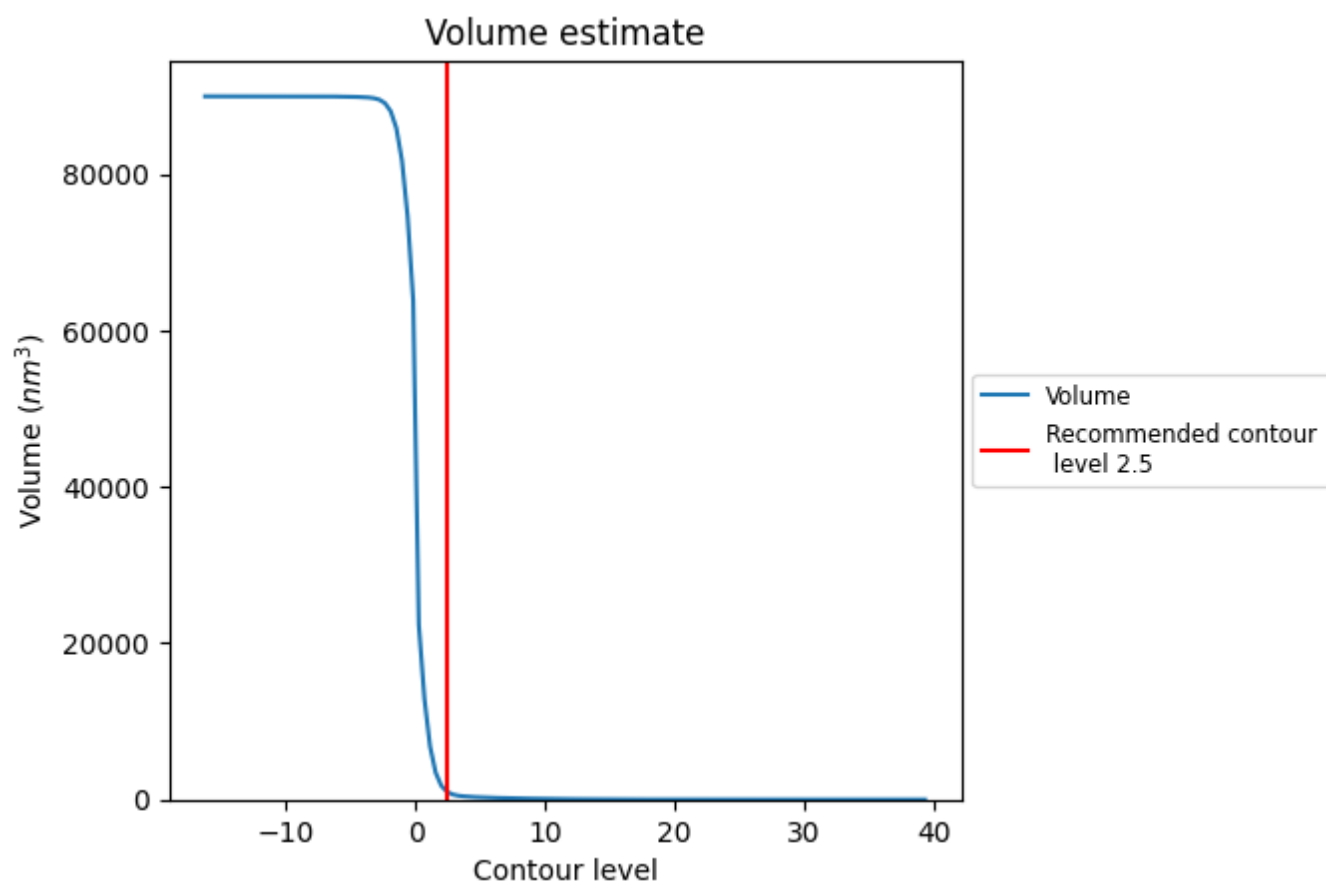
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

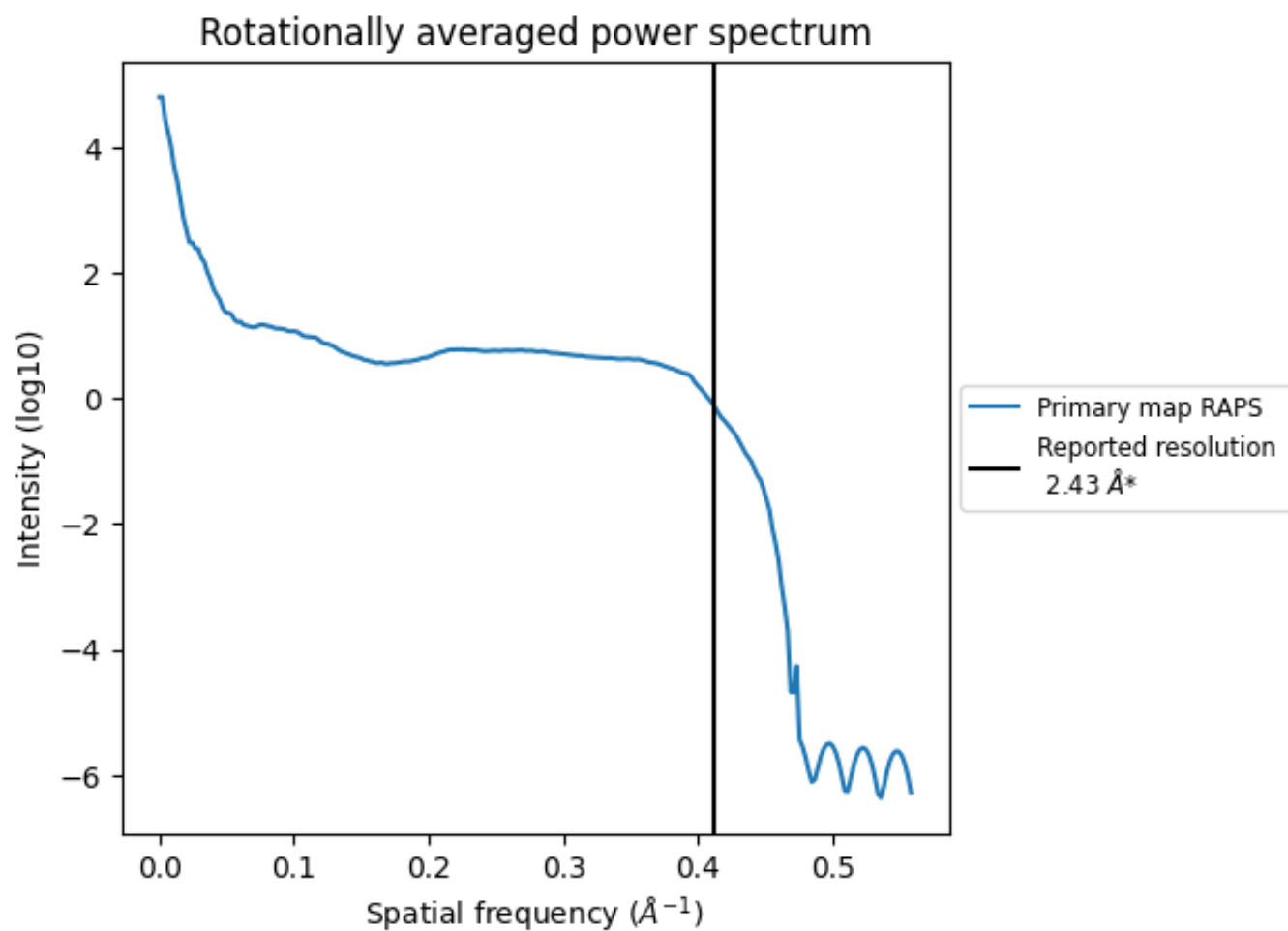
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 948 nm^3 ; this corresponds to an approximate mass of 856 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 ⓘ

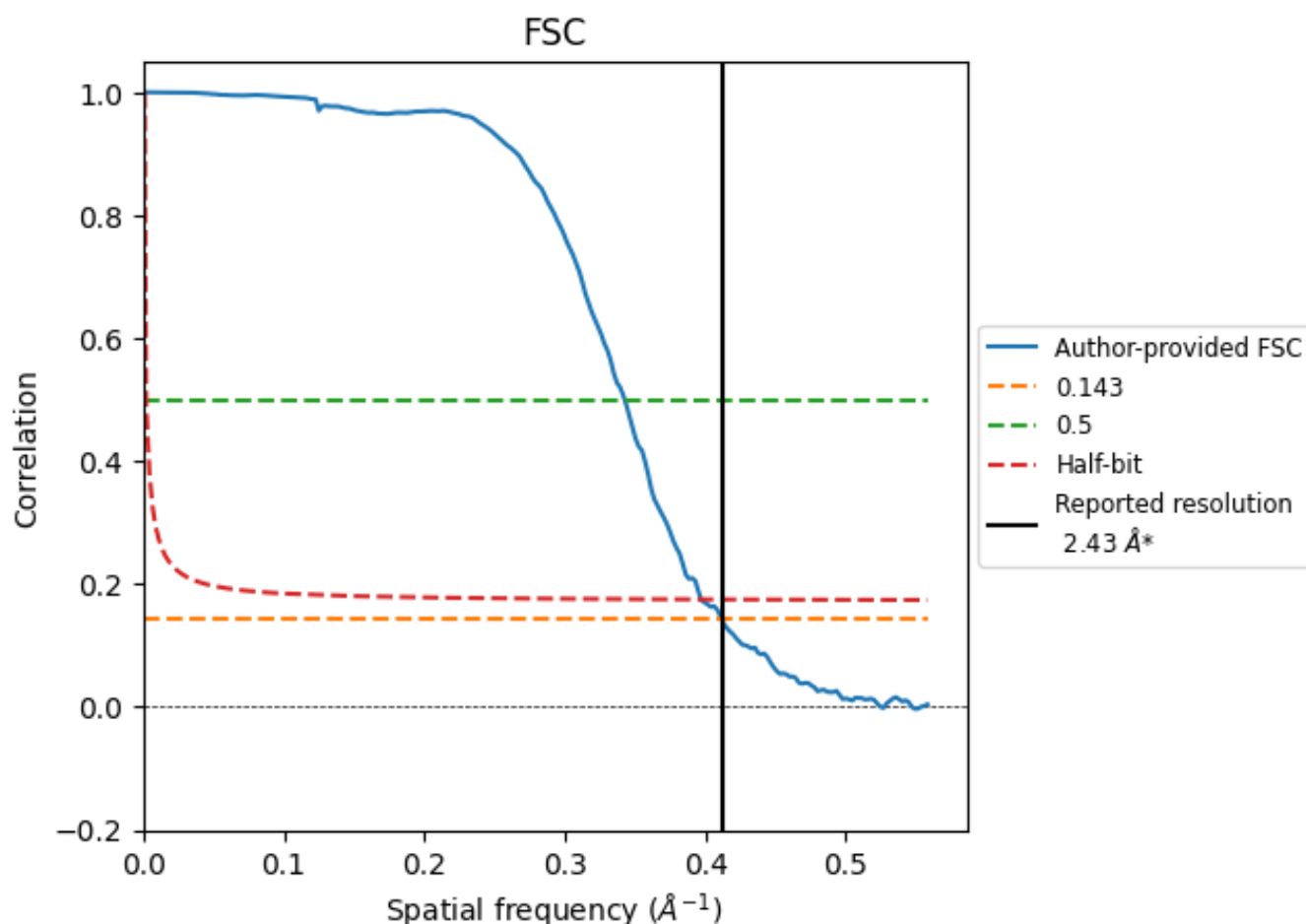


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8.2 Resolution estimates [i](#)

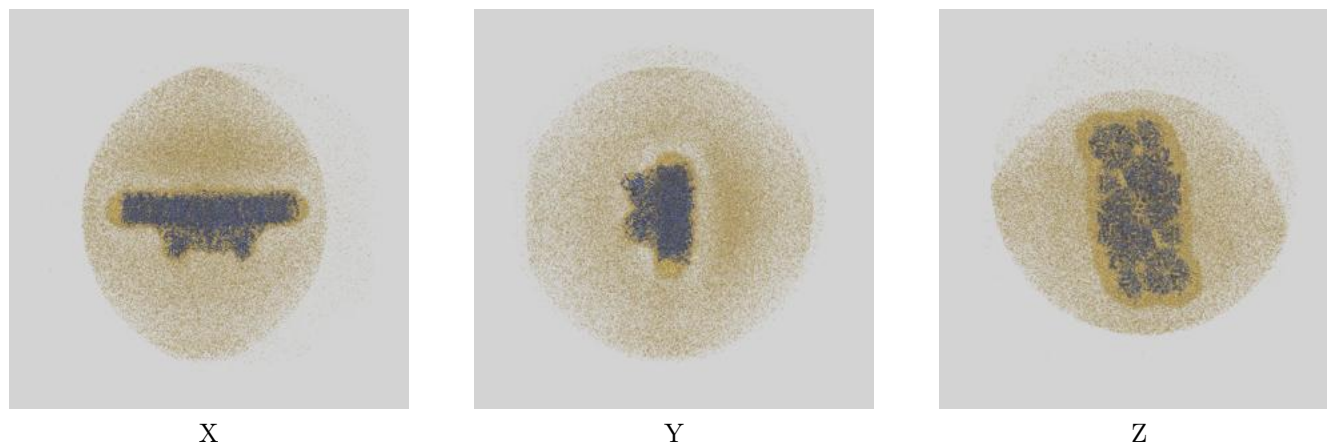
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.43	2.92	2.52
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

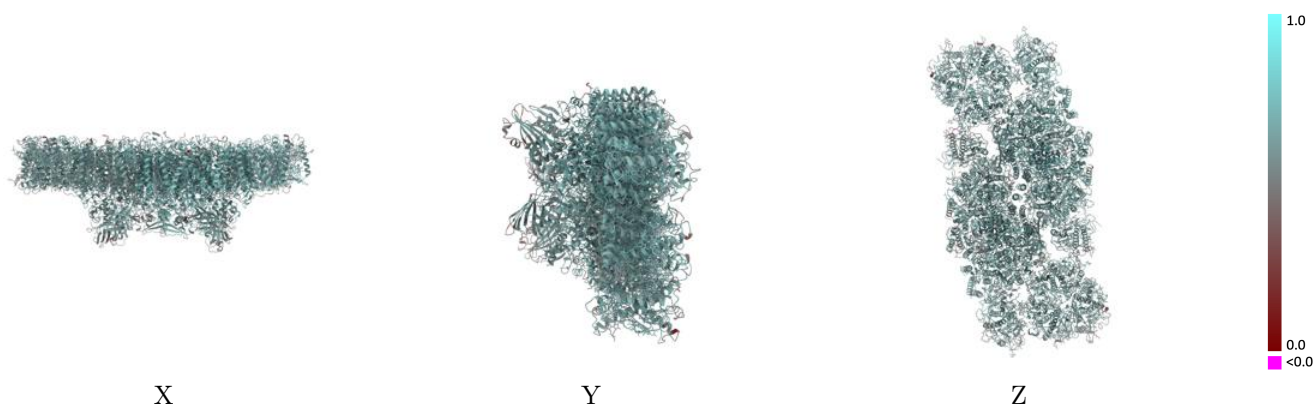
This section contains information regarding the fit between EMDB map EMD-13429 and PDB model 7PI0. Per-residue inclusion information can be found in section [3](#) on page [47](#).

9.1 Map-model overlay [i](#)



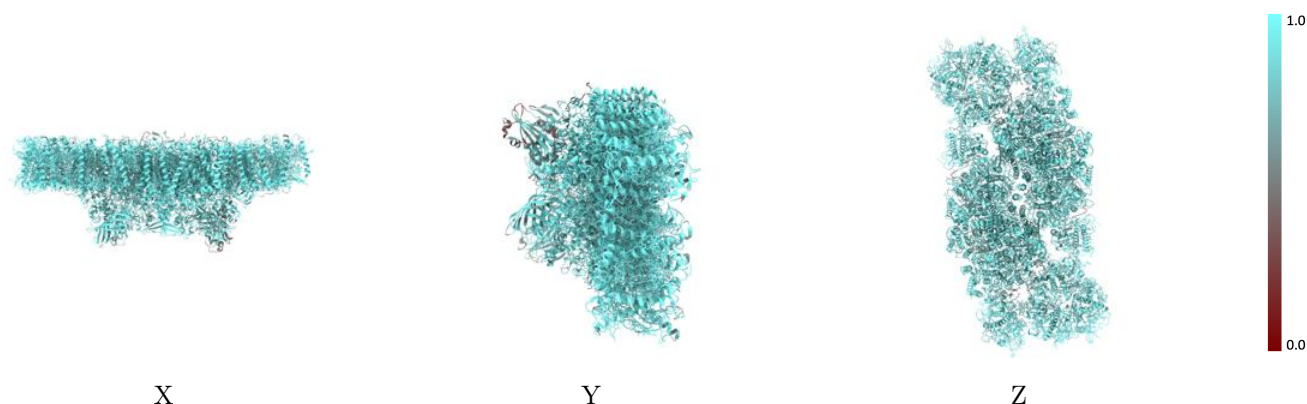
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



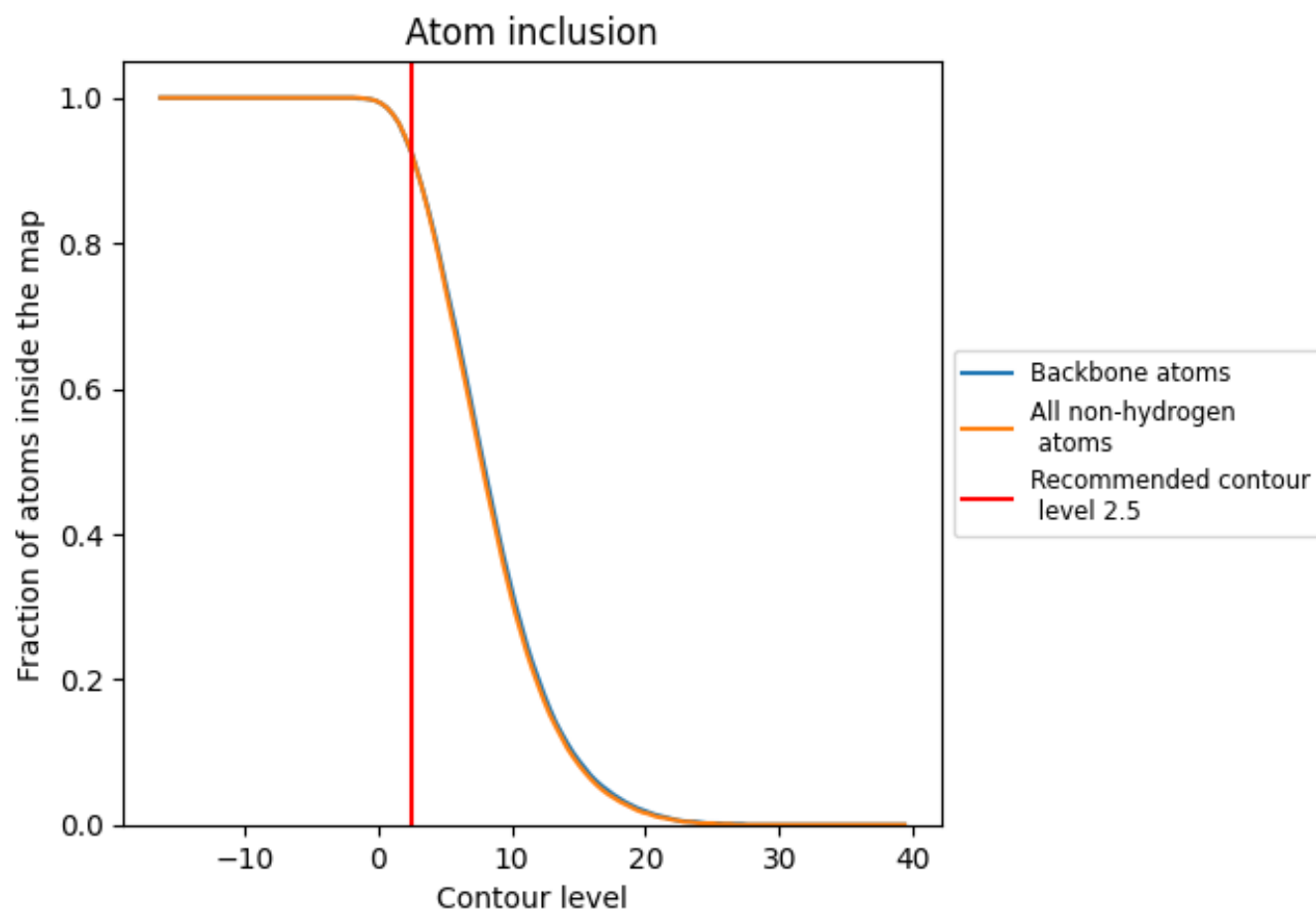
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9250	 0.6230
A	 0.9700	 0.6740
B	 0.9620	 0.6610
C	 0.9500	 0.6650
D	 0.9640	 0.6760
E	 0.9400	 0.6310
F	 0.9510	 0.6330
G	 0.9000	 0.6040
H	 0.9590	 0.6480
I	 0.9530	 0.6540
J	 0.9210	 0.6230
K	 0.9490	 0.6590
L	 0.9470	 0.6280
M	 0.9380	 0.6120
N	 0.9070	 0.6180
O	 0.8920	 0.5830
P	 0.6080	 0.5280
R	 0.8970	 0.5670
S	 0.9130	 0.6180
T	 0.9340	 0.6320
U	 0.8300	 0.5380
V	 0.9290	 0.6250
W	 0.8820	 0.5940
X	 0.8950	 0.5910
Y	 0.9250	 0.6340
Z	 0.9580	 0.6380
a	 0.9590	 0.6550
b	 0.9560	 0.6450
c	 0.9430	 0.6440
d	 0.9590	 0.6520
e	 0.9330	 0.5960
f	 0.9160	 0.6000
g	 0.9360	 0.5770
h	 0.9610	 0.6250
i	 0.9360	 0.6510



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Chain	Atom inclusion	Q-score
j	 0.9070	 0.6080
k	 0.9560	 0.6300
l	 0.9570	 0.6330
m	 0.9490	 0.6100
n	 0.9410	 0.6030
o	 0.8940	 0.5620
p	 0.7120	 0.5100
r	 0.9090	 0.5520
s	 0.9200	 0.5880
t	 0.9300	 0.6340
u	 0.7940	 0.5130
v	 0.9170	 0.6030
w	 0.8730	 0.5780
x	 0.8860	 0.5720
y	 0.9390	 0.6210
z	 0.9540	 0.6120