



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:40 AM UTC

PDB ID : 8JZE / pdb_00008jze
EMDB ID : EMD-36742
Title : PSI-AcpPCI supercomplex from Symbiodinium
Authors : Li, Z.H.; Li, X.Y.; Wang, W.D.
Deposited on : 2023-07-05
Resolution : 2.99 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:

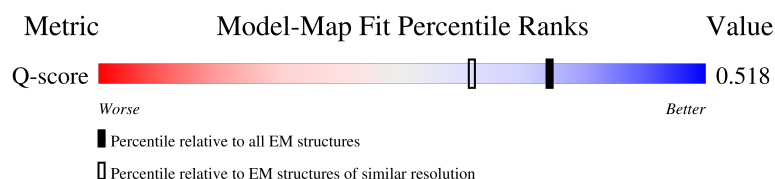
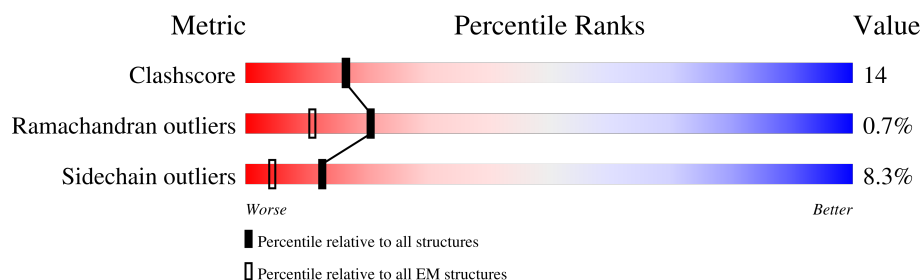
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



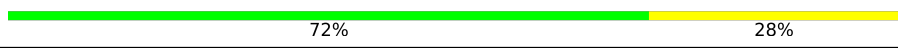
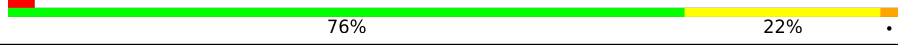
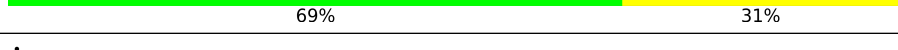
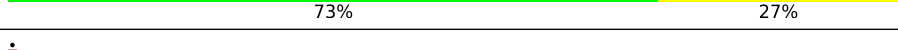
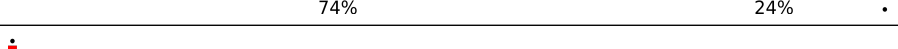
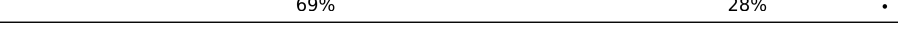
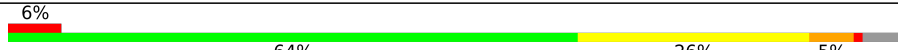
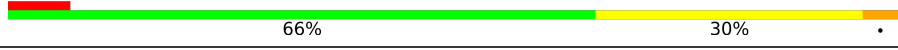
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13287 (2.49 - 3.49)

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	I	200	 6% 71% 26% .
2	K	177	 0% 67% 31% .
3	z	78	 0% 92% 8% .
4	y	131	 0% 97% .

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Mol	Chain	Length	Quality of chain
5	G	224	
6	A	189	
7	c	86	
8	d	218	
9	e	73	
10	f	184	
11	h	131	
12	i	119	
13	j	98	
14	l	250	
15	m	79	
16	a	670	
17	b	663	
18	B	192	
19	D	165	
20	F	176	
21	H	160	
22	J	220	
23	L	185	
24	M	173	
25	N	160	
26	O	161	
27	P	160	

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
30	CLA	A	307	X	-	-	-
30	CLA	A	308	X	-	-	-
30	CLA	A	309	X	-	-	-
30	CLA	A	310	X	-	-	-
30	CLA	A	311	X	-	-	-
30	CLA	A	312	X	-	-	-
30	CLA	A	313	X	-	-	-
30	CLA	A	315	X	-	-	-
30	CLA	A	316	X	-	-	-
30	CLA	A	317	X	-	-	-
30	CLA	A	319	X	-	-	-
30	CLA	A	320	X	-	-	-
30	CLA	B	301	X	-	-	-
30	CLA	B	307	X	-	-	-
30	CLA	B	308	X	-	-	-
30	CLA	B	309	X	-	-	-
30	CLA	B	310	X	-	-	-
30	CLA	B	311	X	-	-	-
30	CLA	B	312	X	-	-	-
30	CLA	B	313	X	-	-	-
30	CLA	B	315	X	-	-	-
30	CLA	B	316	X	-	-	-
30	CLA	B	317	X	-	-	-
30	CLA	D	308	X	-	-	-
30	CLA	D	309	X	-	-	-
30	CLA	D	311	X	-	-	-
30	CLA	D	312	X	-	-	-
30	CLA	D	313	X	-	-	-
30	CLA	D	314	X	-	-	-
30	CLA	D	316	X	-	-	-
30	CLA	F	307	X	-	-	-
30	CLA	F	308	X	-	-	-
30	CLA	F	310	X	-	-	-
30	CLA	F	311	X	-	-	-
30	CLA	F	312	X	-	-	-
30	CLA	F	313	X	-	-	-
30	CLA	F	315	X	-	-	-
30	CLA	G	509	X	-	-	-
30	CLA	G	510	X	-	-	-
30	CLA	G	511	X	-	-	-
30	CLA	G	512	X	-	-	-
30	CLA	G	513	X	-	-	-
30	CLA	G	514	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	G	516	X	-	-	-
30	CLA	G	517	X	-	-	-
30	CLA	G	518	X	-	-	-
30	CLA	G	519	X	-	-	-
30	CLA	G	520	X	-	-	-
30	CLA	H	304	X	-	-	-
30	CLA	H	305	X	-	-	-
30	CLA	H	307	X	-	-	-
30	CLA	H	308	X	-	-	-
30	CLA	H	309	X	-	-	-
30	CLA	H	312	X	-	-	-
30	CLA	I	306	X	-	-	-
30	CLA	I	307	X	-	-	-
30	CLA	I	308	X	-	-	-
30	CLA	I	309	X	-	-	-
30	CLA	I	310	X	-	-	-
30	CLA	I	311	X	-	-	-
30	CLA	I	312	X	-	-	-
30	CLA	I	313	X	-	-	-
30	CLA	I	315	X	-	-	-
30	CLA	I	316	X	-	-	-
30	CLA	I	319	X	-	-	-
30	CLA	I	321	X	-	-	-
30	CLA	J	301	X	-	-	-
30	CLA	J	306	X	-	-	-
30	CLA	J	307	X	-	-	-
30	CLA	J	308	X	-	-	-
30	CLA	J	309	X	-	-	-
30	CLA	J	310	X	-	-	-
30	CLA	J	311	X	-	-	-
30	CLA	J	312	X	-	-	-
30	CLA	J	314	X	-	-	-
30	CLA	J	315	X	-	-	-
30	CLA	K	306	X	-	-	-
30	CLA	K	307	X	-	-	-
30	CLA	K	308	X	-	-	-
30	CLA	K	309	X	-	-	-
30	CLA	K	310	X	-	-	-
30	CLA	K	311	X	-	-	-
30	CLA	K	312	X	-	-	-
30	CLA	K	313	X	-	-	-
30	CLA	K	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	K	316	X	-	-	-
30	CLA	L	308	X	-	-	-
30	CLA	L	309	X	-	-	-
30	CLA	L	310	X	-	-	-
30	CLA	L	311	X	-	-	-
30	CLA	L	312	X	-	-	-
30	CLA	L	313	X	-	-	-
30	CLA	L	314	X	-	-	-
30	CLA	L	316	X	-	-	-
30	CLA	L	317	X	-	-	-
30	CLA	L	318	X	-	-	-
30	CLA	M	308	X	-	-	-
30	CLA	M	309	X	-	-	-
30	CLA	M	310	X	-	-	-
30	CLA	M	311	X	-	-	-
30	CLA	M	312	X	-	-	-
30	CLA	M	313	X	-	-	-
30	CLA	M	315	X	-	-	-
30	CLA	M	316	X	-	-	-
30	CLA	M	317	X	-	-	-
30	CLA	M	318	X	-	-	-
30	CLA	N	304	X	-	-	-
30	CLA	N	305	X	-	-	-
30	CLA	N	307	X	-	-	-
30	CLA	N	309	X	-	-	-
30	CLA	N	310	X	-	-	-
30	CLA	O	308	X	-	-	-
30	CLA	O	309	X	-	-	-
30	CLA	O	311	X	-	-	-
30	CLA	O	313	X	-	-	-
30	CLA	O	314	X	-	-	-
30	CLA	O	316	X	-	-	-
30	CLA	P	209	X	-	-	-
30	CLA	P	210	X	-	-	-
30	CLA	P	212	X	-	-	-
30	CLA	P	214	X	-	-	-
30	CLA	P	215	X	-	-	-
30	CLA	P	217	X	-	-	-
30	CLA	a	701	X	-	-	-
30	CLA	a	702	X	-	-	-
30	CLA	a	703	X	-	-	-
30	CLA	a	704	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	a	705	X	-	-	-
30	CLA	a	706	X	-	-	-
30	CLA	a	707	X	-	-	-
30	CLA	a	708	X	-	-	-
30	CLA	a	709	X	-	-	-
30	CLA	a	710	X	-	-	-
30	CLA	a	711	X	-	-	-
30	CLA	a	712	X	-	-	-
30	CLA	a	713	X	-	-	-
30	CLA	a	714	X	-	-	-
30	CLA	a	715	X	-	-	-
30	CLA	a	716	X	-	-	-
30	CLA	a	717	X	-	-	-
30	CLA	a	718	X	-	-	-
30	CLA	a	719	X	-	-	-
30	CLA	a	720	X	-	-	-
30	CLA	a	721	X	-	-	-
30	CLA	a	722	X	-	-	-
30	CLA	a	723	X	-	-	-
30	CLA	a	724	X	-	-	-
30	CLA	a	725	X	-	-	-
30	CLA	a	726	X	-	-	-
30	CLA	a	727	X	-	-	-
30	CLA	a	728	X	-	-	-
30	CLA	a	729	X	-	-	-
30	CLA	a	730	X	-	-	-
30	CLA	a	731	X	-	-	-
30	CLA	a	735	X	-	-	-
30	CLA	a	738	X	-	-	-
30	CLA	b	701	X	-	-	-
30	CLA	b	703	X	-	-	-
30	CLA	b	704	X	-	-	-
30	CLA	b	705	X	-	-	-
30	CLA	b	706	X	-	-	-
30	CLA	b	707	X	-	-	-
30	CLA	b	708	X	-	-	-
30	CLA	b	709	X	-	-	-
30	CLA	b	710	X	-	-	-
30	CLA	b	711	X	-	-	-
30	CLA	b	712	X	-	-	-
30	CLA	b	713	X	-	-	-
30	CLA	b	714	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	b	715	X	-	-	-
30	CLA	b	716	X	-	-	-
30	CLA	b	717	X	-	-	-
30	CLA	b	718	X	-	-	-
30	CLA	b	719	X	-	-	-
30	CLA	b	720	X	-	-	-
30	CLA	b	721	X	-	-	-
30	CLA	b	722	X	-	-	-
30	CLA	b	723	X	-	-	-
30	CLA	b	724	X	-	-	-
30	CLA	b	725	X	-	-	-
30	CLA	b	726	X	-	-	-
30	CLA	b	727	X	-	-	-
30	CLA	b	728	X	-	-	-
30	CLA	f	301	X	-	-	-
30	CLA	f	302	X	-	-	-
30	CLA	f	303	X	-	-	-
30	CLA	h	202	X	-	-	-
30	CLA	j	104	X	-	-	-
30	CLA	j	106	X	-	-	-
30	CLA	l	303	X	-	-	-
30	CLA	l	304	X	-	-	-
30	CLA	l	305	X	-	-	-
30	CLA	l	308	X	-	-	-
30	CLA	l	309	X	-	-	-
30	CLA	l	311	X	-	-	-
30	CLA	l	312	X	-	-	-
30	CLA	l	313	X	-	-	-
30	CLA	m	202	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 55927 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 Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	200	Total	C	N	O	S	0	0
			1480	961	250	259	10		

- Molecule 2 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	177	Total	C	N	O	S	0	0
			1349	872	227	238	12		

- Molecule 3 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	z	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 4 is a protein called Photosystem I unk.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	y	131	Total	C	N	O	0	0
			655	393	131	131		

- Molecule 5 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	217	Total	C	N	O	S	0	0
			1572	1004	269	289	10		

- Molecule 6 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	186	Total	C	N	O	S	0	0
			1346	870	225	242	9		

- Molecule 7 is a protein called Photosystem I PsuC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	86	Total	C	N	O	S	0	0
			653	403	109	132	9		

- Molecule 8 is a protein called Photosystem I PsuD.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	218	Total	C	N	O	S	0	0
			1731	1096	307	315	13		

- Molecule 9 is a protein called Photosystem I PsuE.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	e	73	Total	C	N	O	0	0
			587	384	99	104		

- Molecule 10 is a protein called Photosystem I PsuF.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	184	Total	C	N	O	S	0	0
			1450	930	252	260	8		

- Molecule 11 is a protein called Photosystem I PsuR.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	131	Total	C	N	O	S	0	0
			1066	704	165	193	4		

- Molecule 12 is a protein called Photosystem I PsuI.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	119	Total	C	N	O	S	0	0
			964	620	167	175	2		

- Molecule 13 is a protein called Photosystem I PsuJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	j	98	Total	C	N	O	0	0
			783	505	125	153		

- Molecule 14 is a protein called Photosystem I Psal.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	250	Total	C	N	O	S	0	0
			1943	1267	312	354	10		

- Molecule 15 is a protein called Photosystem I Psam.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	m	79	Total	C	N	O	S	0	0
			582	373	100	107	2		

- Molecule 16 is a protein called Photosystem I PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	670	Total	C	N	O	S	0	0
			5194	3393	875	910	16		

- Molecule 17 is a protein called Photosystem I PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	663	Total	C	N	O	S	0	0
			5199	3408	851	928	12		

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	192	Total	C	N	O	S	0	0
			1452	934	241	265	12		

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D	160	Total	C	N	O	S	0	0
			1158	728	195	228	7		

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2,

acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	F	169	Total	C	N	O	S	0	0
			1237	777	209	239	12		

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	160	Total	C	N	O	S	0	0
			1202	769	198	228	7		

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	220	Total	C	N	O	S	0	0
			1496	938	261	290	7		

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	185	Total	C	N	O	S	0	0
			1427	924	239	258	6		

- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	168	Total	C	N	O	S	0	0
			1211	773	208	225	5		

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	153	Total	C	N	O	S	0	0
			993	607	179	202	5		

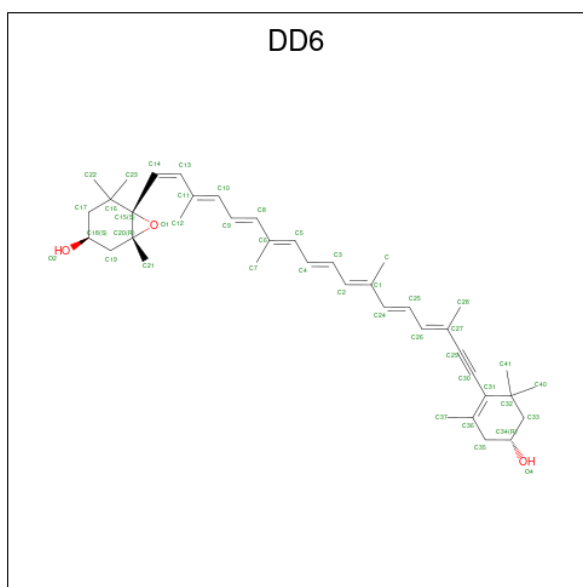
- Molecule 26 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	161	Total	C	N	O	S	0	0
			1073	670	189	207	7		

- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	159	Total	C	N	O	S	0	0
			1113	693	191	223	6		

- Molecule 28 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) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	I	1	Total	C	O	0
			43	40	3	
28	I	1	Total	C	O	0
			43	40	3	
28	I	1	Total	C	O	0
			43	40	3	
28	I	1	Total	C	O	0
			43	40	3	
28	K	1	Total	C	O	0
			43	40	3	
28	K	1	Total	C	O	0
			43	40	3	

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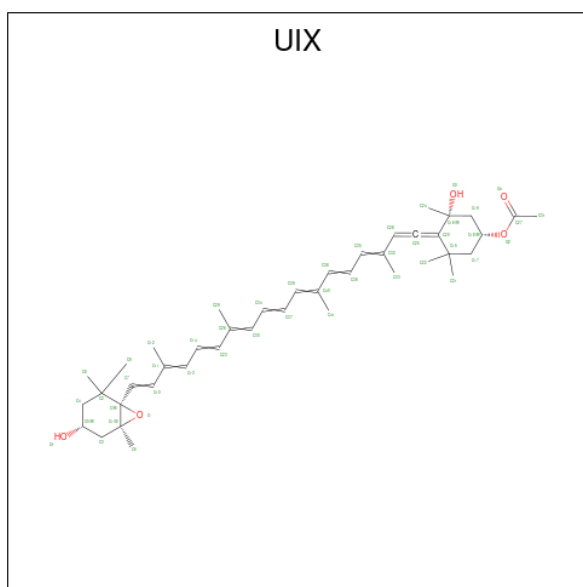
Mol	Chain	Residues	Atoms			AltConf
28	K	1	Total 43	C 40	O 3	0
28	K	1	Total 43	C 40	O 3	0
28	K	1	Total 43	C 40	O 3	0
28	G	1	Total 43	C 40	O 3	0
28	G	1	Total 43	C 40	O 3	0
28	G	1	Total 43	C 40	O 3	0
28	G	1	Total 43	C 40	O 3	0
28	A	1	Total 43	C 40	O 3	0
28	A	1	Total 43	C 40	O 3	0
28	A	1	Total 43	C 40	O 3	0
28	A	1	Total 43	C 40	O 3	0
28	h	1	Total 43	C 40	O 3	0
28	b	1	Total 43	C 40	O 3	0
28	B	1	Total 42	C 39	O 3	0
28	B	1	Total 43	C 40	O 3	0
28	B	1	Total 43	C 40	O 3	0
28	B	1	Total 43	C 40	O 3	0
28	D	1	Total 43	C 40	O 3	0
28	F	1	Total 43	C 40	O 3	0
28	F	1	Total 43	C 40	O 3	0
28	H	1	Total 43	C 40	O 3	0

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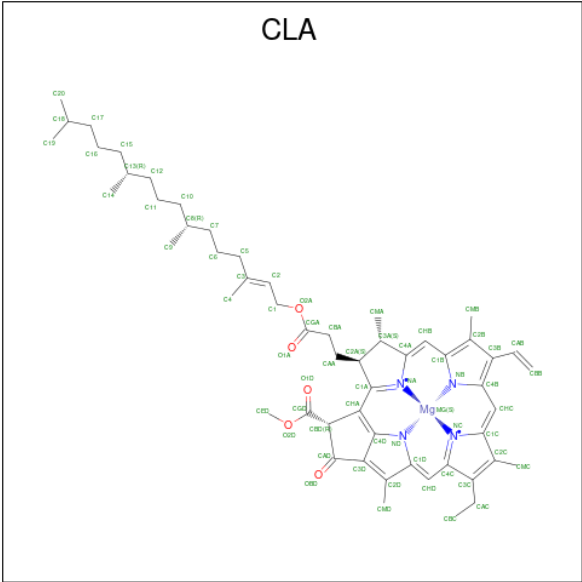
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			43	40	3	
28	J	1	Total	C	O	0
			43	40	3	
28	J	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	L	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	M	1	Total	C	O	0
			43	40	3	
28	N	1	Total	C	O	0
			43	40	3	
28	O	1	Total	C	O	0
			43	40	3	
28	P	1	Total	C	O	0
			43	40	3	

- Molecule 29 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (CCD ID: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	I	1	Total	C	O	0
			47	42	5	
29	K	1	Total	C	O	0
			47	42	5	
29	G	1	Total	C	O	0
			47	42	5	
29	A	1	Total	C	O	0
			47	42	5	
29	h	1	Total	C	O	0
			47	42	5	
29	B	1	Total	C	O	0
			47	42	5	
29	J	1	Total	C	O	0
			47	42	5	
29	O	1	Total	C	O	0
			47	42	5	
29	P	1	Total	C	O	0
			47	42	5	

- Molecule 30 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	I	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	K	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
30	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	h	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	j	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	j	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	l	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	l	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
30	l	1	Total 45	C 36	N 4	O 5		0
30	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	l	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	m	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	b	1	Total 48	C 38	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
30	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
30	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
30	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
30	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	D	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	F	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
30	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	J	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	J	1	Total 56	C 46	Mg 1	N 4	O 5	0
30	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	J	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	J	1	Total 53	C 43	Mg 1	N 4	O 5	0

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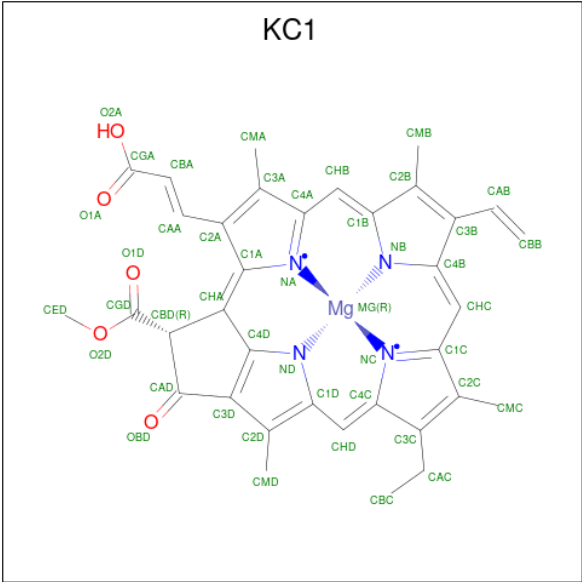
Mol	Chain	Residues	Atoms					AltConf
30	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	J	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	L	1	Total 47	C 39	Mg 1	N 4	O 3	0
30	L	1	Total 53	C 43	Mg 1	N 4	O 5	0
30	L	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	L	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	L	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	L	1	Total 53	C 43	Mg 1	N 4	O 5	0
30	L	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	L	1	Total 52	C 42	Mg 1	N 4	O 5	0
30	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	M	1	Total 53	C 43	Mg 1	N 4	O 5	0
30	M	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	M	1	Total 48	C 38	Mg 1	N 4	O 5	0
30	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	M	1	Total 48	C 38	Mg 1	N 4	O 5	0
30	M	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	M	1	Total 41	C 33	Mg 1	N 4	O 3	0
30	M	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
30	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 31 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



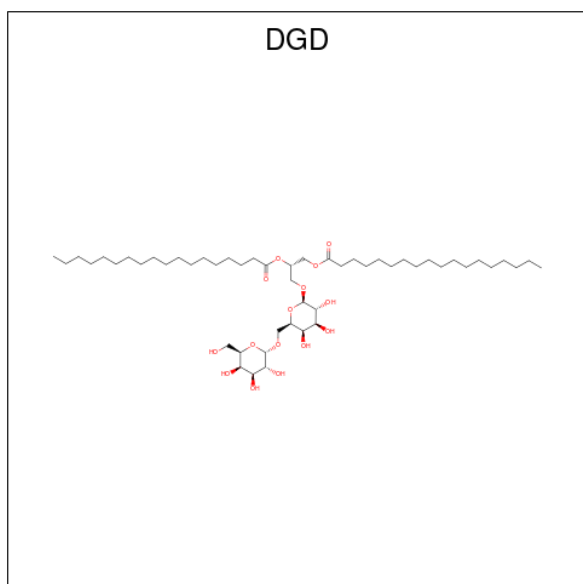
Mol	Chain	Residues	Atoms					AltConf
31	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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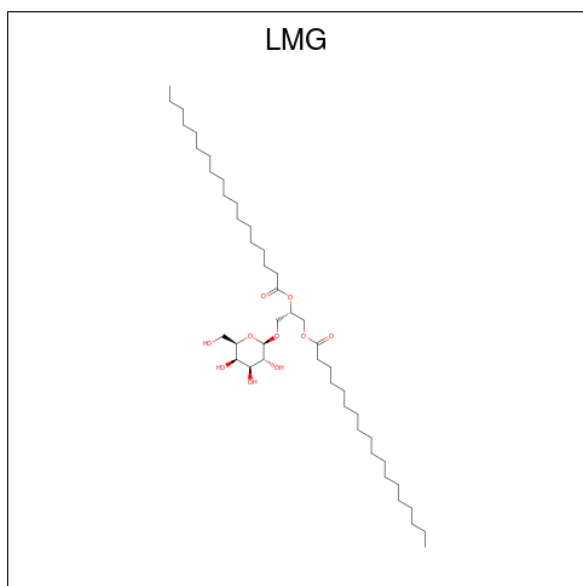
Mol	Chain	Residues	Atoms					AltConf
31	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
32	I	1	Total	C	O	0
			39	24	15	
32	y	1	Total	C	O	0
			54	39	15	
32	G	1	Total	C	O	0
			45	30	15	
32	G	1	Total	C	O	0
			44	29	15	
32	j	1	Total	C	O	0
			41	26	15	
32	l	1	Total	C	O	0
			50	35	15	
32	L	1	Total	C	O	0
			38	23	15	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



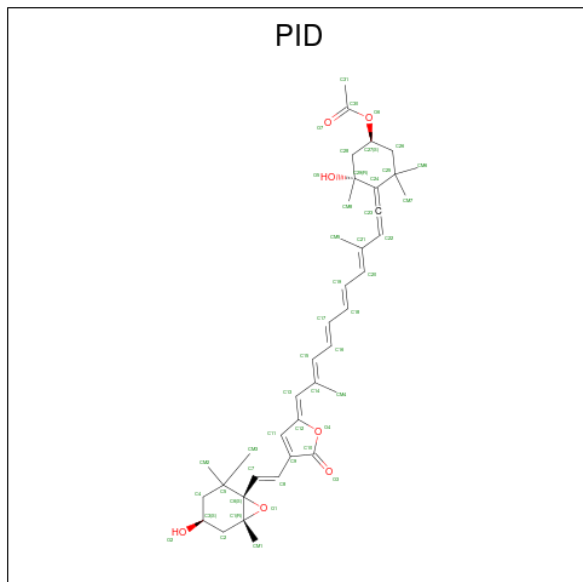
Mol	Chain	Residues	Atoms			AltConf
33	I	1	Total	C	O	0
			36	26	10	
33	I	1	Total	C	O	0
			38	28	10	
33	K	1	Total	C	O	0
			43	33	10	
33	j	1	Total	C	O	0
			35	25	10	

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Mol	Chain	Residues	Atoms			AltConf
33	b	1	Total	C	O	0
			44	34	10	
33	b	1	Total	C	O	0
			31	21	10	
33	B	1	Total	C	O	0
			37	27	10	
33	D	1	Total	C	O	0
			49	39	10	
33	P	1	Total	C	O	0
			27	17	10	

- Molecule 34 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	G	1	Total	C	O	0
			46	39	7	
34	G	1	Total	C	O	0
			46	39	7	
34	j	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	
34	D	1	Total	C	O	0
			46	39	7	

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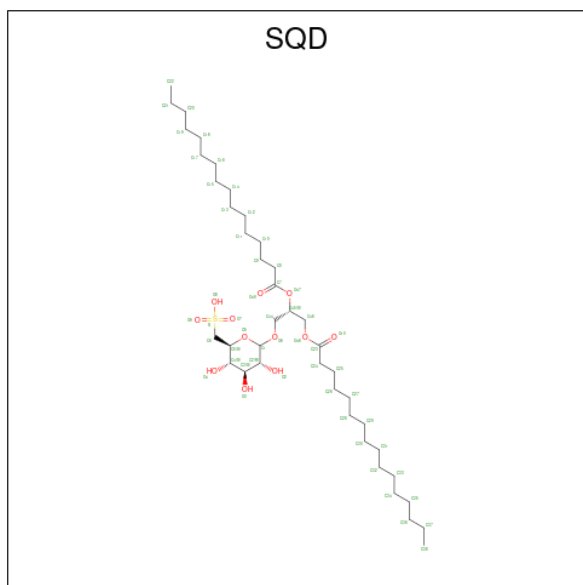
Mol	Chain	Residues	Atoms			AltConf
34	D	1	Total 46	C 39	O 7	0
34	D	1	Total 46	C 39	O 7	0
34	D	1	Total 46	C 39	O 7	0
34	F	1	Total 46	C 39	O 7	0
34	F	1	Total 46	C 39	O 7	0
34	F	1	Total 46	C 39	O 7	0
34	F	1	Total 46	C 39	O 7	0
34	H	1	Total 46	C 39	O 7	0
34	H	1	Total 46	C 39	O 7	0
34	M	1	Total 46	C 39	O 7	0
34	N	1	Total 46	C 39	O 7	0
34	N	1	Total 46	C 39	O 7	0
34	O	1	Total 46	C 39	O 7	0
34	O	1	Total 46	C 39	O 7	0
34	O	1	Total 46	C 39	O 7	0
34	O	1	Total 46	C 39	O 7	0
34	O	1	Total 46	C 39	O 7	0
34	P	1	Total 46	C 39	O 7	0
34	P	1	Total 46	C 39	O 7	0
34	P	1	Total 46	C 39	O 7	0
34	P	1	Total 46	C 39	O 7	0

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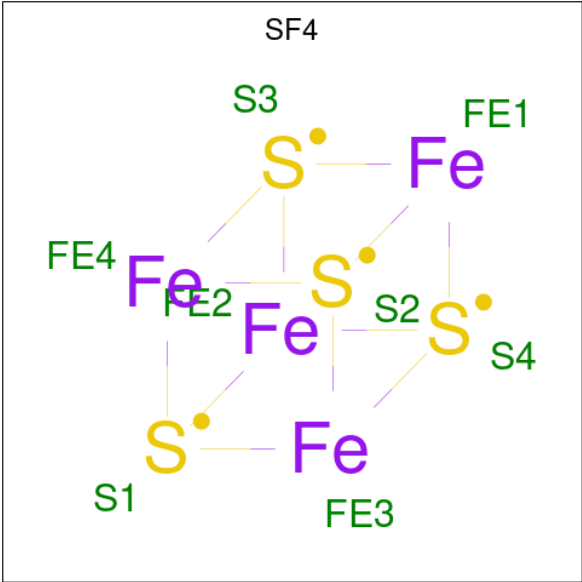
Mol	Chain	Residues	Atoms			AltConf
34	P	1	Total	C	O	0
			46	39	7	

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



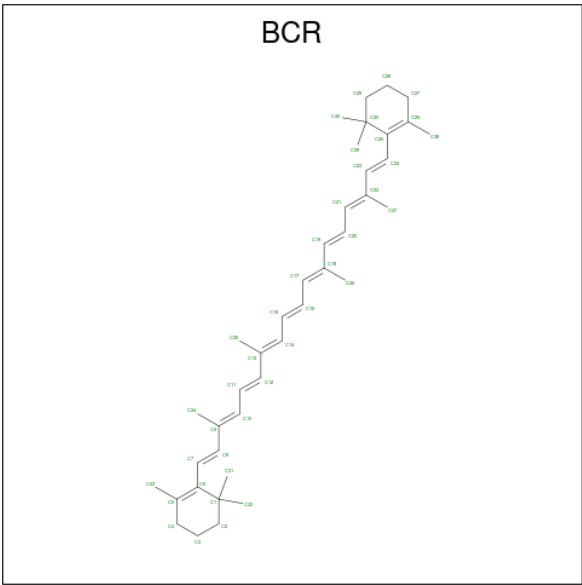
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
36	c	1	Total	Fe	S	0
			8	4	4	
36	c	1	Total	Fe	S	0
			8	4	4	
36	a	1	Total	Fe	S	0
			8	4	4	

- Molecule 37 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



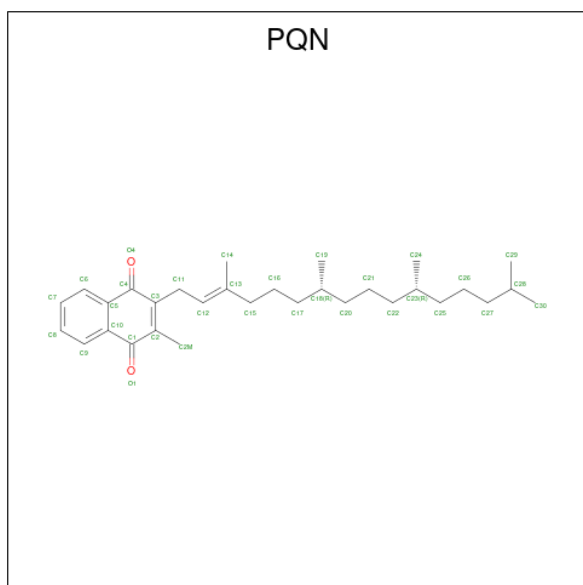
Mol	Chain	Residues	Atoms		AltConf
37	f	1	Total	C	0
			40	40	

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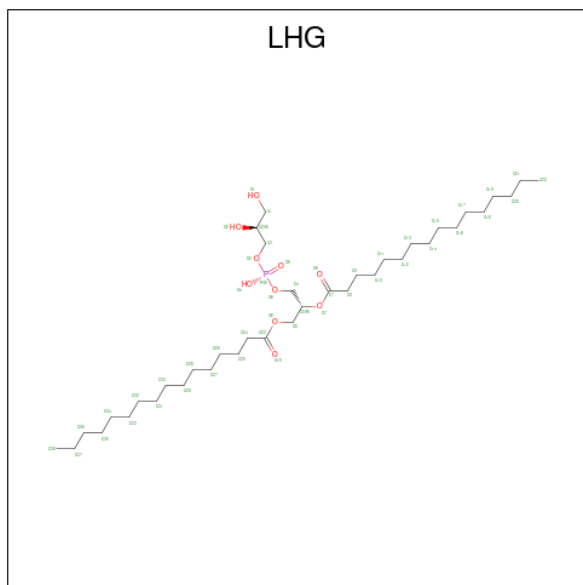
Mol	Chain	Residues	Atoms	AltConf
37	i	1	Total C 40 40	0
37	j	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	l	1	Total C 40 40	0
37	m	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	a	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	b	1	Total C 40 40	0

- Molecule 38 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
38	a	1	Total	C	O	0
			33	31	2	
38	b	1	Total	C	O	0
			33	31	2	

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

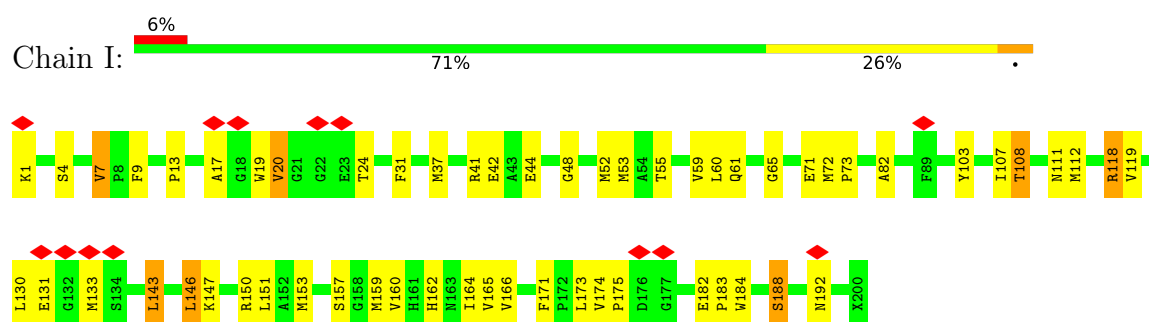


Mol	Chain	Residues	Atoms				AltConf
39	a	1	Total	C	O	P	0
			48	37	10	1	

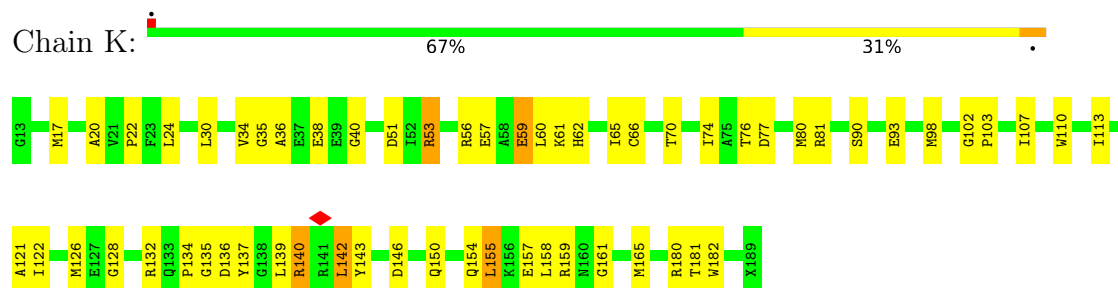
3 Residue-property plots [i](#)

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

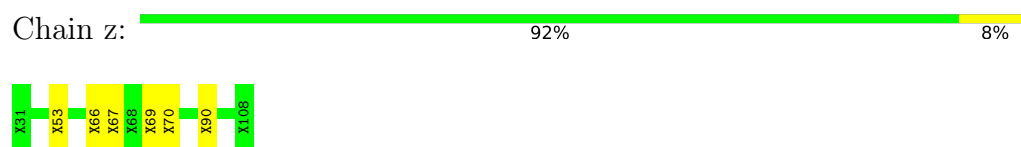
- Molecule 1: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7



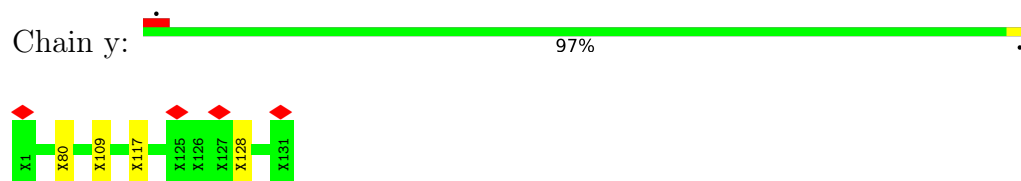
- Molecule 2: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6



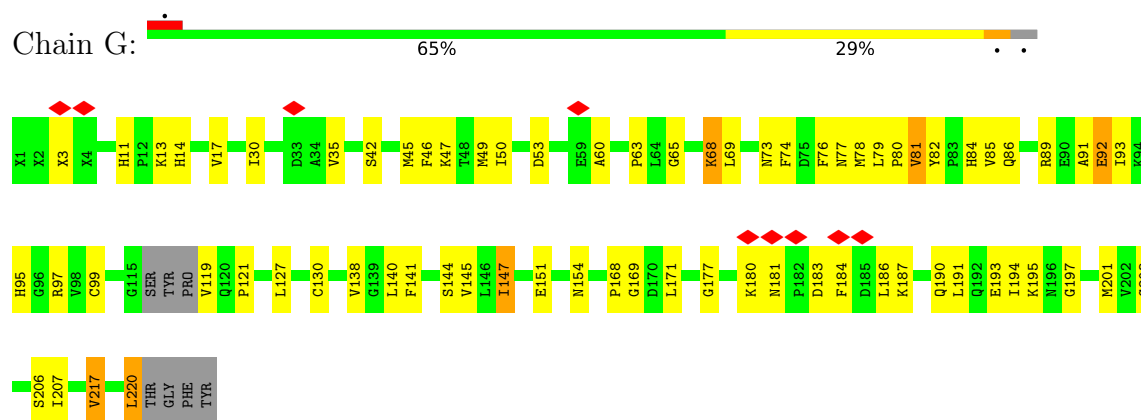
- Molecule 3: Photosystem I unk



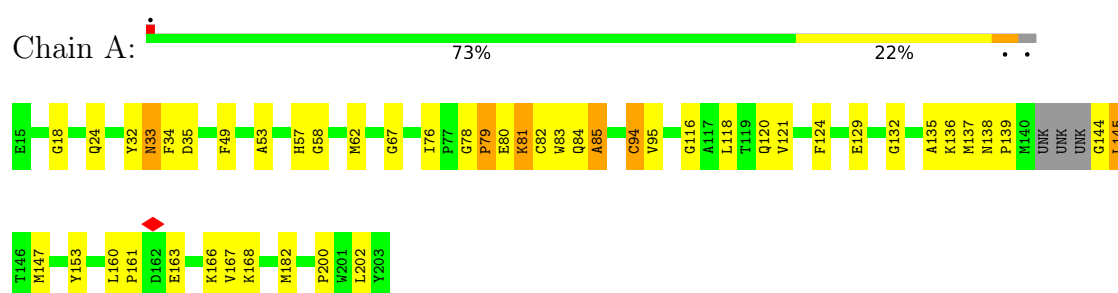
- Molecule 4: Photosystem I unk



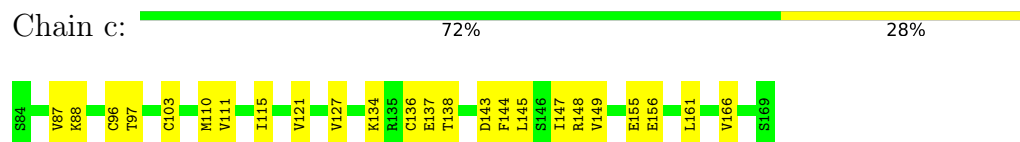
- Molecule 5: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8



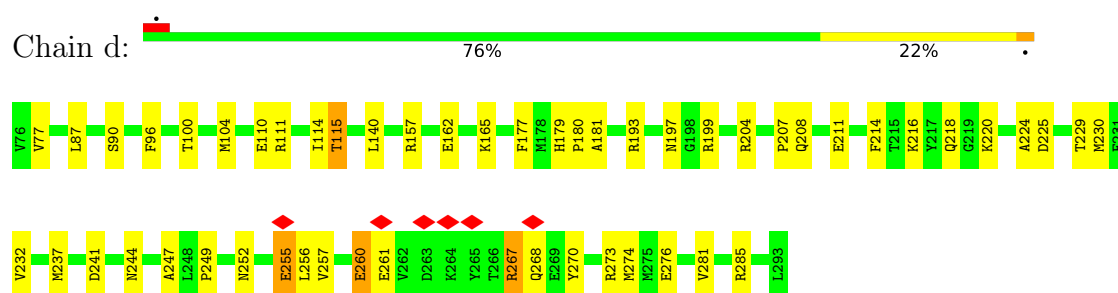
- Molecule 6: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10



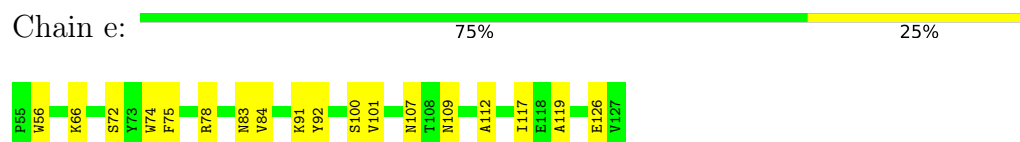
- Molecule 7: Photosystem I PsuC



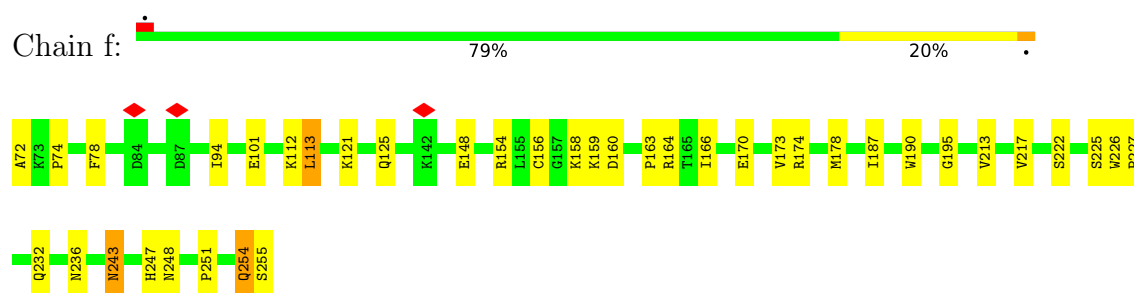
- Molecule 8: Photosystem I PsuD



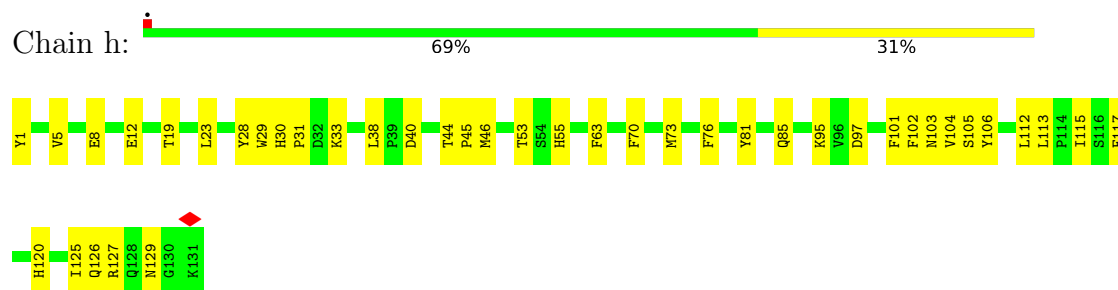
- Molecule 9: Photosystem I PsuE



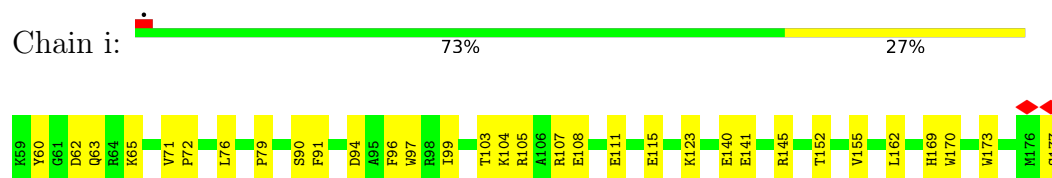
- Molecule 10: Photosystem I PsuF



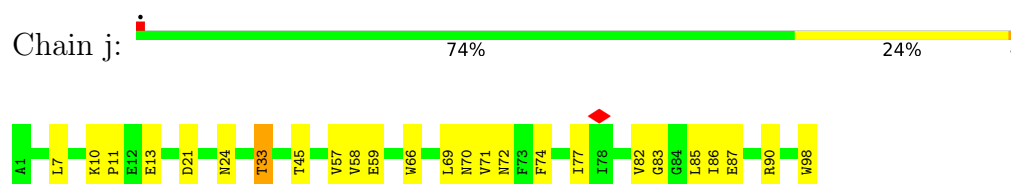
- Molecule 11: Photosystem I Psal



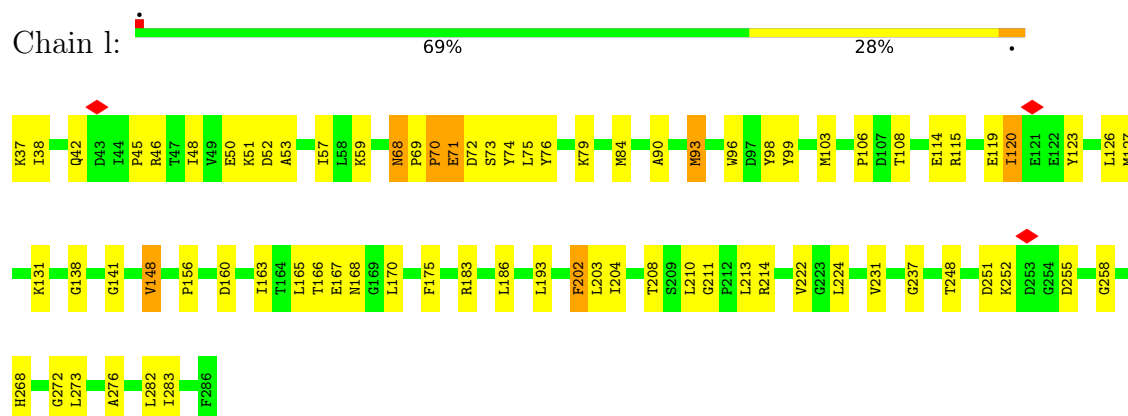
- Molecule 12: Photosystem I Psal



- Molecule 13: Photosystem I PsalJ



- Molecule 14: Photosystem I PsalL



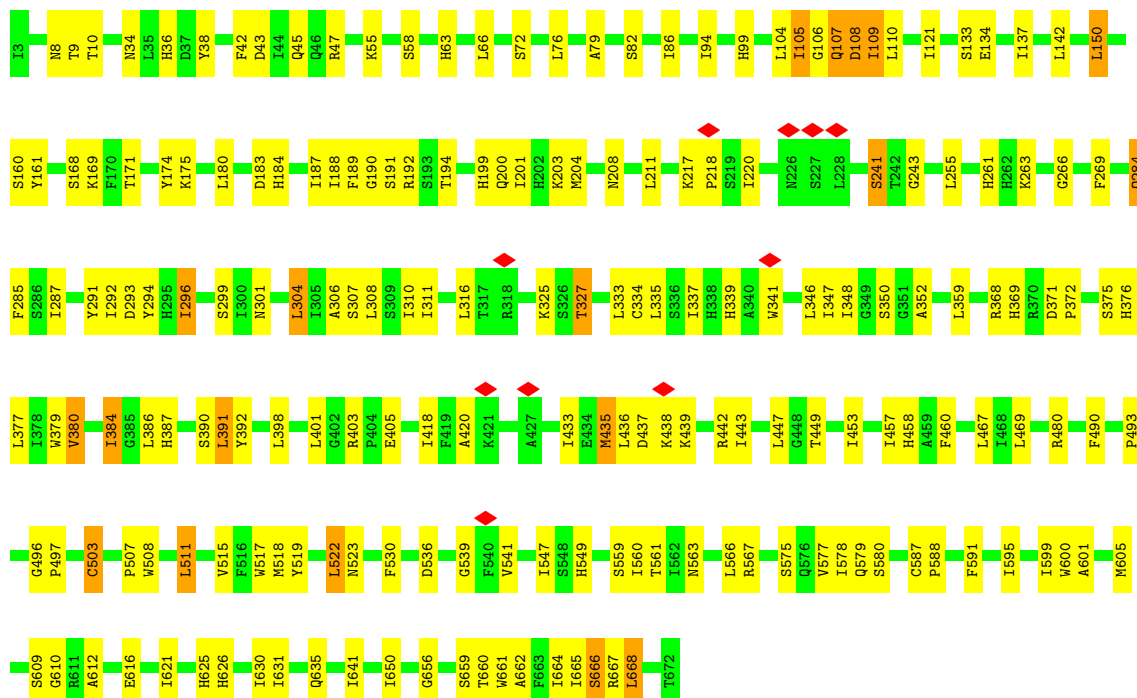
- Molecule 15: Photosystem I PsalM

Chain m:  76% 24%



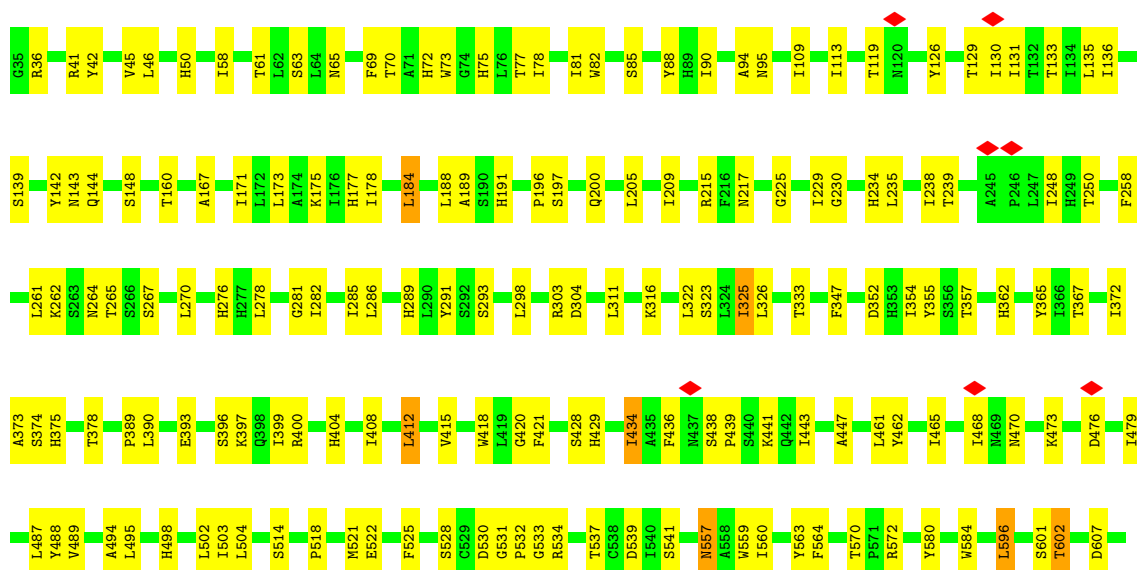
• Molecule 16: Photosystem I PsuA

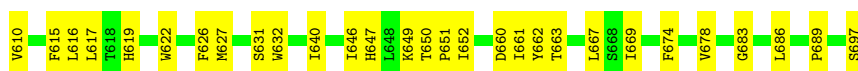
Chain a:  70% 27%



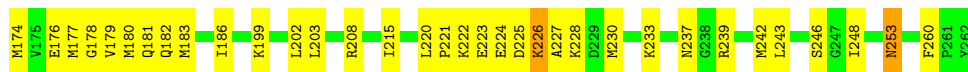
• Molecule 17: Photosystem I PsuB

Chain b:  70% 29%

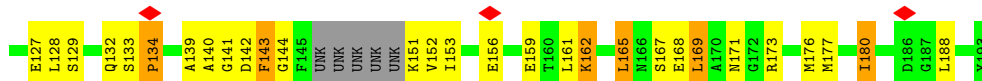




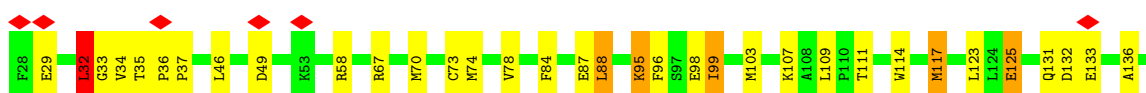
- Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11



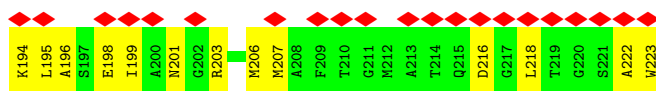
- Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9



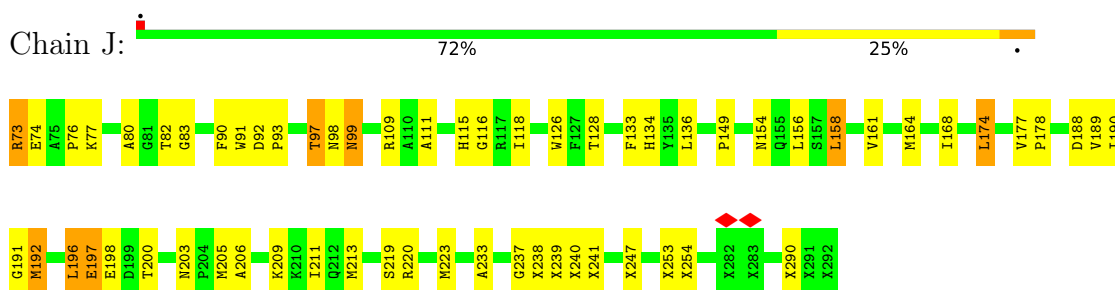
- Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2



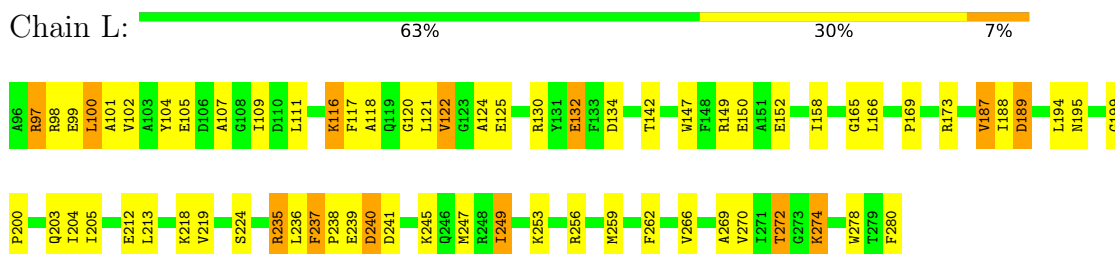
- Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12



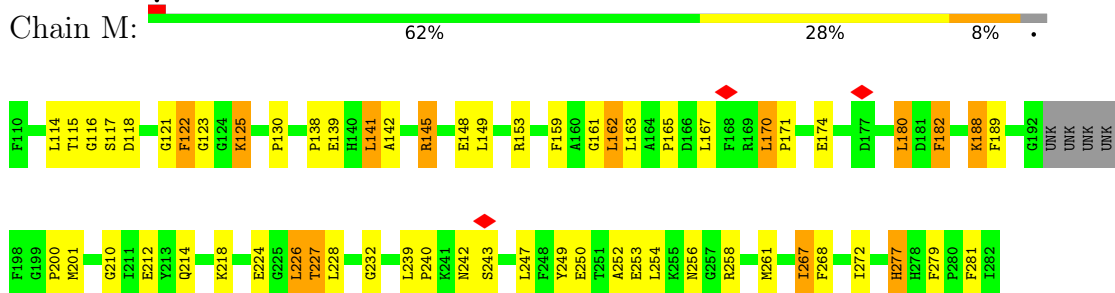
- Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3



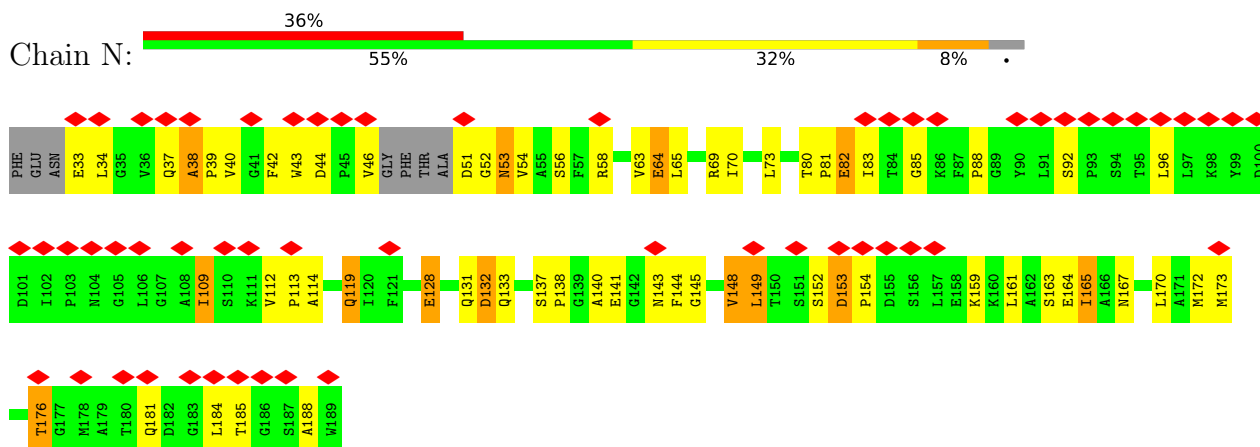
- Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5



- Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4

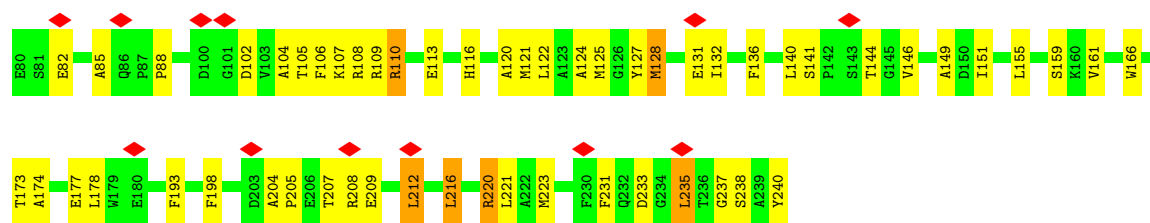


- Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13

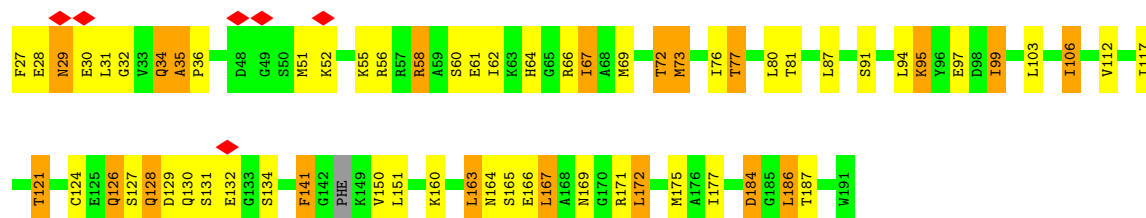


- Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15





- Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46321	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	1.690	Depositor
Minimum map value	-0.344	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.235	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, DGD, DD6, LMG, PID, LHG, SF4, CLA, SQD, KC1, PQN, UX

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	I	0.13	0/1484	0.33	0/2019
2	K	0.14	0/1357	0.33	1/1838 (0.1%)
5	G	0.35	0/1562	0.52	1/2122 (0.0%)
6	A	0.37	0/1276	0.53	0/1725
7	c	0.12	0/663	0.31	0/902
8	d	0.11	0/1767	0.30	0/2375
9	e	0.24	0/608	0.29	0/833
10	f	0.16	0/1489	0.33	0/2016
11	h	0.12	0/1101	0.27	0/1493
12	i	0.17	0/992	0.32	0/1346
13	j	0.14	0/801	0.31	0/1092
14	l	0.20	0/1998	0.35	0/2706
15	m	0.13	0/590	0.29	0/793
16	a	0.26	0/5344	0.41	2/7280 (0.0%)
17	b	0.19	0/5362	0.33	0/7335
18	B	0.17	0/1382	0.36	1/1862 (0.1%)
19	D	0.25	0/1178	0.47	0/1592
20	F	0.24	0/1263	0.54	4/1708 (0.2%)
21	H	0.19	0/1232	0.42	1/1665 (0.1%)
22	J	0.17	0/1246	0.39	0/1699
23	L	0.24	0/1462	0.43	0/1985
24	M	0.20	0/1241	0.35	0/1681
25	N	0.23	0/1005	0.51	0/1370
26	O	0.12	0/1091	0.40	0/1491
27	P	0.28	0/1128	0.45	0/1523
All	All	0.22	0/38622	0.39	10/52451 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	F	145	LYS	N-CA-C	8.92	123.26	112.38
16	a	391	LEU	N-CA-C	-6.93	103.78	111.82
21	H	110	MET	N-CA-C	-6.54	104.15	111.28
20	F	148	PHE	CA-C-N	-6.02	113.74	119.76
20	F	148	PHE	C-N-CA	-6.02	113.74	119.76

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	I	1480	0	1381	53	0
2	K	1349	0	1323	54	0
3	z	390	0	87	4	0
4	y	655	0	136	3	0
5	G	1572	0	1440	51	0
6	A	1346	0	1242	40	0
7	c	653	0	629	22	0
8	d	1731	0	1741	42	0
9	e	587	0	575	17	0
10	f	1450	0	1437	30	0
11	h	1066	0	1018	33	0
12	i	964	0	941	25	0
13	j	783	0	774	22	0
14	l	1943	0	1919	65	0
15	m	582	0	603	15	0
16	a	5194	0	5023	159	0
17	b	5199	0	5053	172	0
18	B	1452	0	1368	40	0
19	D	1158	0	1114	53	0
20	F	1237	0	1188	37	0
21	H	1202	0	1182	47	0
22	J	1496	0	1233	47	0
23	L	1427	0	1392	51	0
24	M	1211	0	1090	43	0
25	N	993	0	844	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	O	1073	0	956	37	0
27	P	1113	0	1050	49	0
28	A	172	0	0	2	0
28	B	171	0	0	1	0
28	D	43	0	0	0	0
28	F	86	0	0	1	0
28	G	172	0	0	5	0
28	H	43	0	0	1	0
28	I	172	0	0	2	0
28	J	129	0	0	5	0
28	K	215	0	0	0	0
28	L	215	0	0	2	0
28	M	215	0	0	2	0
28	N	43	0	0	0	0
28	O	43	0	0	0	0
28	P	43	0	0	0	0
28	b	43	0	0	0	0
28	h	43	0	0	0	0
29	A	47	0	0	1	0
29	B	47	0	0	0	0
29	G	47	0	0	0	0
29	I	47	0	0	2	0
29	J	47	0	0	1	0
29	K	47	0	0	1	0
29	O	47	0	0	0	0
29	P	47	0	0	0	0
29	h	47	0	0	0	0
30	A	597	0	493	23	0
30	B	587	0	532	20	0
30	D	317	0	229	18	0
30	F	317	0	227	22	0
30	G	592	0	530	22	0
30	H	343	0	278	15	0
30	I	637	0	554	31	0
30	J	552	0	456	29	0
30	K	496	0	398	18	0
30	L	503	0	411	21	0
30	M	481	0	370	19	0
30	N	256	0	216	10	0
30	O	297	0	245	14	0
30	P	297	0	245	18	0
30	a	1870	0	1786	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	1563	0	1526	106	0
30	f	147	0	115	10	0
30	h	55	0	49	0	0
30	j	113	0	104	8	0
30	l	493	0	471	25	0
30	m	60	0	59	2	0
31	A	90	0	0	0	0
31	B	45	0	0	0	0
31	D	90	0	0	1	0
31	F	90	0	0	2	0
31	G	45	0	0	0	0
31	H	90	0	0	1	0
31	I	45	0	0	0	0
31	J	45	0	0	0	0
31	K	45	0	0	0	0
31	L	90	0	0	0	0
31	M	90	0	0	1	0
31	N	135	0	0	1	0
31	O	135	0	0	4	0
31	P	135	0	0	1	0
32	G	89	0	94	2	0
32	I	39	0	36	0	0
32	L	38	0	34	2	0
32	j	41	0	40	3	0
32	l	50	0	58	0	0
32	y	54	0	66	1	0
33	B	37	0	44	1	0
33	D	49	0	64	5	0
33	I	74	0	88	2	0
33	K	43	0	56	0	0
33	P	27	0	24	0	0
33	b	75	0	90	5	0
33	j	35	0	40	4	0
34	D	276	0	300	12	0
34	F	184	0	200	13	0
34	G	92	0	100	6	0
34	H	92	0	100	8	0
34	M	46	0	50	1	0
34	N	92	0	100	4	0
34	O	230	0	250	23	0
34	P	230	0	250	17	0
34	j	46	0	50	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	50	0	64	8	0
36	a	8	0	0	1	0
36	c	16	0	0	2	0
37	a	80	0	112	5	0
37	b	120	0	168	15	0
37	f	40	0	56	4	0
37	i	40	0	56	7	0
37	j	40	0	56	5	0
37	l	120	0	168	10	0
37	m	40	0	56	4	0
38	a	33	0	46	5	0
38	b	33	0	46	4	0
39	a	48	0	69	3	0
All	All	55927	0	49064	1485	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 14.

The worst 5 of 1485 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)
10:f:72:ALA:N	17:b:462:TYR:HH	1.46	1.12
30:K:308:CLA:H2A	30:K:308:CLA:HED3	1.53	0.88
17:b:468:ILE:HG22	17:b:470:ASN:H	1.36	0.87
30:b:712:CLA:H12	18:B:124:ILE:HD11	1.56	0.87
26:O:221:LEU:HG	34:O:305:PID:H13	1.56	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	191/200 (96%)	163 (85%)	28 (15%)	0	100	100
2	K	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
5	G	204/224 (91%)	175 (86%)	27 (13%)	2 (1%)	12	45
6	A	162/189 (86%)	144 (89%)	14 (9%)	4 (2%)	4	23
7	c	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
8	d	216/218 (99%)	197 (91%)	19 (9%)	0	100	100
9	e	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	f	182/184 (99%)	177 (97%)	4 (2%)	1 (0%)	24	60
11	h	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
12	i	117/119 (98%)	105 (90%)	12 (10%)	0	100	100
13	j	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
14	l	248/250 (99%)	235 (95%)	12 (5%)	1 (0%)	30	65
15	m	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
16	a	668/670 (100%)	622 (93%)	43 (6%)	3 (0%)	30	65
17	b	661/663 (100%)	613 (93%)	47 (7%)	1 (0%)	43	76
18	B	171/192 (89%)	153 (90%)	15 (9%)	3 (2%)	6	31
19	D	156/165 (94%)	131 (84%)	22 (14%)	3 (2%)	6	30
20	F	165/176 (94%)	153 (93%)	10 (6%)	2 (1%)	10	40
21	H	158/160 (99%)	140 (89%)	16 (10%)	2 (1%)	9	38
22	J	164/220 (74%)	146 (89%)	17 (10%)	1 (1%)	21	56
23	L	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
24	M	164/173 (95%)	151 (92%)	13 (8%)	0	100	100
25	N	149/160 (93%)	119 (80%)	24 (16%)	6 (4%)	2	14
26	O	159/161 (99%)	130 (82%)	25 (16%)	4 (2%)	4	23
27	P	155/160 (97%)	135 (87%)	19 (12%)	1 (1%)	21	56
All	All	4901/5113 (96%)	4446 (91%)	421 (9%)	34 (1%)	20	53

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	121	PRO
6	A	85	ALA
14	l	70	PRO
16	a	47	ARG

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Mol	Chain	Res	Type
16	a	218	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	139/155 (90%)	131 (94%)	8 (6%)	18	51
2	K	133/138 (96%)	126 (95%)	7 (5%)	20	54
5	G	147/171 (86%)	136 (92%)	11 (8%)	12	41
6	A	122/129 (95%)	117 (96%)	5 (4%)	27	61
7	c	76/76 (100%)	75 (99%)	1 (1%)	61	81
8	d	182/184 (99%)	176 (97%)	6 (3%)	33	67
9	e	63/63 (100%)	63 (100%)	0	100	100
10	f	148/148 (100%)	145 (98%)	3 (2%)	48	76
11	h	112/114 (98%)	111 (99%)	1 (1%)	70	85
12	i	100/101 (99%)	99 (99%)	1 (1%)	68	84
13	j	88/89 (99%)	84 (96%)	4 (4%)	24	59
14	l	199/201 (99%)	189 (95%)	10 (5%)	22	56
15	m	60/63 (95%)	59 (98%)	1 (2%)	53	78
16	a	540/592 (91%)	517 (96%)	23 (4%)	26	60
17	b	557/581 (96%)	540 (97%)	17 (3%)	35	68
18	B	142/146 (97%)	123 (87%)	19 (13%)	4	18
19	D	116/123 (94%)	91 (78%)	25 (22%)	1	6
20	F	126/140 (90%)	106 (84%)	20 (16%)	2	13
21	H	123/123 (100%)	111 (90%)	12 (10%)	7	30
22	J	124/136 (91%)	107 (86%)	17 (14%)	3	17
23	L	140/145 (97%)	115 (82%)	25 (18%)	2	10
24	M	106/128 (83%)	86 (81%)	20 (19%)	1	9
25	N	80/124 (64%)	52 (65%)	28 (35%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	O	89/124 (72%)	70 (79%)	19 (21%)	1	6
27	P	105/123 (85%)	72 (69%)	33 (31%)	0	1
All	All	3817/4117 (93%)	3501 (92%)	316 (8%)	12	37

5 of 316 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	M	227	THR
27	P	31	LEU
25	N	37	GLN
25	N	173	MET
27	P	121	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
20	F	166	ASN
20	F	191	ASN
23	L	268	GLN
14	l	280	HIS
13	j	72	ASN

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](#)

342 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	b	721	28	50,54,73	1.37	8 (16%)	59,90,113	1.34	4 (6%)
30	CLA	b	723	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	7 (10%)
31	KC1	M	314	24	49,53,53	1.34	5 (10%)	61,89,89	1.73	14 (22%)
30	CLA	P	209	-	51,55,73	1.37	6 (11%)	60,91,113	1.39	5 (8%)
30	CLA	P	210	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	6 (7%)
28	DD6	I	302	-	40,45,45	1.61	2 (5%)	51,67,67	2.17	18 (35%)
30	CLA	P	214	-	50,54,73	1.34	8 (16%)	59,90,113	1.34	4 (6%)
30	CLA	a	701	-	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
33	LMG	j	101	-	35,35,55	0.88	1 (2%)	43,43,63	1.23	4 (9%)
30	CLA	B	317	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
28	DD6	G	502	-	40,45,45	1.54	2 (5%)	51,67,67	1.87	11 (21%)
28	DD6	h	203	-	40,45,45	1.55	2 (5%)	51,67,67	1.86	12 (23%)
28	DD6	M	305	-	40,45,45	1.56	3 (7%)	51,67,67	1.88	16 (31%)
30	CLA	M	309	24	59,63,73	1.28	6 (10%)	70,101,113	1.31	5 (7%)
31	KC1	D	315	19	49,53,53	1.32	6 (12%)	61,89,89	1.73	15 (24%)
29	UIX	J	305	-	43,49,49	1.35	4 (9%)	53,74,74	2.37	18 (33%)
28	DD6	I	301	-	40,45,45	1.57	2 (5%)	51,67,67	2.17	17 (33%)
30	CLA	D	309	-	50,54,73	1.36	7 (14%)	59,90,113	1.42	4 (6%)
34	PID	O	304	-	43,49,49	1.23	3 (6%)	52,76,76	1.70	11 (21%)
30	CLA	a	716	-	51,55,73	1.35	7 (13%)	60,91,113	1.40	5 (8%)
28	DD6	F	301	-	40,45,45	1.53	2 (5%)	51,67,67	2.31	16 (31%)
30	CLA	J	310	-	50,54,73	1.39	8 (16%)	59,90,113	1.36	3 (5%)
28	DD6	O	303	-	40,45,45	1.60	3 (7%)	51,67,67	2.02	13 (25%)
28	DD6	A	305	31	40,45,45	1.52	2 (5%)	51,67,67	1.89	14 (27%)
30	CLA	m	202	-	64,68,73	1.22	7 (10%)	76,107,113	1.33	6 (7%)
30	CLA	j	106	-	62,66,73	1.24	8 (12%)	73,104,113	1.32	6 (8%)
28	DD6	B	302	-	39,44,45	1.74	2 (5%)	49,65,67	2.08	17 (34%)
30	CLA	K	308	2	58,62,73	1.27	6 (10%)	68,99,113	1.34	6 (8%)
30	CLA	L	318	-	50,54,73	1.37	8 (16%)	59,90,113	1.42	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DD6	b	731	30	40,45,45	1.61	2 (5%)	51,67,67	1.98	17 (33%)
30	CLA	G	518	-	50,54,73	1.39	8 (16%)	59,90,113	1.44	5 (8%)
30	CLA	a	711	-	49,53,73	1.38	6 (12%)	58,89,113	1.45	7 (12%)
30	CLA	b	708	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
30	CLA	A	311	6	50,54,73	1.37	6 (12%)	59,90,113	1.38	4 (6%)
30	CLA	A	309	-	59,63,73	1.27	6 (10%)	70,101,113	1.32	8 (11%)
30	CLA	G	513	5	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
31	KC1	D	310	-	49,53,53	1.34	6 (12%)	61,89,89	1.73	13 (21%)
28	DD6	M	304	-	40,45,45	1.59	3 (7%)	51,67,67	1.92	14 (27%)
30	CLA	b	714	-	50,54,73	1.37	7 (14%)	59,90,113	1.42	5 (8%)
30	CLA	a	715	-	49,53,73	1.39	8 (16%)	58,89,113	1.45	4 (6%)
31	KC1	P	211	-	49,53,53	1.33	5 (10%)	61,89,89	1.73	14 (22%)
34	PID	D	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.46	9 (17%)
30	CLA	l	308	-	45,49,73	1.43	7 (15%)	54,84,113	1.45	5 (9%)
33	LMG	D	317	-	48,48,55	0.76	1 (2%)	55,55,63	1.28	5 (9%)
34	PID	D	304	-	43,49,49	1.23	3 (6%)	52,76,76	1.72	7 (13%)
30	CLA	D	308	-	51,55,73	1.36	6 (11%)	60,91,113	1.37	5 (8%)
30	CLA	b	727	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	5 (6%)
37	BCR	m	201	-	41,41,41	0.68	0	56,56,56	2.35	17 (30%)
30	CLA	B	313	18	69,73,73	1.17	6 (8%)	82,113,113	1.27	4 (4%)
34	PID	F	302	-	43,49,49	1.24	3 (6%)	52,76,76	1.59	7 (13%)
33	LMG	b	733	-	44,44,55	0.81	1 (2%)	52,52,63	1.31	7 (13%)
30	CLA	h	202	-	59,63,73	1.28	7 (11%)	70,101,113	1.33	5 (7%)
34	PID	O	307	-	43,49,49	1.26	3 (6%)	52,76,76	1.28	5 (9%)
30	CLA	l	311	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
28	DD6	P	204	-	40,45,45	1.53	2 (5%)	51,67,67	2.04	15 (29%)
30	CLA	B	311	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	5 (6%)
30	CLA	A	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.47	5 (9%)
30	CLA	a	720	-	66,70,73	1.21	7 (10%)	78,109,113	1.29	6 (7%)
30	CLA	J	312	-	57,61,73	1.28	8 (14%)	67,98,113	1.42	7 (10%)
30	CLA	H	312	-	50,54,73	1.38	7 (14%)	59,90,113	1.39	4 (6%)
30	CLA	F	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.45	5 (8%)
28	DD6	M	303	-	40,45,45	1.75	4 (10%)	51,67,67	2.19	18 (35%)
34	PID	P	206	-	43,49,49	1.24	3 (6%)	52,76,76	1.82	11 (21%)
30	CLA	b	722	-	69,73,73	1.18	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
34	PID	P	203	-	43,49,49	1.26	3 (6%)	52,76,76	1.32	6 (11%)
30	CLA	b	711	-	59,63,73	1.27	5 (8%)	70,101,113	1.31	6 (8%)
30	CLA	L	312	-	50,54,73	1.36	7 (14%)	59,90,113	1.39	4 (6%)
30	CLA	H	304	-	51,55,73	1.36	7 (13%)	60,91,113	1.38	5 (8%)
30	CLA	N	304	-	51,55,73	1.36	7 (13%)	60,91,113	1.40	5 (8%)
30	CLA	M	318	-	50,54,73	1.38	8 (16%)	59,90,113	1.37	4 (6%)
28	DD6	I	303	-	40,45,45	1.82	5 (12%)	51,67,67	2.02	16 (31%)
28	DD6	K	305	-	40,45,45	1.51	2 (5%)	51,67,67	1.86	15 (29%)
30	CLA	N	305	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
34	PID	F	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.91	9 (17%)
30	CLA	D	314	-	50,54,73	1.40	8 (16%)	59,90,113	1.45	6 (10%)
30	CLA	a	735	-	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
31	KC1	M	307	30	49,53,53	1.36	6 (12%)	61,89,89	1.79	14 (22%)
38	PQN	a	732	-	34,34,34	1.61	2 (5%)	43,45,45	1.15	5 (11%)
30	CLA	a	708	-	55,59,73	1.32	7 (12%)	64,96,113	1.39	6 (9%)
34	PID	H	302	-	43,49,49	1.29	3 (6%)	52,76,76	1.39	9 (17%)
30	CLA	G	517	-	50,54,73	1.36	7 (14%)	59,90,113	1.38	4 (6%)
33	LMG	B	318	-	37,37,55	0.84	0	45,45,63	1.33	6 (13%)
34	PID	G	506	-	43,49,49	1.29	3 (6%)	52,76,76	1.35	7 (13%)
30	CLA	F	308	-	50,54,73	1.35	8 (16%)	59,90,113	1.40	4 (6%)
28	DD6	L	304	-	40,45,45	1.55	2 (5%)	51,67,67	1.81	12 (23%)
34	PID	N	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.44	6 (11%)
30	CLA	a	725	-	65,69,73	1.21	7 (10%)	77,108,113	1.30	6 (7%)
33	LMG	I	318	-	36,36,55	0.89	1 (2%)	44,44,63	1.25	3 (6%)
30	CLA	N	309	25	50,54,73	1.36	7 (14%)	59,90,113	1.42	4 (6%)
30	CLA	P	212	-	55,59,73	1.32	7 (12%)	64,96,113	1.38	5 (7%)
30	CLA	J	309	-	60,64,73	1.25	9 (15%)	71,102,113	1.40	6 (8%)
30	CLA	a	738	22	50,54,73	1.37	7 (14%)	59,90,113	1.44	5 (8%)
30	CLA	H	311	-	45,49,73	1.44	7 (15%)	54,84,113	1.45	5 (9%)
30	CLA	H	305	-	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
30	CLA	J	308	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	6 (10%)
28	DD6	I	305	-	40,45,45	1.80	4 (10%)	51,67,67	2.24	17 (33%)
35	SQD	A	318	-	48,50,54	0.41	1 (2%)	58,61,65	0.58	0
30	CLA	a	729	-	60,64,73	1.26	6 (10%)	71,102,113	1.30	5 (7%)
28	DD6	K	304	-	40,45,45	1.56	2 (5%)	51,67,67	1.99	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	O	311	-	55,59,73	1.31	7 (12%)	64,96,113	1.34	5 (7%)
34	PID	O	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.47	5 (9%)
28	DD6	D	303	-	40,45,45	1.49	2 (5%)	51,67,67	1.83	14 (27%)
30	CLA	a	704	-	69,73,73	1.18	7 (10%)	82,113,113	1.17	2 (2%)
30	CLA	b	706	-	52,56,73	1.36	6 (11%)	61,92,113	1.37	6 (9%)
34	PID	M	301	-	43,49,49	1.22	3 (6%)	52,76,76	1.68	9 (17%)
34	PID	P	208	-	43,49,49	1.25	3 (6%)	52,76,76	1.42	6 (11%)
30	CLA	a	709	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
30	CLA	A	320	-	50,54,73	1.37	7 (14%)	59,90,113	1.41	4 (6%)
30	CLA	a	728	-	59,63,73	1.27	8 (13%)	70,101,113	1.34	6 (8%)
30	CLA	a	705	30	59,63,73	1.28	7 (11%)	70,101,113	1.37	7 (10%)
28	DD6	B	304	-	40,45,45	1.54	2 (5%)	51,67,67	1.88	11 (21%)
37	BCR	l	307	-	41,41,41	0.67	0	56,56,56	2.02	19 (33%)
28	DD6	L	303	-	40,45,45	1.50	2 (5%)	51,67,67	1.94	14 (27%)
33	LMG	P	201	-	27,27,55	0.99	1 (3%)	35,35,63	1.19	4 (11%)
30	CLA	J	316	-	50,54,73	1.37	7 (14%)	59,90,113	1.37	4 (6%)
30	CLA	l	305	-	69,73,73	1.18	7 (10%)	82,113,113	1.25	4 (4%)
30	CLA	F	310	-	50,54,73	1.36	6 (12%)	59,90,113	1.46	5 (8%)
30	CLA	b	716	-	54,58,73	1.32	7 (12%)	64,95,113	1.40	5 (7%)
30	CLA	f	301	-	59,63,73	1.27	7 (11%)	70,101,113	1.32	5 (7%)
30	CLA	b	726	-	51,55,73	1.36	7 (13%)	60,91,113	1.36	5 (8%)
30	CLA	L	313	-	59,63,73	1.27	8 (13%)	70,101,113	1.30	5 (7%)
31	KC1	A	314	6	49,53,53	1.33	6 (12%)	61,89,89	1.73	14 (22%)
28	DD6	K	301	-	40,45,45	1.52	2 (5%)	51,67,67	1.93	15 (29%)
28	DD6	G	505	-	40,45,45	1.83	3 (7%)	51,67,67	2.32	19 (37%)
37	BCR	a	734	-	41,41,41	0.65	0	56,56,56	2.08	20 (35%)
28	DD6	K	303	-	40,45,45	1.65	3 (7%)	51,67,67	1.73	12 (23%)
30	CLA	P	215	-	51,55,73	1.36	8 (15%)	60,91,113	1.52	7 (11%)
31	KC1	A	306	30,28	49,53,53	1.34	6 (12%)	61,89,89	1.71	13 (21%)
30	CLA	O	308	-	51,55,73	1.36	6 (11%)	60,91,113	1.39	5 (8%)
30	CLA	K	307	-	50,54,73	1.34	7 (14%)	59,90,113	1.42	5 (8%)
30	CLA	L	310	-	59,63,73	1.27	7 (11%)	70,101,113	1.33	6 (8%)
30	CLA	B	315	-	45,49,73	1.41	7 (15%)	54,84,113	1.52	5 (9%)
30	CLA	H	307	-	55,59,73	1.32	7 (12%)	64,96,113	1.40	6 (9%)
30	CLA	A	316	-	51,55,73	1.35	7 (13%)	60,91,113	1.39	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	K	312	-	52,56,73	1.34	8 (15%)	61,92,113	1.38	5 (8%)
34	PID	P	205	-	43,49,49	1.24	3 (6%)	52,76,76	1.64	8 (15%)
30	CLA	a	731	-	69,73,73	1.18	7 (10%)	82,113,113	1.27	6 (7%)
29	UIX	I	304	-	43,49,49	1.42	6 (13%)	53,74,74	2.50	16 (30%)
31	KC1	P	216	27	49,53,53	1.33	6 (12%)	61,89,89	1.70	12 (19%)
38	PQN	b	729	-	34,34,34	1.58	2 (5%)	43,45,45	1.28	5 (11%)
30	CLA	G	520	-	53,57,73	1.32	7 (13%)	61,93,113	1.35	7 (11%)
34	PID	G	507	-	43,49,49	1.25	3 (6%)	52,76,76	1.34	7 (13%)
33	LMG	I	320	-	38,38,55	0.81	0	46,46,63	1.29	6 (13%)
31	KC1	O	315	26	49,53,53	1.34	5 (10%)	61,89,89	1.68	13 (21%)
37	BCR	l	302	-	41,41,41	0.68	0	56,56,56	2.20	22 (39%)
30	CLA	I	310	-	52,56,73	1.34	6 (11%)	61,92,113	1.42	6 (9%)
30	CLA	G	512	-	64,68,73	1.22	7 (10%)	76,107,113	1.31	5 (6%)
30	CLA	b	710	-	56,60,73	1.32	8 (14%)	65,97,113	1.36	5 (7%)
30	CLA	G	516	5	45,49,73	1.44	6 (13%)	54,84,113	1.48	5 (9%)
34	PID	F	306	-	43,49,49	1.24	3 (6%)	52,76,76	1.43	5 (9%)
29	UIX	h	201	-	43,49,49	1.41	4 (9%)	53,74,74	2.48	20 (37%)
30	CLA	a	717	-	61,65,73	1.26	7 (11%)	72,103,113	1.31	7 (9%)
30	CLA	B	312	-	55,59,73	1.32	7 (12%)	64,96,113	1.36	5 (7%)
30	CLA	G	510	-	69,73,73	1.16	6 (8%)	82,113,113	1.28	7 (8%)
30	CLA	j	104	-	59,63,73	1.29	7 (11%)	70,101,113	1.31	6 (8%)
30	CLA	L	309	-	57,61,73	1.29	6 (10%)	67,98,113	1.36	6 (8%)
30	CLA	b	715	-	64,68,73	1.22	5 (7%)	76,107,113	1.31	5 (6%)
31	KC1	O	312	-	49,53,53	1.33	5 (10%)	61,89,89	1.73	14 (22%)
28	DD6	J	304	-	40,45,45	1.80	4 (10%)	51,67,67	2.14	19 (37%)
28	DD6	A	303	-	40,45,45	1.49	2 (5%)	51,67,67	1.79	13 (25%)
37	BCR	b	702	-	41,41,41	0.66	0	56,56,56	2.19	16 (28%)
32	DGD	j	103	-	42,42,67	1.06	2 (4%)	56,56,81	1.01	3 (5%)
30	CLA	b	701	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)
30	CLA	I	308	-	64,68,73	1.22	8 (12%)	76,107,113	1.28	7 (9%)
30	CLA	A	307	31	49,53,73	1.41	6 (12%)	58,89,113	1.44	4 (6%)
30	CLA	b	718	-	55,59,73	1.33	7 (12%)	64,96,113	1.42	6 (9%)
30	CLA	b	707	-	69,73,73	1.18	5 (7%)	82,113,113	1.28	6 (7%)
28	DD6	H	303	-	40,45,45	1.54	3 (7%)	51,67,67	1.92	14 (27%)
30	CLA	I	321	30	56,60,73	1.31	6 (10%)	65,97,113	1.47	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	N	307	-	55,59,73	1.32	8 (14%)	64,96,113	1.34	5 (7%)
34	PID	N	302	-	43,49,49	1.31	3 (6%)	52,76,76	1.64	10 (19%)
31	KC1	F	309	20	49,53,53	1.35	6 (12%)	61,89,89	1.79	14 (22%)
29	UIX	O	306	-	43,49,49	1.39	4 (9%)	53,74,74	2.89	20 (37%)
28	DD6	K	318	-	40,45,45	1.54	2 (5%)	51,67,67	2.05	12 (23%)
30	CLA	O	316	-	45,49,73	1.44	7 (15%)	54,84,113	1.50	5 (9%)
30	CLA	M	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.55	8 (14%)
30	CLA	b	712	-	58,62,73	1.36	9 (15%)	71,100,113	1.38	7 (9%)
28	DD6	A	302	-	40,45,45	1.60	3 (7%)	51,67,67	2.10	15 (29%)
30	CLA	B	309	18	69,73,73	1.17	6 (8%)	82,113,113	1.26	6 (7%)
28	DD6	L	306	-	40,45,45	1.54	2 (5%)	51,67,67	2.03	15 (29%)
32	DGD	I	317	-	40,40,67	1.10	2 (5%)	54,54,81	1.01	4 (7%)
30	CLA	I	315	-	56,60,73	1.31	7 (12%)	65,97,113	1.37	7 (10%)
30	CLA	a	719	-	51,55,73	1.36	8 (15%)	60,91,113	1.35	5 (8%)
30	CLA	J	315	-	50,54,73	1.37	6 (12%)	59,90,113	1.41	4 (6%)
30	CLA	F	315	-	45,49,73	1.43	6 (13%)	54,84,113	1.53	6 (11%)
28	DD6	L	302	-	40,45,45	1.48	2 (5%)	51,67,67	1.97	16 (31%)
30	CLA	L	317	-	56,60,73	1.32	7 (12%)	65,97,113	1.37	6 (9%)
30	CLA	J	306	-	50,54,73	1.37	8 (16%)	59,90,113	1.42	4 (6%)
30	CLA	a	706	16	62,66,73	1.23	7 (11%)	73,104,113	1.31	5 (6%)
30	CLA	K	316	-	50,54,73	1.37	8 (16%)	59,90,113	1.41	5 (8%)
30	CLA	a	724	-	69,73,73	1.19	8 (11%)	82,113,113	1.29	8 (9%)
28	DD6	M	302	-	40,45,45	1.75	3 (7%)	51,67,67	2.23	19 (37%)
30	CLA	P	217	-	45,49,73	1.43	8 (17%)	54,84,113	1.49	5 (9%)
30	CLA	l	304	-	64,68,73	1.22	6 (9%)	76,107,113	1.34	5 (6%)
31	KC1	I	314	1	49,53,53	1.33	6 (12%)	61,89,89	1.74	15 (24%)
28	DD6	F	303	-	40,45,45	1.55	2 (5%)	51,67,67	2.03	14 (27%)
31	KC1	N	308	-	49,53,53	1.43	6 (12%)	61,89,89	2.04	15 (24%)
31	KC1	F	314	20	49,53,53	1.35	5 (10%)	61,89,89	1.72	13 (21%)
30	CLA	b	728	-	69,73,73	1.18	7 (10%)	82,113,113	1.28	5 (6%)
30	CLA	M	308	31	57,61,73	1.29	7 (12%)	67,98,113	1.38	6 (8%)
30	CLA	l	313	14	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
30	CLA	a	721	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
36	SF4	c	202	7	0,12,12	-	-	-	-	-
30	CLA	I	312	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	I	313	-	59,63,73	1.26	7 (11%)	70,101,113	1.35	7 (10%)
30	CLA	a	727	-	50,54,73	1.38	7 (14%)	59,90,113	1.38	4 (6%)
34	PID	H	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.58	7 (13%)
31	KC1	K	314	2	49,53,53	1.33	6 (12%)	61,89,89	1.69	12 (19%)
30	CLA	B	316	-	50,54,73	1.37	6 (12%)	59,90,113	1.35	4 (6%)
30	CLA	F	312	-	50,54,73	1.32	8 (16%)	59,90,113	1.37	4 (6%)
30	CLA	l	310	-	39,50,73	2.85	11 (28%)	32,76,113	1.72	6 (18%)
31	KC1	O	310	-	49,53,53	1.33	6 (12%)	61,89,89	1.73	14 (22%)
30	CLA	D	311	-	50,54,73	1.36	6 (12%)	59,90,113	1.41	4 (6%)
30	CLA	l	309	-	45,49,73	1.42	5 (11%)	54,84,113	1.47	5 (9%)
30	CLA	J	314	-	45,49,73	1.43	6 (13%)	54,84,113	1.47	6 (11%)
30	CLA	I	307	-	50,54,73	1.37	6 (12%)	59,90,113	1.39	4 (6%)
30	CLA	F	313	-	50,54,73	1.37	7 (14%)	59,90,113	1.47	6 (10%)
31	KC1	B	314	18	49,53,53	1.33	5 (10%)	61,89,89	1.71	13 (21%)
30	CLA	M	316	-	56,60,73	1.31	8 (14%)	65,97,113	1.36	4 (6%)
30	CLA	l	312	-	50,54,73	1.37	7 (14%)	59,90,113	1.34	4 (6%)
30	CLA	O	314	-	51,55,73	1.36	8 (15%)	60,91,113	1.48	6 (10%)
30	CLA	f	303	10	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)
39	LHG	a	733	-	47,47,48	0.27	0	50,53,54	0.33	0
30	CLA	H	309	-	51,55,73	1.36	7 (13%)	60,91,113	1.40	5 (8%)
31	KC1	H	306	-	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
30	CLA	a	710	16	59,63,73	1.28	8 (13%)	70,101,113	1.36	7 (10%)
30	CLA	b	713	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
28	DD6	M	306	-	40,45,45	1.70	2 (5%)	51,67,67	2.22	20 (39%)
30	CLA	K	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.50	7 (12%)
30	CLA	B	307	18	53,57,73	1.35	7 (13%)	61,93,113	1.37	5 (8%)
31	KC1	P	213	-	49,53,53	1.34	6 (12%)	61,89,89	1.75	14 (22%)
29	UIX	K	302	-	43,49,49	1.40	4 (9%)	53,74,74	2.71	22 (41%)
37	BCR	b	732	-	41,41,41	0.72	0	56,56,56	1.90	18 (32%)
30	CLA	A	313	-	59,63,73	1.26	6 (10%)	70,101,113	1.32	6 (8%)
31	KC1	N	306	-	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
30	CLA	a	703	-	59,63,73	1.25	10 (16%)	70,101,113	1.44	8 (11%)
30	CLA	a	723	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	5 (6%)
34	PID	D	307	-	43,49,49	1.22	4 (9%)	52,76,76	1.37	5 (9%)
30	CLA	M	310	-	52,56,73	1.35	7 (13%)	61,92,113	1.39	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	b	709	-	64,68,73	1.22	7 (10%)	76,107,113	1.32	7 (9%)
30	CLA	J	301	-	64,68,73	1.22	7 (10%)	76,107,113	1.29	5 (6%)
30	CLA	a	726	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	8 (9%)
30	CLA	b	720	-	57,61,73	1.28	7 (12%)	67,98,113	1.32	5 (7%)
28	DD6	G	508	-	40,45,45	1.55	2 (5%)	51,67,67	2.02	14 (27%)
30	CLA	b	703	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	6 (7%)
32	DGD	l	301	-	51,51,67	0.96	2 (3%)	65,65,81	0.89	2 (3%)
28	DD6	G	504	-	40,45,45	1.83	6 (15%)	51,67,67	2.12	20 (39%)
30	CLA	G	509	5	55,59,73	1.32	6 (10%)	64,96,113	1.38	5 (7%)
34	PID	F	305	-	43,49,49	1.24	4 (9%)	52,76,76	1.83	8 (15%)
30	CLA	b	704	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
30	CLA	J	311	22	51,55,73	1.36	5 (9%)	60,91,113	1.41	6 (10%)
30	CLA	b	717	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
30	CLA	l	303	14	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
33	LMG	b	734	-	31,31,55	0.98	1 (3%)	39,39,63	1.18	4 (10%)
30	CLA	A	319	-	50,54,73	1.36	7 (14%)	59,90,113	1.34	4 (6%)
34	PID	D	306	-	43,49,49	1.25	3 (6%)	52,76,76	1.37	5 (9%)
30	CLA	K	306	2	53,57,73	1.34	7 (13%)	61,93,113	1.41	6 (9%)
28	DD6	L	305	-	40,45,45	1.54	2 (5%)	51,67,67	1.93	14 (27%)
30	CLA	a	722	-	62,66,73	1.23	7 (11%)	73,104,113	1.29	8 (10%)
31	KC1	H	310	-	49,53,53	1.35	5 (10%)	61,89,89	1.72	13 (21%)
32	DGD	G	521	-	45,45,67	1.03	2 (4%)	59,59,81	1.46	8 (13%)
29	UIX	A	304	-	43,49,49	1.36	4 (9%)	53,74,74	2.42	22 (41%)
30	CLA	a	707	-	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
30	CLA	D	312	19	50,54,73	1.37	8 (16%)	59,90,113	1.36	4 (6%)
31	KC1	G	515	5	49,53,53	1.35	6 (12%)	61,89,89	1.70	14 (22%)
30	CLA	G	514	-	57,61,73	1.28	8 (14%)	67,98,113	1.38	6 (8%)
36	SF4	c	201	7	0,12,12	-	-	-	-	-
31	KC1	J	313	-	49,53,53	1.34	6 (12%)	61,89,89	1.71	12 (19%)
30	CLA	H	308	-	50,54,73	1.38	7 (14%)	59,90,113	1.40	4 (6%)
31	KC1	L	315	-	49,53,53	1.35	5 (10%)	61,89,89	1.75	14 (22%)
31	KC1	N	311	25	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
37	BCR	b	730	-	41,41,41	0.70	0	56,56,56	2.27	20 (35%)
30	CLA	a	702	-	69,73,73	1.19	9 (13%)	82,113,113	1.32	5 (6%)
28	DD6	B	303	-	40,45,45	1.51	1 (2%)	51,67,67	1.89	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	J	307	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	4 (4%)
30	CLA	O	313	-	50,54,73	1.34	6 (12%)	59,90,113	1.36	5 (8%)
29	UIX	P	207	-	43,49,49	1.40	5 (11%)	53,74,74	2.79	21 (39%)
30	CLA	G	511	-	59,63,73	1.28	7 (11%)	70,101,113	1.32	5 (7%)
37	BCR	f	304	-	41,41,41	0.68	0	56,56,56	2.08	17 (30%)
34	PID	O	305	-	43,49,49	1.31	4 (9%)	52,76,76	1.52	8 (15%)
30	CLA	K	313	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	7 (10%)
30	CLA	A	312	-	59,63,73	1.27	7 (11%)	70,101,113	1.29	5 (7%)
32	DGD	L	301	-	39,39,67	0.96	2 (5%)	53,53,81	0.99	3 (5%)
30	CLA	A	310	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	5 (6%)
28	DD6	A	301	-	40,45,45	1.52	2 (5%)	51,67,67	2.05	14 (27%)
30	CLA	f	302	-	50,54,73	1.37	7 (14%)	59,90,113	1.39	5 (8%)
30	CLA	a	718	-	50,54,73	1.36	5 (10%)	59,90,113	1.41	4 (6%)
30	CLA	L	308	31	49,55,73	1.37	6 (12%)	62,91,113	1.39	7 (11%)
29	UIX	B	305	-	43,49,49	1.36	4 (9%)	53,74,74	2.39	17 (32%)
30	CLA	G	519	-	63,67,73	1.23	7 (11%)	74,105,113	1.30	4 (5%)
30	CLA	K	311	-	56,60,73	1.31	7 (12%)	65,97,113	1.34	6 (9%)
37	BCR	j	102	-	41,41,41	0.66	0	56,56,56	2.03	17 (30%)
37	BCR	l	306	-	41,41,41	0.68	0	56,56,56	1.92	12 (21%)
30	CLA	K	310	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
33	LMG	K	317	-	43,43,55	0.81	1 (2%)	51,51,63	1.32	6 (11%)
30	CLA	b	725	-	69,73,73	1.17	6 (8%)	82,113,113	1.25	6 (7%)
30	CLA	M	317	-	50,54,73	1.36	6 (12%)	59,90,113	1.43	5 (8%)
30	CLA	A	317	-	45,49,73	1.42	8 (17%)	54,84,113	1.48	6 (11%)
28	DD6	J	303	-	40,45,45	1.86	3 (7%)	51,67,67	2.45	16 (31%)
30	CLA	O	309	-	69,73,73	1.18	8 (11%)	82,113,113	1.30	6 (7%)
28	DD6	J	302	-	40,45,45	1.55	1 (2%)	51,67,67	2.06	14 (27%)
30	CLA	I	316	-	59,63,73	1.25	5 (8%)	70,101,113	1.34	6 (8%)
30	CLA	a	714	-	49,53,73	1.40	6 (12%)	58,89,113	1.43	5 (8%)
34	PID	D	302	-	43,49,49	1.26	3 (6%)	52,76,76	1.40	9 (17%)
30	CLA	D	313	19	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
31	KC1	L	307	30	49,53,53	1.33	5 (10%)	61,89,89	1.73	15 (24%)
30	CLA	a	712	30	64,68,73	1.21	8 (12%)	76,107,113	1.30	6 (7%)
28	DD6	N	303	-	40,45,45	1.54	2 (5%)	51,67,67	2.07	17 (33%)
30	CLA	A	308	-	59,63,73	1.26	6 (10%)	70,101,113	1.33	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PID	O	302	-	43,49,49	1.27	3 (6%)	52,76,76	1.27	6 (11%)
30	CLA	b	719	-	50,54,73	1.37	8 (16%)	59,90,113	1.44	4 (6%)
30	CLA	M	312	-	52,56,73	1.35	8 (15%)	61,92,113	1.40	6 (9%)
34	PID	P	202	-	43,49,49	1.23	3 (6%)	52,76,76	1.53	6 (11%)
30	CLA	B	310	-	59,63,73	1.28	7 (11%)	70,101,113	1.32	7 (10%)
37	BCR	a	736	-	41,41,41	0.70	0	56,56,56	2.04	18 (32%)
30	CLA	I	311	1	59,63,73	1.28	6 (10%)	70,101,113	1.34	6 (8%)
30	CLA	B	308	-	49,53,73	1.40	5 (10%)	58,89,113	1.45	4 (6%)
34	PID	D	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.44	7 (13%)
30	CLA	a	713	-	64,68,73	1.22	7 (10%)	76,107,113	1.28	6 (7%)
34	PID	j	105	-	43,49,49	1.28	4 (9%)	52,76,76	1.54	11 (21%)
30	CLA	b	705	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
28	DD6	B	306	-	40,45,45	1.55	2 (5%)	51,67,67	1.95	19 (37%)
30	CLA	M	313	-	50,54,73	1.37	7 (14%)	59,90,113	1.37	4 (6%)
36	SF4	a	737	16,17	0,12,12	-	-	-	-	-
30	CLA	L	314	-	57,61,73	1.29	7 (12%)	67,98,113	1.36	6 (8%)
32	DGD	G	501	-	46,46,67	1.03	2 (4%)	60,60,81	1.01	4 (6%)
30	CLA	F	307	-	50,54,73	1.37	8 (16%)	59,90,113	1.43	4 (6%)
30	CLA	L	311	-	59,63,73	1.27	6 (10%)	70,101,113	1.34	5 (7%)
30	CLA	D	316	-	45,49,73	1.42	7 (15%)	54,84,113	1.46	5 (9%)
30	CLA	I	319	30	49,53,73	1.39	7 (14%)	58,89,113	1.46	7 (12%)
30	CLA	I	306	1	53,57,73	1.33	7 (13%)	61,93,113	1.43	6 (9%)
30	CLA	I	309	-	59,63,73	1.28	8 (13%)	70,101,113	1.33	6 (8%)
30	CLA	M	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.38	4 (6%)
37	BCR	i	201	-	41,41,41	0.78	2 (4%)	56,56,56	2.14	21 (37%)
30	CLA	B	301	-	64,68,73	1.23	7 (10%)	76,107,113	1.25	5 (6%)
29	UIX	G	503	-	43,49,49	1.33	4 (9%)	53,74,74	2.33	19 (35%)
30	CLA	N	310	-	51,55,73	1.37	7 (13%)	60,91,113	1.50	6 (10%)
30	CLA	b	724	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
30	CLA	L	316	-	45,49,73	1.43	7 (15%)	54,84,113	1.49	5 (9%)
30	CLA	a	730	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
30	CLA	K	309	-	54,58,73	1.31	7 (12%)	64,95,113	1.40	7 (10%)
32	DGD	y	201	-	55,55,67	0.93	2 (3%)	69,69,81	0.97	3 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	721	28	1/1/11/20	1/17/93/115	-
30	CLA	b	723	-	1/1/12/20	9/21/97/115	-
31	KC1	M	314	24	-	9/15/71/71	-
30	CLA	P	209	-	1/1/11/20	6/18/94/115	-
30	CLA	P	210	-	1/1/15/20	13/39/115/115	-
30	CLA	P	214	-	1/1/11/20	3/17/93/115	-
28	DD6	I	302	-	-	5/26/80/80	0/3/3/3
30	CLA	a	701	-	1/1/11/20	2/15/91/115	-
33	LMG	j	101	-	-	14/30/50/70	0/1/1/1
30	CLA	B	317	-	1/1/11/20	7/15/91/115	-
28	DD6	G	502	-	-	6/26/80/80	0/3/3/3
28	DD6	h	203	-	-	1/26/80/80	0/3/3/3
30	CLA	M	309	24	1/1/13/20	5/27/103/115	-
28	DD6	M	305	-	-	1/26/80/80	0/3/3/3
31	KC1	D	315	19	-	4/15/71/71	-
29	UIX	J	305	-	-	11/31/87/87	0/3/3/3
28	DD6	I	301	-	-	3/26/80/80	0/3/3/3
30	CLA	D	309	-	1/1/11/20	7/17/93/115	-
34	PID	O	304	-	-	3/24/93/93	0/4/4/4
30	CLA	a	716	-	1/1/11/20	6/18/94/115	-
28	DD6	F	301	-	-	2/26/80/80	0/3/3/3
30	CLA	J	310	-	1/1/11/20	8/17/93/115	-
28	DD6	O	303	-	-	0/26/80/80	0/3/3/3
30	CLA	m	202	-	1/1/14/20	10/33/109/115	-
28	DD6	A	305	31	-	1/26/80/80	0/3/3/3
30	CLA	j	106	-	1/1/13/20	11/31/107/115	-
28	DD6	B	302	-	-	3/24/78/80	0/3/3/3
30	CLA	K	308	2	1/1/12/20	10/26/102/115	-
30	CLA	L	318	-	1/1/11/20	8/17/93/115	-
28	DD6	b	731	30	-	3/26/80/80	0/3/3/3
30	CLA	G	518	-	1/1/11/20	7/17/93/115	-
30	CLA	a	711	-	1/1/11/20	6/15/91/115	-
30	CLA	b	708	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	A	311	6	1/1/11/20	5/17/93/115	-
30	CLA	A	309	-	1/1/13/20	5/27/103/115	-
30	CLA	G	513	5	1/1/15/20	7/39/115/115	-
31	KC1	D	310	-	-	10/15/71/71	-
28	DD6	M	304	-	-	0/26/80/80	0/3/3/3
30	CLA	b	714	-	1/1/11/20	3/17/93/115	-
30	CLA	a	715	-	1/1/11/20	7/15/91/115	-
31	KC1	P	211	-	-	9/15/71/71	-
34	PID	D	305	-	-	2/24/93/93	0/4/4/4
30	CLA	l	308	-	1/1/10/20	3/10/86/115	-
33	LMG	D	317	-	-	17/41/61/70	0/1/1/1
34	PID	D	304	-	-	3/24/93/93	0/4/4/4
30	CLA	D	308	-	1/1/11/20	4/18/94/115	-
30	CLA	b	727	-	1/1/15/20	7/39/115/115	-
37	BCR	m	201	-	-	5/29/63/63	0/2/2/2
30	CLA	B	313	18	1/1/15/20	9/39/115/115	-
34	PID	F	302	-	-	2/24/93/93	0/4/4/4
33	LMG	b	733	-	-	18/39/59/70	0/1/1/1
30	CLA	h	202	-	1/1/13/20	9/27/103/115	-
34	PID	O	307	-	-	4/24/93/93	0/4/4/4
30	CLA	l	311	-	1/1/15/20	14/39/115/115	-
28	DD6	P	204	-	-	1/26/80/80	0/3/3/3
30	CLA	B	311	-	1/1/15/20	21/39/115/115	-
30	CLA	A	315	-	1/1/10/20	4/10/86/115	-
30	CLA	a	720	-	1/1/14/20	7/36/112/115	-
30	CLA	J	312	-	1/1/12/20	6/25/101/115	-
30	CLA	H	312	-	1/1/11/20	9/17/93/115	-
30	CLA	F	311	-	1/1/11/20	7/17/93/115	-
28	DD6	M	303	-	-	2/26/80/80	0/3/3/3
34	PID	P	206	-	-	3/24/93/93	0/4/4/4
30	CLA	b	722	-	1/1/15/20	7/39/115/115	-
34	PID	P	203	-	-	2/24/93/93	0/4/4/4
30	CLA	b	711	-	1/1/13/20	11/27/103/115	-
30	CLA	L	312	-	1/1/11/20	7/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	H	304	-	1/1/11/20	6/18/94/115	-
30	CLA	N	304	-	1/1/11/20	4/18/94/115	-
30	CLA	M	318	-	1/1/11/20	9/17/93/115	-
28	DD6	I	303	-	-	2/26/80/80	0/3/3/3
28	DD6	K	305	-	-	4/26/80/80	0/3/3/3
30	CLA	N	305	-	1/1/15/20	9/39/115/115	-
34	PID	F	304	-	-	3/24/93/93	0/4/4/4
30	CLA	D	314	-	1/1/11/20	8/17/93/115	-
30	CLA	a	735	-	1/1/15/20	18/39/115/115	-
31	KC1	M	307	30	-	6/15/71/71	-
38	PQN	a	732	-	-	8/23/43/43	0/2/2/2
30	CLA	a	708	-	1/1/12/20	5/23/99/115	-
34	PID	H	302	-	-	2/24/93/93	0/4/4/4
30	CLA	G	517	-	1/1/11/20	4/17/93/115	-
33	LMG	B	318	-	-	15/32/52/70	0/1/1/1
34	PID	G	506	-	-	3/24/93/93	0/4/4/4
30	CLA	F	308	-	1/1/11/20	3/17/93/115	-
28	DD6	L	304	-	-	0/26/80/80	0/3/3/3
34	PID	N	301	-	-	6/24/93/93	0/4/4/4
30	CLA	a	725	-	1/1/14/20	13/35/111/115	-
33	LMG	I	318	-	-	21/31/51/70	0/1/1/1
30	CLA	N	309	25	1/1/11/20	4/17/93/115	-
30	CLA	P	212	-	1/1/12/20	9/23/99/115	-
30	CLA	J	309	-	1/1/13/20	10/29/105/115	-
30	CLA	a	738	22	1/1/11/20	4/17/93/115	-
30	CLA	H	311	-	-	6/10/86/115	-
30	CLA	H	305	-	1/1/15/20	8/39/115/115	-
30	CLA	J	308	-	1/1/11/20	9/17/93/115	-
28	DD6	I	305	-	-	5/26/80/80	0/3/3/3
35	SQD	A	318	-	-	5/45/65/69	0/1/1/1
30	CLA	a	729	-	1/1/13/20	8/29/105/115	-
28	DD6	K	304	-	-	1/26/80/80	0/3/3/3
30	CLA	O	311	-	1/1/12/20	4/23/99/115	-
34	PID	O	301	-	-	4/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DD6	D	303	-	-	6/26/80/80	0/3/3/3
30	CLA	a	704	-	1/1/15/20	6/39/115/115	-
30	CLA	b	706	-	1/1/11/20	4/19/95/115	-
34	PID	M	301	-	-	1/24/93/93	0/4/4/4
34	PID	P	208	-	-	2/24/93/93	0/4/4/4
30	CLA	a	709	-	1/1/15/20	16/39/115/115	-
30	CLA	A	320	-	1/1/11/20	6/17/93/115	-
30	CLA	a	728	-	1/1/13/20	8/27/103/115	-
30	CLA	a	705	30	1/1/13/20	8/27/103/115	-
28	DD6	B	304	-	-	0/26/80/80	0/3/3/3
37	BCR	l	307	-	-	0/29/63/63	0/2/2/2
28	DD6	L	303	-	-	0/26/80/80	0/3/3/3
33	LMG	P	201	-	-	9/22/42/70	0/1/1/1
30	CLA	J	316	-	-	3/17/93/115	-
30	CLA	l	305	-	1/1/15/20	12/39/115/115	-
30	CLA	F	310	-	1/1/11/20	8/17/93/115	-
30	CLA	b	716	-	1/1/12/20	4/21/97/115	-
30	CLA	f	301	-	1/1/13/20	11/27/103/115	-
30	CLA	b	726	-	1/1/11/20	2/18/94/115	-
30	CLA	L	313	-	1/1/13/20	11/27/103/115	-
31	KC1	A	314	6	-	5/15/71/71	-
28	DD6	K	301	-	-	5/26/80/80	0/3/3/3
28	DD6	G	505	-	-	4/26/80/80	0/3/3/3
37	BCR	a	734	-	-	2/29/63/63	0/2/2/2
28	DD6	K	303	-	-	0/26/80/80	0/3/3/3
30	CLA	P	215	-	1/1/11/20	7/18/94/115	-
31	KC1	A	306	30,28	-	7/15/71/71	-
30	CLA	O	308	-	1/1/11/20	6/18/94/115	-
30	CLA	K	307	-	1/1/11/20	2/17/93/115	-
30	CLA	L	310	-	1/1/13/20	0/27/103/115	-
30	CLA	B	315	-	1/1/10/20	4/10/86/115	-
30	CLA	H	307	-	1/1/12/20	5/23/99/115	-
30	CLA	A	316	-	1/1/11/20	4/18/94/115	-
30	CLA	K	312	-	1/1/11/20	5/19/95/115	-
34	PID	P	205	-	-	3/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	a	731	-	1/1/15/20	13/39/115/115	-
29	UIX	I	304	-	-	4/31/87/87	0/3/3/3
31	KC1	P	216	27	-	8/15/71/71	-
38	PQN	b	729	-	-	4/23/43/43	0/2/2/2
30	CLA	G	520	-	1/1/11/20	5/20/96/115	-
34	PID	G	507	-	-	0/24/93/93	1/4/4/4
33	LMG	I	320	-	-	14/33/53/70	0/1/1/1
31	KC1	O	315	26	-	6/15/71/71	-
37	BCR	l	302	-	-	3/29/63/63	0/2/2/2
30	CLA	I	310	-	1/1/11/20	8/19/95/115	-
30	CLA	G	512	-	1/1/14/20	11/33/109/115	-
30	CLA	b	710	-	1/1/12/20	4/24/100/115	-
30	CLA	G	516	5	1/1/10/20	6/10/86/115	-
34	PID	F	306	-	-	0/24/93/93	0/4/4/4
29	UIX	h	201	-	-	2/31/87/87	0/3/3/3
30	CLA	a	717	-	1/1/13/20	13/30/106/115	-
30	CLA	B	312	-	1/1/12/20	4/23/99/115	-
30	CLA	G	510	-	1/1/15/20	10/39/115/115	-
30	CLA	j	104	-	1/1/13/20	6/27/103/115	-
30	CLA	L	309	-	1/1/12/20	7/25/101/115	-
30	CLA	b	715	-	1/1/14/20	12/33/109/115	-
31	KC1	O	312	-	-	9/15/71/71	-
28	DD6	J	304	-	-	2/26/80/80	0/3/3/3
28	DD6	A	303	-	-	1/26/80/80	0/3/3/3
37	BCR	b	702	-	-	2/29/63/63	0/2/2/2
32	DGD	j	103	-	-	8/30/70/95	0/2/2/2
30	CLA	b	701	-	1/1/15/20	13/39/115/115	-
30	CLA	I	308	-	1/1/14/20	12/33/109/115	-
30	CLA	A	307	31	1/1/11/20	1/15/91/115	-
30	CLA	b	718	-	1/1/12/20	3/23/99/115	-
30	CLA	b	707	-	1/1/15/20	18/39/115/115	-
30	CLA	I	321	30	1/1/12/20	8/24/100/115	-
28	DD6	H	303	-	-	1/26/80/80	0/3/3/3
30	CLA	N	307	-	1/1/12/20	3/23/99/115	-
34	PID	N	302	-	-	2/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	KC1	F	309	20	-	9/15/71/71	-
29	UIX	O	306	-	-	4/31/87/87	0/3/3/3
28	DD6	K	318	-	-	4/26/80/80	0/3/3/3
30	CLA	O	316	-	1/1/10/20	4/10/86/115	-
30	CLA	M	315	-	1/1/10/20	4/10/86/115	-
30	CLA	b	712	-	1/1/13/20	9/25/101/115	-
30	CLA	B	309	18	1/1/15/20	19/39/115/115	-
28	DD6	A	302	-	-	3/26/80/80	0/3/3/3
28	DD6	L	306	-	-	3/26/80/80	0/3/3/3
32	DGD	I	317	-	-	3/28/68/95	0/2/2/2
30	CLA	I	315	-	1/1/12/20	8/24/100/115	-
30	CLA	a	719	-	1/1/11/20	7/18/94/115	-
30	CLA	J	315	-	1/1/11/20	3/17/93/115	-
30	CLA	F	315	-	1/1/10/20	4/10/86/115	-
28	DD6	L	302	-	-	4/26/80/80	0/3/3/3
30	CLA	L	317	-	1/1/12/20	11/24/100/115	-
30	CLA	J	306	-	1/1/11/20	6/17/93/115	-
30	CLA	a	706	16	1/1/13/20	15/31/107/115	-
30	CLA	K	316	-	1/1/11/20	3/17/93/115	-
30	CLA	a	724	-	1/1/15/20	13/39/115/115	-
30	CLA	P	217	-	1/1/10/20	4/10/86/115	-
28	DD6	M	302	-	-	3/26/80/80	0/3/3/3
30	CLA	l	304	-	1/1/14/20	9/33/109/115	-
31	KC1	I	314	1	-	9/15/71/71	-
28	DD6	F	303	-	-	2/26/80/80	0/3/3/3
31	KC1	N	308	-	-	8/15/71/71	-
31	KC1	F	314	20	-	5/15/71/71	-
30	CLA	b	728	-	1/1/15/20	9/39/115/115	-
30	CLA	M	308	31	1/1/12/20	10/25/101/115	-
30	CLA	l	313	14	1/1/15/20	20/39/115/115	-
30	CLA	a	721	-	1/1/15/20	18/39/115/115	-
36	SF4	c	202	7	-	-	0/6/5/5
30	CLA	I	312	-	1/1/15/20	15/39/115/115	-
30	CLA	I	313	-	1/1/13/20	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	a	727	-	1/1/11/20	9/17/93/115	-
34	PID	H	301	-	-	4/24/93/93	0/4/4/4
31	KC1	K	314	2	-	9/15/71/71	-
30	CLA	B	316	-	1/1/11/20	9/17/93/115	-
30	CLA	F	312	-	1/1/11/20	3/17/93/115	-
30	CLA	l	310	-	-	10/15/65/115	0/5/5/9
31	KC1	O	310	-	-	7/15/71/71	-
30	CLA	D	311	-	1/1/11/20	3/17/93/115	-
30	CLA	l	309	-	1/1/10/20	3/10/86/115	-
30	CLA	J	314	-	1/1/10/20	2/10/86/115	-
30	CLA	I	307	-	1/1/11/20	7/17/93/115	-
30	CLA	F	313	-	1/1/11/20	5/17/93/115	-
31	KC1	B	314	18	-	7/15/71/71	-
30	CLA	M	316	-	1/1/12/20	10/24/100/115	-
30	CLA	l	312	-	1/1/11/20	6/17/93/115	-
30	CLA	O	314	-	1/1/11/20	8/18/94/115	-
30	CLA	f	303	10	1/1/11/20	8/17/93/115	-
39	LHG	a	733	-	-	16/52/52/53	-
30	CLA	H	309	-	1/1/11/20	8/18/94/115	-
31	KC1	H	306	-	-	4/15/71/71	-
30	CLA	a	710	16	1/1/13/20	6/27/103/115	-
30	CLA	b	713	-	1/1/15/20	8/39/115/115	-
28	DD6	M	306	-	-	5/26/80/80	0/3/3/3
30	CLA	K	315	-	1/1/10/20	2/10/86/115	-
30	CLA	B	307	18	1/1/11/20	3/20/96/115	-
31	KC1	P	213	-	-	8/15/71/71	-
29	UIX	K	302	-	-	5/31/87/87	0/3/3/3
37	BCR	b	732	-	-	0/29/63/63	0/2/2/2
30	CLA	A	313	-	1/1/13/20	10/27/103/115	-
31	KC1	N	306	-	-	6/15/71/71	-
30	CLA	a	703	-	1/1/13/20	6/27/103/115	-
30	CLA	a	723	-	1/1/15/20	13/39/115/115	-
34	PID	D	307	-	-	4/24/93/93	0/4/4/4
30	CLA	M	310	-	1/1/11/20	8/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	709	-	1/1/14/20	8/33/109/115	-
30	CLA	J	301	-	1/1/14/20	12/33/109/115	-
30	CLA	a	726	-	1/1/15/20	13/39/115/115	-
30	CLA	b	720	-	1/1/12/20	9/25/101/115	-
28	DD6	G	508	-	-	1/26/80/80	0/3/3/3
30	CLA	b	703	-	1/1/15/20	12/39/115/115	-
32	DGD	l	301	-	-	8/39/79/95	0/2/2/2
28	DD6	G	504	-	-	5/26/80/80	0/3/3/3
30	CLA	G	509	5	1/1/12/20	4/23/99/115	-
34	PID	F	305	-	-	8/24/93/93	0/4/4/4
30	CLA	b	704	-	1/1/15/20	19/39/115/115	-
30	CLA	J	311	22	1/1/11/20	7/18/94/115	-
30	CLA	b	717	-	1/1/15/20	18/39/115/115	-
30	CLA	l	303	14	1/1/15/20	14/39/115/115	-
33	LMG	b	734	-	-	12/26/46/70	0/1/1/1
30	CLA	A	319	-	1/1/11/20	9/17/93/115	-
34	PID	D	306	-	-	8/24/93/93	0/4/4/4
30	CLA	K	306	2	1/1/11/20	4/20/96/115	-
28	DD6	L	305	-	-	3/26/80/80	0/3/3/3
30	CLA	a	722	-	1/1/13/20	8/31/107/115	-
31	KC1	H	310	-	-	6/15/71/71	-
32	DGD	G	521	-	-	18/33/73/95	0/2/2/2
29	UIX	A	304	-	-	0/31/87/87	0/3/3/3
30	CLA	a	707	-	1/1/15/20	17/39/115/115	-
30	CLA	D	312	19	1/1/11/20	7/17/93/115	-
31	KC1	G	515	5	-	6/15/71/71	-
30	CLA	G	514	-	1/1/12/20	11/25/101/115	-
36	SF4	c	201	7	-	-	0/6/5/5
31	KC1	J	313	-	-	7/15/71/71	-
30	CLA	H	308	-	1/1/11/20	4/17/93/115	-
31	KC1	L	315	-	-	8/15/71/71	-
31	KC1	N	311	25	-	7/15/71/71	-
37	BCR	b	730	-	-	6/29/63/63	0/2/2/2
30	CLA	a	702	-	1/1/15/20	11/39/115/115	-
28	DD6	B	303	-	-	2/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	J	307	-	1/1/15/20	19/39/115/115	-
30	CLA	O	313	-	1/1/11/20	3/17/93/115	-
29	UIX	P	207	-	-	8/31/87/87	0/3/3/3
30	CLA	G	511	-	1/1/13/20	4/27/103/115	-
37	BCR	f	304	-	-	2/29/63/63	0/2/2/2
34	PID	O	305	-	-	16/24/93/93	0/4/4/4
30	CLA	K	313	-	1/1/13/20	7/27/103/115	-
30	CLA	A	312	-	1/1/13/20	6/27/103/115	-
32	DGD	L	301	-	-	1/26/66/95	0/2/2/2
30	CLA	A	310	-	1/1/15/20	15/39/115/115	-
30	CLA	f	302	-	1/1/11/20	6/17/93/115	-
28	DD6	A	301	-	-	3/26/80/80	0/3/3/3
30	CLA	a	718	-	1/1/11/20	9/17/93/115	-
30	CLA	L	308	31	1/1/11/20	9/15/91/115	-
29	UIX	B	305	-	-	2/31/87/87	0/3/3/3
30	CLA	G	519	-	1/1/13/20	13/32/108/115	-
30	CLA	K	311	-	1/1/12/20	11/24/100/115	-
37	BCR	j	102	-	-	5/29/63/63	0/2/2/2
37	BCR	l	306	-	-	7/29/63/63	0/2/2/2
30	CLA	K	310	-	1/1/13/20	5/27/103/115	-
33	LMG	K	317	-	-	19/38/58/70	0/1/1/1
30	CLA	b	725	-	1/1/15/20	9/39/115/115	-
30	CLA	M	317	-	1/1/11/20	8/17/93/115	-
30	CLA	A	317	-	1/1/10/20	0/10/86/115	-
28	DD6	J	303	-	-	2/26/80/80	0/3/3/3
30	CLA	O	309	-	1/1/15/20	1/39/115/115	-
30	CLA	a	714	-	1/1/11/20	4/15/91/115	-
30	CLA	I	316	-	1/1/13/20	13/27/103/115	-
28	DD6	J	302	-	-	3/26/80/80	0/3/3/3
34	PID	D	302	-	-	3/24/93/93	0/4/4/4
30	CLA	D	313	19	1/1/11/20	2/15/91/115	-
31	KC1	L	307	30	-	6/15/71/71	-
30	CLA	a	712	30	1/1/14/20	8/33/109/115	-
30	CLA	A	308	-	1/1/13/20	4/27/103/115	-
28	DD6	N	303	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PID	O	302	-	-	2/24/93/93	0/4/4/4
30	CLA	b	719	-	1/1/11/20	9/17/93/115	-
30	CLA	M	312	-	1/1/11/20	5/19/95/115	-
34	PID	P	202	-	-	3/24/93/93	0/4/4/4
30	CLA	B	310	-	1/1/13/20	8/27/103/115	-
37	BCR	a	736	-	-	2/29/63/63	0/2/2/2
30	CLA	I	311	1	1/1/13/20	10/27/103/115	-
30	CLA	B	308	-	1/1/11/20	5/15/91/115	-
34	PID	D	301	-	-	2/24/93/93	0/4/4/4
30	CLA	a	713	-	1/1/14/20	11/33/109/115	-
34	PID	j	105	-	-	4/24/93/93	0/4/4/4
30	CLA	b	705	-	1/1/15/20	11/39/115/115	-
28	DD6	B	306	-	-	2/26/80/80	0/3/3/3
30	CLA	M	313	-	1/1/11/20	2/17/93/115	-
36	SF4	a	737	16,17	-	-	0/6/5/5
30	CLA	L	314	-	1/1/12/20	6/25/101/115	-
32	DGD	G	501	-	-	10/34/74/95	0/2/2/2
30	CLA	F	307	-	1/1/11/20	3/17/93/115	-
30	CLA	L	311	-	1/1/13/20	5/27/103/115	-
30	CLA	D	316	-	1/1/10/20	0/10/86/115	-
30	CLA	I	319	30	1/1/11/20	7/15/91/115	-
30	CLA	I	306	1	1/1/11/20	9/20/96/115	-
30	CLA	I	309	-	1/1/13/20	6/27/103/115	-
30	CLA	M	311	-	1/1/11/20	4/17/93/115	-
37	BCR	i	201	-	-	8/29/63/63	0/2/2/2
30	CLA	B	301	-	1/1/14/20	10/33/109/115	-
29	UIX	G	503	-	-	5/31/87/87	0/3/3/3
30	CLA	N	310	-	1/1/11/20	10/18/94/115	-
30	CLA	b	724	-	1/1/15/20	15/39/115/115	-
30	CLA	L	316	-	1/1/10/20	4/10/86/115	-
30	CLA	a	730	-	1/1/15/20	4/39/115/115	-
30	CLA	K	309	-	1/1/12/20	2/21/97/115	-
32	DGD	y	201	-	-	7/43/83/95	0/2/2/2

The worst 5 of 1826 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	I	310	CLA	C1B-C2B	9.21	1.49	1.39
28	J	303	DD6	C30-C31	-9.00	1.25	1.42
28	I	305	DD6	C30-C31	-8.99	1.25	1.42
28	G	505	DD6	C30-C31	-8.98	1.25	1.42
28	M	306	DD6	C30-C31	-8.97	1.25	1.42

The worst 5 of 2771 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	I	304	UIX	C6-C1-C	-9.10	107.33	122.30
37	m	201	BCR	C7-C8-C9	-8.31	113.94	126.23
29	O	306	UIX	C14-C13-C11	-7.75	116.40	127.28
30	I	304	CLA	C4A-NA-C1A	7.44	110.07	106.68
30	O	314	CLA	C4A-NA-C1A	7.35	110.03	106.68

5 of 198 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	I	306	CLA	ND
30	I	307	CLA	ND
30	I	308	CLA	ND
30	I	309	CLA	ND
30	I	310	CLA	ND

5 of 2247 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	K	301	DD6	C12-C11-C13-C14
28	G	502	DD6	C-C1-C24-C25
28	G	502	DD6	C2-C1-C24-C25
28	G	504	DD6	C10-C11-C13-C14
28	G	504	DD6	C12-C11-C13-C14

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	G	507	PID	C24-C25-C26-C27-C28-C29

264 monomers are involved in 671 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	b	721	CLA	2	0
30	b	723	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	P	209	CLA	2	0
30	P	210	CLA	4	0
30	P	214	CLA	3	0
33	j	101	LMG	4	0
30	B	317	CLA	2	0
30	M	309	CLA	8	0
29	J	305	UIX	1	0
28	I	301	DD6	1	0
30	D	309	CLA	2	0
34	O	304	PID	1	0
30	a	716	CLA	3	0
28	F	301	DD6	1	0
30	J	310	CLA	3	0
28	A	305	DD6	1	0
30	m	202	CLA	2	0
30	j	106	CLA	3	0
28	B	302	DD6	1	0
30	K	308	CLA	3	0
30	G	518	CLA	1	0
30	a	711	CLA	3	0
30	b	708	CLA	2	0
30	A	311	CLA	1	0
30	A	309	CLA	2	0
30	G	513	CLA	4	0
31	D	310	KC1	1	0
30	b	714	CLA	1	0
34	D	305	PID	3	0
30	l	308	CLA	1	0
33	D	317	LMG	5	0
34	D	304	PID	2	0
30	D	308	CLA	1	0
30	b	727	CLA	6	0
37	m	201	BCR	4	0
30	B	313	CLA	4	0
34	F	302	PID	2	0
33	b	733	LMG	2	0
34	O	307	PID	5	0
30	l	311	CLA	4	0
30	B	311	CLA	2	0
30	A	315	CLA	1	0
30	a	720	CLA	2	0
30	J	312	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	H	312	CLA	1	0
30	F	311	CLA	1	0
28	M	303	DD6	2	0
34	P	206	PID	4	0
30	b	722	CLA	4	0
34	P	203	PID	5	0
30	L	312	CLA	1	0
30	H	304	CLA	3	0
30	M	318	CLA	1	0
30	N	305	CLA	2	0
34	F	304	PID	6	0
30	D	314	CLA	10	0
30	a	735	CLA	5	0
31	M	307	KC1	1	0
38	a	732	PQN	5	0
30	a	708	CLA	2	0
34	H	302	PID	5	0
30	G	517	CLA	6	0
33	B	318	LMG	1	0
34	G	506	PID	2	0
30	F	308	CLA	1	0
28	L	304	DD6	1	0
34	N	301	PID	1	0
30	a	725	CLA	5	0
30	N	309	CLA	4	0
30	J	309	CLA	3	0
30	a	738	CLA	1	0
30	H	311	CLA	2	0
30	H	305	CLA	4	0
30	J	308	CLA	3	0
28	I	305	DD6	1	0
35	A	318	SQD	8	0
30	a	729	CLA	3	0
30	O	311	CLA	1	0
34	O	301	PID	1	0
30	a	704	CLA	5	0
30	b	706	CLA	3	0
34	M	301	PID	1	0
34	P	208	PID	2	0
30	a	709	CLA	5	0
30	A	320	CLA	3	0
30	a	728	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	a	705	CLA	2	0
37	l	307	BCR	3	0
30	J	316	CLA	4	0
30	l	305	CLA	3	0
30	F	310	CLA	5	0
30	b	716	CLA	4	0
30	f	301	CLA	5	0
30	b	726	CLA	1	0
30	L	313	CLA	7	0
28	G	505	DD6	1	0
37	a	734	BCR	3	0
30	P	215	CLA	6	0
30	O	308	CLA	1	0
30	K	307	CLA	1	0
30	B	315	CLA	2	0
30	H	307	CLA	1	0
30	A	316	CLA	1	0
30	K	312	CLA	2	0
34	P	205	PID	2	0
30	a	731	CLA	6	0
29	I	304	UIX	2	0
38	b	729	PQN	4	0
30	G	520	CLA	3	0
34	G	507	PID	5	0
33	I	320	LMG	2	0
31	O	315	KC1	3	0
37	l	302	BCR	3	0
30	I	310	CLA	4	0
30	b	710	CLA	6	0
34	F	306	PID	2	0
30	a	717	CLA	4	0
30	G	510	CLA	4	0
30	j	104	CLA	5	0
30	L	309	CLA	1	0
30	b	715	CLA	5	0
31	O	312	KC1	1	0
28	J	304	DD6	3	0
28	A	303	DD6	1	0
37	b	702	BCR	6	0
32	j	103	DGD	3	0
30	b	701	CLA	7	0
30	I	308	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	b	718	CLA	4	0
30	b	707	CLA	5	0
28	H	303	DD6	1	0
30	I	321	CLA	3	0
30	N	307	CLA	1	0
34	N	302	PID	3	0
31	F	309	KC1	2	0
30	O	316	CLA	2	0
30	M	315	CLA	2	0
30	b	712	CLA	4	0
30	B	309	CLA	4	0
30	I	315	CLA	1	0
30	a	719	CLA	4	0
30	F	315	CLA	1	0
30	L	317	CLA	5	0
30	J	306	CLA	1	0
30	a	706	CLA	7	0
30	K	316	CLA	1	0
30	a	724	CLA	3	0
30	P	217	CLA	3	0
30	l	304	CLA	3	0
31	N	308	KC1	1	0
30	b	728	CLA	3	0
30	M	308	CLA	2	0
30	l	313	CLA	6	0
30	a	721	CLA	6	0
36	c	202	SF4	1	0
30	I	312	CLA	2	0
30	I	313	CLA	3	0
30	a	727	CLA	1	0
34	H	301	PID	3	0
30	B	316	CLA	1	0
30	F	312	CLA	5	0
30	l	310	CLA	1	0
30	D	311	CLA	2	0
30	I	307	CLA	2	0
30	F	313	CLA	8	0
30	M	316	CLA	1	0
30	l	312	CLA	3	0
30	O	314	CLA	5	0
30	f	303	CLA	1	0
39	a	733	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	H	309	CLA	2	0
30	a	710	CLA	4	0
30	b	713	CLA	6	0
30	B	307	CLA	1	0
31	P	213	KC1	1	0
29	K	302	UIX	1	0
37	b	732	BCR	4	0
30	A	313	CLA	4	0
30	a	703	CLA	5	0
30	a	723	CLA	7	0
30	M	310	CLA	2	0
30	b	709	CLA	7	0
30	J	301	CLA	5	0
30	a	726	CLA	6	0
30	b	720	CLA	8	0
28	G	508	DD6	1	0
30	b	703	CLA	6	0
28	G	504	DD6	3	0
30	G	509	CLA	1	0
34	F	305	PID	3	0
30	b	704	CLA	14	0
30	J	311	CLA	2	0
30	b	717	CLA	6	0
30	l	303	CLA	5	0
33	b	734	LMG	3	0
30	A	319	CLA	2	0
34	D	306	PID	1	0
30	K	306	CLA	1	0
28	L	305	DD6	1	0
30	a	722	CLA	5	0
31	H	310	KC1	1	0
29	A	304	UIX	1	0
30	a	707	CLA	7	0
30	D	312	CLA	2	0
30	G	514	CLA	3	0
36	c	201	SF4	1	0
30	H	308	CLA	2	0
37	b	730	BCR	5	0
30	a	702	CLA	5	0
30	J	307	CLA	11	0
30	O	313	CLA	2	0
30	G	511	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	f	304	BCR	4	0
34	O	305	PID	14	0
30	K	313	CLA	5	0
30	A	312	CLA	3	0
32	L	301	DGD	2	0
30	A	310	CLA	4	0
30	f	302	CLA	4	0
30	a	718	CLA	1	0
30	L	308	CLA	2	0
30	G	519	CLA	1	0
30	K	311	CLA	2	0
37	j	102	BCR	5	0
37	l	306	BCR	4	0
30	K	310	CLA	1	0
30	b	725	CLA	4	0
30	M	317	CLA	2	0
30	A	317	CLA	2	0
28	J	303	DD6	2	0
30	O	309	CLA	3	0
30	I	316	CLA	3	0
30	a	714	CLA	3	0
34	D	302	PID	2	0
30	D	313	CLA	1	0
30	a	712	CLA	1	0
30	A	308	CLA	3	0
34	O	302	PID	2	0
30	M	312	CLA	1	0
34	P	202	PID	5	0
30	B	310	CLA	1	0
37	a	736	BCR	2	0
30	I	311	CLA	5	0
30	B	308	CLA	1	0
34	D	301	PID	4	0
30	a	713	CLA	3	0
34	j	105	PID	4	0
30	b	705	CLA	4	0
30	M	313	CLA	3	0
36	a	737	SF4	1	0
30	L	314	CLA	4	0
32	G	501	DGD	2	0
30	F	307	CLA	1	0
30	I	319	CLA	2	0

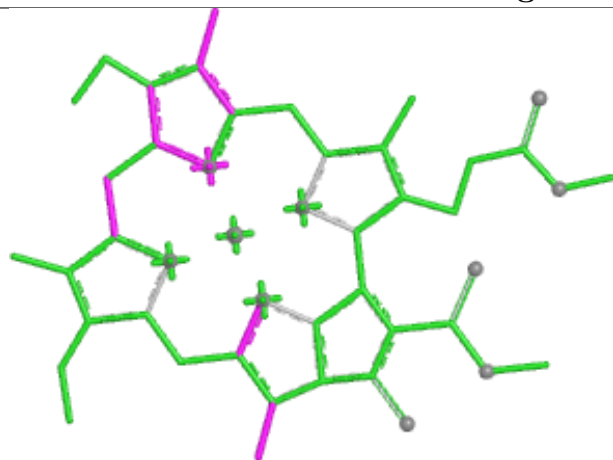
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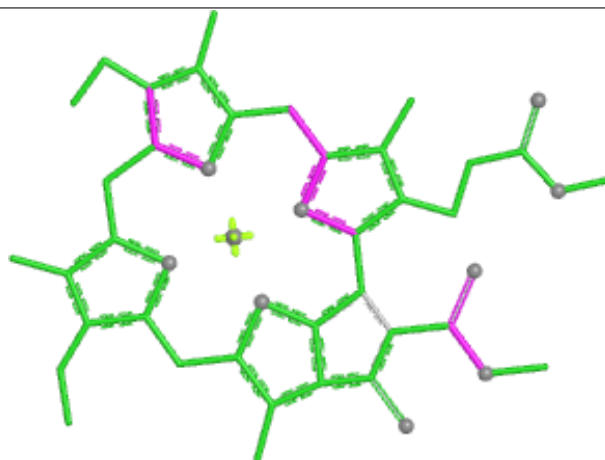
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	I	306	CLA	2	0
30	I	309	CLA	1	0
37	i	201	BCR	7	0
30	B	301	CLA	3	0
30	N	310	CLA	3	0
30	b	724	CLA	4	0
30	L	316	CLA	1	0
30	a	730	CLA	6	0
30	K	309	CLA	2	0
32	y	201	DGD	1	0

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.

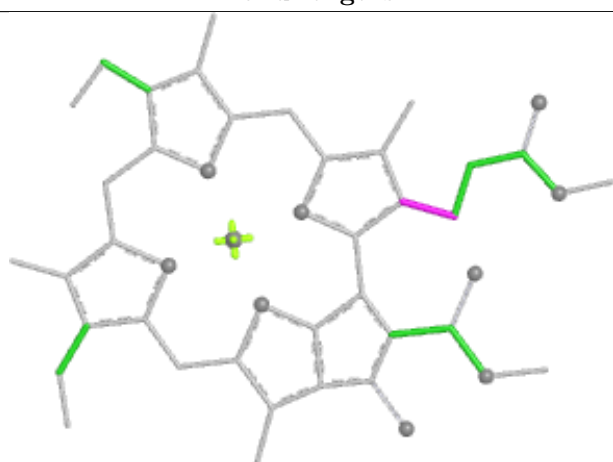
Ligand CLA b 721



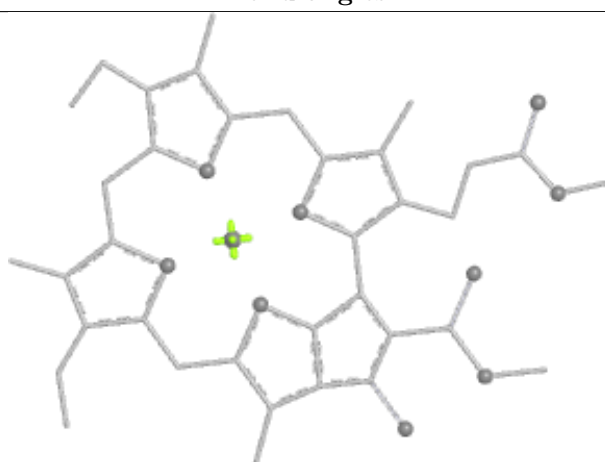
Bond lengths



Bond angles

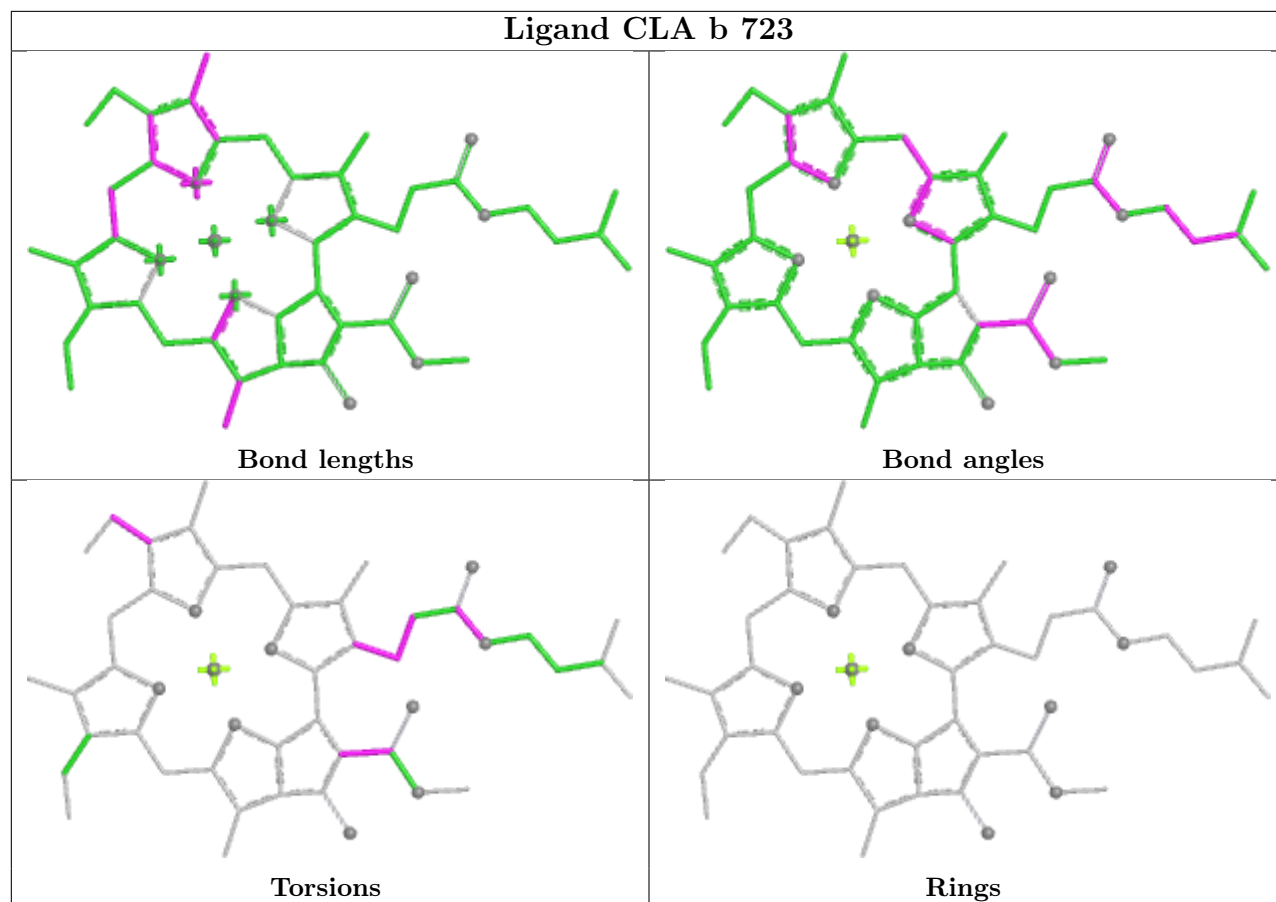


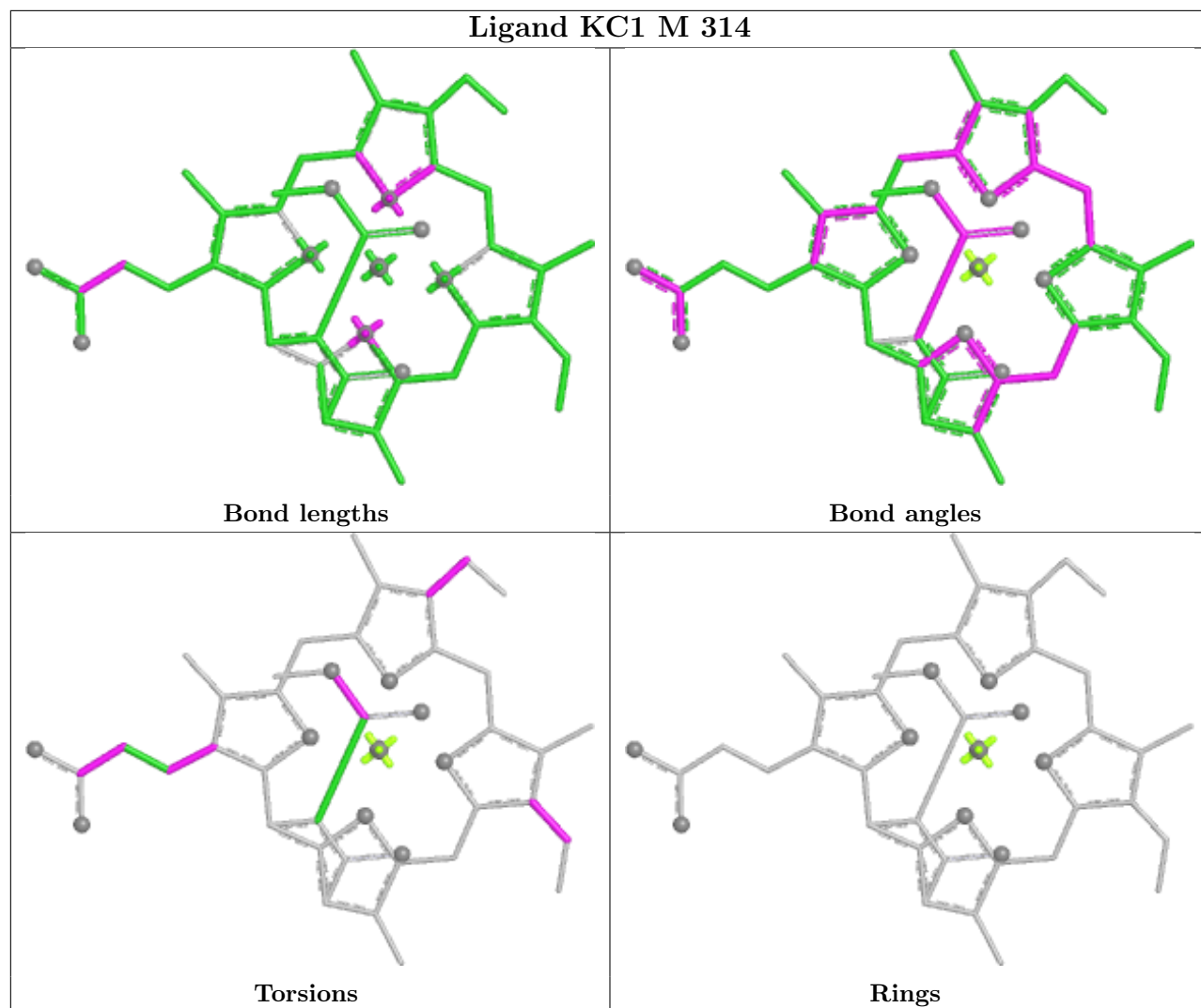
Torsions



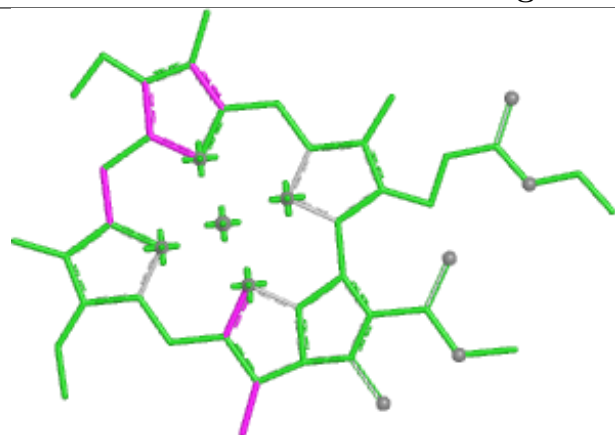
Rings

Ligand CLA b 723

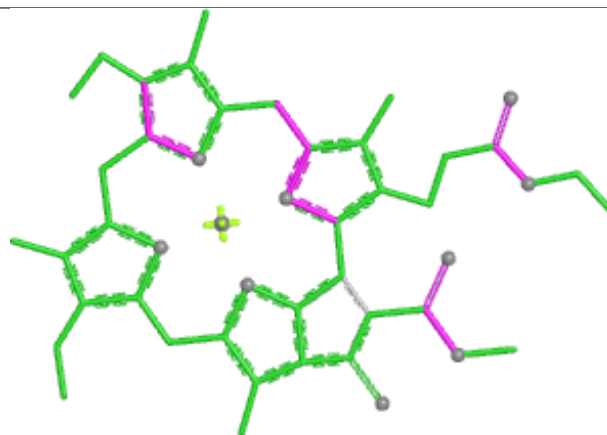




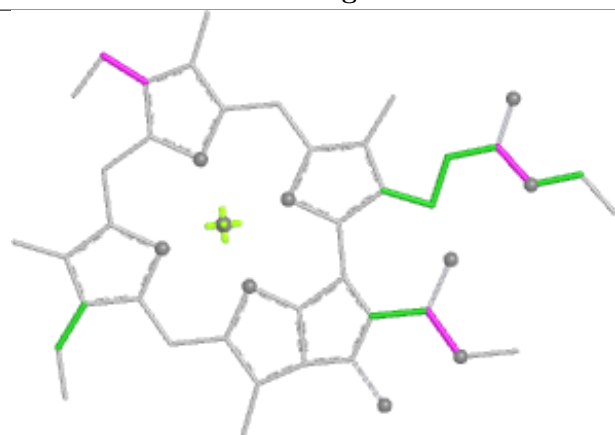
Ligand CLA P 209



Bond lengths



Bond angles

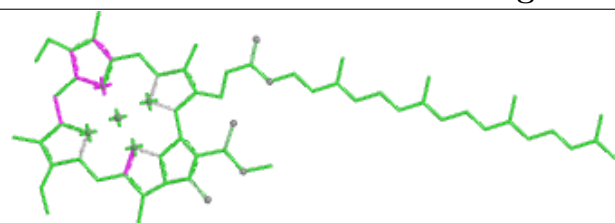


Torsions

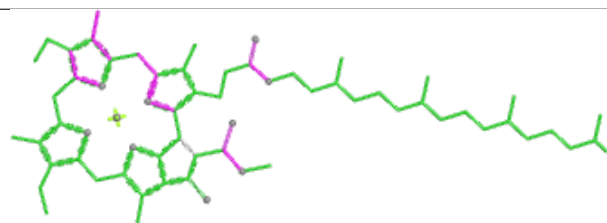


Rings

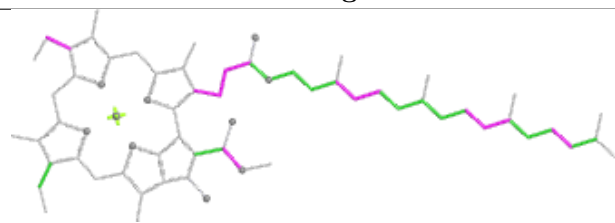
Ligand CLA P 210



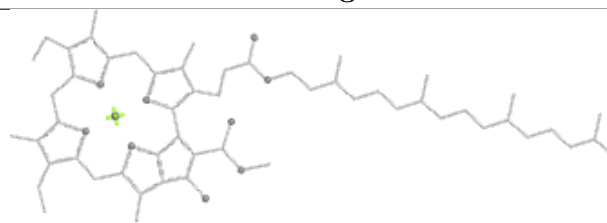
Bond lengths



Bond angles

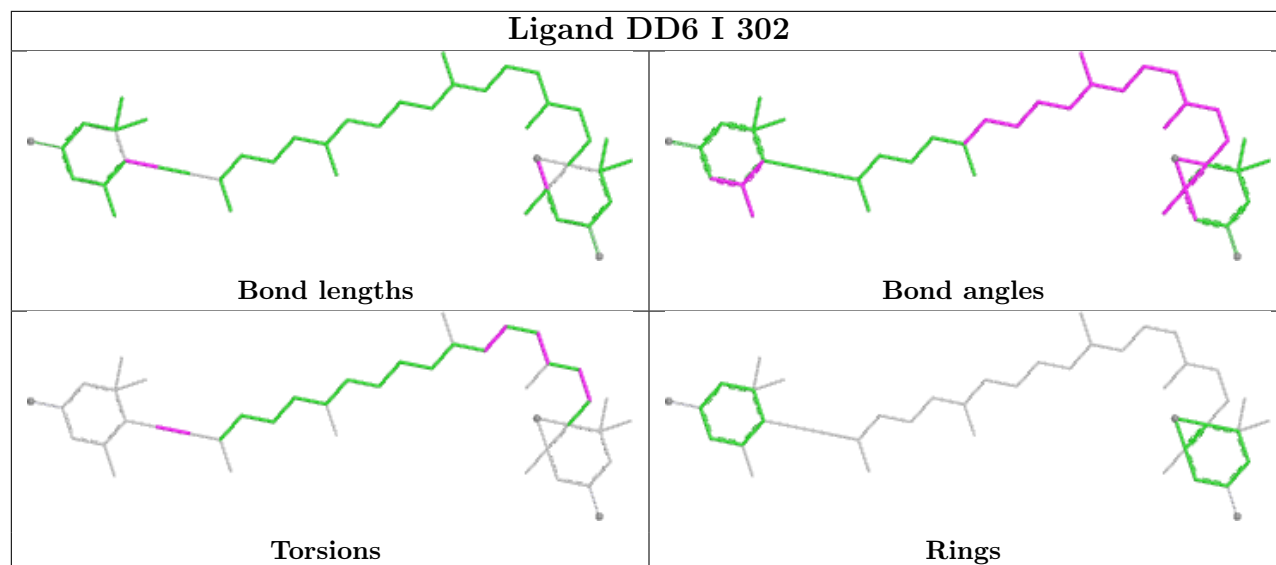


Torsions

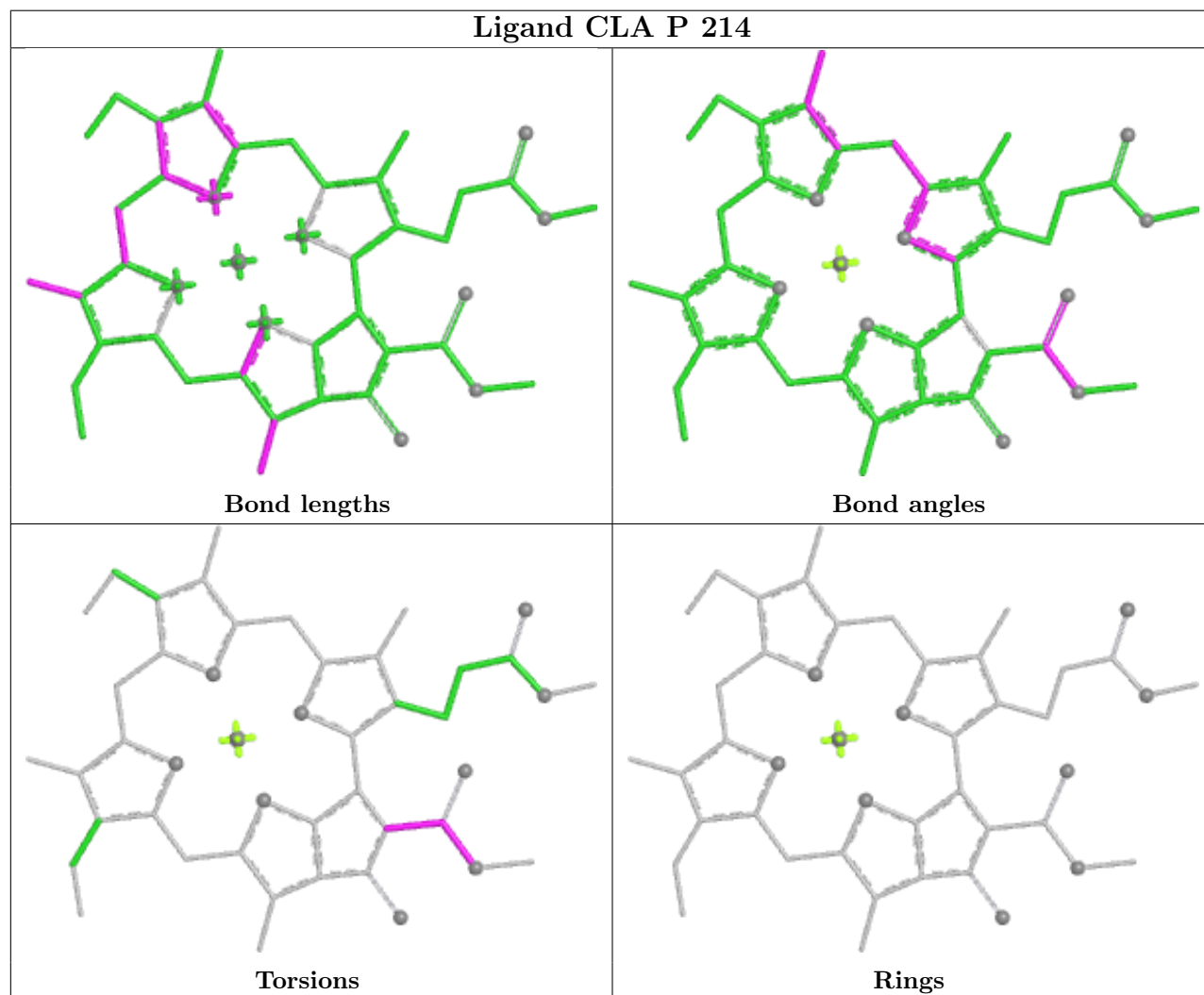


Rings

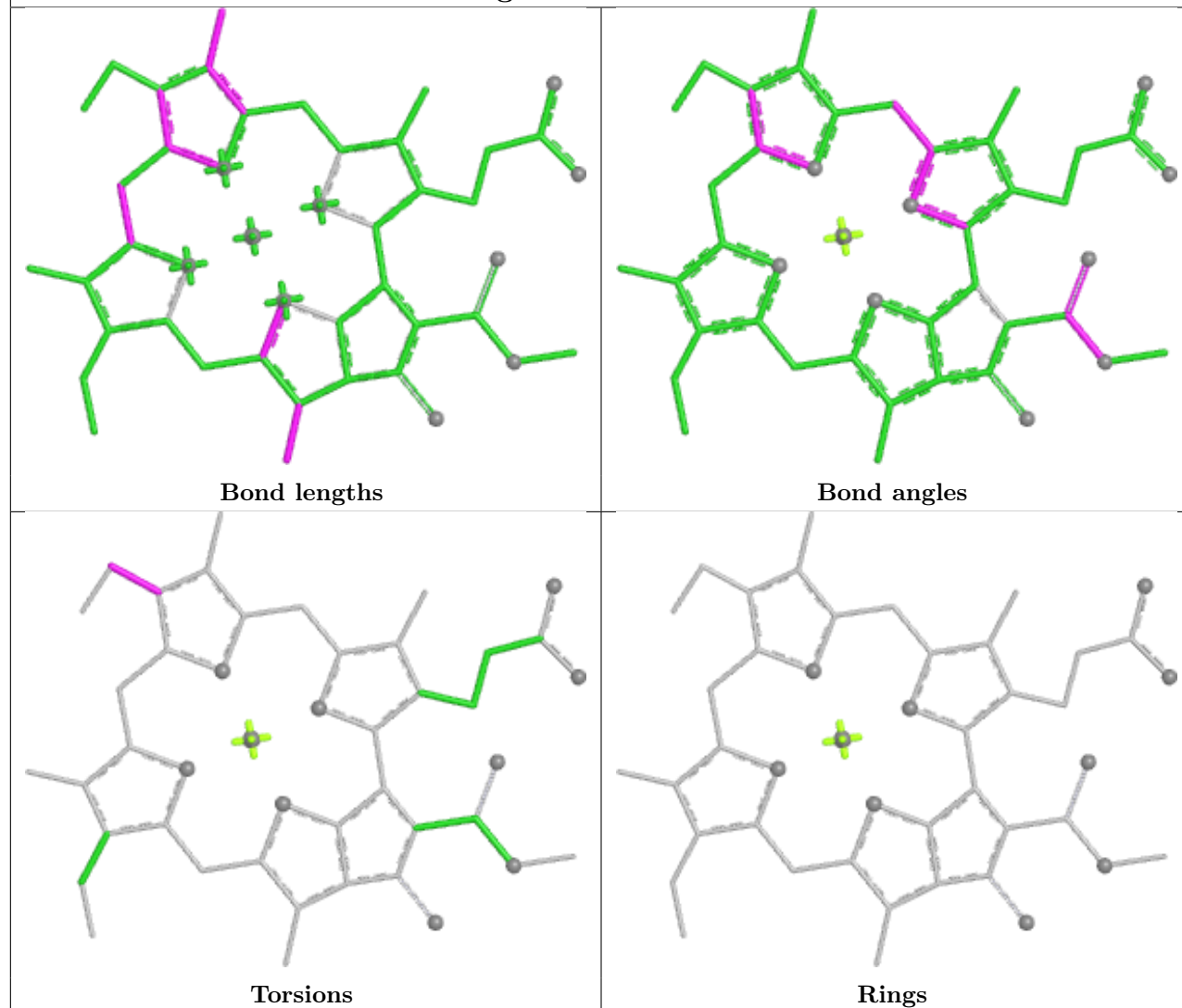
Ligand DD6 I 302



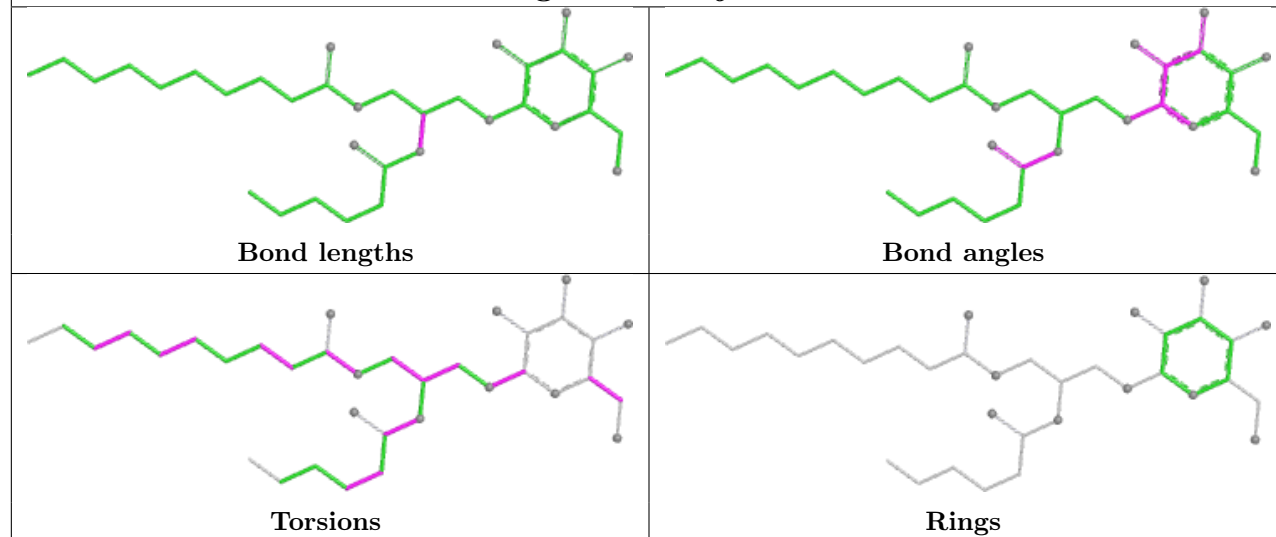
Ligand CLA P 214



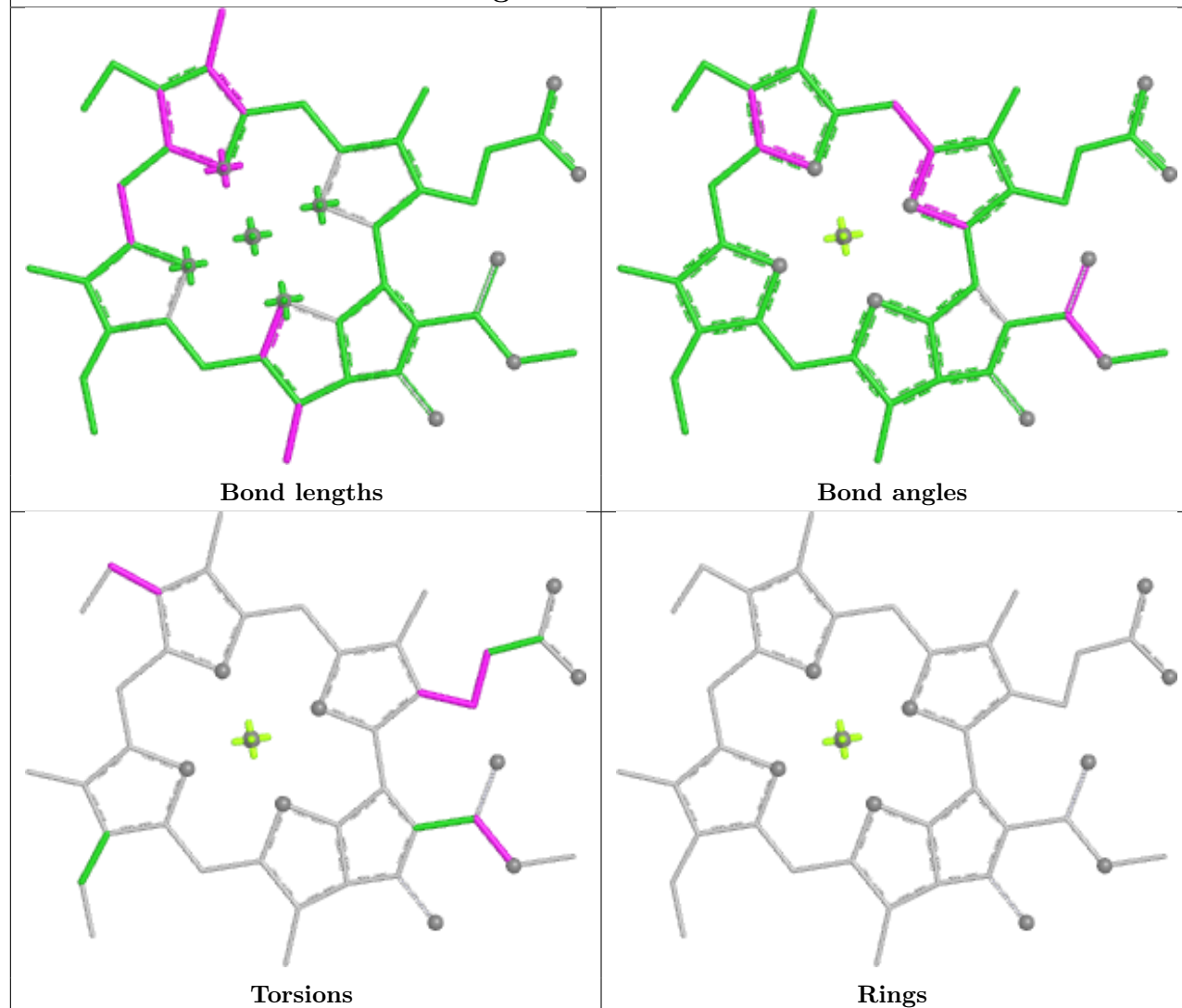
Ligand CLA a 701



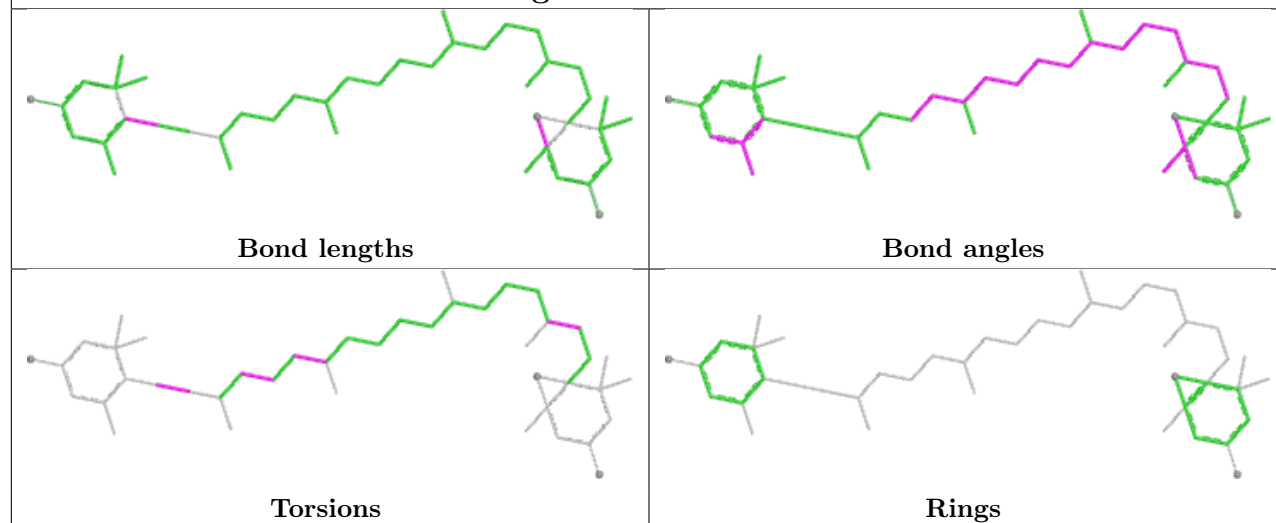
Ligand LMG j 101

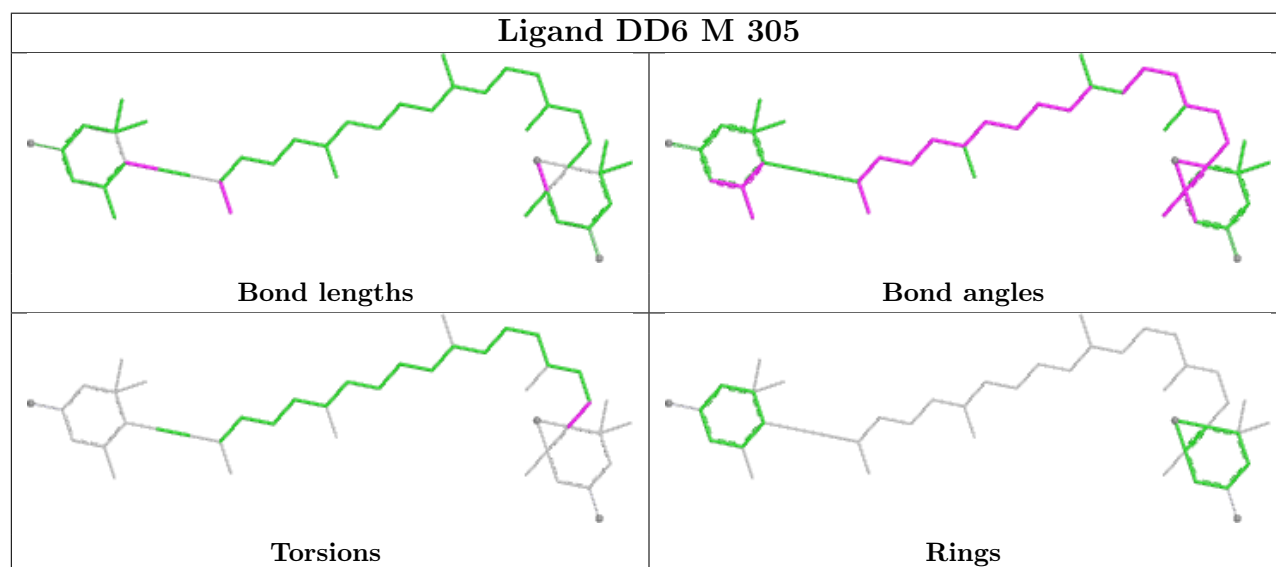
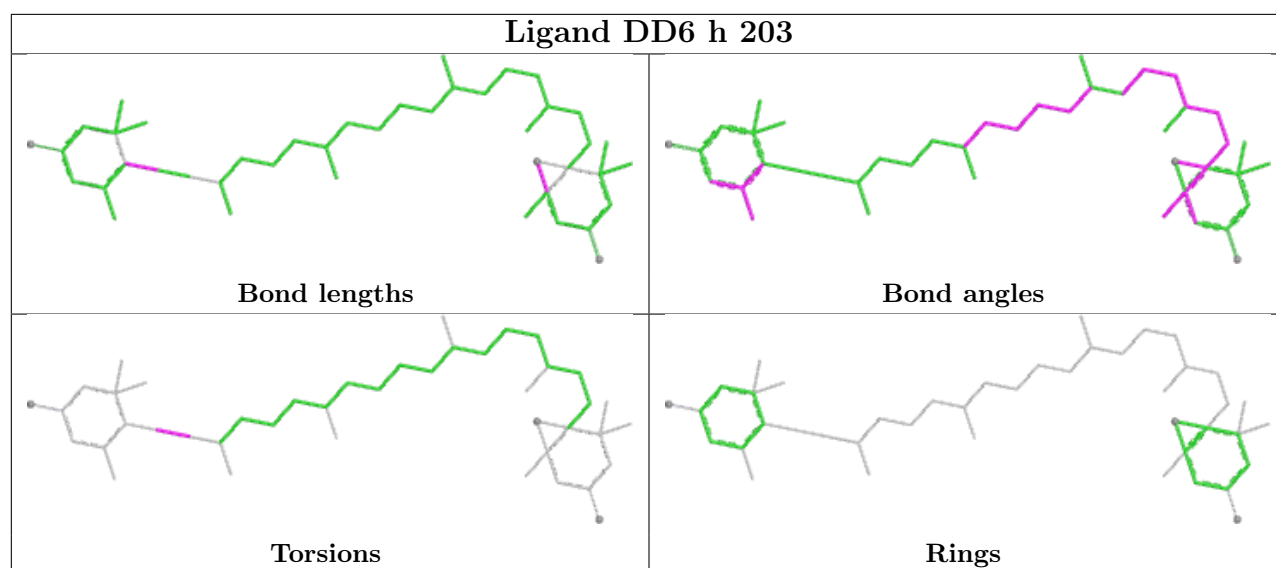


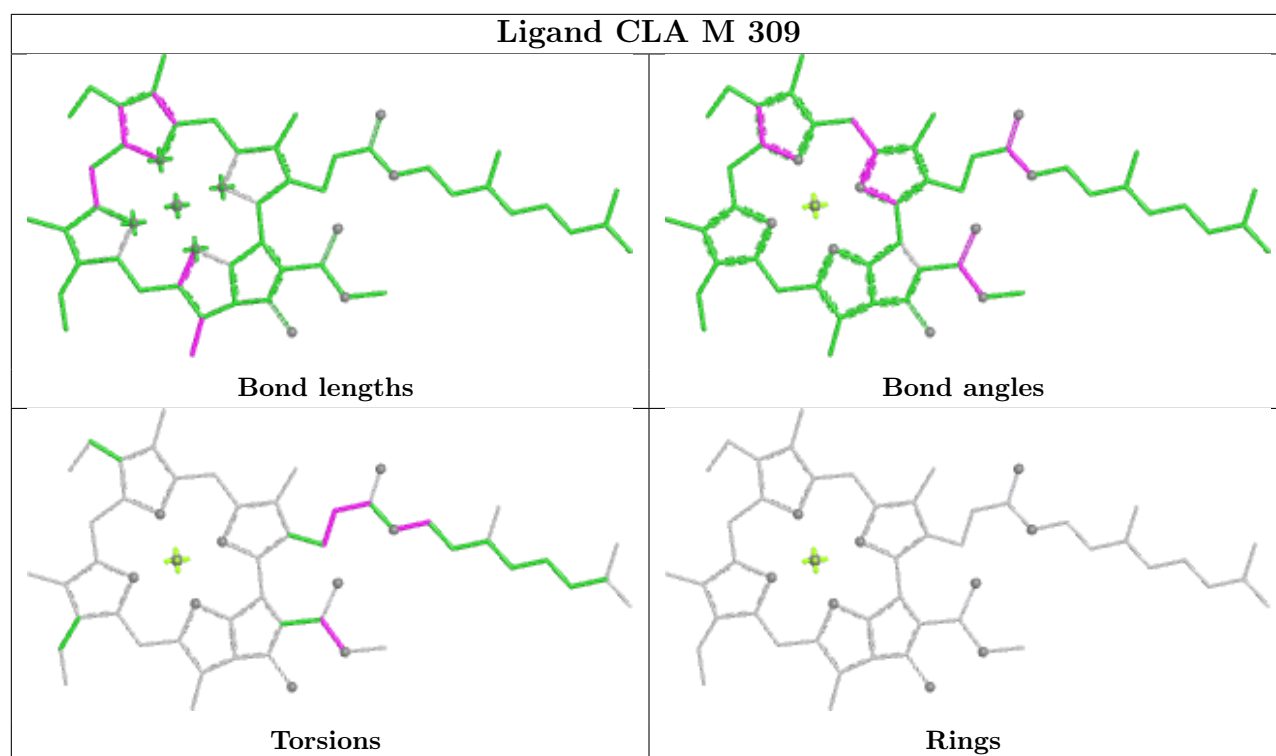
Ligand CLA B 317



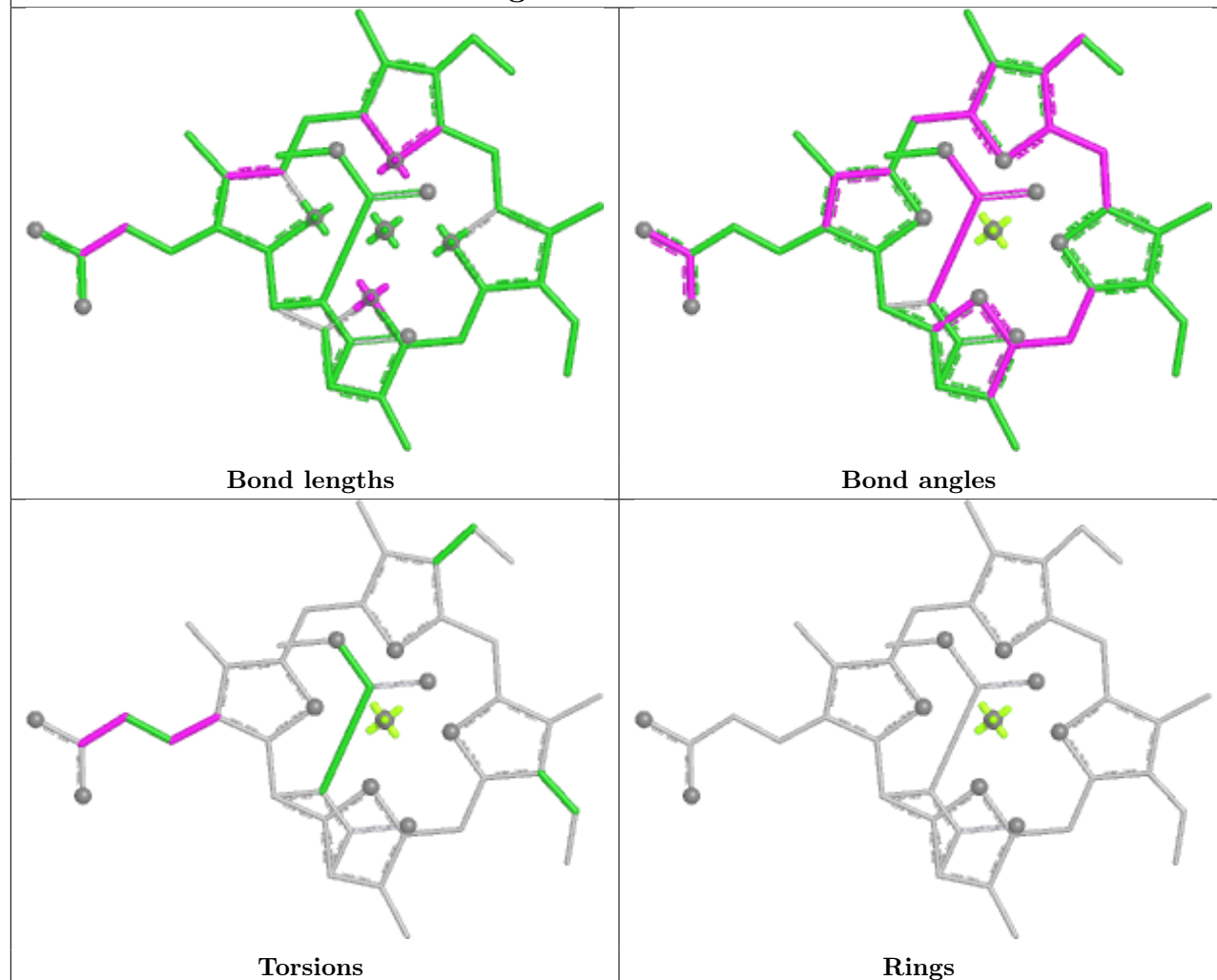
Ligand DD6 G 502



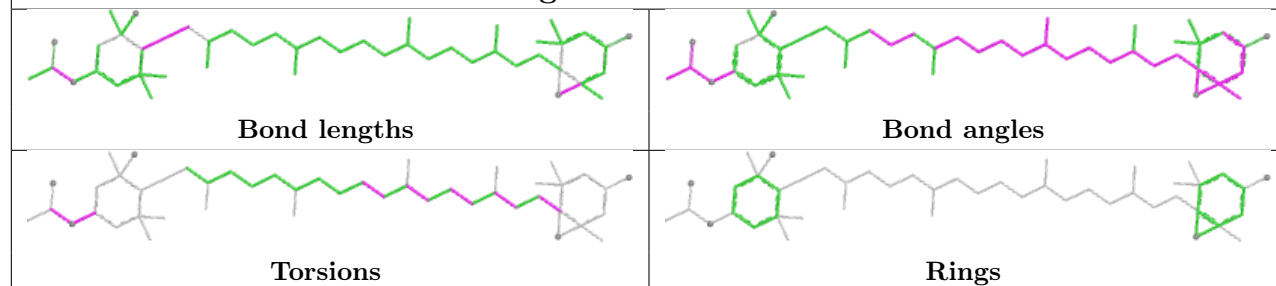


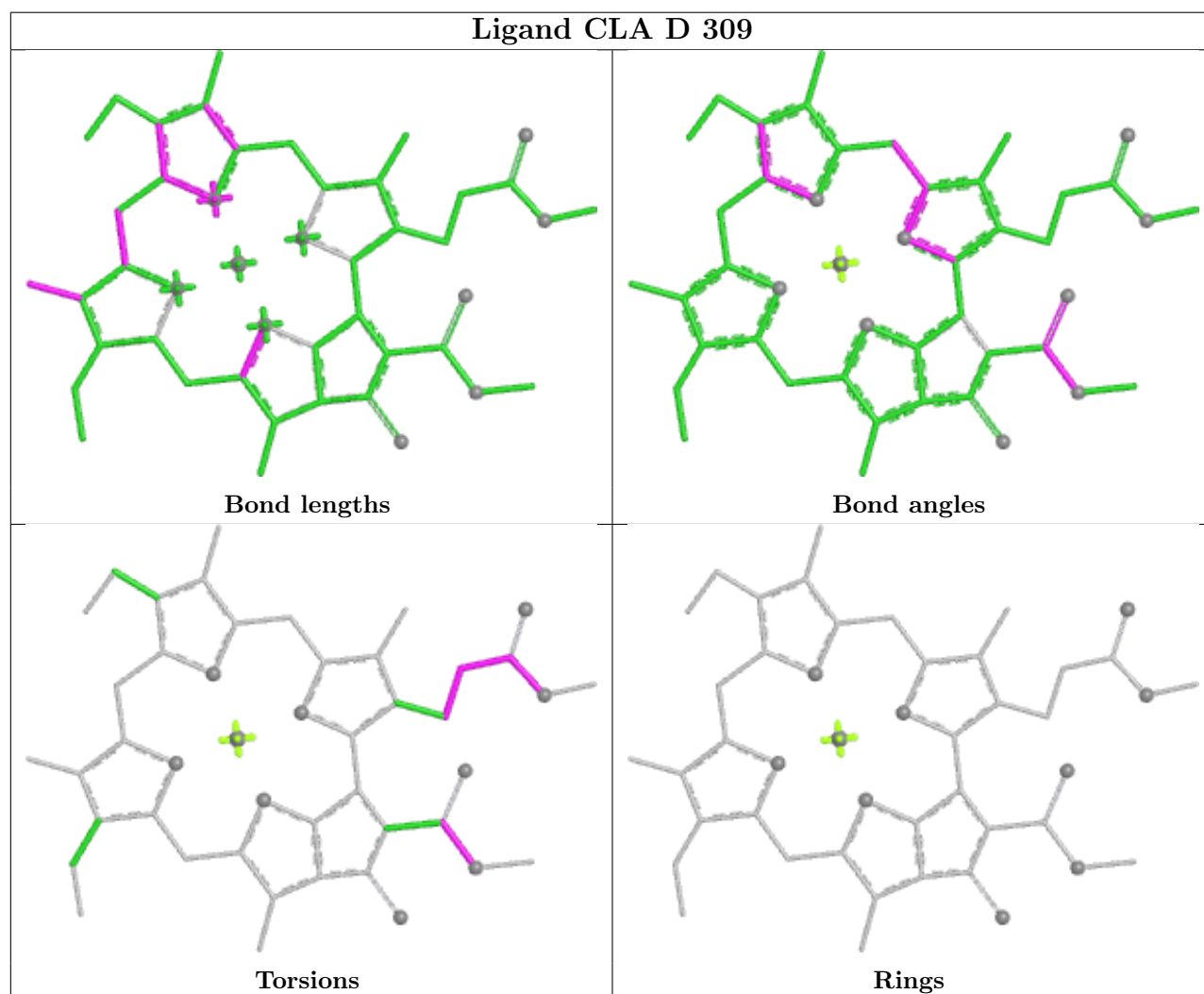
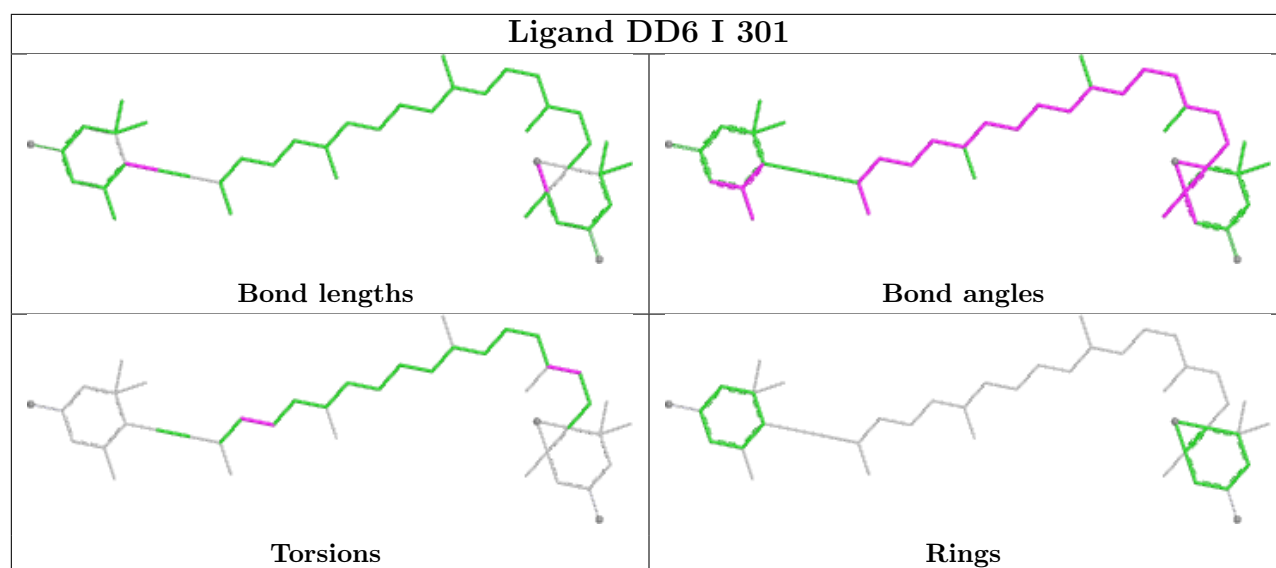


Ligand KC1 D 315

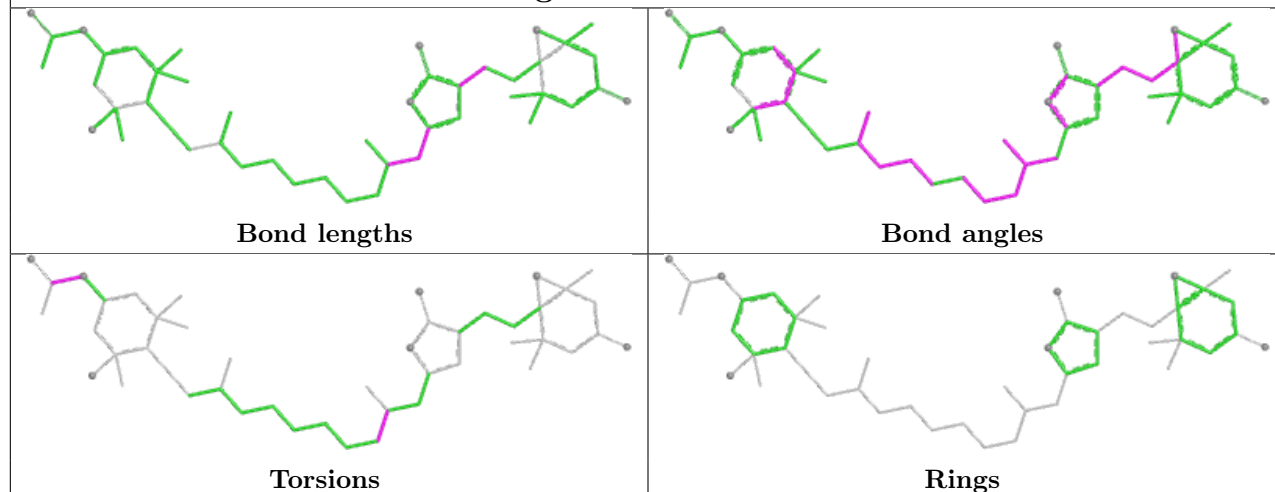


Ligand UIX J 305

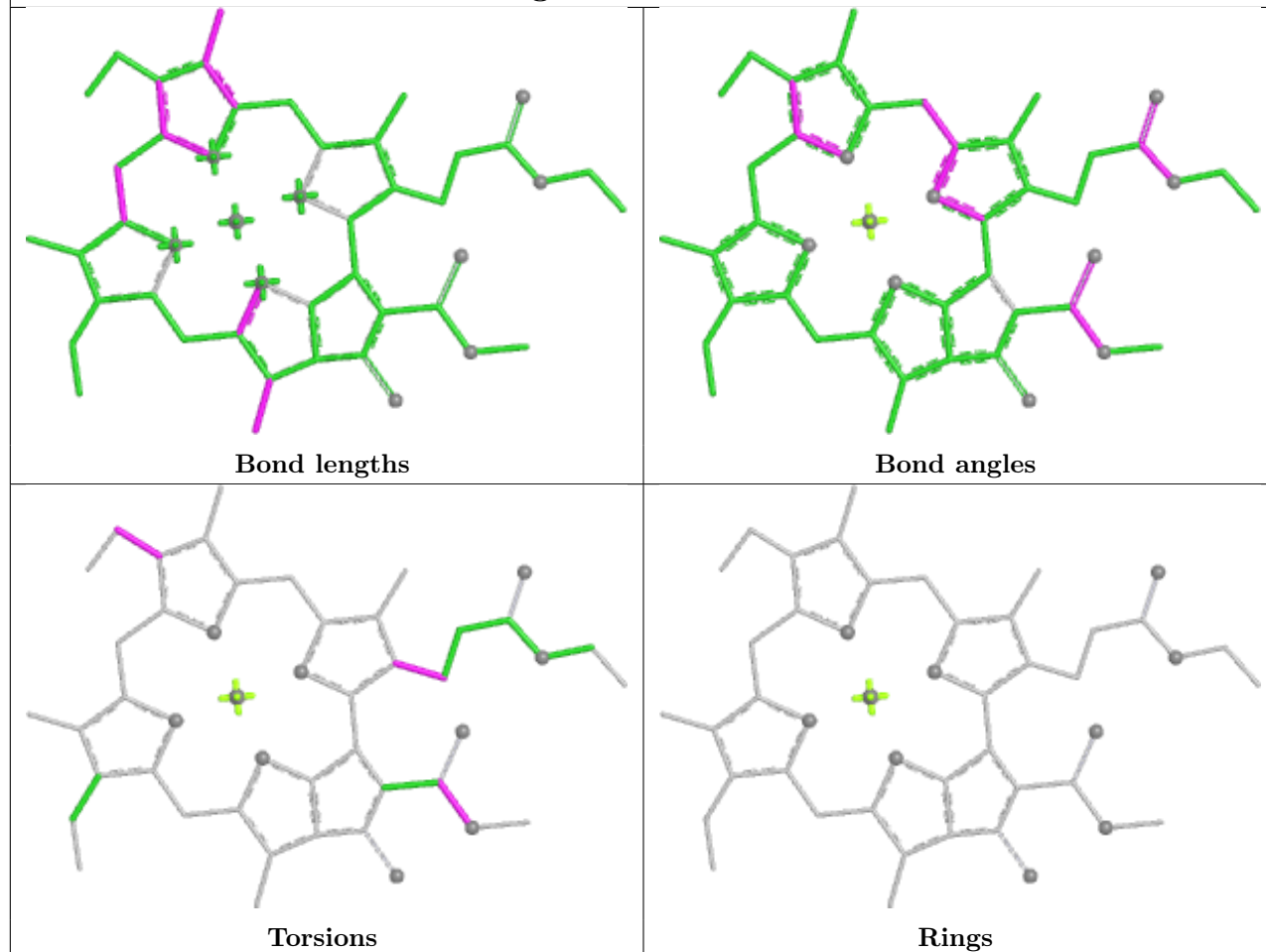


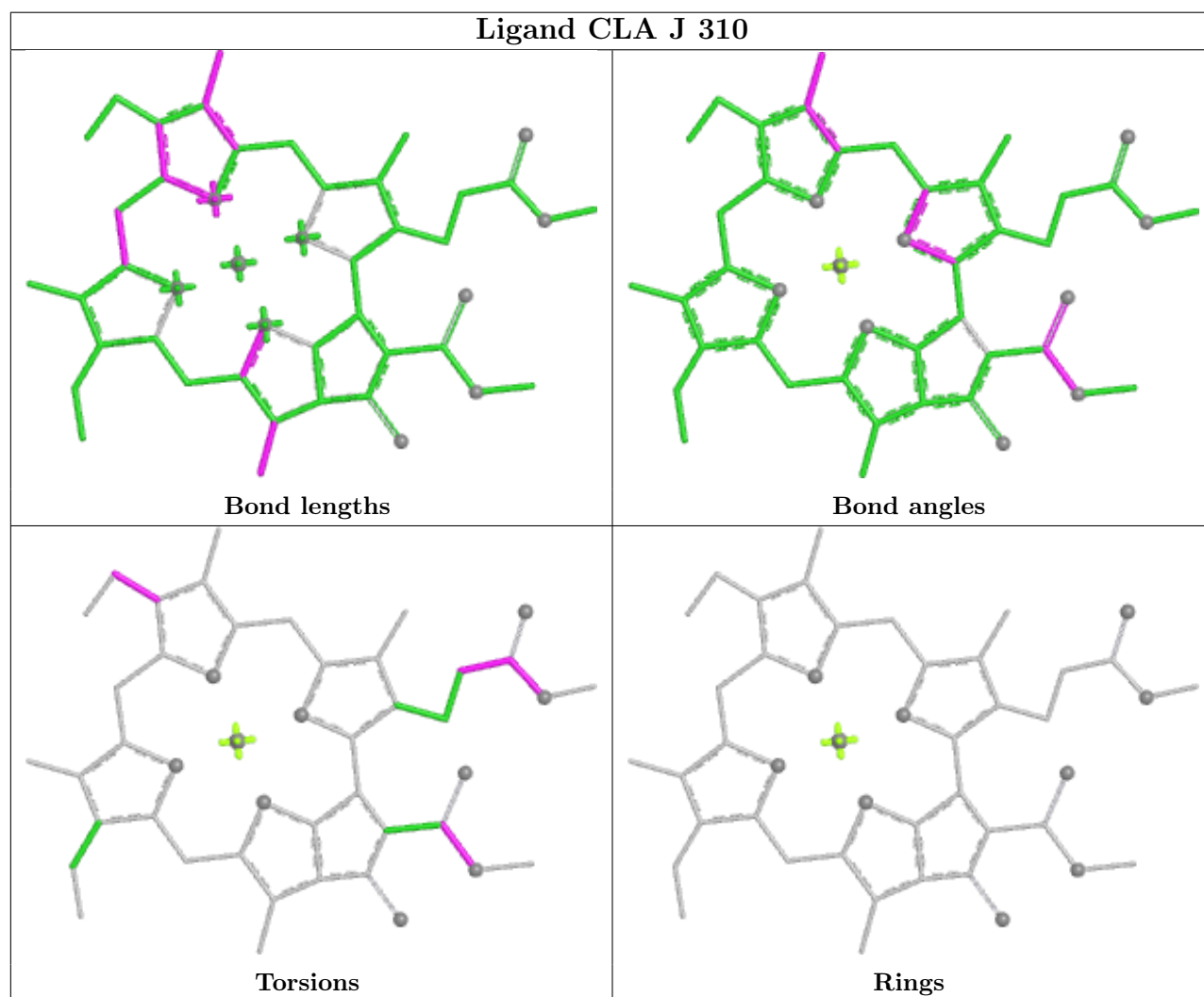
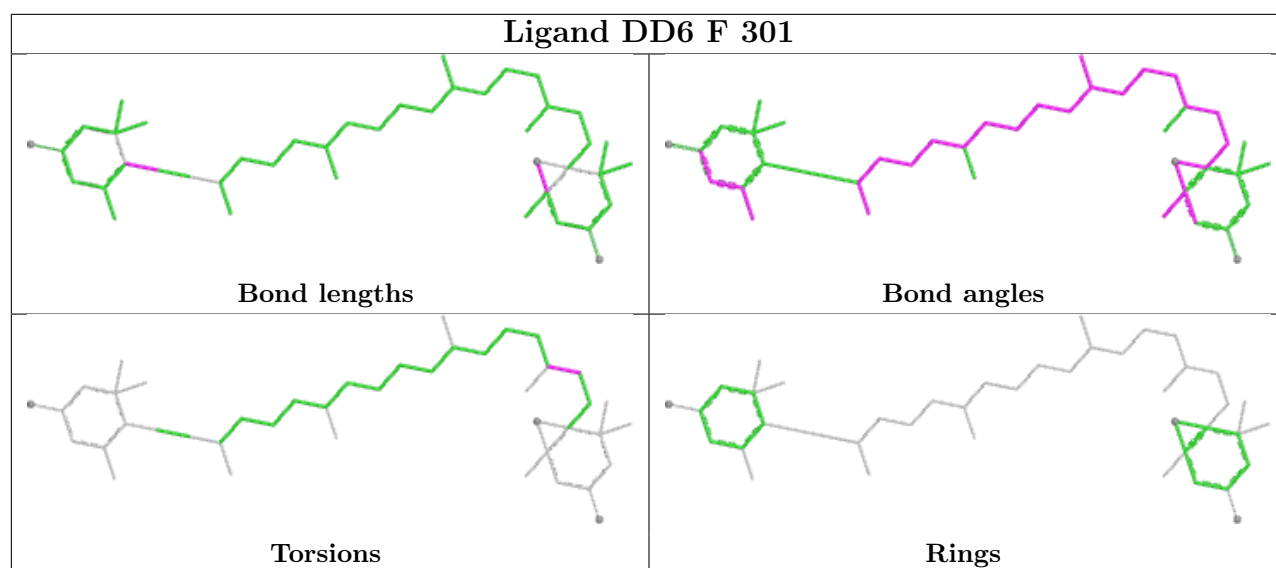


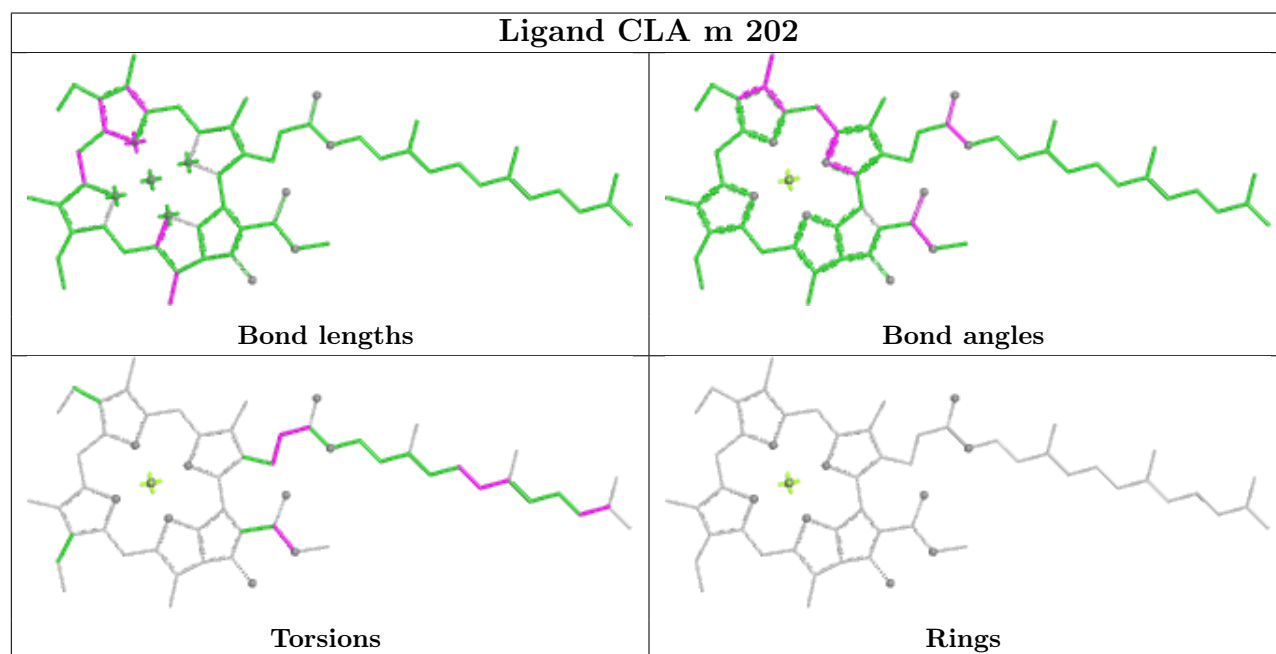
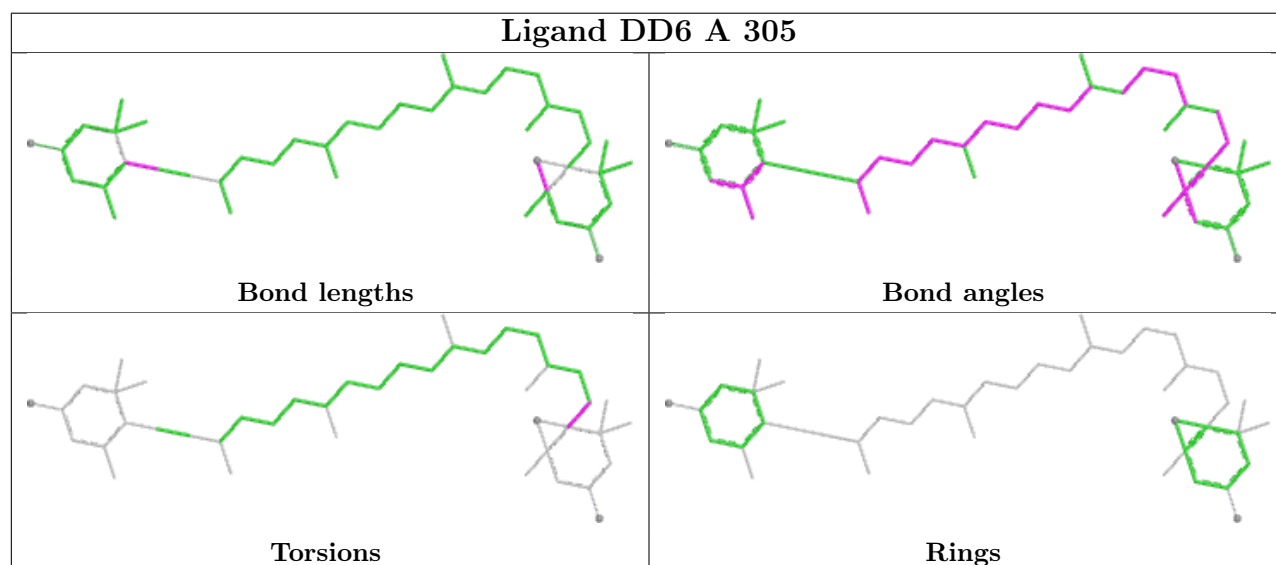
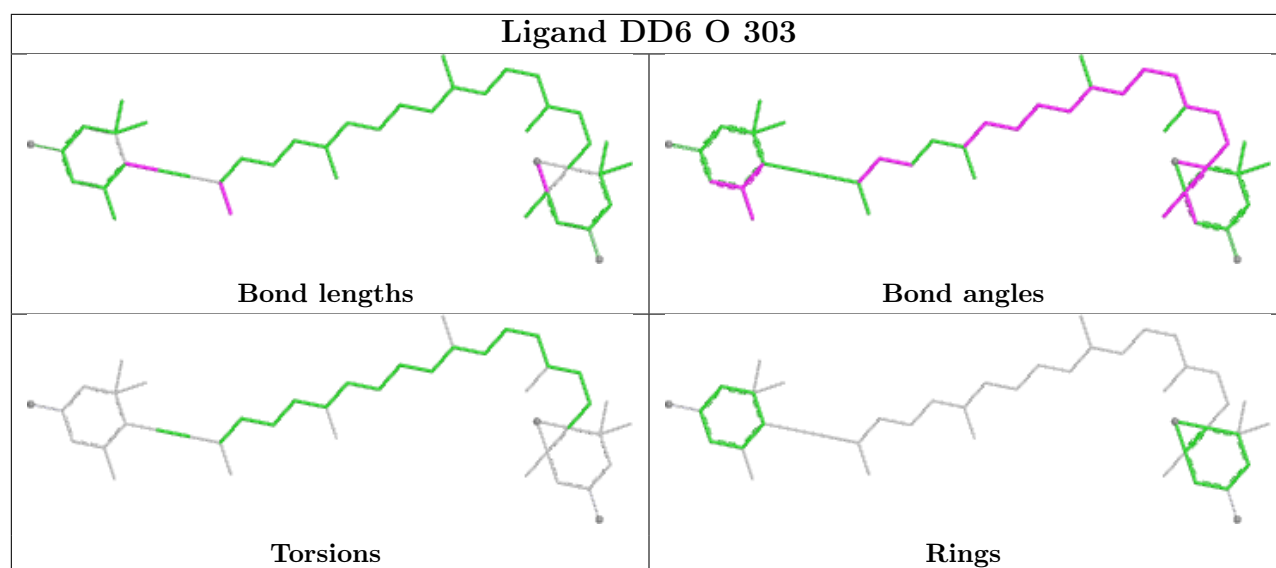
Ligand PID O 304

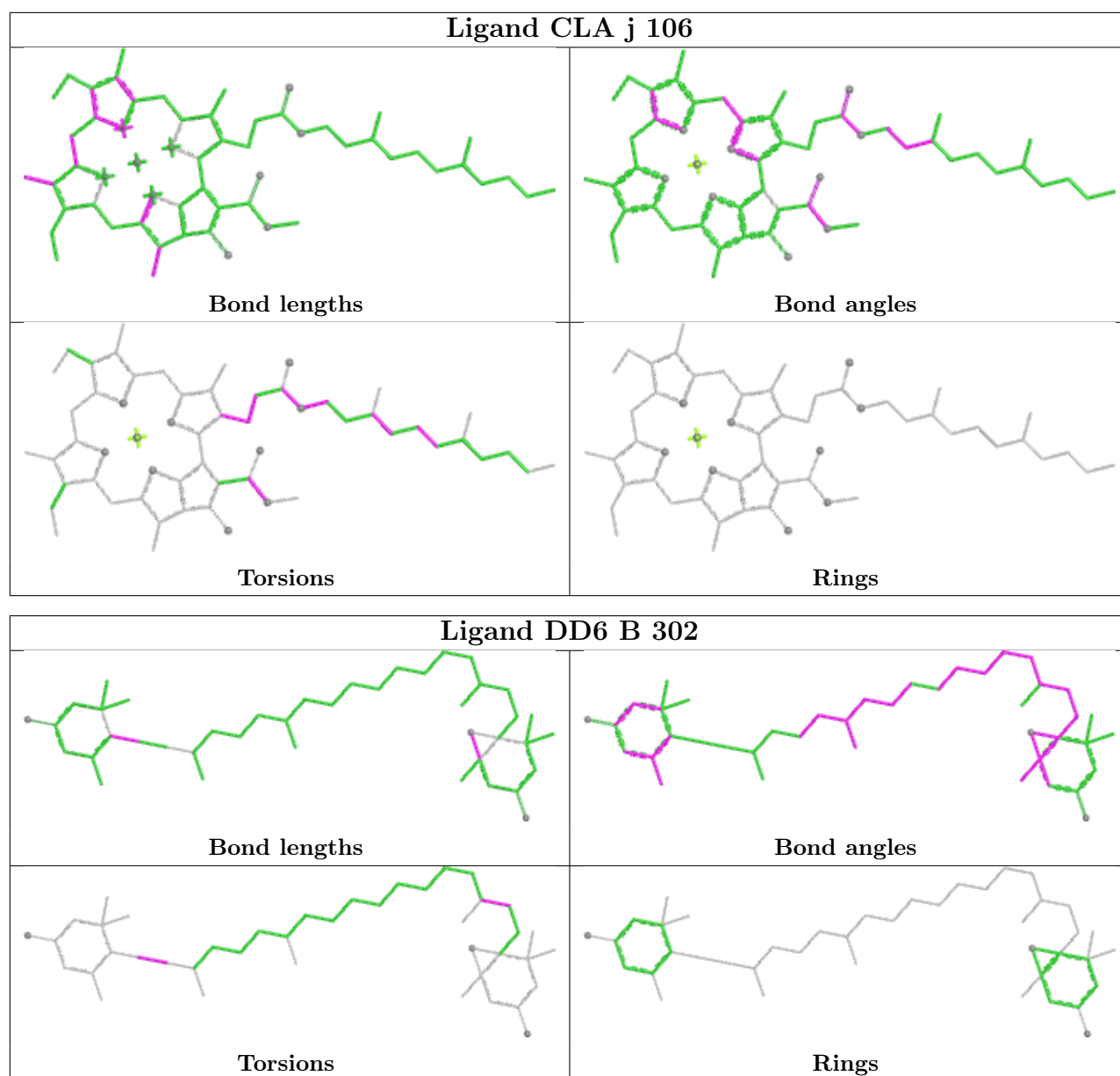


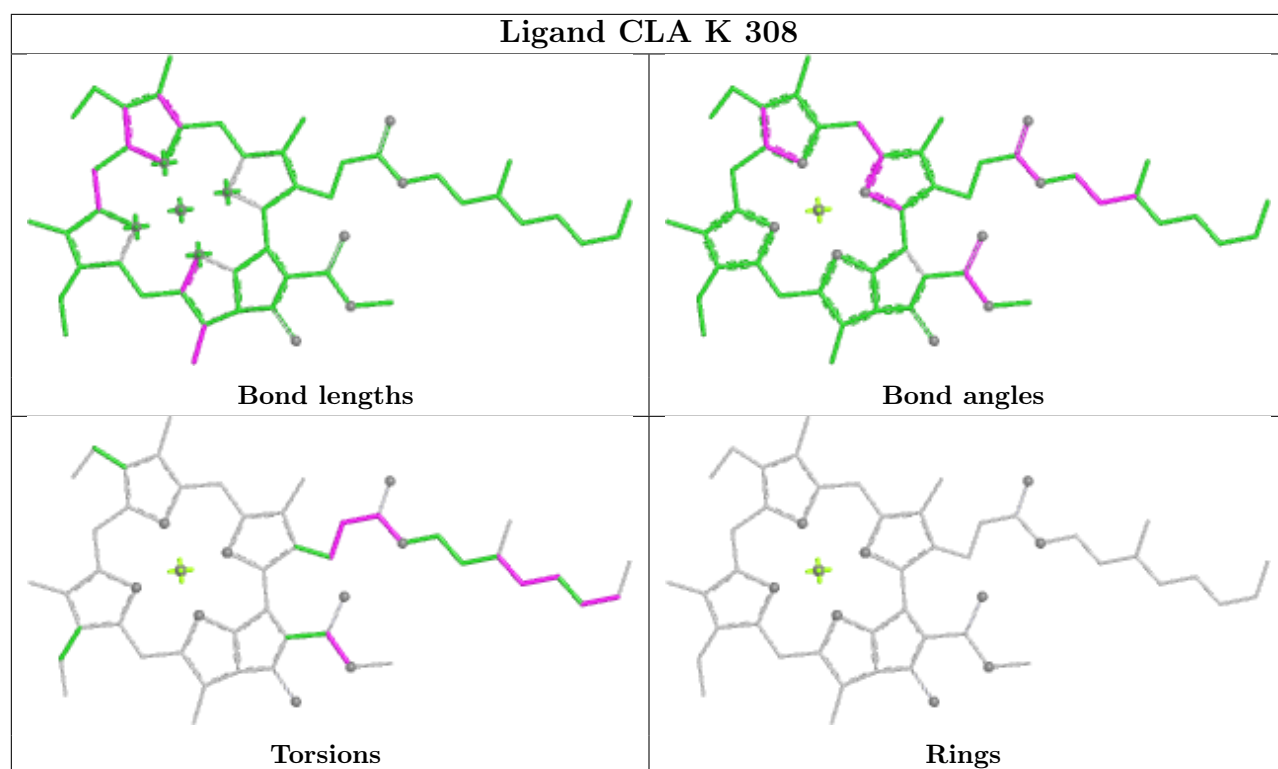
Ligand CLA a 716



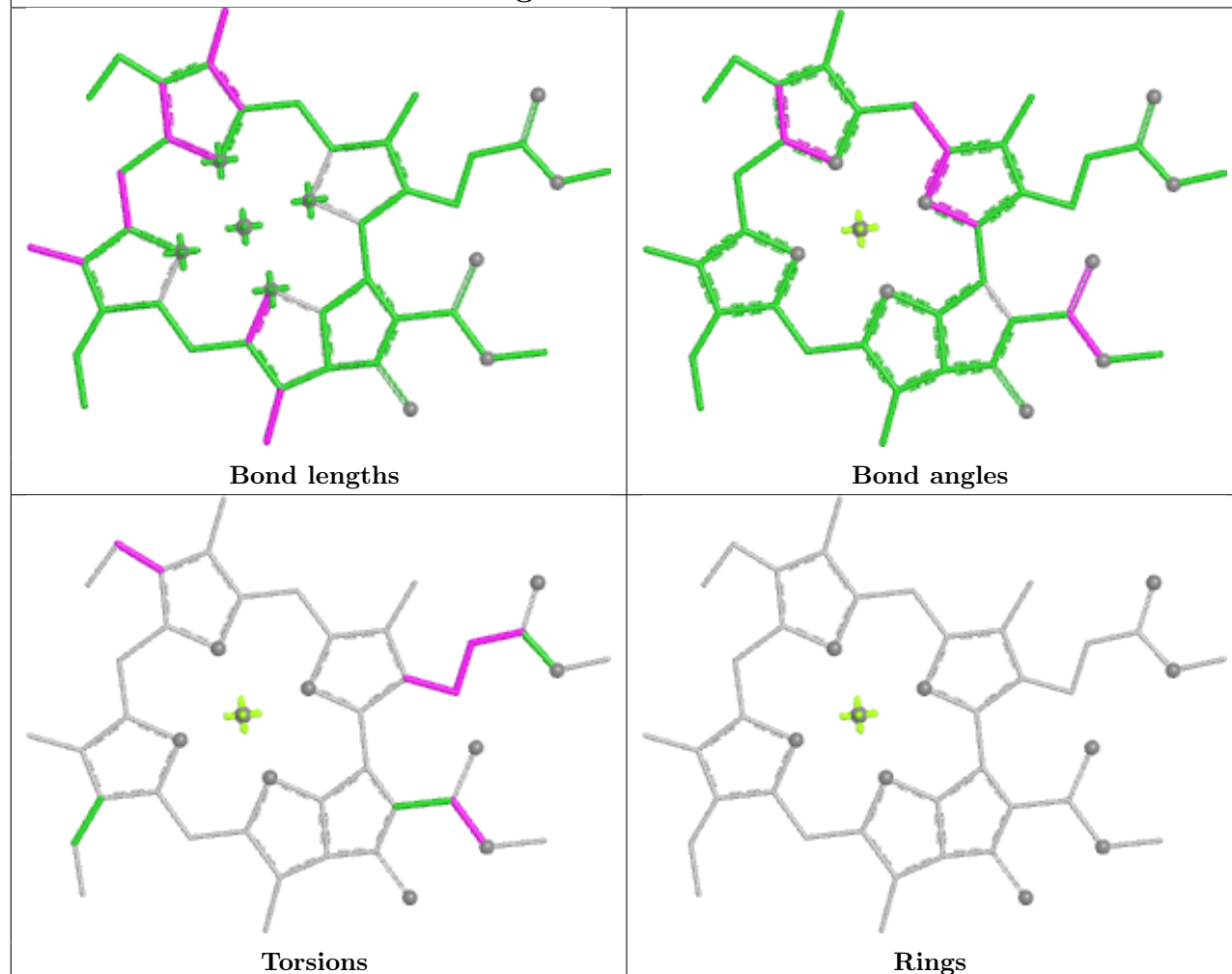




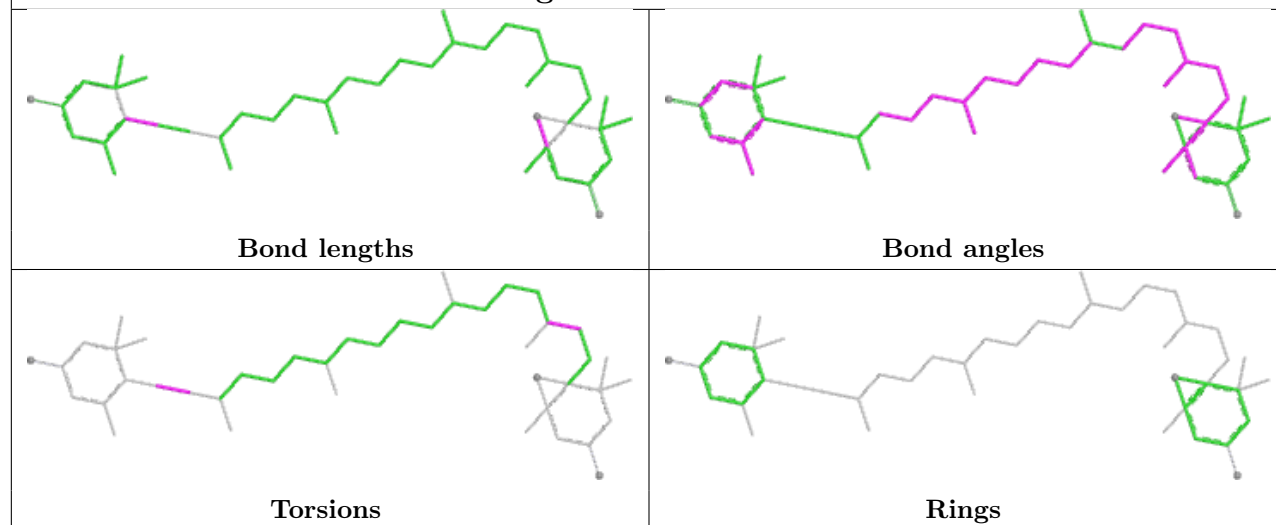


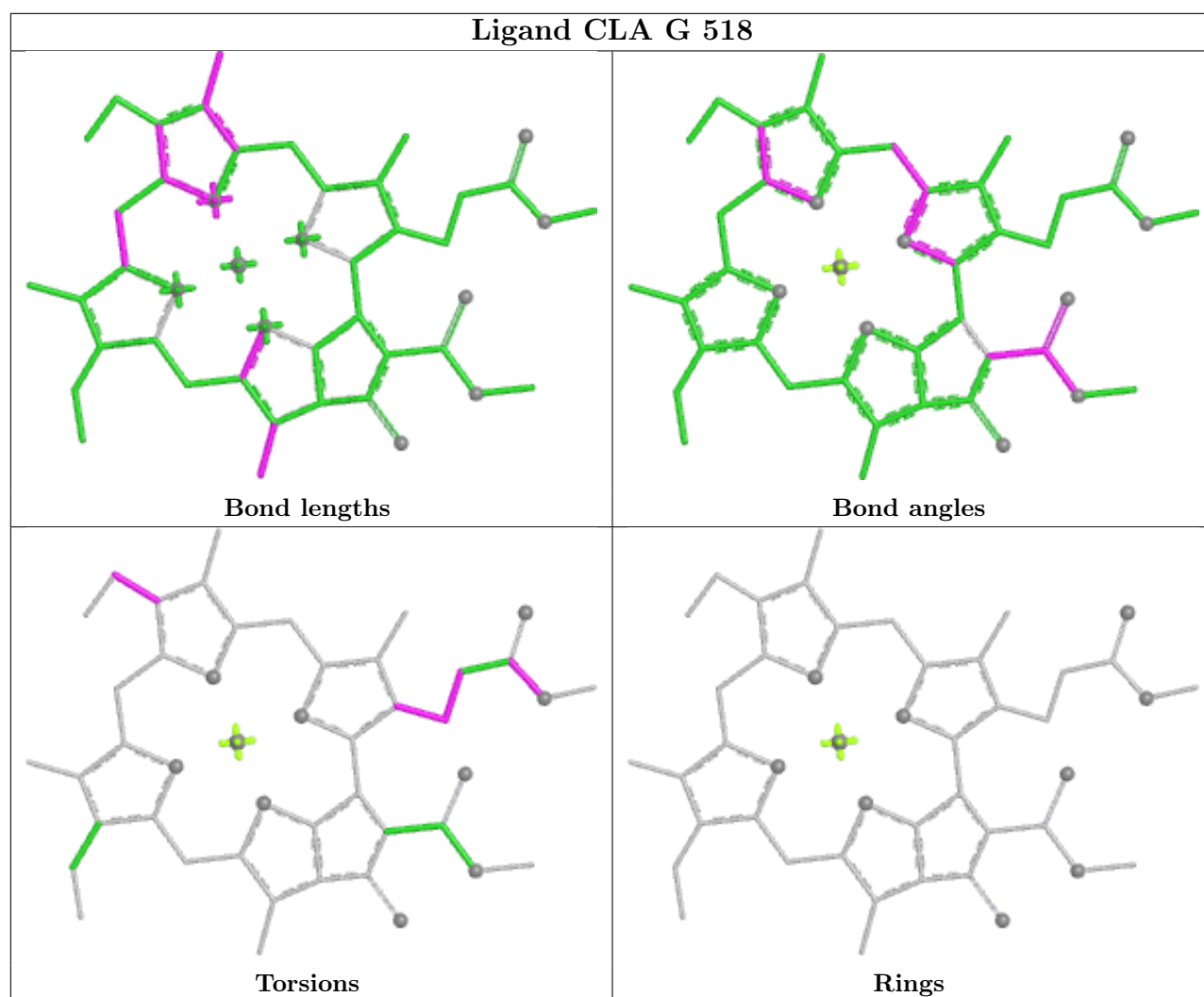


Ligand CLA L 318

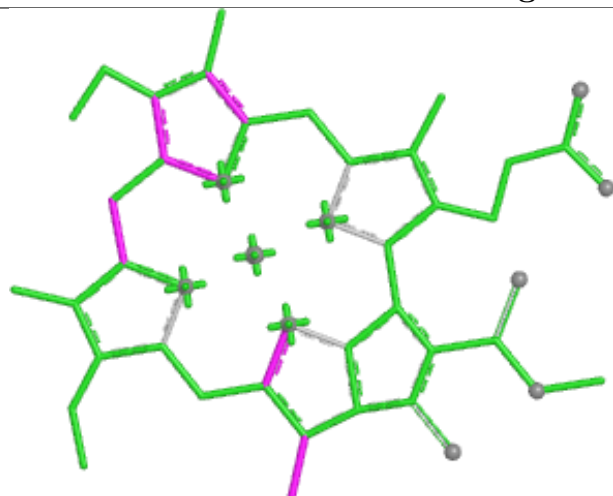


Ligand DD6 b 731

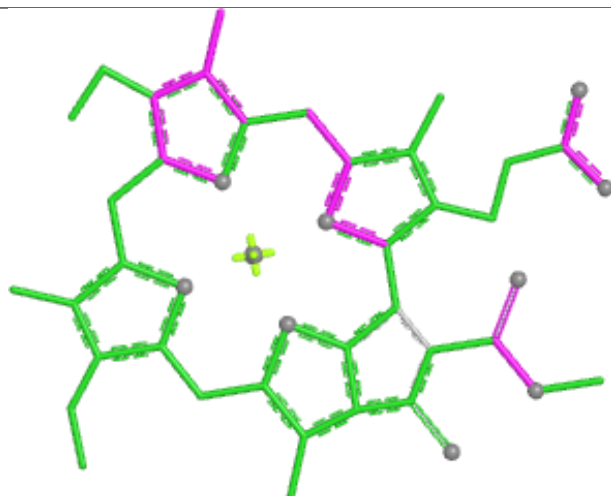




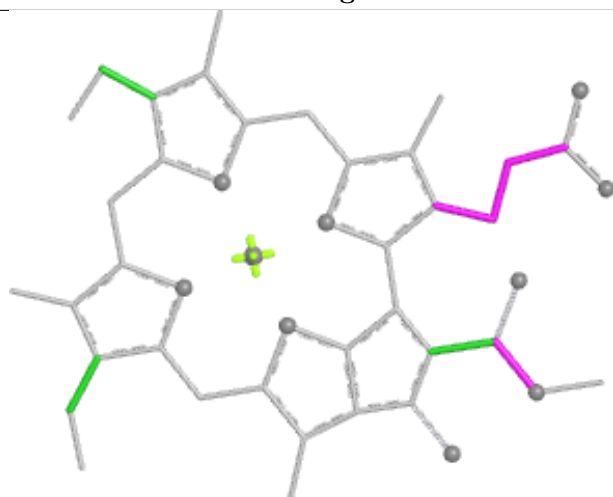
Ligand CLA a 711



Bond lengths



Bond angles

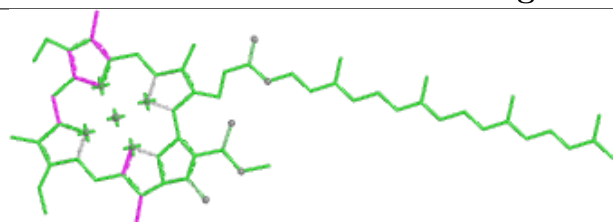


Torsions

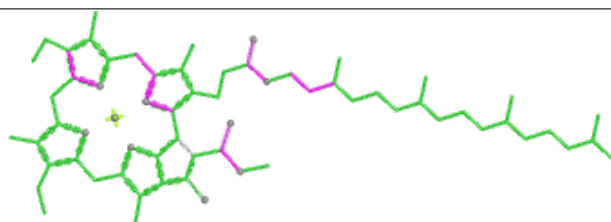


Rings

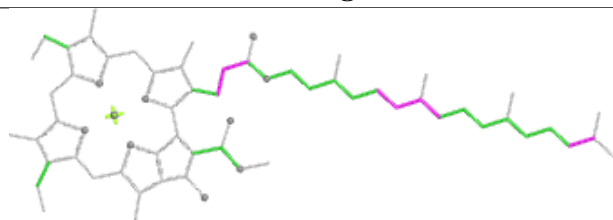
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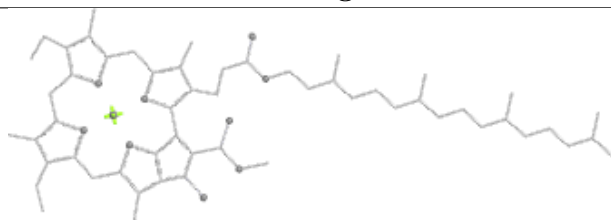
Bond lengths



Bond angles

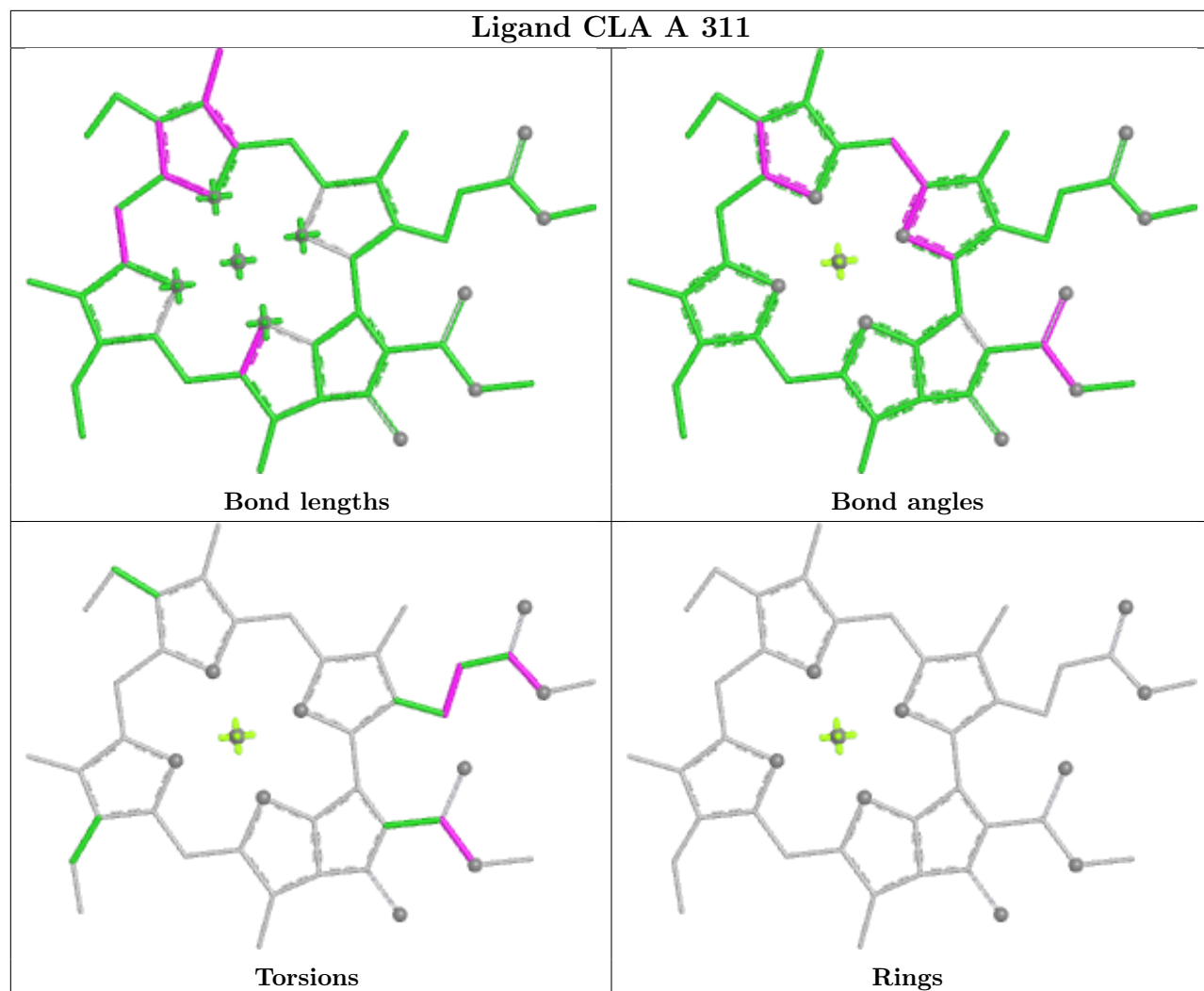


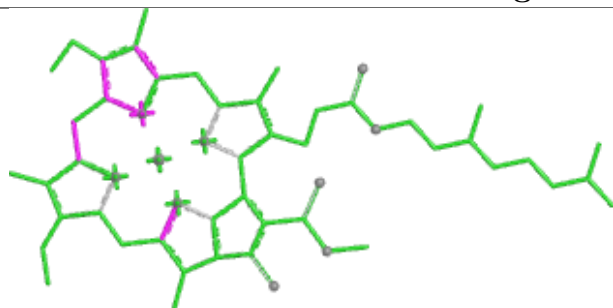
Torsions



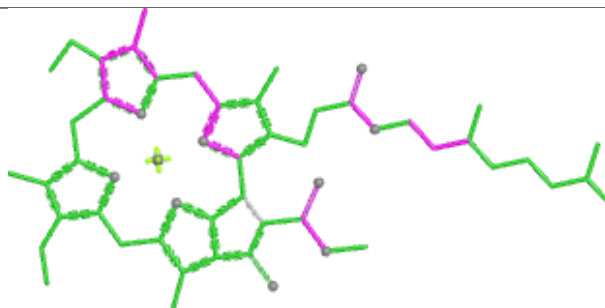
Rings

Ligand CLA A 311

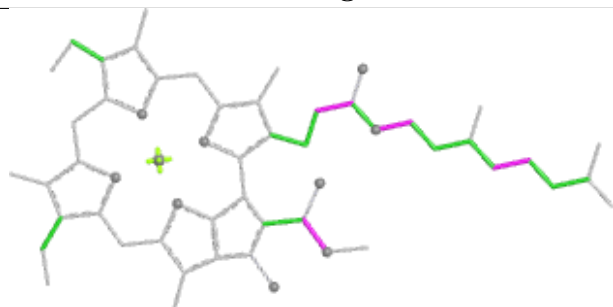


Ligand CLA A 309

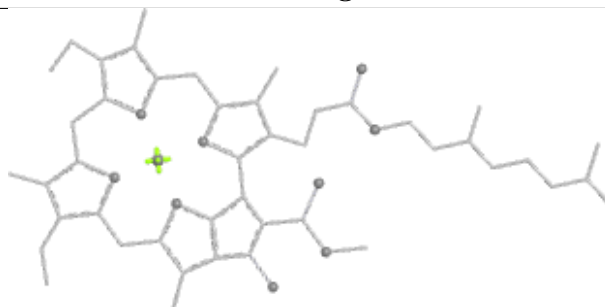
Bond lengths



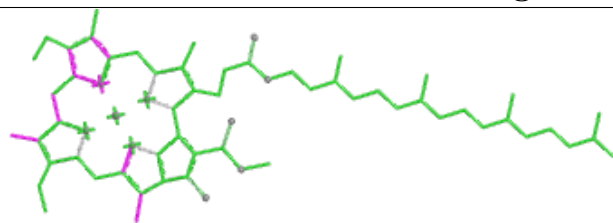
Bond angles



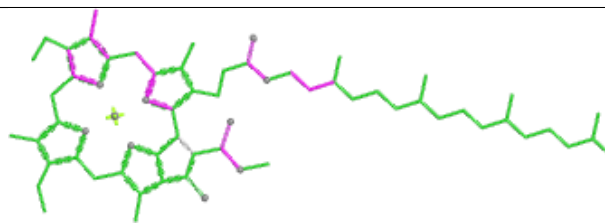
Torsions



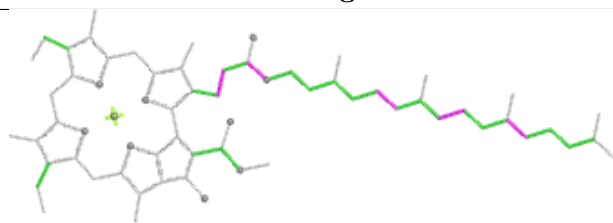
Rings

Ligand CLA G 513

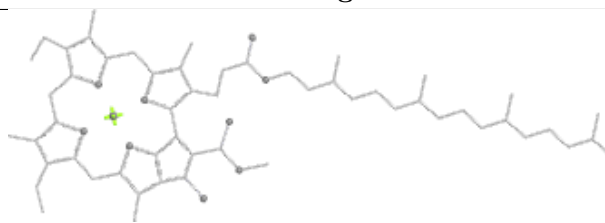
Bond lengths



Bond angles

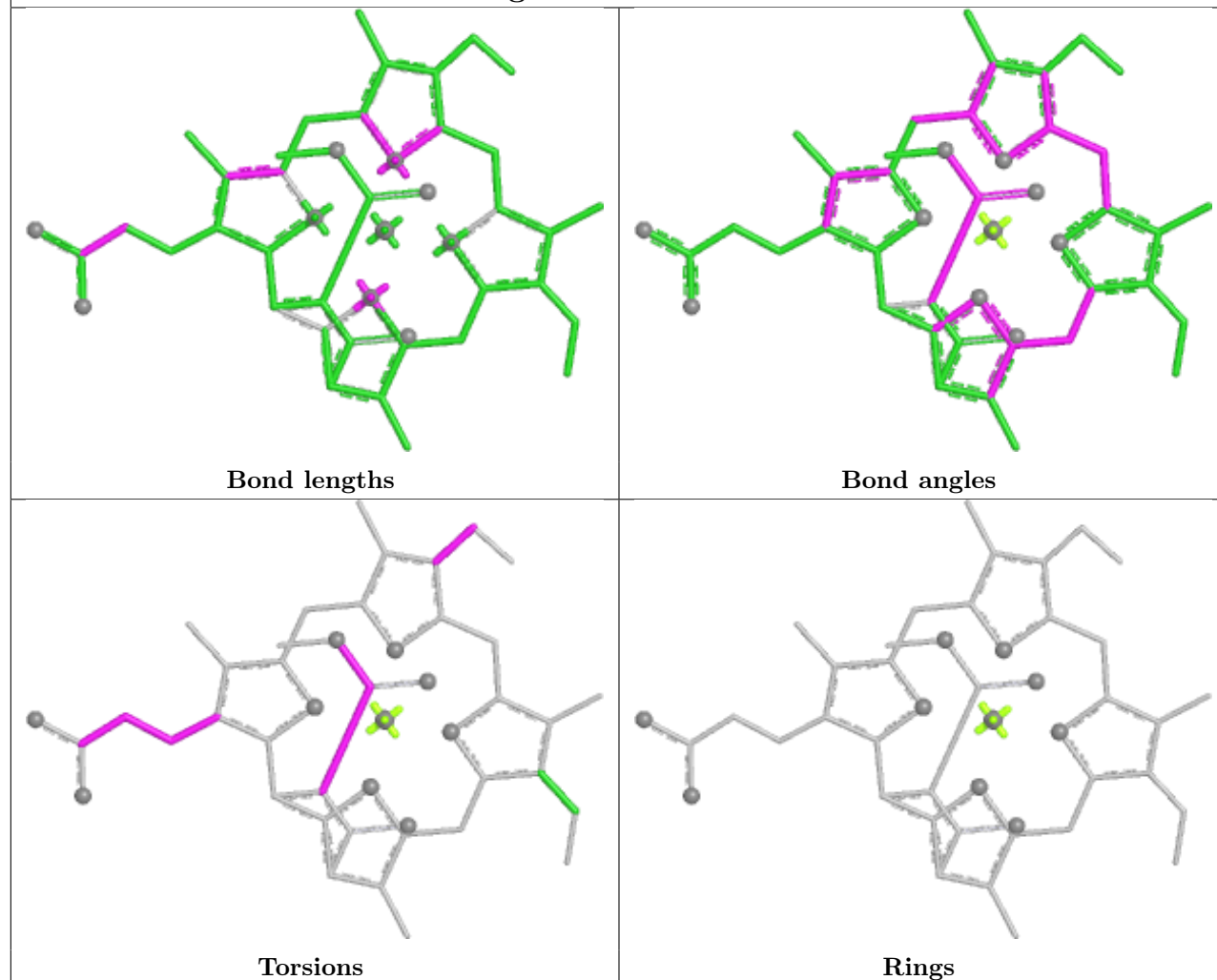


Torsions

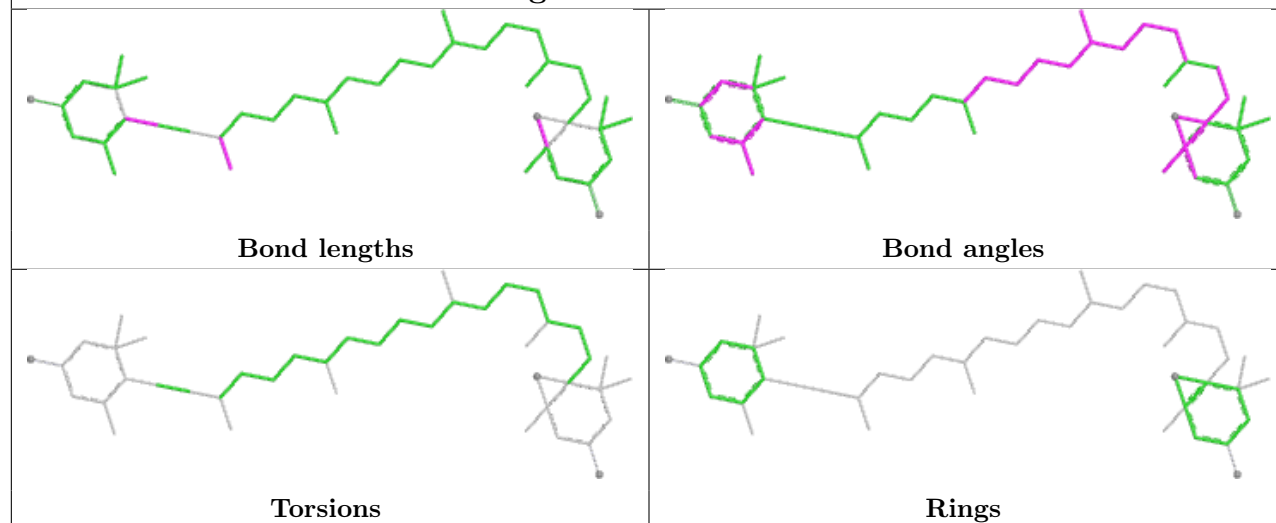


Rings

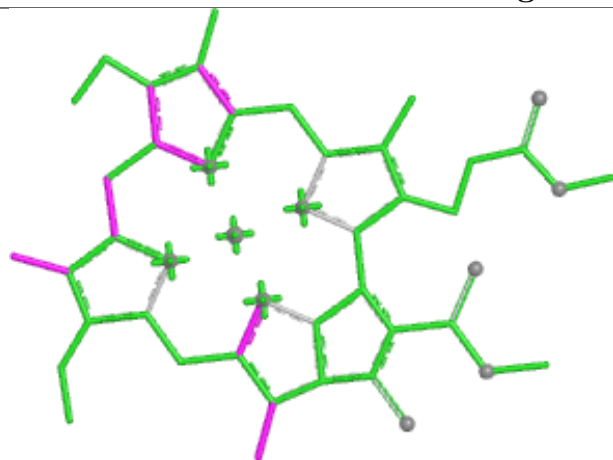
Ligand KC1 D 310



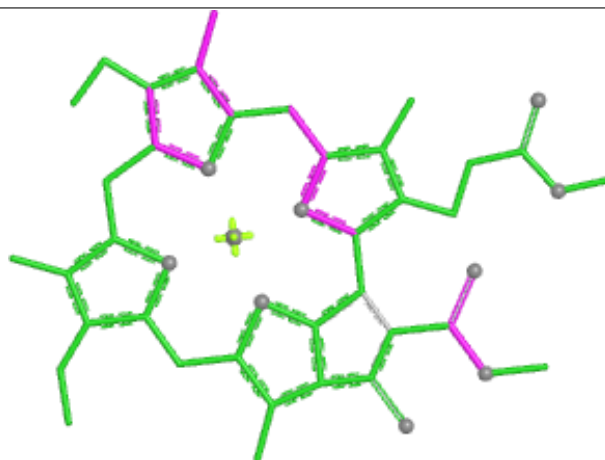
Ligand DD6 M 304



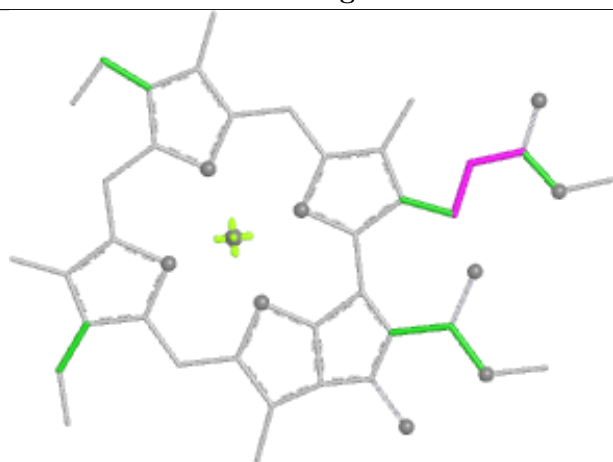
Ligand CLA b 714



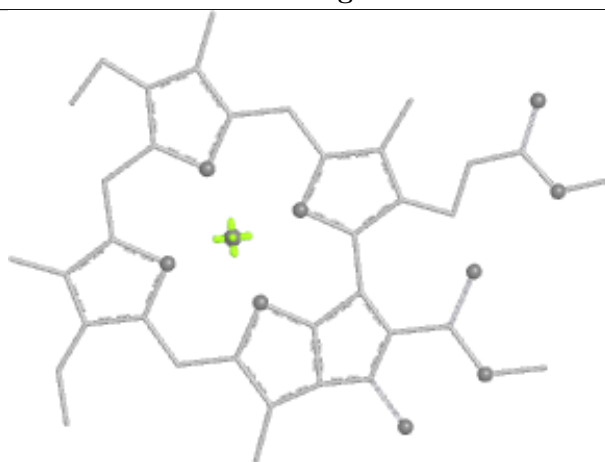
Bond lengths



Bond angles

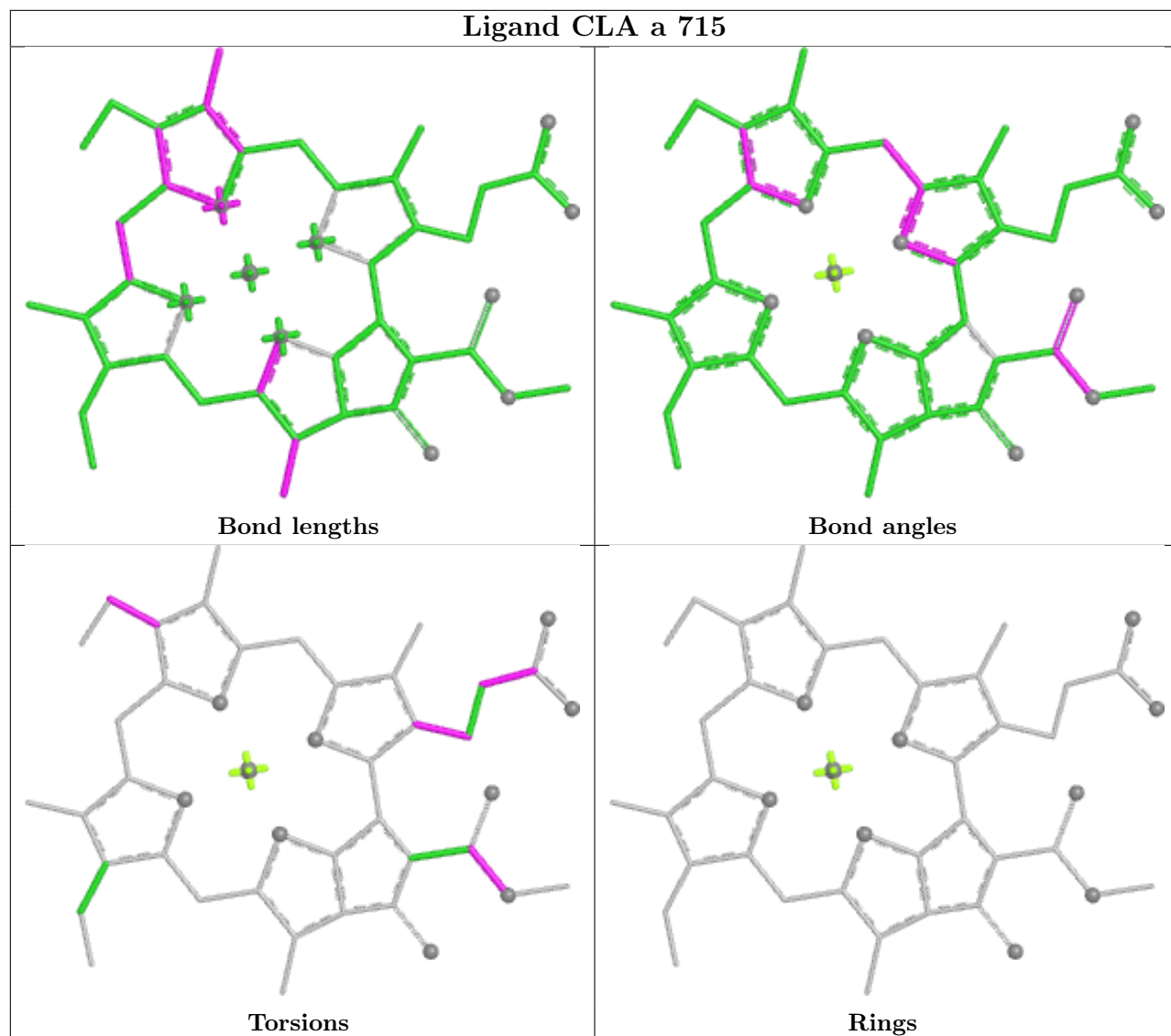


Torsions

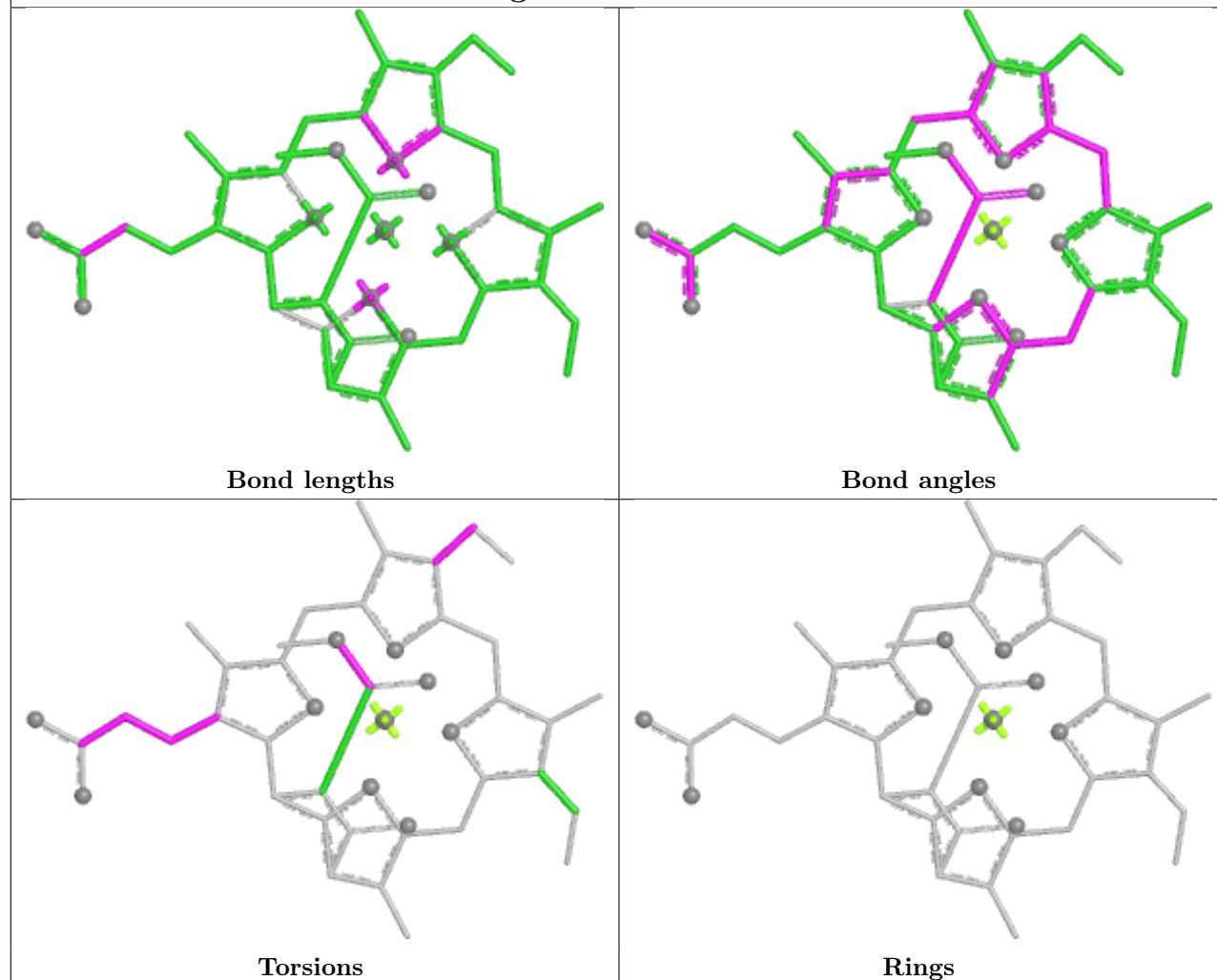


Rings

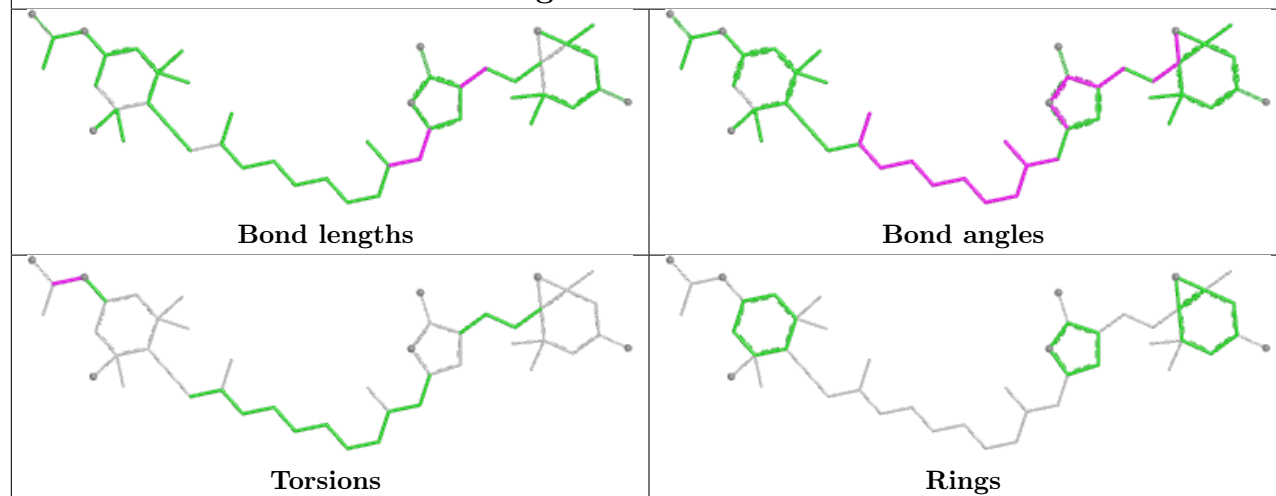
Ligand CLA a 715



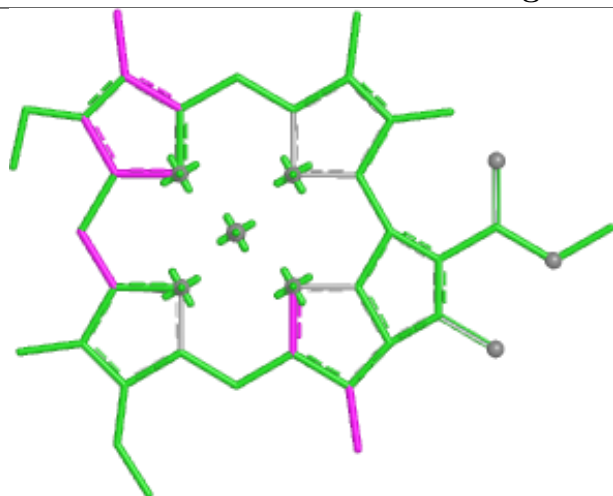
Ligand KC1 P 211



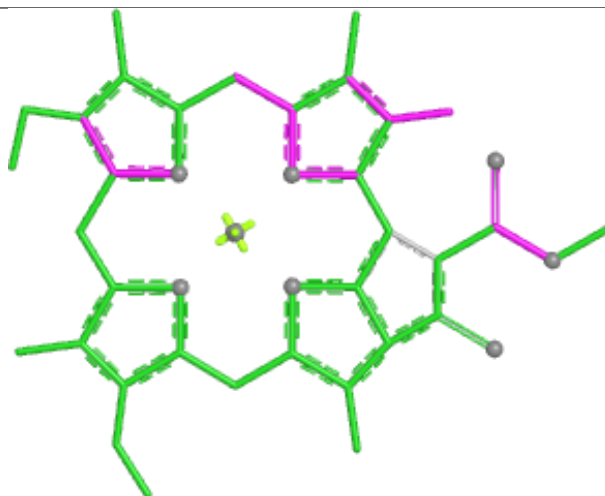
Ligand PID D 305



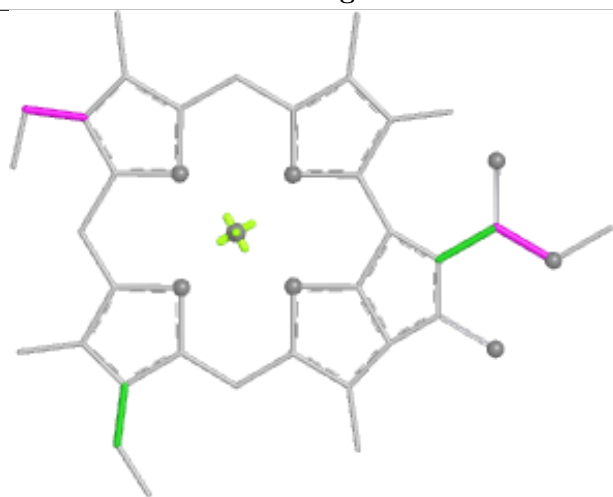
Ligand CLA 1 308



Bond lengths



Bond angles



Torsions



Rings

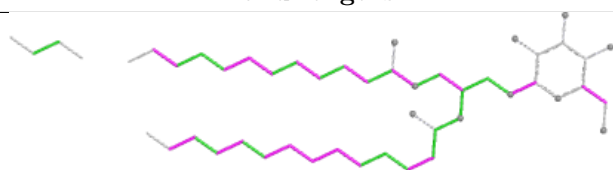
Ligand LMG D 317



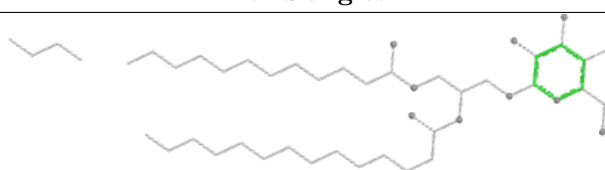
Bond lengths



Bond angles

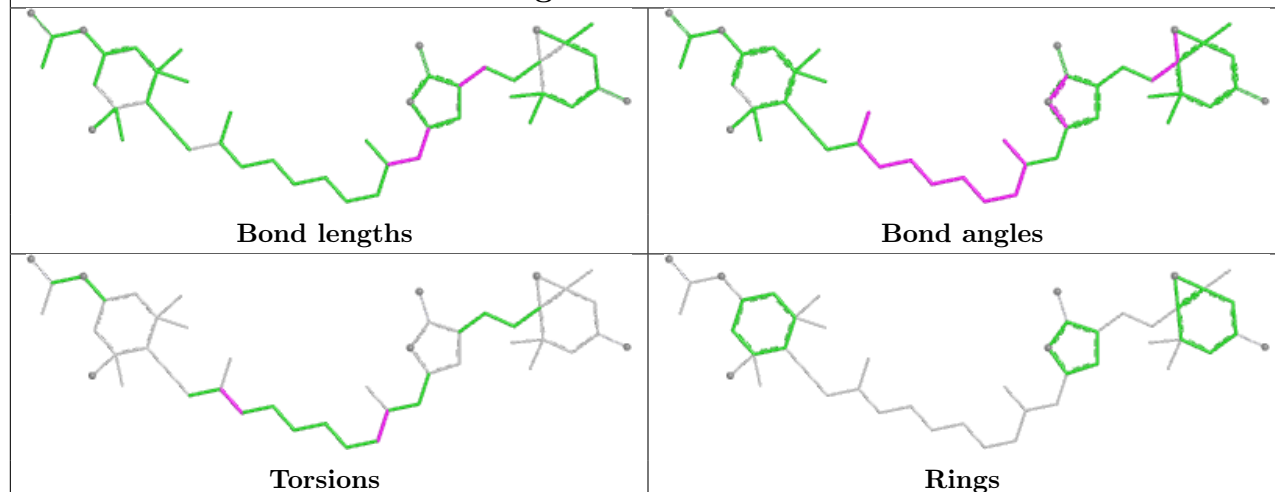


Torsions

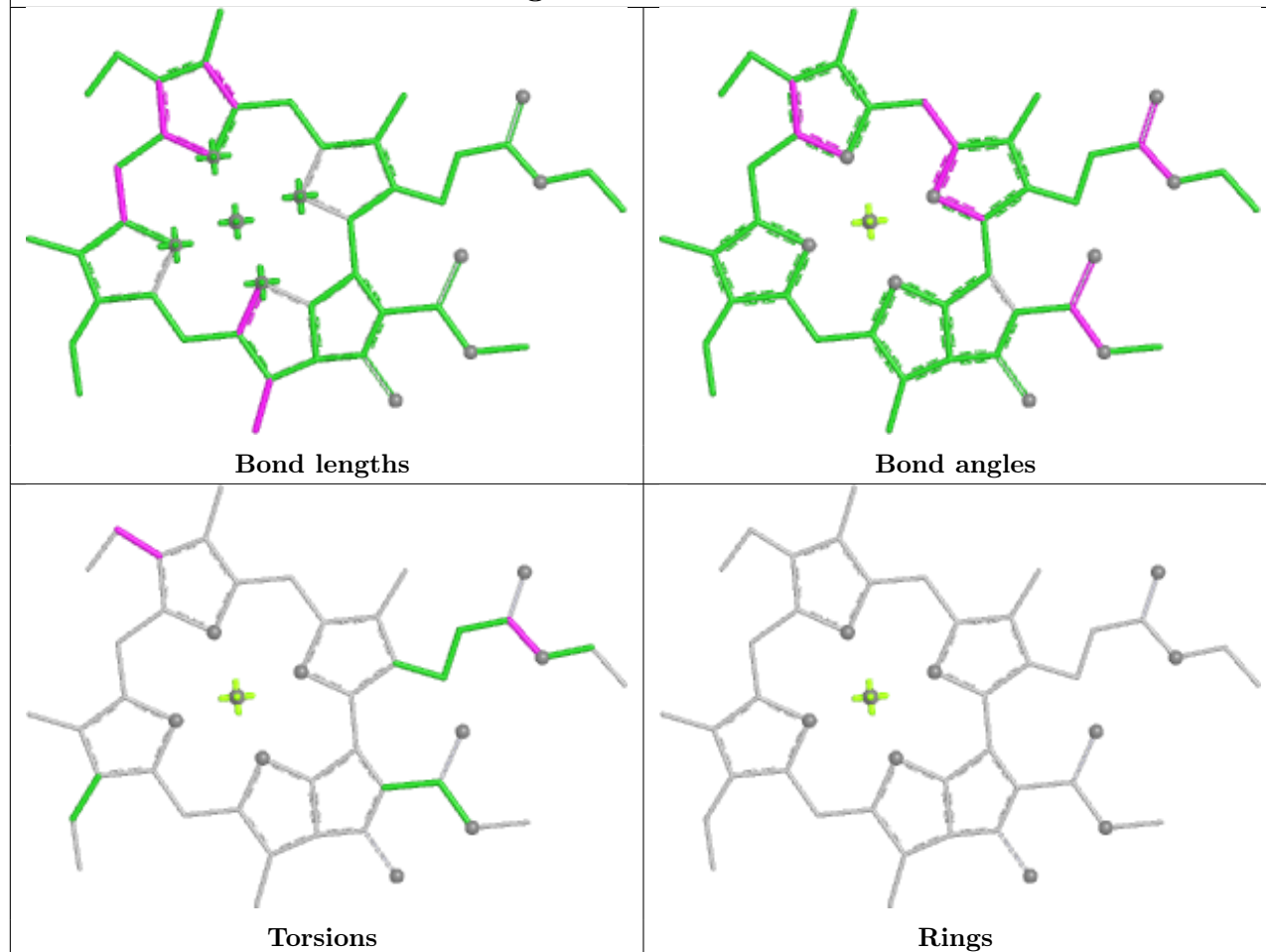


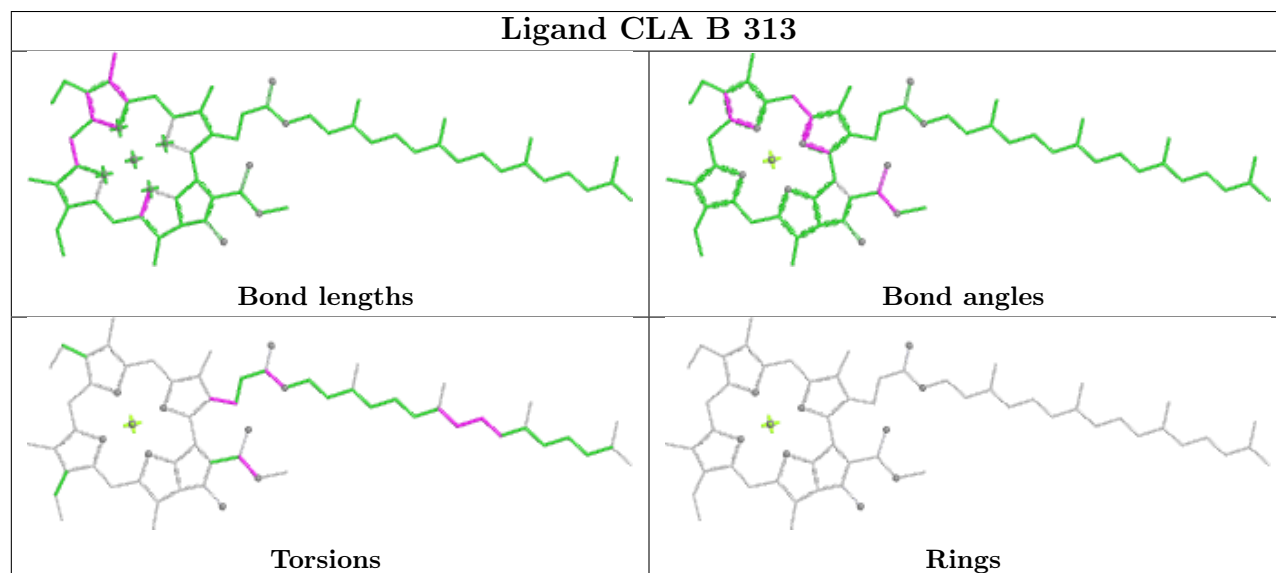
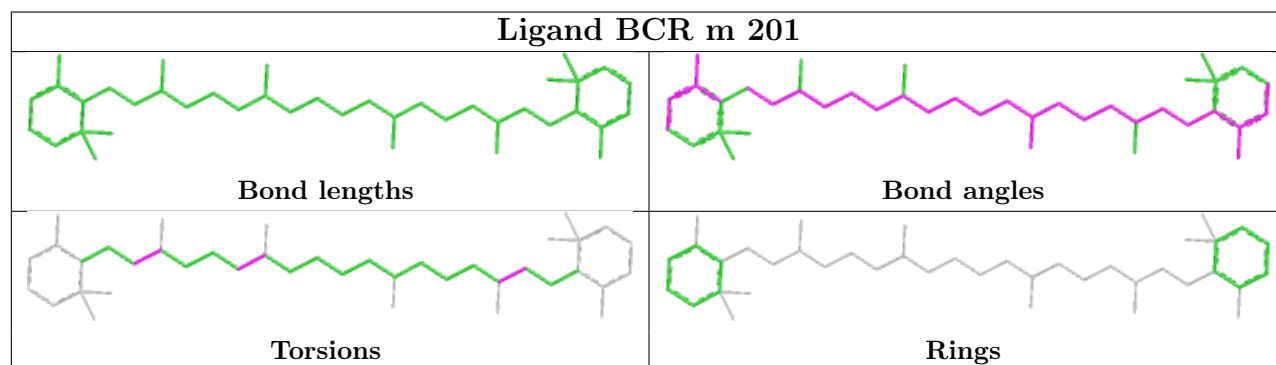
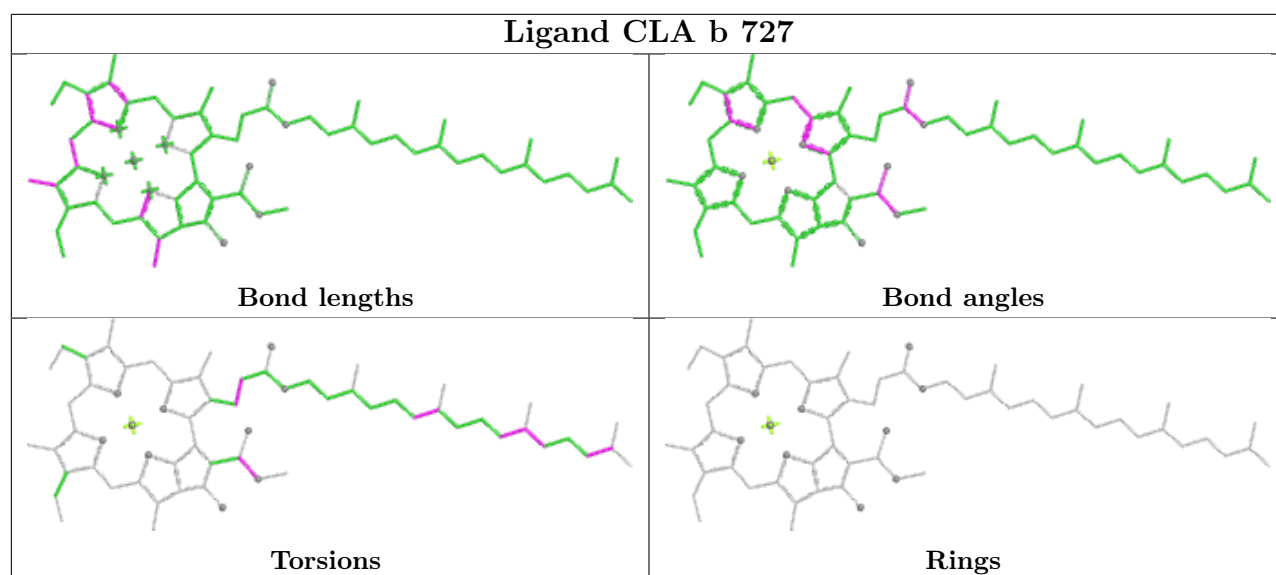
Rings

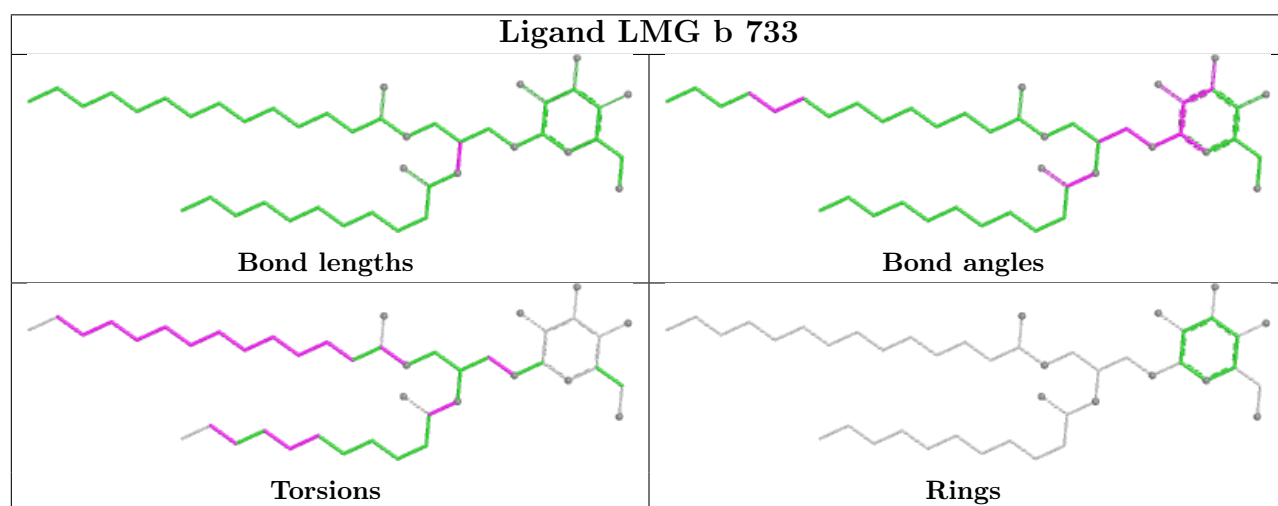
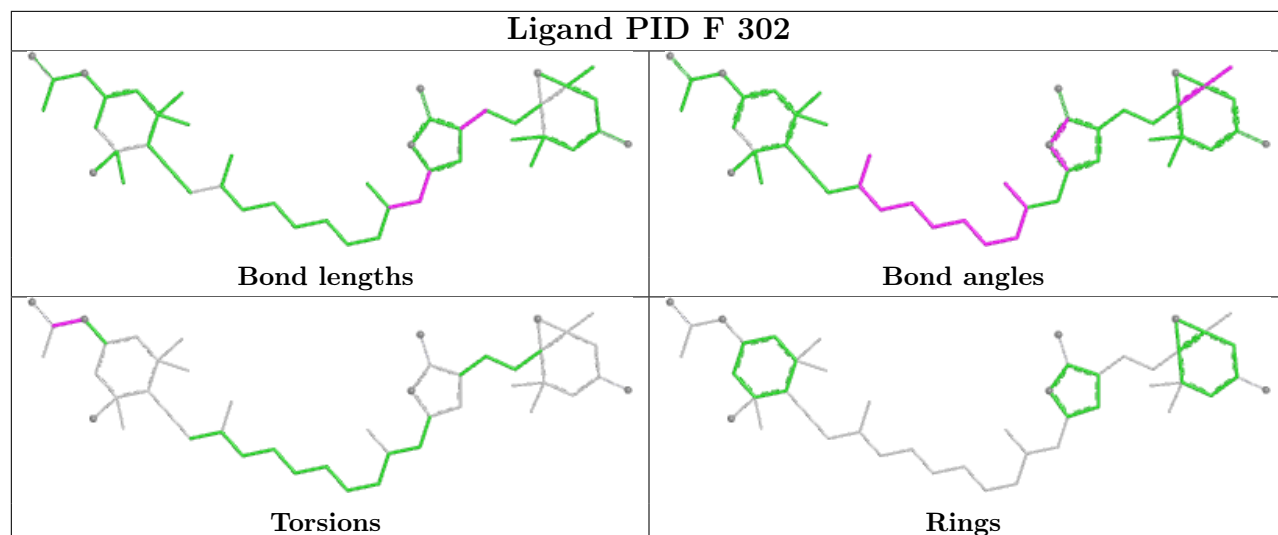
Ligand PID D 304



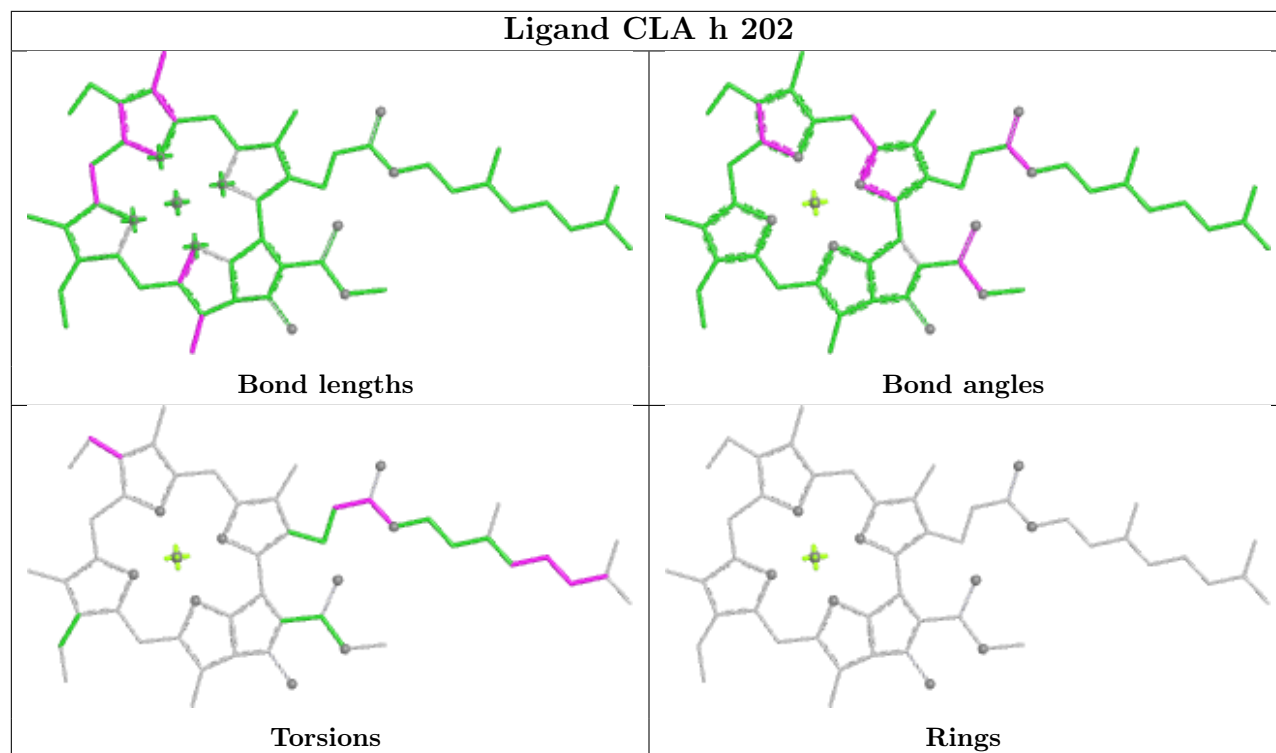
Ligand CLA D 308



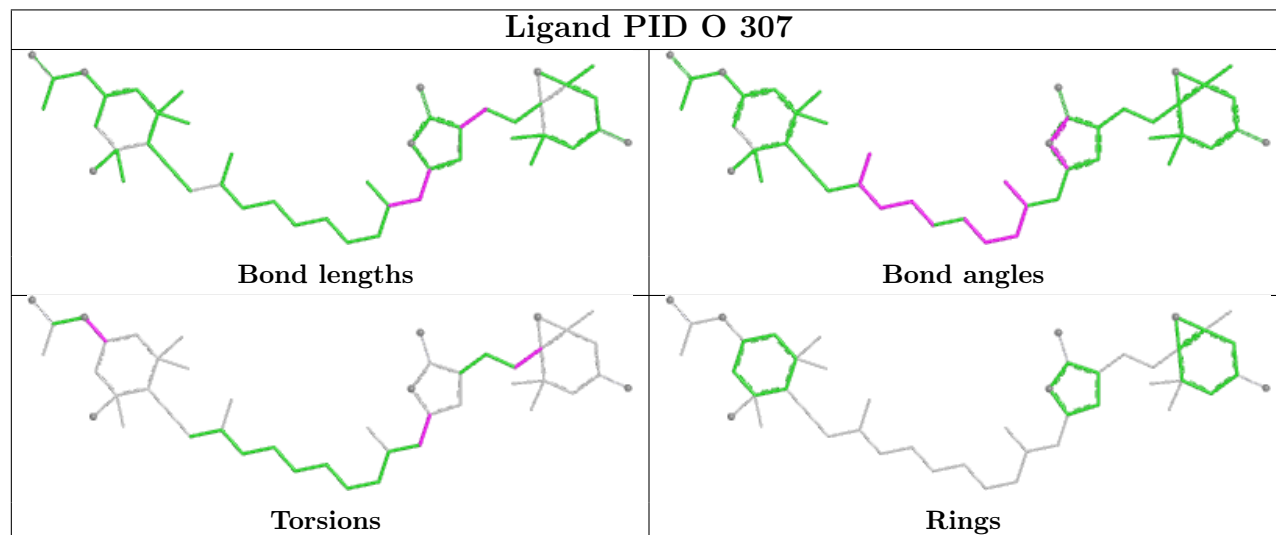


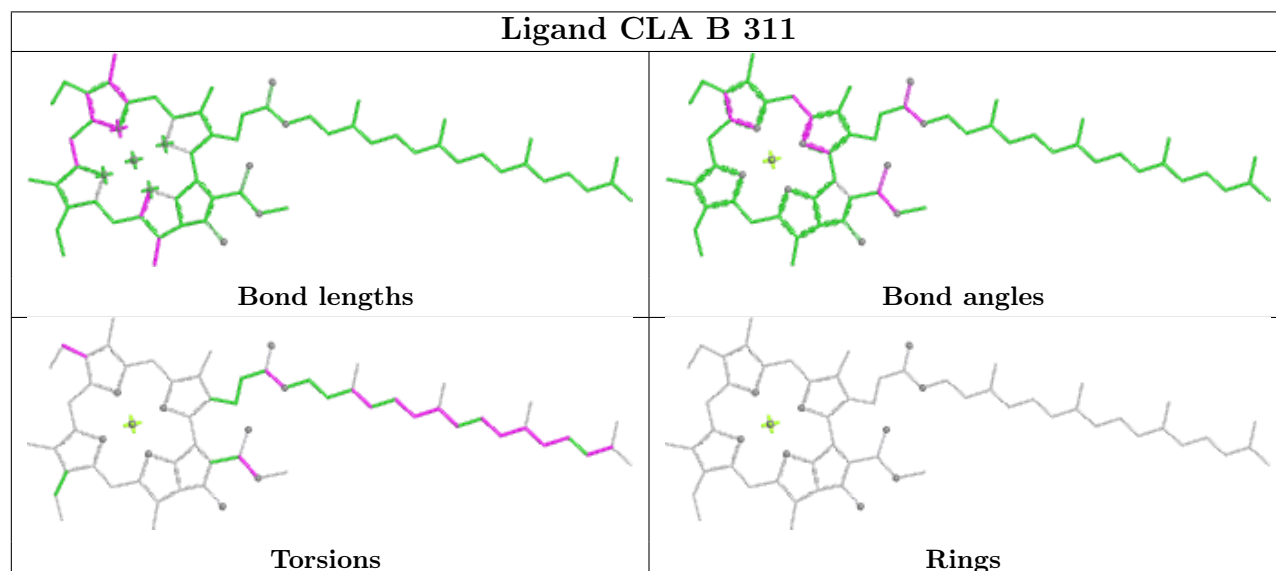
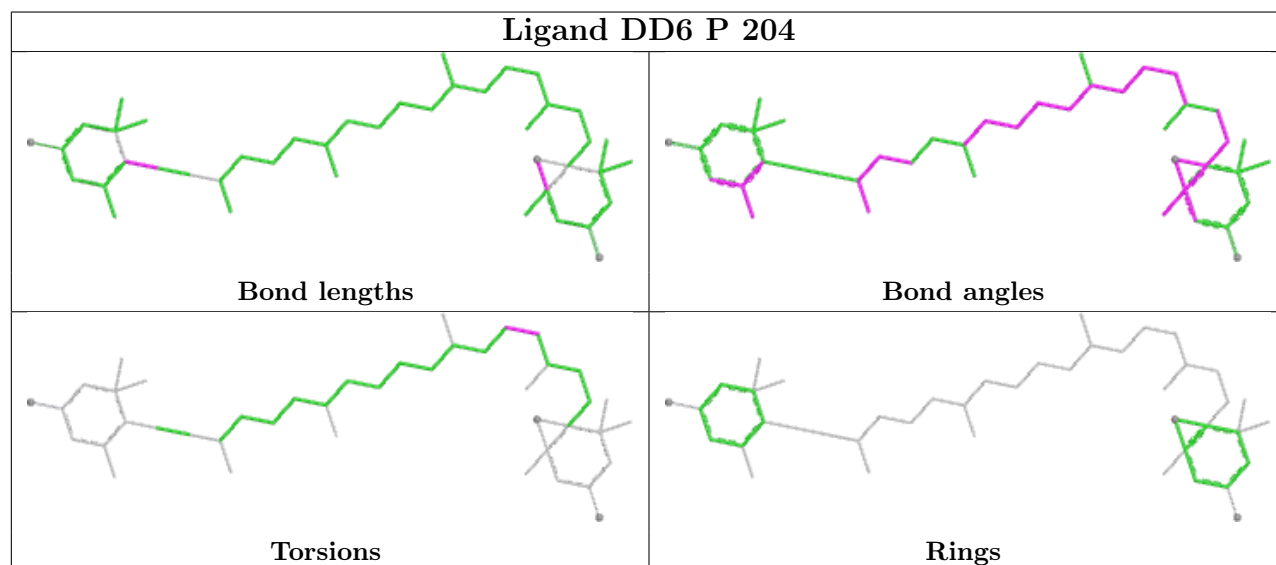
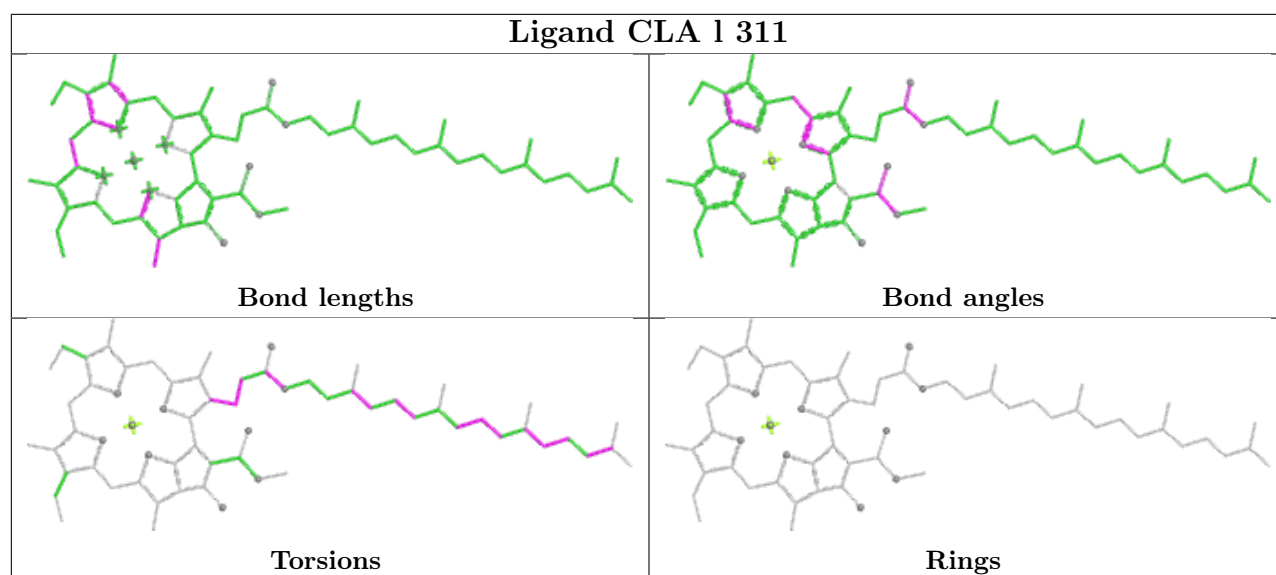


Ligand CLA h 202

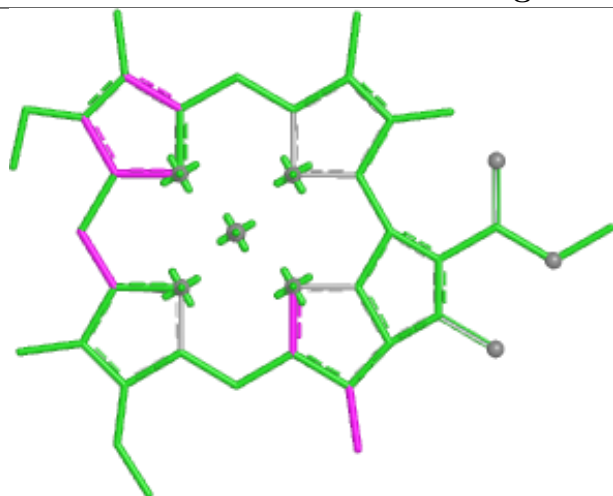


Ligand PID O 307

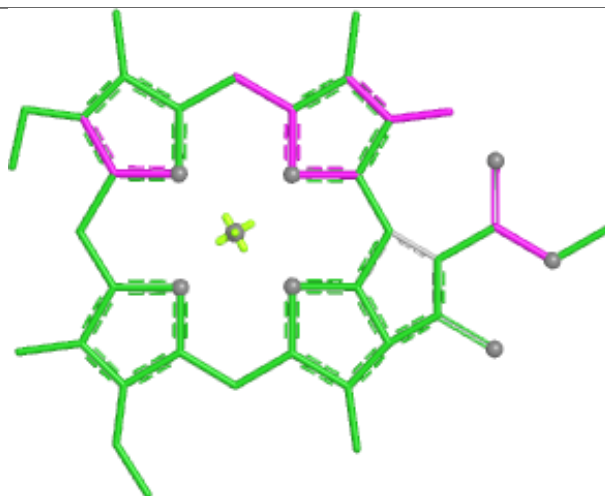




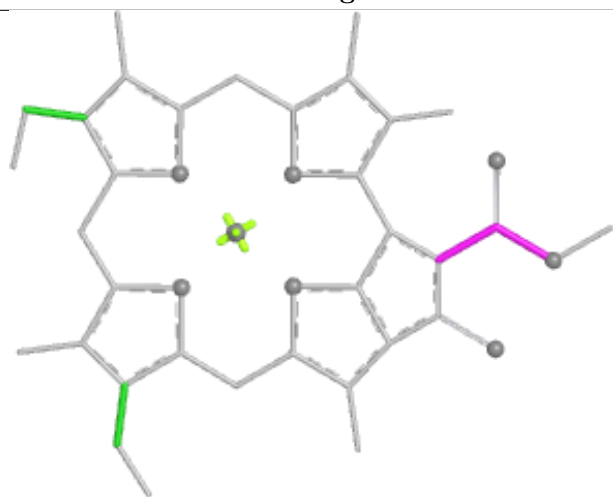
Ligand CLA A 315



Bond lengths



Bond angles

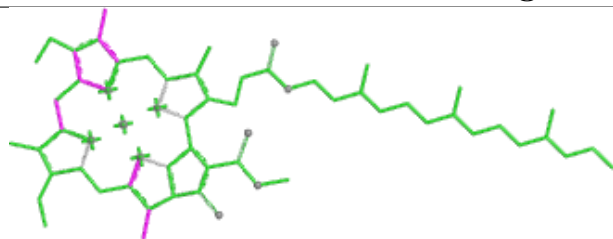


Torsions

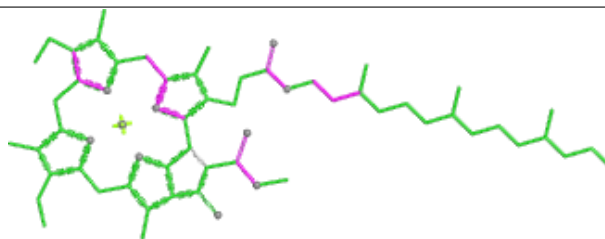


Rings

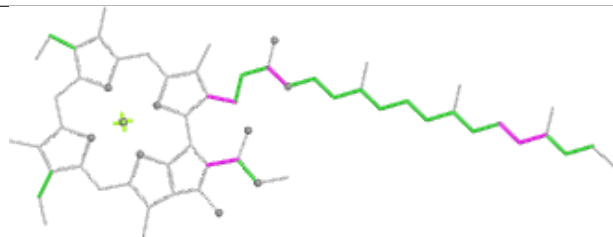
Ligand CLA a 720



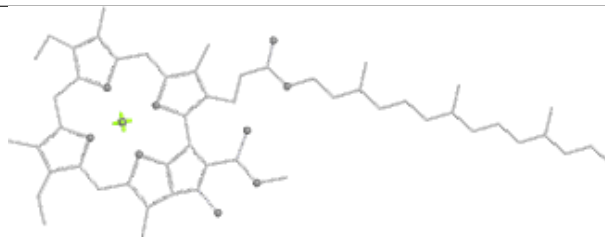
Bond lengths



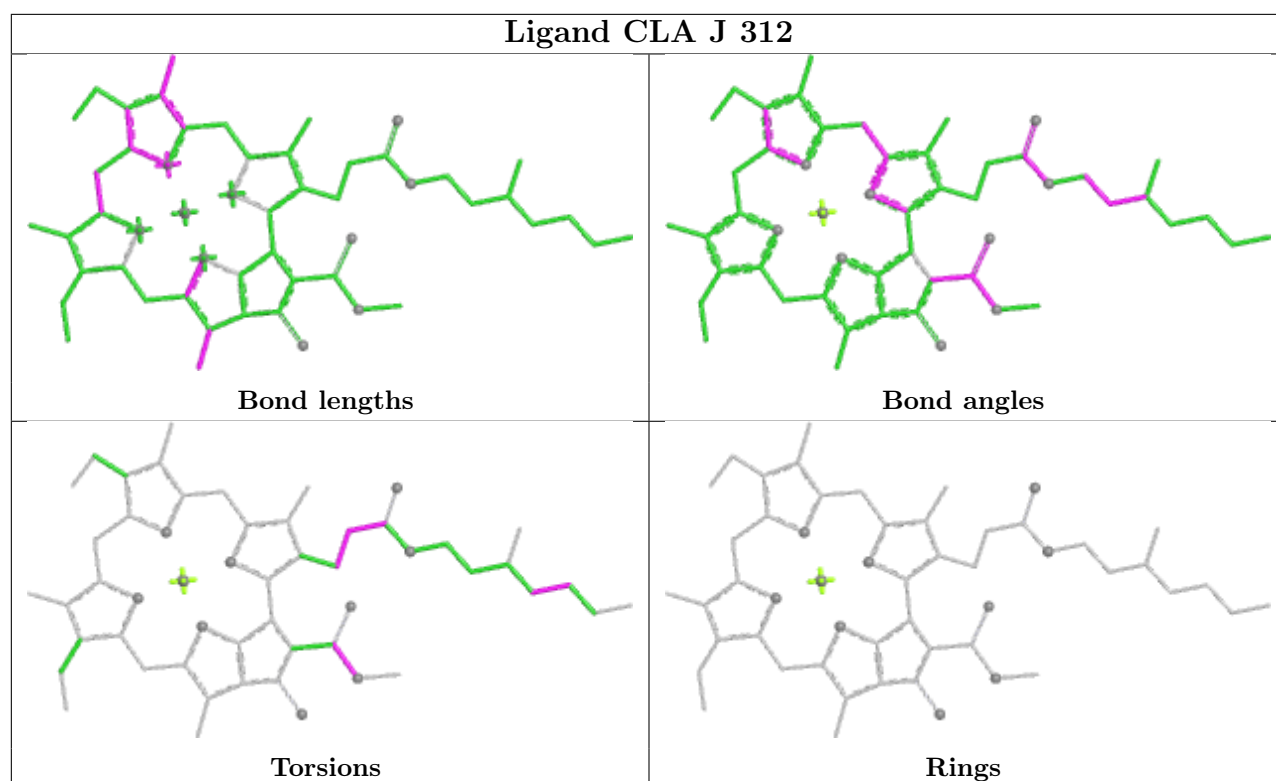
Bond angles



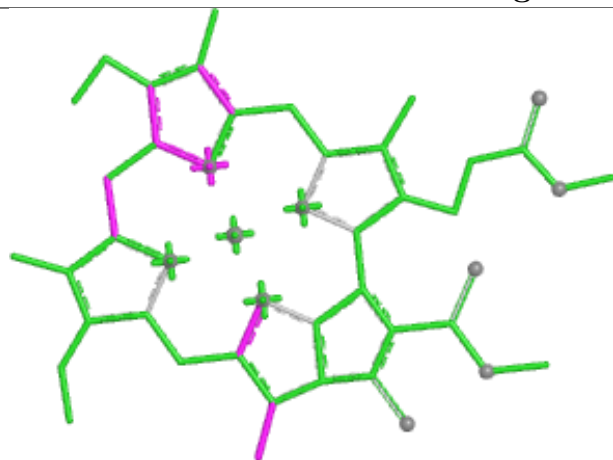
Torsions



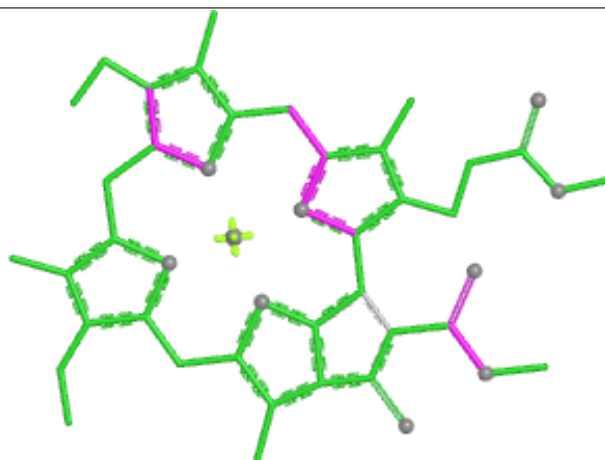
Rings



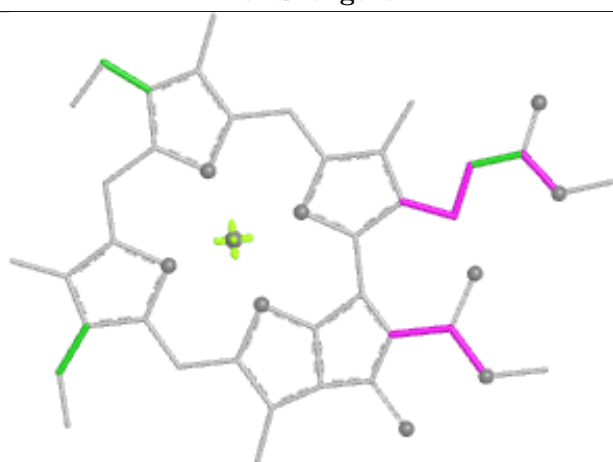
Ligand CLA H 312



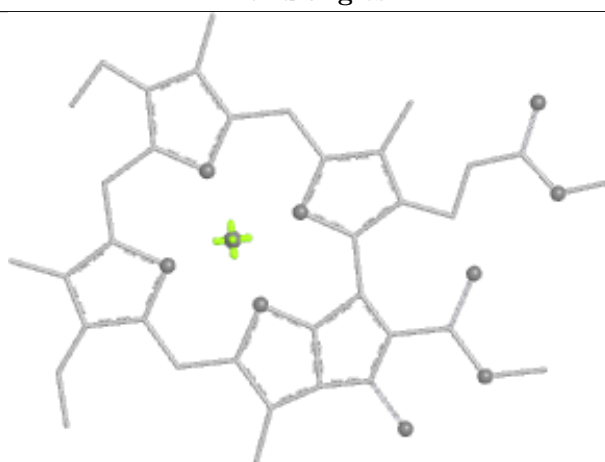
Bond lengths



Bond angles

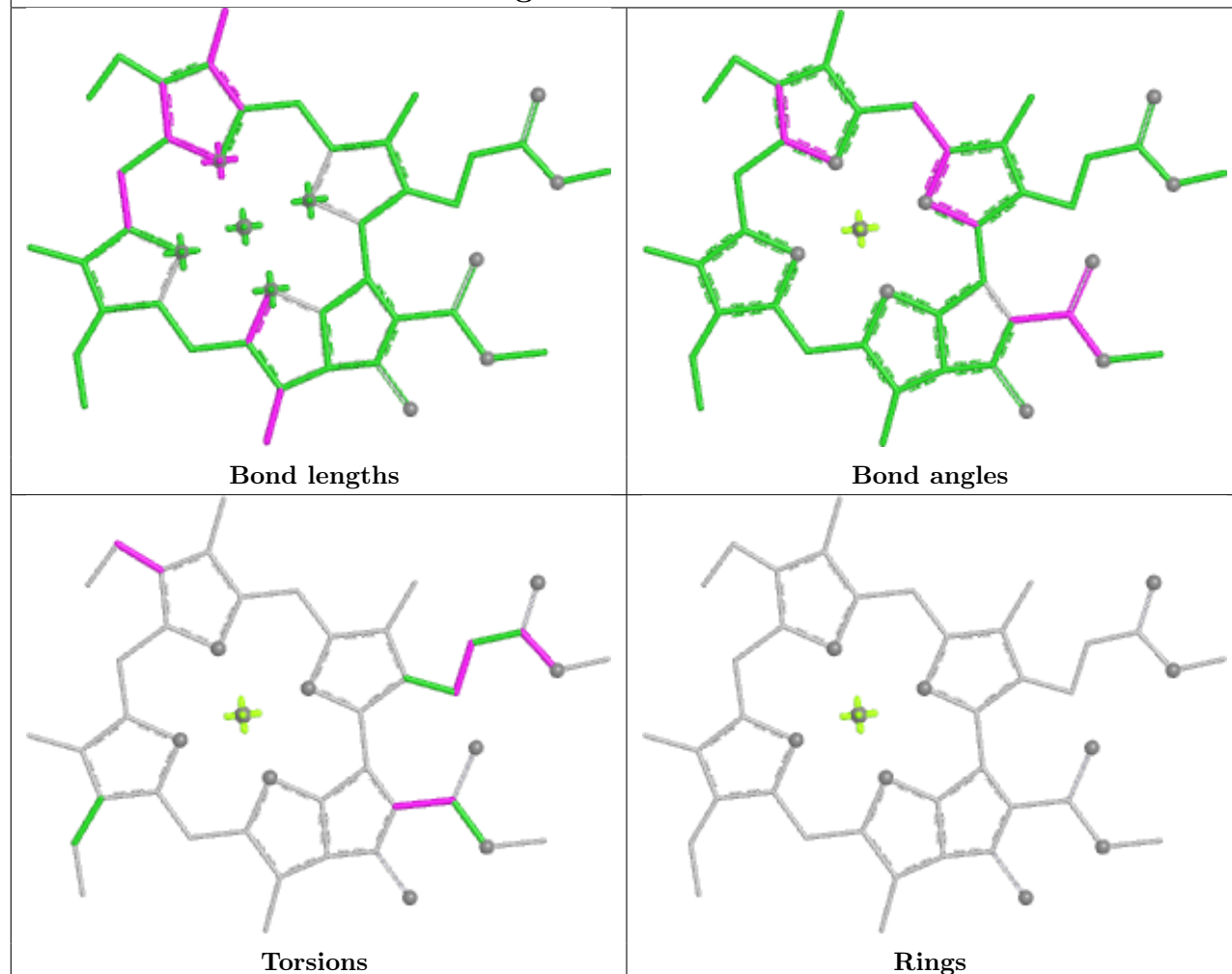


Torsions

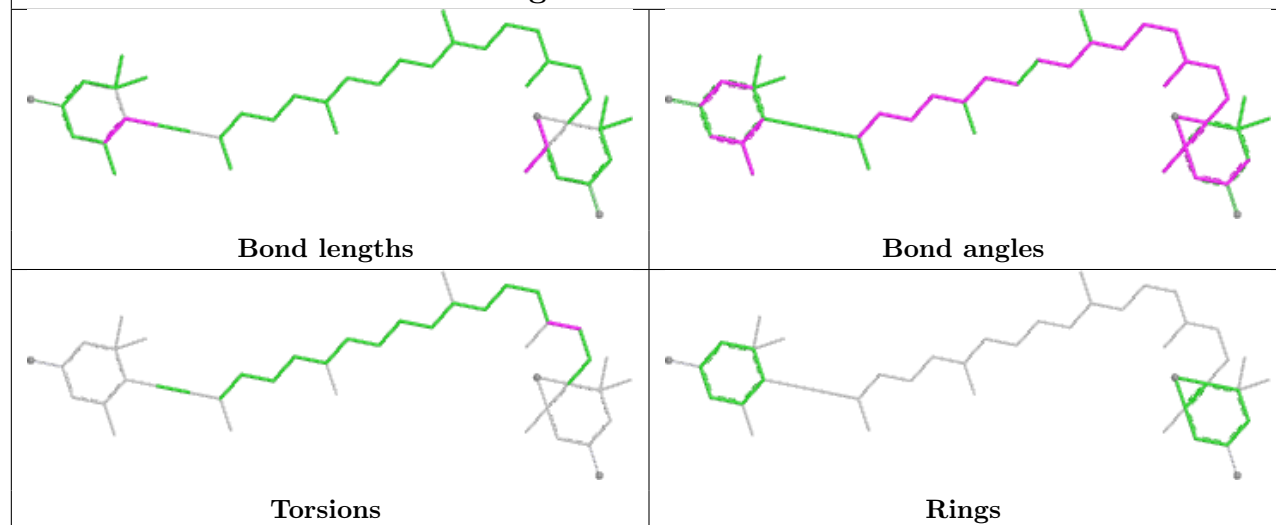


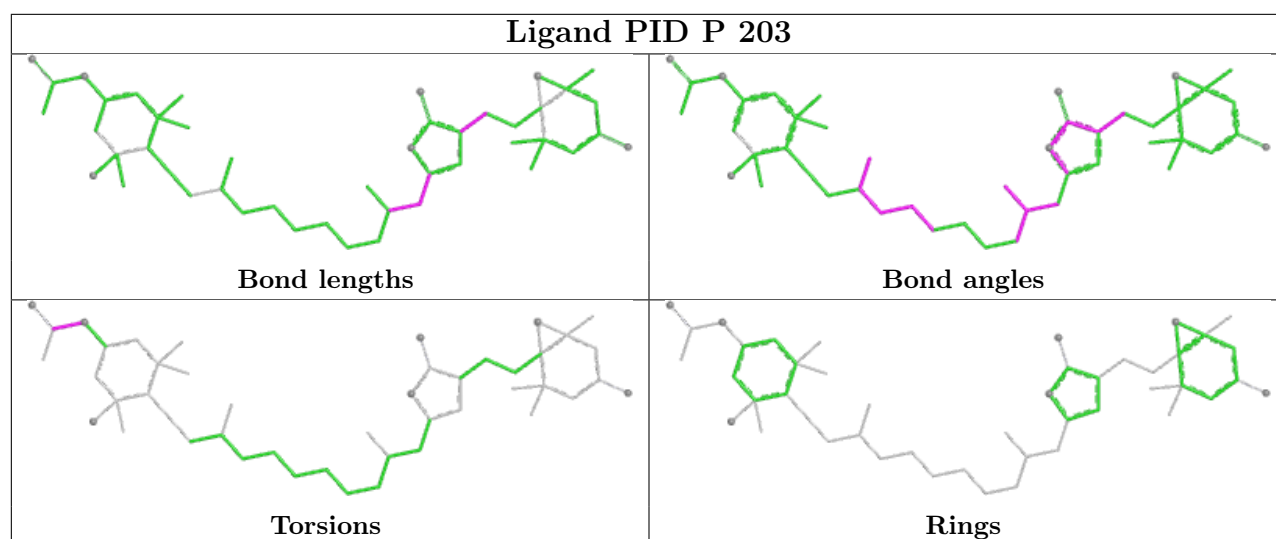
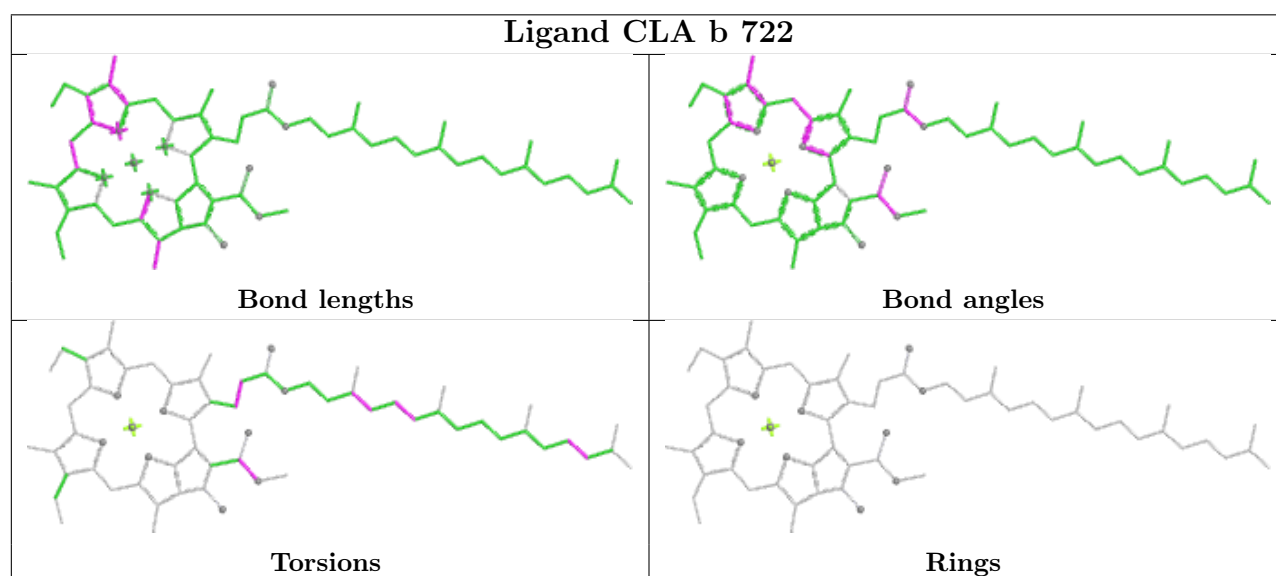
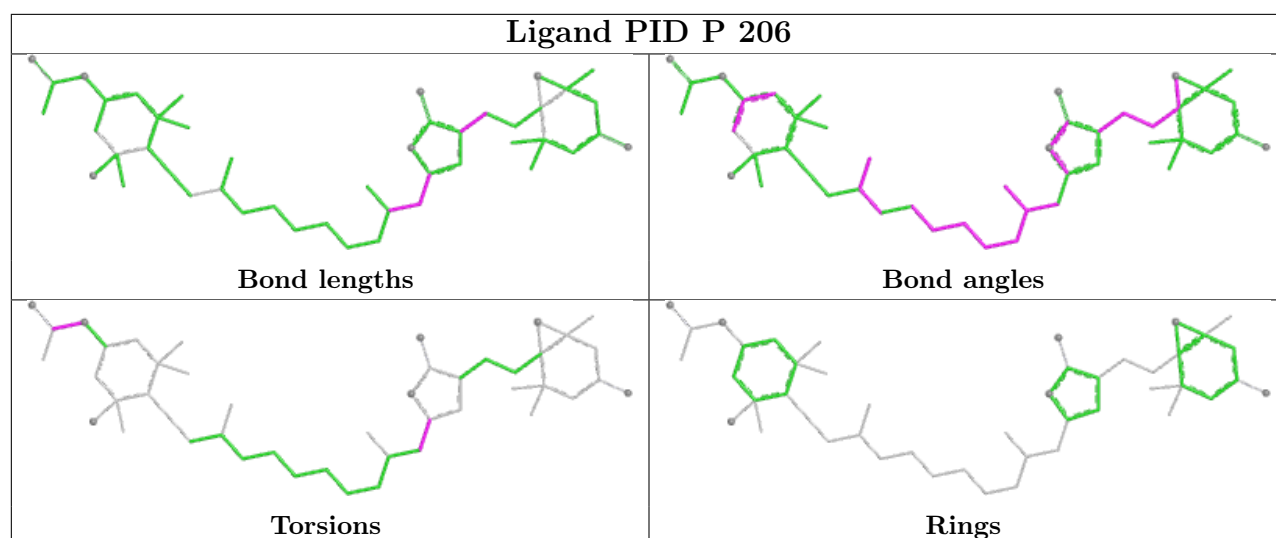
Rings

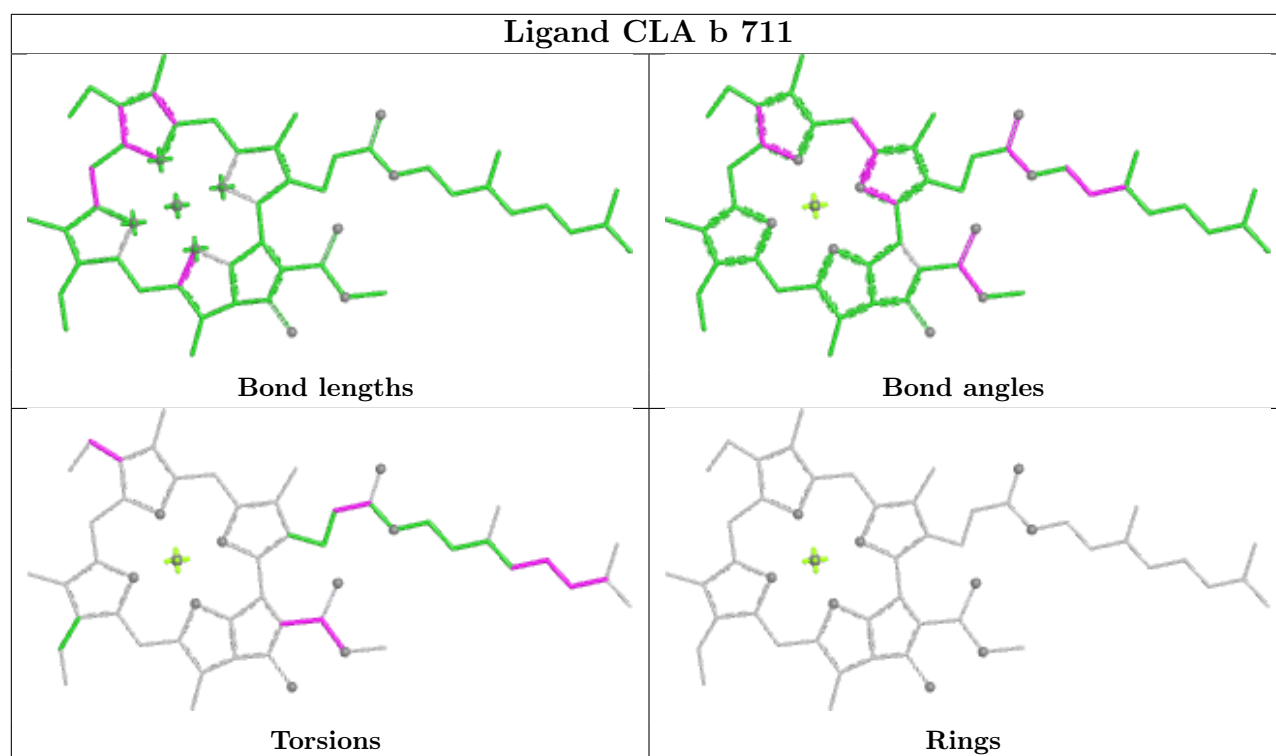
Ligand CLA F 311



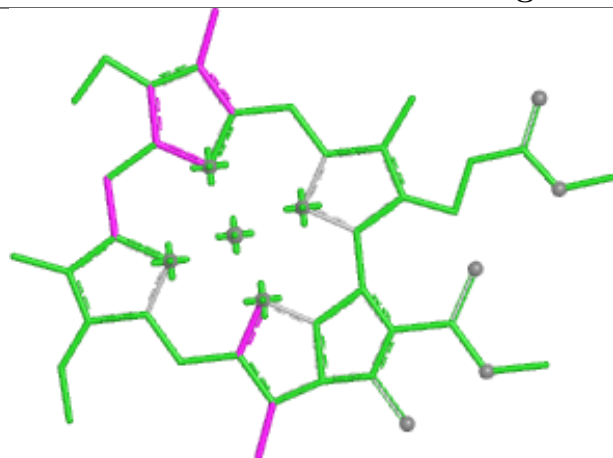
Ligand DD6 M 303



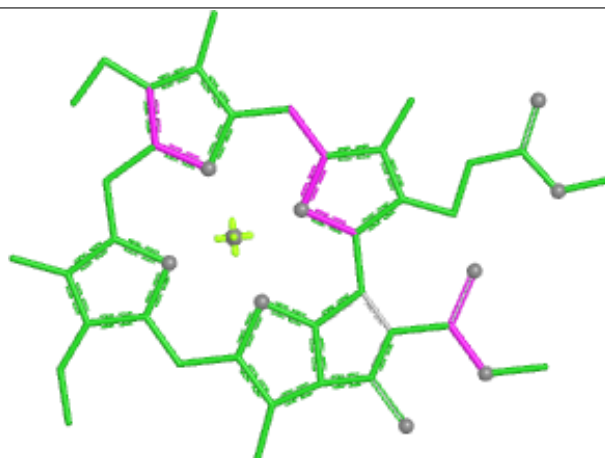




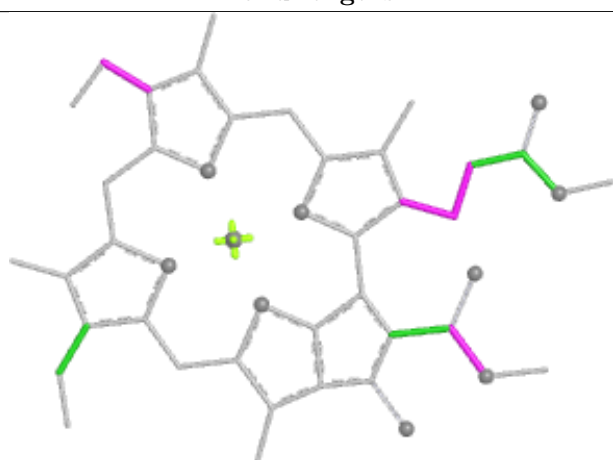
Ligand CLA L 312



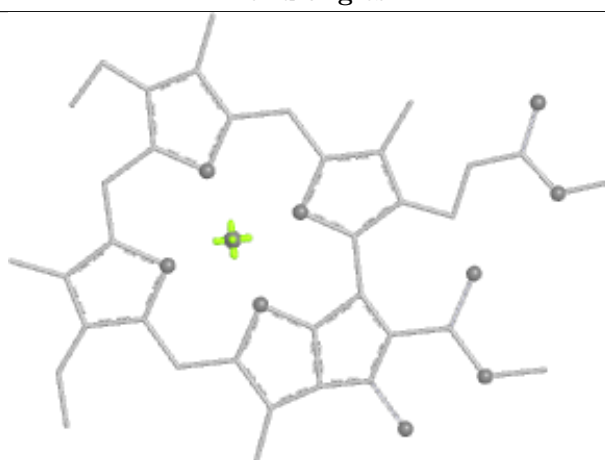
Bond lengths



Bond angles

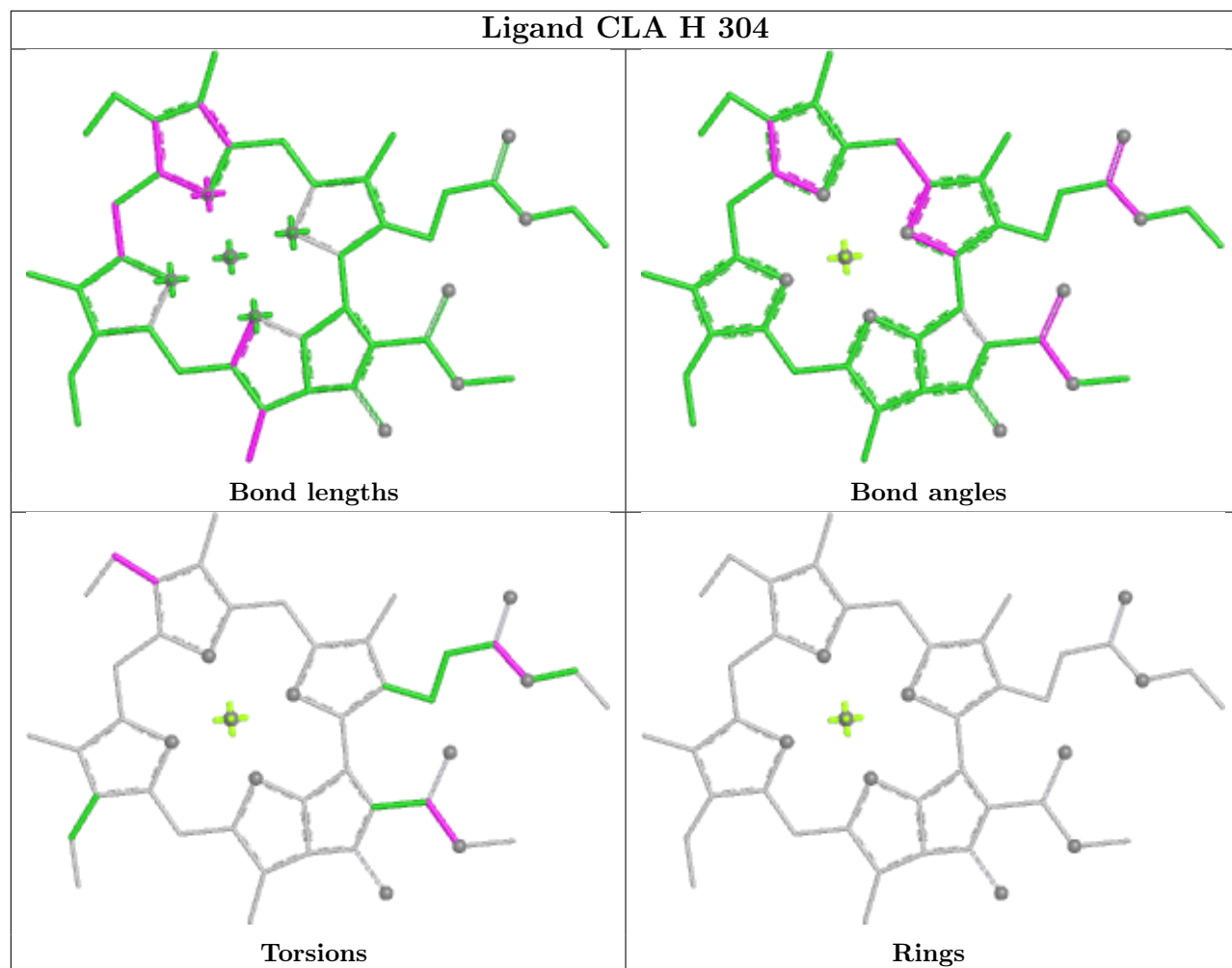


Torsions

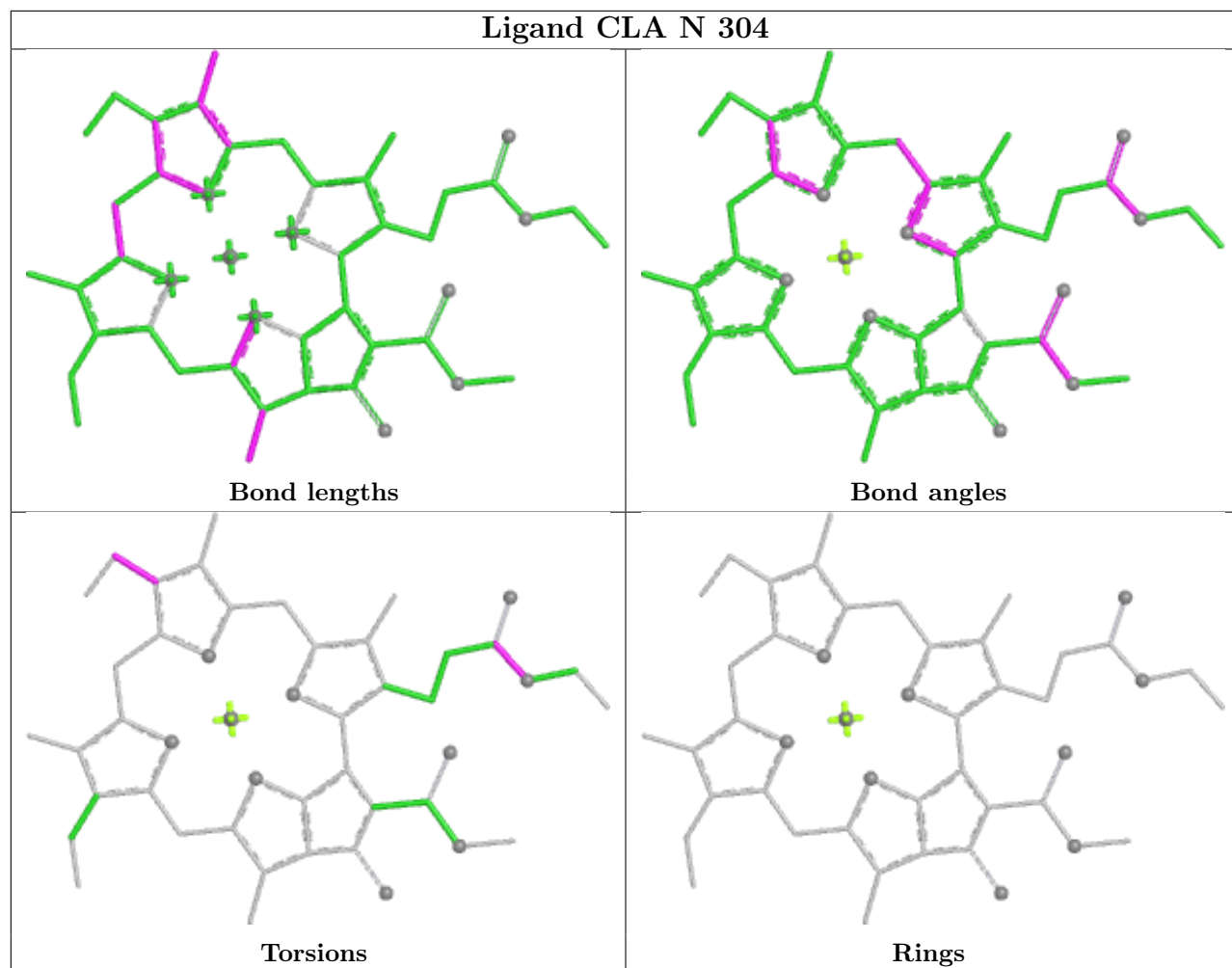


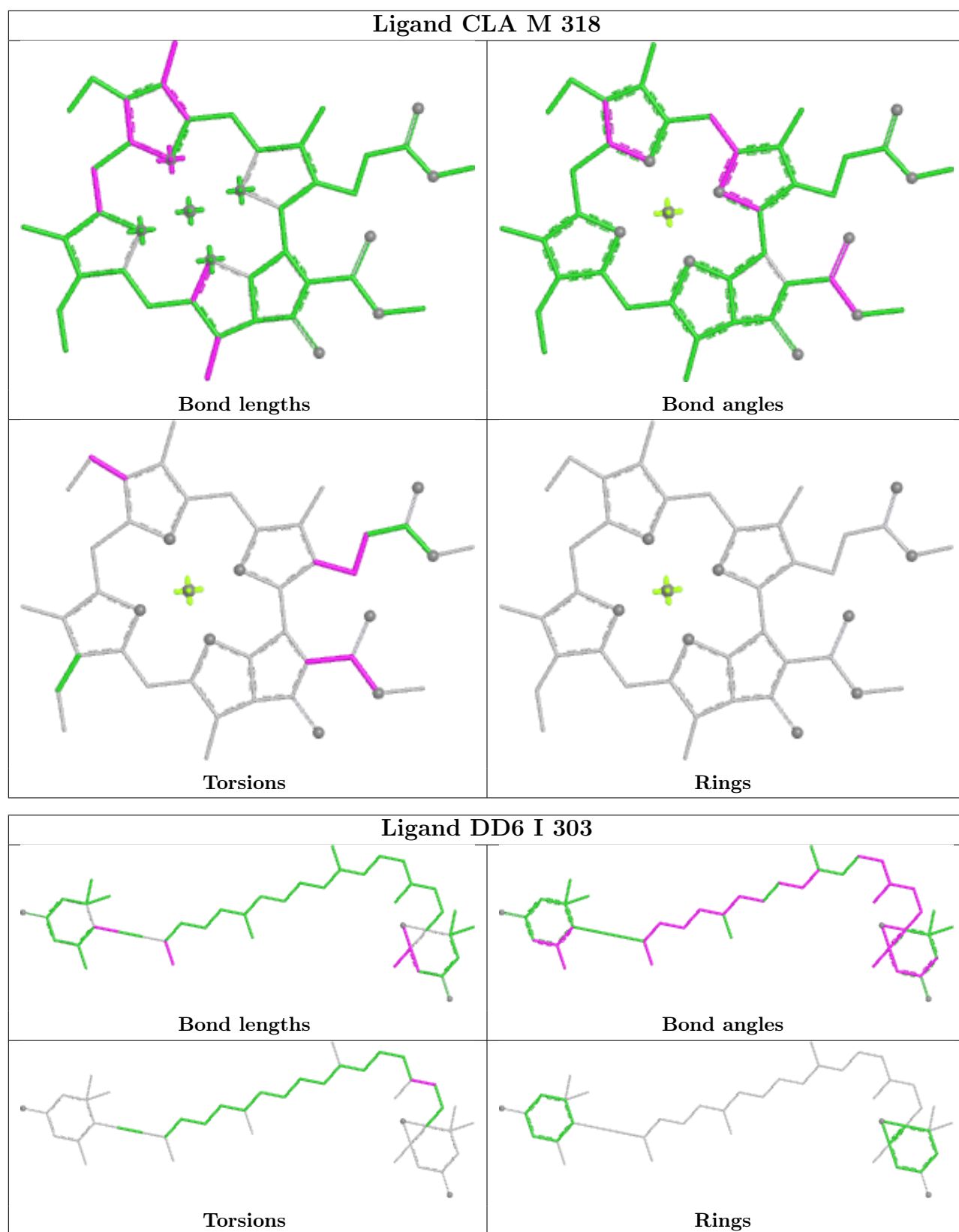
Rings

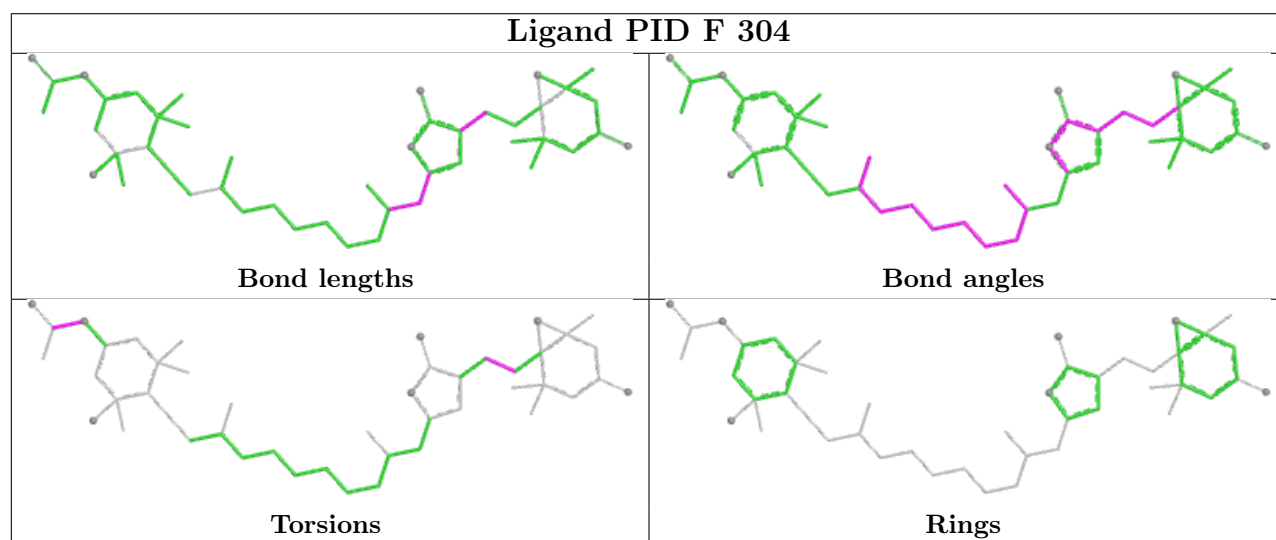
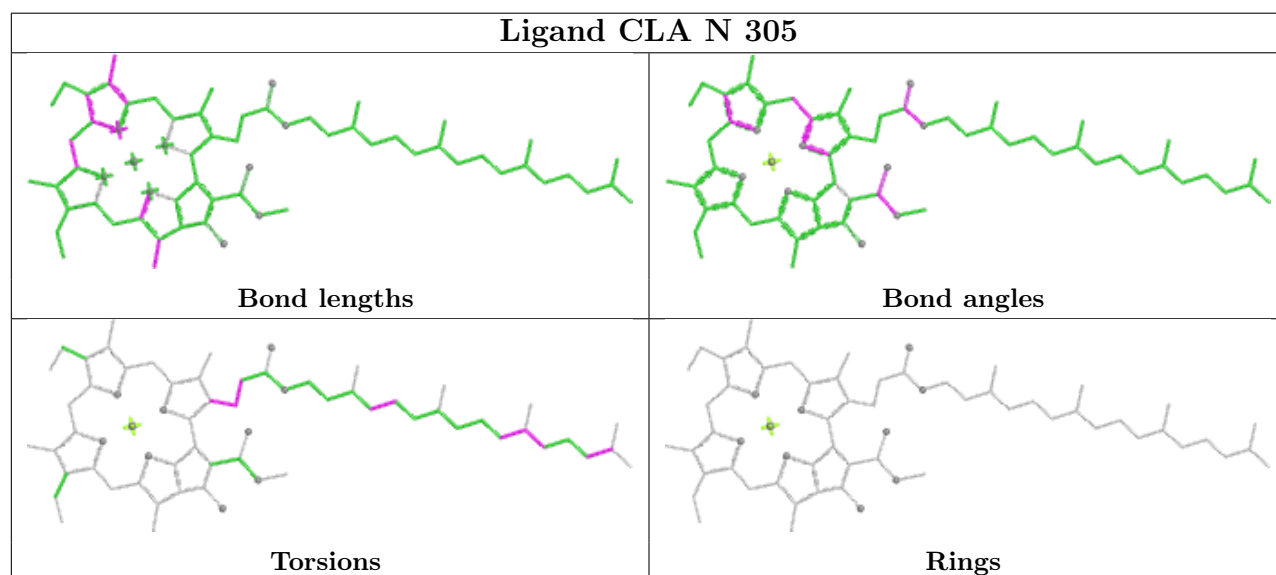
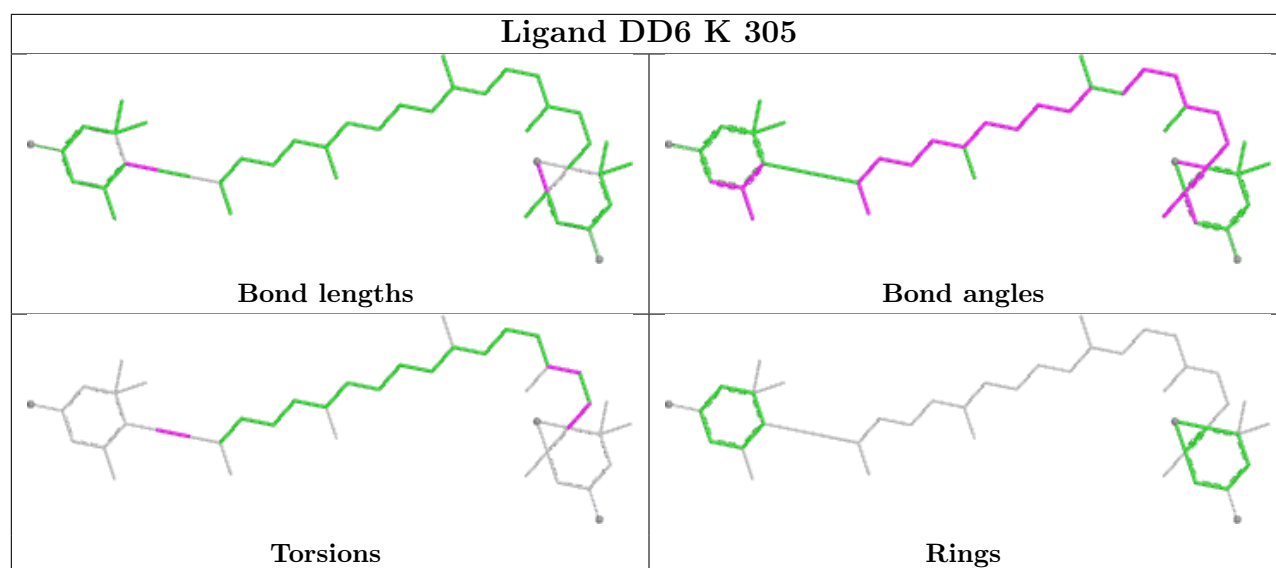
Ligand CLA H 304



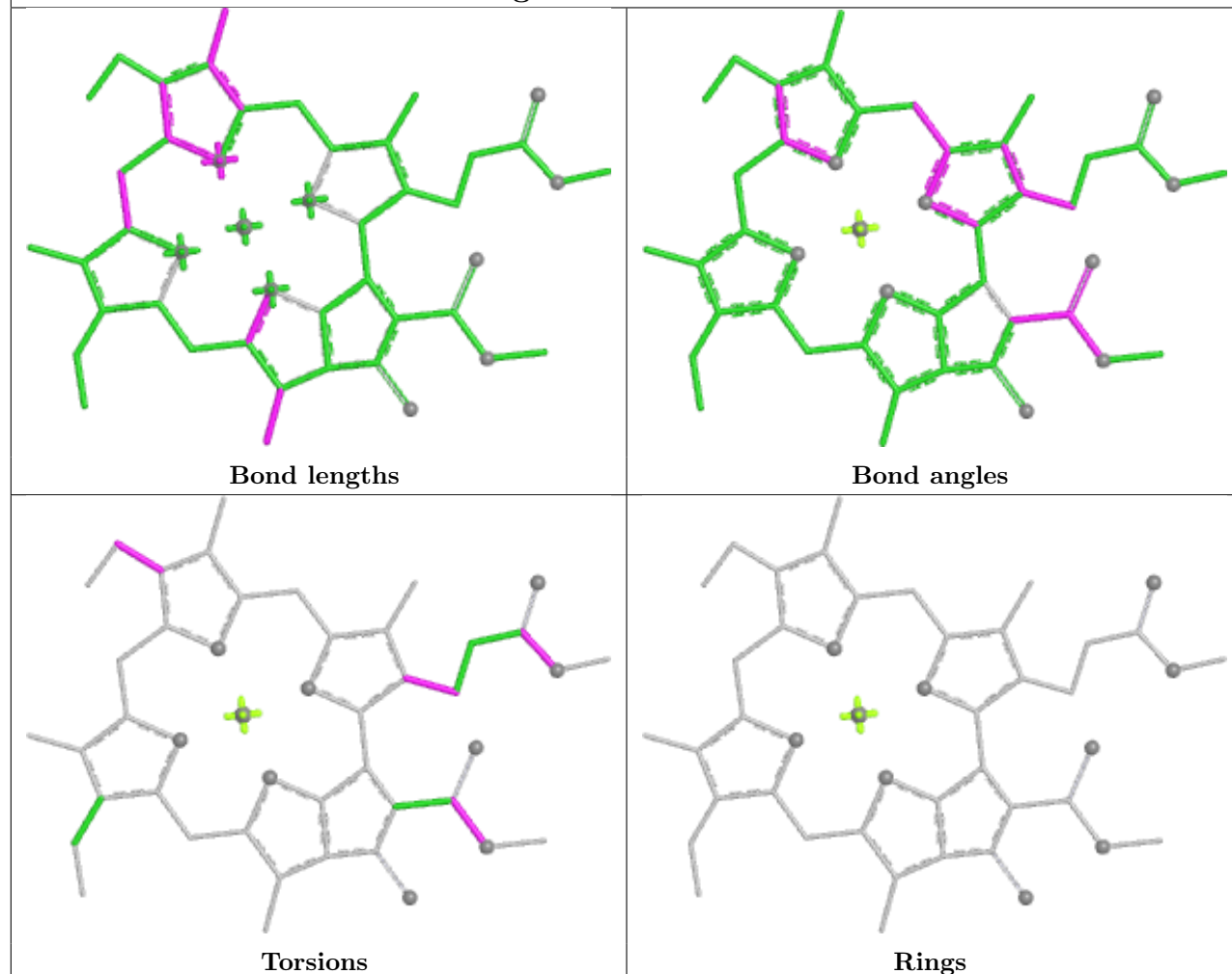
Ligand CLA N 304



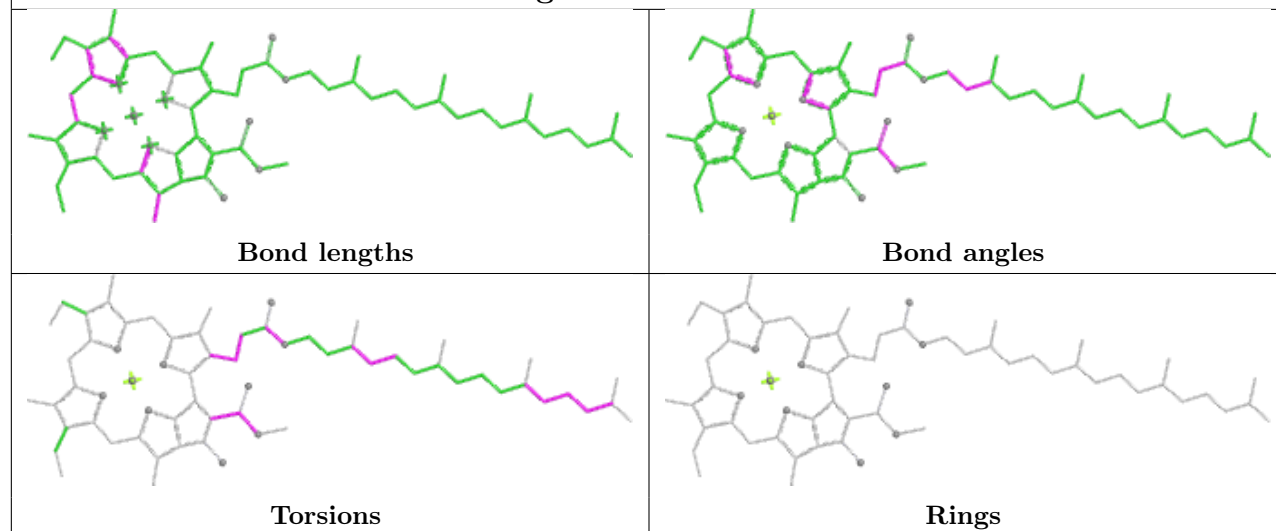


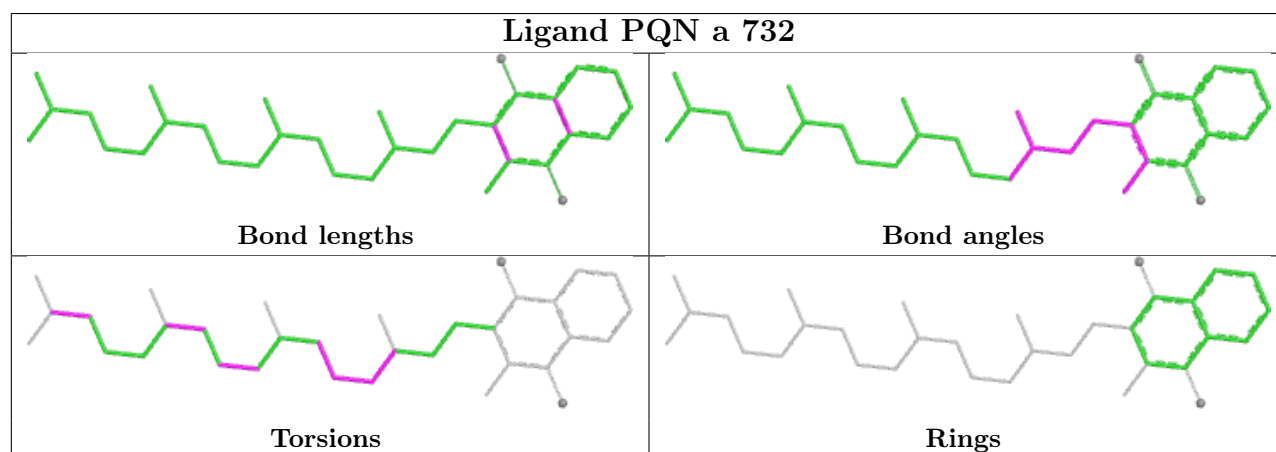
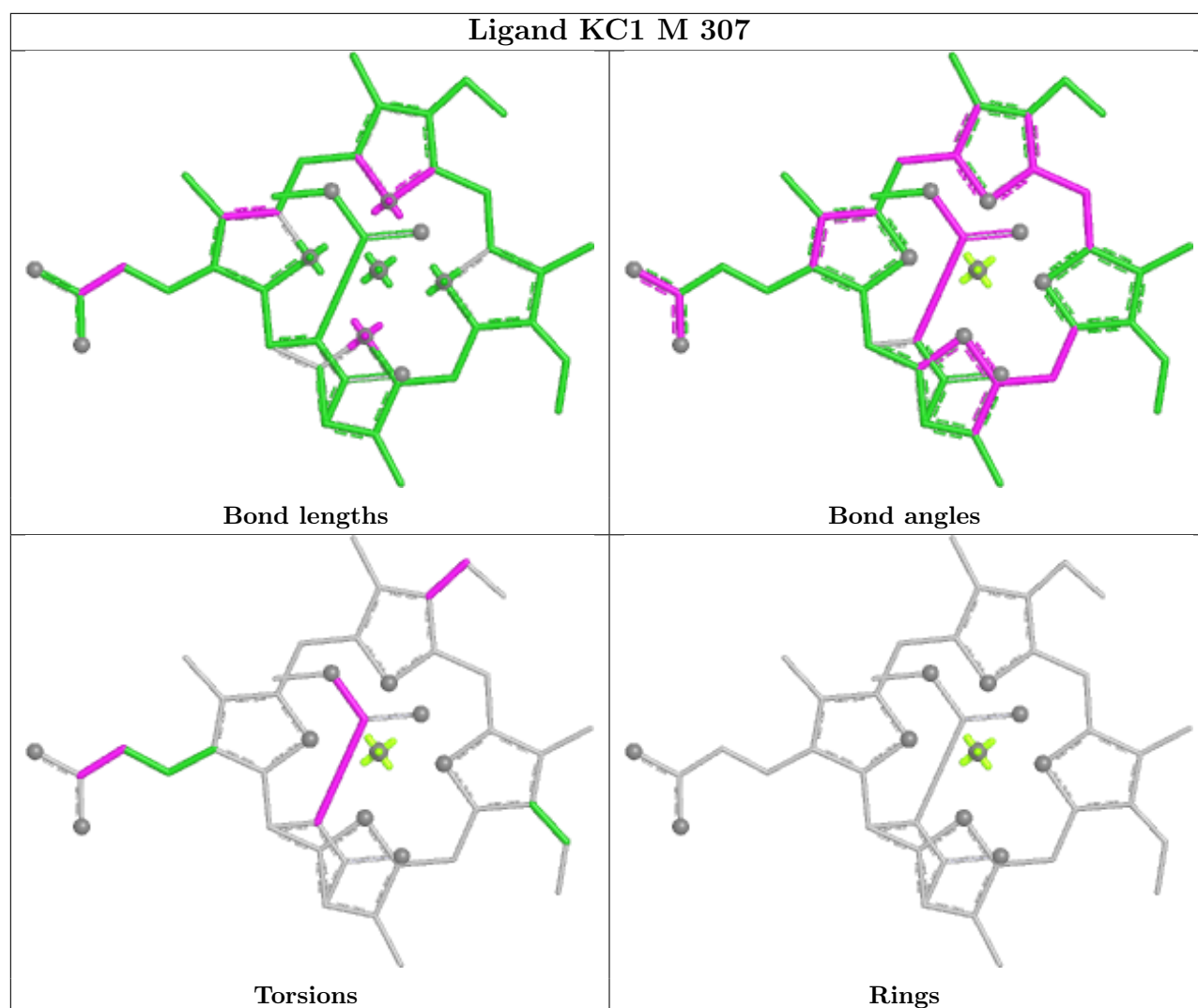


Ligand CLA D 314

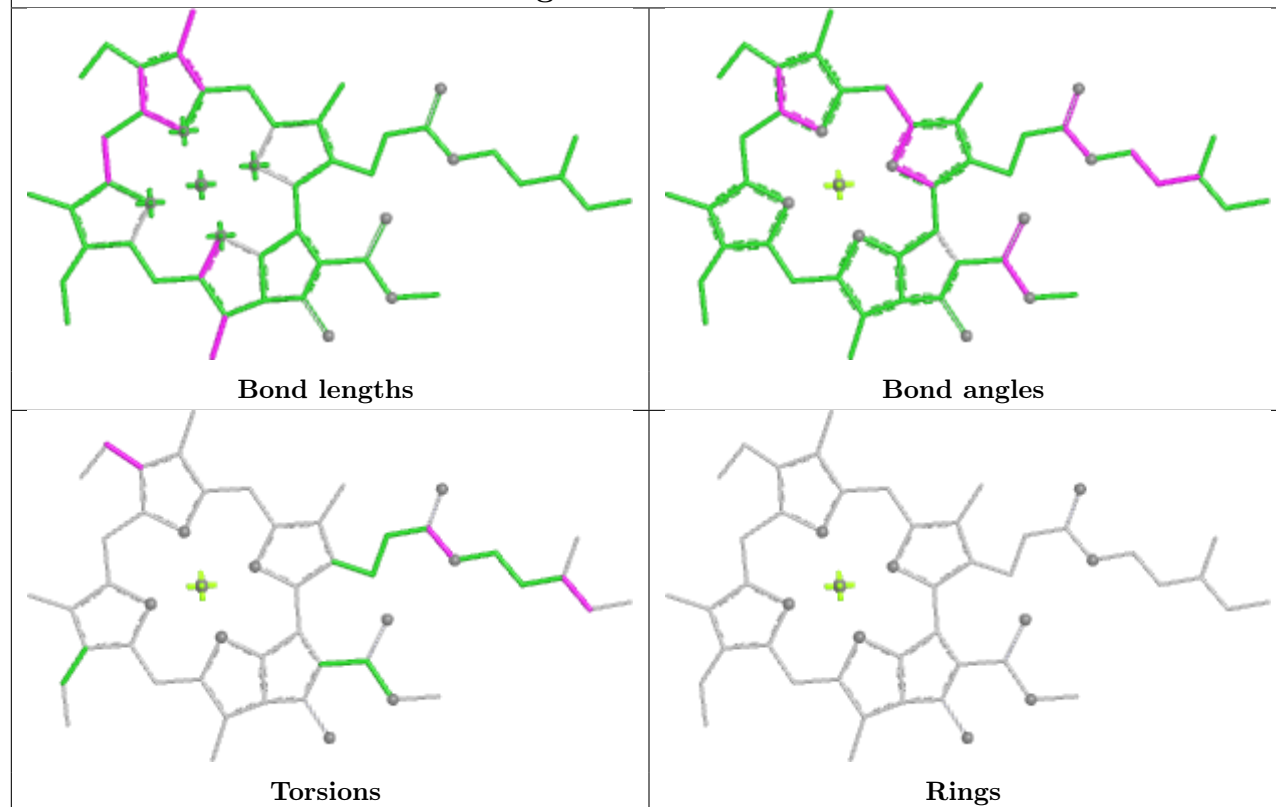


Ligand CLA a 735

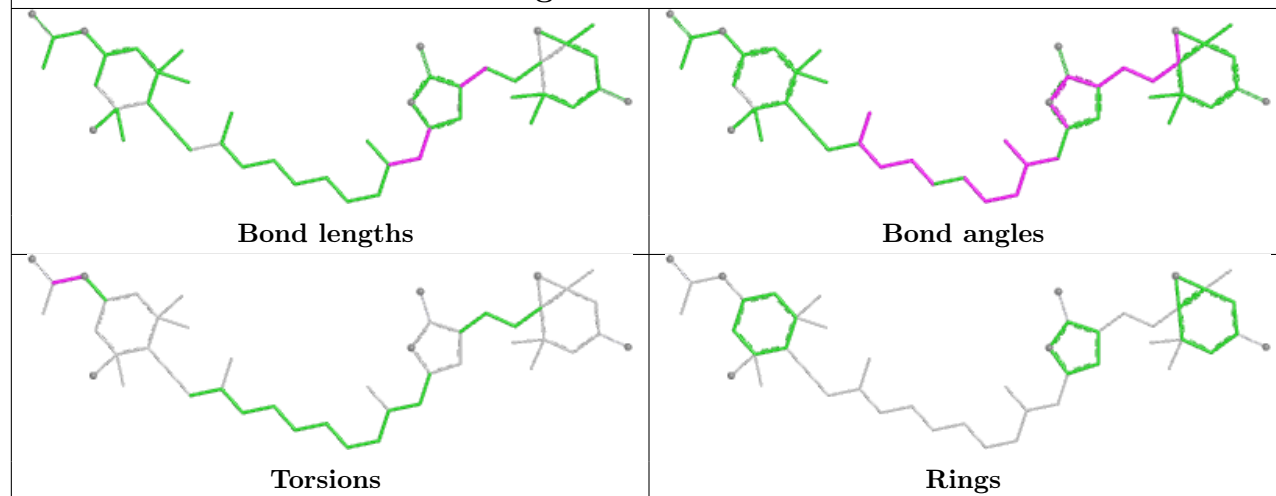




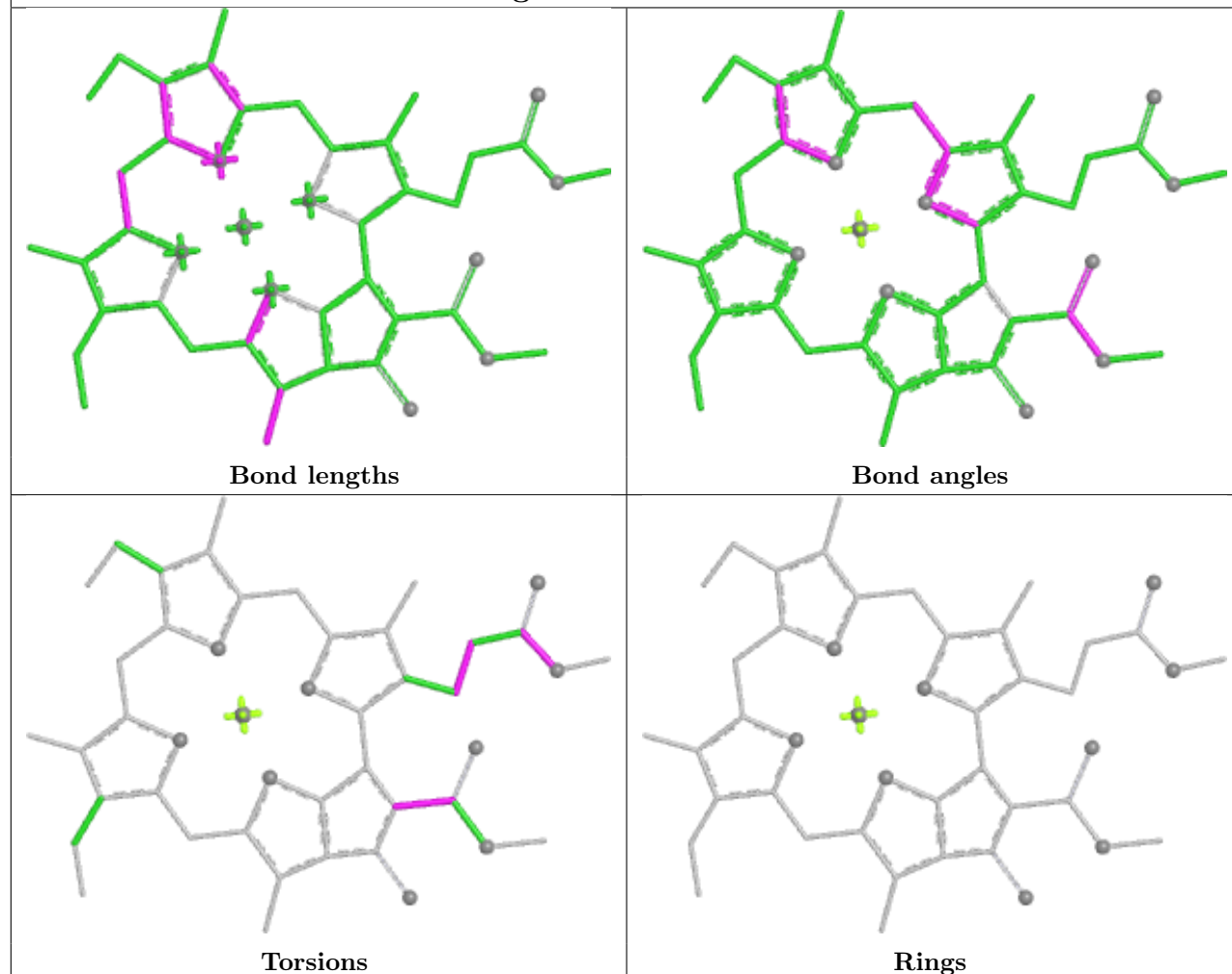
Ligand CLA a 708



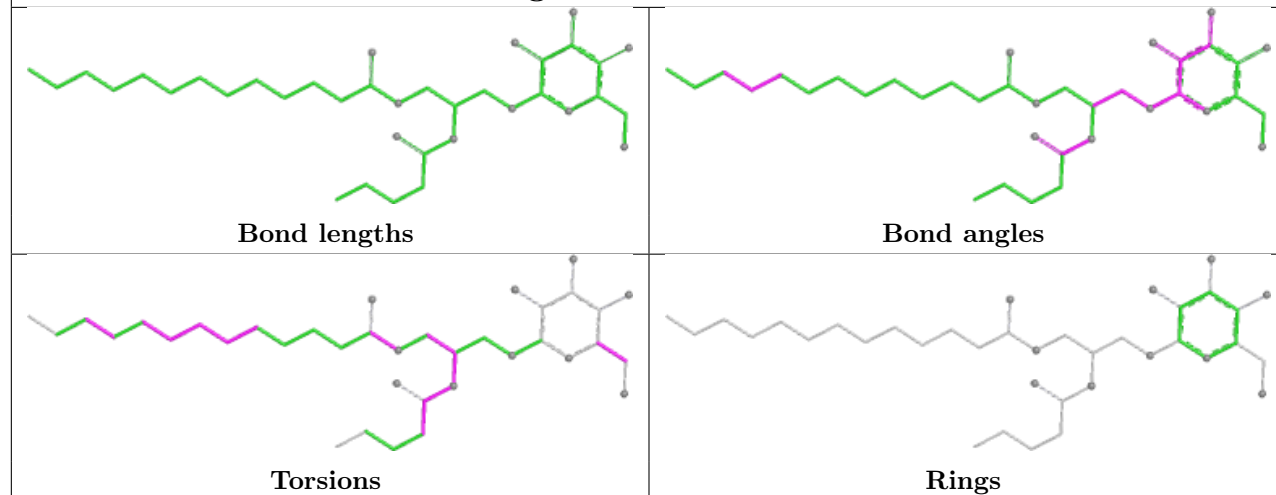
Ligand PID H 302



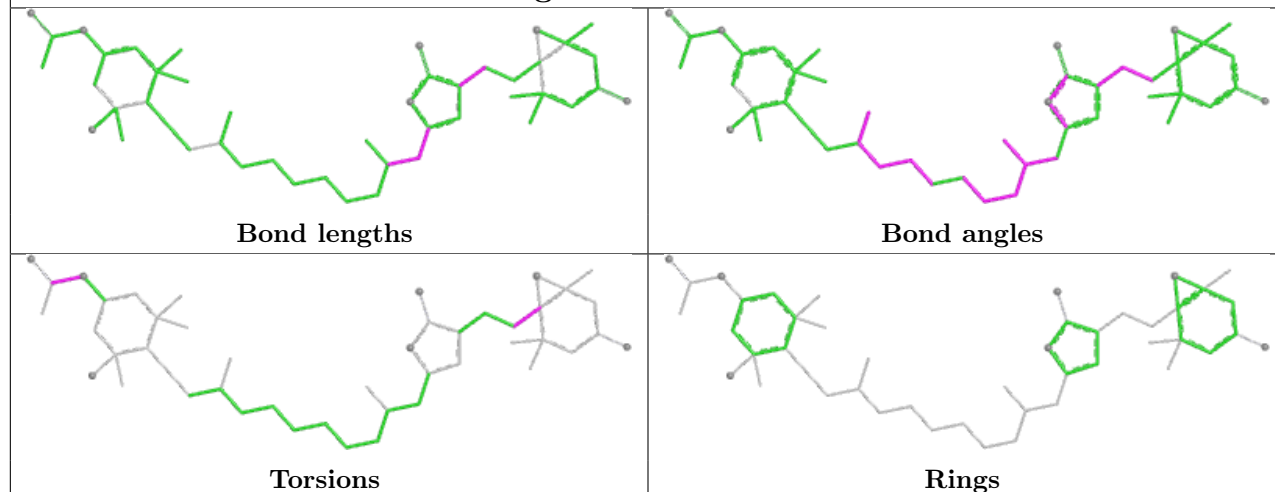
Ligand CLA G 517



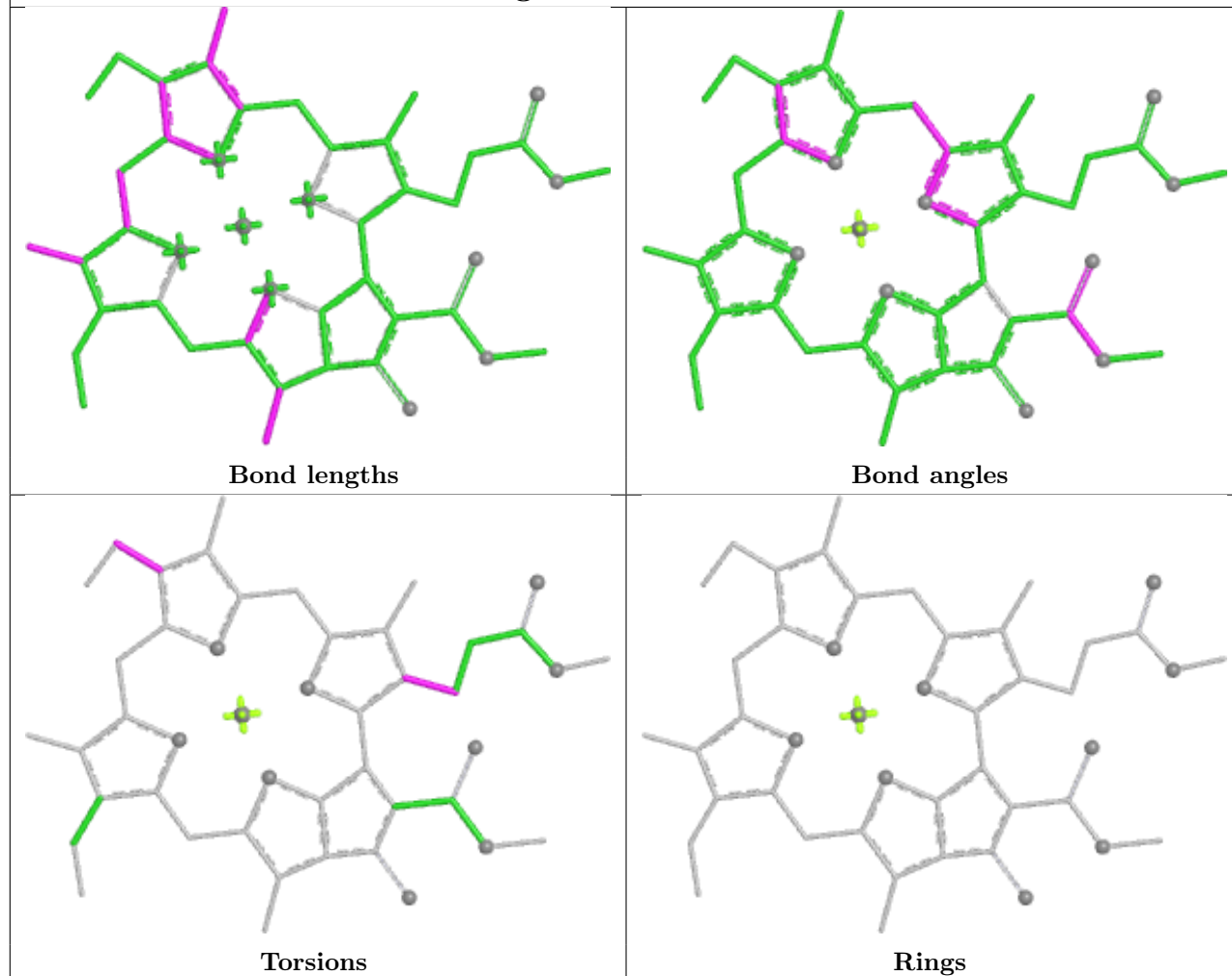
Ligand LMG B 318

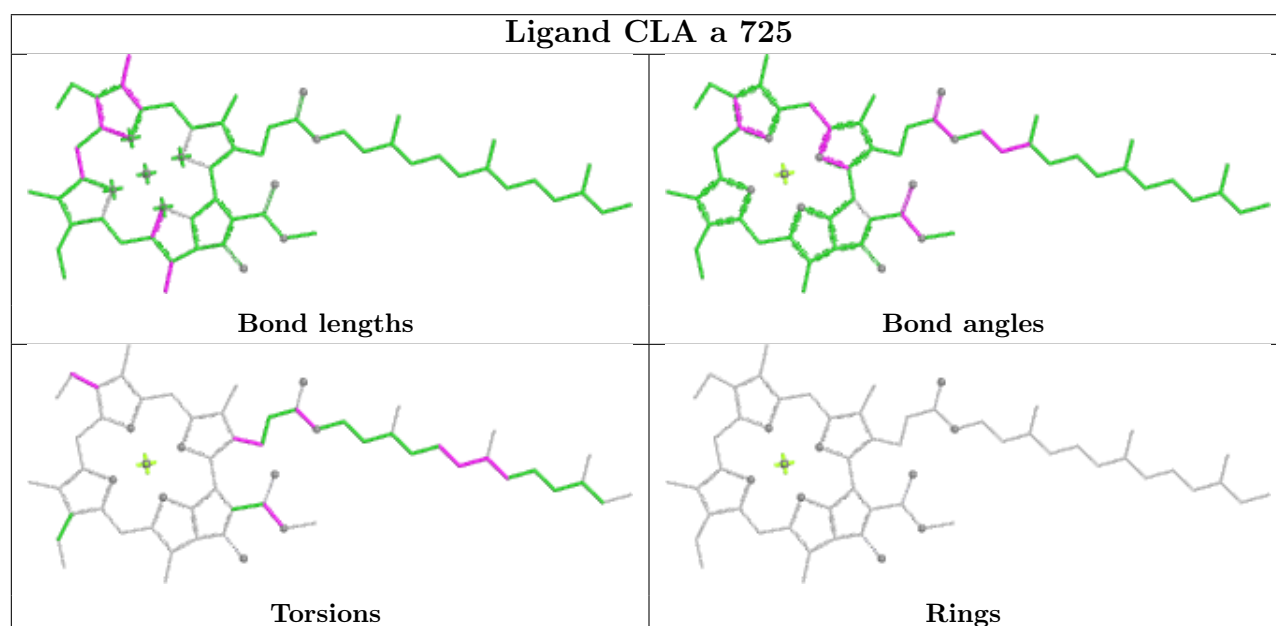
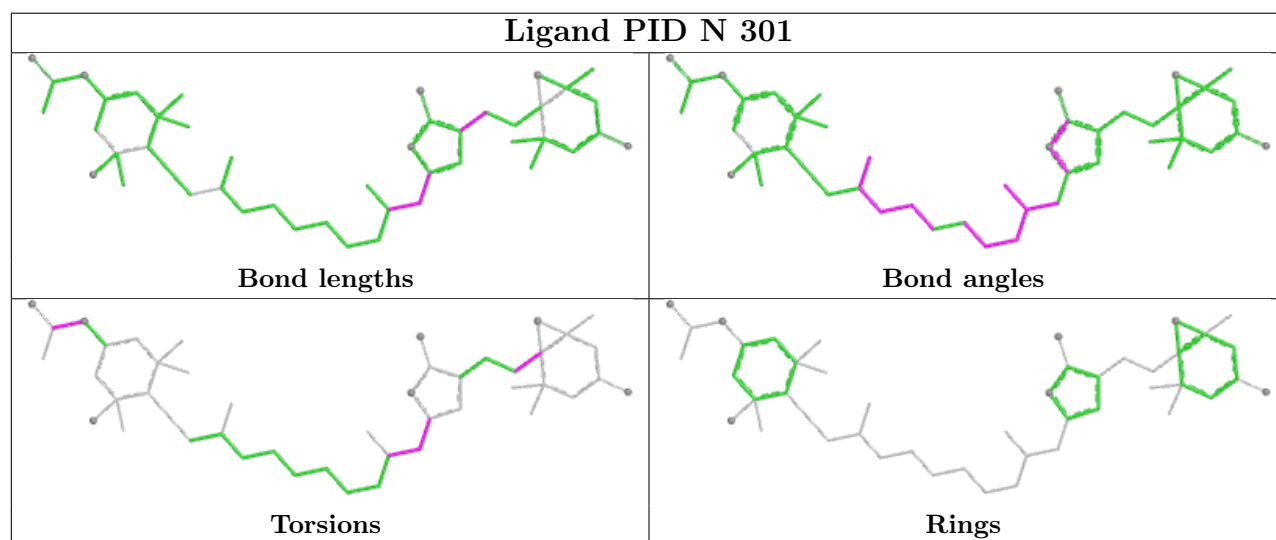
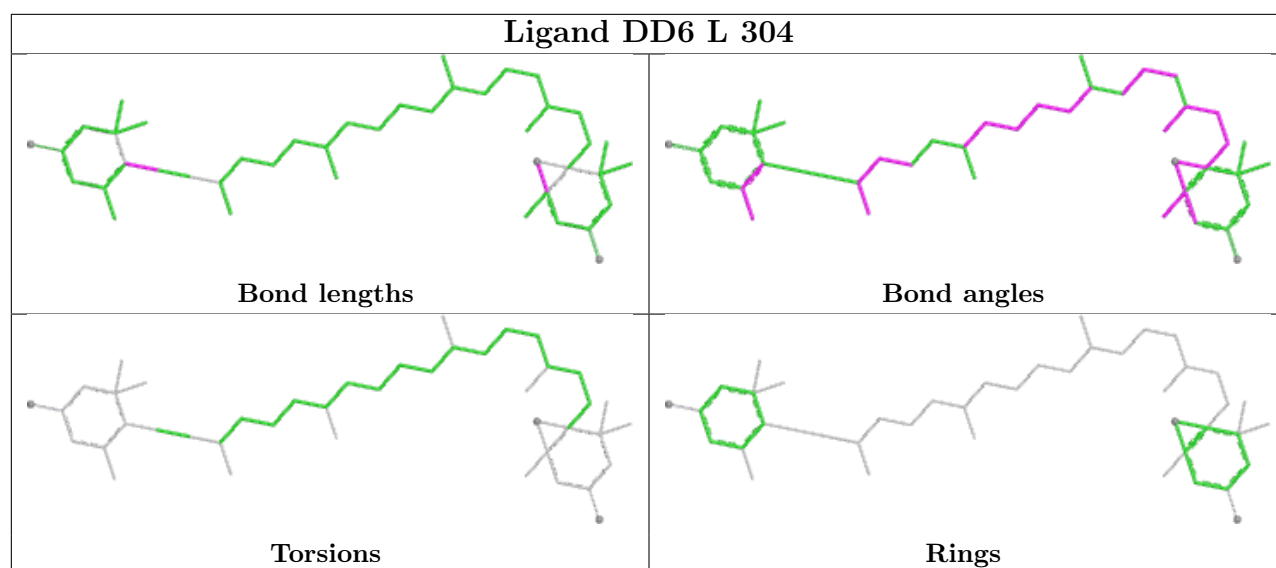


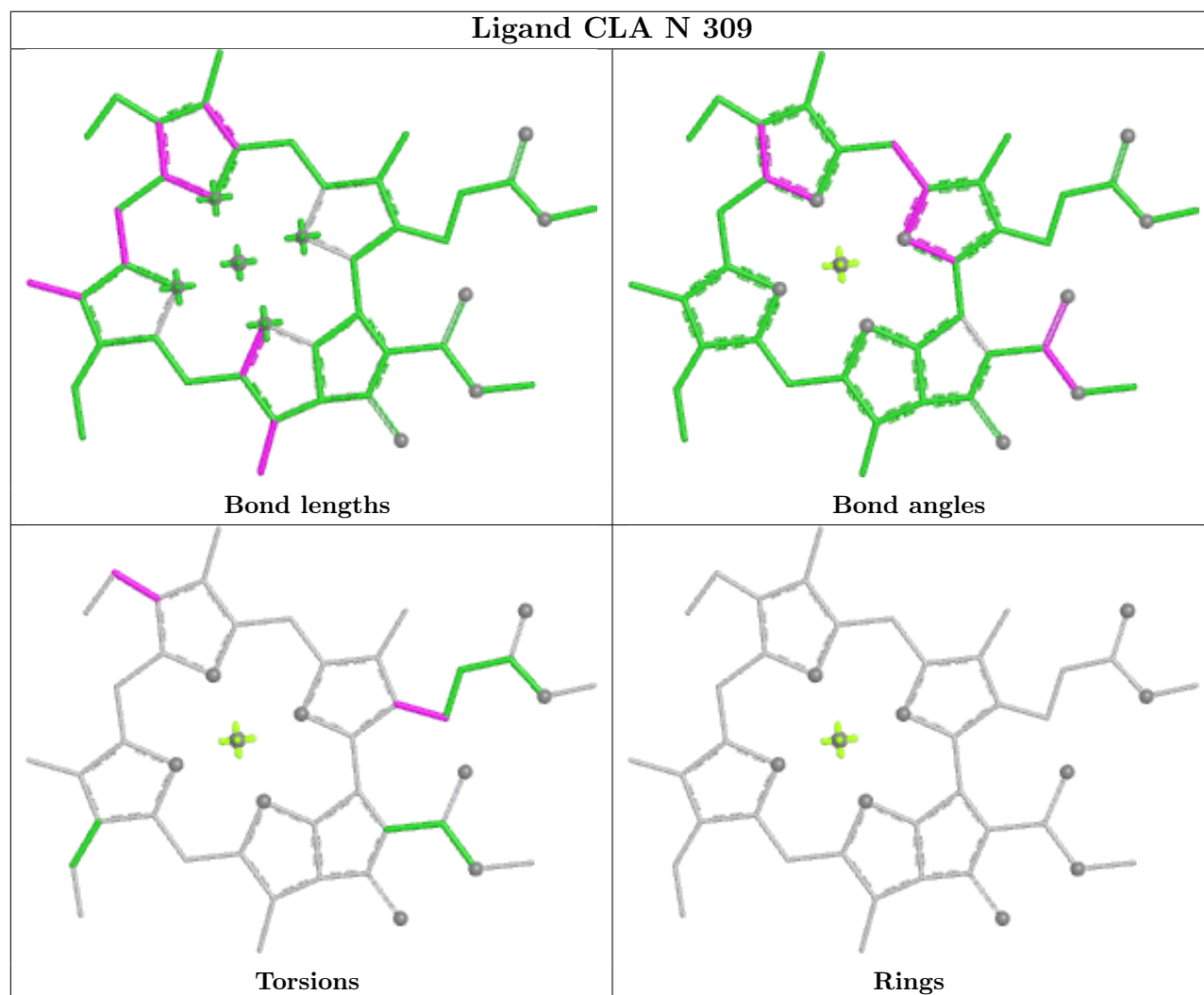
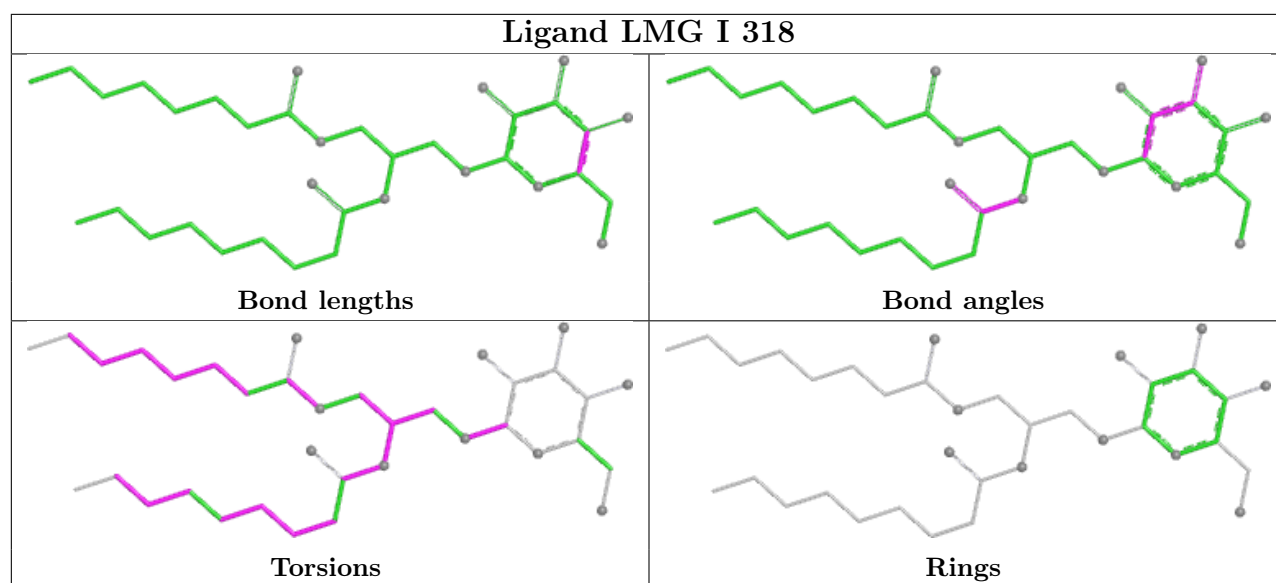
Ligand PID G 506



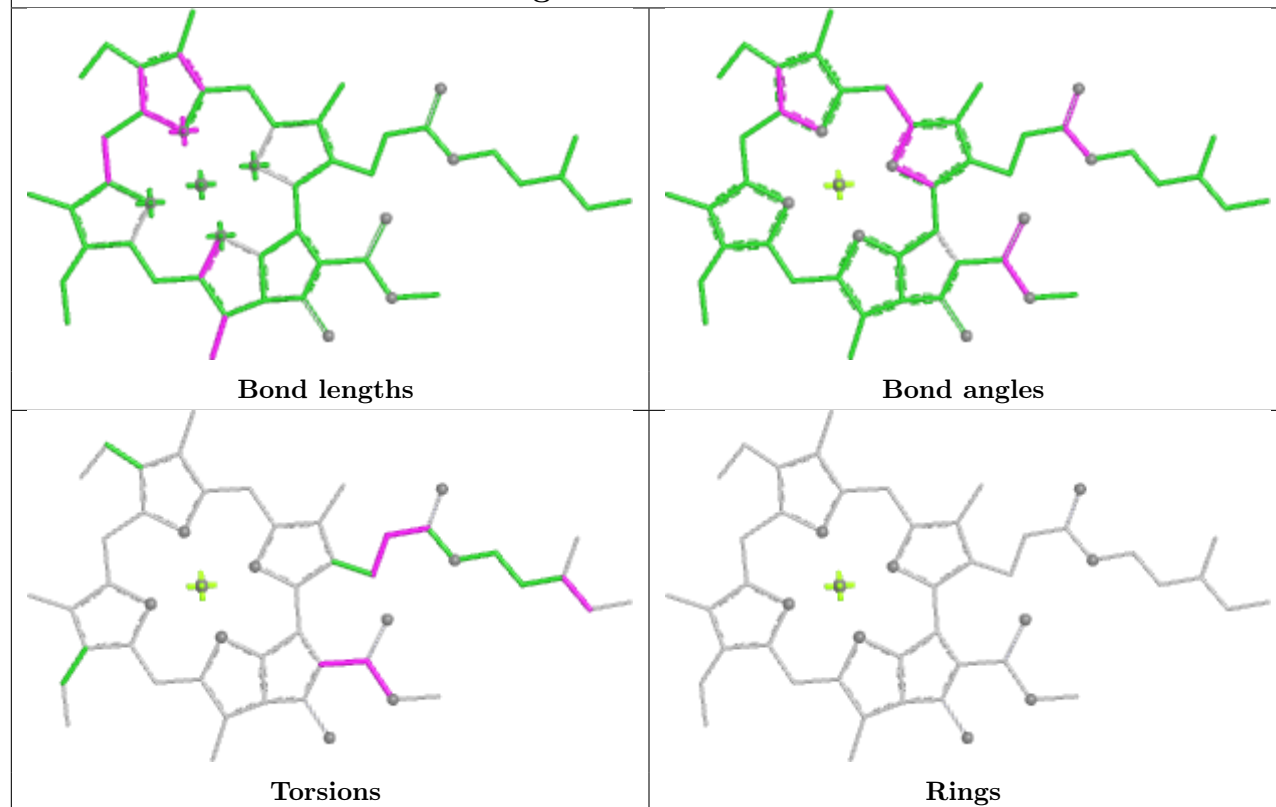
Ligand CLA F 308



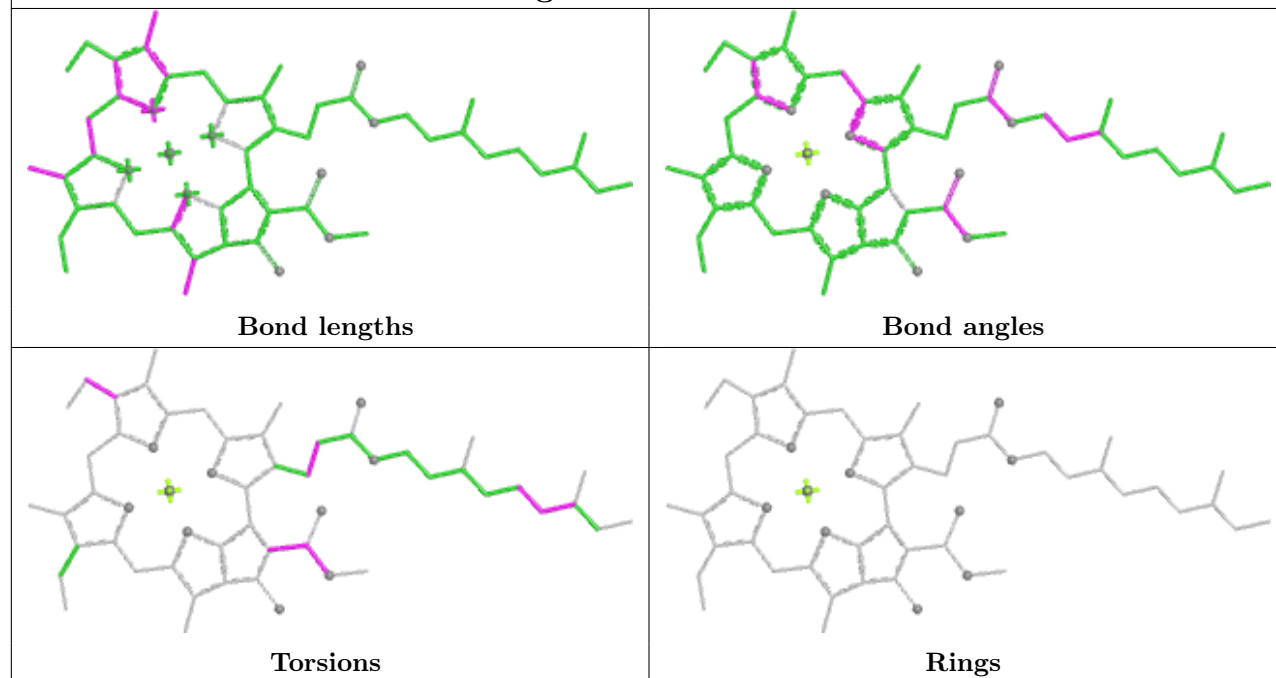




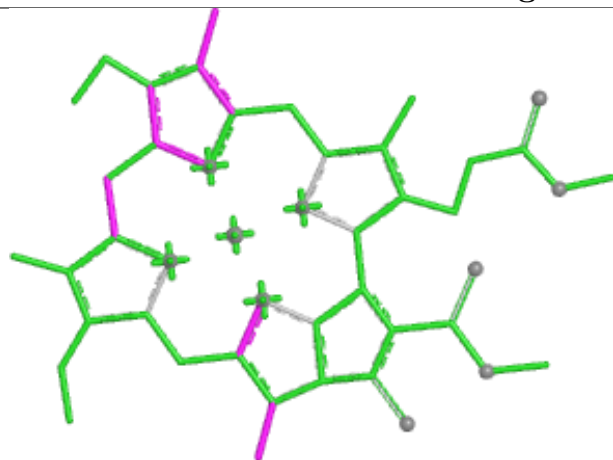
Ligand CLA P 212



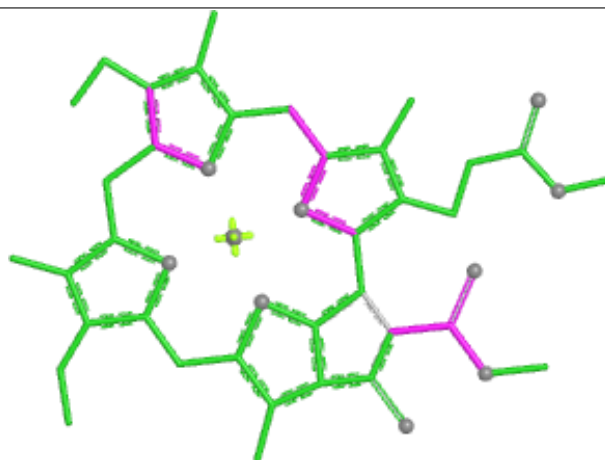
Ligand CLA J 309



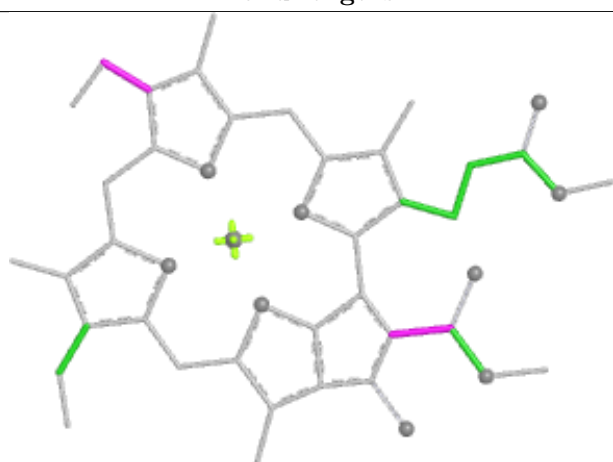
Ligand CLA a 738



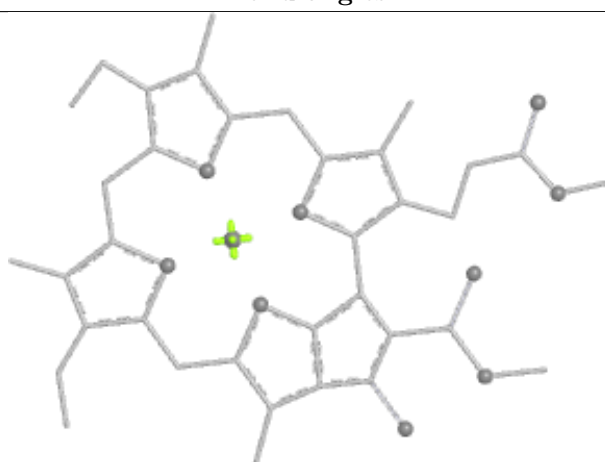
Bond lengths



Bond angles

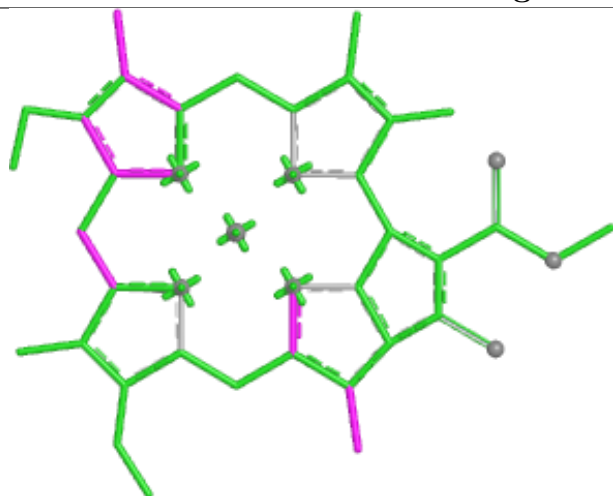


Torsions

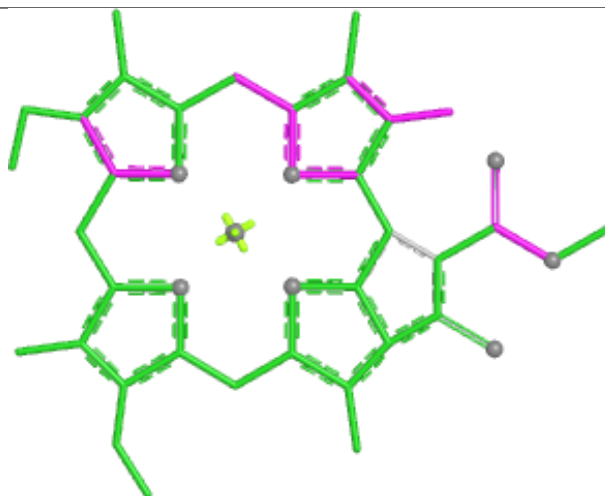


Rings

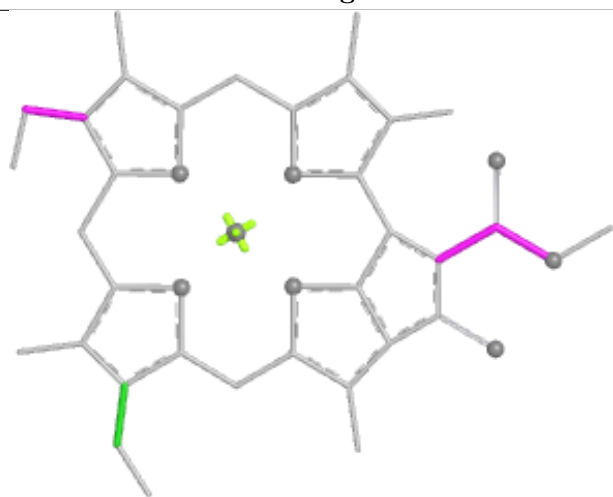
Ligand CLA H 311



Bond lengths



Bond angles

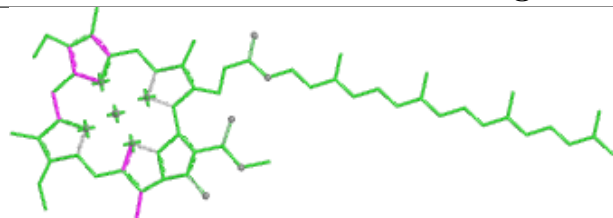


Torsions

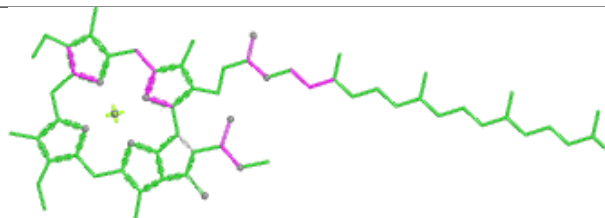


Rings

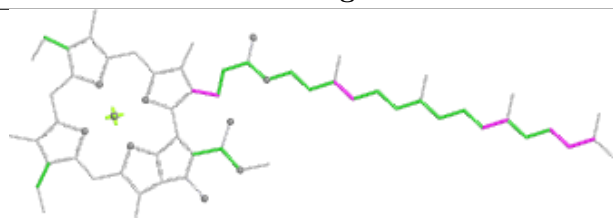
Ligand CLA H 305



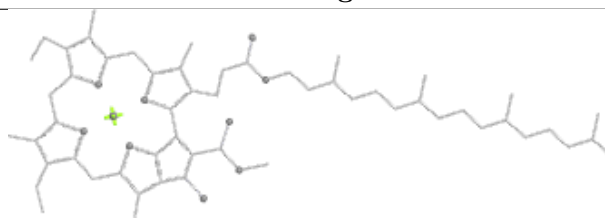
Bond lengths



Bond angles

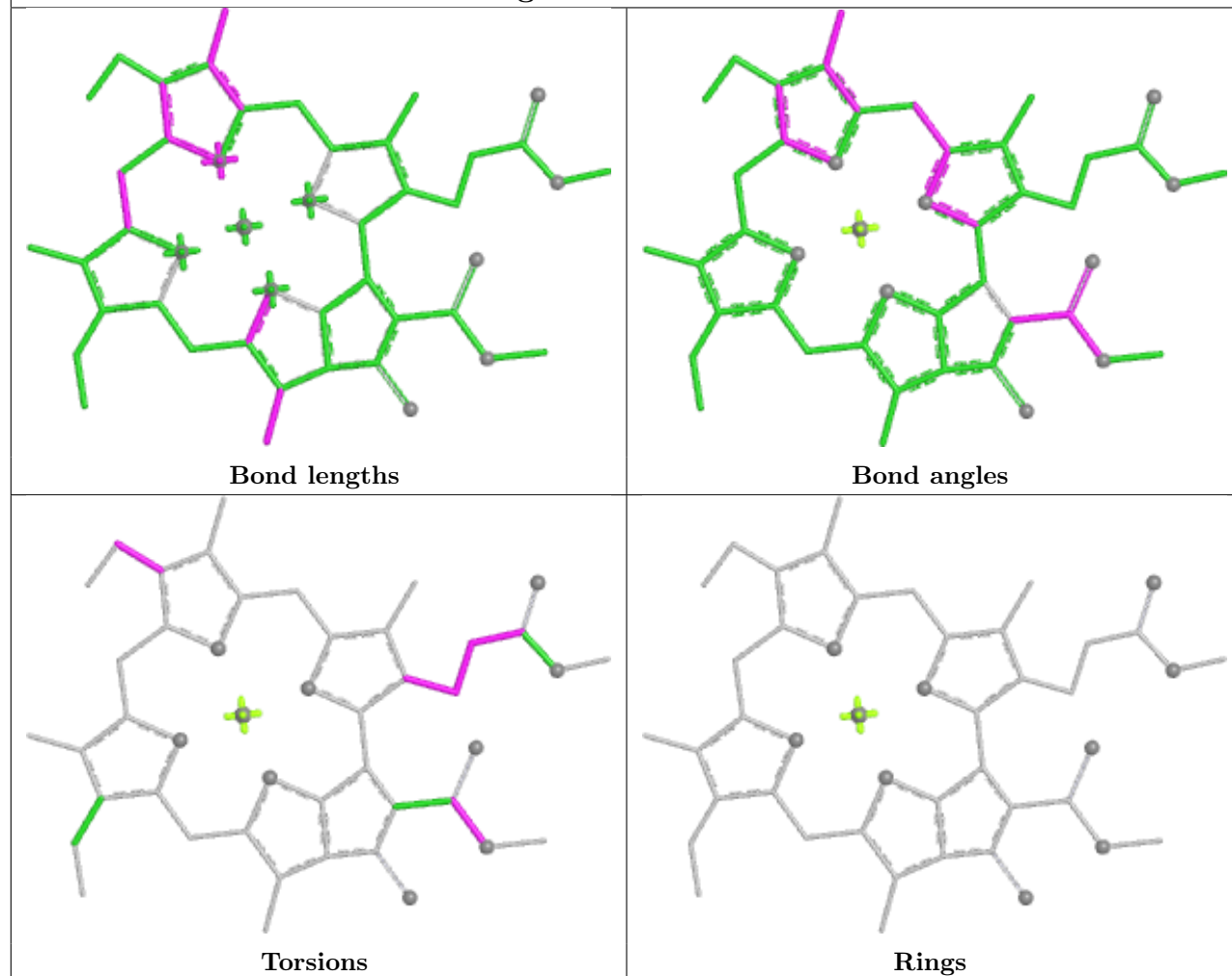


Torsions

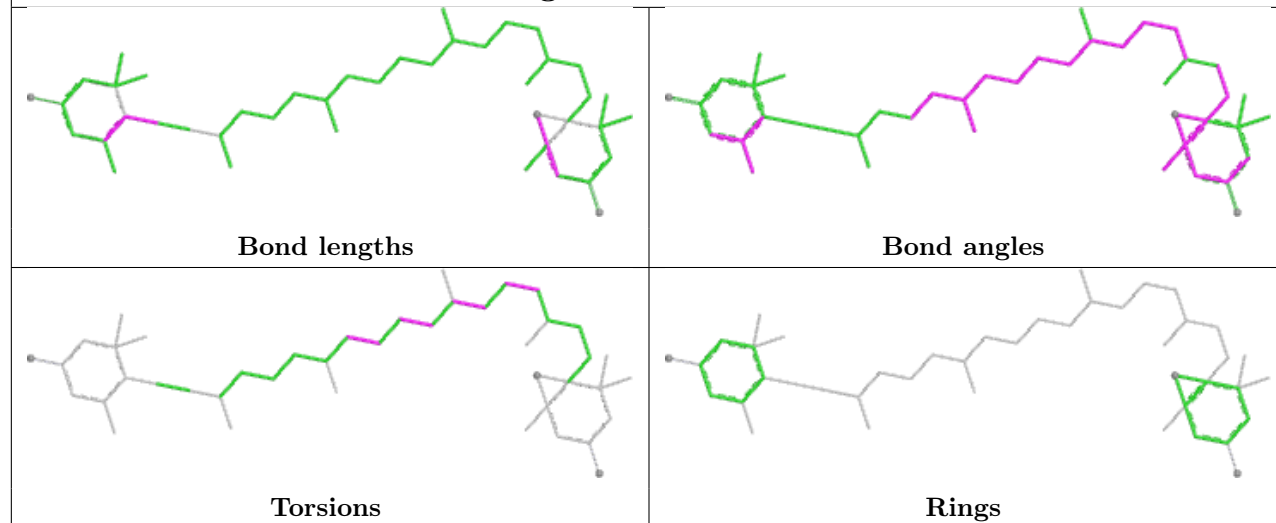


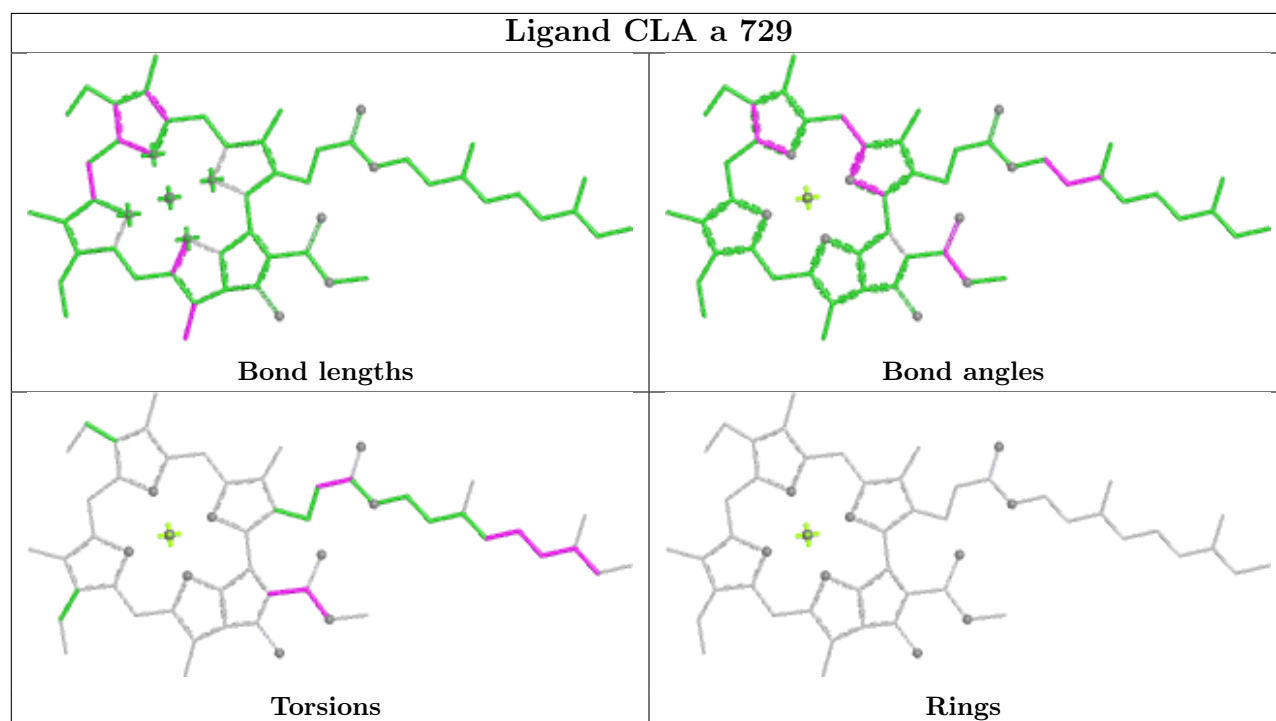
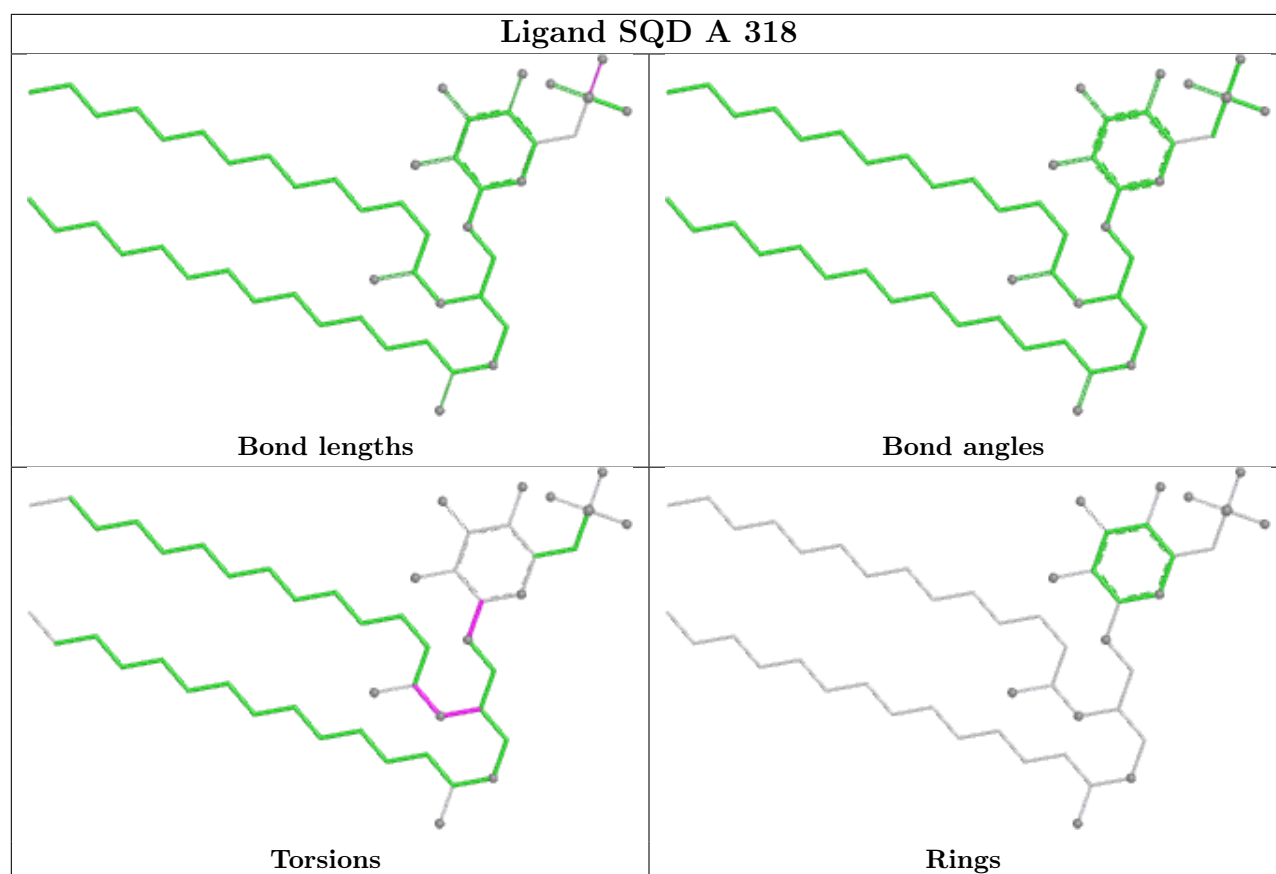
Rings

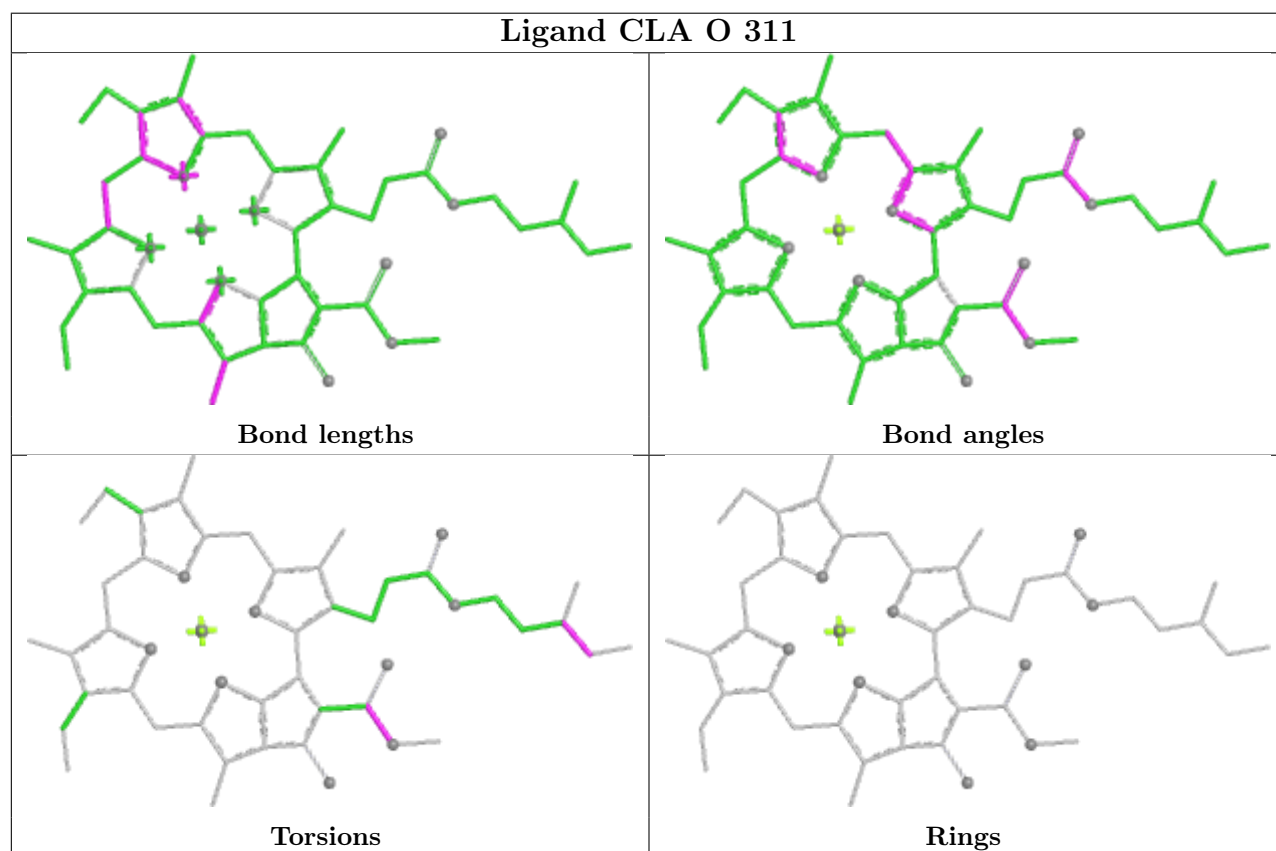
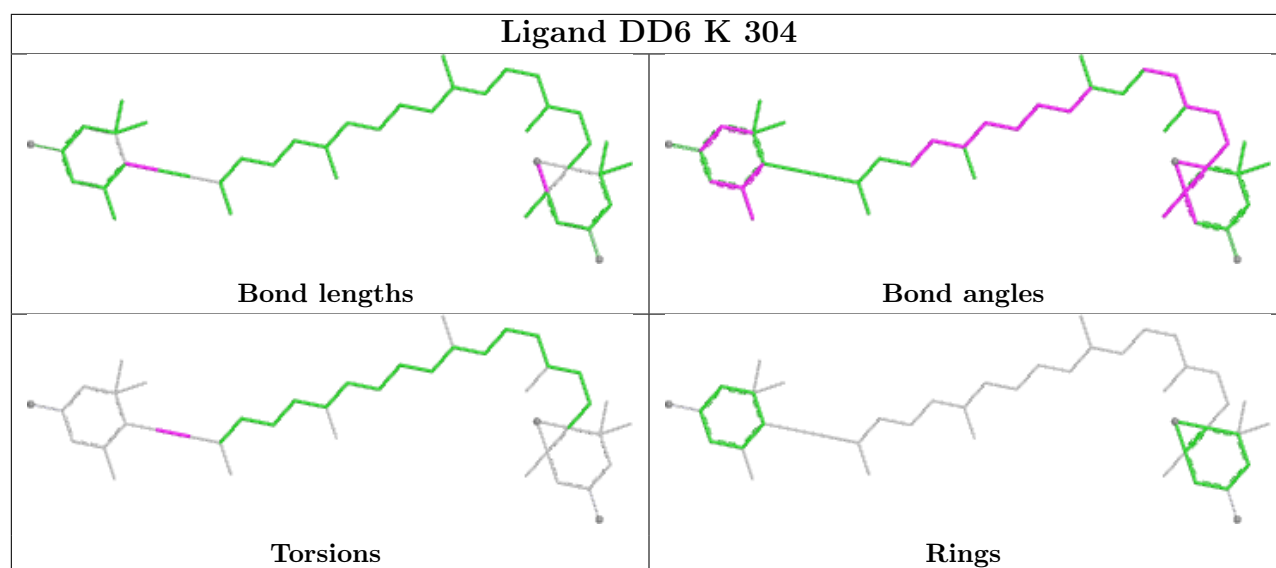
Ligand CLA J 308

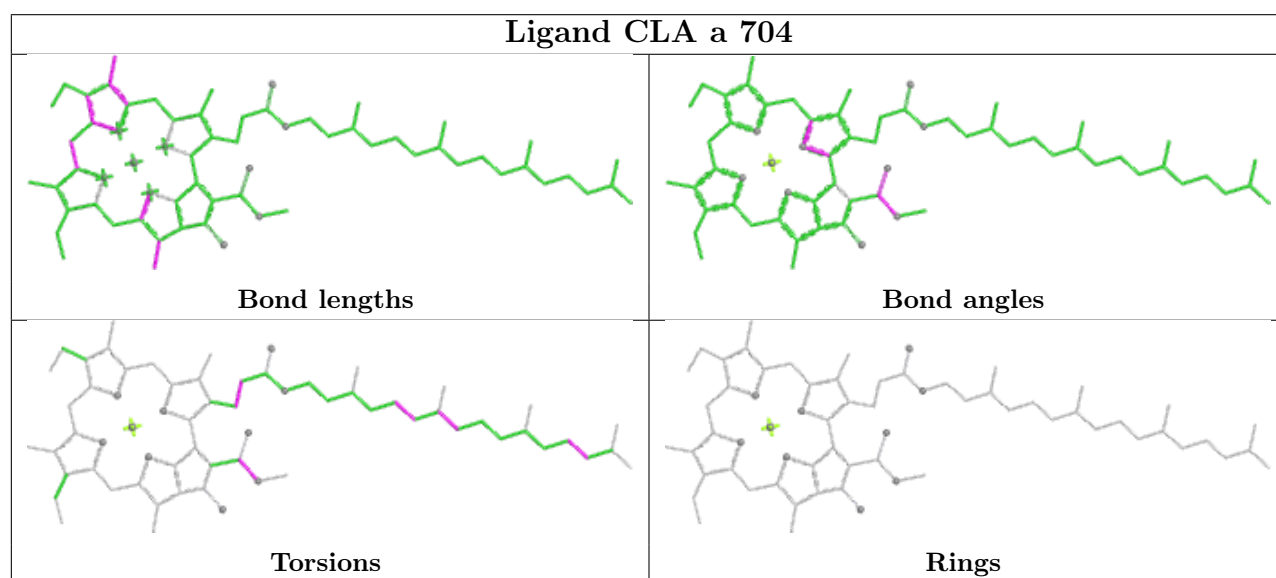
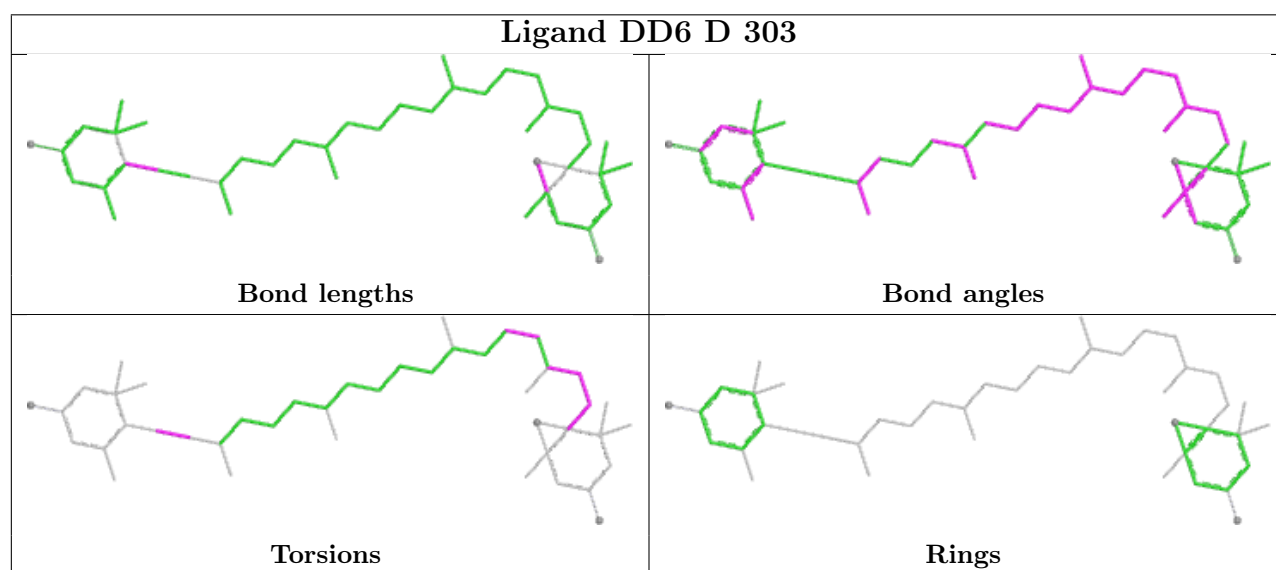
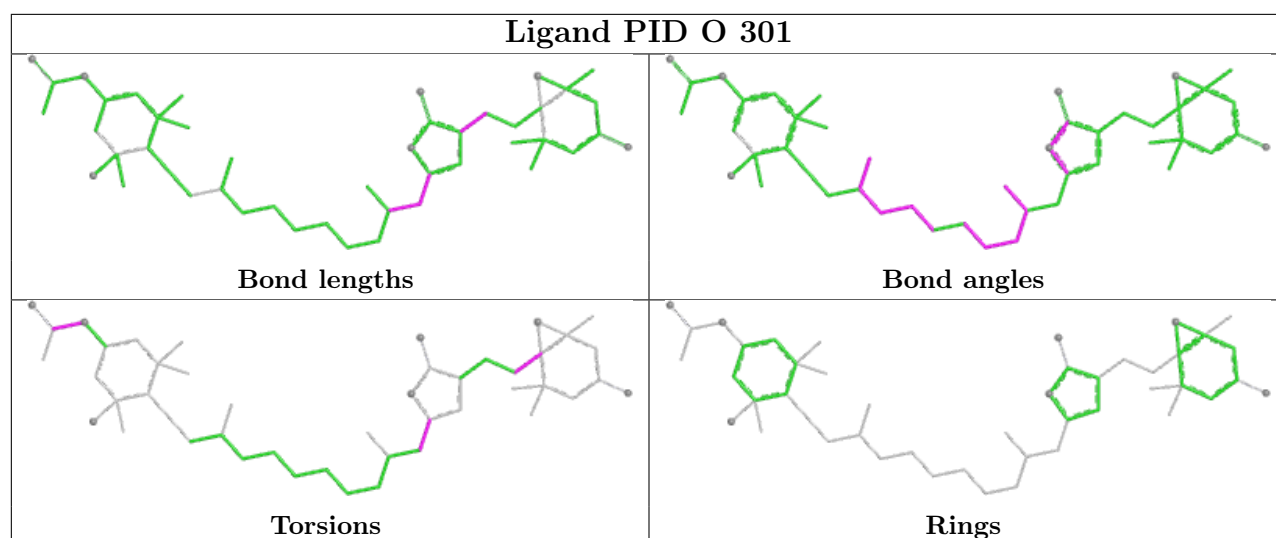


Ligand DD6 I 305

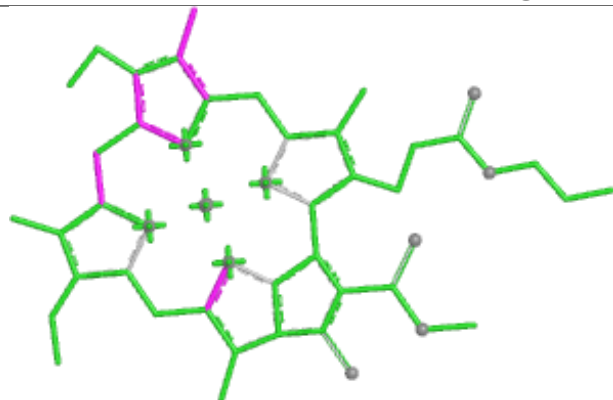




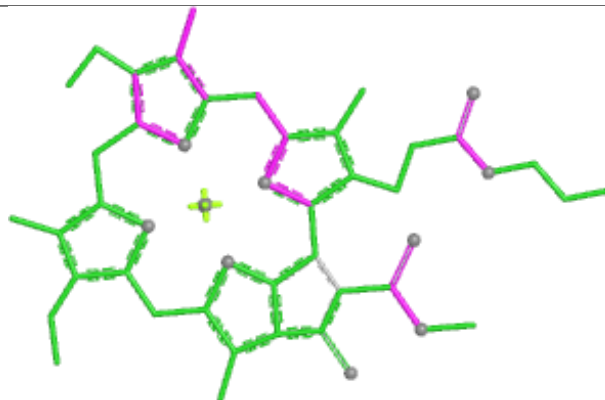




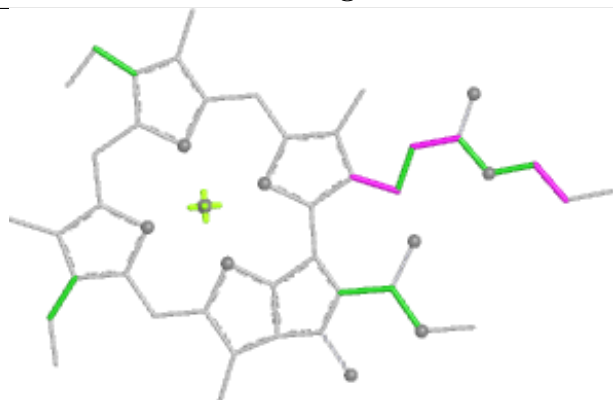
Ligand CLA b 706



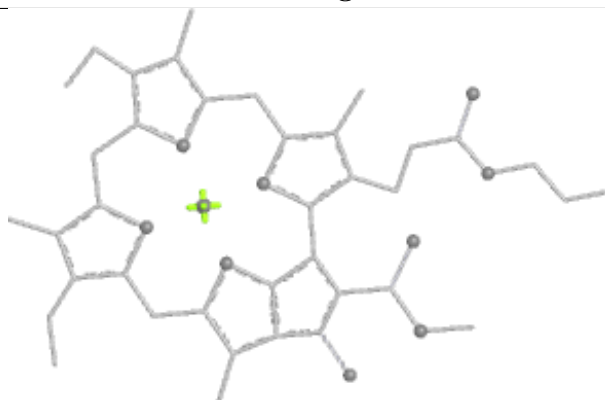
Bond lengths



Bond angles

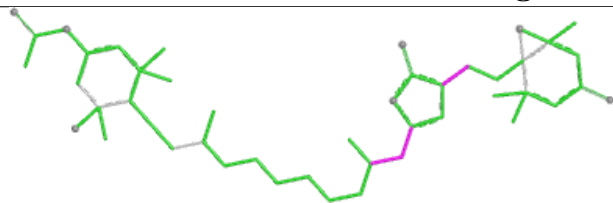


Torsions

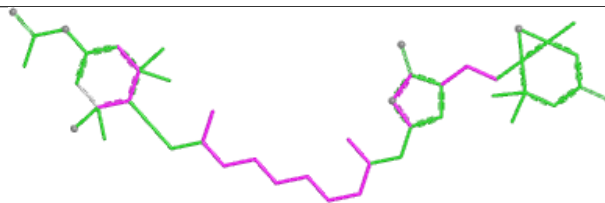


Rings

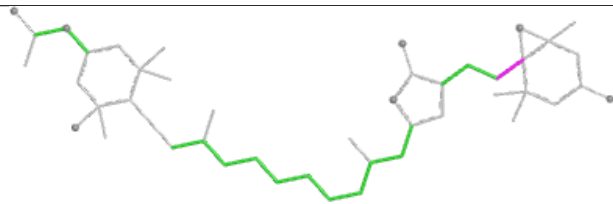
Ligand PID M 301



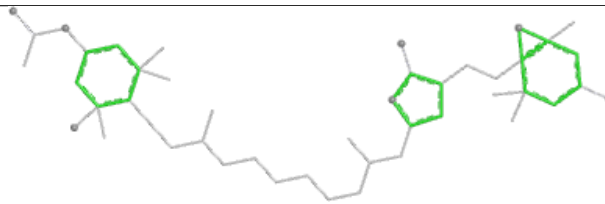
Bond lengths



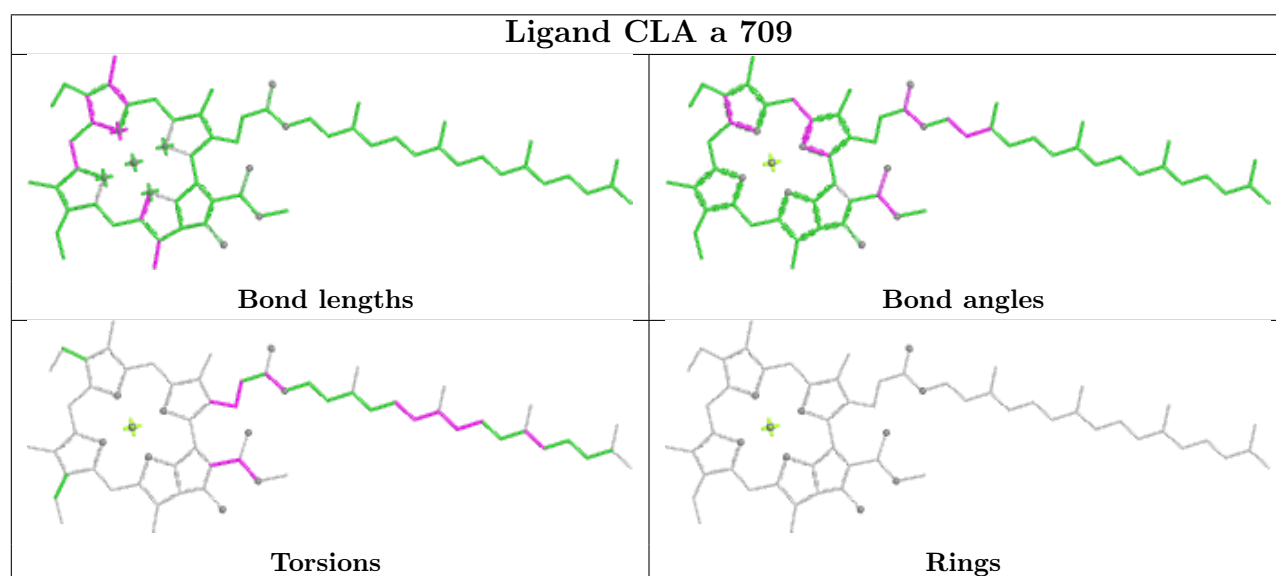
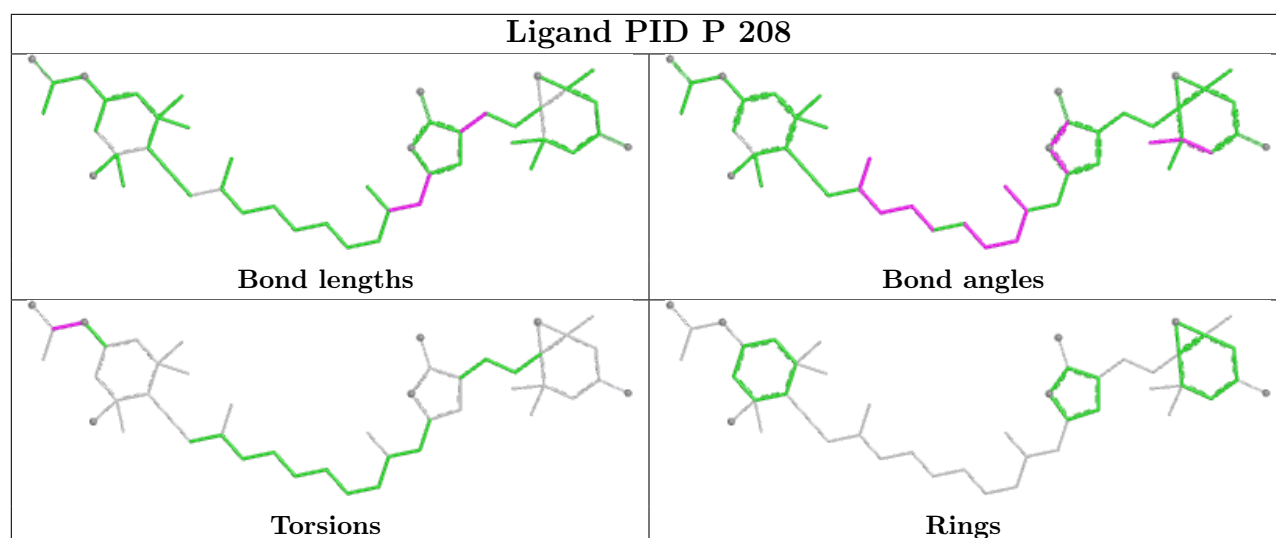
Bond angles



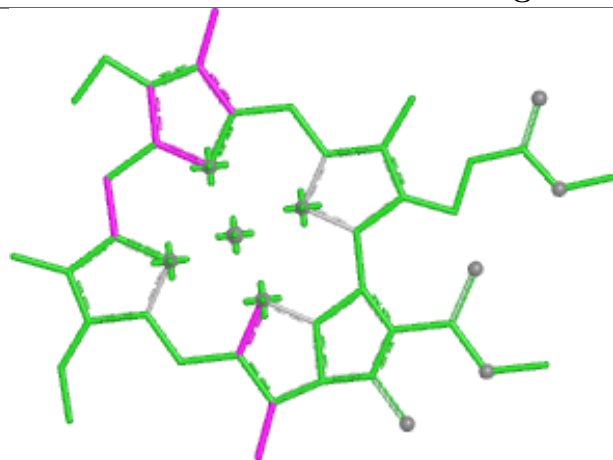
Torsions



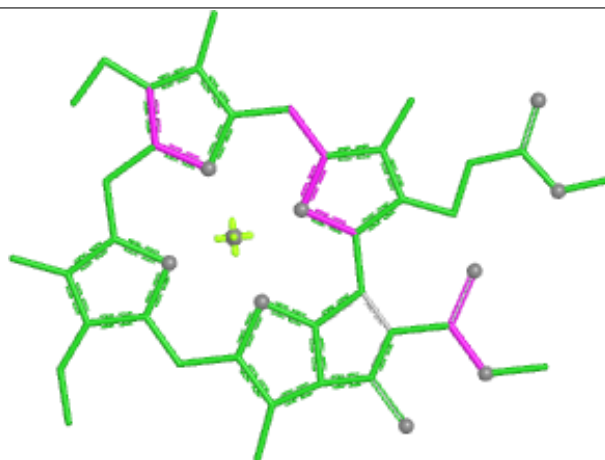
Rings



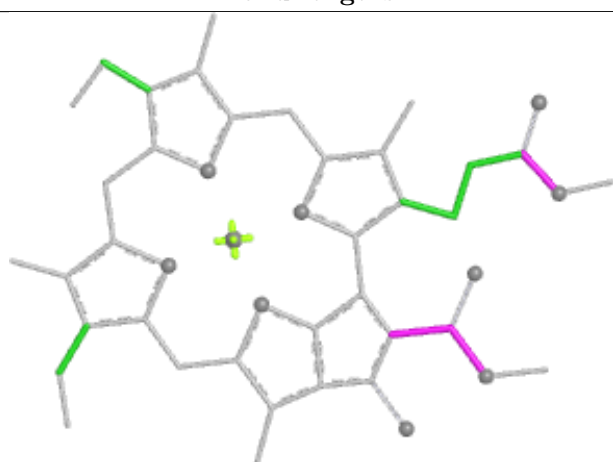
Ligand CLA A 320



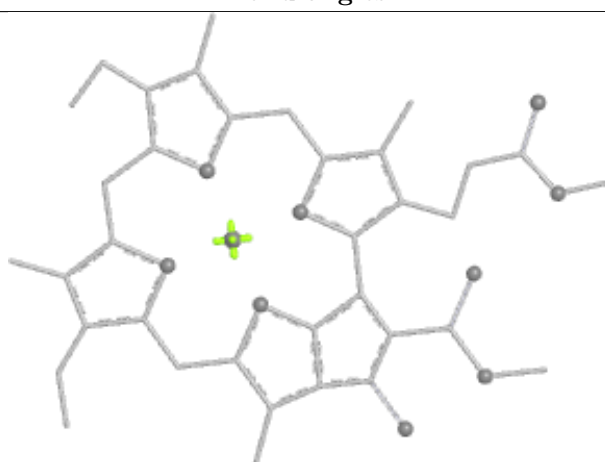
Bond lengths



Bond angles

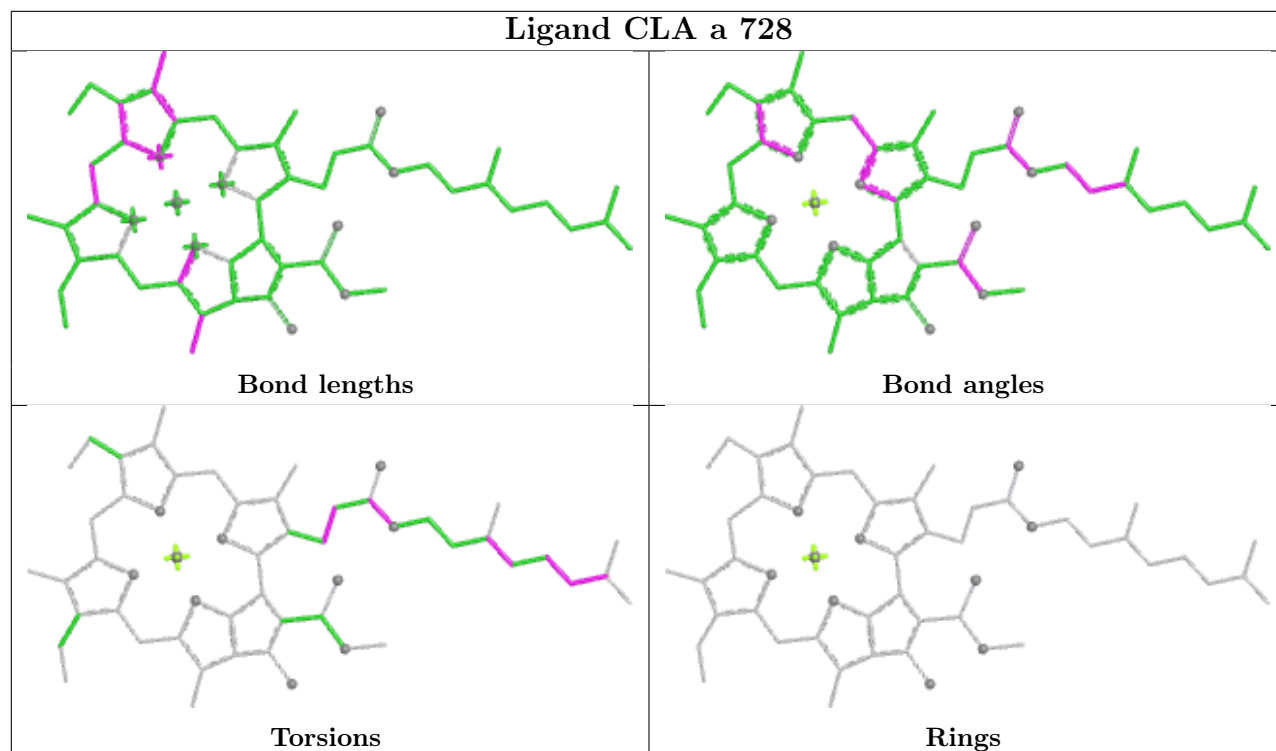


Torsions

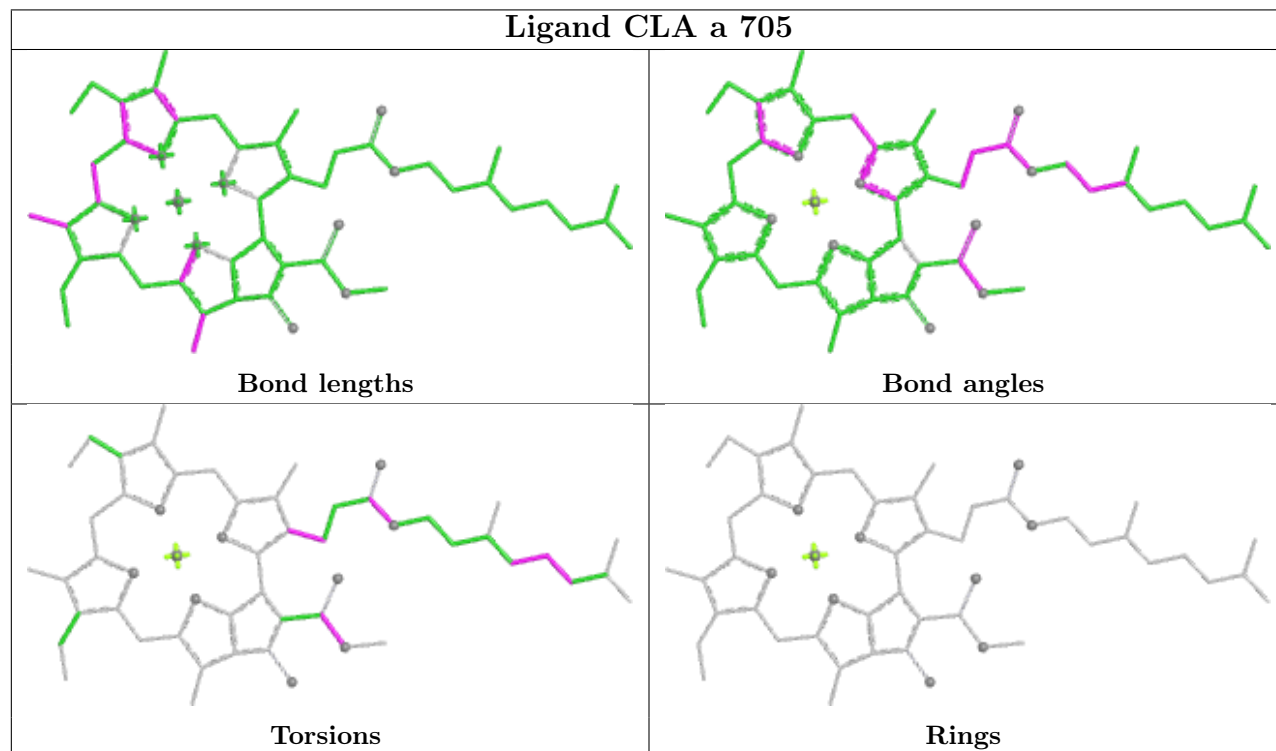


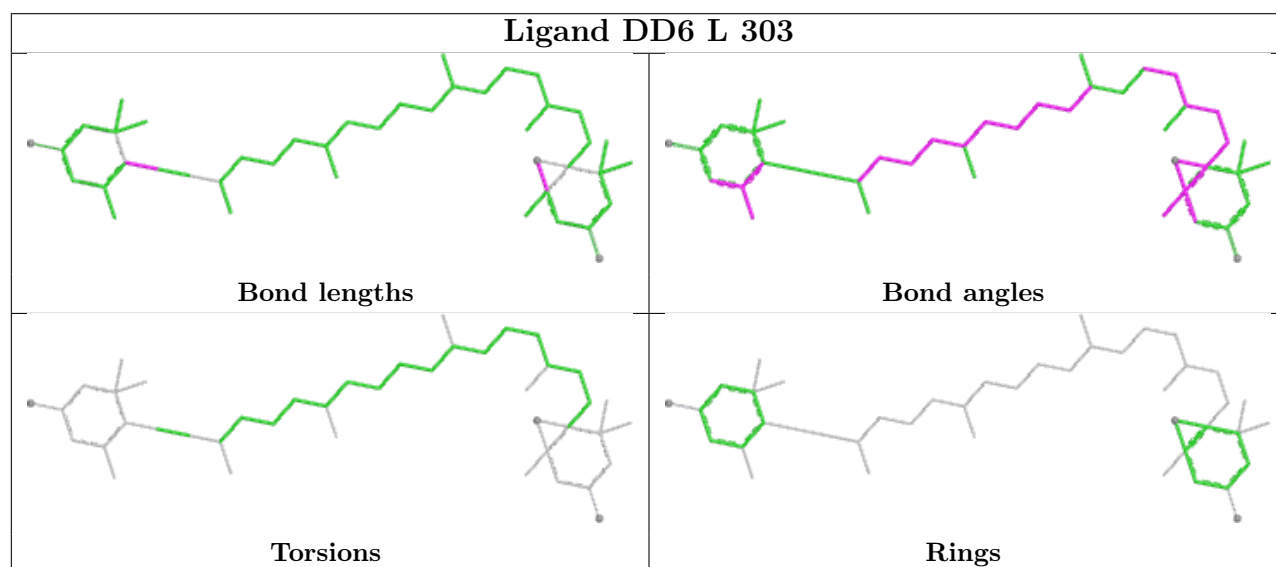
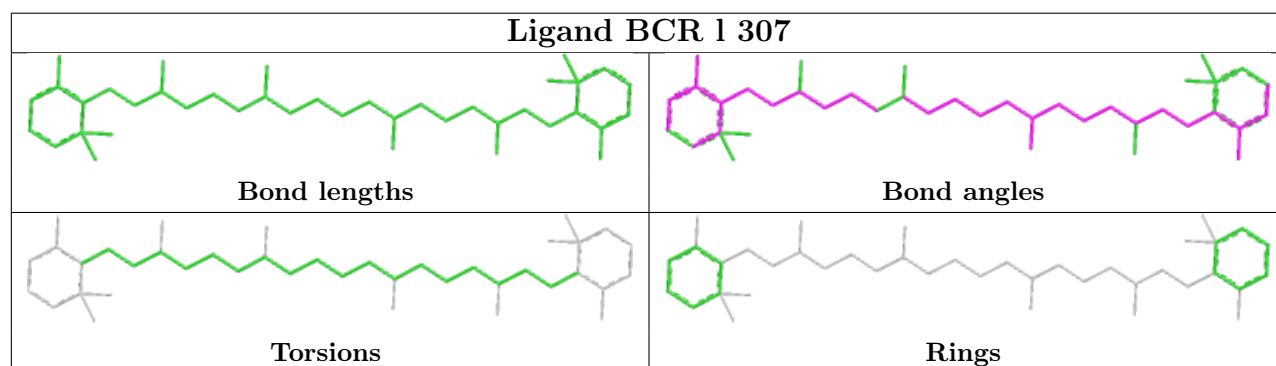
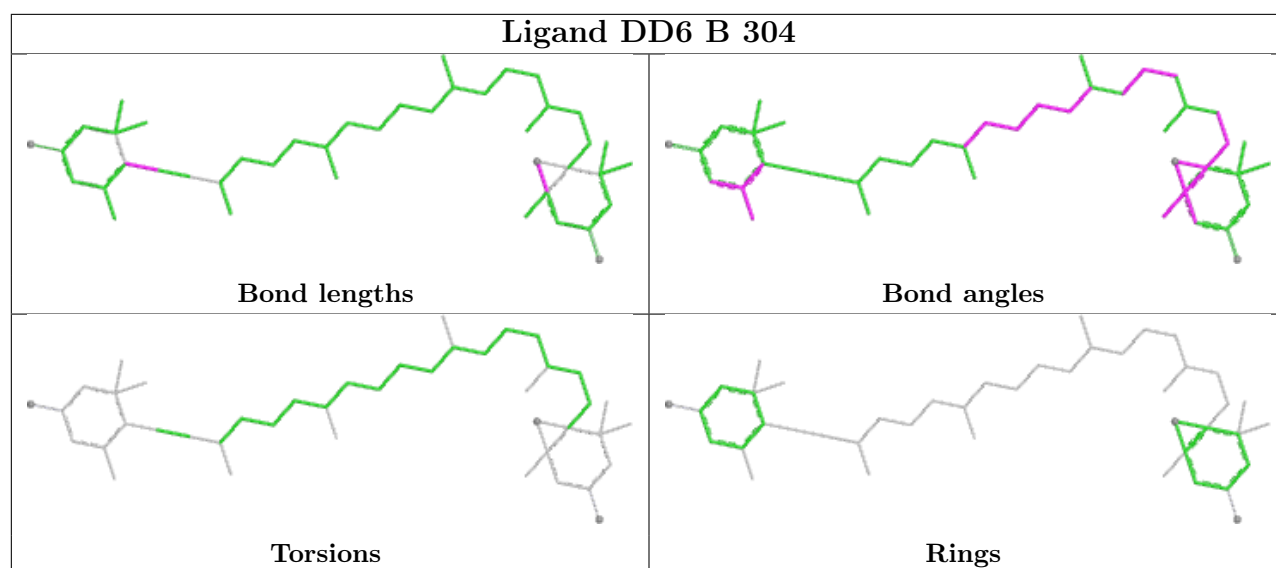
Rings

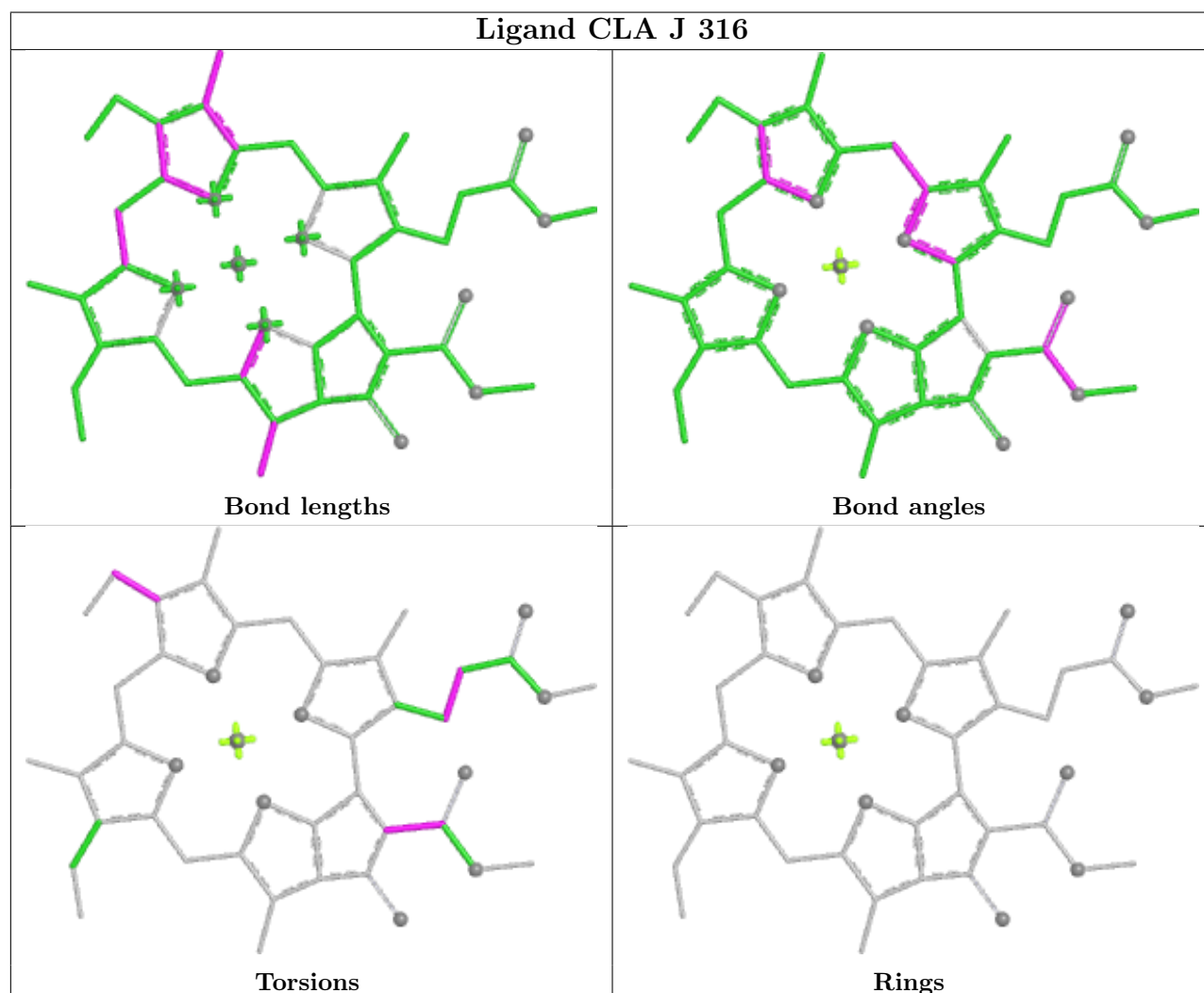
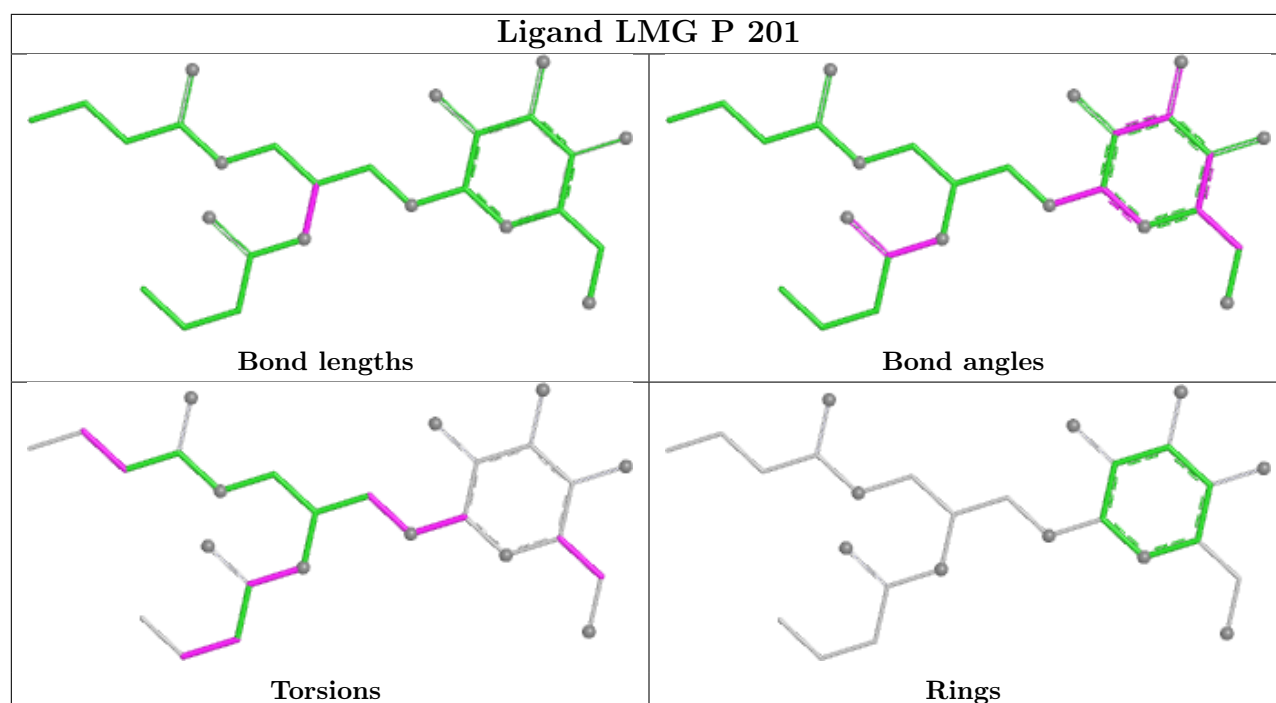
Ligand CLA a 728



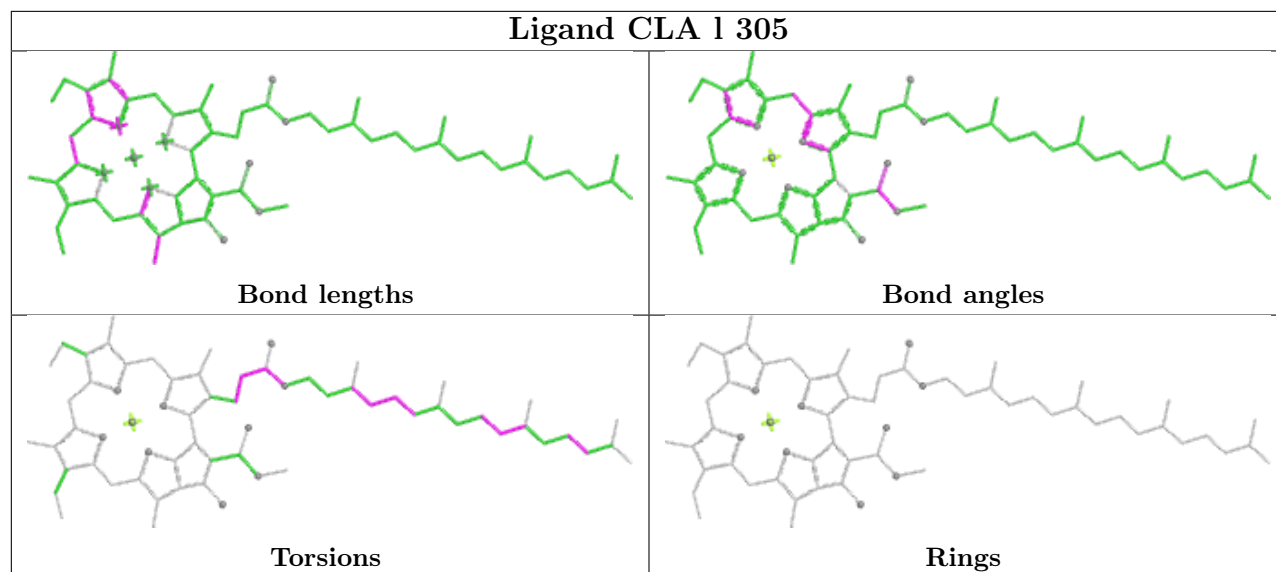
Ligand CLA a 705



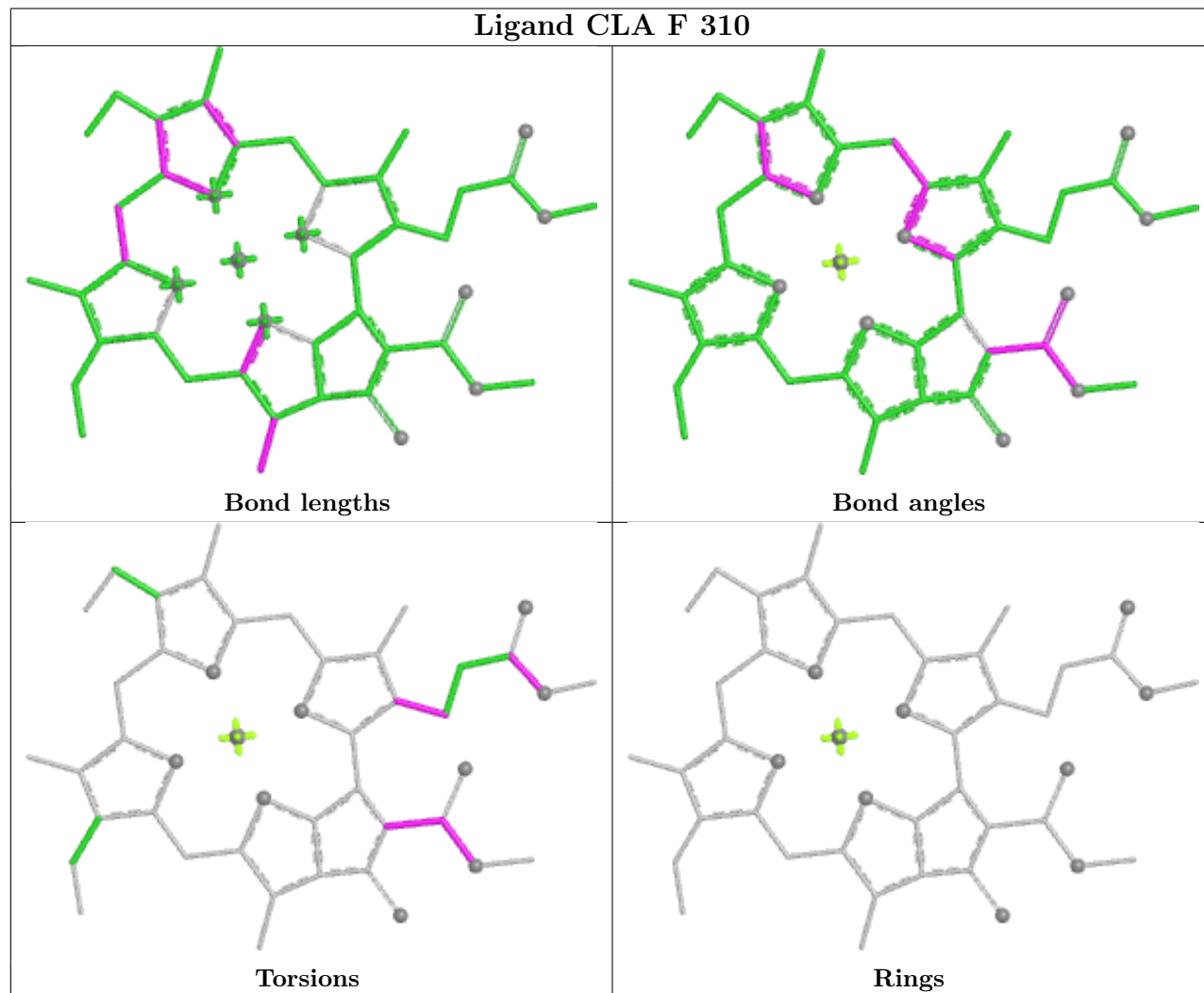




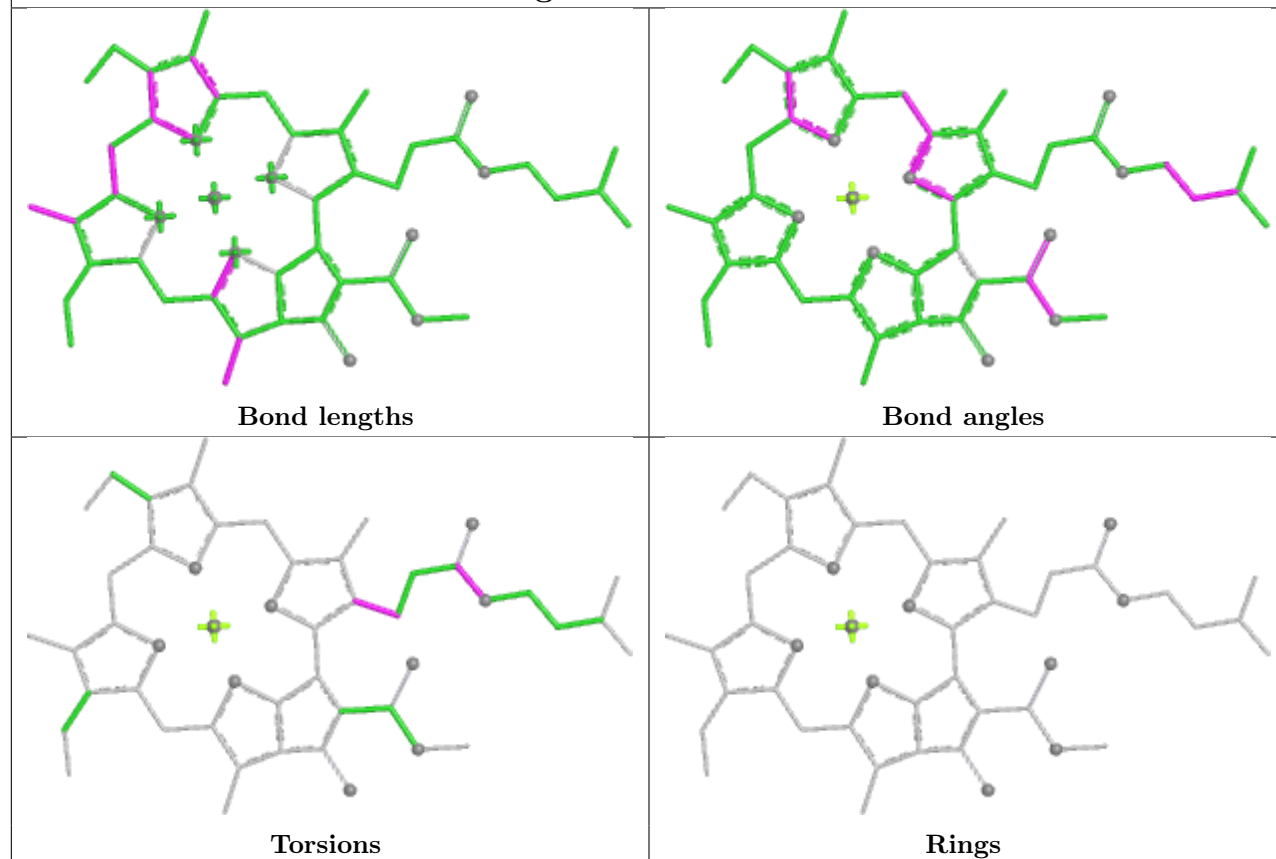
Ligand CLA I 305



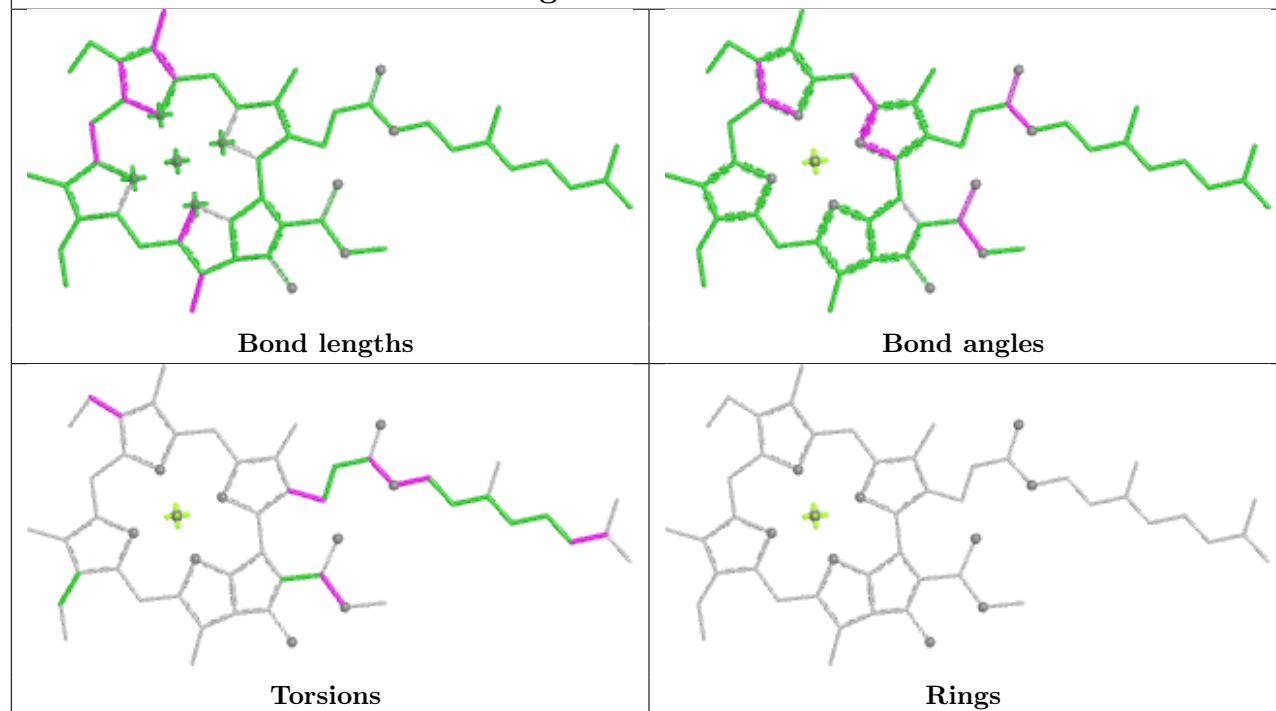
Ligand CLA F 310



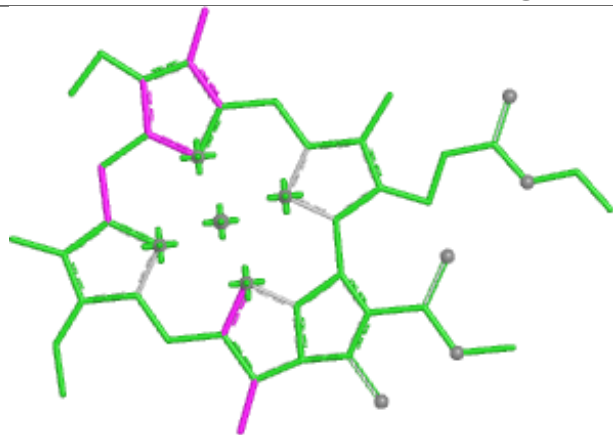
Ligand CLA b 716



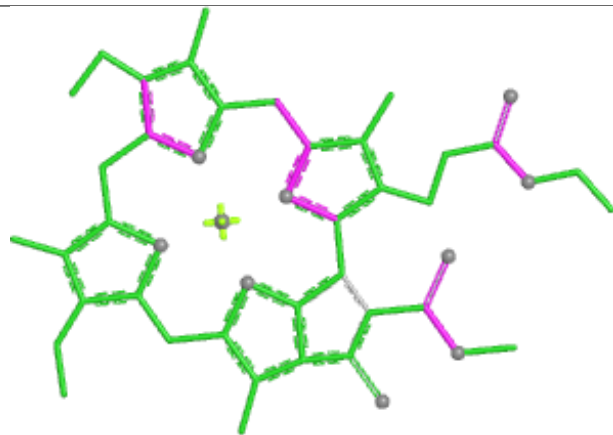
Ligand CLA f 301



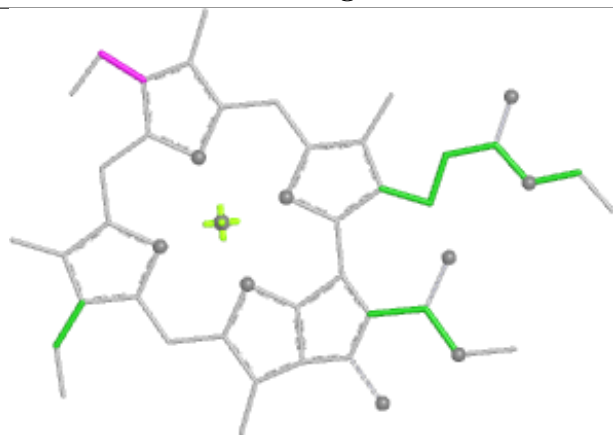
Ligand CLA b 726



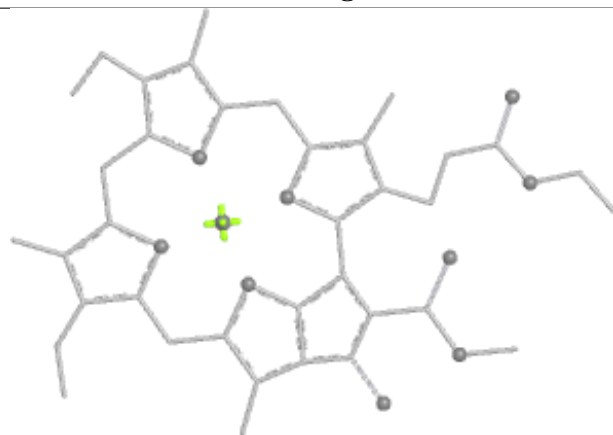
Bond lengths



Bond angles

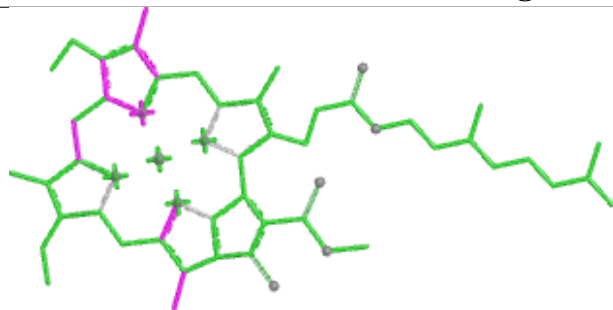


Torsions

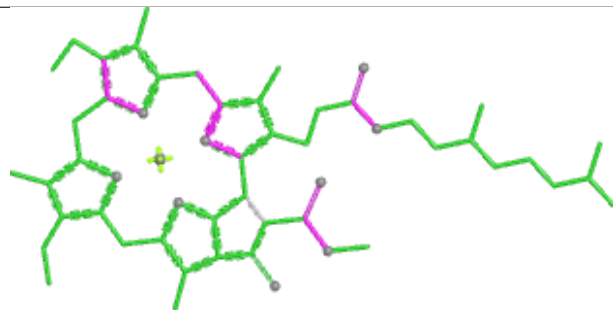


Rings

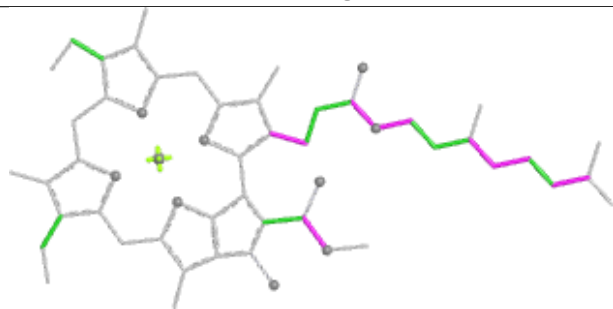
Ligand CLA L 313



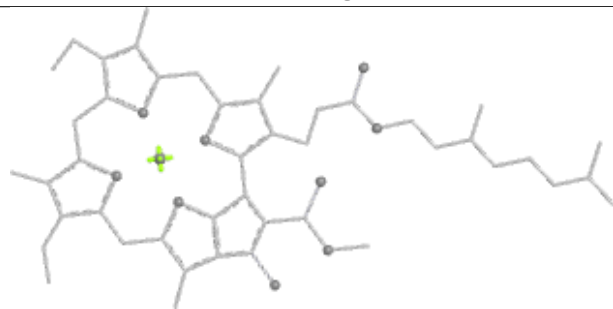
Bond lengths



Bond angles

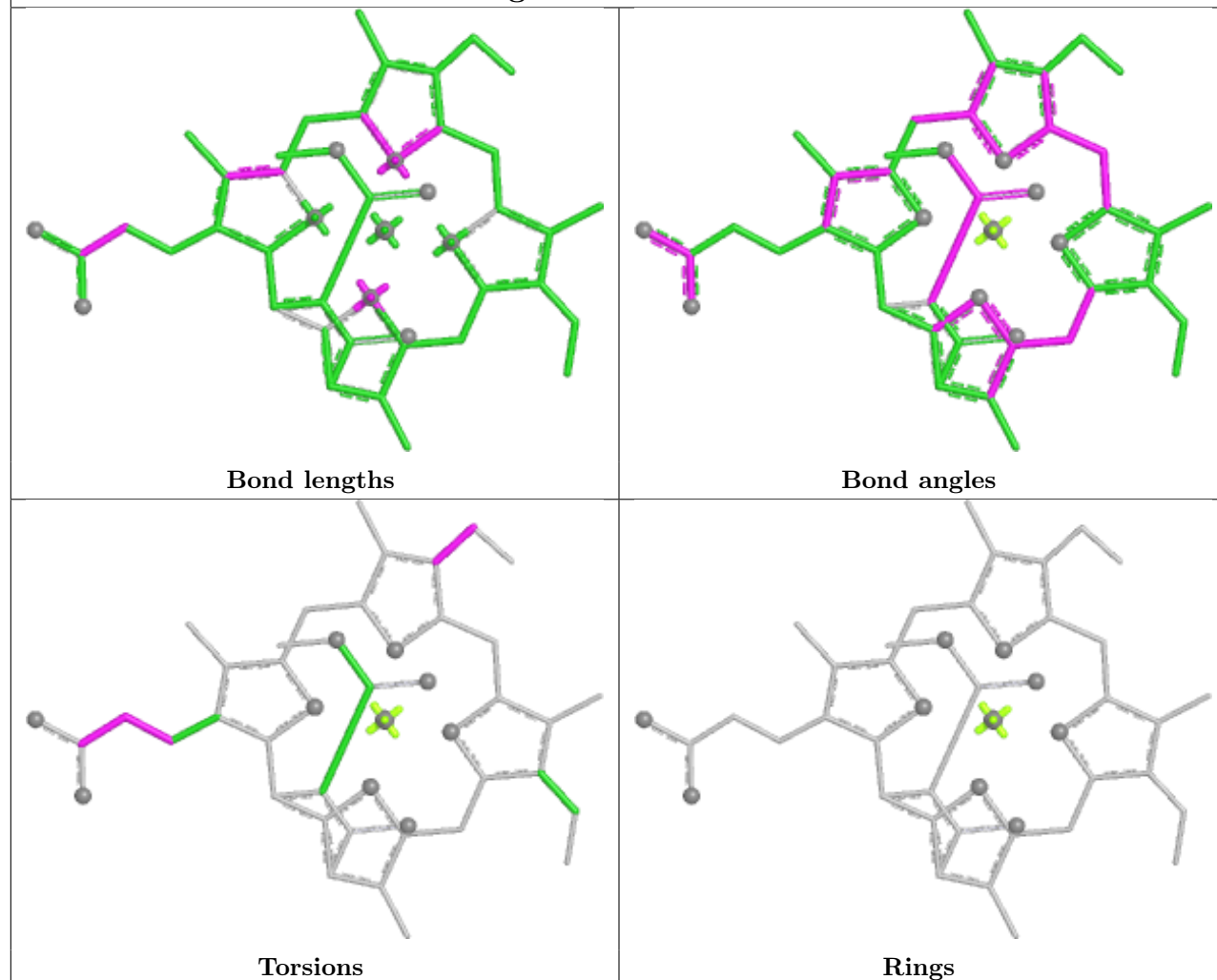


Torsions

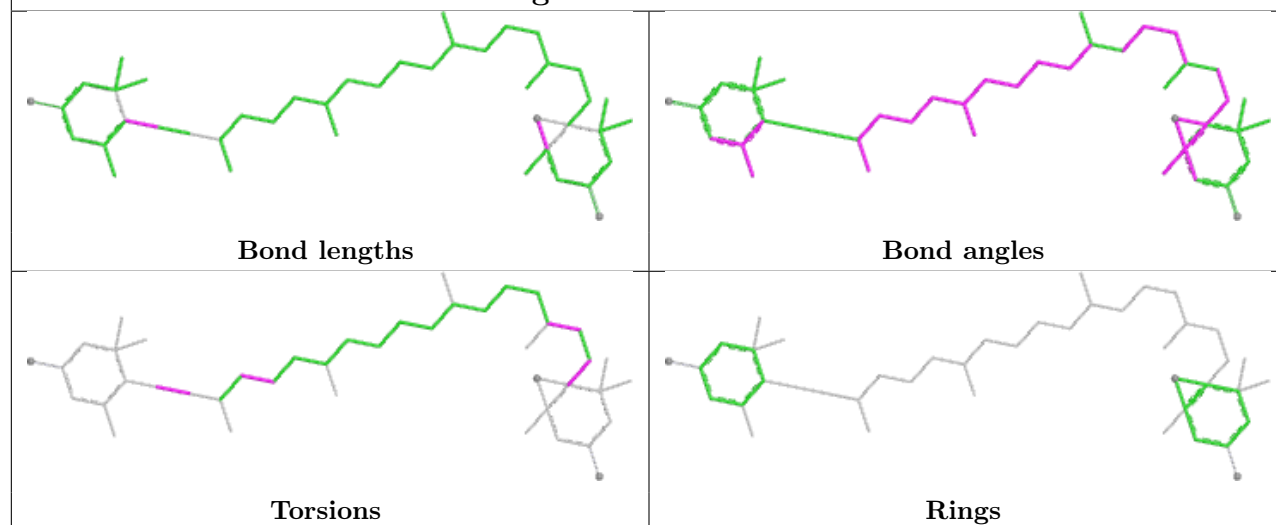


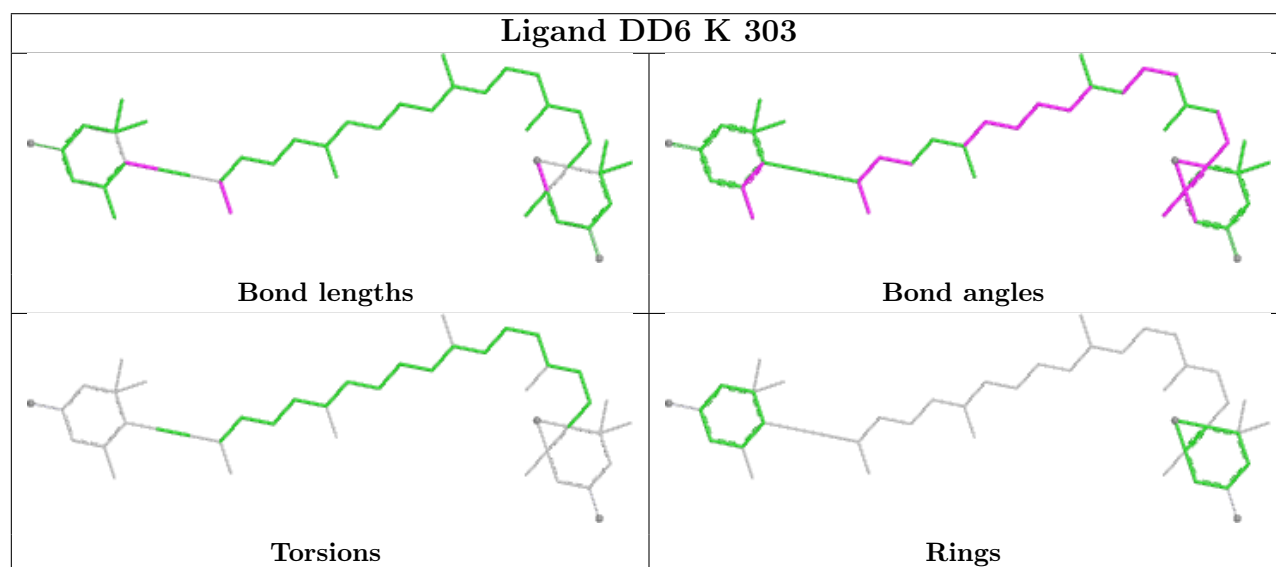
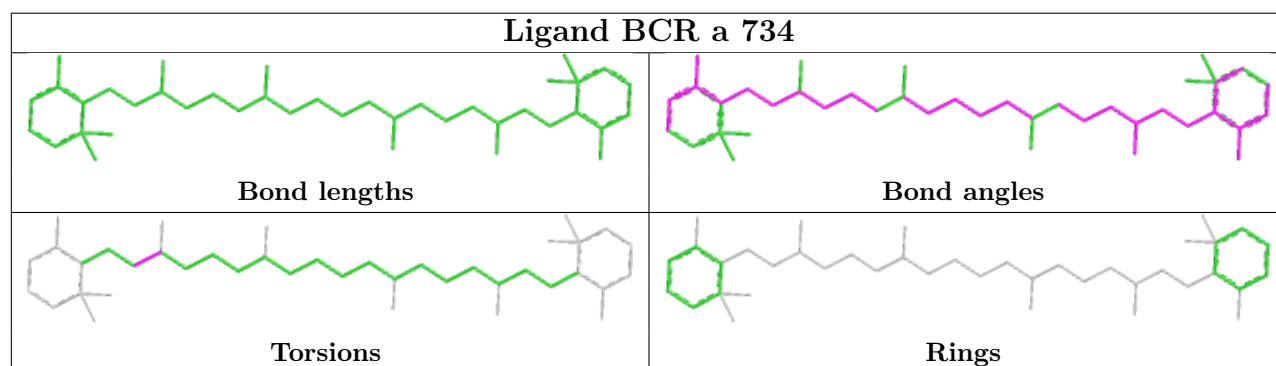
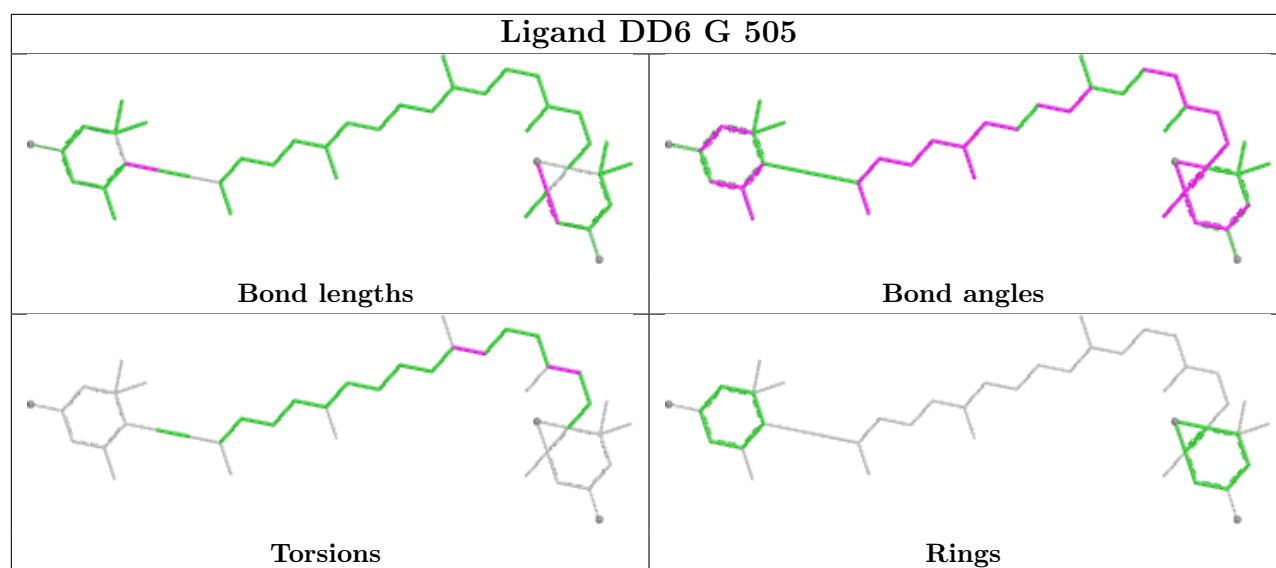
Rings

Ligand KC1 A 314

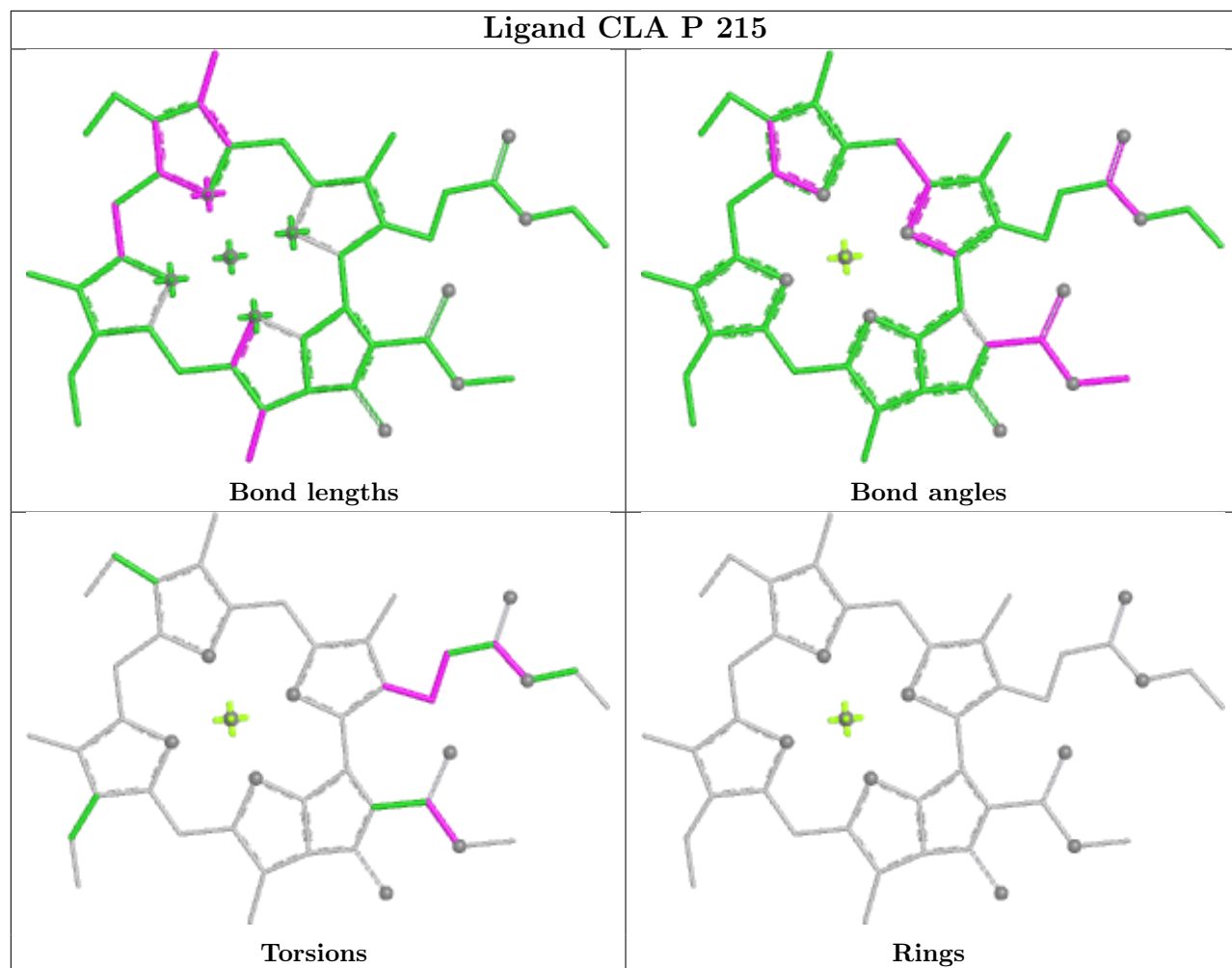


Ligand DD6 K 301

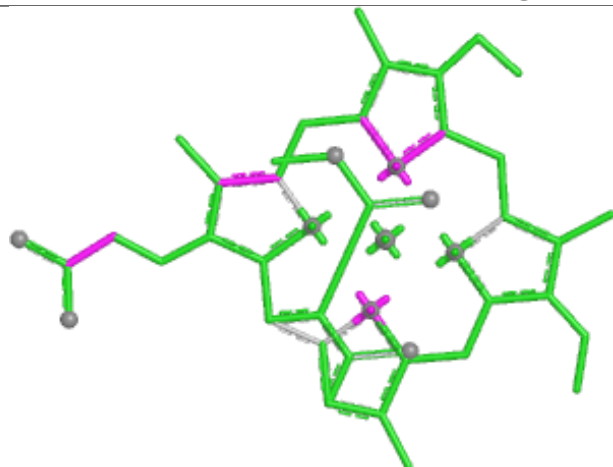




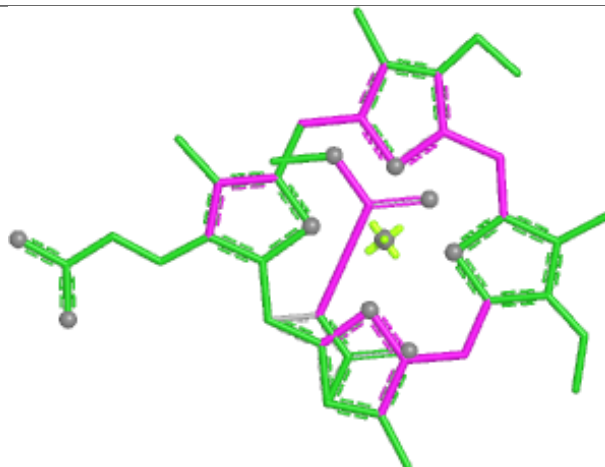
Ligand CLA P 215



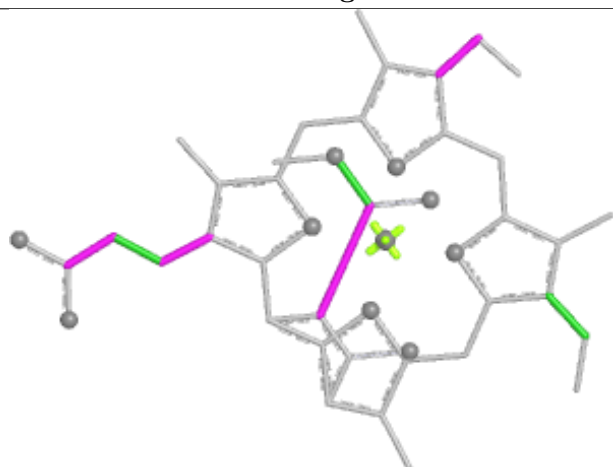
Ligand KC1 A 306



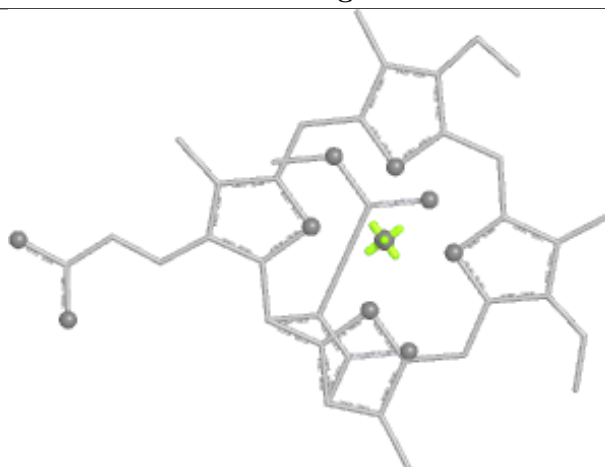
Bond lengths



Bond angles

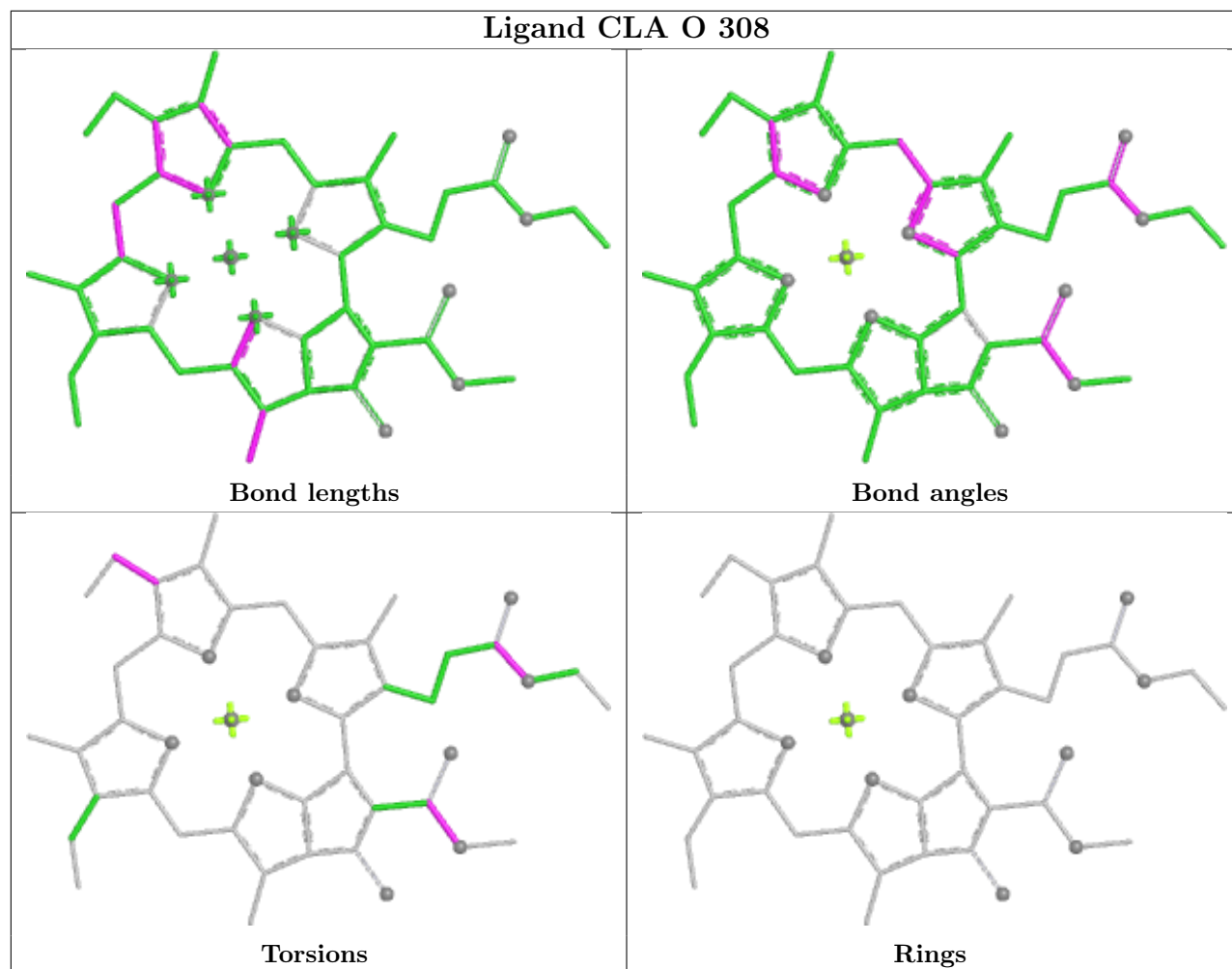


Torsions

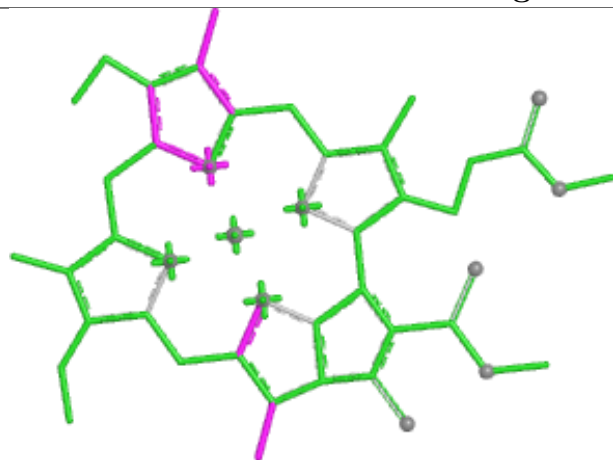


Rings

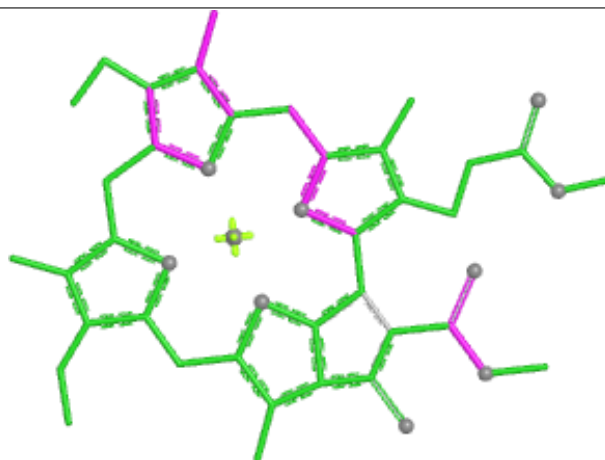
Ligand CLA O 308



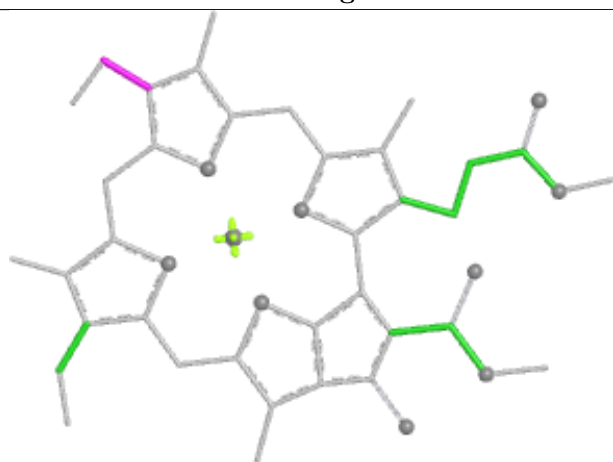
Ligand CLA K 307



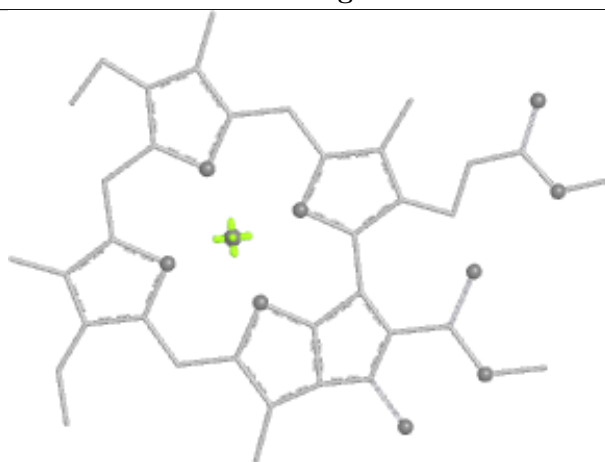
Bond lengths



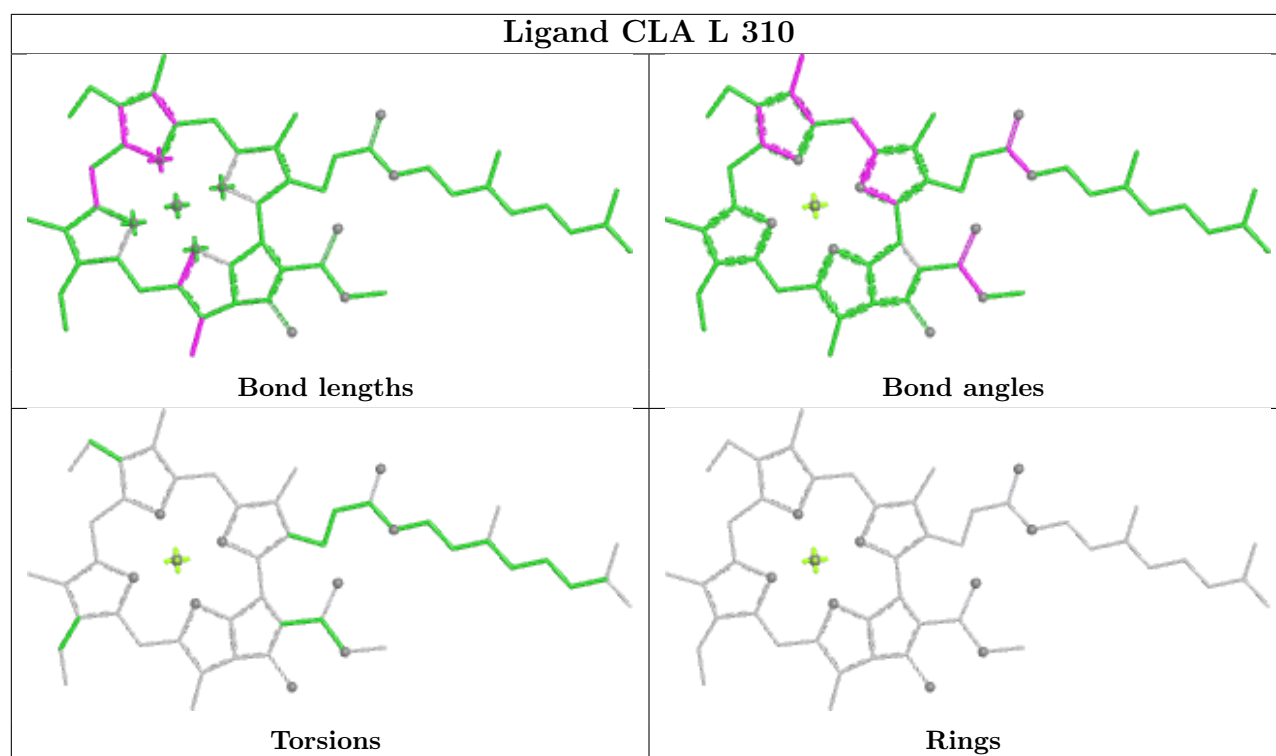
Bond angles



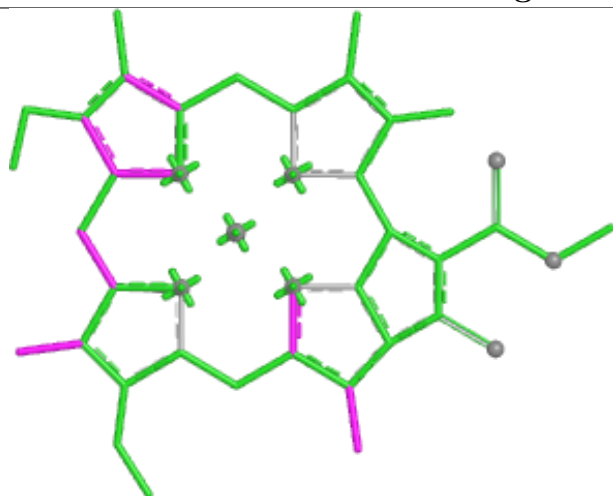
Torsions



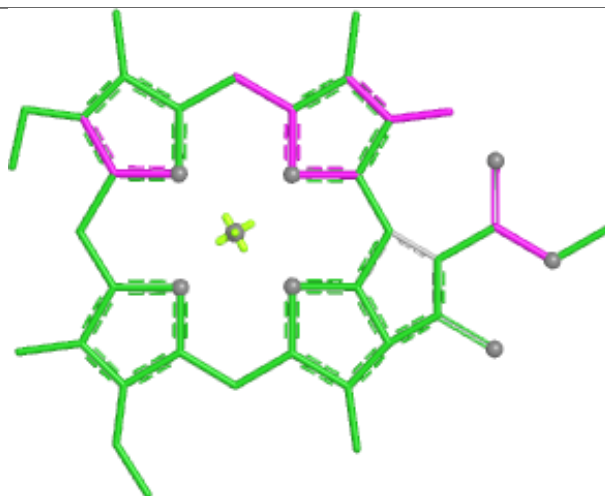
Rings



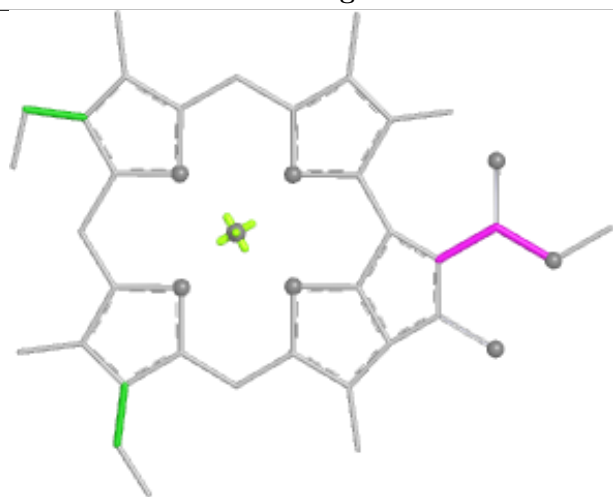
Ligand CLA B 315



Bond lengths



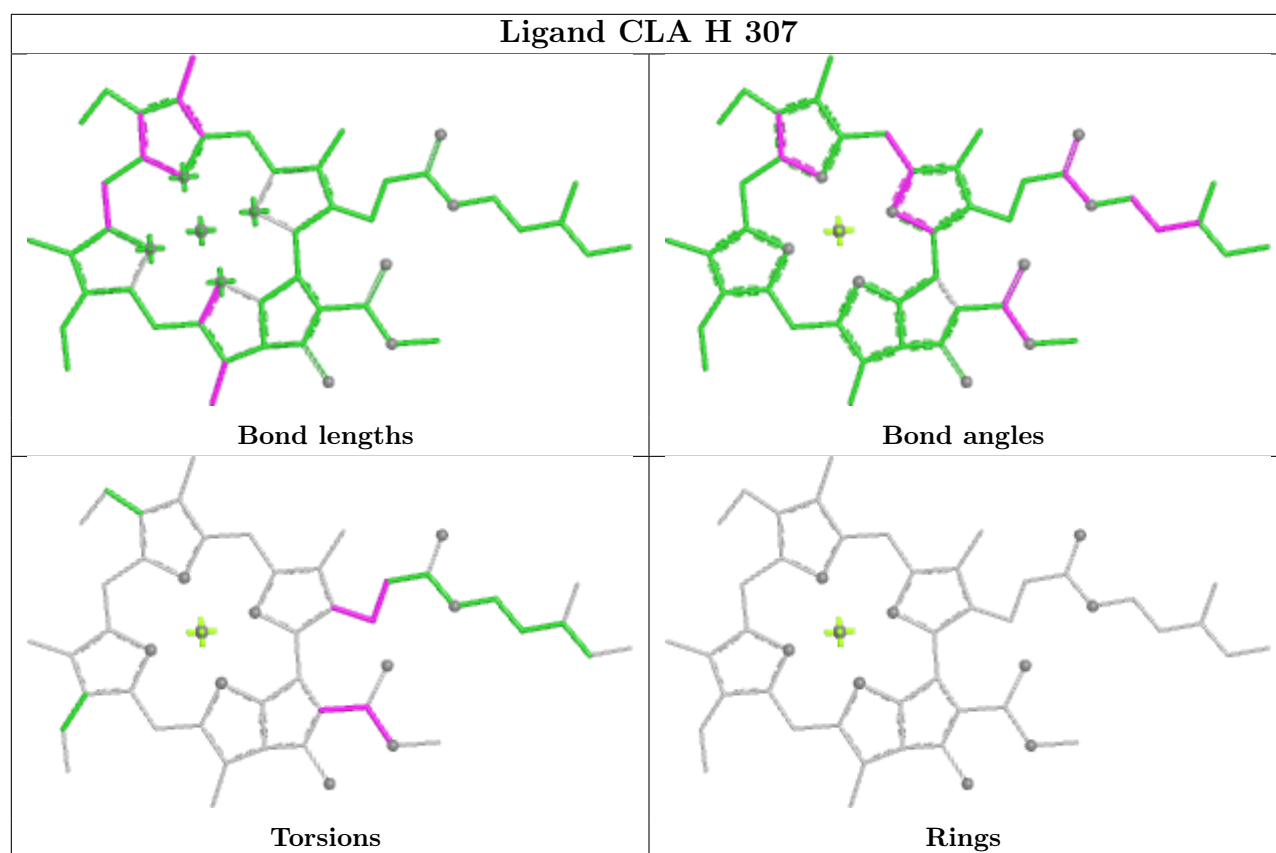
Bond angles



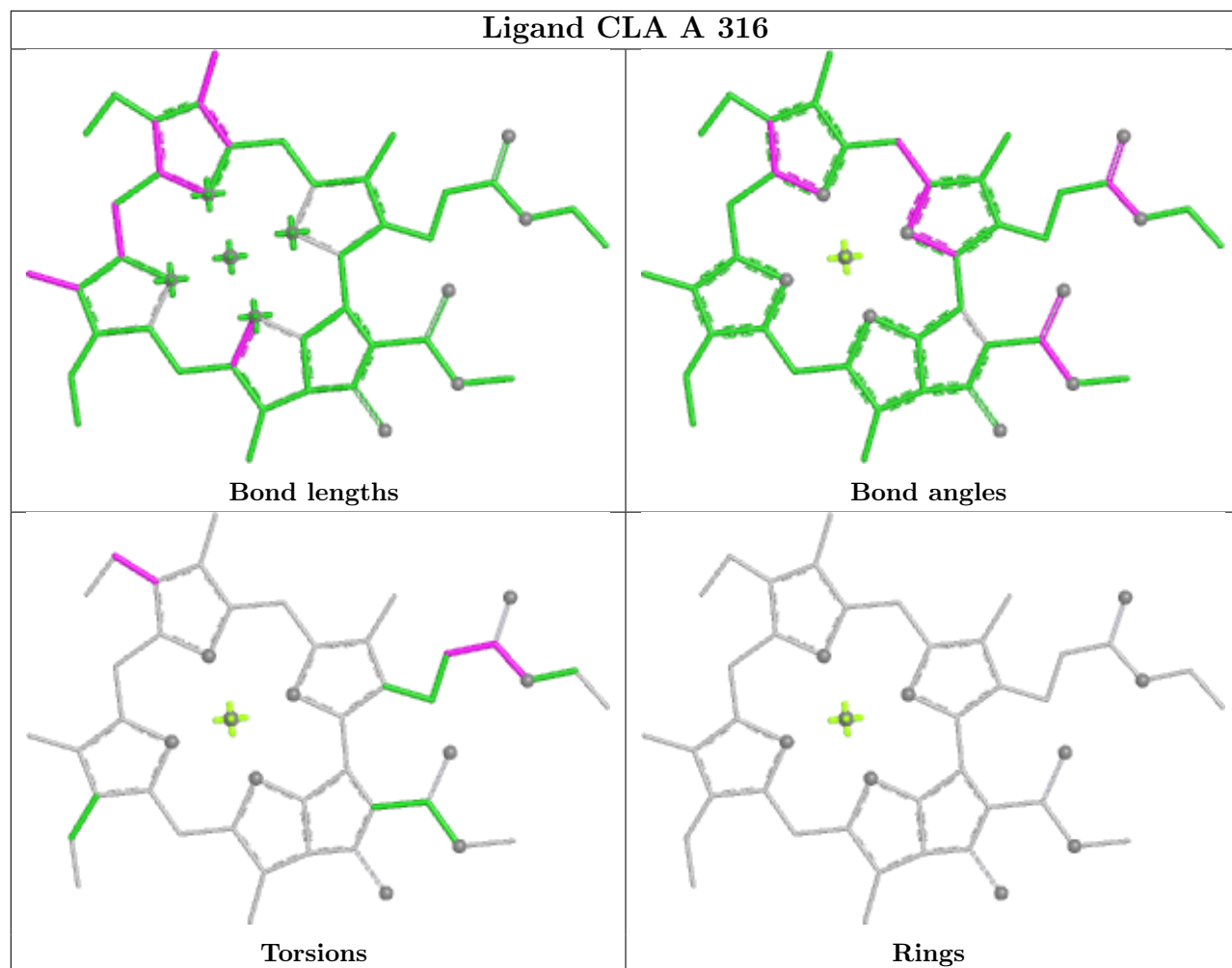
Torsions



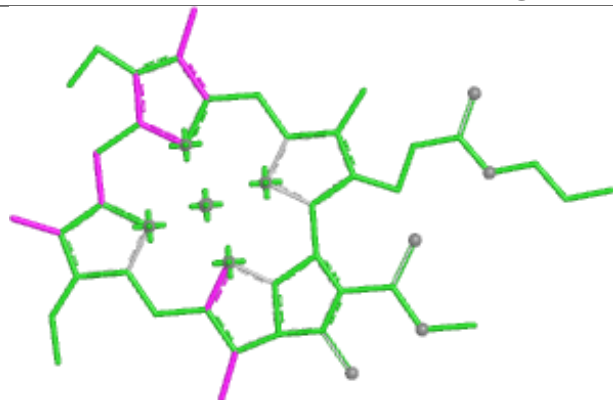
Rings



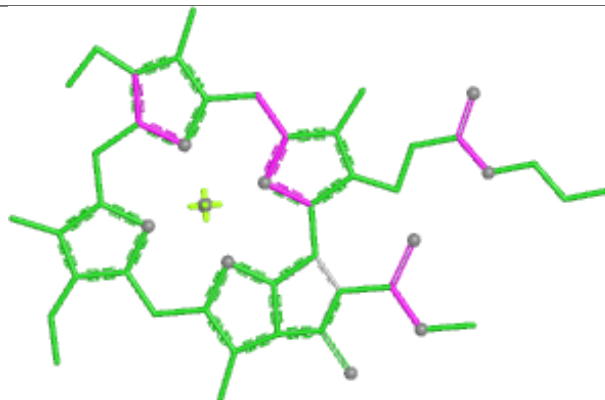
Ligand CLA A 316



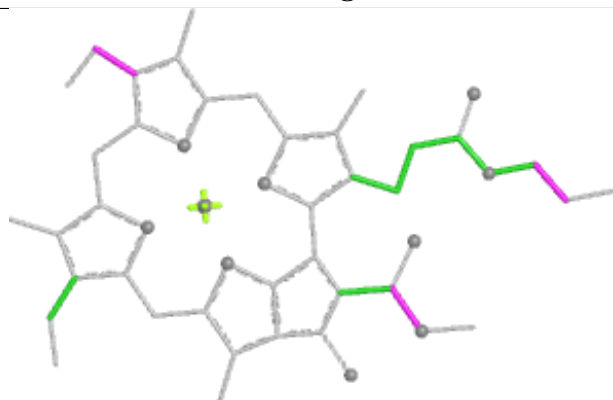
Ligand CLA K 312



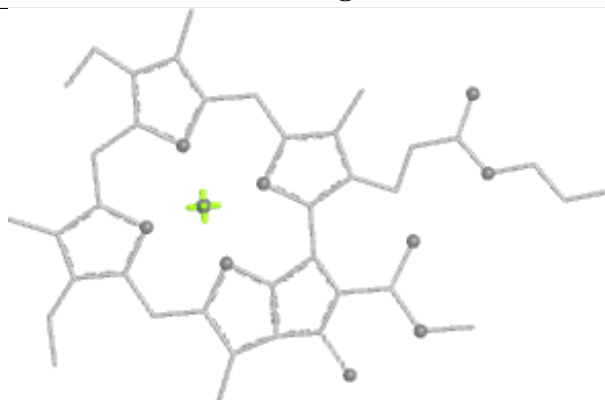
Bond lengths



Bond angles

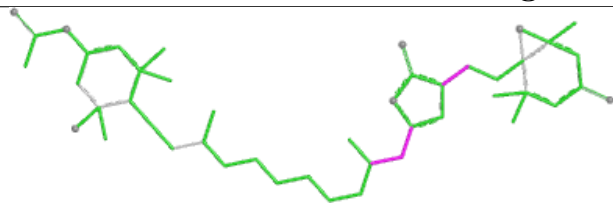


Torsions

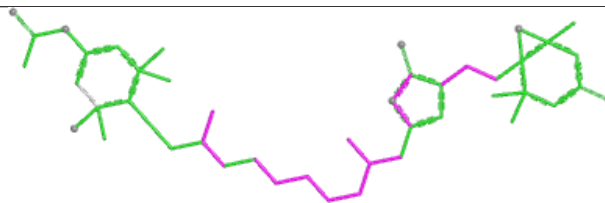


Rings

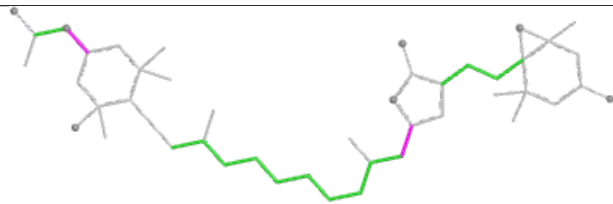
Ligand PID P 205



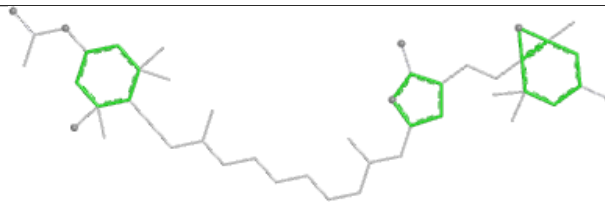
Bond lengths



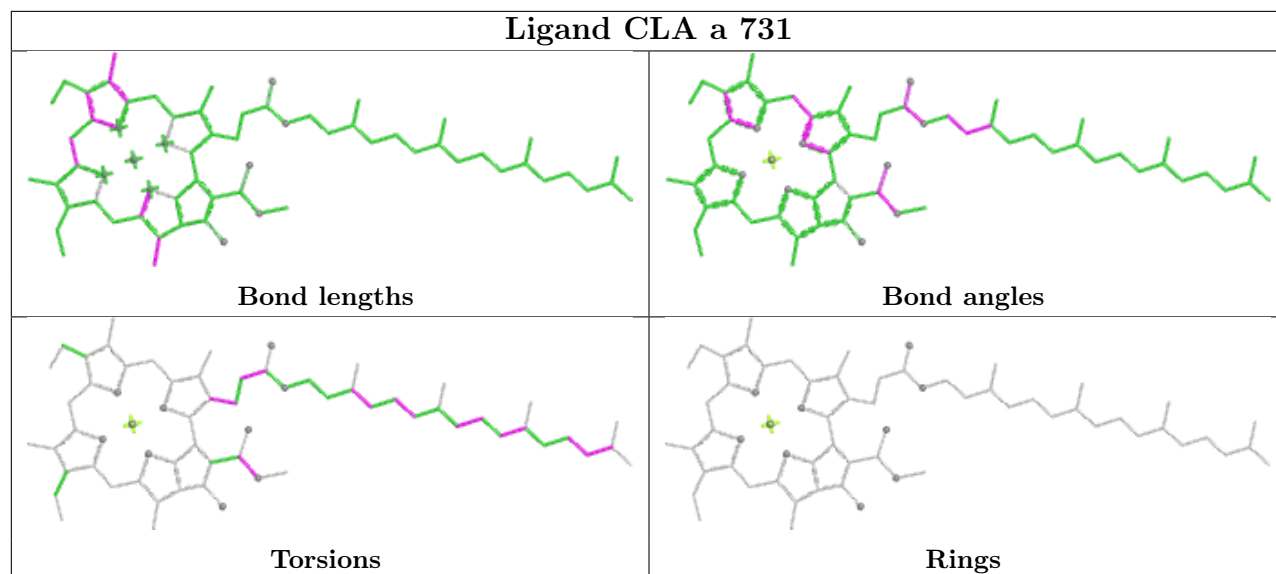
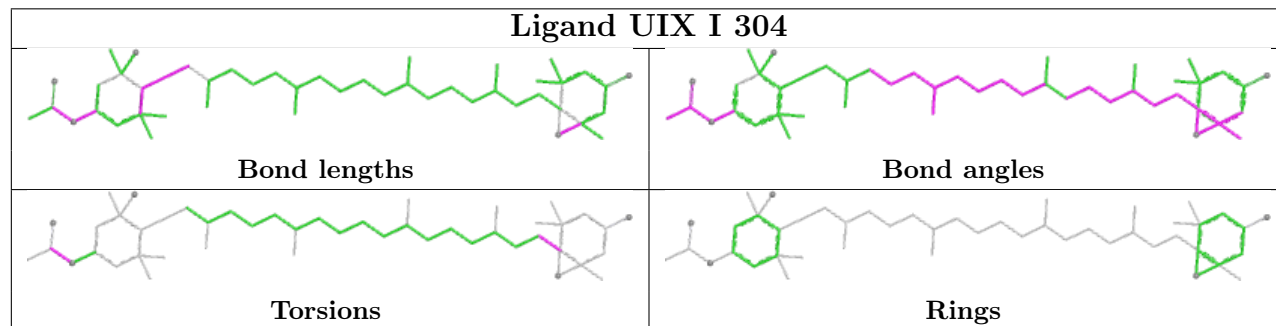
Bond angles



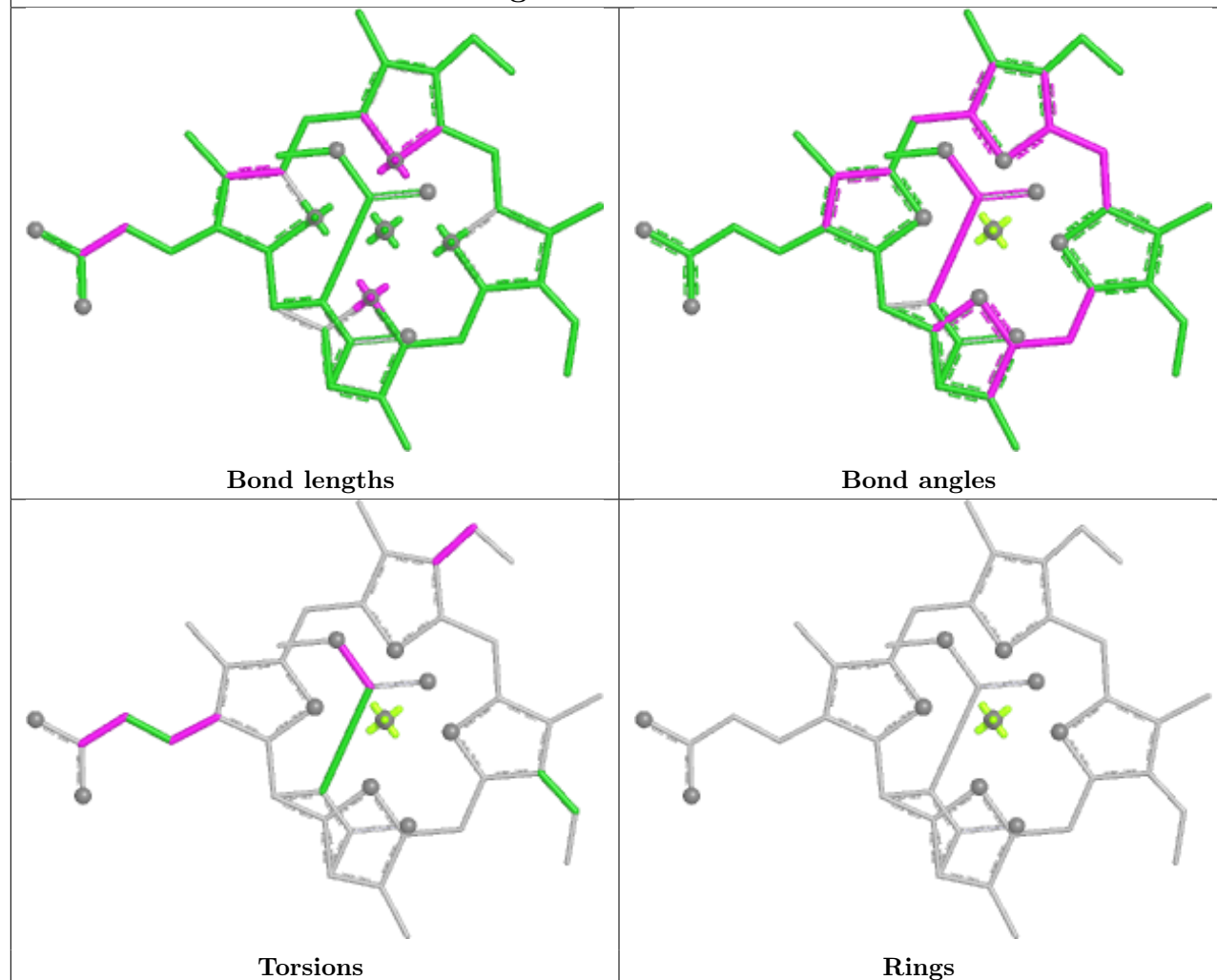
Torsions



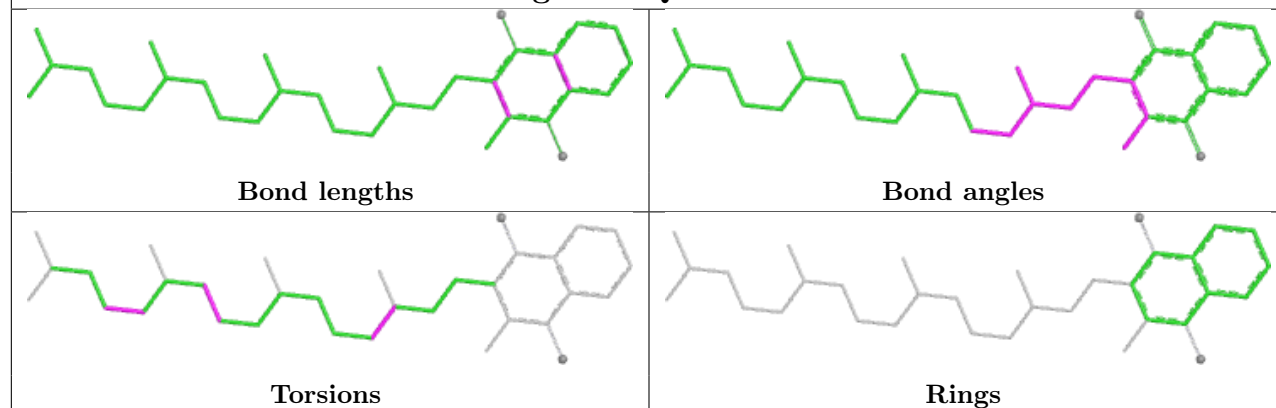
Rings

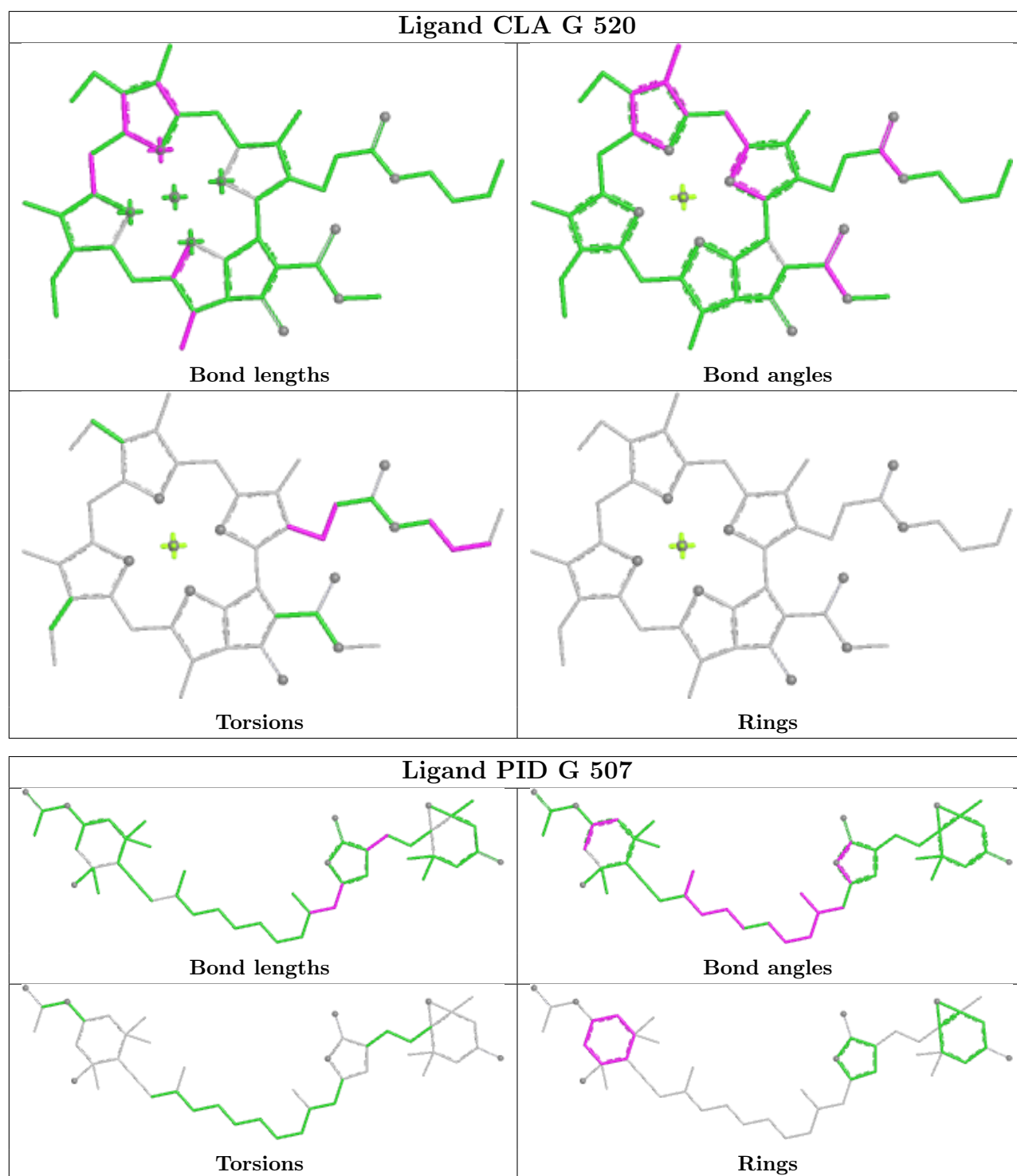
Ligand CLA a 731**Ligand UIX I 304**

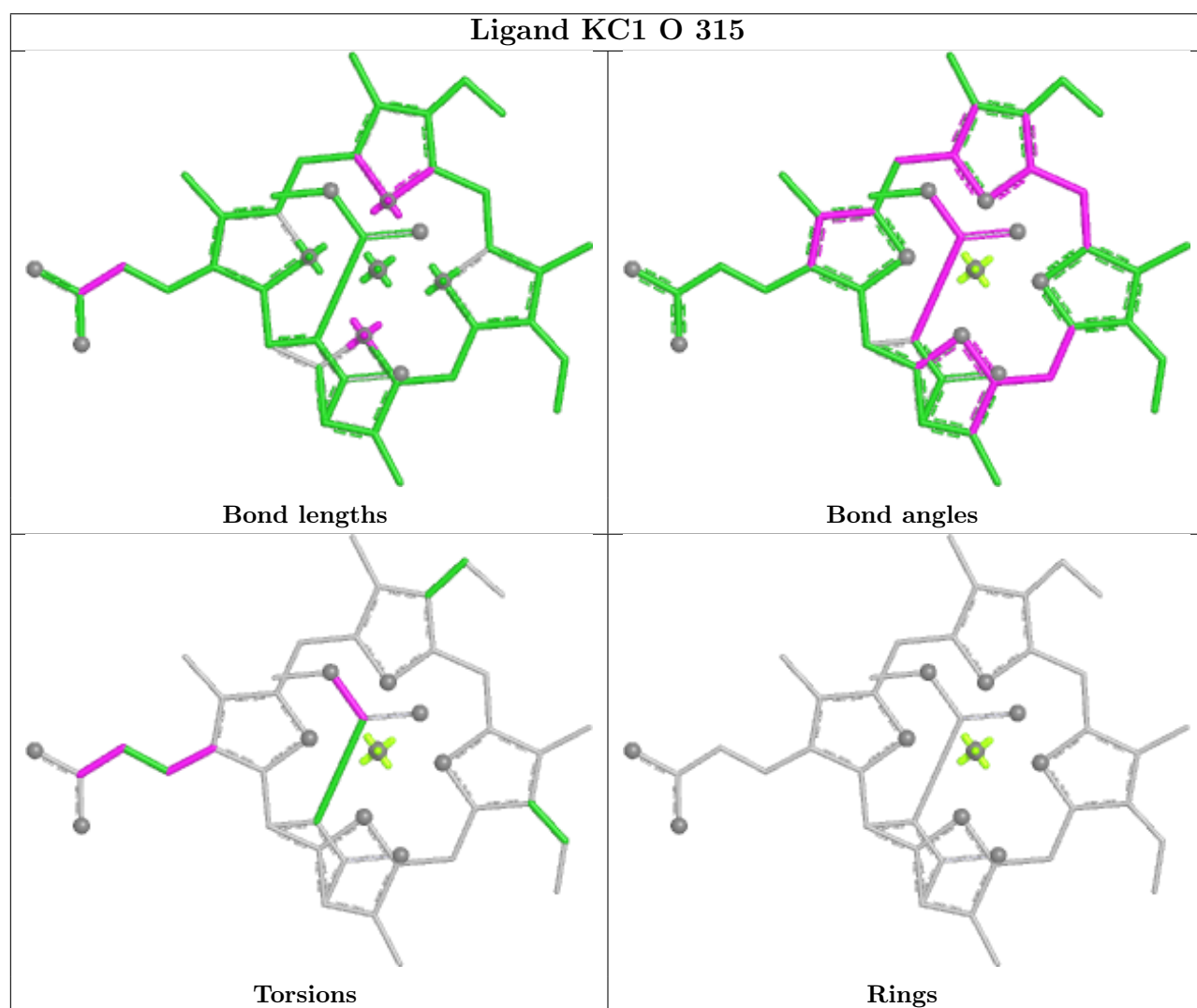
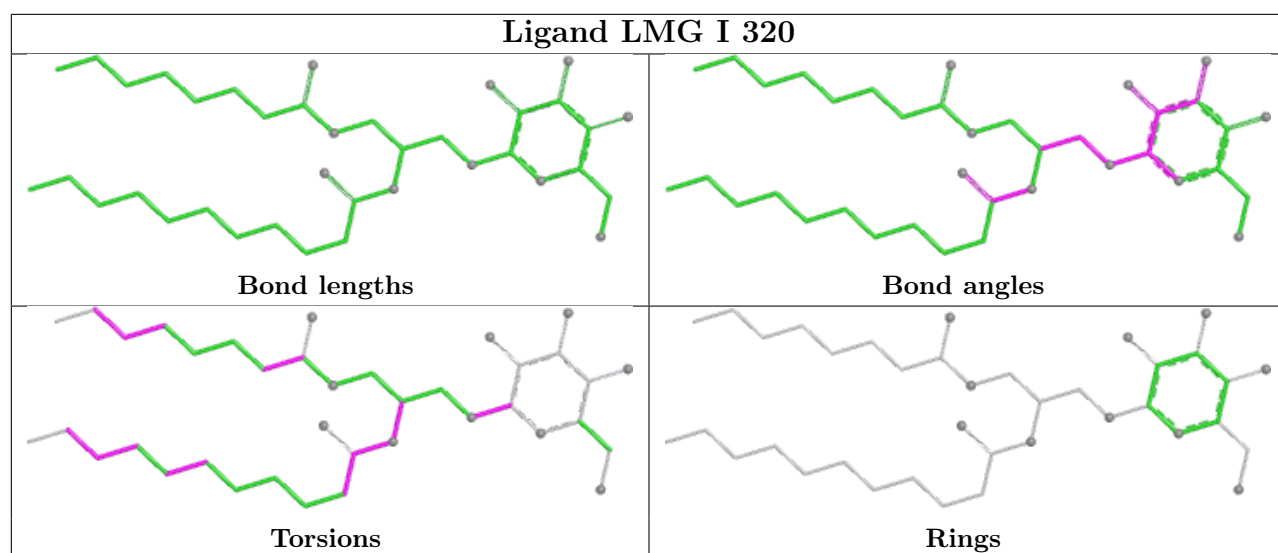
Ligand KC1 P 216

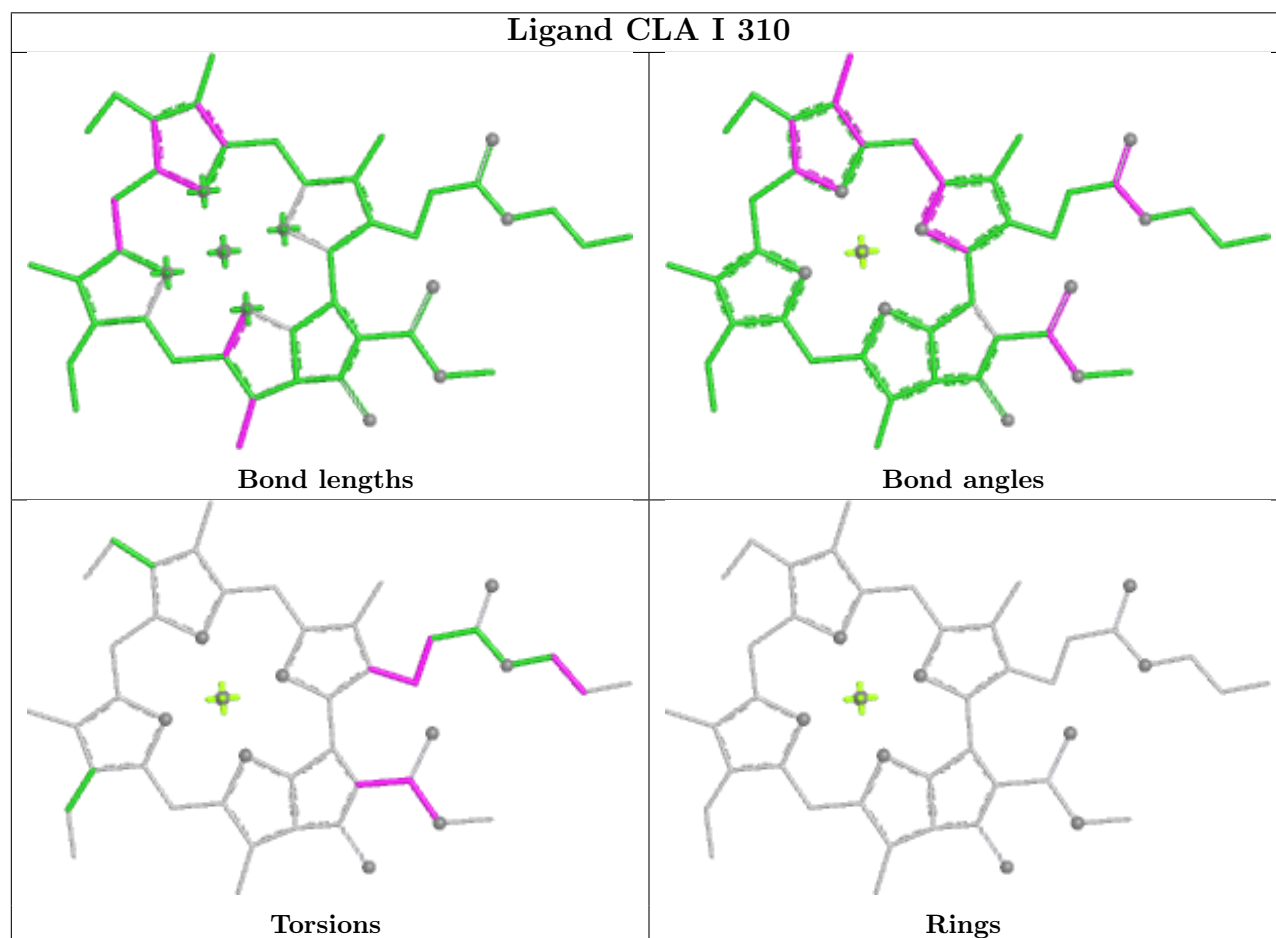
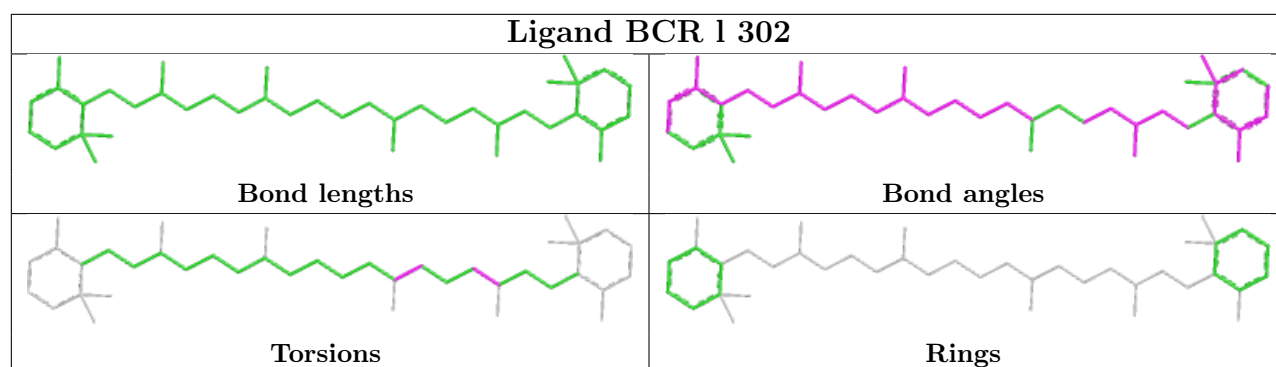


Ligand PQN b 729

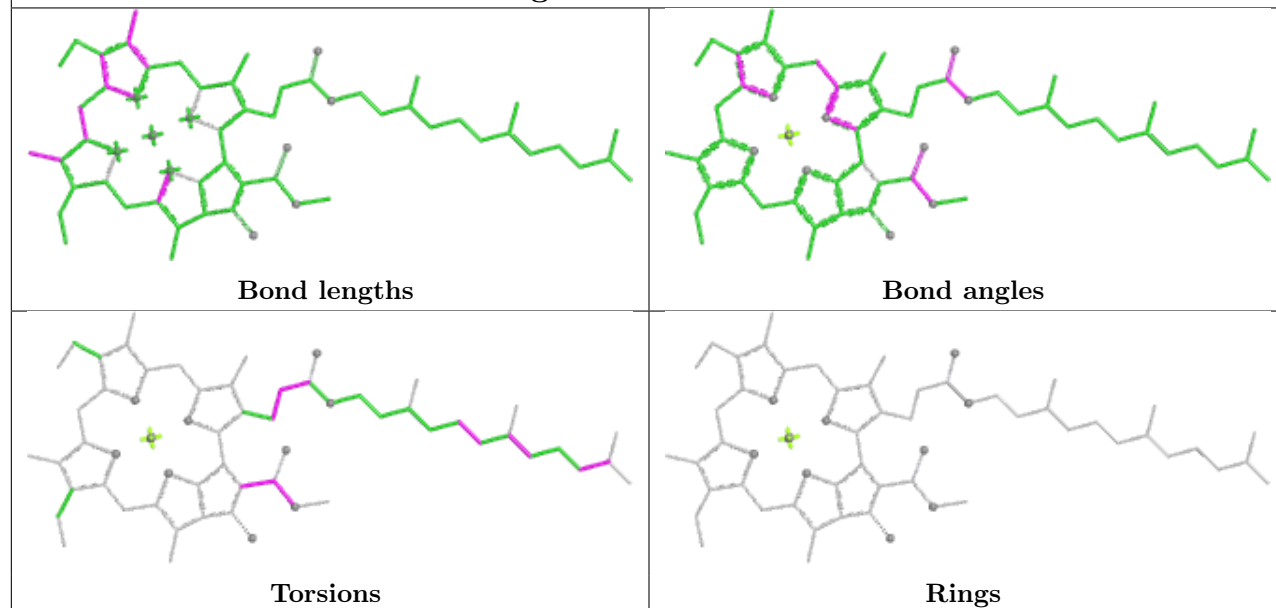




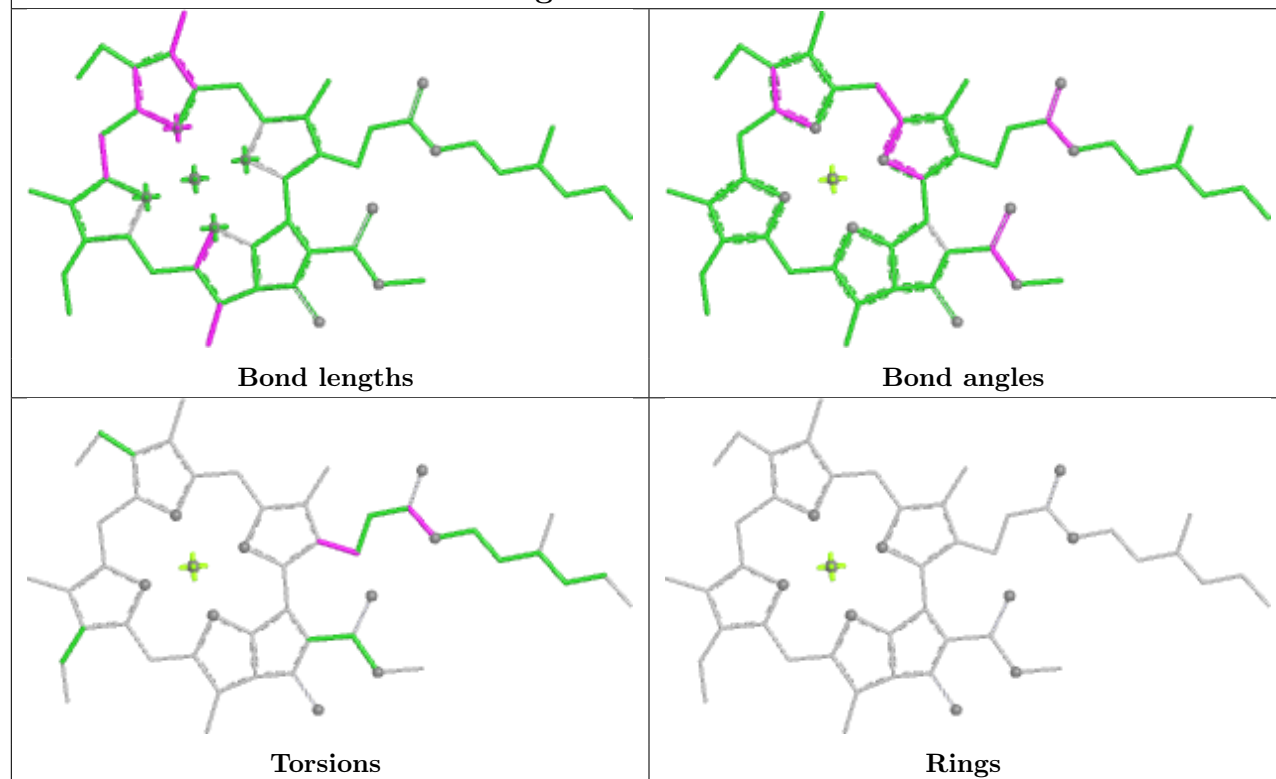




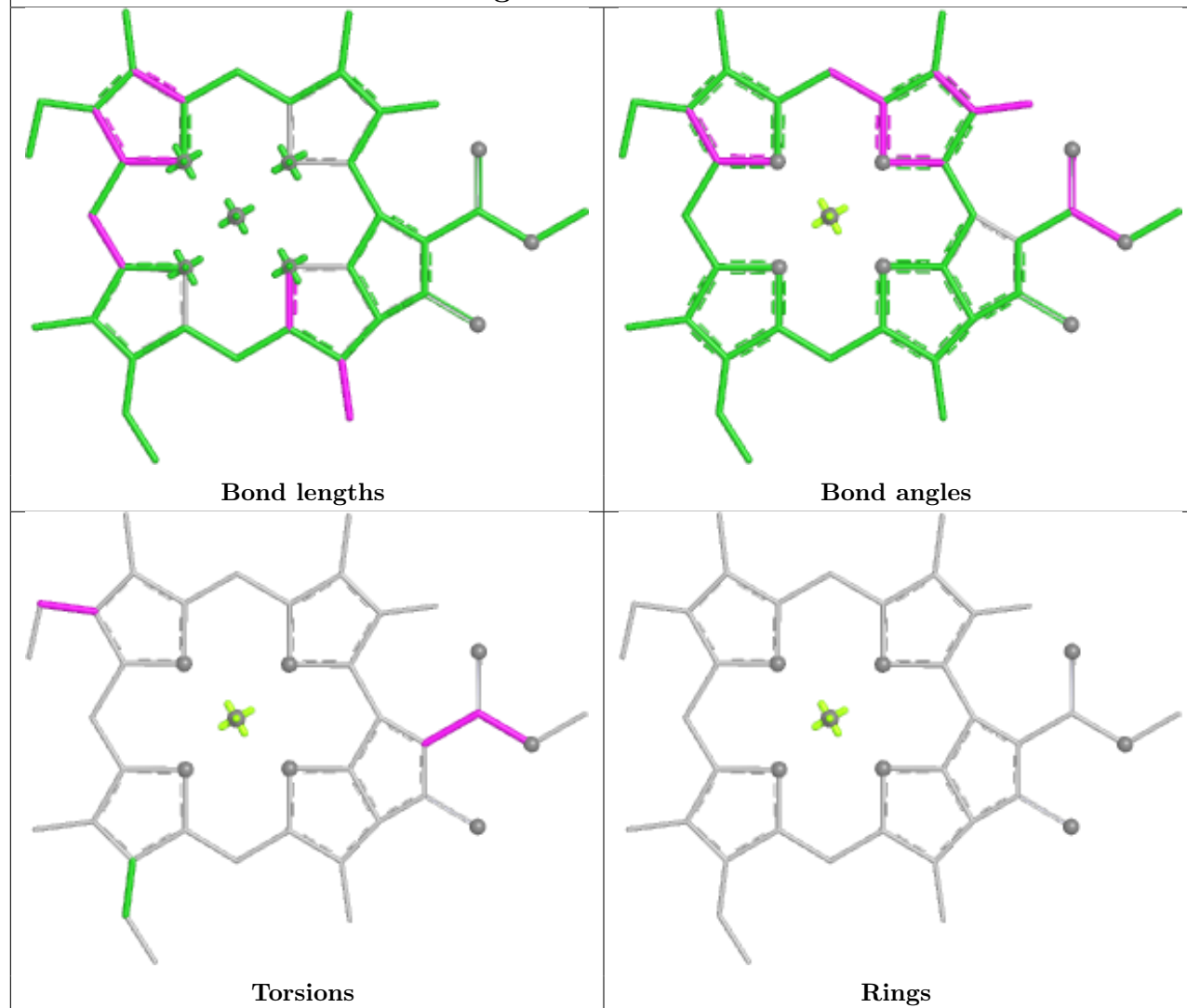
Ligand CLA G 512



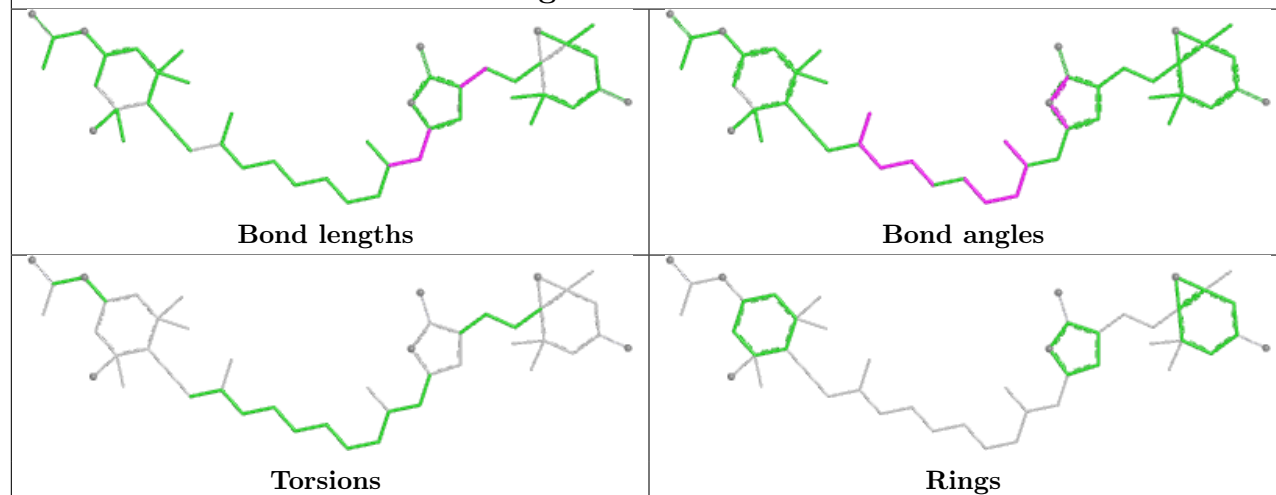
Ligand CLA b 710

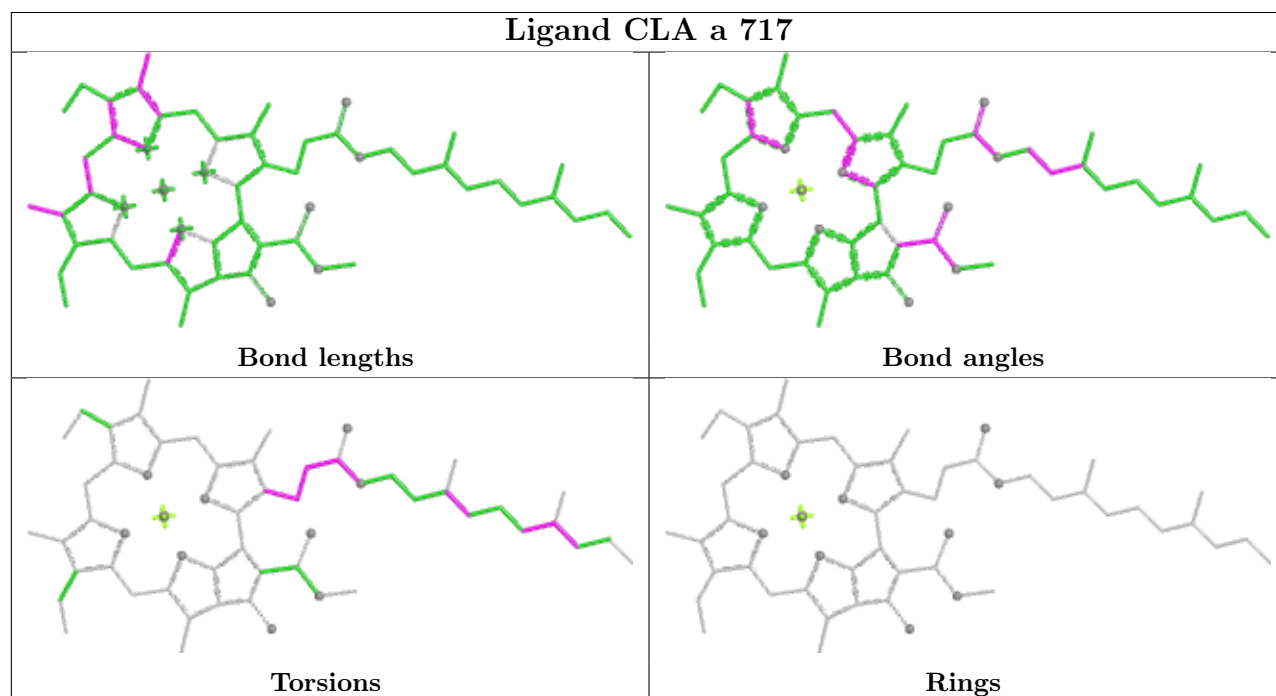
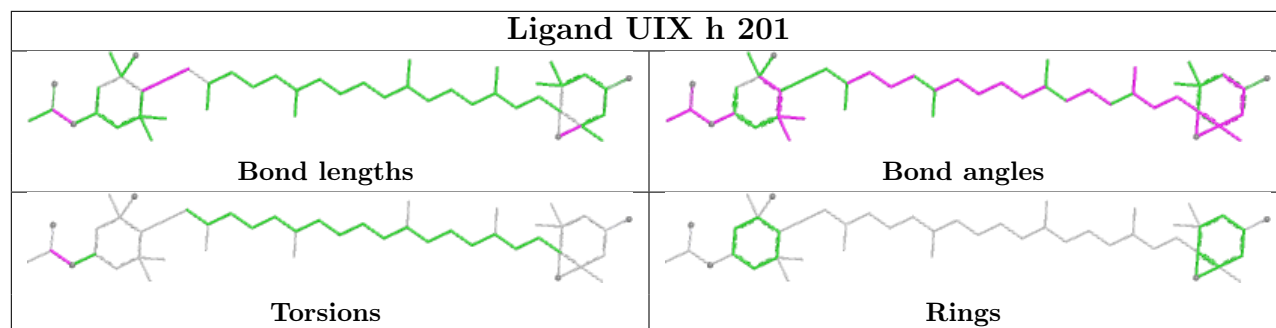


Ligand CLA G 516

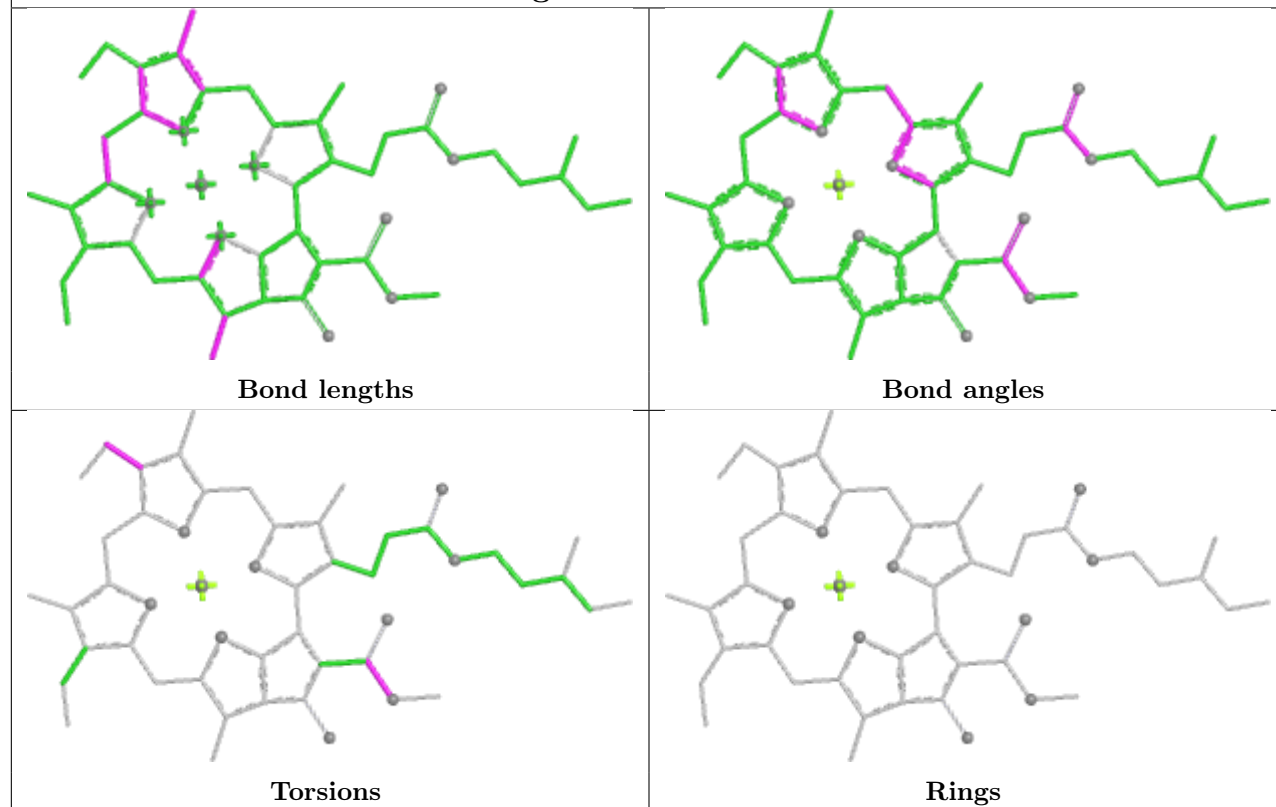


Ligand PID F 306

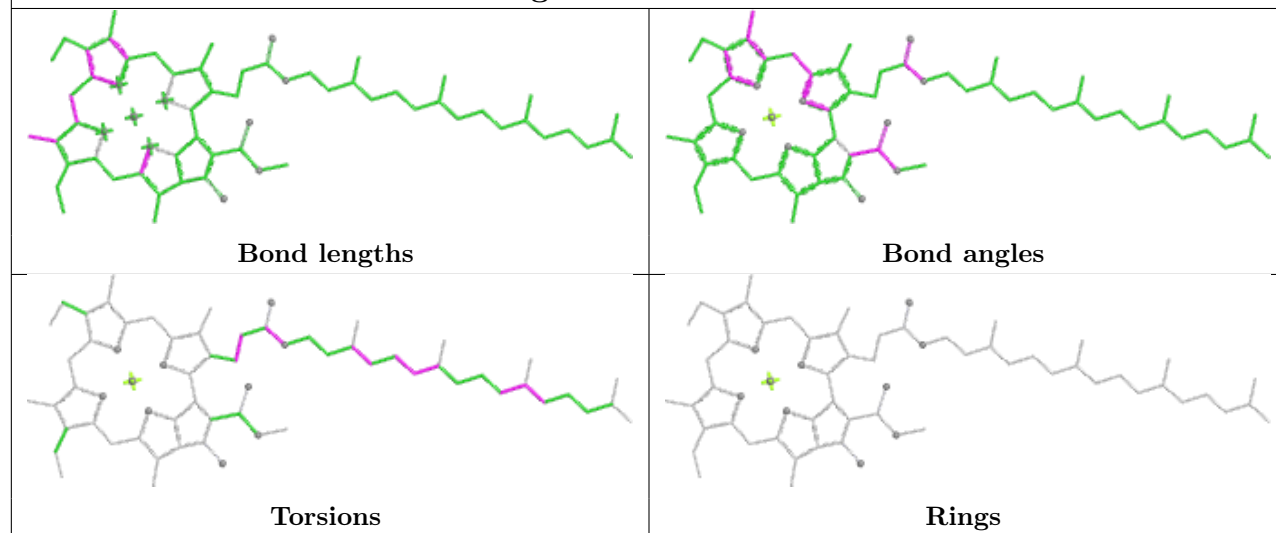




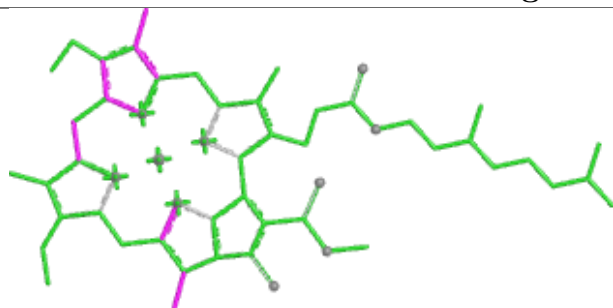
Ligand CLA B 312



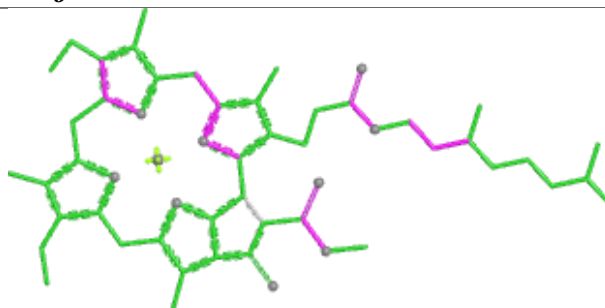
Ligand CLA G 510



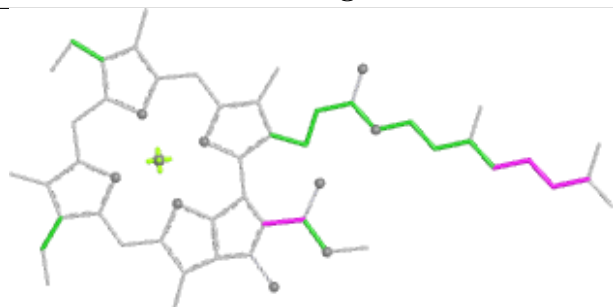
Ligand CLA j 104



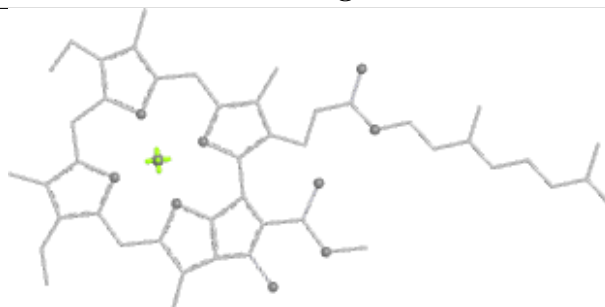
Bond lengths



Bond angles

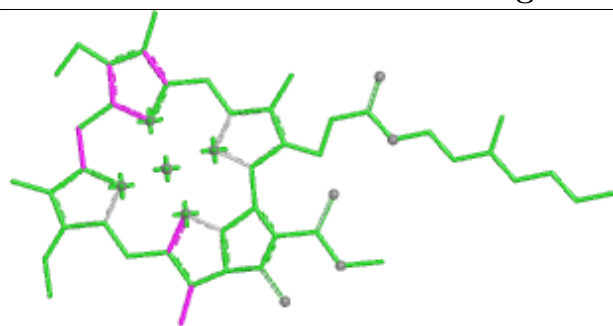


Torsions

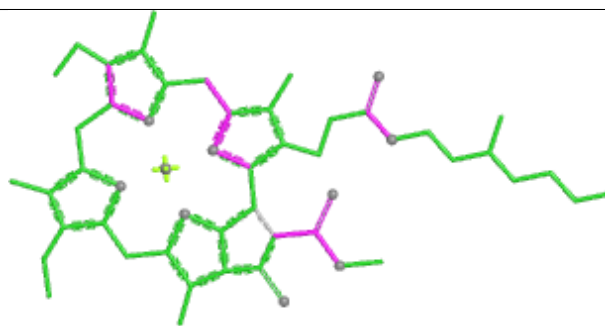


Rings

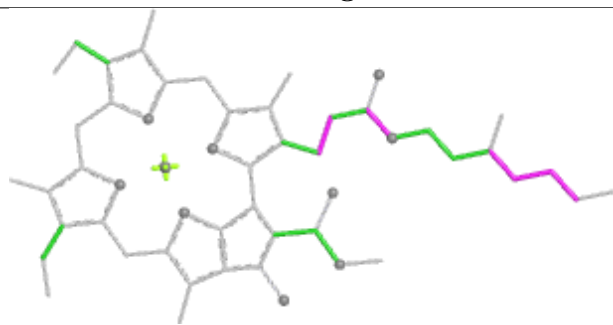
Ligand CLA L 309



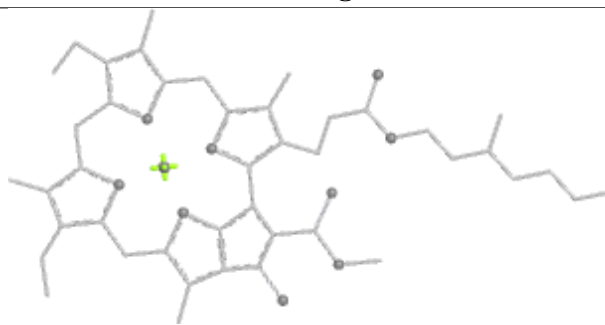
Bond lengths



Bond angles

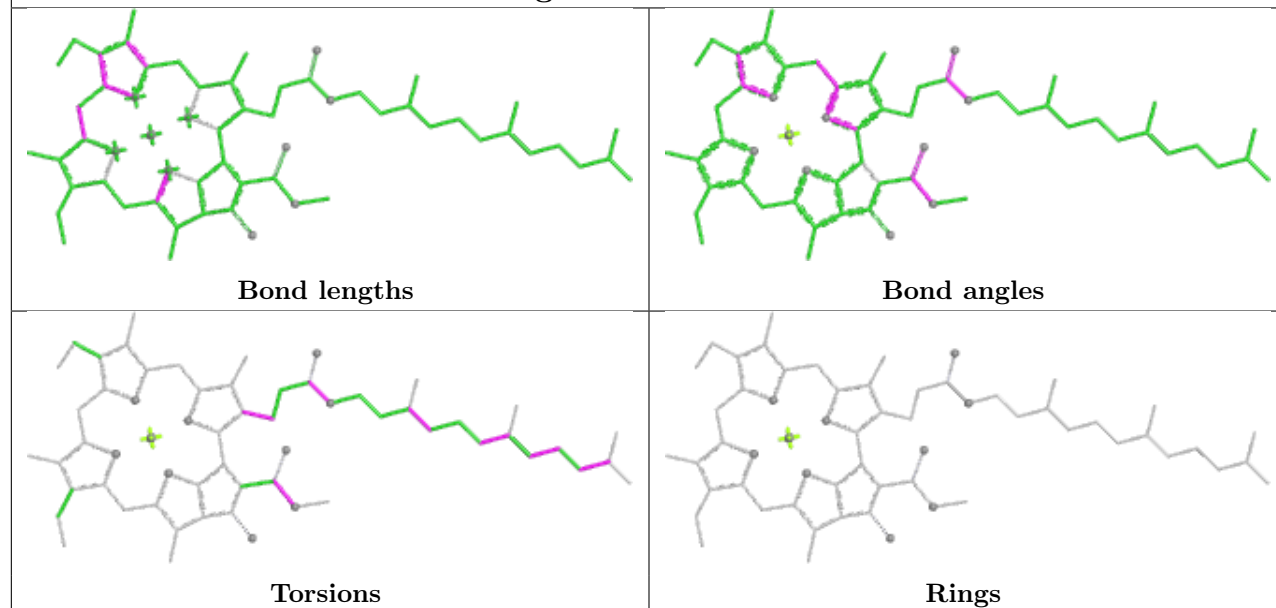


Torsions

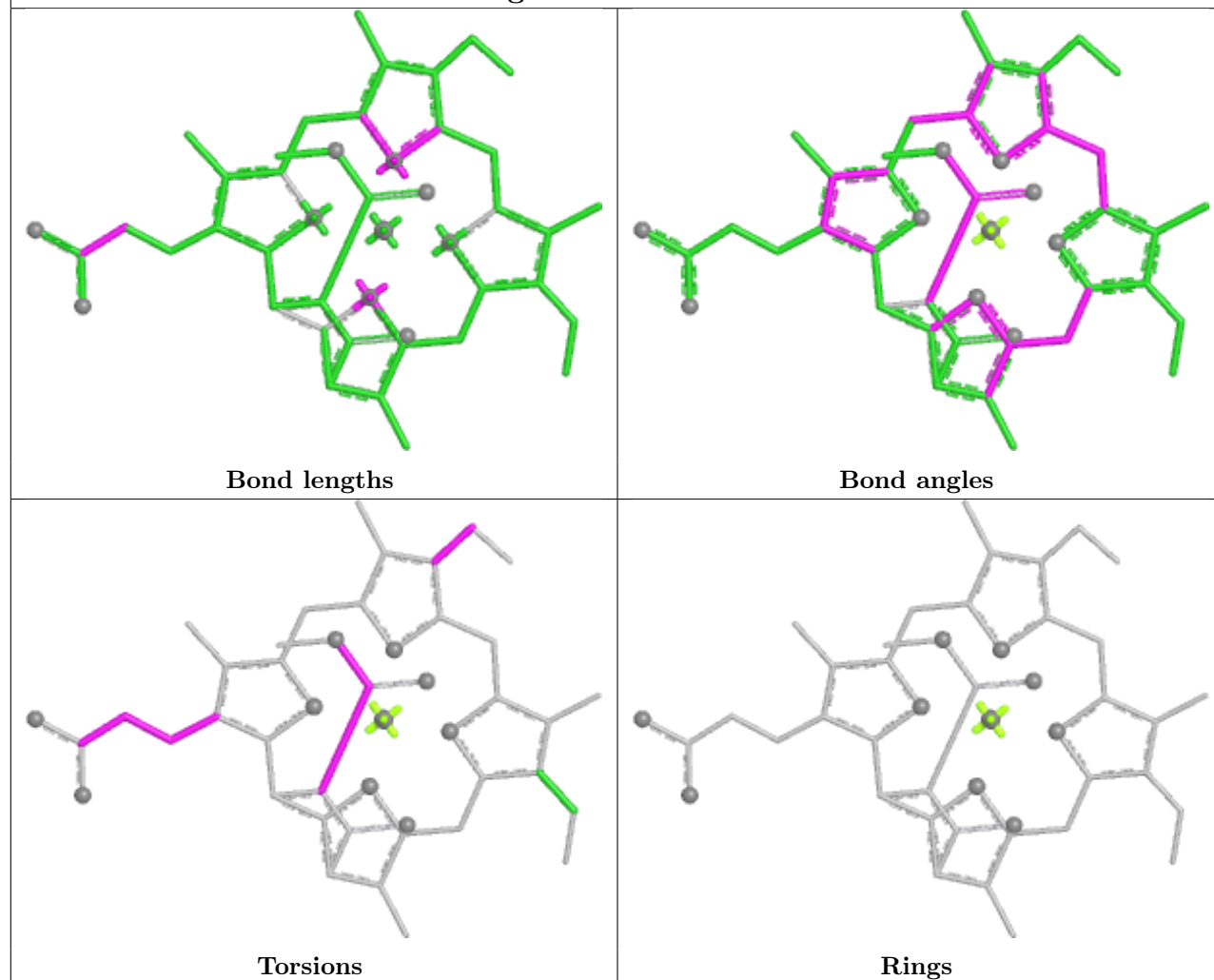


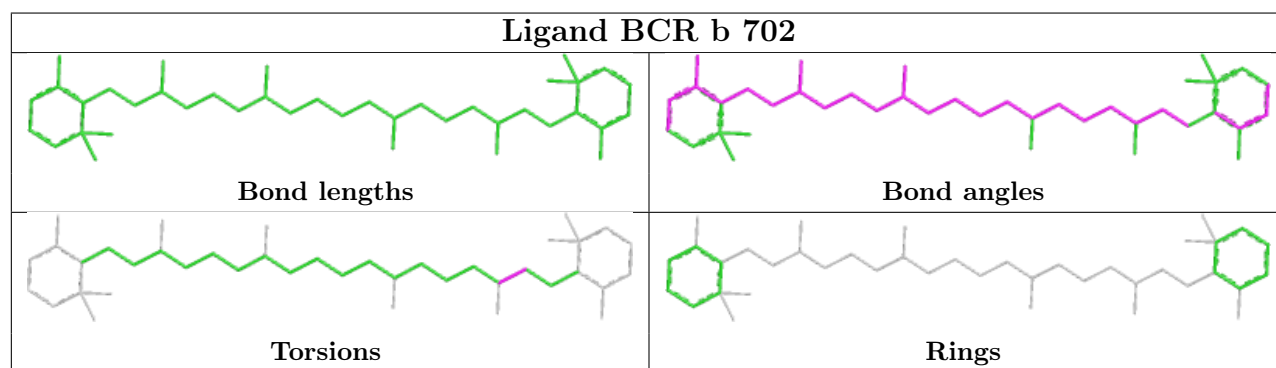
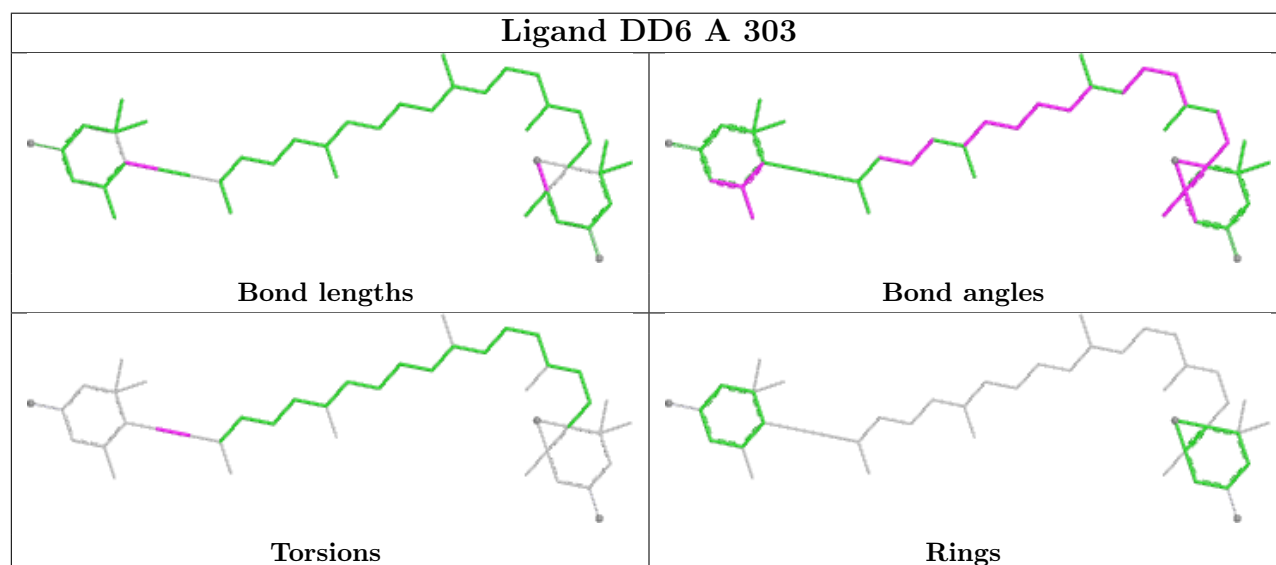
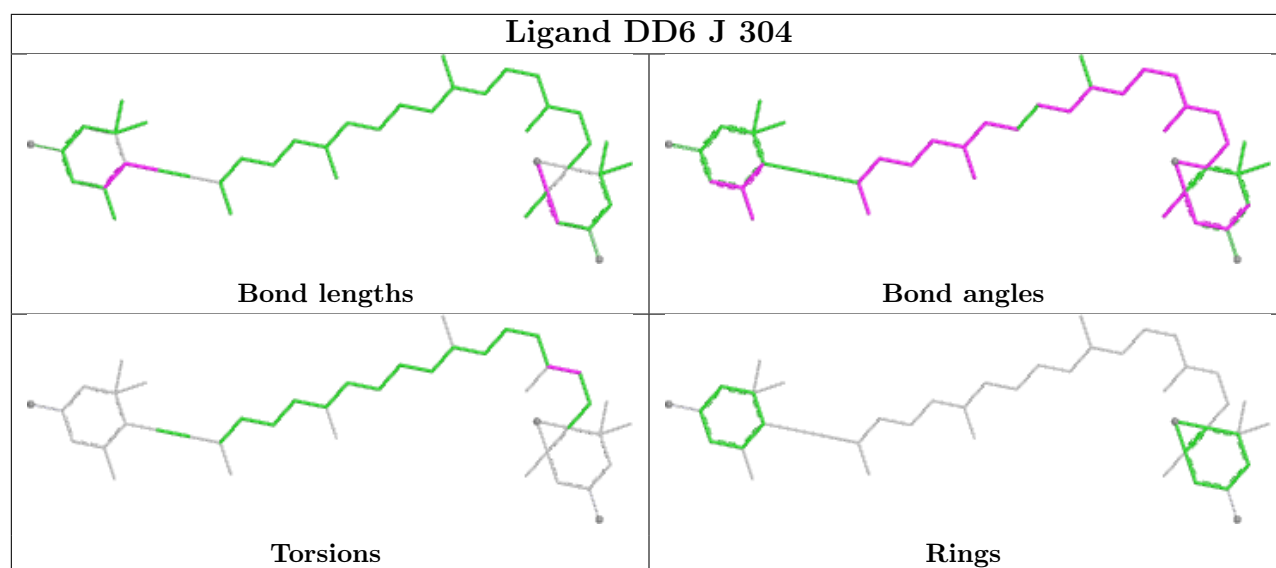
Rings

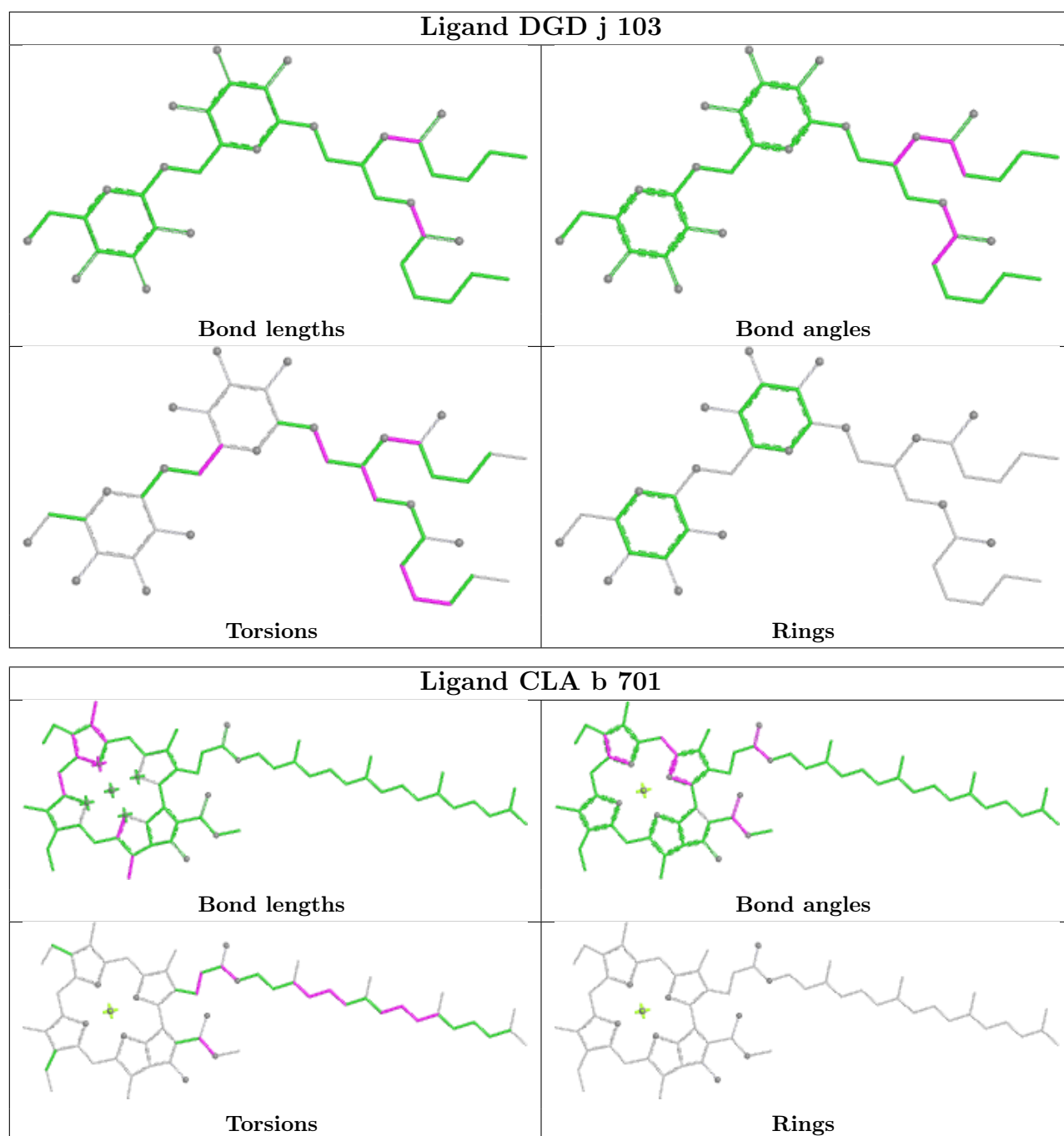
Ligand CLA b 715



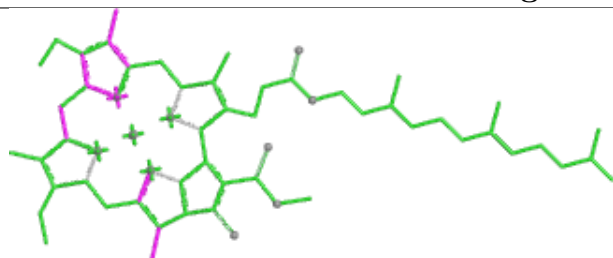
Ligand KC1 O 312



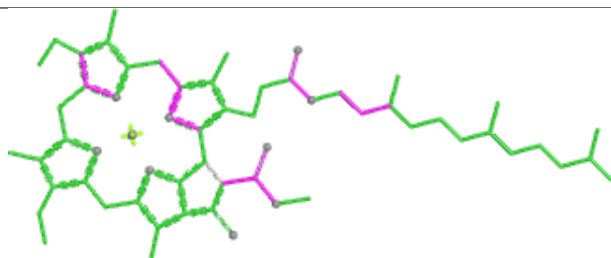




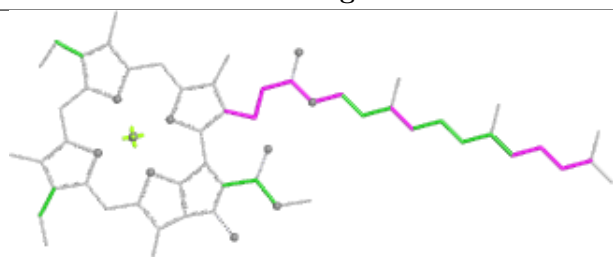
Ligand CLA I 308



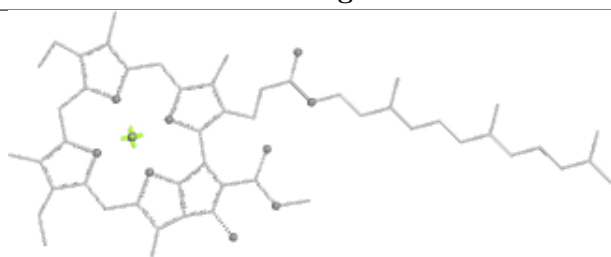
Bond lengths



Bond angles

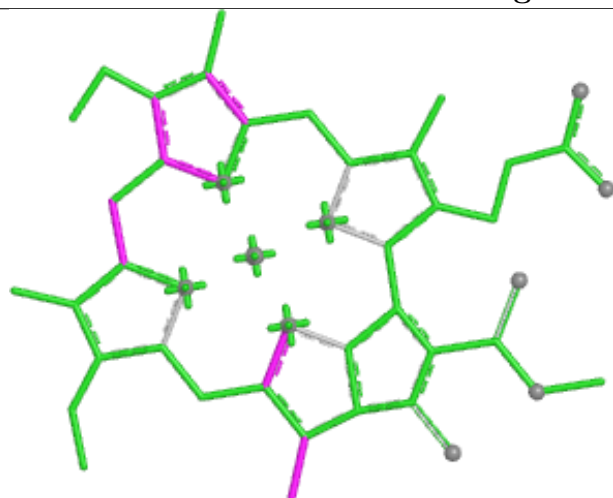


Torsions

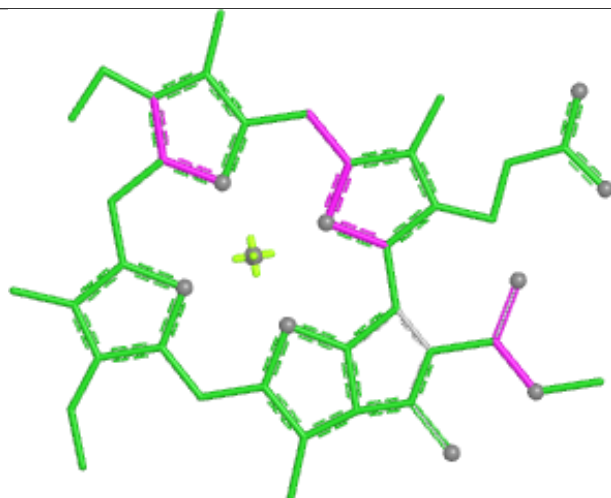


Rings

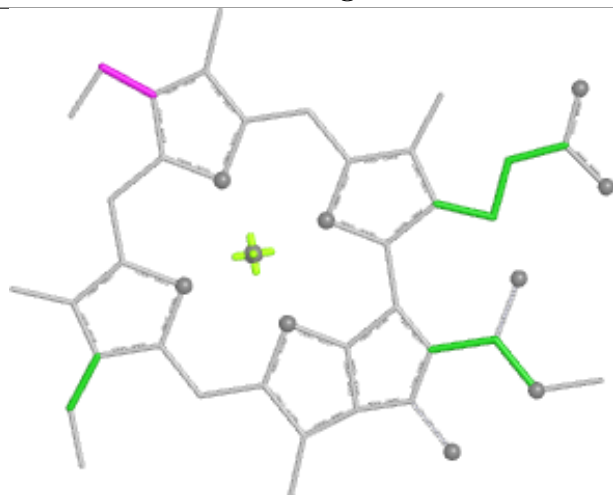
Ligand CLA A 307



Bond lengths



Bond angles

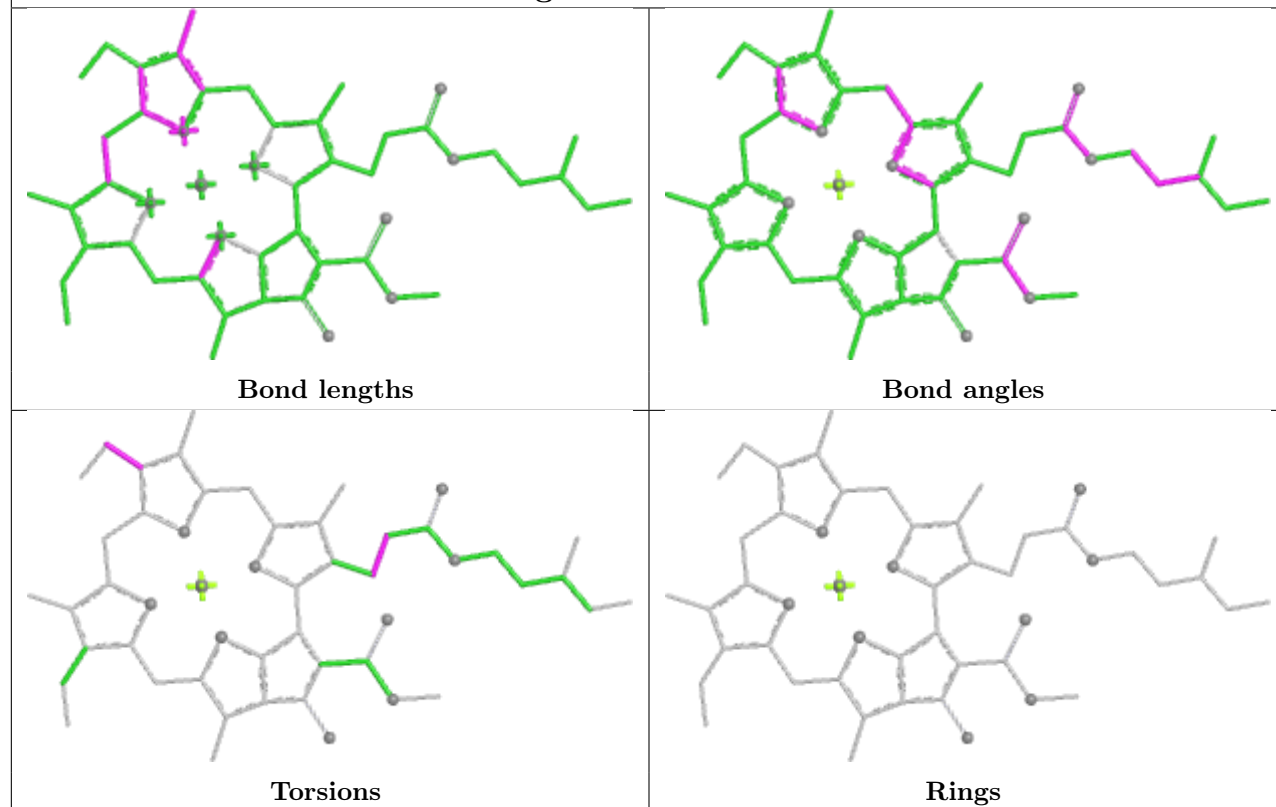


Torsions

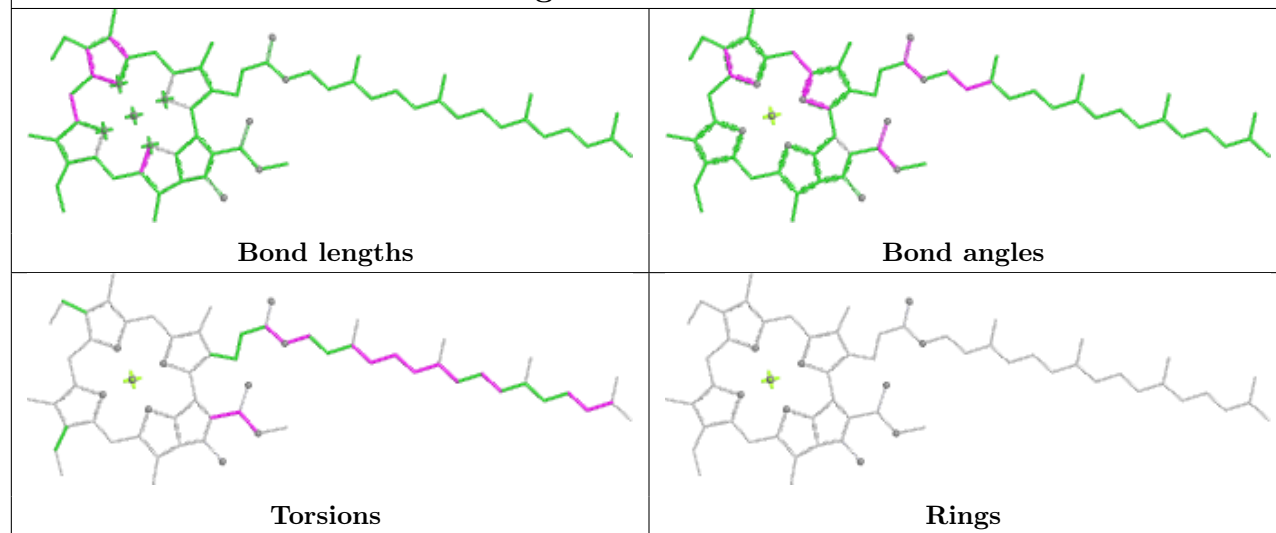


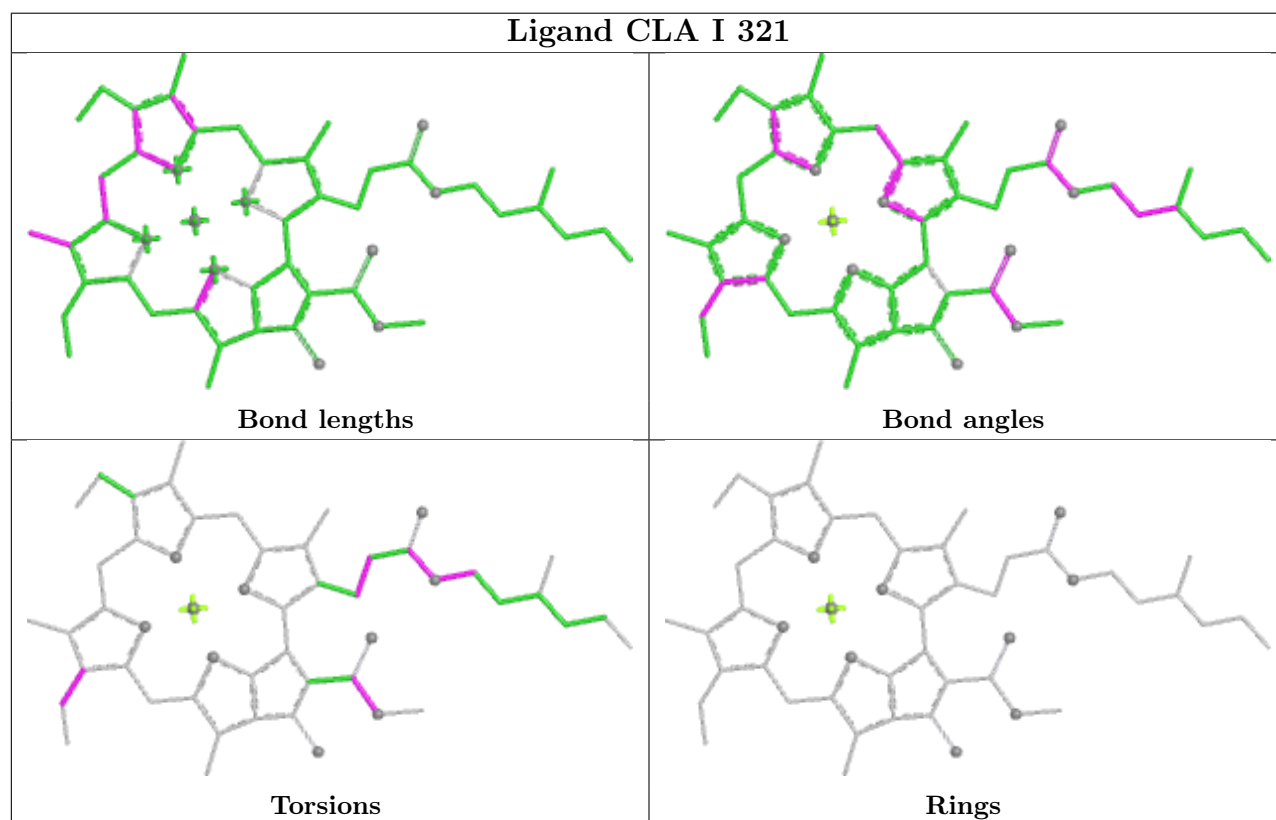
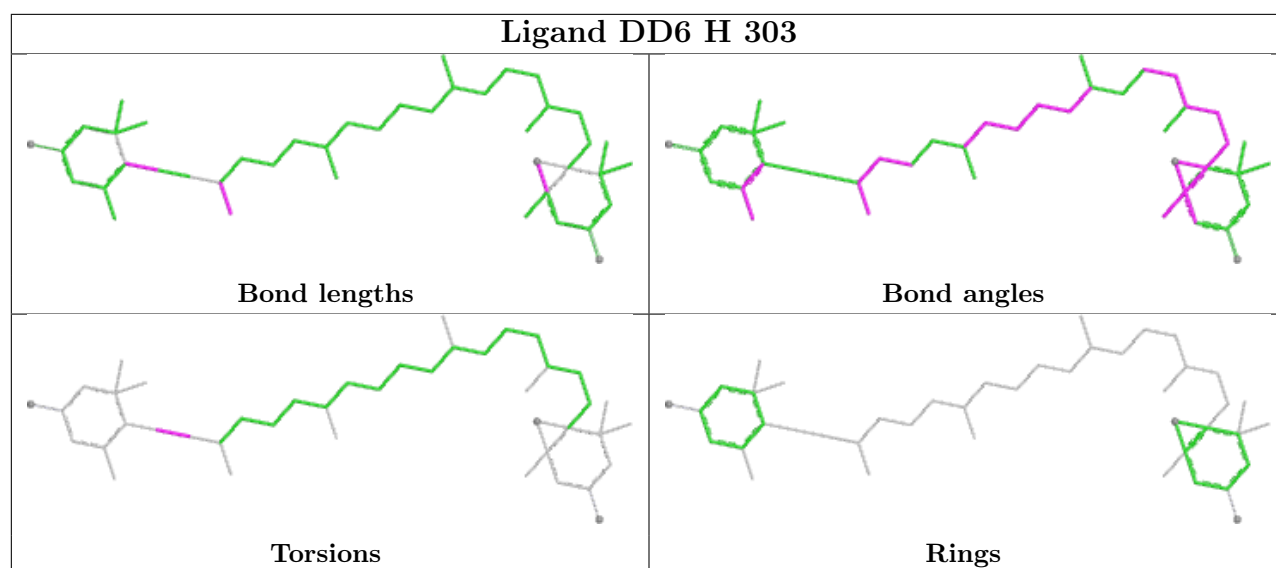
Rings

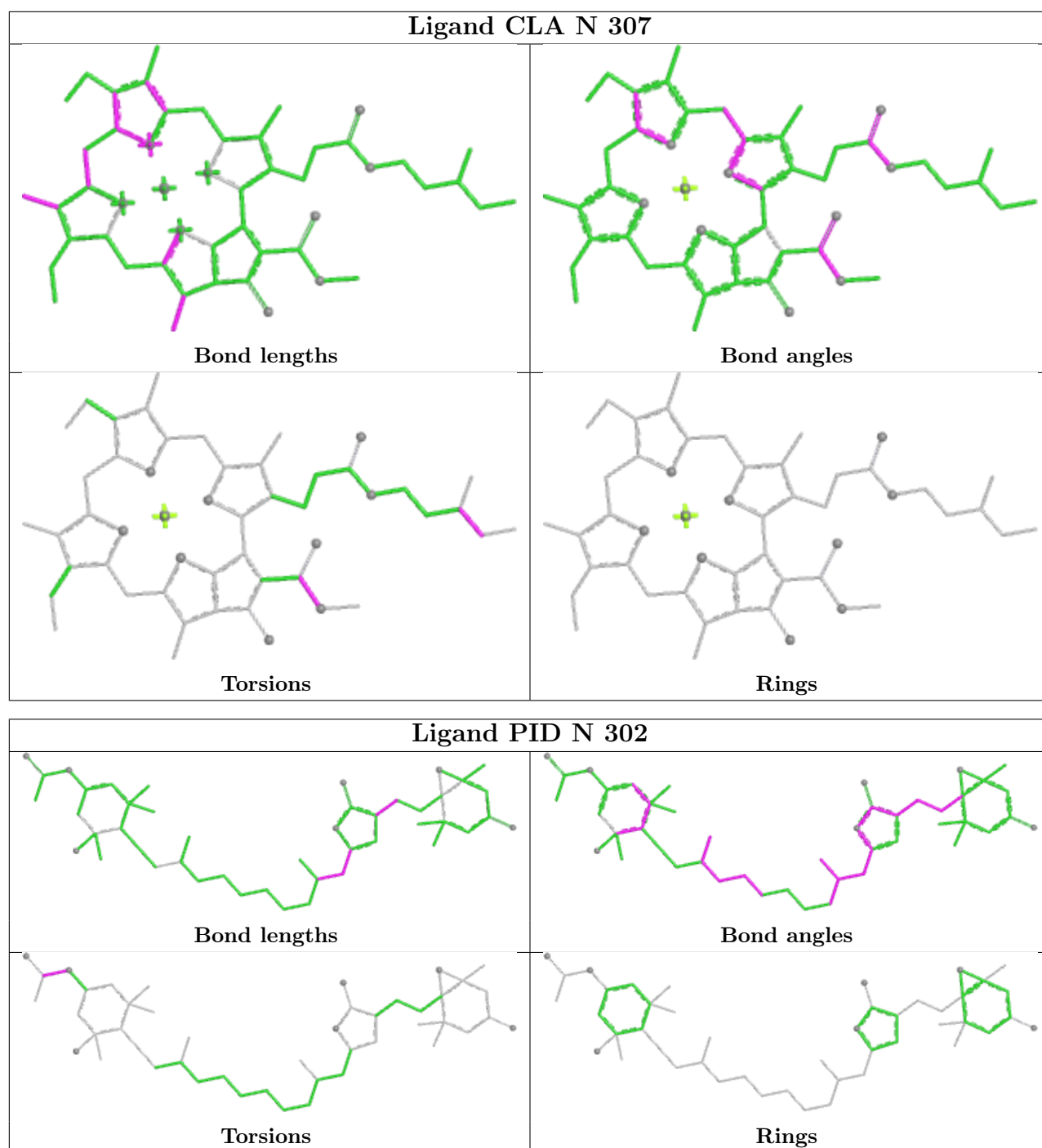
Ligand CLA b 718



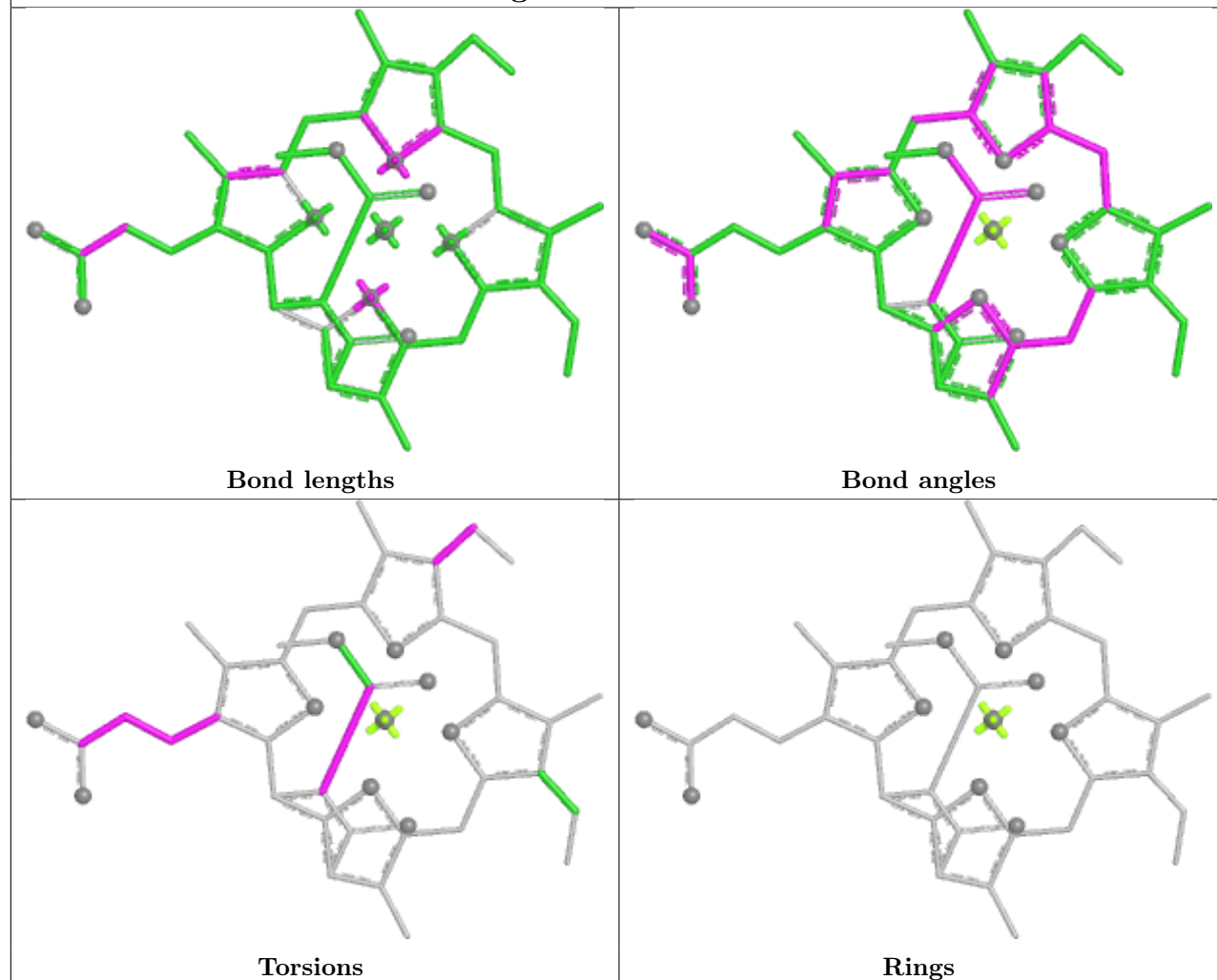
Ligand CLA b 707



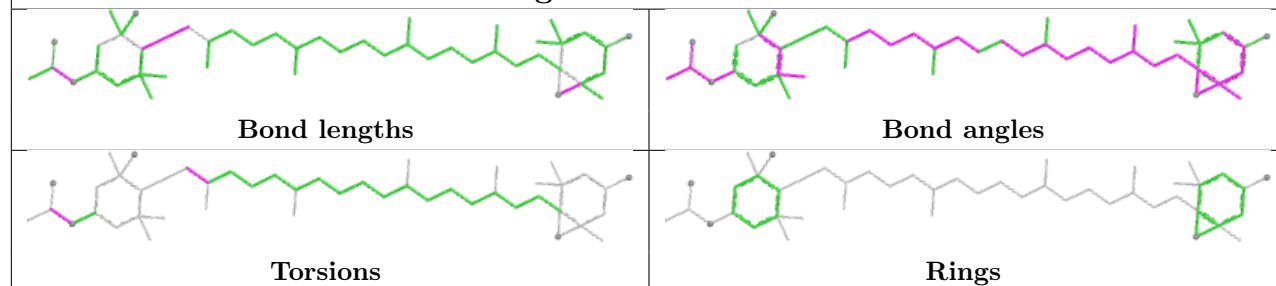


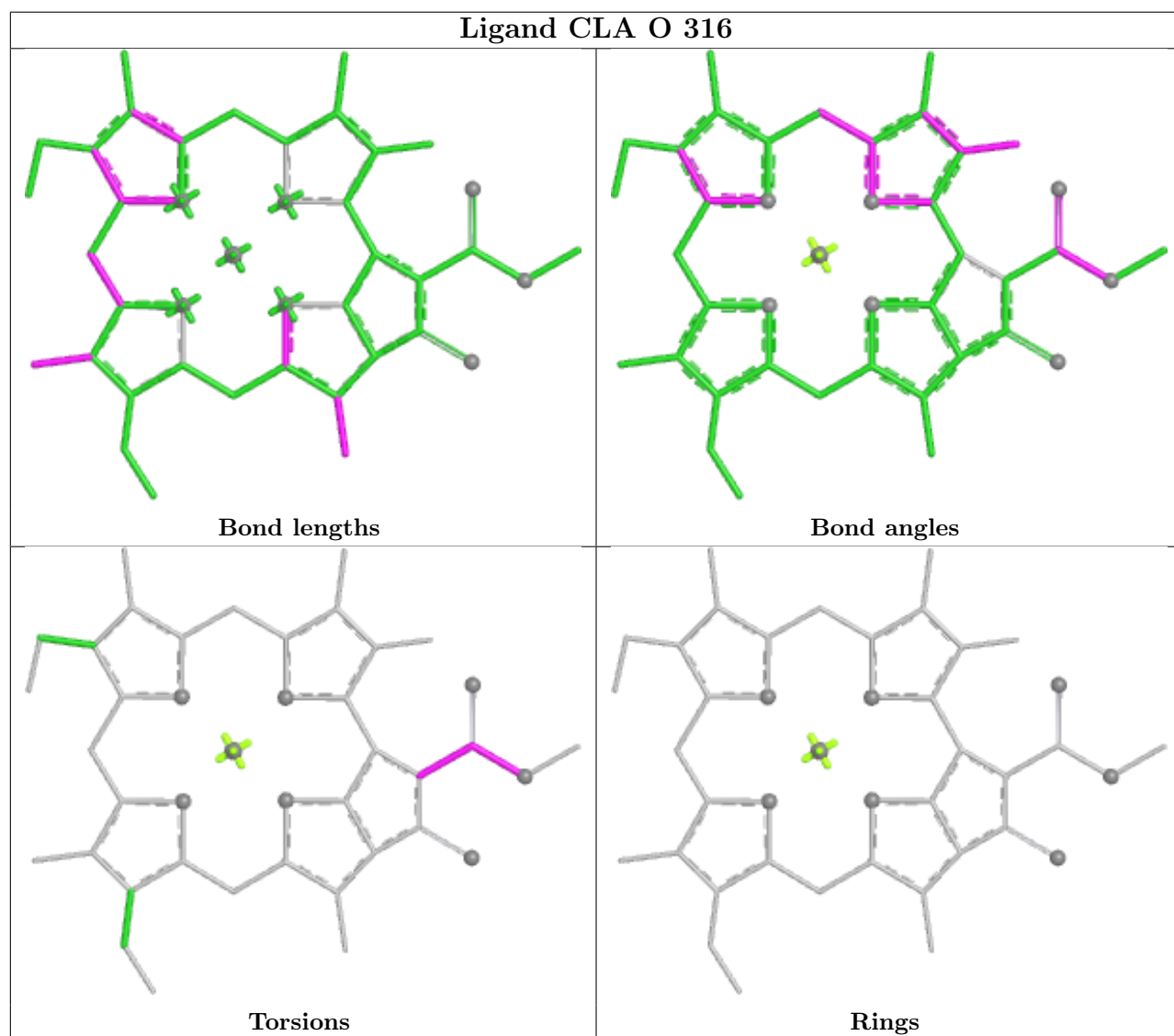
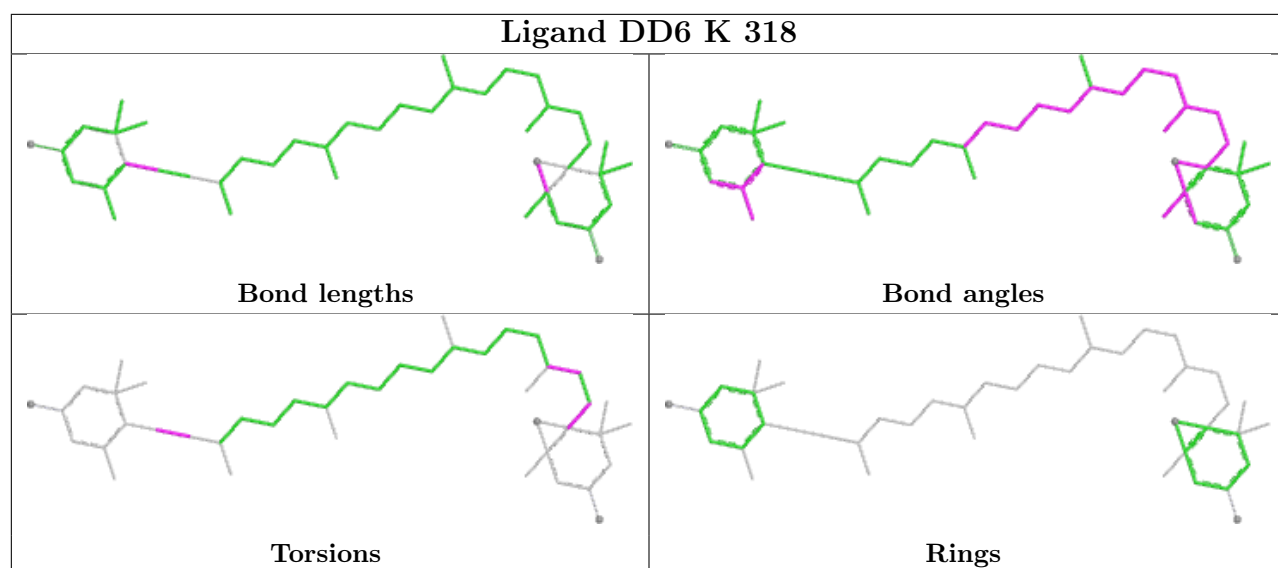


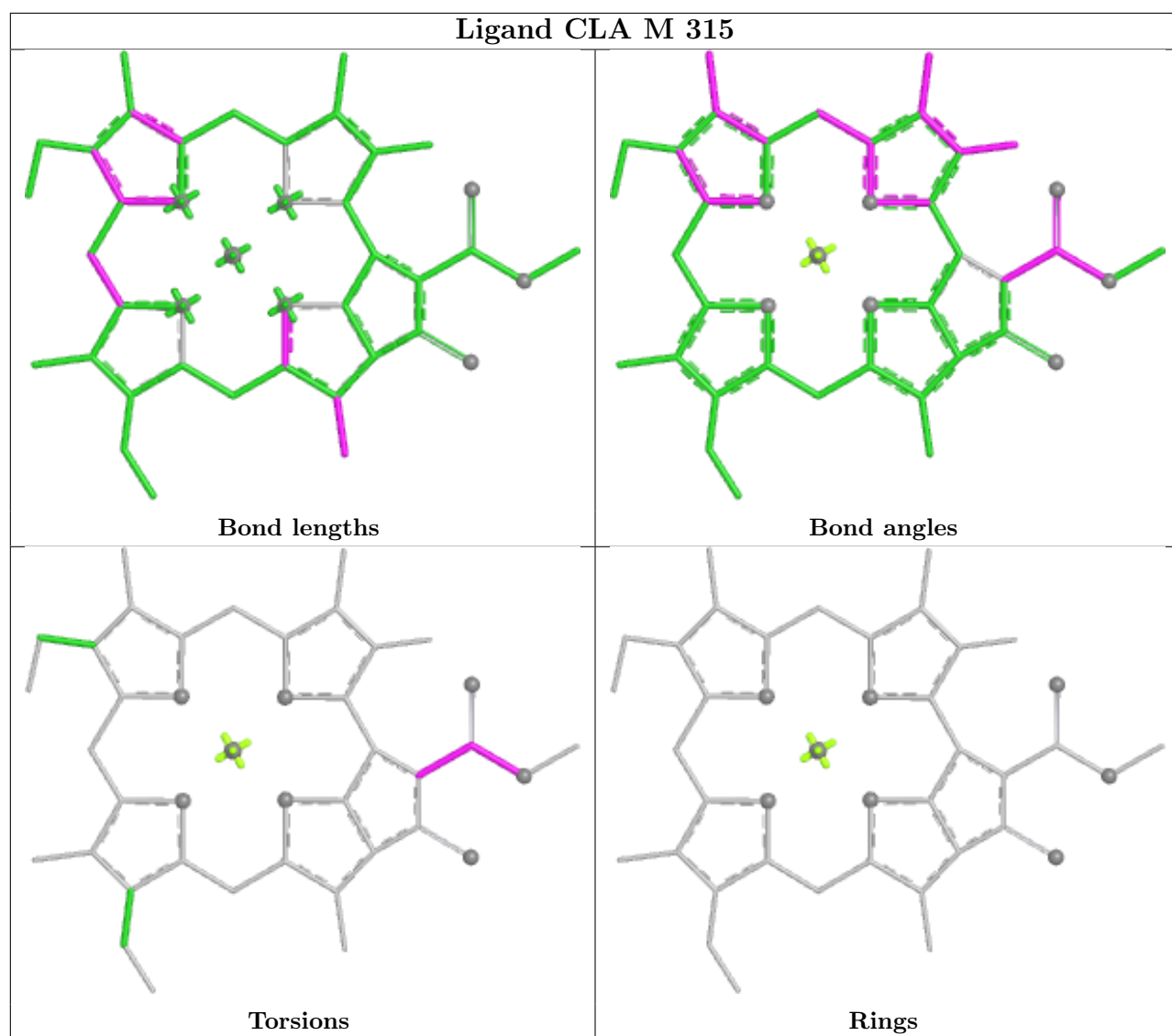
Ligand KC1 F 309



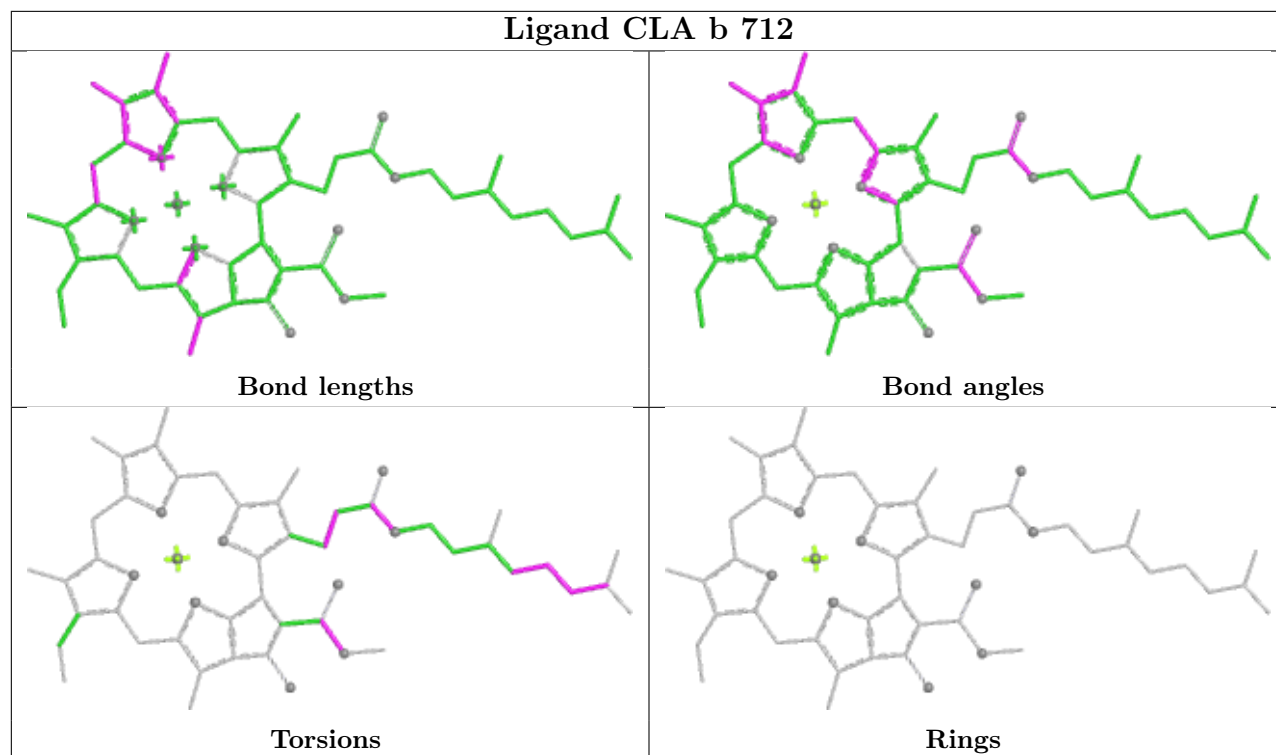
Ligand UIX O 306



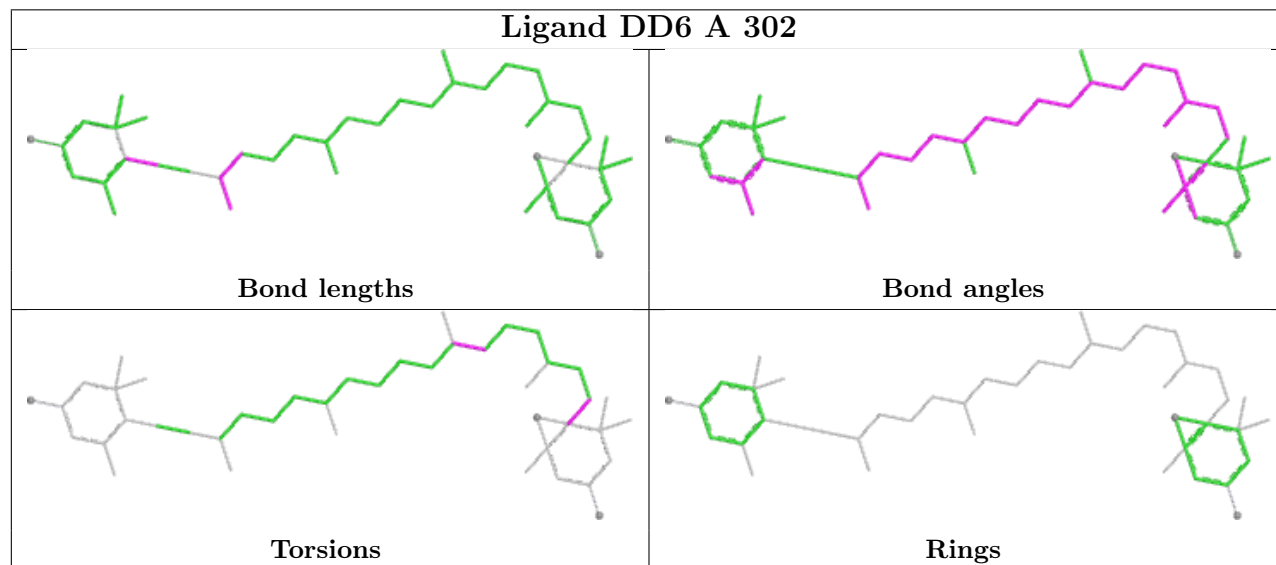


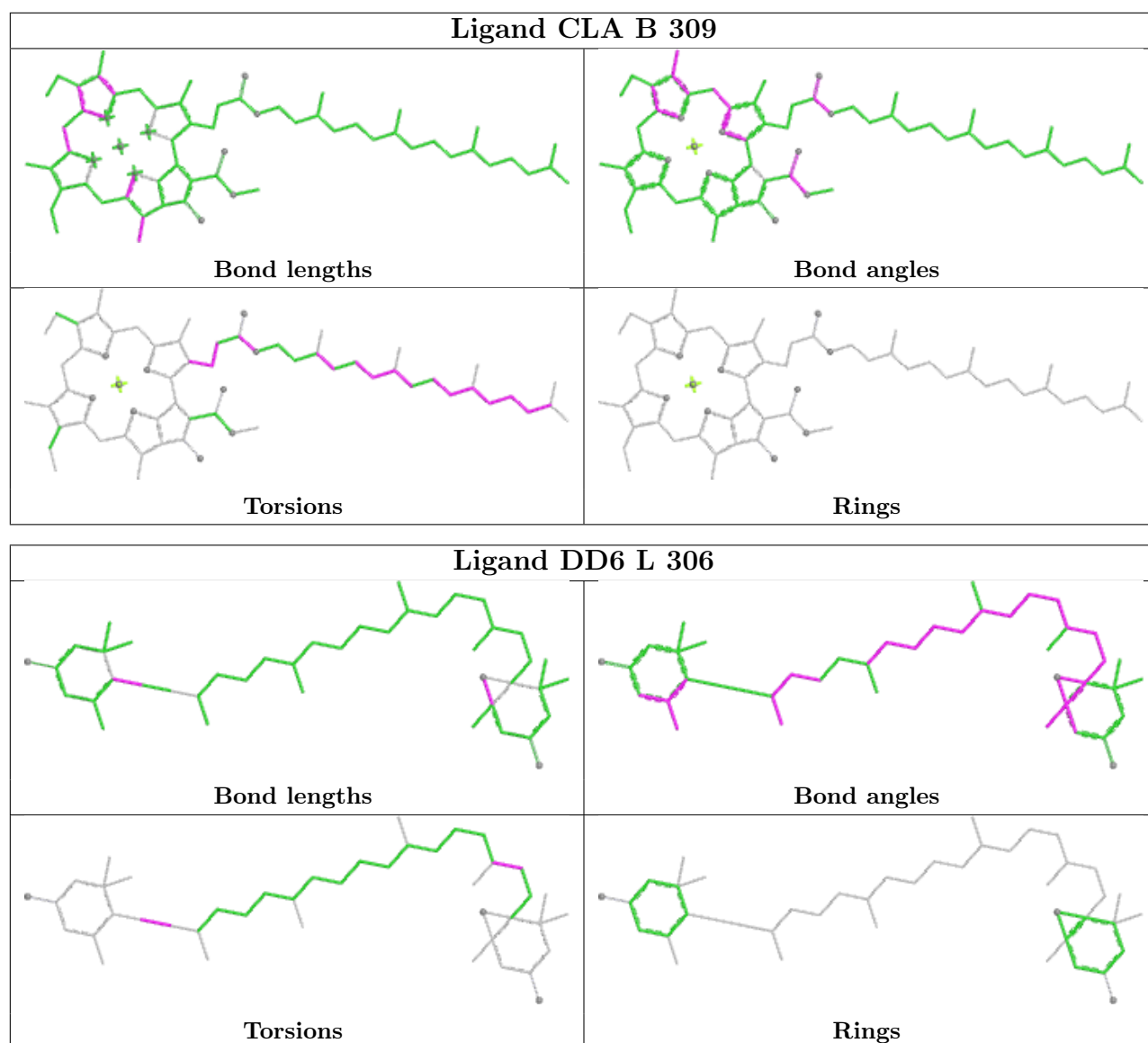


Ligand CLA b 712

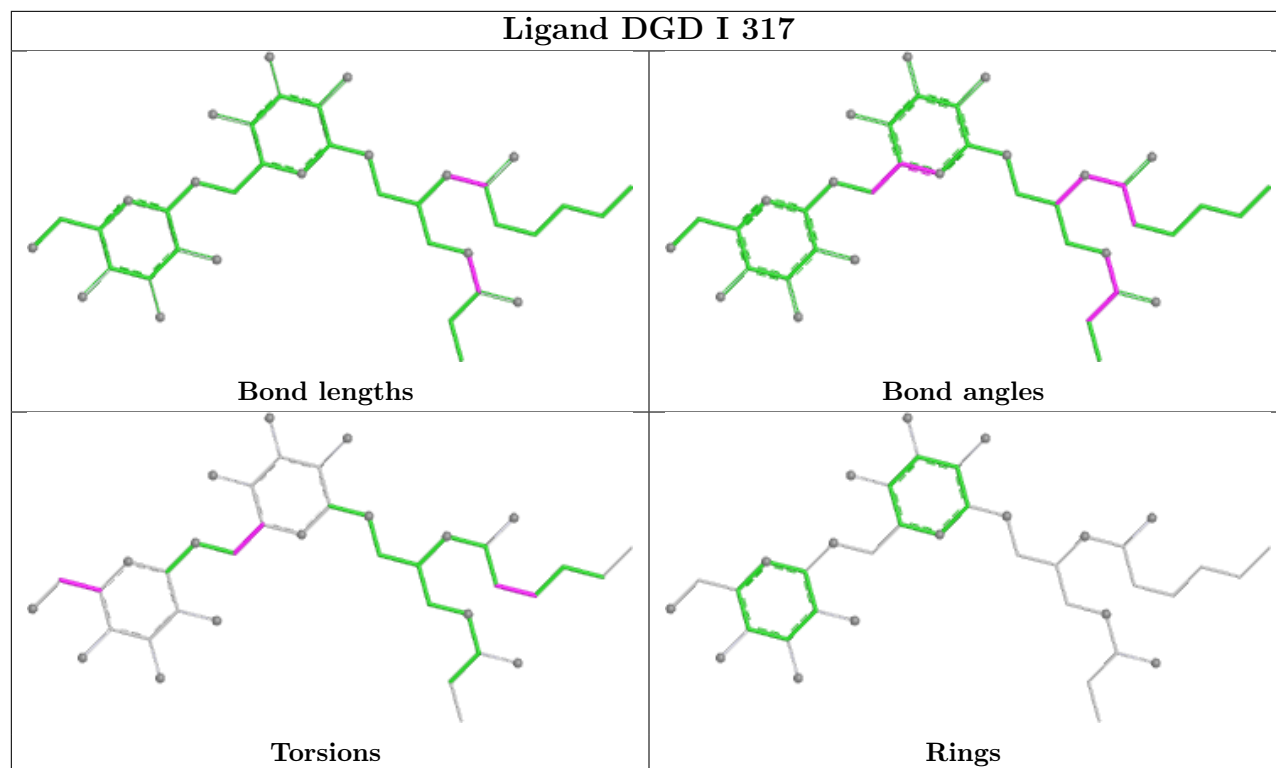


Ligand DD6 A 302

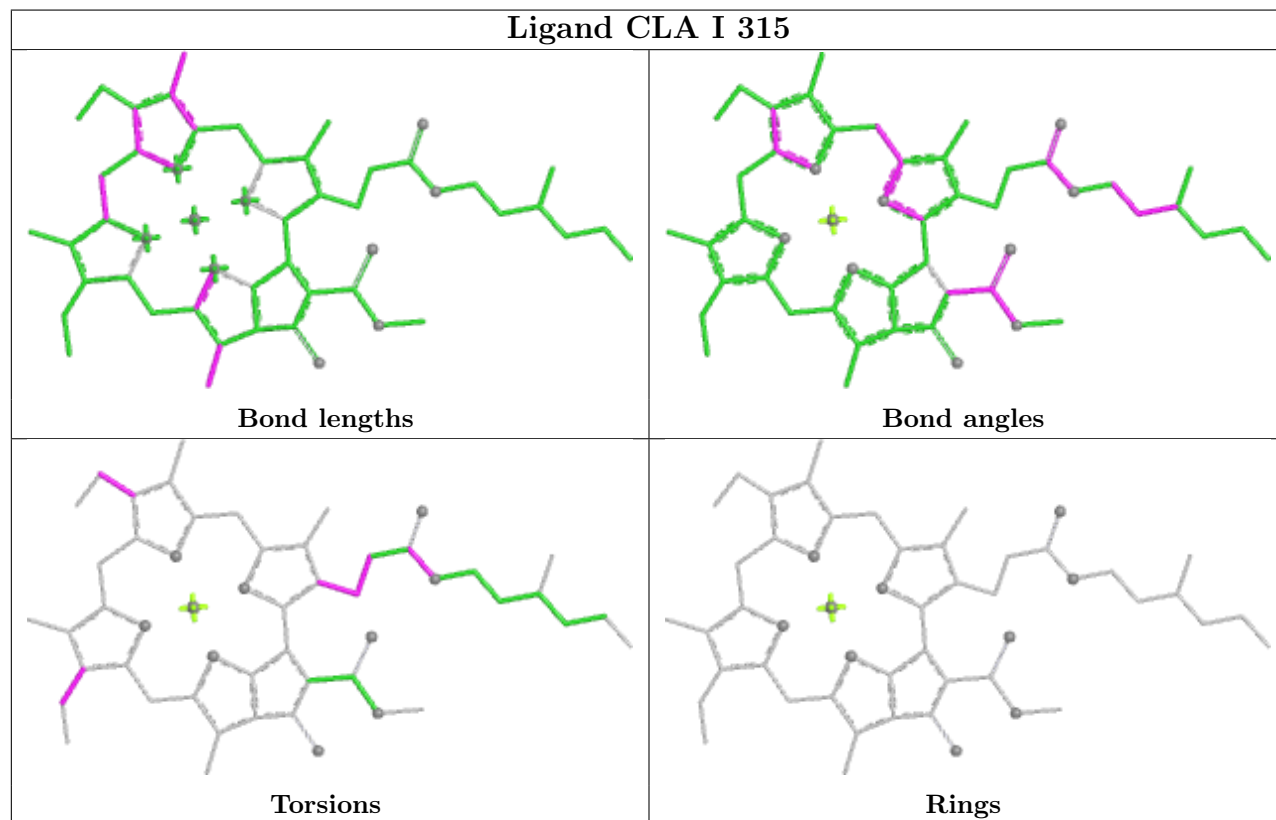




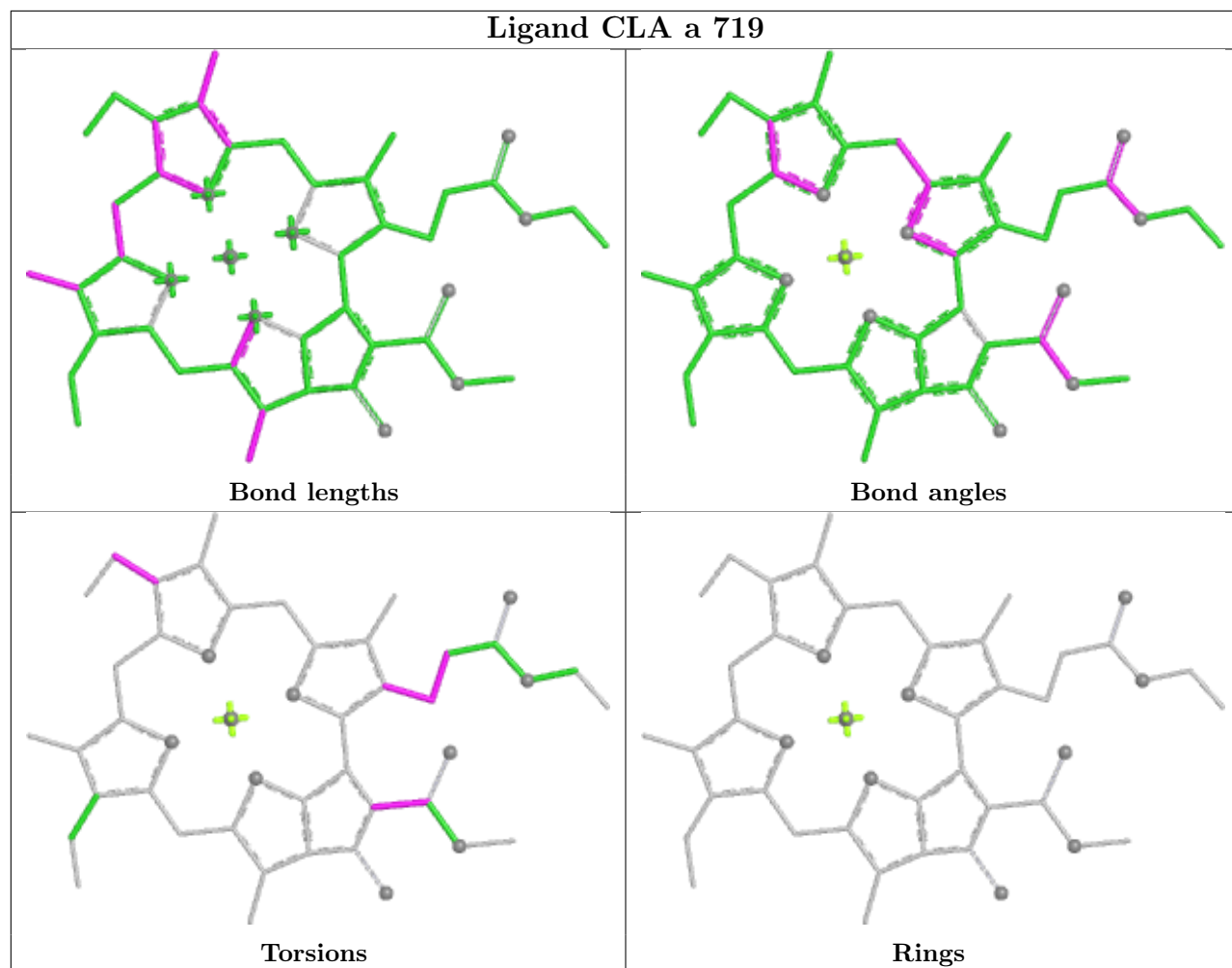
Ligand DGD I 317



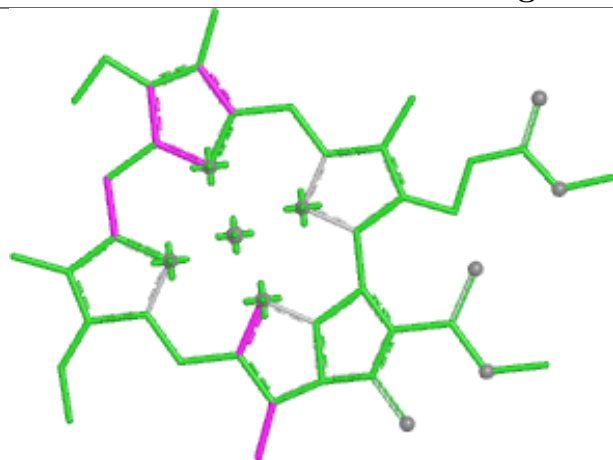
Ligand CLA I 315



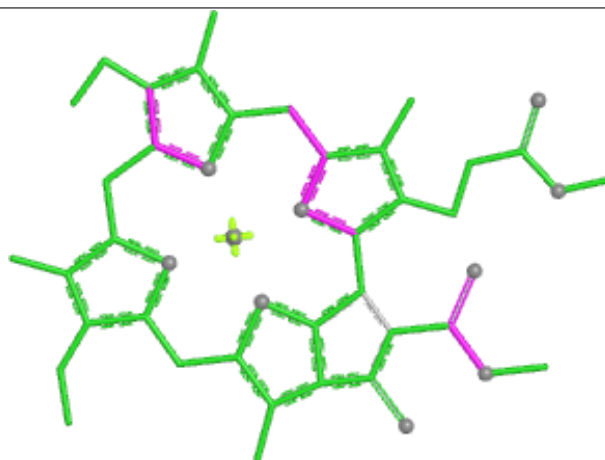
Ligand CLA a 719



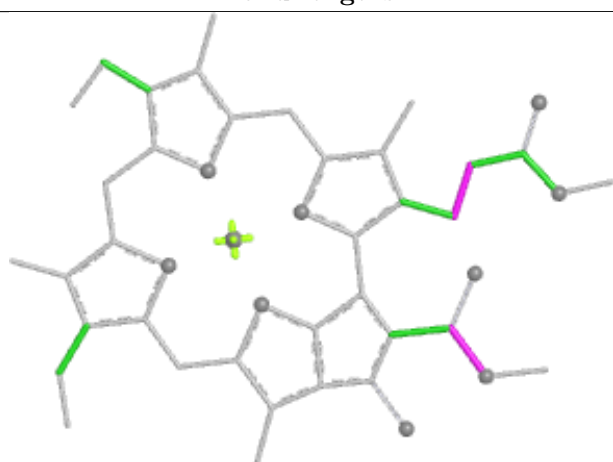
Ligand CLA J 315



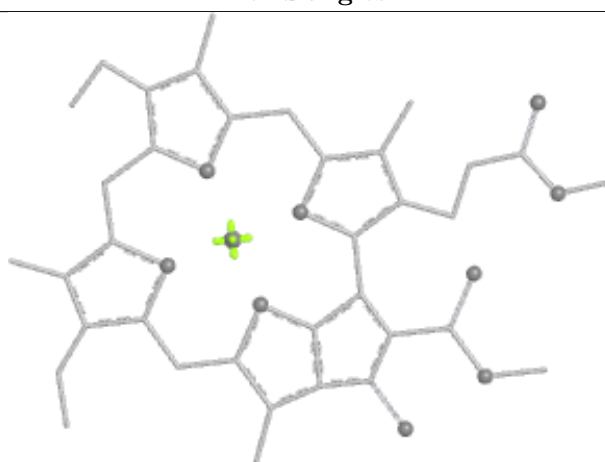
Bond lengths



Bond angles

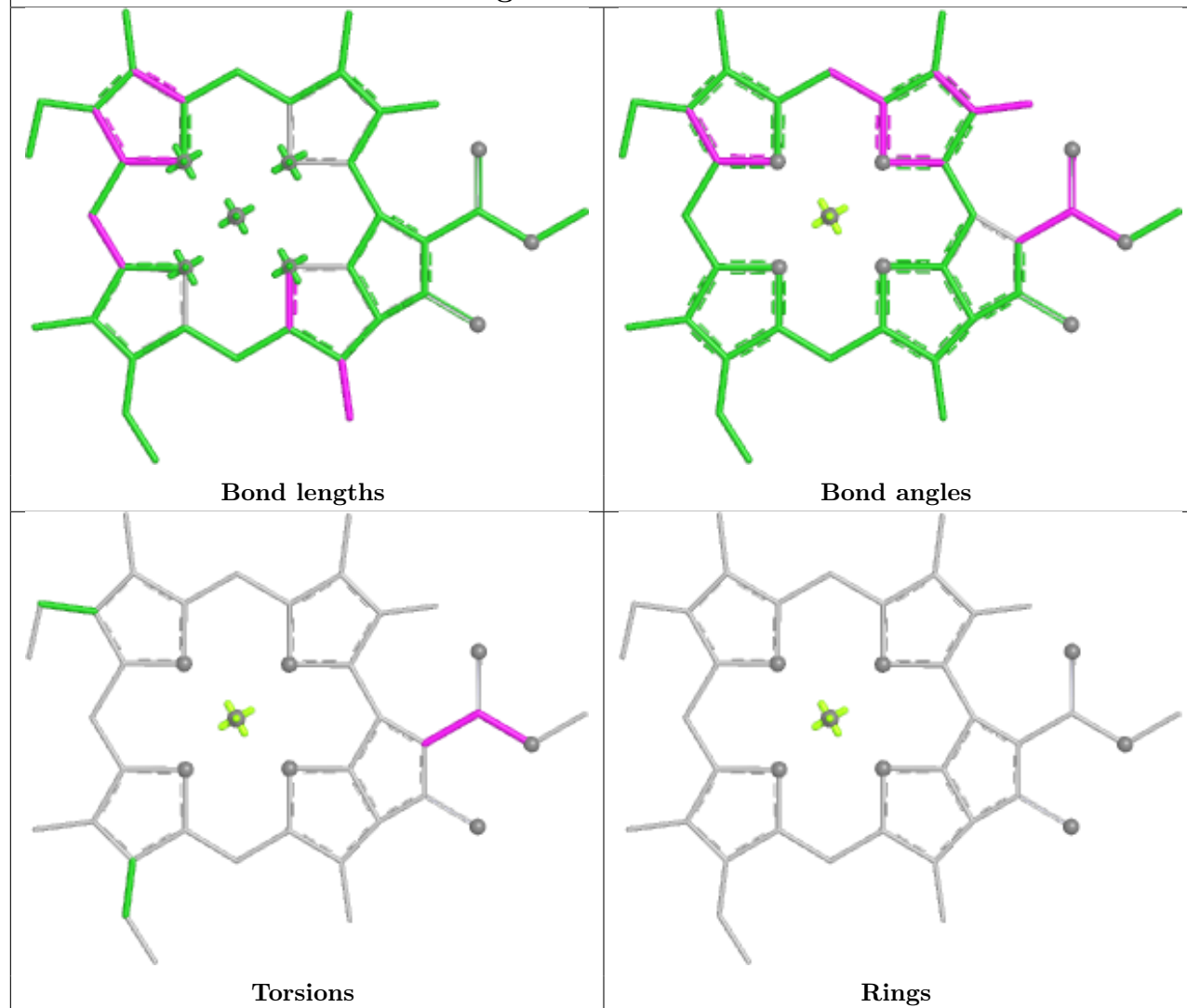


Torsions

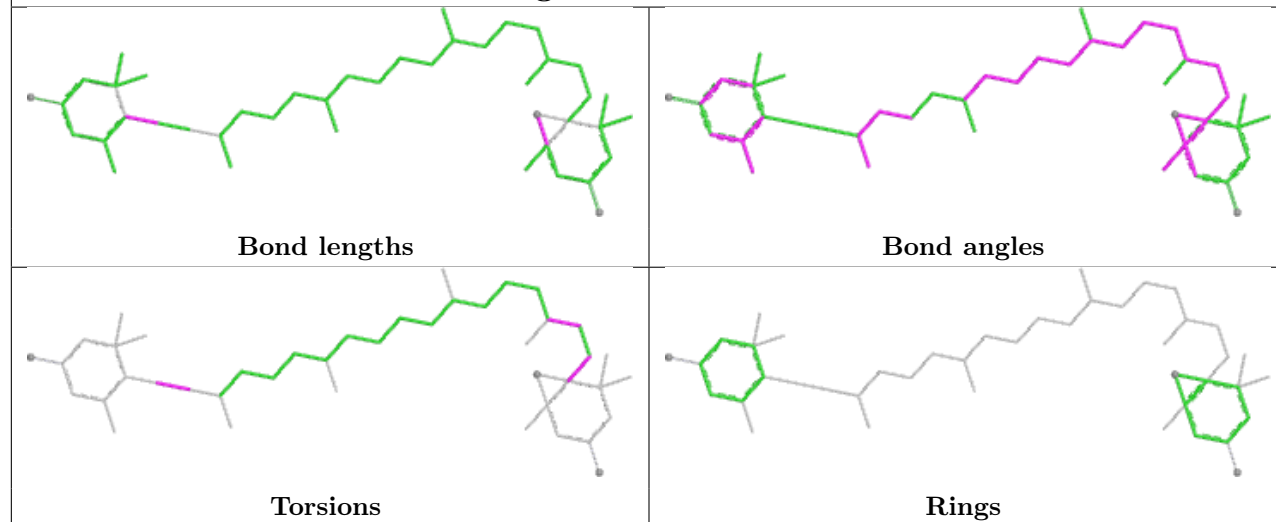


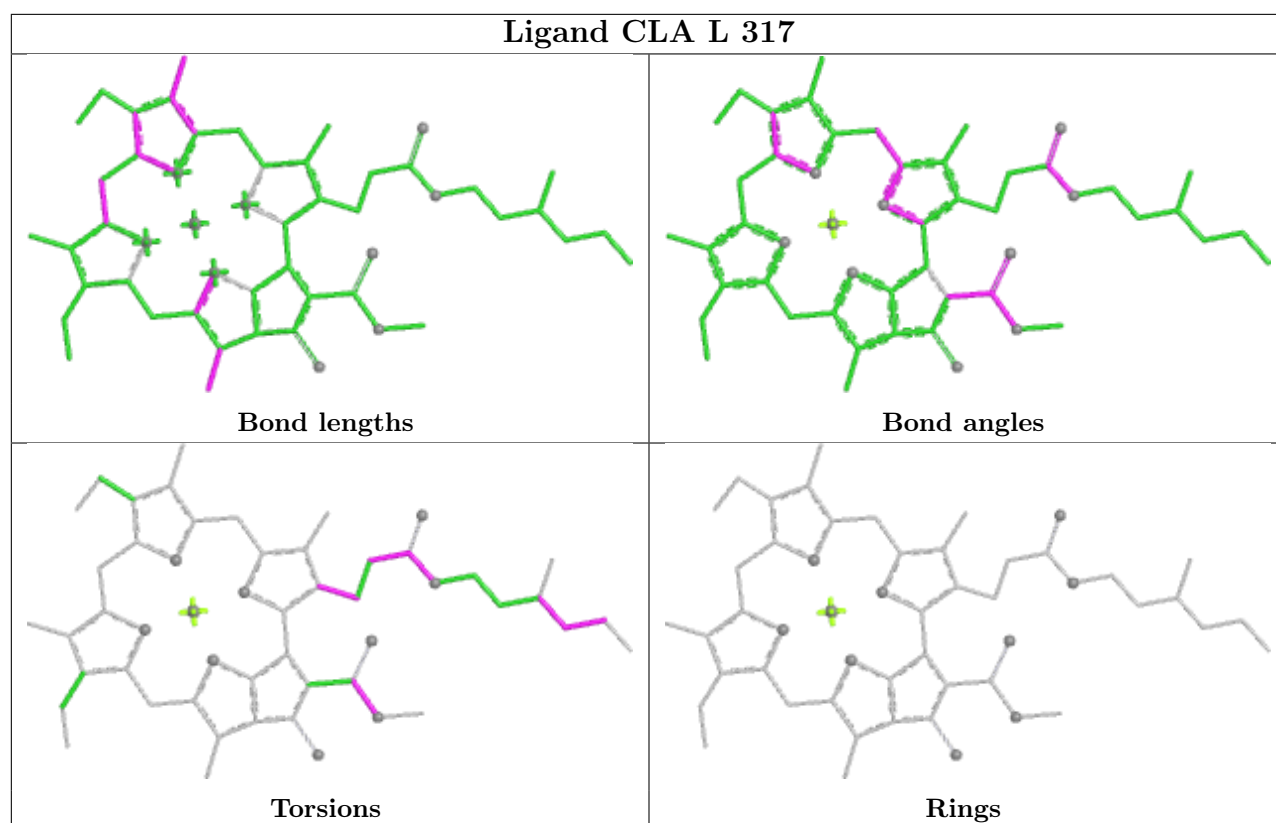
Rings

Ligand CLA F 315

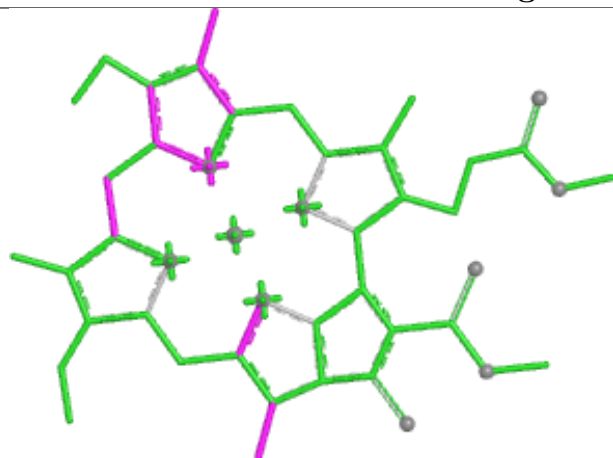


Ligand DD6 L 302

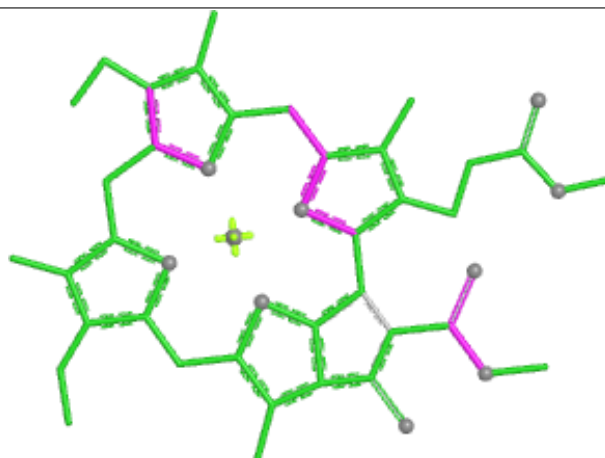




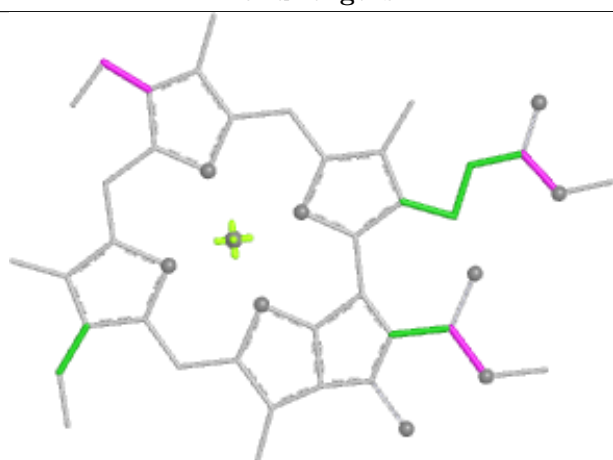
Ligand CLA J 306



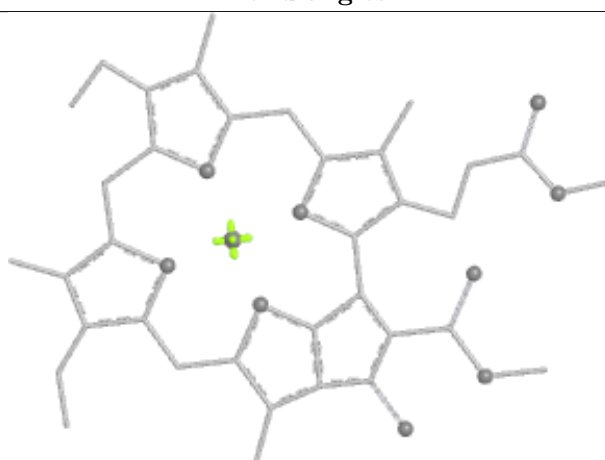
Bond lengths



Bond angles

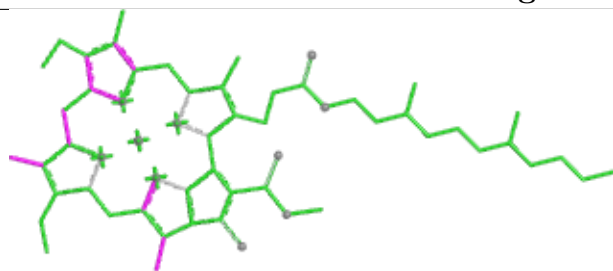


Torsions

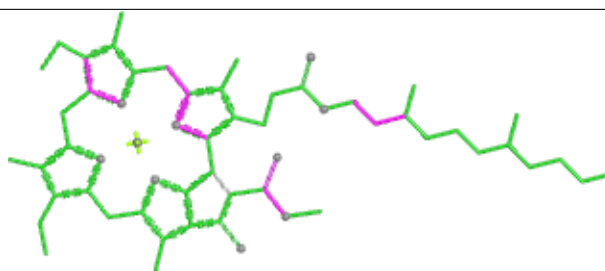


Rings

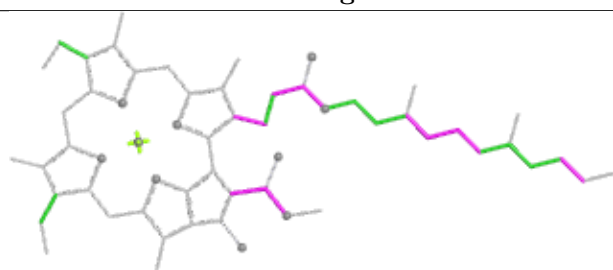
Ligand CLA a 706



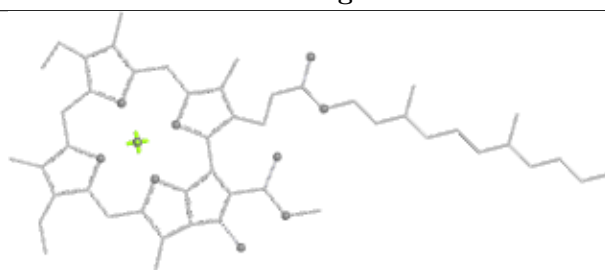
Bond lengths



Bond angles

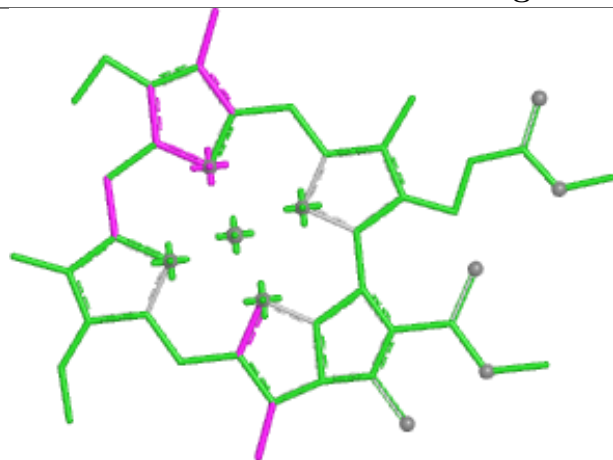


Torsions

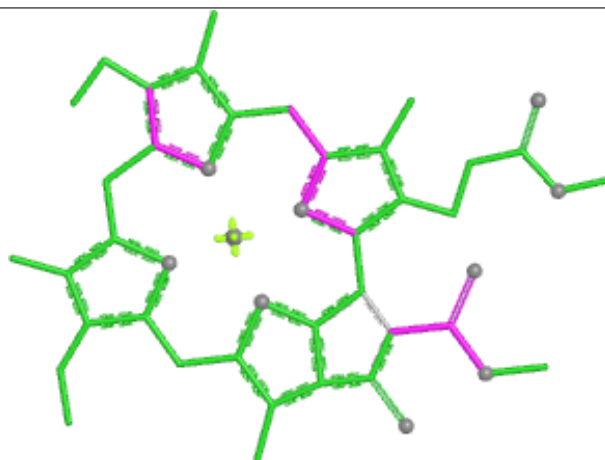


Rings

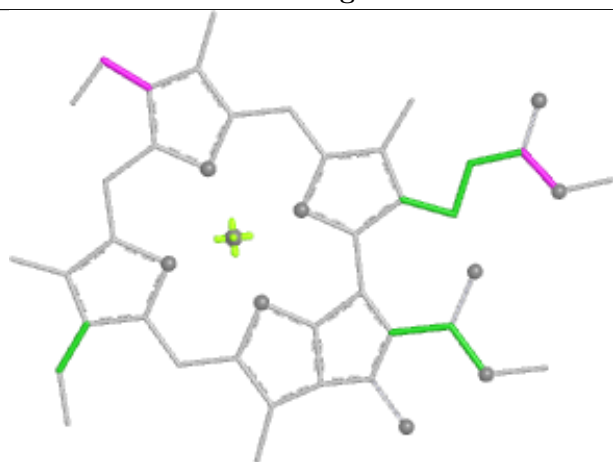
Ligand CLA K 316



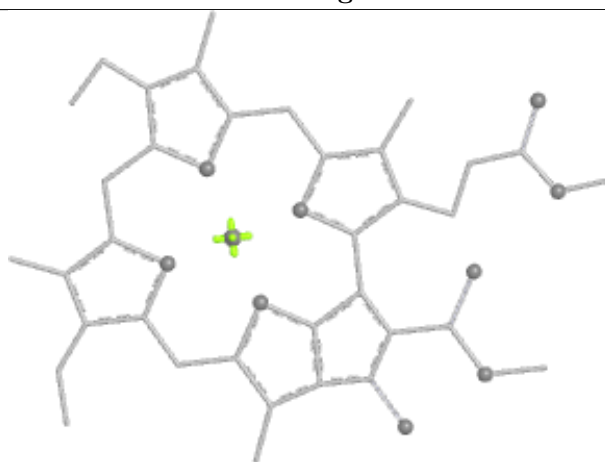
Bond lengths



Bond angles

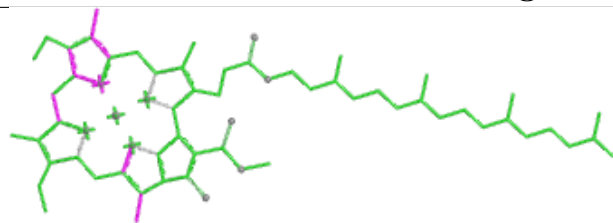


Torsions

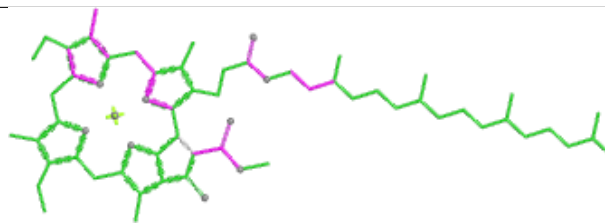


Rings

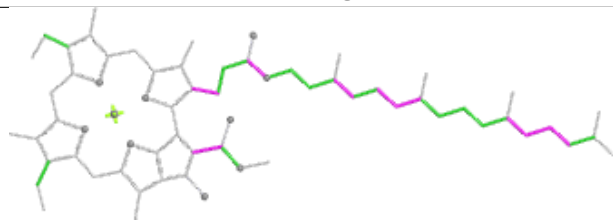
Ligand CLA a 724



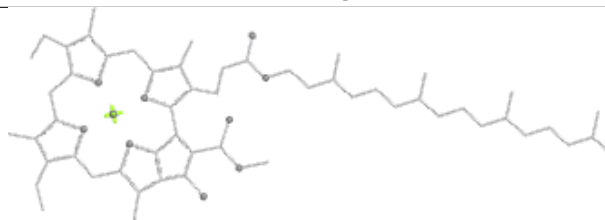
Bond lengths



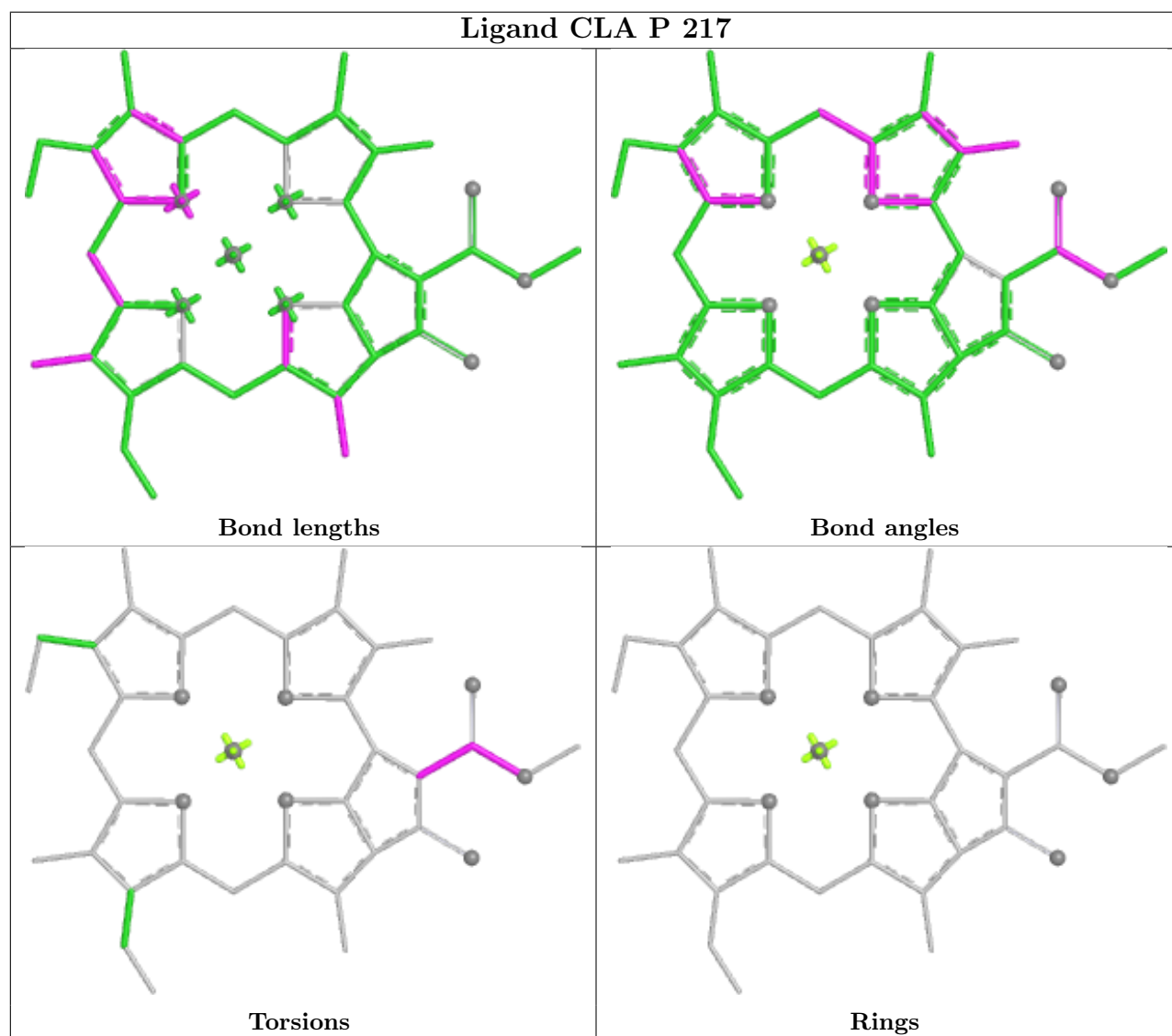
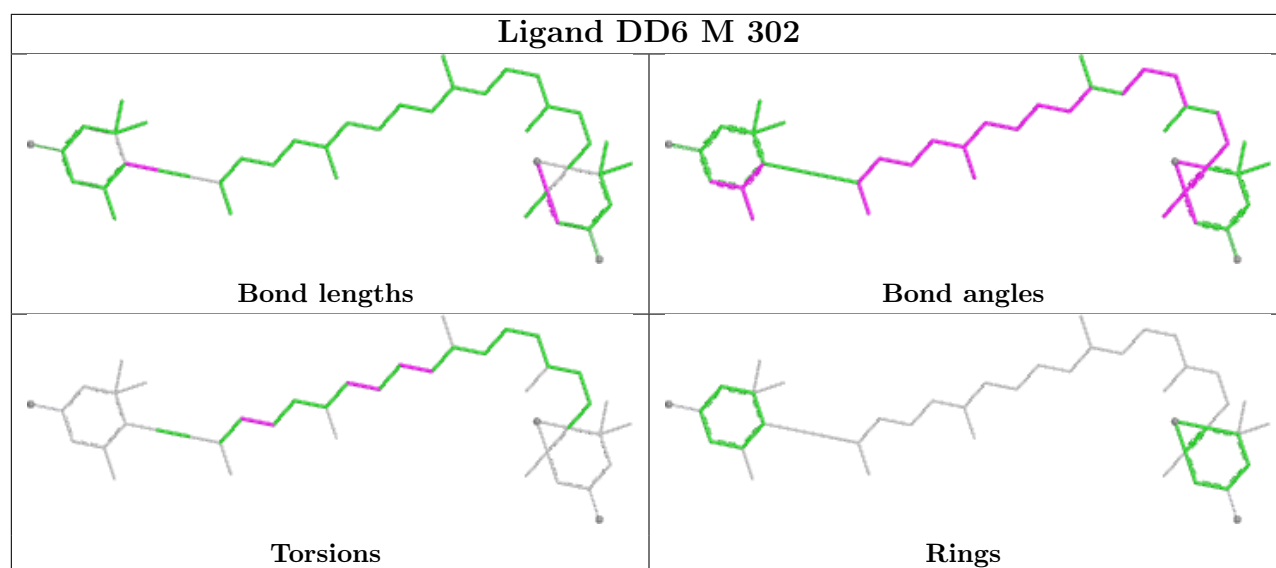
Bond angles



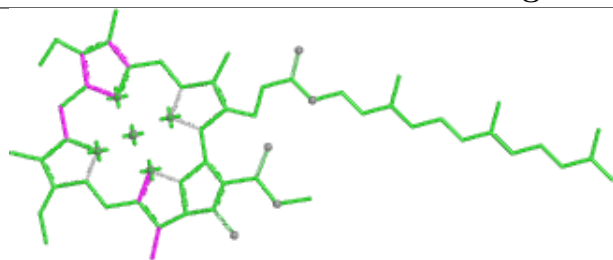
Torsions



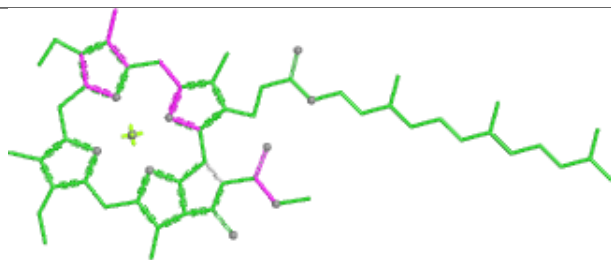
Rings



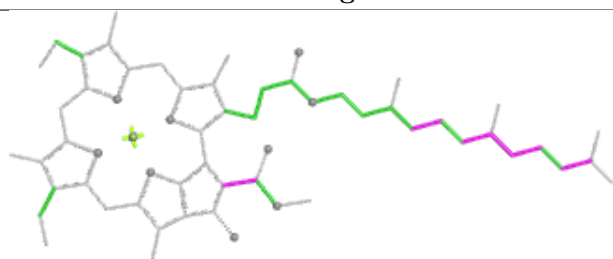
Ligand CLA I 304



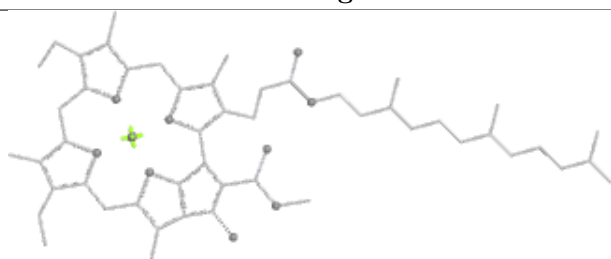
Bond lengths



Bond angles

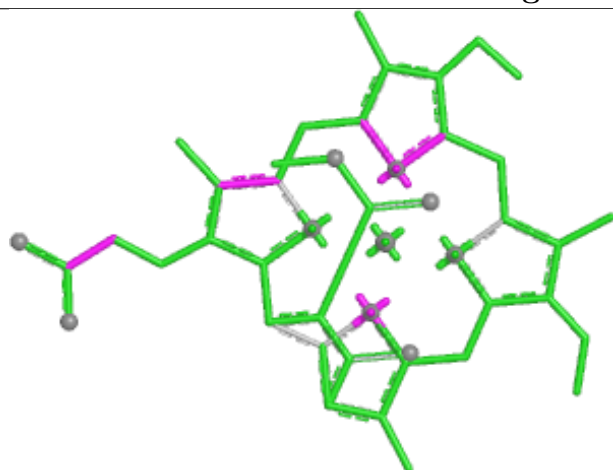


Torsions

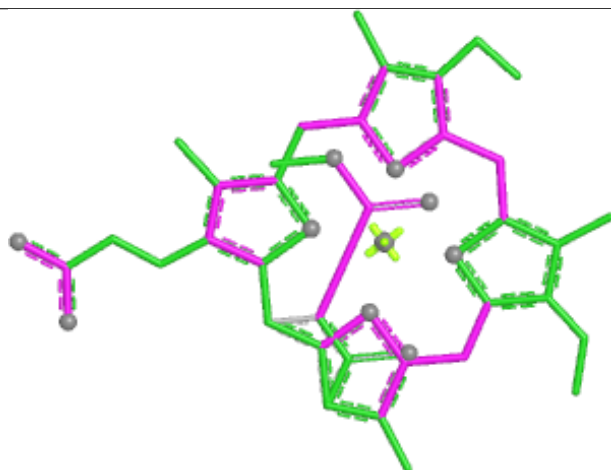


Rings

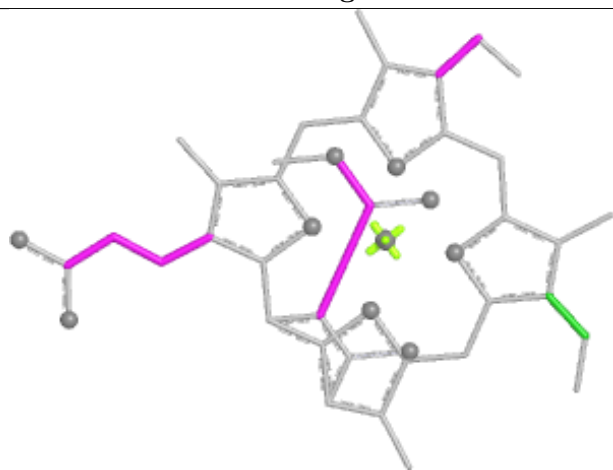
Ligand KC1 I 314



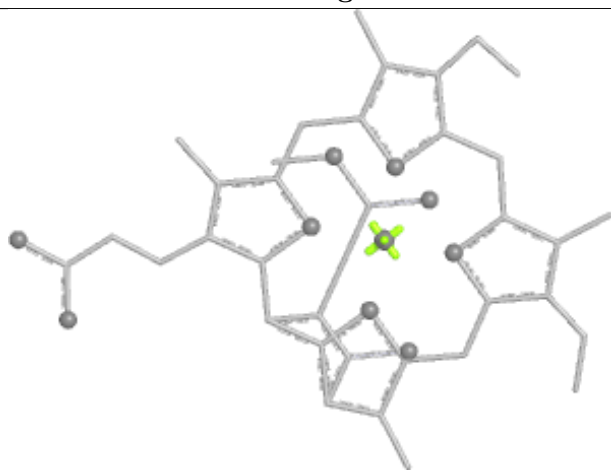
Bond lengths



Bond angles

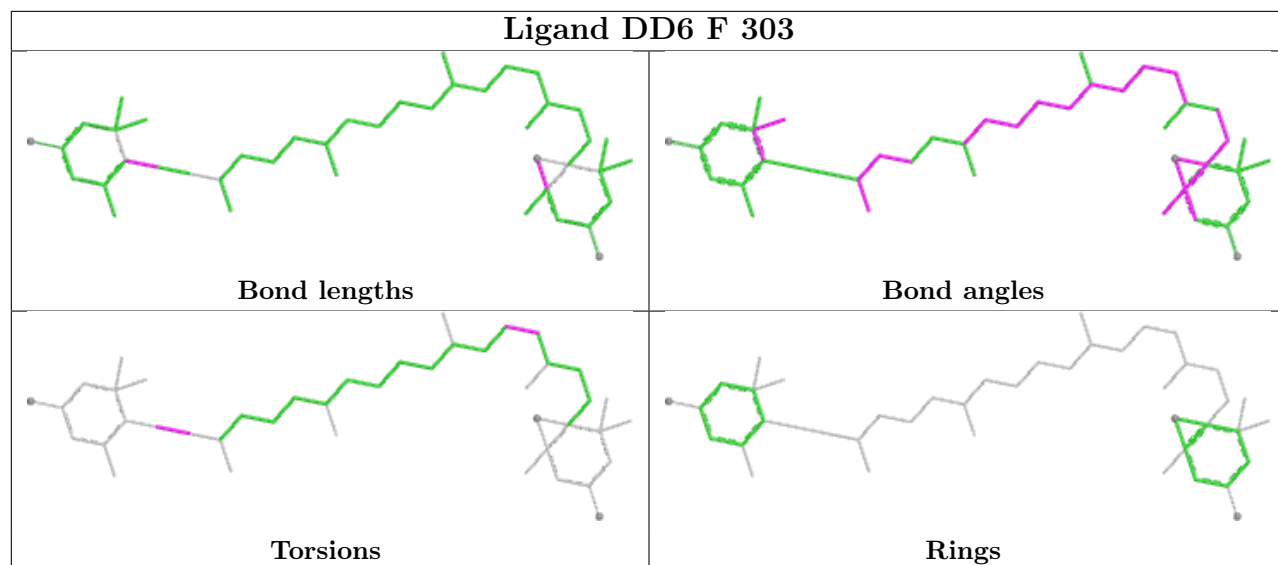


Torsions

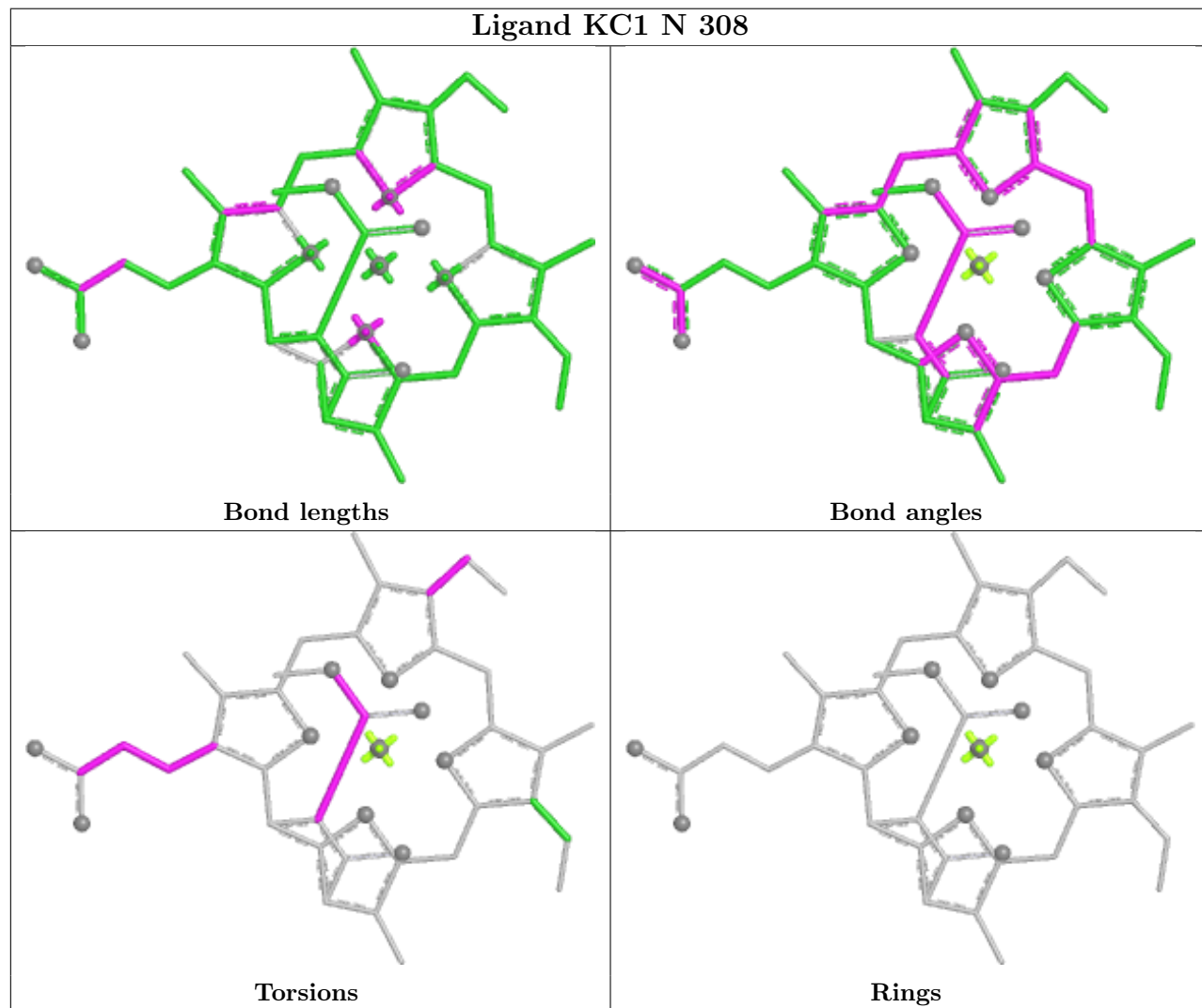


Rings

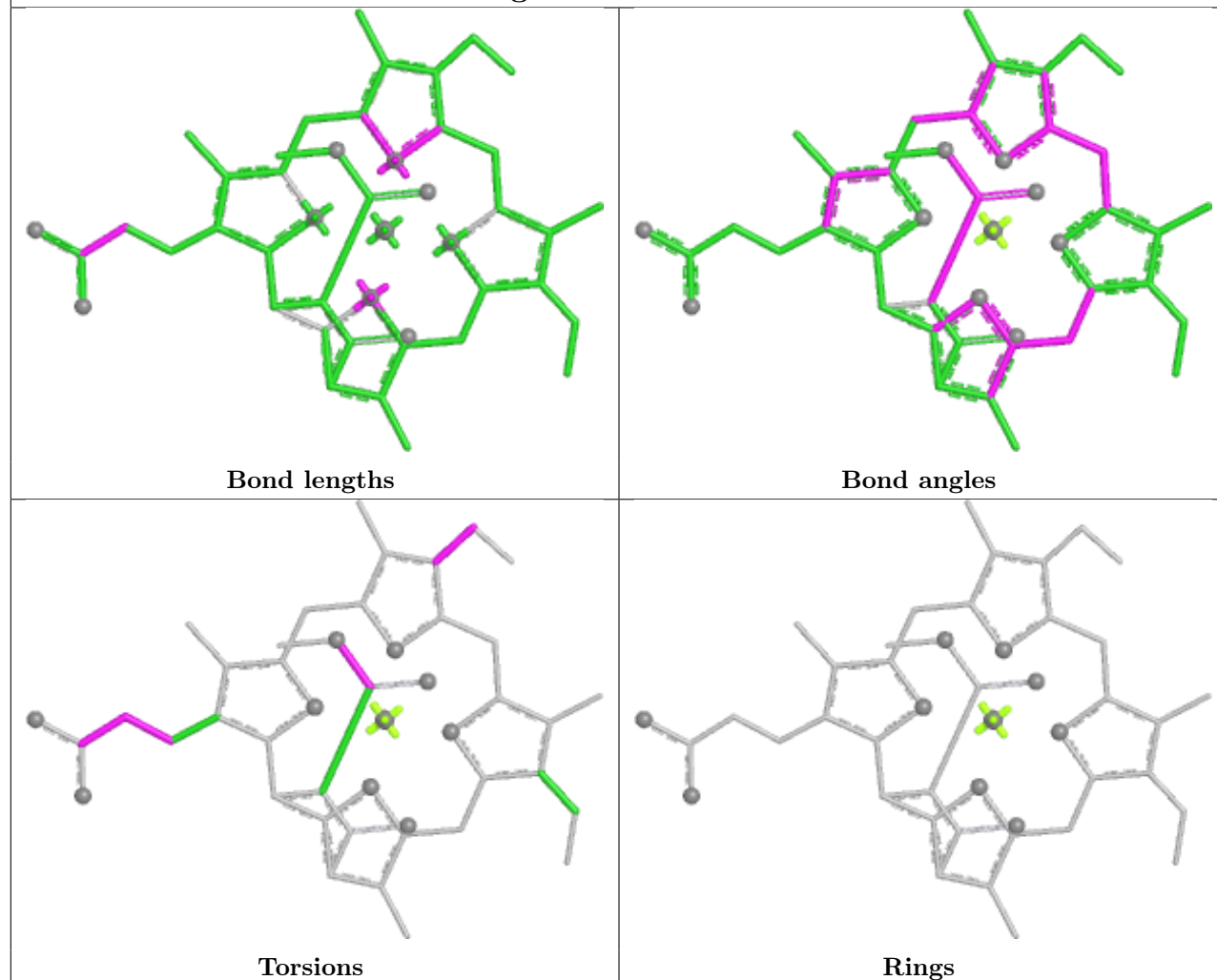
Ligand DD6 F 303



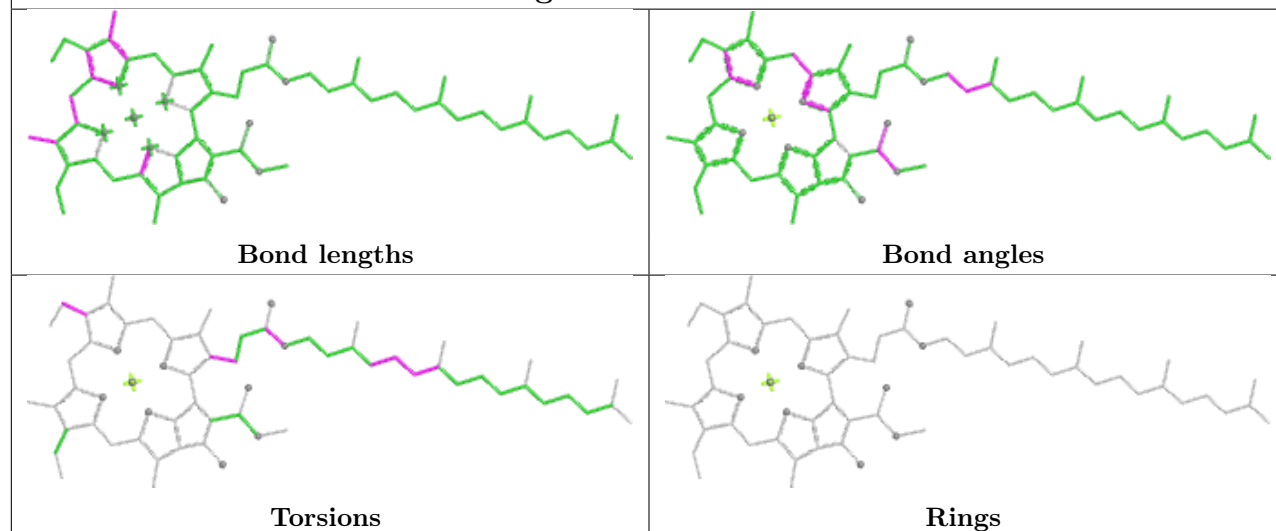
Ligand KC1 N 308

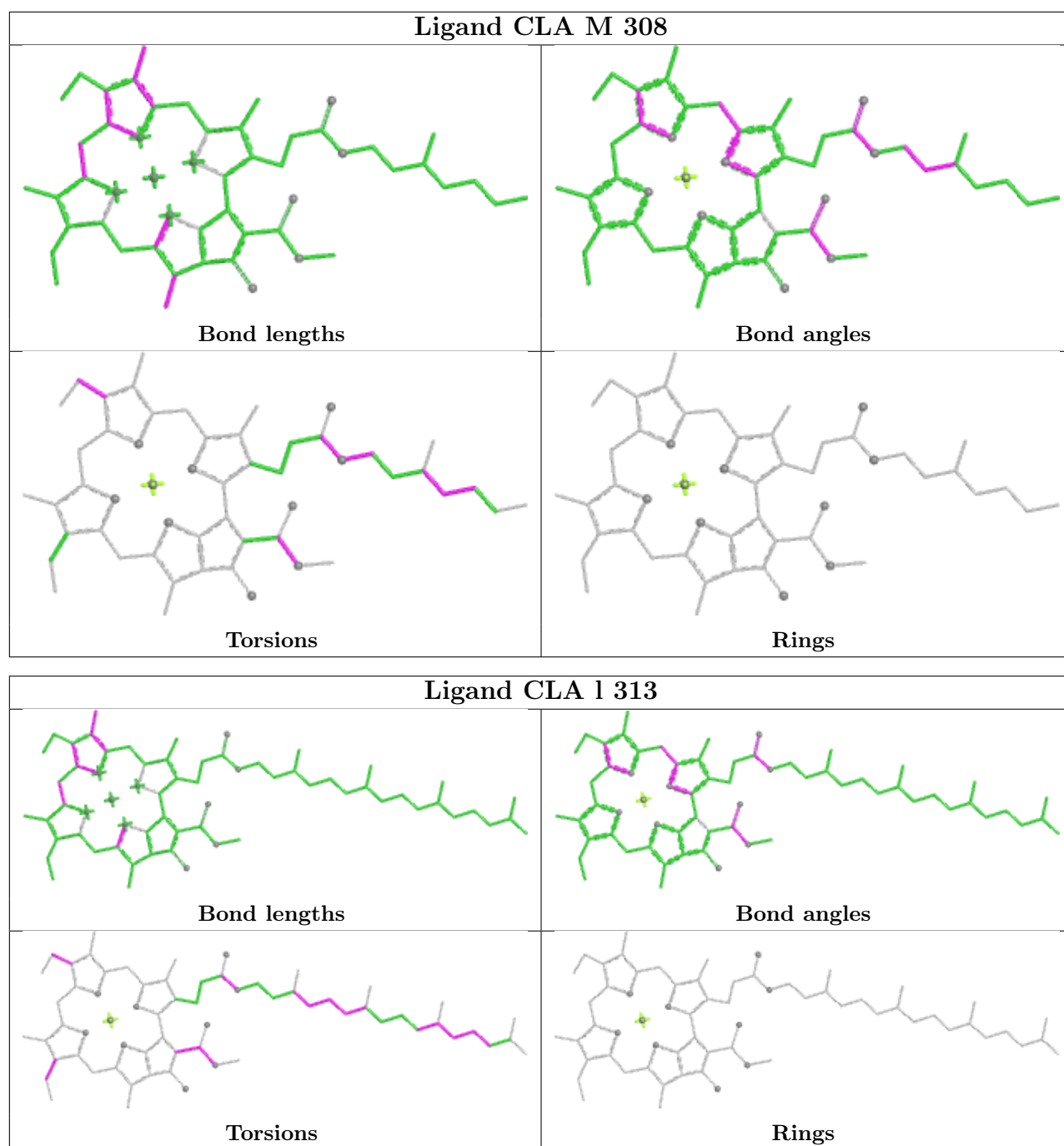


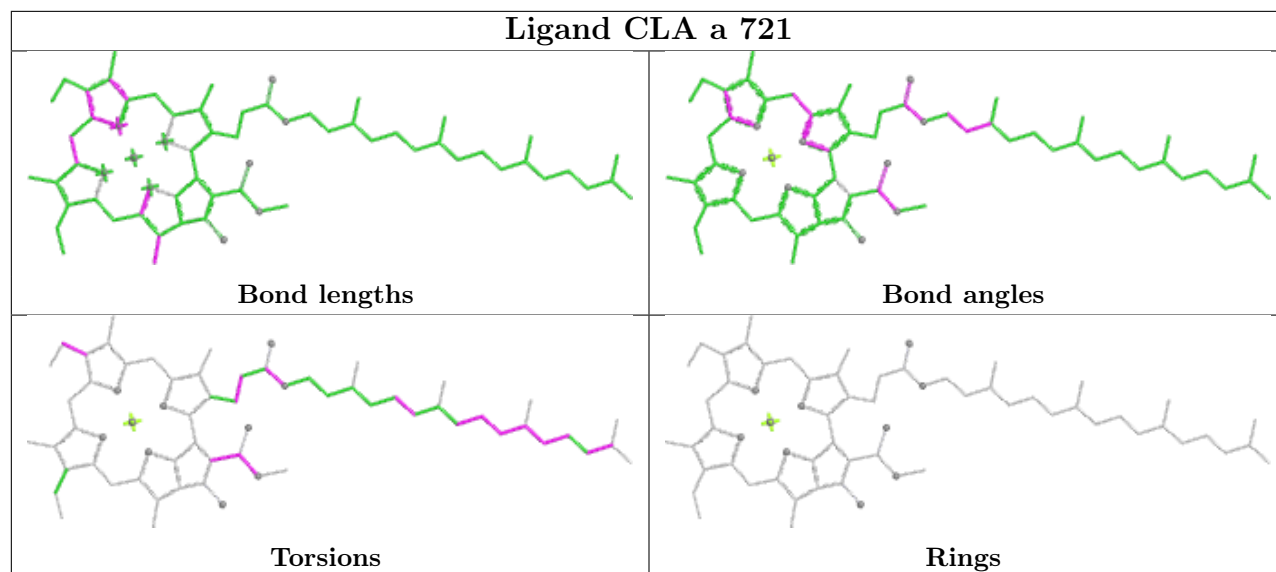
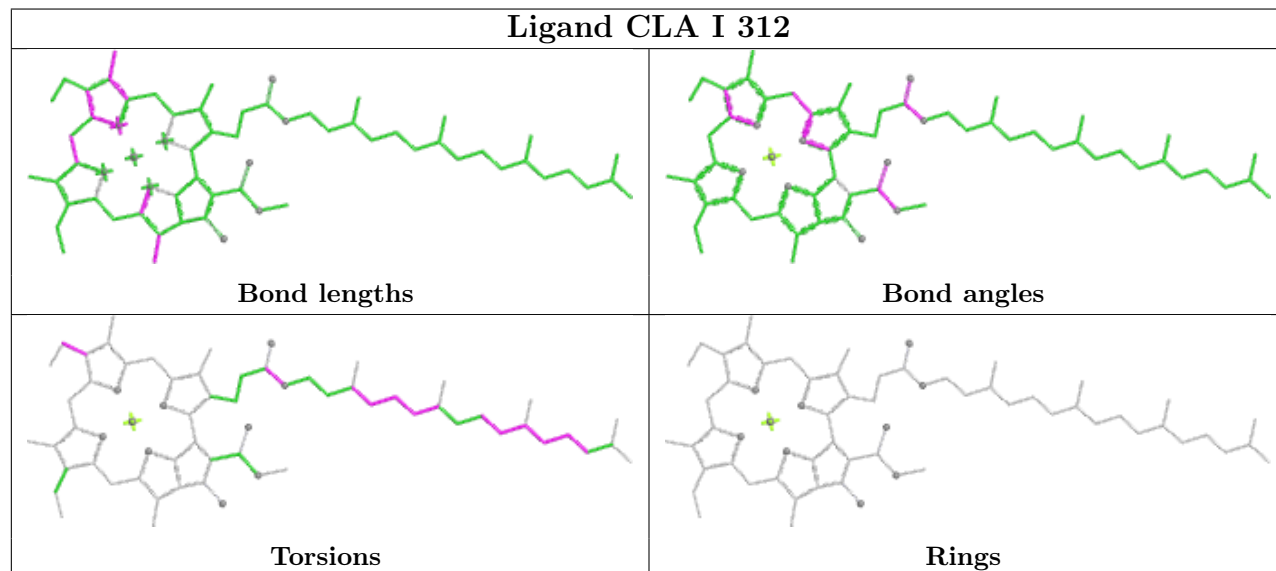
Ligand KC1 F 314

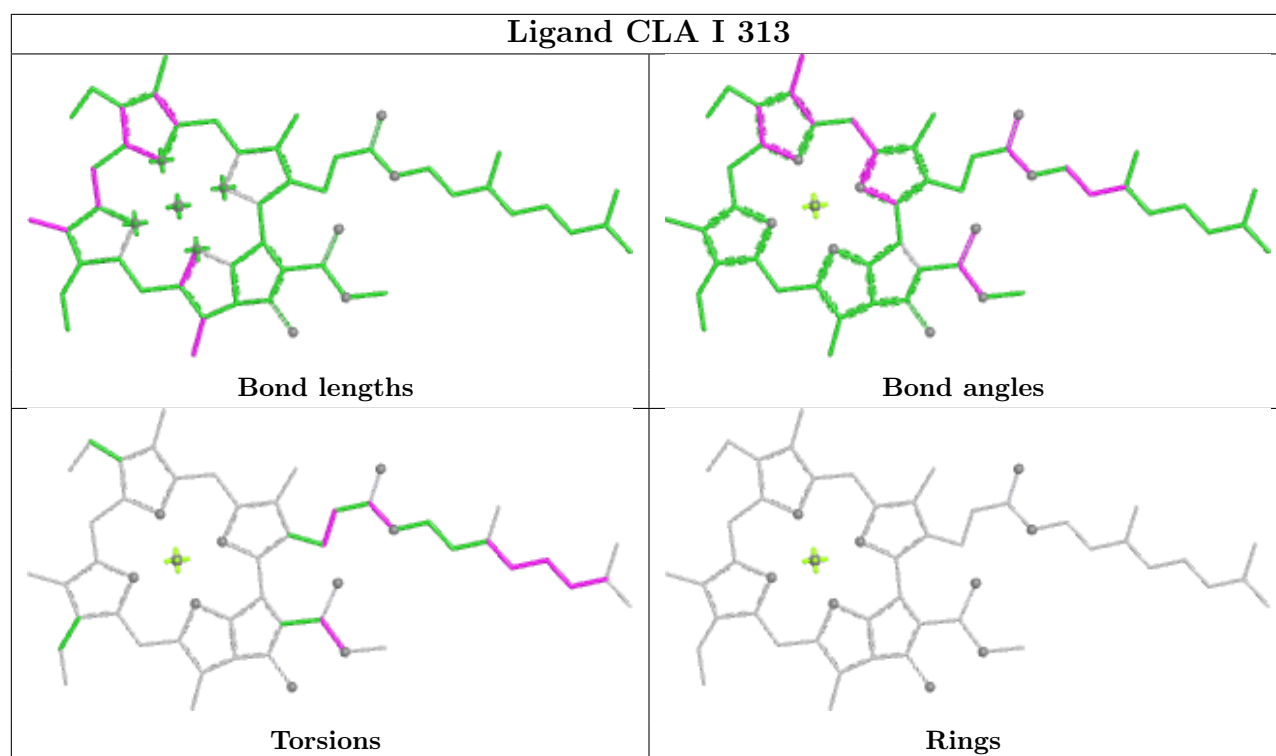


Ligand CLA b 728

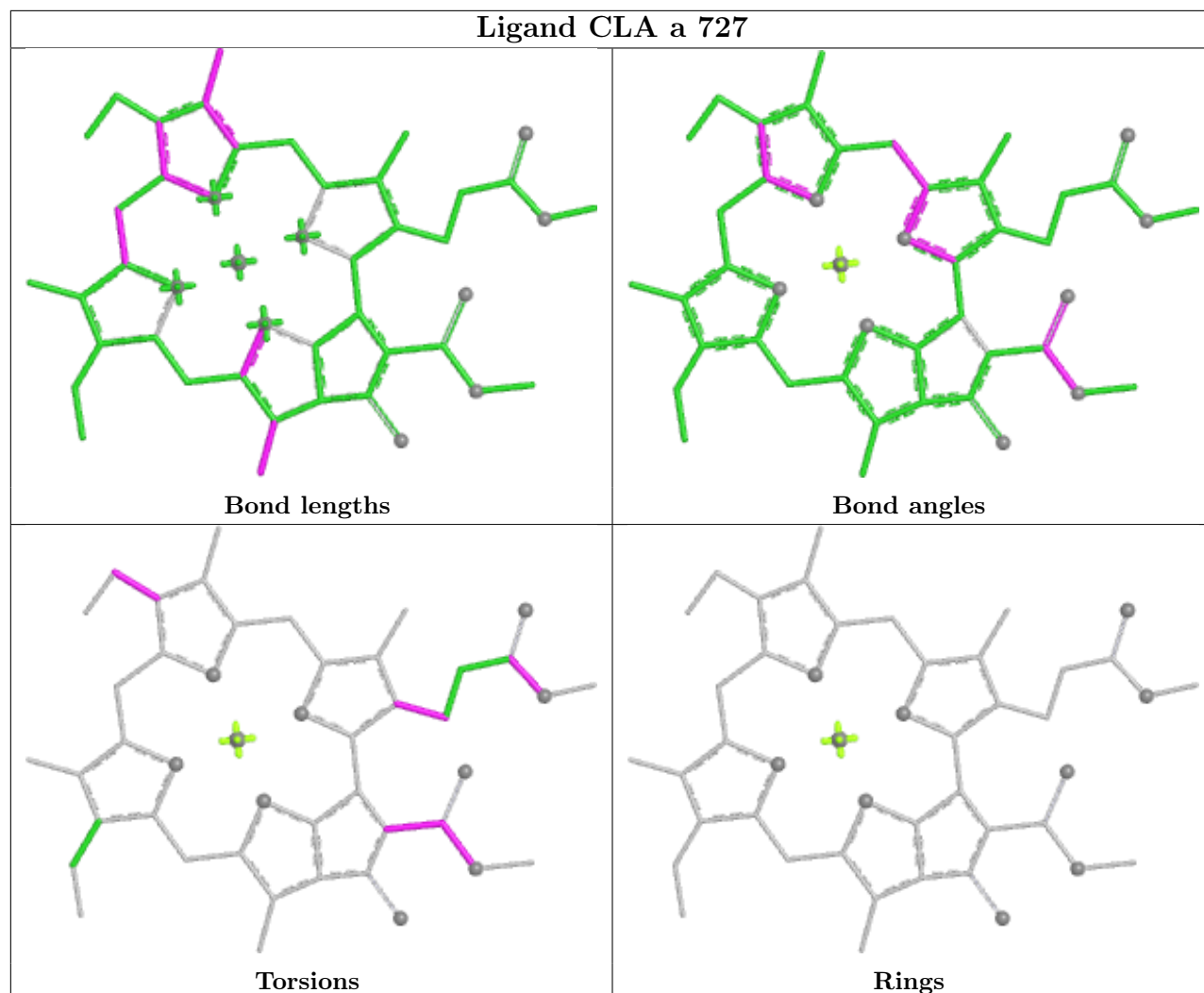




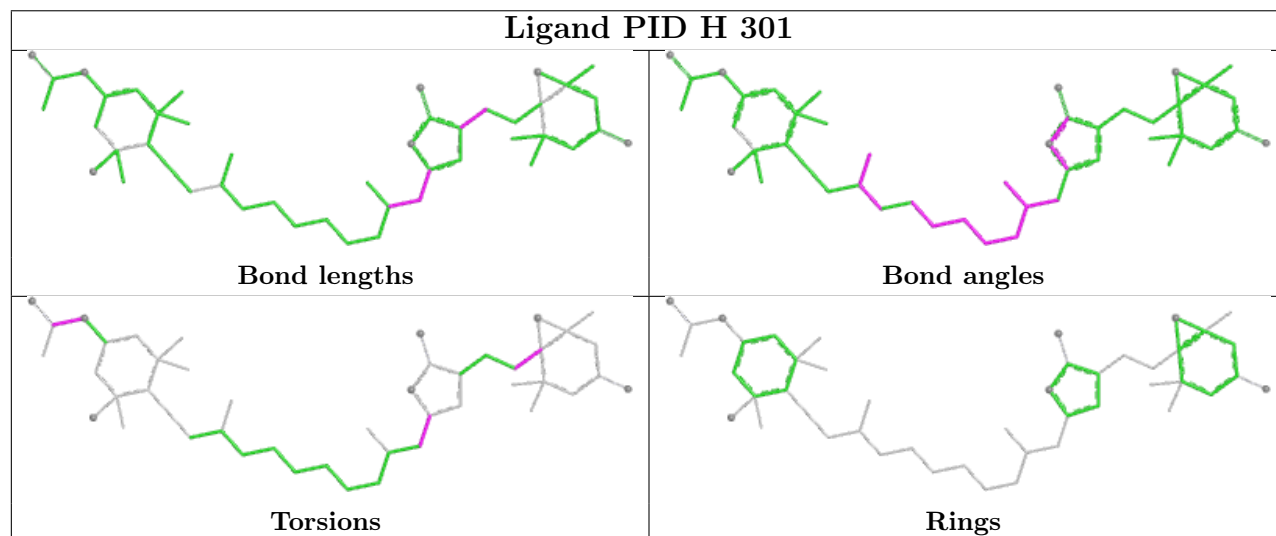
Ligand CLA a 721**Ligand CLA I 312**



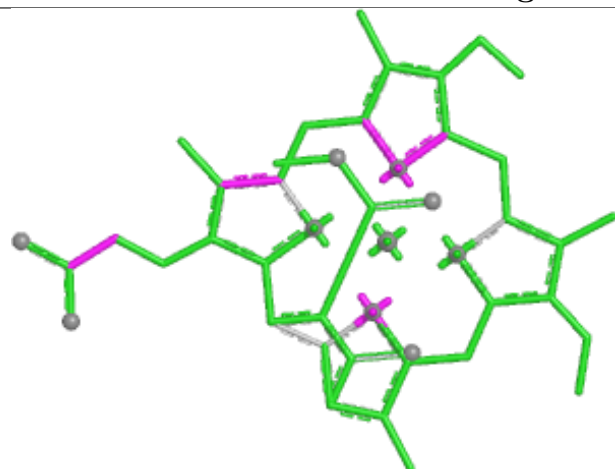
Ligand CLA a 727



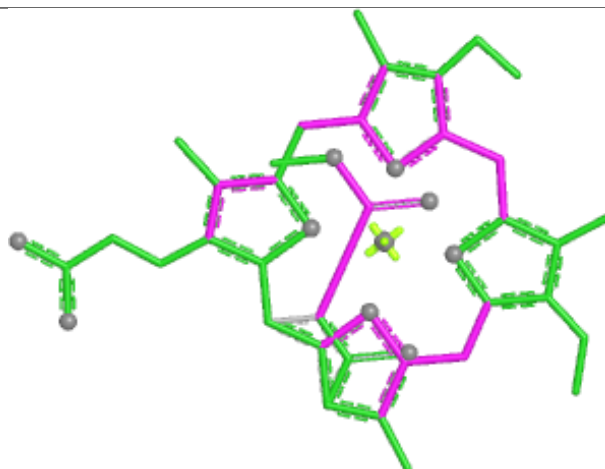
Ligand PID H 301



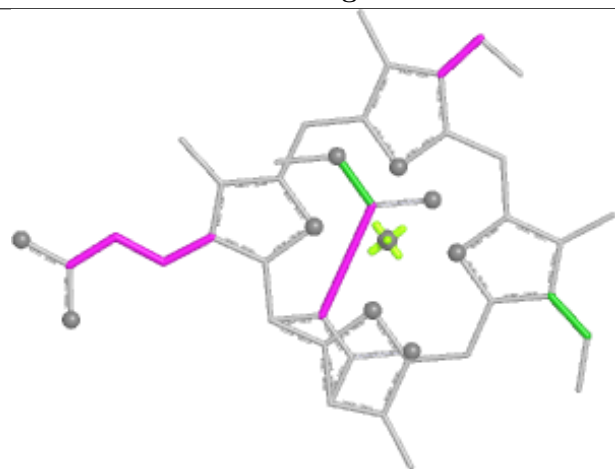
Ligand KC1 K 314



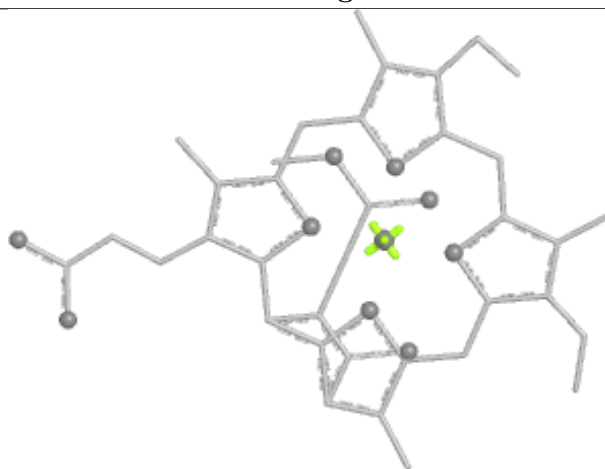
Bond lengths



Bond angles

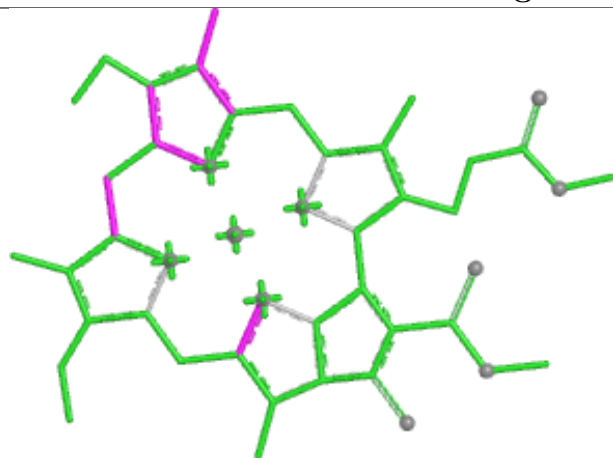


Torsions

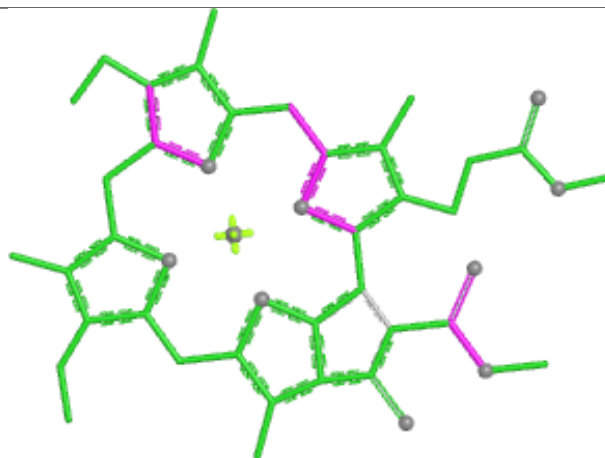


Rings

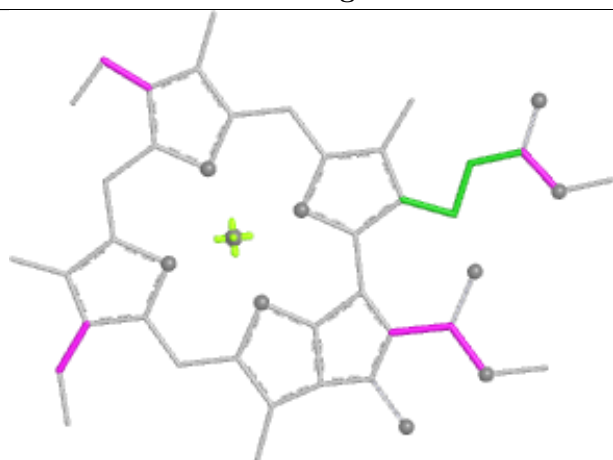
Ligand CLA B 316



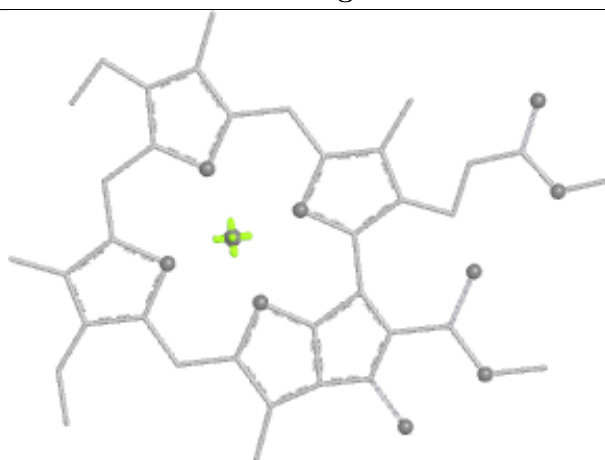
Bond lengths



Bond angles

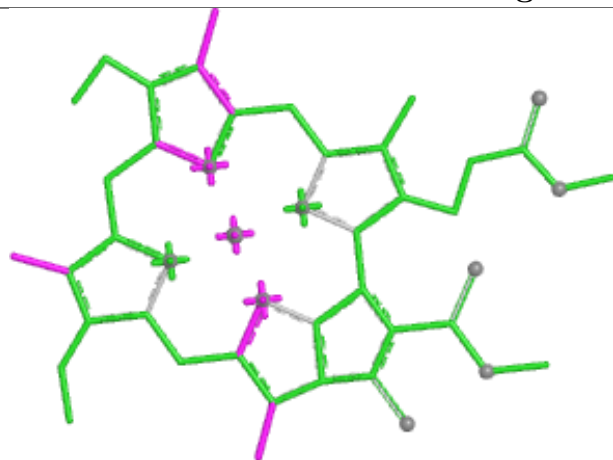


Torsions

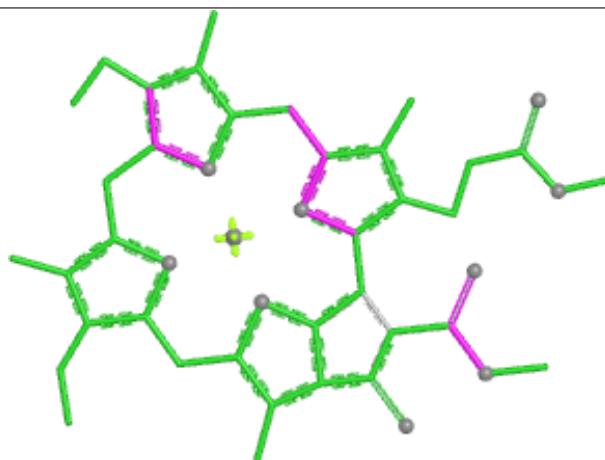


Rings

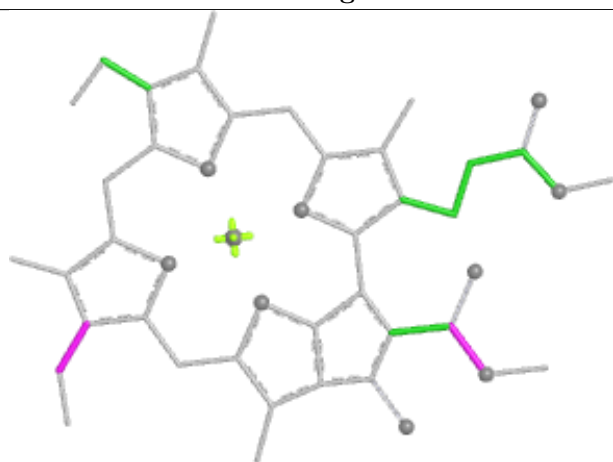
Ligand CLA F 312



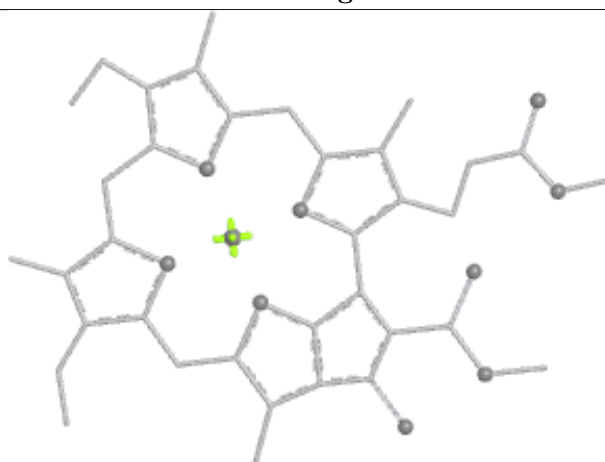
Bond lengths



Bond angles

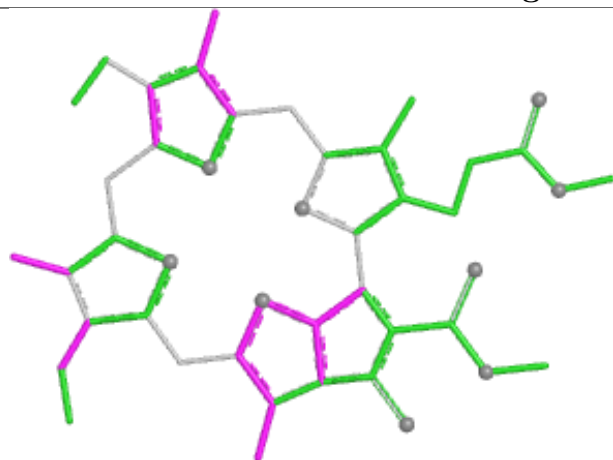


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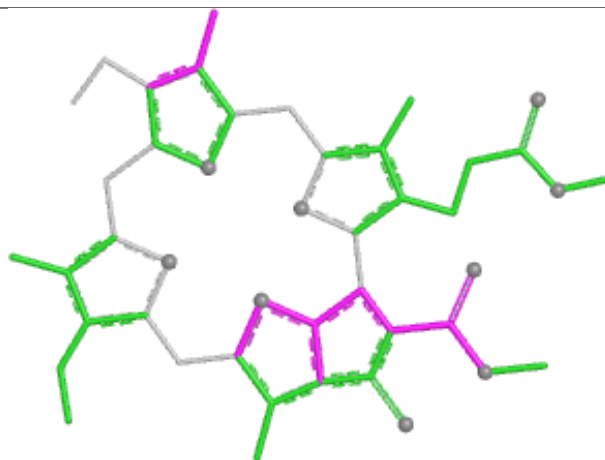


Rings

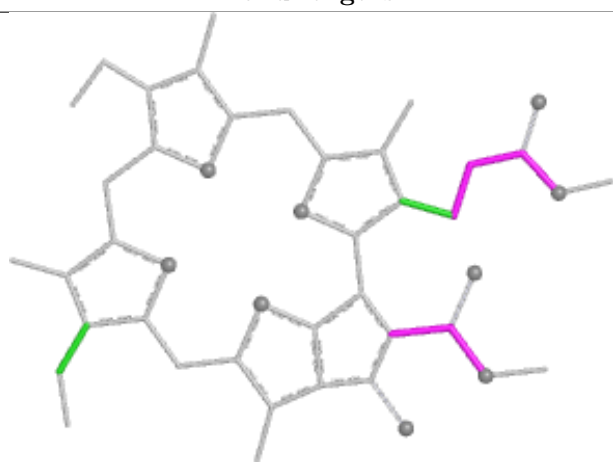
Ligand CLA 1 310



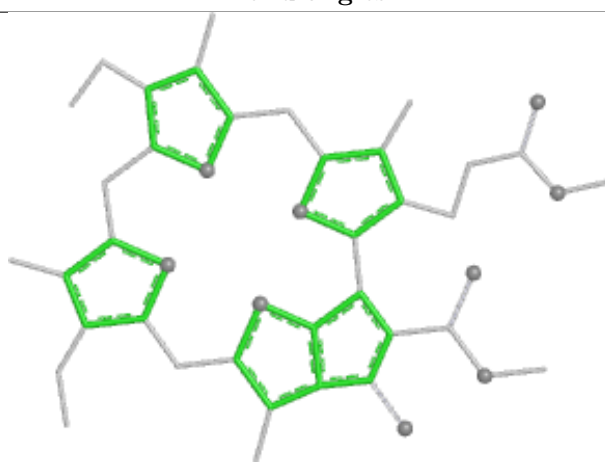
Bond lengths



Bond angles

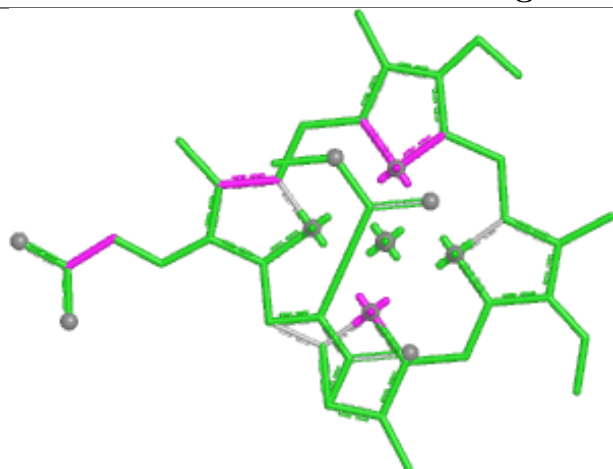


Torsions

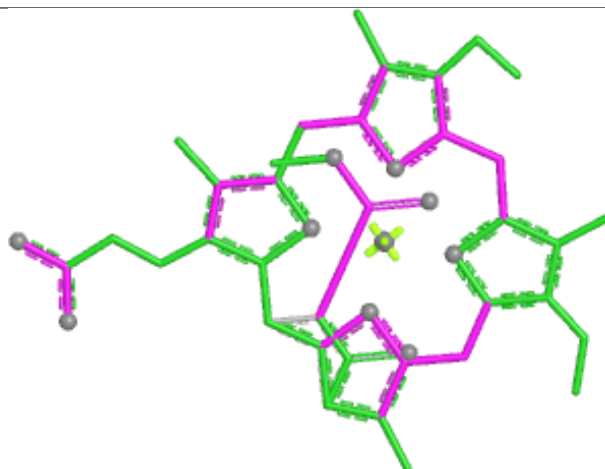


Rings

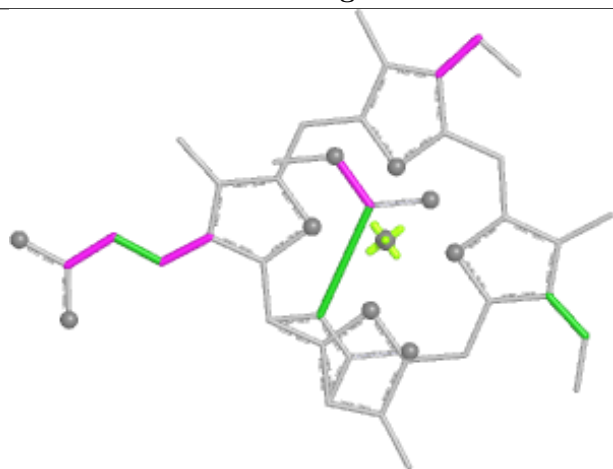
Ligand KC1 O 310



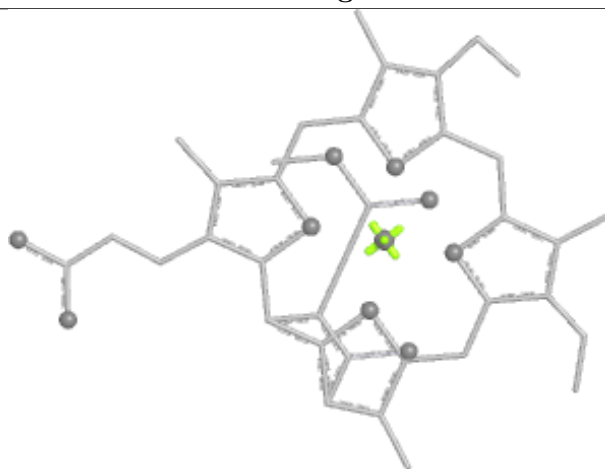
Bond lengths



Bond angles

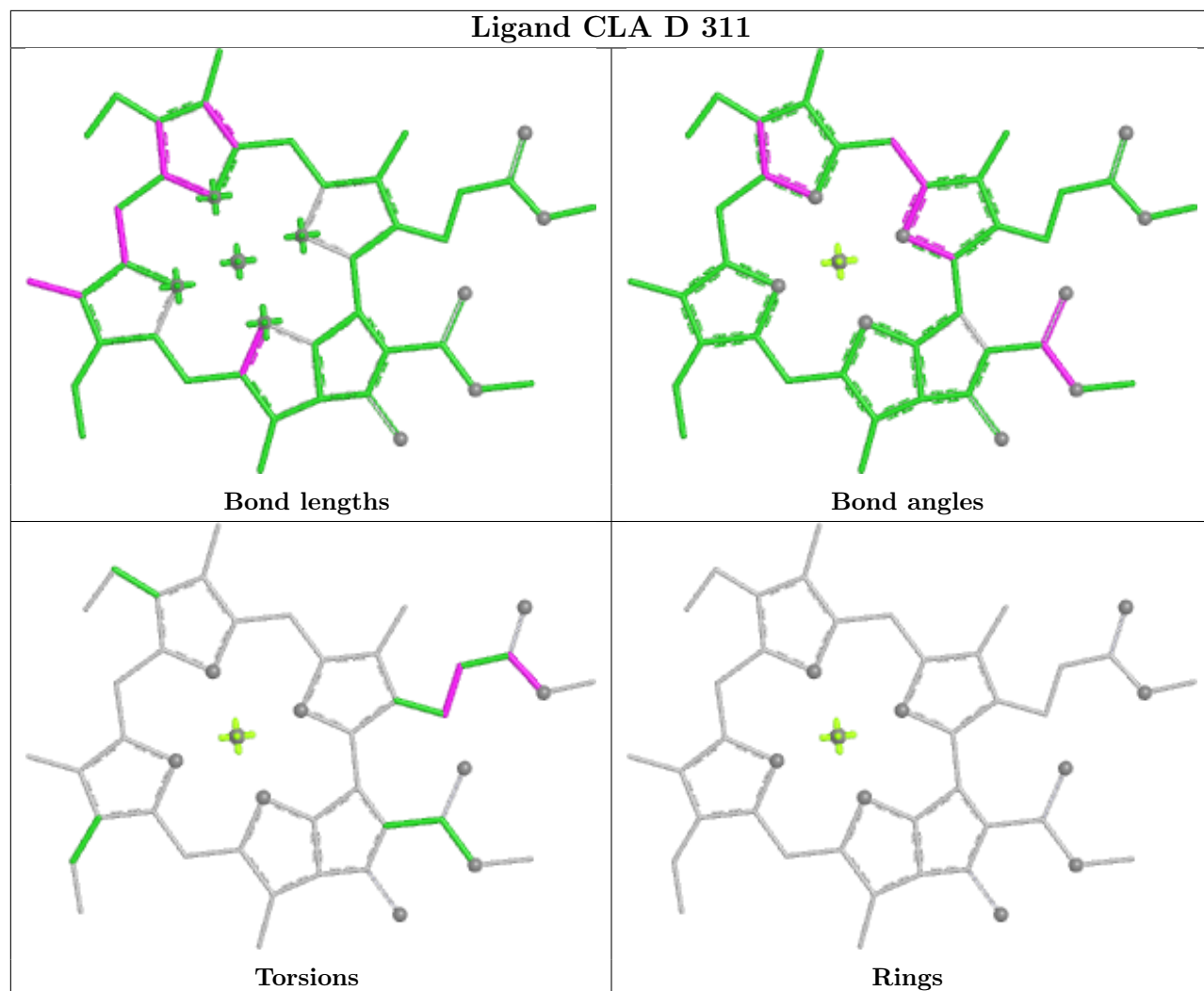


Torsions

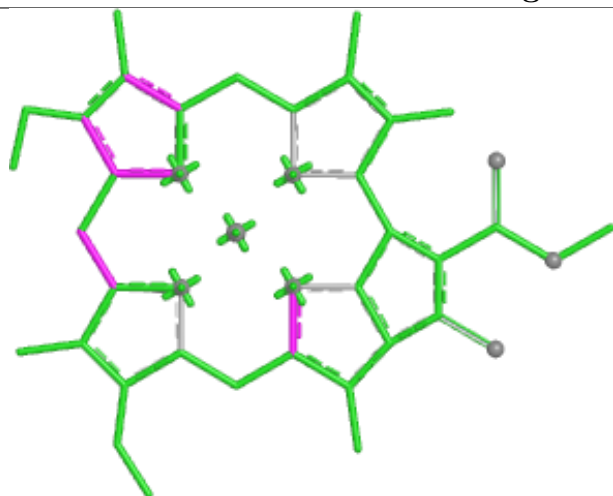


Rings

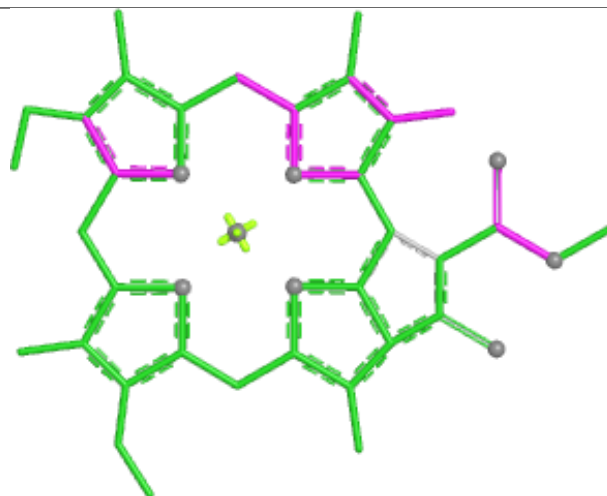
Ligand CLA D 311



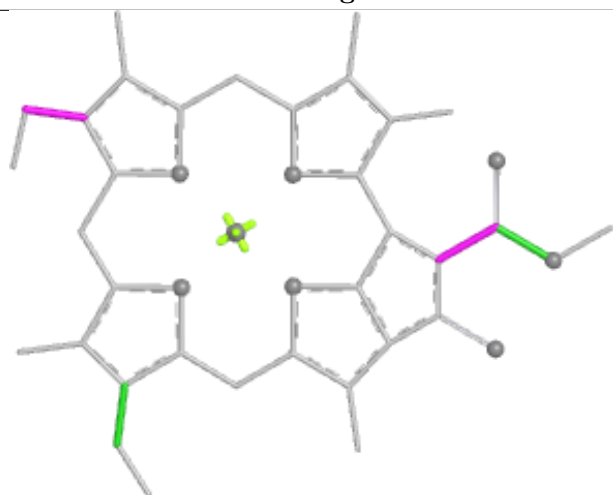
Ligand CLA 1 309



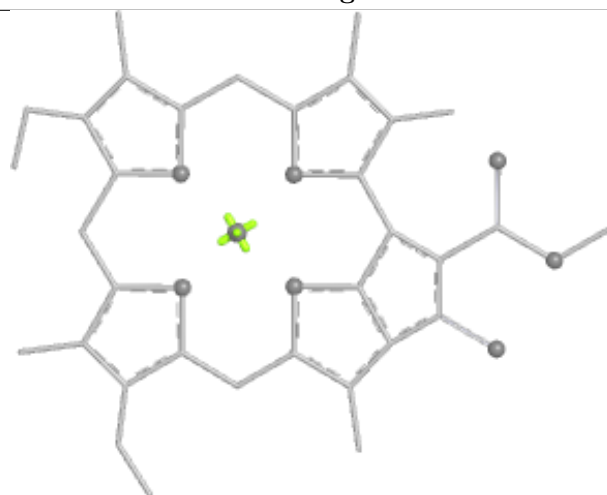
Bond lengths



Bond angles

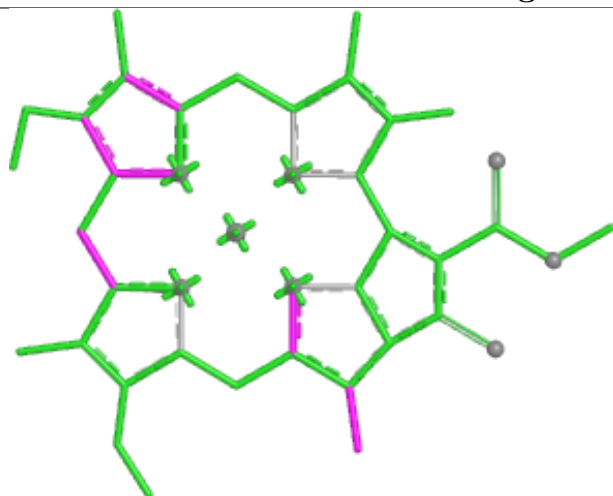


Torsions

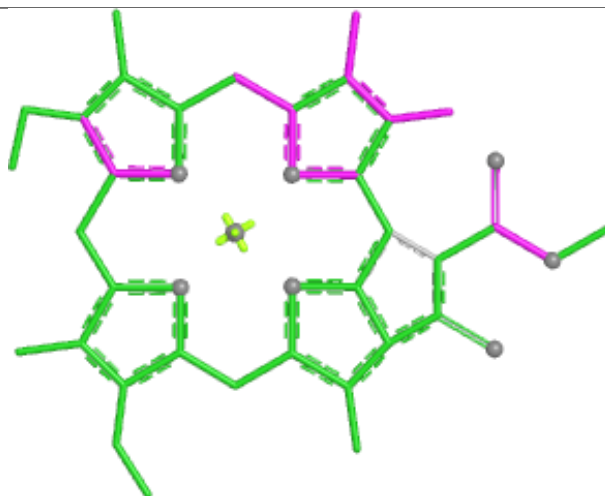


Rings

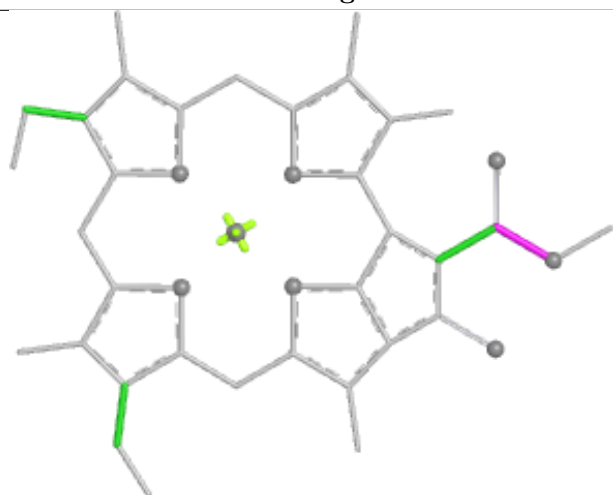
Ligand CLA J 314



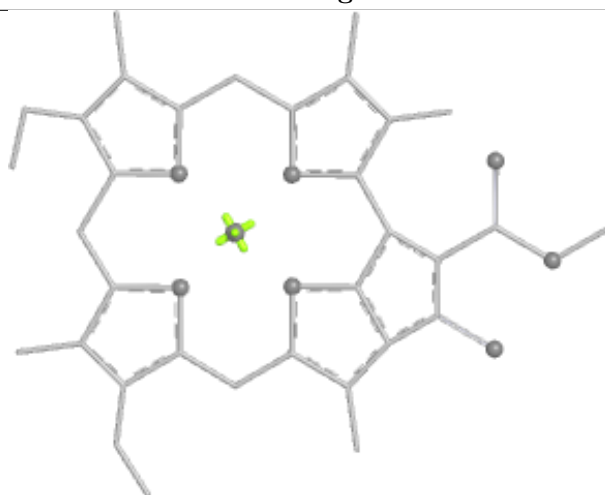
Bond lengths



Bond angles

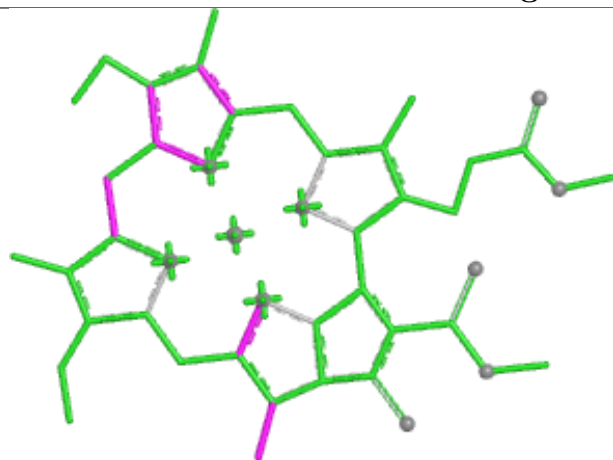


Torsions

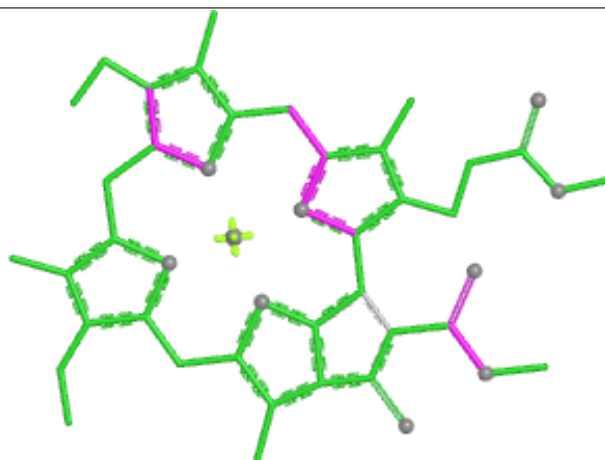


Rings

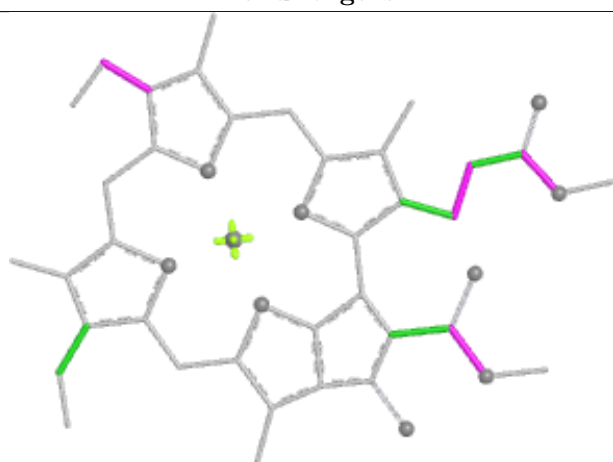
Ligand CLA I 307



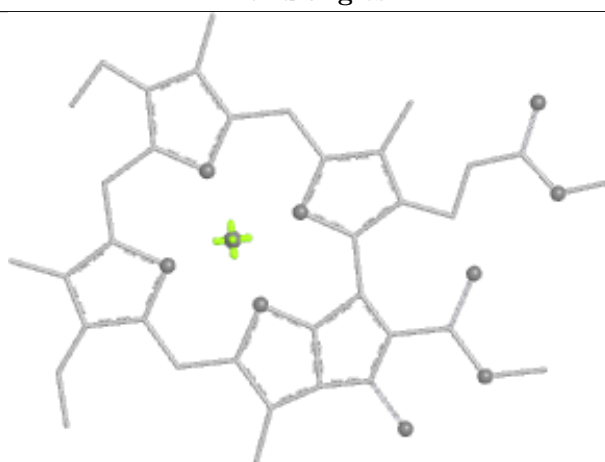
Bond lengths



Bond angles

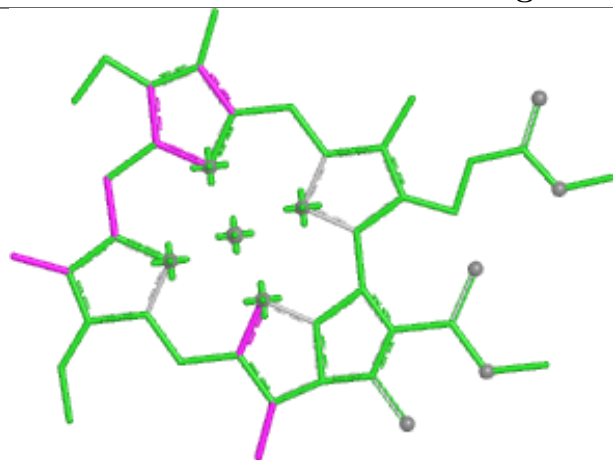


Torsions

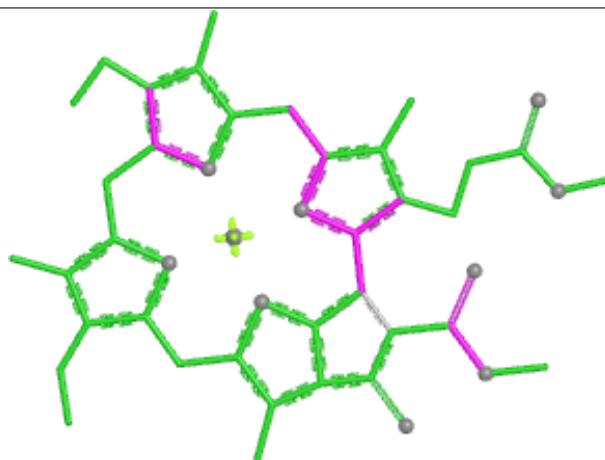


Rings

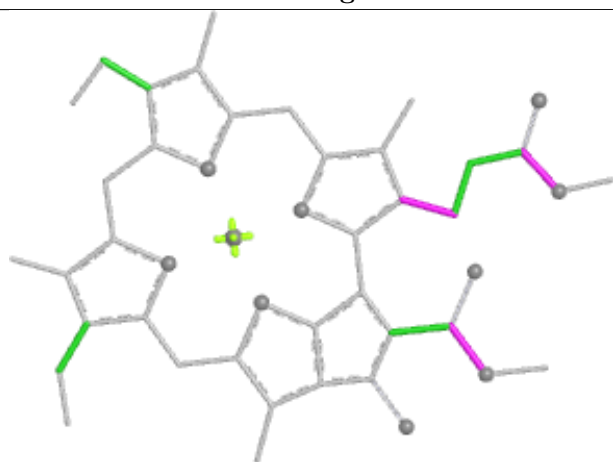
Ligand CLA F 313



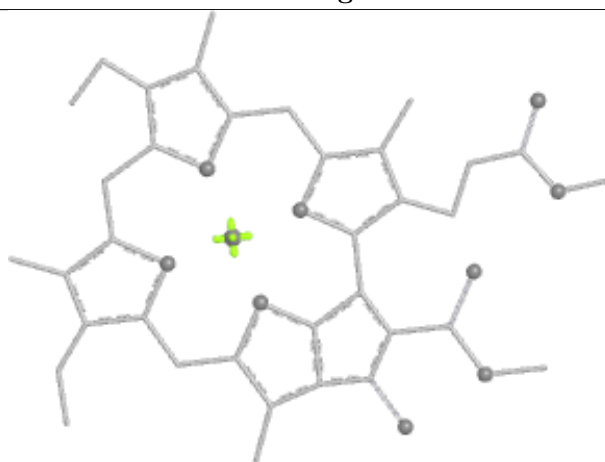
Bond lengths



Bond angles

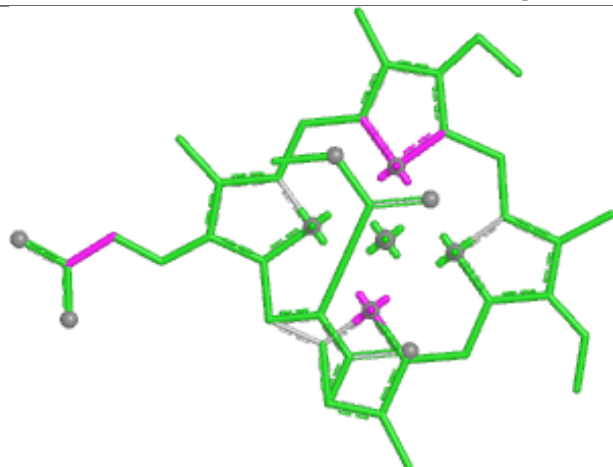


Torsions

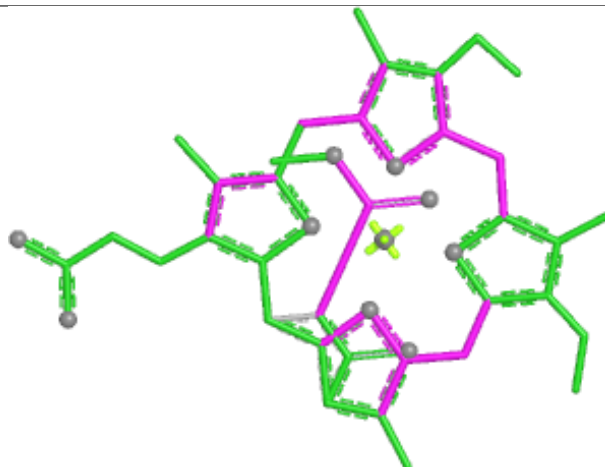


Rings

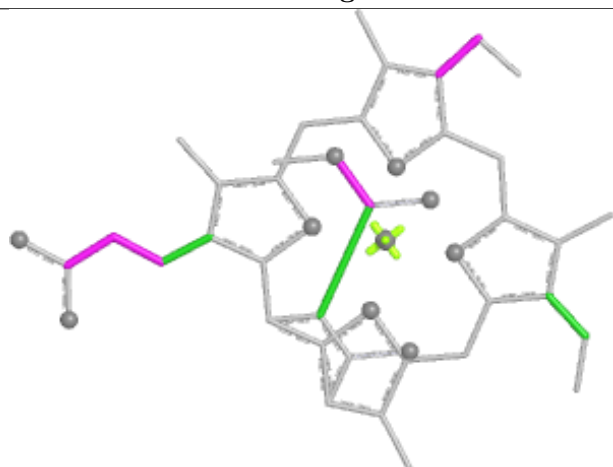
Ligand KC1 B 314



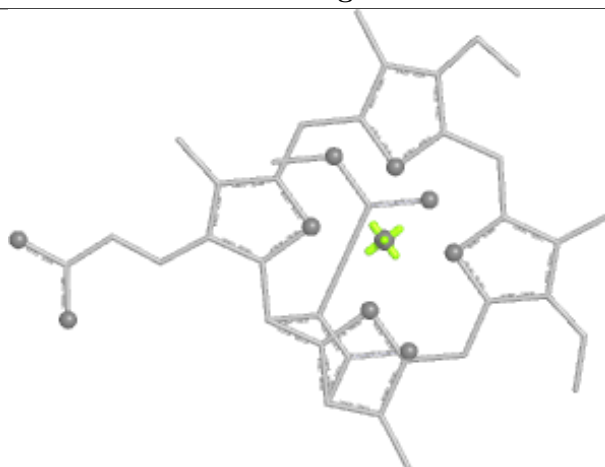
Bond lengths



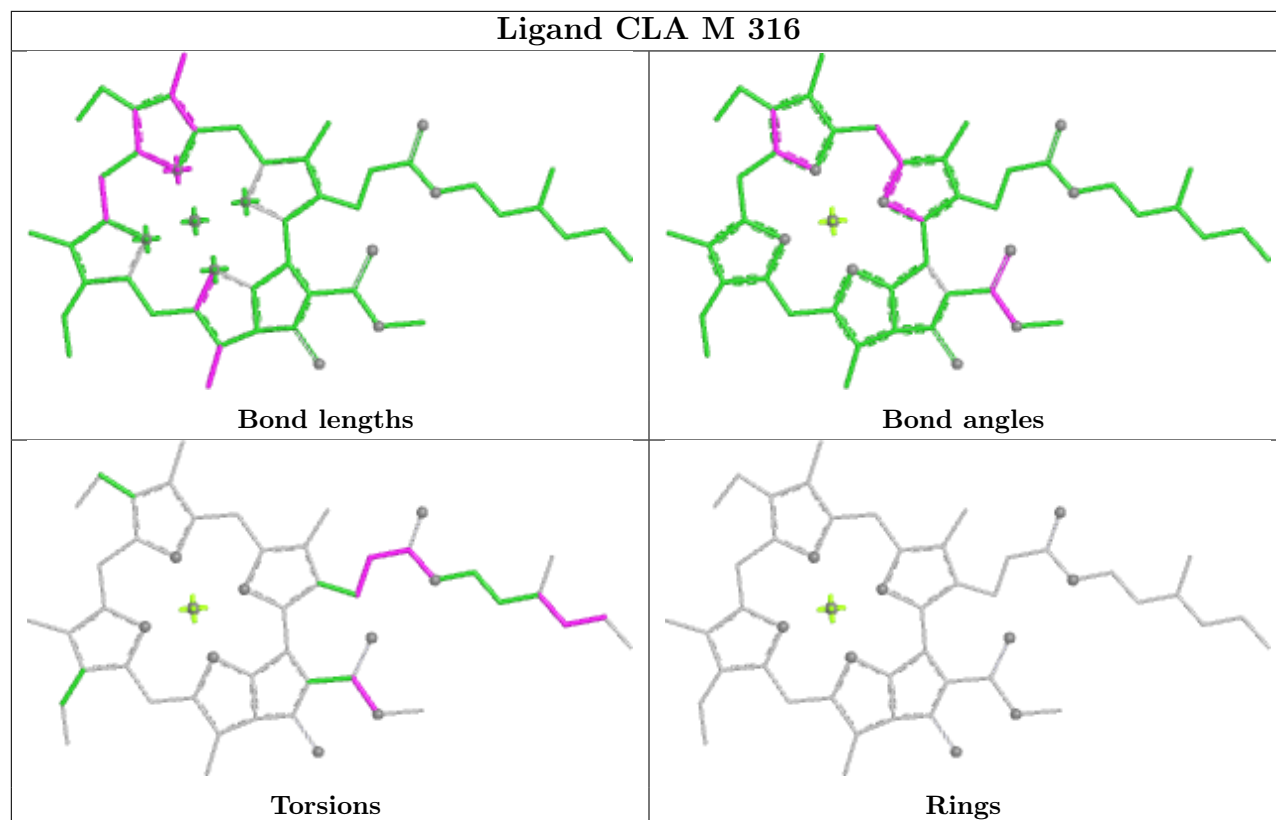
Bond angles



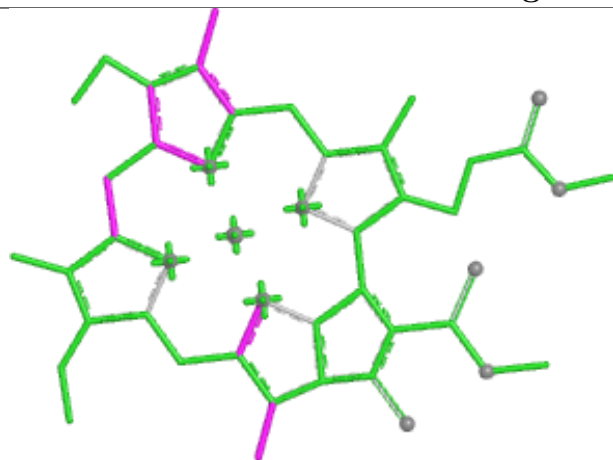
Torsions



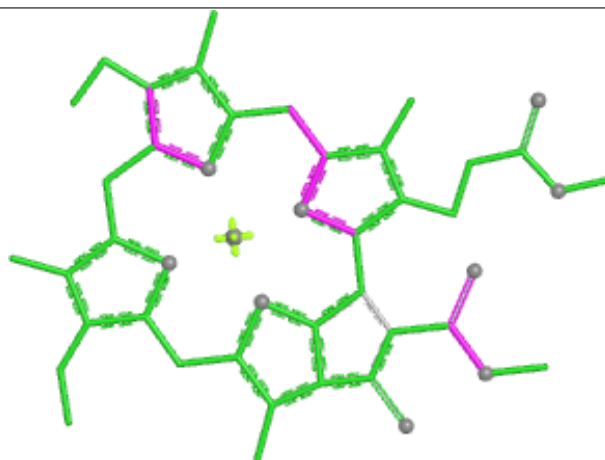
Rings



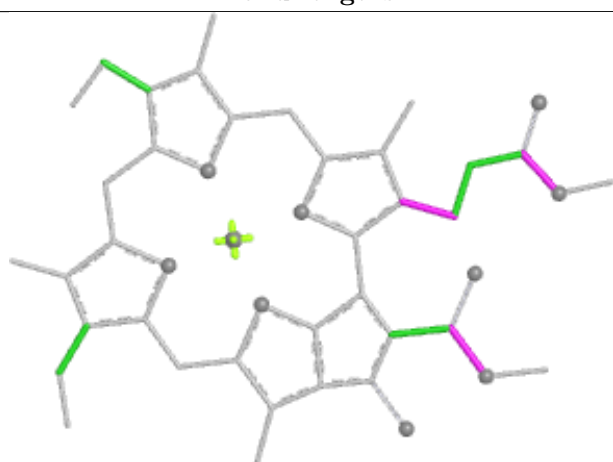
Ligand CLA 1 312



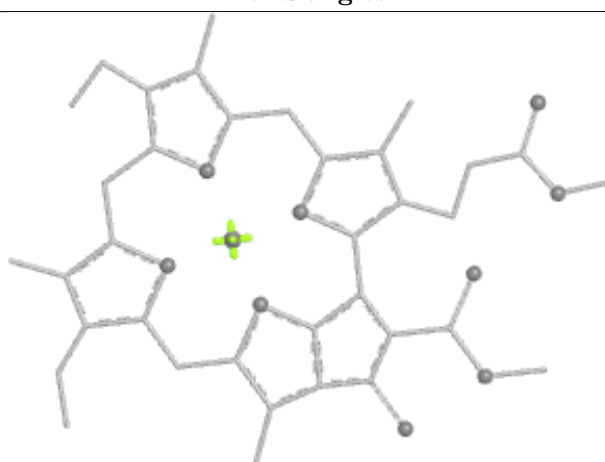
Bond lengths



Bond angles

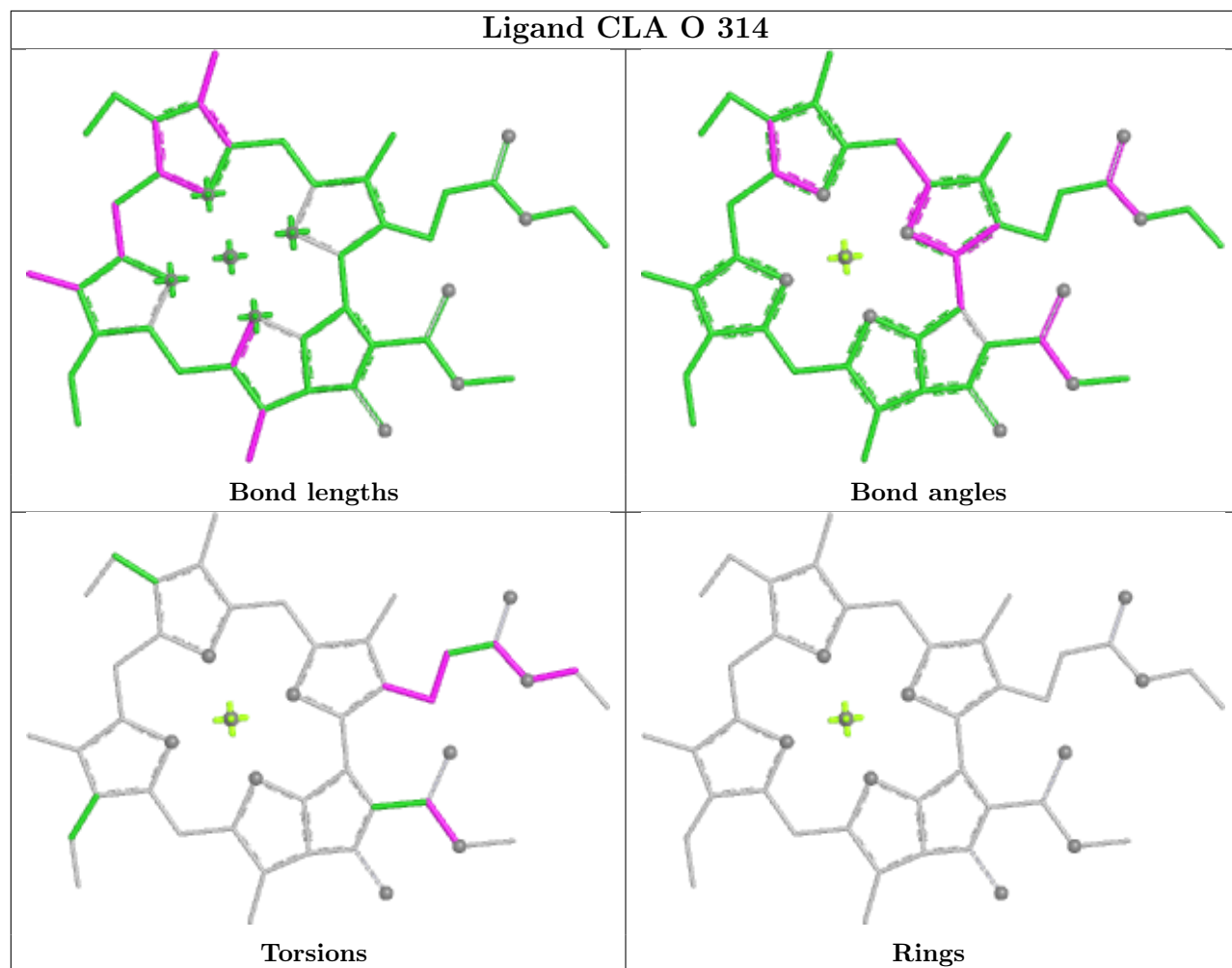


Torsions

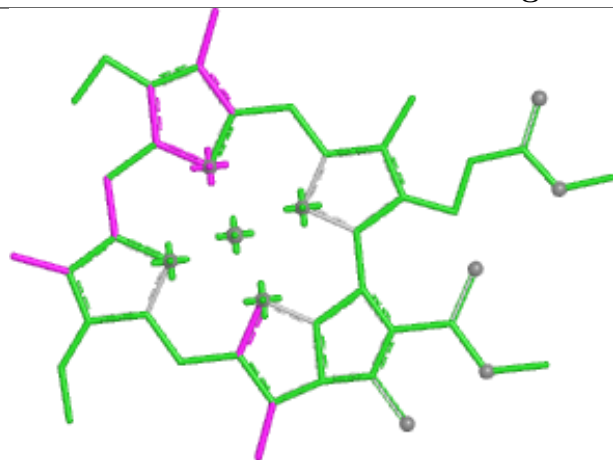


Rings

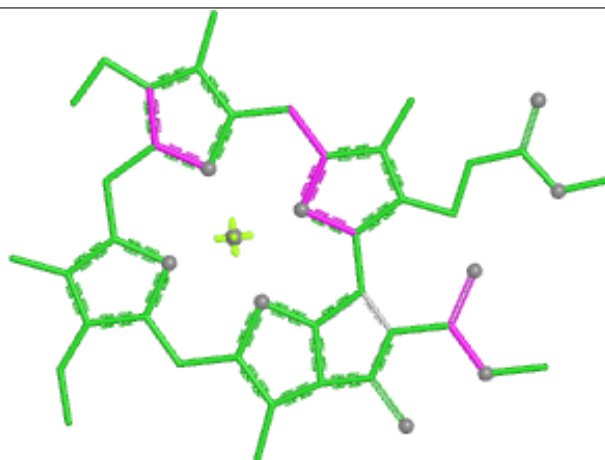
Ligand CLA O 314



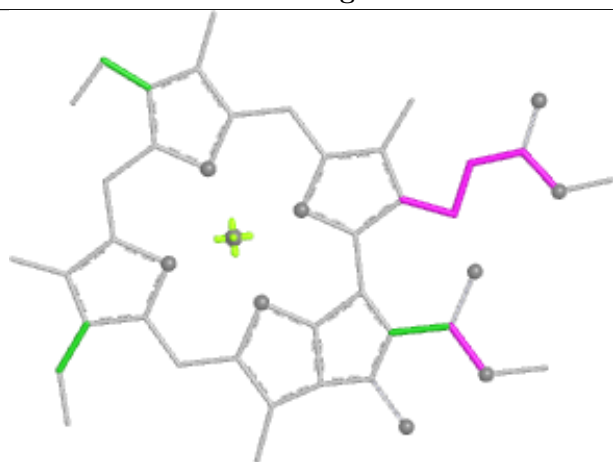
Ligand CLA f 303



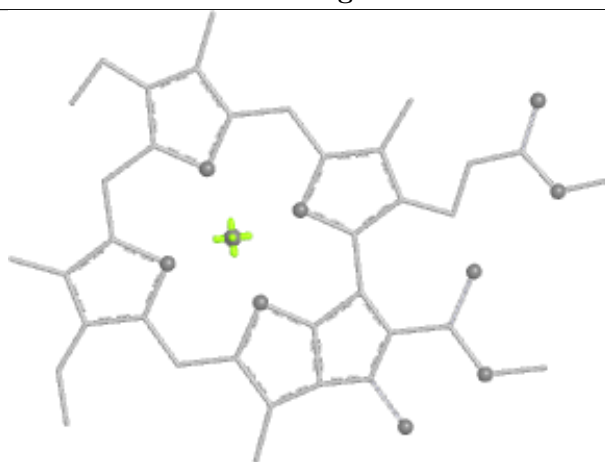
Bond lengths



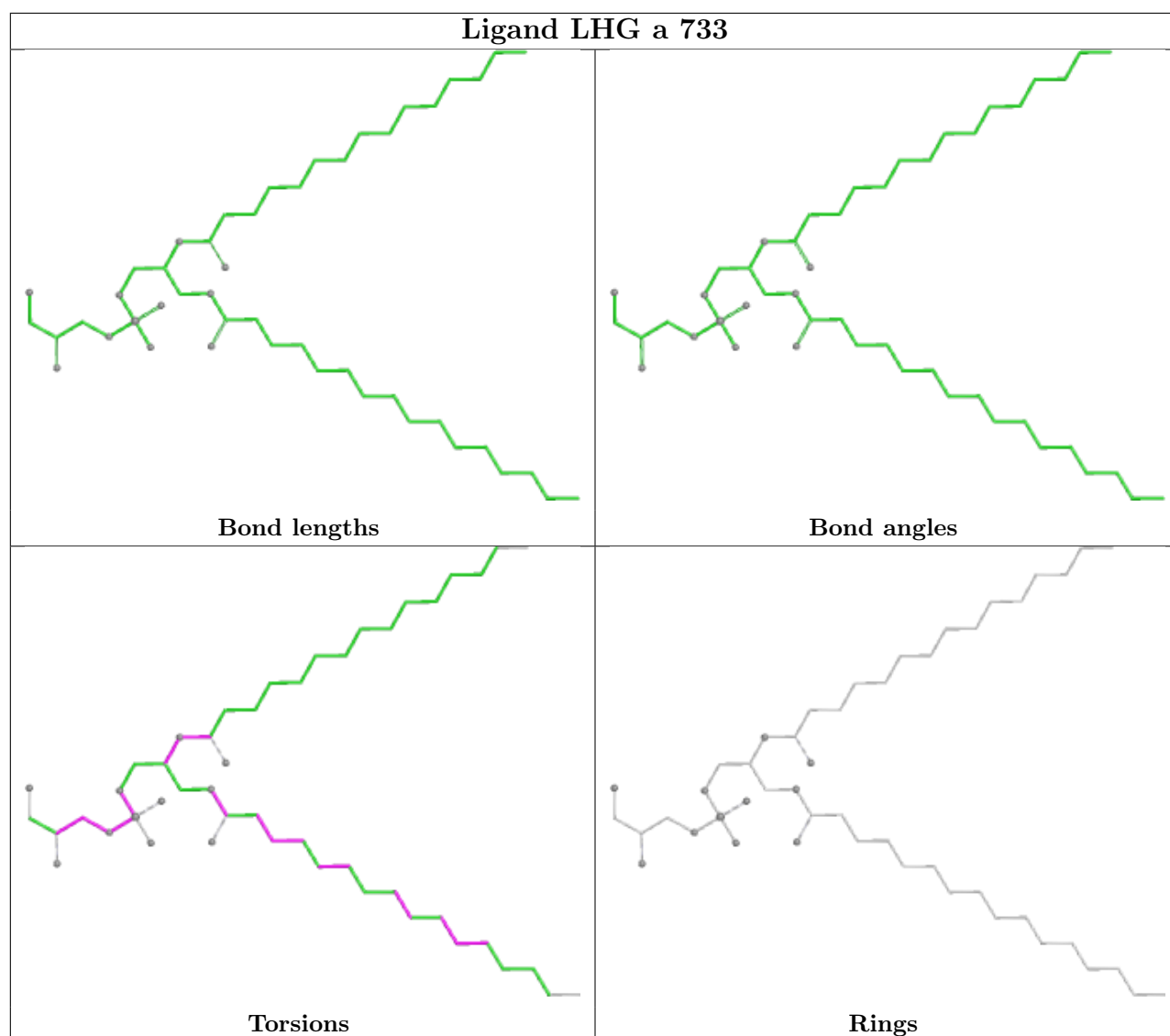
Bond angles



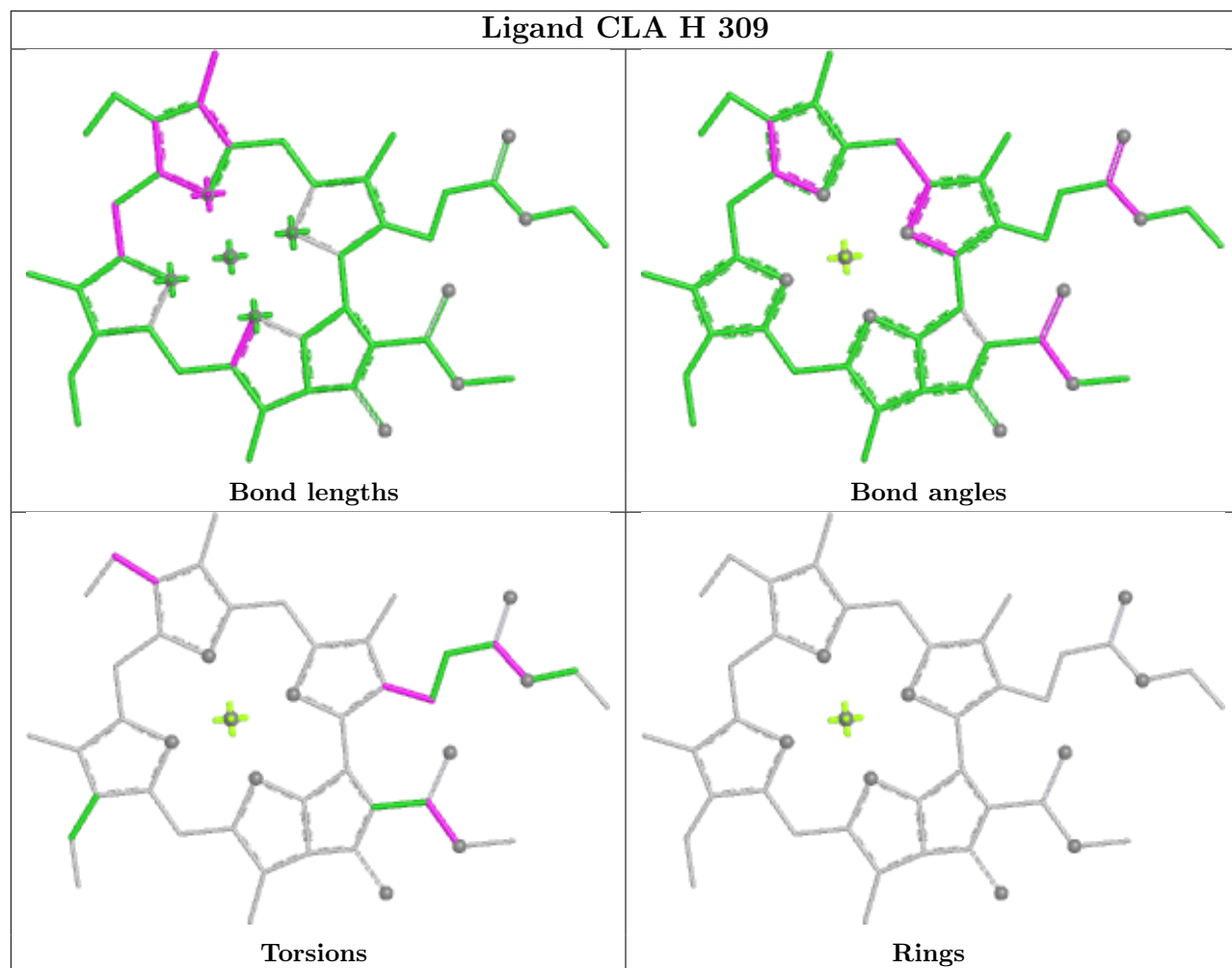
Torsions



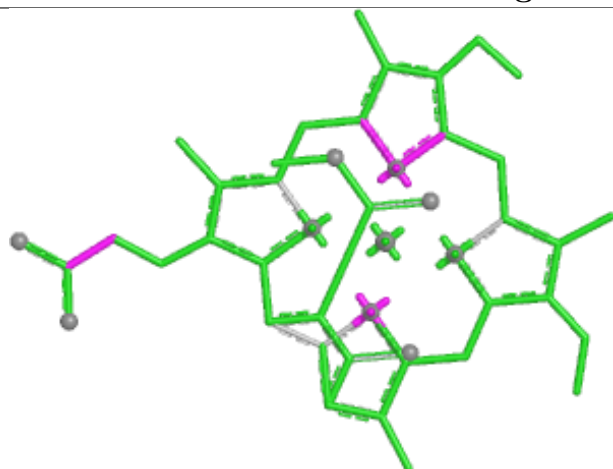
Rings



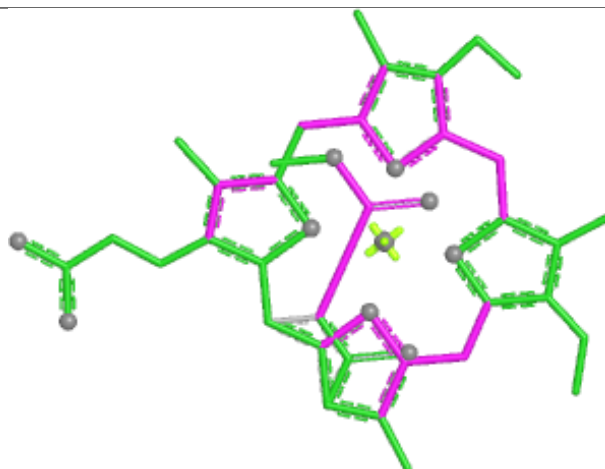
Ligand CLA H 309



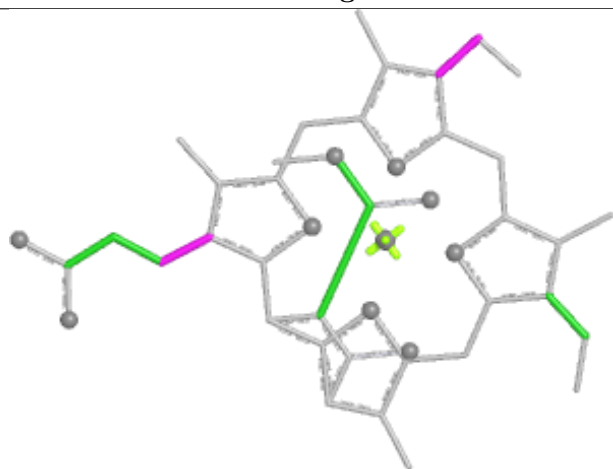
Ligand KC1 H 306



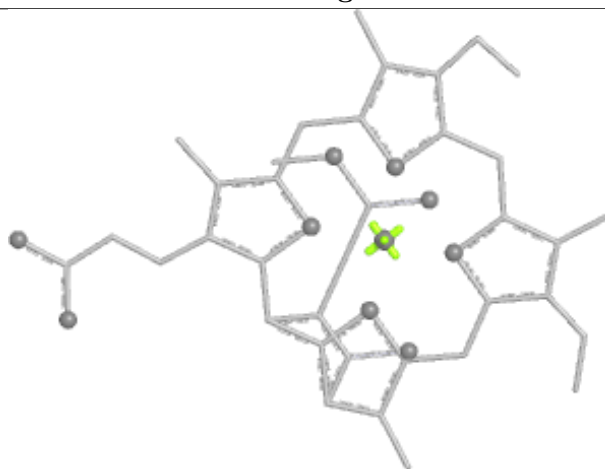
Bond lengths



Bond angles

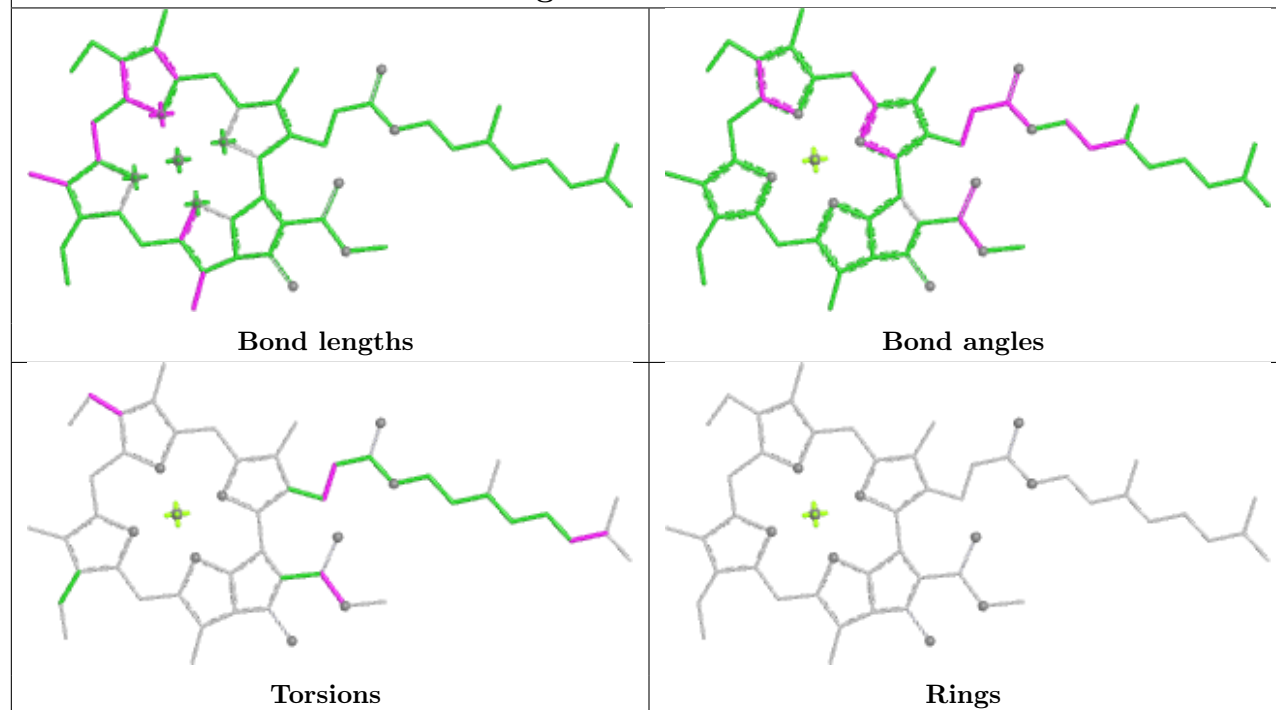


Torsions

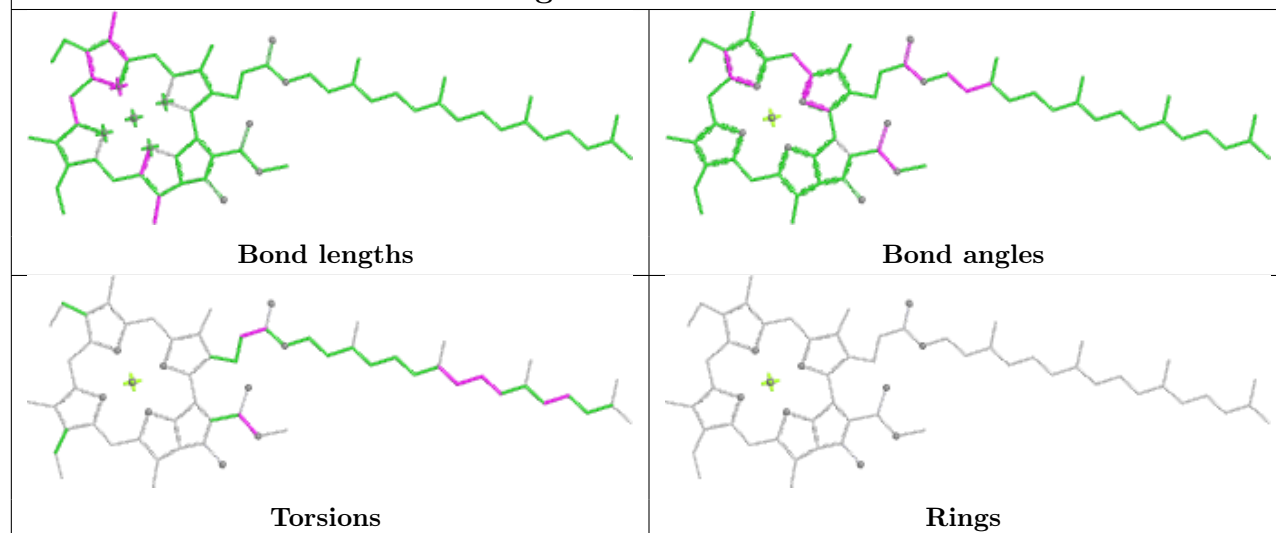


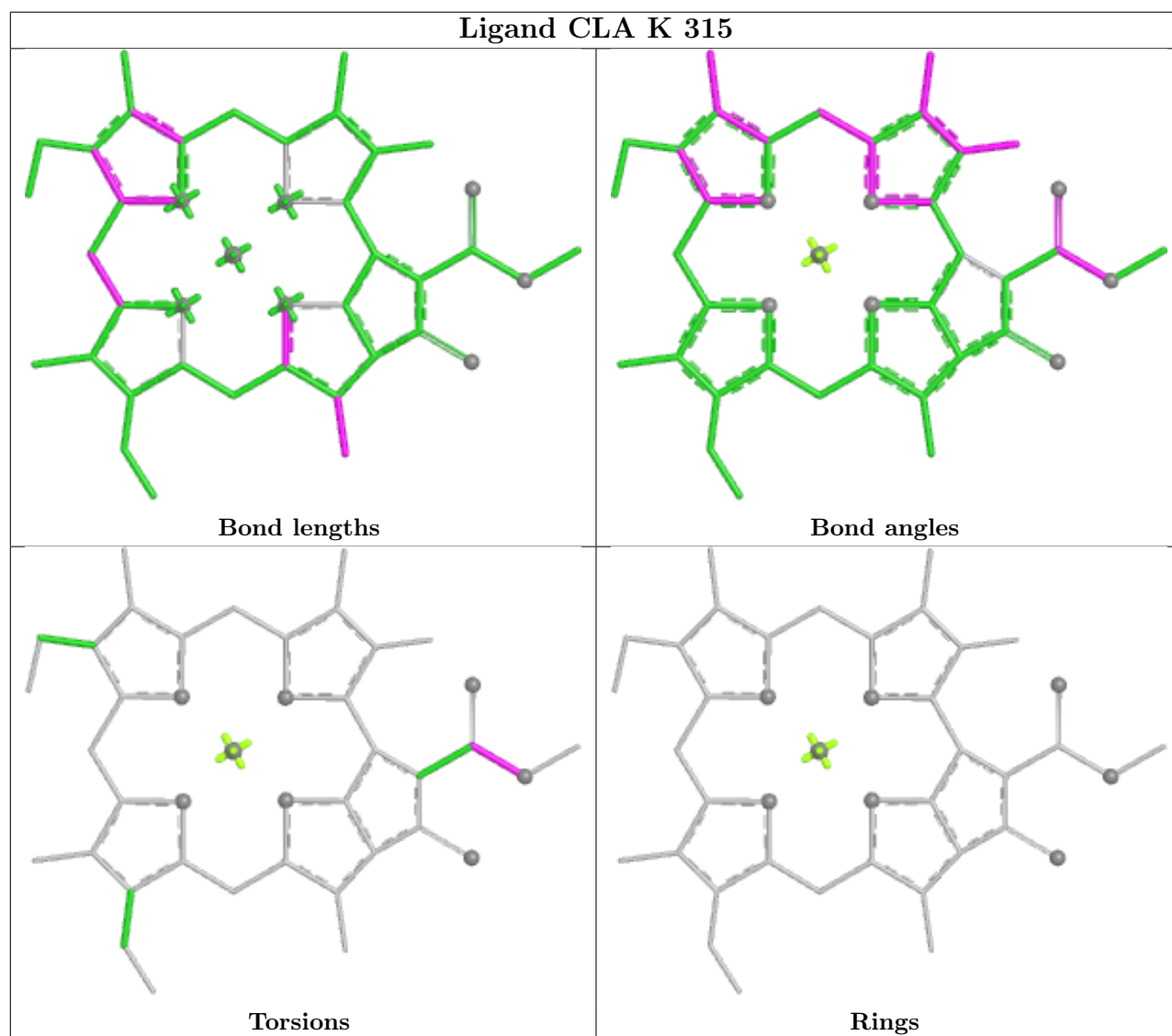
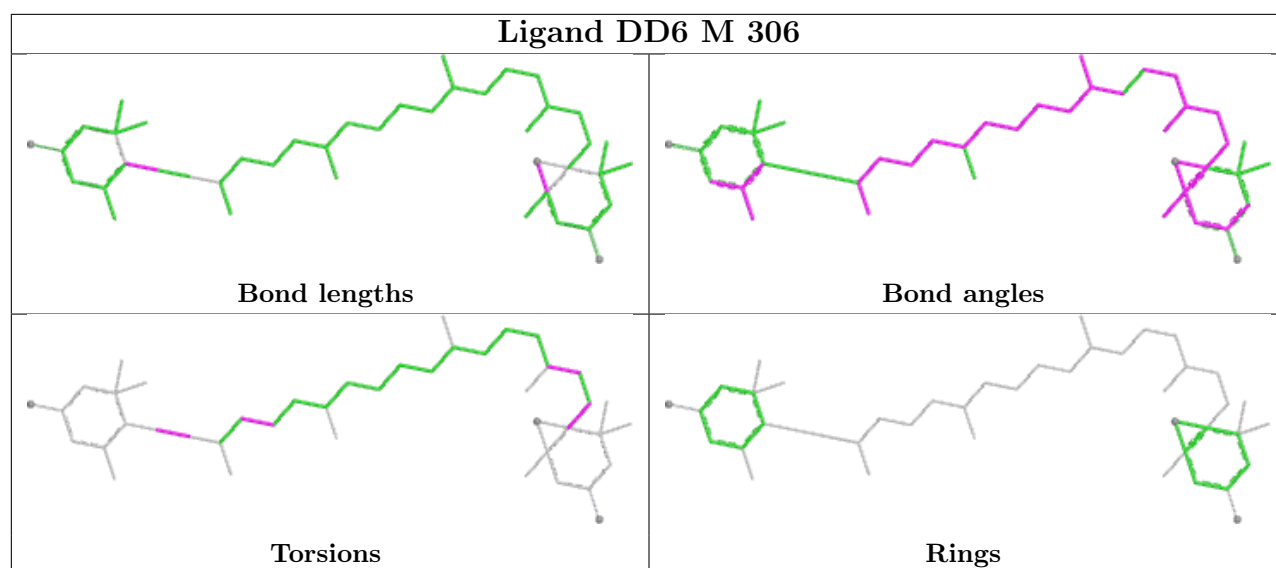
Rings

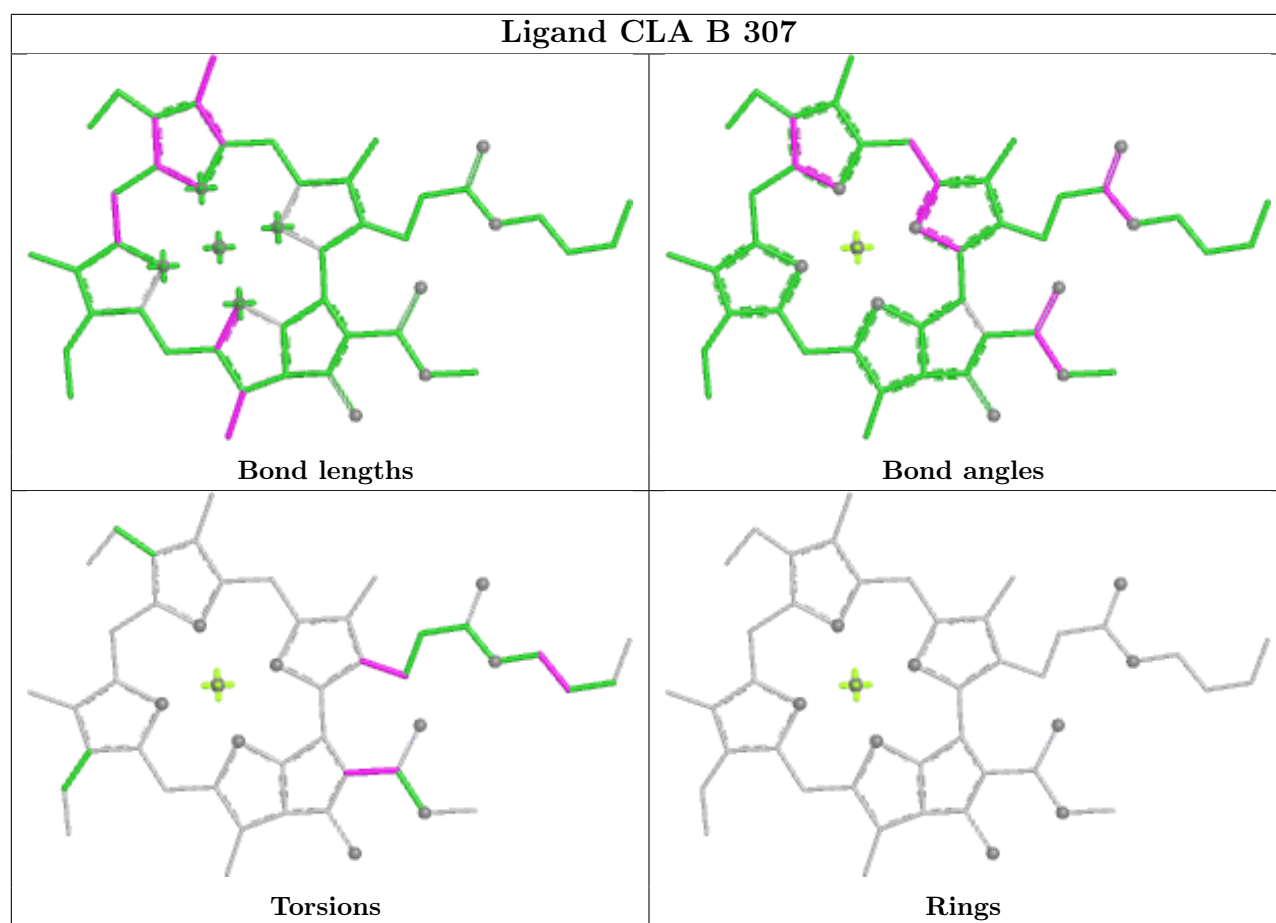
Ligand CLA a 710



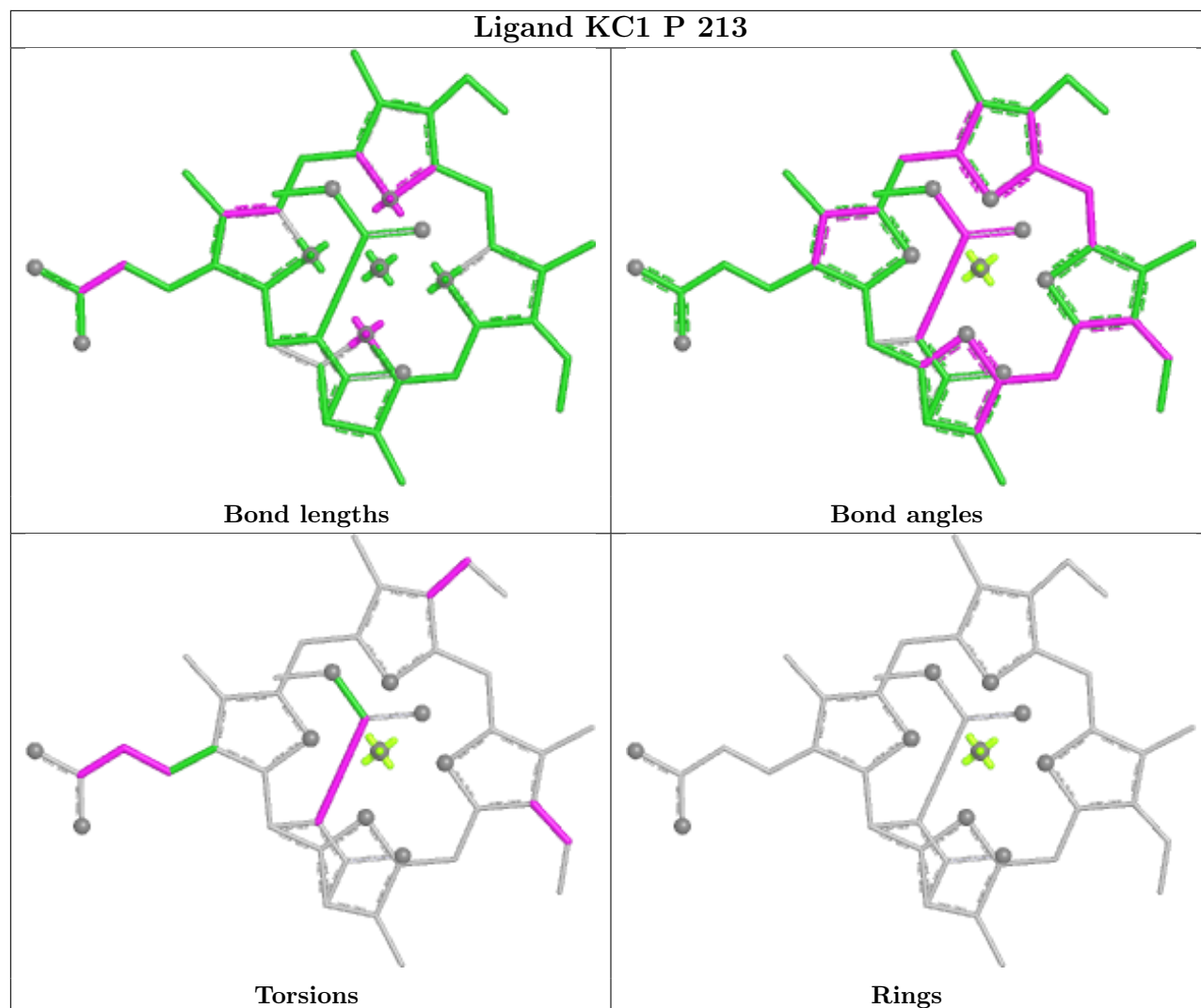
Ligand CLA b 713



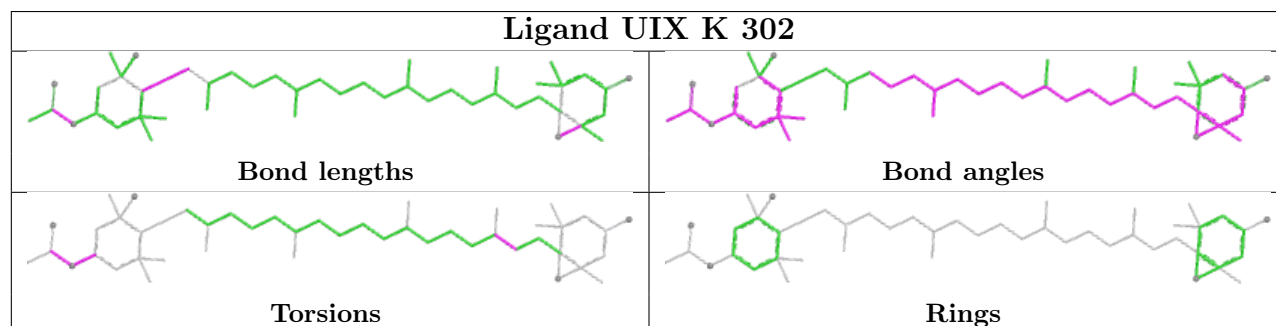




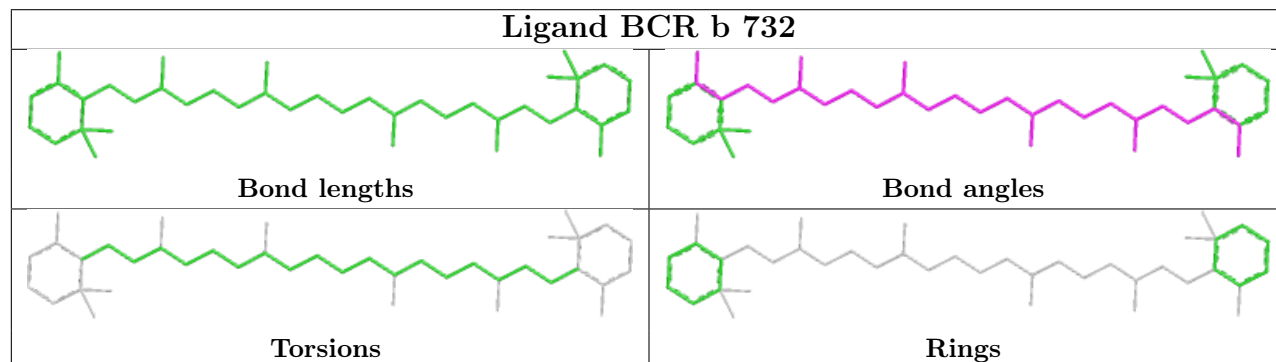
Ligand KC1 P 213

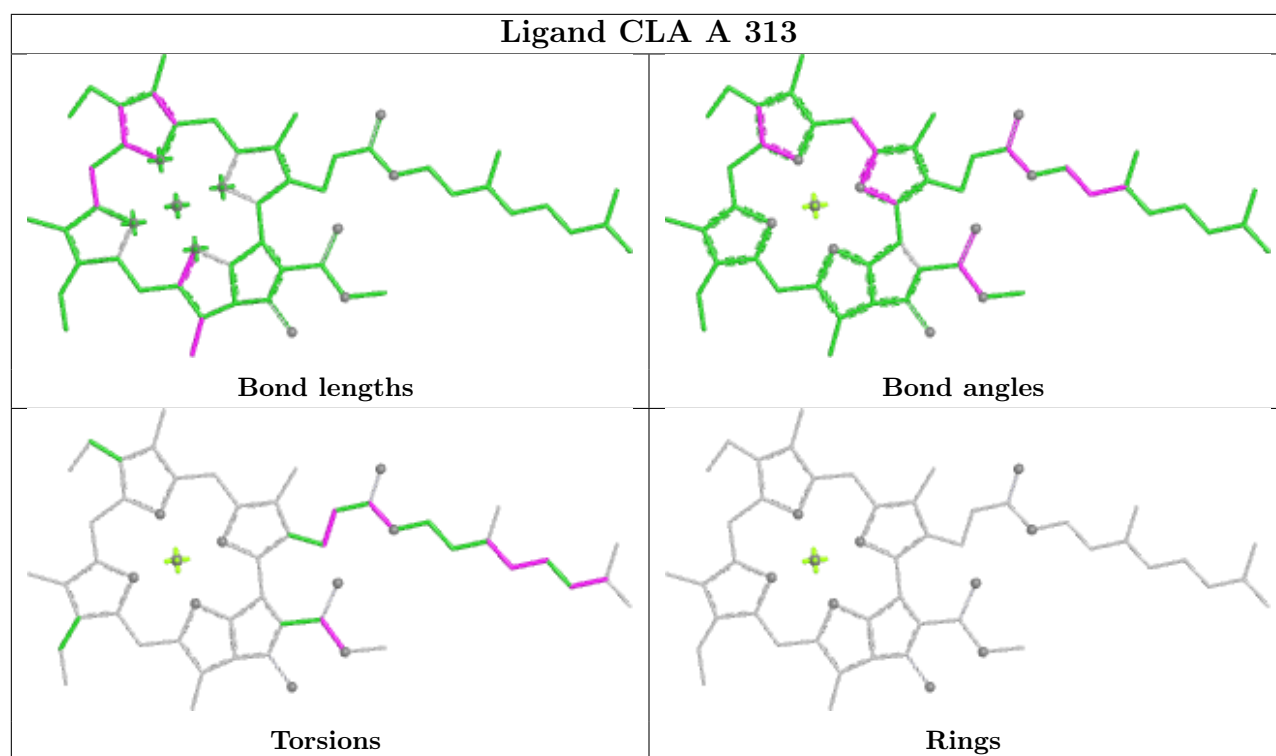


Ligand UIX K 302

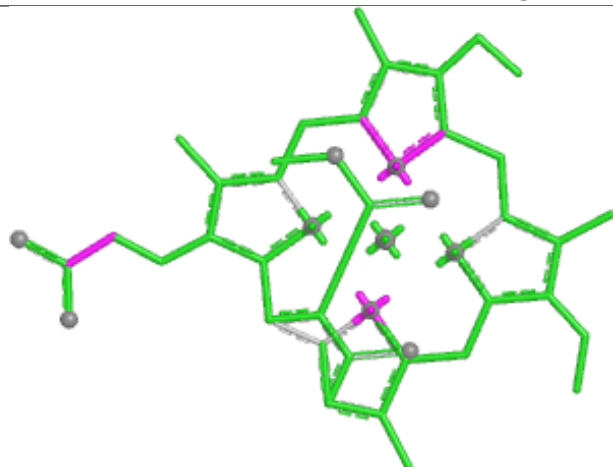


Ligand BCR b 732

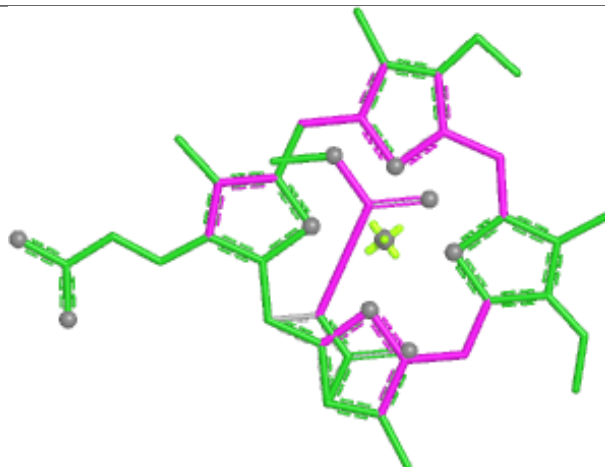




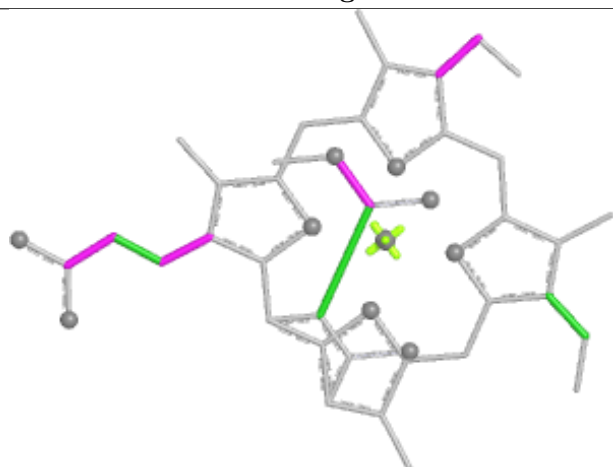
Ligand KC1 N 306



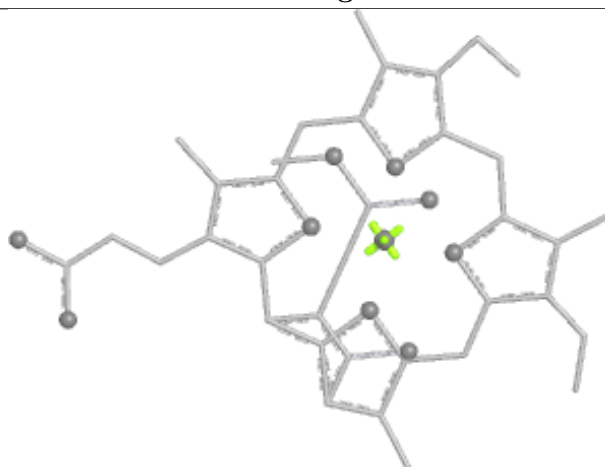
Bond lengths



Bond angles

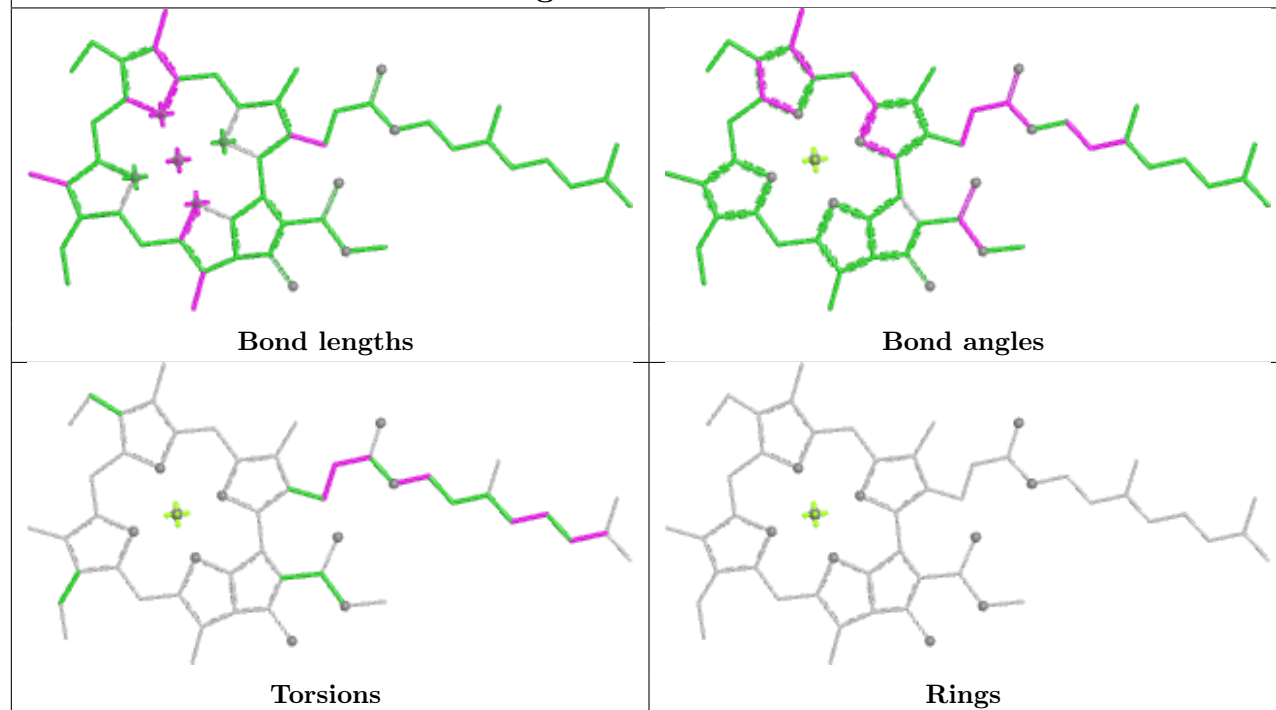


Torsions

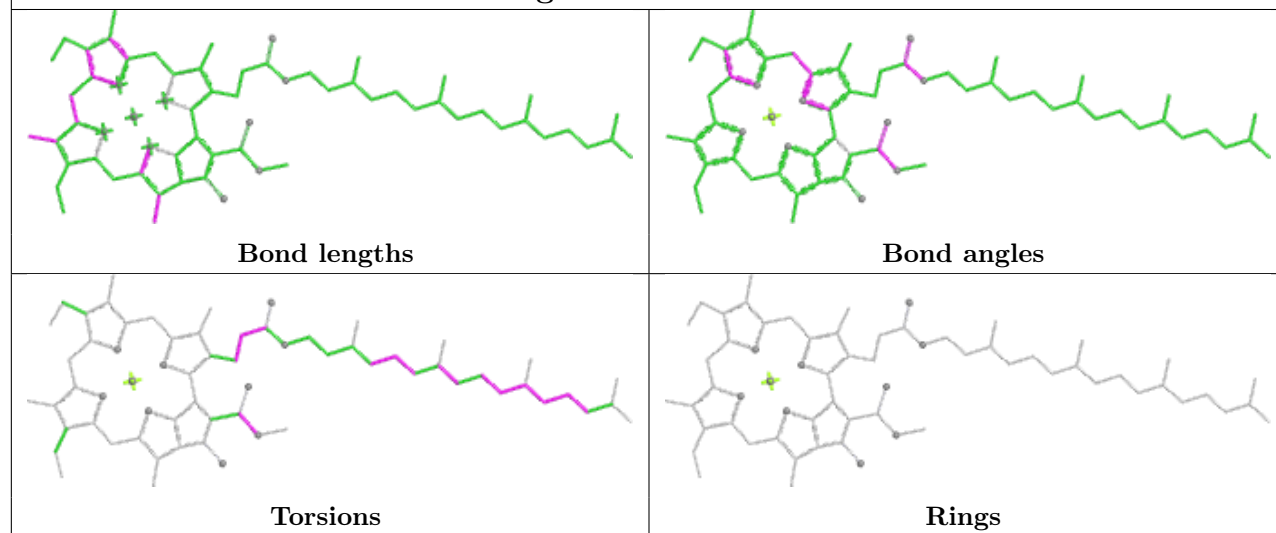


Rings

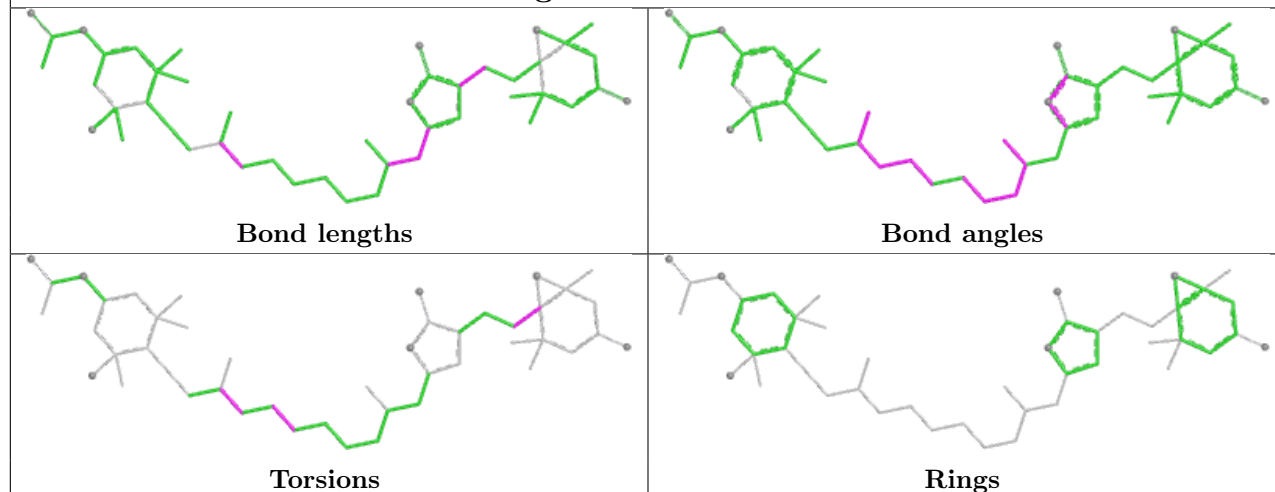
Ligand CLA a 703



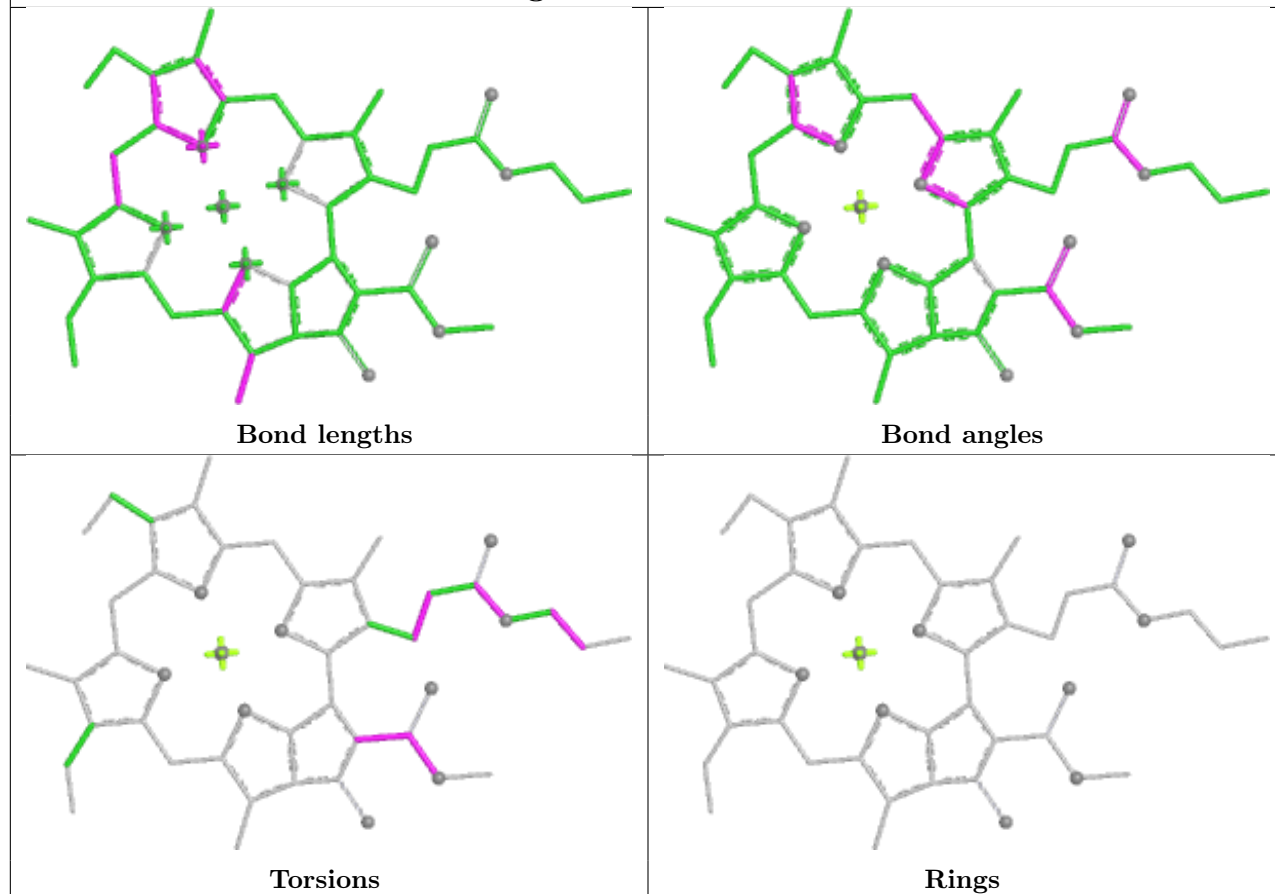
Ligand CLA a 723



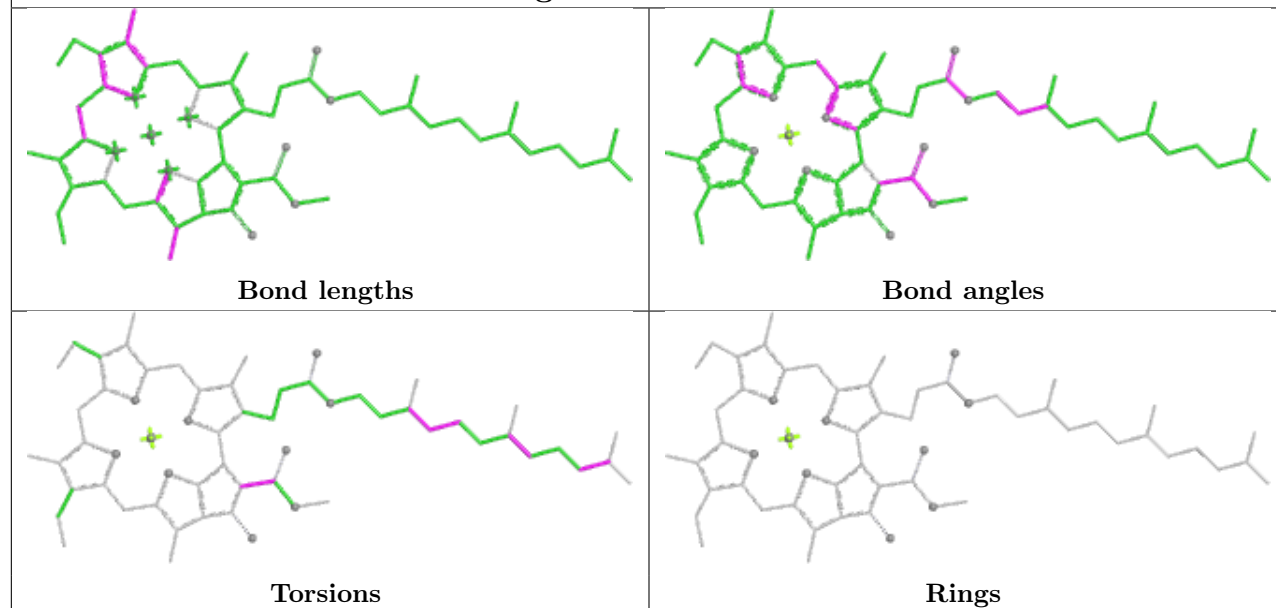
Ligand PID D 307



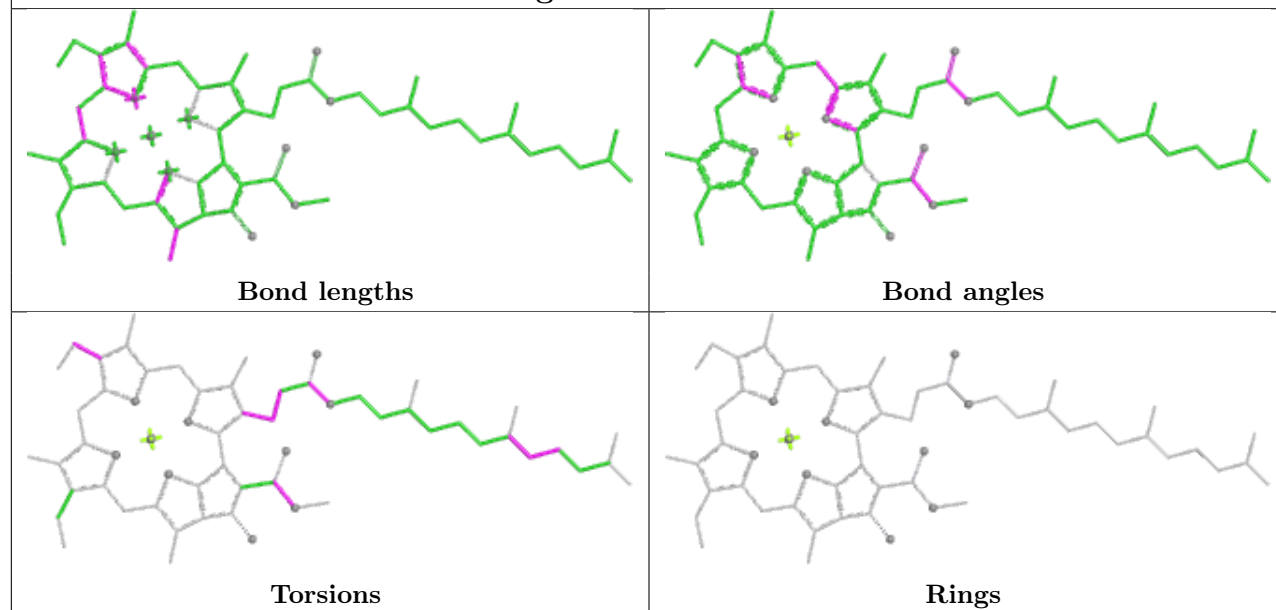
Ligand CLA M 310

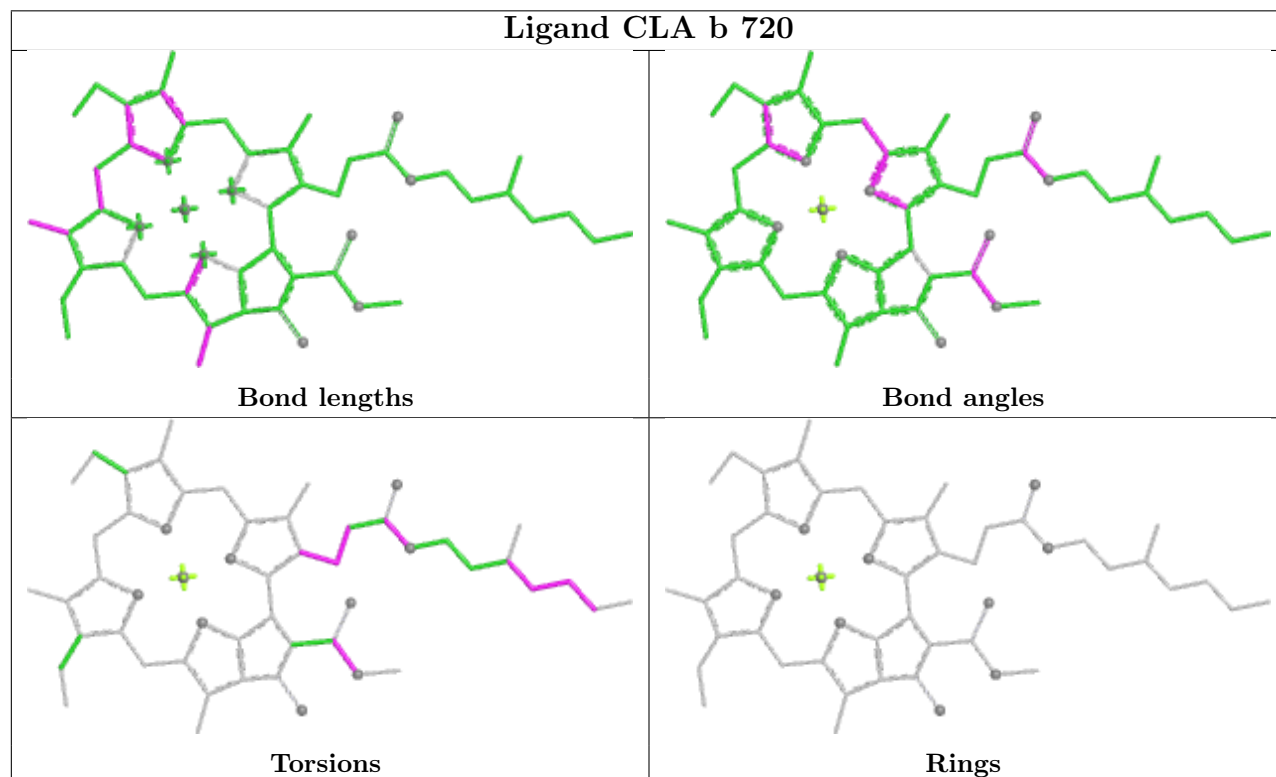
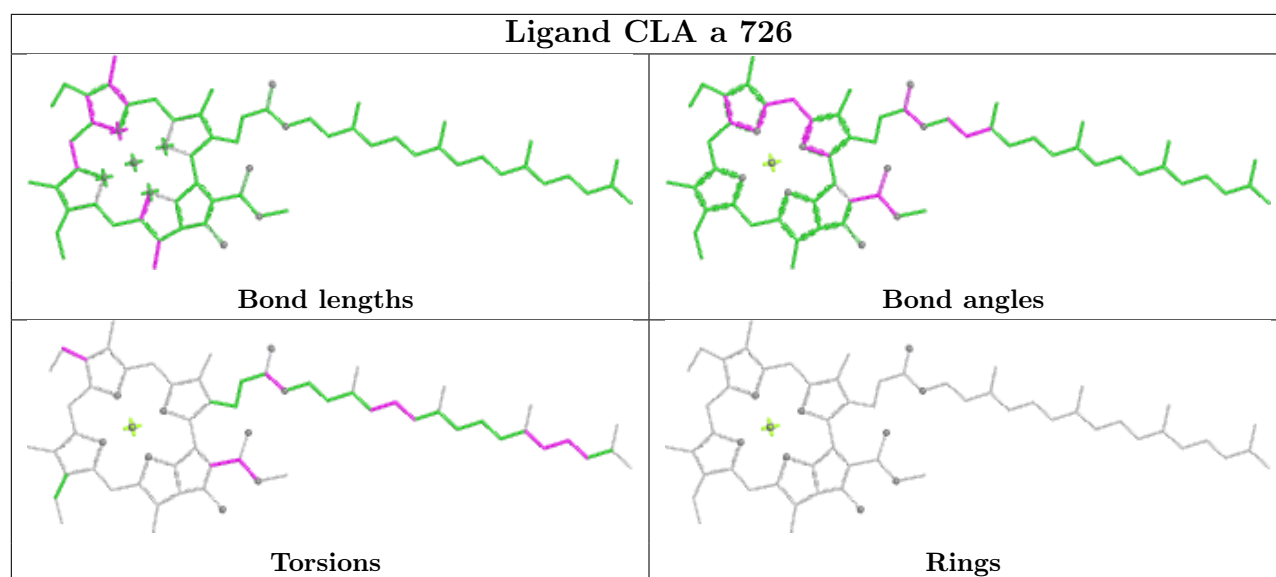


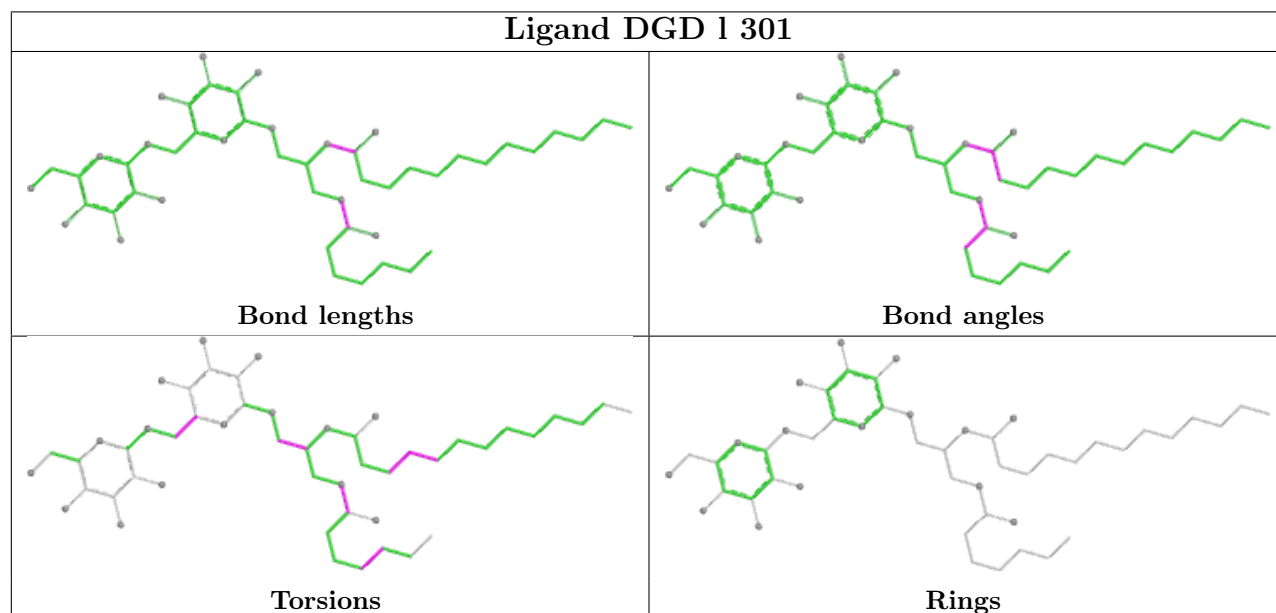
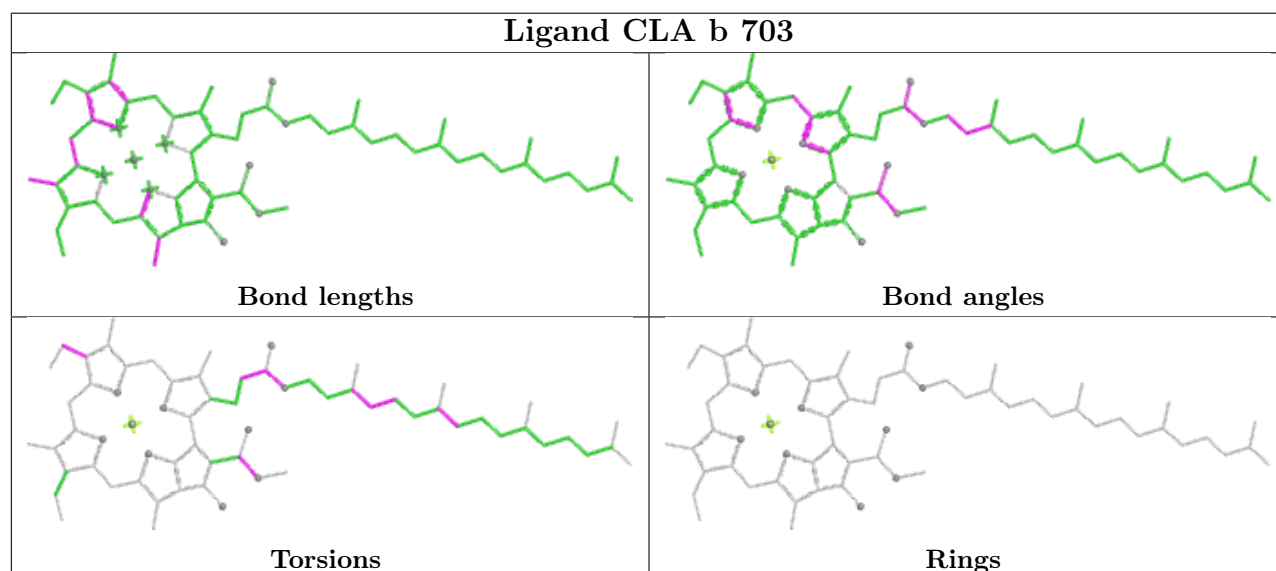
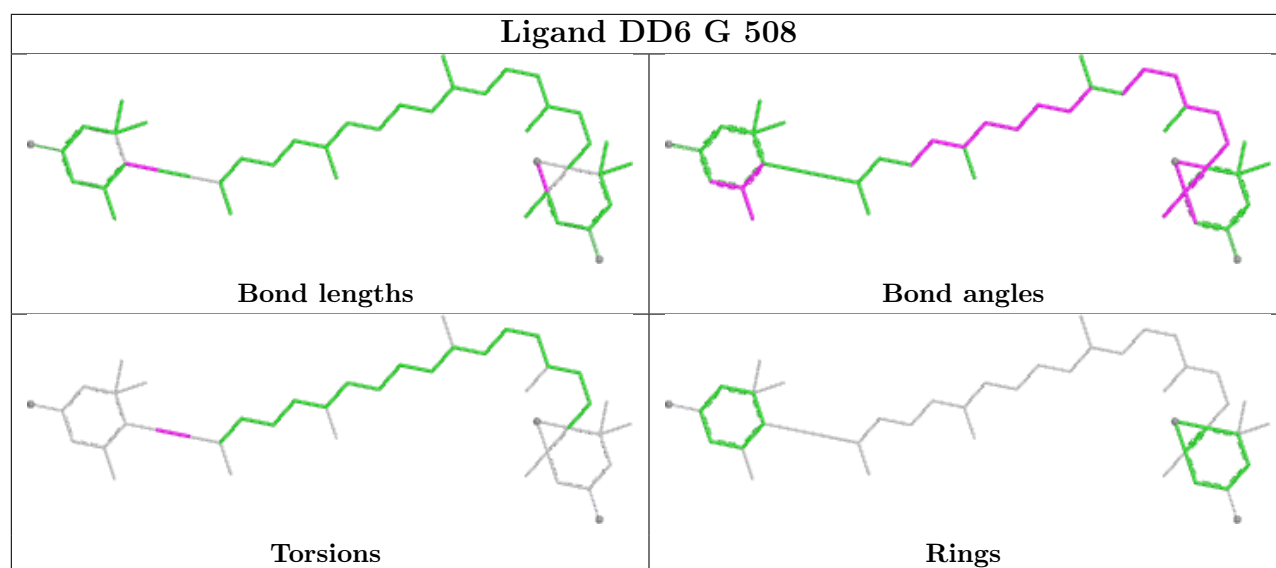
Ligand CLA b 709

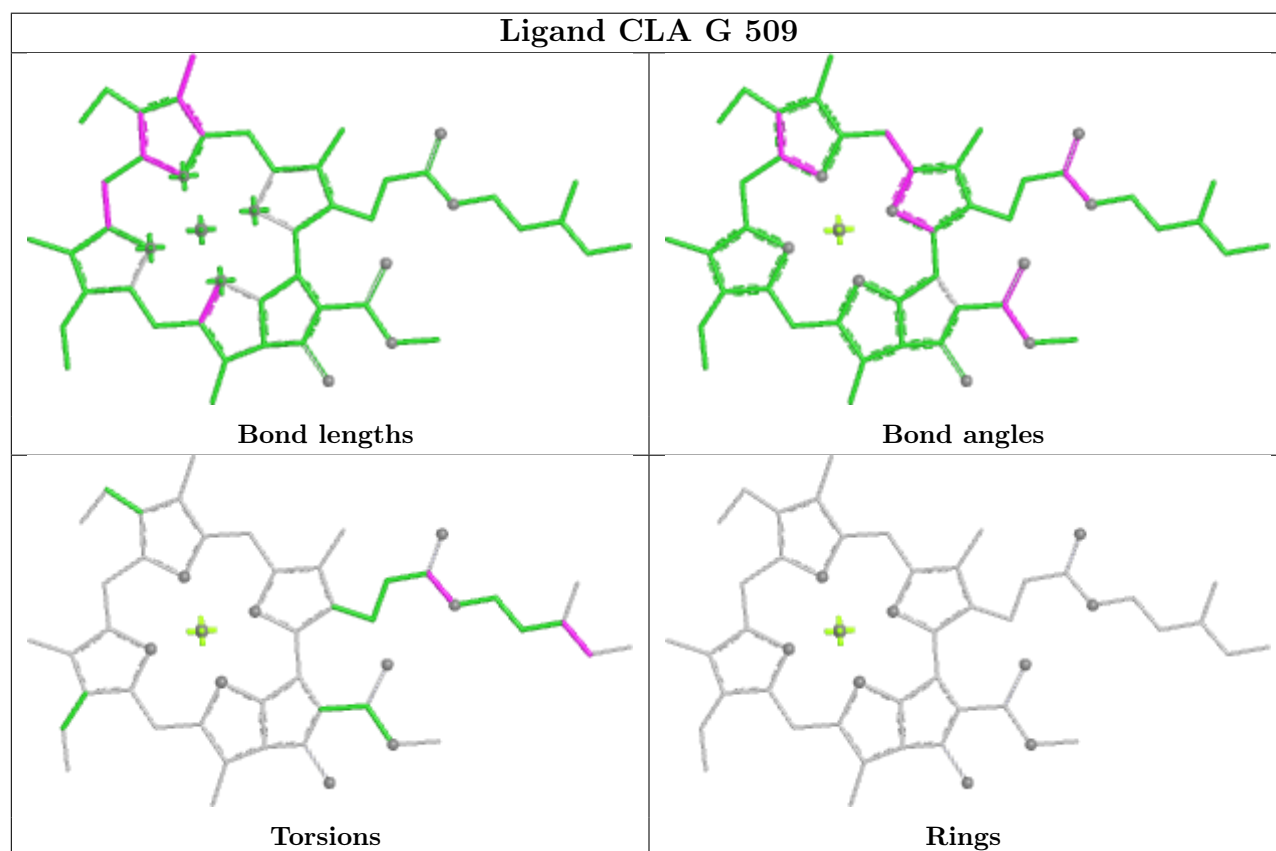
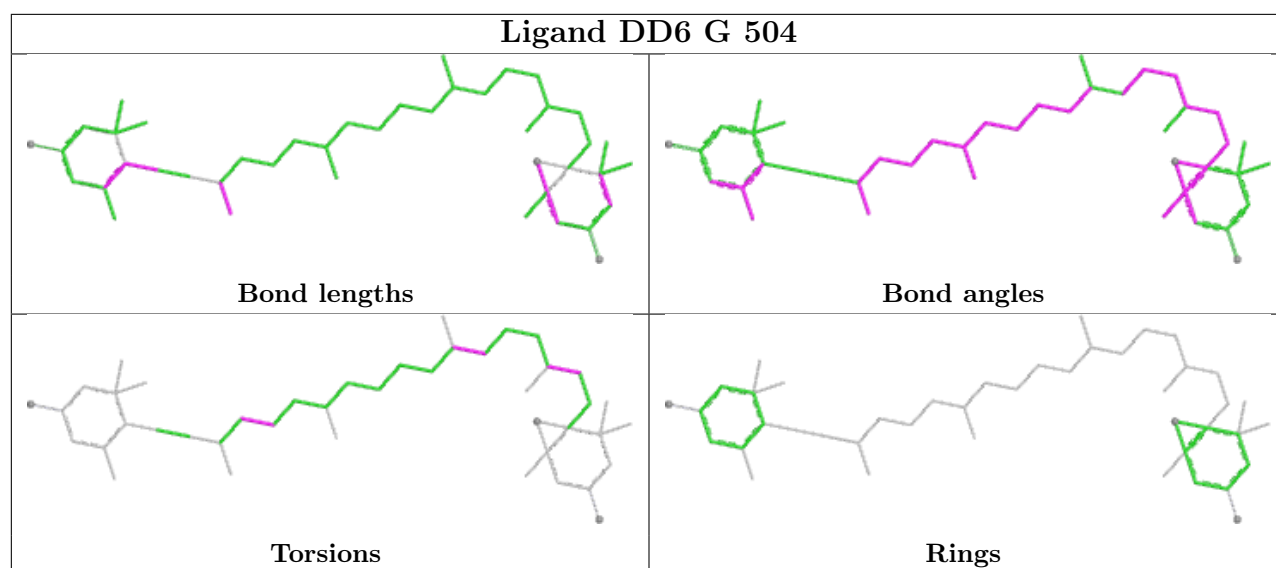


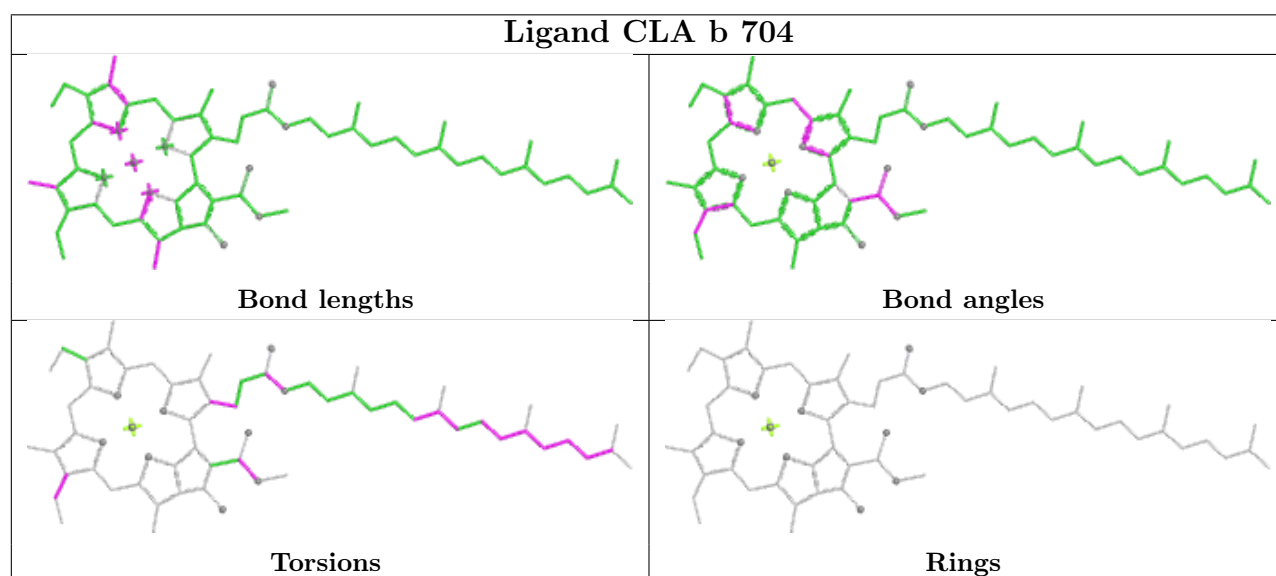
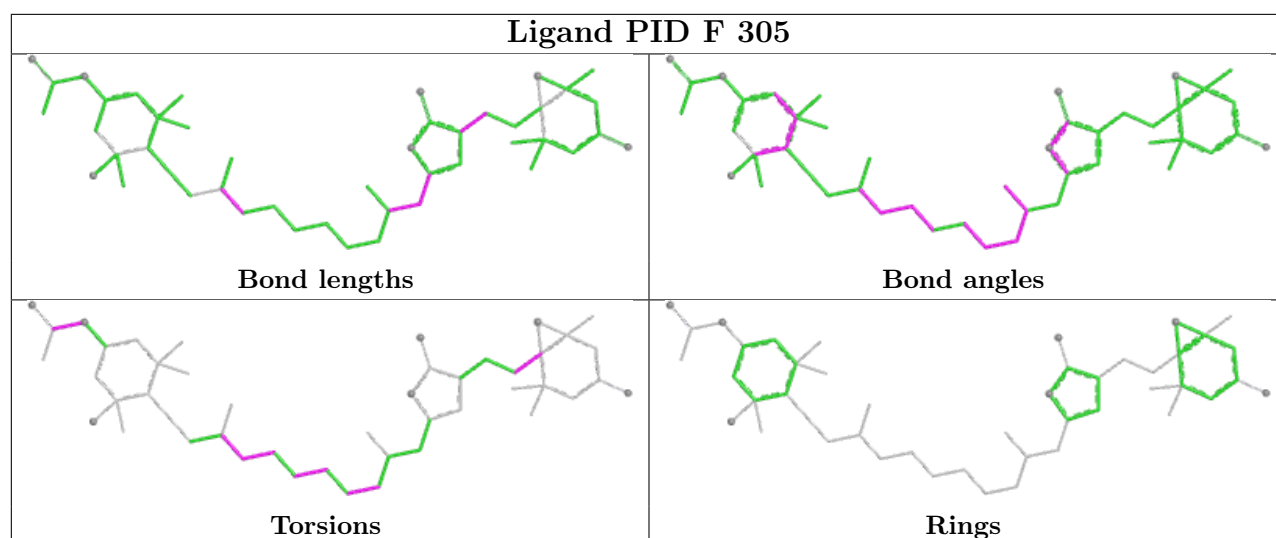
Ligand CLA J 301



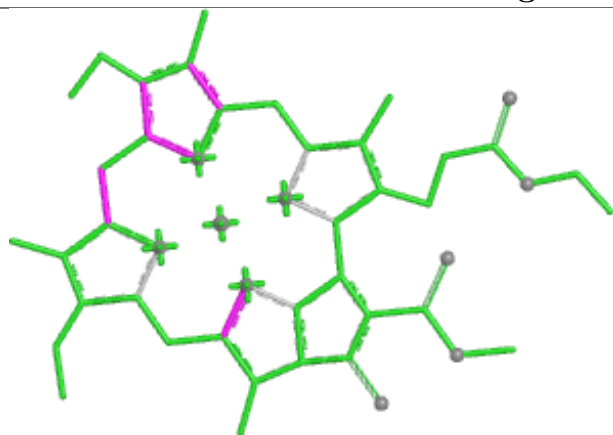




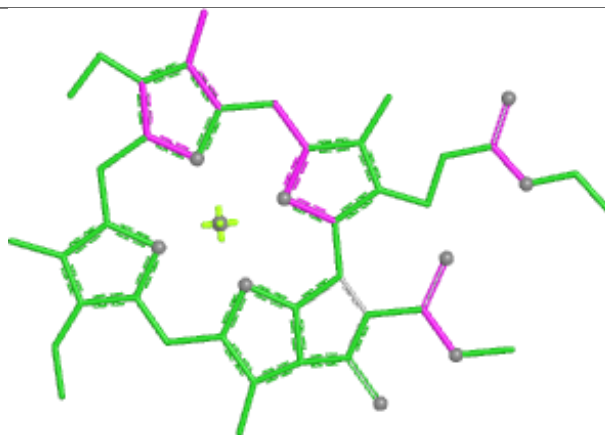




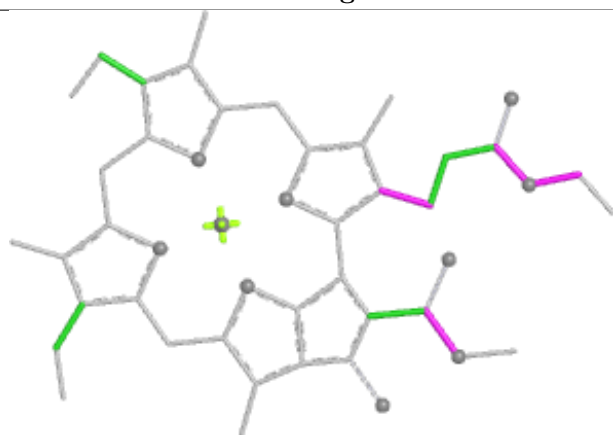
Ligand CLA J 311



Bond lengths



Bond angles

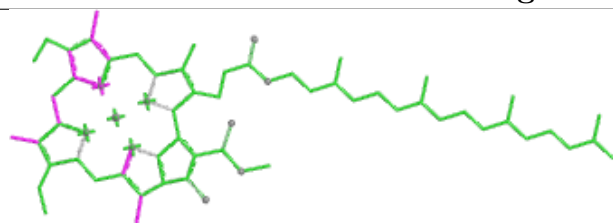


Torsions

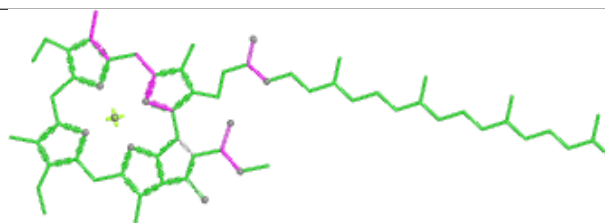


Rings

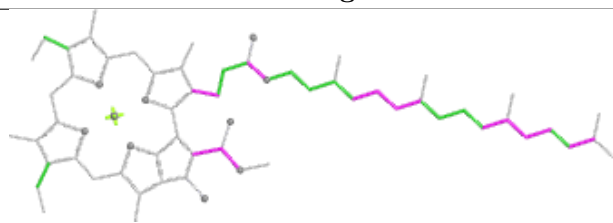
Ligand CLA b 717



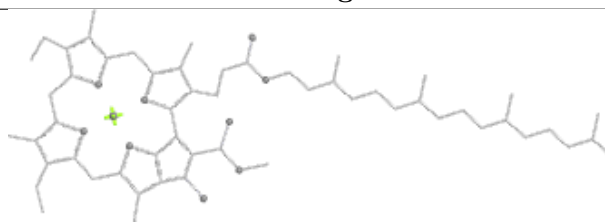
Bond lengths



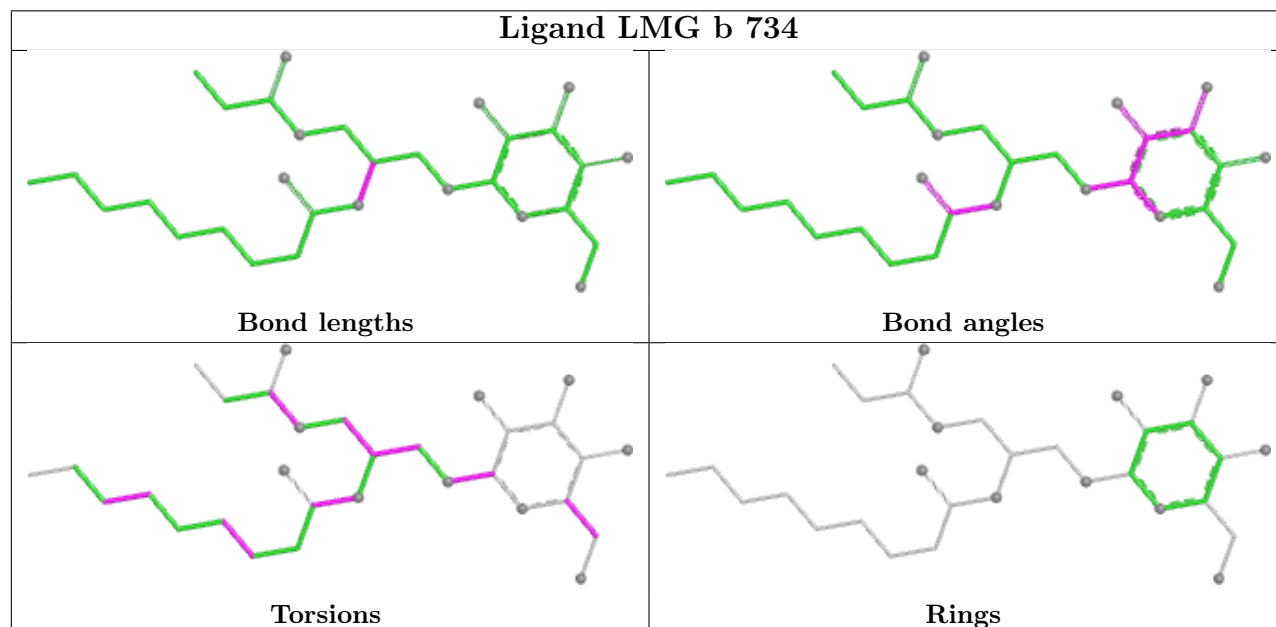
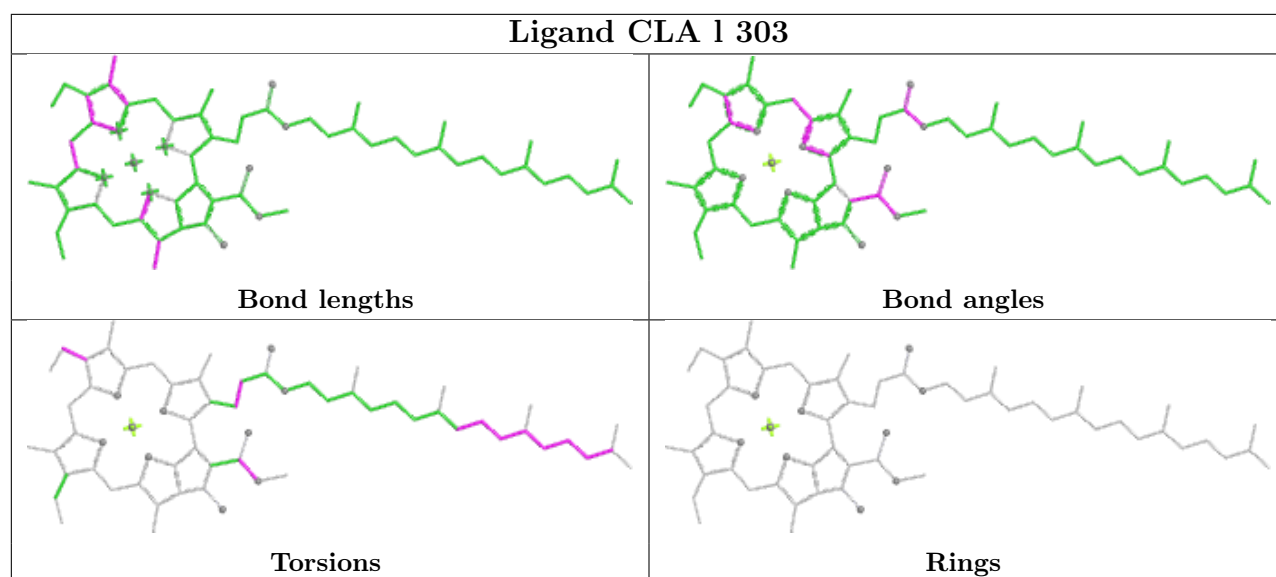
Bond angles



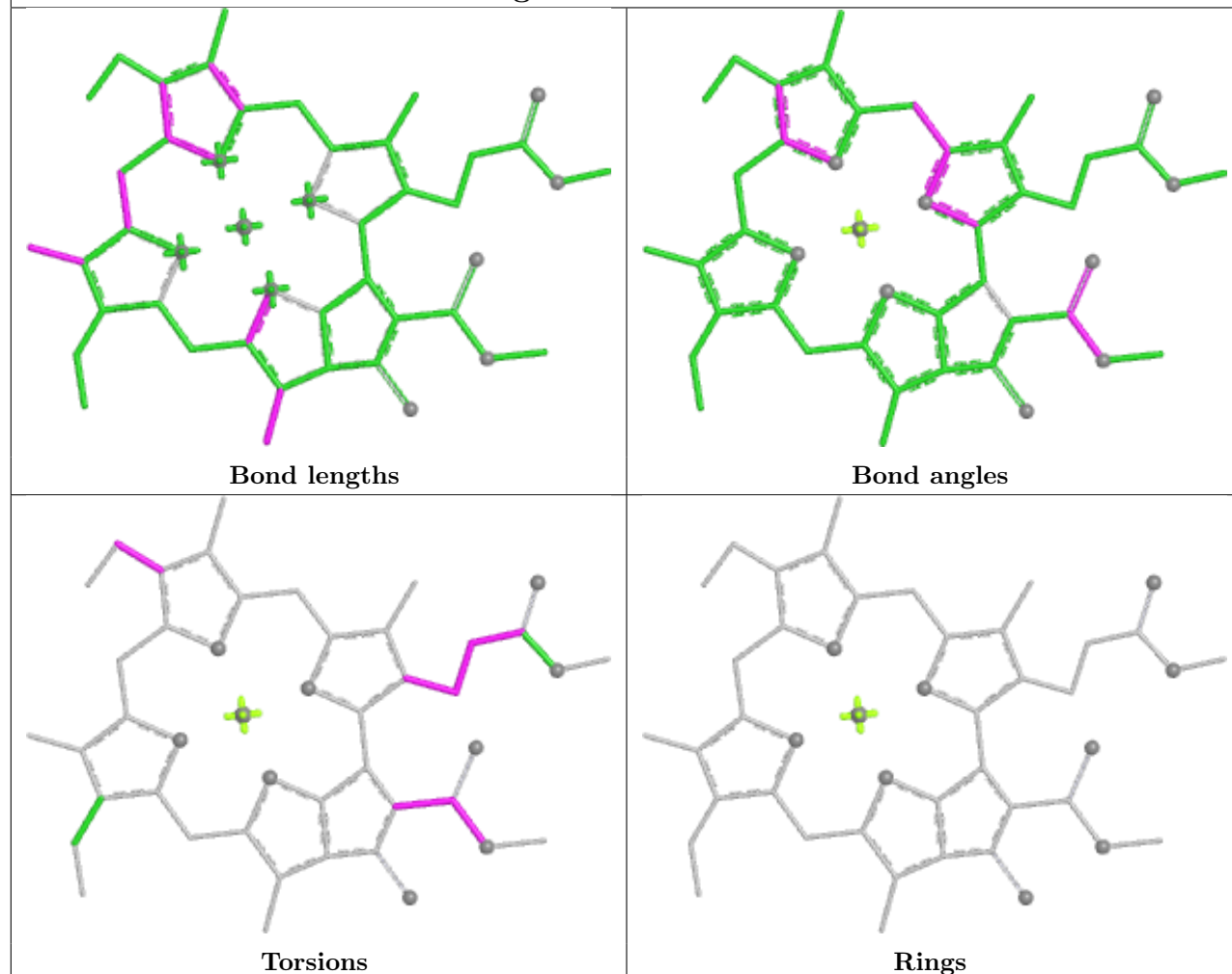
Torsions



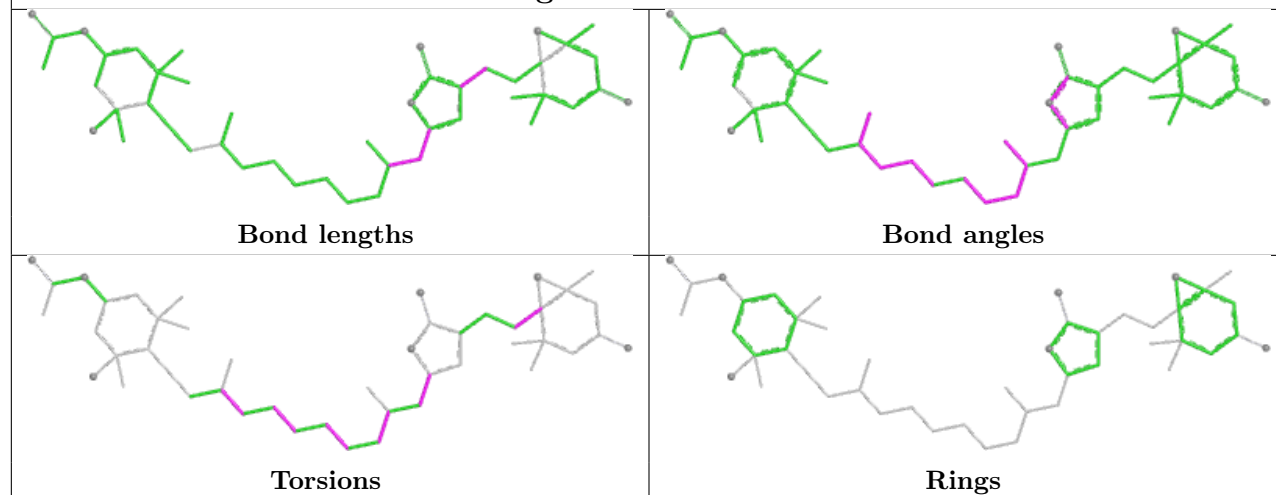
Rings



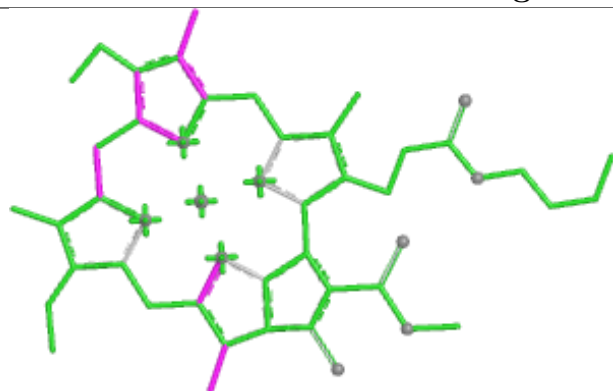
Ligand CLA A 319



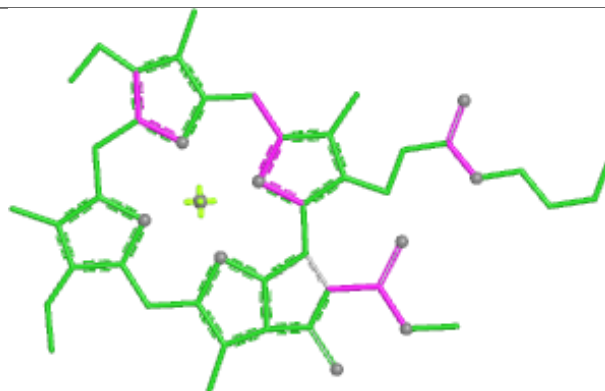
Ligand PID D 306



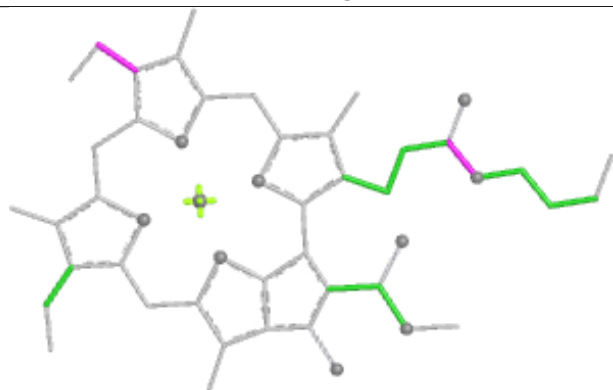
Ligand CLA K 306



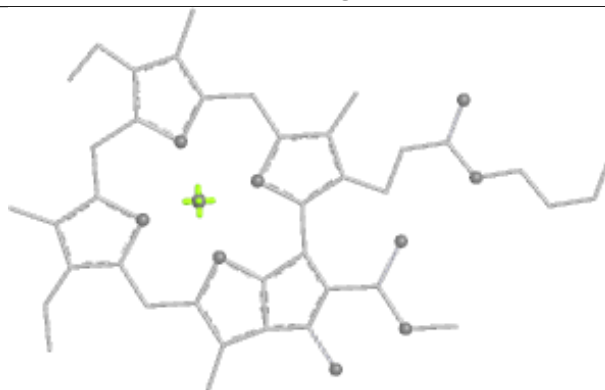
Bond lengths



Bond angles



Torsions

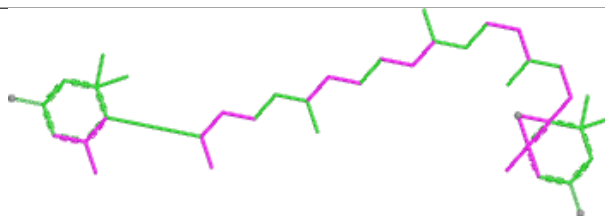


Rings

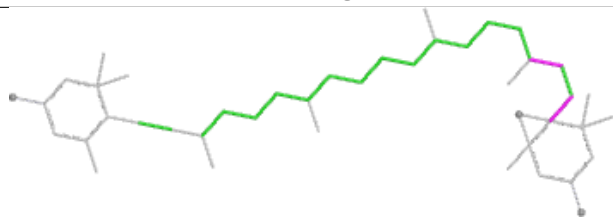
Ligand DD6 L 305



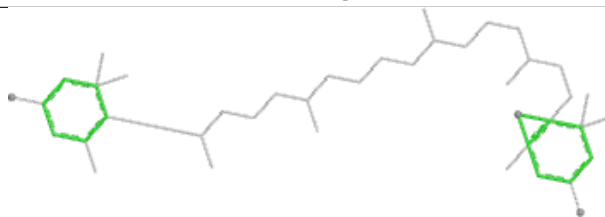
Bond lengths



Bond angles

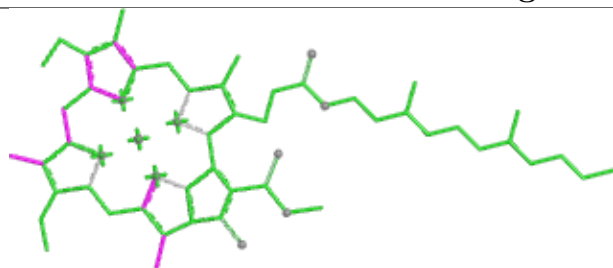


Torsions

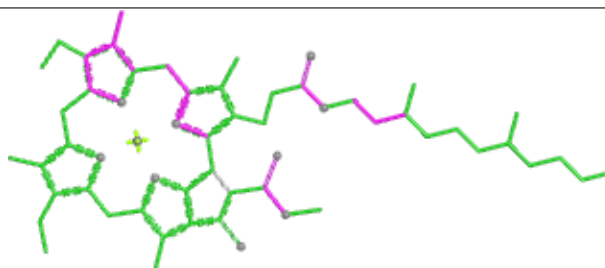


Rings

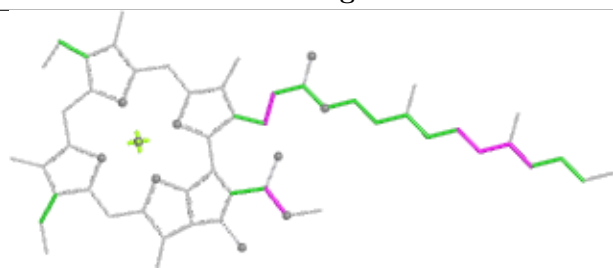
Ligand CLA a 722



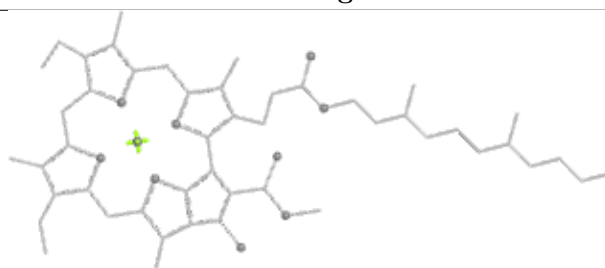
Bond lengths



Bond angles

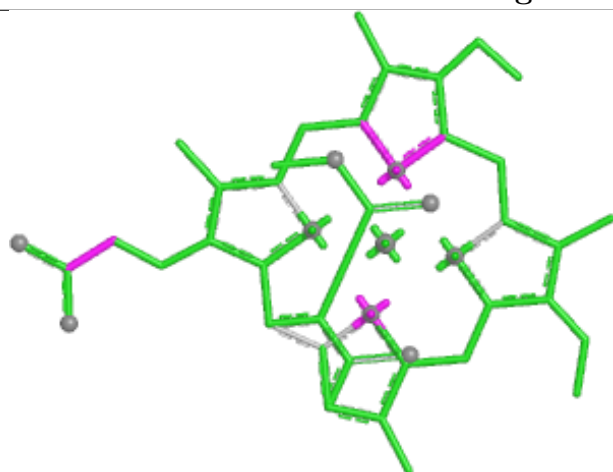


Torsions

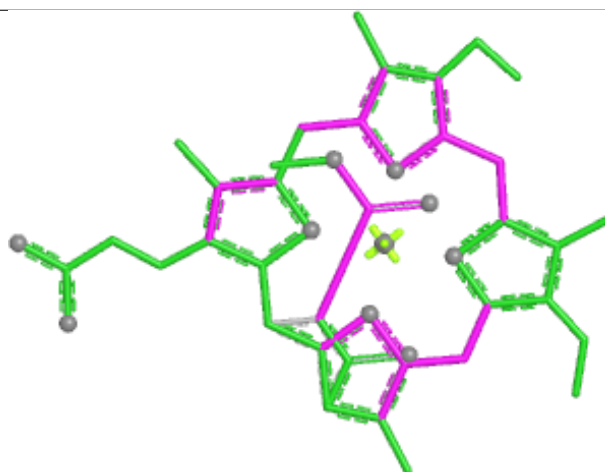


Rings

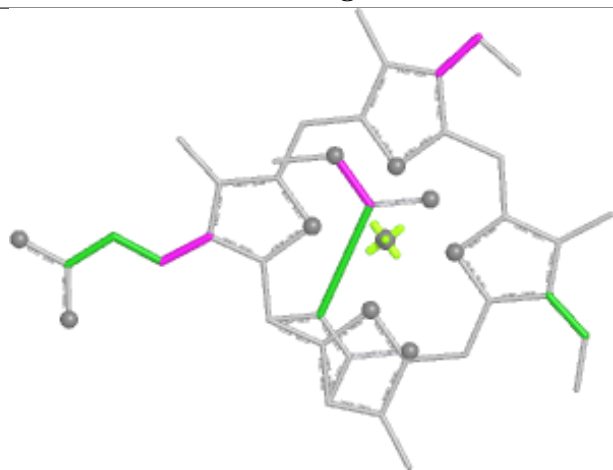
Ligand KC1 H 310



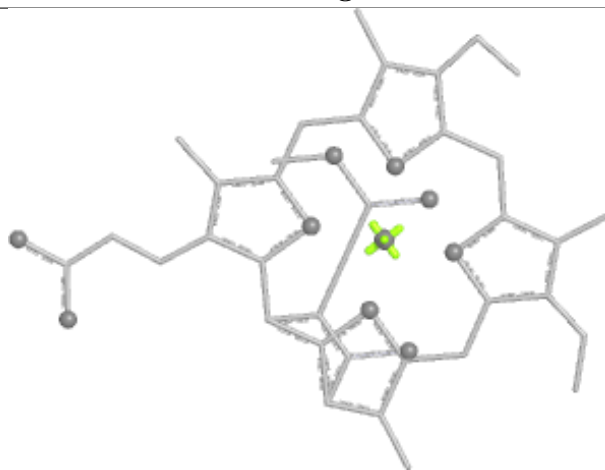
Bond lengths



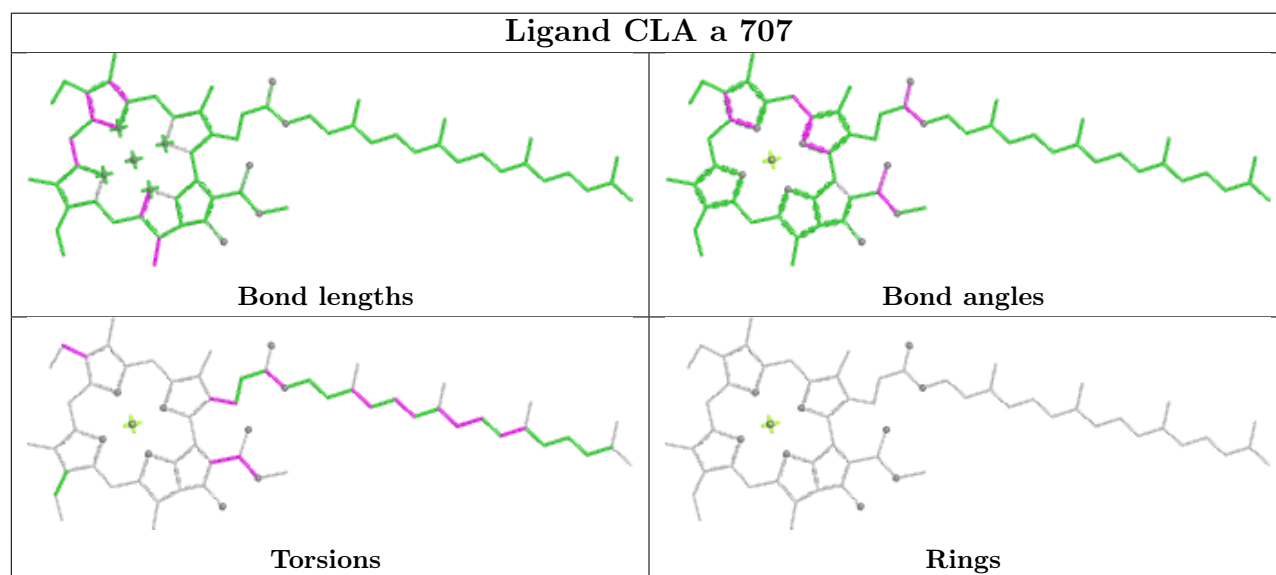
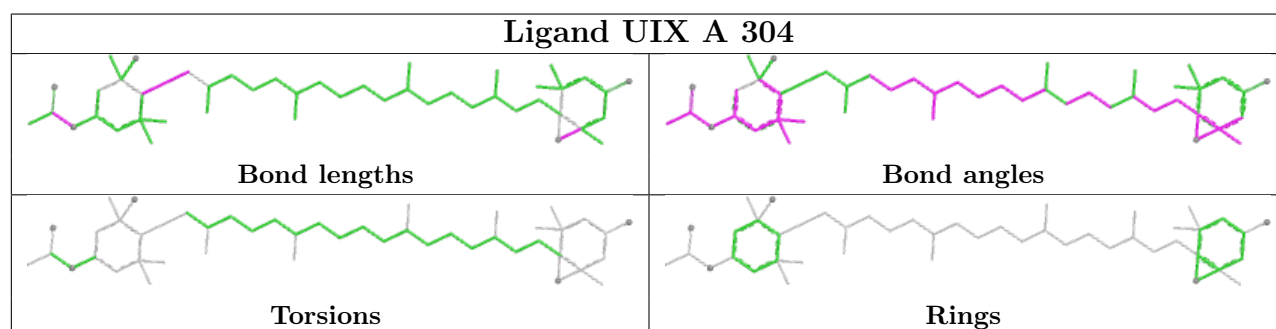
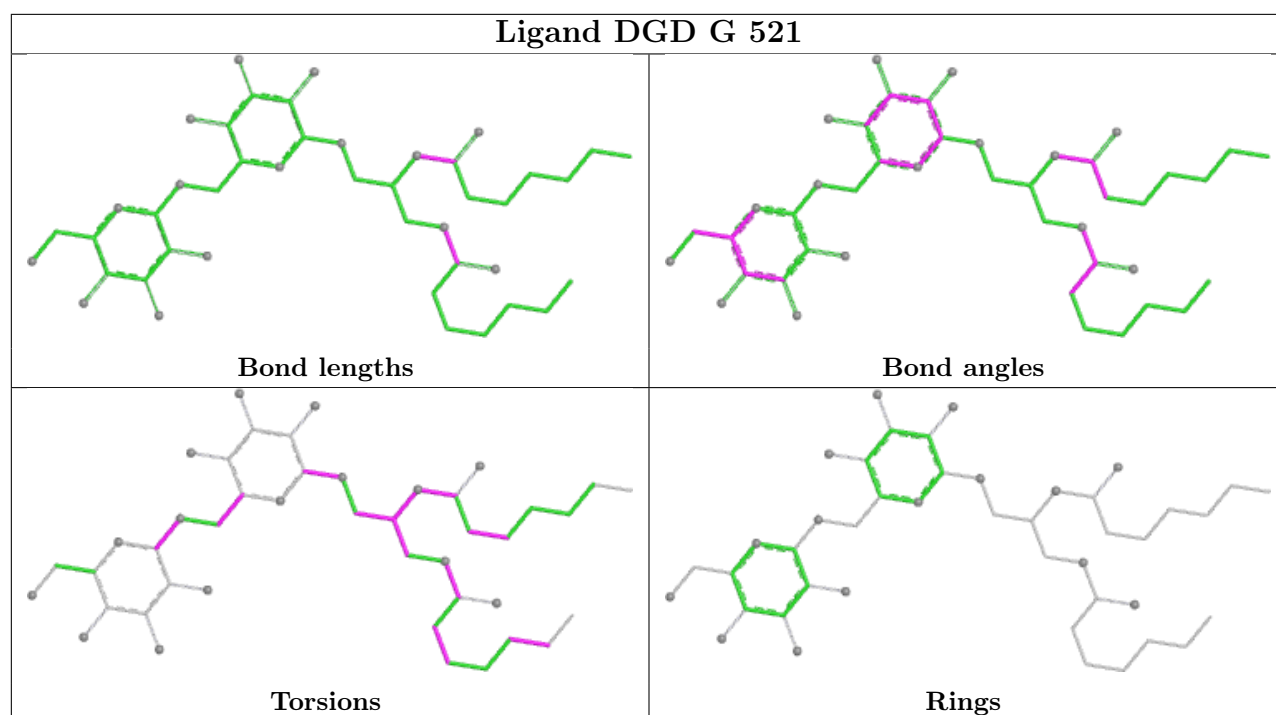
Bond angles



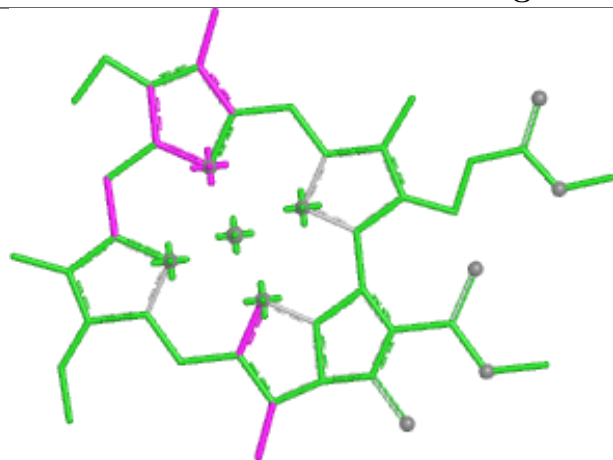
Torsions



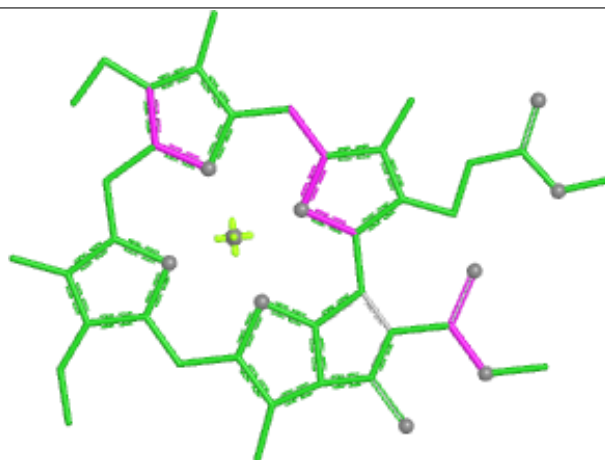
Rings



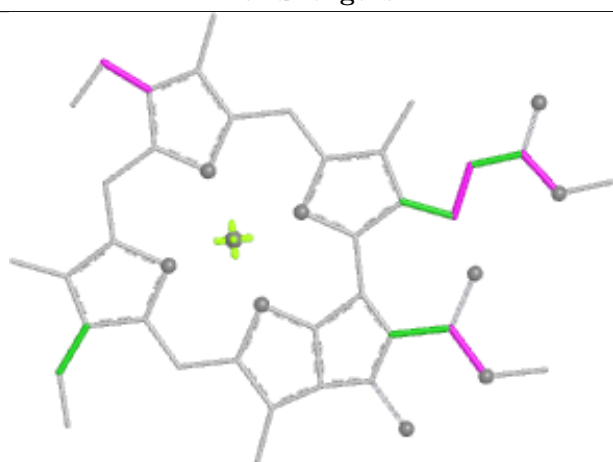
Ligand CLA D 312



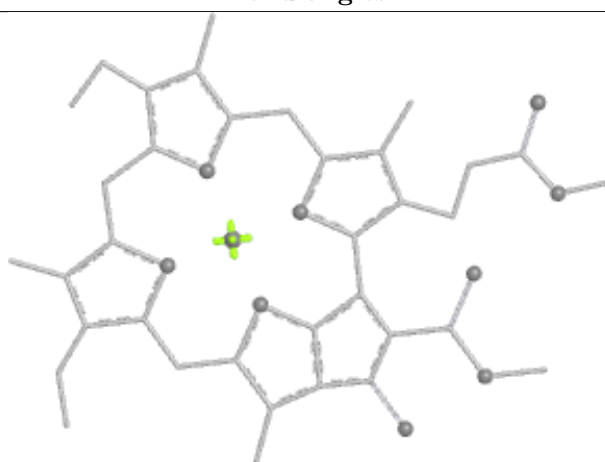
Bond lengths



Bond angles

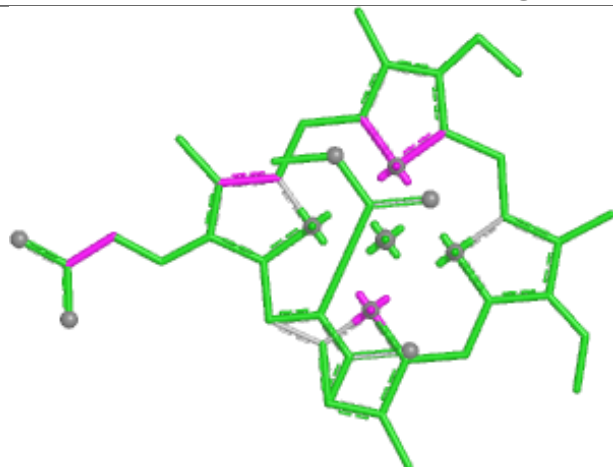


Torsions

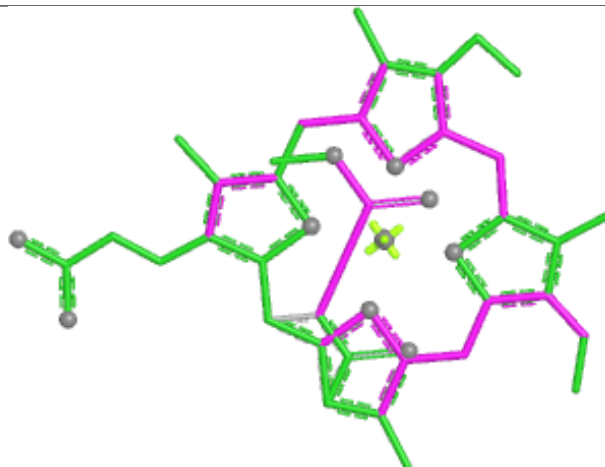


Rings

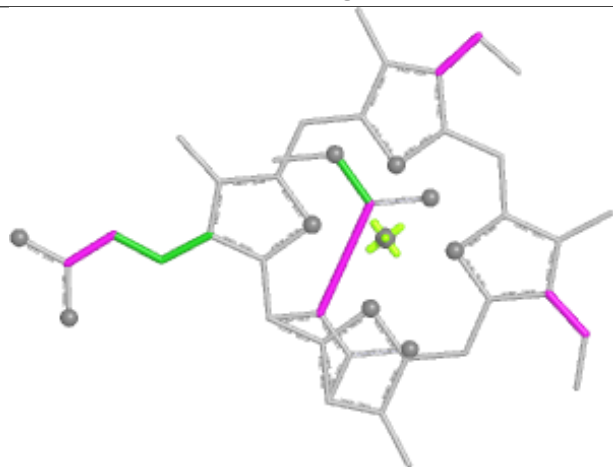
Ligand KC1 G 515



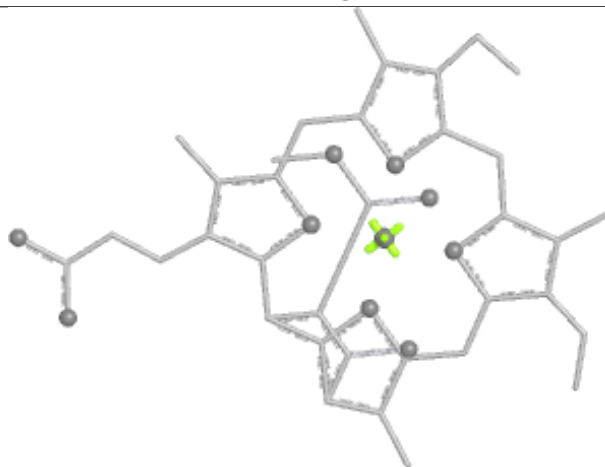
Bond lengths



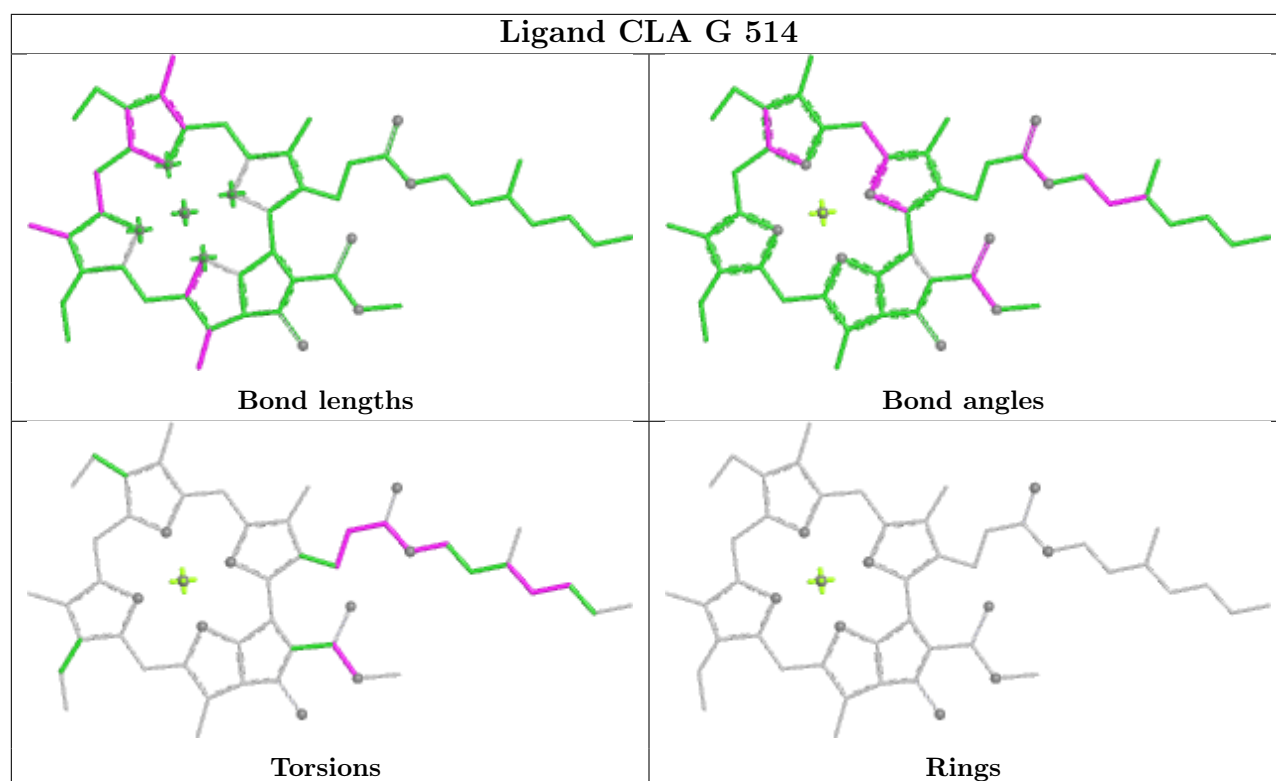
Bond angles



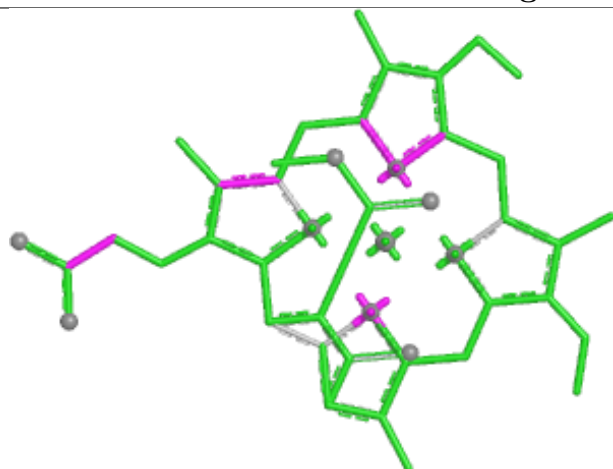
Torsions



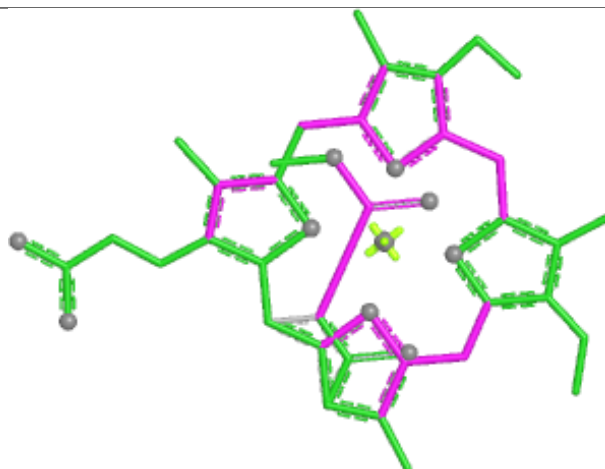
Rings



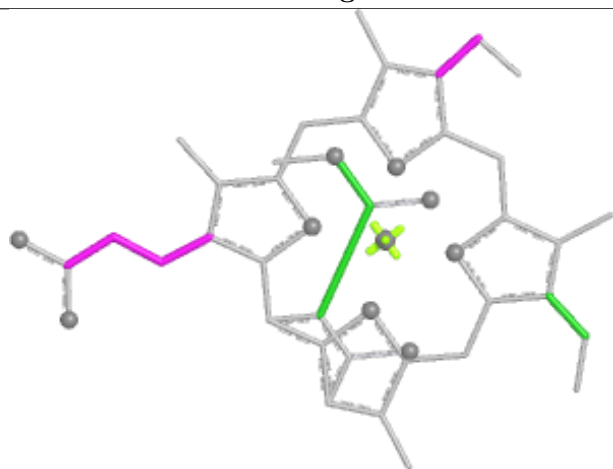
Ligand KC1 J 313



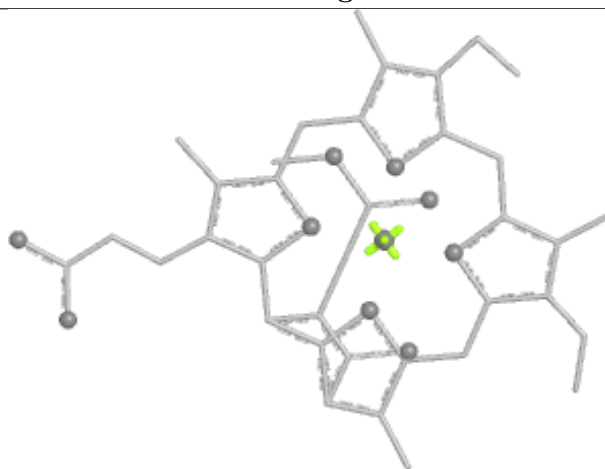
Bond lengths



Bond angles

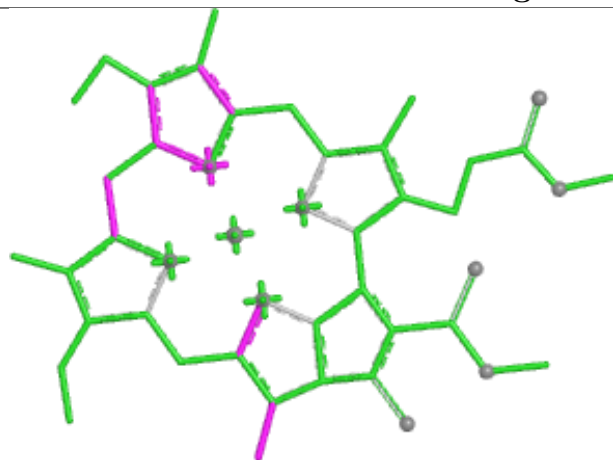


Torsions

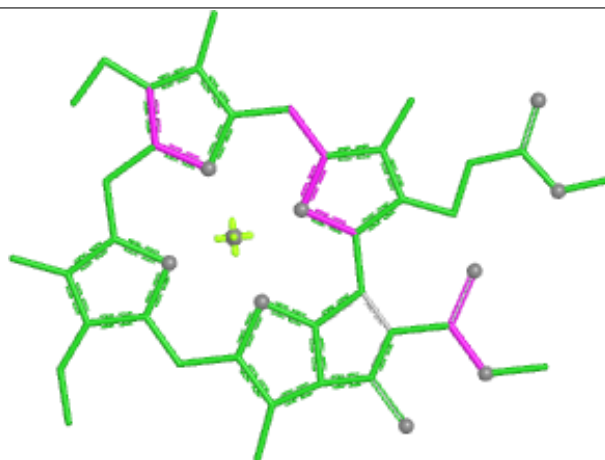


Rings

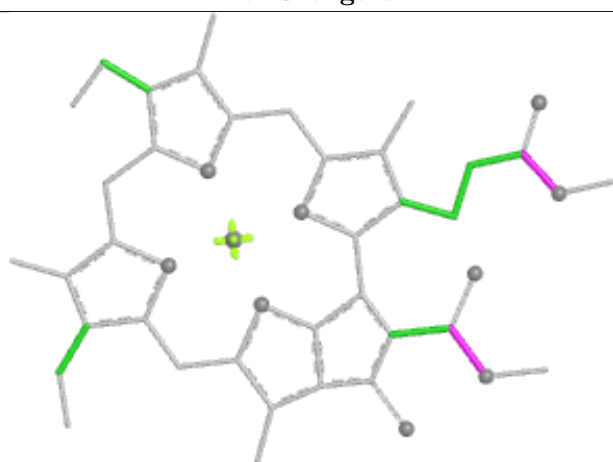
Ligand CLA H 308



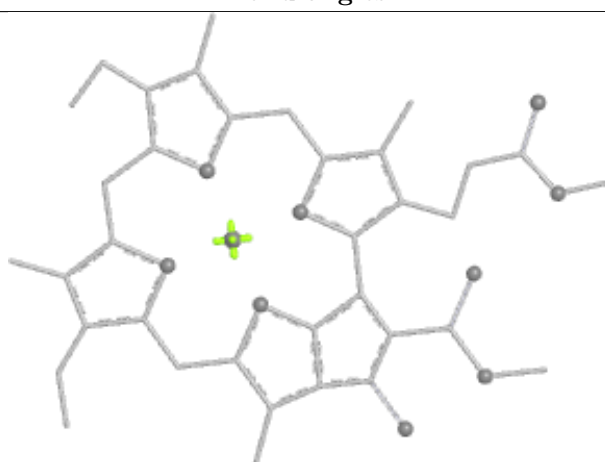
Bond lengths



Bond angles

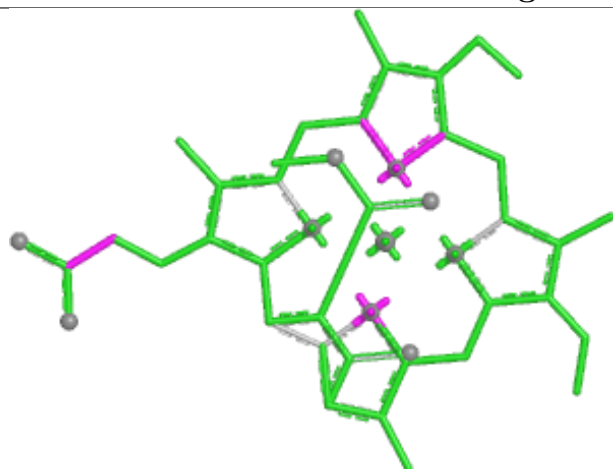


Torsions

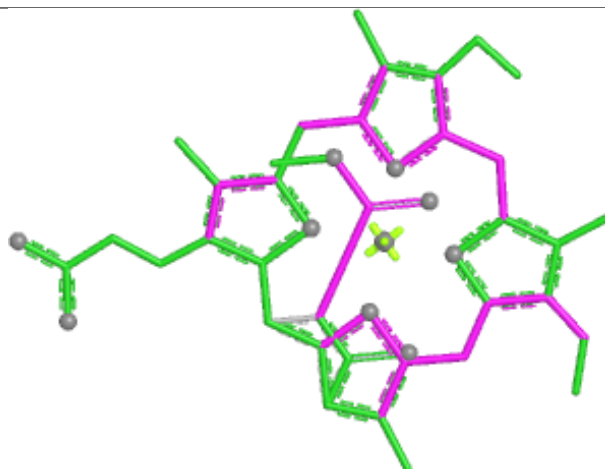


Rings

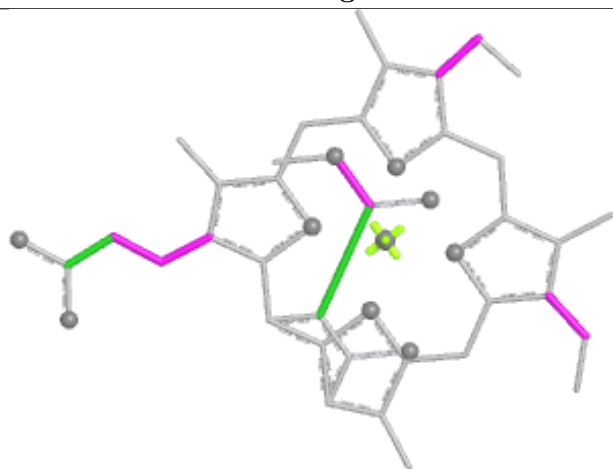
Ligand KC1 L 315



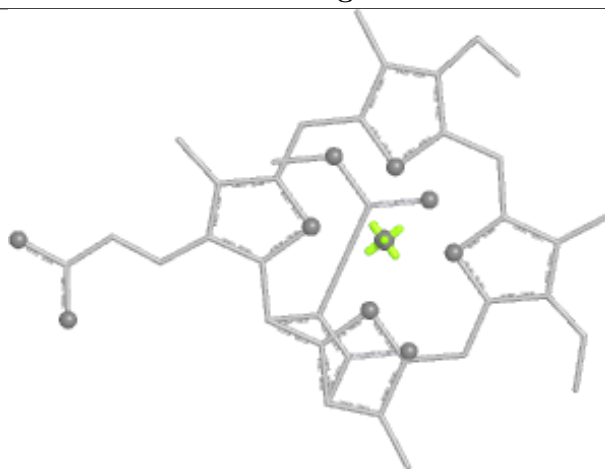
Bond lengths



Bond angles

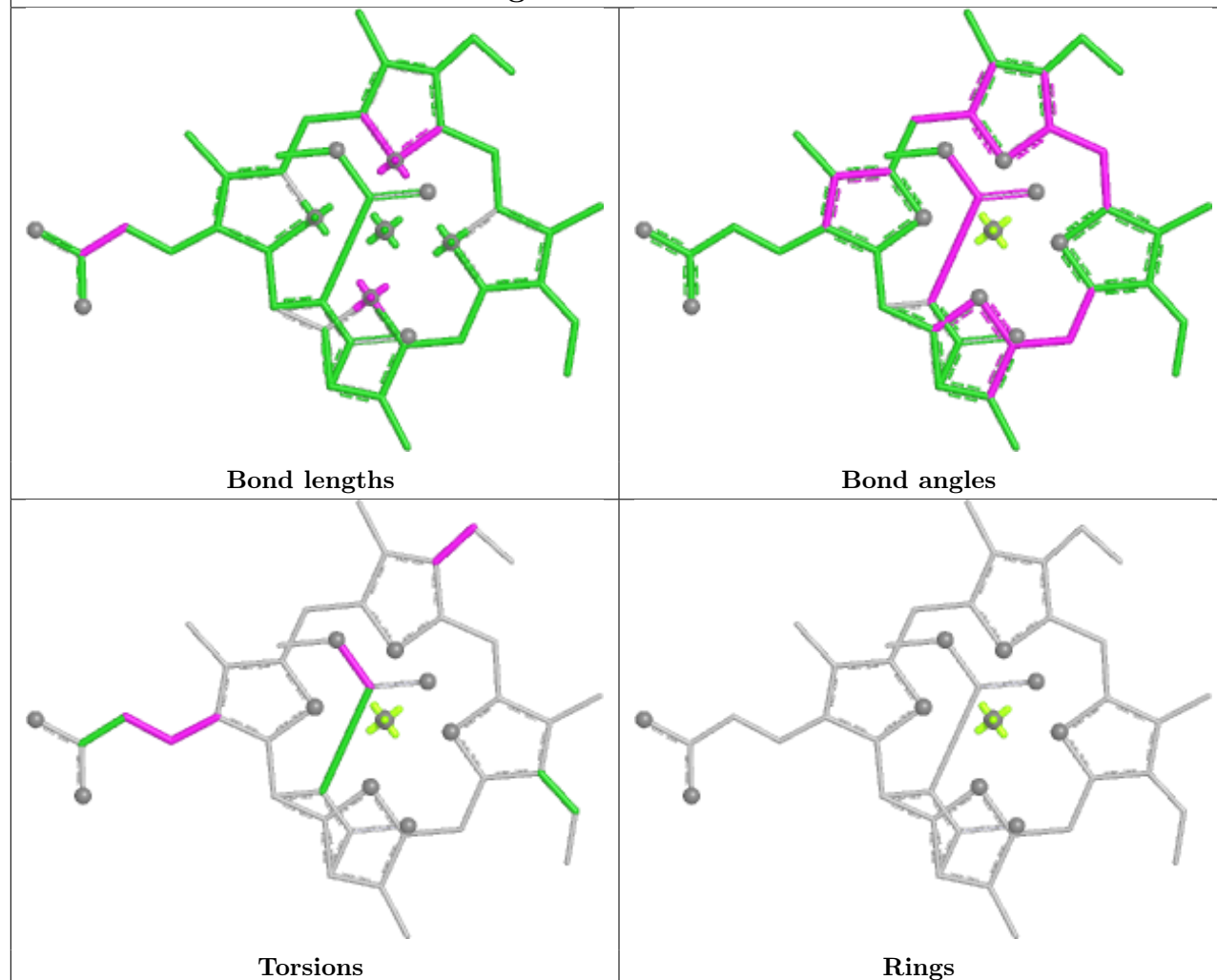


Torsions

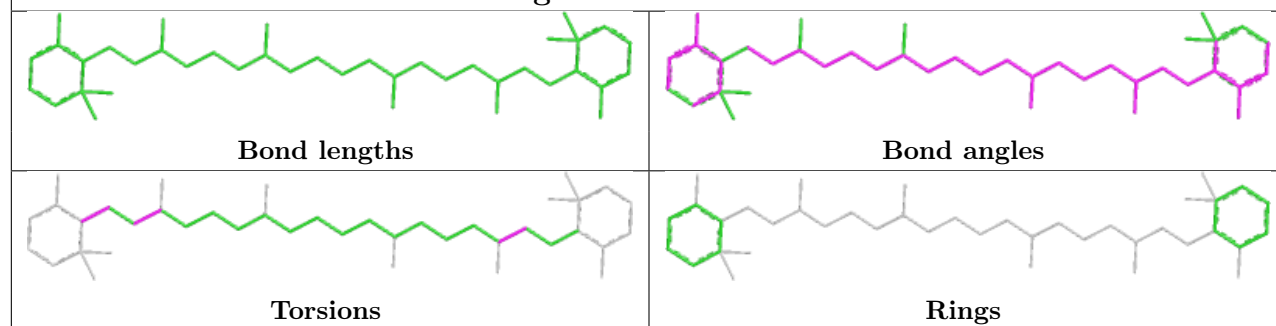


Rings

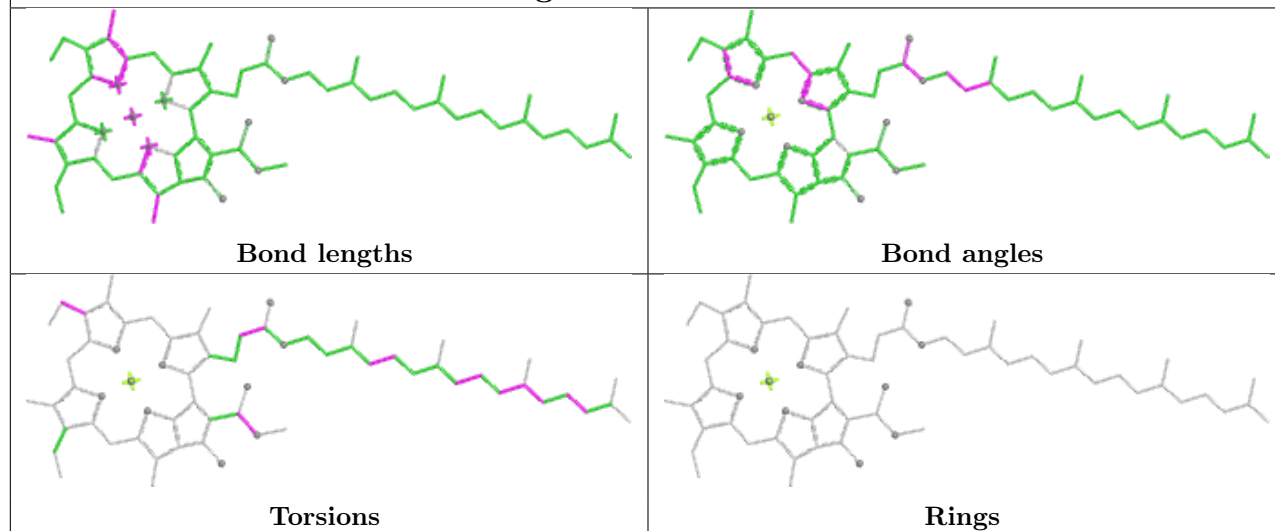
Ligand KC1 N 311



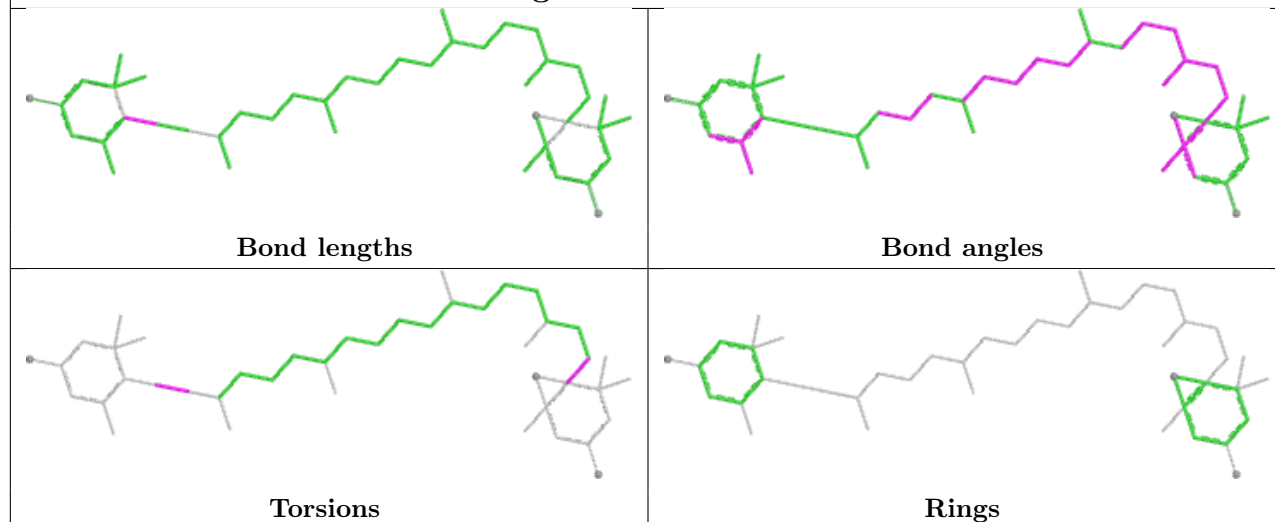
Ligand BCR b 730



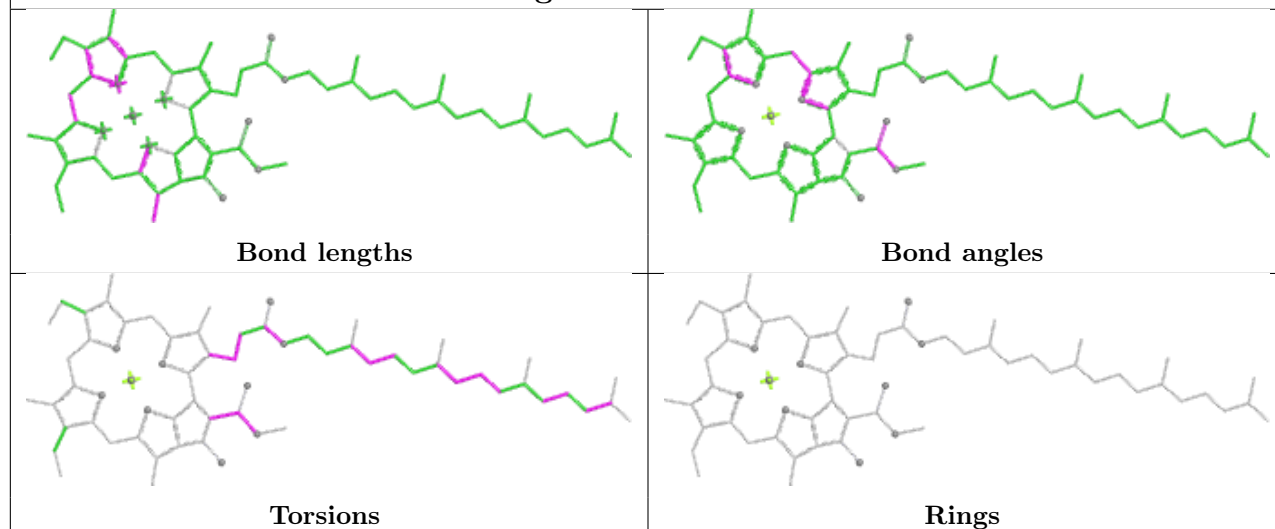
Ligand CLA a 702



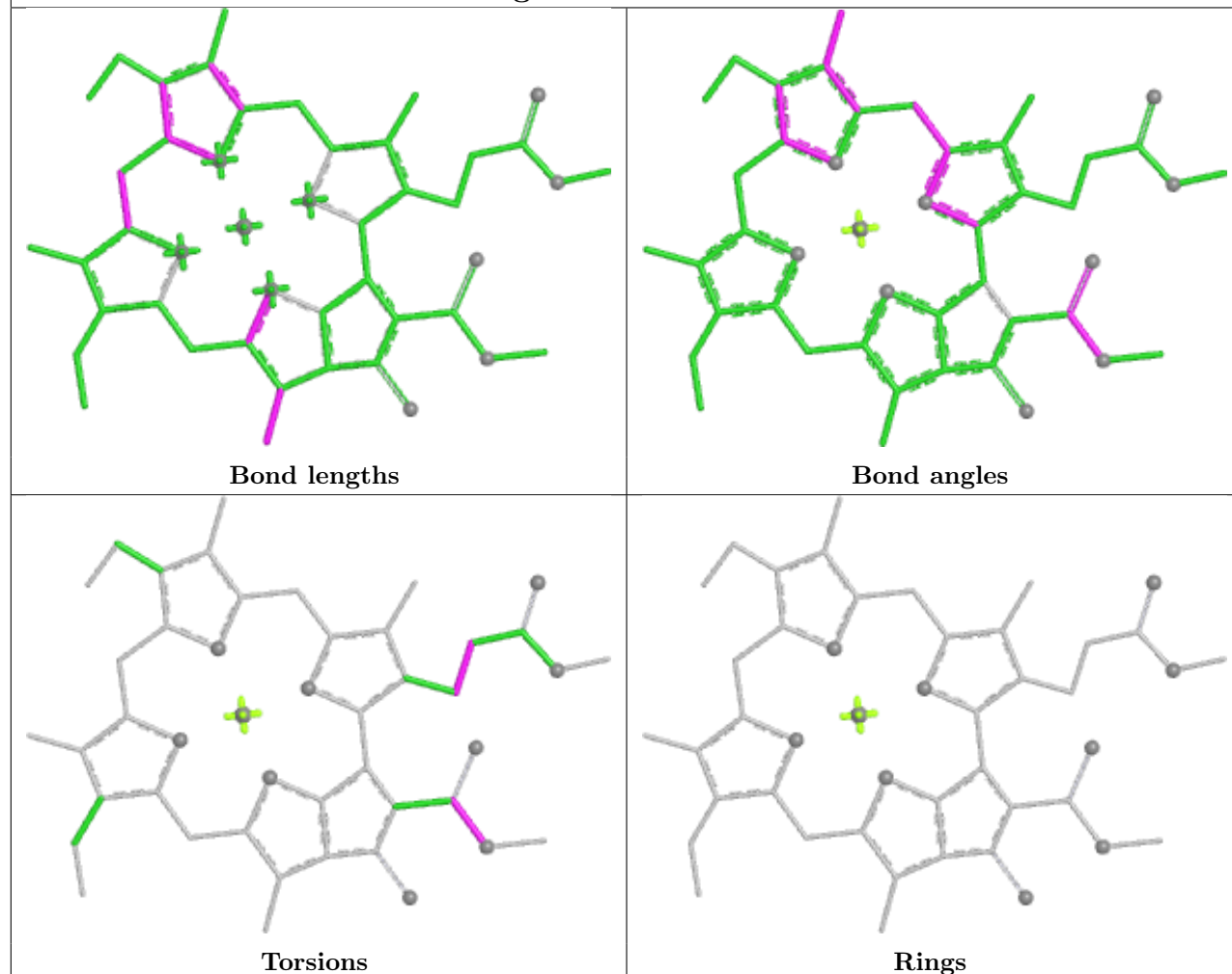
Ligand DD6 B 303



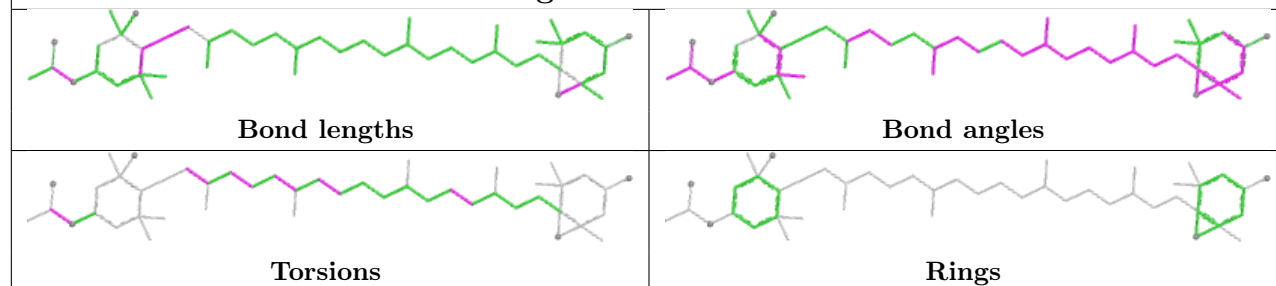
Ligand CLA J 307

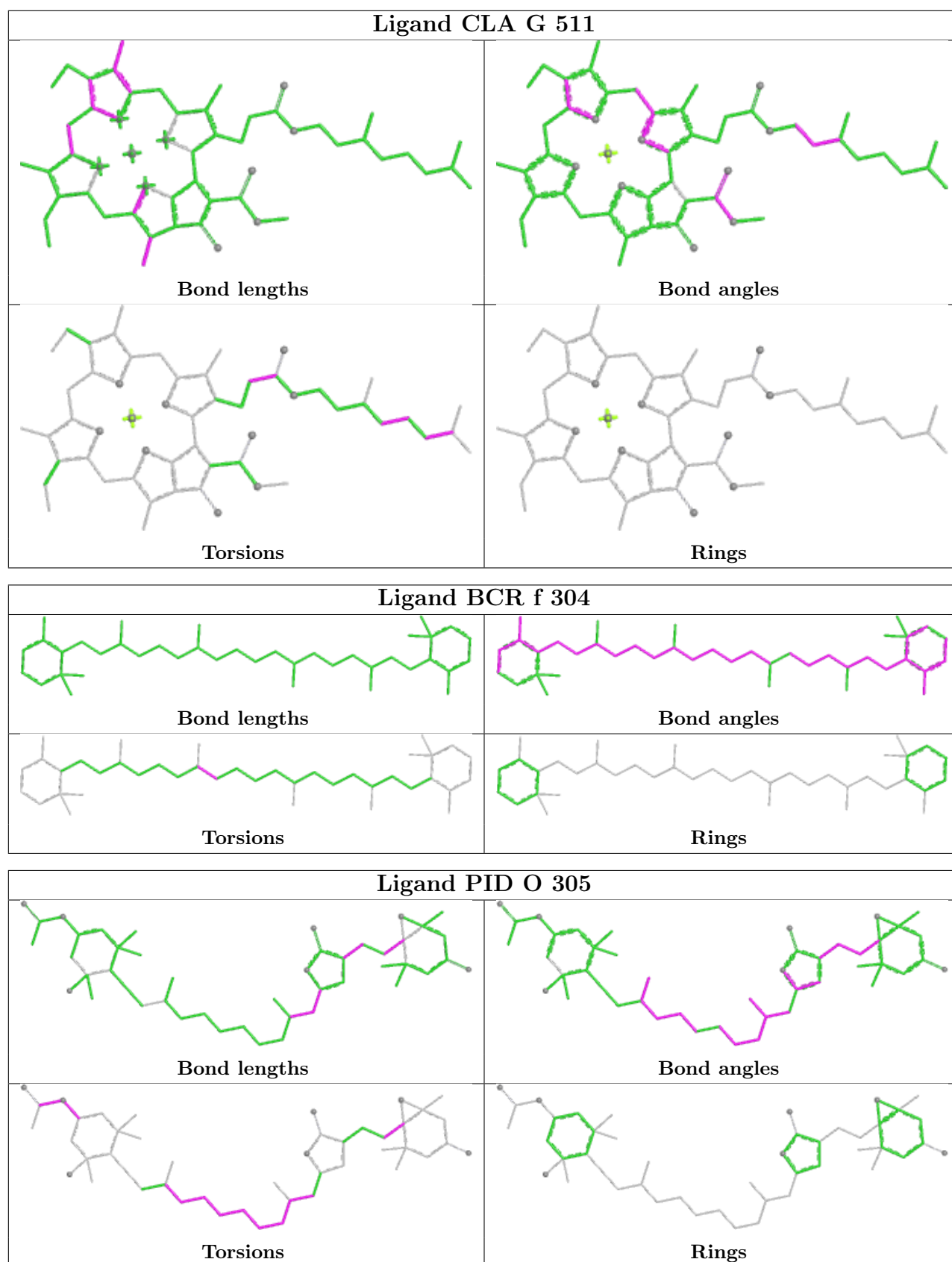


Ligand CLA O 313

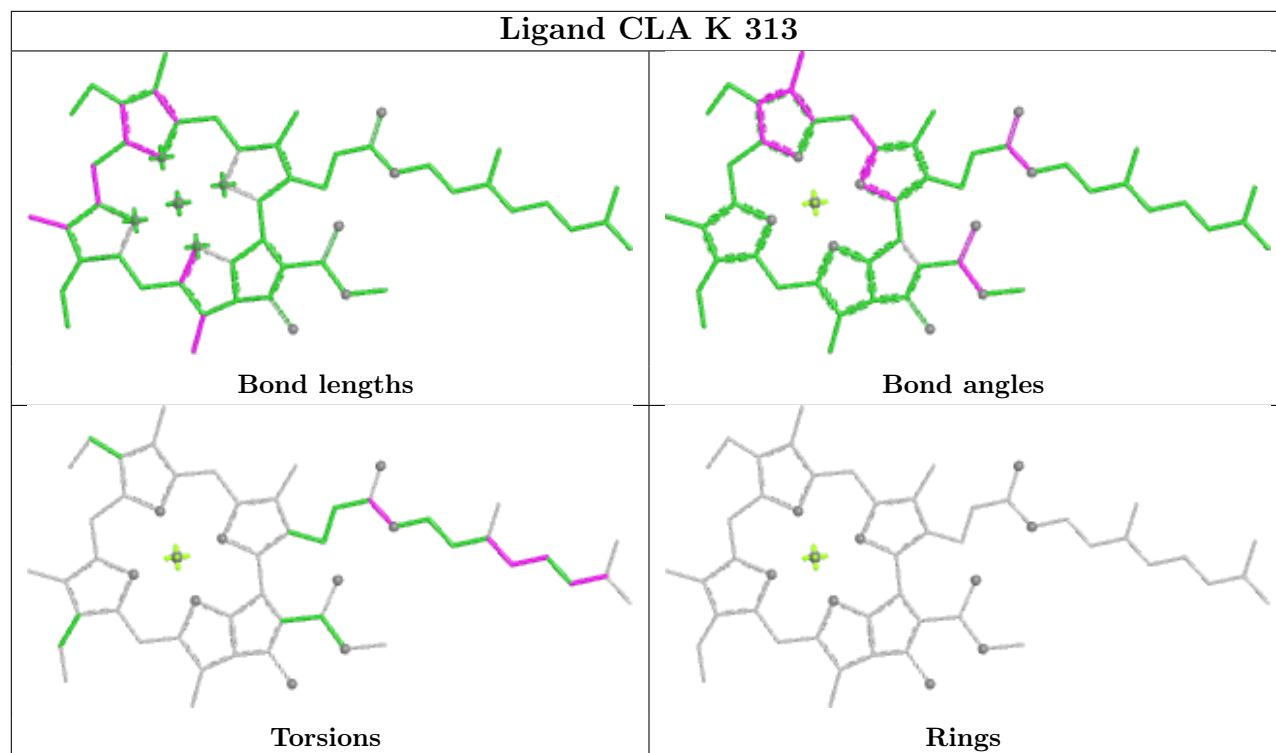


Ligand UIX P 207

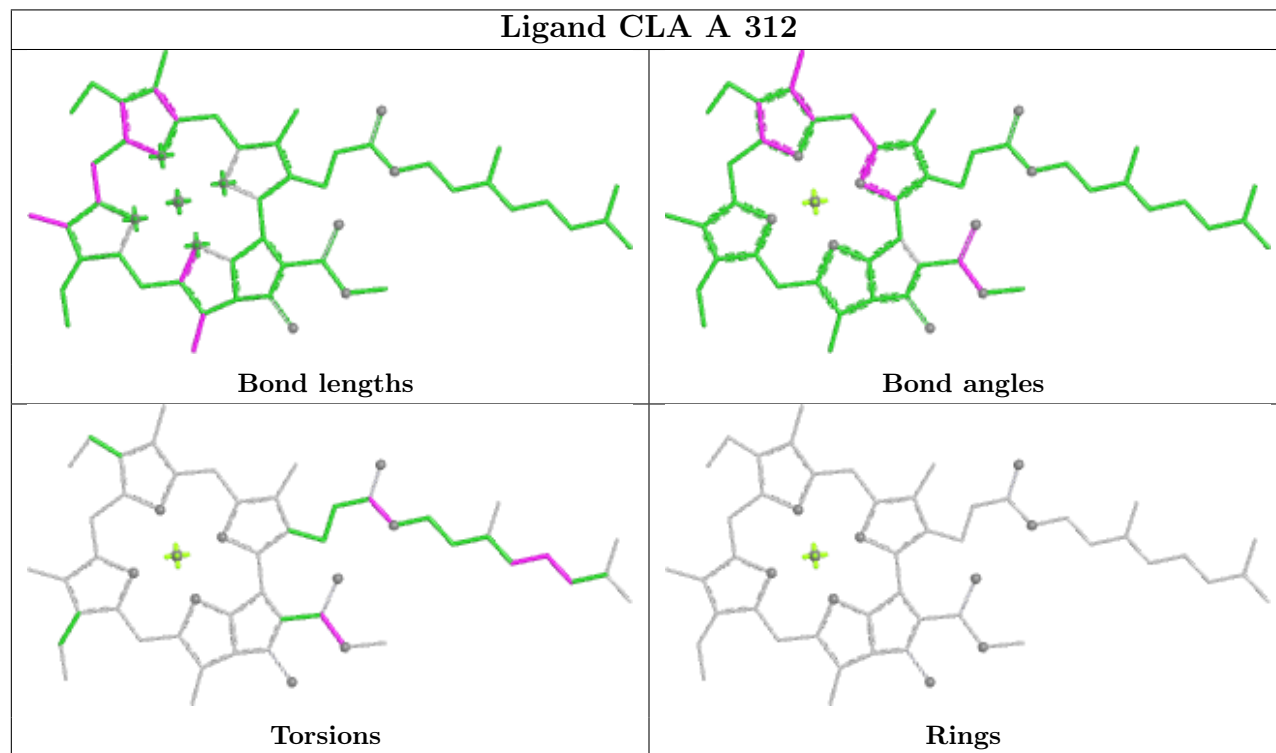


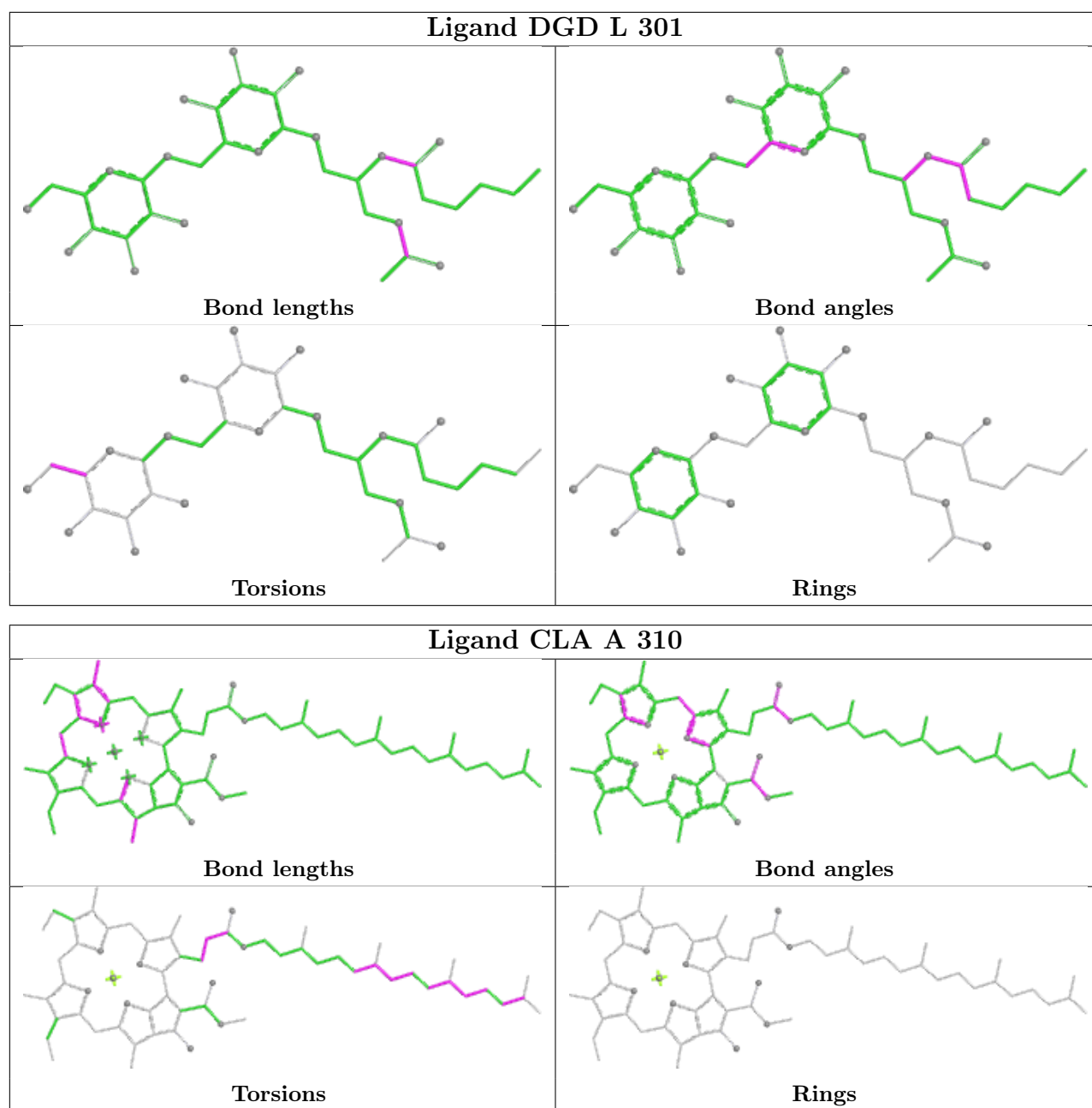


Ligand CLA K 313

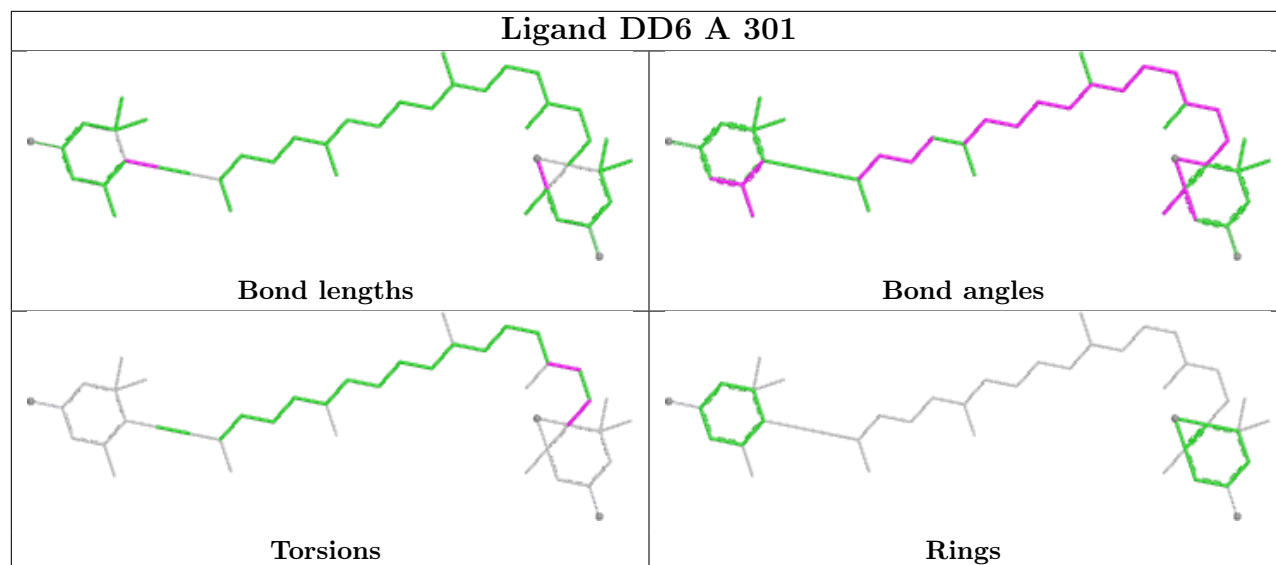


Ligand CLA A 312

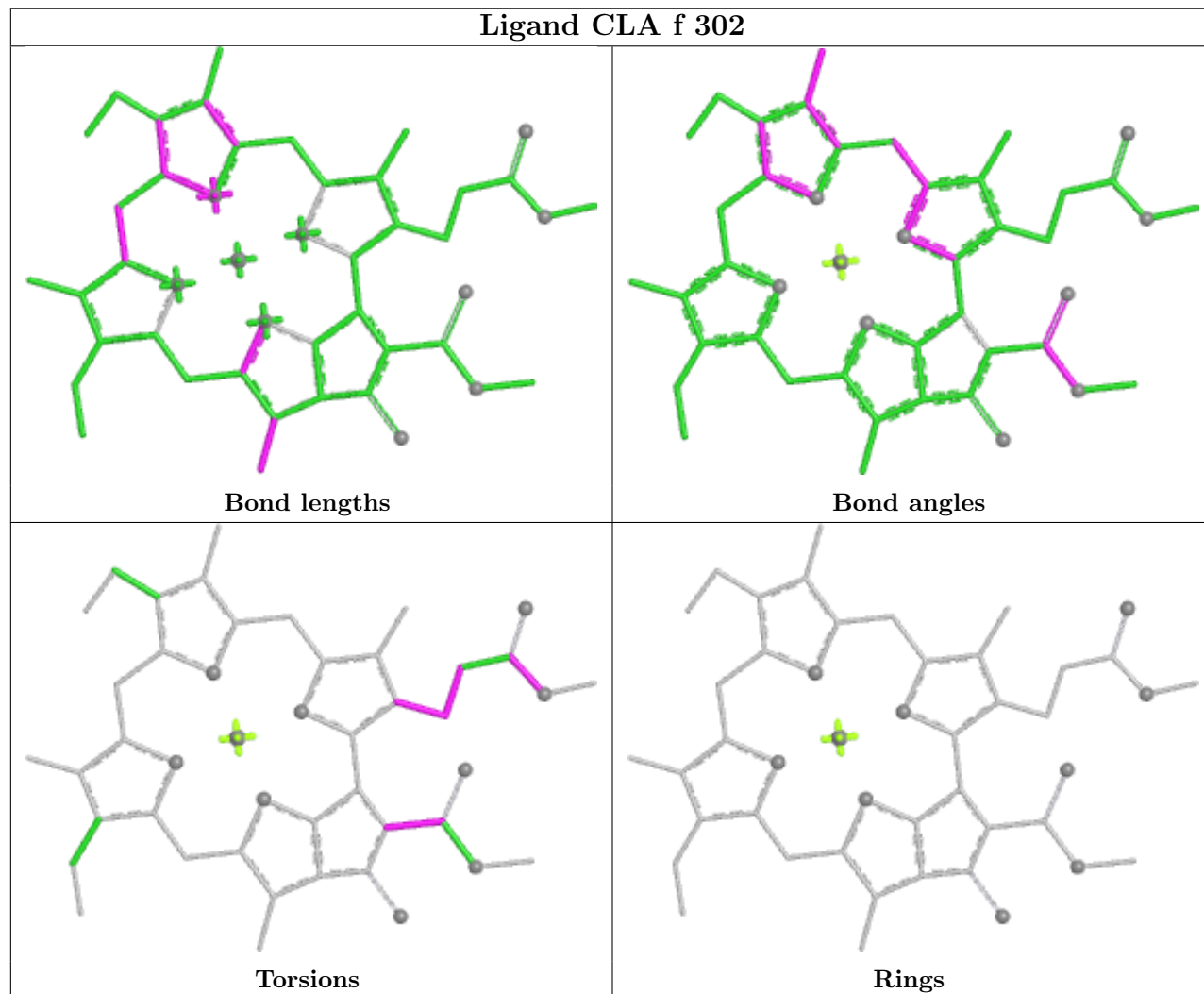




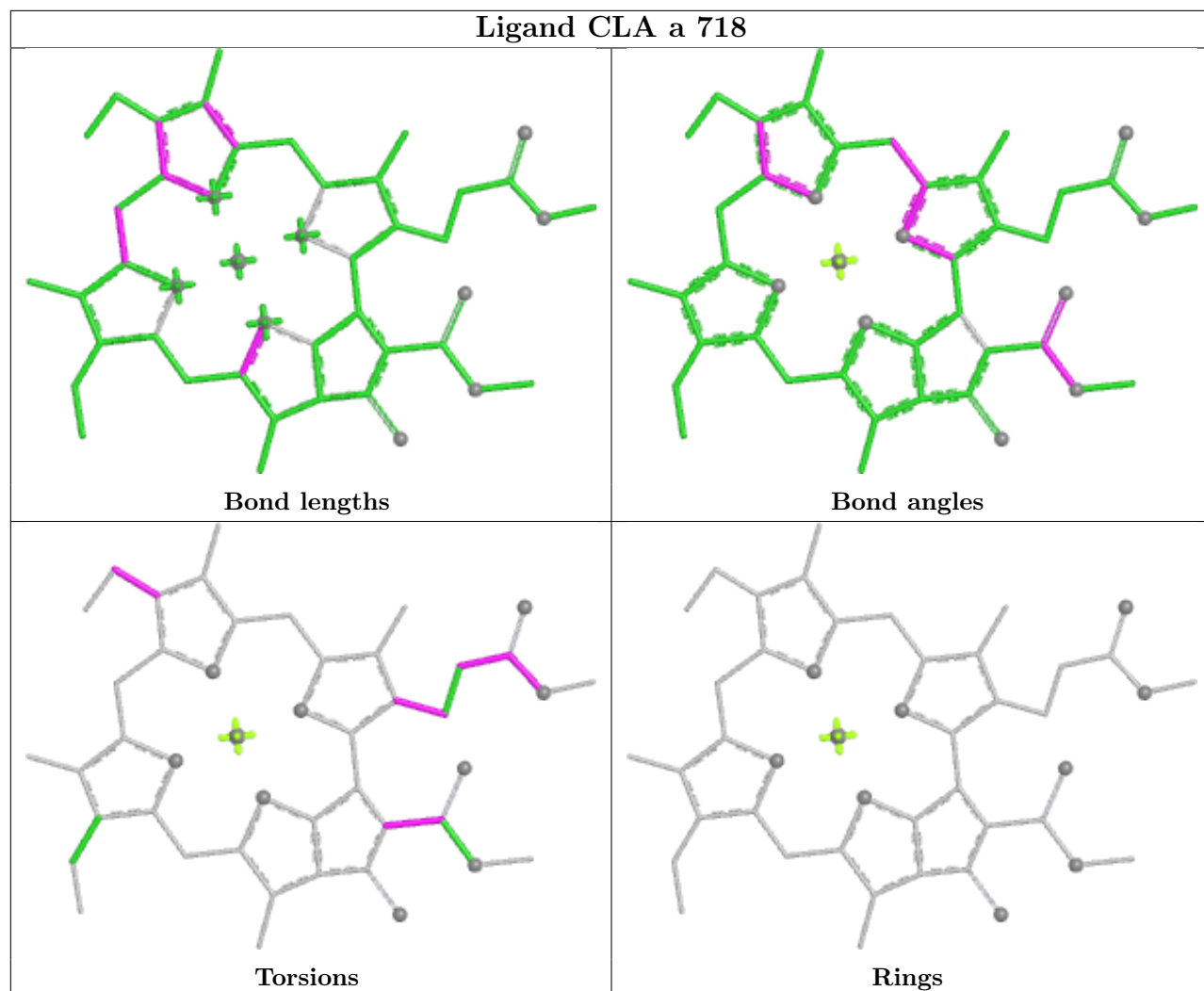
Ligand DD6 A 301



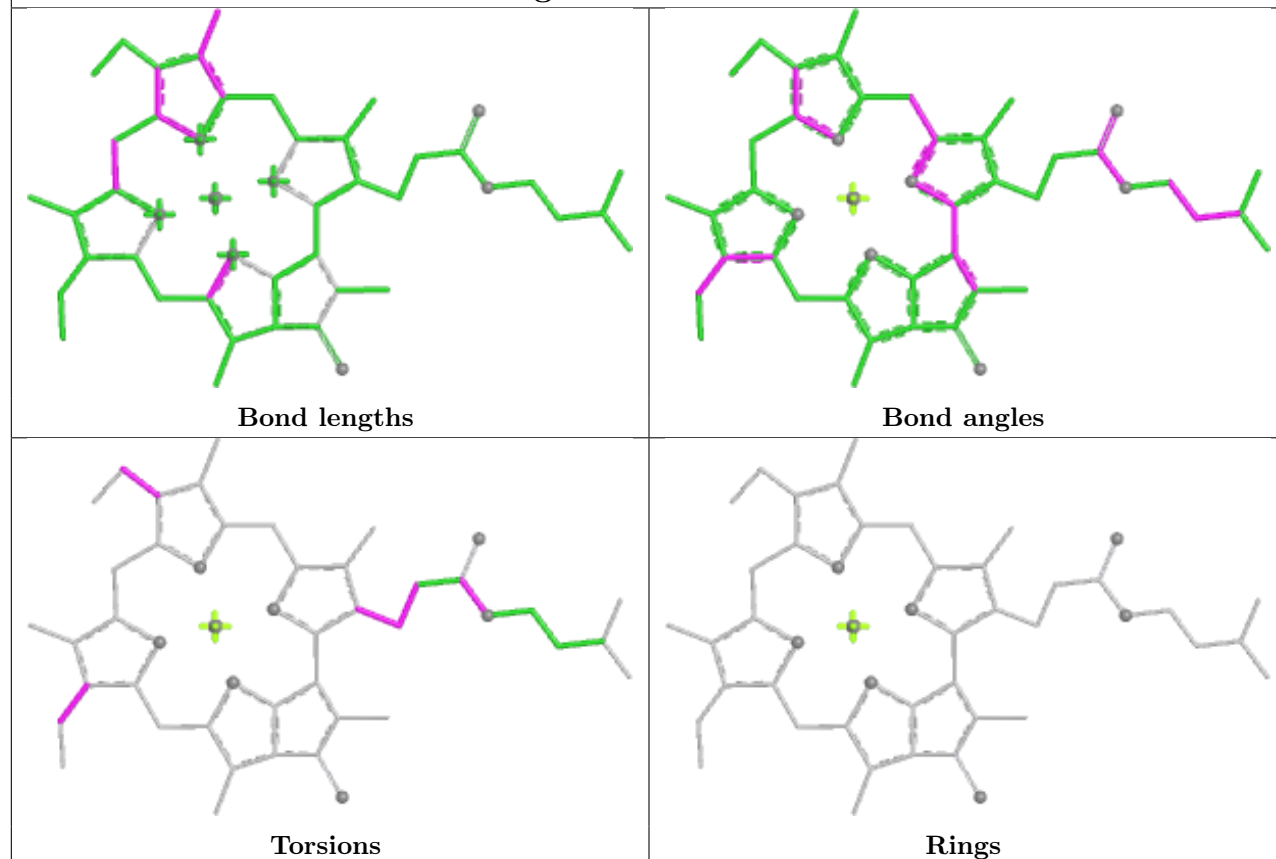
Ligand CLA f 302



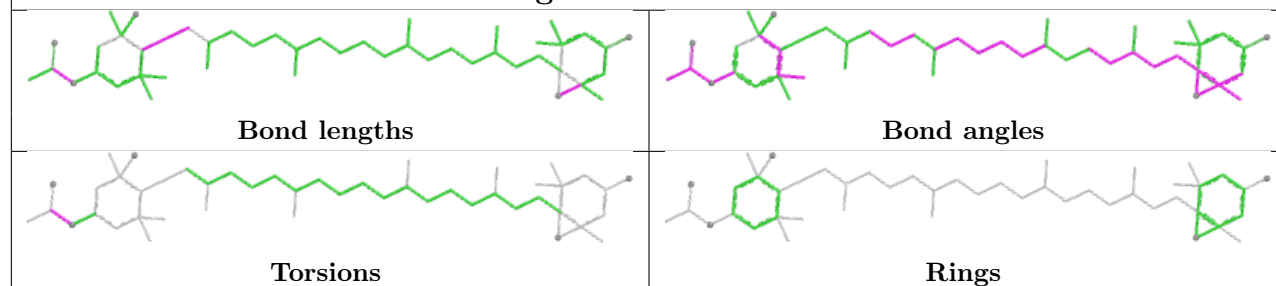
Ligand CLA a 718

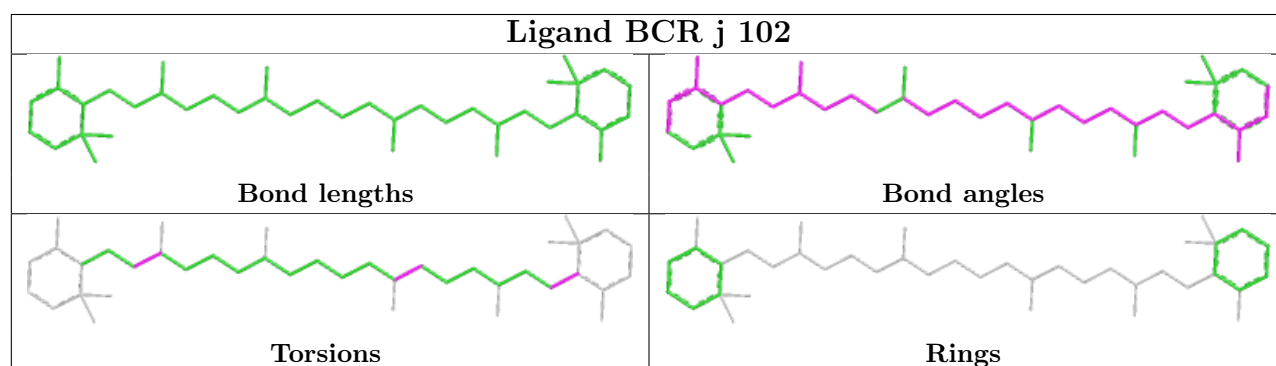
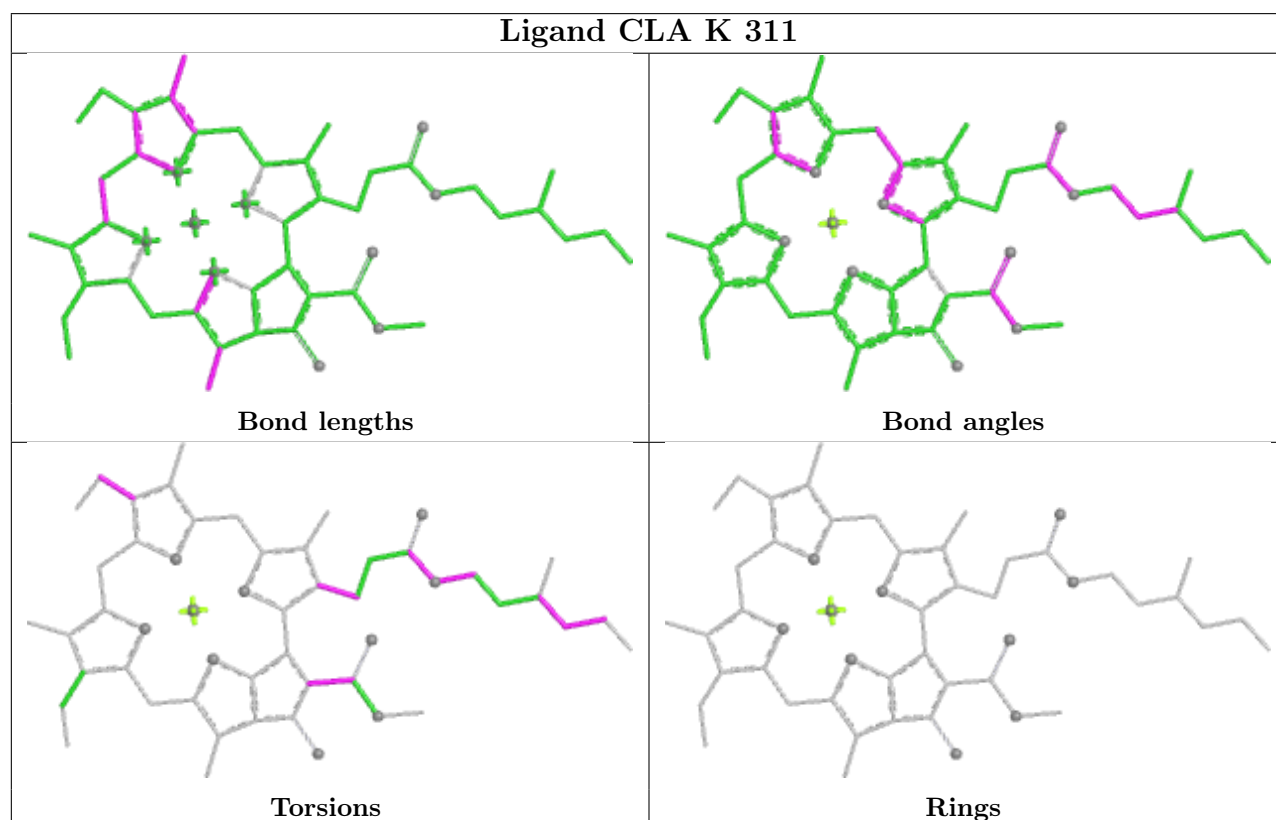
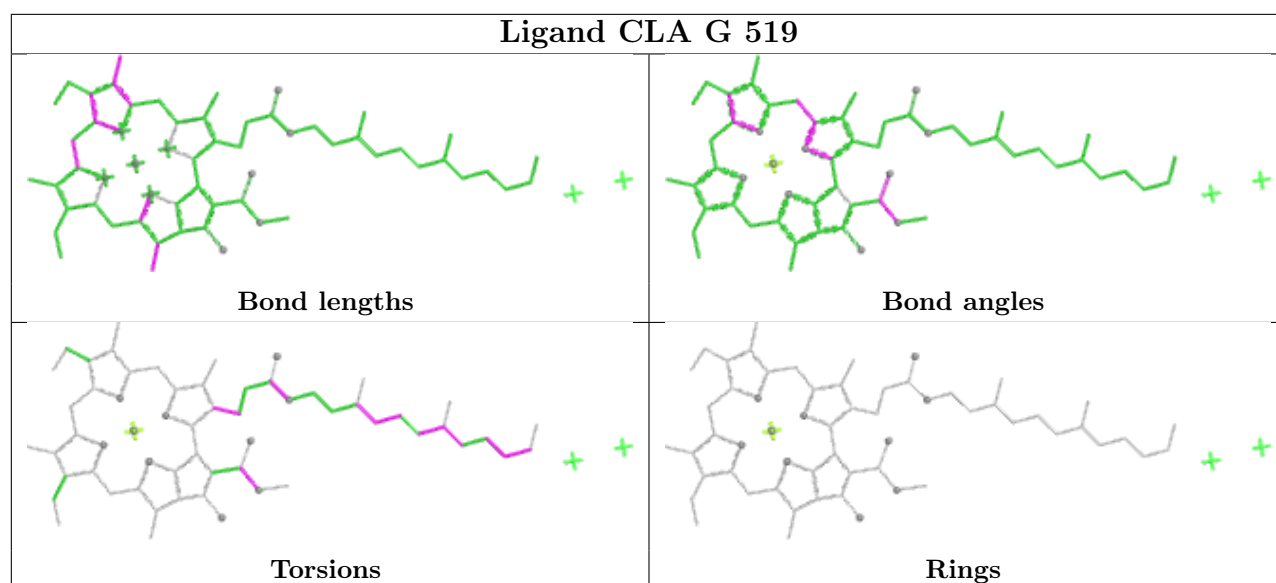


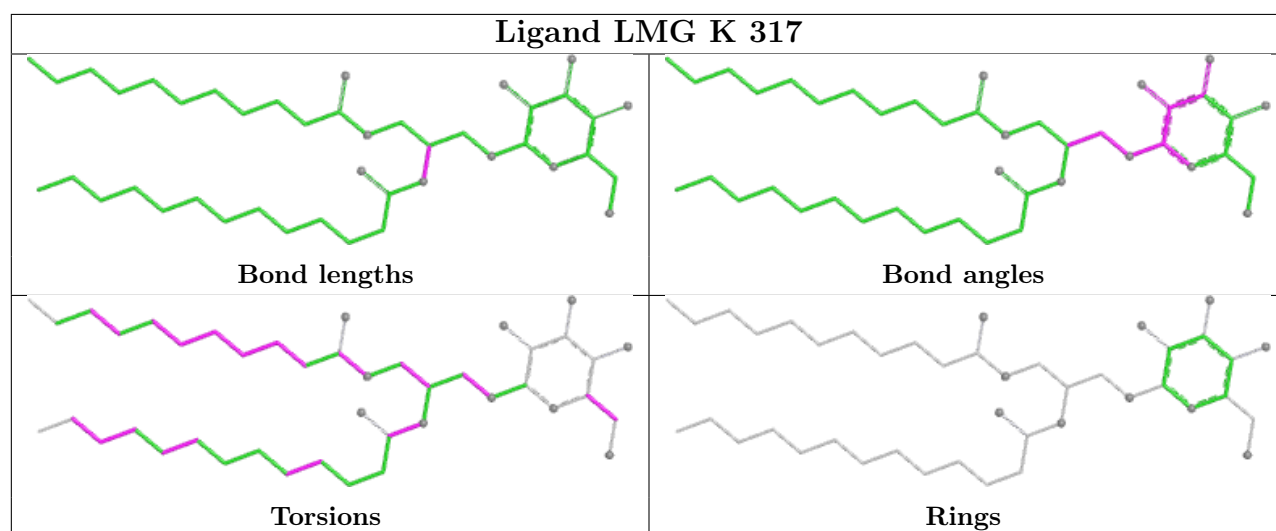
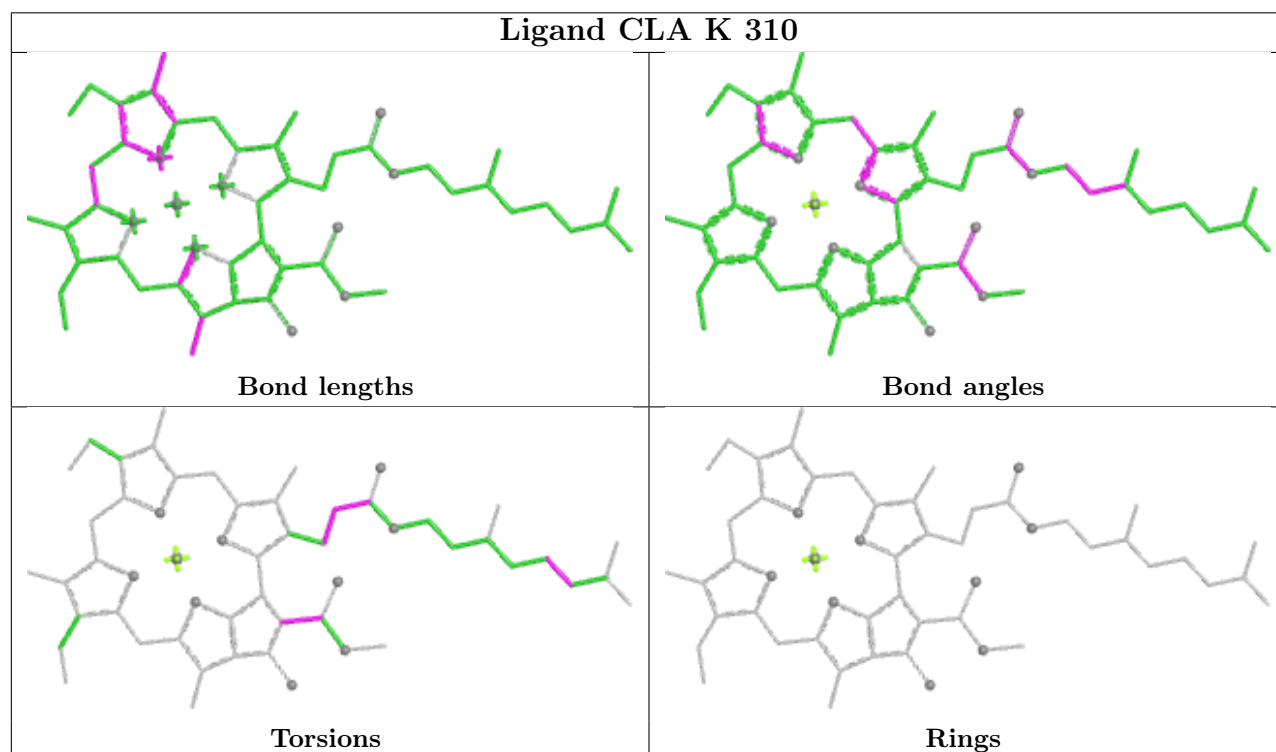
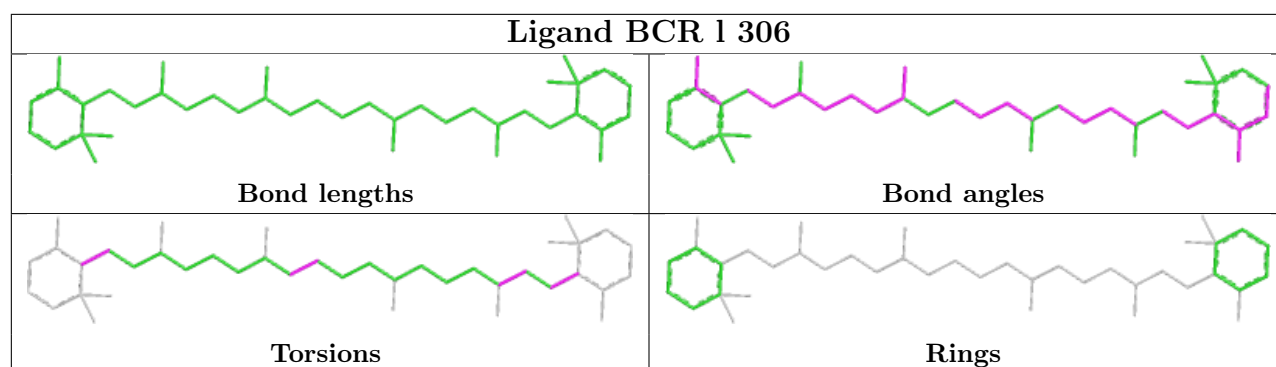
Ligand CLA L 308



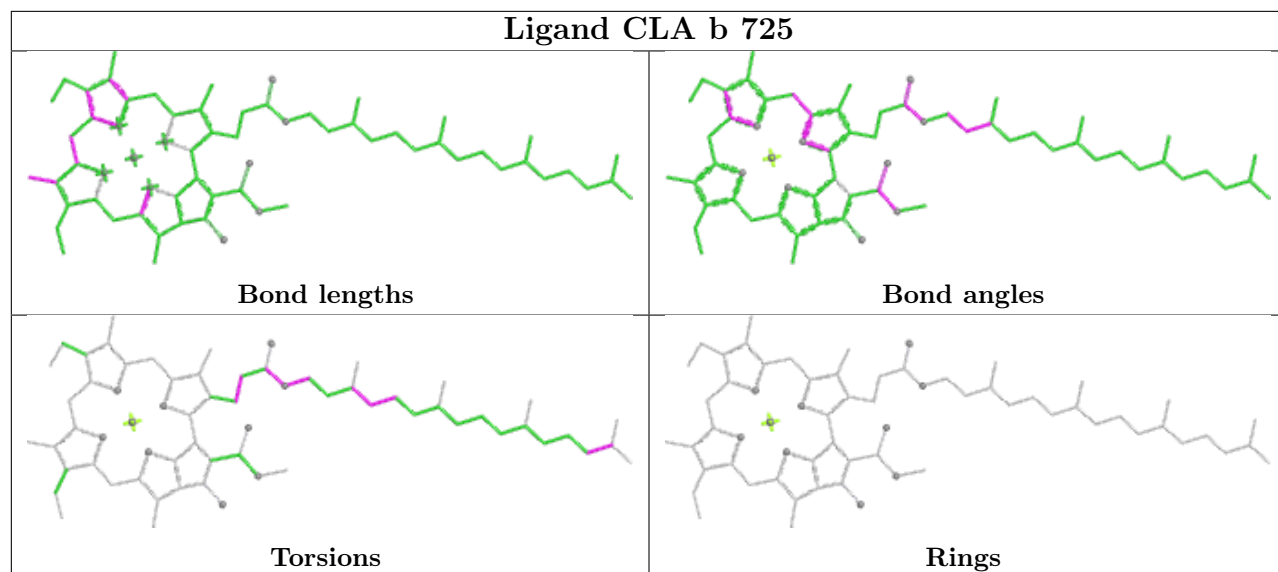
Ligand UIX B 305



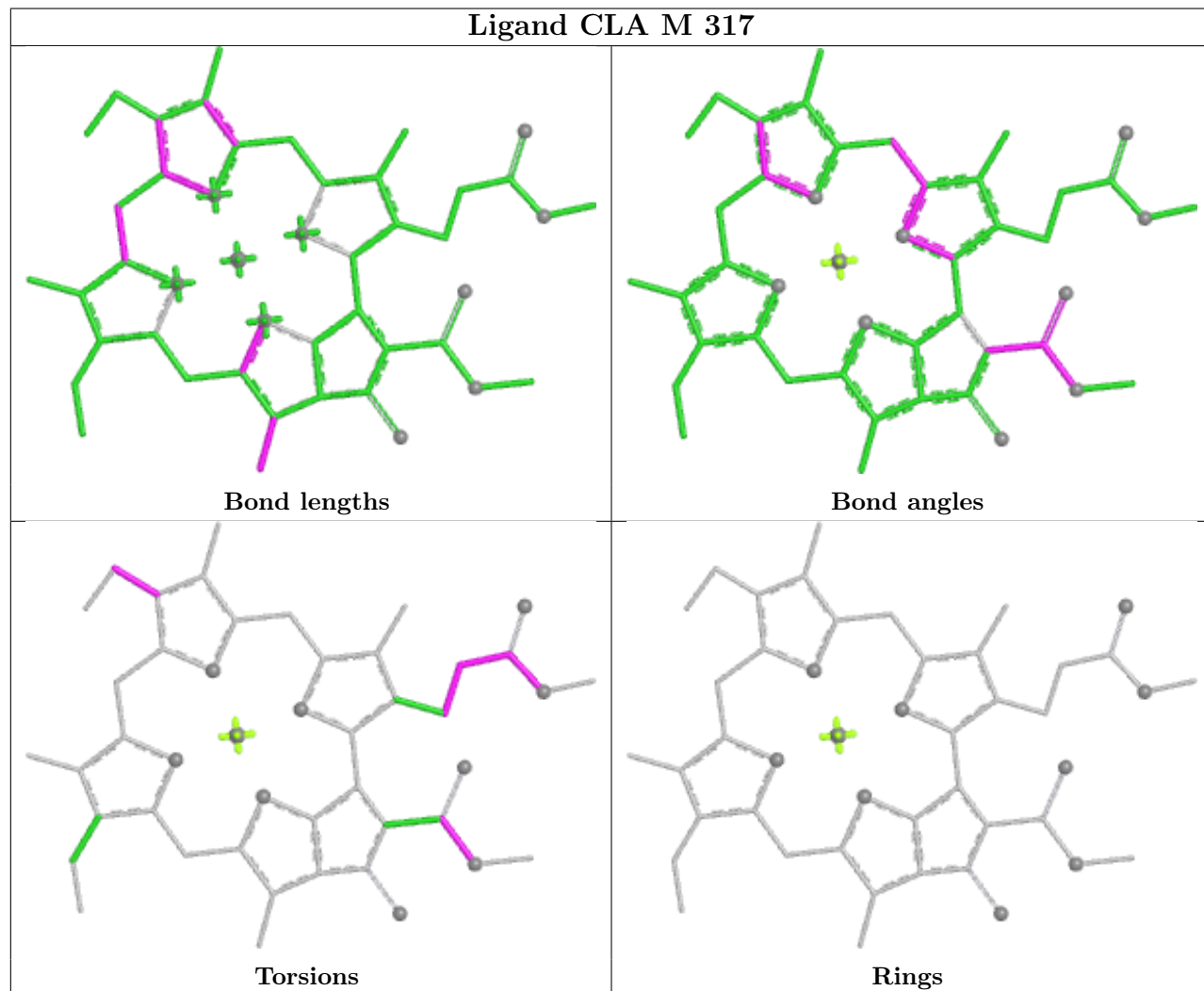




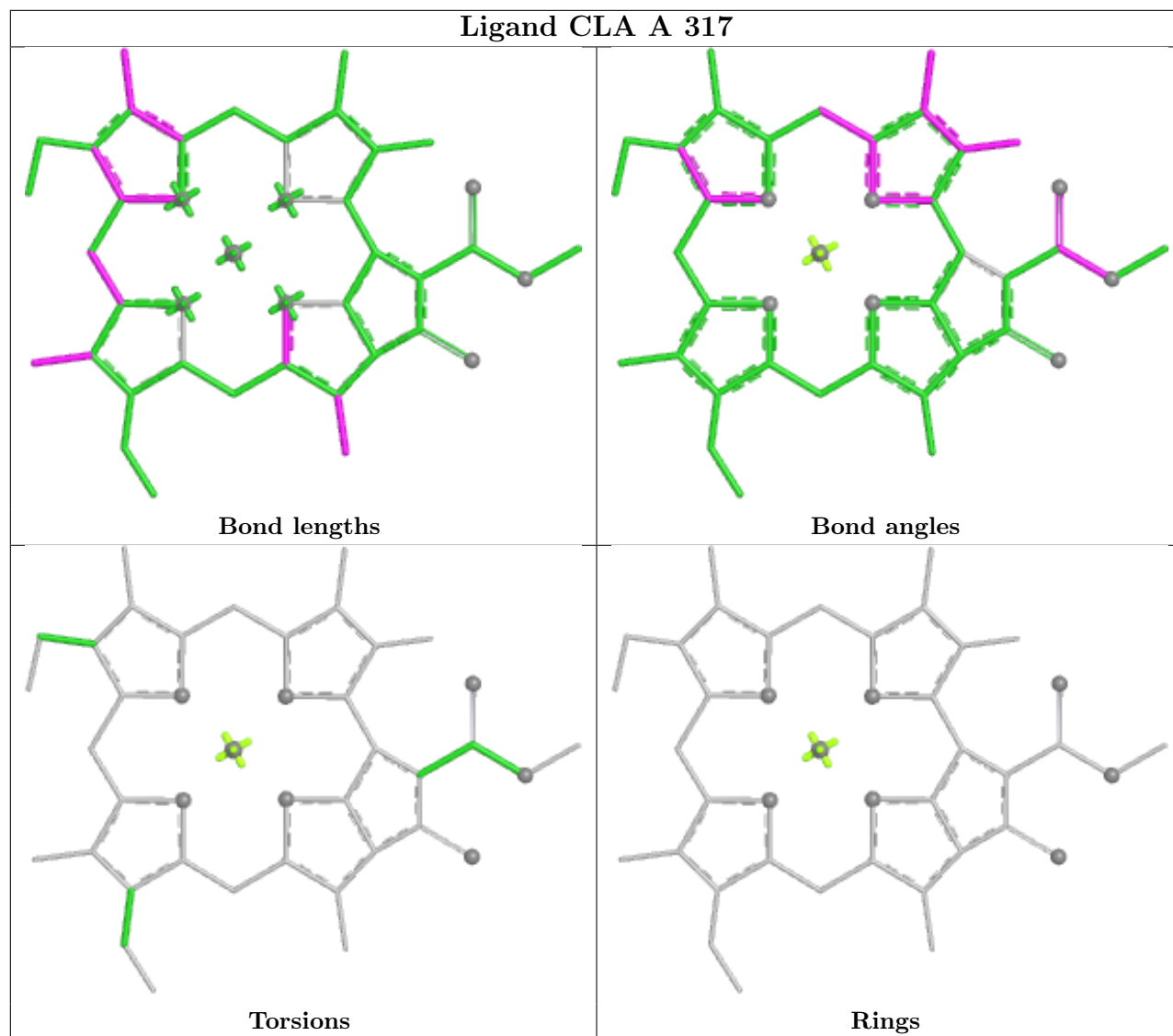
Ligand CLA b 725



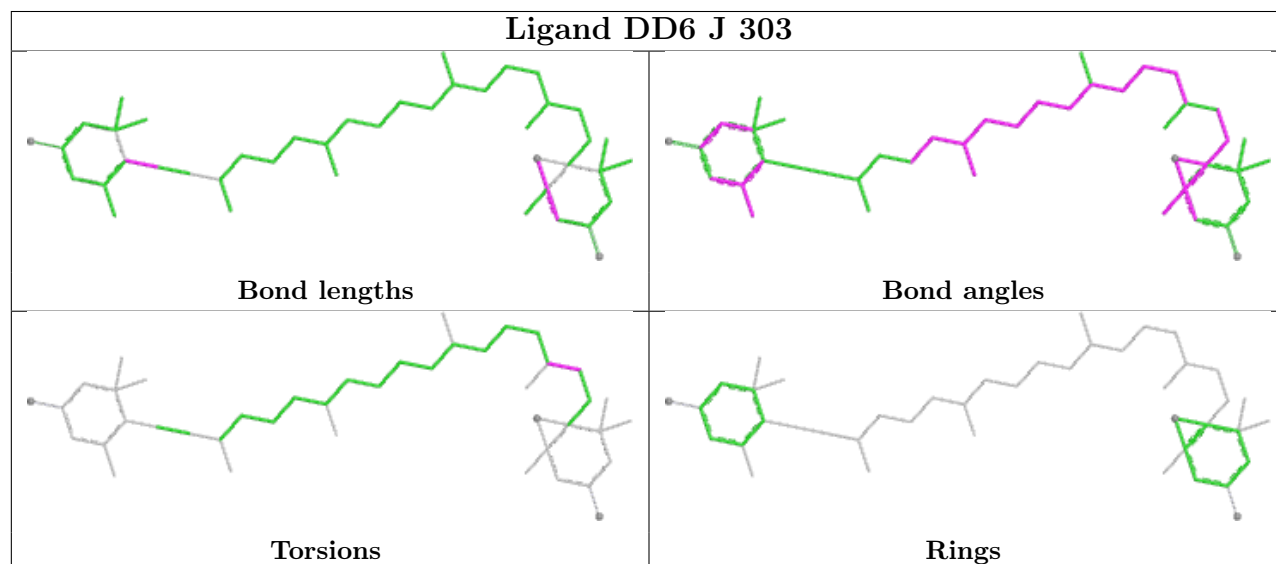
Ligand CLA M 317

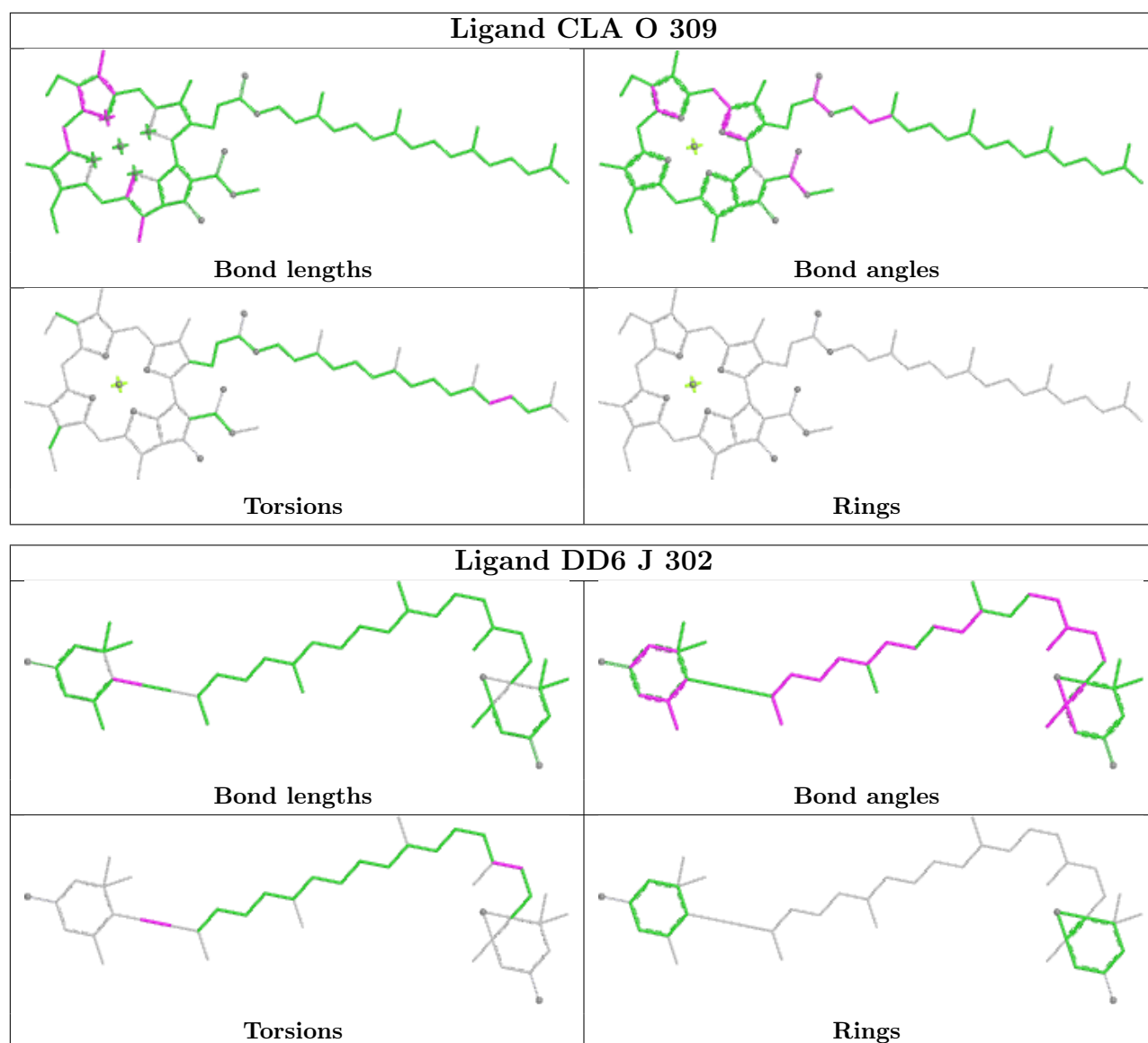


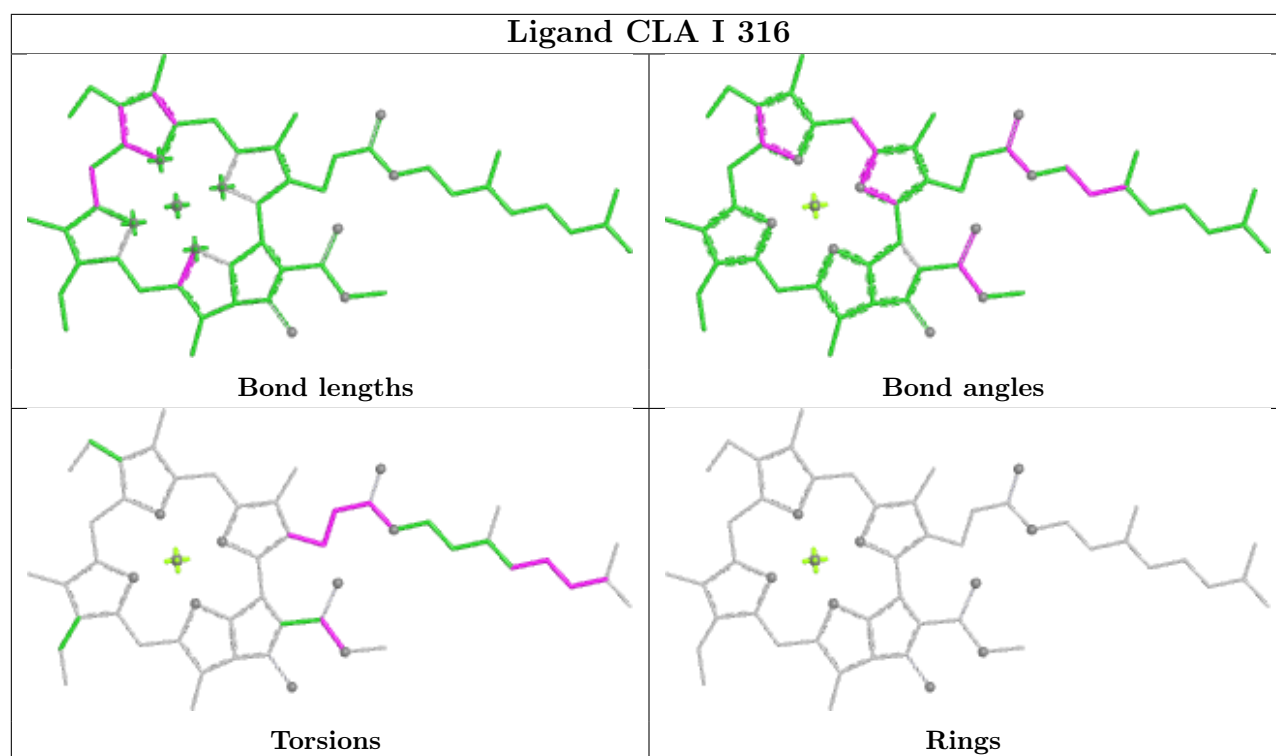
Ligand CLA A 317



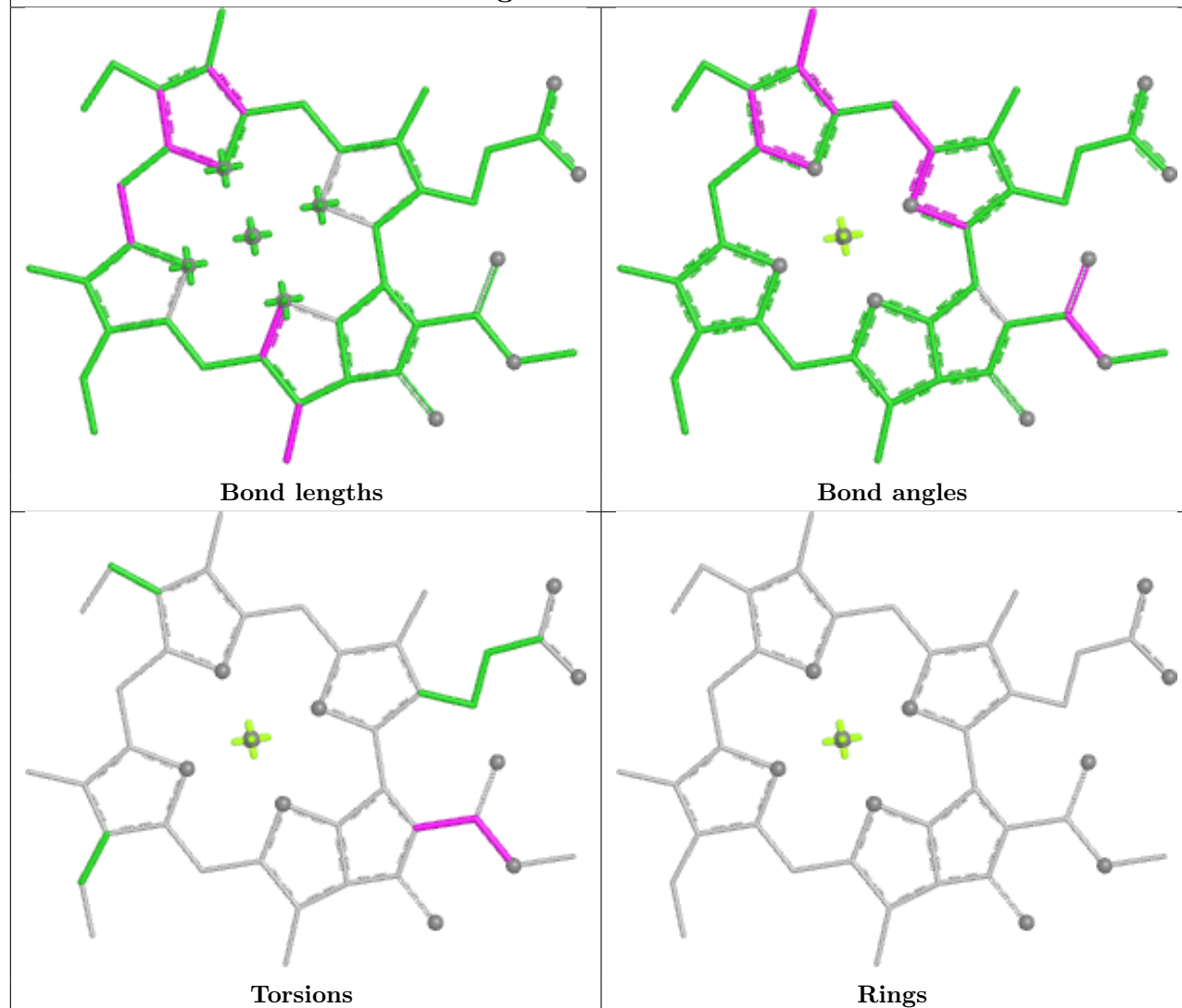
Ligand DD6 J 303



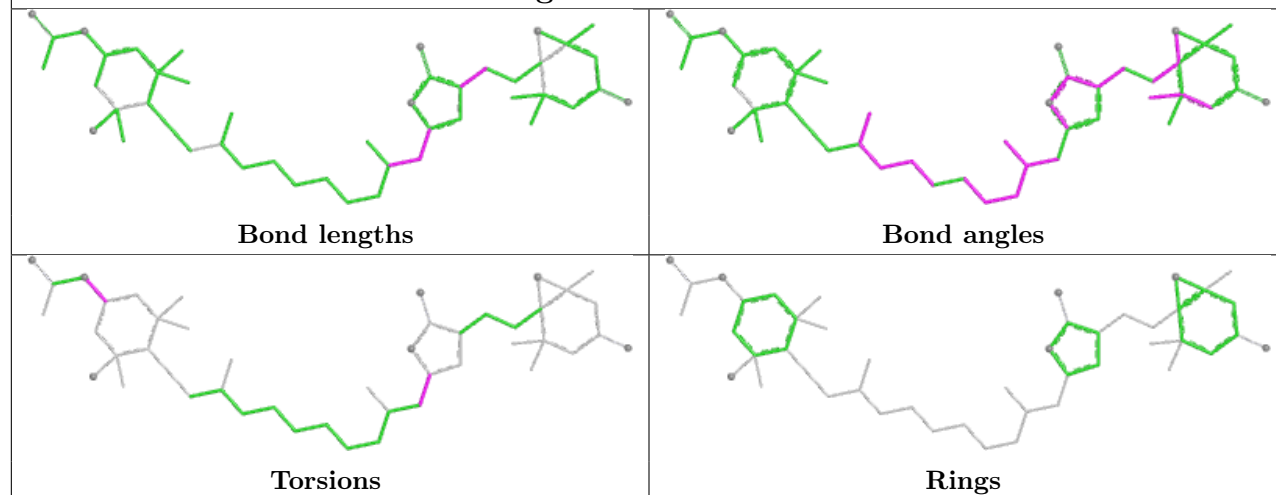




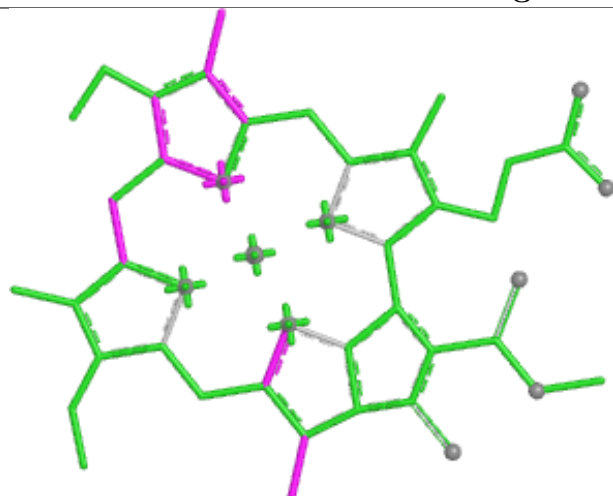
Ligand CLA a 714



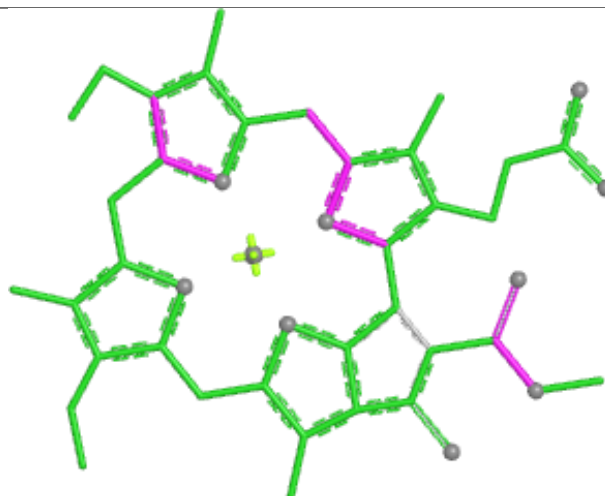
Ligand PID D 302



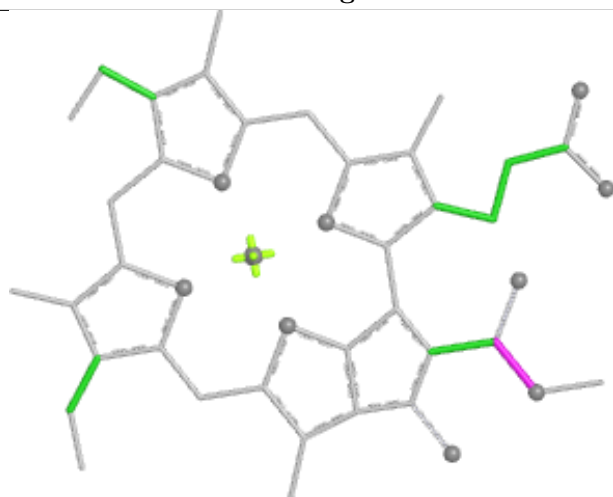
Ligand CLA D 313



Bond lengths



Bond angles

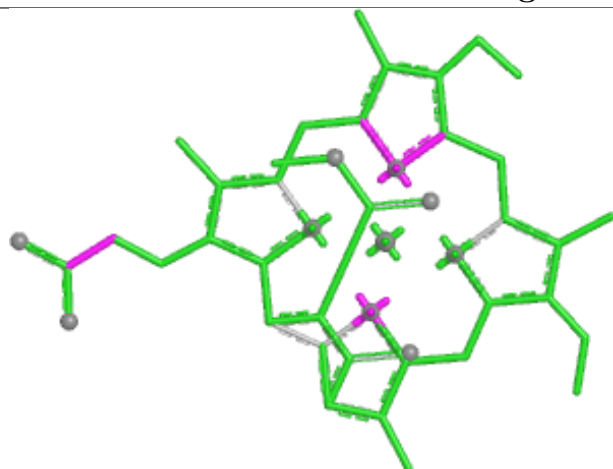


Torsions

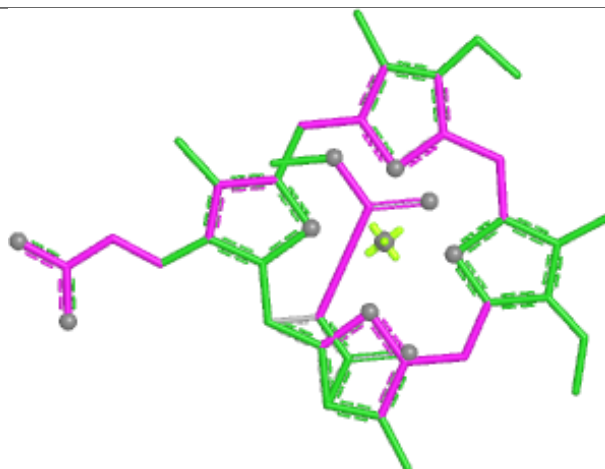


Rings

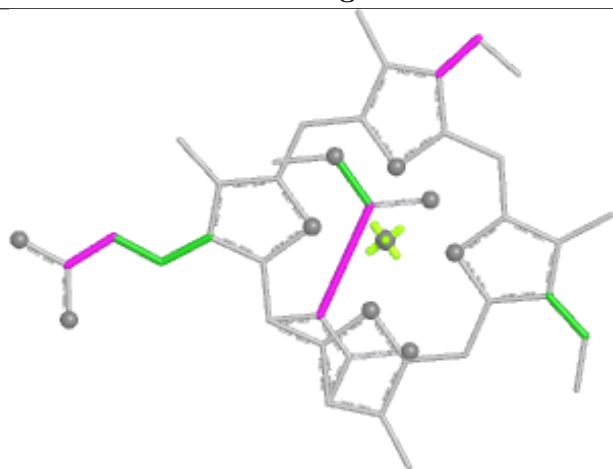
Ligand KC1 L 307



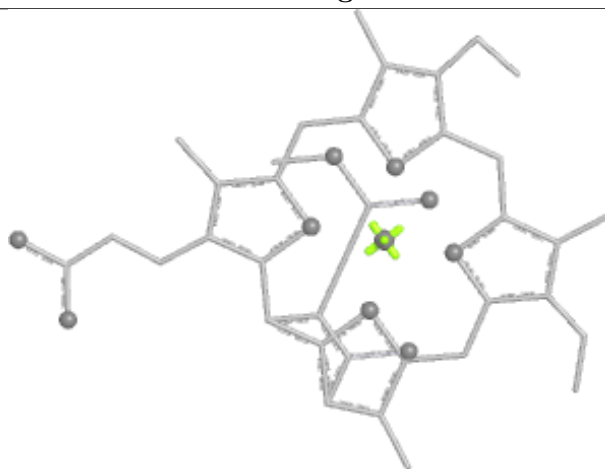
Bond lengths



Bond angles

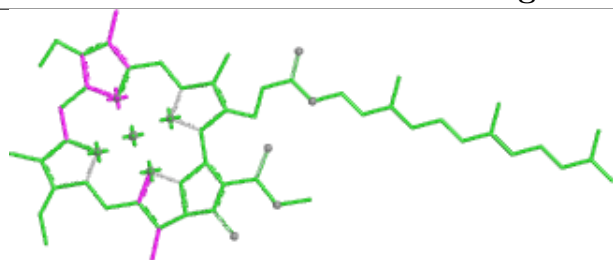


Torsions

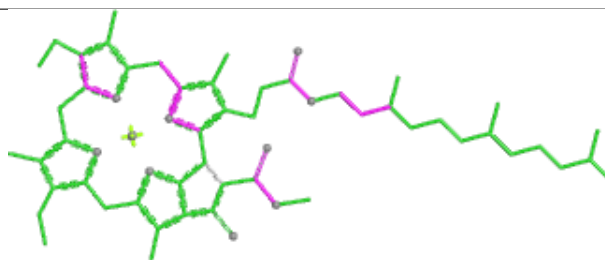


Rings

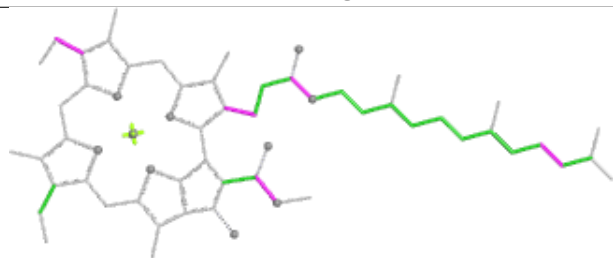
Ligand CLA a 712



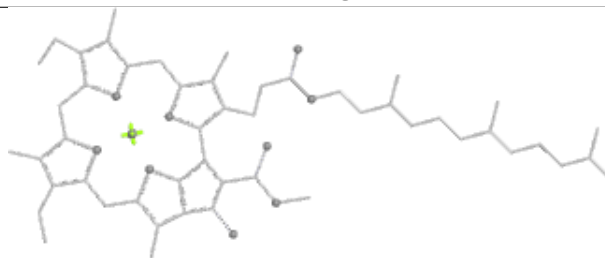
Bond lengths



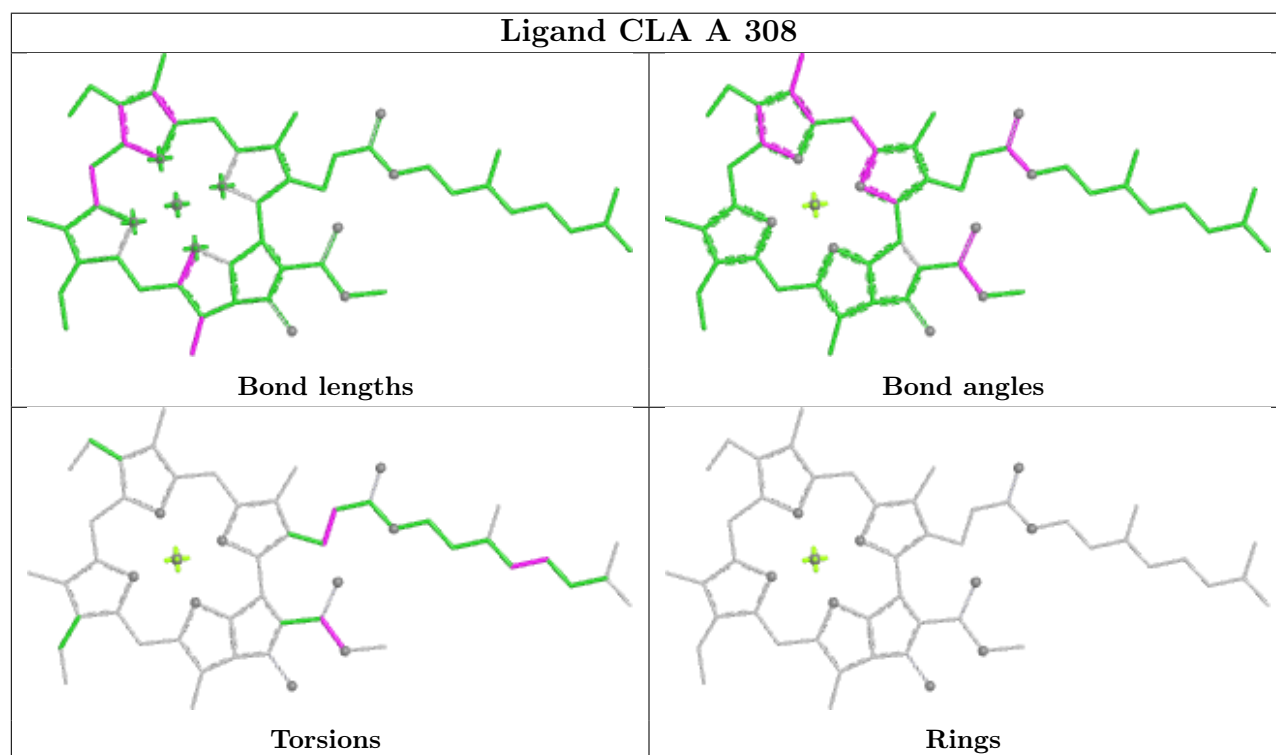
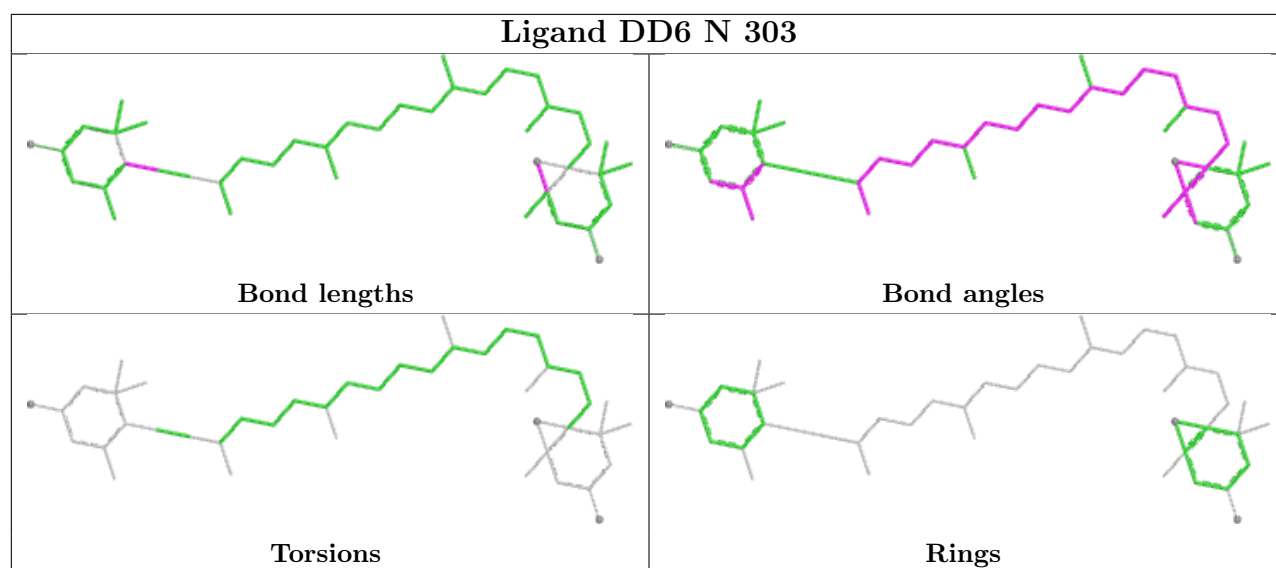
Bond angles



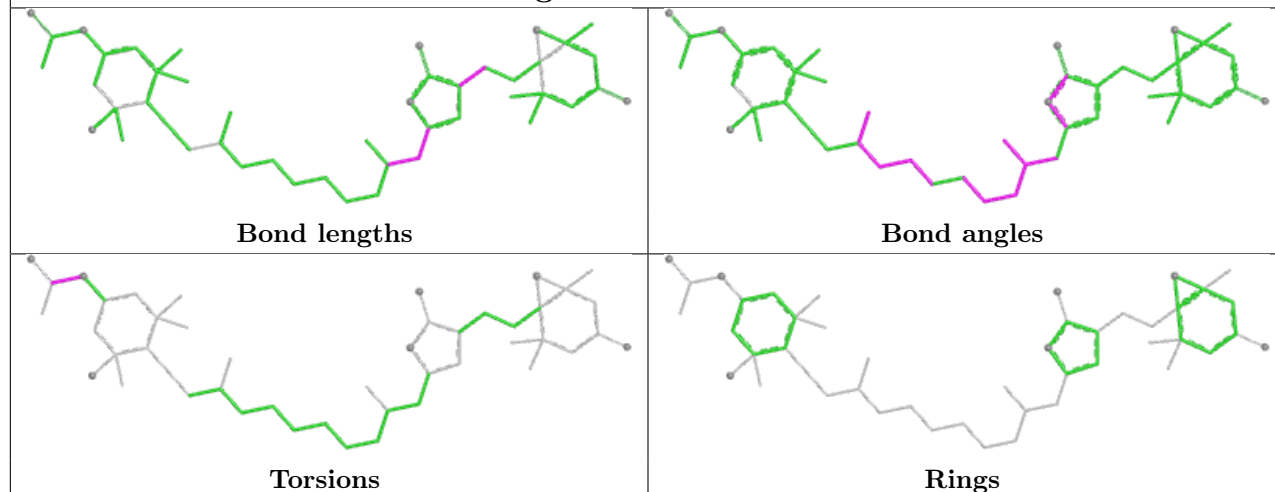
Torsions



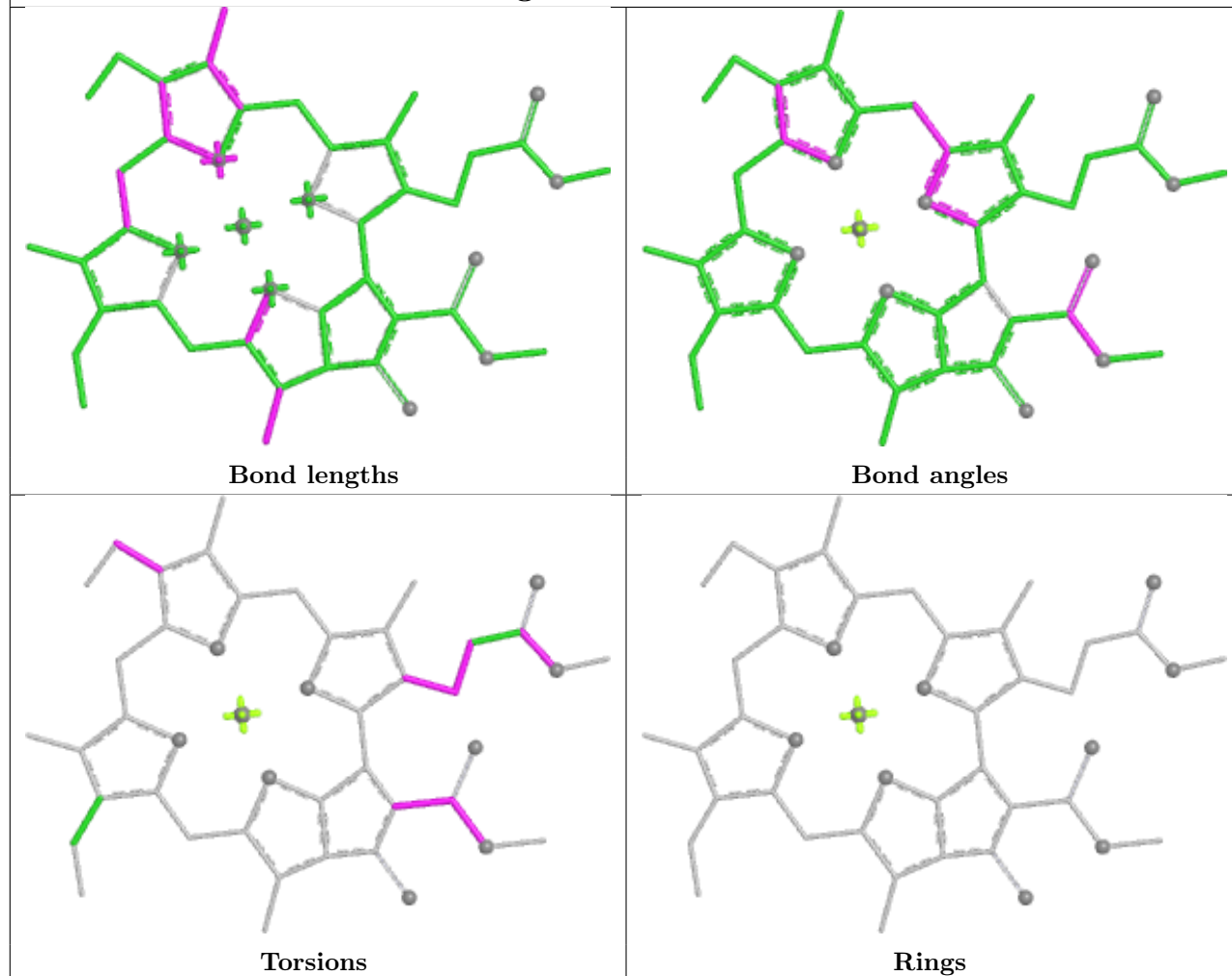
Rings

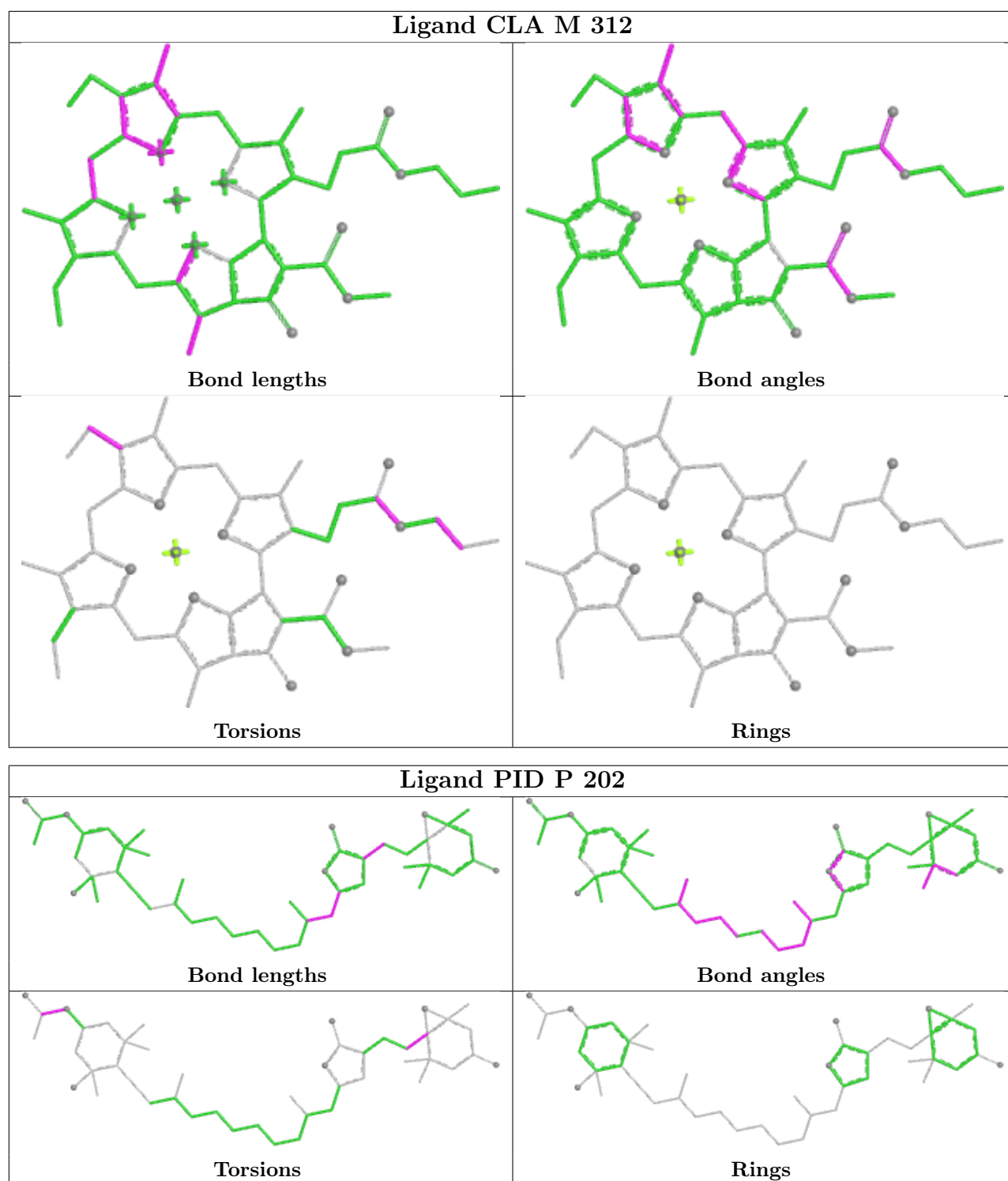


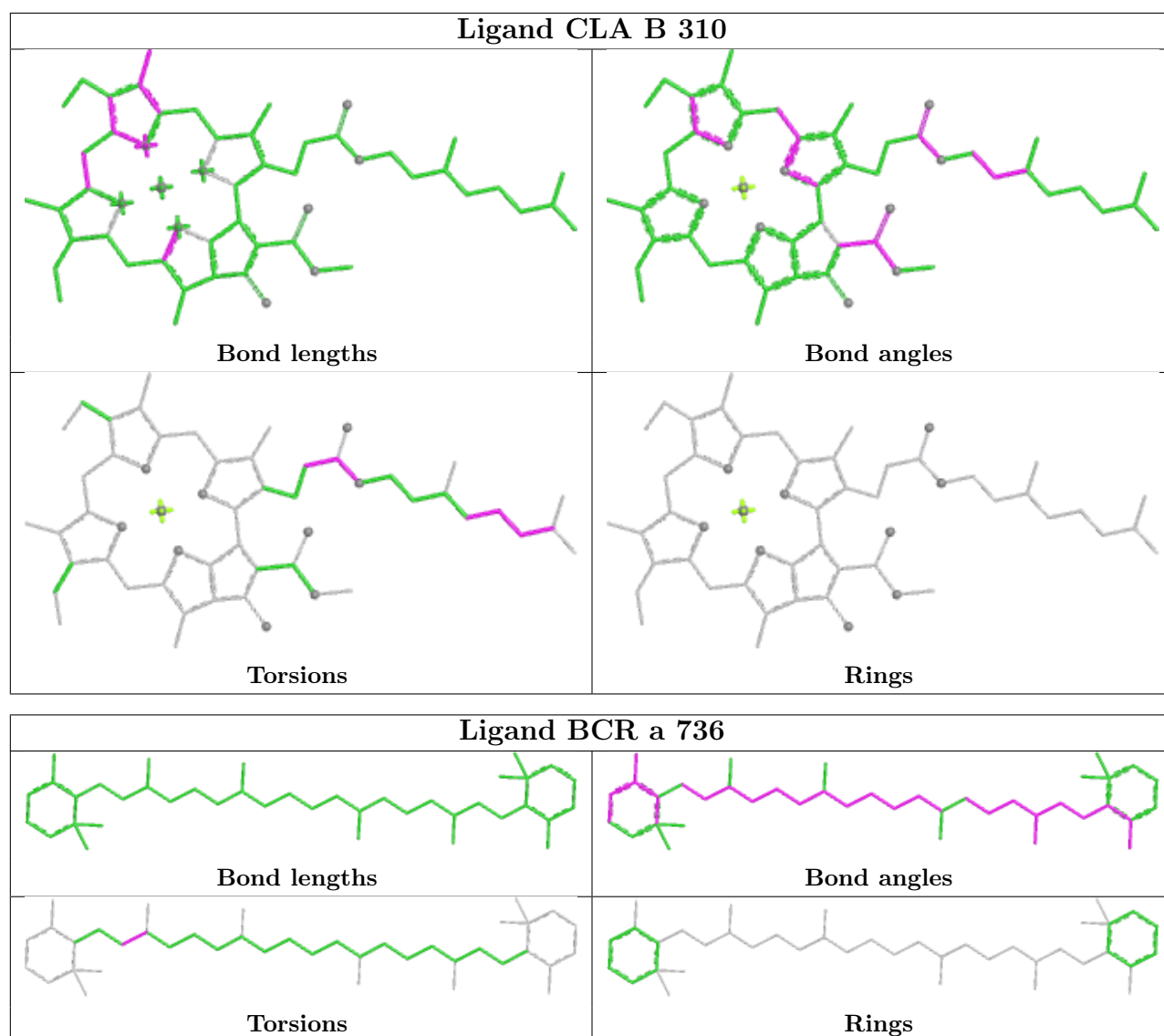
Ligand PID O 302

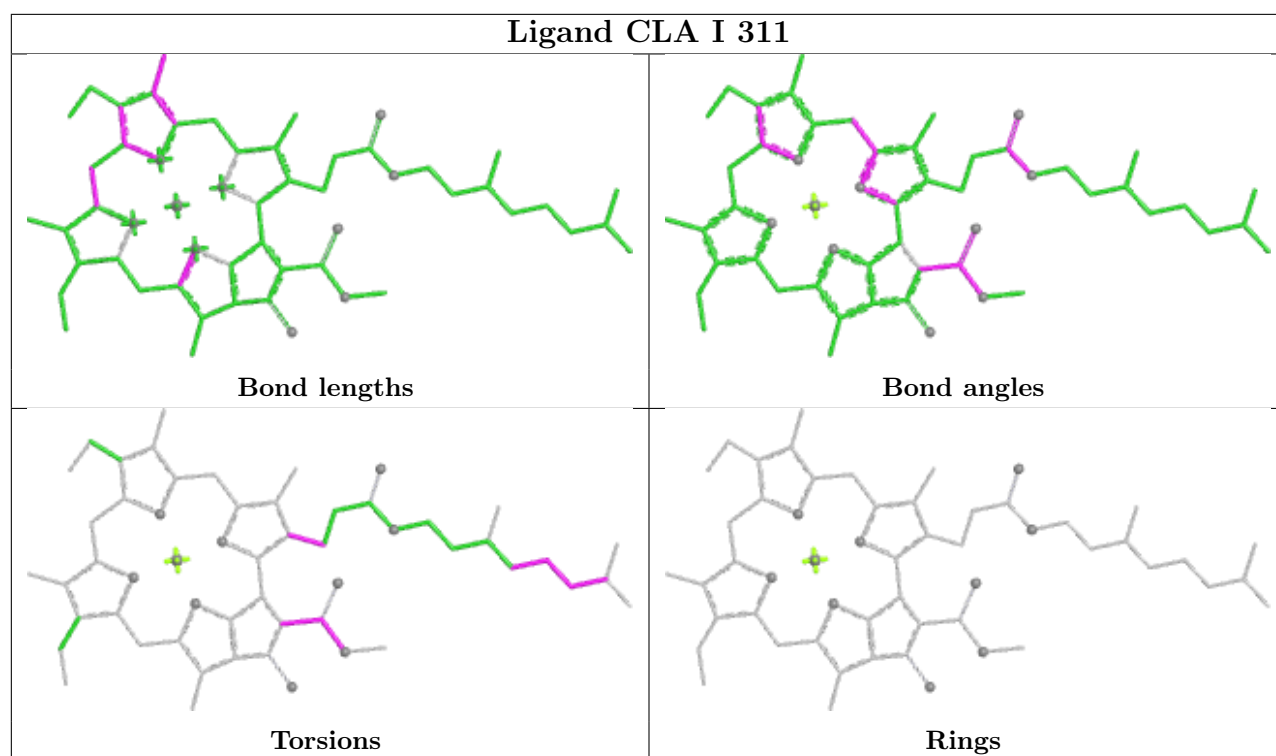


Ligand CLA b 719

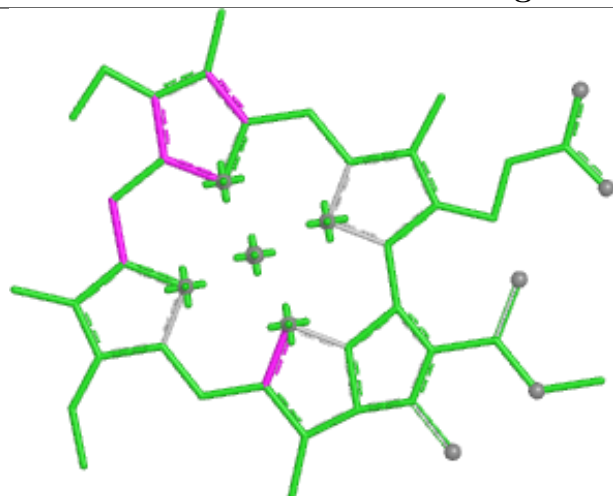




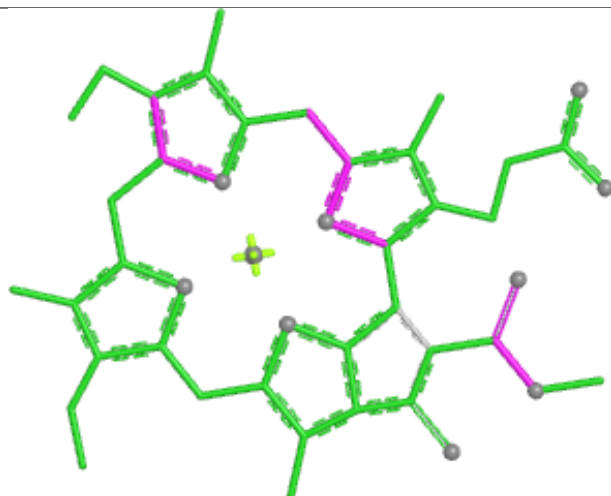




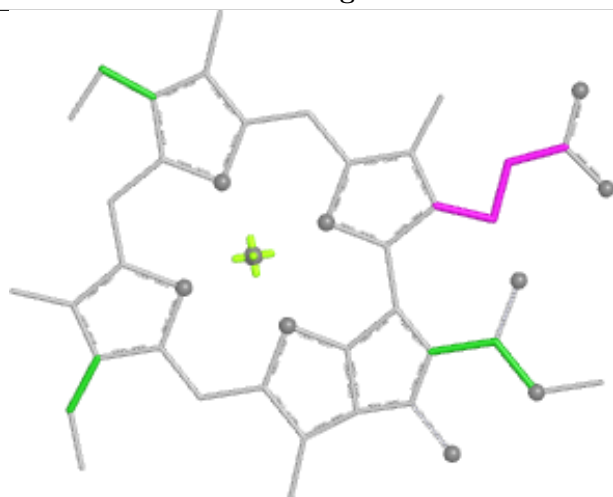
Ligand CLA B 308



Bond lengths



Bond angles

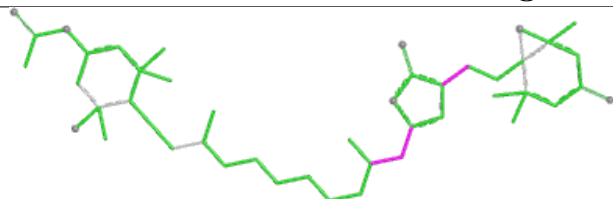


Torsions

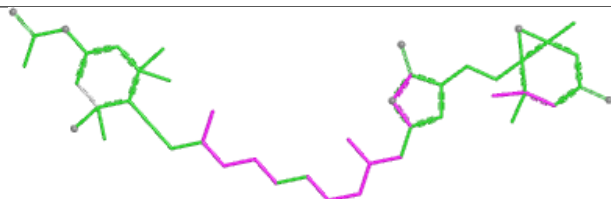


Rings

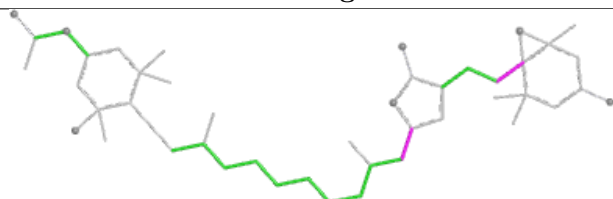
Ligand PID D 301



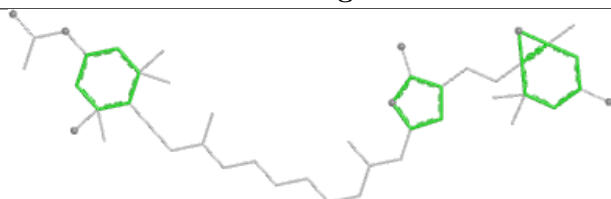
Bond lengths



Bond angles

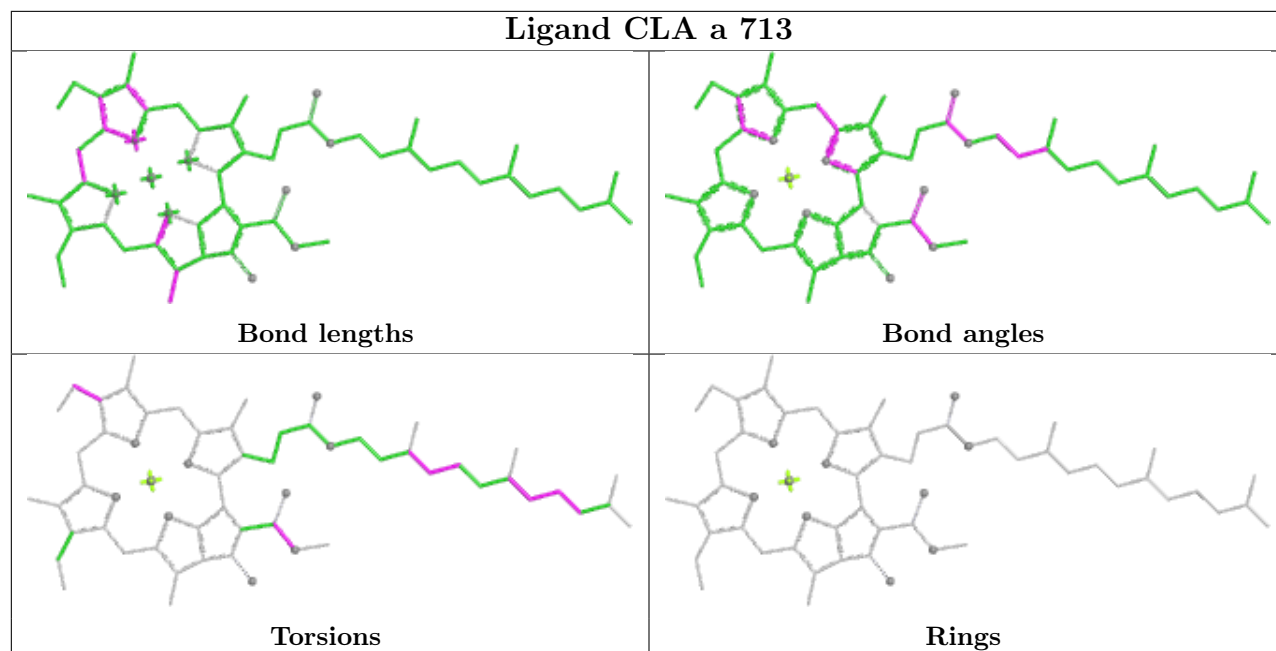


Torsions

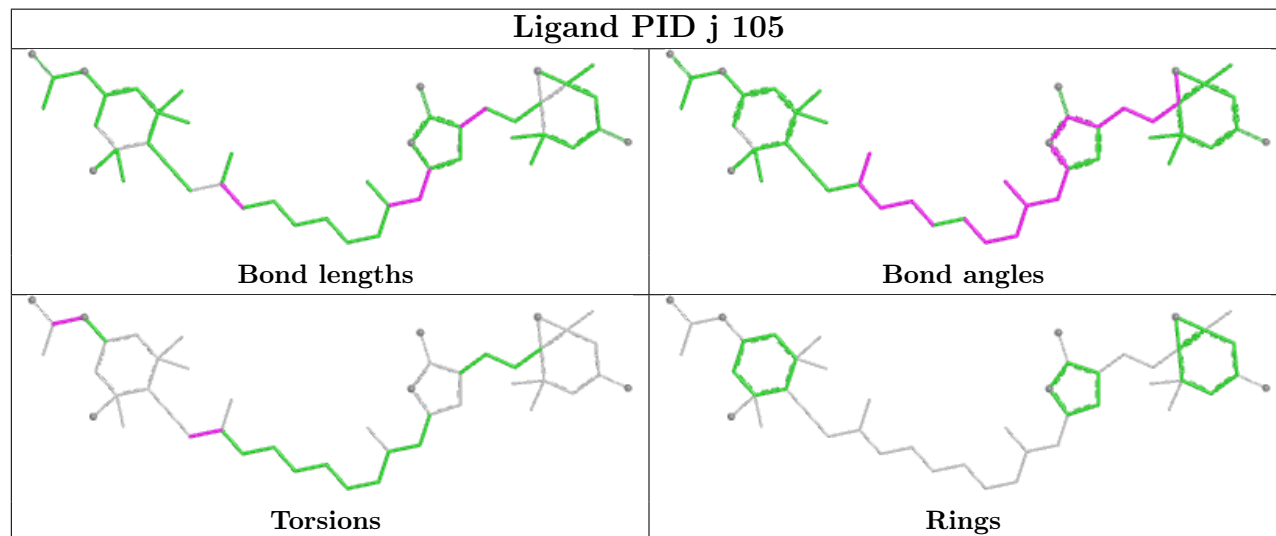


Rings

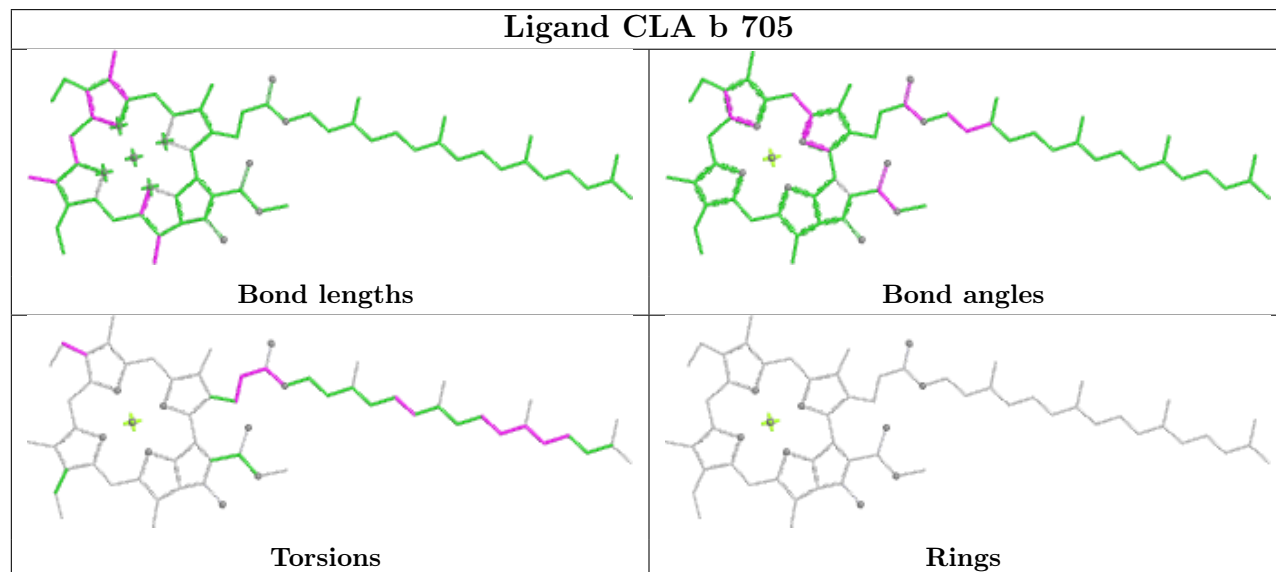
Ligand CLA a 713

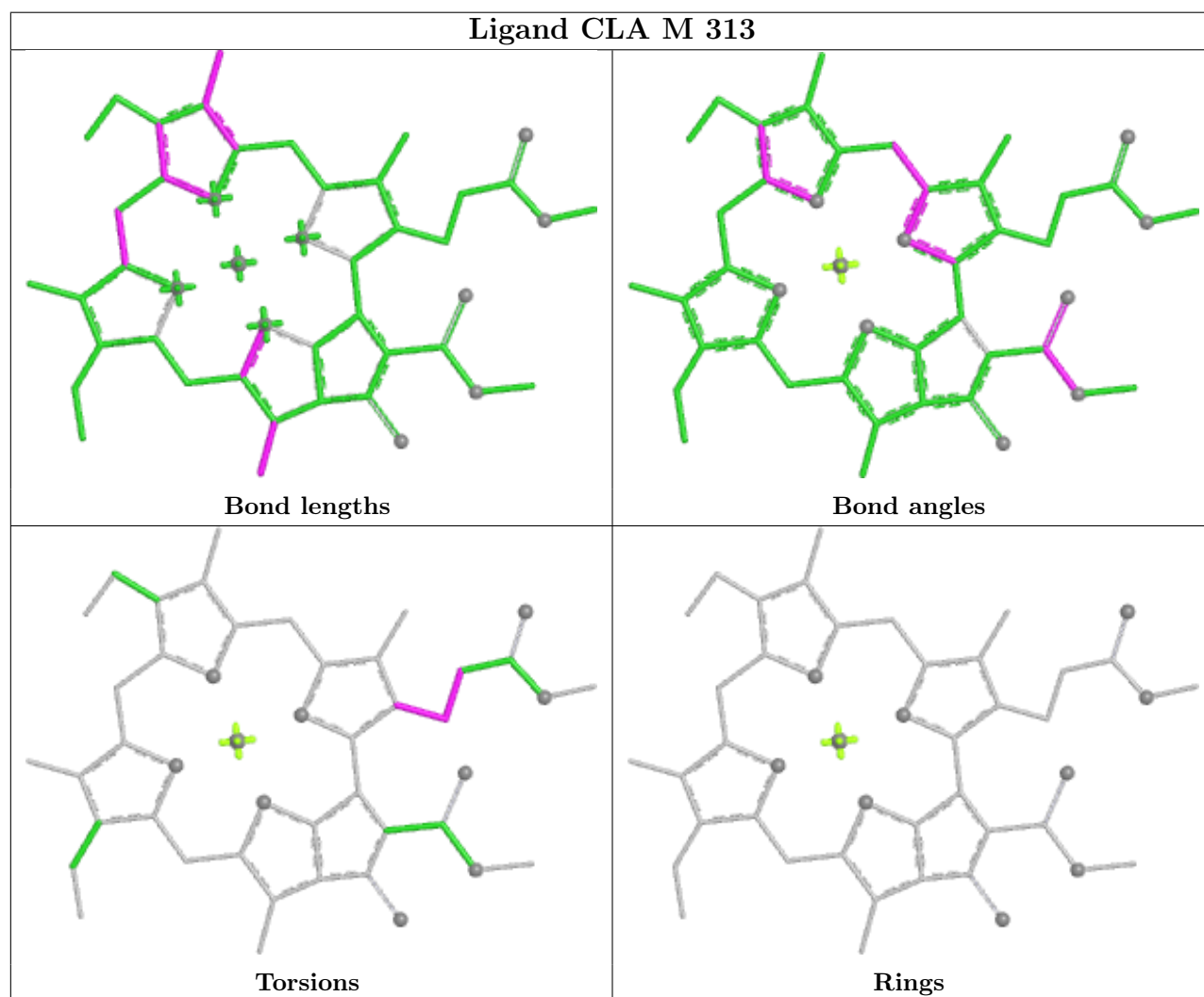
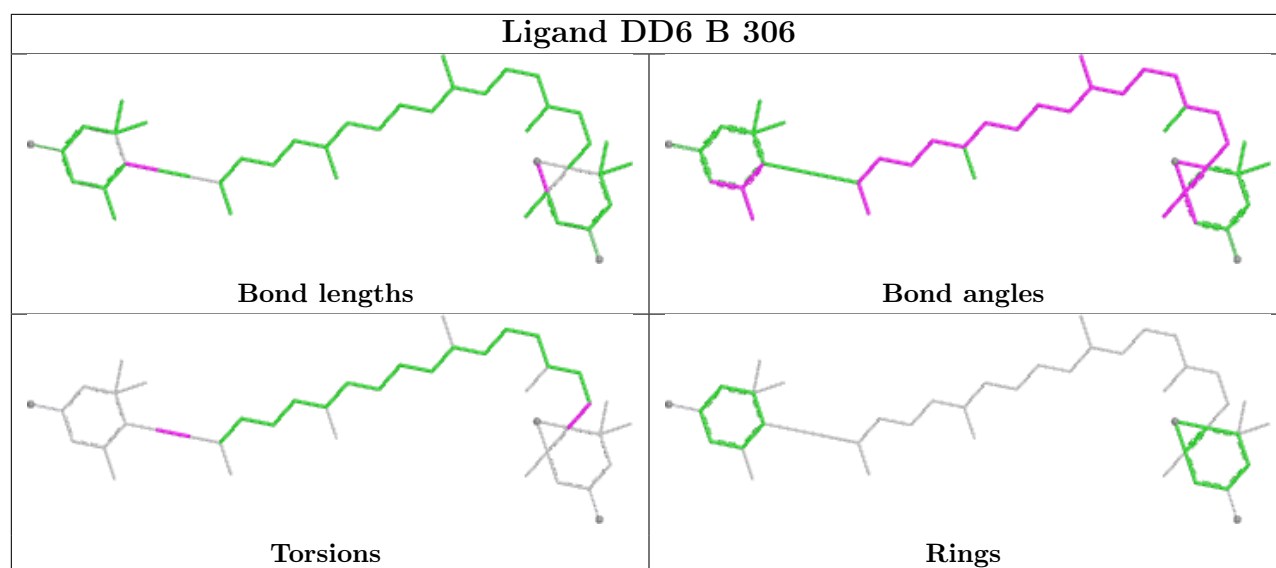


Ligand PID j 105

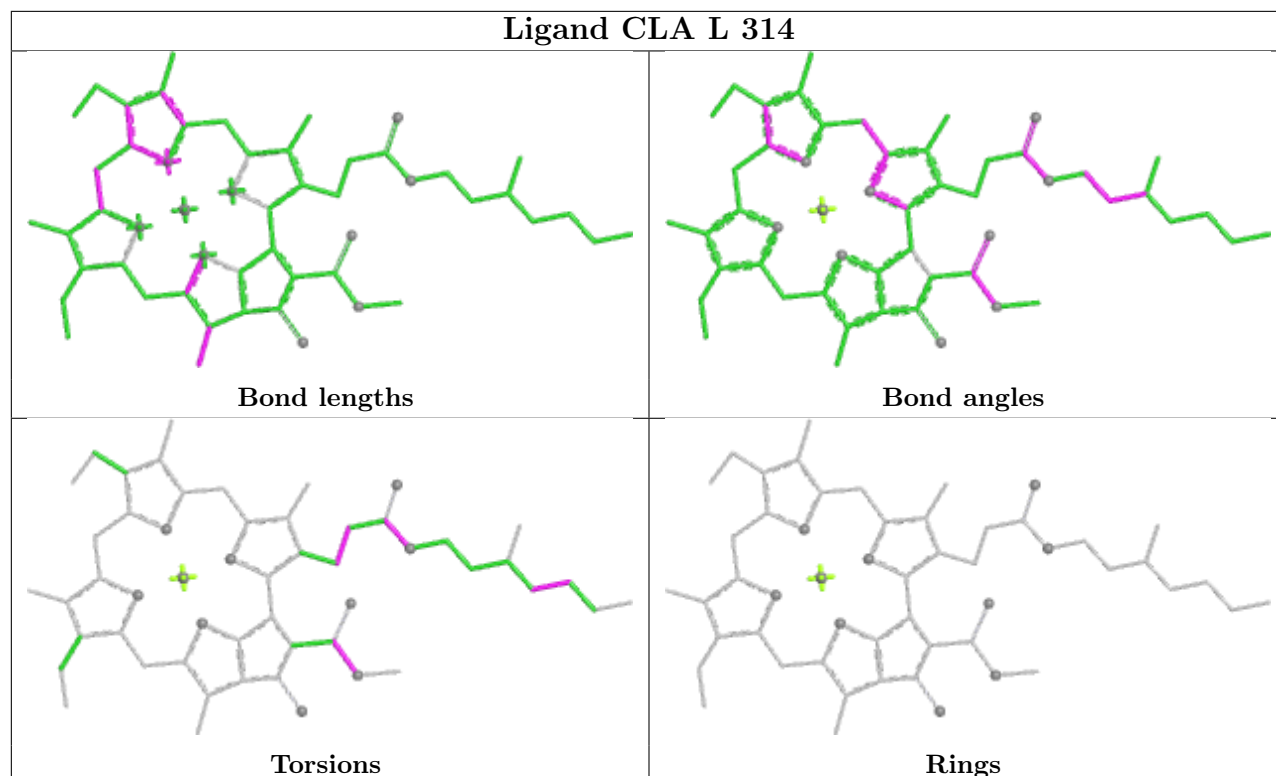


Ligand CLA b 705

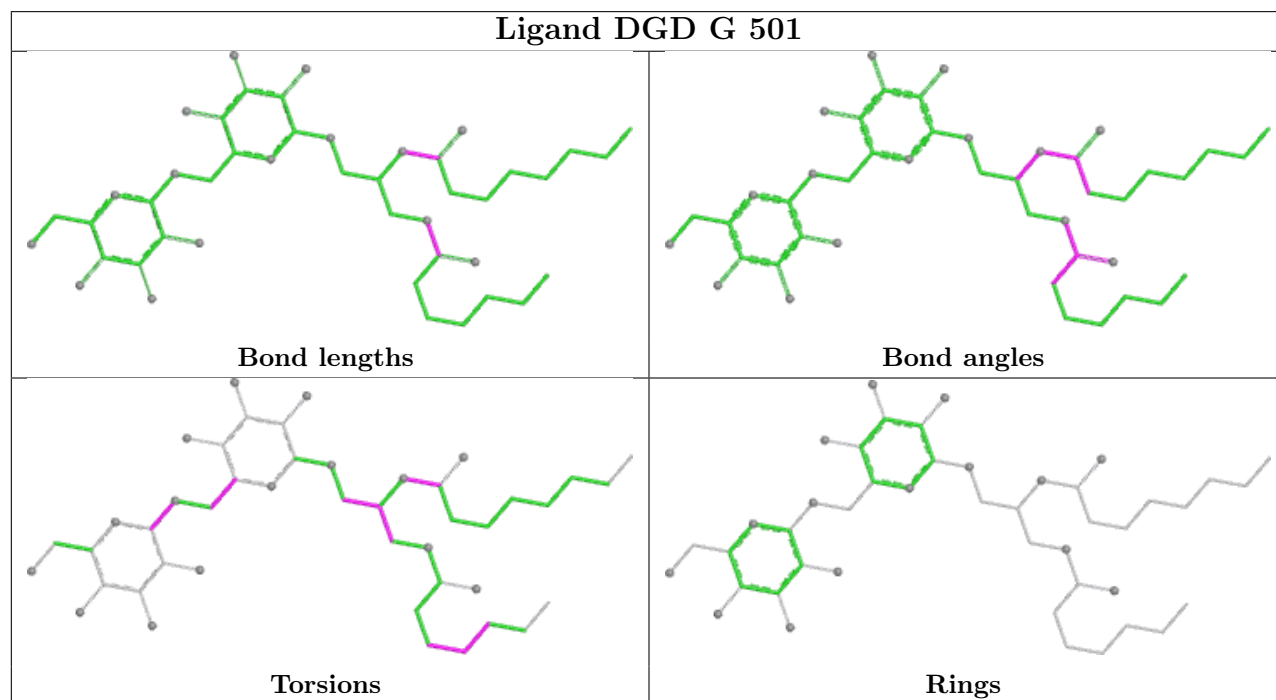




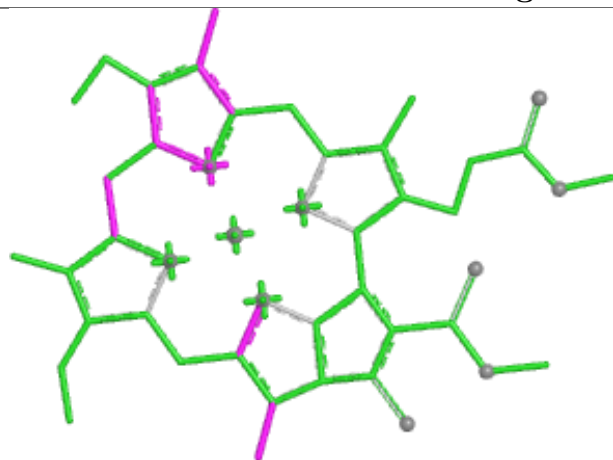
Ligand CLA L 314



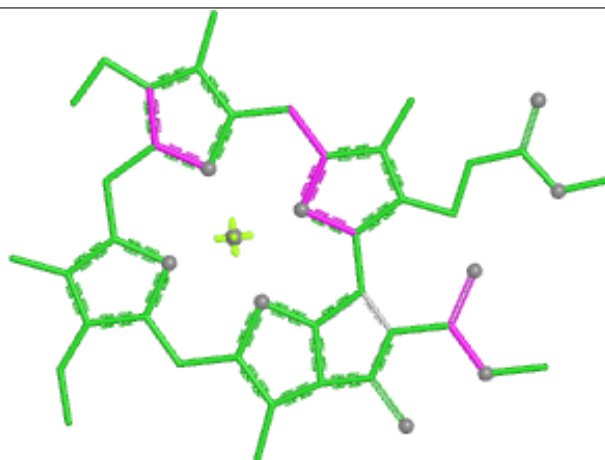
Ligand DGD G 501



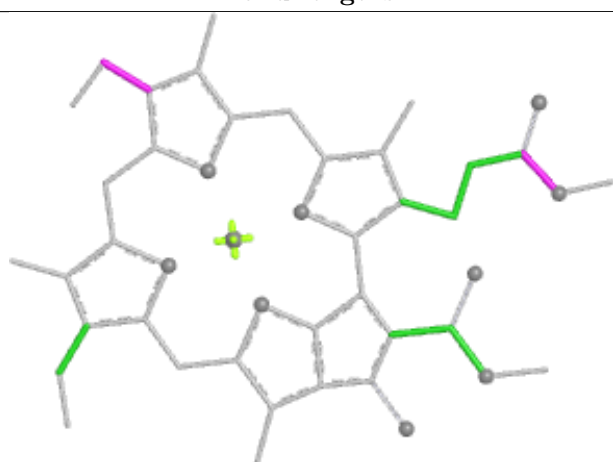
Ligand CLA F 307



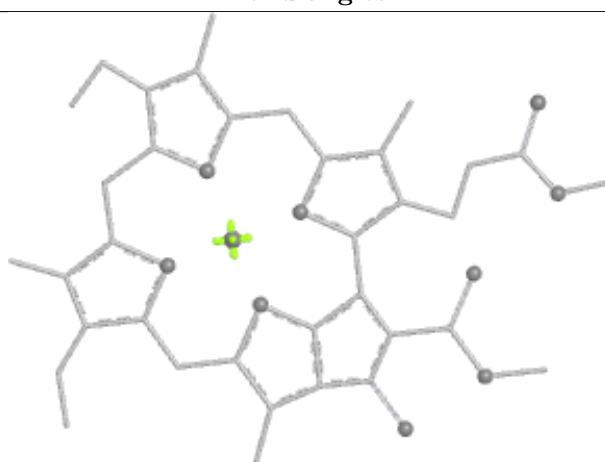
Bond lengths



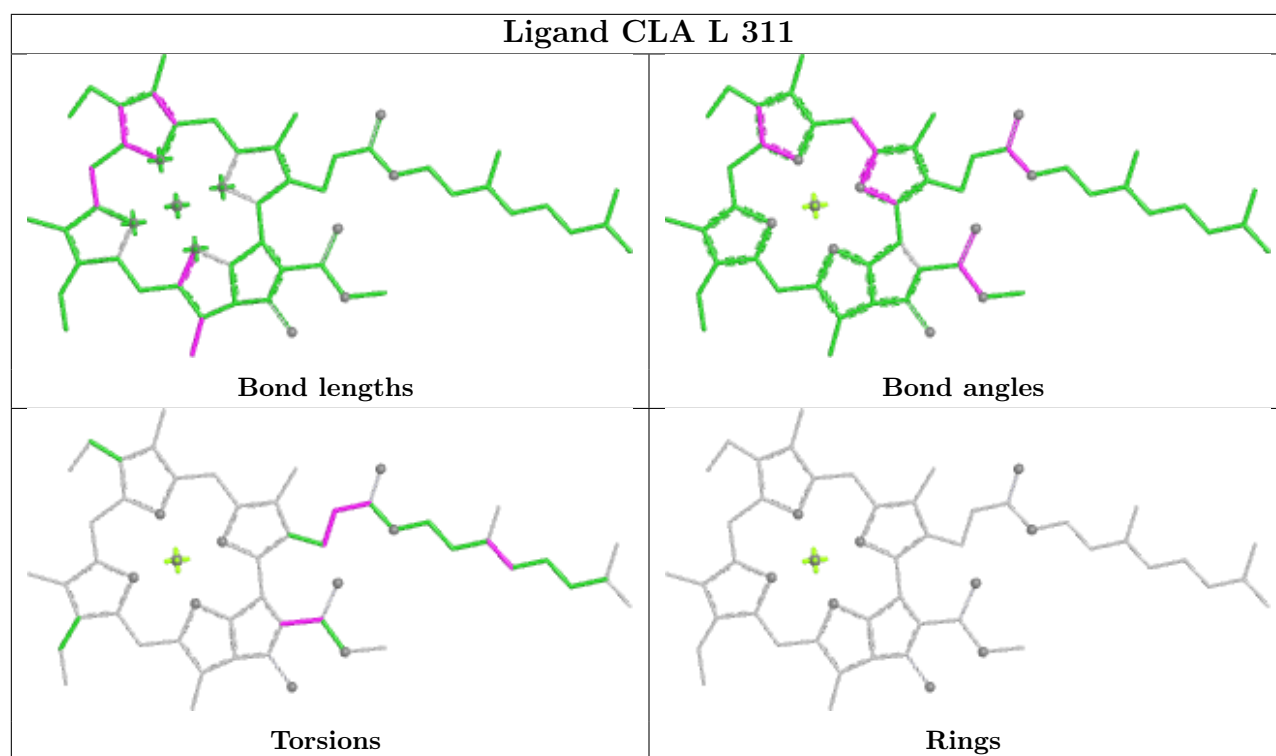
Bond angles



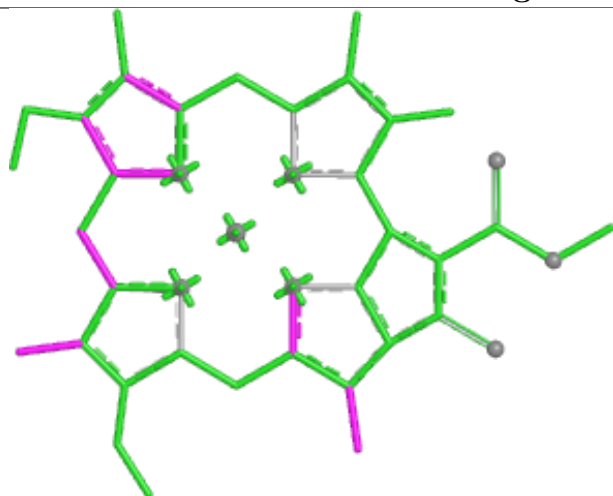
Torsions



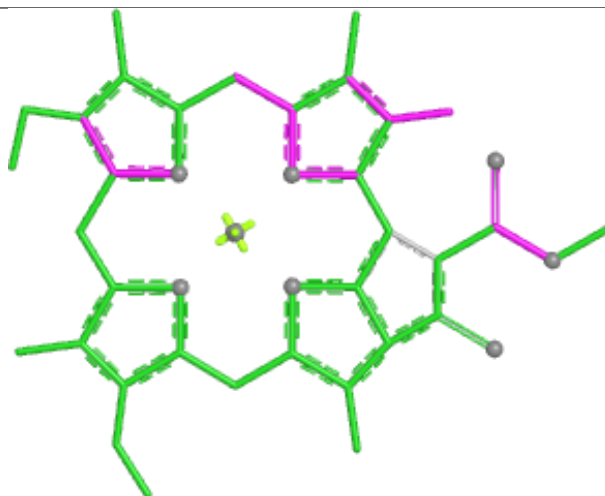
Rings



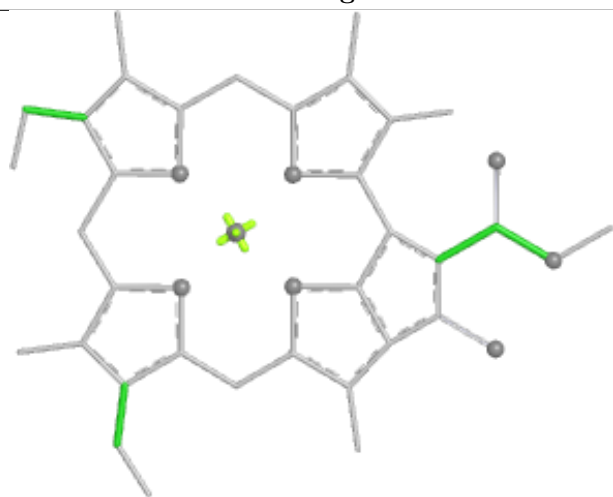
Ligand CLA D 316



Bond lengths



Bond angles

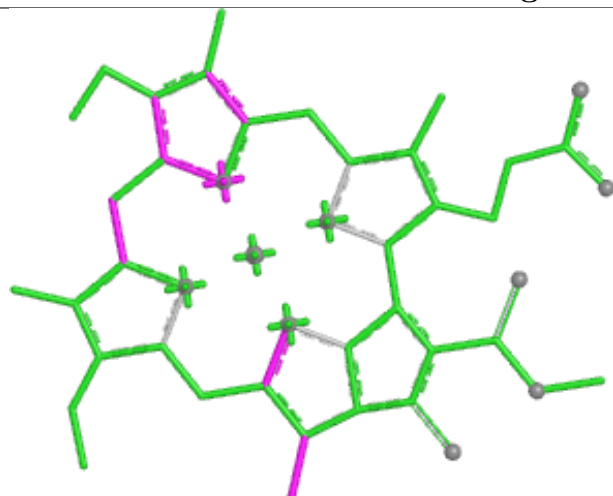


Torsions

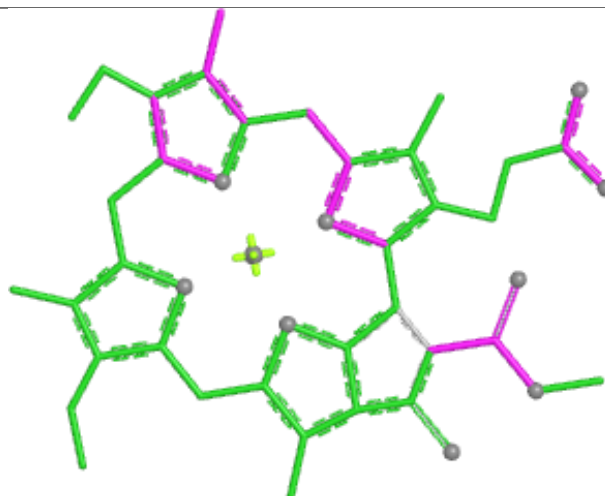


Rings

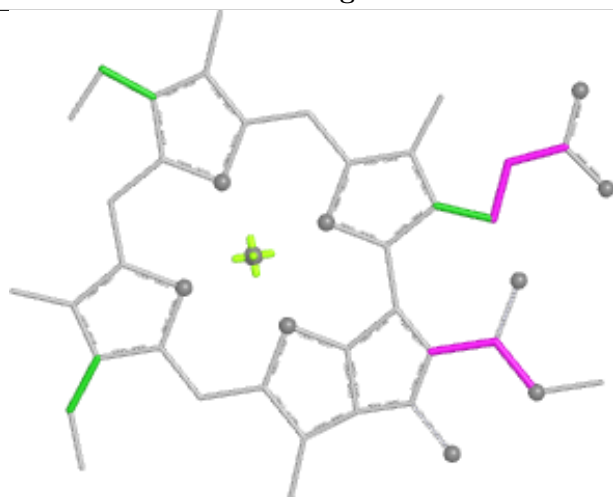
Ligand CLA I 319



Bond lengths



Bond angles

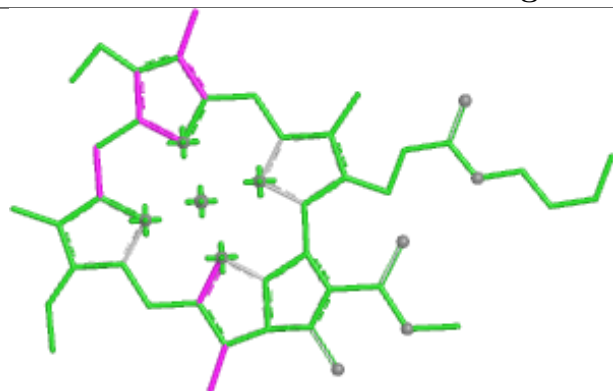


Torsions

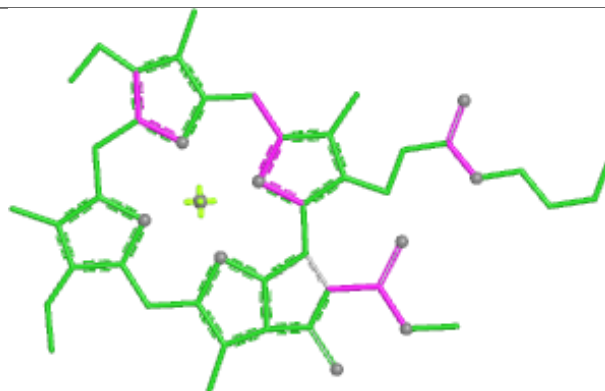


Rings

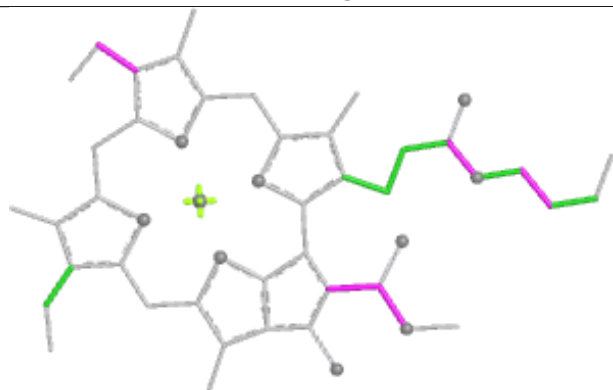
Ligand CLA I 306



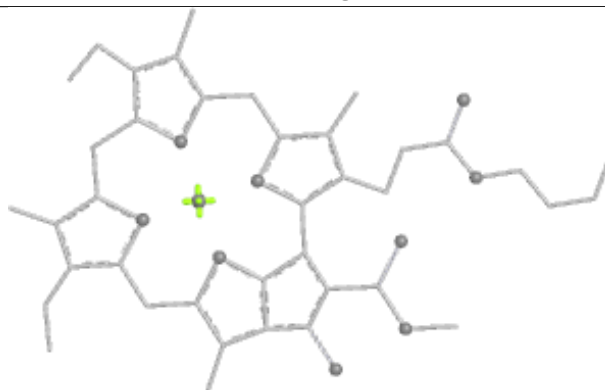
Bond lengths



Bond angles

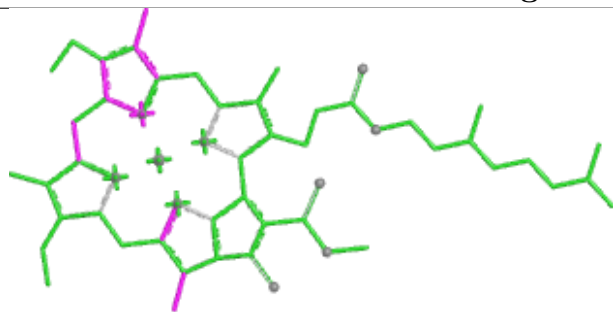


Torsions

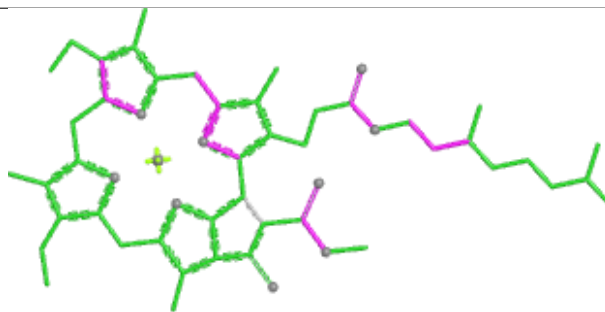


Rings

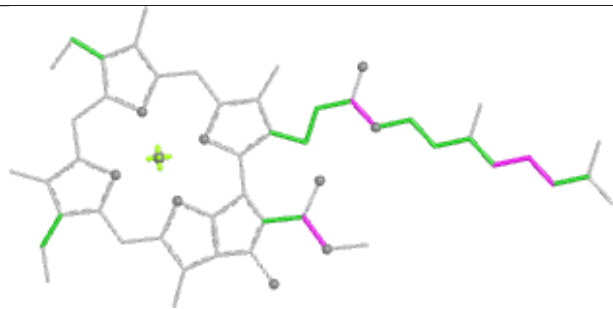
Ligand CLA I 309



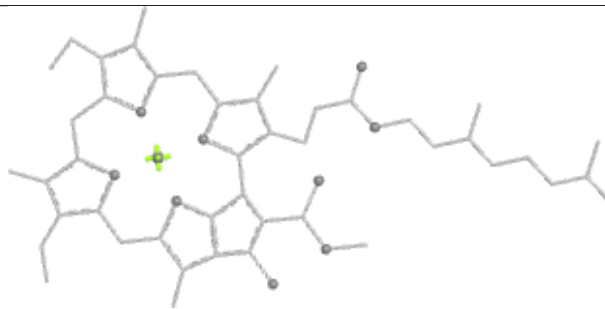
Bond lengths



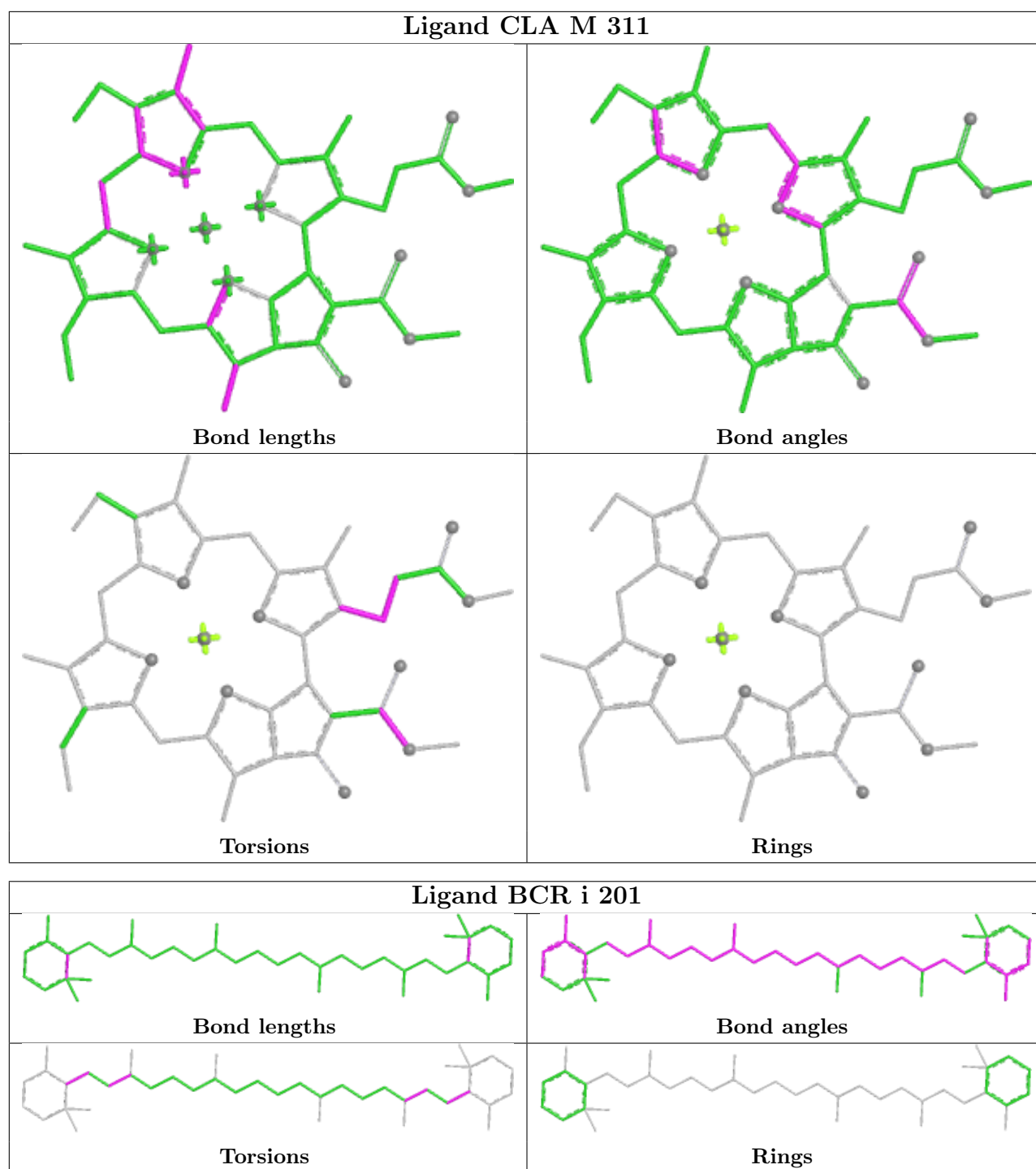
Bond angles

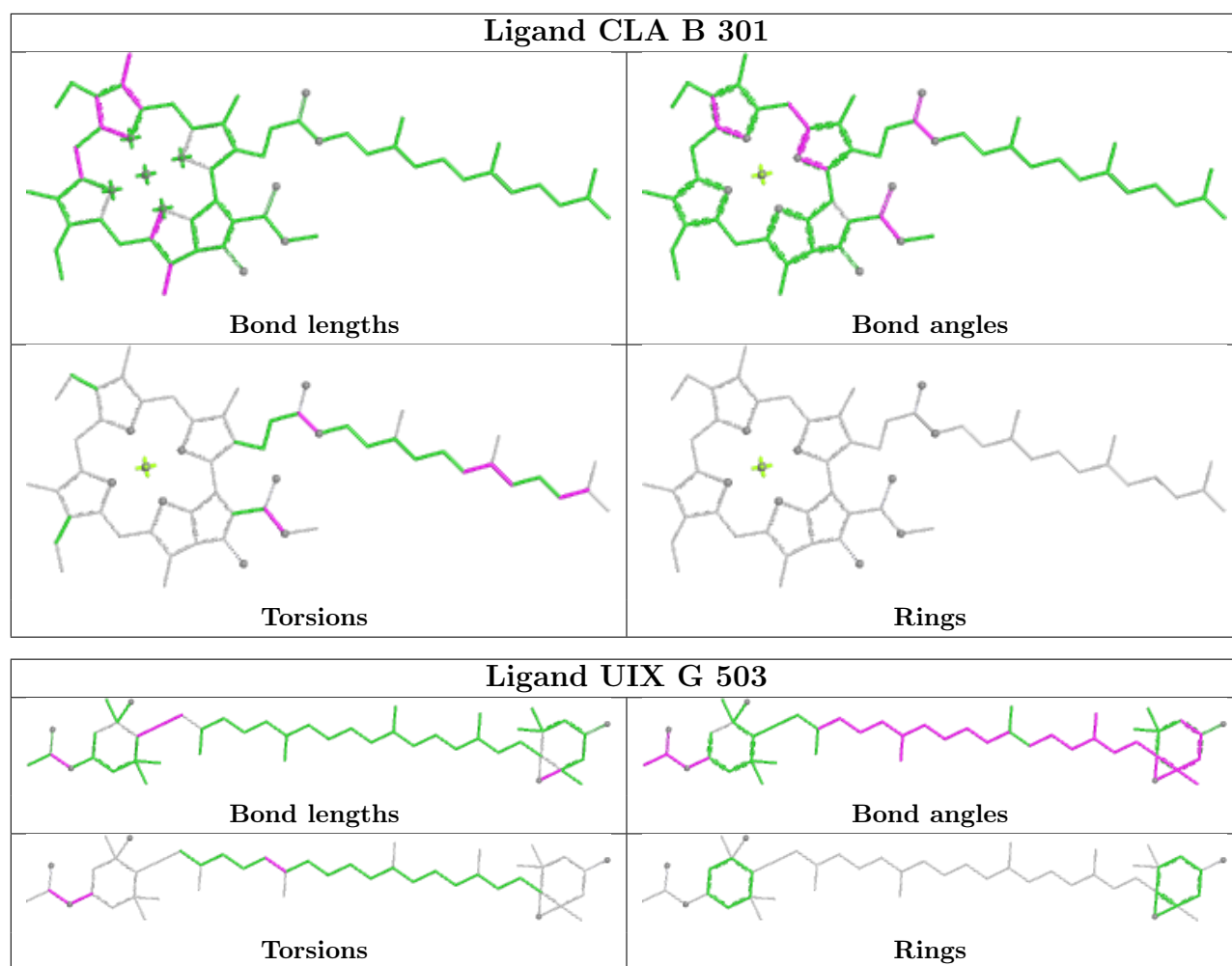


Torsions

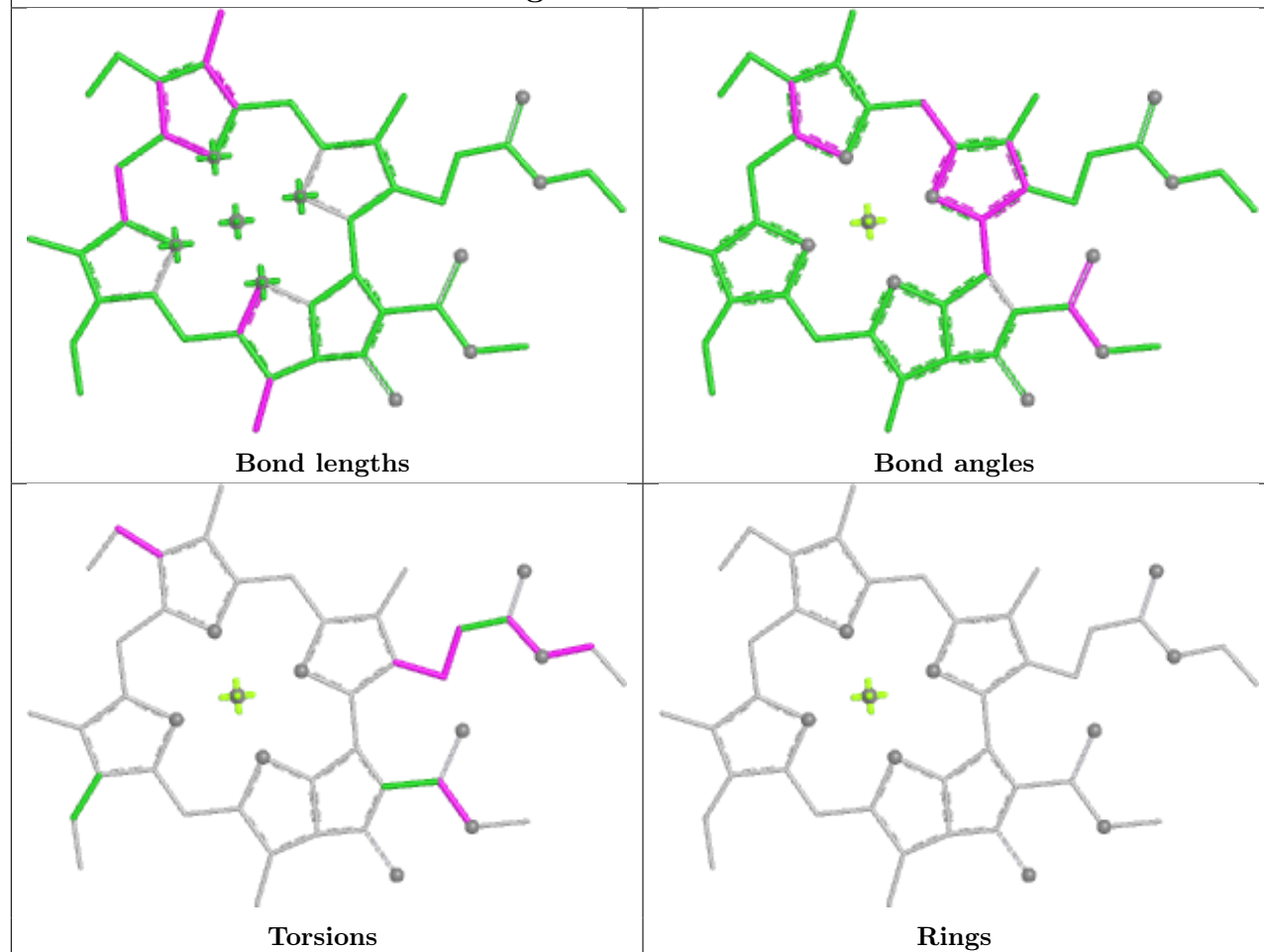


Rings

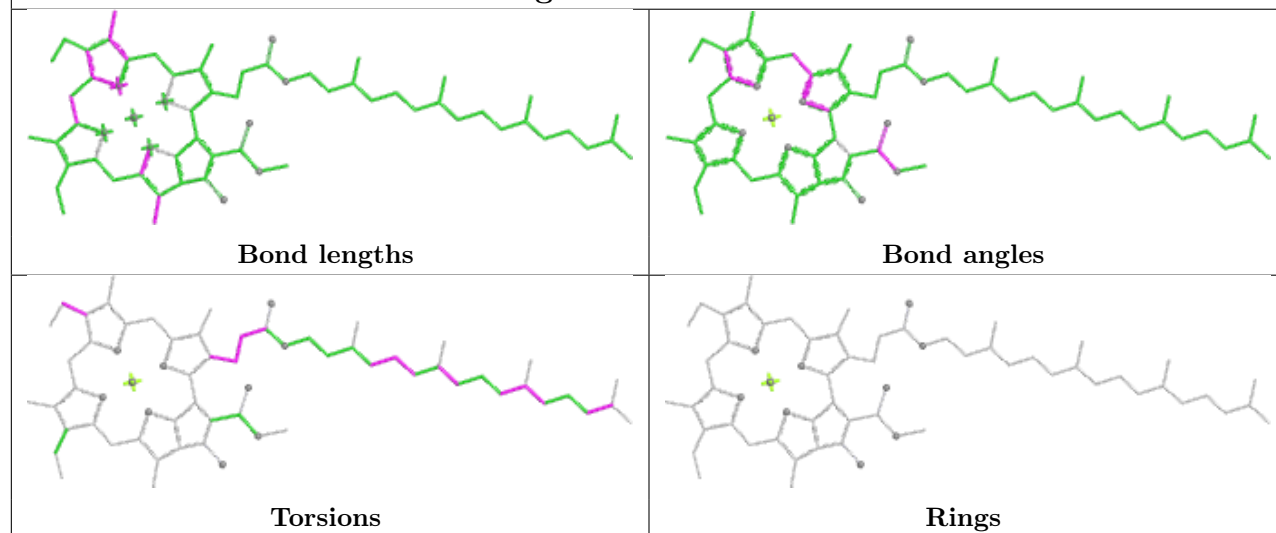




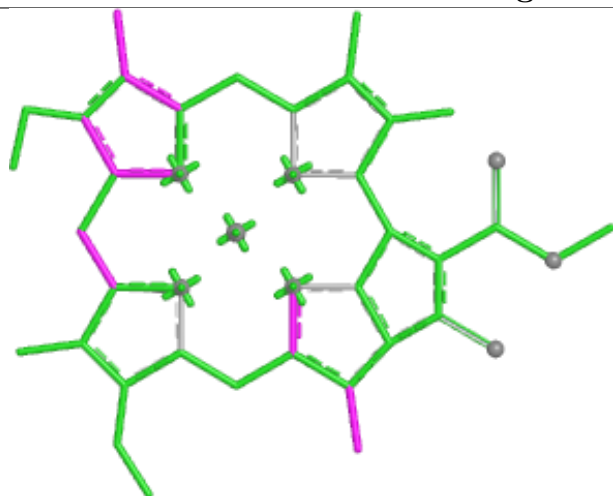
Ligand CLA N 310



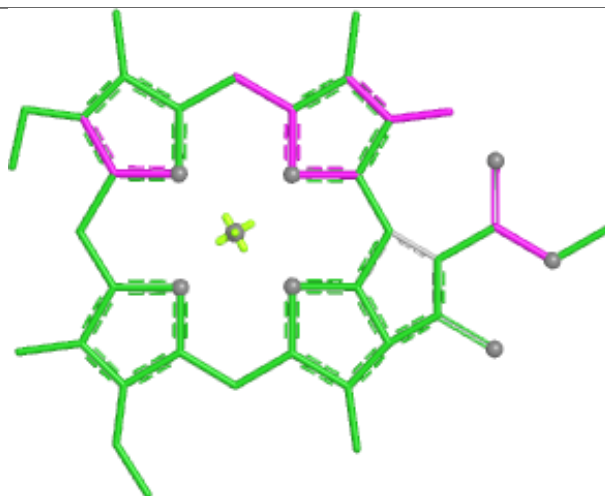
Ligand CLA b 724



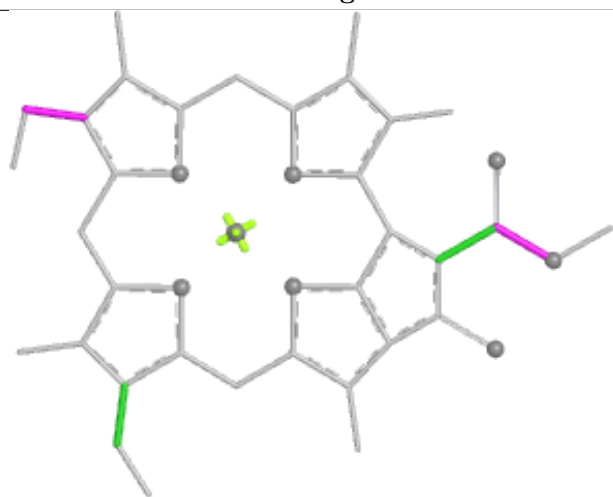
Ligand CLA L 316



Bond lengths



Bond angles

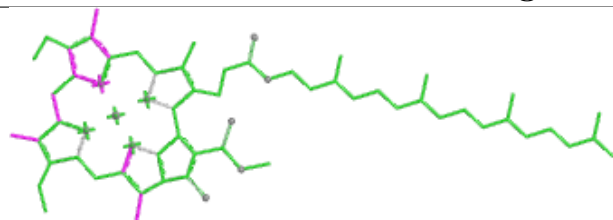


Torsions

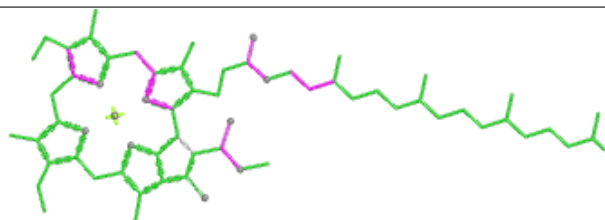


Rings

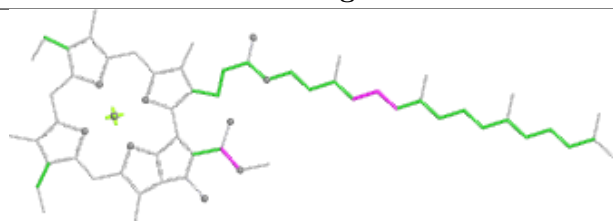
Ligand CLA a 730



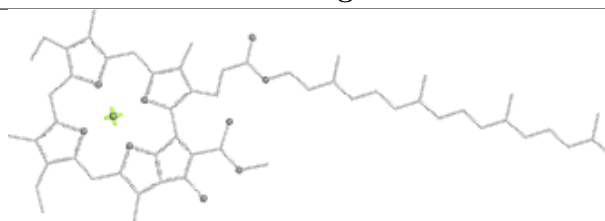
Bond lengths



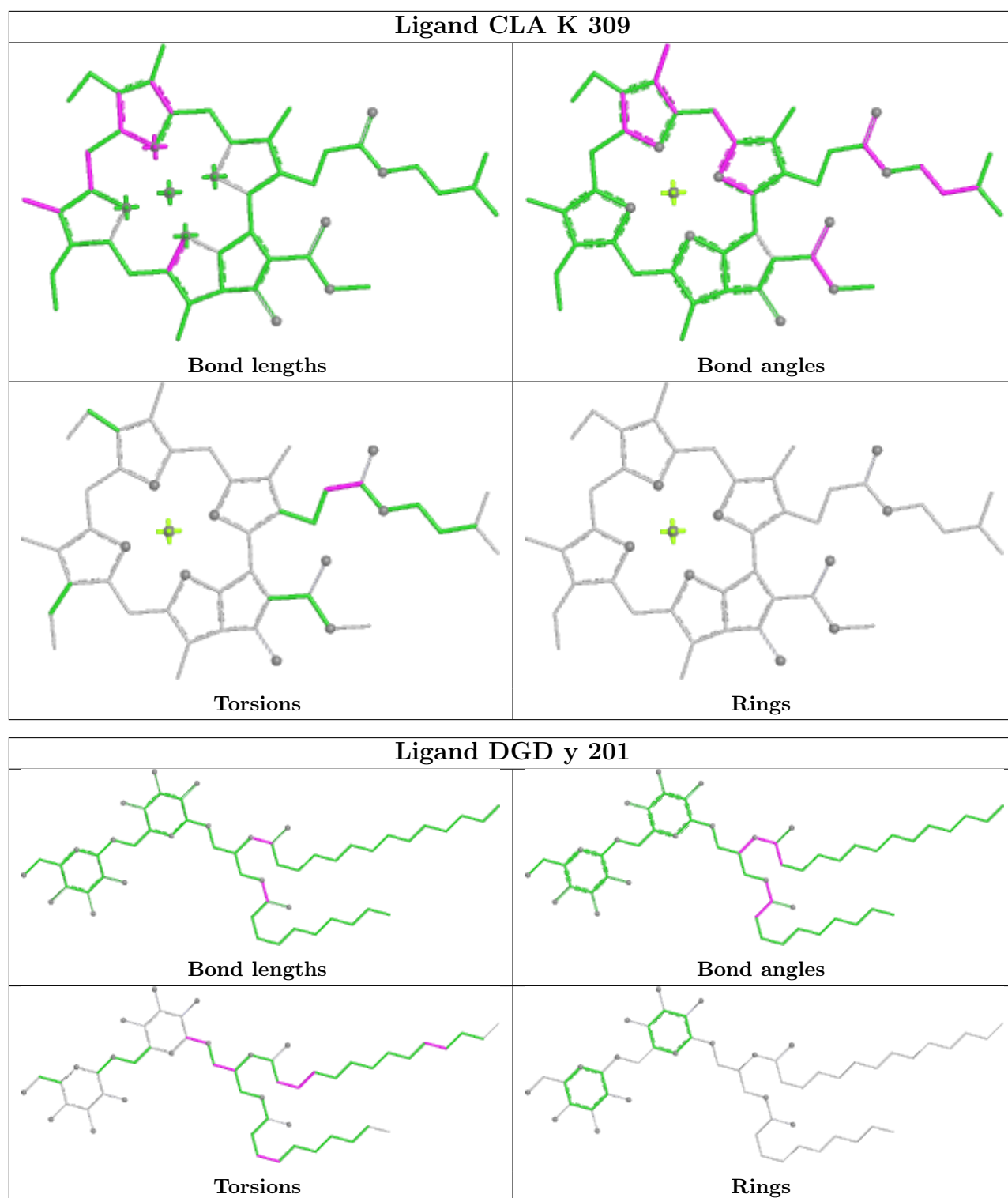
Bond angles



Torsions



Rings



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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

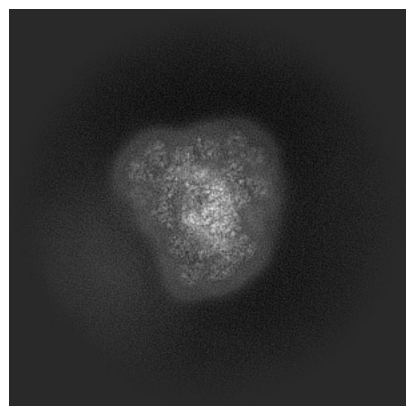
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36742. These allow visual inspection of the internal detail of the map and identification of artifacts.

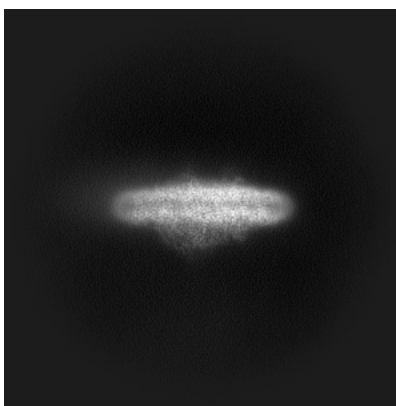
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

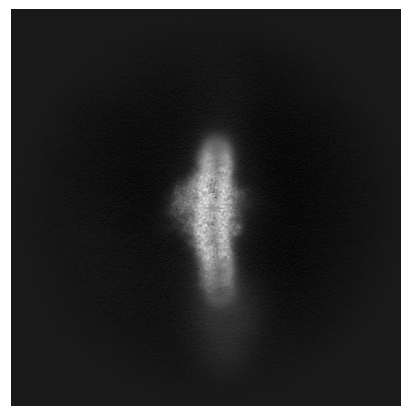
6.1.1 Primary map



X

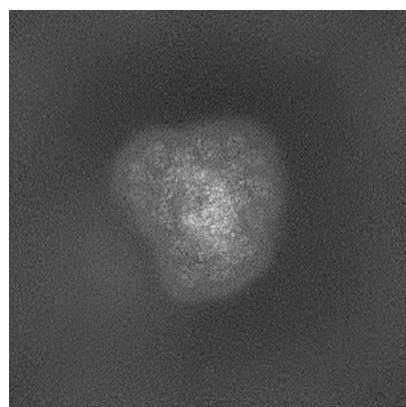


Y

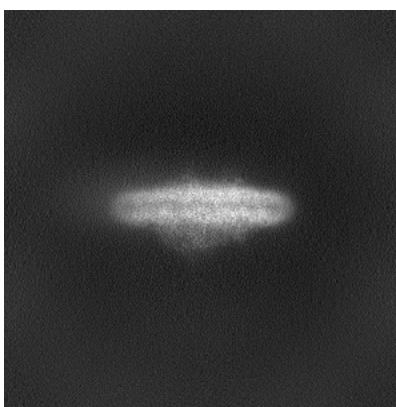


Z

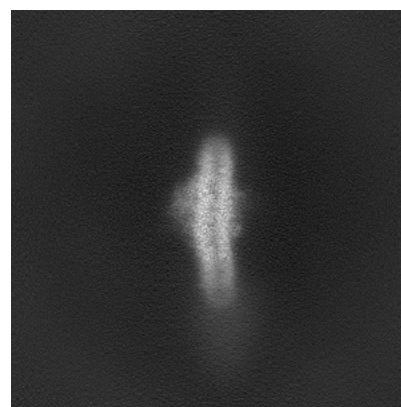
6.1.2 Raw map



X



Y

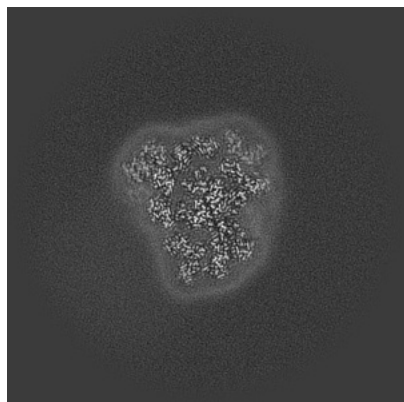


Z

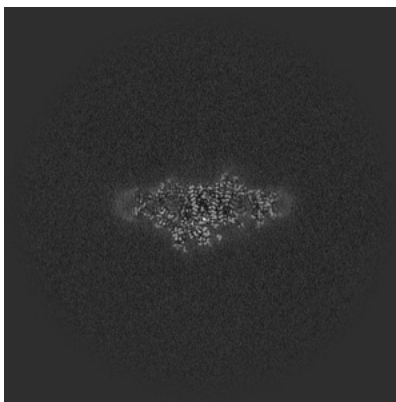
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

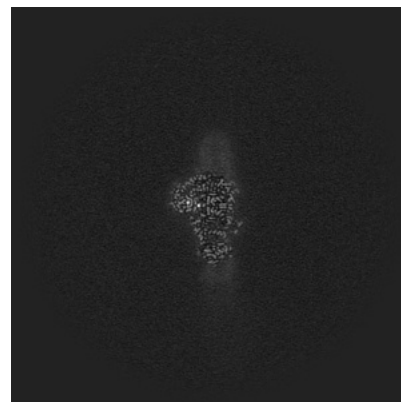
6.2.1 Primary map



X Index: 256

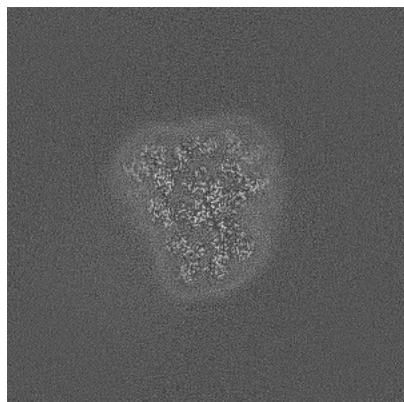


Y Index: 256

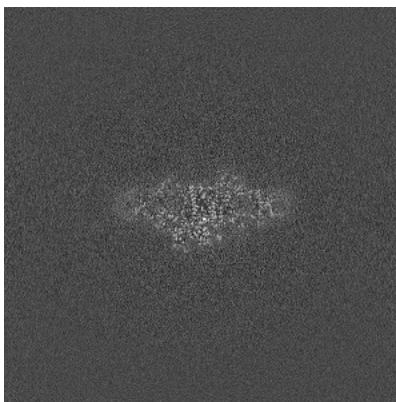


Z Index: 256

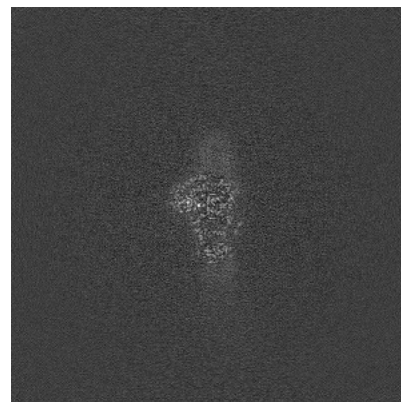
6.2.2 Raw map



X Index: 256



Y Index: 256

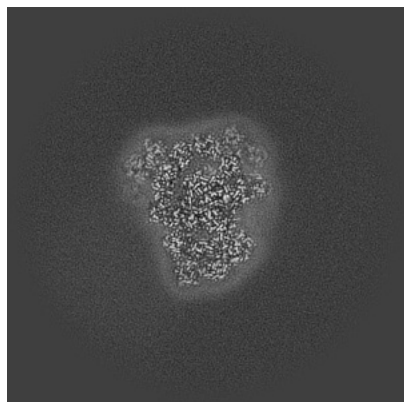


Z Index: 256

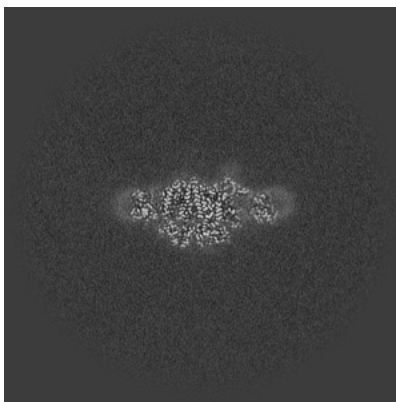
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

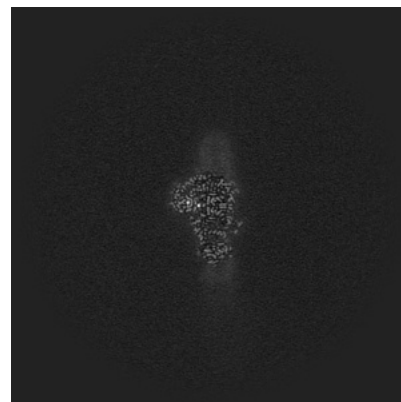
6.3.1 Primary map



X Index: 250

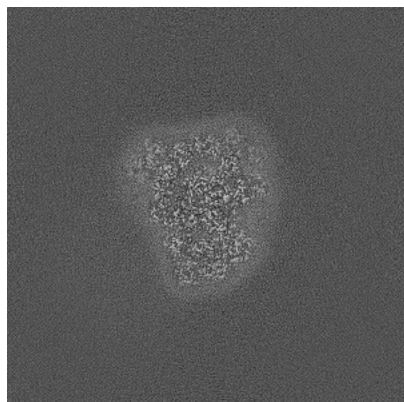


Y Index: 264

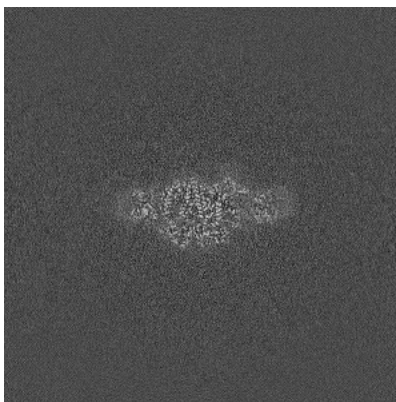


Z Index: 256

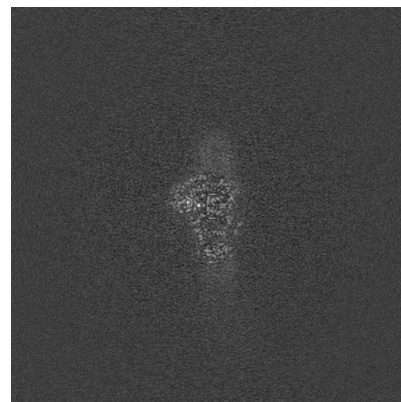
6.3.2 Raw map



X Index: 250



Y Index: 264

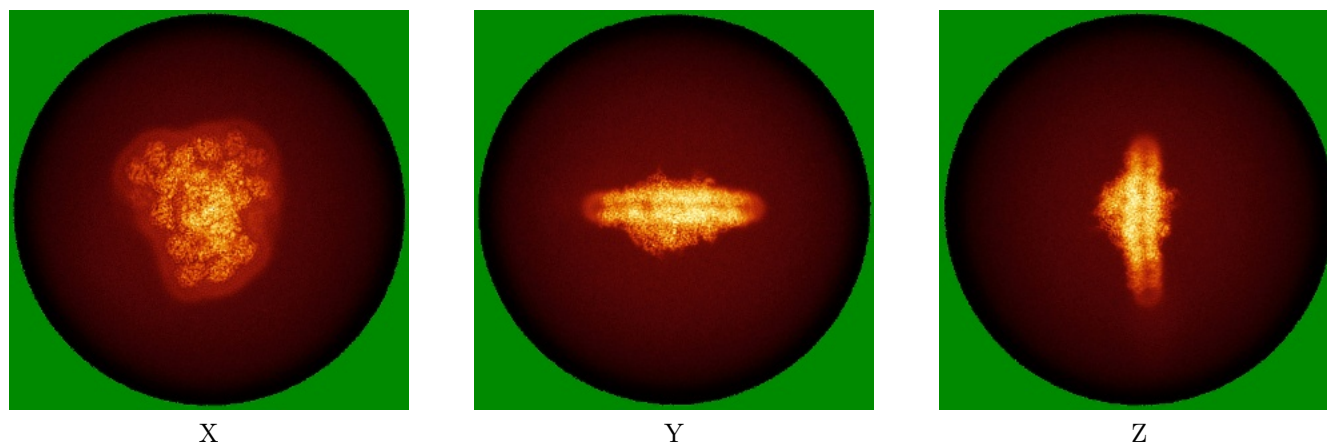


Z Index: 256

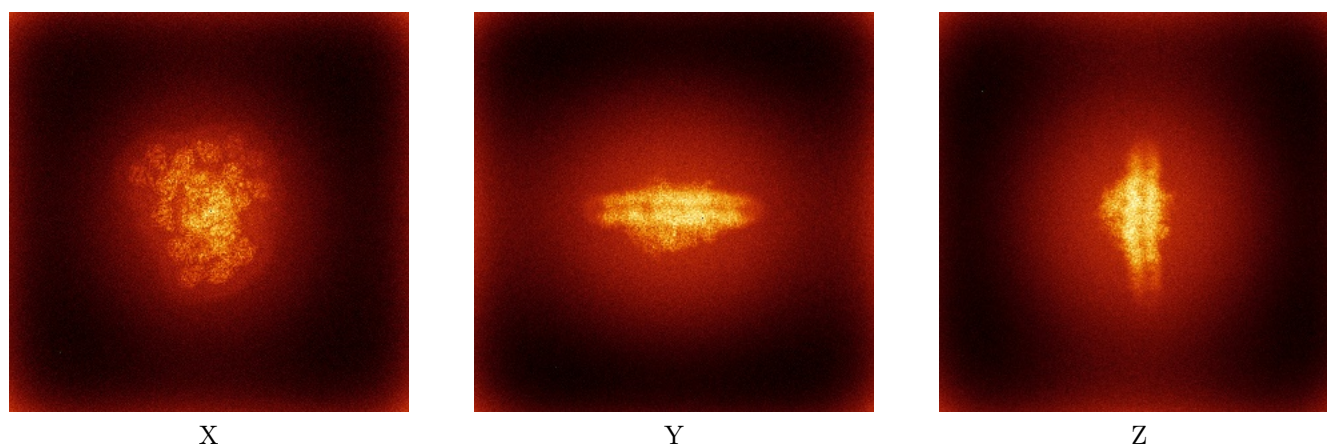
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

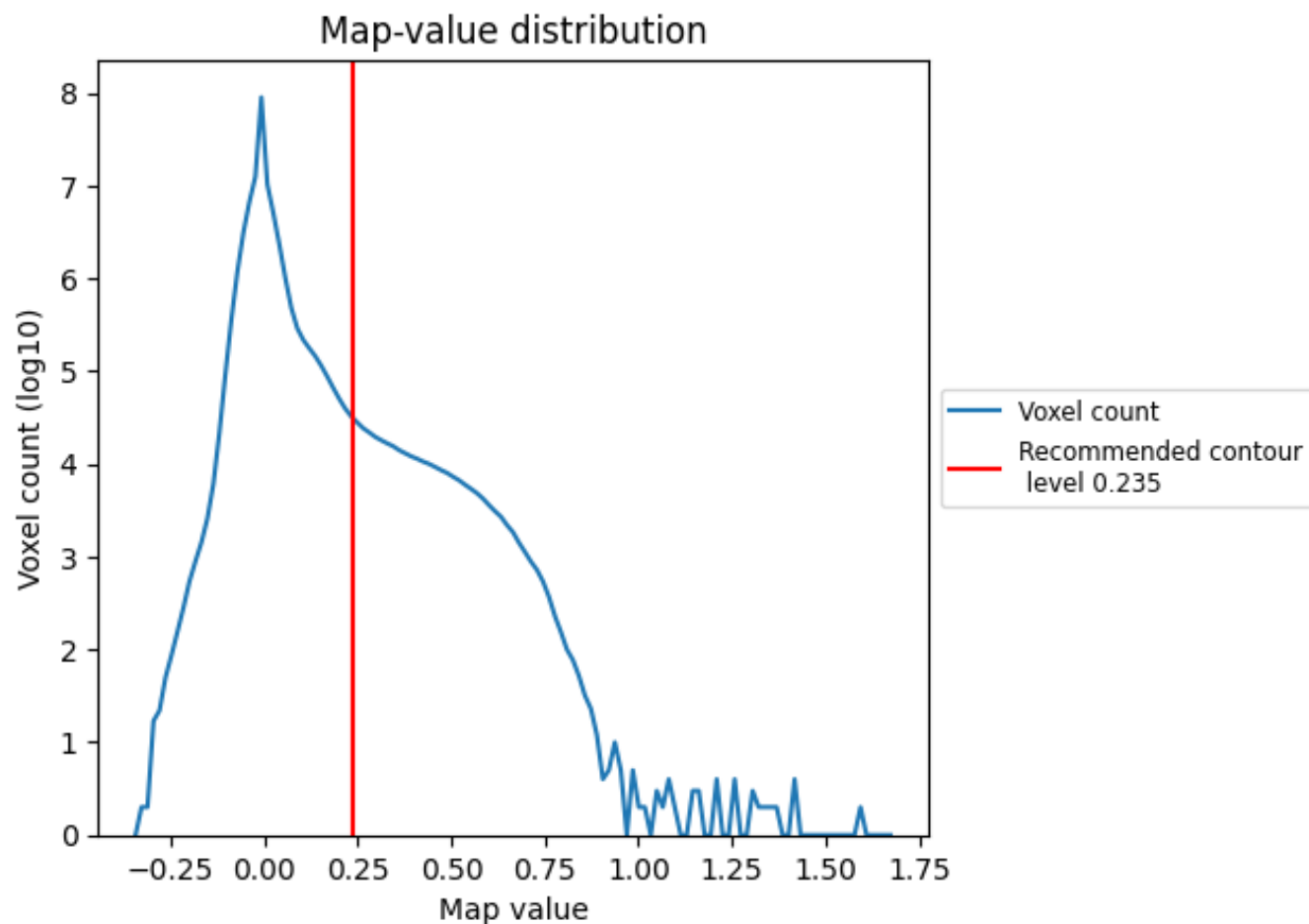
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

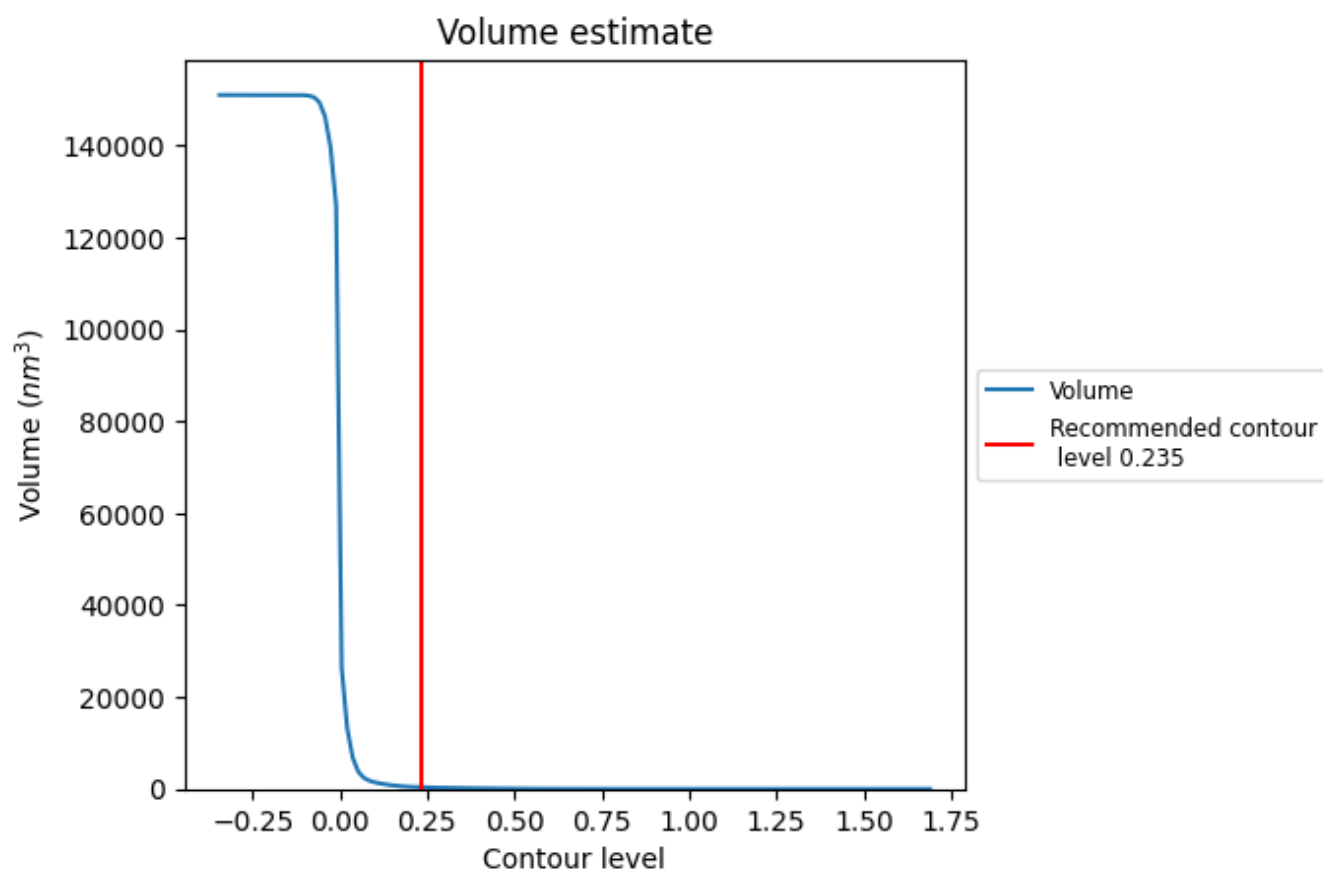
This section contains the results of statistical analysis of the map.

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.

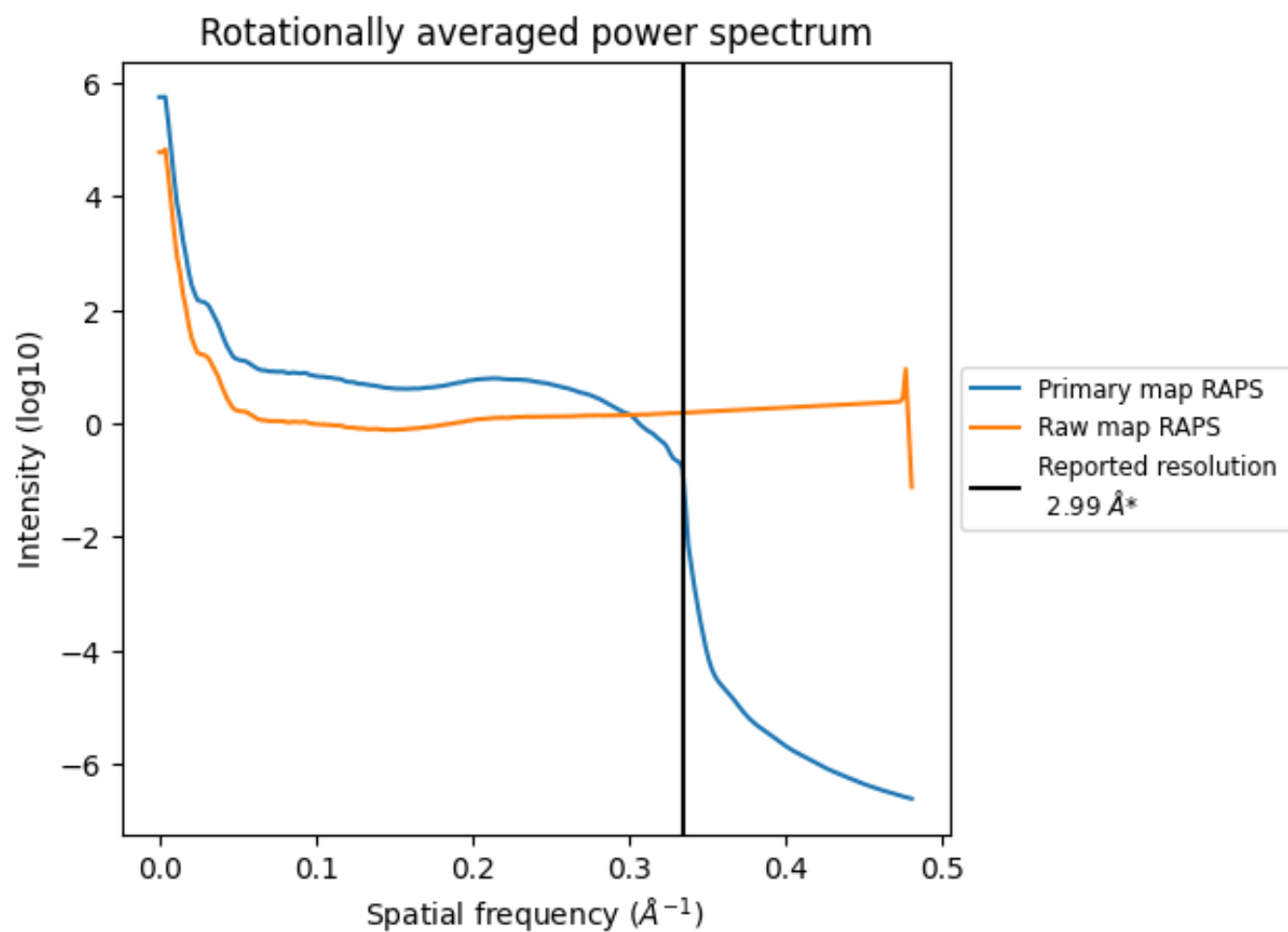
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm^3 ; this corresponds to an approximate mass of 328 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 ⓘ

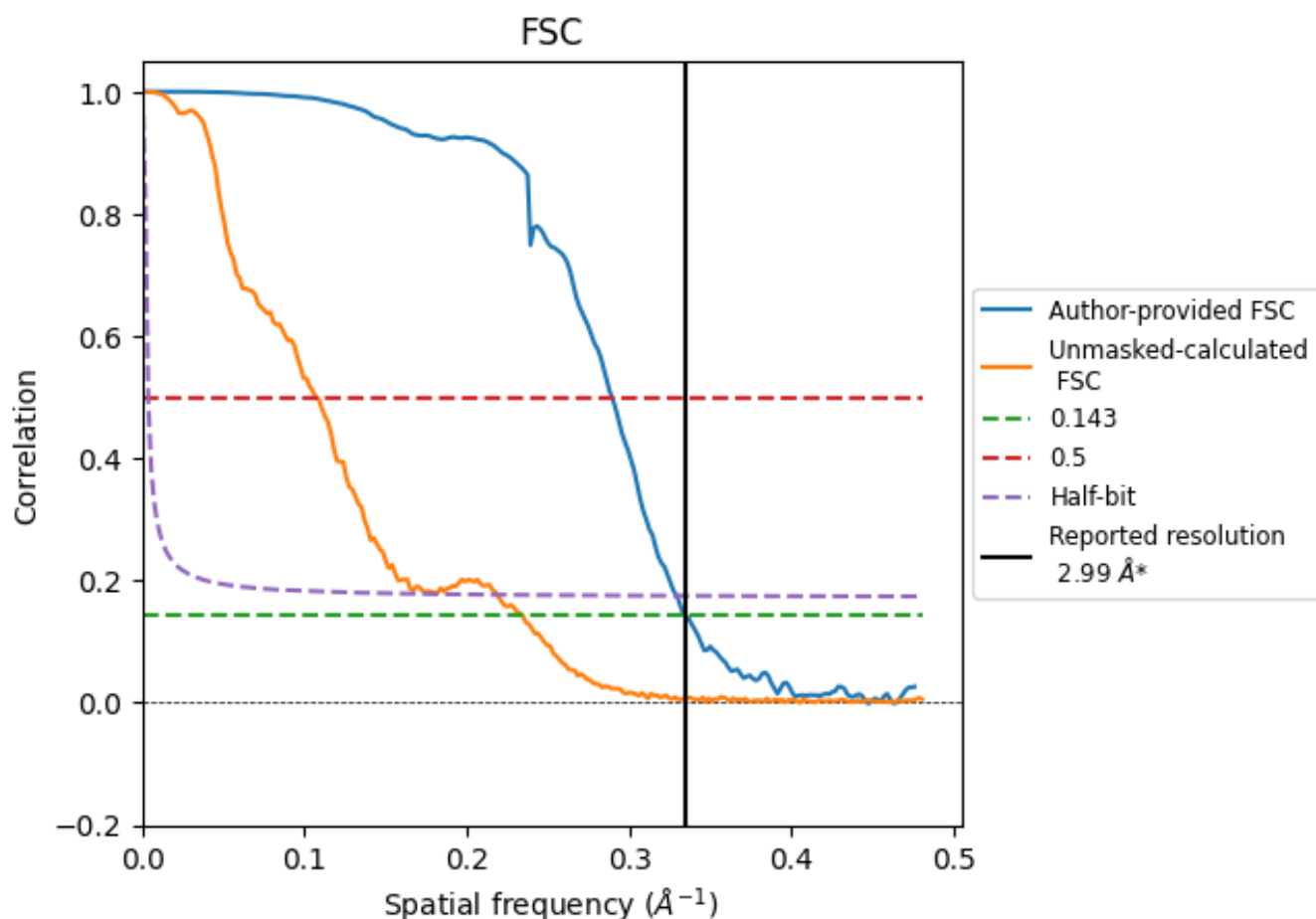


*Reported resolution corresponds to spatial frequency of $0.334 \text{ \AA}^{-1}$

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 0.334 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.45	3.03
Unmasked-calculated*	4.27	9.35	4.57

*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 4.27 differs from the reported value 2.99 by more than 10 %

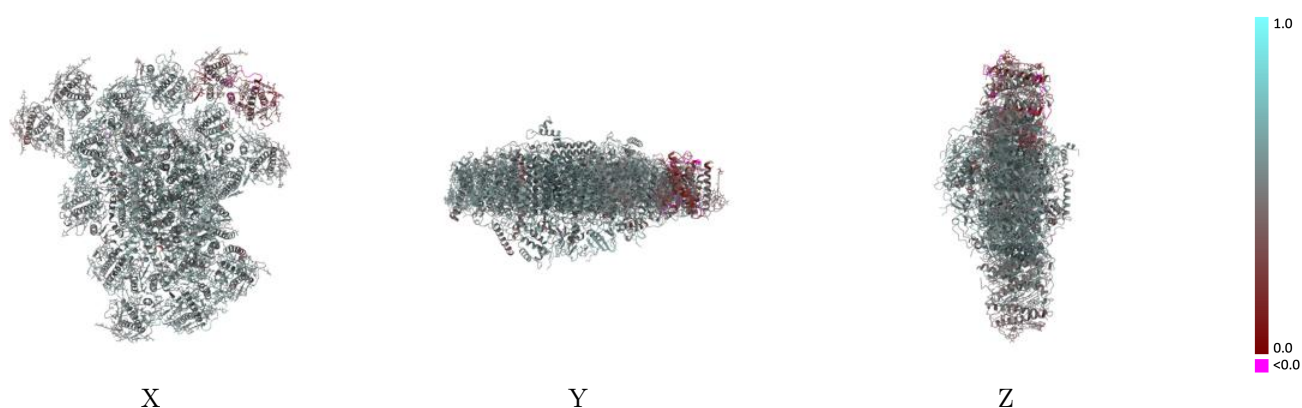
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-36742 and PDB model 8JZE. Per-residue inclusion information can be found in section 3 on page 36.

9.1 Map-model overlay [i](#)

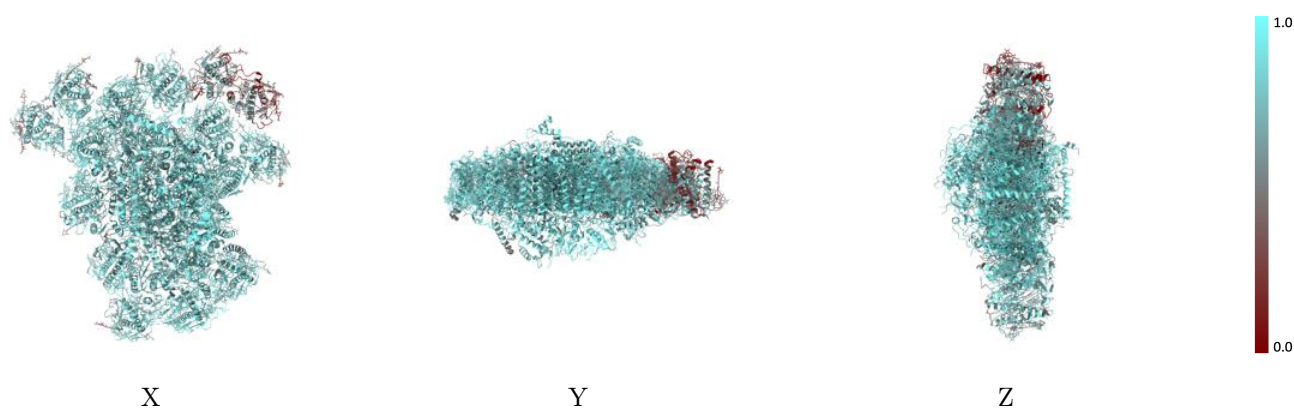
This section was not generated.

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



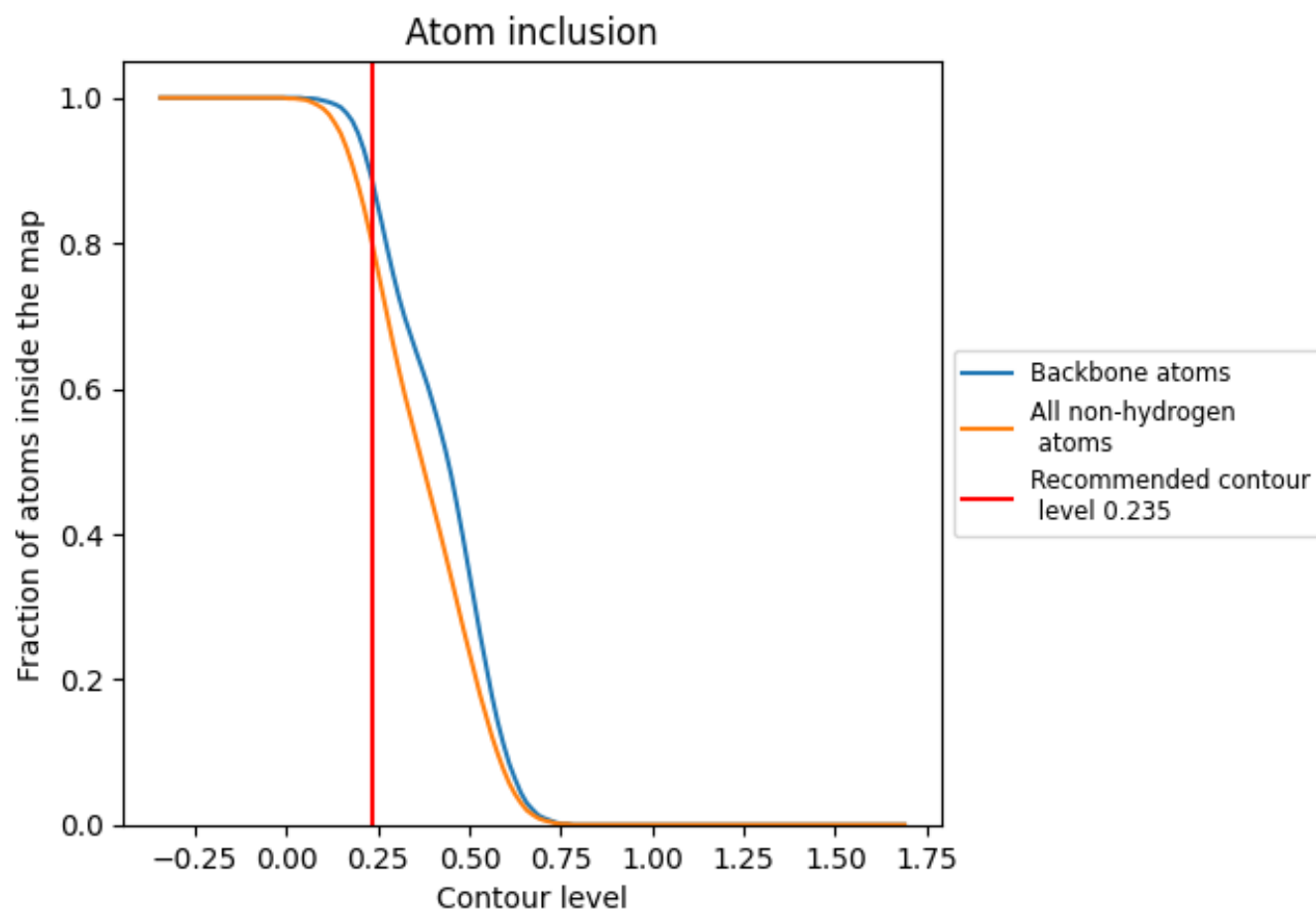
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.235).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% 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 (0.235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.5180
A	 0.8360	 0.5390
B	 0.7940	 0.5260
D	 0.7490	 0.5080
F	 0.7320	 0.4980
G	 0.8000	 0.5170
H	 0.3060	 0.2340
I	 0.7850	 0.5140
J	 0.8410	 0.5330
K	 0.8600	 0.5510
L	 0.8440	 0.5460
M	 0.7800	 0.5200
N	 0.4940	 0.3650
O	 0.6780	 0.4560
P	 0.7250	 0.4850
a	 0.8560	 0.5470
b	 0.8710	 0.5530
c	 0.9280	 0.5570
d	 0.8550	 0.5450
e	 0.8990	 0.5640
f	 0.8330	 0.5420
h	 0.8660	 0.5480
i	 0.8360	 0.5320
j	 0.7800	 0.5310
l	 0.8610	 0.5490
m	 0.8270	 0.5380
y	 0.8670	 0.5260
z	 0.9150	 0.5230

