



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 03:23 PM UTC

PDB ID : 8IWH / pdb_00008iwh
EMDB ID : EMD-35766
Title : Structure and characteristics of a photosystem II supercomplex containing monomeric LHGX and dimeric FCPH antennae from the diatom *Thalassiosira pseudonana*
Authors : Feng, Y.; Li, Z.H.; Wang, W.D.; Shen, J.R.
Deposited on : 2023-03-30
Resolution : 2.68 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

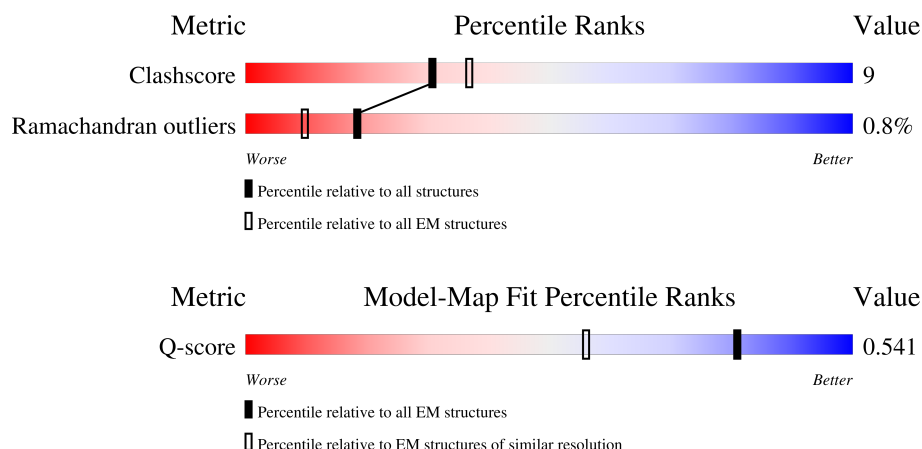
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.68 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.



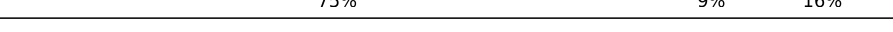
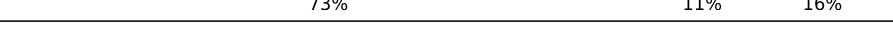
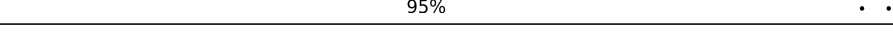
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	9255 (2.18 - 3.18)

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	333	88% 11% .
1	a	333	93% 7%
2	B	509	86% 7% 6%
2	b	509	83% 11% 6%
3	C	470	85% 11% .

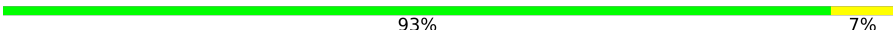
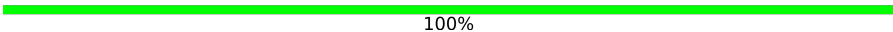
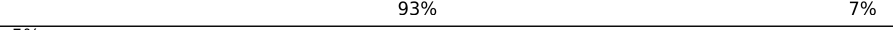
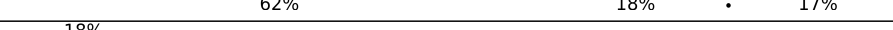
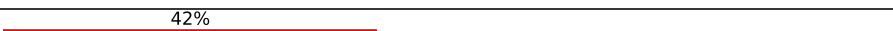
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Mol	Chain	Length	Quality of chain
3	c	470	
4	D	351	
4	d	351	
5	E	84	
5	e	84	
6	F	43	
6	f	43	
7	G	176	
7	g	176	
8	H	66	
8	h	66	
9	I	34	
9	i	34	
10	J	39	
10	j	39	
11	K	44	
11	k	44	
12	L	38	
12	l	38	
13	M	113	
13	m	113	
14	N	30	
14	n	30	
15	O	305	
15	o	305	

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Mol	Chain	Length	Quality of chain
16	T	28	
16	t	28	
17	U	148	
17	u	148	
18	V	162	
18	v	162	
19	W	54	
19	w	54	
20	X	38	
20	x	38	
21	Z	61	
21	z	61	
22	3	220	
23	4	196	
24	5	192	
25	6	199	
26	0	199	
26	7	199	
27	Y	34	
27	y	34	
28	Q	211	
28	q	211	
29	1	193	
29	2	193	
29	8	193	

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Mol	Chain	Length	Quality of chain
29	9	193	

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
33	CLA	0	304	X	-	-	-
33	CLA	0	305	X	-	-	-
33	CLA	0	307	X	-	-	-
33	CLA	0	308	X	-	-	-
33	CLA	0	309	X	-	-	-
33	CLA	0	310	X	-	-	-
33	CLA	0	311	X	-	-	-
33	CLA	0	312	X	-	-	-
33	CLA	0	313	X	-	-	-
33	CLA	1	305	X	-	-	-
33	CLA	1	306	X	-	-	-
33	CLA	1	307	X	-	-	-
33	CLA	1	308	X	-	-	-
33	CLA	1	309	X	-	-	-
33	CLA	1	310	X	-	-	-
33	CLA	1	311	X	-	-	-
33	CLA	1	312	X	-	-	-
33	CLA	1	313	X	-	-	-
33	CLA	1	314	X	-	-	-
33	CLA	1	315	X	-	-	-
33	CLA	1	316	X	-	-	-
33	CLA	2	305	X	-	-	-
33	CLA	2	306	X	-	-	-
33	CLA	2	307	X	-	-	-
33	CLA	2	308	X	-	-	-
33	CLA	2	309	X	-	-	-
33	CLA	2	310	X	-	-	-
33	CLA	2	311	X	-	-	-
33	CLA	2	312	X	-	-	-
33	CLA	2	314	X	-	-	-
33	CLA	2	315	X	-	-	-
33	CLA	2	316	X	-	-	-
33	CLA	2	317	X	-	-	-
33	CLA	3	302	X	-	-	-
33	CLA	3	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	3	304	X	-	-	-
33	CLA	3	305	X	-	-	-
33	CLA	3	306	X	-	-	-
33	CLA	3	307	X	-	-	-
33	CLA	3	308	X	-	-	-
33	CLA	3	309	X	-	-	-
33	CLA	3	311	X	-	-	-
33	CLA	3	312	X	-	-	-
33	CLA	3	313	X	-	-	-
33	CLA	3	319	X	-	-	-
33	CLA	4	305	X	-	-	-
33	CLA	4	306	X	-	-	-
33	CLA	4	308	X	-	-	-
33	CLA	4	309	X	-	-	-
33	CLA	4	310	X	-	-	-
33	CLA	4	311	X	-	-	-
33	CLA	4	312	X	-	-	-
33	CLA	4	313	X	-	-	-
33	CLA	4	314	X	-	-	-
33	CLA	4	315	X	-	-	-
33	CLA	4	316	X	-	-	-
33	CLA	5	308	X	-	-	-
33	CLA	5	309	X	-	-	-
33	CLA	5	311	X	-	-	-
33	CLA	5	312	X	-	-	-
33	CLA	5	313	X	-	-	-
33	CLA	5	314	X	-	-	-
33	CLA	5	316	X	-	-	-
33	CLA	5	317	X	-	-	-
33	CLA	6	307	X	-	-	-
33	CLA	6	308	X	-	-	-
33	CLA	6	310	X	-	-	-
33	CLA	6	311	X	-	-	-
33	CLA	6	312	X	-	-	-
33	CLA	6	313	X	-	-	-
33	CLA	6	315	X	-	-	-
33	CLA	6	316	X	-	-	-
33	CLA	7	304	X	-	-	-
33	CLA	7	305	X	-	-	-
33	CLA	7	307	X	-	-	-
33	CLA	7	308	X	-	-	-
33	CLA	7	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	7	310	X	-	-	-
33	CLA	7	311	X	-	-	-
33	CLA	7	312	X	-	-	-
33	CLA	7	313	X	-	-	-
33	CLA	7	314	X	-	-	-
33	CLA	8	305	X	-	-	-
33	CLA	8	306	X	-	-	-
33	CLA	8	307	X	-	-	-
33	CLA	8	308	X	-	-	-
33	CLA	8	309	X	-	-	-
33	CLA	8	310	X	-	-	-
33	CLA	8	311	X	-	-	-
33	CLA	8	312	X	-	-	-
33	CLA	8	313	X	-	-	-
33	CLA	8	314	X	-	-	-
33	CLA	8	315	X	-	-	-
33	CLA	8	316	X	-	-	-
33	CLA	9	305	X	-	-	-
33	CLA	9	306	X	-	-	-
33	CLA	9	307	X	-	-	-
33	CLA	9	308	X	-	-	-
33	CLA	9	309	X	-	-	-
33	CLA	9	310	X	-	-	-
33	CLA	9	311	X	-	-	-
33	CLA	9	312	X	-	-	-
33	CLA	9	313	X	-	-	-
33	CLA	9	314	X	-	-	-
33	CLA	9	315	X	-	-	-
33	CLA	9	316	X	-	-	-
33	CLA	9	317	X	-	-	-
33	CLA	A	404	X	-	-	-
33	CLA	A	405	X	-	-	-
33	CLA	A	408	X	-	-	-
33	CLA	B	601	X	-	-	-
33	CLA	B	602	X	-	-	-
33	CLA	B	603	X	-	-	-
33	CLA	B	604	X	-	-	-
33	CLA	B	605	X	-	-	-
33	CLA	B	606	X	-	-	-
33	CLA	B	607	X	-	-	-
33	CLA	B	608	X	-	-	-
33	CLA	B	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	B	610	X	-	-	-
33	CLA	B	611	X	-	-	-
33	CLA	B	612	X	-	-	-
33	CLA	B	613	X	-	-	-
33	CLA	B	614	X	-	-	-
33	CLA	B	615	X	-	-	-
33	CLA	B	616	X	-	-	-
33	CLA	C	501	X	-	-	-
33	CLA	C	502	X	-	-	-
33	CLA	C	503	X	-	-	-
33	CLA	C	504	X	-	-	-
33	CLA	C	505	X	-	-	-
33	CLA	C	506	X	-	-	-
33	CLA	C	507	X	-	-	-
33	CLA	C	508	X	-	-	-
33	CLA	C	509	X	-	-	-
33	CLA	C	510	X	-	-	-
33	CLA	C	511	X	-	-	-
33	CLA	C	512	X	-	-	-
33	CLA	C	513	X	-	-	-
33	CLA	D	402	X	-	-	-
33	CLA	D	405	X	-	-	-
33	CLA	D	406	X	-	-	-
33	CLA	H	103	X	-	-	-
33	CLA	W	303	X	-	-	-
33	CLA	Z	101	X	-	-	-
33	CLA	a	407	X	-	-	-
33	CLA	a	408	X	-	-	-
33	CLA	a	411	X	-	-	-
33	CLA	b	602	X	-	-	-
33	CLA	b	603	X	-	-	-
33	CLA	b	604	X	-	-	-
33	CLA	b	605	X	-	-	-
33	CLA	b	606	X	-	-	-
33	CLA	b	607	X	-	-	-
33	CLA	b	608	X	-	-	-
33	CLA	b	609	X	-	-	-
33	CLA	b	610	X	-	-	-
33	CLA	b	611	X	-	-	-
33	CLA	b	612	X	-	-	-
33	CLA	b	613	X	-	-	-
33	CLA	b	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	b	615	X	-	-	-
33	CLA	b	616	X	-	-	-
33	CLA	b	617	X	-	-	-
33	CLA	c	501	X	-	-	-
33	CLA	c	502	X	-	-	-
33	CLA	c	503	X	-	-	-
33	CLA	c	504	X	-	-	-
33	CLA	c	505	X	-	-	-
33	CLA	c	506	X	-	-	-
33	CLA	c	507	X	-	-	-
33	CLA	c	508	X	-	-	-
33	CLA	c	509	X	-	-	-
33	CLA	c	510	X	-	-	-
33	CLA	c	511	X	-	-	-
33	CLA	c	512	X	-	-	-
33	CLA	c	513	X	-	-	-
33	CLA	d	401	X	-	-	-
33	CLA	d	402	X	-	-	-
33	CLA	d	409	X	-	-	-
33	CLA	w	303	X	-	-	-
33	CLA	z	101	X	-	-	-
35	BCT	A	410	-	-	X	-
35	BCT	a	402	-	-	X	-

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 75511 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	333	Total	C	N	O	S	0	0
			2614	1709	427	462	16		
1	a	333	Total	C	N	O	S	0	0
			2614	1709	427	462	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	478	Total	C	N	O	S	0	0
			3772	2466	639	654	13		
2	b	478	Total	C	N	O	S	0	0
			3772	2466	639	654	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3489	2277	588	608	16		
3	c	450	Total	C	N	O	S	0	0
			3489	2277	588	608	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2699	1784	442	463	10		
4	d	341	Total	C	N	O	S	0	0
			2699	1784	442	463	10		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	76	Total	C	N	O	0	0
			626	407	103	116		
5	e	76	Total	C	N	O	0	0
			626	407	103	116		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	31	Total	C	N	O	S	0	0
			253	173	42	37	1		
6	f	31	Total	C	N	O	S	0	0
			253	173	42	37	1		

- Molecule 7 is a protein called Photosystem II Psb31 protein domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	120	Total	C	N	O	0	0
			890	556	160	174		
7	g	120	Total	C	N	O	0	0
			890	556	160	174		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			512	339	82	89	2		
8	h	65	Total	C	N	O	S	0	0
			512	339	82	89	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total 279	C 188	N 43	O 47	S 1	0	0
9	i	34	Total 279	C 188	N 43	O 47	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	33	Total	C	N	O	0	0
			243	165	37	41		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	33	Total	C	N	O	0	0
			243	165	37	41		

- 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
			303	213	45	45		
11	k	37	Total	C	N	O	0	0
			303	213	45	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	37	Total	C	N	O	0	0
			302	203	47	52		
12	l	37	Total	C	N	O	0	0
			302	203	47	52		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	41	Total	C	N	O	0	0
			317	208	51	58		
13	m	41	Total	C	N	O	0	0
			317	208	51	58		

- Molecule 14 is a protein called Photosystem II subunit, PsbN..

Mol	Chain	Residues	Atoms				AltConf	Trace
14	n	30	Total	C	N	O	0	0
			150	90	30	30		
14	N	30	Total	C	N	O	0	0
			150	90	30	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	248	Total	C	N	O	S	0	0
			1867	1176	309	374	8		
15	o	248	Total	C	N	O	S	0	0
			1867	1176	309	374	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	28	Total	C	N	O	S	0	0
			233	161	34	36	2		
16	t	28	Total	C	N	O	S	0	0
			233	161	34	36	2		

- Molecule 17 is a protein called PS II complex 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	92	Total	C	N	O	S	0	0
			708	451	121	134	2		
17	u	92	Total	C	N	O	S	0	0
			708	451	121	134	2		

- Molecule 18 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	135	Total	C	N	O	S	0	0
			1029	640	179	206	4		
18	v	135	Total	C	N	O	S	0	0
			1029	640	179	206	4		

- Molecule 19 is a protein called Photosystem II subunit, PsbW.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	W	54	Total	C	N	O	0	0
			434	281	64	89		
19	w	54	Total	C	N	O	0	0
			434	281	64	89		

- Molecule 20 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	35	Total	C	N	O	S	0	0
			248	160	41	46	1		
20	x	35	Total	C	N	O	S	0	0
			248	160	41	46	1		

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			453	301	68	83	1		
21	z	61	Total	C	N	O	S	0	0
			453	301	68	83	1		

- Molecule 22 is a protein called Fucoxanthin chl a/c protein, lhca clade.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	220	Total	C	N	O	S	0	0
			1710	1110	281	315	4		

- Molecule 23 is a protein called Fucoxanthin-chlorophyll a-c binding protein, plastid.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4	163	Total	C	N	O	S	0	0
			1249	809	204	232	4		

- Molecule 24 is a protein called Fucoxanthin chlorophyll a/c protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	160	Total	C	N	O	S	0	0
			1229	780	217	227	5		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	168	Total	C	N	O	S	0	0
			1296	833	219	238	6		

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c protein-LI818 clade.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	165	Total	C	N	O	S	0	0
			1269	819	213	233	4		
26	0	165	Total	C	N	O	S	0	0
			1269	819	213	233	4		

- Molecule 27 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	34	Total	C	N	O	S	0	0
			251	167	41	41	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	y	34	Total	C	N	O	S	0	0
			251	167	41	41	2		

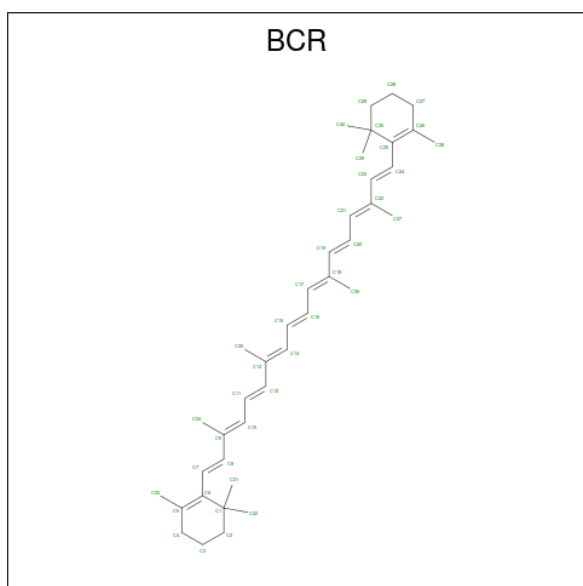
- Molecule 28 is a protein called Photosystem II subunit, PsbQ..

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	156	Total	C	N	O	S	0	0
			1198	757	202	237	2		
28	q	156	Total	C	N	O	S	0	0
			1198	757	202	237	2		

- Molecule 29 is a protein called Fucoxanthin chlorophyll a/c light-harvesting protein, major type.

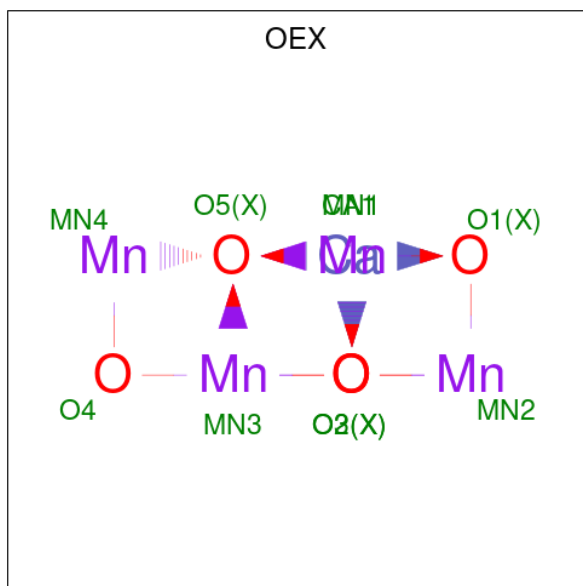
Mol	Chain	Residues	Atoms					AltConf	Trace
29	9	163	Total	C	N	O	S	0	0
			1214	788	206	218	2		
29	2	163	Total	C	N	O	S	0	0
			1214	788	206	218	2		
29	8	163	Total	C	N	O	S	0	0
			1206	783	206	216	1		
29	1	163	Total	C	N	O	S	0	0
			1206	783	206	216	1		

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	C	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	D	1	Total C 40 40	0
30	d	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	h	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	k	1	Total C 40 40	0
30	k	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0
30	b	1	Total C 40 40	0

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

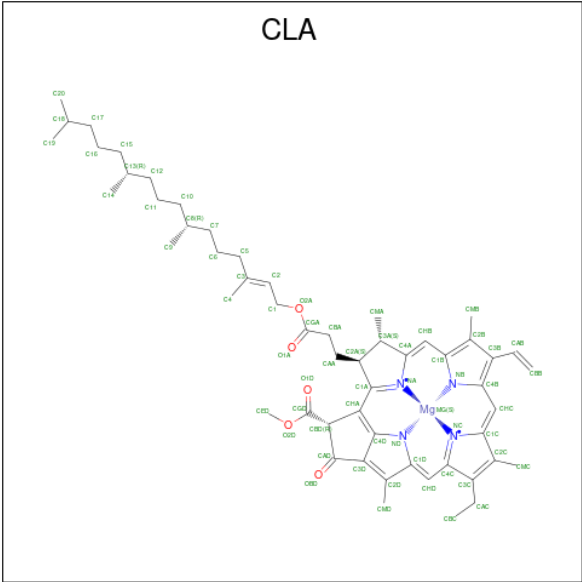


Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
31	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 32 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 33 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
33	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	D	1	Total 59	C 49	Mg 1	N 4	O 5	0
33	D	1	Total 57	C 47	Mg 1	N 4	O 5	0
33	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	d	1	Total 57	C 47	Mg 1	N 4	O 5	0
33	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	d	1	Total 59	C 49	Mg 1	N 4	O 5	0
33	H	1	Total 43	C 35	Mg 1	N 4	O 3	0
33	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	Z	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	z	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 48	C 38	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
33	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
33	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	4	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	4	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
33	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	5	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
33	6	1	Total 54	C 44	Mg 1	N 4	O 5	0
33	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
33	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	6	1	Total 39	C 30	Mg 1	N 4	O 4	0
33	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 34	C 28	Mg 1	N 4	O 1	0
33	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
33	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	b	1	Total 61	C 52	Mg 1	N 4	O 4	0
33	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 64	C 54	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	0	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	0	1	Total 34	C 28	Mg 1	N 4	O 1	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	9	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	2	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	2	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	8	1	Total 45	C 35	Mg 1	N 4	O 5	0

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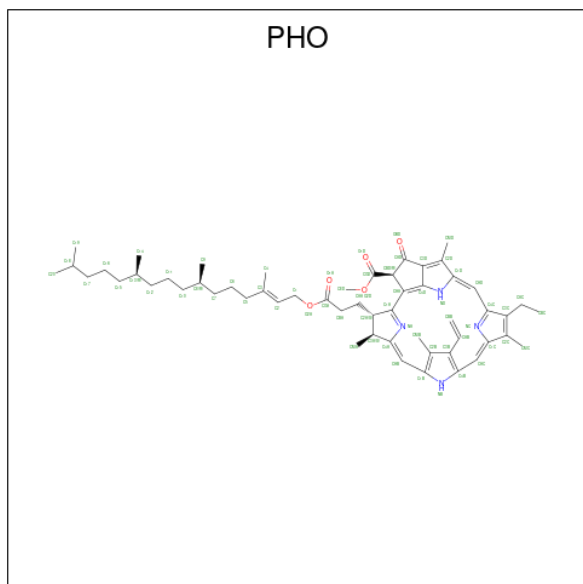
Mol	Chain	Residues	Atoms					AltConf
33	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	8	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	8	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	8	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	8	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
33	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
33	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	1	1	Total 36	C 30	Mg 1	N 4	O 1	0
33	1	1	Total 38	C 32	Mg 1	N 4	O 1	0
33	1	1	Total 38	C 32	Mg 1	N 4	O 1	0

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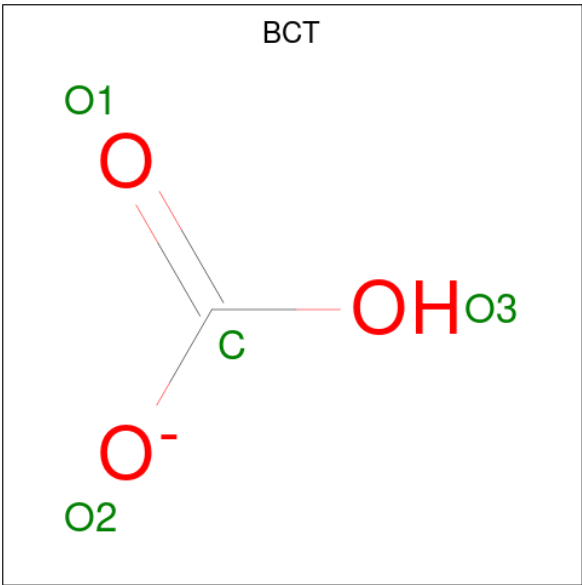
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
33	1	1	38	32	1	4	1	0

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



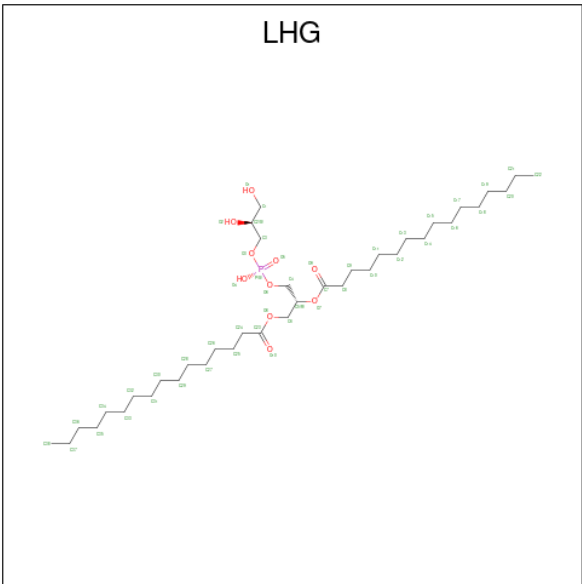
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
34	A	1	64	55	4	5	0
34	A	1	64	55	4	5	0
34	a	1	64	55	4	5	0
34	a	1	64	55	4	5	0

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



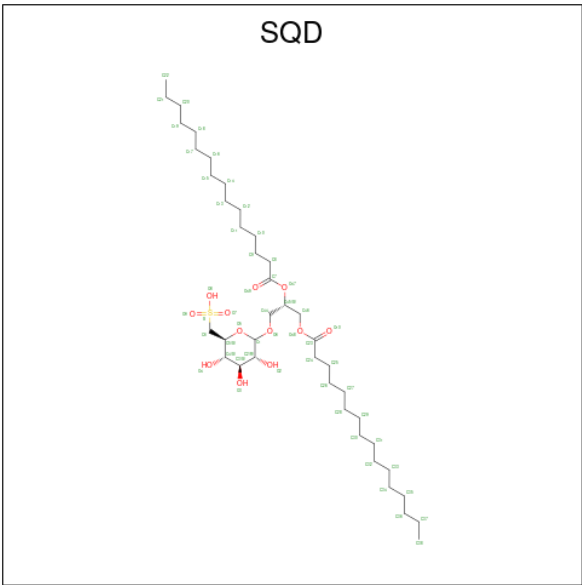
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	P	0
			43	32	10	1	

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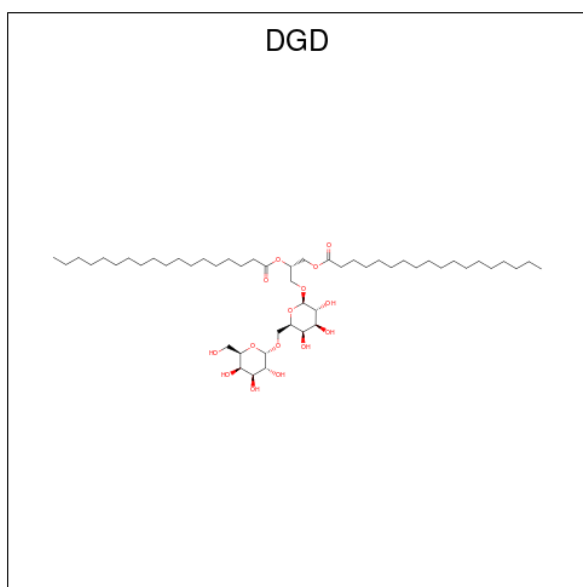
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	P	0
			49	38	10	1	
36	A	1	Total	C	O	P	0
			49	38	10	1	
36	D	1	Total	C	O	P	0
			48	38	9	1	
36	D	1	Total	C	O	P	0
			42	31	10	1	
36	d	1	Total	C	O	P	0
			48	38	9	1	
36	d	1	Total	C	O	P	0
			42	31	10	1	
36	H	1	Total	C	O	P	0
			42	31	10	1	
36	h	1	Total	C	O	P	0
			42	31	10	1	
36	W	1	Total	C	O	P	0
			35	24	10	1	
36	w	1	Total	C	O	P	0
			35	24	10	1	
36	3	1	Total	C	O	P	0
			27	16	10	1	
36	3	1	Total	C	O	P	0
			49	38	10	1	
36	4	1	Total	C	O	P	0
			49	38	10	1	
36	5	1	Total	C	O	P	0
			33	24	8	1	
36	7	1	Total	C	O	P	0
			28	19	8	1	
36	a	1	Total	C	O	P	0
			43	32	10	1	
36	a	1	Total	C	O	P	0
			49	38	10	1	
36	b	1	Total	C	O	P	0
			49	38	10	1	
36	0	1	Total	C	O	P	0
			28	19	8	1	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



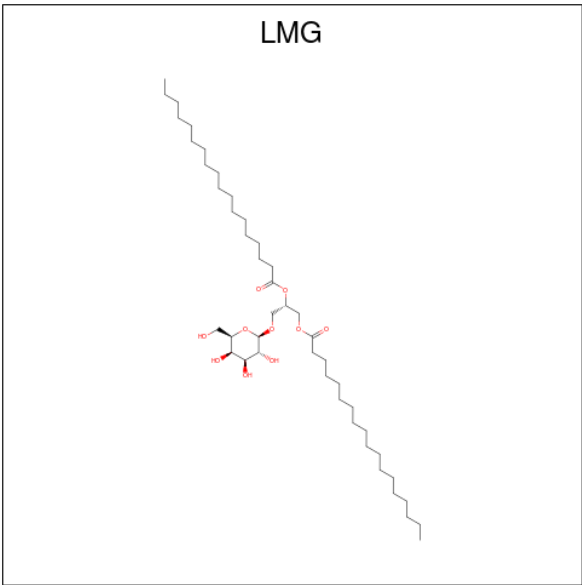
Mol	Chain	Residues	Atoms				AltConf
37	A	1	Total	C	O	S	0
			40	27	12	1	
37	B	1	Total	C	O	S	0
			54	41	12	1	
37	D	1	Total	C	O	S	0
			54	41	12	1	
37	i	1	Total	C	O	S	0
			40	27	12	1	
37	L	1	Total	C	O	S	0
			54	41	12	1	
37	l	1	Total	C	O	S	0
			54	41	12	1	
37	T	1	Total	C	O	S	0
			40	27	12	1	
37	T	1	Total	C	O	S	0
			54	41	12	1	
37	t	1	Total	C	O	S	0
			40	27	12	1	
37	7	1	Total	C	O	S	0
			48	35	12	1	
37	a	1	Total	C	O	S	0
			54	41	12	1	
37	0	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			53	39	14	
38	C	1	Total	C	O	0
			55	40	15	
38	C	1	Total	C	O	0
			56	41	15	
38	C	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			55	40	15	
38	c	1	Total	C	O	0
			56	41	15	
38	c	1	Total	C	O	0
			55	40	15	
38	H	1	Total	C	O	0
			62	47	15	
38	h	1	Total	C	O	0
			62	47	15	
38	3	1	Total	C	O	0
			39	34	5	
38	a	1	Total	C	O	0
			53	39	14	

- Molecule 39 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			51	41	10	
39	B	1	Total	C	O	0
			28	18	10	
39	C	1	Total	C	O	0
			46	36	10	
39	C	1	Total	C	O	0
			48	38	10	
39	C	1	Total	C	O	0
			27	17	10	
39	C	1	Total	C	O	0
			23	13	10	
39	c	1	Total	C	O	0
			48	38	10	
39	c	1	Total	C	O	0
			27	17	10	
39	D	1	Total	C	O	0
			40	30	10	
39	D	1	Total	C	O	0
			46	36	10	
39	d	1	Total	C	O	0
			46	36	10	
39	d	1	Total	C	O	0
			37	27	10	
39	M	1	Total	C	O	0
			40	30	10	
39	m	1	Total	C	O	0
			40	30	10	

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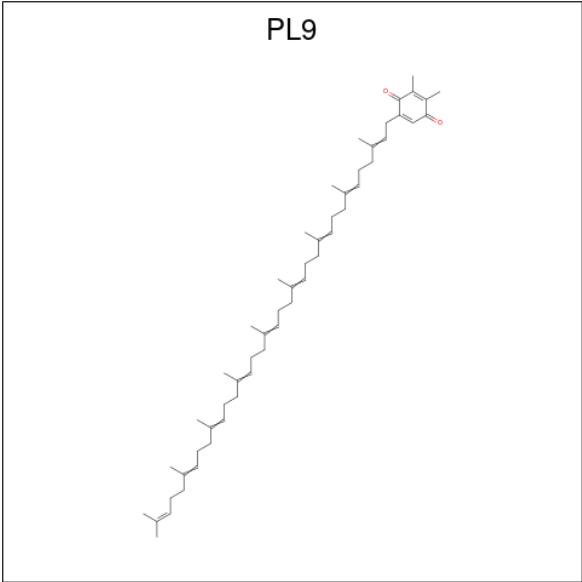
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Mol	Chain	Residues	Atoms			AltConf
39	W	1	Total	C	O	0
			48	38	10	
39	w	1	Total	C	O	0
			48	38	10	
39	3	1	Total	C	O	0
			31	21	10	
39	5	1	Total	C	O	0
			31	21	10	
39	7	1	Total	C	O	0
			55	45	10	
39	b	1	Total	C	O	0
			51	41	10	
39	b	1	Total	C	O	0
			28	18	10	
39	b	1	Total	C	O	0
			40	30	10	
39	Q	1	Total	C	O	0
			37	27	10	
39	q	1	Total	C	O	0
			46	36	10	
39	q	1	Total	C	O	0
			37	27	10	
39	0	1	Total	C	O	0
			42	32	10	

- Molecule 40 is FE (II) ION (CCD ID: FE2) (formula: Fe).

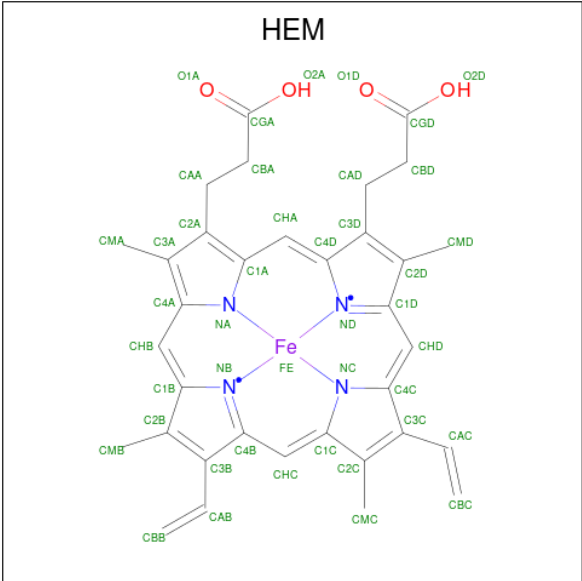
Mol	Chain	Residues	Atoms		AltConf
40	D	1	Total	Fe	0
			1	1	
40	d	1	Total	Fe	0
			1	1	

- Molecule 41 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



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

- Molecule 42 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



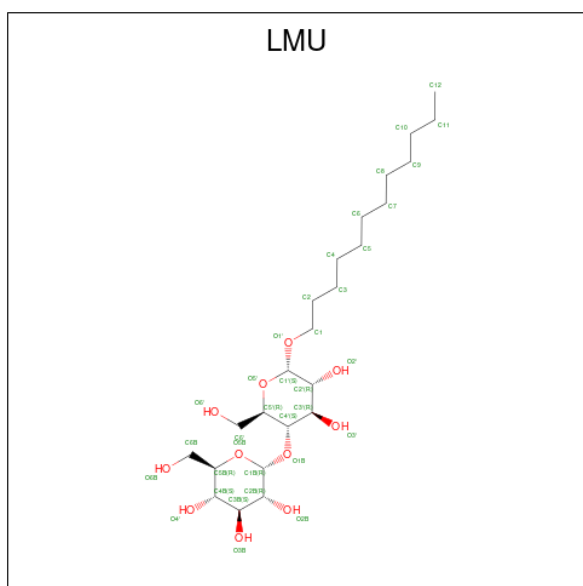
Mol	Chain	Residues	Atoms					AltConf
42	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 43 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
43	T	1	Total	C	O	0
			31	20	11	
43	t	1	Total	C	O	0
			31	20	11	
43	w	1	Total	C	O	0
			35	24	11	
43	3	1	Total	C	O	0
			35	24	11	
43	4	1	Total	C	O	0
			35	24	11	
43	5	1	Total	C	O	0
			31	20	11	

- Molecule 44 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
44	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
44	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
44	6	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 45 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).



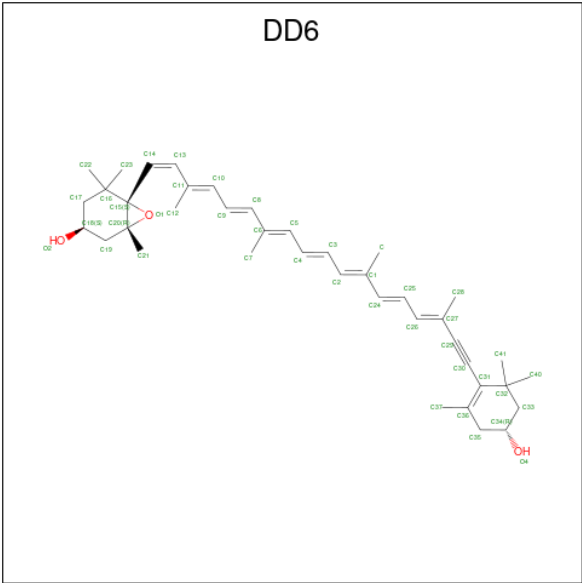
Mol	Chain	Residues	Atoms			AltConf
45	3	1	Total	C	O	0
			48	42	6	
45	4	1	Total	C	O	0
			48	42	6	
45	4	1	Total	C	O	0
			48	42	6	
45	4	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			47	41	6	
45	5	1	Total	C	O	0
			48	42	6	
45	5	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	6	1	Total	C	O	0
			48	42	6	
45	7	1	Total	C	O	0
			48	42	6	
45	7	1	Total	C	O	0
			48	42	6	
45	0	1	Total	C	O	0
			48	42	6	
45	0	1	Total	C	O	0
			48	42	6	
45	9	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	C	O	0
			48	42	6	
45	2	1	Total	C	O	0
			48	42	6	
45	2	1	Total	C	O	0
			48	42	6	
45	8	1	Total	C	O	0
			48	42	6	
45	8	1	Total	C	O	0
			48	42	6	
45	1	1	Total	C	O	0
			48	42	6	
45	1	1	Total	C	O	0
			48	42	6	

- Molecule 46 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: C₄₀H₅₄O₃).



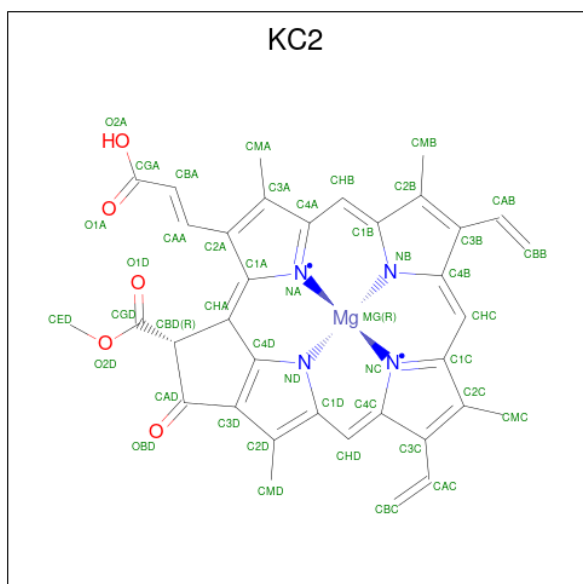
Mol	Chain	Residues	Atoms			AltConf
46	3	1	Total	C	O	0
			43	40	3	
46	4	1	Total	C	O	0
			43	40	3	
46	9	1	Total	C	O	0
			43	40	3	
46	9	1	Total	C	O	0
			43	40	3	

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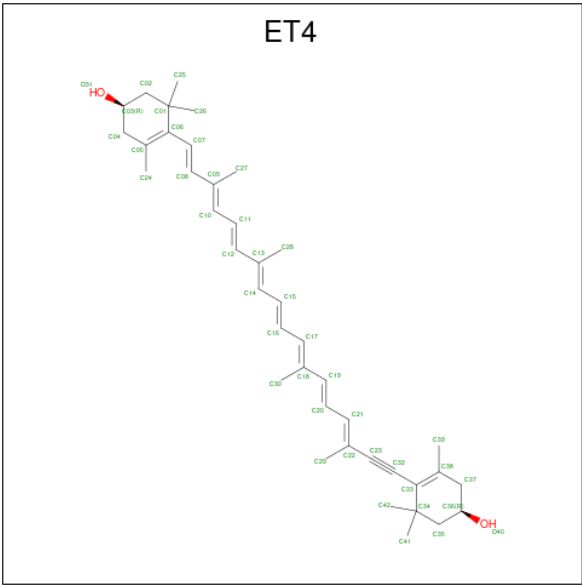
Mol	Chain	Residues	Atoms			AltConf
46	2	1	Total	C	O	0
			43	40	3	
46	2	1	Total	C	O	0
			43	40	3	
46	8	1	Total	C	O	0
			43	40	3	
46	8	1	Total	C	O	0
			43	40	3	
46	1	1	Total	C	O	0
			43	40	3	
46	1	1	Total	C	O	0
			43	40	3	

- Molecule 47 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
47	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 48 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: C₄₀H₅₄O₂).

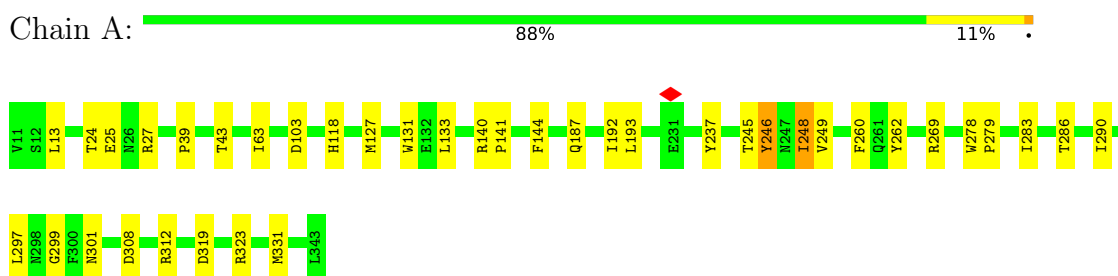


Mol	Chain	Residues	Atoms			AltConf
48	7	1	Total	C	O	0
			42	40	2	
48	0	1	Total	C	O	0
			42	40	2	

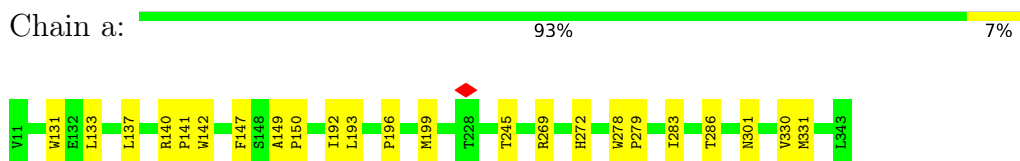
3 Residue-property plots

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.

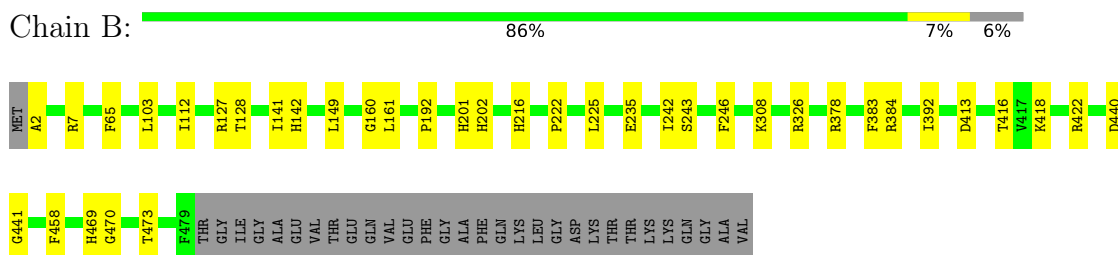
- Molecule 1: Photosystem II protein D1



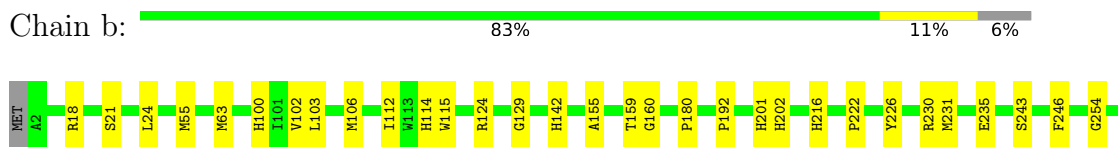
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



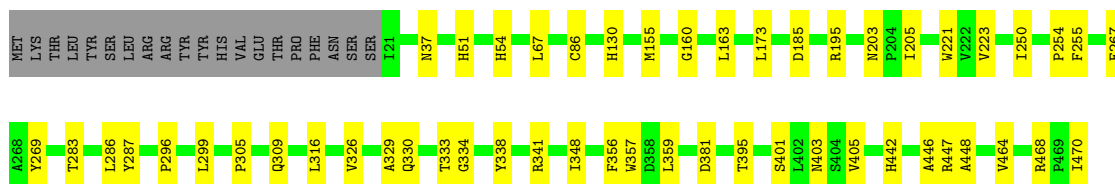
- Molecule 2: Photosystem II CP47 reaction center protein





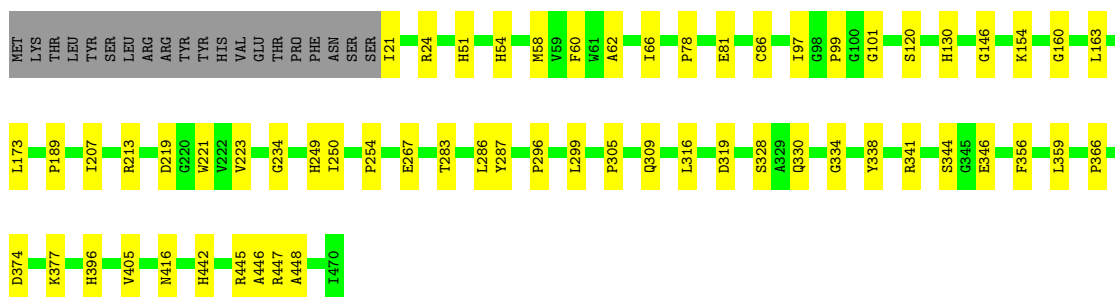
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 85% 11% .



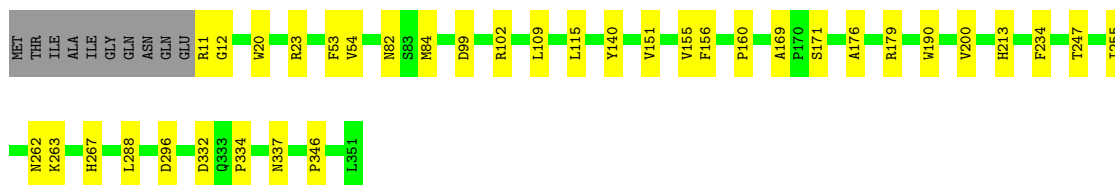
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 83% 13% .



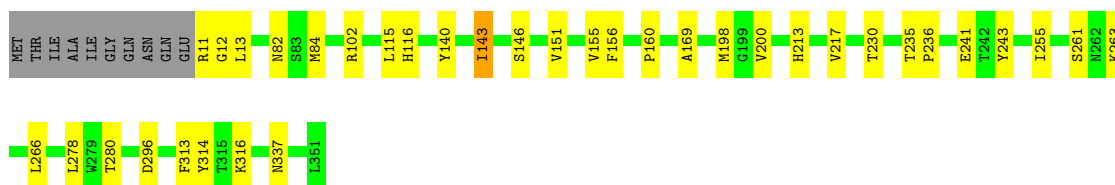
- Molecule 4: Photosystem II D2 protein

Chain D: 87% 10% .



- Molecule 4: Photosystem II D2 protein

Chain d: 87% 10% .



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  77% 13% 10%



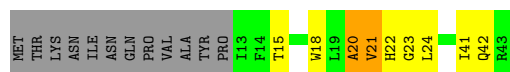
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  70% 20% 10%



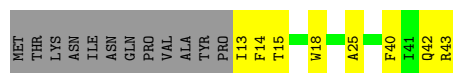
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  51% 16% 5% 28%



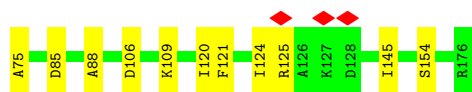
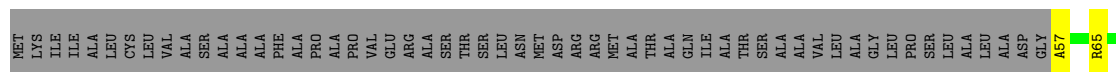
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  53% 19% 28%



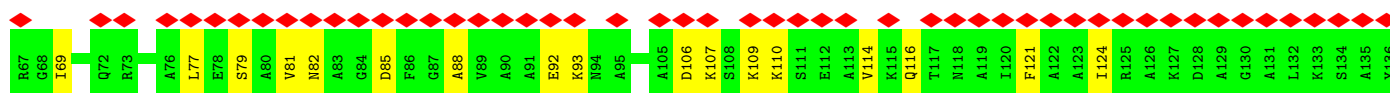
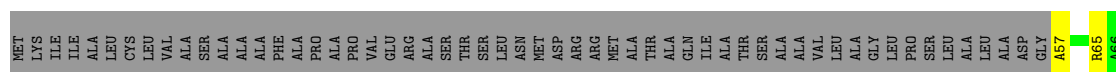
- Molecule 7: Photosystem II Psb31 protein domain-containing protein

Chain G:  61% 7% 32%



- Molecule 7: Photosystem II Psb31 protein domain-containing protein

Chain g:  44% 55% 14% 32%





• Molecule 8: Photosystem II reaction center protein H

Chain H: 88% 11% .



• Molecule 8: Photosystem II reaction center protein H

Chain h: 91% 8% .



• Molecule 9: Photosystem II reaction center protein I

Chain I: 91% 9%



• Molecule 9: Photosystem II reaction center protein I

Chain i: 85% 15%



• Molecule 10: Photosystem II reaction center protein J

Chain J: 67% 15% . 15%



• Molecule 10: Photosystem II reaction center protein J

Chain j: 77% 8% 15%



• Molecule 11: Photosystem II reaction center protein K

Chain K: 75% 9% 16%



- Molecule 11: Photosystem II reaction center protein K

Chain k: 73% 11% 16%



- Molecule 12: Photosystem II reaction center protein L

Chain L: 95% . .



- Molecule 12: Photosystem II reaction center protein L

Chain l: 87% 11% .



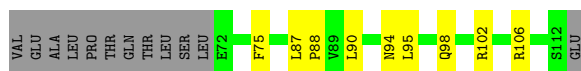
- Molecule 13: Photosystem II reaction center M protein, plastid

Chain M: 27% 9% 64%



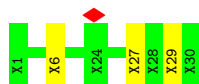
- Molecule 13: Photosystem II reaction center M protein, plastid

Chain m: 28% 8% 64%



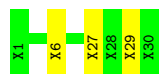
- Molecule 14: Photosystem II subunit, PsbN.

Chain n: 90% 10%



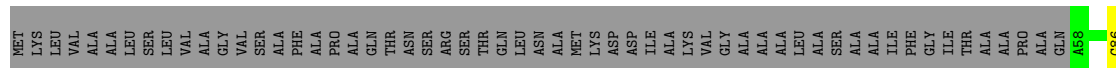
- Molecule 14: Photosystem II subunit, PsbN.

Chain N:  90% 10%



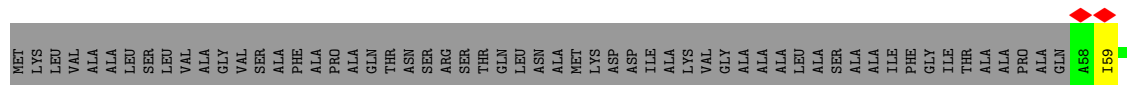
- Molecule 15: Oxygen-evolving enhancer protein 1

Chain O:  72% 10% 19%



- Molecule 15: Oxygen-evolving enhancer protein 1

Chain o:  69% 13% 19%



- Molecule 16: Photosystem II reaction center protein T

Chain T:  93% 7%



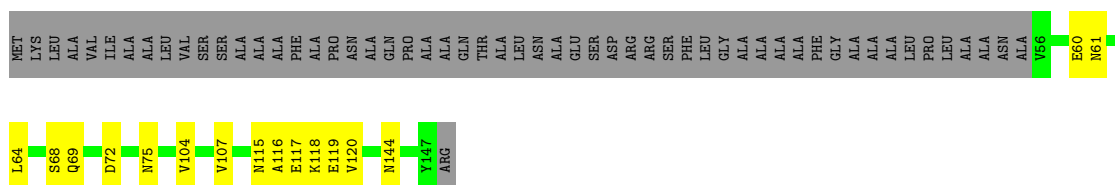
- Molecule 16: Photosystem II reaction center protein T

Chain t:  100%

There are no outlier residues recorded for this chain.

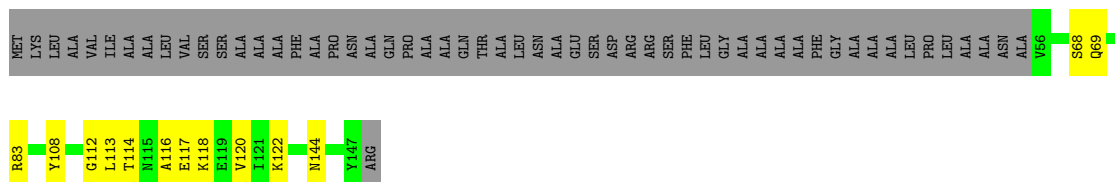
- Molecule 17: PS II complex 12 kDa extrinsic protein

Chain U:  51% 11% 38%



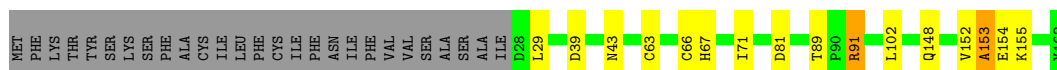
- Molecule 17: PS II complex 12 kDa extrinsic protein

Chain u: 53% 9% 38%



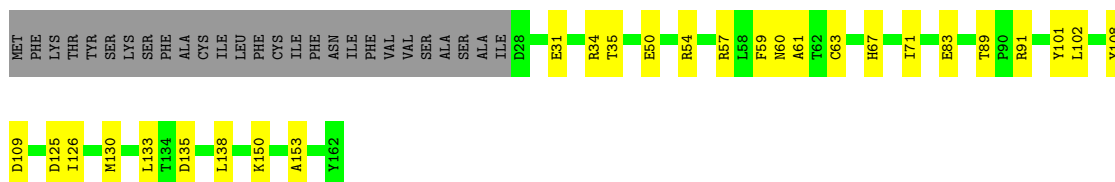
- Molecule 18: Cytochrome c-550

Chain V: 73% 9% 17%



- Molecule 18: Cytochrome c-550

Chain v: 67% 17% 17%



- Molecule 19: Photosystem II subunit, PsbW

Chain W: 91% 9%



- Molecule 19: Photosystem II subunit, PsbW

Chain w: 91% 9%



- Molecule 20: Photosystem II reaction center X protein

Chain X:  74% 18% 8%



- Molecule 20: Photosystem II reaction center X protein

Chain x:  82% 11% 8%



- Molecule 21: Photosystem II reaction center protein Z

Chain Z:  93% 7%



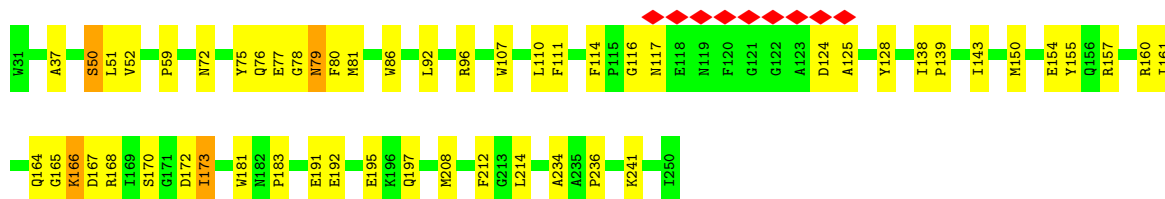
- Molecule 21: Photosystem II reaction center protein Z

Chain z:  5% 89% 11%



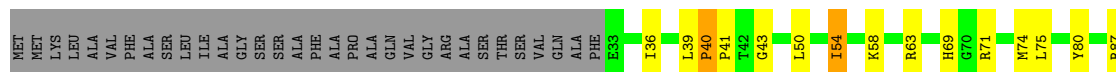
- Molecule 22: Fucoxanthin chl a/c protein, lhca clade

Chain 3:  75% 23% 2%

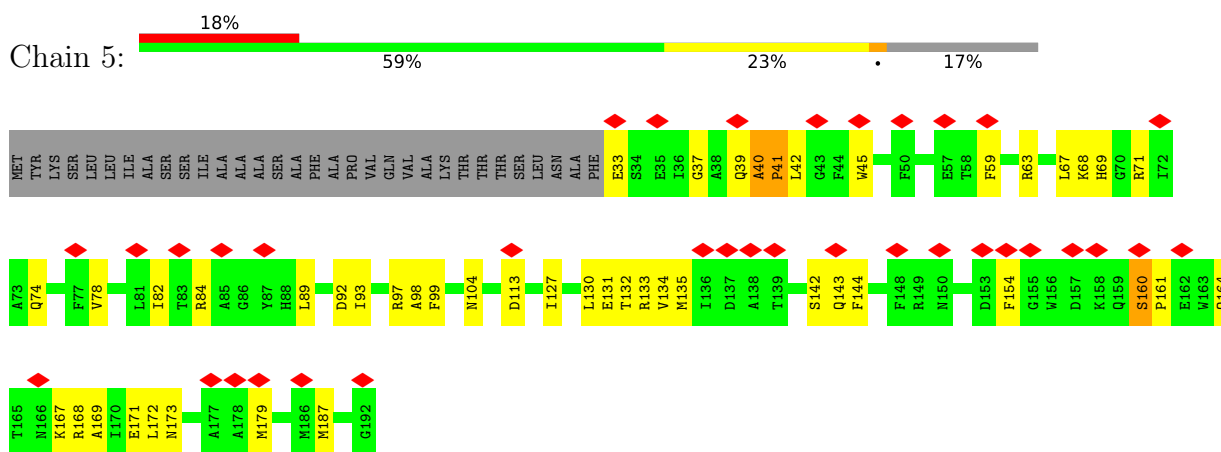


- Molecule 23: Fucoxanthin-chlorophyll a-c binding protein, plastid

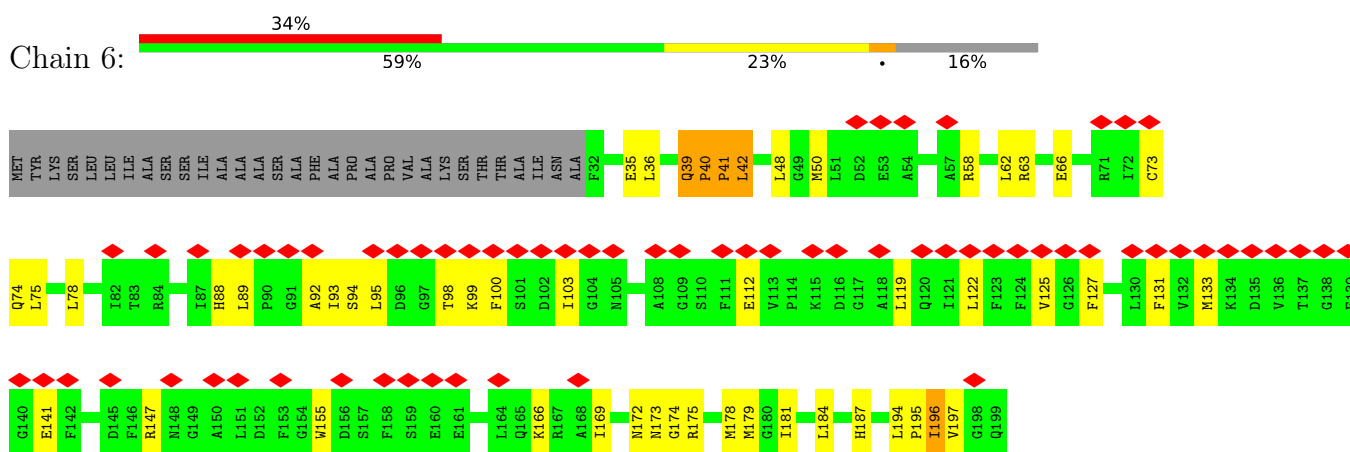
Chain 4:  62% 18% 17%



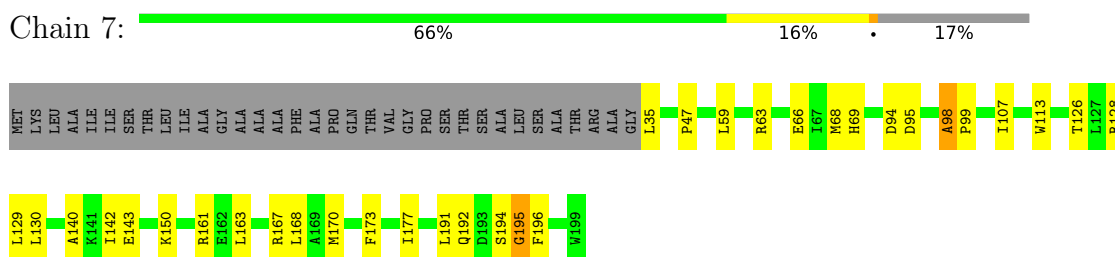
- Molecule 24: Fucoxanthin chlorophyll a/c protein 6



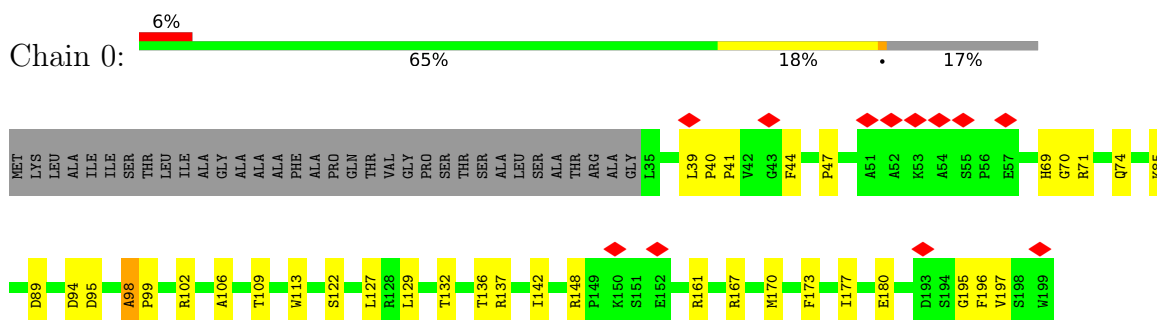
• Molecule 25: Fucoxanthin chlorophyll a/c protein 5



• Molecule 26: Fucoxanthin chlorophyll a/c protein-LI818 clade



• Molecule 26: Fucoxanthin chlorophyll a/c protein-LI818 clade



• Molecule 27: Photosystem II reaction center protein Ycf12

Chain Y:  91% 9%



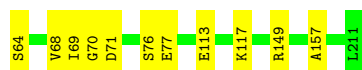
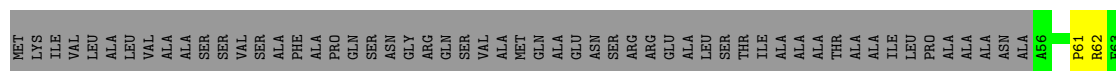
- Molecule 27: Photosystem II reaction center protein Ycf12

Chain y:  88% 12%



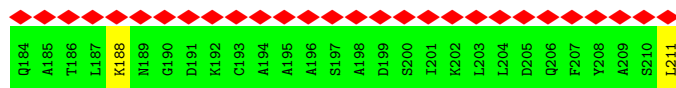
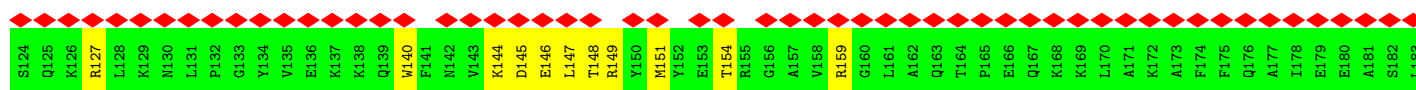
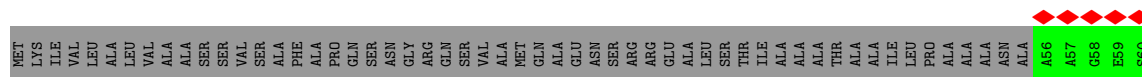
- Molecule 28: Photosystem II subunit, PsbQ.

Chain Q:  68% 6% 26%



- Molecule 28: Photosystem II subunit, PsbQ.

Chain q:  66% 60% 14% 26%



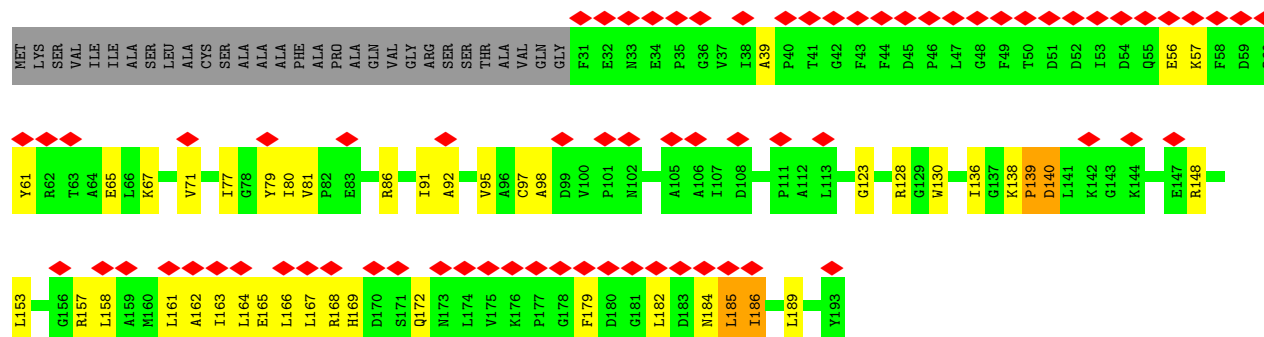
- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type

Chain 9:  60% 23% 16%

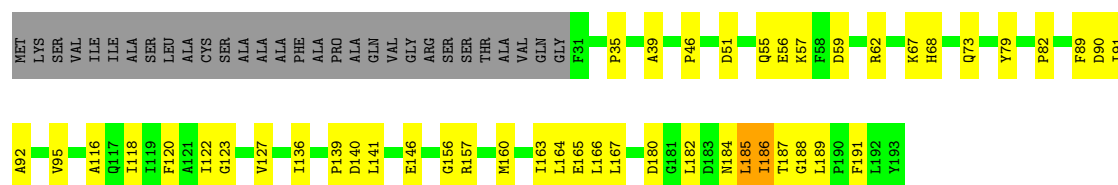




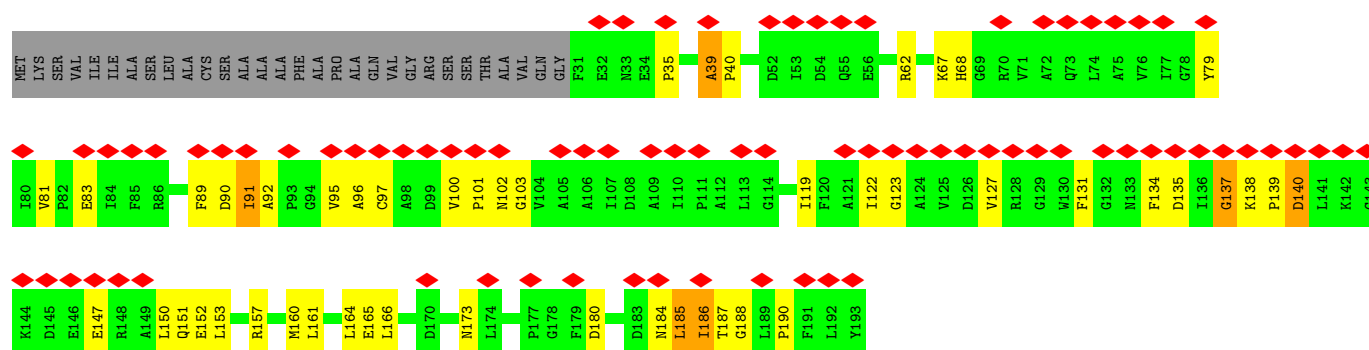
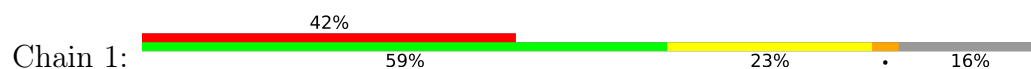
- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type



- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type



- Molecule 29: Fucoxanthin chlorophyll a/c light-harvesting protein, major type



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97098	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.719	Depositor
Minimum map value	-0.241	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.088	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, A86, KC1, LMU, HEM, FE2, DGD, DD6, PL9, LMG, BCT, LHG, KC2, PHO, BCR, SQD, OEX, CL, ET4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/2697	0.39	1/3674 (0.0%)
1	a	0.22	0/2697	0.35	0/3674
2	B	0.25	0/3901	0.33	0/5308
2	b	0.22	0/3901	0.29	0/5308
3	C	0.22	0/3604	0.32	0/4909
3	c	0.20	0/3604	0.31	0/4909
4	D	0.22	0/2791	0.32	0/3804
4	d	0.27	0/2791	0.43	2/3804 (0.1%)
5	E	0.17	0/644	0.29	0/878
5	e	0.16	0/644	0.32	0/878
6	F	0.41	0/261	0.61	0/352
6	f	0.16	0/261	0.29	0/352
7	G	0.11	0/900	0.26	0/1207
7	g	0.11	0/900	0.26	0/1207
8	H	0.19	0/522	0.29	0/712
8	h	0.19	0/522	0.29	0/712
9	I	0.24	0/286	0.32	0/386
9	i	0.19	0/286	0.31	0/386
10	J	0.40	0/249	0.69	1/339 (0.3%)
10	j	0.11	0/249	0.27	0/339
11	K	0.23	0/315	0.44	0/432
11	k	0.22	0/315	0.38	0/432
12	L	0.33	0/311	0.40	0/423
12	l	0.20	0/311	0.23	0/423
13	M	0.19	0/322	0.27	0/435
13	m	0.19	0/322	0.28	0/435
15	O	0.32	0/1896	0.46	0/2549
15	o	0.32	0/1896	0.45	0/2549
16	T	0.19	0/239	0.24	0/323
16	t	0.17	0/239	0.23	0/323
17	U	0.19	0/722	0.34	0/982

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	u	0.28	0/722	0.40	0/982
18	V	0.31	0/1047	0.43	0/1422
18	v	0.34	0/1047	0.46	0/1422
19	W	0.22	0/446	0.32	0/606
19	w	0.18	0/446	0.29	0/606
20	X	0.18	0/248	0.25	0/336
20	x	0.18	0/248	0.26	0/336
21	Z	0.15	0/461	0.26	0/633
21	z	0.12	0/461	0.28	0/633
22	3	0.26	0/1765	0.41	0/2405
23	4	0.35	0/1282	0.56	2/1746 (0.1%)
24	5	0.24	0/1255	0.39	1/1696 (0.1%)
25	6	0.37	1/1324 (0.1%)	0.62	1/1780 (0.1%)
26	0	0.15	0/1298	0.35	0/1764
26	7	0.29	0/1298	0.46	1/1764 (0.1%)
27	Y	0.15	0/253	0.31	0/341
27	y	0.11	0/253	0.23	0/341
28	Q	0.15	0/1220	0.27	0/1638
28	q	0.23	0/1220	0.41	0/1638
29	1	0.29	0/1237	0.47	0/1687
29	2	0.31	0/1246	0.53	1/1700 (0.1%)
29	8	0.29	0/1237	0.50	0/1687
29	9	0.32	0/1246	0.49	1/1700 (0.1%)
All	All	0.25	1/59858 (0.0%)	0.39	11/81307 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	39	GLN	N-CA	5.18	1.49	1.46

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	40	PRO	N-CA-C	10.12	123.04	110.70
23	4	40	PRO	N-CA-C	9.97	122.86	110.70
1	A	248	ILE	N-CA-C	9.52	120.13	110.23
29	2	136	ILE	N-CA-C	-7.48	104.20	112.80
24	5	41	PRO	N-CA-CB	6.03	109.58	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2614	0	2513	35	0
1	a	2614	0	2513	20	0
2	B	3772	0	3654	39	0
2	b	3772	0	3654	40	0
3	C	3489	0	3398	46	0
3	c	3489	0	3398	51	0
4	D	2699	0	2600	30	0
4	d	2699	0	2600	40	0
5	E	626	0	610	12	0
5	e	626	0	610	14	0
6	F	253	0	259	9	0
6	f	253	0	259	8	0
7	G	890	0	896	11	0
7	g	890	0	896	16	0
8	H	512	0	540	8	0
8	h	512	0	540	4	0
9	I	279	0	293	2	0
9	i	279	0	293	4	0
10	J	243	0	253	5	0
10	j	243	0	253	2	0
11	K	303	0	310	4	0
11	k	303	0	310	4	0
12	L	302	0	301	1	0
12	l	302	0	301	4	0
13	M	317	0	323	11	0
13	m	317	0	323	13	0
14	N	150	0	34	2	0
14	n	150	0	34	2	0
15	O	1867	0	1862	18	0
15	o	1867	0	1862	27	0
16	T	233	0	244	2	0
16	t	233	0	244	0	0
17	U	708	0	707	11	0
17	u	708	0	707	10	0
18	V	1029	0	1028	15	0
18	v	1029	0	1028	33	0
19	W	434	0	383	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	w	434	0	383	8	0
20	X	248	0	278	4	0
20	x	248	0	278	3	0
21	Z	453	0	482	3	0
21	z	453	0	482	5	0
22	3	1710	0	1623	59	0
23	4	1249	0	1219	55	0
24	5	1229	0	1184	47	0
25	6	1296	0	1269	64	0
26	0	1269	0	1261	26	0
26	7	1269	0	1262	29	0
27	Y	251	0	289	3	0
27	y	251	0	289	2	0
28	Q	1198	0	1175	9	0
28	q	1198	0	1175	37	0
29	1	1206	0	1119	43	0
29	2	1214	0	1138	40	0
29	8	1206	0	1120	41	0
29	9	1214	0	1137	44	0
30	A	80	0	112	6	0
30	B	120	0	168	6	0
30	C	80	0	112	6	0
30	D	40	0	56	1	0
30	H	40	0	56	1	0
30	K	80	0	112	9	0
30	a	80	0	112	6	0
30	b	120	0	168	7	0
30	c	80	0	112	6	0
30	d	40	0	56	1	0
30	h	40	0	56	5	0
30	k	80	0	112	7	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	0	478	0	445	16	0
33	1	543	0	422	23	0
33	2	598	0	471	32	0
33	3	702	0	698	35	0
33	4	603	0	556	36	0
33	5	401	0	340	44	0
33	6	396	0	328	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	7	521	0	475	23	0
33	8	543	0	422	21	0
33	9	598	0	471	19	0
33	A	174	0	170	2	0
33	B	987	0	1039	26	0
33	C	806	0	853	19	0
33	D	176	0	164	3	0
33	H	43	0	30	3	0
33	W	65	0	72	6	0
33	Z	51	0	41	1	0
33	a	174	0	170	0	0
33	b	987	0	1039	29	0
33	c	806	0	853	22	0
33	d	176	0	164	6	0
33	w	65	0	72	5	0
33	z	51	0	41	1	0
34	A	128	0	148	2	0
34	a	128	0	148	2	0
35	A	4	0	1	2	0
35	a	4	0	1	3	0
36	0	28	0	29	0	0
36	3	76	0	98	2	0
36	4	49	0	74	2	0
36	5	33	0	42	1	0
36	7	28	0	29	1	0
36	A	141	0	207	4	0
36	D	90	0	128	1	0
36	H	42	0	54	0	0
36	W	35	0	40	2	0
36	a	92	0	133	2	0
36	b	49	0	74	0	0
36	d	90	0	128	1	0
36	h	42	0	54	2	0
36	w	35	0	40	0	0
37	0	48	0	63	1	0
37	7	48	0	62	0	0
37	A	40	0	44	0	0
37	B	54	0	78	3	0
37	D	54	0	77	2	0
37	L	54	0	78	2	0
37	T	94	0	125	2	0
37	a	54	0	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	i	40	0	44	1	0
37	l	54	0	78	2	0
37	t	40	0	47	2	0
38	3	39	0	62	3	0
38	A	53	0	64	3	0
38	C	166	0	206	7	0
38	H	62	0	82	0	0
38	a	53	0	64	2	0
38	c	166	0	206	10	0
38	h	62	0	82	1	0
39	0	42	0	54	2	0
39	3	31	0	32	0	0
39	5	31	0	32	0	0
39	7	55	0	86	1	0
39	B	79	0	98	0	0
39	C	144	0	168	3	0
39	D	86	0	112	2	0
39	M	40	0	50	1	0
39	Q	37	0	44	0	0
39	W	48	0	66	2	0
39	b	119	0	148	6	0
39	c	75	0	90	4	0
39	d	83	0	106	4	0
39	m	40	0	50	2	0
39	q	83	0	106	5	0
39	w	48	0	66	1	0
40	D	1	0	0	0	0
40	d	1	0	0	0	0
41	D	55	0	80	0	0
41	d	55	0	80	1	0
42	F	43	0	30	9	0
42	V	43	0	30	2	0
42	e	43	0	30	4	0
42	v	43	0	30	5	0
43	3	35	0	46	5	0
43	4	35	0	46	13	0
43	5	31	0	35	11	0
43	T	31	0	35	1	0
43	t	31	0	35	1	0
43	w	35	0	46	5	0
44	3	45	0	0	0	0
44	5	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	6	45	0	0	6	0
45	0	96	0	0	1	0
45	1	96	0	0	8	0
45	2	96	0	0	7	0
45	3	48	0	0	2	0
45	4	144	0	0	11	0
45	5	335	0	0	31	0
45	6	288	0	0	18	0
45	7	96	0	0	2	0
45	8	96	0	0	3	0
45	9	96	0	0	1	0
46	1	86	0	0	5	0
46	2	86	0	0	19	0
46	3	43	0	0	1	0
46	4	43	0	0	1	0
46	8	86	0	0	8	0
46	9	86	0	0	5	0
47	0	45	0	0	0	0
47	4	45	0	0	2	0
47	5	45	0	0	16	0
47	6	45	0	0	0	0
47	7	45	0	0	0	0
48	0	42	0	0	2	0
48	7	42	0	0	2	0
All	All	75511	0	72563	1313	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 1313 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)
2:B:243:SER:HA	2:B:246:PHE:CE1	1.47	1.47
25:6:179:MET:SD	45:6:301:A86:C8	2.21	1.28
29:2:158:LEU:HD11	46:2:304:DD6:C	1.72	1.20
18:v:89:THR:OG1	18:v:109:ASP:HA	1.40	1.20
25:6:179:MET:HE1	45:6:301:A86:C10	1.71	1.19

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	331/333 (99%)	311 (94%)	19 (6%)	1 (0%)	36	57
1	a	331/333 (99%)	314 (95%)	17 (5%)	0	100	100
2	B	476/509 (94%)	463 (97%)	13 (3%)	0	100	100
2	b	476/509 (94%)	464 (98%)	12 (2%)	0	100	100
3	C	448/470 (95%)	430 (96%)	18 (4%)	0	100	100
3	c	448/470 (95%)	433 (97%)	15 (3%)	0	100	100
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	74/84 (88%)	69 (93%)	5 (7%)	0	100	100
5	e	74/84 (88%)	71 (96%)	3 (4%)	0	100	100
6	F	29/43 (67%)	26 (90%)	0	3 (10%)	0	0
6	f	29/43 (67%)	29 (100%)	0	0	100	100
7	G	118/176 (67%)	108 (92%)	10 (8%)	0	100	100
7	g	118/176 (67%)	108 (92%)	10 (8%)	0	100	100
8	H	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
8	h	63/66 (96%)	56 (89%)	7 (11%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
9	i	32/34 (94%)	32 (100%)	0	0	100	100
10	J	31/39 (80%)	29 (94%)	2 (6%)	0	100	100
10	j	31/39 (80%)	29 (94%)	2 (6%)	0	100	100
11	K	35/44 (80%)	34 (97%)	1 (3%)	0	100	100
11	k	35/44 (80%)	34 (97%)	1 (3%)	0	100	100
12	L	35/38 (92%)	35 (100%)	0	0	100	100
12	l	35/38 (92%)	35 (100%)	0	0	100	100
13	M	39/113 (34%)	39 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	39/113 (34%)	38 (97%)	1 (3%)	0	100	100
15	O	246/305 (81%)	230 (94%)	14 (6%)	2 (1%)	16	34
15	o	246/305 (81%)	228 (93%)	16 (6%)	2 (1%)	16	34
16	T	26/28 (93%)	26 (100%)	0	0	100	100
16	t	26/28 (93%)	26 (100%)	0	0	100	100
17	U	90/148 (61%)	88 (98%)	2 (2%)	0	100	100
17	u	90/148 (61%)	82 (91%)	8 (9%)	0	100	100
18	V	133/162 (82%)	125 (94%)	6 (4%)	2 (2%)	8	19
18	v	133/162 (82%)	123 (92%)	7 (5%)	3 (2%)	5	11
19	W	52/54 (96%)	47 (90%)	5 (10%)	0	100	100
19	w	52/54 (96%)	49 (94%)	3 (6%)	0	100	100
20	X	33/38 (87%)	31 (94%)	1 (3%)	1 (3%)	3	7
20	x	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
21	Z	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
21	z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
22	3	218/220 (99%)	186 (85%)	27 (12%)	5 (2%)	5	11
23	4	161/196 (82%)	139 (86%)	16 (10%)	6 (4%)	2	5
24	5	158/192 (82%)	137 (87%)	18 (11%)	3 (2%)	6	15
25	6	166/199 (83%)	136 (82%)	27 (16%)	3 (2%)	6	15
26	0	163/199 (82%)	148 (91%)	13 (8%)	2 (1%)	10	24
26	7	163/199 (82%)	148 (91%)	13 (8%)	2 (1%)	10	24
27	Y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
27	y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
28	Q	154/211 (73%)	145 (94%)	9 (6%)	0	100	100
28	q	154/211 (73%)	144 (94%)	10 (6%)	0	100	100
29	1	161/193 (83%)	128 (80%)	26 (16%)	7 (4%)	2	4
29	2	161/193 (83%)	141 (88%)	14 (9%)	6 (4%)	2	5
29	8	161/193 (83%)	144 (89%)	13 (8%)	4 (2%)	4	10
29	9	161/193 (83%)	138 (86%)	17 (11%)	6 (4%)	2	5
All	All	7423/8659 (86%)	6918 (93%)	447 (6%)	58 (1%)	18	34

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	4	99	THR
24	5	41	PRO
25	6	42	LEU
25	6	196	ILE
29	9	39	ALA

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 347 ligands modelled in this entry, 4 are monoatomic - leaving 343 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	$\# Z > 2$
39	LMG	B	621	-	28,28,55	0.97	0	36,36,63	1.31	4 (11%)
33	CLA	c	506	-	49,53,73	1.36	9 (18%)	58,89,113	1.41	5 (8%)
36	LHG	w	301	-	34,34,48	0.75	2 (5%)	37,40,54	1.26	4 (10%)
33	CLA	9	314	-	40,46,73	1.47	9 (22%)	52,80,113	1.45	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	c	508	-	69,73,73	1.15	9 (13%)	82,113,113	1.23	5 (6%)
33	CLA	C	502	-	68,72,73	1.17	10 (14%)	80,111,113	1.24	5 (6%)
33	CLA	4	315	-	51,55,73	1.35	8 (15%)	60,91,113	1.43	6 (10%)
45	A86	4	301	-	47,50,50	1.54	6 (12%)	51,76,76	2.55	16 (31%)
33	CLA	2	312	-	49,53,73	1.40	9 (18%)	58,89,113	1.41	4 (6%)
36	LHG	3	317	33	26,26,48	0.86	1 (3%)	29,32,54	1.35	4 (13%)
33	CLA	6	315	-	45,49,73	1.41	8 (17%)	54,84,113	1.50	5 (9%)
33	CLA	c	507	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
33	CLA	b	605	-	65,69,73	1.19	9 (13%)	77,108,113	1.35	8 (10%)
33	CLA	B	604	-	65,69,73	1.19	8 (12%)	77,108,113	1.34	7 (9%)
39	LMG	C	520	-	48,48,55	0.81	1 (2%)	56,56,63	1.34	6 (10%)
30	BCR	k	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
38	DGD	C	518	-	56,56,67	0.99	2 (3%)	70,70,81	1.40	9 (12%)
33	CLA	3	302	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
45	A86	6	306	-	47,50,50	1.43	5 (10%)	51,76,76	7.47	22 (43%)
33	CLA	4	306	23	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
33	CLA	2	305	-	45,49,73	1.43	8 (17%)	54,84,113	1.44	6 (11%)
46	DD6	2	304	-	40,45,45	1.56	2 (5%)	51,67,67	2.18	12 (23%)
33	CLA	B	615	-	69,73,73	1.17	9 (13%)	82,113,113	1.22	5 (6%)
33	CLA	5	317	-	40,46,73	1.47	7 (17%)	52,80,113	1.47	5 (9%)
33	CLA	4	313	23	45,49,73	1.40	8 (17%)	54,84,113	1.48	5 (9%)
33	CLA	2	308	-	59,63,73	1.26	7 (11%)	70,101,113	1.34	6 (8%)
39	LMG	B	620	-	51,51,55	0.75	1 (1%)	59,59,63	1.36	6 (10%)
36	LHG	H	104	-	41,41,48	0.68	1 (2%)	44,47,54	1.33	5 (11%)
33	CLA	B	606	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	7 (8%)
33	CLA	C	513	-	53,57,73	1.30	9 (16%)	61,93,113	1.45	8 (13%)
45	A86	4	304	-	47,50,50	1.46	5 (10%)	51,76,76	2.51	18 (35%)
45	A86	1	301	-	47,50,50	1.45	6 (12%)	51,76,76	2.35	15 (29%)
33	CLA	2	309	-	48,51,73	1.47	10 (20%)	56,86,113	1.52	6 (10%)
33	CLA	a	407	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	5 (6%)
39	LMG	q	302	-	37,37,55	0.84	1 (2%)	45,45,63	1.28	5 (11%)
30	BCR	k	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.24	7 (12%)
34	PHO	A	406	-	58,69,69	2.09	10 (17%)	55,99,99	1.48	7 (12%)
33	CLA	B	614	-	68,72,73	1.15	9 (13%)	80,111,113	1.26	6 (7%)
46	DD6	9	304	-	40,45,45	1.56	2 (5%)	51,67,67	2.18	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	3	309	36	55,59,73	1.30	9 (16%)	64,96,113	1.37	6 (9%)
33	CLA	3	311	-	45,49,73	1.40	9 (20%)	54,84,113	1.50	5 (9%)
45	A86	6	304	-	47,50,50	1.46	5 (10%)	51,76,76	11.60	22 (43%)
33	CLA	b	606	-	69,73,73	1.15	9 (13%)	82,113,113	1.17	5 (6%)
30	BCR	b	620	-	41,41,41	1.19	4 (9%)	56,56,56	1.22	5 (8%)
39	LMG	q	301	-	46,46,55	0.76	1 (2%)	54,54,63	1.33	6 (11%)
36	LHG	h	103	-	41,41,48	0.70	1 (2%)	44,47,54	1.33	5 (11%)
33	CLA	b	611	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
33	CLA	C	508	-	69,73,73	1.14	9 (13%)	82,113,113	1.25	7 (8%)
33	CLA	9	309	29	48,51,73	1.48	10 (20%)	56,86,113	1.52	5 (8%)
30	BCR	c	515	-	41,41,41	0.81	1 (2%)	56,56,56	1.98	14 (25%)
45	A86	5	304	-	47,50,50	1.46	5 (10%)	51,76,76	10.37	24 (47%)
37	SQD	L	101	-	52,54,54	0.96	4 (7%)	62,65,65	1.44	9 (14%)
33	CLA	C	507	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	5 (6%)
33	CLA	c	511	3	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
33	CLA	1	309	-	48,51,73	1.49	9 (18%)	56,86,113	1.50	6 (10%)
38	DGD	3	320	-	38,38,67	0.65	1 (2%)	40,40,81	1.51	6 (15%)
45	A86	6	303	-	47,50,50	1.49	6 (12%)	51,76,76	8.05	26 (50%)
47	KC2	6	309	-	49,53,53	1.74	9 (18%)	60,89,89	1.99	14 (23%)
33	CLA	C	505	-	69,73,73	1.16	9 (13%)	82,113,113	1.17	6 (7%)
30	BCR	B	617	-	41,41,41	1.23	3 (7%)	56,56,56	1.23	7 (12%)
33	CLA	3	304	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
38	DGD	A	415	-	54,54,67	0.99	3 (5%)	67,67,81	1.46	12 (17%)
31	OEX	A	402	1,3	0,15,15	-	-	-	-	-
30	BCR	A	409	-	41,41,41	1.18	3 (7%)	56,56,56	1.16	4 (7%)
33	CLA	8	311	29	59,63,73	1.26	9 (15%)	70,101,113	1.32	6 (8%)
36	LHG	W	302	-	34,34,48	0.76	2 (5%)	37,40,54	1.25	4 (10%)
41	PL9	D	408	-	55,55,55	1.34	5 (9%)	68,69,69	1.47	12 (17%)
33	CLA	5	309	24	59,63,73	1.26	8 (13%)	70,101,113	1.36	6 (8%)
45	A86	2	302	-	47,50,50	1.55	7 (14%)	51,76,76	2.68	19 (37%)
36	LHG	A	414	-	48,48,48	0.67	1 (2%)	51,54,54	1.29	6 (11%)
39	LMG	C	519	-	46,46,55	0.77	1 (2%)	54,54,63	1.38	7 (12%)
33	CLA	9	307	-	48,52,73	1.48	8 (16%)	59,88,113	1.40	5 (8%)
33	CLA	8	306	29	49,53,73	1.37	9 (18%)	58,89,113	1.44	6 (10%)
37	SQD	l	101	-	52,54,54	0.96	4 (7%)	62,65,65	1.40	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	3	308	22	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
36	LHG	D	411	-	41,41,48	0.66	1 (2%)	44,47,54	1.31	4 (9%)
39	LMG	b	622	-	28,28,55	0.98	0	36,36,63	1.31	5 (13%)
39	LMG	C	522	-	23,23,55	1.36	3 (13%)	31,31,63	1.51	7 (22%)
48	ET4	0	302	-	41,43,43	2.09	13 (31%)	52,60,60	2.45	18 (34%)
45	A86	9	302	-	47,50,50	1.55	7 (14%)	51,76,76	2.68	19 (37%)
38	DGD	c	517	-	57,57,67	0.96	2 (3%)	71,71,81	1.46	12 (16%)
33	CLA	7	310	26	49,53,73	1.38	8 (16%)	58,89,113	1.43	6 (10%)
38	DGD	c	516	-	56,56,67	0.96	2 (3%)	70,70,81	1.45	11 (15%)
33	CLA	b	602	-	51,55,73	1.31	9 (17%)	60,91,113	1.43	5 (8%)
47	KC2	4	307	-	49,53,53	1.59	10 (20%)	60,89,89	2.28	17 (28%)
33	CLA	8	305	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	5 (9%)
33	CLA	8	308	-	59,63,73	1.25	8 (13%)	70,101,113	1.41	7 (10%)
43	LMU	T	102	-	32,32,36	0.35	0	43,43,47	0.85	0
33	CLA	1	308	-	59,63,73	1.26	6 (10%)	70,101,113	1.36	7 (10%)
33	CLA	b	604	-	68,72,73	1.15	9 (13%)	80,111,113	1.24	6 (7%)
36	LHG	A	411	-	42,42,48	0.70	1 (2%)	45,48,54	1.23	4 (8%)
33	CLA	3	313	-	65,69,73	1.20	8 (12%)	77,108,113	1.27	5 (6%)
36	LHG	D	409	-	44,47,48	0.57	1 (2%)	44,51,54	1.18	5 (11%)
45	A86	6	305	-	47,50,50	1.47	6 (12%)	51,76,76	9.14	23 (45%)
33	CLA	B	602	-	64,69,73	1.17	9 (14%)	73,106,113	1.23	6 (8%)
45	A86	4	302	-	47,50,50	1.46	6 (12%)	51,76,76	12.38	29 (56%)
33	CLA	4	308	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
33	CLA	b	613	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	8 (9%)
37	SQD	A	413	-	38,40,54	1.12	3 (7%)	48,51,65	1.69	11 (22%)
36	LHG	a	403	-	42,42,48	0.69	1 (2%)	45,48,54	1.24	5 (11%)
43	LMU	4	317	-	36,36,36	0.38	0	47,47,47	0.87	2 (4%)
46	DD6	9	303	-	40,45,45	1.59	2 (5%)	51,67,67	2.20	13 (25%)
33	CLA	2	311	29	59,63,73	1.26	8 (13%)	70,101,113	1.31	4 (5%)
33	CLA	4	309	23	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
33	CLA	4	311	23	64,68,73	1.20	9 (14%)	76,107,113	1.27	5 (6%)
45	A86	7	301	-	47,50,50	1.62	8 (17%)	51,76,76	2.60	19 (37%)
39	LMG	m	201	-	40,40,55	0.86	2 (5%)	48,48,63	1.29	5 (10%)
39	LMG	Q	301	-	37,37,55	0.87	1 (2%)	45,45,63	1.27	4 (8%)
30	BCR	C	515	-	41,41,41	0.76	0	56,56,56	1.90	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	6	316	-	41,46,73	1.66	6 (14%)	50,79,113	1.60	8 (16%)
45	A86	5	306	-	47,50,50	1.47	6 (12%)	51,76,76	7.76	25 (49%)
33	CLA	3	312	-	60,64,73	1.26	8 (13%)	71,102,113	1.33	5 (7%)
33	CLA	a	408	-	53,57,73	1.30	9 (16%)	61,93,113	1.45	6 (9%)
37	SQD	B	622	-	52,54,54	0.96	4 (7%)	62,65,65	1.71	10 (16%)
36	LHG	4	318	-	48,48,48	0.58	0	51,54,54	1.28	6 (11%)
37	SQD	t	102	-	38,40,54	1.15	3 (7%)	48,51,65	1.96	12 (25%)
33	CLA	d	402	-	64,68,73	1.19	8 (12%)	76,107,113	1.39	7 (9%)
36	LHG	b	601	-	48,48,48	0.66	1 (2%)	51,54,54	1.30	6 (11%)
37	SQD	i	101	-	38,40,54	1.12	3 (7%)	48,51,65	1.66	10 (20%)
33	CLA	1	305	-	45,49,73	1.42	8 (17%)	54,84,113	1.47	5 (9%)
33	CLA	9	316	29	40,46,73	1.48	8 (20%)	52,80,113	1.48	5 (9%)
33	CLA	6	313	25	50,54,73	1.36	7 (14%)	59,90,113	1.36	5 (8%)
38	DGD	h	102	-	63,63,67	0.90	2 (3%)	77,77,81	1.39	9 (11%)
46	DD6	1	304	-	40,45,45	1.62	3 (7%)	51,67,67	2.31	14 (27%)
33	CLA	B	613	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
38	DGD	H	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.39	10 (12%)
33	CLA	3	305	-	52,56,73	1.33	9 (17%)	61,92,113	1.42	6 (9%)
36	LHG	7	316	-	27,27,48	0.90	2 (7%)	30,32,54	1.75	4 (13%)
33	CLA	7	307	-	69,73,73	1.13	9 (13%)	82,113,113	1.30	7 (8%)
30	BCR	c	514	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	8 (14%)
33	CLA	2	314	-	40,46,73	1.47	8 (20%)	52,80,113	1.47	5 (9%)
33	CLA	8	315	29	40,46,73	1.45	8 (20%)	52,80,113	1.52	6 (11%)
33	CLA	b	614	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
33	CLA	6	312	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	4 (4%)
37	SQD	0	316	-	46,48,54	1.03	4 (8%)	56,59,65	1.45	8 (14%)
45	A86	5	303	-	47,50,50	1.46	5 (10%)	51,76,76	11.25	23 (45%)
36	LHG	3	318	-	48,48,48	0.63	1 (2%)	51,54,54	1.28	6 (11%)
39	LMG	7	315	-	55,55,55	0.73	1 (1%)	63,63,63	1.35	6 (9%)
33	CLA	1	315	-	40,46,73	1.46	8 (20%)	52,80,113	1.50	5 (9%)
33	CLA	b	612	-	68,72,73	1.15	9 (13%)	80,111,113	1.32	6 (7%)
33	CLA	8	312	-	49,53,73	1.39	9 (18%)	58,89,113	1.46	4 (6%)
45	A86	0	303	-	47,50,50	1.52	6 (12%)	51,76,76	2.45	15 (29%)
33	CLA	3	306	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
43	LMU	w	302	-	36,36,36	0.35	0	47,47,47	1.02	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LHG	a	404	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
42	HEM	V	201	18	50,50,50	1.61	9 (18%)	67,82,82	1.67	14 (20%)
33	CLA	c	504	-	68,72,73	1.16	8 (11%)	80,111,113	1.31	6 (7%)
45	A86	5	305	-	46,49,50	1.62	7 (15%)	46,74,76	7.59	22 (47%)
30	BCR	b	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	6 (10%)
33	CLA	8	316	29	40,46,73	1.47	8 (20%)	52,80,113	1.50	5 (9%)
33	CLA	A	405	-	53,57,73	1.30	8 (15%)	61,93,113	1.46	6 (9%)
44	KC1	3	310	-	49,53,53	1.33	6 (12%)	61,89,89	1.74	13 (21%)
39	LMG	0	314	-	42,42,55	0.91	2 (4%)	50,50,63	1.27	3 (6%)
33	CLA	9	311	29	59,63,73	1.27	8 (13%)	70,101,113	1.35	6 (8%)
39	LMG	b	623	-	40,40,55	0.85	1 (2%)	48,48,63	1.31	5 (10%)
33	CLA	c	501	-	69,73,73	1.15	9 (13%)	82,113,113	1.20	6 (7%)
33	CLA	B	608	-	69,73,73	1.14	9 (13%)	82,113,113	1.26	5 (6%)
33	CLA	c	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
30	BCR	B	619	-	41,41,41	1.20	3 (7%)	56,56,56	1.21	4 (7%)
33	CLA	w	303	-	69,73,73	1.16	7 (10%)	82,113,113	1.26	6 (7%)
33	CLA	A	408	-	64,68,73	1.19	8 (12%)	76,107,113	1.30	6 (7%)
33	CLA	9	313	-	39,44,73	1.58	10 (25%)	50,77,113	1.60	7 (14%)
33	CLA	5	314	24	59,63,73	1.26	8 (13%)	70,101,113	1.30	6 (8%)
33	CLA	7	304	-	51,55,73	1.34	9 (17%)	60,91,113	1.42	4 (6%)
33	CLA	c	503	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	7 (8%)
42	HEM	F	101	6	50,50,50	1.37	7 (14%)	67,82,82	1.03	2 (2%)
33	CLA	c	512	-	68,72,73	1.15	9 (13%)	80,111,113	1.28	5 (6%)
33	CLA	1	306	29	49,53,73	1.38	9 (18%)	58,89,113	1.44	5 (8%)
39	LMG	c	520	-	27,27,55	1.02	0	35,35,63	1.18	5 (14%)
33	CLA	1	307	-	48,52,73	1.49	8 (16%)	59,88,113	1.43	5 (8%)
39	LMG	d	406	-	46,46,55	0.80	1 (2%)	54,54,63	1.36	5 (9%)
35	BCT	a	402	40	3,3,3	1.25	0	2,3,3	4.32	2 (100%)
39	LMG	W	301	-	48,48,55	0.79	1 (2%)	56,56,63	1.36	6 (10%)
33	CLA	9	312	-	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
30	BCR	h	101	-	41,41,41	1.17	4 (9%)	56,56,56	1.20	3 (5%)
33	CLA	B	601	-	51,55,73	1.33	9 (17%)	60,91,113	1.39	5 (8%)
44	KC1	6	314	25	49,53,53	1.39	7 (14%)	61,89,89	1.71	13 (21%)
46	DD6	2	303	-	40,45,45	1.58	2 (5%)	51,67,67	2.19	13 (25%)
33	CLA	9	306	-	49,53,73	1.38	9 (18%)	58,89,113	1.44	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	A86	6	301	-	47,50,50	1.46	7 (14%)	51,76,76	12.04	26 (50%)
30	BCR	H	101	-	41,41,41	1.18	4 (9%)	56,56,56	1.19	3 (5%)
33	CLA	C	504	-	68,72,73	1.14	9 (13%)	80,111,113	1.29	6 (7%)
36	LHG	d	407	-	41,41,48	0.68	1 (2%)	44,47,54	1.31	5 (11%)
33	CLA	4	314	23	60,64,73	1.24	8 (13%)	71,102,113	1.28	7 (9%)
33	CLA	8	313	29	39,44,73	1.56	10 (25%)	50,77,113	1.56	7 (14%)
33	CLA	c	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
33	CLA	C	503	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
38	DGD	c	518	-	56,56,67	0.94	2 (3%)	70,70,81	1.38	8 (11%)
30	BCR	d	403	-	41,41,41	1.15	3 (7%)	56,56,56	1.20	5 (8%)
33	CLA	4	305	-	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
33	CLA	4	316	-	56,60,73	1.28	9 (16%)	65,97,113	1.39	6 (9%)
46	DD6	3	315	-	40,45,45	1.55	2 (5%)	51,67,67	1.87	14 (27%)
45	A86	5	301	-	47,50,50	1.47	6 (12%)	51,76,76	11.11	26 (50%)
46	DD6	4	303	-	40,45,45	1.61	3 (7%)	51,67,67	2.83	16 (31%)
33	CLA	7	312	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	5 (6%)
33	CLA	B	616	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	6 (7%)
36	LHG	5	318	-	32,32,48	0.84	2 (6%)	35,37,54	1.75	6 (17%)
39	LMG	C	521	-	27,27,55	1.06	1 (3%)	35,35,63	1.16	5 (14%)
30	BCR	D	407	-	41,41,41	1.20	3 (7%)	56,56,56	1.21	7 (12%)
33	CLA	2	307	-	48,52,73	1.49	10 (20%)	59,88,113	1.41	5 (8%)
33	CLA	6	308	25	58,62,73	1.28	8 (13%)	68,99,113	1.35	6 (8%)
33	CLA	C	506	-	49,53,73	1.37	9 (18%)	58,89,113	1.40	5 (8%)
33	CLA	D	405	-	61,65,73	1.31	10 (16%)	74,103,113	1.35	8 (10%)
33	CLA	a	411	-	64,68,73	1.19	7 (10%)	76,107,113	1.37	7 (9%)
33	CLA	5	313	-	69,73,73	1.17	7 (10%)	82,113,113	1.24	7 (8%)
33	CLA	C	510	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	7 (8%)
33	CLA	B	610	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
33	CLA	9	310	29	69,73,73	1.17	8 (11%)	82,113,113	1.25	7 (8%)
33	CLA	5	316	-	45,49,73	1.42	8 (17%)	54,84,113	1.46	5 (9%)
33	CLA	6	310	-	56,60,73	1.29	8 (14%)	65,97,113	1.37	6 (9%)
45	A86	1	302	-	47,50,50	1.49	5 (10%)	51,76,76	2.55	18 (35%)
46	DD6	1	303	-	40,45,45	1.54	2 (5%)	51,67,67	2.06	13 (25%)
34	PHO	a	409	-	58,69,69	2.09	10 (17%)	55,99,99	1.48	7 (12%)
43	LMU	5	320	-	32,32,36	0.37	0	43,43,47	0.75	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	7	309	26	69,73,73	1.16	9 (13%)	82,113,113	1.26	7 (8%)
33	CLA	8	310	29	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
36	LHG	A	412	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
45	A86	6	302	-	47,50,50	1.37	5 (10%)	51,76,76	10.82	24 (47%)
33	CLA	5	312	-	50,54,73	1.37	9 (18%)	59,90,113	1.39	4 (6%)
39	LMG	b	621	-	51,51,55	0.75	1 (1%)	59,59,63	1.34	7 (11%)
33	CLA	W	303	-	69,73,73	1.15	8 (11%)	82,113,113	1.30	8 (9%)
33	CLA	7	313	26	36,42,73	1.69	6 (16%)	45,73,113	1.64	7 (15%)
33	CLA	1	314	-	40,46,73	1.48	8 (20%)	52,80,113	1.44	5 (9%)
41	PL9	d	404	-	55,55,55	1.29	5 (9%)	68,69,69	1.46	11 (16%)
33	CLA	d	401	-	61,65,73	1.32	10 (16%)	74,103,113	1.33	8 (10%)
34	PHO	A	407	-	58,69,69	2.11	10 (17%)	55,99,99	1.45	7 (12%)
33	CLA	8	309	-	48,51,73	1.47	10 (20%)	56,86,113	1.53	5 (8%)
33	CLA	C	501	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	6 (7%)
33	CLA	0	309	26	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
33	CLA	0	311	-	55,59,73	1.30	8 (14%)	64,96,113	1.45	6 (9%)
43	LMU	t	101	-	32,32,36	0.35	0	43,43,47	0.81	0
30	BCR	a	412	-	41,41,41	1.19	3 (7%)	56,56,56	1.17	4 (7%)
43	LMU	3	301	-	36,36,36	0.38	0	47,47,47	0.83	1 (2%)
33	CLA	2	310	29	69,73,73	1.17	8 (11%)	82,113,113	1.26	8 (9%)
37	SQD	T	103	-	52,54,54	0.94	2 (3%)	62,65,65	1.52	11 (17%)
33	CLA	1	312	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
39	LMG	3	316	-	31,31,55	0.93	0	39,39,63	1.26	5 (12%)
46	DD6	8	303	-	40,45,45	1.53	2 (5%)	51,67,67	2.06	13 (25%)
39	LMG	c	519	-	48,48,55	0.85	2 (4%)	56,56,63	1.29	6 (10%)
39	LMG	d	410	-	37,37,55	0.86	1 (2%)	45,45,63	1.29	6 (13%)
39	LMG	5	319	-	31,31,55	0.95	0	39,39,63	1.34	5 (12%)
33	CLA	1	316	29	40,46,73	1.48	8 (20%)	52,80,113	1.48	5 (9%)
33	CLA	9	305	-	45,49,73	1.42	8 (17%)	54,84,113	1.45	5 (9%)
45	A86	8	301	-	47,50,50	1.50	5 (10%)	51,76,76	2.56	19 (37%)
33	CLA	4	312	-	55,59,73	1.29	9 (16%)	64,96,113	1.36	5 (7%)
33	CLA	2	306	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	5 (8%)
33	CLA	7	311	-	55,59,73	1.29	8 (14%)	64,96,113	1.44	6 (9%)
36	LHG	d	405	-	44,47,48	0.54	1 (2%)	44,51,54	1.18	5 (11%)
33	CLA	c	513	-	53,57,73	1.31	9 (16%)	61,93,113	1.44	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	D	406	-	64,68,73	1.18	9 (14%)	76,107,113	1.38	8 (10%)
33	CLA	0	304	-	51,55,73	1.33	8 (15%)	60,91,113	1.43	5 (8%)
33	CLA	0	312	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
33	CLA	9	317	-	59,63,73	1.28	9 (15%)	70,101,113	1.35	5 (7%)
33	CLA	A	404	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
38	DGD	a	401	-	54,54,67	1.00	4 (7%)	67,67,81	1.47	13 (19%)
33	CLA	B	605	-	69,73,73	1.14	9 (13%)	82,113,113	1.18	6 (7%)
38	DGD	C	517	-	57,57,67	0.99	2 (3%)	71,71,81	1.46	10 (14%)
37	SQD	a	413	-	52,54,54	0.94	3 (5%)	62,65,65	1.54	11 (17%)
31	OEX	a	405	1,3	0,15,15	-	-	-	-	-
44	KC1	5	315	-	49,53,53	1.36	5 (10%)	61,89,89	1.71	13 (21%)
30	BCR	K	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.26	6 (10%)
33	CLA	1	313	29	39,44,73	1.57	10 (25%)	50,77,113	1.58	7 (14%)
33	CLA	b	608	-	45,49,73	1.37	9 (20%)	54,84,113	1.53	7 (12%)
33	CLA	8	307	-	48,52,73	1.47	10 (20%)	59,88,113	1.44	6 (10%)
33	CLA	9	308	-	59,63,73	1.26	9 (15%)	70,101,113	1.35	6 (8%)
33	CLA	b	603	-	64,69,73	1.18	7 (10%)	73,106,113	1.07	7 (9%)
33	CLA	c	502	-	68,72,73	1.16	9 (13%)	80,111,113	1.26	5 (6%)
30	BCR	A	401	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	7 (12%)
33	CLA	9	315	-	40,46,73	1.46	8 (20%)	52,80,113	1.48	5 (9%)
39	LMG	D	410	-	46,46,55	0.81	1 (2%)	54,54,63	1.35	4 (7%)
45	A86	9	301	-	47,50,50	1.50	5 (10%)	51,76,76	2.59	18 (35%)
34	PHO	a	410	-	58,69,69	2.10	10 (17%)	55,99,99	1.49	7 (12%)
33	CLA	2	317	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	5 (7%)
33	CLA	C	509	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
45	A86	7	303	-	47,50,50	1.49	5 (10%)	51,76,76	2.60	15 (29%)
39	LMG	M	201	-	40,40,55	0.85	2 (5%)	48,48,63	1.32	5 (10%)
30	BCR	K	102	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	7 (12%)
33	CLA	b	617	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
33	CLA	Z	101	-	55,59,73	1.30	9 (16%)	64,96,113	1.38	5 (7%)
33	CLA	3	307	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
33	CLA	7	308	26	45,49,73	1.39	9 (20%)	54,84,113	1.44	5 (9%)
33	CLA	b	609	-	69,73,73	1.14	9 (13%)	82,113,113	1.27	5 (6%)
33	CLA	3	303	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	5 (6%)
45	A86	2	301	-	47,50,50	1.50	5 (10%)	51,76,76	2.58	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	5	308	-	50,54,73	1.36	7 (14%)	59,90,113	1.37	4 (6%)
45	A86	8	302	-	47,50,50	1.49	5 (10%)	51,76,76	2.55	18 (35%)
33	CLA	3	319	-	59,63,73	1.26	9 (15%)	70,101,113	1.33	5 (7%)
37	SQD	D	403	-	52,54,54	0.95	3 (5%)	62,65,65	1.42	9 (14%)
33	CLA	b	615	-	68,72,73	1.15	9 (13%)	80,111,113	1.28	6 (7%)
39	LMG	D	404	-	40,40,55	0.82	1 (2%)	48,48,63	1.32	5 (10%)
42	HEM	v	201	18	50,50,50	1.32	7 (14%)	67,82,82	1.21	5 (7%)
33	CLA	1	311	29	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
33	CLA	B	611	-	68,72,73	1.15	9 (13%)	80,111,113	1.26	8 (10%)
33	CLA	4	310	-	50,54,73	1.36	9 (18%)	59,90,113	1.40	6 (10%)
33	CLA	H	103	26	45,51,73	1.40	8 (17%)	57,86,113	1.40	4 (7%)
30	BCR	b	618	-	41,41,41	1.23	3 (7%)	56,56,56	1.24	7 (12%)
33	CLA	D	402	-	63,67,73	1.20	9 (14%)	74,105,113	1.35	7 (9%)
33	CLA	b	607	-	69,73,73	1.14	8 (11%)	82,113,113	1.26	5 (6%)
33	CLA	0	310	-	49,53,73	1.38	7 (14%)	58,89,113	1.45	5 (8%)
33	CLA	B	612	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
45	A86	3	314	-	47,50,50	1.46	5 (10%)	51,76,76	2.53	18 (35%)
36	LHG	0	315	-	27,27,48	0.93	2 (7%)	30,32,54	1.72	4 (13%)
48	ET4	7	302	-	41,43,43	2.02	11 (26%)	52,60,60	2.38	17 (32%)
30	BCR	a	414	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	7 (12%)
33	CLA	b	616	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
33	CLA	b	610	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)
45	A86	5	302	-	47,50,50	1.48	7 (14%)	51,76,76	11.77	25 (49%)
33	CLA	6	307	-	57,61,73	1.29	7 (12%)	67,98,113	1.42	7 (10%)
33	CLA	2	316	29	40,46,73	1.48	7 (17%)	52,80,113	1.46	5 (9%)
33	CLA	0	307	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
30	BCR	B	618	-	41,41,41	1.16	2 (4%)	56,56,56	1.18	4 (7%)
39	LMG	w	304	-	48,48,55	0.77	1 (2%)	56,56,63	1.33	6 (10%)
47	KC2	0	306	-	49,53,53	1.69	9 (18%)	60,89,89	2.09	18 (30%)
45	A86	5	307	-	47,50,50	1.45	6 (12%)	51,76,76	12.72	23 (45%)
33	CLA	C	512	-	68,72,73	1.15	9 (13%)	80,111,113	1.30	5 (6%)
33	CLA	7	305	26	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
33	CLA	0	308	-	45,49,73	1.40	8 (17%)	54,84,113	1.47	6 (11%)
33	CLA	B	609	-	69,73,73	1.13	8 (11%)	82,113,113	1.24	7 (8%)
33	CLA	0	305	26	69,73,73	1.17	8 (11%)	82,113,113	1.31	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CLA	c	505	-	69,73,73	1.15	9 (13%)	82,113,113	1.19	5 (6%)
33	CLA	B	607	-	45,49,73	1.38	9 (20%)	54,84,113	1.53	6 (11%)
33	CLA	7	314	-	45,51,73	1.38	9 (20%)	57,86,113	1.41	5 (8%)
33	CLA	B	603	-	68,72,73	1.15	9 (13%)	80,111,113	1.23	6 (7%)
38	DGD	C	516	-	56,56,67	0.98	2 (3%)	70,70,81	1.44	11 (15%)
37	SQD	7	317	-	46,48,54	1.04	5 (10%)	56,59,65	1.48	10 (17%)
33	CLA	1	310	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
47	KC2	5	310	-	49,53,53	1.68	9 (18%)	60,89,89	2.11	18 (30%)
33	CLA	8	314	-	40,46,73	1.47	8 (20%)	52,80,113	1.46	5 (9%)
33	CLA	5	311	-	59,63,73	1.26	6 (10%)	70,101,113	1.33	5 (7%)
47	KC2	7	306	-	49,53,53	1.69	9 (18%)	60,89,89	2.11	16 (26%)
35	BCT	A	410	40	3,3,3	1.18	0	2,3,3	4.08	2 (100%)
33	CLA	C	511	3	69,73,73	1.15	9 (13%)	82,113,113	1.29	5 (6%)
33	CLA	2	313	29	39,44,73	1.70	7 (17%)	50,77,113	1.46	8 (16%)
45	A86	0	301	-	47,50,50	1.62	8 (17%)	51,76,76	2.61	19 (37%)
30	BCR	C	514	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	8 (14%)
37	SQD	T	101	-	38,40,54	1.15	4 (10%)	48,51,65	1.95	12 (25%)
42	HEM	e	101	6	50,50,50	1.60	9 (18%)	67,82,82	1.70	12 (17%)
33	CLA	d	409	-	63,67,73	1.20	9 (14%)	74,105,113	1.37	9 (12%)
33	CLA	2	315	-	40,46,73	1.48	8 (20%)	52,80,113	1.50	5 (9%)
33	CLA	6	311	-	50,54,73	1.37	7 (14%)	59,90,113	1.43	5 (8%)
46	DD6	8	304	-	40,45,45	1.58	2 (5%)	51,67,67	2.46	14 (27%)
33	CLA	z	101	-	55,59,73	1.32	9 (16%)	64,96,113	1.37	4 (6%)
33	CLA	0	313	-	36,42,73	1.69	6 (16%)	45,73,113	1.62	7 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LMG	B	621	-	-	6/23/43/70	0/1/1/1
33	CLA	c	506	-	1/1/11/20	4/15/91/115	-
36	LHG	w	301	-	-	20/39/39/53	-
33	CLA	9	314	-	1/1/9/20	2/4/80/115	-
33	CLA	c	508	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	C	502	-	1/1/14/20	16/37/113/115	-
33	CLA	4	315	-	1/1/11/20	4/18/94/115	-
45	A86	4	301	-	-	9/34/90/90	0/3/3/3
33	CLA	2	312	-	1/1/11/20	4/15/91/115	-
36	LHG	3	317	33	-	12/31/31/53	-
33	CLA	6	315	-	1/1/10/20	4/10/86/115	-
33	CLA	c	507	-	1/1/15/20	15/39/115/115	-
33	CLA	b	605	-	1/1/14/20	4/35/111/115	-
33	CLA	B	604	-	1/1/14/20	8/35/111/115	-
39	LMG	C	520	-	-	19/43/63/70	0/1/1/1
30	BCR	k	101	-	-	24/29/63/63	0/2/2/2
38	DGD	C	518	-	-	13/44/84/95	0/2/2/2
33	CLA	3	302	-	1/1/15/20	17/39/115/115	-
45	A86	6	306	-	-	8/34/90/90	0/3/3/3
33	CLA	4	306	23	1/1/15/20	5/39/115/115	-
33	CLA	2	305	-	1/1/10/20	2/10/86/115	-
46	DD6	2	304	-	-	10/26/80/80	0/3/3/3
33	CLA	B	615	-	1/1/15/20	8/39/115/115	-
33	CLA	5	317	-	1/1/9/20	2/4/80/115	-
33	CLA	4	313	23	1/1/10/20	0/10/86/115	-
33	CLA	2	308	-	1/1/13/20	11/27/103/115	-
39	LMG	B	620	-	-	19/46/66/70	0/1/1/1
36	LHG	H	104	-	-	20/46/46/53	-
33	CLA	B	606	-	1/1/15/20	7/39/115/115	-
33	CLA	C	513	-	1/1/11/20	6/20/96/115	-
45	A86	4	304	-	-	3/34/90/90	0/3/3/3
45	A86	1	301	-	-	5/34/90/90	0/3/3/3
33	CLA	2	309	-	1/1/11/20	4/13/89/115	-
33	CLA	a	407	-	1/1/15/20	8/39/115/115	-
39	LMG	q	302	-	-	18/32/52/70	0/1/1/1
30	BCR	k	102	-	-	4/29/63/63	0/2/2/2
34	PHO	A	406	-	-	13/37/103/103	0/5/6/6
33	CLA	B	614	-	1/1/14/20	11/37/113/115	-
46	DD6	9	304	-	-	10/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	3	309	36	1/1/12/20	6/23/99/115	-
33	CLA	3	311	-	1/1/10/20	2/10/86/115	-
45	A86	6	304	-	-	8/34/90/90	0/3/3/3
33	CLA	b	606	-	1/1/15/20	9/39/115/115	-
30	BCR	b	620	-	-	6/29/63/63	0/2/2/2
39	LMG	q	301	-	-	22/41/61/70	0/1/1/1
36	LHG	h	103	-	-	18/46/46/53	-
33	CLA	b	611	-	1/1/15/20	6/39/115/115	-
33	CLA	C	508	-	1/1/15/20	7/39/115/115	-
33	CLA	9	309	29	1/1/11/20	3/13/89/115	-
30	BCR	c	515	-	-	6/29/63/63	0/2/2/2
45	A86	5	304	-	-	8/34/90/90	0/3/3/3
37	SQD	L	101	-	-	23/49/69/69	0/1/1/1
33	CLA	C	507	-	1/1/15/20	15/39/115/115	-
33	CLA	c	511	3	1/1/15/20	7/39/115/115	-
33	CLA	1	309	-	1/1/11/20	5/13/89/115	-
38	DGD	3	320	-	-	20/40/40/95	-
45	A86	6	303	-	-	8/34/90/90	0/3/3/3
47	KC2	6	309	-	-	8/15/71/71	-
33	CLA	C	505	-	1/1/15/20	15/39/115/115	-
30	BCR	B	617	-	-	2/29/63/63	0/2/2/2
33	CLA	3	304	-	1/1/15/20	10/39/115/115	-
38	DGD	A	415	-	-	24/43/79/95	0/2/2/2
30	BCR	A	409	-	-	2/29/63/63	0/2/2/2
33	CLA	8	311	29	1/1/13/20	4/27/103/115	-
36	LHG	W	302	-	-	23/39/39/53	-
41	PL9	D	408	-	-	5/53/73/73	0/1/1/1
33	CLA	5	309	24	1/1/13/20	5/27/103/115	-
45	A86	2	302	-	-	8/34/90/90	0/3/3/3
36	LHG	A	414	-	-	17/53/53/53	-
39	LMG	C	519	-	-	18/41/61/70	0/1/1/1
33	CLA	9	307	-	1/1/11/20	5/13/89/115	-
33	CLA	8	306	29	1/1/11/20	3/15/91/115	-
37	SQD	l	101	-	-	21/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	3	308	22	1/1/15/20	14/39/115/115	-
36	LHG	D	411	-	-	19/46/46/53	-
39	LMG	b	622	-	-	4/23/43/70	0/1/1/1
39	LMG	C	522	-	-	7/16/36/70	0/1/1/1
48	ET4	0	302	-	-	13/25/67/67	0/2/2/2
45	A86	9	302	-	-	8/34/90/90	0/3/3/3
38	DGD	c	517	-	-	22/45/85/95	0/2/2/2
33	CLA	7	310	26	1/1/11/20	6/15/91/115	-
38	DGD	c	516	-	-	15/44/84/95	0/2/2/2
33	CLA	b	602	-	1/1/11/20	6/18/94/115	-
47	KC2	4	307	-	-	7/15/71/71	-
33	CLA	8	305	-	1/1/10/20	2/10/86/115	-
33	CLA	8	308	-	1/1/13/20	11/27/103/115	-
43	LMU	T	102	-	-	9/17/57/61	0/2/2/2
33	CLA	1	308	-	1/1/13/20	7/27/103/115	-
33	CLA	b	604	-	1/1/14/20	12/37/113/115	-
36	LHG	A	411	-	-	15/47/47/53	-
33	CLA	3	313	-	1/1/14/20	15/35/111/115	-
36	LHG	D	409	-	-	18/47/51/53	-
45	A86	6	305	-	-	8/34/90/90	0/3/3/3
33	CLA	B	602	-	1/1/12/20	11/29/107/115	-
45	A86	4	302	-	-	9/34/90/90	0/3/3/3
33	CLA	4	308	-	1/1/15/20	8/39/115/115	-
33	CLA	b	613	-	1/1/15/20	15/39/115/115	-
37	SQD	A	413	-	-	13/35/55/69	0/1/1/1
36	LHG	a	403	-	-	13/47/47/53	-
43	LMU	4	317	-	-	14/21/61/61	0/2/2/2
46	DD6	9	303	-	-	4/26/80/80	0/3/3/3
33	CLA	2	311	29	1/1/13/20	6/27/103/115	-
33	CLA	4	309	23	1/1/15/20	3/39/115/115	-
33	CLA	4	311	23	1/1/14/20	13/33/109/115	-
45	A86	7	301	-	-	8/34/90/90	0/3/3/3
39	LMG	m	201	-	-	16/35/55/70	0/1/1/1
39	LMG	Q	301	-	-	16/32/52/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	C	515	-	-	9/29/63/63	0/2/2/2
33	CLA	6	316	-	1/1/9/20	2/8/80/115	-
45	A86	5	306	-	-	8/34/90/90	0/3/3/3
33	CLA	3	312	-	1/1/13/20	10/29/105/115	-
33	CLA	a	408	-	1/1/11/20	4/20/96/115	-
37	SQD	B	622	-	-	22/49/69/69	0/1/1/1
36	LHG	4	318	-	-	31/53/53/53	-
37	SQD	t	102	-	-	18/34/54/69	0/1/1/1
33	CLA	d	402	-	1/1/14/20	9/33/109/115	-
36	LHG	b	601	-	-	19/53/53/53	-
37	SQD	i	101	-	-	10/35/55/69	0/1/1/1
33	CLA	1	305	-	1/1/10/20	4/10/86/115	-
33	CLA	9	316	29	1/1/9/20	2/4/80/115	-
33	CLA	6	313	25	1/1/11/20	5/17/93/115	-
38	DGD	h	102	-	-	16/51/91/95	0/2/2/2
46	DD6	1	304	-	-	7/26/80/80	0/3/3/3
33	CLA	B	613	-	1/1/15/20	13/39/115/115	-
38	DGD	H	102	-	-	16/51/91/95	0/2/2/2
33	CLA	3	305	-	1/1/11/20	8/19/95/115	-
36	LHG	7	316	-	-	15/29/29/53	-
33	CLA	7	307	-	1/1/15/20	13/39/115/115	-
30	BCR	c	514	-	-	2/29/63/63	0/2/2/2
33	CLA	2	314	-	1/1/9/20	2/4/80/115	-
33	CLA	8	315	29	1/1/9/20	0/4/80/115	-
33	CLA	b	614	-	1/1/15/20	11/39/115/115	-
33	CLA	6	312	-	1/1/15/20	11/39/115/115	-
37	SQD	0	316	-	-	13/43/63/69	0/1/1/1
45	A86	5	303	-	-	8/34/90/90	0/3/3/3
36	LHG	3	318	-	-	21/53/53/53	-
39	LMG	7	315	-	-	26/50/70/70	0/1/1/1
33	CLA	1	315	-	1/1/9/20	0/4/80/115	-
33	CLA	b	612	-	1/1/14/20	6/37/113/115	-
33	CLA	8	312	-	1/1/11/20	4/15/91/115	-
45	A86	0	303	-	-	3/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	3	306	-	1/1/15/20	16/39/115/115	-
43	LMU	w	302	-	-	13/21/61/61	0/2/2/2
36	LHG	a	404	-	-	26/53/53/53	-
42	HEM	V	201	18	-	6/14/54/54	-
33	CLA	c	504	-	1/1/14/20	11/37/113/115	-
45	A86	5	305	-	-	8/33/89/90	0/3/3/3
33	CLA	8	316	29	1/1/9/20	2/4/80/115	-
30	BCR	b	619	-	-	5/29/63/63	0/2/2/2
33	CLA	A	405	-	1/1/11/20	3/20/96/115	-
44	KC1	3	310	-	-	9/15/71/71	-
39	LMG	0	314	-	-	20/37/57/70	0/1/1/1
33	CLA	9	311	29	1/1/13/20	6/27/103/115	-
39	LMG	b	623	-	-	22/35/55/70	0/1/1/1
33	CLA	c	501	-	1/1/15/20	19/39/115/115	-
33	CLA	B	608	-	1/1/15/20	5/39/115/115	-
33	CLA	c	510	-	1/1/15/20	10/39/115/115	-
30	BCR	B	619	-	-	6/29/63/63	0/2/2/2
33	CLA	w	303	-	1/1/15/20	18/39/115/115	-
33	CLA	A	408	-	1/1/14/20	7/33/109/115	-
33	CLA	9	313	-	1/1/9/20	2/2/78/115	-
33	CLA	5	314	24	1/1/13/20	4/27/103/115	-
33	CLA	7	304	-	1/1/11/20	7/18/94/115	-
33	CLA	c	503	-	1/1/15/20	12/39/115/115	-
42	HEM	F	101	6	-	3/14/54/54	-
33	CLA	c	512	-	1/1/14/20	10/37/113/115	-
33	CLA	1	306	29	1/1/11/20	4/15/91/115	-
39	LMG	c	520	-	-	7/21/41/70	0/1/1/1
33	CLA	1	307	-	1/1/11/20	3/13/89/115	-
39	LMG	d	406	-	-	17/41/61/70	0/1/1/1
39	LMG	W	301	-	-	18/43/63/70	0/1/1/1
33	CLA	9	312	-	1/1/11/20	5/15/91/115	-
30	BCR	h	101	-	-	3/29/63/63	0/2/2/2
33	CLA	B	601	-	1/1/11/20	7/18/94/115	-
44	KC1	6	314	25	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	DD6	2	303	-	-	4/26/80/80	0/3/3/3
33	CLA	9	306	-	1/1/11/20	4/15/91/115	-
45	A86	6	301	-	-	7/34/90/90	0/3/3/3
30	BCR	H	101	-	-	2/29/63/63	0/2/2/2
33	CLA	C	504	-	1/1/14/20	12/37/113/115	-
36	LHG	d	407	-	-	18/46/46/53	-
33	CLA	4	314	23	1/1/13/20	4/29/105/115	-
33	CLA	8	313	29	1/1/9/20	0/2/78/115	-
33	CLA	c	509	-	1/1/15/20	5/39/115/115	-
33	CLA	C	503	-	1/1/15/20	13/39/115/115	-
38	DGD	c	518	-	-	15/44/84/95	0/2/2/2
30	BCR	d	403	-	-	4/29/63/63	0/2/2/2
33	CLA	4	305	-	1/1/13/20	5/27/103/115	-
33	CLA	4	316	-	1/1/12/20	4/24/100/115	-
46	DD6	3	315	-	-	5/26/80/80	0/3/3/3
45	A86	5	301	-	-	10/34/90/90	0/3/3/3
46	DD6	4	303	-	-	3/26/80/80	0/3/3/3
33	CLA	7	312	-	1/1/15/20	15/39/115/115	-
33	CLA	B	616	-	1/1/15/20	12/39/115/115	-
36	LHG	5	318	-	-	13/34/34/53	-
39	LMG	C	521	-	-	4/21/41/70	0/1/1/1
30	BCR	D	407	-	-	2/29/63/63	0/2/2/2
33	CLA	2	307	-	1/1/11/20	6/13/89/115	-
33	CLA	6	308	25	1/1/12/20	3/26/102/115	-
33	CLA	C	506	-	1/1/11/20	4/15/91/115	-
33	CLA	D	405	-	1/1/13/20	5/28/104/115	-
33	CLA	a	411	-	1/1/14/20	4/33/109/115	-
33	CLA	5	313	-	1/1/15/20	12/39/115/115	-
33	CLA	C	510	-	1/1/15/20	6/39/115/115	-
33	CLA	B	610	-	1/1/15/20	5/39/115/115	-
33	CLA	9	310	29	1/1/15/20	14/39/115/115	-
33	CLA	5	316	-	1/1/10/20	2/10/86/115	-
33	CLA	6	310	-	1/1/12/20	3/24/100/115	-
45	A86	1	302	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	DD6	1	303	-	-	4/26/80/80	0/3/3/3
34	PHO	a	409	-	-	12/37/103/103	0/5/6/6
43	LMU	5	320	-	-	8/17/57/61	0/2/2/2
33	CLA	7	309	26	1/1/15/20	16/39/115/115	-
33	CLA	8	310	29	1/1/15/20	18/39/115/115	-
36	LHG	A	412	-	-	26/53/53/53	-
45	A86	6	302	-	-	8/34/90/90	0/3/3/3
33	CLA	5	312	-	1/1/11/20	9/17/93/115	-
39	LMG	b	621	-	-	21/46/66/70	0/1/1/1
33	CLA	W	303	-	1/1/15/20	17/39/115/115	-
33	CLA	7	313	26	1/1/8/20	0/2/74/115	-
33	CLA	1	314	-	1/1/9/20	2/4/80/115	-
41	PL9	d	404	-	-	7/53/73/73	0/1/1/1
33	CLA	d	401	-	1/1/13/20	5/28/104/115	-
34	PHO	A	407	-	-	8/37/103/103	0/5/6/6
33	CLA	8	309	-	1/1/11/20	3/13/89/115	-
33	CLA	C	501	-	1/1/15/20	19/39/115/115	-
33	CLA	0	309	26	1/1/15/20	13/39/115/115	-
33	CLA	0	311	-	1/1/12/20	7/23/99/115	-
43	LMU	t	101	-	-	12/17/57/61	0/2/2/2
30	BCR	a	412	-	-	3/29/63/63	0/2/2/2
43	LMU	3	301	-	-	17/21/61/61	0/2/2/2
33	CLA	2	310	29	1/1/15/20	12/39/115/115	-
37	SQD	T	103	-	-	22/49/69/69	0/1/1/1
33	CLA	1	312	-	1/1/11/20	6/15/91/115	-
39	LMG	3	316	-	-	6/26/46/70	0/1/1/1
46	DD6	8	303	-	-	4/26/80/80	0/3/3/3
39	LMG	c	519	-	-	21/43/63/70	0/1/1/1
39	LMG	d	410	-	-	18/32/52/70	0/1/1/1
39	LMG	5	319	-	-	13/26/46/70	0/1/1/1
33	CLA	1	316	29	1/1/9/20	2/4/80/115	-
33	CLA	9	305	-	1/1/10/20	2/10/86/115	-
45	A86	8	301	-	-	8/34/90/90	0/3/3/3
33	CLA	4	312	-	1/1/12/20	7/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	2	306	-	1/1/11/20	5/15/91/115	-
33	CLA	7	311	-	1/1/12/20	10/23/99/115	-
36	LHG	d	405	-	-	21/47/51/53	-
33	CLA	c	513	-	1/1/11/20	6/20/96/115	-
33	CLA	D	406	-	1/1/14/20	9/33/109/115	-
33	CLA	0	304	-	1/1/11/20	9/18/94/115	-
33	CLA	0	312	-	1/1/15/20	17/39/115/115	-
33	CLA	9	317	-	1/1/13/20	7/27/103/115	-
33	CLA	A	404	-	1/1/15/20	9/39/115/115	-
38	DGD	a	401	-	-	28/43/79/95	0/2/2/2
33	CLA	B	605	-	1/1/15/20	14/39/115/115	-
38	DGD	C	517	-	-	18/45/85/95	0/2/2/2
37	SQD	a	413	-	-	19/49/69/69	0/1/1/1
44	KC1	5	315	-	-	7/15/71/71	-
30	BCR	K	101	-	-	18/29/63/63	0/2/2/2
33	CLA	1	313	29	1/1/9/20	2/2/78/115	-
33	CLA	b	608	-	1/1/10/20	2/10/86/115	-
33	CLA	8	307	-	1/1/11/20	5/13/89/115	-
33	CLA	9	308	-	1/1/13/20	11/27/103/115	-
33	CLA	b	603	-	1/1/12/20	7/29/107/115	-
33	CLA	c	502	-	1/1/14/20	13/37/113/115	-
30	BCR	A	401	-	-	5/29/63/63	0/2/2/2
33	CLA	9	315	-	1/1/9/20	2/4/80/115	-
39	LMG	D	410	-	-	15/41/61/70	0/1/1/1
45	A86	9	301	-	-	7/34/90/90	0/3/3/3
34	PHO	a	410	-	-	3/37/103/103	0/5/6/6
33	CLA	2	317	-	1/1/13/20	8/27/103/115	-
33	CLA	C	509	-	1/1/15/20	8/39/115/115	-
45	A86	7	303	-	-	6/34/90/90	0/3/3/3
39	LMG	M	201	-	-	15/35/55/70	0/1/1/1
30	BCR	K	102	-	-	4/29/63/63	0/2/2/2
33	CLA	b	617	-	1/1/15/20	18/39/115/115	-
33	CLA	Z	101	-	1/1/12/20	4/23/99/115	-
33	CLA	3	307	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	7	308	26	1/1/10/20	3/10/86/115	-
33	CLA	b	609	-	1/1/15/20	4/39/115/115	-
33	CLA	3	303	-	1/1/15/20	13/39/115/115	-
45	A86	2	301	-	-	7/34/90/90	0/3/3/3
33	CLA	5	308	-	1/1/11/20	6/17/93/115	-
45	A86	8	302	-	-	8/34/90/90	0/3/3/3
33	CLA	3	319	-	1/1/13/20	9/27/103/115	-
37	SQD	D	403	-	-	21/49/69/69	0/1/1/1
33	CLA	b	615	-	1/1/14/20	12/37/113/115	-
39	LMG	D	404	-	-	20/35/55/70	0/1/1/1
42	HEM	v	201	18	-	6/14/54/54	-
33	CLA	1	311	29	1/1/13/20	5/27/103/115	-
33	CLA	B	611	-	1/1/14/20	10/37/113/115	-
33	CLA	4	310	-	1/1/11/20	5/17/93/115	-
33	CLA	H	103	26	1/1/10/20	4/11/87/115	-
30	BCR	b	618	-	-	2/29/63/63	0/2/2/2
33	CLA	D	402	-	1/1/13/20	2/32/108/115	-
33	CLA	b	607	-	1/1/15/20	8/39/115/115	-
33	CLA	0	310	-	1/1/11/20	8/15/91/115	-
33	CLA	B	612	-	1/1/15/20	12/39/115/115	-
45	A86	3	314	-	-	7/34/90/90	0/3/3/3
36	LHG	0	315	-	-	17/29/29/53	-
48	ET4	7	302	-	-	11/25/67/67	0/2/2/2
30	BCR	a	414	-	-	4/29/63/63	0/2/2/2
33	CLA	b	616	-	1/1/15/20	7/39/115/115	-
33	CLA	b	610	-	1/1/15/20	9/39/115/115	-
45	A86	5	302	-	-	8/34/90/90	0/3/3/3
33	CLA	6	307	-	1/1/12/20	4/25/101/115	-
33	CLA	2	316	29	1/1/9/20	2/4/80/115	-
33	CLA	0	307	-	1/1/15/20	14/39/115/115	-
30	BCR	B	618	-	-	3/29/63/63	0/2/2/2
39	LMG	w	304	-	-	20/43/63/70	0/1/1/1
47	KC2	0	306	-	-	10/15/71/71	-
45	A86	5	307	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	C	512	-	1/1/14/20	14/37/113/115	-
33	CLA	7	305	26	1/1/15/20	18/39/115/115	-
33	CLA	0	308	-	1/1/10/20	2/10/86/115	-
33	CLA	B	609	-	1/1/15/20	10/39/115/115	-
33	CLA	0	305	26	1/1/15/20	16/39/115/115	-
33	CLA	c	505	-	1/1/15/20	15/39/115/115	-
33	CLA	B	607	-	1/1/10/20	2/10/86/115	-
33	CLA	7	314	-	1/1/10/20	4/11/87/115	-
33	CLA	B	603	-	1/1/14/20	10/37/113/115	-
38	DGD	C	516	-	-	20/44/84/95	0/2/2/2
37	SQD	7	317	-	-	13/43/63/69	0/1/1/1
33	CLA	1	310	-	1/1/15/20	16/39/115/115	-
47	KC2	5	310	-	-	6/15/71/71	-
33	CLA	8	314	-	1/1/9/20	2/4/80/115	-
33	CLA	5	311	-	1/1/13/20	5/27/103/115	-
47	KC2	7	306	-	-	8/15/71/71	-
33	CLA	C	511	3	1/1/15/20	7/39/115/115	-
33	CLA	2	313	29	-	0/2/78/115	-
45	A86	0	301	-	-	8/34/90/90	0/3/3/3
30	BCR	C	514	-	-	0/29/63/63	0/2/2/2
37	SQD	T	101	-	-	17/34/54/69	0/1/1/1
42	HEM	e	101	6	-	9/14/54/54	-
33	CLA	d	409	-	1/1/13/20	4/32/108/115	-
33	CLA	2	315	-	1/1/9/20	2/4/80/115	-
33	CLA	6	311	-	1/1/11/20	11/17/93/115	-
46	DD6	8	304	-	-	10/26/80/80	0/3/3/3
33	CLA	z	101	-	1/1/12/20	6/23/99/115	-
33	CLA	0	313	-	1/1/8/20	0/2/74/115	-

The worst 5 of 2089 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	410	PHO	C1B-C2B	9.44	1.49	1.39
34	A	407	PHO	C1B-C2B	9.43	1.49	1.39
34	a	409	PHO	C1B-C2B	9.33	1.49	1.39
34	A	406	PHO	C1B-C2B	9.33	1.49	1.39
46	1	304	DD6	C30-C31	-8.85	1.25	1.42

The worst 5 of 2660 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	5	302	A86	C23-C16-C22	-72.53	2.00	107.37
45	6	304	A86	C23-C16-C22	-72.36	2.25	107.37
45	5	303	A86	C23-C16-C22	-71.86	2.97	107.37
45	4	302	A86	C23-C16-C22	-71.36	3.70	107.37
45	5	307	A86	C23-C16-C22	-69.94	5.76	107.37

5 of 182 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	A	404	CLA	ND
33	A	405	CLA	ND
33	A	408	CLA	ND
33	B	601	CLA	ND
33	B	602	CLA	ND

5 of 3206 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	B	619	BCR	C7-C8-C9-C10
30	B	619	BCR	C21-C22-C23-C24
30	B	619	BCR	C37-C22-C23-C24
30	B	619	BCR	C22-C23-C24-C25
30	C	515	BCR	C7-C8-C9-C10

There are no ring outliers.

259 monomers are involved in 635 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	c	506	CLA	3	0
33	9	314	CLA	2	0
33	c	508	CLA	5	0
33	C	502	CLA	1	0
33	4	315	CLA	1	0
45	4	301	A86	4	0
33	2	312	CLA	1	0
33	c	507	CLA	1	0
33	b	605	CLA	2	0
33	B	604	CLA	5	0
39	C	520	LMG	2	0
30	k	101	BCR	4	0
38	C	518	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	3	302	CLA	1	0
33	4	306	CLA	6	0
46	2	304	DD6	13	0
33	B	615	CLA	4	0
33	4	313	CLA	3	0
33	2	308	CLA	4	0
33	B	606	CLA	1	0
33	C	513	CLA	2	0
45	1	301	A86	3	0
33	2	309	CLA	3	0
39	q	302	LMG	3	0
30	k	102	BCR	3	0
34	A	406	PHO	1	0
46	9	304	DD6	4	0
33	3	309	CLA	1	0
45	6	304	A86	5	0
33	b	606	CLA	3	0
30	b	620	BCR	2	0
39	q	301	LMG	4	0
36	h	103	LHG	2	0
33	b	611	CLA	1	0
33	C	508	CLA	1	0
30	c	515	BCR	2	0
45	5	304	A86	3	0
37	L	101	SQD	2	0
33	C	507	CLA	2	0
33	c	511	CLA	1	0
38	3	320	DGD	3	0
30	B	617	BCR	1	0
33	3	304	CLA	4	0
38	A	415	DGD	3	0
30	A	409	BCR	2	0
33	8	311	CLA	7	0
36	W	302	LHG	2	0
33	5	309	CLA	3	0
45	2	302	A86	6	0
39	C	519	LMG	1	0
33	9	307	CLA	2	0
37	l	101	SQD	2	0
33	3	308	CLA	1	0
39	b	622	LMG	1	0
48	0	302	ET4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	9	302	A86	1	0
38	c	517	DGD	3	0
33	7	310	CLA	8	0
38	c	516	DGD	5	0
33	b	602	CLA	3	0
47	4	307	KC2	2	0
33	8	308	CLA	3	0
43	T	102	LMU	1	0
33	1	308	CLA	3	0
33	b	604	CLA	3	0
36	A	411	LHG	1	0
33	3	313	CLA	6	0
36	D	409	LHG	1	0
33	B	602	CLA	2	0
45	4	302	A86	7	0
33	4	308	CLA	8	0
36	a	403	LHG	1	0
43	4	317	LMU	13	0
46	9	303	DD6	1	0
33	2	311	CLA	10	0
33	4	309	CLA	2	0
33	4	311	CLA	2	0
45	7	301	A86	2	0
39	m	201	LMG	2	0
30	C	515	BCR	3	0
45	5	306	A86	2	0
33	3	312	CLA	4	0
37	B	622	SQD	3	0
36	4	318	LHG	2	0
37	t	102	SQD	2	0
33	d	402	CLA	5	0
37	i	101	SQD	1	0
33	1	305	CLA	1	0
33	6	313	CLA	2	0
38	h	102	DGD	1	0
46	1	304	DD6	3	0
33	B	613	CLA	2	0
36	7	316	LHG	1	0
33	7	307	CLA	3	0
30	c	514	BCR	4	0
33	b	614	CLA	3	0
37	0	316	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	5	303	A86	1	0
36	3	318	LHG	2	0
39	7	315	LMG	1	0
33	3	306	CLA	1	0
43	w	302	LMU	5	0
36	a	404	LHG	1	0
42	V	201	HEM	2	0
33	c	504	CLA	2	0
45	5	305	A86	2	0
30	b	619	BCR	2	0
39	0	314	LMG	2	0
33	9	311	CLA	3	0
39	b	623	LMG	4	0
33	c	501	CLA	2	0
33	B	608	CLA	1	0
33	c	510	CLA	1	0
30	B	619	BCR	3	0
33	w	303	CLA	5	0
33	A	408	CLA	1	0
33	5	314	CLA	8	0
33	7	304	CLA	2	0
33	c	503	CLA	3	0
42	F	101	HEM	9	0
33	c	512	CLA	1	0
33	1	306	CLA	2	0
33	1	307	CLA	3	0
39	d	406	LMG	1	0
35	a	402	BCT	3	0
39	W	301	LMG	2	0
30	h	101	BCR	5	0
33	B	601	CLA	1	0
44	6	314	KC1	6	0
46	2	303	DD6	6	0
45	6	301	A86	10	0
30	H	101	BCR	1	0
33	C	504	CLA	1	0
33	4	314	CLA	2	0
33	c	509	CLA	2	0
33	C	503	CLA	4	0
38	c	518	DGD	2	0
30	d	403	BCR	1	0
33	4	305	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	3	315	DD6	1	0
45	5	301	A86	9	0
46	4	303	DD6	1	0
33	7	312	CLA	4	0
33	B	616	CLA	1	0
36	5	318	LHG	1	0
30	D	407	BCR	1	0
33	6	308	CLA	2	0
33	C	506	CLA	1	0
33	D	405	CLA	1	0
33	5	313	CLA	14	0
33	C	510	CLA	2	0
33	9	310	CLA	5	0
33	5	316	CLA	10	0
33	6	310	CLA	1	0
45	1	302	A86	5	0
46	1	303	DD6	2	0
34	a	409	PHO	1	0
43	5	320	LMU	11	0
33	7	309	CLA	2	0
33	8	310	CLA	9	0
36	A	412	LHG	3	0
45	6	302	A86	3	0
33	5	312	CLA	2	0
39	b	621	LMG	1	0
33	W	303	CLA	6	0
33	1	314	CLA	1	0
41	d	404	PL9	1	0
33	d	401	CLA	1	0
34	A	407	PHO	1	0
33	C	501	CLA	2	0
33	0	311	CLA	2	0
43	t	101	LMU	1	0
30	a	412	BCR	4	0
43	3	301	LMU	5	0
33	2	310	CLA	4	0
37	T	103	SQD	1	0
33	1	312	CLA	2	0
46	8	303	DD6	1	0
39	c	519	LMG	4	0
39	d	410	LMG	3	0
33	4	312	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	2	306	CLA	7	0
33	7	311	CLA	1	0
36	d	405	LHG	1	0
33	c	513	CLA	1	0
33	D	406	CLA	2	0
33	0	304	CLA	4	0
33	0	312	CLA	1	0
33	A	404	CLA	1	0
38	a	401	DGD	2	0
33	B	605	CLA	4	0
38	C	517	DGD	3	0
37	a	413	SQD	1	0
30	K	101	BCR	6	0
33	1	313	CLA	3	0
33	8	307	CLA	2	0
33	9	308	CLA	6	0
33	b	603	CLA	2	0
33	c	502	CLA	2	0
30	A	401	BCR	4	0
33	9	315	CLA	1	0
34	a	410	PHO	1	0
33	C	509	CLA	2	0
39	M	201	LMG	1	0
30	K	102	BCR	3	0
33	b	617	CLA	5	0
33	Z	101	CLA	1	0
33	3	307	CLA	18	0
33	7	308	CLA	1	0
33	b	609	CLA	1	0
33	3	303	CLA	2	0
45	2	301	A86	1	0
33	5	308	CLA	3	0
45	8	302	A86	3	0
33	3	319	CLA	2	0
37	D	403	SQD	2	0
33	b	615	CLA	1	0
39	D	404	LMG	2	0
42	v	201	HEM	5	0
33	1	311	CLA	3	0
33	B	611	CLA	1	0
33	4	310	CLA	9	0
33	H	103	CLA	3	0

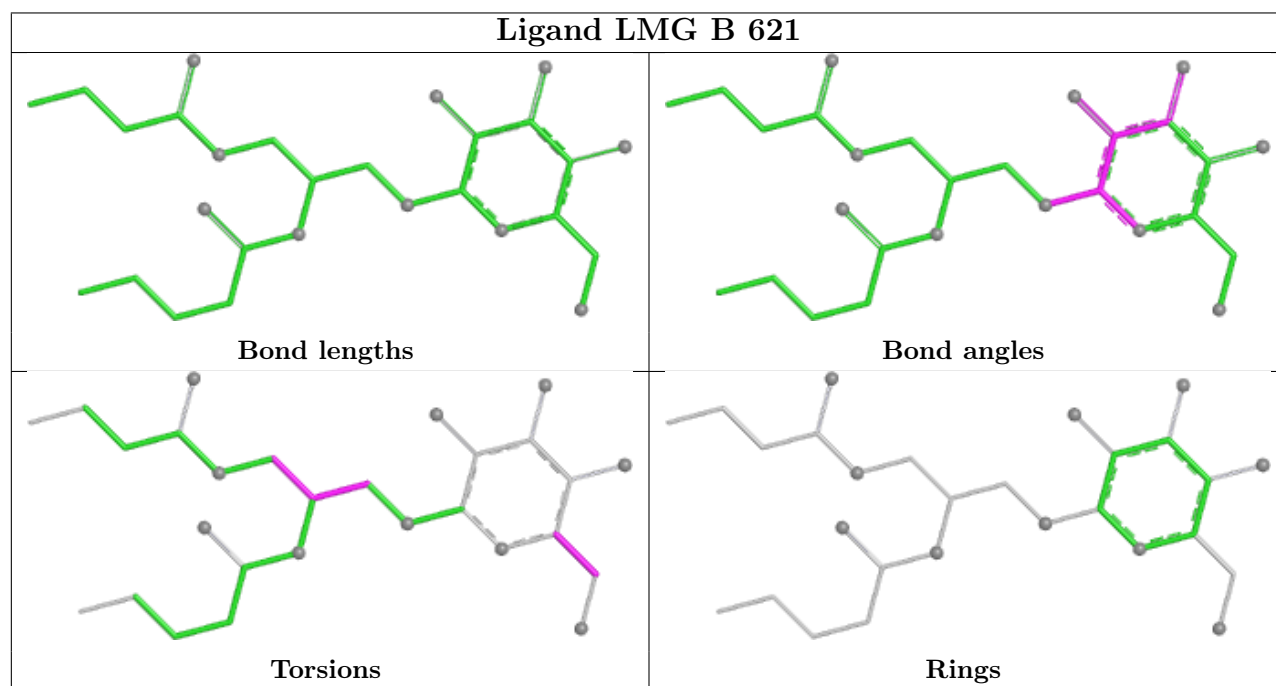
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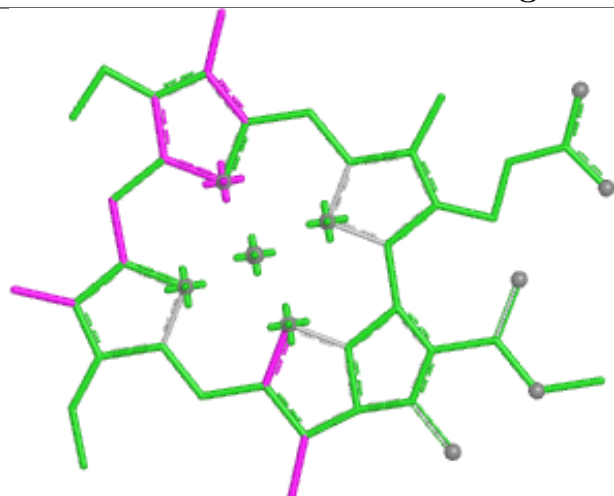
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	b	618	BCR	3	0
33	b	607	CLA	3	0
33	0	310	CLA	2	0
33	B	612	CLA	1	0
45	3	314	A86	2	0
48	7	302	ET4	2	0
30	a	414	BCR	2	0
33	b	616	CLA	1	0
33	b	610	CLA	3	0
45	5	302	A86	14	0
33	6	307	CLA	5	0
33	0	307	CLA	3	0
30	B	618	BCR	2	0
39	w	304	LMG	1	0
33	C	512	CLA	1	0
33	7	305	CLA	4	0
33	0	308	CLA	2	0
33	B	609	CLA	3	0
33	0	305	CLA	3	0
33	B	607	CLA	1	0
33	B	603	CLA	2	0
38	C	516	DGD	3	0
33	1	310	CLA	5	0
47	5	310	KC2	16	0
33	5	311	CLA	4	0
35	A	410	BCT	2	0
33	C	511	CLA	1	0
33	2	313	CLA	2	0
45	0	301	A86	1	0
30	C	514	BCR	3	0
37	T	101	SQD	1	0
42	e	101	HEM	4	0
33	2	315	CLA	1	0
33	6	311	CLA	1	0
46	8	304	DD6	7	0
33	z	101	CLA	1	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

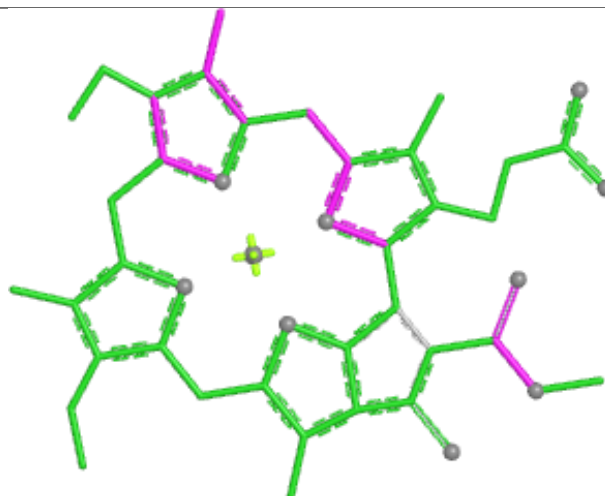
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



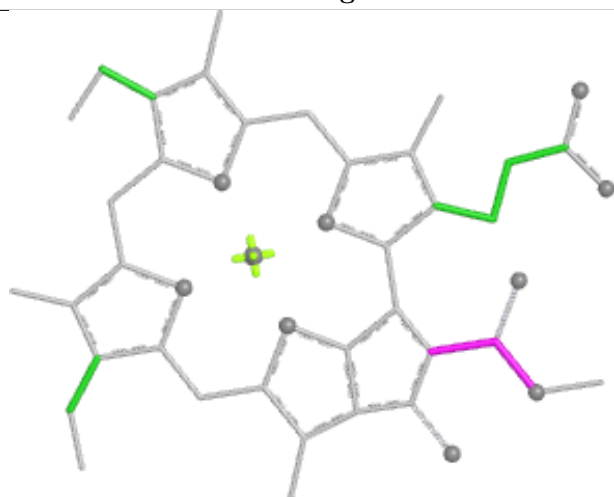
Ligand CLA c 506



Bond lengths



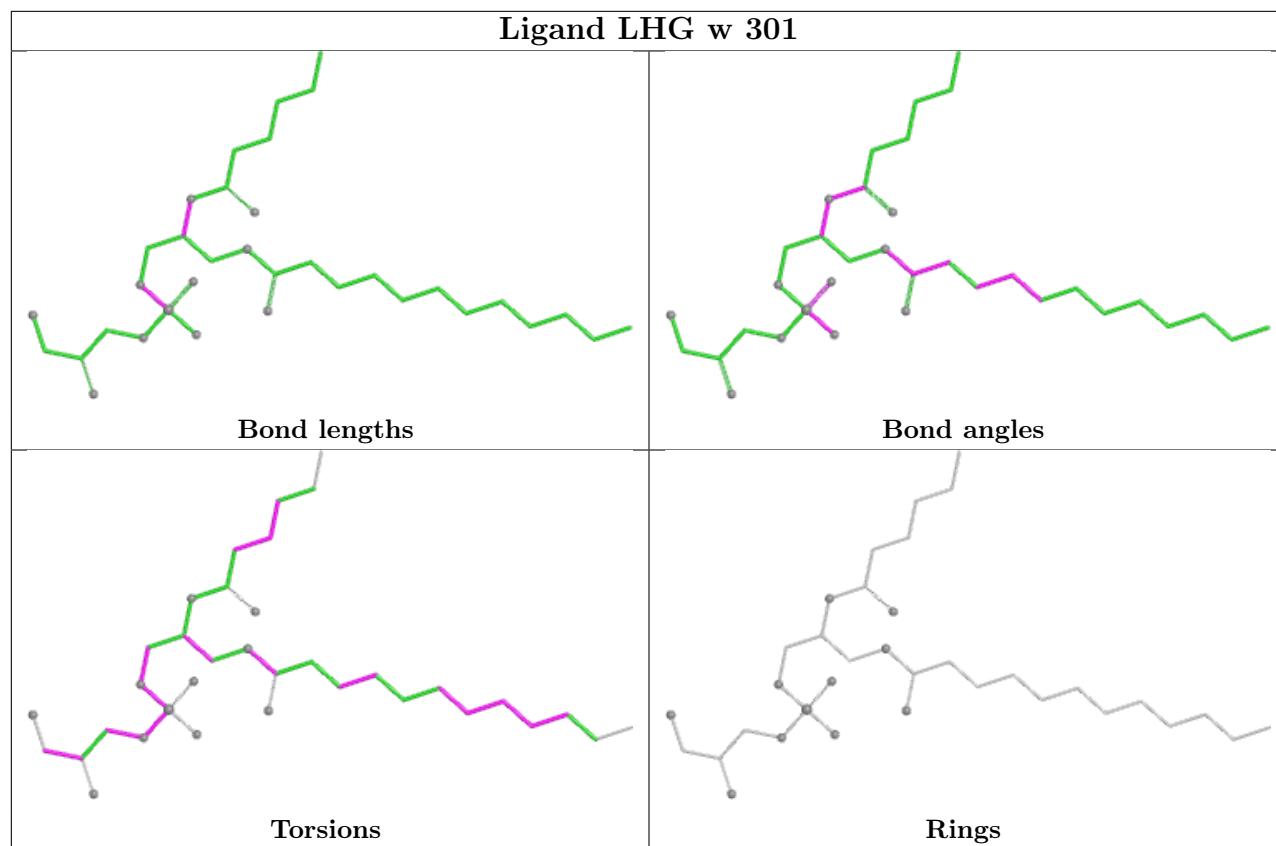
Bond angles



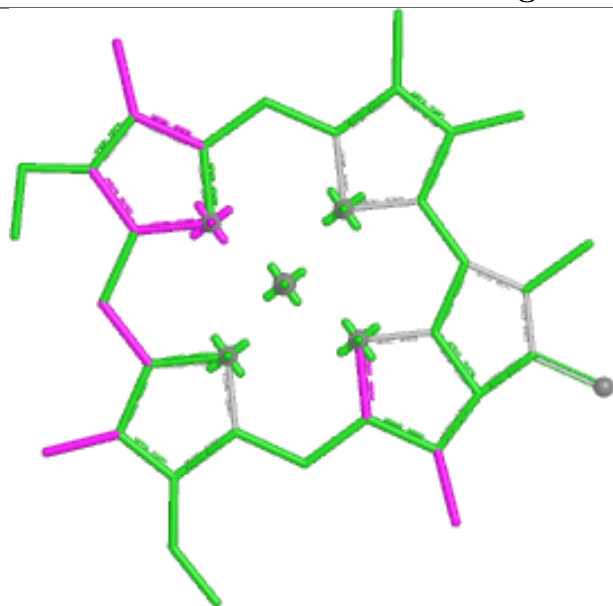
Torsions



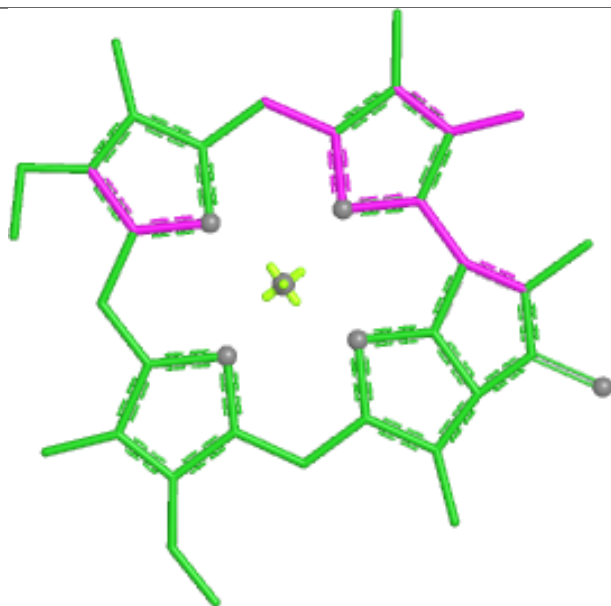
Rings



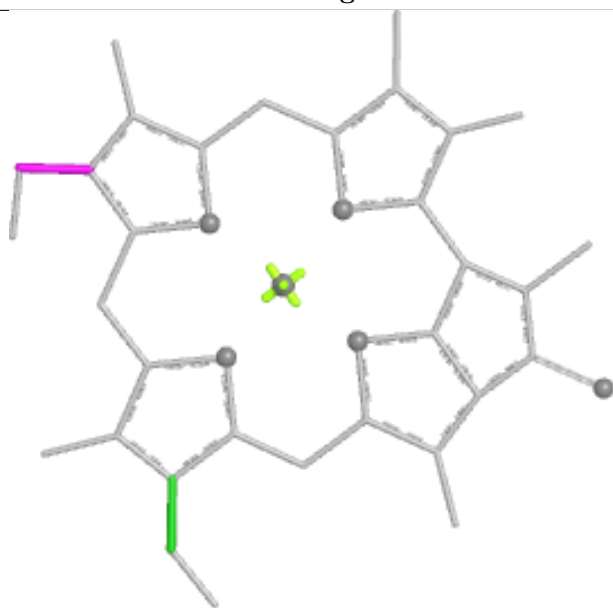
Ligand CLA 9 314



Bond lengths



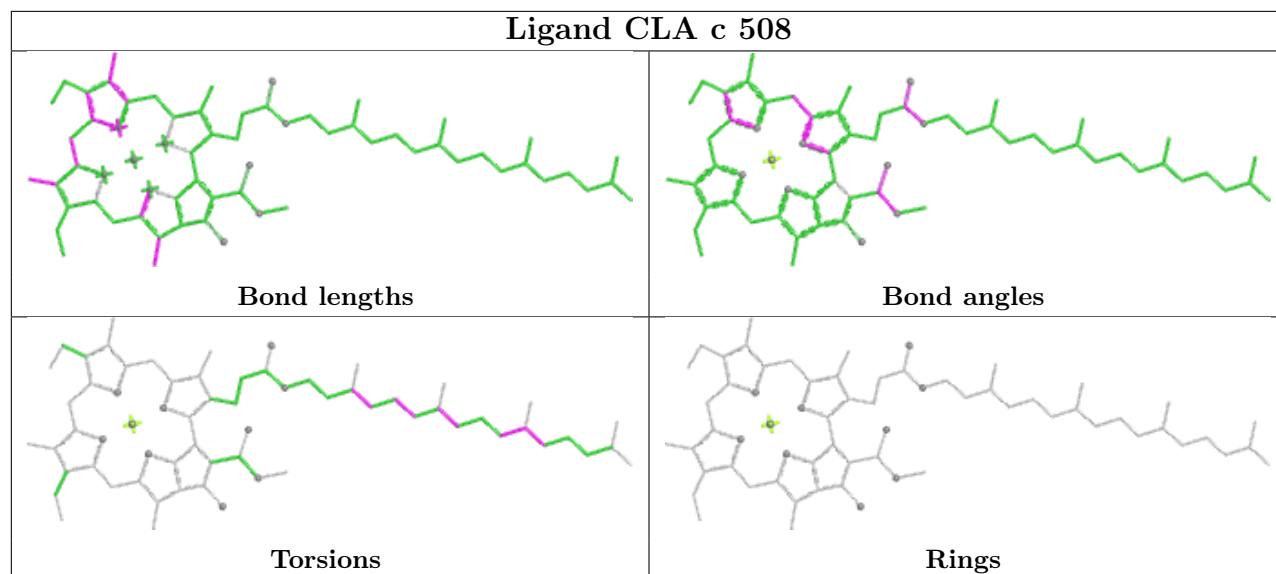
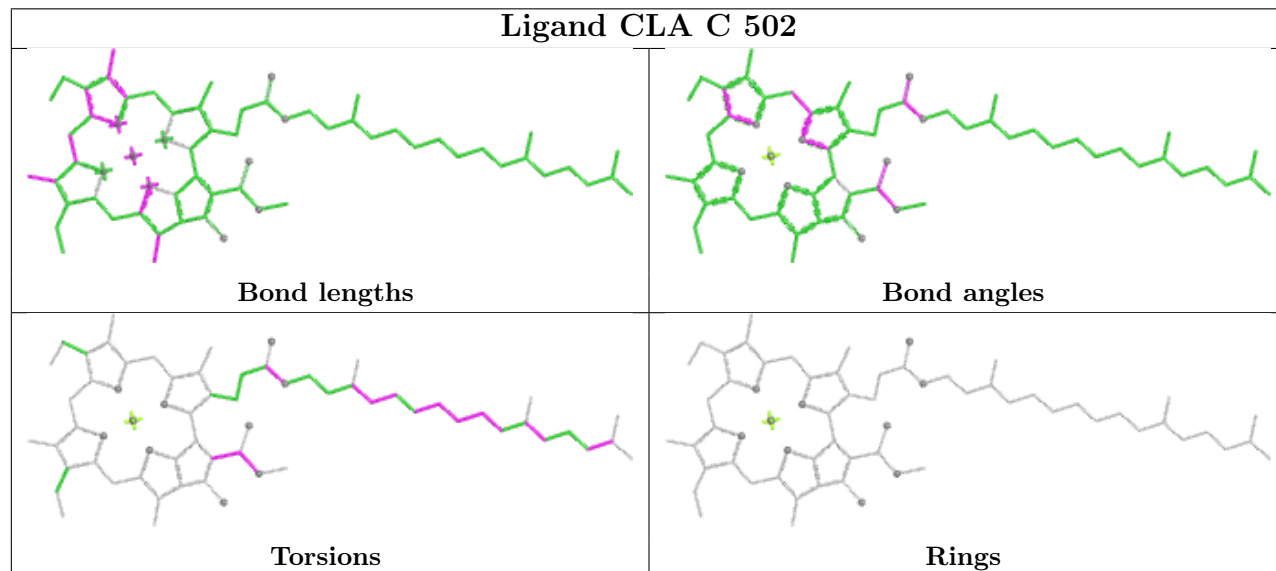
Bond angles



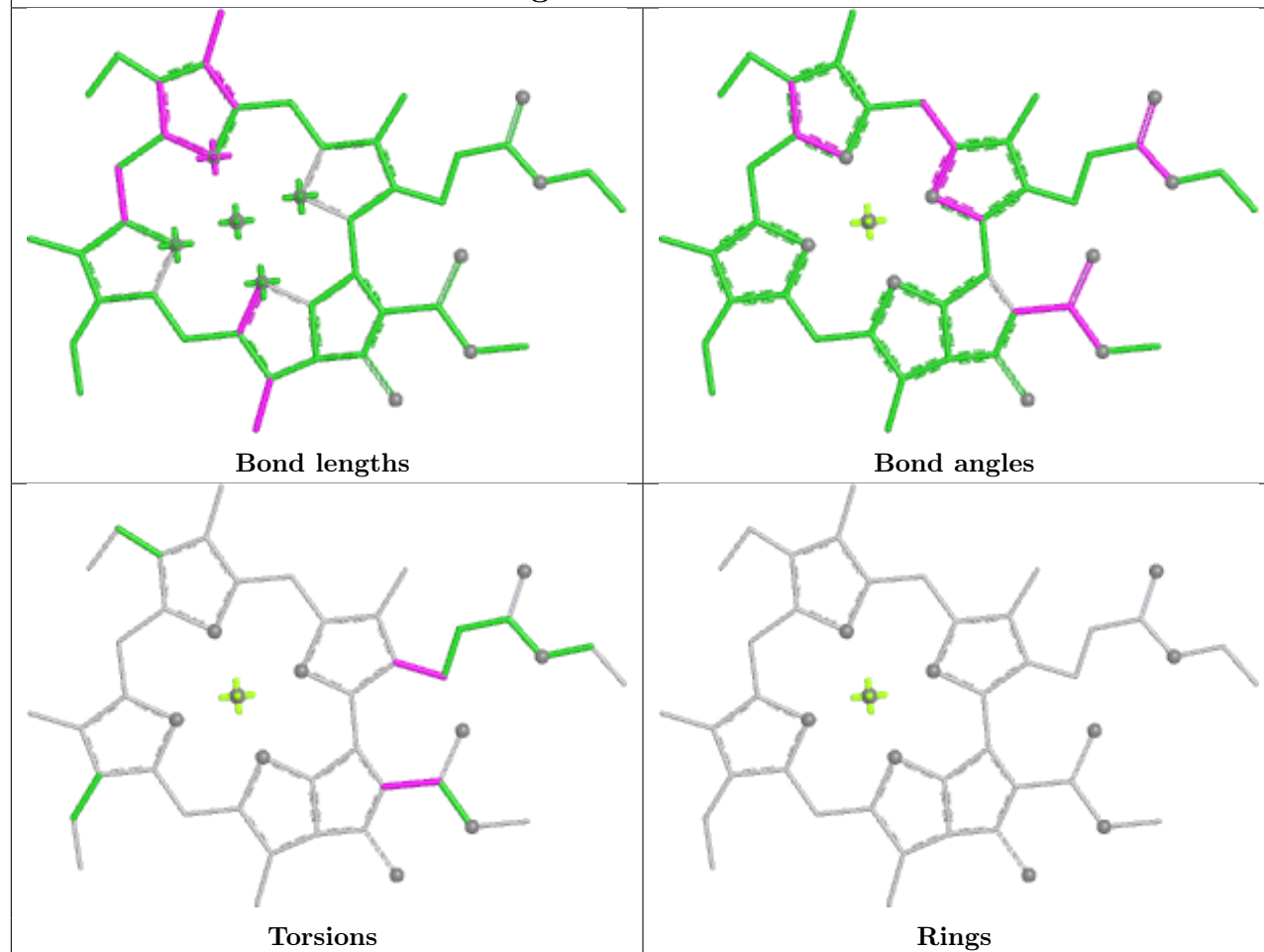
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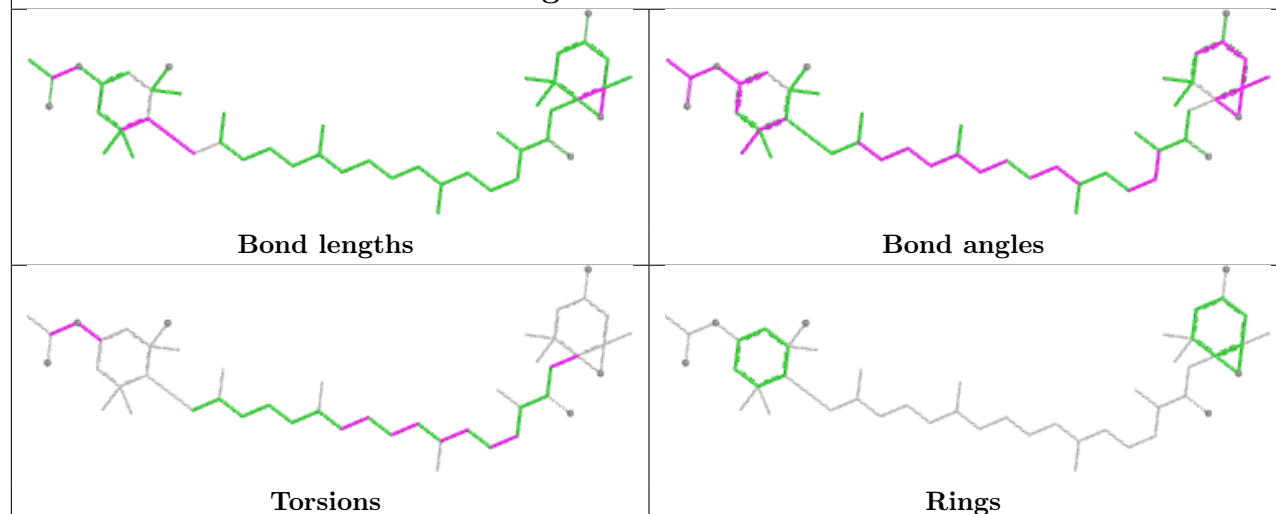
Rings

Ligand CLA c 508**Ligand CLA C 502**

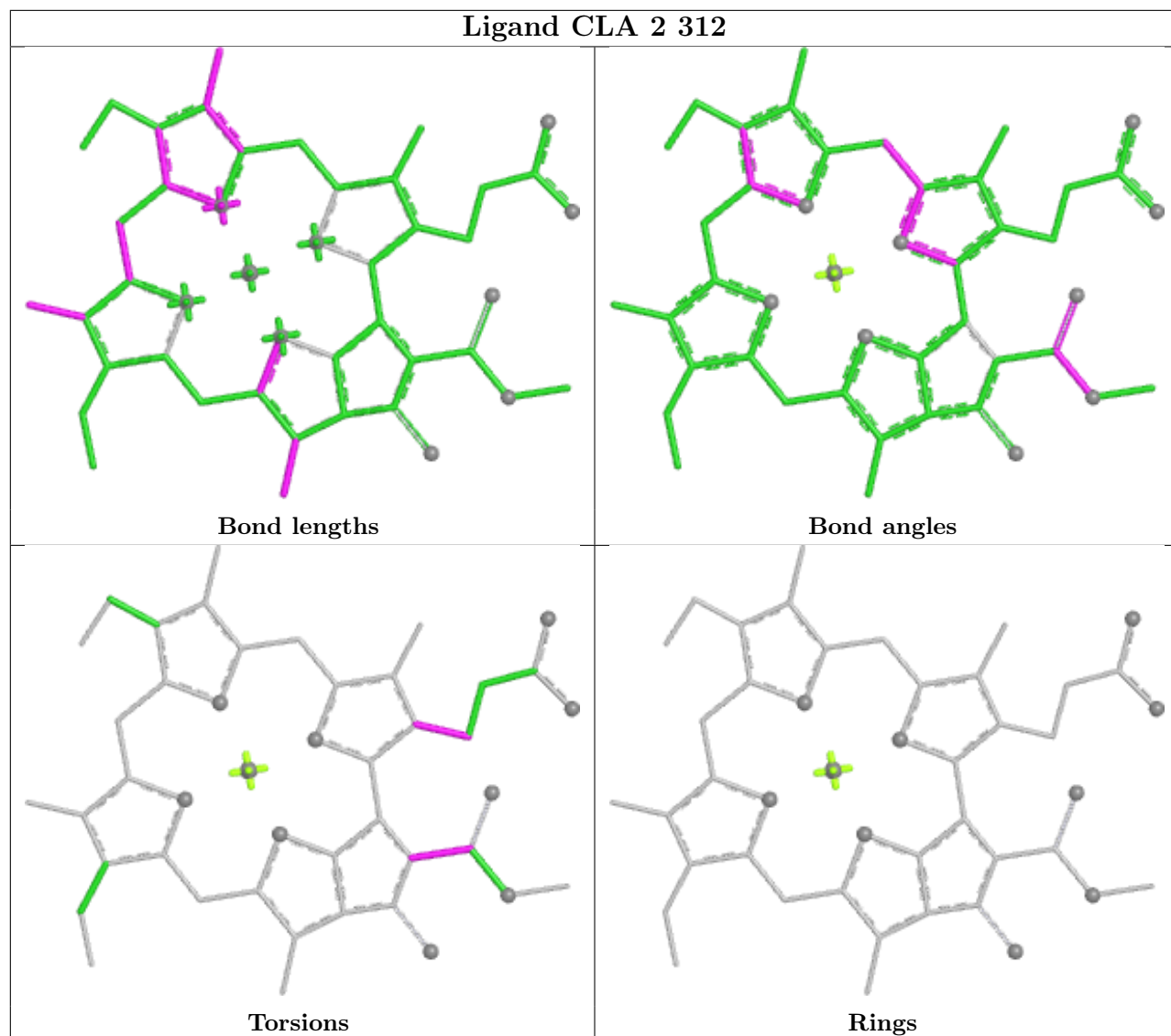
Ligand CLA 4 315

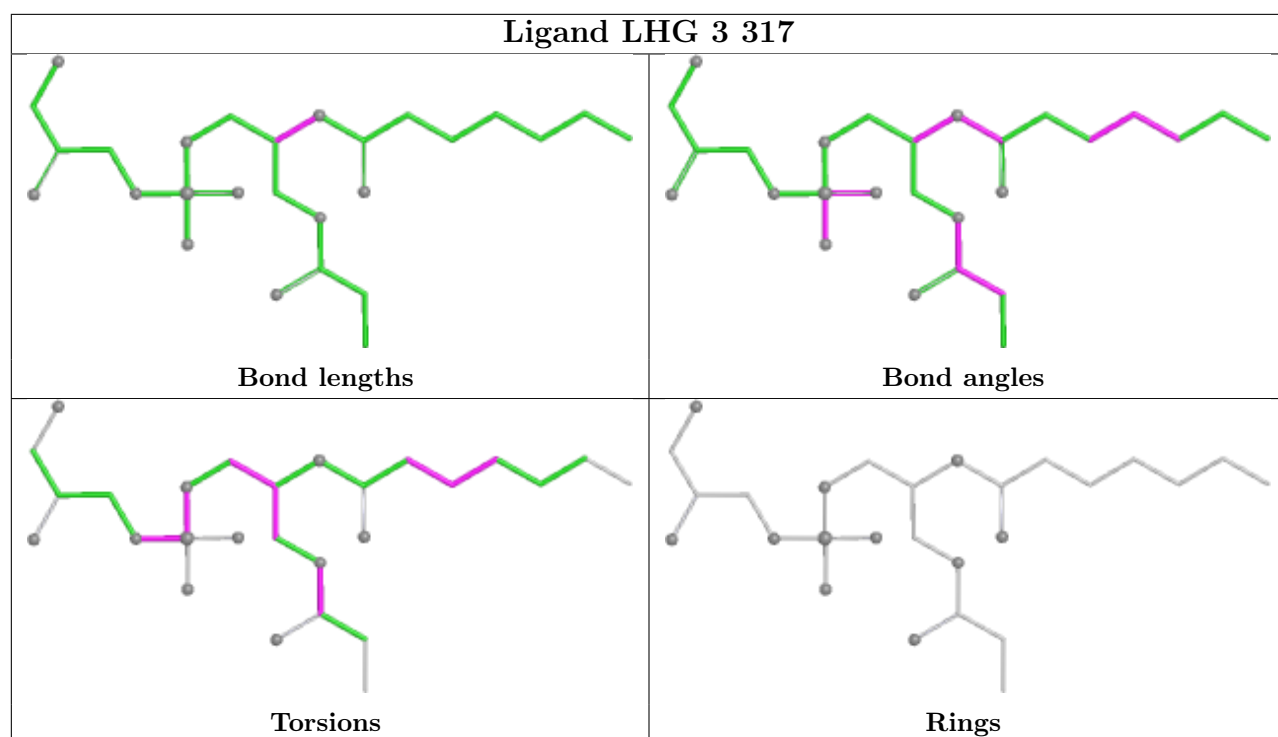


Ligand A86 4 301

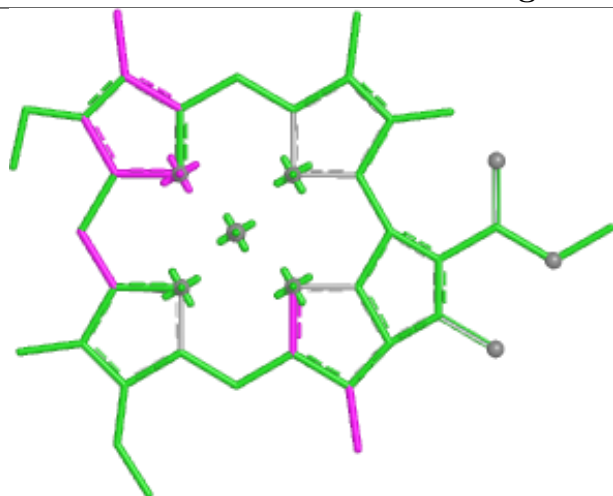


Ligand CLA 2 312

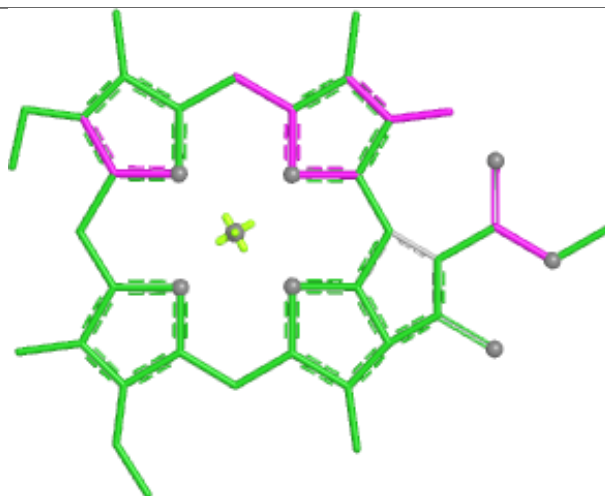




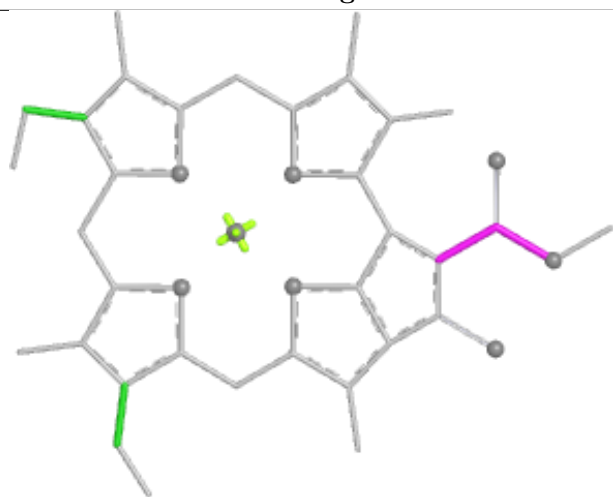
Ligand CLA 6 315



Bond lengths



Bond angles

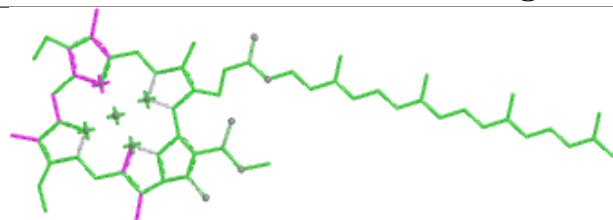


Torsions

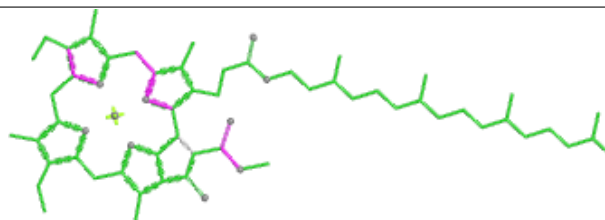


Rings

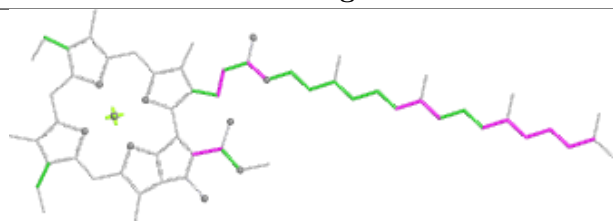
Ligand CLA c 507



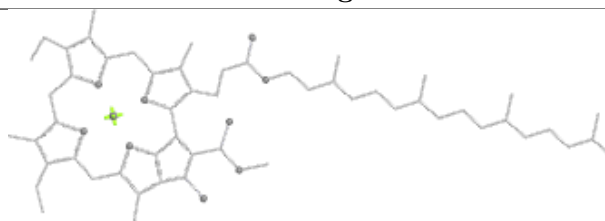
Bond lengths



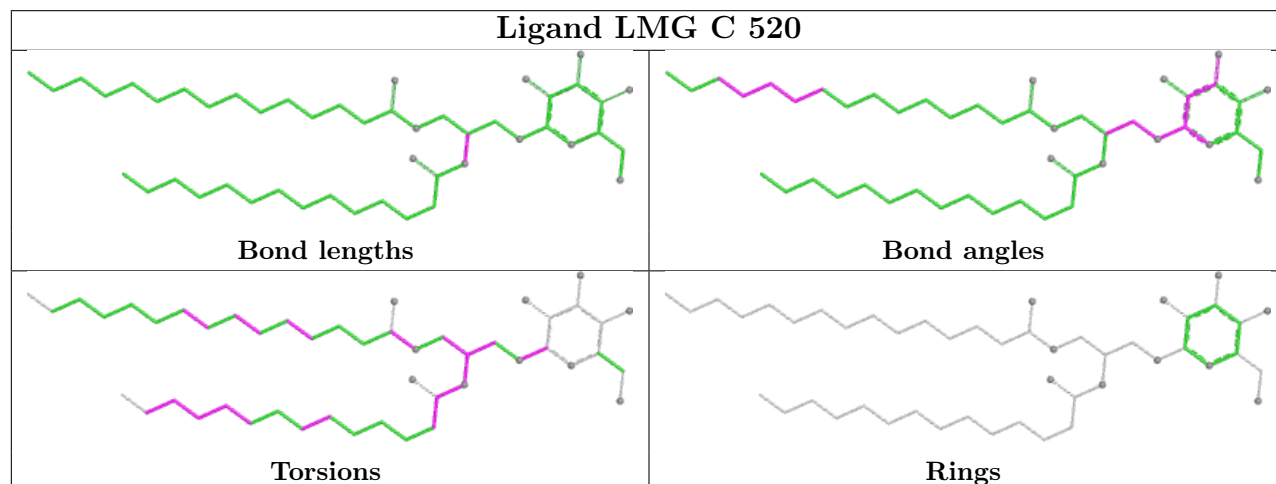
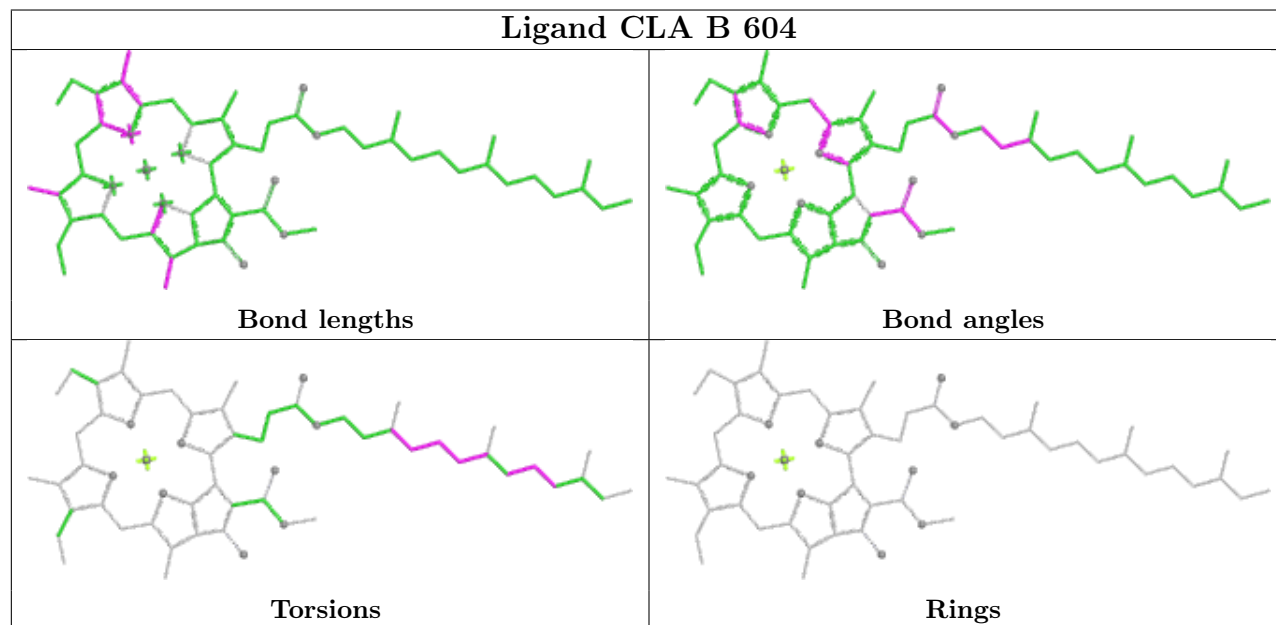
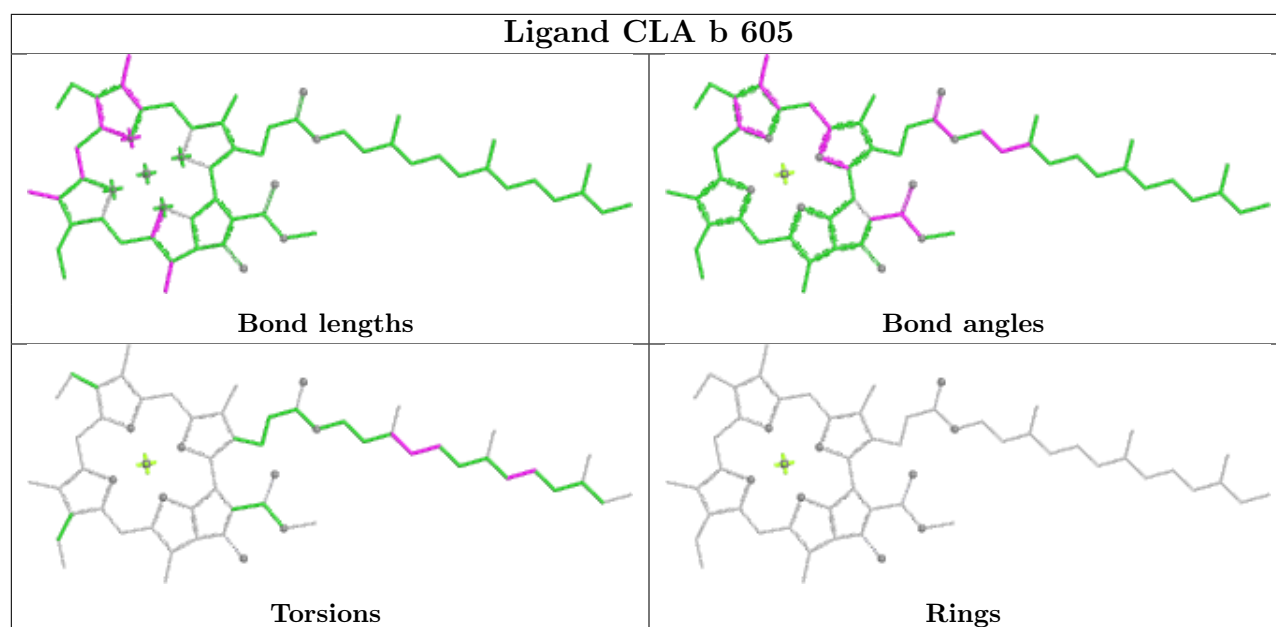
Bond angles

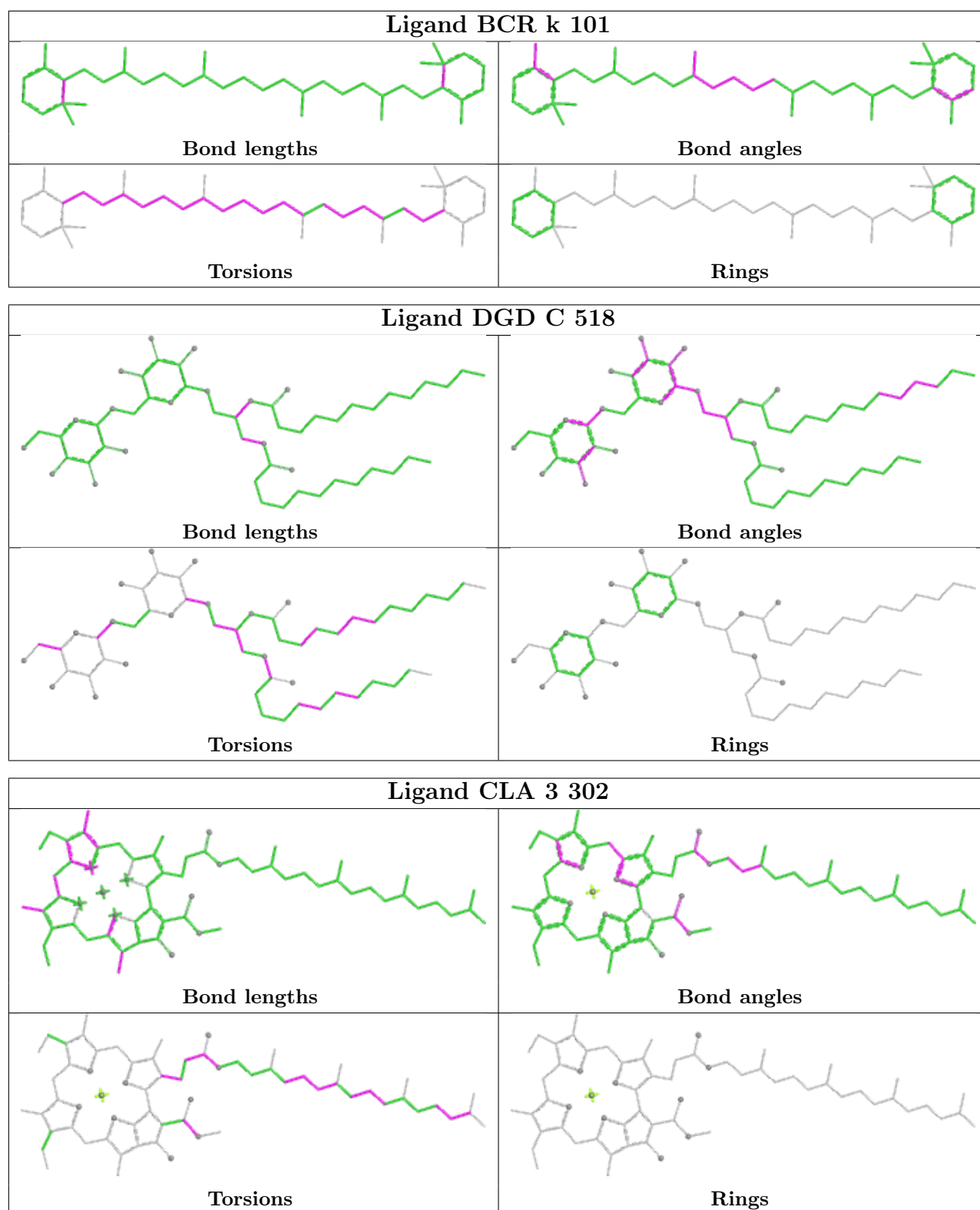


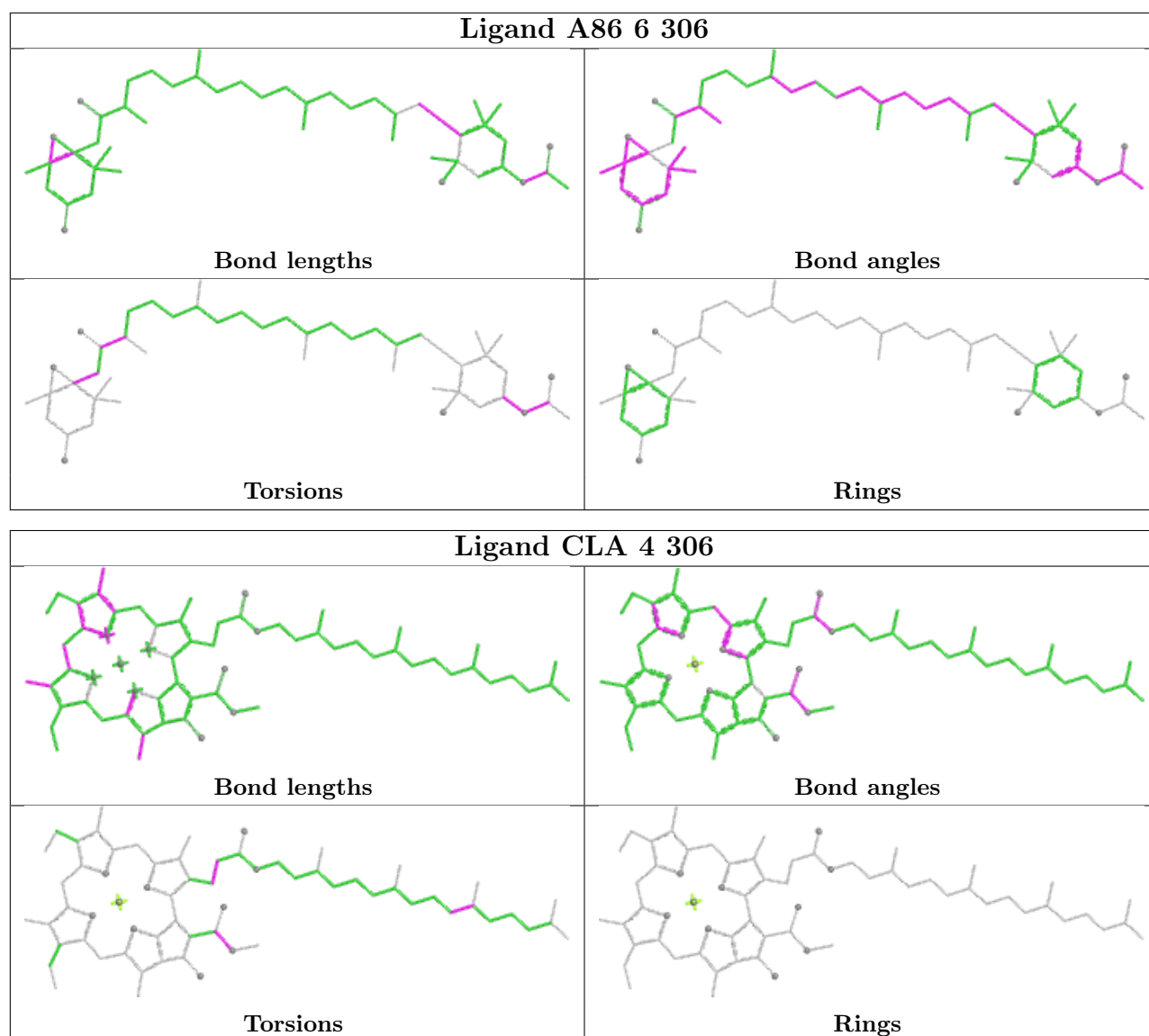
Torsions



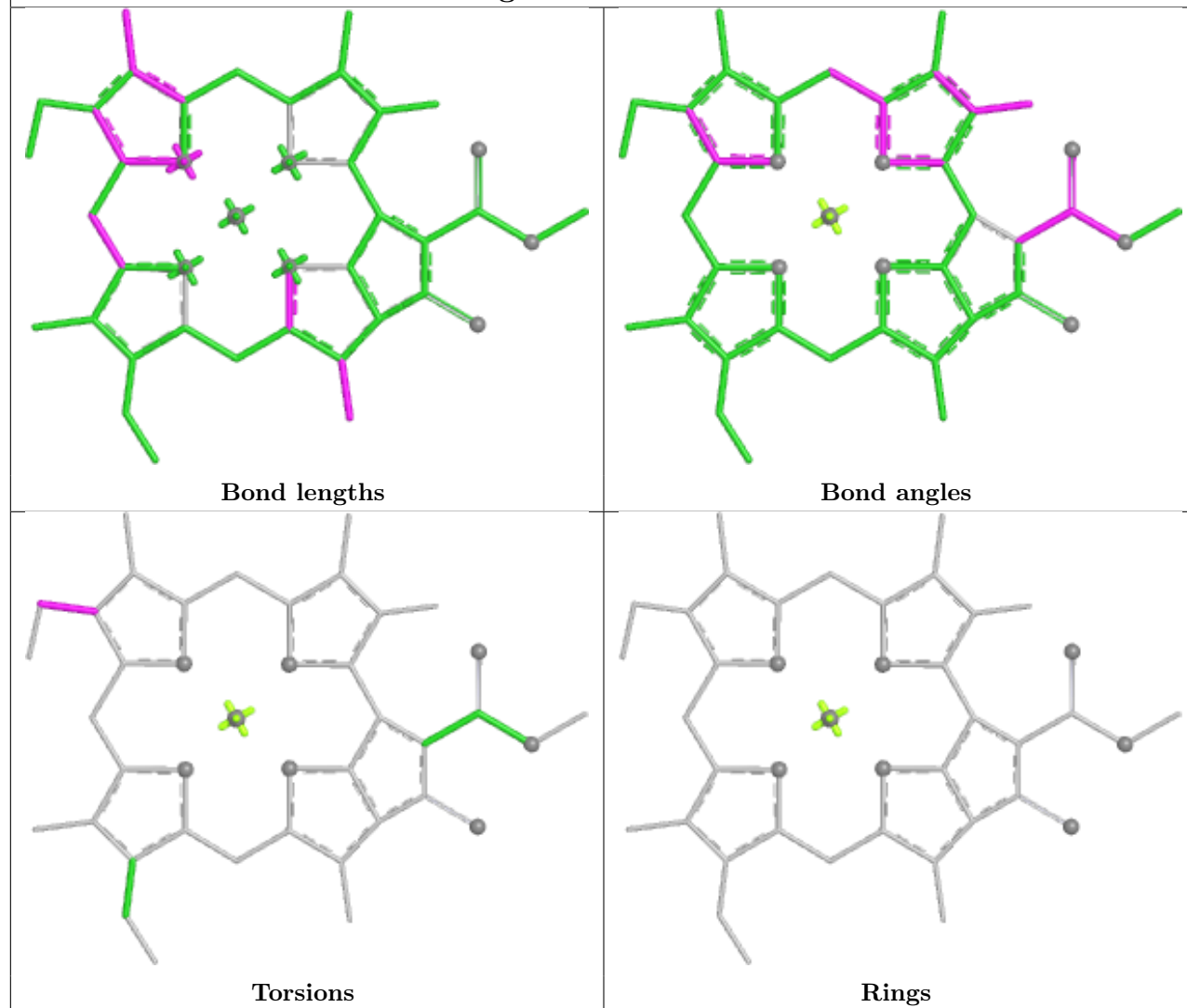
Rings



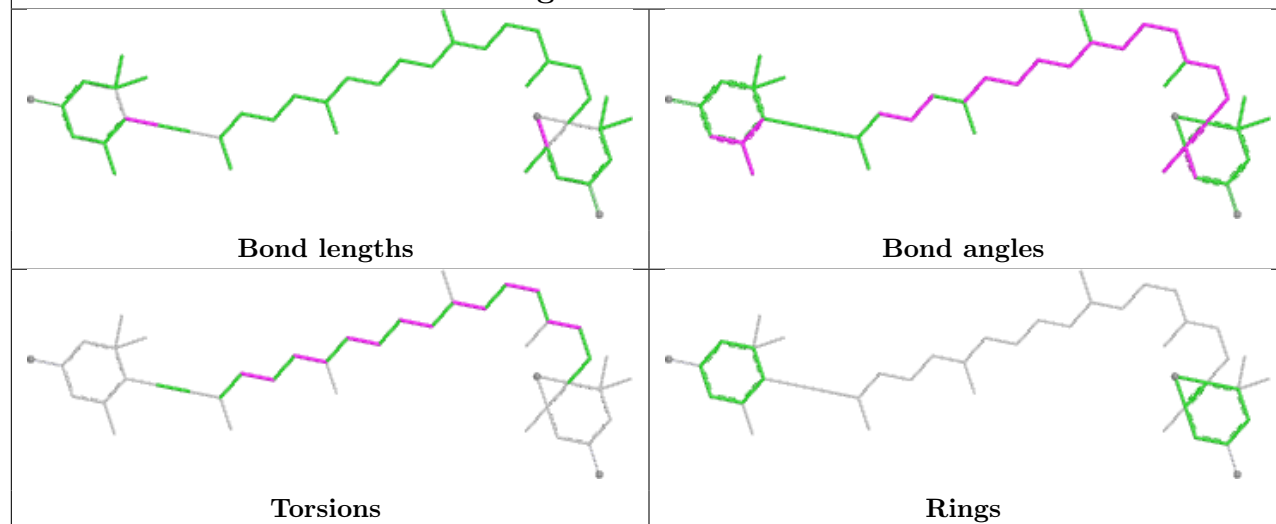


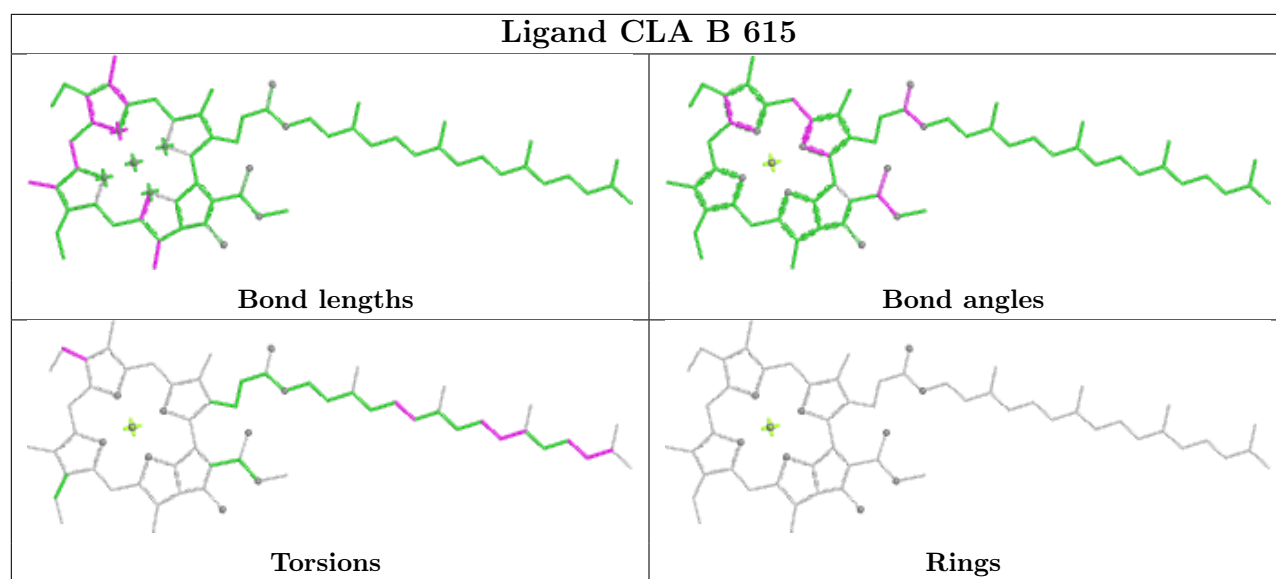


Ligand CLA 2 305

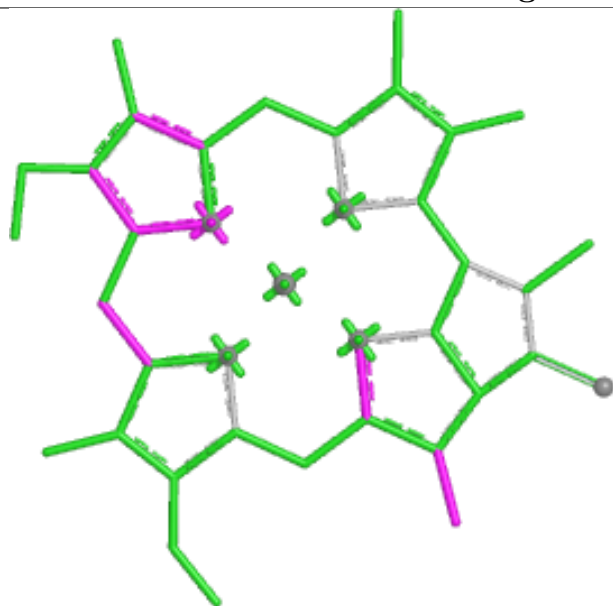


Ligand DD6 2 304

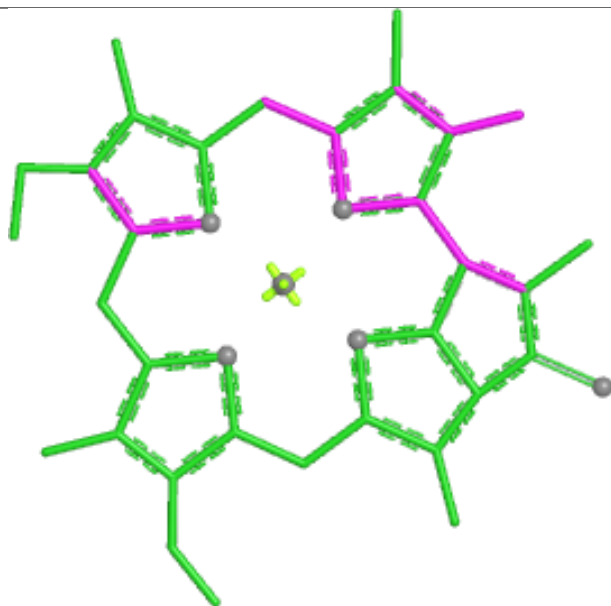




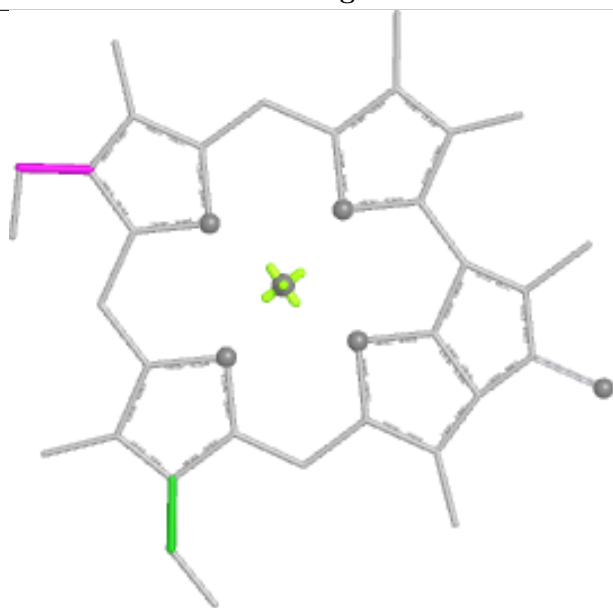
Ligand CLA 5 317



Bond lengths



Bond angles

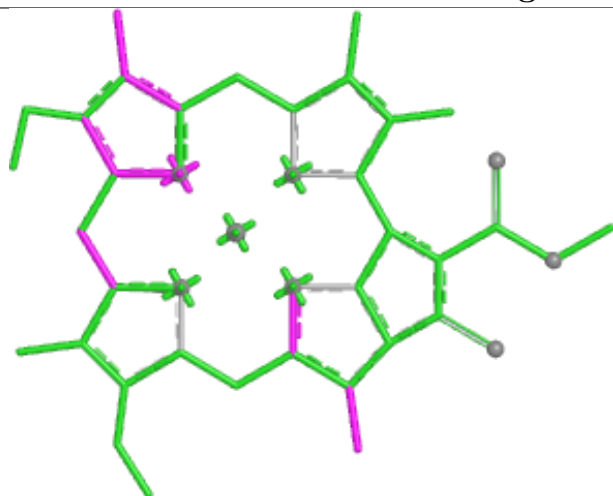


Torsions

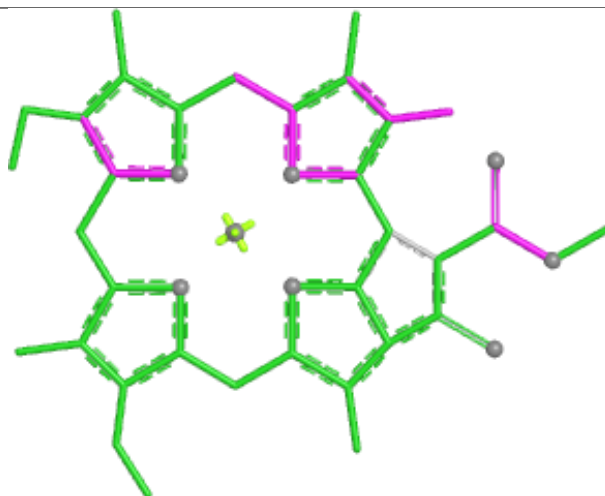


Rings

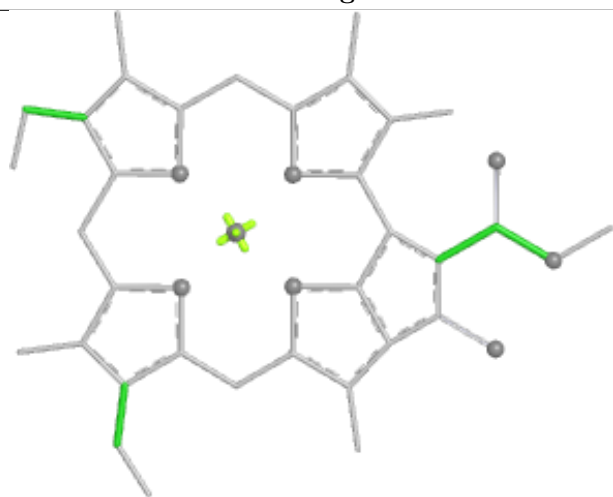
Ligand CLA 4 313



Bond lengths



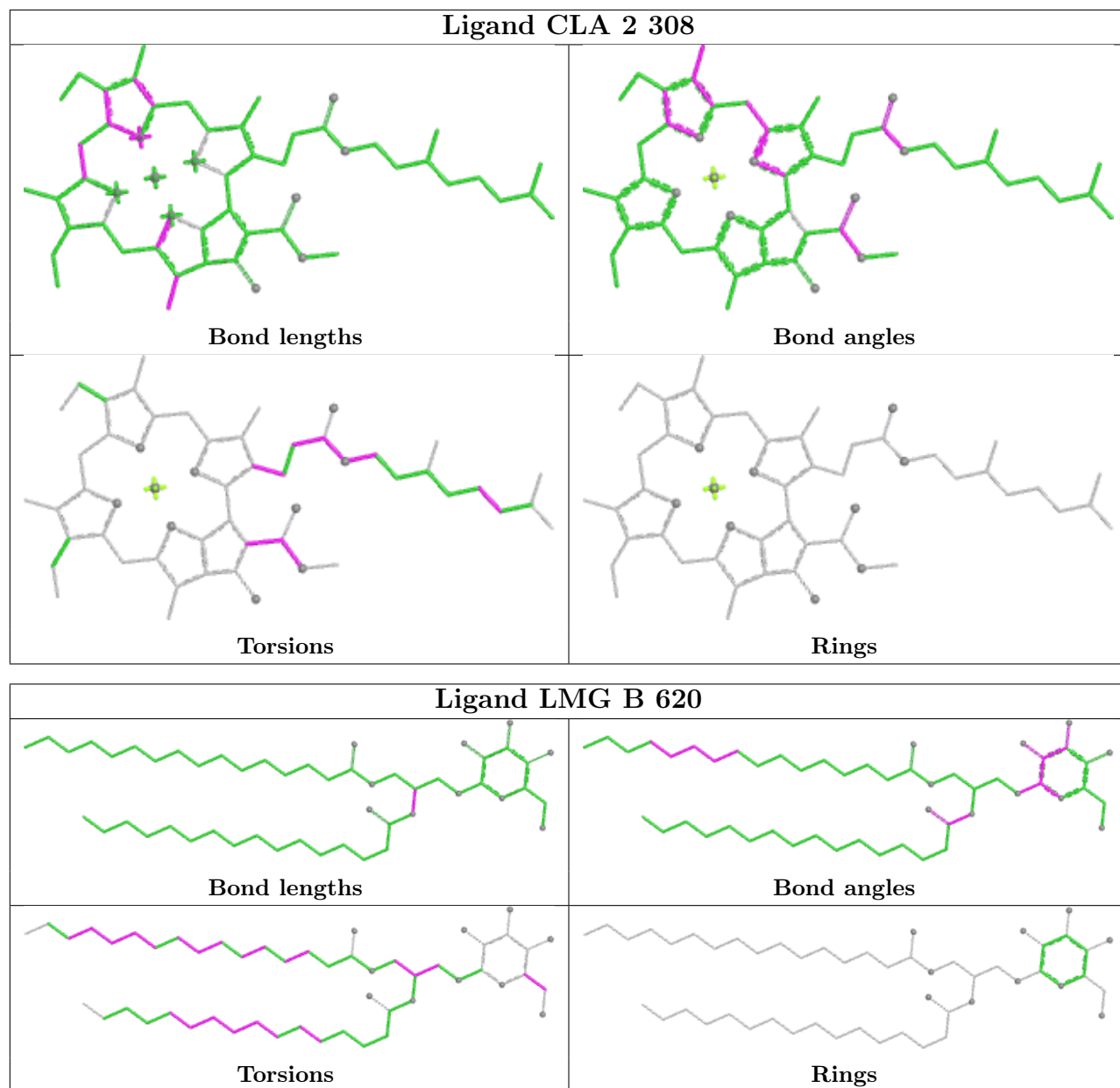
Bond angles

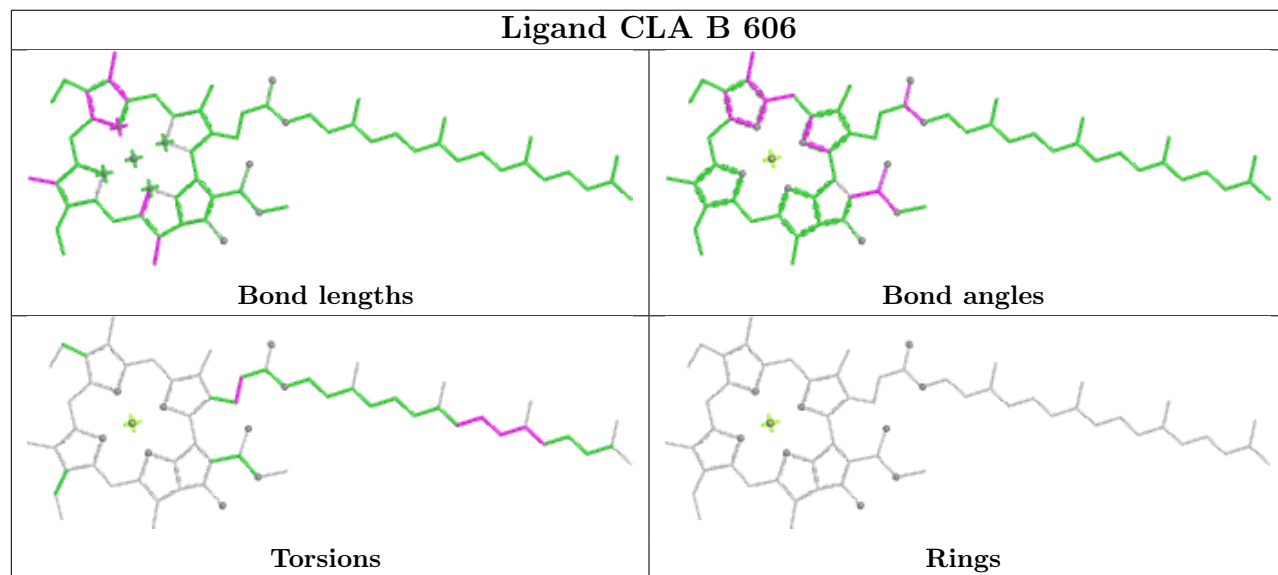
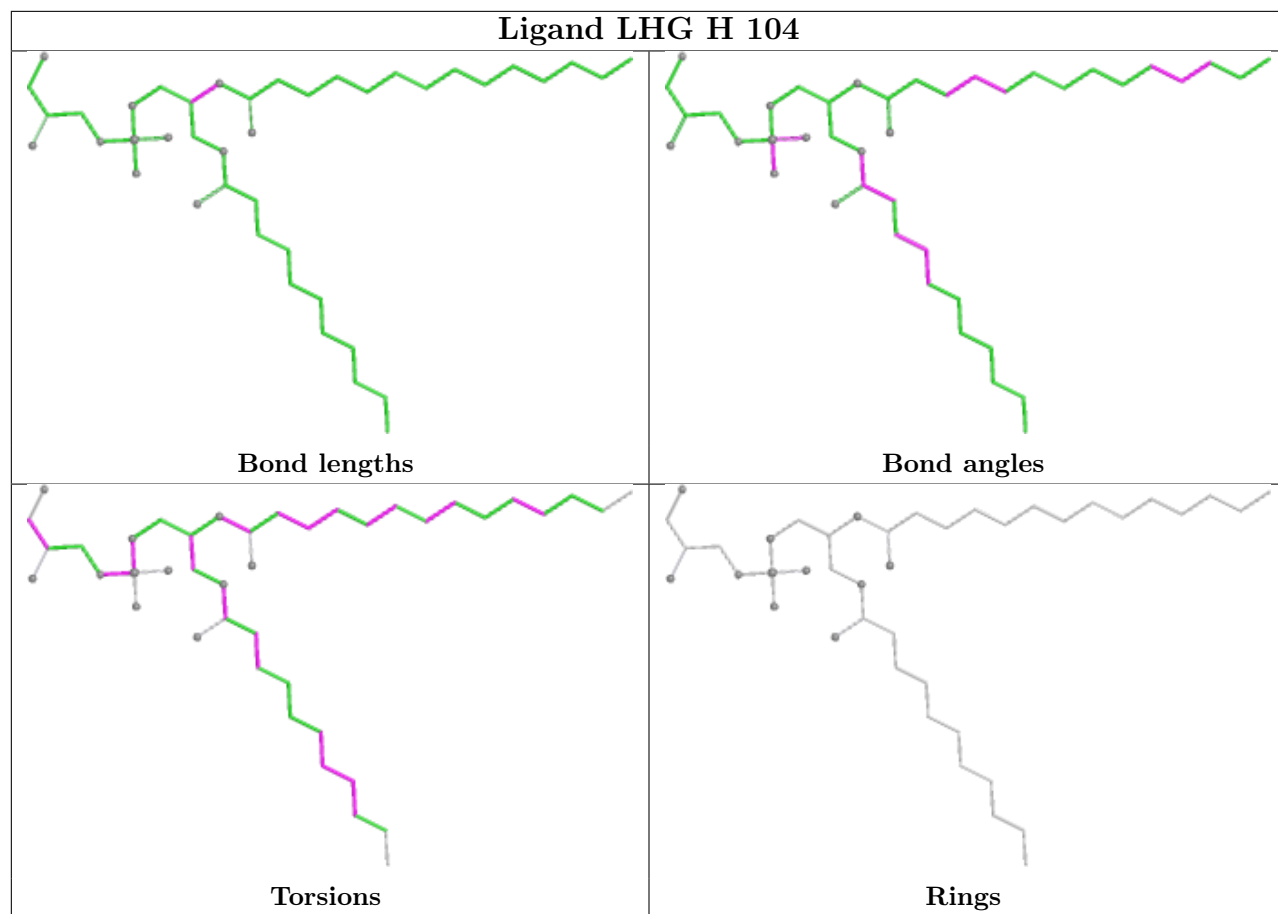


Torsions

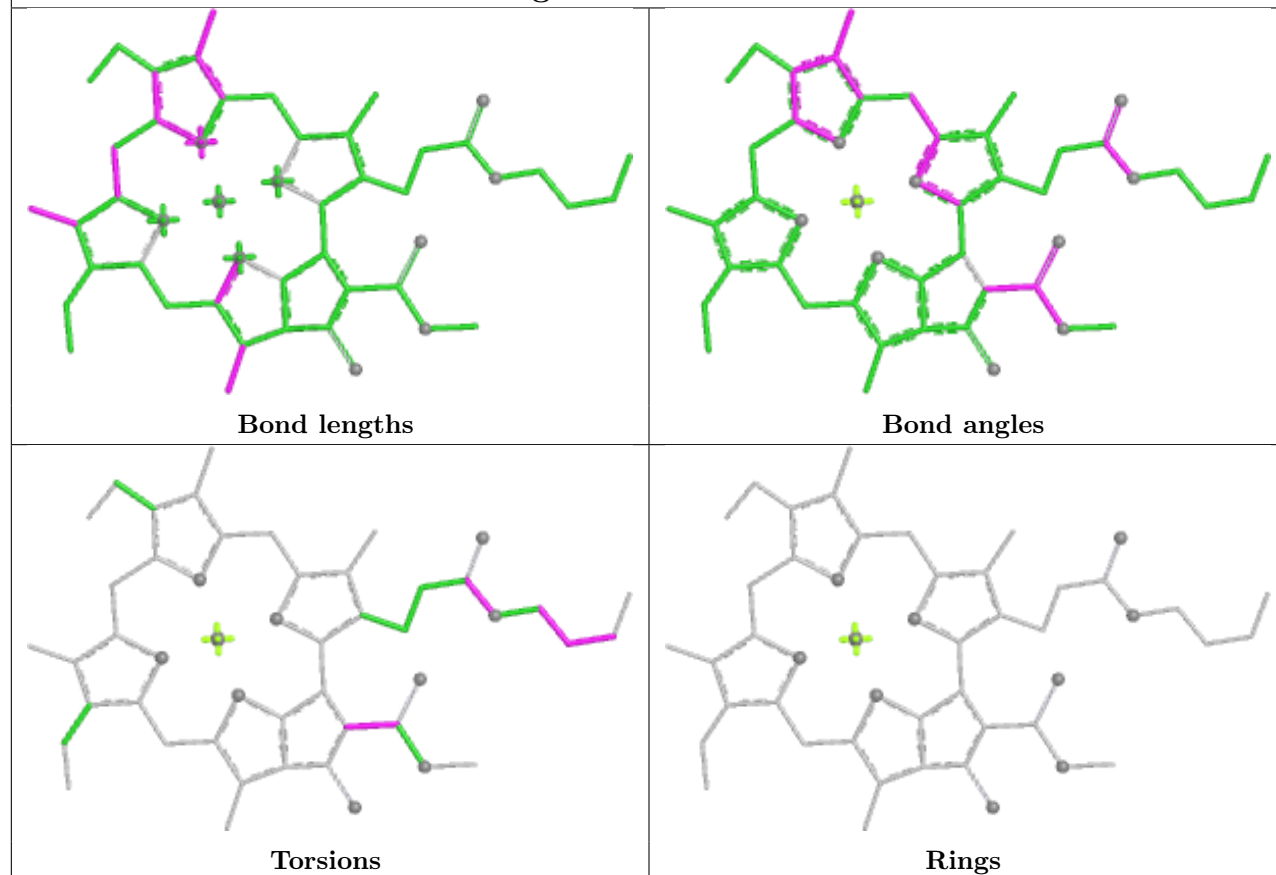


Rings

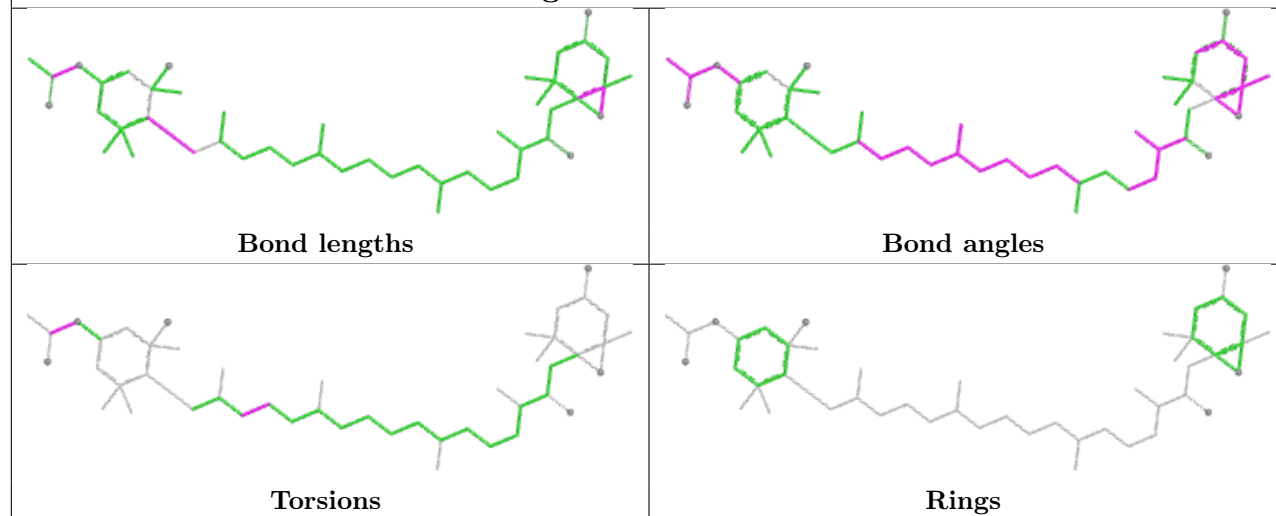


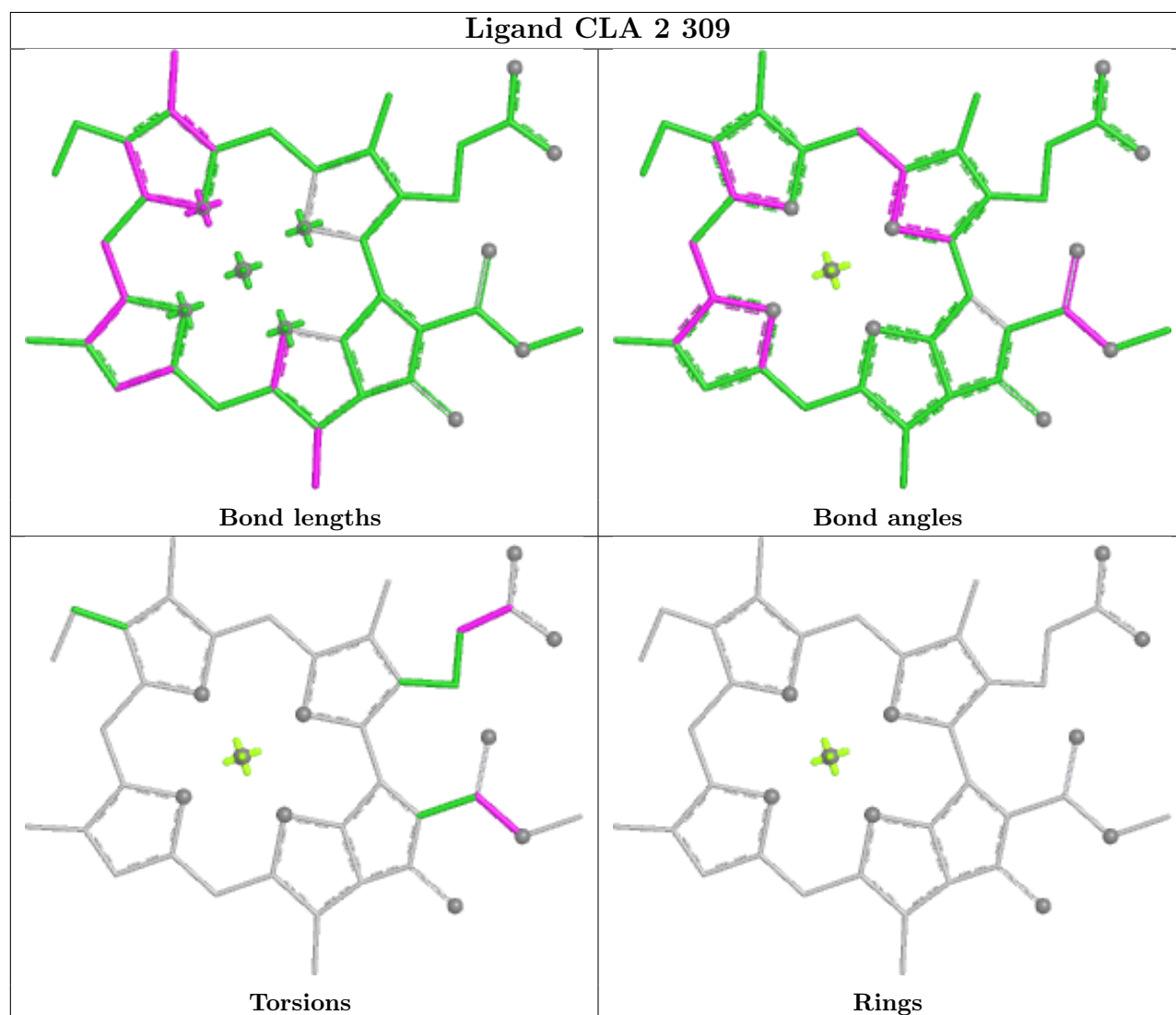
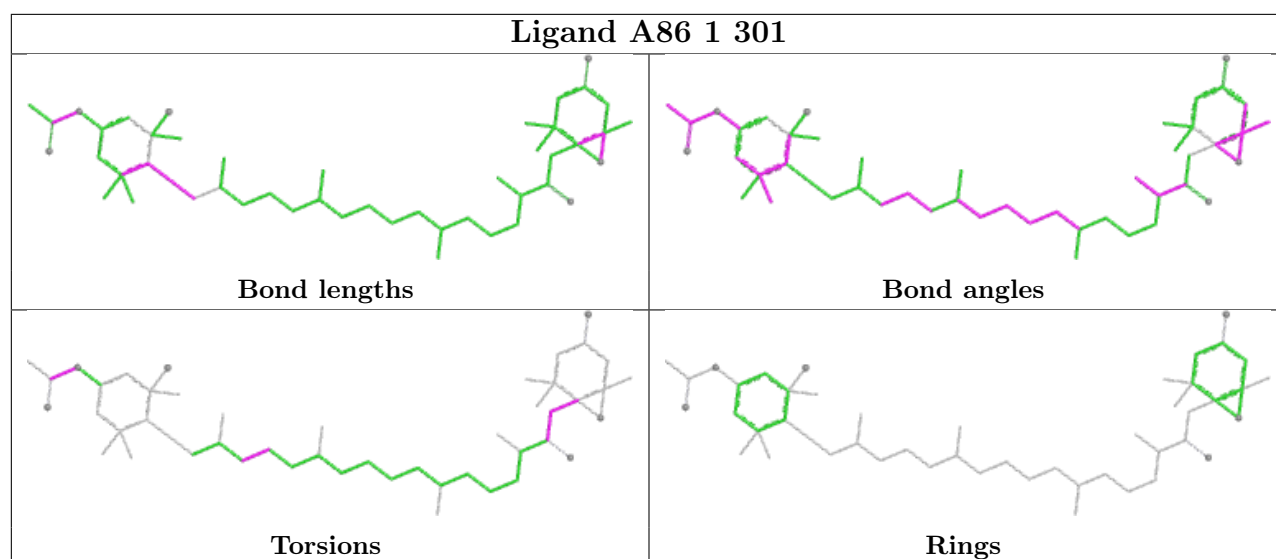


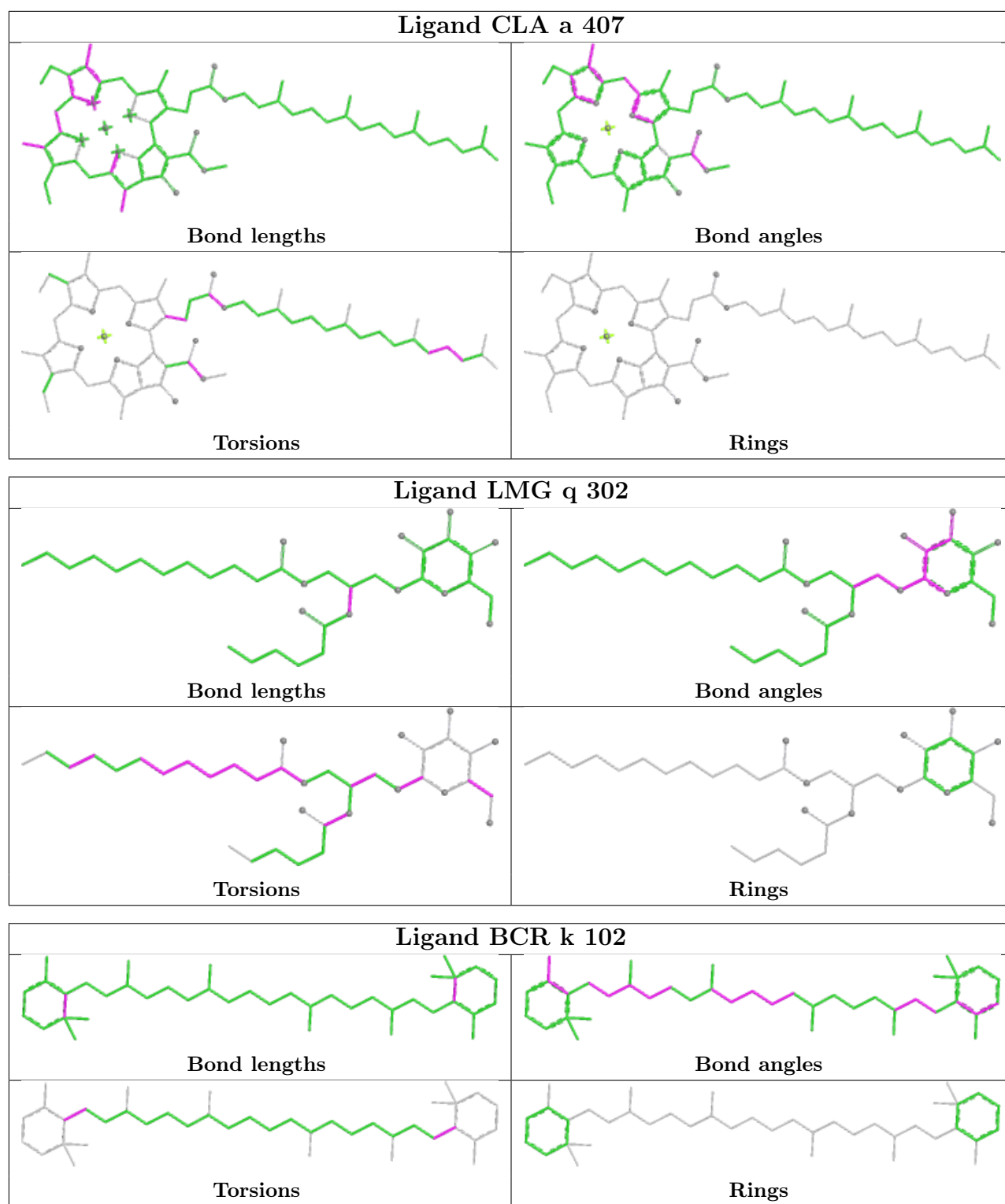
Ligand CLA C 513

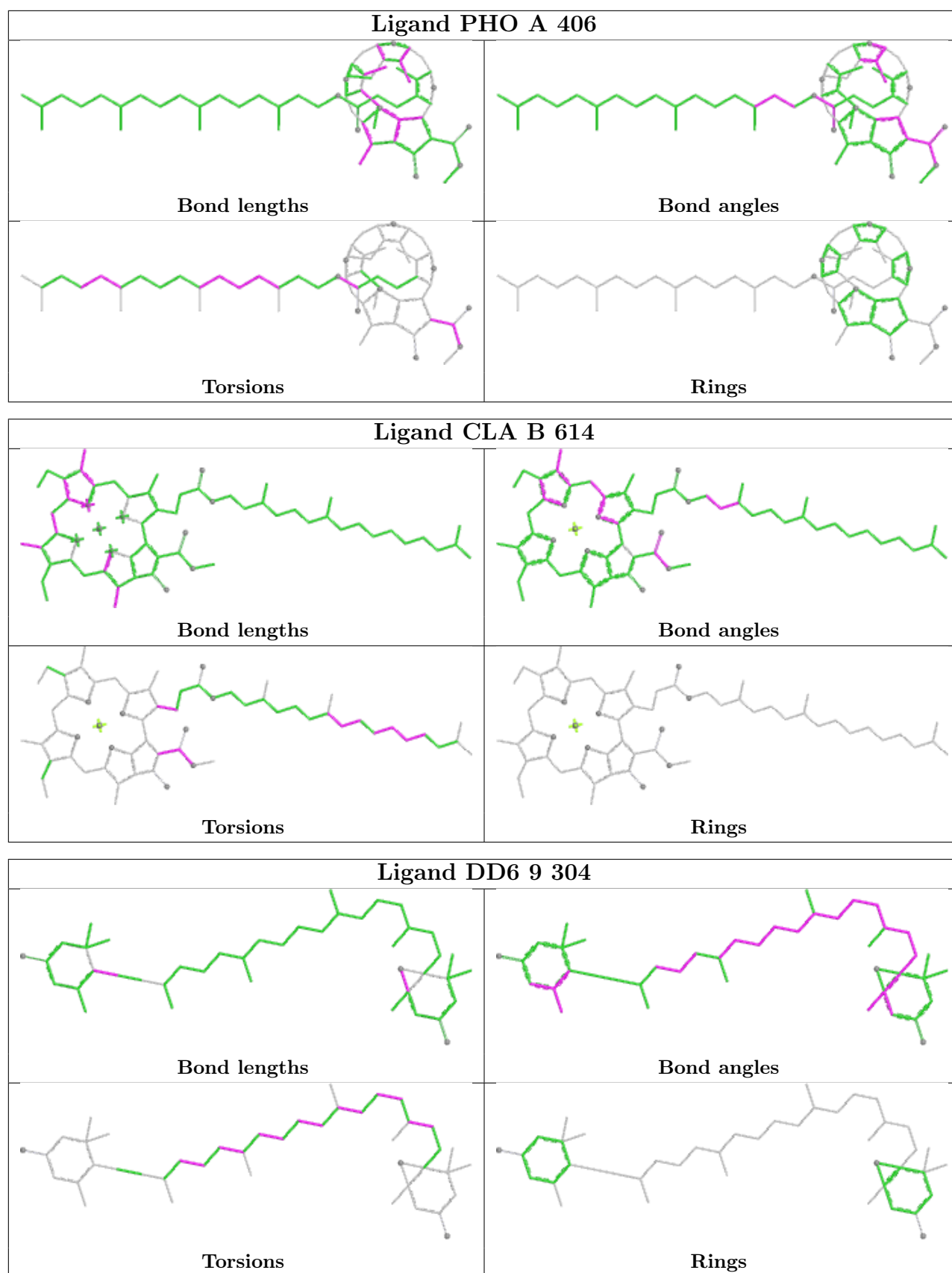


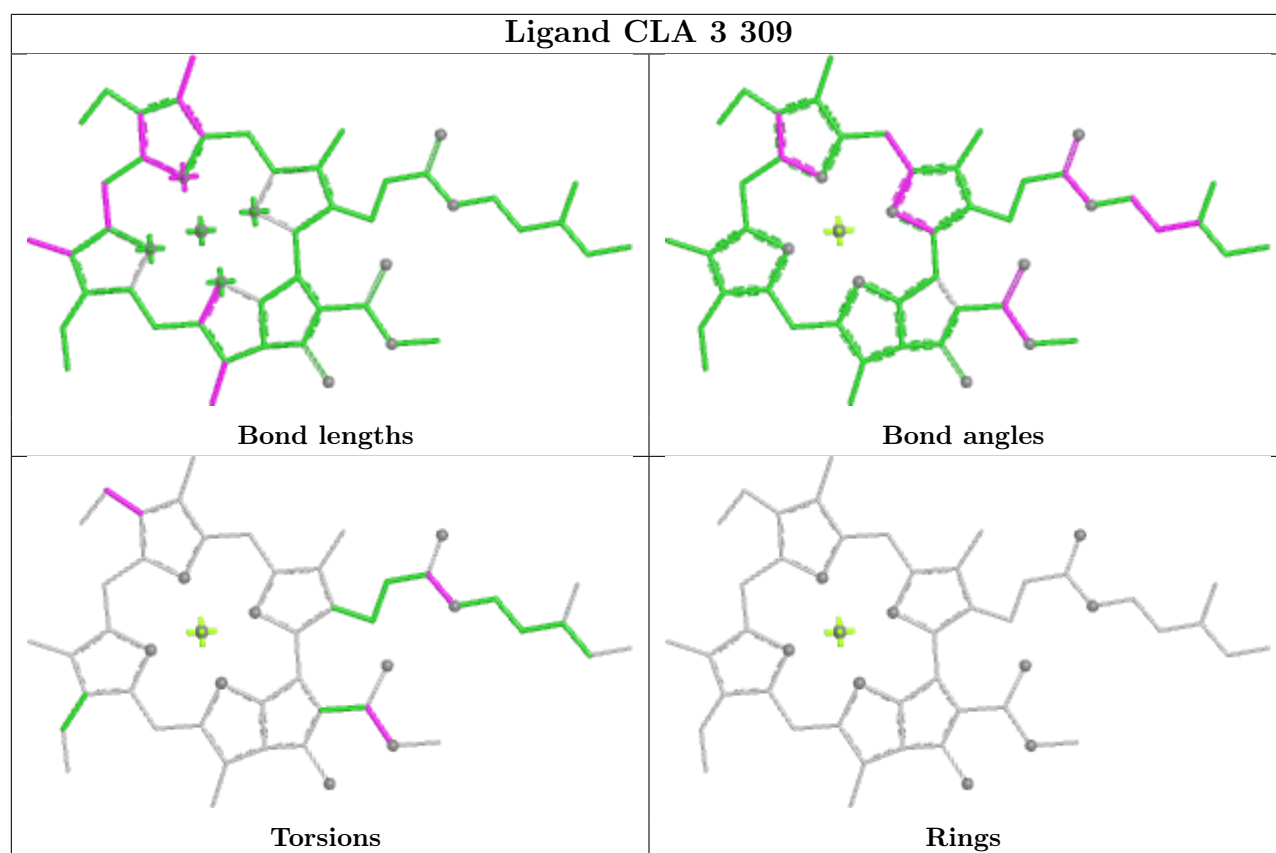
Ligand A86 4 304



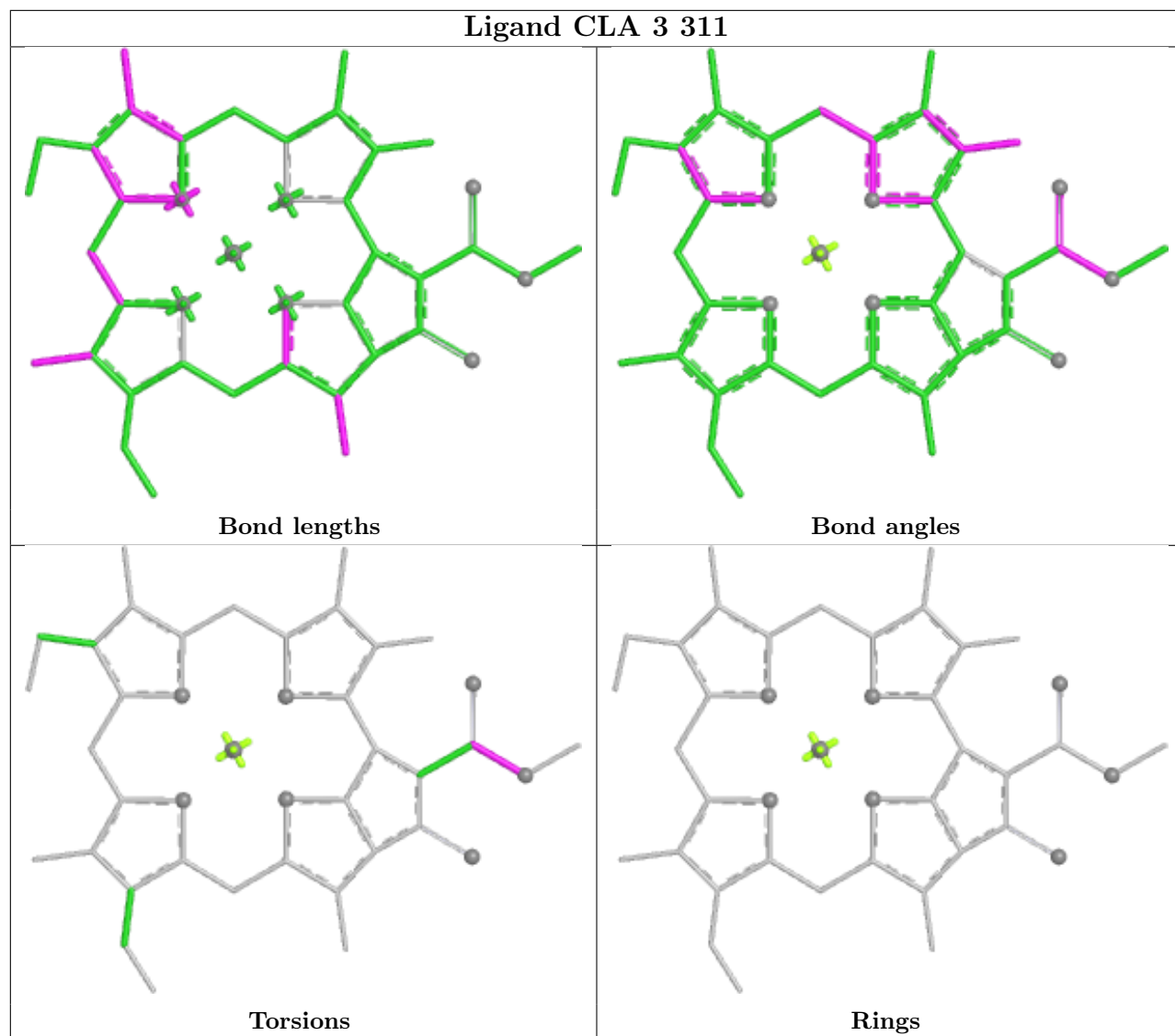




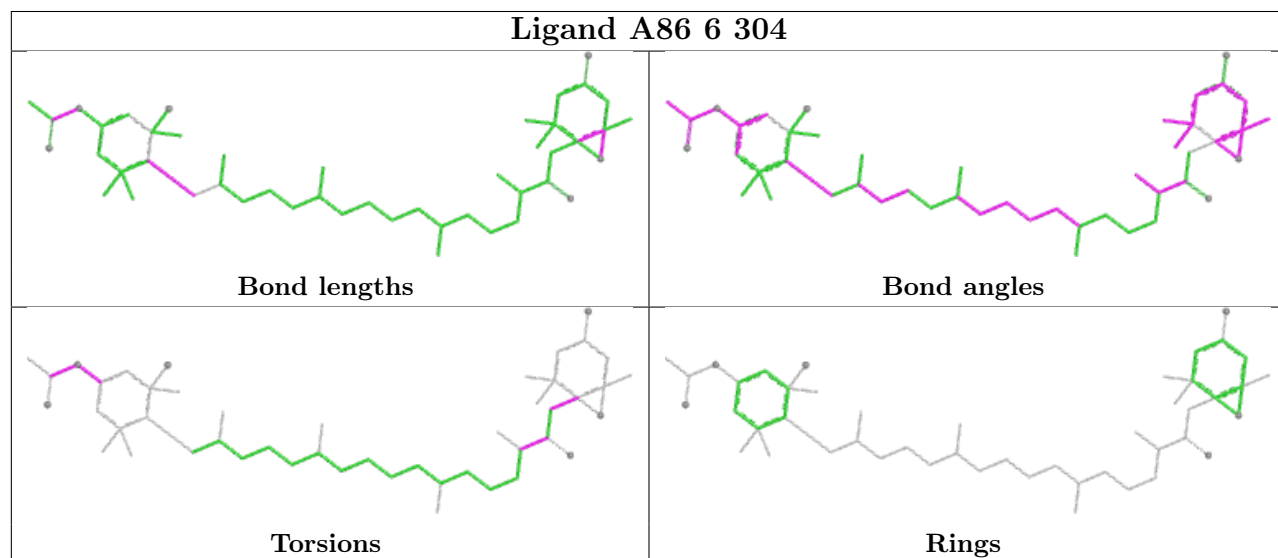


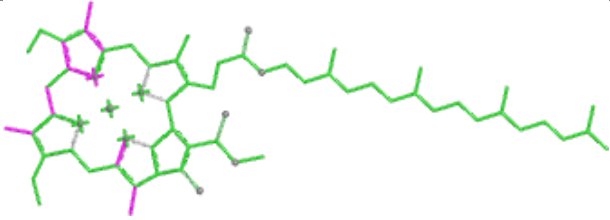
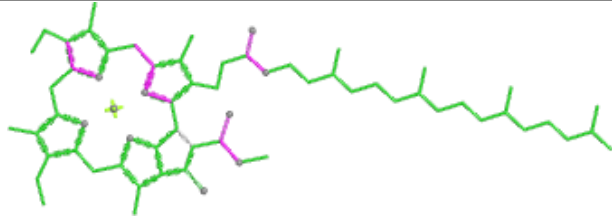
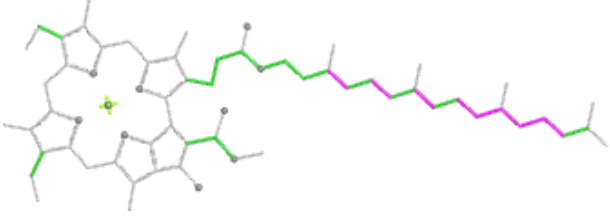
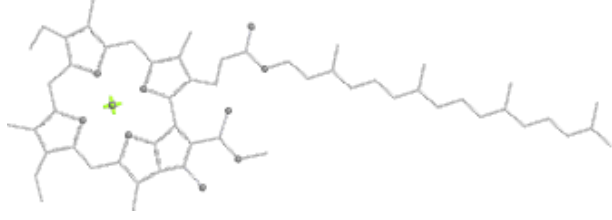
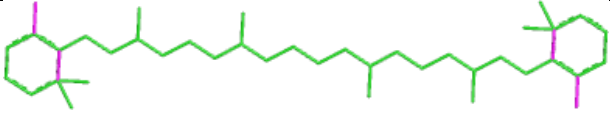
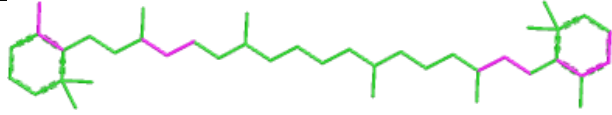
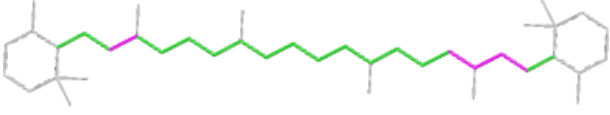
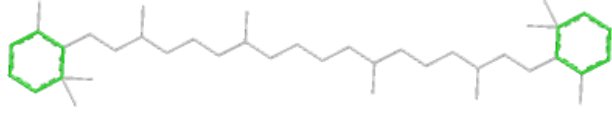
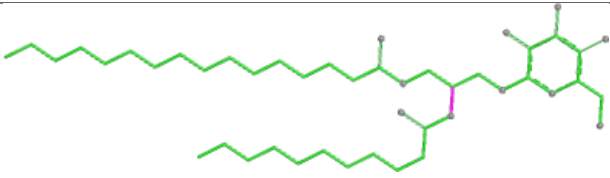
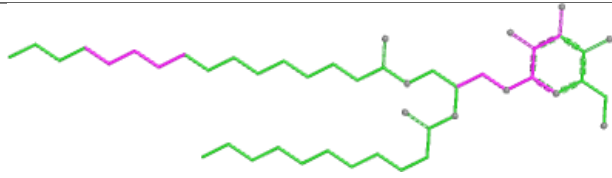
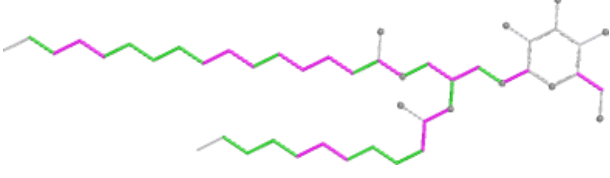
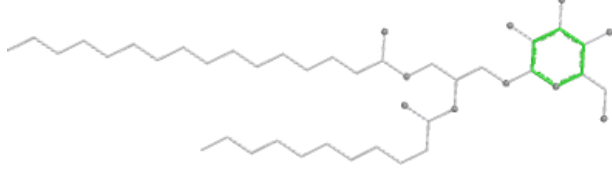


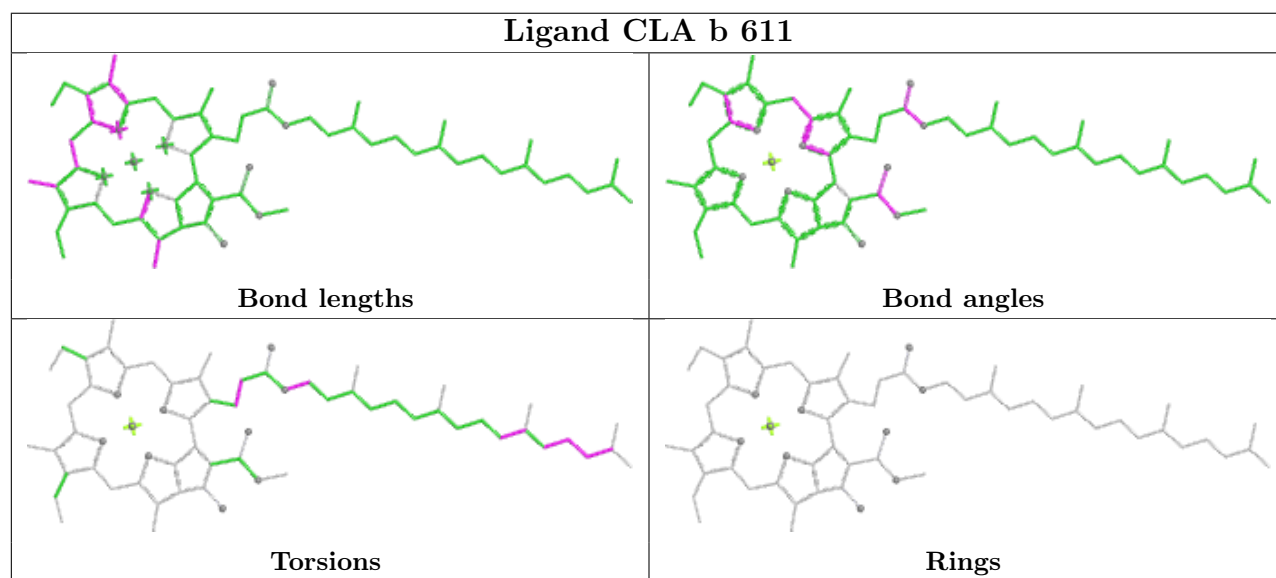
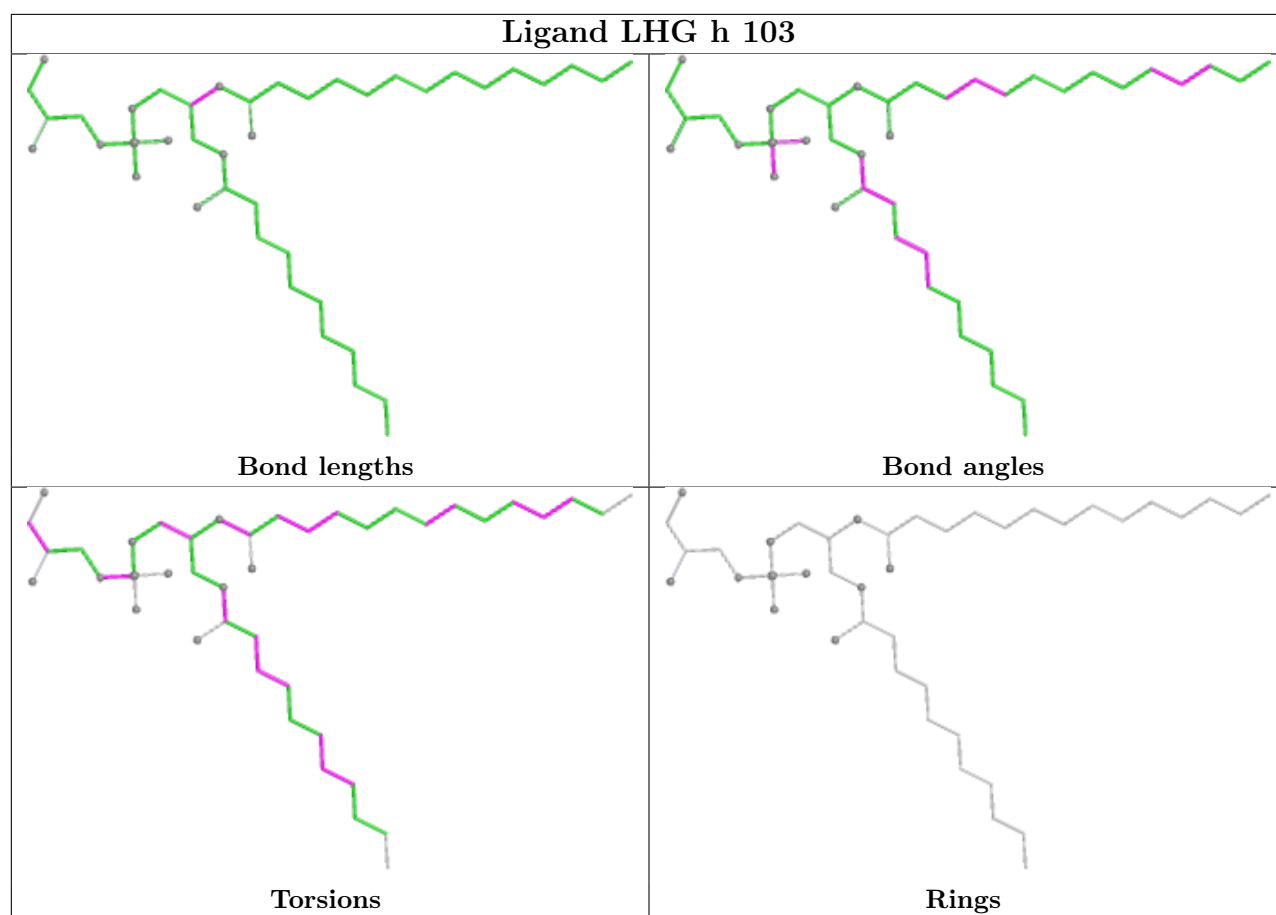
Ligand CLA 3 311



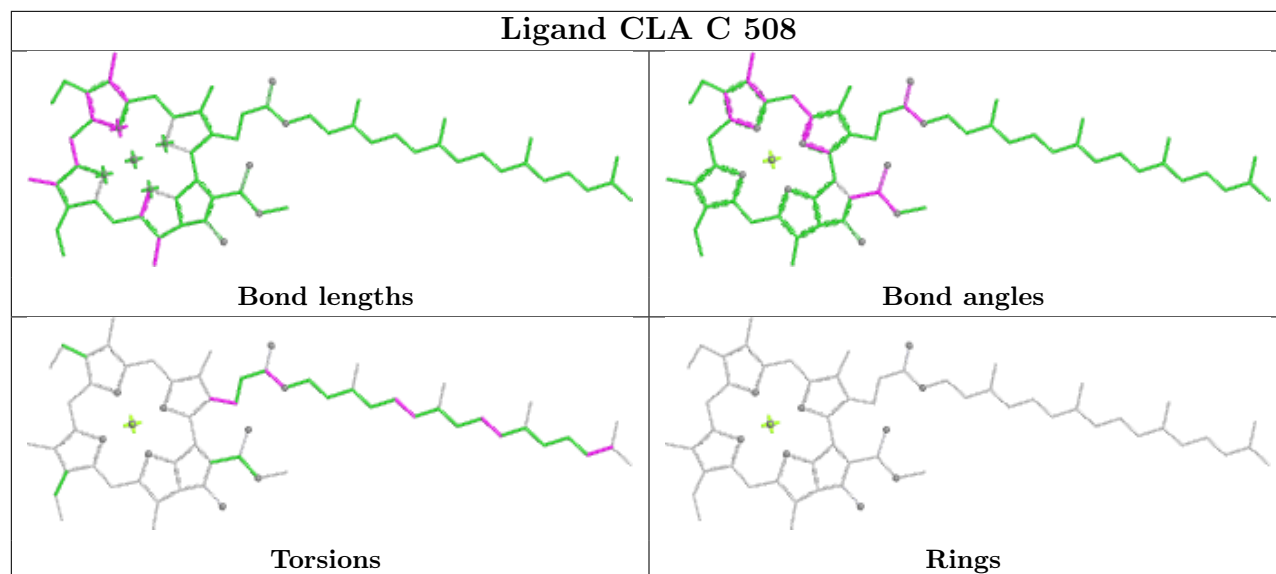
Ligand A86 6 304



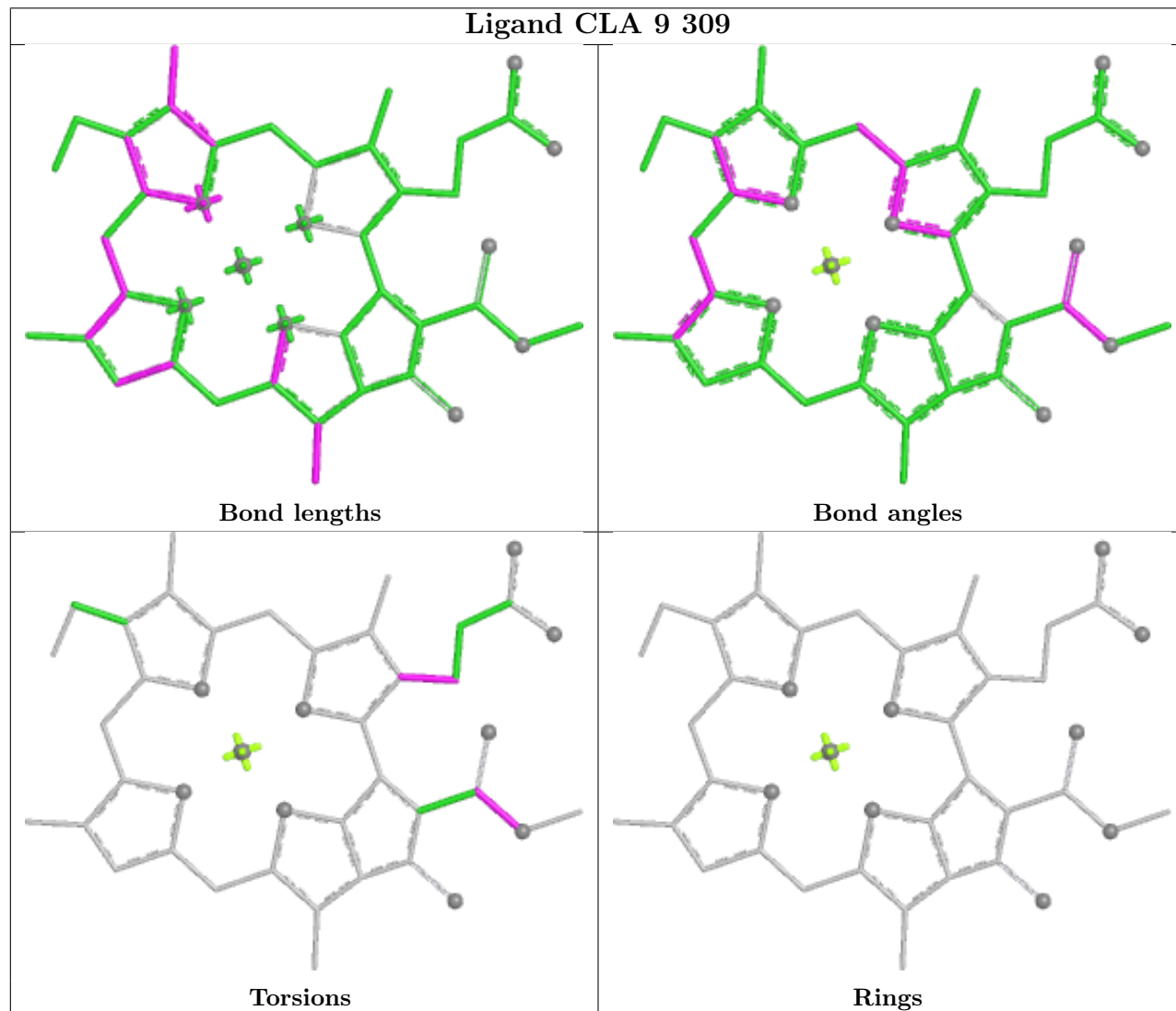
Ligand CLA b 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 620	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG q 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

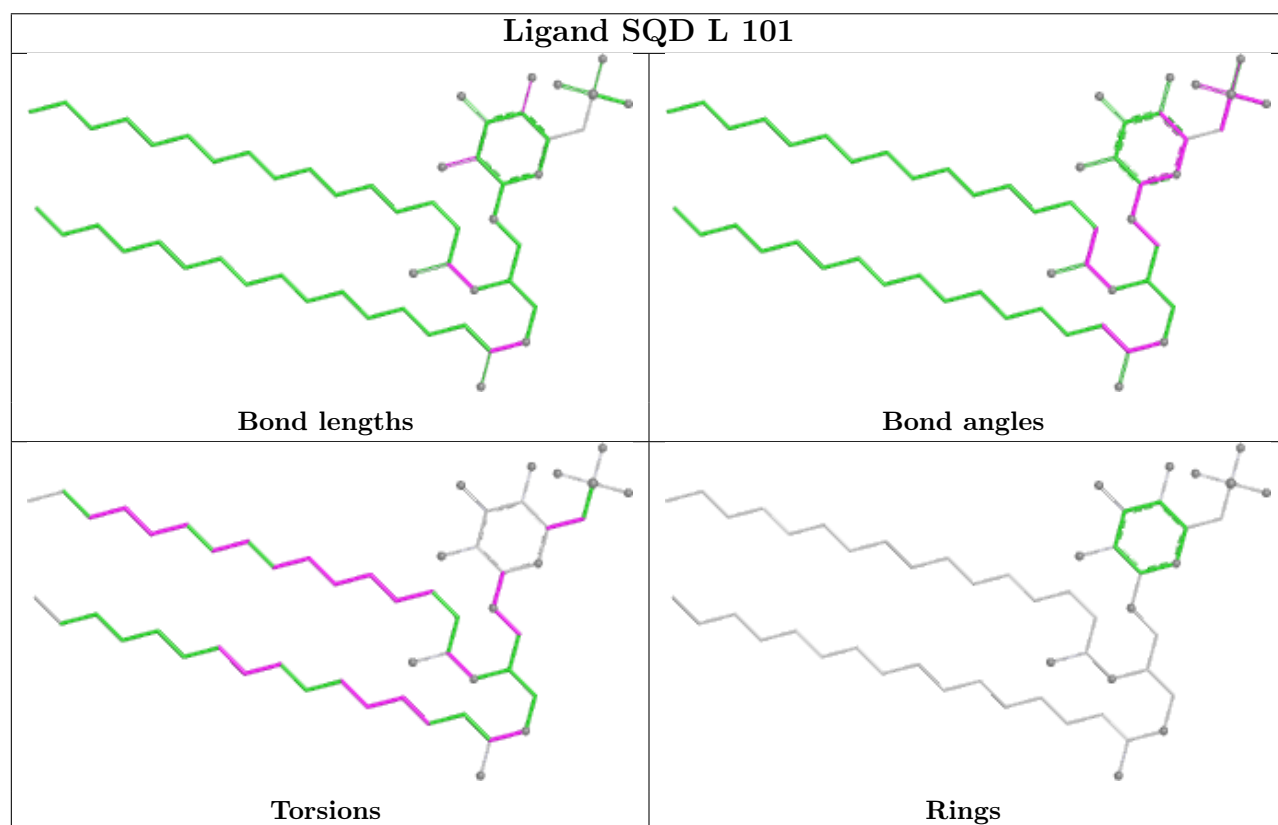
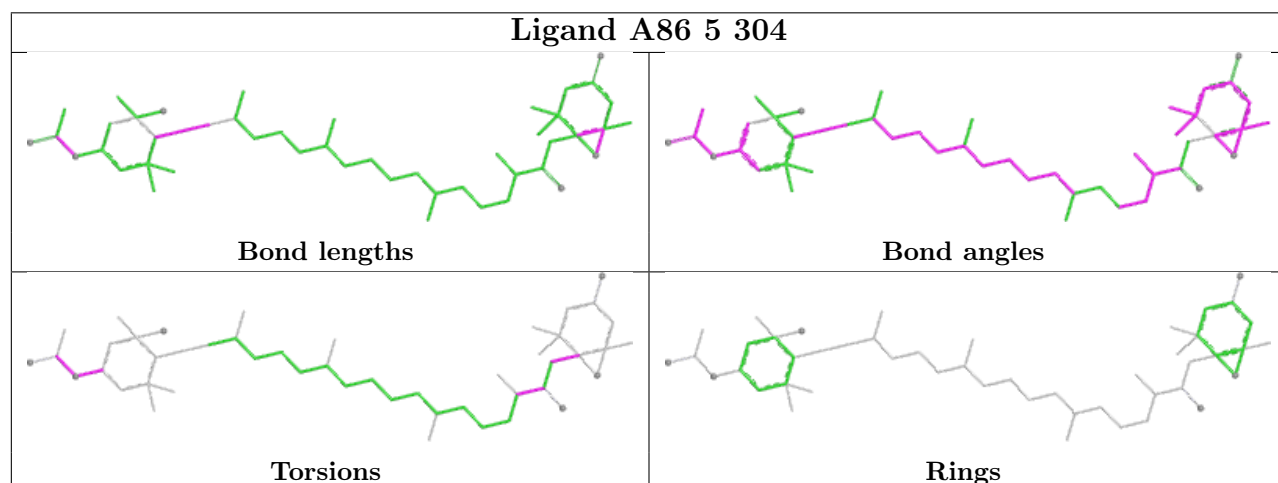
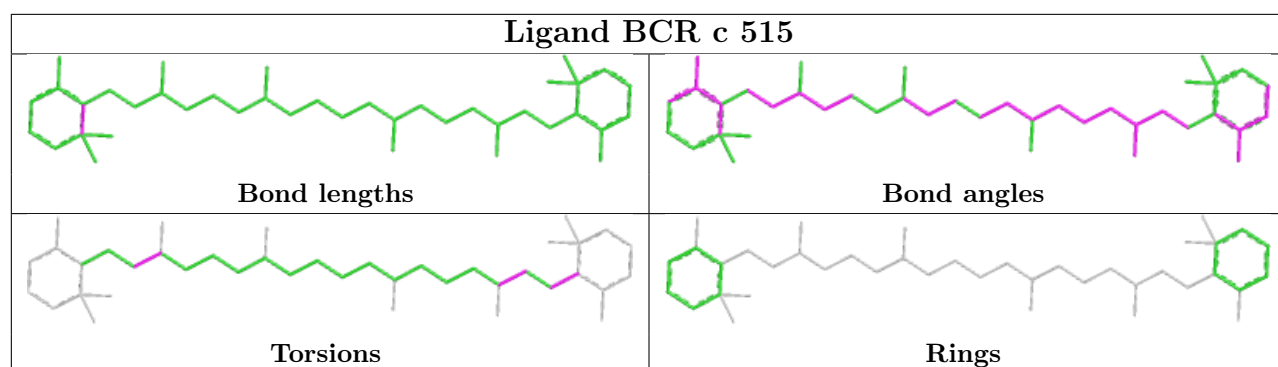


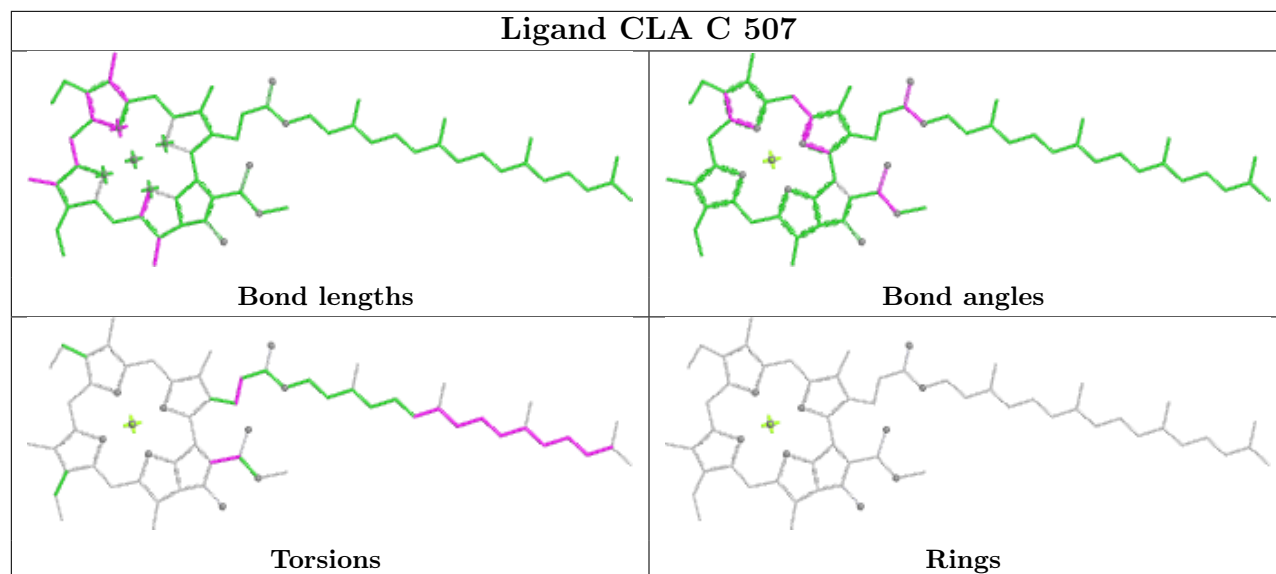
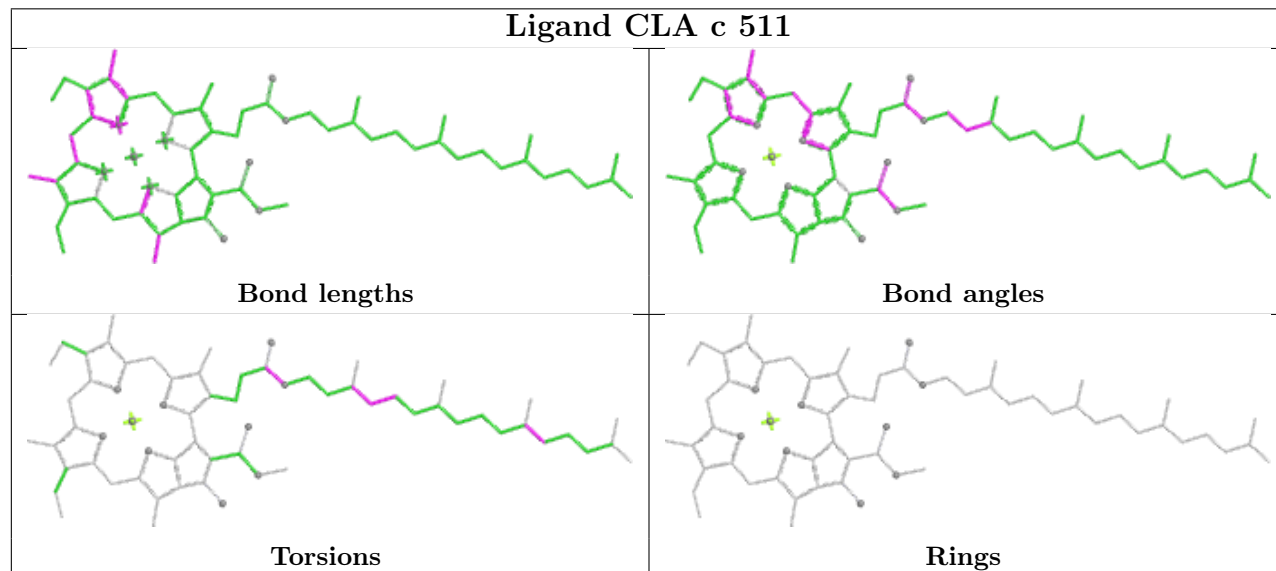
Ligand CLA C 508

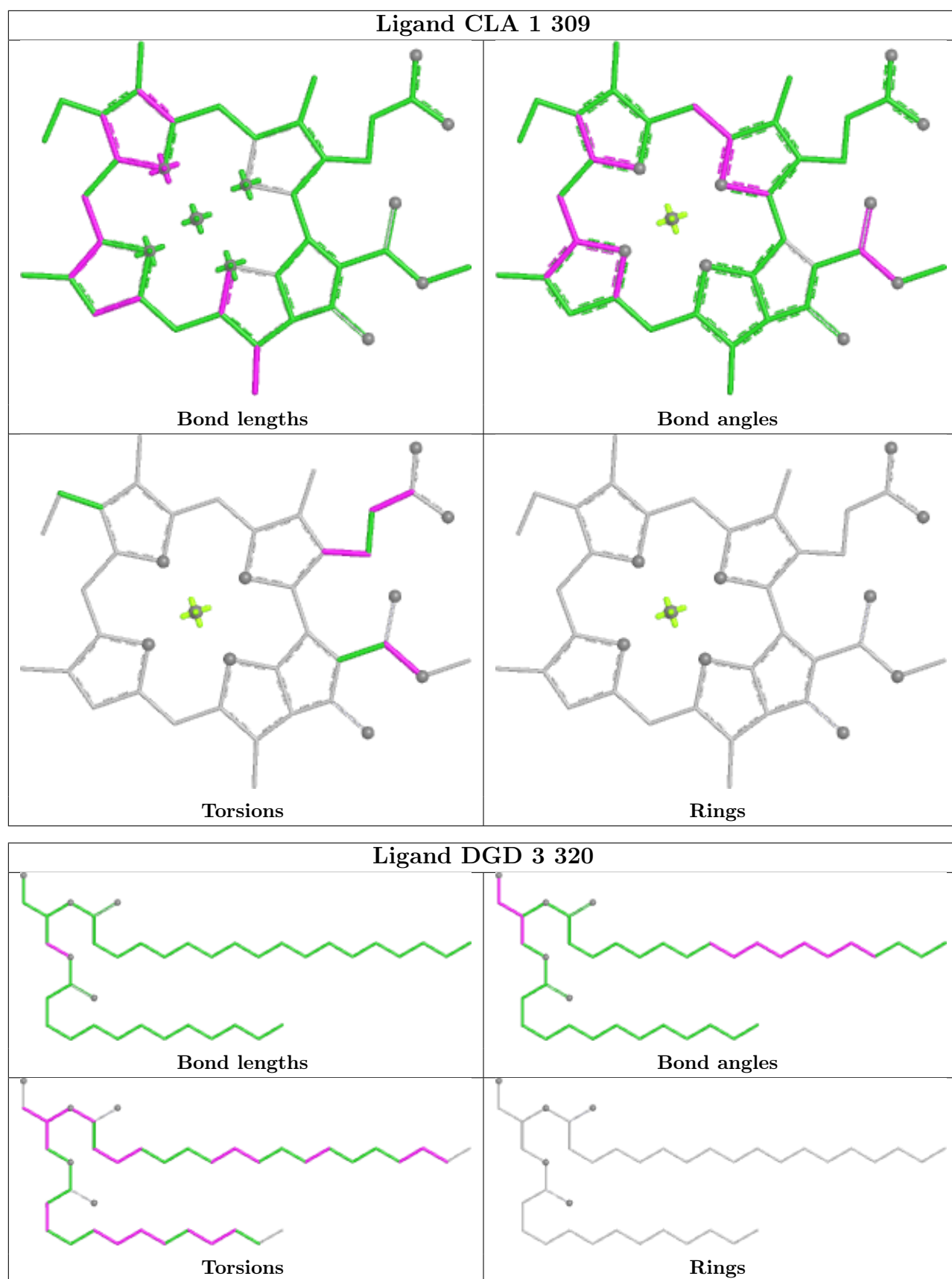


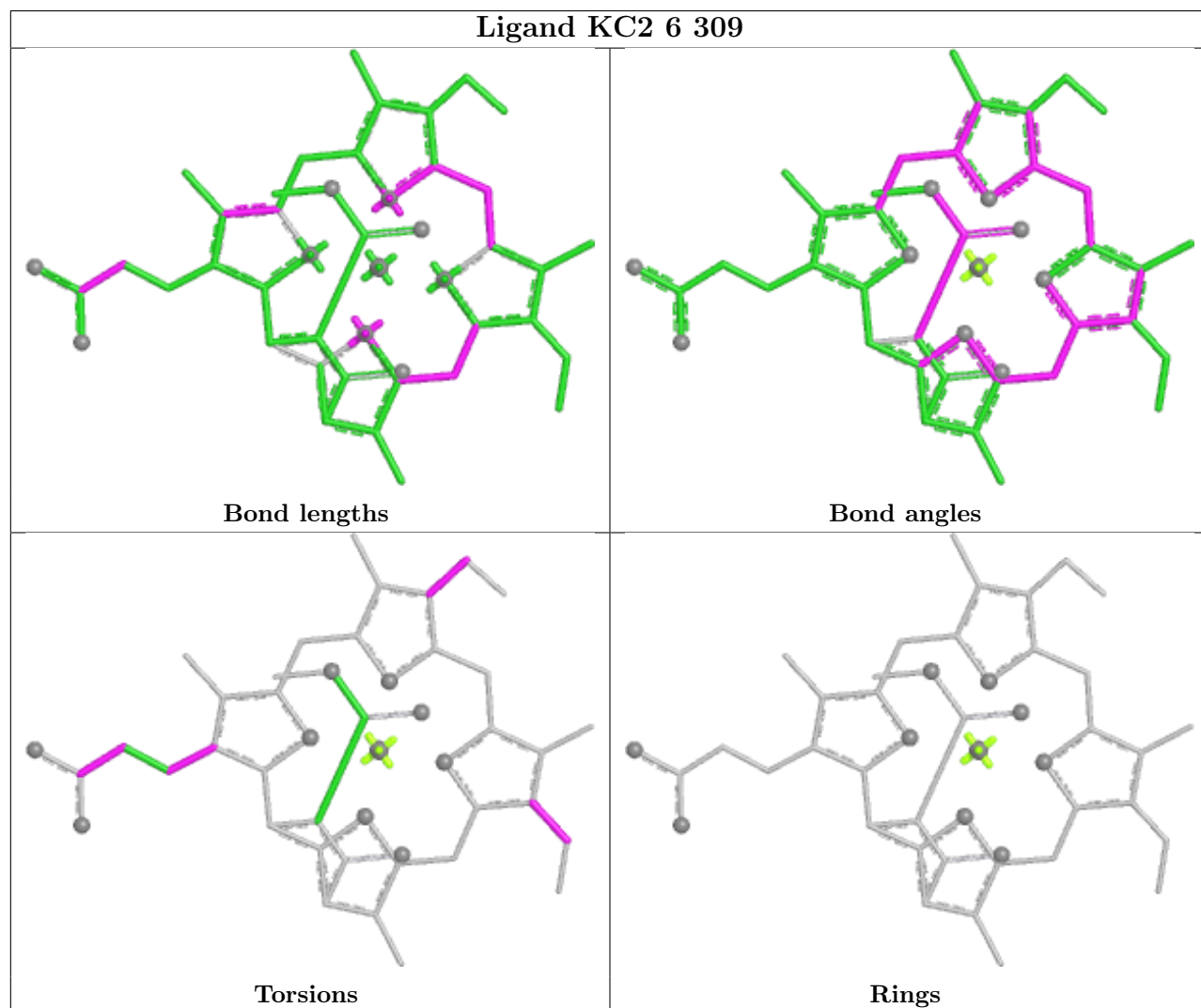
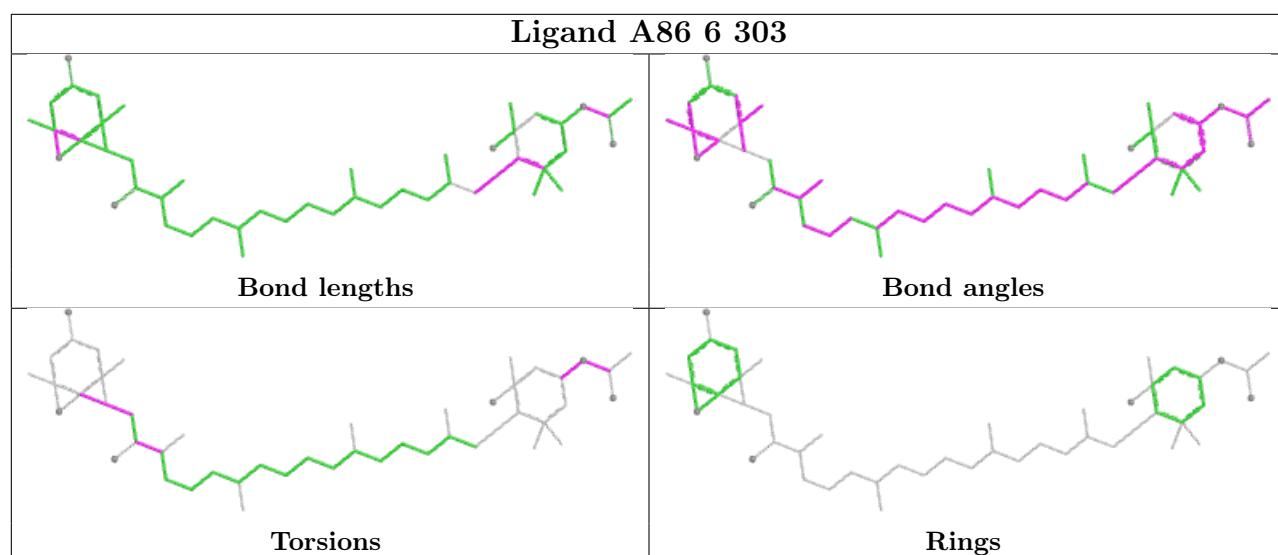
Ligand CLA 9 309

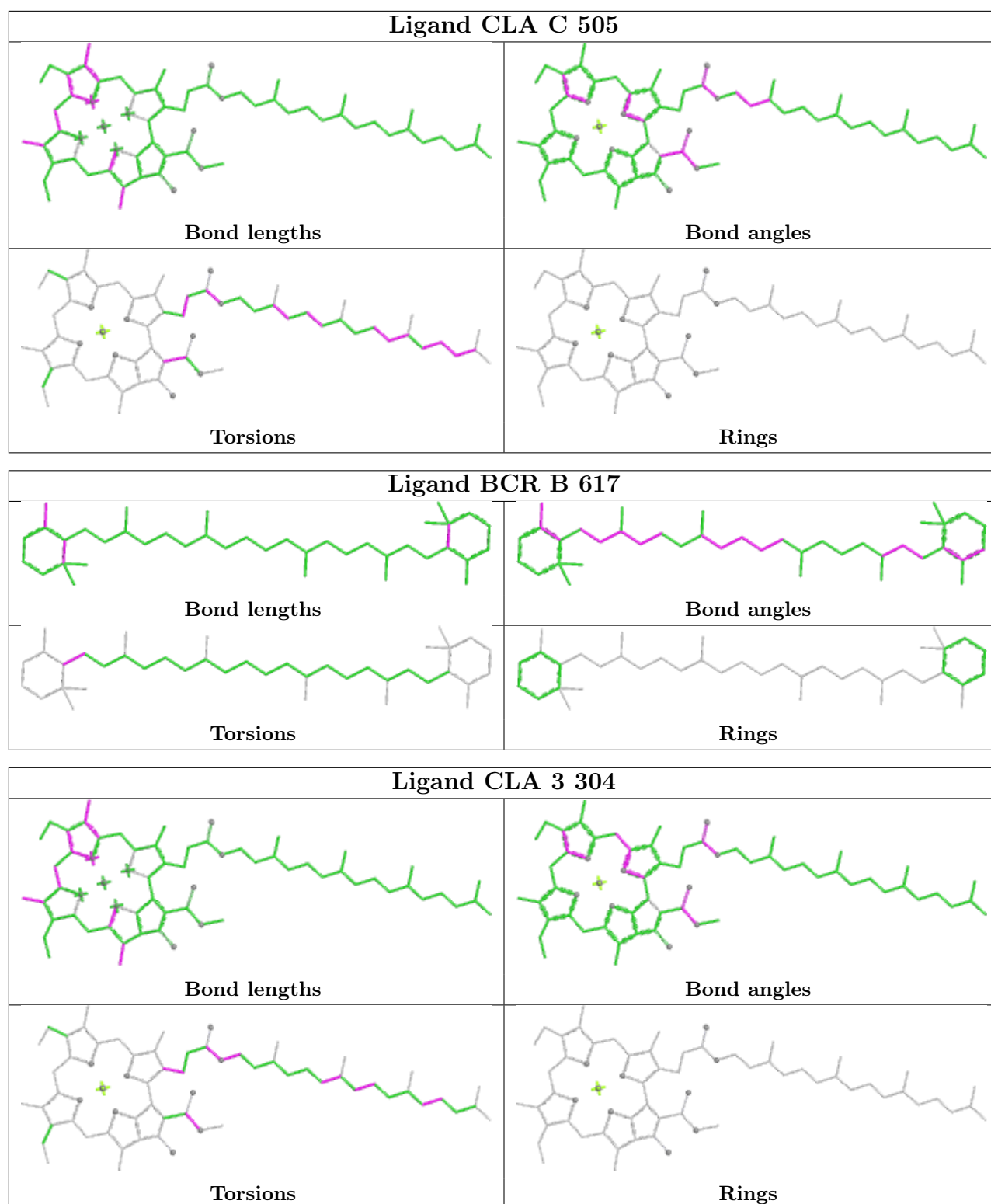


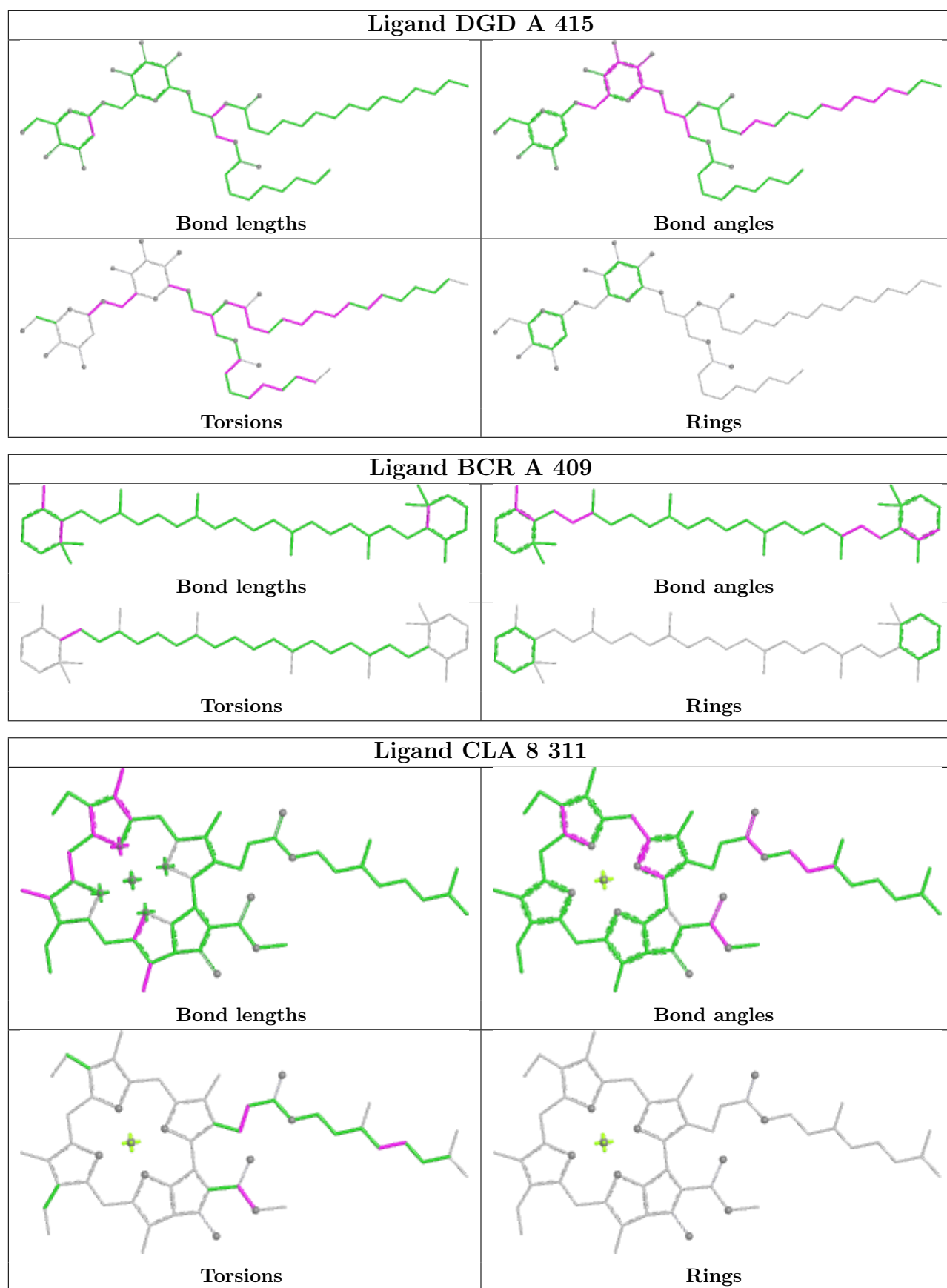


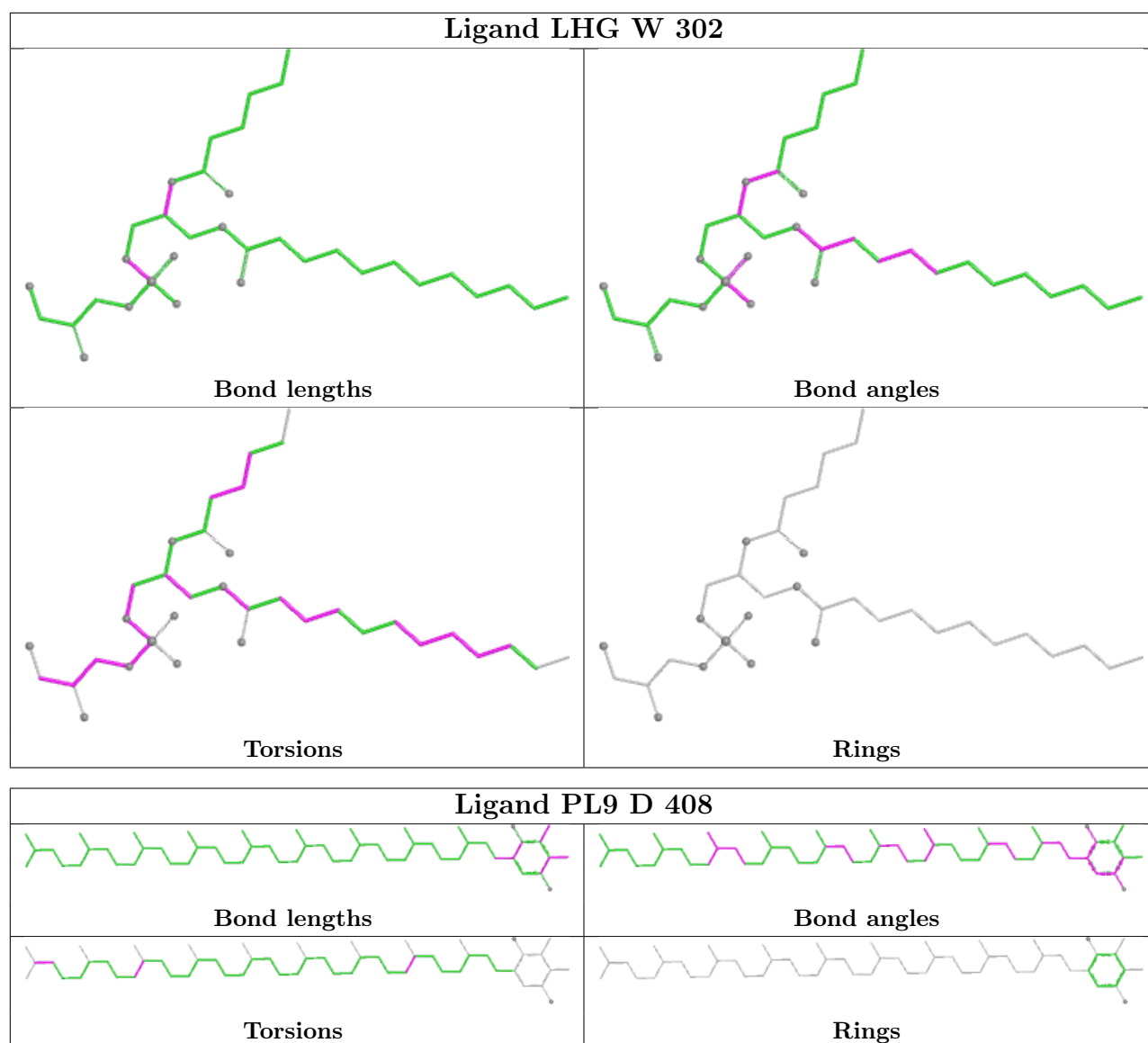
Ligand CLA C 507**Ligand CLA c 511**



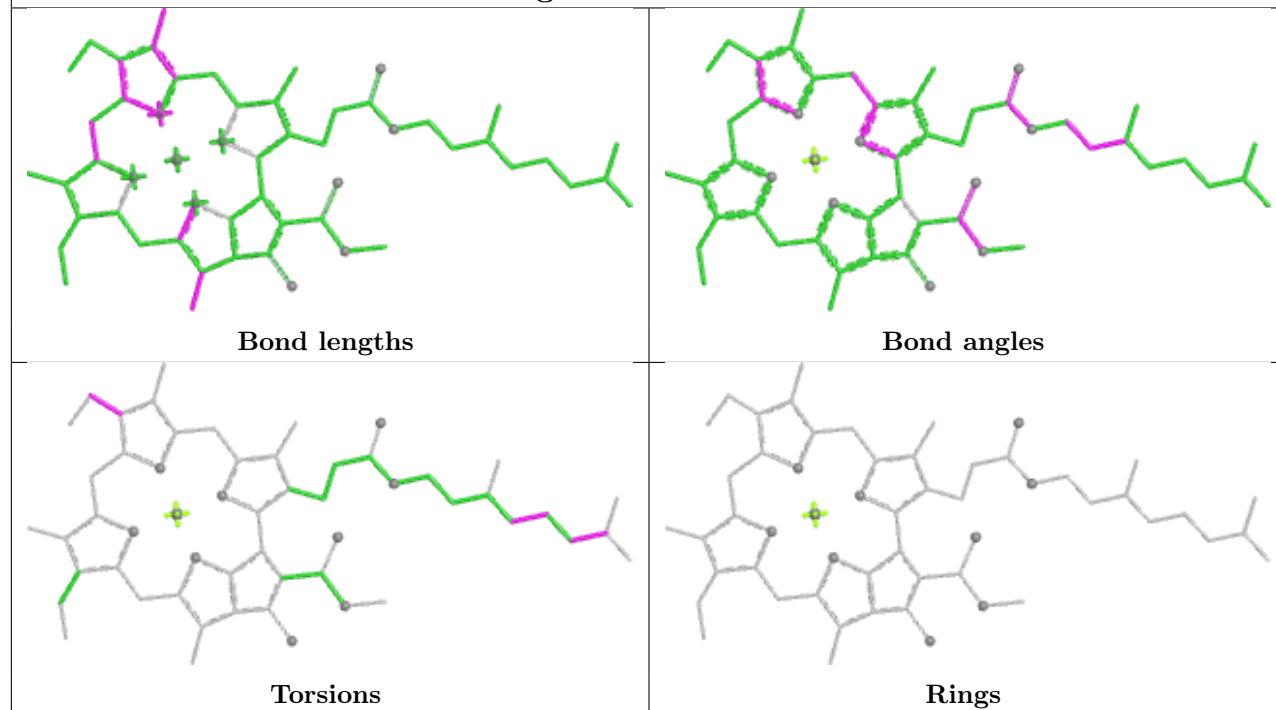




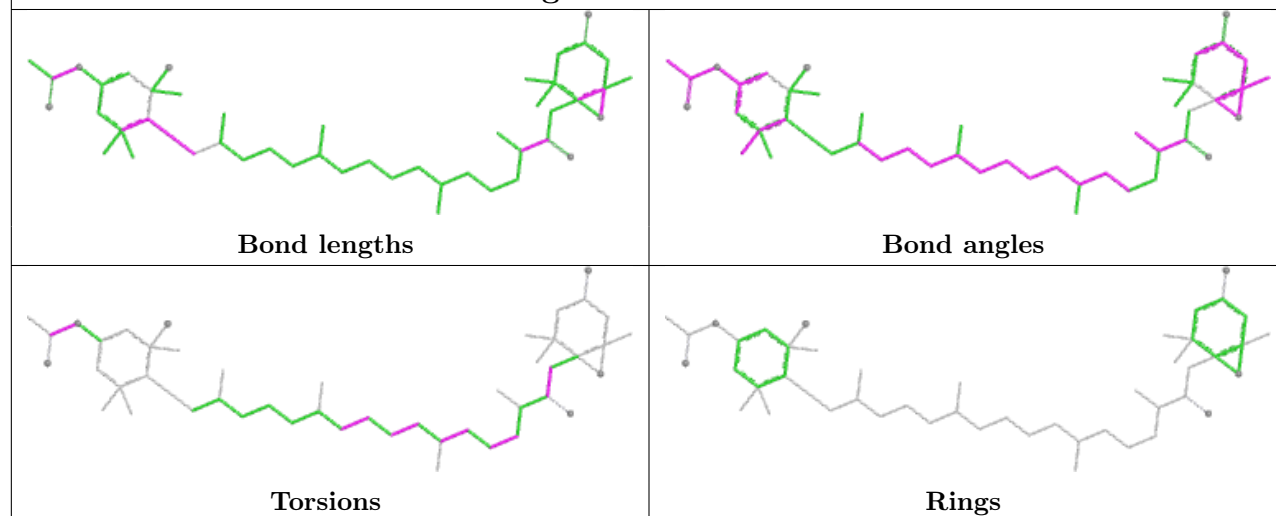


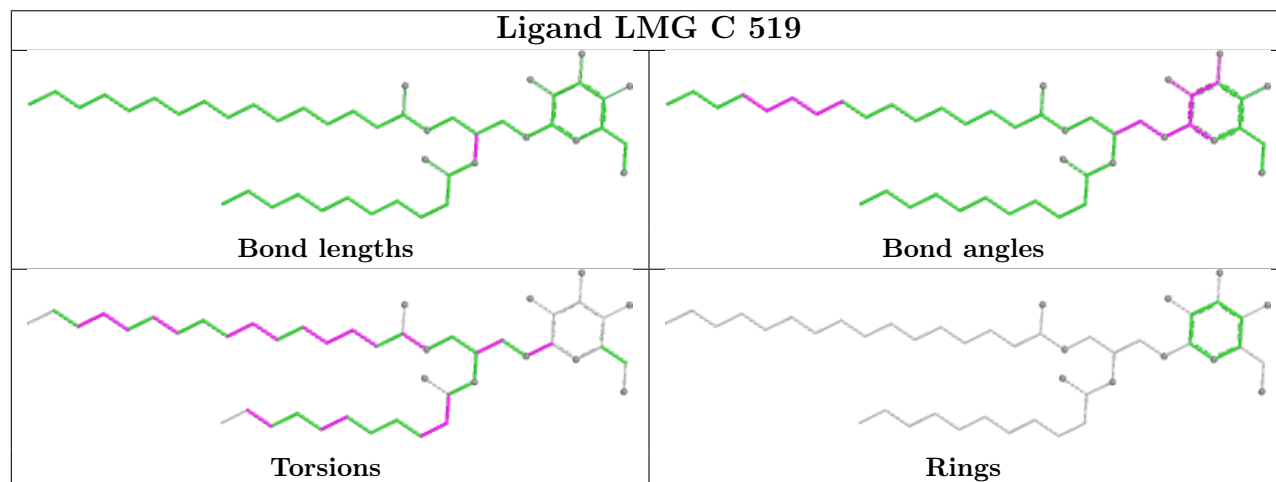
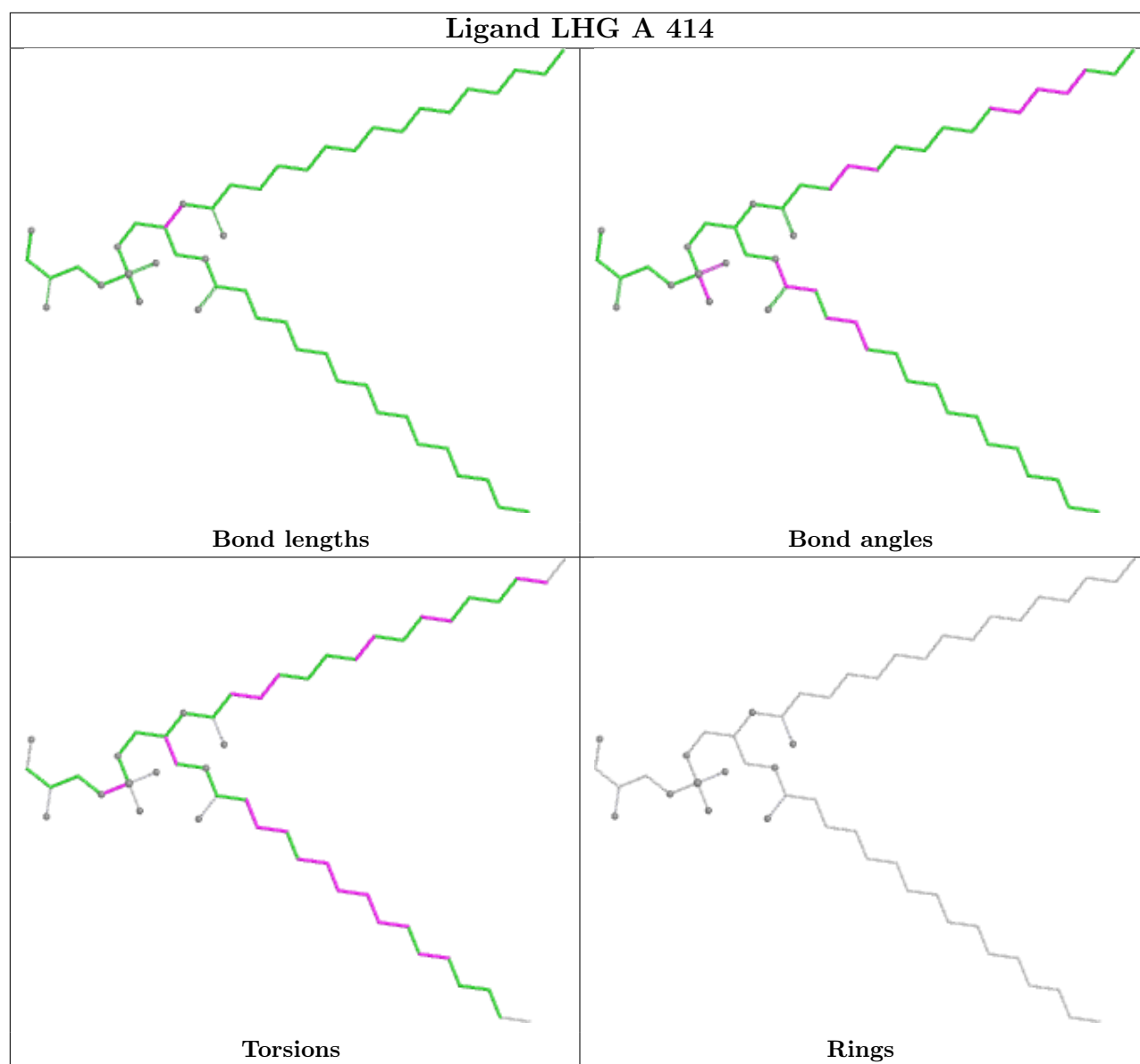


Ligand CLA 5 309

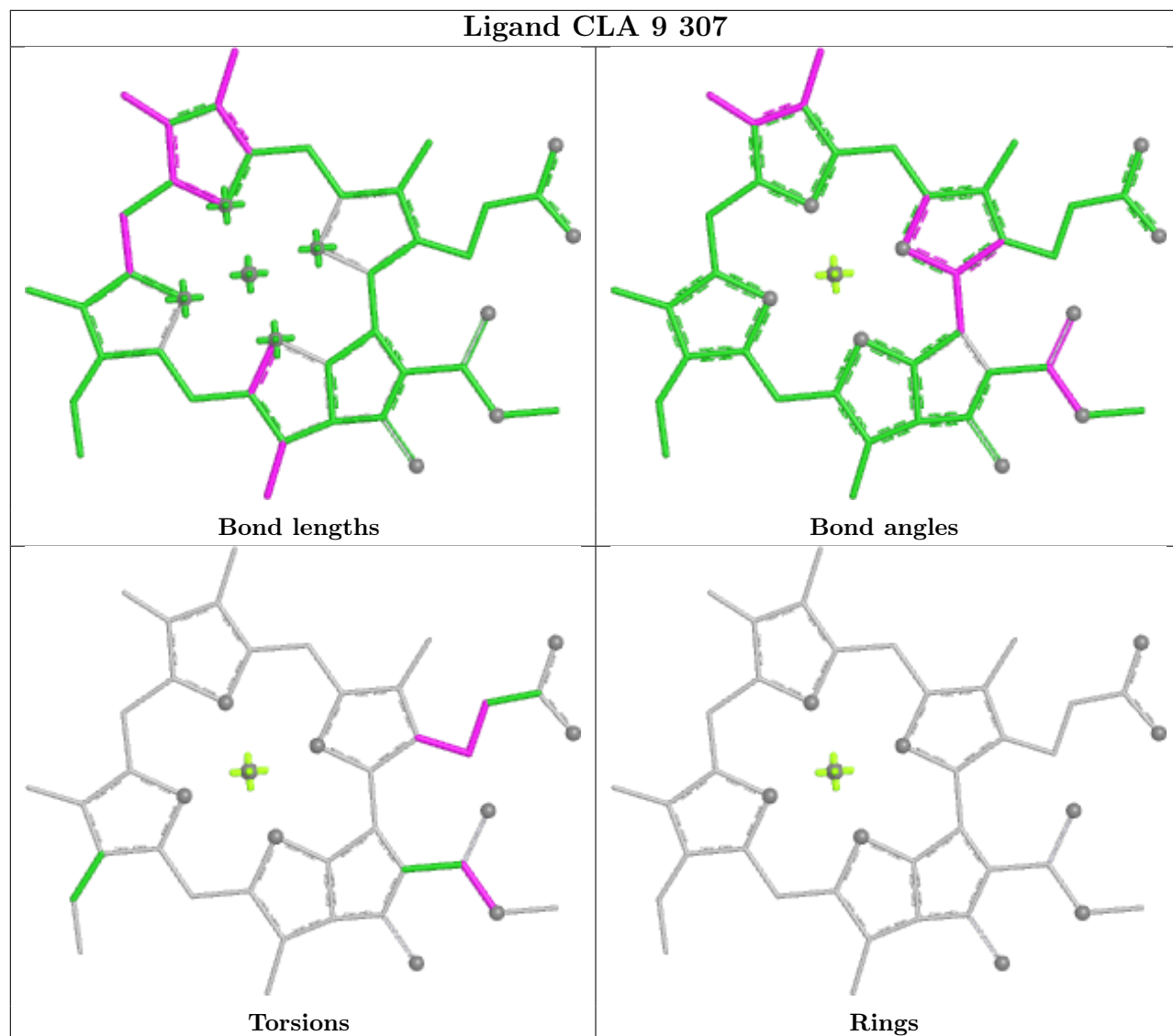


Ligand A86 2 302

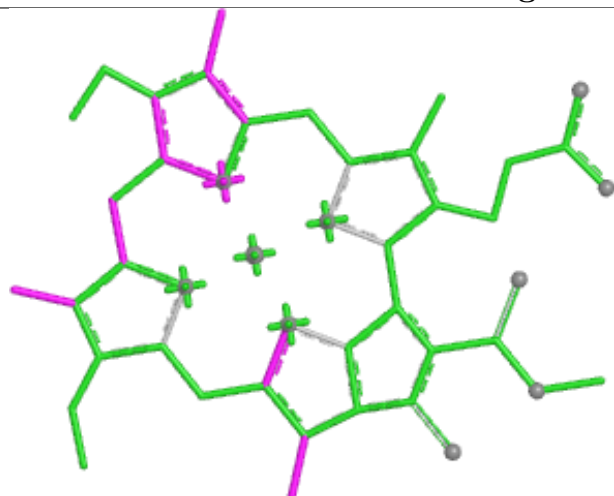




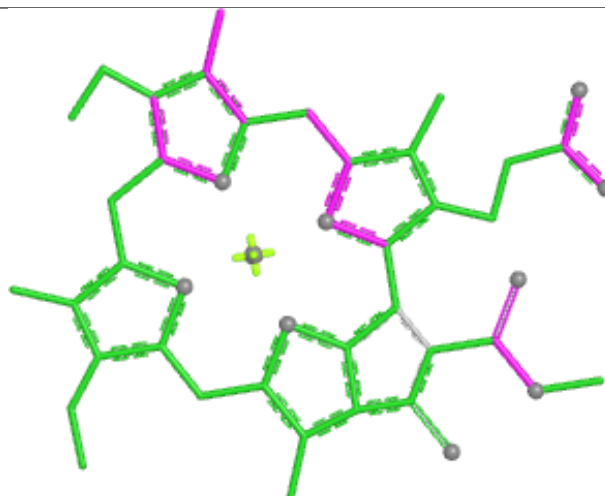
Ligand CLA 9 307



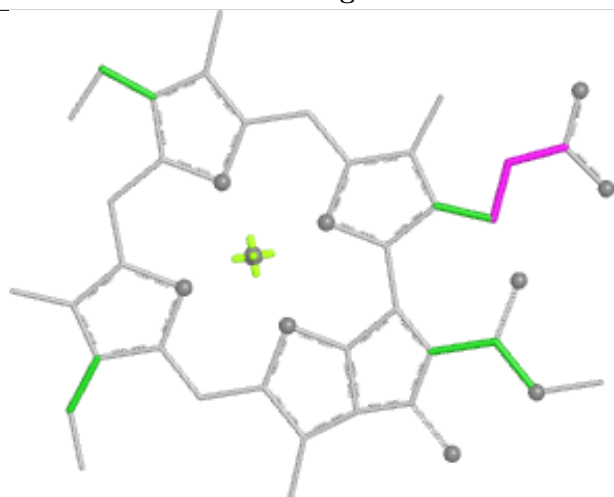
Ligand CLA 8 306



Bond lengths



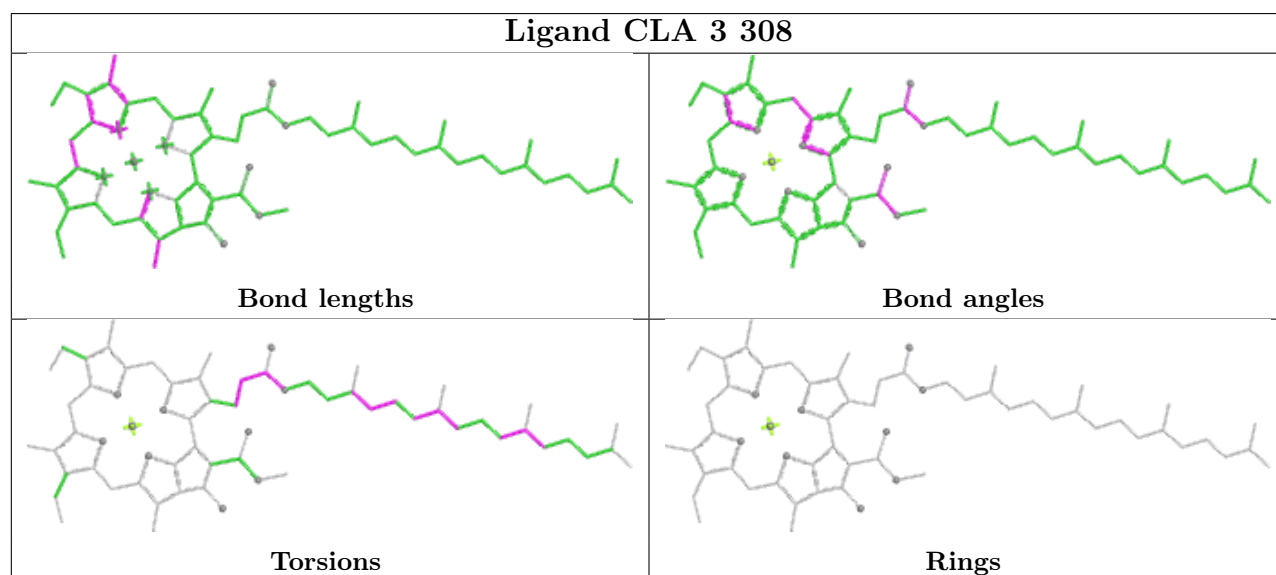
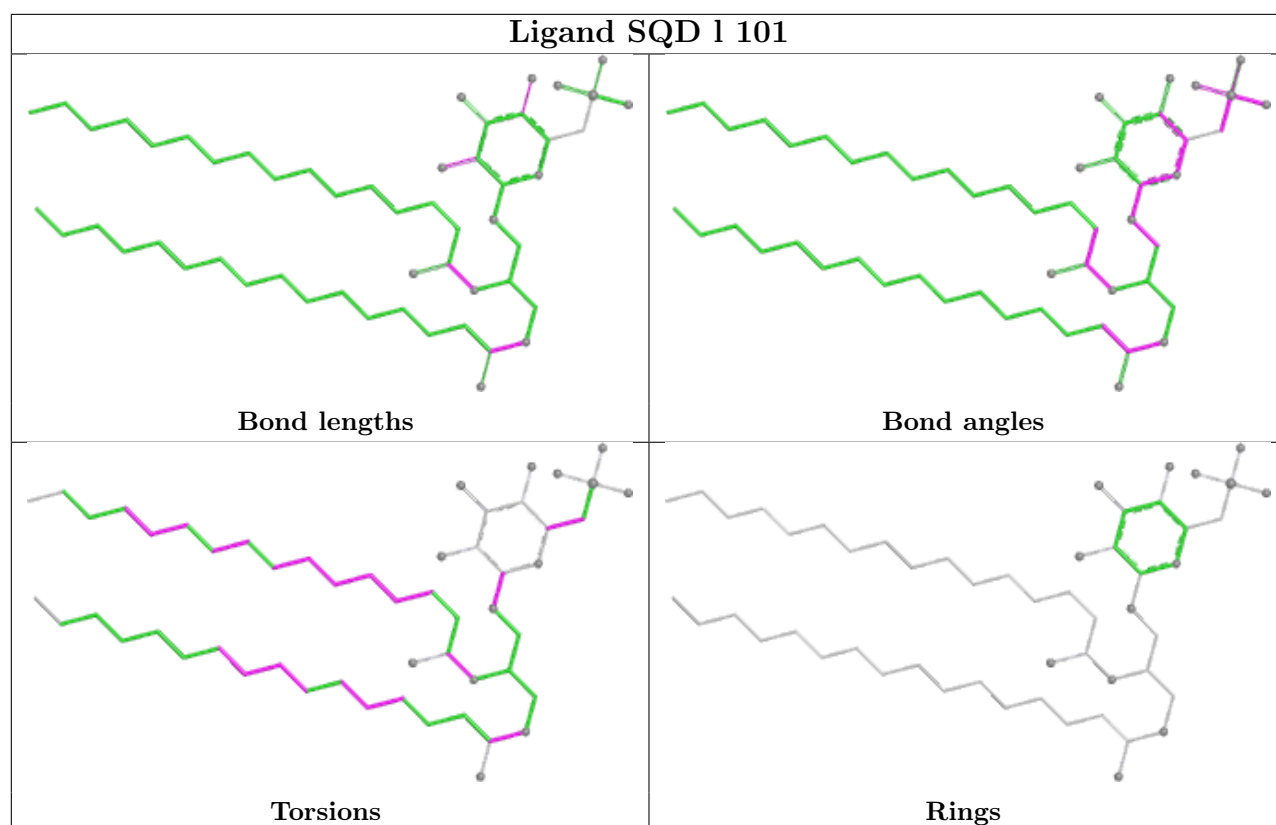
Bond angles

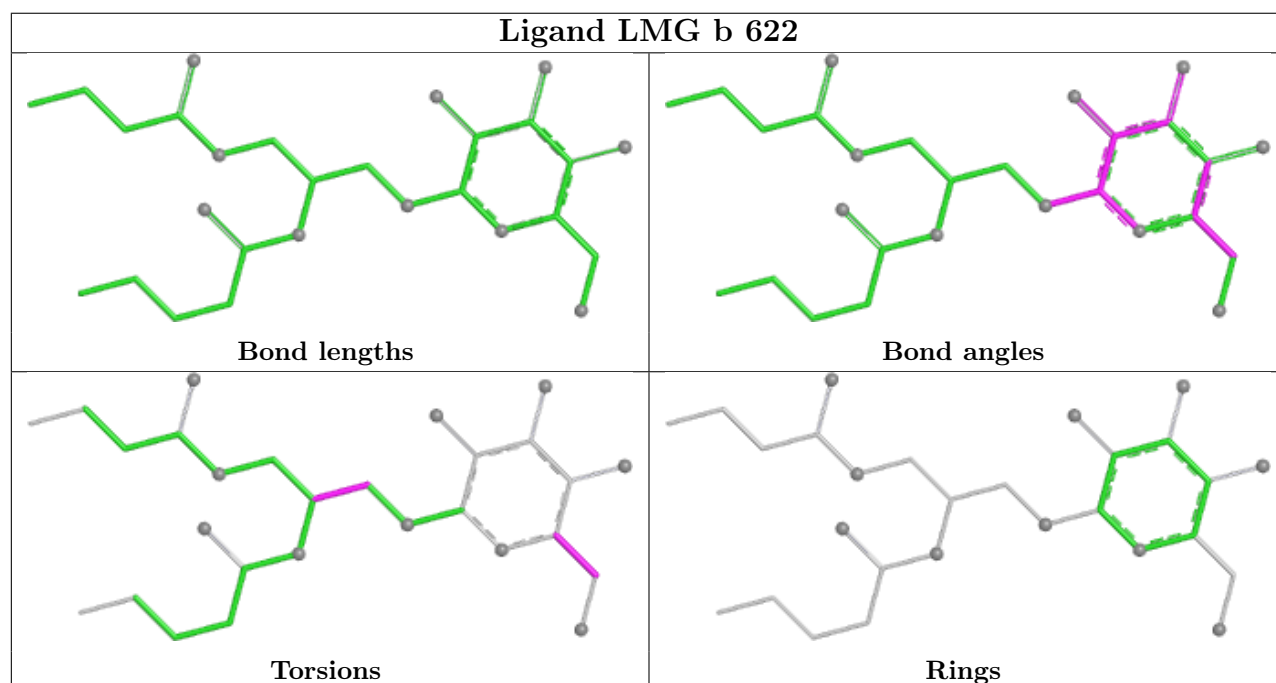
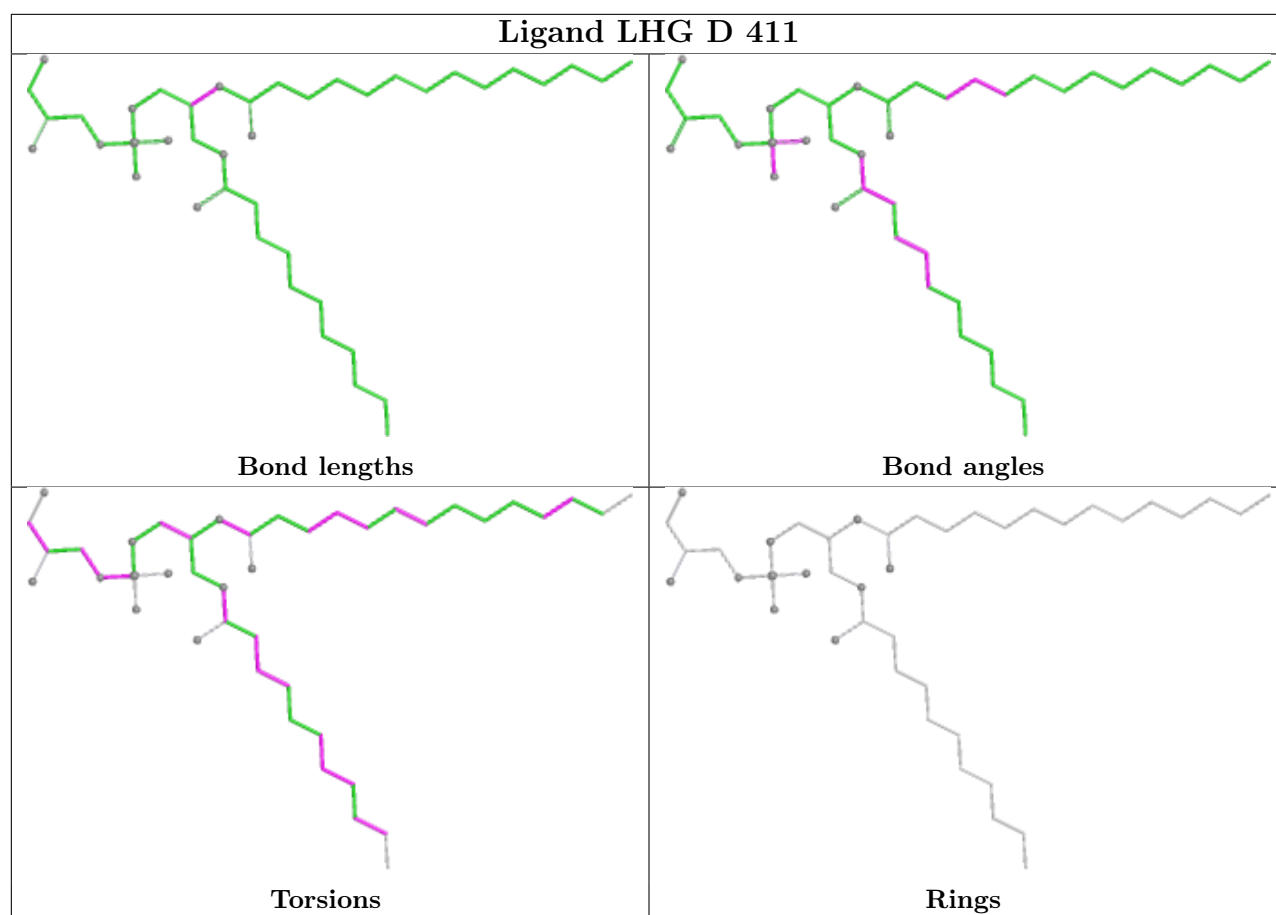


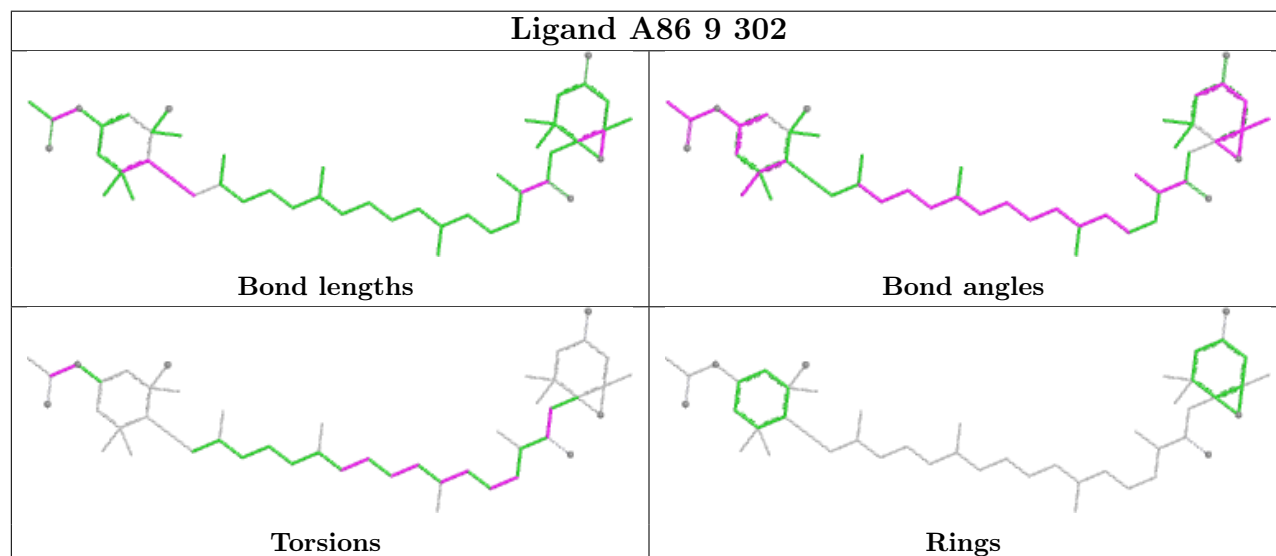
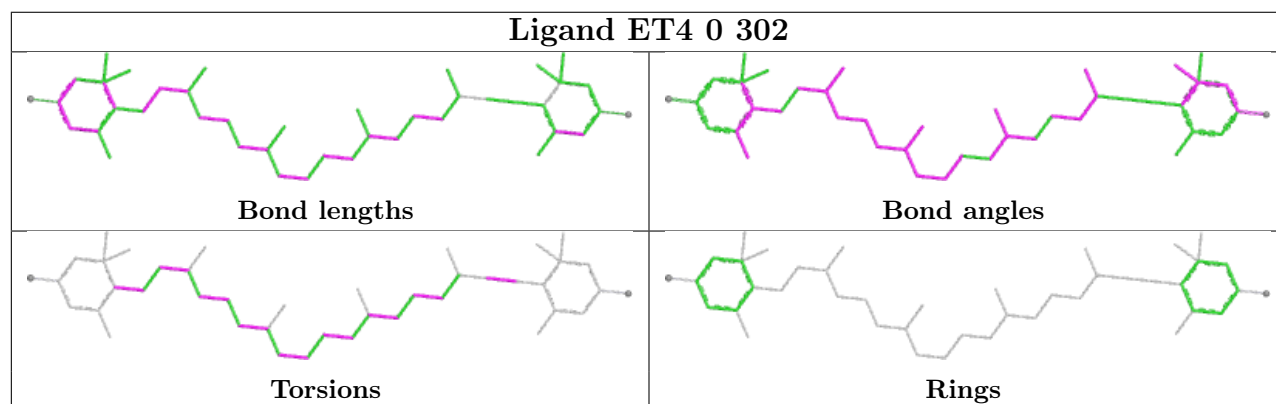
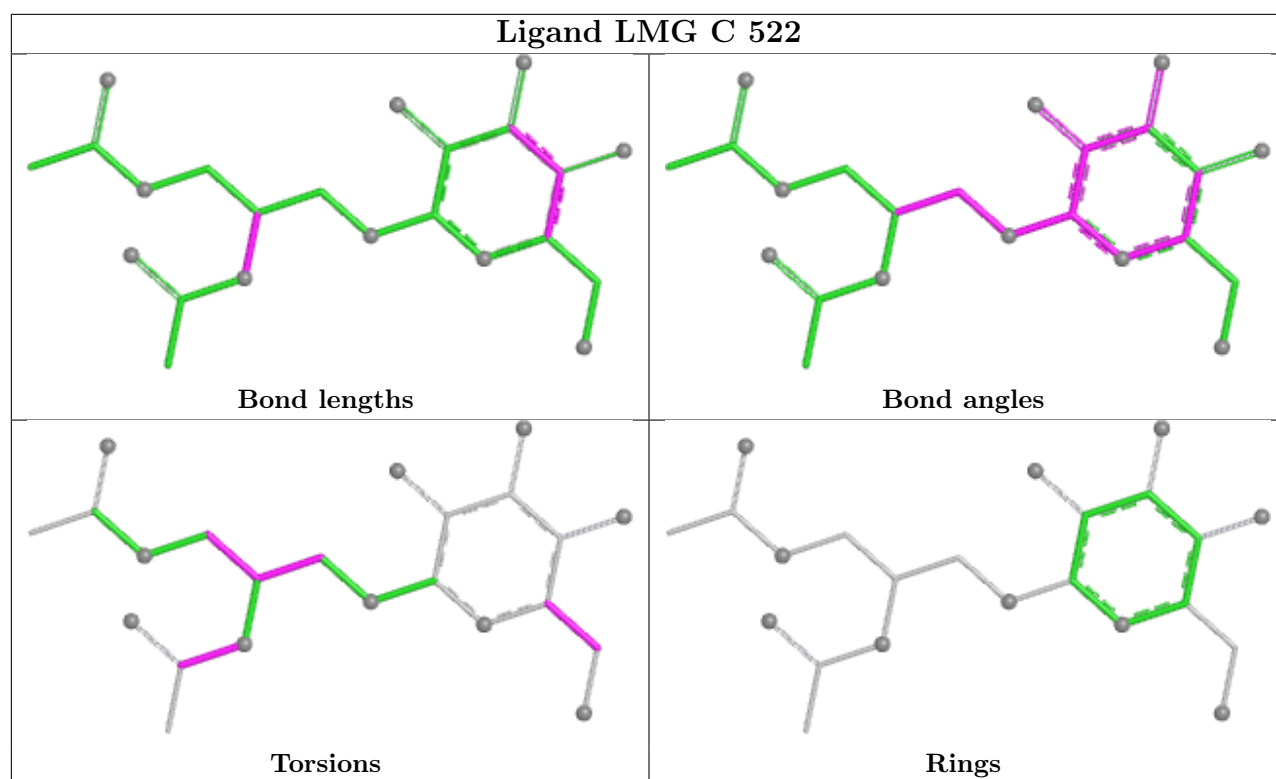
Torsions

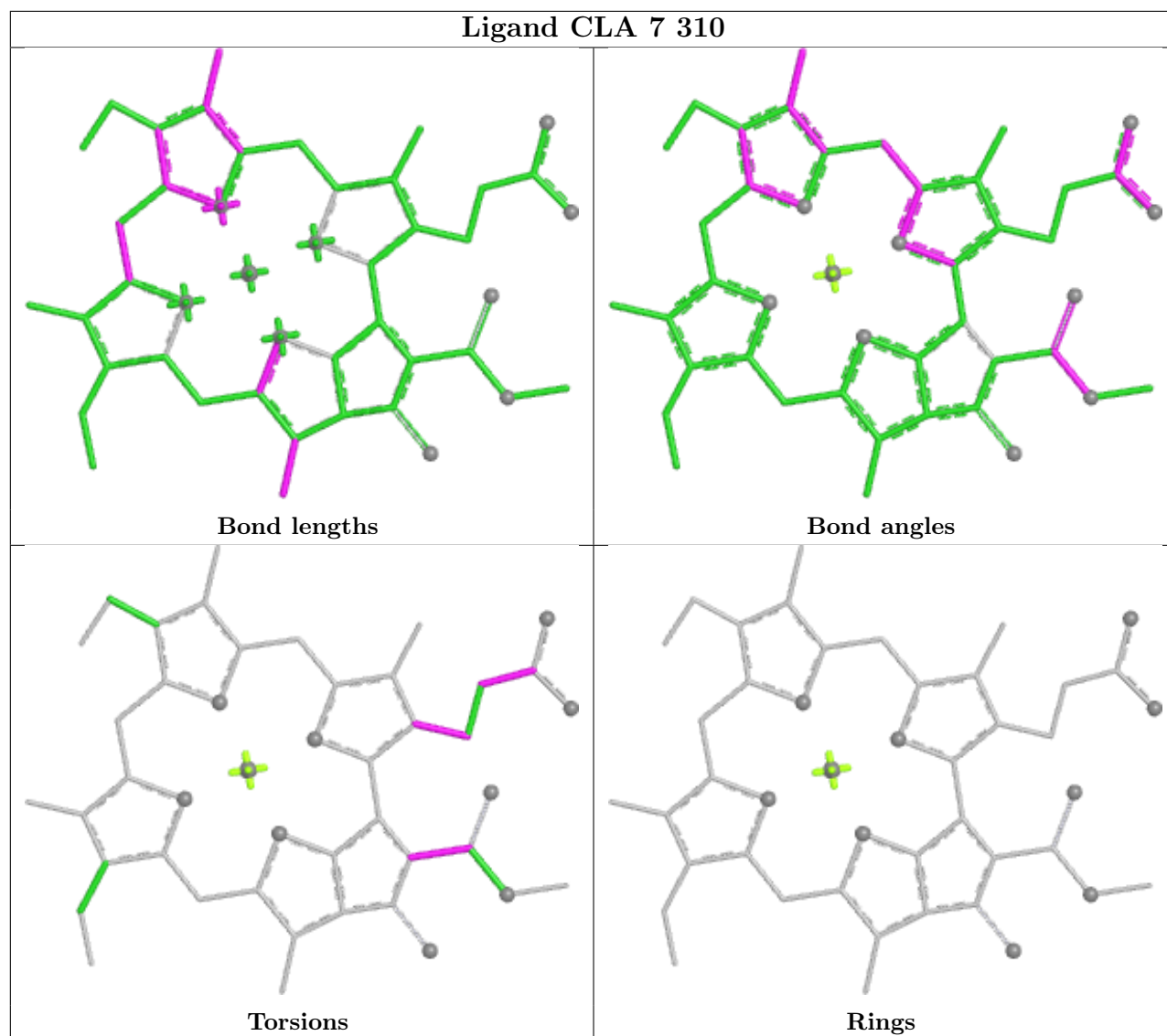
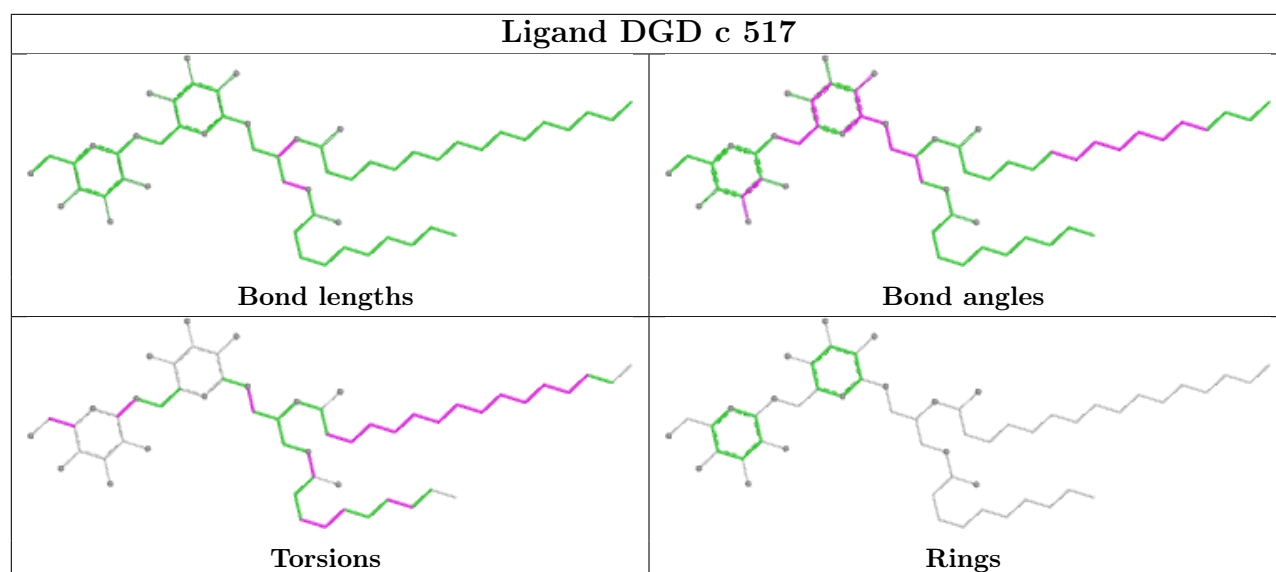


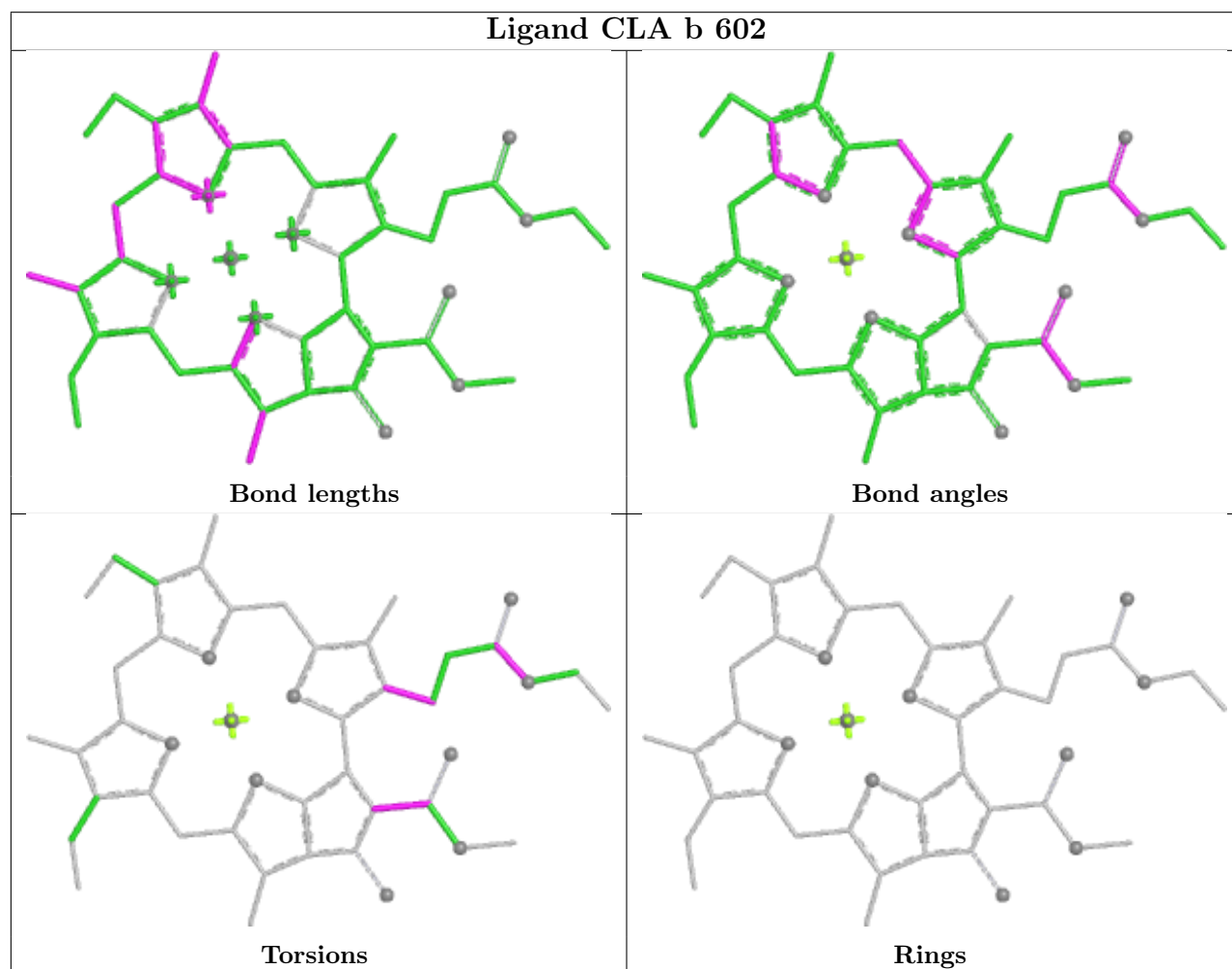
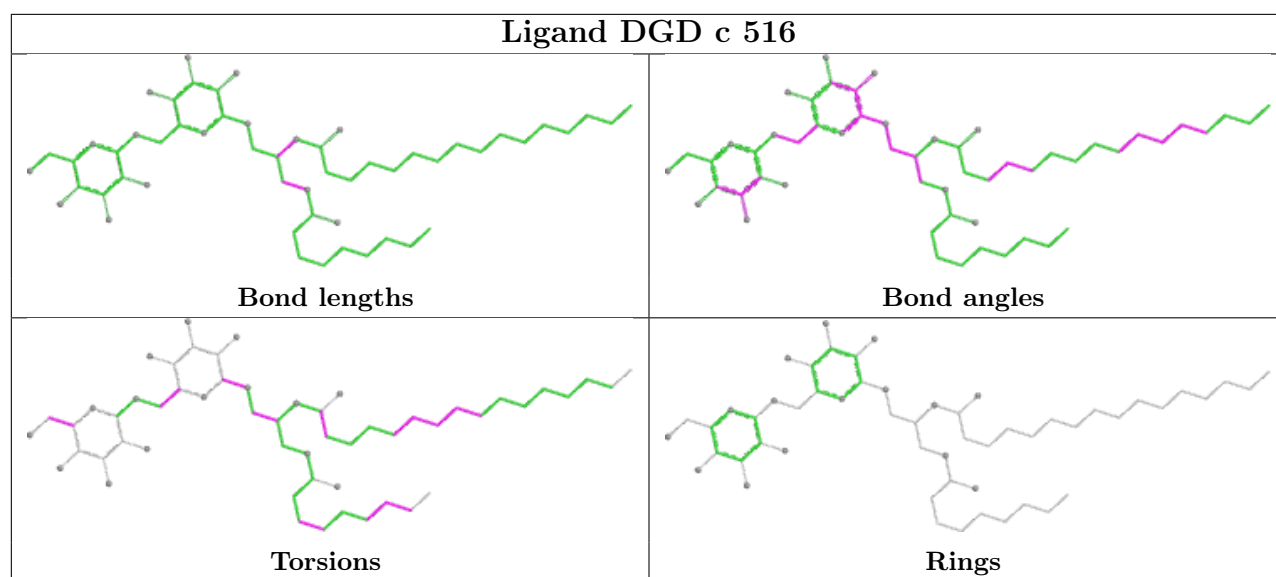
Rings



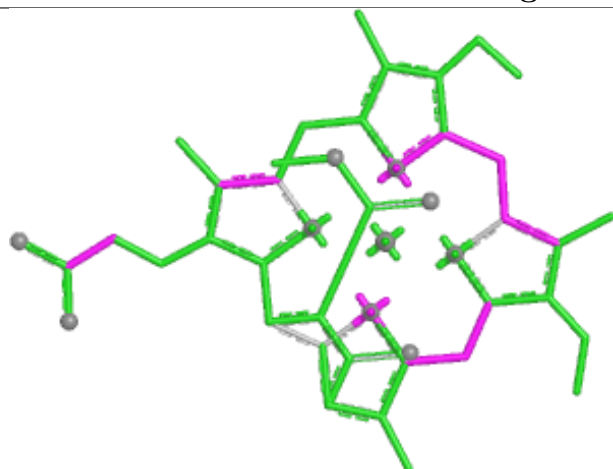




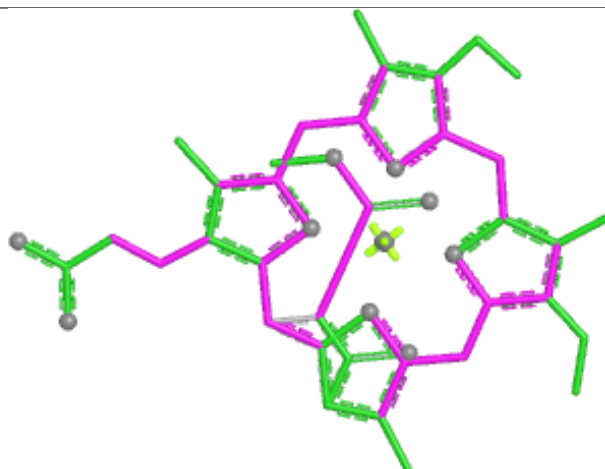




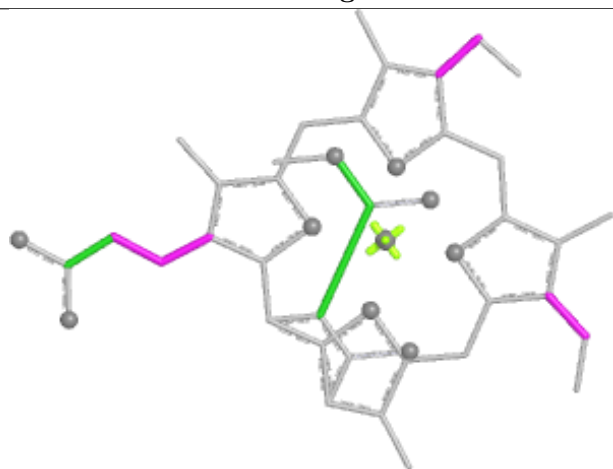
Ligand KC2 4 307



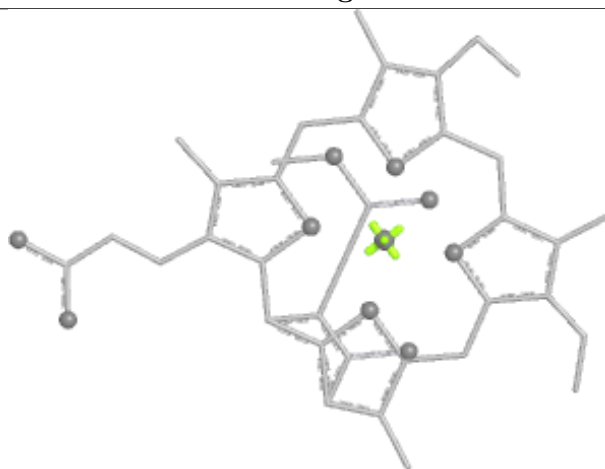
Bond lengths



Bond angles

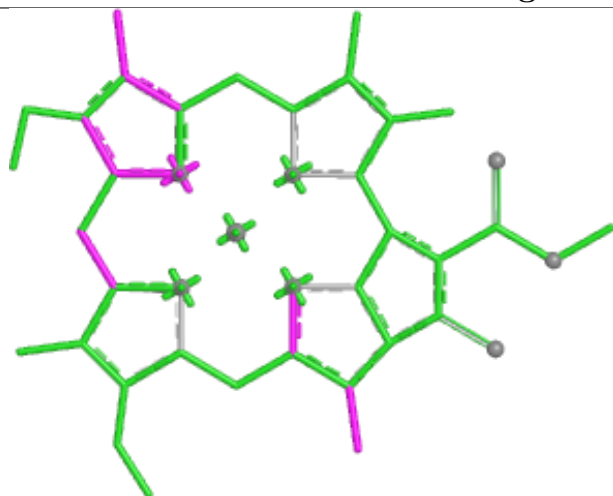


Torsions

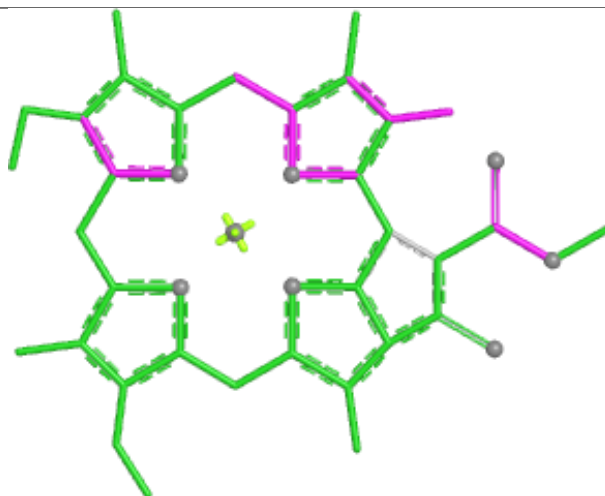


Rings

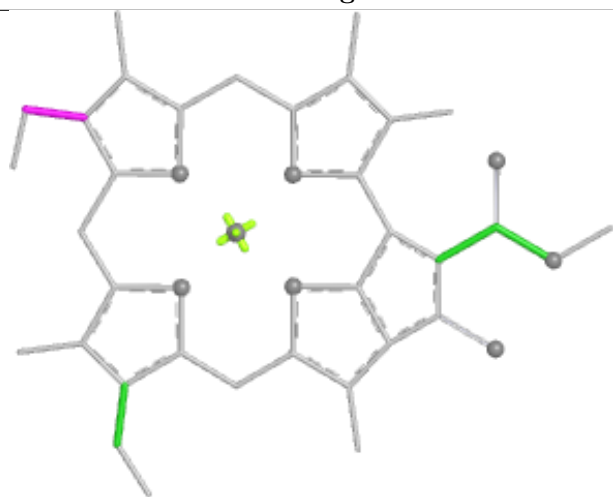
Ligand CLA 8 305



Bond lengths



Bond angles

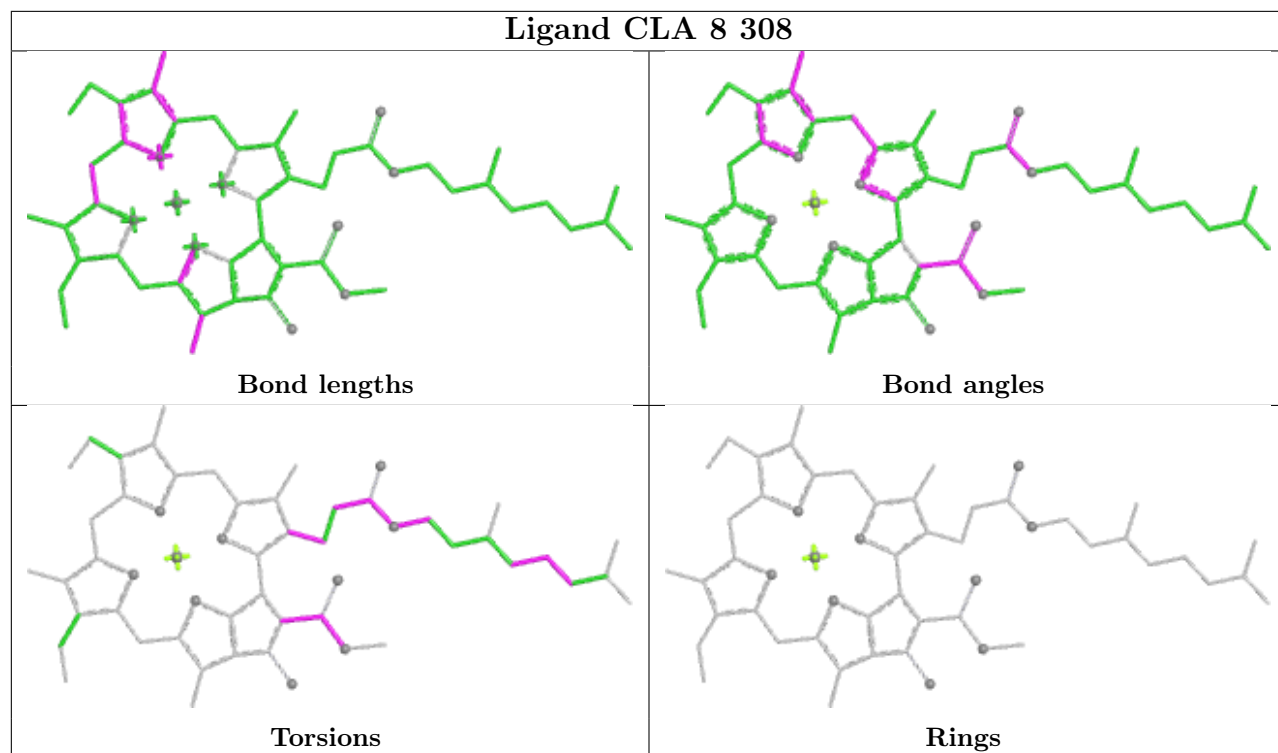


Torsions

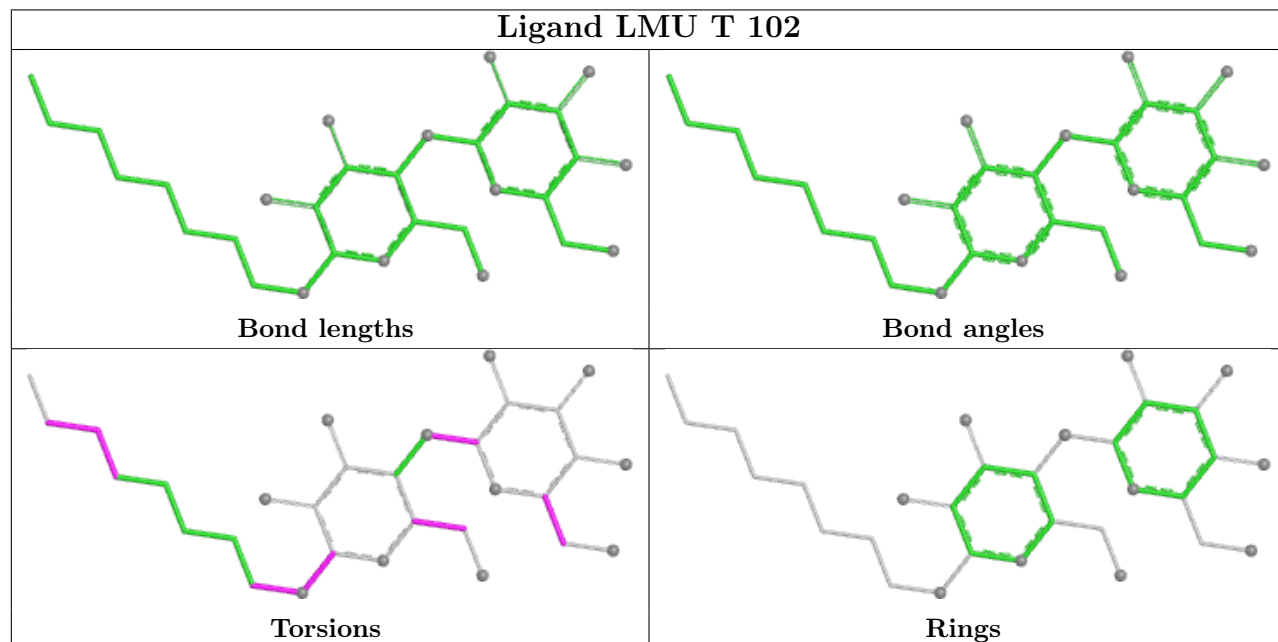


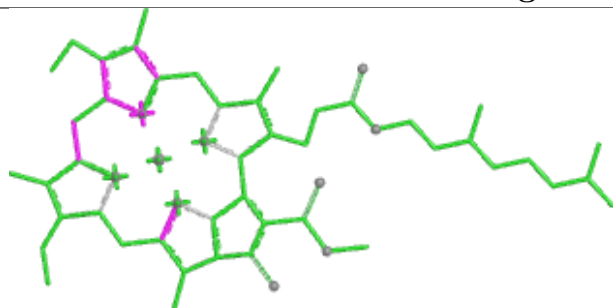
Rings

Ligand CLA 8 308

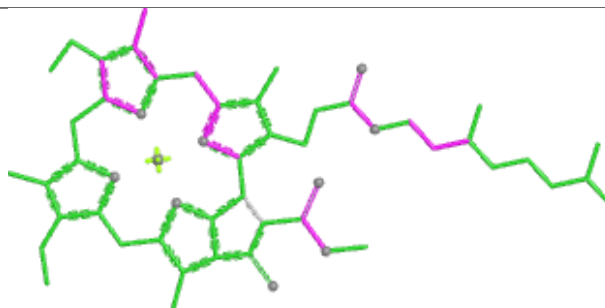


Ligand LMU T 102

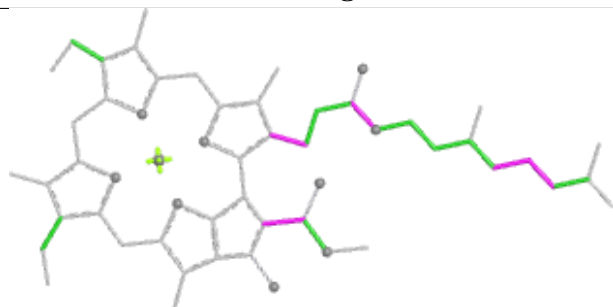


Ligand CLA 1 308

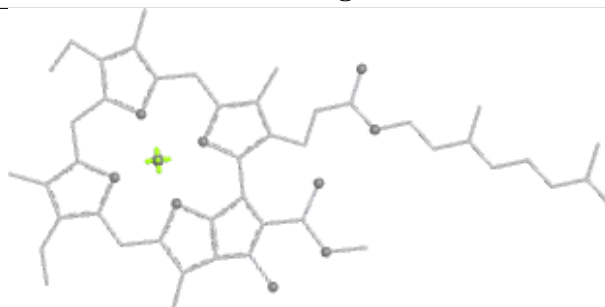
Bond lengths



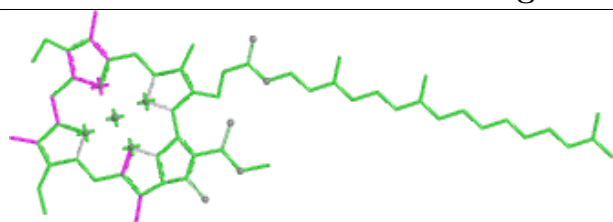
Bond angles



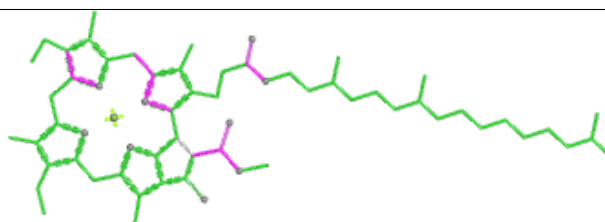
Torsions



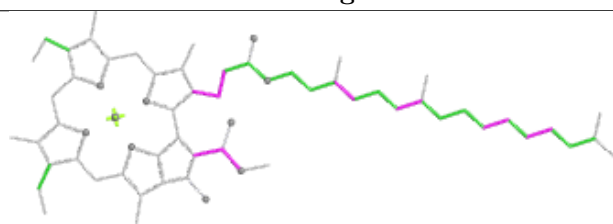
Rings

Ligand CLA b 604

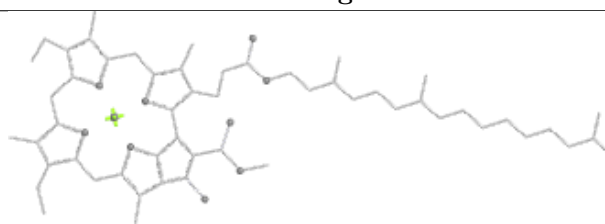
Bond lengths



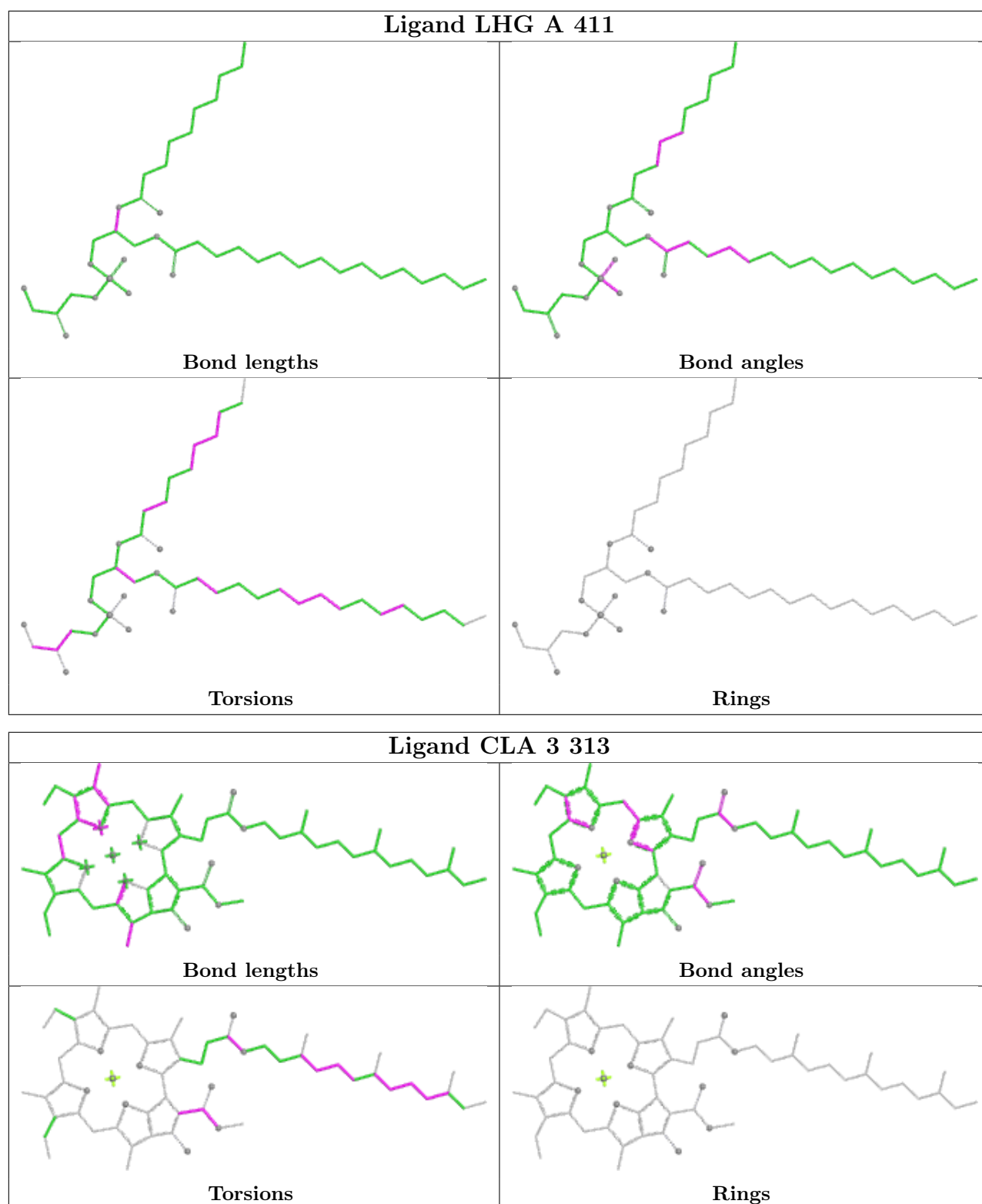
Bond angles

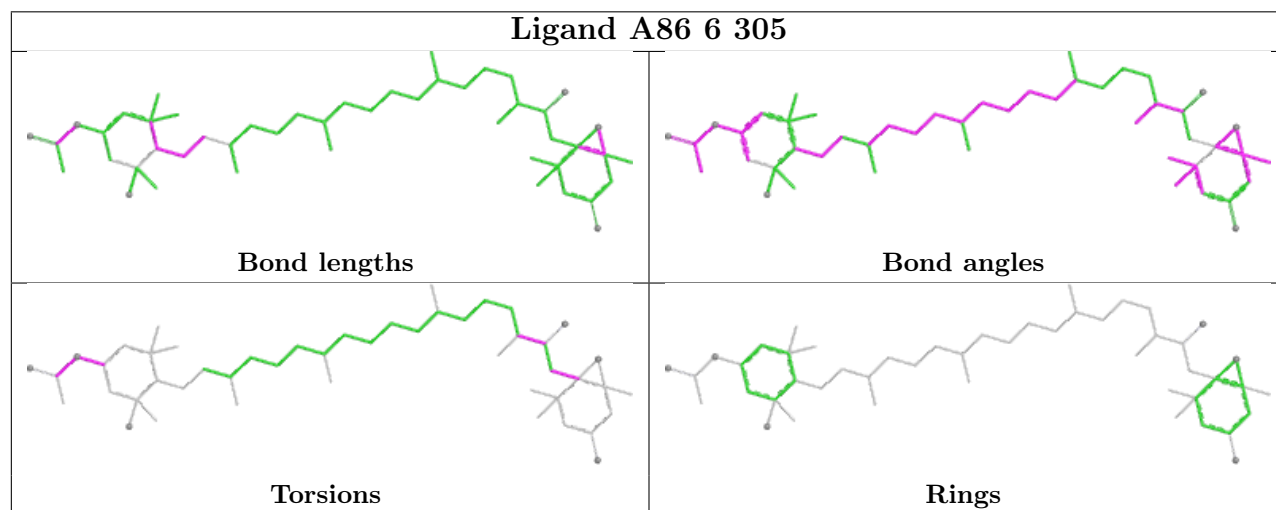
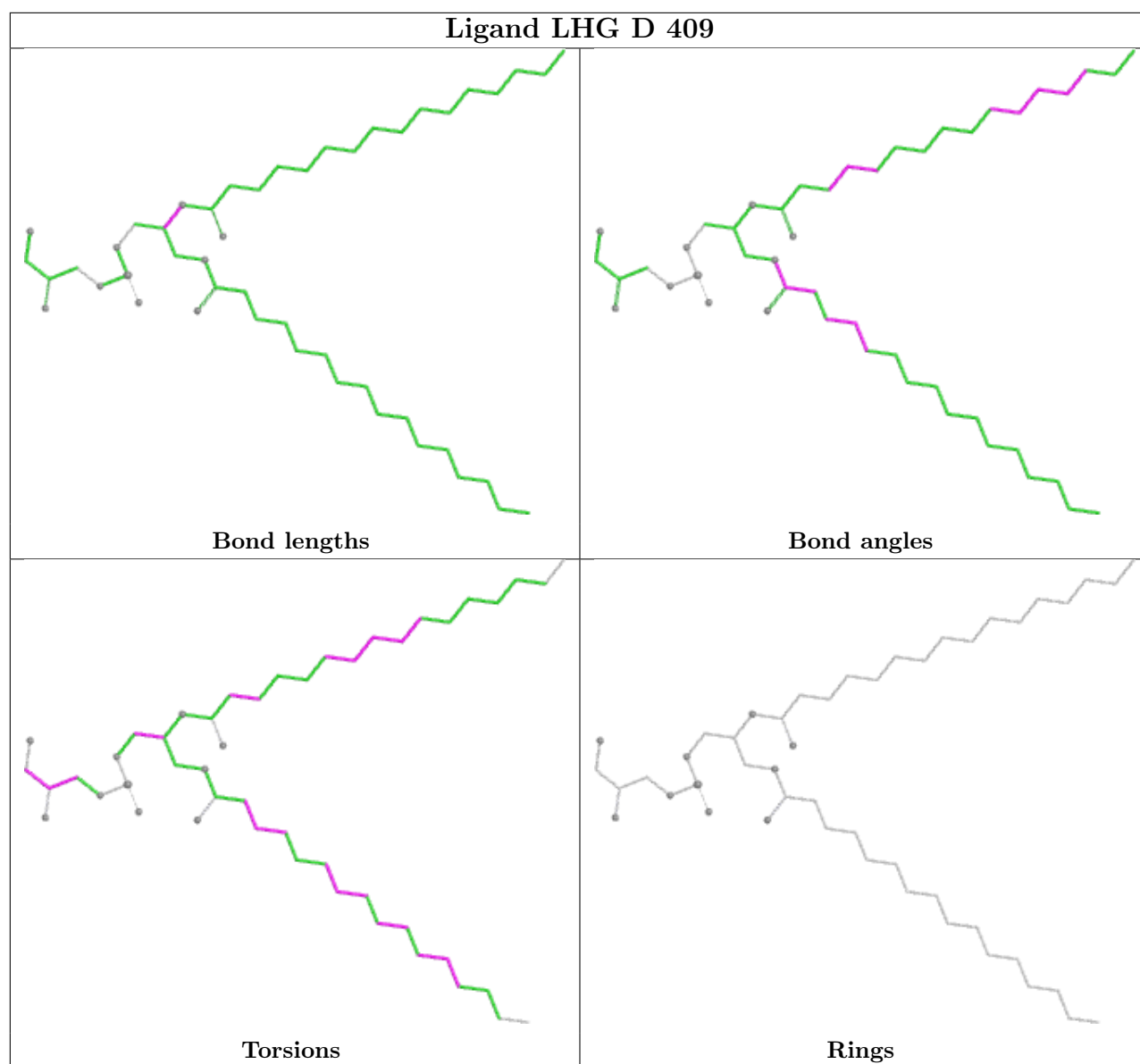


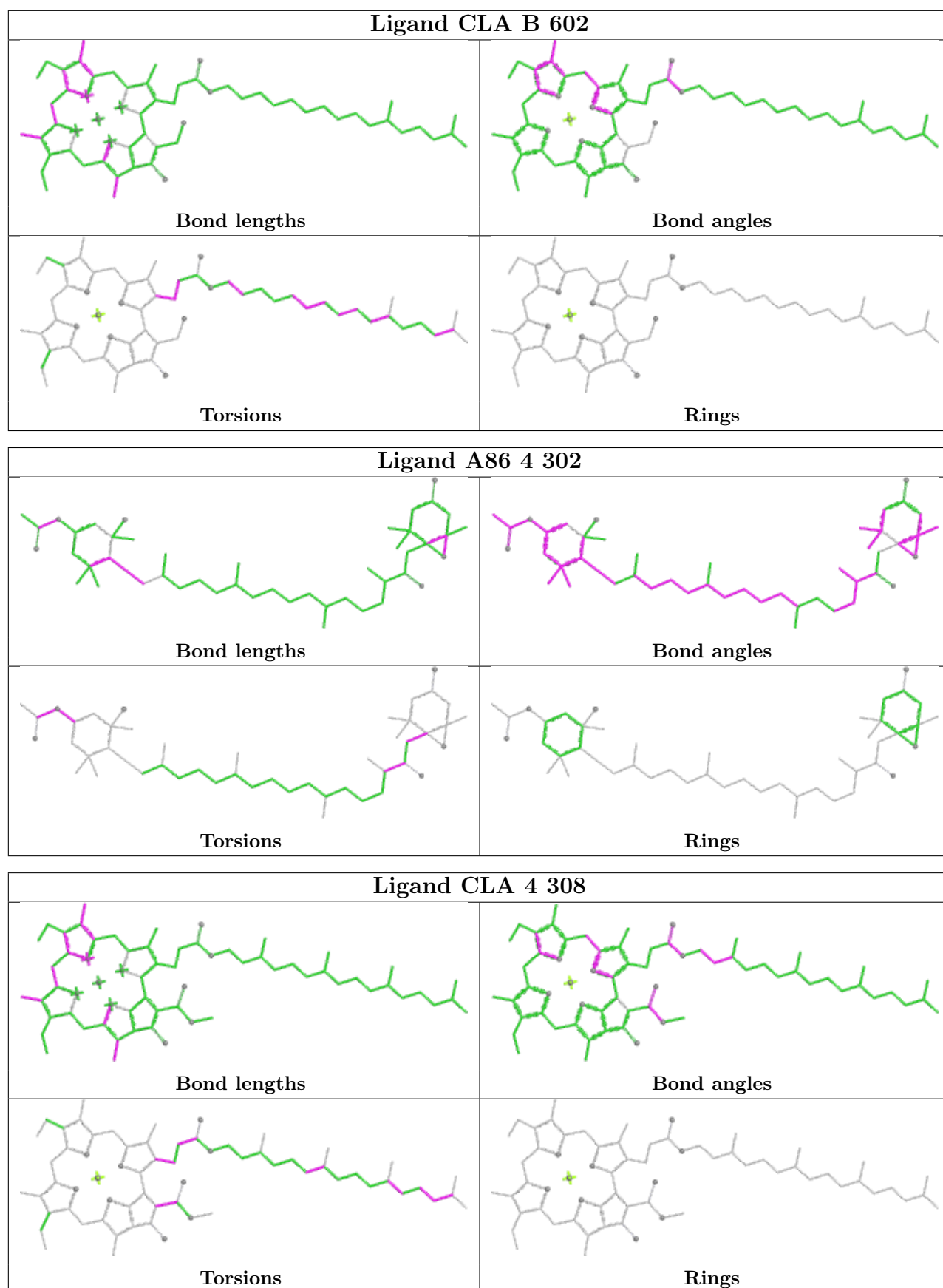
Torsions

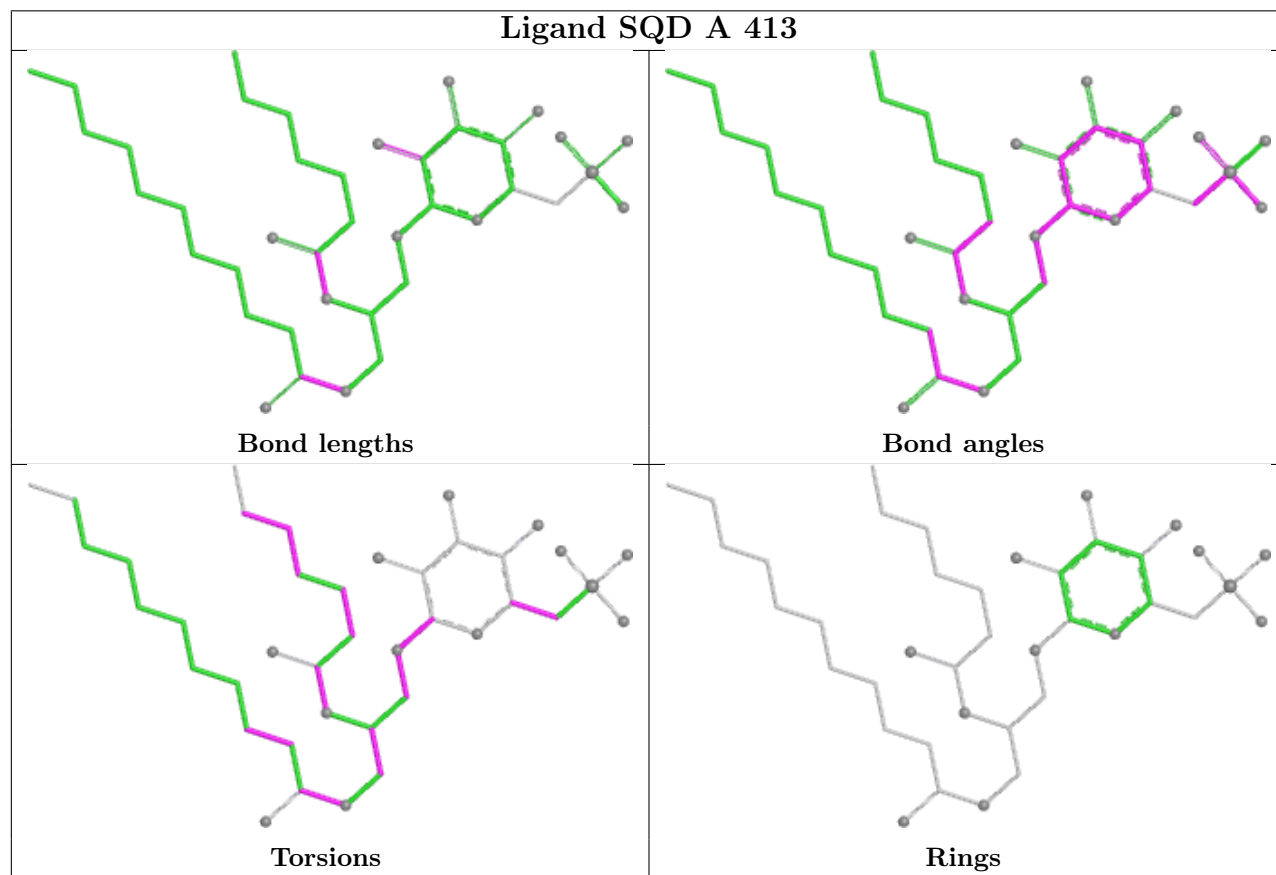
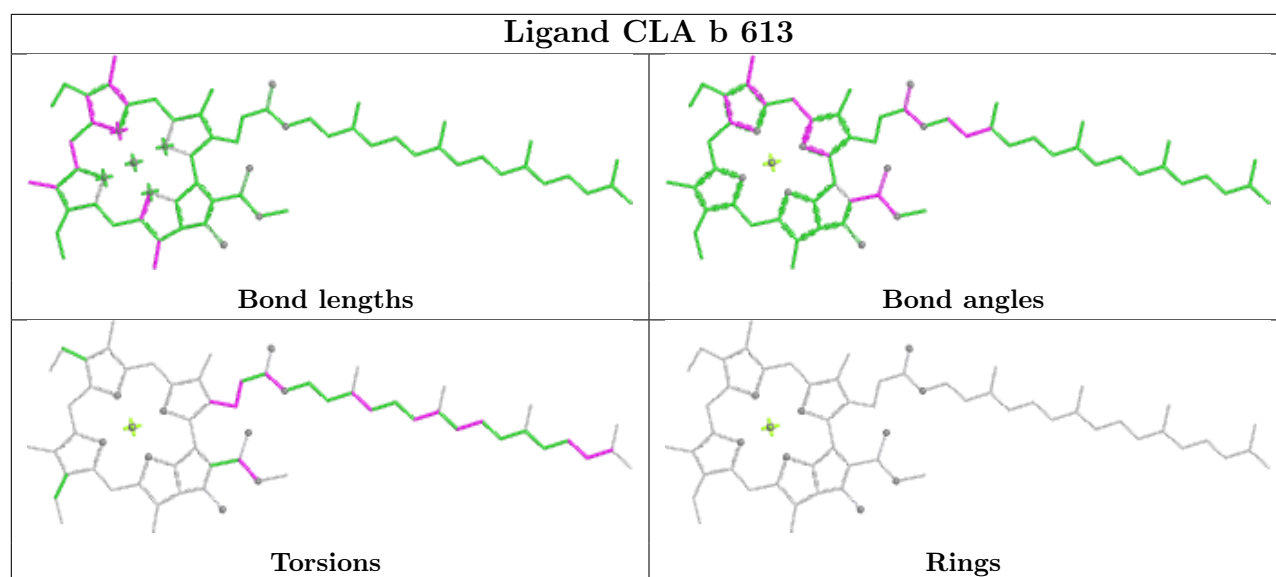


Rings

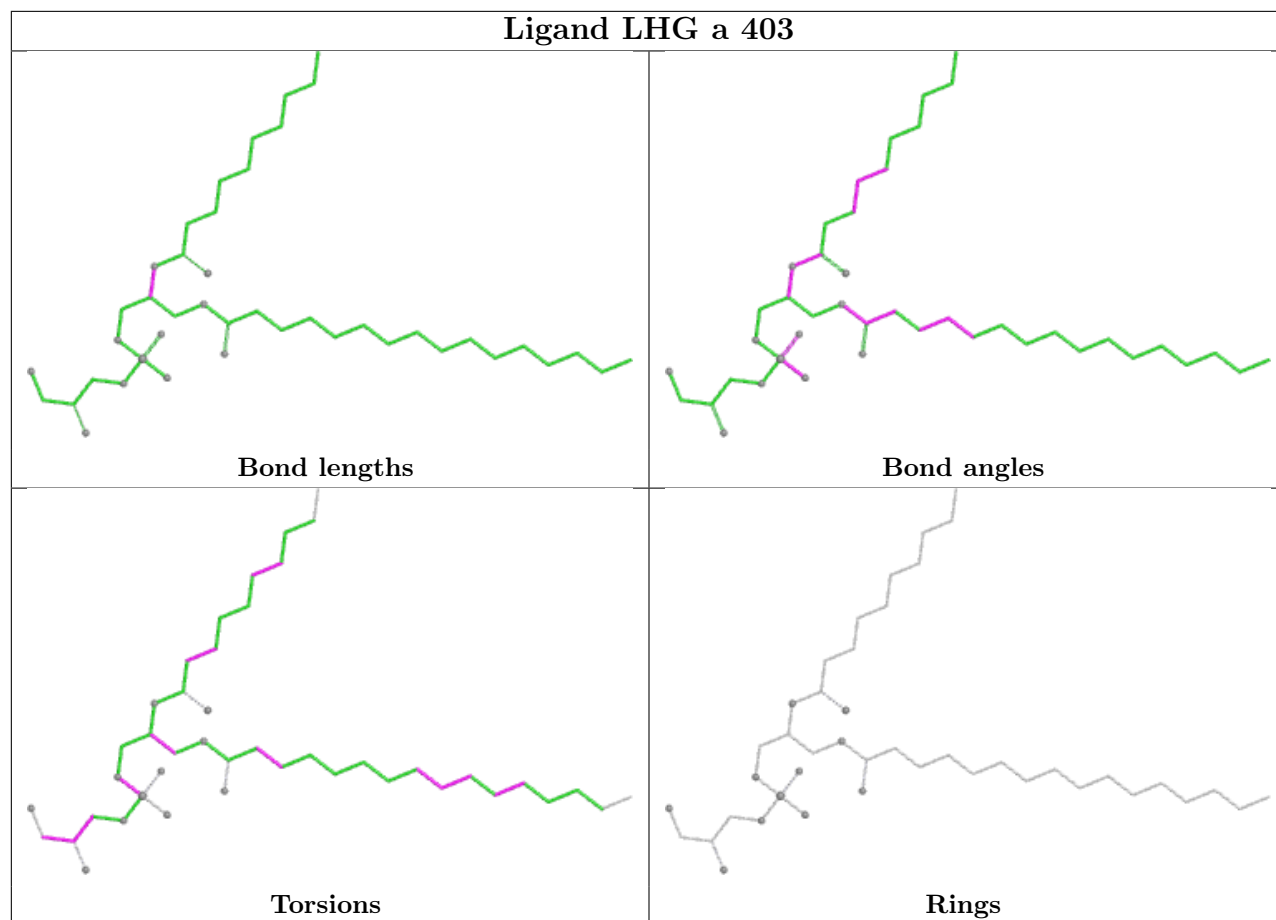




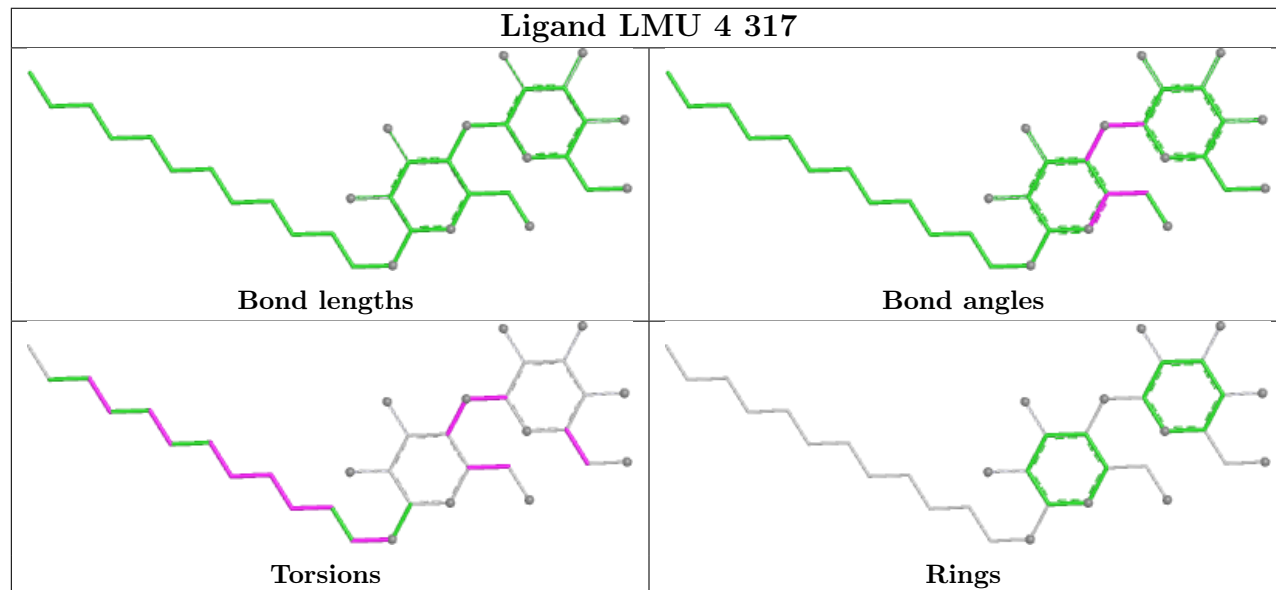


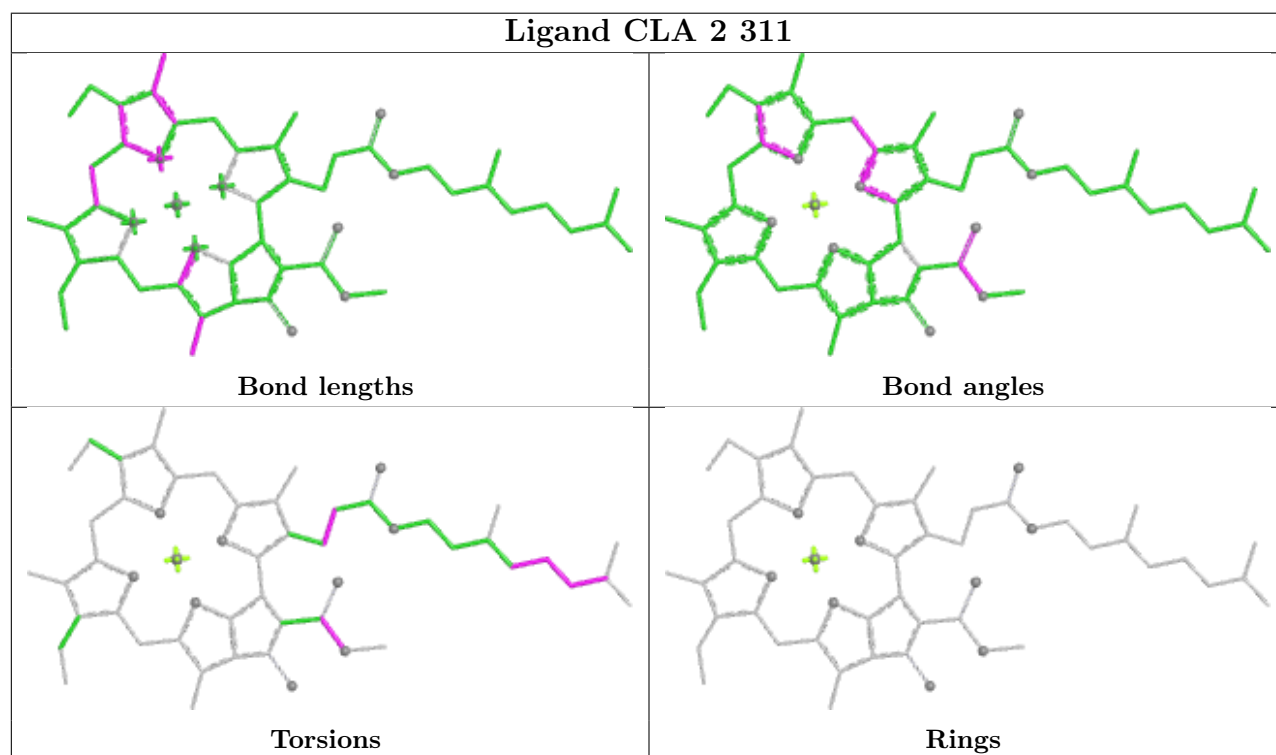
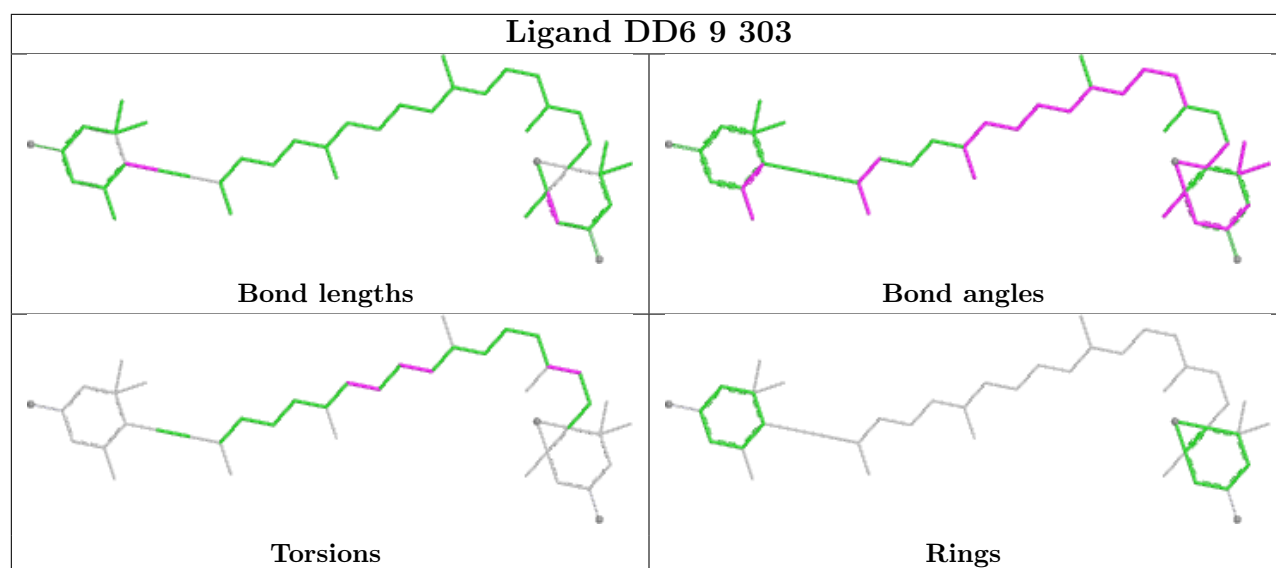


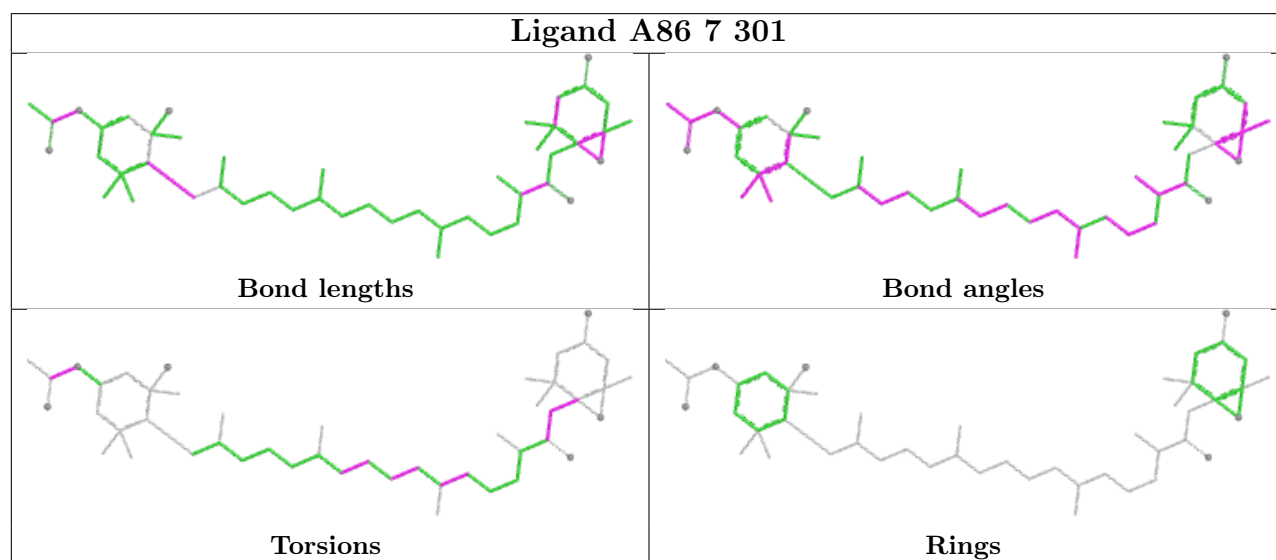
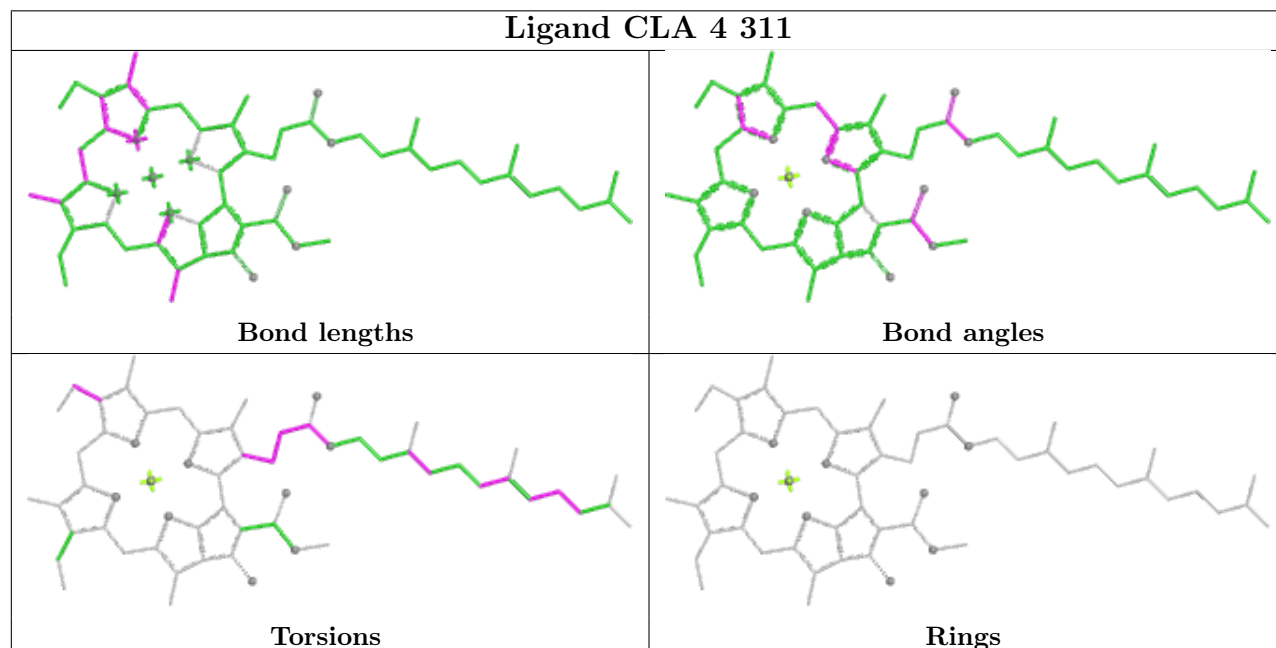
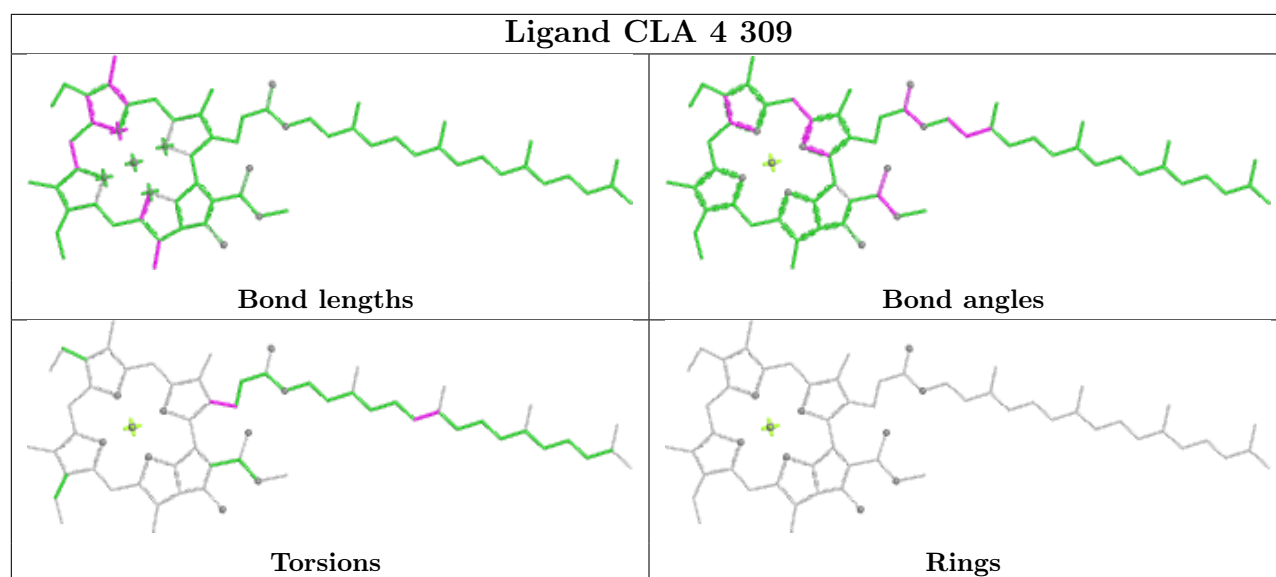
Ligand LHG a 403

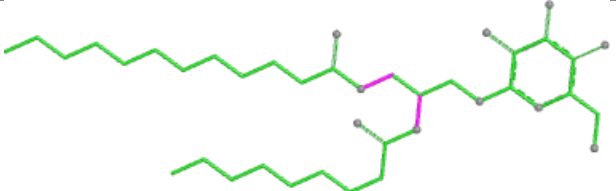
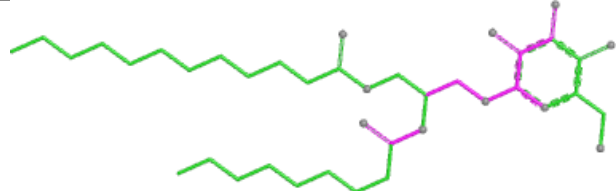
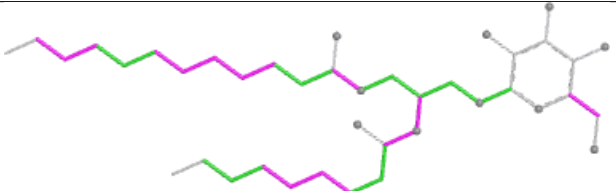
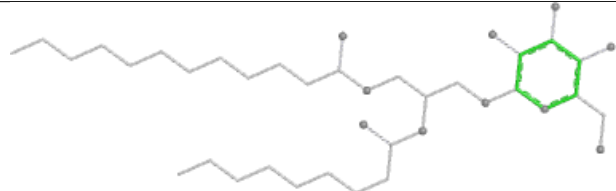


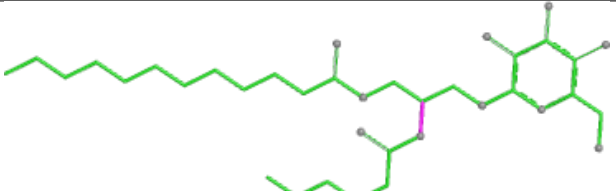
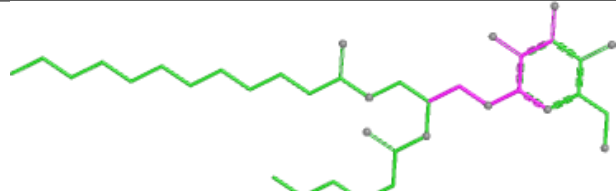
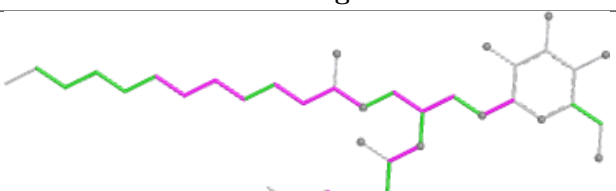
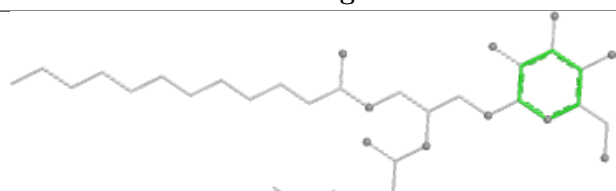
Ligand LMU 4 317

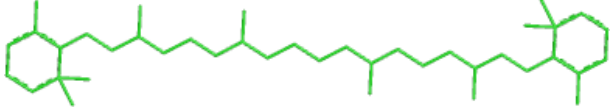
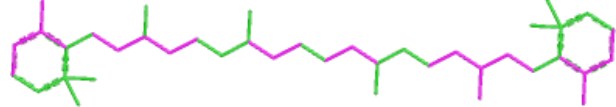
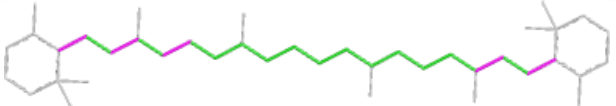
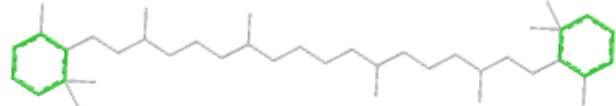




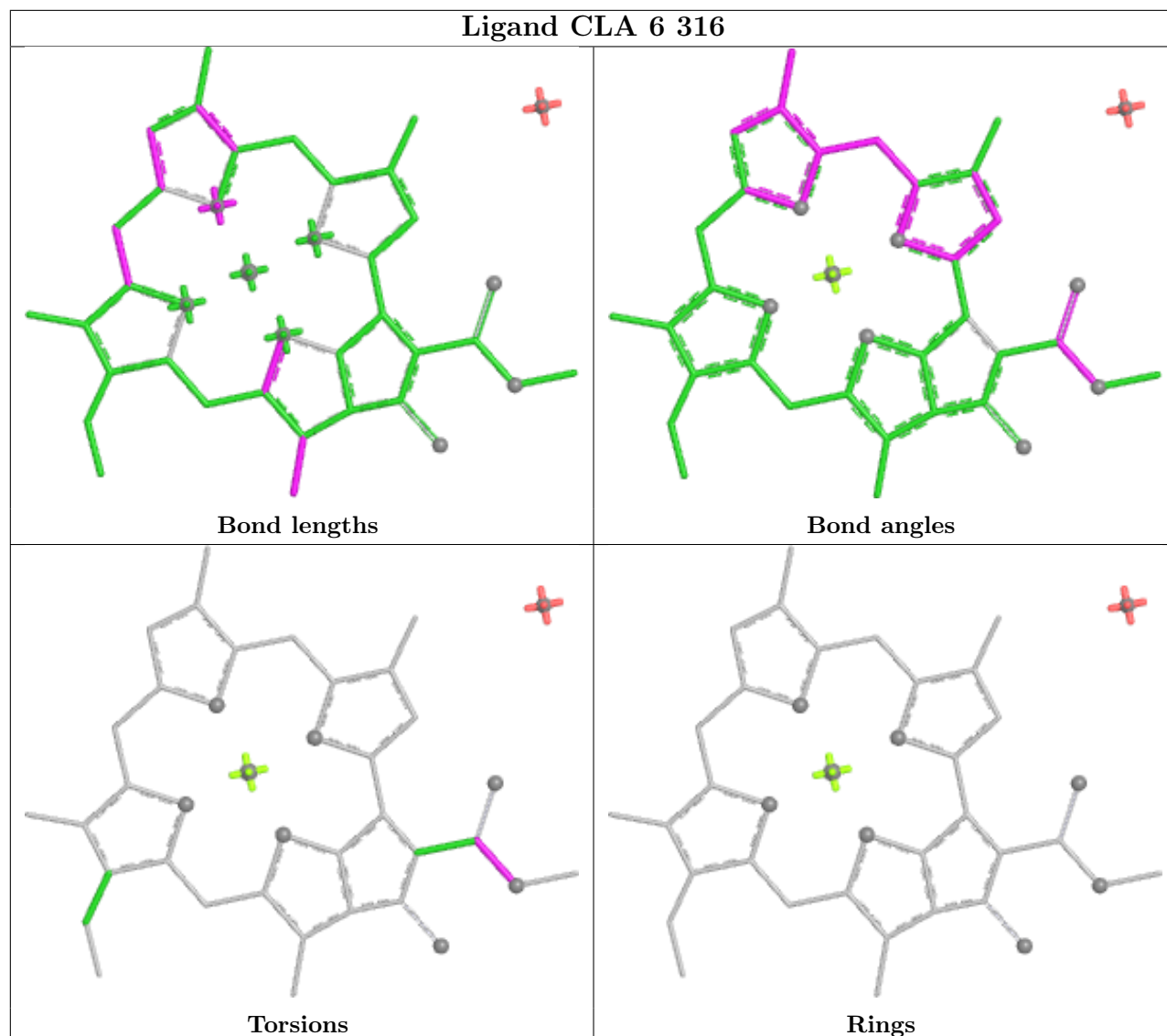


Ligand LMG m 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

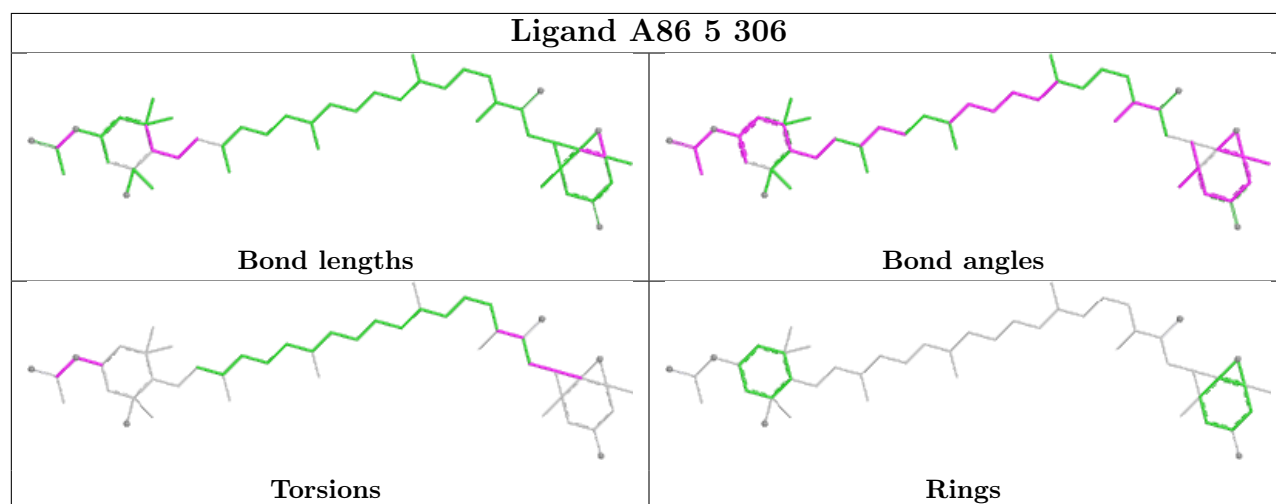
Ligand LMG Q 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

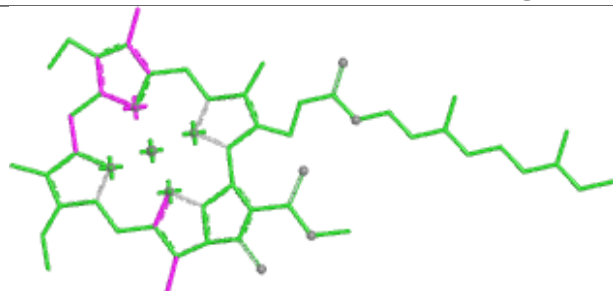
Ligand CLA 6 316



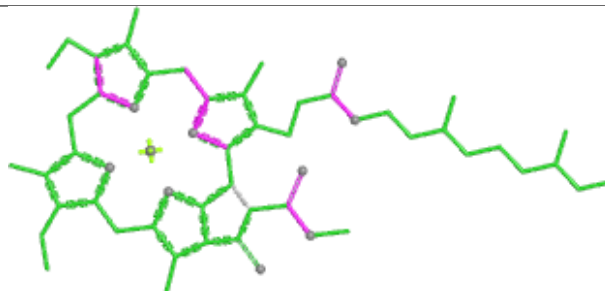
Ligand A86 5 306



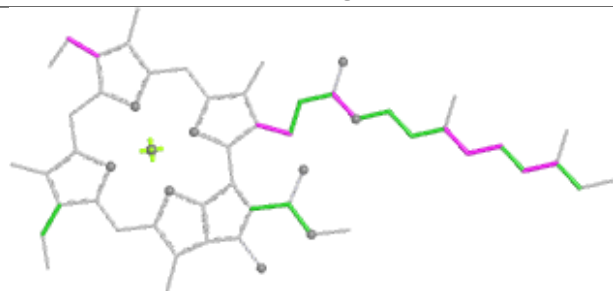
Ligand CLA 3 312



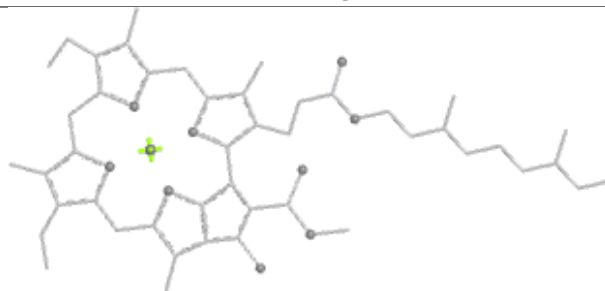
Bond lengths



Bond angles

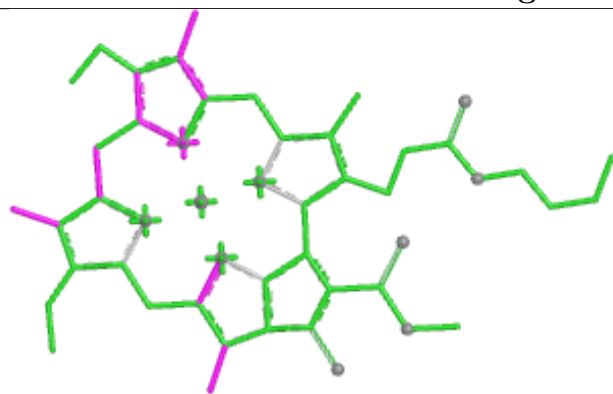


Torsions

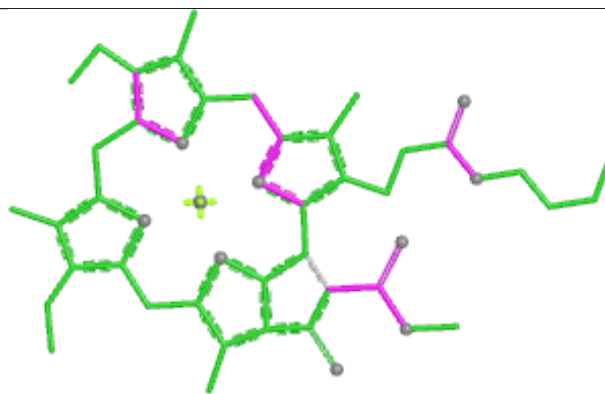


Rings

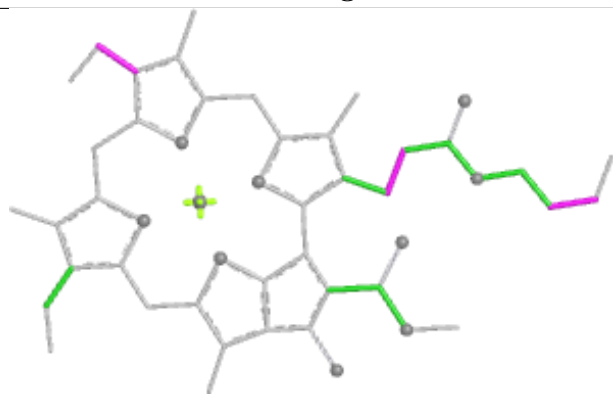
Ligand CLA a 408



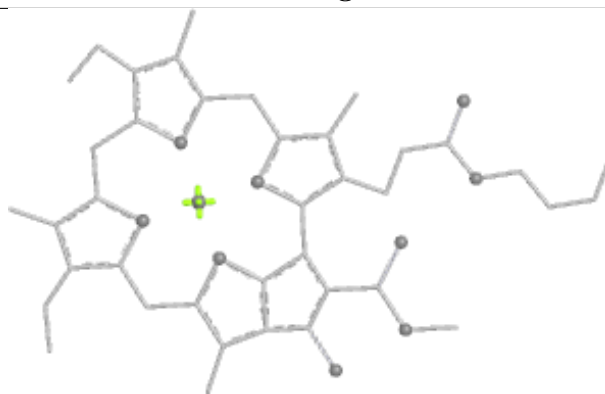
Bond lengths



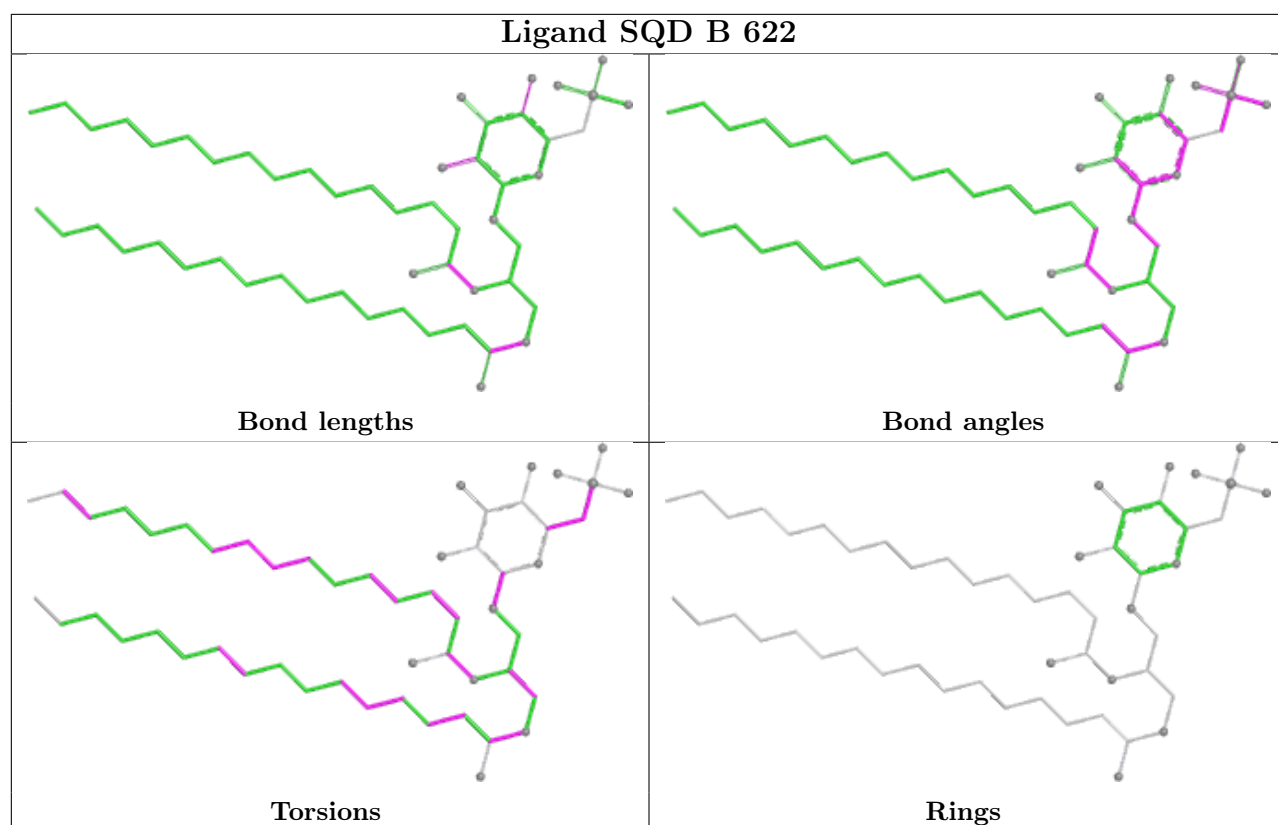
Bond angles

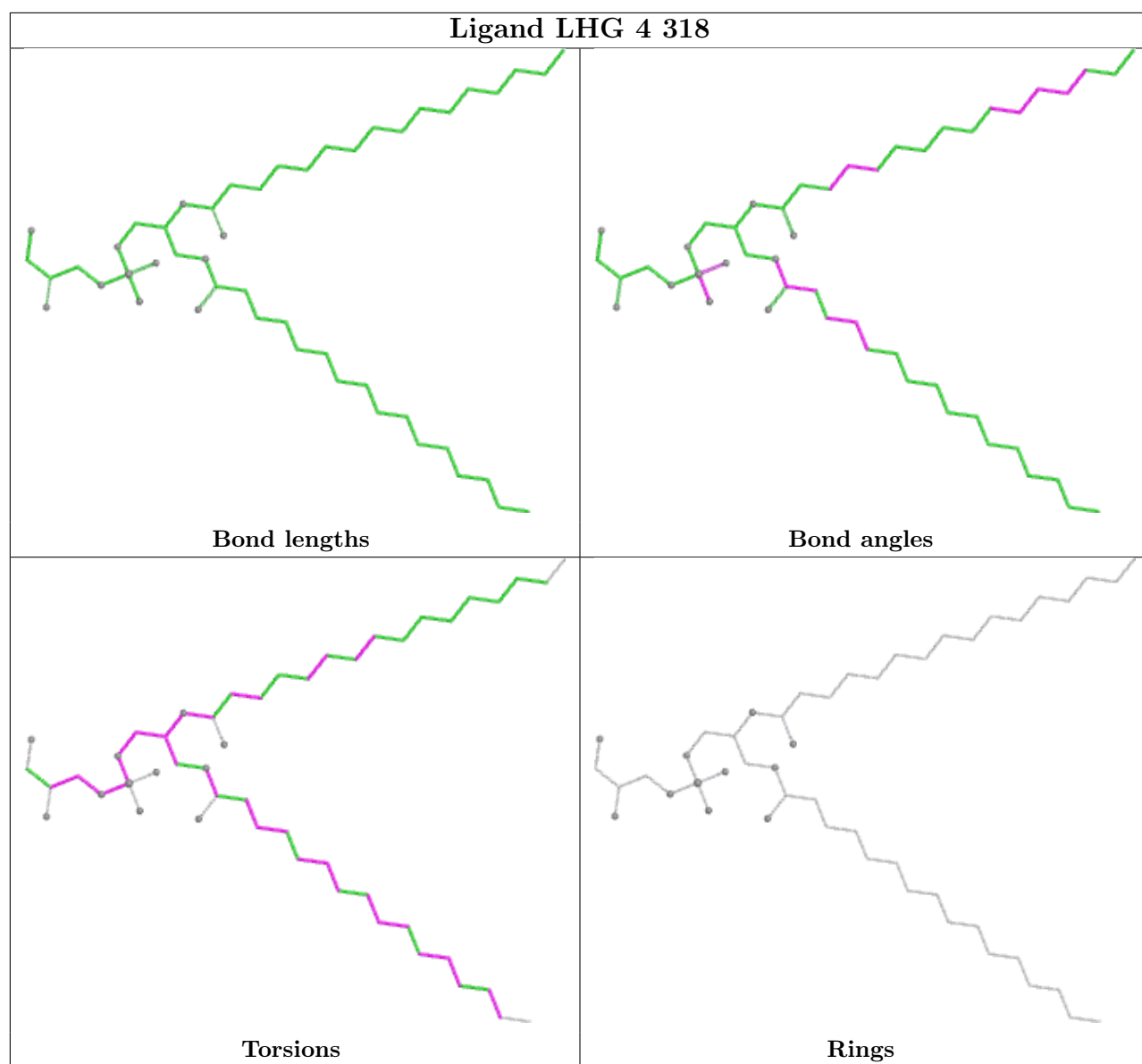


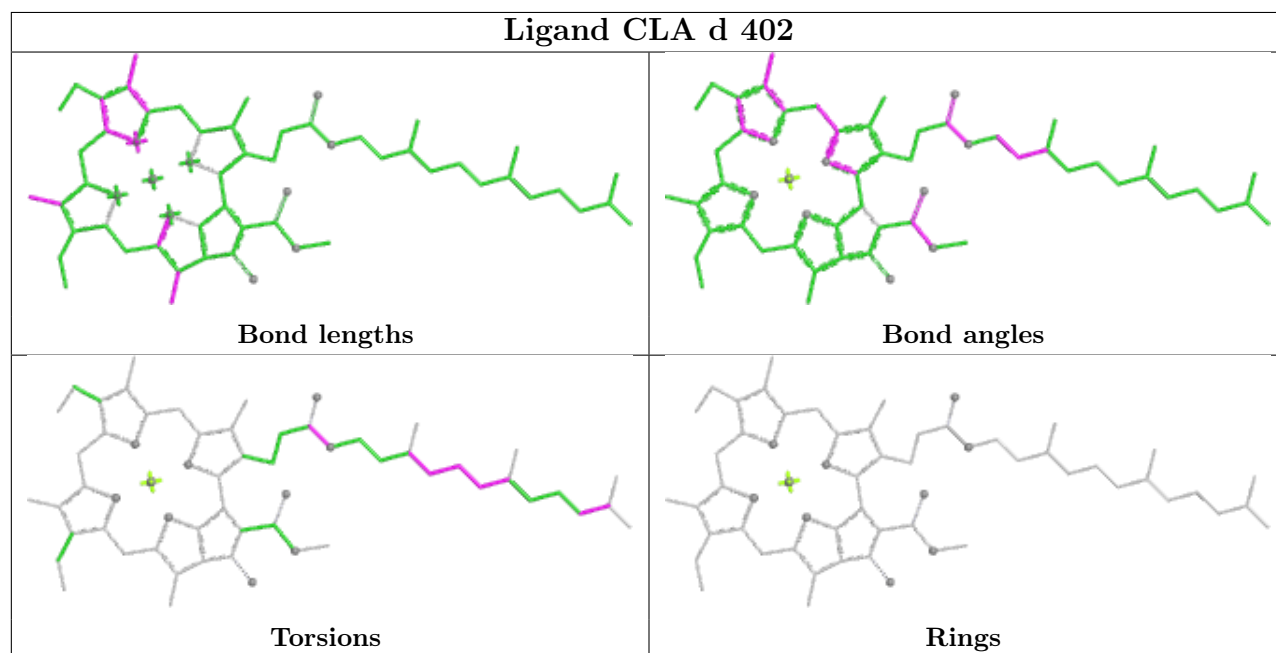
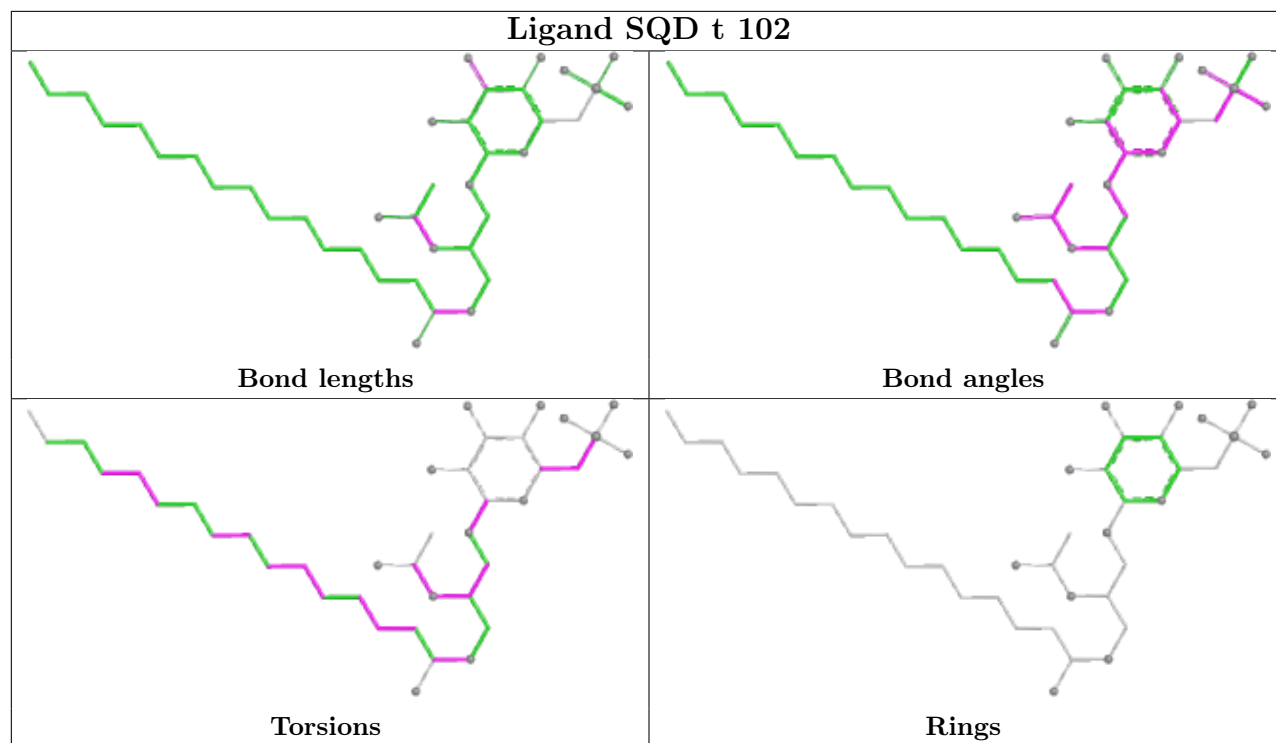
Torsions

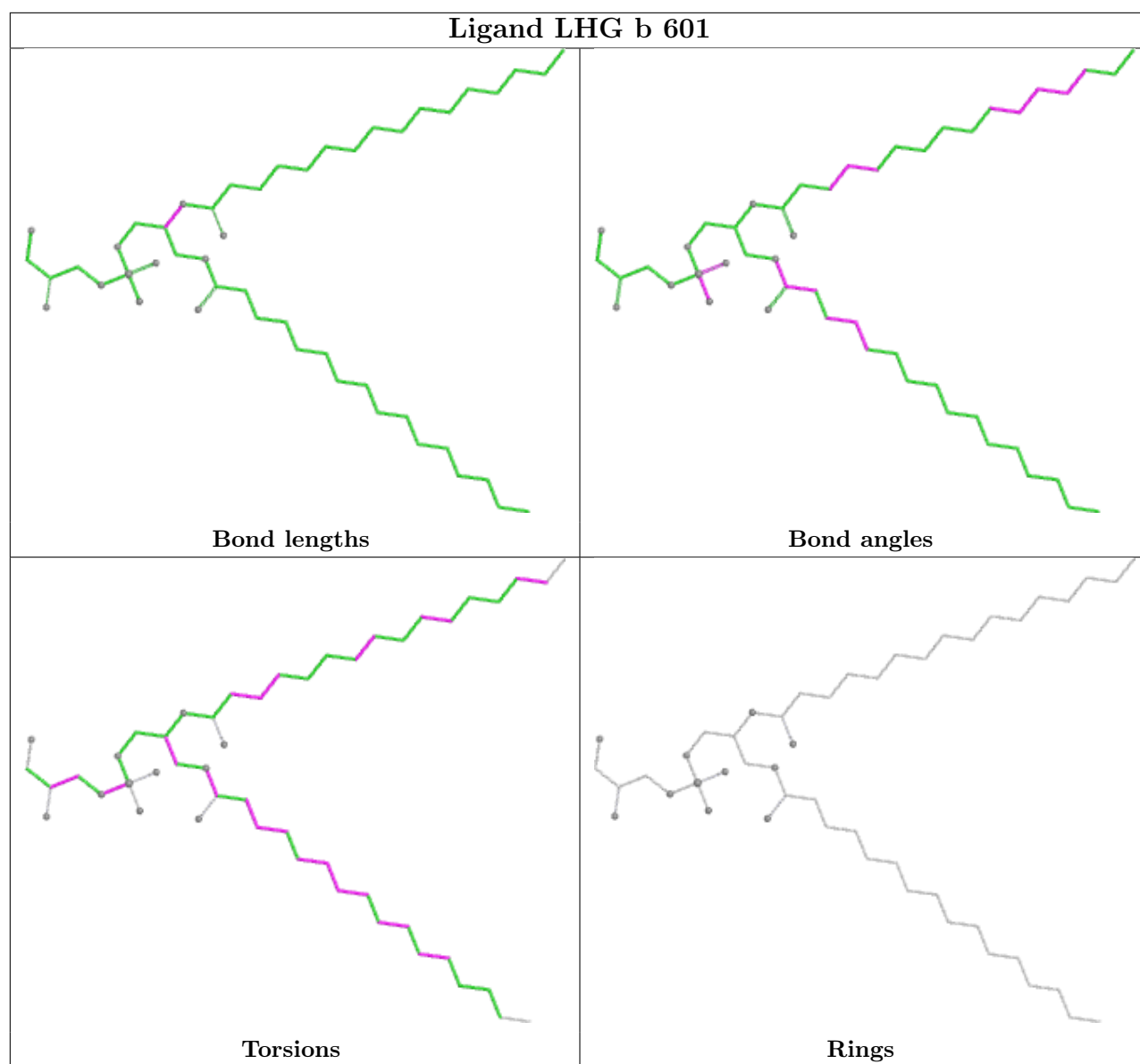


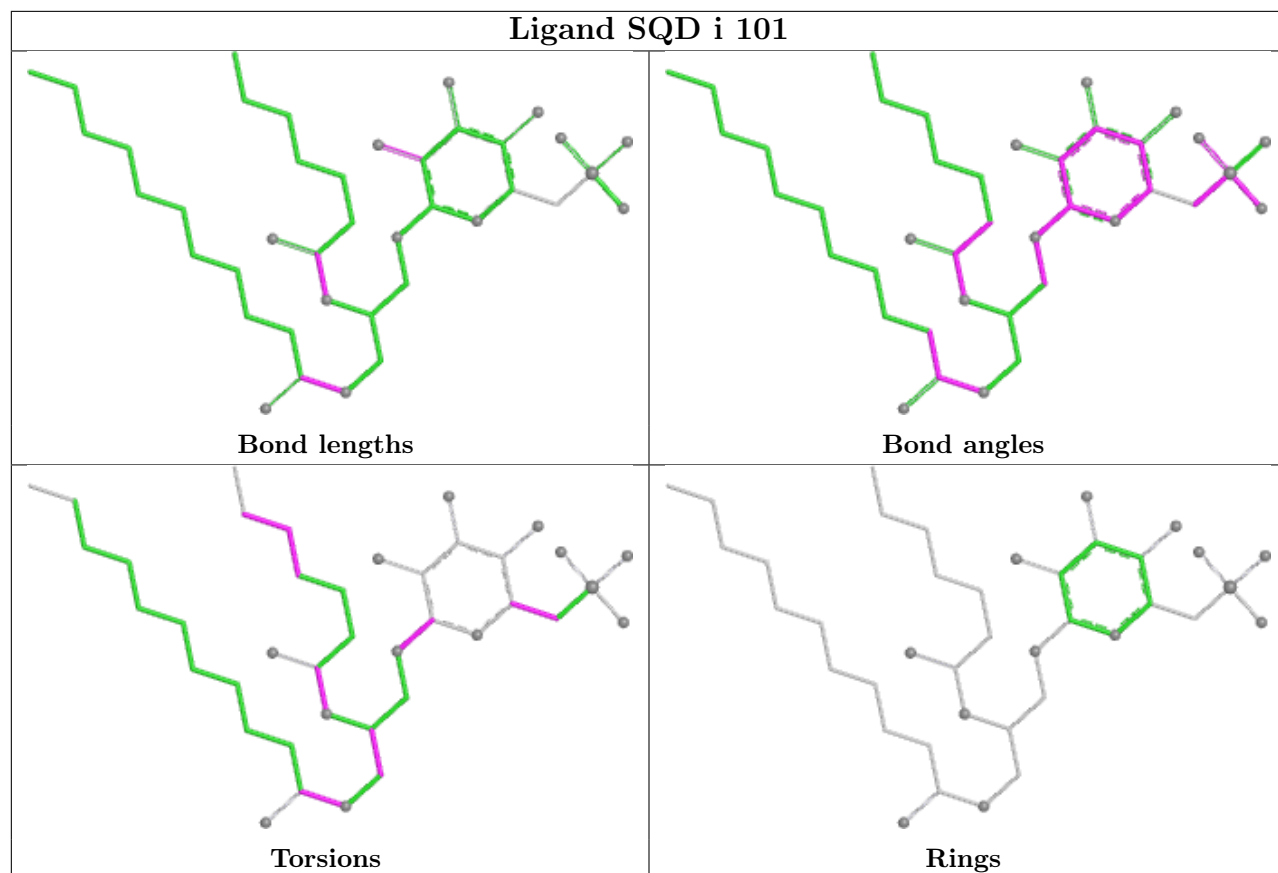
Rings



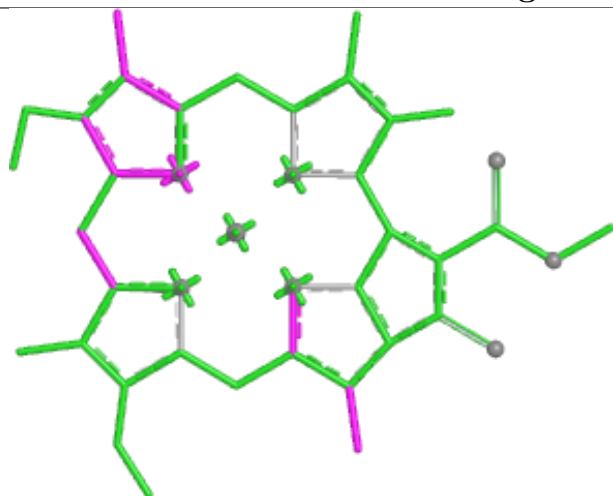




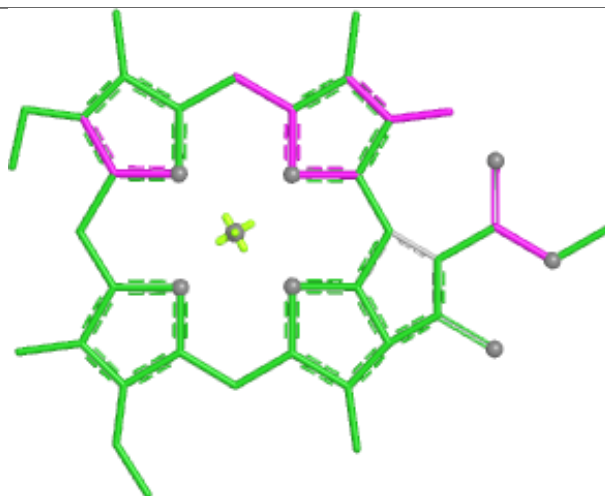




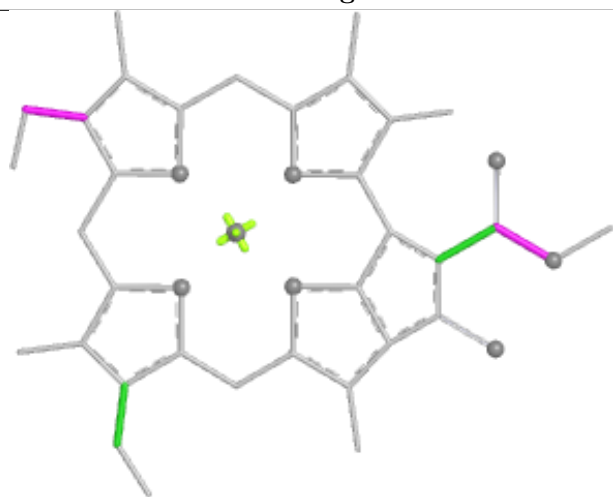
Ligand CLA 1 305



Bond lengths



Bond angles

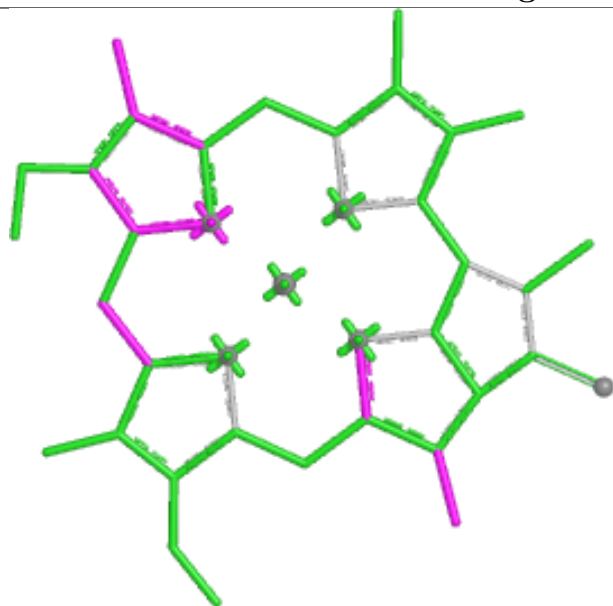


Torsions

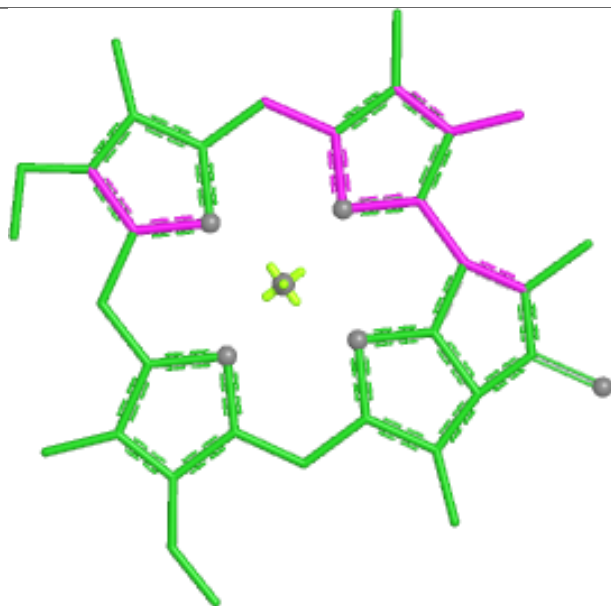


Rings

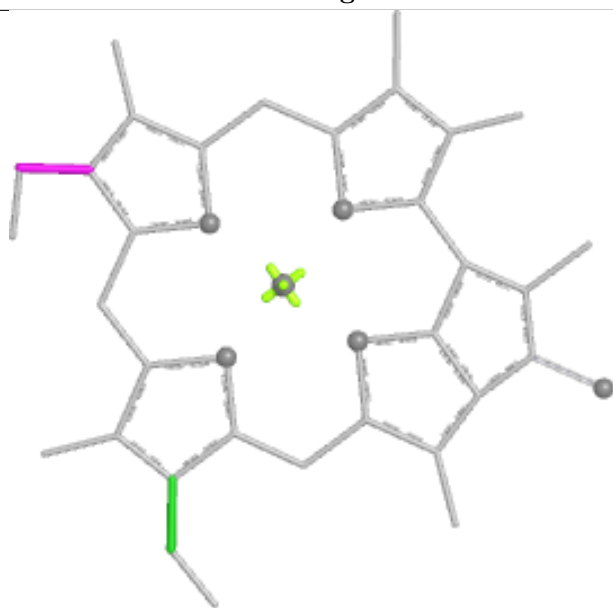
Ligand CLA 9 316



Bond lengths



Bond angles

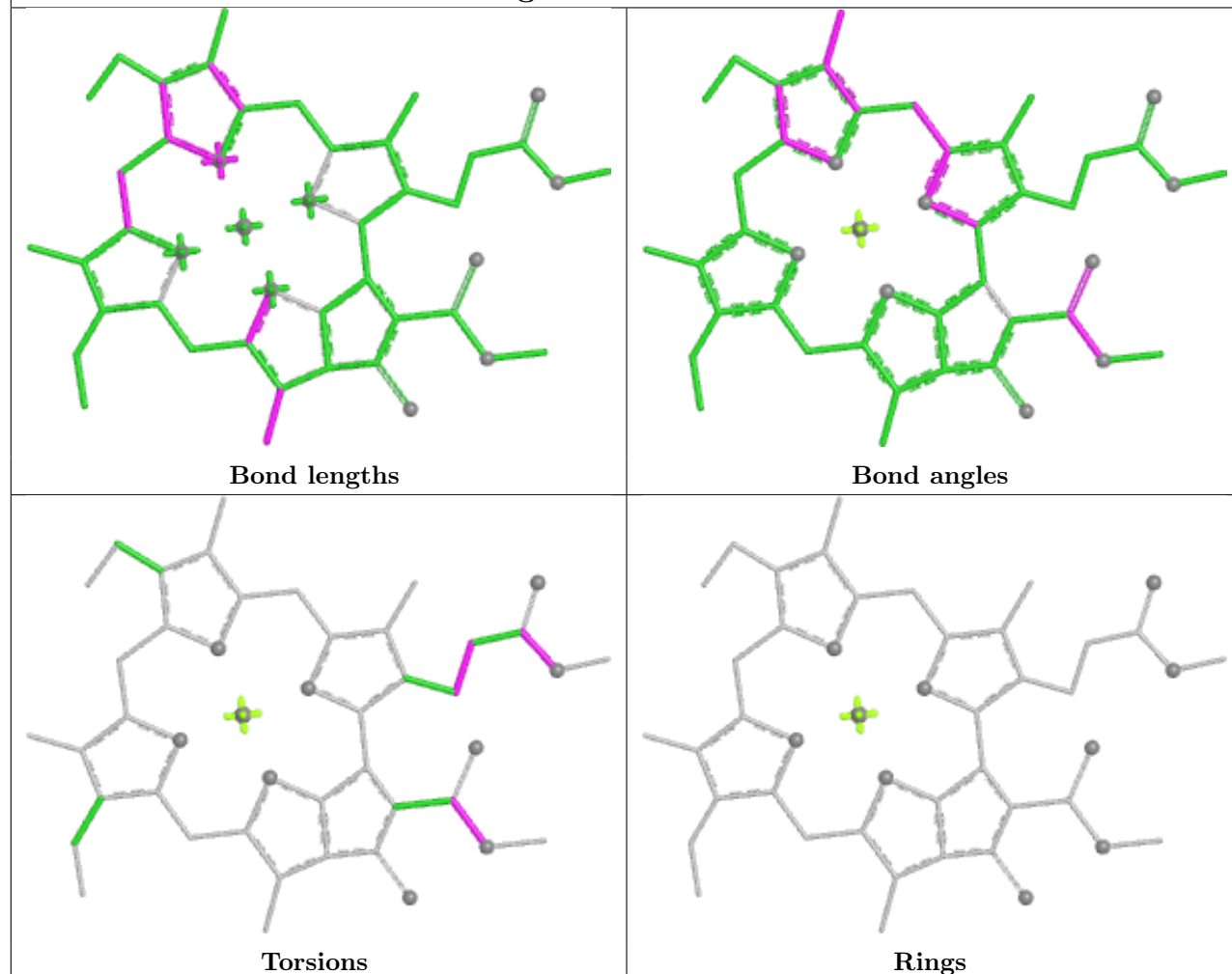


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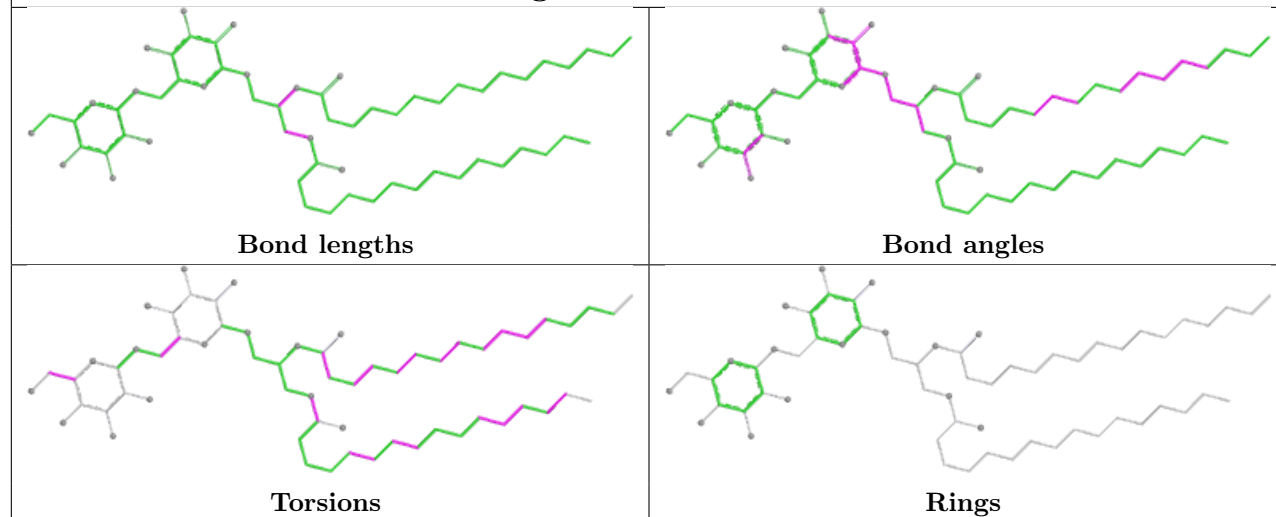


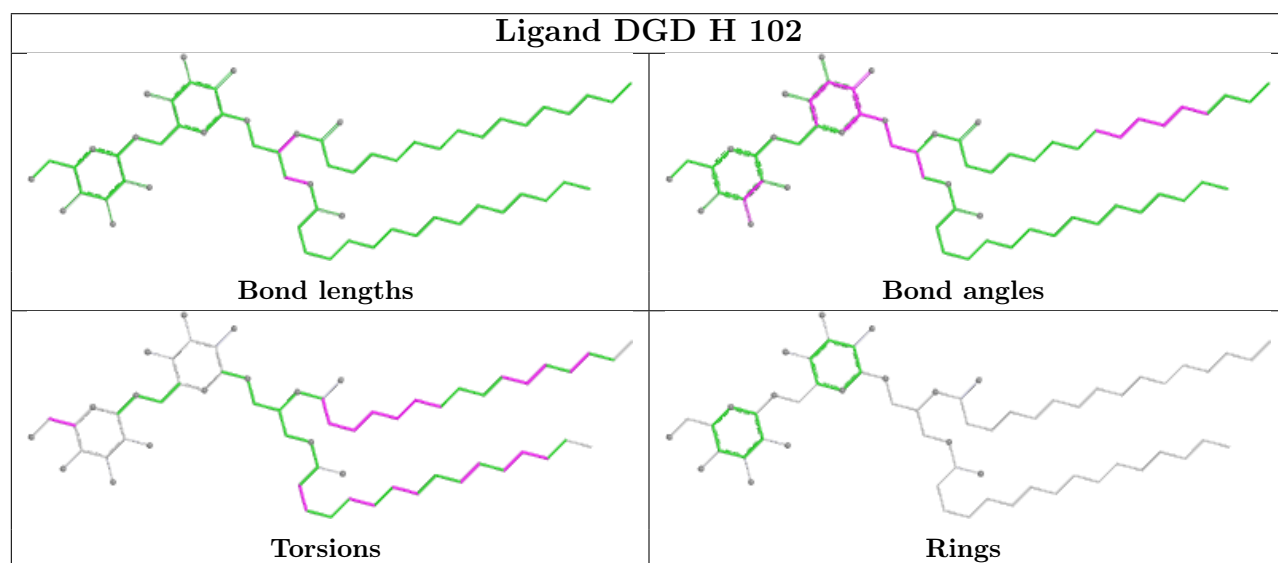
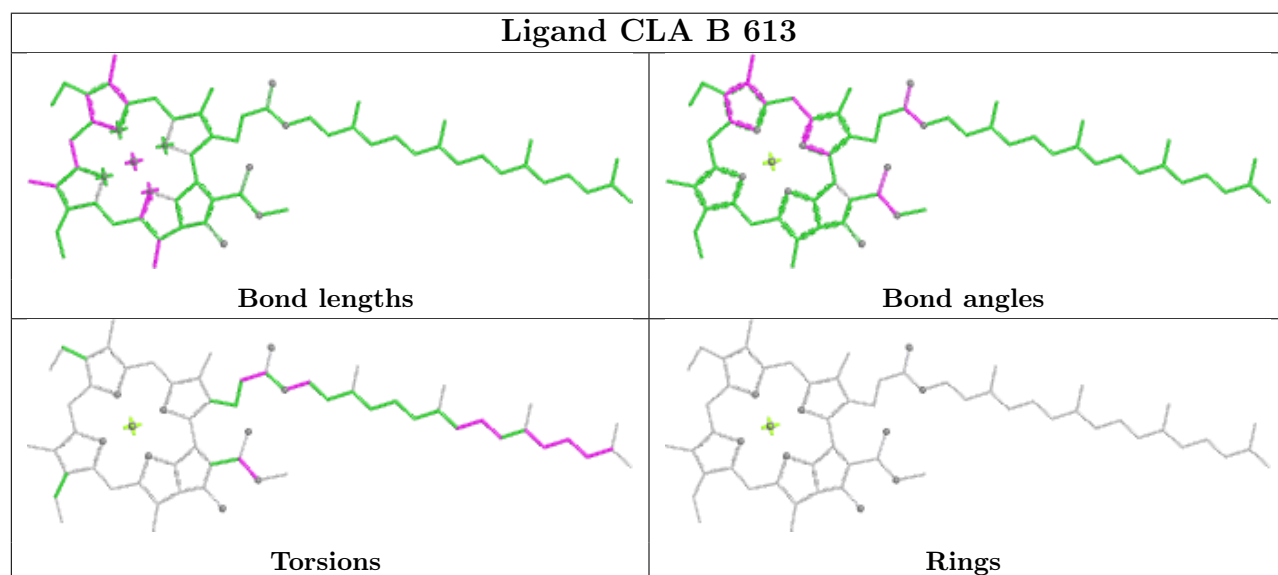
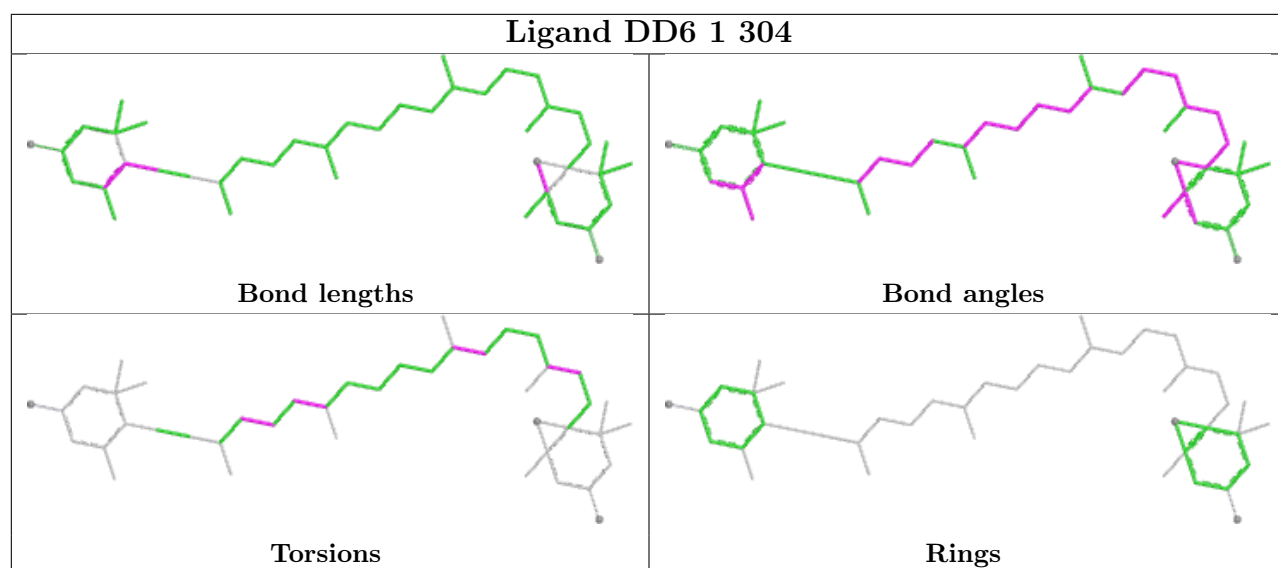
Rings

Ligand CLA 6 313

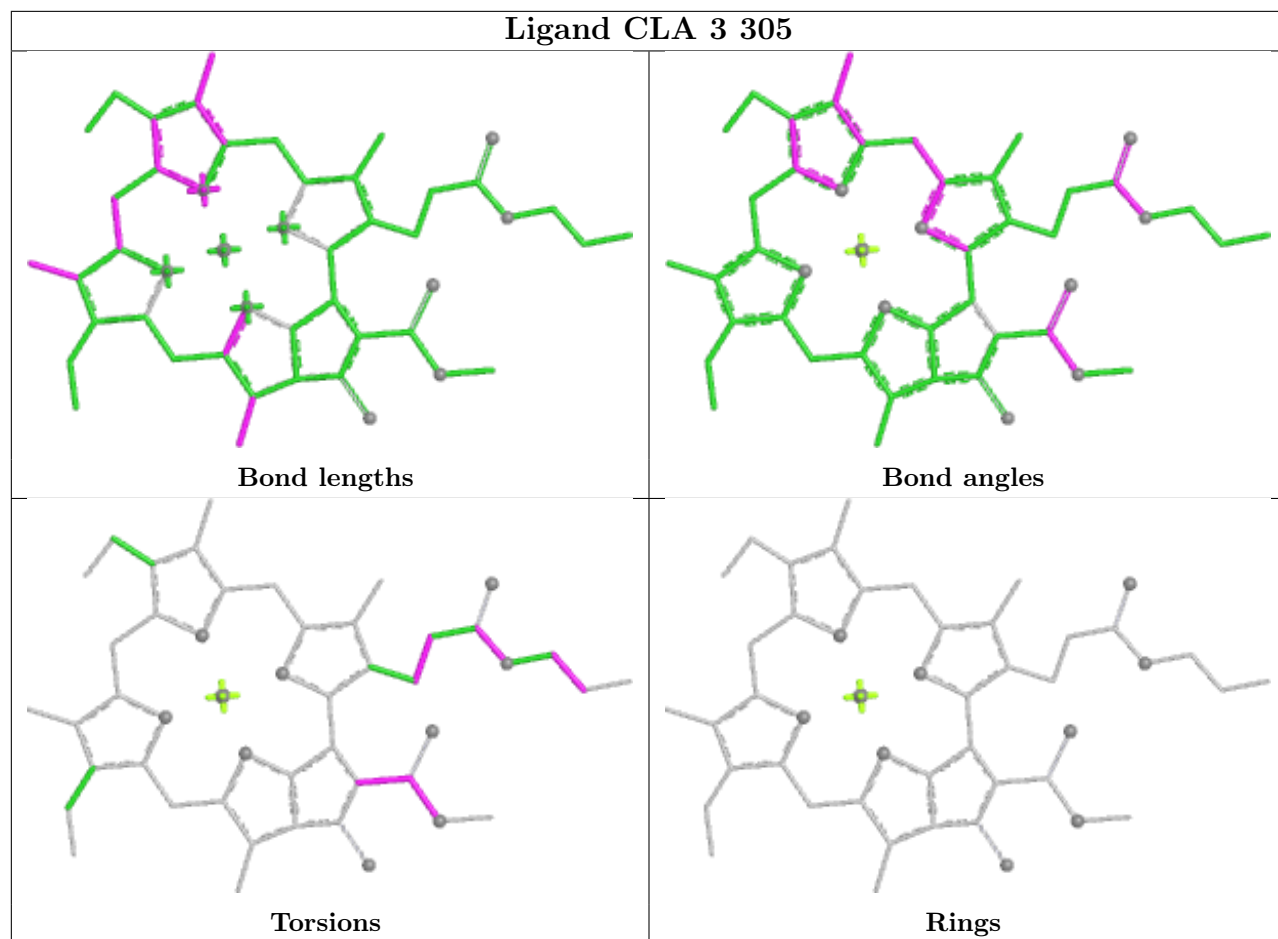


Ligand DGD h 102

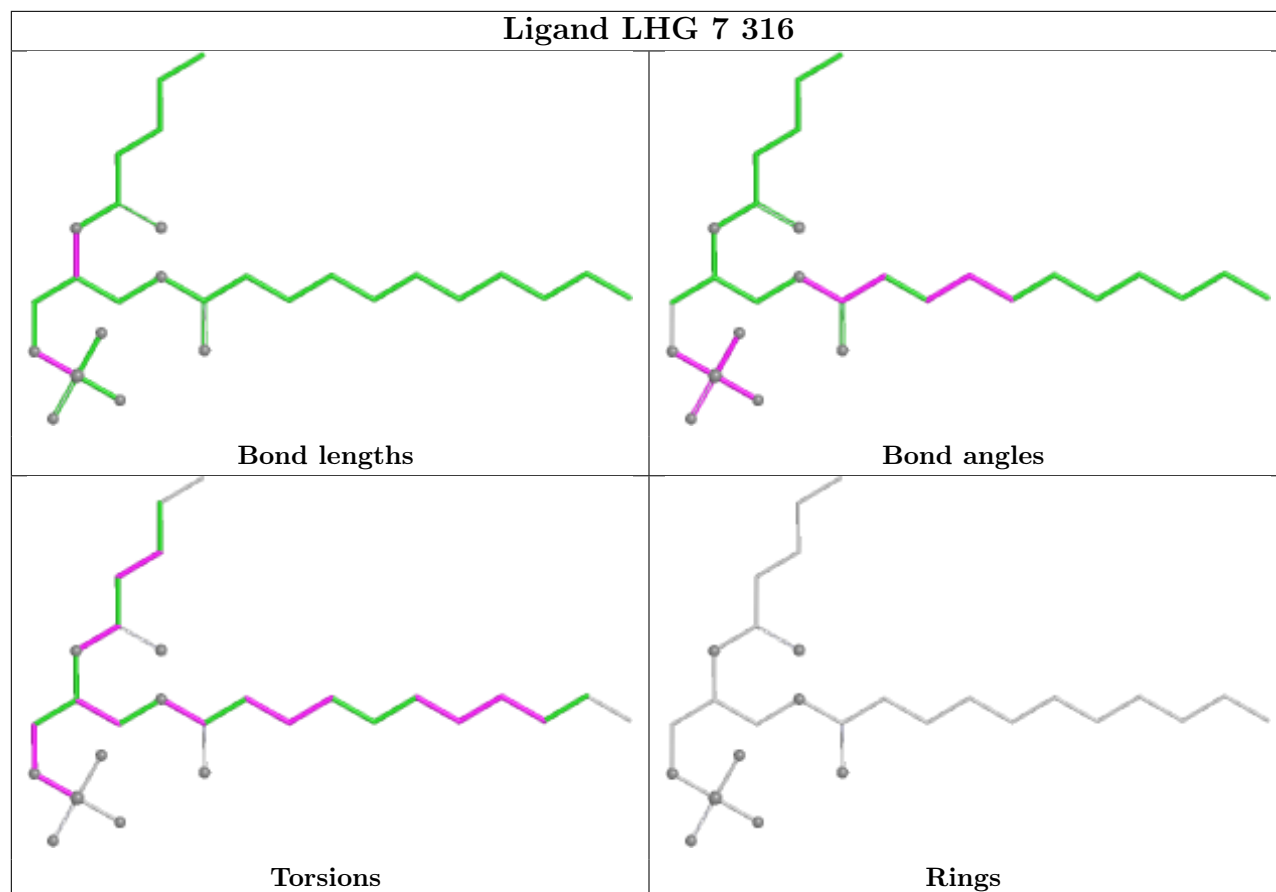




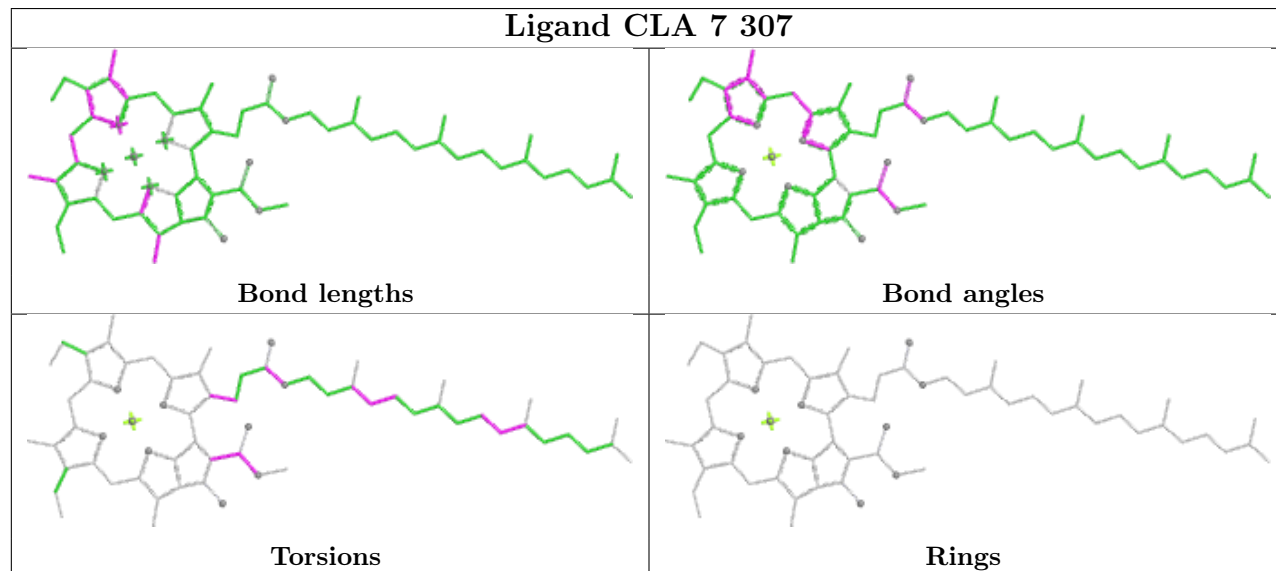
Ligand CLA 3 305

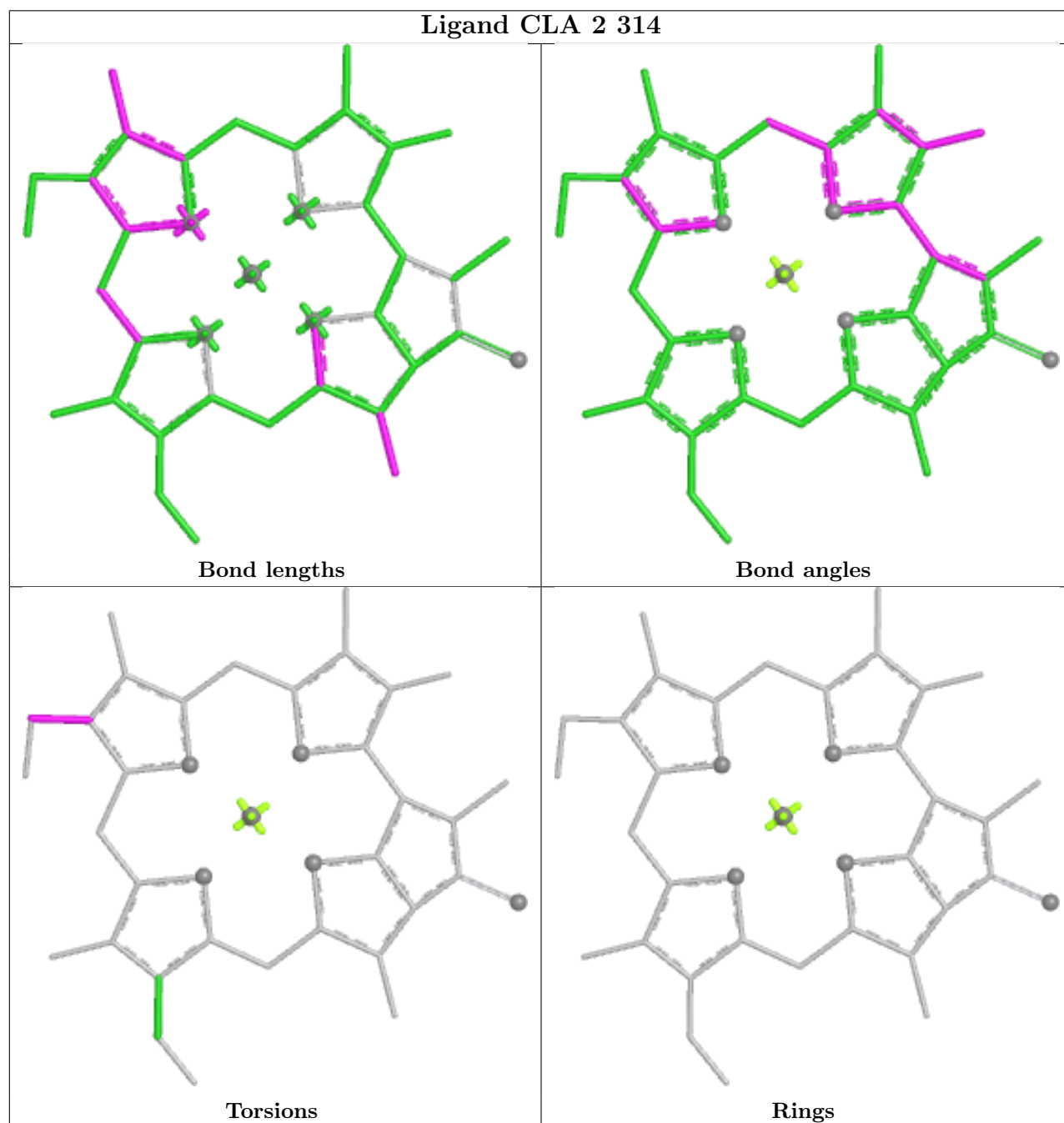
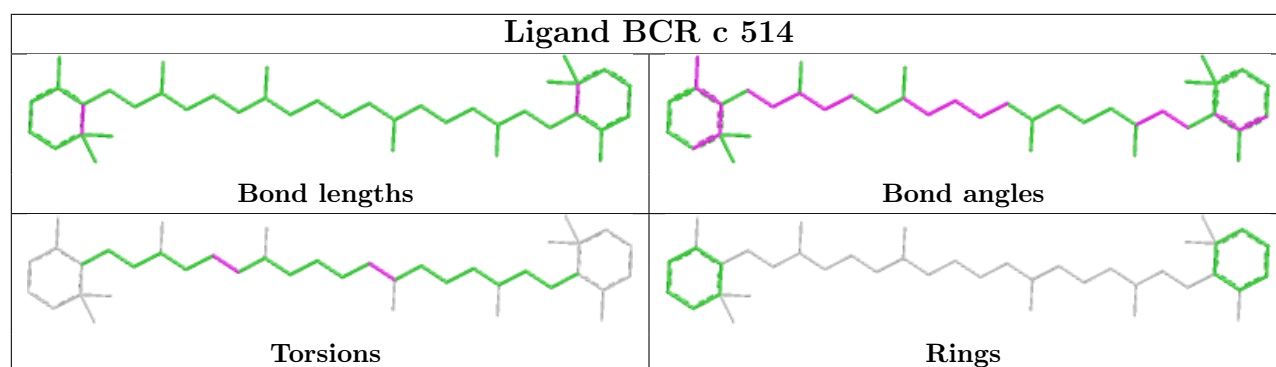


Ligand LHG 7 316

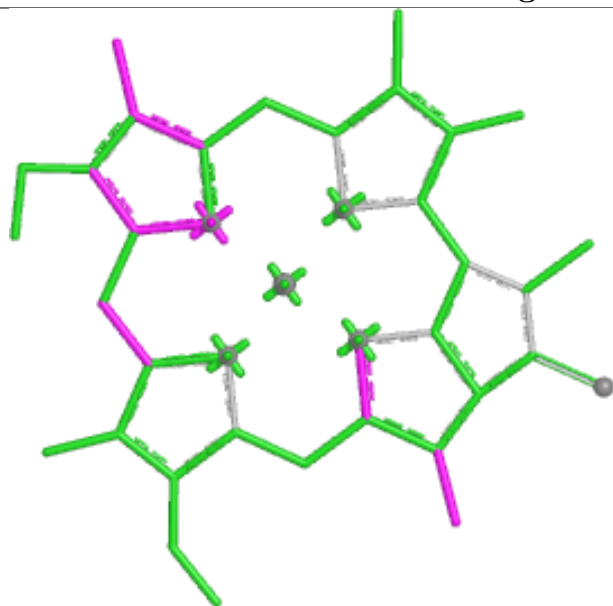


Ligand CLA 7 307

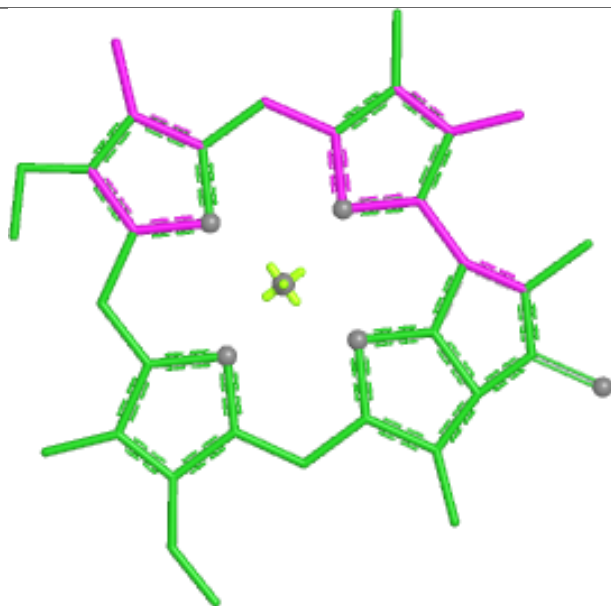




Ligand CLA 8 315



Bond lengths



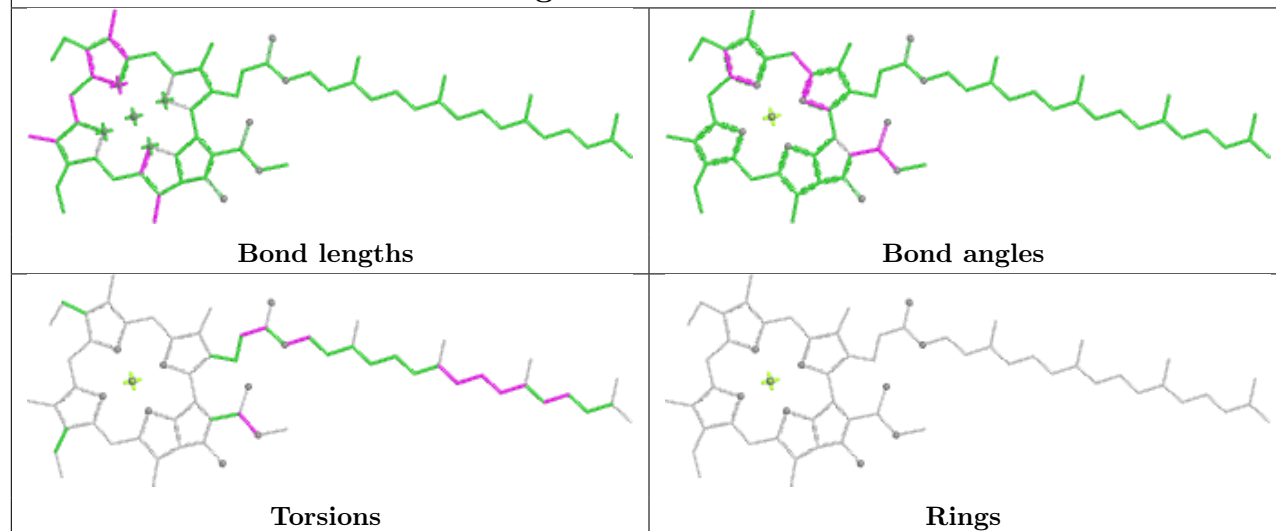
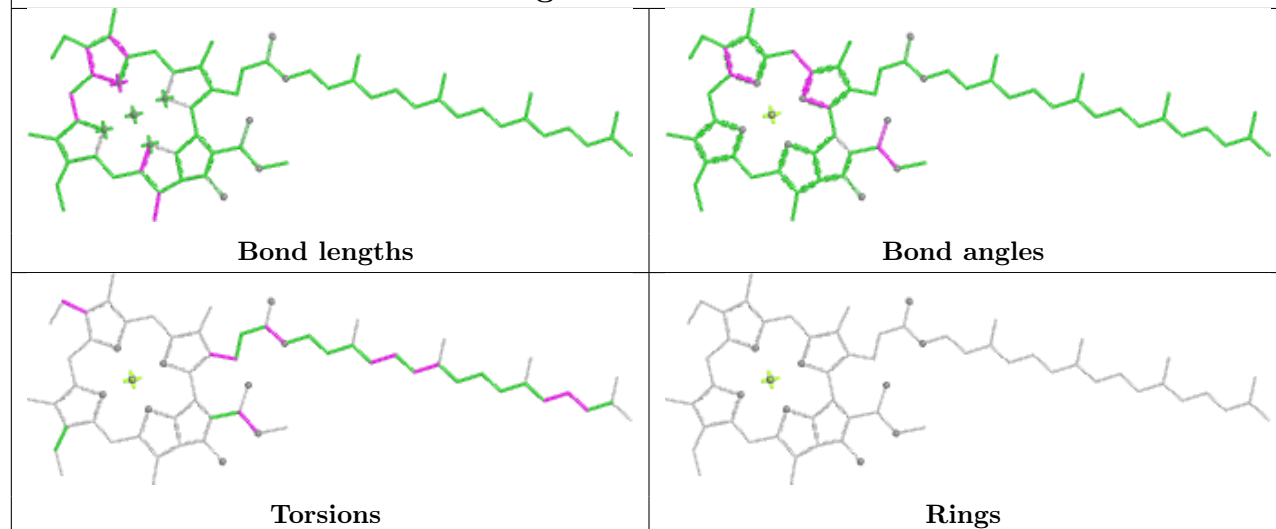
Bond angles

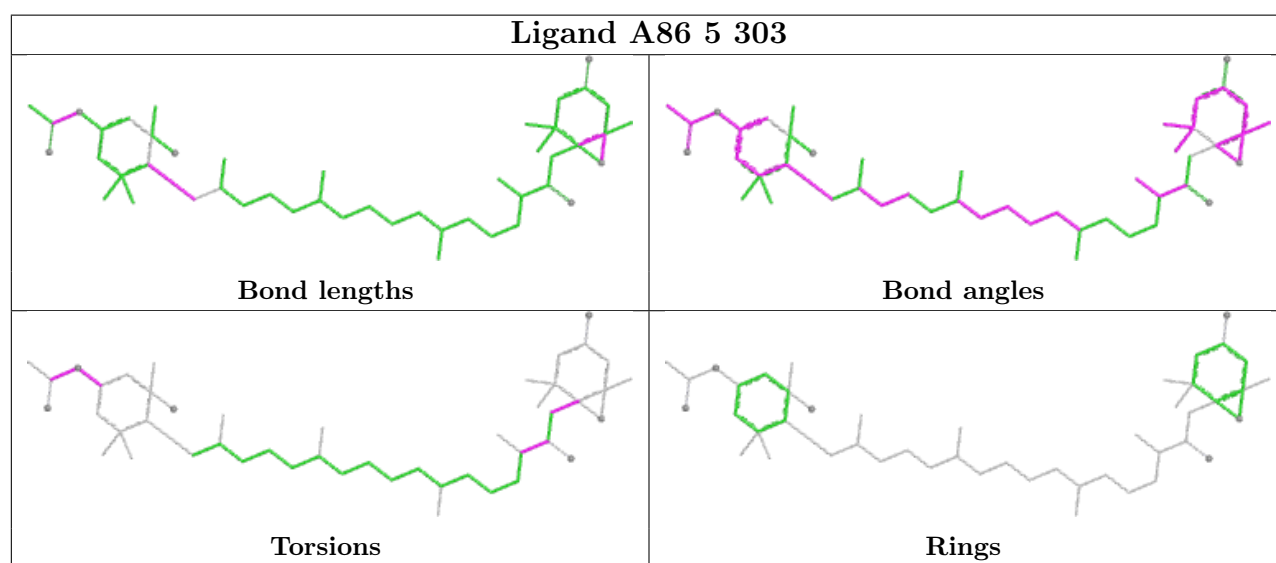
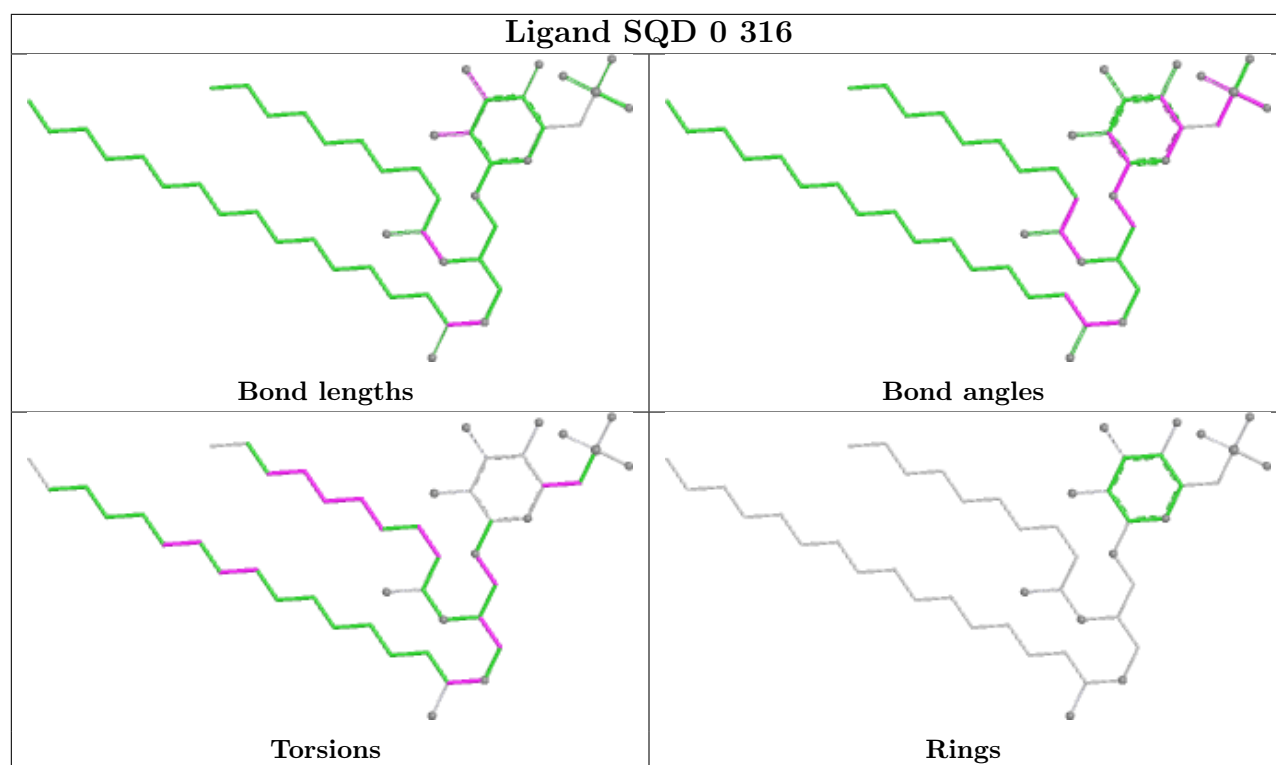


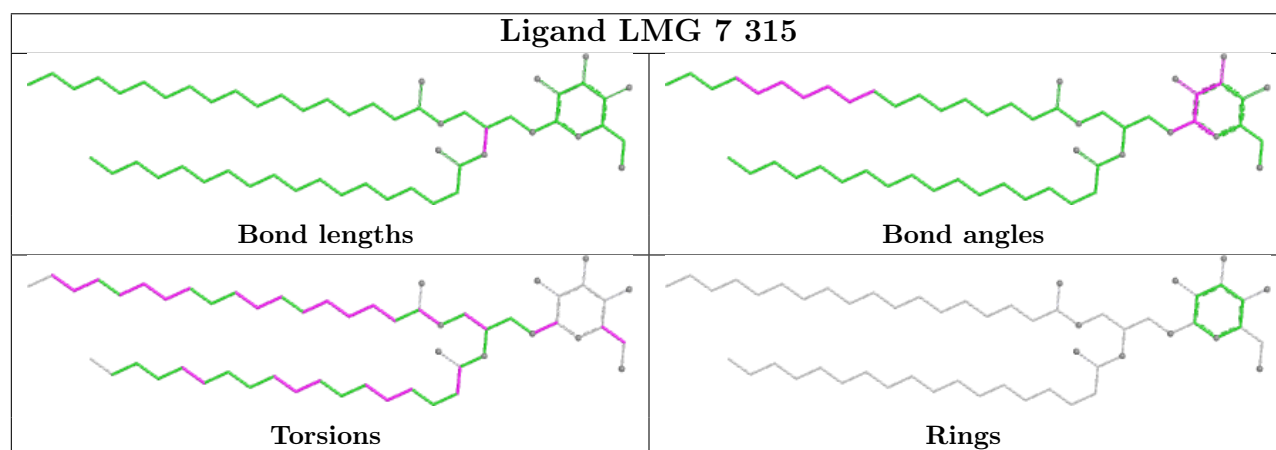
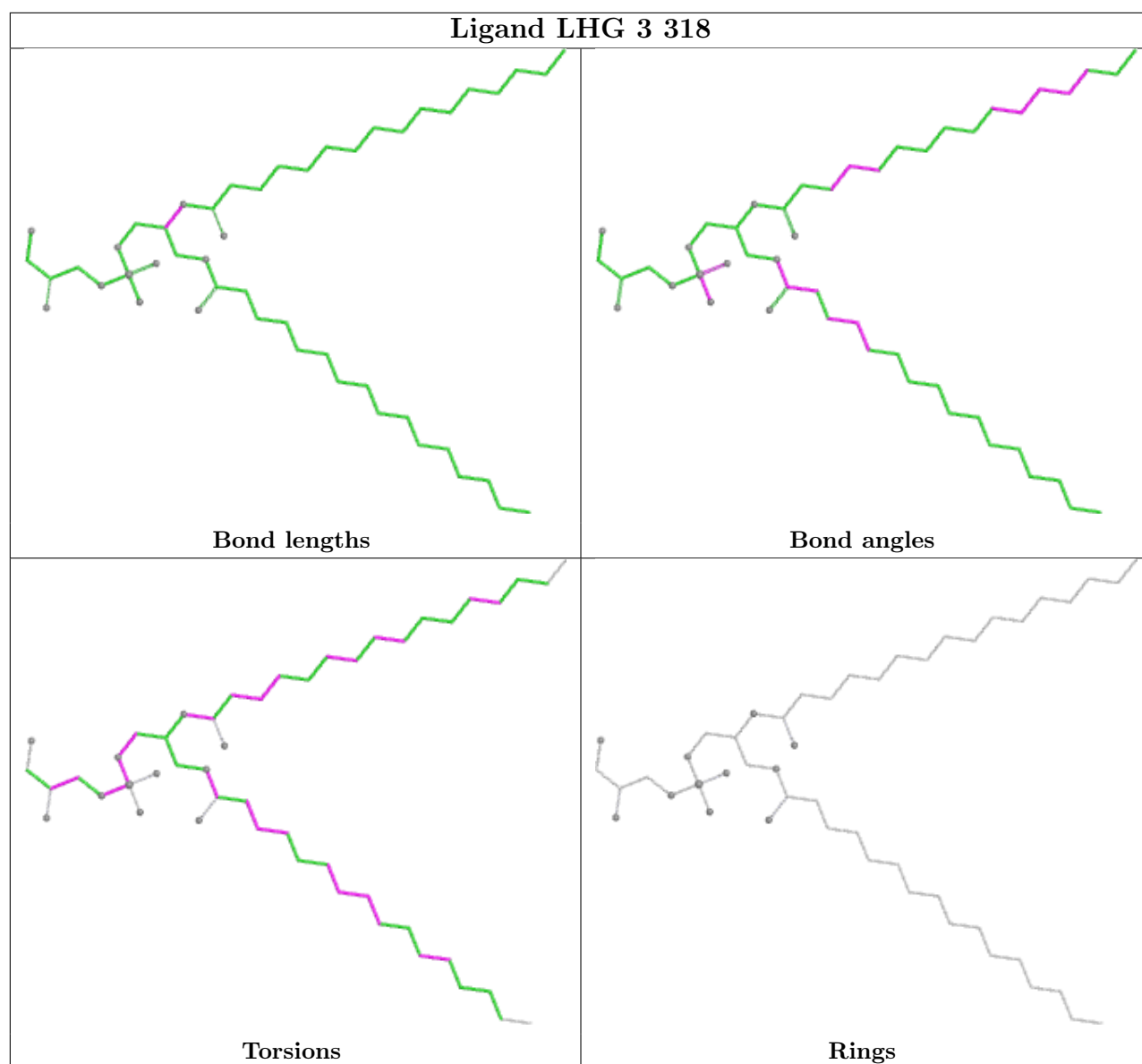
Torsions



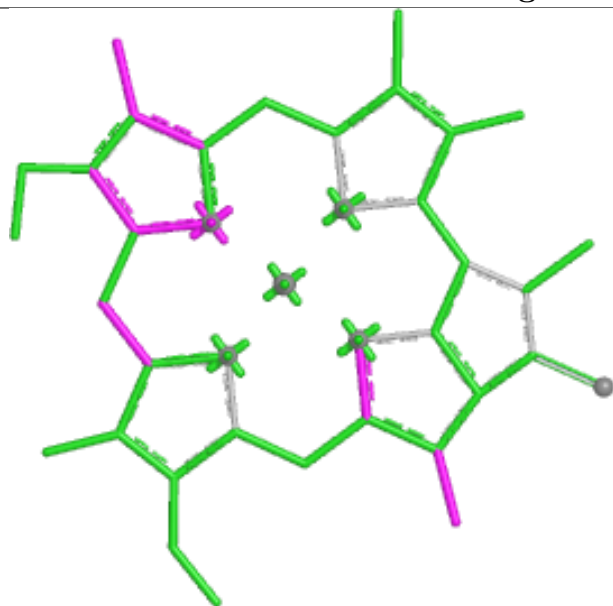
Rings

Ligand CLA b 614**Ligand CLA 6 312**

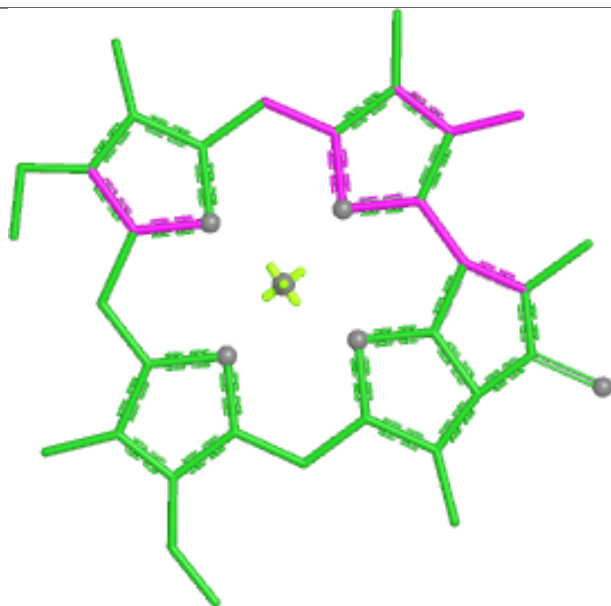




Ligand CLA 1 315



Bond lengths



Bond angles

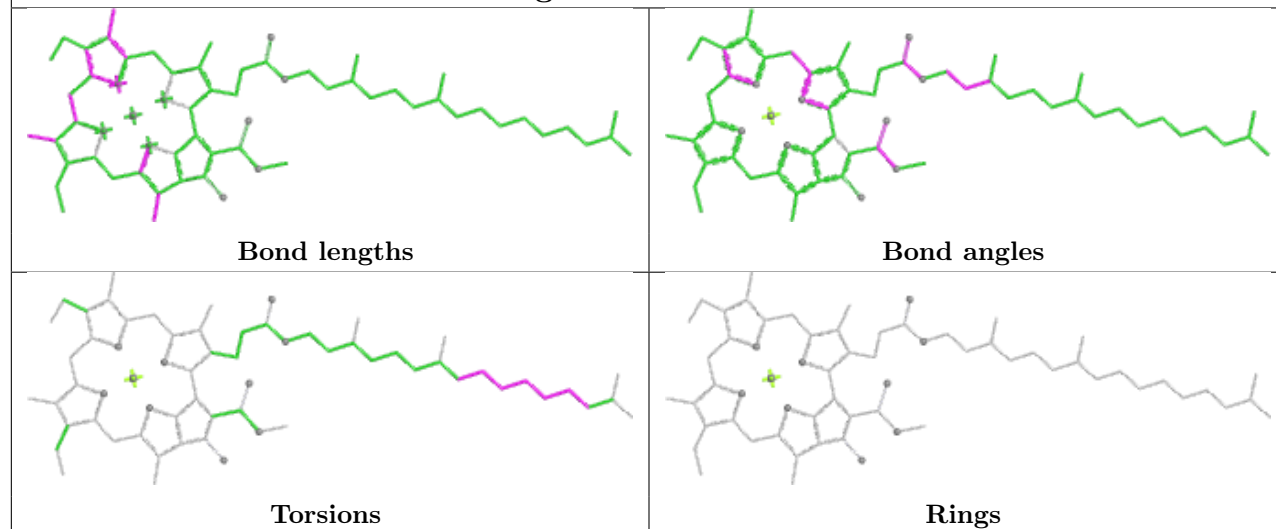


Torsions

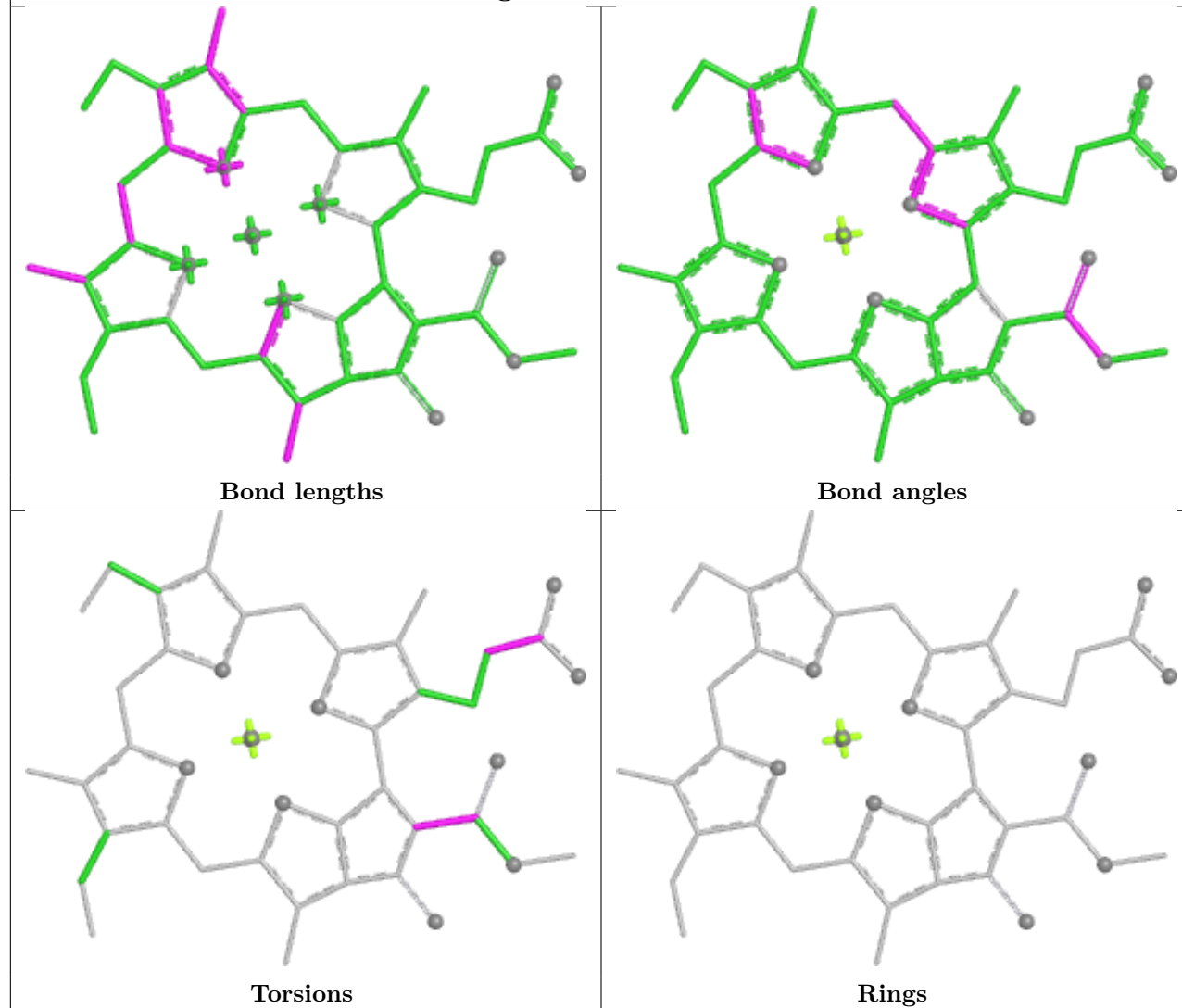


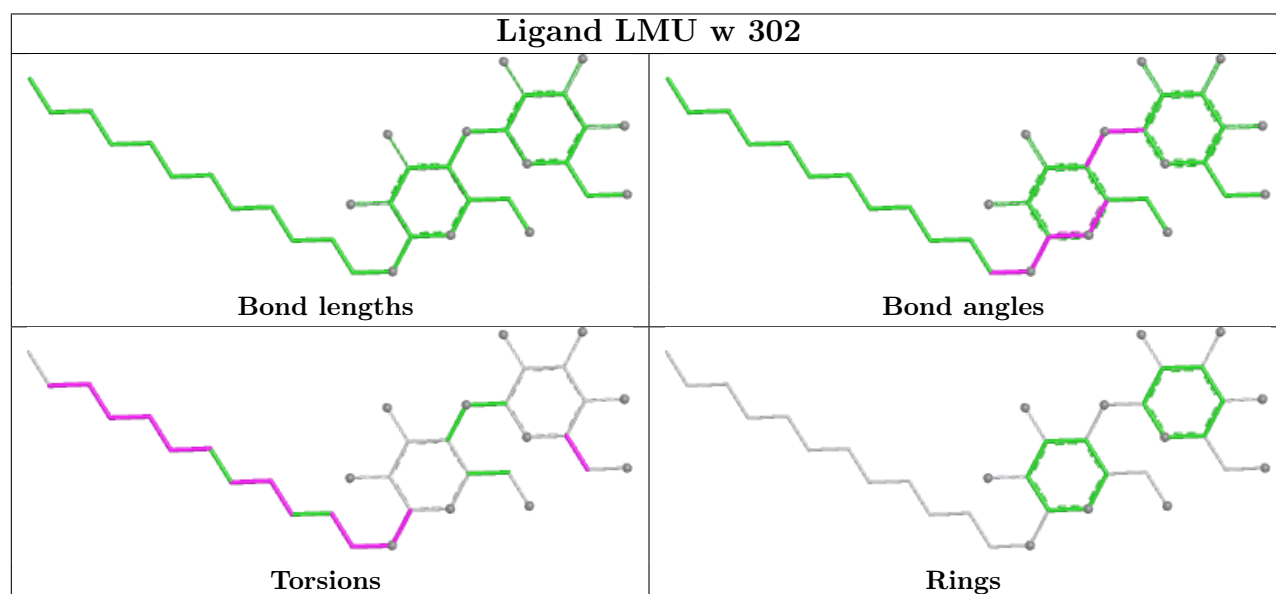
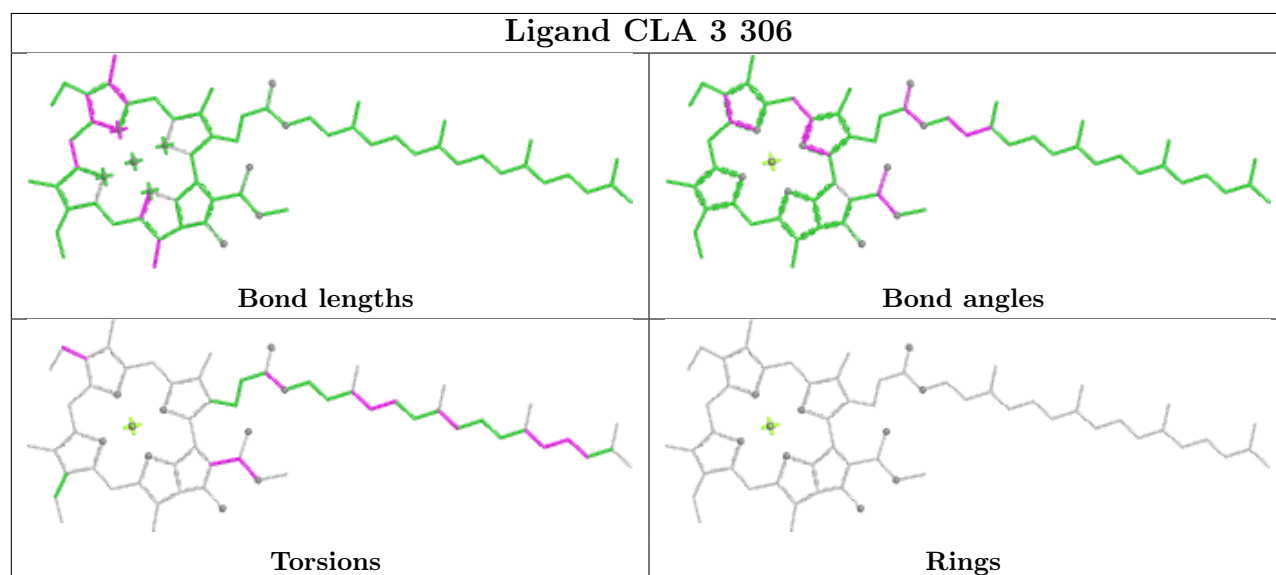
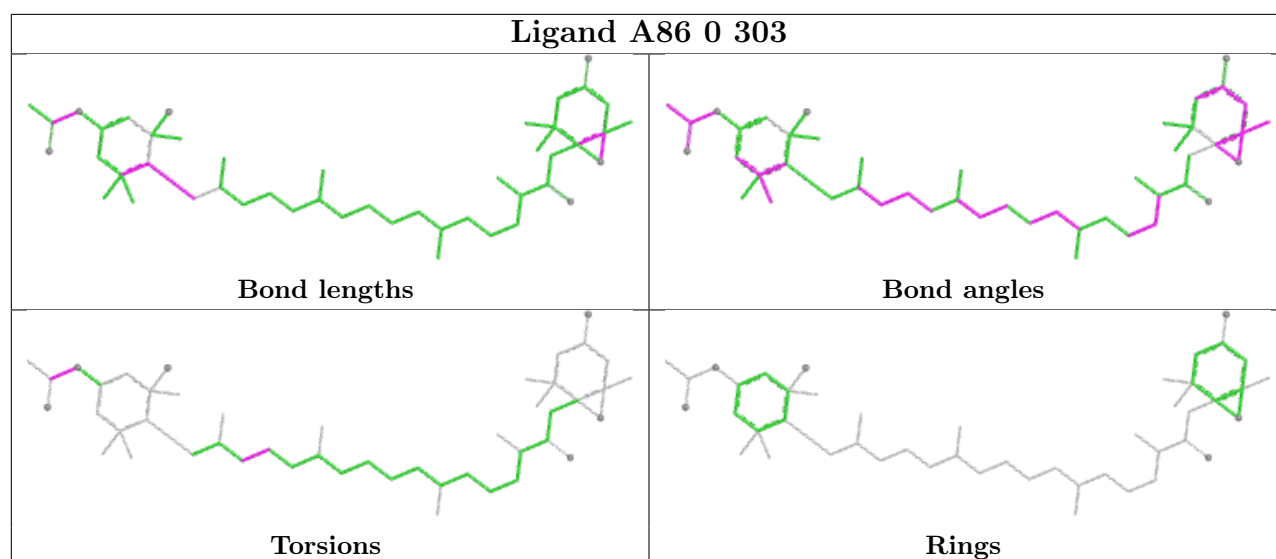
Rings

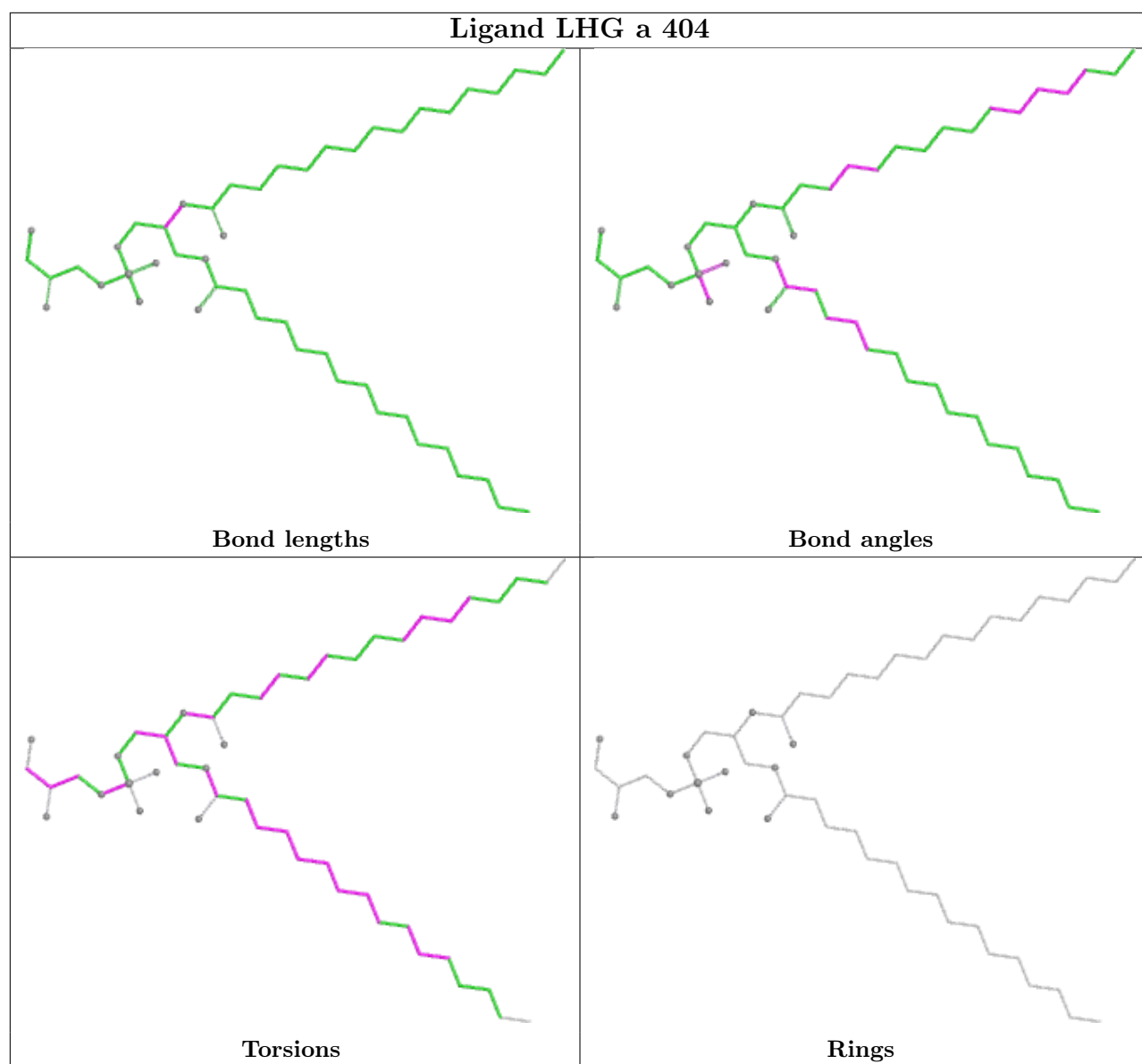
Ligand CLA b 612

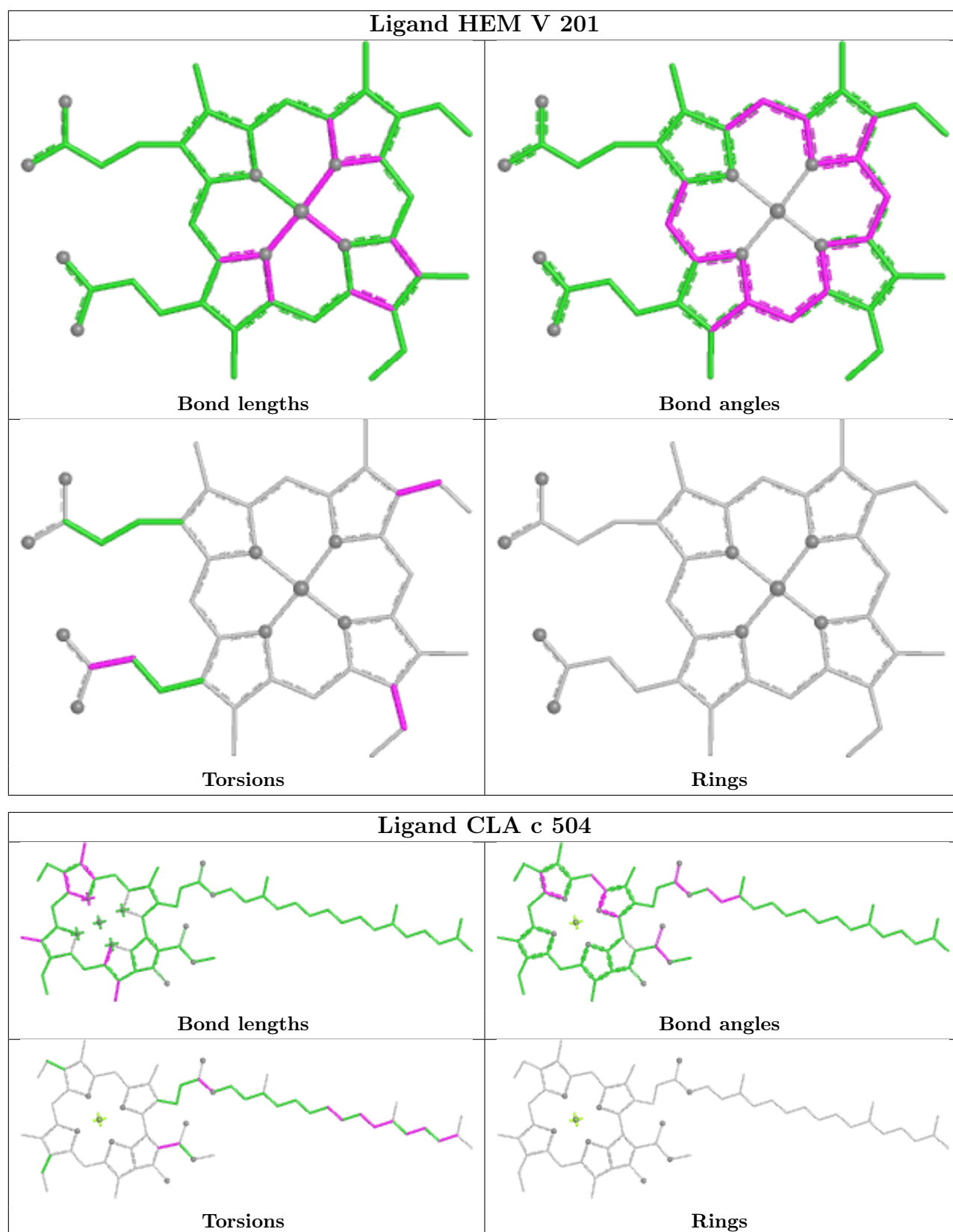


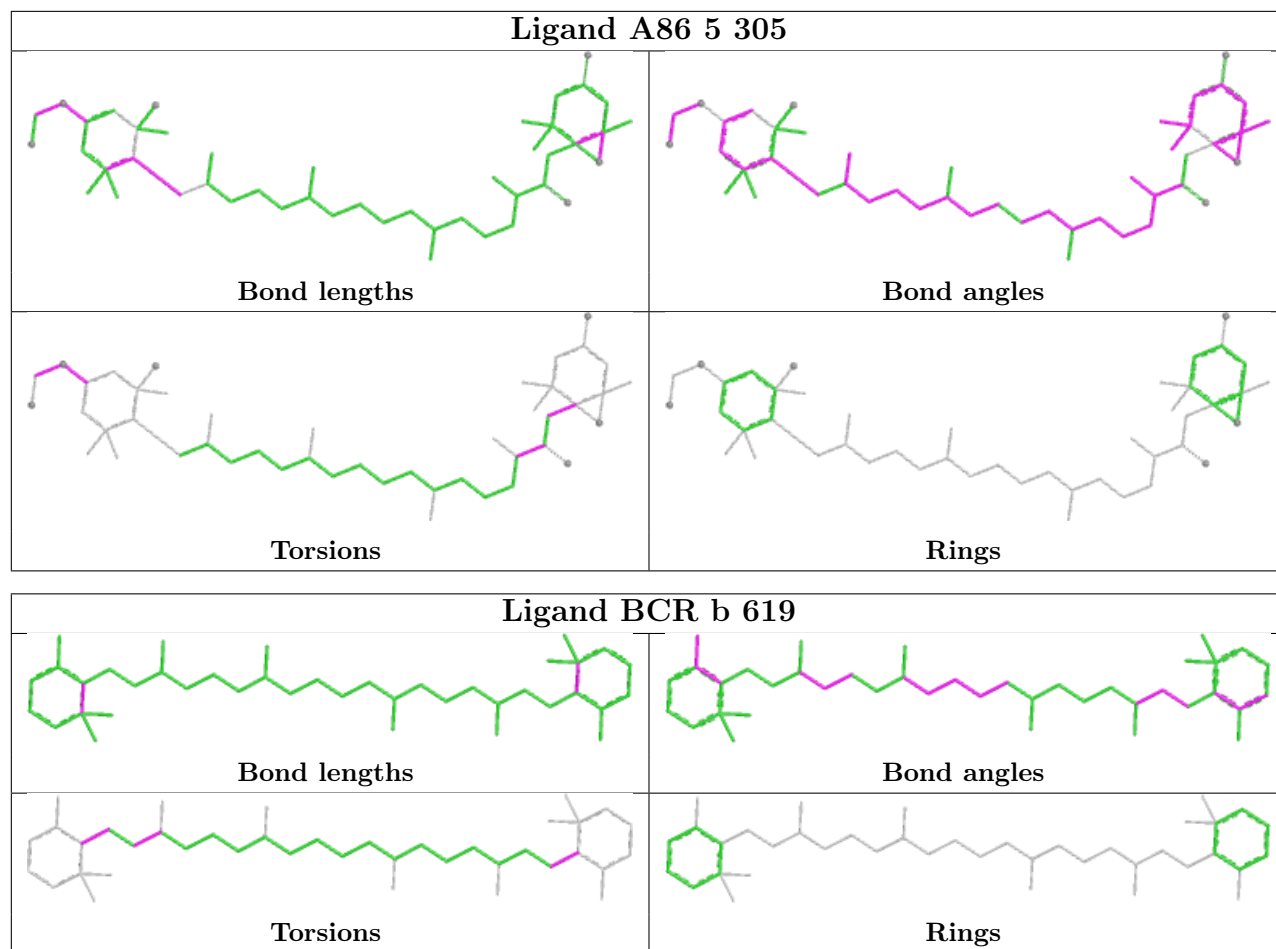
Ligand CLA 8 312



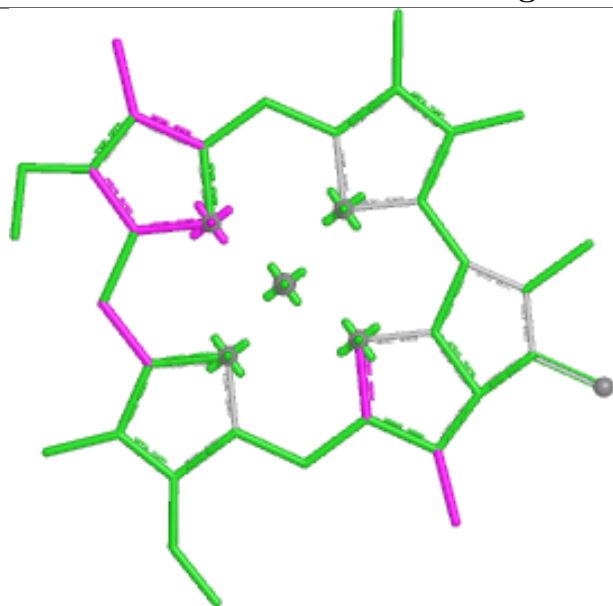




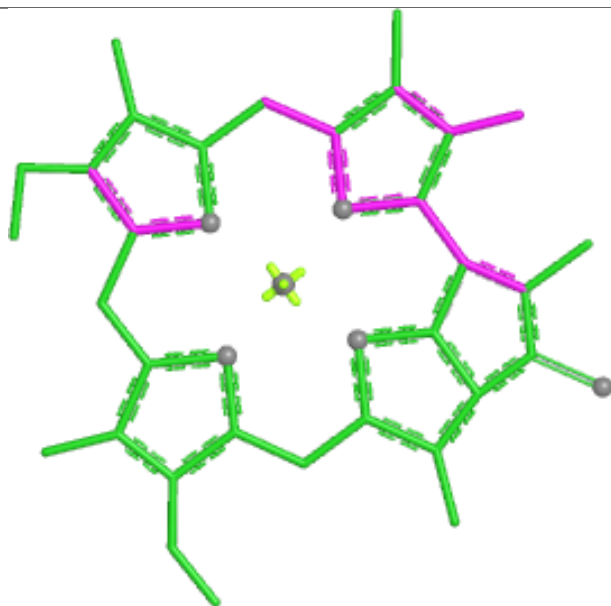




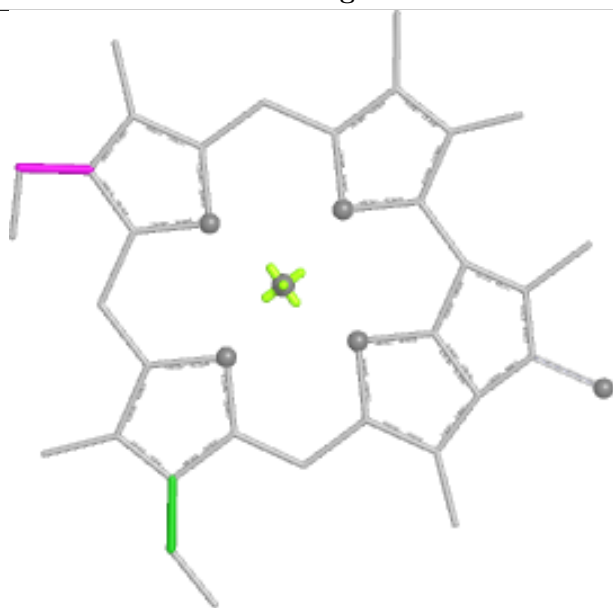
Ligand CLA 8 316



Bond lengths



Bond angles

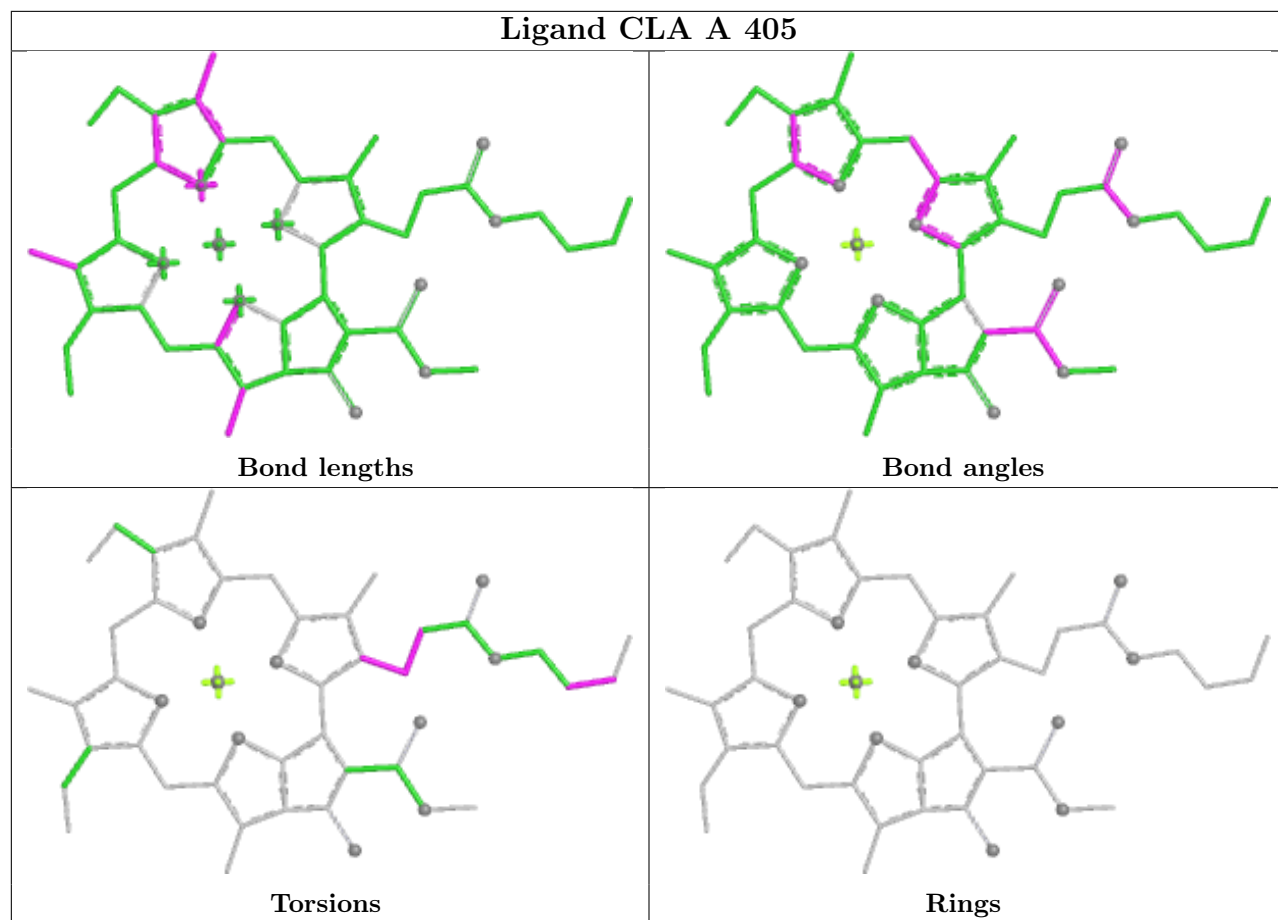


Torsions

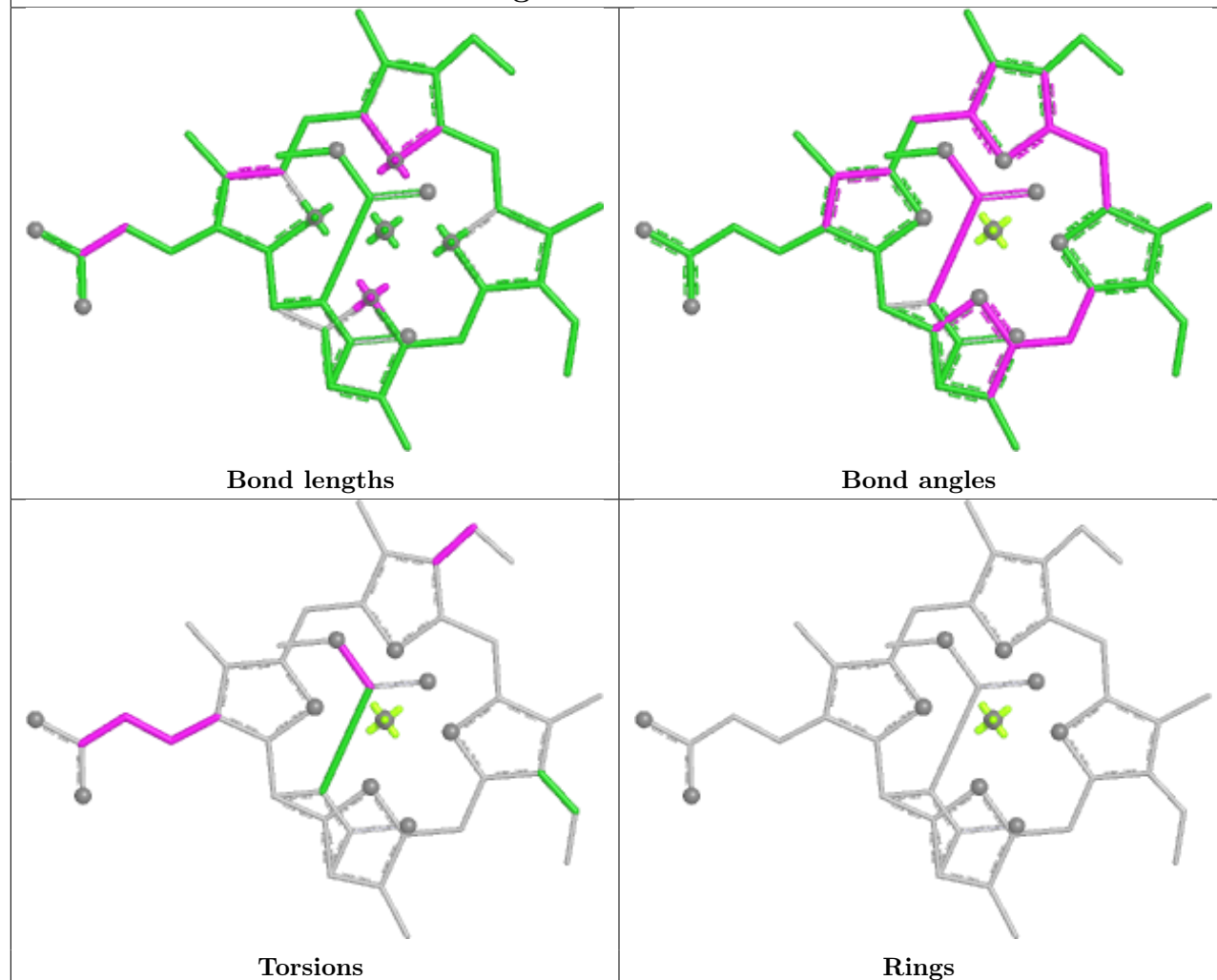


Rings

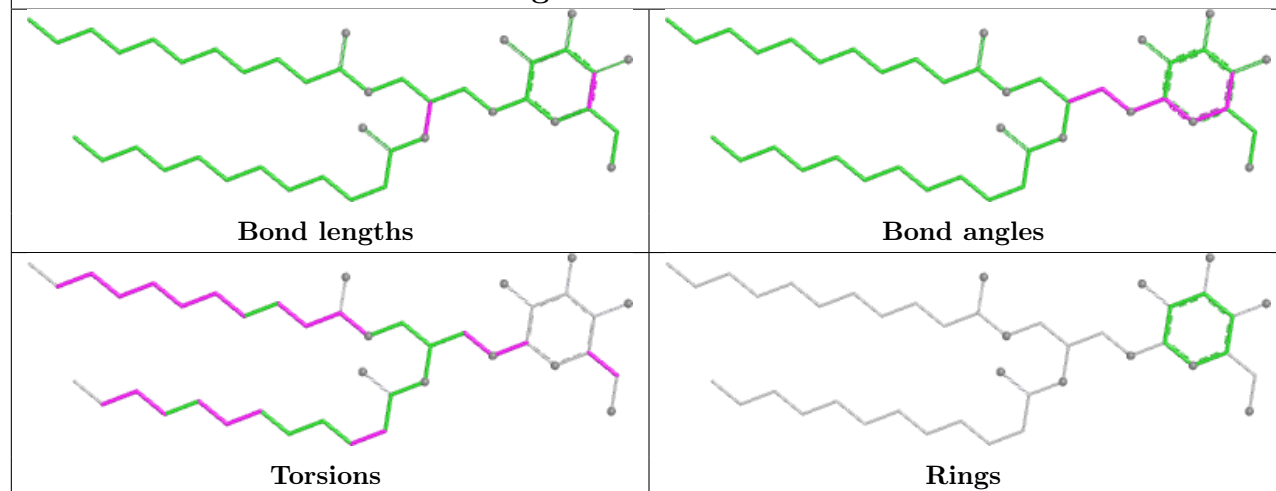
Ligand CLA A 405

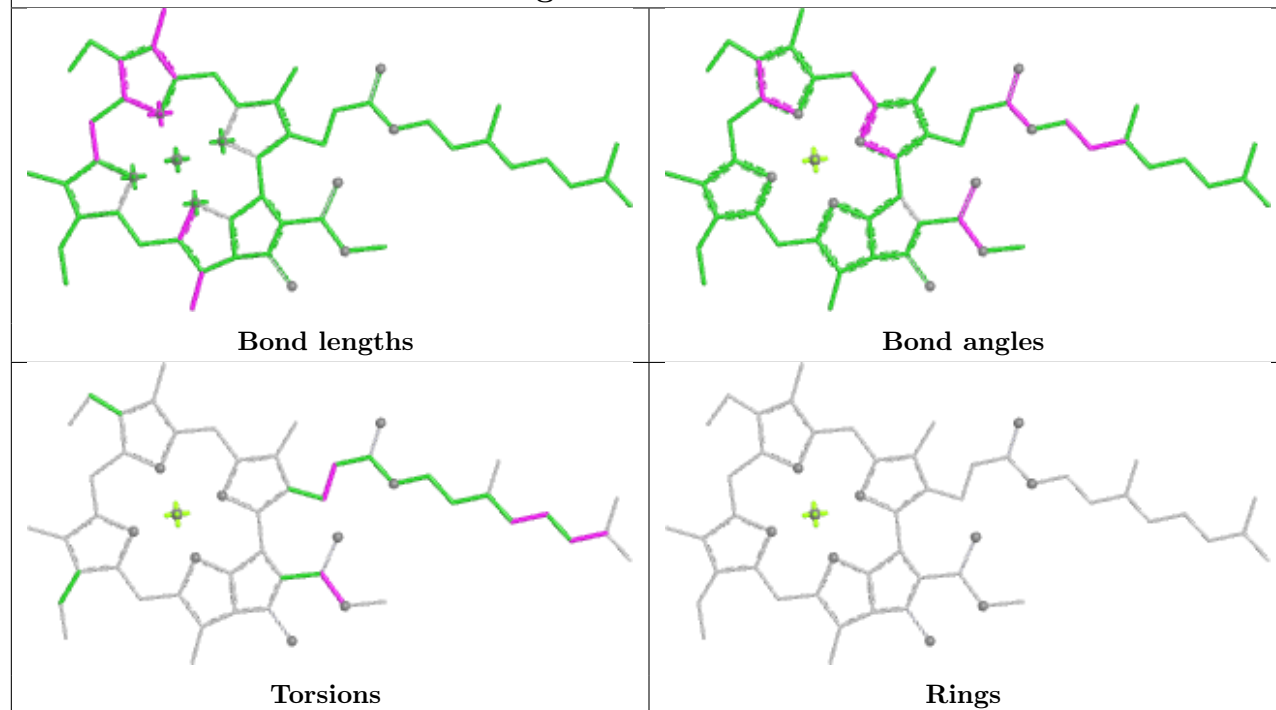
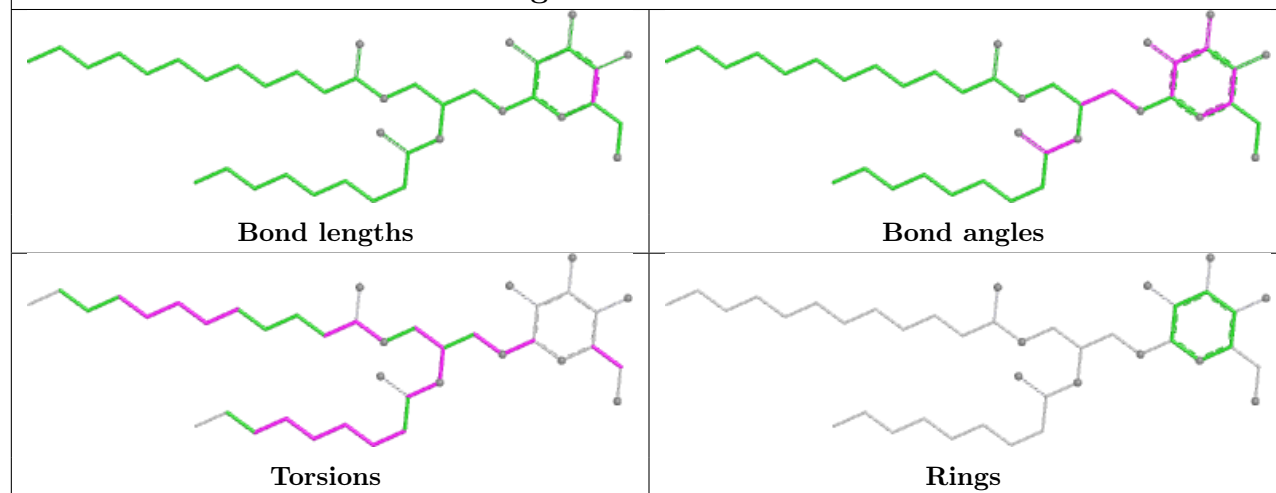


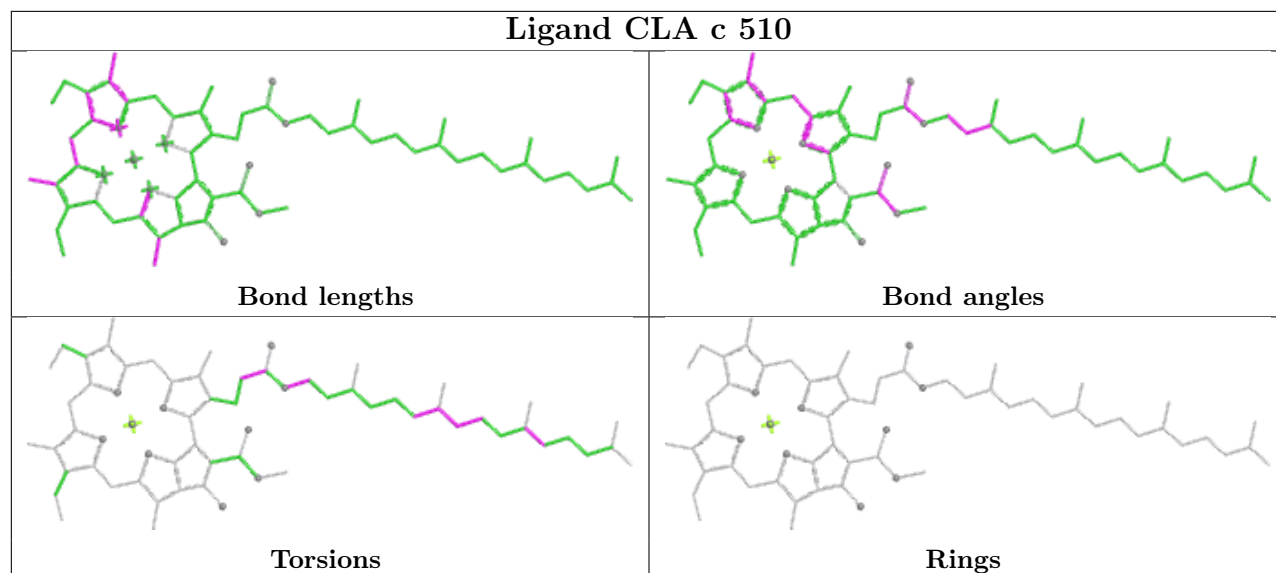
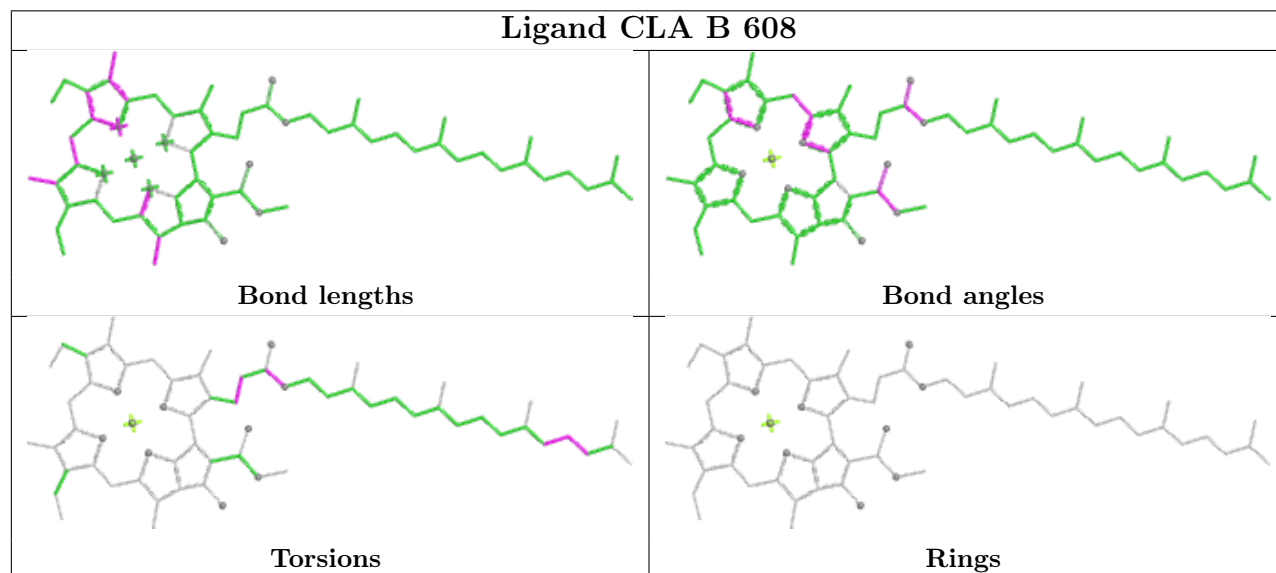
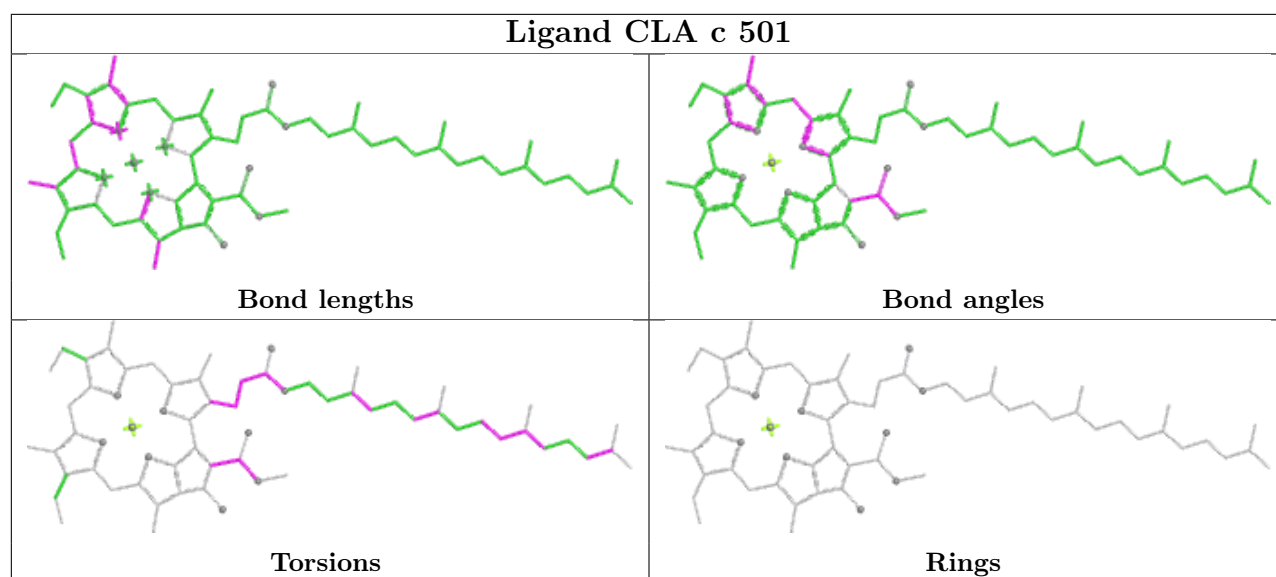
Ligand KC1 3 310

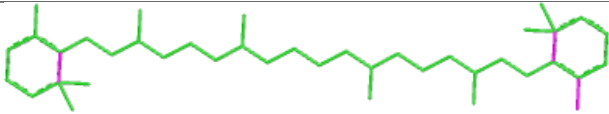
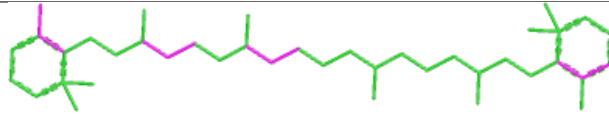
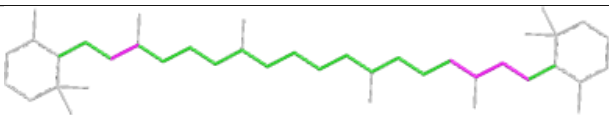
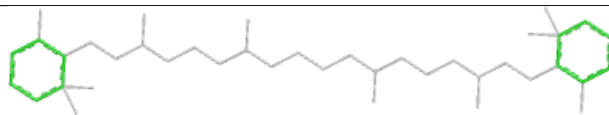


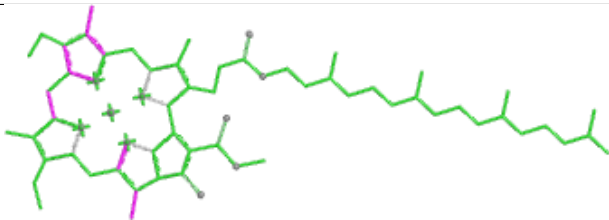
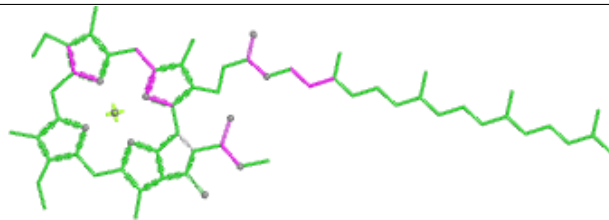
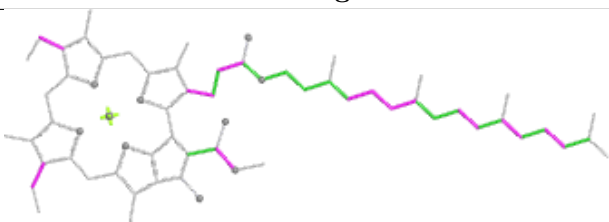
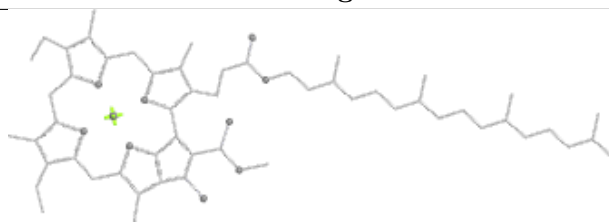
Ligand LMG 0 314

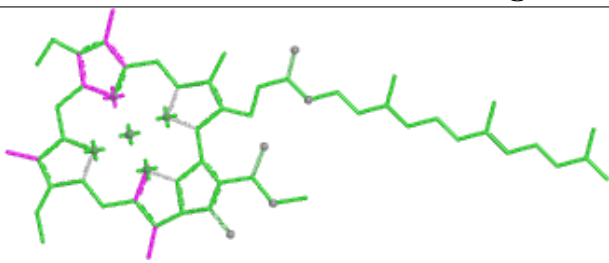
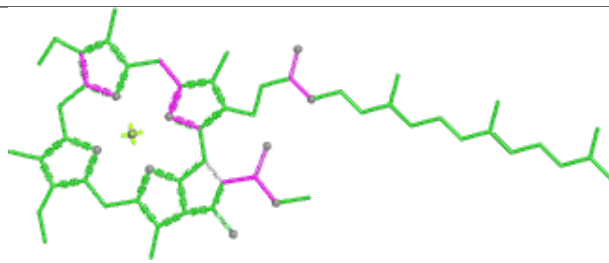
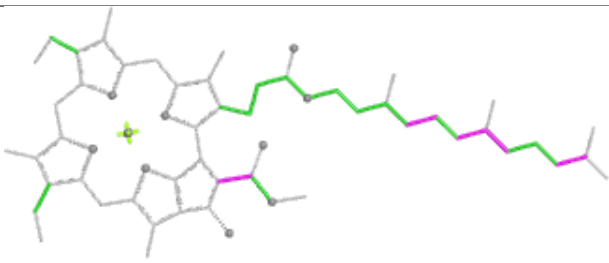
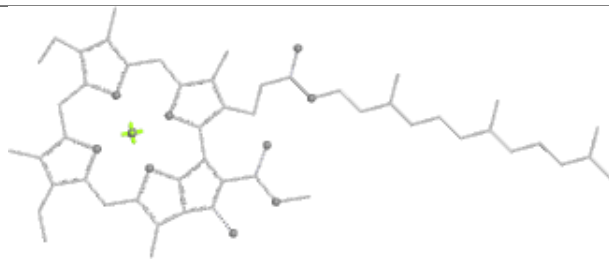


Ligand CLA 9 311**Ligand LMG b 623**

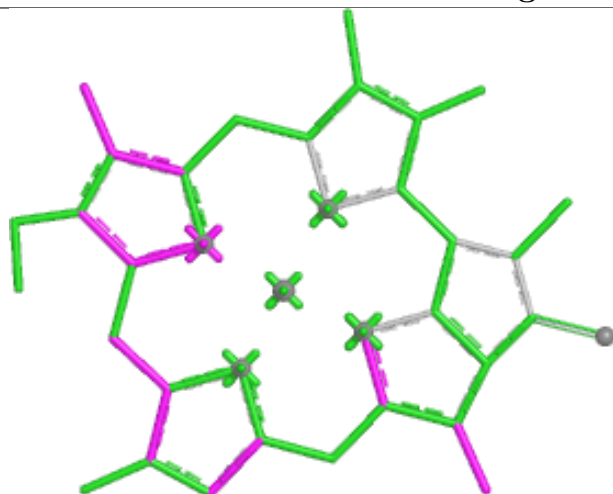


Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

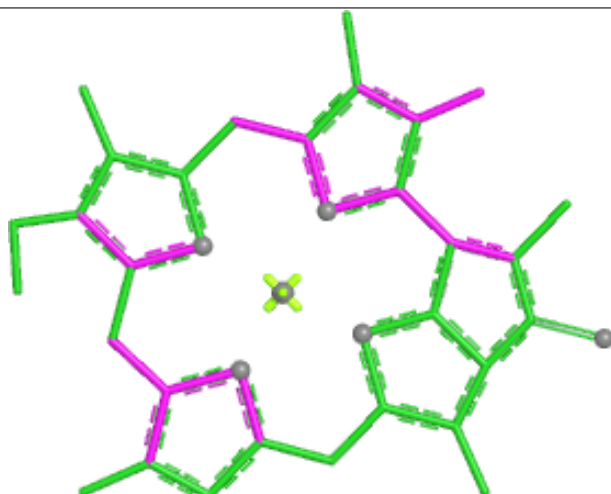
Ligand CLA w 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

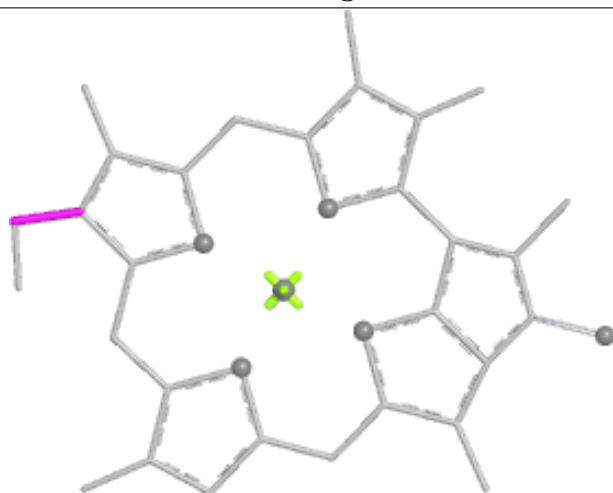
Ligand CLA 9 313



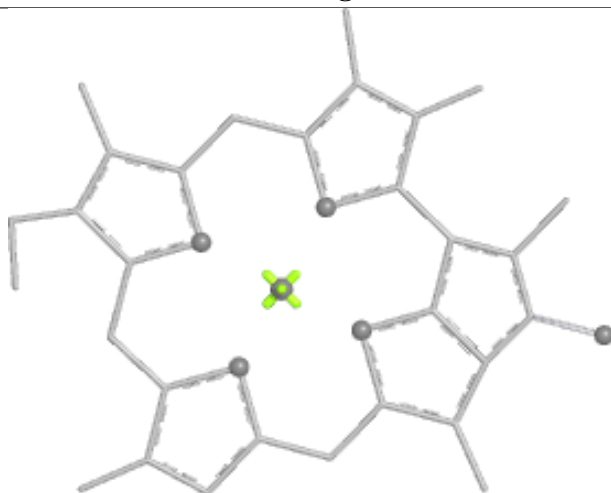
Bond lengths



Bond angles

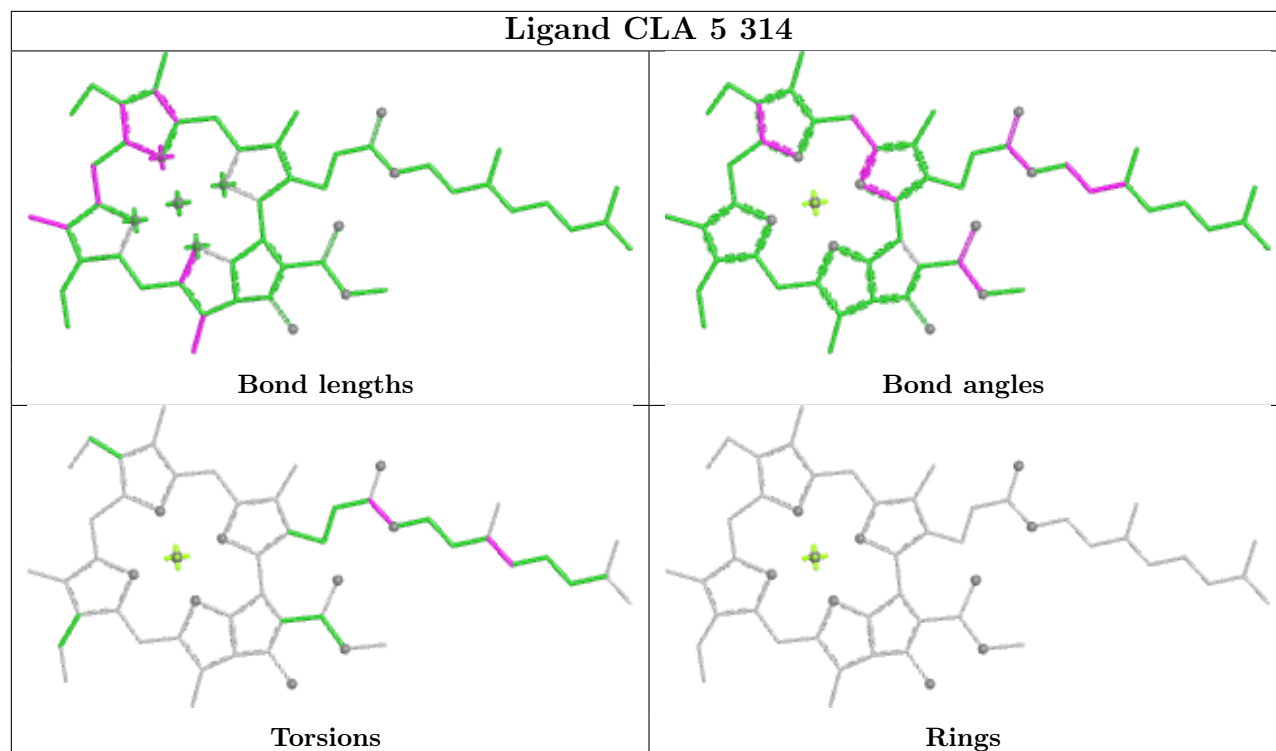


Torsions

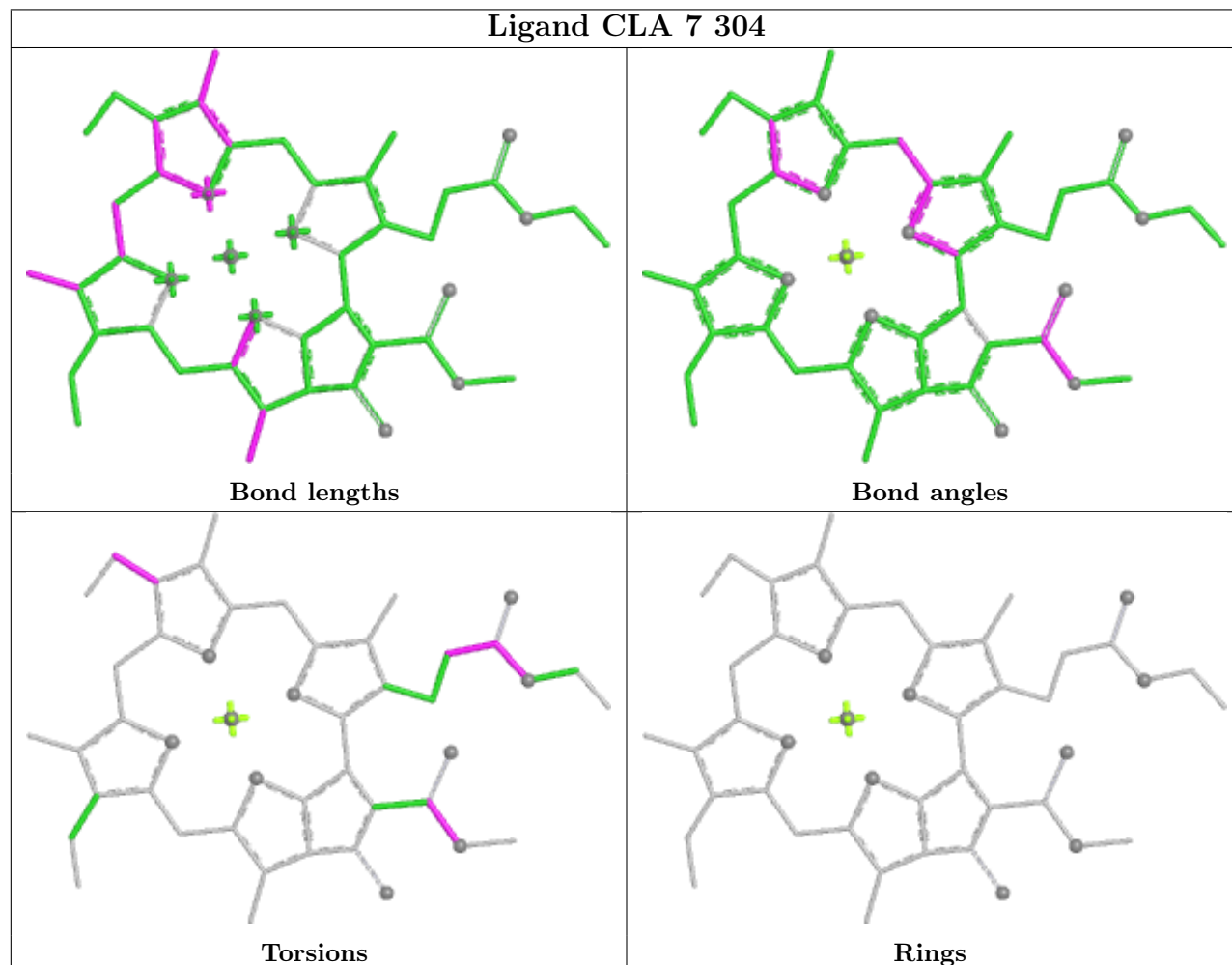


Rings

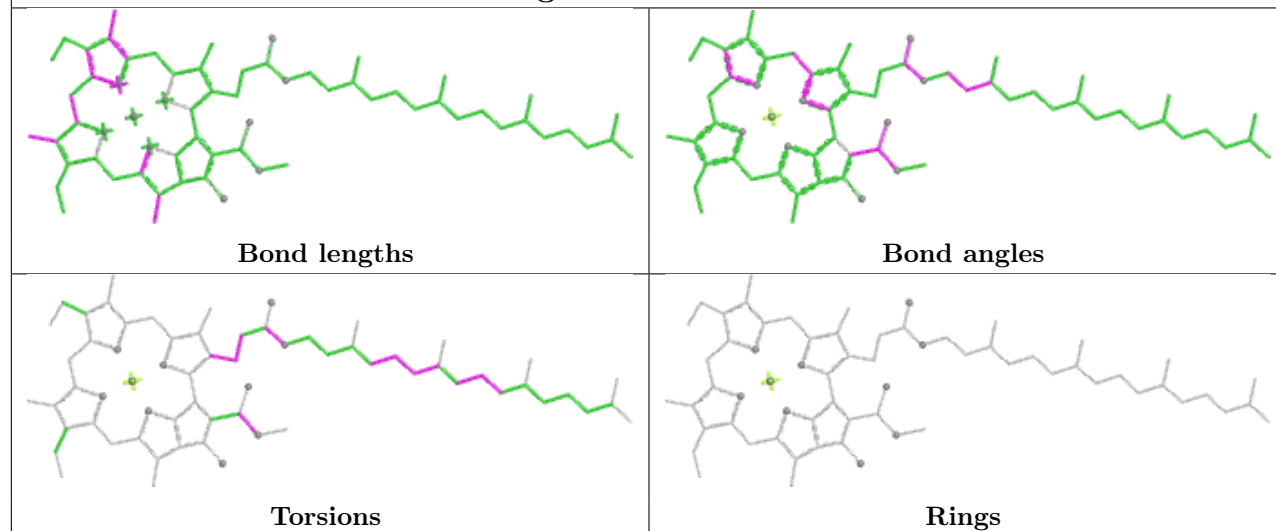
Ligand CLA 5 314



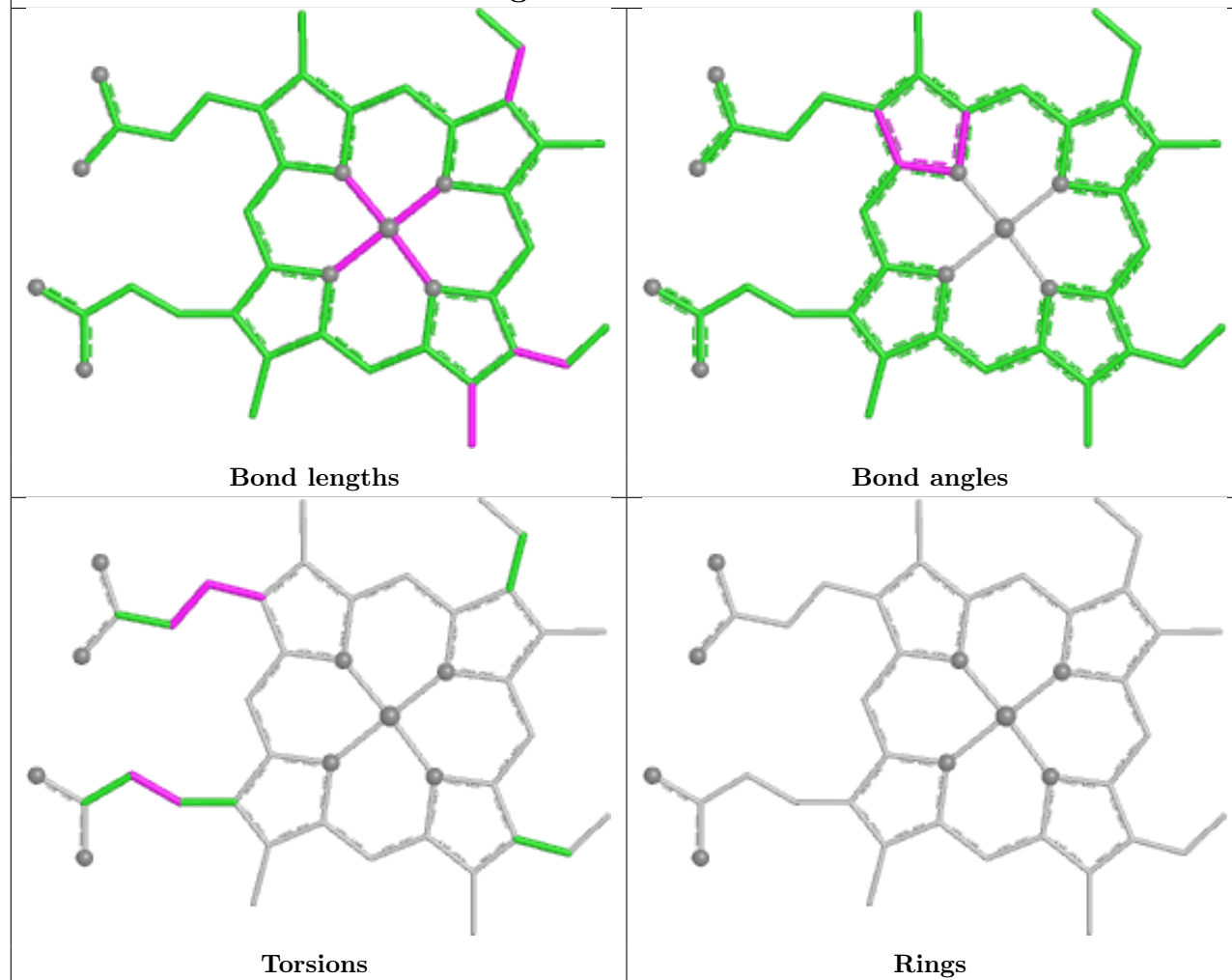
Ligand CLA 7 304

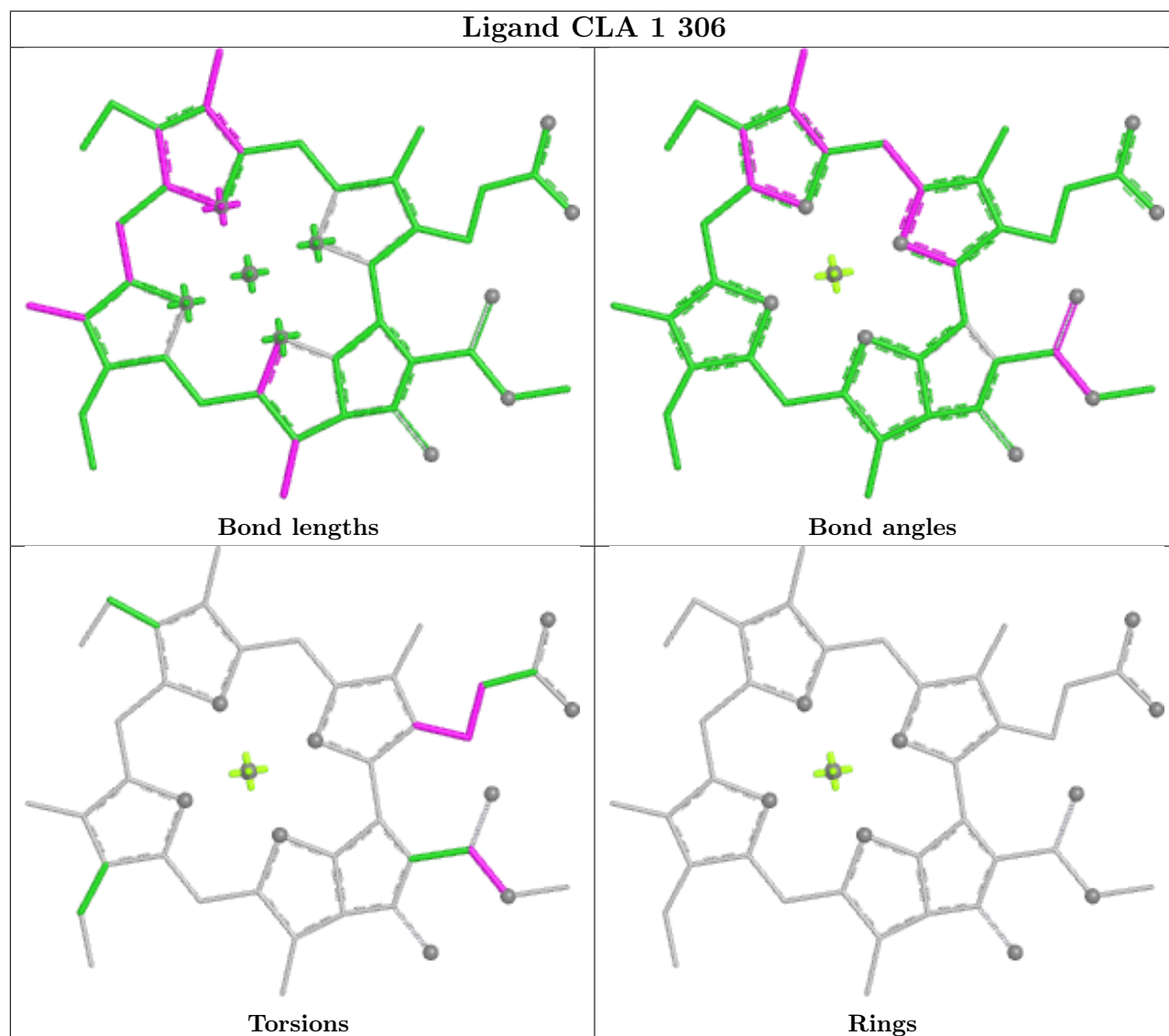
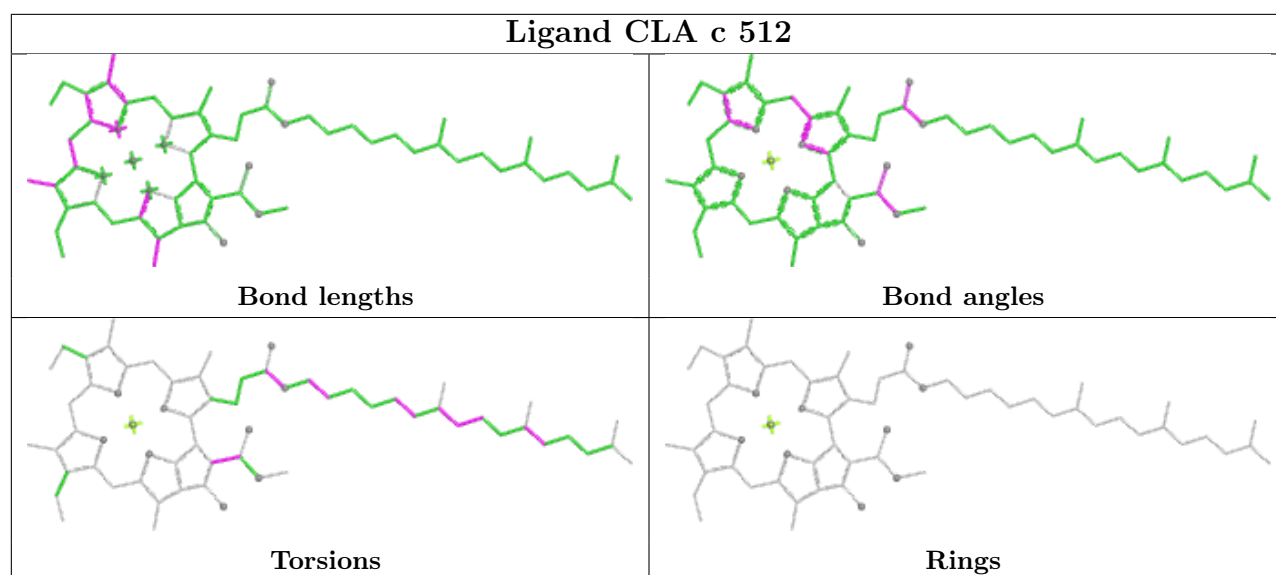


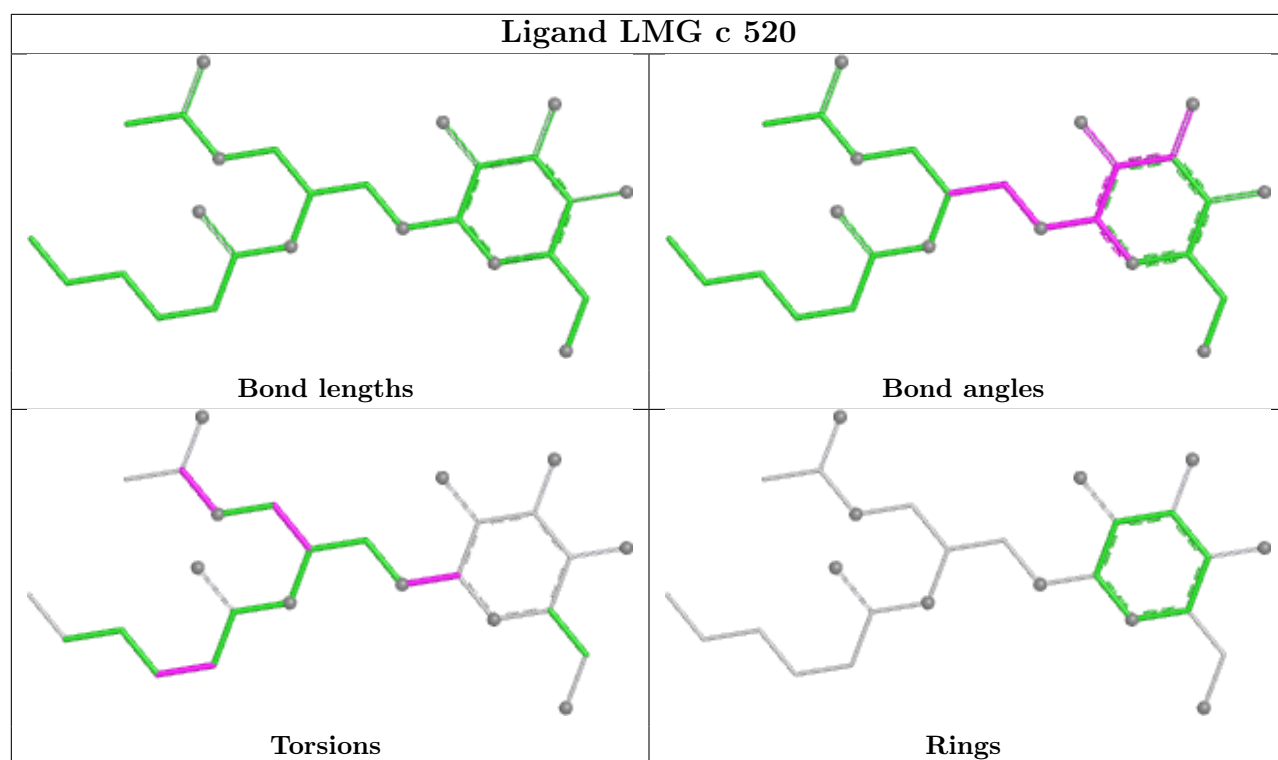
Ligand CLA c 503



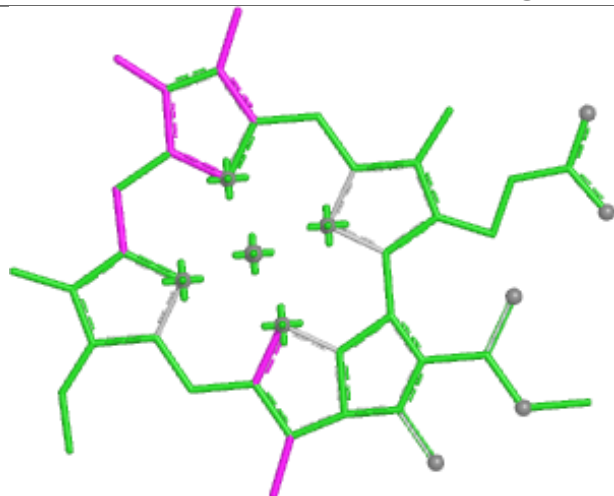
Ligand HEM F 101



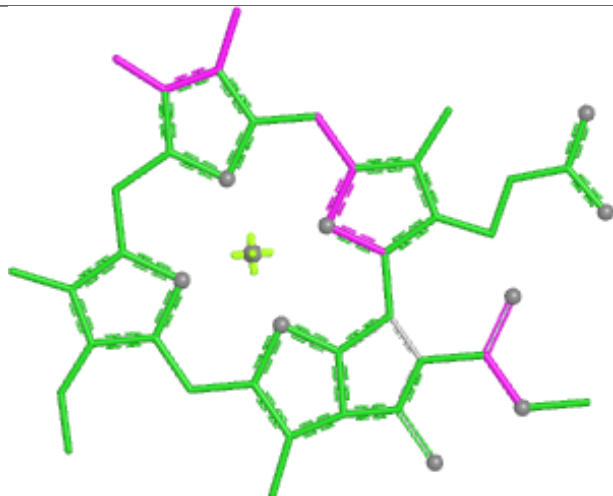




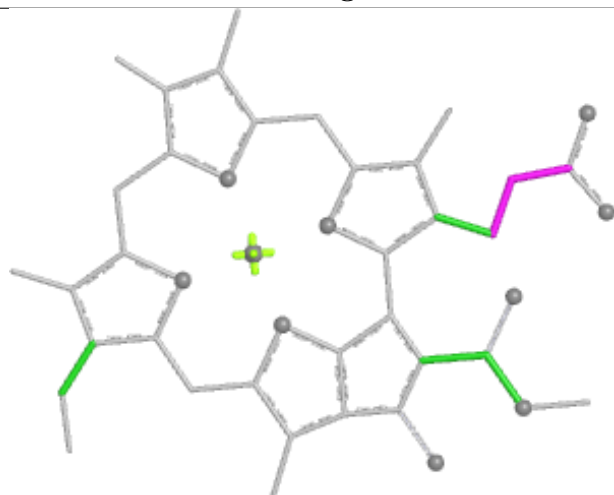
Ligand CLA 1 307



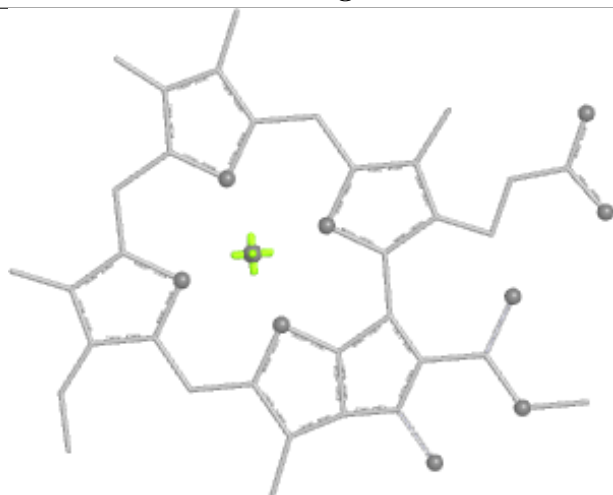
Bond lengths



Bond angles

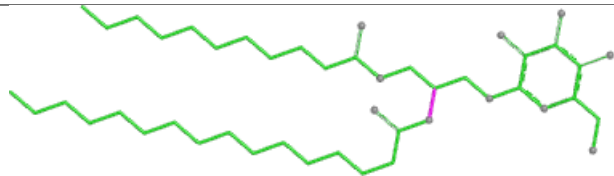


Torsions

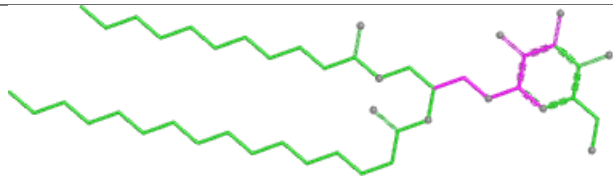


Rings

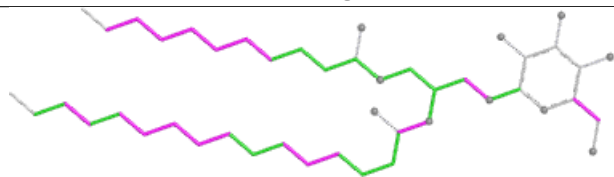
Ligand LMG d 406



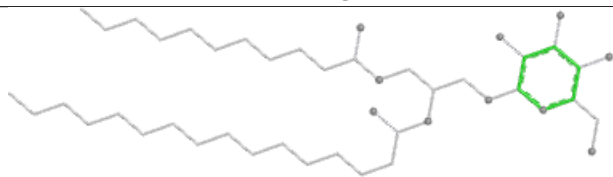
Bond lengths



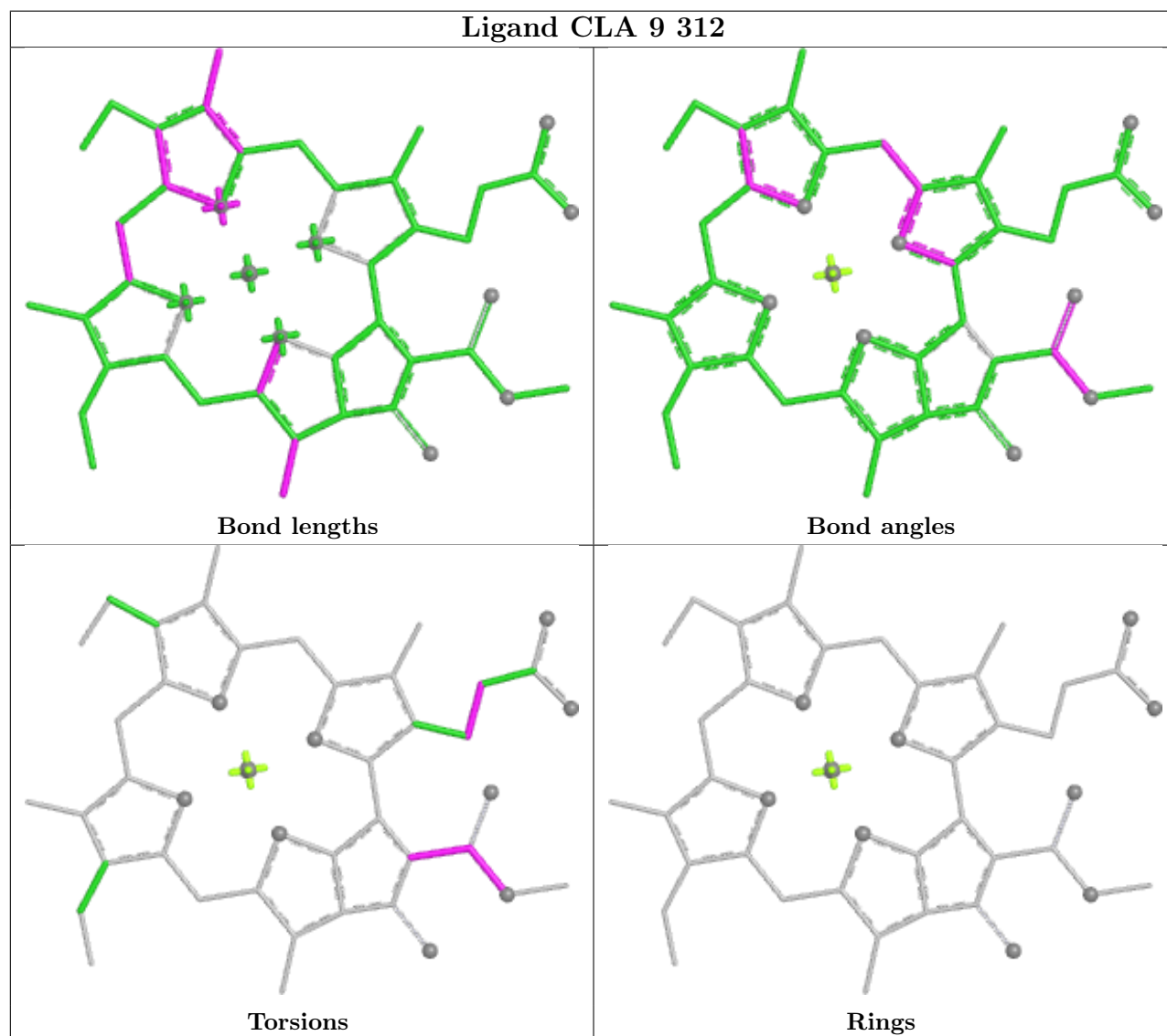
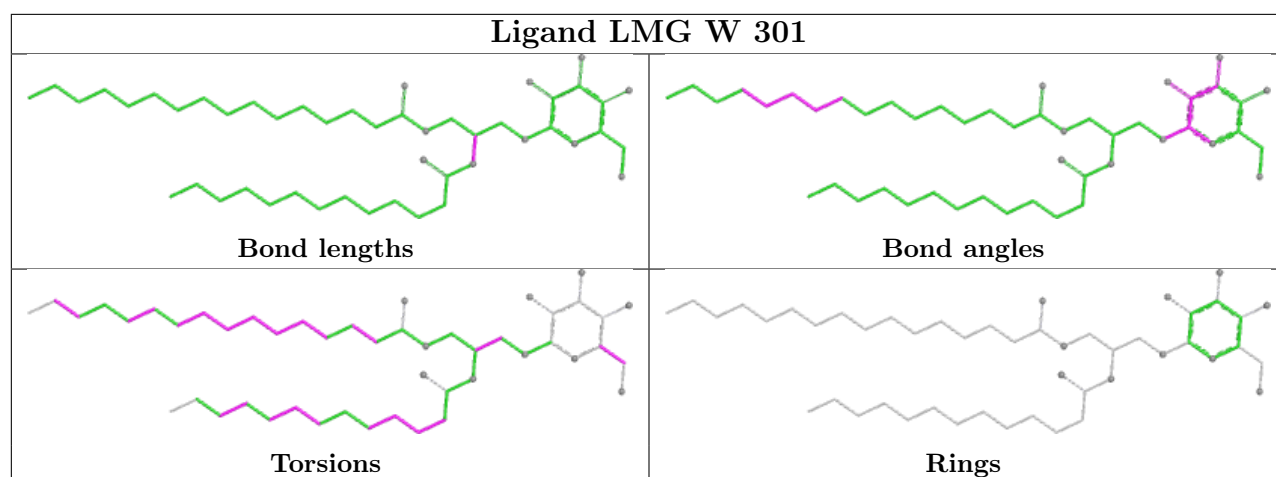
Bond angles

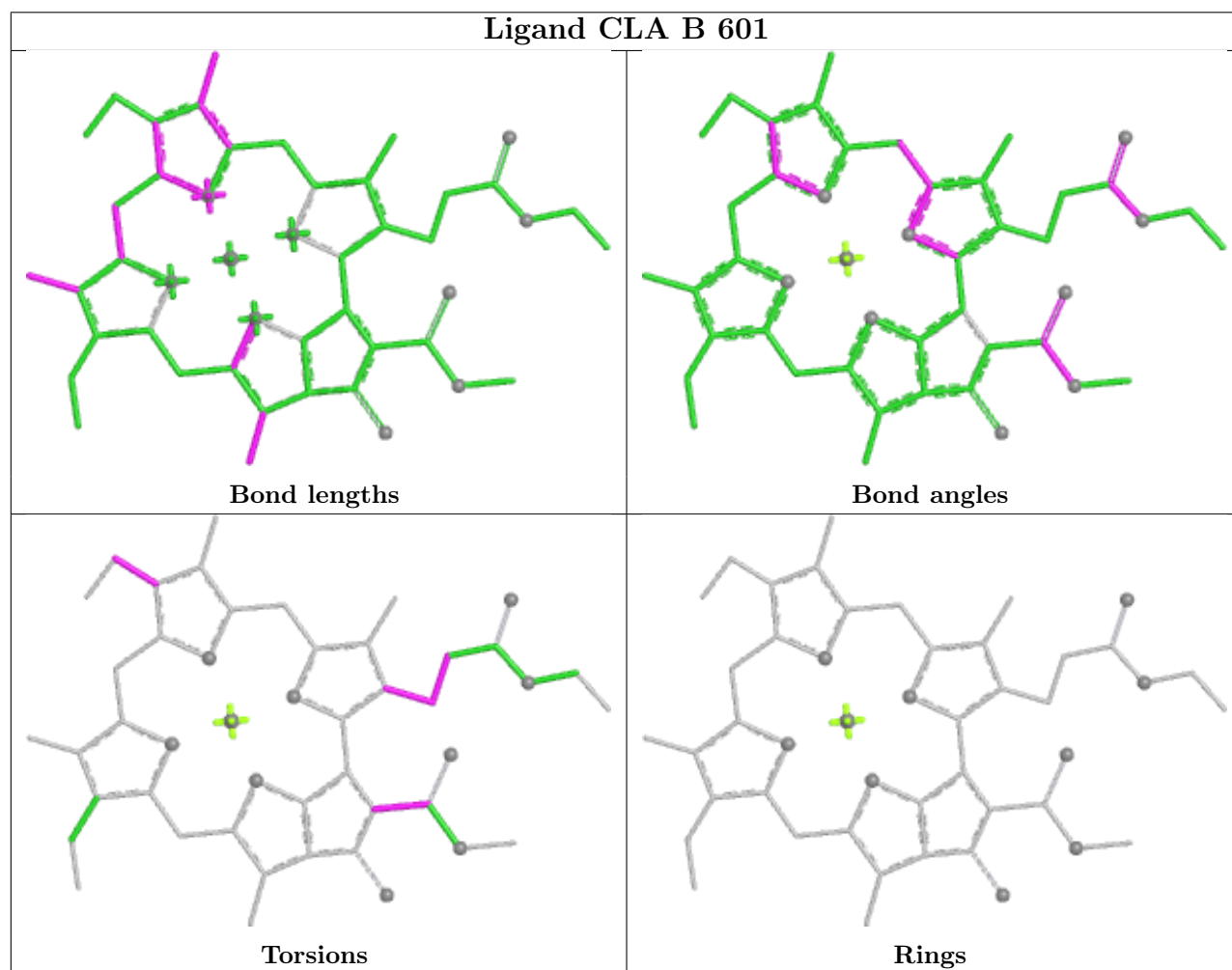
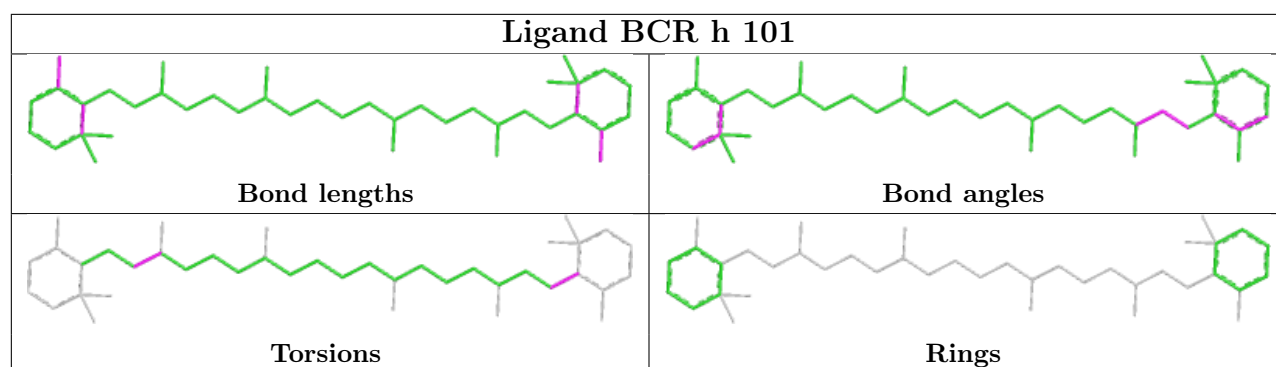


Torsions

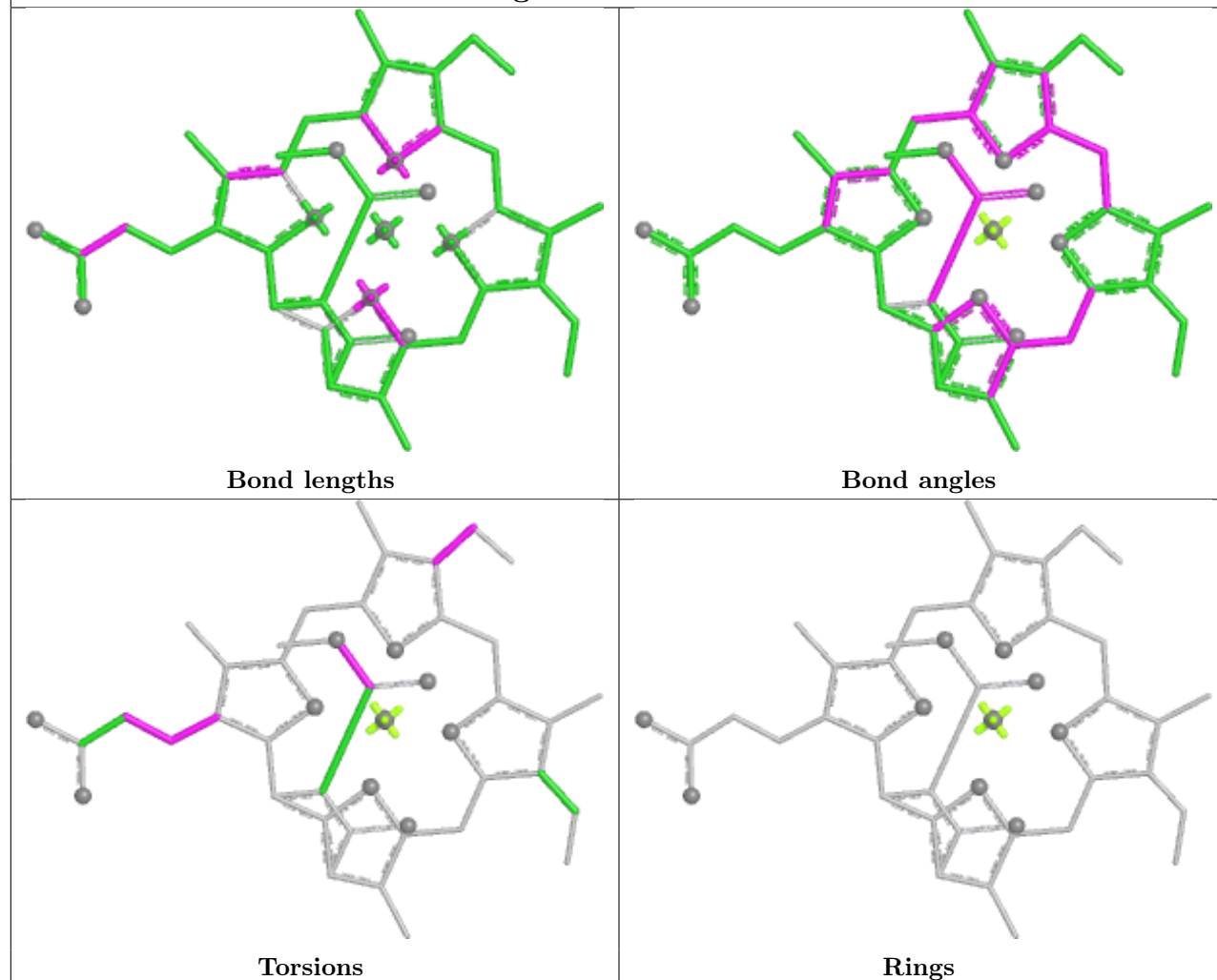


Rings

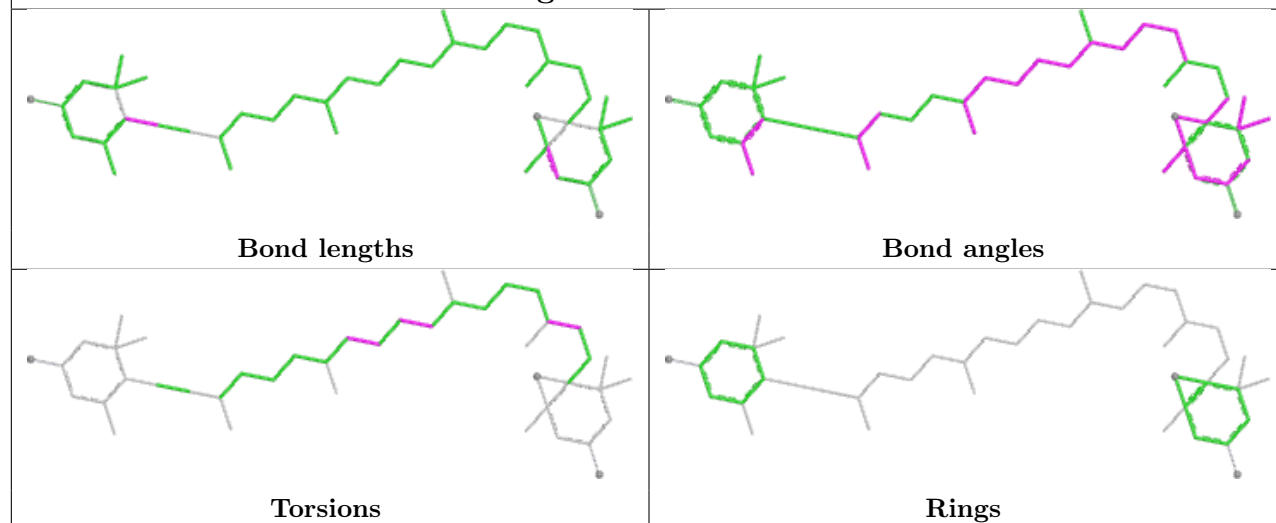




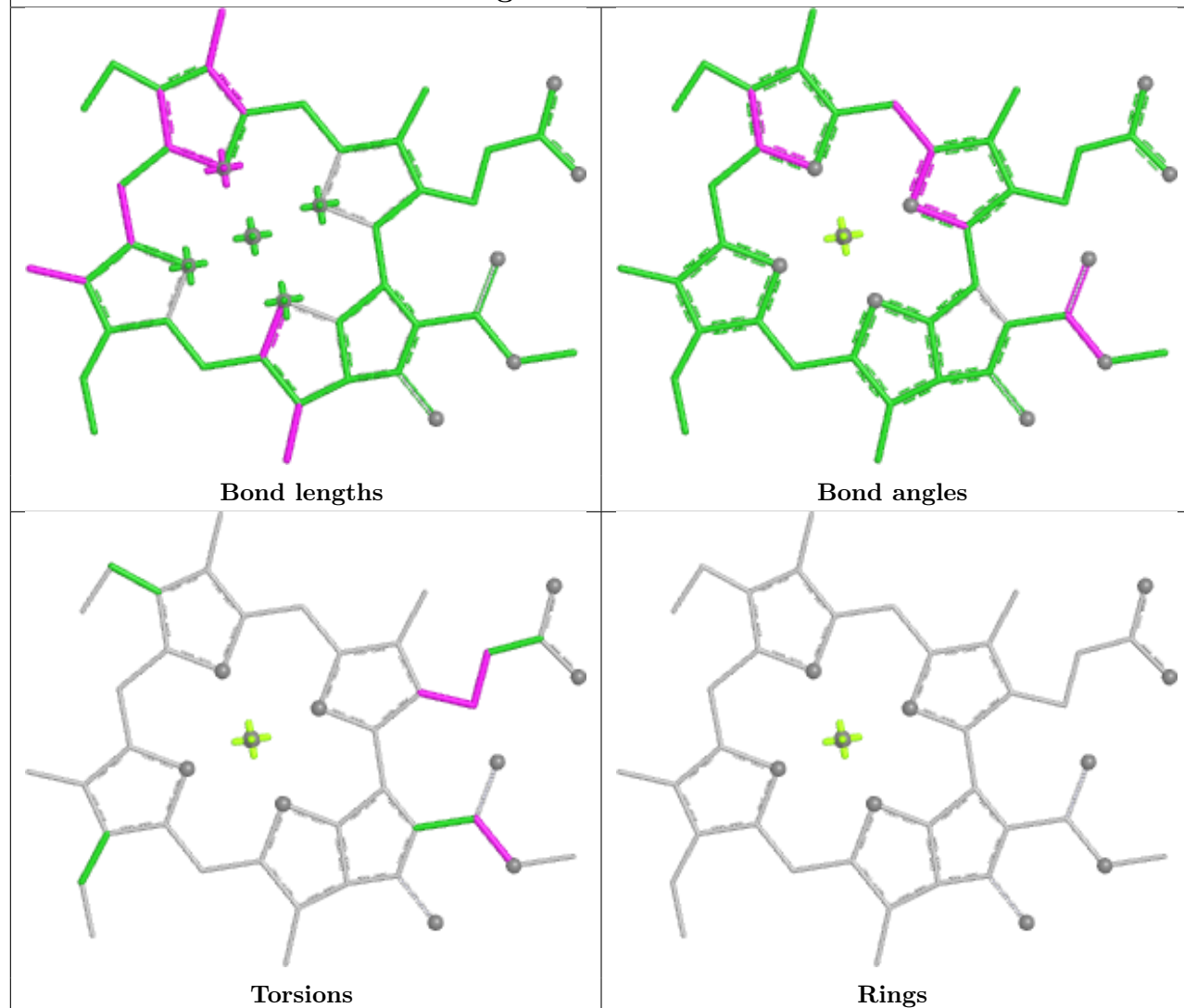
Ligand KC1 6 314



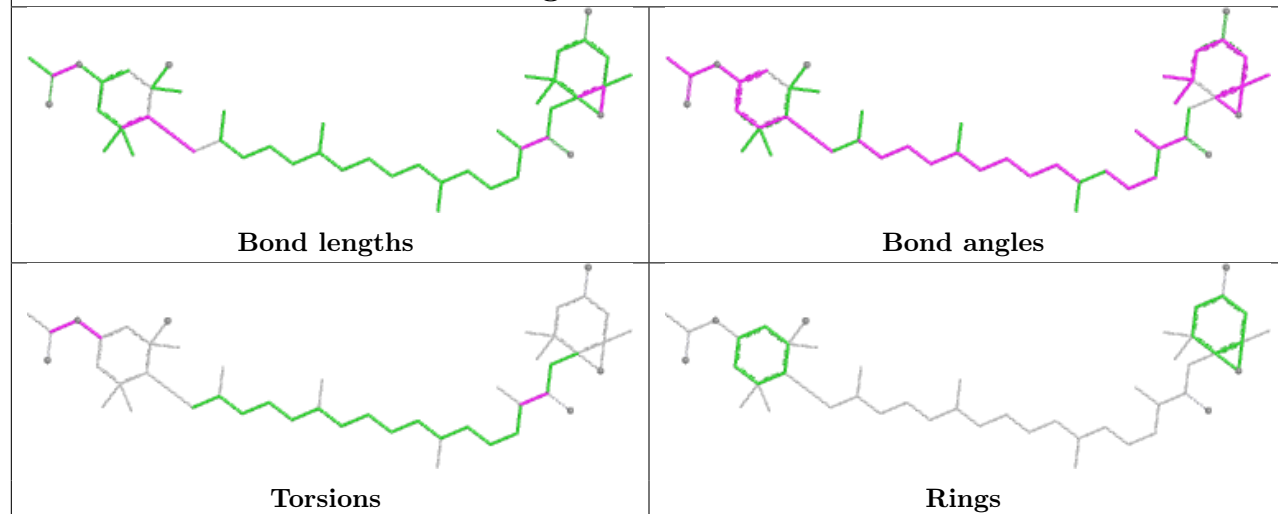
Ligand DD6 2 303

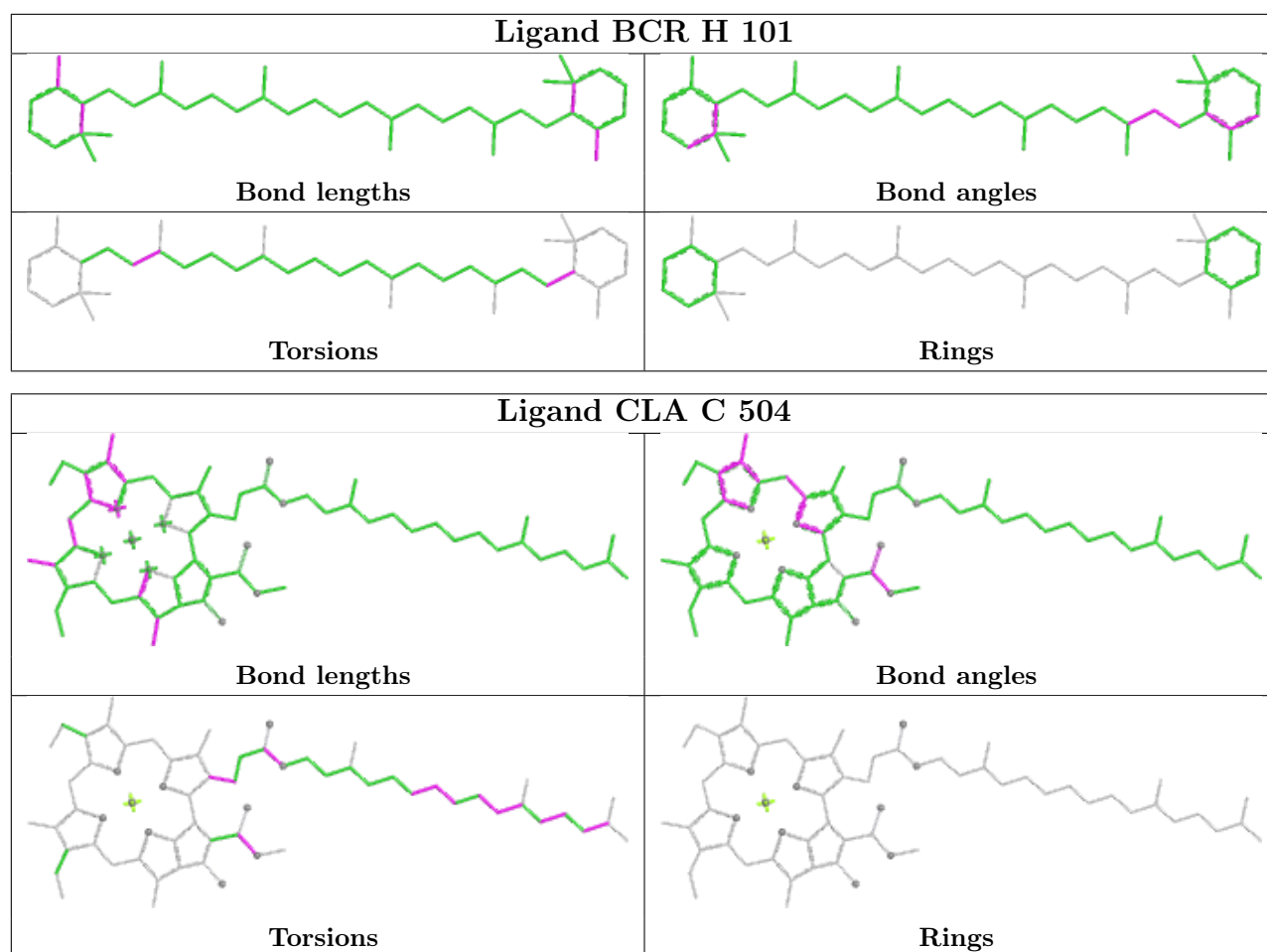


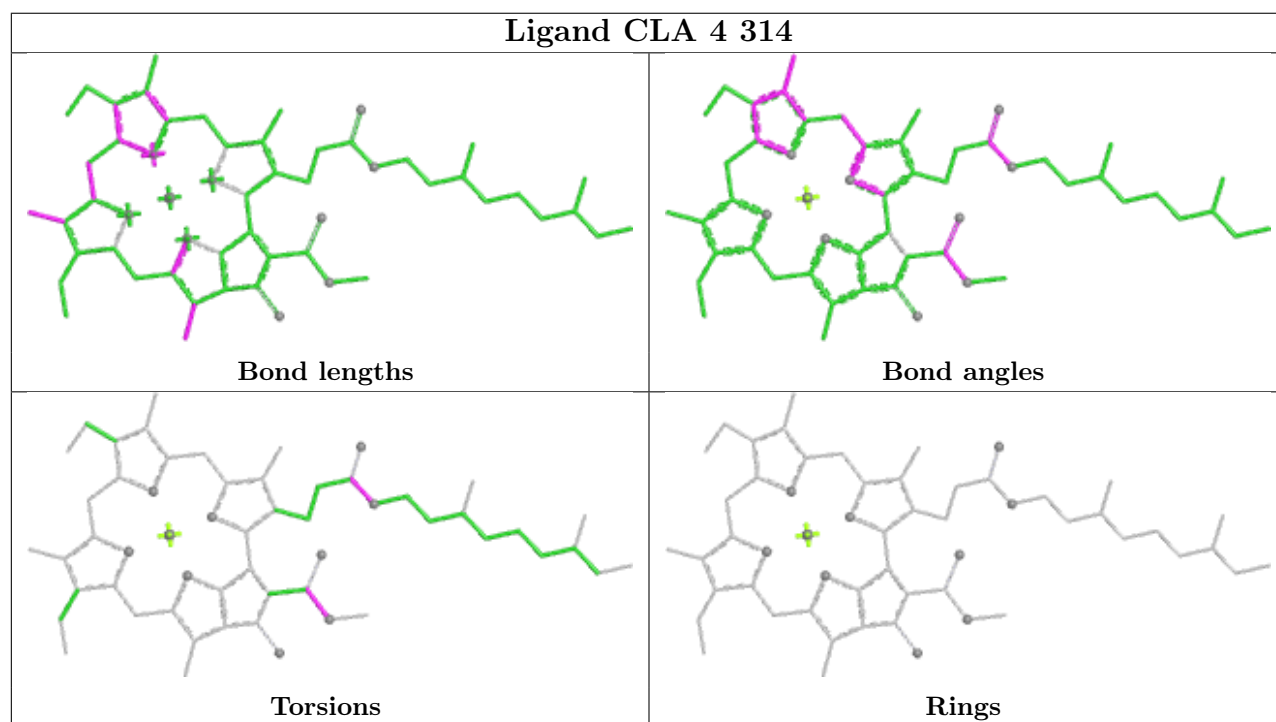
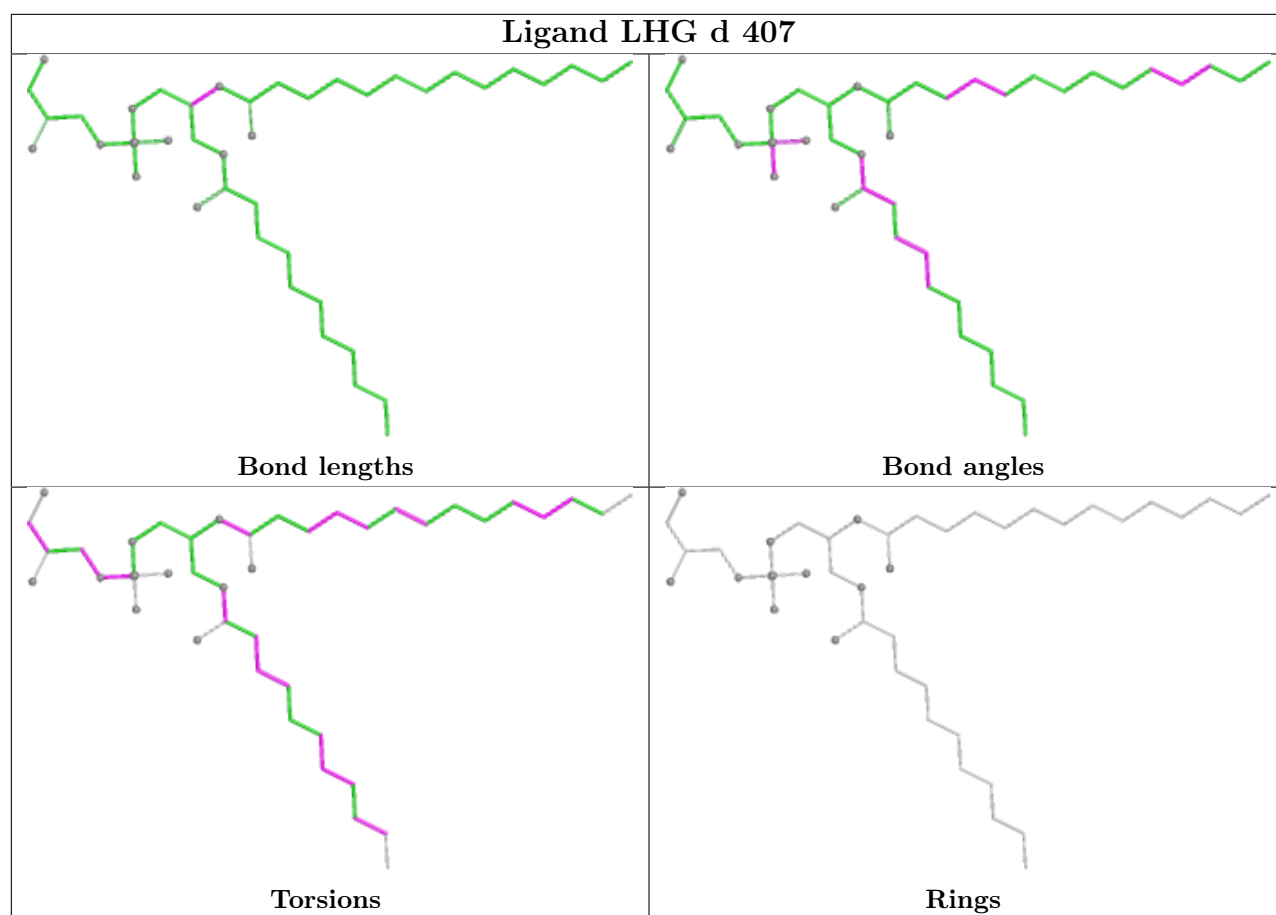
Ligand CLA 9 306



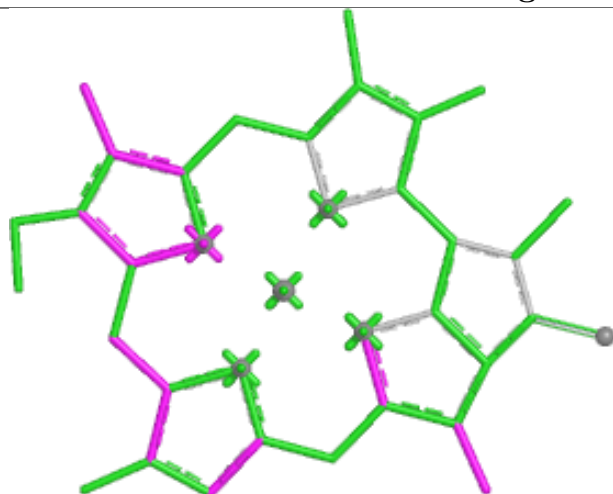
Ligand A86 6 301



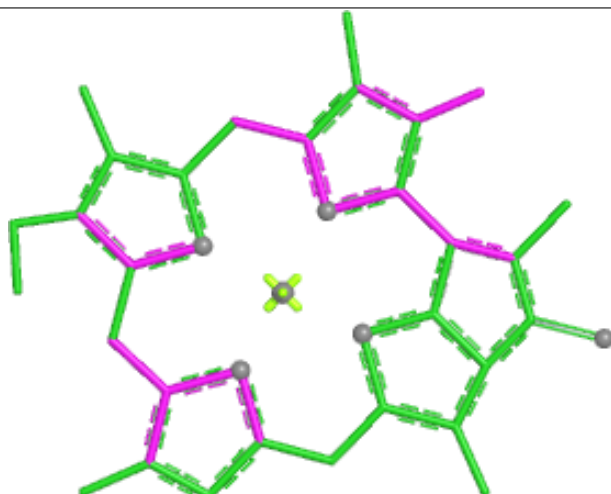




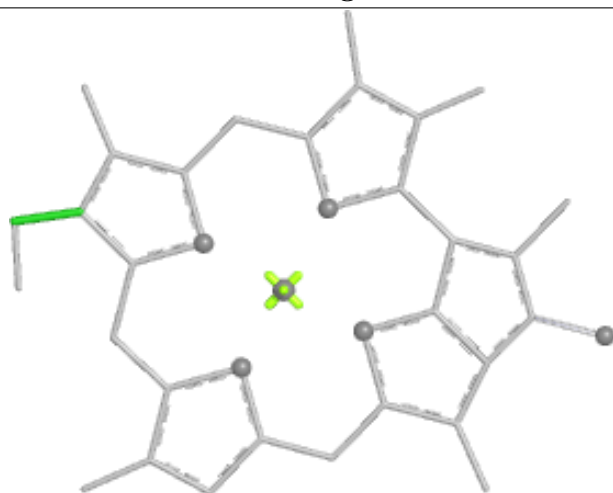
Ligand CLA 8 313



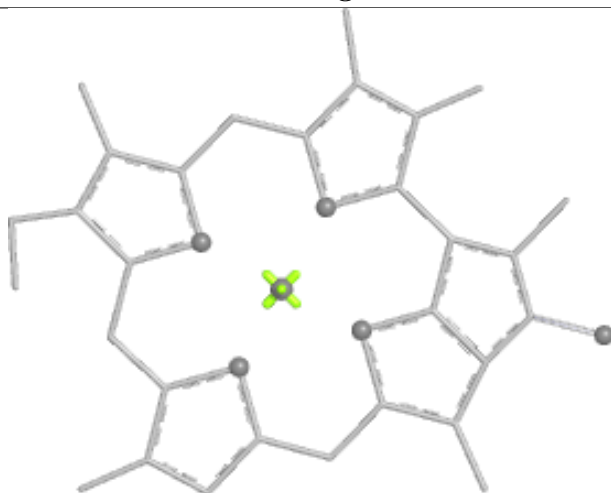
Bond lengths



Bond angles

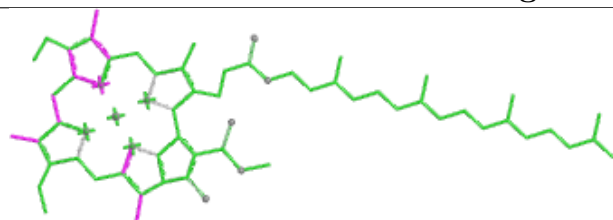


Torsions

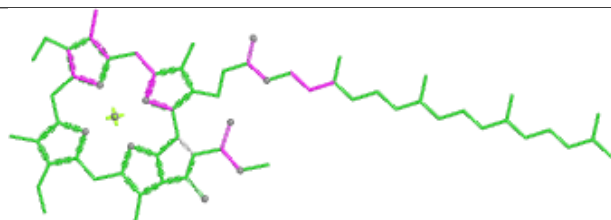


Rings

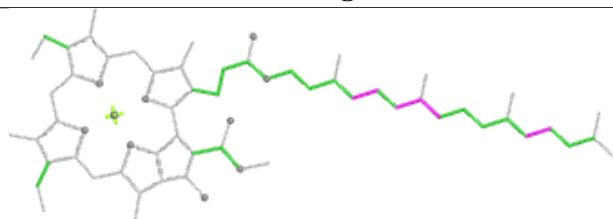
Ligand CLA c 509



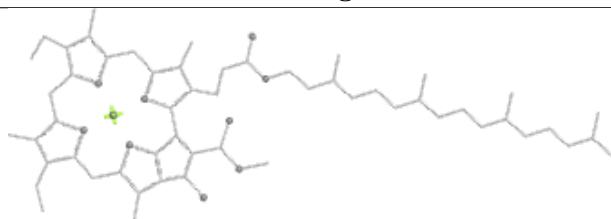
Bond lengths



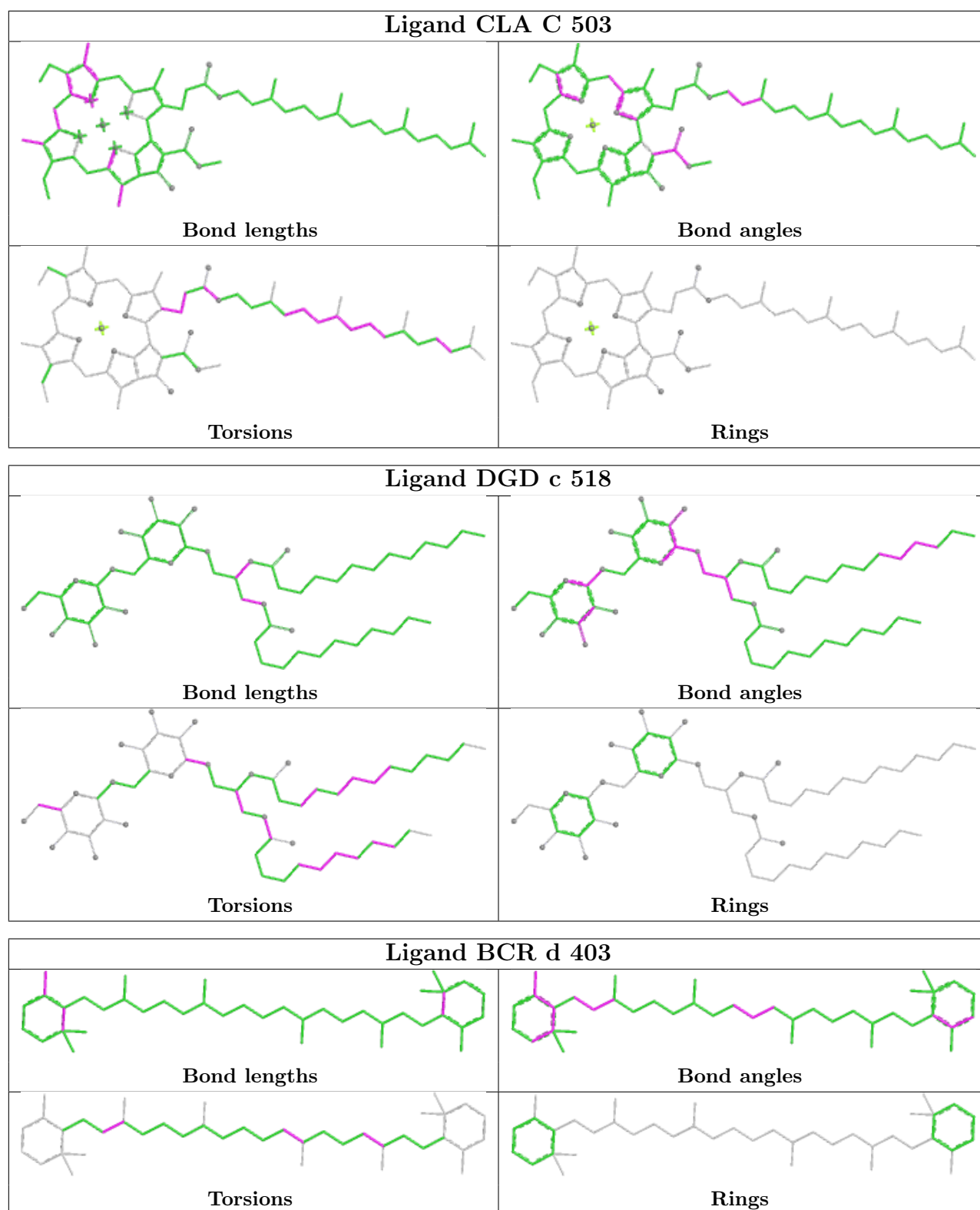
Bond angles



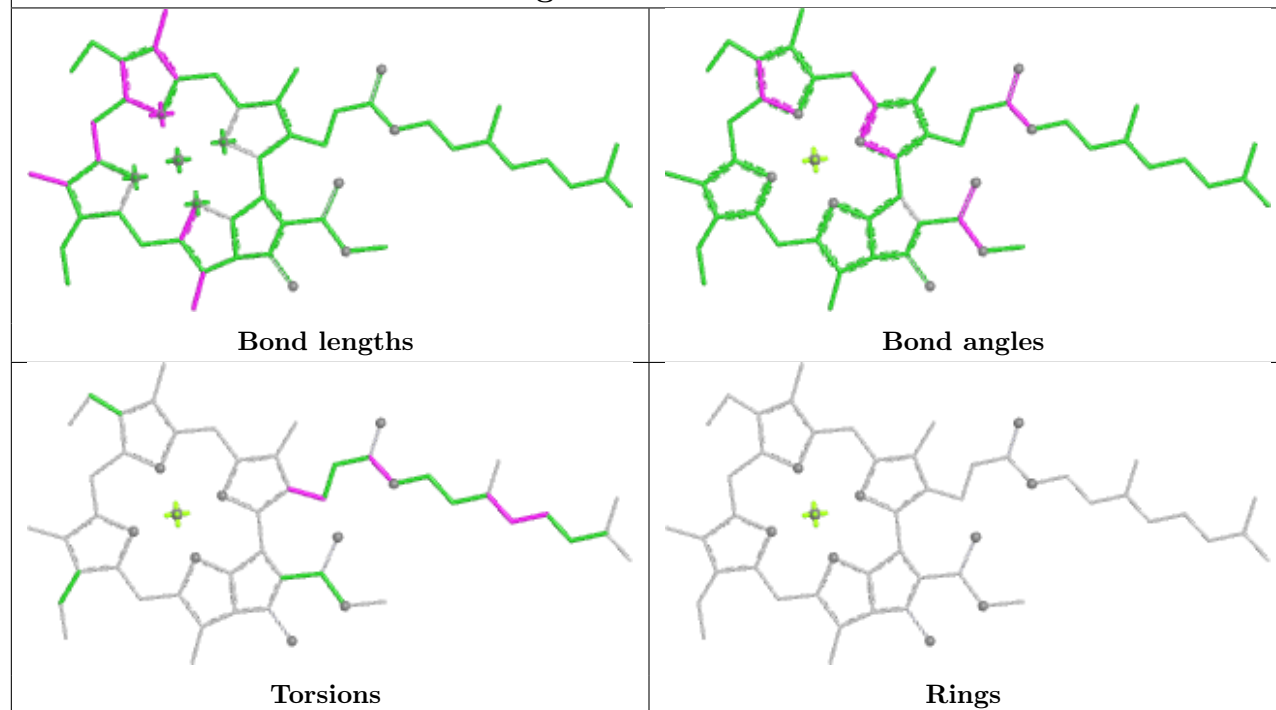
Torsions



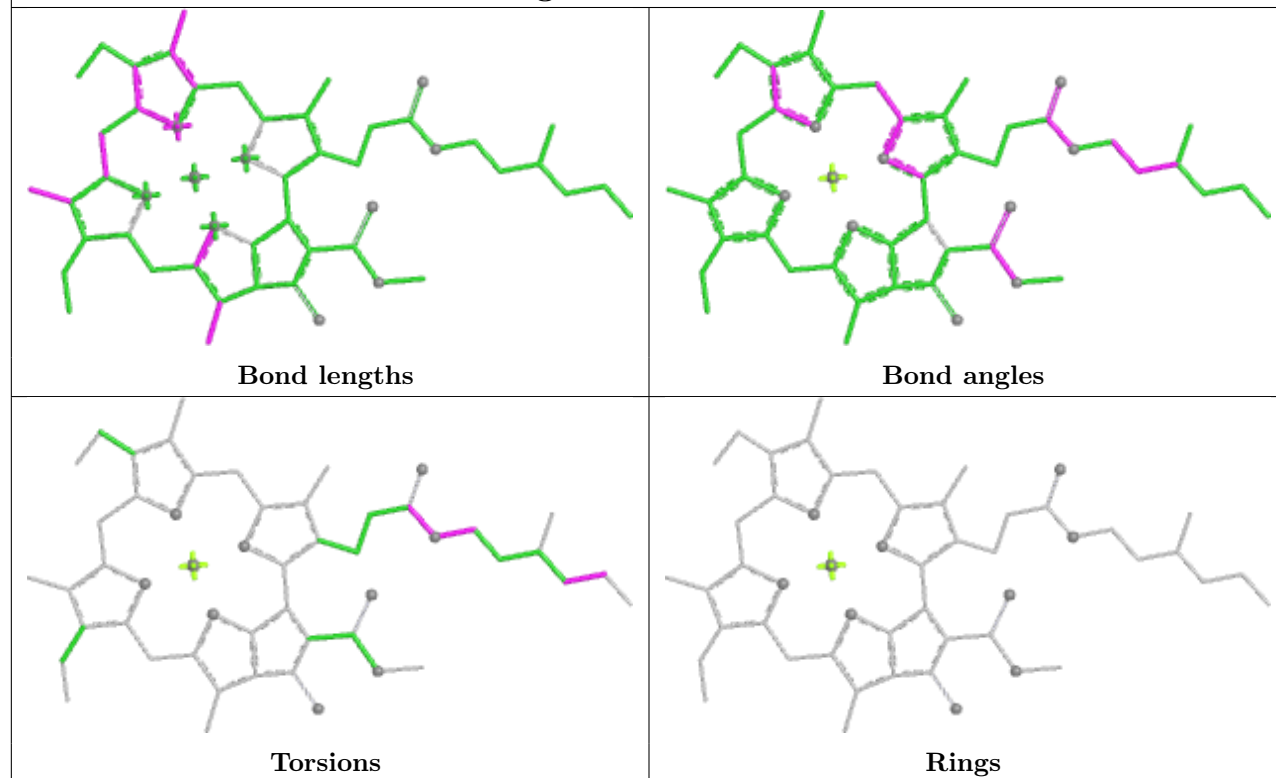
Rings



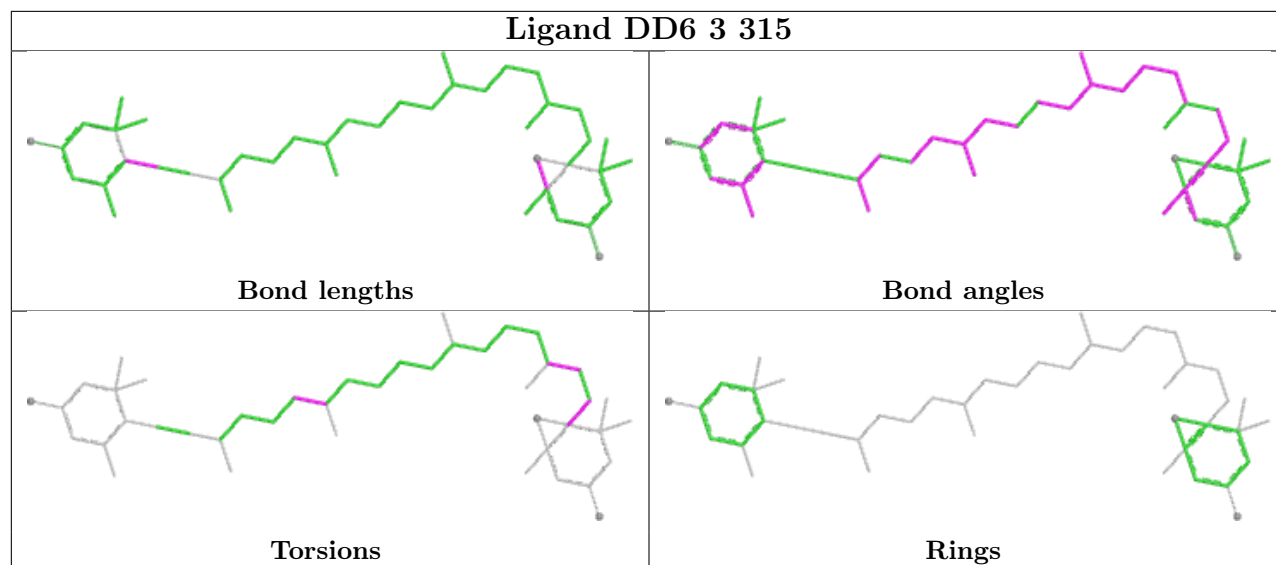
Ligand CLA 4 305



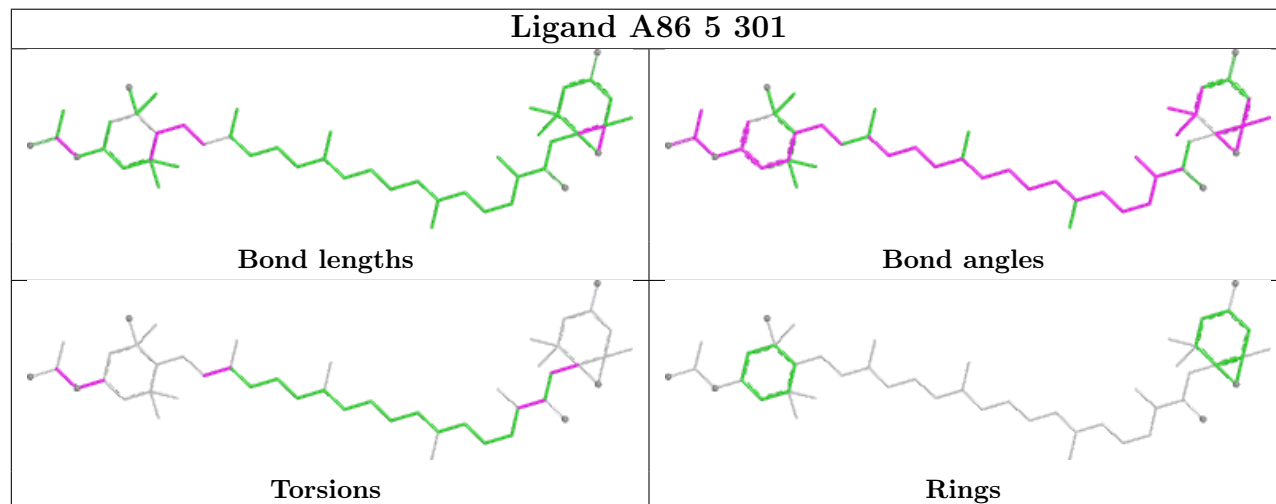
Ligand CLA 4 316



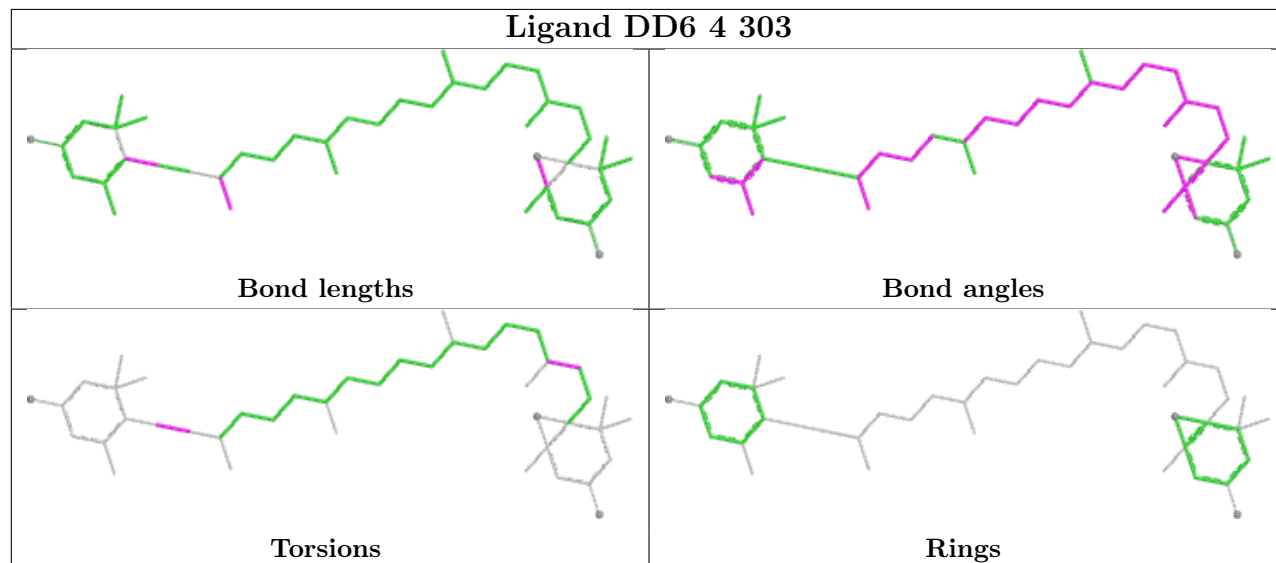
Ligand DD6 3 315

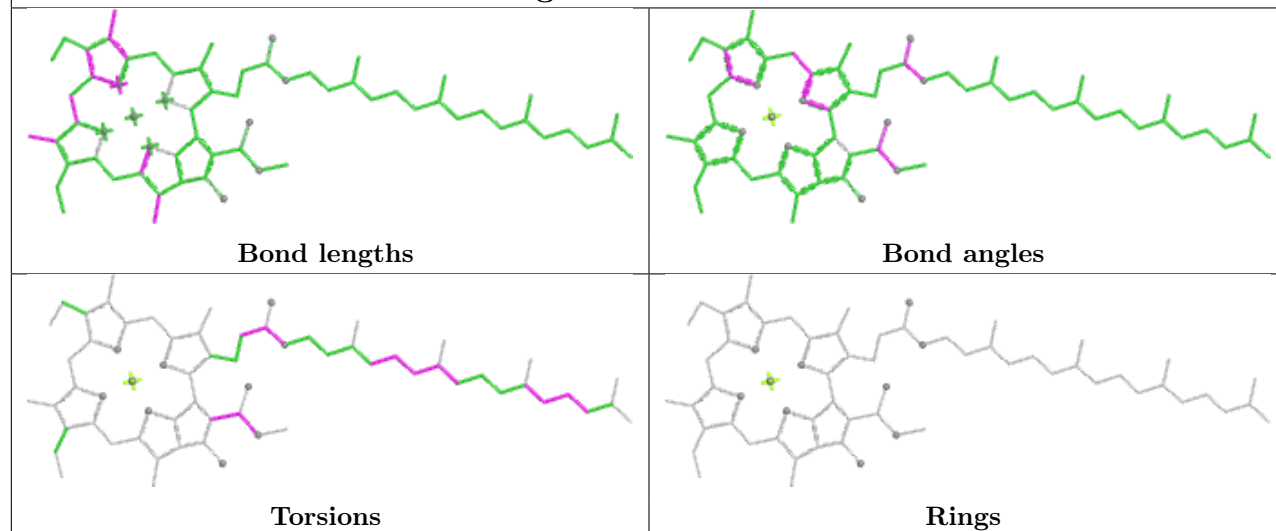
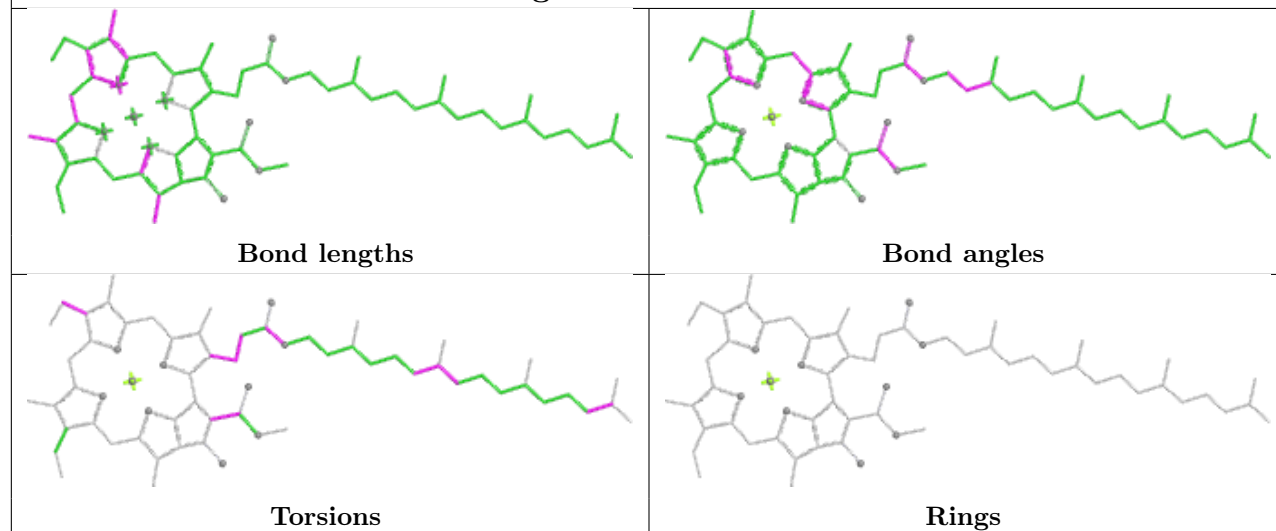
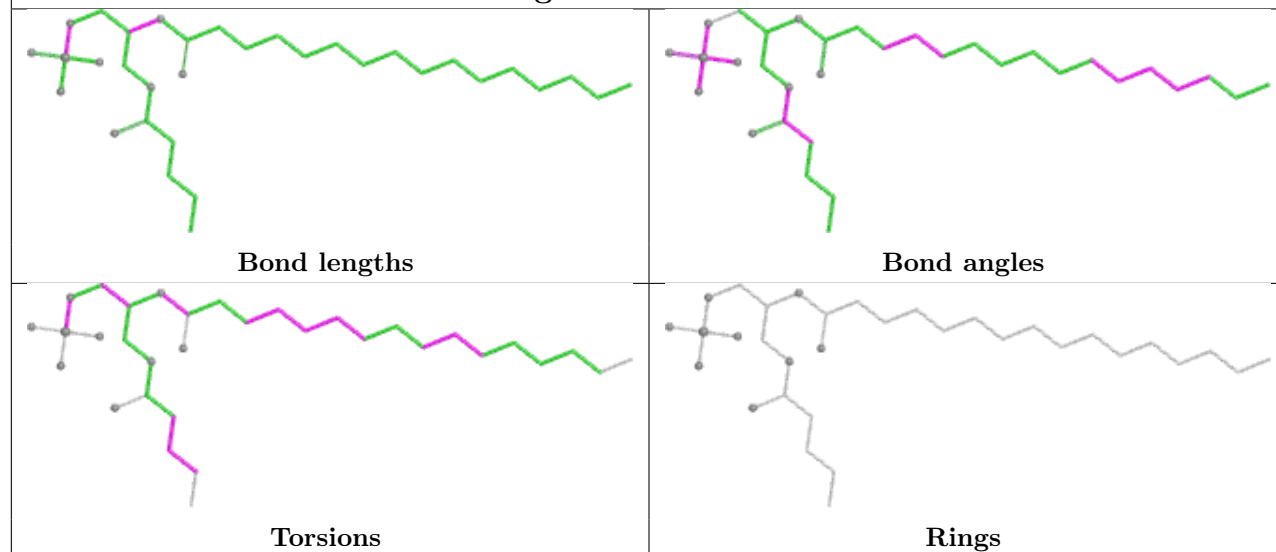


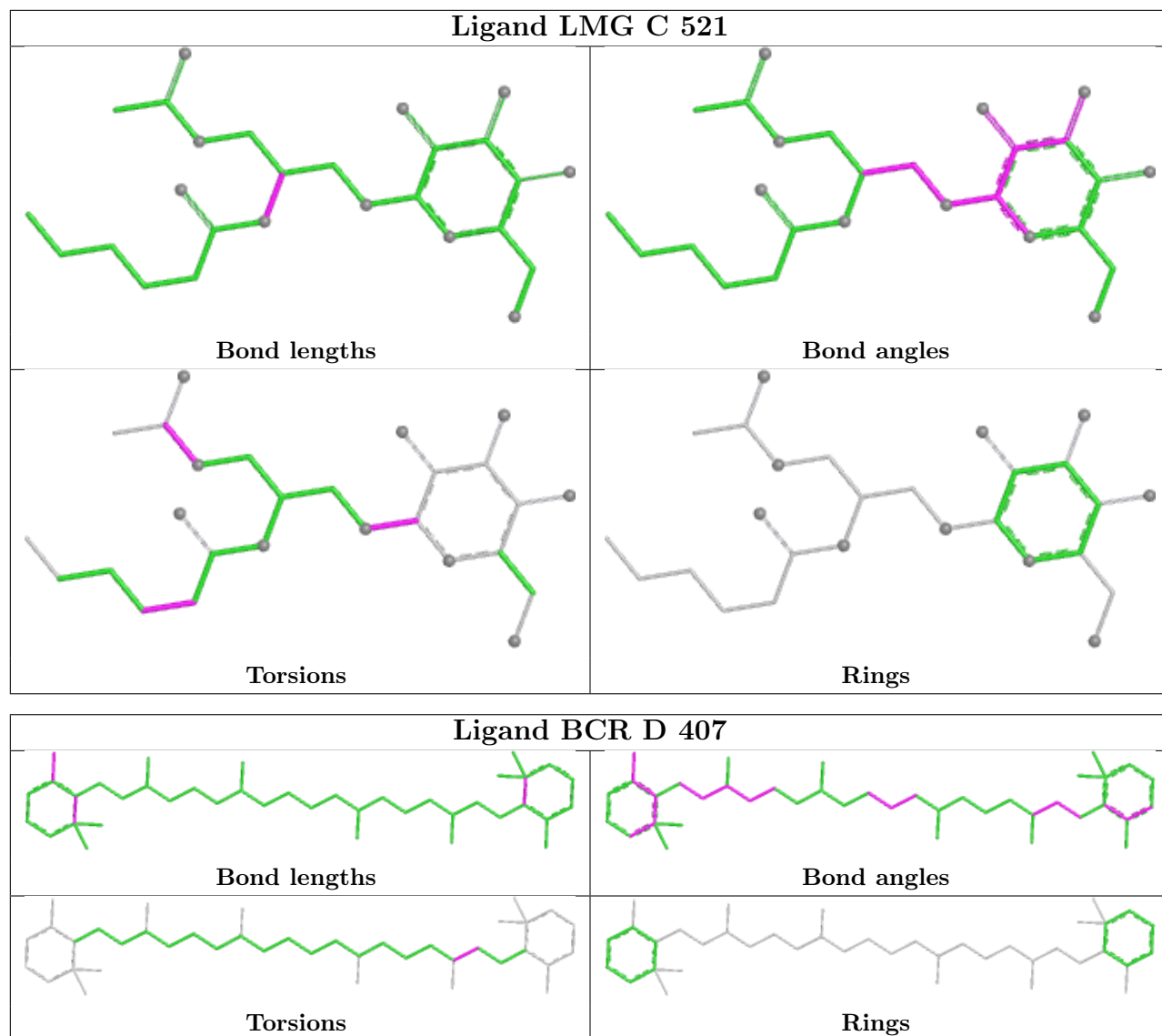
Ligand A86 5 301



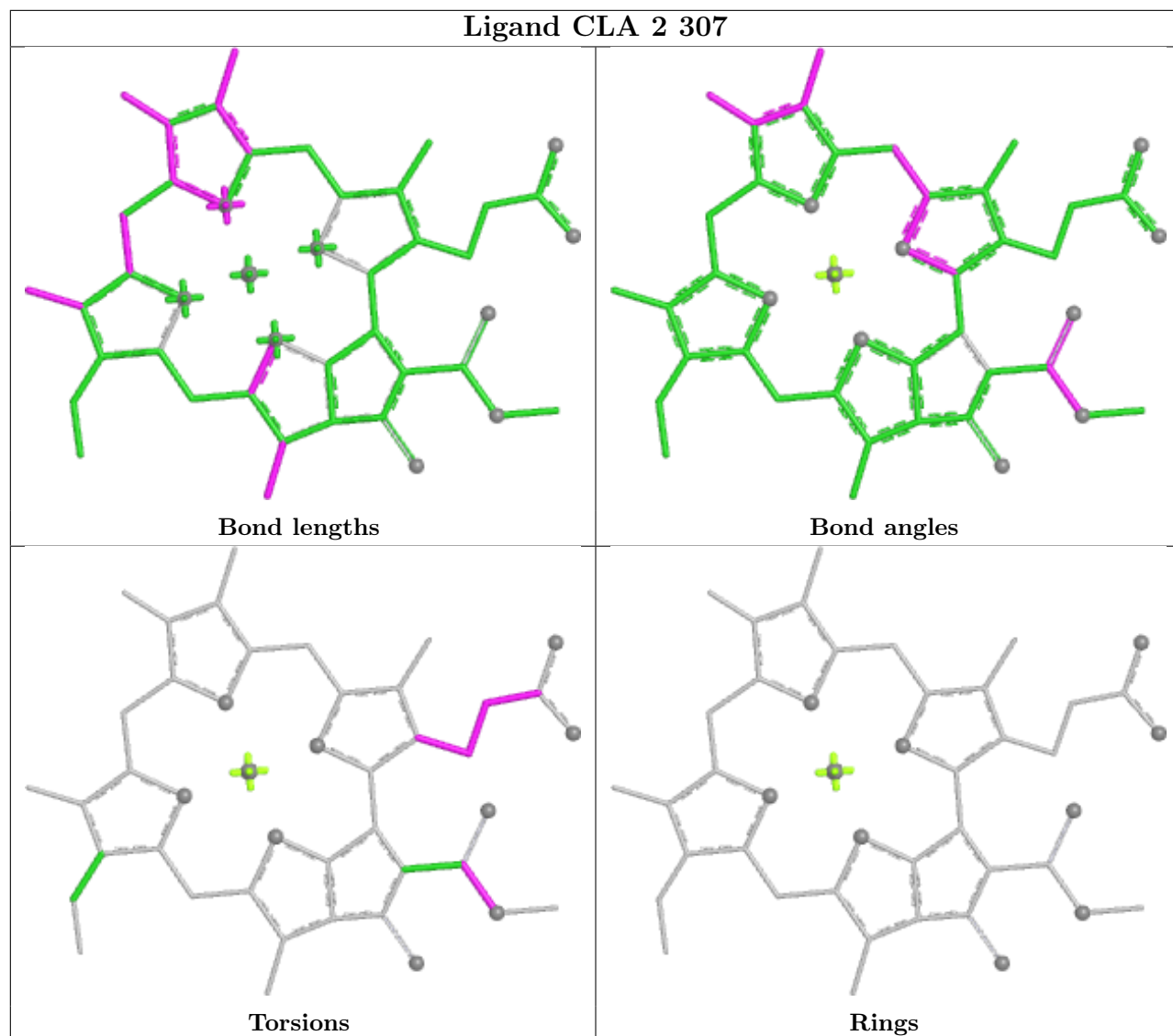
Ligand DD6 4 303

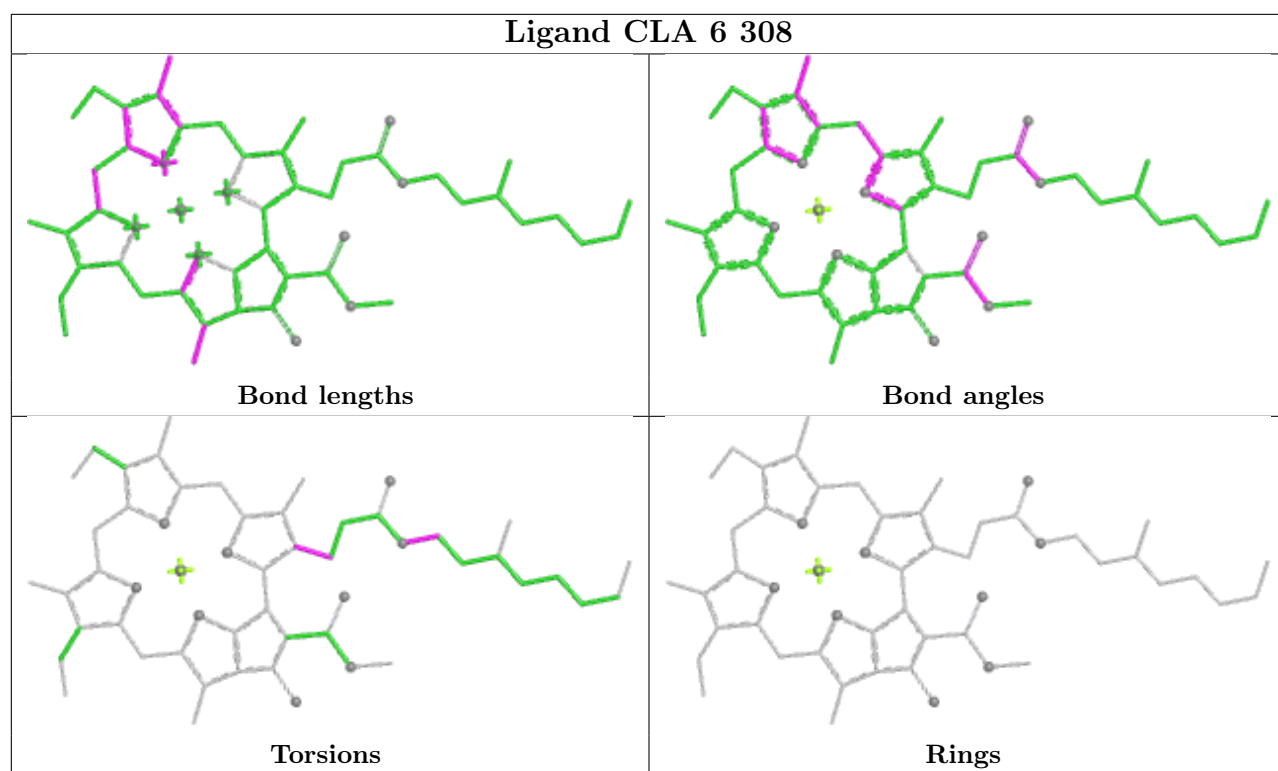


Ligand CLA 7 312**Ligand CLA B 616****Ligand LHG 5 318**

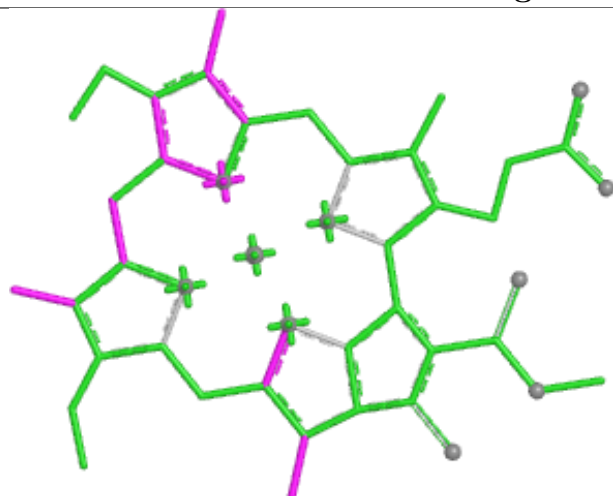


Ligand CLA 2 307

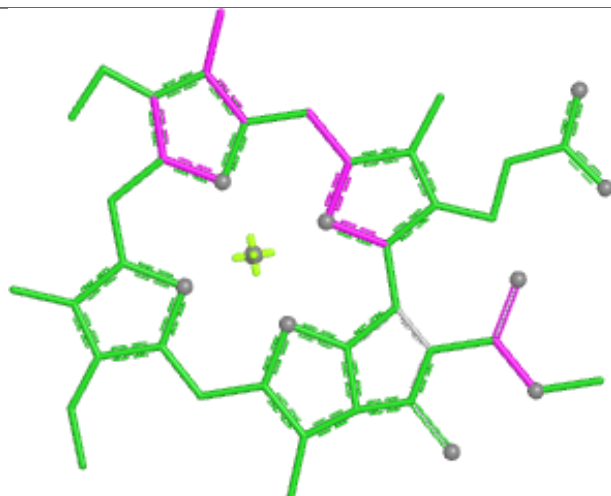




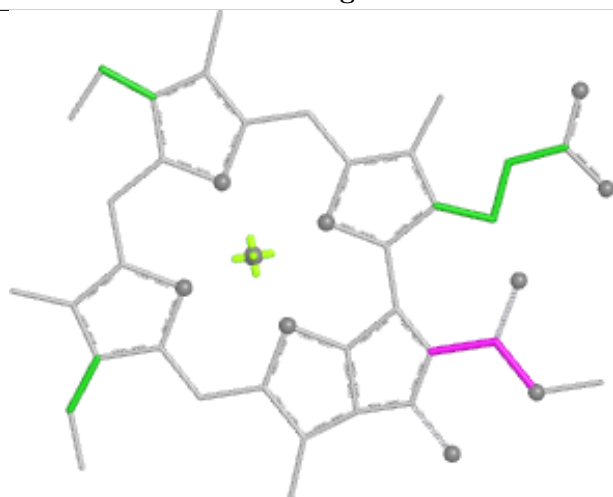
Ligand CLA C 506



Bond lengths



Bond angles

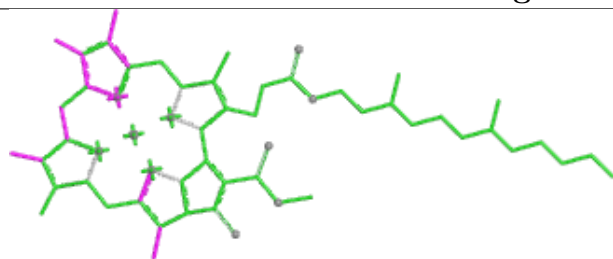


Torsions

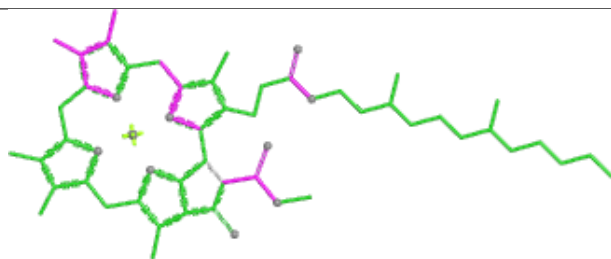


Rings

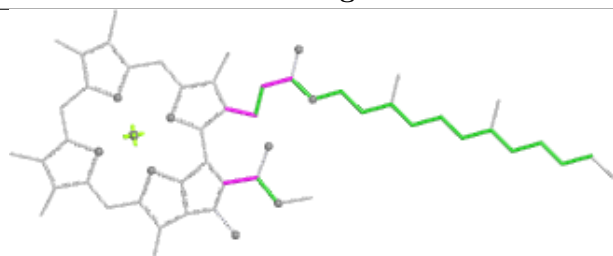
Ligand CLA D 405



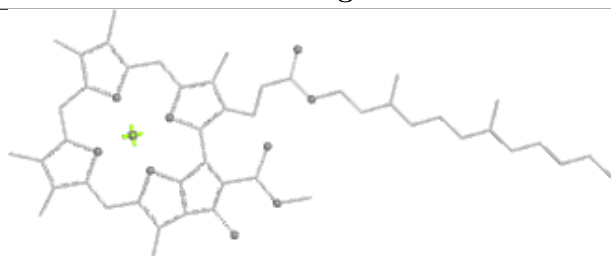
Bond lengths



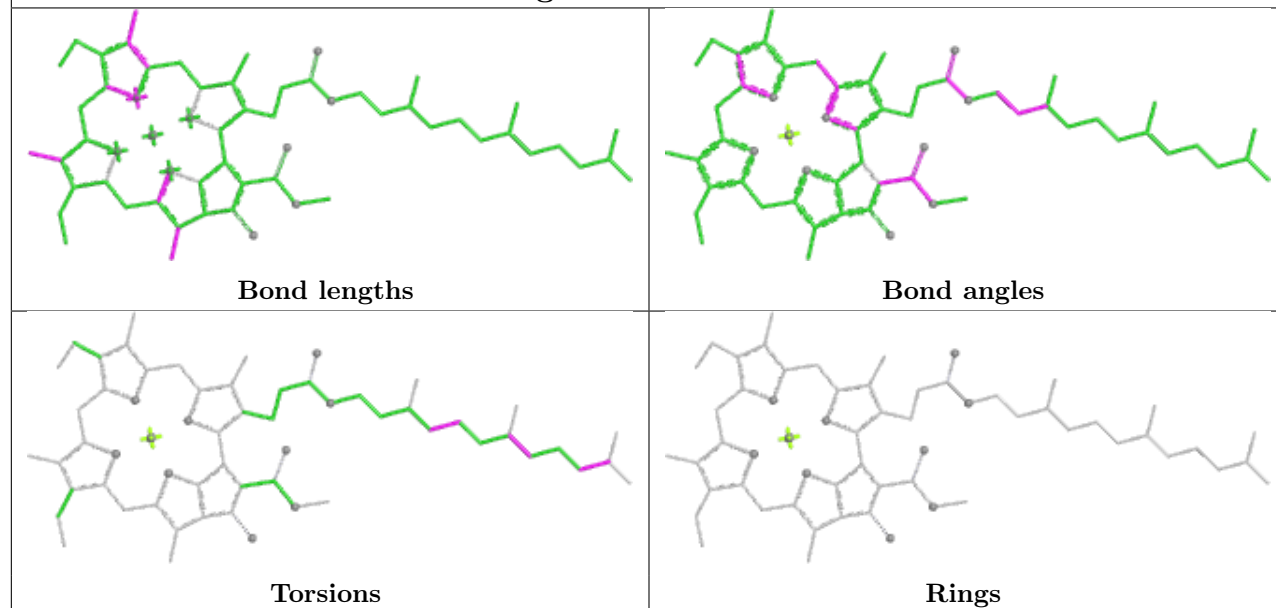
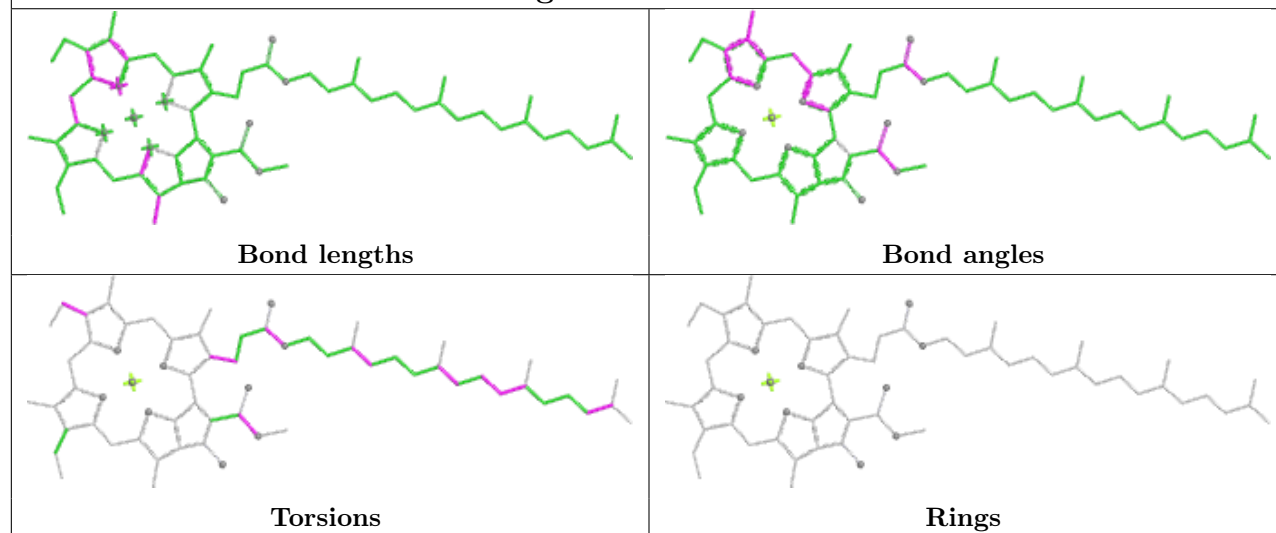
Bond angles

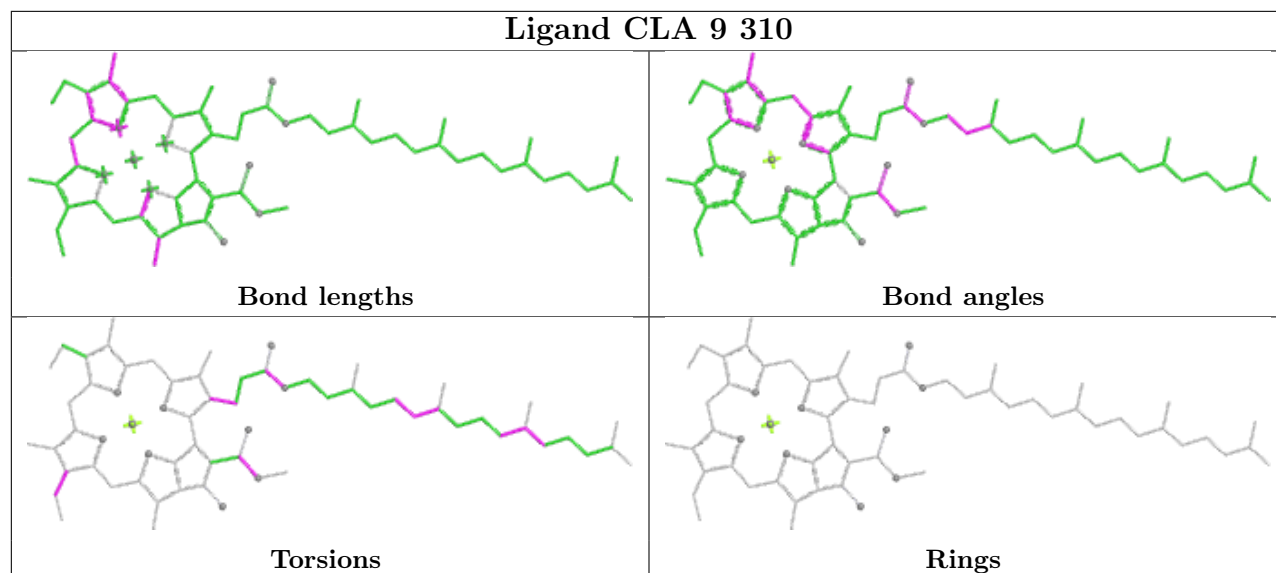
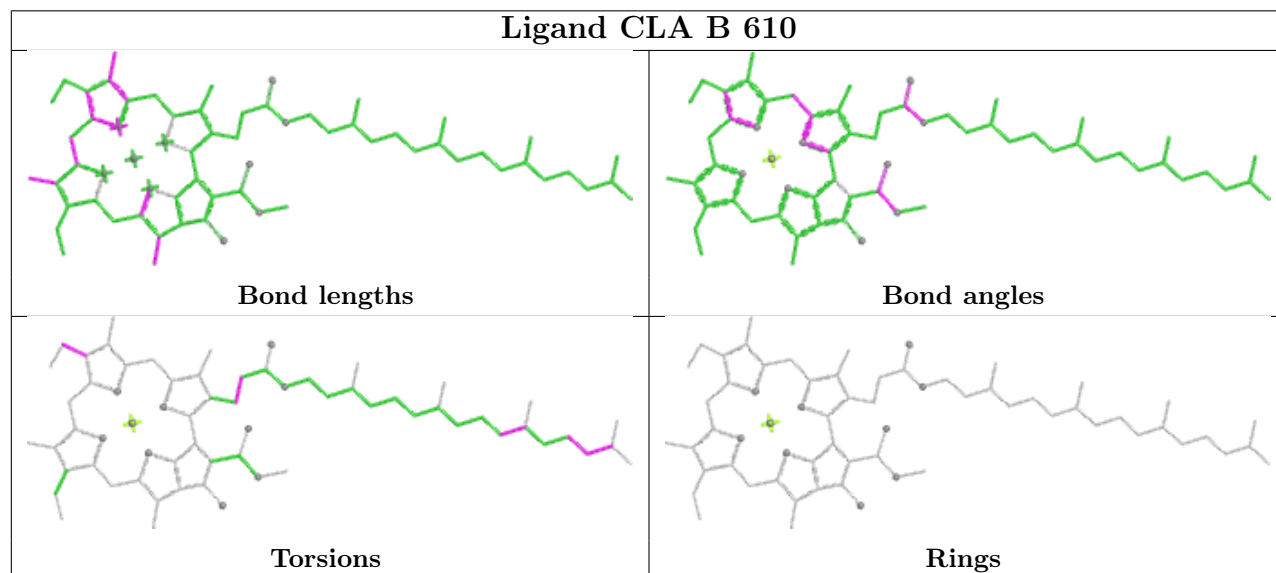
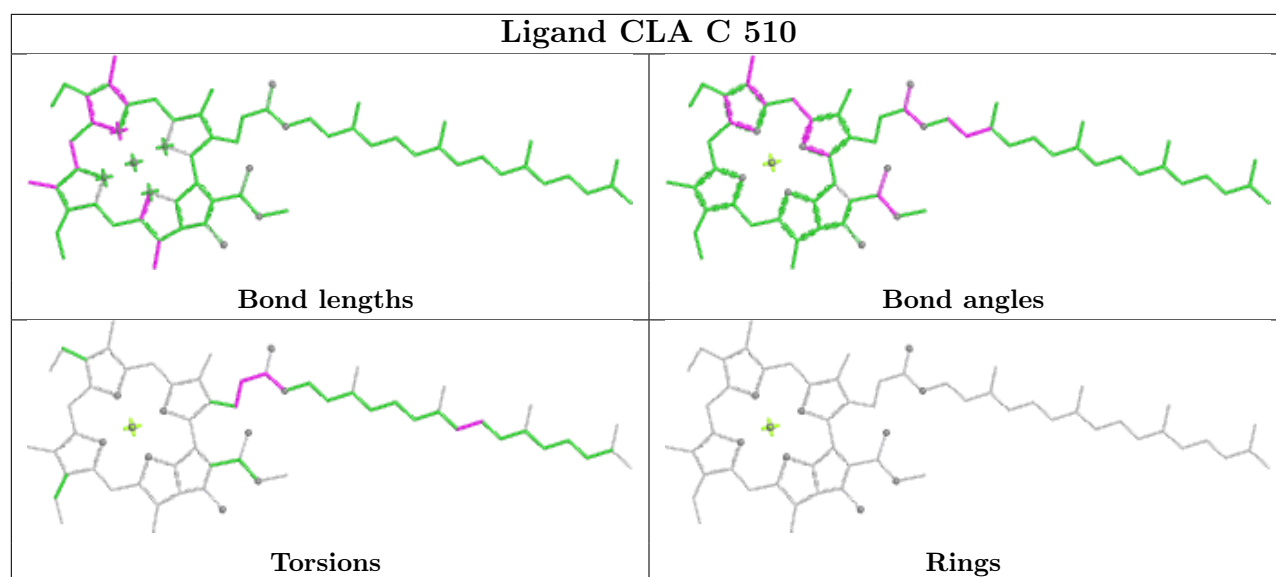


Torsions

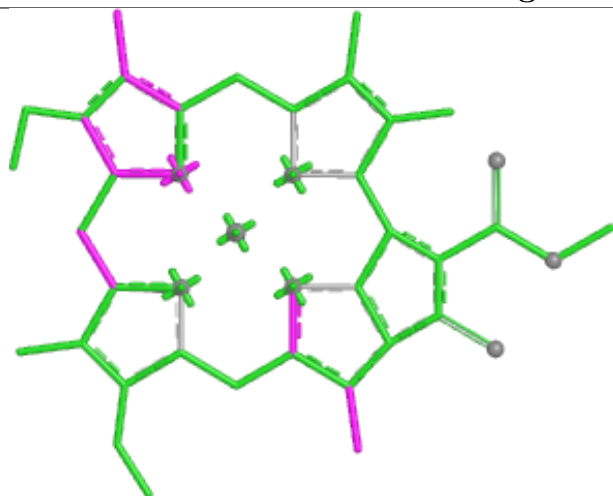


Rings

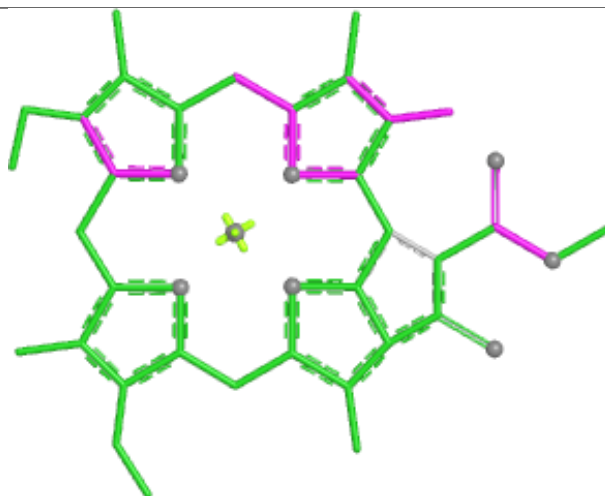
Ligand CLA a 411**Ligand CLA 5 313**



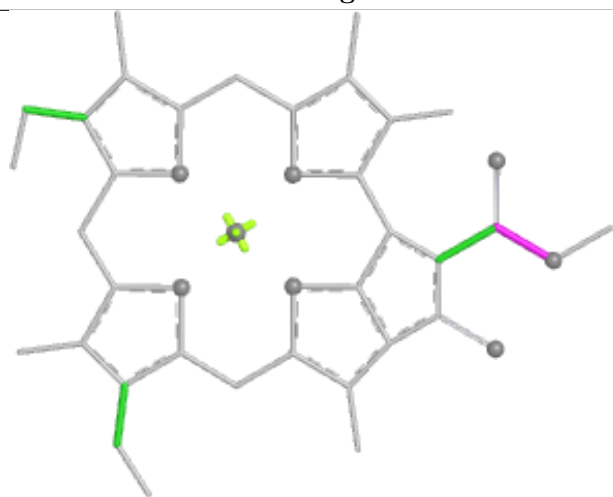
Ligand CLA 5 316



Bond lengths



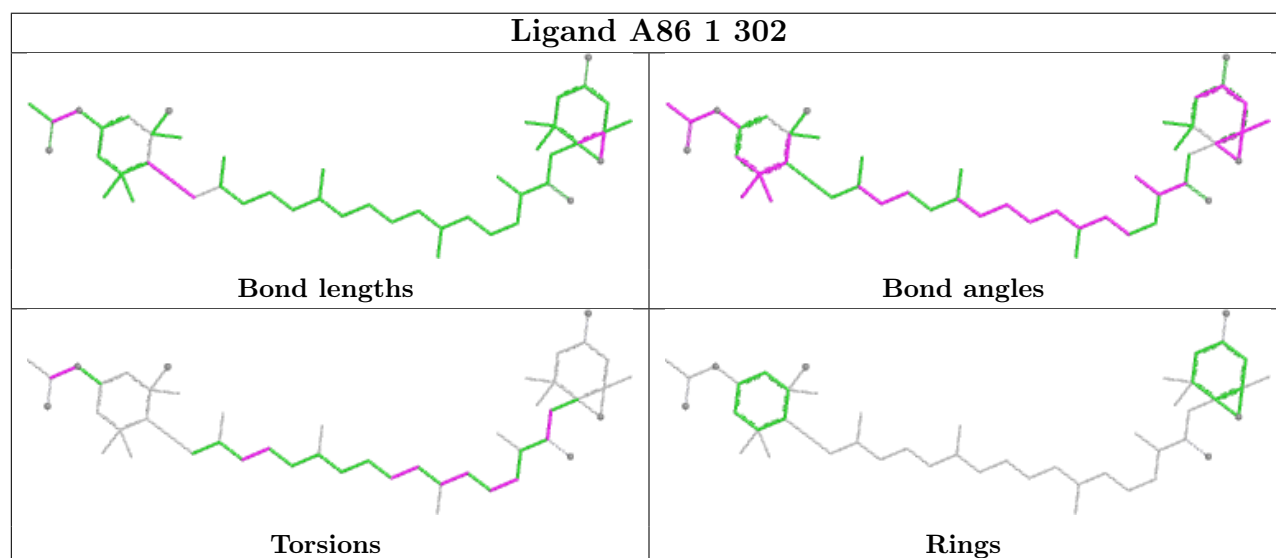
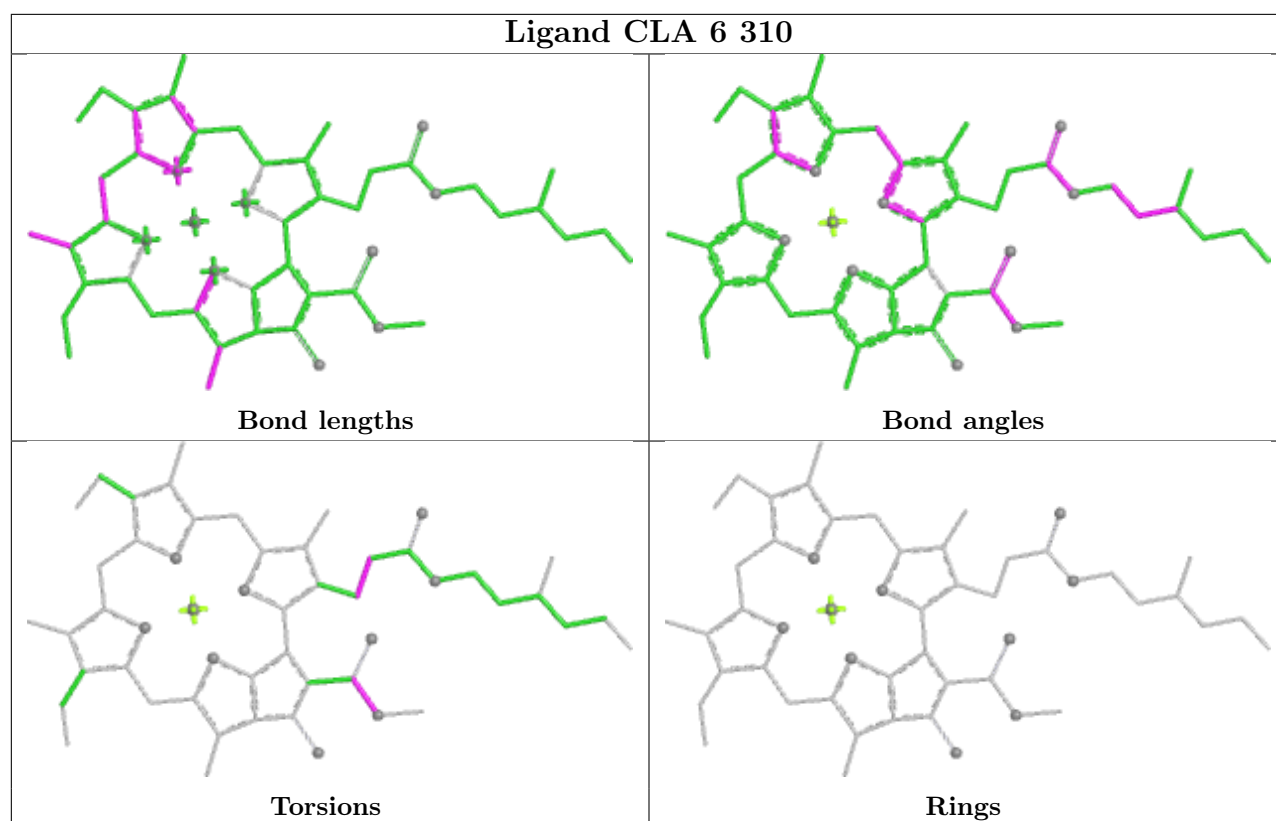
Bond angles

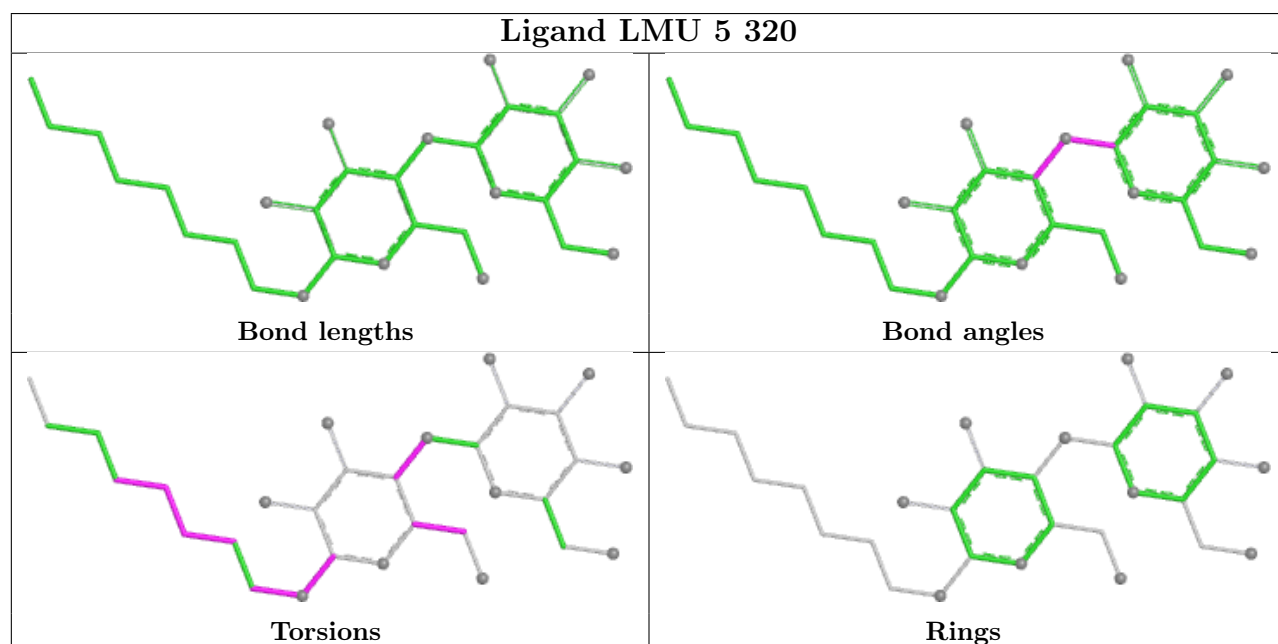
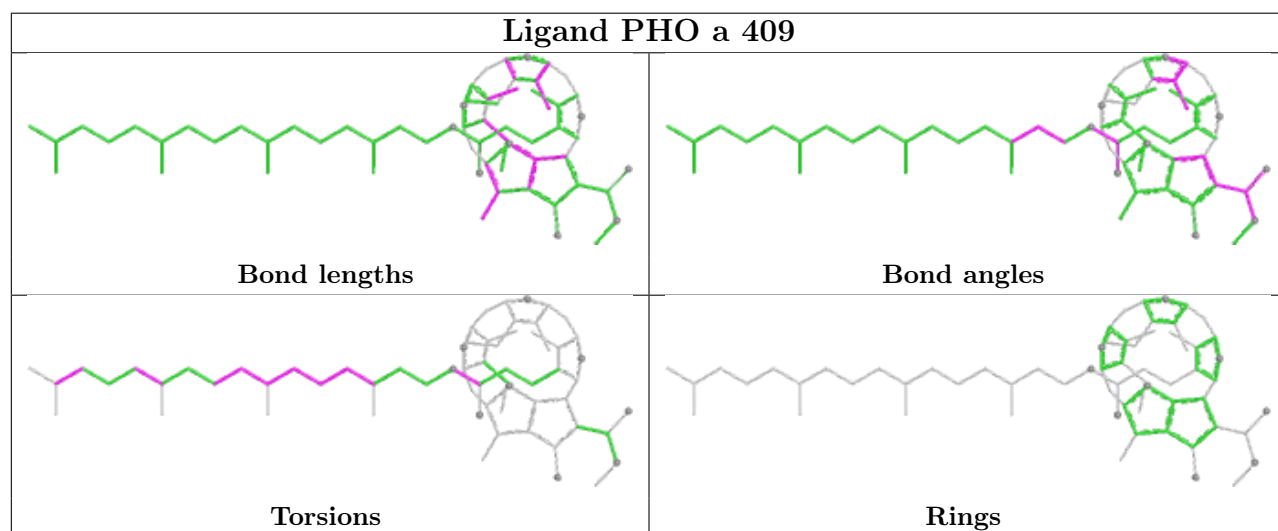
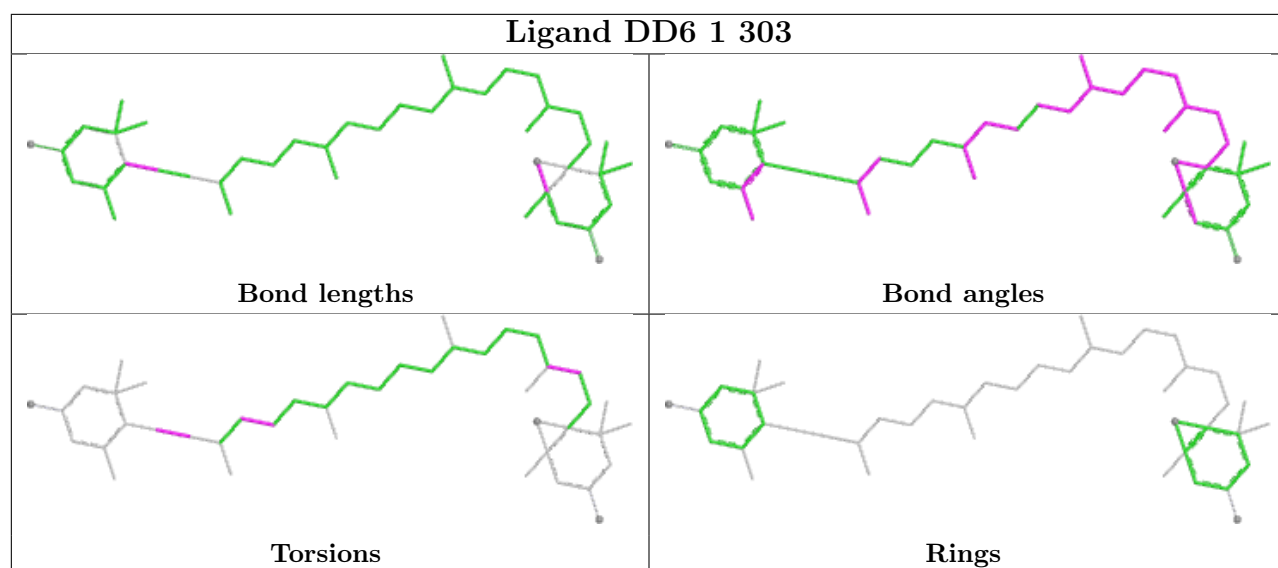


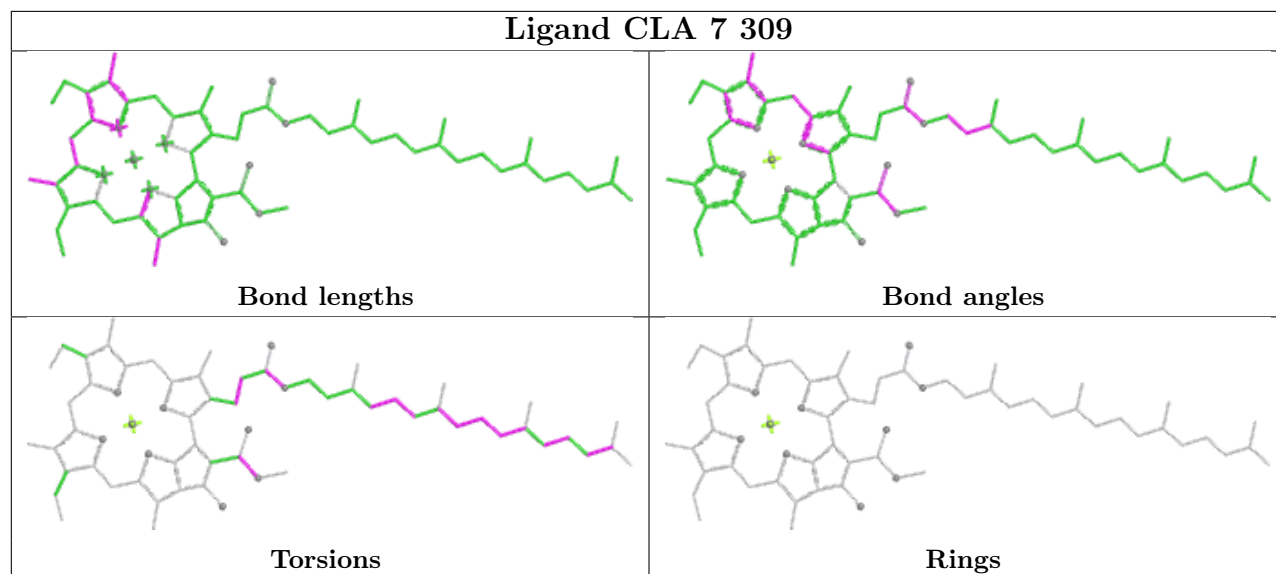
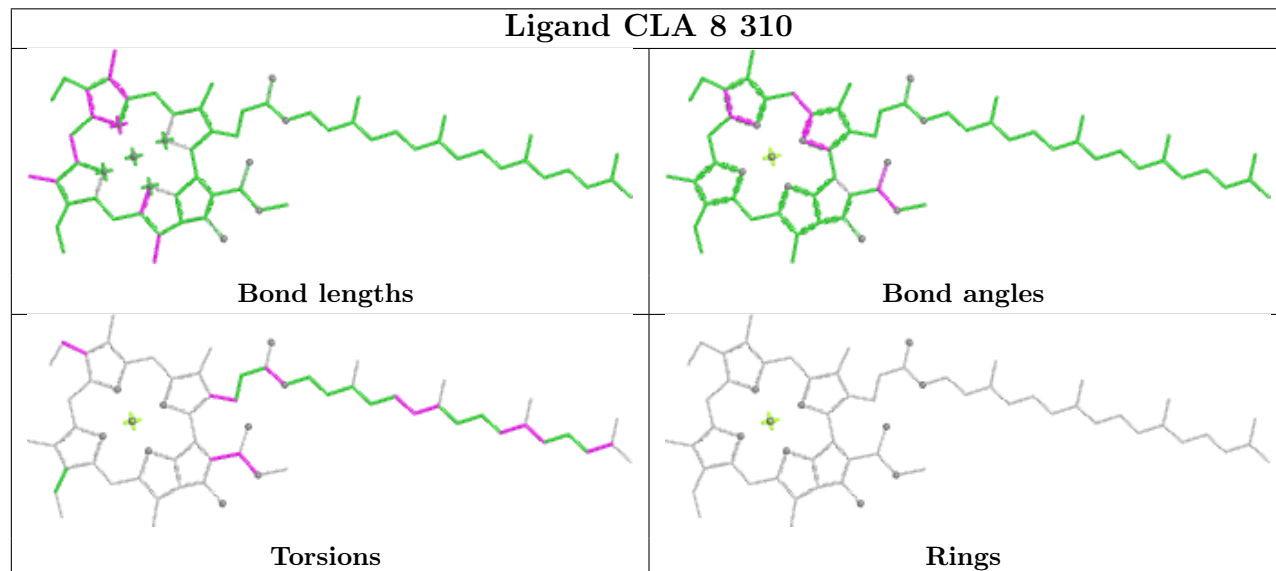
Torsions

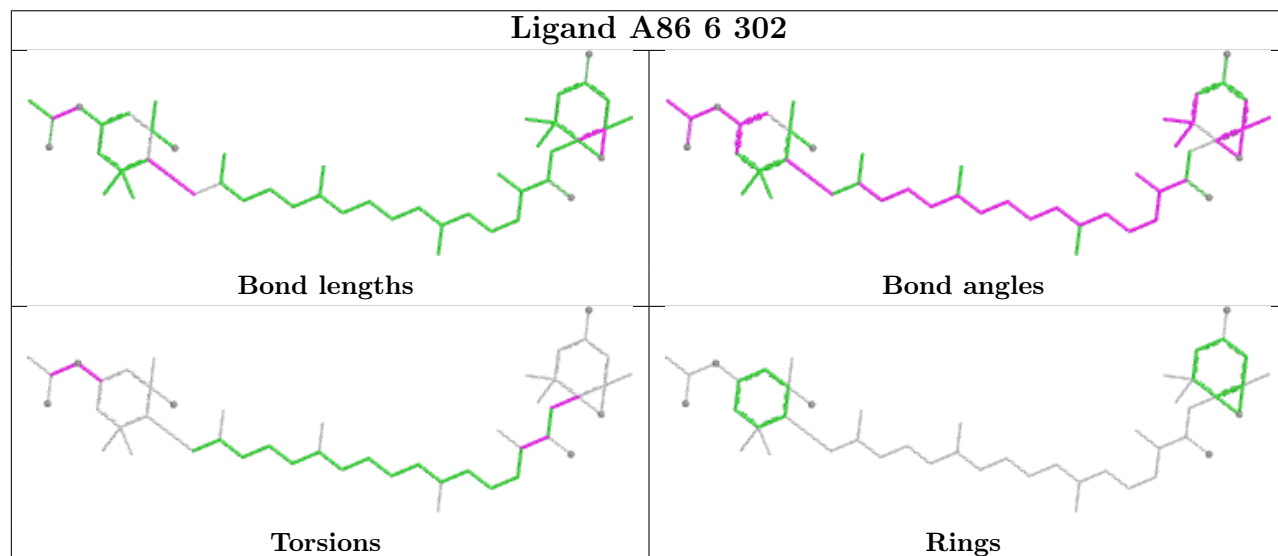
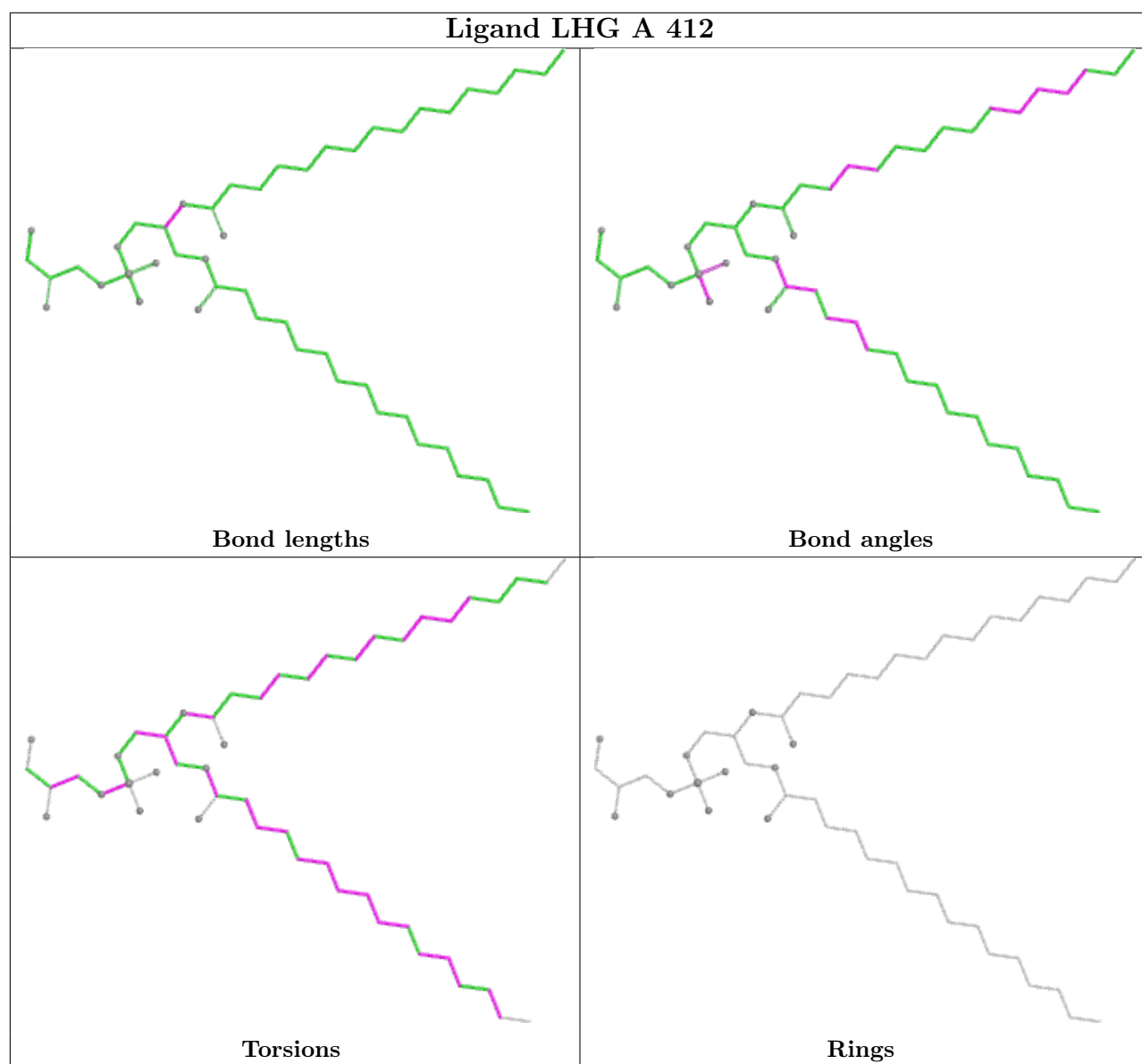


Rings

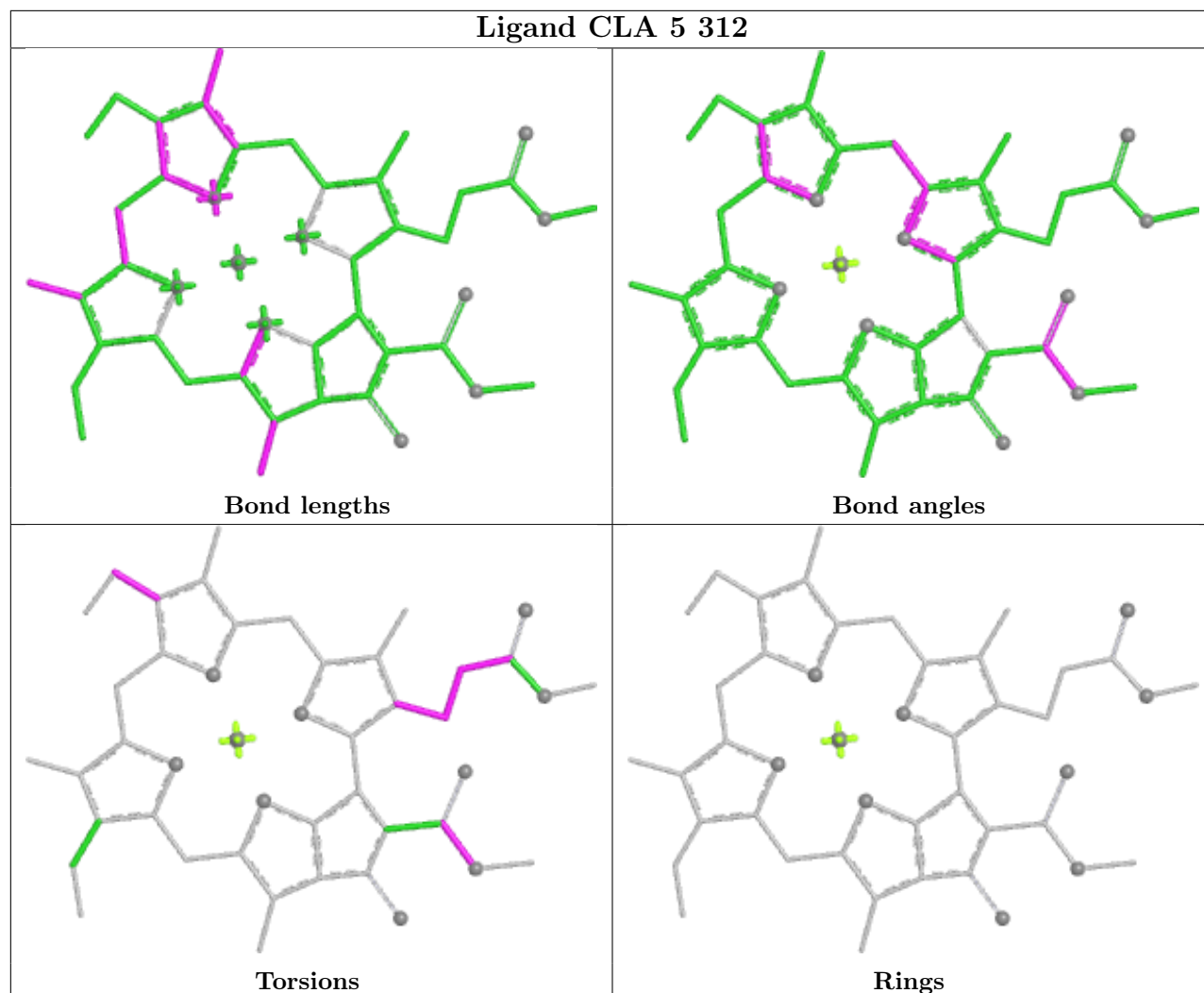




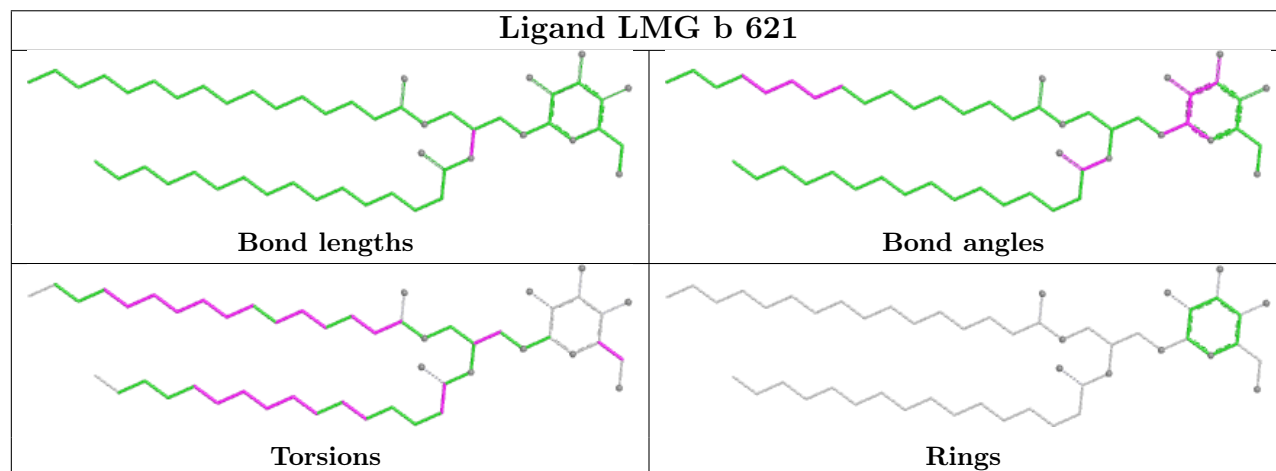
Ligand CLA 7 309**Ligand CLA 8 310**

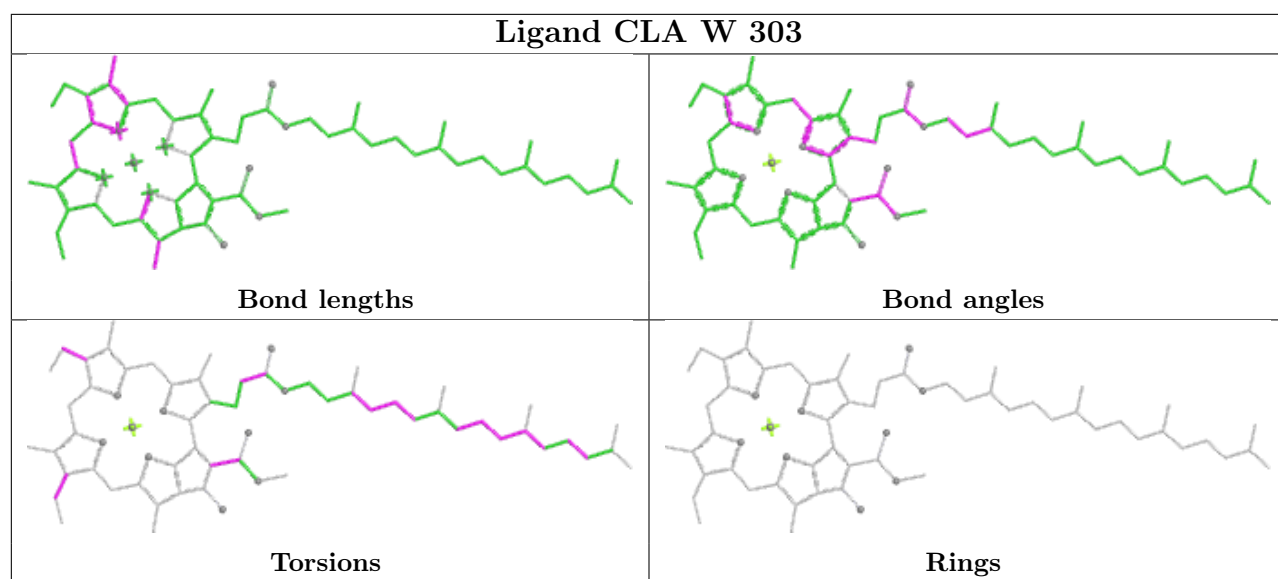


Ligand CLA 5 312

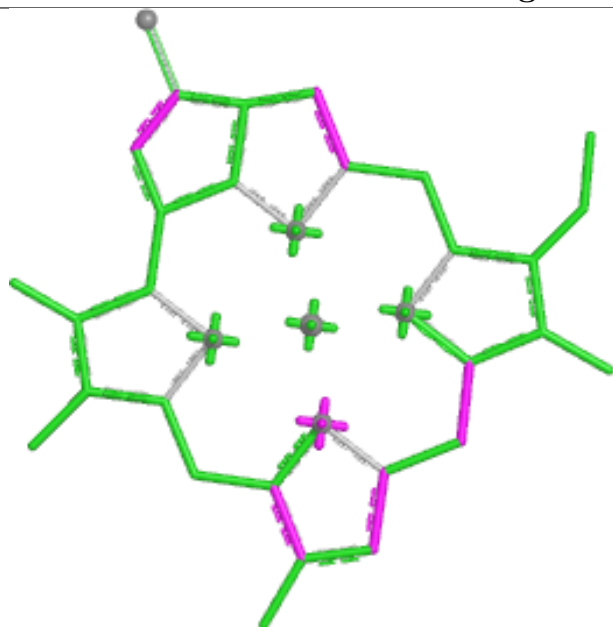


Ligand LMG b 621

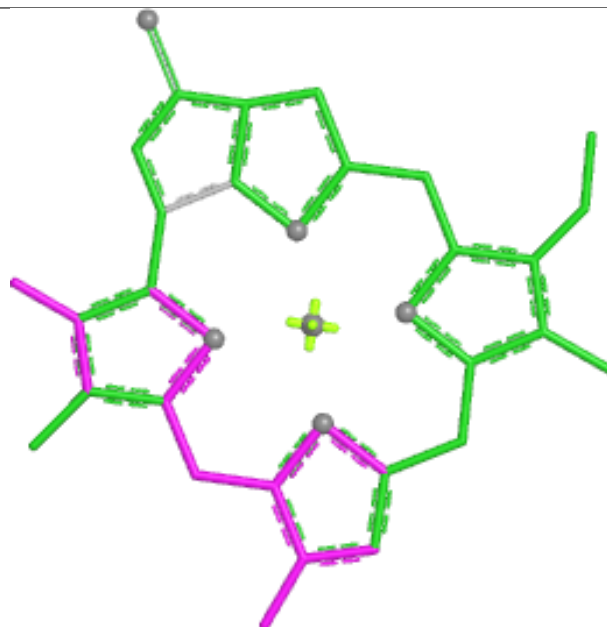




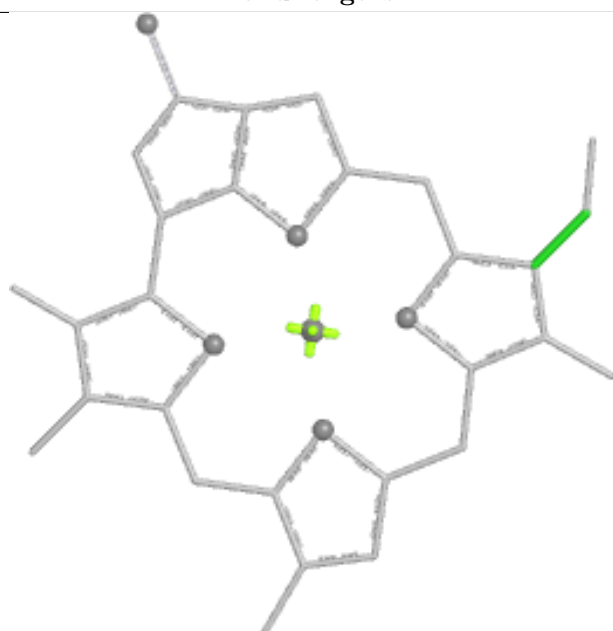
Ligand CLA 7 313



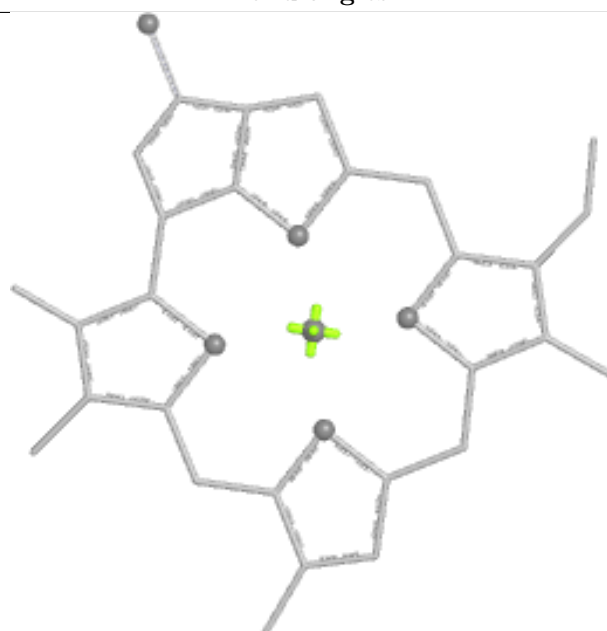
Bond lengths



Bond angles

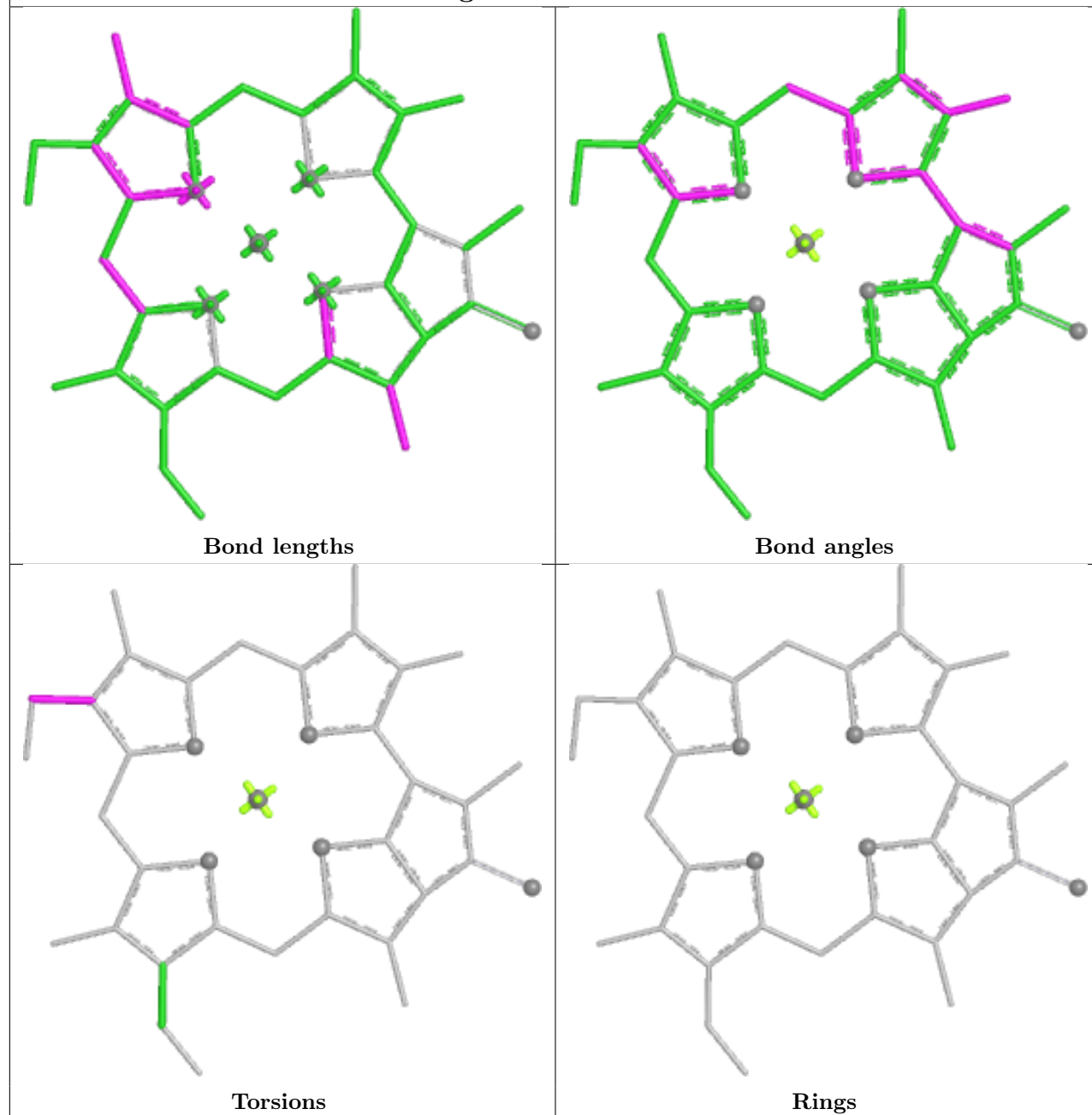


Torsions

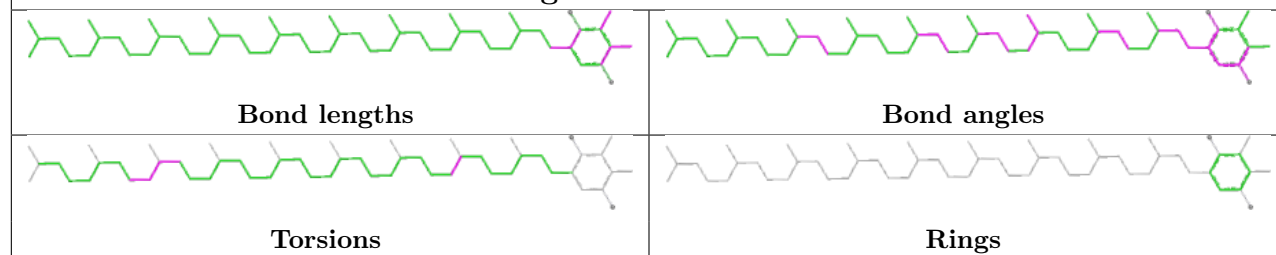


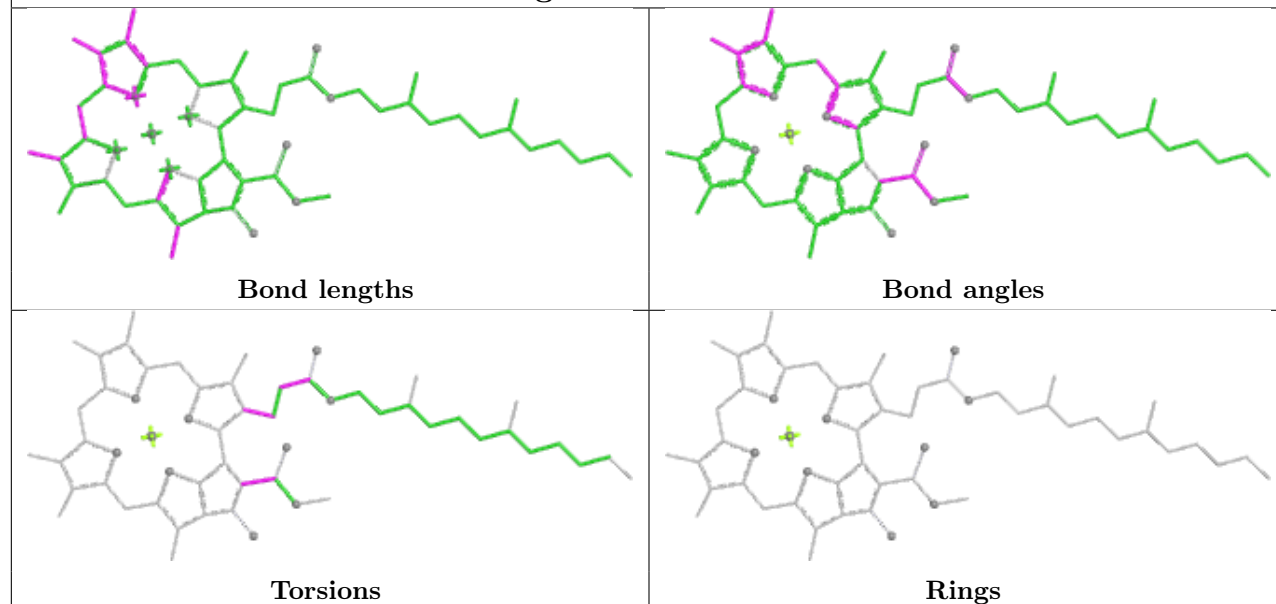
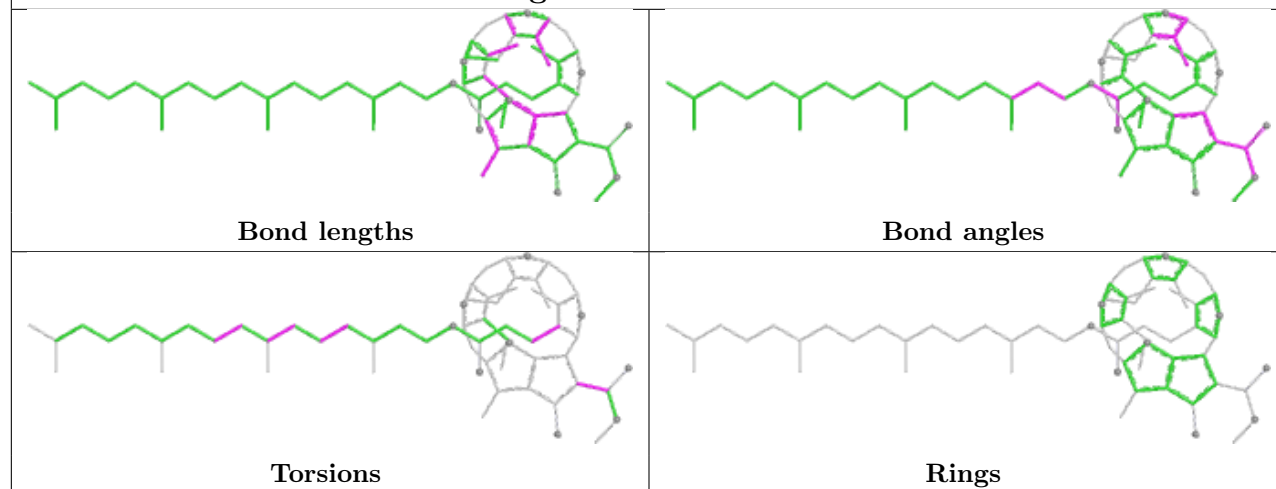
Rings

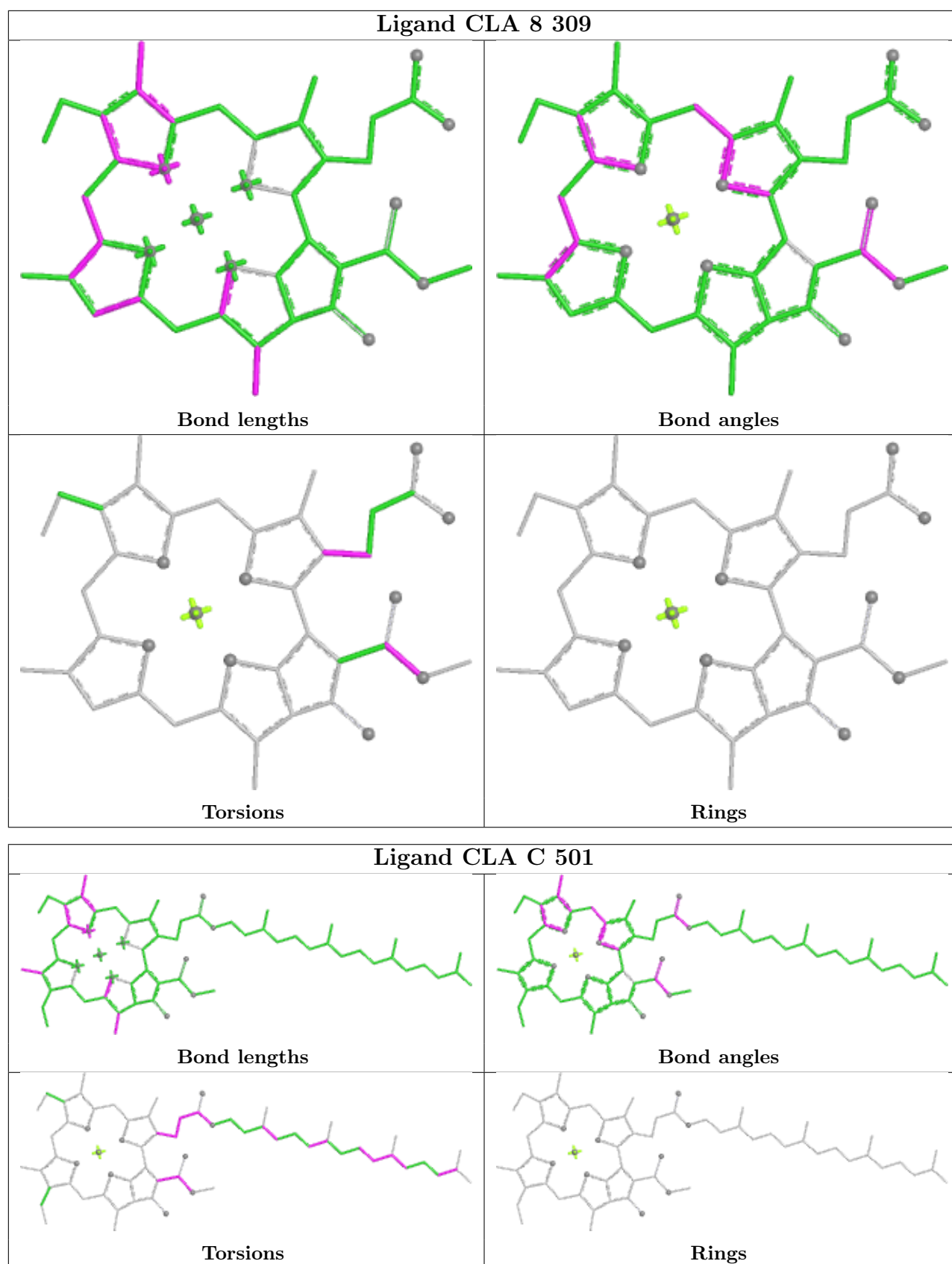
Ligand CLA 1 314



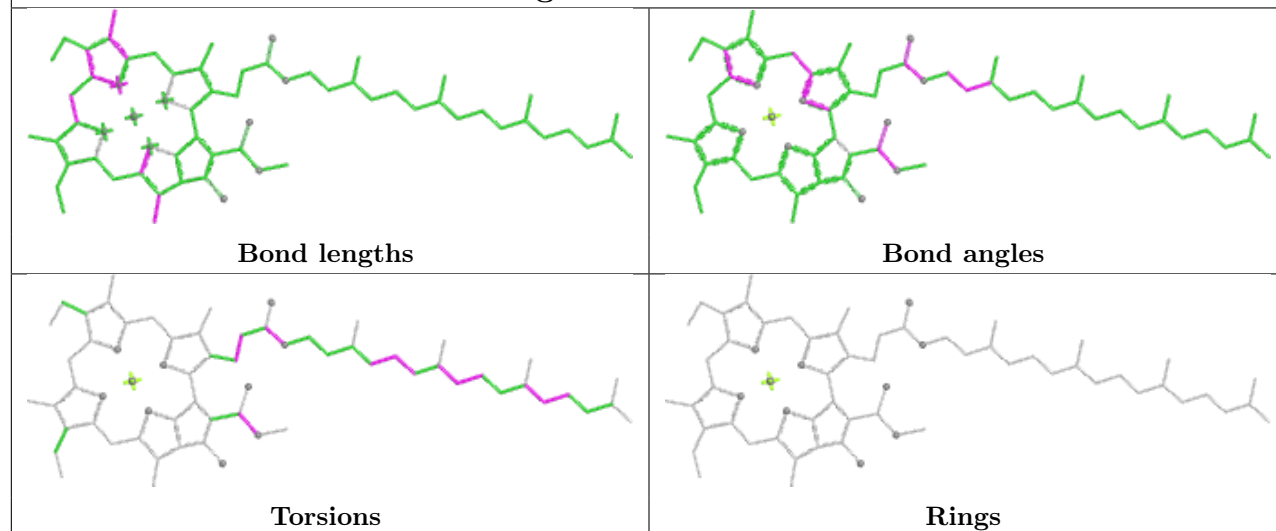
Ligand PL9 d 404



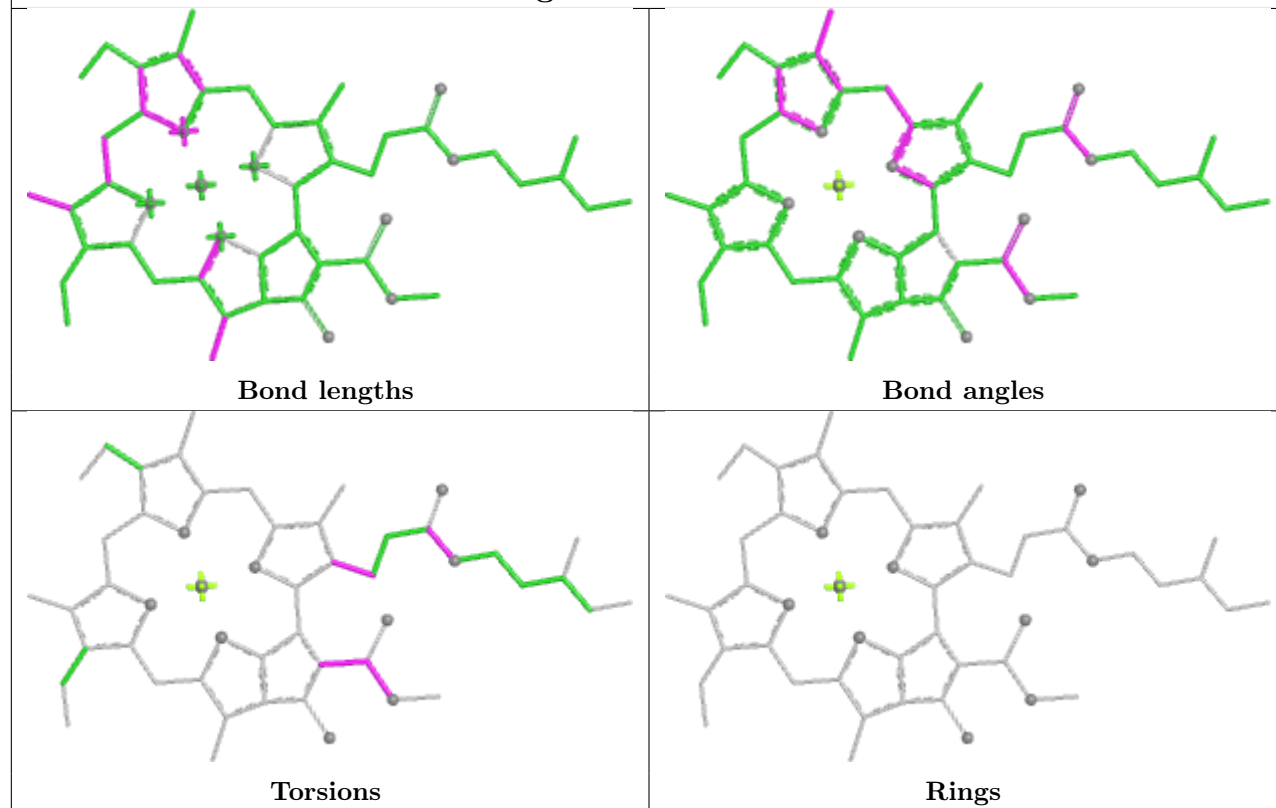
Ligand CLA d 401**Ligand PHO A 407**

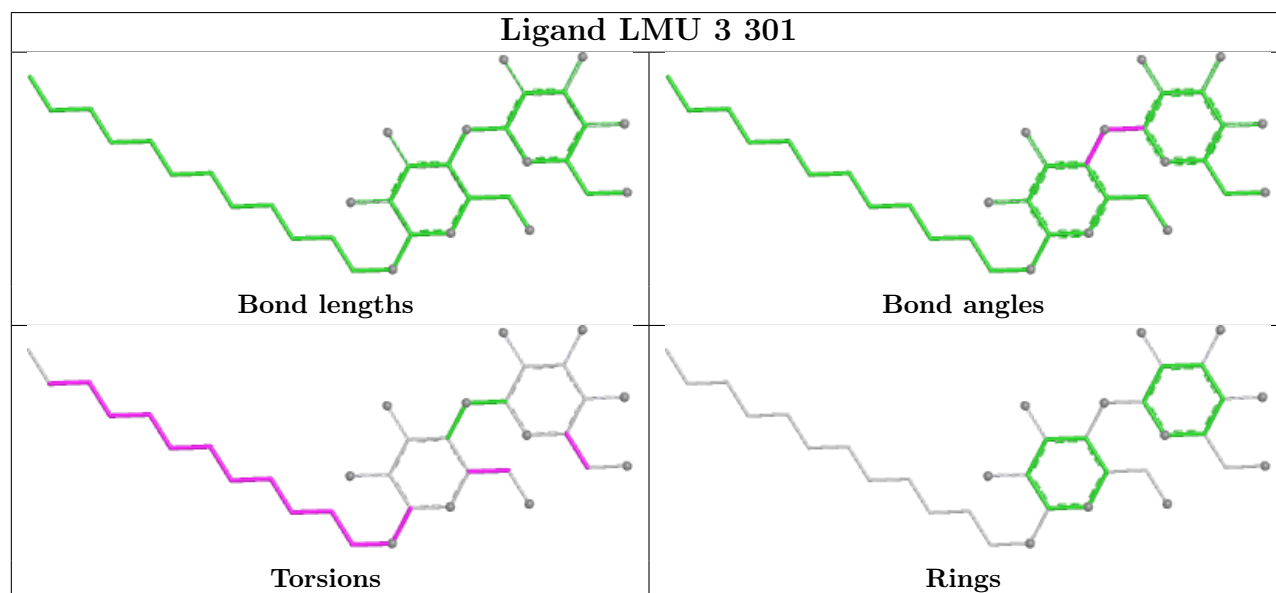
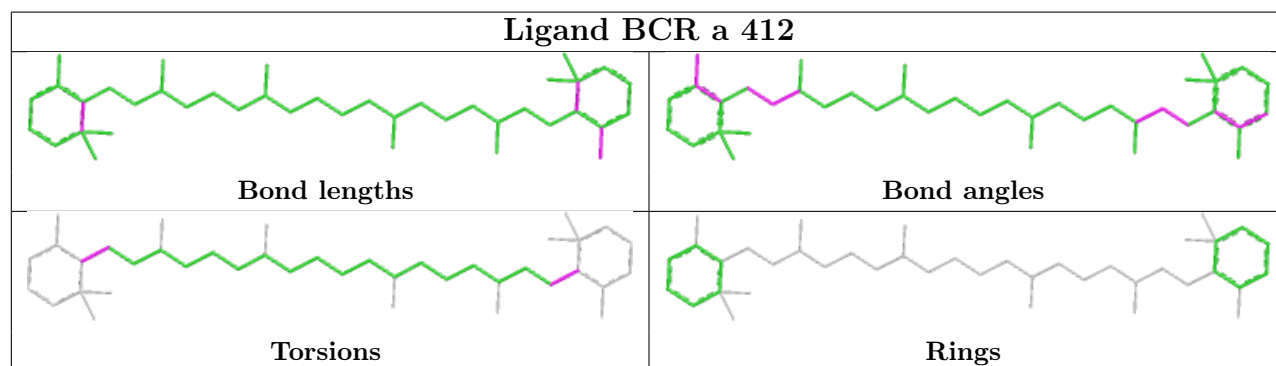
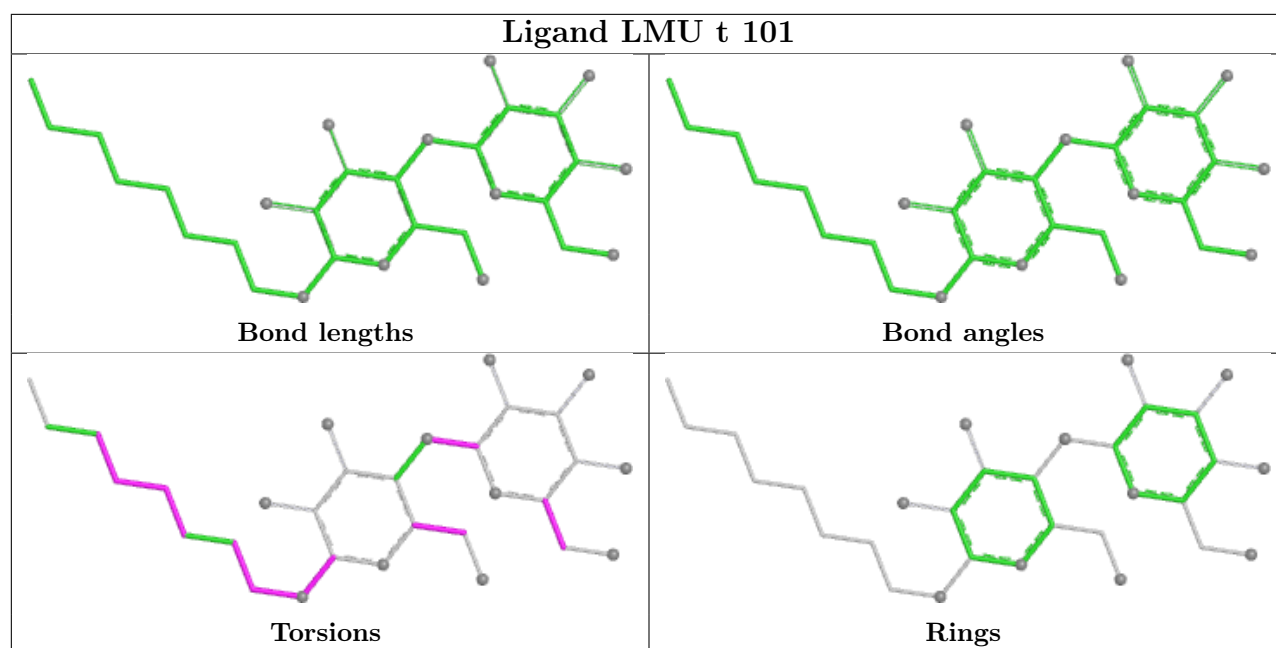


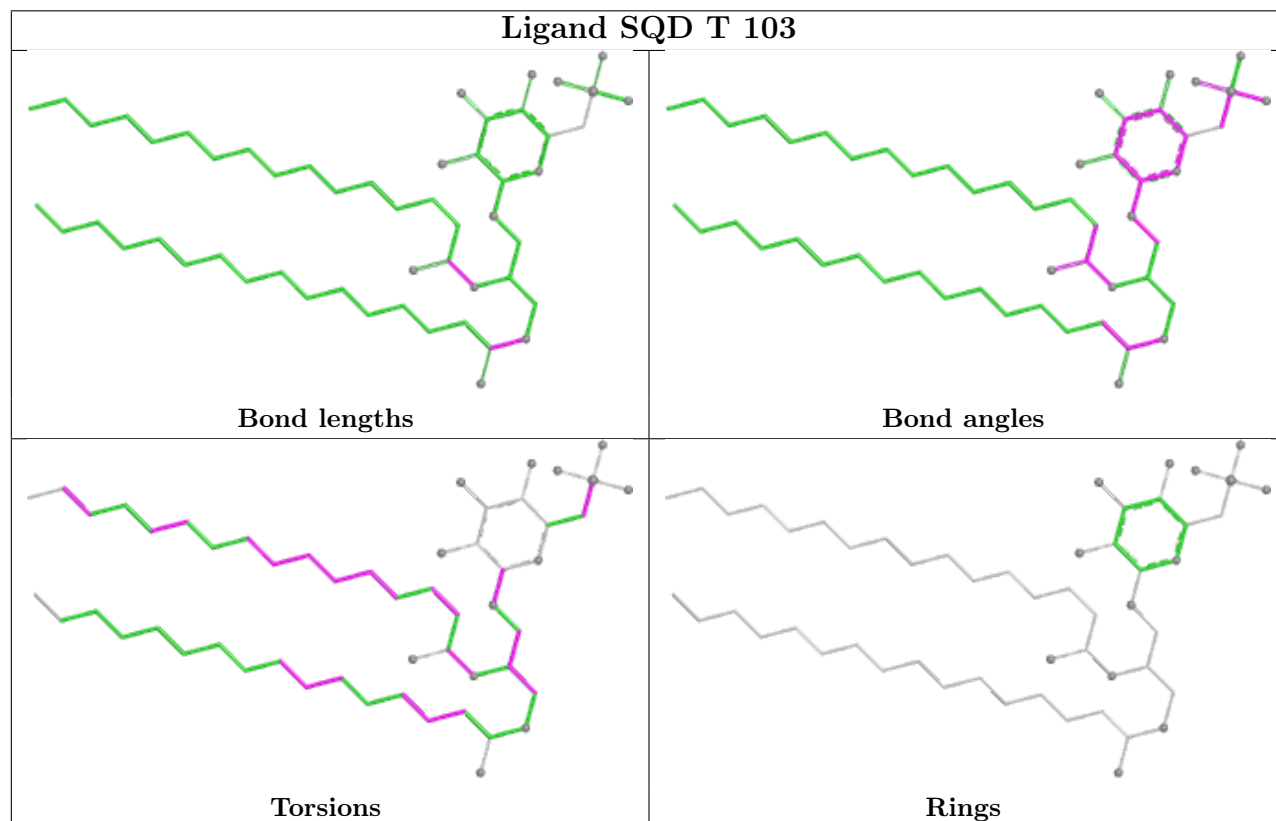
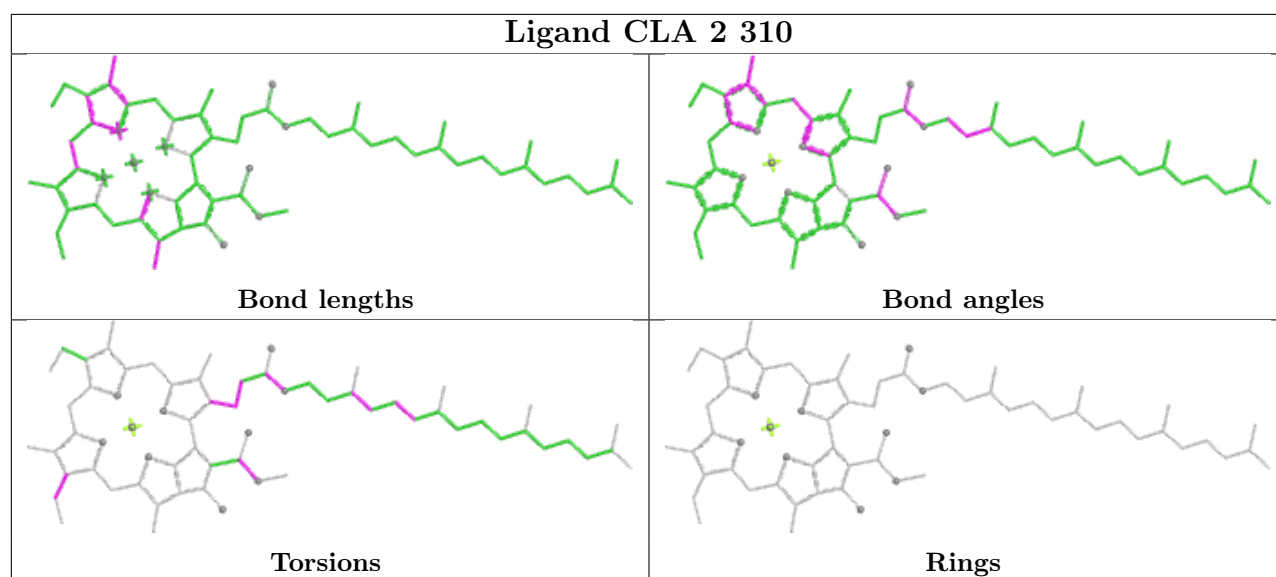
Ligand CLA 0 309



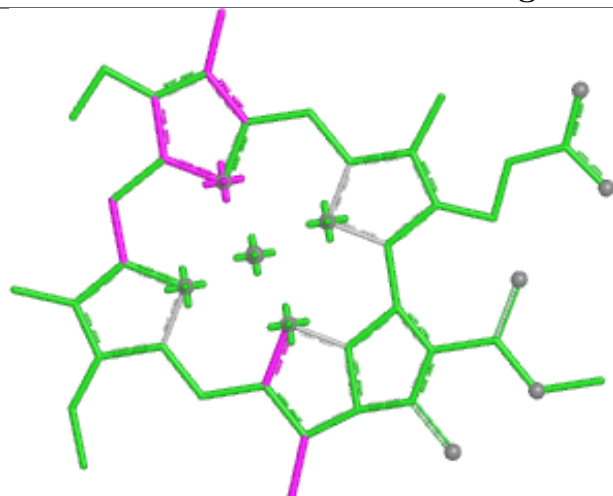
Ligand CLA 0 311



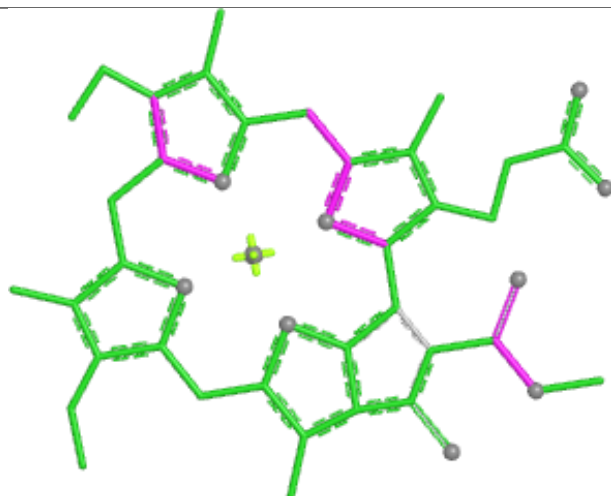




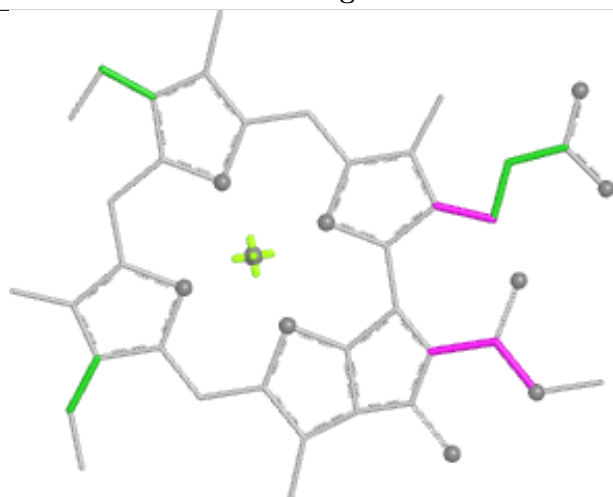
Ligand CLA 1 312



Bond lengths



Bond angles

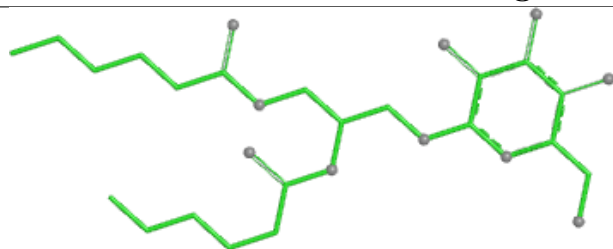


Torsions

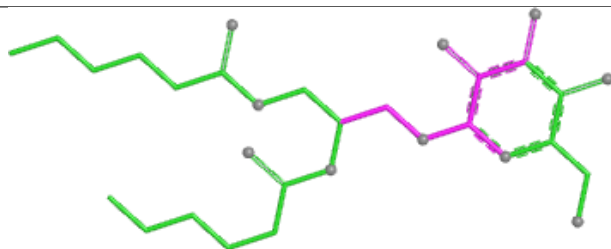


Rings

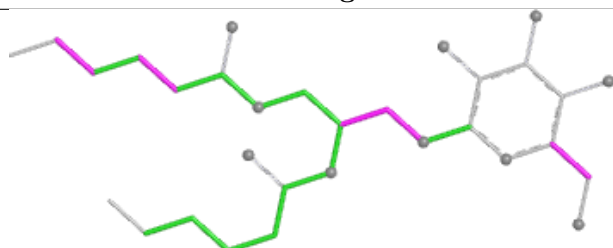
Ligand LMG 3 316



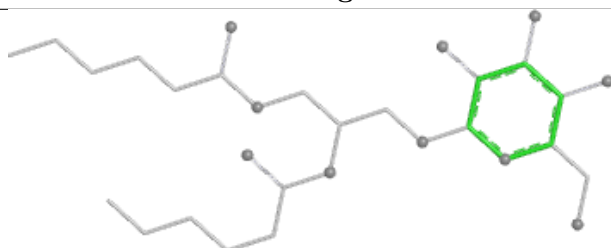
Bond lengths



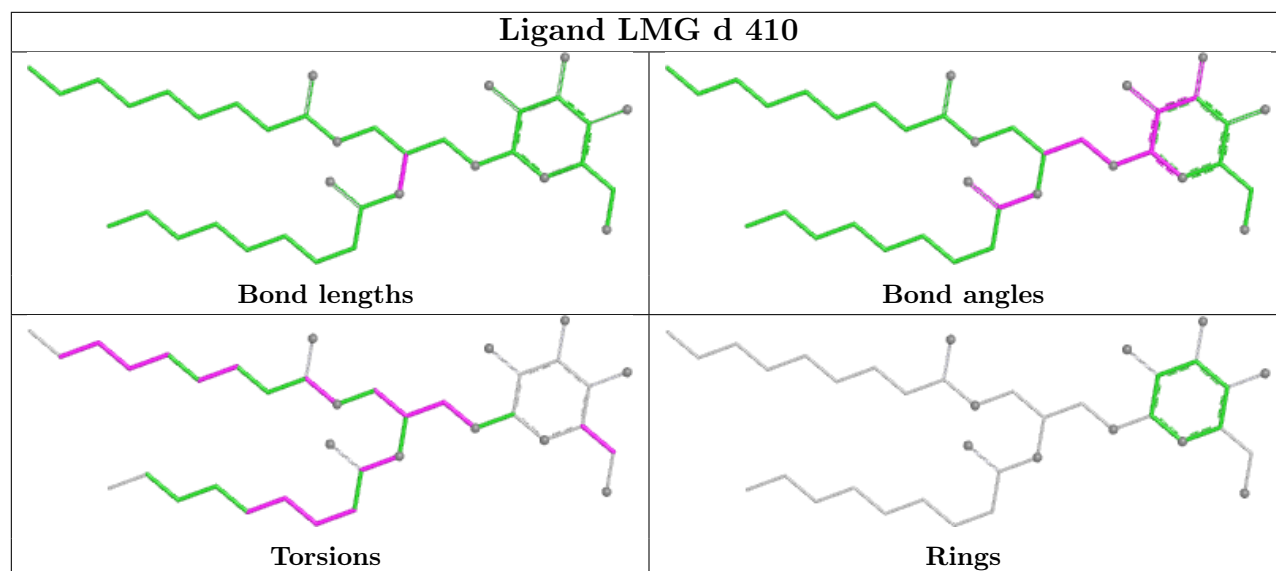
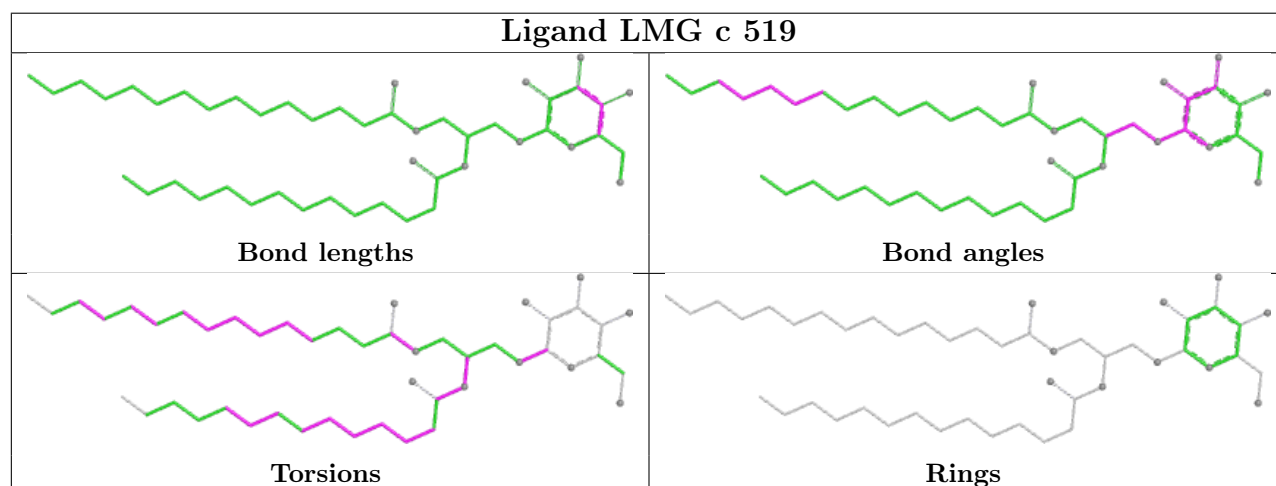
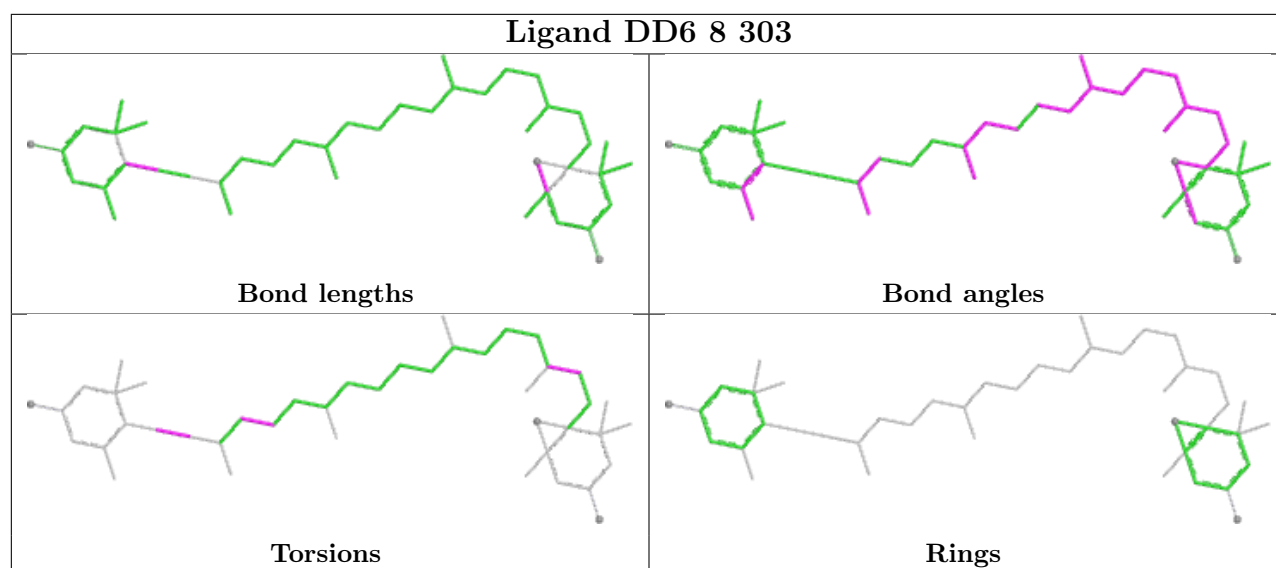
Bond angles

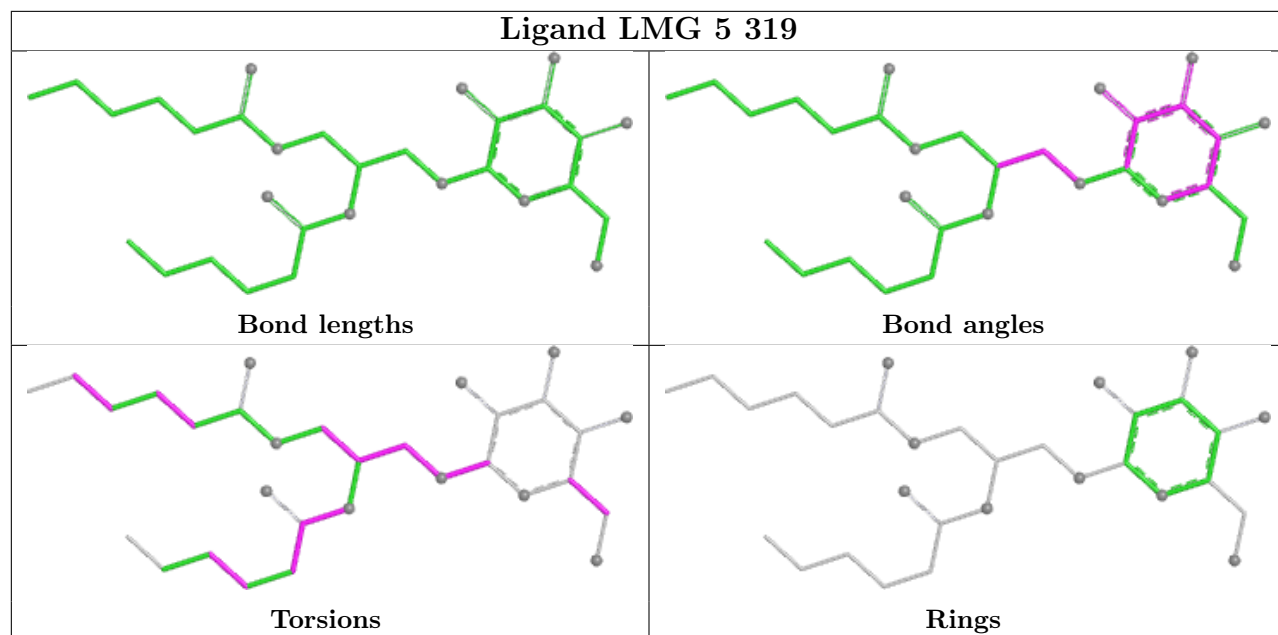


Torsions

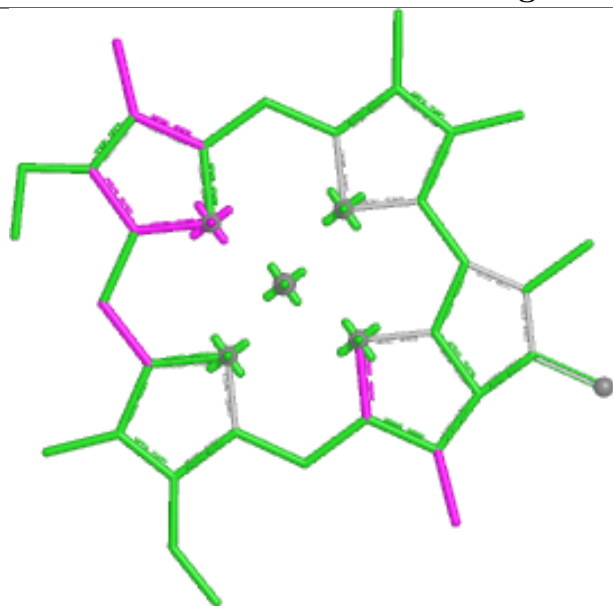


Rings

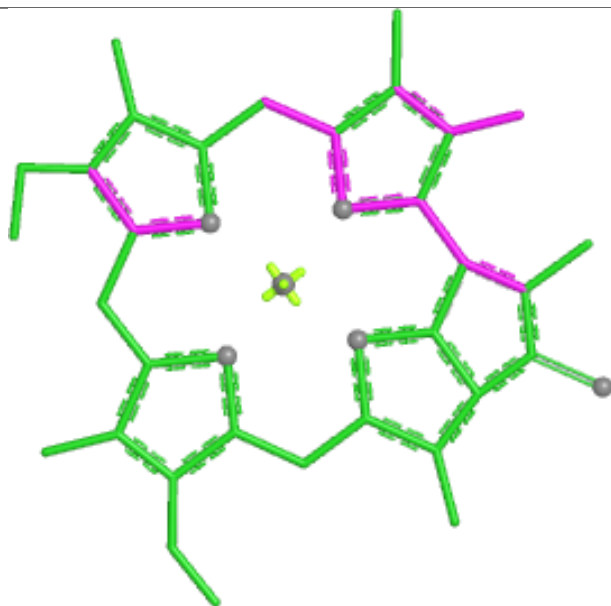




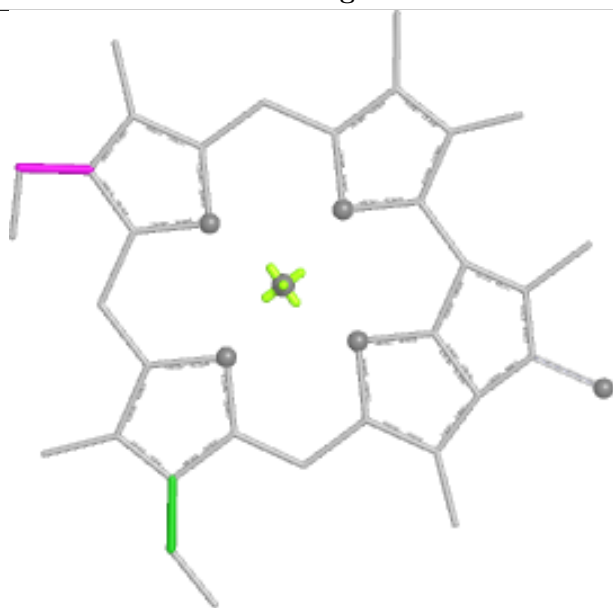
Ligand CLA 1 316



Bond lengths



Bond angles

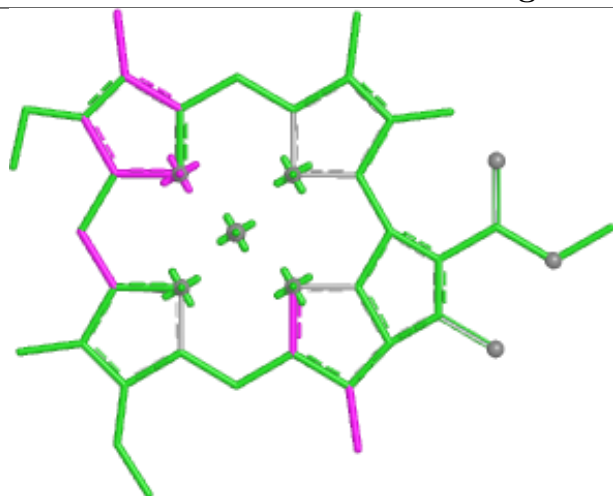


Torsions

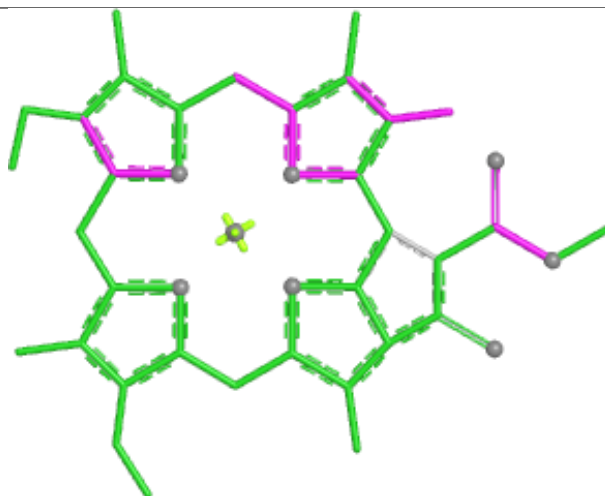


Rings

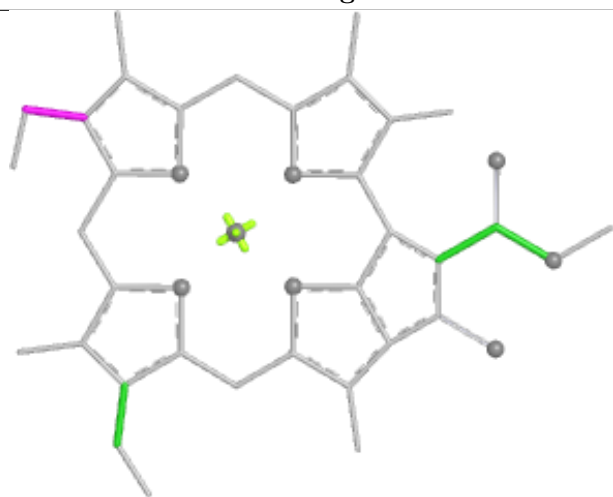
Ligand CLA 9 305



Bond lengths



Bond angles

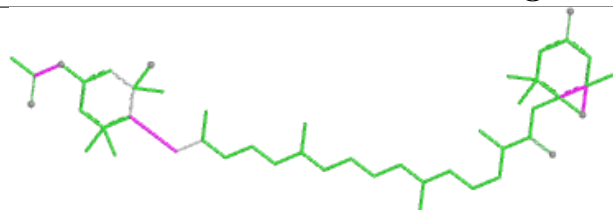


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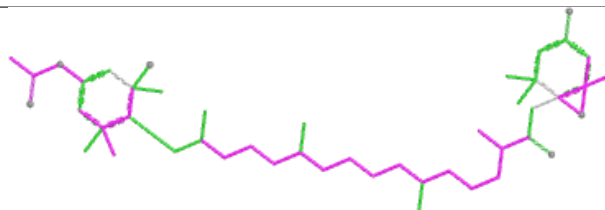


Rings

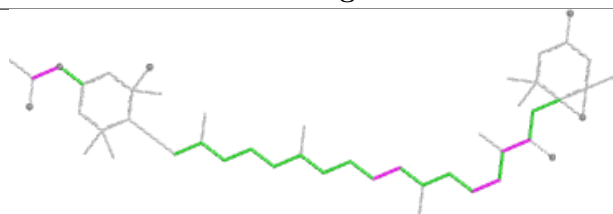
Ligand A86 8 301



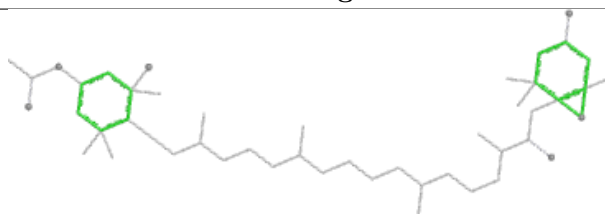
Bond lengths



Bond angles

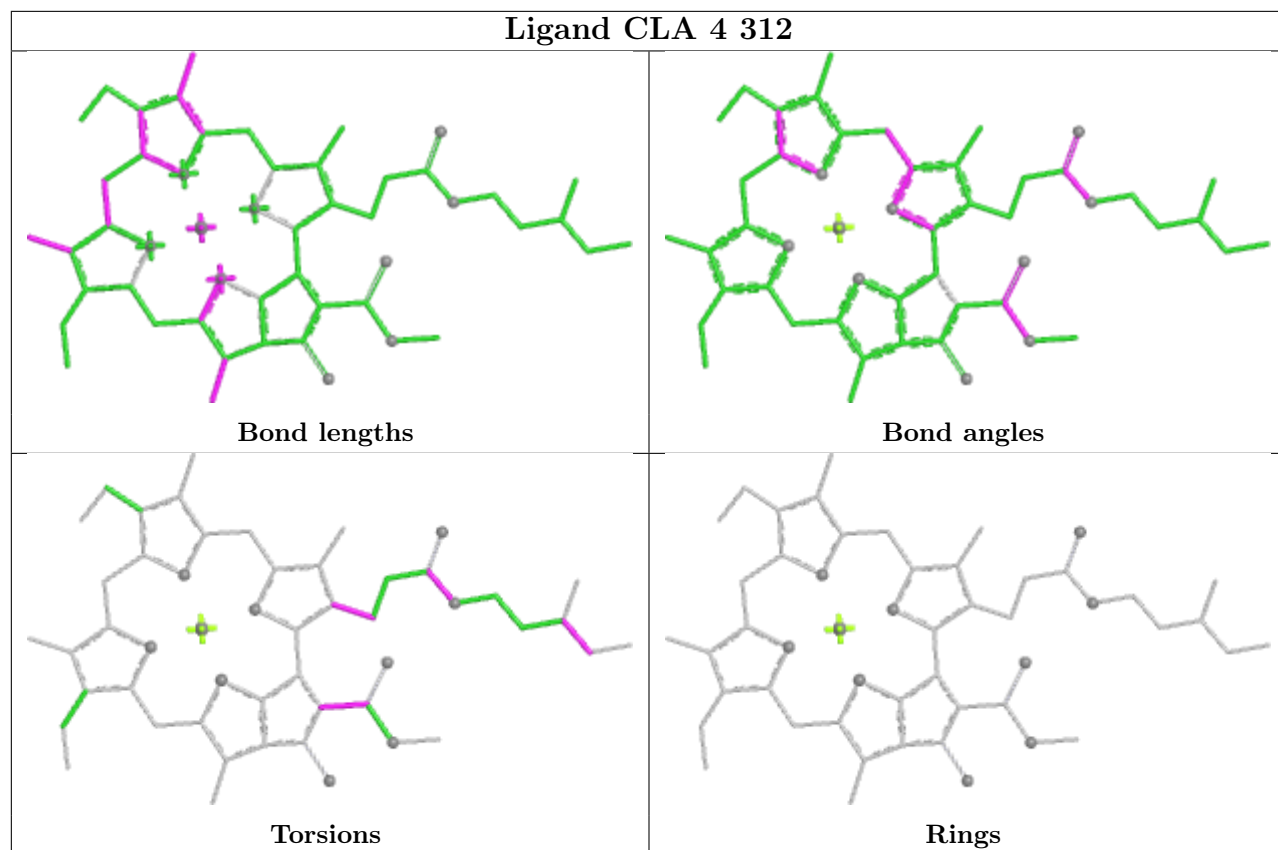


Torsions

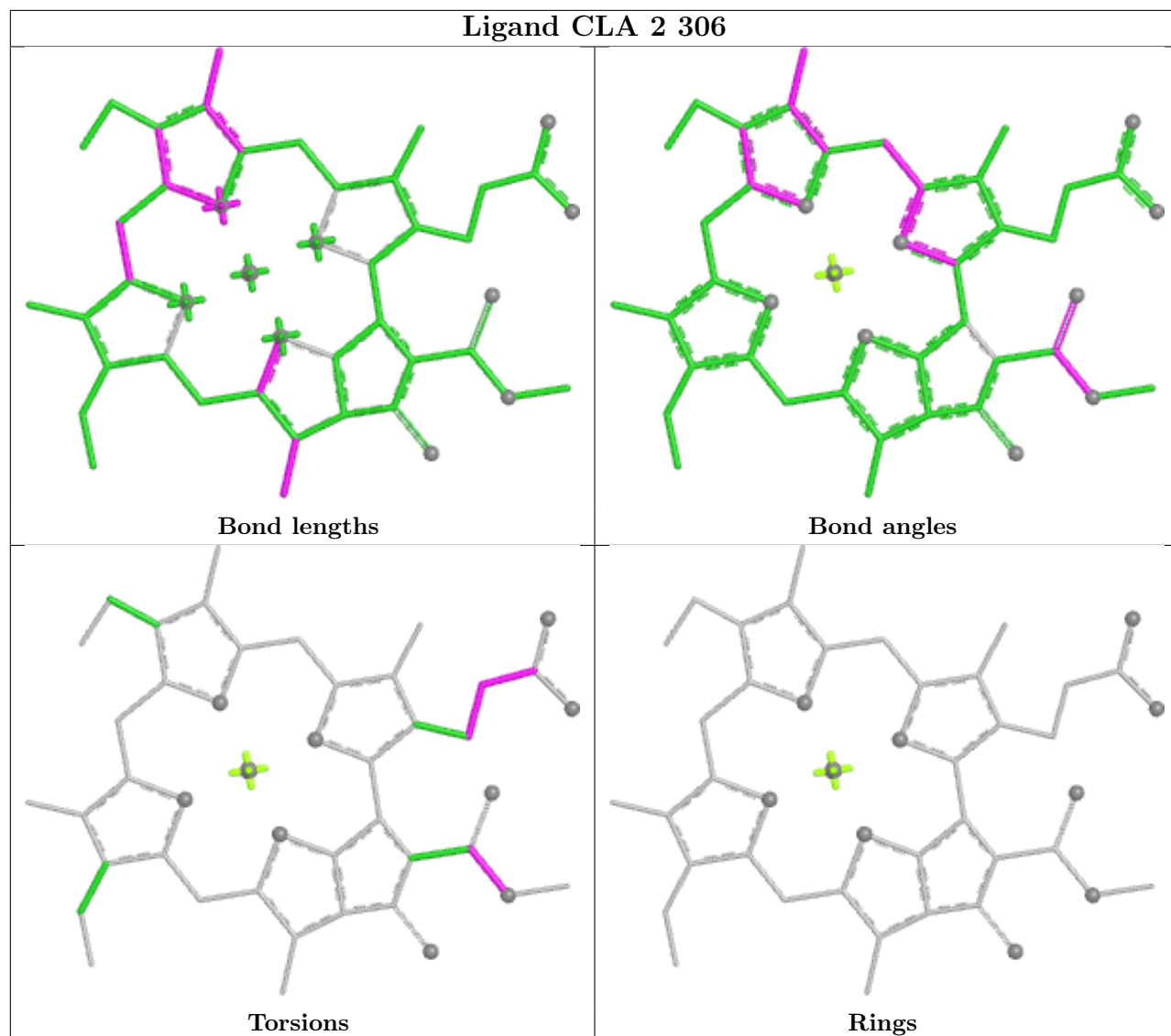


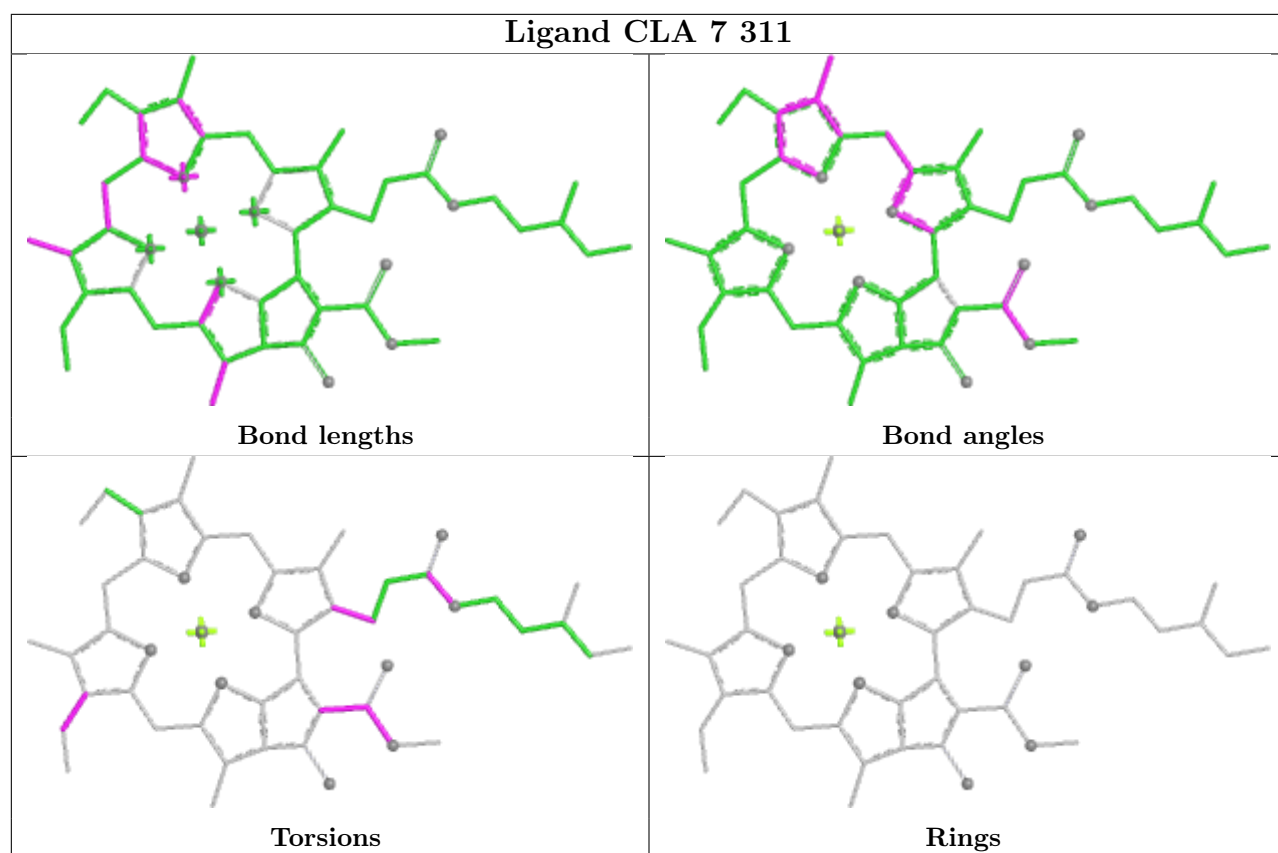
Rings

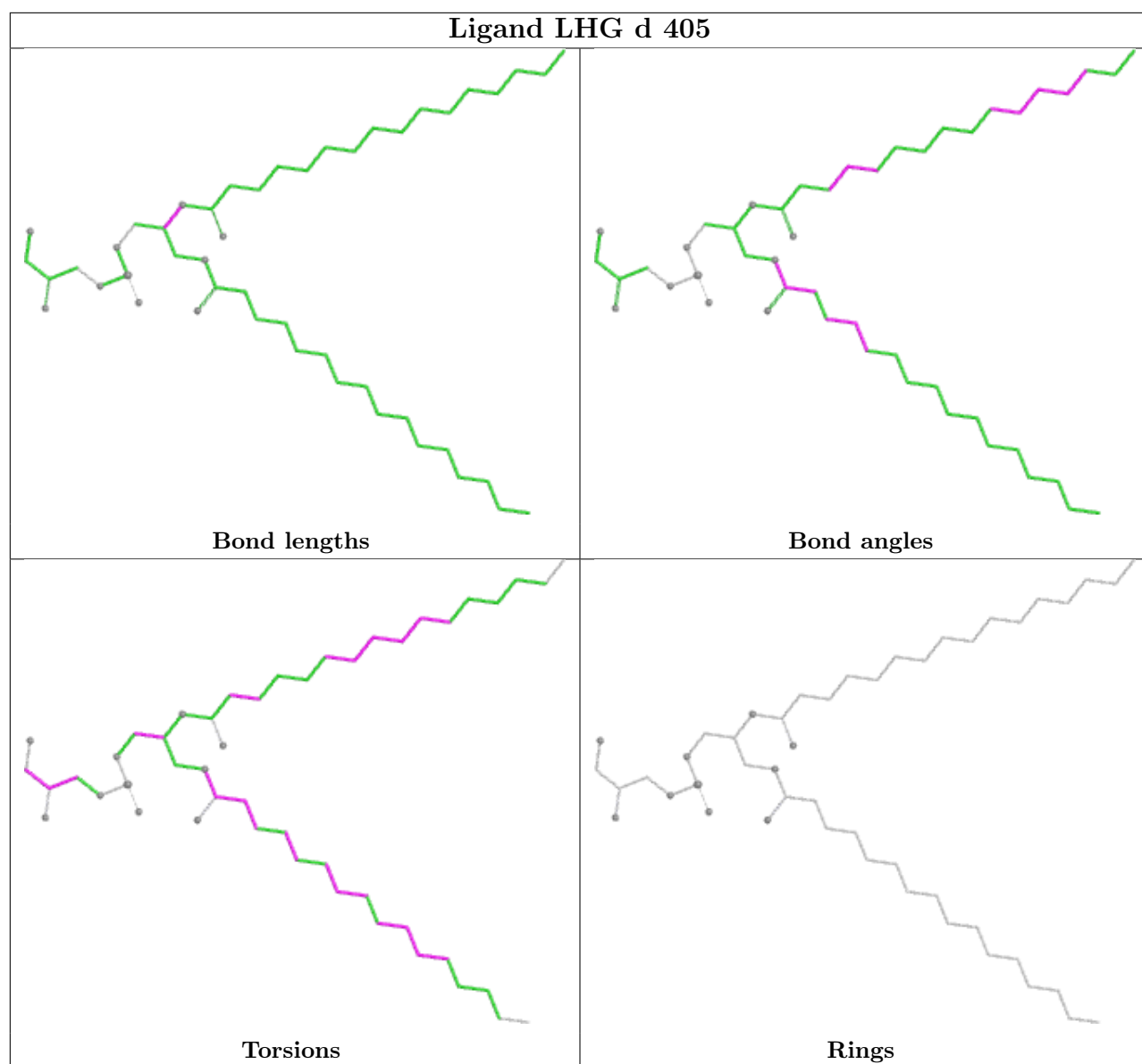
Ligand CLA 4 312



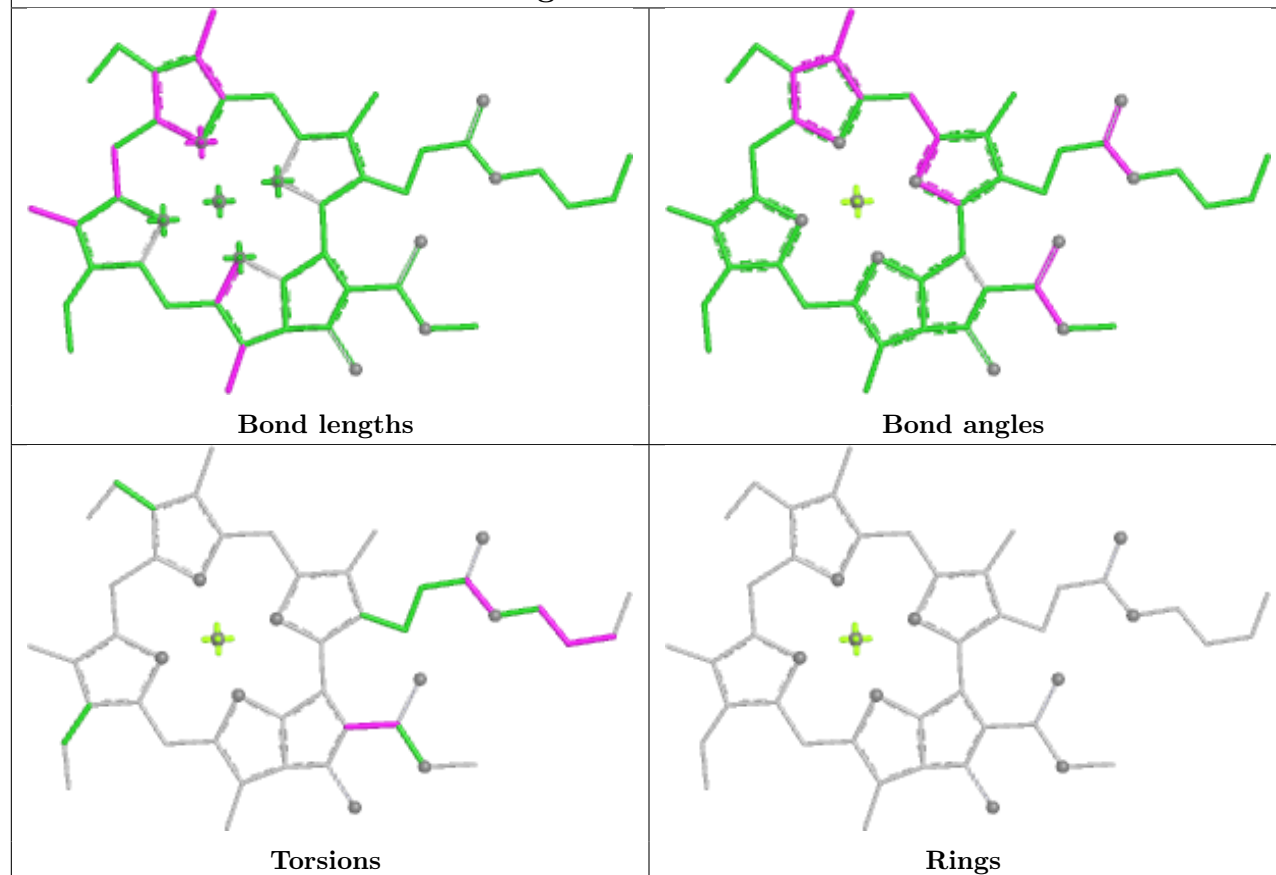
Ligand CLA 2 306



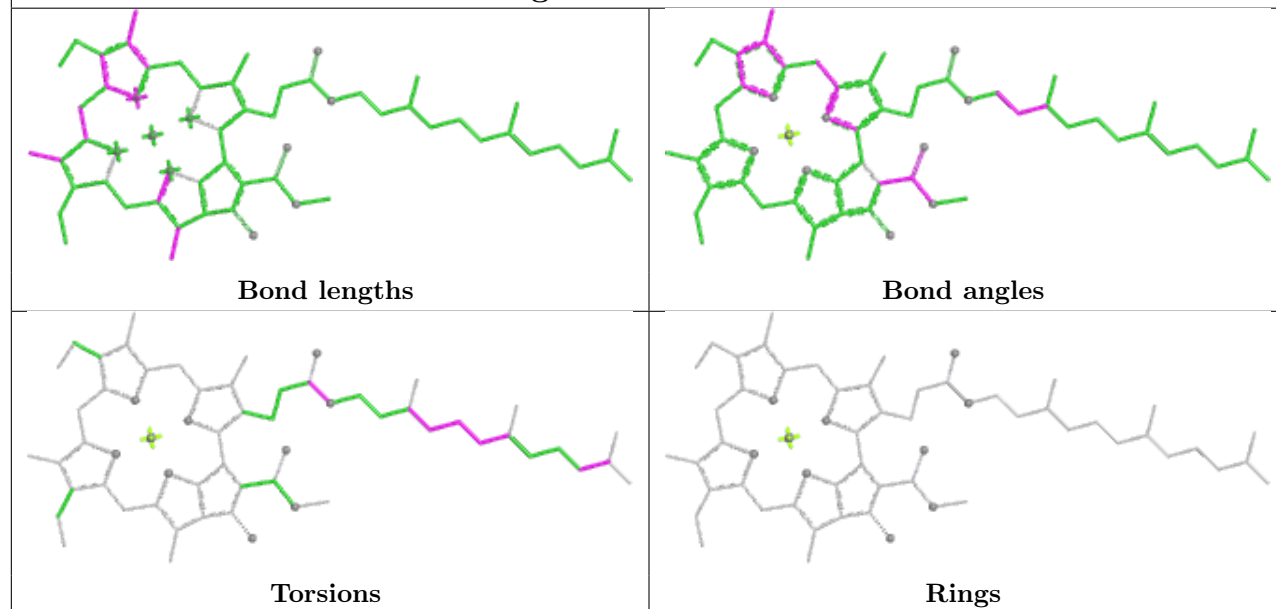




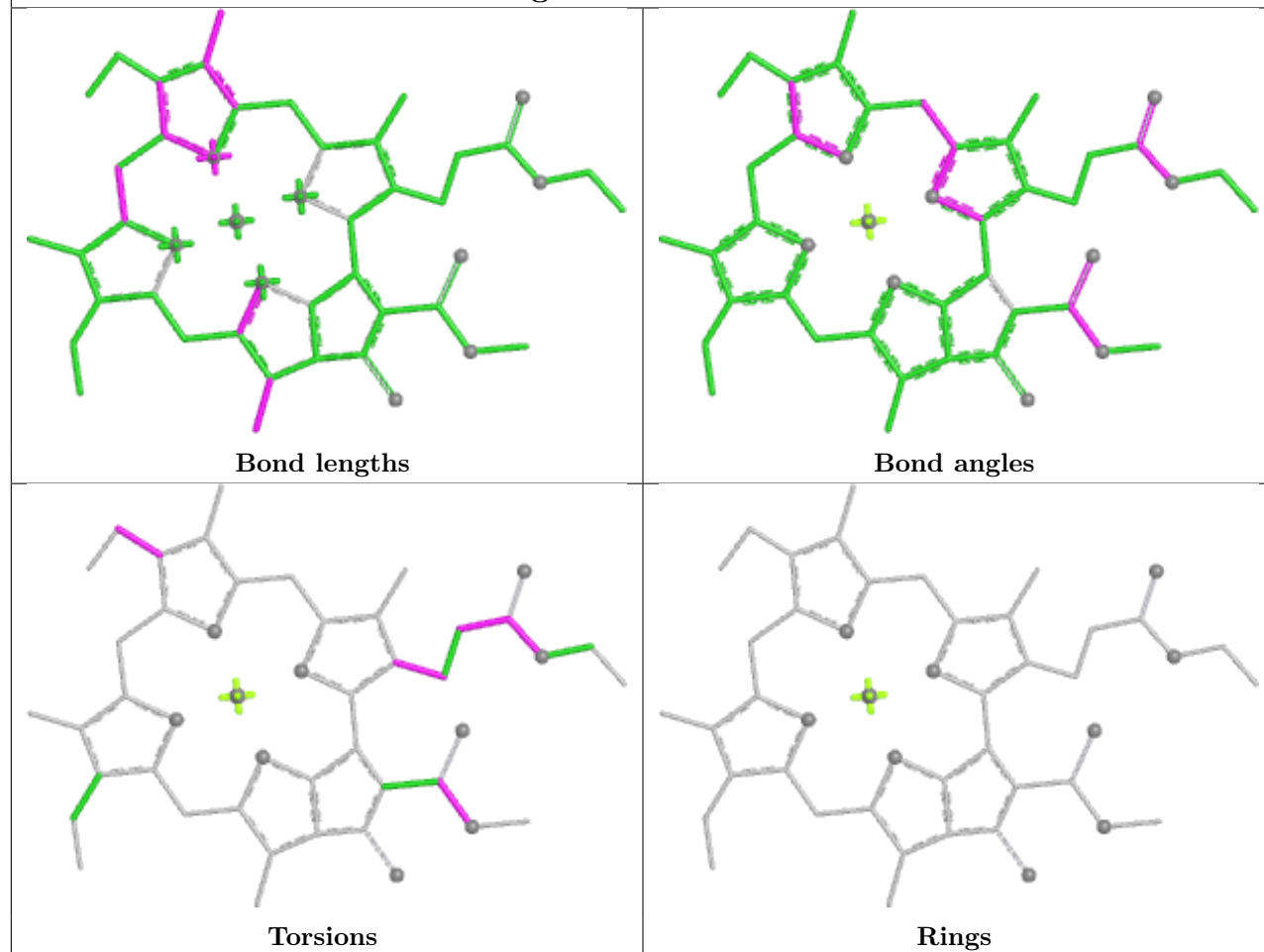
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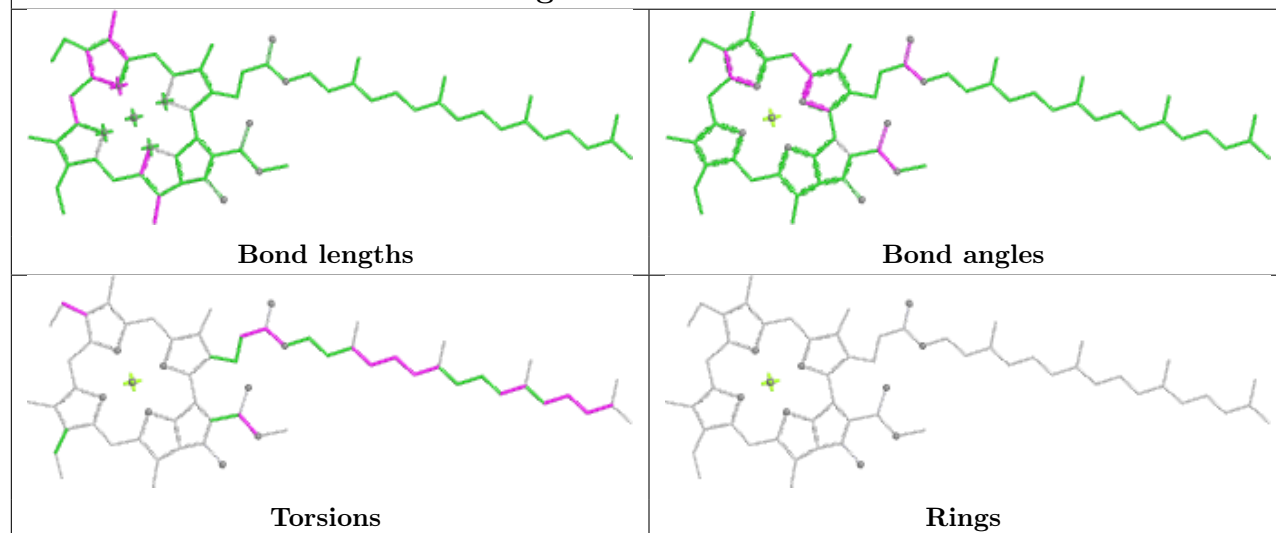
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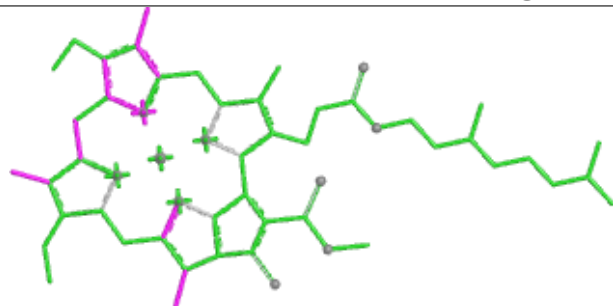


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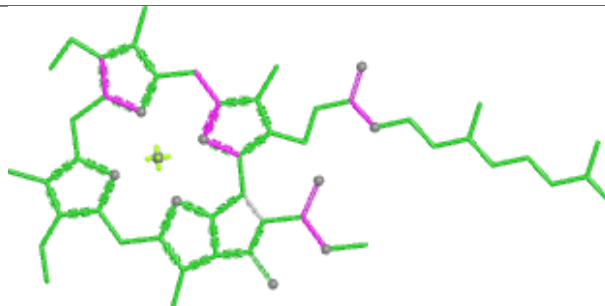


Ligand CLA 0 312

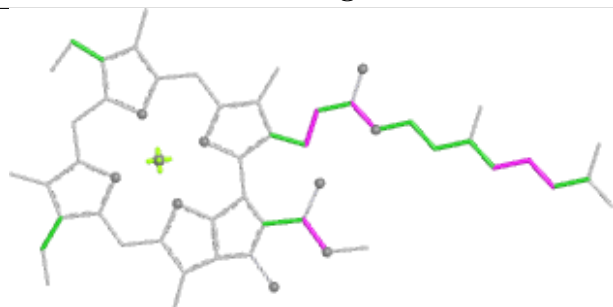


Ligand CLA 9 317

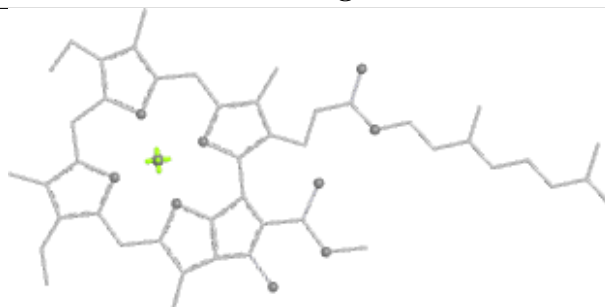
Bond lengths



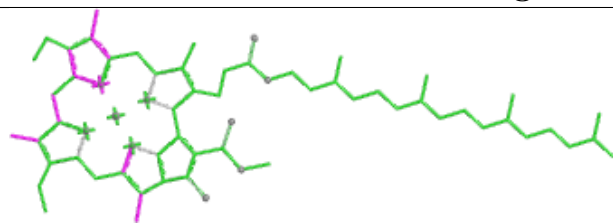
Bond angles



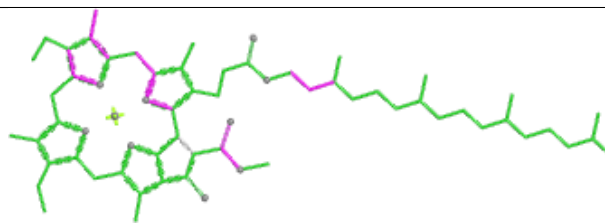
Torsions



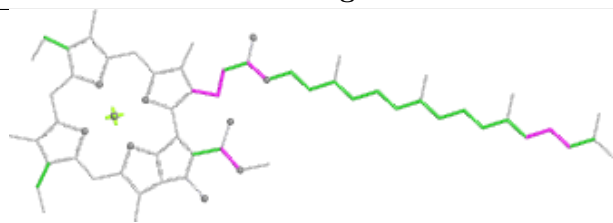
Rings

Ligand CLA A 404

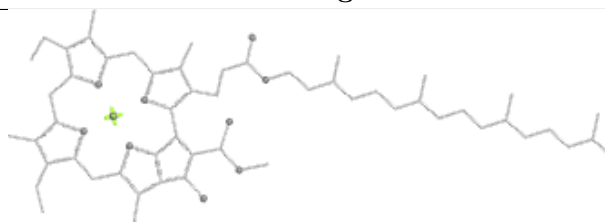
Bond lengths



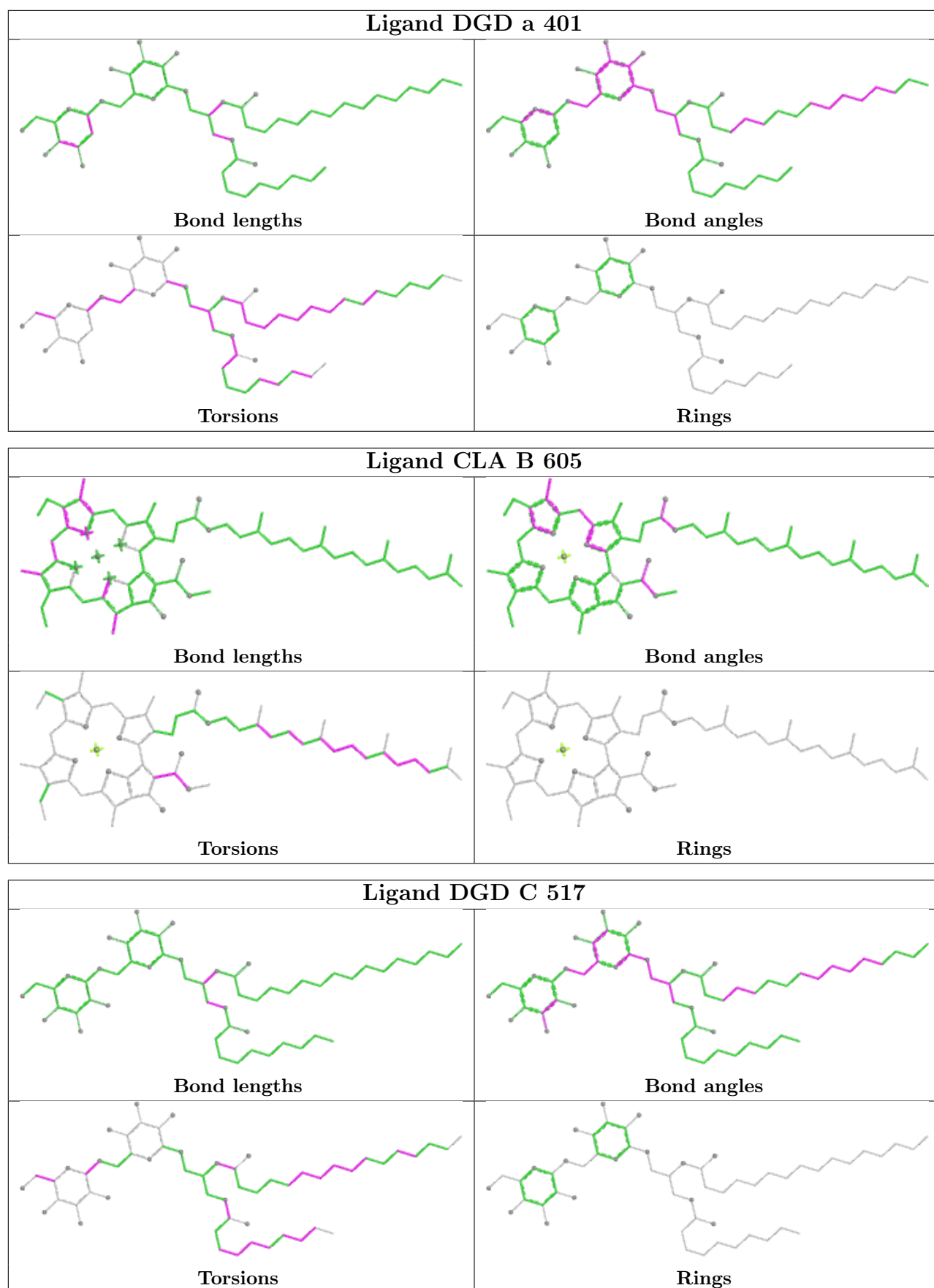
Bond angles

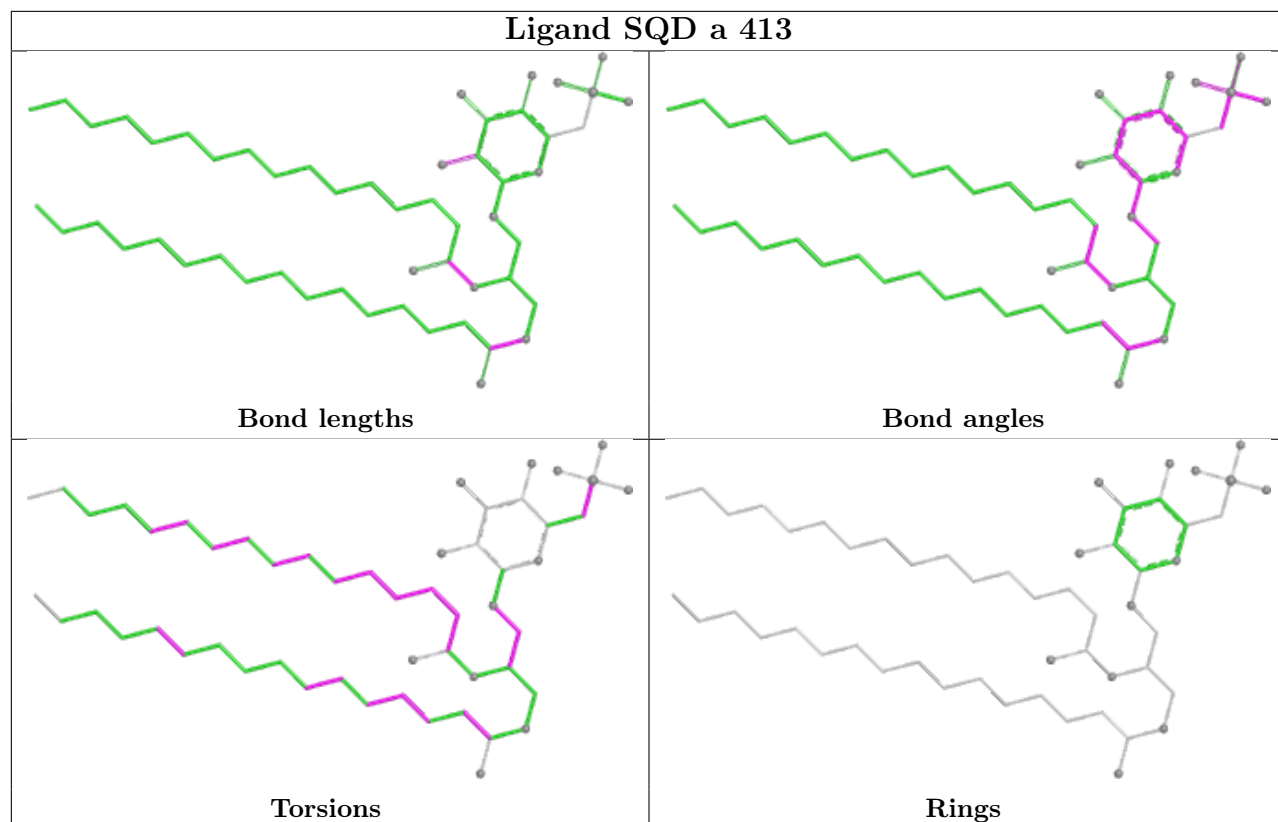


Torsions

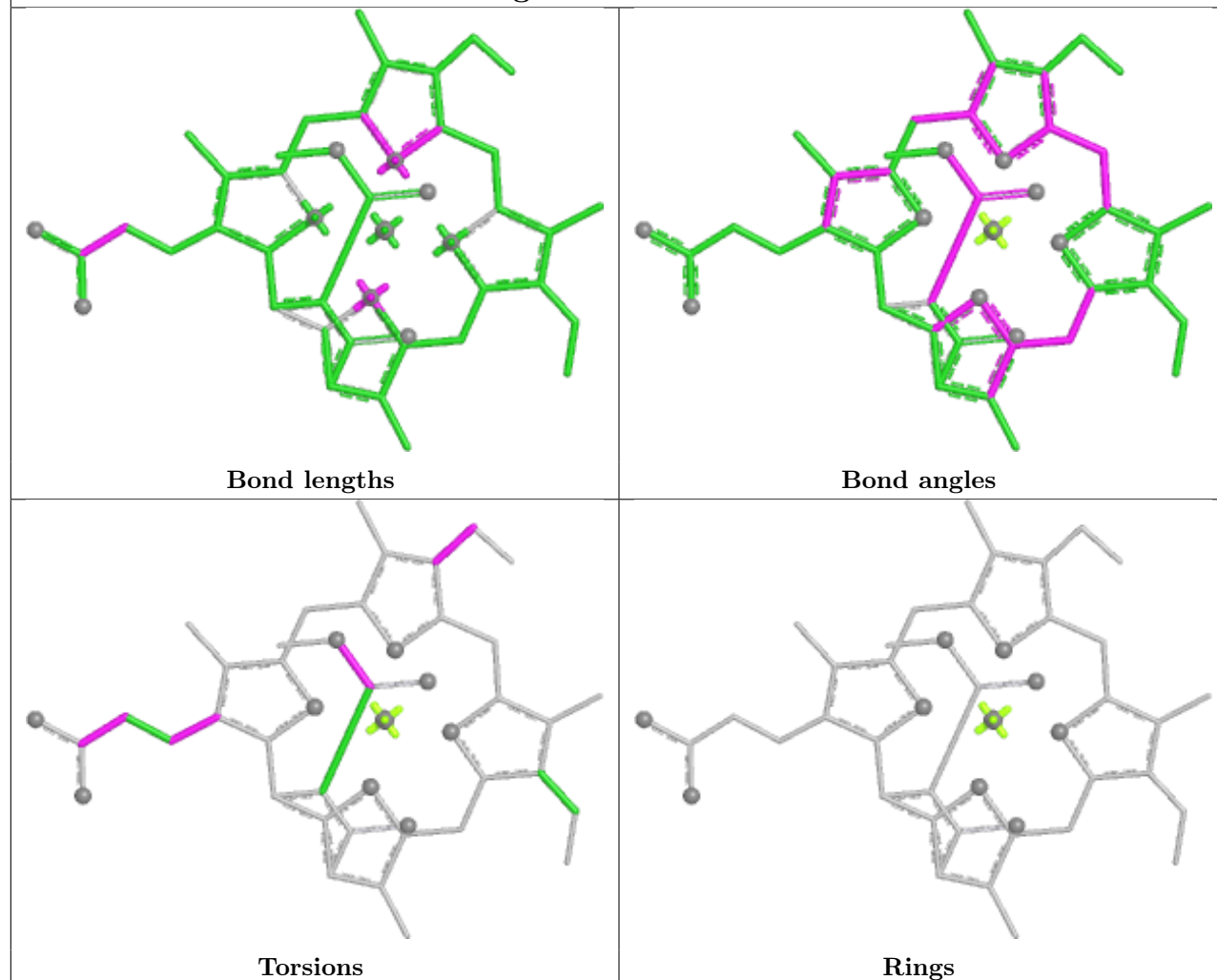


Rings

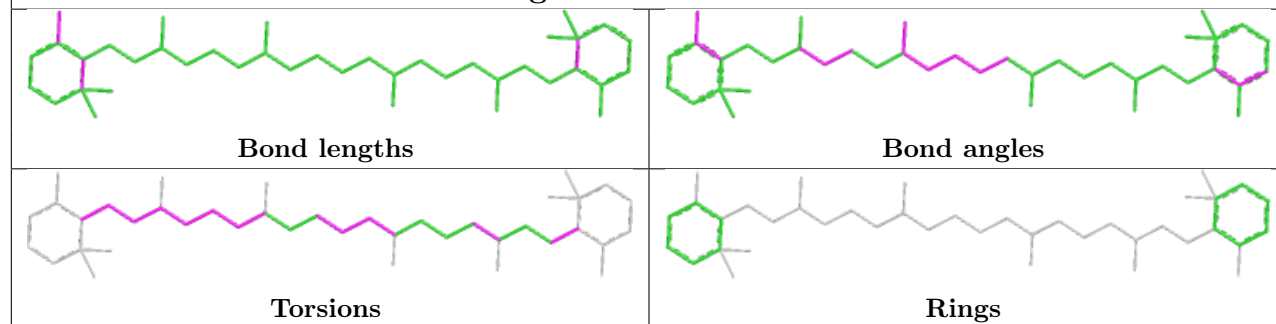




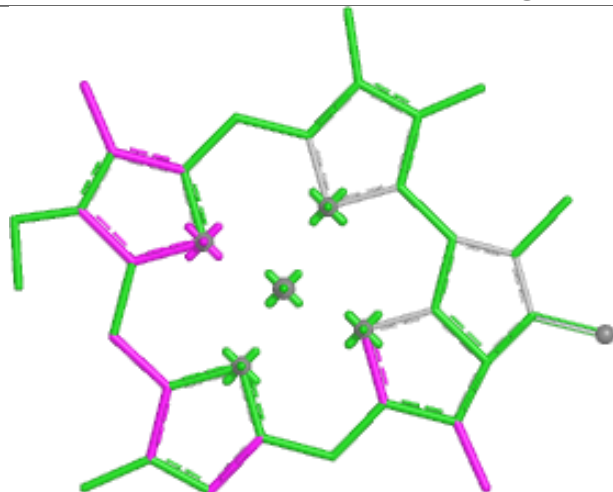
Ligand KC1 5 315



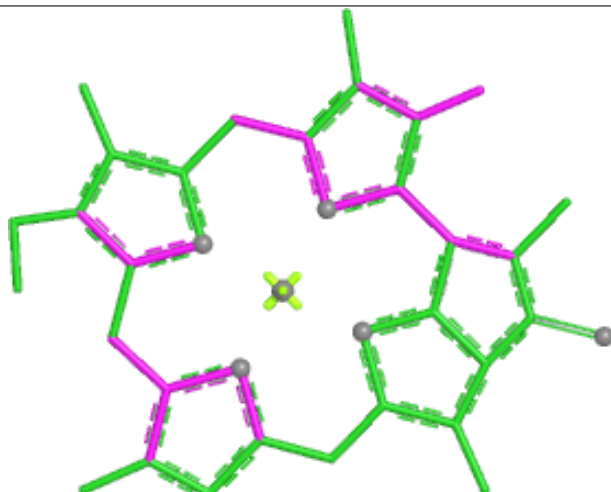
Ligand BCR K 101



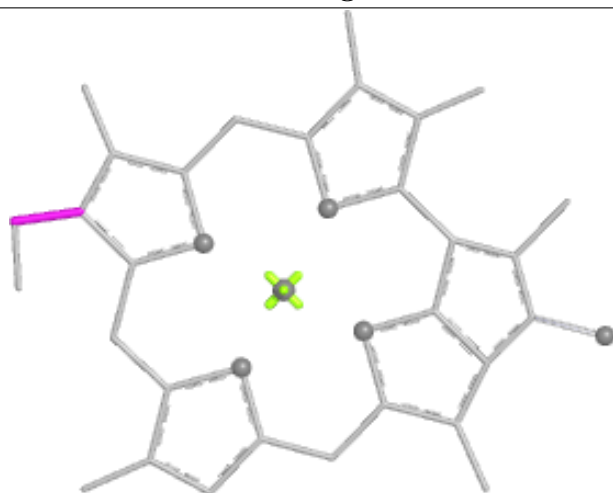
Ligand CLA 1 313



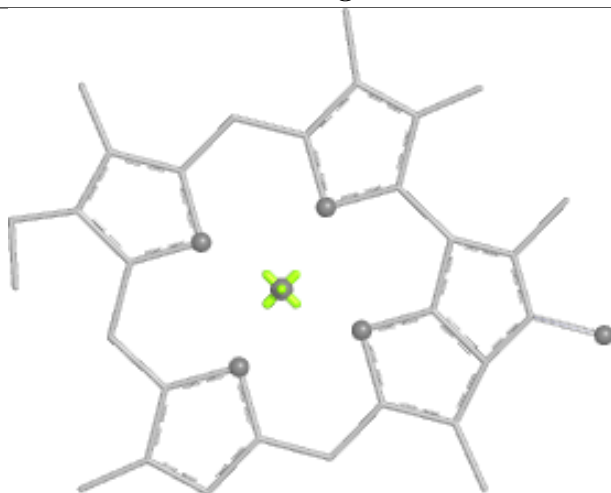
Bond lengths



Bond angles

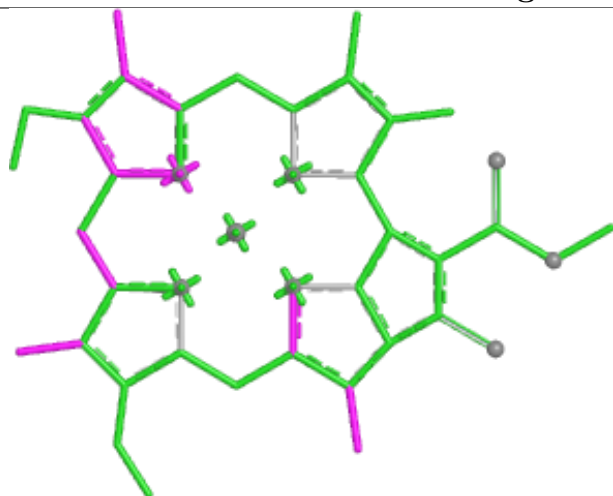


Torsions

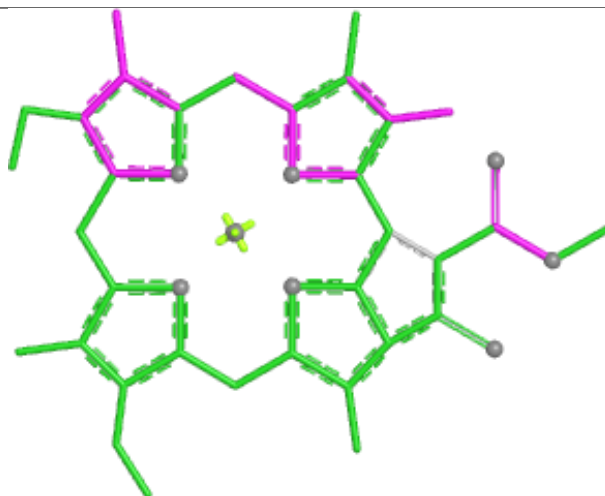


Rings

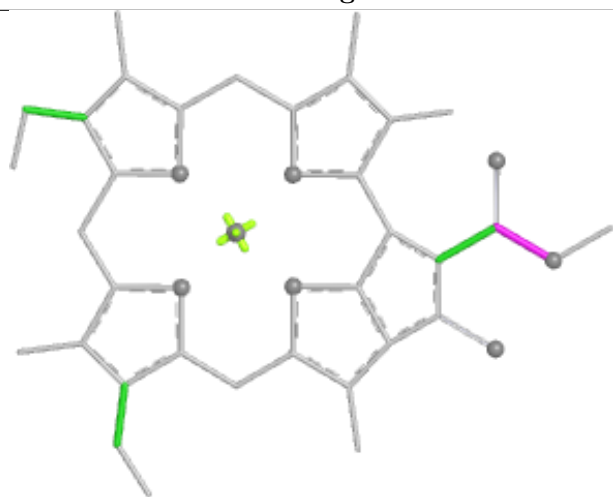
Ligand CLA b 608



Bond lengths



Bond angles

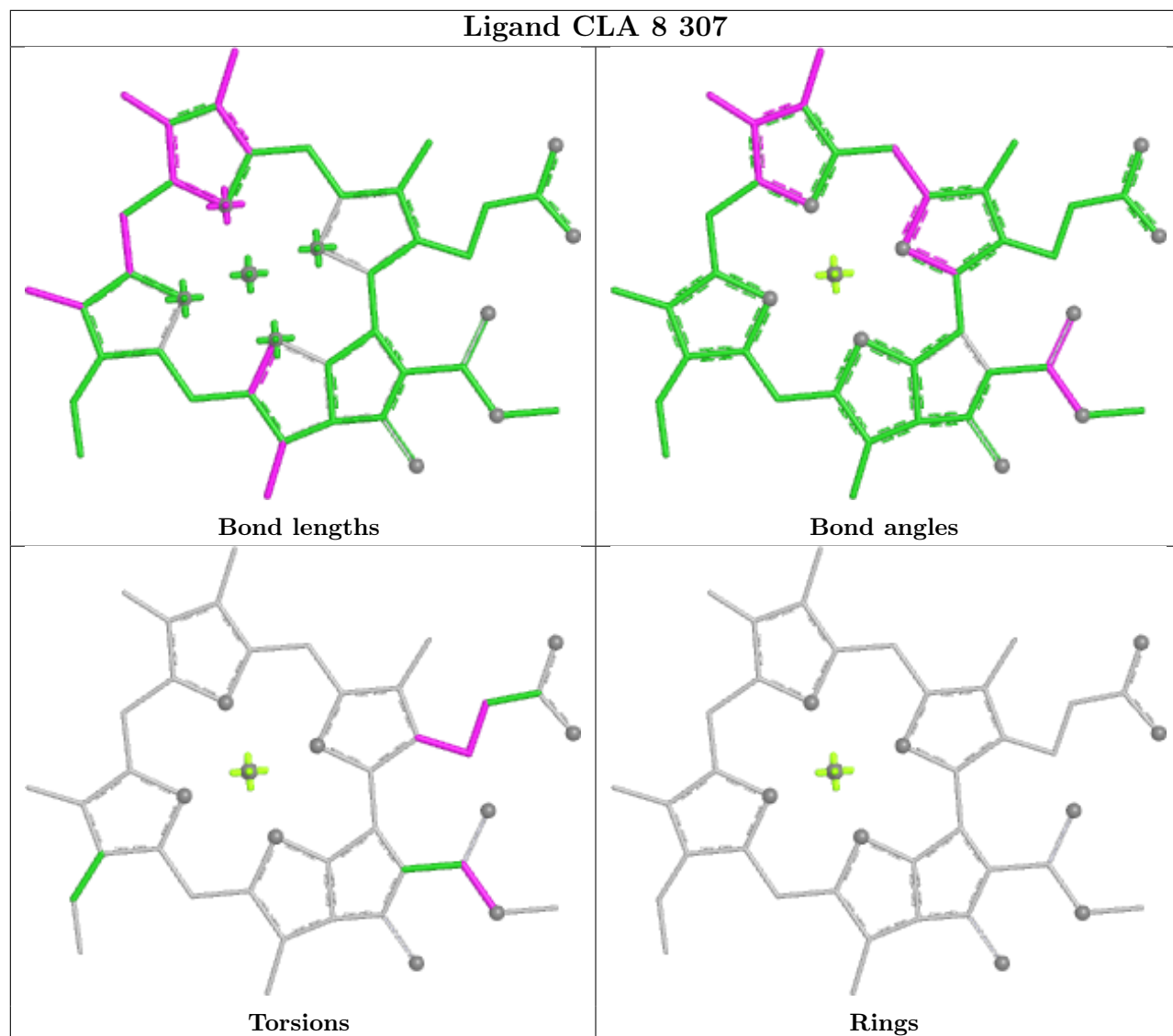


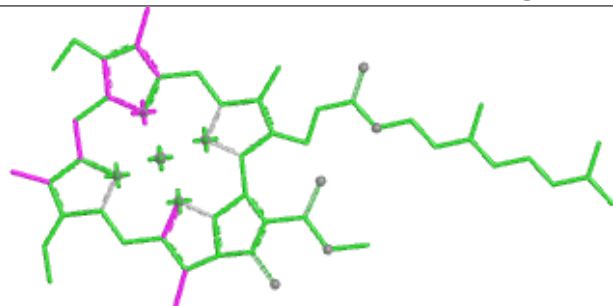
Torsions



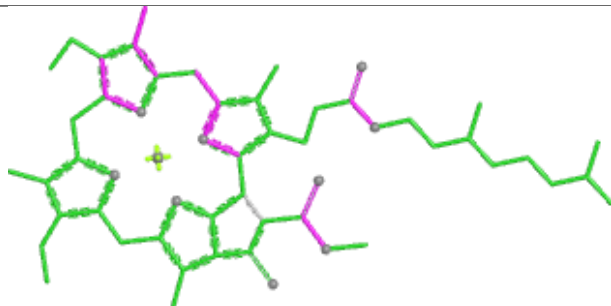
Rings

Ligand CLA 8 307

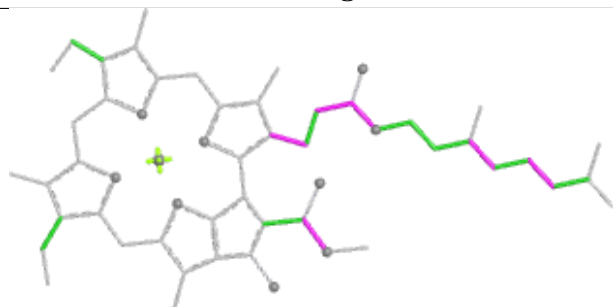


Ligand CLA 9 308

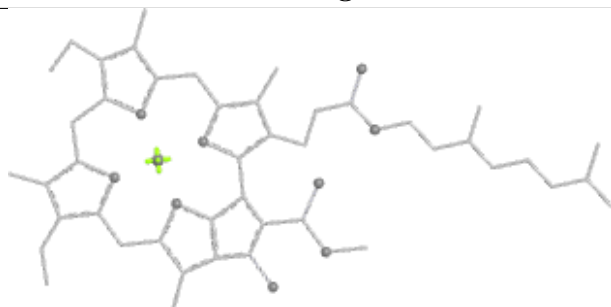
Bond lengths



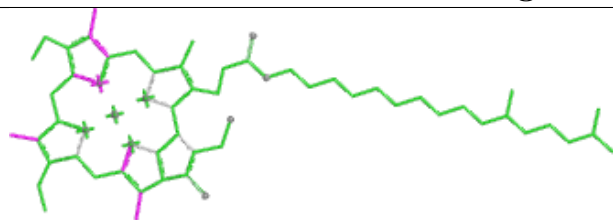
Bond angles



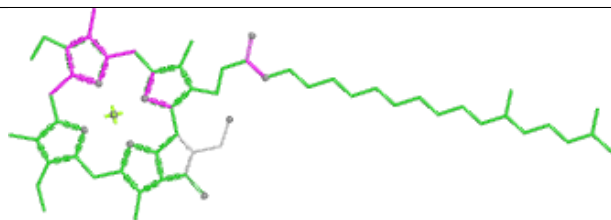
Torsions



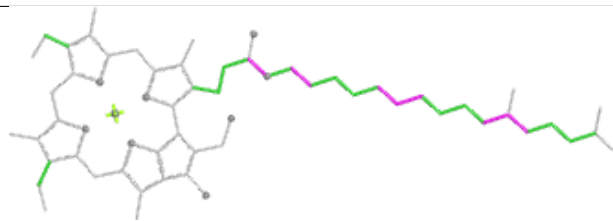
Rings

Ligand CLA b 603

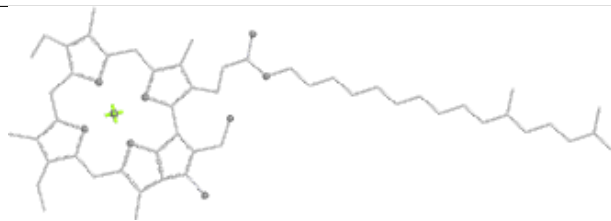
Bond lengths



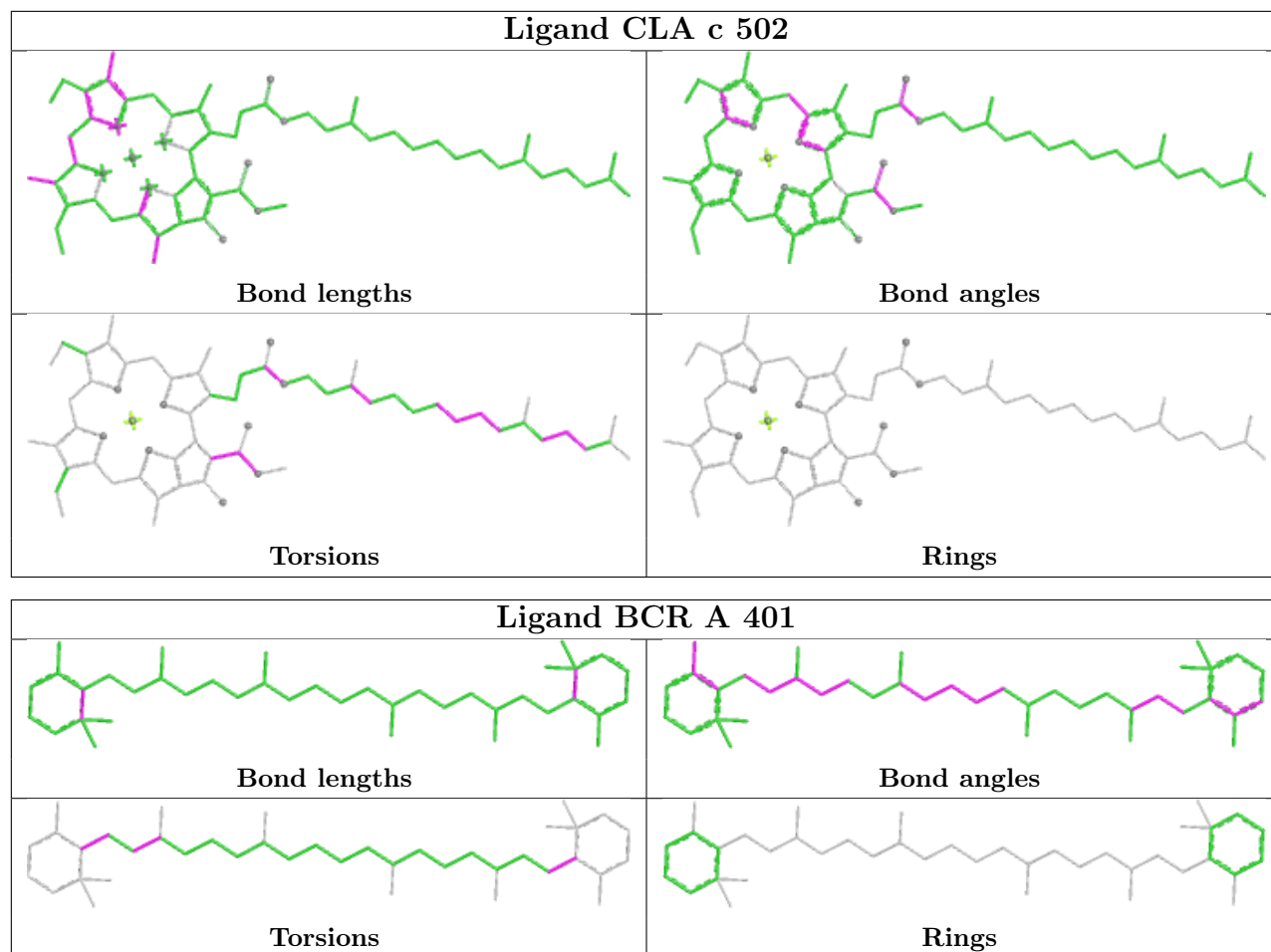
Bond angles



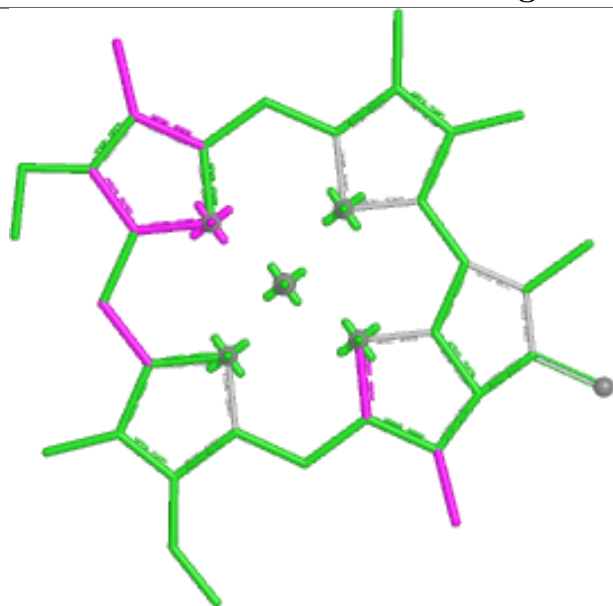
Torsions



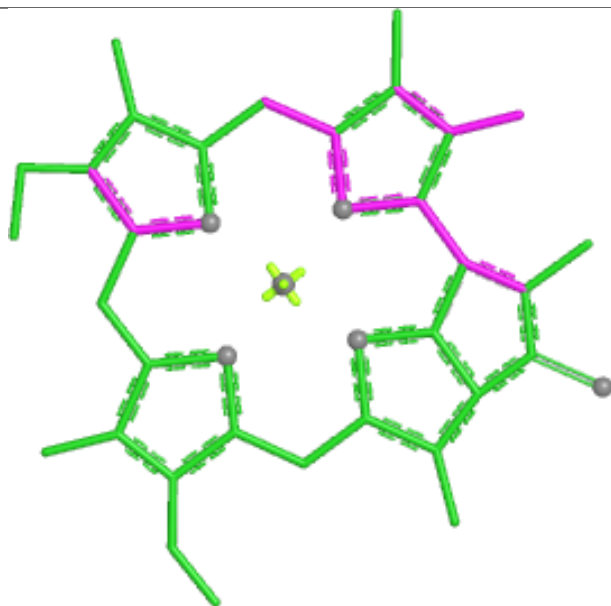
Rings



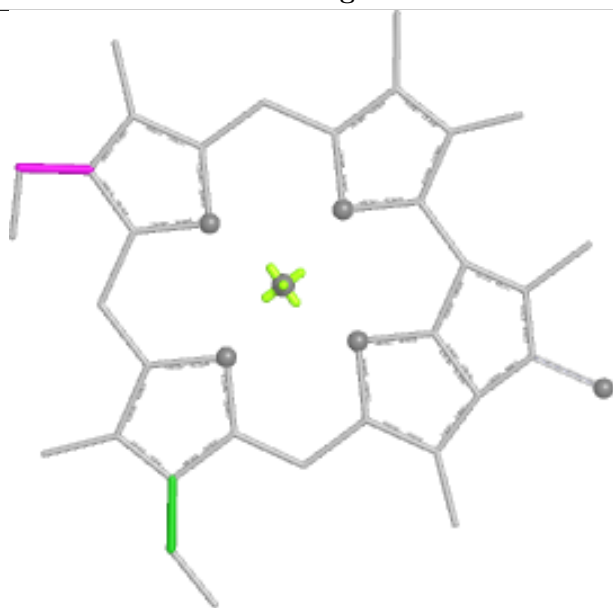
Ligand CLA 9 315



Bond lengths



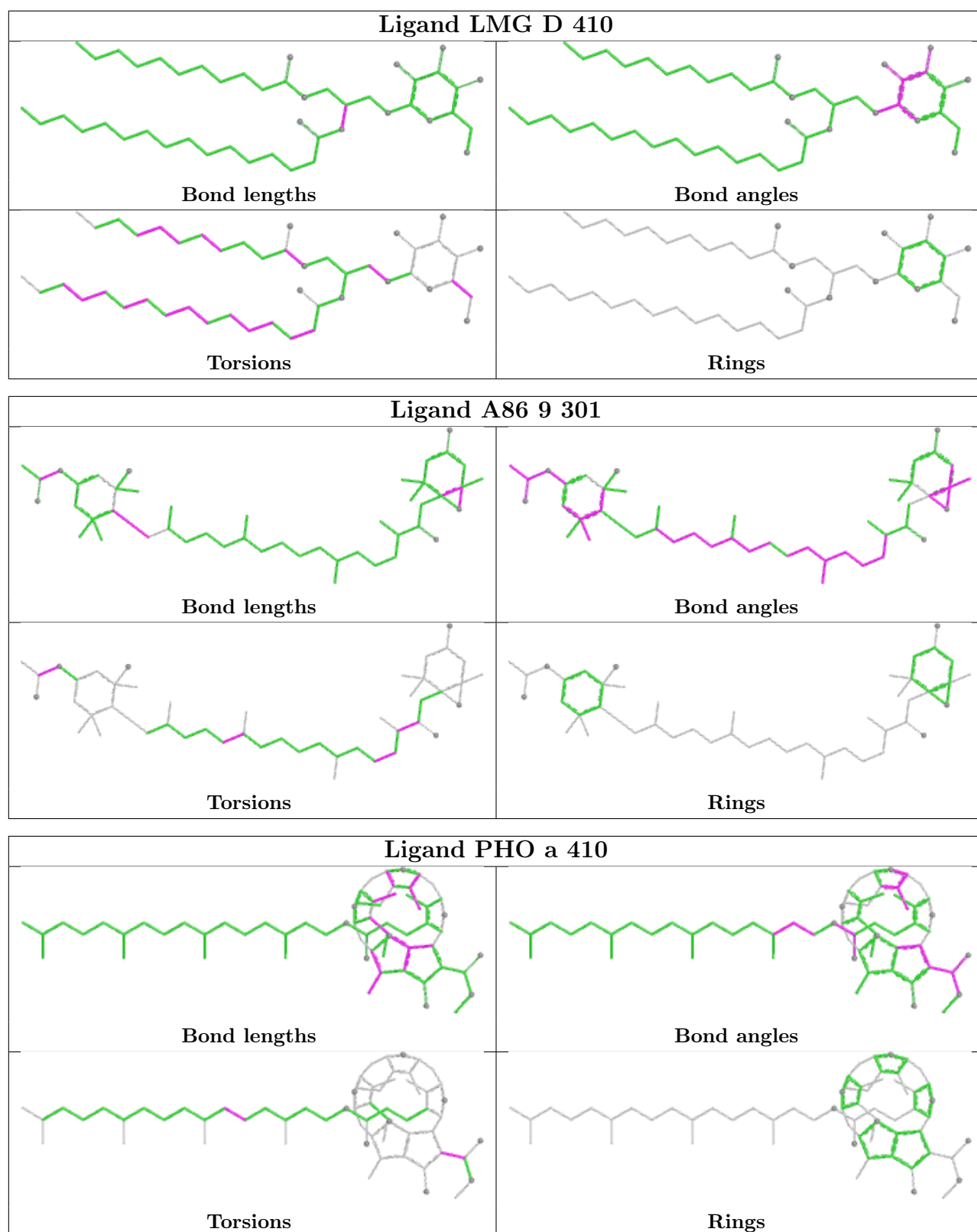
Bond angles



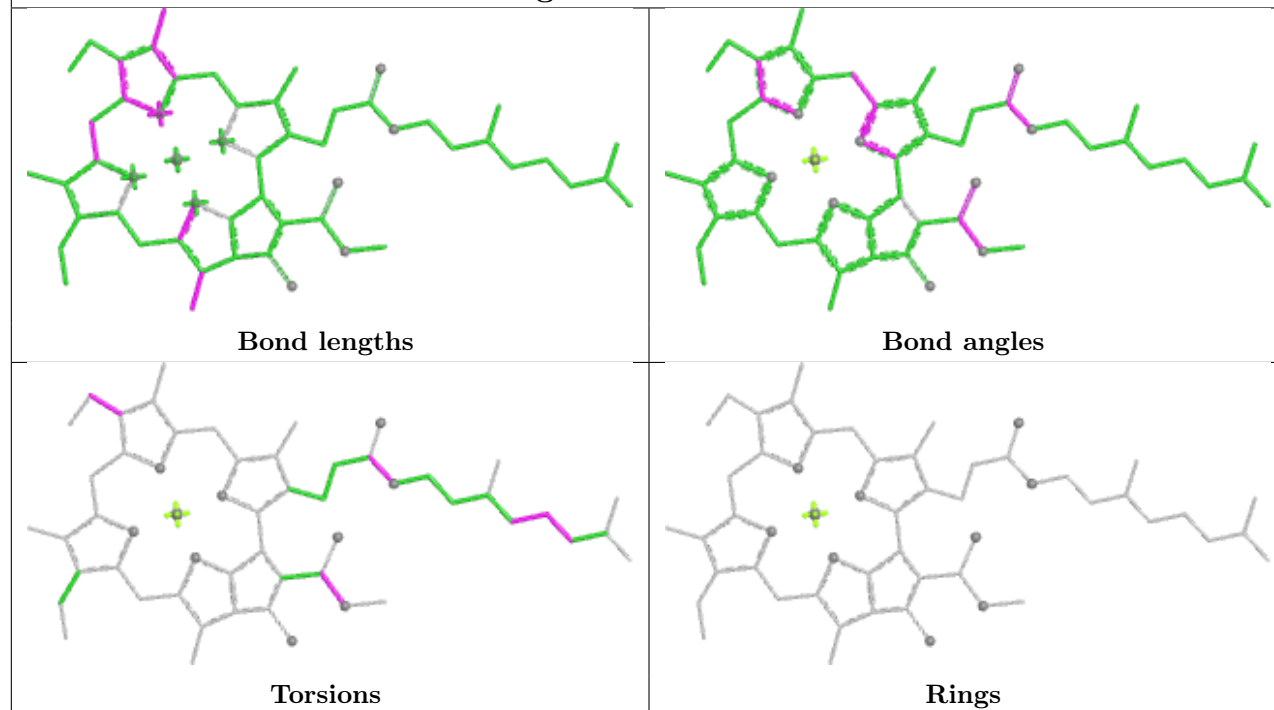
Torsions



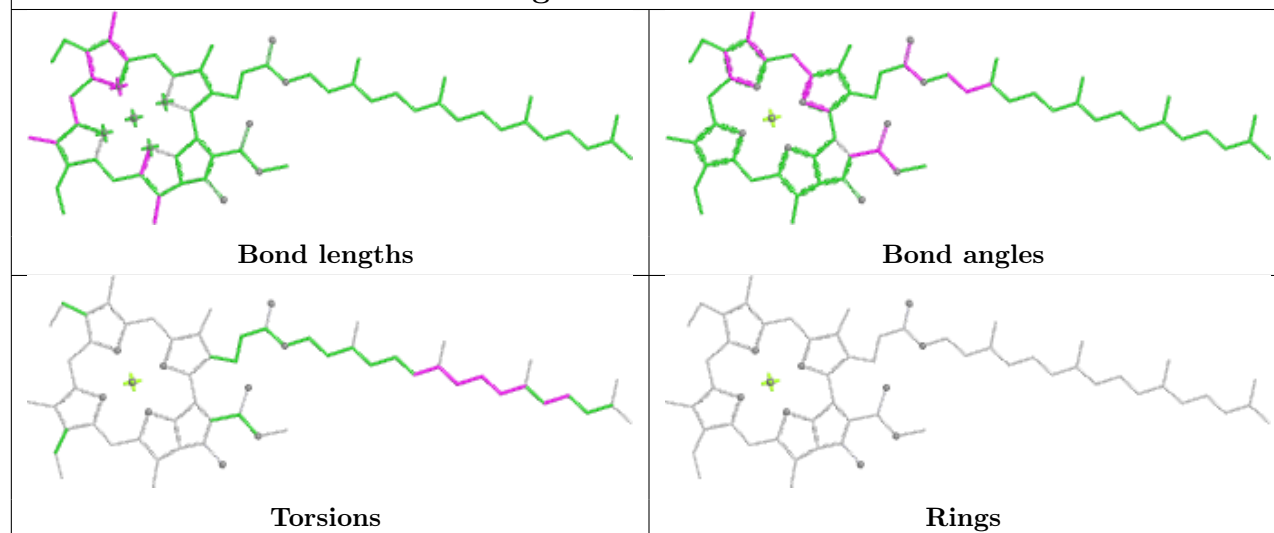
Rings

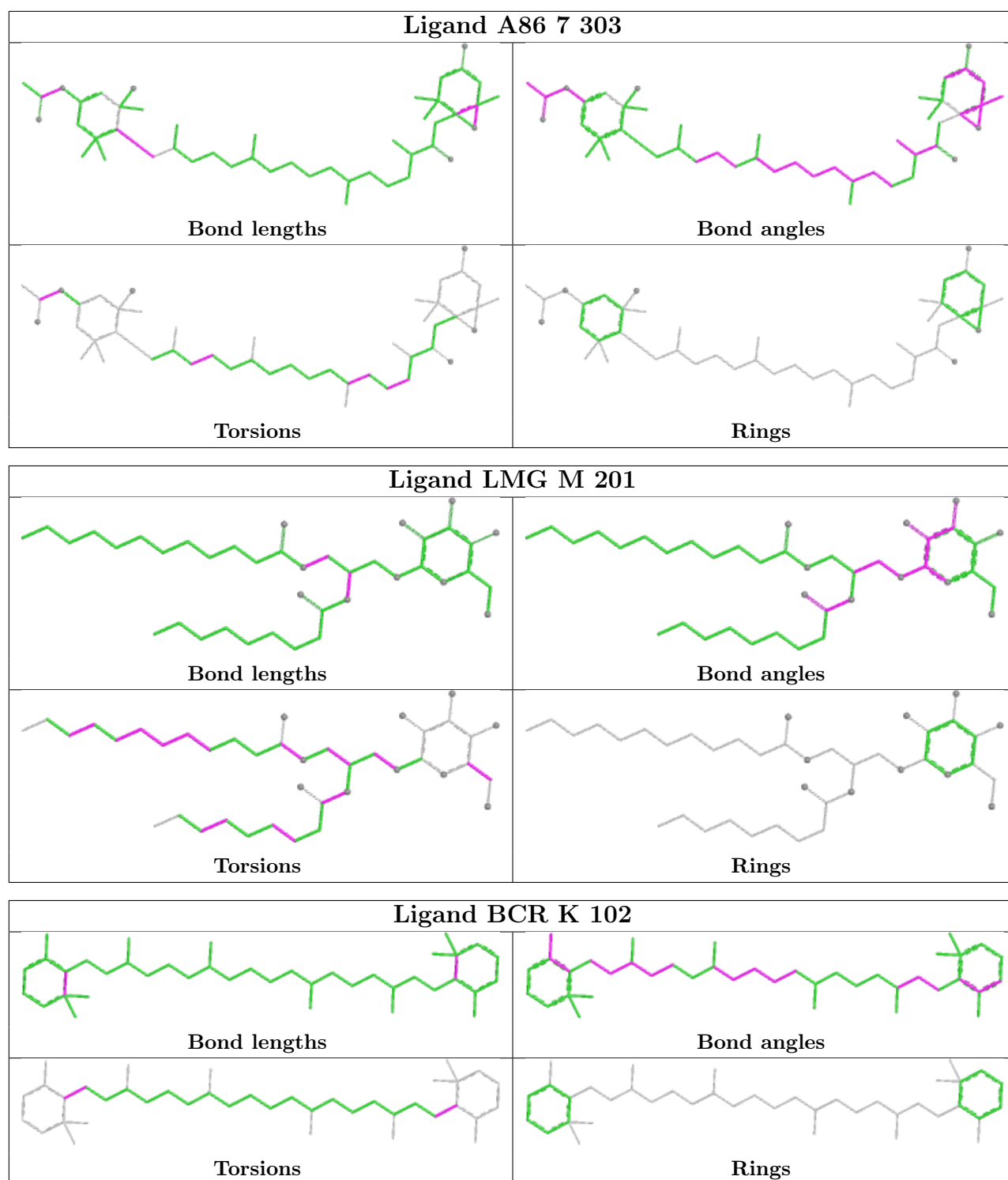


Ligand CLA 2 317

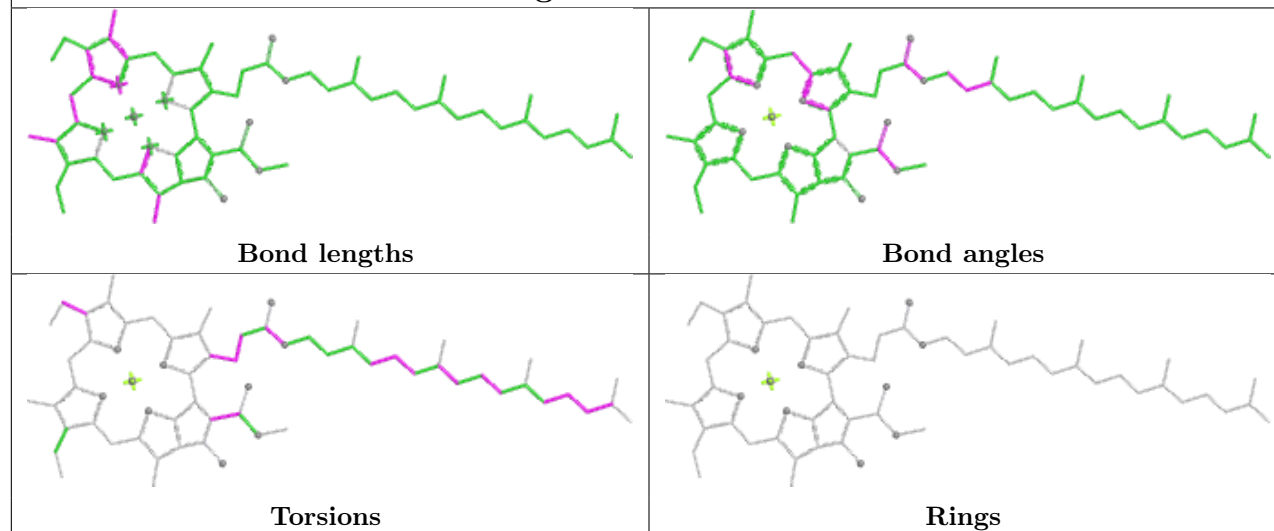


Ligand CLA C 509

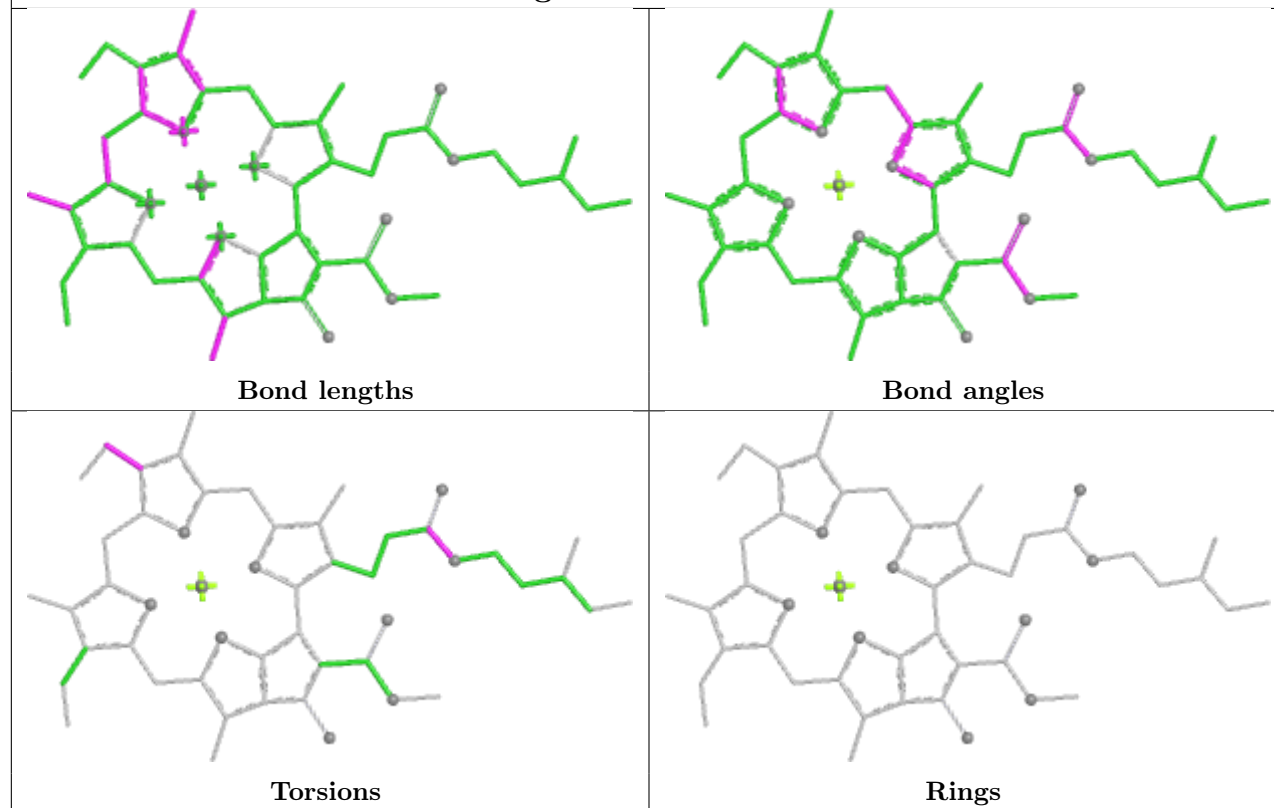




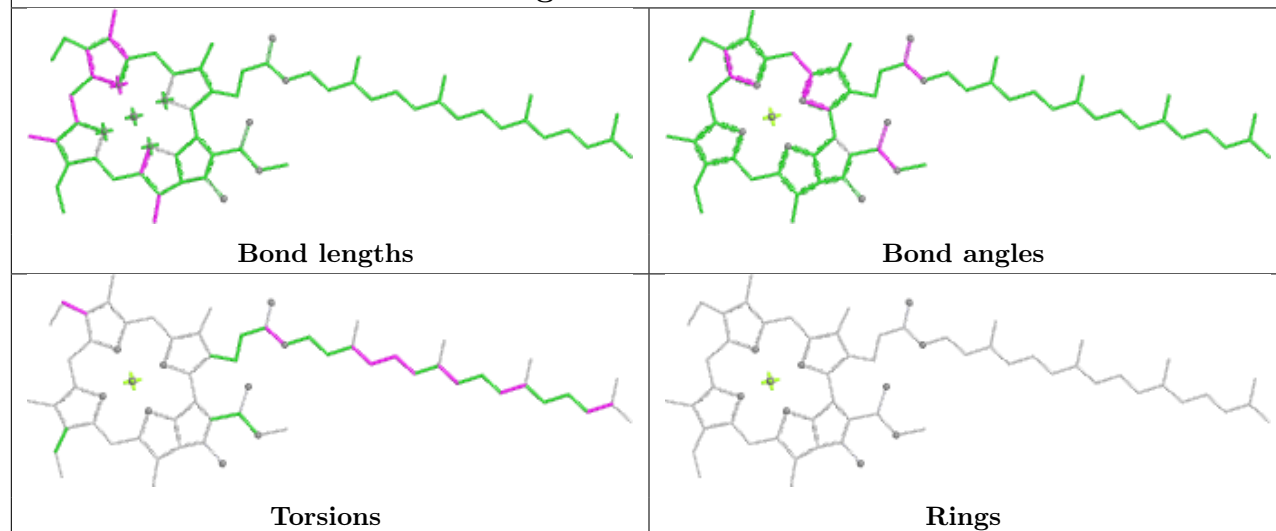
Ligand CLA b 617



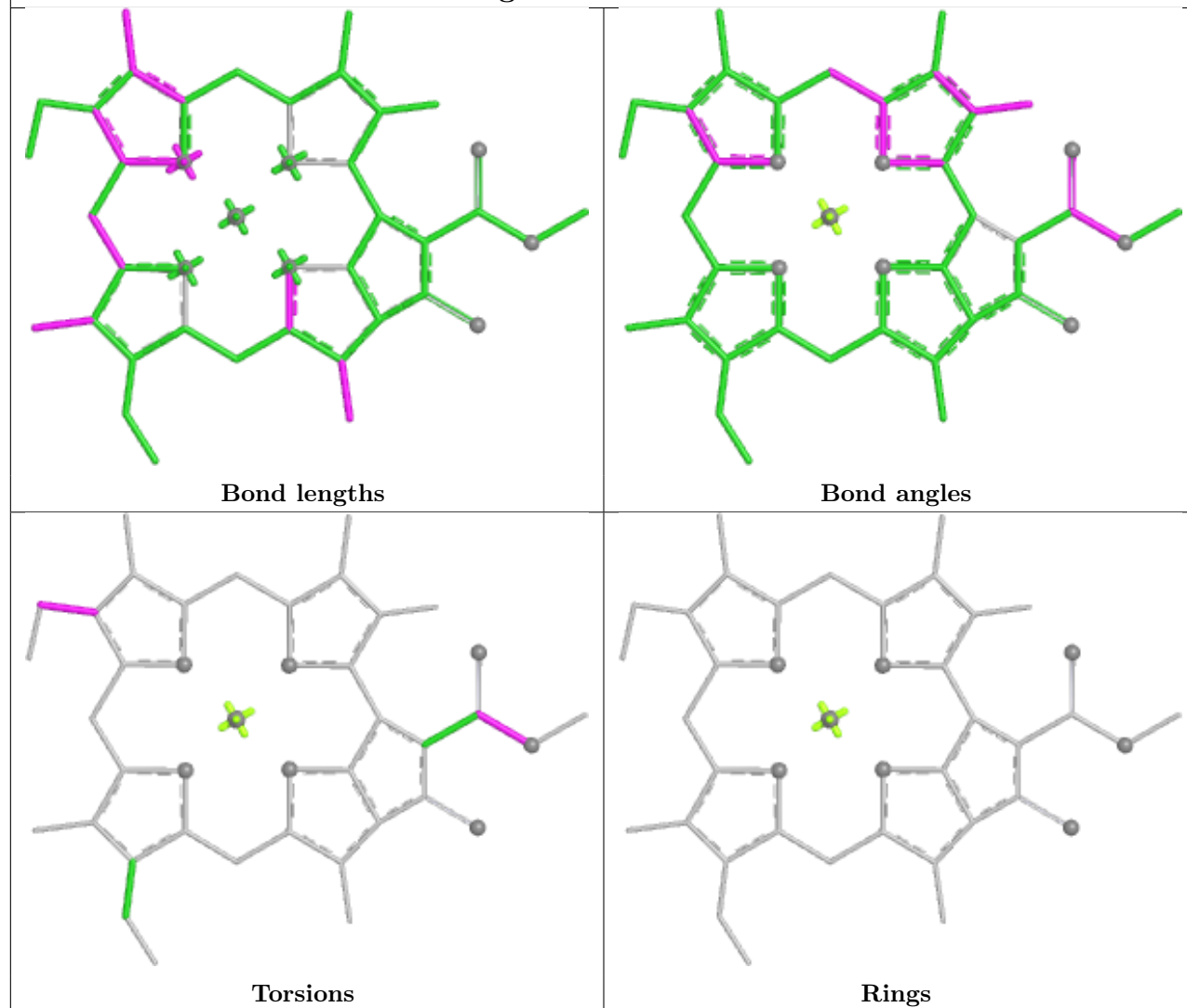
Ligand CLA Z 101

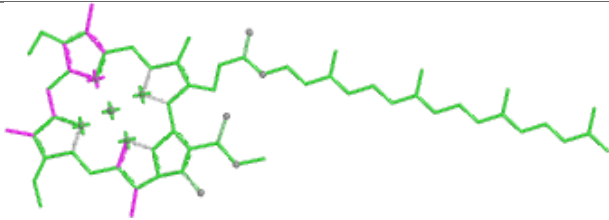
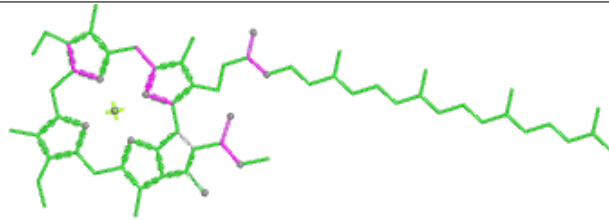
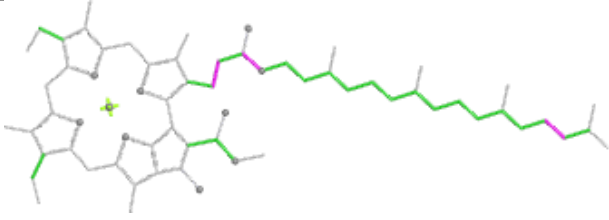
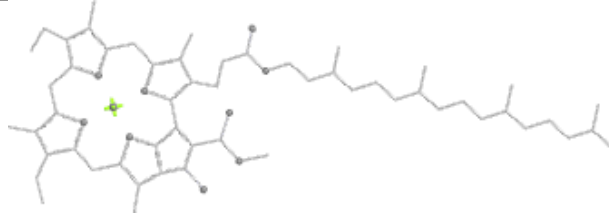


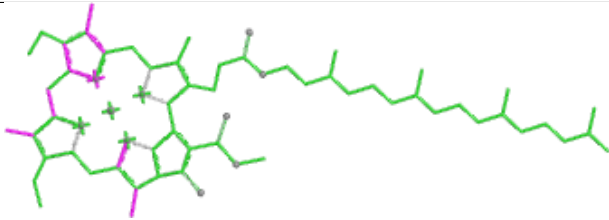
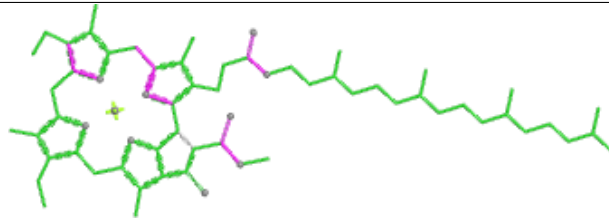
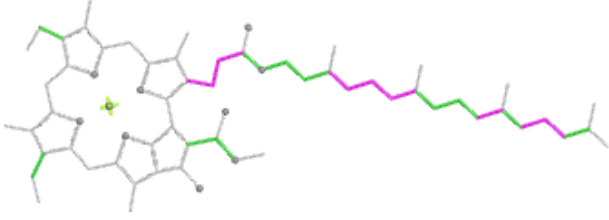
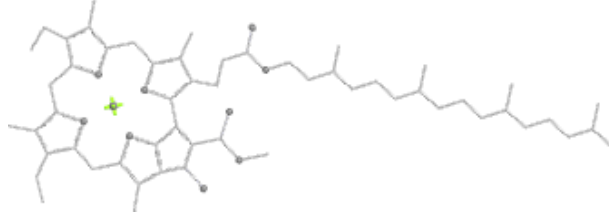
Ligand CLA 3 307

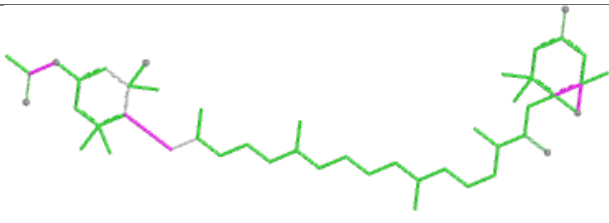
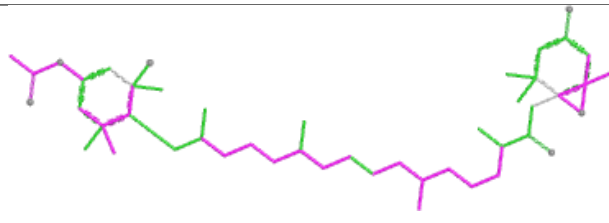
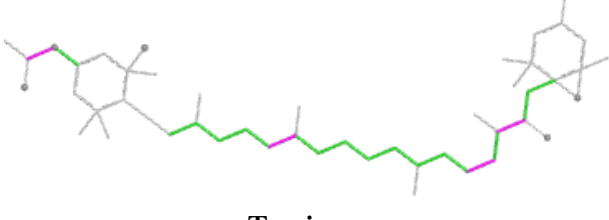
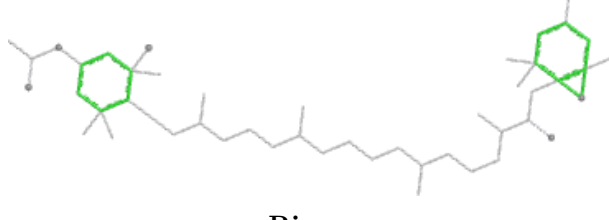


Ligand CLA 7 308

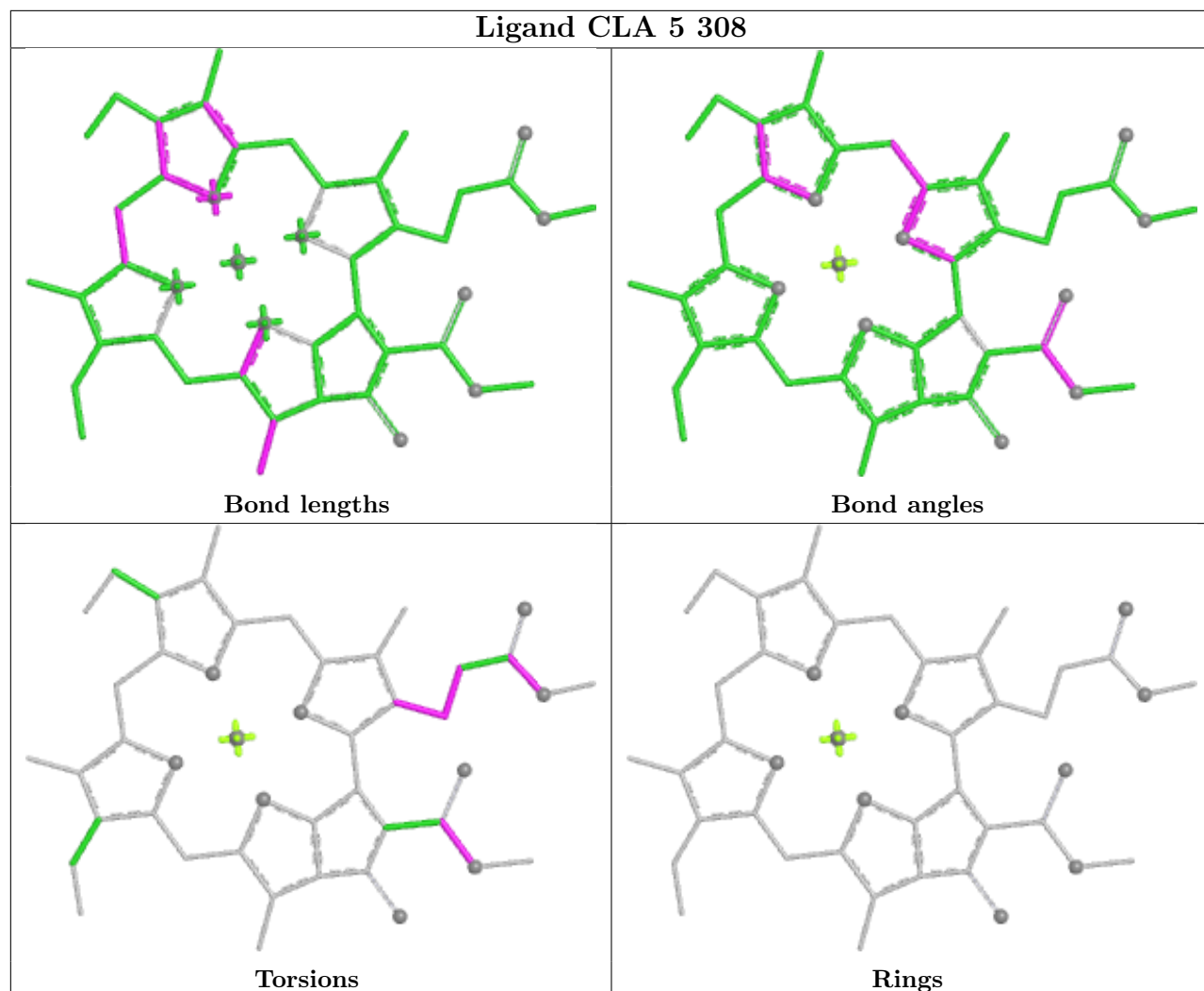


Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

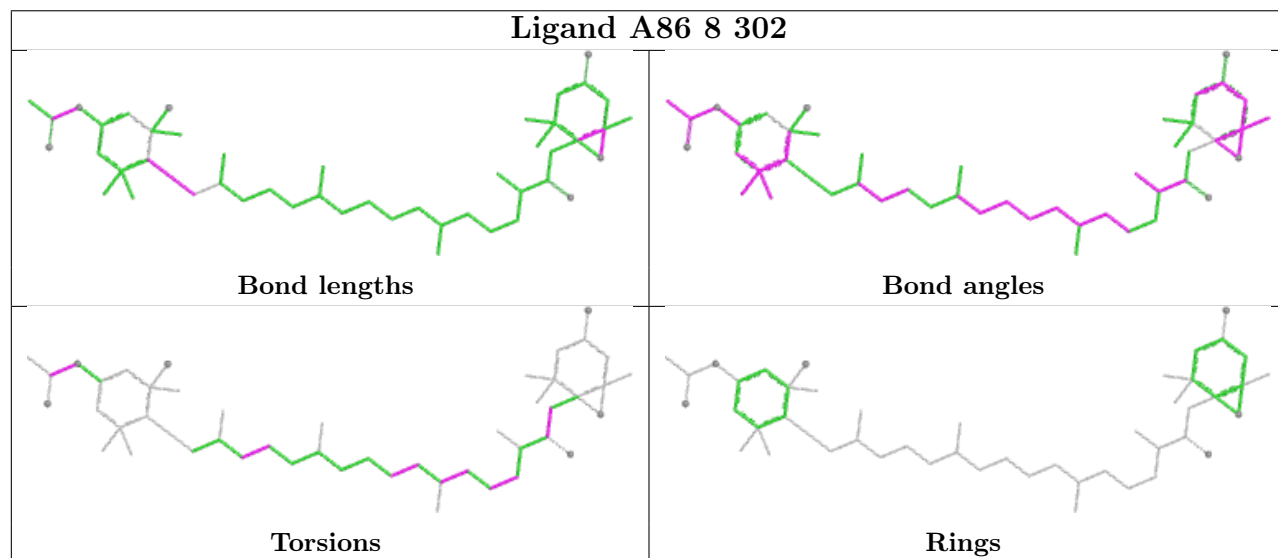
Ligand CLA 3 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A86 2 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

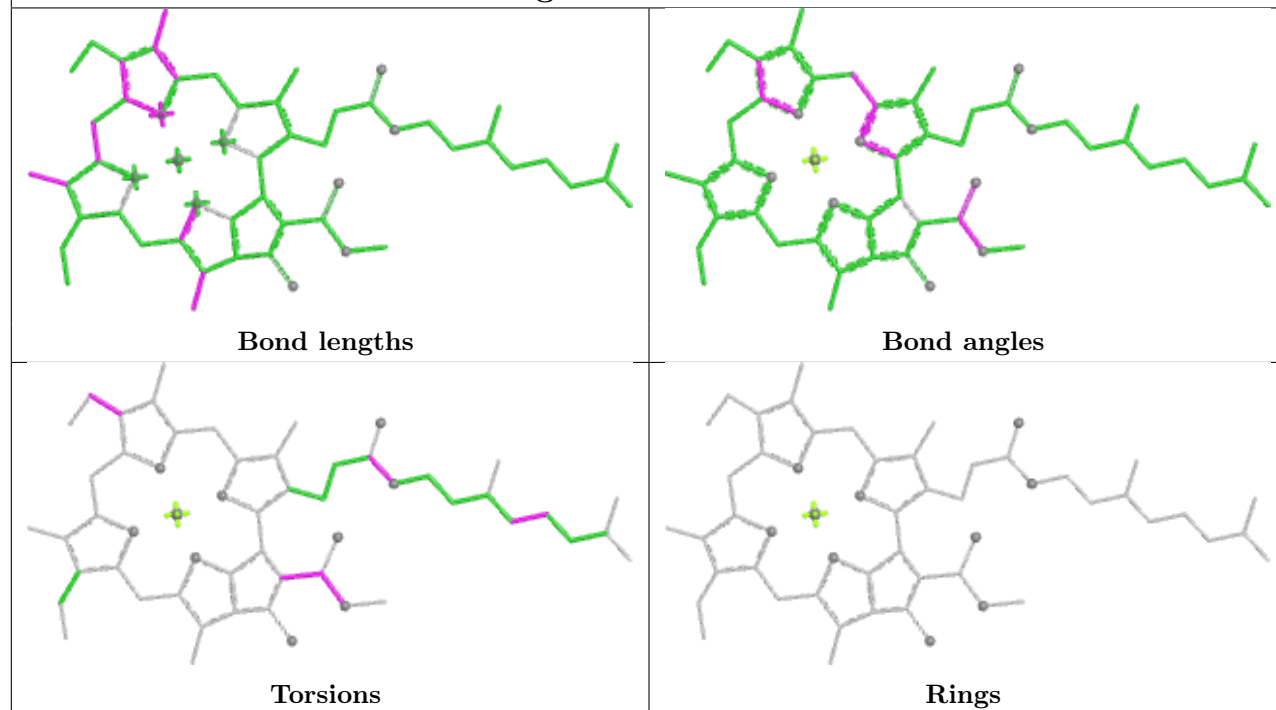
Ligand CLA 5 308



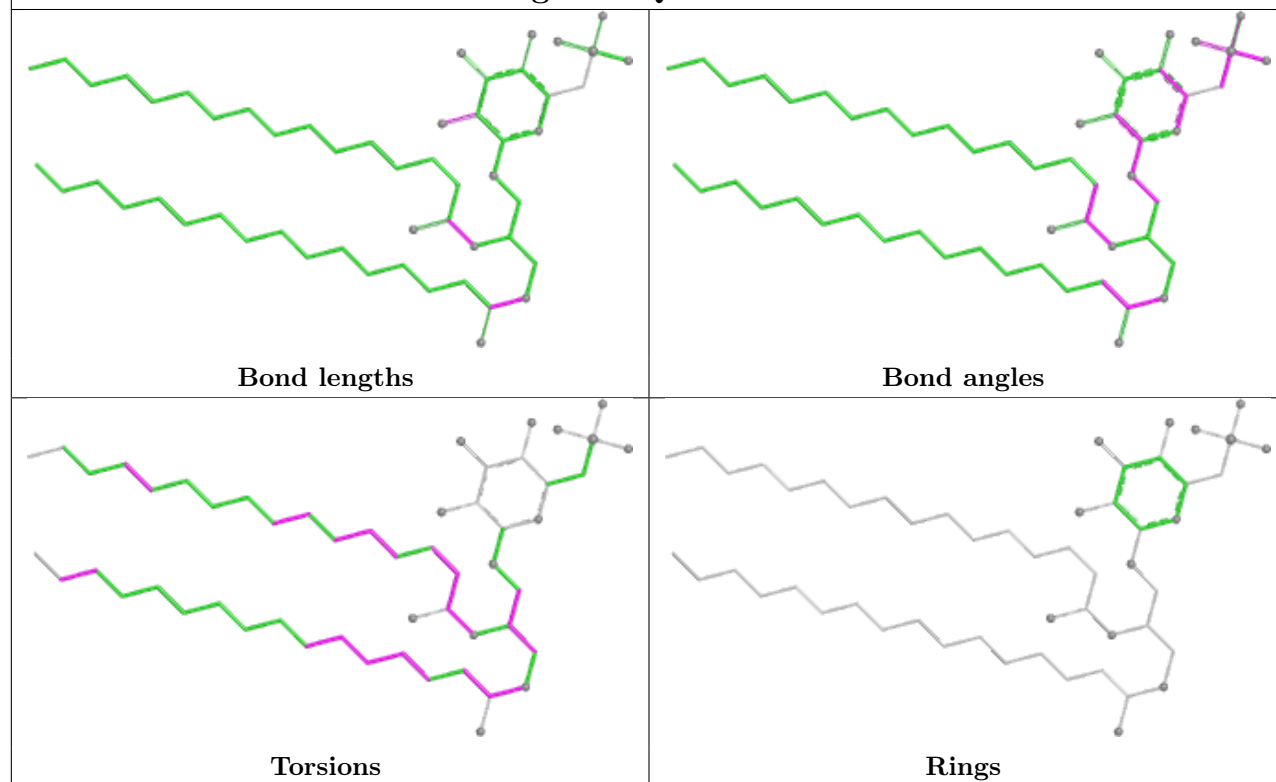
Ligand A86 8 302

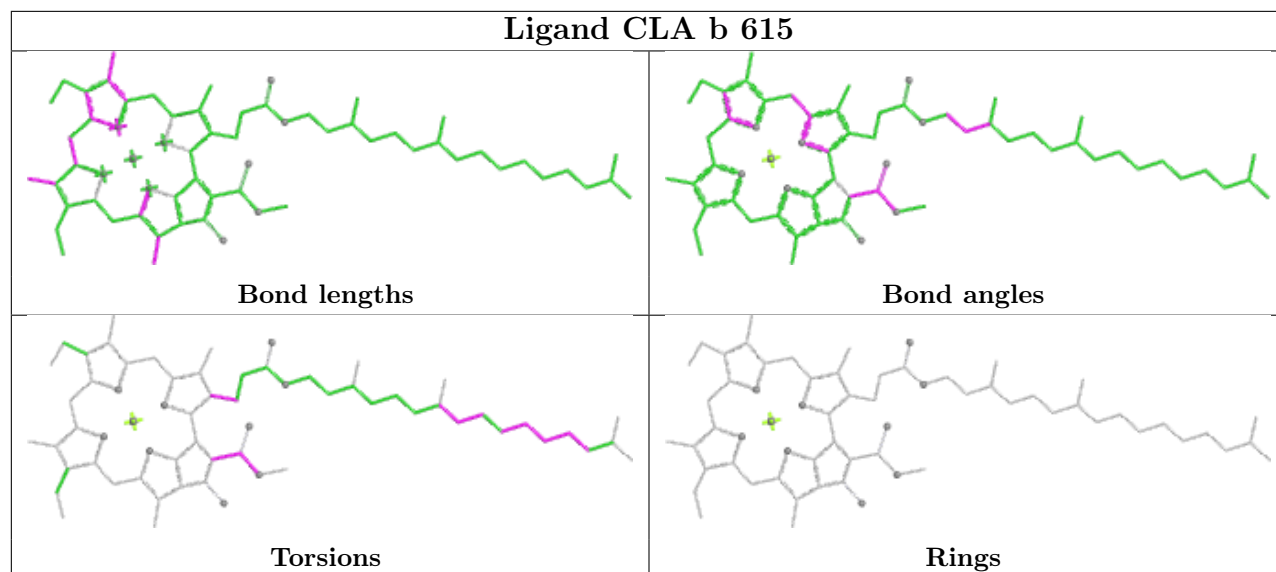
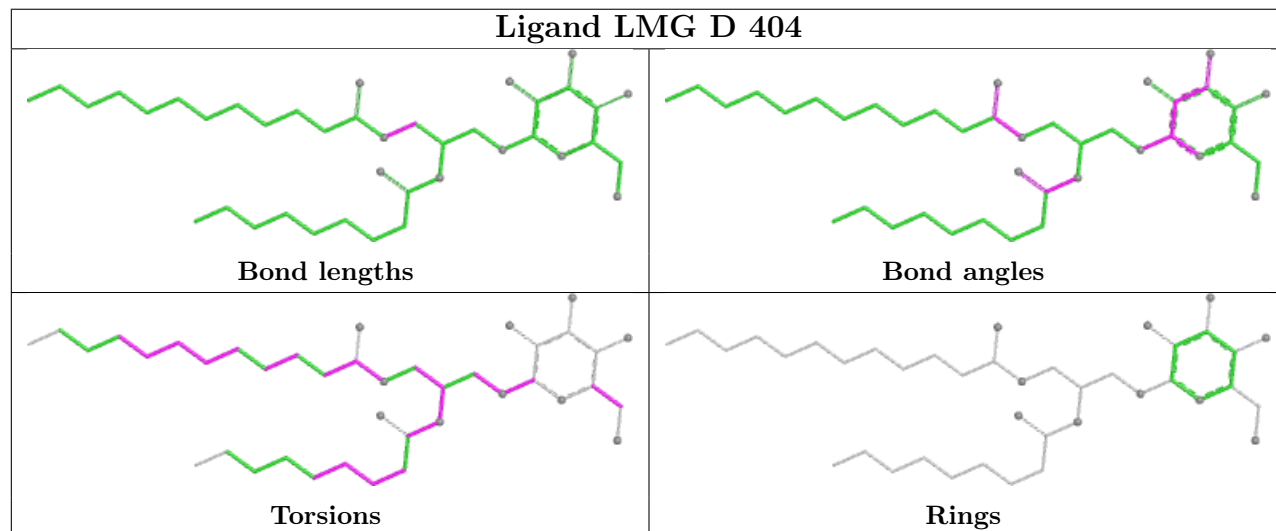


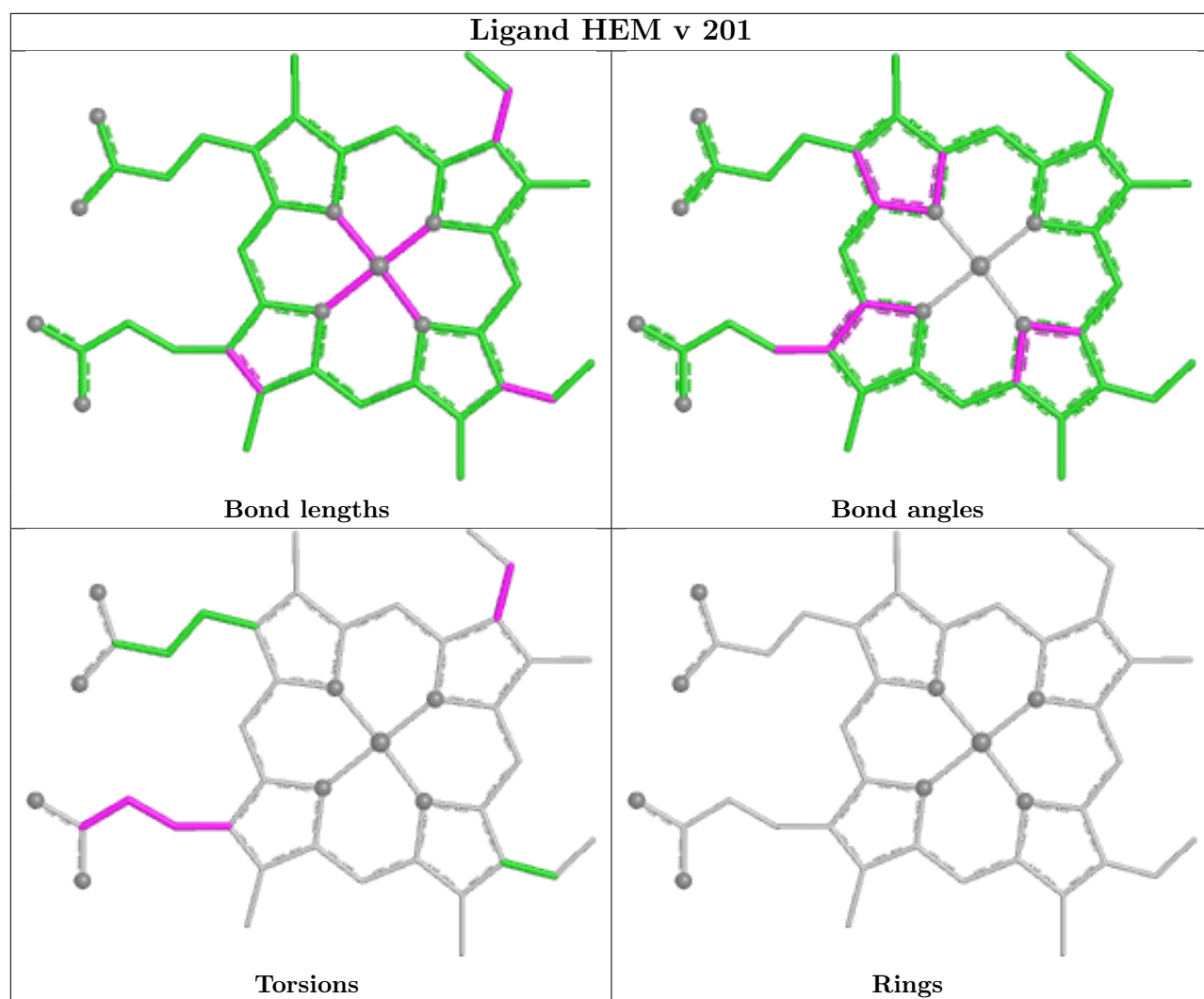
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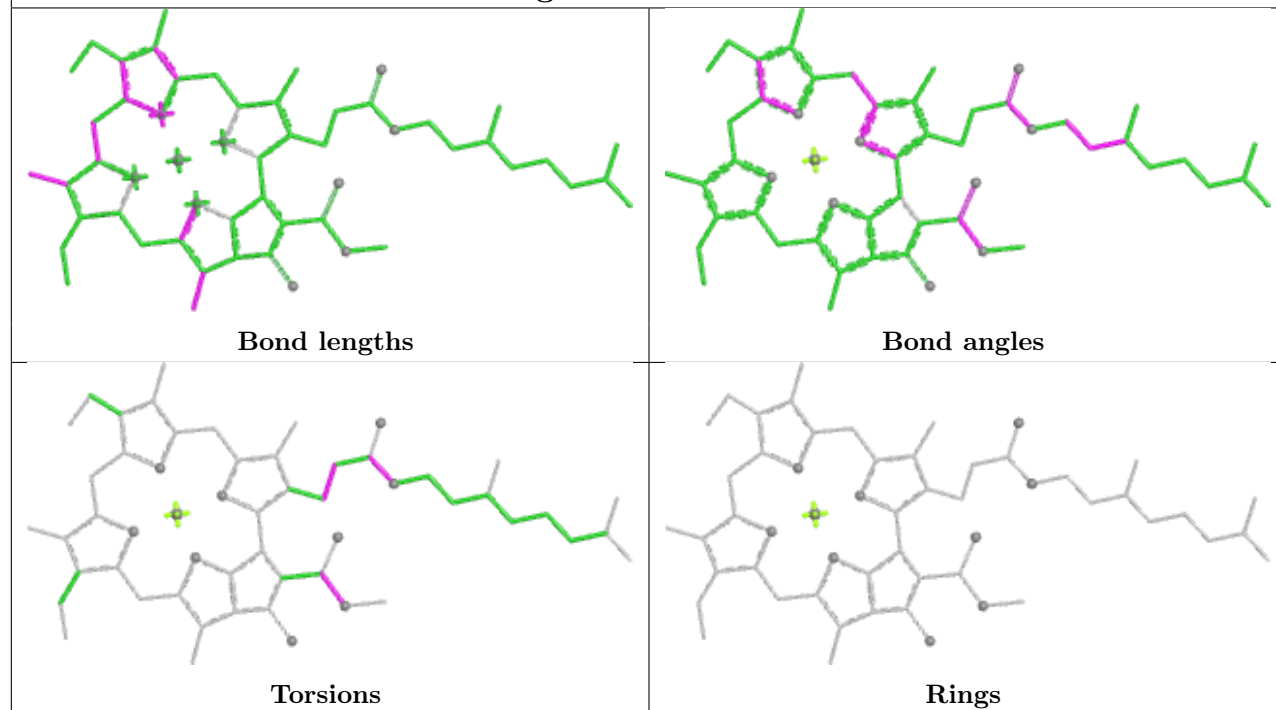
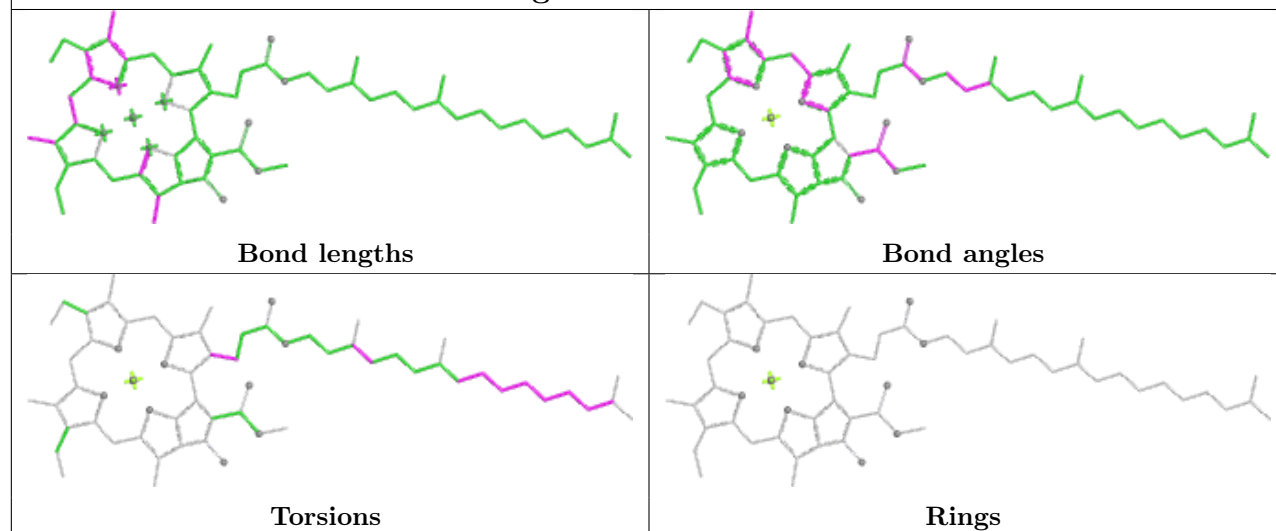


Ligand SQD D 403

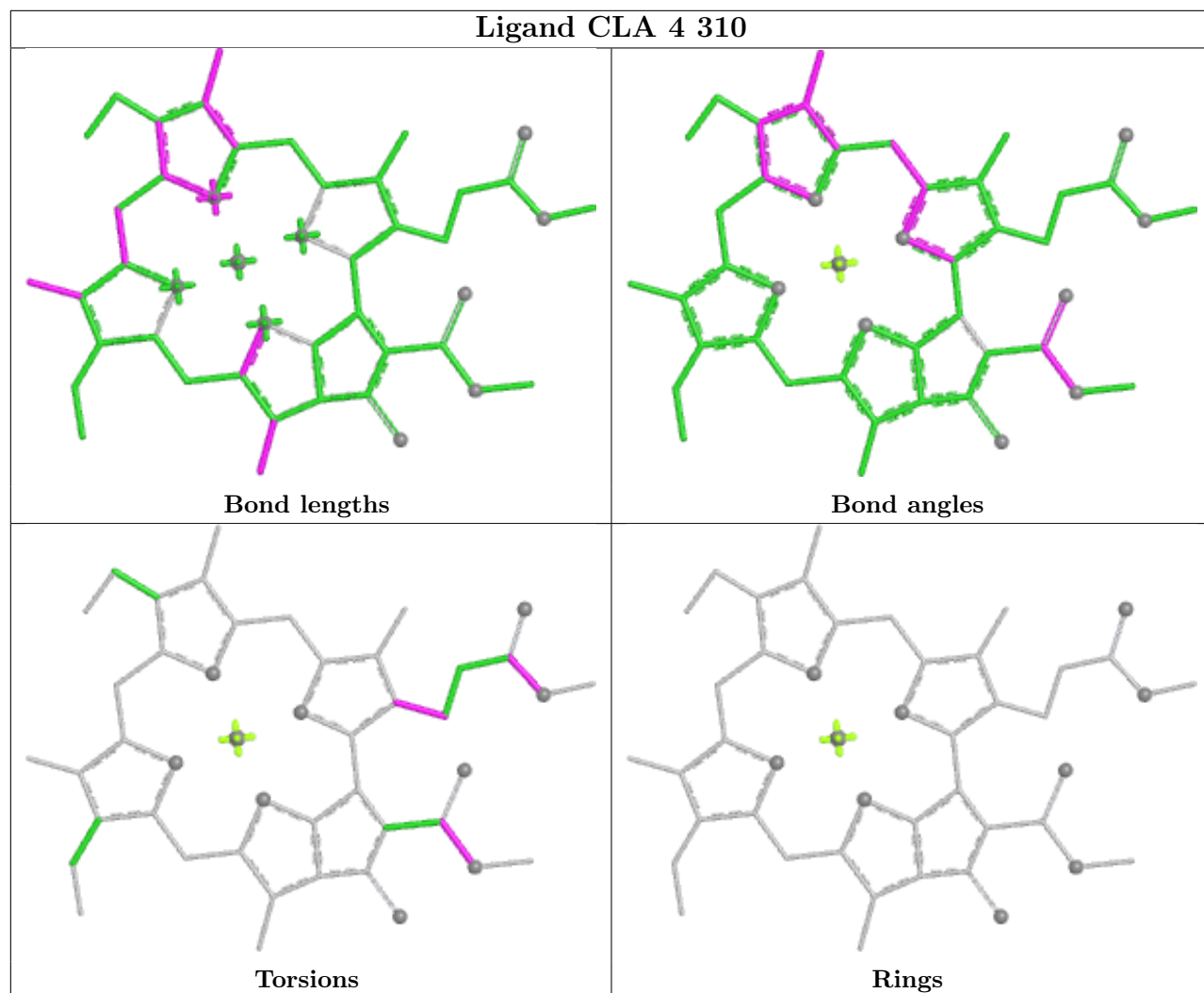


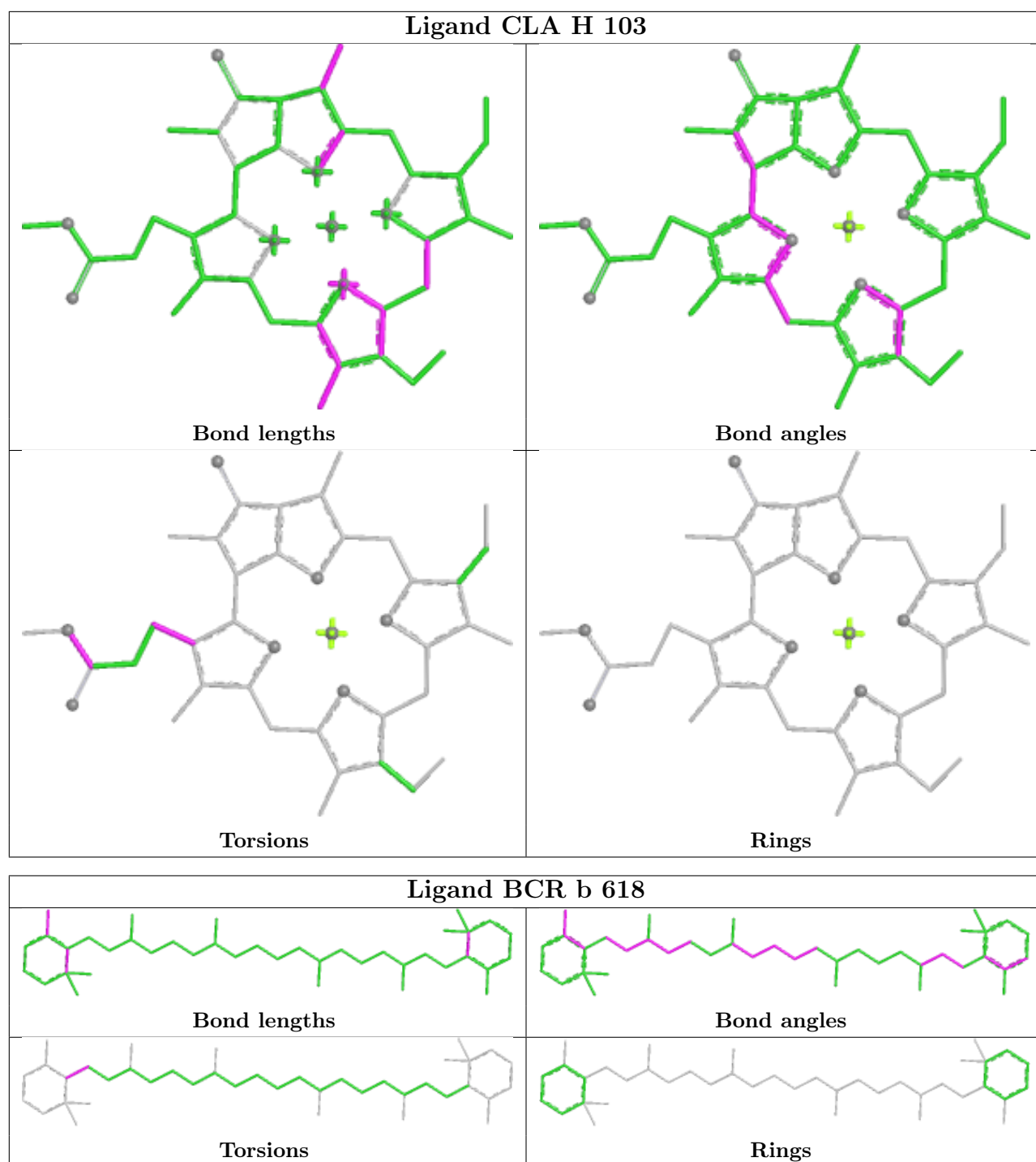
Ligand CLA b 615**Ligand LMG D 404**



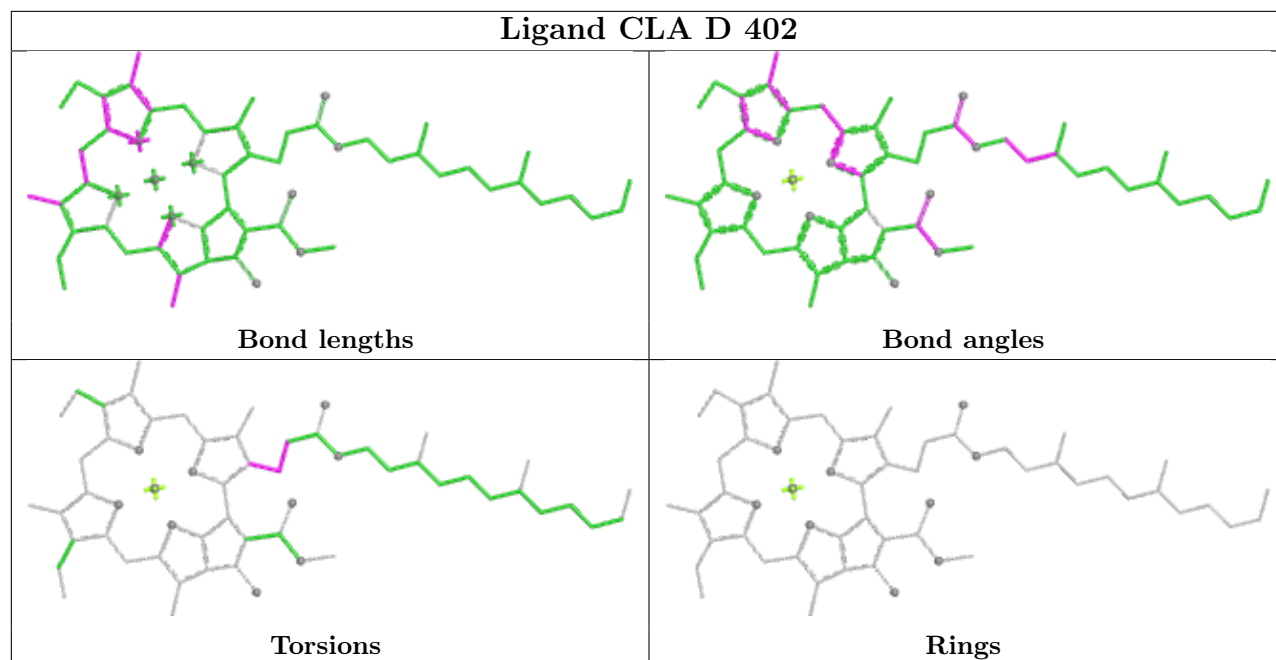
Ligand CLA 1 311**Ligand CLA B 611**

Ligand CLA 4 310

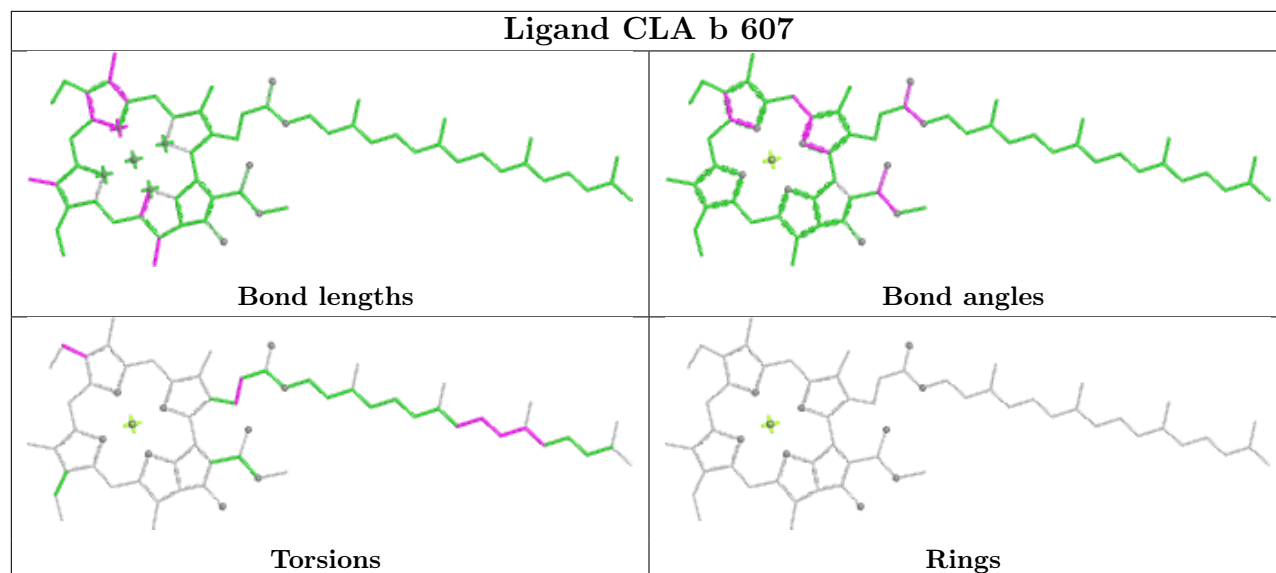




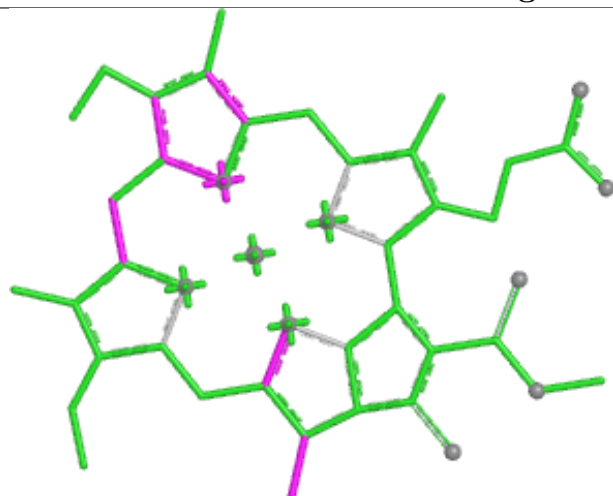
Ligand CLA D 402



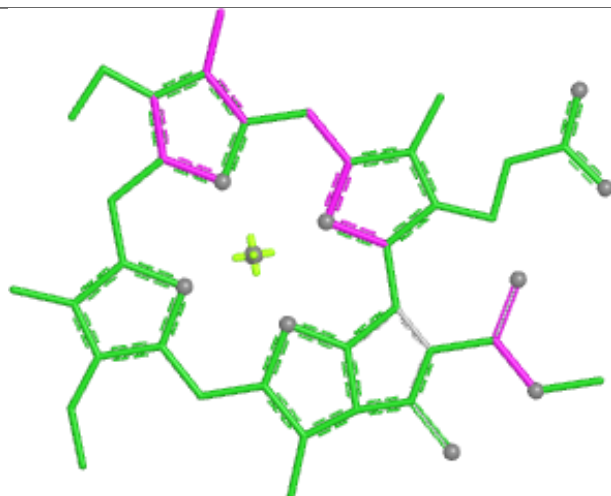
Ligand CLA b 607



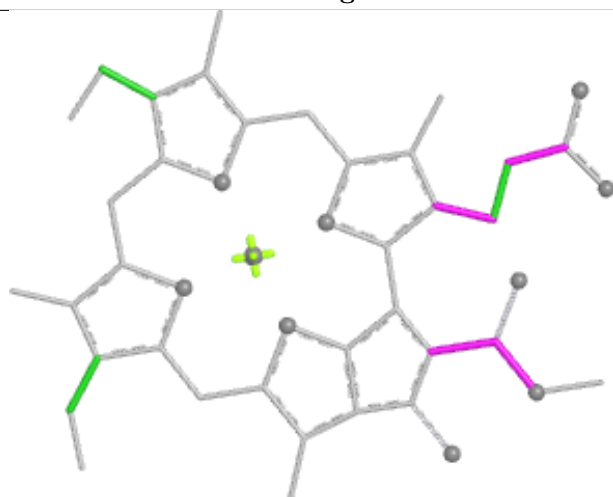
Ligand CLA 0 310



Bond lengths



Bond angles

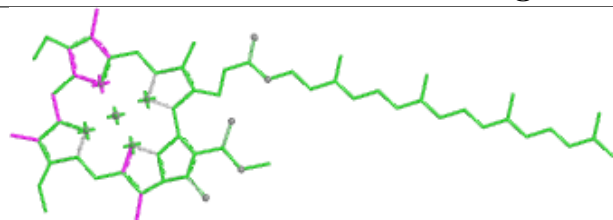


Torsions

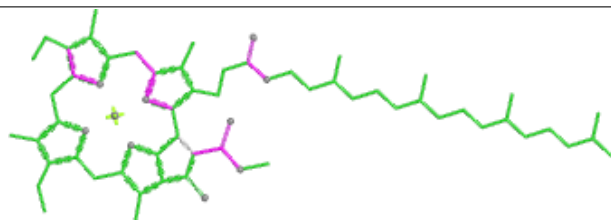


Rings

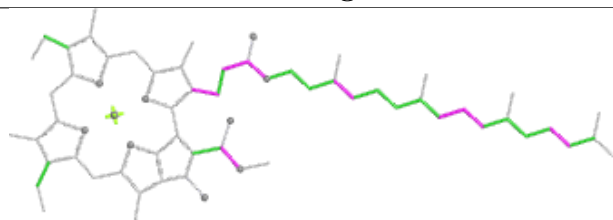
Ligand CLA B 612



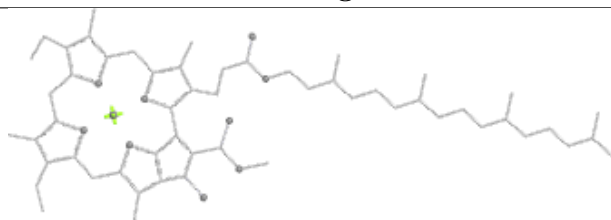
Bond lengths



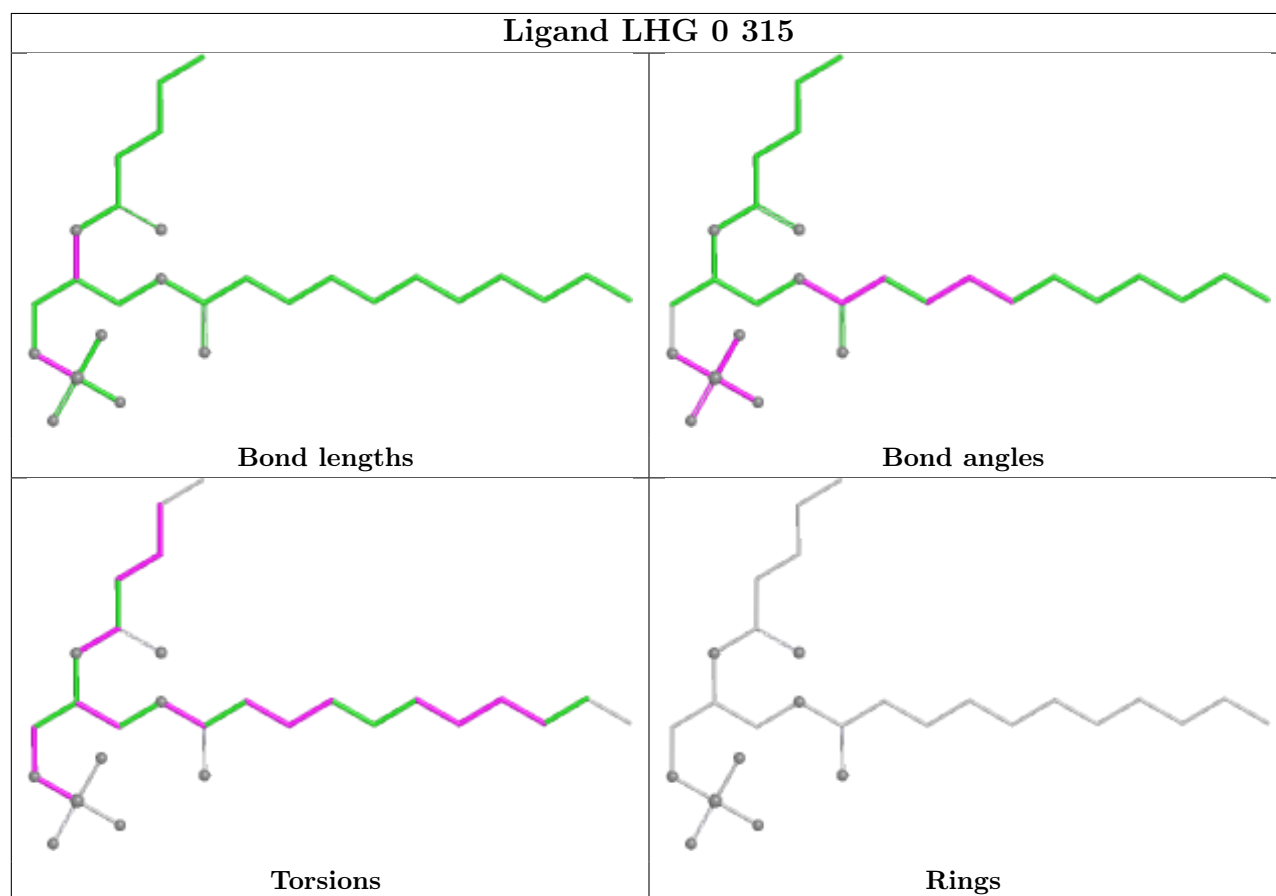
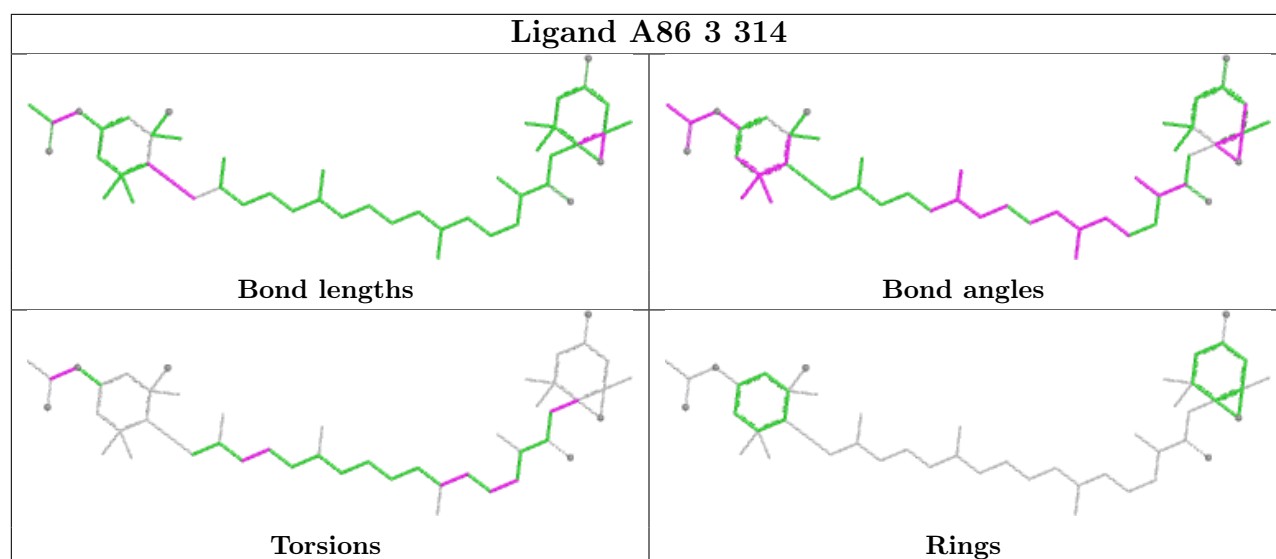
Bond angles

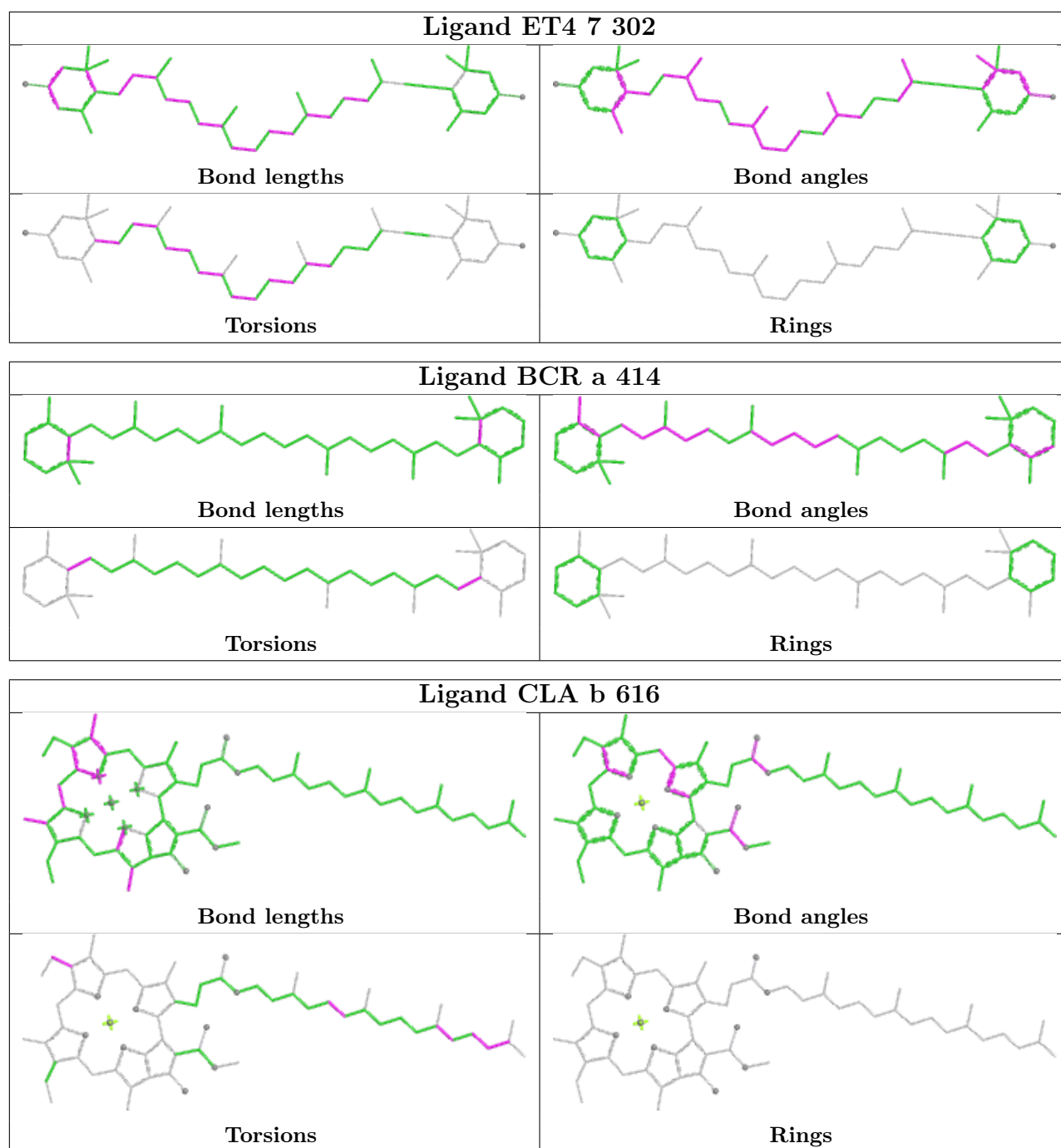


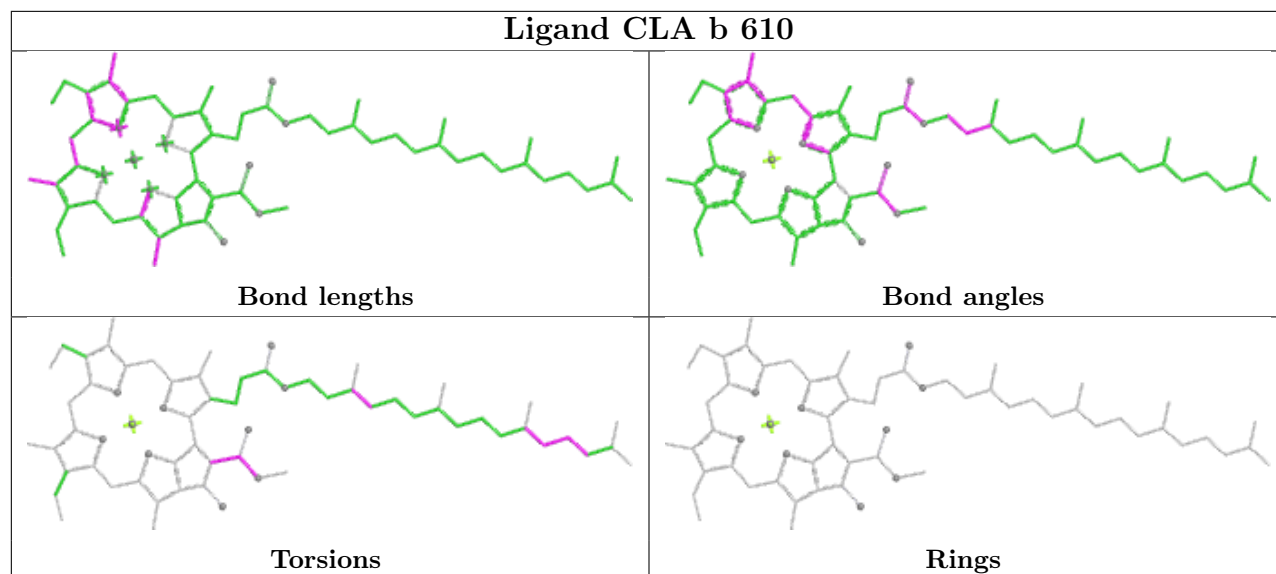
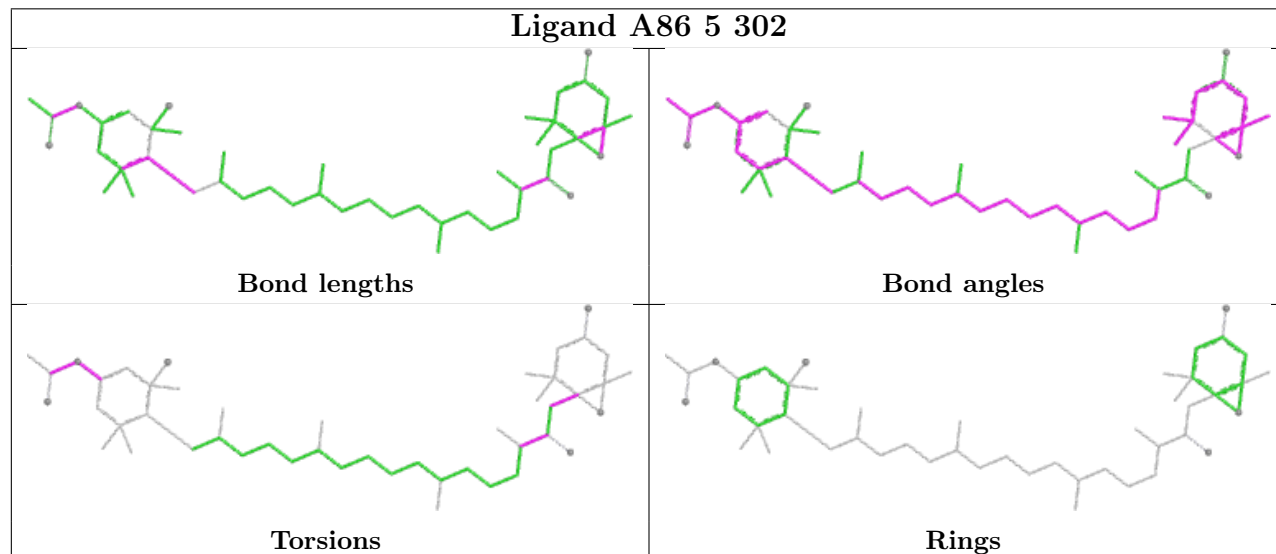
Torsions

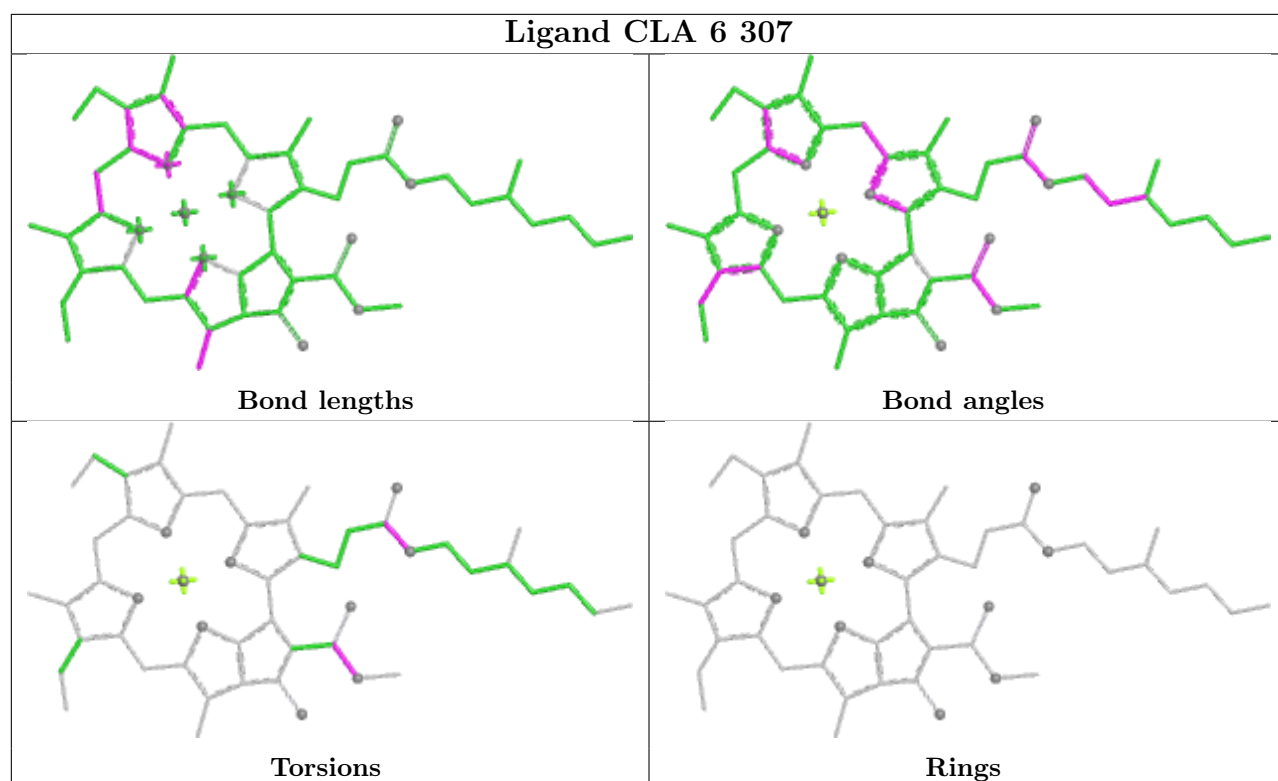


Rings

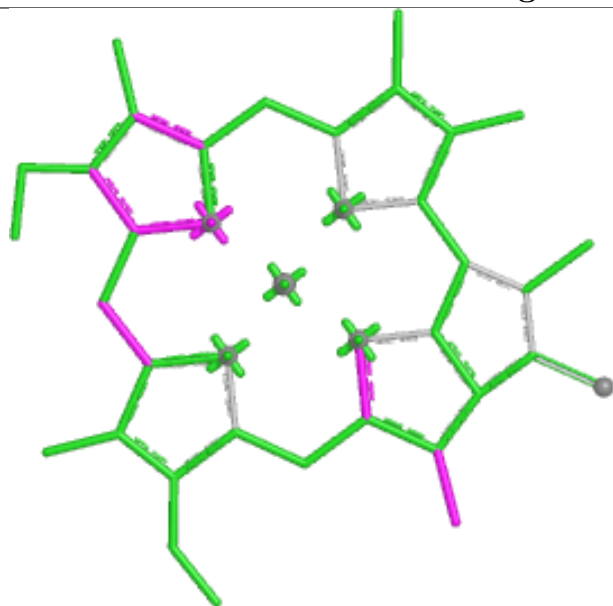




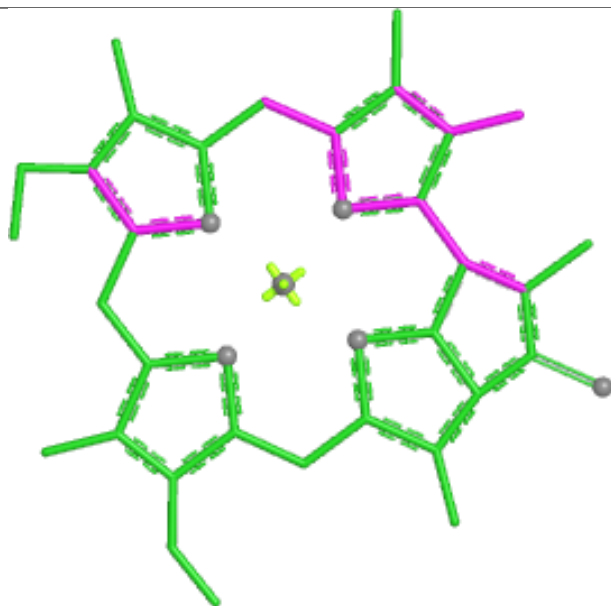
Ligand CLA b 610**Ligand A86 5 302**



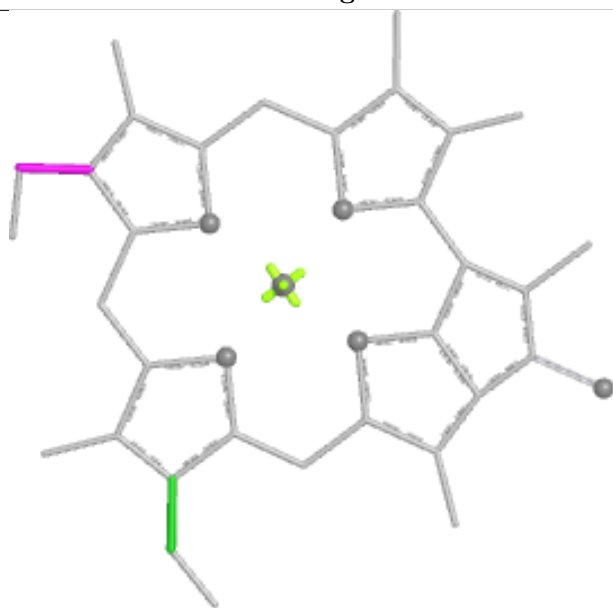
Ligand CLA 2 316



Bond lengths



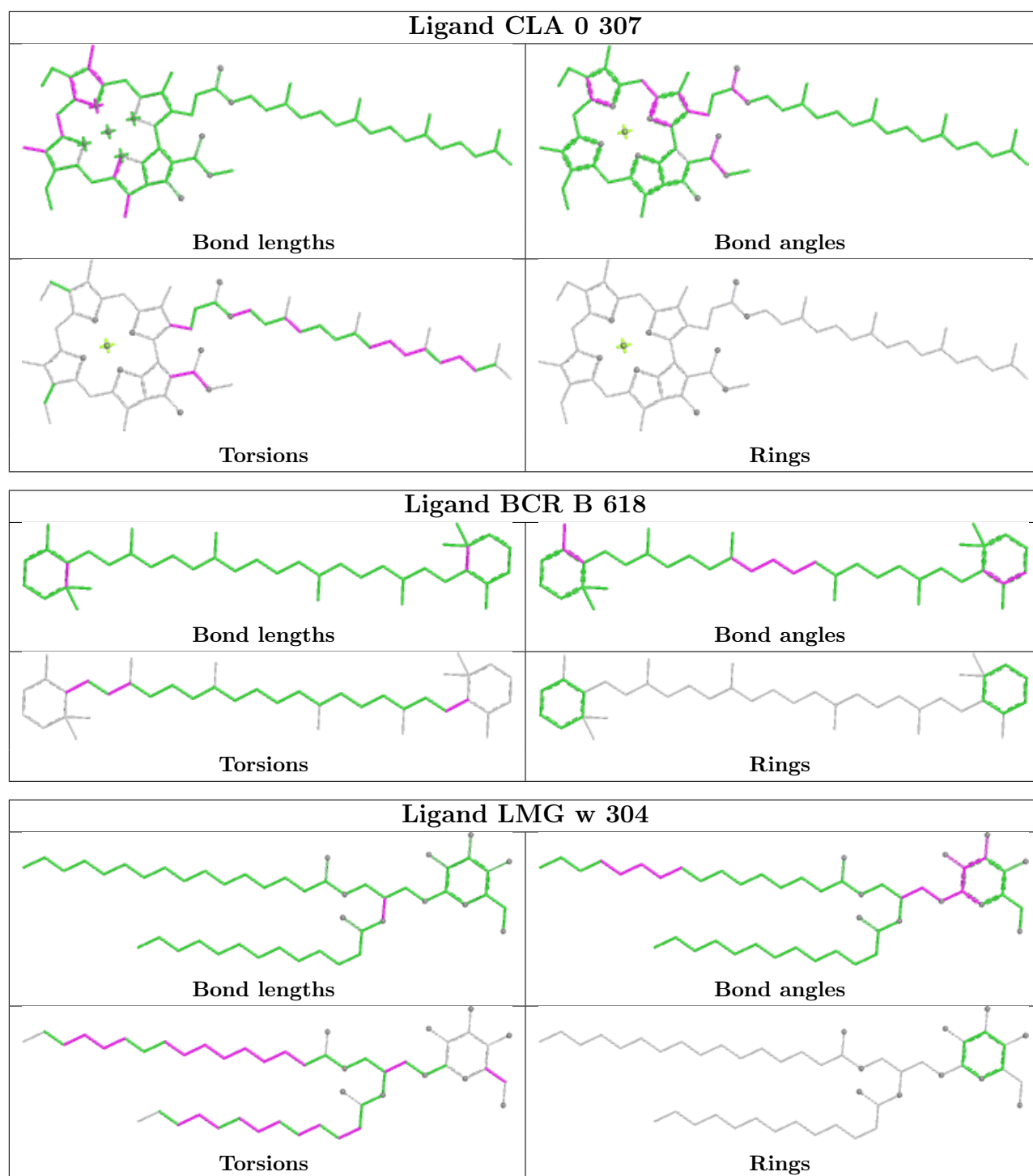
Bond angles



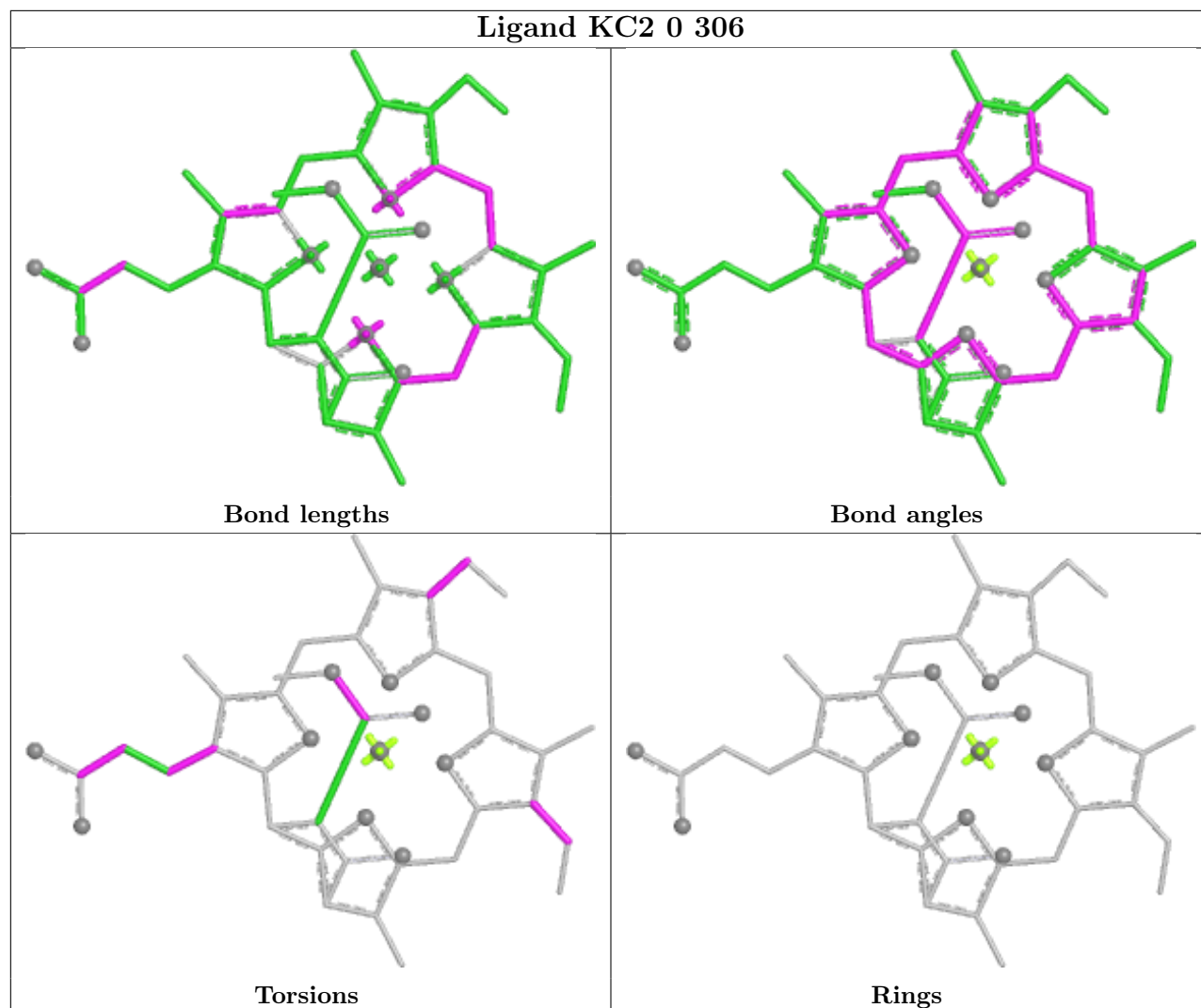
Torsions



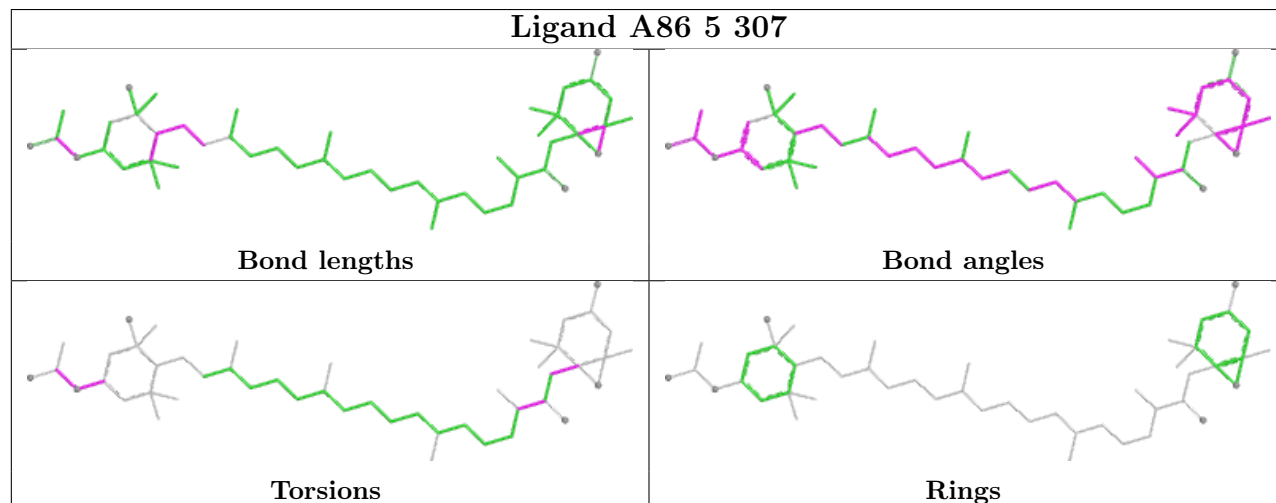
Rings

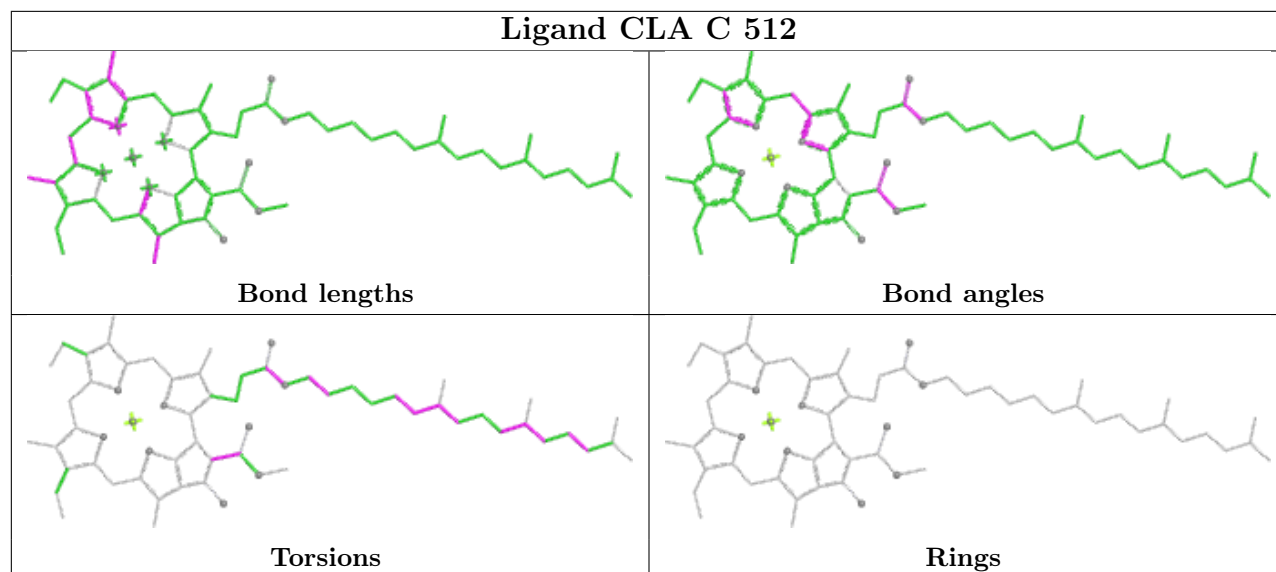
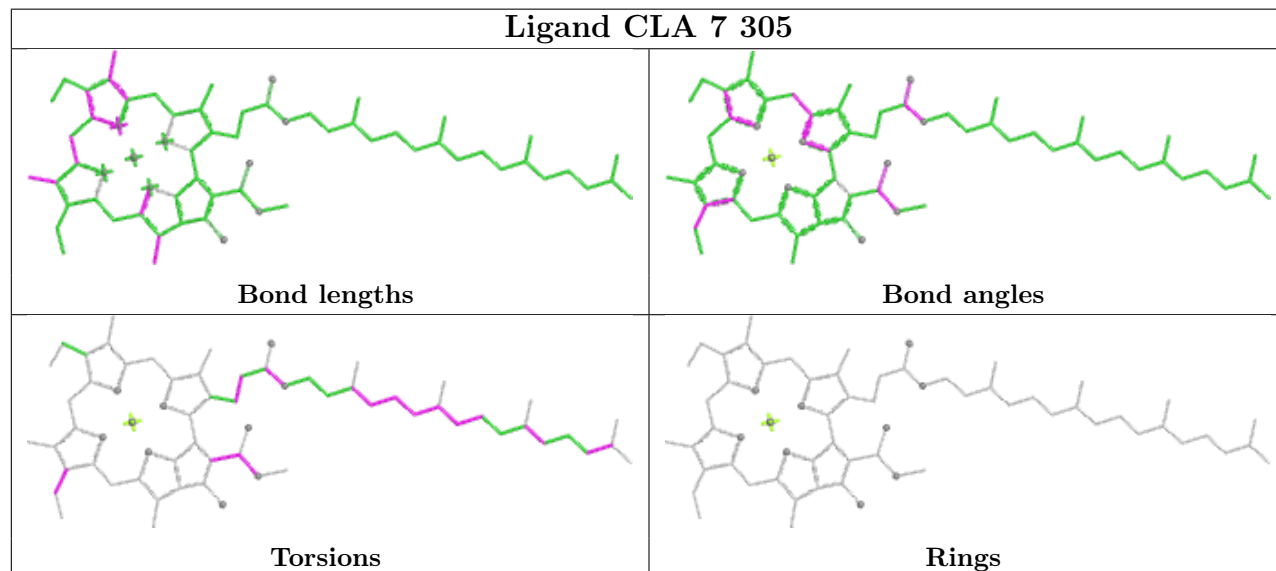


Ligand KC2 0 306

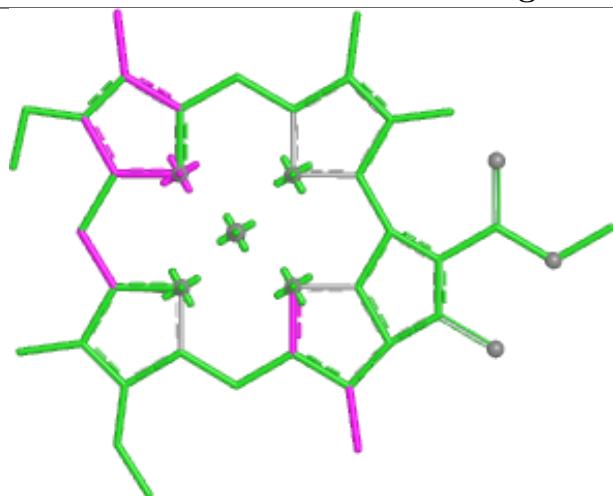


Ligand A86 5 307

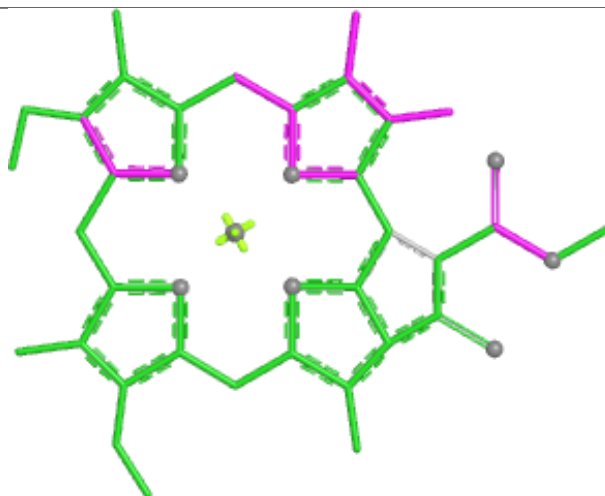


Ligand CLA C 512**Ligand CLA 7 305**

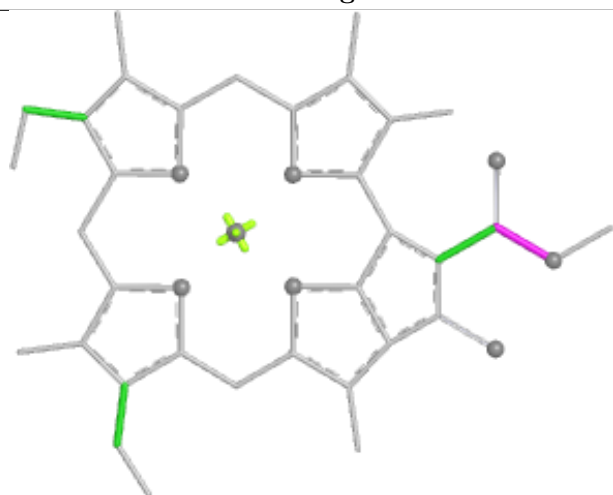
Ligand CLA 0 308



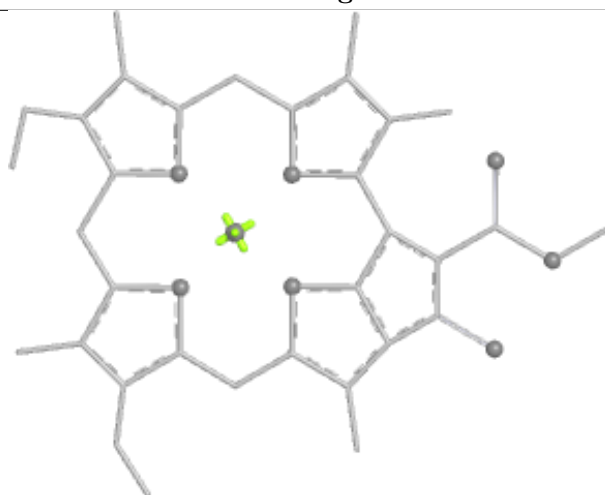
Bond lengths



Bond angles

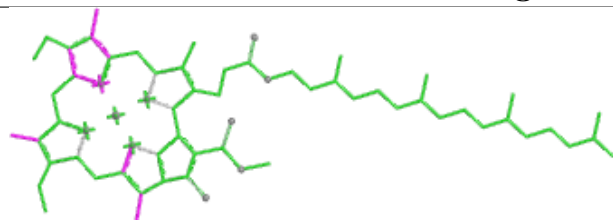


Torsions

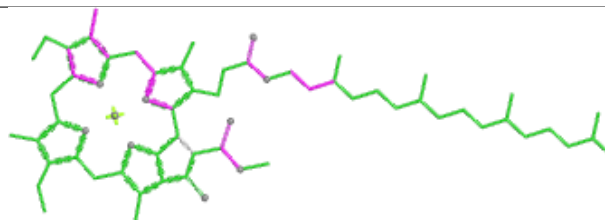


Rings

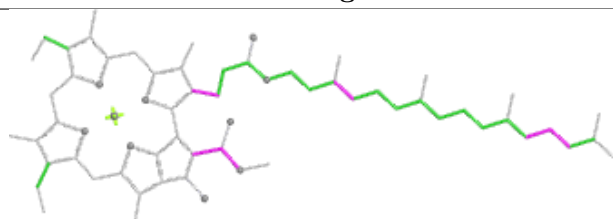
Ligand CLA B 609



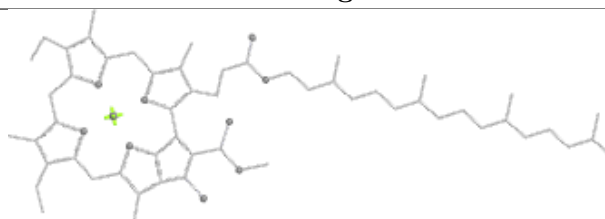
Bond lengths



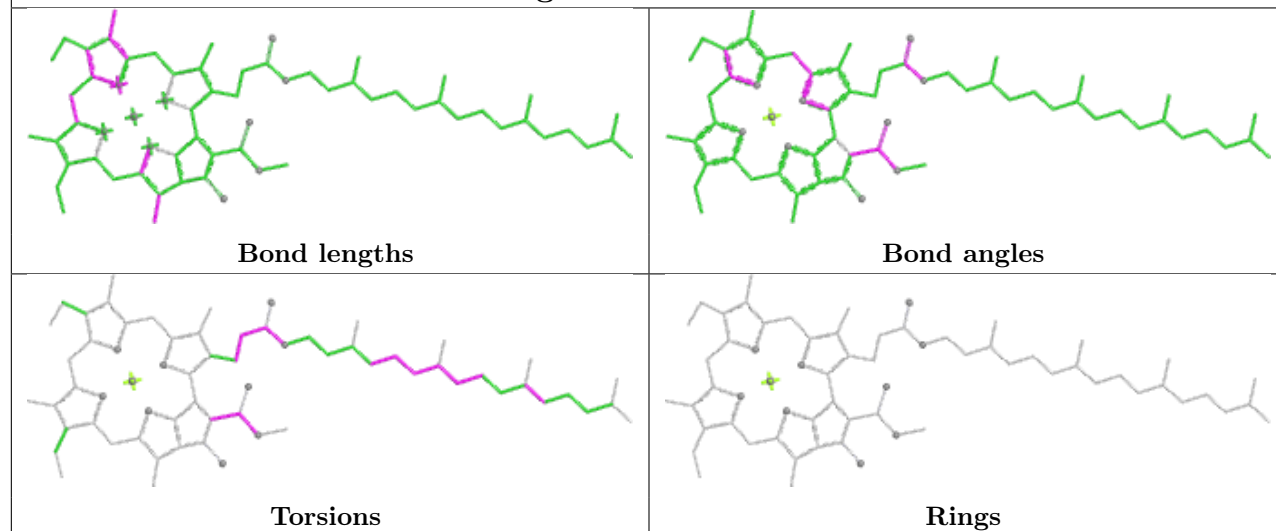
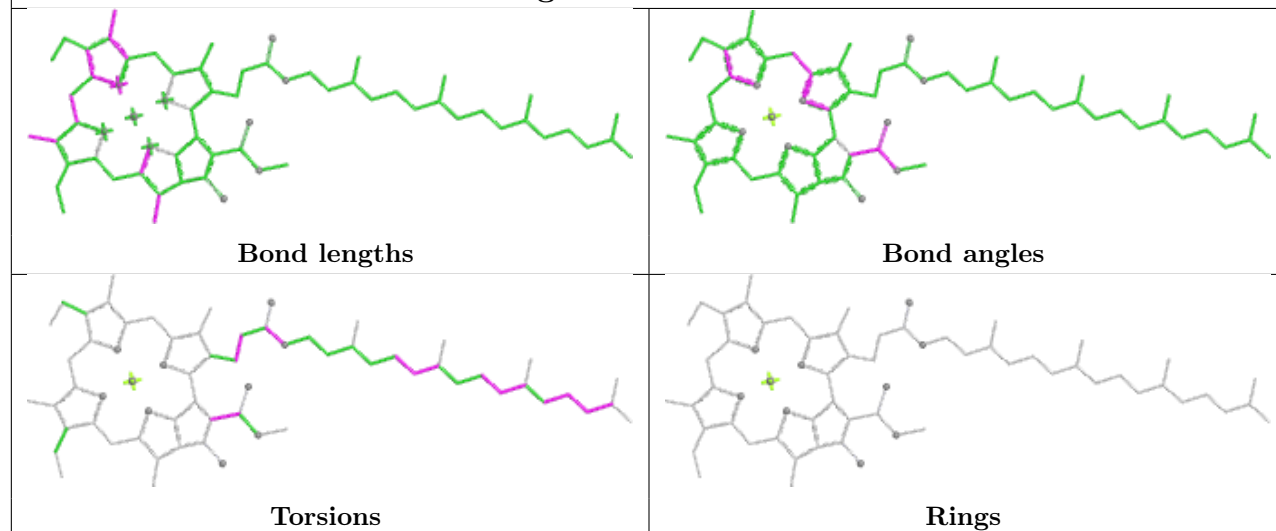
Bond angles



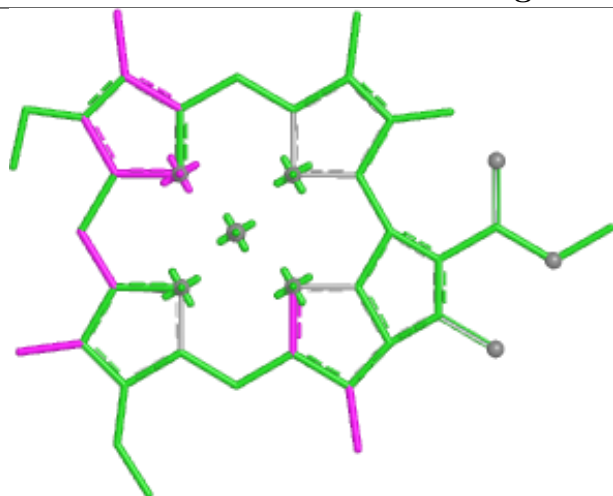
Torsions



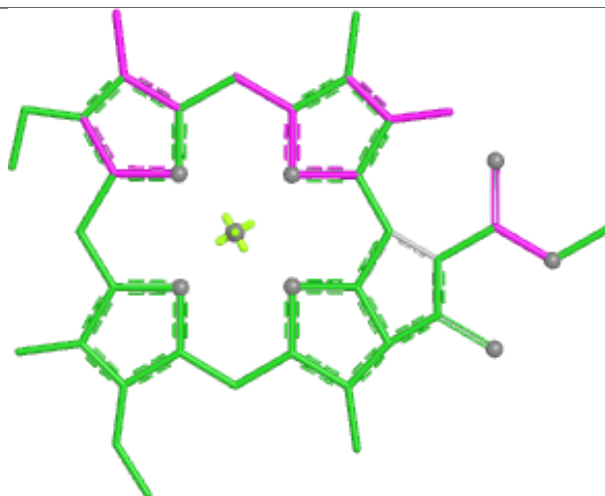
Rings

Ligand CLA 0 305**Ligand CLA c 505**

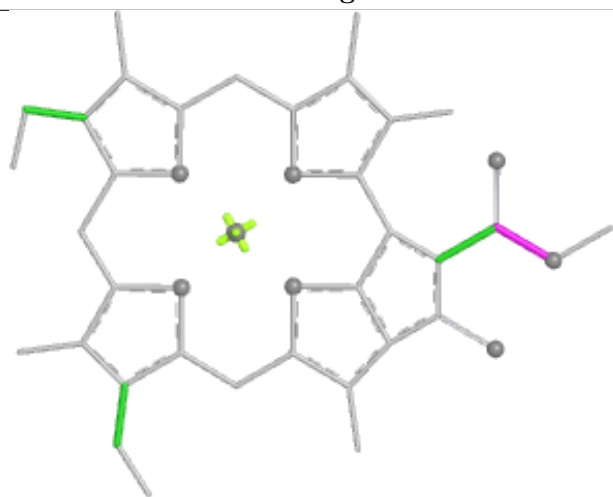
Ligand CLA B 607



Bond lengths



Bond angles

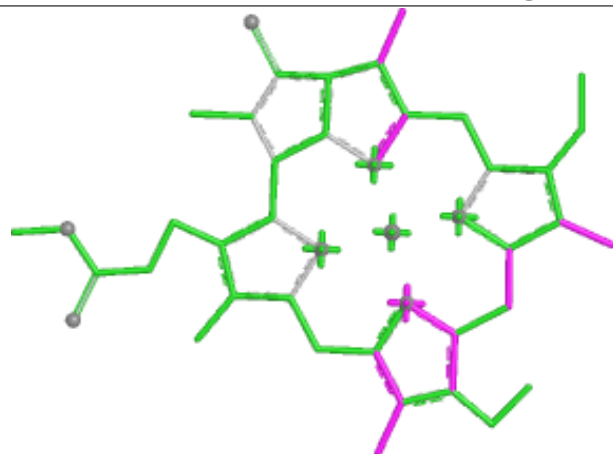


Torsions

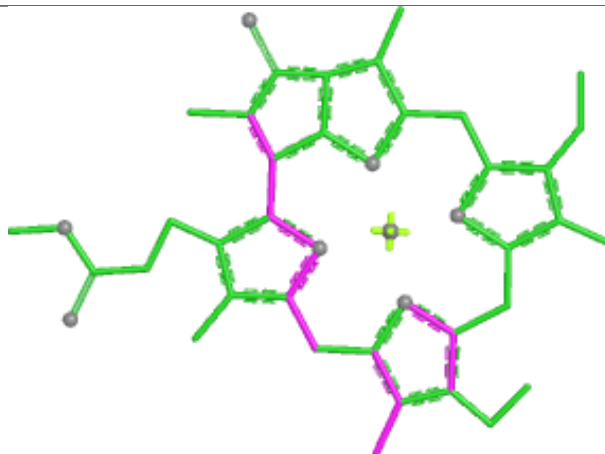


Rings

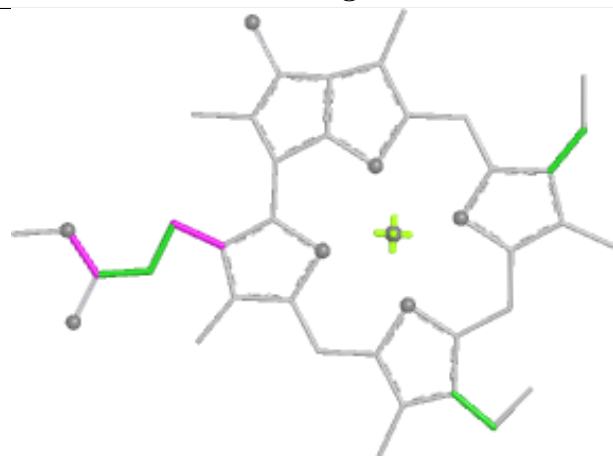
Ligand CLA 7 314



Bond lengths



Bond angles

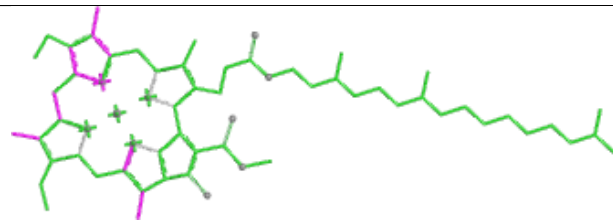


Torsions

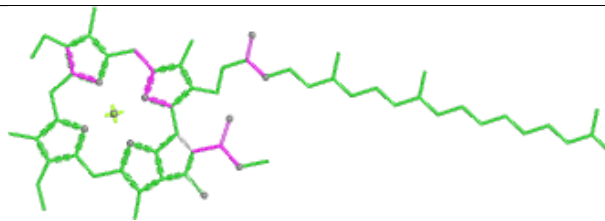


Rings

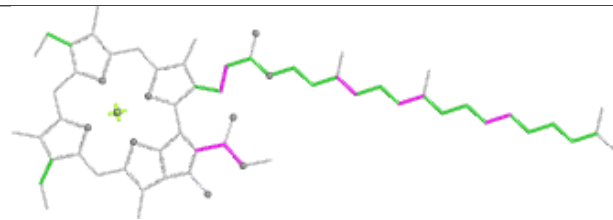
Ligand CLA B 603



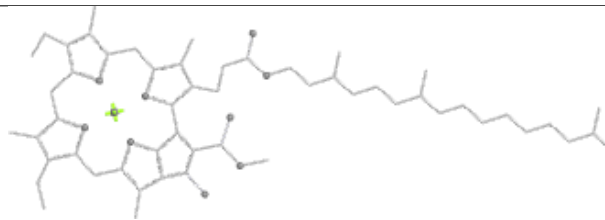
Bond lengths



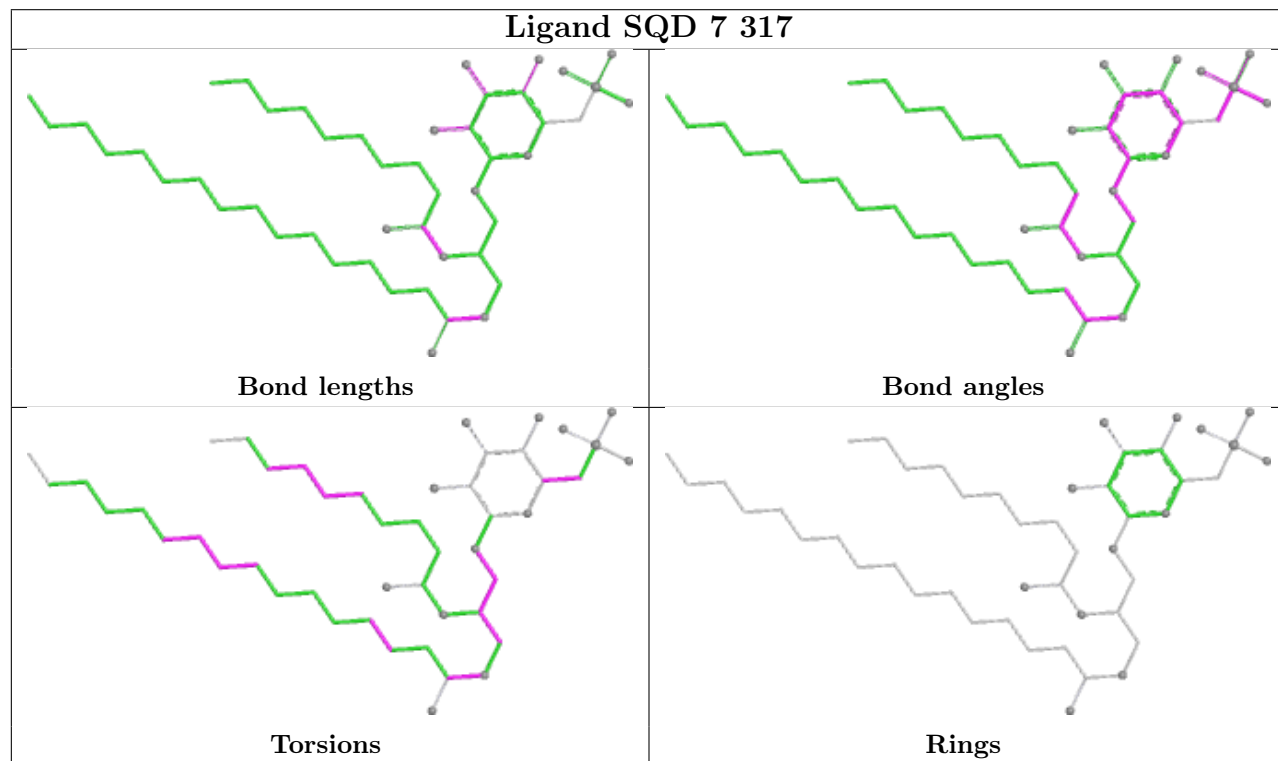
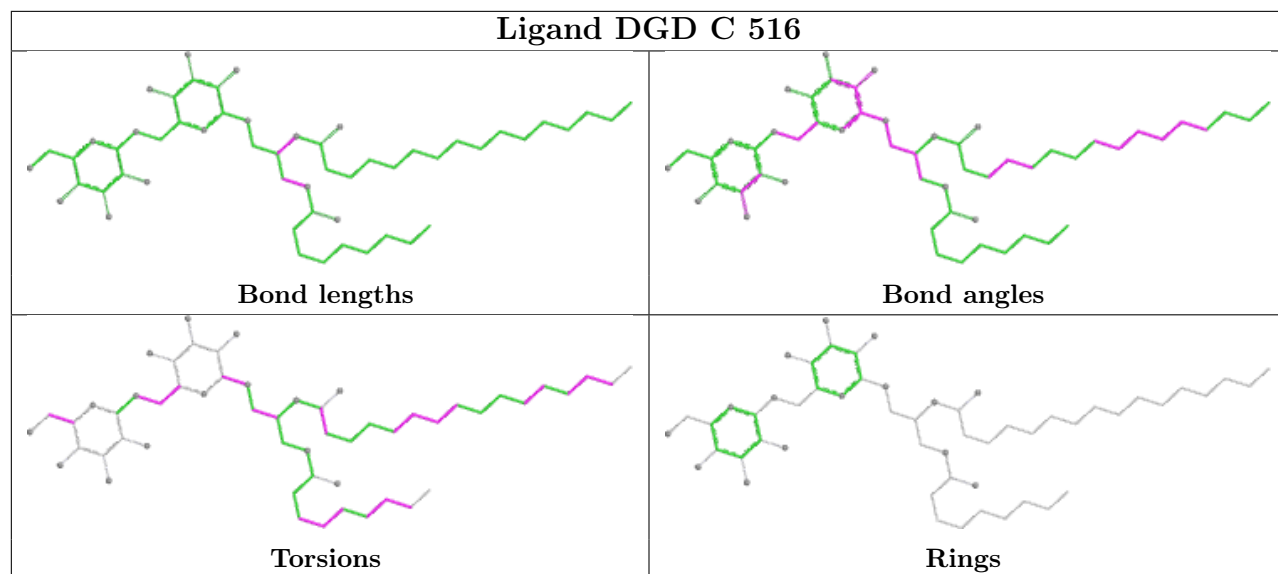
Bond angles



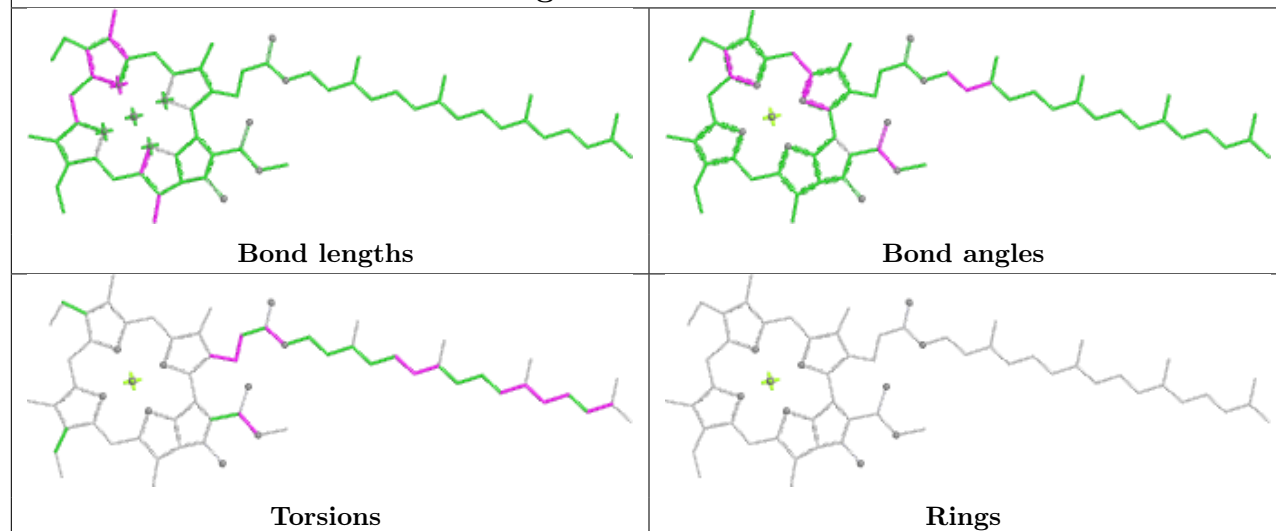
Torsions



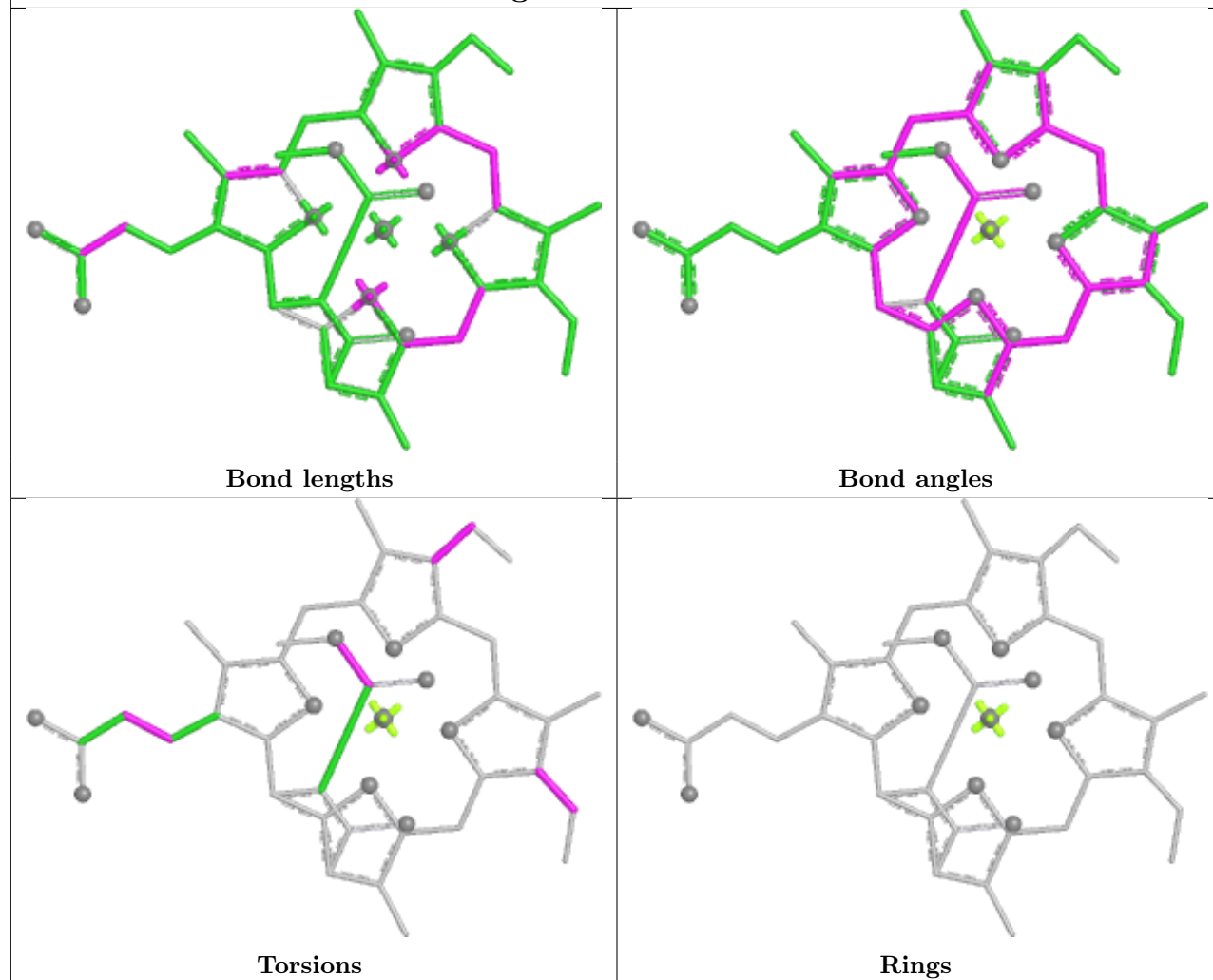
Rings



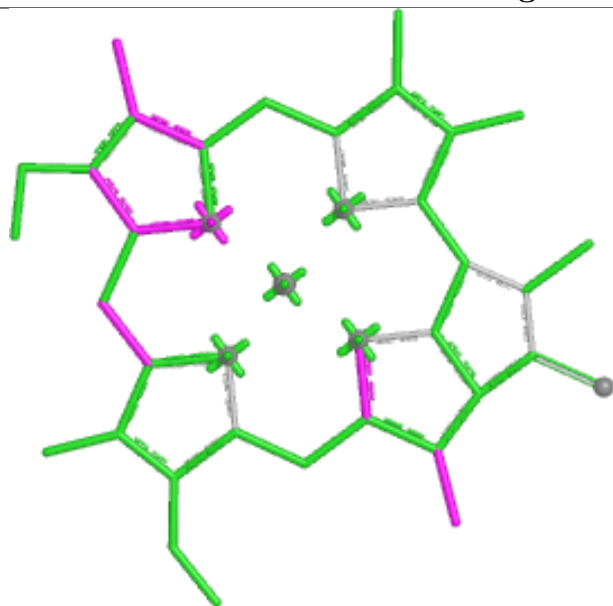
Ligand CLA 1 310



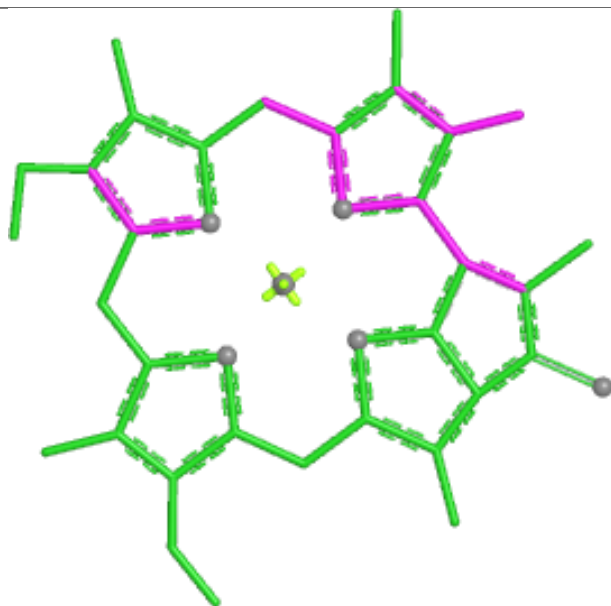
Ligand KC2 5 310



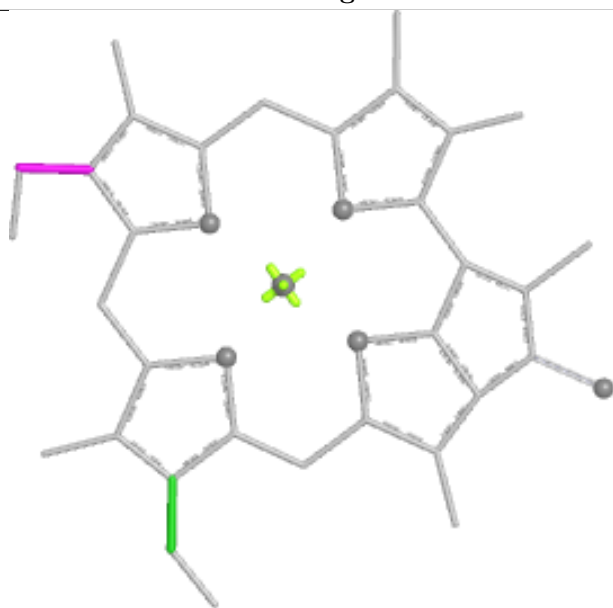
Ligand CLA 8 314



Bond lengths



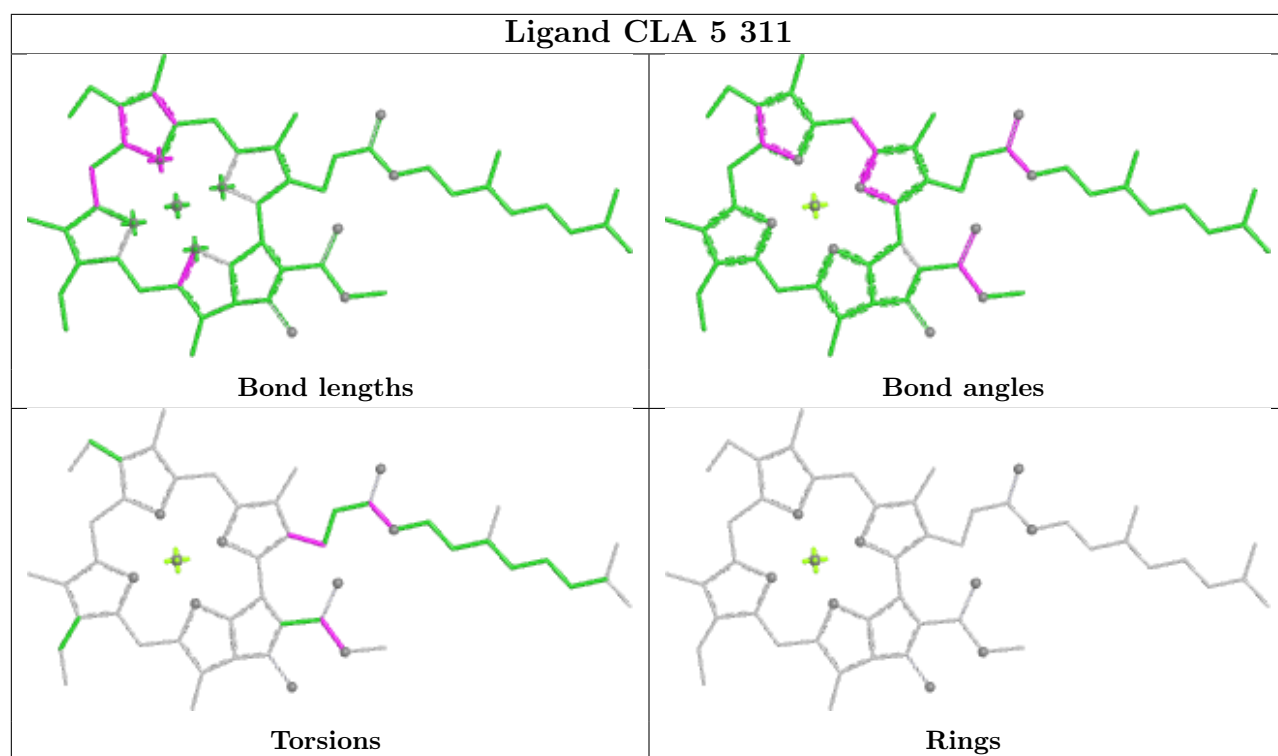
Bond angles



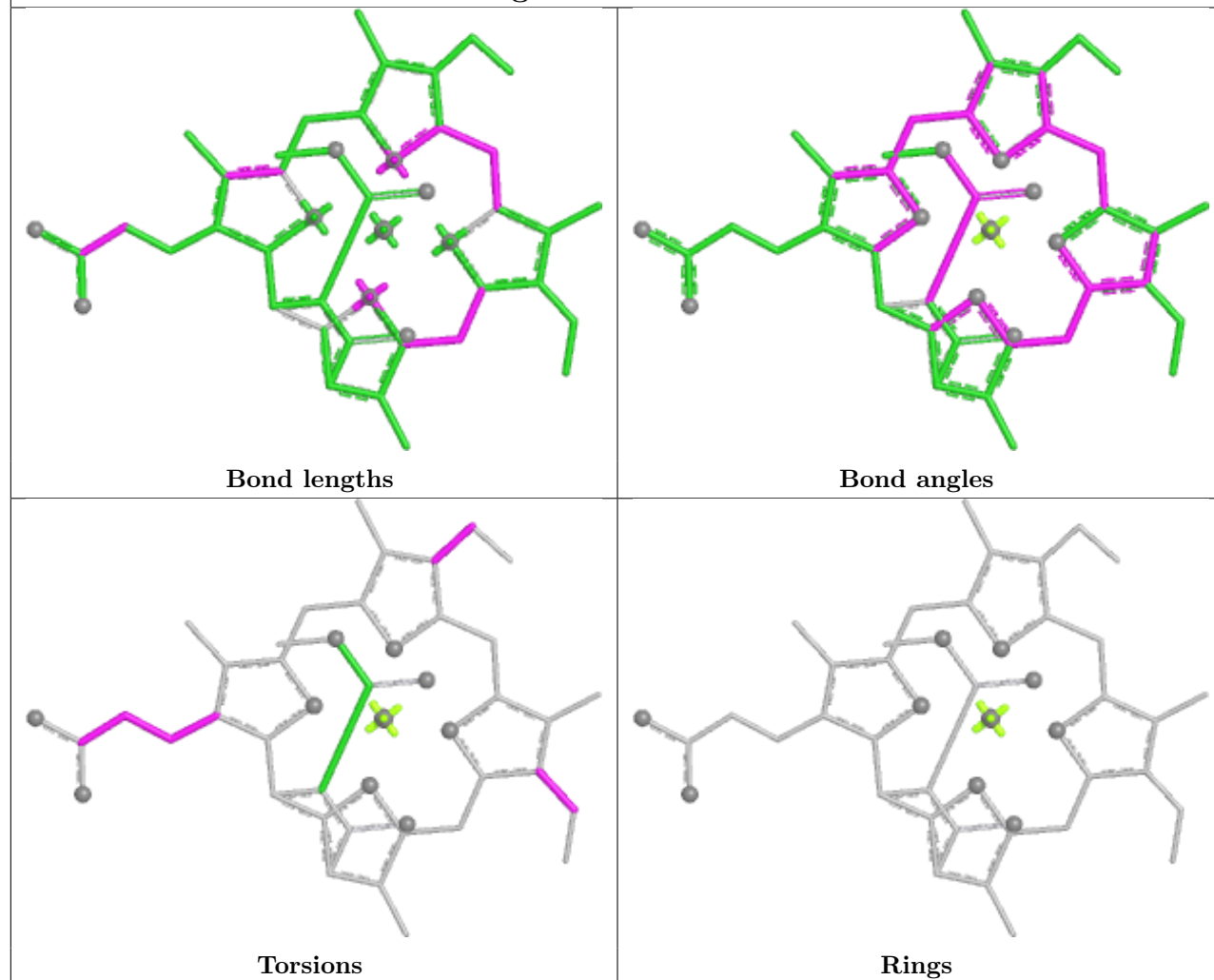
Torsions



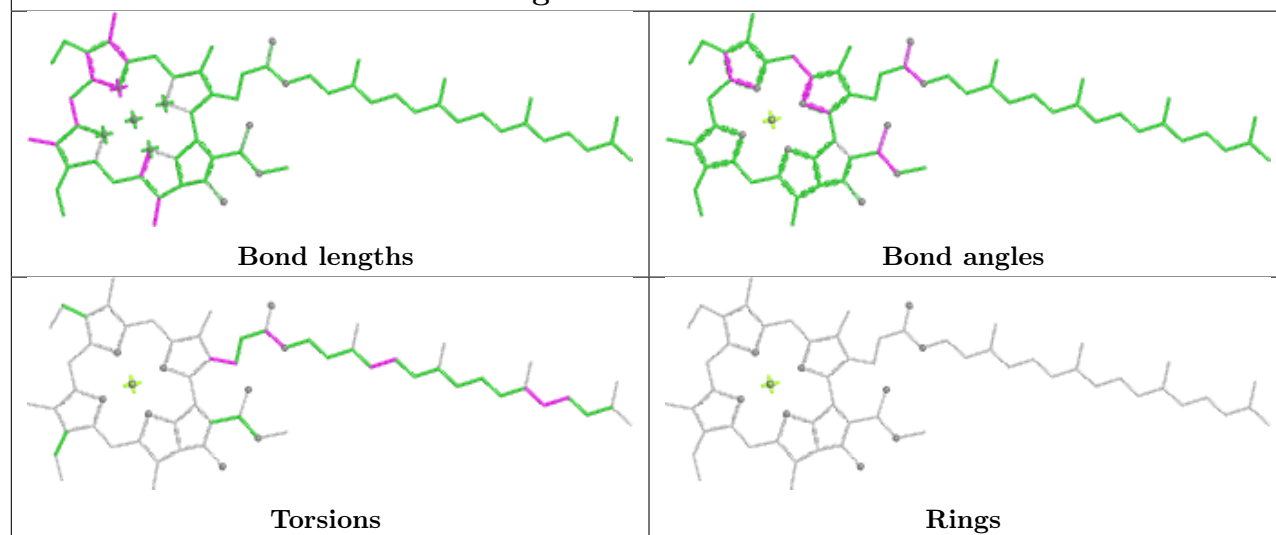
Rings



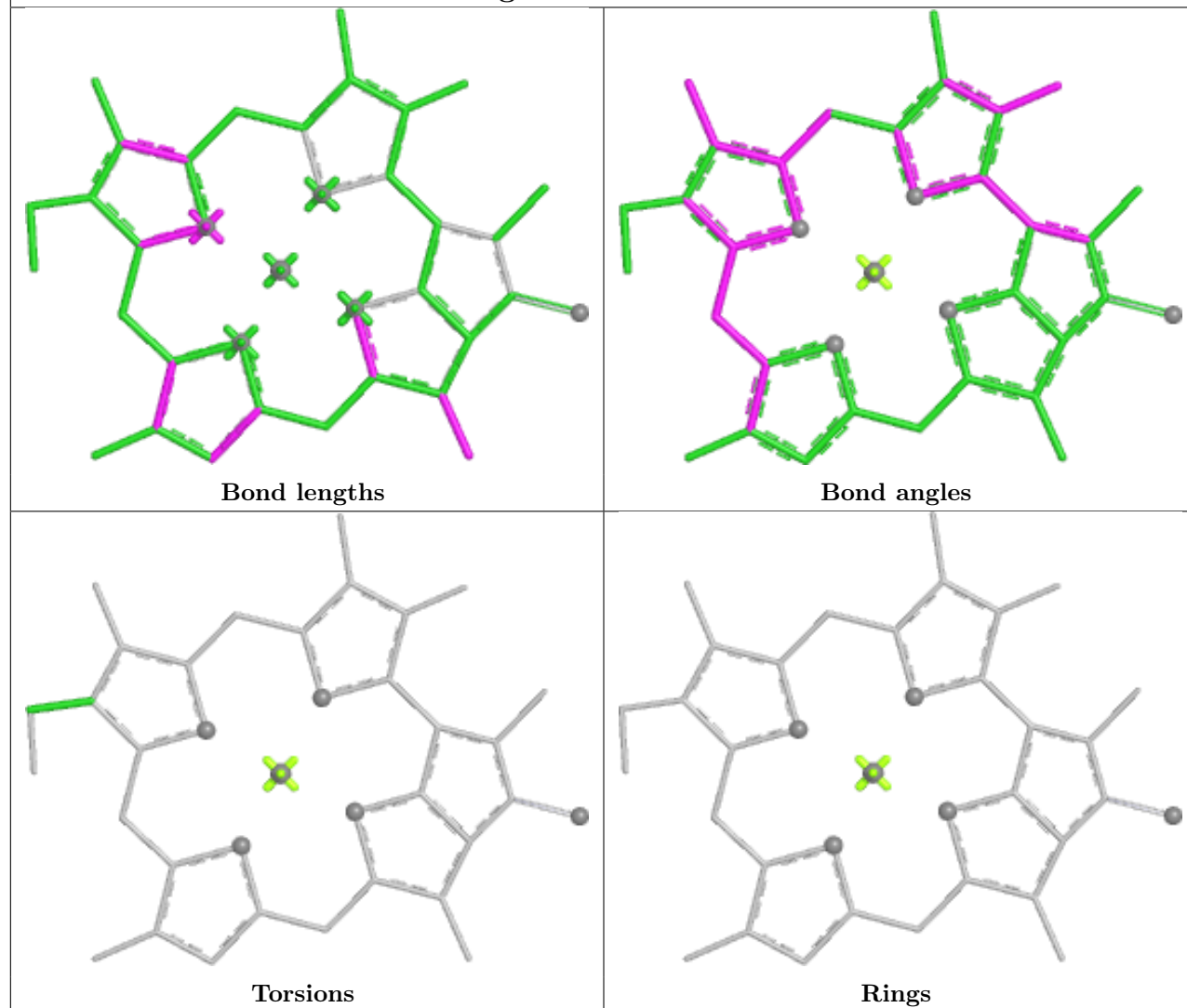
Ligand KC2 7 306



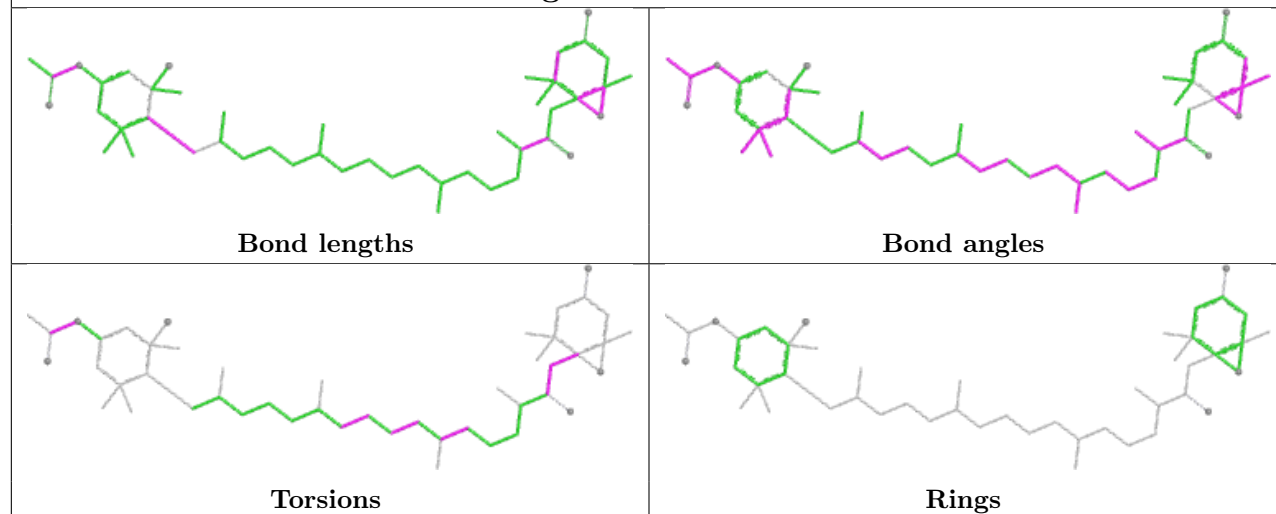
Ligand CLA C 511

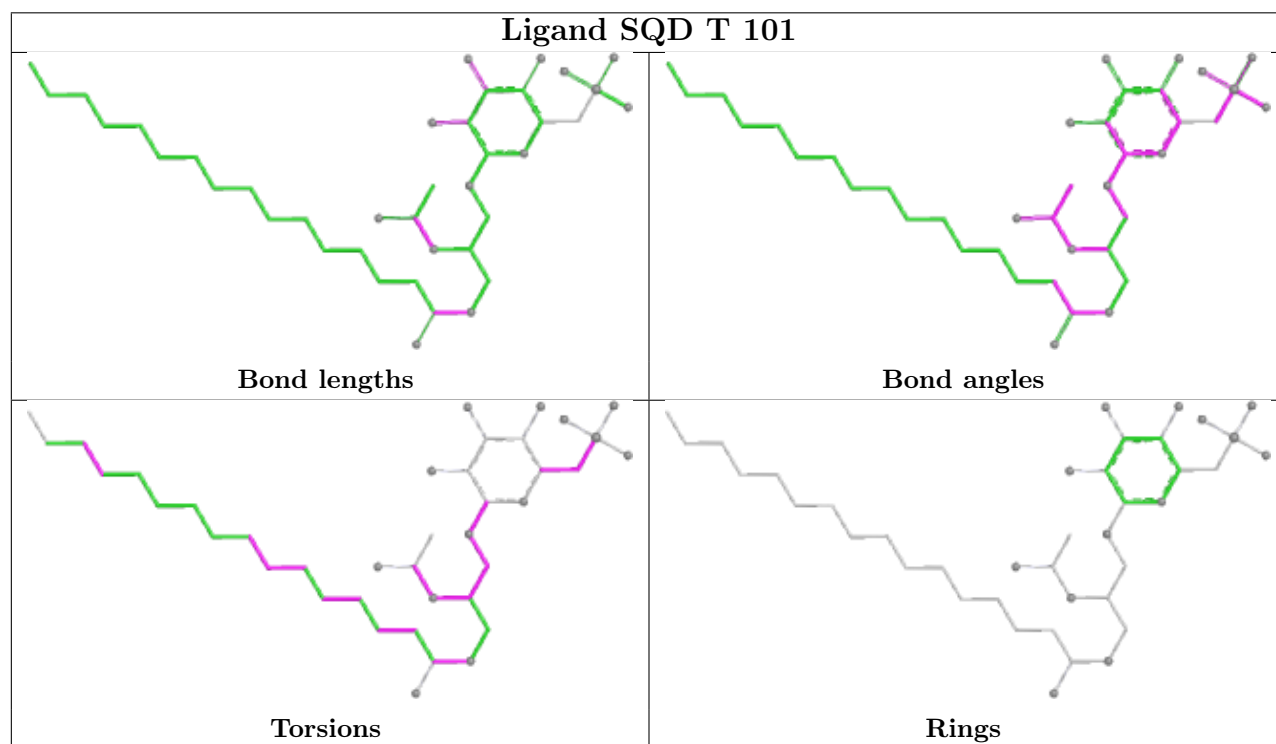
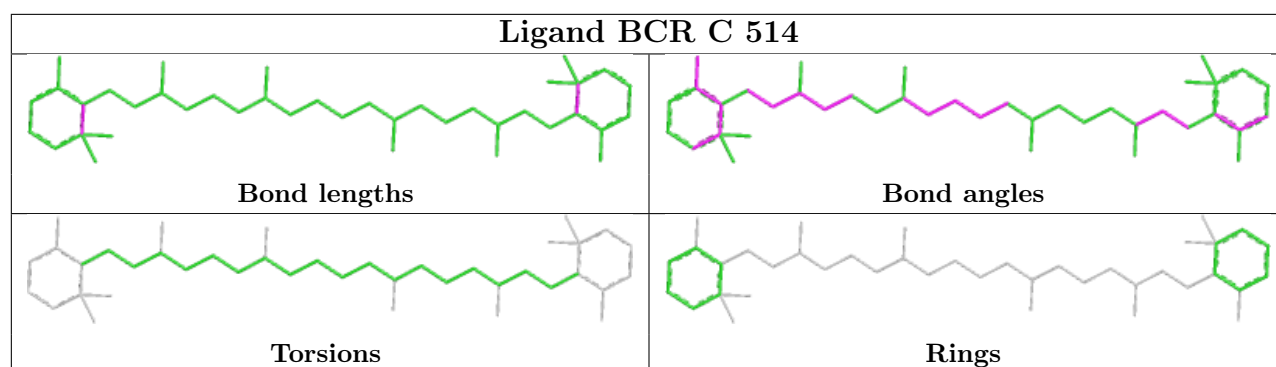


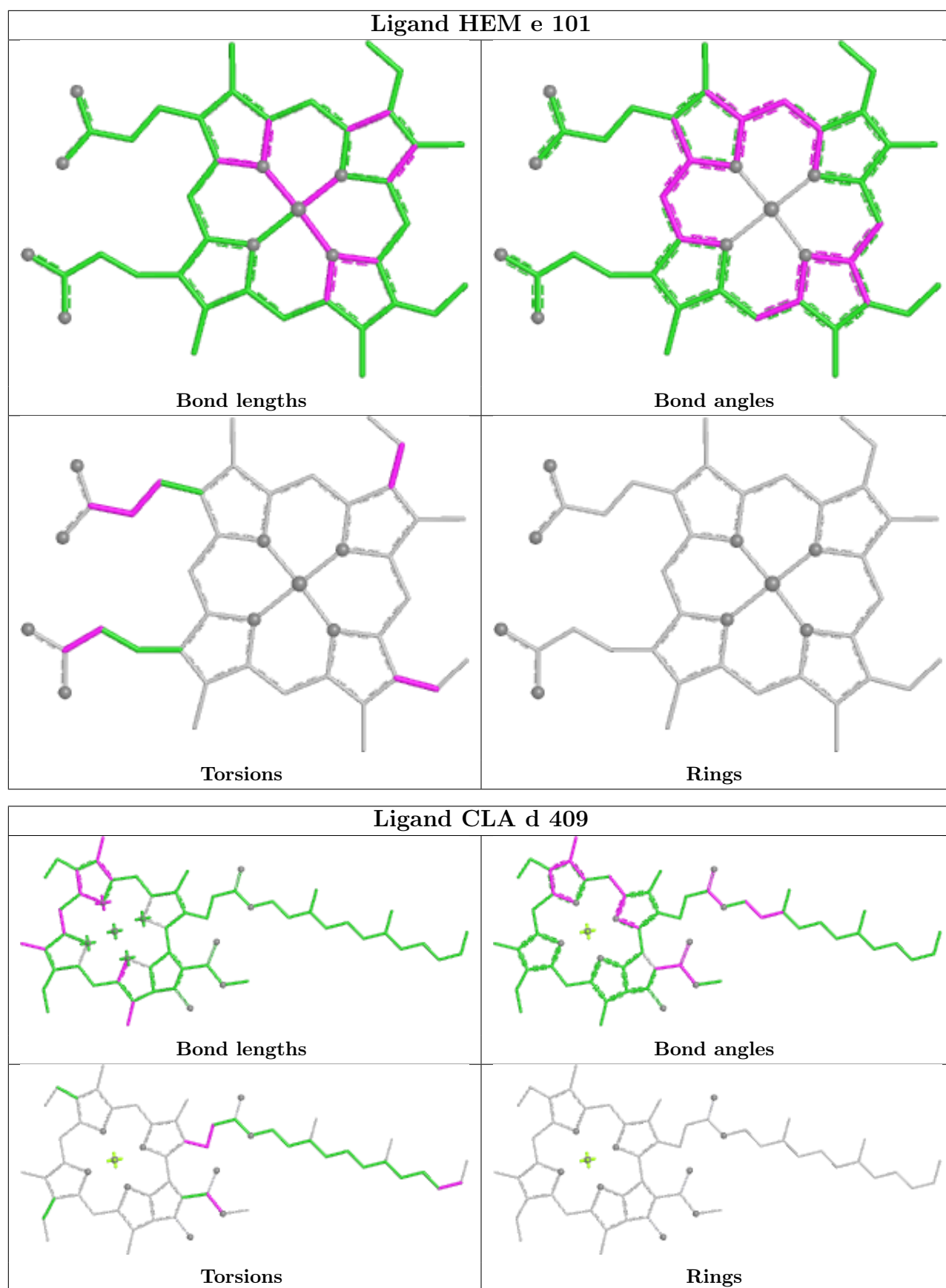
Ligand CLA 2 313



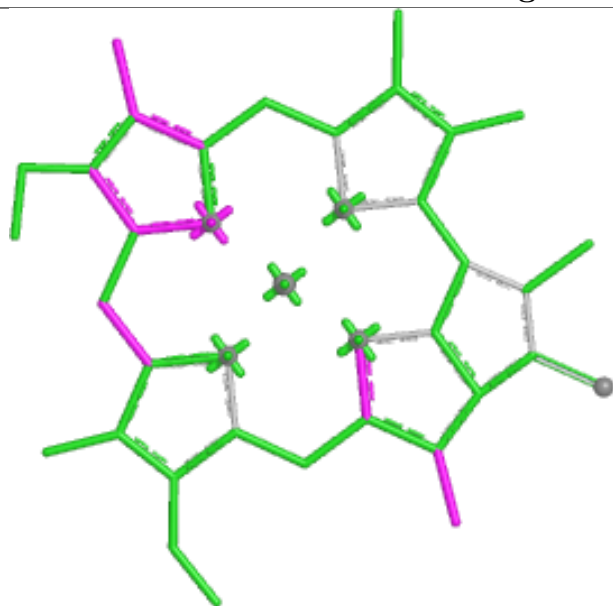
Ligand A86 0 301



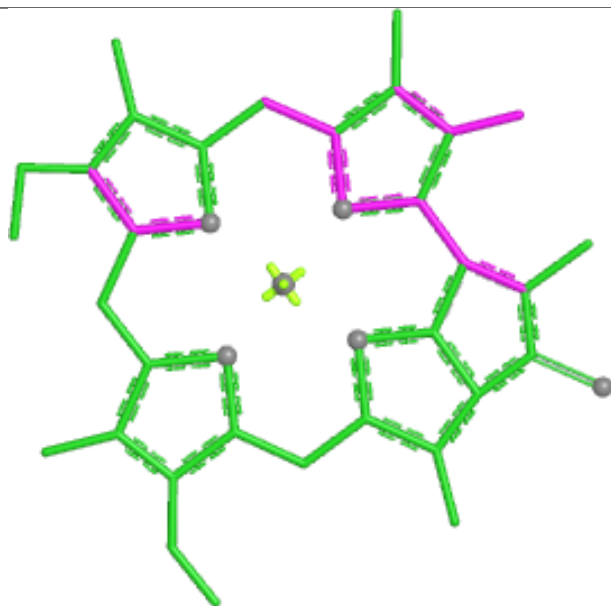




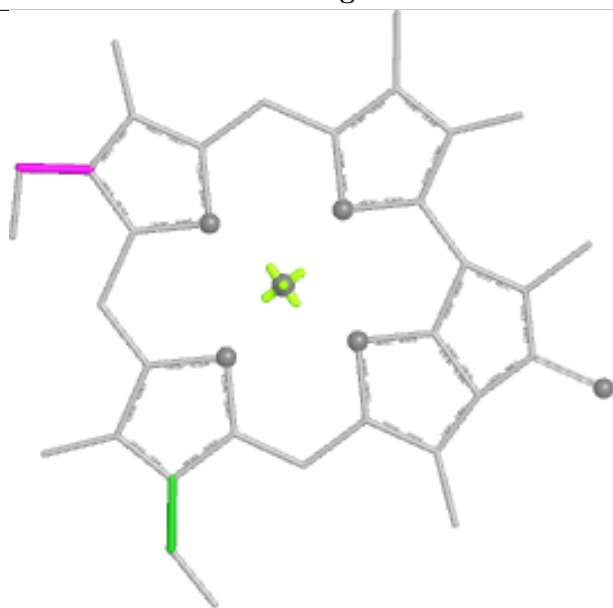
Ligand CLA 2 315



Bond lengths



Bond angles

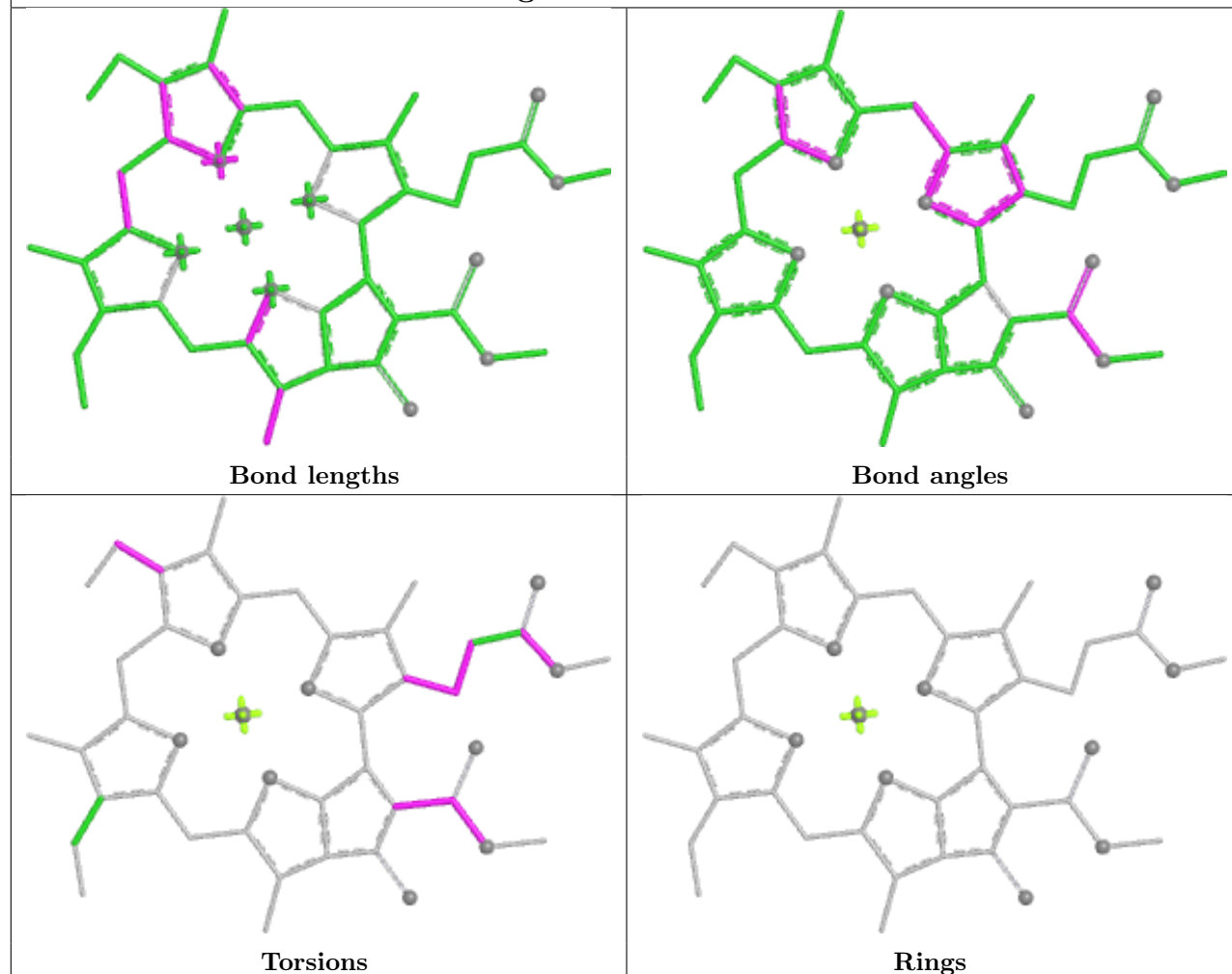


Torsions

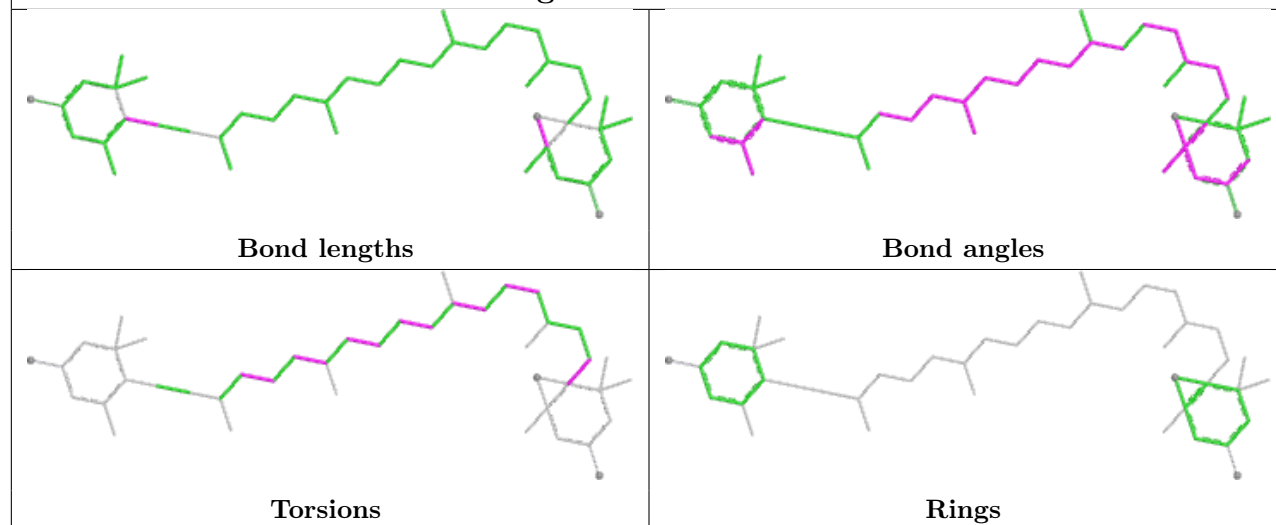


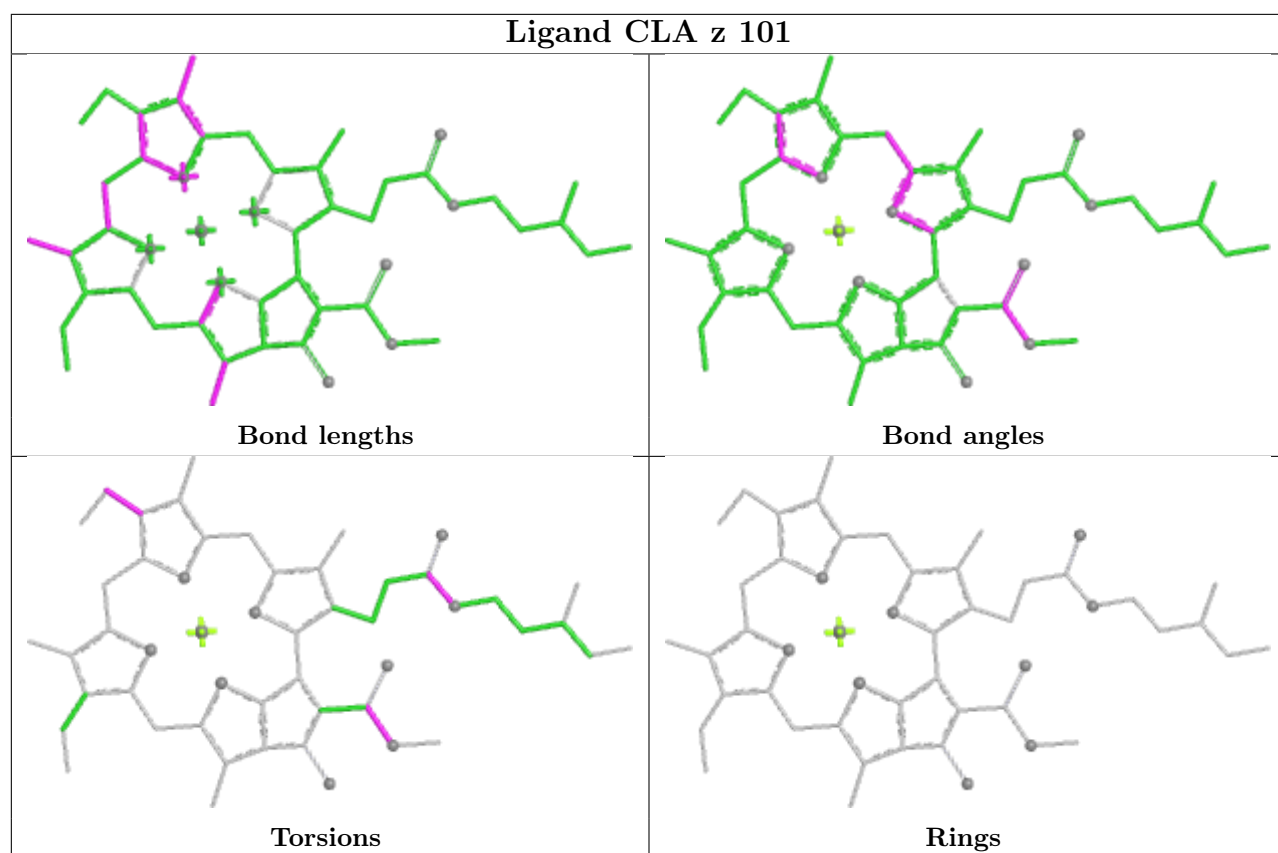
Rings

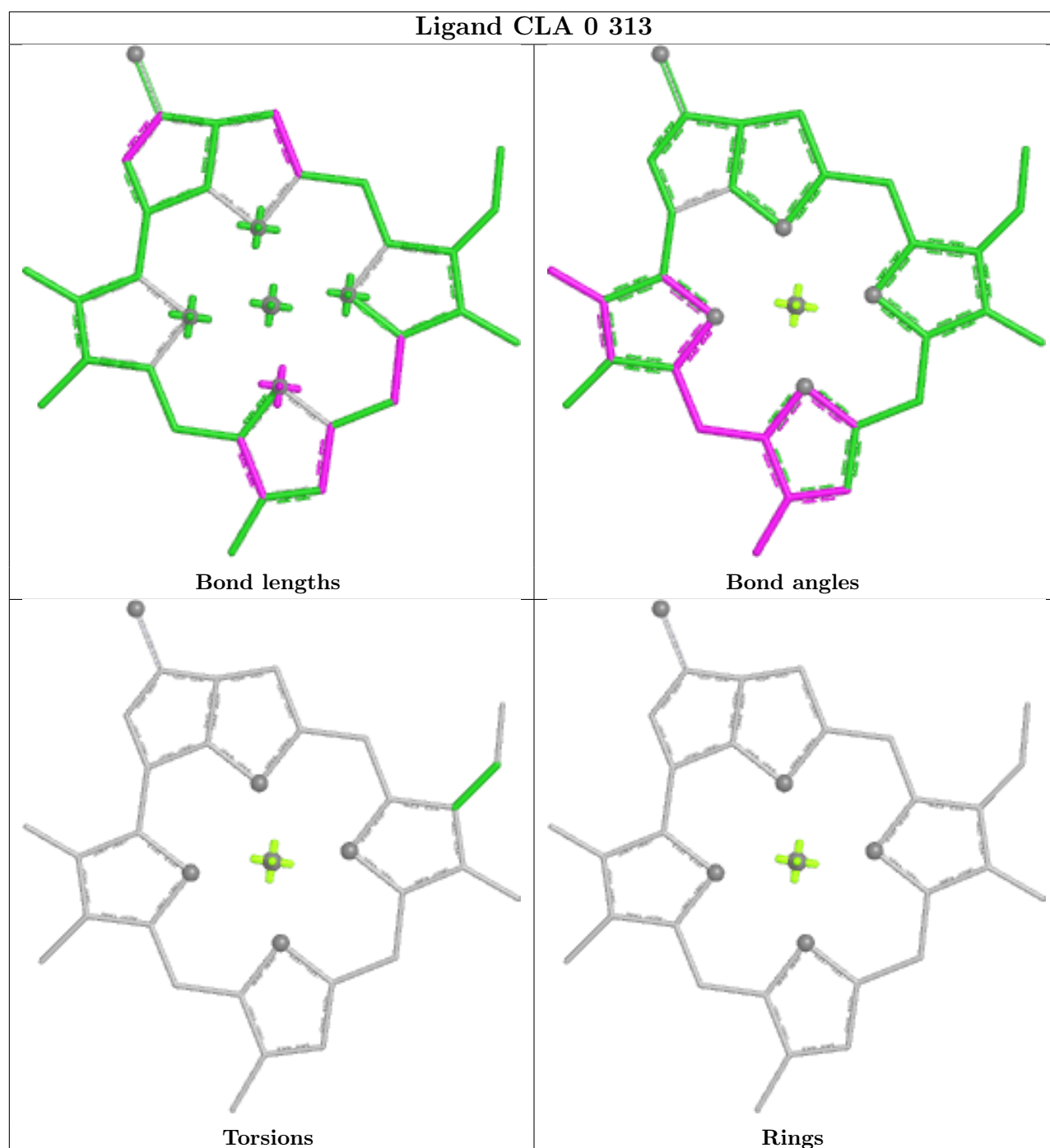
Ligand CLA 6 311



Ligand DD6 8 304







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

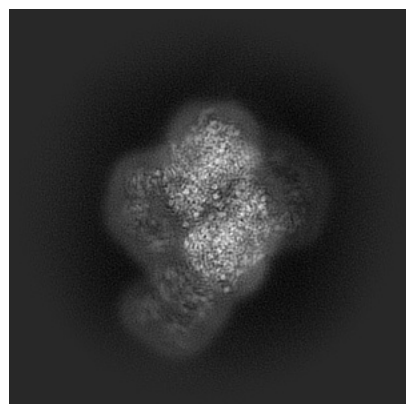
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35766. These allow visual inspection of the internal detail of the map and identification of artifacts.

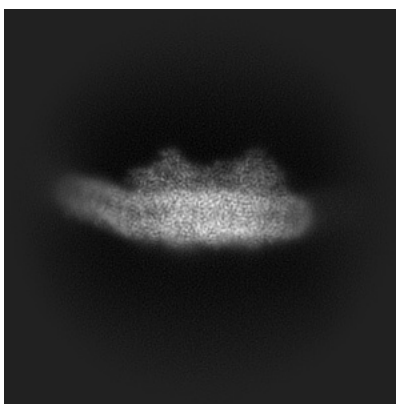
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

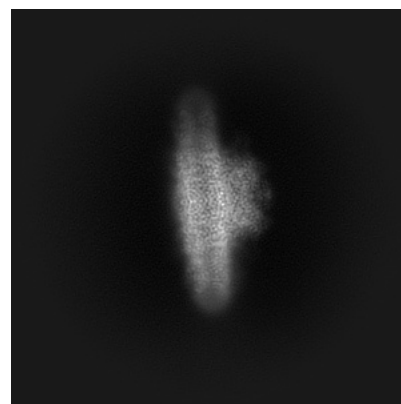
6.1.1 Primary map



X

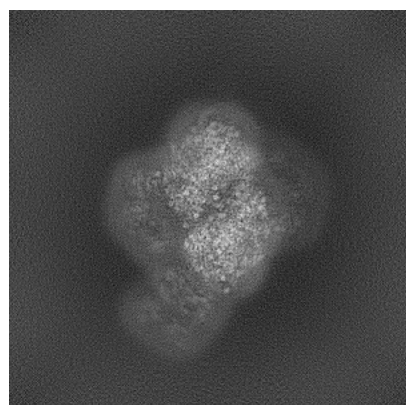


Y

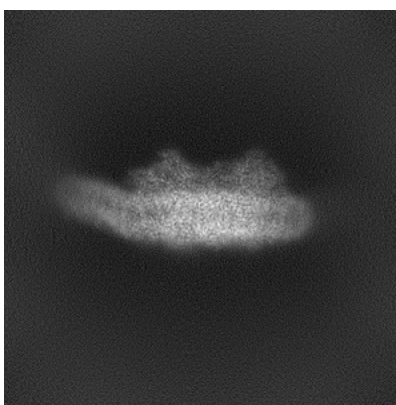


Z

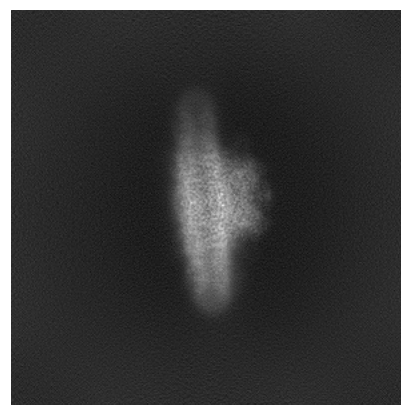
6.1.2 Raw map



X



Y

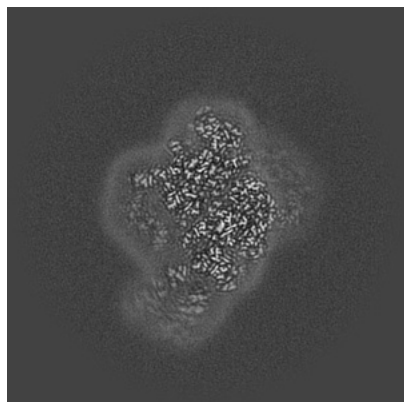


Z

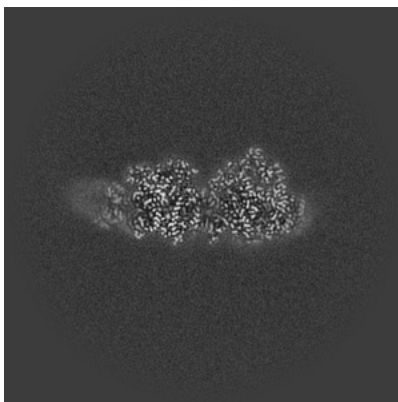
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

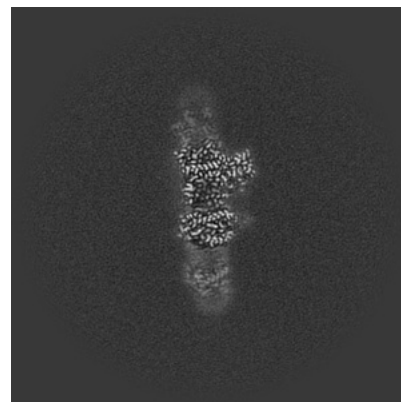
6.2.1 Primary map



X Index: 250

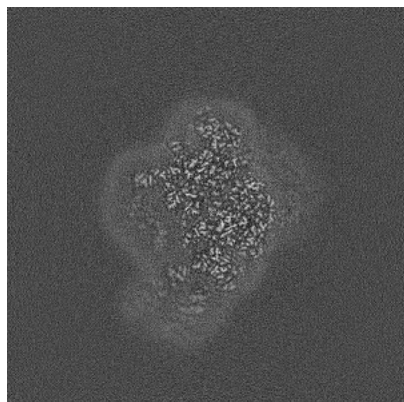


Y Index: 250

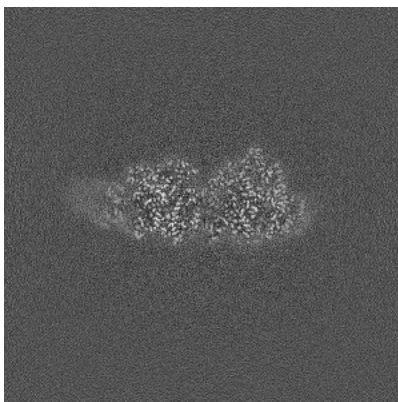


Z Index: 250

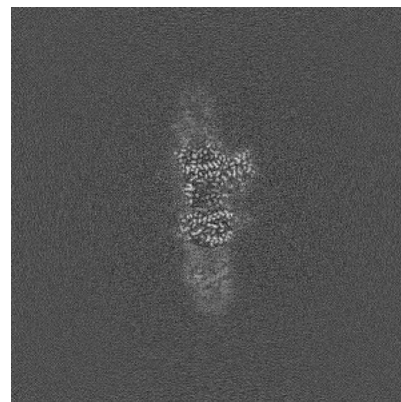
6.2.2 Raw map



X Index: 250



Y Index: 250

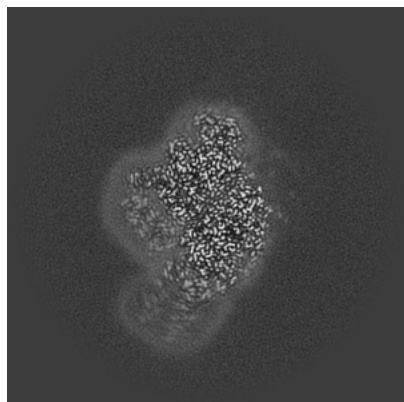


Z Index: 250

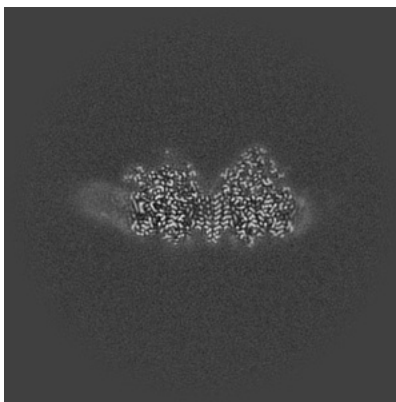
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

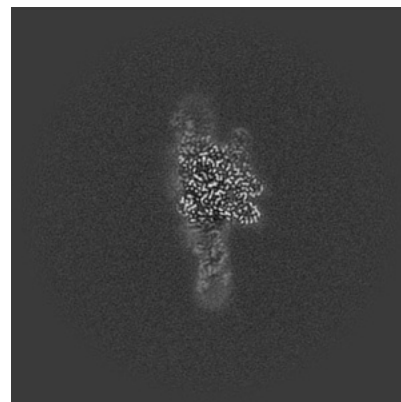
6.3.1 Primary map



X Index: 259

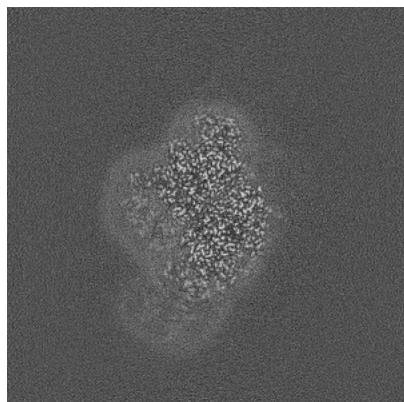


Y Index: 259

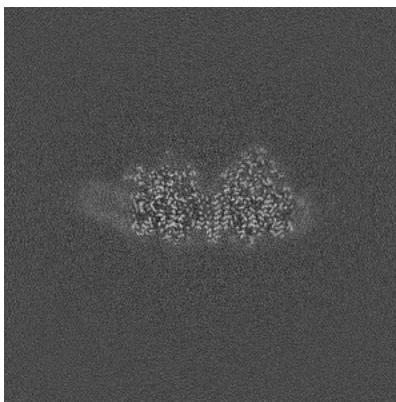


Z Index: 223

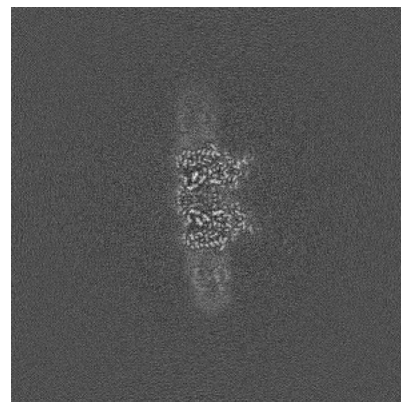
6.3.2 Raw map



X Index: 259



Y Index: 259

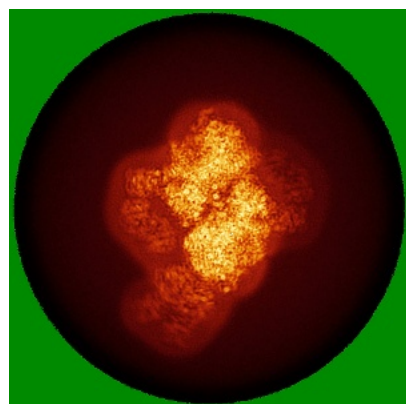


Z Index: 260

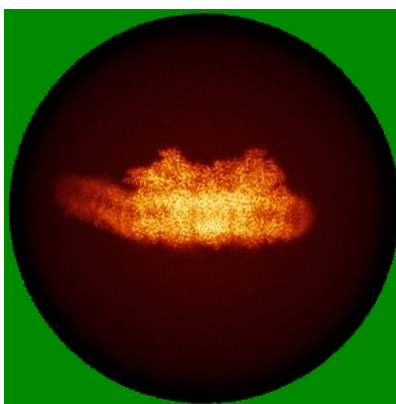
The images above show the largest variance slices of the map in three orthogonal directions.

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

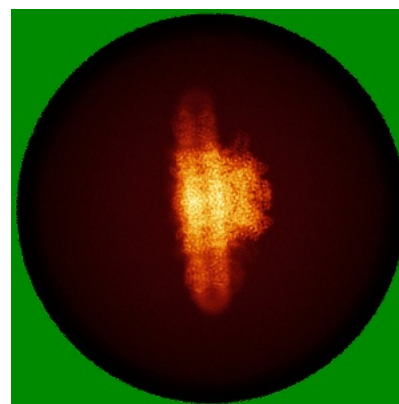
6.4.1 Primary map



X

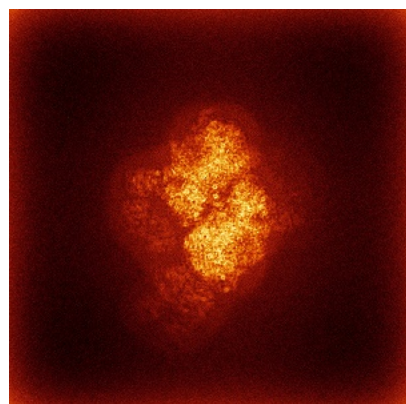


Y

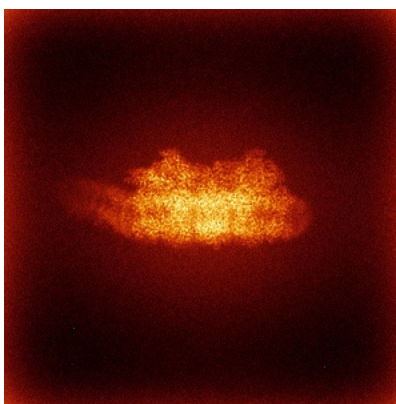


Z

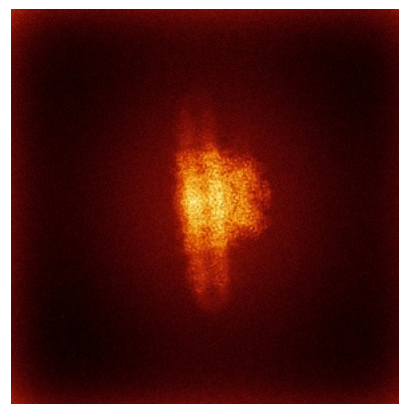
6.4.2 Raw map



X



Y

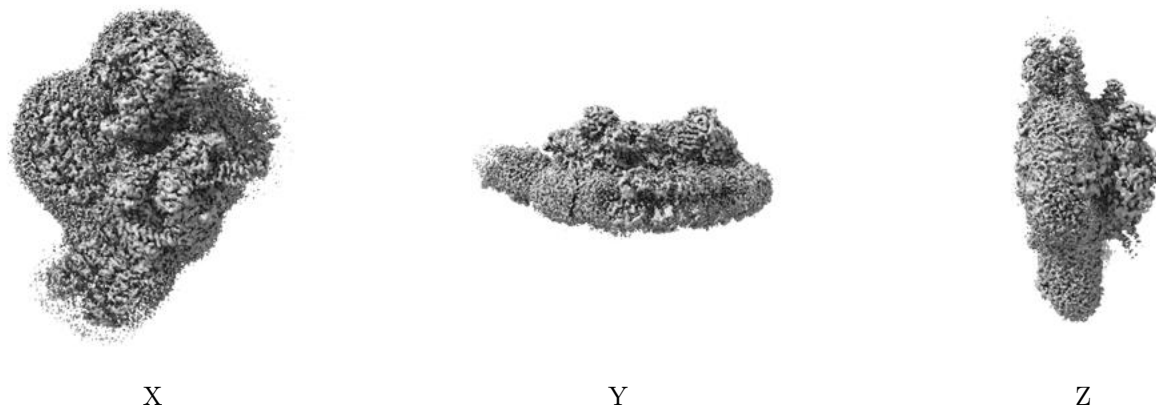


Z

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

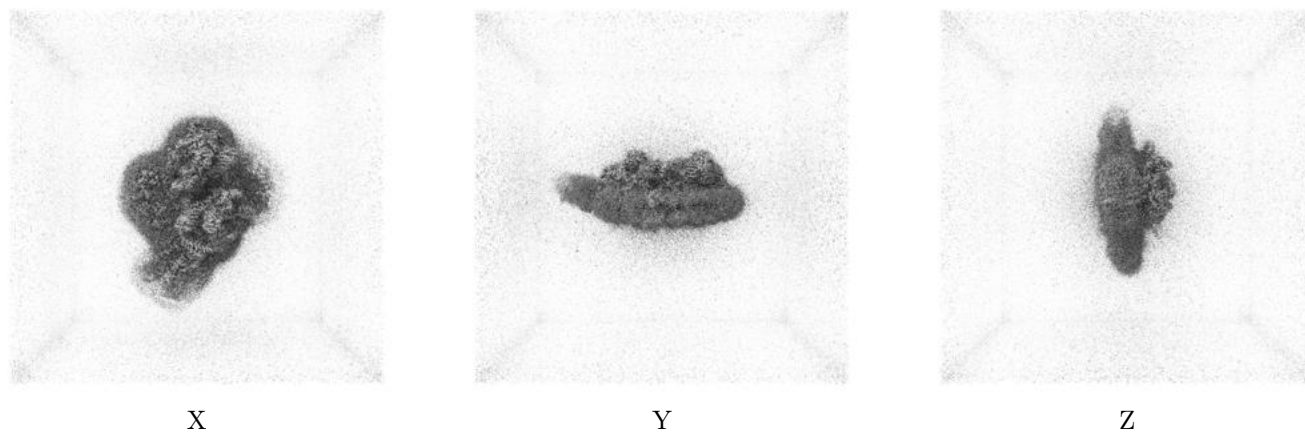
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

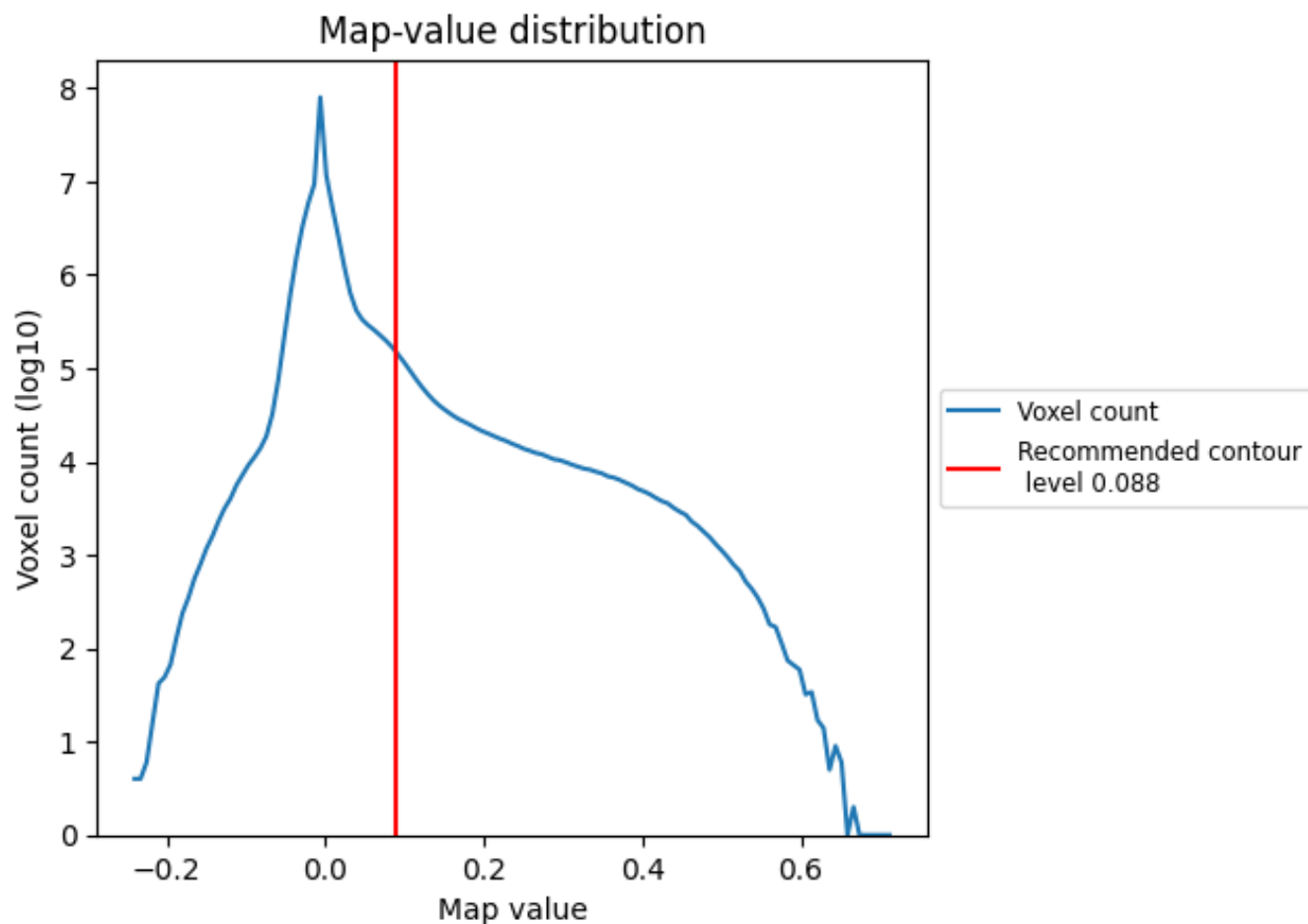
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

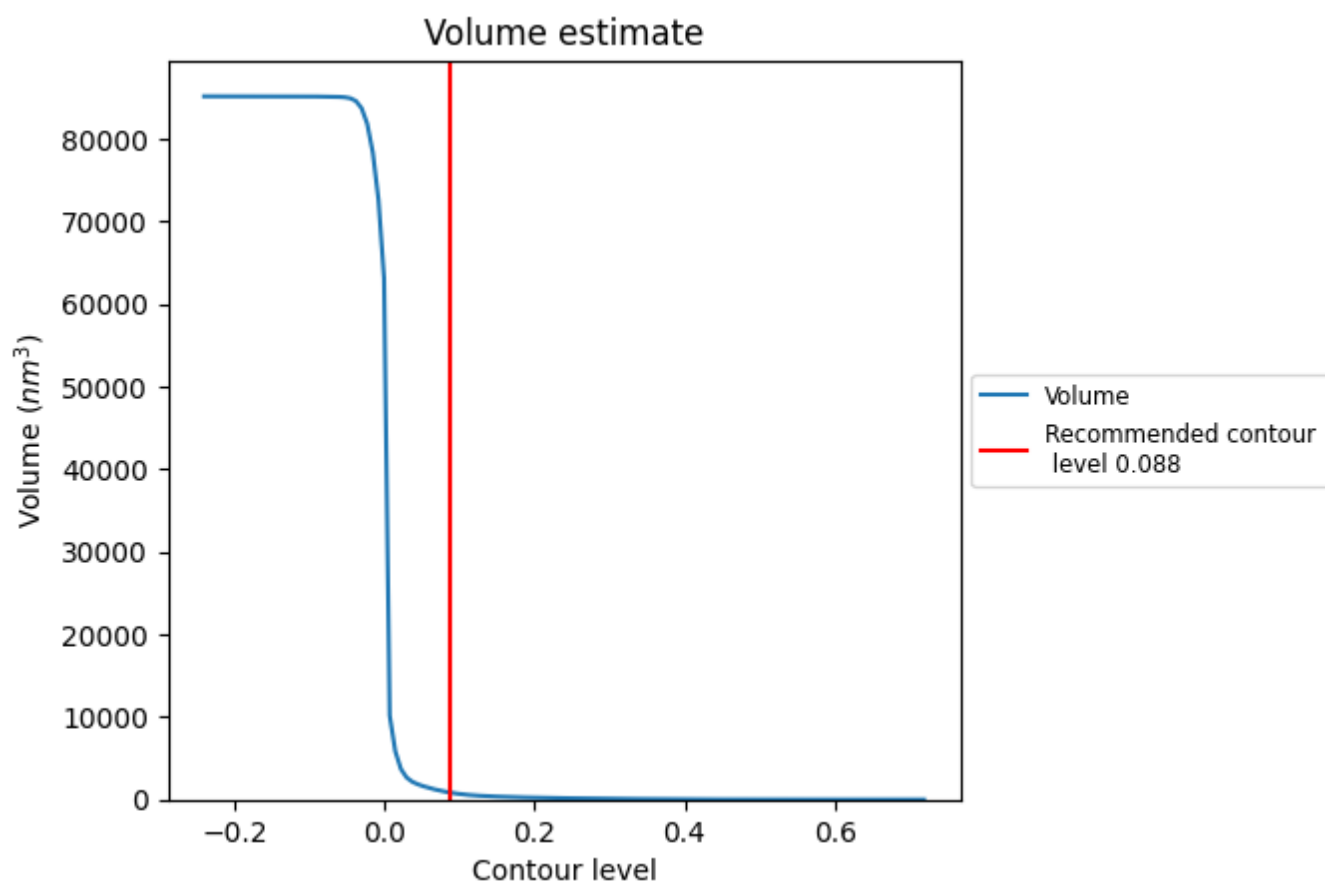
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

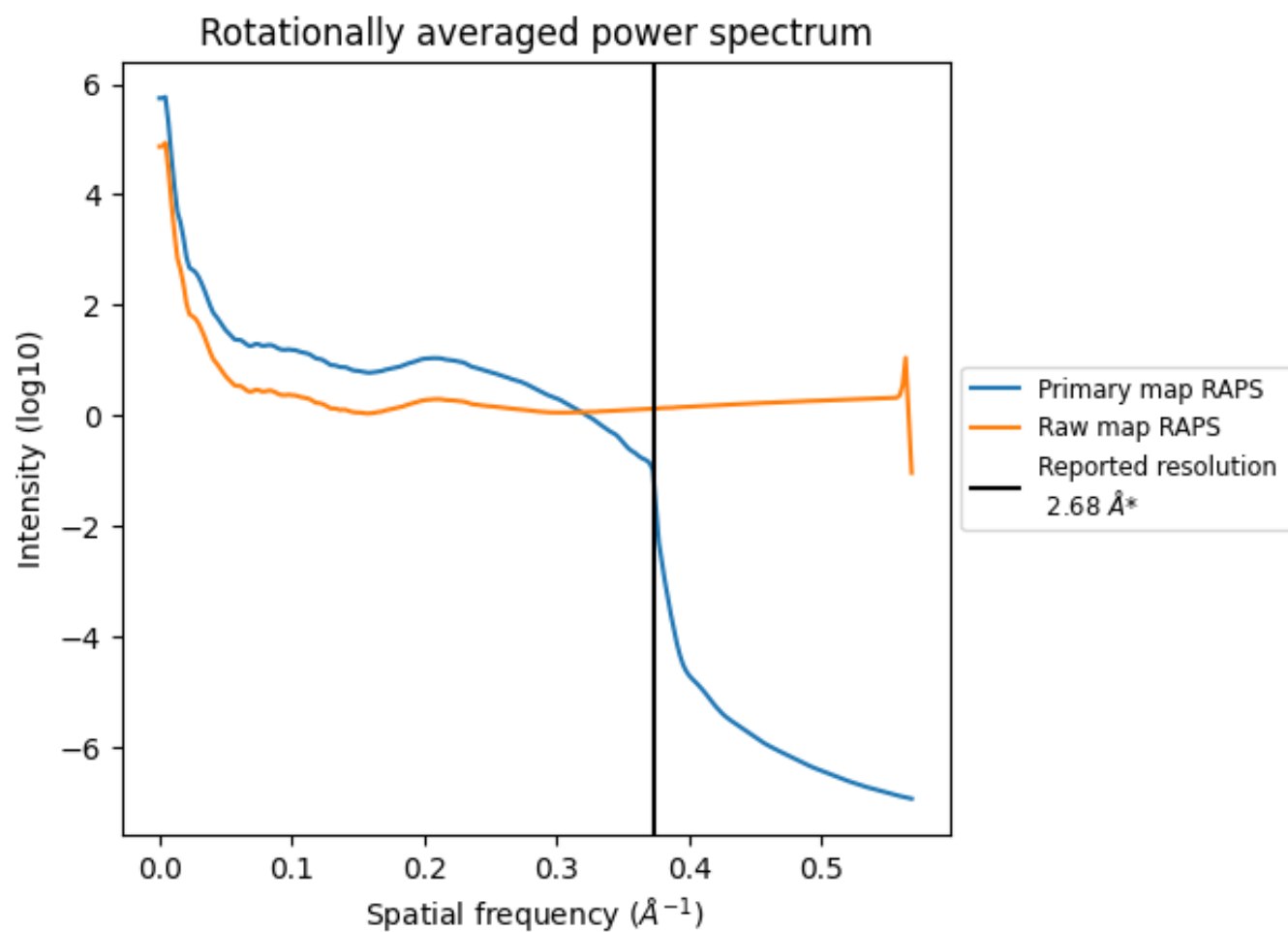
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 833 nm³; this corresponds to an approximate mass of 752 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 ⓘ

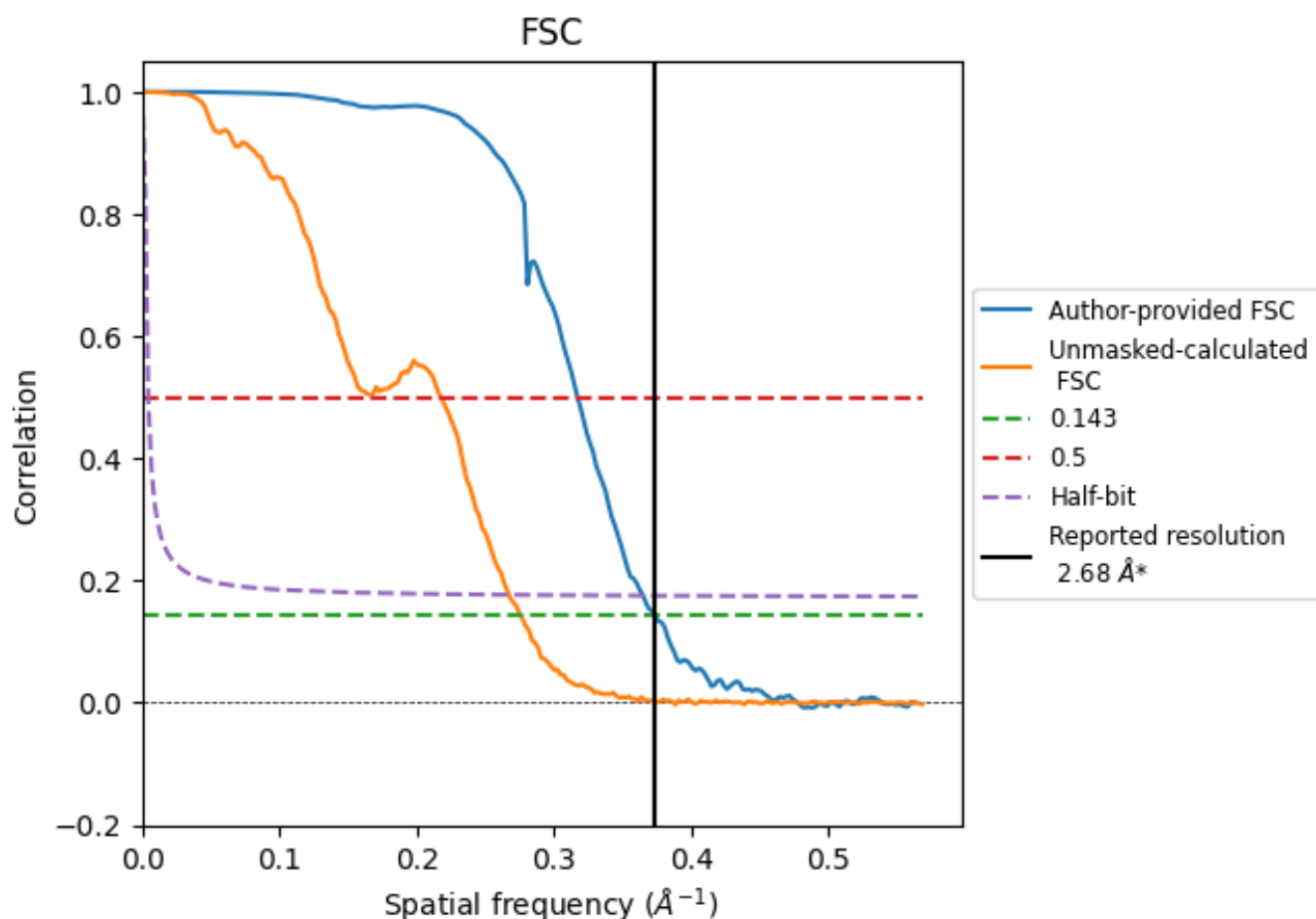


*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

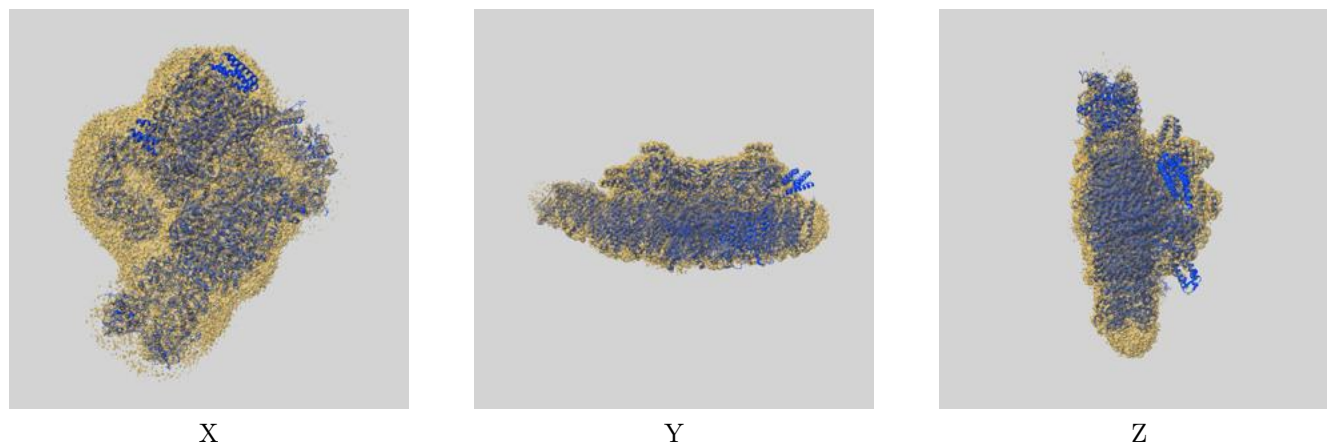
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	3.15	2.74
Unmasked-calculated*	3.63	4.59	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

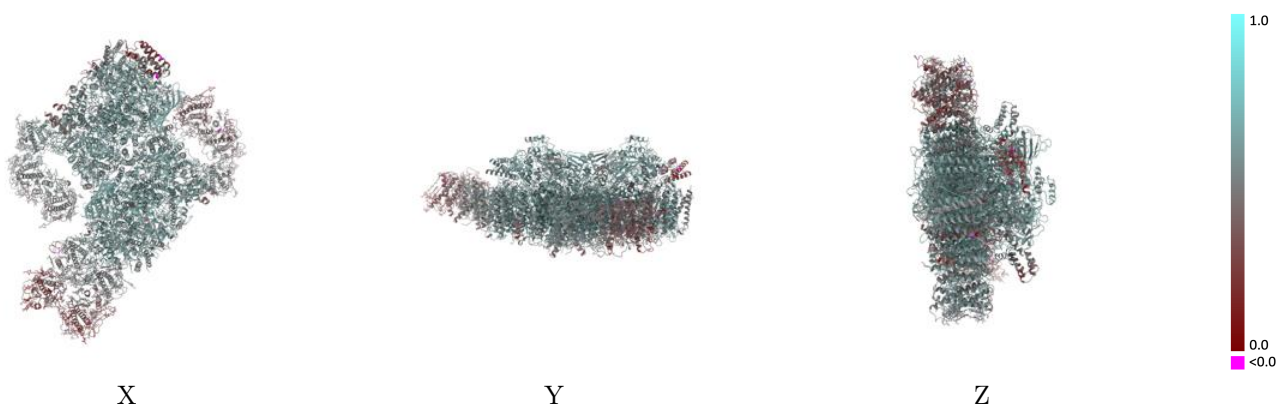
This section contains information regarding the fit between EMDB map EMD-35766 and PDB model 8IWH. Per-residue inclusion information can be found in section 3 on page 41.

9.1 Map-model overlay [i](#)



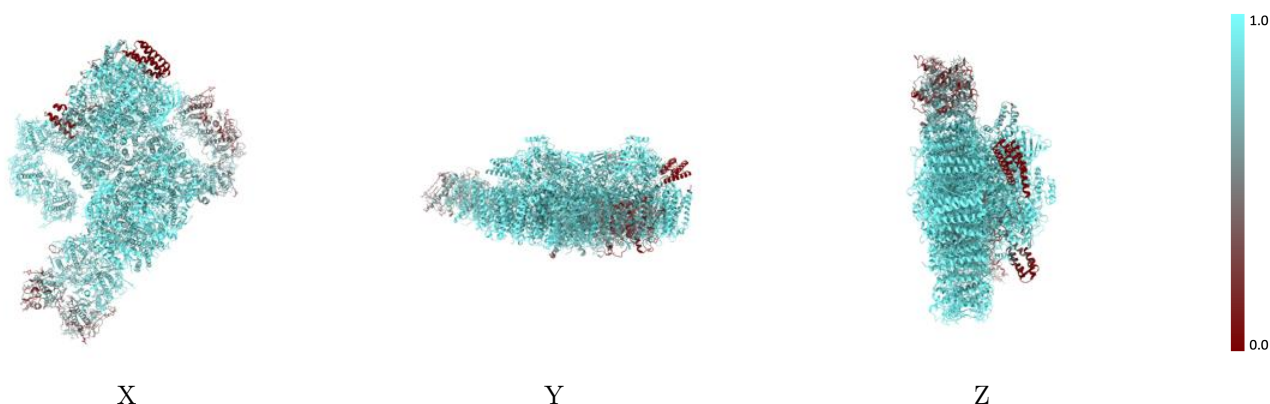
The images above show the 3D surface view of the map at the recommended contour level 0.088 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



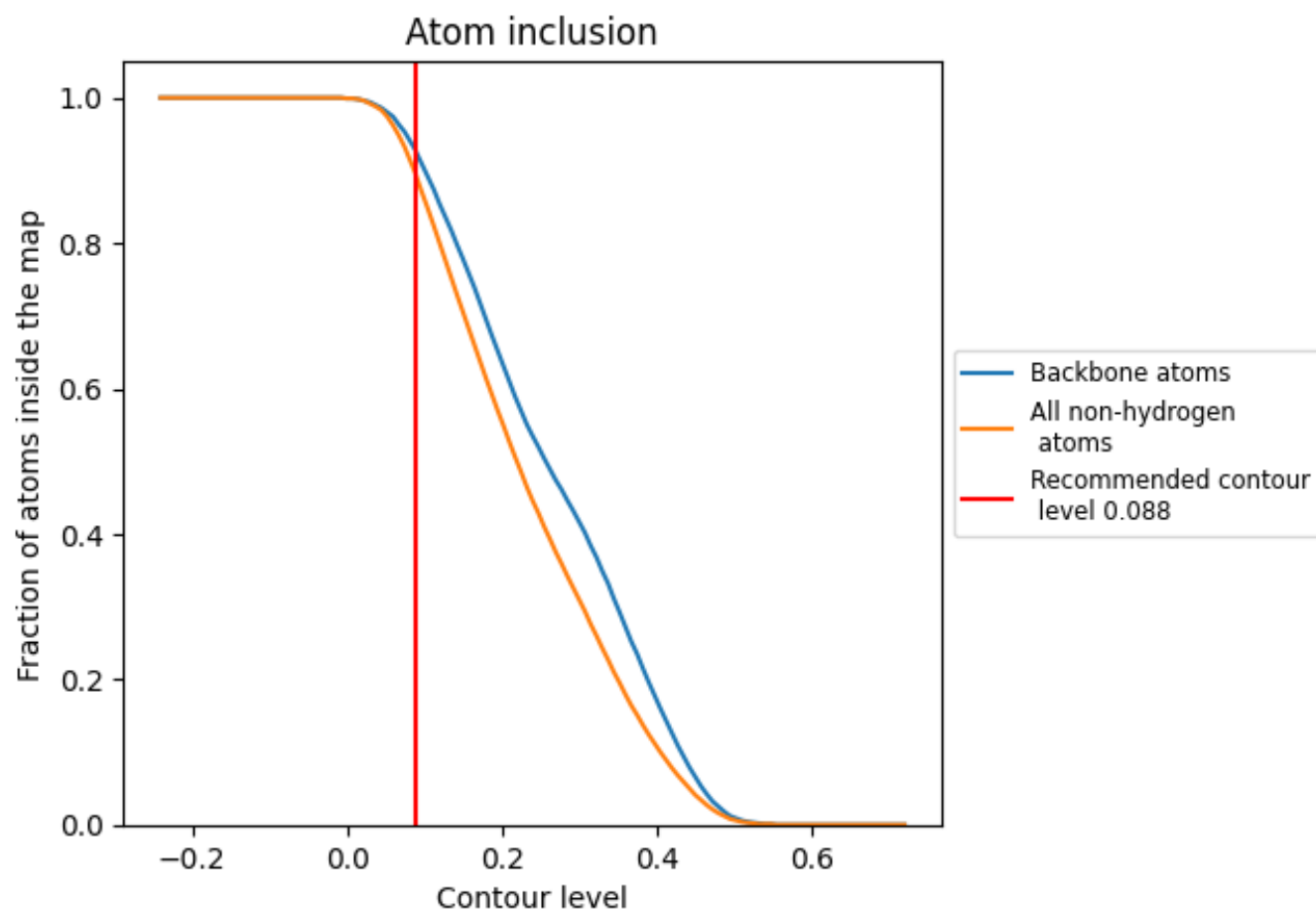
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.088).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.5410
0	 0.7820	 0.5060
1	 0.4420	 0.4020
2	 0.5170	 0.3360
3	 0.9120	 0.4840
4	 0.9310	 0.4850
5	 0.5590	 0.3090
6	 0.5250	 0.2970
7	 0.9750	 0.5430
8	 0.9550	 0.4950
9	 0.9390	 0.4550
A	 0.9800	 0.5990
B	 0.9920	 0.6150
C	 0.9920	 0.6110
D	 0.9880	 0.6130
E	 0.9710	 0.5170
F	 0.9930	 0.5420
G	 0.7830	 0.5380
H	 0.9830	 0.5900
I	 0.9930	 0.6130
J	 0.9410	 0.5150
K	 0.9840	 0.5810
L	 0.9970	 0.6040
M	 0.9940	 0.6050
N	 0.9600	 0.4960
O	 0.9680	 0.6000
Q	 0.9690	 0.5810
T	 0.9860	 0.5800
U	 0.9870	 0.5970
V	 0.9890	 0.5950
W	 0.9620	 0.5820
X	 0.9840	 0.5500
Y	 0.9760	 0.5170
Z	 0.9760	 0.5180
a	 0.9740	 0.5910



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Chain	Atom inclusion	Q-score
b	 0.9910	 0.6160
c	 0.9870	 0.5950
d	 0.9920	 0.6130
e	 0.9720	 0.5010
f	 0.9640	 0.5140
g	 0.3360	 0.4630
h	 0.9850	 0.6030
i	 0.9900	 0.5840
j	 0.9160	 0.4460
k	 0.9810	 0.5700
l	 0.9940	 0.6040
m	 0.9920	 0.5980
n	 0.9600	 0.4800
o	 0.9480	 0.5870
q	 0.1580	 0.3360
t	 0.9870	 0.5710
u	 0.9740	 0.5960
v	 0.9680	 0.5730
w	 0.9360	 0.5310
x	 0.9760	 0.5460
y	 0.8920	 0.4190
z	 0.9220	 0.4740