



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 02:35 AM UTC

PDB ID : 8JZF / pdb_00008jzf
EMDB ID : EMD-36743
Title : PSI-AcpPCI supercomplex from Symbiodinium
Authors : Li, X.Y.; Li, Z.H.; Wang, W.D.
Deposited on : 2023-07-05
Resolution : 2.70 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:

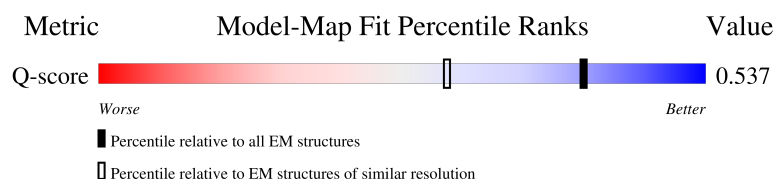
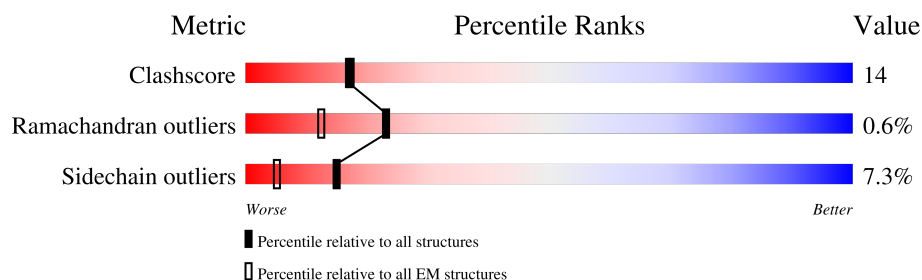
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.70 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.



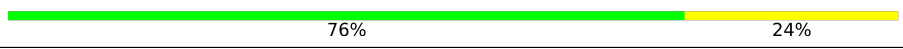
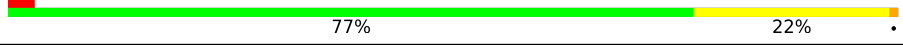
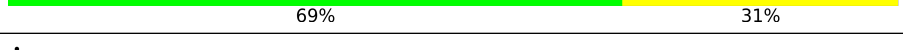
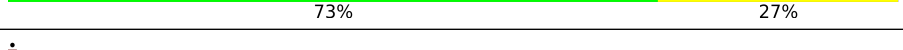
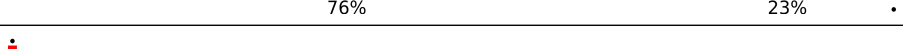
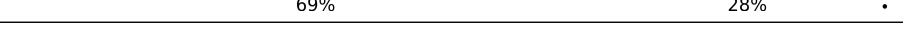
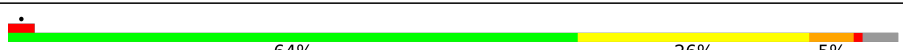
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	
2	K	177	
3	z	78	
4	y	131	

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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	

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
28	CLA	A	307	X	-	-	-
28	CLA	A	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	A	309	X	-	-	-
28	CLA	A	310	X	-	-	-
28	CLA	A	311	X	-	-	-
28	CLA	A	312	X	-	-	-
28	CLA	A	313	X	-	-	-
28	CLA	A	315	X	-	-	-
28	CLA	A	316	X	-	-	-
28	CLA	A	317	X	-	-	-
28	CLA	A	319	X	-	-	-
28	CLA	A	320	X	-	-	-
28	CLA	B	301	X	-	-	-
28	CLA	B	307	X	-	-	-
28	CLA	B	308	X	-	-	-
28	CLA	B	309	X	-	-	-
28	CLA	B	310	X	-	-	-
28	CLA	B	311	X	-	-	-
28	CLA	B	312	X	-	-	-
28	CLA	B	313	X	-	-	-
28	CLA	B	315	X	-	-	-
28	CLA	B	316	X	-	-	-
28	CLA	B	317	X	-	-	-
28	CLA	D	308	X	-	-	-
28	CLA	D	309	X	-	-	-
28	CLA	D	311	X	-	-	-
28	CLA	D	312	X	-	-	-
28	CLA	D	313	X	-	-	-
28	CLA	D	314	X	-	-	-
28	CLA	D	316	X	-	-	-
28	CLA	F	307	X	-	-	-
28	CLA	F	308	X	-	-	-
28	CLA	F	310	X	-	-	-
28	CLA	F	311	X	-	-	-
28	CLA	F	312	X	-	-	-
28	CLA	F	313	X	-	-	-
28	CLA	F	315	X	-	-	-
28	CLA	G	509	X	-	-	-
28	CLA	G	510	X	-	-	-
28	CLA	G	511	X	-	-	-
28	CLA	G	512	X	-	-	-
28	CLA	G	513	X	-	-	-
28	CLA	G	514	X	-	-	-
28	CLA	G	516	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	L	308	X	-	-	-
28	CLA	L	309	X	-	-	-
28	CLA	L	310	X	-	-	-
28	CLA	L	311	X	-	-	-
28	CLA	L	312	X	-	-	-
28	CLA	L	313	X	-	-	-
28	CLA	L	314	X	-	-	-
28	CLA	L	316	X	-	-	-
28	CLA	L	317	X	-	-	-
28	CLA	L	318	X	-	-	-
28	CLA	M	308	X	-	-	-
28	CLA	M	309	X	-	-	-
28	CLA	M	310	X	-	-	-
28	CLA	M	311	X	-	-	-
28	CLA	M	312	X	-	-	-
28	CLA	M	313	X	-	-	-
28	CLA	M	315	X	-	-	-
28	CLA	M	316	X	-	-	-
28	CLA	M	317	X	-	-	-
28	CLA	M	318	X	-	-	-
28	CLA	N	304	X	-	-	-
28	CLA	N	305	X	-	-	-
28	CLA	N	307	X	-	-	-
28	CLA	N	309	X	-	-	-
28	CLA	N	310	X	-	-	-
28	CLA	a	701	X	-	-	-
28	CLA	a	702	X	-	-	-
28	CLA	a	703	X	-	-	-
28	CLA	a	704	X	-	-	-
28	CLA	a	705	X	-	-	-
28	CLA	a	706	X	-	-	-
28	CLA	a	707	X	-	-	-
28	CLA	a	708	X	-	-	-
28	CLA	a	709	X	-	-	-
28	CLA	a	710	X	-	-	-
28	CLA	a	711	X	-	-	-
28	CLA	a	712	X	-	-	-
28	CLA	a	713	X	-	-	-
28	CLA	a	714	X	-	-	-
28	CLA	a	715	X	-	-	-
28	CLA	a	716	X	-	-	-
28	CLA	a	717	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	b	728	X	-	-	-
28	CLA	f	301	X	-	-	-
28	CLA	f	302	X	-	-	-
28	CLA	f	303	X	-	-	-
28	CLA	h	202	X	-	-	-
28	CLA	j	104	X	-	-	-
28	CLA	j	106	X	-	-	-
28	CLA	l	303	X	-	-	-
28	CLA	l	304	X	-	-	-
28	CLA	l	305	X	-	-	-
28	CLA	l	308	X	-	-	-
28	CLA	l	309	X	-	-	-
28	CLA	l	311	X	-	-	-
28	CLA	l	312	X	-	-	-
28	CLA	l	313	X	-	-	-
28	CLA	m	202	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 52237 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		

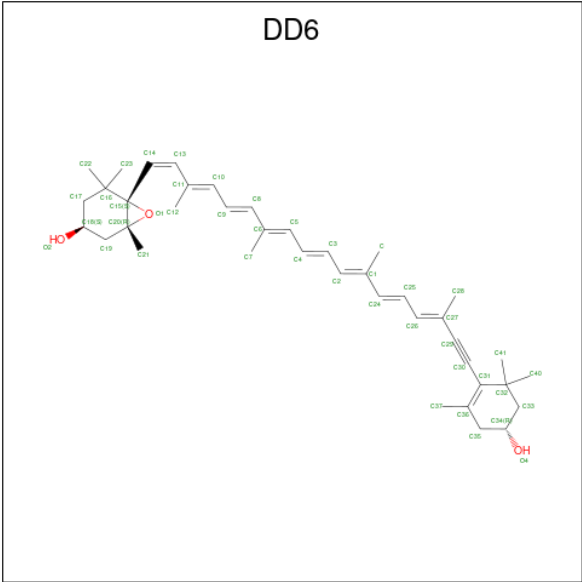
- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

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 (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
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	I	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	K	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	G	1	Total	C	O	0
			43	40	3	
26	A	1	Total	C	O	0
			43	40	3	

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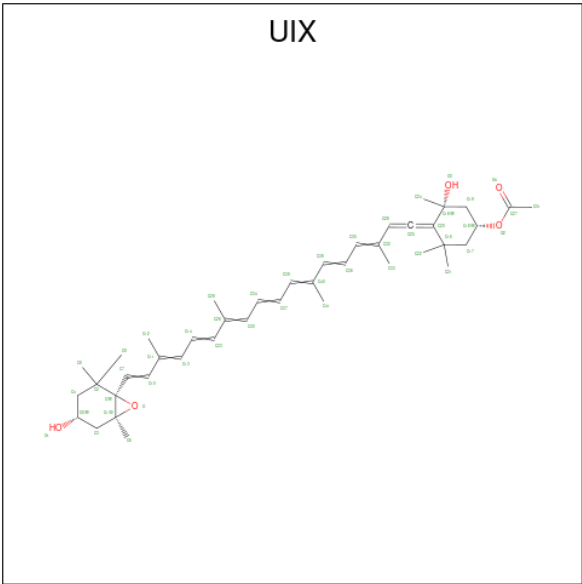
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total 43	C 40	O 3	0
26	A	1	Total 43	C 40	O 3	0
26	A	1	Total 43	C 40	O 3	0
26	h	1	Total 43	C 40	O 3	0
26	b	1	Total 43	C 40	O 3	0
26	B	1	Total 42	C 39	O 3	0
26	B	1	Total 43	C 40	O 3	0
26	B	1	Total 43	C 40	O 3	0
26	B	1	Total 43	C 40	O 3	0
26	B	1	Total 43	C 40	O 3	0
26	D	1	Total 43	C 40	O 3	0
26	F	1	Total 43	C 40	O 3	0
26	F	1	Total 43	C 40	O 3	0
26	H	1	Total 43	C 40	O 3	0
26	J	1	Total 43	C 40	O 3	0
26	J	1	Total 43	C 40	O 3	0
26	J	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0
26	L	1	Total 43	C 40	O 3	0

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Mol	Chain	Residues	Atoms			AltConf
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	M	1	Total	C	O	0
			43	40	3	
26	N	1	Total	C	O	0
			43	40	3	

- Molecule 27 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).



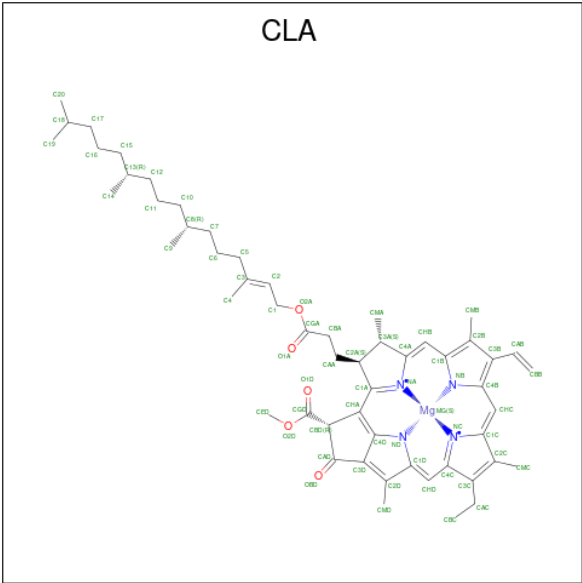
Mol	Chain	Residues	Atoms			AltConf
27	I	1	Total	C	O	0
			47	42	5	
27	K	1	Total	C	O	0
			47	42	5	
27	G	1	Total	C	O	0
			47	42	5	

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Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			47	42	5	
27	h	1	Total	C	O	0
			47	42	5	
27	B	1	Total	C	O	0
			47	42	5	
27	J	1	Total	C	O	0
			47	42	5	

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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

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Mol	Chain	Residues	Atoms					AltConf
28	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	G	1	Total 61	C 51	Mg 1	N 4	O 5	0
28	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	h	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	j	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	l	1	Total	C	N	O		0
			45	36	4	5		
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	m	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
28	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
28	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	D	1	Total 47	C 37	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	H	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	H	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	H	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	J	1	Total 60	C 50	Mg 1	N 4	O 5	0

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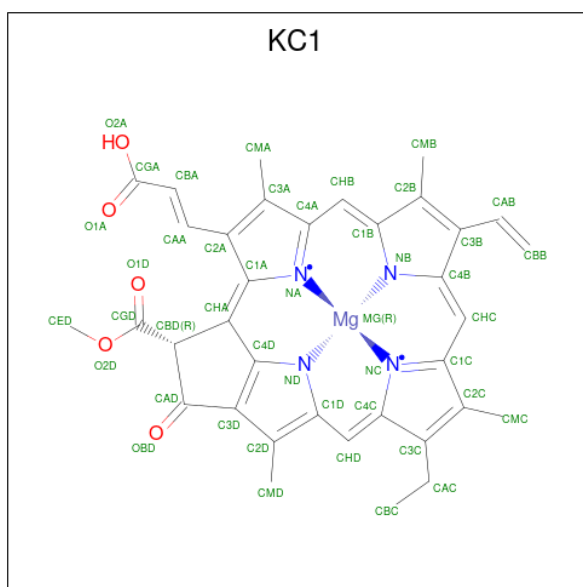
Mol	Chain	Residues	Atoms					AltConf
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			47	39	1	4	3	
28	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	M	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
28	M	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

- Molecule 29 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



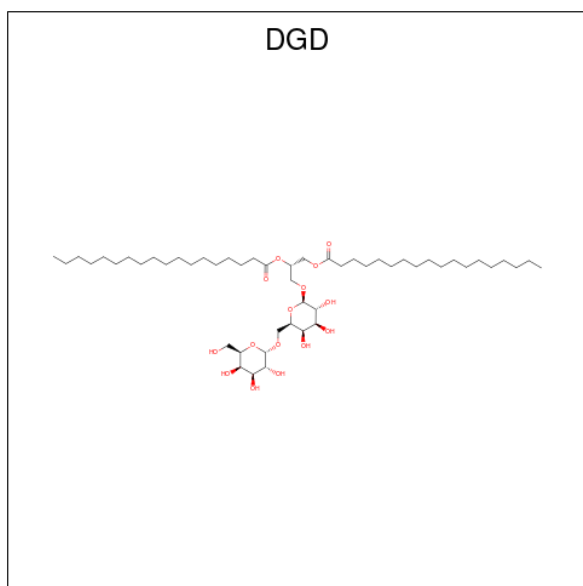
Mol	Chain	Residues	Atoms					AltConf
29	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	D	1	Total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

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

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



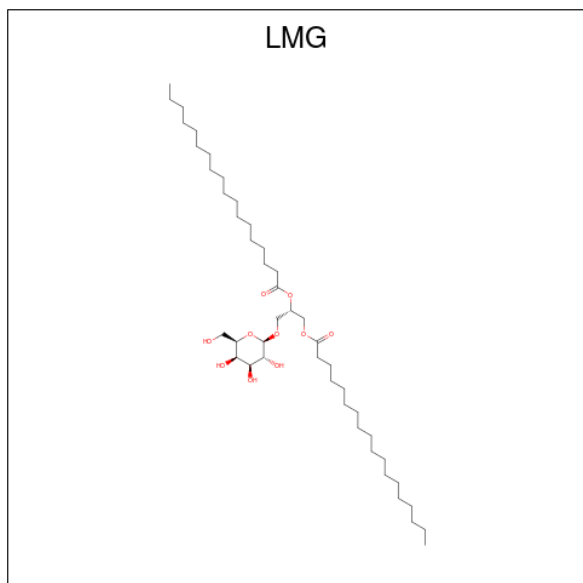
Mol	Chain	Residues	Atoms			AltConf
30	I	1	Total	C	O	0
			39	24	15	
30	y	1	Total	C	O	0
			54	39	15	
30	G	1	Total	C	O	0
			45	30	15	
30	G	1	Total	C	O	0
			44	29	15	
30	j	1	Total	C	O	0
			41	26	15	

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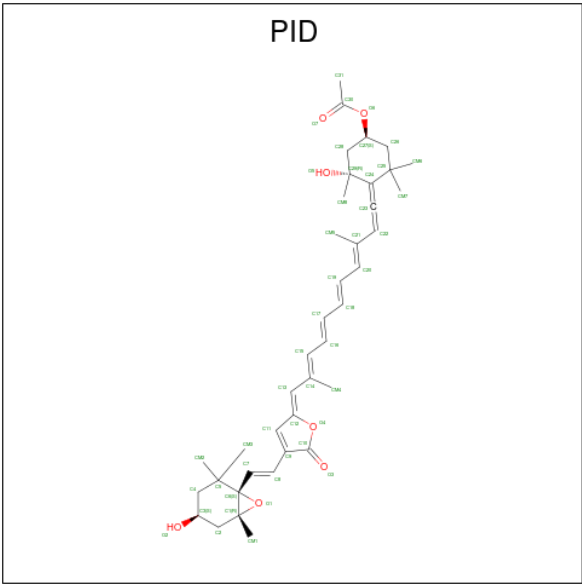
Mol	Chain	Residues	Atoms			AltConf
30	l	1	Total	C	O	0
			50	35	15	
30	L	1	Total	C	O	0
			38	23	15	

- Molecule 31 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
31	I	1	Total	C	O	0
			36	26	10	
31	I	1	Total	C	O	0
			38	28	10	
31	K	1	Total	C	O	0
			27	17	10	
31	K	1	Total	C	O	0
			43	33	10	
31	j	1	Total	C	O	0
			35	25	10	
31	b	1	Total	C	O	0
			44	34	10	
31	b	1	Total	C	O	0
			31	21	10	
31	B	1	Total	C	O	0
			37	27	10	
31	D	1	Total	C	O	0
			49	39	10	

- Molecule 32 is PERIDININ (CCD ID: PID) (formula: C₃₉H₅₀O₇) (labeled as "Ligand of Interest" by depositor).



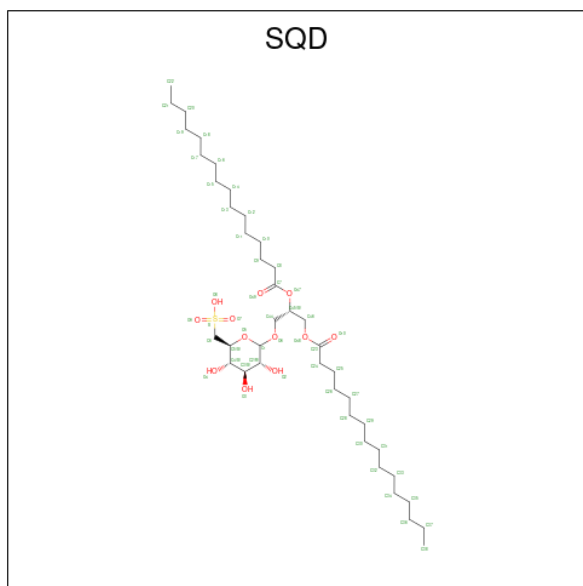
Mol	Chain	Residues	Atoms			AltConf
32	G	1	Total	C	O	0
			46	39	7	
32	G	1	Total	C	O	0
			46	39	7	
32	j	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0
			46	39	7	
32	D	1	Total	C	O	0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

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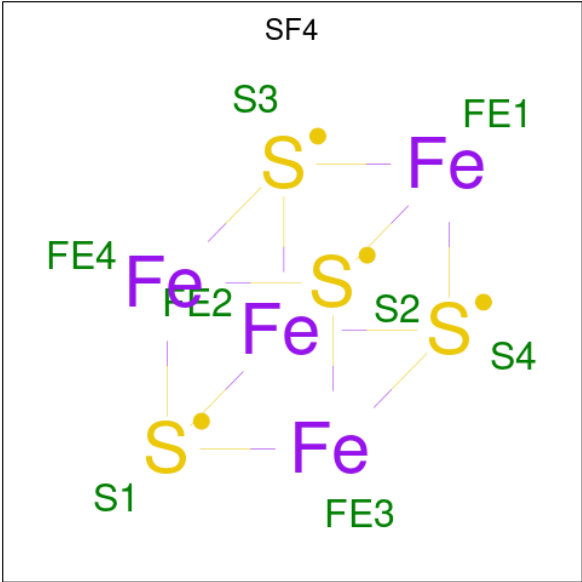
Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total	C	O	0
			46	39	7	
32	H	1	Total	C	O	0
			46	39	7	
32	H	1	Total	C	O	0
			46	39	7	
32	M	1	Total	C	O	0
			46	39	7	
32	N	1	Total	C	O	0
			46	39	7	
32	N	1	Total	C	O	0
			46	39	7	

- Molecule 33 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).



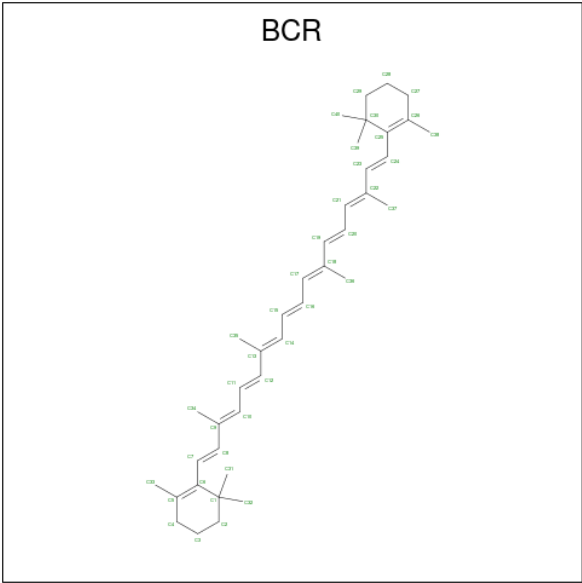
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 34 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 35 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



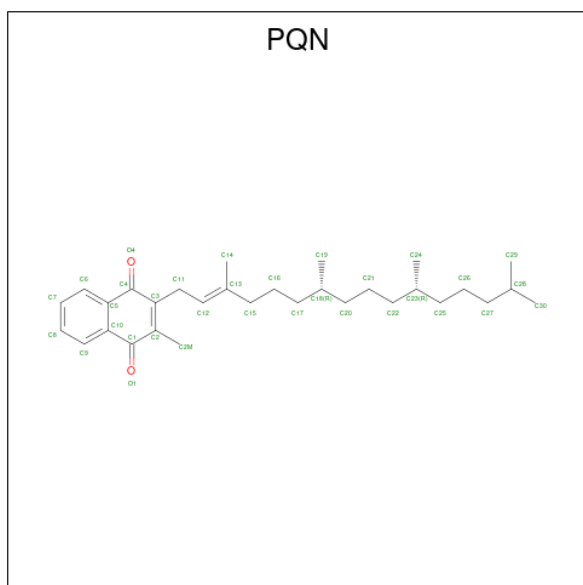
Mol	Chain	Residues	Atoms		AltConf
35	f	1	Total	C	0
			40	40	

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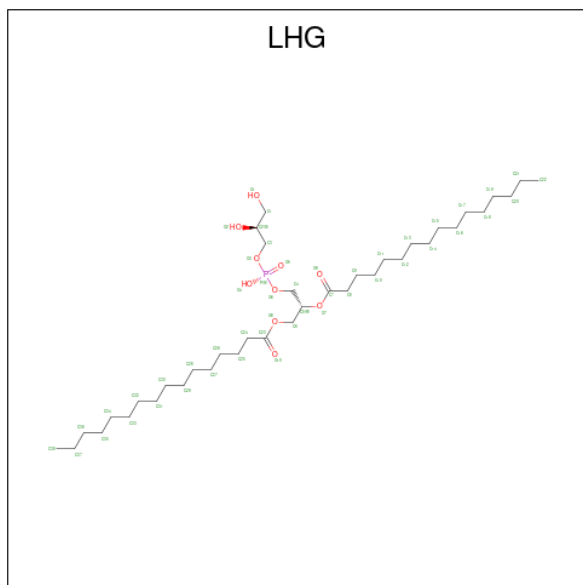
Mol	Chain	Residues	Atoms	AltConf
35	i	1	Total C 40 40	0
35	j	1	Total C 40 40	0
35	l	1	Total C 40 40	0
35	l	1	Total C 40 40	0
35	l	1	Total C 40 40	0
35	m	1	Total C 40 40	0
35	a	1	Total C 40 40	0
35	a	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0

- Molecule 36 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

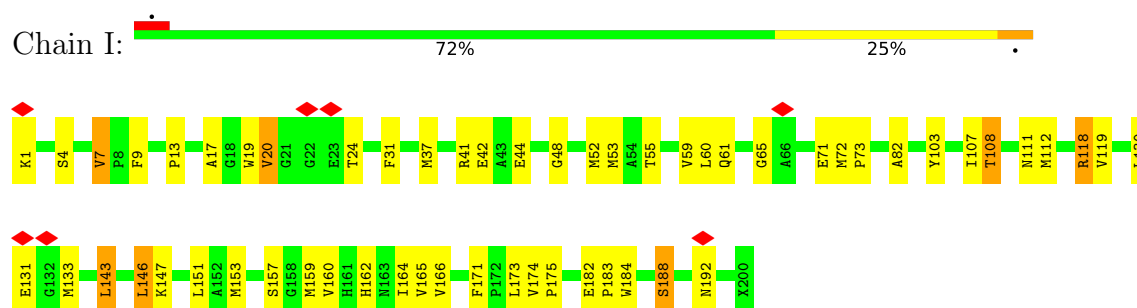


Mol	Chain	Residues	Atoms				AltConf
37	a	1	Total	C	O	P	0
			48	37	10	1	

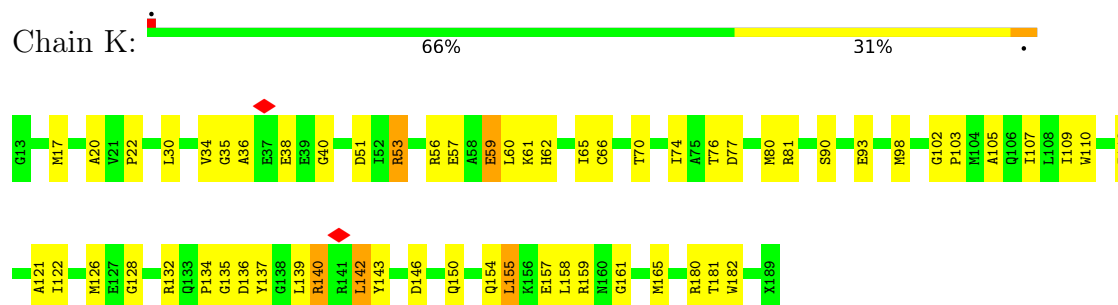
3 Residue-property plots

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

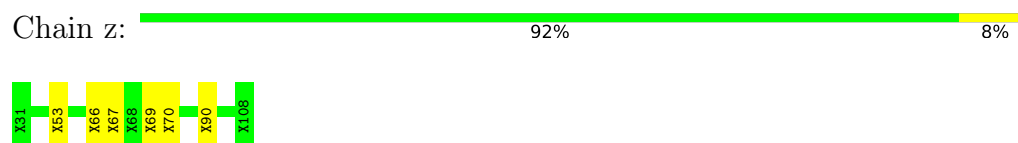
- Molecule 1: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7



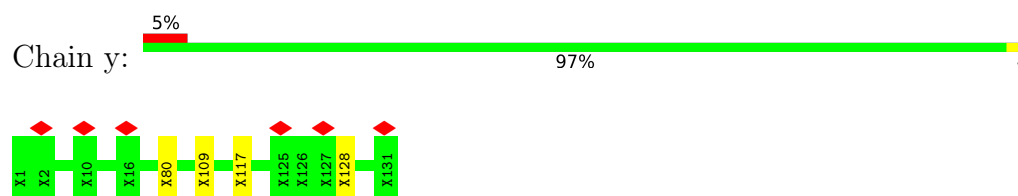
- Molecule 2: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6



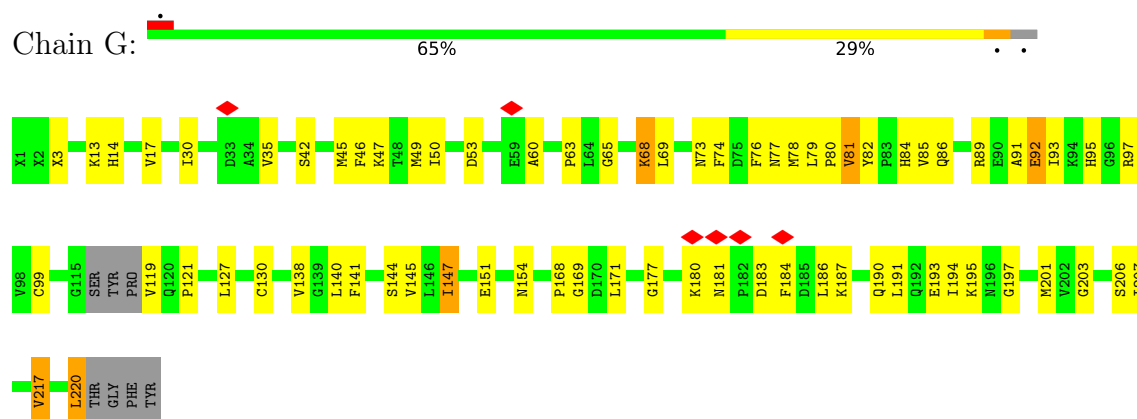
- Molecule 3: Photosystem I unk



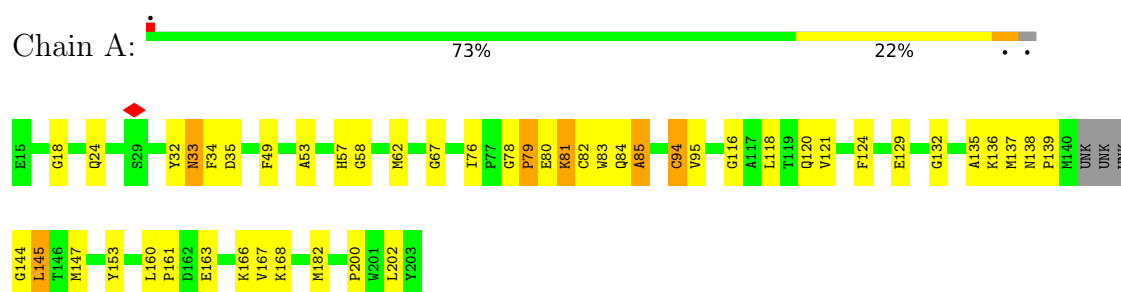
- Molecule 4: Photosystem I unk



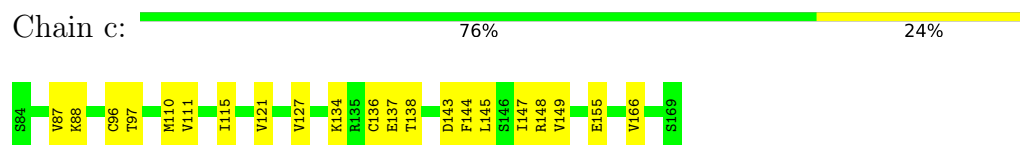
- Molecule 5: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8



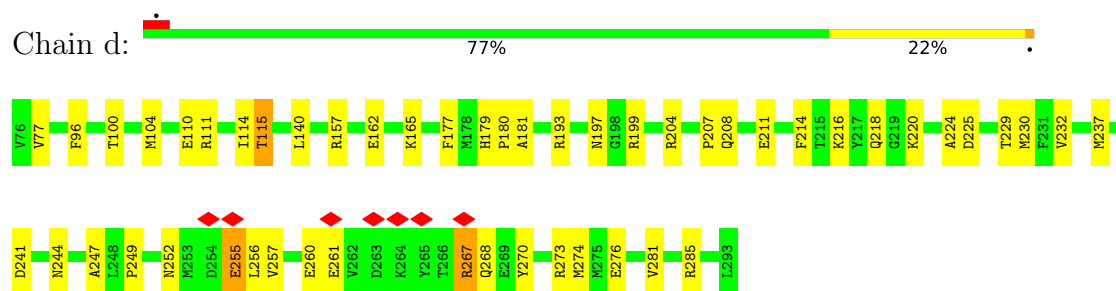
- Molecule 6: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10



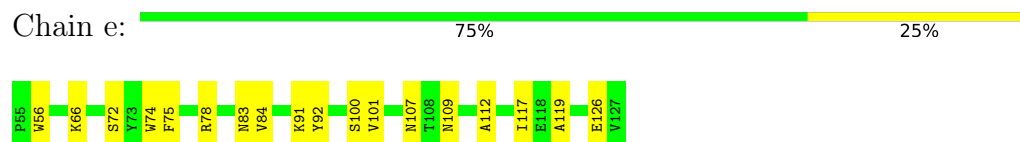
- Molecule 7: Photosystem I Psac



- Molecule 8: Photosystem I Psad

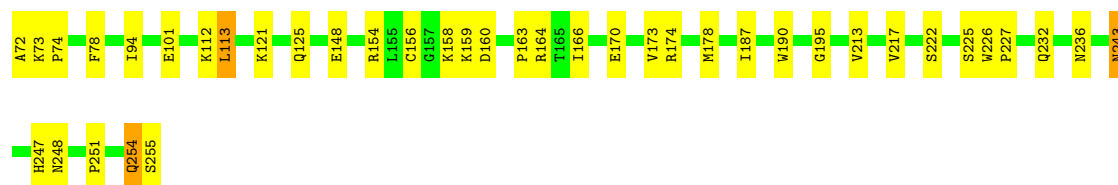


- Molecule 9: Photosystem I Psae



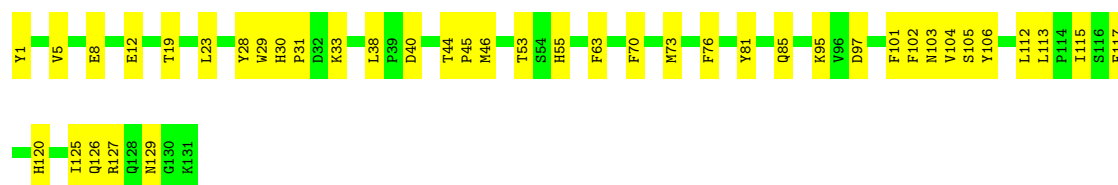
- Molecule 10: Photosystem I Psaf

Chain f:  78% 20%



- Molecule 11: Photosystem I Psar

Chain h:  69% 31%



- Molecule 12: Photosystem I Psal

Chain i:  73% 27%



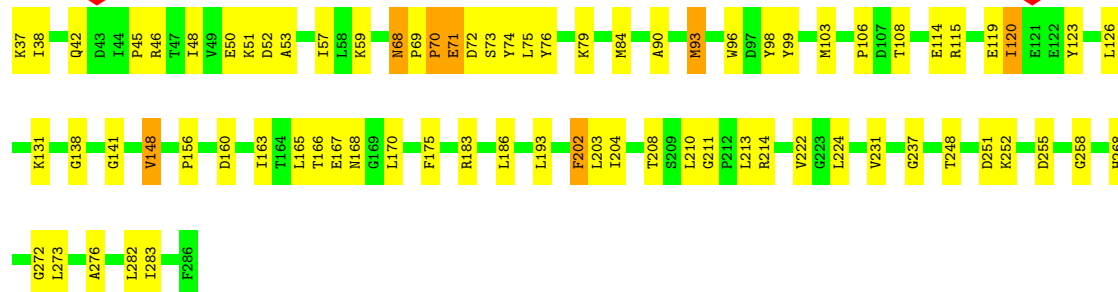
- Molecule 13: Photosystem I Psaj

Chain j:  76% 23%



- Molecule 14: Photosystem I Psal

Chain l:  69% 28%



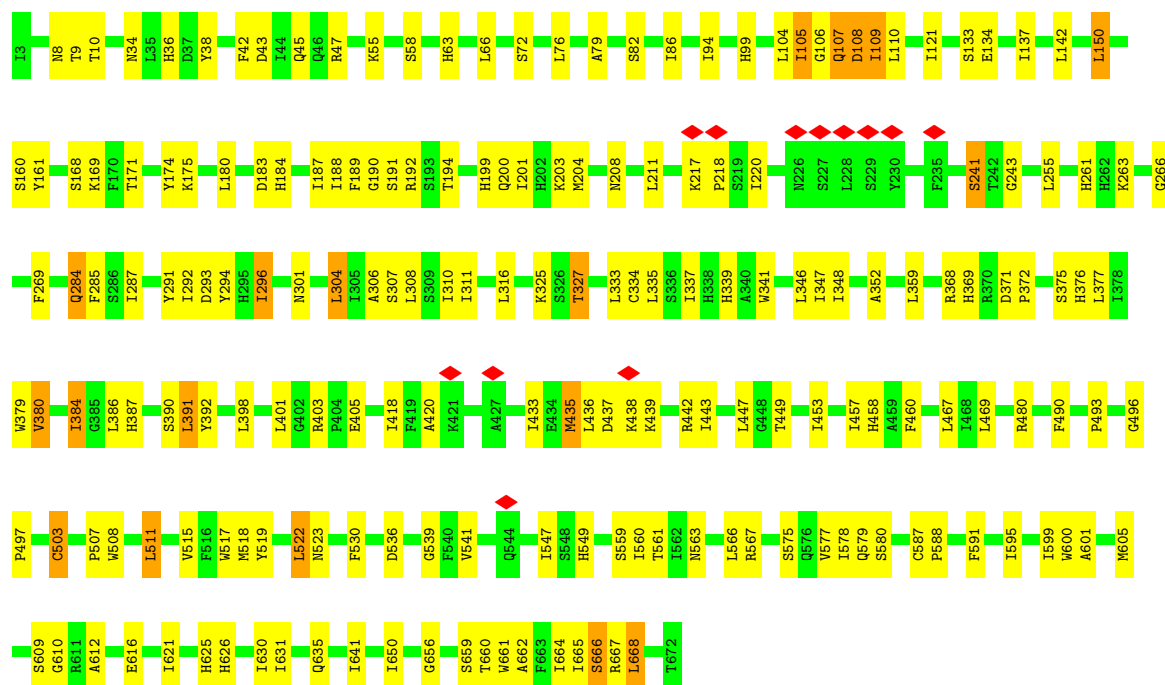
- Molecule 15: Photosystem I Psam

Chain m:  75% 25%



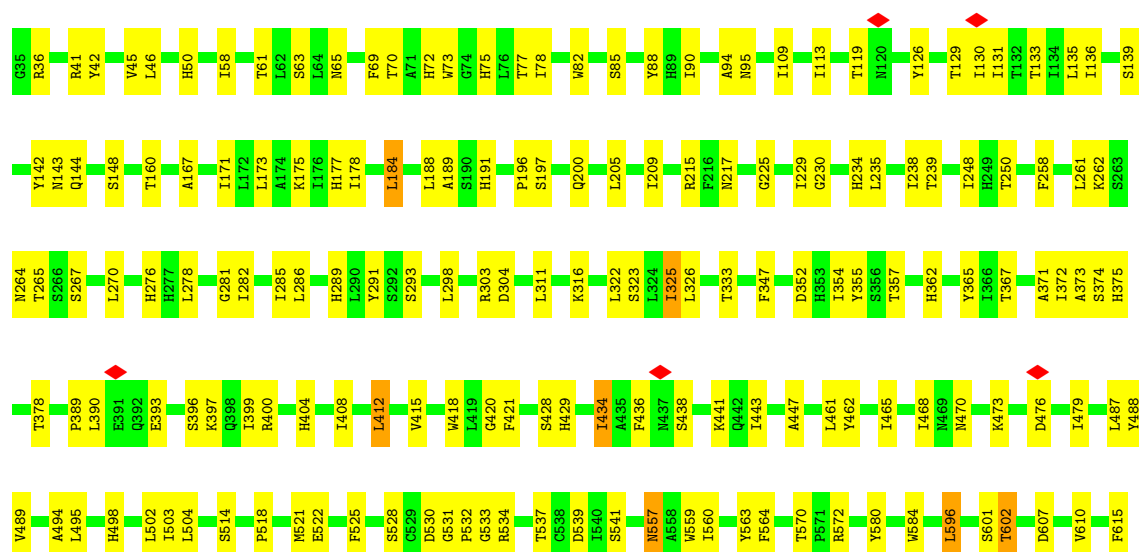
• Molecule 16: Photosystem I PsA

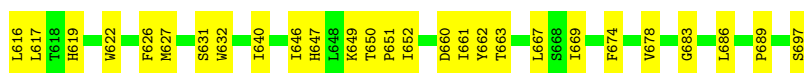
Chain a:  71% 26% .



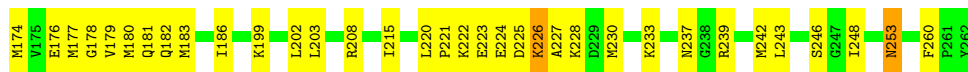
• Molecule 17: Photosystem I PsbB

Chain b:  70% 29% .

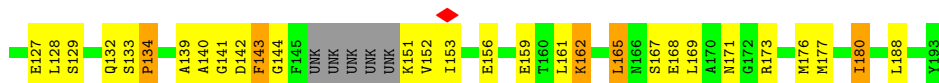




- Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11



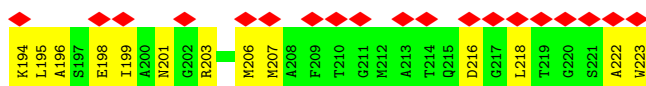
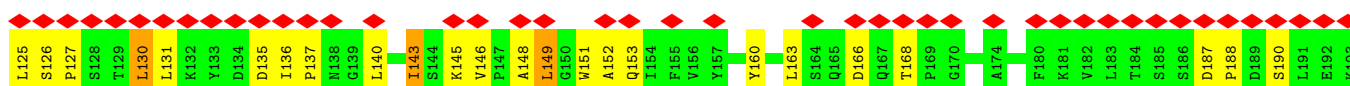
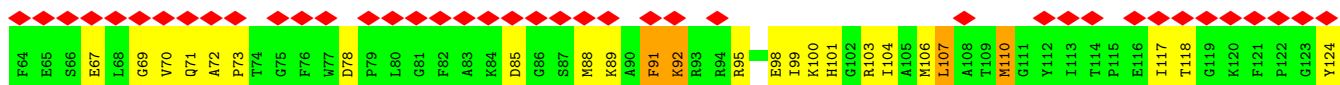
- Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9



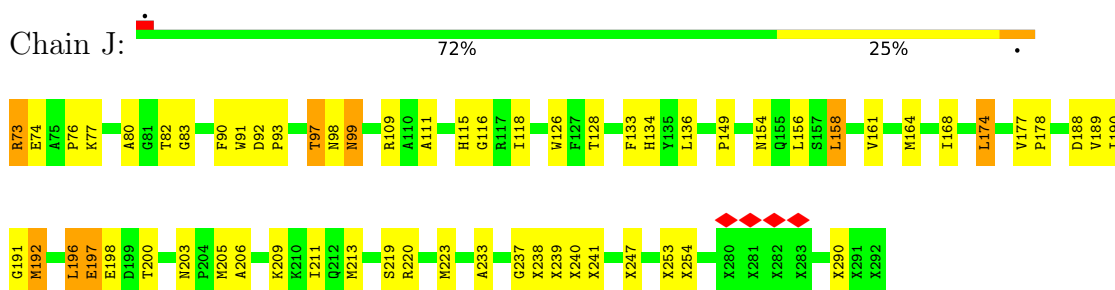
- Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2



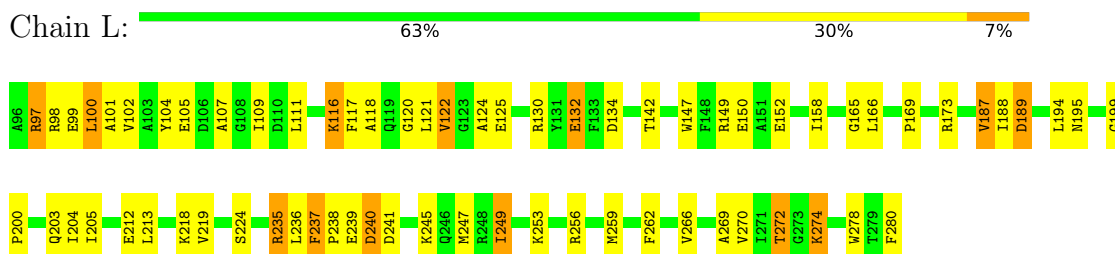
- Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12



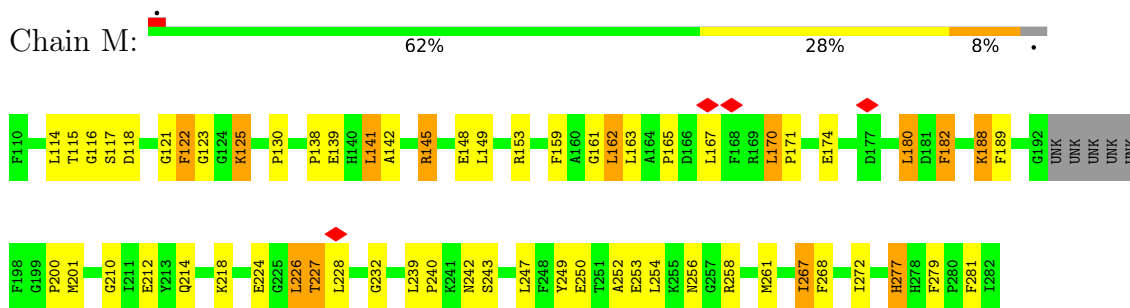
- Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3



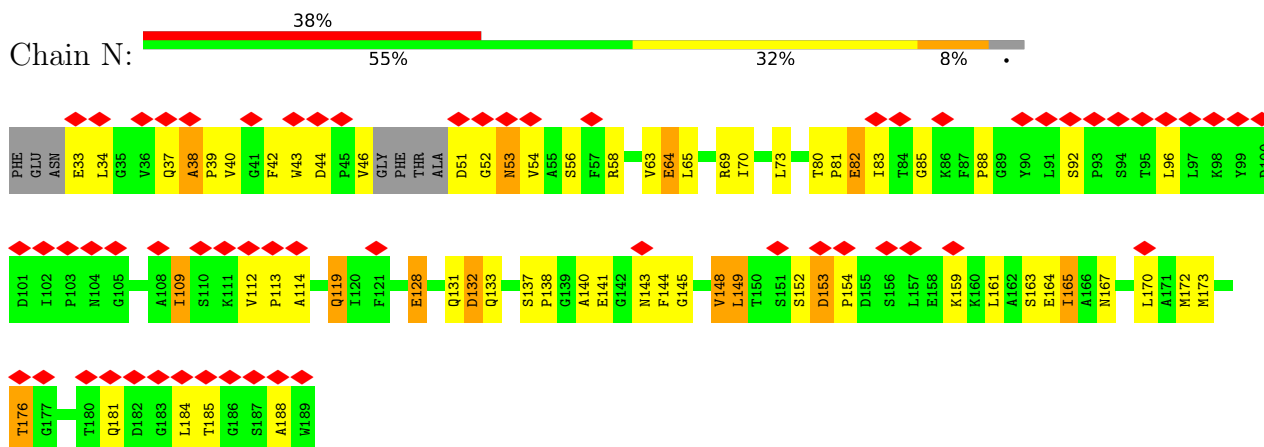
- Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5



- 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	216895	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	1.628	Depositor
Minimum map value	-0.312	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.215	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

5.1 Standard geometry

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

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	0.15	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	0.30	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	0.33	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	0.20	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	0.18	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
All	All	0.22	0/36403	0.39	10/49437 (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	8.96	123.31	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	391	LEU	N-CA-C	-6.94	103.77	111.82
21	H	110	MET	N-CA-C	-6.52	104.18	111.28
20	F	146	TYR	N-CA-C	-6.00	104.41	113.89
20	F	148	PHE	CA-C-N	-5.99	113.77	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	52	0
2	K	1349	0	1323	55	0
3	z	390	0	87	4	0
4	y	655	0	136	3	0
5	G	1572	0	1440	49	0
6	A	1346	0	1242	40	0
7	c	653	0	629	21	0
8	d	1731	0	1741	40	0
9	e	587	0	575	15	0
10	f	1450	0	1437	31	0
11	h	1066	0	1018	34	0
12	i	964	0	941	27	0
13	j	783	0	774	21	0
14	l	1943	0	1919	66	0
15	m	582	0	603	16	0
16	a	5194	0	5023	158	0
17	b	5199	0	5053	171	0
18	B	1452	0	1368	40	0
19	D	1158	0	1114	51	0
20	F	1237	0	1188	36	0
21	H	1202	0	1182	46	0
22	J	1496	0	1233	48	0
23	L	1427	0	1392	51	0
24	M	1211	0	1090	42	0
25	N	993	0	844	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	172	0	0	2	0
26	B	171	0	0	1	0
26	D	43	0	0	0	0
26	F	86	0	0	1	0
26	G	172	0	0	5	0
26	H	43	0	0	1	0
26	I	172	0	0	2	0
26	J	129	0	0	5	0
26	K	215	0	0	0	0
26	L	215	0	0	2	0
26	M	215	0	0	2	0
26	N	43	0	0	0	0
26	b	43	0	0	0	0
26	h	43	0	0	0	0
27	A	47	0	0	1	0
27	B	47	0	0	0	0
27	G	47	0	0	0	0
27	I	47	0	0	2	0
27	J	47	0	0	1	0
27	K	47	0	0	1	0
27	h	47	0	0	0	0
28	A	597	0	493	22	0
28	B	587	0	532	20	0
28	D	317	0	229	18	0
28	F	317	0	227	22	0
28	G	592	0	530	22	0
28	H	343	0	278	15	0
28	I	637	0	554	30	0
28	J	552	0	456	29	0
28	K	496	0	398	17	0
28	L	503	0	411	21	0
28	M	481	0	370	18	0
28	N	256	0	216	10	0
28	a	1870	0	1786	112	0
28	b	1563	0	1526	105	0
28	f	147	0	115	10	0
28	h	55	0	49	0	0
28	j	113	0	104	8	0
28	l	493	0	471	26	0
28	m	60	0	59	2	0
29	A	90	0	0	0	0
29	B	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	D	90	0	0	1	0
29	F	90	0	0	2	0
29	G	45	0	0	0	0
29	H	90	0	0	1	0
29	I	45	0	0	0	0
29	J	45	0	0	0	0
29	K	45	0	0	0	0
29	L	90	0	0	0	0
29	M	90	0	0	1	0
29	N	135	0	0	1	0
30	G	89	0	94	2	0
30	I	39	0	36	0	0
30	L	38	0	34	2	0
30	j	41	0	40	4	0
30	l	50	0	58	0	0
30	y	54	0	66	1	0
31	B	37	0	44	1	0
31	D	49	0	64	5	0
31	I	74	0	88	1	0
31	K	70	0	80	0	0
31	b	75	0	90	4	0
31	j	35	0	40	5	0
32	D	276	0	300	12	0
32	F	184	0	200	12	0
32	G	92	0	100	6	0
32	H	92	0	100	8	0
32	M	46	0	50	1	0
32	N	92	0	100	3	0
32	j	46	0	50	5	0
33	A	50	0	64	8	0
34	a	8	0	0	1	0
34	c	16	0	0	1	0
35	a	80	0	112	5	0
35	b	120	0	168	14	0
35	f	40	0	56	3	0
35	i	40	0	56	5	0
35	j	40	0	56	5	0
35	l	120	0	168	11	0
35	m	40	0	56	5	0
36	a	33	0	46	5	0
36	b	33	0	46	4	0
37	a	48	0	69	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	52237	0	46068	1357	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 1357 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
28:K:308:CLA:H2A	28:K:308:CLA:HED3	1.53	0.89
28:b:712:CLA:H12	18:B:124:ILE:HD11	1.56	0.87
17:b:468:ILE:HG22	17:b:470:ASN:H	1.36	0.87
18:B:124:ILE:HG21	28:B:301:CLA:HHB	1.61	0.82

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%)	164 (86%)	27 (14%)	0	100	100
2	K	171/177 (97%)	160 (94%)	11 (6%)	0	100	100
5	G	204/224 (91%)	176 (86%)	26 (13%)	2 (1%)	12	32
6	A	162/189 (86%)	144 (89%)	14 (9%)	4 (2%)	4	11
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	48
11	h	129/131 (98%)	120 (93%)	9 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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	54
15	m	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
16	a	668/670 (100%)	622 (93%)	43 (6%)	3 (0%)	30	54
17	b	661/663 (100%)	613 (93%)	47 (7%)	1 (0%)	43	68
18	B	171/192 (89%)	153 (90%)	15 (9%)	3 (2%)	6	18
19	D	156/165 (94%)	130 (83%)	23 (15%)	3 (2%)	6	17
20	F	165/176 (94%)	153 (93%)	10 (6%)	2 (1%)	10	27
21	H	158/160 (99%)	140 (89%)	16 (10%)	2 (1%)	9	25
22	J	164/220 (74%)	146 (89%)	17 (10%)	1 (1%)	21	44
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	5
All	All	4587/4792 (96%)	4182 (91%)	376 (8%)	29 (1%)	23	44

5 of 29 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
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	42
2	K	133/138 (96%)	127 (96%)	6 (4%)	24	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	147/171 (86%)	136 (92%)	11 (8%)	12	31
6	A	122/129 (95%)	117 (96%)	5 (4%)	27	56
7	c	76/76 (100%)	75 (99%)	1 (1%)	61	83
8	d	182/184 (99%)	176 (97%)	6 (3%)	33	63
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	87
12	i	100/101 (99%)	99 (99%)	1 (1%)	68	86
13	j	88/89 (99%)	84 (96%)	4 (4%)	24	52
14	l	199/201 (99%)	189 (95%)	10 (5%)	22	48
15	m	60/63 (95%)	59 (98%)	1 (2%)	53	79
16	a	540/592 (91%)	517 (96%)	23 (4%)	26	54
17	b	557/581 (96%)	540 (97%)	17 (3%)	35	65
18	B	142/146 (97%)	123 (87%)	19 (13%)	4	9
19	D	116/123 (94%)	91 (78%)	25 (22%)	1	3
20	F	126/140 (90%)	106 (84%)	20 (16%)	2	7
21	H	123/123 (100%)	111 (90%)	12 (10%)	7	19
22	J	124/136 (91%)	107 (86%)	17 (14%)	3	9
23	L	140/145 (97%)	115 (82%)	25 (18%)	2	5
24	M	106/128 (83%)	86 (81%)	20 (19%)	1	4
25	N	80/124 (64%)	52 (65%)	28 (35%)	0	0
All	All	3623/3870 (94%)	3360 (93%)	263 (7%)	15	32

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	M	247	LEU
25	N	40	VAL
25	N	176	THR
18	B	91	VAL
17	b	651	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
20	F	131	GLN
20	F	166	ASN
22	J	232	GLN
16	a	46	GLN
14	l	280	HIS

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](#)

310 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$
28	CLA	N	309	25	50,54,73	1.35	7 (14%)	59,90,113	1.41	4 (6%)
26	DD6	L	302	-	40,45,45	1.48	2 (5%)	51,67,67	1.97	16 (31%)
26	DD6	F	303	-	40,45,45	1.55	2 (5%)	51,67,67	2.03	14 (27%)
28	CLA	M	316	-	56,60,73	1.32	8 (14%)	65,97,113	1.36	4 (6%)
28	CLA	L	313	-	59,63,73	1.28	7 (11%)	70,101,113	1.31	5 (7%)
28	CLA	a	723	-	69,73,73	1.17	9 (13%)	82,113,113	1.22	5 (6%)
28	CLA	b	710	-	56,60,73	1.32	8 (14%)	65,97,113	1.36	5 (7%)
28	CLA	F	315	-	45,49,73	1.43	6 (13%)	54,84,113	1.52	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	G	512	-	64,68,73	1.23	7 (10%)	76,107,113	1.32	5 (6%)
28	CLA	K	313	-	59,63,73	1.25	6 (10%)	70,101,113	1.32	7 (10%)
32	PID	G	507	-	43,49,49	1.25	3 (6%)	52,76,76	1.34	7 (13%)
32	PID	D	304	-	43,49,49	1.23	3 (6%)	52,76,76	1.72	7 (13%)
28	CLA	G	516	5	45,49,73	1.43	6 (13%)	54,84,113	1.48	5 (9%)
28	CLA	M	309	24	59,63,73	1.27	6 (10%)	70,101,113	1.30	5 (7%)
29	KC1	I	314	1	49,53,53	1.32	6 (12%)	61,89,89	1.75	15 (24%)
31	LMG	I	320	-	38,38,55	0.80	0	46,46,63	1.29	6 (13%)
28	CLA	H	304	-	51,55,73	1.36	6 (11%)	60,91,113	1.38	5 (8%)
26	DD6	L	304	-	40,45,45	1.55	2 (5%)	51,67,67	1.81	12 (23%)
28	CLA	l	312	-	50,54,73	1.36	7 (14%)	59,90,113	1.34	4 (6%)
28	CLA	M	308	29	57,61,73	1.30	8 (14%)	67,98,113	1.38	6 (8%)
28	CLA	H	308	-	50,54,73	1.38	7 (14%)	59,90,113	1.41	4 (6%)
28	CLA	L	316	-	45,49,73	1.42	7 (15%)	54,84,113	1.48	5 (9%)
31	LMG	K	318	-	43,43,55	0.81	1 (2%)	51,51,63	1.32	6 (11%)
31	LMG	I	318	-	36,36,55	0.89	1 (2%)	44,44,63	1.25	3 (6%)
31	LMG	j	101	-	35,35,55	0.87	1 (2%)	43,43,63	1.23	4 (9%)
28	CLA	B	308	-	49,53,73	1.39	5 (10%)	58,89,113	1.44	4 (6%)
28	CLA	L	312	-	50,54,73	1.37	7 (14%)	59,90,113	1.40	4 (6%)
29	KC1	G	515	5	49,53,53	1.35	6 (12%)	61,89,89	1.71	14 (22%)
28	CLA	I	308	-	64,68,73	1.23	8 (12%)	76,107,113	1.29	7 (9%)
28	CLA	a	728	-	59,63,73	1.27	8 (13%)	70,101,113	1.34	6 (8%)
28	CLA	B	310	-	59,63,73	1.27	7 (11%)	70,101,113	1.32	7 (10%)
28	CLA	a	729	-	60,64,73	1.26	6 (10%)	71,102,113	1.30	6 (8%)
26	DD6	h	203	-	40,45,45	1.55	2 (5%)	51,67,67	1.86	12 (23%)
28	CLA	b	715	-	64,68,73	1.22	5 (7%)	76,107,113	1.31	6 (7%)
26	DD6	L	305	-	40,45,45	1.55	2 (5%)	51,67,67	1.93	14 (27%)
28	CLA	F	307	-	50,54,73	1.37	8 (16%)	59,90,113	1.43	4 (6%)
29	KC1	N	306	-	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
26	DD6	M	304	-	40,45,45	1.59	3 (7%)	51,67,67	1.92	14 (27%)
28	CLA	I	312	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	5 (6%)
26	DD6	B	306	-	40,45,45	1.55	2 (5%)	51,67,67	1.95	19 (37%)
28	CLA	a	718	-	50,54,73	1.36	6 (12%)	59,90,113	1.41	4 (6%)
28	CLA	a	715	-	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
28	CLA	a	725	-	65,69,73	1.21	7 (10%)	77,108,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	319	-	50,54,73	1.36	7 (14%)	59,90,113	1.35	4 (6%)
26	DD6	M	303	-	40,45,45	1.76	4 (10%)	51,67,67	2.19	18 (35%)
28	CLA	N	305	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
27	UIX	I	304	-	43,49,49	1.41	6 (13%)	53,74,74	2.50	16 (30%)
31	LMG	K	317	-	27,27,55	0.99	1 (3%)	35,35,63	1.19	4 (11%)
32	PID	F	305	-	43,49,49	1.25	4 (9%)	52,76,76	1.83	8 (15%)
28	CLA	L	314	-	57,61,73	1.29	8 (14%)	67,98,113	1.36	6 (8%)
28	CLA	H	311	-	45,49,73	1.44	7 (15%)	54,84,113	1.44	5 (9%)
36	PQN	a	732	-	34,34,34	1.60	2 (5%)	43,45,45	1.15	4 (9%)
28	CLA	B	313	18	69,73,73	1.16	7 (10%)	82,113,113	1.27	4 (4%)
28	CLA	K	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.49	7 (12%)
29	KC1	F	309	20	49,53,53	1.35	6 (12%)	61,89,89	1.79	14 (22%)
28	CLA	l	311	-	69,73,73	1.18	6 (8%)	82,113,113	1.26	5 (6%)
26	DD6	L	306	-	40,45,45	1.54	2 (5%)	51,67,67	2.03	15 (29%)
28	CLA	a	708	-	55,59,73	1.32	7 (12%)	64,96,113	1.38	6 (9%)
28	CLA	G	517	-	50,54,73	1.36	6 (12%)	59,90,113	1.39	4 (6%)
28	CLA	K	307	-	50,54,73	1.34	7 (14%)	59,90,113	1.42	5 (8%)
28	CLA	a	713	-	64,68,73	1.21	7 (10%)	76,107,113	1.27	6 (7%)
28	CLA	J	311	22	51,55,73	1.36	6 (11%)	60,91,113	1.41	6 (10%)
28	CLA	D	314	-	50,54,73	1.40	8 (16%)	59,90,113	1.46	6 (10%)
28	CLA	a	735	-	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
28	CLA	h	202	-	59,63,73	1.28	7 (11%)	70,101,113	1.33	5 (7%)
30	DGD	L	301	-	39,39,67	0.96	2 (5%)	53,53,81	0.99	2 (3%)
28	CLA	G	511	-	59,63,73	1.28	7 (11%)	70,101,113	1.32	5 (7%)
29	KC1	H	310	-	49,53,53	1.35	5 (10%)	61,89,89	1.72	13 (21%)
28	CLA	M	312	-	52,56,73	1.35	8 (15%)	61,92,113	1.40	6 (9%)
28	CLA	D	308	-	51,55,73	1.36	7 (13%)	60,91,113	1.37	4 (6%)
26	DD6	B	304	-	40,45,45	1.54	2 (5%)	51,67,67	1.88	12 (23%)
34	SF4	c	201	7	0,12,12	-	-	-	-	-
28	CLA	l	313	14	69,73,73	1.19	6 (8%)	82,113,113	1.29	5 (6%)
28	CLA	M	318	-	50,54,73	1.38	8 (16%)	59,90,113	1.37	4 (6%)
35	BCR	a	734	-	41,41,41	0.65	0	56,56,56	2.08	20 (35%)
32	PID	D	305	-	43,49,49	1.26	3 (6%)	52,76,76	1.46	9 (17%)
26	DD6	G	505	-	40,45,45	1.84	3 (7%)	51,67,67	2.31	19 (37%)
28	CLA	B	316	-	50,54,73	1.37	7 (14%)	59,90,113	1.35	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	b	703	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	6 (7%)
30	DGD	I	317	-	40,40,67	1.10	2 (5%)	54,54,81	1.00	4 (7%)
30	DGD	y	201	-	55,55,67	0.93	2 (3%)	69,69,81	0.97	3 (4%)
28	CLA	a	716	-	51,55,73	1.35	6 (11%)	60,91,113	1.40	5 (8%)
28	CLA	a	705	28	59,63,73	1.27	7 (11%)	70,101,113	1.38	7 (10%)
28	CLA	G	520	-	53,57,73	1.32	7 (13%)	61,93,113	1.35	7 (11%)
28	CLA	M	317	-	50,54,73	1.36	6 (12%)	59,90,113	1.43	5 (8%)
28	CLA	b	708	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
26	DD6	M	302	-	40,45,45	1.74	3 (7%)	51,67,67	2.23	18 (35%)
28	CLA	K	308	2	58,62,73	1.27	6 (10%)	68,99,113	1.33	6 (8%)
28	CLA	A	308	-	59,63,73	1.26	7 (11%)	70,101,113	1.32	6 (8%)
30	DGD	j	103	-	42,42,67	1.06	2 (4%)	56,56,81	1.01	3 (5%)
28	CLA	D	311	-	50,54,73	1.36	5 (10%)	59,90,113	1.41	4 (6%)
28	CLA	a	724	-	69,73,73	1.19	8 (11%)	82,113,113	1.29	8 (9%)
28	CLA	a	720	-	66,70,73	1.20	7 (10%)	78,109,113	1.29	6 (7%)
33	SQD	A	318	-	48,50,54	0.41	1 (2%)	58,61,65	0.58	0
28	CLA	b	718	-	55,59,73	1.34	6 (10%)	64,96,113	1.41	6 (9%)
26	DD6	K	301	-	40,45,45	1.53	2 (5%)	51,67,67	1.93	15 (29%)
28	CLA	a	707	-	69,73,73	1.19	6 (8%)	82,113,113	1.21	5 (6%)
28	CLA	f	302	-	50,54,73	1.37	7 (14%)	59,90,113	1.39	5 (8%)
29	KC1	N	311	25	49,53,53	1.33	5 (10%)	61,89,89	1.72	13 (21%)
28	CLA	A	312	-	59,63,73	1.27	7 (11%)	70,101,113	1.30	5 (7%)
28	CLA	L	310	-	59,63,73	1.27	6 (10%)	70,101,113	1.33	6 (8%)
26	DD6	I	301	-	40,45,45	1.57	2 (5%)	51,67,67	2.17	17 (33%)
28	CLA	A	310	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	5 (6%)
28	CLA	a	706	16	62,66,73	1.23	7 (11%)	73,104,113	1.31	4 (5%)
28	CLA	l	303	14	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
35	BCR	l	307	-	41,41,41	0.68	0	56,56,56	2.03	19 (33%)
28	CLA	f	301	-	59,63,73	1.27	7 (11%)	70,101,113	1.32	5 (7%)
34	SF4	a	737	17,16	0,12,12	-	-	-	-	-
28	CLA	I	310	-	52,56,73	1.34	6 (11%)	61,92,113	1.42	6 (9%)
28	CLA	a	702	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	5 (6%)
29	KC1	A	314	6	49,53,53	1.33	6 (12%)	61,89,89	1.73	14 (22%)
28	CLA	l	305	-	69,73,73	1.19	8 (11%)	82,113,113	1.26	4 (4%)
27	UIX	J	305	-	43,49,49	1.35	4 (9%)	53,74,74	2.38	18 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	307	29	49,53,73	1.41	6 (12%)	58,89,113	1.44	4 (6%)
29	KC1	A	306	26,28	49,53,53	1.34	6 (12%)	61,89,89	1.70	13 (21%)
37	LHG	a	733	-	47,47,48	0.27	0	50,53,54	0.33	0
32	PID	F	306	-	43,49,49	1.23	3 (6%)	52,76,76	1.43	5 (9%)
28	CLA	m	202	-	64,68,73	1.22	7 (10%)	76,107,113	1.33	6 (7%)
28	CLA	D	309	-	50,54,73	1.35	6 (12%)	59,90,113	1.41	4 (6%)
28	CLA	G	519	-	63,67,73	1.23	7 (11%)	74,105,113	1.30	4 (5%)
35	BCR	a	736	-	41,41,41	0.70	0	56,56,56	2.04	18 (32%)
26	DD6	A	303	-	40,45,45	1.49	2 (5%)	51,67,67	1.80	13 (25%)
28	CLA	I	319	28	49,53,73	1.38	7 (14%)	58,89,113	1.46	7 (12%)
32	PID	N	302	-	43,49,49	1.31	3 (6%)	52,76,76	1.64	10 (19%)
28	CLA	K	309	-	54,58,73	1.31	7 (12%)	64,95,113	1.40	6 (9%)
29	KC1	M	307	28	49,53,53	1.36	6 (12%)	61,89,89	1.80	14 (22%)
28	CLA	b	709	-	64,68,73	1.22	8 (12%)	76,107,113	1.32	7 (9%)
28	CLA	K	310	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	5 (7%)
28	CLA	A	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.47	5 (9%)
28	CLA	b	707	-	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
28	CLA	I	306	1	53,57,73	1.33	6 (11%)	61,93,113	1.43	6 (9%)
28	CLA	K	316	-	50,54,73	1.37	8 (16%)	59,90,113	1.42	5 (8%)
26	DD6	J	303	-	40,45,45	1.87	3 (7%)	51,67,67	2.45	16 (31%)
28	CLA	a	703	-	59,63,73	1.25	10 (16%)	70,101,113	1.45	8 (11%)
26	DD6	M	305	-	40,45,45	1.56	3 (7%)	51,67,67	1.88	16 (31%)
27	UIX	h	201	-	43,49,49	1.41	4 (9%)	53,74,74	2.48	20 (37%)
28	CLA	J	312	-	57,61,73	1.28	9 (15%)	67,98,113	1.42	7 (10%)
26	DD6	K	304	-	40,45,45	1.55	2 (5%)	51,67,67	1.99	15 (29%)
28	CLA	H	307	-	55,59,73	1.31	9 (16%)	64,96,113	1.39	6 (9%)
35	BCR	b	730	-	41,41,41	0.70	0	56,56,56	2.27	20 (35%)
28	CLA	a	731	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
28	CLA	f	303	10	50,54,73	1.36	8 (16%)	59,90,113	1.39	4 (6%)
28	CLA	L	309	-	57,61,73	1.29	5 (8%)	67,98,113	1.37	6 (8%)
28	CLA	N	304	-	51,55,73	1.37	7 (13%)	60,91,113	1.40	5 (8%)
28	CLA	a	726	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	7 (8%)
26	DD6	A	301	-	40,45,45	1.53	2 (5%)	51,67,67	2.05	14 (27%)
28	CLA	I	307	-	50,54,73	1.36	6 (12%)	59,90,113	1.39	4 (6%)
28	CLA	K	311	-	56,60,73	1.31	7 (12%)	65,97,113	1.34	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	a	727	-	50,54,73	1.37	7 (14%)	59,90,113	1.36	4 (6%)
28	CLA	K	306	2	53,57,73	1.34	7 (13%)	61,93,113	1.41	6 (9%)
26	DD6	N	303	-	40,45,45	1.53	2 (5%)	51,67,67	2.07	17 (33%)
28	CLA	I	309	-	59,63,73	1.28	7 (11%)	70,101,113	1.33	6 (8%)
32	PID	D	307	-	43,49,49	1.22	4 (9%)	52,76,76	1.36	5 (9%)
26	DD6	M	306	-	40,45,45	1.70	2 (5%)	51,67,67	2.22	20 (39%)
28	CLA	b	706	-	52,56,73	1.36	6 (11%)	61,92,113	1.37	6 (9%)
26	DD6	G	502	-	40,45,45	1.53	2 (5%)	51,67,67	1.87	11 (21%)
26	DD6	D	303	-	40,45,45	1.49	2 (5%)	51,67,67	1.83	14 (27%)
28	CLA	A	313	-	59,63,73	1.26	6 (10%)	70,101,113	1.32	6 (8%)
28	CLA	l	308	-	45,49,73	1.43	7 (15%)	54,84,113	1.45	5 (9%)
28	CLA	b	712	-	58,62,73	1.36	9 (15%)	71,100,113	1.38	6 (8%)
28	CLA	B	307	18	53,57,73	1.35	7 (13%)	61,93,113	1.37	5 (8%)
26	DD6	J	304	-	40,45,45	1.80	4 (10%)	51,67,67	2.14	19 (37%)
28	CLA	G	518	-	50,54,73	1.39	8 (16%)	59,90,113	1.44	5 (8%)
28	CLA	j	106	-	62,66,73	1.24	8 (12%)	73,104,113	1.33	6 (8%)
28	CLA	J	307	-	69,73,73	1.17	7 (10%)	82,113,113	1.31	4 (4%)
28	CLA	l	310	-	39,50,73	2.85	12 (30%)	32,76,113	1.72	6 (18%)
32	PID	F	304	-	43,49,49	1.24	3 (6%)	52,76,76	1.90	9 (17%)
28	CLA	b	728	-	69,73,73	1.18	7 (10%)	82,113,113	1.29	5 (6%)
26	DD6	J	302	-	40,45,45	1.54	1 (2%)	51,67,67	2.07	14 (27%)
28	CLA	J	301	-	64,68,73	1.22	7 (10%)	76,107,113	1.29	5 (6%)
35	BCR	b	732	-	41,41,41	0.72	0	56,56,56	1.90	18 (32%)
27	UIX	B	305	-	43,49,49	1.36	4 (9%)	53,74,74	2.39	17 (32%)
28	CLA	a	722	-	62,66,73	1.24	7 (11%)	73,104,113	1.30	8 (10%)
26	DD6	L	303	-	40,45,45	1.50	2 (5%)	51,67,67	1.94	14 (27%)
28	CLA	A	316	-	51,55,73	1.35	7 (13%)	60,91,113	1.38	5 (8%)
28	CLA	H	312	-	50,54,73	1.38	7 (14%)	59,90,113	1.39	4 (6%)
28	CLA	a	701	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
28	CLA	B	311	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	5 (6%)
28	CLA	G	513	5	69,73,73	1.18	8 (11%)	82,113,113	1.27	7 (8%)
28	CLA	D	313	19	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
28	CLA	I	311	1	59,63,73	1.28	6 (10%)	70,101,113	1.34	6 (8%)
28	CLA	A	309	-	59,63,73	1.27	6 (10%)	70,101,113	1.32	6 (8%)
27	UIX	A	304	-	43,49,49	1.36	4 (9%)	53,74,74	2.42	21 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	A	305	29	40,45,45	1.52	2 (5%)	51,67,67	1.89	14 (27%)
28	CLA	a	721	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
30	DGD	G	521	-	45,45,67	1.03	2 (4%)	59,59,81	1.46	8 (13%)
28	CLA	a	704	-	69,73,73	1.18	7 (10%)	82,113,113	1.17	2 (2%)
28	CLA	b	727	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
29	KC1	H	306	-	49,53,53	1.32	5 (10%)	61,89,89	1.72	13 (21%)
35	BCR	b	702	-	41,41,41	0.66	0	56,56,56	2.19	16 (28%)
28	CLA	L	308	29	49,55,73	1.38	7 (14%)	62,91,113	1.39	7 (11%)
31	LMG	B	318	-	37,37,55	0.85	0	45,45,63	1.34	6 (13%)
28	CLA	I	315	-	56,60,73	1.31	7 (12%)	65,97,113	1.37	7 (10%)
28	CLA	J	314	-	45,49,73	1.43	6 (13%)	54,84,113	1.48	6 (11%)
28	CLA	b	711	-	59,63,73	1.27	5 (8%)	70,101,113	1.31	6 (8%)
27	UIX	G	503	-	43,49,49	1.33	4 (9%)	53,74,74	2.33	19 (35%)
28	CLA	b	713	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	6 (7%)
28	CLA	a	711	-	49,53,73	1.38	7 (14%)	58,89,113	1.46	7 (12%)
28	CLA	a	714	-	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
32	PID	H	301	-	43,49,49	1.24	3 (6%)	52,76,76	1.58	7 (13%)
32	PID	G	506	-	43,49,49	1.28	3 (6%)	52,76,76	1.35	7 (13%)
35	BCR	l	306	-	41,41,41	0.68	0	56,56,56	1.93	12 (21%)
28	CLA	a	719	-	51,55,73	1.36	9 (17%)	60,91,113	1.36	5 (8%)
28	CLA	L	318	-	50,54,73	1.36	8 (16%)	59,90,113	1.41	4 (6%)
28	CLA	a	712	28	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
28	CLA	G	510	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	7 (8%)
29	KC1	K	314	2	49,53,53	1.33	6 (12%)	61,89,89	1.70	12 (19%)
26	DD6	H	303	-	40,45,45	1.54	3 (7%)	51,67,67	1.92	13 (25%)
28	CLA	J	315	-	50,54,73	1.37	7 (14%)	59,90,113	1.41	4 (6%)
26	DD6	G	508	-	40,45,45	1.55	2 (5%)	51,67,67	2.01	14 (27%)
26	DD6	A	302	-	40,45,45	1.59	3 (7%)	51,67,67	2.10	15 (29%)
29	KC1	N	308	-	49,53,53	1.43	6 (12%)	61,89,89	2.04	15 (24%)
28	CLA	B	317	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
26	DD6	B	302	-	39,44,45	1.74	2 (5%)	49,65,67	2.08	17 (34%)
35	BCR	i	201	-	41,41,41	0.78	2 (4%)	56,56,56	2.14	21 (37%)
26	DD6	K	303	-	40,45,45	1.65	3 (7%)	51,67,67	1.73	13 (25%)
32	PID	M	301	-	43,49,49	1.22	3 (6%)	52,76,76	1.68	9 (17%)
29	KC1	D	310	-	49,53,53	1.34	6 (12%)	61,89,89	1.74	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	I	316	-	59,63,73	1.25	5 (8%)	70,101,113	1.34	7 (10%)
28	CLA	M	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.38	4 (6%)
28	CLA	F	308	-	50,54,73	1.35	8 (16%)	59,90,113	1.39	4 (6%)
31	LMG	D	317	-	48,48,55	0.76	1 (2%)	55,55,63	1.29	5 (9%)
28	CLA	I	313	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	7 (10%)
29	KC1	F	314	20	49,53,53	1.35	5 (10%)	61,89,89	1.73	13 (21%)
26	DD6	B	303	-	40,45,45	1.51	2 (5%)	51,67,67	1.89	13 (25%)
26	DD6	I	303	-	40,45,45	1.83	5 (12%)	51,67,67	2.02	16 (31%)
31	LMG	b	733	-	44,44,55	0.82	1 (2%)	52,52,63	1.31	7 (13%)
28	CLA	G	514	-	57,61,73	1.28	8 (14%)	67,98,113	1.37	6 (8%)
32	PID	D	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.44	7 (13%)
28	CLA	F	310	-	50,54,73	1.36	6 (12%)	59,90,113	1.47	5 (8%)
28	CLA	G	509	5	55,59,73	1.32	6 (10%)	64,96,113	1.38	5 (7%)
28	CLA	l	309	-	45,49,73	1.43	6 (13%)	54,84,113	1.47	5 (9%)
28	CLA	b	721	26	50,54,73	1.37	8 (16%)	59,90,113	1.34	4 (6%)
28	CLA	b	701	-	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)
28	CLA	N	310	-	51,55,73	1.38	7 (13%)	60,91,113	1.51	6 (10%)
28	CLA	l	304	-	64,68,73	1.21	5 (7%)	76,107,113	1.34	5 (6%)
28	CLA	F	312	-	50,54,73	1.33	8 (16%)	59,90,113	1.37	4 (6%)
28	CLA	K	312	-	52,56,73	1.35	8 (15%)	61,92,113	1.38	5 (8%)
28	CLA	b	705	-	69,73,73	1.17	7 (10%)	82,113,113	1.26	6 (7%)
35	BCR	j	102	-	41,41,41	0.65	0	56,56,56	2.02	16 (28%)
26	DD6	K	319	-	40,45,45	1.54	2 (5%)	51,67,67	2.05	13 (25%)
28	CLA	b	725	-	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
28	CLA	L	311	-	59,63,73	1.27	6 (10%)	70,101,113	1.34	5 (7%)
28	CLA	b	724	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
28	CLA	b	720	-	57,61,73	1.27	7 (12%)	67,98,113	1.32	5 (7%)
28	CLA	I	321	28	56,60,73	1.31	6 (10%)	65,97,113	1.46	7 (10%)
28	CLA	B	312	-	55,59,73	1.32	7 (12%)	64,96,113	1.37	5 (7%)
32	PID	N	301	-	43,49,49	1.25	3 (6%)	52,76,76	1.44	6 (11%)
29	KC1	M	314	24	49,53,53	1.34	5 (10%)	61,89,89	1.73	14 (22%)
26	DD6	K	305	-	40,45,45	1.51	2 (5%)	51,67,67	1.86	15 (29%)
26	DD6	G	504	-	40,45,45	1.83	6 (15%)	51,67,67	2.12	19 (37%)
28	CLA	H	305	-	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
28	CLA	N	307	-	55,59,73	1.32	8 (14%)	64,96,113	1.35	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DD6	b	731	28	40,45,45	1.61	2 (5%)	51,67,67	1.98	17 (33%)
28	CLA	J	310	-	50,54,73	1.39	8 (16%)	59,90,113	1.37	4 (6%)
28	CLA	a	717	-	61,65,73	1.26	8 (13%)	72,103,113	1.30	7 (9%)
28	CLA	B	301	-	64,68,73	1.23	6 (9%)	76,107,113	1.26	5 (6%)
28	CLA	b	723	-	54,58,73	1.32	8 (14%)	64,95,113	1.38	7 (10%)
32	PID	D	302	-	43,49,49	1.26	3 (6%)	52,76,76	1.40	9 (17%)
26	DD6	I	305	-	40,45,45	1.80	4 (10%)	51,67,67	2.24	17 (33%)
28	CLA	H	309	-	51,55,73	1.35	6 (11%)	60,91,113	1.40	5 (8%)
26	DD6	I	302	-	40,45,45	1.60	2 (5%)	51,67,67	2.16	18 (35%)
28	CLA	M	315	-	45,49,73	1.42	6 (13%)	54,84,113	1.56	8 (14%)
28	CLA	J	308	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	6 (10%)
30	DGD	l	301	-	51,51,67	0.96	2 (3%)	65,65,81	0.89	2 (3%)
36	PQN	b	729	-	34,34,34	1.58	2 (5%)	43,45,45	1.28	5 (11%)
32	PID	j	105	-	43,49,49	1.28	4 (9%)	52,76,76	1.54	11 (21%)
28	CLA	a	730	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
32	PID	H	302	-	43,49,49	1.29	3 (6%)	52,76,76	1.39	9 (17%)
28	CLA	a	738	22	50,54,73	1.37	5 (10%)	59,90,113	1.45	5 (8%)
30	DGD	G	501	-	46,46,67	1.02	2 (4%)	60,60,81	1.01	4 (6%)
35	BCR	m	201	-	41,41,41	0.68	0	56,56,56	2.35	17 (30%)
35	BCR	l	302	-	41,41,41	0.68	0	56,56,56	2.20	22 (39%)
26	DD6	F	301	-	40,45,45	1.53	2 (5%)	51,67,67	2.31	16 (31%)
28	CLA	D	312	19	50,54,73	1.37	8 (16%)	59,90,113	1.37	4 (6%)
28	CLA	F	313	-	50,54,73	1.38	7 (14%)	59,90,113	1.48	6 (10%)
29	KC1	D	315	19	49,53,53	1.32	6 (12%)	61,89,89	1.73	15 (24%)
28	CLA	a	710	16	59,63,73	1.28	8 (13%)	70,101,113	1.35	7 (10%)
28	CLA	J	309	-	60,64,73	1.25	8 (13%)	71,102,113	1.39	6 (8%)
28	CLA	A	320	-	50,54,73	1.38	8 (16%)	59,90,113	1.41	4 (6%)
28	CLA	J	306	-	50,54,73	1.37	7 (14%)	59,90,113	1.42	4 (6%)
28	CLA	F	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.44	5 (8%)
29	KC1	B	314	18	49,53,53	1.33	5 (10%)	61,89,89	1.71	13 (21%)
28	CLA	j	104	-	59,63,73	1.29	7 (11%)	70,101,113	1.30	6 (8%)
28	CLA	b	704	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
28	CLA	b	716	-	54,58,73	1.32	7 (12%)	64,95,113	1.39	5 (7%)
28	CLA	b	717	-	69,73,73	1.19	8 (11%)	82,113,113	1.22	5 (6%)
28	CLA	D	316	-	45,49,73	1.43	7 (15%)	54,84,113	1.47	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	M	310	-	52,56,73	1.35	6 (11%)	61,92,113	1.39	5 (8%)
32	PID	F	302	-	43,49,49	1.24	3 (6%)	52,76,76	1.59	7 (13%)
28	CLA	b	714	-	50,54,73	1.37	7 (14%)	59,90,113	1.42	5 (8%)
35	BCR	f	304	-	41,41,41	0.67	0	56,56,56	2.08	17 (30%)
27	UIX	K	302	-	43,49,49	1.40	4 (9%)	53,74,74	2.71	22 (41%)
28	CLA	b	726	-	51,55,73	1.36	7 (13%)	60,91,113	1.36	5 (8%)
28	CLA	a	709	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
28	CLA	B	315	-	45,49,73	1.41	7 (15%)	54,84,113	1.52	5 (9%)
28	CLA	M	313	-	50,54,73	1.37	7 (14%)	59,90,113	1.37	4 (6%)
31	LMG	b	734	-	31,31,55	0.99	1 (3%)	39,39,63	1.18	4 (10%)
29	KC1	J	313	-	49,53,53	1.34	6 (12%)	61,89,89	1.71	13 (21%)
34	SF4	c	202	7	0,12,12	-	-	-	-	-
32	PID	D	306	-	43,49,49	1.25	3 (6%)	52,76,76	1.37	5 (9%)
28	CLA	b	719	-	50,54,73	1.37	8 (16%)	59,90,113	1.44	4 (6%)
29	KC1	L	307	28	49,53,53	1.33	5 (10%)	61,89,89	1.74	15 (24%)
28	CLA	J	316	-	50,54,73	1.38	7 (14%)	59,90,113	1.38	4 (6%)
28	CLA	A	311	6	50,54,73	1.37	7 (14%)	59,90,113	1.38	4 (6%)
28	CLA	L	317	-	56,60,73	1.32	7 (12%)	65,97,113	1.37	6 (9%)
28	CLA	B	309	18	69,73,73	1.17	6 (8%)	82,113,113	1.26	6 (7%)
28	CLA	A	317	-	45,49,73	1.42	7 (15%)	54,84,113	1.49	6 (11%)
29	KC1	L	315	-	49,53,53	1.35	6 (12%)	61,89,89	1.75	14 (22%)
28	CLA	b	722	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	7 (8%)

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
28	CLA	N	309	25	1/1/11/20	4/17/93/115	-
26	DD6	L	302	-	-	4/26/80/80	0/3/3/3
28	CLA	M	316	-	1/1/12/20	10/24/100/115	-
26	DD6	F	303	-	-	2/26/80/80	0/3/3/3
28	CLA	L	313	-	1/1/13/20	11/27/103/115	-
28	CLA	a	723	-	1/1/15/20	13/39/115/115	-
28	CLA	b	710	-	1/1/12/20	4/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	F	315	-	1/1/10/20	4/10/86/115	-
28	CLA	G	512	-	1/1/14/20	11/33/109/115	-
28	CLA	K	313	-	1/1/13/20	7/27/103/115	-
32	PID	G	507	-	-	0/24/93/93	1/4/4/4
32	PID	D	304	-	-	3/24/93/93	0/4/4/4
28	CLA	G	516	5	1/1/10/20	6/10/86/115	-
28	CLA	M	309	24	1/1/13/20	5/27/103/115	-
29	KC1	I	314	1	-	9/15/71/71	-
31	LMG	I	320	-	-	14/33/53/70	0/1/1/1
28	CLA	H	304	-	1/1/11/20	6/18/94/115	-
28	CLA	l	312	-	1/1/11/20	6/17/93/115	-
26	DD6	L	304	-	-	0/26/80/80	0/3/3/3
28	CLA	M	308	29	1/1/12/20	10/25/101/115	-
28	CLA	H	308	-	1/1/11/20	4/17/93/115	-
28	CLA	L	316	-	1/1/10/20	4/10/86/115	-
31	LMG	K	318	-	-	19/38/58/70	0/1/1/1
31	LMG	I	318	-	-	21/31/51/70	0/1/1/1
31	LMG	j	101	-	-	14/30/50/70	0/1/1/1
28	CLA	B	308	-	1/1/11/20	5/15/91/115	-
28	CLA	L	312	-	1/1/11/20	7/17/93/115	-
29	KC1	G	515	5	-	6/15/71/71	-
28	CLA	I	308	-	1/1/14/20	12/33/109/115	-
28	CLA	a	728	-	1/1/13/20	8/27/103/115	-
28	CLA	B	310	-	1/1/13/20	8/27/103/115	-
28	CLA	a	729	-	1/1/13/20	7/29/105/115	-
26	DD6	h	203	-	-	1/26/80/80	0/3/3/3
28	CLA	b	715	-	1/1/14/20	12/33/109/115	-
26	DD6	L	305	-	-	3/26/80/80	0/3/3/3
28	CLA	F	307	-	1/1/11/20	3/17/93/115	-
29	KC1	N	306	-	-	6/15/71/71	-
26	DD6	M	304	-	-	0/26/80/80	0/3/3/3
28	CLA	I	312	-	1/1/15/20	15/39/115/115	-
26	DD6	B	306	-	-	2/26/80/80	0/3/3/3
28	CLA	a	718	-	1/1/11/20	9/17/93/115	-
28	CLA	a	715	-	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	a	725	-	1/1/14/20	13/35/111/115	-
28	CLA	A	319	-	1/1/11/20	9/17/93/115	-
28	CLA	N	305	-	1/1/15/20	9/39/115/115	-
26	DD6	M	303	-	-	2/26/80/80	0/3/3/3
27	UIX	I	304	-	-	4/31/87/87	0/3/3/3
31	LMG	K	317	-	-	9/22/42/70	0/1/1/1
32	PID	F	305	-	-	8/24/93/93	0/4/4/4
28	CLA	L	314	-	1/1/12/20	6/25/101/115	-
28	CLA	H	311	-	-	6/10/86/115	-
36	PQN	a	732	-	-	8/23/43/43	0/2/2/2
28	CLA	B	313	18	1/1/15/20	9/39/115/115	-
28	CLA	K	315	-	1/1/10/20	2/10/86/115	-
29	KC1	F	309	20	-	9/15/71/71	-
28	CLA	l	311	-	1/1/15/20	14/39/115/115	-
26	DD6	L	306	-	-	3/26/80/80	0/3/3/3
28	CLA	a	708	-	1/1/12/20	5/23/99/115	-
28	CLA	G	517	-	1/1/11/20	4/17/93/115	-
28	CLA	K	307	-	1/1/11/20	2/17/93/115	-
28	CLA	a	713	-	1/1/14/20	11/33/109/115	-
28	CLA	J	311	22	1/1/11/20	7/18/94/115	-
28	CLA	D	314	-	1/1/11/20	8/17/93/115	-
28	CLA	a	735	-	1/1/15/20	18/39/115/115	-
28	CLA	h	202	-	1/1/13/20	9/27/103/115	-
30	DGD	L	301	-	-	1/26/66/95	0/2/2/2
28	CLA	G	511	-	1/1/13/20	4/27/103/115	-
29	KC1	H	310	-	-	6/15/71/71	-
28	CLA	M	312	-	1/1/11/20	5/19/95/115	-
28	CLA	D	308	-	1/1/11/20	4/18/94/115	-
26	DD6	B	304	-	-	0/26/80/80	0/3/3/3
34	SF4	c	201	7	-	-	0/6/5/5
28	CLA	l	313	14	1/1/15/20	20/39/115/115	-
26	DD6	G	505	-	-	4/26/80/80	0/3/3/3
35	BCR	a	734	-	-	2/29/63/63	0/2/2/2
32	PID	D	305	-	-	2/24/93/93	0/4/4/4
28	CLA	M	318	-	1/1/11/20	9/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	316	-	1/1/11/20	9/17/93/115	-
28	CLA	b	703	-	1/1/15/20	12/39/115/115	-
30	DGD	I	317	-	-	3/28/68/95	0/2/2/2
30	DGD	y	201	-	-	7/43/83/95	0/2/2/2
28	CLA	a	716	-	1/1/11/20	6/18/94/115	-
28	CLA	a	705	28	1/1/13/20	8/27/103/115	-
28	CLA	G	520	-	1/1/11/20	5/20/96/115	-
28	CLA	M	317	-	1/1/11/20	8/17/93/115	-
28	CLA	b	708	-	1/1/15/20	10/39/115/115	-
26	DD6	M	302	-	-	3/26/80/80	0/3/3/3
28	CLA	K	308	2	1/1/12/20	10/26/102/115	-
28	CLA	A	308	-	1/1/13/20	4/27/103/115	-
30	DGD	j	103	-	-	8/30/70/95	0/2/2/2
28	CLA	D	311	-	1/1/11/20	3/17/93/115	-
28	CLA	a	724	-	1/1/15/20	13/39/115/115	-
28	CLA	a	720	-	1/1/14/20	7/36/112/115	-
33	SQD	A	318	-	-	5/45/65/69	0/1/1/1
28	CLA	b	718	-	1/1/12/20	3/23/99/115	-
28	CLA	a	707	-	1/1/15/20	17/39/115/115	-
26	DD6	K	301	-	-	5/26/80/80	0/3/3/3
28	CLA	f	302	-	1/1/11/20	6/17/93/115	-
29	KC1	N	311	25	-	7/15/71/71	-
28	CLA	A	312	-	1/1/13/20	6/27/103/115	-
28	CLA	L	310	-	1/1/13/20	0/27/103/115	-
26	DD6	I	301	-	-	3/26/80/80	0/3/3/3
28	CLA	A	310	-	1/1/15/20	15/39/115/115	-
28	CLA	a	706	16	1/1/13/20	15/31/107/115	-
28	CLA	l	303	14	1/1/15/20	14/39/115/115	-
35	BCR	l	307	-	-	0/29/63/63	0/2/2/2
28	CLA	f	301	-	1/1/13/20	11/27/103/115	-
34	SF4	a	737	17,16	-	-	0/6/5/5
28	CLA	I	310	-	1/1/11/20	8/19/95/115	-
28	CLA	a	702	-	1/1/15/20	11/39/115/115	-
29	KC1	A	314	6	-	5/15/71/71	-
28	CLA	l	305	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	A	307	29	1/1/11/20	1/15/91/115	-
27	UIX	J	305	-	-	11/31/87/87	0/3/3/3
29	KC1	A	306	26,28	-	7/15/71/71	-
37	LHG	a	733	-	-	16/52/52/53	-
32	PID	F	306	-	-	0/24/93/93	0/4/4/4
28	CLA	m	202	-	1/1/14/20	10/33/109/115	-
28	CLA	D	309	-	1/1/11/20	7/17/93/115	-
28	CLA	G	519	-	1/1/13/20	13/32/108/115	-
35	BCR	a	736	-	-	2/29/63/63	0/2/2/2
26	DD6	A	303	-	-	1/26/80/80	0/3/3/3
28	CLA	I	319	28	1/1/11/20	7/15/91/115	-
32	PID	N	302	-	-	2/24/93/93	0/4/4/4
28	CLA	K	309	-	1/1/12/20	2/21/97/115	-
29	KC1	M	307	28	-	6/15/71/71	-
28	CLA	b	709	-	1/1/14/20	8/33/109/115	-
28	CLA	K	310	-	1/1/13/20	5/27/103/115	-
28	CLA	A	315	-	1/1/10/20	4/10/86/115	-
28	CLA	b	707	-	1/1/15/20	18/39/115/115	-
28	CLA	I	306	1	1/1/11/20	9/20/96/115	-
28	CLA	K	316	-	1/1/11/20	3/17/93/115	-
26	DD6	J	303	-	-	2/26/80/80	0/3/3/3
28	CLA	a	703	-	1/1/13/20	6/27/103/115	-
26	DD6	M	305	-	-	1/26/80/80	0/3/3/3
28	CLA	J	312	-	1/1/12/20	6/25/101/115	-
27	UIX	h	201	-	-	2/31/87/87	0/3/3/3
26	DD6	K	304	-	-	1/26/80/80	0/3/3/3
28	CLA	H	307	-	1/1/12/20	5/23/99/115	-
35	BCR	b	730	-	-	6/29/63/63	0/2/2/2
28	CLA	a	731	-	1/1/15/20	13/39/115/115	-
28	CLA	f	303	10	1/1/11/20	8/17/93/115	-
28	CLA	L	309	-	1/1/12/20	7/25/101/115	-
28	CLA	N	304	-	1/1/11/20	4/18/94/115	-
28	CLA	a	726	-	1/1/15/20	13/39/115/115	-
26	DD6	A	301	-	-	3/26/80/80	0/3/3/3
28	CLA	K	311	-	1/1/12/20	11/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	I	307	-	1/1/11/20	7/17/93/115	-
28	CLA	a	727	-	1/1/11/20	9/17/93/115	-
28	CLA	K	306	2	1/1/11/20	4/20/96/115	-
26	DD6	N	303	-	-	0/26/80/80	0/3/3/3
28	CLA	I	309	-	1/1/13/20	6/27/103/115	-
32	PID	D	307	-	-	4/24/93/93	0/4/4/4
26	DD6	M	306	-	-	4/26/80/80	0/3/3/3
28	CLA	b	706	-	1/1/11/20	4/19/95/115	-
26	DD6	G	502	-	-	6/26/80/80	0/3/3/3
26	DD6	D	303	-	-	6/26/80/80	0/3/3/3
28	CLA	A	313	-	1/1/13/20	10/27/103/115	-
28	CLA	l	308	-	1/1/10/20	3/10/86/115	-
28	CLA	b	712	-	1/1/13/20	9/25/101/115	-
28	CLA	B	307	18	1/1/11/20	3/20/96/115	-
26	DD6	J	304	-	-	2/26/80/80	0/3/3/3
28	CLA	G	518	-	1/1/11/20	7/17/93/115	-
28	CLA	j	106	-	1/1/13/20	10/31/107/115	-
28	CLA	J	307	-	1/1/15/20	19/39/115/115	-
28	CLA	l	310	-	-	10/15/65/115	0/5/5/9
32	PID	F	304	-	-	3/24/93/93	0/4/4/4
28	CLA	b	728	-	1/1/15/20	9/39/115/115	-
26	DD6	J	302	-	-	3/26/80/80	0/3/3/3
28	CLA	J	301	-	1/1/14/20	12/33/109/115	-
35	BCR	b	732	-	-	0/29/63/63	0/2/2/2
27	UIX	B	305	-	-	2/31/87/87	0/3/3/3
28	CLA	a	722	-	1/1/13/20	8/31/107/115	-
26	DD6	L	303	-	-	0/26/80/80	0/3/3/3
28	CLA	A	316	-	1/1/11/20	4/18/94/115	-
28	CLA	H	312	-	1/1/11/20	9/17/93/115	-
28	CLA	a	701	-	1/1/11/20	2/15/91/115	-
28	CLA	B	311	-	1/1/15/20	21/39/115/115	-
28	CLA	G	513	5	1/1/15/20	7/39/115/115	-
28	CLA	D	313	19	1/1/11/20	2/15/91/115	-
28	CLA	I	311	1	1/1/13/20	10/27/103/115	-
28	CLA	A	309	-	1/1/13/20	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	UIX	A	304	-	-	0/31/87/87	0/3/3/3
26	DD6	A	305	29	-	1/26/80/80	0/3/3/3
28	CLA	a	721	-	1/1/15/20	18/39/115/115	-
30	DGD	G	521	-	-	18/33/73/95	0/2/2/2
28	CLA	a	704	-	1/1/15/20	6/39/115/115	-
28	CLA	b	727	-	1/1/15/20	7/39/115/115	-
29	KC1	H	306	-	-	4/15/71/71	-
35	BCR	b	702	-	-	2/29/63/63	0/2/2/2
28	CLA	L	308	29	1/1/11/20	9/15/91/115	-
31	LMG	B	318	-	-	15/32/52/70	0/1/1/1
28	CLA	I	315	-	1/1/12/20	8/24/100/115	-
28	CLA	J	314	-	1/1/10/20	2/10/86/115	-
28	CLA	b	711	-	1/1/13/20	11/27/103/115	-
28	CLA	b	713	-	1/1/15/20	8/39/115/115	-
27	UIX	G	503	-	-	5/31/87/87	0/3/3/3
28	CLA	a	711	-	1/1/11/20	6/15/91/115	-
28	CLA	a	714	-	1/1/11/20	4/15/91/115	-
32	PID	H	301	-	-	4/24/93/93	0/4/4/4
32	PID	G	506	-	-	3/24/93/93	0/4/4/4
35	BCR	l	306	-	-	7/29/63/63	0/2/2/2
28	CLA	a	719	-	1/1/11/20	7/18/94/115	-
28	CLA	L	318	-	1/1/11/20	8/17/93/115	-
28	CLA	a	712	28	1/1/14/20	8/33/109/115	-
28	CLA	G	510	-	1/1/15/20	10/39/115/115	-
29	KC1	K	314	2	-	9/15/71/71	-
26	DD6	H	303	-	-	1/26/80/80	0/3/3/3
28	CLA	J	315	-	1/1/11/20	3/17/93/115	-
26	DD6	G	508	-	-	1/26/80/80	0/3/3/3
26	DD6	A	302	-	-	3/26/80/80	0/3/3/3
29	KC1	N	308	-	-	8/15/71/71	-
28	CLA	B	317	-	1/1/11/20	7/15/91/115	-
26	DD6	B	302	-	-	3/24/78/80	0/3/3/3
35	BCR	i	201	-	-	8/29/63/63	0/2/2/2
26	DD6	K	303	-	-	0/26/80/80	0/3/3/3
32	PID	M	301	-	-	1/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	KC1	D	310	-	-	10/15/71/71	-
28	CLA	I	316	-	1/1/13/20	13/27/103/115	-
28	CLA	M	311	-	1/1/11/20	4/17/93/115	-
28	CLA	F	308	-	1/1/11/20	3/17/93/115	-
31	LMG	D	317	-	-	17/41/61/70	0/1/1/1
28	CLA	I	313	-	1/1/13/20	11/27/103/115	-
29	KC1	F	314	20	-	5/15/71/71	-
26	DD6	B	303	-	-	2/26/80/80	0/3/3/3
26	DD6	I	303	-	-	2/26/80/80	0/3/3/3
31	LMG	b	733	-	-	19/39/59/70	0/1/1/1
28	CLA	G	514	-	1/1/12/20	11/25/101/115	-
32	PID	D	301	-	-	2/24/93/93	0/4/4/4
28	CLA	F	310	-	1/1/11/20	8/17/93/115	-
28	CLA	G	509	5	1/1/12/20	4/23/99/115	-
28	CLA	l	309	-	1/1/10/20	3/10/86/115	-
28	CLA	b	721	26	1/1/11/20	1/17/93/115	-
28	CLA	b	701	-	1/1/15/20	13/39/115/115	-
28	CLA	N	310	-	1/1/11/20	10/18/94/115	-
28	CLA	l	304	-	1/1/14/20	9/33/109/115	-
28	CLA	F	312	-	1/1/11/20	3/17/93/115	-
28	CLA	K	312	-	1/1/11/20	5/19/95/115	-
28	CLA	b	705	-	1/1/15/20	11/39/115/115	-
35	BCR	j	102	-	-	5/29/63/63	0/2/2/2
26	DD6	K	319	-	-	4/26/80/80	0/3/3/3
28	CLA	b	725	-	1/1/15/20	9/39/115/115	-
28	CLA	L	311	-	1/1/13/20	5/27/103/115	-
28	CLA	b	724	-	1/1/15/20	15/39/115/115	-
28	CLA	b	720	-	1/1/12/20	9/25/101/115	-
28	CLA	I	321	28	1/1/12/20	8/24/100/115	-
28	CLA	B	312	-	1/1/12/20	4/23/99/115	-
32	PID	N	301	-	-	6/24/93/93	0/4/4/4
29	KC1	M	314	24	-	9/15/71/71	-
26	DD6	K	305	-	-	4/26/80/80	0/3/3/3
26	DD6	G	504	-	-	5/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	H	305	-	1/1/15/20	8/39/115/115	-
28	CLA	N	307	-	1/1/12/20	3/23/99/115	-
26	DD6	b	731	28	-	3/26/80/80	0/3/3/3
28	CLA	J	310	-	1/1/11/20	8/17/93/115	-
28	CLA	a	717	-	1/1/13/20	13/30/106/115	-
28	CLA	B	301	-	1/1/14/20	10/33/109/115	-
28	CLA	b	723	-	1/1/12/20	9/21/97/115	-
32	PID	D	302	-	-	3/24/93/93	0/4/4/4
26	DD6	I	305	-	-	5/26/80/80	0/3/3/3
28	CLA	H	309	-	1/1/11/20	8/18/94/115	-
28	CLA	M	315	-	1/1/10/20	5/10/86/115	-
26	DD6	I	302	-	-	5/26/80/80	0/3/3/3
28	CLA	J	308	-	1/1/11/20	9/17/93/115	-
30	DGD	l	301	-	-	8/39/79/95	0/2/2/2
36	PQN	b	729	-	-	4/23/43/43	0/2/2/2
32	PID	j	105	-	-	4/24/93/93	0/4/4/4
28	CLA	a	730	-	1/1/15/20	4/39/115/115	-
32	PID	H	302	-	-	2/24/93/93	0/4/4/4
28	CLA	a	738	22	1/1/11/20	4/17/93/115	-
30	DGD	G	501	-	-	10/34/74/95	0/2/2/2
35	BCR	m	201	-	-	5/29/63/63	0/2/2/2
35	BCR	l	302	-	-	3/29/63/63	0/2/2/2
28	CLA	D	312	19	1/1/11/20	7/17/93/115	-
26	DD6	F	301	-	-	2/26/80/80	0/3/3/3
28	CLA	F	313	-	1/1/11/20	5/17/93/115	-
29	KC1	D	315	19	-	4/15/71/71	-
28	CLA	a	710	16	1/1/13/20	6/27/103/115	-
28	CLA	J	309	-	1/1/13/20	9/29/105/115	-
28	CLA	A	320	-	1/1/11/20	6/17/93/115	-
28	CLA	J	306	-	1/1/11/20	6/17/93/115	-
28	CLA	F	311	-	1/1/11/20	7/17/93/115	-
29	KC1	B	314	18	-	7/15/71/71	-
28	CLA	j	104	-	1/1/13/20	6/27/103/115	-
28	CLA	b	704	-	1/1/15/20	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	b	716	-	1/1/12/20	4/21/97/115	-
28	CLA	b	717	-	1/1/15/20	18/39/115/115	-
28	CLA	D	316	-	1/1/10/20	0/10/86/115	-
28	CLA	M	310	-	1/1/11/20	8/19/95/115	-
32	PID	F	302	-	-	2/24/93/93	0/4/4/4
28	CLA	b	714	-	1/1/11/20	3/17/93/115	-
35	BCR	f	304	-	-	2/29/63/63	0/2/2/2
27	UIX	K	302	-	-	5/31/87/87	0/3/3/3
28	CLA	b	726	-	1/1/11/20	2/18/94/115	-
28	CLA	a	709	-	1/1/15/20	16/39/115/115	-
28	CLA	B	315	-	1/1/10/20	4/10/86/115	-
28	CLA	M	313	-	1/1/11/20	2/17/93/115	-
31	LMG	b	734	-	-	12/26/46/70	0/1/1/1
29	KC1	J	313	-	-	7/15/71/71	-
34	SF4	c	202	7	-	-	0/6/5/5
32	PID	D	306	-	-	8/24/93/93	0/4/4/4
28	CLA	b	719	-	1/1/11/20	9/17/93/115	-
29	KC1	L	307	28	-	6/15/71/71	-
28	CLA	J	316	-	-	3/17/93/115	-
28	CLA	A	311	6	1/1/11/20	5/17/93/115	-
28	CLA	L	317	-	1/1/12/20	11/24/100/115	-
28	CLA	B	309	18	1/1/15/20	19/39/115/115	-
28	CLA	A	317	-	1/1/10/20	0/10/86/115	-
29	KC1	L	315	-	-	8/15/71/71	-
28	CLA	b	722	-	1/1/15/20	7/39/115/115	-

The worst 5 of 1669 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	l	310	CLA	C1B-C2B	9.21	1.49	1.39
26	I	305	DD6	C30-C31	-9.00	1.25	1.42
26	J	303	DD6	C30-C31	-8.99	1.25	1.42
26	M	306	DD6	C30-C31	-8.99	1.25	1.42
26	G	505	DD6	C30-C31	-8.96	1.25	1.42

The worst 5 of 2478 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	I	304	UIX	C6-C1-C	-9.09	107.34	122.30
35	m	201	BCR	C7-C8-C9	-8.29	113.98	126.23
28	l	304	CLA	C4A-NA-C1A	7.47	110.09	106.68
27	G	503	UIX	C6-C1-C	-7.23	110.40	122.30
27	I	304	UIX	O-C1-C3	7.23	120.27	113.49

5 of 186 chirality outliers are listed below:

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

5 of 2075 torsion outliers are listed below:

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

All (1) ring outliers are listed below:

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

238 monomers are involved in 601 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	N	309	CLA	4	0
28	M	316	CLA	1	0
28	L	313	CLA	7	0
28	a	723	CLA	7	0
28	b	710	CLA	6	0
28	F	315	CLA	1	0
28	K	313	CLA	5	0
32	G	507	PID	5	0
32	D	304	PID	2	0
28	M	309	CLA	7	0
31	I	320	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	H	304	CLA	3	0
26	L	304	DD6	1	0
28	l	312	CLA	2	0
28	M	308	CLA	2	0
28	H	308	CLA	2	0
28	L	316	CLA	1	0
31	j	101	LMG	5	0
28	B	308	CLA	1	0
28	L	312	CLA	1	0
28	I	308	CLA	4	0
28	a	728	CLA	3	0
28	B	310	CLA	1	0
28	a	729	CLA	3	0
28	b	715	CLA	5	0
26	L	305	DD6	1	0
28	F	307	CLA	1	0
28	I	312	CLA	2	0
28	a	718	CLA	1	0
28	a	725	CLA	5	0
28	A	319	CLA	1	0
26	M	303	DD6	2	0
28	N	305	CLA	2	0
27	I	304	UIX	2	0
32	F	305	PID	3	0
28	L	314	CLA	3	0
28	H	311	CLA	2	0
36	a	732	PQN	5	0
28	B	313	CLA	4	0
29	F	309	KC1	2	0
28	l	311	CLA	5	0
28	a	708	CLA	2	0
28	G	517	CLA	6	0
28	K	307	CLA	1	0
28	a	713	CLA	3	0
28	J	311	CLA	2	0
28	D	314	CLA	10	0
28	a	735	CLA	5	0
30	L	301	DGD	2	0
28	G	511	CLA	2	0
29	H	310	KC1	1	0
28	M	312	CLA	1	0
28	D	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	l	313	CLA	6	0
28	M	318	CLA	1	0
35	a	734	BCR	3	0
32	D	305	PID	3	0
26	G	505	DD6	1	0
28	B	316	CLA	1	0
28	b	703	CLA	6	0
30	y	201	DGD	1	0
28	a	716	CLA	3	0
28	a	705	CLA	2	0
28	G	520	CLA	3	0
28	M	317	CLA	2	0
28	b	708	CLA	2	0
28	K	308	CLA	3	0
28	A	308	CLA	3	0
30	j	103	DGD	4	0
28	D	311	CLA	2	0
28	a	724	CLA	3	0
28	a	720	CLA	2	0
33	A	318	SQD	8	0
28	b	718	CLA	4	0
28	a	707	CLA	7	0
28	f	302	CLA	4	0
28	A	312	CLA	3	0
26	I	301	DD6	1	0
28	A	310	CLA	4	0
28	a	706	CLA	7	0
28	l	303	CLA	5	0
35	l	307	BCR	4	0
28	f	301	CLA	5	0
34	a	737	SF4	1	0
28	I	310	CLA	3	0
28	a	702	CLA	5	0
28	l	305	CLA	4	0
27	J	305	UIX	1	0
37	a	733	LHG	3	0
32	F	306	PID	2	0
28	m	202	CLA	2	0
28	D	309	CLA	2	0
28	G	519	CLA	1	0
35	a	736	BCR	2	0
26	A	303	DD6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	I	319	CLA	2	0
32	N	302	PID	2	0
28	K	309	CLA	2	0
29	M	307	KC1	1	0
28	b	709	CLA	7	0
28	K	310	CLA	1	0
28	A	315	CLA	1	0
28	b	707	CLA	5	0
28	I	306	CLA	2	0
28	K	316	CLA	1	0
26	J	303	DD6	2	0
28	a	703	CLA	5	0
28	J	312	CLA	2	0
28	H	307	CLA	1	0
35	b	730	BCR	4	0
28	a	731	CLA	6	0
28	f	303	CLA	1	0
28	L	309	CLA	2	0
28	a	726	CLA	6	0
28	I	307	CLA	2	0
28	K	311	CLA	2	0
28	a	727	CLA	1	0
28	I	309	CLA	1	0
28	b	706	CLA	3	0
28	A	313	CLA	4	0
28	l	308	CLA	1	0
28	b	712	CLA	4	0
28	B	307	CLA	1	0
26	J	304	DD6	3	0
28	G	518	CLA	1	0
28	j	106	CLA	3	0
28	J	307	CLA	11	0
28	l	310	CLA	1	0
32	F	304	PID	6	0
28	b	728	CLA	3	0
28	J	301	CLA	5	0
35	b	732	BCR	4	0
28	a	722	CLA	5	0
28	A	316	CLA	1	0
28	H	312	CLA	1	0
28	B	311	CLA	2	0
28	G	513	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	D	313	CLA	1	0
28	I	311	CLA	5	0
28	A	309	CLA	2	0
27	A	304	UIX	1	0
26	A	305	DD6	1	0
28	a	721	CLA	6	0
28	a	704	CLA	6	0
28	b	727	CLA	6	0
35	b	702	BCR	6	0
28	L	308	CLA	2	0
31	B	318	LMG	1	0
28	I	315	CLA	1	0
28	b	713	CLA	6	0
28	a	711	CLA	3	0
28	a	714	CLA	3	0
32	H	301	PID	3	0
32	G	506	PID	2	0
35	l	306	BCR	4	0
28	a	719	CLA	4	0
28	a	712	CLA	2	0
28	G	510	CLA	4	0
26	H	303	DD6	1	0
26	G	508	DD6	1	0
29	N	308	KC1	1	0
28	B	317	CLA	2	0
26	B	302	DD6	1	0
35	i	201	BCR	5	0
32	M	301	PID	1	0
29	D	310	KC1	1	0
28	I	316	CLA	3	0
28	F	308	CLA	1	0
31	D	317	LMG	5	0
28	I	313	CLA	3	0
31	b	733	LMG	2	0
28	G	514	CLA	3	0
32	D	301	PID	4	0
28	F	310	CLA	5	0
28	G	509	CLA	1	0
28	b	721	CLA	2	0
28	b	701	CLA	7	0
28	N	310	CLA	3	0
28	l	304	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	F	312	CLA	5	0
28	K	312	CLA	2	0
28	b	705	CLA	5	0
35	j	102	BCR	5	0
28	b	725	CLA	4	0
28	b	724	CLA	3	0
28	b	720	CLA	7	0
28	I	321	CLA	3	0
32	N	301	PID	1	0
26	G	504	DD6	3	0
28	H	305	CLA	4	0
28	N	307	CLA	1	0
28	J	310	CLA	3	0
28	a	717	CLA	4	0
28	B	301	CLA	3	0
28	b	723	CLA	3	0
32	D	302	PID	2	0
26	I	305	DD6	1	0
28	H	309	CLA	2	0
28	M	315	CLA	2	0
28	J	308	CLA	3	0
36	b	729	PQN	4	0
32	j	105	PID	5	0
28	a	730	CLA	6	0
32	H	302	PID	5	0
28	a	738	CLA	1	0
30	G	501	DGD	2	0
35	m	201	BCR	5	0
35	l	302	BCR	3	0
26	F	301	DD6	1	0
28	D	312	CLA	2	0
28	F	313	CLA	8	0
28	a	710	CLA	4	0
28	J	309	CLA	3	0
28	A	320	CLA	3	0
28	J	306	CLA	1	0
28	F	311	CLA	1	0
28	j	104	CLA	5	0
28	b	704	CLA	15	0
28	b	716	CLA	3	0
28	b	717	CLA	6	0
28	M	310	CLA	2	0

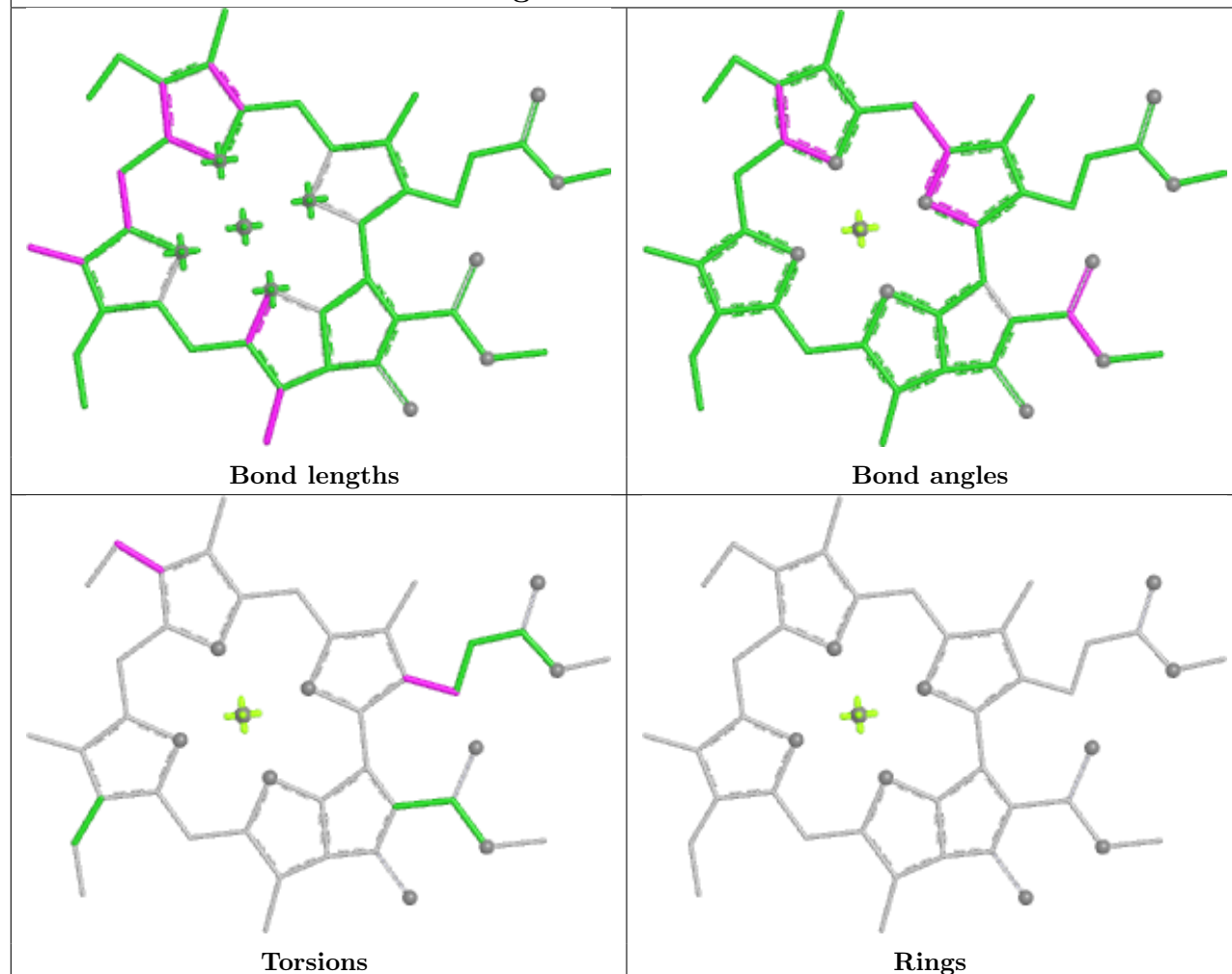
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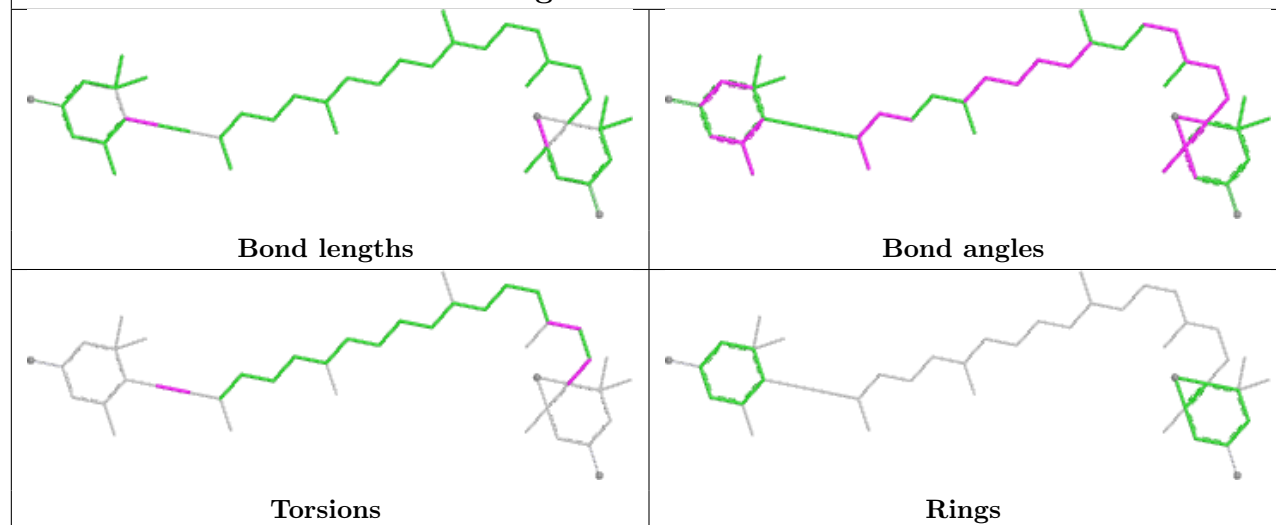
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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28	b	714	CLA	1	0
35	f	304	BCR	3	0
27	K	302	UIX	1	0
28	b	726	CLA	1	0
28	a	709	CLA	5	0
28	B	315	CLA	2	0
28	M	313	CLA	3	0
31	b	734	LMG	2	0
34	c	202	SF4	1	0
32	D	306	PID	1	0
28	J	316	CLA	4	0
28	A	311	CLA	1	0
28	L	317	CLA	5	0
28	B	309	CLA	4	0
28	A	317	CLA	2	0
28	b	722	CLA	4	0

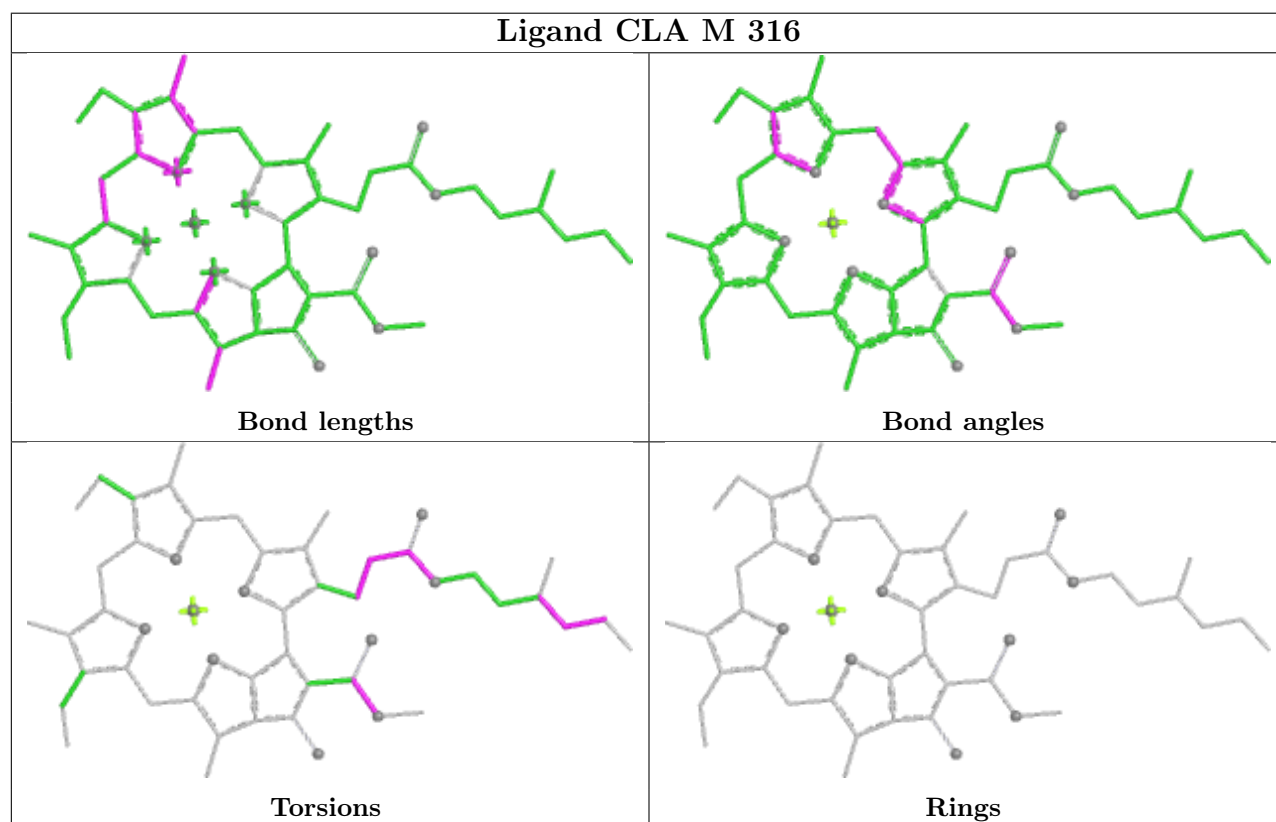
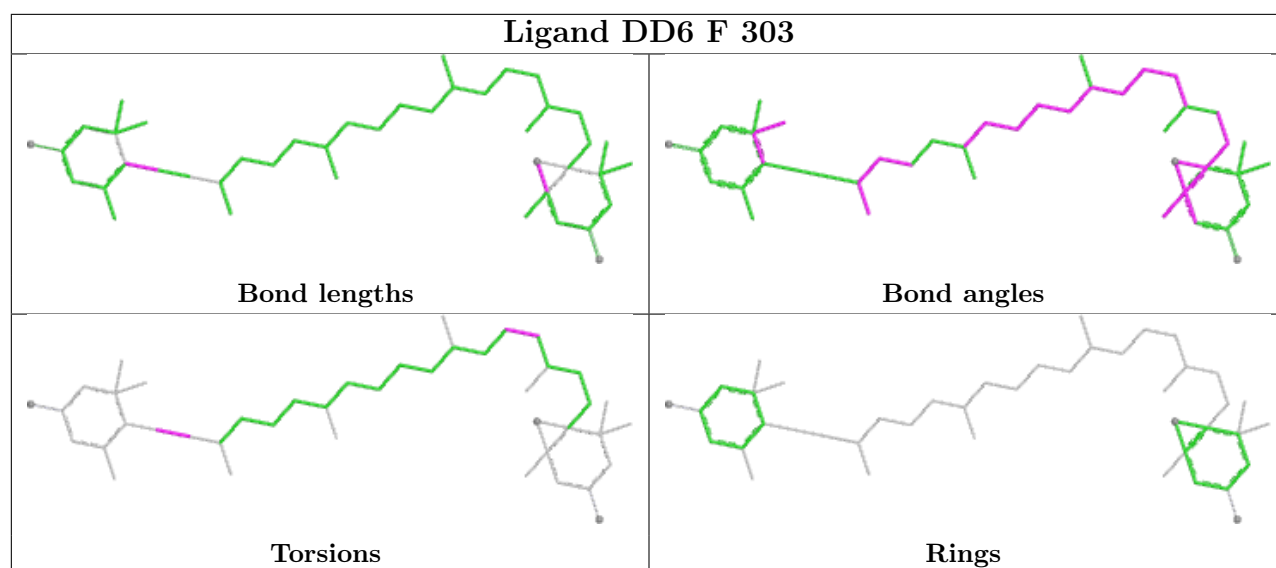
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

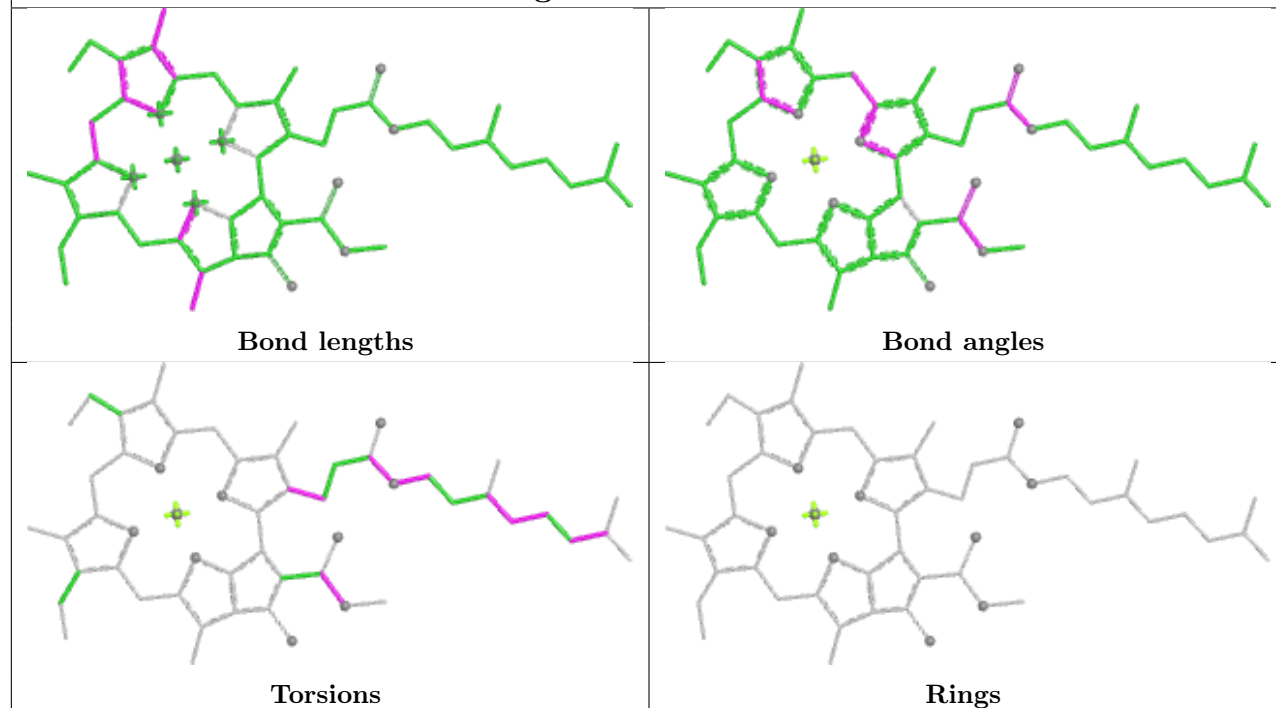
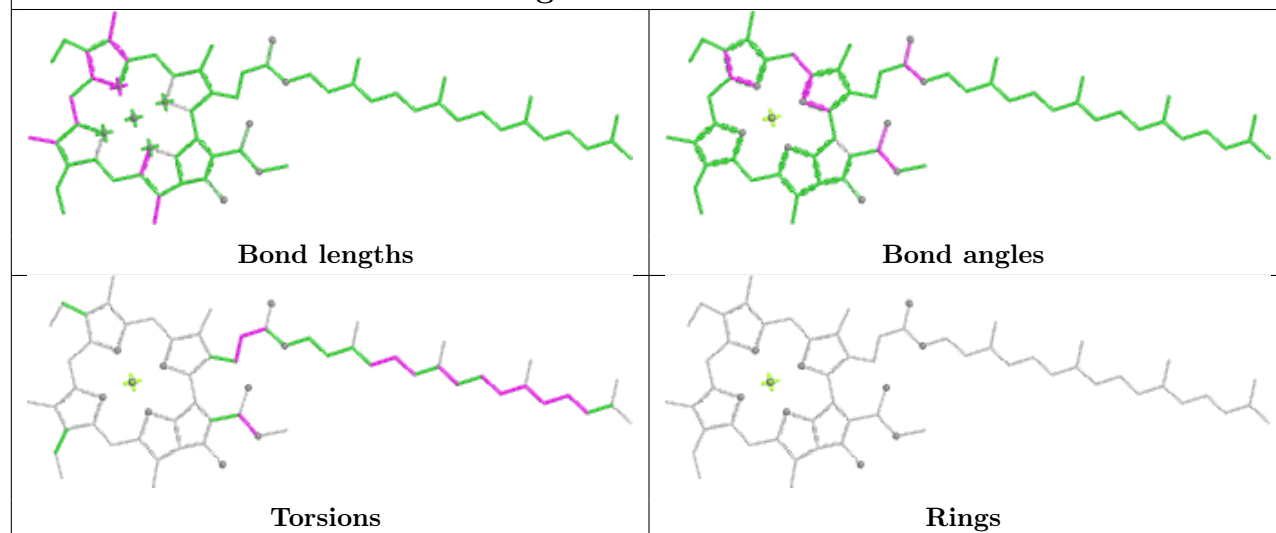
Ligand CLA N 309

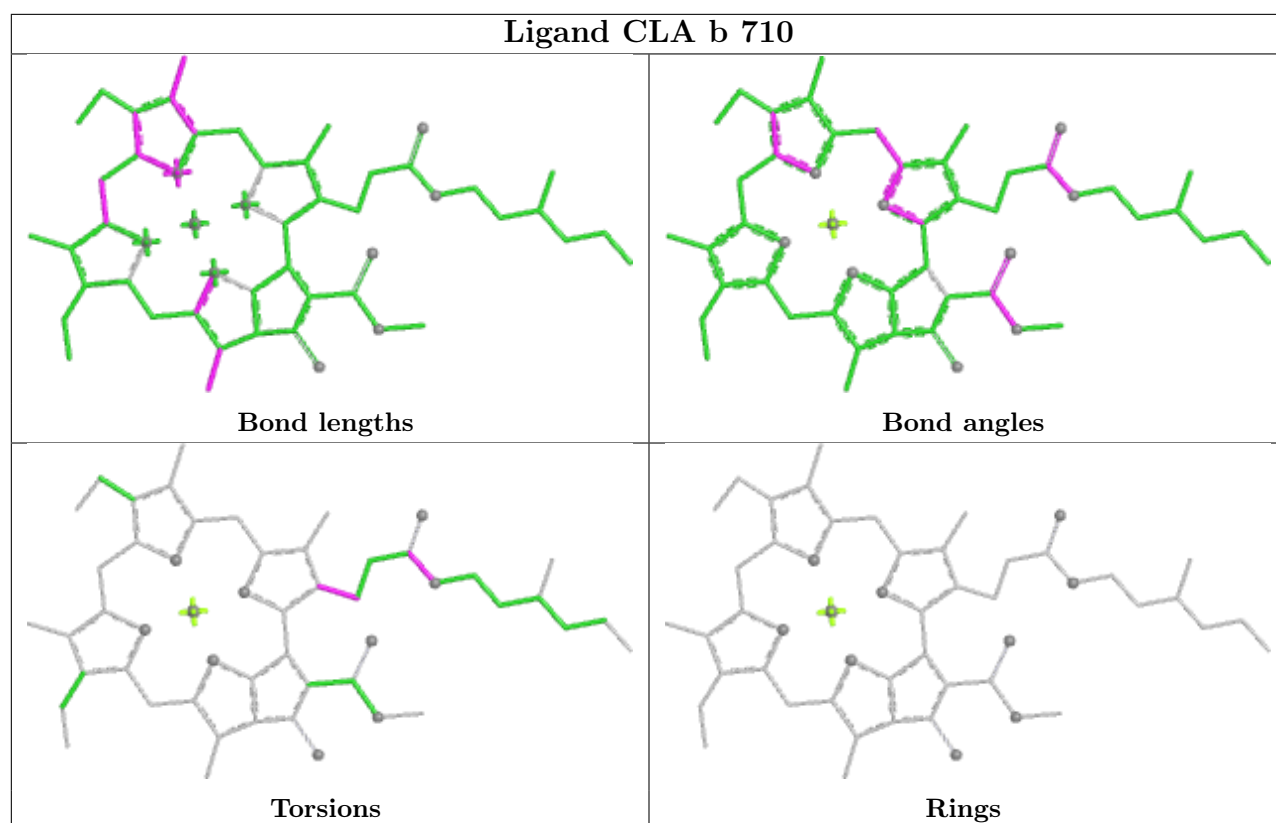


Ligand DD6 L 302

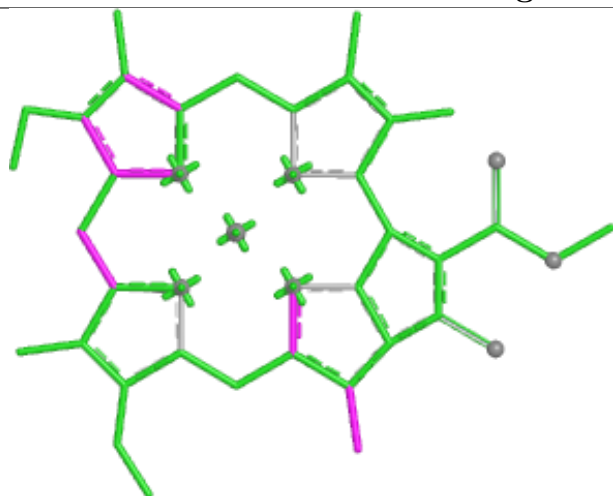




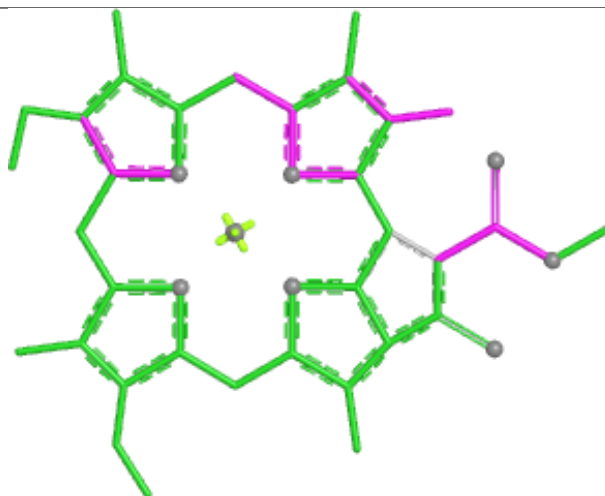
Ligand CLA L 313**Ligand CLA a 723**



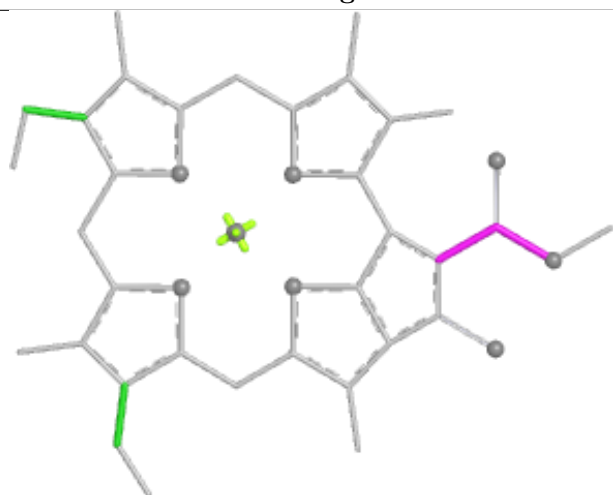
Ligand CLA F 315



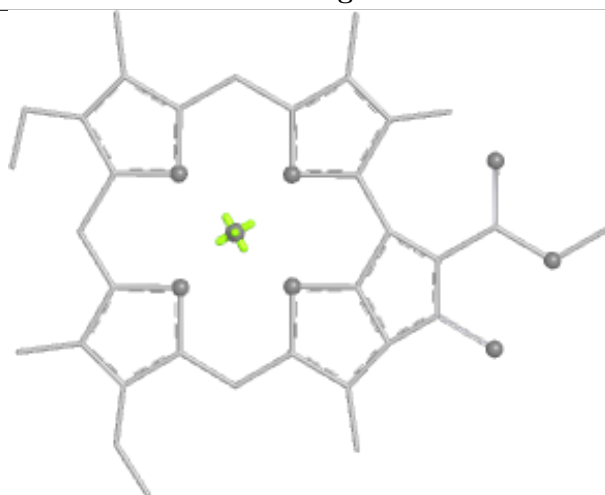
Bond lengths



Bond angles

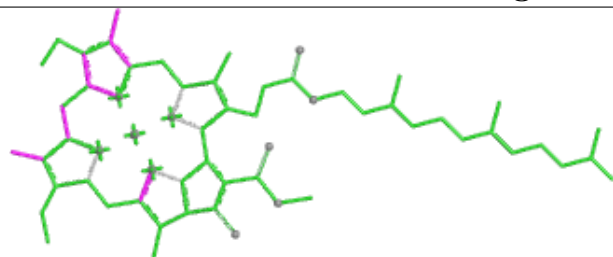


Torsions

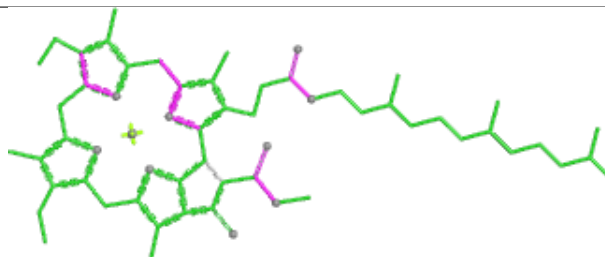


Rings

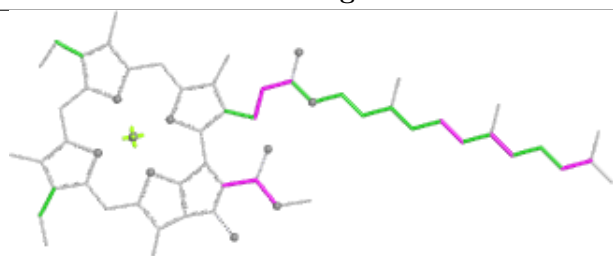
Ligand CLA G 512



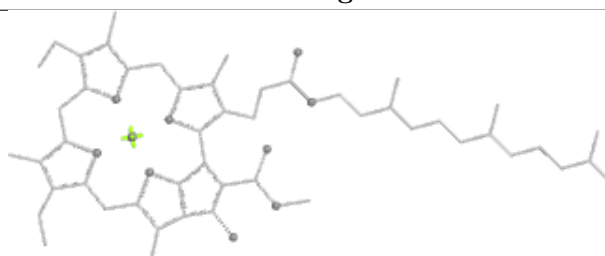
Bond lengths



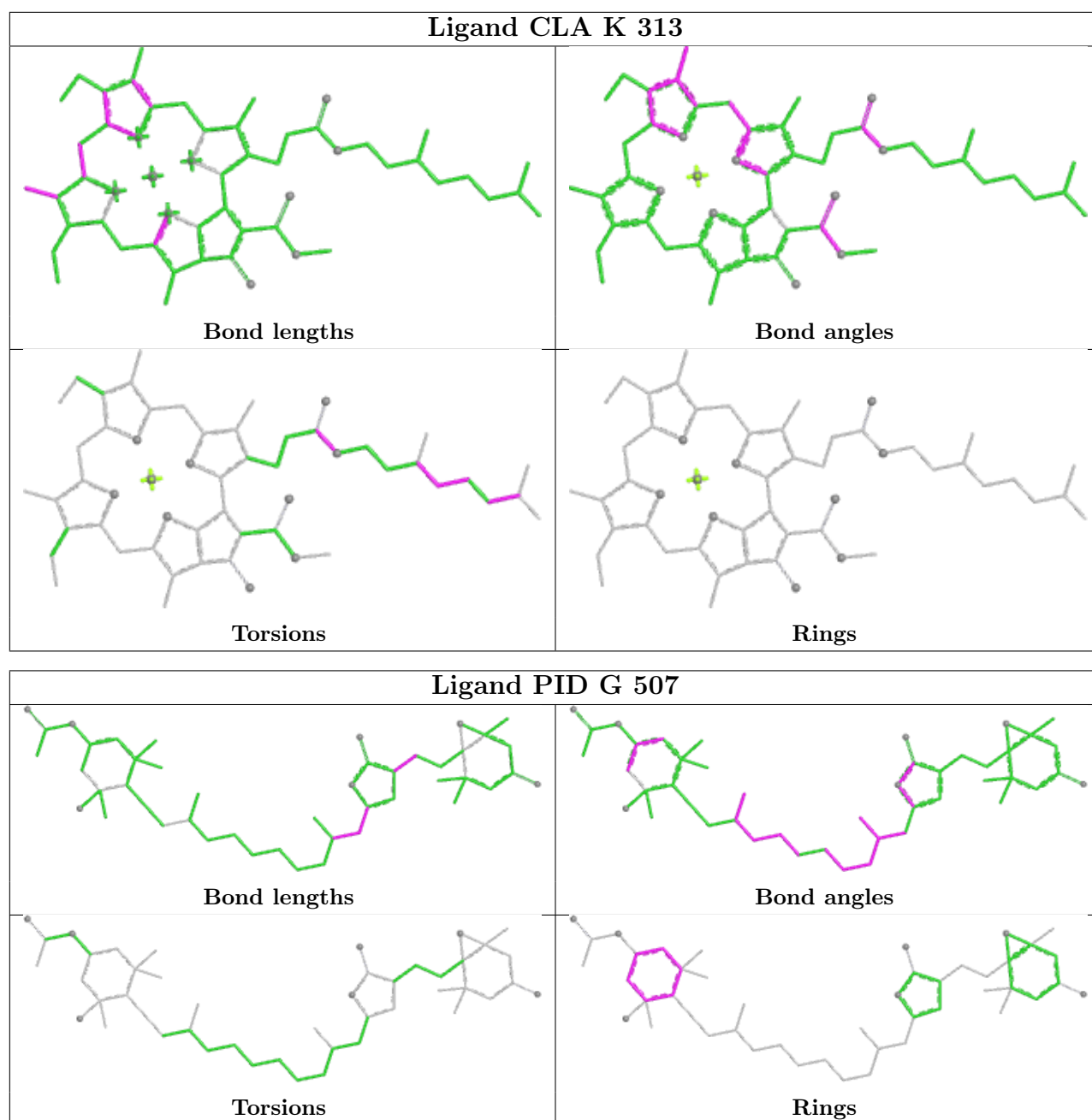
Bond angles

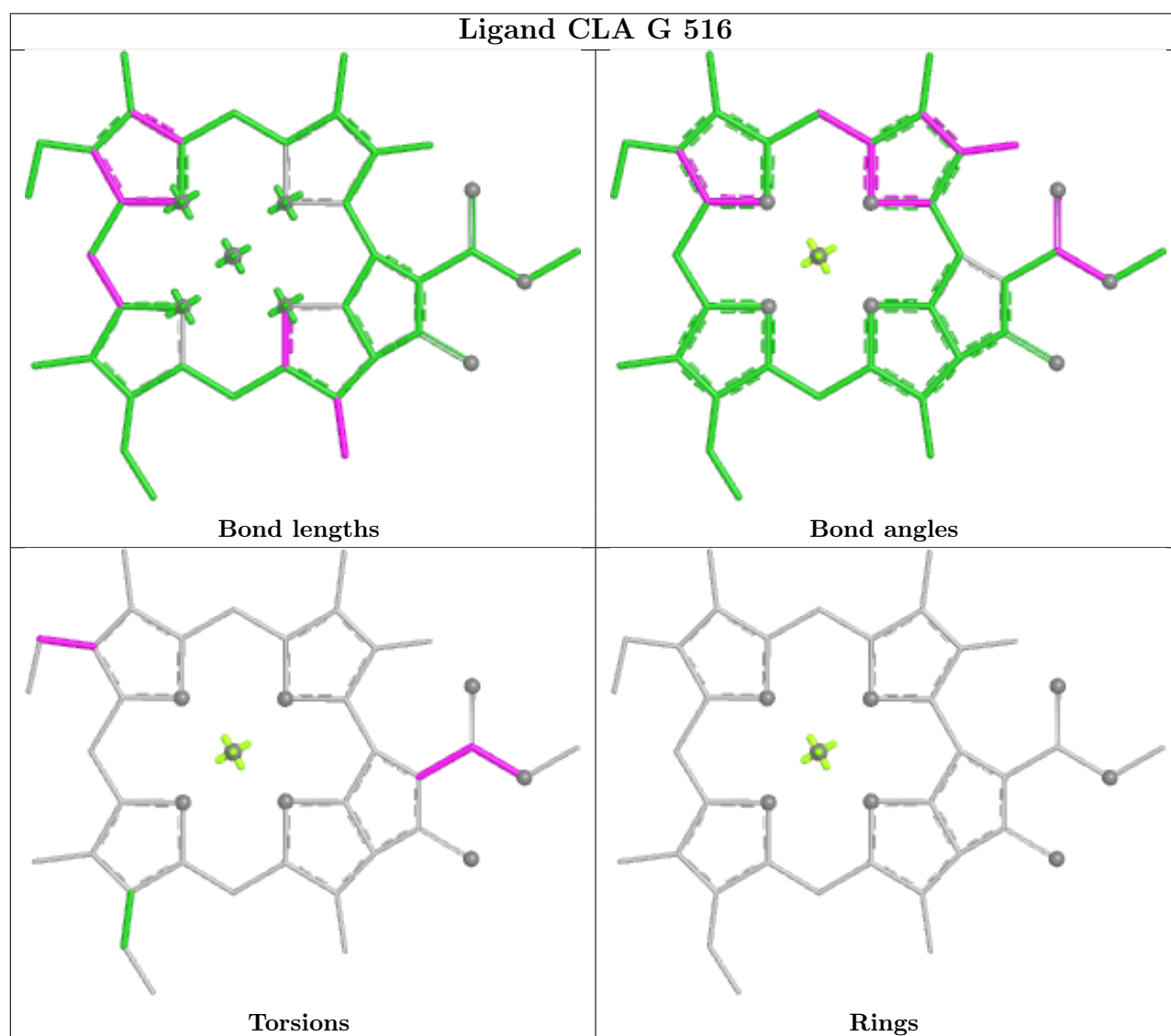
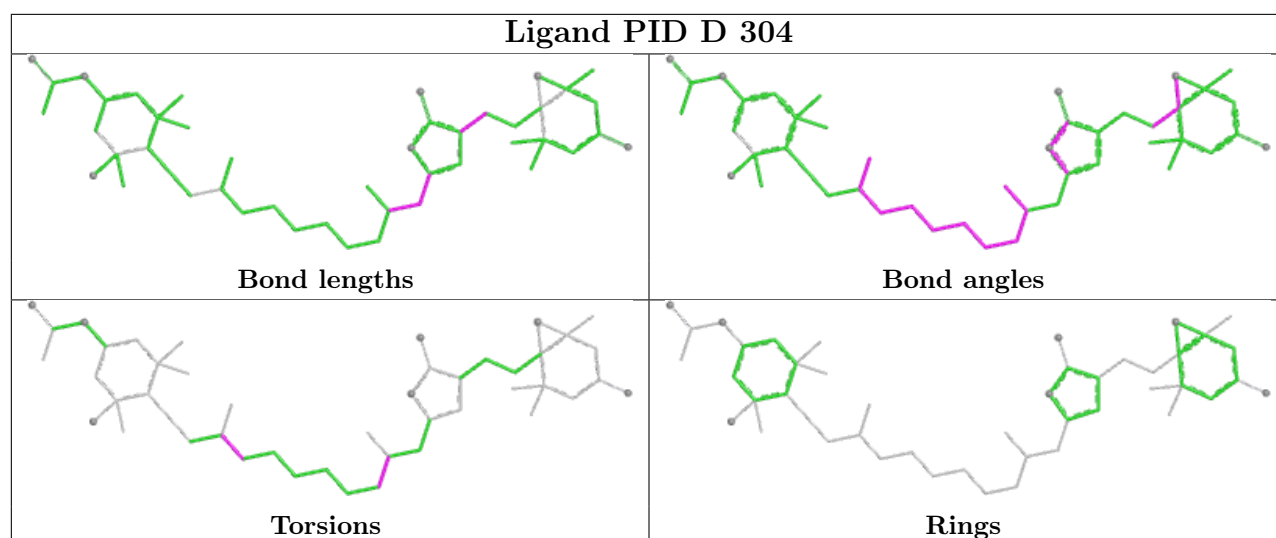


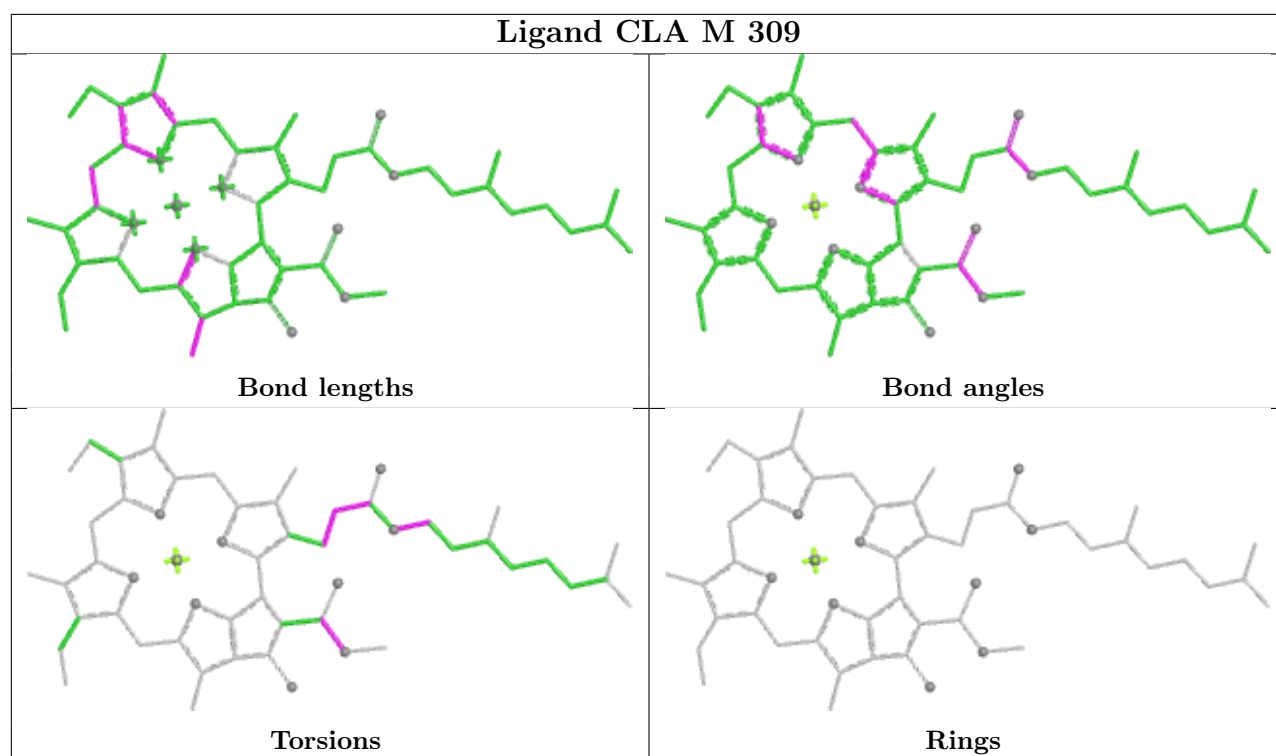
Torsions



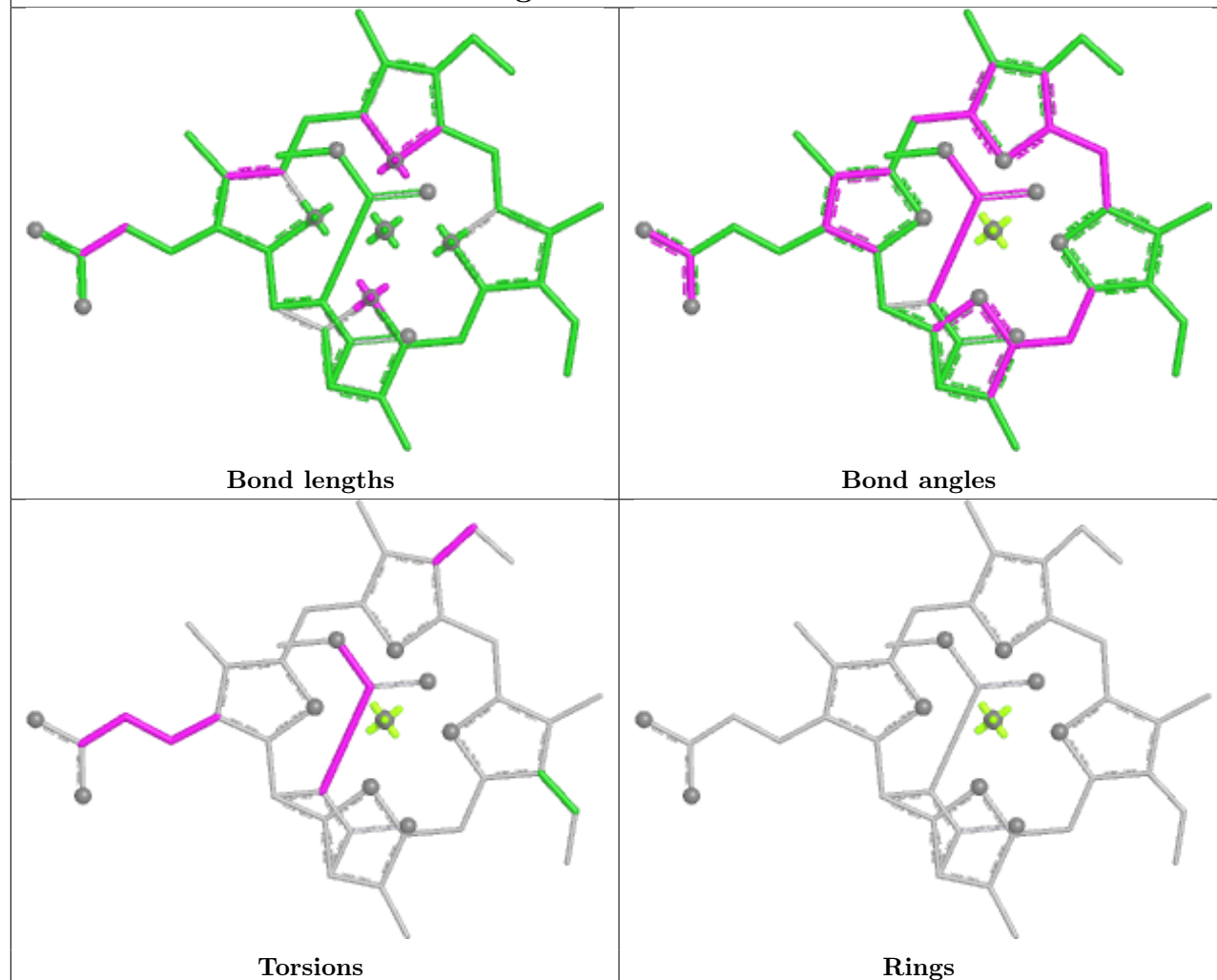
Rings



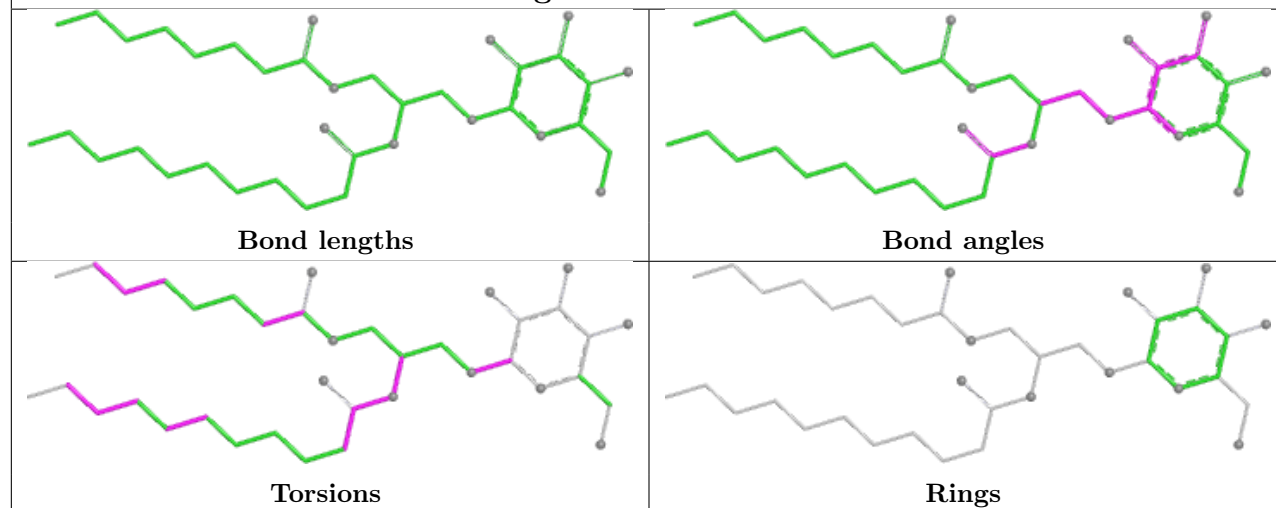


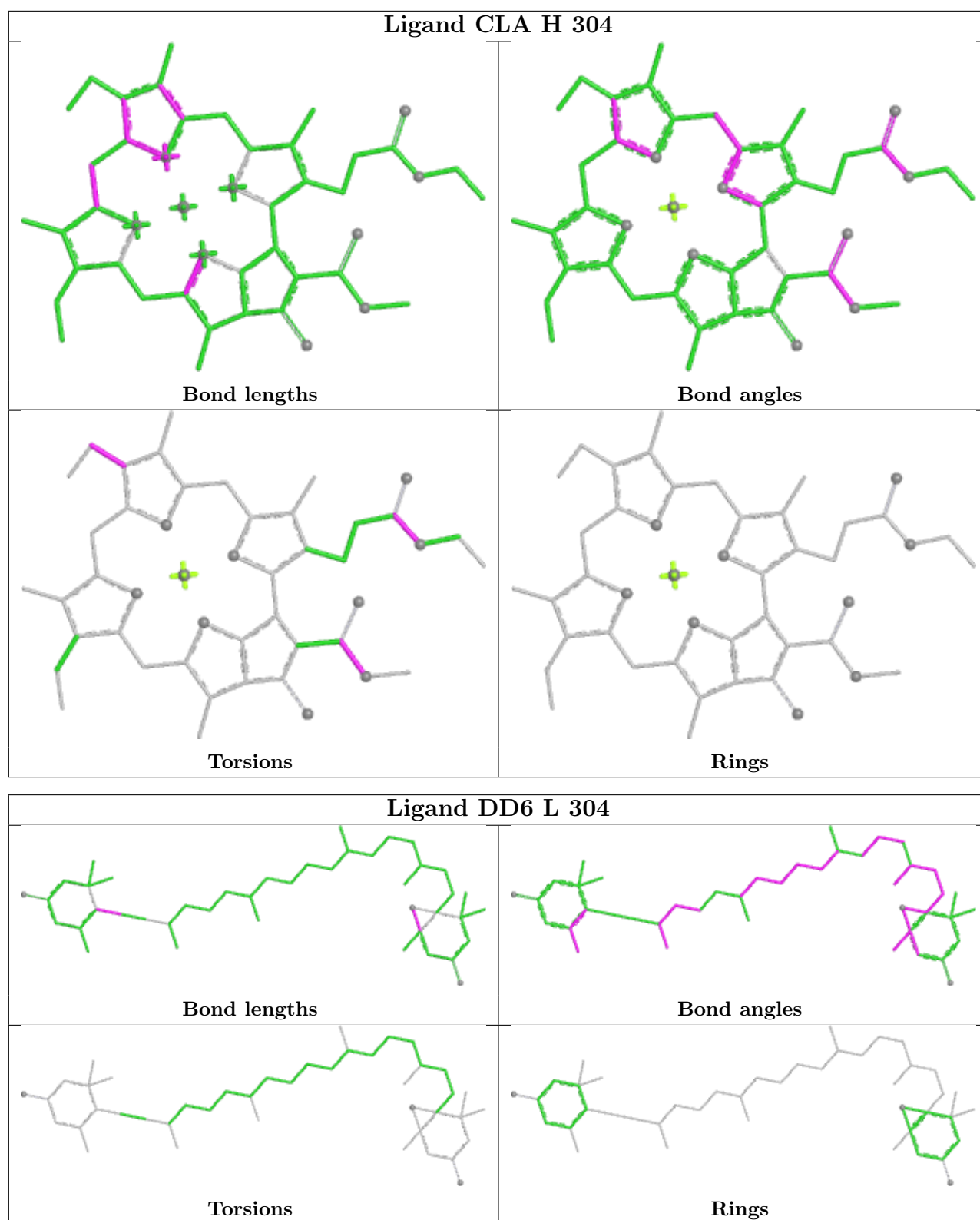


Ligand KC1 I 314

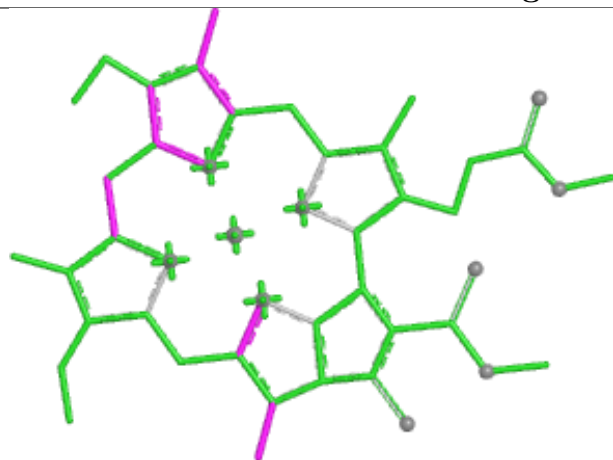


Ligand LMG I 320

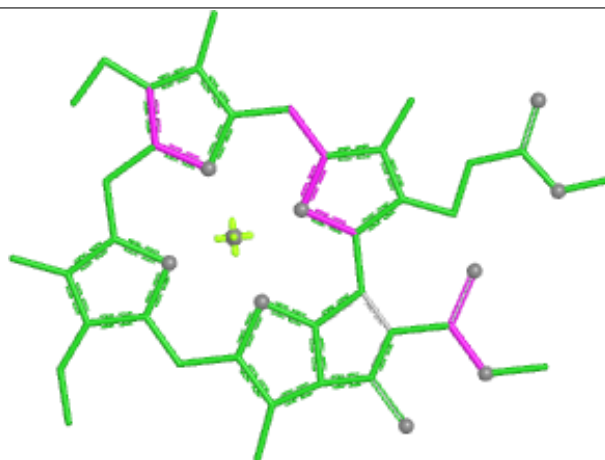




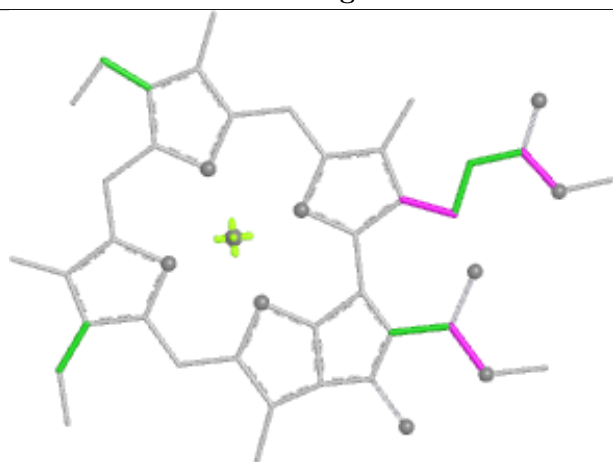
Ligand CLA 1 312



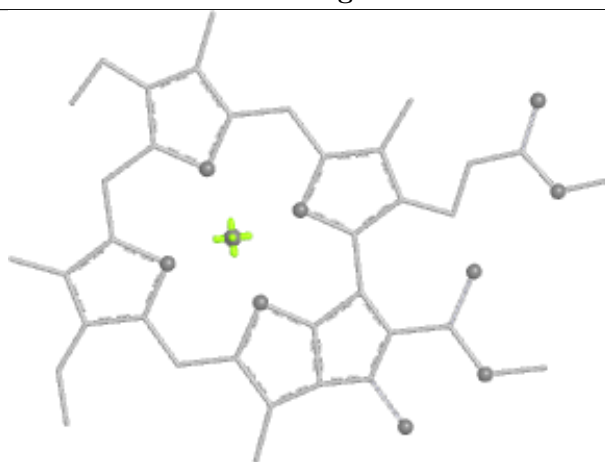
Bond lengths



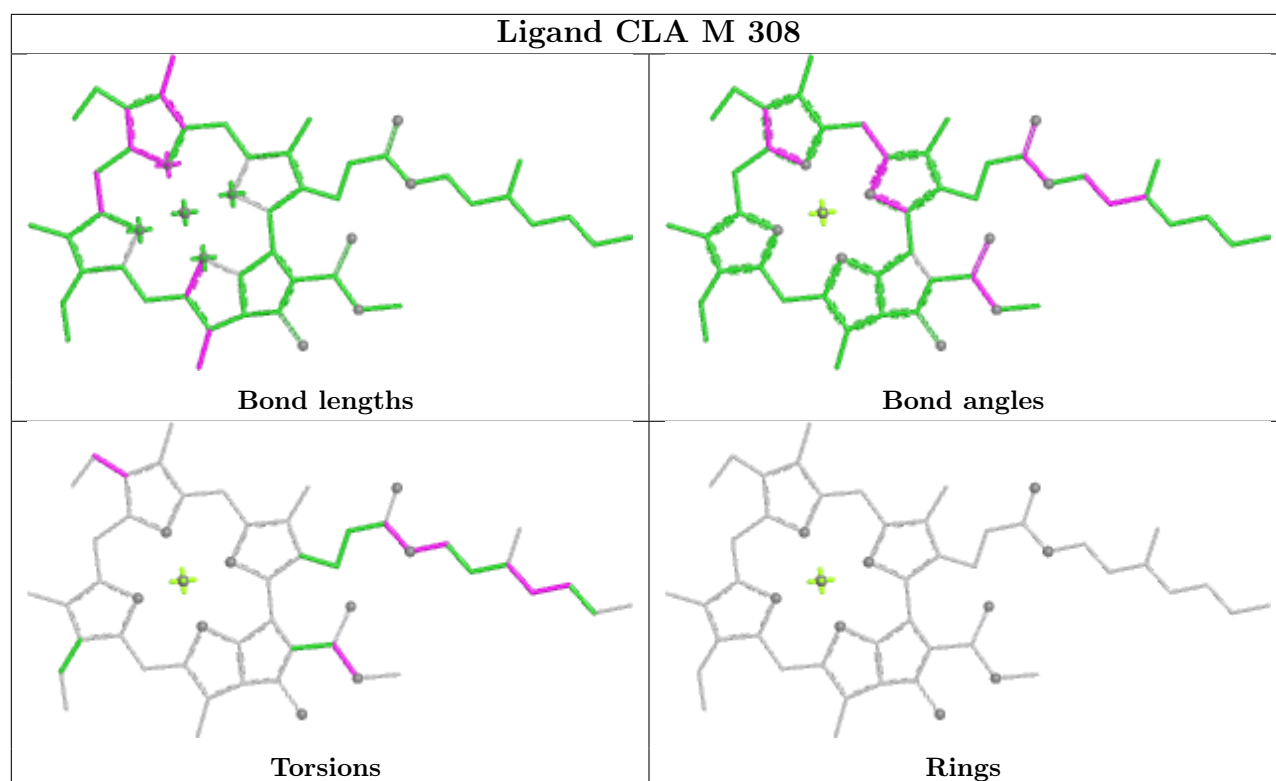
Bond angles



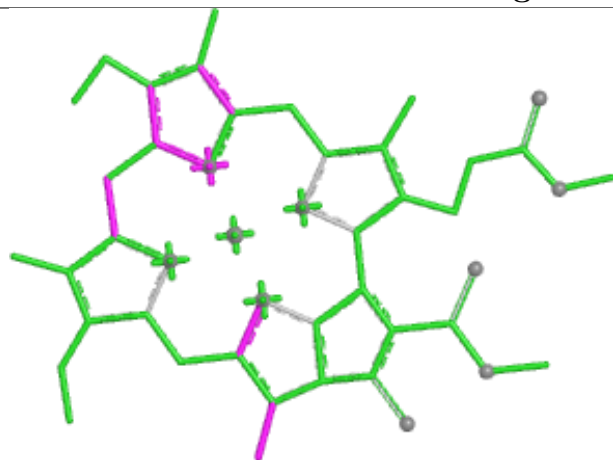
Torsions



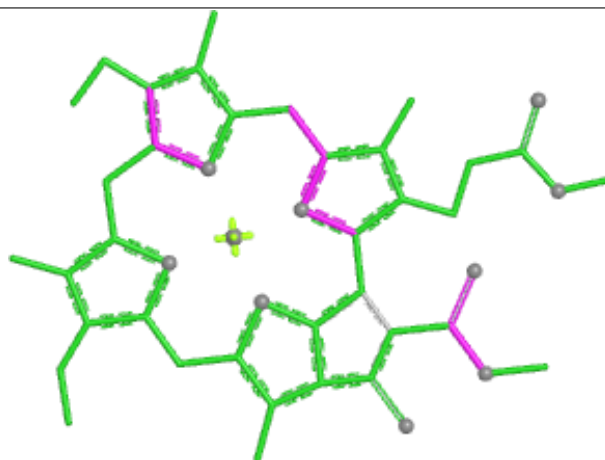
Rings



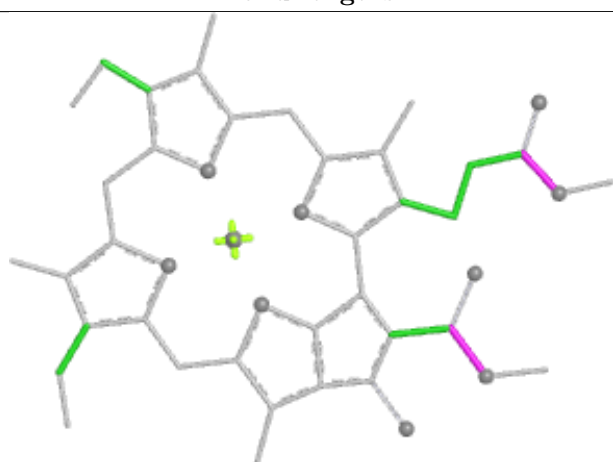
Ligand CLA H 308



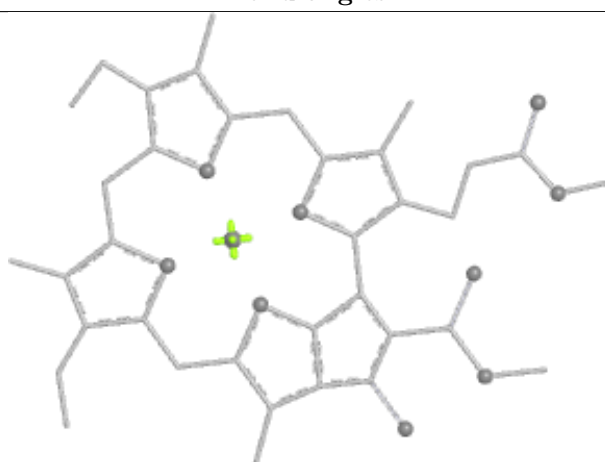
Bond lengths



Bond angles

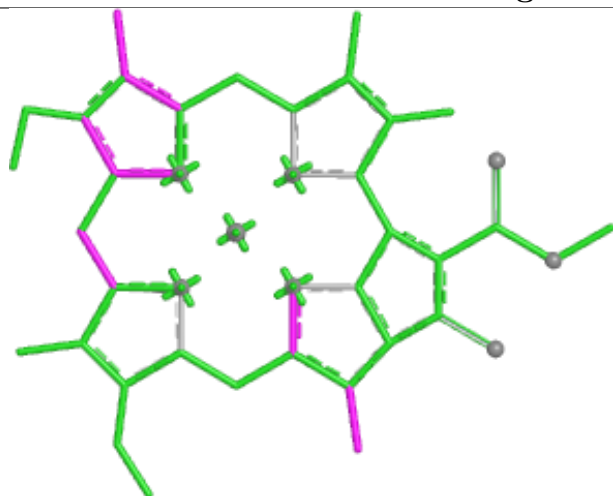


Torsions

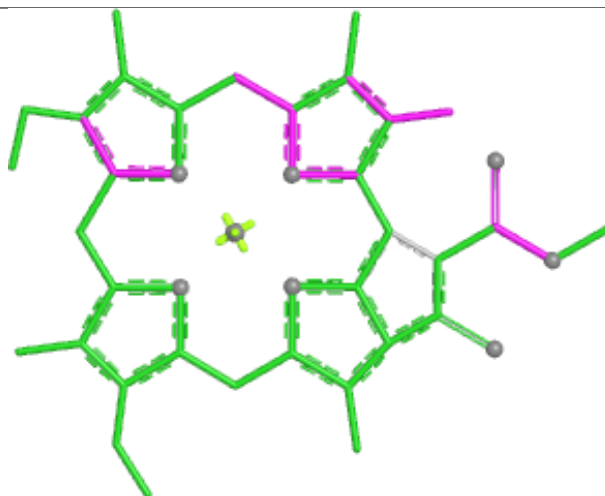


Rings

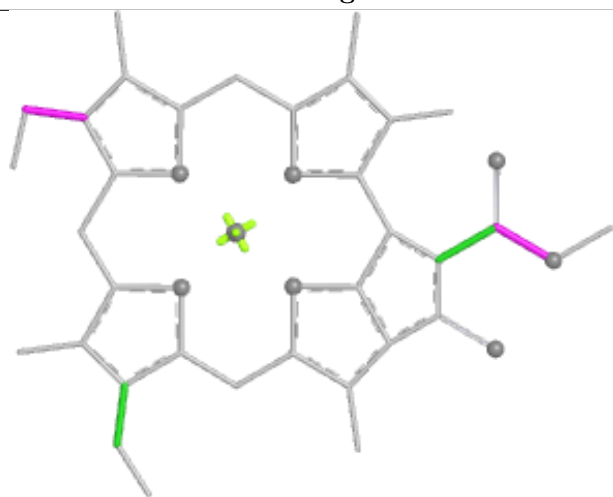
Ligand CLA L 316



Bond lengths



Bond angles

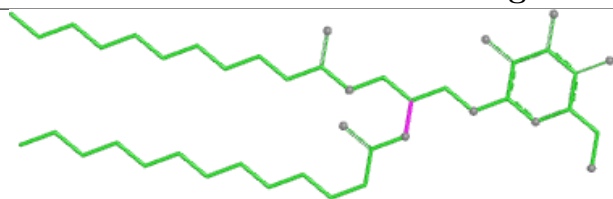


Torsions

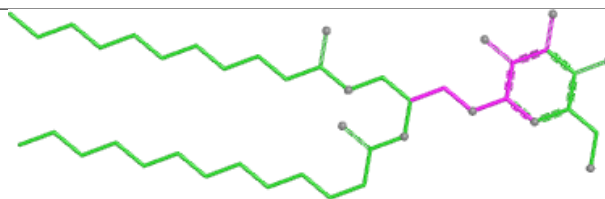


Rings

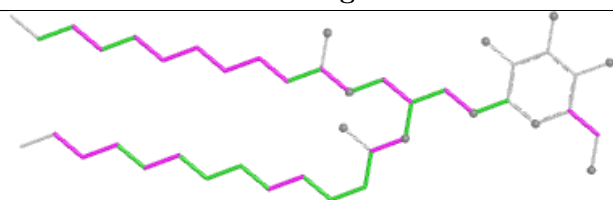
Ligand LMG K 318



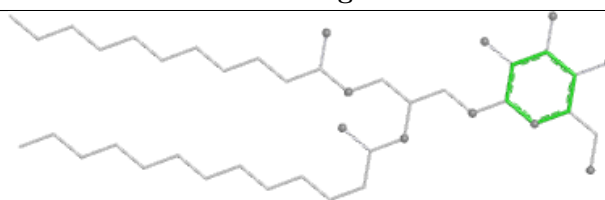
Bond lengths



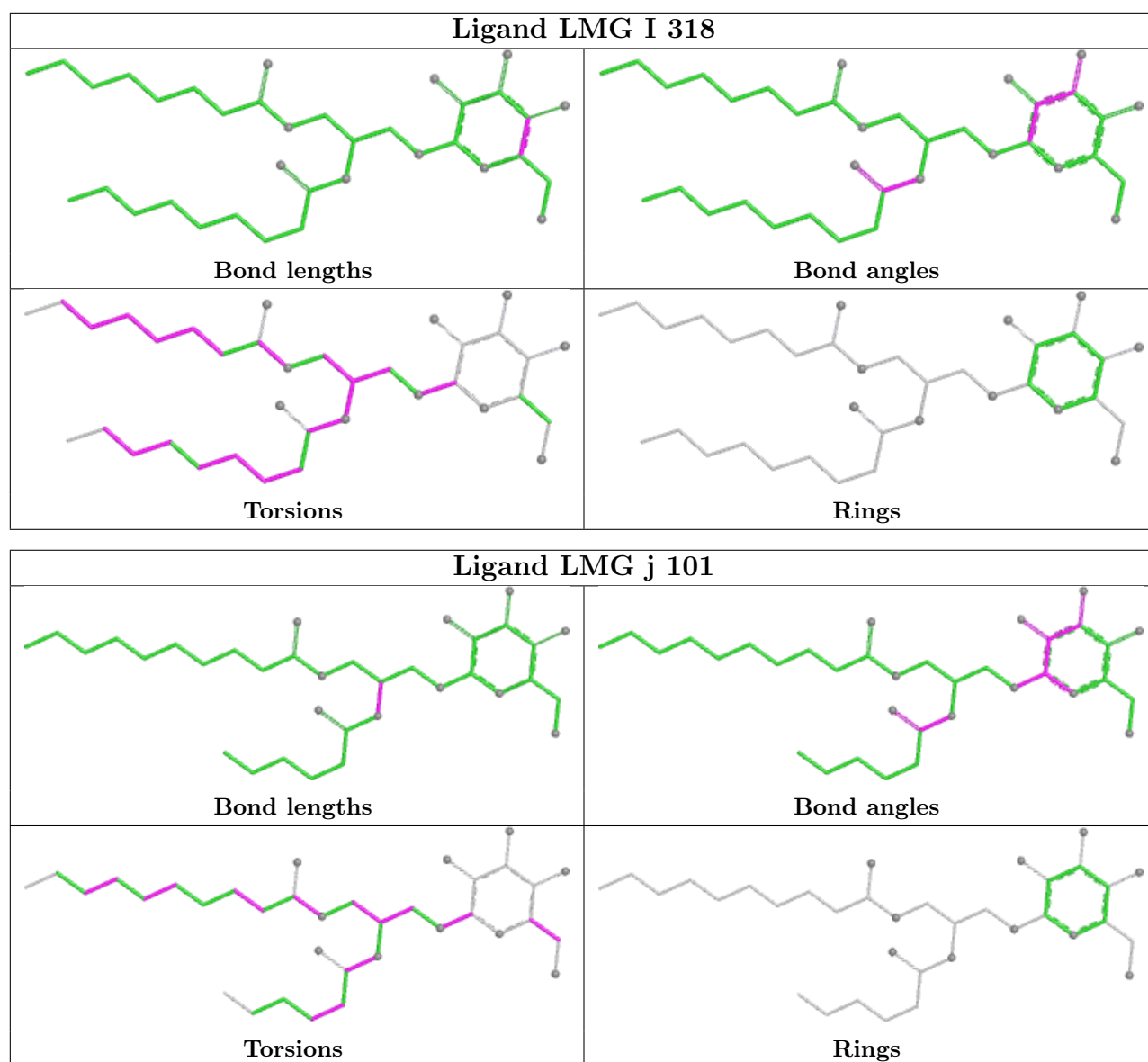
Bond angles



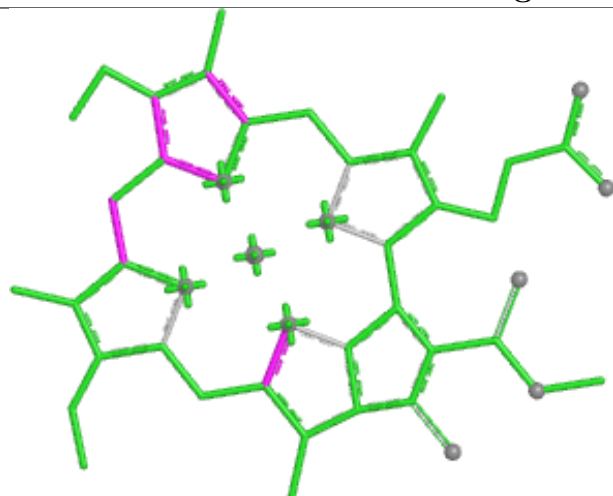
Torsions



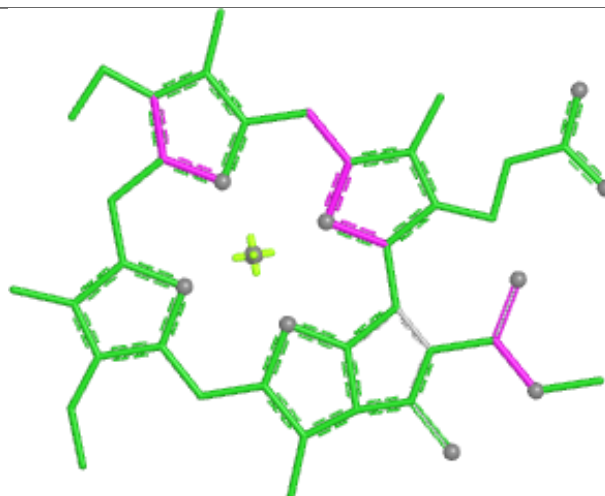
Rings



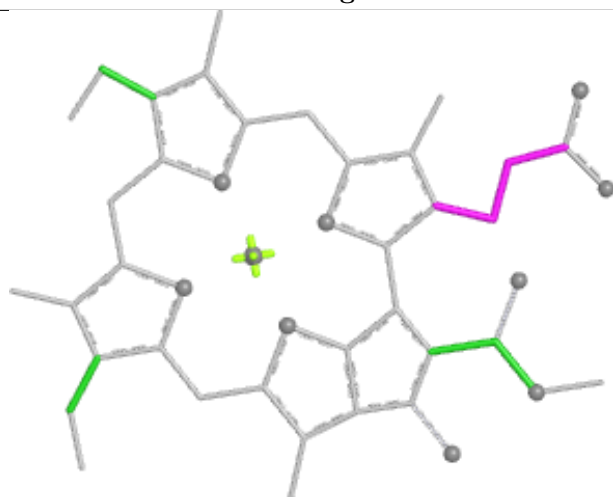
Ligand CLA B 308



Bond lengths



Bond angles

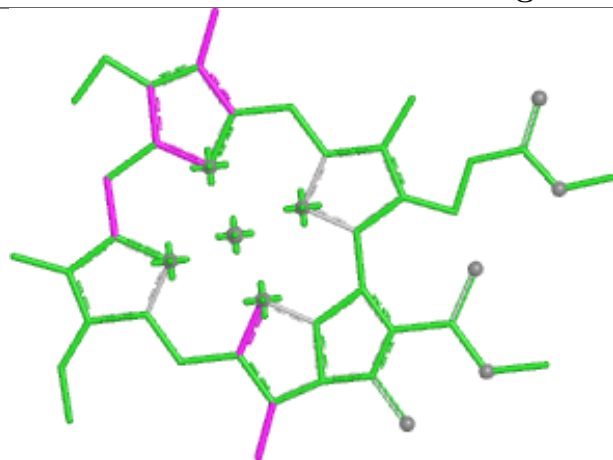


Torsions

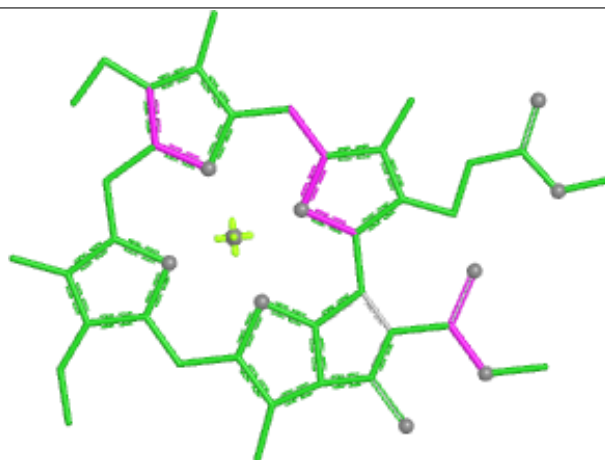


Rings

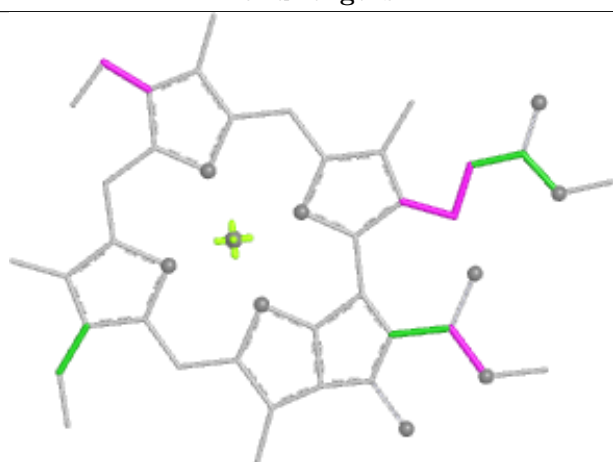
Ligand CLA L 312



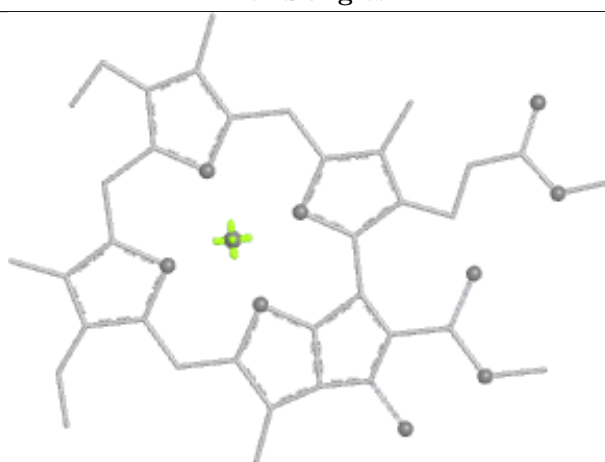
Bond lengths



Bond angles

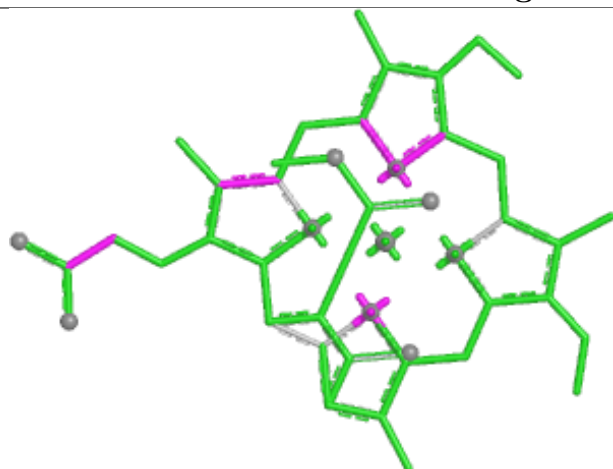


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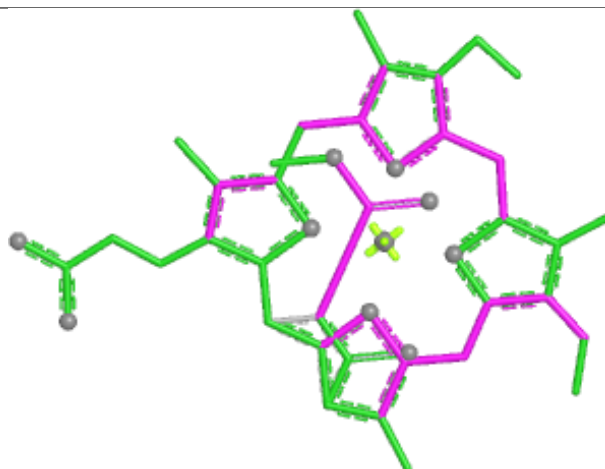


Rings

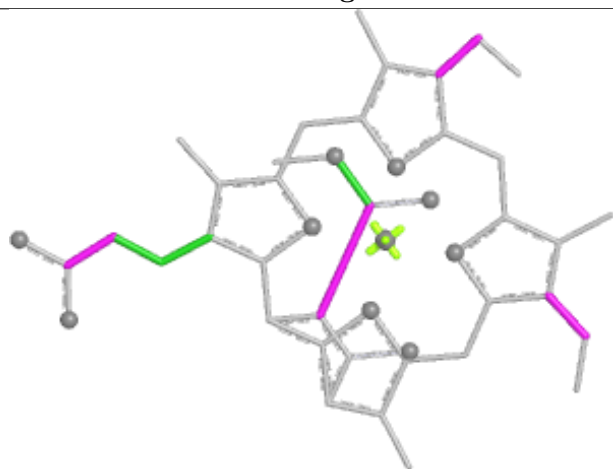
Ligand KC1 G 515



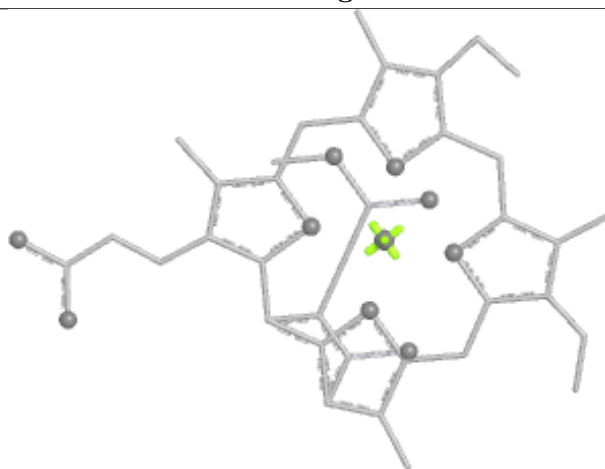
Bond lengths



Bond angles

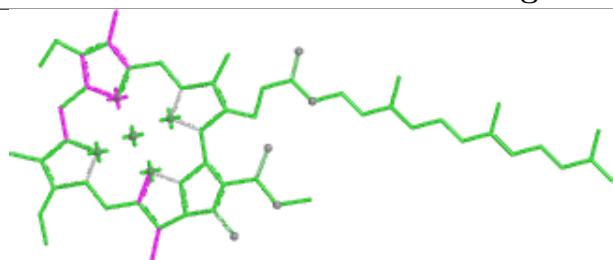


Torsions

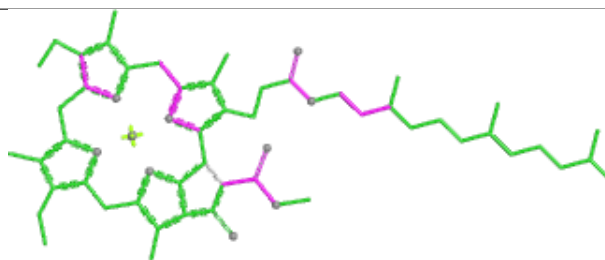


Rings

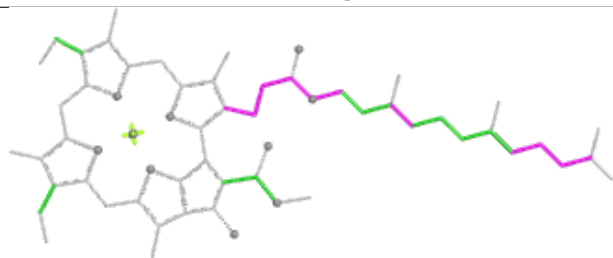
Ligand CLA I 308



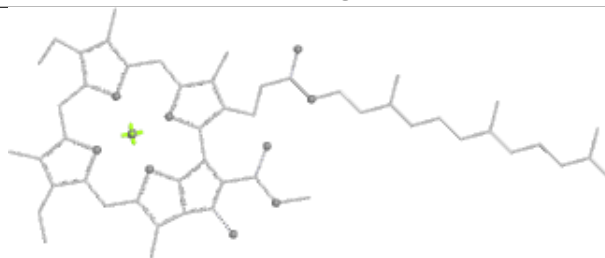
Bond lengths



Bond angles

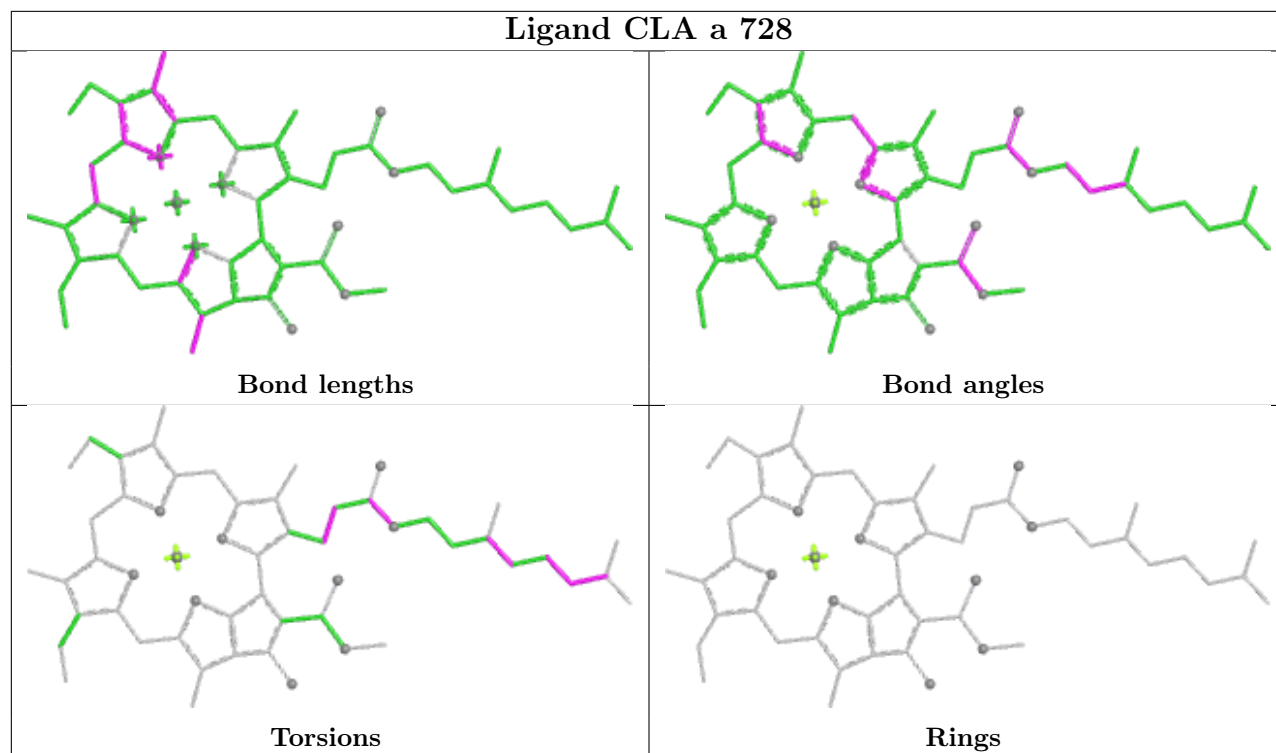


Torsions

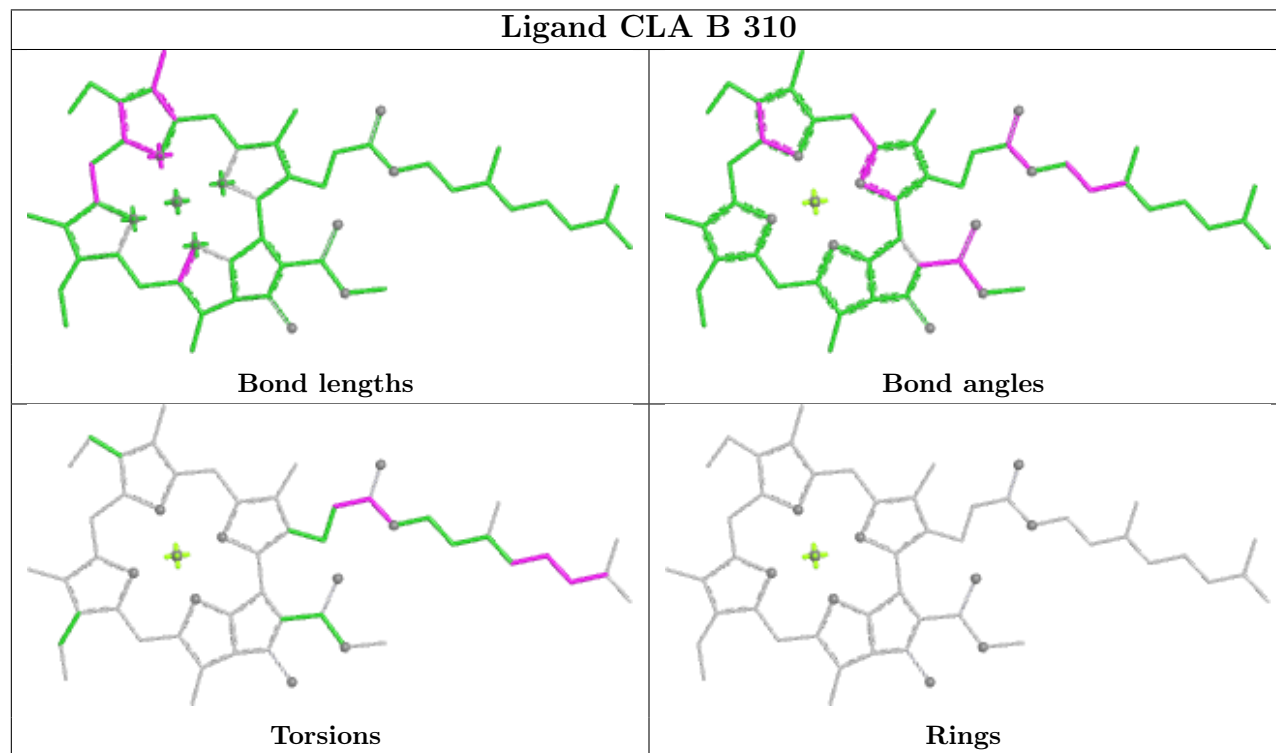


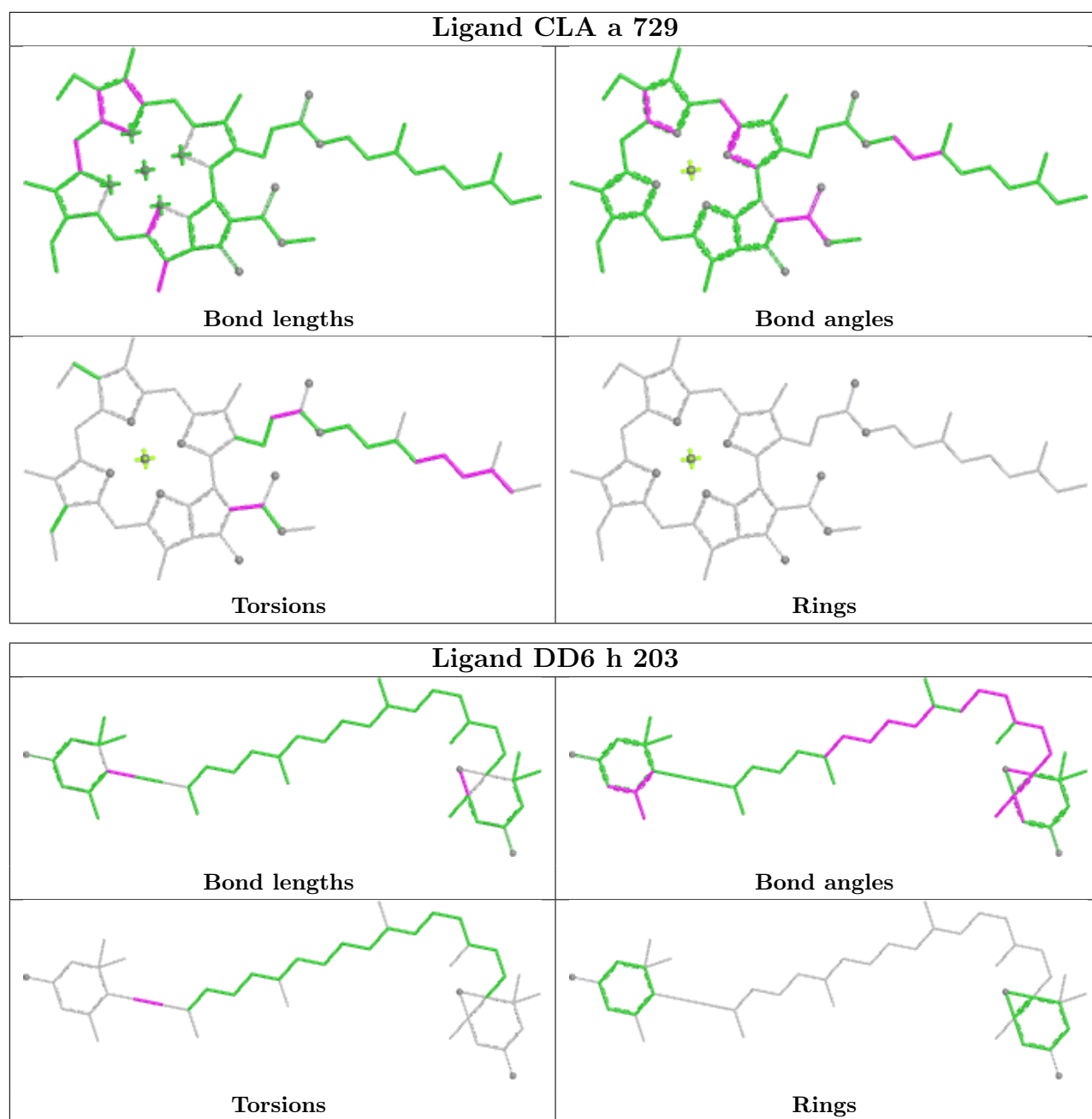
Rings

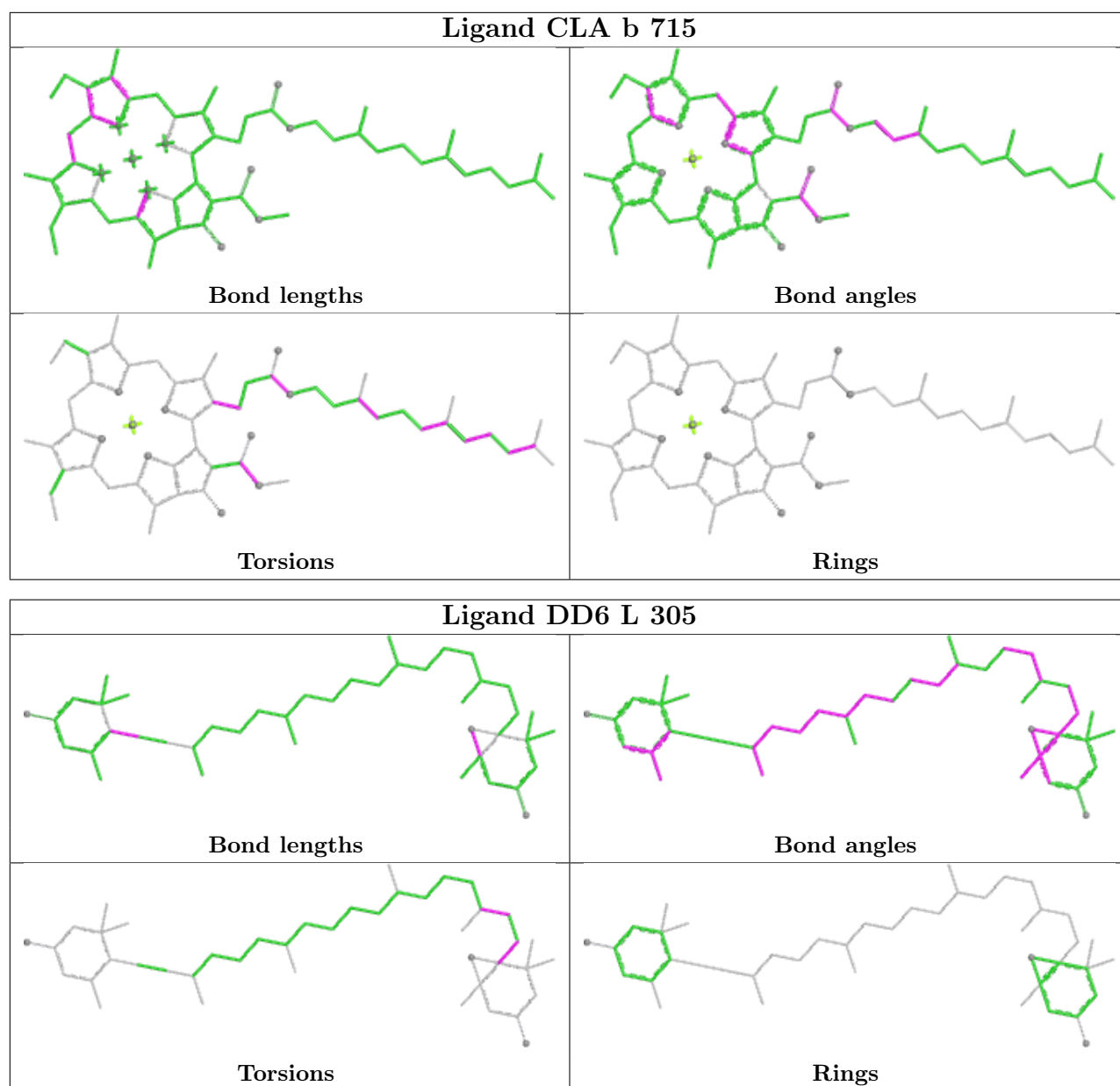
Ligand CLA a 728



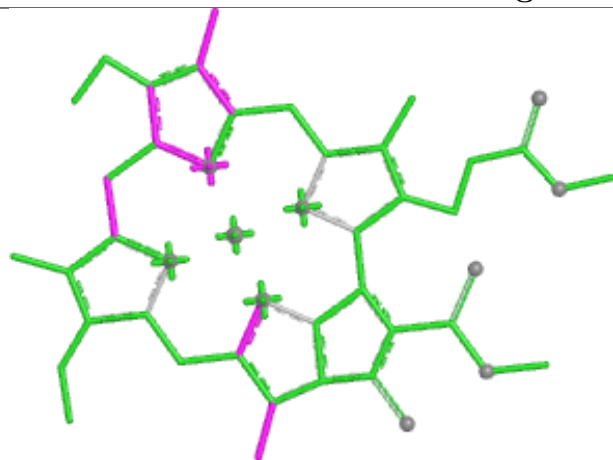
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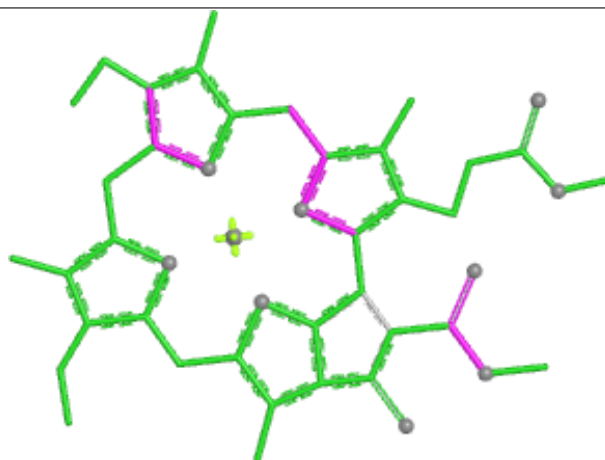




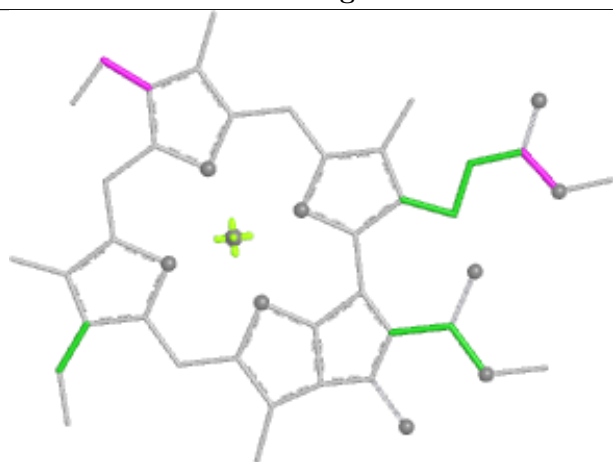
Ligand CLA F 307



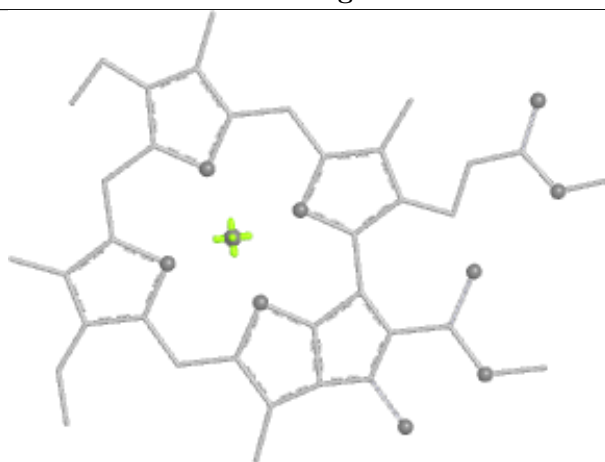
Bond lengths



Bond angles

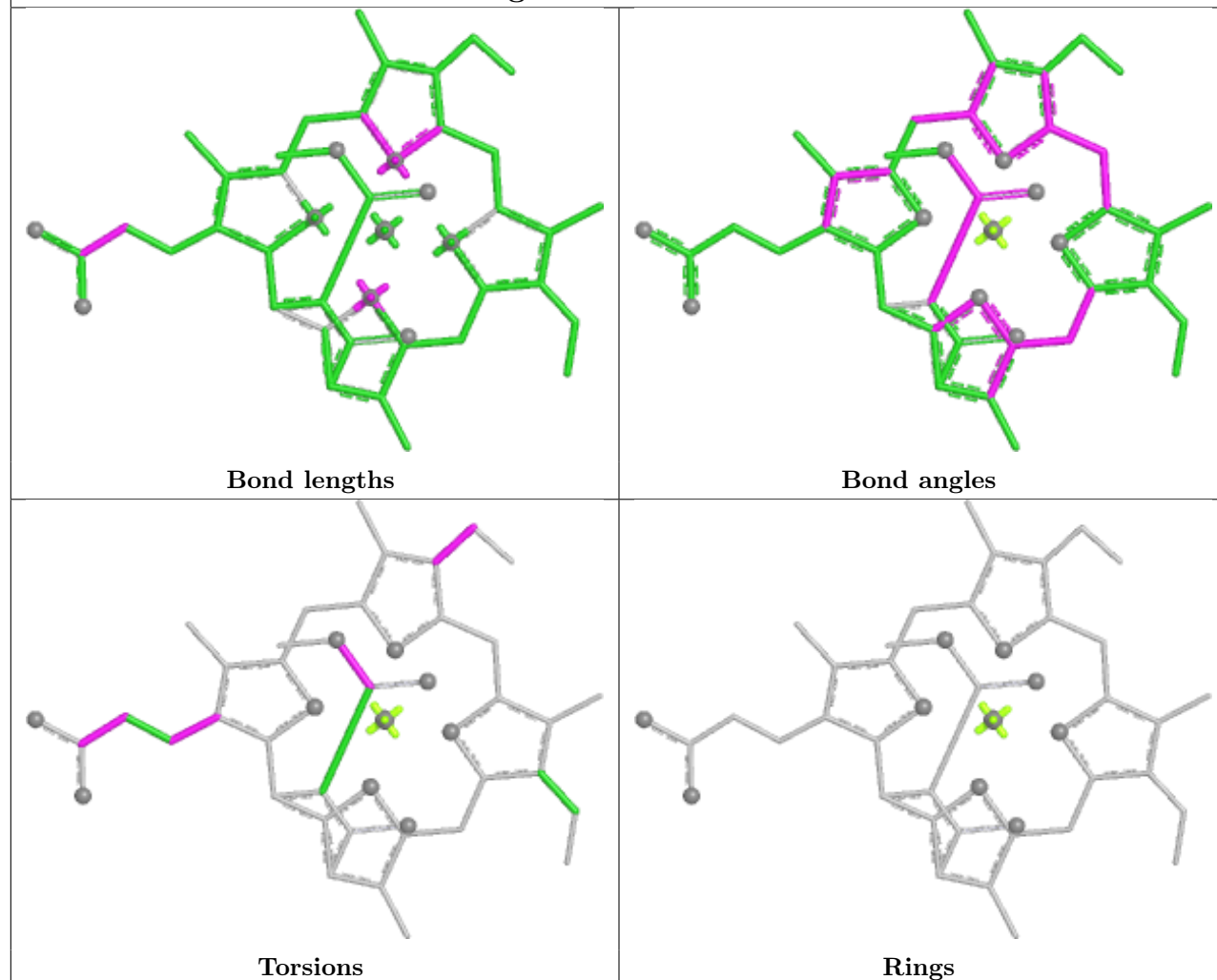


Torsions

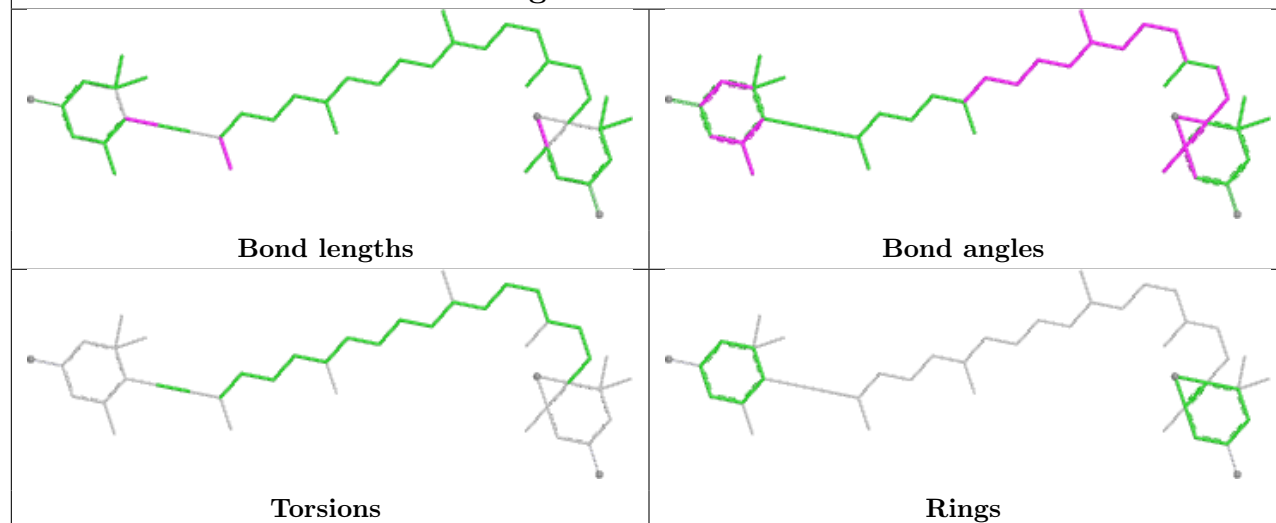


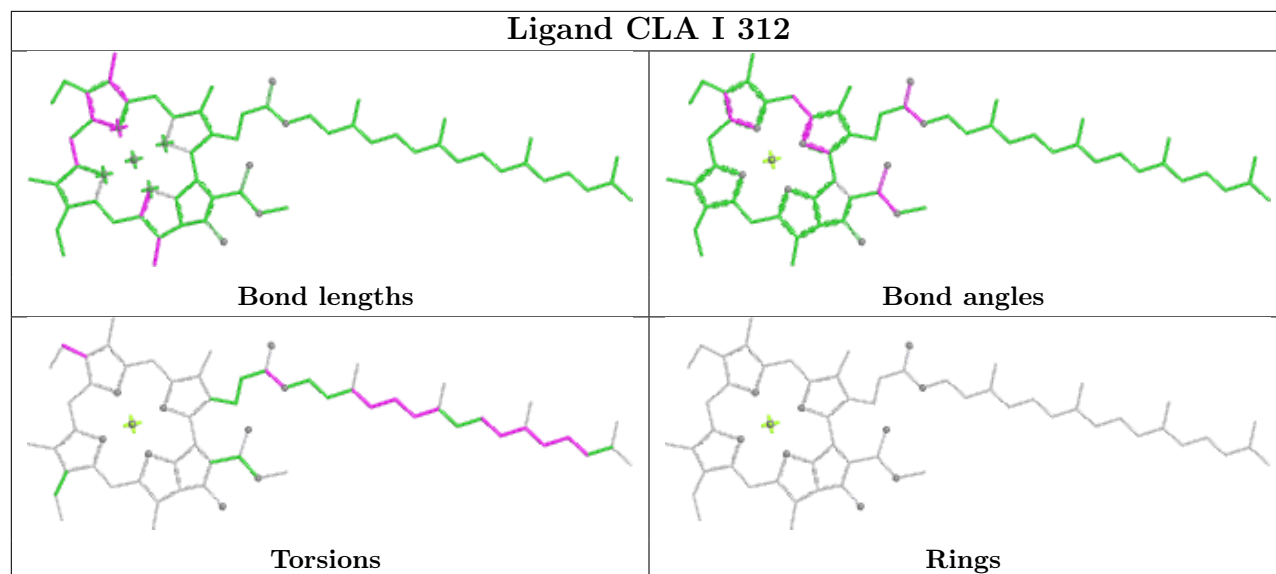
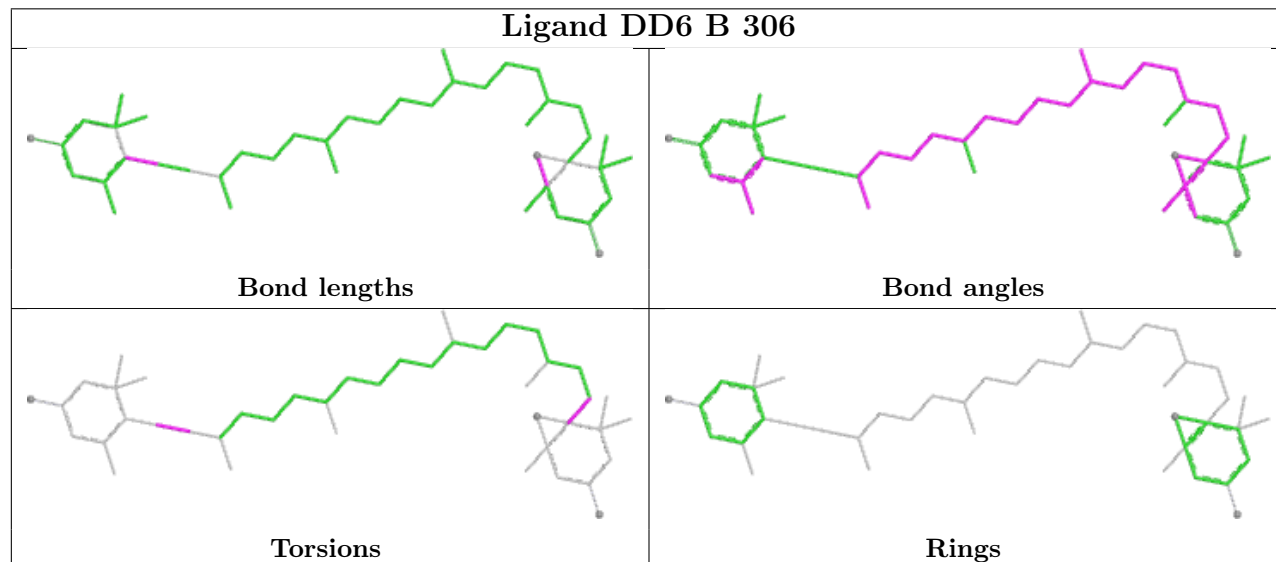
Rings

Ligand KC1 N 306

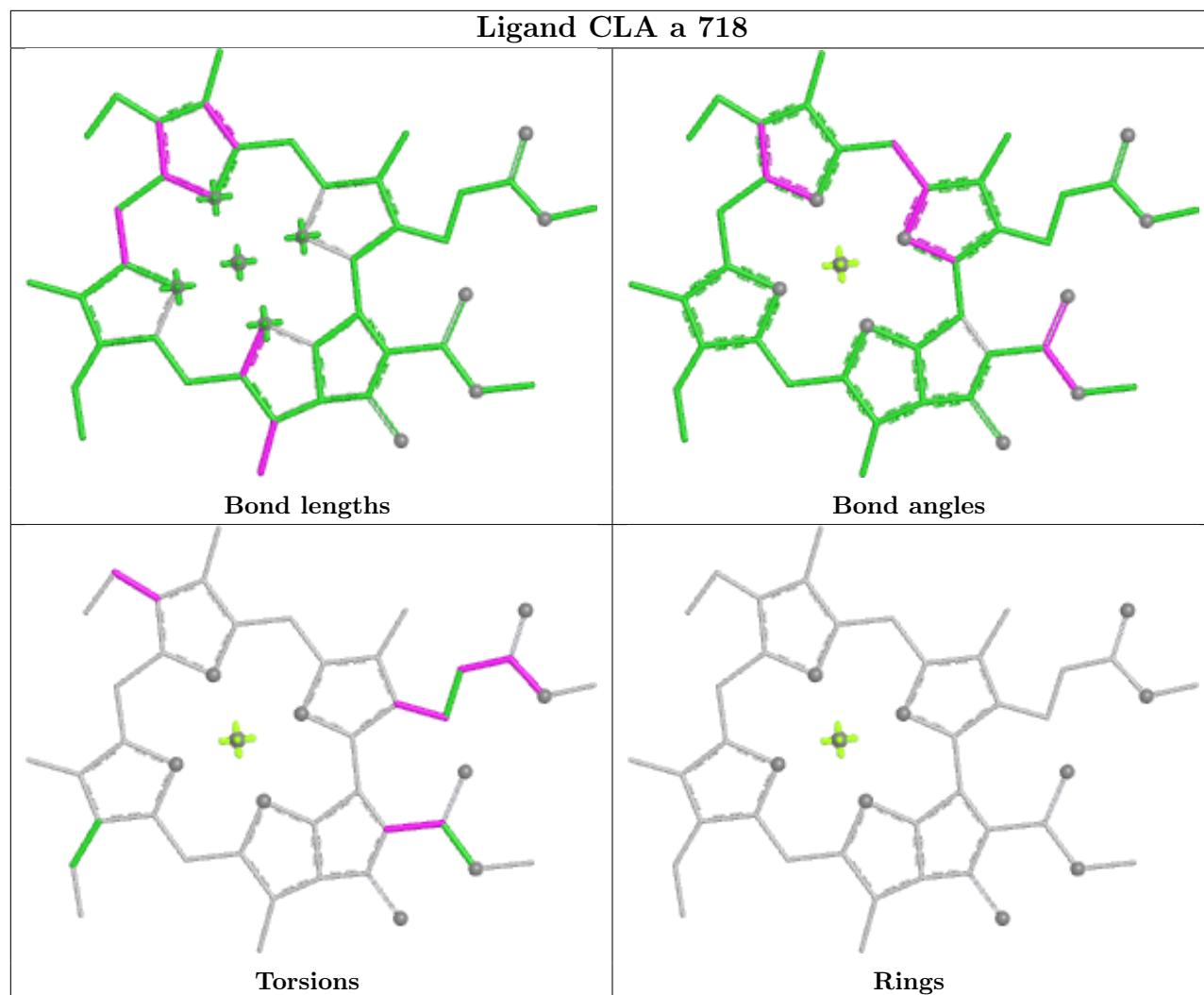


Ligand DD6 M 304

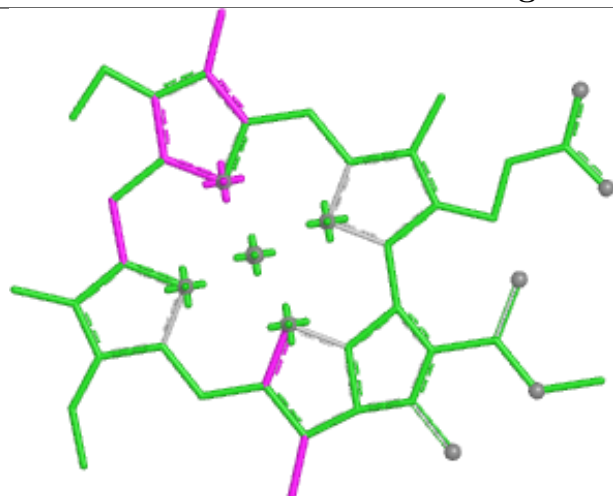


Ligand CLA I 312**Ligand DD6 B 306**

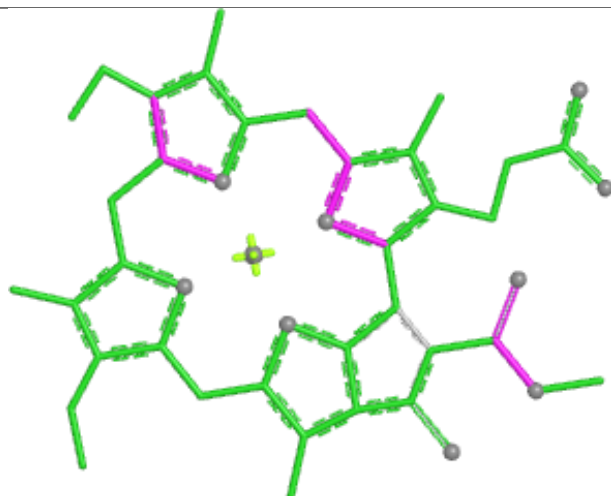
Ligand CLA a 718



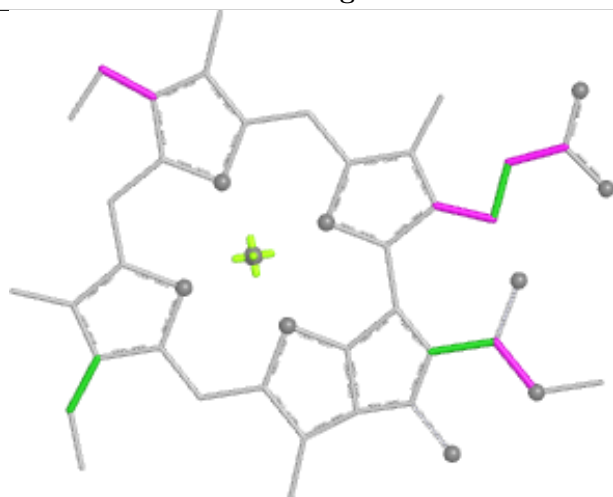
Ligand CLA a 715



Bond lengths



Bond angles

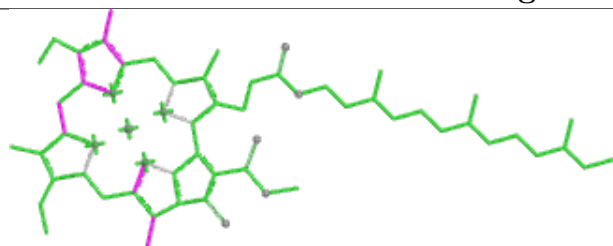


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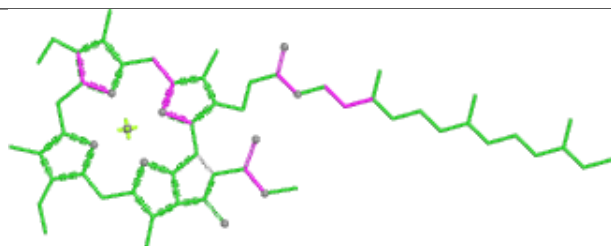


Rings

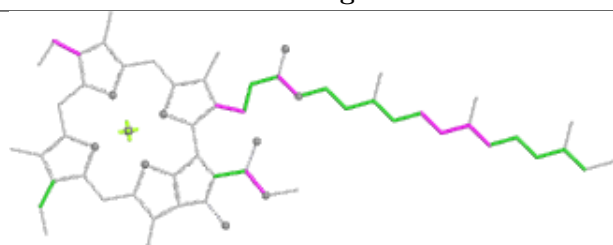
Ligand CLA a 725



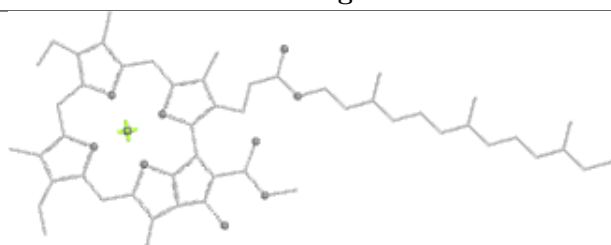
Bond lengths



Bond angles

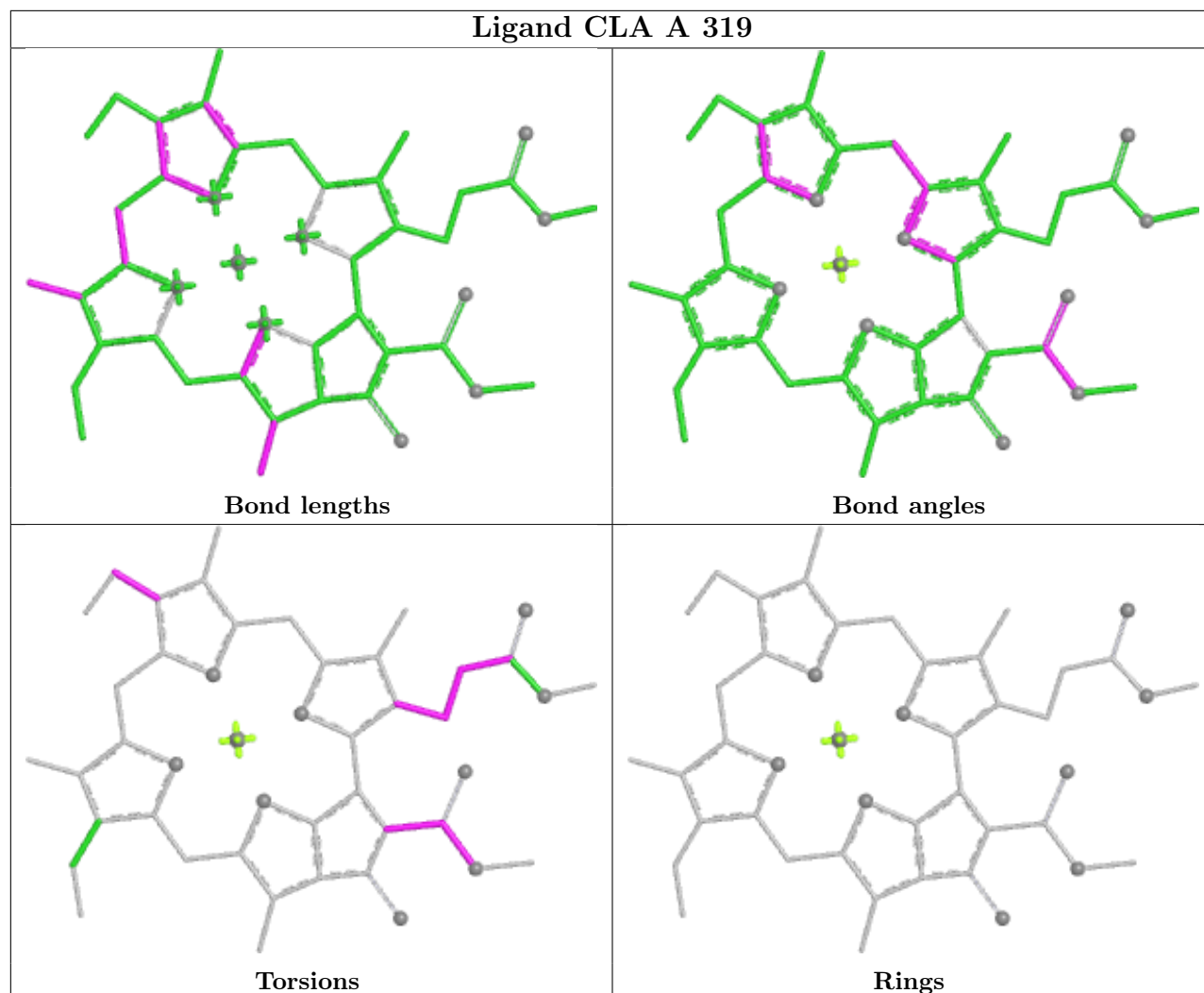


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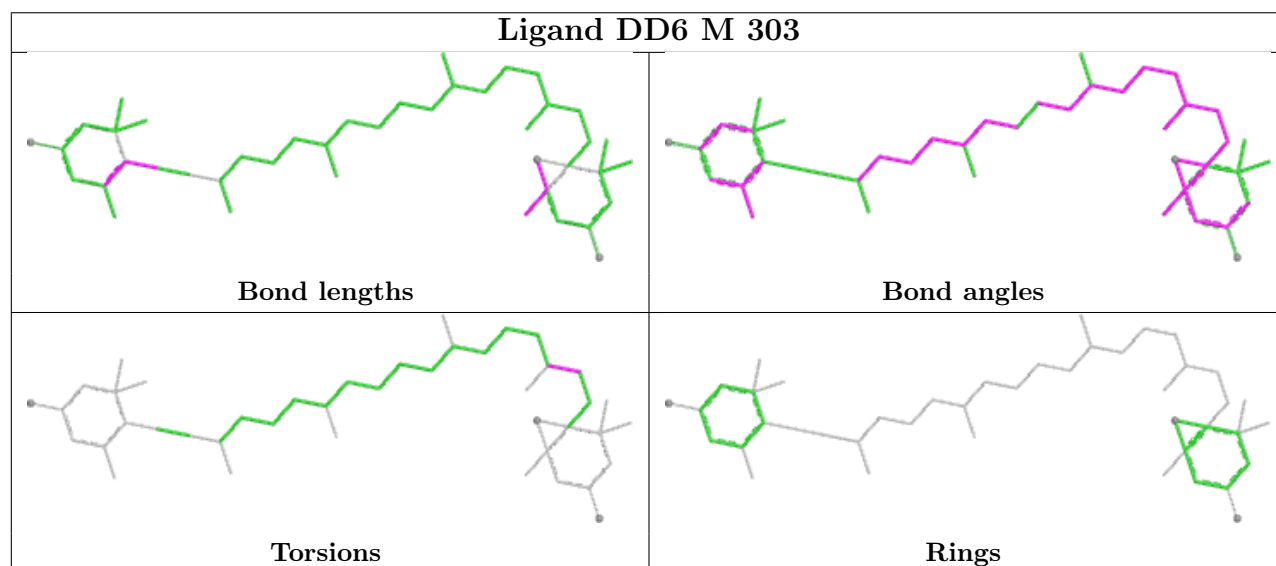


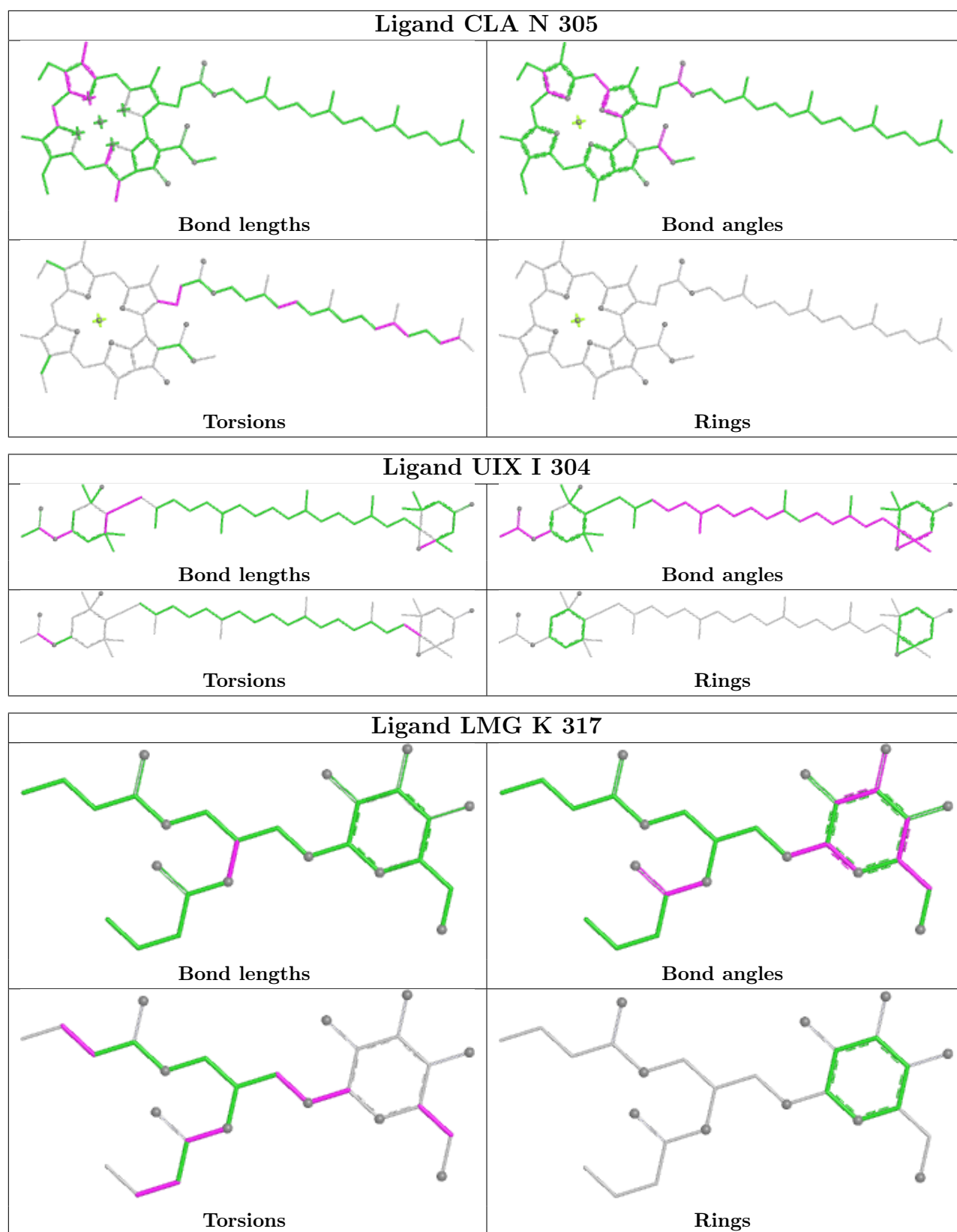
Rings

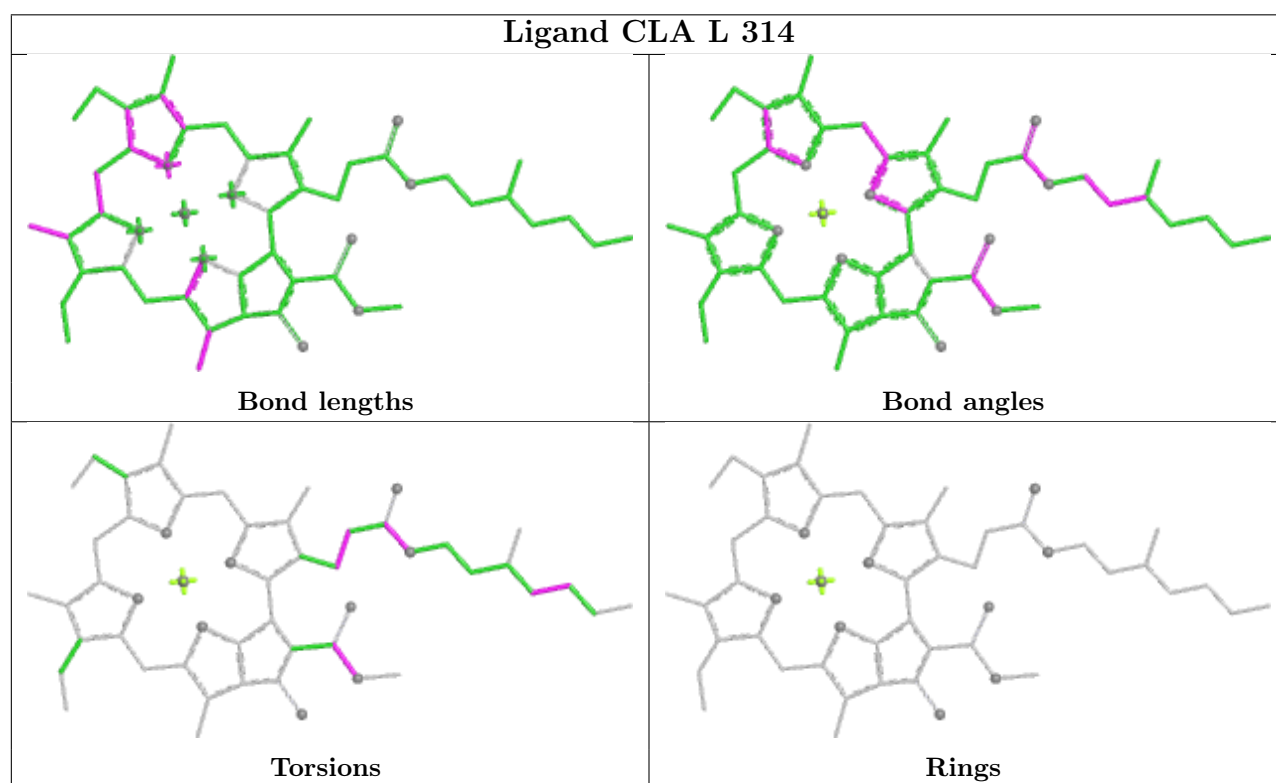
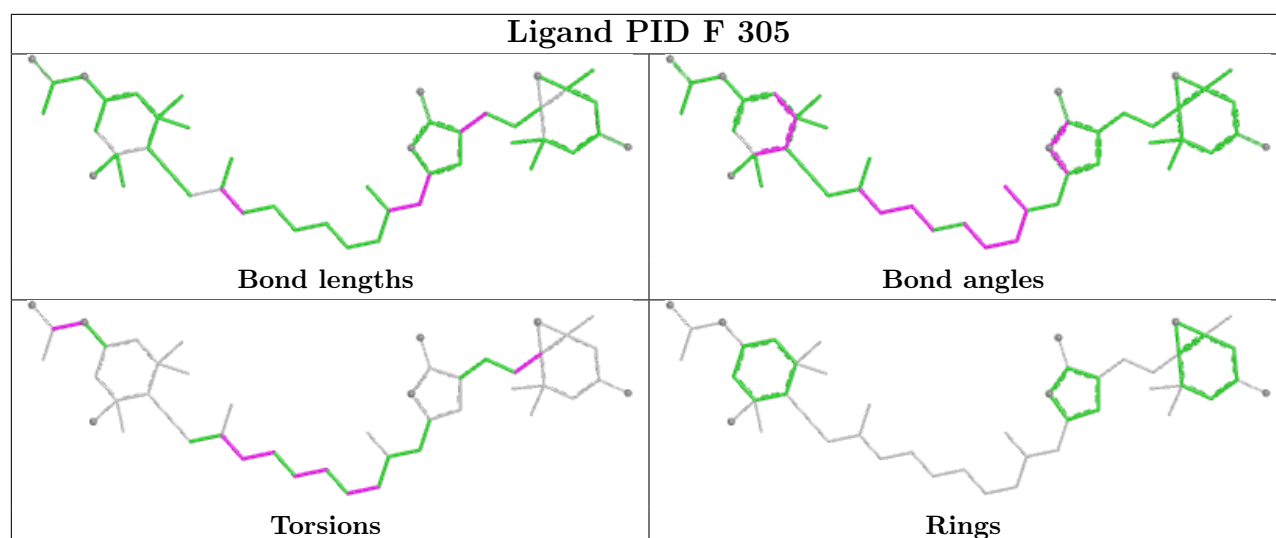
Ligand CLA A 319



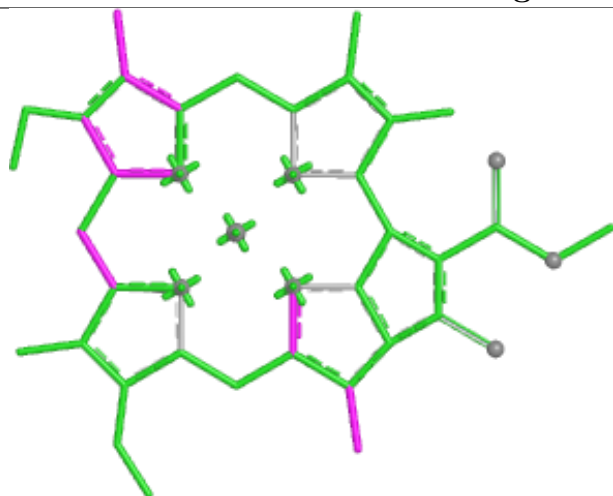
Ligand DD6 M 303



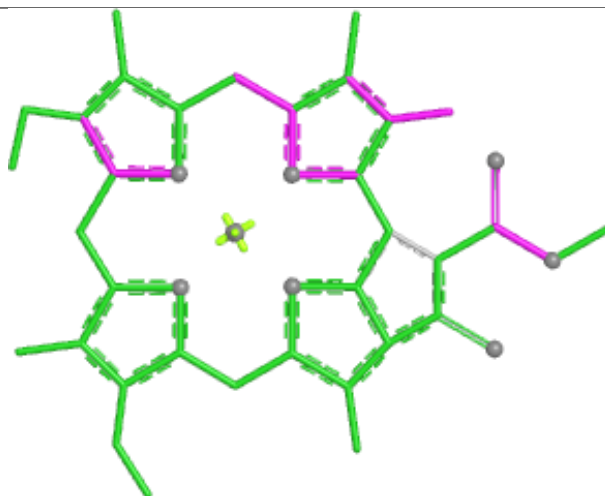




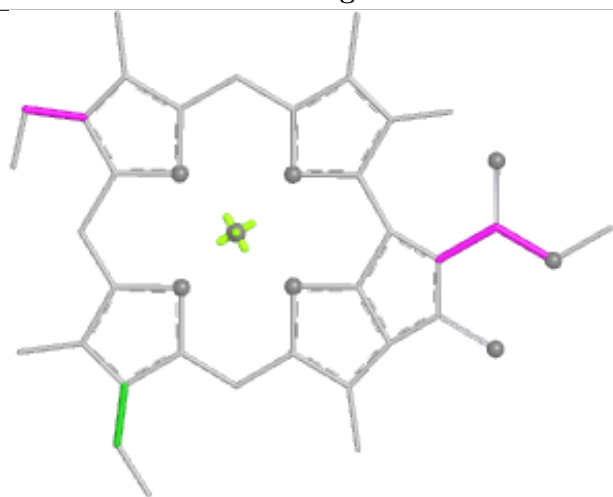
Ligand CLA H 311



Bond lengths



Bond angles

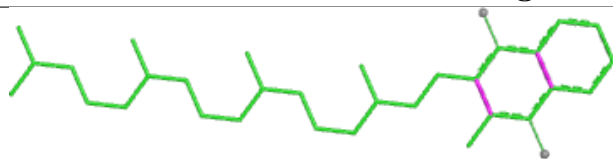


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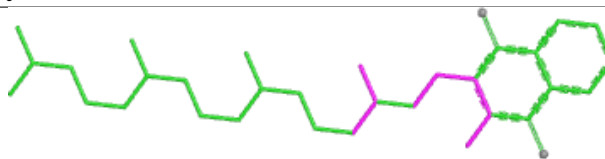


Rings

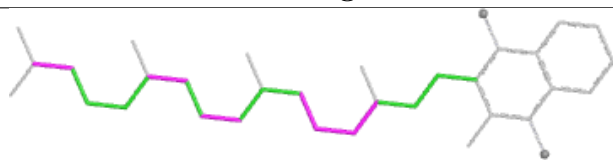
Ligand PQN a 732



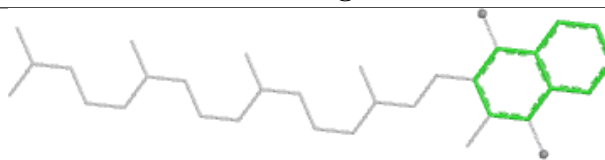
Bond lengths



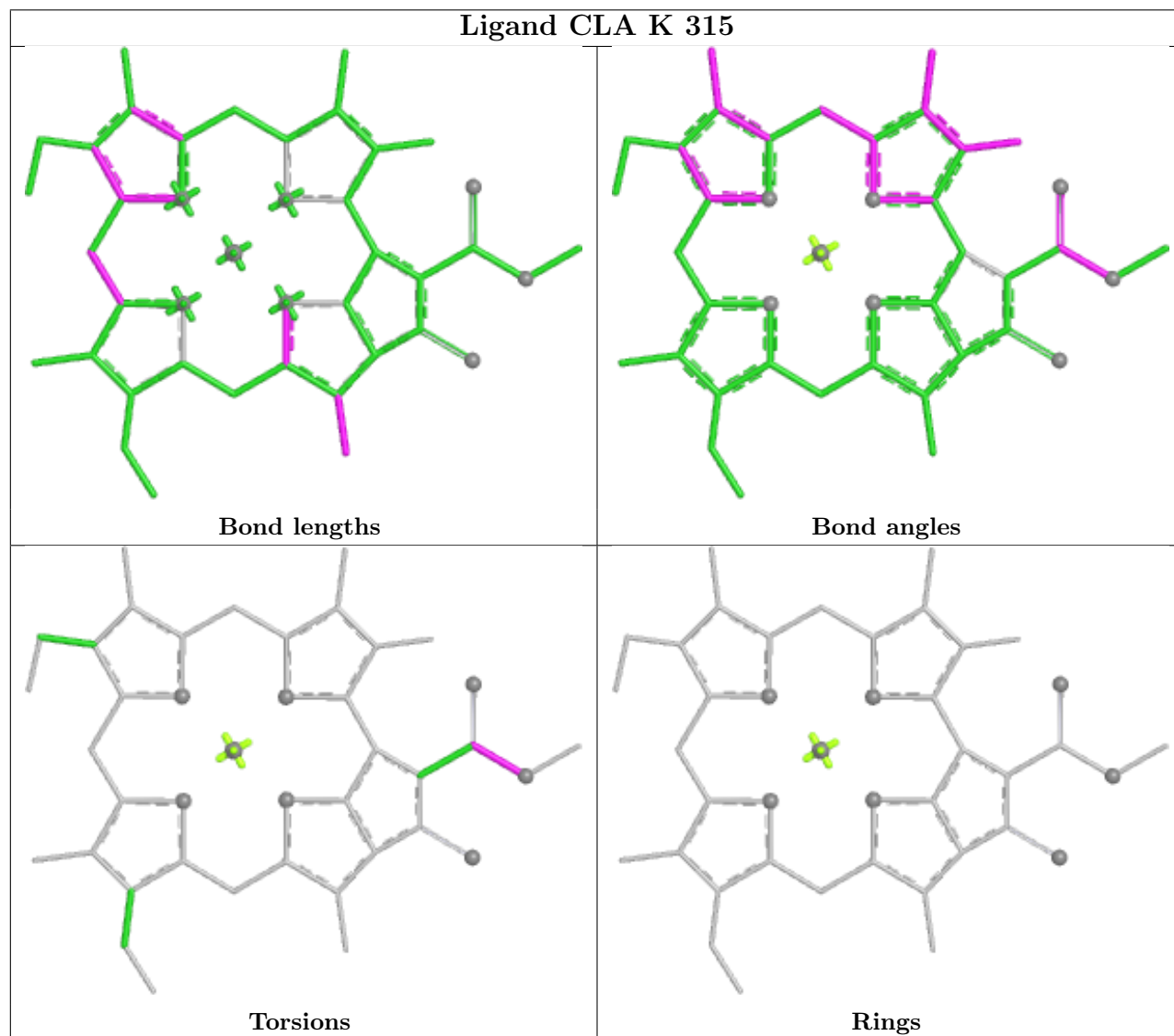
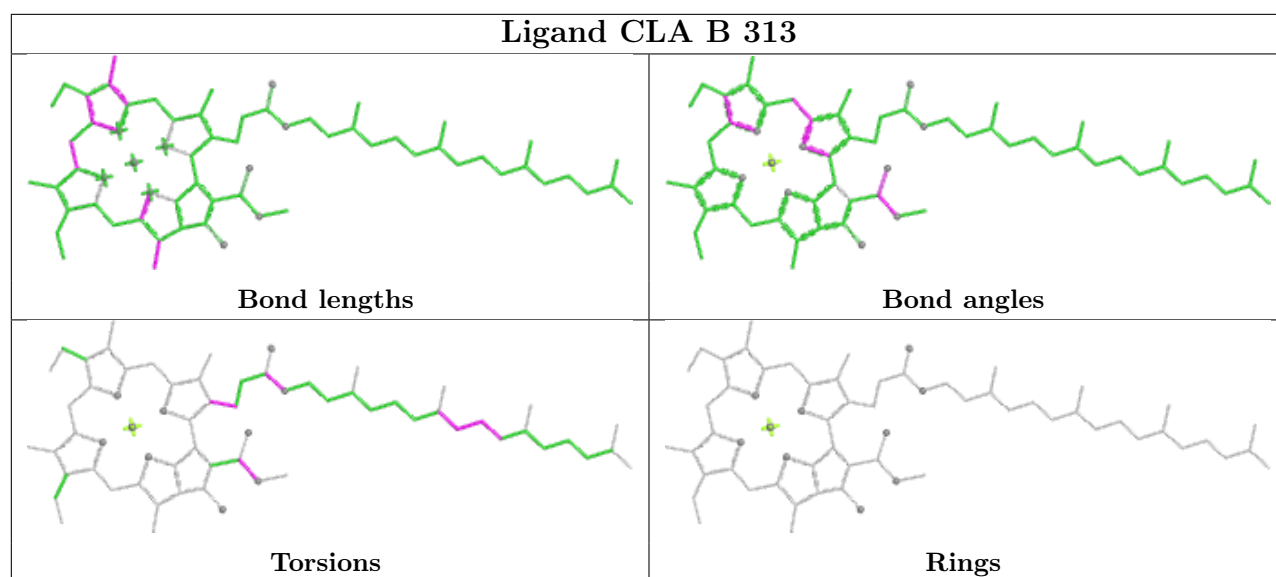
Bond angles



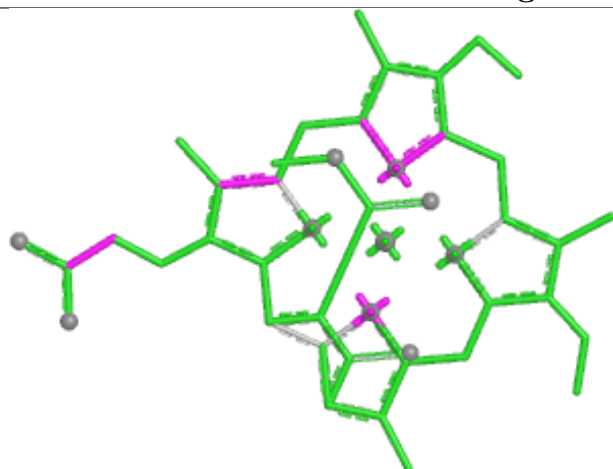
Torsions



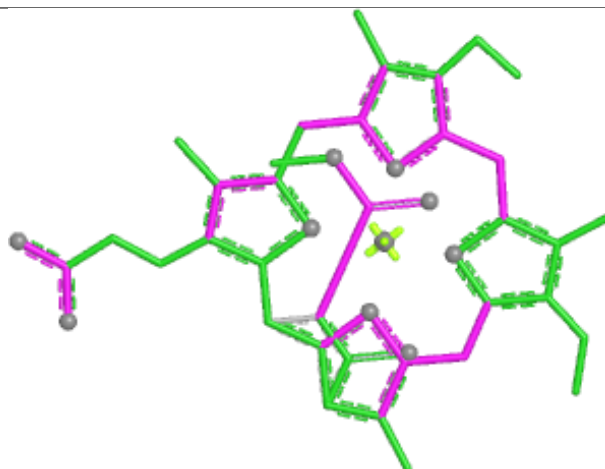
Rings



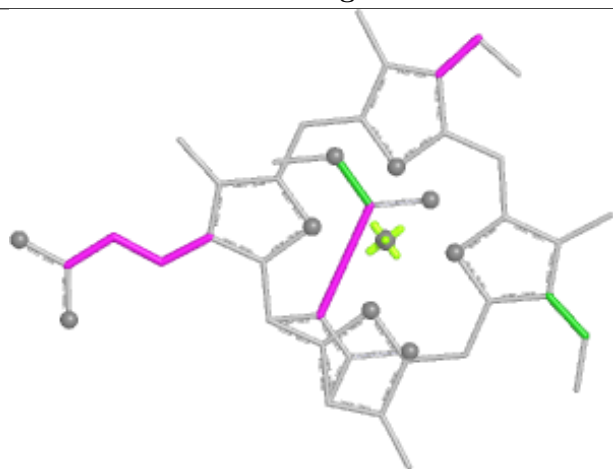
Ligand KC1 F 309



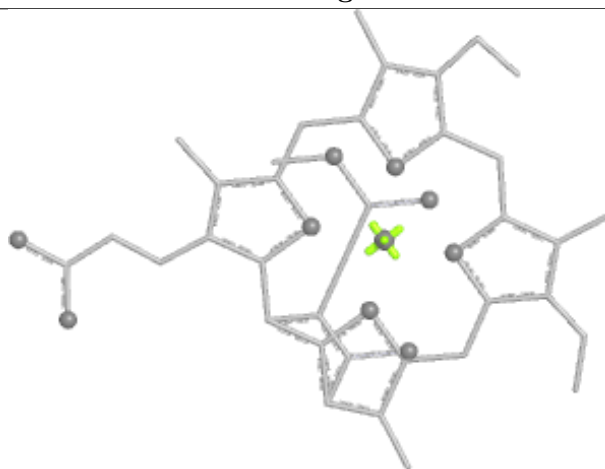
Bond lengths



Bond angles

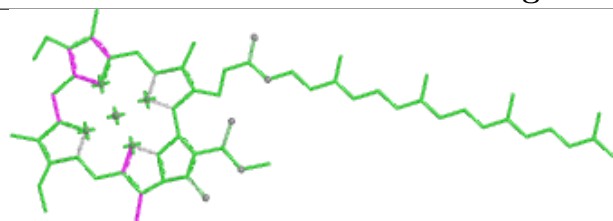


Torsions

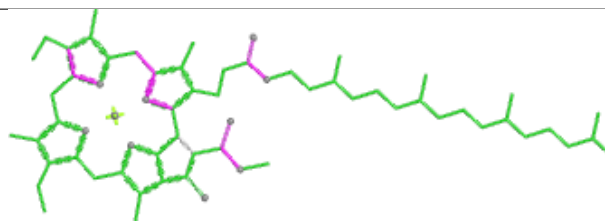


Rings

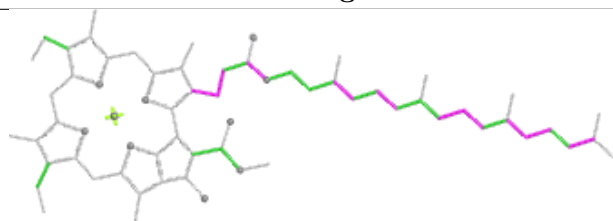
Ligand CLA I 311



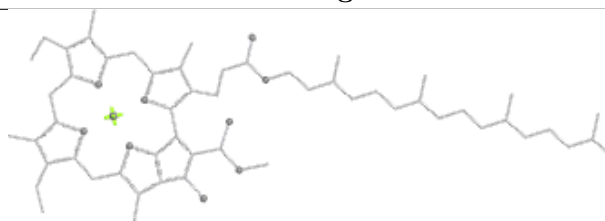
Bond lengths



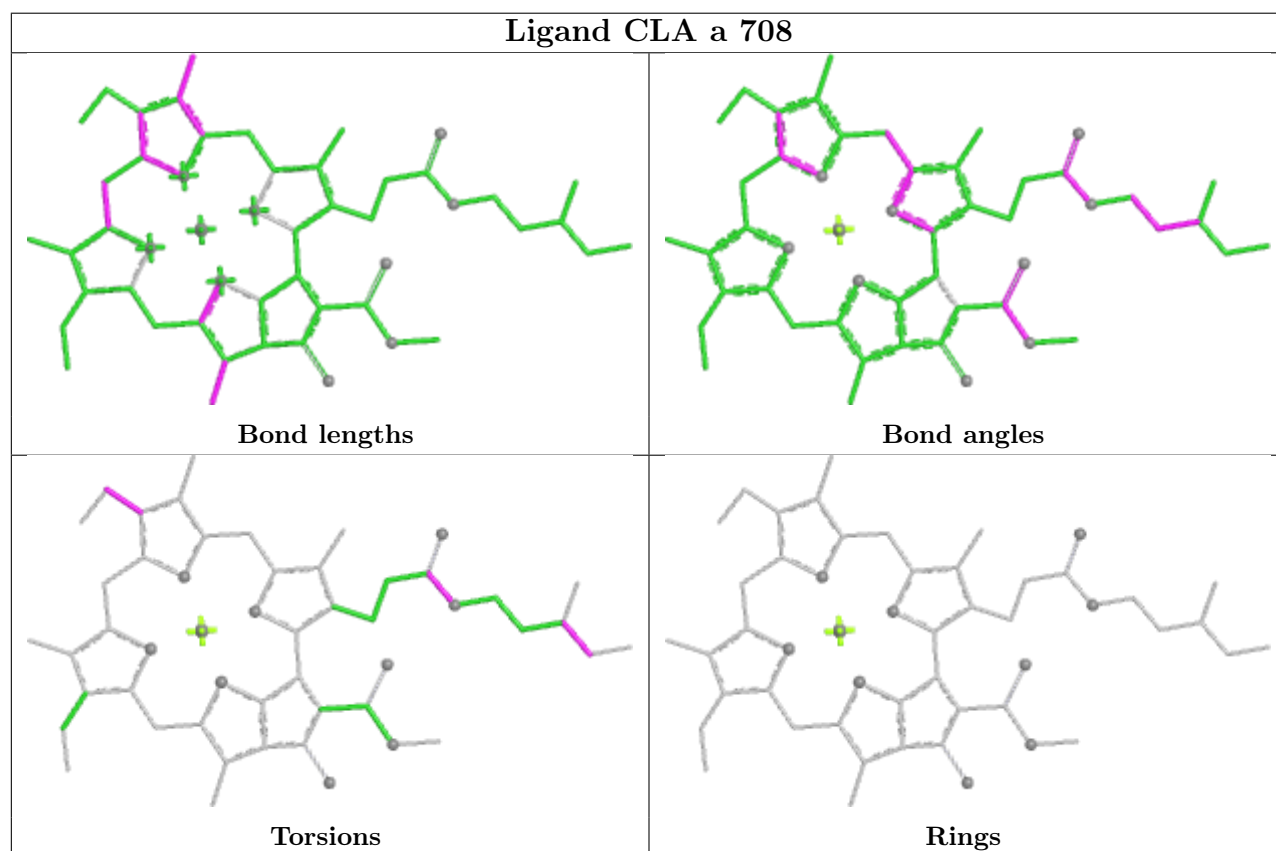
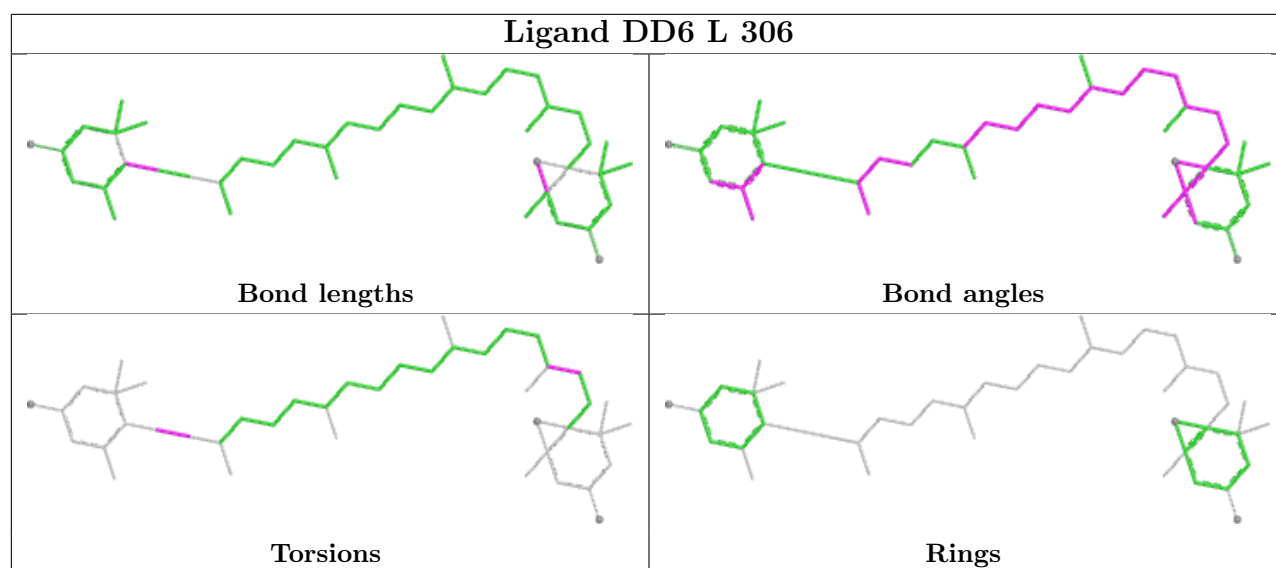
Bond angles

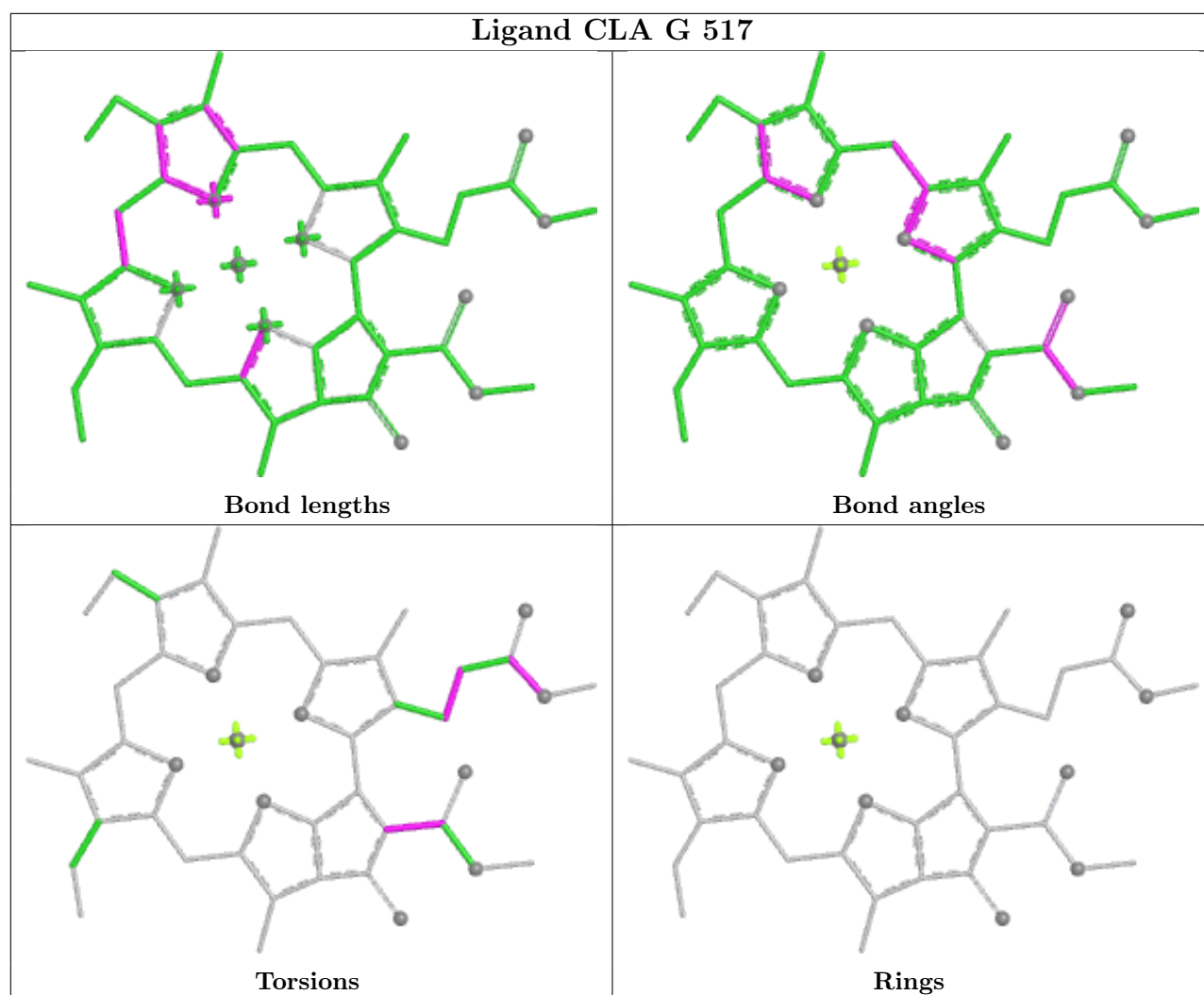


Torsions

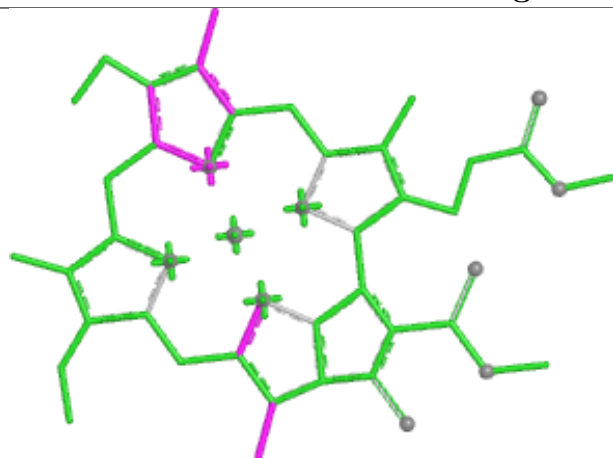


Rings

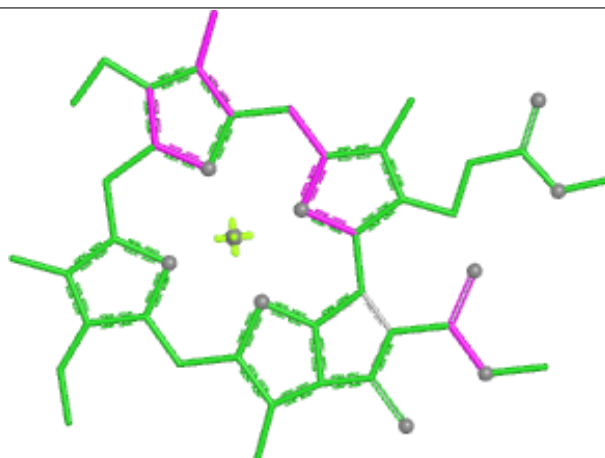




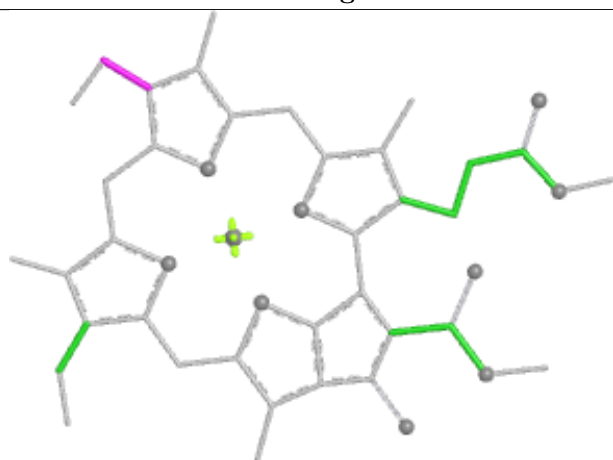
Ligand CLA K 307



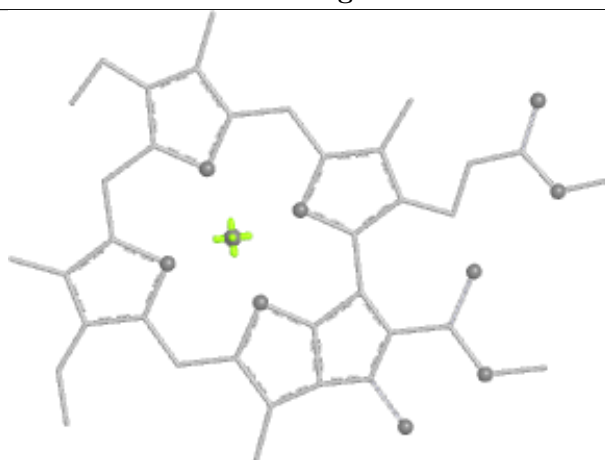
Bond lengths



Bond angles

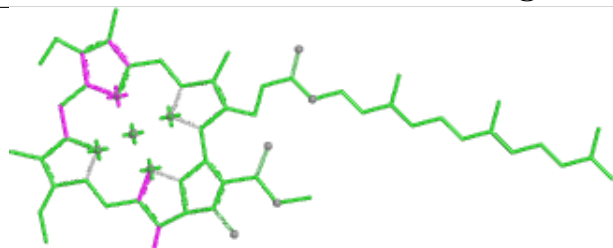


Torsions

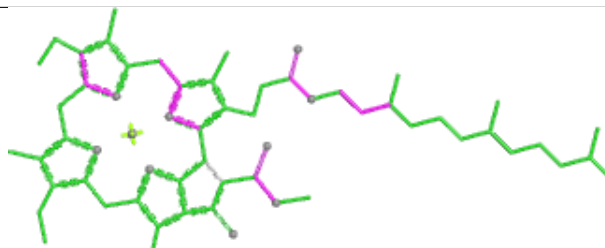


Rings

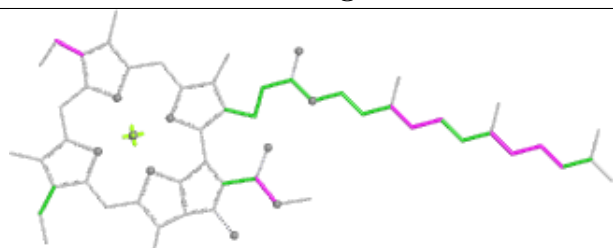
Ligand CLA a 713



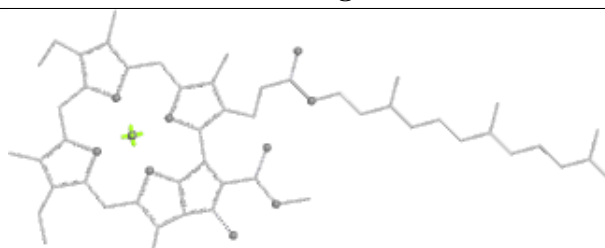
Bond lengths



Bond angles

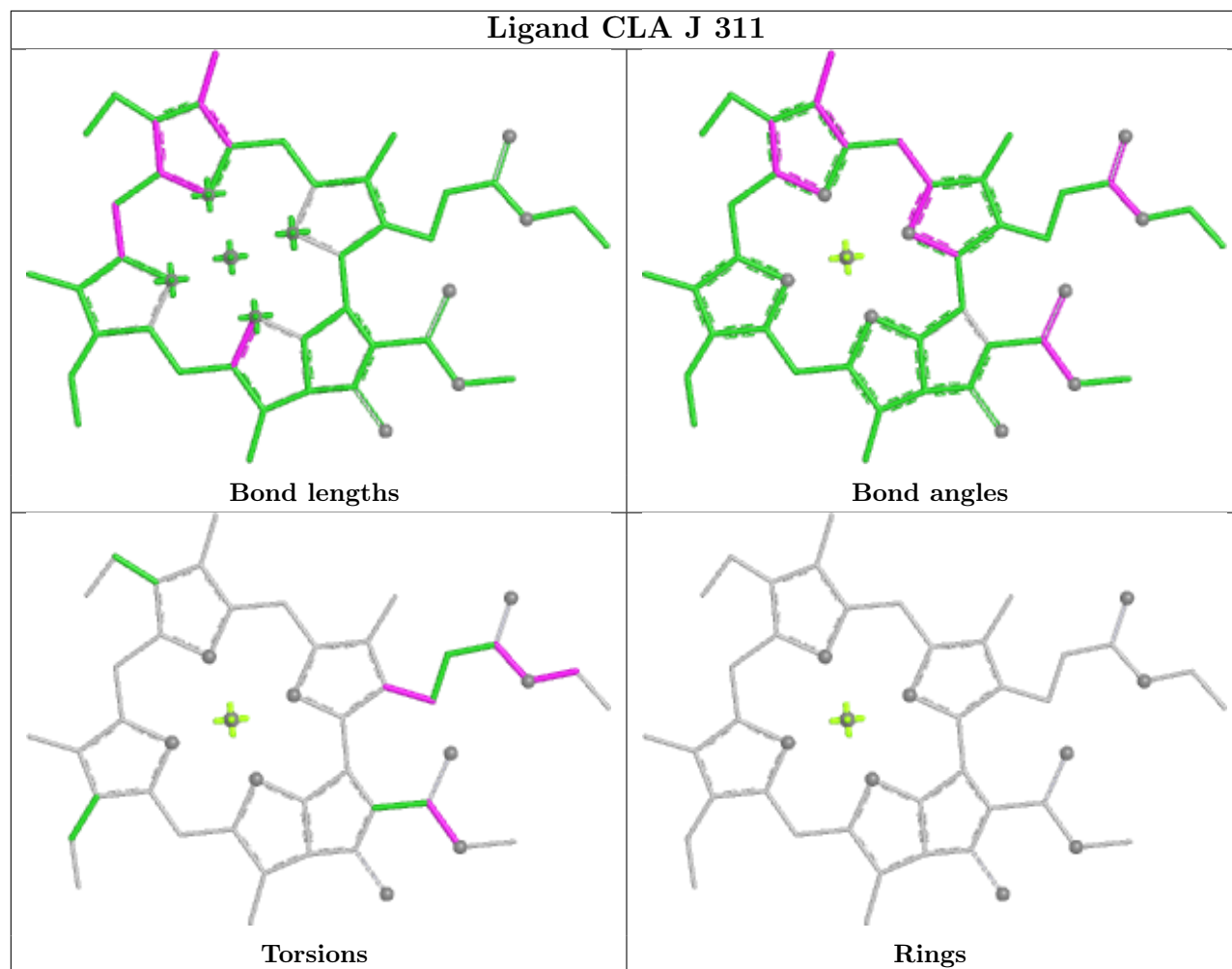


Torsions

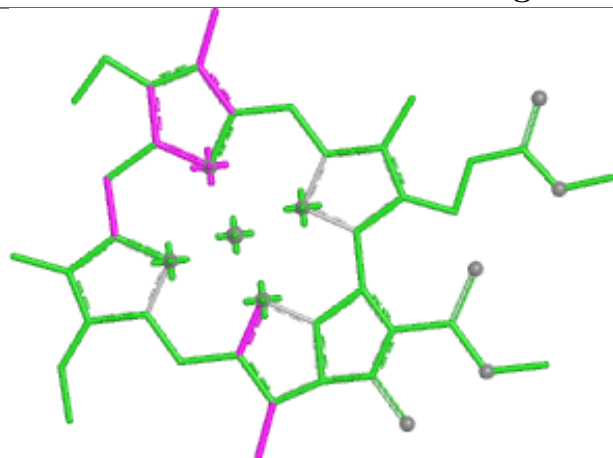


Rings

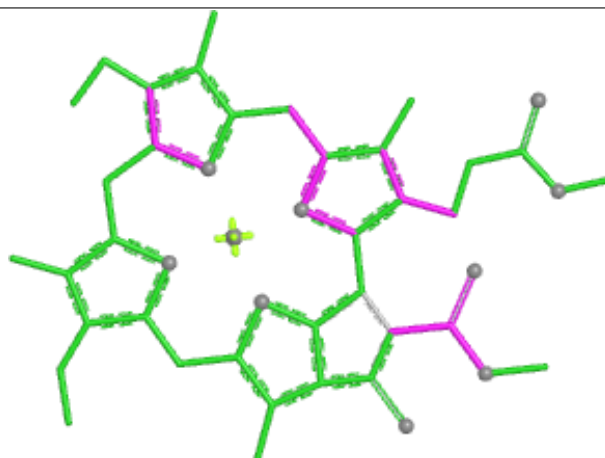
Ligand CLA J 311



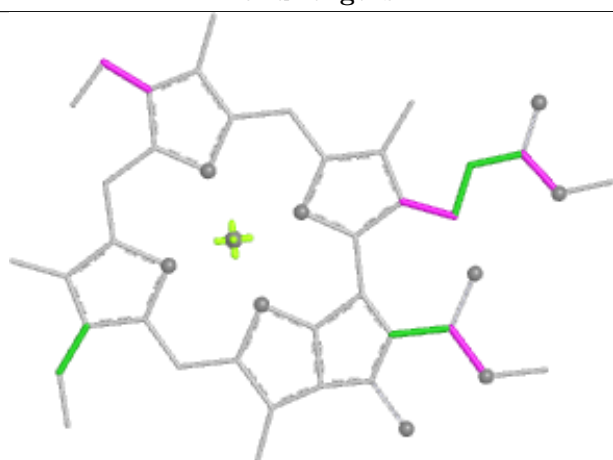
Ligand CLA D 314



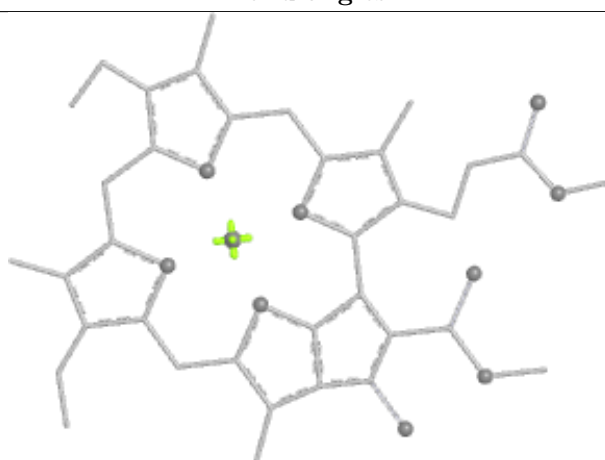
Bond lengths



Bond angles

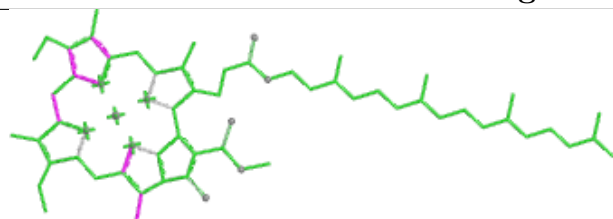


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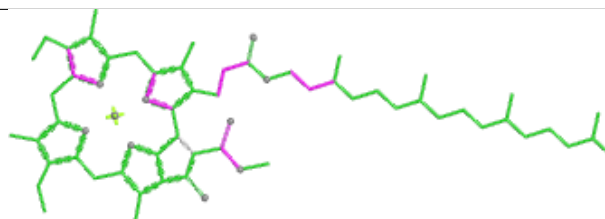


Rings

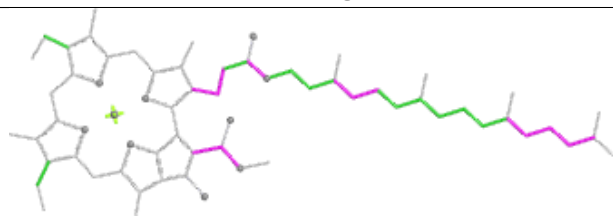
Ligand CLA a 735



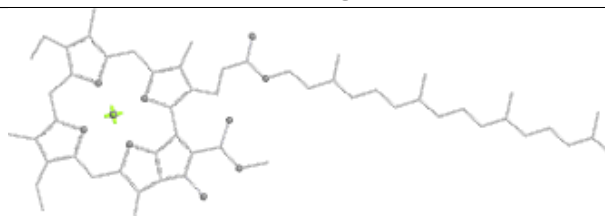
Bond lengths



Bond angles

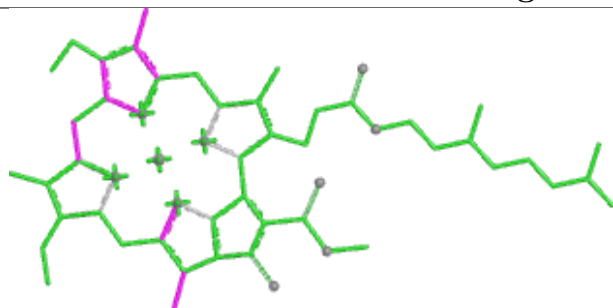


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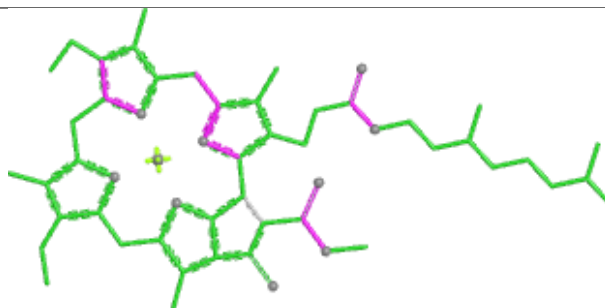


Rings

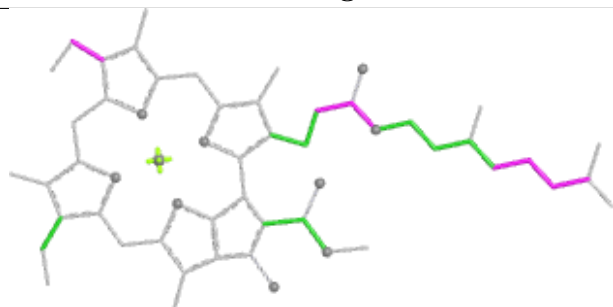
Ligand CLA h 202



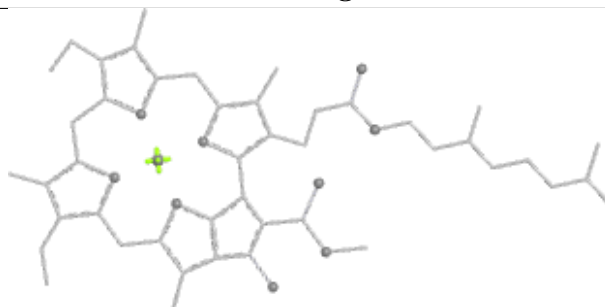
Bond lengths



Bond angles

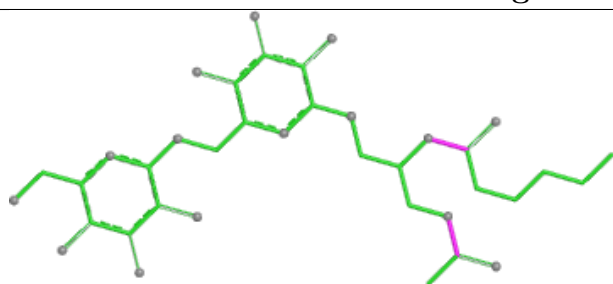


Torsions

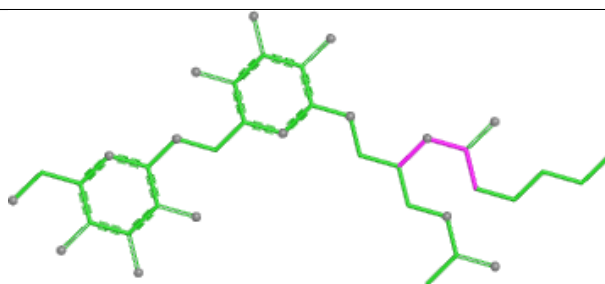


Rings

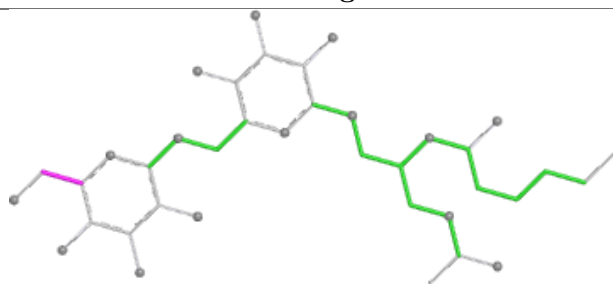
Ligand DGD L 301



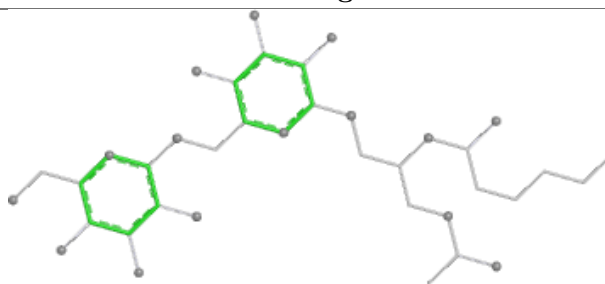
Bond lengths



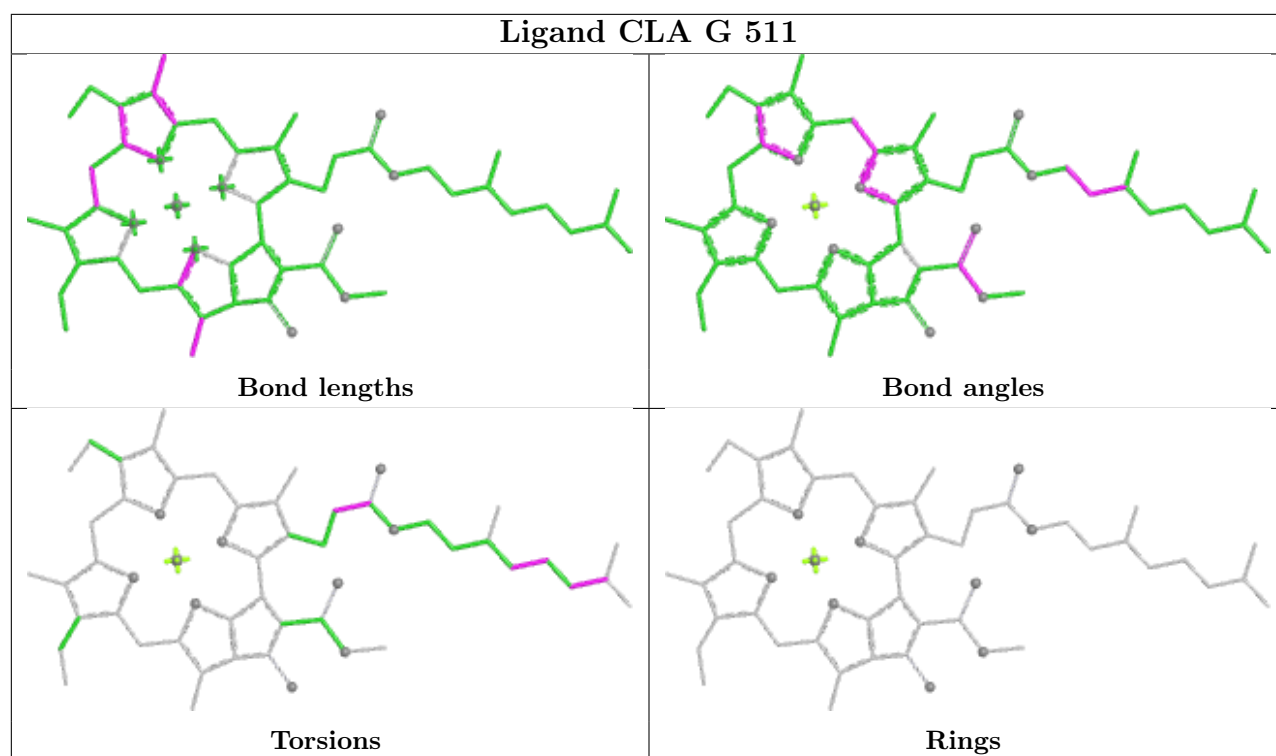
Bond angles



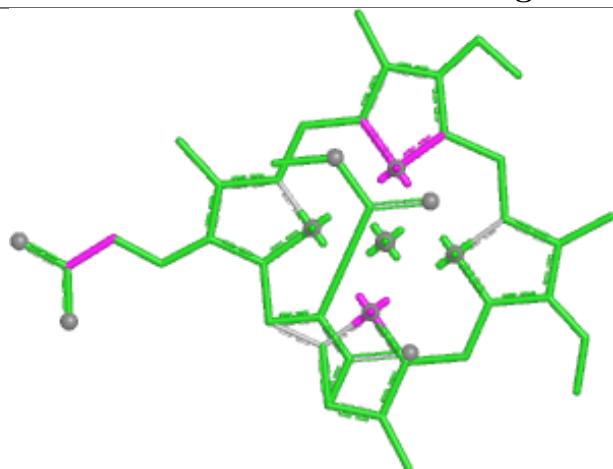
Torsions



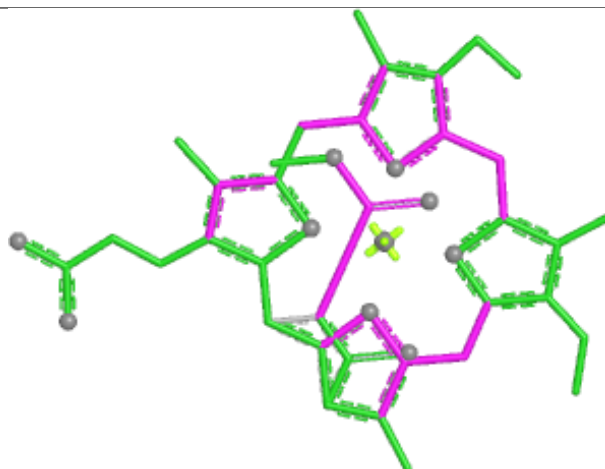
Rings



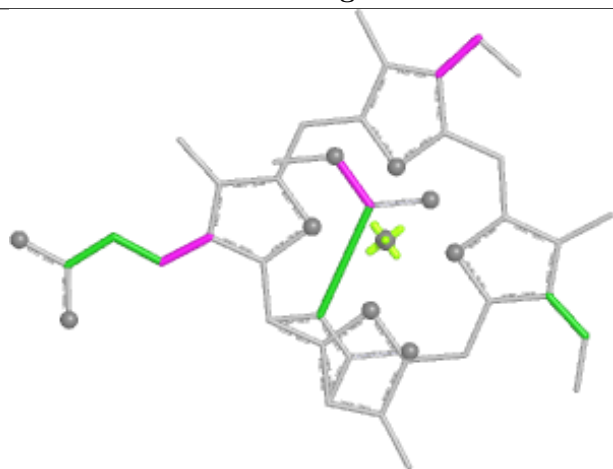
Ligand KC1 H 310



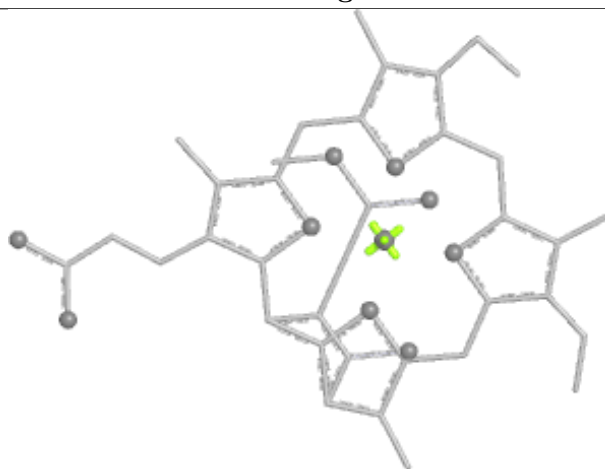
Bond lengths



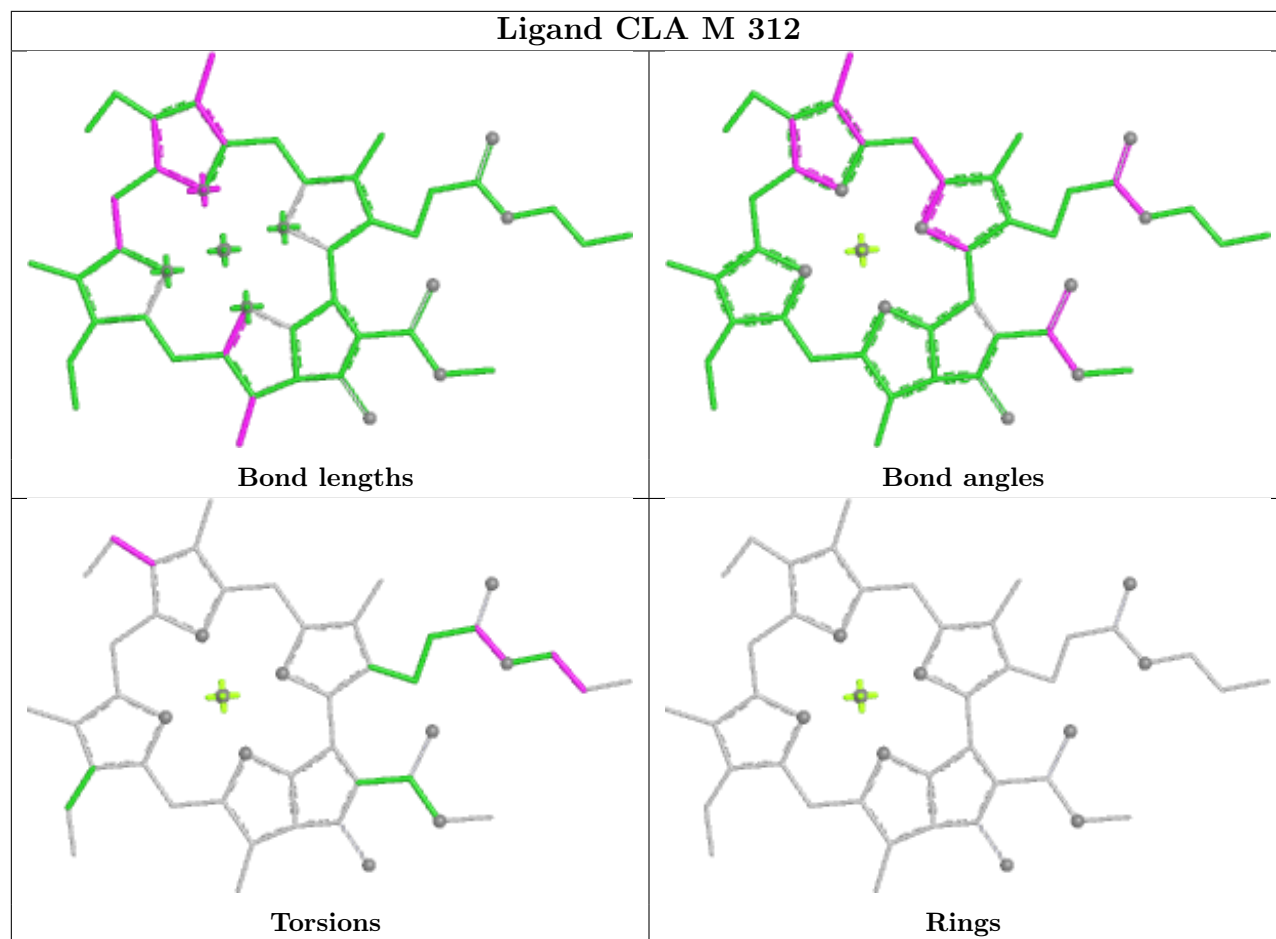
Bond angles



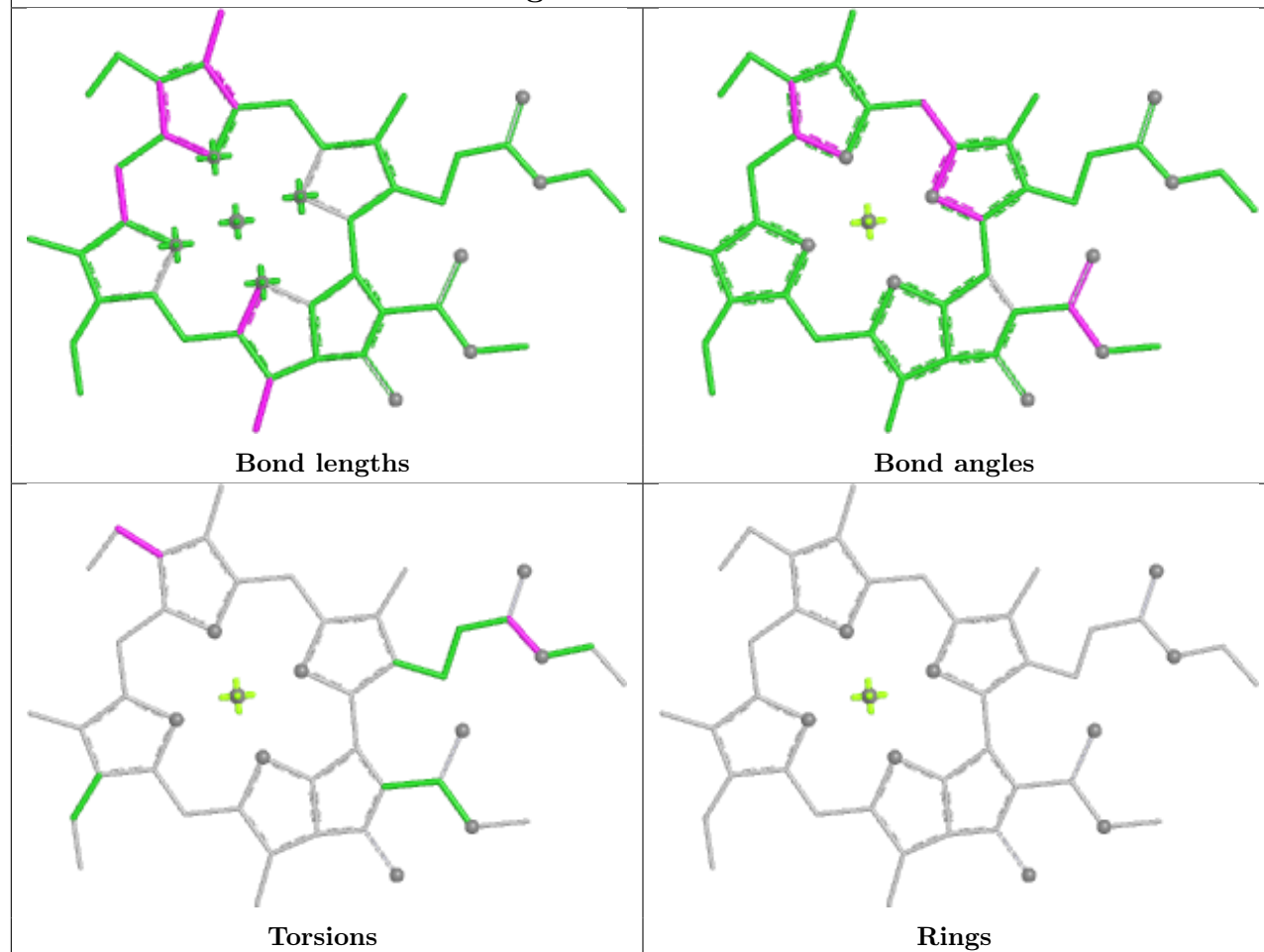
Torsions



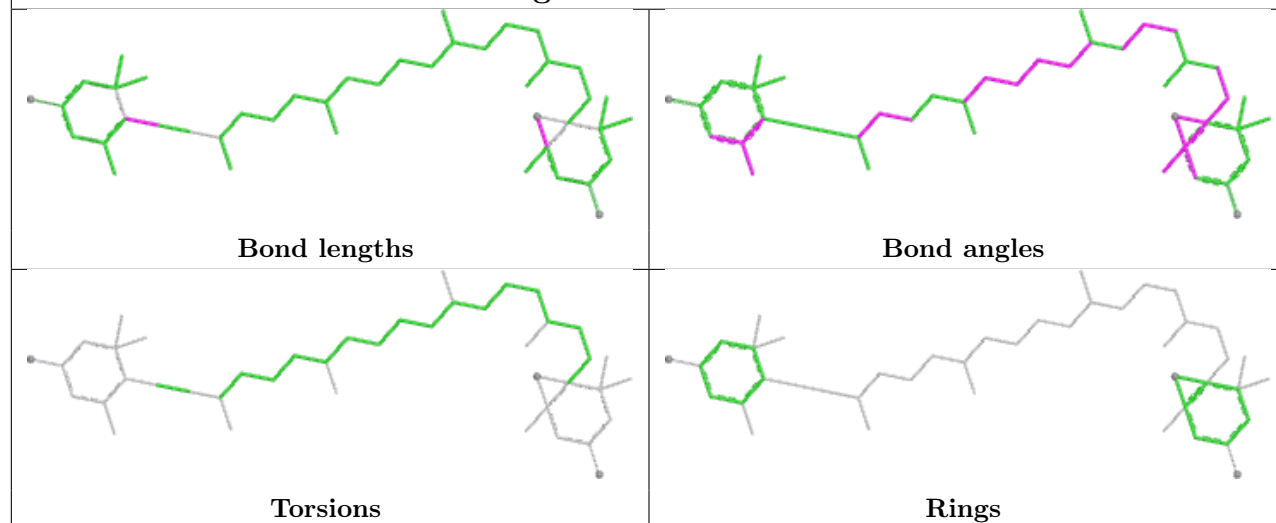
Rings



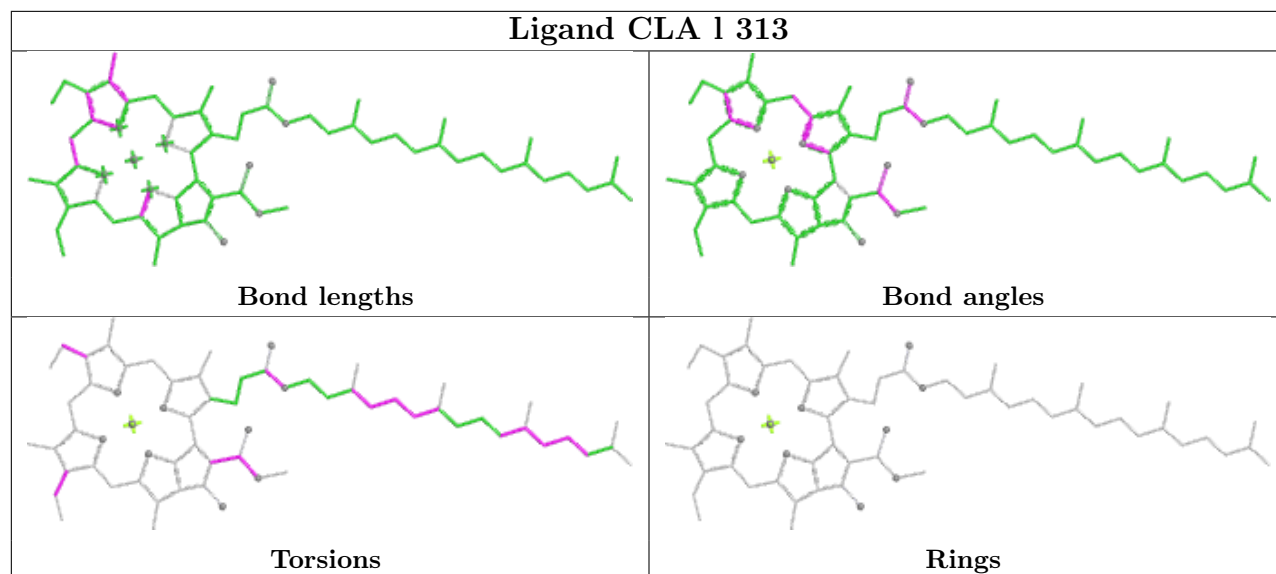
Ligand CLA D 308



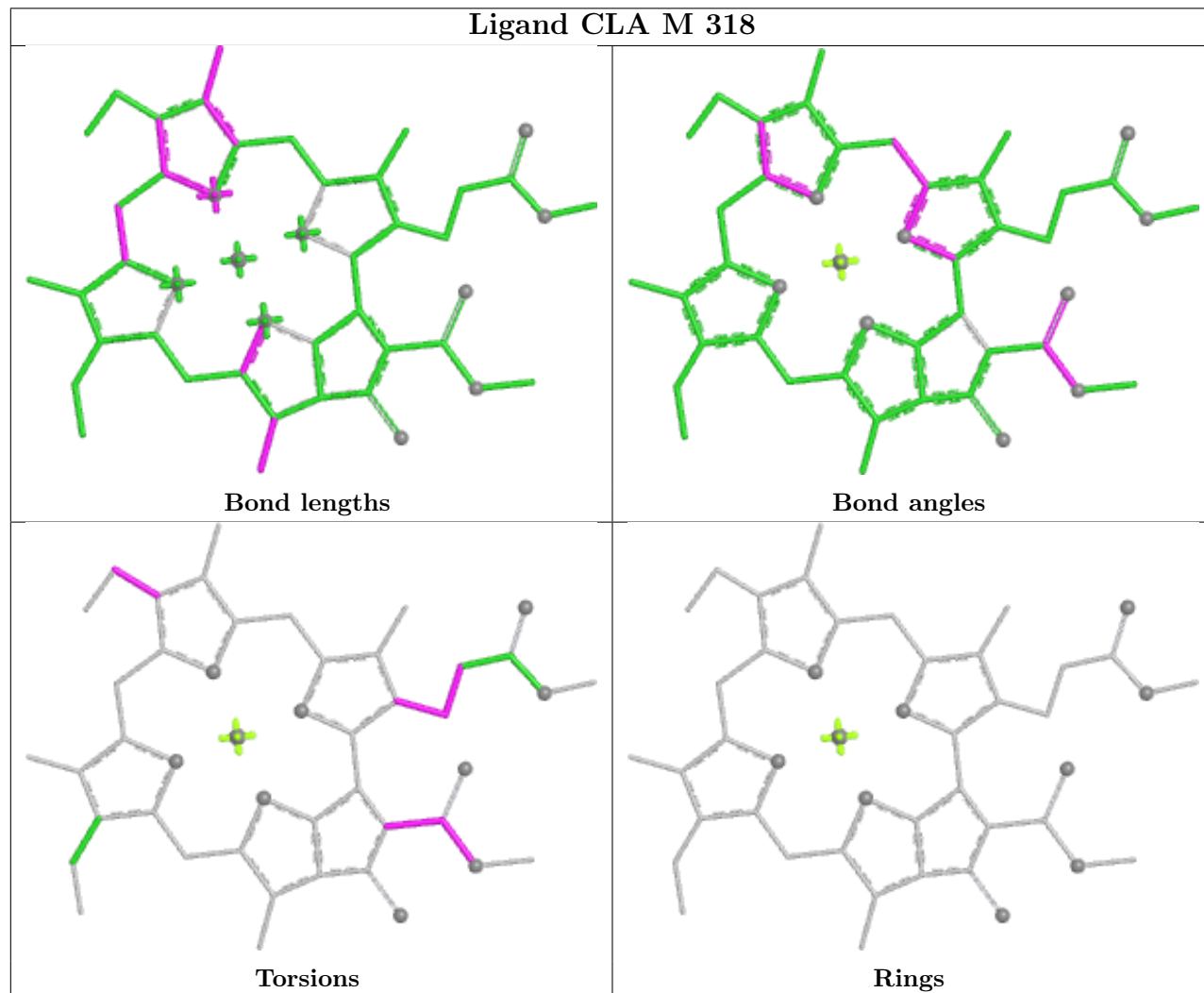
Ligand DD6 B 304

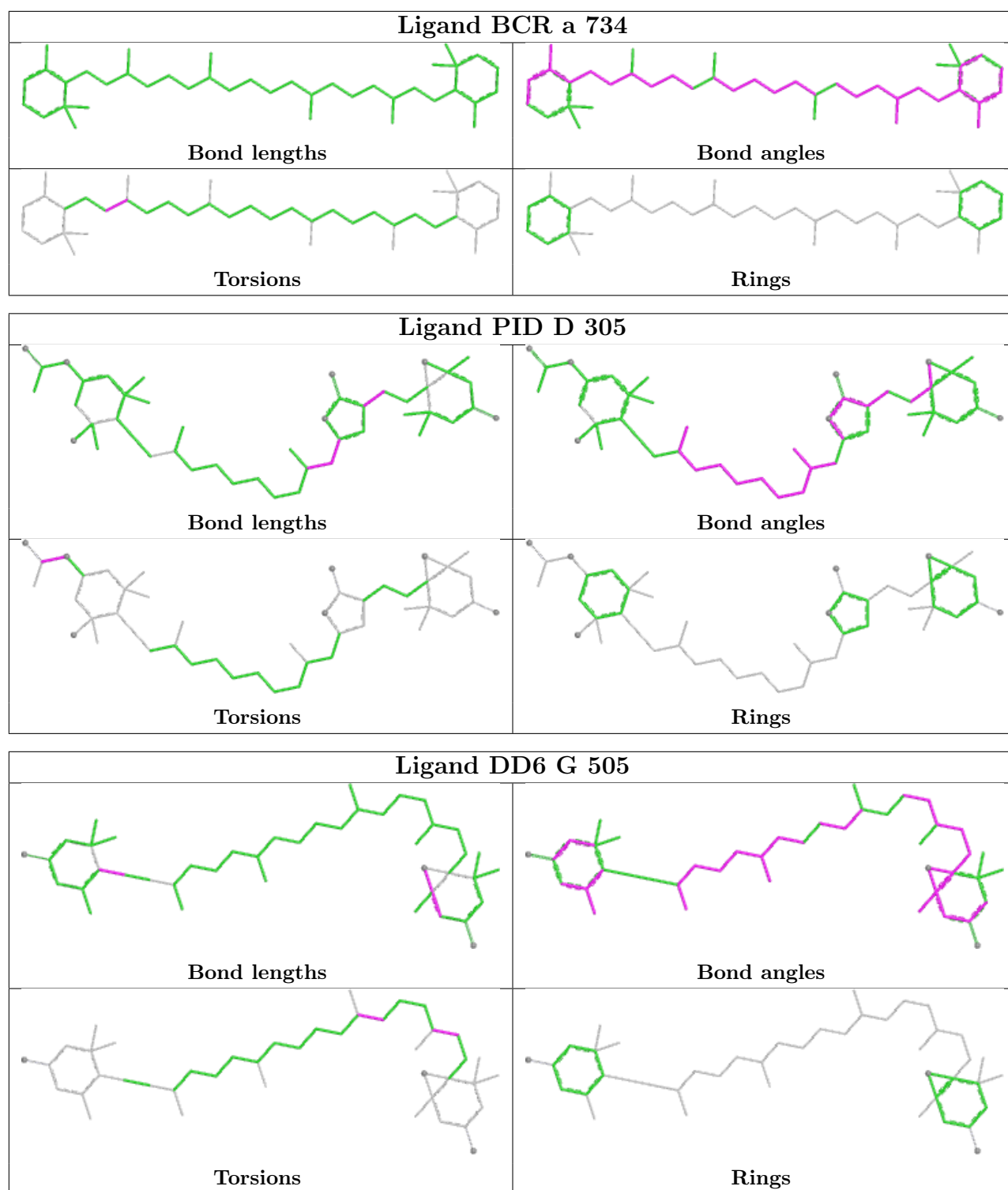


Ligand CLA I 313

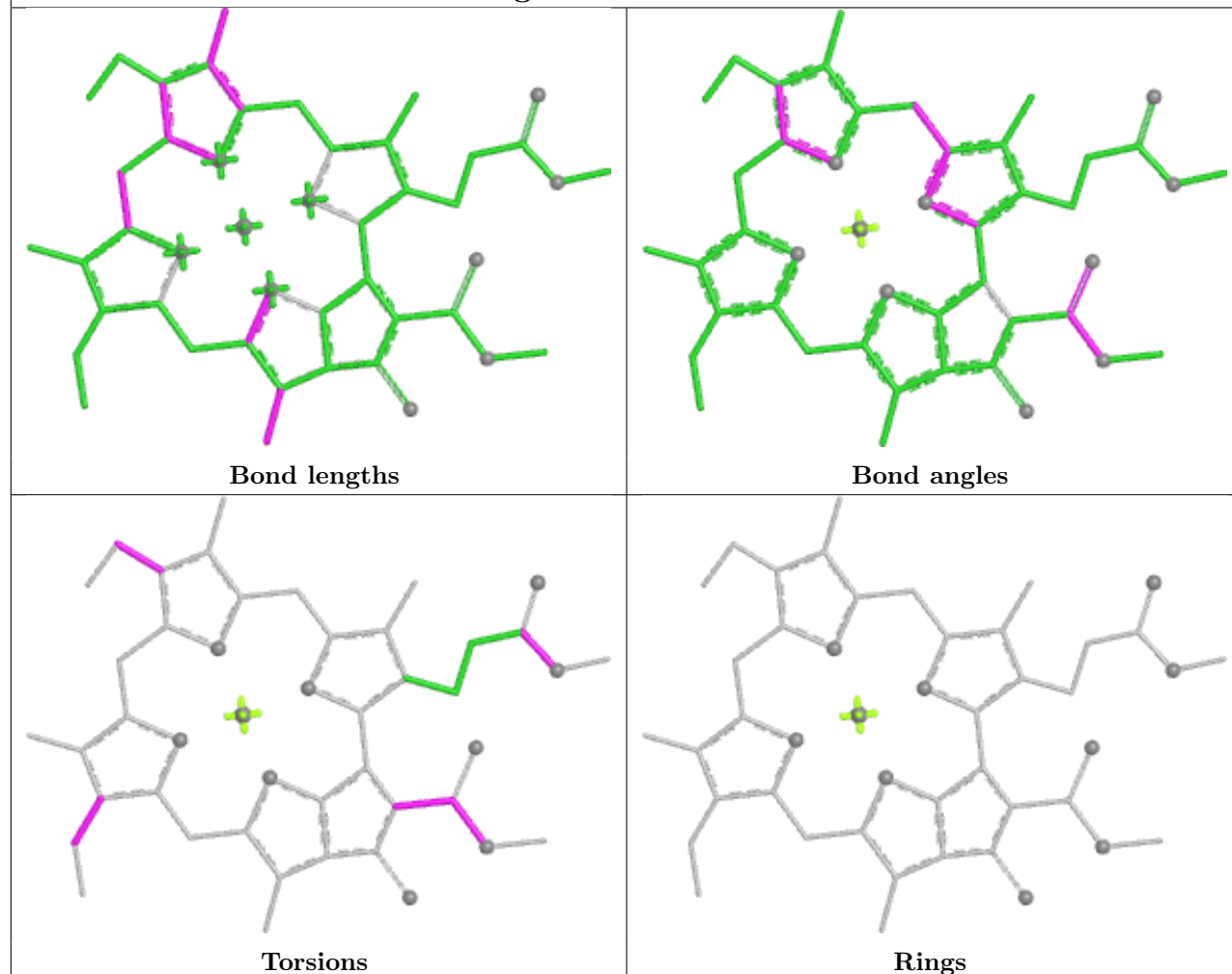


Ligand CLA M 318

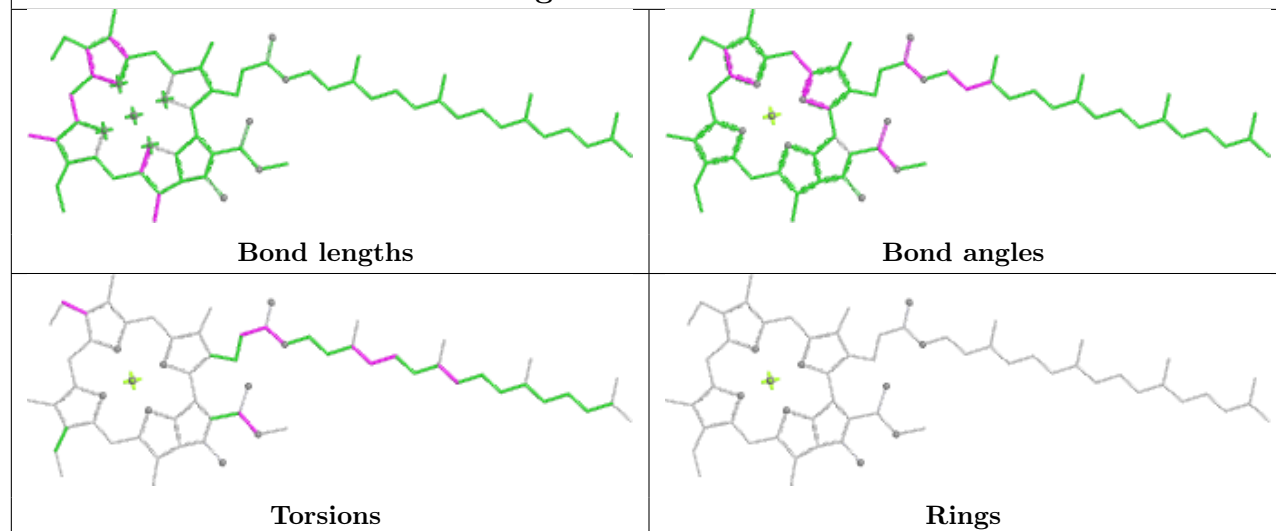


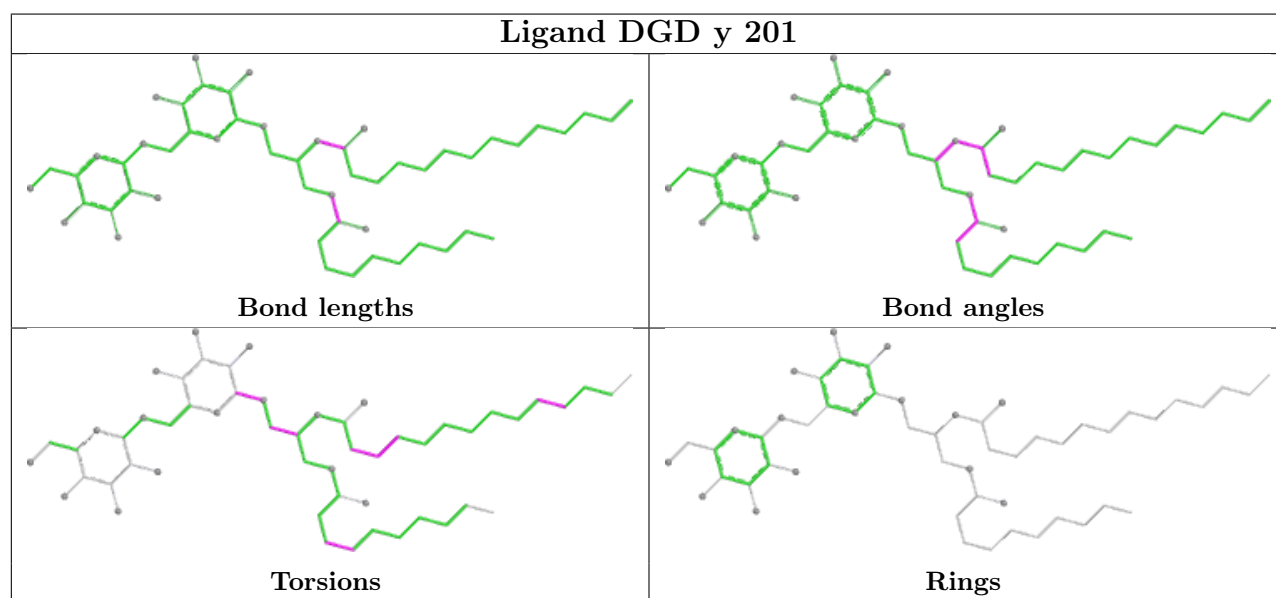
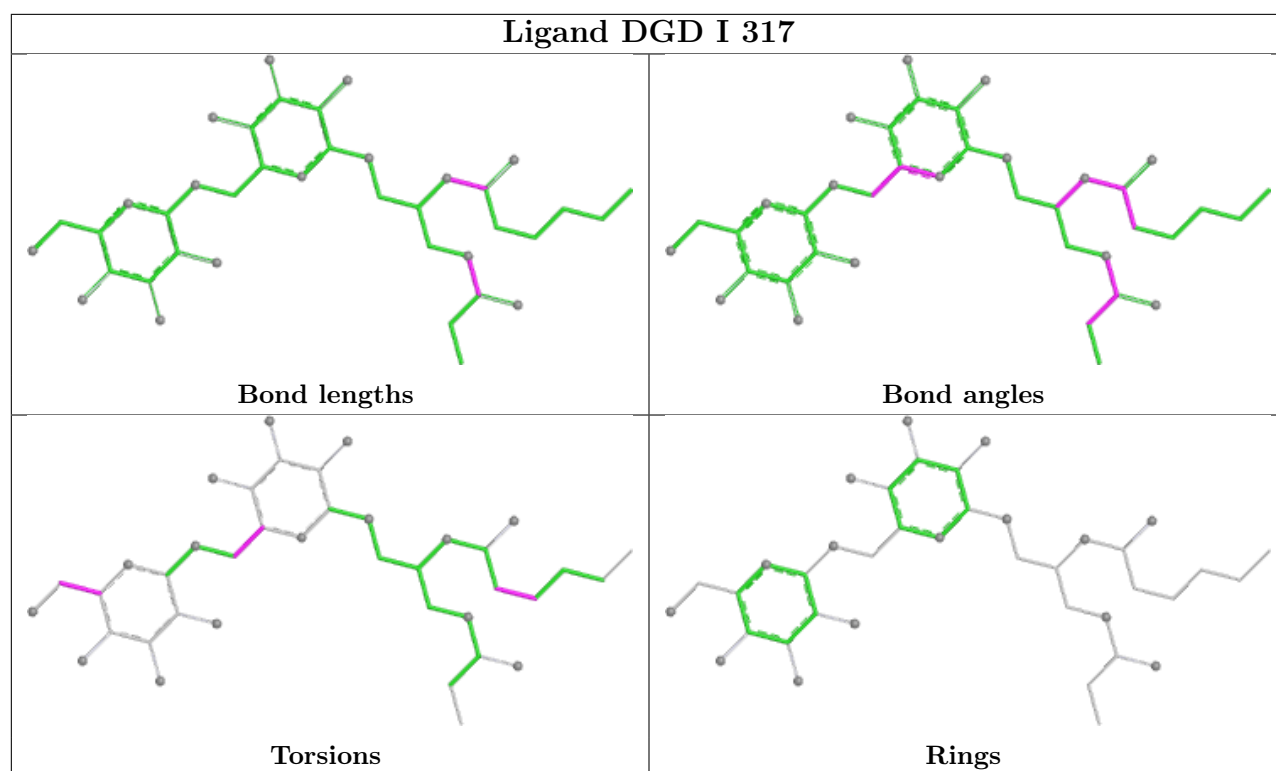


Ligand CLA B 316

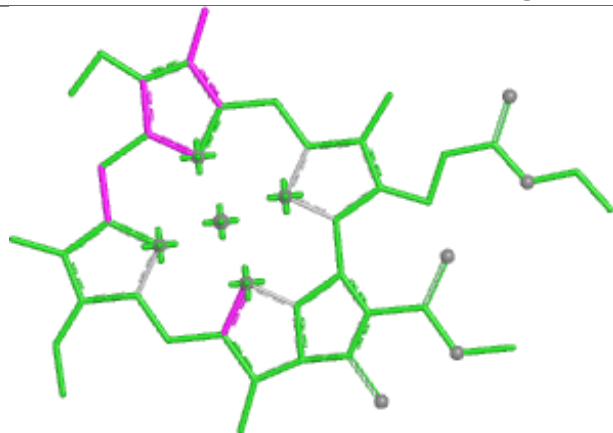


Ligand CLA b 703

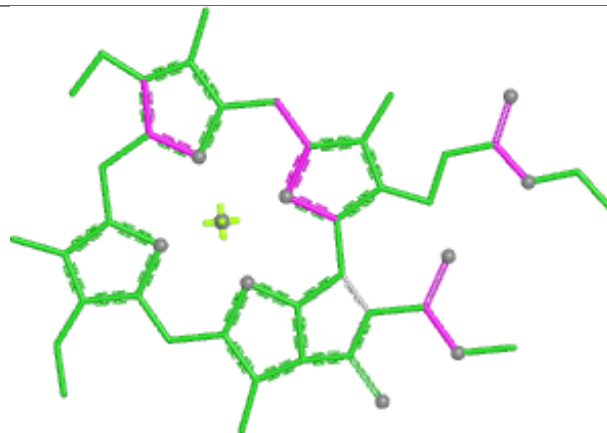




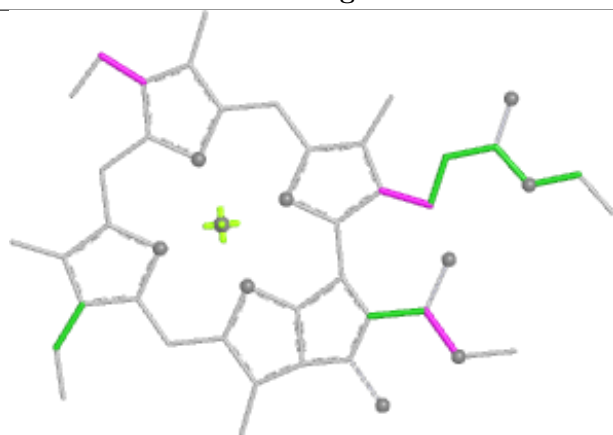
Ligand CLA a 716



Bond lengths



Bond angles

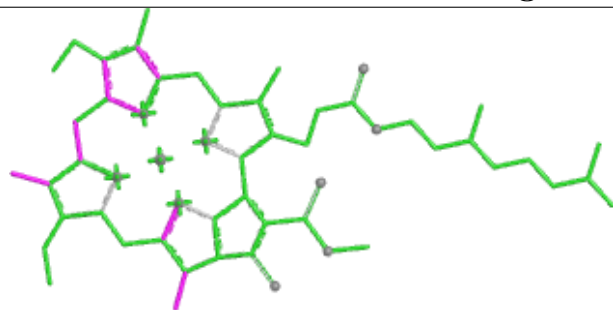


Torsions

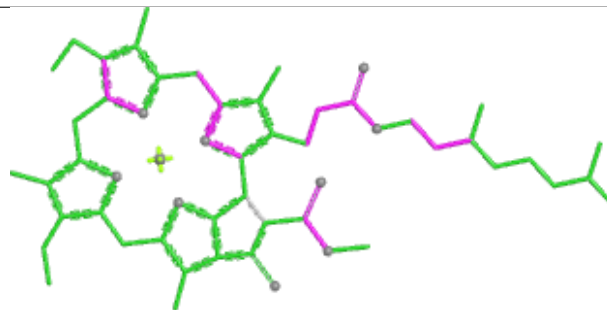


Rings

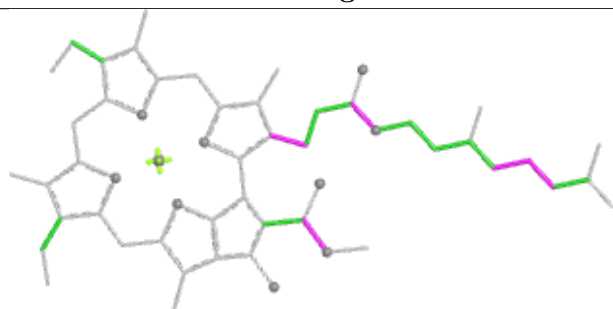
Ligand CLA a 705



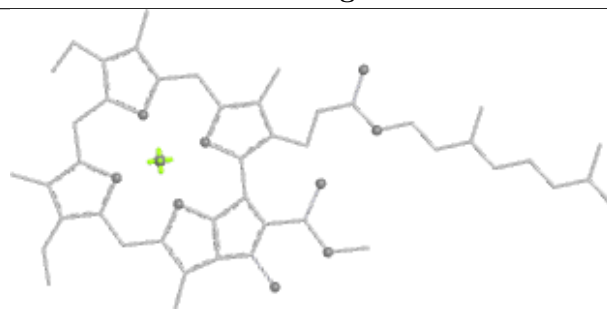
Bond lengths



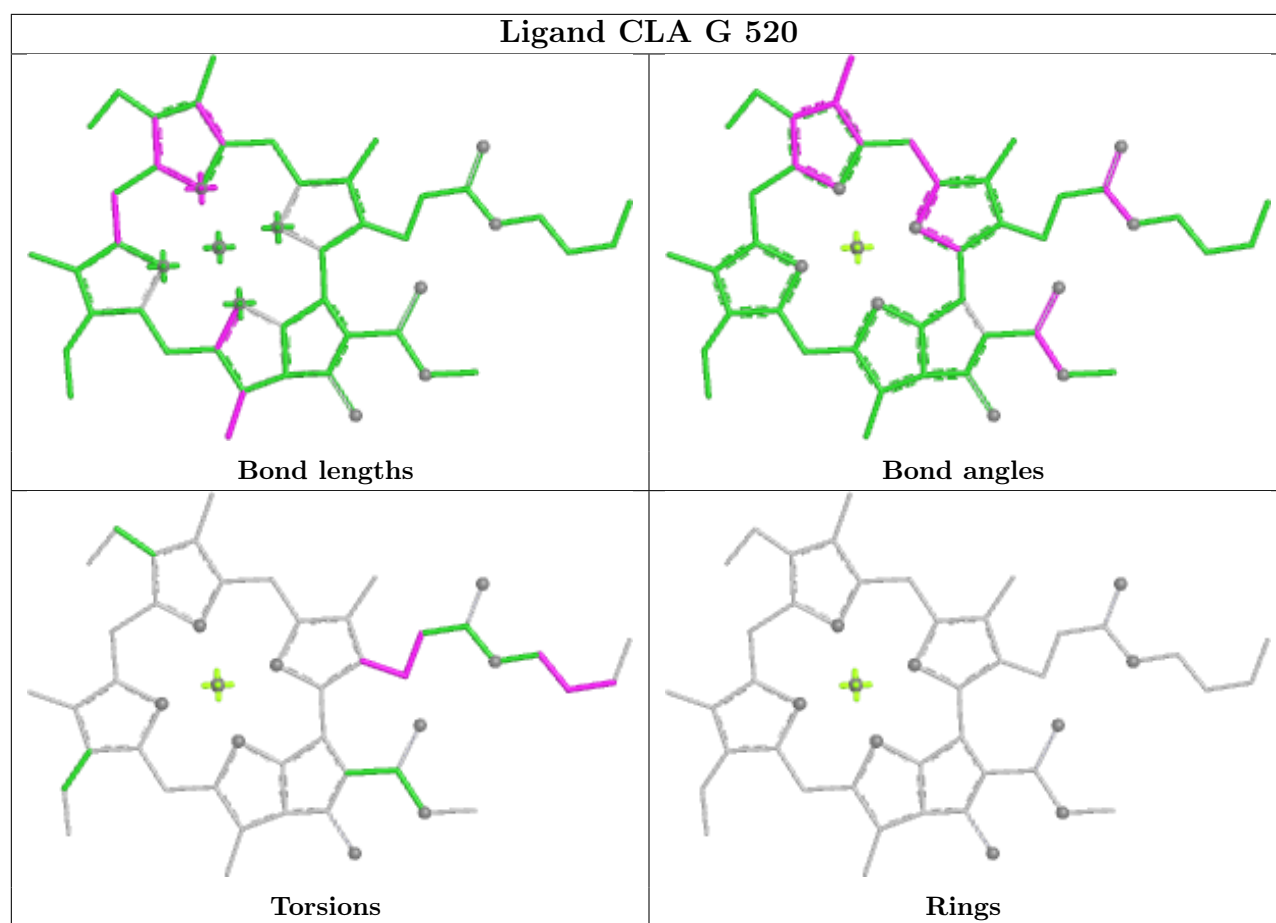
Bond angles

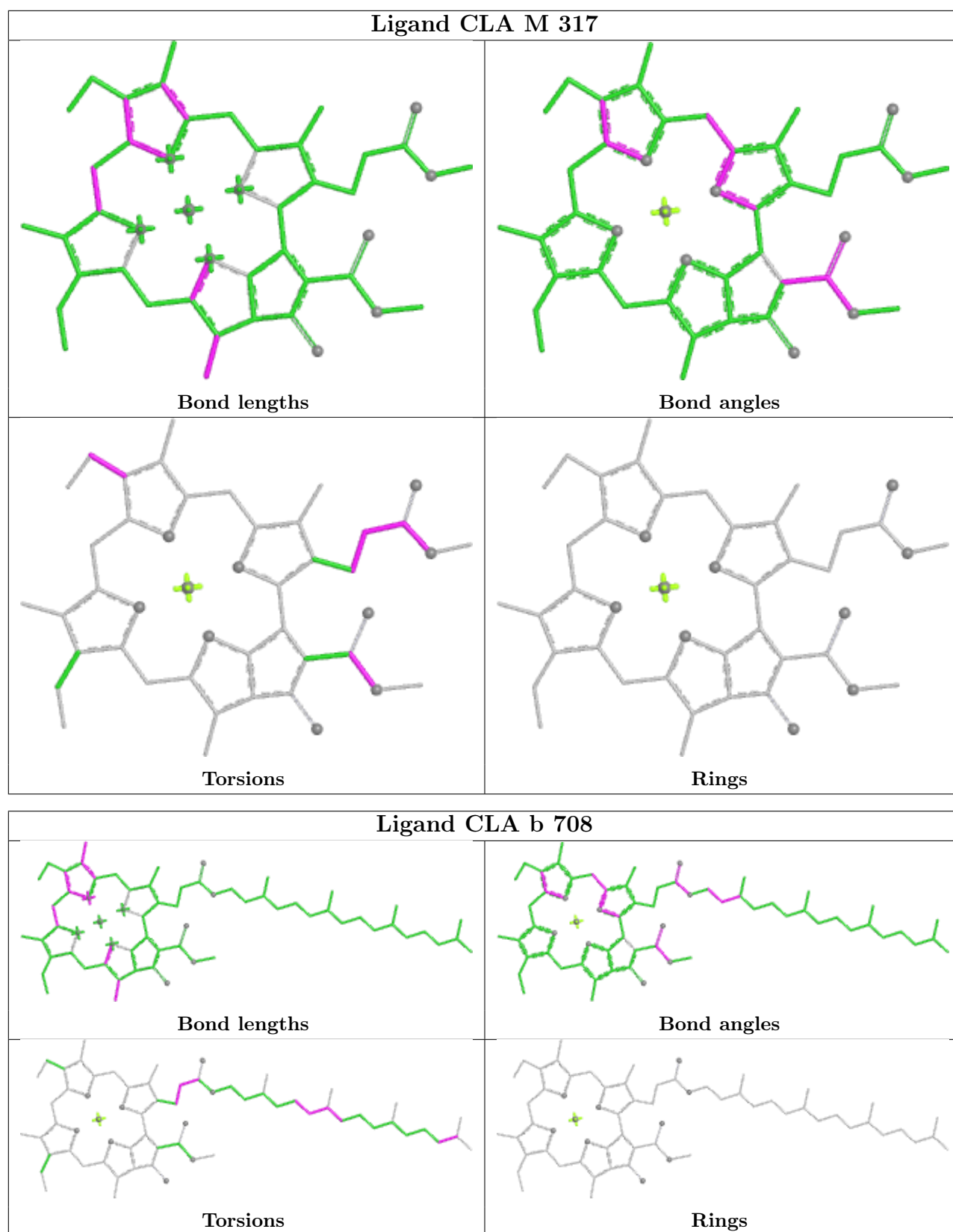


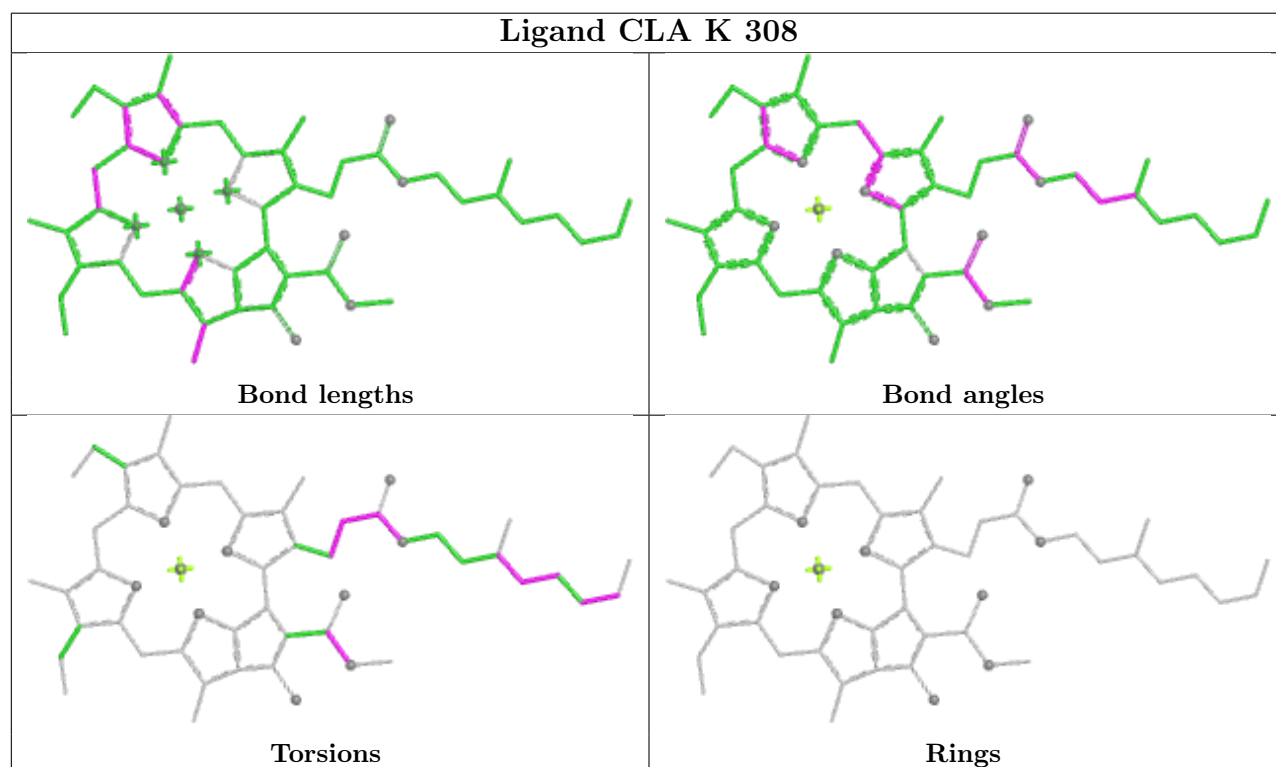
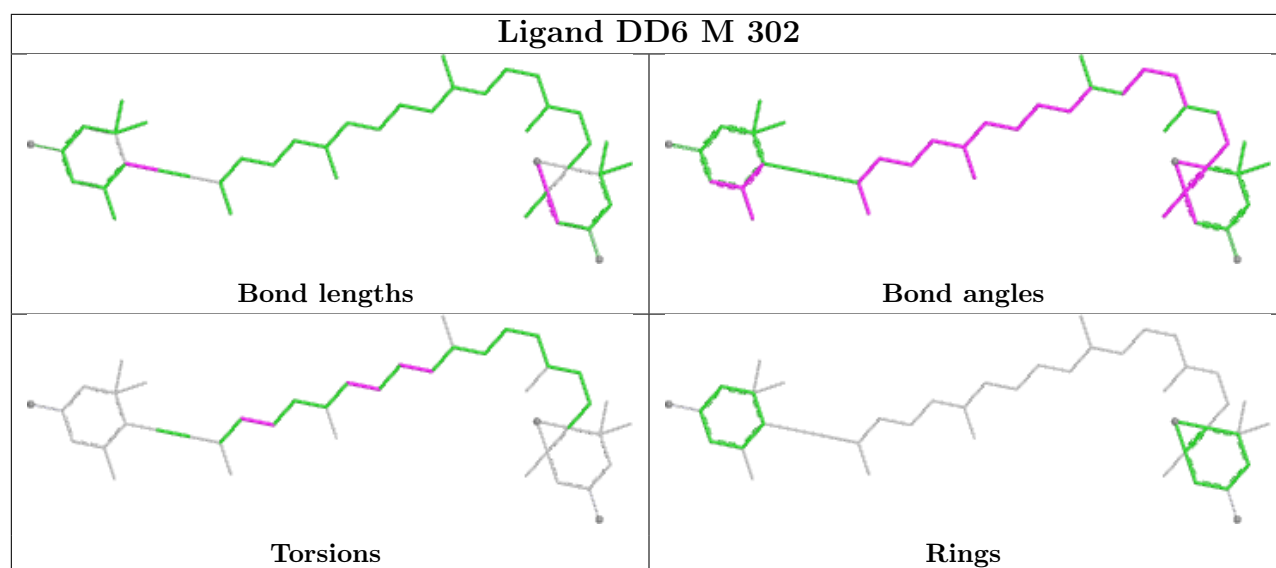
Torsions



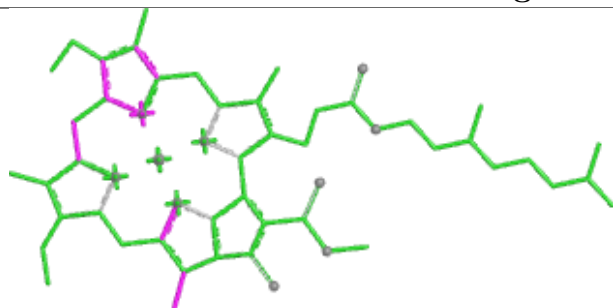
Rings



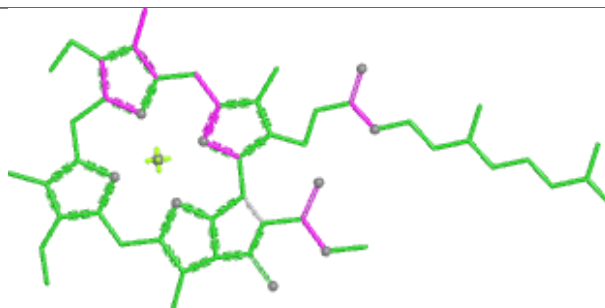




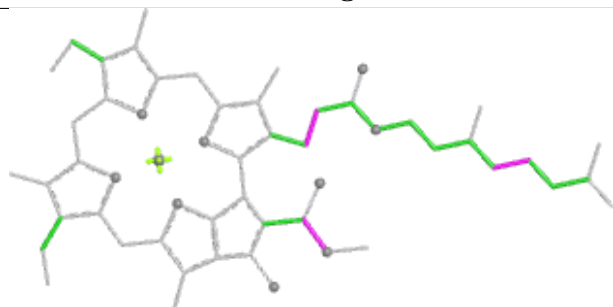
Ligand CLA A 308



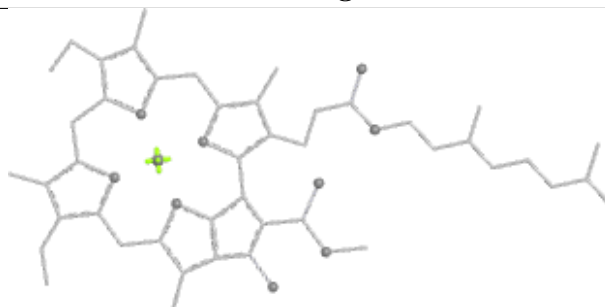
Bond lengths



Bond angles

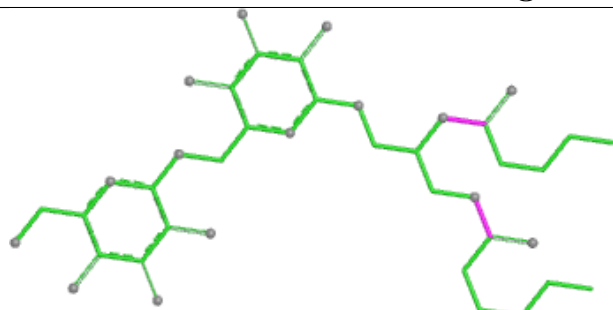


Torsions

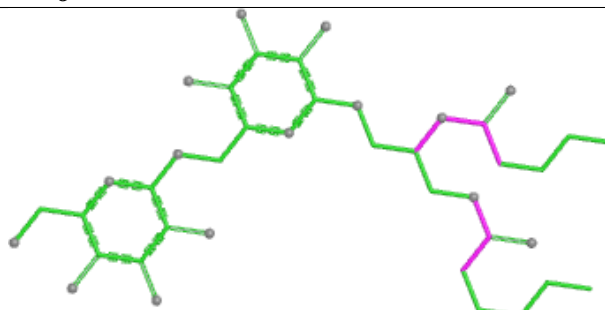


Rings

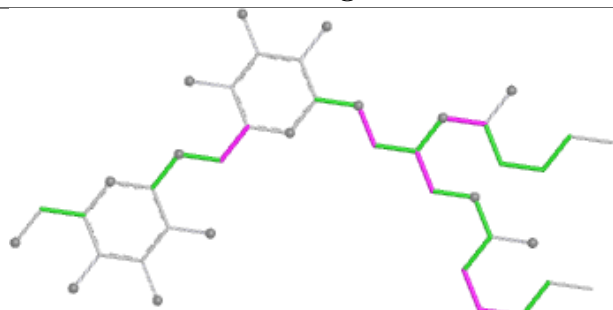
Ligand DGD j 103



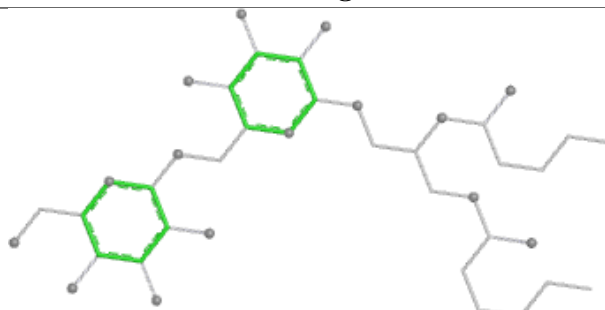
Bond lengths



Bond angles

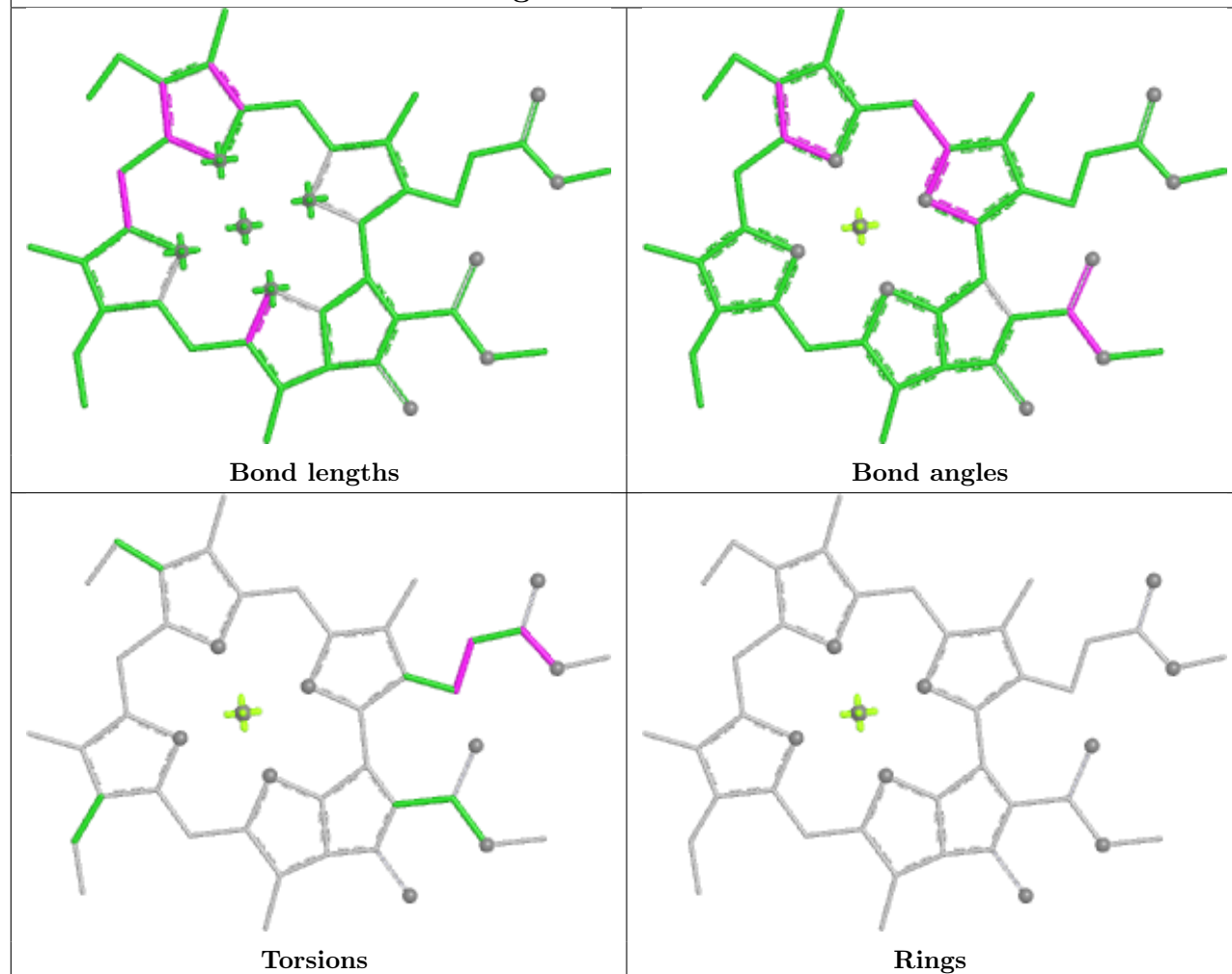


Torsions

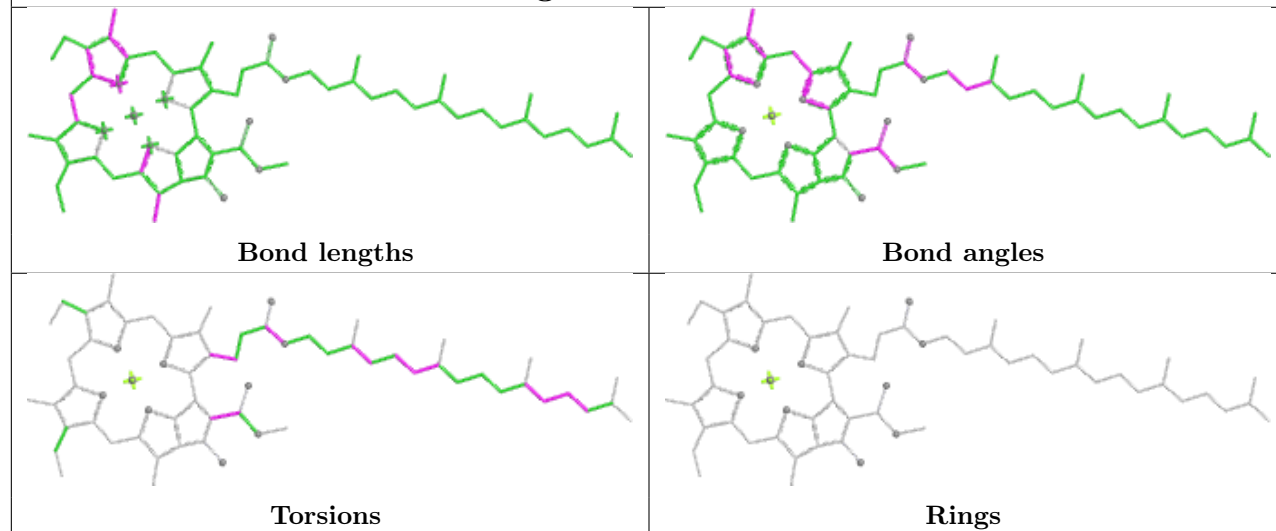


Rings

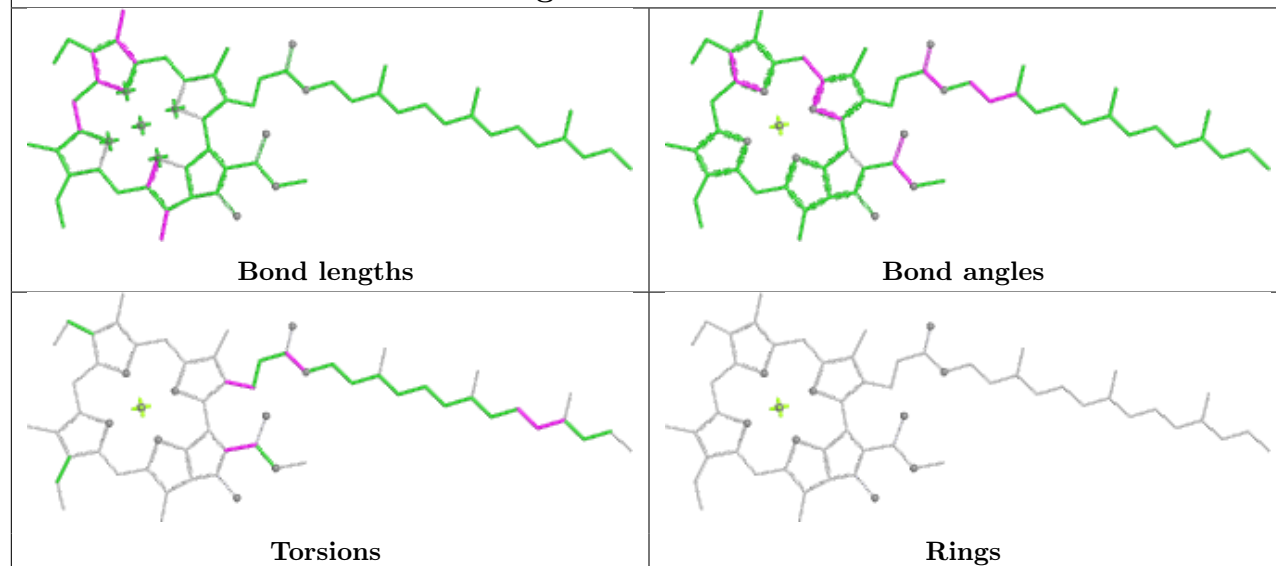
Ligand CLA D 311



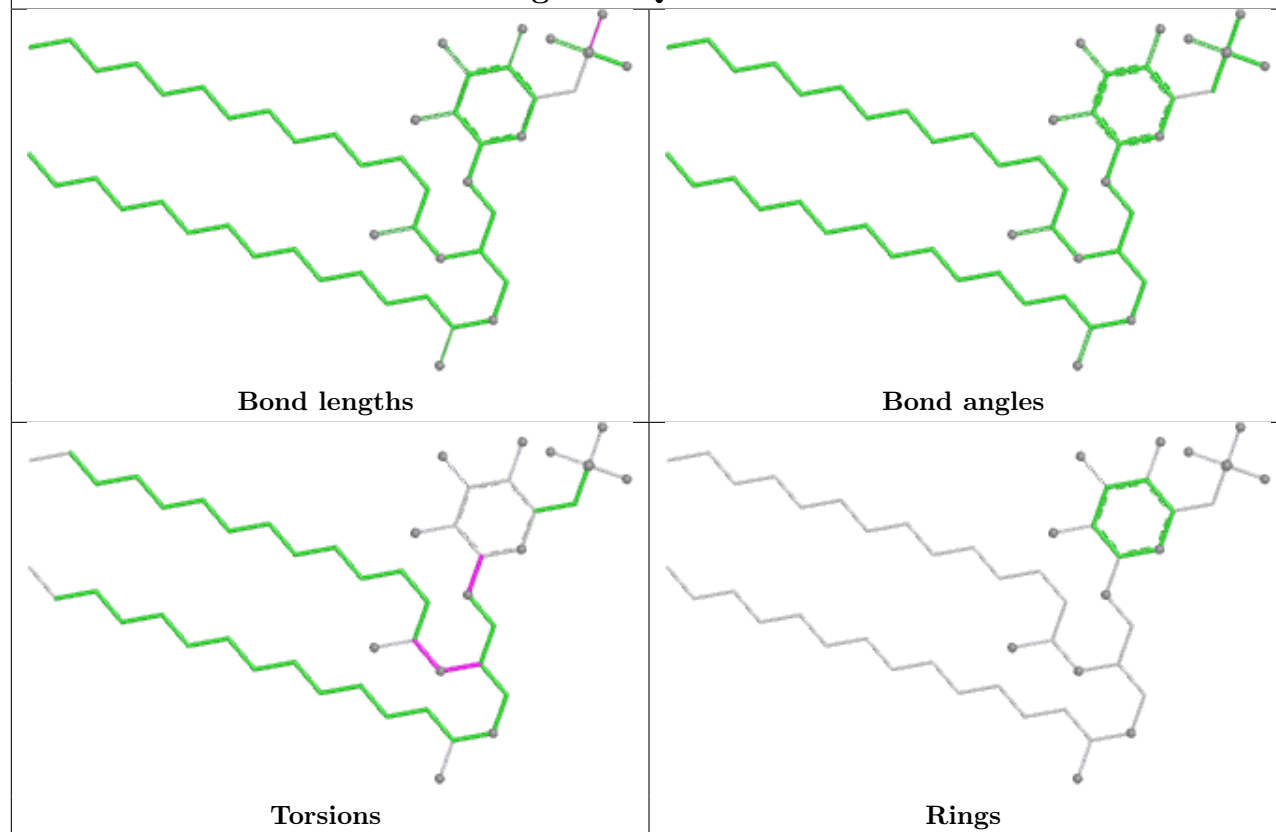
Ligand CLA a 724

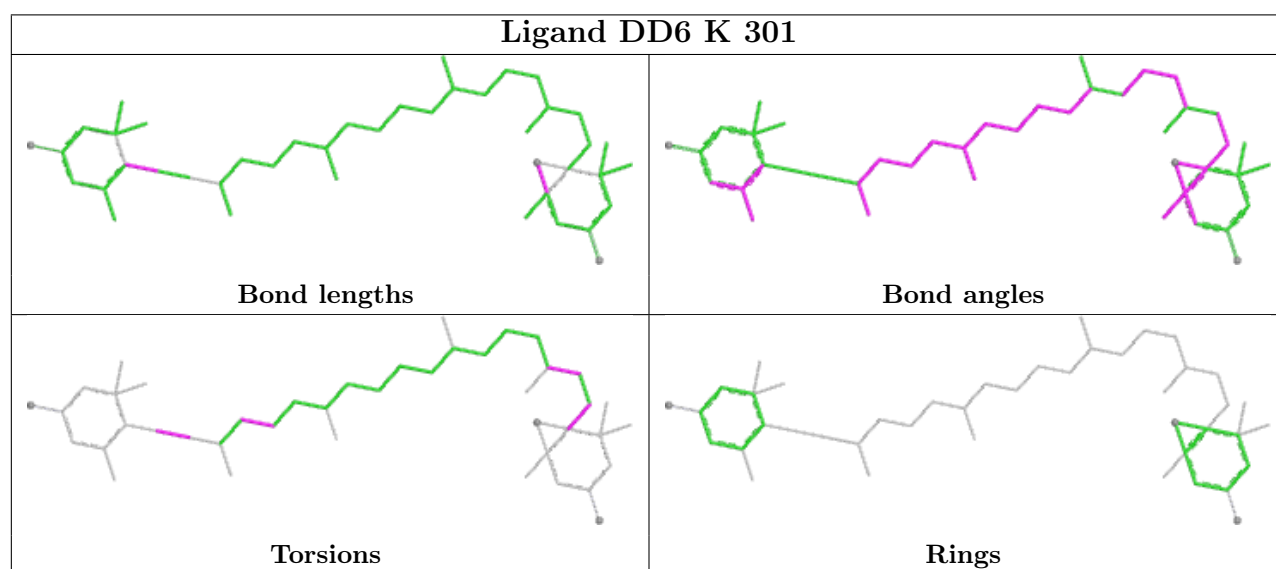
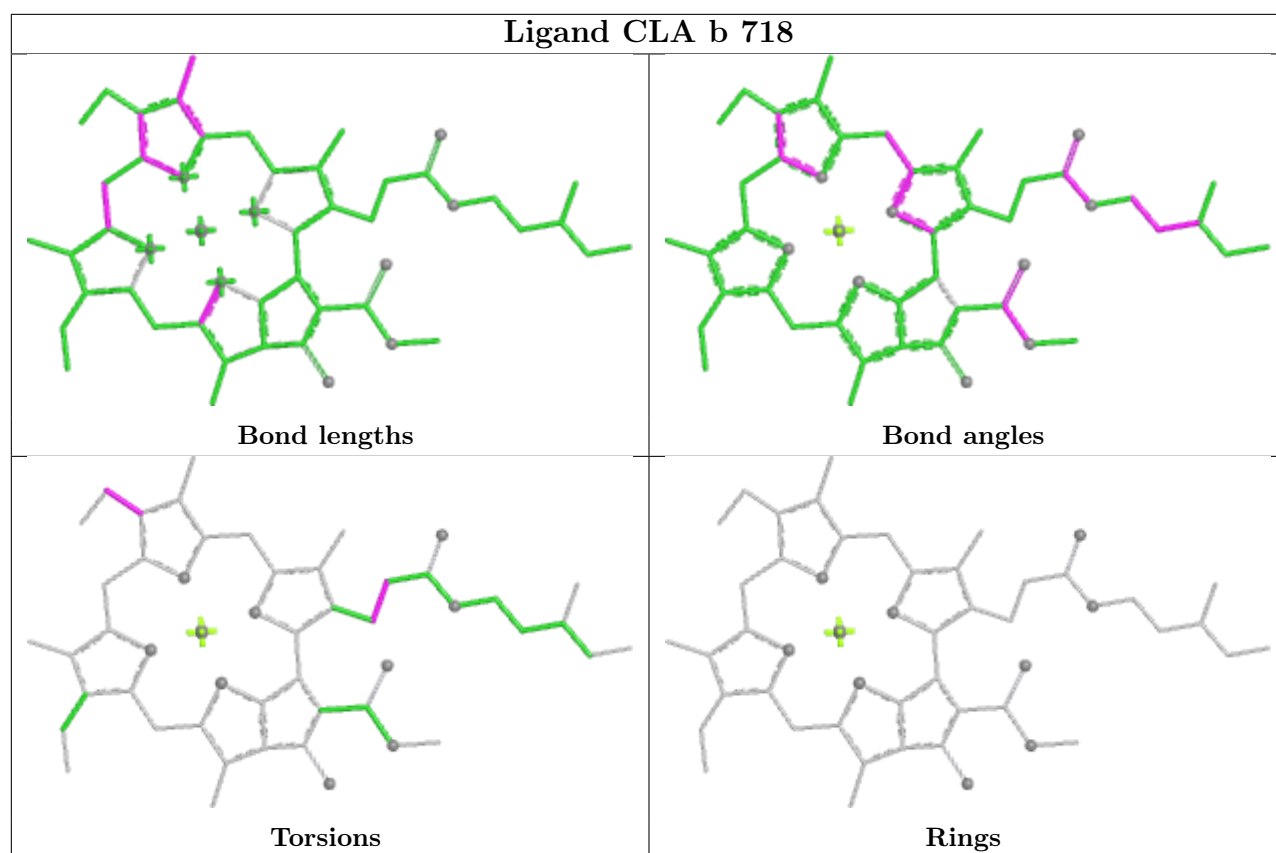


Ligand CLA a 720

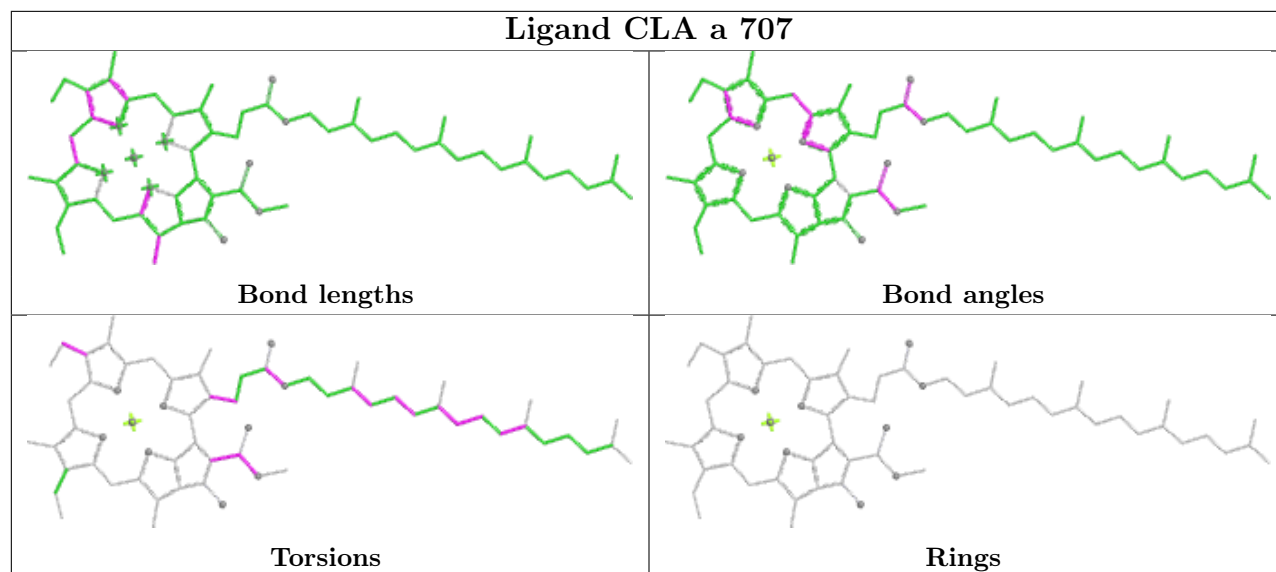


Ligand SQD A 318

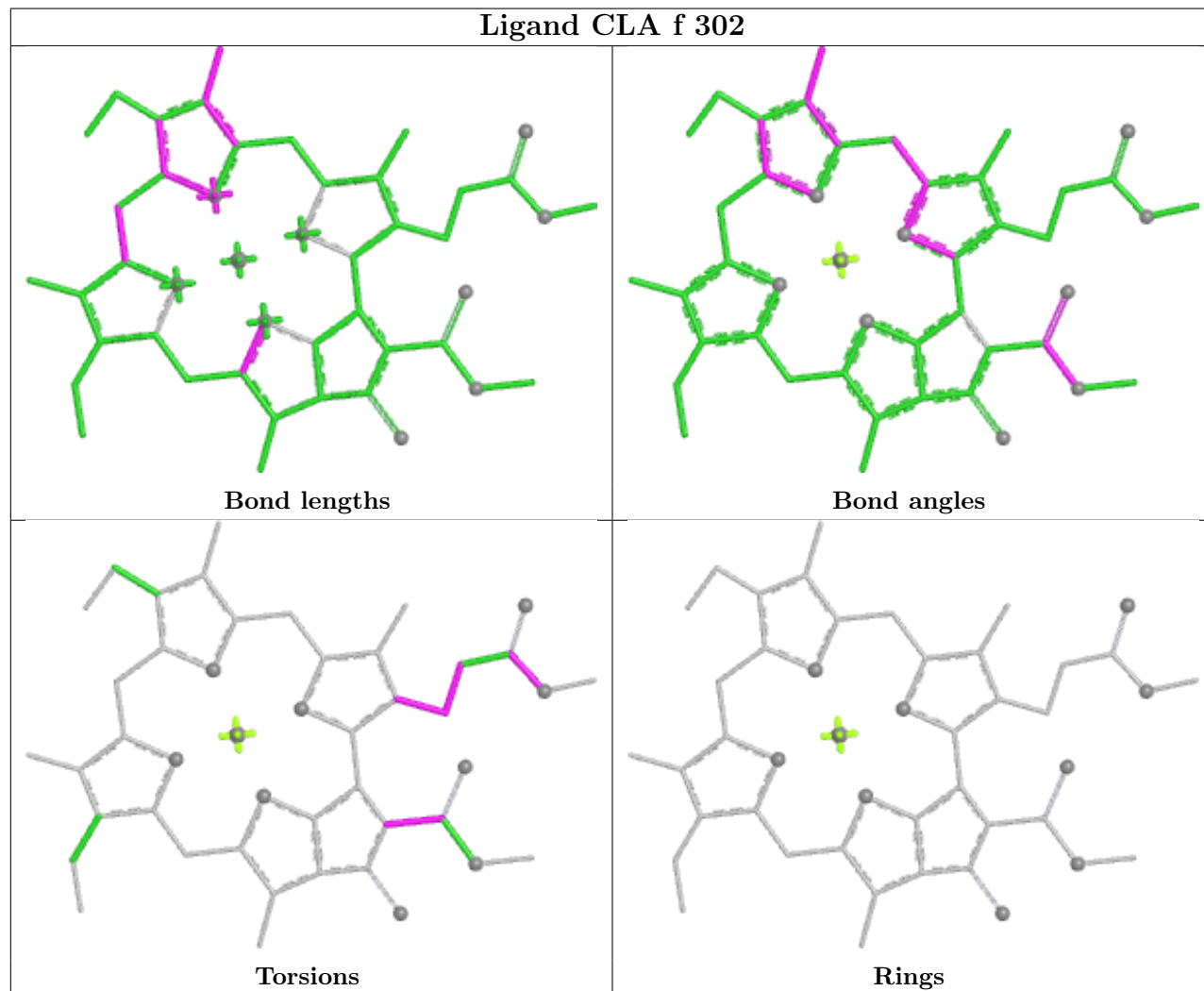




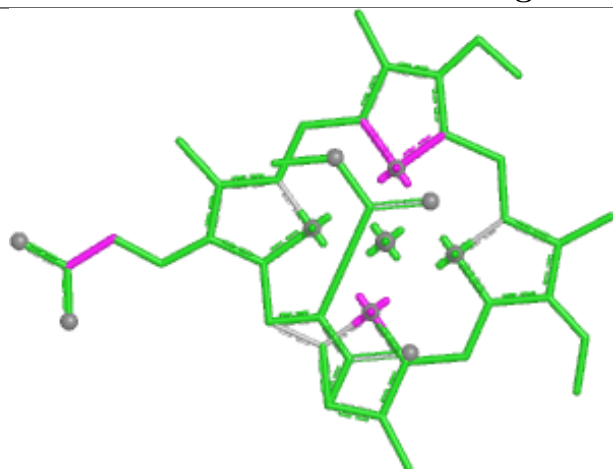
Ligand CLA a 707



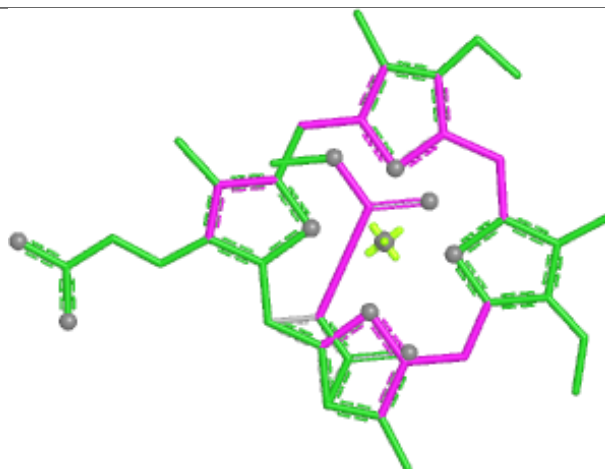
Ligand CLA f 302



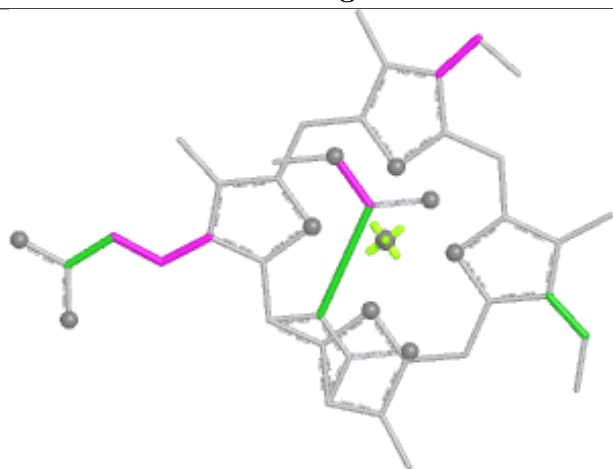
Ligand KC1 N 311



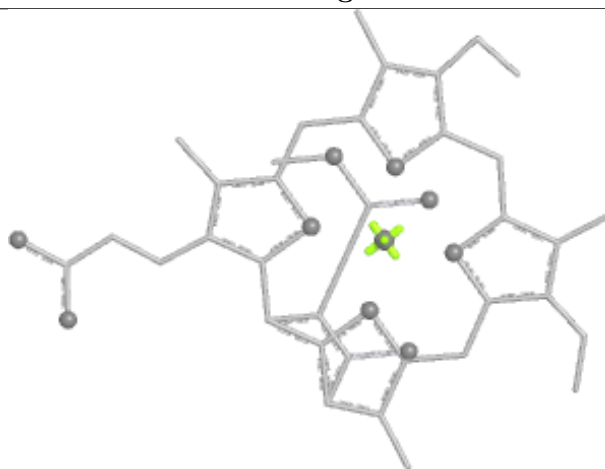
Bond lengths



Bond angles

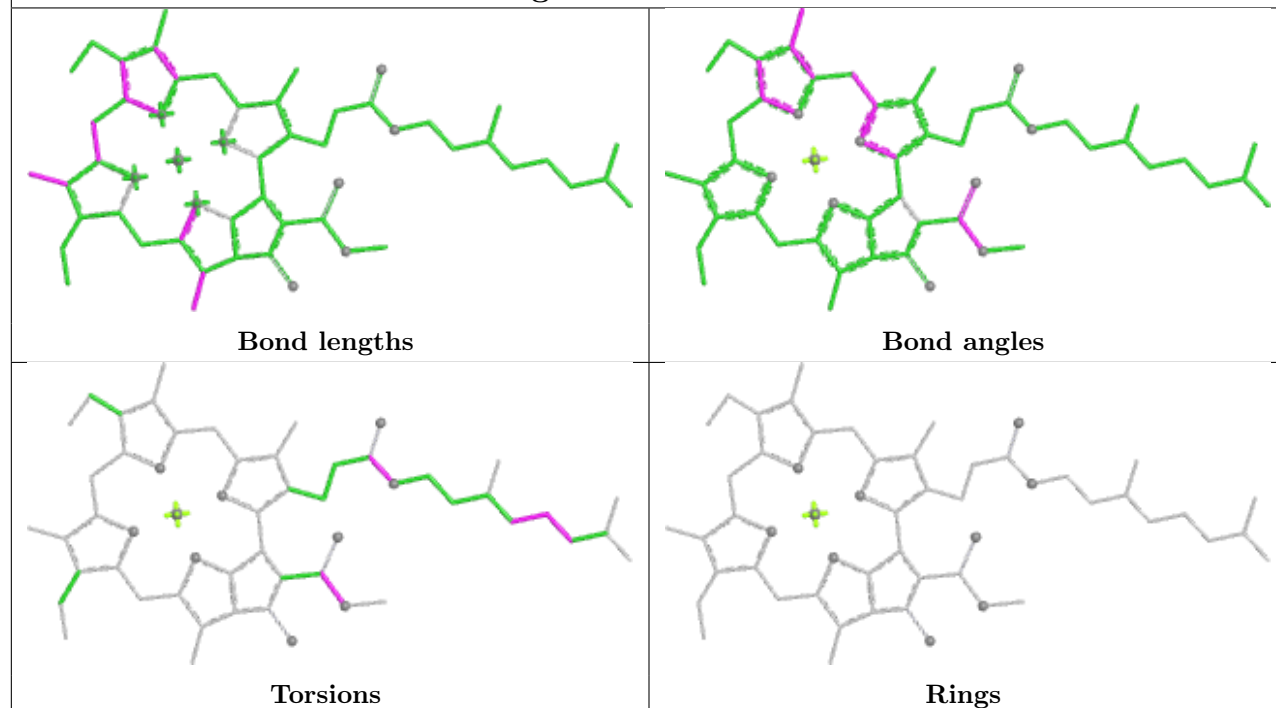


Torsions

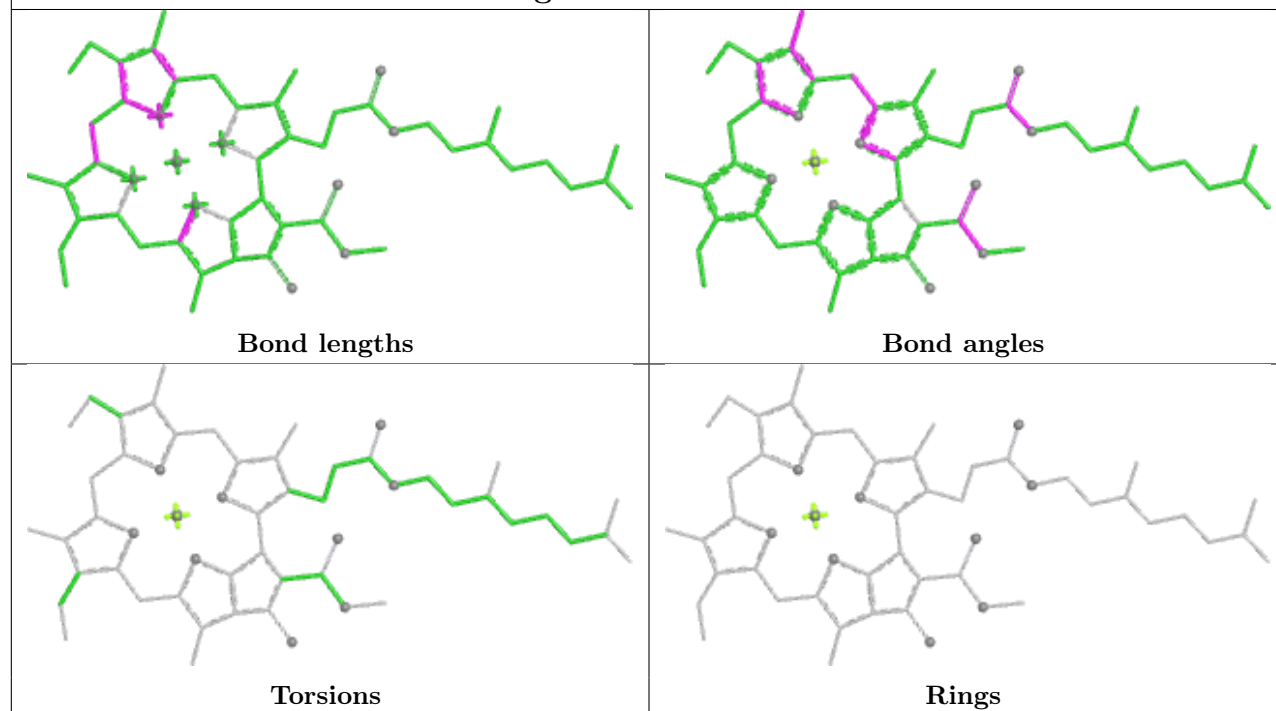


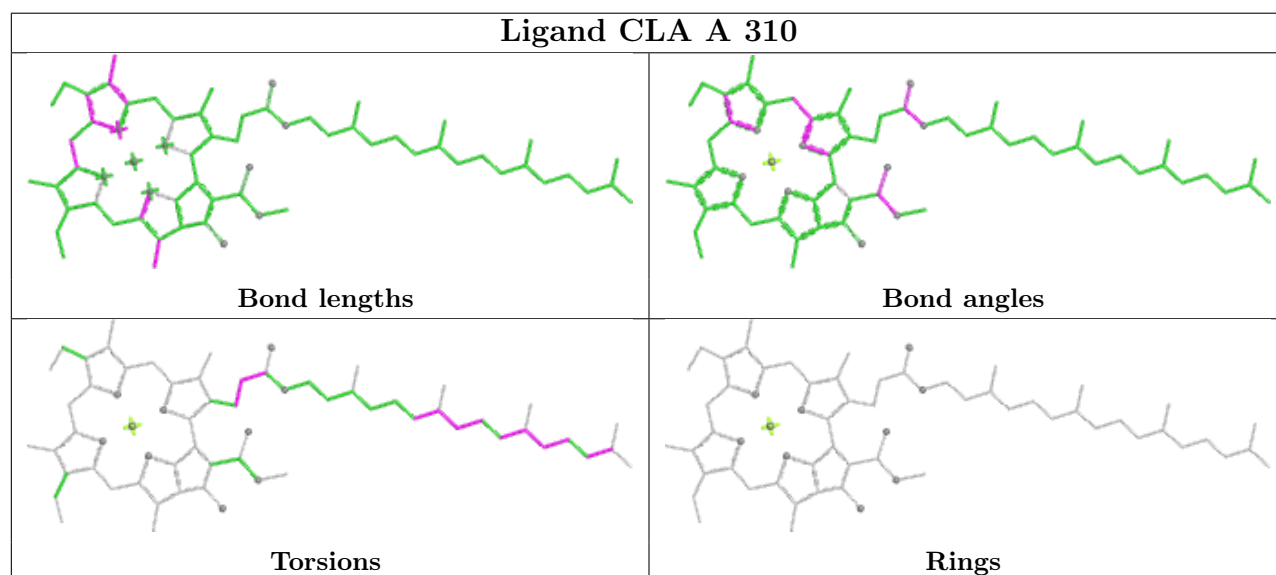
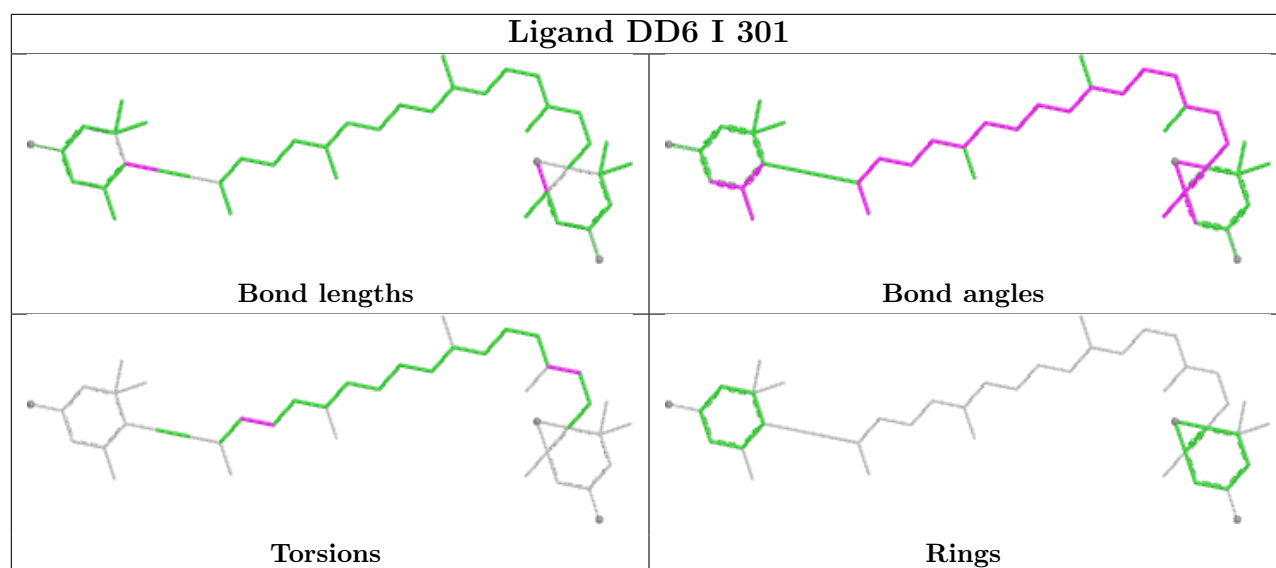
Rings

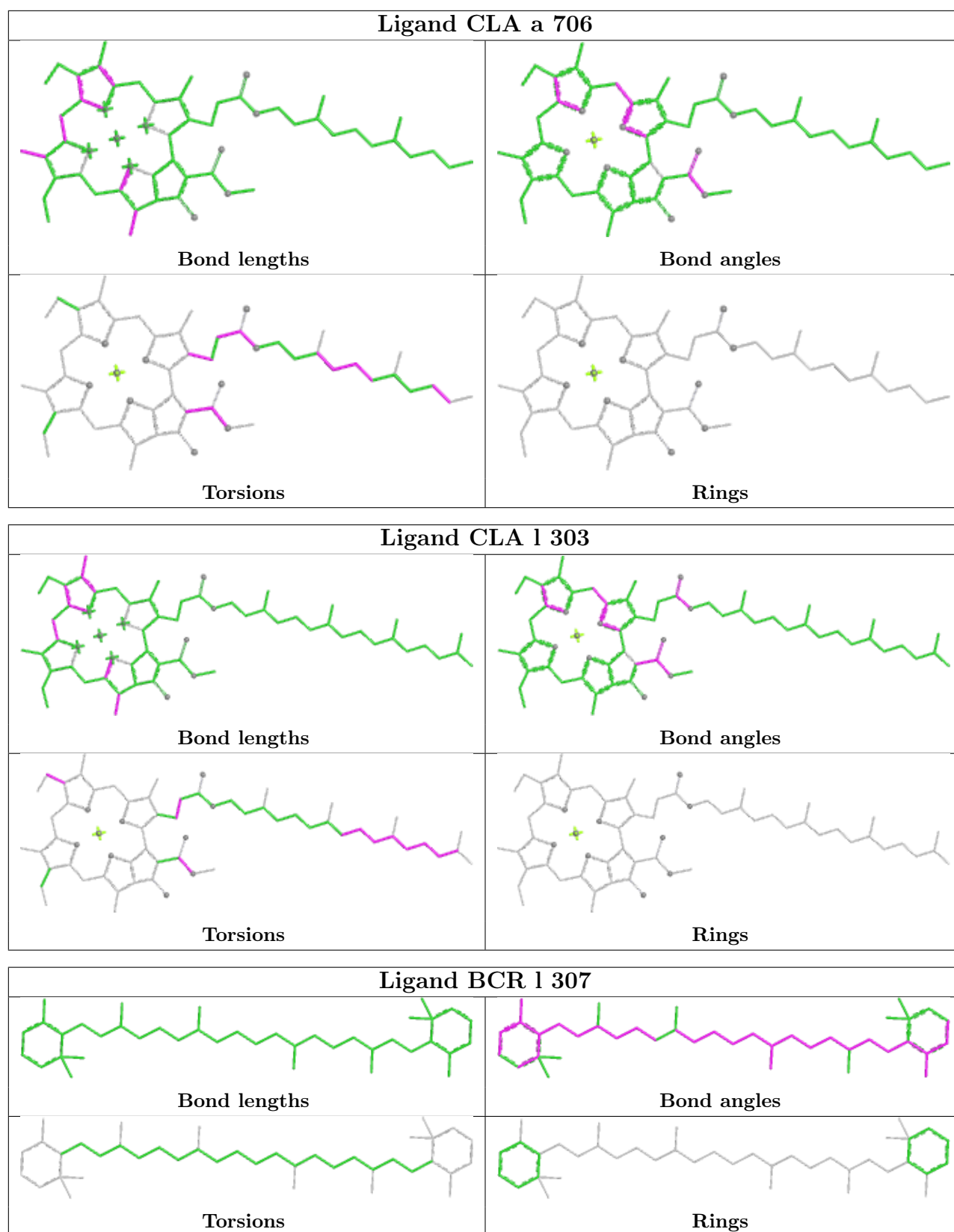
Ligand CLA A 312



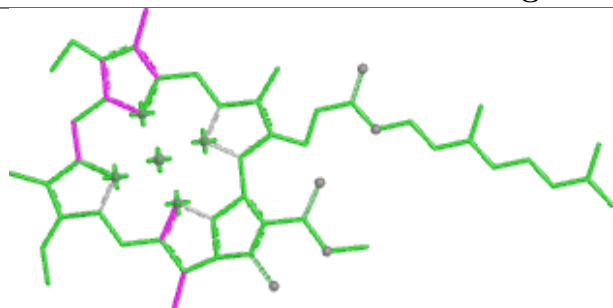
Ligand CLA L 310



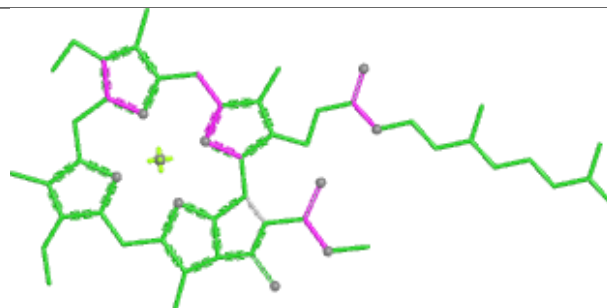




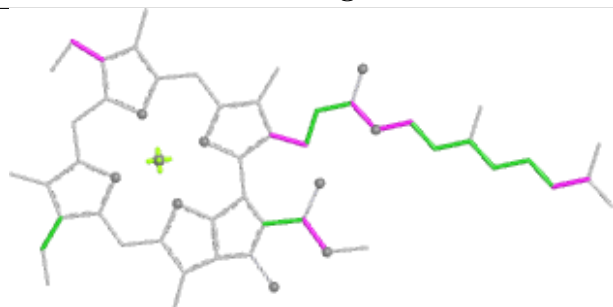
Ligand CLA f 301



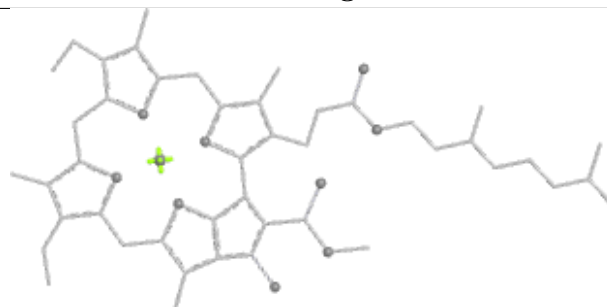
Bond lengths



Bond angles

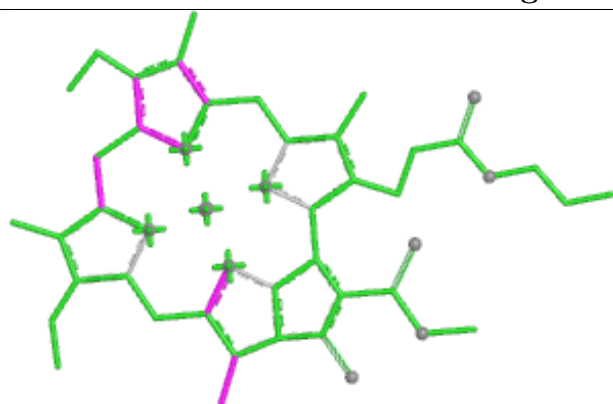


Torsions

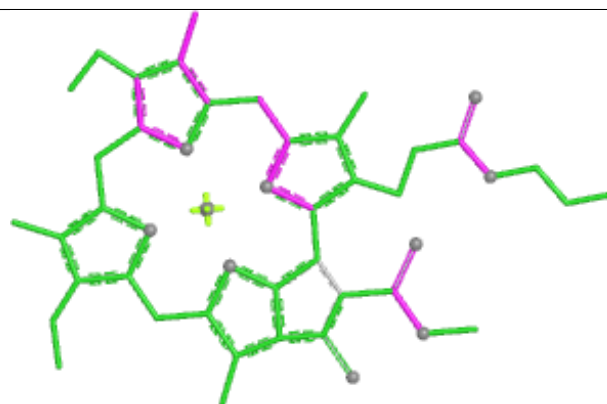


Rings

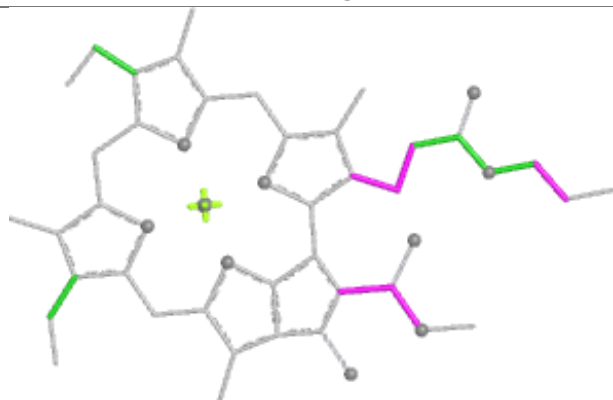
Ligand CLA I 310



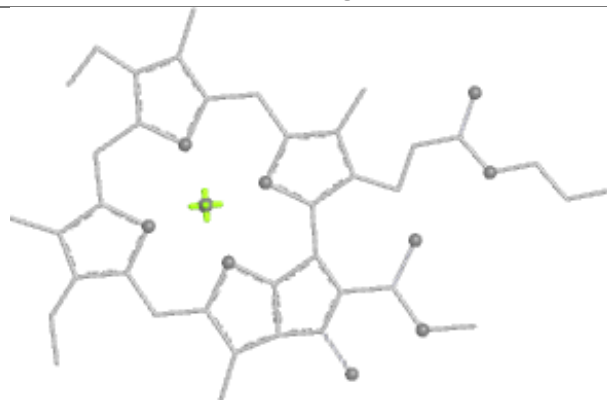
Bond lengths



Bond angles

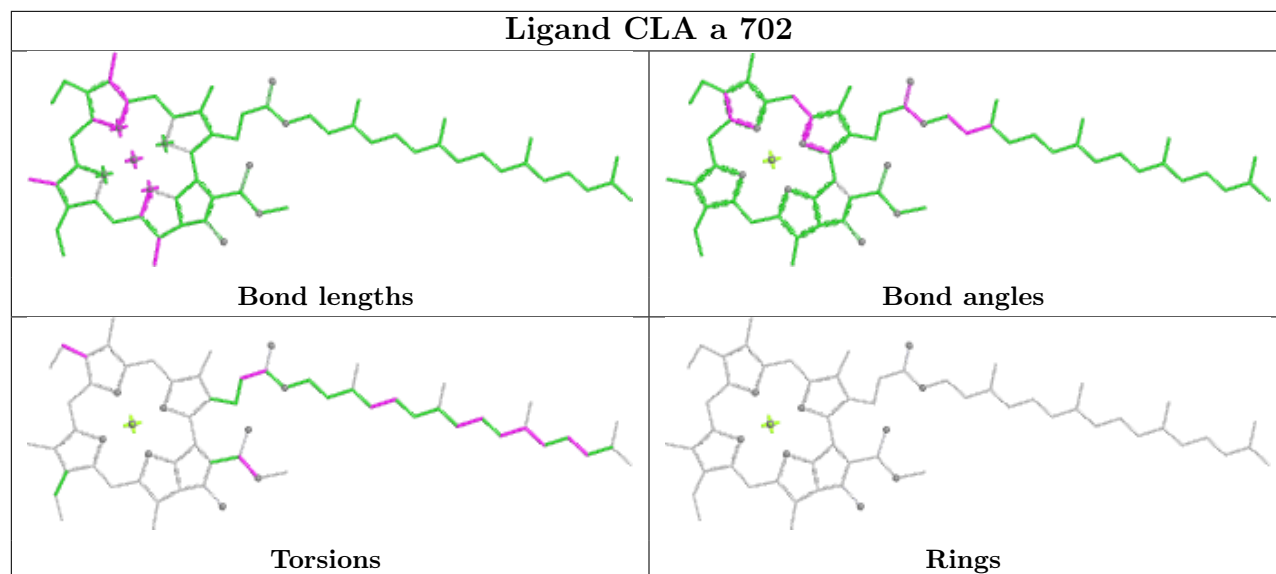


Torsions

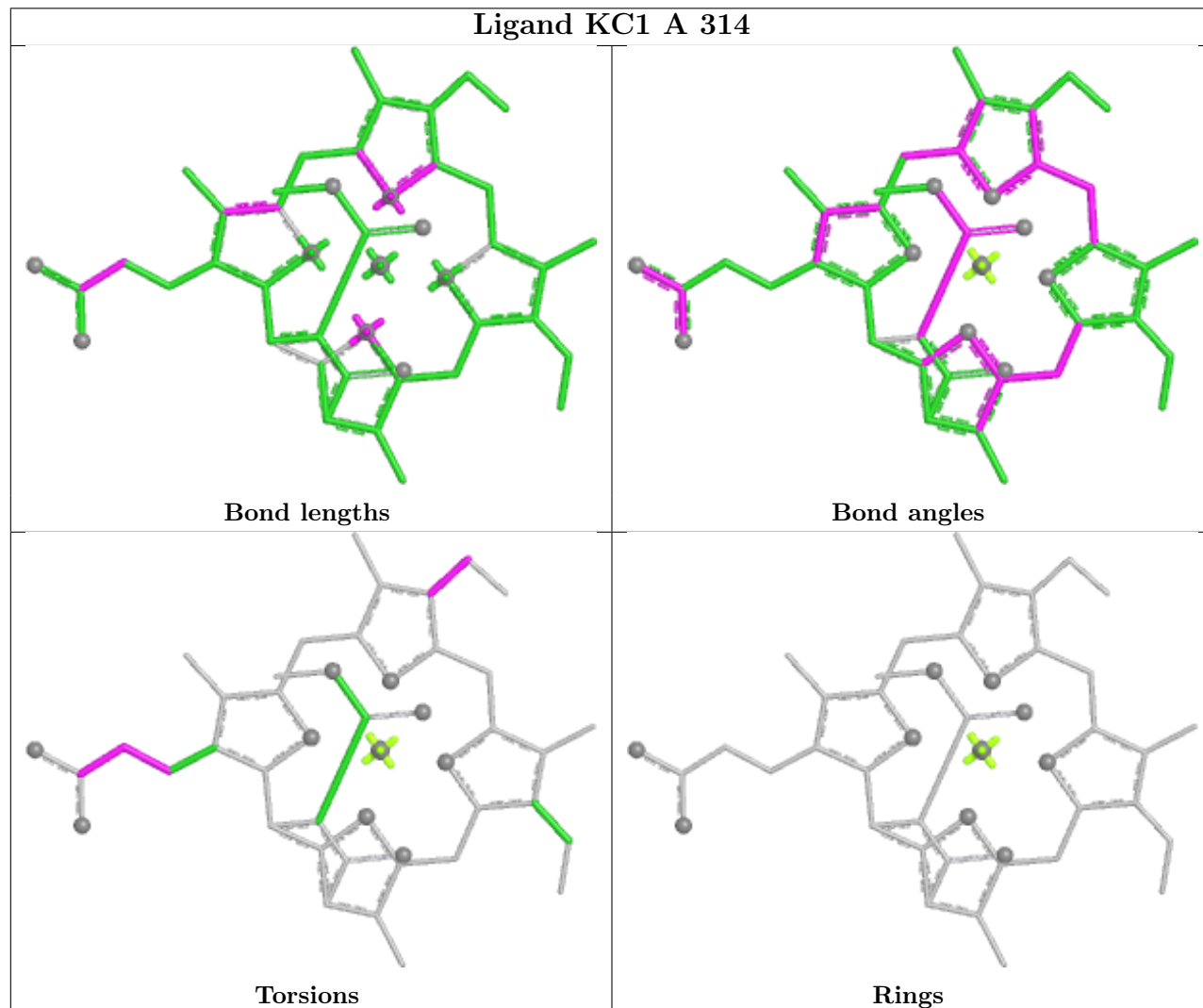


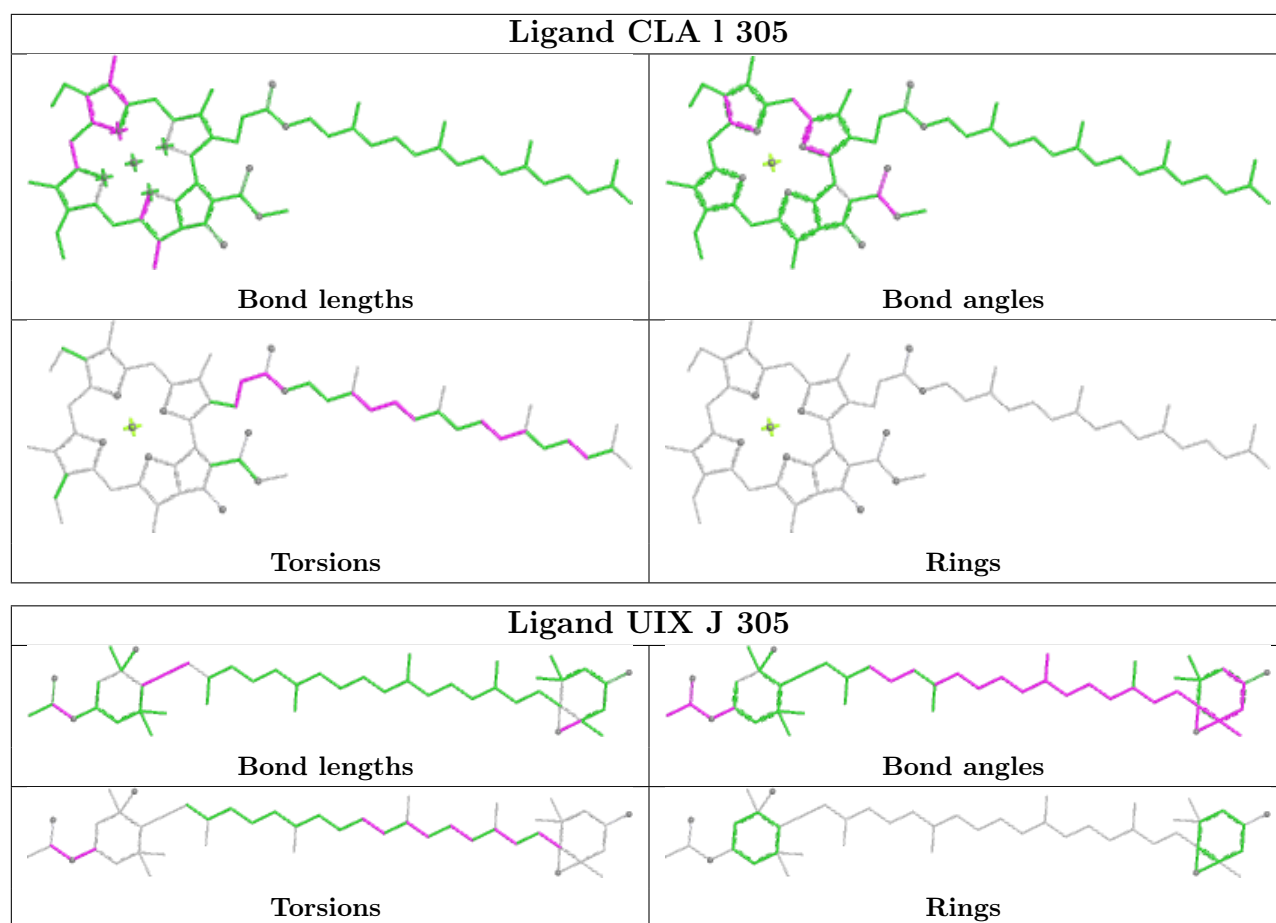
Rings

Ligand CLA a 702

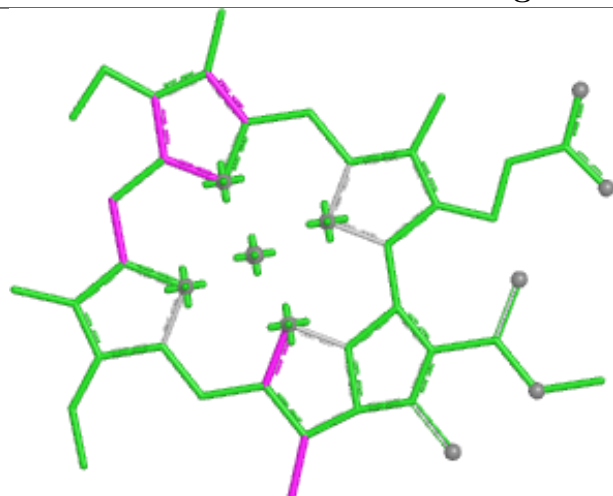


Ligand KC1 A 314

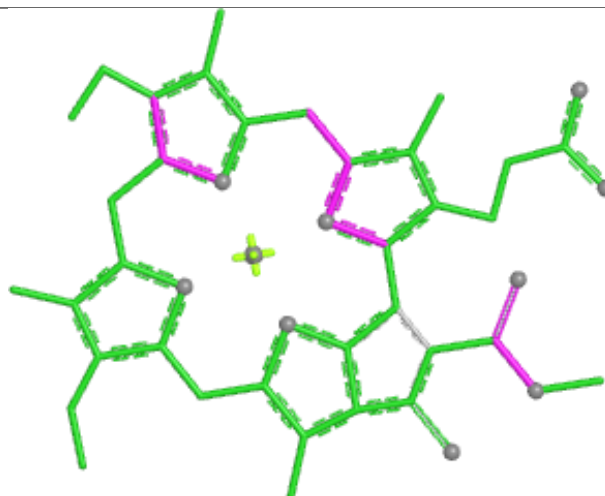




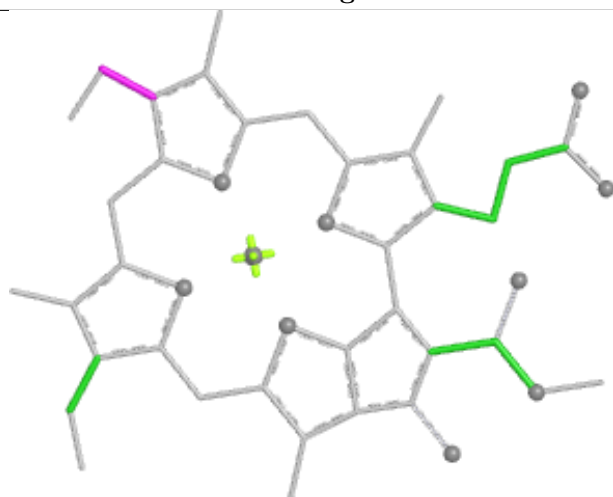
Ligand CLA A 307



Bond lengths



Bond angles

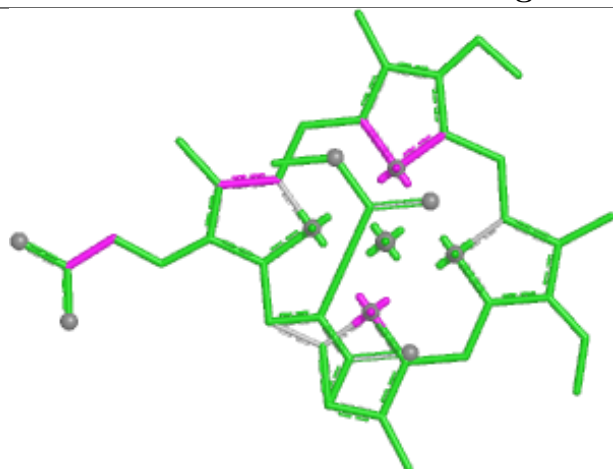


Torsions

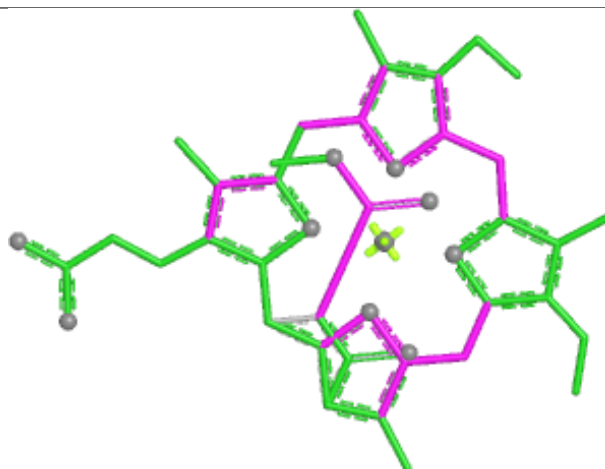


Rings

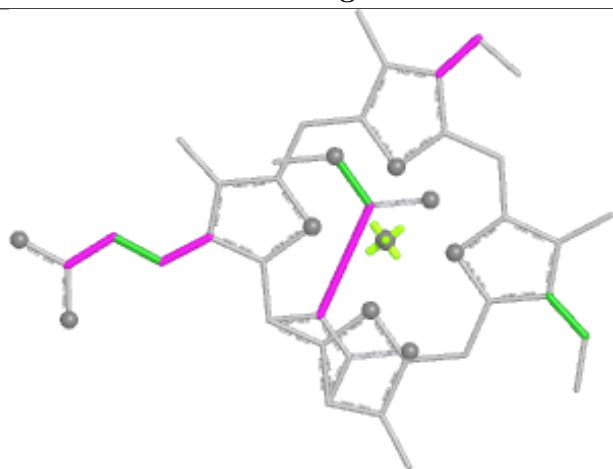
Ligand KC1 A 306



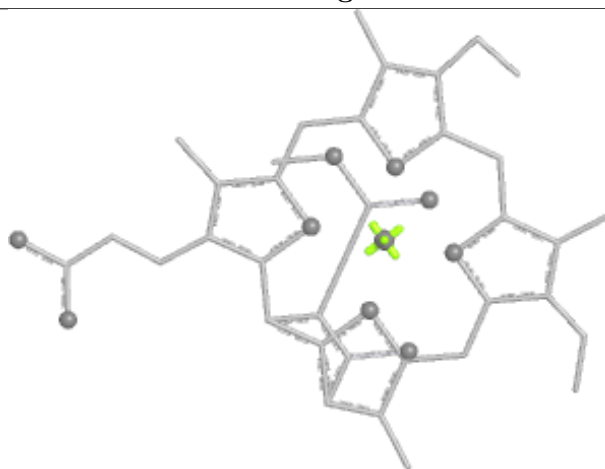
Bond lengths



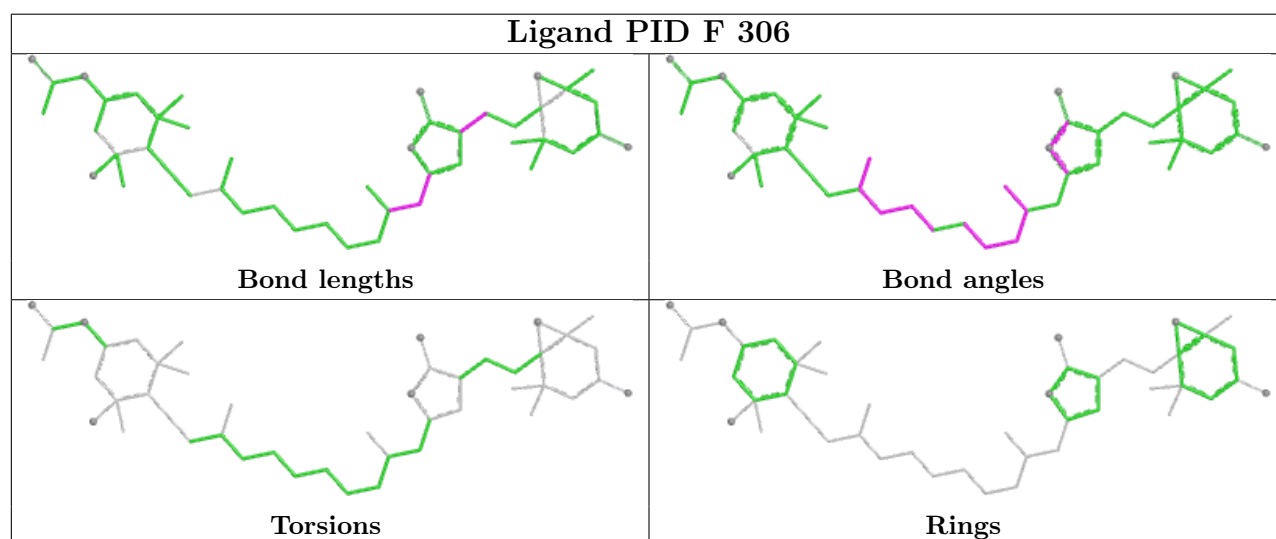
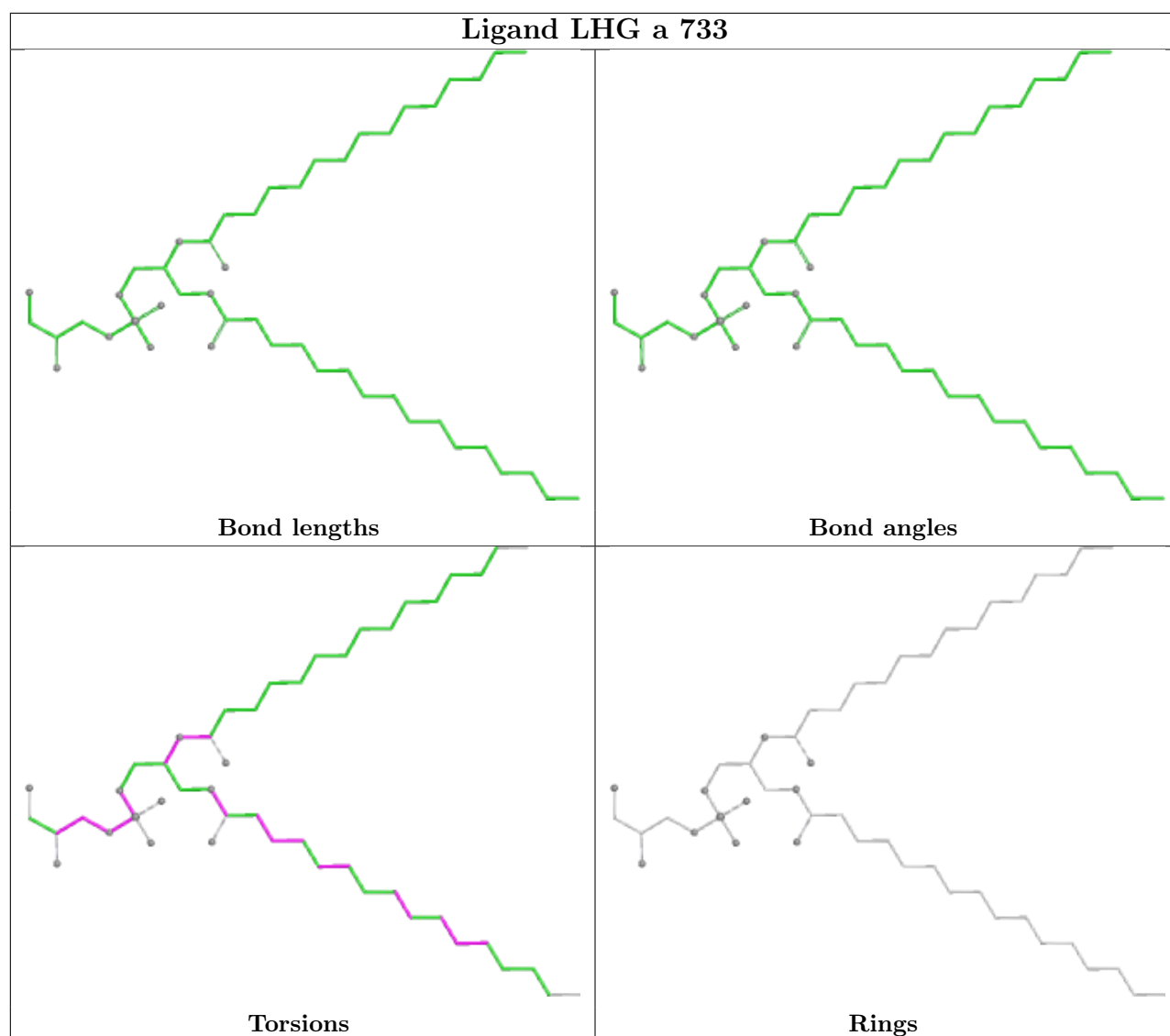
Bond angles

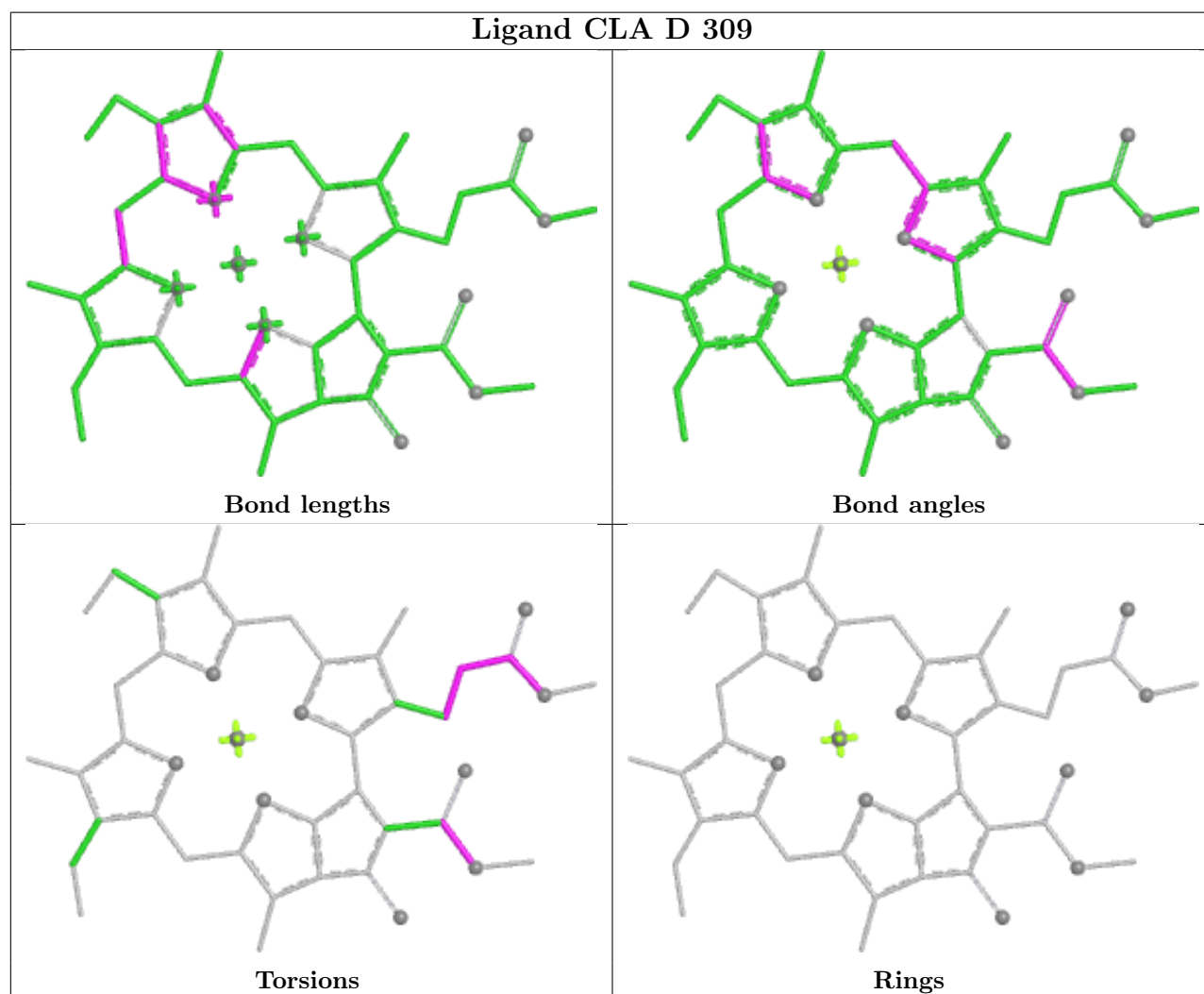
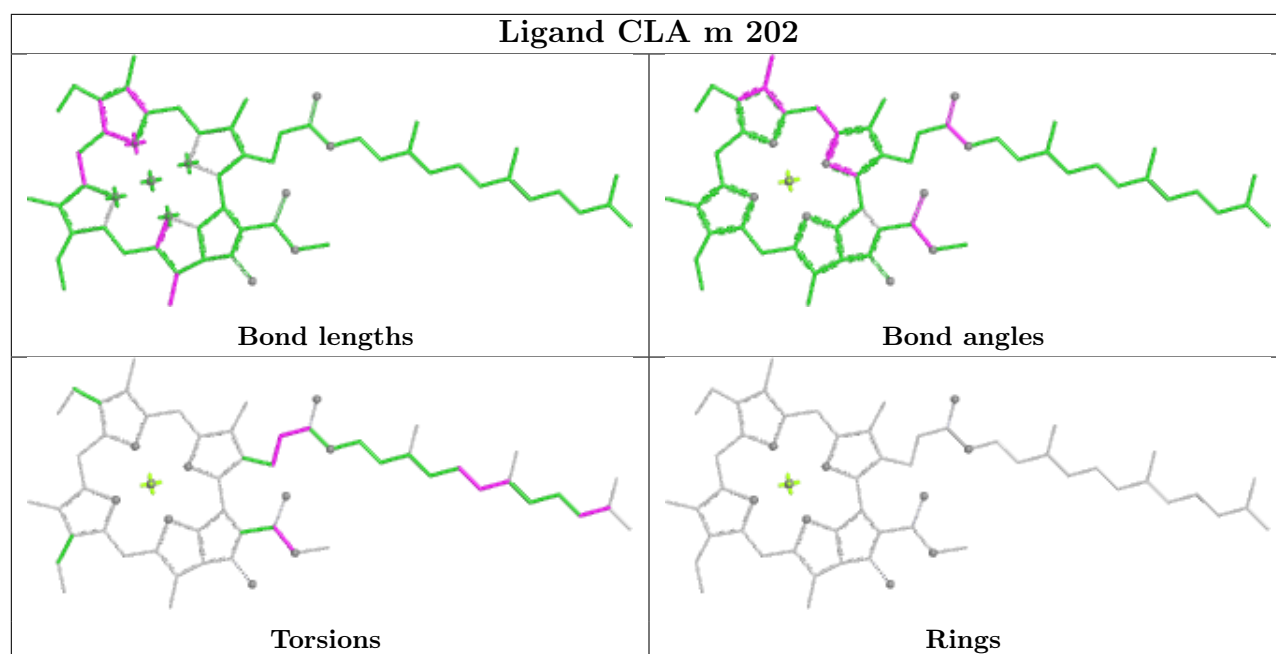


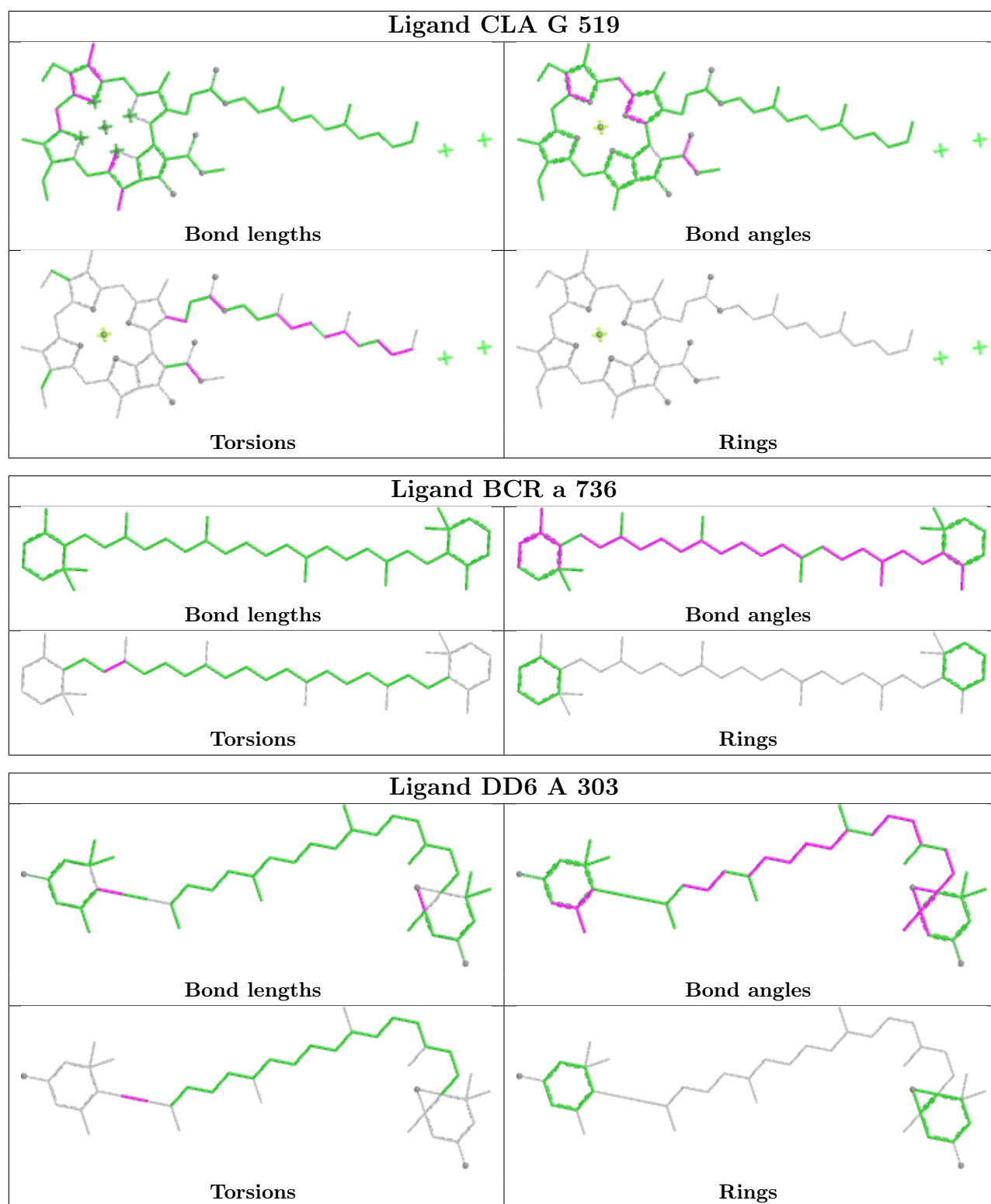
Torsions



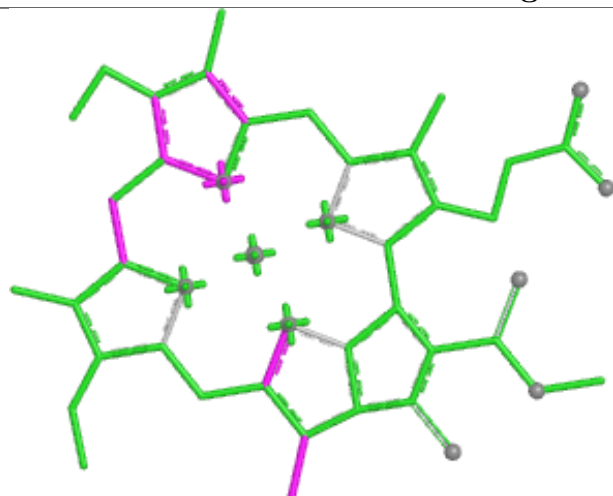
Rings



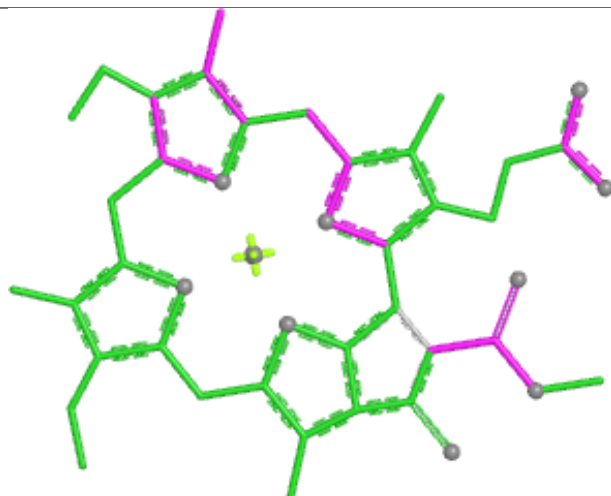




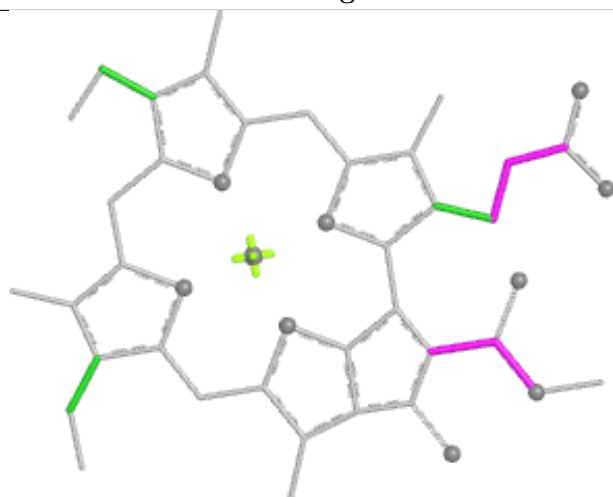
Ligand CLA I 319



Bond lengths



Bond angles

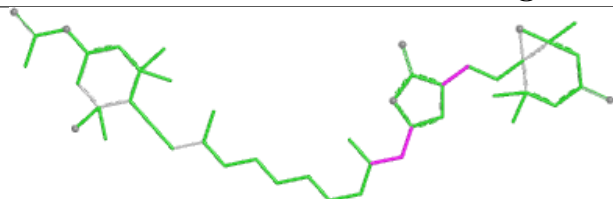


Torsions

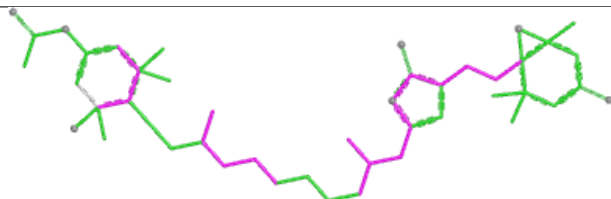


Rings

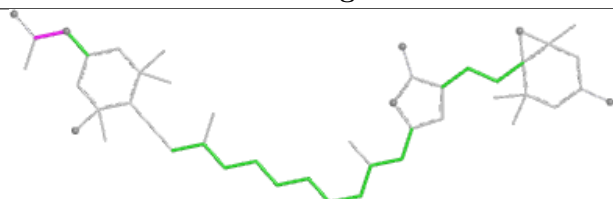
Ligand PID N 302



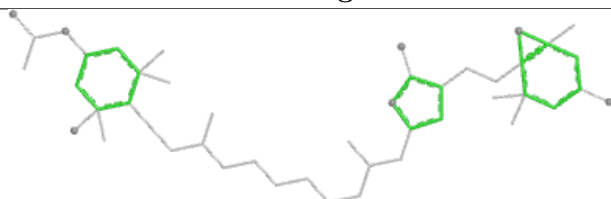
Bond lengths



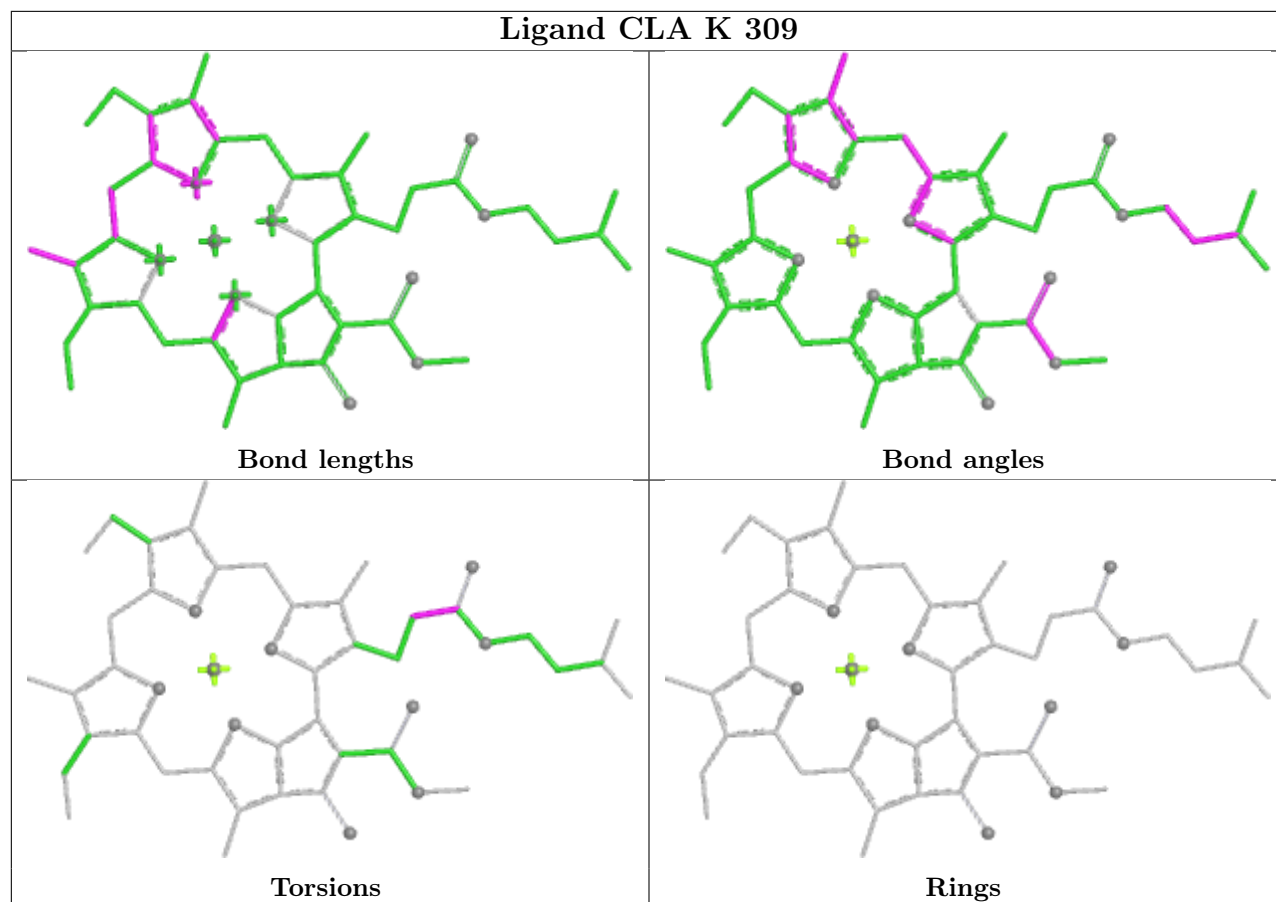
Bond angles

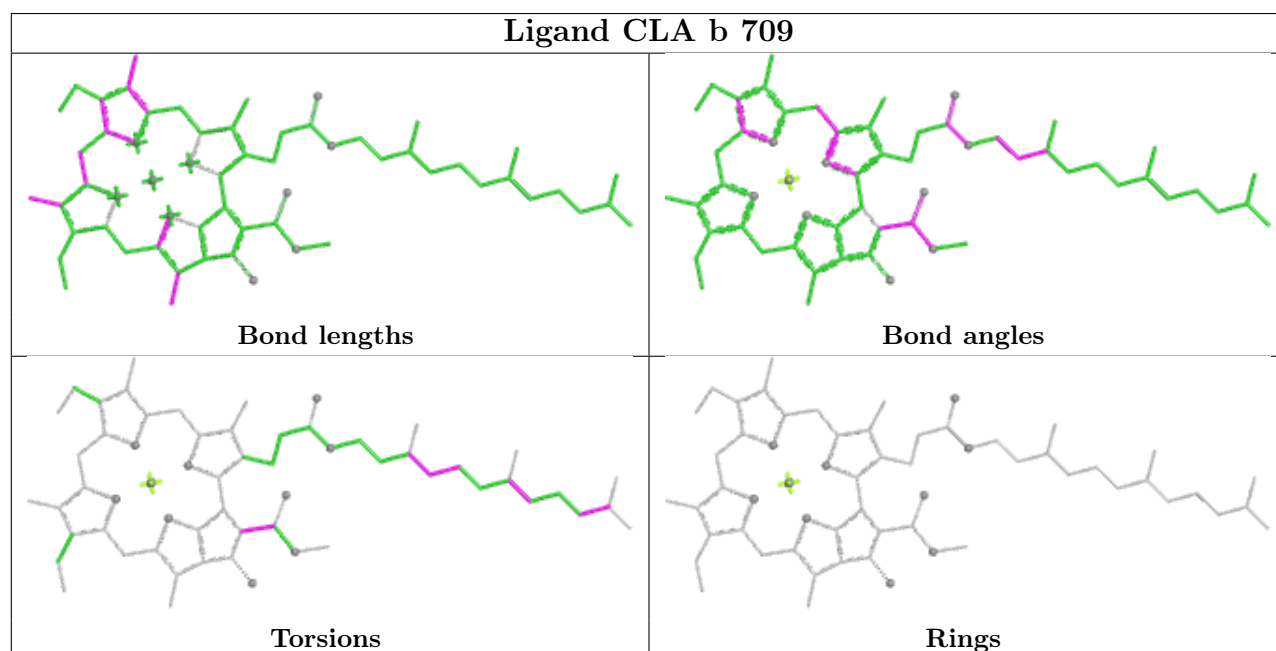
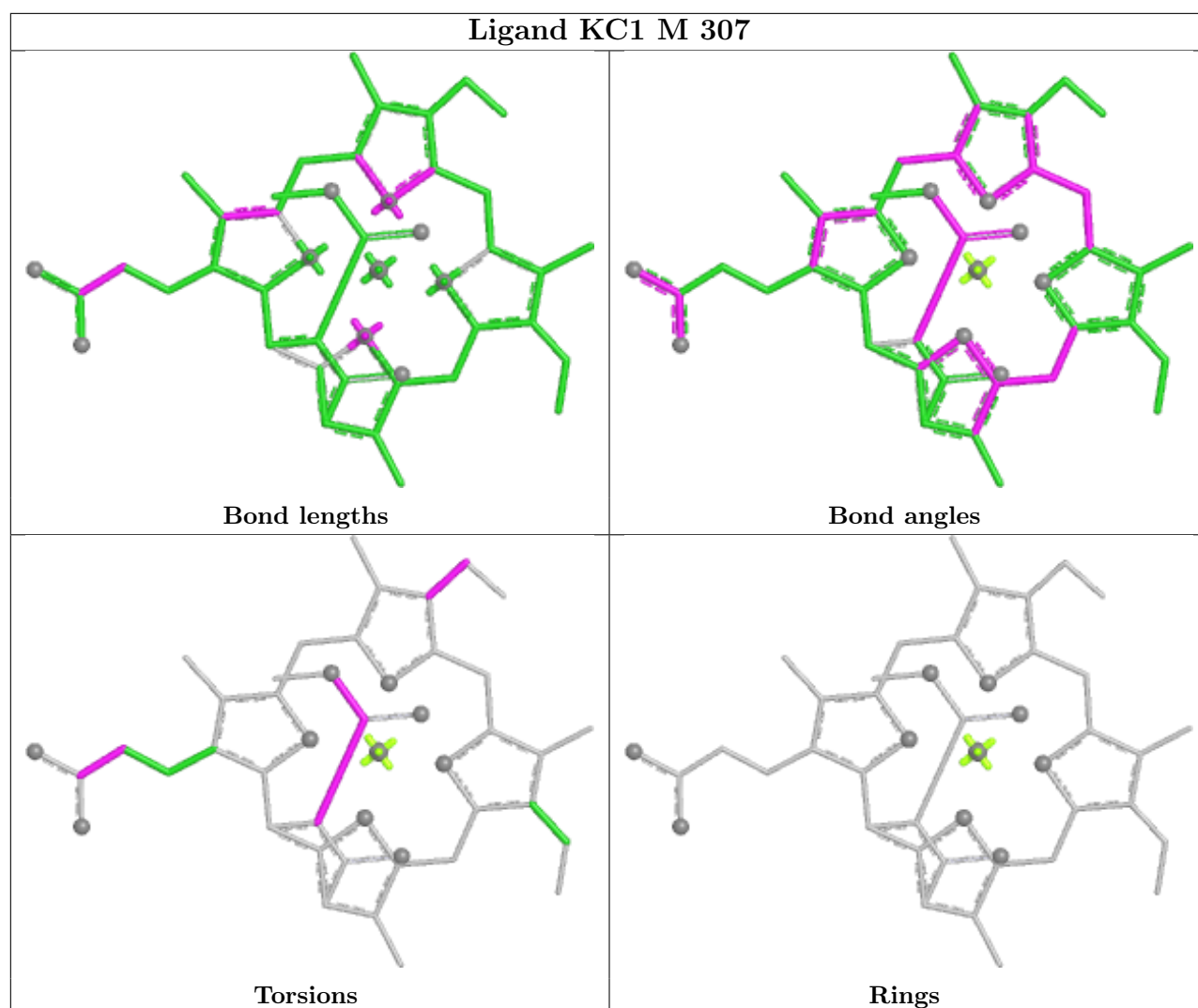


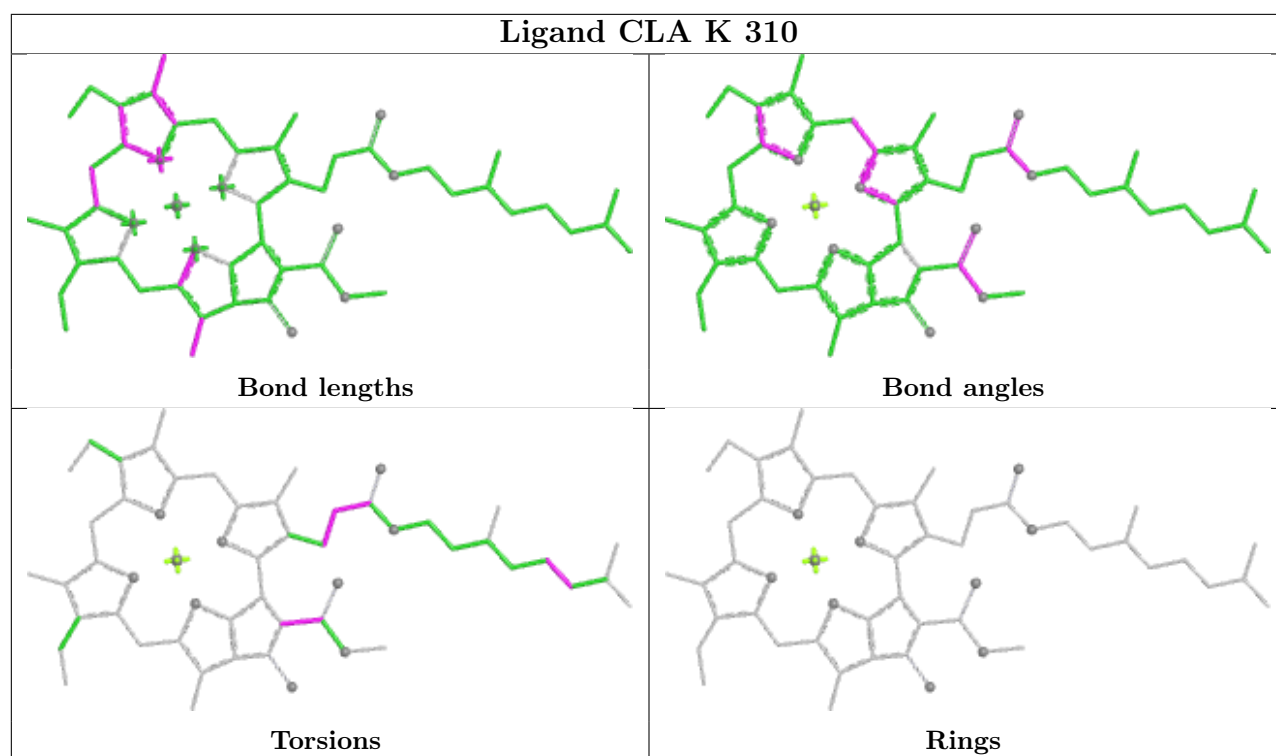
Torsions



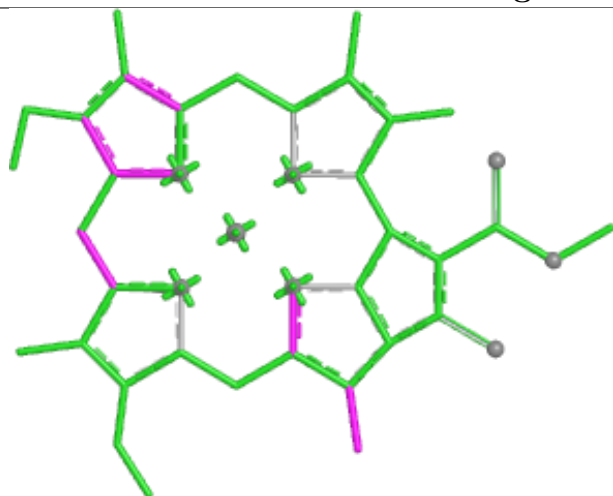
Rings



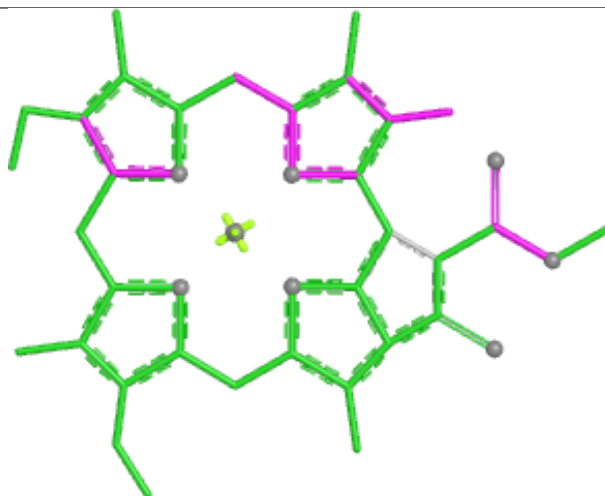




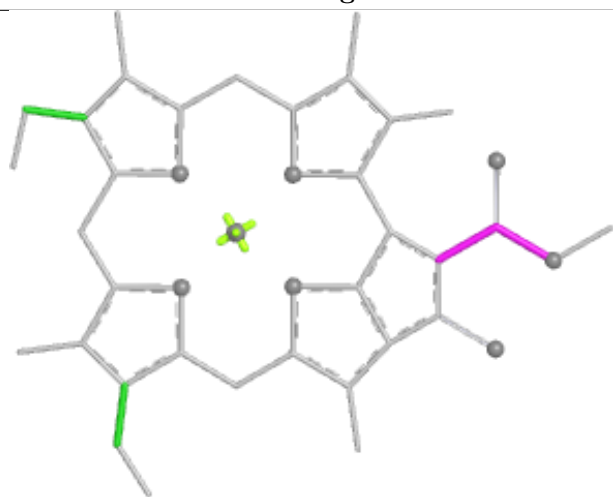
Ligand CLA A 315



Bond lengths



Bond angles

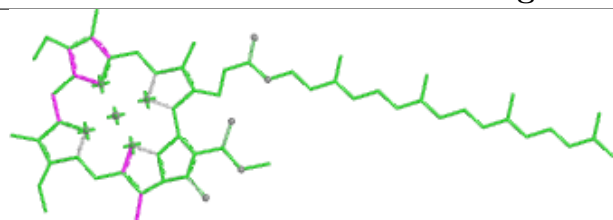


Torsions

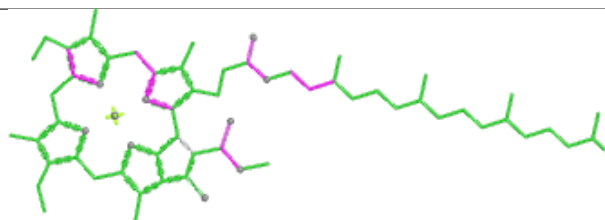


Rings

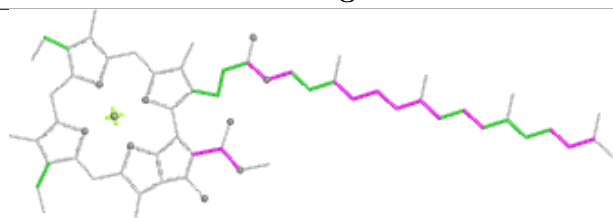
Ligand CLA b 707



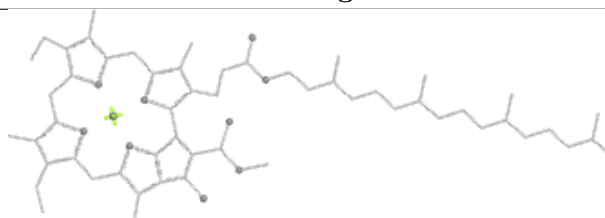
Bond lengths



Bond angles

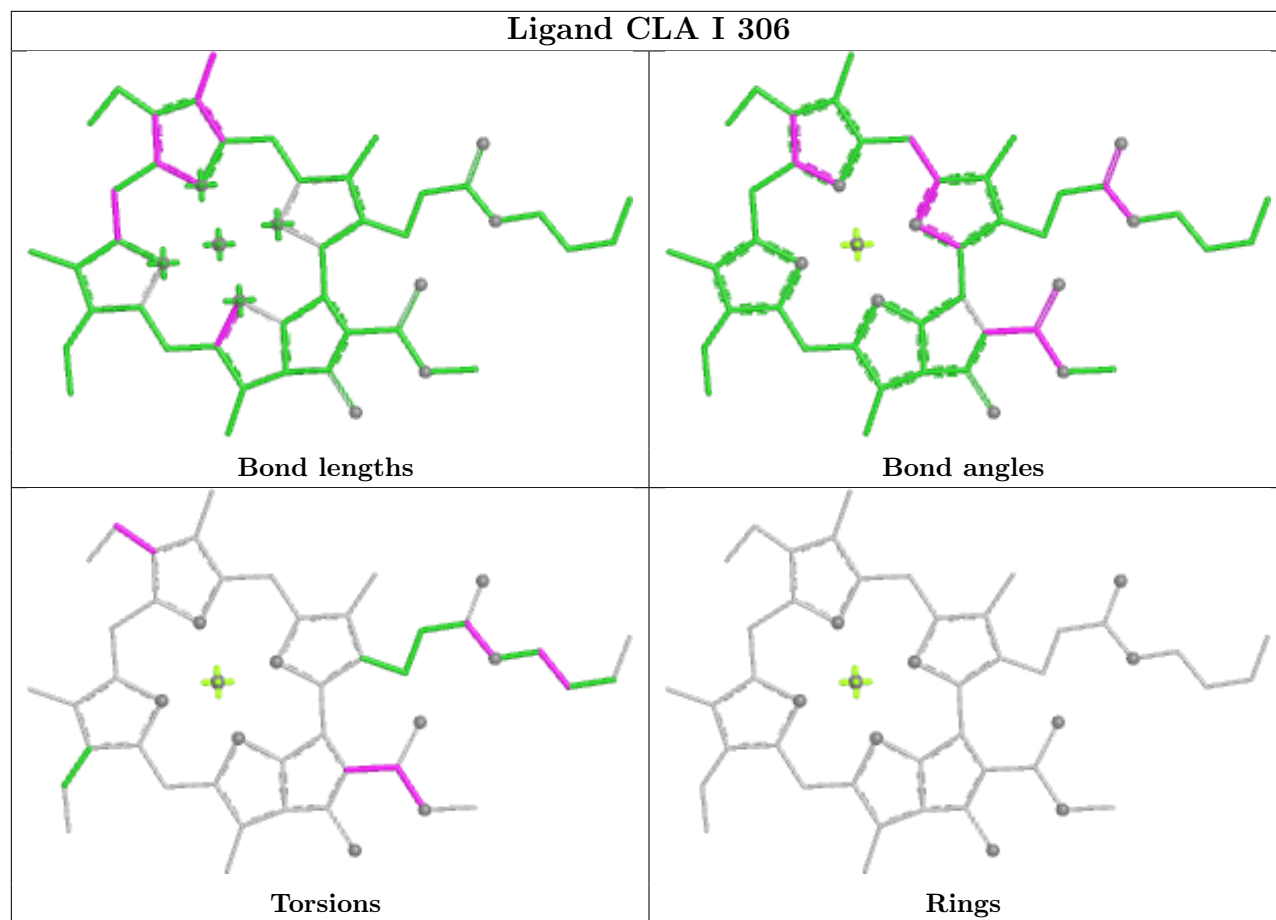


Torsions

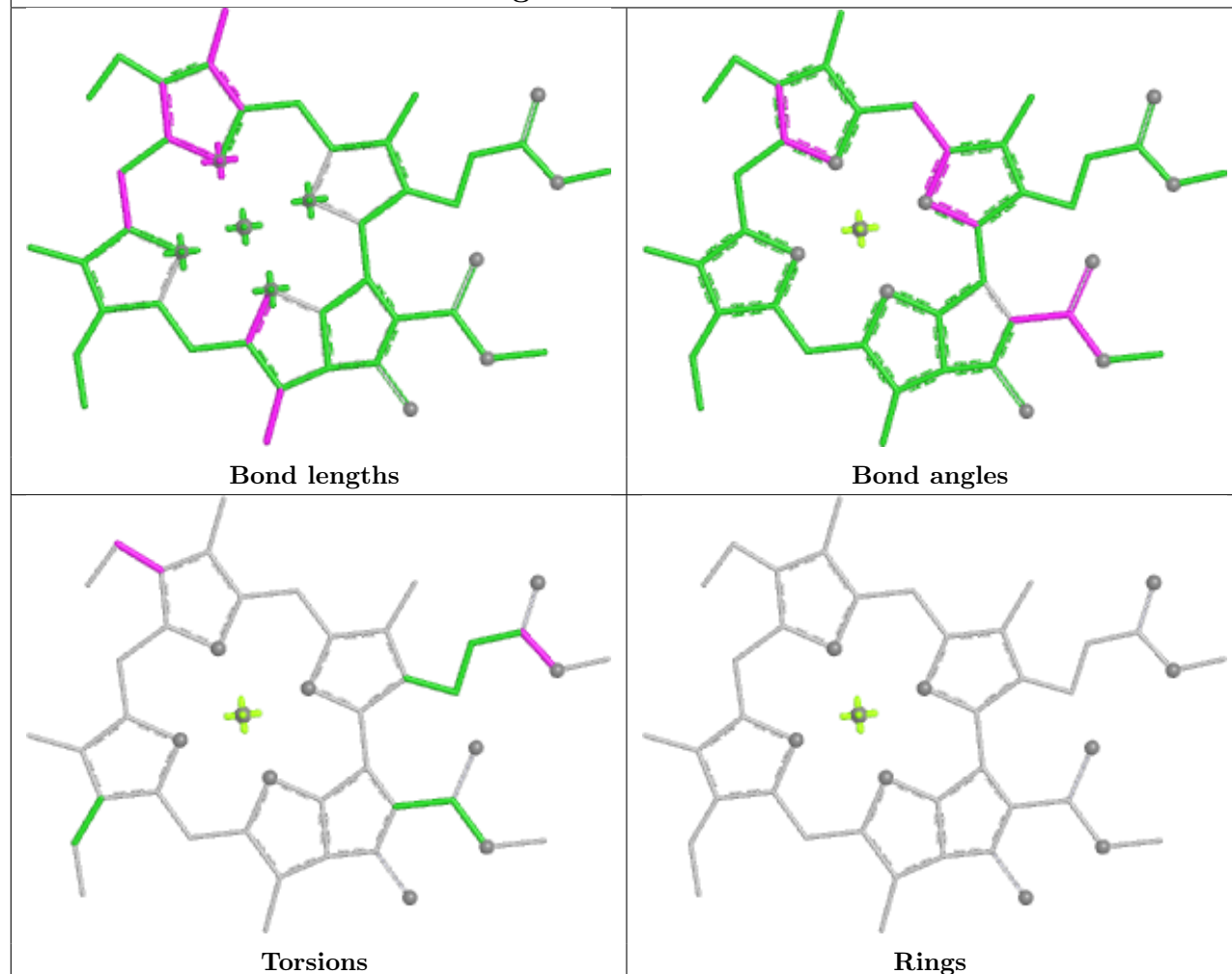


Rings

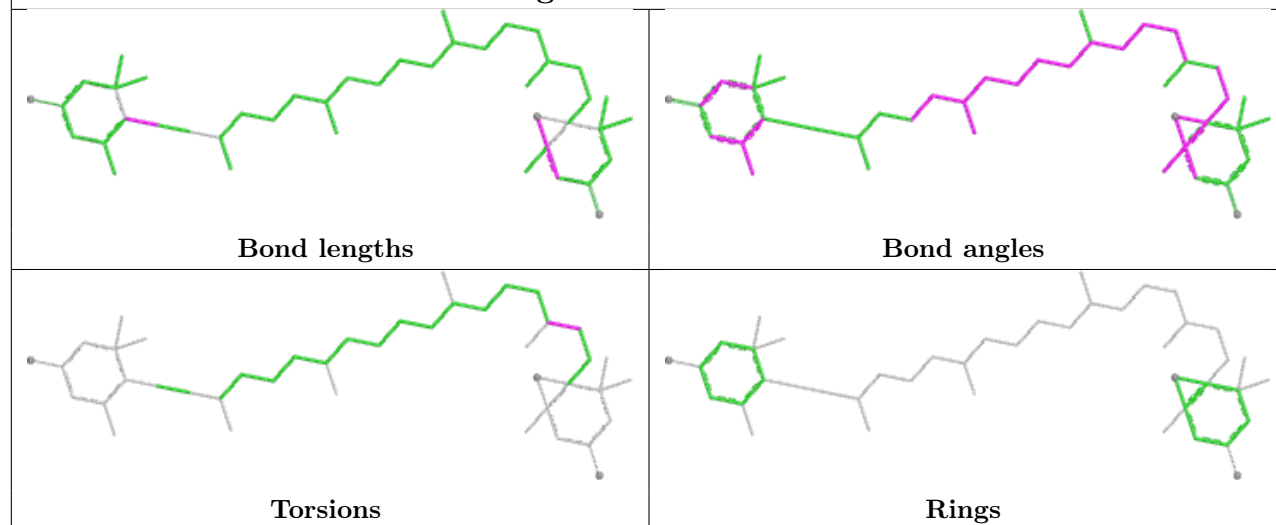
Ligand CLA I 306

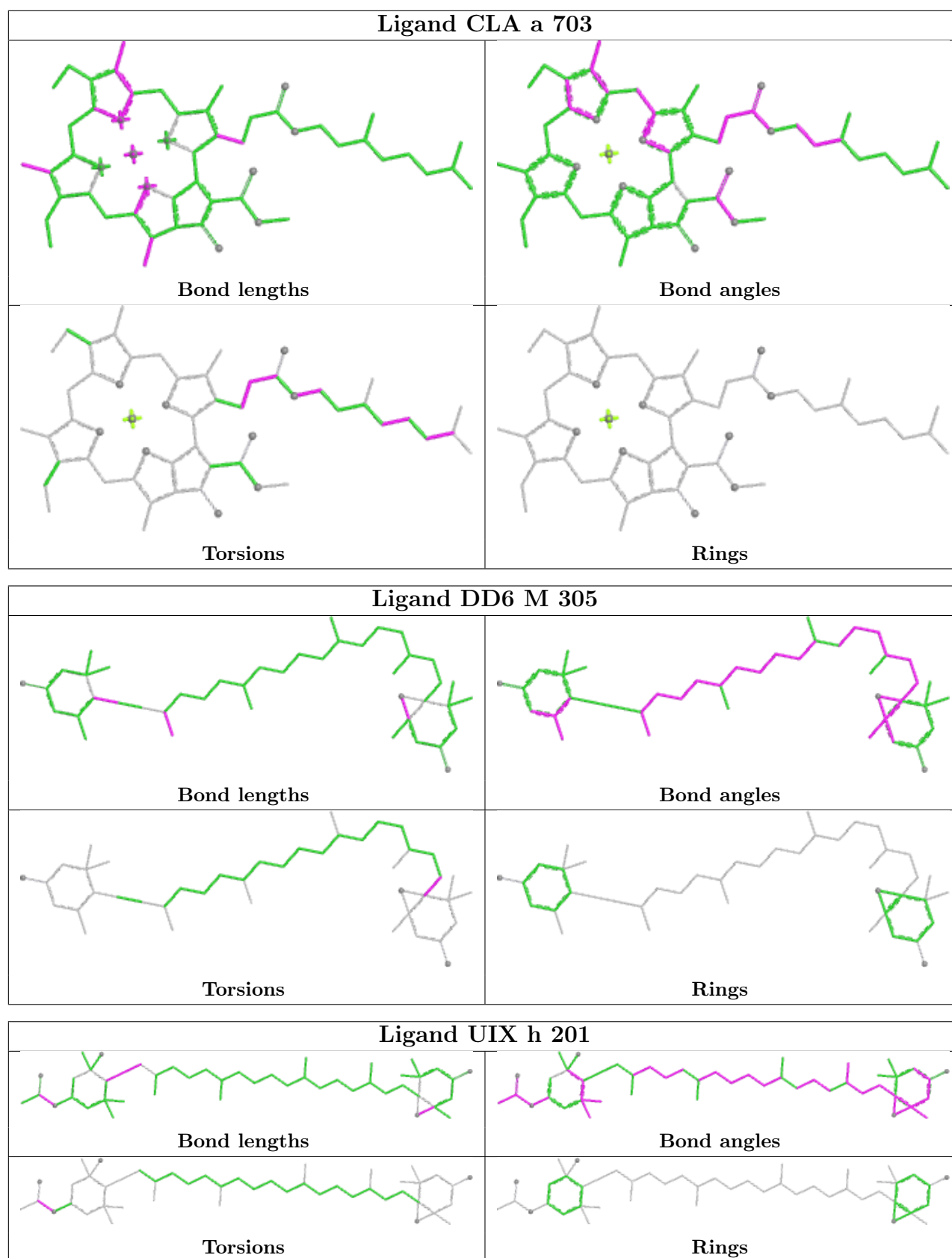


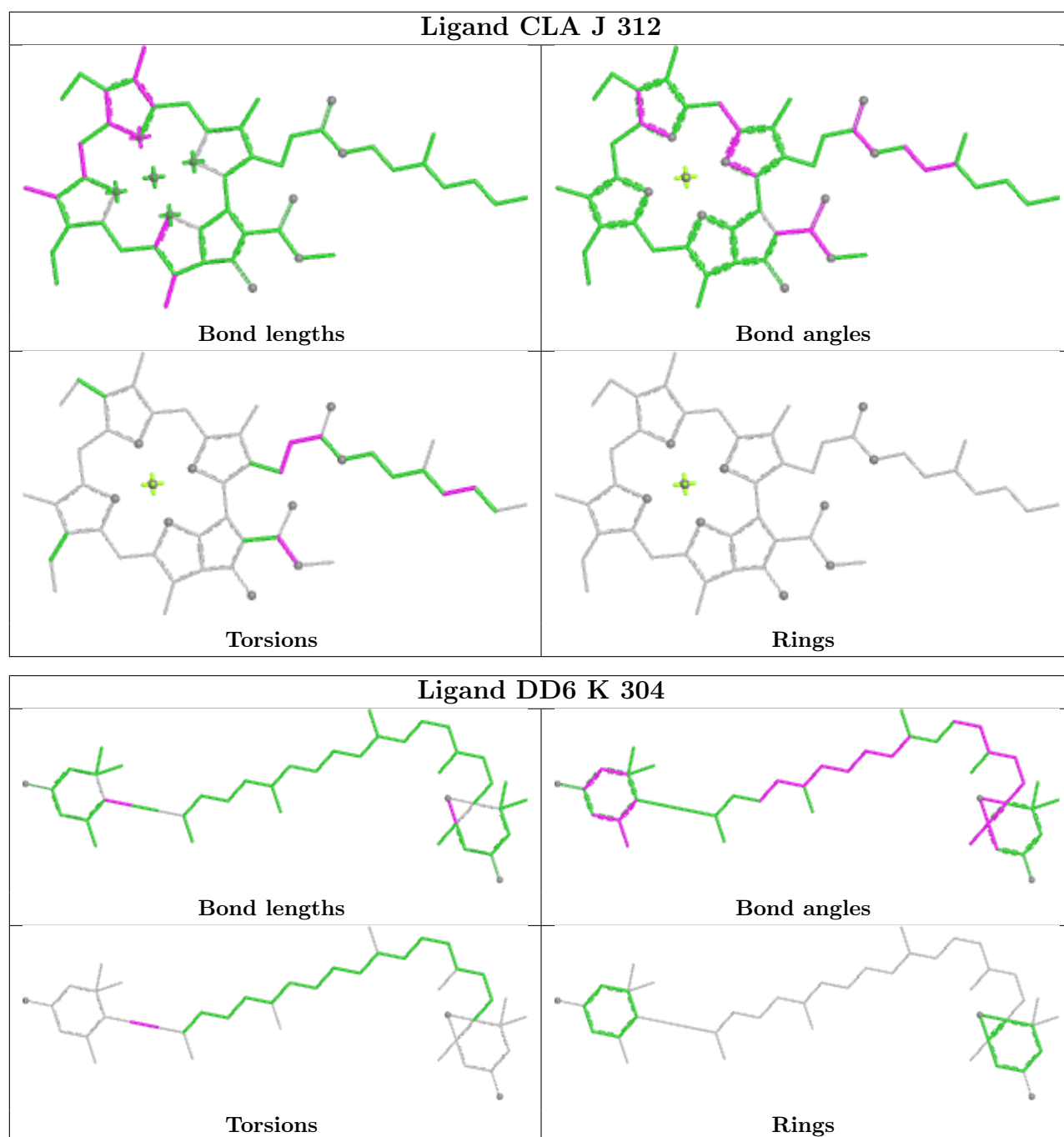
Ligand CLA K 316

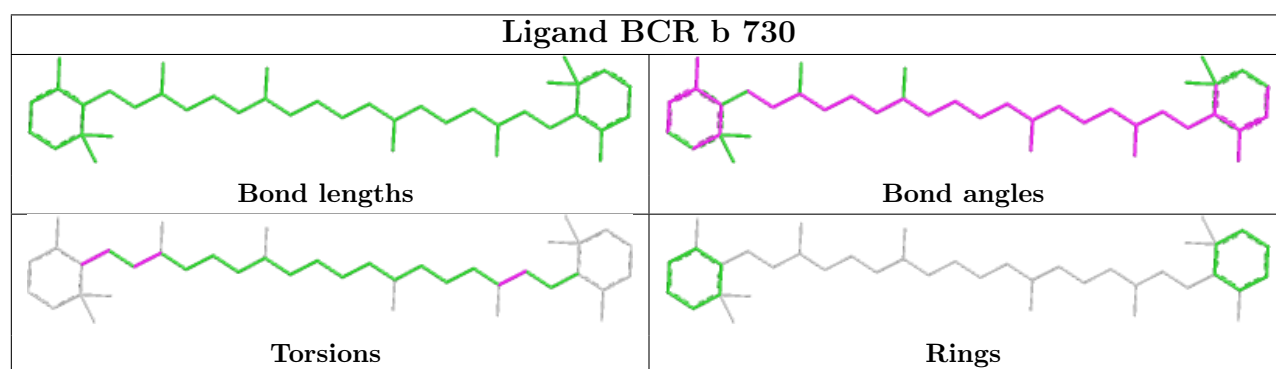
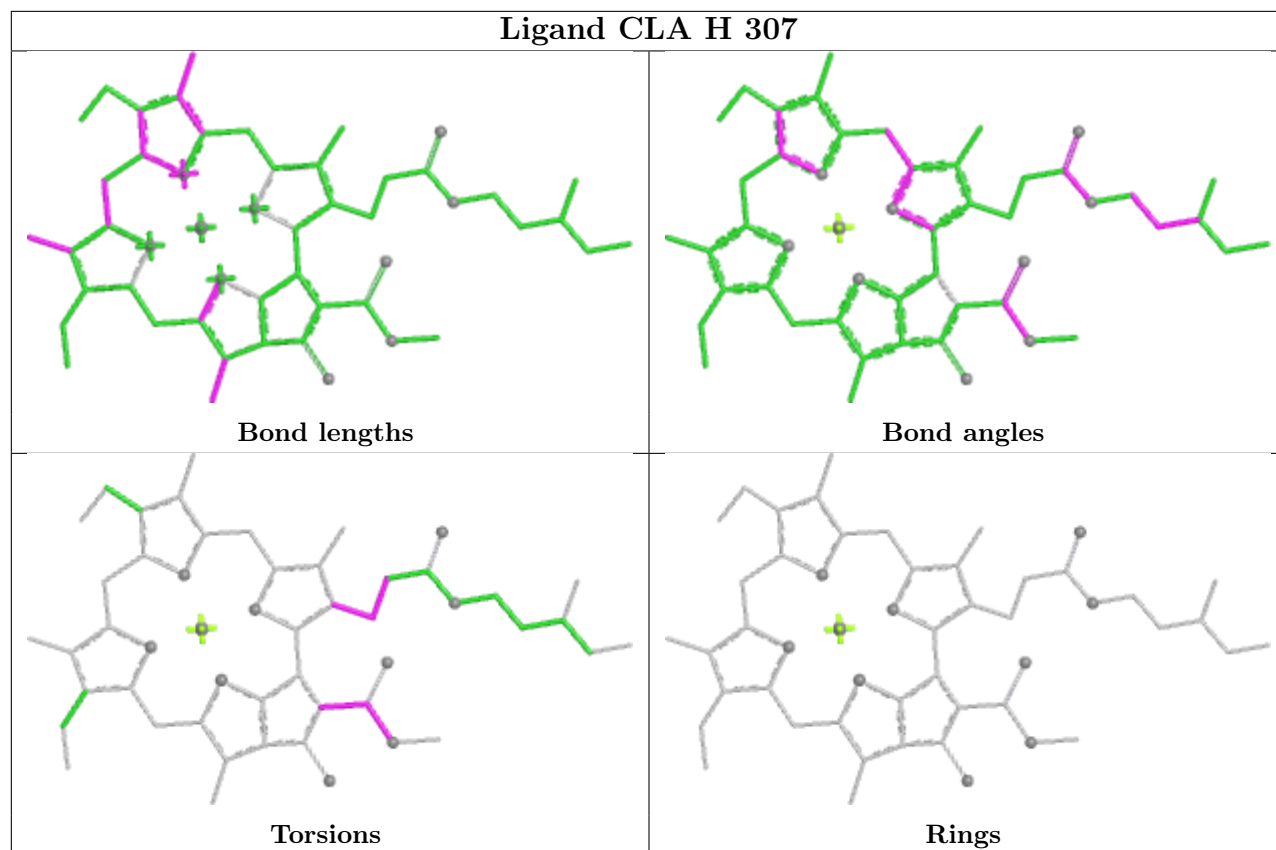


Ligand DD6 J 303

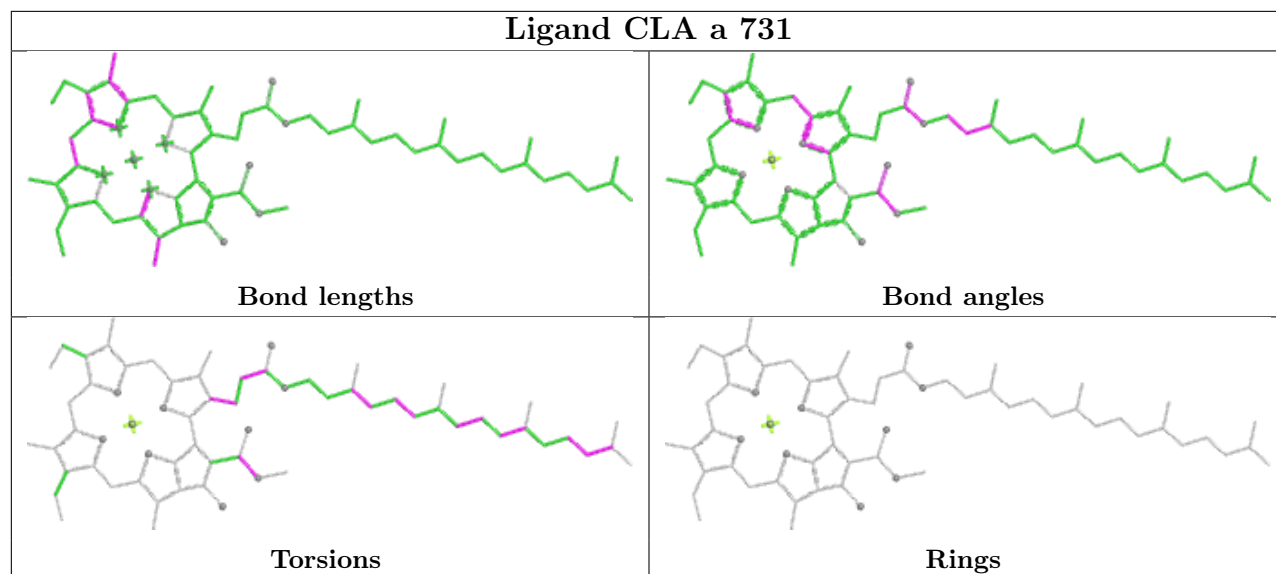




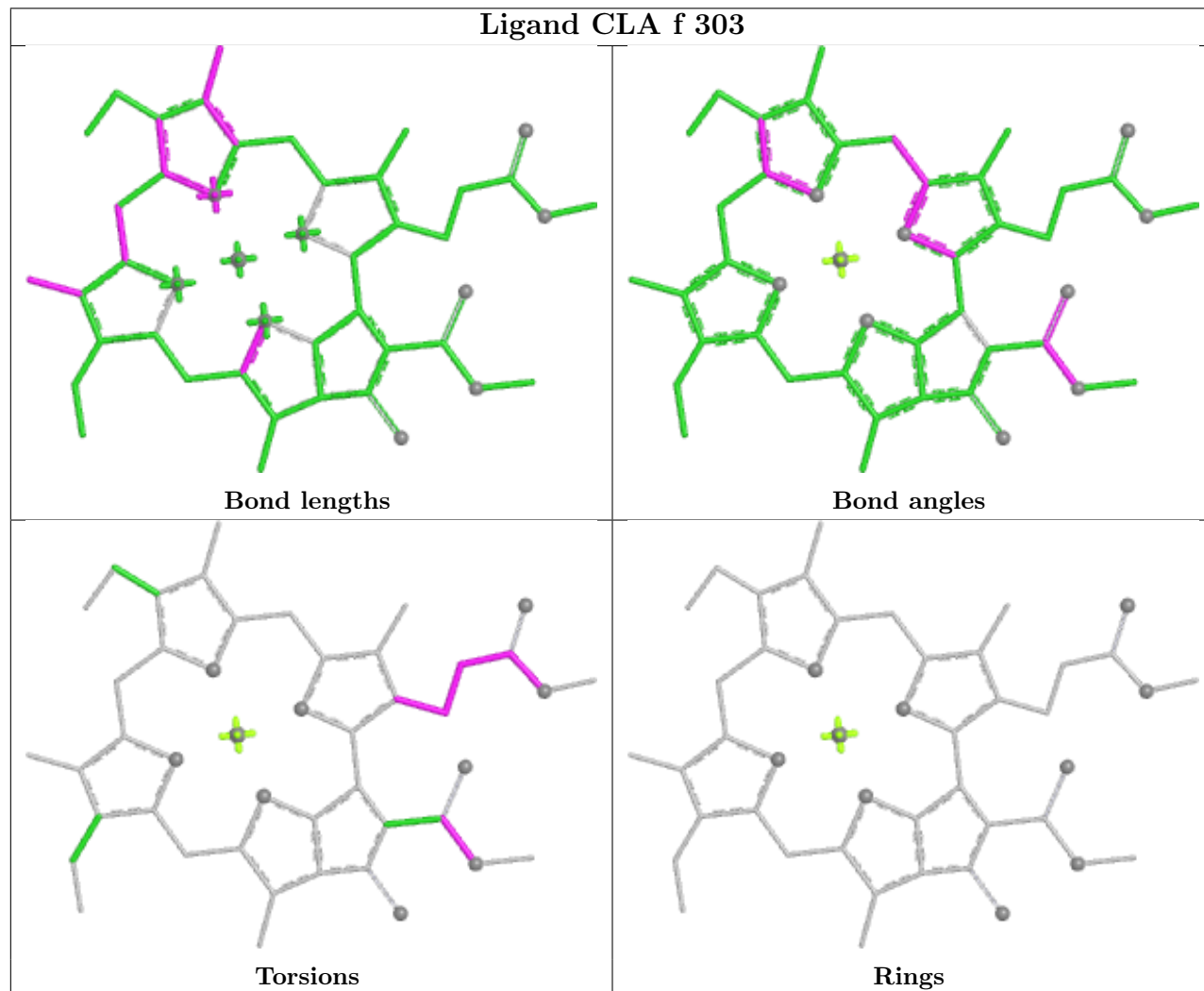




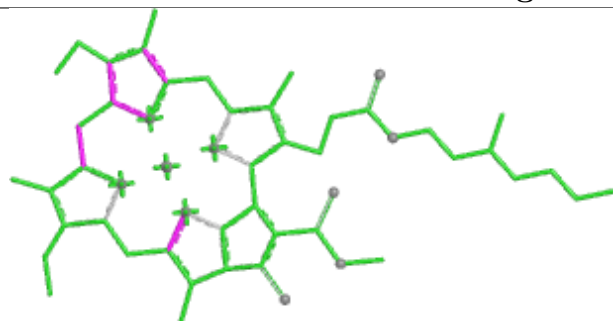
Ligand CLA a 731



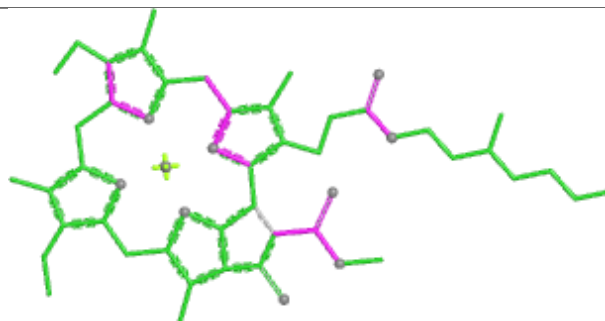
Ligand CLA f 303



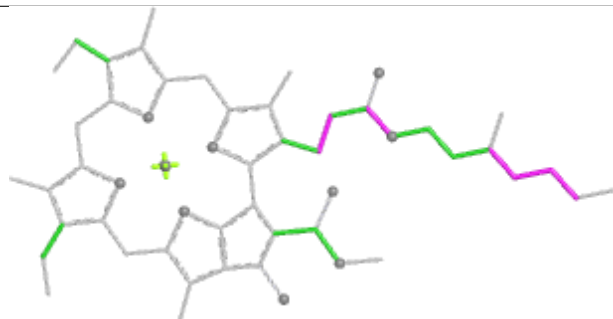
Ligand CLA L 309



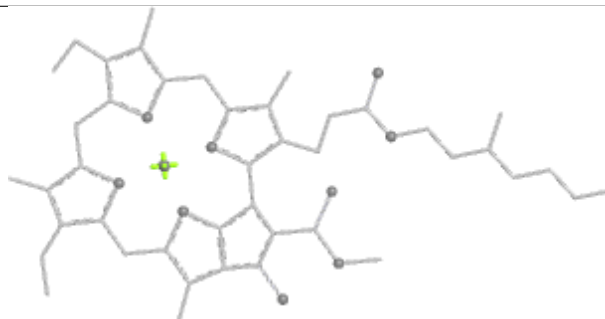
Bond lengths



Bond angles

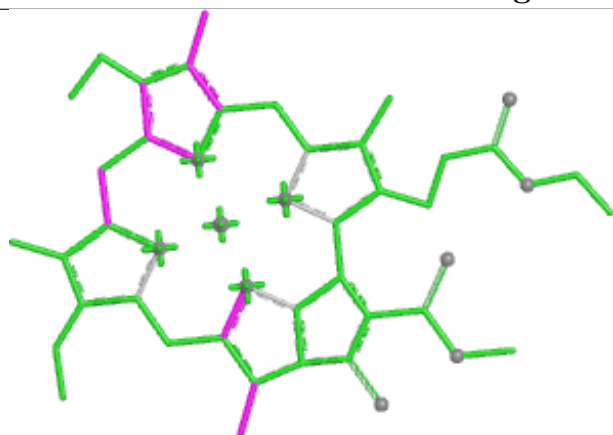


Torsions

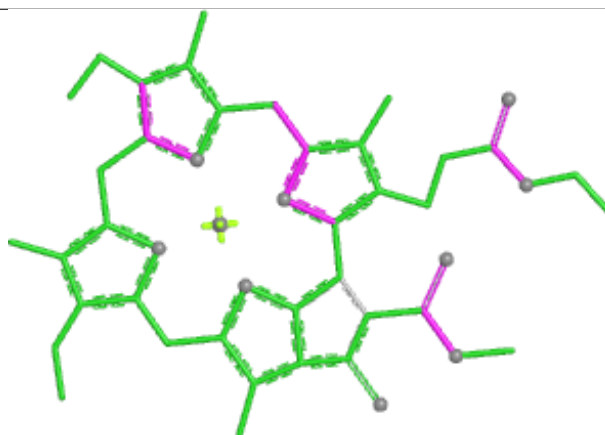


Rings

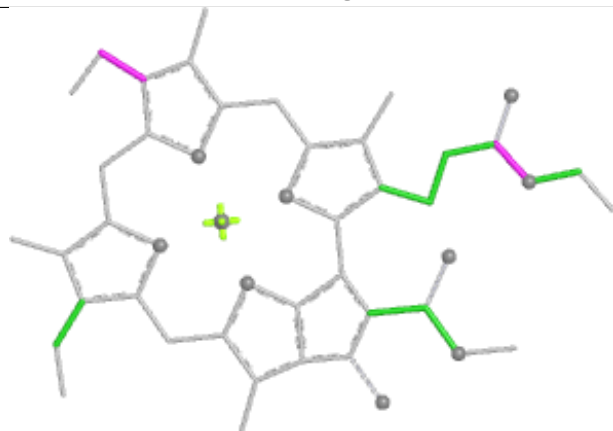
Ligand CLA N 304



Bond lengths



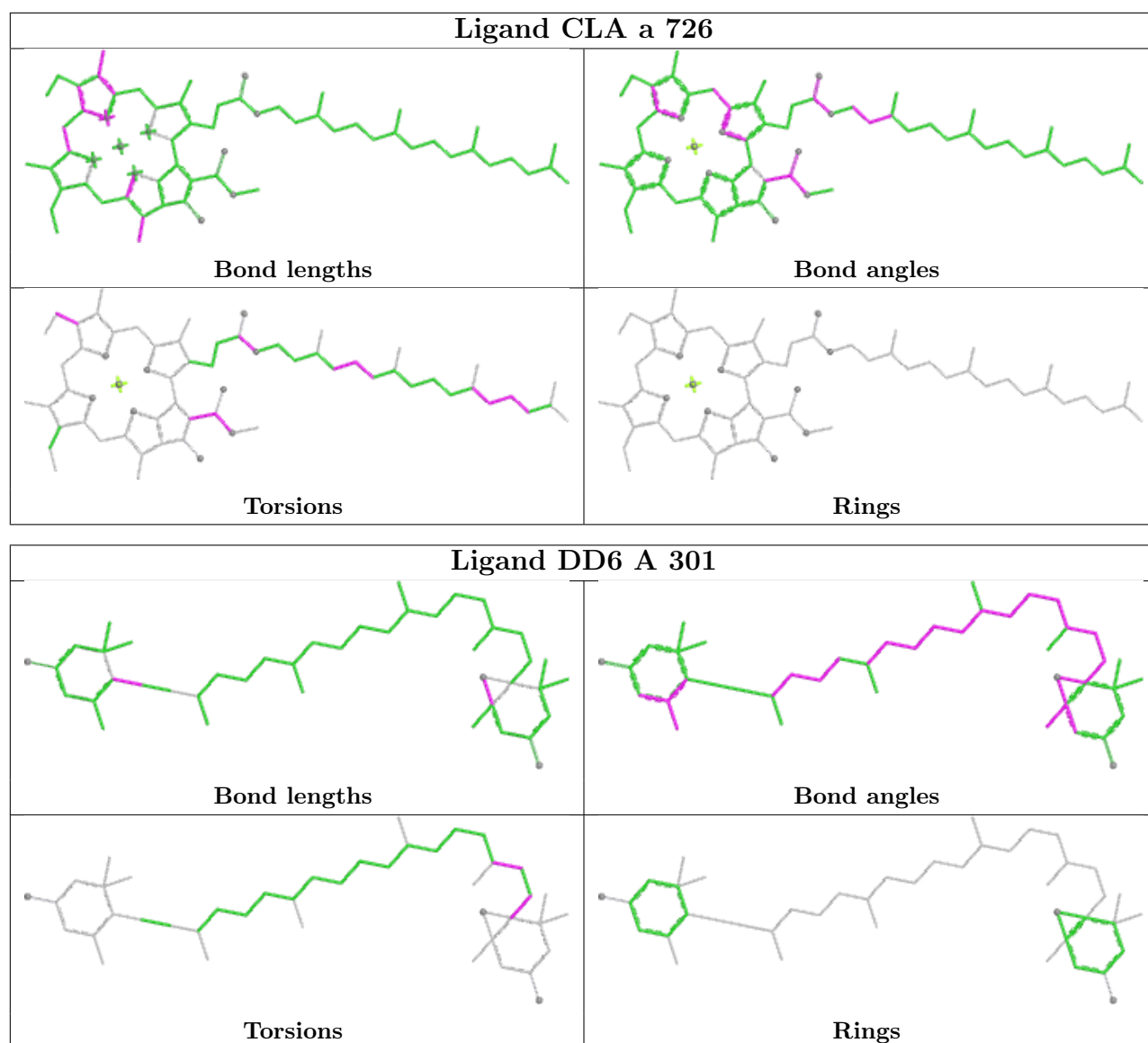
Bond angles



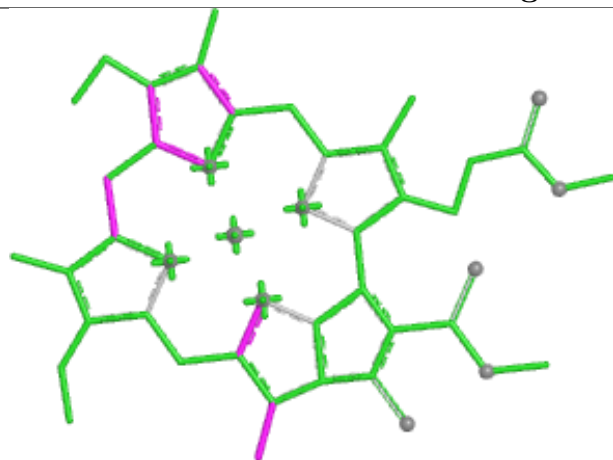
Torsions



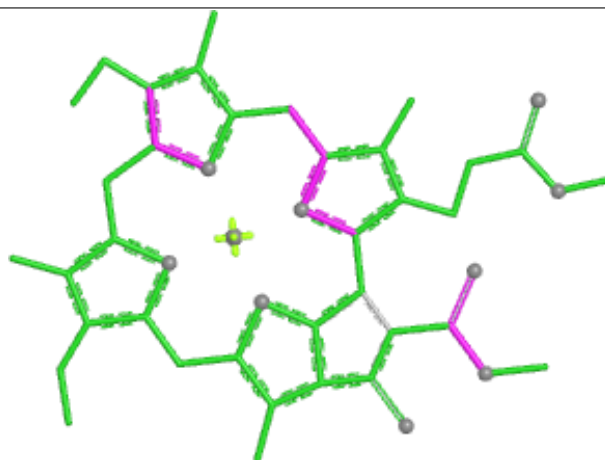
Rings



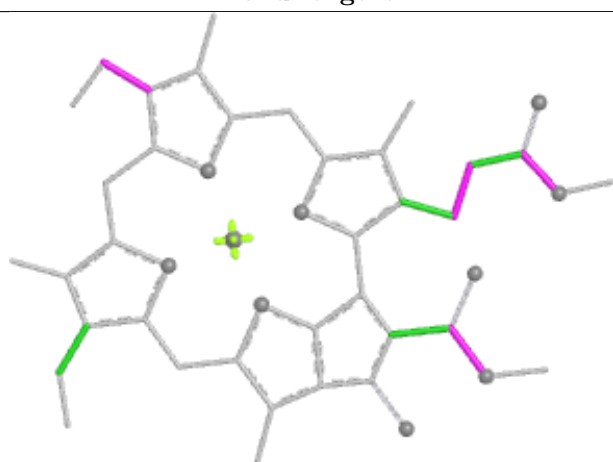
Ligand CLA I 307



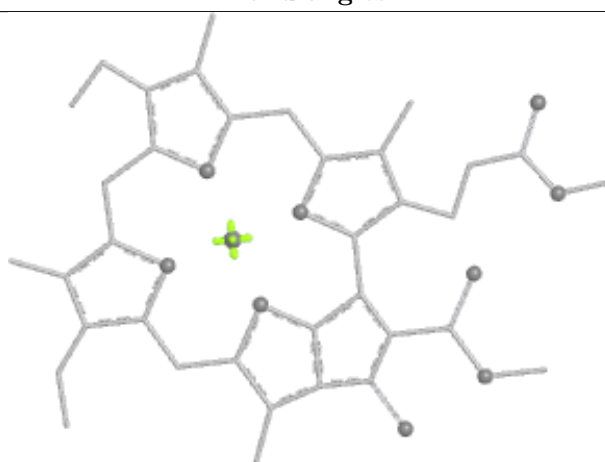
Bond lengths



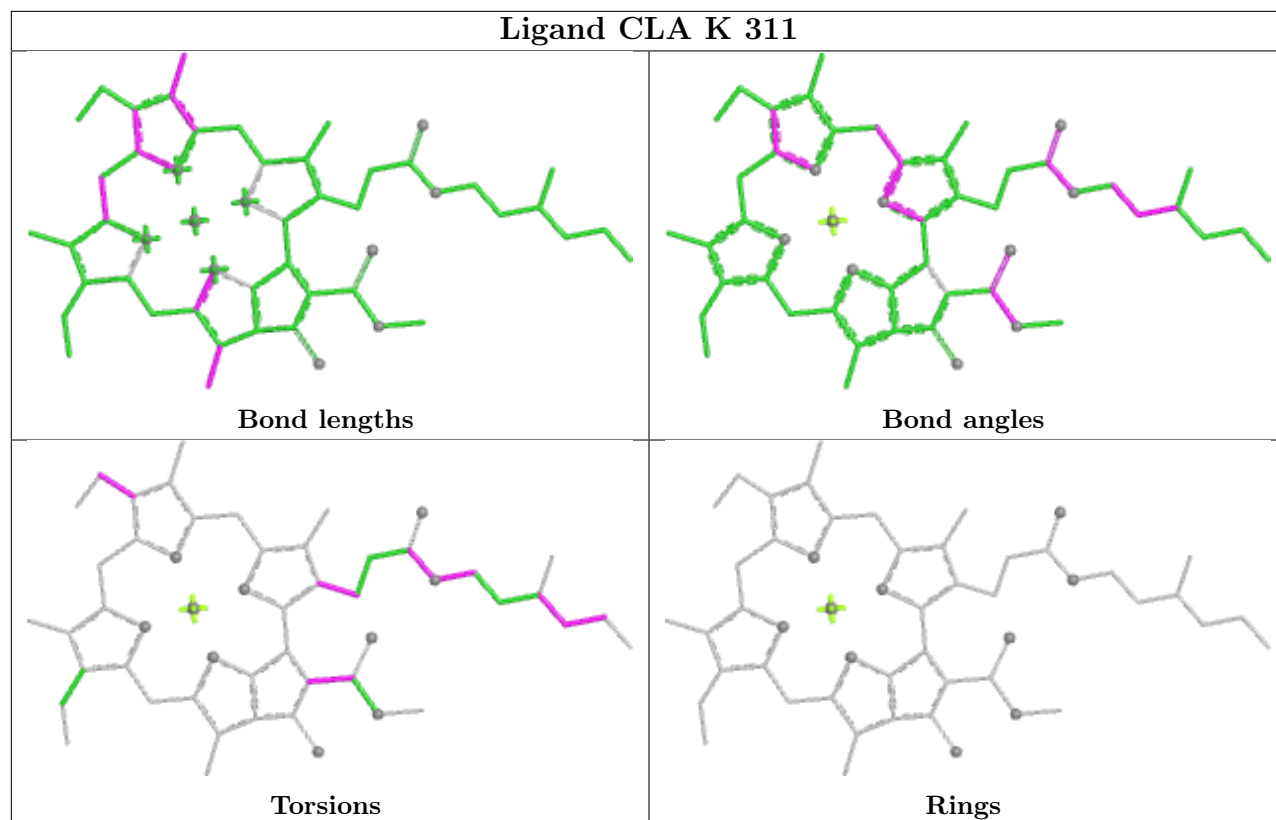
Bond angles



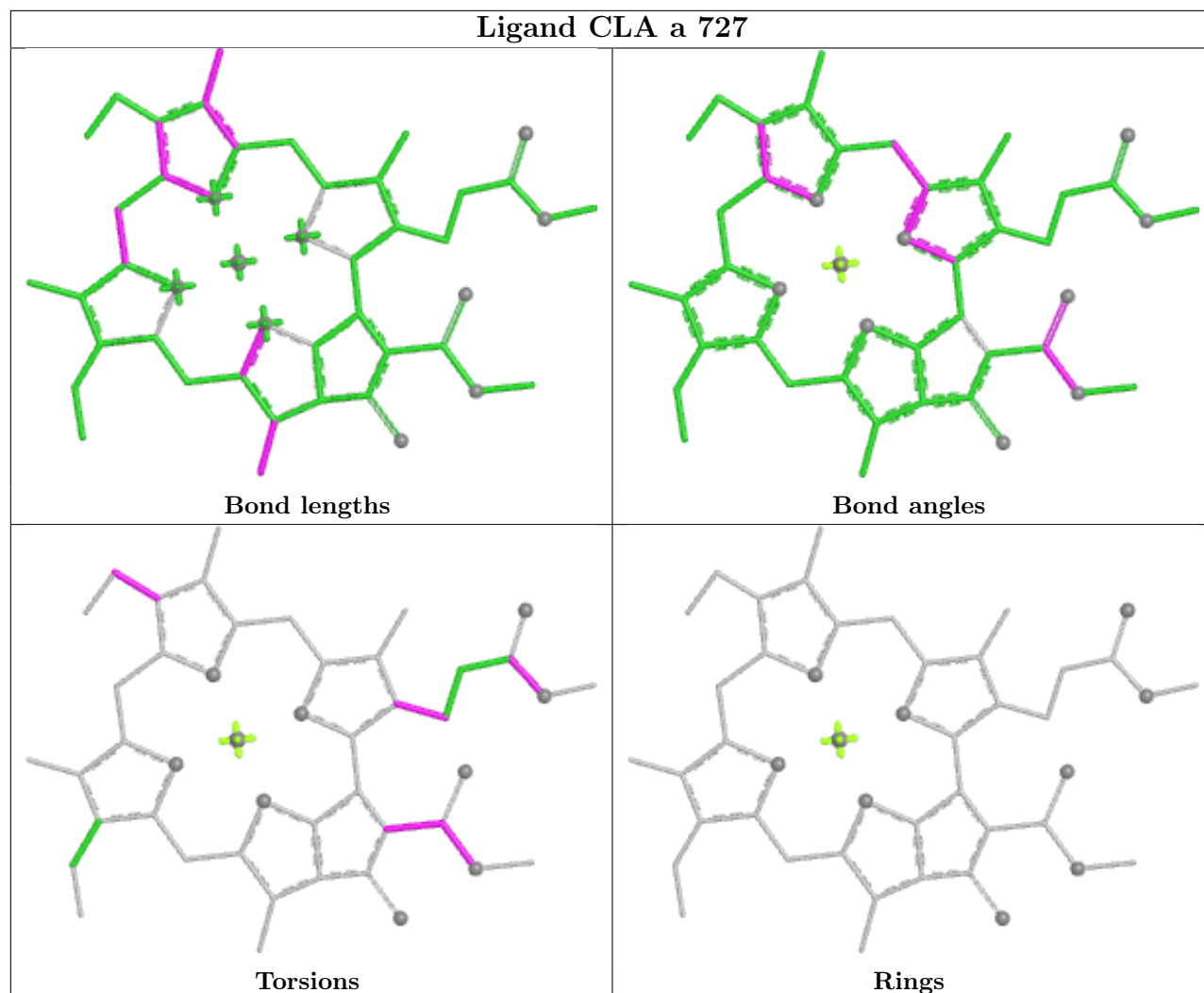
Torsions



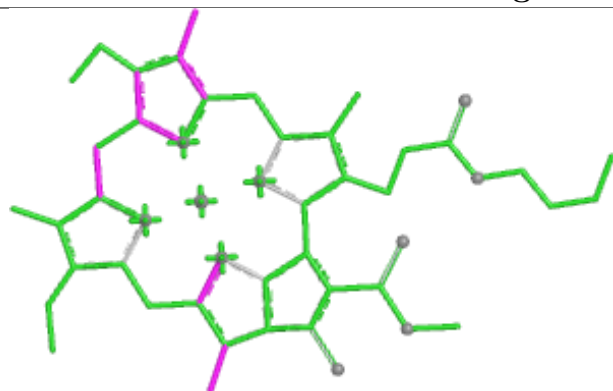
Rings



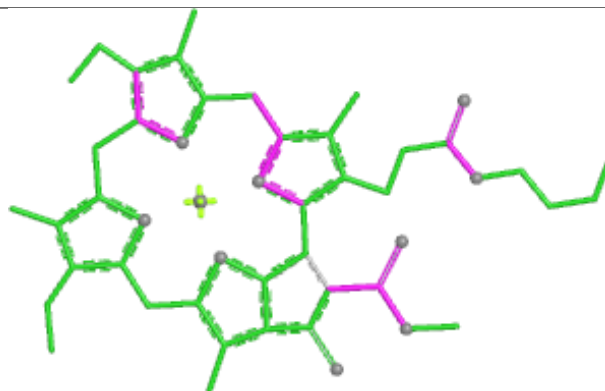
Ligand CLA a 727



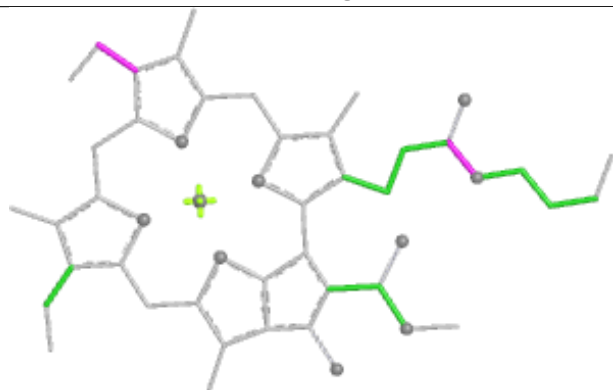
Ligand CLA K 306



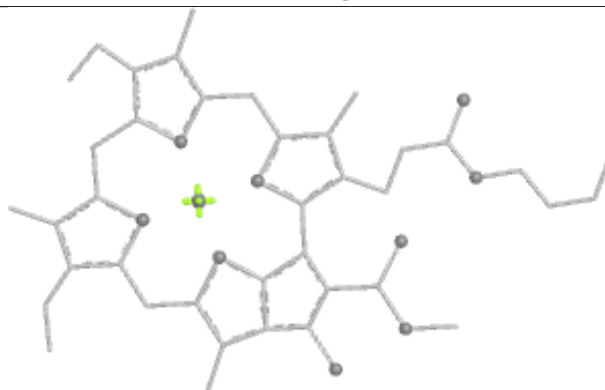
Bond lengths



Bond angles



Torsions

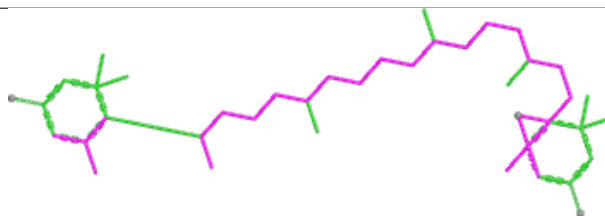


Rings

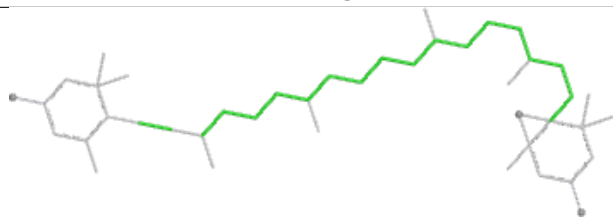
Ligand DD6 N 303



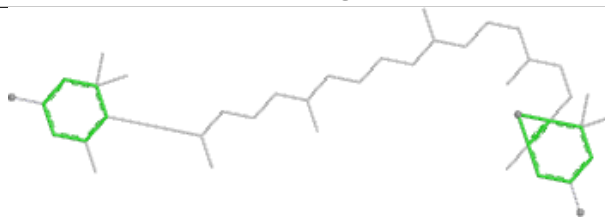
Bond lengths



Bond angles

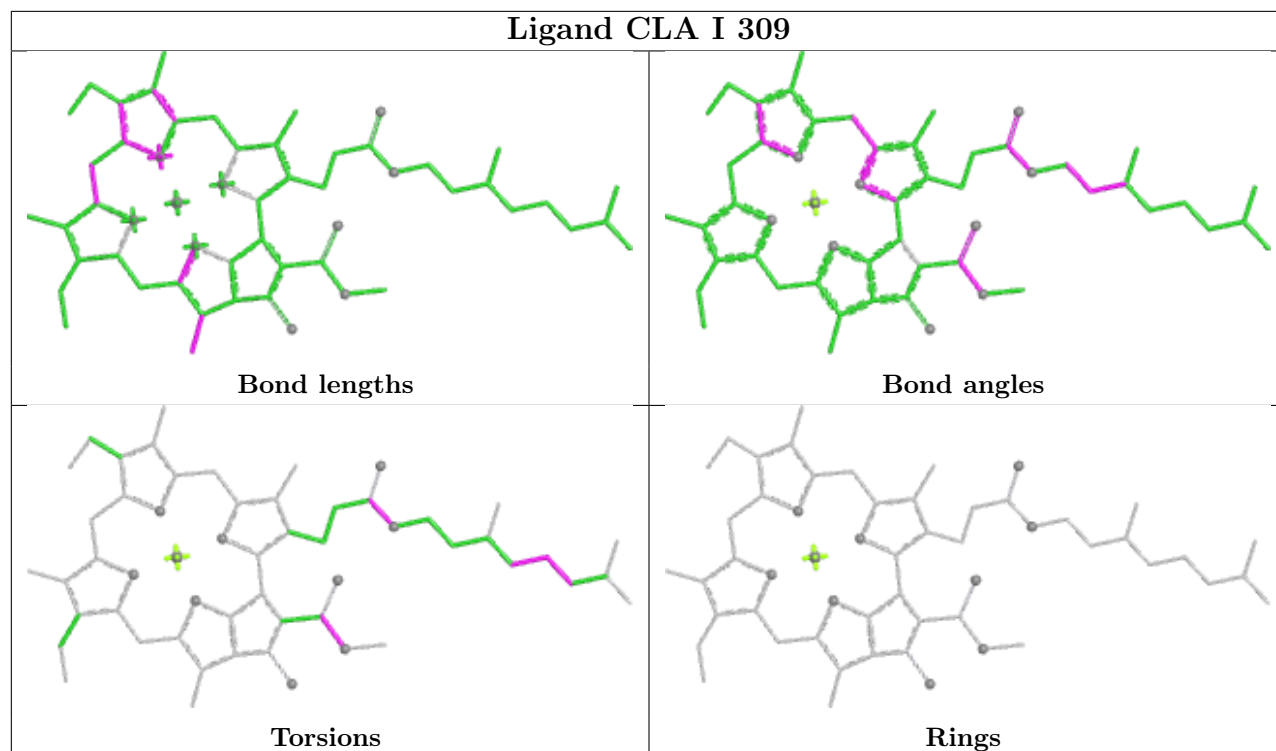


Torsions

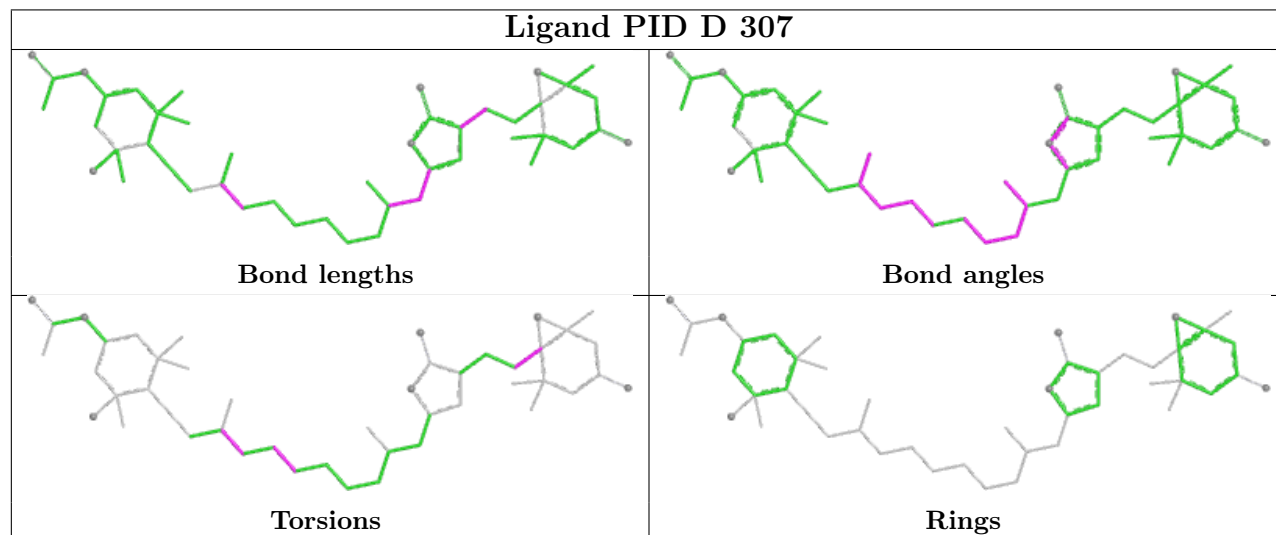


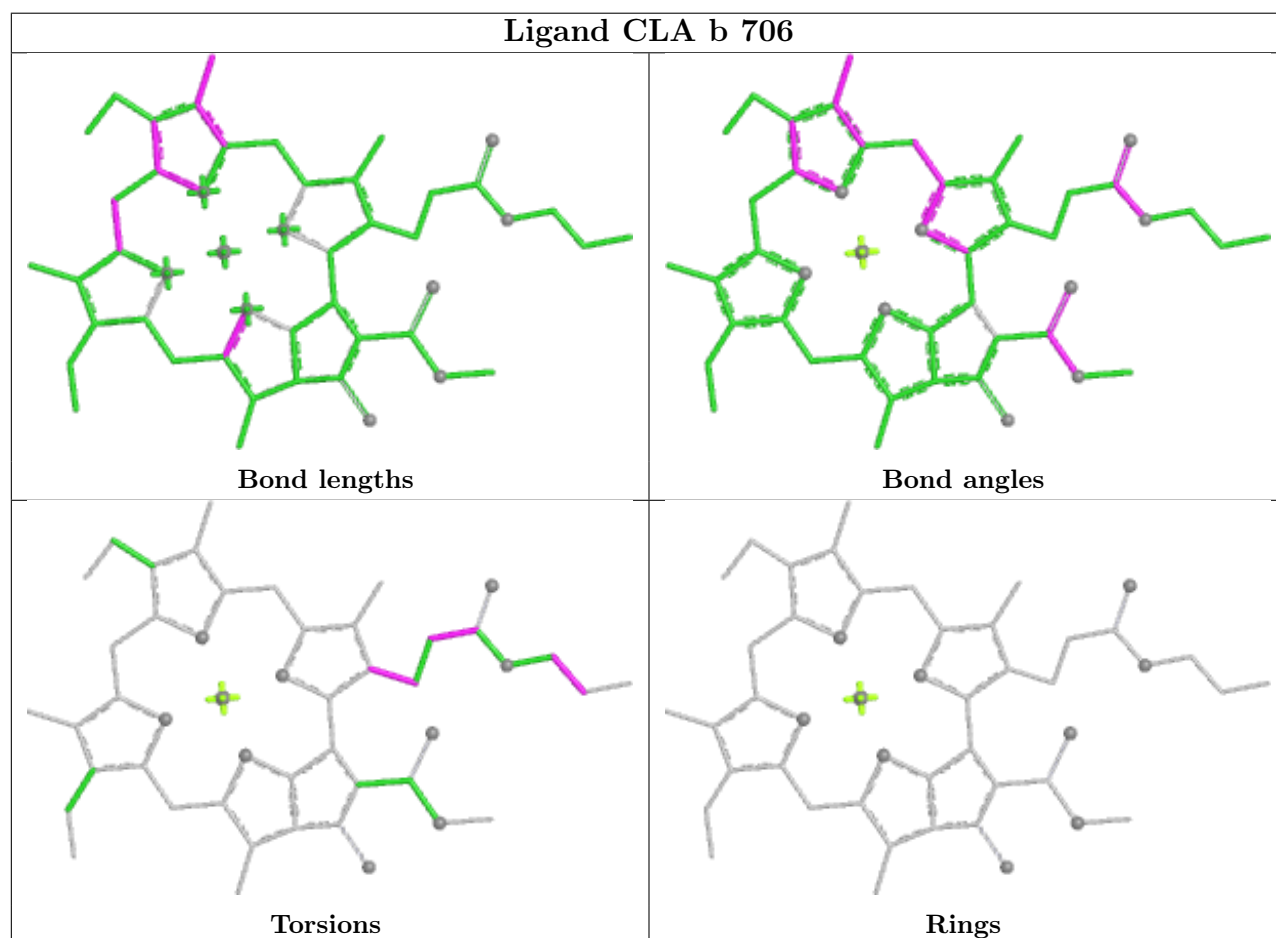
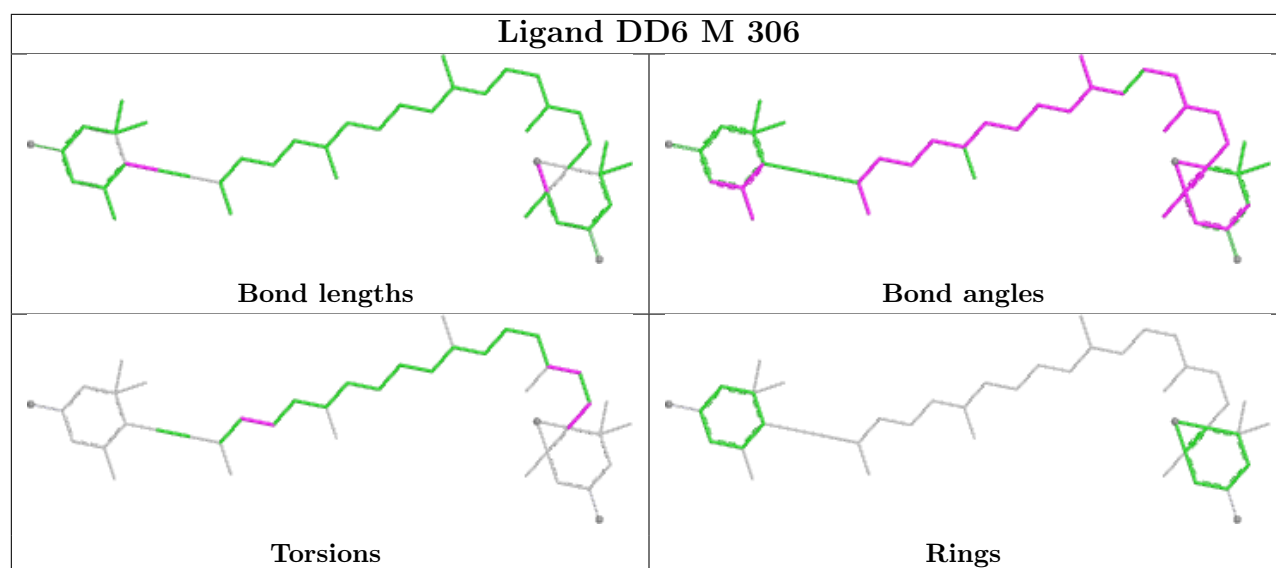
Rings

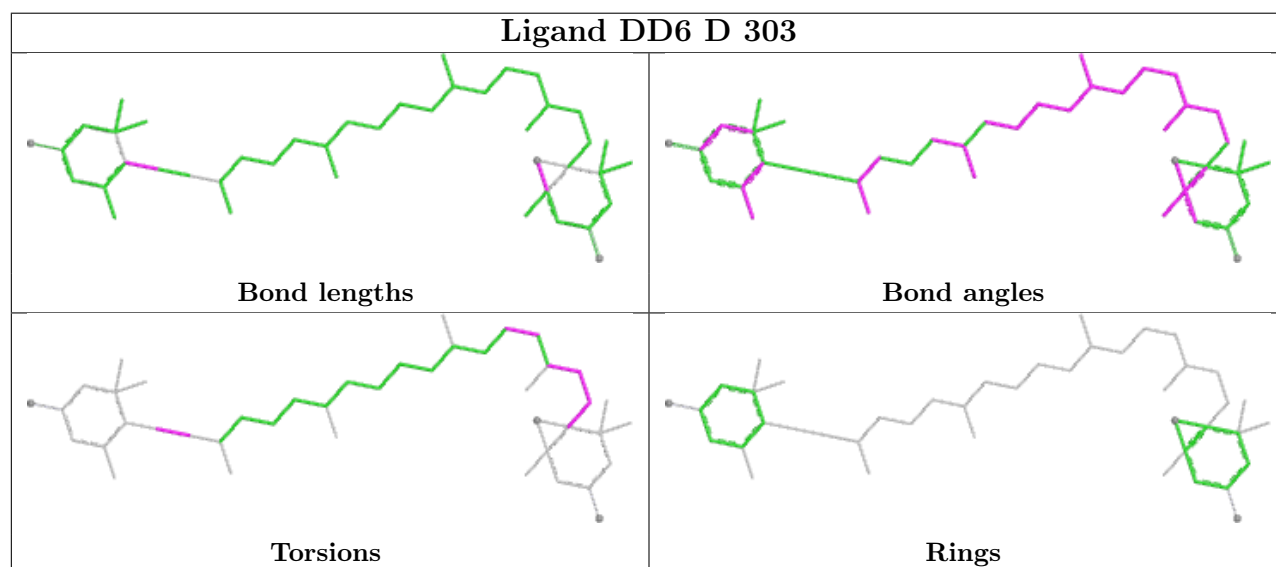
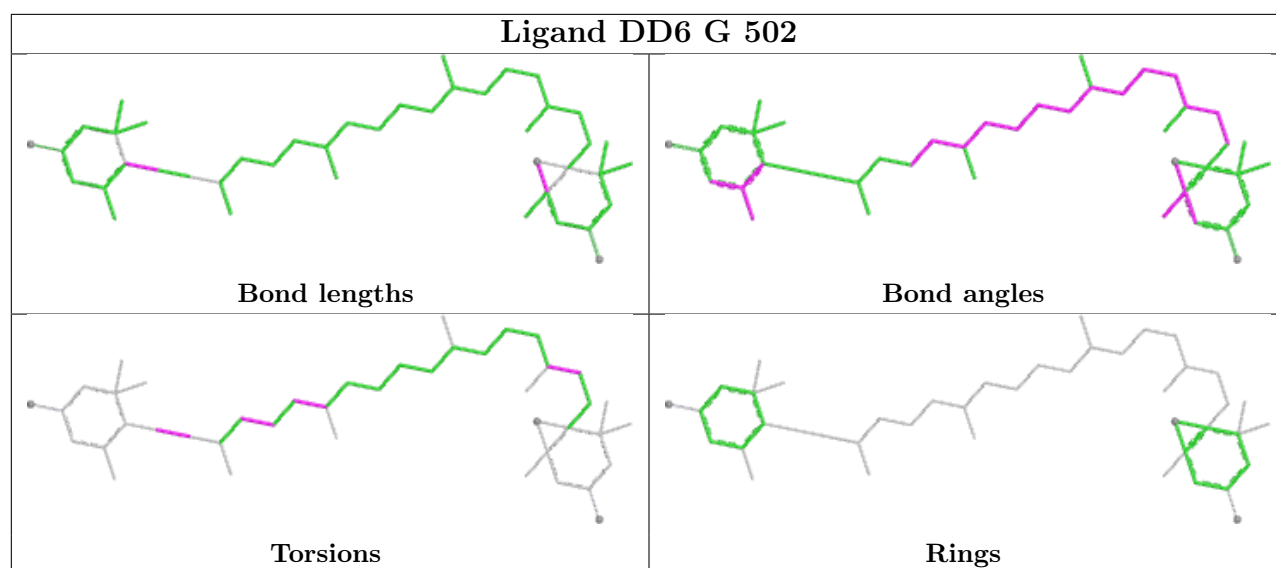
Ligand CLA I 309

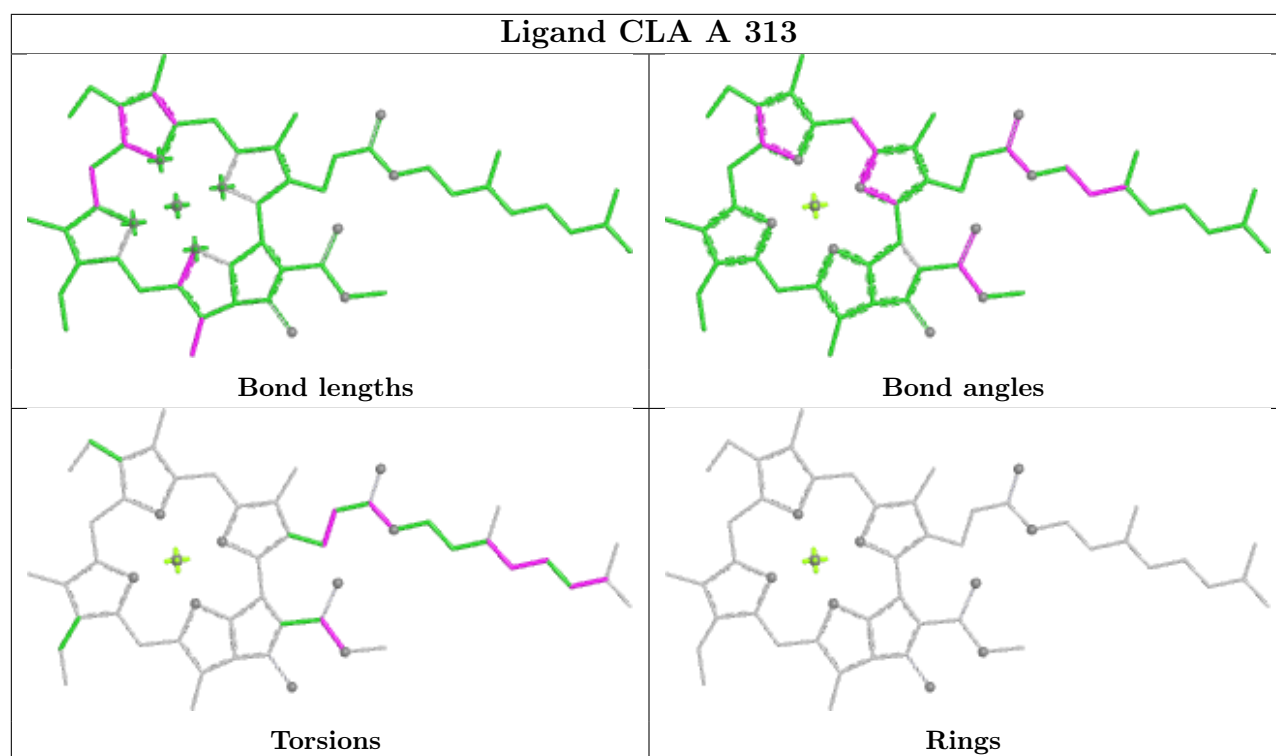


Ligand PID D 307

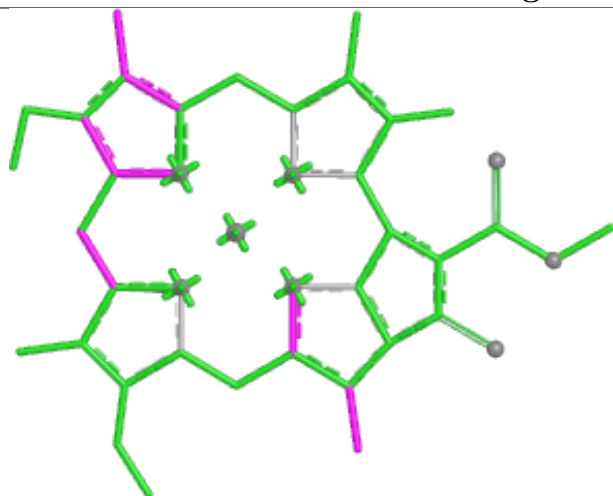




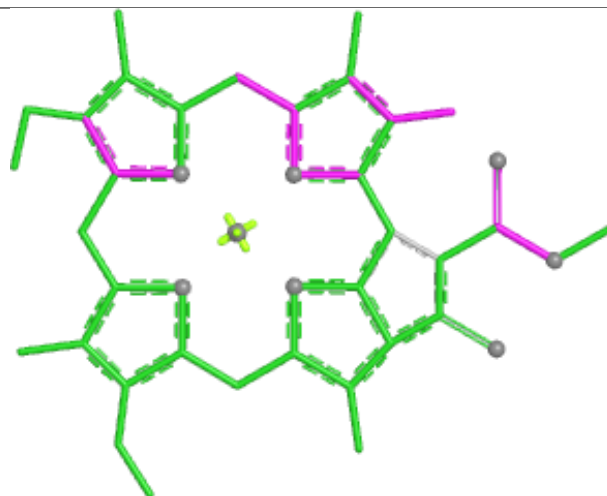




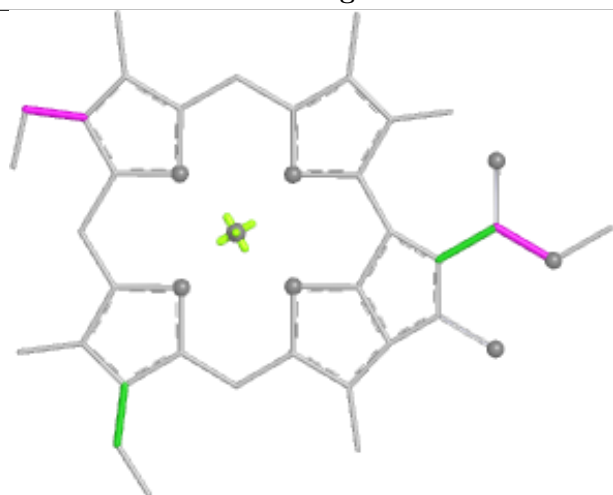
Ligand CLA 1 308



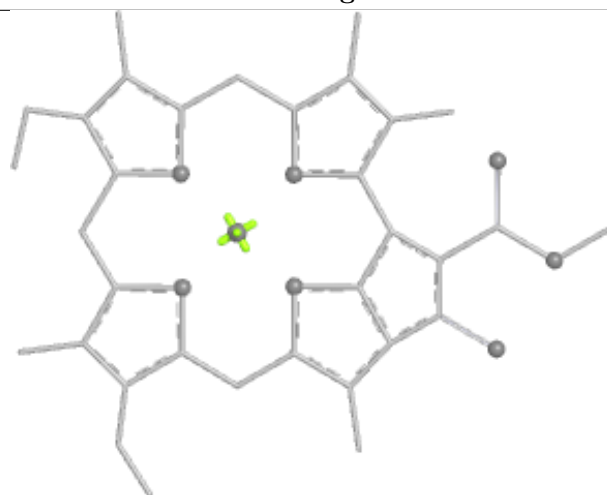
Bond lengths



Bond angles

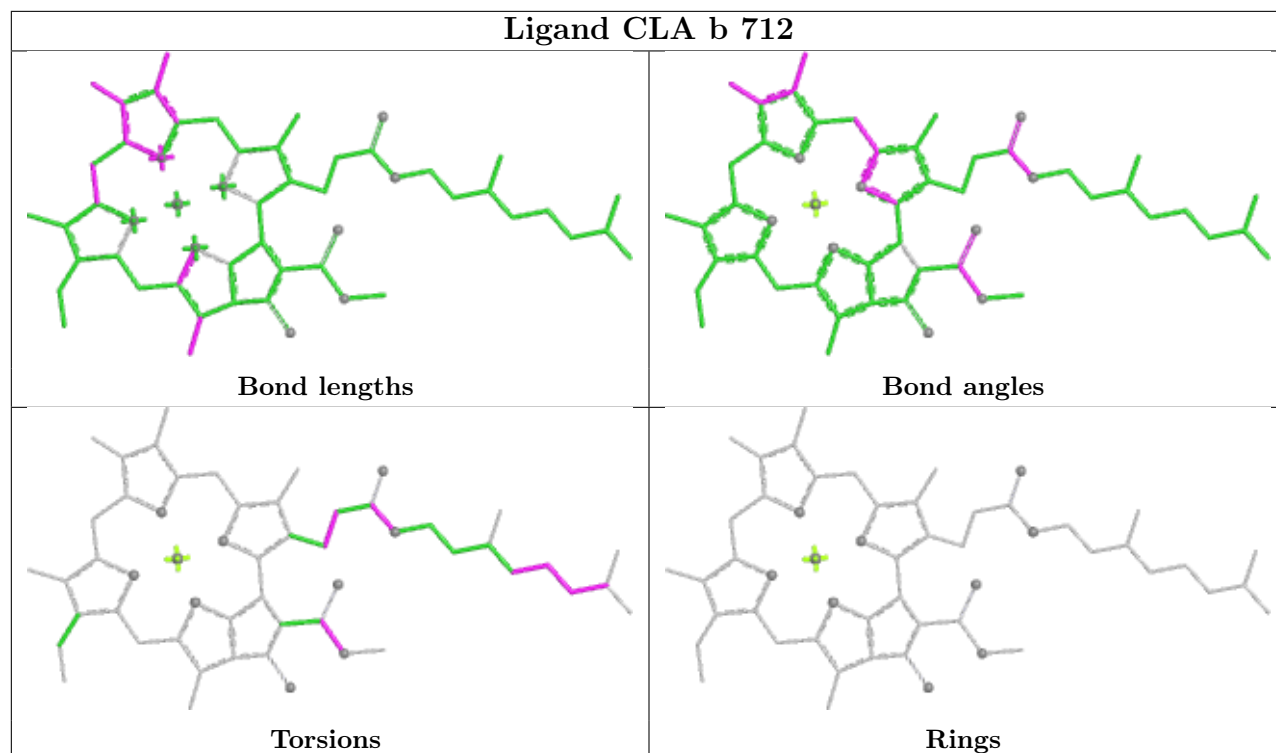


Torsions

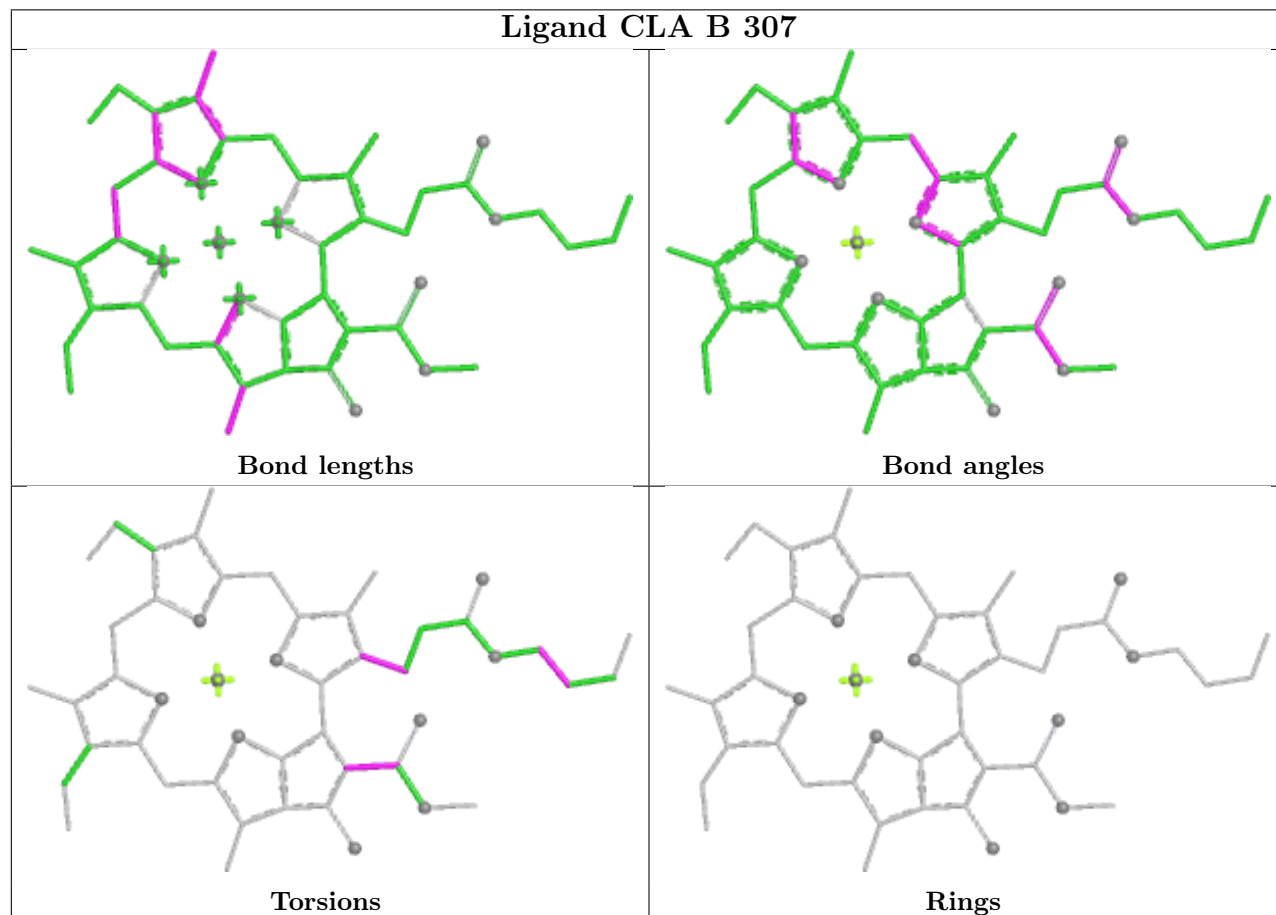


Rings

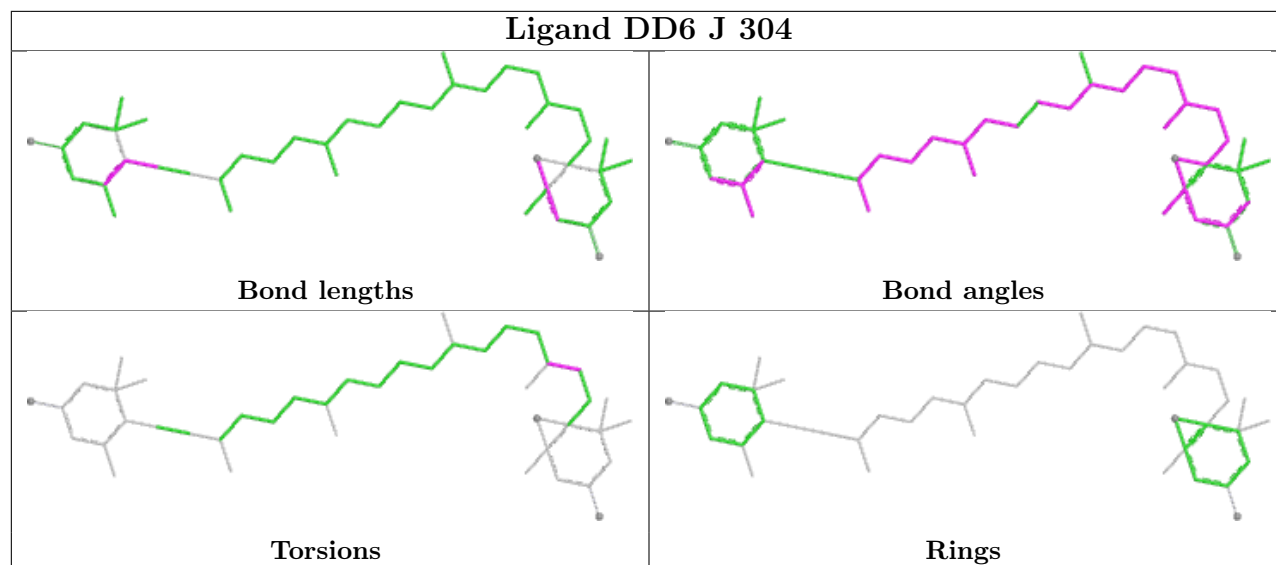
Ligand CLA b 712



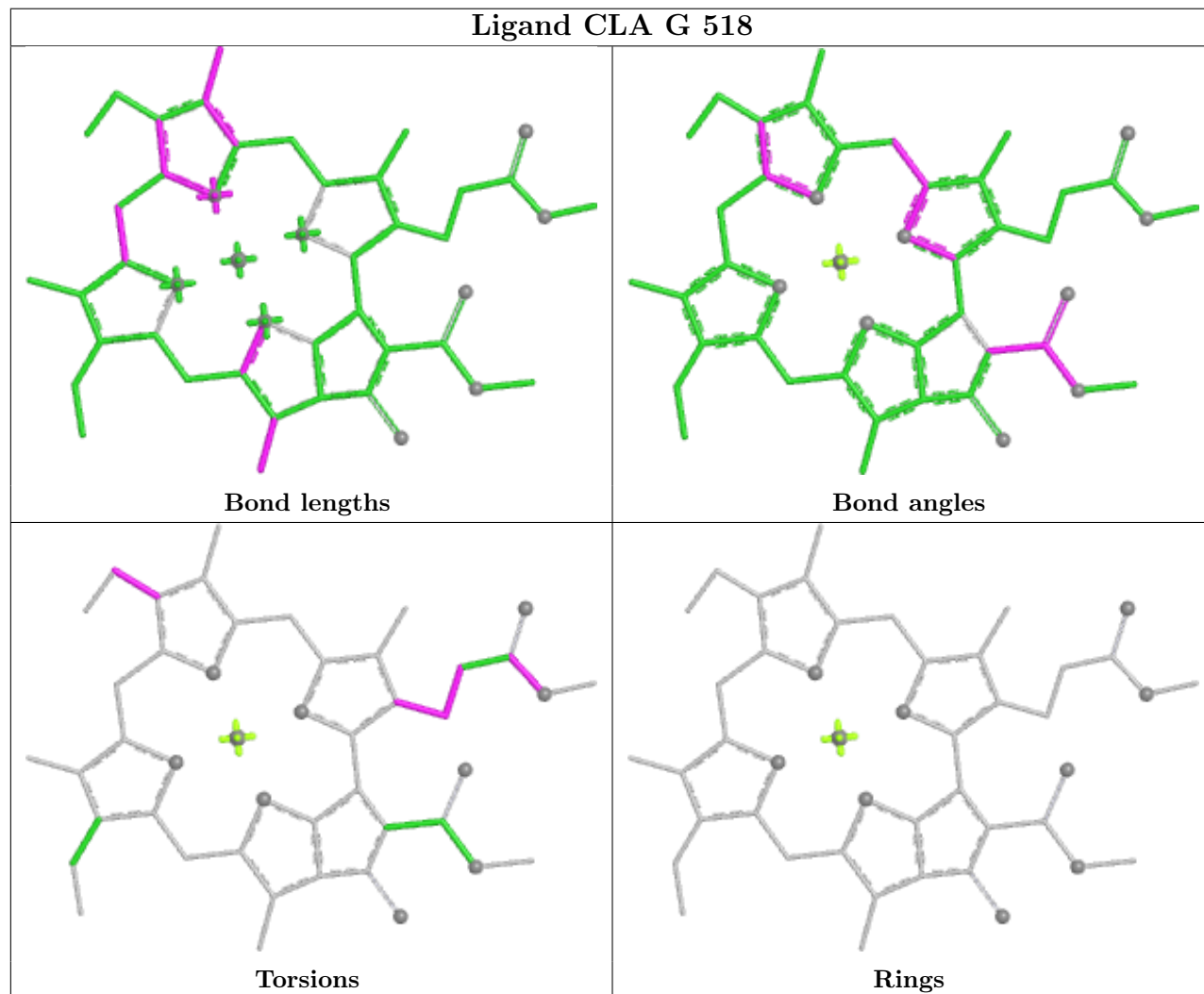
Ligand CLA B 307



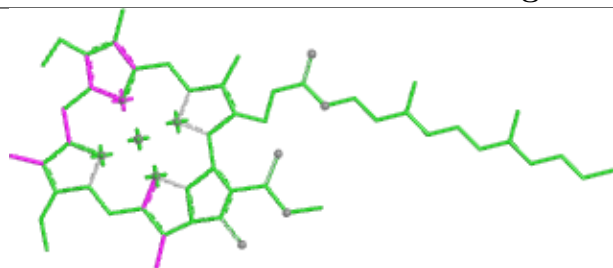
Ligand DD6 J 304



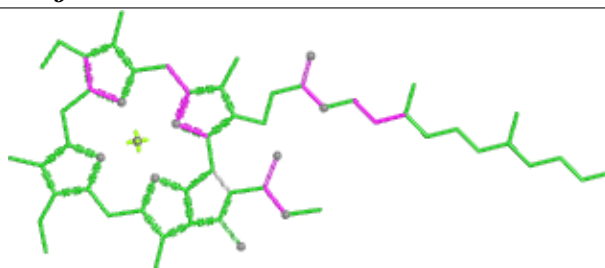
Ligand CLA G 518



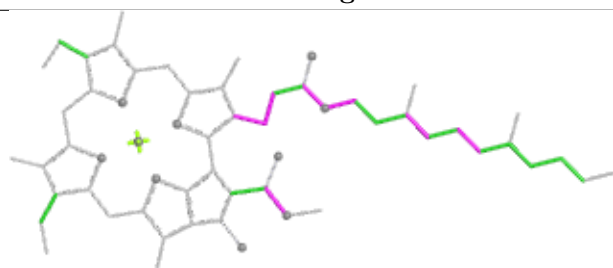
Ligand CLA j 106



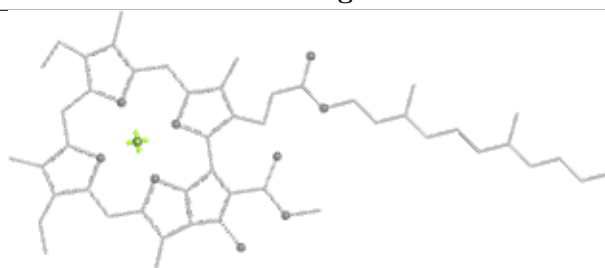
Bond lengths



Bond angles

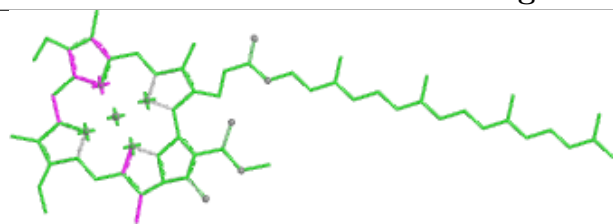


Torsions

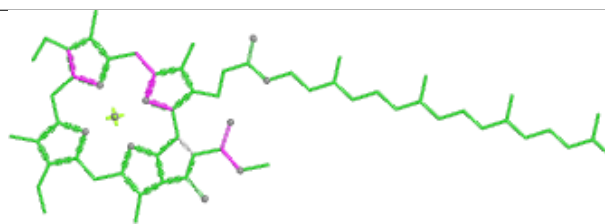


Rings

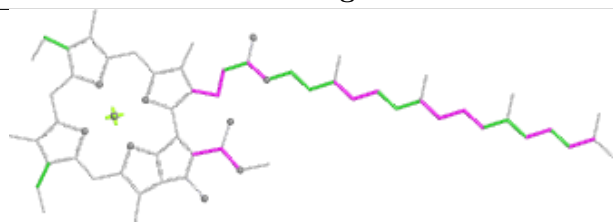
Ligand CLA J 307



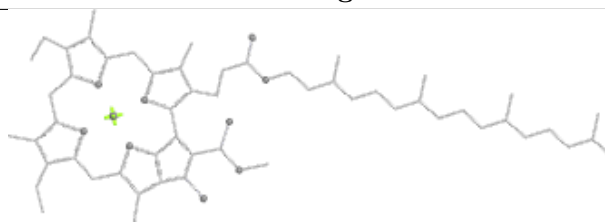
Bond lengths



Bond angles

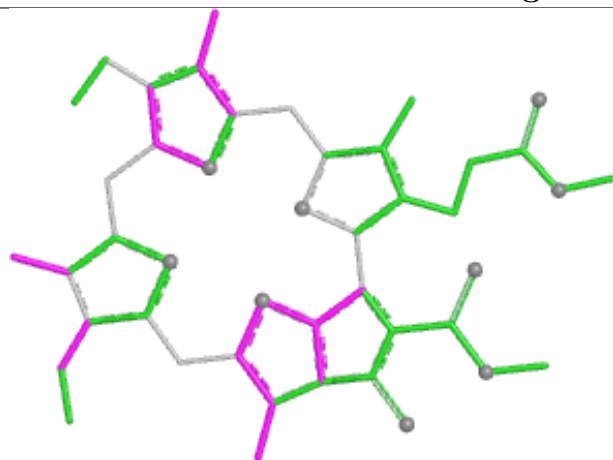


Torsions

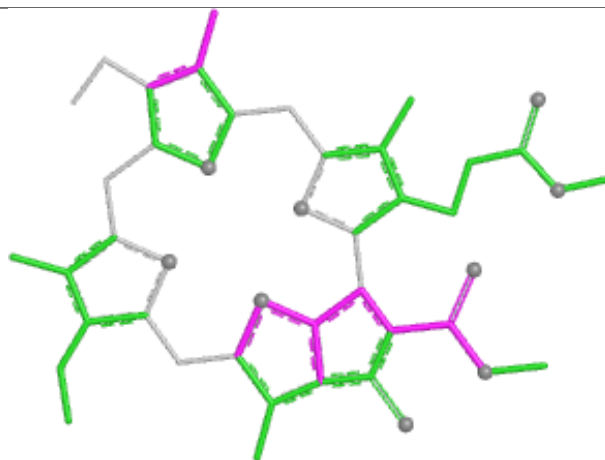


Rings

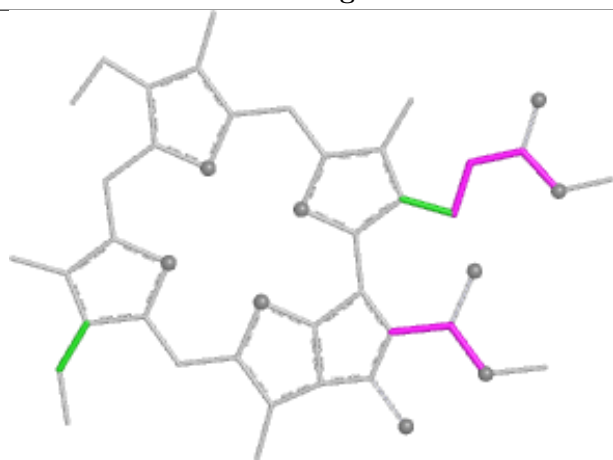
Ligand CLA I 310



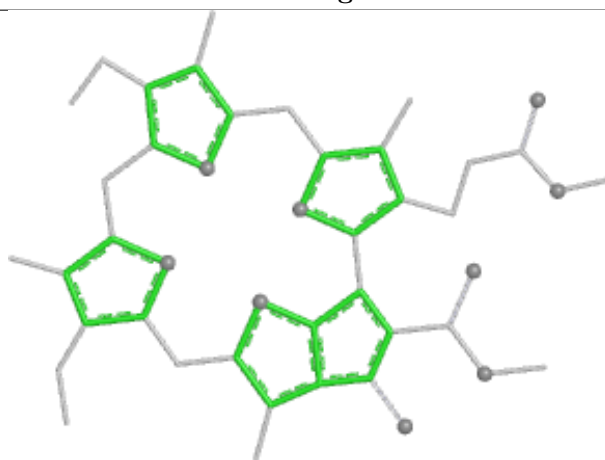
Bond lengths



Bond angles

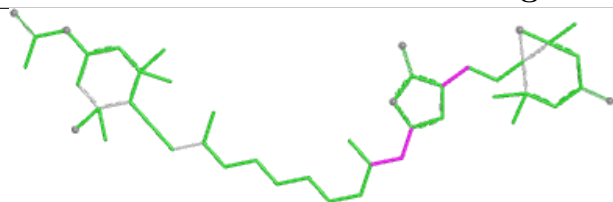


Torsions

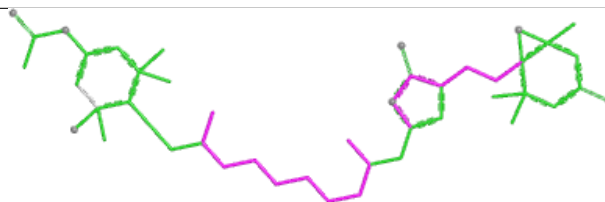


Rings

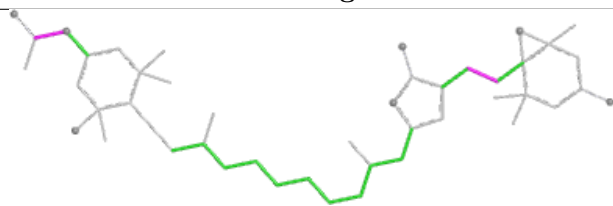
Ligand PID F 304



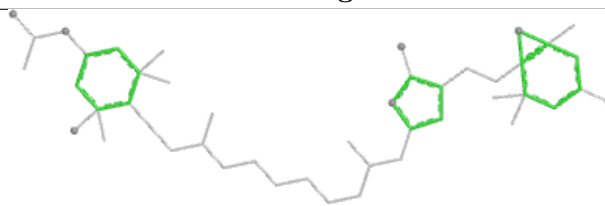
Bond lengths



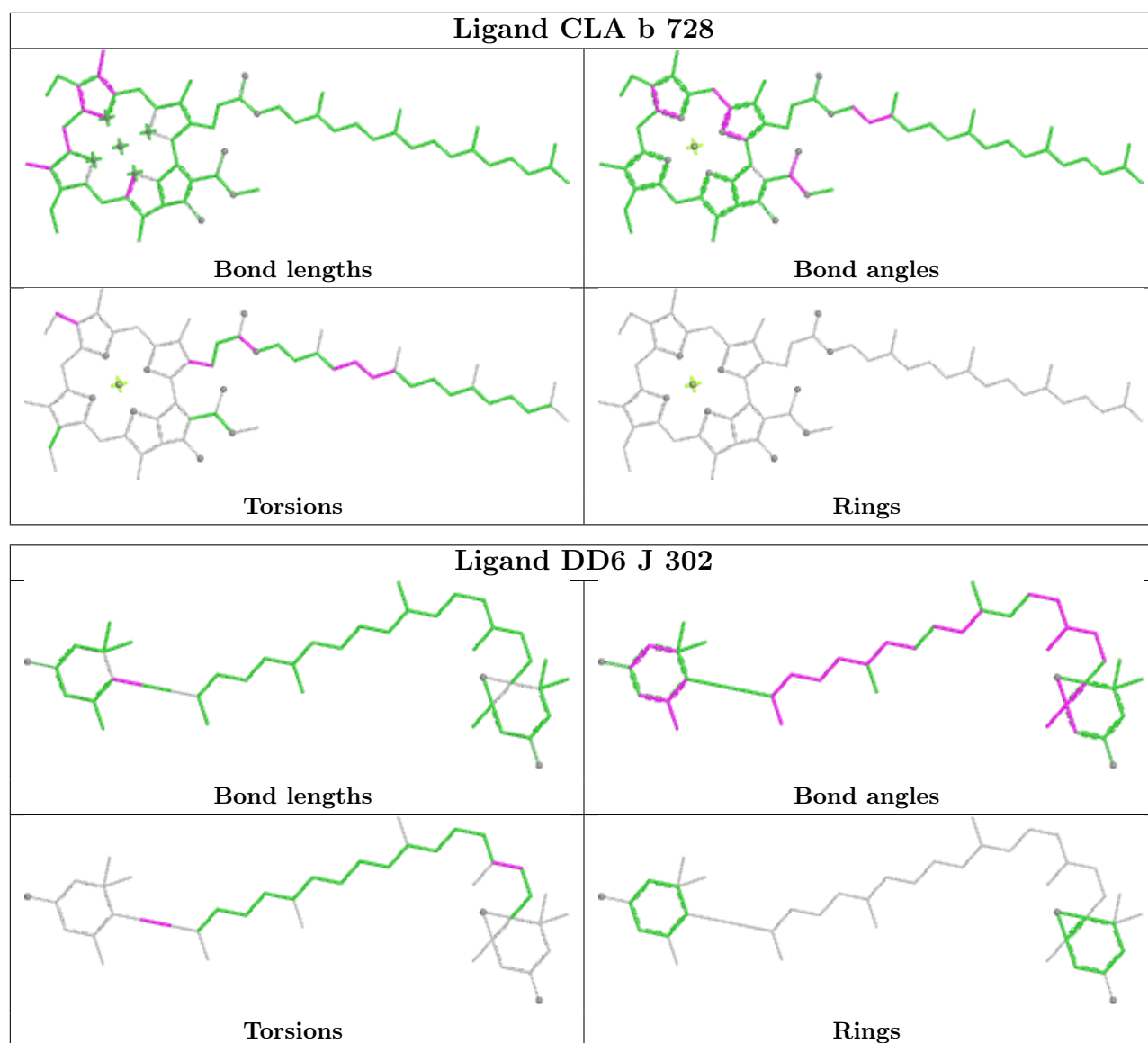
Bond angles

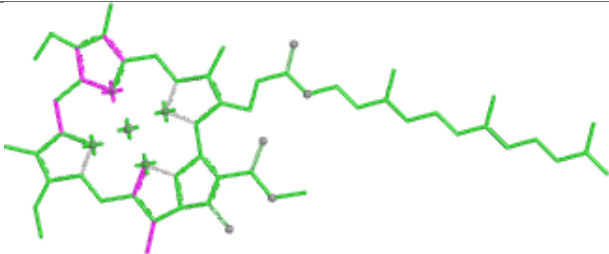
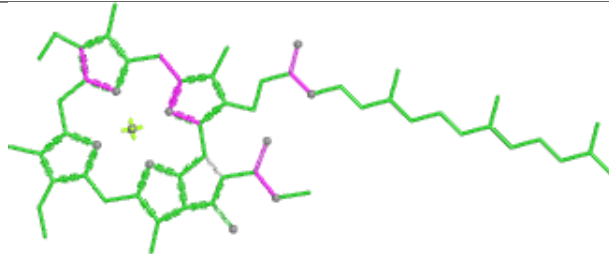
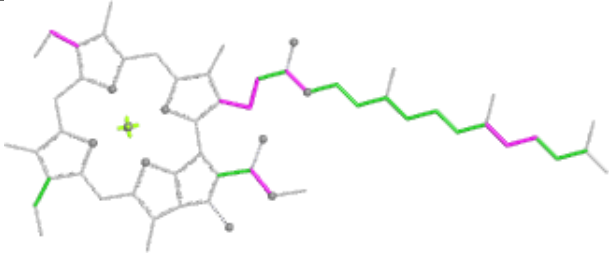
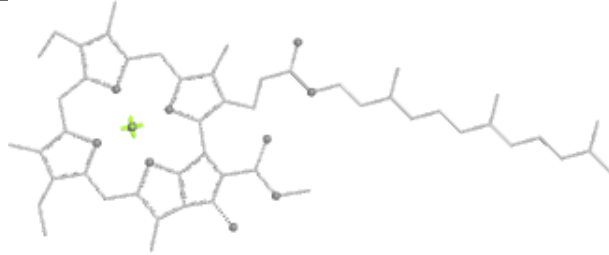


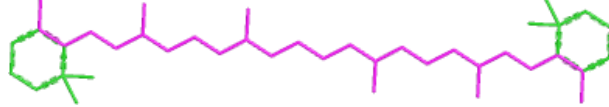
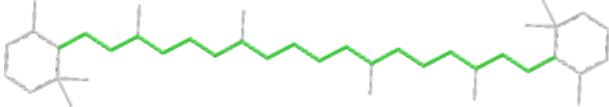
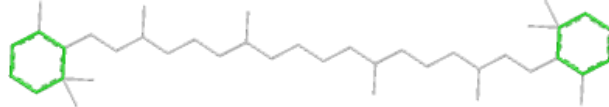
Torsions

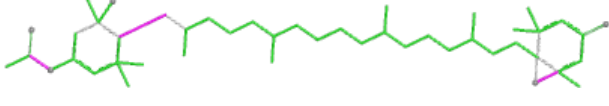
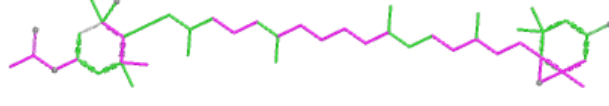
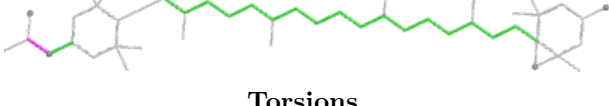


Rings

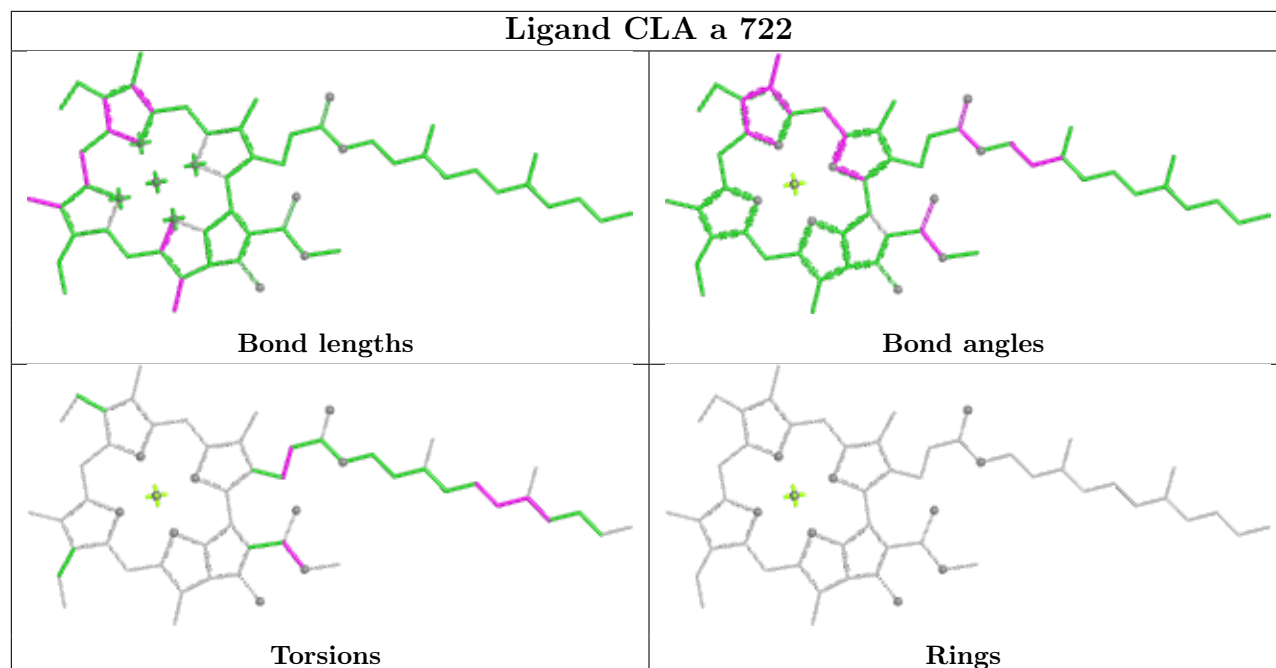


Ligand CLA J 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

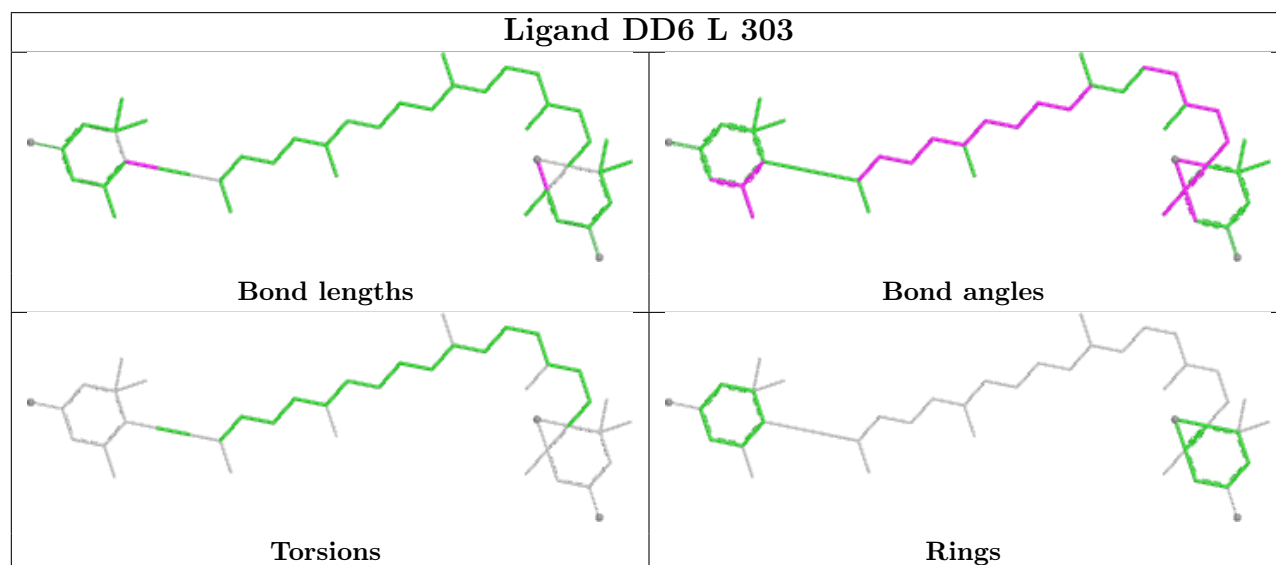
Ligand BCR b 732	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand UIX B 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

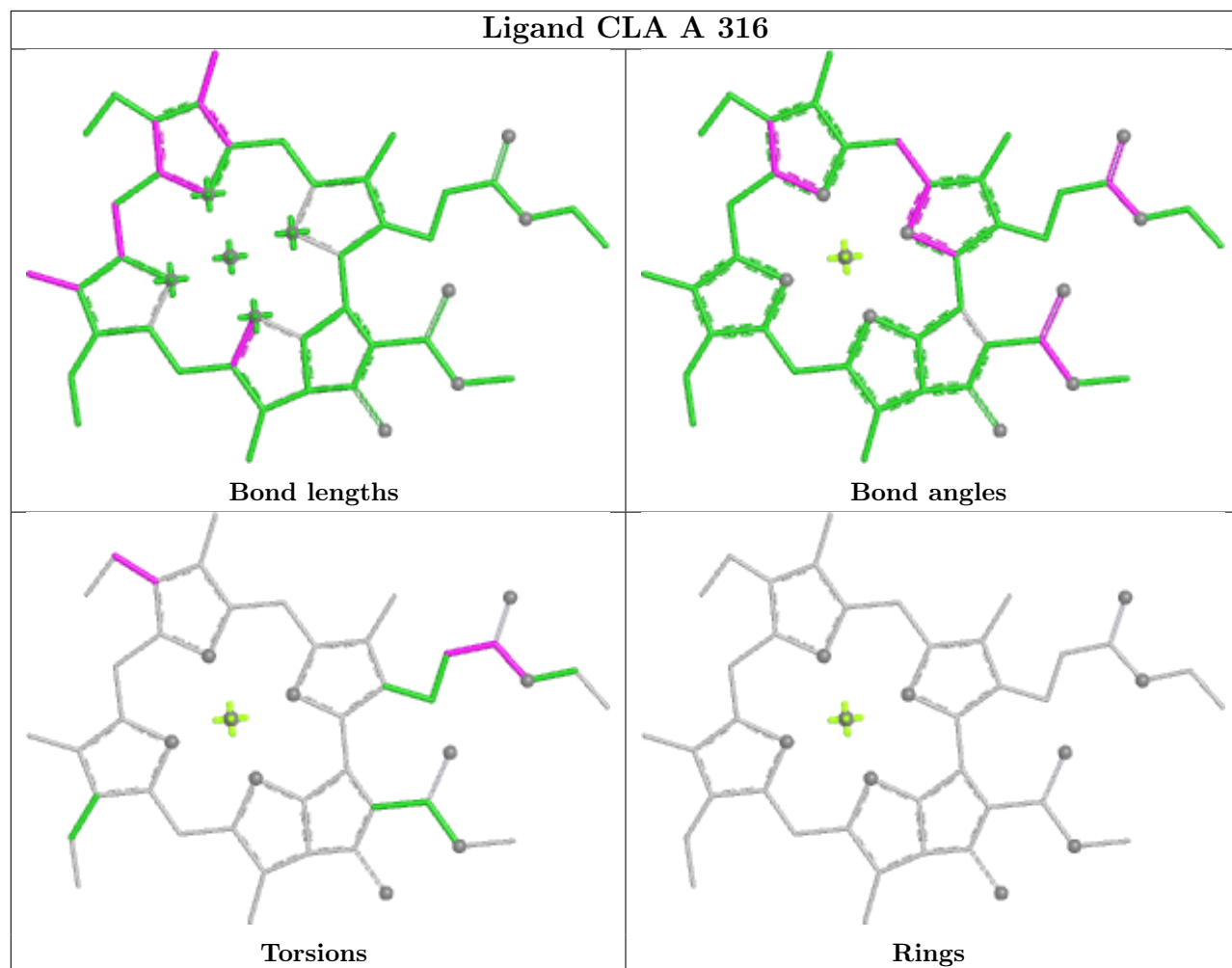
Ligand CLA a 722

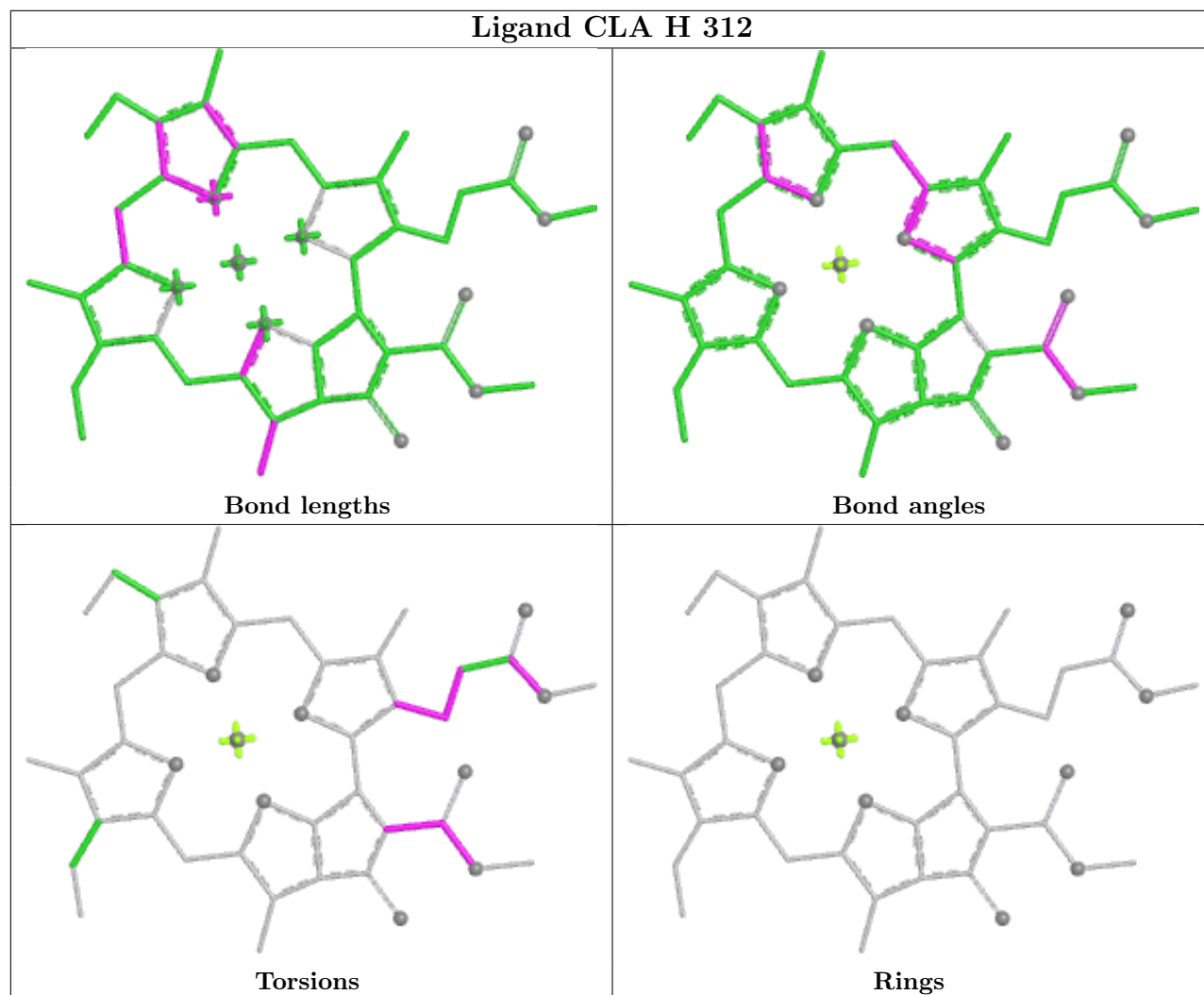


Ligand DD6 L 303

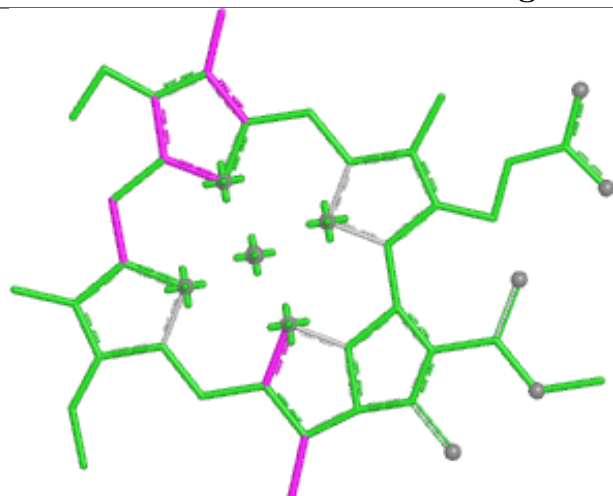


Ligand CLA A 316

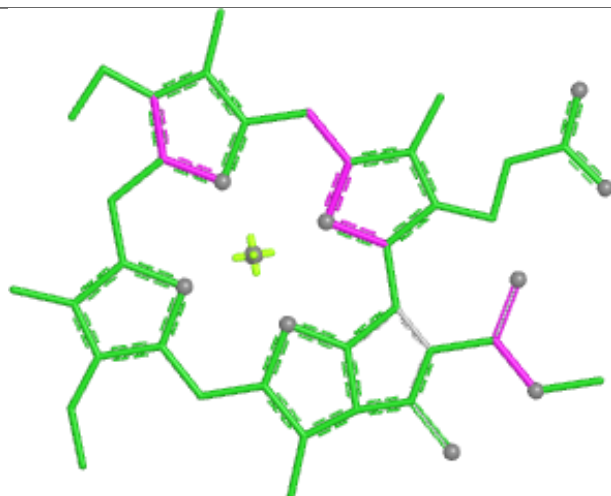




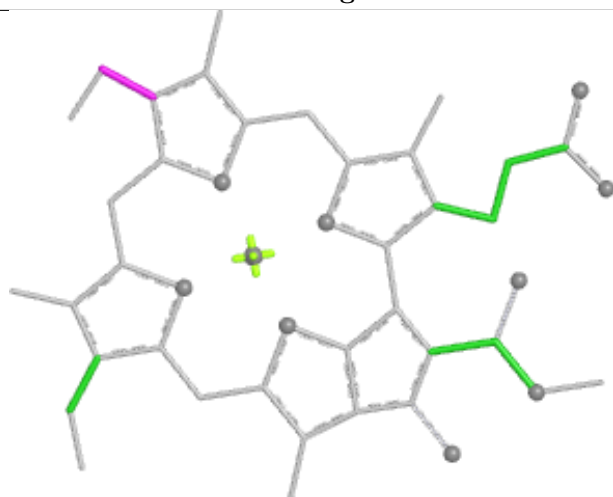
Ligand CLA a 701



Bond lengths



Bond angles

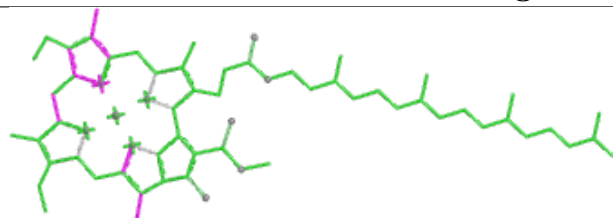


Torsions

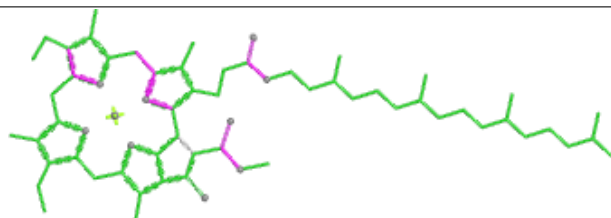


Rings

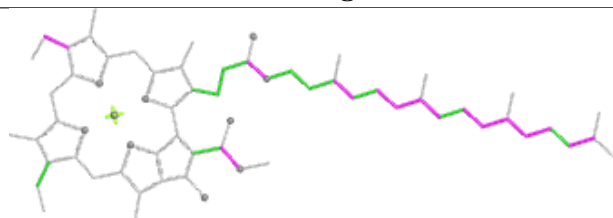
Ligand CLA B 311



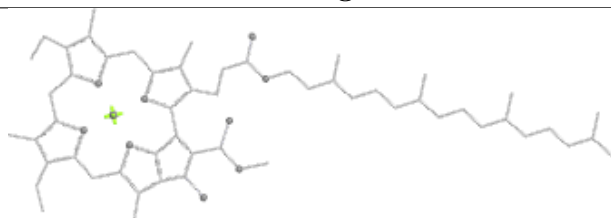
Bond lengths



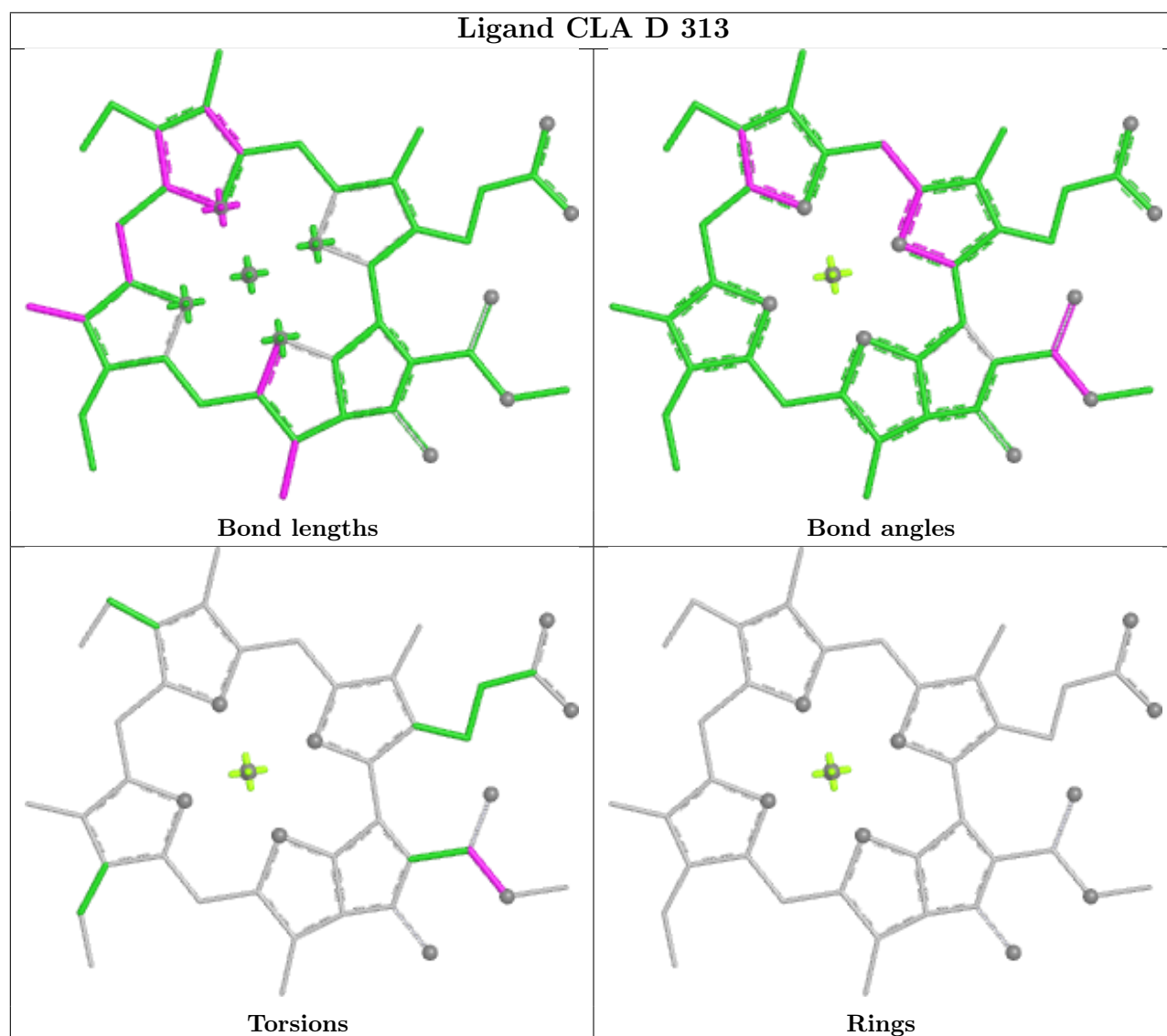
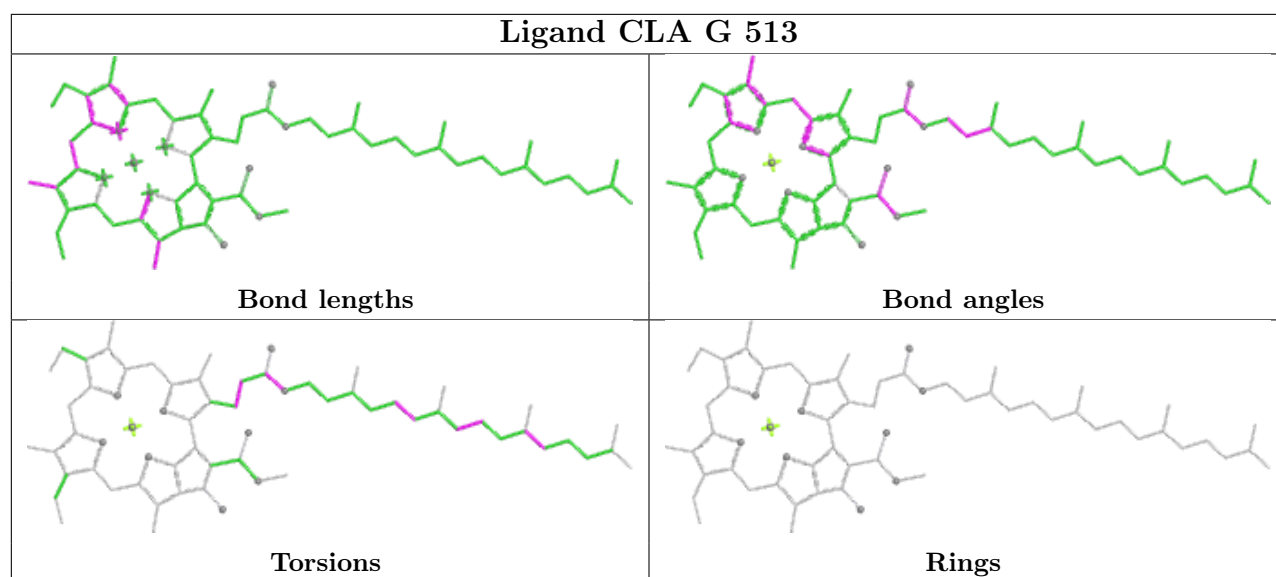
Bond angles

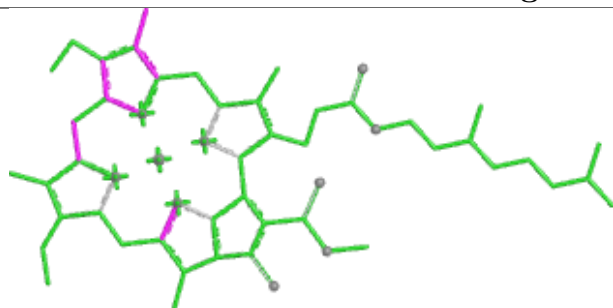


Torsions

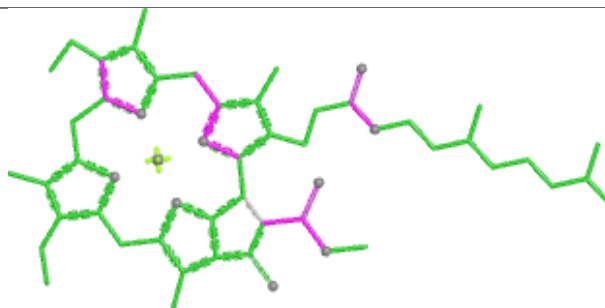


Rings

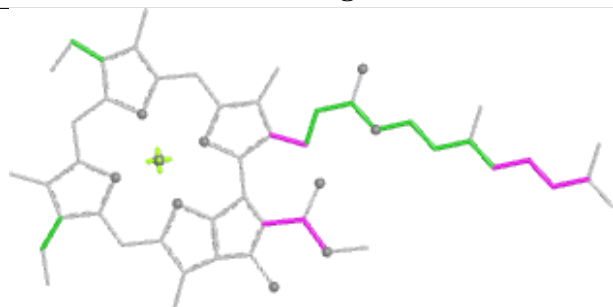


Ligand CLA I 311

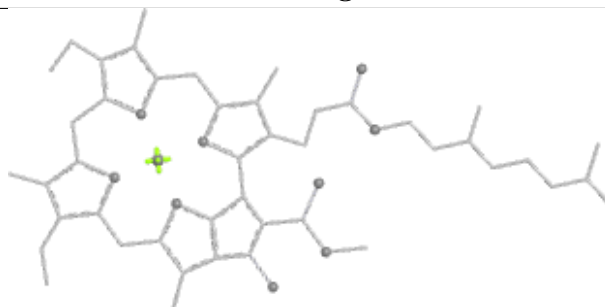
Bond lengths



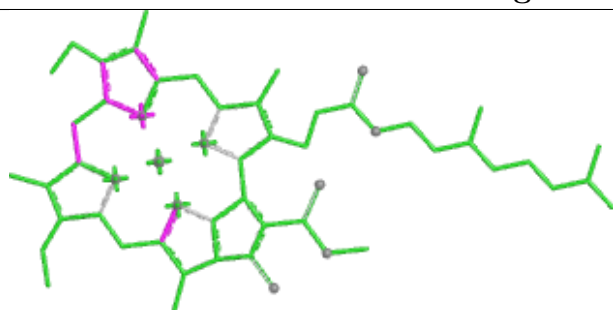
Bond angles



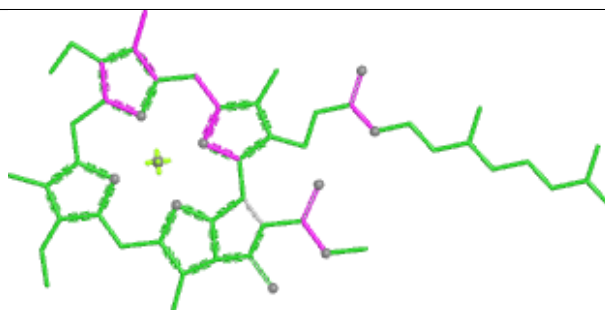
Torsions



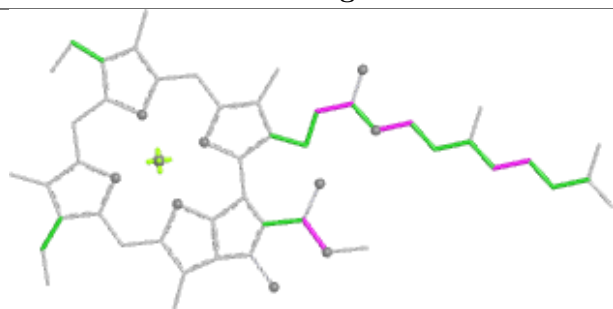
Rings

Ligand CLA A 309

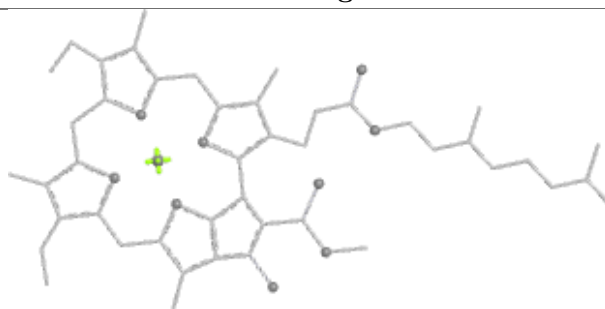
Bond lengths



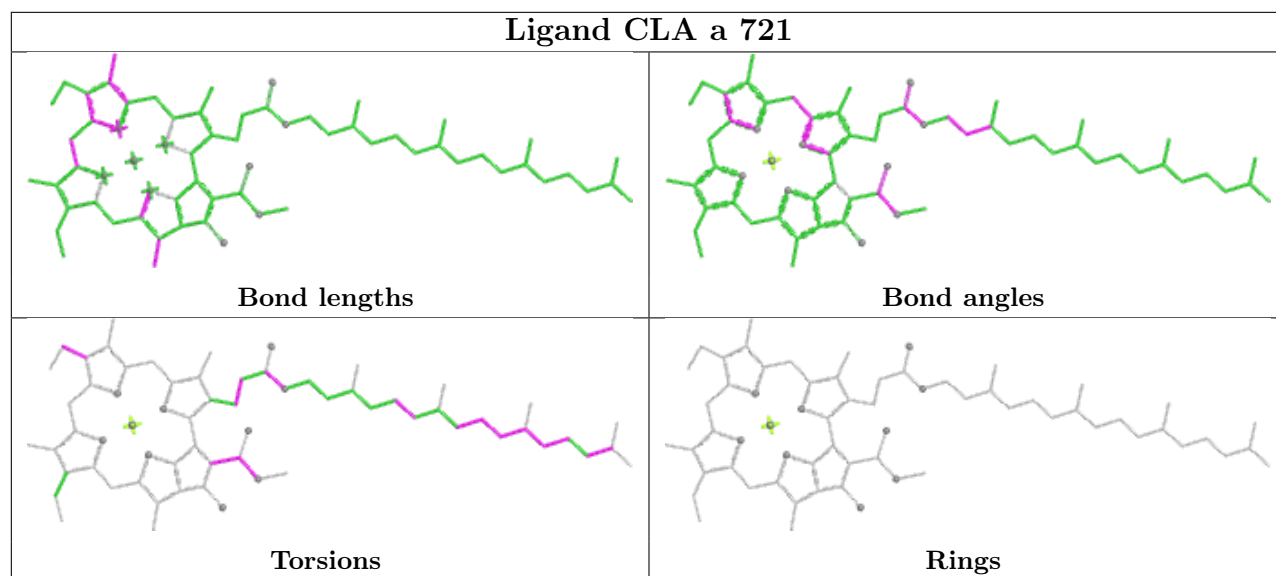
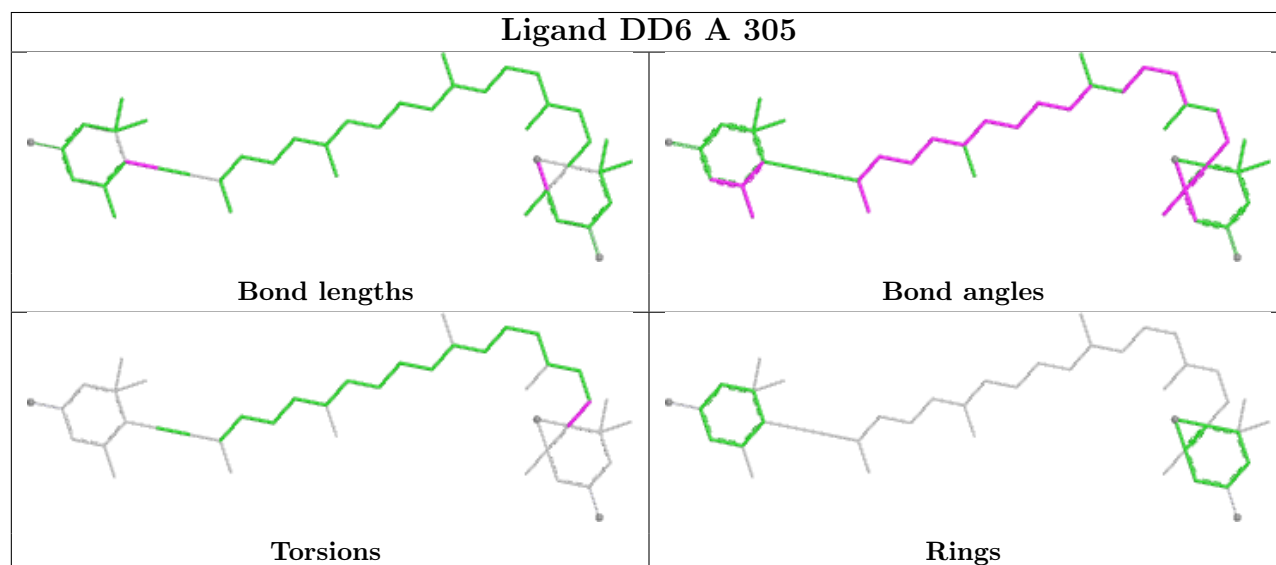
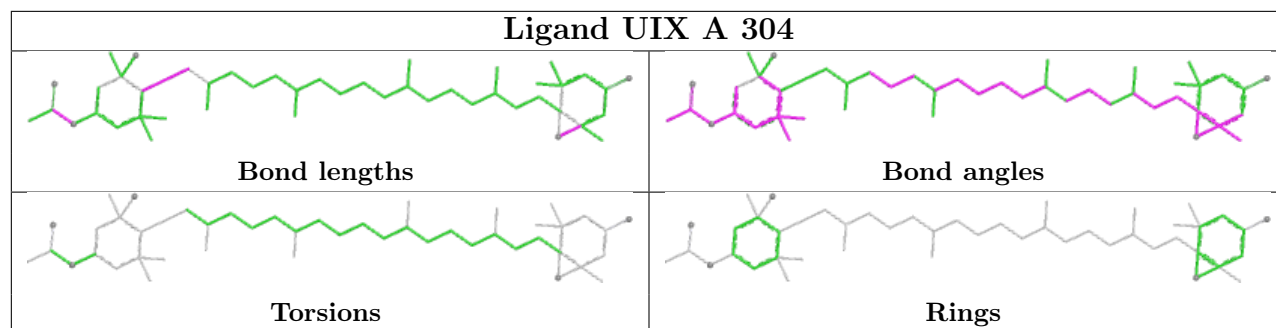
Bond angles

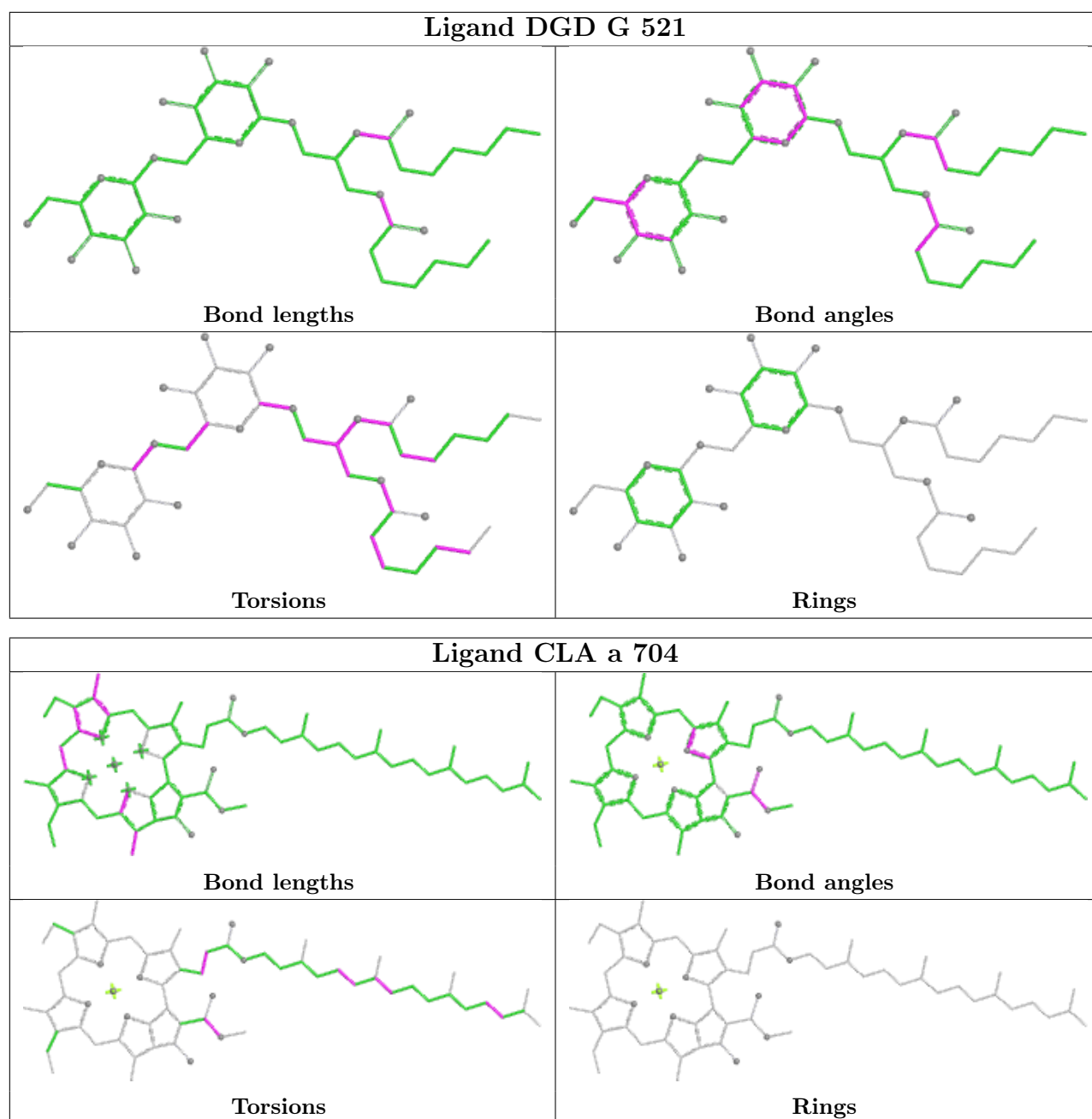


Torsions

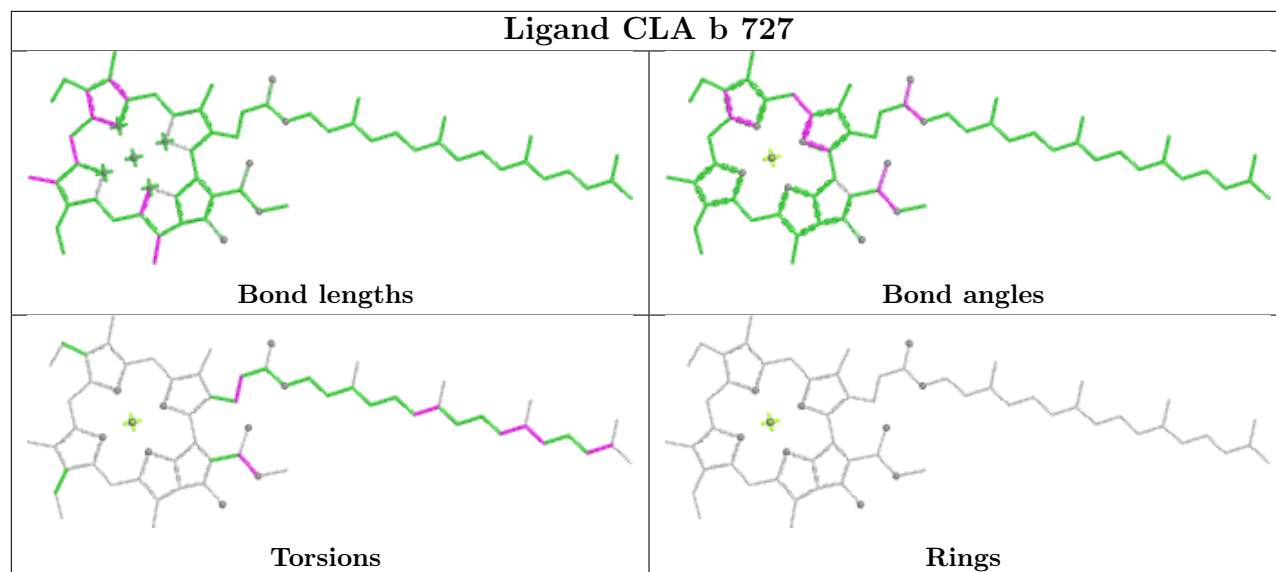


Rings

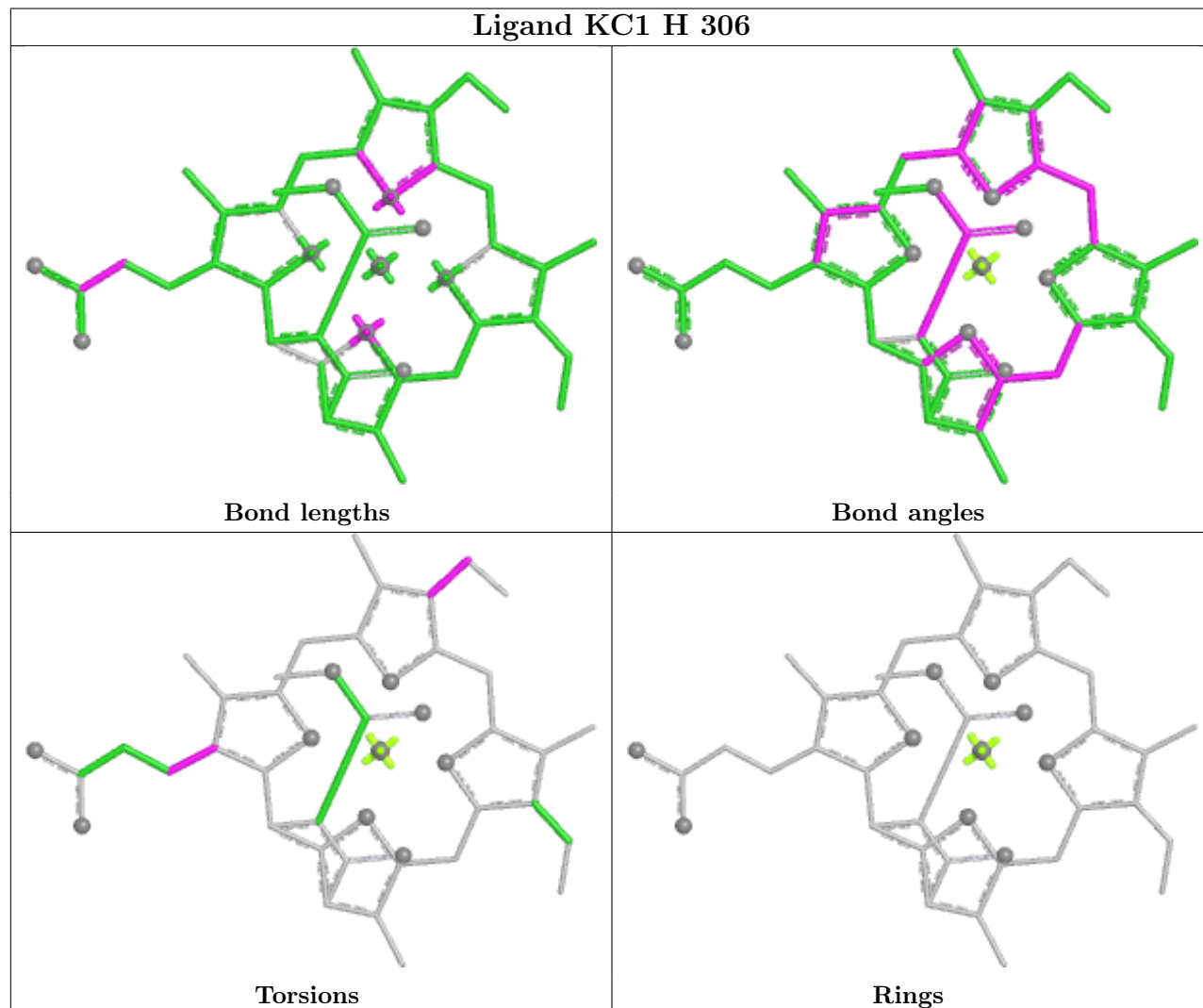


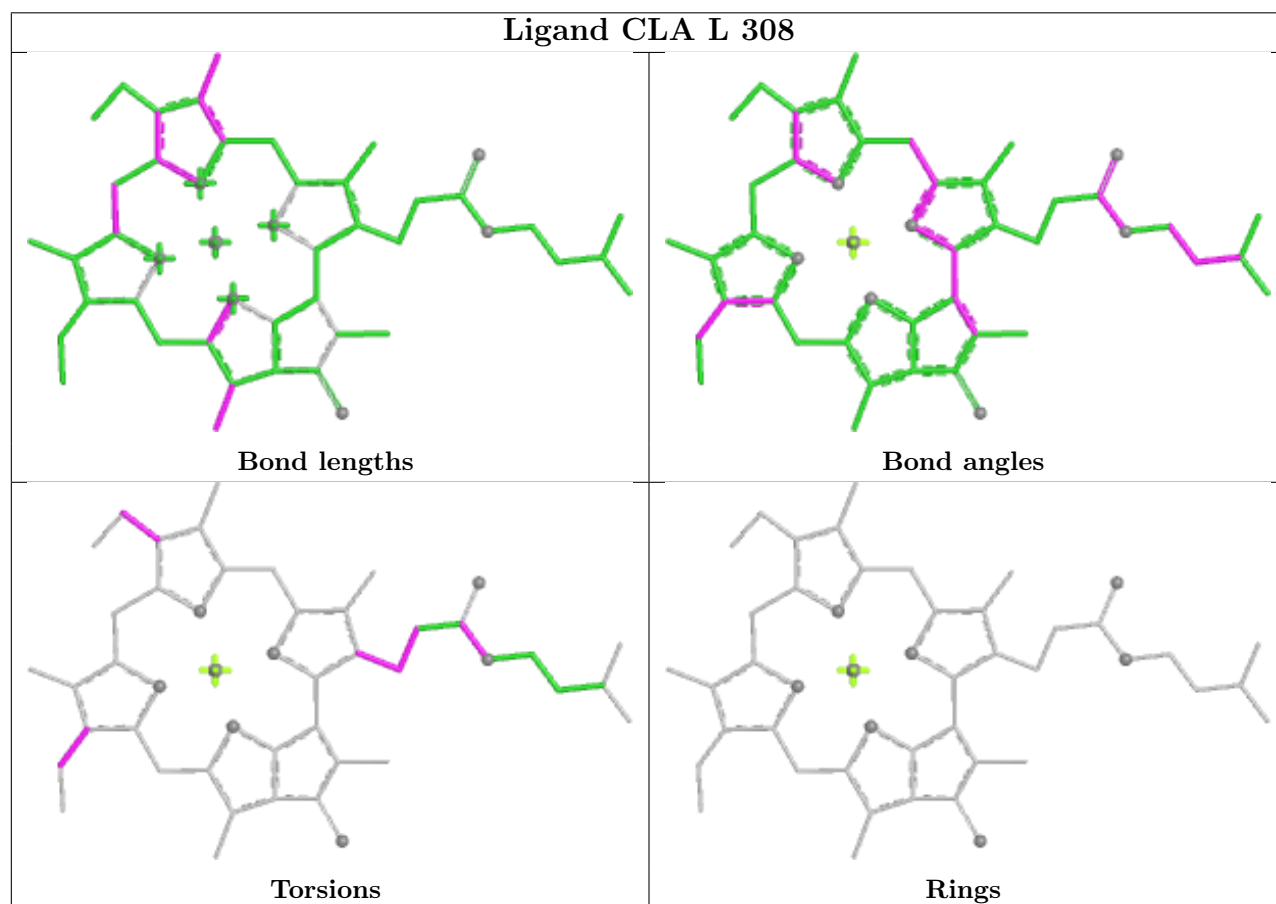
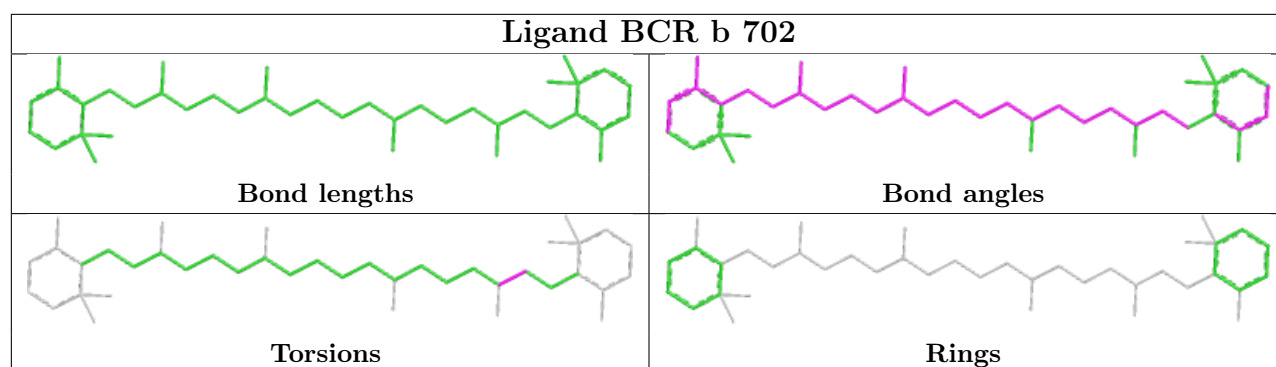


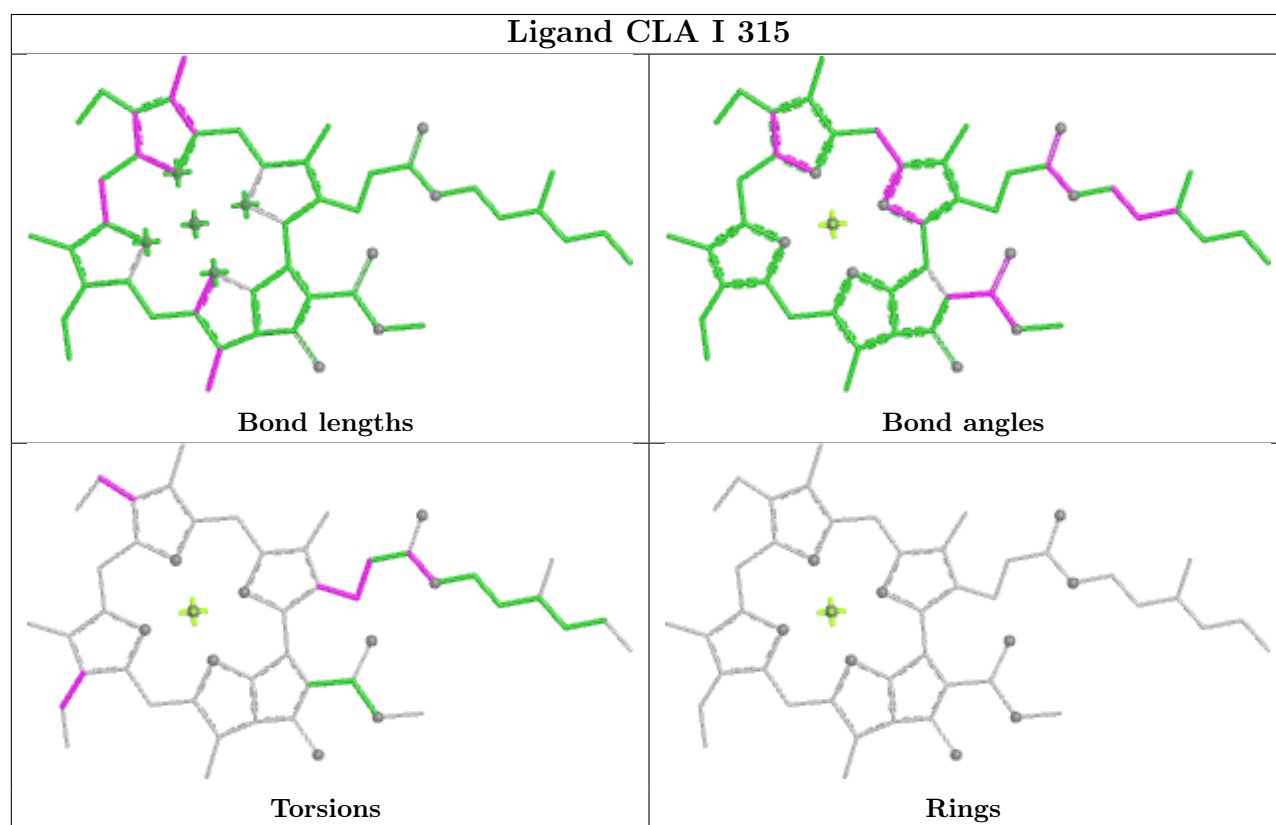
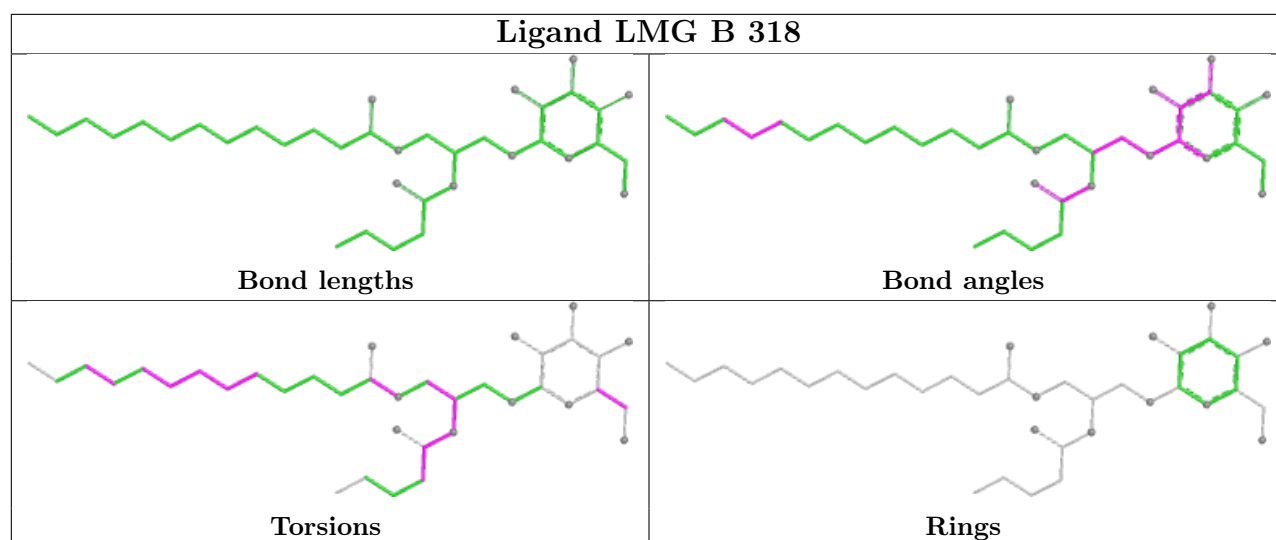
Ligand CLA b 727



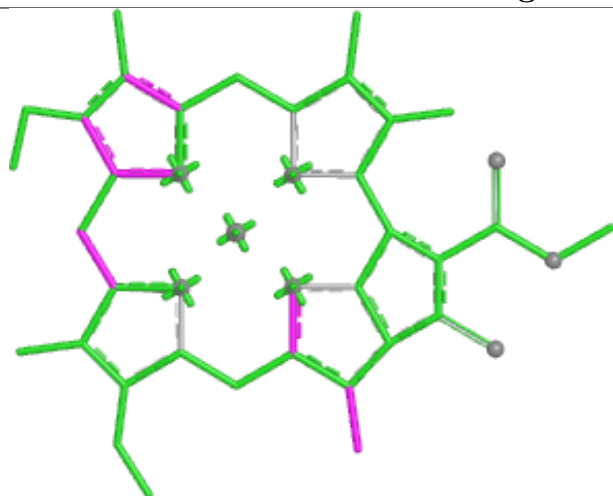
Ligand KC1 H 306



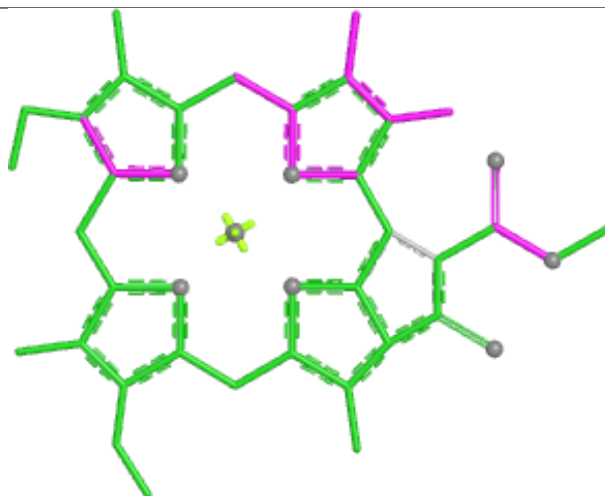




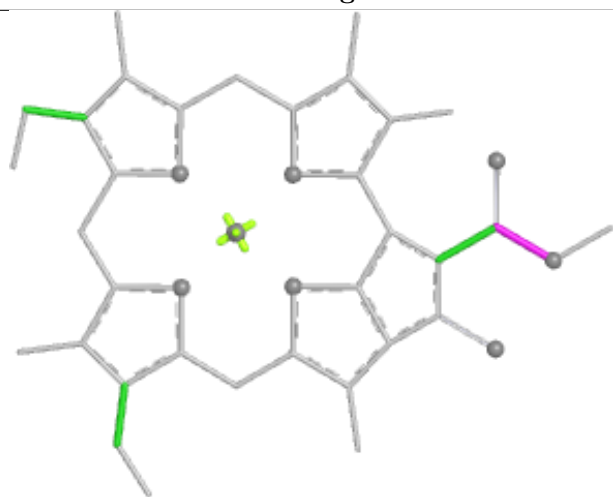
Ligand CLA J 314



Bond lengths



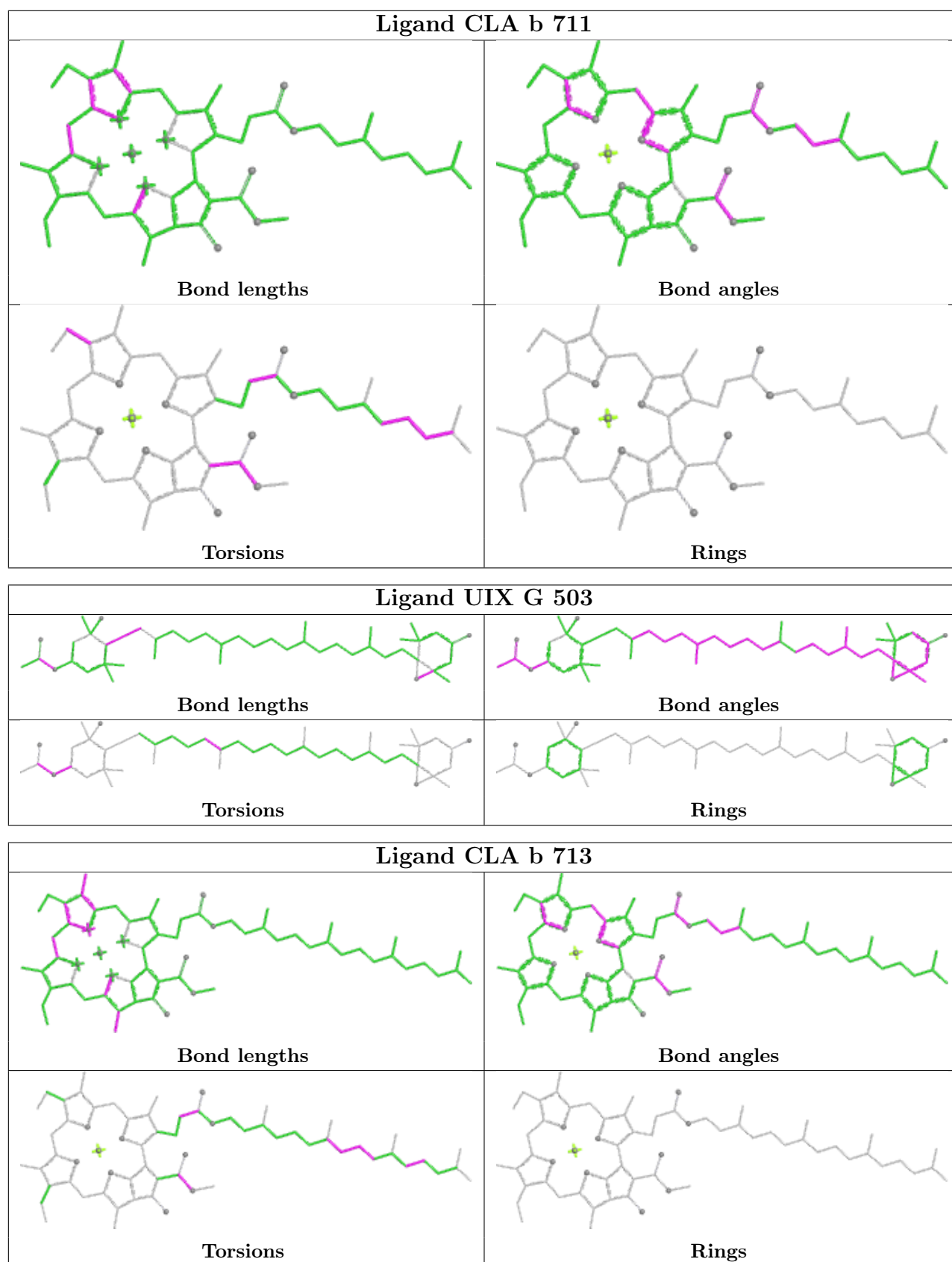
Bond angles



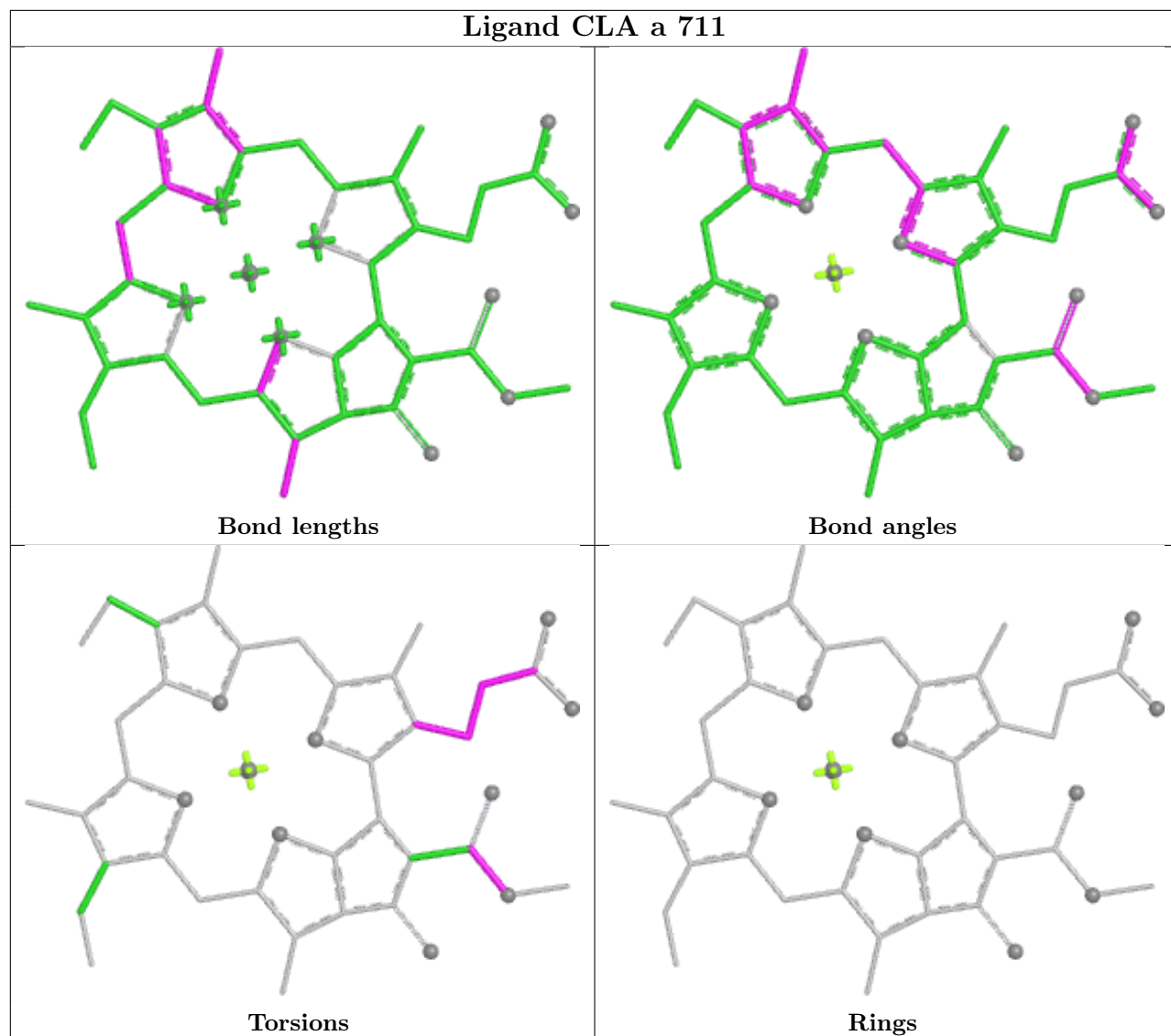
Torsions



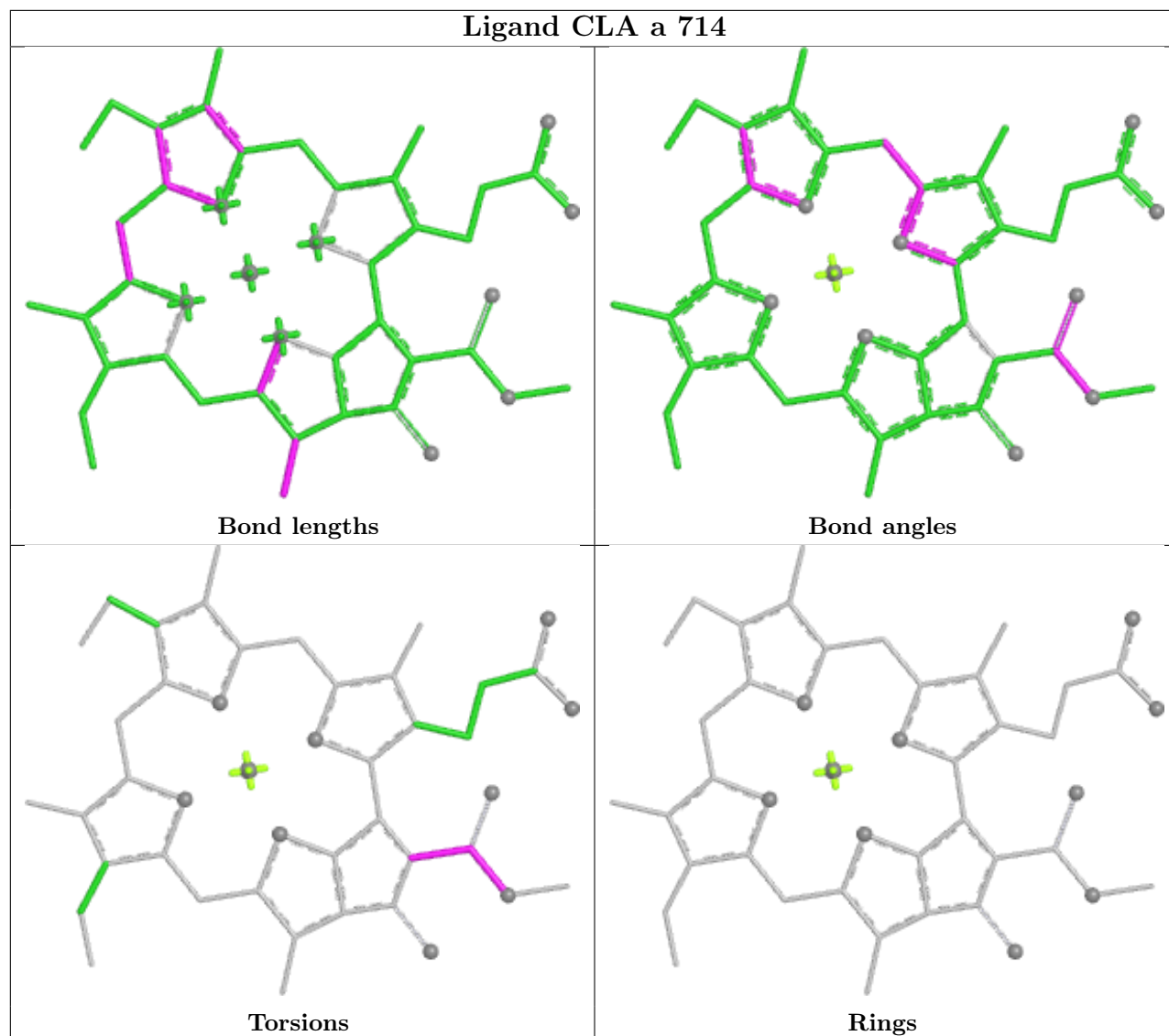
Rings



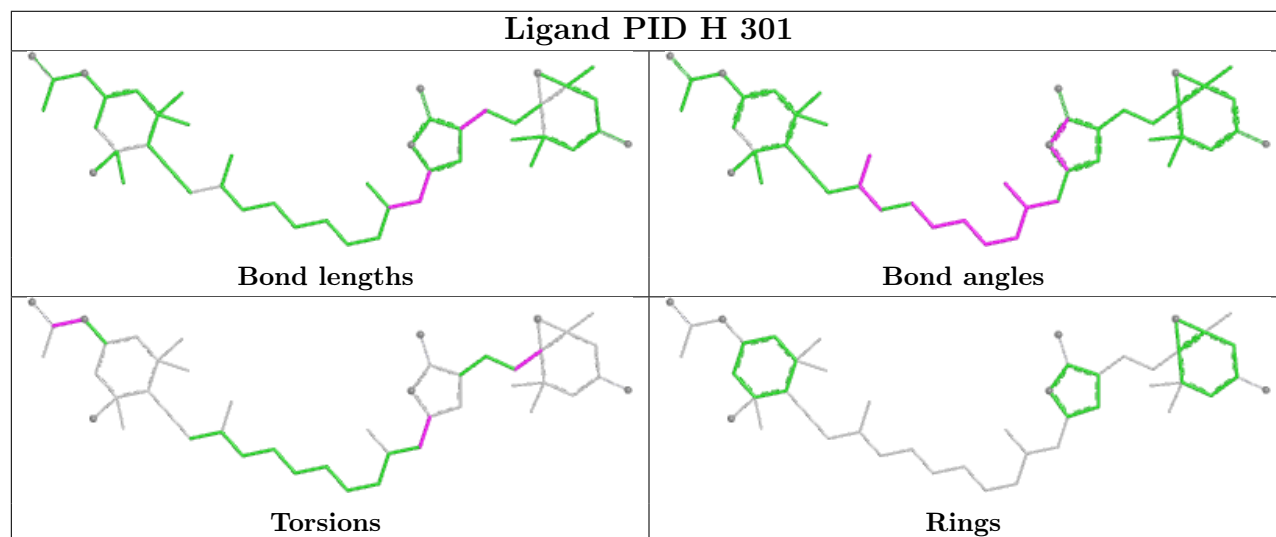
Ligand CLA a 711

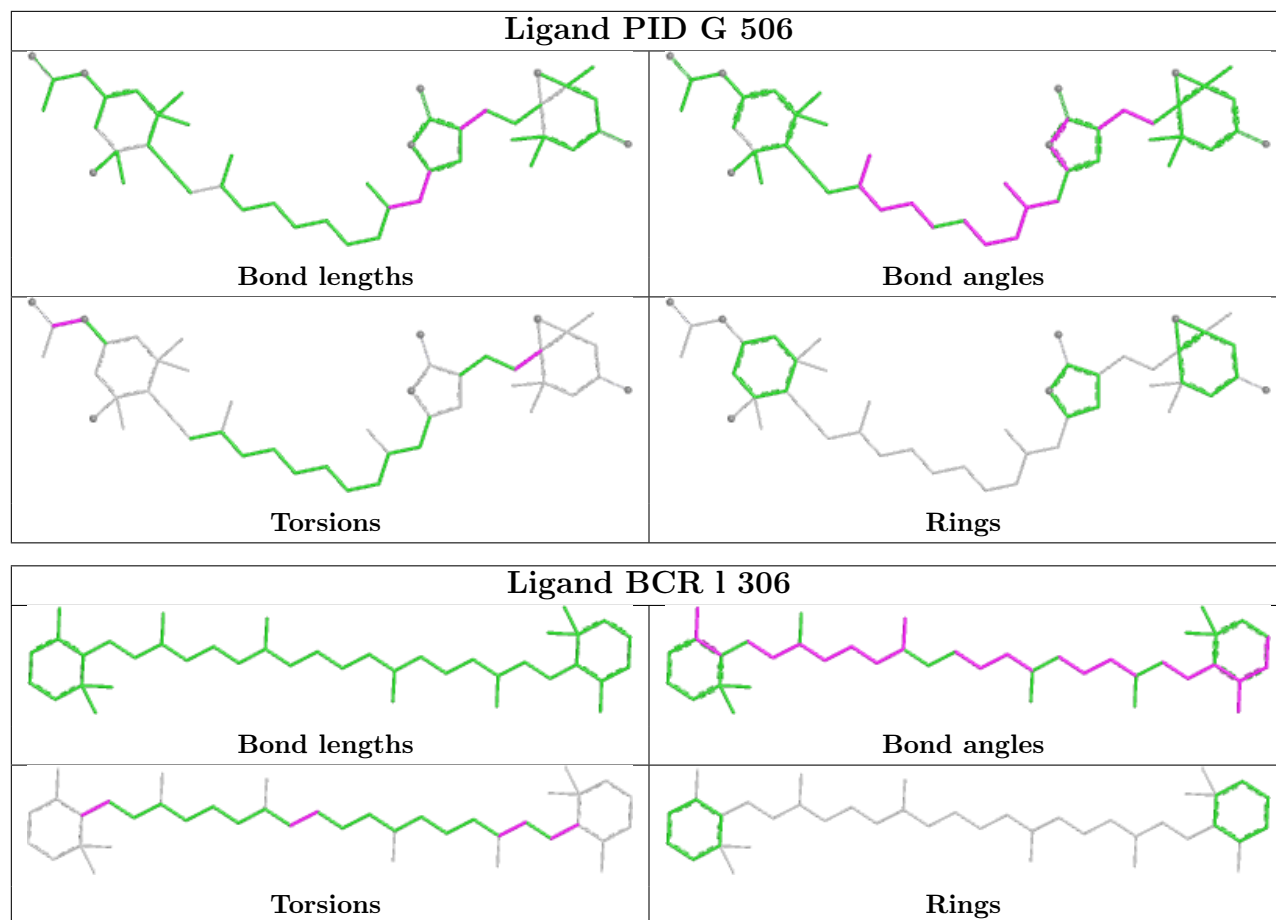


Ligand CLA a 714

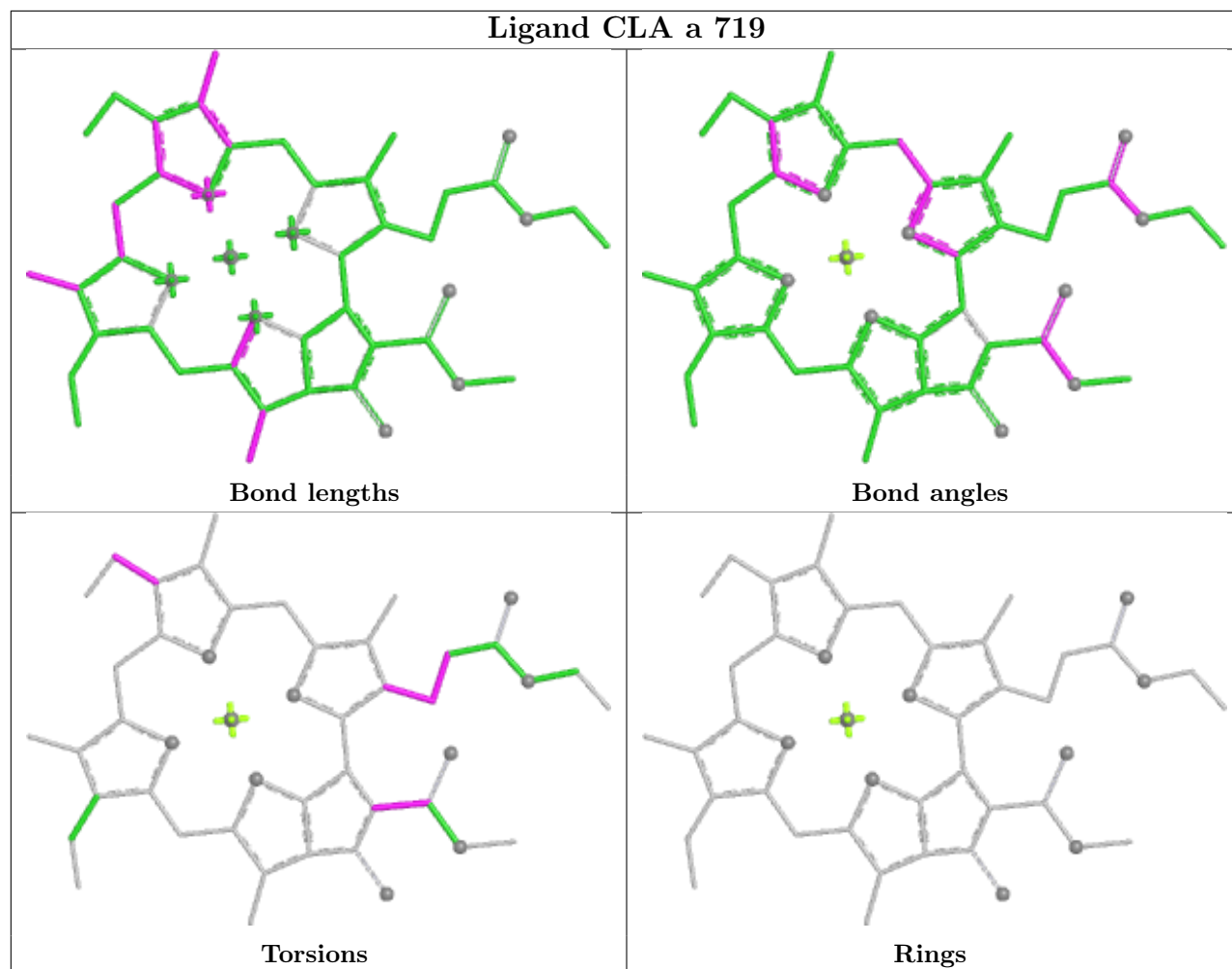


Ligand PID H 301

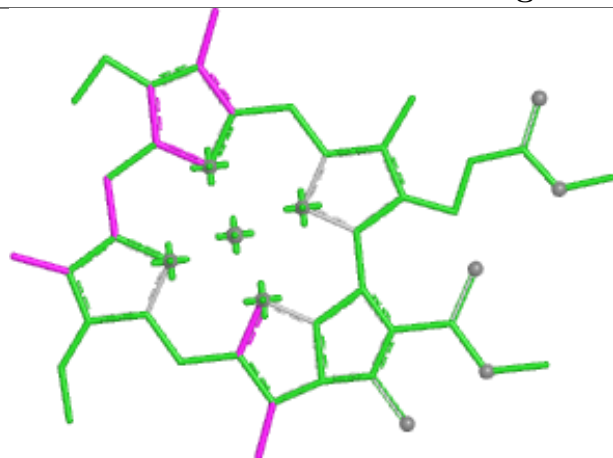




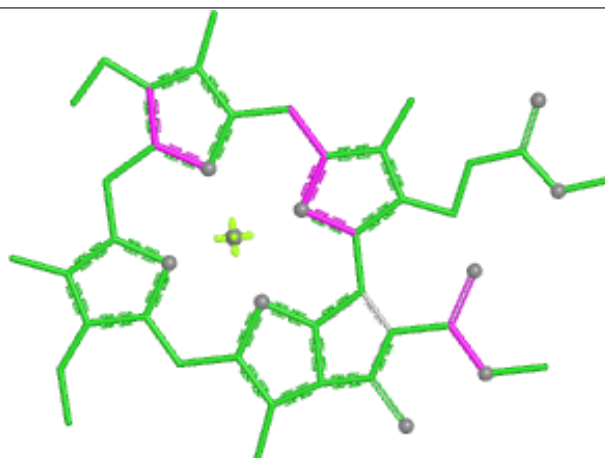
Ligand CLA a 719



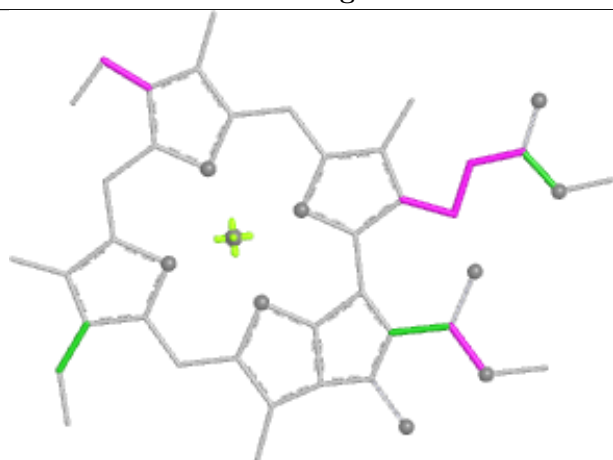
Ligand CLA L 318



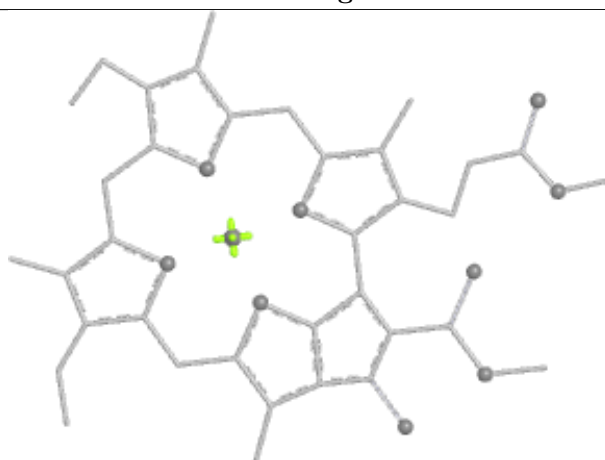
Bond lengths



Bond angles

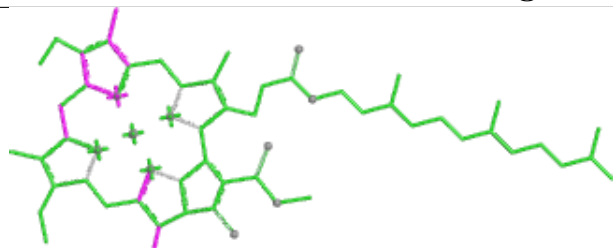


Torsions

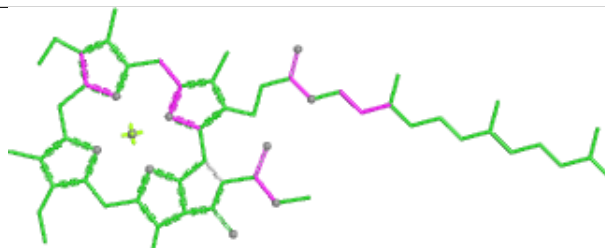


Rings

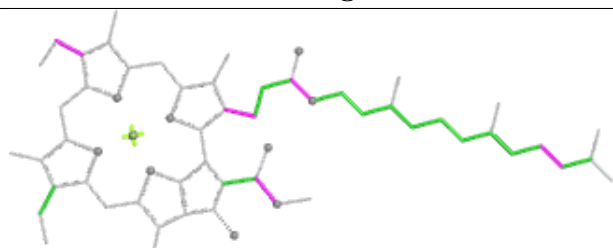
Ligand CLA a 712



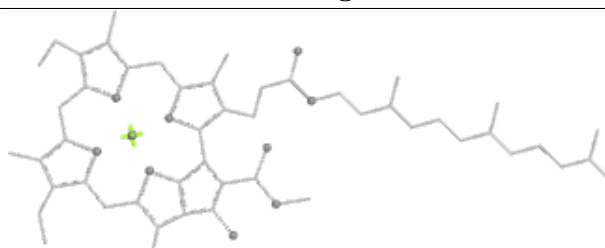
Bond lengths



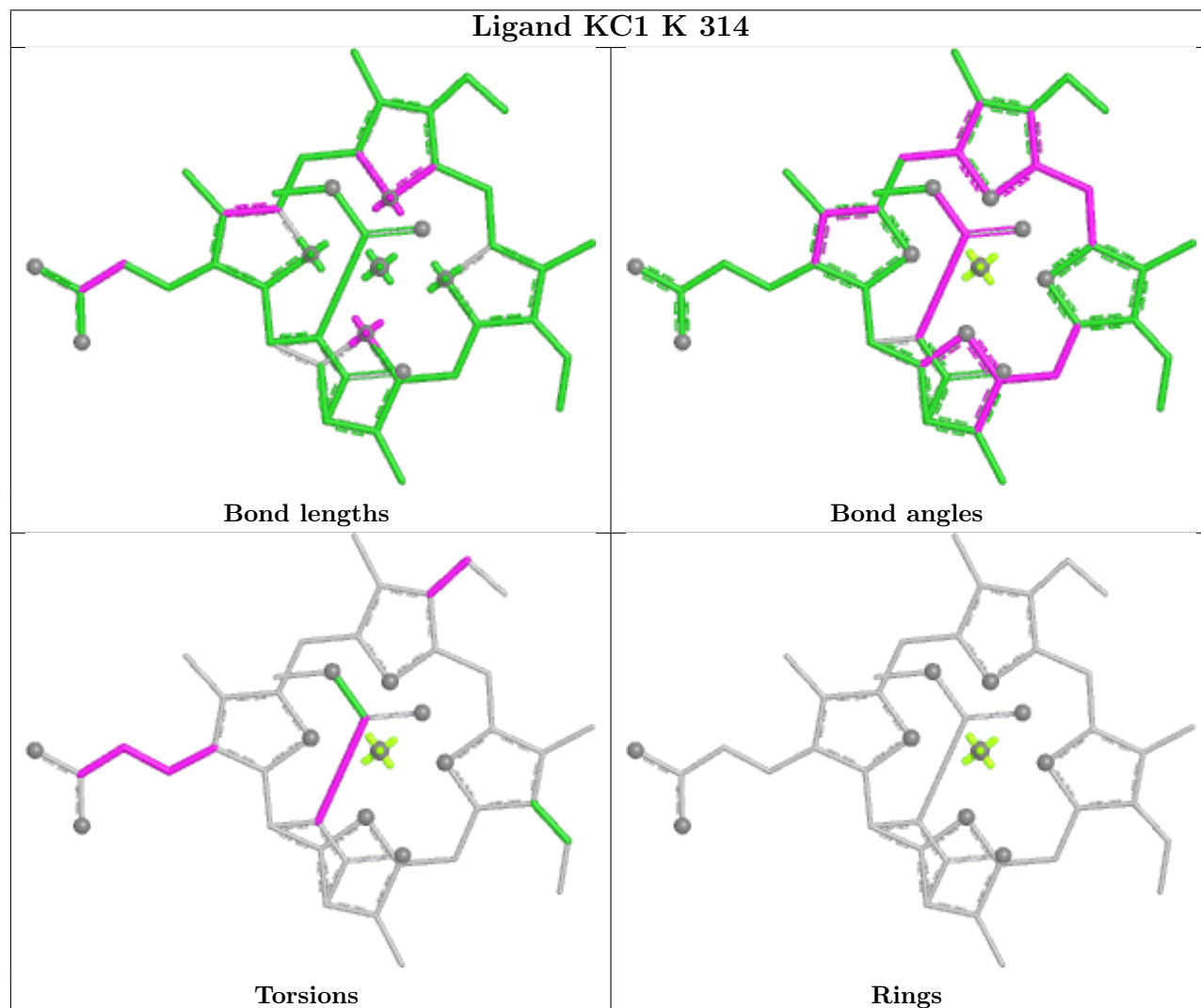
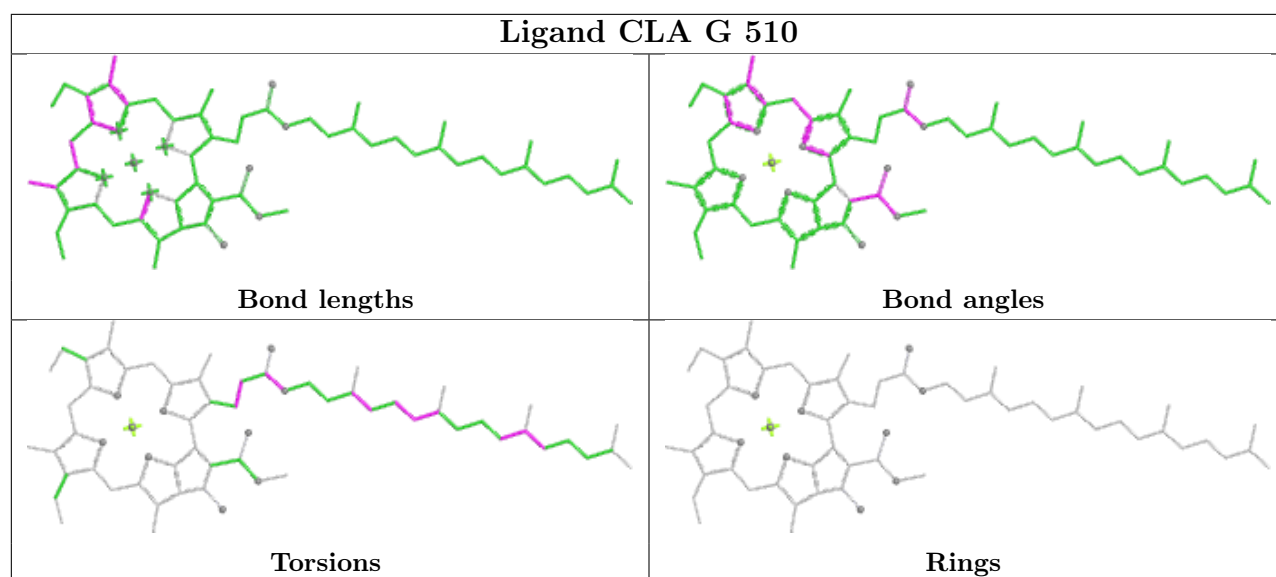
Bond angles

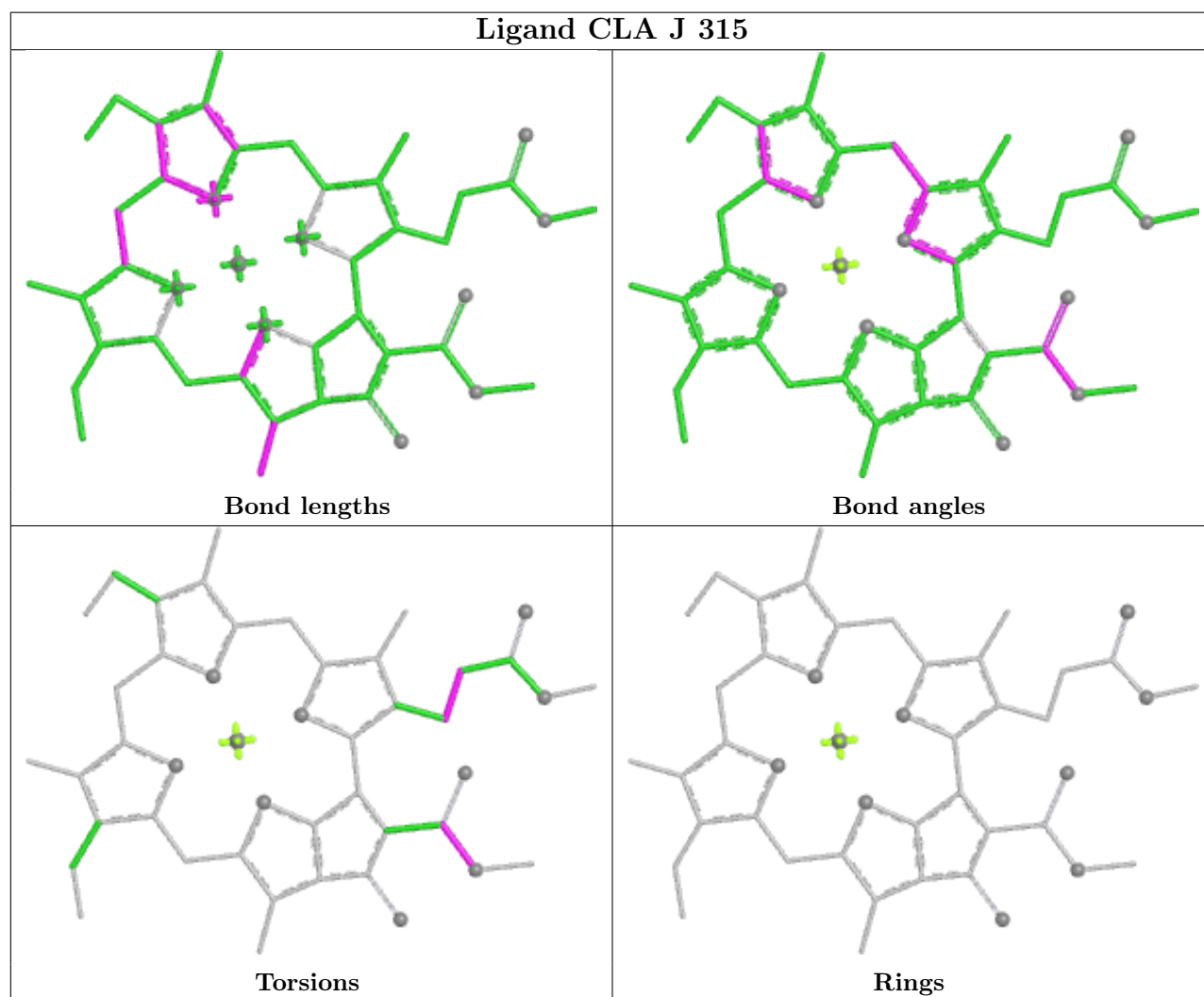
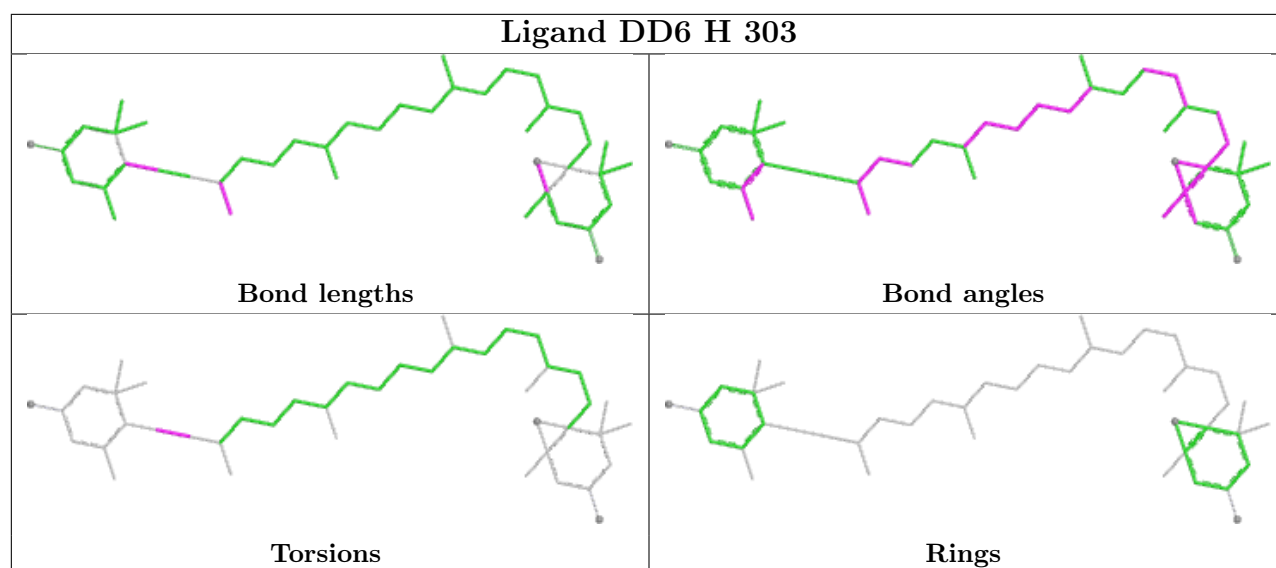


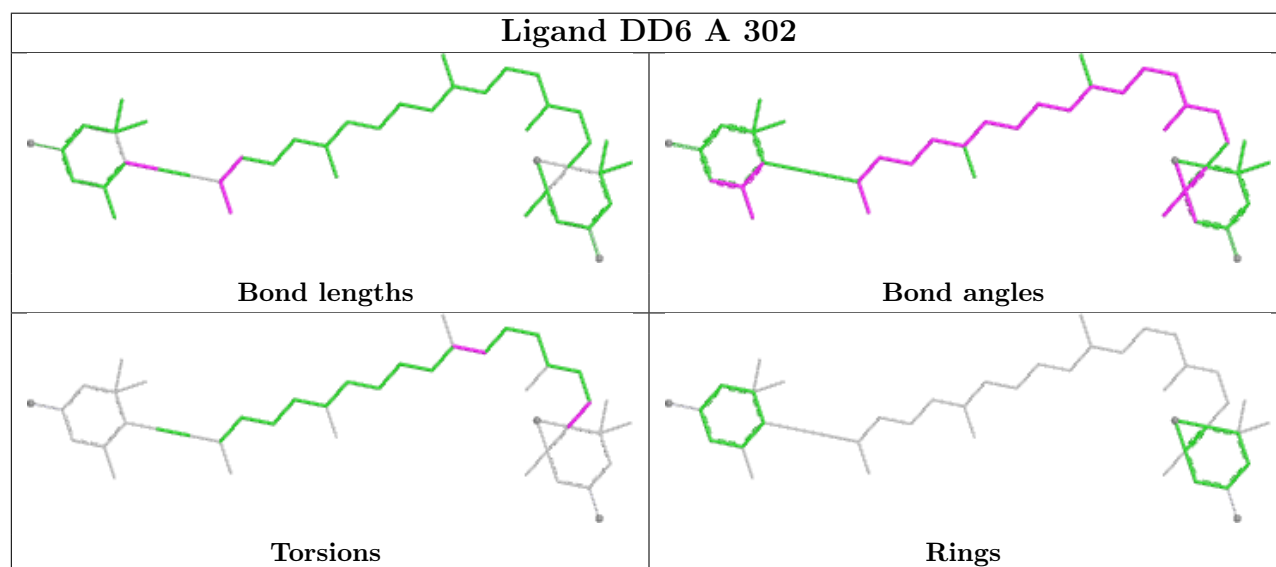
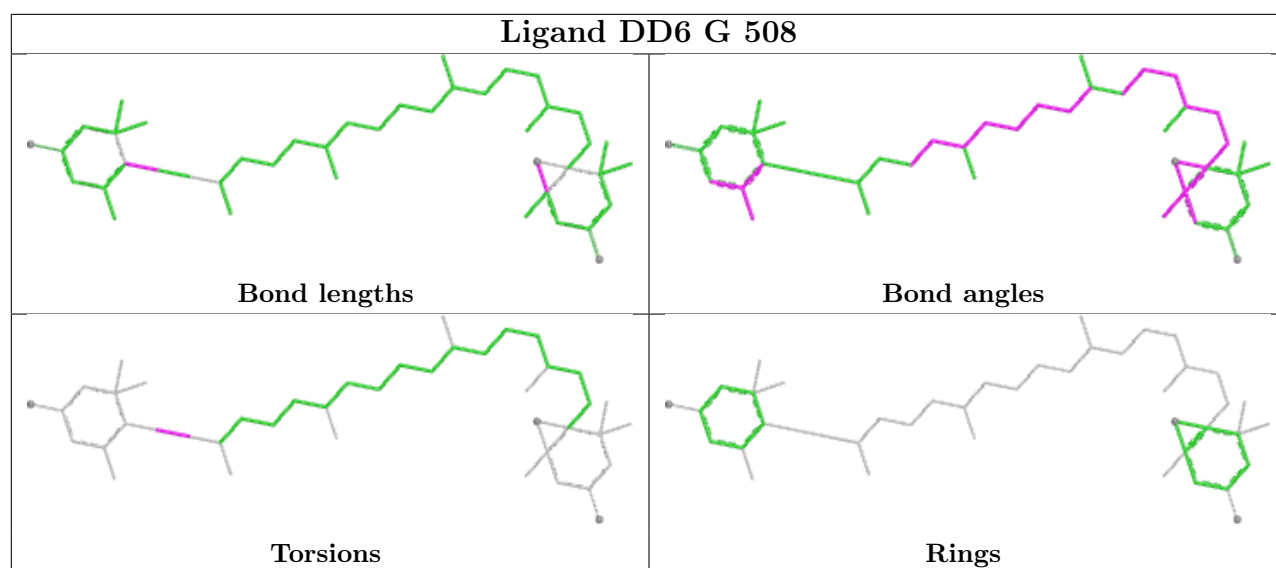
Torsions



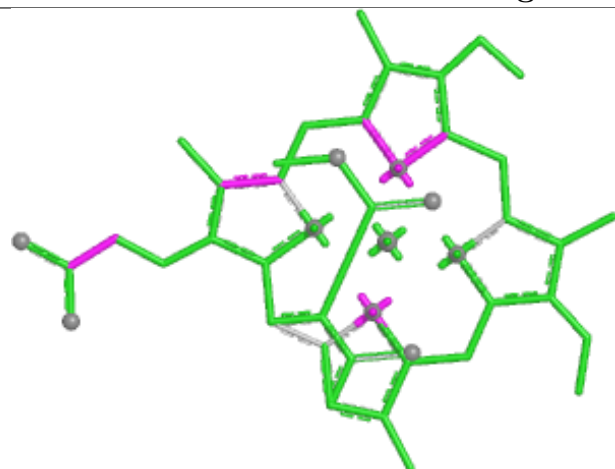
Rings



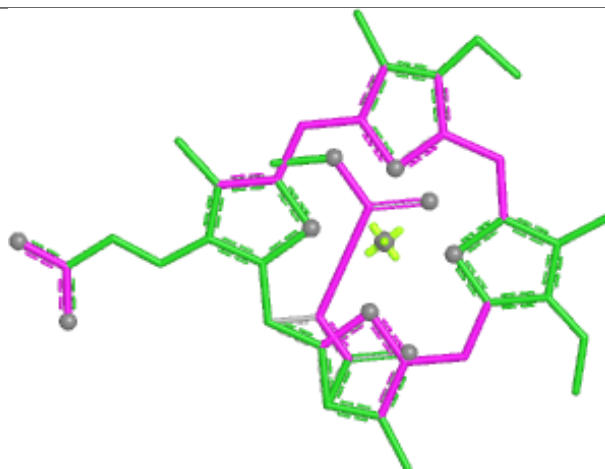




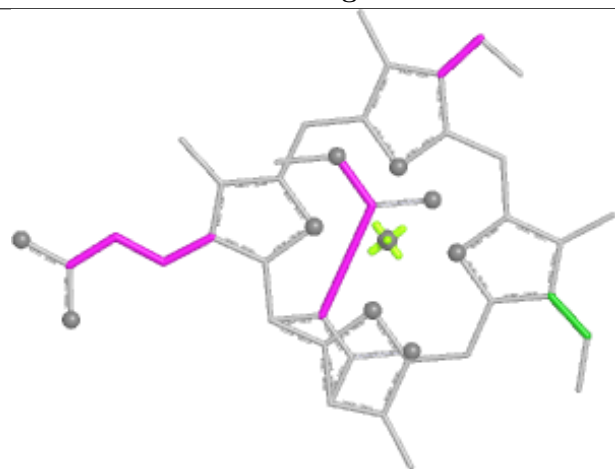
Ligand KC1 N 308



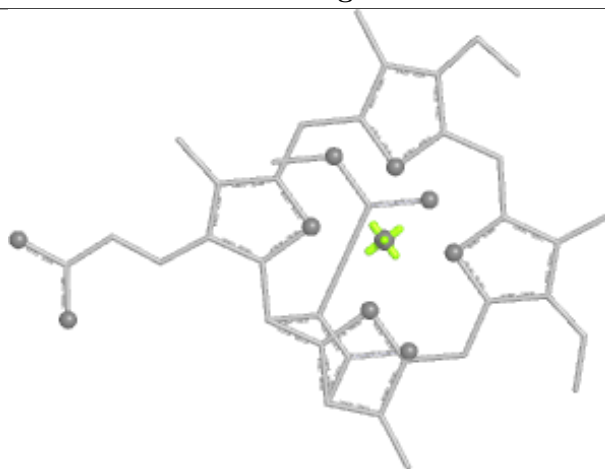
Bond lengths



Bond angles

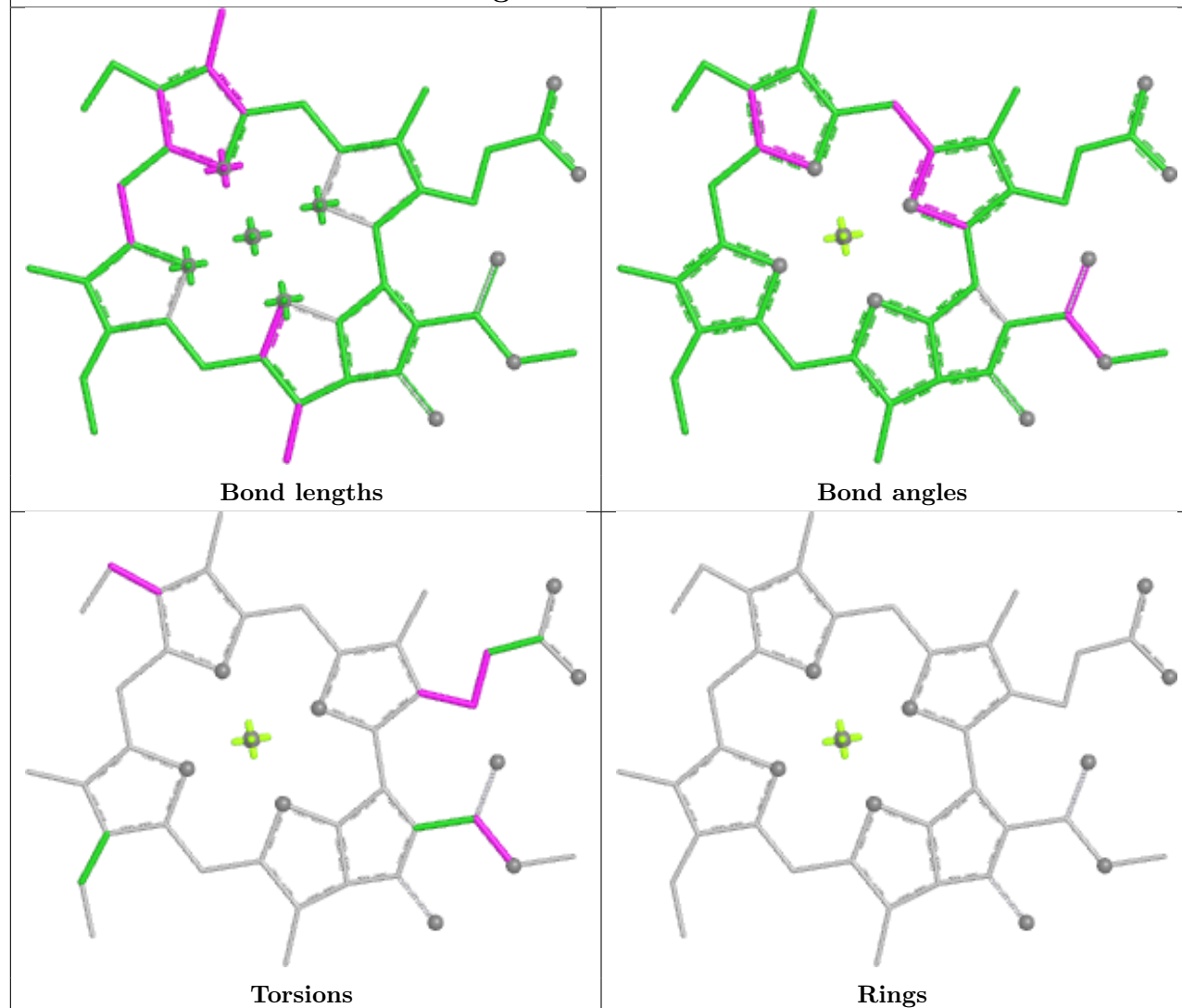


Torsions

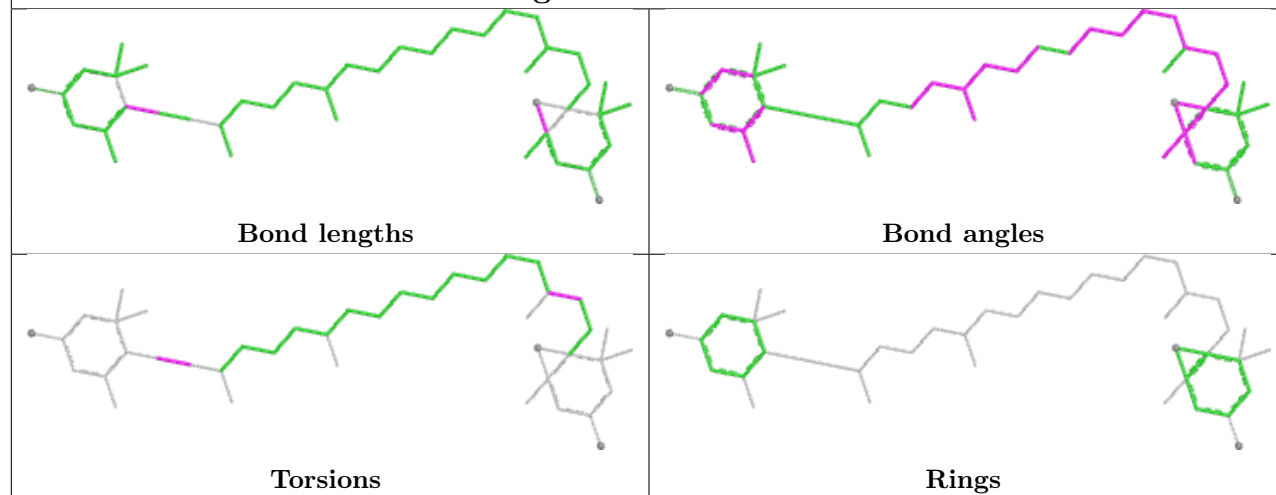


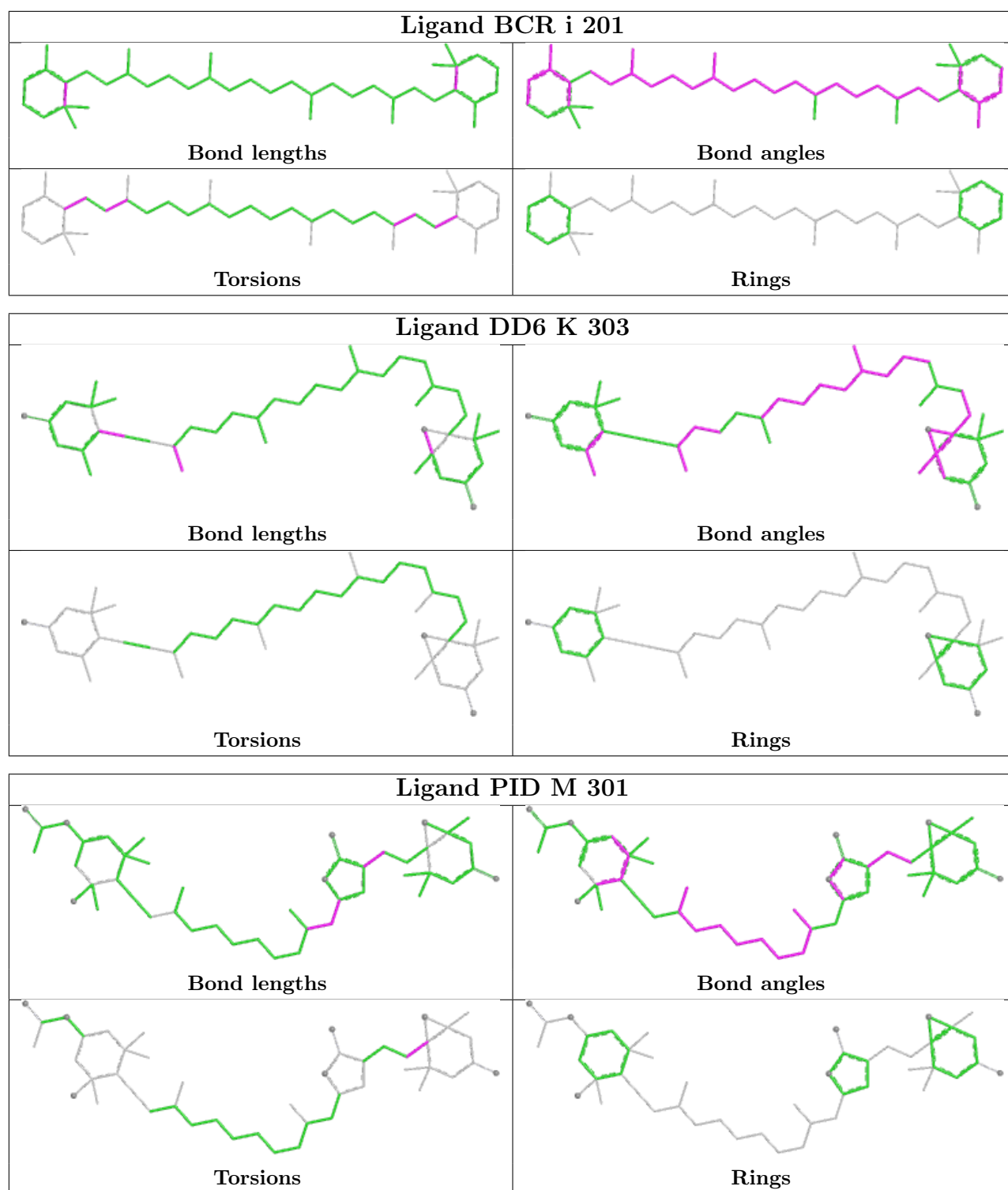
Rings

Ligand CLA B 317

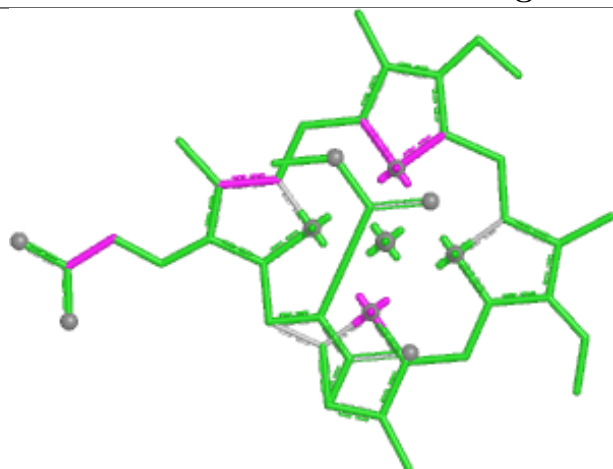


Ligand DD6 B 302

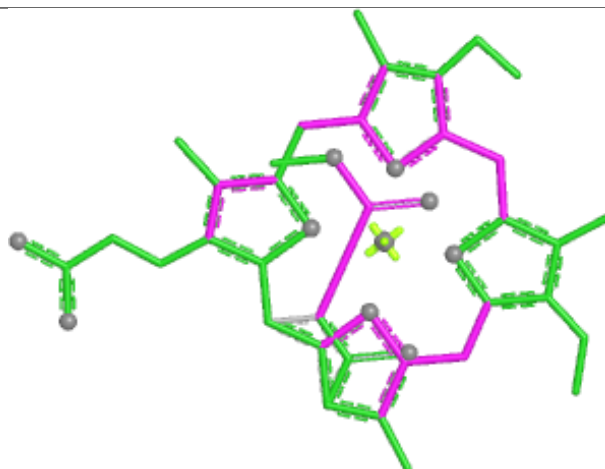




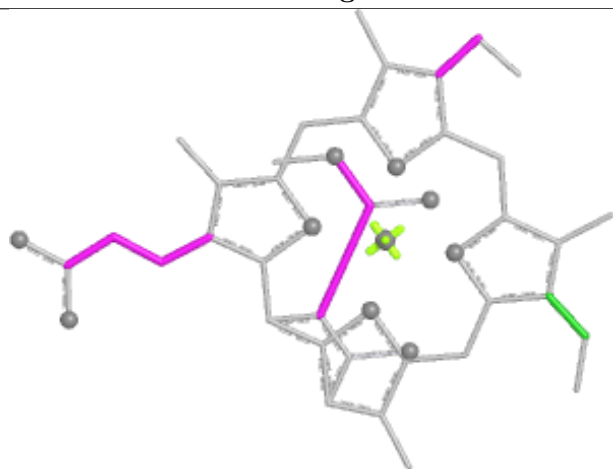
Ligand KC1 D 310



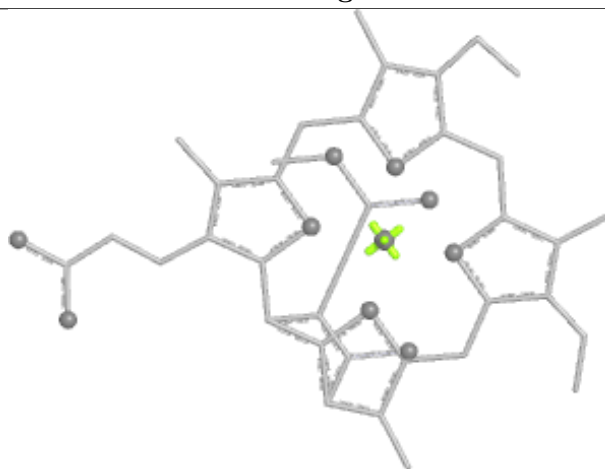
Bond lengths



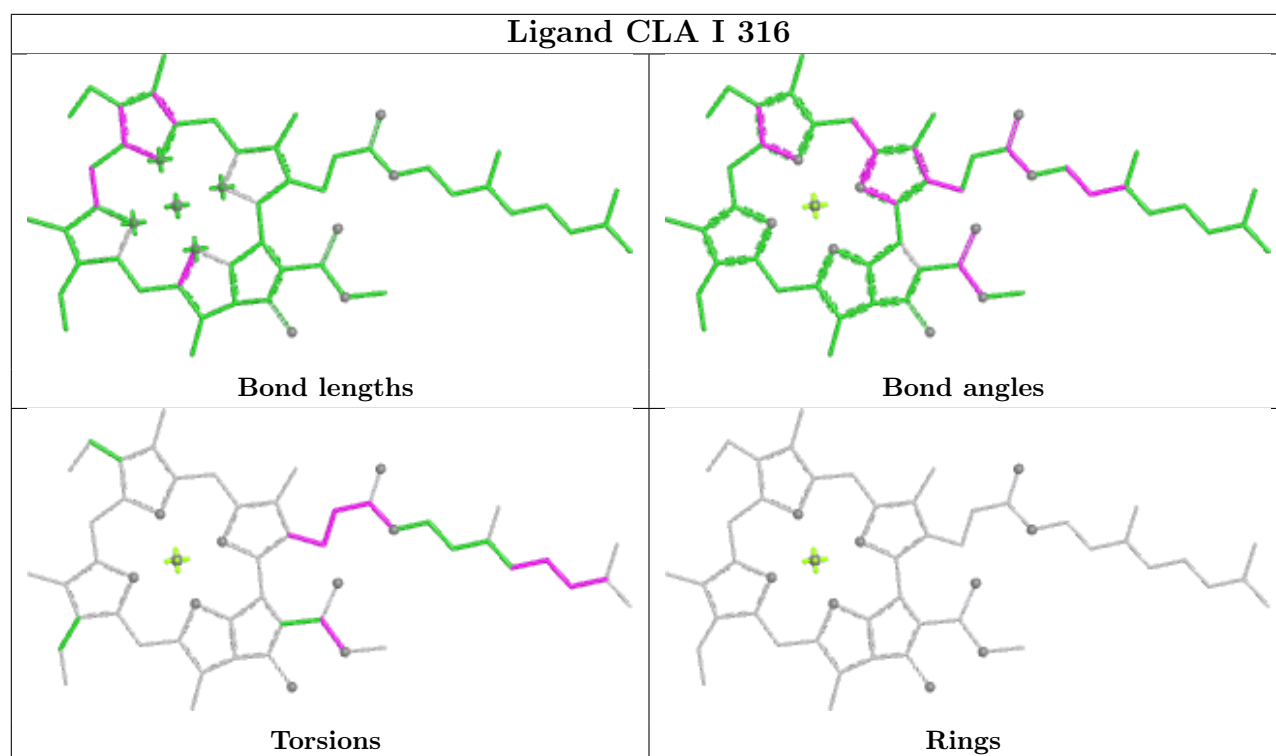
Bond angles

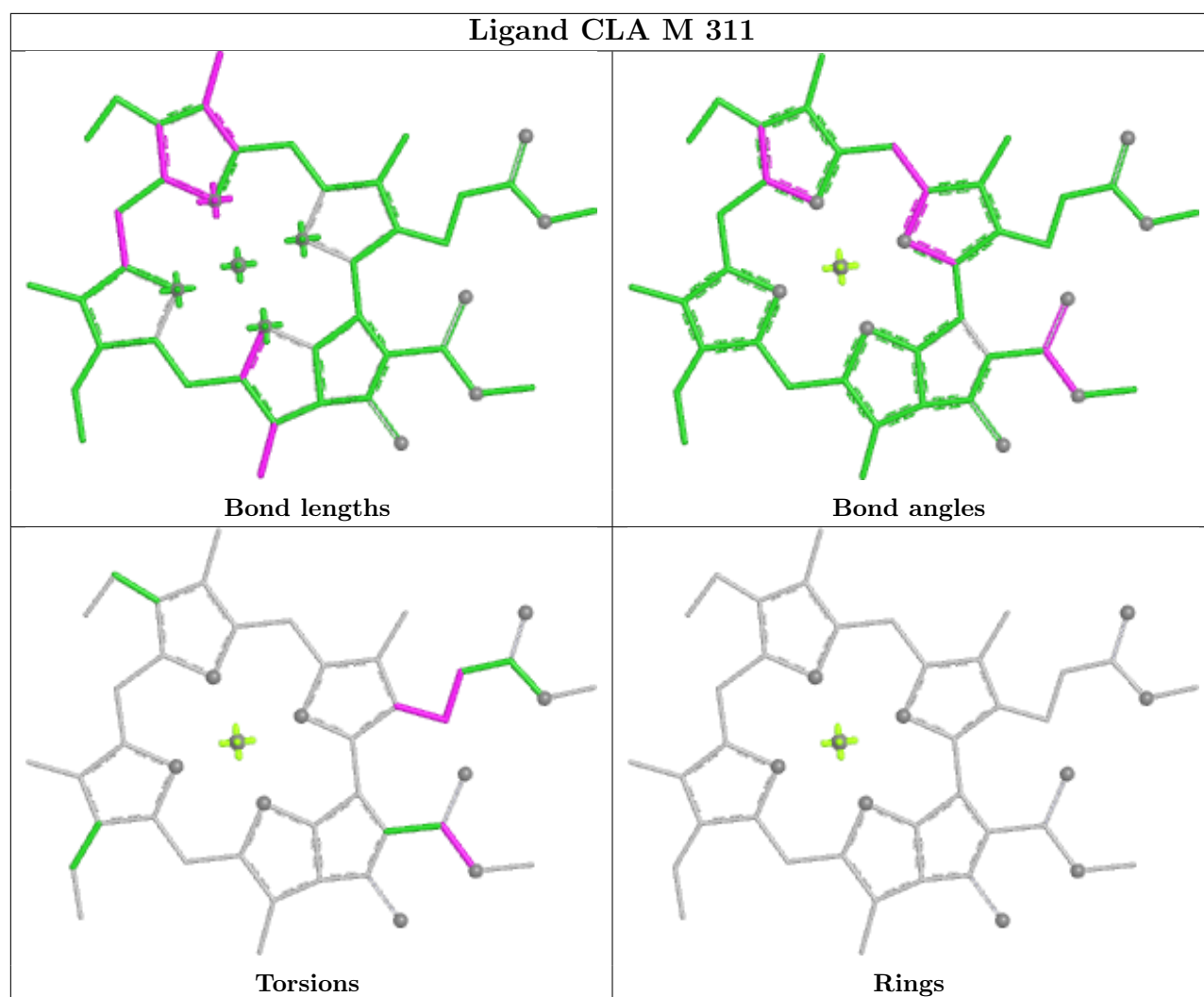


Torsions

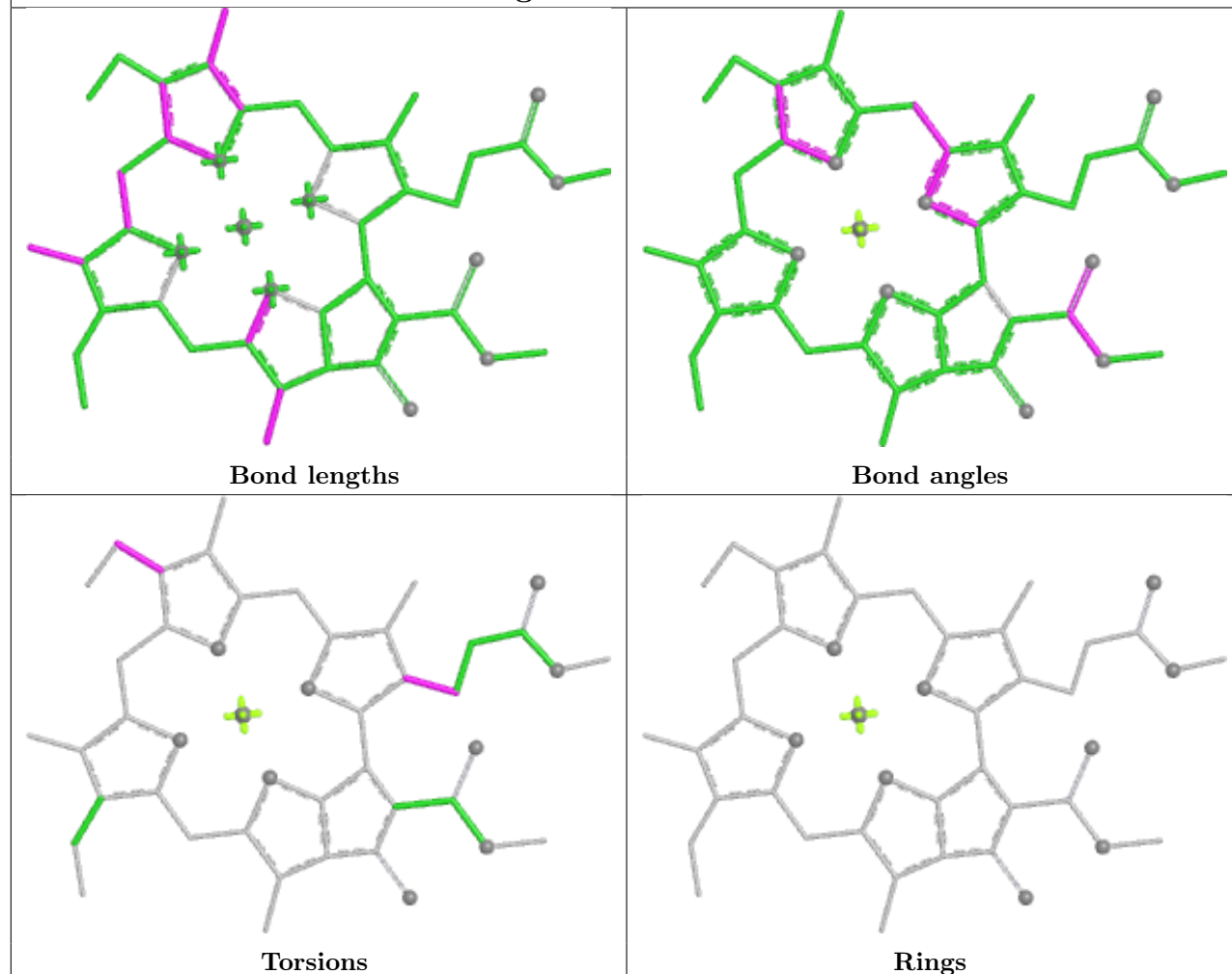


Rings

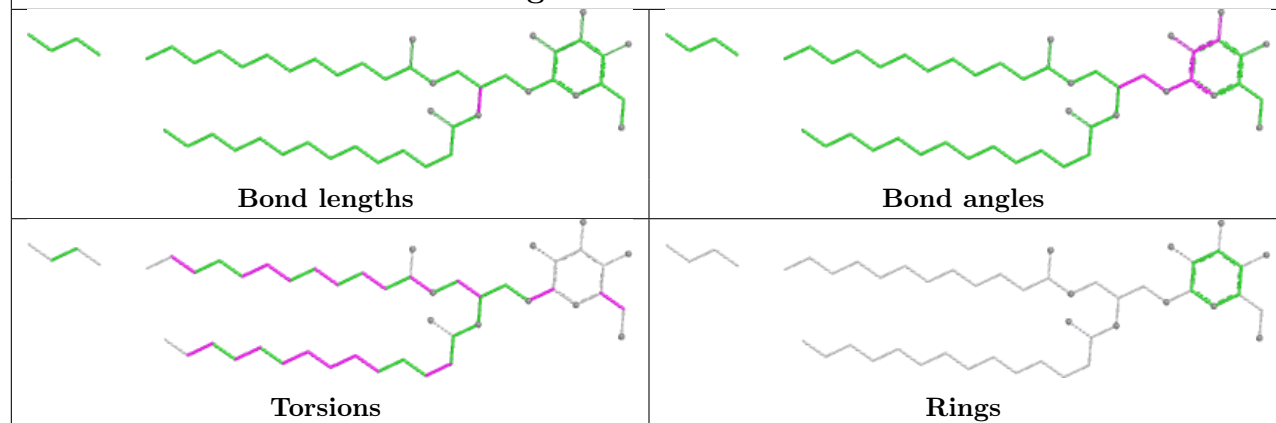


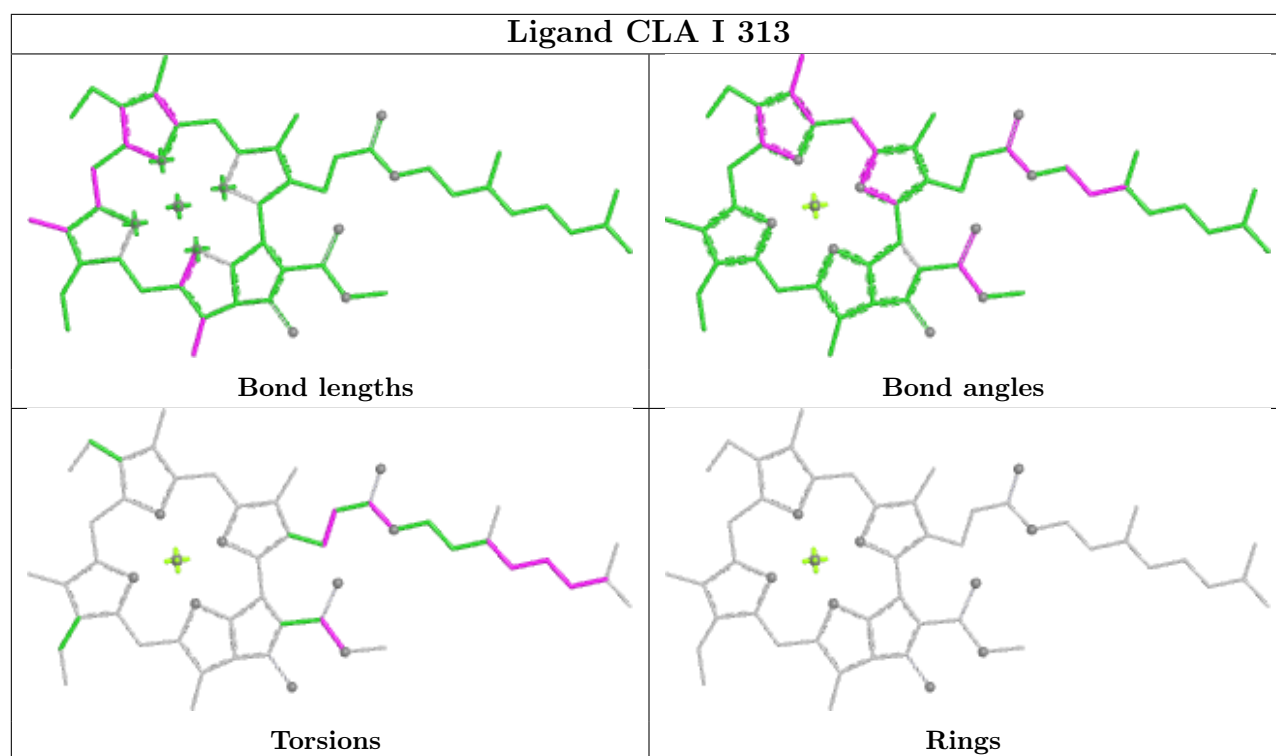


Ligand CLA F 308

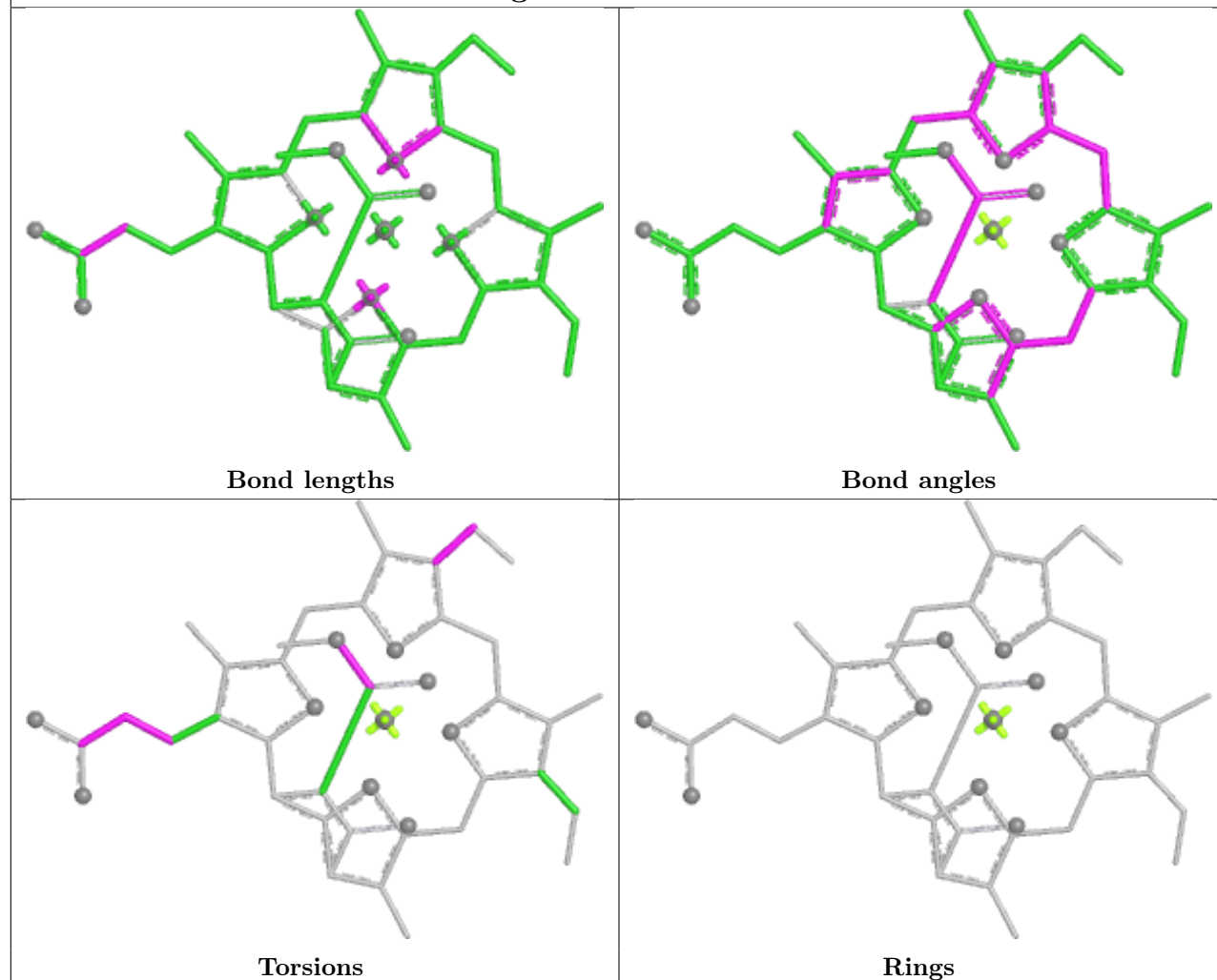


Ligand LMG D 317

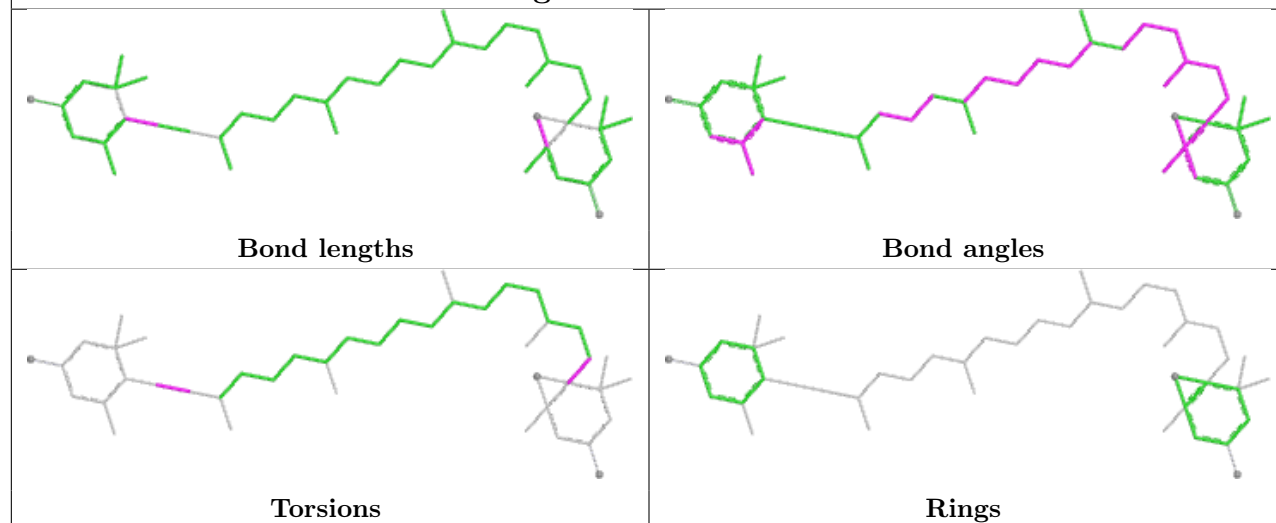


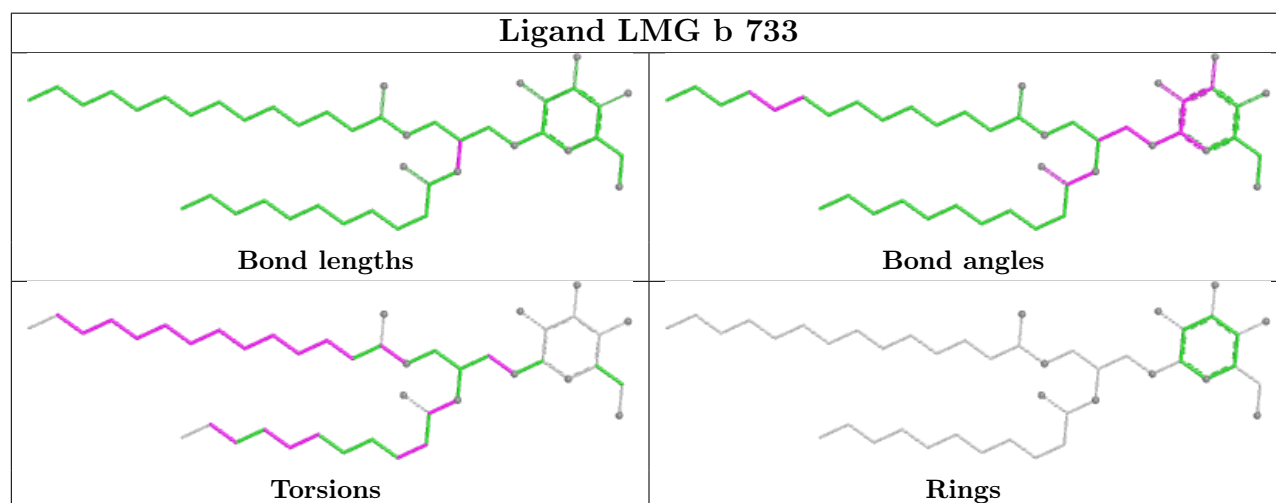
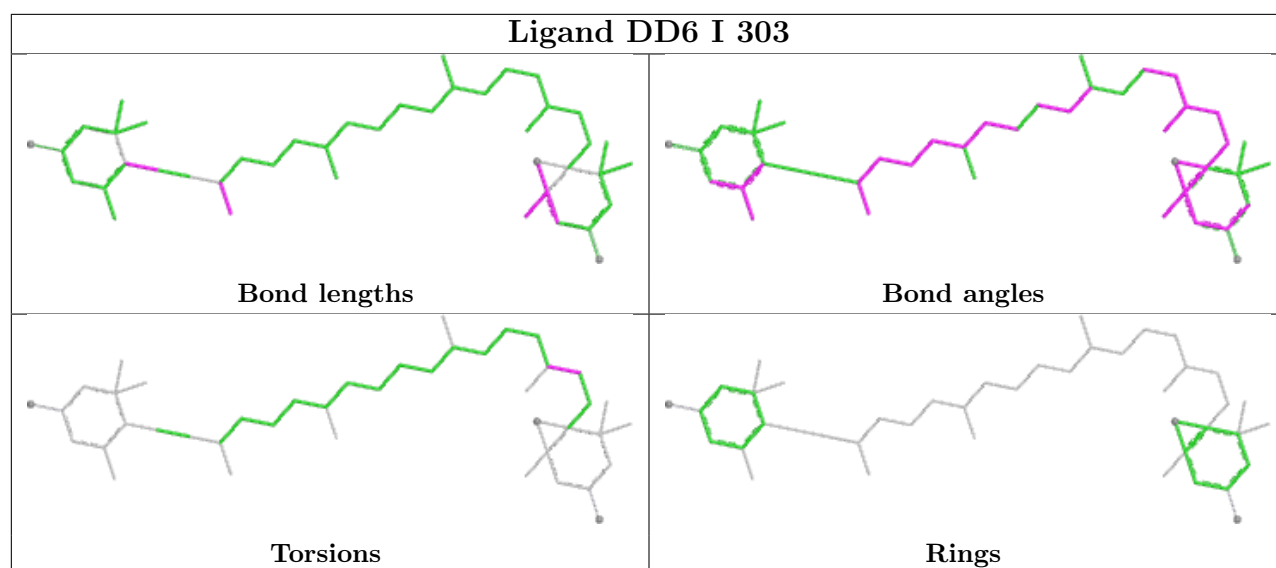


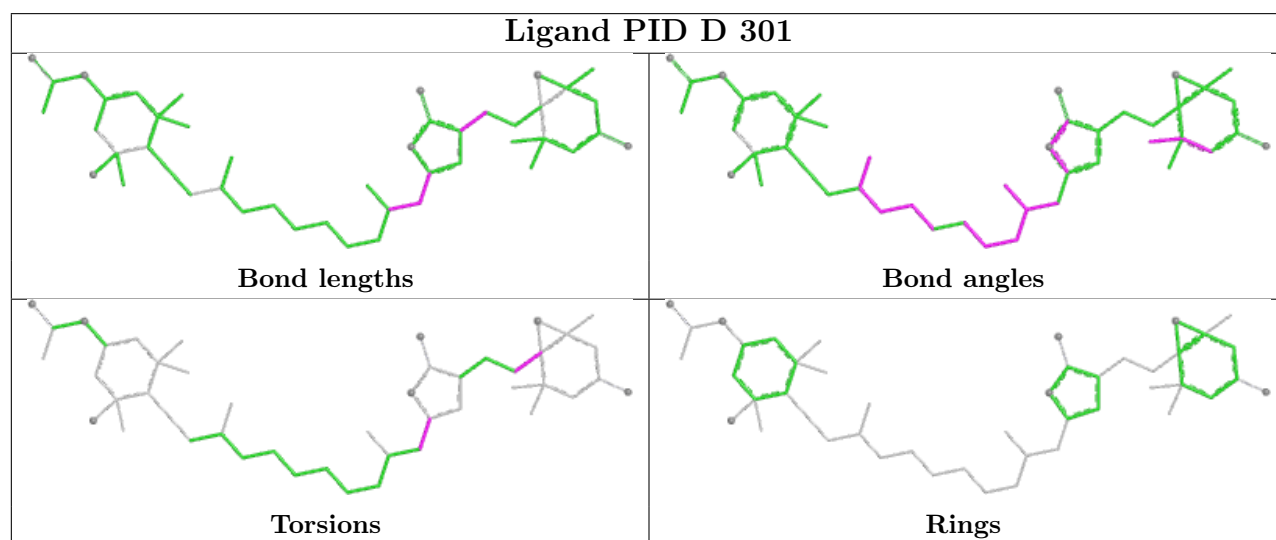
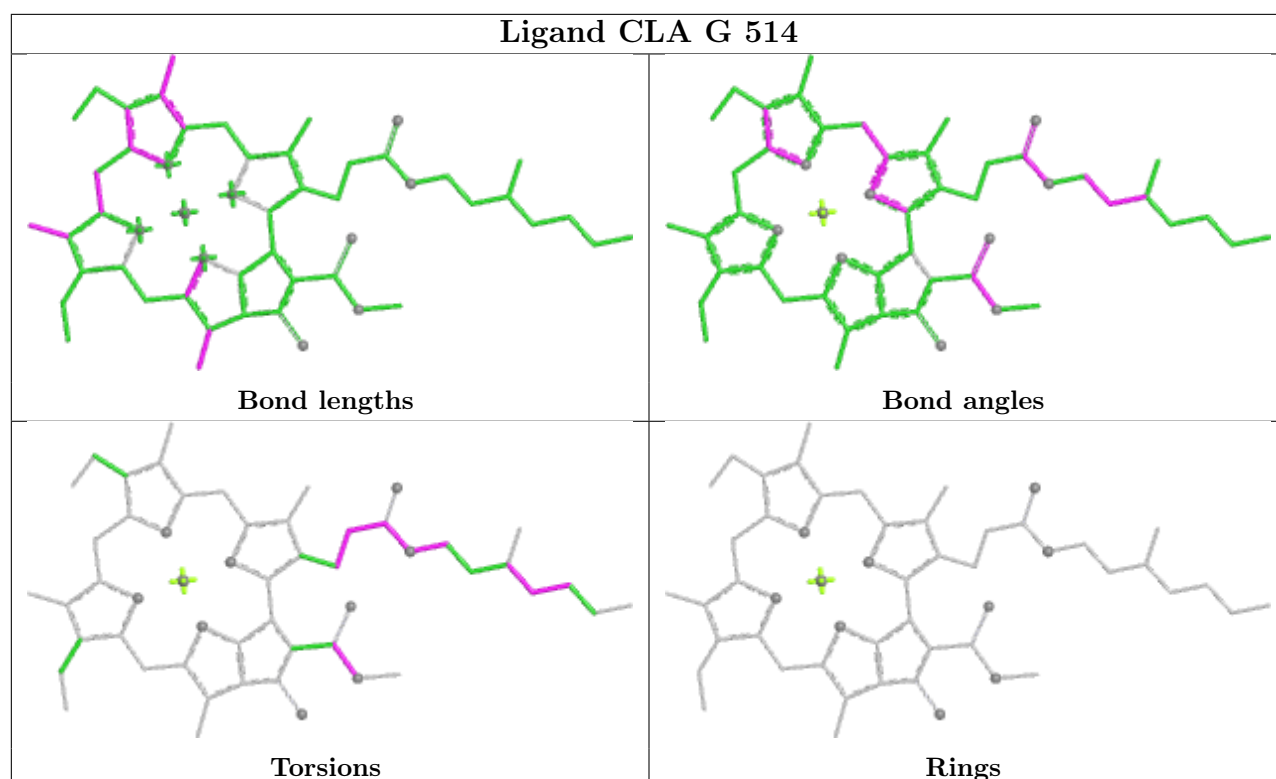
Ligand KC1 F 314



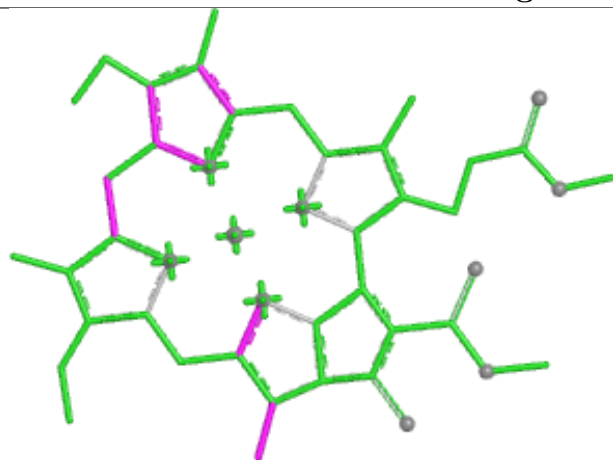
Ligand DD6 B 303



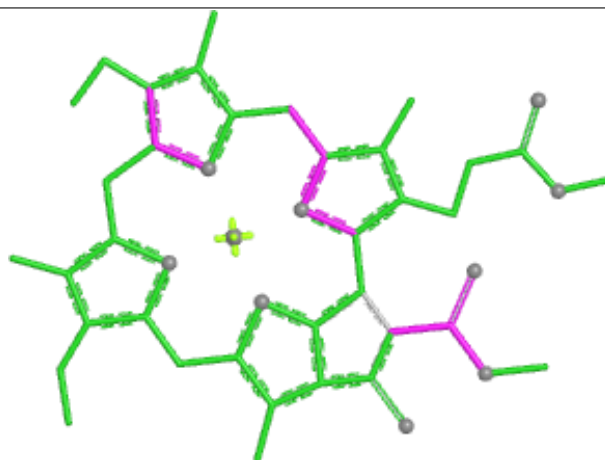




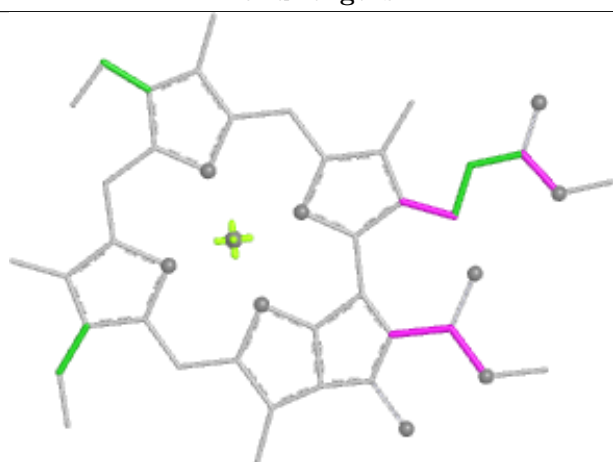
Ligand CLA F 310



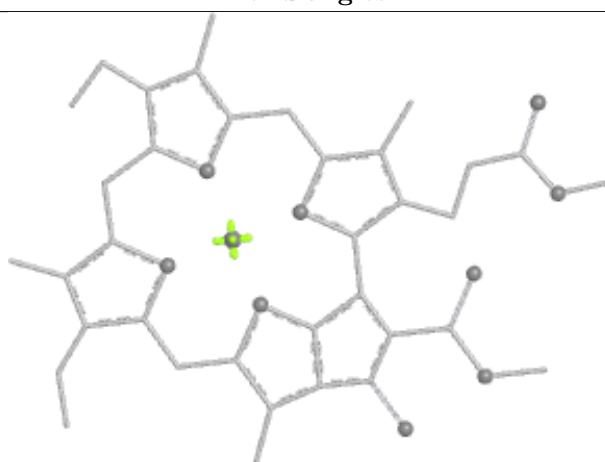
Bond lengths



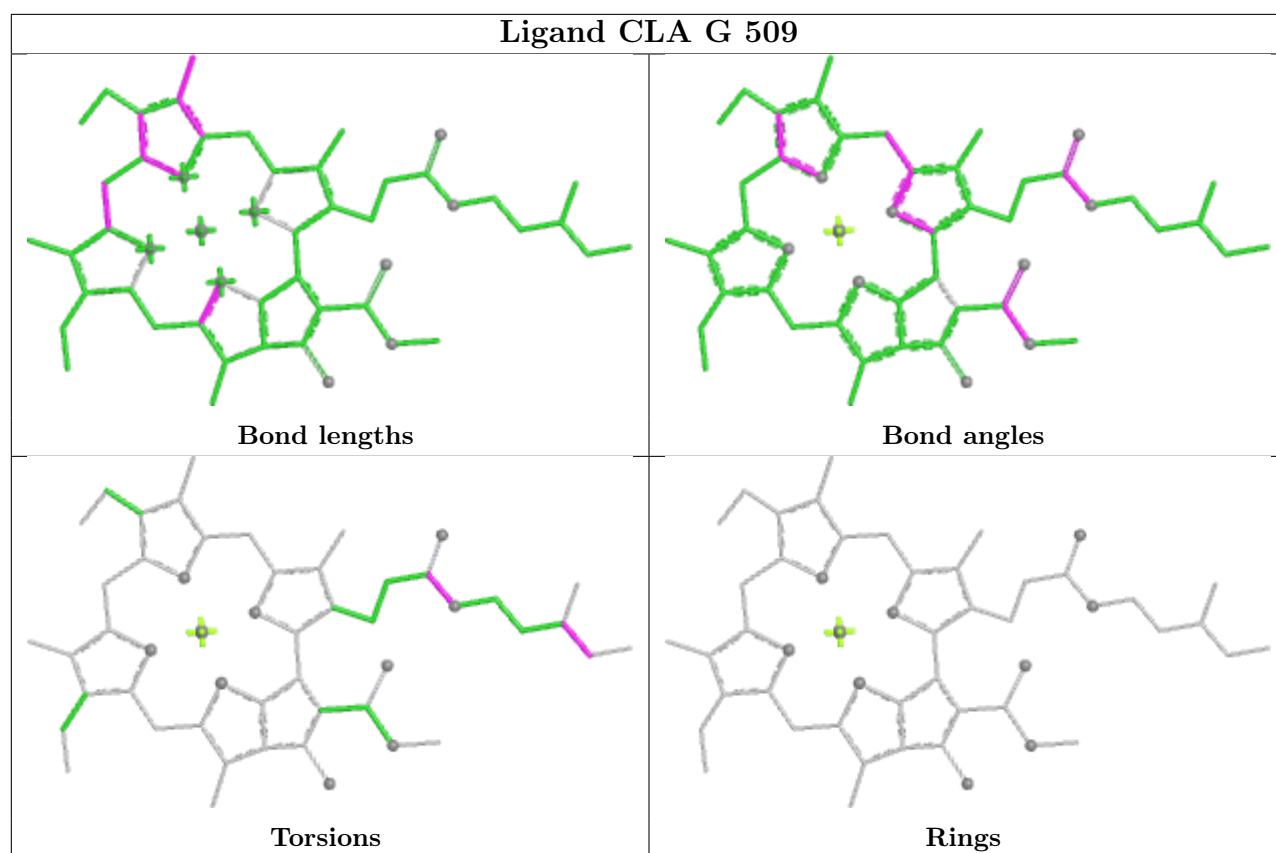
Bond angles



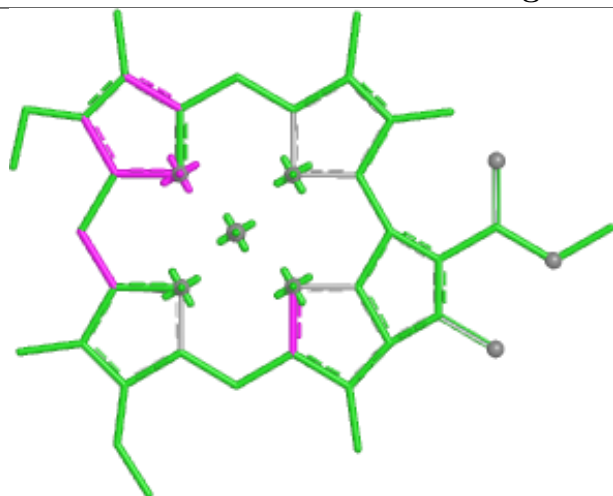
Torsions



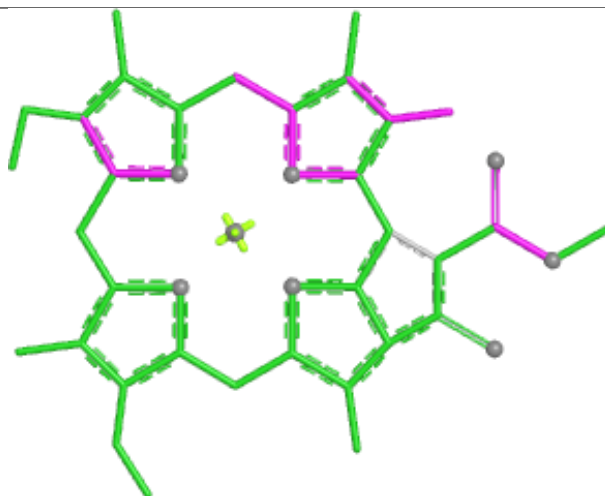
Rings



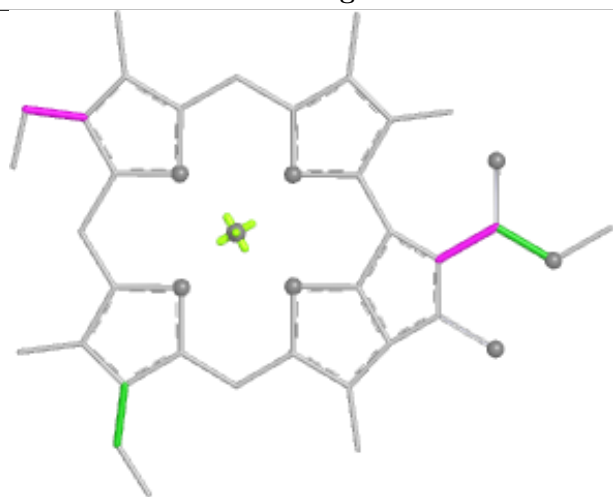
Ligand CLA 1 309



Bond lengths



Bond angles

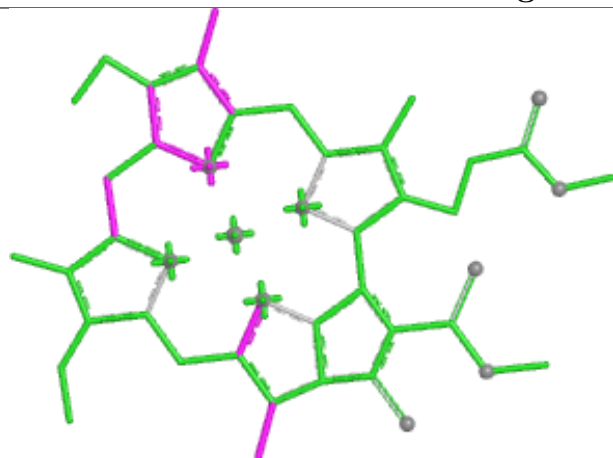


Torsions

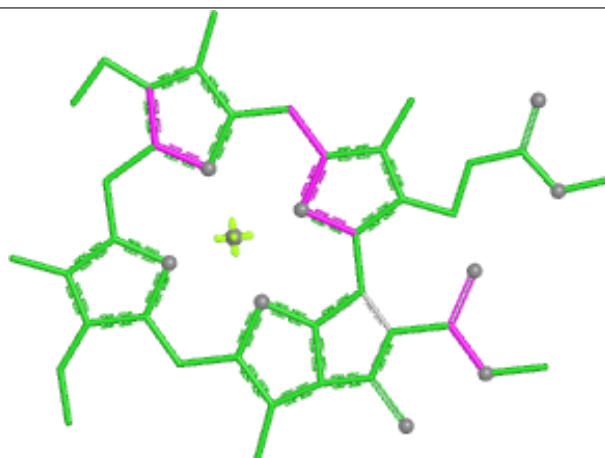


Rings

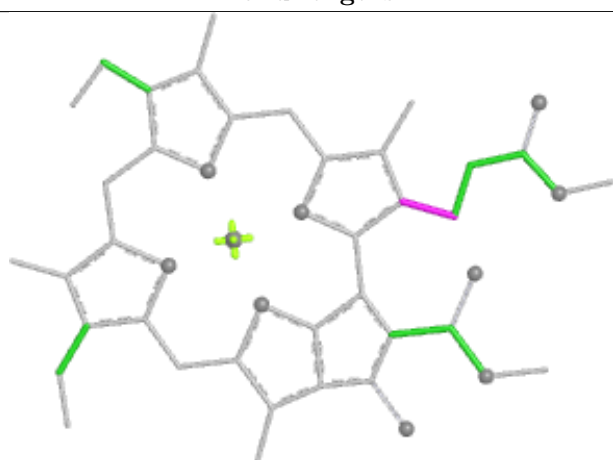
Ligand CLA b 721



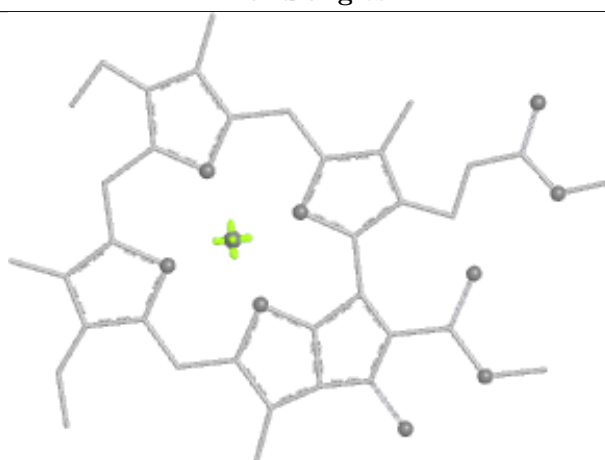
Bond lengths



Bond angles

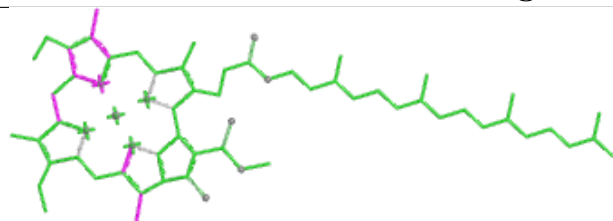


Torsions

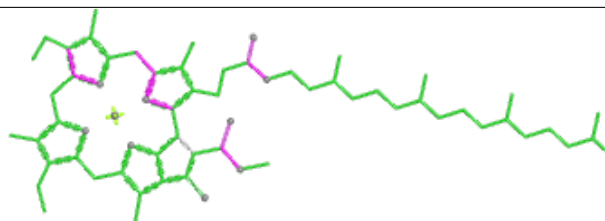


Rings

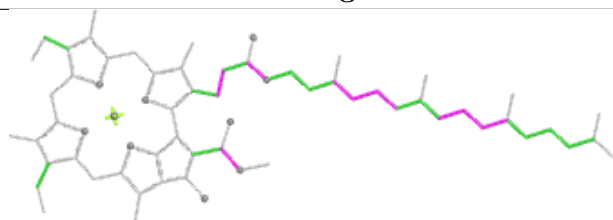
Ligand CLA b 701



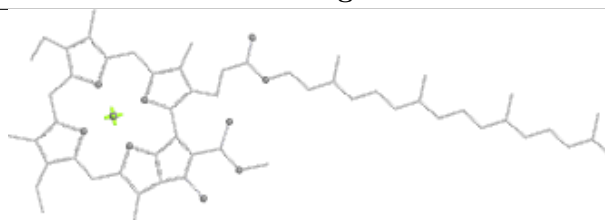
Bond lengths



Bond angles

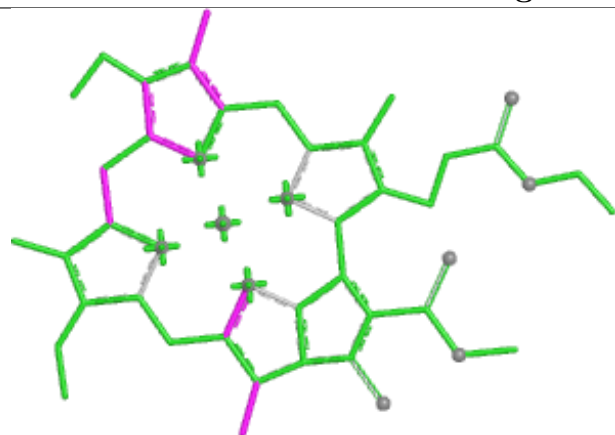


Torsions

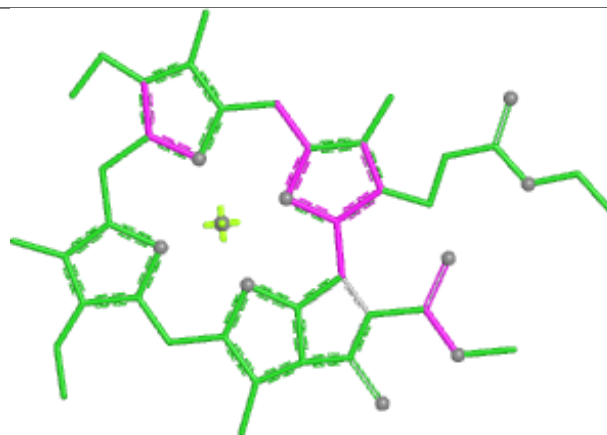


Rings

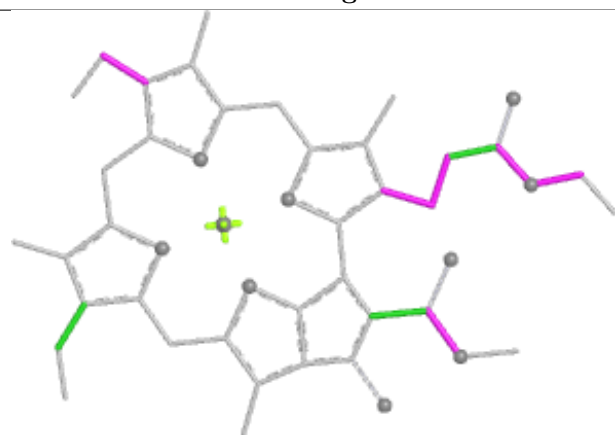
Ligand CLA N 310



Bond lengths



Bond angles

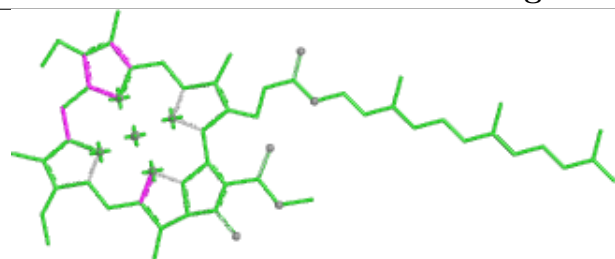


Torsions

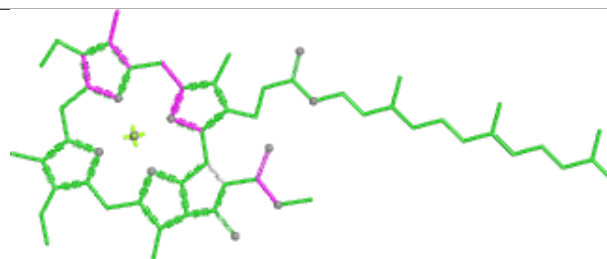


Rings

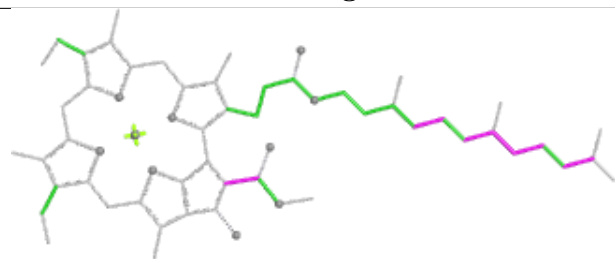
Ligand CLA I 304



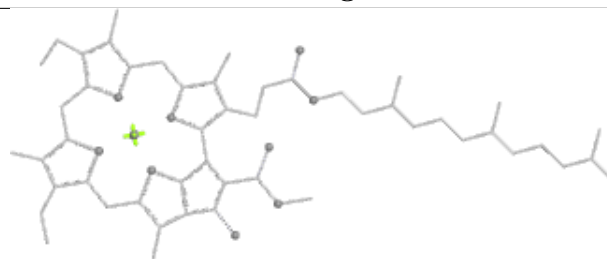
Bond lengths



Bond angles

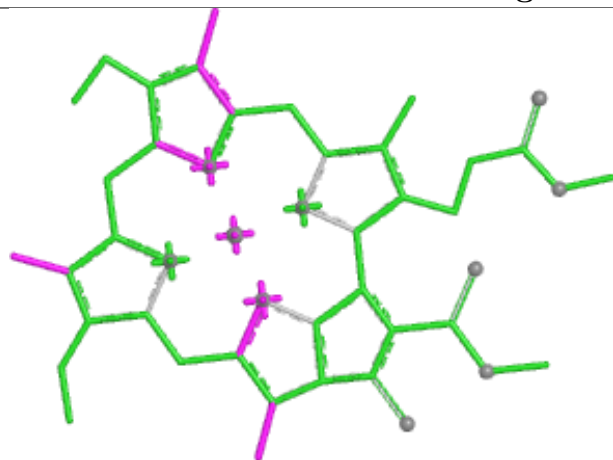


Torsions

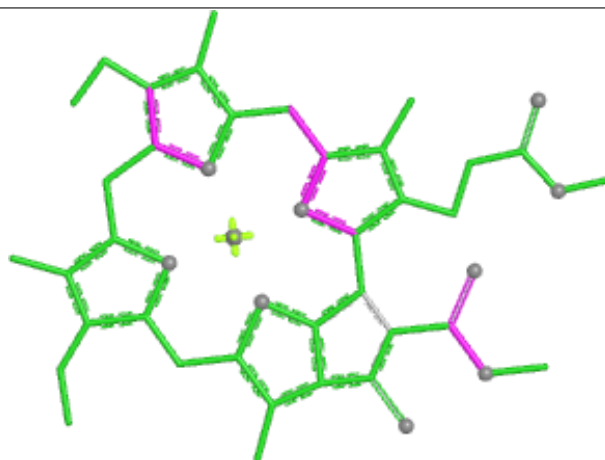


Rings

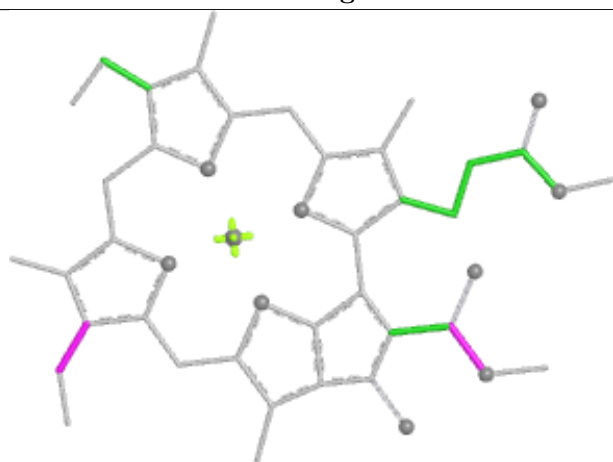
Ligand CLA F 312



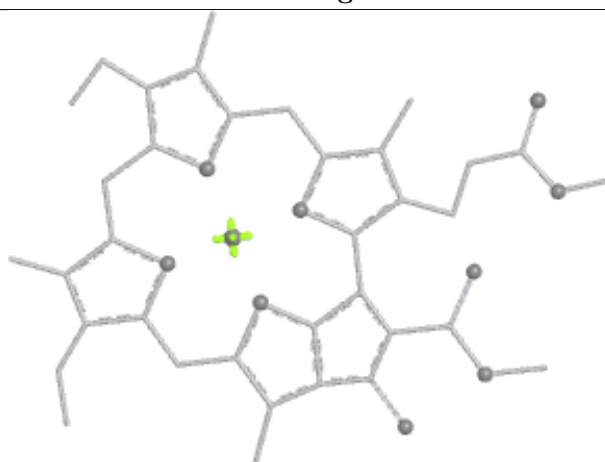
Bond lengths



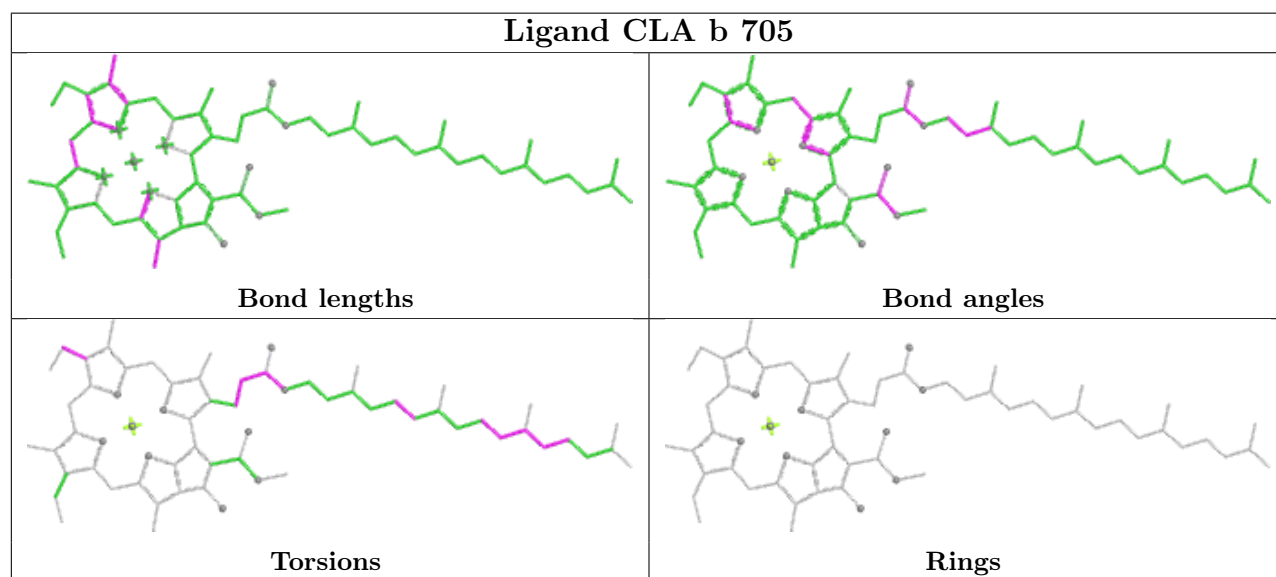
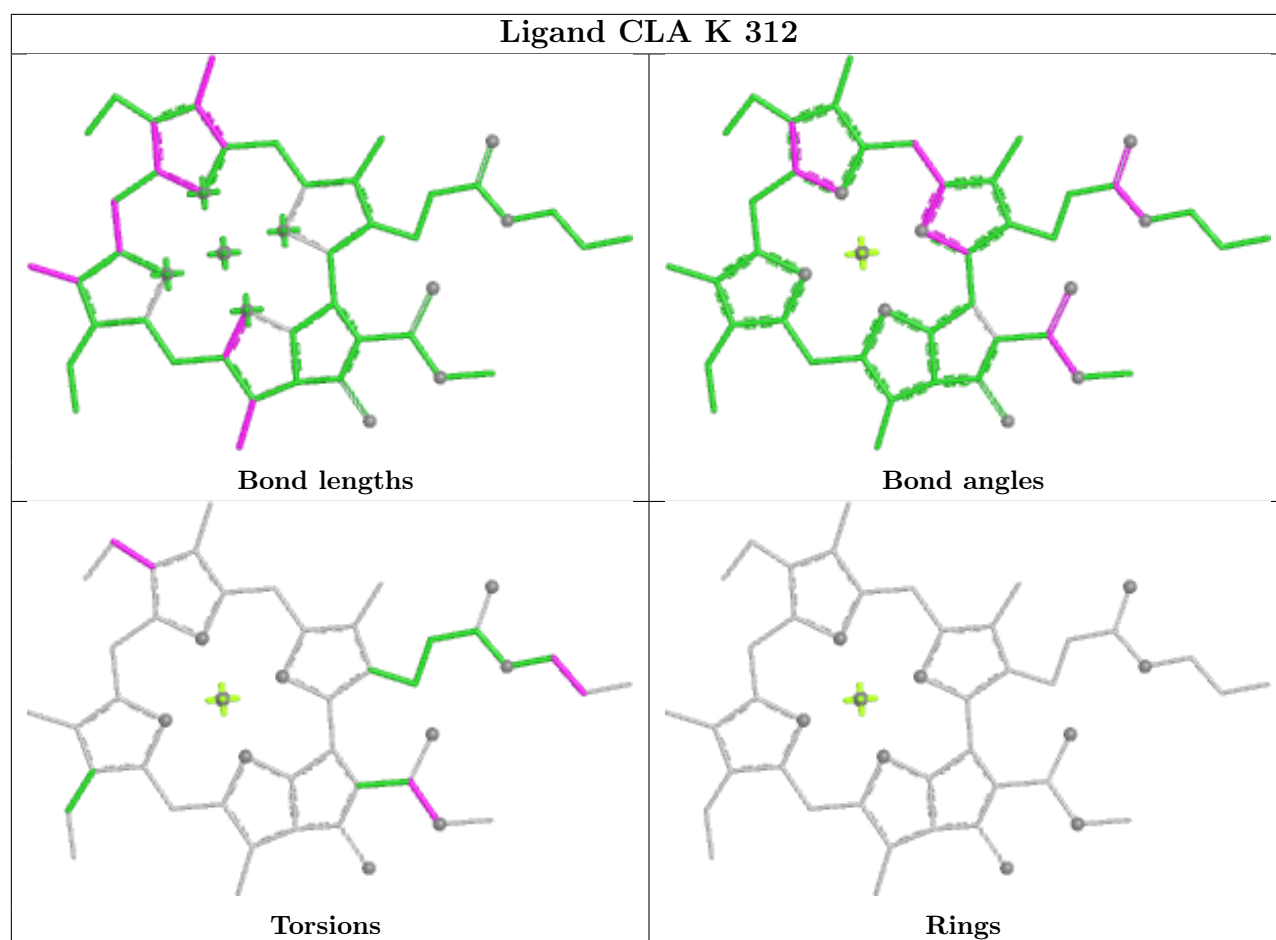
Bond angles

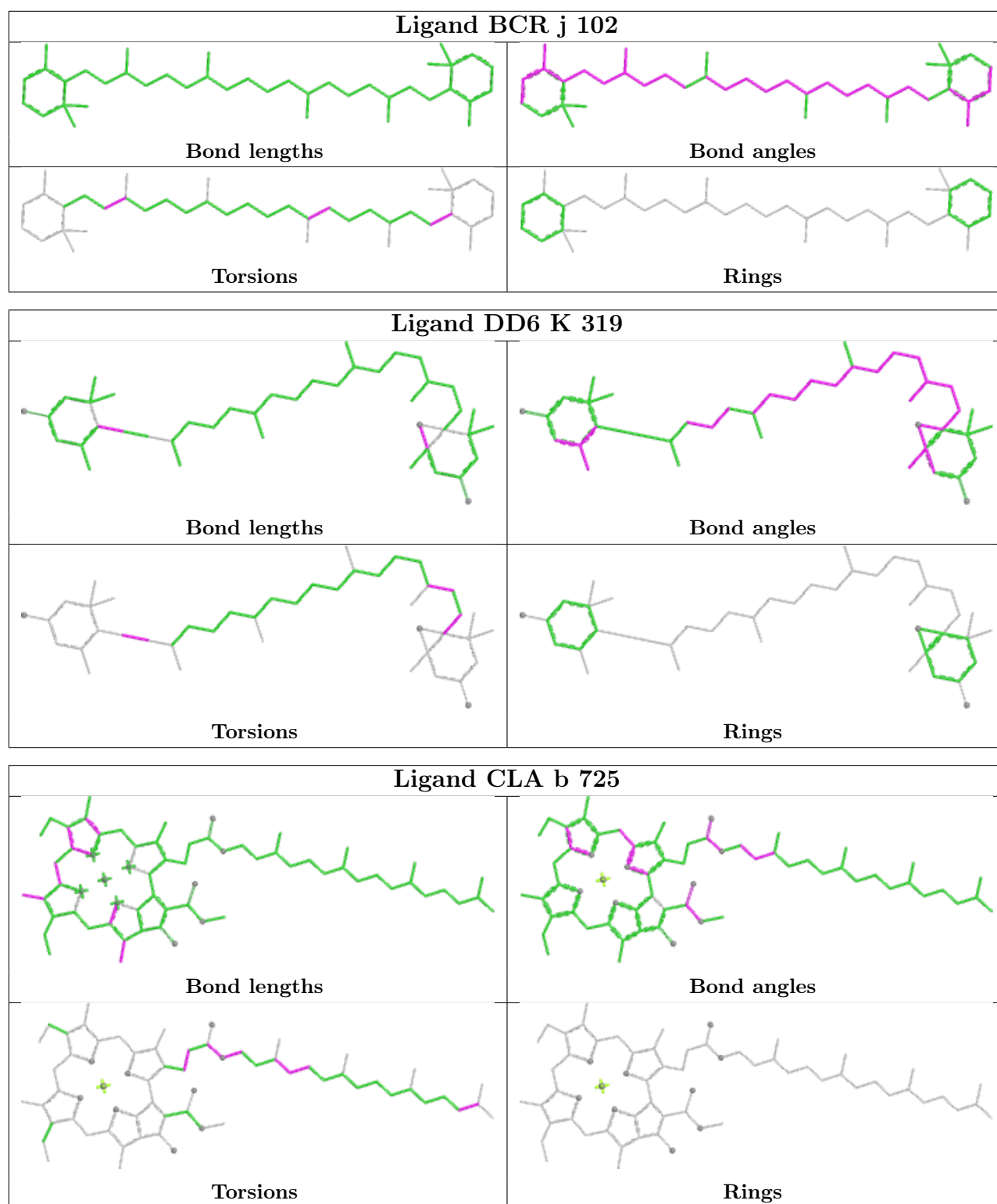


Torsions

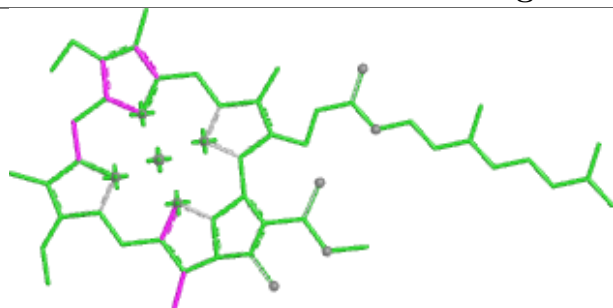


Rings

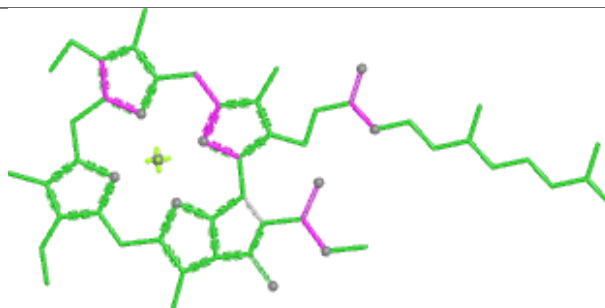




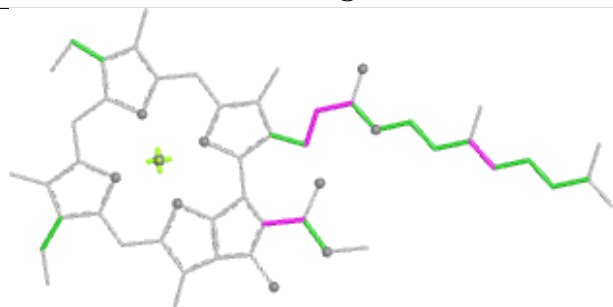
Ligand CLA L 311



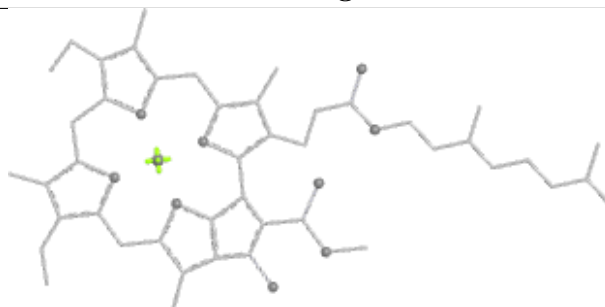
Bond lengths



Bond angles

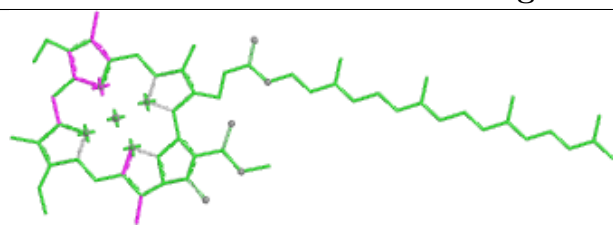


Torsions

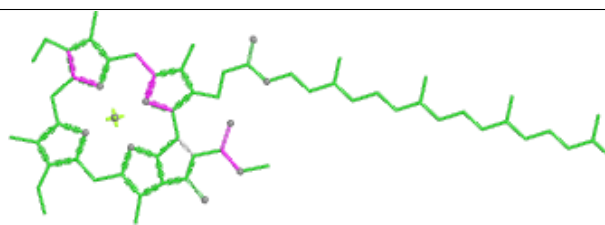


Rings

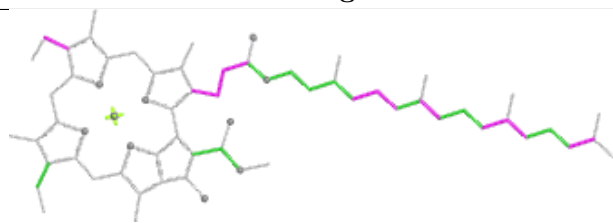
Ligand CLA b 724



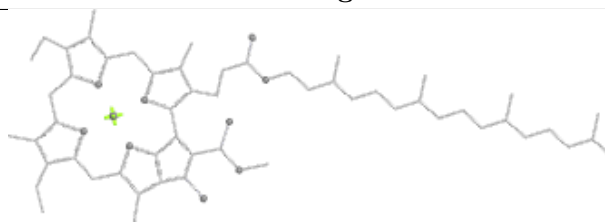
Bond lengths



Bond angles

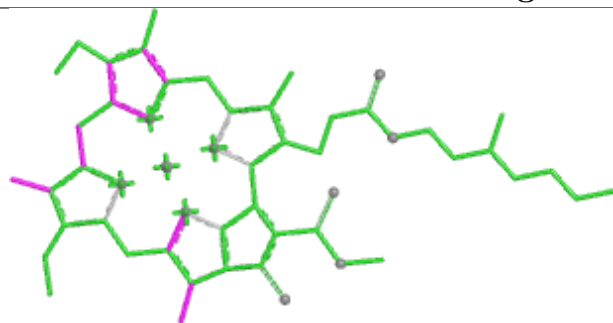


Torsions

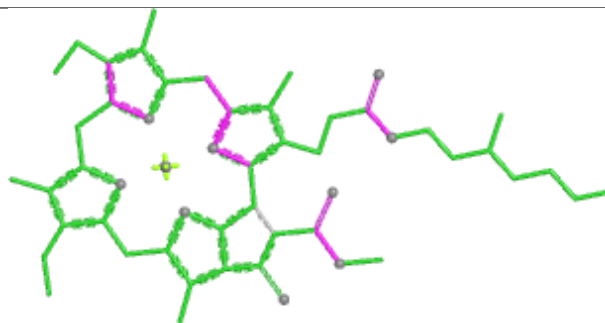


Rings

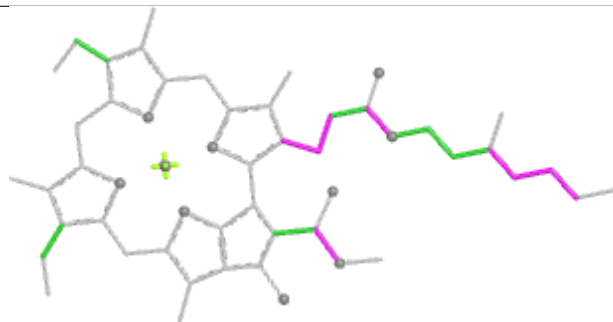
Ligand CLA b 720



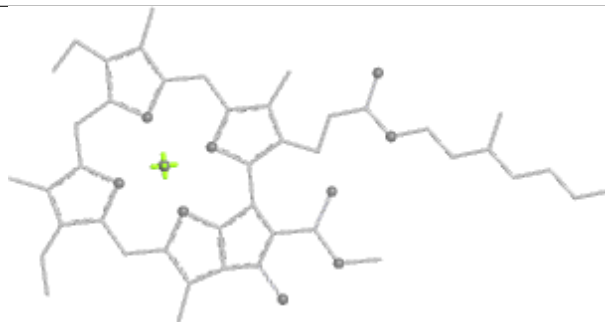
Bond lengths



Bond angles

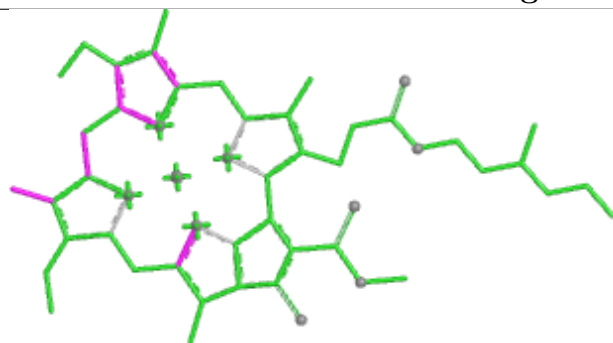


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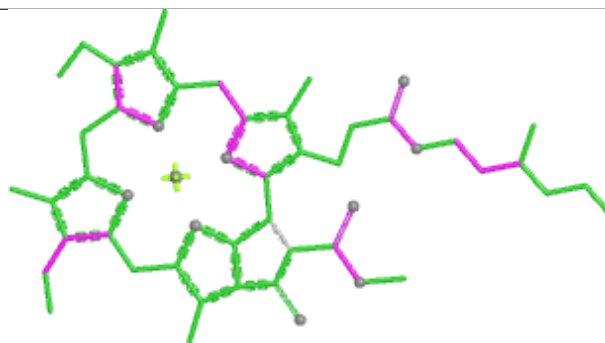


Rings

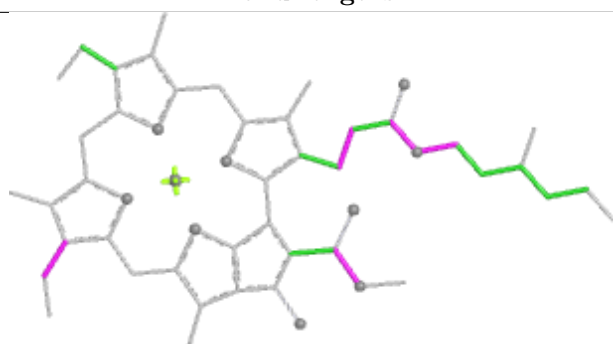
Ligand CLA I 321



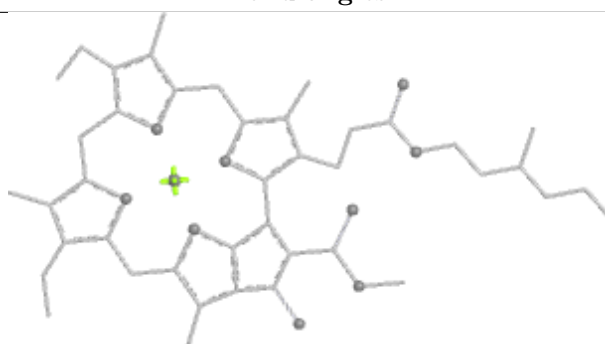
Bond lengths



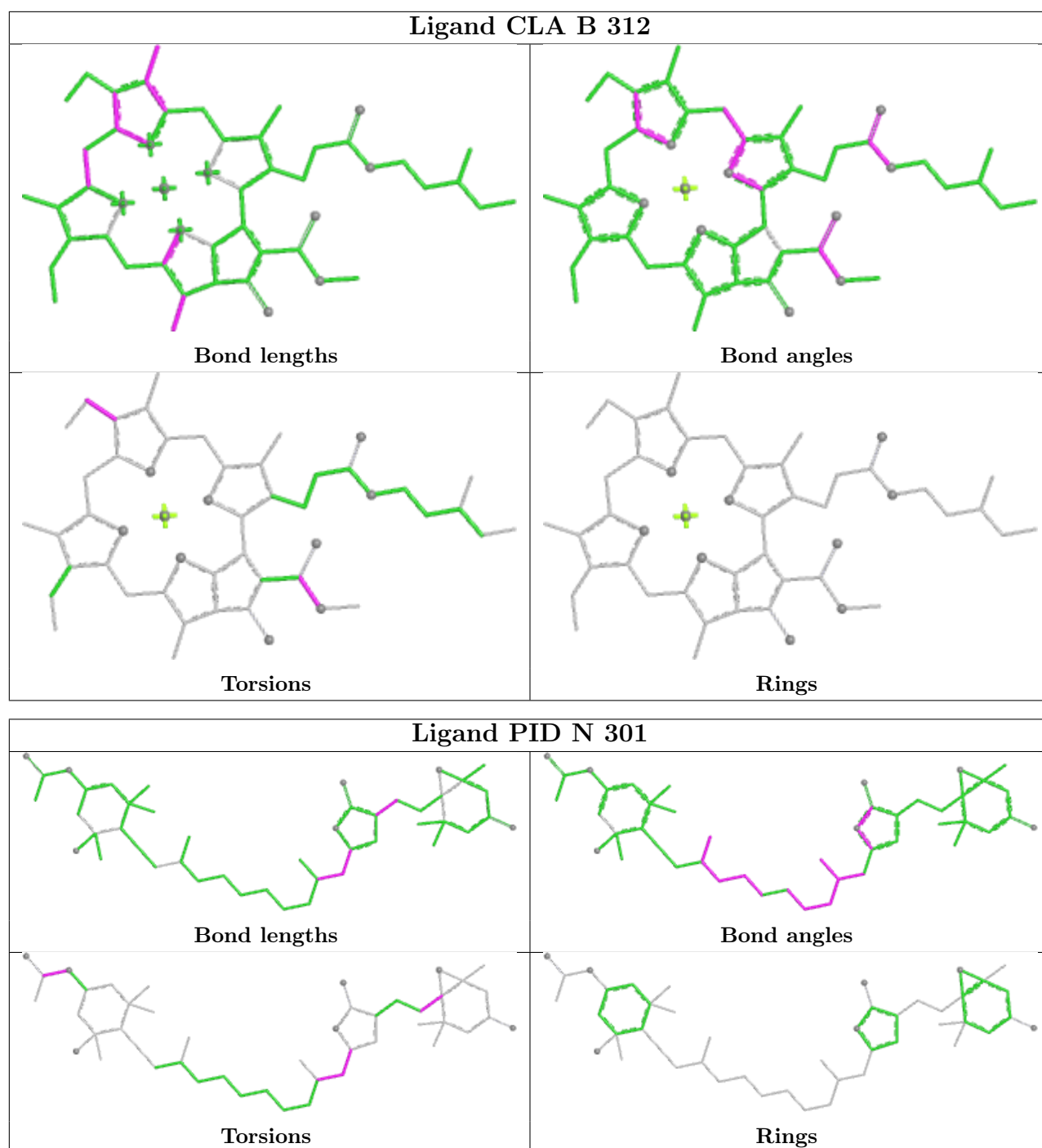
Bond angles

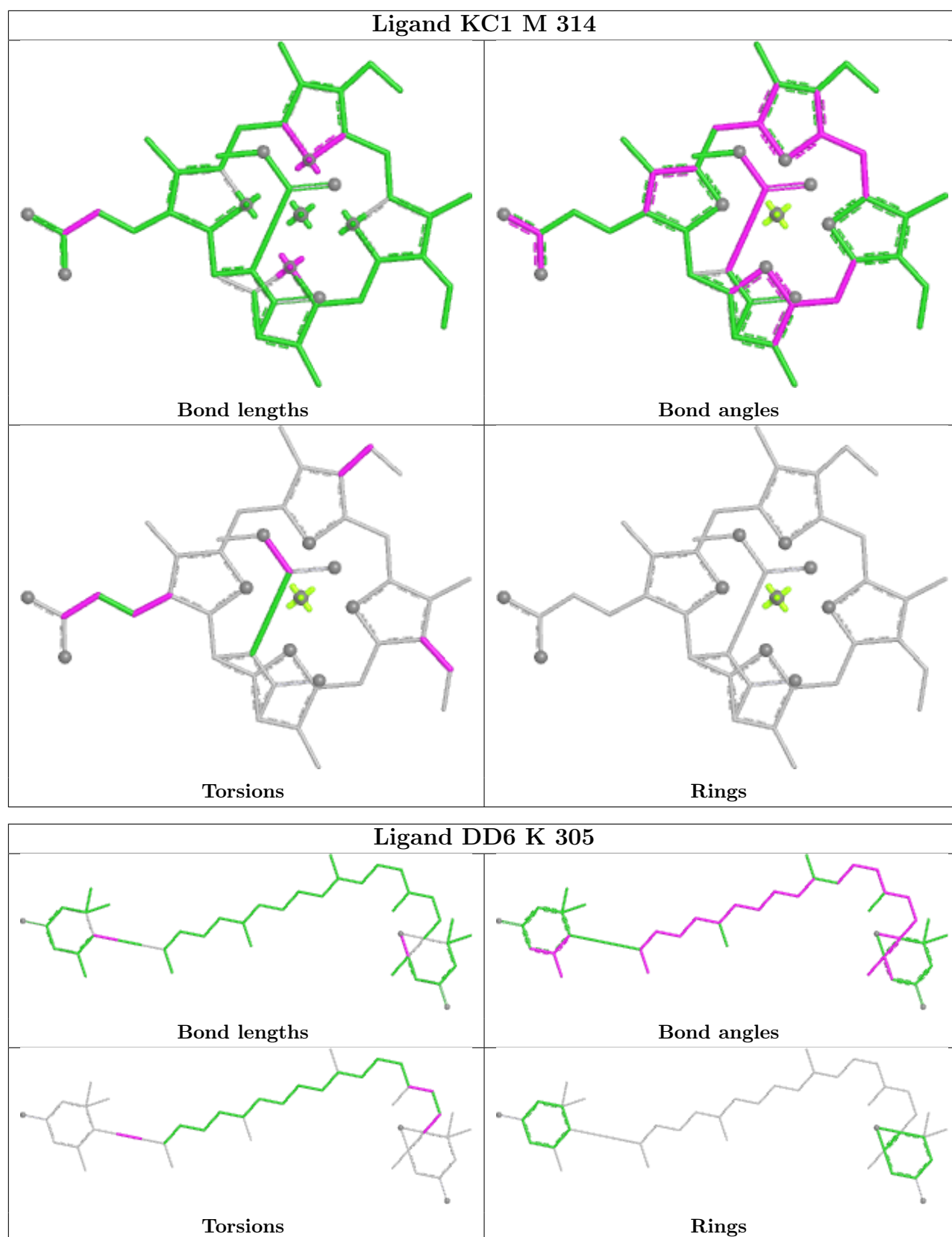


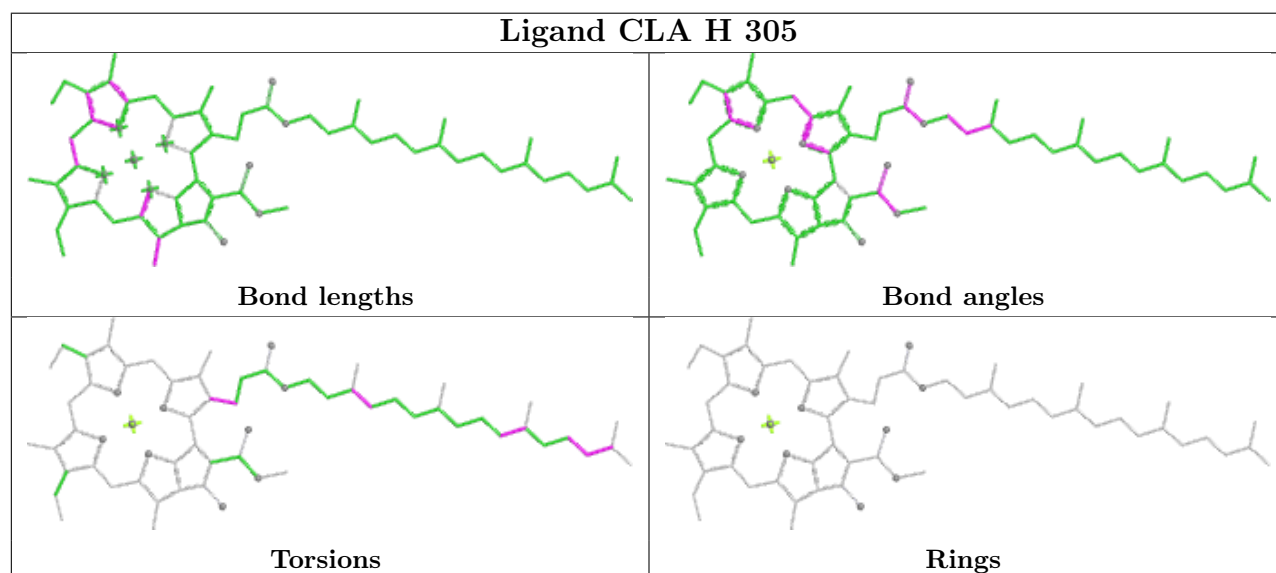
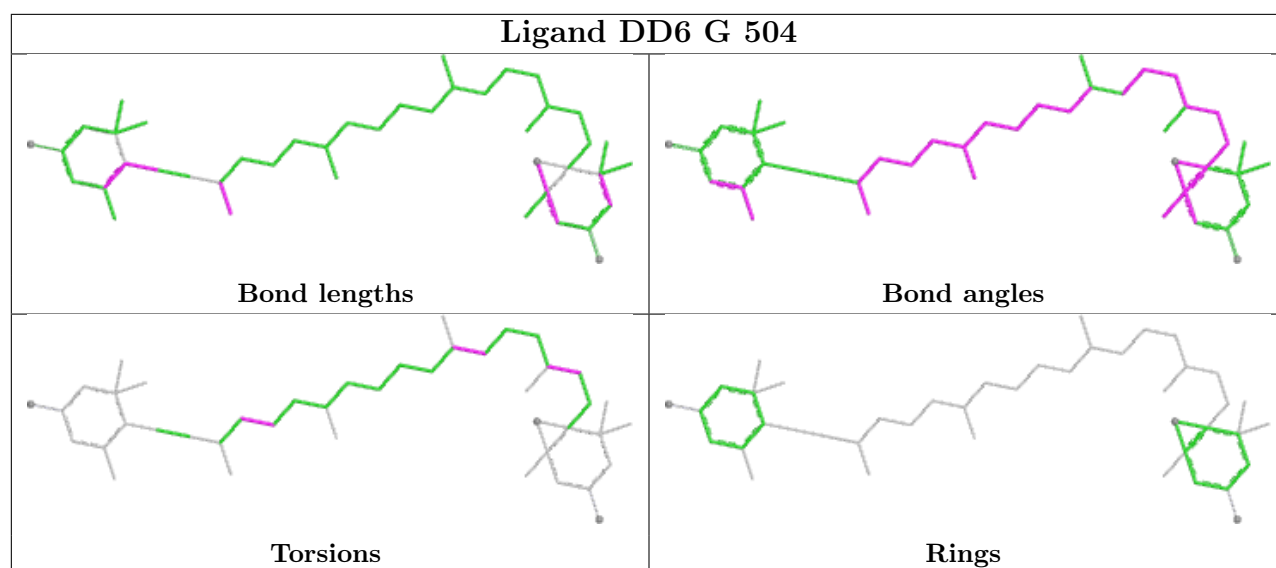
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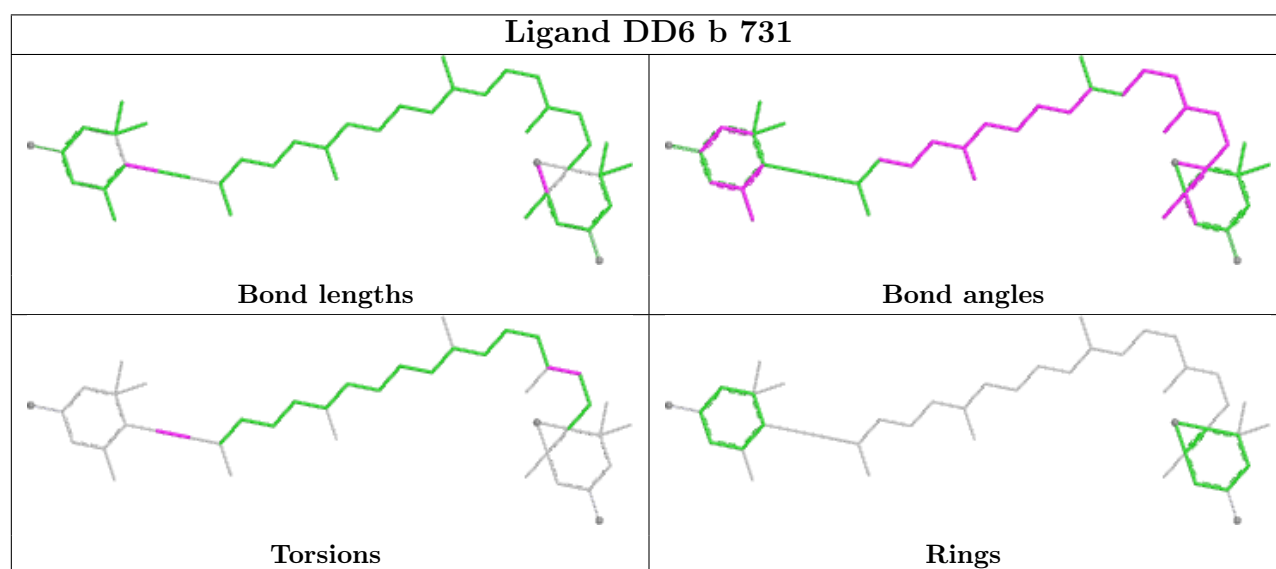
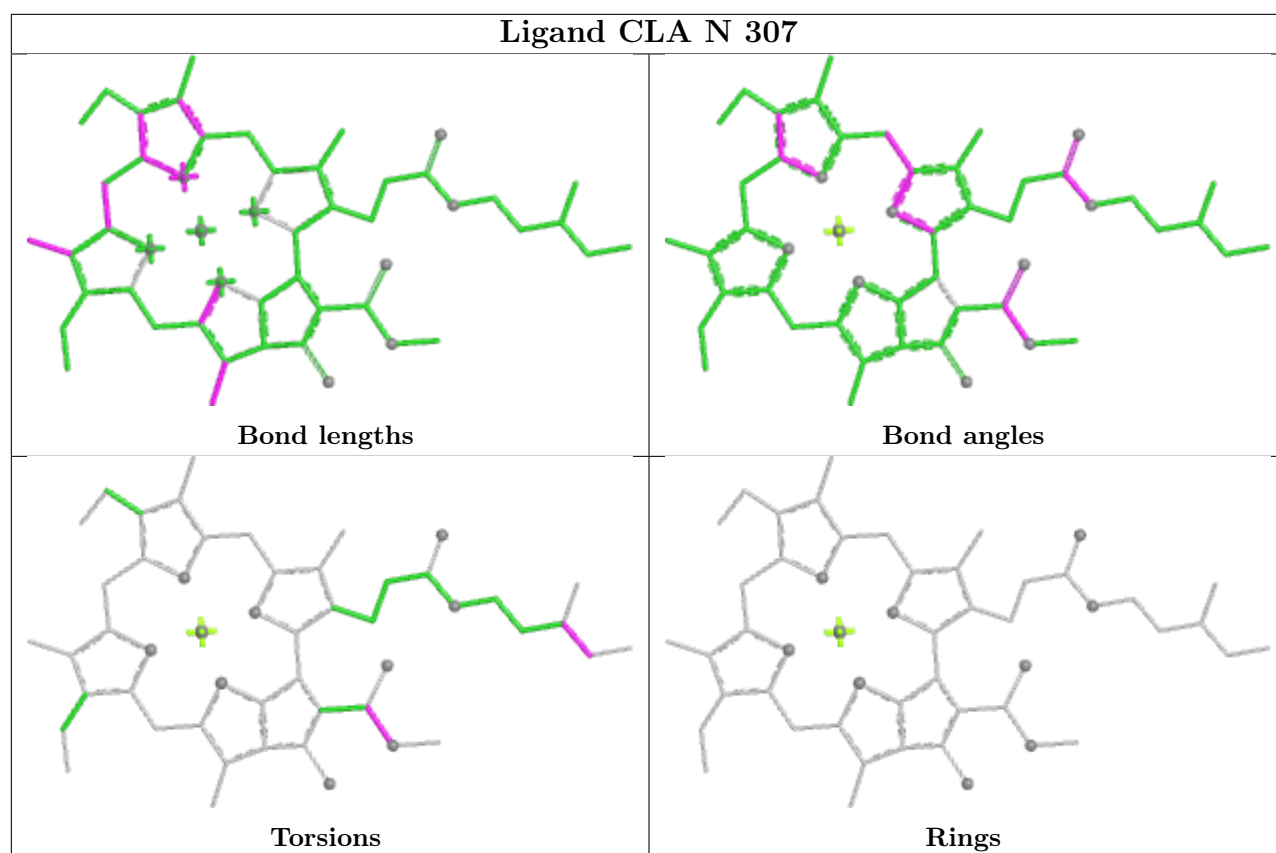


Rings

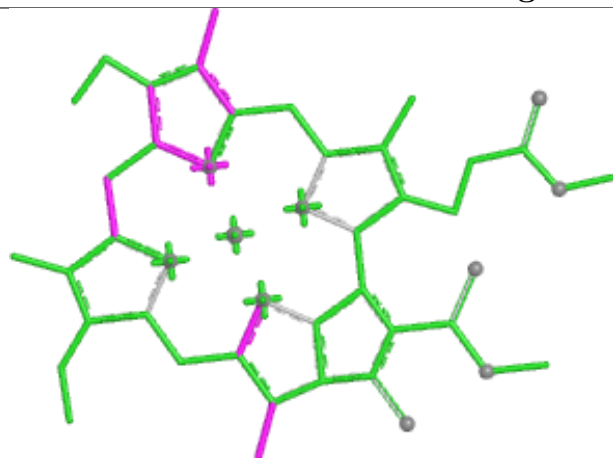




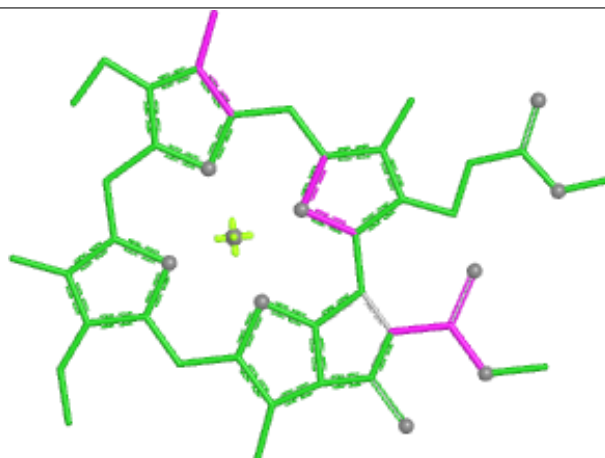




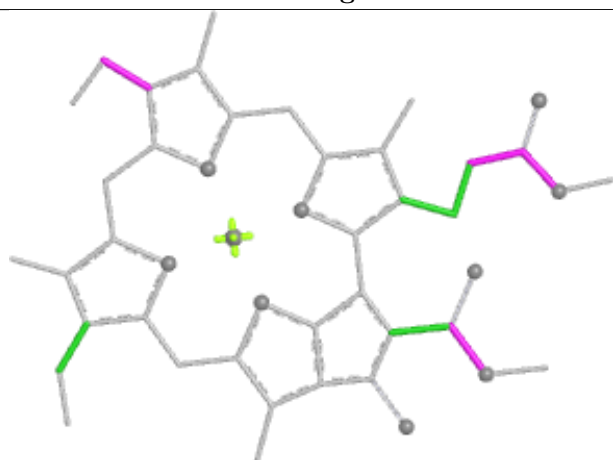
Ligand CLA J 310



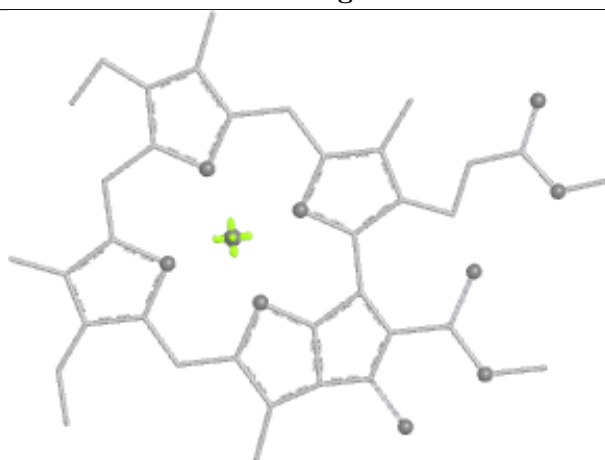
Bond lengths



Bond angles

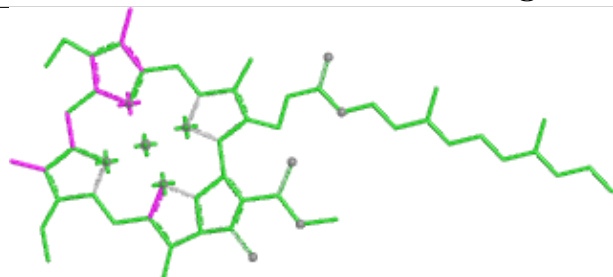


Torsions

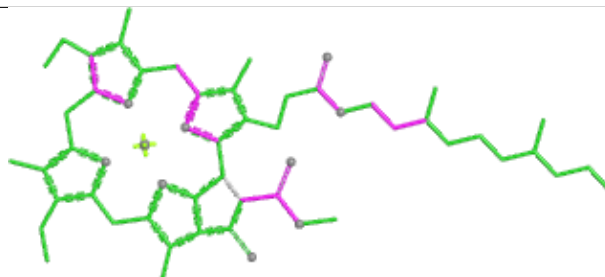


Rings

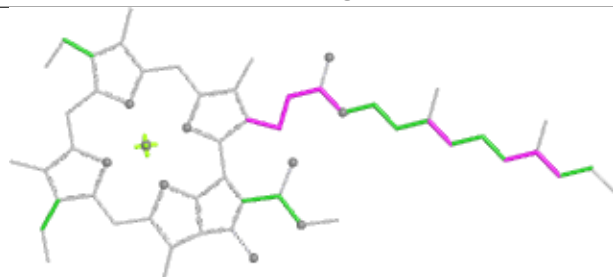
Ligand CLA a 717



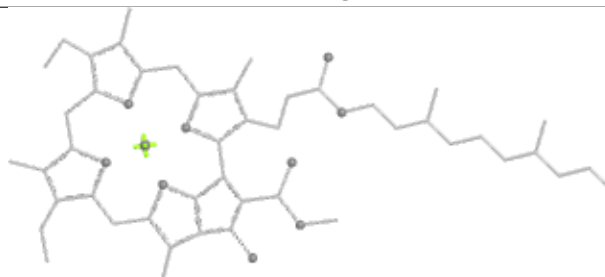
Bond lengths



Bond angles

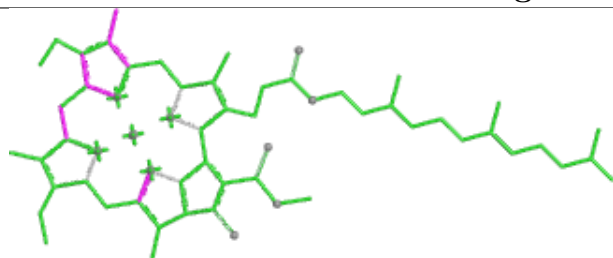


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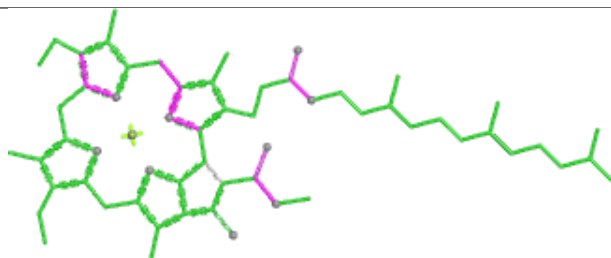


Rings

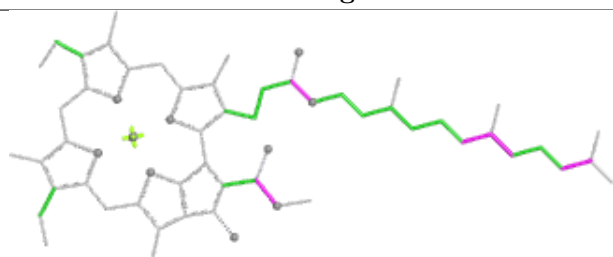
Ligand CLA B 301



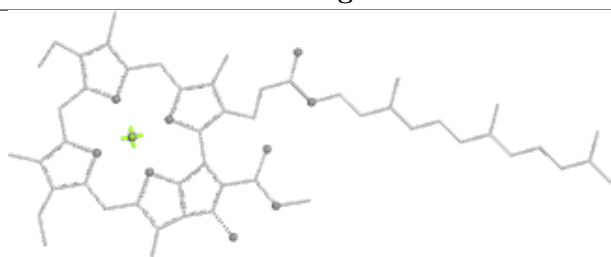
Bond lengths



Bond angles

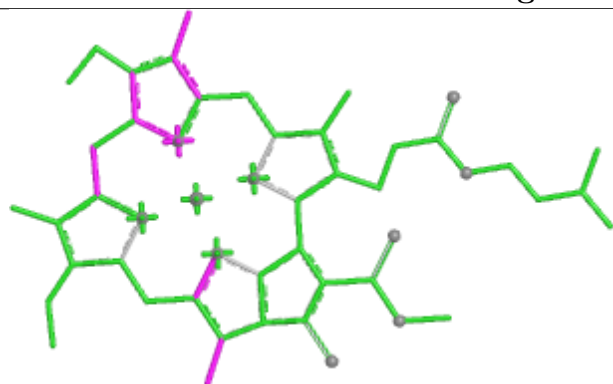


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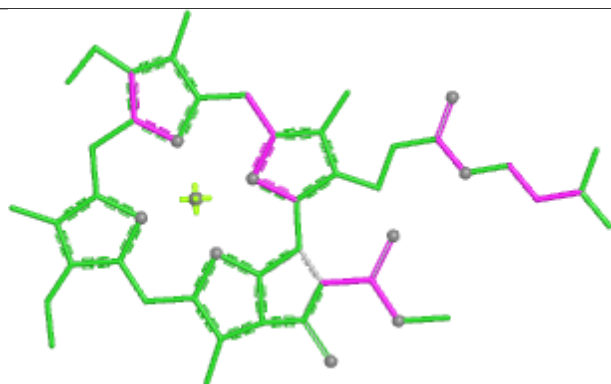


Rings

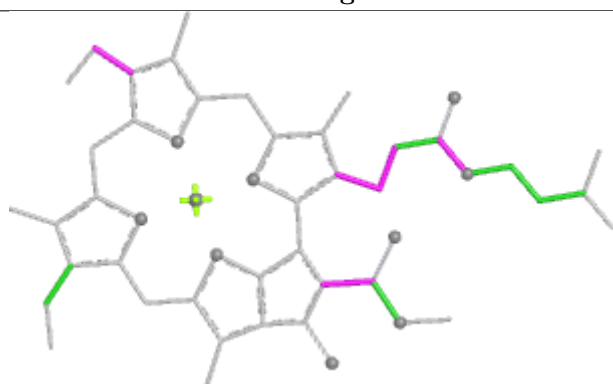
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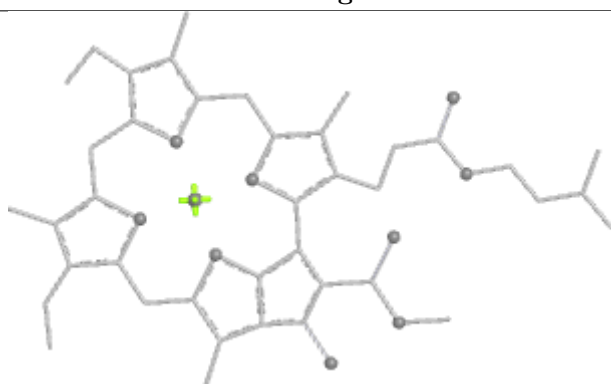
Bond lengths



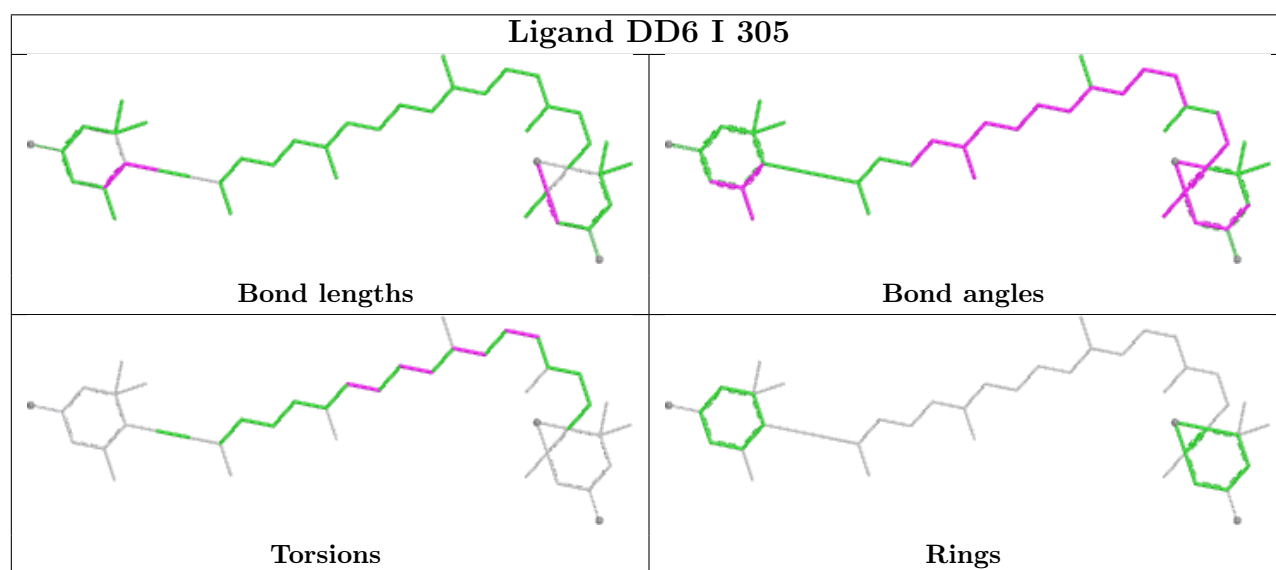
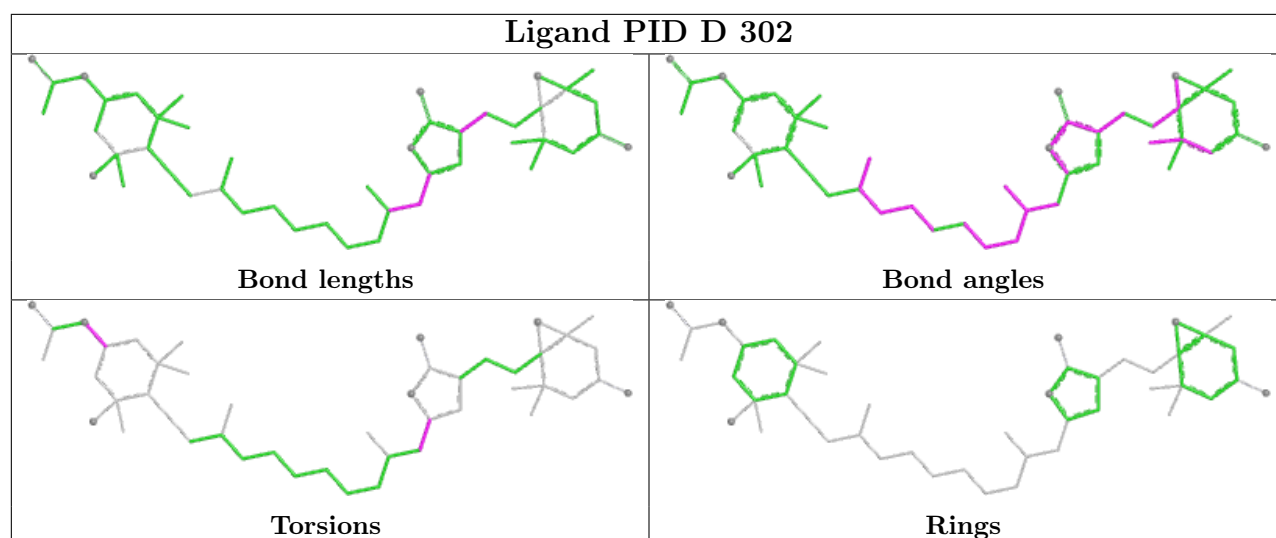
Bond angles



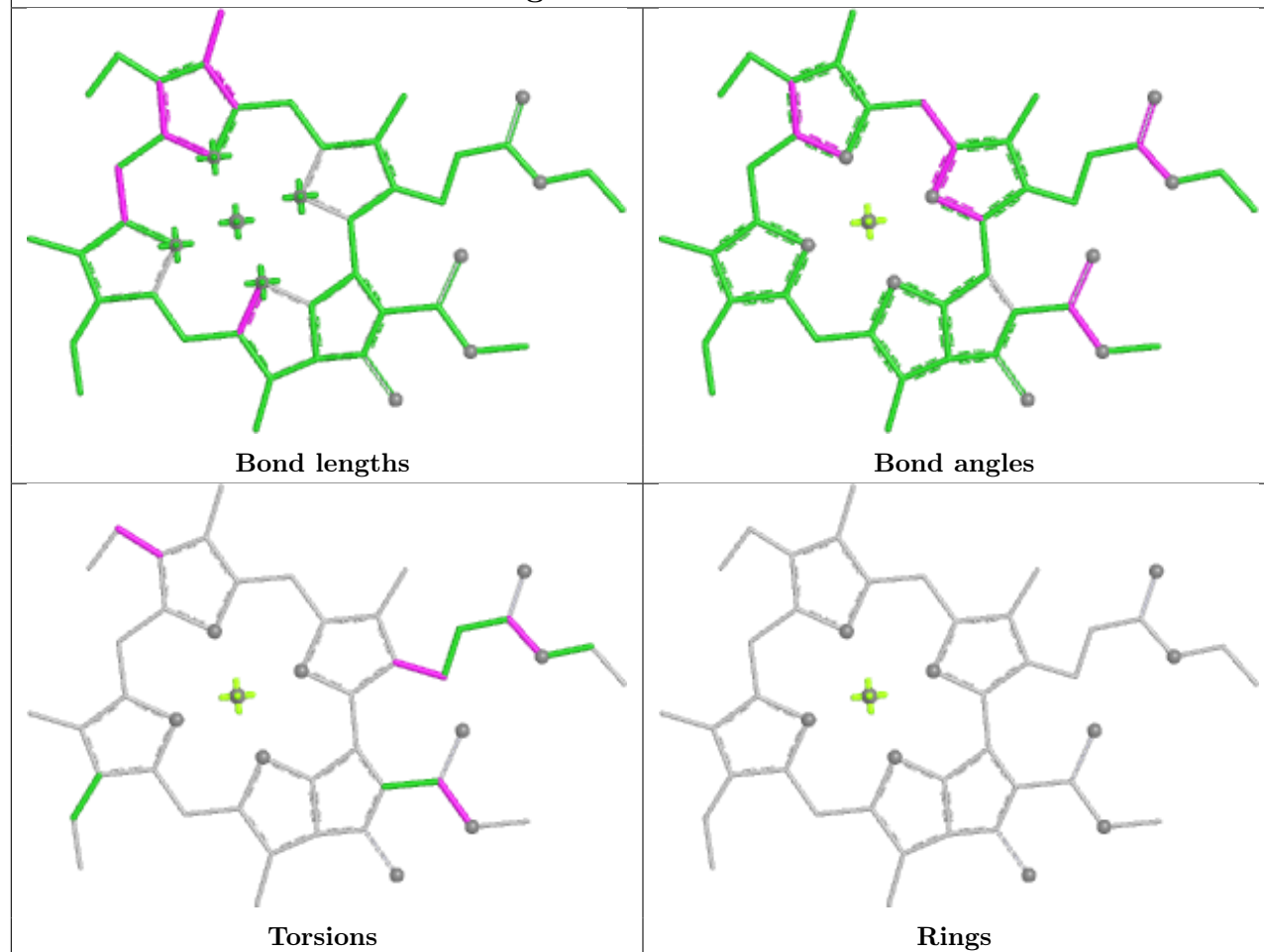
Torsions



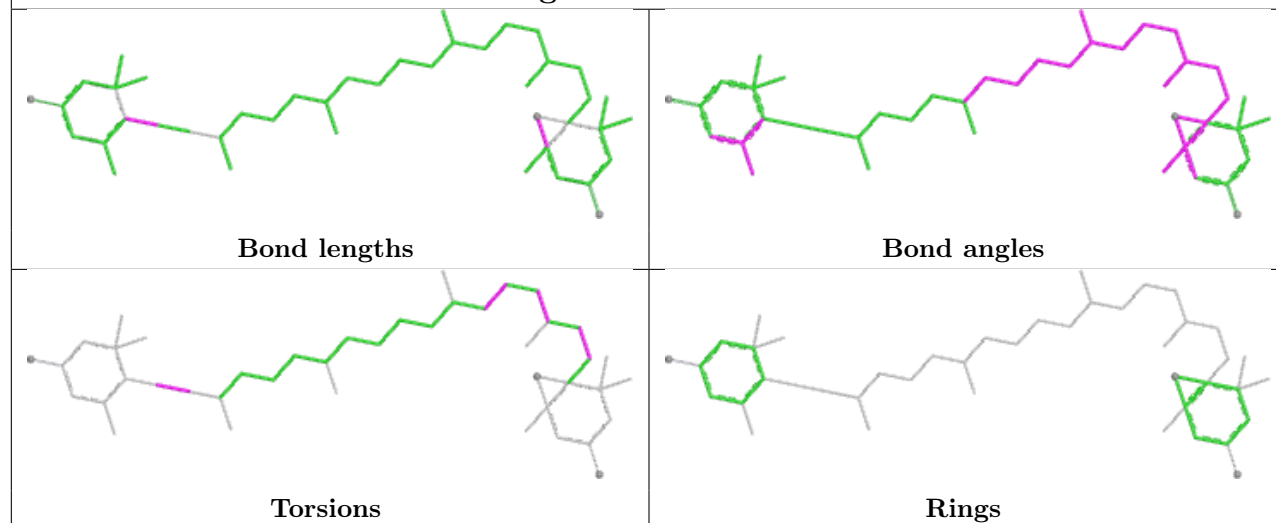
Rings

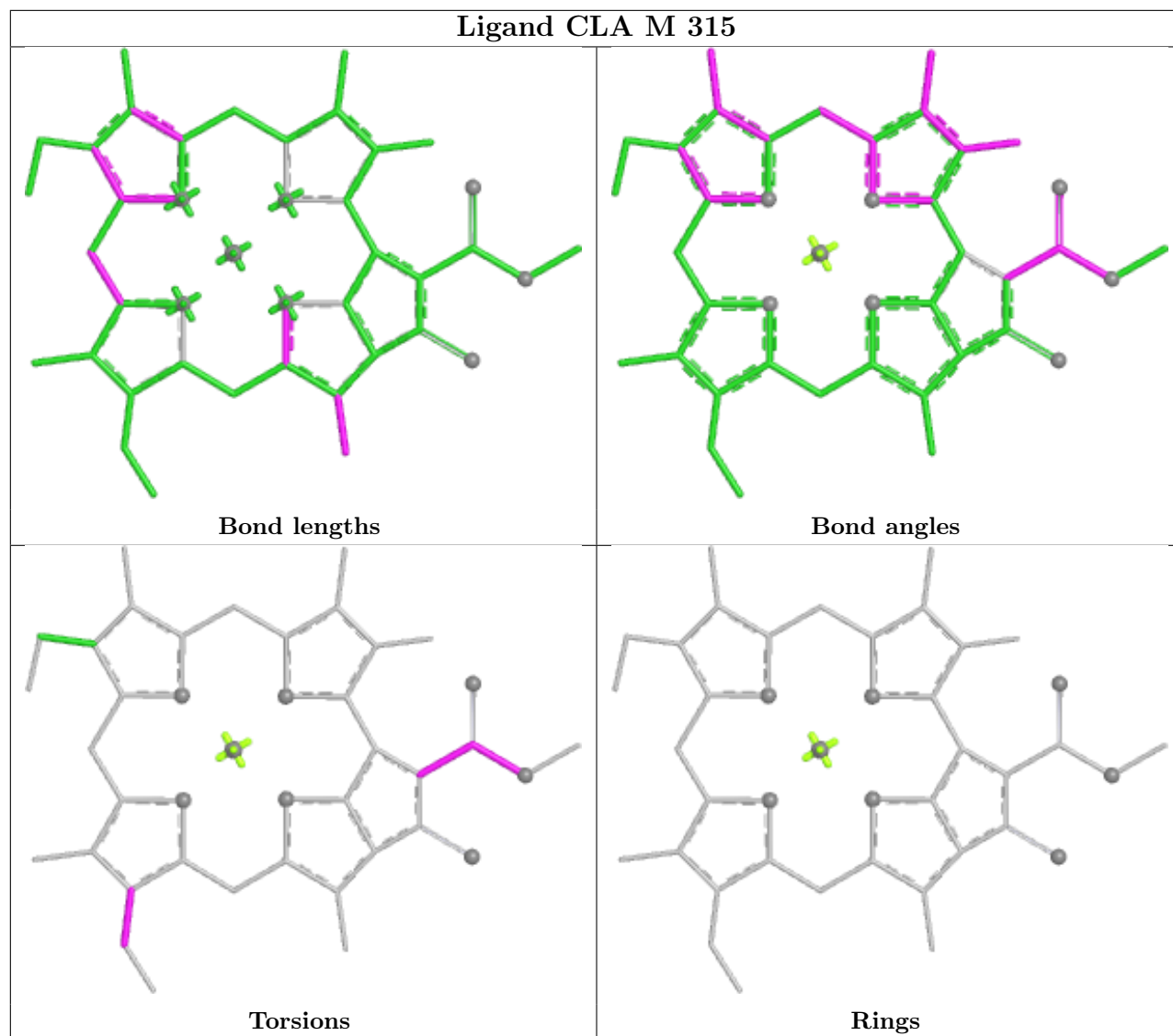


Ligand CLA H 309

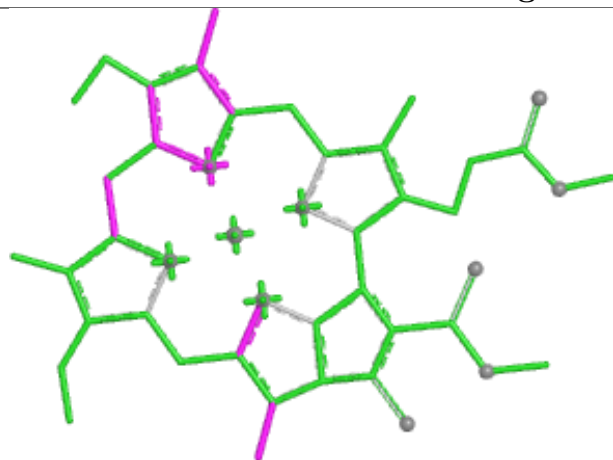


Ligand DD6 I 302

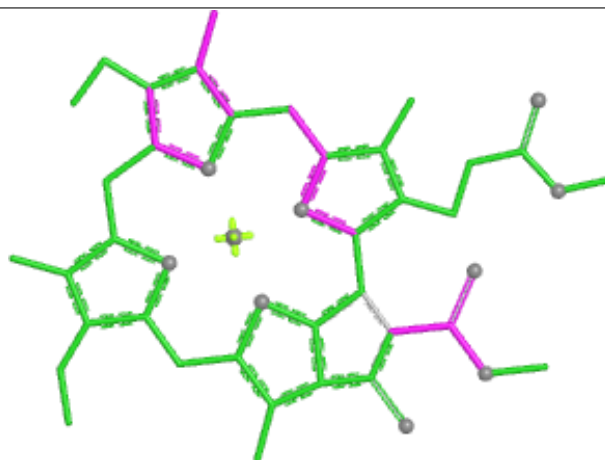




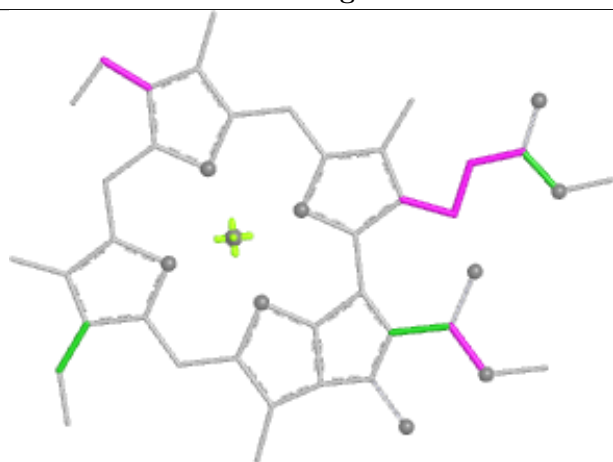
Ligand CLA J 308



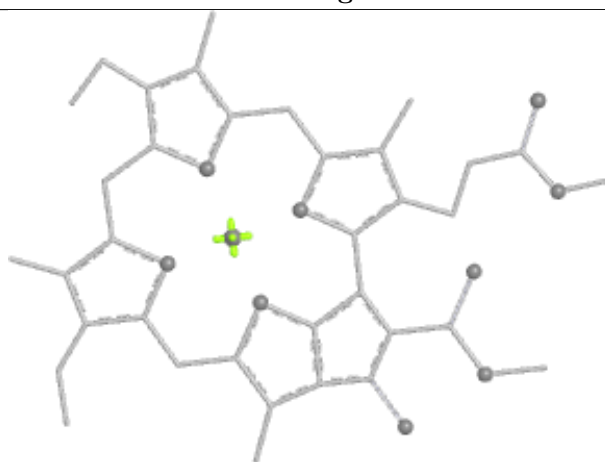
Bond lengths



Bond angles

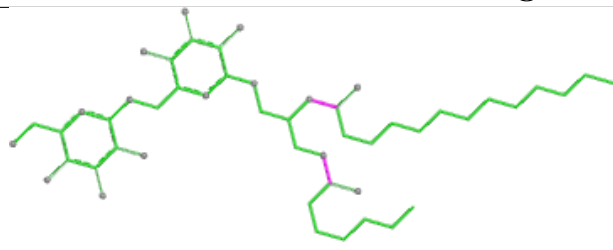


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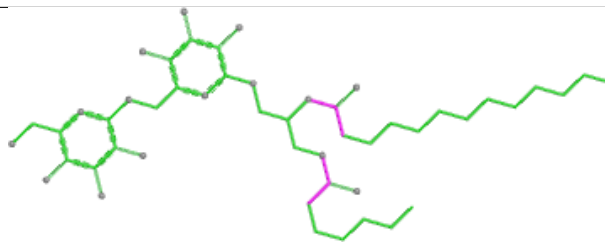


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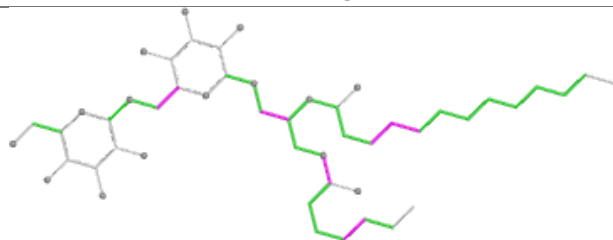
Ligand DGD 1 301



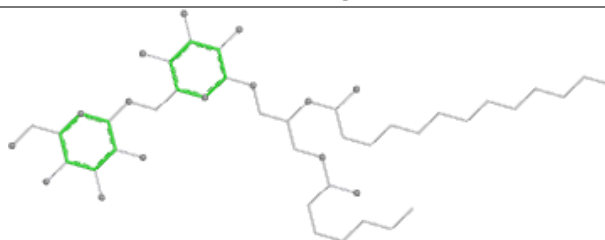
Bond lengths



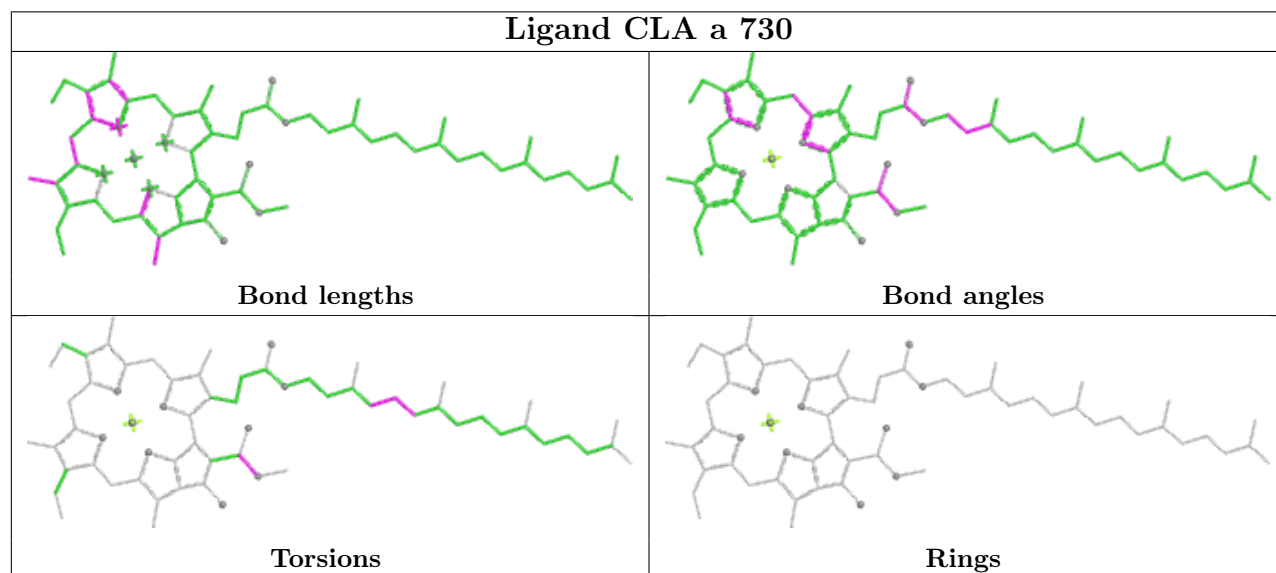
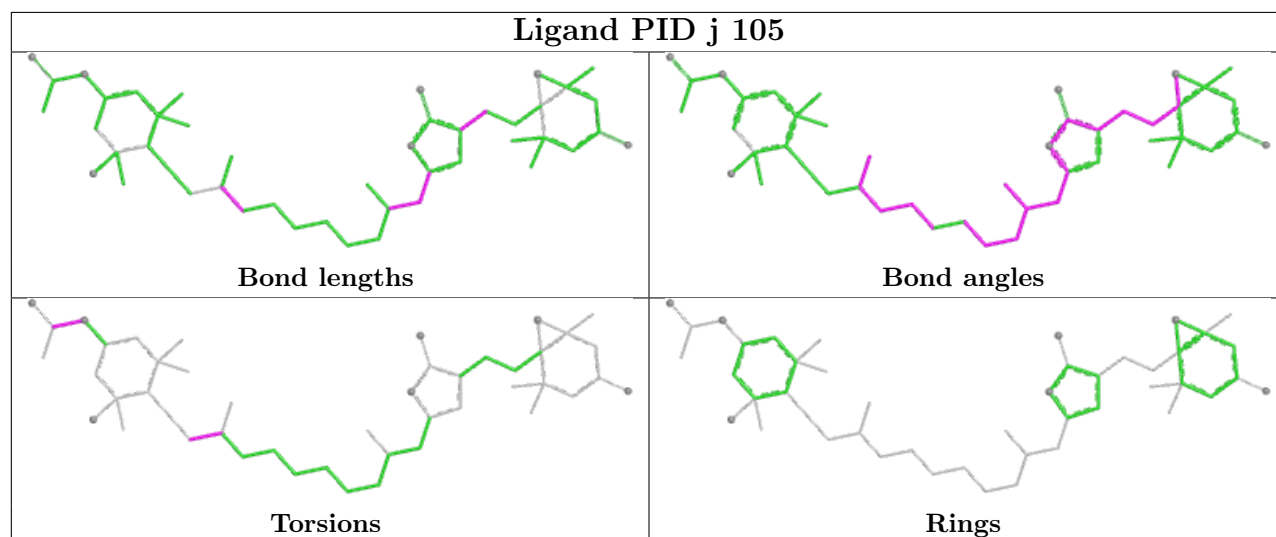
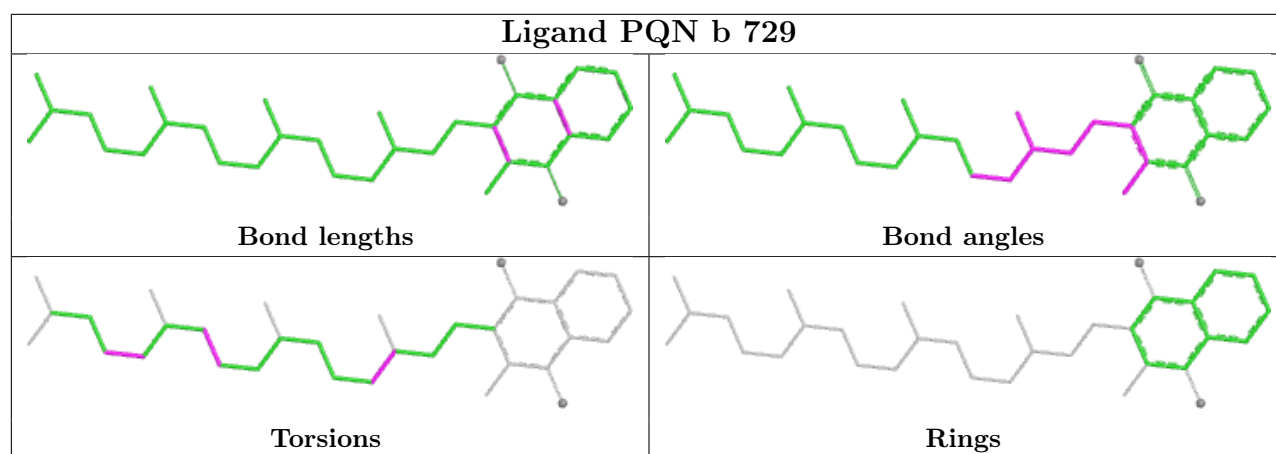
Bond angles



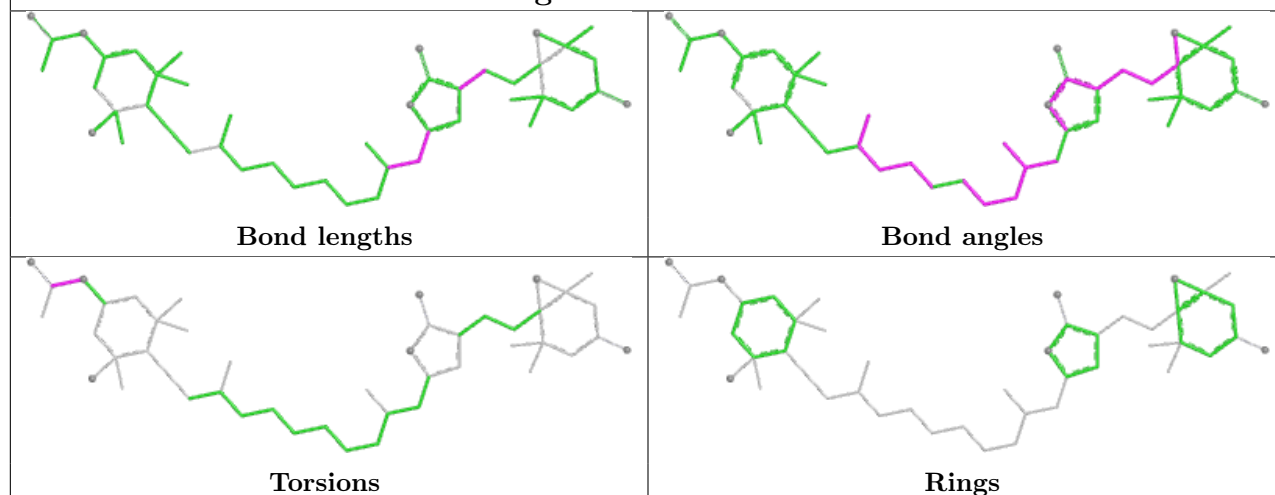
Torsions



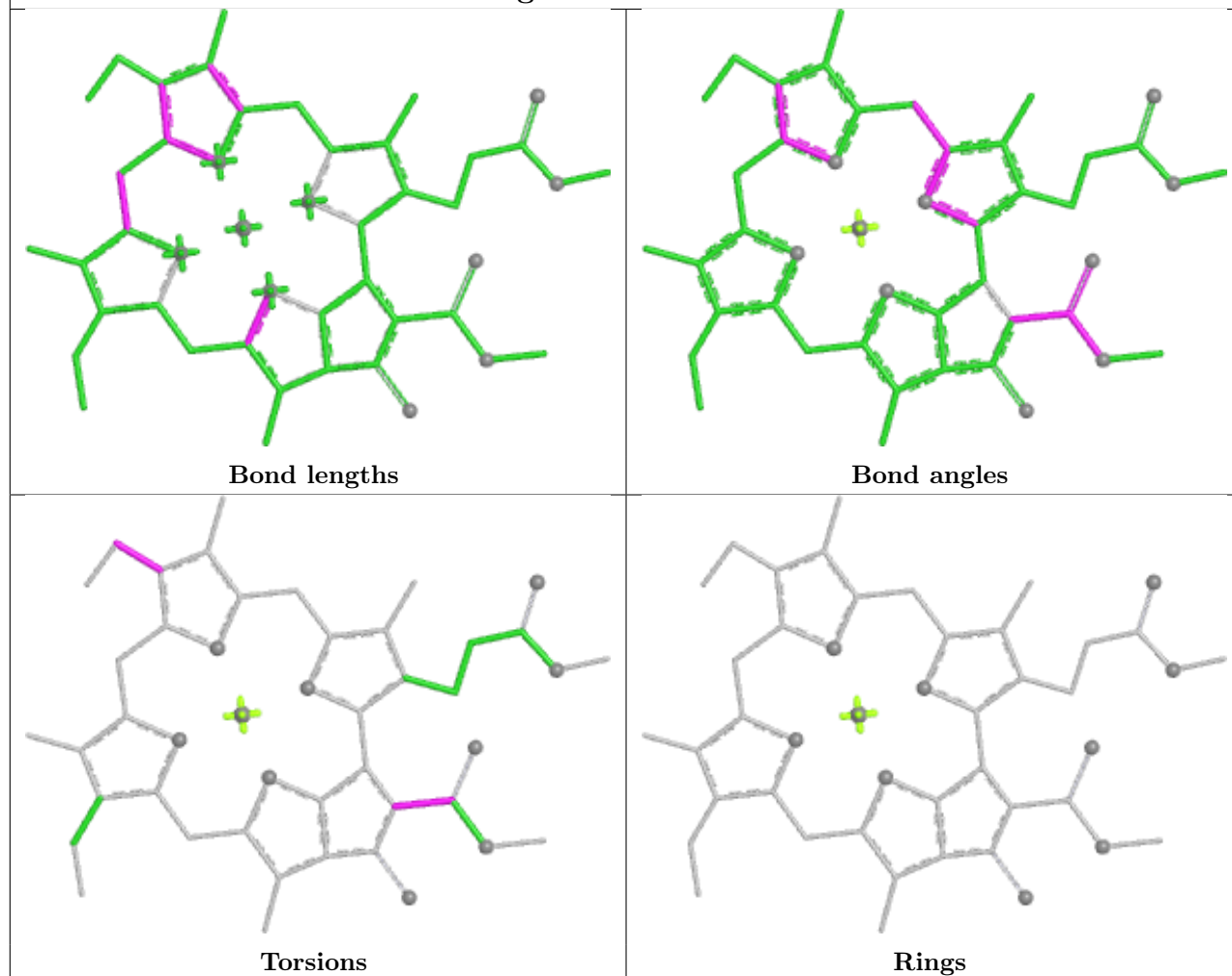
Rings

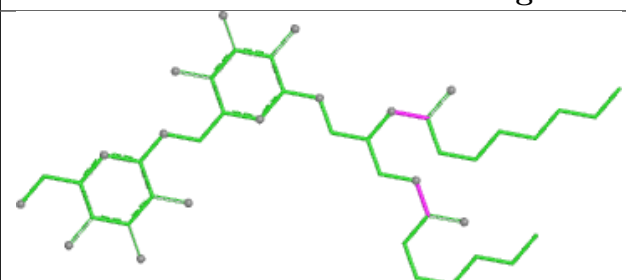
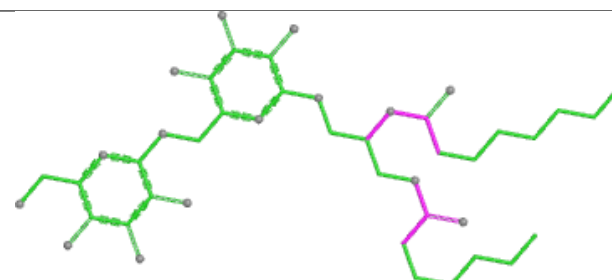
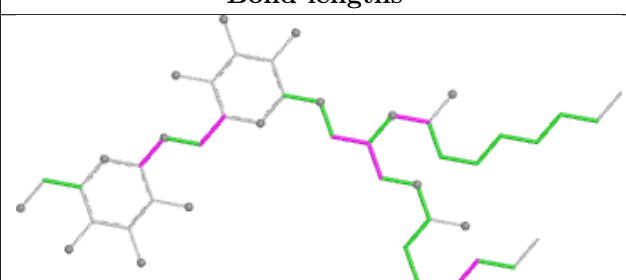
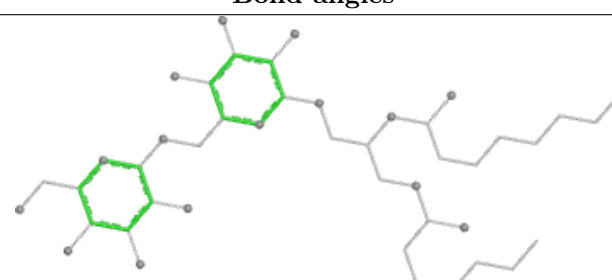


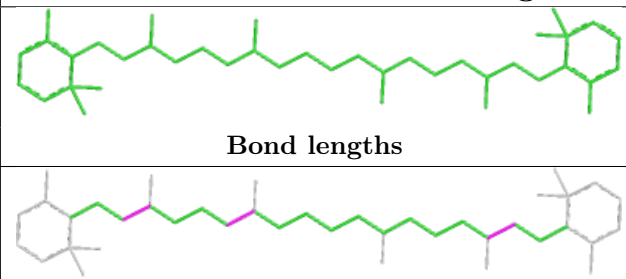
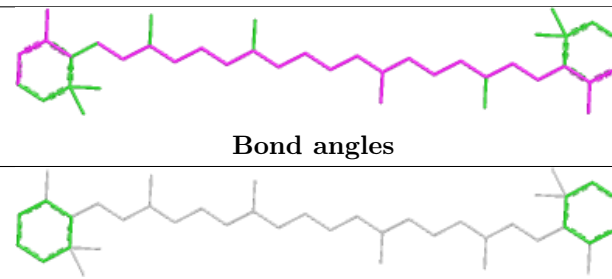
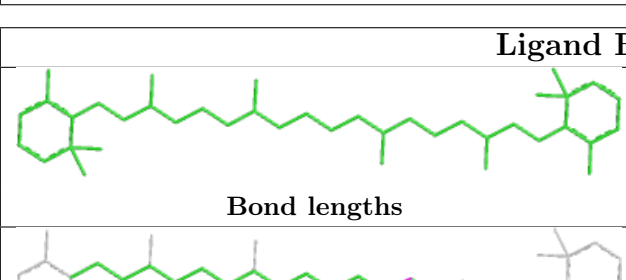
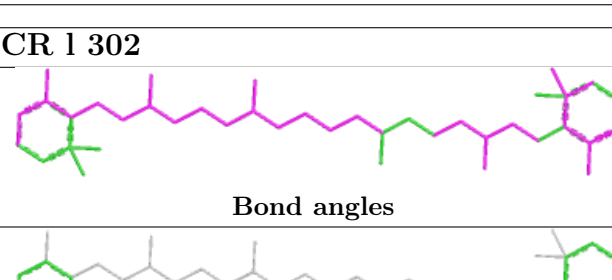
Ligand PID H 302

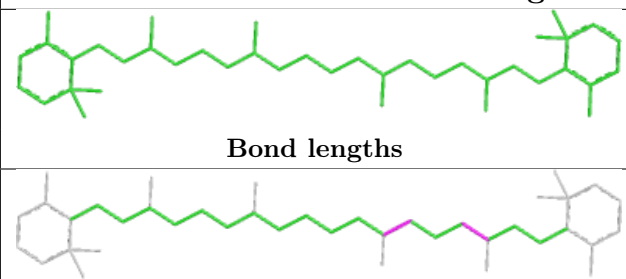
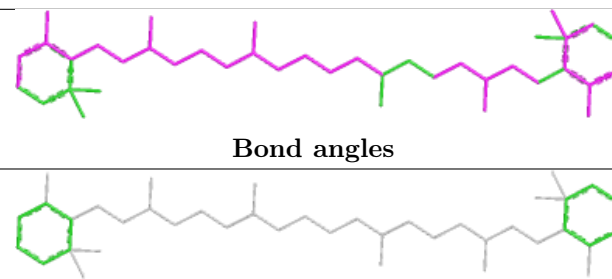
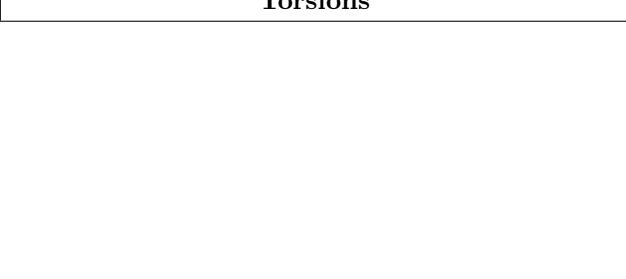
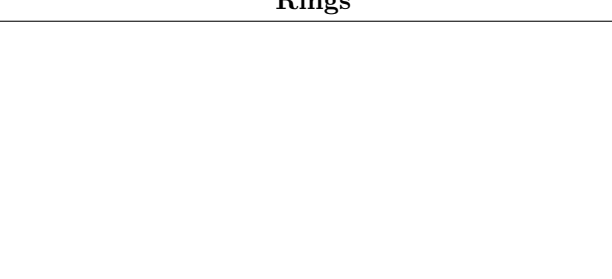


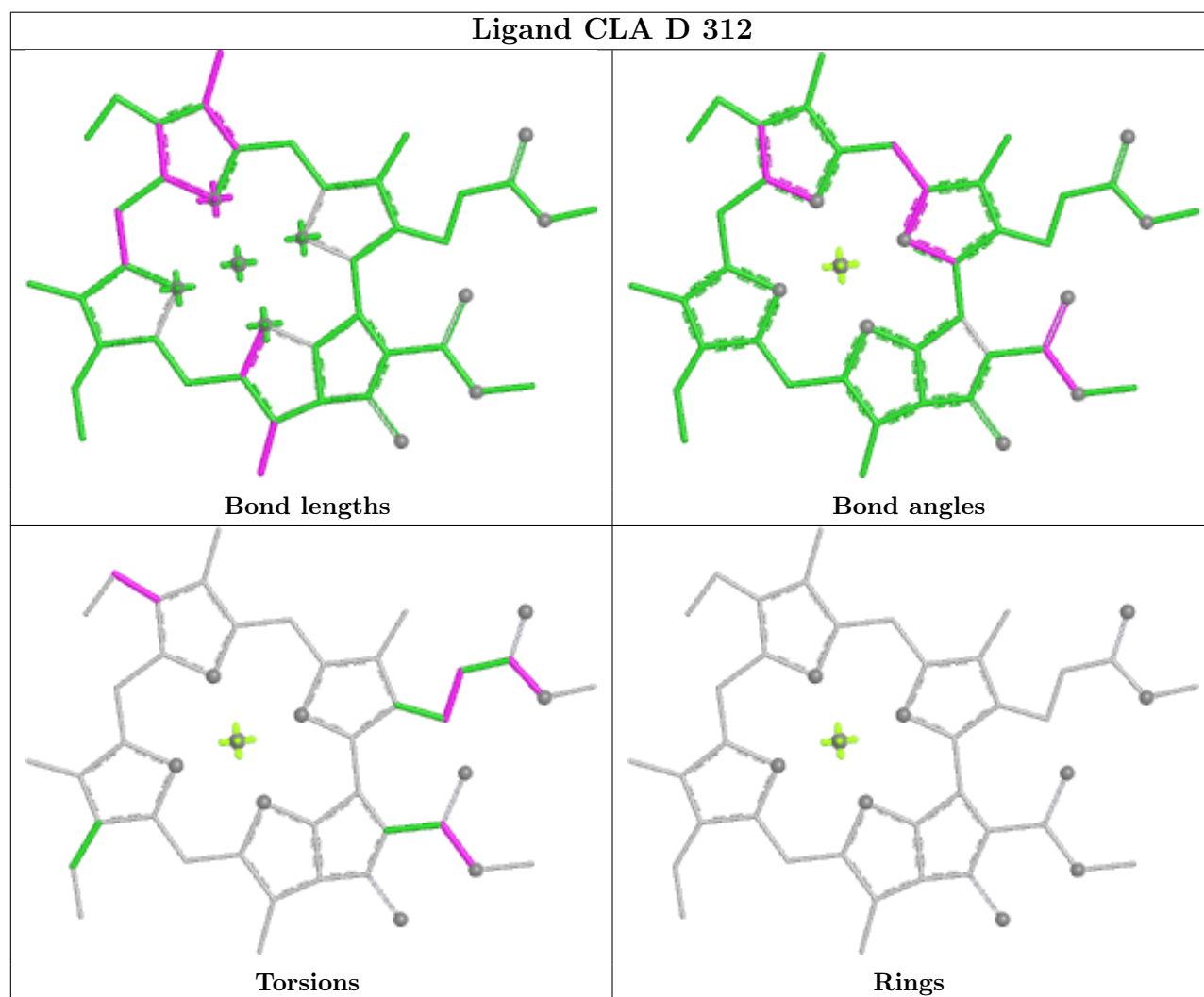
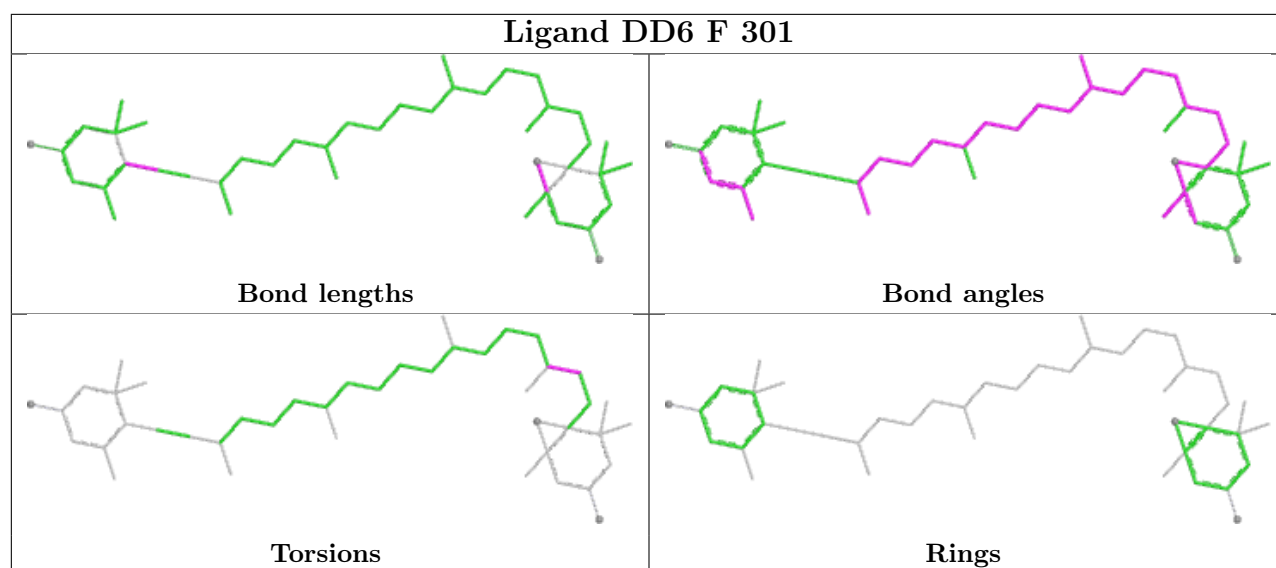
Ligand CLA a 738



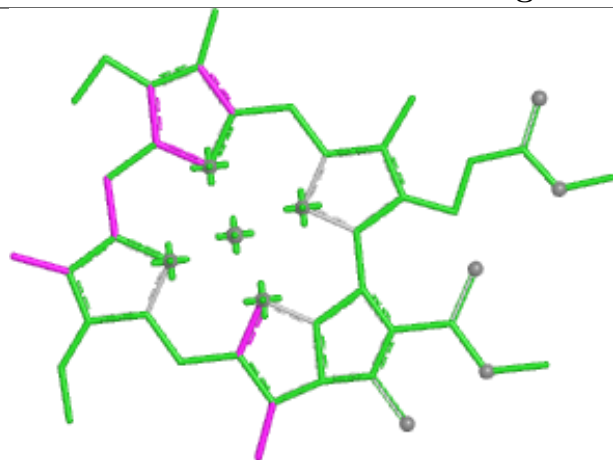
Ligand DGD G 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR m 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

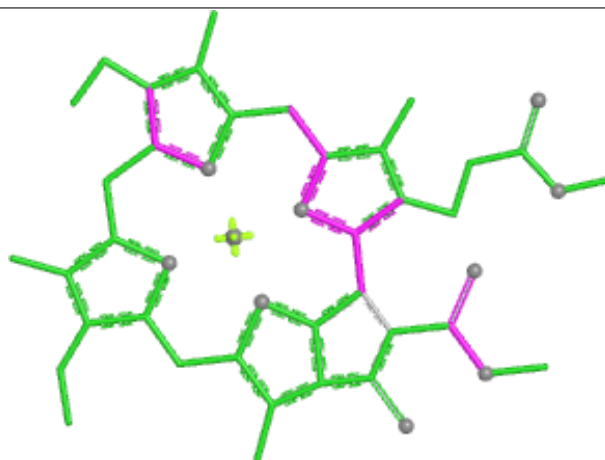
Ligand BCR 1 302	
	
Bond lengths	Bond angles
	
Torsions	Rings



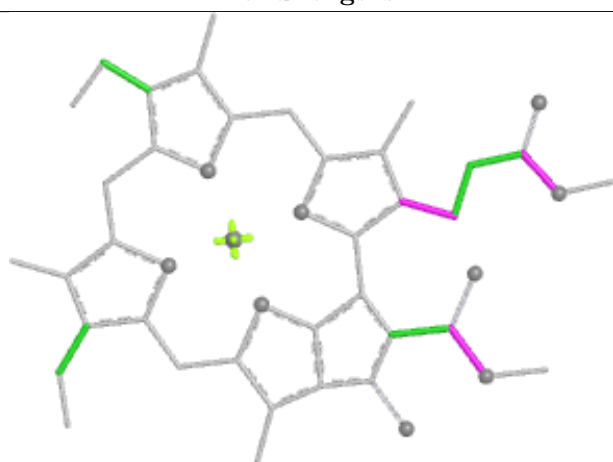
Ligand CLA F 313



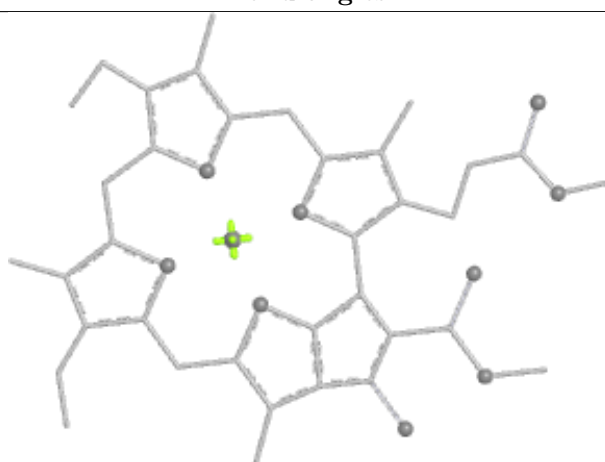
Bond lengths



Bond angles

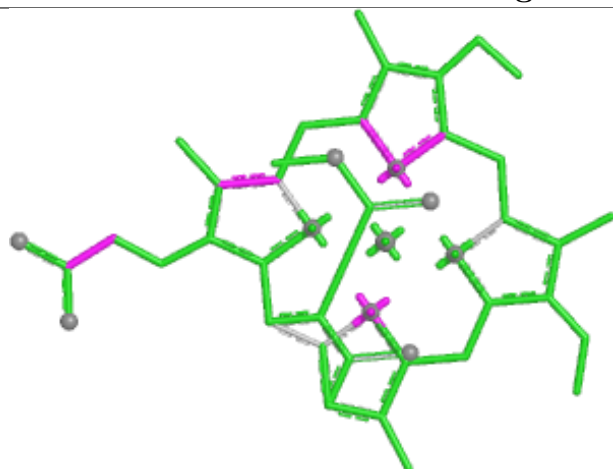


Torsions

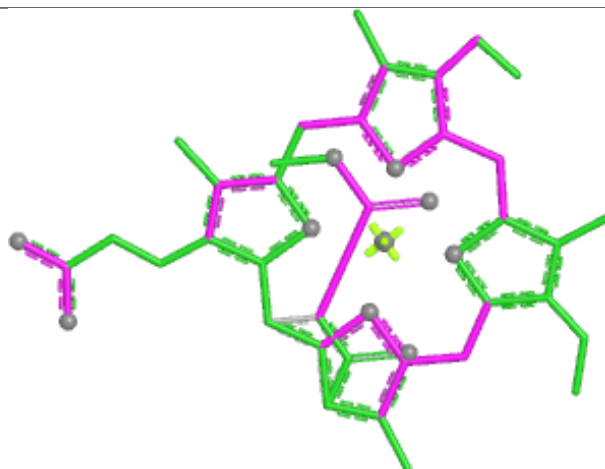


Rings

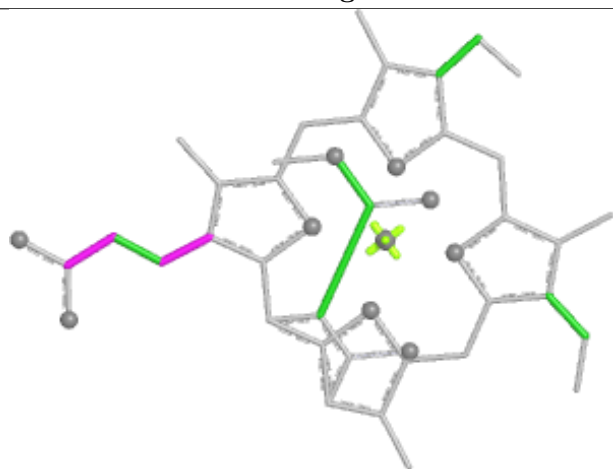
Ligand KC1 D 315



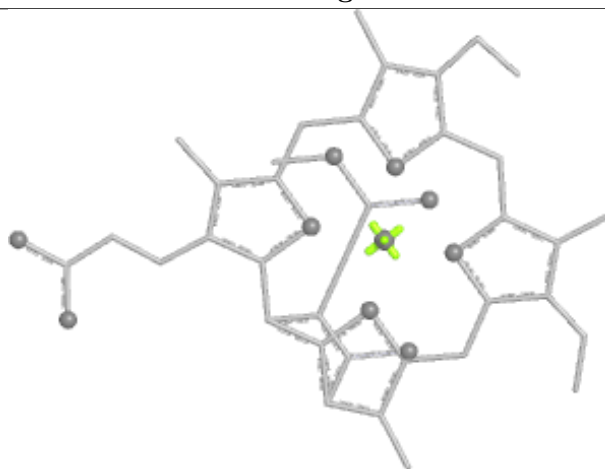
Bond lengths



Bond angles

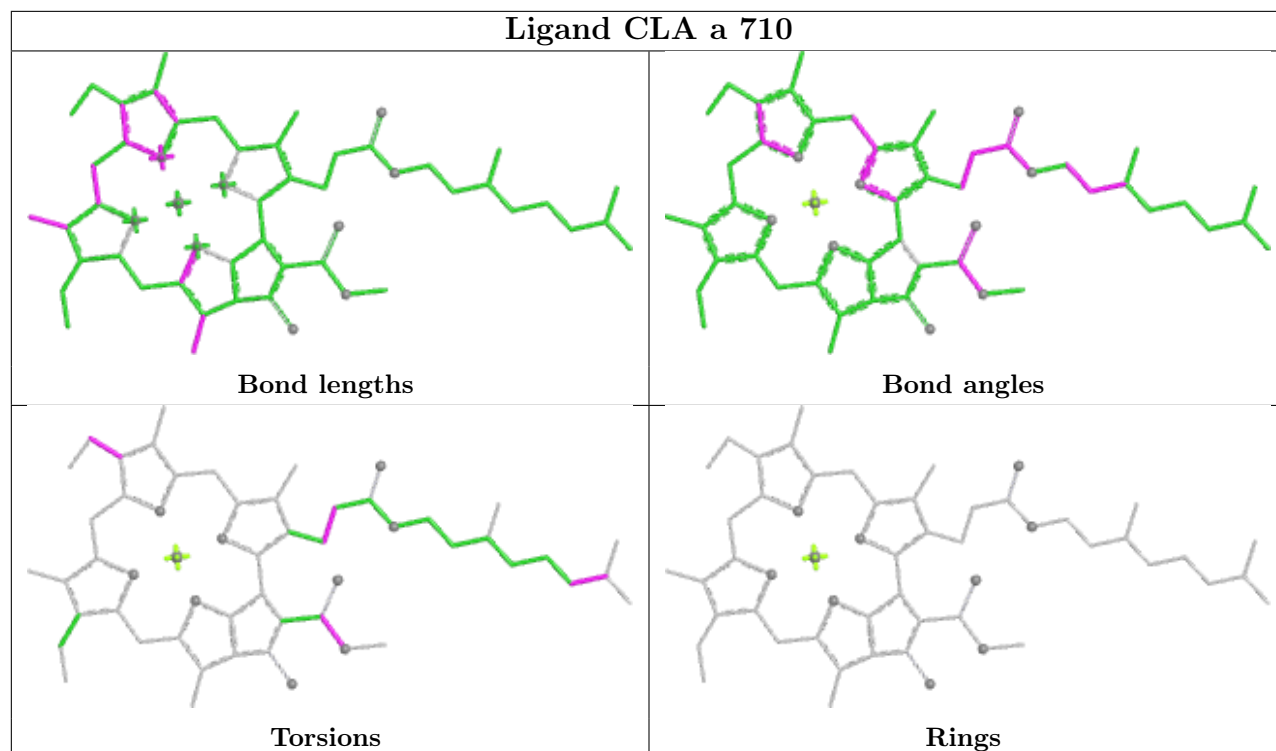


Torsions

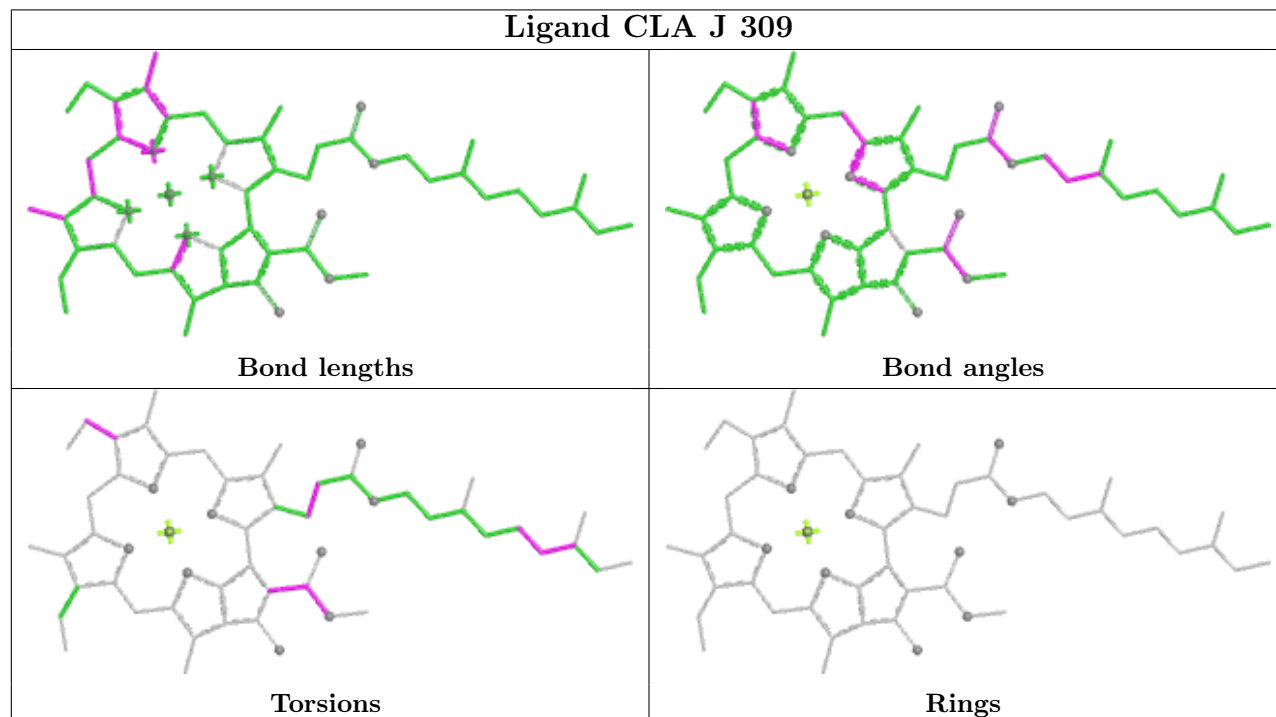


Rings

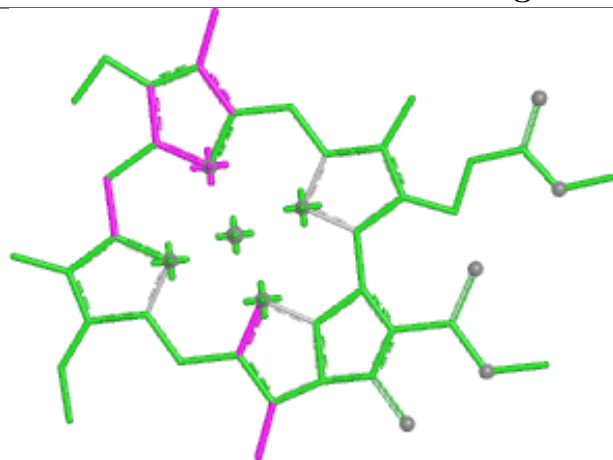
Ligand CLA a 710



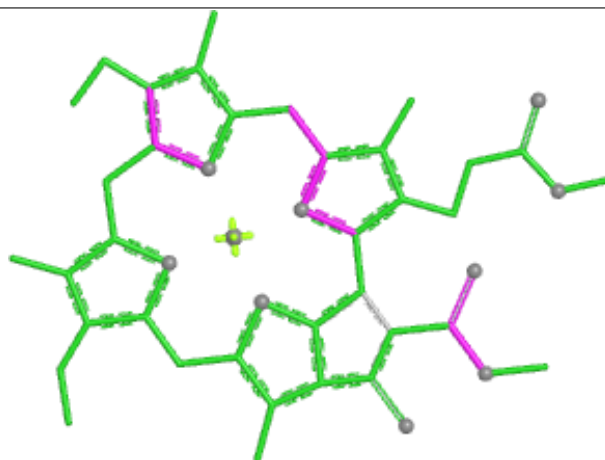
Ligand CLA J 309



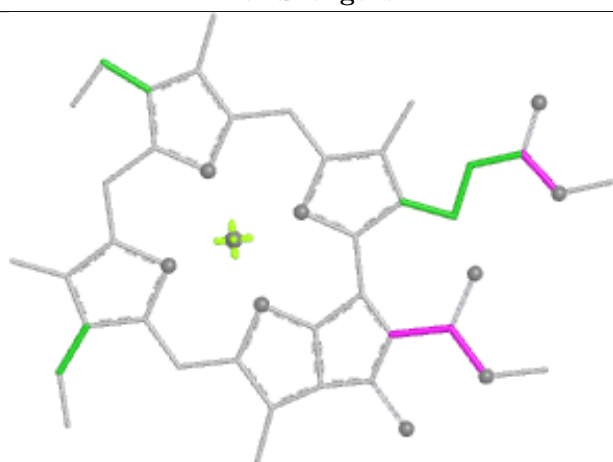
Ligand CLA A 320



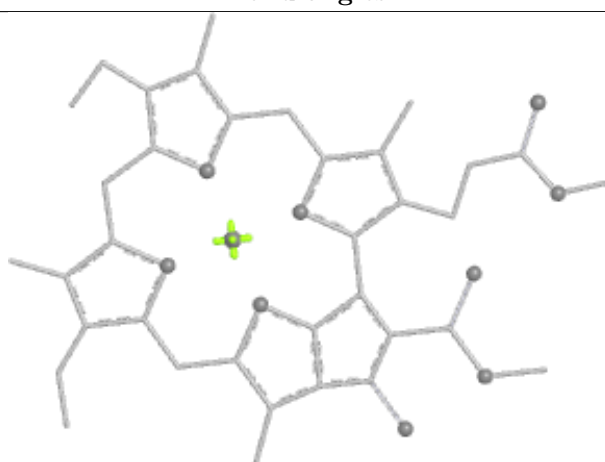
Bond lengths



Bond angles

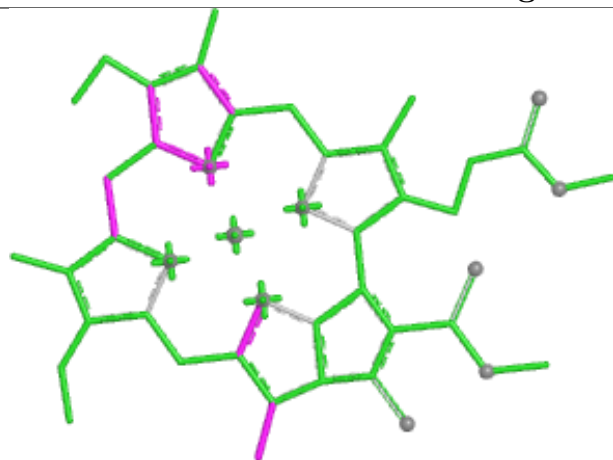


Torsions

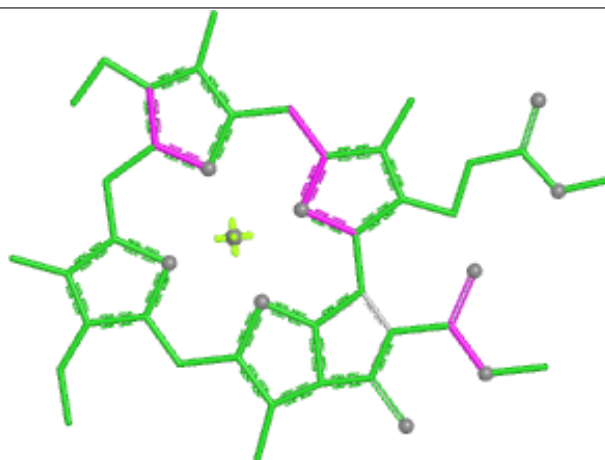


Rings

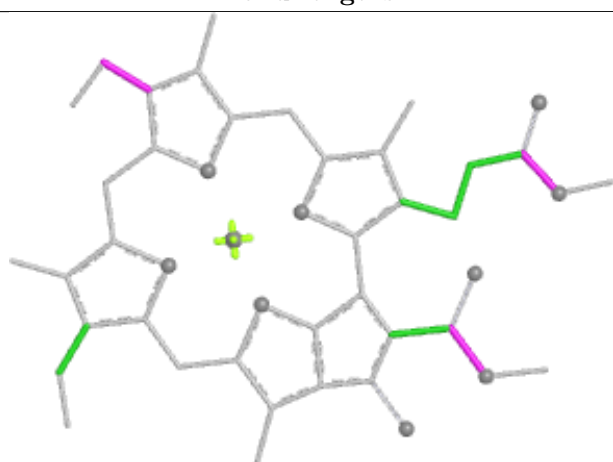
Ligand CLA J 306



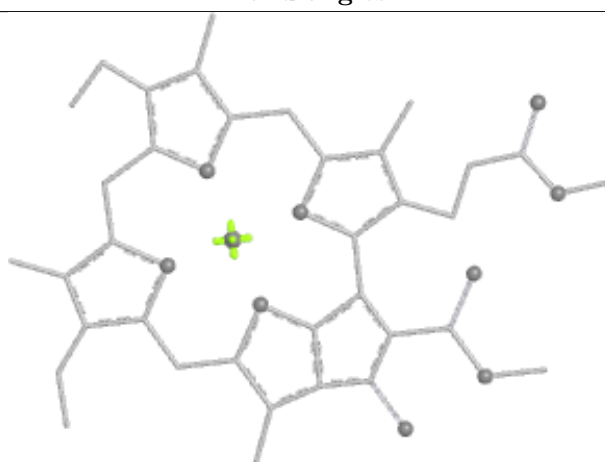
Bond lengths



Bond angles

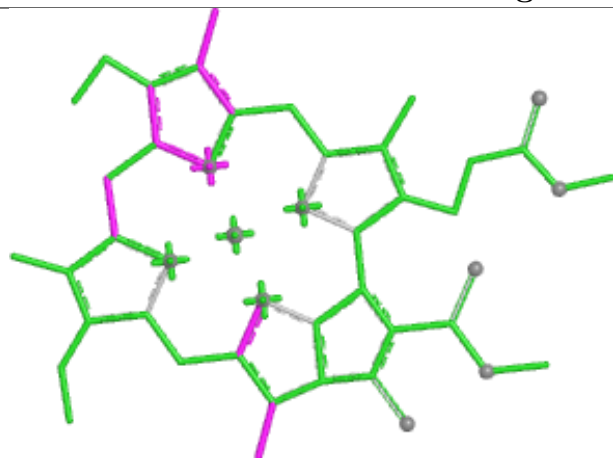


Torsions

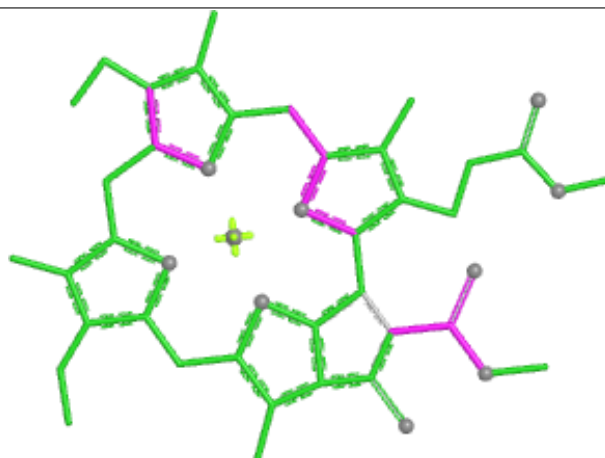


Rings

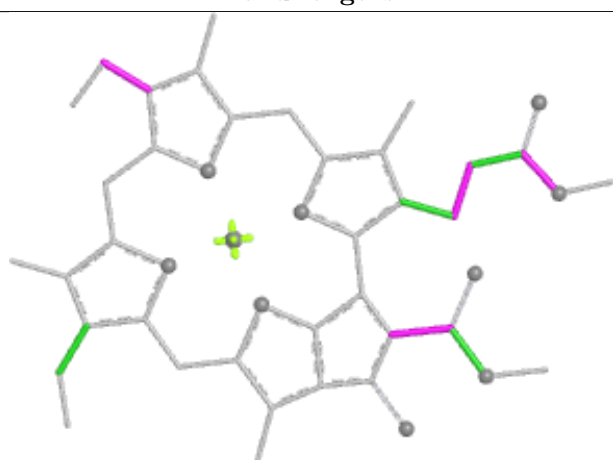
Ligand CLA F 311



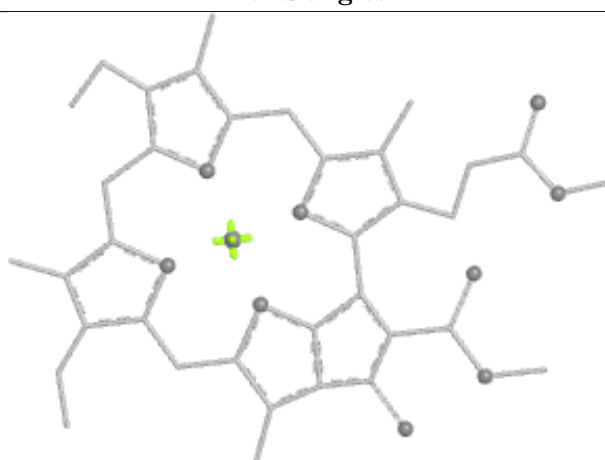
Bond lengths



Bond angles

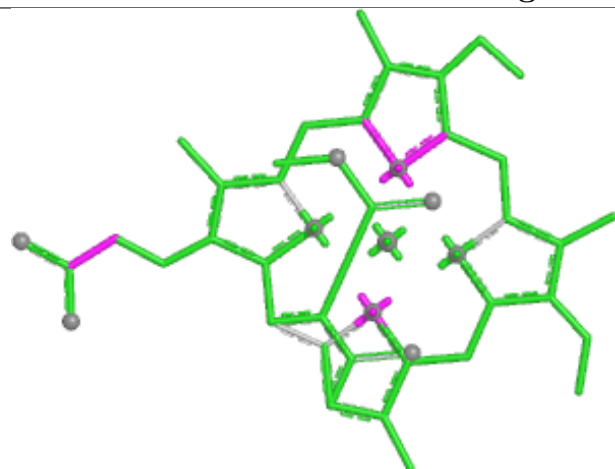


Torsions

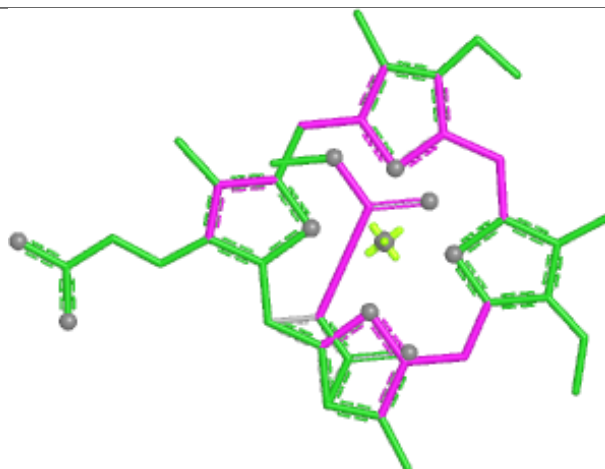


Rings

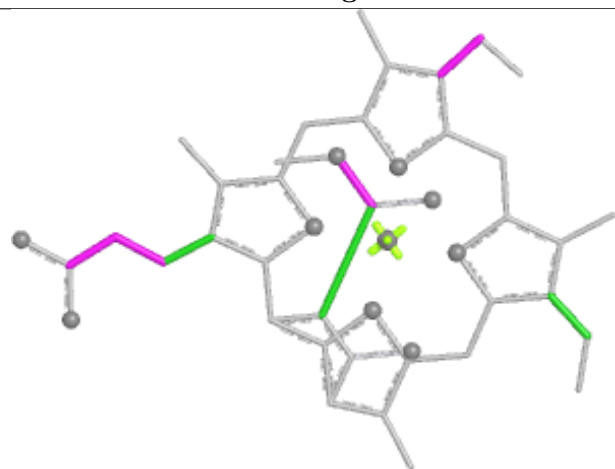
Ligand KC1 B 314



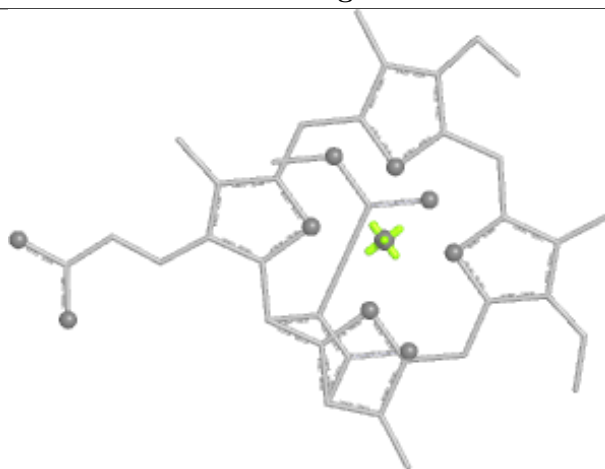
Bond lengths



Bond angles

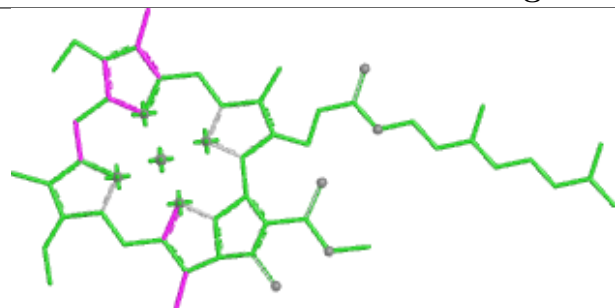


Torsions

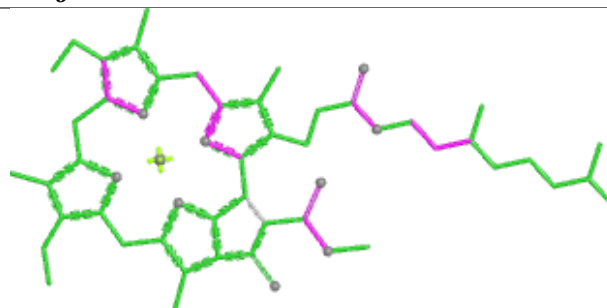


Rings

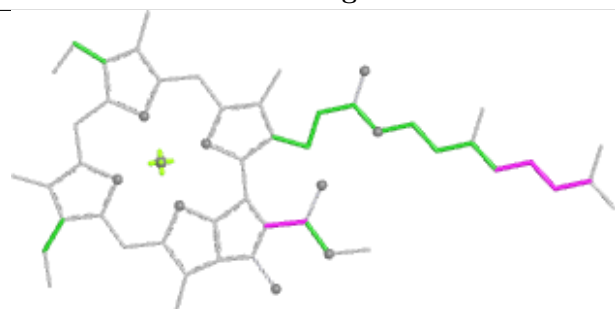
Ligand CLA j 104



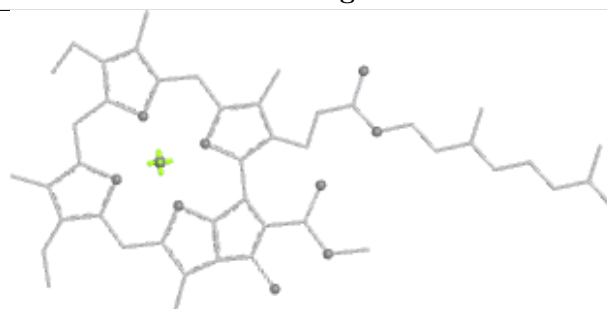
Bond lengths



Bond angles

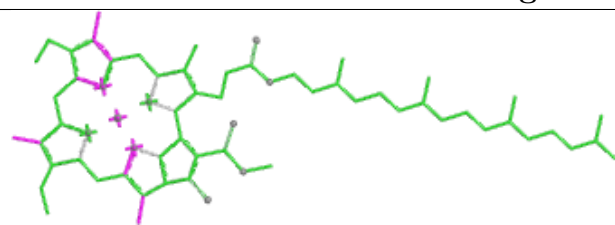


Torsions

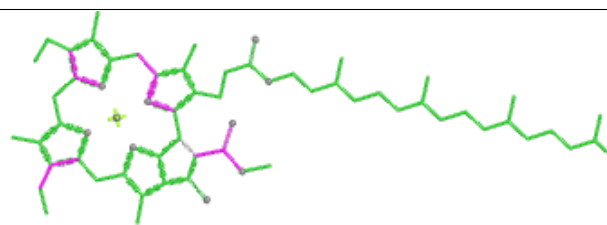


Rings

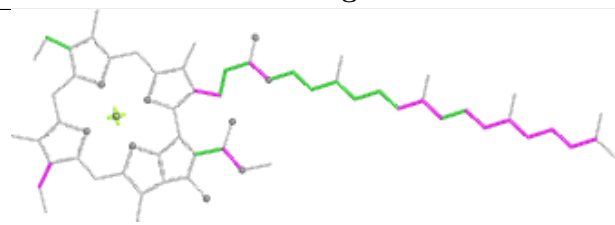
Ligand CLA b 704



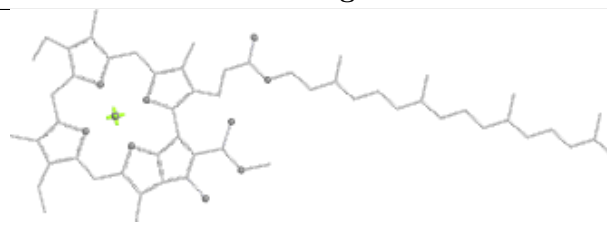
Bond lengths



Bond angles

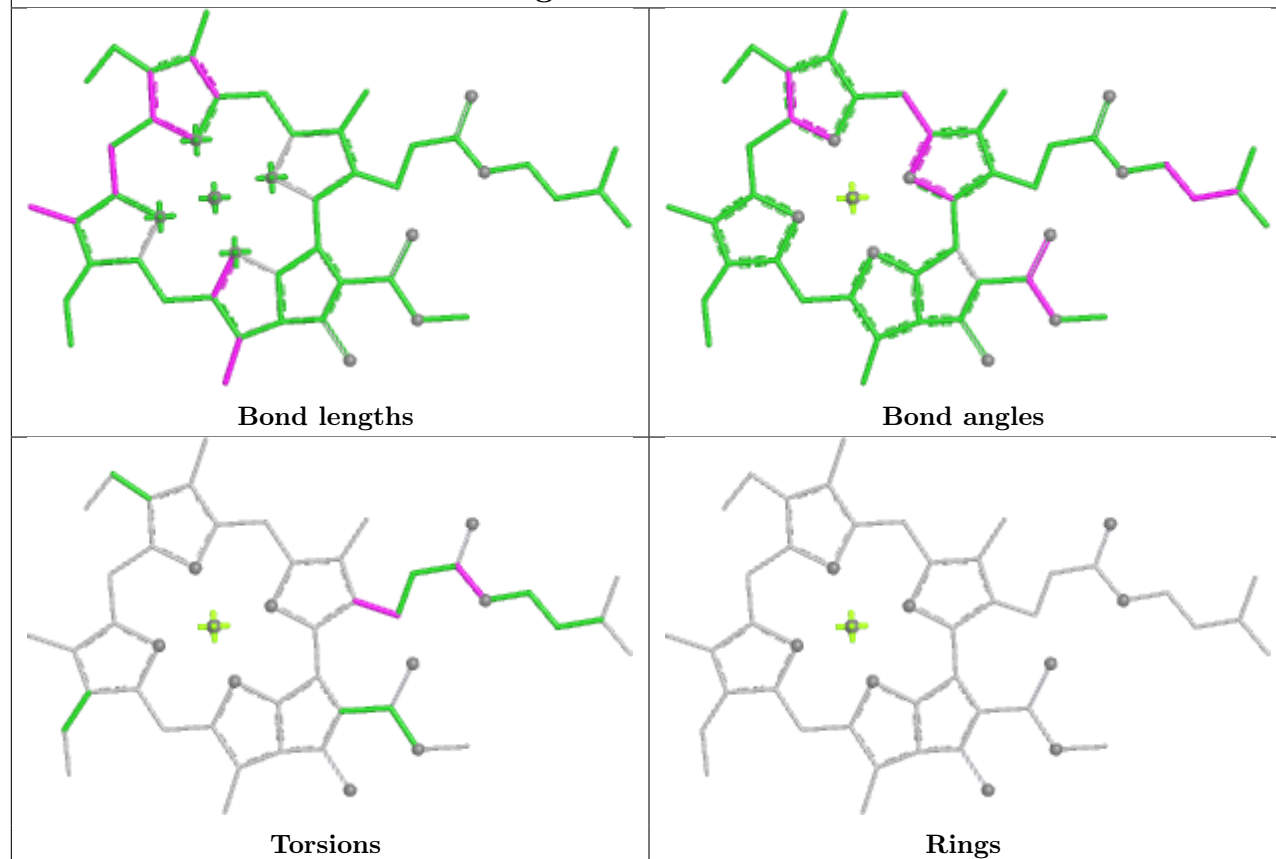


Torsions

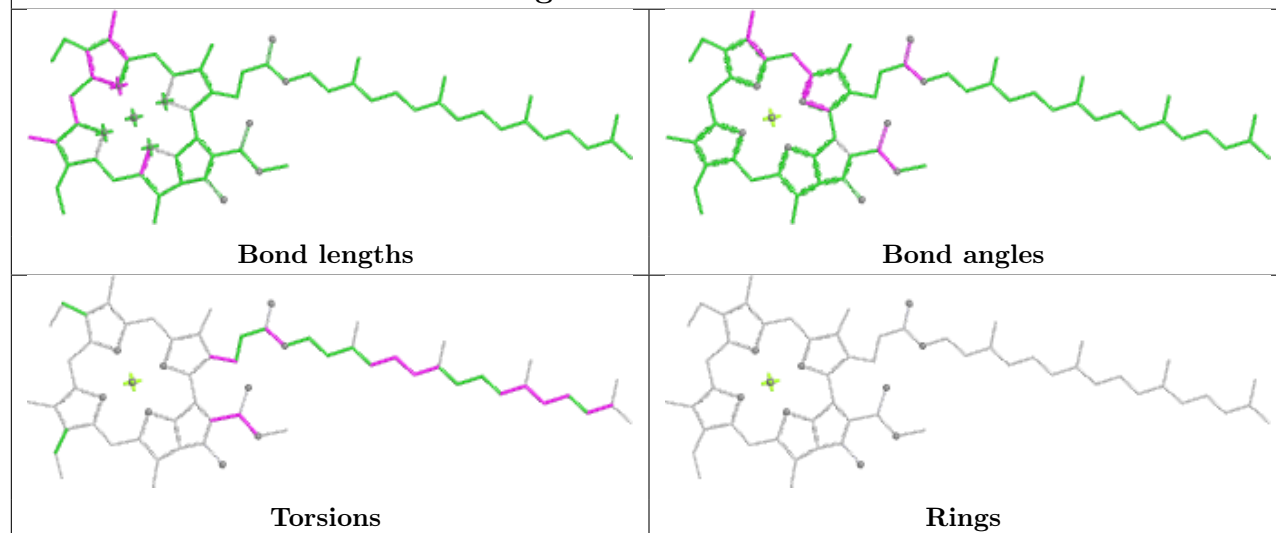


Rings

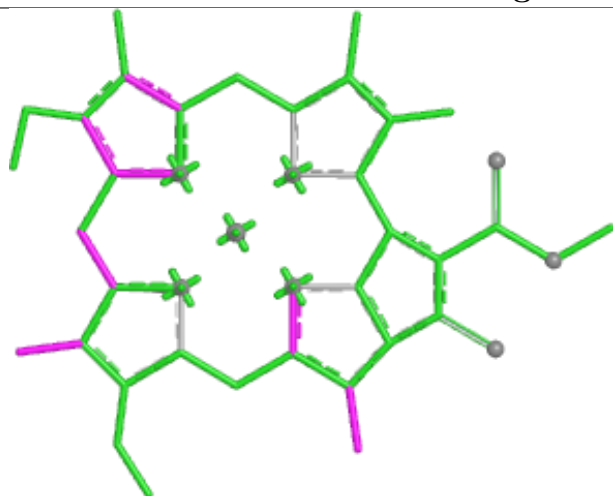
Ligand CLA b 716



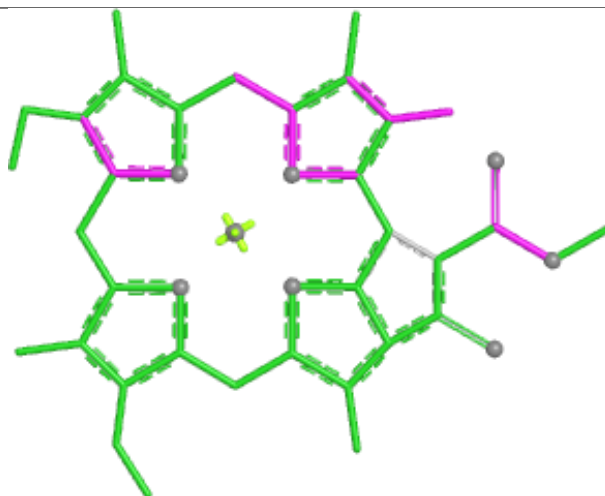
Ligand CLA b 717



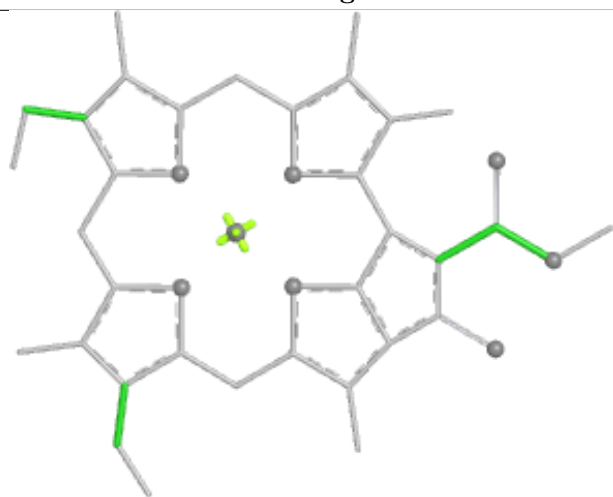
Ligand CLA D 316



Bond lengths



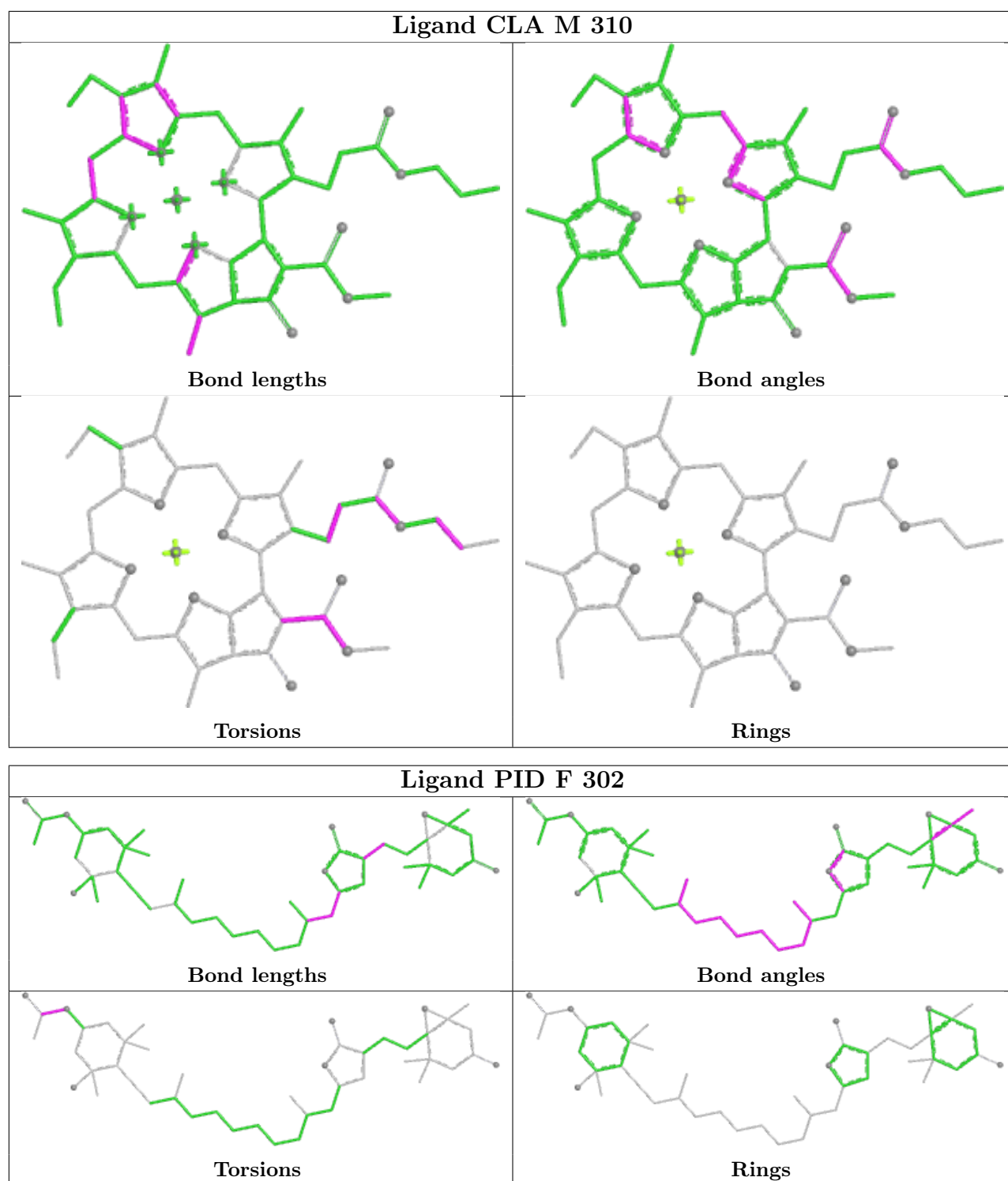
Bond angles

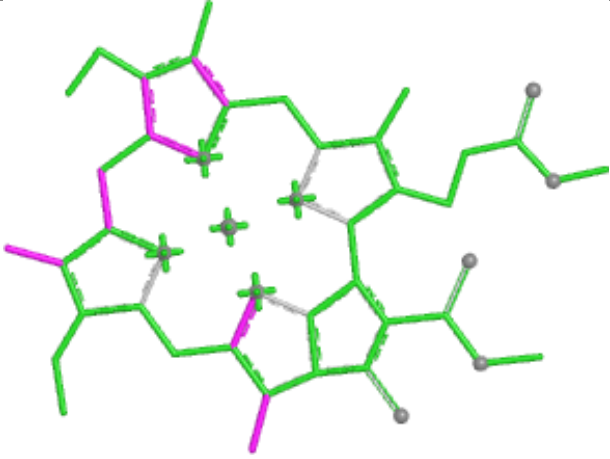
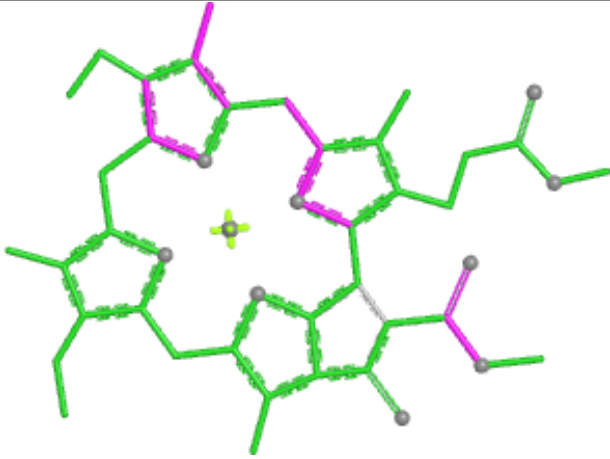
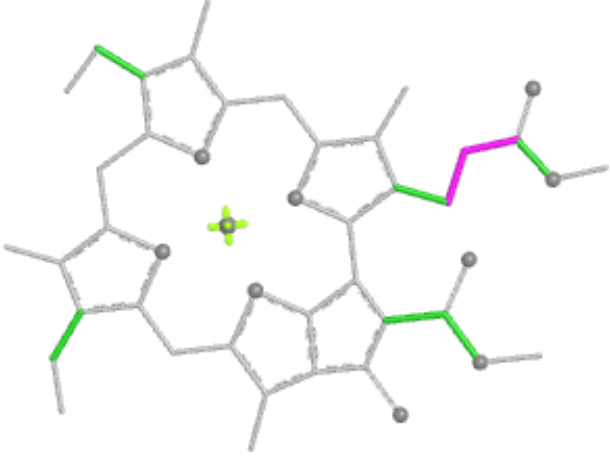
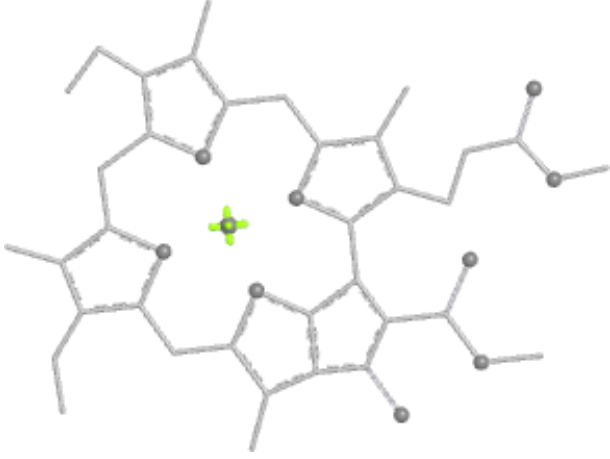
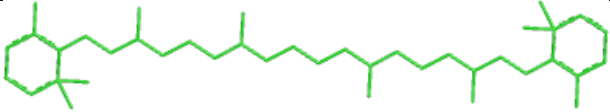
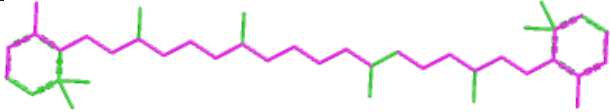
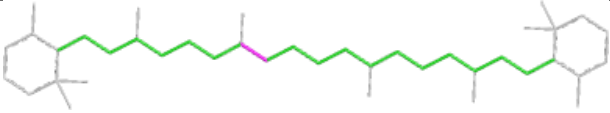
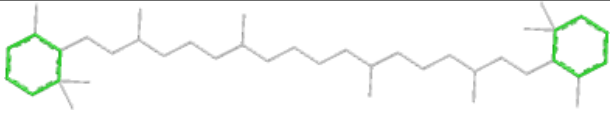
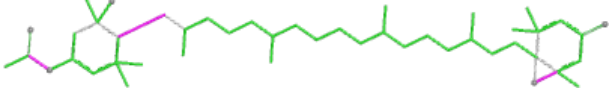
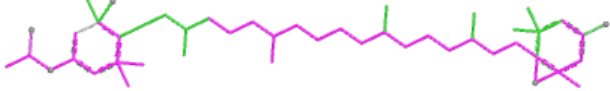
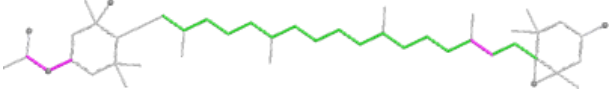
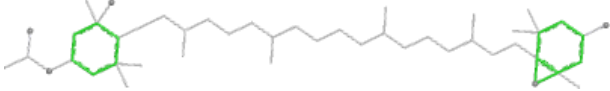


Torsions

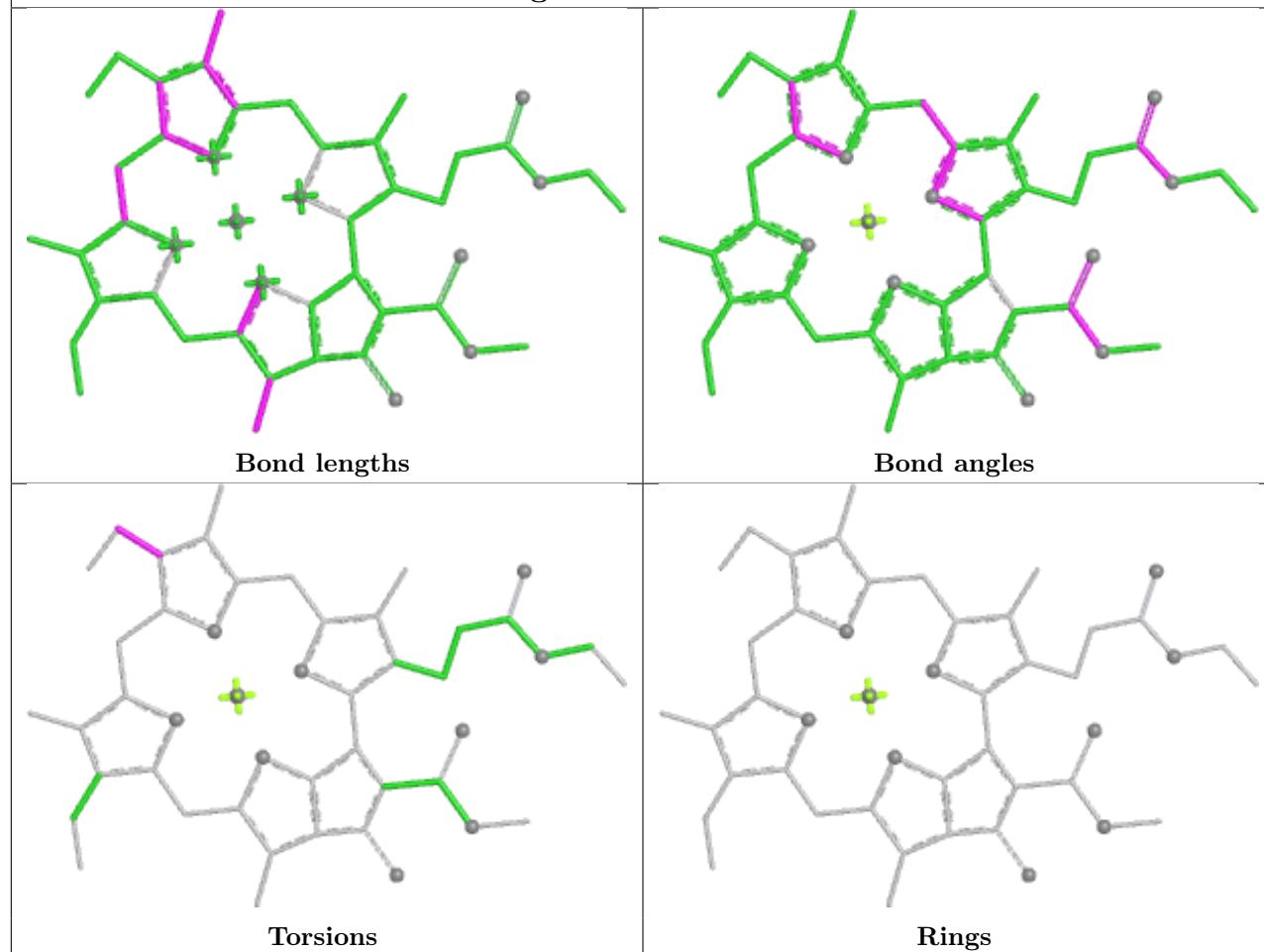


Rings

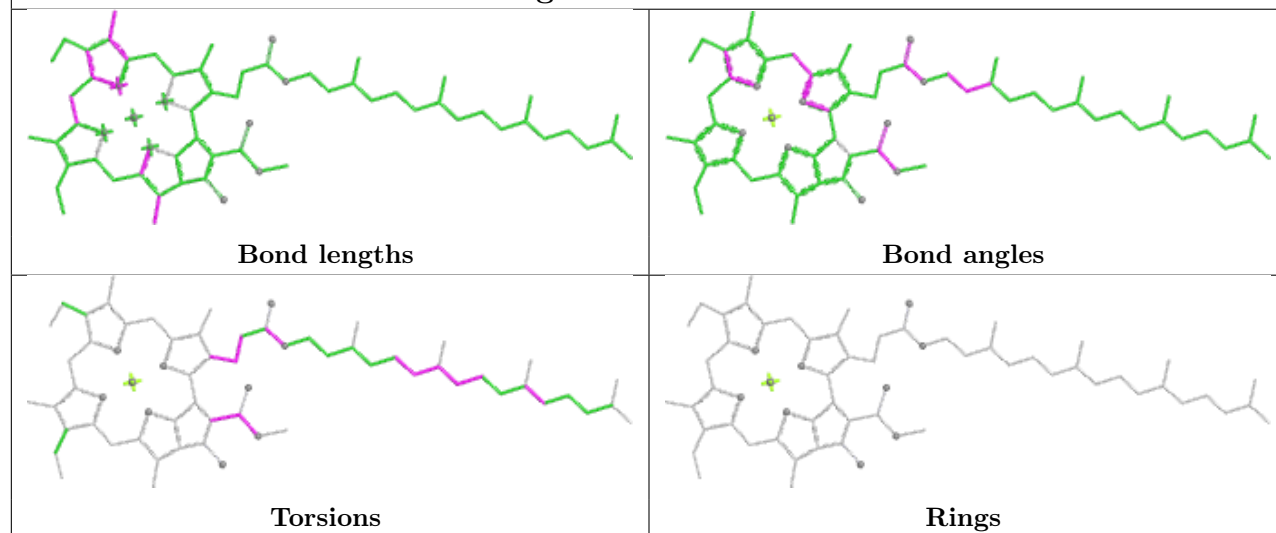


Ligand CLA b 714	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR f 304	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand UIX K 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

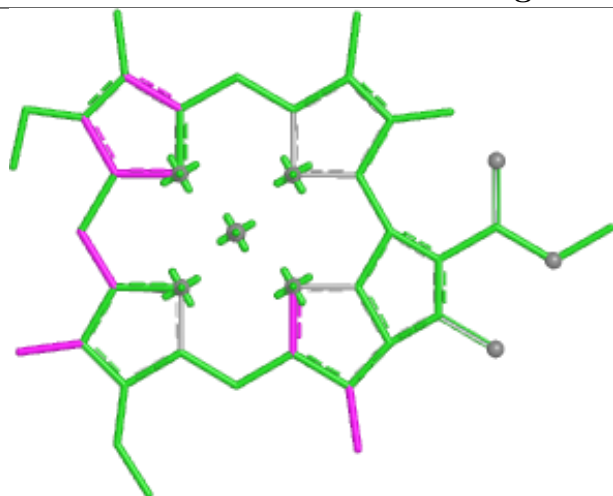
Ligand CLA b 726



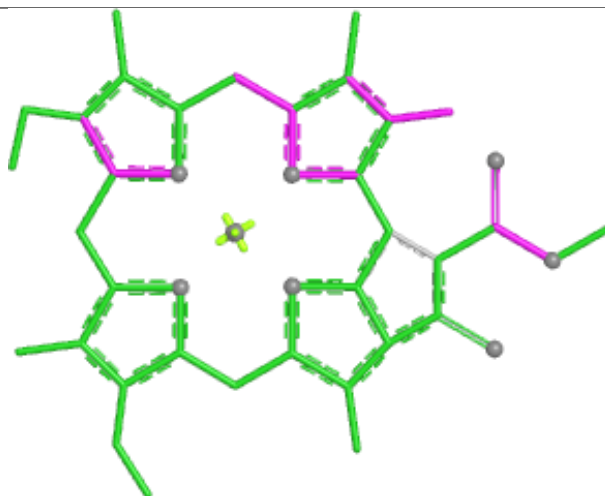
Ligand CLA a 709



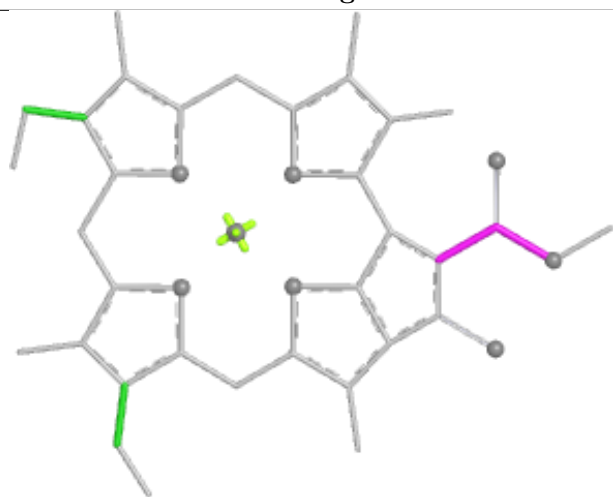
Ligand CLA B 315



Bond lengths



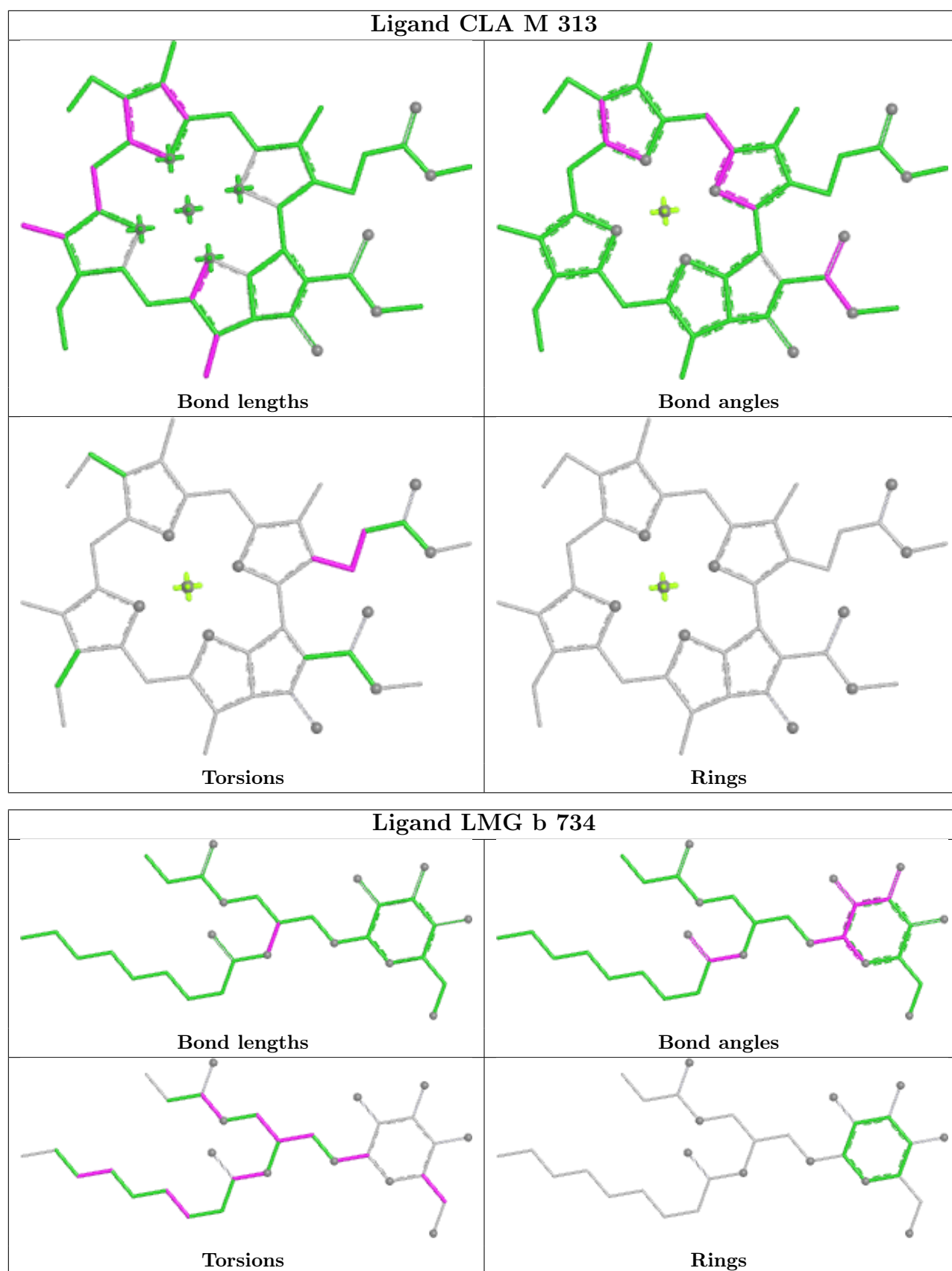
Bond angles



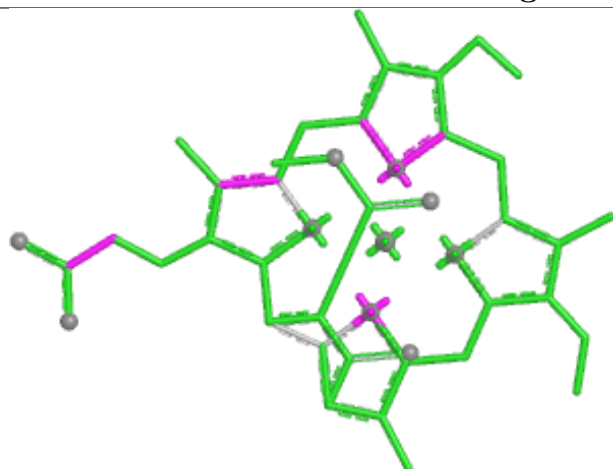
Torsions



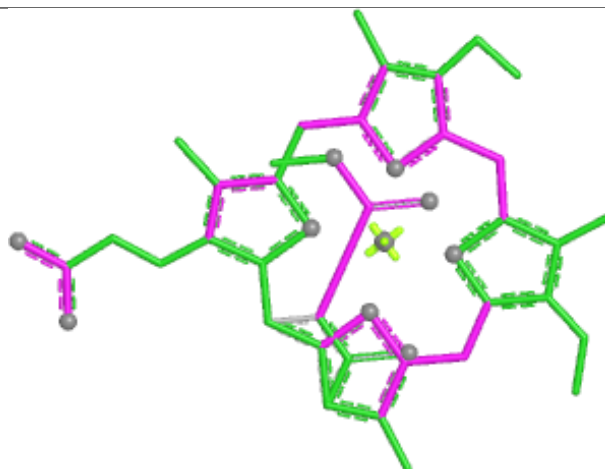
Rings



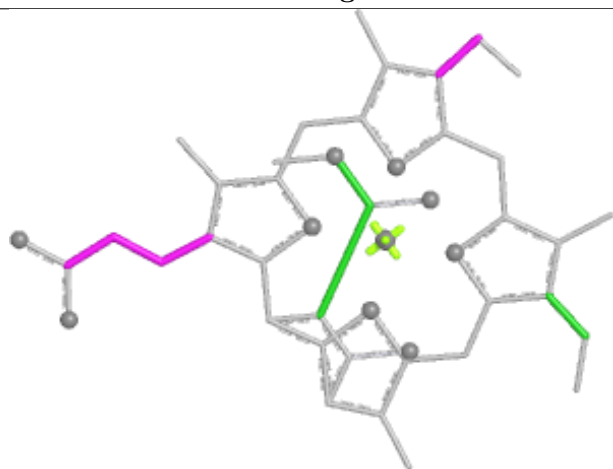
Ligand KC1 J 313



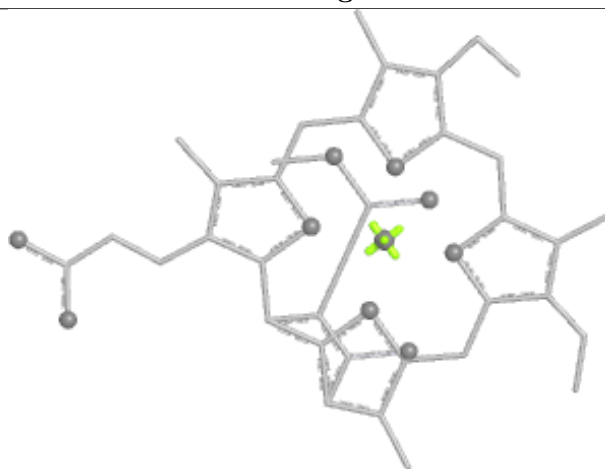
Bond lengths



Bond angles

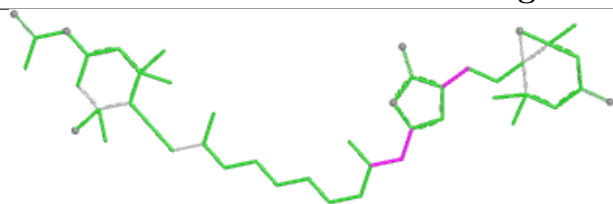


Torsions

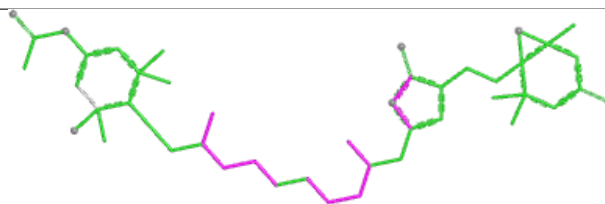


Rings

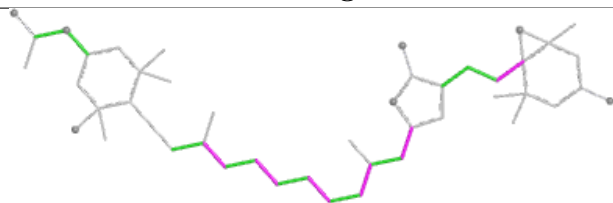
Ligand PID D 306



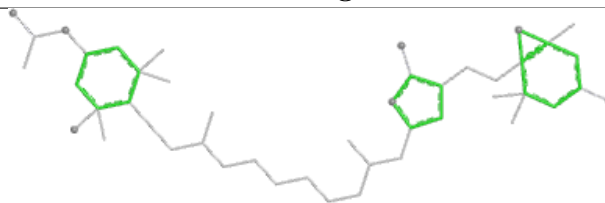
Bond lengths



Bond angles

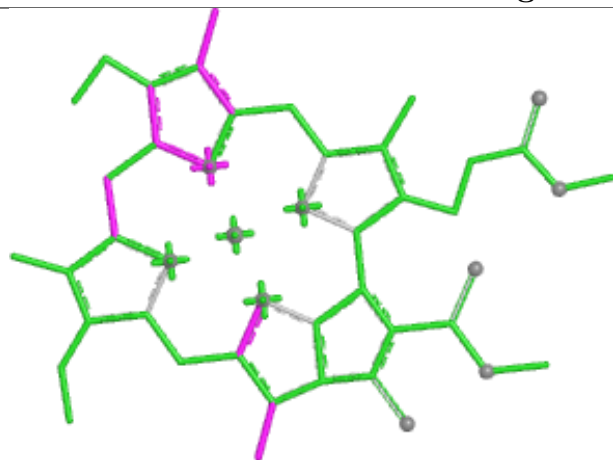


Torsions

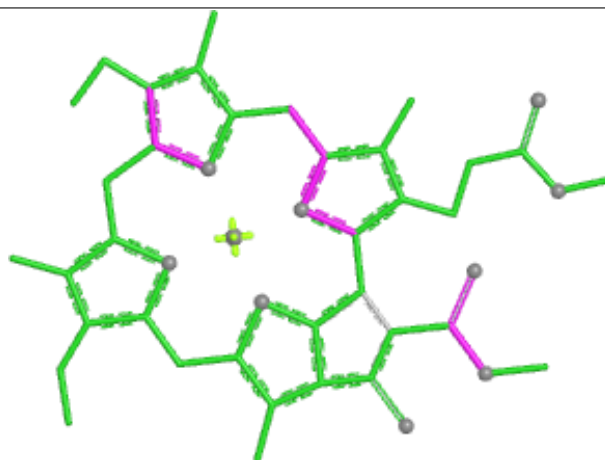


Rings

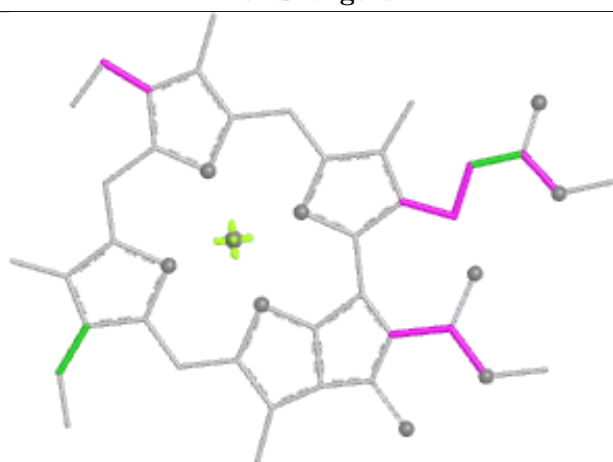
Ligand CLA b 719



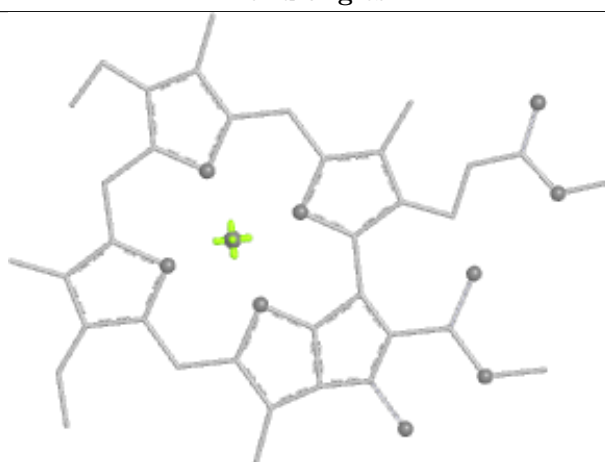
Bond lengths



Bond angles

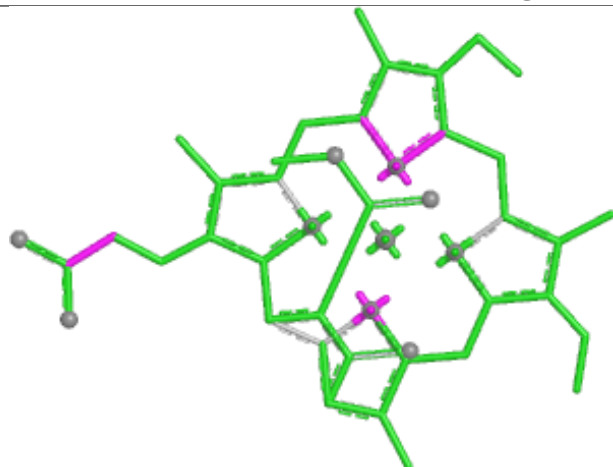


Torsions

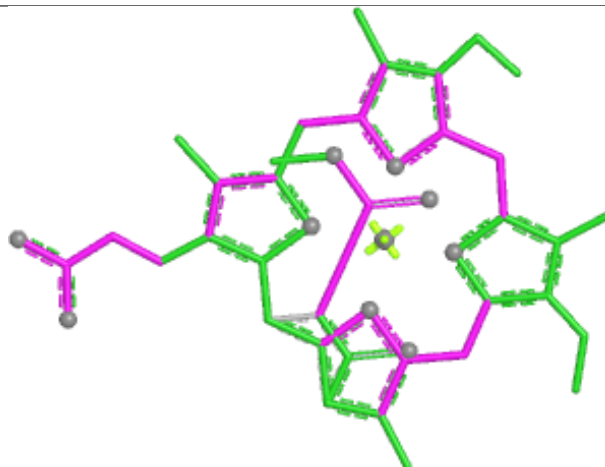


Rings

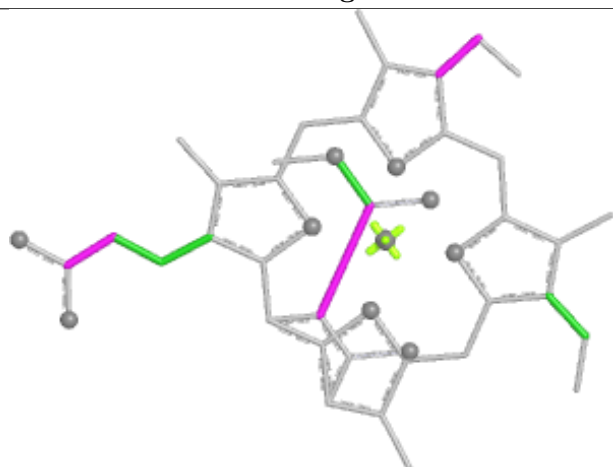
Ligand KC1 L 307



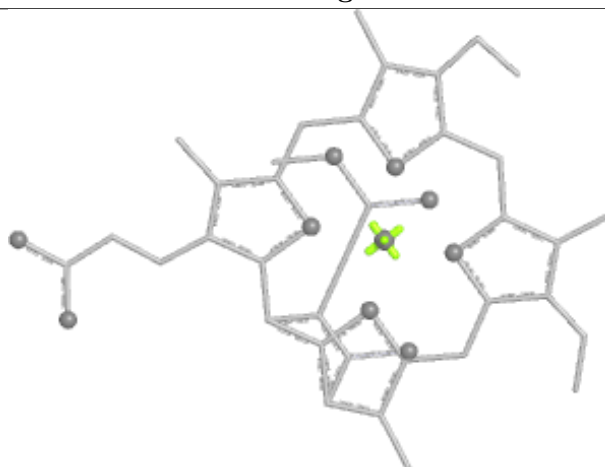
Bond lengths



Bond angles

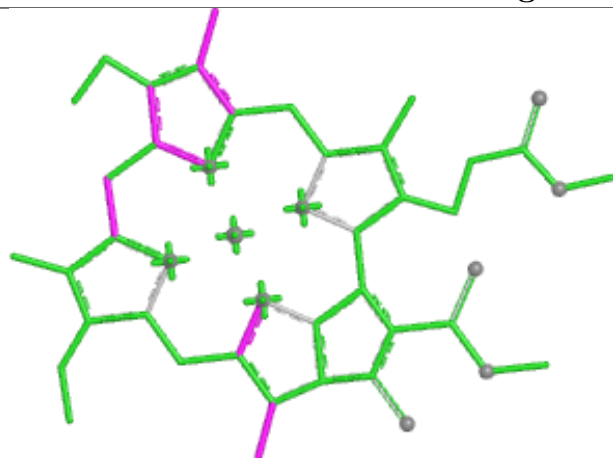


Torsions

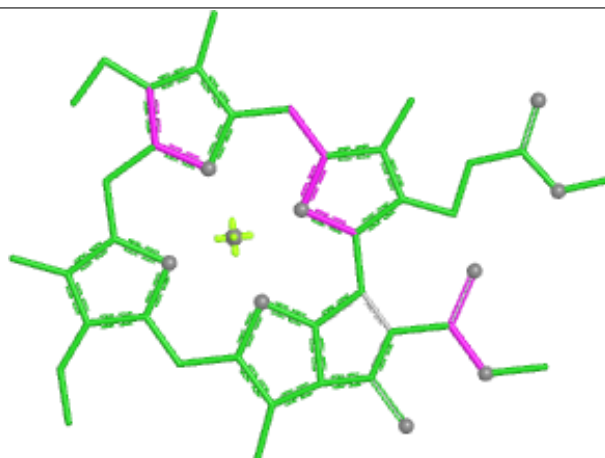


Rings

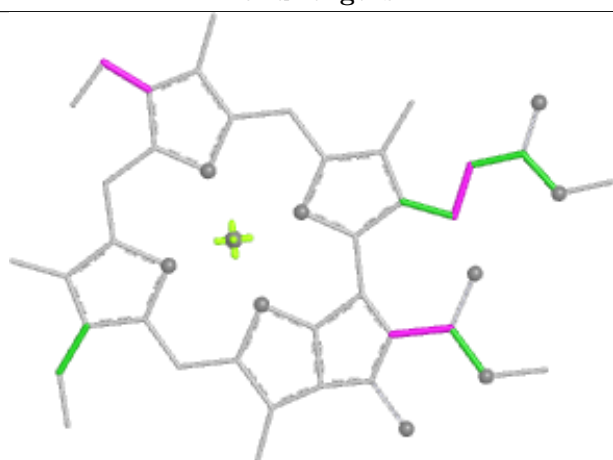
Ligand CLA J 316



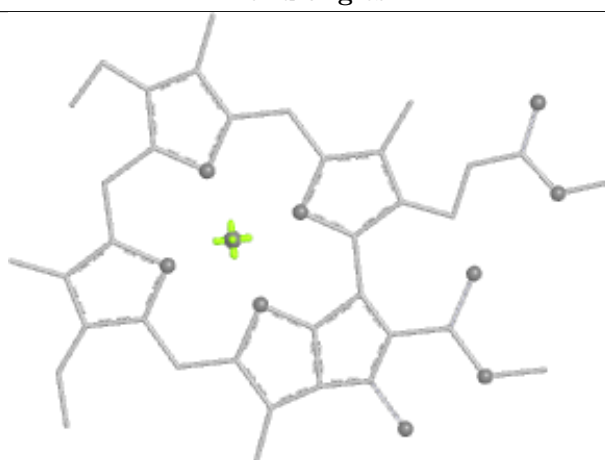
Bond lengths



Bond angles

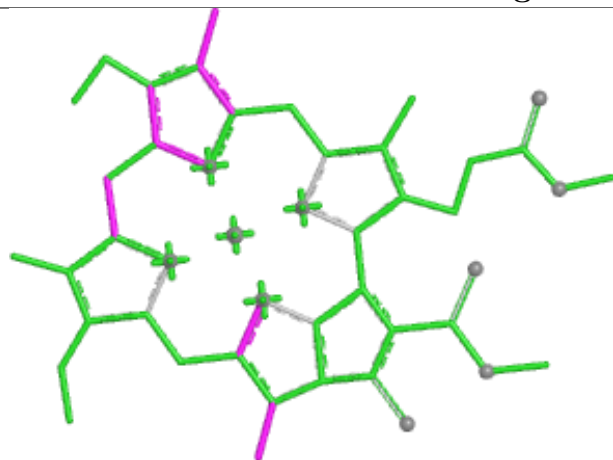


Torsions

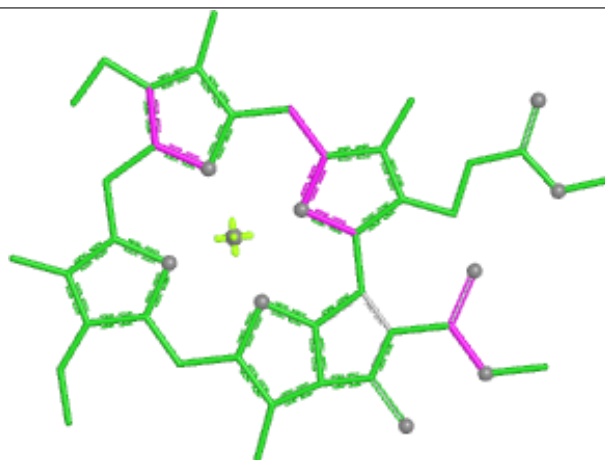


Rings

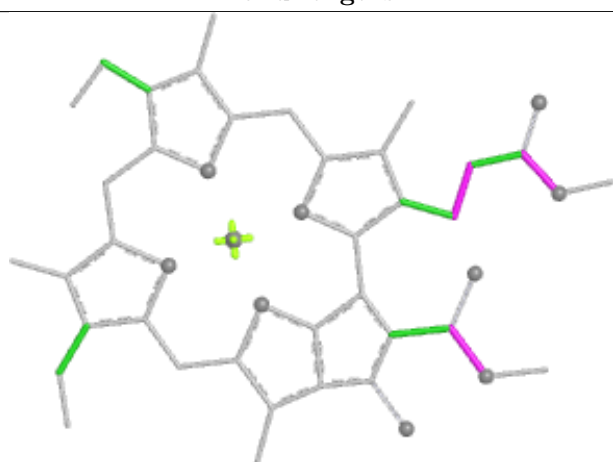
Ligand CLA A 311



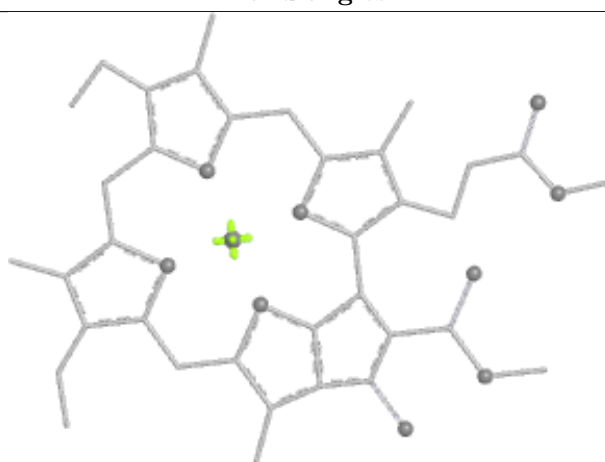
Bond lengths



Bond angles

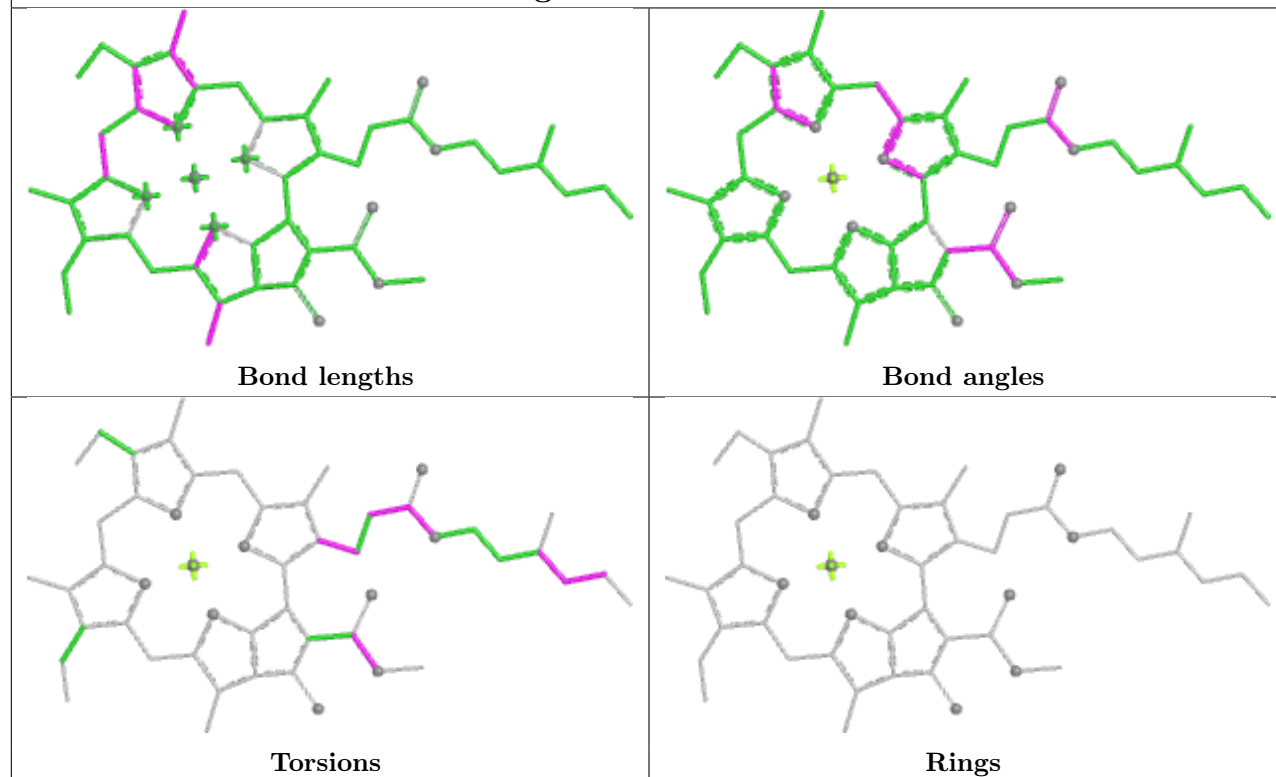


Torsions

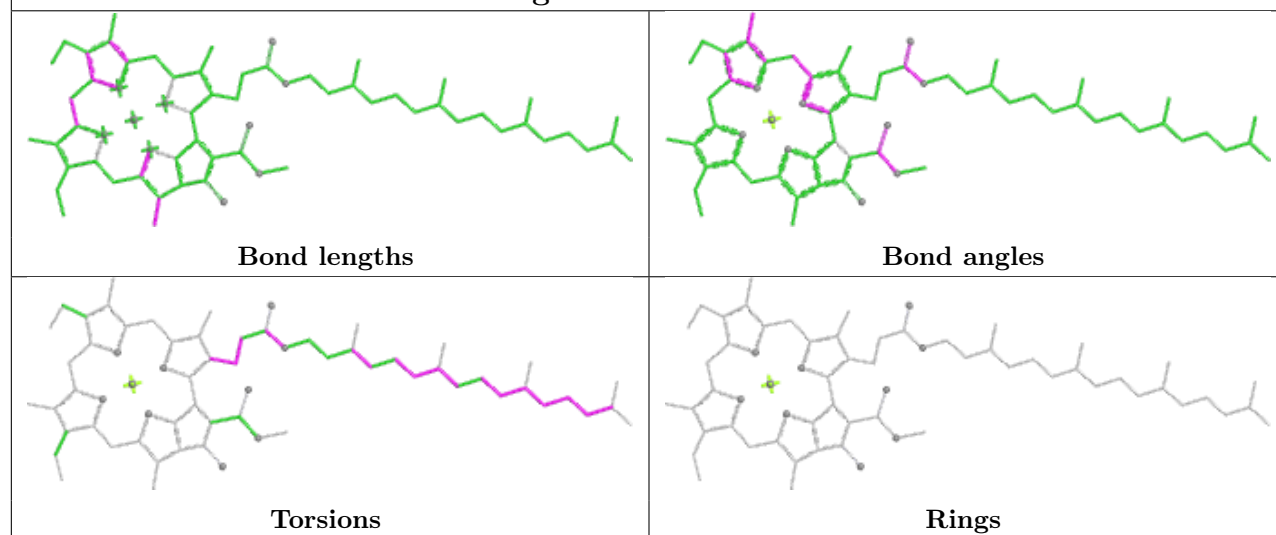


Rings

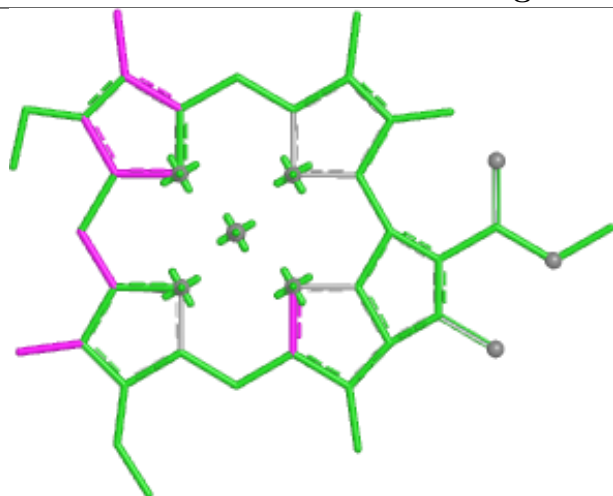
Ligand CLA L 317



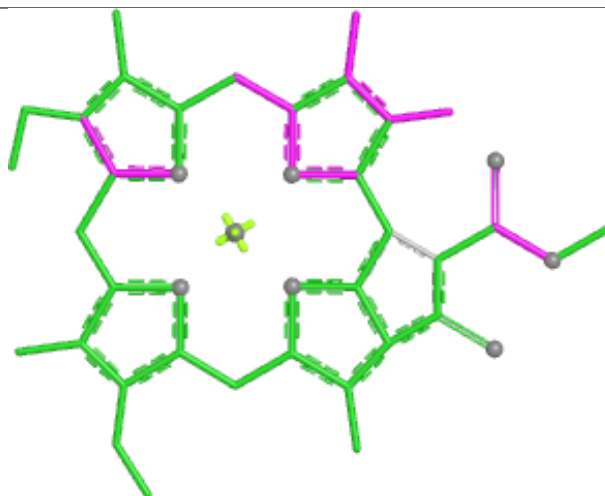
Ligand CLA B 309



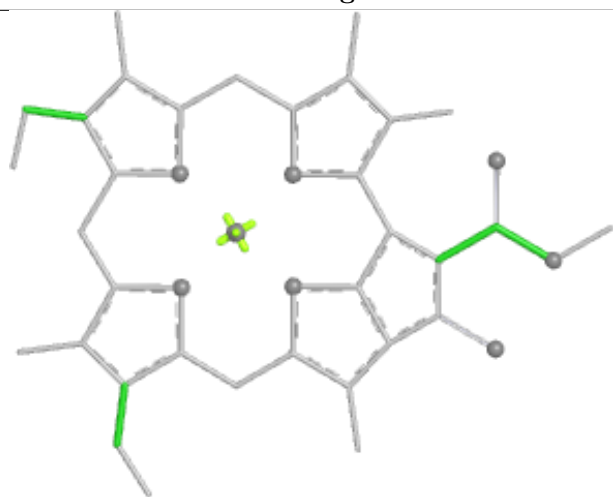
Ligand CLA A 317



Bond lengths



Bond angles

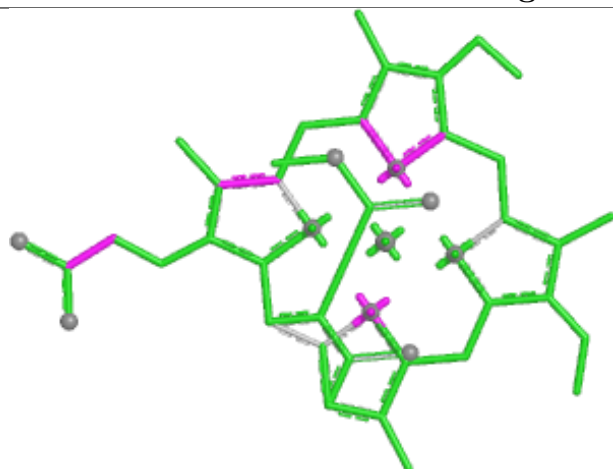


Torsions

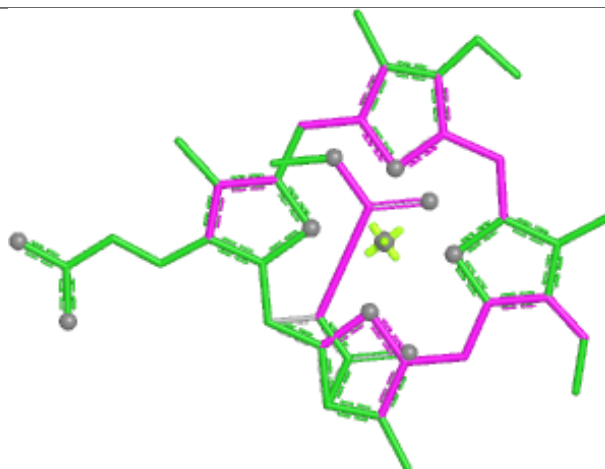


Rings

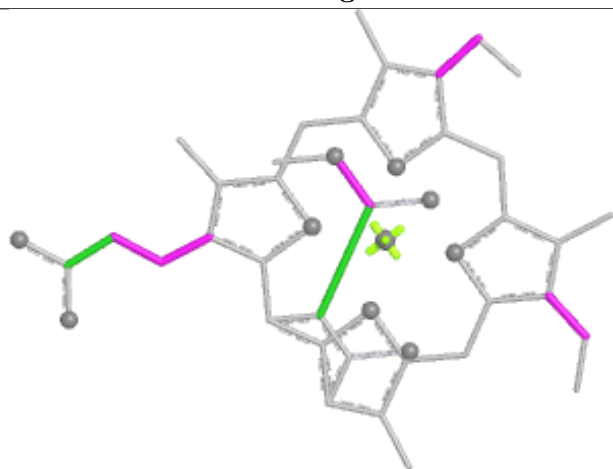
Ligand KC1 L 315



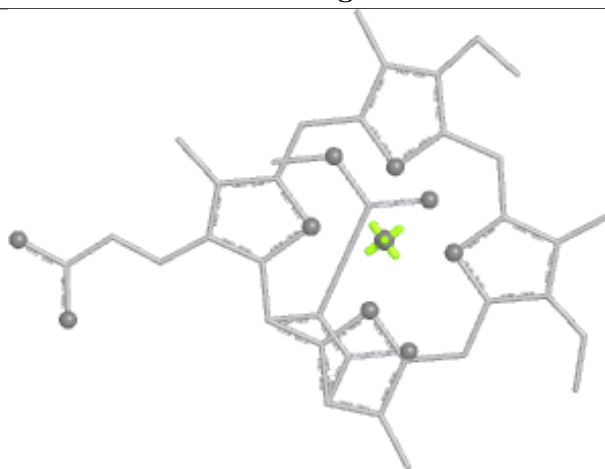
Bond lengths



Bond angles

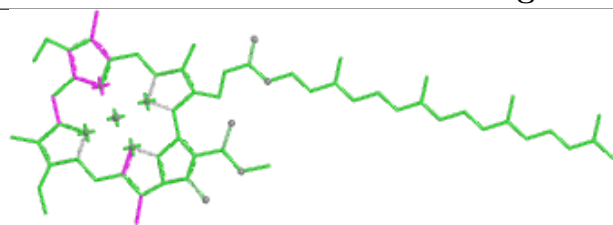


Torsions

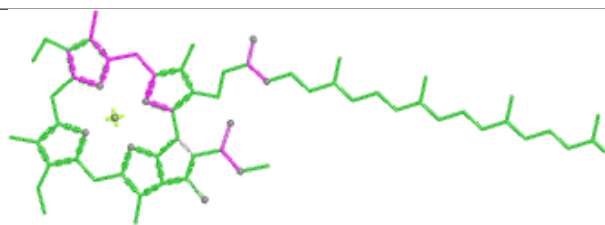


Rings

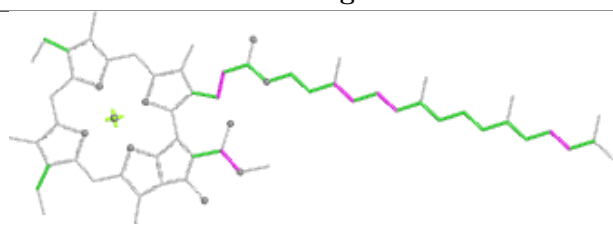
Ligand CLA b 722



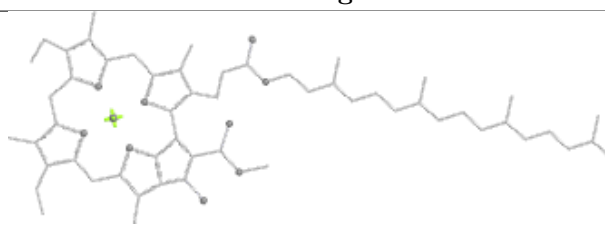
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

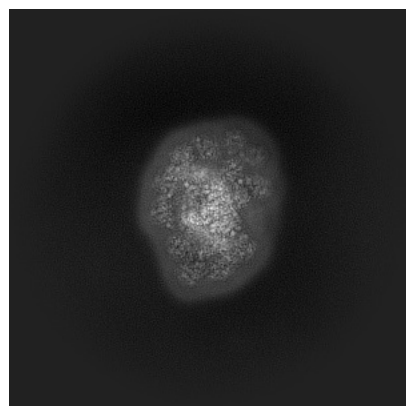
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36743. These allow visual inspection of the internal detail of the map and identification of artifacts.

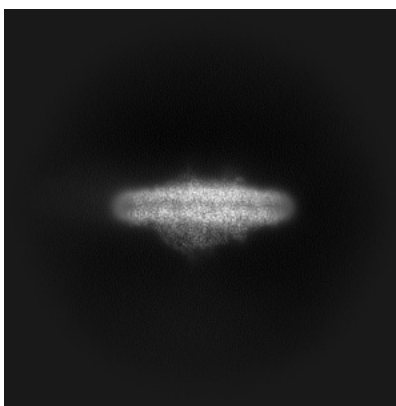
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

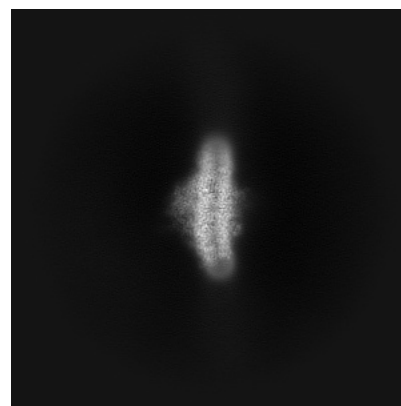
6.1.1 Primary map



X

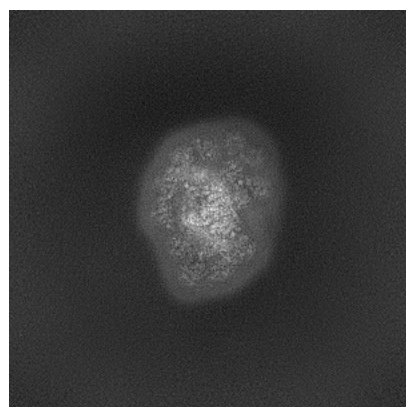


Y

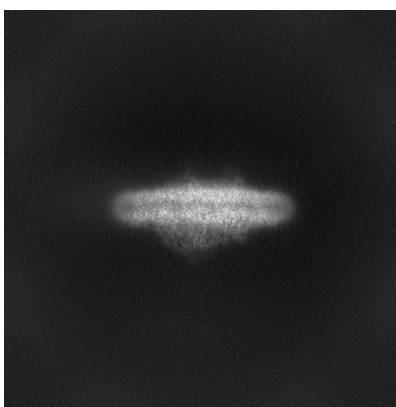


Z

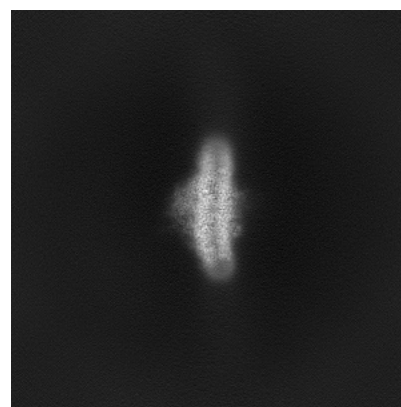
6.1.2 Raw map



X



Y

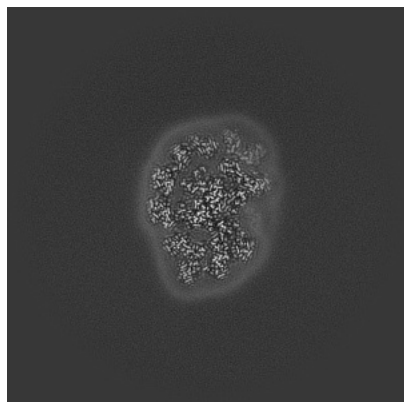


Z

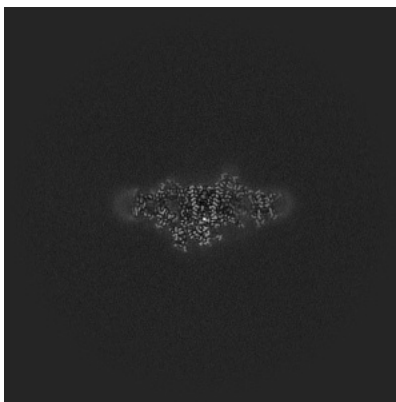
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

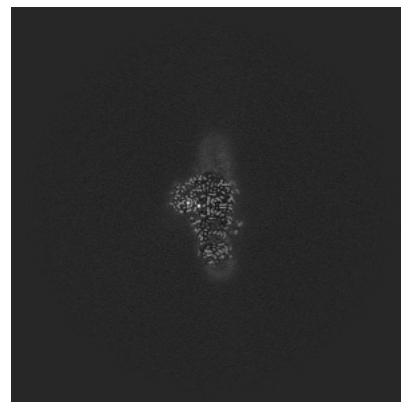
6.2.1 Primary map



X Index: 256

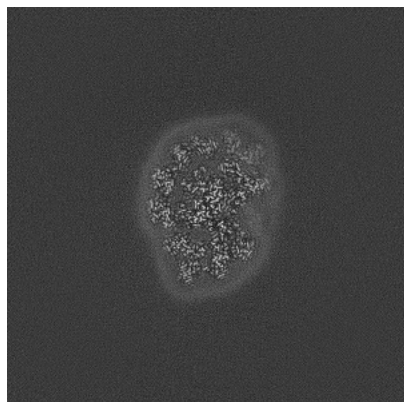


Y Index: 256

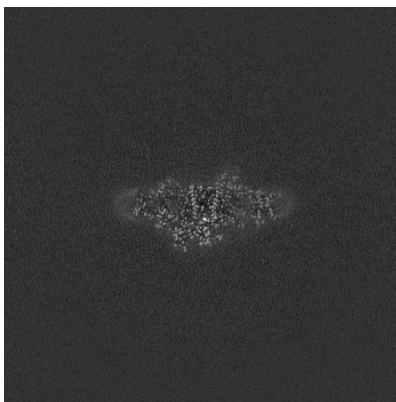


Z Index: 256

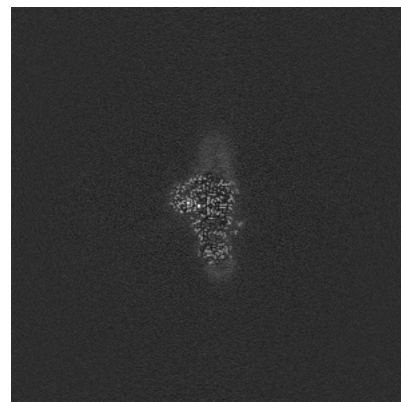
6.2.2 Raw map



X Index: 256



Y Index: 256

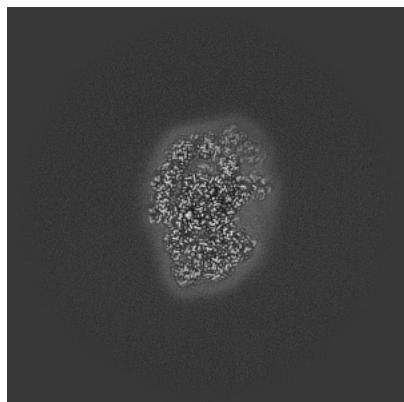


Z Index: 256

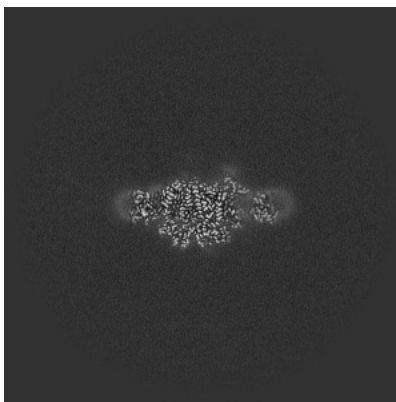
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

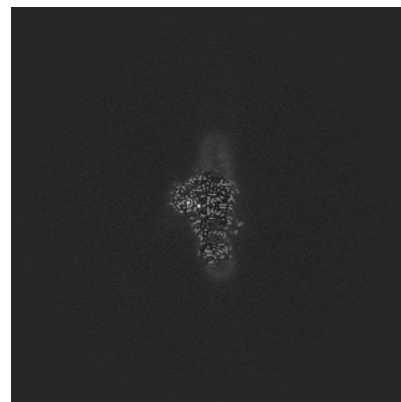
6.3.1 Primary map



X Index: 248

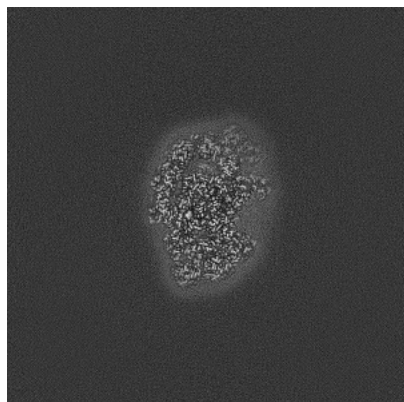


Y Index: 263

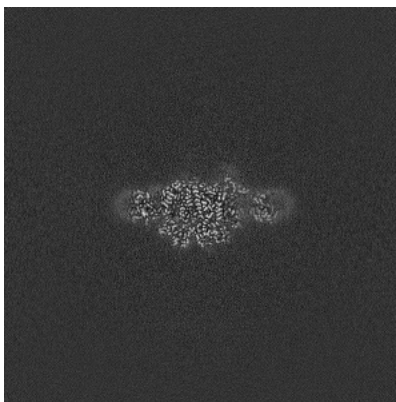


Z Index: 256

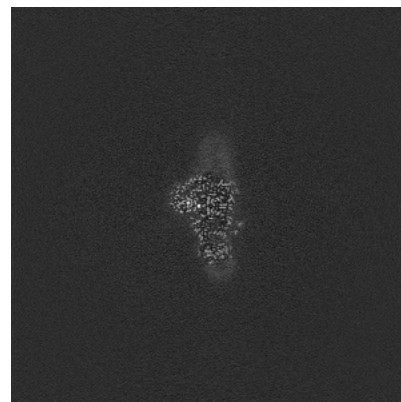
6.3.2 Raw map



X Index: 248



Y Index: 263

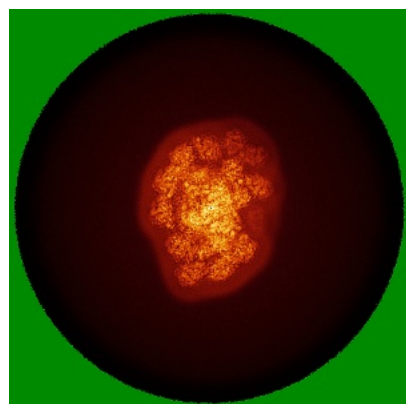


Z Index: 256

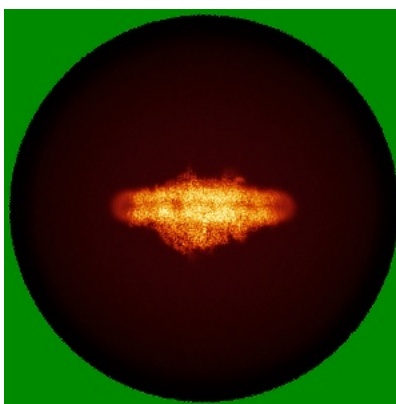
The images above show the largest variance slices of the map in three orthogonal directions.

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

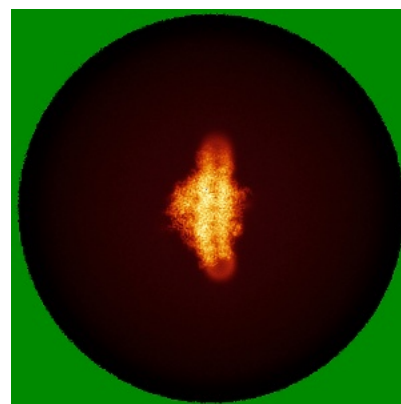
6.4.1 Primary map



X

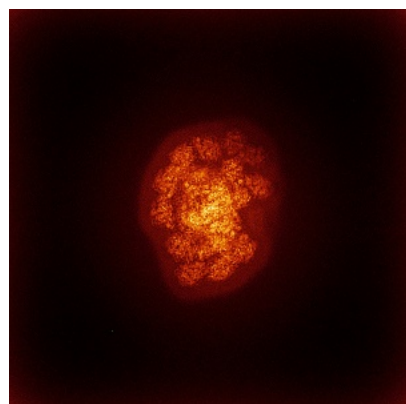


Y

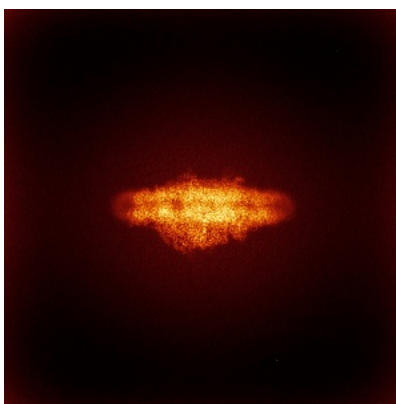


Z

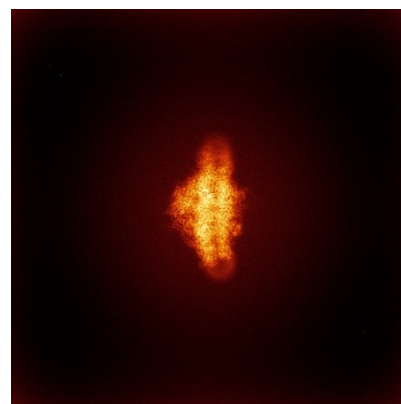
6.4.2 Raw map



X



Y

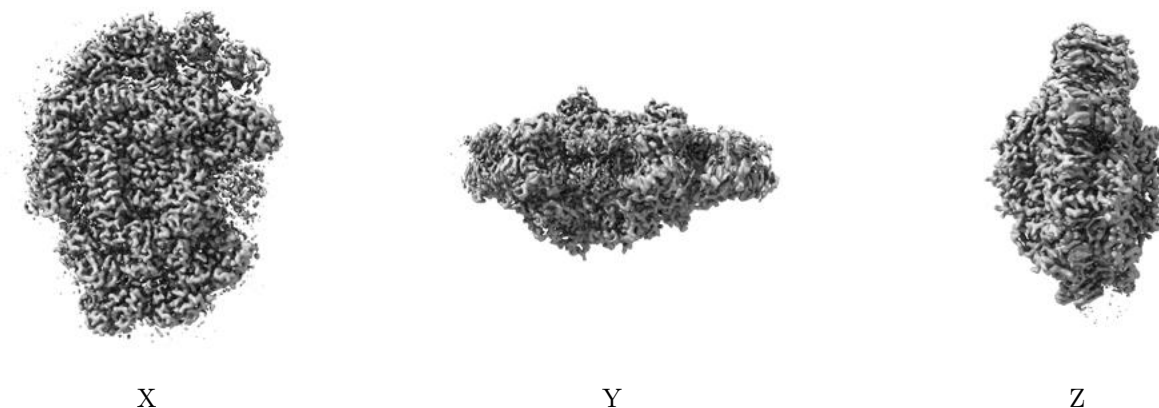


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.215. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

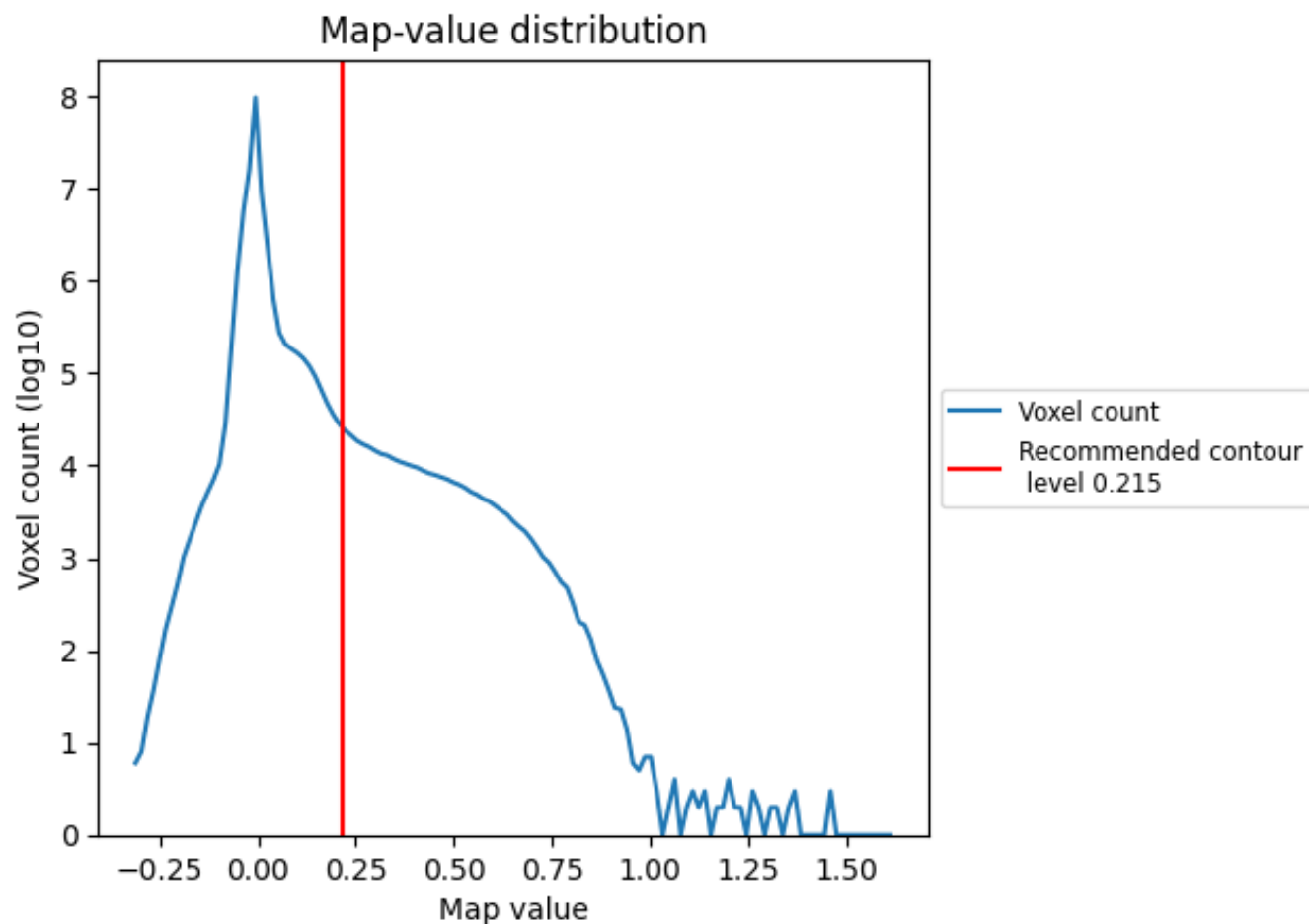
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

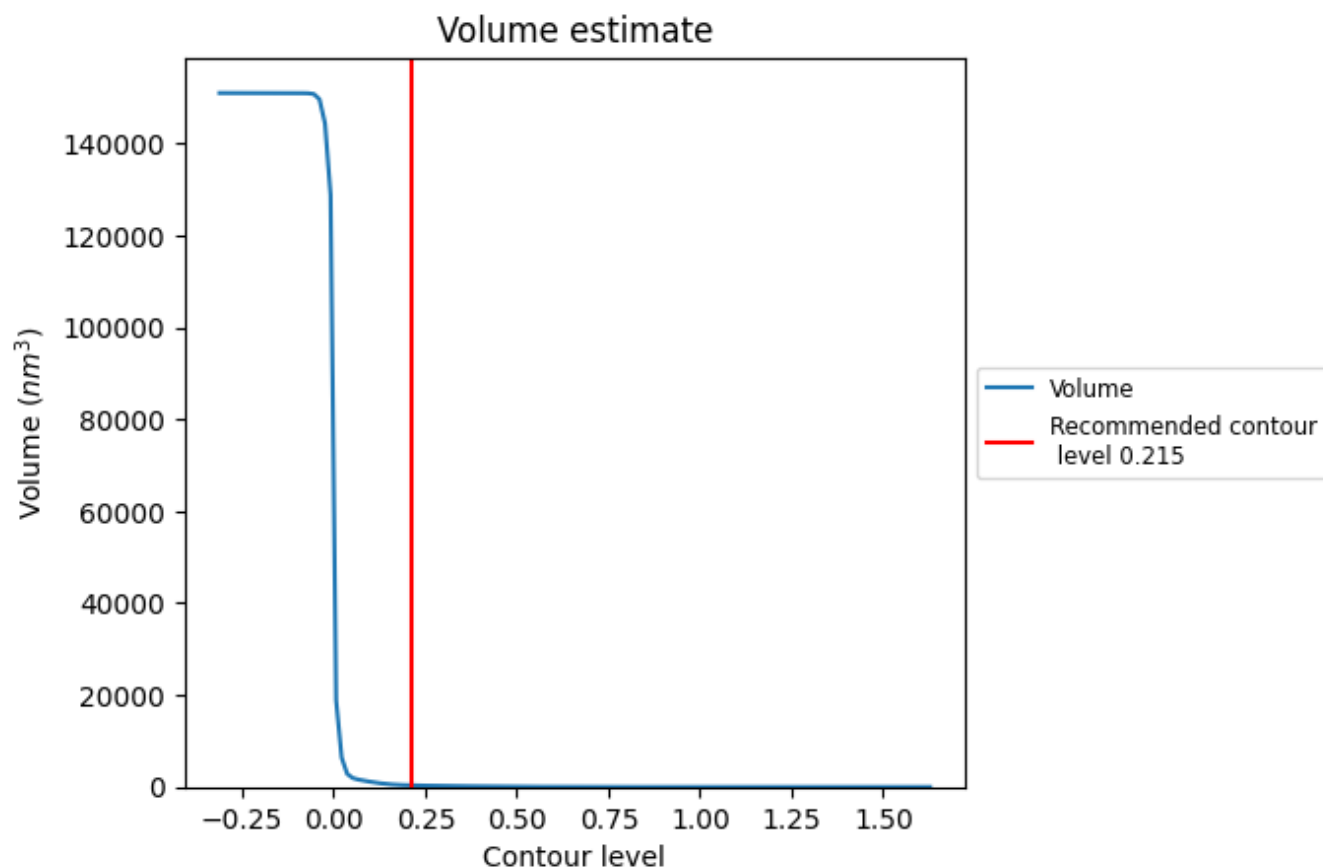
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

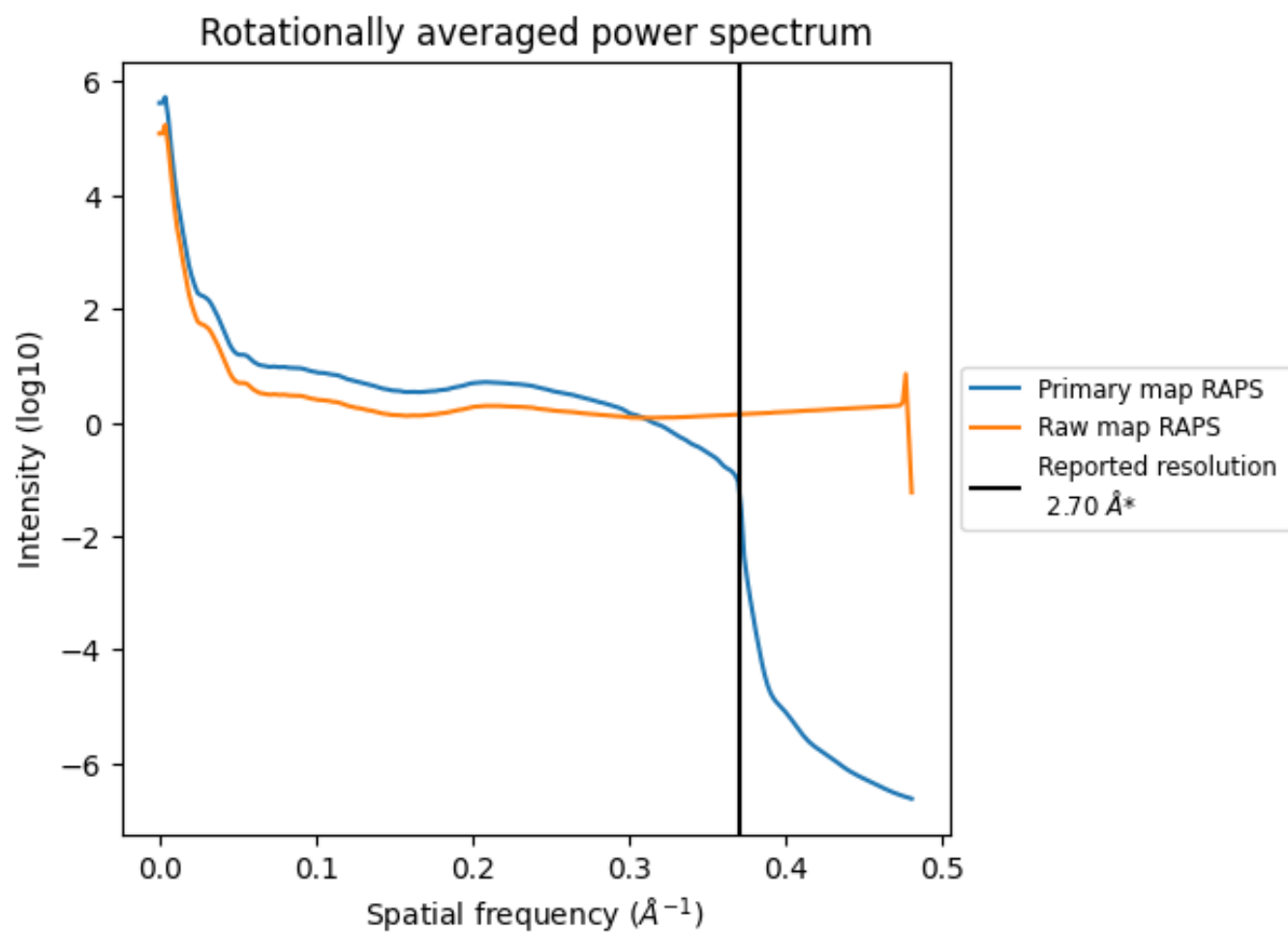
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm^3 ; this corresponds to an approximate mass of 311 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 ⓘ

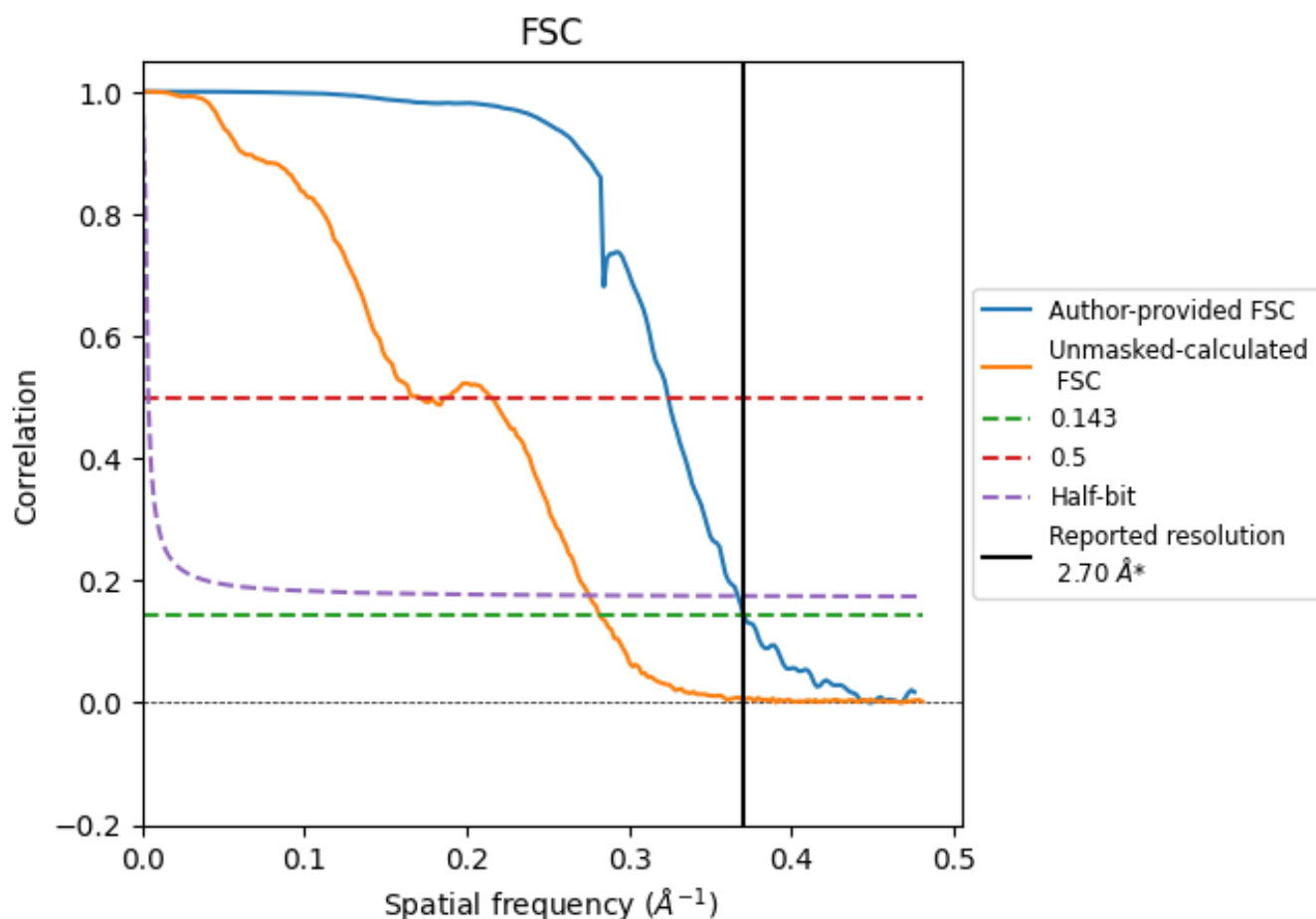


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.370 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.09	2.72
Unmasked-calculated*	3.55	5.84	3.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.55 differs from the reported value 2.7 by more than 10 %

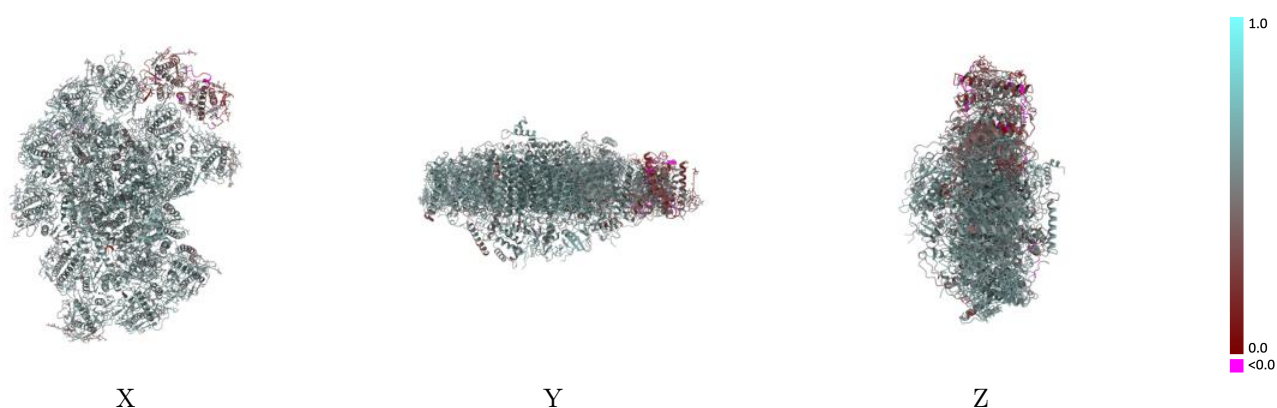
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36743 and PDB model 8JZF. Per-residue inclusion information can be found in section 3 on page 34.

9.1 Map-model overlay [i](#)

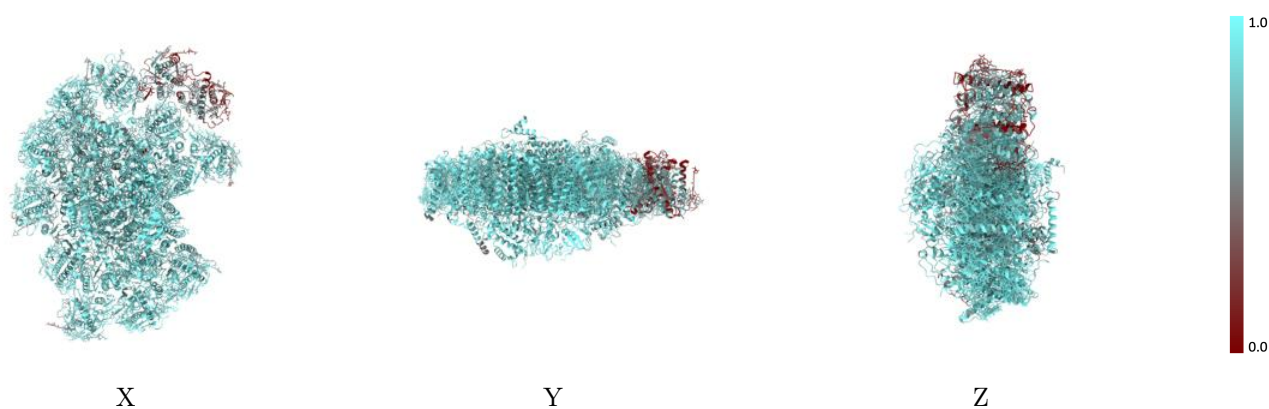
This section was not generated.

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



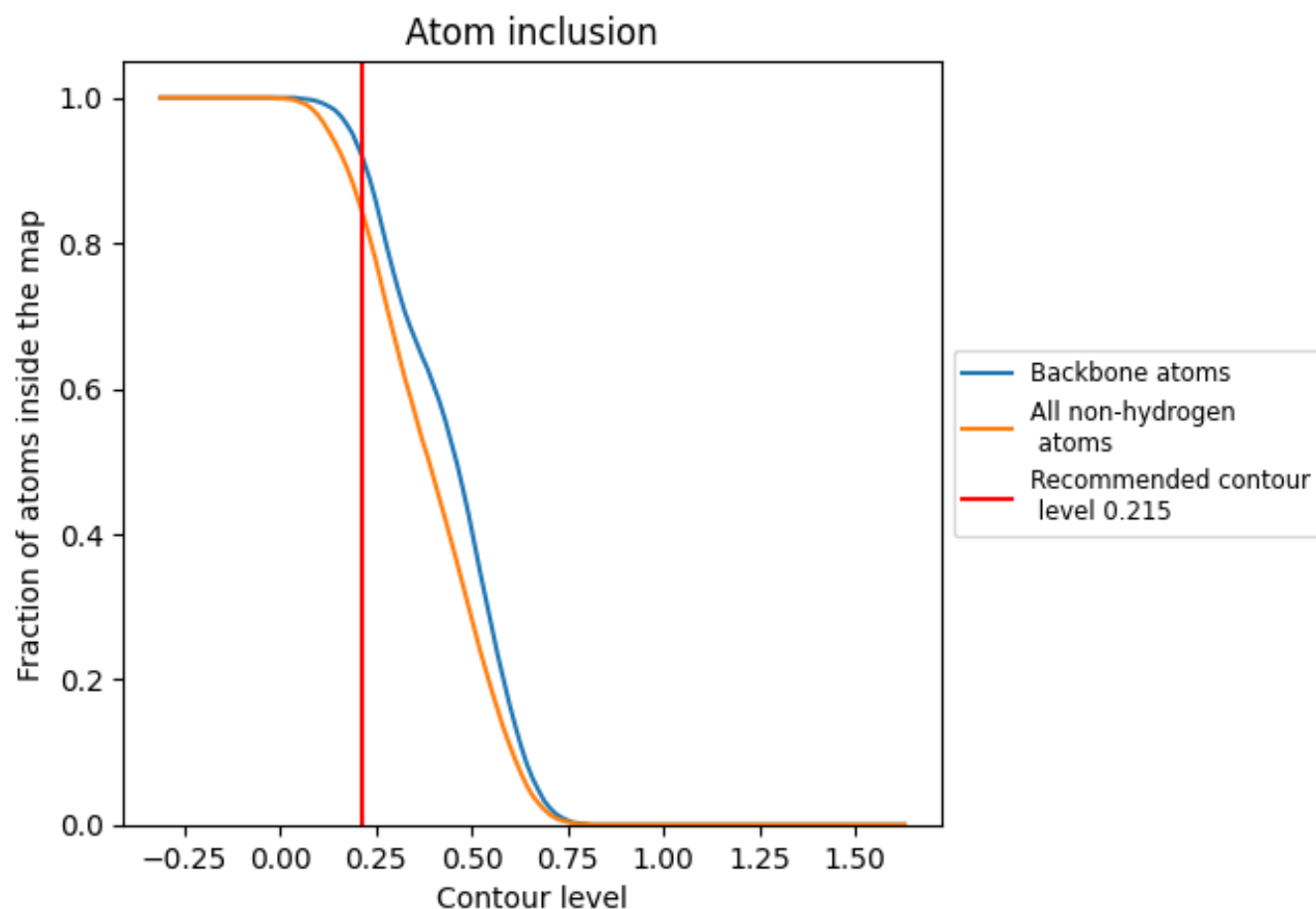
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.215).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5370
A	 0.8820	 0.5560
B	 0.8450	 0.5390
D	 0.8150	 0.5140
F	 0.7870	 0.5140
G	 0.8470	 0.5260
H	 0.3050	 0.2360
I	 0.8220	 0.5280
J	 0.8630	 0.5390
K	 0.8900	 0.5620
L	 0.8750	 0.5590
M	 0.8060	 0.5270
N	 0.4790	 0.3450
a	 0.8860	 0.5680
b	 0.9240	 0.5820
c	 0.9440	 0.5790
d	 0.8820	 0.5540
e	 0.9230	 0.5830
f	 0.8710	 0.5580
h	 0.9130	 0.5770
i	 0.8730	 0.5480
j	 0.8130	 0.5390
l	 0.9020	 0.5690
m	 0.8750	 0.5550
y	 0.8730	 0.5410
z	 0.9050	 0.5070

