



# wwPDB EM Validation Summary Report ⓘ

May 1, 2025 – 12:56 PM JST

PDB ID : 9KQB / pdb\_00009kqb  
EMDB ID : EMD-62499  
Title : PSII-FCPII supercomplex from haptophyte *Chrysotila roscoffensis*  
Authors : La Rocca, R.; Kato, K.; Tsai, P.-C.; Nakajima, Y.; Akita, F.; Shen, J.-R.  
Deposited on : 2024-11-25  
Resolution : 2.22 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

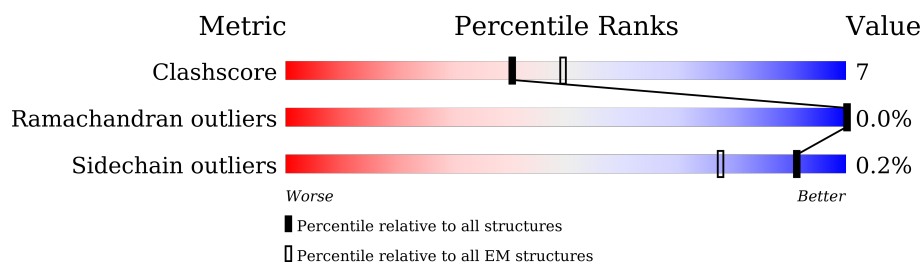
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.22 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.











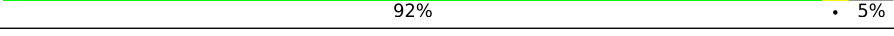

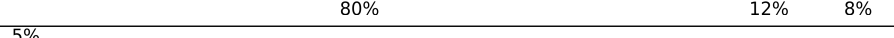
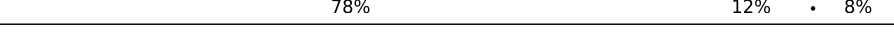

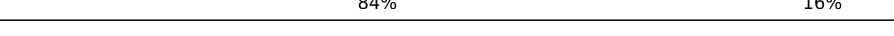


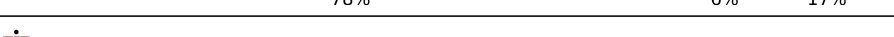

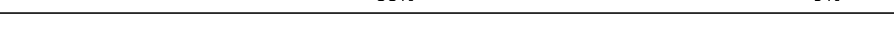






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1	166	 80% 17% 2% 1%
1	5	166	 68% 25% 6% 1%
1	7	166	 86% 13% 1%
1	g	166	 78% 16% 6% 1%
2	6	167	 74% 17% 8% 1%
2	J	167	 74% 18% 8% 1%
3	A	360	 78% 13% 9% 1%
3	a	360	 79% 12% 9% 1%

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Mol	Chain	Length	Quality of chain
4	B	509	
4	b	509	
5	E	82	
5	e	82	
6	F	42	
6	f	42	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	K	40	
9	k	40	
10	L	38	
10	l	38	
11	M	130	
11	m	130	
12	N	36	
12	n	36	
13	T	32	
13	t	32	
14	W	53	
14	w	53	
15	X	36	
15	x	36	
16	2	225	

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Mol	Chain	Length	Quality of chain
16	8	225	
17	D	351	
17	d	351	
18	C	445	
18	c	445	
19	3	216	
19	9	216	
20	4	167	
20	G	167	

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
21	CLA	1	301	X	-	-	-
21	CLA	1	302	X	-	-	-
21	CLA	1	303	X	-	-	-
21	CLA	1	304	X	-	-	-
21	CLA	1	306	X	-	-	-
21	CLA	1	307	X	-	-	-
21	CLA	1	309	X	-	-	-
21	CLA	2	301	X	-	-	-
21	CLA	2	302	X	-	-	-
21	CLA	2	303	X	-	-	-
21	CLA	2	305	X	-	-	-
21	CLA	3	301	X	-	-	-
21	CLA	3	302	X	-	-	-
21	CLA	4	300	X	-	-	-
21	CLA	4	301	X	-	-	-
21	CLA	4	303	X	-	-	-
21	CLA	4	304	X	-	-	-
21	CLA	5	302	X	-	-	-
21	CLA	5	303	X	-	-	-
21	CLA	5	305	X	-	-	-
21	CLA	5	306	X	-	-	-
21	CLA	5	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	6	300	X	-	-	-
21	CLA	6	301	X	-	-	-
21	CLA	6	302	X	-	-	-
21	CLA	6	303	X	-	-	-
21	CLA	6	304	X	-	-	-
21	CLA	6	305	X	-	-	-
21	CLA	6	306	X	-	-	-
21	CLA	6	307	X	-	-	-
21	CLA	6	308	X	-	-	-
21	CLA	7	300	X	-	-	-
21	CLA	7	301	X	-	-	-
21	CLA	7	302	X	-	-	-
21	CLA	7	303	X	-	-	-
21	CLA	7	304	X	-	-	-
21	CLA	7	305	X	-	-	-
21	CLA	7	306	X	-	-	-
21	CLA	7	307	X	-	-	-
21	CLA	7	308	X	-	-	-
21	CLA	8	302	X	-	-	-
21	CLA	8	303	X	-	-	-
21	CLA	8	306	X	-	-	-
21	CLA	8	307	X	-	-	-
21	CLA	9	300	X	-	-	-
21	CLA	9	302	X	-	-	-
21	CLA	9	303	X	-	-	-
21	CLA	9	304	X	-	-	-
21	CLA	B	602	X	-	-	-
21	CLA	B	603	X	-	-	-
21	CLA	B	604	X	-	-	-
21	CLA	B	610	X	-	-	-
21	CLA	B	612	X	-	-	-
21	CLA	B	613	X	-	-	-
21	CLA	B	614	X	-	-	-
21	CLA	B	615	X	-	-	-
21	CLA	B	616	X	-	-	-
21	CLA	C	503	X	-	-	-
21	CLA	C	508	X	-	-	-
21	CLA	C	509	X	-	-	-
21	CLA	C	511	X	-	-	-
21	CLA	C	512	X	-	-	-
21	CLA	C	514	X	-	-	-
21	CLA	D	404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	D	406	X	-	-	-
21	CLA	G	300	X	-	-	-
21	CLA	G	301	X	-	-	-
21	CLA	G	303	X	-	-	-
21	CLA	G	304	X	-	-	-
21	CLA	J	300	X	-	-	-
21	CLA	J	301	X	-	-	-
21	CLA	J	302	X	-	-	-
21	CLA	J	304	X	-	-	-
21	CLA	J	305	X	-	-	-
21	CLA	J	306	X	-	-	-
21	CLA	J	307	X	-	-	-
21	CLA	J	308	X	-	-	-
21	CLA	b	603	X	-	-	-
21	CLA	b	604	X	-	-	-
21	CLA	b	605	X	-	-	-
21	CLA	b	611	X	-	-	-
21	CLA	b	613	X	-	-	-
21	CLA	b	614	X	-	-	-
21	CLA	b	615	X	-	-	-
21	CLA	b	616	X	-	-	-
21	CLA	b	617	X	-	-	-
21	CLA	b	623	X	-	-	-
21	CLA	c	502	X	-	-	-
21	CLA	c	507	X	-	-	-
21	CLA	c	508	X	-	-	-
21	CLA	c	510	X	-	-	-
21	CLA	c	511	X	-	-	-
21	CLA	c	512	X	-	-	-
21	CLA	c	513	X	-	-	-
21	CLA	d	404	X	-	-	-
21	CLA	d	405	X	-	-	-
21	CLA	g	302	X	-	-	-
21	CLA	g	303	X	-	-	-
21	CLA	g	305	X	-	-	-
21	CLA	g	306	X	-	-	-
21	CLA	g	309	X	-	-	-

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 61348 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 Fucoxanthin chlorophyll a/c binding protein II (FCPII-1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	164	Total	C	N	O	S	0	0
			1281	834	206	238	3		
1	7	164	Total	C	N	O	S	0	0
			1278	833	206	236	3		
1	5	156	Total	C	N	O	S	0	0
			1217	789	198	227	3		
1	g	156	Total	C	N	O	S	0	0
			1217	789	198	227	3		

- Molecule 2 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPII-5).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	6	154	Total	C	N	O	S	0	0
			1191	778	197	213	3		
2	J	154	Total	C	N	O	S	0	0
			1191	778	197	213	3		

- Molecule 3 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	328	Total	C	N	O	S	0	0
			2565	1678	418	454	15		
3	a	329	Total	C	N	O	S	0	0
			2575	1684	421	455	15		

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	484	Total	C	N	O	S	0	0
			3796	2479	647	657	13		
4	b	484	Total	C	N	O	S	0	0
			3796	2479	647	657	13		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	LEU	MET	conflict	UNP Q4G3C5
B	146	ALA	SER	conflict	UNP Q4G3C5
B	161	ALA	THR	conflict	UNP Q4G3C5
B	174	VAL	ILE	conflict	UNP Q4G3C5
B	187	PRO	ALA	conflict	UNP Q4G3C5
B	210	ILE	LEU	conflict	UNP Q4G3C5
B	290	ALA	SER	conflict	UNP Q4G3C5
B	292	ILE	LEU	conflict	UNP Q4G3C5
b	106	LEU	MET	conflict	UNP Q4G3C5
b	146	ALA	SER	conflict	UNP Q4G3C5
b	161	ALA	THR	conflict	UNP Q4G3C5
b	174	VAL	ILE	conflict	UNP Q4G3C5
b	187	PRO	ALA	conflict	UNP Q4G3C5
b	210	ILE	LEU	conflict	UNP Q4G3C5
b	290	ALA	SER	conflict	UNP Q4G3C5
b	292	ILE	LEU	conflict	UNP Q4G3C5

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	66	Total	C	N	O	0	0
			539	352	89	98		
5	e	66	Total	C	N	O	0	0
			539	352	89	98		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	32	Total	C	N	O	S	0	0
			265	181	43	40	1		
6	f	32	Total	C	N	O	S	0	0
			265	181	43	40	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H (psbH).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	64	Total	C	N	O	S	0	0
			502	333	80	87	2		
7	h	64	Total	C	N	O	S	0	0
			502	333	80	87	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I (psbI).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	36	Total	C	N	O	S	0	0
			298	201	46	50	1		
8	i	36	Total	C	N	O	S	0	0
			298	201	46	50	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K (psbK).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	37	Total	C	N	O	S	0	0
			295	203	45	46	1		
9	k	37	Total	C	N	O	S	0	0
			295	203	45	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	38	Total	C	N	O	S	0	0
			312	210	48	53	1		
10	l	38	Total	C	N	O	S	0	0
			312	210	48	53	1		

- Molecule 11 is a protein called Photosystem II reaction center protein M (psbM).

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	53	Total	C	N	O	0	0
			397	261	63	73		
11	m	53	Total	C	N	O	0	0
			397	261	63	73		

- Molecule 12 is a protein called Photosystem II reaction center protein Psb36.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	N	30	Total	C	N	O	0	0
			202	133	31	38		
12	n	30	Total	C	N	O	0	0
			202	133	31	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	31	Total	C	N	O	S	0	0
			258	181	38	38	1		
13	t	31	Total	C	N	O	S	0	0
			258	181	38	38	1		

- Molecule 14 is a protein called Photosystem II reaction center protein W (psbW).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	44	Total	C	N	O	S	0	0
			342	217	55	70			
14	w	44	Total	C	N	O	S	0	0
			342	217	55	70			

- Molecule 15 is a protein called Photosystem II reaction center protein X (psbX).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	34	Total	C	N	O	S	0	0
			240	161	34	44	1		
15	x	34	Total	C	N	O	S	0	0
			240	161	34	44	1		

- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPII-2).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	211	Total	C	N	O	S	0	0
			1657	1074	280	296	7		
16	8	212	Total	C	N	O	S	0	0
			1664	1079	281	297	7		

- Molecule 17 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	333	Total	C	N	O	S	0	0
			2644	1750	431	452	11		
17	d	327	Total	C	N	O	S	0	0
			2597	1720	424	442	11		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	282	SER	ALA	conflict	UNP Q4G395
D	283	LEU	ILE	conflict	UNP Q4G395

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Chain	Residue	Modelled	Actual	Comment	Reference
D	294	SER	ALA	conflict	UNP Q4G395
d	282	SER	ALA	conflict	UNP Q4G395
d	283	LEU	ILE	conflict	UNP Q4G395
d	294	SER	ALA	conflict	UNP Q4G395

- Molecule 18 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	C	416	Total	C	N	O	S	0	0
			3268	2148	547	560	13		
18	c	416	Total	C	N	O	S	0	0
			3268	2148	547	560	13		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	79	ASP	ASN	conflict	UNP A0A075DWU3
C	144	SER	CYS	conflict	UNP A0A075DWU3
C	170	ILE	VAL	conflict	UNP A0A075DWU3
C	172	THR	SER	conflict	UNP A0A075DWU3
C	253	VAL	GLY	conflict	UNP A0A075DWU3
C	259	SER	ALA	conflict	UNP A0A075DWU3
C	399	THR	CYS	conflict	UNP A0A075DWU3
C	400	THR	CYS	conflict	UNP A0A075DWU3
c	79	ASP	ASN	conflict	UNP A0A075DWU3
c	144	SER	CYS	conflict	UNP A0A075DWU3
c	170	ILE	VAL	conflict	UNP A0A075DWU3
c	172	THR	SER	conflict	UNP A0A075DWU3
c	253	VAL	GLY	conflict	UNP A0A075DWU3
c	259	SER	ALA	conflict	UNP A0A075DWU3
c	399	THR	CYS	conflict	UNP A0A075DWU3
c	400	THR	CYS	conflict	UNP A0A075DWU3

- Molecule 19 is a protein called Light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	98	Total	C	N	O	S	0	0
			770	495	136	133	6		
19	3	98	Total	C	N	O	S	0	0
			770	495	136	133	6		

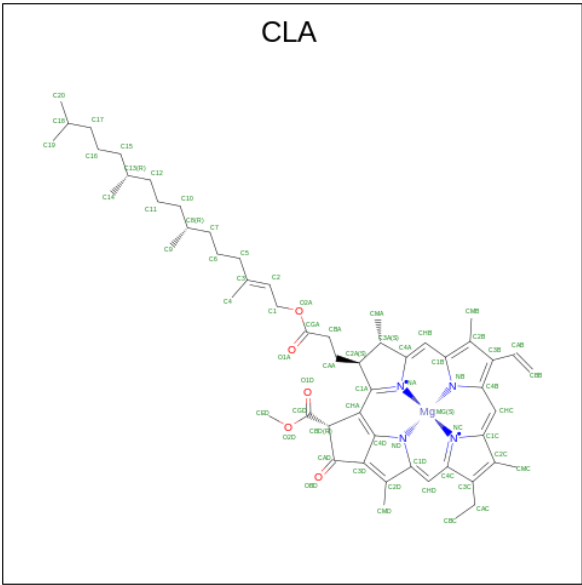
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	8	LEU	PHE	conflict	UNP A0A7S4BJL5
9	77	MET	ILE	conflict	UNP A0A7S4BJL5
3	8	LEU	PHE	conflict	UNP A0A7S4BJL5
3	77	MET	ILE	conflict	UNP A0A7S4BJL5

- Molecule 20 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPII-4).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	104	Total	C	N	O	S	0	0
			822	532	140	147	3		
20	G	104	Total	C	N	O	S	0	0
			822	532	140	147	3		

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	1	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	6	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	6	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	7	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	B	1	Total 61	C 52	Mg 1	N 4	O 4	0
21	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	J	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	J	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	J	1	Total 43	C 33	Mg 1	N 4	O 5	0
21	J	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	J	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	b	1	Total 61	C 52	Mg 1	N 4	O 4	0
21	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	2	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	8	1	Total 58	C 48	Mg 1	N 4	O 5	0
21	8	1	Total 43	C 35	Mg 1	N 4	O 3	0
21	D	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	D	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	d	1	Total 59	C 49	Mg 1	N 4	O 5	0
21	d	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	c	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	c	1	Total 64	C 54	Mg 1	N 4	O 5	0
21	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	9	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	9	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	3	1	Total 57	C 47	Mg 1	N 4	O 5	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0

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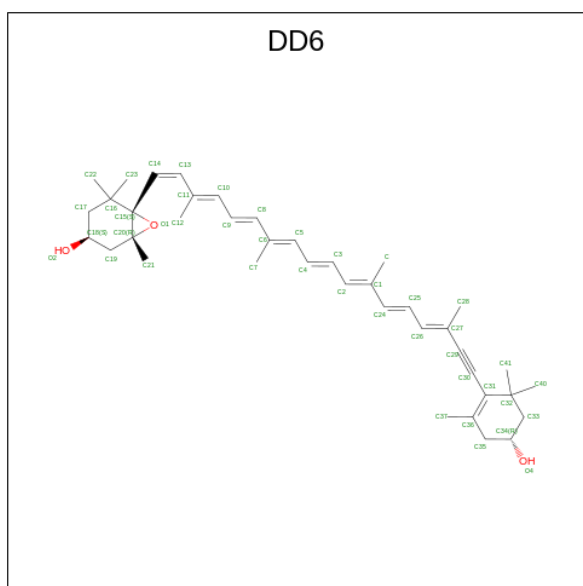
Mol	Chain	Residues	Atoms					AltConf
21	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	5	1	Total 48	C 38	Mg 1	N 4	O 5	0
21	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	g	1	Total 54	C 44	Mg 1	N 4	O 5	0
21	g	1	Total 41	C 33	Mg 1	N 4	O 3	0
21	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	G	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

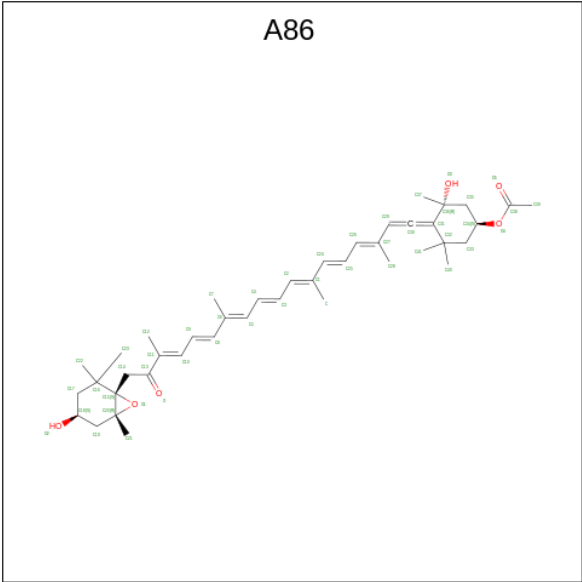
- Molecule 22 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula:  $C_{40}H_{54}O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			43	40	3	
22	7	1	Total	C	O	0
			43	40	3	
22	5	1	Total	C	O	0
			43	40	3	
22	g	1	Total	C	O	0
			43	40	3	

- Molecule 23 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula:  $C_{42}H_{58}O_6$ ) (labeled as "Ligand of Interest" by depositor).





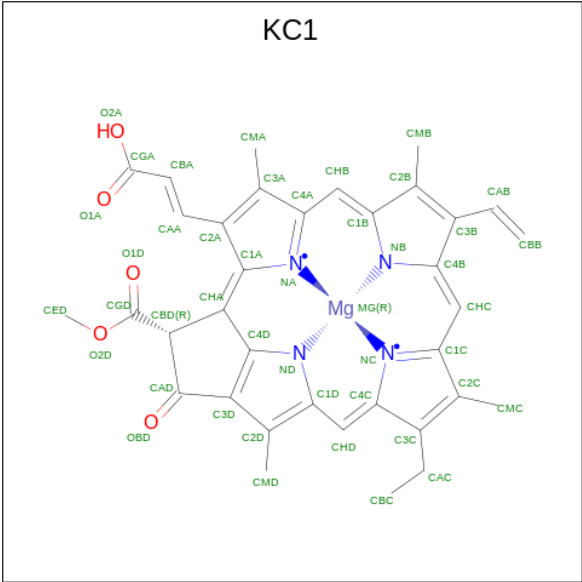
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			48	42	6	
23	1	1	Total	C	O	0
			48	42	6	
23	1	1	Total	C	O	0
			48	42	6	
23	6	1	Total	C	O	0
			48	42	6	
23	6	1	Total	C	O	0
			48	42	6	
23	7	1	Total	C	O	0
			48	42	6	
23	7	1	Total	C	O	0
			48	42	6	
23	7	1	Total	C	O	0
			44	40	4	
23	J	1	Total	C	O	0
			48	42	6	
23	J	1	Total	C	O	0
			48	42	6	
23	W	1	Total	C	O	0
			48	42	6	
23	2	1	Total	C	O	0
			48	42	6	
23	2	1	Total	C	O	0
			48	42	6	
23	2	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
23	2	1	Total	C	O	0
			48	42	6	
23	2	1	Total	C	O	0
			48	42	6	
23	2	1	Total	C	O	0
			48	42	6	
23	8	1	Total	C	O	0
			48	42	6	
23	8	1	Total	C	O	0
			48	42	6	
23	8	1	Total	C	O	0
			48	42	6	
23	8	1	Total	C	O	0
			48	42	6	
23	8	1	Total	C	O	0
			48	42	6	
23	4	1	Total	C	O	0
			48	42	6	
23	5	1	Total	C	O	0
			48	42	6	
23	5	1	Total	C	O	0
			48	42	6	
23	g	1	Total	C	O	0
			48	42	6	
23	g	1	Total	C	O	0
			48	42	6	
23	G	1	Total	C	O	0
			48	42	6	

- Molecule 24 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
24	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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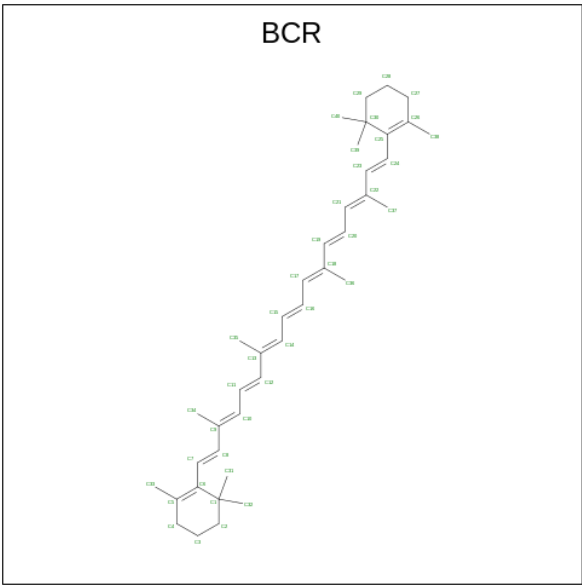
Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	4	1	Total 38	C 30	Mg 1	N 4	O 3	0
24	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	G	1	Total 38	C 30	Mg 1	N 4	O 3	0
24	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	G	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	G	1	45	35	1	4	5	0

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



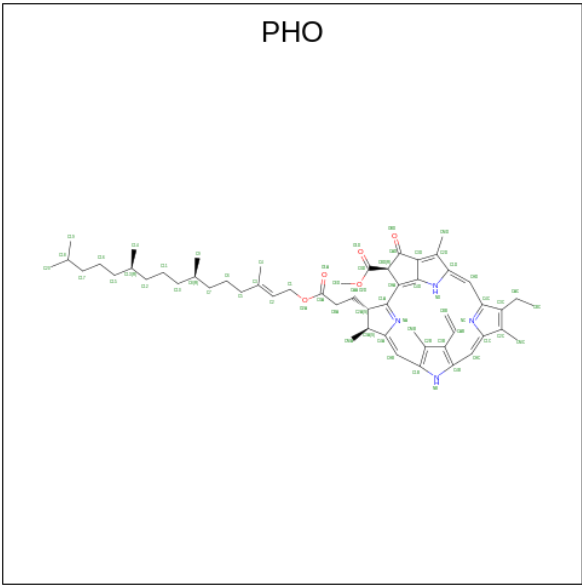
Mol	Chain	Residues	Atoms		AltConf
25	1	1	Total	C	0
			40	40	
25	A	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	B	1	Total	C	0
			40	40	
25	H	1	Total	C	0
			40	40	
25	M	1	Total	C	0
			40	40	
25	a	1	Total	C	0
			40	40	
25	b	1	Total	C	0
			40	40	
25	b	1	Total	C	0
			40	40	
25	h	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
25	h	1	Total C 40 40	0
25	m	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	d	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	c	1	Total C 40 40	0

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>) (labeled as "Lig- and of Interest" by depositor).



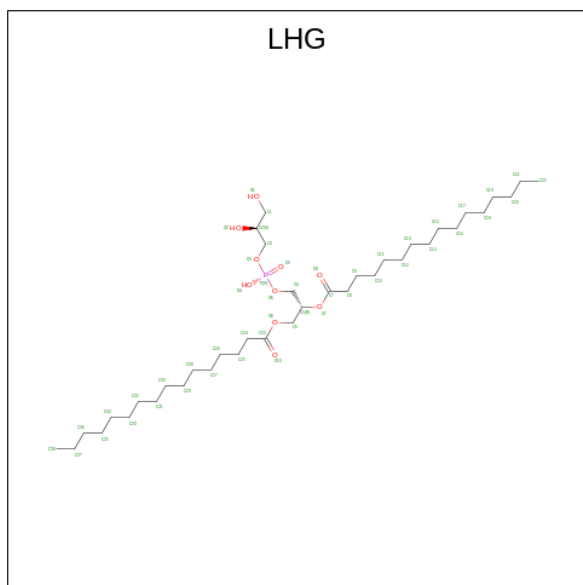
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C N O 64 55 4 5	0
26	a	1	Total C N O 64 55 4 5	0
26	D	1	Total C N O 64 55 4 5	0

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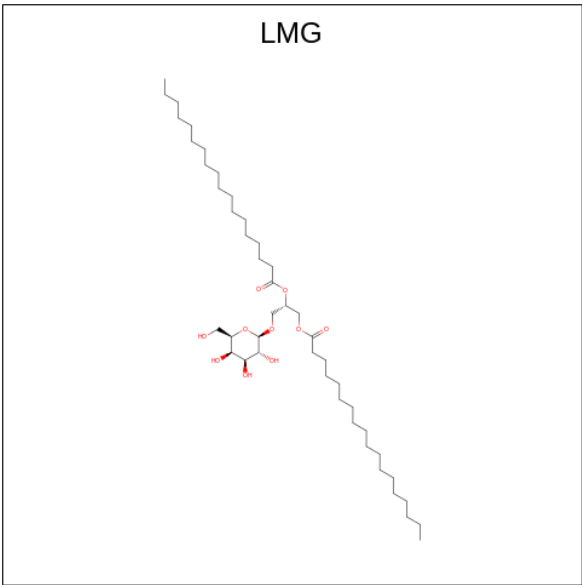
Mol	Chain	Residues	Atoms				AltConf
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 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
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	B	1	Total	C	O	P	0
			49	38	10	1	
27	a	1	Total	C	O	P	0
			49	38	10	1	
27	l	1	Total	C	O	P	0
			49	38	10	1	
27	D	1	Total	C	O	P	0
			43	32	10	1	
27	D	1	Total	C	O	P	0
			48	38	9	1	
27	d	1	Total	C	O	P	0
			43	32	10	1	
27	d	1	Total	C	O	P	0
			48	38	9	1	

- Molecule 28 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
28	A	1	Total	C	O	0
			48	38	10	
28	B	1	Total	C	O	0
			51	41	10	
28	B	1	Total	C	O	0
			28	18	10	
28	B	1	Total	C	O	0
			37	27	10	
28	B	1	Total	C	O	0
			43	33	10	
28	B	1	Total	C	O	0
			40	30	10	
28	L	1	Total	C	O	0
			40	30	10	
28	M	1	Total	C	O	0
			40	30	10	
28	N	1	Total	C	O	0
			24	15	9	
28	a	1	Total	C	O	0
			48	38	10	
28	b	1	Total	C	O	0
			51	41	10	
28	b	1	Total	C	O	0
			28	18	10	
28	b	1	Total	C	O	0
			35	25	10	
28	b	1	Total	C	O	0
			37	27	10	

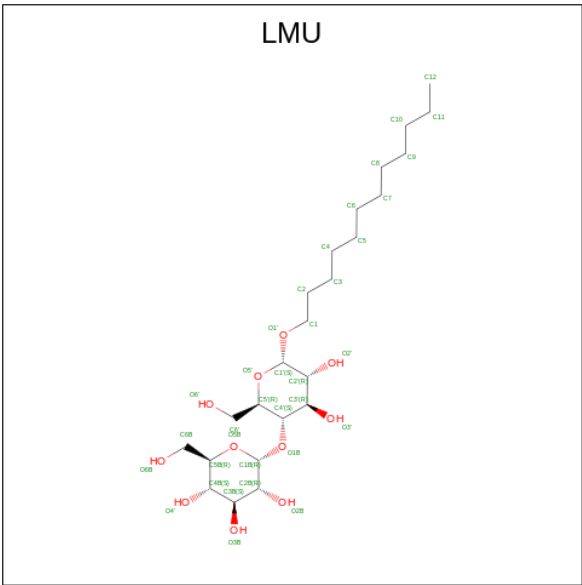
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Mol	Chain	Residues	Atoms			AltConf
28	b	1	Total	C	O	0
			43	33	10	
28	b	1	Total	C	O	0
			37	27	10	
28	f	1	Total	C	O	0
			46	36	10	
28	2	1	Total	C	O	0
			46	36	10	
28	8	1	Total	C	O	0
			24	15	9	
28	8	1	Total	C	O	0
			51	41	10	
28	D	1	Total	C	O	0
			46	36	10	

- Molecule 29 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



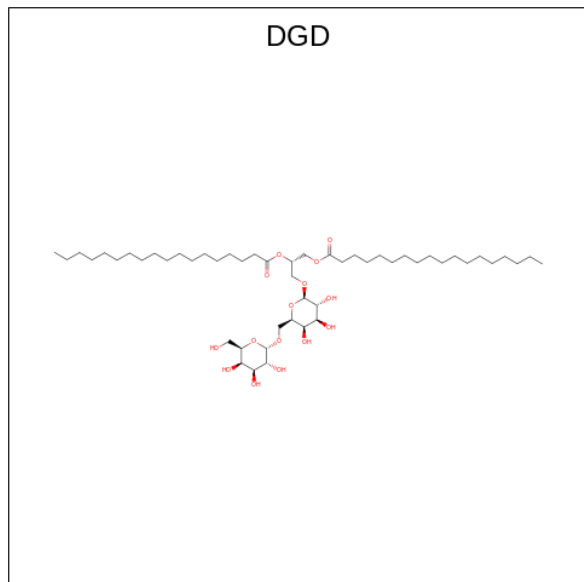
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			35	24	11	
29	a	1	Total	C	O	0
			35	24	11	
29	2	1	Total	C	O	0
			35	24	11	
29	8	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
29	D	1	Total	C	O	0
			35	24	11	
29	5	1	Total	C	O	0
			32	21	11	
29	5	1	Total	C	O	0
			23	13	10	
29	g	1	Total	C	O	0
			32	21	11	
29	g	1	Total	C	O	0
			24	13	11	

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



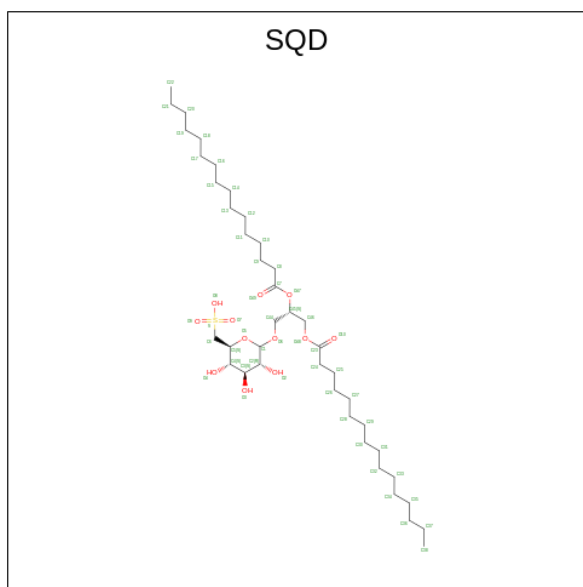
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			53	39	14	
30	H	1	Total	C	O	0
			62	47	15	
30	b	1	Total	C	O	0
			53	39	14	
30	h	1	Total	C	O	0
			62	47	15	
30	C	1	Total	C	O	0
			55	40	15	
30	C	1	Total	C	O	0
			39	26	13	

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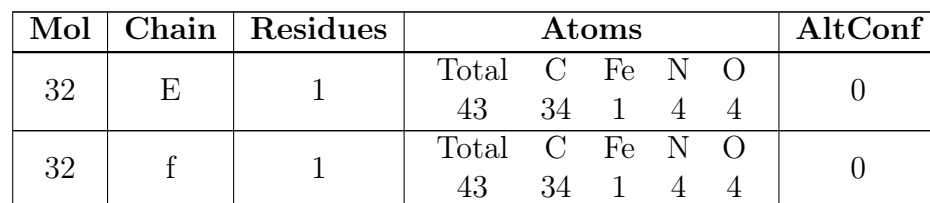
Mol	Chain	Residues	Atoms			AltConf
30	c	1	Total	C	O	0
			55	40	15	
30	c	1	Total	C	O	0
			39	26	13	

- Molecule 31 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
31	B	1	Total	C	O	S	0
			49	36	12	1	
31	B	1	Total	C	O	S	0
			54	41	12	1	
31	X	1	Total	C	O	S	0
			37	24	12	1	
31	b	1	Total	C	O	S	0
			54	41	12	1	
31	C	1	Total	C	O	S	0
			51	38	12	1	

- Molecule 32 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



- BCT
- 
- The diagram shows the chemical structure of Bicarbonate (BCT). A central carbon atom (labeled 'C' in green) is bonded to three oxygen atoms and one hydrogen atom. One oxygen atom (labeled 'O1' in green) is double-bonded to the carbon. Another oxygen atom (labeled 'O2' in green) is single-bonded to the carbon and carries a negative charge (O<sup>-</sup>). The third oxygen atom (labeled 'O3' in green) is single-bonded to the carbon and is part of a hydroxyl group (OH). The hydrogen atom is also labeled 'O3' in green. The bonds are shown in grey, with red lines indicating the double bond and the single bonds to the negatively charged oxygen and the hydroxyl group.

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



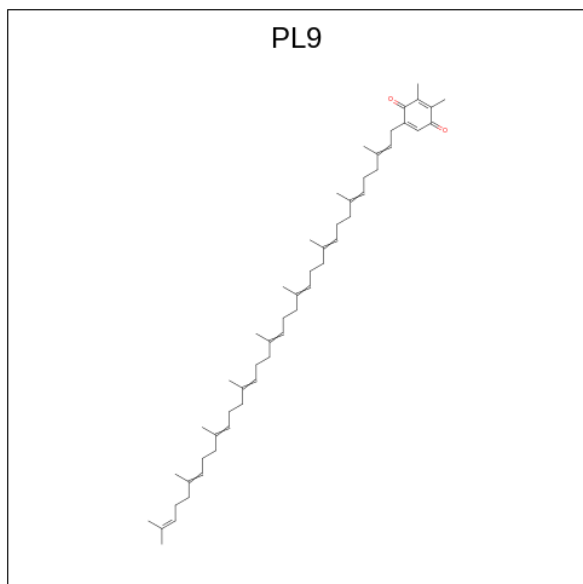
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
33	d	1	Total	C	O	0
			4	1	3	

- Molecule 34 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 35 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	6	3	Total O 3 3	0
36	A	15	Total O 15 15	0
36	B	29	Total O 29 29	0
36	E	1	Total O 1 1	0
36	H	5	Total O 5 5	0
36	J	1	Total O 1 1	0
36	L	1	Total O 1 1	0
36	M	2	Total O 2 2	0
36	T	3	Total O 3 3	0
36	X	2	Total O 2 2	0
36	a	15	Total O 15 15	0
36	b	28	Total O 28 28	0
36	e	2	Total O 2 2	0
36	h	5	Total O 5 5	0
36	l	1	Total O 1 1	0
36	m	2	Total O 2 2	0
36	t	3	Total O 3 3	0
36	x	2	Total O 2 2	0
36	2	3	Total O 3 3	0
36	D	25	Total O 25 25	0
36	d	23	Total O 23 23	0
36	C	5	Total O 5 5	0

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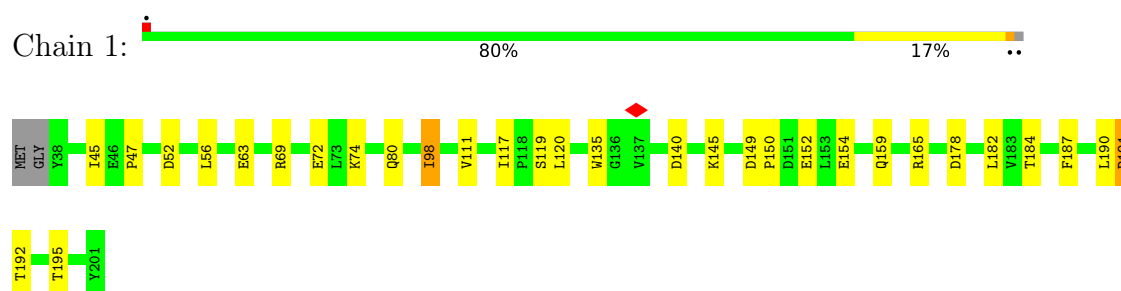
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
36	c	4	Total	O	0
			4	4	
36	5	1	Total	O	0
			1	1	

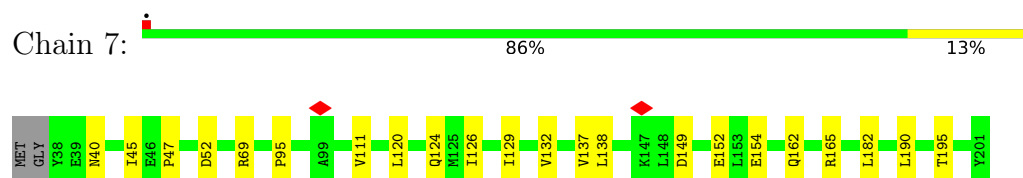
### 3 Residue-property plots [i](#)

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

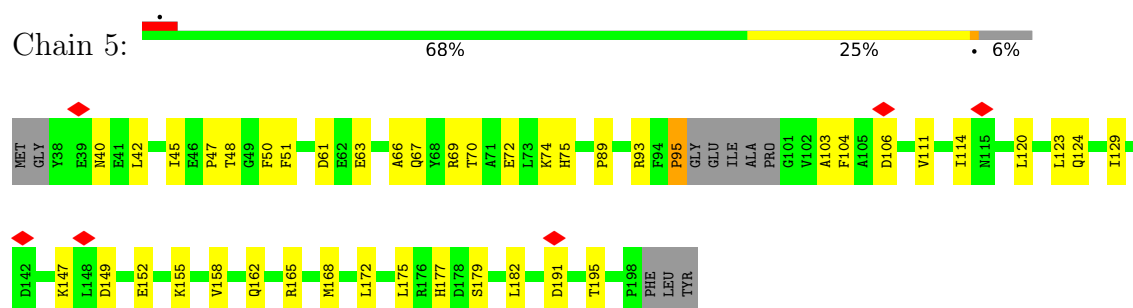
- Molecule 1: Fucoxanthin chlorophyll a/c binding protein II (FCPII-1)



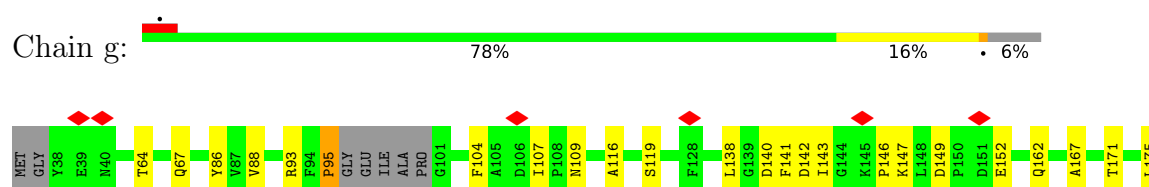
- Molecule 1: Fucoxanthin chlorophyll a/c binding protein II (FCPII-1)



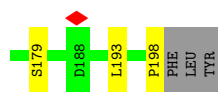
- Molecule 1: Fucoxanthin chlorophyll a/c binding protein II (FCPII-1)



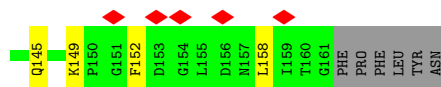
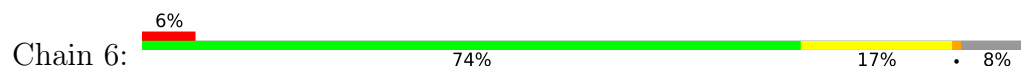
- Molecule 1: Fucoxanthin chlorophyll a/c binding protein II (FCPII-1)



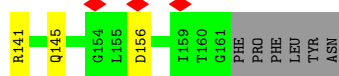
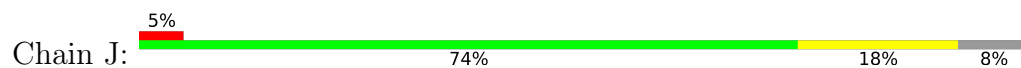




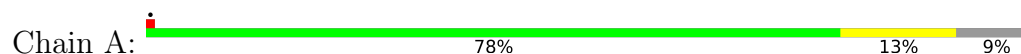
- Molecule 2: Fucoxanthin chlorophyll a/c binding protein II (FCPII-5)



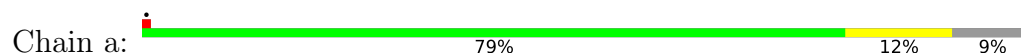
- Molecule 2: Fucoxanthin chlorophyll a/c binding protein II (FCPII-5)



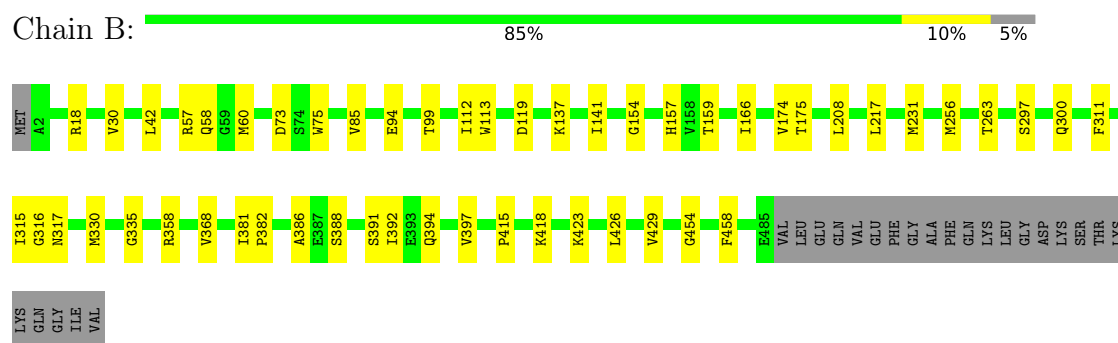
- Molecule 3: Photosystem II protein D1



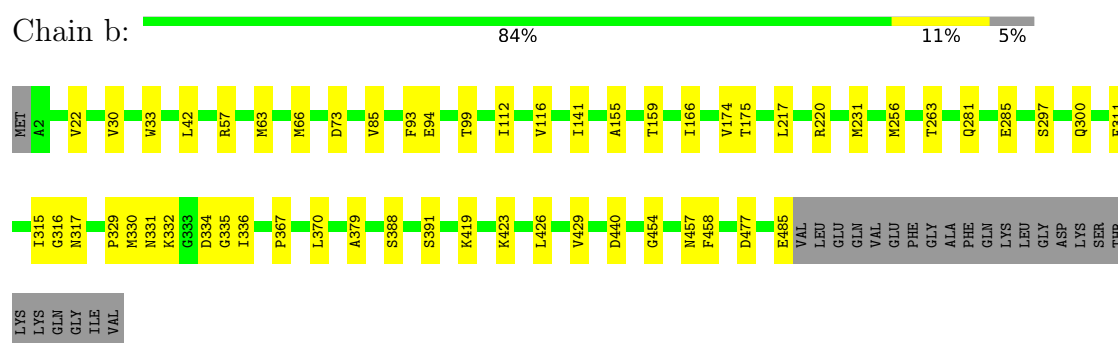
- Molecule 3: Photosystem II protein D1



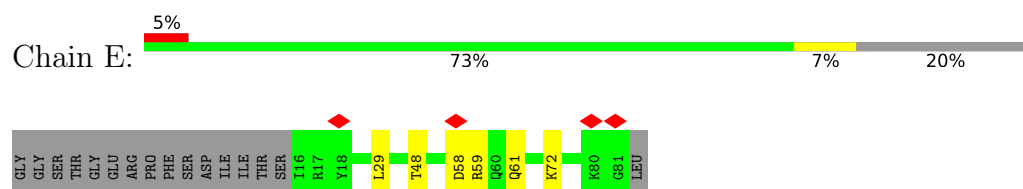
- Molecule 4: Photosystem II CP47 reaction center protein



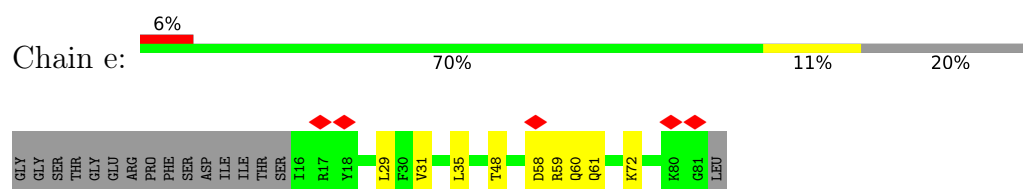
- Molecule 4: Photosystem II CP47 reaction center protein



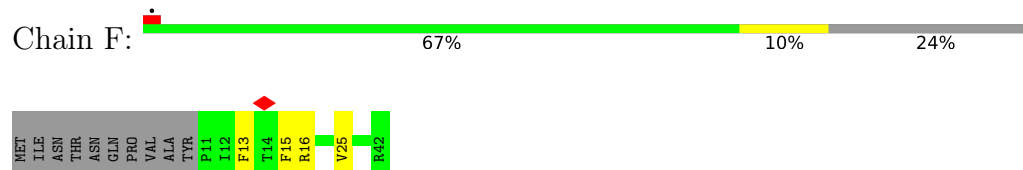
- Molecule 5: Cytochrome b559 subunit alpha



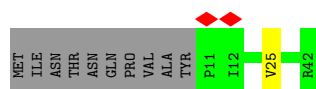
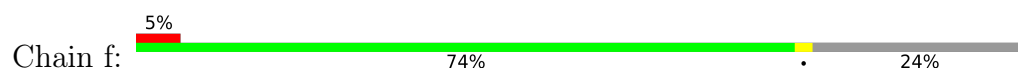
- Molecule 5: Cytochrome b559 subunit alpha



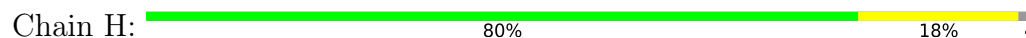
- Molecule 6: Cytochrome b559 subunit beta



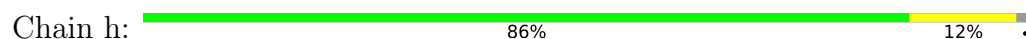
- Molecule 6: Cytochrome b559 subunit beta



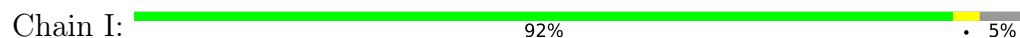
- Molecule 7: Photosystem II reaction center protein H (psbH)



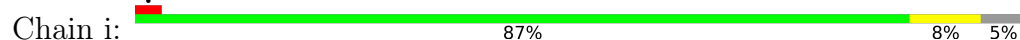
- Molecule 7: Photosystem II reaction center protein H (psbH)



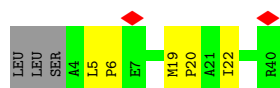
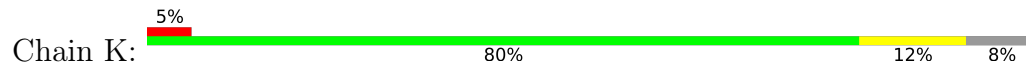
- Molecule 8: Photosystem II reaction center protein I (psbI)



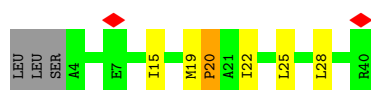
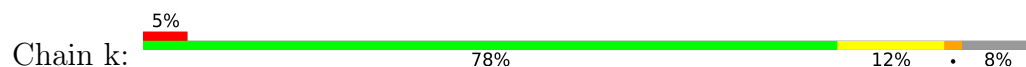
- Molecule 8: Photosystem II reaction center protein I (psbI)




- Molecule 9: Photosystem II reaction center protein K (psbK)



- Molecule 9: Photosystem II reaction center protein K (psbK)




- Molecule 10: Photosystem II reaction center protein L

Chain L:  82% 18%



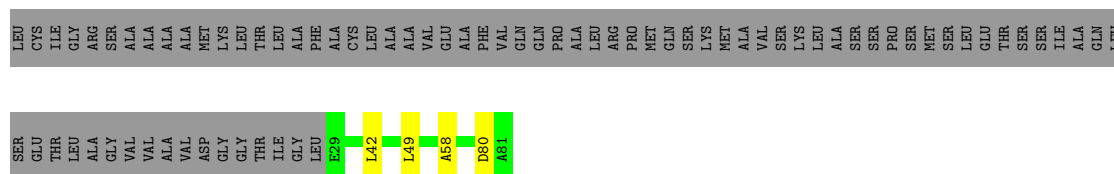
- Molecule 10: Photosystem II reaction center protein L

Chain l:  84% 16%




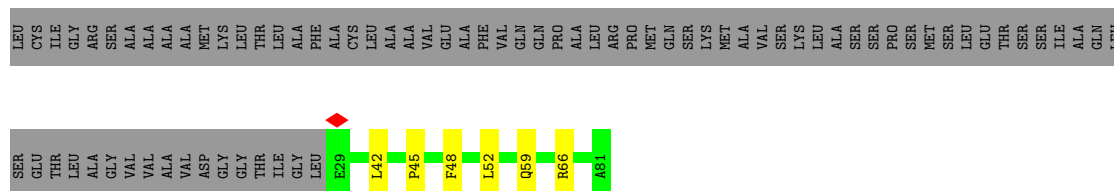
- Molecule 11: Photosystem II reaction center protein M (psbM)

Chain M:  38% 59%




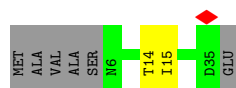
- Molecule 11: Photosystem II reaction center protein M (psbM)

Chain m:  36% 5% 59%




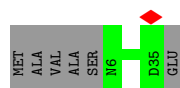
- Molecule 12: Photosystem II reaction center protein Psb36

Chain N:  78% 6% 17%




- Molecule 12: Photosystem II reaction center protein Psb36

Chain n:  83% 17%




- Molecule 13: Photosystem II reaction center protein T

Chain T:  88% 9%



- Molecule 13: Photosystem II reaction center protein T

Chain t:  91% 6%



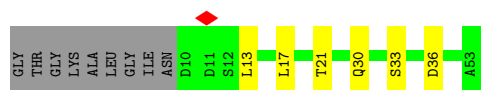
- Molecule 14: Photosystem II reaction center protein W (psbW)

Chain W:  66% 17% 17%




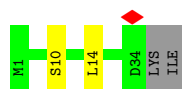
- Molecule 14: Photosystem II reaction center protein W (psbW)

Chain w:  72% 11% 17%




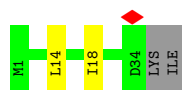
- Molecule 15: Photosystem II reaction center protein X (psbX)

Chain X:  89% 6% 6%




- Molecule 15: Photosystem II reaction center protein X (psbX)

Chain x:  89% 6% 6%



- Molecule 16: Fucoxanthin chlorophyll a/c binding protein II (FCPII-2)

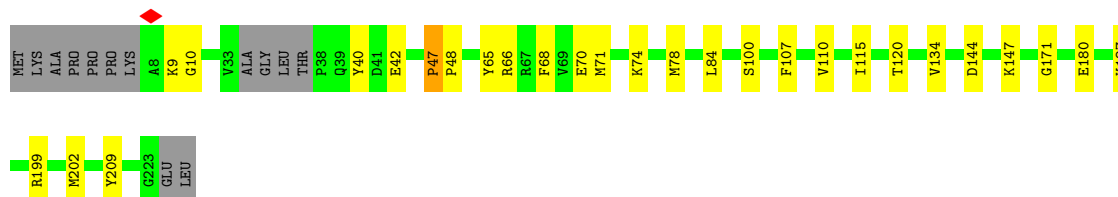
Chain 2:  78% 15% 6%





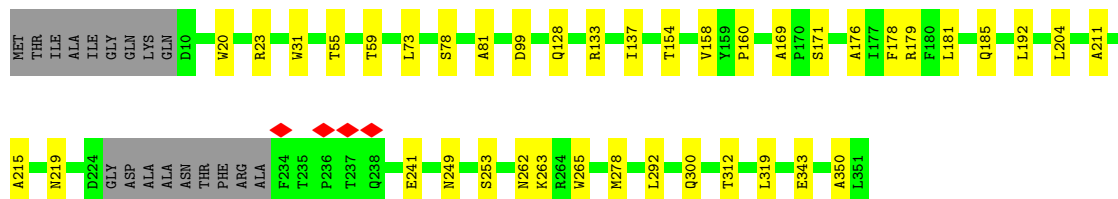
- Molecule 16: Fucoxanthin chlorophyll a/c binding protein II (FCPII-2)

Chain 8: 82% 12% 6%



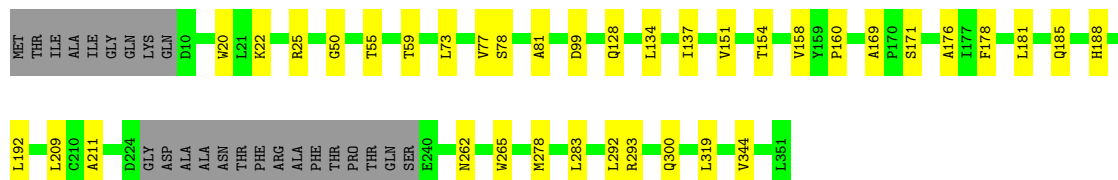
- Molecule 17: Photosystem II D2 protein

Chain D: 83% 11% 5%



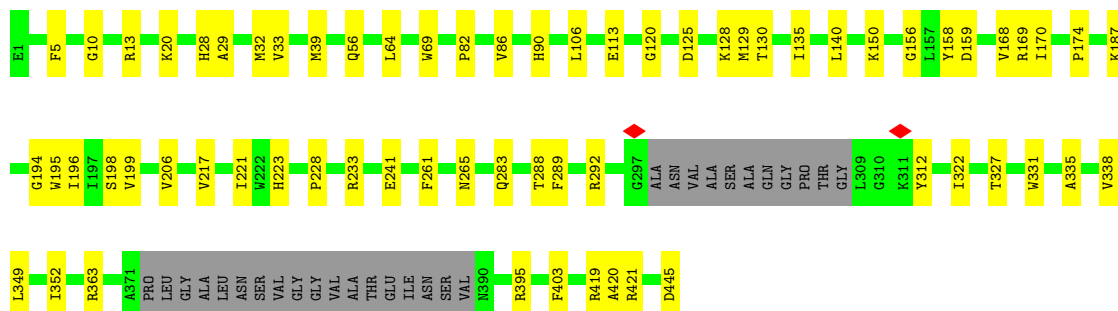
- Molecule 17: Photosystem II D2 protein

Chain d: 83% 11% 7%

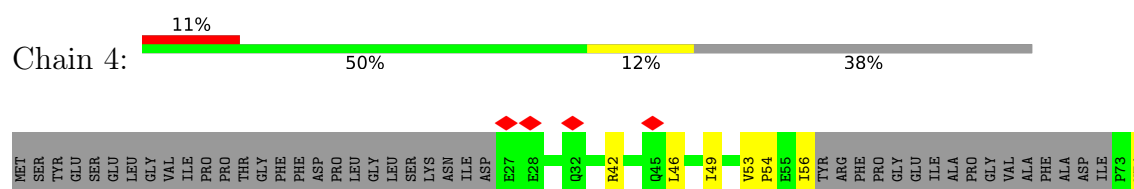


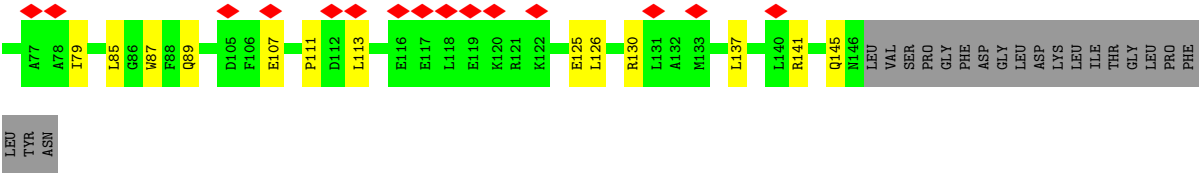
- Molecule 18: Photosystem II CP43 reaction center protein

Chain C: 79% 15% 7%

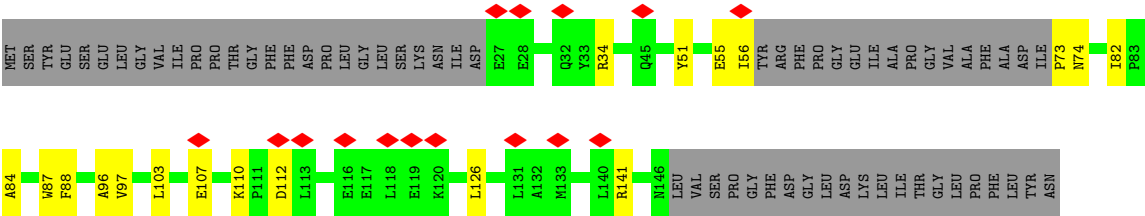


- Molecule 18: Photosystem II CP43 reaction center protein





● Molecule 20: Fucoxanthin chlorophyll a/c binding protein II (FCPII-4)





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	38582	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.298	Depositor
Minimum map value	-0.110	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	1	0.23	0/1314	0.49	0/1791
1	5	0.57	1/1246 (0.1%)	0.71	2/1696 (0.1%)
1	7	0.29	1/1311 (0.1%)	0.49	1/1787 (0.1%)
1	g	0.65	2/1246 (0.2%)	0.77	3/1696 (0.2%)
2	6	0.29	0/1223	0.57	0/1665
2	J	0.24	0/1223	0.52	0/1665
3	A	0.21	0/2648	0.45	0/3609
3	a	0.21	0/2659	0.45	0/3624
4	B	0.23	1/3923 (0.0%)	0.38	1/5341 (0.0%)
4	b	0.17	0/3923	0.37	0/5341
5	E	0.17	0/554	0.44	0/753
5	e	0.18	0/554	0.42	0/753
6	F	0.22	0/274	0.65	0/371
6	f	0.16	0/274	0.48	0/371
7	H	0.16	0/512	0.42	0/699
7	h	0.16	0/512	0.42	0/699
8	I	0.19	0/306	0.43	0/413
8	i	0.19	0/306	0.43	0/413
9	K	0.42	0/306	0.70	1/420 (0.2%)
9	k	0.59	1/306 (0.3%)	0.61	0/420
10	L	0.20	0/322	0.35	0/438
10	l	0.17	0/322	0.31	0/438
11	M	0.20	0/406	0.45	0/555
11	m	0.18	0/406	0.44	0/555
12	N	0.17	0/205	0.46	0/280
12	n	0.20	0/205	0.56	0/280
13	T	0.16	0/265	0.33	0/359
13	t	0.15	0/265	0.30	0/359
14	W	0.13	0/350	0.39	0/477
14	w	0.13	0/350	0.45	0/477
15	X	0.21	0/243	0.54	0/334
15	x	0.21	0/243	0.48	0/334

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2	0.20	0/1702	0.46	1/2314 (0.0%)
16	8	0.18	0/1710	0.46	1/2325 (0.0%)
17	D	0.16	0/2733	0.38	0/3724
17	d	0.16	0/2684	0.39	0/3656
18	C	0.18	0/3379	0.40	0/4604
18	c	0.18	0/3379	0.39	0/4604
19	3	0.19	0/785	0.53	0/1057
19	9	0.18	0/785	0.48	0/1057
20	4	0.24	0/840	0.57	0/1136
20	G	0.22	0/840	0.50	0/1136
All	All	0.24	6/47039 (0.0%)	0.46	10/64026 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	95	PRO	N-CD	19.50	1.75	1.47
1	5	95	PRO	N-CD	17.70	1.72	1.47
4	B	415	PRO	N-CD	10.63	1.62	1.47
9	k	20	PRO	N-CD	-8.29	1.36	1.47
1	7	95	PRO	N-CD	7.15	1.57	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	95	PRO	CA-N-CD	-17.29	87.79	112.00
1	5	95	PRO	CA-N-CD	-11.82	95.46	112.00
1	g	95	PRO	N-CD-CG	-7.59	91.82	103.20
1	5	95	PRO	N-CD-CG	-7.31	92.23	103.20
1	g	198	PRO	CA-N-CD	-7.09	102.07	112.00

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	1	1281	0	1258	26	0
1	5	1217	0	1196	34	0
1	7	1278	0	1256	18	0
1	g	1217	0	1196	23	0
2	6	1191	0	1187	26	0
2	J	1191	0	1187	23	0
3	A	2565	0	2446	42	0
3	a	2575	0	2453	36	0
4	B	3796	0	3687	38	0
4	b	3796	0	3687	40	0
5	E	539	0	527	6	0
5	e	539	0	527	10	0
6	F	265	0	273	3	0
6	f	265	0	273	1	0
7	H	502	0	524	10	0
7	h	502	0	524	6	0
8	I	298	0	308	1	0
8	i	298	0	308	2	0
9	K	295	0	304	3	0
9	k	295	0	304	7	0
10	L	312	0	315	8	0
10	l	312	0	315	5	0
11	M	397	0	397	4	0
11	m	397	0	397	6	0
12	N	202	0	208	2	0
12	n	202	0	208	0	0
13	T	258	0	281	4	0
13	t	258	0	281	2	0
14	W	342	0	304	6	0
14	w	342	0	304	4	0
15	X	240	0	267	1	0
15	x	240	0	267	1	0
16	2	1657	0	1647	32	0
16	8	1664	0	1655	21	0
17	D	2644	0	2553	31	0
17	d	2597	0	2510	28	0
18	C	3268	0	3190	48	0
18	c	3268	0	3190	61	0
19	3	770	0	781	11	0
19	9	770	0	781	15	0
20	4	822	0	818	15	0
20	G	822	0	818	20	0
21	1	558	0	535	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2	317	0	286	11	0
21	3	262	0	229	9	0
21	4	292	0	285	11	0
21	5	457	0	447	12	0
21	6	467	0	412	8	0
21	7	563	0	551	17	0
21	8	308	0	269	12	0
21	9	270	0	237	10	0
21	A	174	0	170	4	0
21	B	1011	0	1082	30	0
21	C	806	0	853	21	0
21	D	176	0	164	7	0
21	G	294	0	289	3	0
21	J	467	0	412	9	0
21	a	174	0	170	5	0
21	b	1002	0	1061	38	0
21	c	798	0	834	24	0
21	d	176	0	164	6	0
21	g	436	0	404	11	0
22	1	43	0	0	1	0
22	5	43	0	0	0	0
22	7	43	0	0	1	0
22	g	43	0	0	0	0
23	1	144	0	0	0	0
23	2	288	0	0	0	0
23	4	48	0	0	0	0
23	5	96	0	0	1	0
23	6	96	0	0	0	0
23	7	140	0	0	0	0
23	8	240	0	0	0	0
23	G	48	0	0	0	0
23	J	96	0	0	0	0
23	W	48	0	0	0	0
23	g	96	0	0	0	0
24	1	90	0	0	0	0
24	2	180	0	0	5	0
24	3	90	0	0	0	0
24	4	173	0	0	0	0
24	5	135	0	0	1	0
24	6	135	0	0	0	0
24	7	90	0	0	0	0
24	8	180	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	9	90	0	0	0	0
24	G	173	0	0	2	0
24	J	135	0	0	1	0
24	g	135	0	0	1	0
25	1	40	0	56	3	0
25	A	40	0	56	5	0
25	B	80	0	112	7	0
25	C	80	0	112	4	0
25	D	40	0	56	1	0
25	H	40	0	56	2	0
25	M	40	0	56	2	0
25	a	40	0	56	5	0
25	b	80	0	112	3	0
25	c	80	0	112	2	0
25	d	40	0	56	1	0
25	h	80	0	112	4	0
25	m	40	0	56	0	0
26	A	64	0	74	2	0
26	D	64	0	74	2	0
26	a	64	0	74	1	0
26	d	64	0	74	2	0
27	A	49	0	74	3	0
27	B	49	0	74	3	0
27	D	91	0	133	6	0
27	a	49	0	74	1	0
27	d	91	0	133	4	0
27	l	49	0	74	2	0
28	2	46	0	65	3	0
28	8	75	0	99	4	0
28	A	48	0	66	1	0
28	B	199	0	248	6	0
28	D	46	0	62	0	0
28	L	40	0	50	1	0
28	M	40	0	50	2	0
28	N	24	0	24	1	0
28	a	48	0	66	2	0
28	b	231	0	282	5	0
28	f	46	0	62	0	0
29	2	35	0	46	0	0
29	5	55	0	55	2	0
29	8	35	0	46	1	0
29	A	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	D	35	0	46	1	0
29	a	35	0	46	0	0
29	g	56	0	58	1	0
30	B	53	0	64	4	0
30	C	94	0	110	1	0
30	H	62	0	82	3	0
30	b	53	0	64	3	0
30	c	94	0	110	4	0
30	h	62	0	82	0	0
31	B	103	0	140	3	0
31	C	51	0	69	1	0
31	X	37	0	38	0	0
31	b	54	0	78	3	0
32	E	43	0	30	1	0
32	f	43	0	30	1	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	D	1	0	0	0	0
34	d	1	0	0	0	0
35	D	55	0	80	2	0
35	d	55	0	80	2	0
36	2	3	0	0	0	0
36	5	1	0	0	0	0
36	6	3	0	0	0	0
36	A	15	0	0	0	0
36	B	29	0	0	1	0
36	C	5	0	0	1	0
36	D	25	0	0	0	0
36	E	1	0	0	0	0
36	H	5	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	M	2	0	0	0	0
36	T	3	0	0	0	0
36	X	2	0	0	0	0
36	a	15	0	0	0	0
36	b	28	0	0	0	0
36	c	4	0	0	0	0
36	d	23	0	0	0	0
36	e	2	0	0	0	0
36	h	5	0	0	0	0
36	l	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	m	2	0	0	0	0
36	t	3	0	0	0	0
36	x	2	0	0	0	0
All	All	61348	0	58108	809	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 7.

The worst 5 of 809 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)
20:G:82:ILE:HD11	20:G:87:TRP:CZ2	1.37	1.52
1:5:95:PRO:N	1:5:95:PRO:CD	1.72	1.39
1:g:95:PRO:CD	1:g:95:PRO:N	1.75	1.32
20:G:82:ILE:CD1	20:G:87:TRP:CZ2	2.33	1.11
20:G:82:ILE:HD11	20:G:87:TRP:CE2	1.88	1.06

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	1	162/166 (98%)	159 (98%)	2 (1%)	1 (1%)	22	22
1	5	152/166 (92%)	145 (95%)	7 (5%)	0	100	100
1	7	162/166 (98%)	160 (99%)	2 (1%)	0	100	100
1	g	152/166 (92%)	140 (92%)	12 (8%)	0	100	100
2	6	152/167 (91%)	147 (97%)	5 (3%)	0	100	100
2	J	152/167 (91%)	147 (97%)	5 (3%)	0	100	100
3	A	326/360 (91%)	316 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	a	327/360 (91%)	321 (98%)	6 (2%)	0	100	100
4	B	482/509 (95%)	476 (99%)	6 (1%)	0	100	100
4	b	482/509 (95%)	472 (98%)	10 (2%)	0	100	100
5	E	64/82 (78%)	64 (100%)	0	0	100	100
5	e	64/82 (78%)	64 (100%)	0	0	100	100
6	F	30/42 (71%)	29 (97%)	1 (3%)	0	100	100
6	f	30/42 (71%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	34/38 (90%)	34 (100%)	0	0	100	100
8	i	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
9	K	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
9	k	35/40 (88%)	35 (100%)	0	0	100	100
10	L	36/38 (95%)	36 (100%)	0	0	100	100
10	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	M	51/130 (39%)	51 (100%)	0	0	100	100
11	m	51/130 (39%)	51 (100%)	0	0	100	100
12	N	28/36 (78%)	28 (100%)	0	0	100	100
12	n	28/36 (78%)	28 (100%)	0	0	100	100
13	T	29/32 (91%)	29 (100%)	0	0	100	100
13	t	29/32 (91%)	29 (100%)	0	0	100	100
14	W	42/53 (79%)	41 (98%)	1 (2%)	0	100	100
14	w	42/53 (79%)	41 (98%)	1 (2%)	0	100	100
15	X	32/36 (89%)	32 (100%)	0	0	100	100
15	x	32/36 (89%)	32 (100%)	0	0	100	100
16	2	207/225 (92%)	203 (98%)	4 (2%)	0	100	100
16	8	208/225 (92%)	200 (96%)	8 (4%)	0	100	100
17	D	329/351 (94%)	321 (98%)	8 (2%)	0	100	100
17	d	323/351 (92%)	318 (98%)	5 (2%)	0	100	100
18	C	410/445 (92%)	400 (98%)	10 (2%)	0	100	100
18	c	410/445 (92%)	399 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	3	92/216 (43%)	89 (97%)	3 (3%)	0	100	100
19	9	92/216 (43%)	89 (97%)	3 (3%)	0	100	100
20	4	100/167 (60%)	97 (97%)	3 (3%)	0	100	100
20	G	100/167 (60%)	98 (98%)	2 (2%)	0	100	100
All	All	5706/6728 (85%)	5573 (98%)	132 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	191	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	134/135 (99%)	133 (99%)	1 (1%)	81	89
1	5	128/135 (95%)	127 (99%)	1 (1%)	79	87
1	7	133/135 (98%)	133 (100%)	0	100	100
1	g	128/135 (95%)	127 (99%)	1 (1%)	79	87
2	6	123/135 (91%)	121 (98%)	2 (2%)	58	71
2	J	123/135 (91%)	123 (100%)	0	100	100
3	A	263/287 (92%)	263 (100%)	0	100	100
3	a	264/287 (92%)	262 (99%)	2 (1%)	79	87
4	B	384/405 (95%)	384 (100%)	0	100	100
4	b	384/405 (95%)	384 (100%)	0	100	100
5	E	58/71 (82%)	58 (100%)	0	100	100
5	e	58/71 (82%)	57 (98%)	1 (2%)	56	69
6	F	28/37 (76%)	28 (100%)	0	100	100
6	f	28/37 (76%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	55/56 (98%)	55 (100%)	0	100	100
7	h	55/56 (98%)	55 (100%)	0	100	100
8	I	35/37 (95%)	35 (100%)	0	100	100
8	i	35/37 (95%)	35 (100%)	0	100	100
9	K	31/34 (91%)	31 (100%)	0	100	100
9	k	31/34 (91%)	31 (100%)	0	100	100
10	L	35/35 (100%)	35 (100%)	0	100	100
10	l	35/35 (100%)	35 (100%)	0	100	100
11	M	41/99 (41%)	41 (100%)	0	100	100
11	m	41/99 (41%)	41 (100%)	0	100	100
12	N	19/23 (83%)	19 (100%)	0	100	100
12	n	19/23 (83%)	19 (100%)	0	100	100
13	T	28/29 (97%)	28 (100%)	0	100	100
13	t	28/29 (97%)	28 (100%)	0	100	100
14	W	33/38 (87%)	33 (100%)	0	100	100
14	w	33/38 (87%)	33 (100%)	0	100	100
15	X	29/31 (94%)	29 (100%)	0	100	100
15	x	29/31 (94%)	29 (100%)	0	100	100
16	2	170/181 (94%)	170 (100%)	0	100	100
16	8	171/181 (94%)	171 (100%)	0	100	100
17	D	272/284 (96%)	272 (100%)	0	100	100
17	d	266/284 (94%)	266 (100%)	0	100	100
18	C	334/353 (95%)	333 (100%)	1 (0%)	91	95
18	c	334/353 (95%)	334 (100%)	0	100	100
19	3	78/177 (44%)	78 (100%)	0	100	100
19	9	78/177 (44%)	78 (100%)	0	100	100
20	4	83/135 (62%)	83 (100%)	0	100	100
20	G	83/135 (62%)	82 (99%)	1 (1%)	67	79
All	All	4717/5434 (87%)	4707 (100%)	10 (0%)	91	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5	155	LYS
1	g	64	THR
20	G	51	TYR
3	a	103	ASP
3	a	259	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
18	c	200	ASN
1	g	159	GLN
19	9	75	GLN
1	5	67	GLN
10	L	7	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 2 are monoatomic - leaving 303 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	b	604	4	61,69,73	2.62	19 (31%)	67,106,113	2.02	18 (26%)
25	BCR	1	317	-	41,41,41	1.01	2 (4%)	56,56,56	1.29	7 (12%)
25	BCR	M	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	4 (7%)
31	SQD	B	626	-	53,54,54	0.95	5 (9%)	62,65,65	1.49	9 (14%)
27	LHG	D	410	-	46,47,48	0.59	0	45,51,54	1.16	5 (11%)
23	A86	2	310	-	44,50,50	1.62	6 (13%)	51,76,76	1.72	11 (21%)
29	LMU	D	412	-	36,36,36	1.22	2 (5%)	47,47,47	1.04	2 (4%)
28	LMG	B	619	-	51,51,55	0.79	1 (1%)	59,59,63	1.33	6 (10%)
24	KC1	g	315	-	48,53,53	3.53	27 (56%)	55,89,89	3.78	30 (54%)
26	PHO	A	403	-	51,69,69	0.99	4 (7%)	47,99,99	1.13	6 (12%)
28	LMG	8	317	-	51,51,55	0.77	1 (1%)	59,59,63	1.34	7 (11%)
26	PHO	d	403	-	51,69,69	0.97	3 (5%)	47,99,99	1.21	5 (10%)
21	CLA	b	610	4	65,73,73	2.75	18 (27%)	76,113,113	2.19	22 (28%)
21	CLA	b	606	4	61,69,73	2.52	19 (31%)	71,108,113	2.41	21 (29%)
28	LMG	2	318	-	46,46,55	0.82	2 (4%)	54,54,63	1.32	7 (12%)
21	CLA	5	306	1	65,73,73	2.38	19 (29%)	76,113,113	2.26	23 (30%)
21	CLA	G	304	20	65,73,73	2.39	20 (30%)	76,113,113	2.17	23 (30%)
25	BCR	D	408	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
28	LMG	8	301	-	24,24,55	0.99	0	31,31,63	1.30	5 (16%)
28	LMG	b	626	-	37,37,55	0.90	0	45,45,63	1.23	6 (13%)
28	LMG	D	411	-	46,46,55	0.79	0	54,54,63	1.34	7 (12%)
23	A86	8	310	-	44,50,50	1.64	5 (11%)	51,76,76	1.71	10 (19%)
21	CLA	c	508	36	65,73,73	2.49	19 (29%)	76,113,113	2.28	21 (27%)
23	A86	J	310	-	44,50,50	1.63	6 (13%)	51,76,76	1.59	11 (21%)
21	CLA	7	309	1	45,53,73	3.92	19 (42%)	52,89,113	2.44	21 (40%)
28	LMG	b	620	-	51,51,55	0.79	1 (1%)	59,59,63	1.31	7 (11%)
24	KC1	J	313	2	48,53,53	3.53	26 (54%)	55,89,89	3.89	32 (58%)
21	CLA	3	303	19	42,50,73	4.30	19 (45%)	48,85,113	2.62	19 (39%)
21	CLA	2	305	-	65,73,73	2.54	20 (30%)	76,113,113	2.23	23 (30%)
21	CLA	8	302	16	65,73,73	2.79	19 (29%)	76,113,113	2.13	25 (32%)
21	CLA	7	300	1	65,73,73	3.45	20 (30%)	76,113,113	2.13	21 (27%)
21	CLA	B	611	4	64,72,73	2.53	19 (29%)	74,111,113	2.22	22 (29%)
25	BCR	b	619	-	41,41,41	1.08	3 (7%)	56,56,56	1.25	6 (10%)
25	BCR	C	516	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	6 (10%)
28	LMG	b	621	-	28,28,55	1.00	1 (3%)	36,36,63	1.30	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	A86	1	312	-	44,50,50	1.63	6 (13%)	51,76,76	1.55	9 (17%)
22	DD6	g	310	-	39,45,45	1.60	7 (17%)	52,67,67	1.63	10 (19%)
29	LMU	5	316	-	24,24,36	1.32	2 (8%)	35,35,47	1.17	2 (5%)
21	CLA	1	310	1	55,63,73	3.77	19 (34%)	64,101,113	2.28	22 (34%)
35	PL9	d	408	-	55,55,55	1.16	5 (9%)	68,69,69	1.50	11 (16%)
21	CLA	d	404	36	59,67,73	2.62	17 (28%)	68,105,113	2.23	22 (32%)
24	KC1	2	315	16	48,53,53	3.54	26 (54%)	55,89,89	3.87	30 (54%)
21	CLA	9	301	19	60,68,73	4.85	20 (33%)	70,107,113	2.28	22 (31%)
25	BCR	c	515	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	6 (10%)
21	CLA	c	510	18	65,73,73	2.33	18 (27%)	76,113,113	2.18	24 (31%)
23	A86	g	312	-	44,50,50	1.64	6 (13%)	51,76,76	1.88	14 (27%)
27	LHG	d	402	-	42,42,48	0.66	1 (2%)	45,48,54	1.20	4 (8%)
29	LMU	2	317	-	36,36,36	1.19	2 (5%)	47,47,47	1.05	3 (6%)
21	CLA	1	301	1	65,73,73	3.38	20 (30%)	76,113,113	2.11	22 (28%)
23	A86	W	101	21	44,50,50	1.56	6 (13%)	51,76,76	1.54	10 (19%)
24	KC1	4	309	20	48,53,53	3.54	26 (54%)	55,89,89	3.74	29 (52%)
21	CLA	B	608	4	65,73,73	2.55	19 (29%)	76,113,113	2.10	21 (27%)
21	CLA	3	300	19	56,64,73	3.39	20 (35%)	65,102,113	2.34	20 (30%)
21	CLA	c	502	18	65,73,73	2.69	19 (29%)	76,113,113	2.21	22 (28%)
31	SQD	X	401	-	36,37,54	1.14	5 (13%)	45,48,65	1.67	11 (24%)
24	KC1	2	316	16	48,53,53	3.52	27 (56%)	55,89,89	3.57	29 (52%)
21	CLA	3	302	19	47,55,73	3.64	19 (40%)	54,91,113	2.36	21 (38%)
21	CLA	2	304	16	41,49,73	3.09	20 (48%)	47,84,113	2.59	20 (42%)
21	CLA	b	611	-	65,73,73	2.85	18 (27%)	76,113,113	2.18	20 (26%)
23	A86	G	305	-	44,50,50	1.67	6 (13%)	51,76,76	1.58	9 (17%)
21	CLA	g	304	-	54,62,73	3.44	20 (37%)	62,99,113	2.26	22 (35%)
21	CLA	b	615	4	64,72,73	2.55	20 (31%)	74,111,113	2.16	23 (31%)
24	KC1	5	314	-	48,53,53	3.50	26 (54%)	55,89,89	3.91	29 (52%)
21	CLA	g	303	1	50,58,73	3.01	20 (40%)	58,95,113	2.53	22 (37%)
24	KC1	3	305	19	48,53,53	3.53	27 (56%)	55,89,89	3.84	31 (56%)
28	LMG	L	101	-	40,40,55	0.82	0	48,48,63	1.24	5 (10%)
21	CLA	a	402	3	65,73,73	2.60	18 (27%)	76,113,113	2.20	24 (31%)
28	LMG	A	407	-	48,48,55	0.76	0	56,56,63	1.31	6 (10%)
21	CLA	B	614	4	64,72,73	2.58	20 (31%)	74,111,113	2.12	23 (31%)
21	CLA	1	303	1	65,73,73	2.91	20 (30%)	76,113,113	2.32	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	h	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	6 (10%)
21	CLA	6	300	2	52,60,73	3.55	20 (38%)	60,97,113	2.34	23 (38%)
21	CLA	B	602	-	47,55,73	3.29	18 (38%)	54,91,113	2.56	21 (38%)
21	CLA	A	401	3	65,73,73	2.61	18 (27%)	76,113,113	2.21	24 (31%)
24	KC1	1	315	-	48,53,53	3.52	27 (56%)	55,89,89	3.81	30 (54%)
31	SQD	B	625	-	48,49,54	1.00	5 (10%)	57,60,65	1.57	8 (14%)
32	HEM	E	101	5	41,50,50	1.48	4 (9%)	45,82,82	1.57	9 (20%)
21	CLA	C	505	18	65,73,73	3.17	20 (30%)	76,113,113	2.23	22 (28%)
21	CLA	J	303	2	44,51,73	8.56	21 (47%)	54,86,113	2.55	23 (42%)
21	CLA	c	514	18	49,57,73	3.26	20 (40%)	55,93,113	2.46	22 (40%)
26	PHO	a	404	-	51,69,69	0.99	4 (7%)	47,99,99	1.13	7 (14%)
28	LMG	f	102	-	46,46,55	0.80	1 (2%)	54,54,63	1.33	7 (12%)
21	CLA	2	302	16	50,58,73	3.43	21 (42%)	58,95,113	4.14	27 (46%)
21	CLA	J	307	-	65,73,73	2.31	20 (30%)	76,113,113	2.10	24 (31%)
21	CLA	C	512	18	65,73,73	2.29	20 (30%)	76,113,113	2.22	24 (31%)
21	CLA	A	402	36	49,57,73	3.46	19 (38%)	55,93,113	2.49	19 (34%)
25	BCR	m	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	4 (7%)
21	CLA	d	405	17	57,65,73	2.64	19 (33%)	70,103,113	2.47	26 (37%)
21	CLA	a	403	36	49,57,73	3.45	19 (38%)	55,93,113	2.48	20 (36%)
21	CLA	B	613	4	65,73,73	2.97	19 (29%)	76,113,113	2.14	23 (30%)
21	CLA	1	304	1	65,73,73	2.94	19 (29%)	76,113,113	2.12	24 (31%)
21	CLA	b	623	-	56,64,73	2.66	19 (33%)	65,102,113	2.32	22 (33%)
21	CLA	5	305	-	41,49,73	3.96	19 (46%)	47,84,113	2.67	22 (46%)
21	CLA	G	300	-	65,73,73	3.27	19 (29%)	76,113,113	2.30	24 (31%)
23	A86	8	312	-	44,50,50	1.66	6 (13%)	51,76,76	1.66	9 (17%)
21	CLA	g	305	-	41,49,73	3.76	20 (48%)	47,84,113	2.50	23 (48%)
24	KC1	G	309	-	48,53,53	3.52	27 (56%)	55,89,89	3.75	30 (54%)
21	CLA	5	307	1	56,64,73	2.89	18 (32%)	65,102,113	2.20	22 (33%)
25	BCR	H	100	-	41,41,41	1.07	2 (4%)	56,56,56	1.33	6 (10%)
21	CLA	2	303	36	51,59,73	2.85	17 (33%)	59,96,113	2.43	23 (38%)
25	BCR	h	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
29	LMU	A	408	-	36,36,36	1.21	2 (5%)	47,47,47	1.08	3 (6%)
35	PL9	D	409	-	55,55,55	1.17	5 (9%)	68,69,69	1.52	10 (14%)
21	CLA	g	307	1	46,54,73	3.56	19 (41%)	53,90,113	2.40	22 (41%)
21	CLA	7	307	-	55,63,73	2.97	18 (32%)	64,101,113	2.39	22 (34%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	2	301	16	65,73,73	2.69	19 (29%)	76,113,113	2.21	26 (34%)
21	CLA	6	305	-	45,53,73	3.18	19 (42%)	52,89,113	2.45	19 (36%)
23	A86	8	308	-	44,50,50	1.66	6 (13%)	51,76,76	1.81	12 (23%)
22	DD6	1	311	-	39,45,45	1.58	8 (20%)	52,67,67	1.63	10 (19%)
27	LHG	B	601	-	48,48,48	0.61	1 (2%)	51,54,54	1.28	6 (11%)
25	BCR	a	406	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	6 (10%)
24	KC1	5	315	-	48,53,53	3.47	25 (52%)	55,89,89	3.82	31 (56%)
21	CLA	1	302	1	65,73,73	2.94	19 (29%)	76,113,113	2.21	22 (28%)
31	SQD	b	602	-	53,54,54	0.95	5 (9%)	62,65,65	1.49	9 (14%)
27	LHG	d	409	-	46,47,48	0.63	1 (2%)	45,51,54	1.19	5 (11%)
24	KC1	J	311	2	48,53,53	3.46	26 (54%)	55,89,89	3.77	31 (56%)
30	DGD	B	624	-	54,54,67	1.09	5 (9%)	67,67,81	1.47	9 (13%)
21	CLA	J	302	2	45,53,73	3.53	19 (42%)	52,89,113	2.47	19 (36%)
21	CLA	4	301	20	55,63,73	3.61	20 (36%)	64,101,113	2.36	21 (32%)
23	A86	7	313	-	40,46,50	1.73	6 (15%)	45,70,76	1.75	10 (22%)
21	CLA	C	513	18	65,73,73	2.67	19 (29%)	76,113,113	2.16	20 (26%)
24	KC1	9	305	19	48,53,53	3.46	24 (50%)	55,89,89	3.87	31 (56%)
29	LMU	8	318	-	36,36,36	1.21	2 (5%)	47,47,47	0.99	1 (2%)
21	CLA	7	308	1	56,64,73	2.90	20 (35%)	65,102,113	2.34	22 (33%)
21	CLA	b	614	4	65,73,73	2.96	19 (29%)	76,113,113	2.14	22 (28%)
21	CLA	J	300	2	52,60,73	3.52	19 (36%)	60,97,113	2.36	23 (38%)
21	CLA	D	404	36	59,67,73	2.66	18 (30%)	68,105,113	2.27	23 (33%)
21	CLA	d	406	17	60,68,73	2.94	19 (31%)	70,107,113	2.25	22 (31%)
21	CLA	c	513	18	64,72,73	2.62	20 (31%)	74,111,113	2.11	19 (25%)
23	A86	2	311	-	44,50,50	1.59	6 (13%)	51,76,76	1.74	11 (21%)
23	A86	6	310	-	44,50,50	1.64	6 (13%)	51,76,76	1.58	10 (19%)
21	CLA	7	303	1	65,73,73	2.96	19 (29%)	76,113,113	2.15	23 (30%)
21	CLA	c	507	18	45,53,73	3.02	19 (42%)	52,89,113	2.47	22 (42%)
23	A86	4	305	-	44,50,50	1.61	6 (13%)	51,76,76	1.71	11 (21%)
28	LMG	M	102	-	40,40,55	0.85	1 (2%)	48,48,63	1.25	5 (10%)
21	CLA	1	306	1	41,49,73	3.09	20 (48%)	47,84,113	2.46	21 (44%)
21	CLA	B	607	4	65,73,73	2.84	19 (29%)	76,113,113	2.22	23 (30%)
23	A86	6	309	-	44,50,50	1.74	7 (15%)	51,76,76	1.87	10 (19%)
21	CLA	A	404	3	60,68,73	3.13	19 (31%)	70,107,113	2.27	23 (32%)
21	CLA	B	612	4	65,73,73	2.68	20 (30%)	76,113,113	2.16	24 (31%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	C	504	18	64,72,73	2.52	19 (29%)	74,111,113	2.25	19 (25%)
21	CLA	3	301	19	60,68,73	3.03	20 (33%)	70,107,113	2.30	24 (34%)
25	BCR	d	407	-	41,41,41	1.05	2 (4%)	56,56,56	1.22	5 (8%)
27	LHG	D	403	-	42,42,48	0.67	1 (2%)	45,48,54	1.19	4 (8%)
21	CLA	c	512	18	65,73,73	2.62	20 (30%)	76,113,113	2.18	21 (27%)
21	CLA	4	303	-	51,59,73	4.02	19 (37%)	59,96,113	2.36	24 (40%)
30	DGD	C	518	-	40,40,67	1.17	1 (2%)	53,53,81	1.40	4 (7%)
24	KC1	g	314	-	48,53,53	3.50	25 (52%)	55,89,89	4.01	31 (56%)
32	HEM	f	101	6	41,50,50	1.55	5 (12%)	45,82,82	1.42	6 (13%)
21	CLA	g	302	1	65,73,73	3.56	20 (30%)	76,113,113	2.16	24 (31%)
24	KC1	4	307	20	48,53,53	3.47	25 (52%)	55,89,89	3.84	30 (54%)
27	LHG	a	401	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
21	CLA	C	514	18	64,72,73	2.63	19 (29%)	74,111,113	2.12	19 (25%)
21	CLA	c	504	18	65,73,73	2.68	20 (30%)	76,113,113	2.15	21 (27%)
29	LMU	a	408	-	36,36,36	1.20	2 (5%)	47,47,47	1.09	3 (6%)
21	CLA	a	405	3	60,68,73	3.63	20 (33%)	70,107,113	2.24	23 (32%)
24	KC1	4	308	20	48,53,53	3.53	27 (56%)	55,89,89	3.90	31 (56%)
27	LHG	A	406	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
23	A86	5	312	-	44,50,50	1.64	6 (13%)	51,76,76	1.53	9 (17%)
23	A86	8	309	-	44,50,50	1.63	6 (13%)	51,76,76	1.47	8 (15%)
21	CLA	7	301	1	65,73,73	2.91	20 (30%)	76,113,113	2.18	20 (26%)
21	CLA	7	304	-	65,73,73	2.59	19 (29%)	76,113,113	2.16	24 (31%)
21	CLA	1	305	-	51,59,73	2.86	19 (37%)	59,96,113	2.37	23 (38%)
21	CLA	c	505	-	56,64,73	2.62	19 (33%)	64,101,113	2.38	22 (34%)
22	DD6	7	310	-	39,45,45	1.56	8 (20%)	52,67,67	1.63	10 (19%)
23	A86	1	314	-	44,50,50	1.60	6 (13%)	51,76,76	1.54	7 (13%)
24	KC1	6	311	2	48,53,53	3.46	26 (54%)	55,89,89	3.78	30 (54%)
29	LMU	g	316	-	25,25,36	1.34	3 (12%)	36,36,47	1.16	3 (8%)
28	LMG	B	627	-	40,40,55	0.94	2 (5%)	48,48,63	1.37	7 (14%)
21	CLA	6	301	2	57,65,73	2.59	20 (35%)	66,103,113	2.33	23 (34%)
23	A86	2	307	-	44,50,50	1.64	6 (13%)	51,76,76	1.72	11 (21%)
30	DGD	H	101	-	63,63,67	0.91	2 (3%)	77,77,81	1.37	8 (10%)
21	CLA	b	617	4	65,73,73	2.46	18 (27%)	76,113,113	2.18	25 (32%)
21	CLA	5	304	-	48,56,73	3.35	20 (41%)	55,92,113	2.51	21 (38%)
21	CLA	b	608	4	65,73,73	2.82	19 (29%)	76,113,113	2.20	23 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	4	300	-	65,73,73	3.16	19 (29%)	76,113,113	2.34	23 (30%)
21	CLA	5	303	1	52,60,73	3.10	19 (36%)	60,97,113	2.49	23 (38%)
28	LMG	b	622	-	35,35,55	1.02	1 (2%)	43,43,63	1.29	3 (6%)
21	CLA	7	302	1	65,73,73	2.93	19 (29%)	76,113,113	2.25	23 (30%)
23	A86	7	312	-	44,50,50	1.64	6 (13%)	51,76,76	1.71	10 (19%)
21	CLA	b	613	4	65,73,73	2.63	20 (30%)	76,113,113	2.14	22 (28%)
25	BCR	B	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	5 (8%)
24	KC1	7	315	1	48,53,53	3.49	26 (54%)	55,89,89	3.81	30 (54%)
21	CLA	1	309	1	56,64,73	3.17	20 (35%)	65,102,113	2.31	22 (33%)
21	CLA	B	604	4	64,72,73	2.55	18 (28%)	74,111,113	2.16	22 (29%)
24	KC1	2	314	16	48,53,53	3.52	26 (54%)	55,89,89	3.77	28 (50%)
21	CLA	7	305	1	41,49,73	3.59	19 (46%)	47,84,113	2.82	20 (42%)
21	CLA	4	304	20	65,73,73	2.39	19 (29%)	76,113,113	2.16	25 (32%)
27	LHG	l	101	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
21	CLA	b	605	4	64,72,73	2.57	18 (28%)	74,111,113	2.15	23 (31%)
21	CLA	B	605	4	61,69,73	2.54	19 (31%)	71,108,113	2.40	22 (30%)
21	CLA	g	308	1	65,73,73	2.54	20 (30%)	76,113,113	2.10	22 (28%)
28	LMG	b	624	-	37,37,55	0.88	1 (2%)	45,45,63	1.25	5 (11%)
24	KC1	1	316	1	48,53,53	3.50	26 (54%)	55,89,89	3.84	29 (52%)
21	CLA	9	304	-	56,64,73	3.92	20 (35%)	65,102,113	2.39	22 (33%)
30	DGD	b	601	-	54,54,67	1.10	5 (9%)	67,67,81	1.44	8 (11%)
33	BCT	d	401	34	2,3,3	1.28	0	2,3,3	4.07	1 (50%)
21	CLA	9	303	19	51,59,73	4.17	19 (37%)	59,96,113	2.67	23 (38%)
21	CLA	6	307	-	65,73,73	2.33	19 (29%)	76,113,113	2.12	26 (34%)
21	CLA	G	303	-	51,59,73	3.77	19 (37%)	59,96,113	2.29	22 (37%)
21	CLA	g	306	1	65,73,73	2.37	18 (27%)	76,113,113	2.23	22 (28%)
24	KC1	5	313	1	48,53,53	3.47	23 (47%)	55,89,89	3.84	31 (56%)
25	BCR	b	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	6 (10%)
21	CLA	B	616	4	65,73,73	2.52	18 (27%)	76,113,113	2.19	25 (32%)
21	CLA	B	609	4	65,73,73	2.71	18 (27%)	76,113,113	2.21	23 (30%)
23	A86	1	313	-	44,50,50	1.65	6 (13%)	51,76,76	1.51	7 (13%)
24	KC1	2	313	16	48,53,53	3.49	27 (56%)	55,89,89	3.69	31 (56%)
24	KC1	g	313	1	48,53,53	3.47	22 (45%)	55,89,89	3.81	28 (50%)
24	KC1	G	307	20	48,53,53	3.46	25 (52%)	55,89,89	4.07	32 (58%)
24	KC1	G	308	20	48,53,53	3.58	27 (56%)	55,89,89	4.01	30 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	BCR	A	405	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	6 (10%)
21	CLA	C	509	36	65,73,73	2.45	18 (27%)	76,113,113	2.27	22 (28%)
33	BCT	D	402	34	2,3,3	1.23	0	2,3,3	4.12	2 (100%)
28	LMG	N	101	-	24,24,55	0.98	0	31,31,63	1.27	5 (16%)
24	KC1	8	315	16	48,53,53	3.53	26 (54%)	55,89,89	3.93	31 (56%)
21	CLA	2	306	16	45,53,73	3.53	18 (40%)	52,89,113	2.60	20 (38%)
30	DGD	h	103	-	63,63,67	0.91	2 (3%)	77,77,81	1.38	8 (10%)
21	CLA	5	302	1	65,73,73	3.46	19 (29%)	76,113,113	2.25	26 (34%)
21	CLA	c	506	18	65,73,73	2.77	18 (27%)	76,113,113	2.24	21 (27%)
21	CLA	c	509	18	65,73,73	2.80	19 (29%)	76,113,113	2.18	24 (31%)
21	CLA	8	307	16	43,51,73	3.52	17 (39%)	49,86,113	2.58	19 (38%)
24	KC1	4	306	20	42,46,53	3.50	24 (57%)	47,79,89	4.51	27 (57%)
31	SQD	C	502	-	50,51,54	0.98	5 (10%)	59,62,65	1.59	11 (18%)
24	KC1	9	306	19	48,53,53	3.57	27 (56%)	55,89,89	3.75	30 (54%)
23	A86	2	309	-	44,50,50	1.64	6 (13%)	51,76,76	1.77	10 (19%)
21	CLA	5	309	1	65,73,73	2.83	20 (30%)	76,113,113	2.51	28 (36%)
24	KC1	G	306	20	42,46,53	3.51	24 (57%)	47,79,89	4.55	29 (61%)
21	CLA	b	607	4	65,73,73	2.51	20 (30%)	76,113,113	2.19	22 (28%)
22	DD6	5	310	-	39,45,45	1.63	8 (20%)	52,67,67	1.62	11 (21%)
21	CLA	g	309	1	50,58,73	4.86	20 (40%)	58,95,113	2.49	25 (43%)
23	A86	2	308	-	44,50,50	1.61	6 (13%)	51,76,76	1.70	11 (21%)
21	CLA	B	606	4	65,73,73	2.50	20 (30%)	76,113,113	2.20	22 (28%)
24	KC1	8	316	16	48,53,53	3.52	27 (56%)	55,89,89	3.58	30 (54%)
21	CLA	6	302	2	45,53,73	3.56	20 (44%)	52,89,113	2.48	20 (38%)
21	CLA	B	610	-	65,73,73	2.79	18 (27%)	76,113,113	2.18	20 (26%)
21	CLA	3	304	19	57,65,73	3.70	20 (35%)	66,103,113	2.30	23 (34%)
21	CLA	8	305	16	41,49,73	3.19	20 (48%)	47,84,113	2.59	20 (42%)
24	KC1	J	312	2	48,53,53	3.52	27 (56%)	55,89,89	3.83	32 (58%)
21	CLA	J	305	-	45,53,73	3.25	19 (42%)	52,89,113	2.45	19 (36%)
25	BCR	c	501	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	6 (10%)
24	KC1	8	313	16	48,53,53	3.51	27 (56%)	55,89,89	3.95	31 (56%)
28	LMG	a	407	-	48,48,55	0.75	0	56,56,63	1.31	5 (8%)
28	LMG	B	620	-	28,28,55	1.00	1 (3%)	36,36,63	1.30	5 (13%)
21	CLA	J	301	2	57,65,73	2.42	20 (35%)	66,103,113	2.40	23 (34%)
23	A86	J	309	-	44,50,50	1.63	5 (11%)	51,76,76	1.64	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	A86	2	312	-	44,50,50	1.64	6 (13%)	51,76,76	1.58	9 (17%)
24	KC1	7	314	1	48,53,53	3.48	26 (54%)	55,89,89	3.81	31 (56%)
21	CLA	8	303	16	50,58,73	3.24	19 (38%)	58,95,113	2.47	24 (41%)
30	DGD	c	517	-	40,40,67	1.16	1 (2%)	53,53,81	1.41	4 (7%)
28	LMG	B	622	-	37,37,55	0.88	0	45,45,63	1.27	5 (11%)
21	CLA	C	510	18	65,73,73	2.74	19 (29%)	76,113,113	2.18	24 (31%)
21	CLA	6	304	2	43,51,73	3.17	17 (39%)	49,86,113	2.63	22 (44%)
23	A86	g	311	-	44,50,50	1.64	6 (13%)	51,76,76	1.50	8 (15%)
21	CLA	6	303	-	44,51,73	3.92	21 (47%)	54,86,113	2.59	19 (35%)
21	CLA	J	306	36	65,73,73	2.75	20 (30%)	76,113,113	2.14	24 (31%)
21	CLA	G	301	20	57,65,73	3.37	20 (35%)	66,103,113	2.31	22 (33%)
21	CLA	C	515	18	49,57,73	3.31	20 (40%)	55,93,113	2.45	22 (40%)
21	CLA	4	302	20	56,64,73	4.55	19 (33%)	65,102,113	2.39	24 (36%)
24	KC1	3	306	19	48,53,53	3.51	27 (56%)	55,89,89	3.90	30 (54%)
30	DGD	c	516	-	56,56,67	1.01	2 (3%)	70,70,81	1.49	7 (10%)
26	PHO	D	401	-	51,69,69	0.97	3 (5%)	47,99,99	1.21	6 (12%)
21	CLA	9	302	19	47,55,73	3.28	20 (42%)	54,91,113	2.48	20 (37%)
21	CLA	6	308	2	52,60,73	2.75	20 (38%)	60,97,113	2.60	25 (41%)
24	KC1	6	313	2	48,53,53	3.51	27 (56%)	55,89,89	3.92	32 (58%)
29	LMU	g	301	-	33,33,36	1.24	2 (6%)	44,44,47	1.30	4 (9%)
21	CLA	9	300	19	56,64,73	3.19	20 (35%)	65,102,113	2.23	22 (33%)
21	CLA	C	508	18	45,53,73	2.94	18 (40%)	52,89,113	2.44	21 (40%)
24	KC1	8	314	16	48,53,53	3.52	26 (54%)	55,89,89	3.81	30 (54%)
21	CLA	8	304	23	51,59,73	2.95	19 (37%)	59,96,113	2.45	22 (37%)
21	CLA	b	616	4	65,73,73	2.74	19 (29%)	76,113,113	2.13	24 (31%)
30	DGD	C	517	-	56,56,67	1.00	3 (5%)	70,70,81	1.49	8 (11%)
25	BCR	B	618	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	7 (12%)
21	CLA	6	306	36	65,73,73	2.77	20 (30%)	76,113,113	2.13	24 (31%)
21	CLA	5	308	1	65,73,73	3.26	20 (30%)	76,113,113	2.19	22 (28%)
21	CLA	1	307	1	41,49,73	3.19	20 (48%)	47,84,113	2.51	21 (44%)
21	CLA	B	615	4	65,73,73	2.79	19 (29%)	76,113,113	2.12	24 (31%)
21	CLA	C	503	18	65,73,73	2.60	20 (30%)	76,113,113	2.20	22 (28%)
24	KC1	6	312	2	48,53,53	3.54	27 (56%)	55,89,89	3.86	32 (58%)
21	CLA	b	612	4	64,72,73	2.51	18 (28%)	74,111,113	2.20	22 (29%)
28	LMG	b	625	-	43,43,55	0.87	1 (2%)	51,51,63	1.22	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	b	609	4	65,73,73	2.55	19 (29%)	76,113,113	2.10	21 (27%)
21	CLA	C	511	18	65,73,73	2.29	18 (27%)	76,113,113	2.19	23 (30%)
21	CLA	D	406	17	57,65,73	2.67	18 (31%)	70,103,113	2.46	26 (37%)
21	CLA	J	304	2	43,51,73	3.26	17 (39%)	49,86,113	2.60	22 (44%)
21	CLA	C	506	-	64,72,73	2.48	19 (29%)	74,111,113	2.22	22 (29%)
21	CLA	c	503	18	64,72,73	2.50	19 (29%)	74,111,113	2.23	20 (27%)
21	CLA	7	306	1	41,49,73	3.15	20 (48%)	47,84,113	2.52	22 (46%)
21	CLA	B	603	4	61,69,73	2.66	19 (31%)	67,106,113	2.04	18 (26%)
28	LMG	B	623	-	43,43,55	0.83	0	51,51,63	1.25	4 (7%)
21	CLA	8	306	-	58,66,73	2.67	20 (34%)	67,104,113	2.22	22 (32%)
21	CLA	1	308	-	54,62,73	3.21	19 (35%)	62,99,113	2.40	23 (37%)
23	A86	5	311	-	44,50,50	1.67	6 (13%)	51,76,76	1.64	10 (19%)
29	LMU	5	301	-	33,33,36	1.25	2 (6%)	44,44,47	1.32	6 (13%)
21	CLA	c	511	18	65,73,73	2.32	20 (30%)	76,113,113	2.19	22 (28%)
21	CLA	B	621	-	65,73,73	2.55	19 (29%)	76,113,113	2.15	22 (28%)
21	CLA	D	407	17	60,68,73	2.98	19 (31%)	70,107,113	2.24	22 (31%)
23	A86	7	311	-	44,50,50	1.63	5 (11%)	51,76,76	1.47	8 (15%)
21	CLA	J	308	2	52,60,73	2.72	20 (38%)	60,97,113	2.63	25 (41%)
23	A86	8	311	-	44,50,50	1.63	6 (13%)	51,76,76	1.58	10 (19%)
21	CLA	G	302	20	56,64,73	7.05	20 (35%)	65,102,113	2.28	23 (35%)
21	CLA	b	603	-	47,55,73	3.30	18 (38%)	54,91,113	2.50	22 (40%)
25	BCR	C	501	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	5 (8%)
21	CLA	C	507	18	65,73,73	2.76	18 (27%)	76,113,113	2.24	22 (28%)

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
21	CLA	b	604	4	1/1/12/20	7/27/107/115	-
25	BCR	1	317	-	-	20/29/63/63	0/2/2/2
25	BCR	M	101	-	-	4/29/63/63	0/2/2/2
31	SQD	B	626	-	-	27/49/69/69	0/1/1/1
27	LHG	D	410	-	-	21/47/51/53	-
23	A86	2	310	-	-	16/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMU	D	412	-	-	13/21/61/61	0/2/2/2
28	LMG	B	619	-	-	20/46/66/70	0/1/1/1
24	KC1	g	315	-	-	9/15/71/71	-
26	PHO	A	403	-	-	12/37/103/103	0/5/6/6
28	LMG	8	317	-	-	22/46/66/70	0/1/1/1
26	PHO	d	403	-	-	4/37/103/103	0/5/6/6
21	CLA	b	610	4	-	5/37/115/115	-
21	CLA	b	606	4	-	13/33/111/115	-
28	LMG	2	318	-	-	17/41/61/70	0/1/1/1
21	CLA	5	306	1	1/1/15/20	14/37/115/115	-
21	CLA	G	304	20	1/1/15/20	16/37/115/115	-
25	BCR	D	408	-	-	8/29/63/63	0/2/2/2
28	LMG	8	301	-	-	8/17/37/70	0/1/1/1
28	LMG	b	626	-	-	11/32/52/70	0/1/1/1
28	LMG	D	411	-	-	22/41/61/70	0/1/1/1
23	A86	8	310	-	-	16/34/90/90	0/3/3/3
21	CLA	c	508	36	1/1/15/20	14/37/115/115	-
23	A86	J	310	-	-	19/34/90/90	0/3/3/3
21	CLA	7	309	1	-	5/13/91/115	-
28	LMG	b	620	-	-	19/46/66/70	0/1/1/1
24	KC1	J	313	2	-	8/15/71/71	-
21	CLA	3	303	19	-	2/10/88/115	-
21	CLA	2	305	-	1/1/15/20	19/37/115/115	-
21	CLA	8	302	16	1/1/15/20	13/37/115/115	-
21	CLA	7	300	1	1/1/15/20	12/37/115/115	-
21	CLA	B	611	4	-	5/35/113/115	-
25	BCR	b	619	-	-	12/29/63/63	0/2/2/2
25	BCR	C	516	-	-	10/29/63/63	0/2/2/2
28	LMG	b	621	-	-	3/23/43/70	0/1/1/1
23	A86	1	312	-	-	23/34/90/90	0/3/3/3
22	DD6	g	310	-	-	10/26/80/80	0/3/3/3
29	LMU	5	316	-	-	1/8/48/61	0/2/2/2
21	CLA	1	310	1	-	10/25/103/115	-
35	PL9	d	408	-	-	7/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	d	404	36	1/1/13/20	7/30/108/115	-
24	KC1	2	315	16	-	7/15/71/71	-
21	CLA	9	301	19	-	11/31/109/115	-
25	BCR	c	515	-	-	9/29/63/63	0/2/2/2
21	CLA	c	510	18	1/1/15/20	8/37/115/115	-
23	A86	g	312	-	-	20/34/90/90	0/3/3/3
27	LHG	d	402	-	-	15/47/47/53	-
29	LMU	2	317	-	-	9/21/61/61	0/2/2/2
21	CLA	1	301	1	1/1/15/20	9/37/115/115	-
23	A86	W	101	21	-	24/34/90/90	0/3/3/3
24	KC1	4	309	20	-	4/15/71/71	-
21	CLA	B	608	4	-	10/37/115/115	-
21	CLA	3	300	19	-	9/27/105/115	-
21	CLA	c	502	18	1/1/15/20	11/37/115/115	-
31	SQD	X	401	-	-	17/32/52/69	0/1/1/1
24	KC1	2	316	16	-	5/15/71/71	-
21	CLA	3	302	19	1/1/11/20	5/16/94/115	-
21	CLA	2	304	16	-	3/8/86/115	-
21	CLA	b	611	-	1/1/15/20	7/37/115/115	-
23	A86	G	305	-	-	15/34/90/90	0/3/3/3
21	CLA	g	304	-	-	12/24/102/115	-
21	CLA	b	615	4	1/1/14/20	13/35/113/115	-
24	KC1	5	314	-	-	7/15/71/71	-
21	CLA	g	303	1	1/1/12/20	8/19/97/115	-
24	KC1	3	305	19	-	6/15/71/71	-
28	LMG	L	101	-	-	19/35/55/70	0/1/1/1
21	CLA	a	402	3	-	8/37/115/115	-
28	LMG	A	407	-	-	23/43/63/70	0/1/1/1
21	CLA	B	614	4	1/1/14/20	14/35/113/115	-
21	CLA	1	303	1	1/1/15/20	15/37/115/115	-
25	BCR	h	101	-	-	25/29/63/63	0/2/2/2
21	CLA	6	300	2	1/1/12/20	6/22/100/115	-
21	CLA	B	602	-	1/1/11/20	5/16/94/115	-
21	CLA	A	401	3	-	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	KC1	1	315	-	-	8/15/71/71	-
31	SQD	B	625	-	-	19/44/64/69	0/1/1/1
32	HEM	E	101	5	-	6/12/54/54	-
21	CLA	C	505	18	-	11/37/115/115	-
21	CLA	J	303	2	-	9/13/89/115	-
21	CLA	c	514	18	-	3/18/96/115	-
26	PHO	a	404	-	-	12/37/103/103	0/5/6/6
28	LMG	f	102	-	-	21/41/61/70	0/1/1/1
21	CLA	2	302	16	1/1/12/20	6/19/97/115	-
21	CLA	J	307	-	1/1/15/20	13/37/115/115	-
21	CLA	C	512	18	1/1/15/20	9/37/115/115	-
21	CLA	A	402	36	-	5/18/96/115	-
25	BCR	m	101	-	-	5/29/63/63	0/2/2/2
21	CLA	d	405	17	1/1/13/20	7/28/104/115	-
21	CLA	a	403	36	-	5/18/96/115	-
21	CLA	B	613	4	1/1/15/20	11/37/115/115	-
21	CLA	1	304	1	1/1/15/20	15/37/115/115	-
21	CLA	b	623	-	1/1/13/20	8/27/105/115	-
21	CLA	5	305	-	1/1/10/20	2/8/86/115	-
21	CLA	G	300	-	1/1/15/20	9/37/115/115	-
23	A86	8	312	-	-	21/34/90/90	0/3/3/3
21	CLA	g	305	-	1/1/10/20	2/8/86/115	-
24	KC1	G	309	-	-	9/15/71/71	-
21	CLA	5	307	1	-	11/27/105/115	-
25	BCR	H	100	-	-	8/29/63/63	0/2/2/2
21	CLA	2	303	36	1/1/12/20	8/21/99/115	-
25	BCR	h	102	-	-	7/29/63/63	0/2/2/2
29	LMU	A	408	-	-	7/21/61/61	0/2/2/2
35	PL9	D	409	-	-	3/53/73/73	0/1/1/1
21	CLA	g	307	1	-	3/15/93/115	-
21	CLA	7	307	-	1/1/13/20	5/25/103/115	-
21	CLA	2	301	16	1/1/15/20	15/37/115/115	-
21	CLA	6	305	-	1/1/11/20	4/13/91/115	-
23	A86	8	308	-	-	24/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DD6	1	311	-	-	5/26/80/80	0/3/3/3
27	LHG	B	601	-	-	23/53/53/53	-
25	BCR	a	406	-	-	6/29/63/63	0/2/2/2
24	KC1	5	315	-	-	5/15/71/71	-
21	CLA	1	302	1	1/1/15/20	13/37/115/115	-
31	SQD	b	602	-	-	26/49/69/69	0/1/1/1
27	LHG	d	409	-	-	21/47/51/53	-
24	KC1	J	311	2	-	7/15/71/71	-
30	DGD	B	624	-	-	20/43/79/95	0/2/2/2
21	CLA	J	302	2	1/1/11/20	3/13/91/115	-
21	CLA	4	301	20	1/1/13/20	9/25/103/115	-
23	A86	7	313	-	-	14/30/84/90	0/3/3/3
21	CLA	C	513	18	-	5/37/115/115	-
24	KC1	9	305	19	-	8/15/71/71	-
29	LMU	8	318	-	-	10/21/61/61	0/2/2/2
21	CLA	7	308	1	1/1/13/20	9/27/105/115	-
21	CLA	b	614	4	1/1/15/20	6/37/115/115	-
21	CLA	J	300	2	1/1/12/20	6/22/100/115	-
21	CLA	D	404	36	1/1/13/20	7/30/108/115	-
21	CLA	d	406	17	-	9/31/109/115	-
21	CLA	c	513	18	1/1/14/20	12/35/113/115	-
23	A86	2	311	-	-	23/34/90/90	0/3/3/3
23	A86	6	310	-	-	19/34/90/90	0/3/3/3
21	CLA	7	303	1	1/1/15/20	15/37/115/115	-
21	CLA	c	507	18	1/1/11/20	5/13/91/115	-
23	A86	4	305	-	-	17/34/90/90	0/3/3/3
28	LMG	M	102	-	-	15/35/55/70	0/1/1/1
21	CLA	1	306	1	1/1/10/20	2/8/86/115	-
21	CLA	B	607	4	-	11/37/115/115	-
23	A86	6	309	-	-	21/34/90/90	0/3/3/3
21	CLA	A	404	3	-	7/31/109/115	-
21	CLA	B	612	4	1/1/15/20	10/37/115/115	-
21	CLA	3	301	19	1/1/14/20	12/31/109/115	-
21	CLA	C	504	18	-	8/35/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	d	407	-	-	7/29/63/63	0/2/2/2
27	LHG	D	403	-	-	19/47/47/53	-
21	CLA	c	512	18	1/1/15/20	6/37/115/115	-
21	CLA	4	303	-	1/1/12/20	9/21/99/115	-
30	DGD	C	518	-	-	16/26/66/95	0/2/2/2
24	KC1	g	314	-	-	7/15/71/71	-
32	HEM	f	101	6	-	5/12/54/54	-
21	CLA	g	302	1	1/1/15/20	11/37/115/115	-
24	KC1	4	307	20	-	8/15/71/71	-
27	LHG	a	401	-	-	30/53/53/53	-
21	CLA	C	514	18	1/1/14/20	8/35/113/115	-
21	CLA	c	504	18	-	14/37/115/115	-
29	LMU	a	408	-	-	8/21/61/61	0/2/2/2
21	CLA	a	405	3	-	8/31/109/115	-
24	KC1	4	308	20	-	6/15/71/71	-
27	LHG	A	406	-	-	29/53/53/53	-
23	A86	5	312	-	-	24/34/90/90	0/3/3/3
23	A86	8	309	-	-	9/34/90/90	0/3/3/3
21	CLA	7	301	1	1/1/15/20	15/37/115/115	-
21	CLA	7	304	-	1/1/15/20	13/37/115/115	-
21	CLA	1	305	-	-	8/21/99/115	-
21	CLA	c	505	-	-	11/26/104/115	-
22	DD6	7	310	-	-	8/26/80/80	0/3/3/3
23	A86	1	314	-	-	20/34/90/90	0/3/3/3
24	KC1	6	311	2	-	9/15/71/71	-
29	LMU	g	316	-	-	4/10/50/61	0/2/2/2
28	LMG	B	627	-	-	19/35/55/70	0/1/1/1
21	CLA	6	301	2	1/1/13/20	14/28/106/115	-
23	A86	2	307	-	-	12/34/90/90	0/3/3/3
30	DGD	H	101	-	-	14/51/91/95	0/2/2/2
21	CLA	b	617	4	1/1/15/20	14/37/115/115	-
21	CLA	5	304	-	-	8/17/95/115	-
21	CLA	4	300	-	1/1/15/20	14/37/115/115	-
21	CLA	5	303	1	1/1/12/20	10/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	608	4	-	13/37/115/115	-
28	LMG	b	622	-	-	16/30/50/70	0/1/1/1
21	CLA	7	302	1	1/1/15/20	12/37/115/115	-
23	A86	7	312	-	-	21/34/90/90	0/3/3/3
21	CLA	b	613	4	1/1/15/20	10/37/115/115	-
25	BCR	B	617	-	-	9/29/63/63	0/2/2/2
24	KC1	7	315	1	-	7/15/71/71	-
21	CLA	1	309	1	1/1/13/20	8/27/105/115	-
21	CLA	B	604	4	1/1/14/20	10/35/113/115	-
24	KC1	2	314	16	-	6/15/71/71	-
21	CLA	7	305	1	1/1/10/20	4/8/86/115	-
21	CLA	4	304	20	1/1/15/20	17/37/115/115	-
27	LHG	l	101	-	-	23/53/53/53	-
21	CLA	b	605	4	1/1/14/20	9/35/113/115	-
21	CLA	B	605	4	-	11/33/111/115	-
21	CLA	g	308	1	-	18/37/115/115	-
28	LMG	b	624	-	-	16/32/52/70	0/1/1/1
24	KC1	1	316	1	-	7/15/71/71	-
21	CLA	9	304	-	1/1/13/20	9/27/105/115	-
30	DGD	b	601	-	-	24/43/79/95	0/2/2/2
21	CLA	9	303	19	1/1/12/20	12/21/99/115	-
21	CLA	6	307	-	1/1/15/20	15/37/115/115	-
21	CLA	G	303	-	1/1/12/20	10/21/99/115	-
21	CLA	g	306	1	1/1/15/20	19/37/115/115	-
24	KC1	5	313	1	-	8/15/71/71	-
25	BCR	b	618	-	-	7/29/63/63	0/2/2/2
21	CLA	B	616	4	1/1/15/20	13/37/115/115	-
21	CLA	B	609	4	-	5/37/115/115	-
23	A86	1	313	-	-	21/34/90/90	0/3/3/3
24	KC1	2	313	16	-	8/15/71/71	-
24	KC1	g	313	1	-	8/15/71/71	-
24	KC1	G	307	20	-	7/15/71/71	-
24	KC1	G	308	20	-	7/15/71/71	-
25	BCR	A	405	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	C	509	36	1/1/15/20	15/37/115/115	-
28	LMG	N	101	-	-	11/17/37/70	0/1/1/1
24	KC1	8	315	16	-	4/15/71/71	-
21	CLA	2	306	16	-	6/13/91/115	-
30	DGD	h	103	-	-	17/51/91/95	0/2/2/2
21	CLA	5	302	1	1/1/15/20	9/37/115/115	-
21	CLA	c	506	18	-	11/37/115/115	-
21	CLA	c	509	18	-	11/37/115/115	-
21	CLA	8	307	16	1/1/10/20	4/11/89/115	-
24	KC1	4	306	20	-	2/8/64/71	-
31	SQD	C	502	-	-	20/46/66/69	0/1/1/1
24	KC1	9	306	19	-	6/15/71/71	-
23	A86	2	309	-	-	21/34/90/90	0/3/3/3
21	CLA	5	309	1	1/1/15/20	18/37/115/115	-
24	KC1	G	306	20	-	0/8/64/71	-
21	CLA	b	607	4	-	8/37/115/115	-
22	DD6	5	310	-	-	8/26/80/80	0/3/3/3
21	CLA	g	309	1	1/1/12/20	8/19/97/115	-
23	A86	2	308	-	-	9/34/90/90	0/3/3/3
21	CLA	B	606	4	-	9/37/115/115	-
24	KC1	8	316	16	-	7/15/71/71	-
21	CLA	6	302	2	1/1/11/20	3/13/91/115	-
21	CLA	B	610	-	1/1/15/20	7/37/115/115	-
21	CLA	3	304	19	-	8/28/106/115	-
21	CLA	8	305	16	-	3/8/86/115	-
24	KC1	J	312	2	-	5/15/71/71	-
21	CLA	J	305	-	1/1/11/20	4/13/91/115	-
25	BCR	c	501	-	-	7/29/63/63	0/2/2/2
24	KC1	8	313	16	-	3/15/71/71	-
28	LMG	a	407	-	-	22/43/63/70	0/1/1/1
28	LMG	B	620	-	-	3/23/43/70	0/1/1/1
21	CLA	J	301	2	1/1/13/20	14/28/106/115	-
23	A86	J	309	-	-	19/34/90/90	0/3/3/3
23	A86	2	312	-	-	19/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	KC1	7	314	1	-	6/15/71/71	-
21	CLA	8	303	16	1/1/12/20	4/19/97/115	-
30	DGD	c	517	-	-	14/26/66/95	0/2/2/2
28	LMG	B	622	-	-	14/32/52/70	0/1/1/1
21	CLA	C	510	18	-	11/37/115/115	-
21	CLA	6	304	2	1/1/10/20	3/11/89/115	-
23	A86	g	311	-	-	20/34/90/90	0/3/3/3
21	CLA	6	303	-	1/1/11/20	6/13/89/115	-
21	CLA	J	306	36	1/1/15/20	13/37/115/115	-
21	CLA	G	301	20	1/1/13/20	6/28/106/115	-
21	CLA	C	515	18	-	3/18/96/115	-
21	CLA	4	302	20	-	14/27/105/115	-
24	KC1	3	306	19	-	5/15/71/71	-
30	DGD	c	516	-	-	20/44/84/95	0/2/2/2
26	PHO	D	401	-	-	0/37/103/103	0/5/6/6
21	CLA	9	302	19	1/1/11/20	3/16/94/115	-
21	CLA	6	308	2	1/1/12/20	8/22/100/115	-
24	KC1	6	313	2	-	7/15/71/71	-
29	LMU	g	301	-	-	8/18/58/61	0/2/2/2
21	CLA	9	300	19	1/1/13/20	8/27/105/115	-
21	CLA	C	508	18	1/1/11/20	3/13/91/115	-
24	KC1	8	314	16	-	6/15/71/71	-
21	CLA	8	304	23	-	9/21/99/115	-
21	CLA	b	616	4	1/1/15/20	7/37/115/115	-
30	DGD	C	517	-	-	19/44/84/95	0/2/2/2
25	BCR	B	618	-	-	8/29/63/63	0/2/2/2
21	CLA	6	306	36	1/1/15/20	11/37/115/115	-
21	CLA	5	308	1	-	11/37/115/115	-
21	CLA	1	307	1	1/1/10/20	4/8/86/115	-
21	CLA	B	615	4	1/1/15/20	6/37/115/115	-
21	CLA	C	503	18	1/1/15/20	11/37/115/115	-
24	KC1	6	312	2	-	4/15/71/71	-
21	CLA	b	612	4	-	6/35/113/115	-
28	LMG	b	625	-	-	22/38/58/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	b	609	4	-	7/37/115/115	-
21	CLA	C	511	18	1/1/15/20	8/37/115/115	-
21	CLA	D	406	17	1/1/13/20	7/28/104/115	-
21	CLA	J	304	2	1/1/10/20	3/11/89/115	-
21	CLA	C	506	-	-	15/35/113/115	-
21	CLA	c	503	18	-	3/35/113/115	-
21	CLA	7	306	1	1/1/10/20	4/8/86/115	-
21	CLA	B	603	4	1/1/12/20	14/27/107/115	-
28	LMG	B	623	-	-	15/38/58/70	0/1/1/1
21	CLA	8	306	-	1/1/13/20	12/29/107/115	-
21	CLA	1	308	-	-	10/24/102/115	-
23	A86	5	311	-	-	10/34/90/90	0/3/3/3
29	LMU	5	301	-	-	8/18/58/61	0/2/2/2
21	CLA	c	511	18	1/1/15/20	8/37/115/115	-
21	CLA	B	621	-	-	18/37/115/115	-
21	CLA	D	407	17	-	9/31/109/115	-
23	A86	7	311	-	-	24/34/90/90	0/3/3/3
21	CLA	J	308	2	1/1/12/20	9/22/100/115	-
23	A86	8	311	-	-	16/34/90/90	0/3/3/3
21	CLA	G	302	20	-	10/27/105/115	-
21	CLA	b	603	-	1/1/11/20	6/16/94/115	-
25	BCR	C	501	-	-	9/29/63/63	0/2/2/2
21	CLA	C	507	18	-	11/37/115/115	-

The worst 5 of 4279 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	303	CLA	MG-ND	-44.39	1.17	2.05
21	G	302	CLA	MG-ND	-34.75	1.36	2.05
21	G	302	CLA	MG-NA	29.57	2.76	2.06
21	4	302	CLA	MG-NC	27.33	2.71	2.06
21	J	303	CLA	MG-NA	26.01	2.68	2.06

The worst 5 of 5336 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	302	CLA	C5-C3-C4	-15.68	79.97	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	302	CLA	C4-C3-C2	-14.73	80.08	122.65
21	2	302	CLA	C5-C3-C2	12.93	160.02	122.65
24	4	308	KC1	CMA-C3A-C4A	-12.33	106.26	125.04
24	G	307	KC1	CMA-C3A-C4A	-11.94	106.86	125.04

5 of 101 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	1	301	CLA	ND
21	1	302	CLA	ND
21	1	303	CLA	ND
21	1	304	CLA	ND
21	1	306	CLA	ND

5 of 3240 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	1	301	CLA	CBD-CGD-O2D-CED
21	1	303	CLA	C1A-C2A-CAA-CBA
21	1	303	CLA	CBD-CGD-O2D-CED
21	1	303	CLA	O1D-CGD-O2D-CED
21	1	304	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

191 monomers are involved in 362 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	b	604	CLA	2	0
25	1	317	BCR	3	0
25	M	101	BCR	2	0
31	B	626	SQD	2	0
27	D	410	LHG	6	0
29	D	412	LMU	1	0
28	B	619	LMG	4	0
24	g	315	KC1	1	0
26	A	403	PHO	2	0
28	8	317	LMG	4	0
26	d	403	PHO	2	0
21	b	610	CLA	3	0
21	b	606	CLA	4	0
28	2	318	LMG	3	0
21	5	306	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	G	304	CLA	2	0
25	D	408	BCR	1	0
28	b	626	LMG	2	0
21	c	508	CLA	3	0
21	7	309	CLA	2	0
28	b	620	LMG	3	0
21	2	305	CLA	1	0
21	8	302	CLA	3	0
21	7	300	CLA	2	0
21	B	611	CLA	2	0
25	b	619	BCR	2	0
25	C	516	BCR	3	0
29	5	316	LMU	1	0
35	d	408	PL9	2	0
21	d	404	CLA	2	0
24	2	315	KC1	4	0
21	9	301	CLA	2	0
25	c	515	BCR	2	0
21	c	510	CLA	1	0
21	1	301	CLA	5	0
21	B	608	CLA	1	0
21	3	300	CLA	3	0
21	c	502	CLA	1	0
21	3	302	CLA	1	0
21	b	611	CLA	2	0
21	g	304	CLA	3	0
21	b	615	CLA	3	0
21	g	303	CLA	2	0
28	L	101	LMG	1	0
21	a	402	CLA	3	0
28	A	407	LMG	1	0
21	B	614	CLA	1	0
21	1	303	CLA	1	0
25	h	101	BCR	3	0
21	6	300	CLA	1	0
31	B	625	SQD	1	0
32	E	101	HEM	1	0
21	J	303	CLA	1	0
26	a	404	PHO	1	0
21	2	302	CLA	3	0
21	J	307	CLA	3	0
21	C	512	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	d	405	CLA	3	0
21	B	613	CLA	2	0
21	1	304	CLA	2	0
21	b	623	CLA	6	0
21	G	300	CLA	1	0
21	5	307	CLA	1	0
25	H	100	BCR	2	0
21	2	303	CLA	3	0
25	h	102	BCR	1	0
35	D	409	PL9	2	0
21	g	307	CLA	1	0
21	2	301	CLA	3	0
22	1	311	DD6	1	0
27	B	601	LHG	3	0
25	a	406	BCR	5	0
24	5	315	KC1	1	0
21	1	302	CLA	1	0
31	b	602	SQD	3	0
27	d	409	LHG	4	0
24	J	311	KC1	1	0
30	B	624	DGD	4	0
21	4	301	CLA	2	0
21	C	513	CLA	4	0
29	8	318	LMU	1	0
21	b	614	CLA	2	0
21	J	300	CLA	1	0
21	D	404	CLA	3	0
21	d	406	CLA	1	0
21	c	513	CLA	2	0
21	7	303	CLA	1	0
21	c	507	CLA	2	0
28	M	102	LMG	2	0
21	B	607	CLA	5	0
21	A	404	CLA	4	0
21	B	612	CLA	3	0
21	C	504	CLA	3	0
21	3	301	CLA	3	0
25	d	407	BCR	1	0
21	c	512	CLA	2	0
30	C	518	DGD	1	0
32	f	101	HEM	1	0
21	g	302	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	a	401	LHG	1	0
21	C	514	CLA	3	0
21	c	504	CLA	4	0
21	a	405	CLA	2	0
27	A	406	LHG	3	0
21	7	301	CLA	3	0
21	7	304	CLA	3	0
21	1	305	CLA	1	0
21	c	505	CLA	1	0
22	7	310	DD6	1	0
28	B	627	LMG	2	0
21	6	301	CLA	3	0
30	H	101	DGD	3	0
21	b	617	CLA	6	0
21	5	304	CLA	1	0
21	b	608	CLA	4	0
21	4	300	CLA	4	0
21	5	303	CLA	4	0
28	b	622	LMG	1	0
21	7	302	CLA	5	0
21	b	613	CLA	2	0
25	B	617	BCR	4	0
21	1	309	CLA	1	0
21	B	604	CLA	1	0
21	7	305	CLA	1	0
21	4	304	CLA	1	0
27	l	101	LHG	2	0
21	b	605	CLA	1	0
21	B	605	CLA	4	0
21	g	308	CLA	2	0
30	b	601	DGD	3	0
21	9	303	CLA	2	0
21	6	307	CLA	3	0
21	g	306	CLA	3	0
25	b	618	BCR	1	0
21	B	616	CLA	4	0
21	B	609	CLA	3	0
24	2	313	KC1	1	0
24	G	307	KC1	2	0
25	A	405	BCR	5	0
21	C	509	CLA	2	0
28	N	101	LMG	1	0

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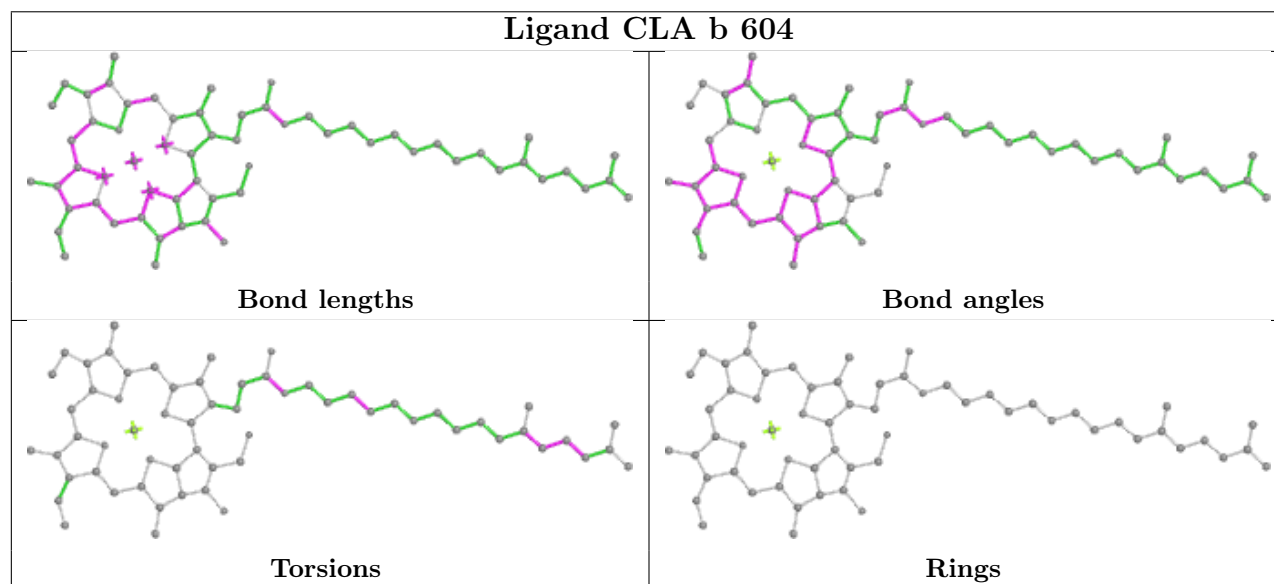
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	306	CLA	1	0
21	5	302	CLA	3	0
21	c	506	CLA	2	0
21	c	509	CLA	3	0
21	8	307	CLA	2	0
31	C	502	SQD	1	0
21	b	607	CLA	4	0
21	B	606	CLA	4	0
21	6	302	CLA	1	0
21	B	610	CLA	1	0
21	3	304	CLA	3	0
24	8	313	KC1	1	0
28	a	407	LMG	2	0
21	J	301	CLA	1	0
21	8	303	CLA	3	0
30	c	517	DGD	1	0
21	C	510	CLA	3	0
21	6	303	CLA	1	0
21	J	306	CLA	3	0
21	4	302	CLA	4	0
30	c	516	DGD	3	0
26	D	401	PHO	2	0
21	9	302	CLA	5	0
29	g	301	LMU	1	0
21	9	300	CLA	2	0
21	C	508	CLA	2	0
21	8	304	CLA	2	0
21	b	616	CLA	3	0
25	B	618	BCR	3	0
21	5	308	CLA	2	0
21	B	615	CLA	2	0
21	C	503	CLA	3	0
21	b	612	CLA	1	0
21	b	609	CLA	1	0
21	C	511	CLA	2	0
21	D	406	CLA	2	0
21	C	506	CLA	2	0
21	c	503	CLA	4	0
21	7	306	CLA	1	0
21	B	603	CLA	2	0
21	8	306	CLA	2	0
21	1	308	CLA	1	0

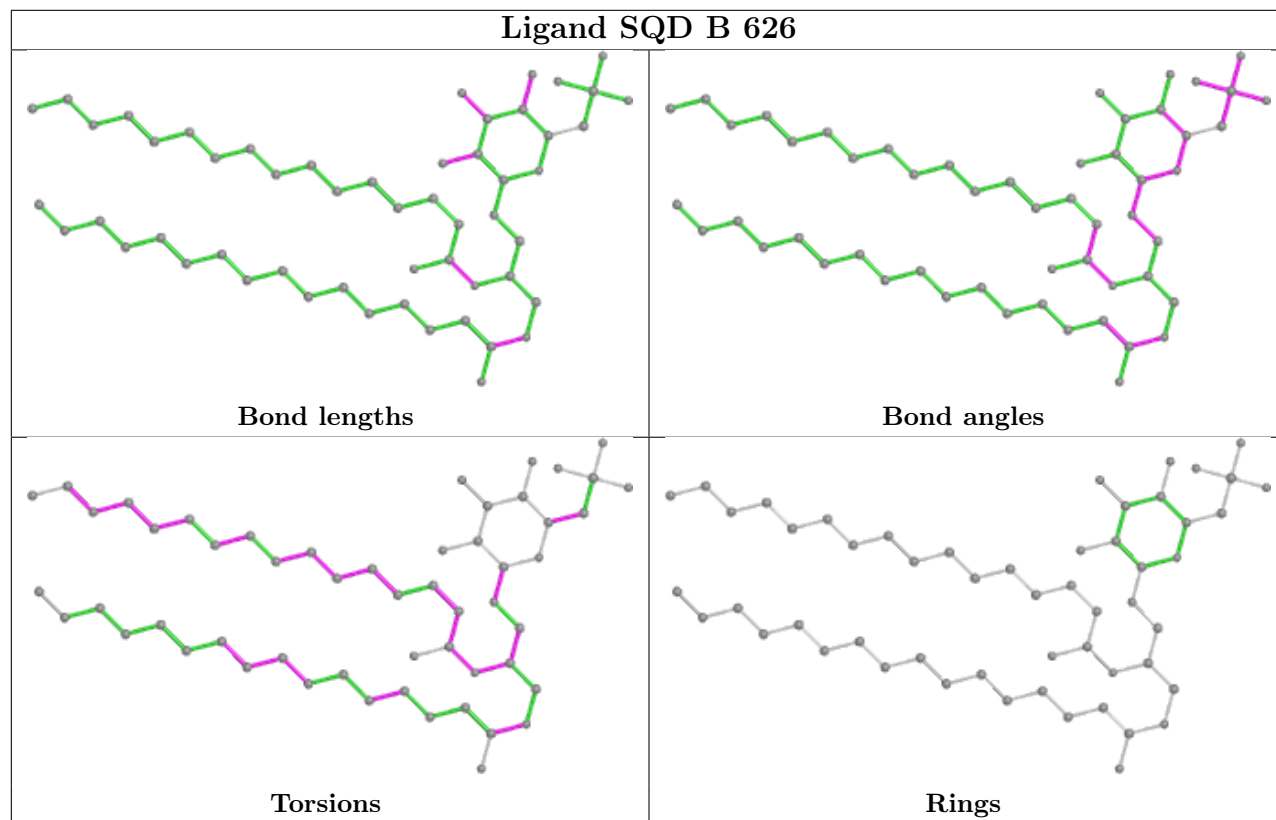
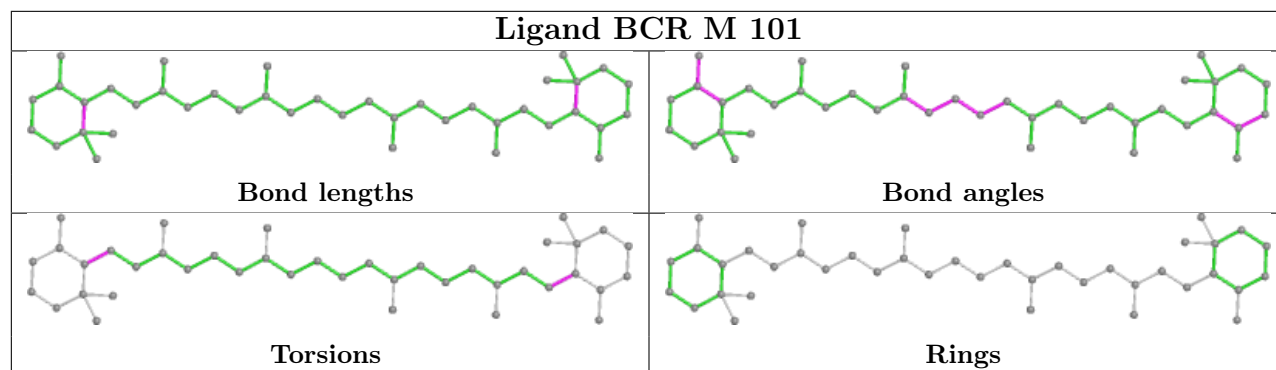
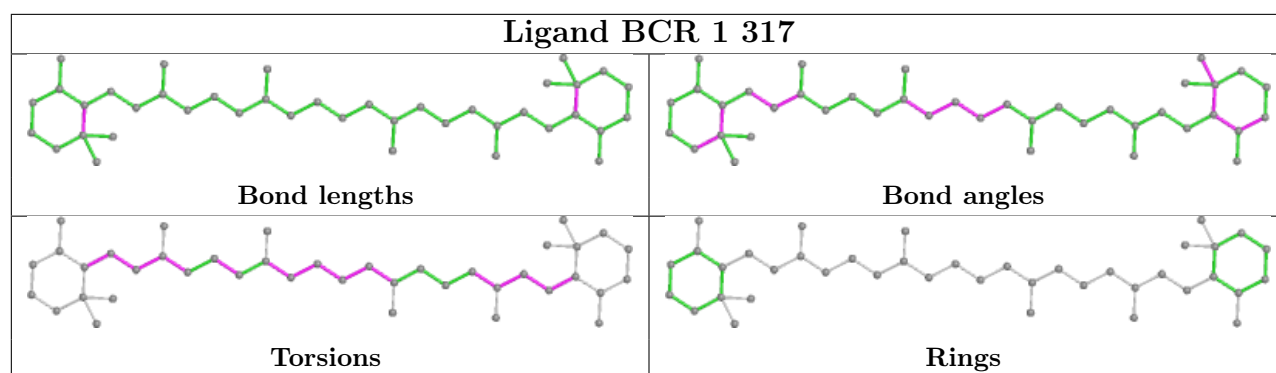
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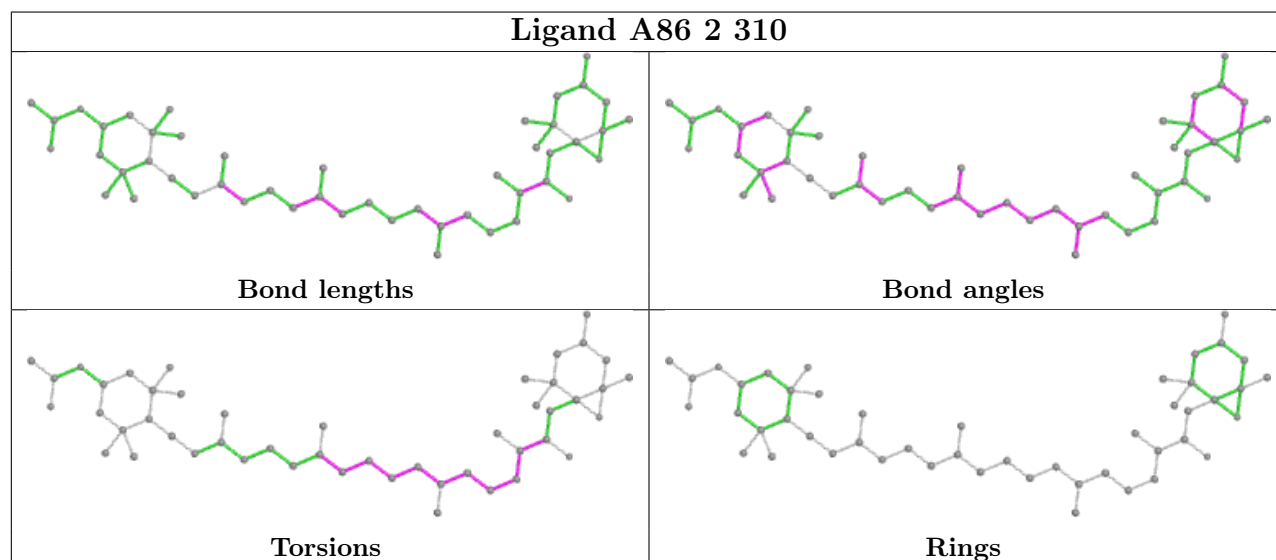
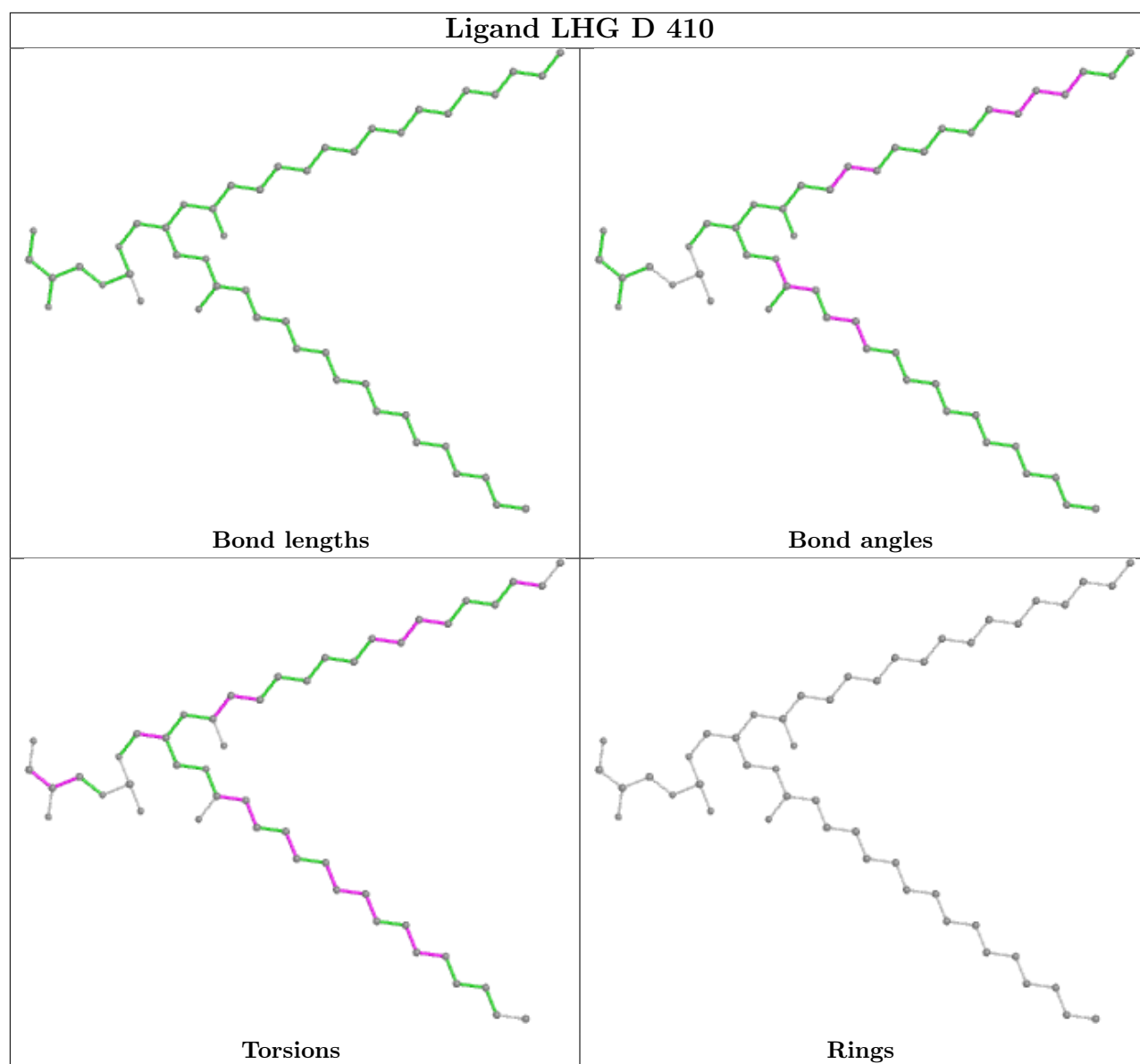
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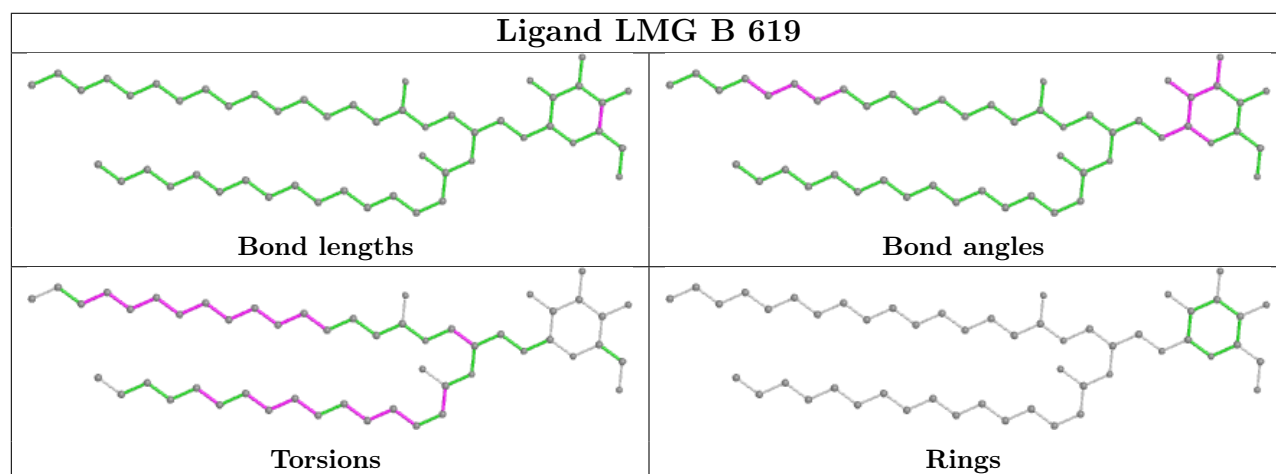
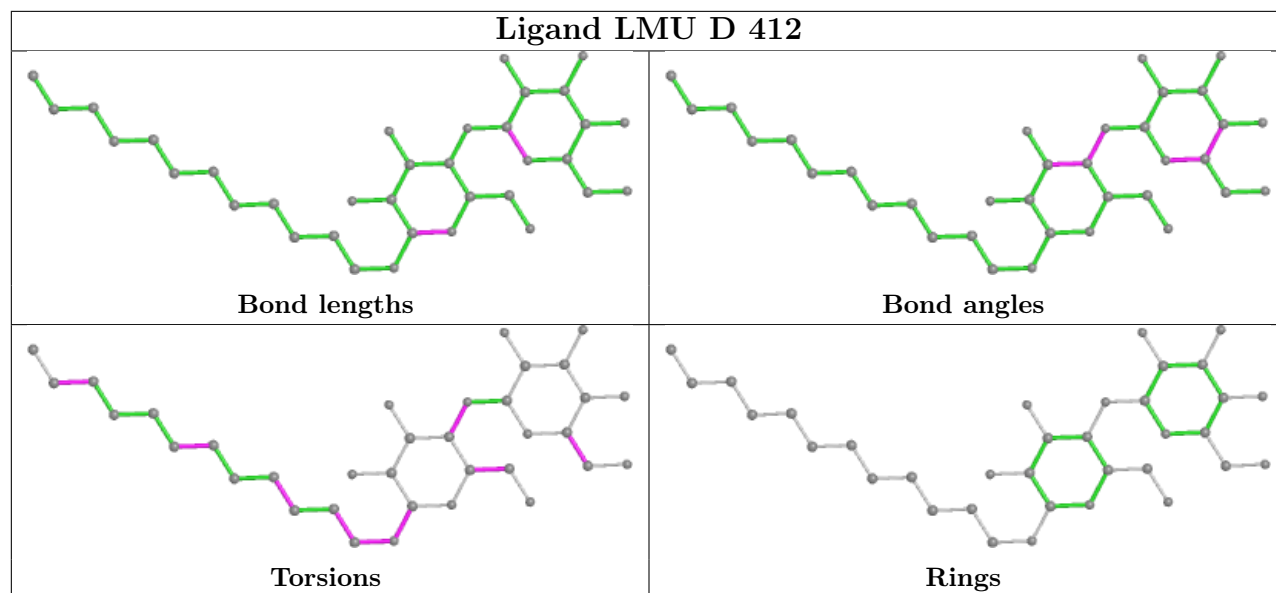
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	5	311	A86	1	0
29	5	301	LMU	1	0
21	c	511	CLA	5	0
21	B	621	CLA	3	0
21	D	407	CLA	2	0
21	b	603	CLA	1	0
25	C	501	BCR	1	0
21	C	507	CLA	1	0

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

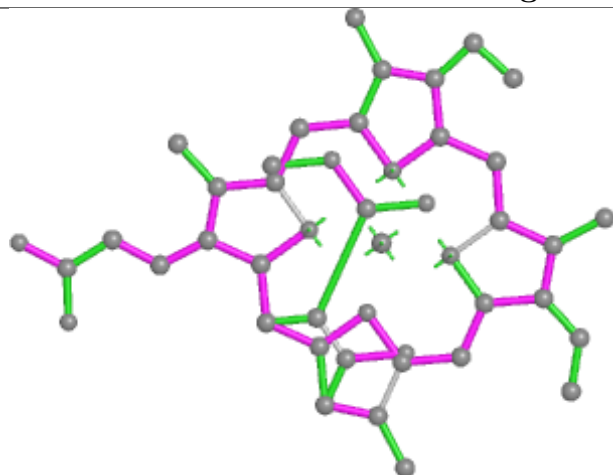




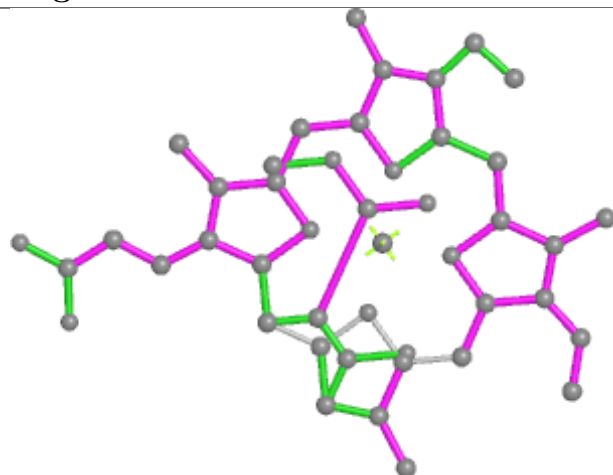




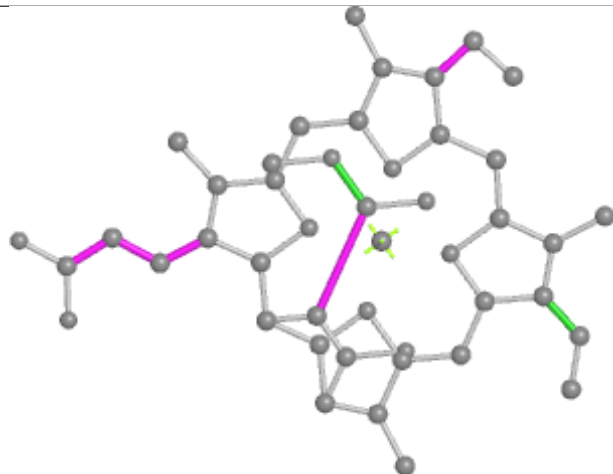
## Ligand KC1 g 315



Bond lengths



Bond angles

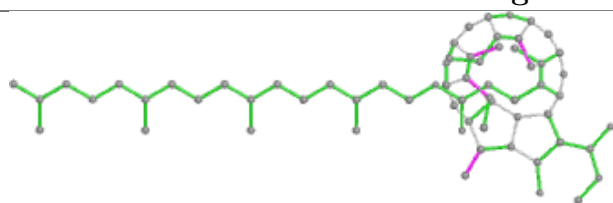


Torsions

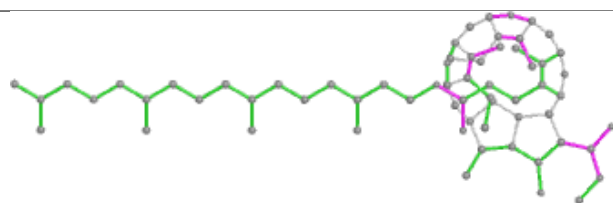


Rings

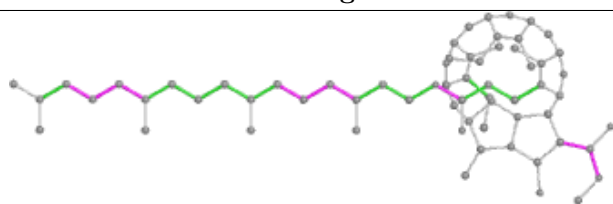
## Ligand PHO A 403



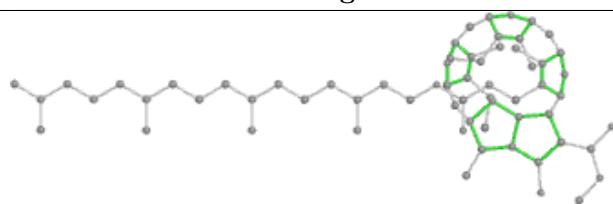
Bond lengths



Bond angles

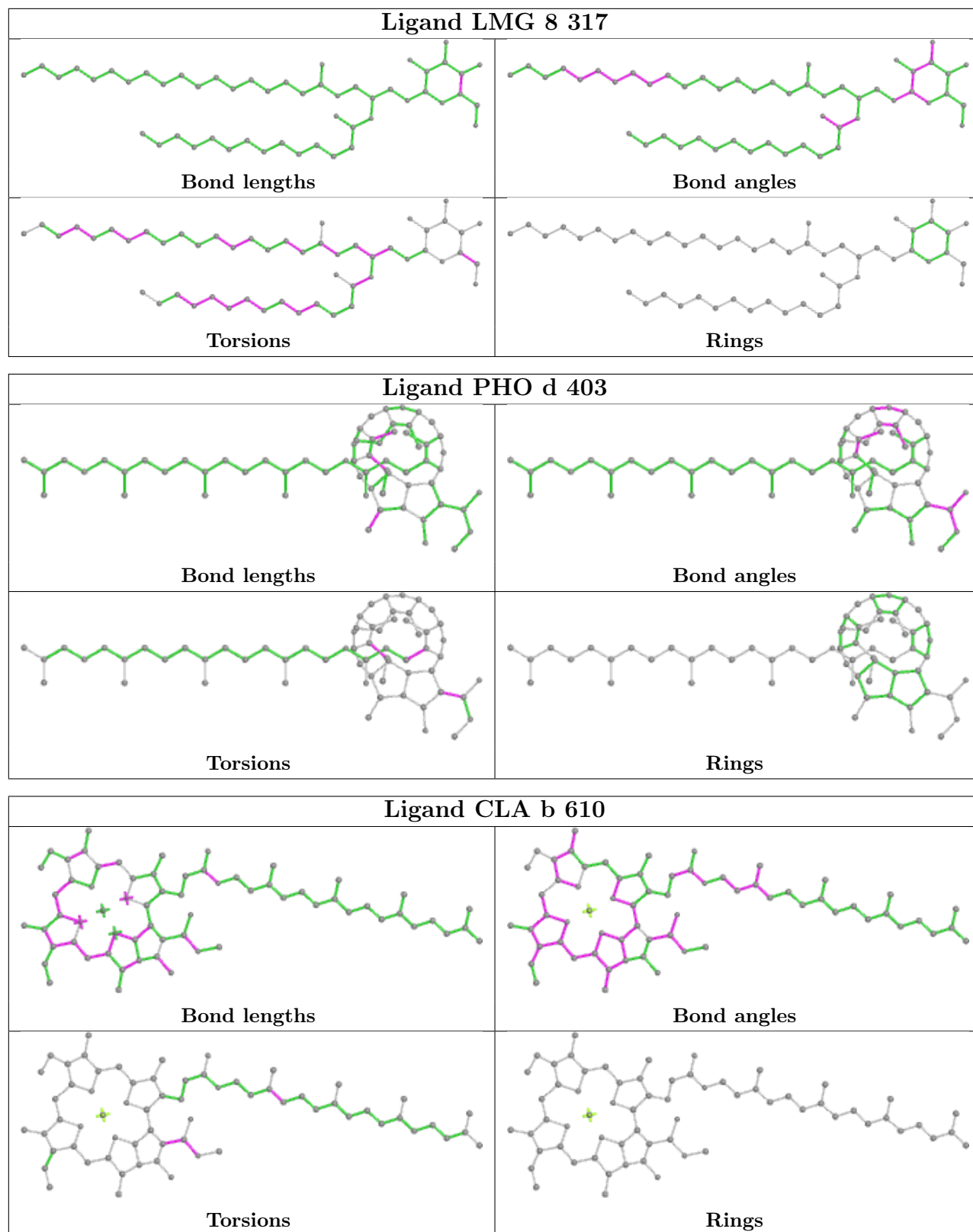


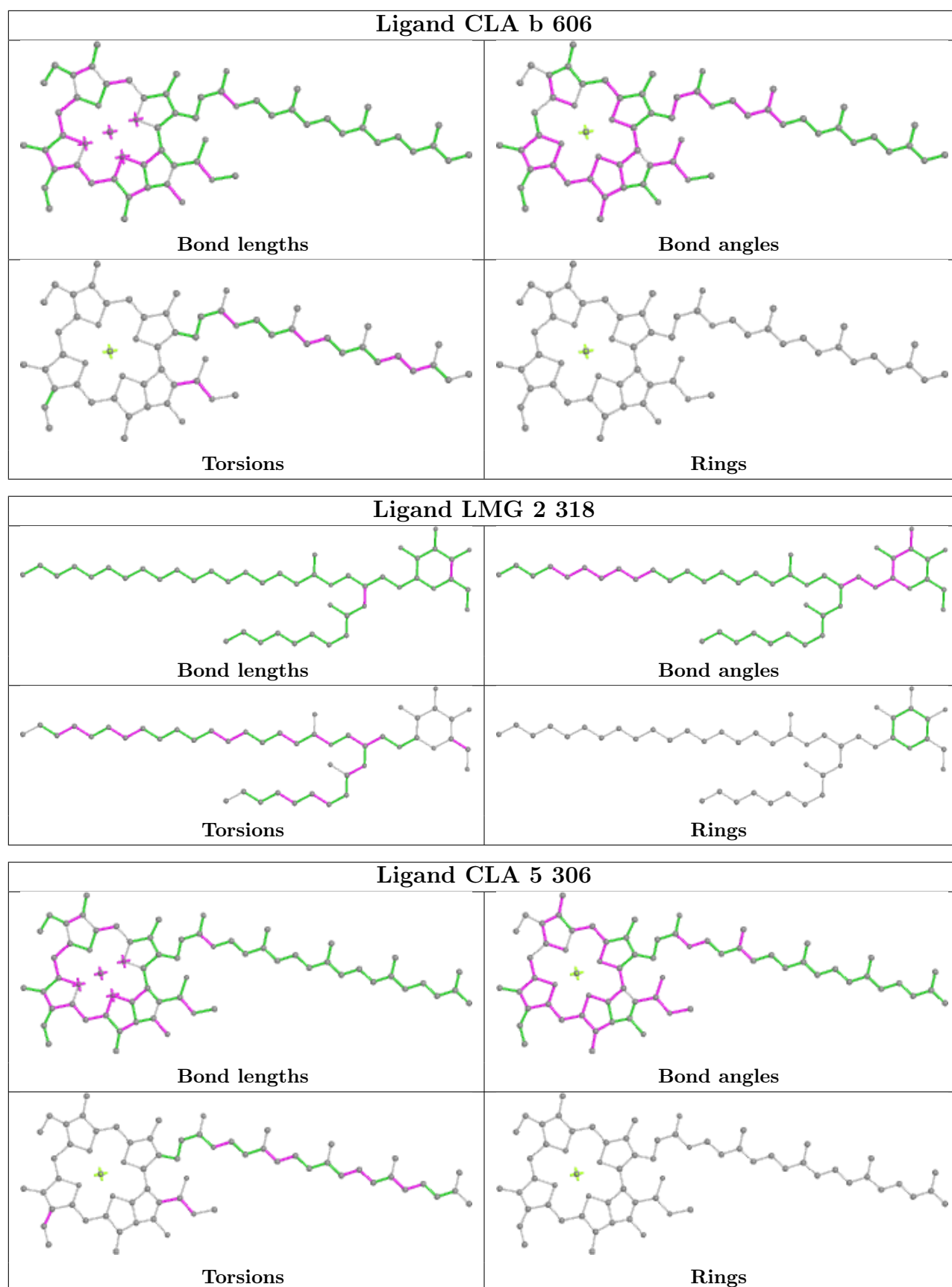
Torsions

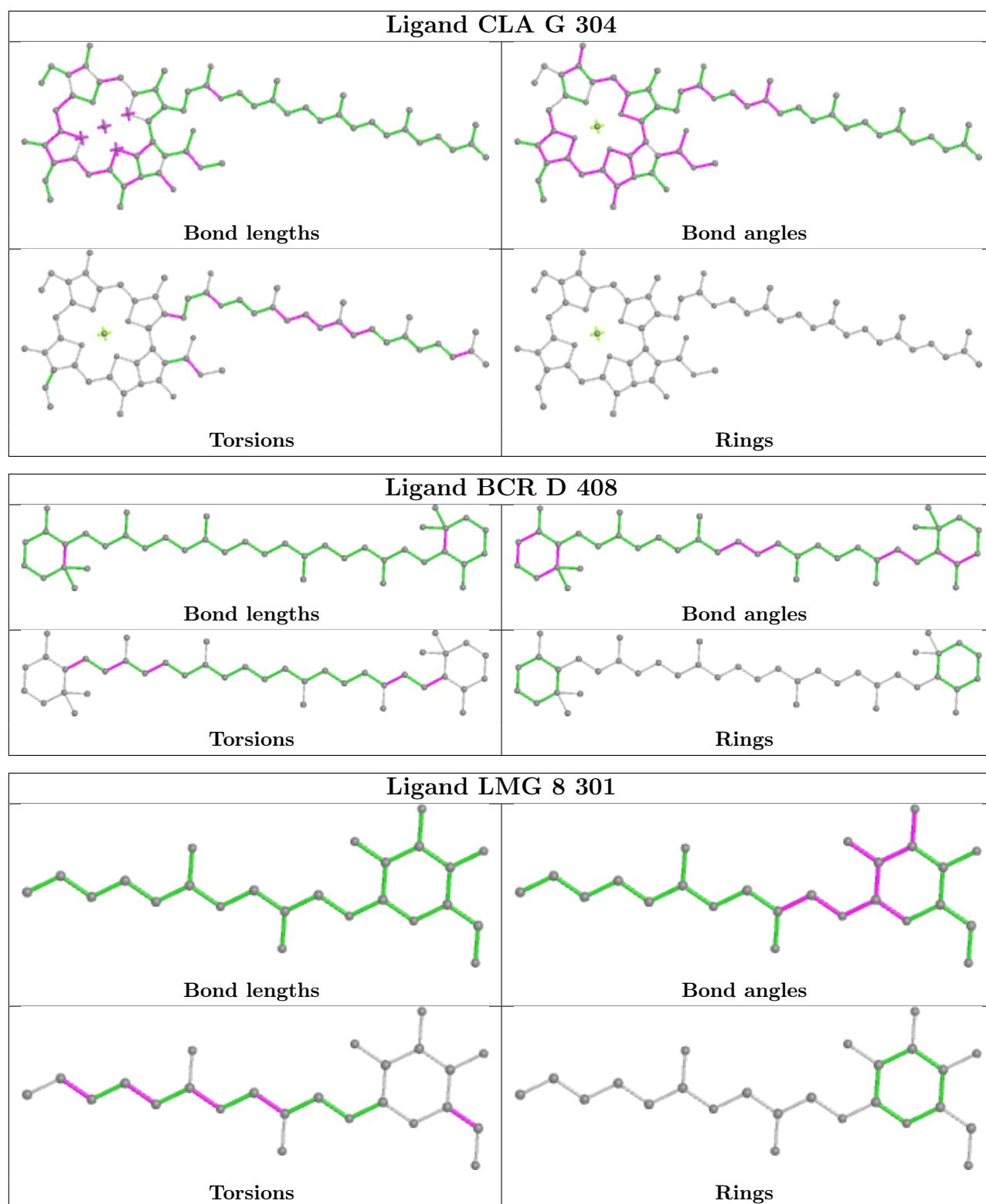


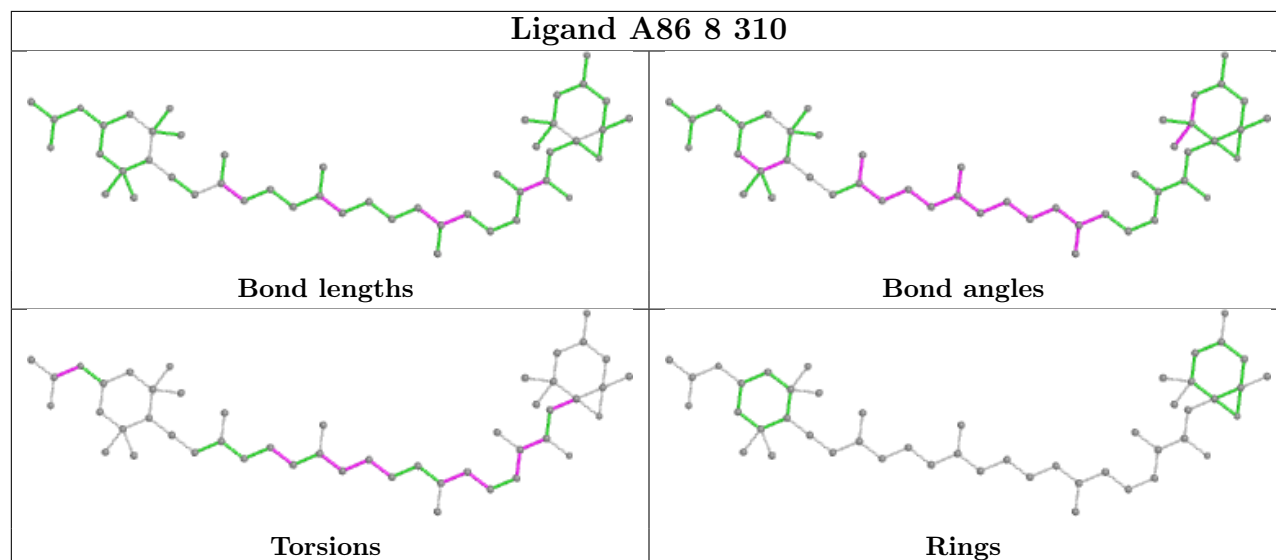
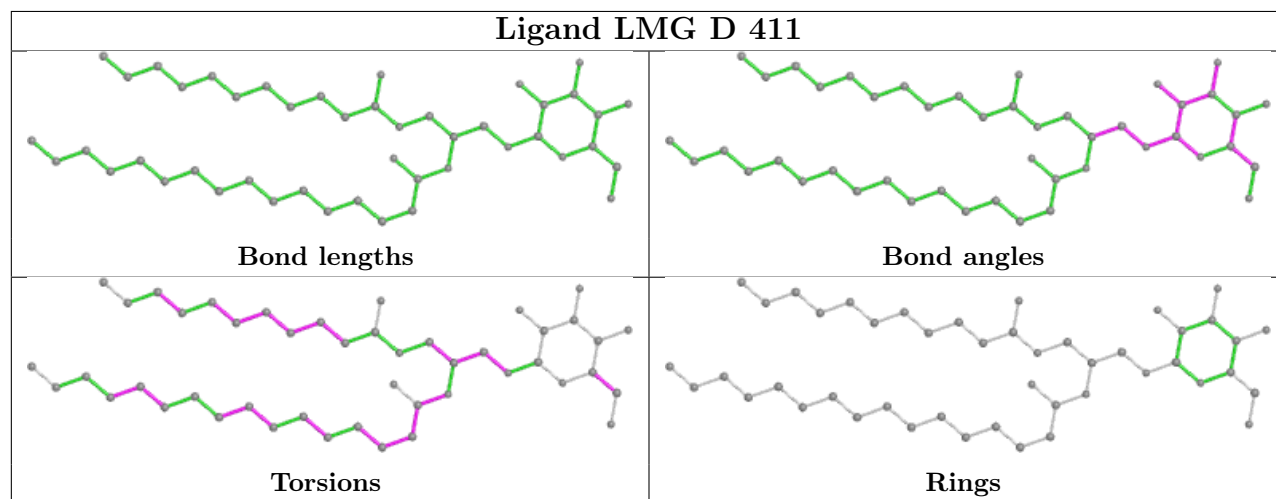
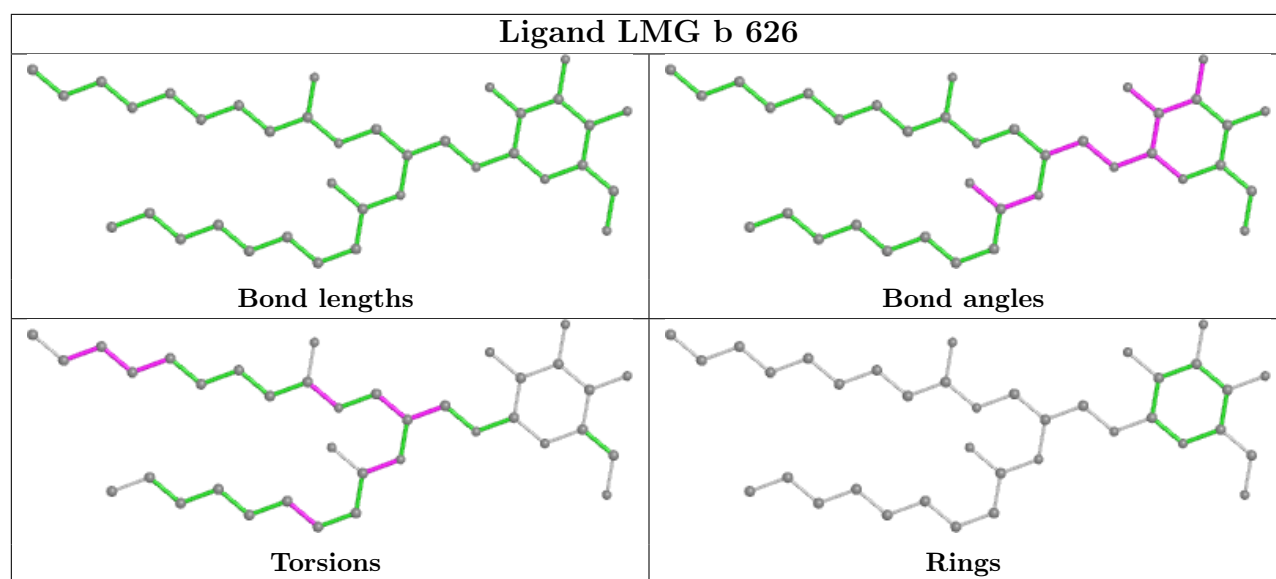
Rings

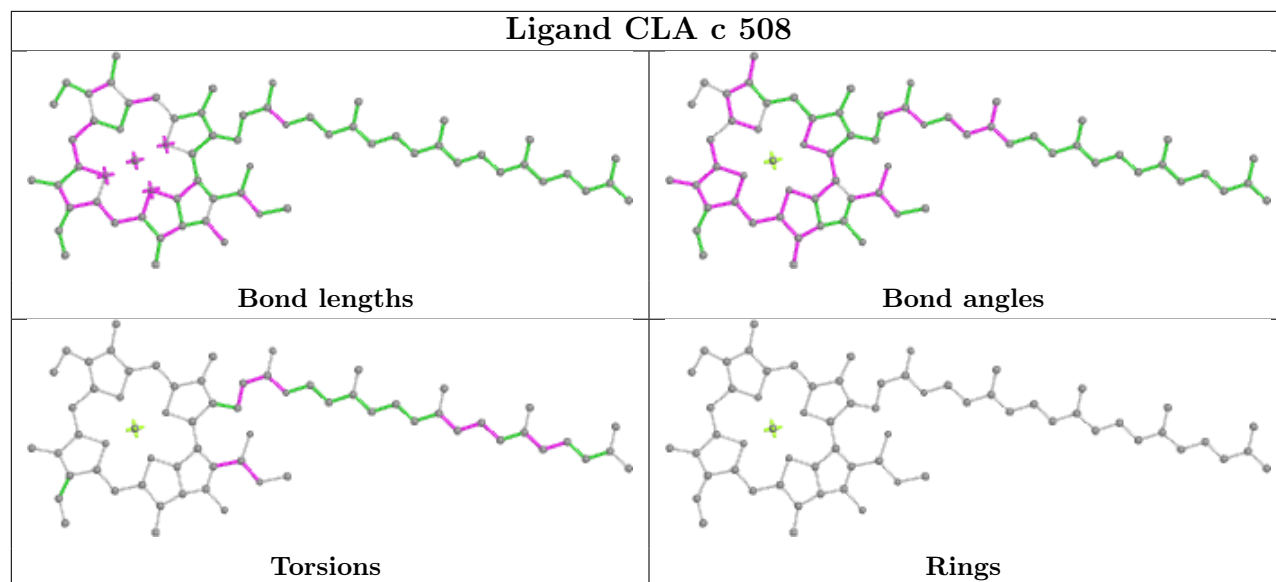
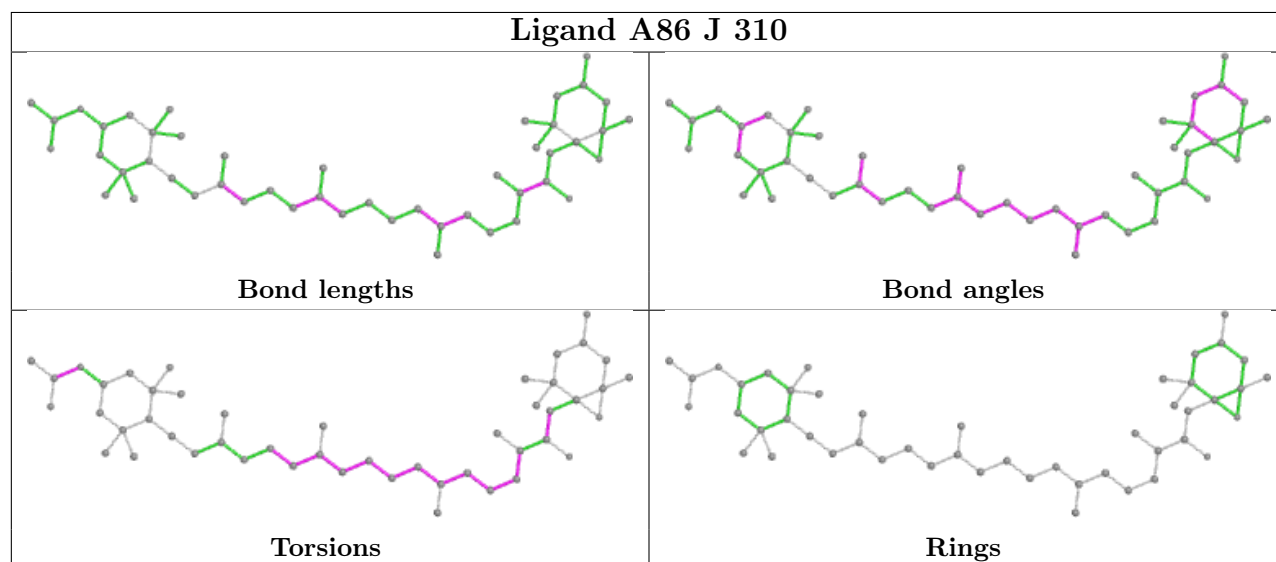




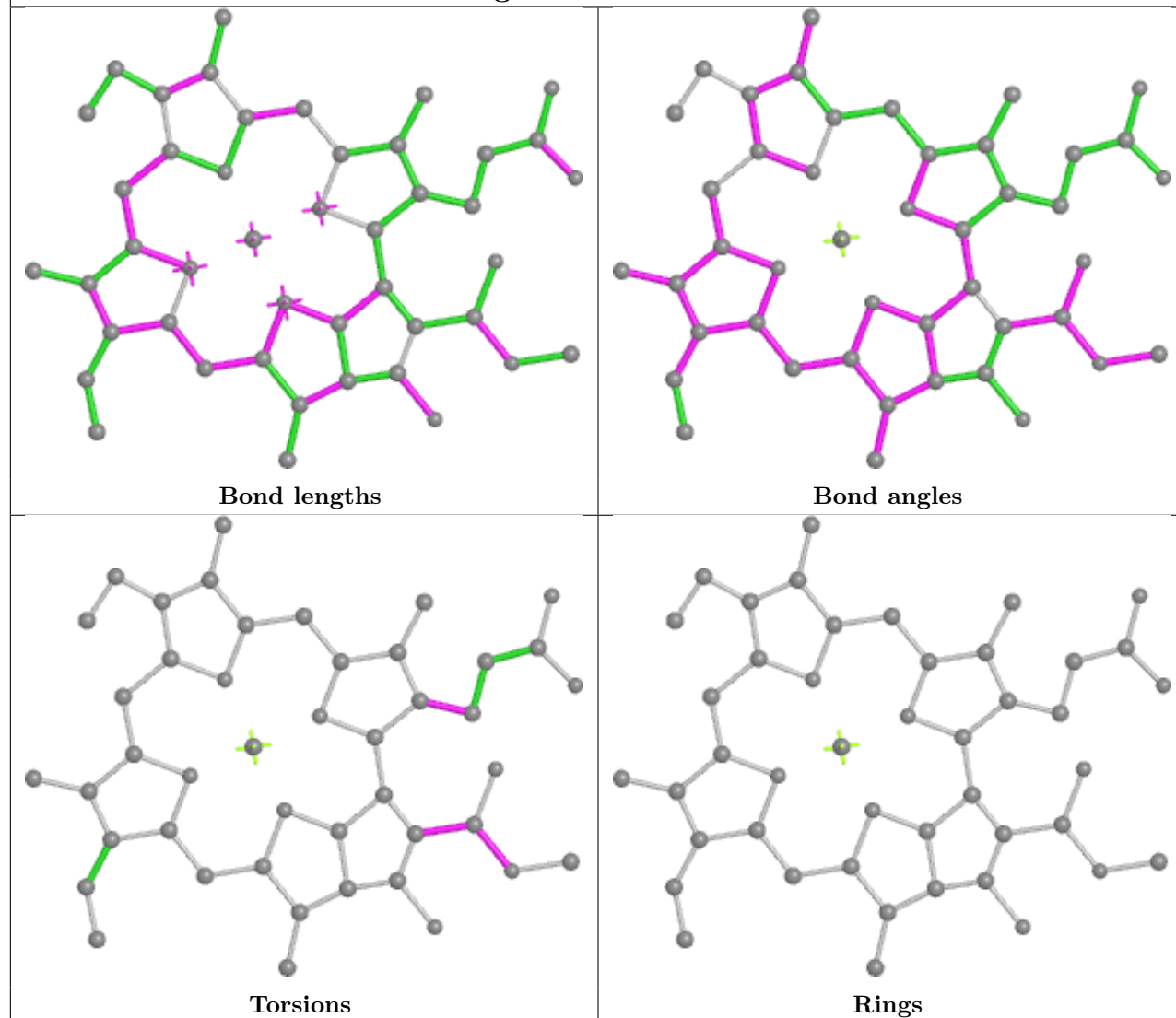




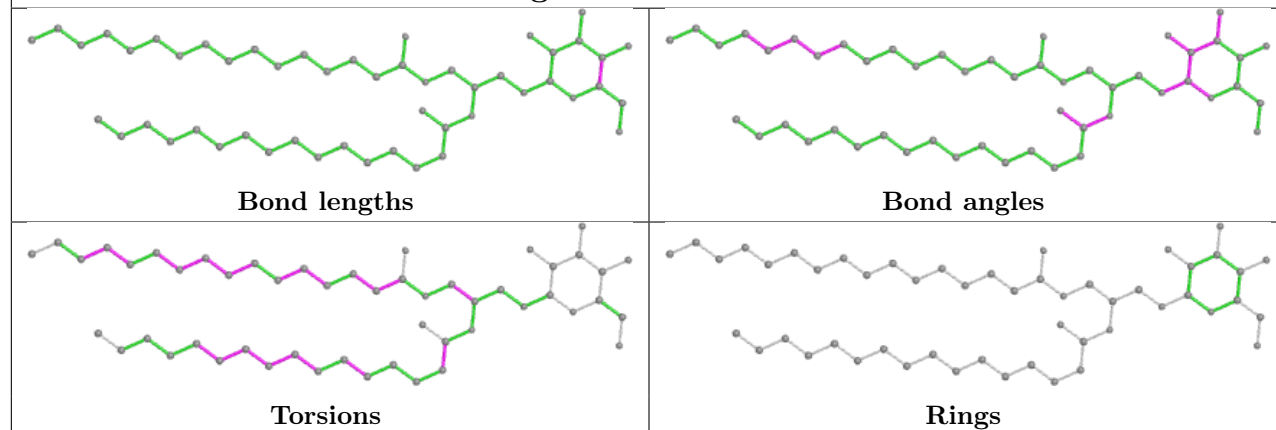


**Ligand CLA c 508****Ligand A86 J 310**

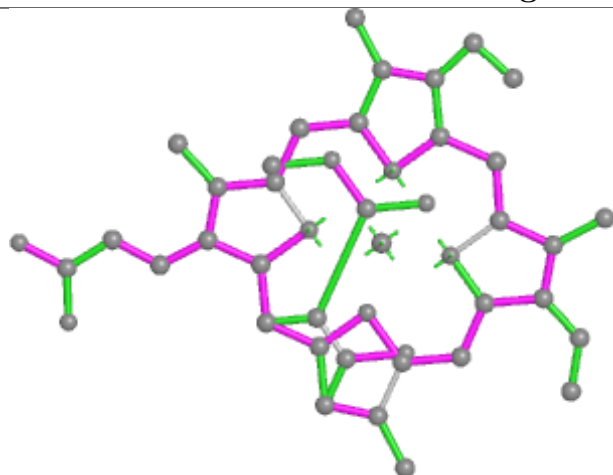
## Ligand CLA 7 309



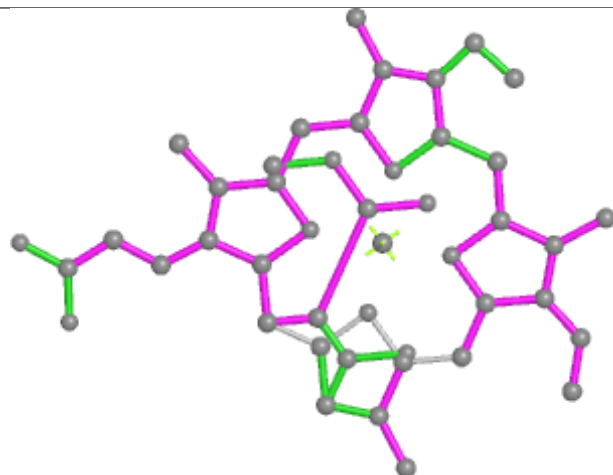
## Ligand LMG b 620



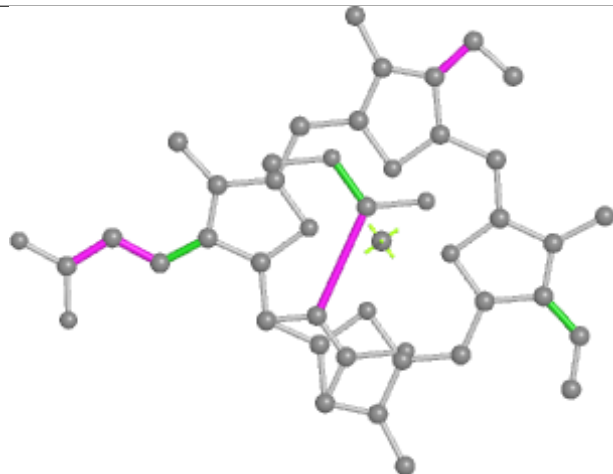
## Ligand KC1 J 313



Bond lengths



Bond angles

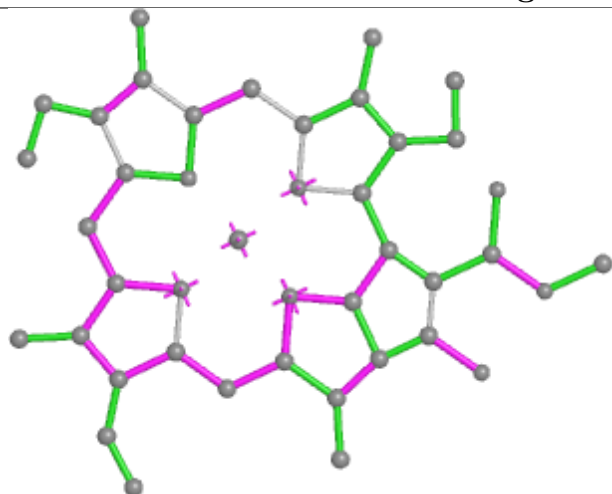


Torsions

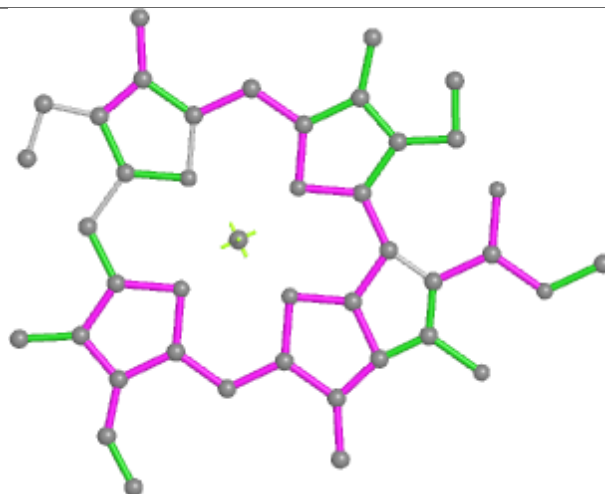


Rings

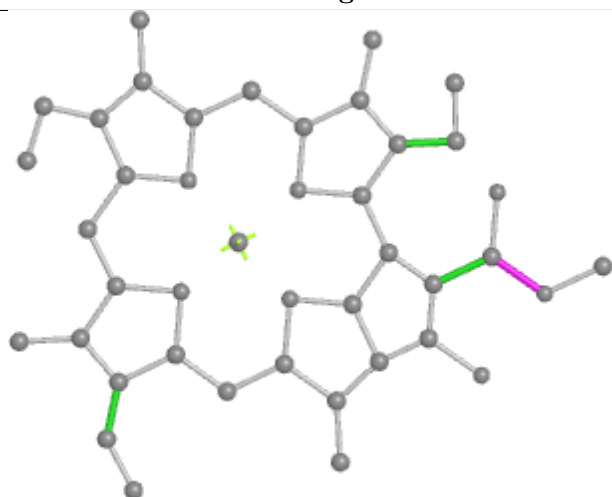
## Ligand CLA 3 303



Bond lengths



Bond angles

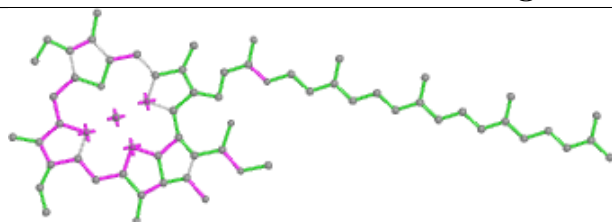


Torsions

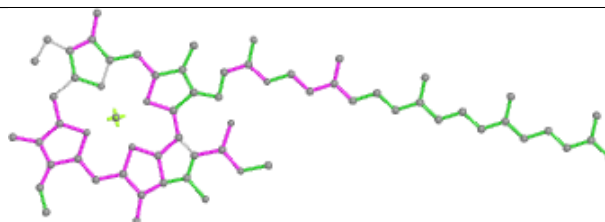


Rings

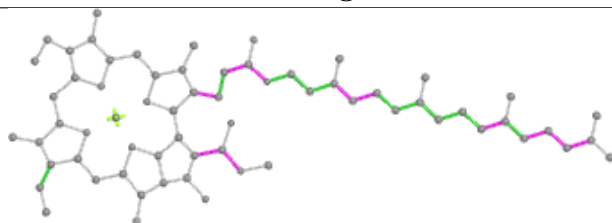
## Ligand CLA 2 305



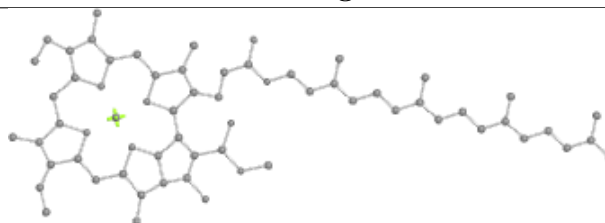
Bond lengths



Bond angles

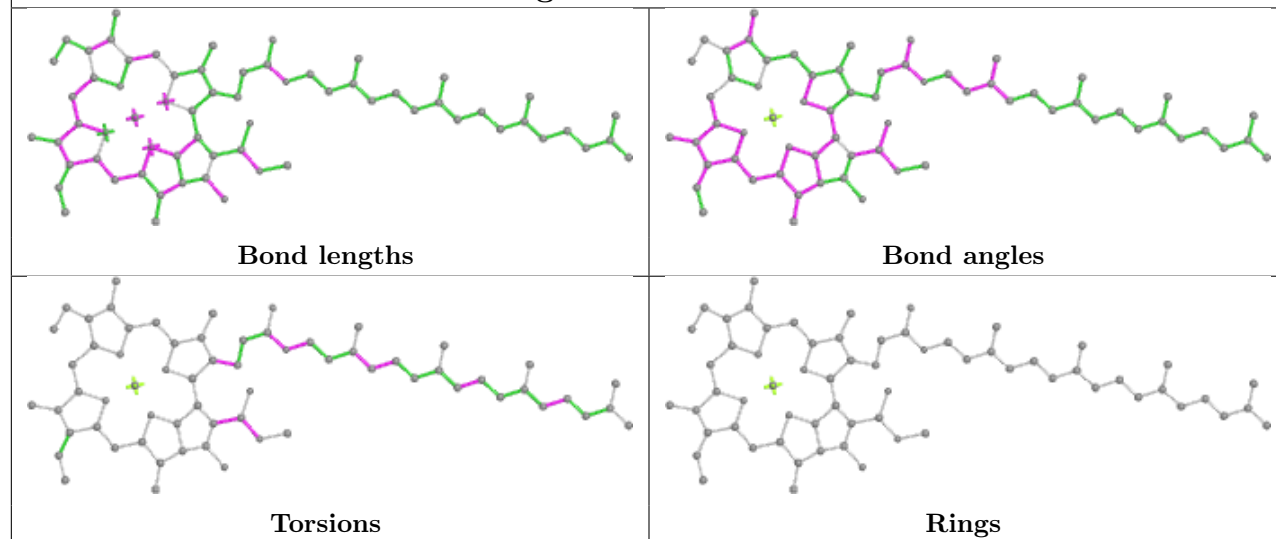
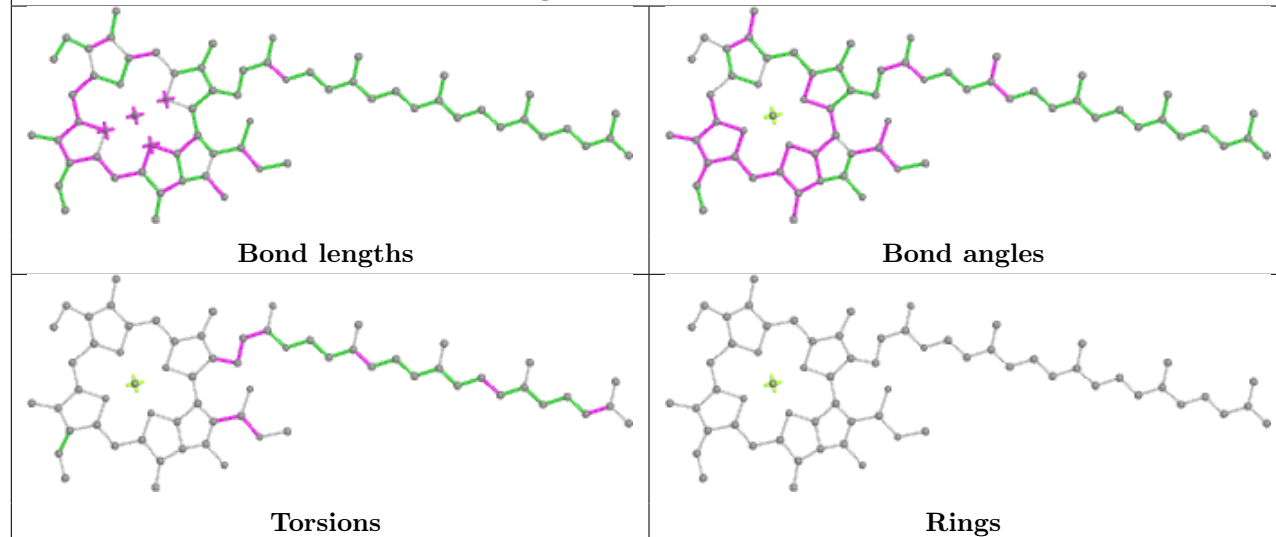
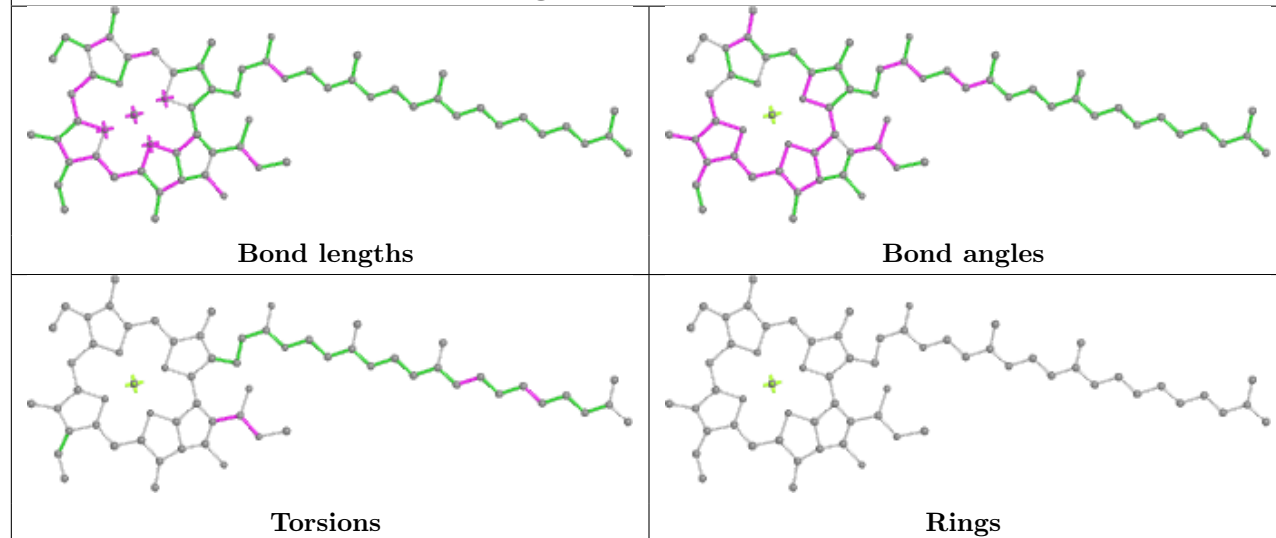


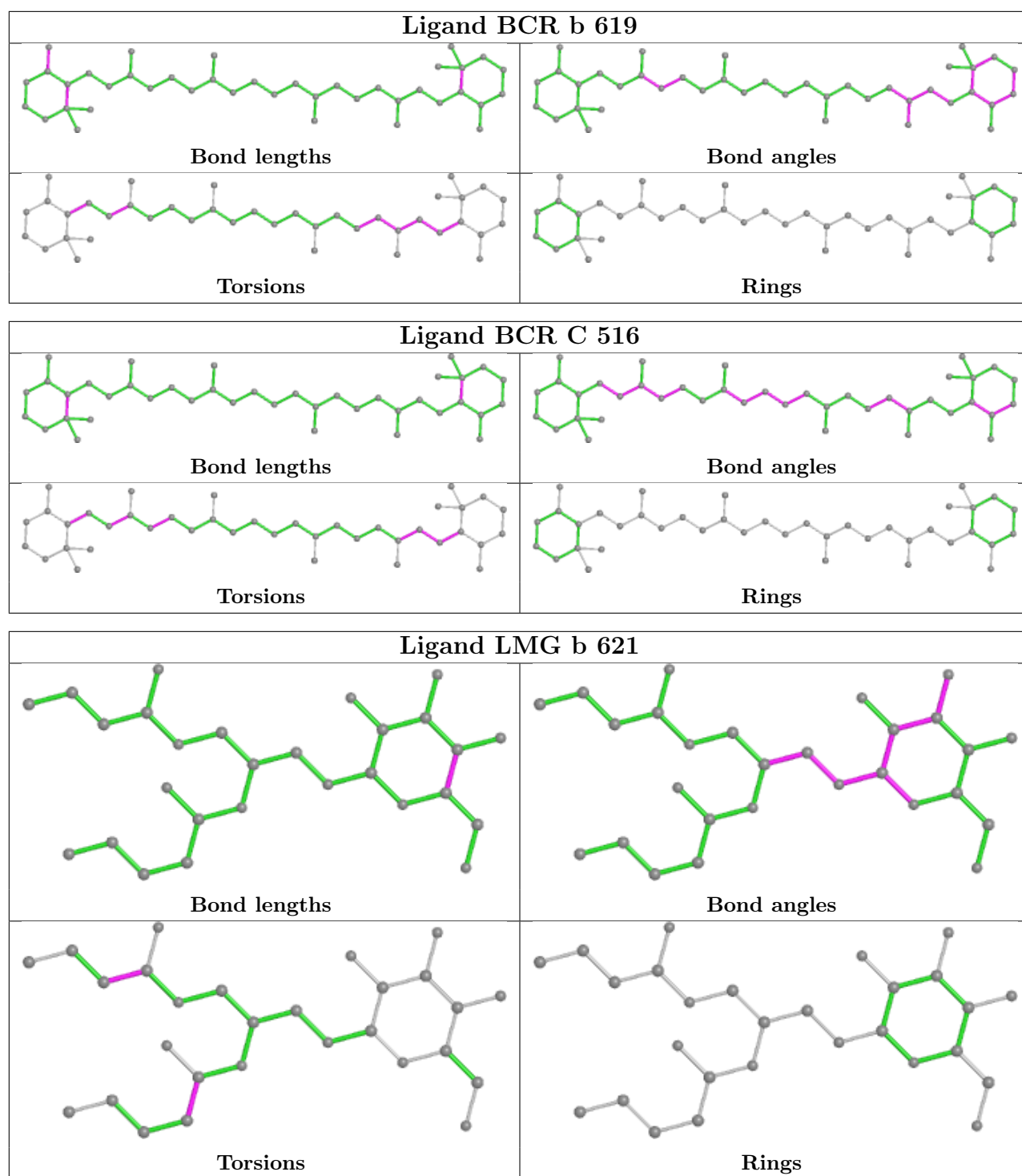
Torsions

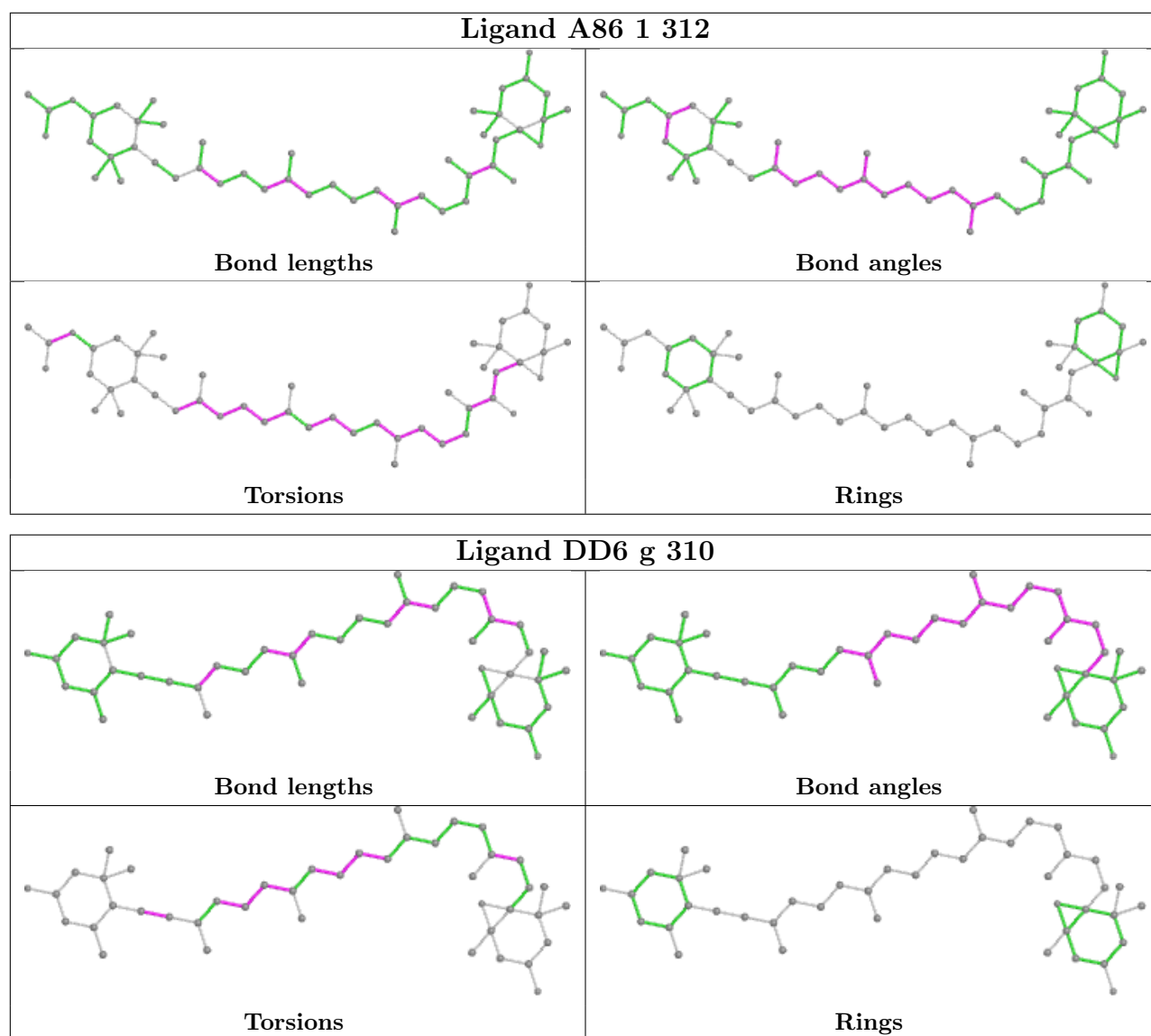


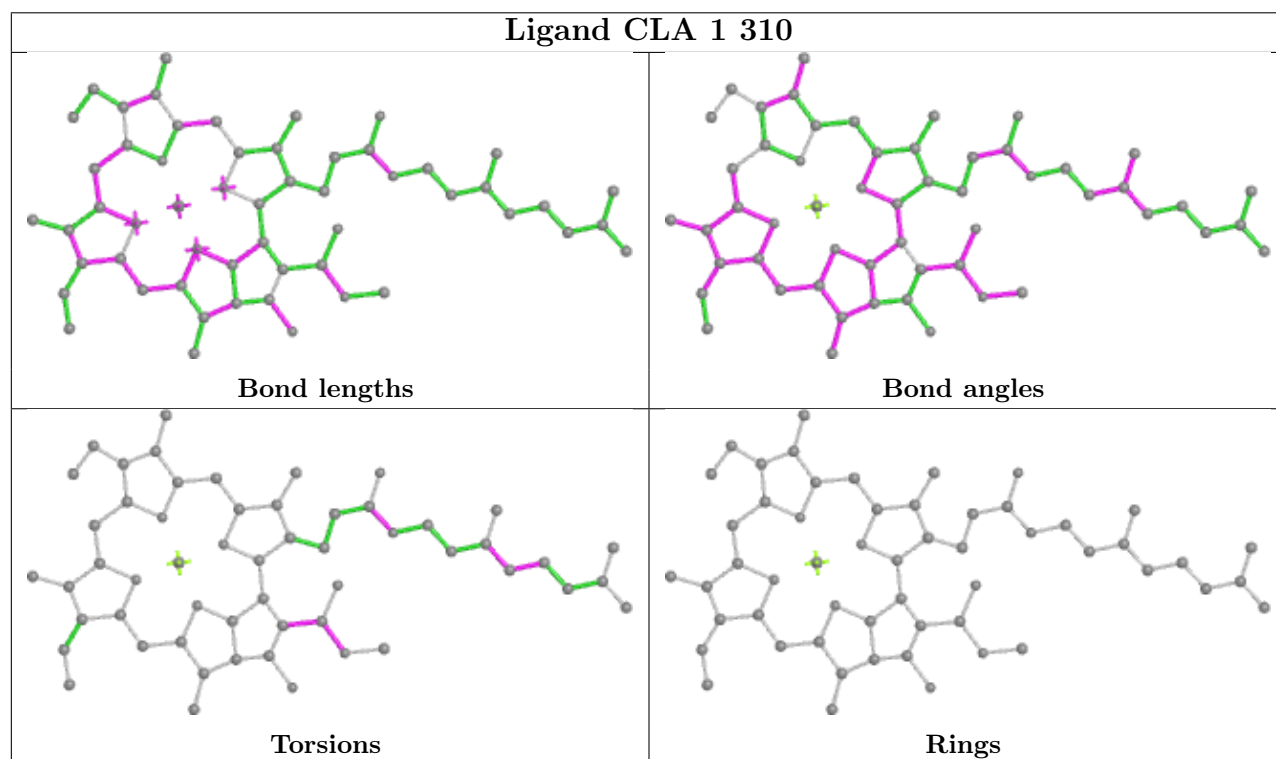
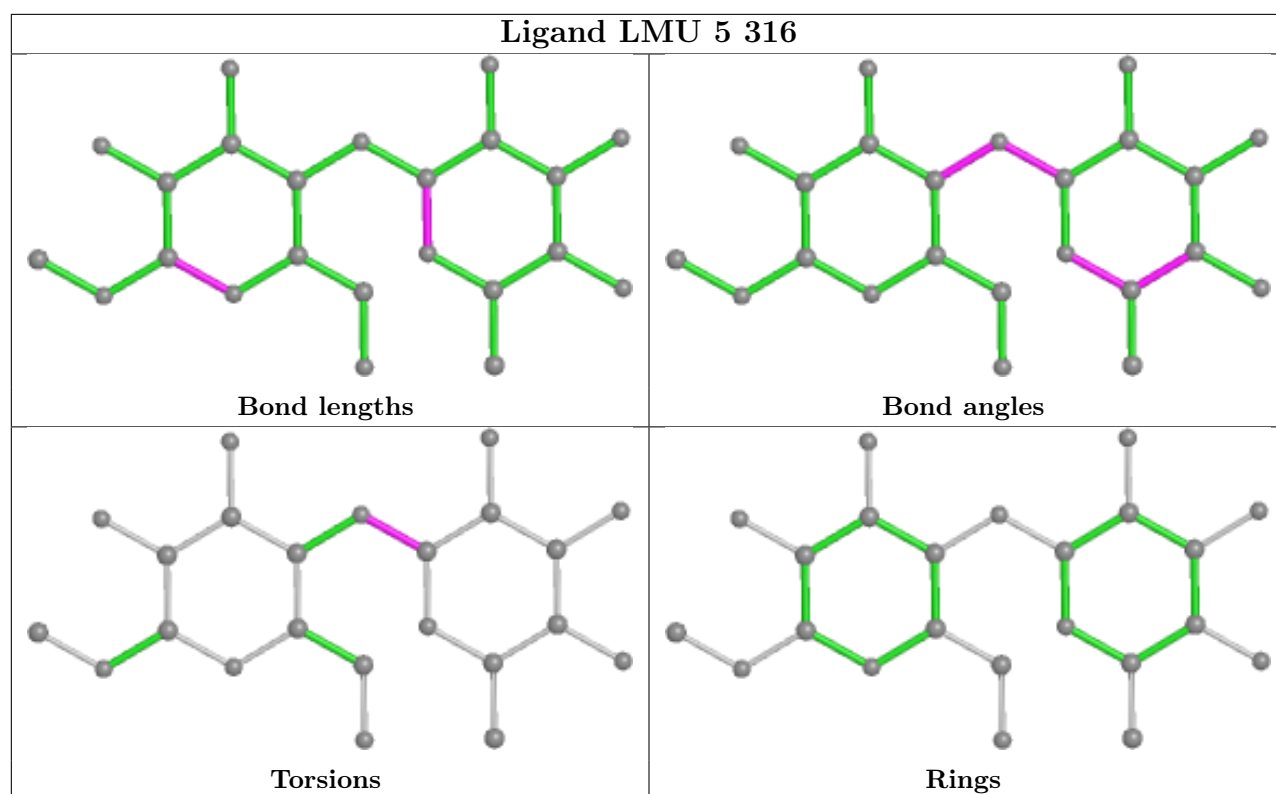
Rings

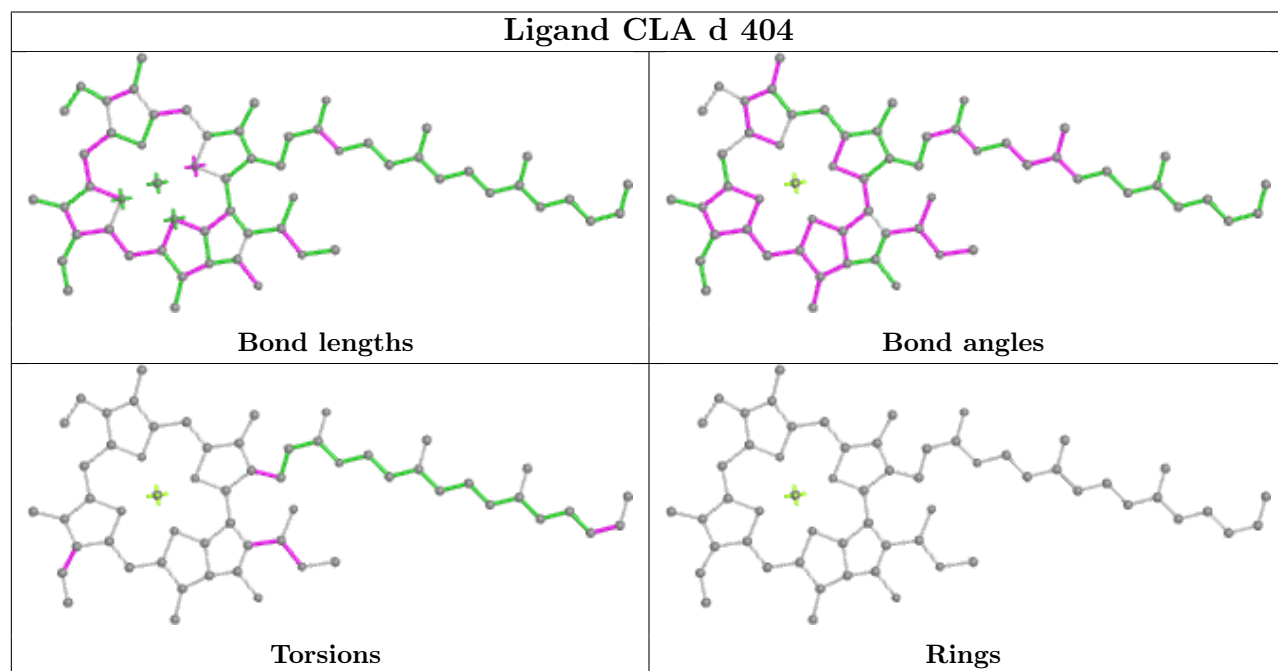
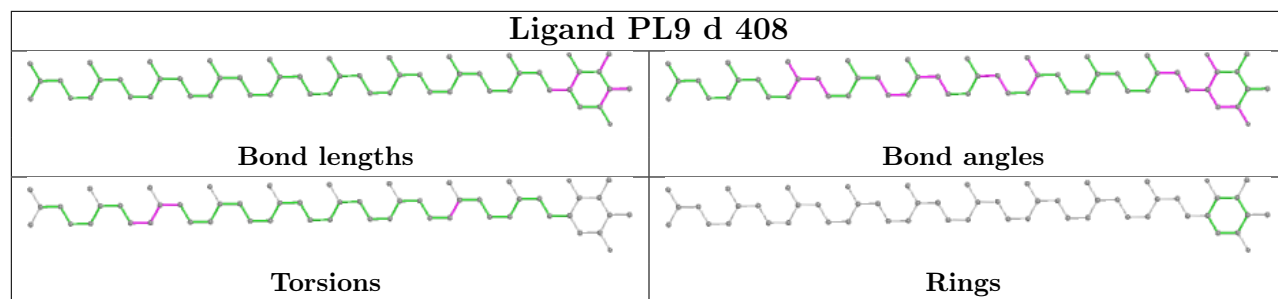


**Ligand CLA 8 302****Ligand CLA 7 300****Ligand CLA B 611**

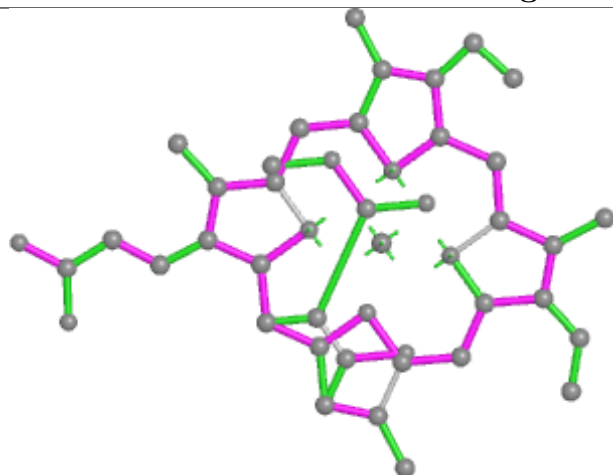




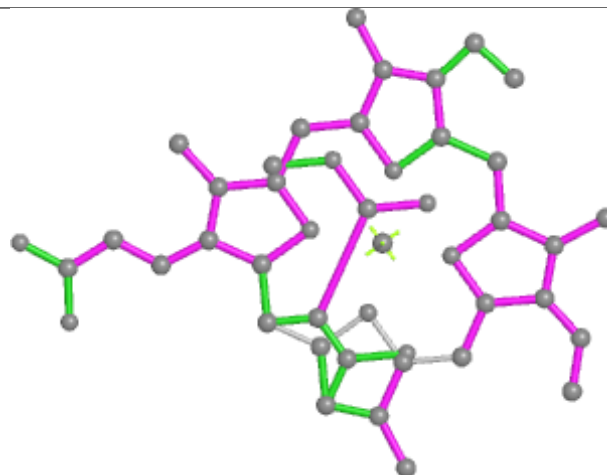




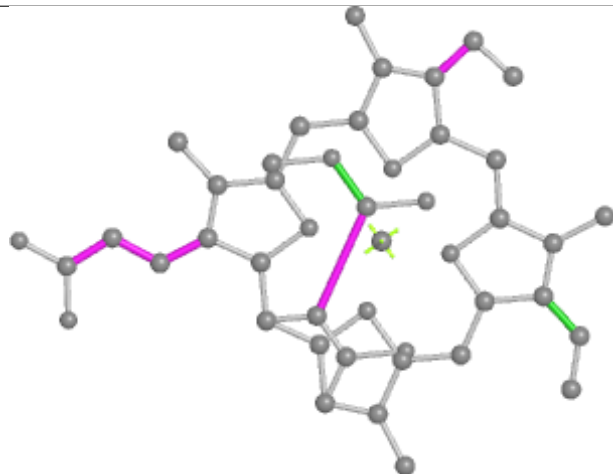
## Ligand KC1 2 315



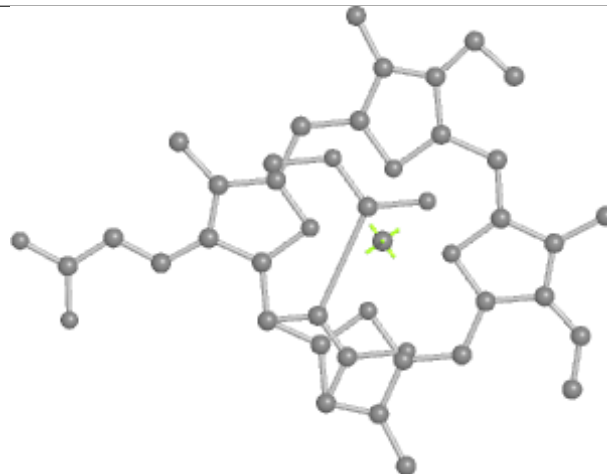
Bond lengths



Bond angles

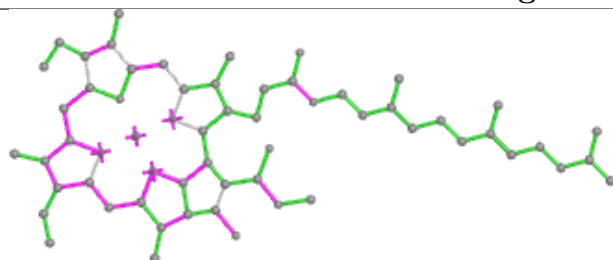


Torsions

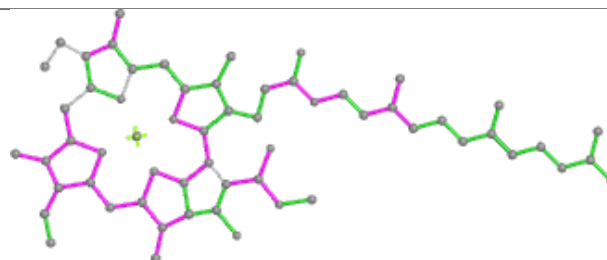


Rings

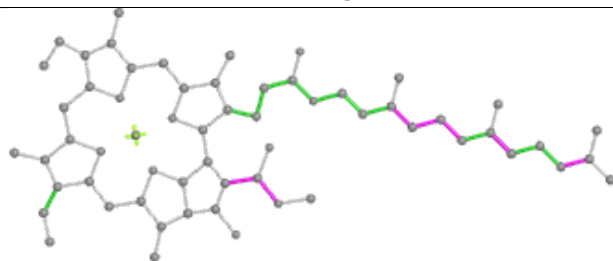
## Ligand CLA 9 301



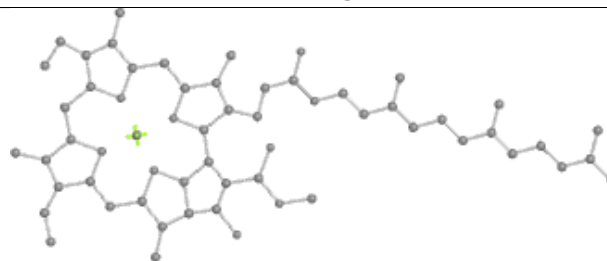
Bond lengths



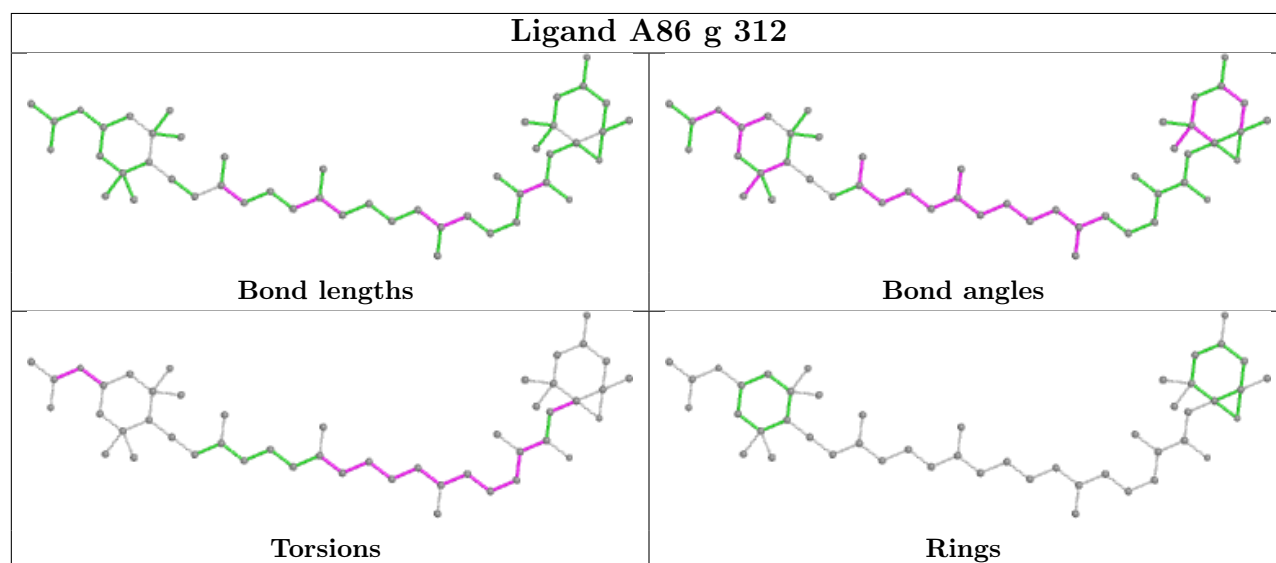
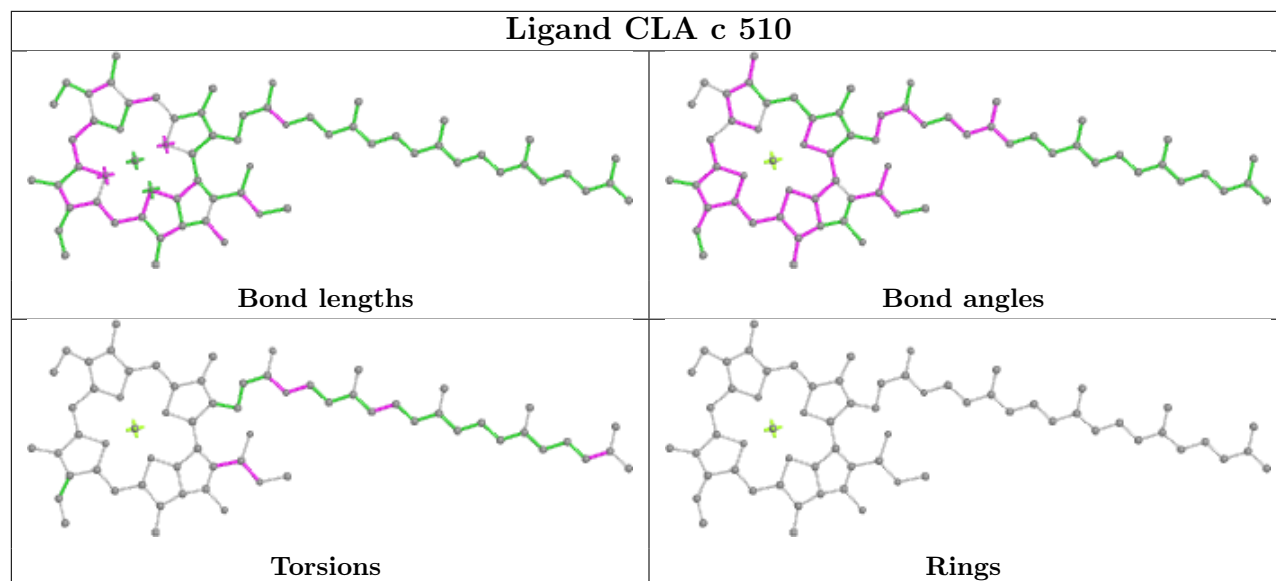
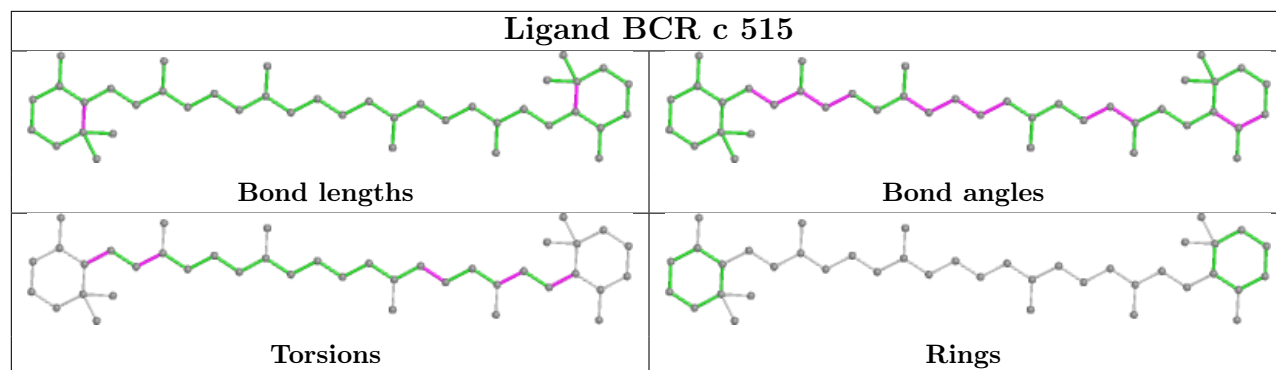
Bond angles



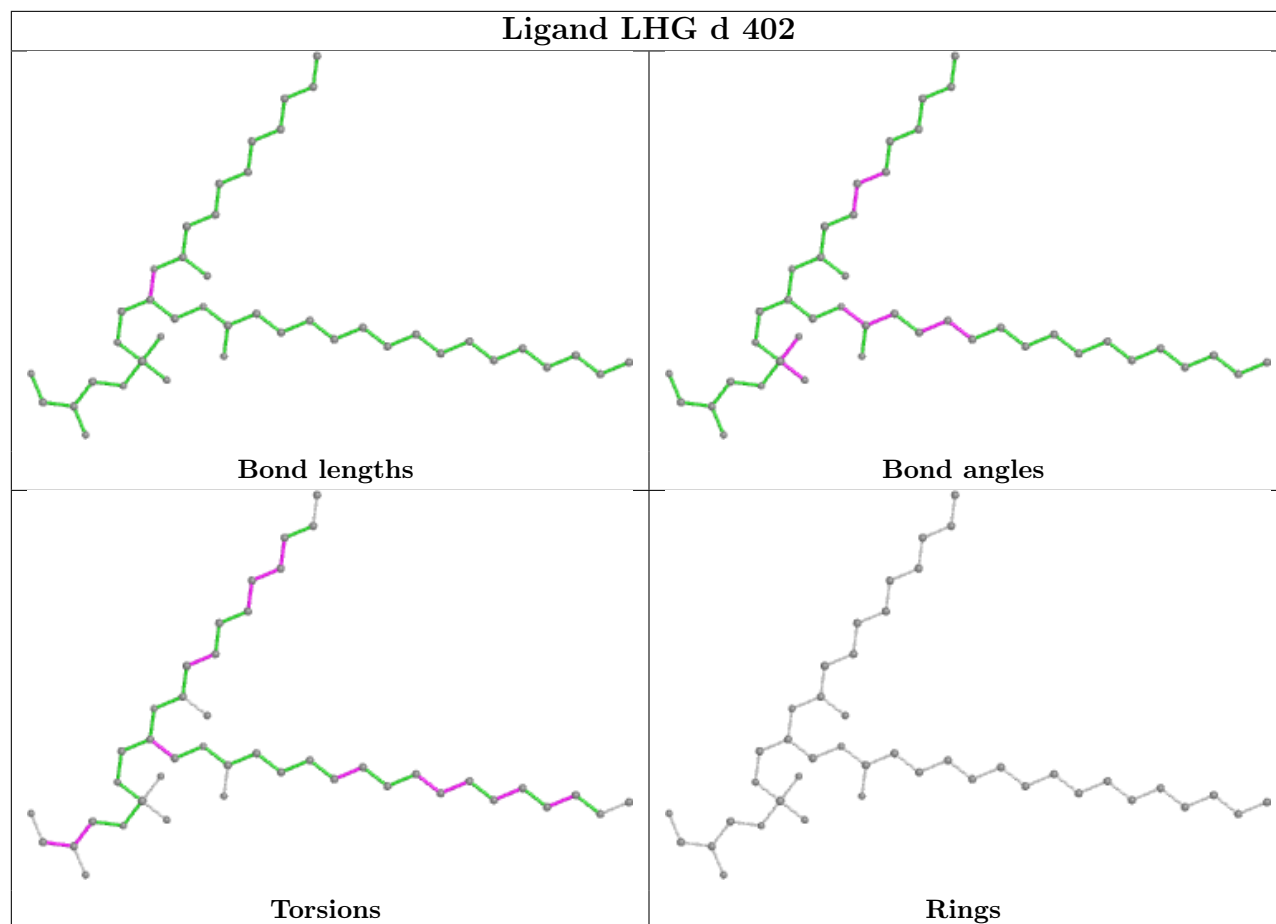
Torsions



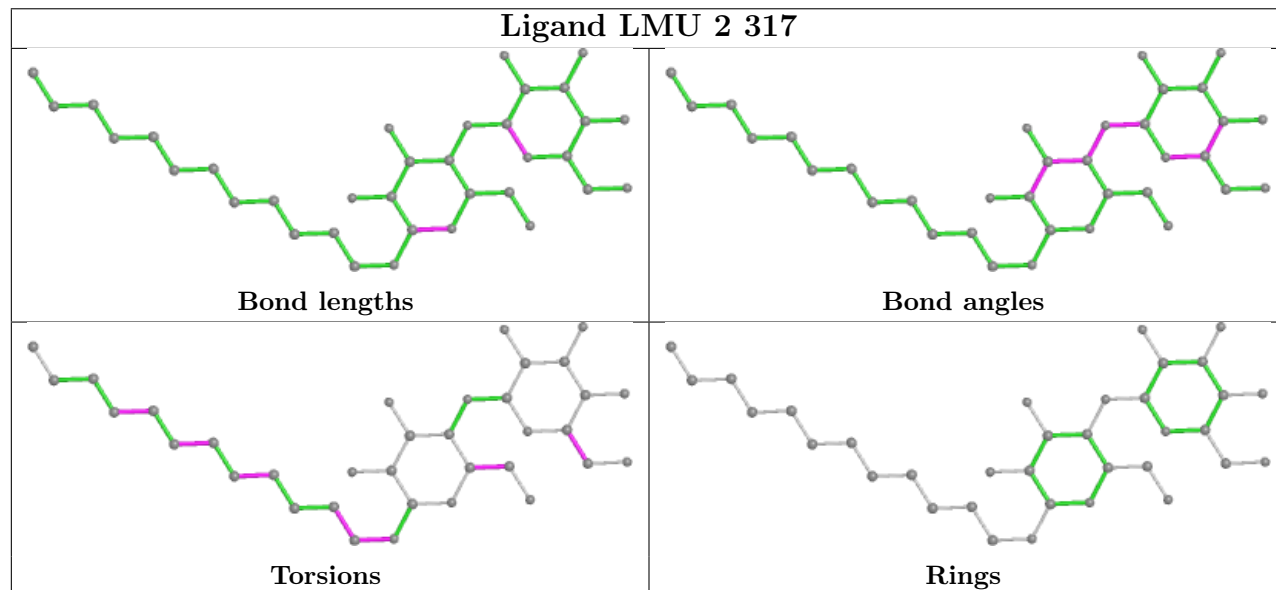
Rings



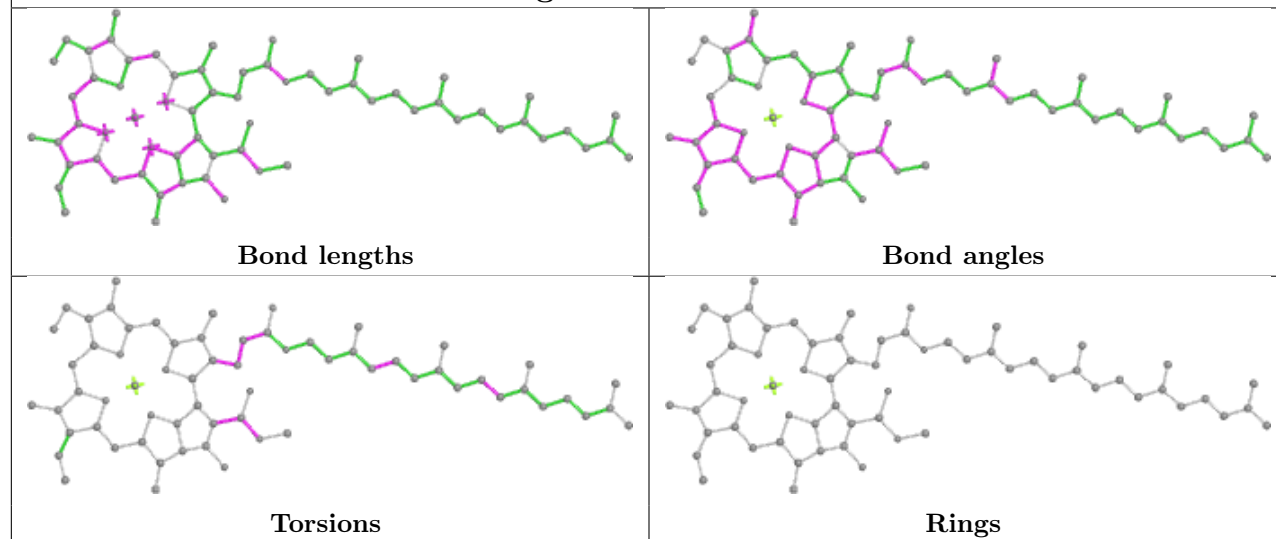
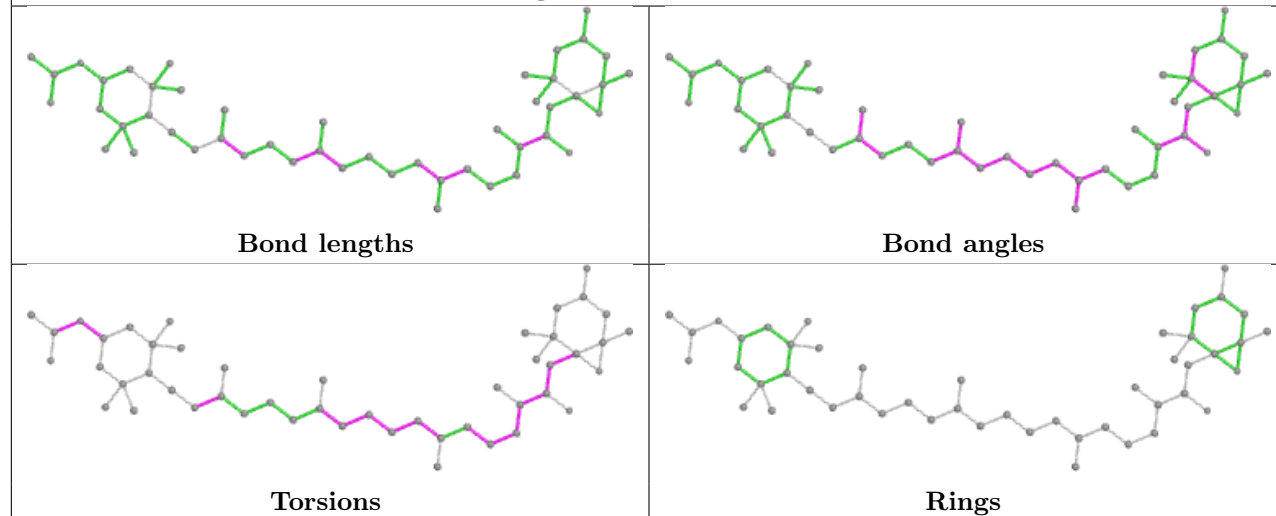
## Ligand LHG d 402



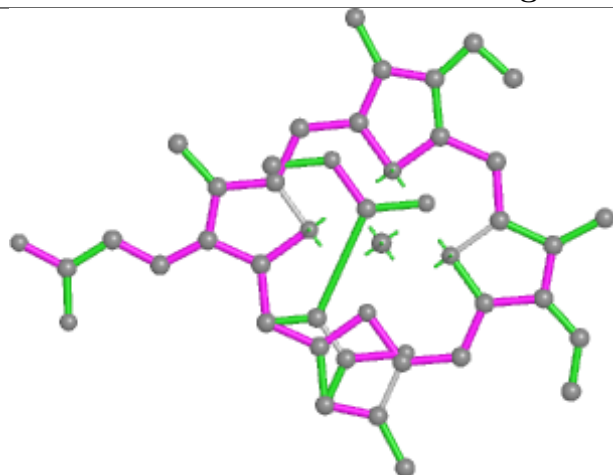
## Ligand LMU 2 317



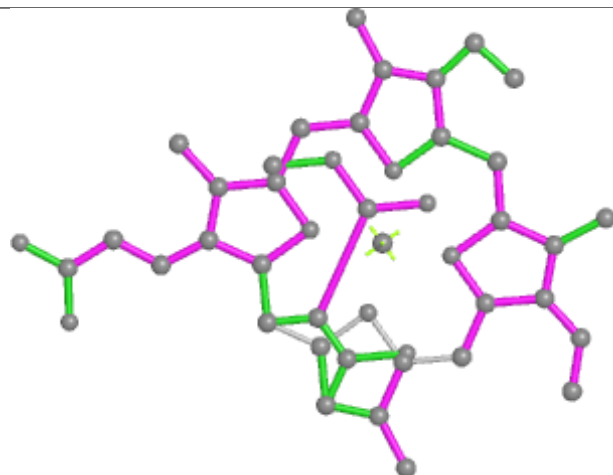


**Ligand CLA 1 301****Ligand A86 W 101**

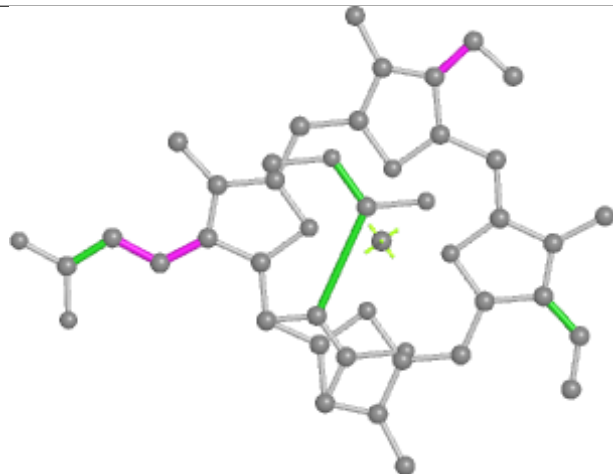
## Ligand KC1 4 309



Bond lengths



Bond angles

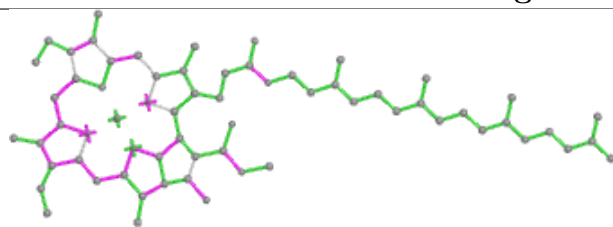


Torsions

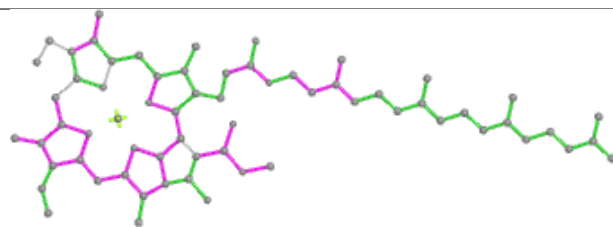


Rings

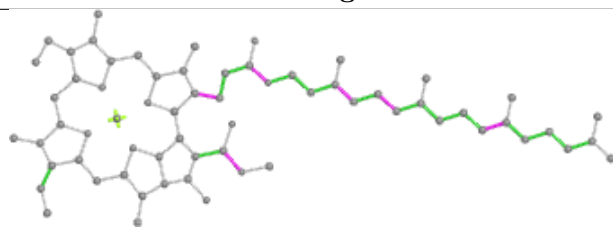
## Ligand CLA B 608



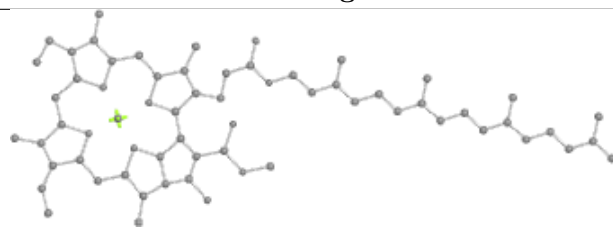
Bond lengths



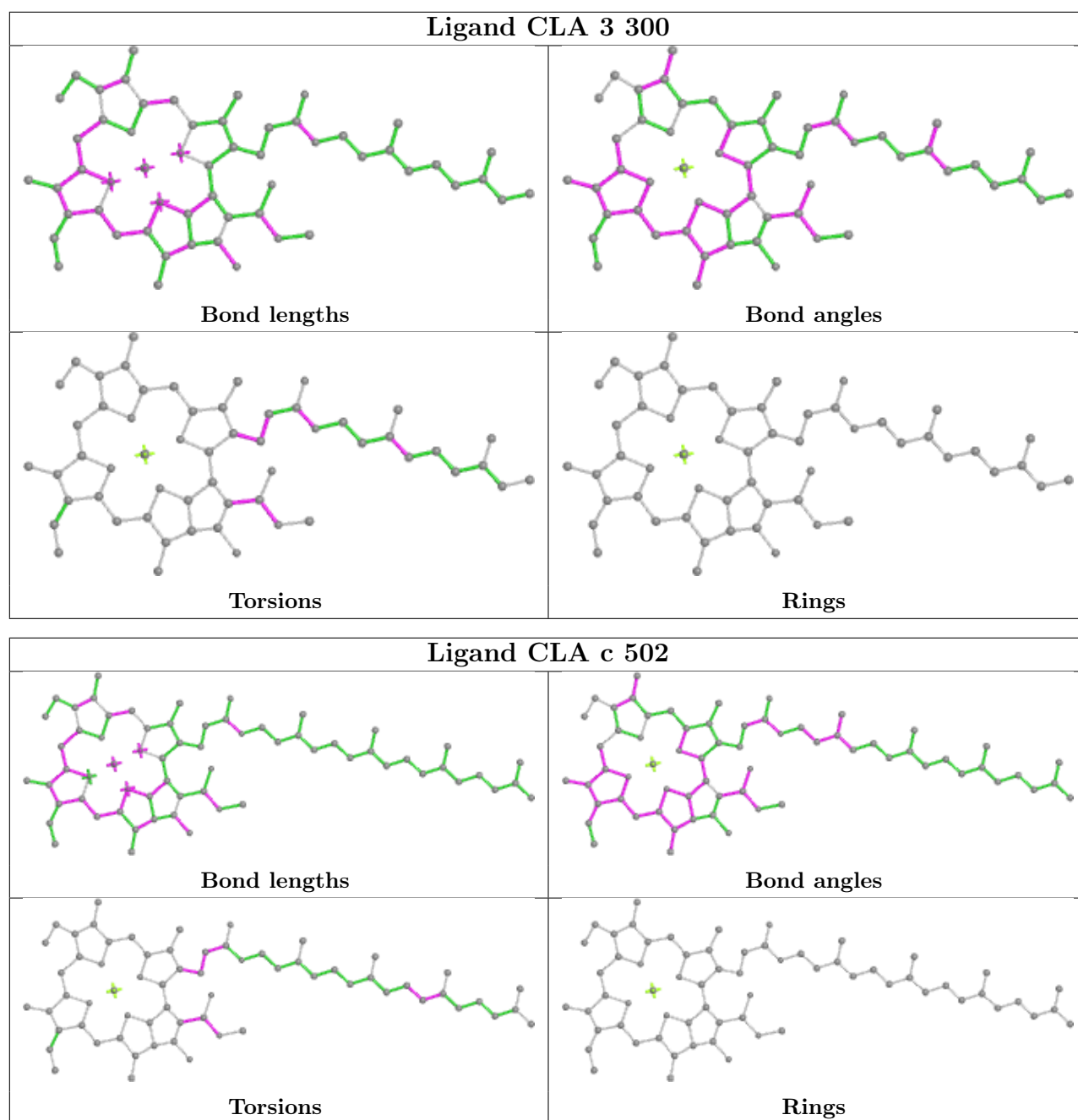
Bond angles



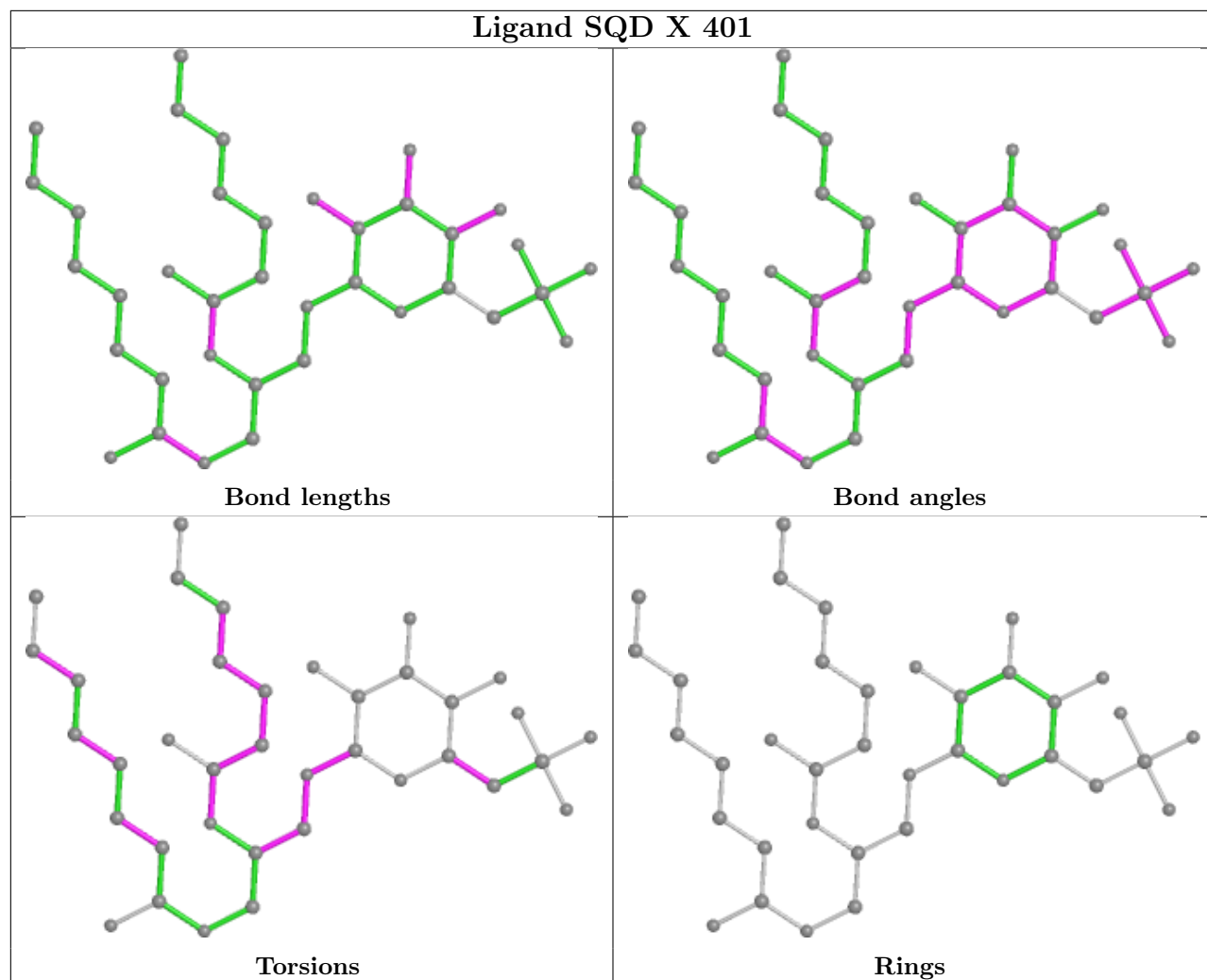
Torsions



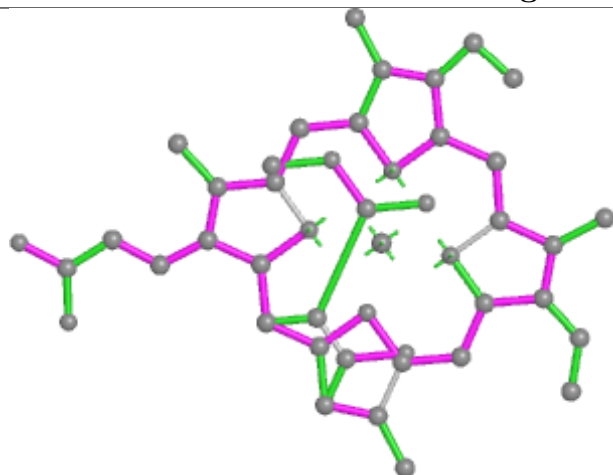
Rings



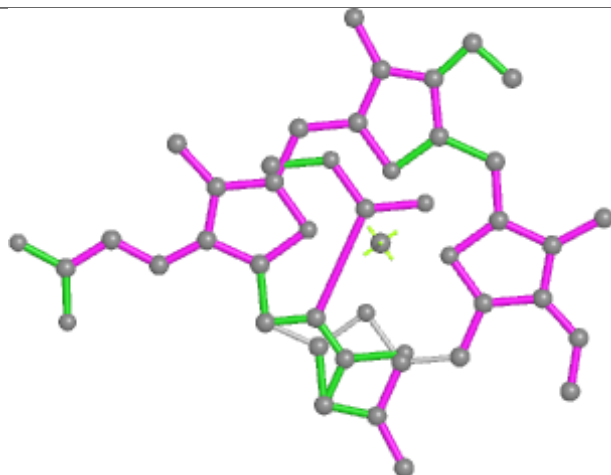
## Ligand SQD X 401



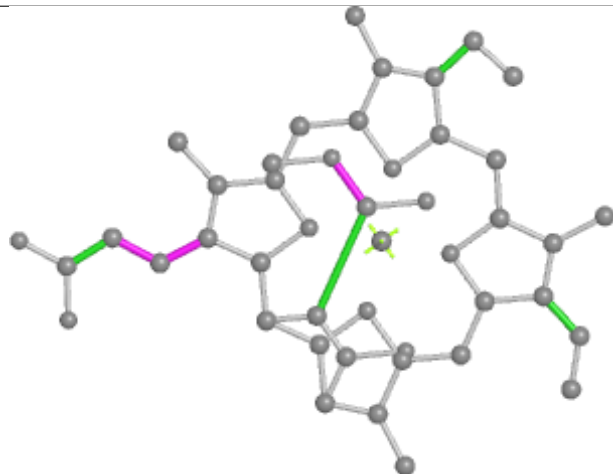
## Ligand KC1 2 316



Bond lengths



Bond angles

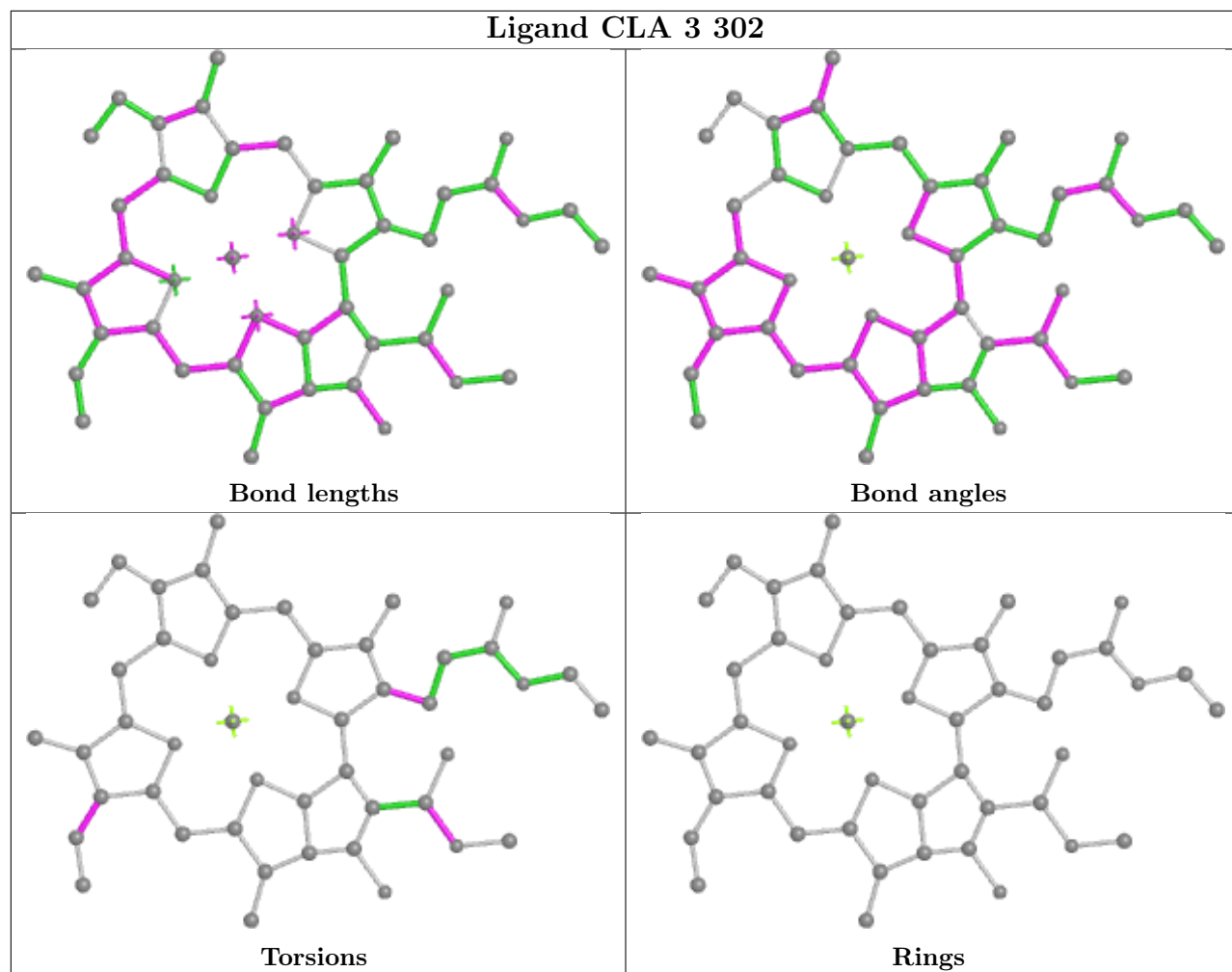


Torsions

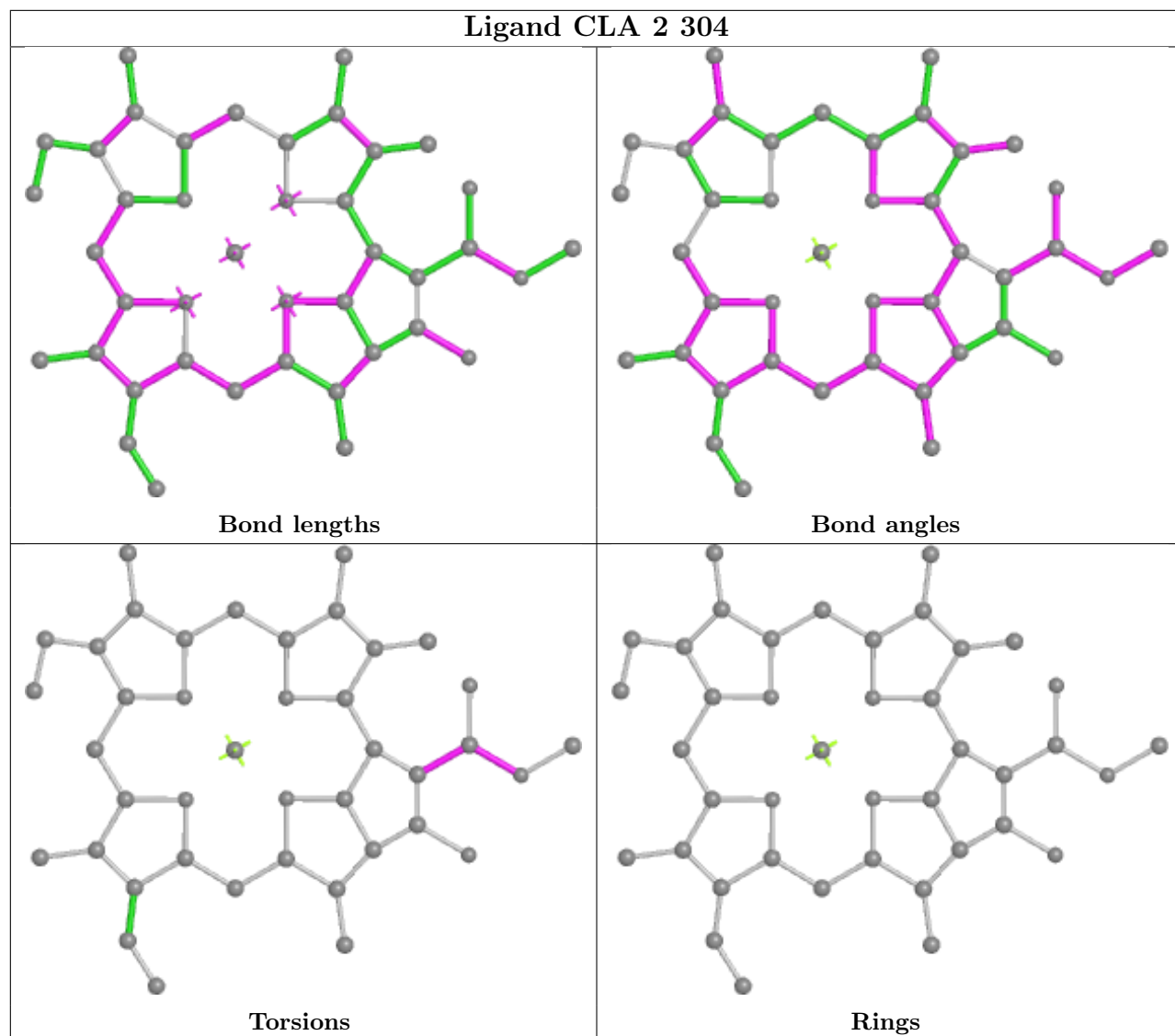


Rings

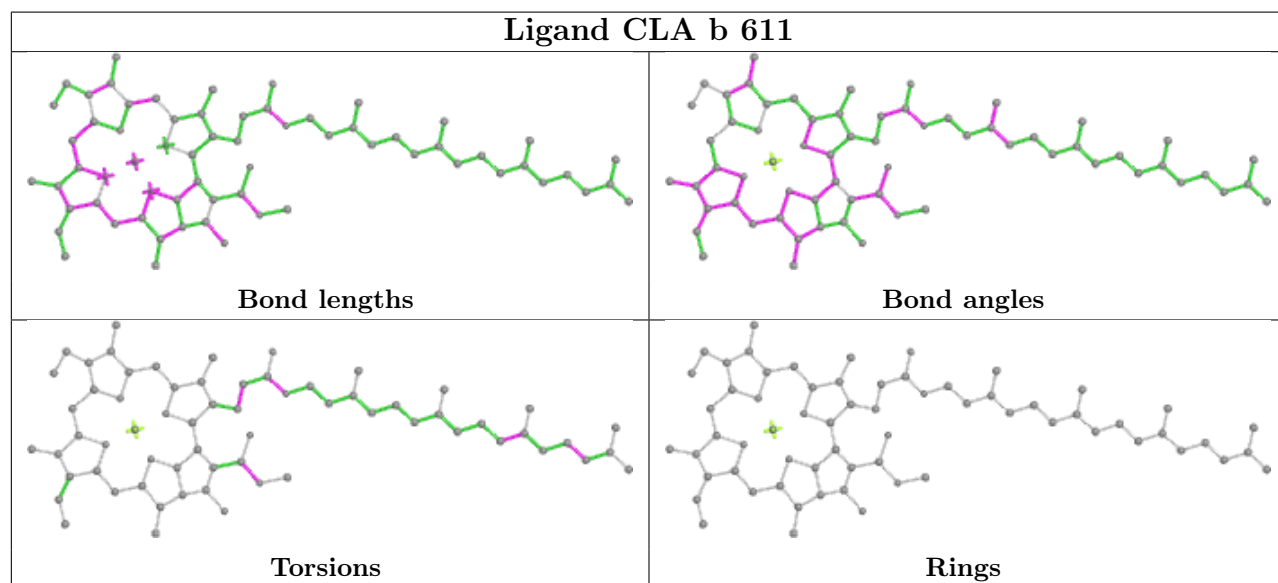
## Ligand CLA 3 302

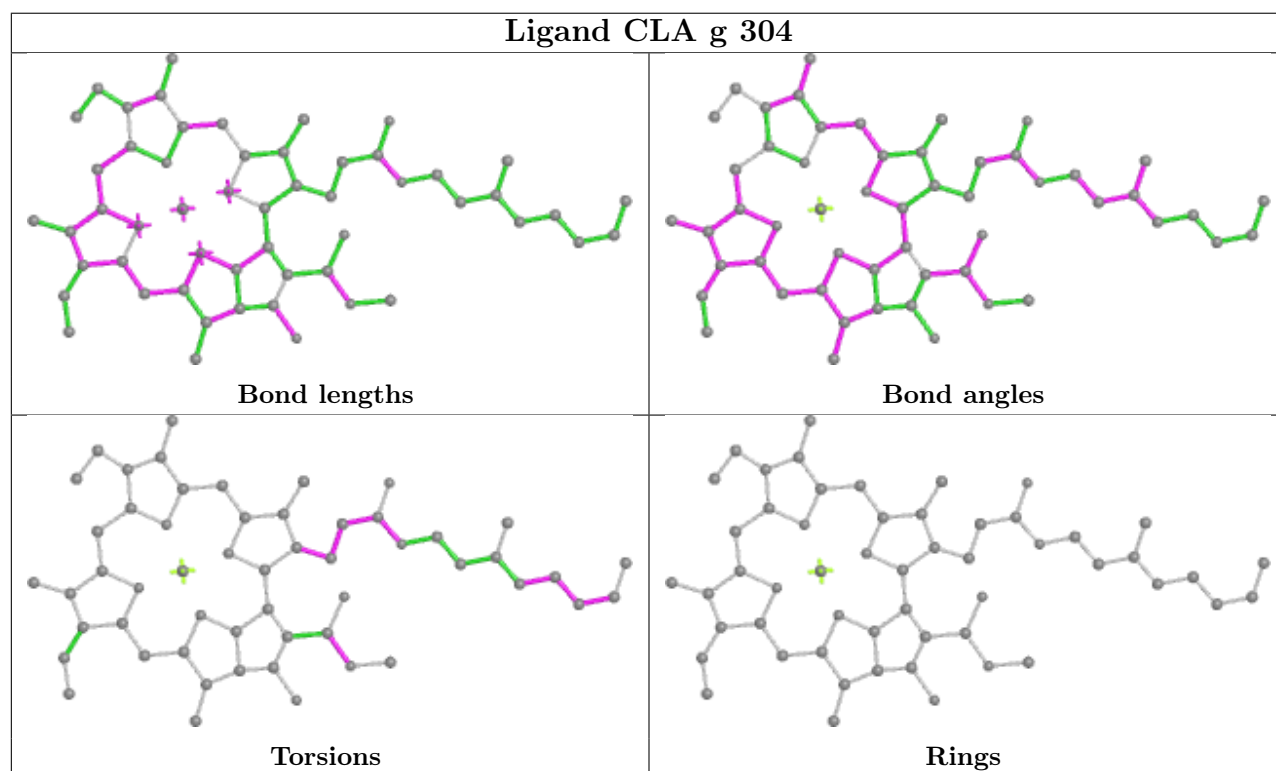
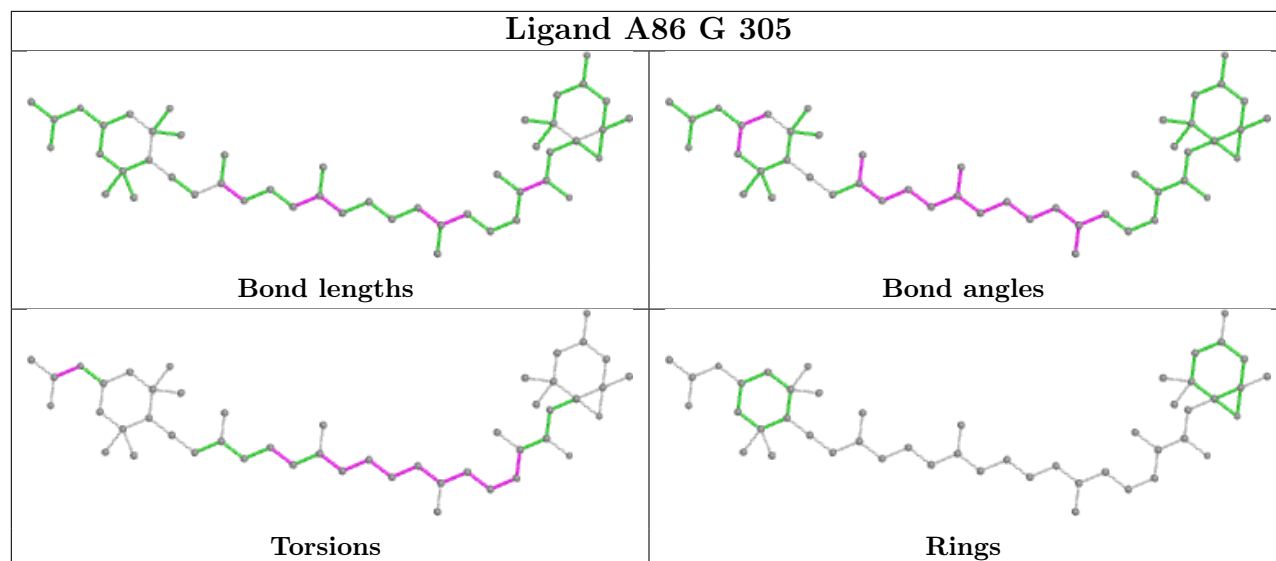


## Ligand CLA 2 304



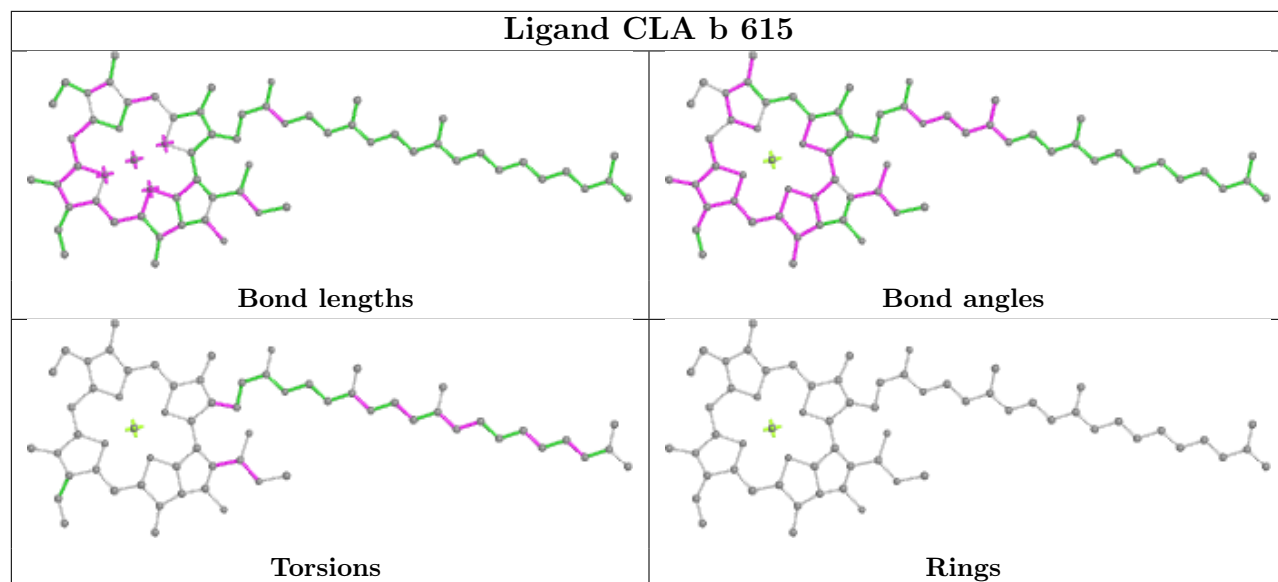
## Ligand CLA b 611



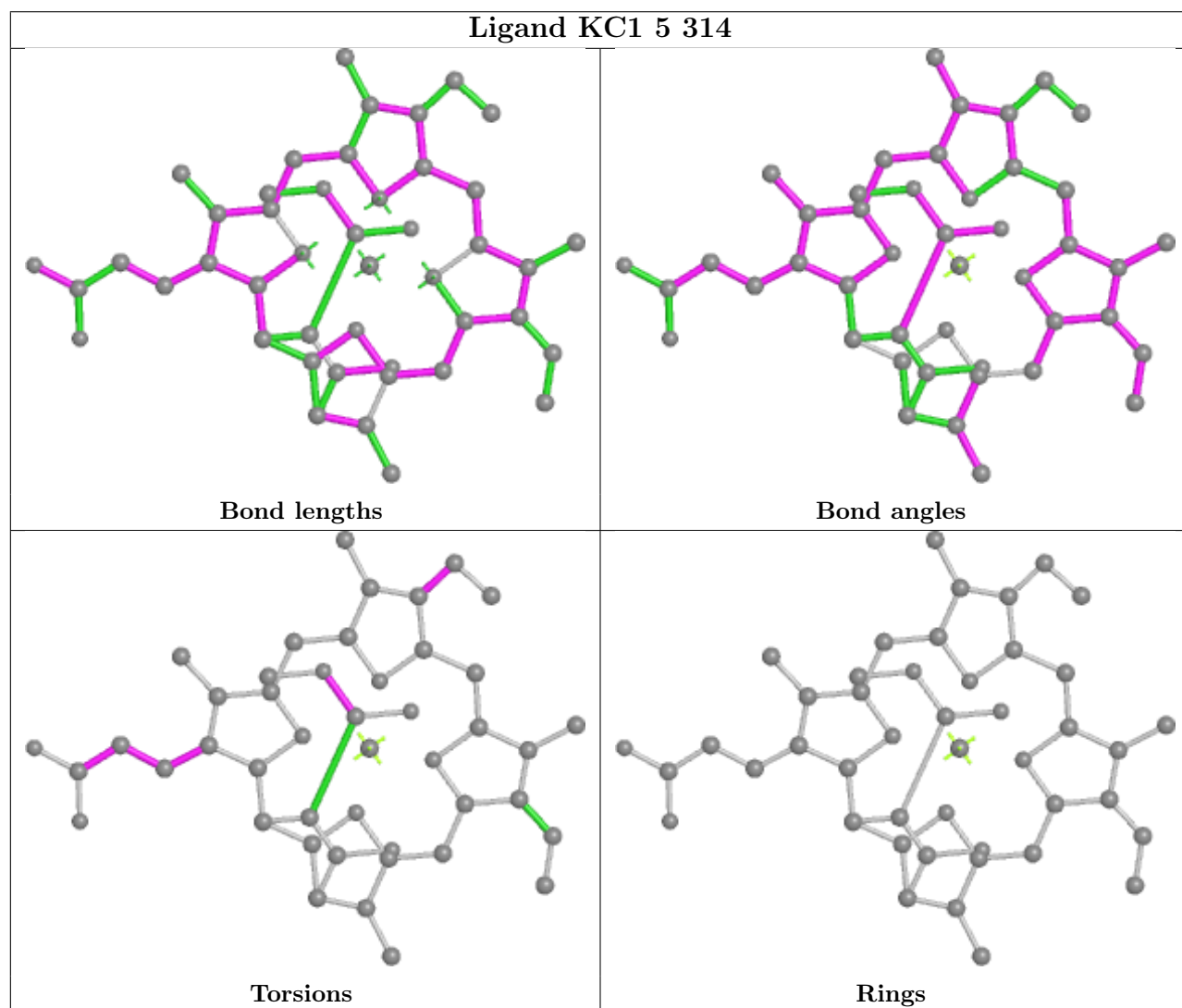




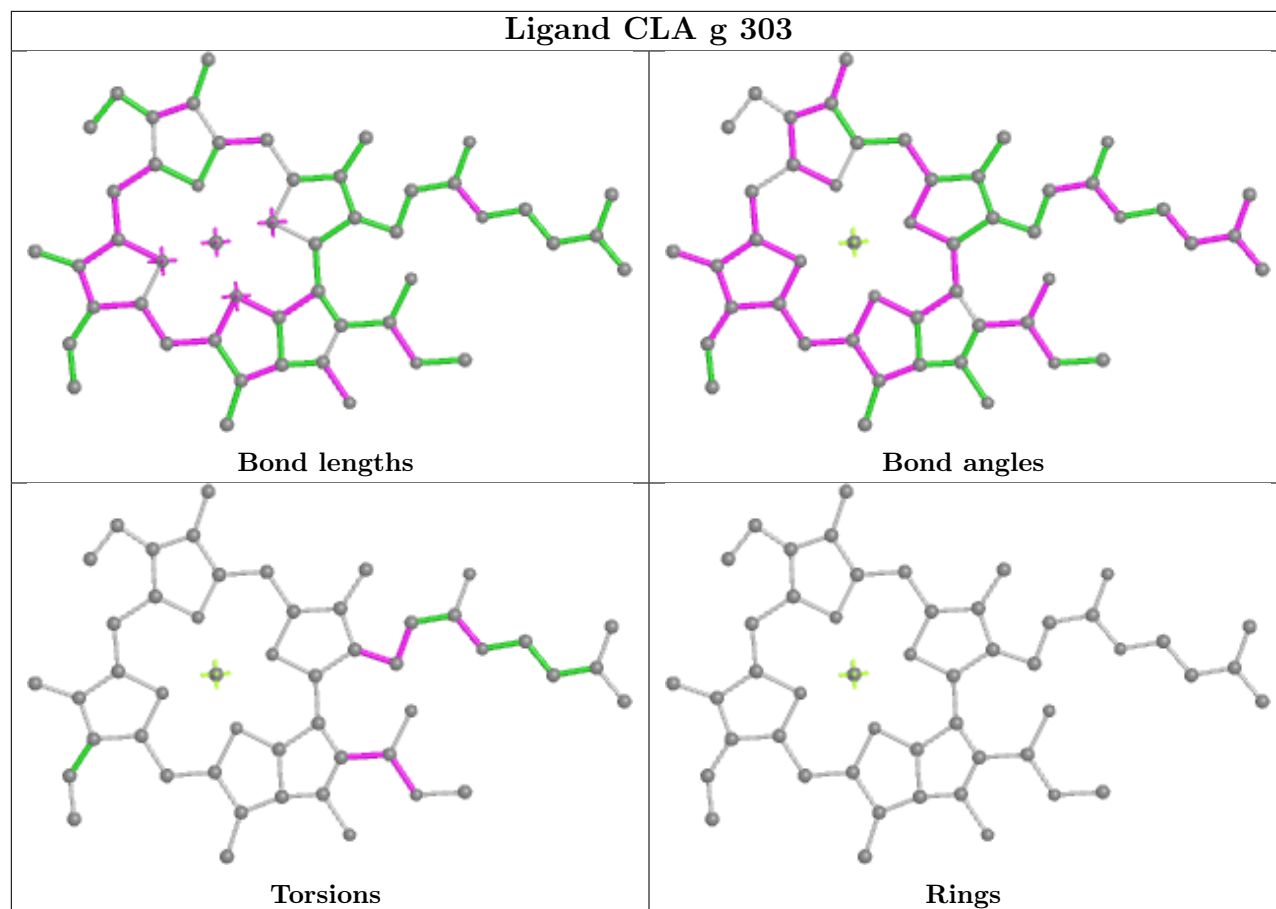
## Ligand CLA b 615



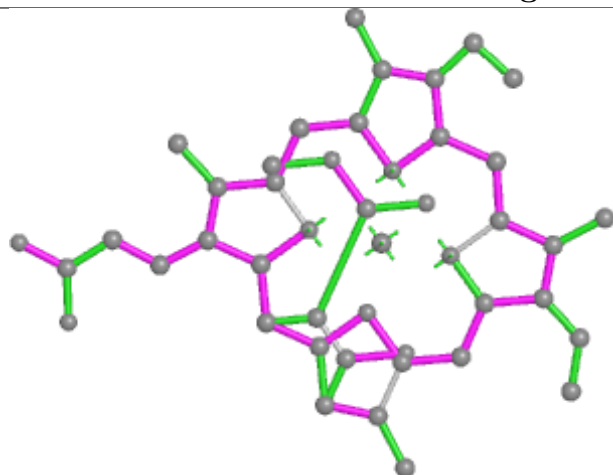
## Ligand KC1 5 314



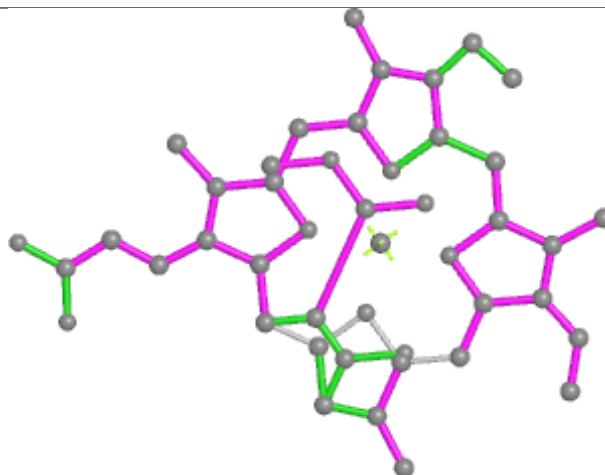
## Ligand CLA g 303



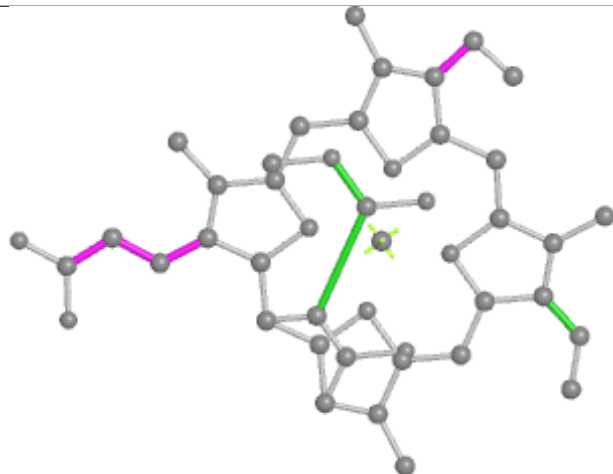
## Ligand KC1 3 305



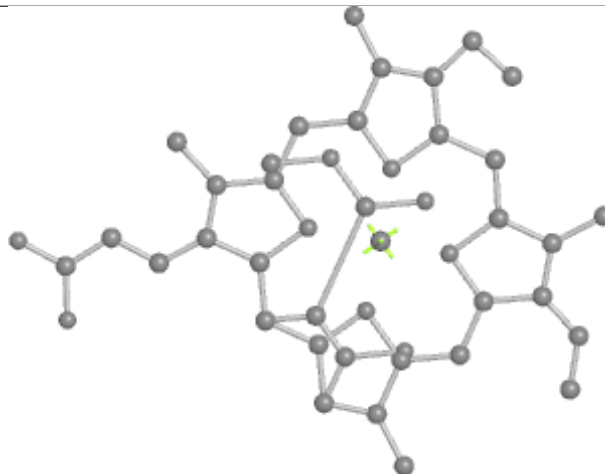
Bond lengths



Bond angles

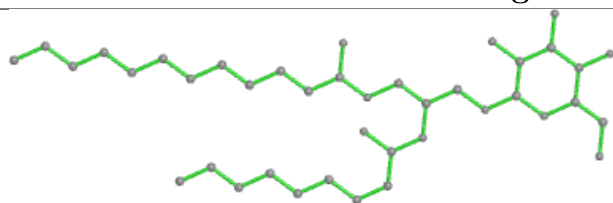


Torsions

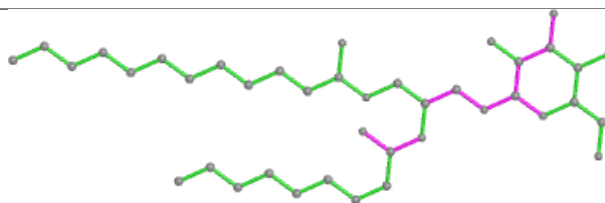


Rings

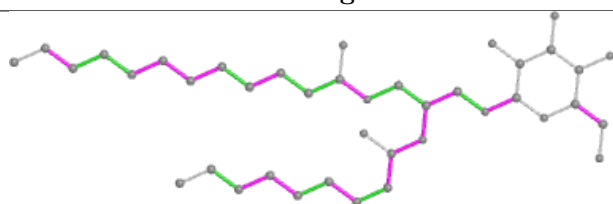
## Ligand LMG L 101



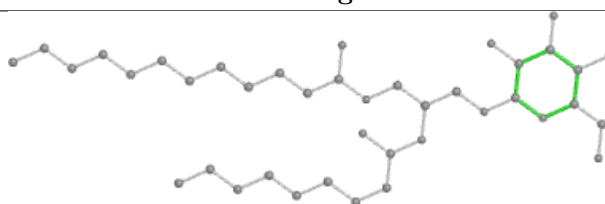
Bond lengths



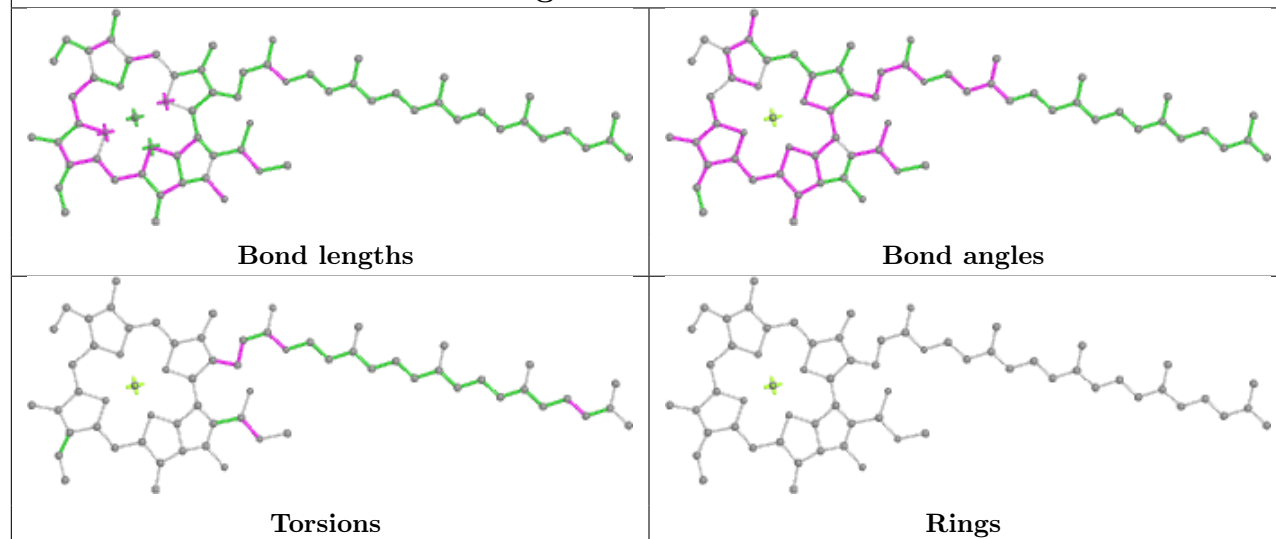
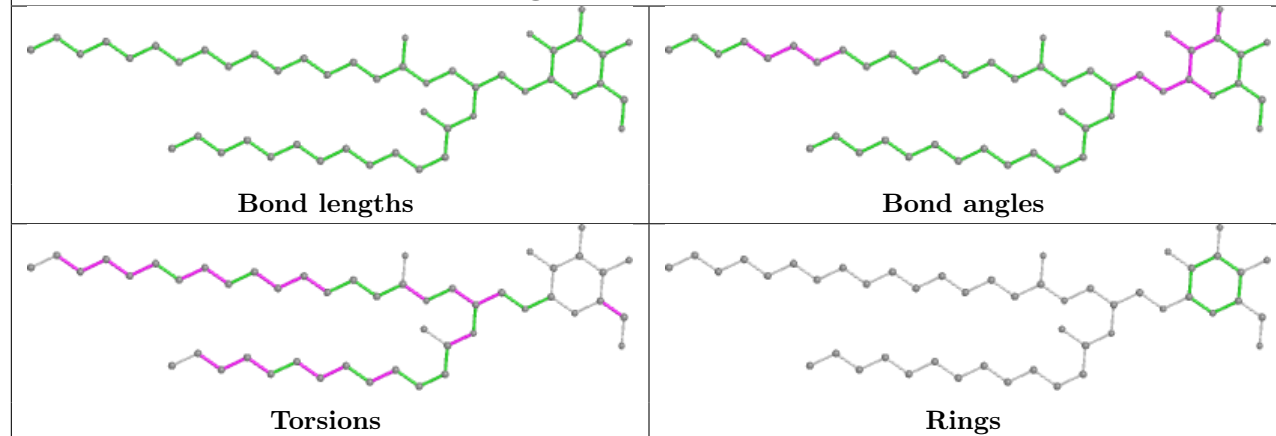
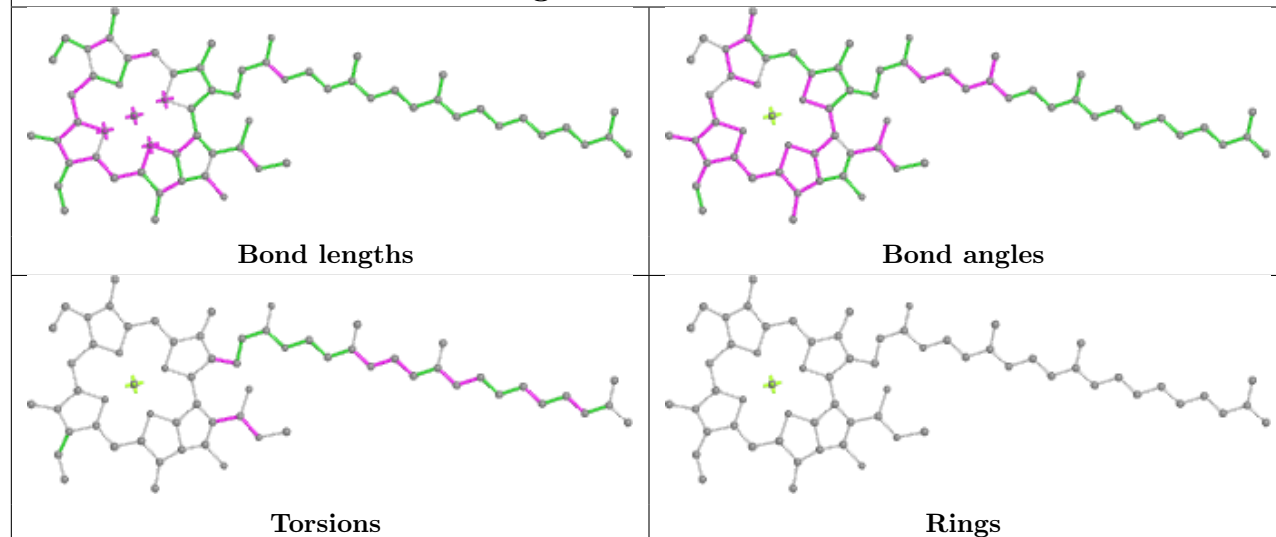
Bond angles



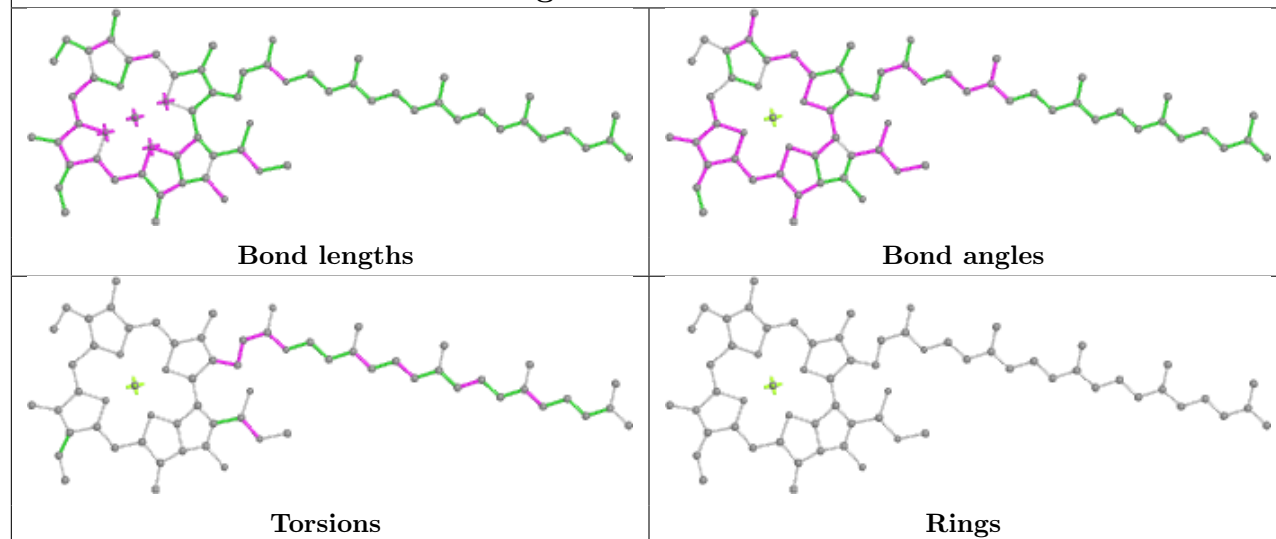
Torsions



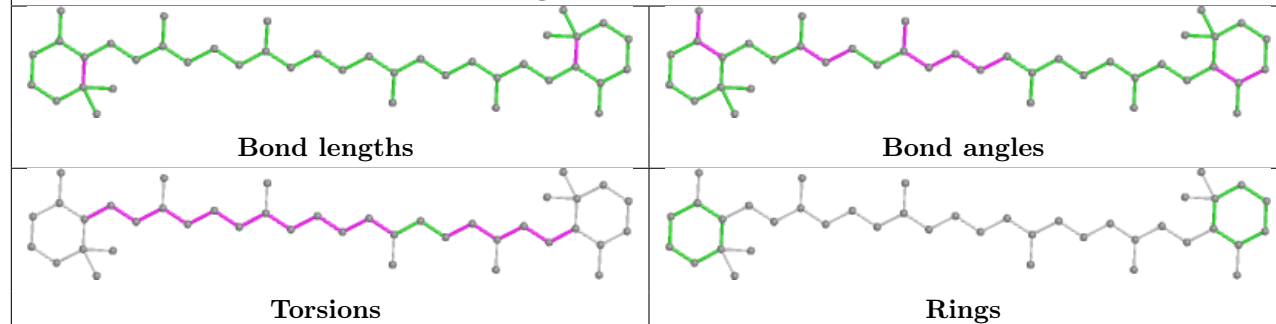
Rings

**Ligand CLA a 402****Ligand LMG A 407****Ligand CLA B 614**

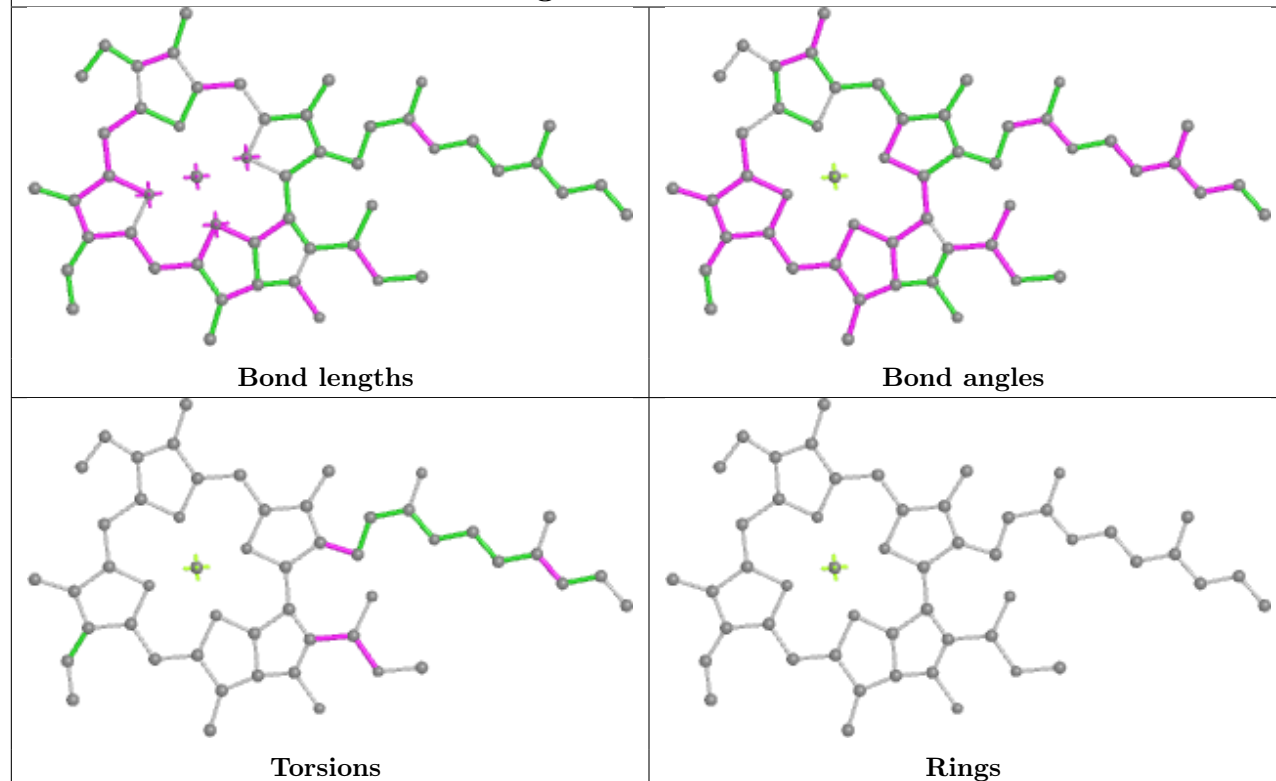
## Ligand CLA 1 303



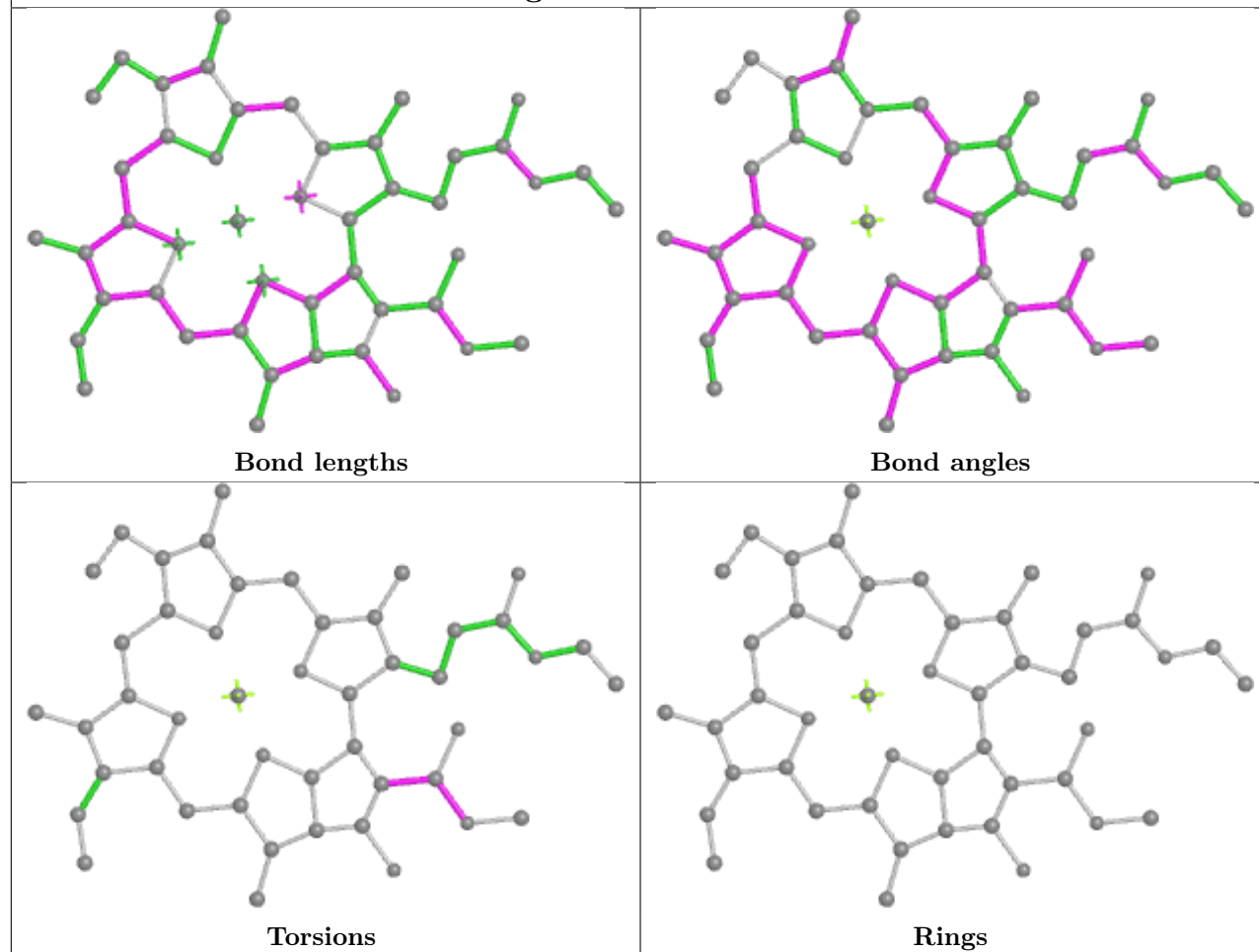
## Ligand BCR h 101



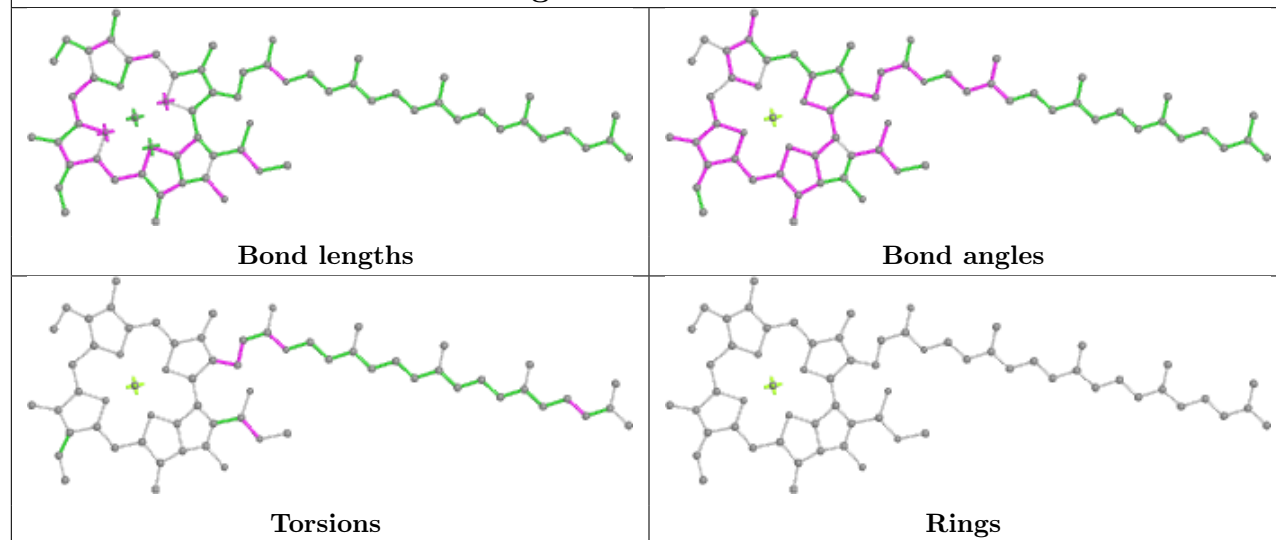
## Ligand CLA 6 300



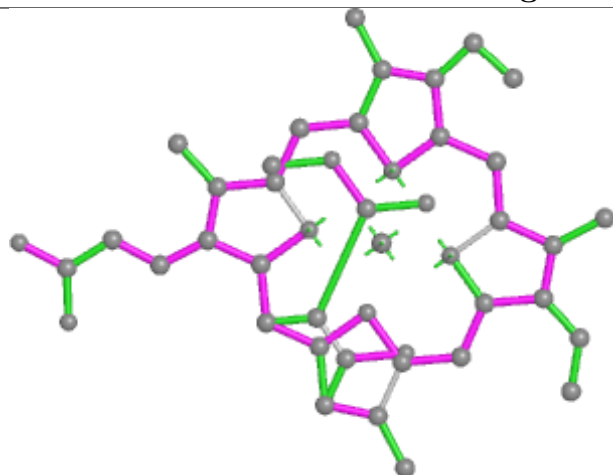
## Ligand CLA B 602



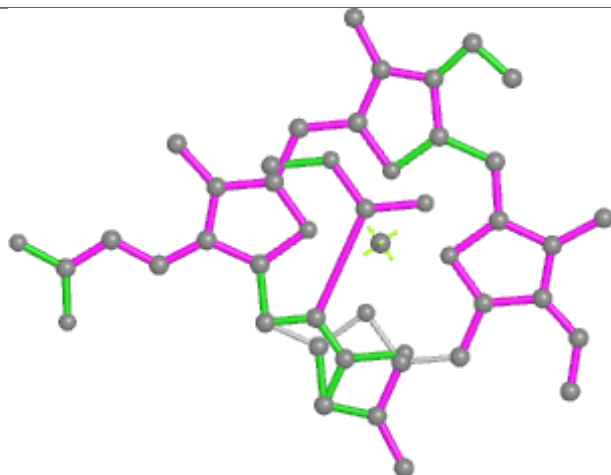
## Ligand CLA A 401



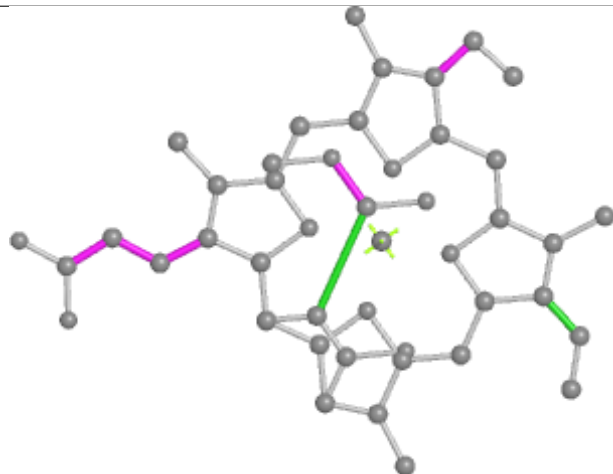
## Ligand KC1 1 315



Bond lengths



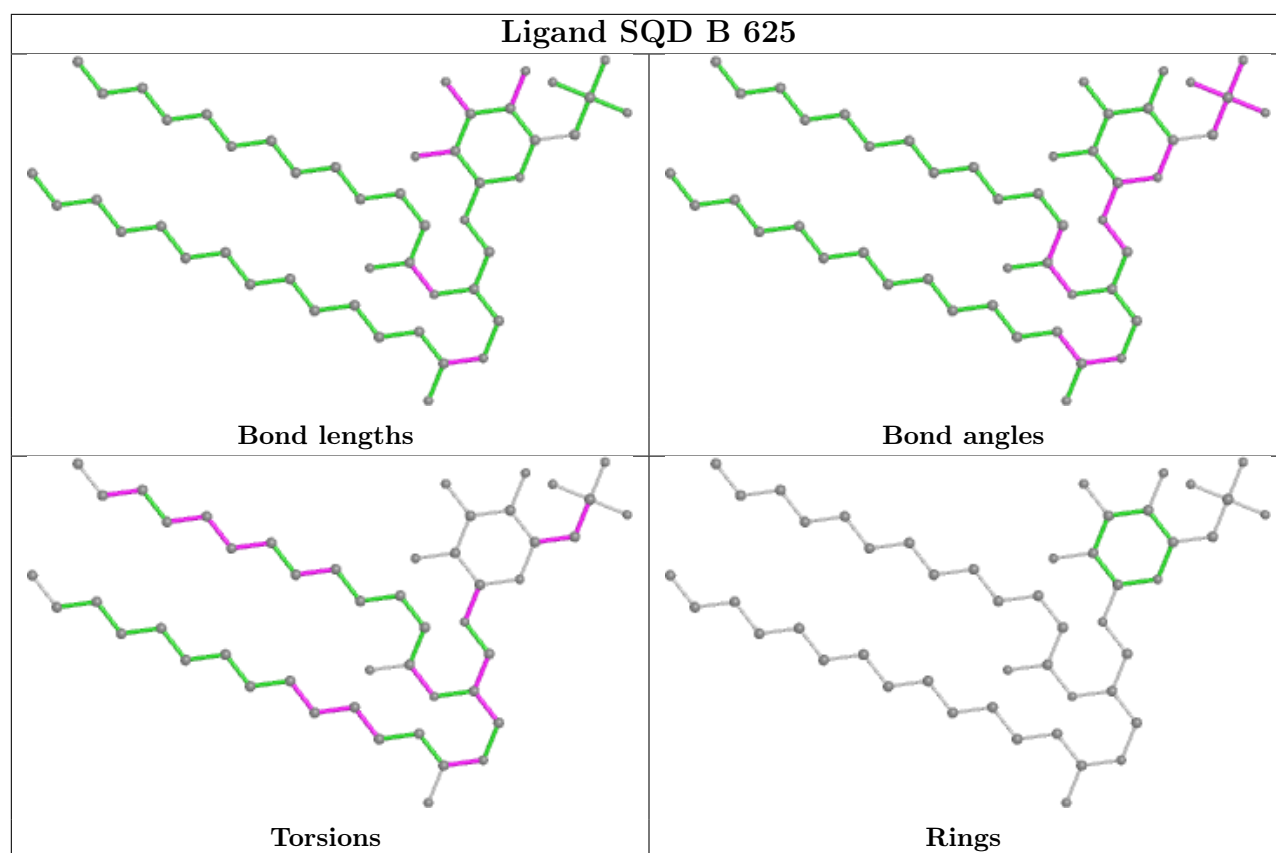
Bond angles



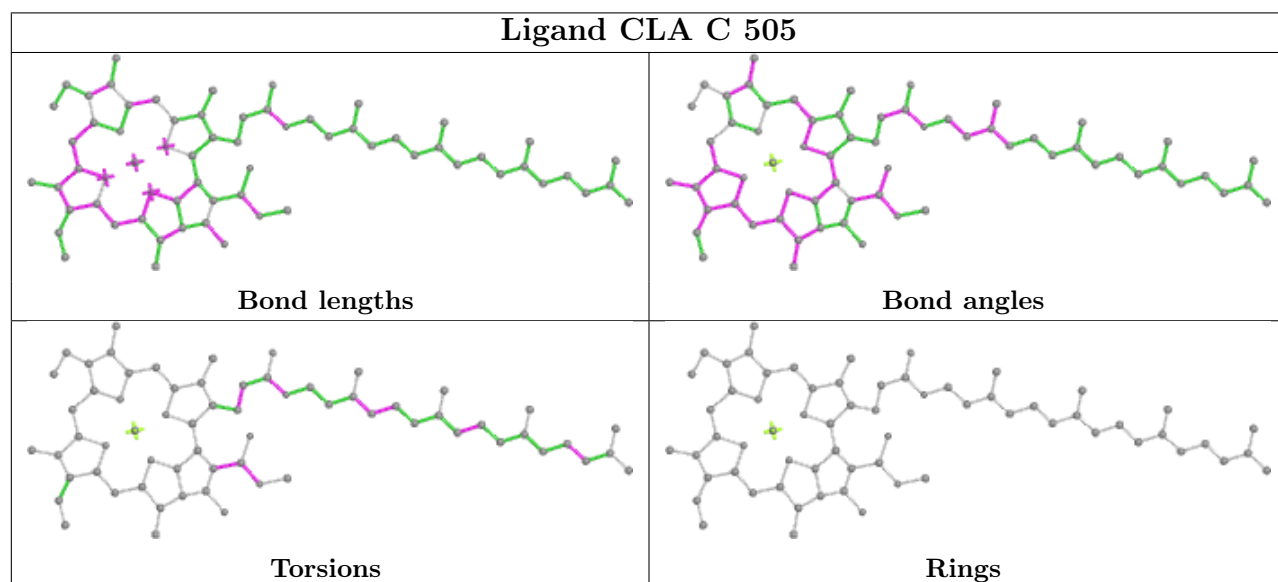
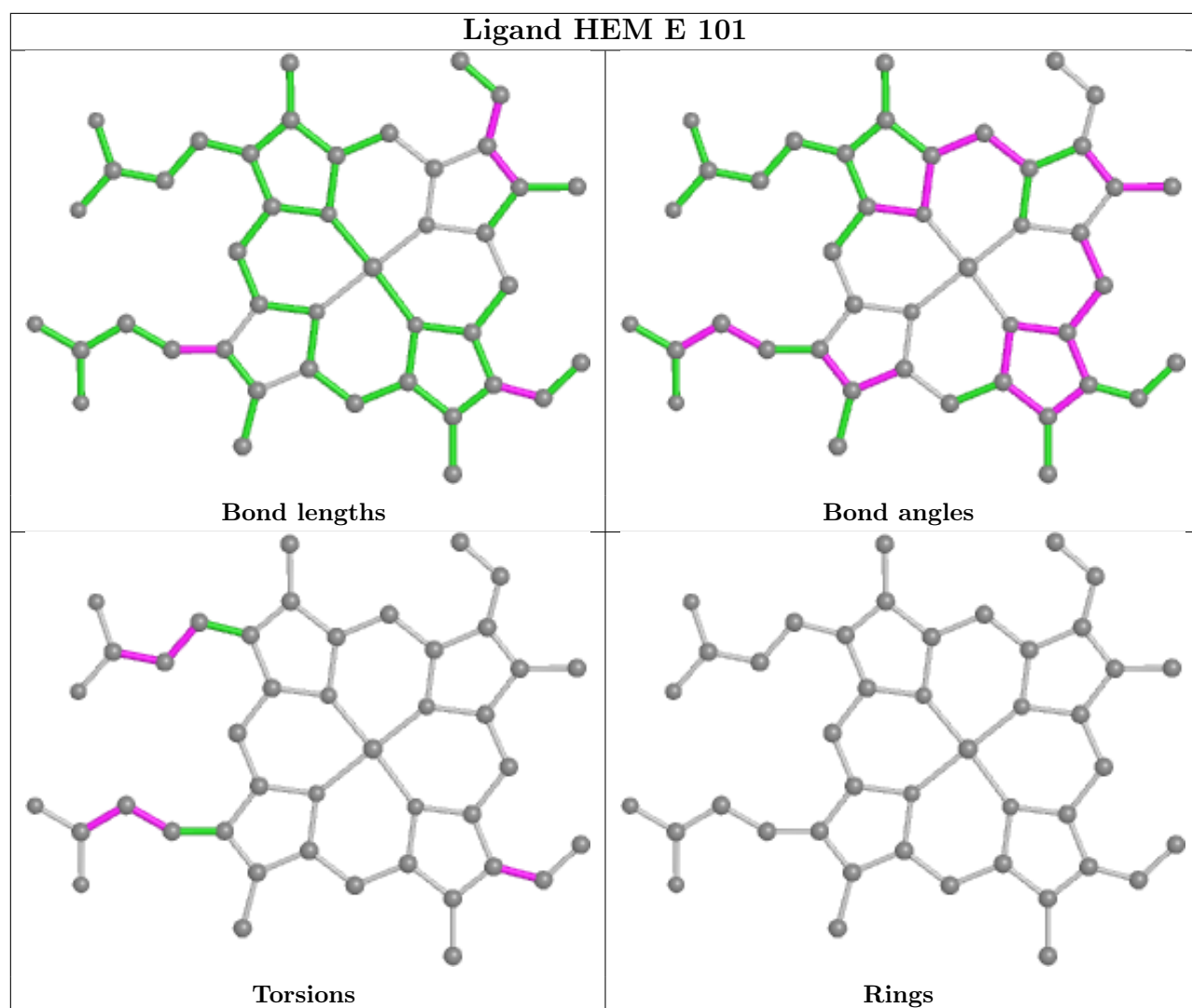
Torsions



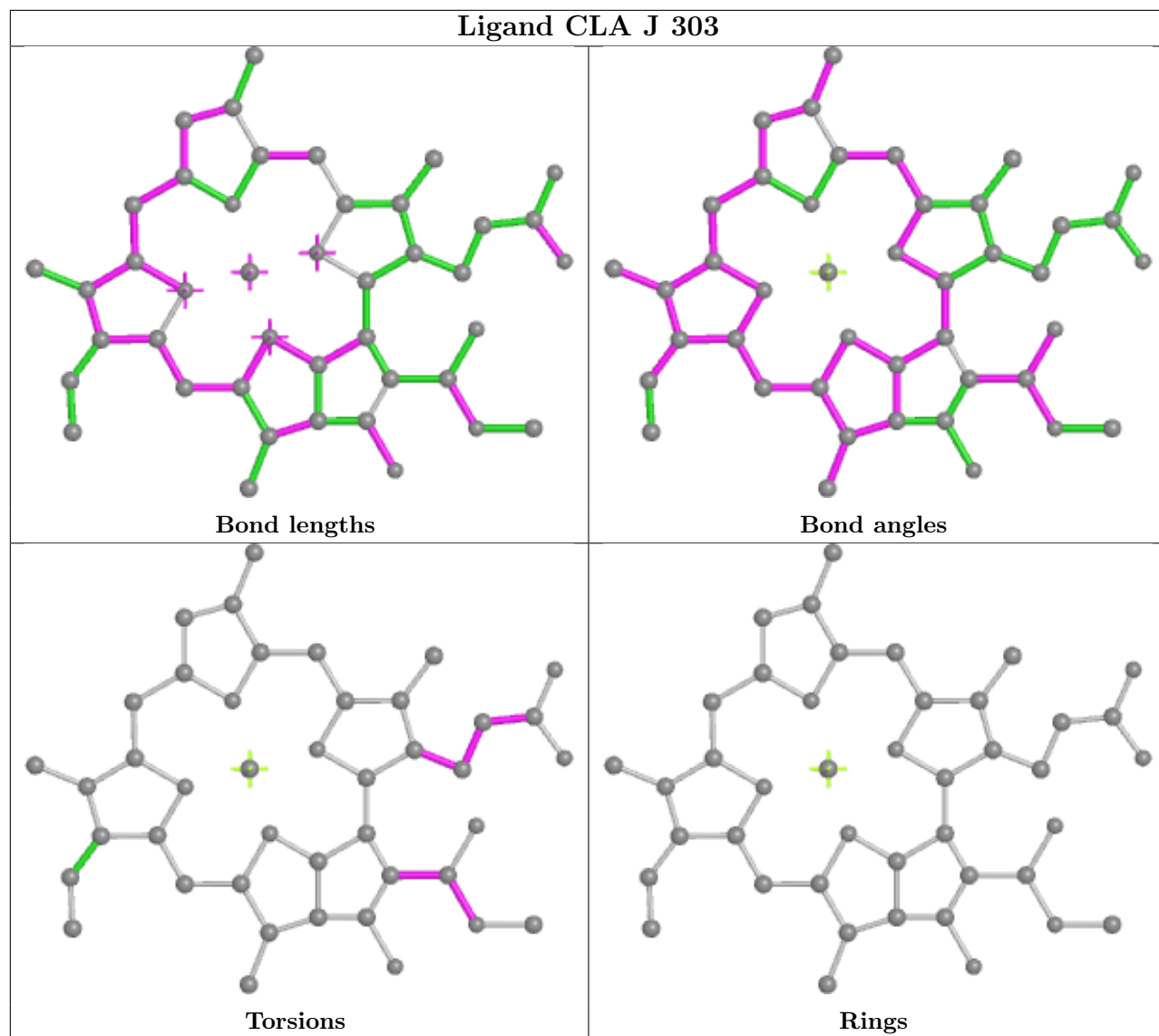
Rings



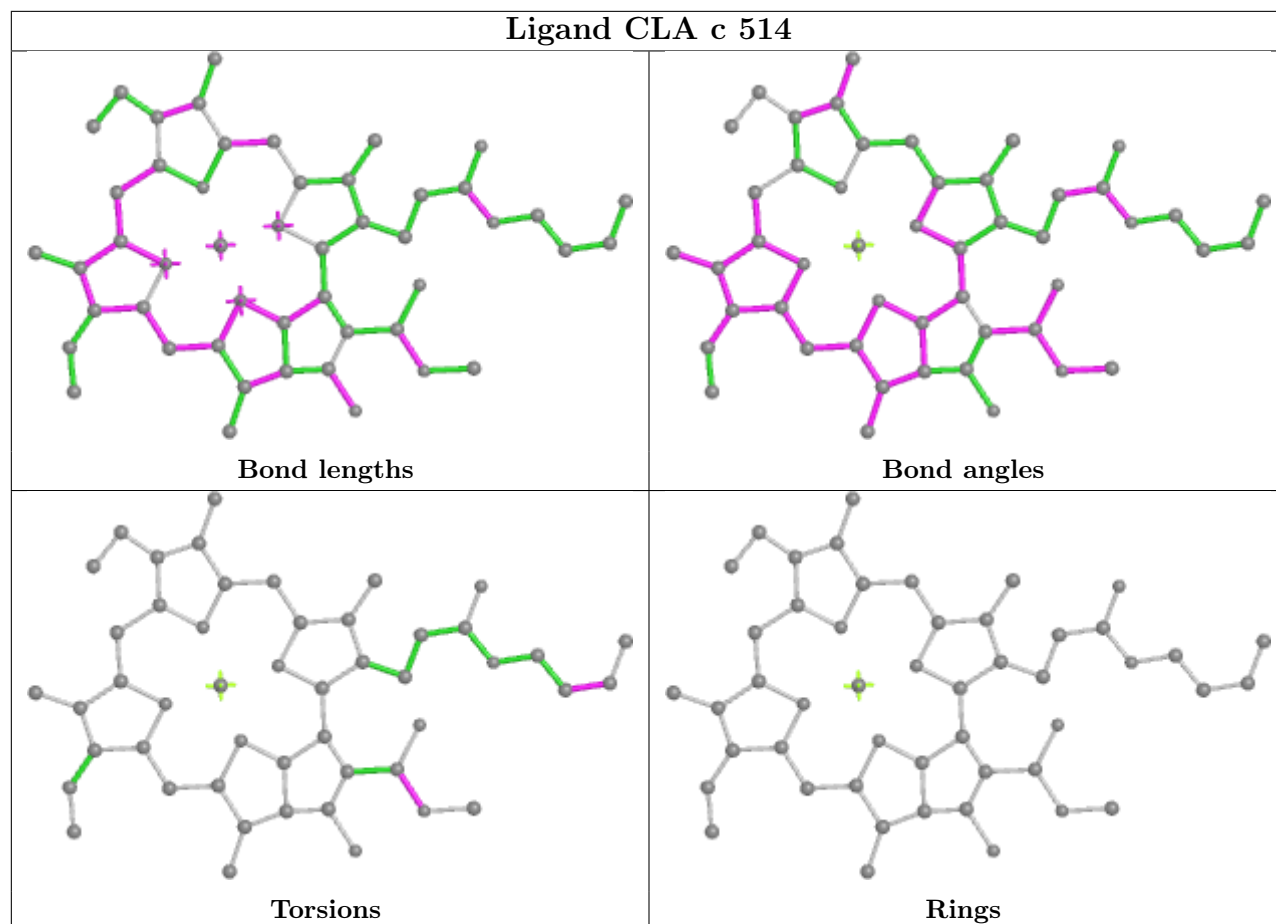




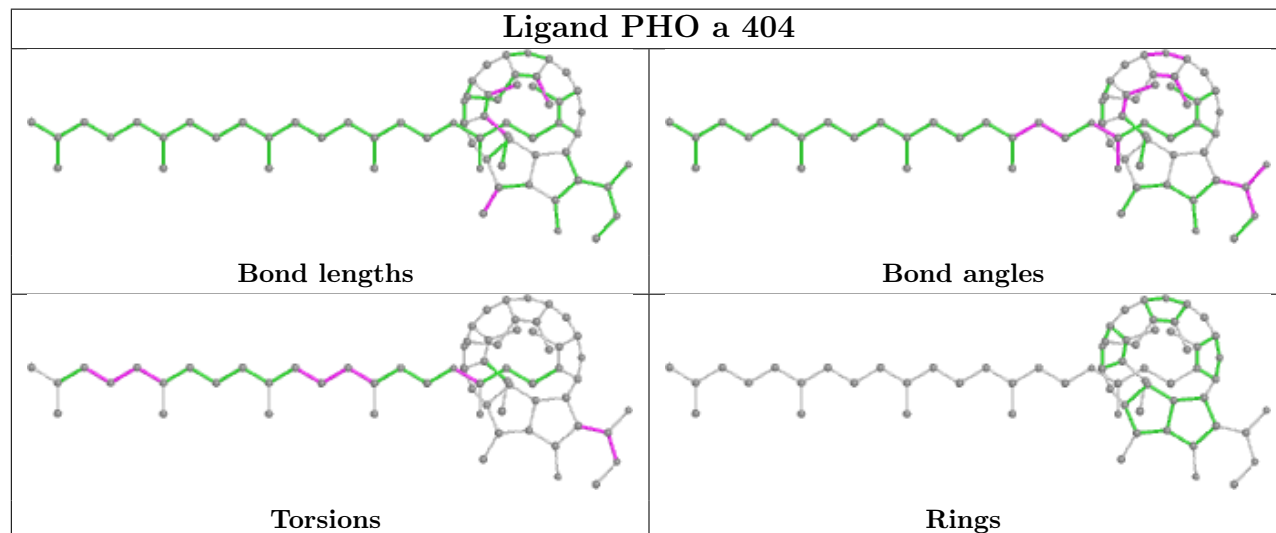
## Ligand CLA J 303



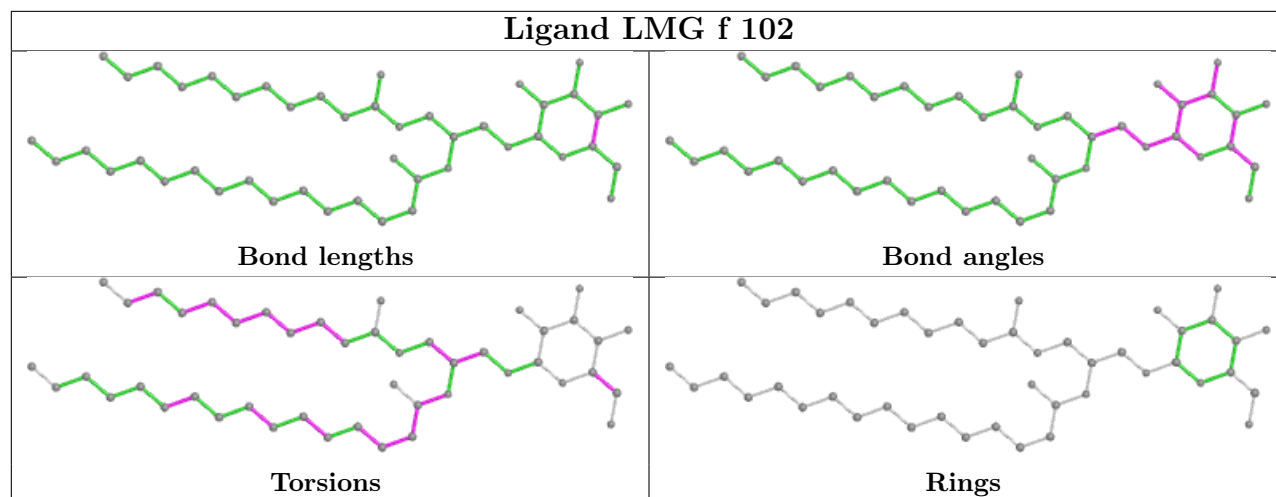
## Ligand CLA c 514



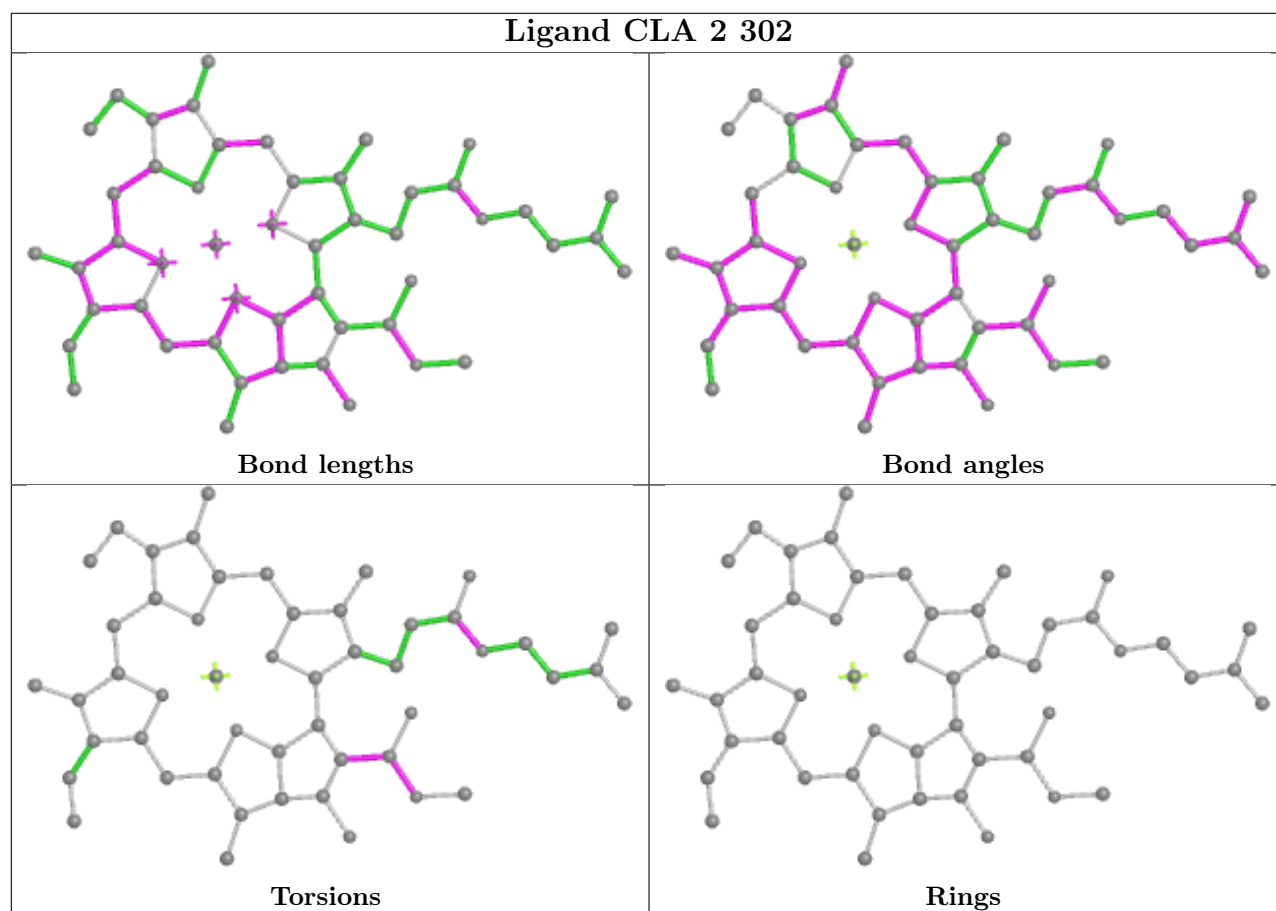
## Ligand PHO a 404

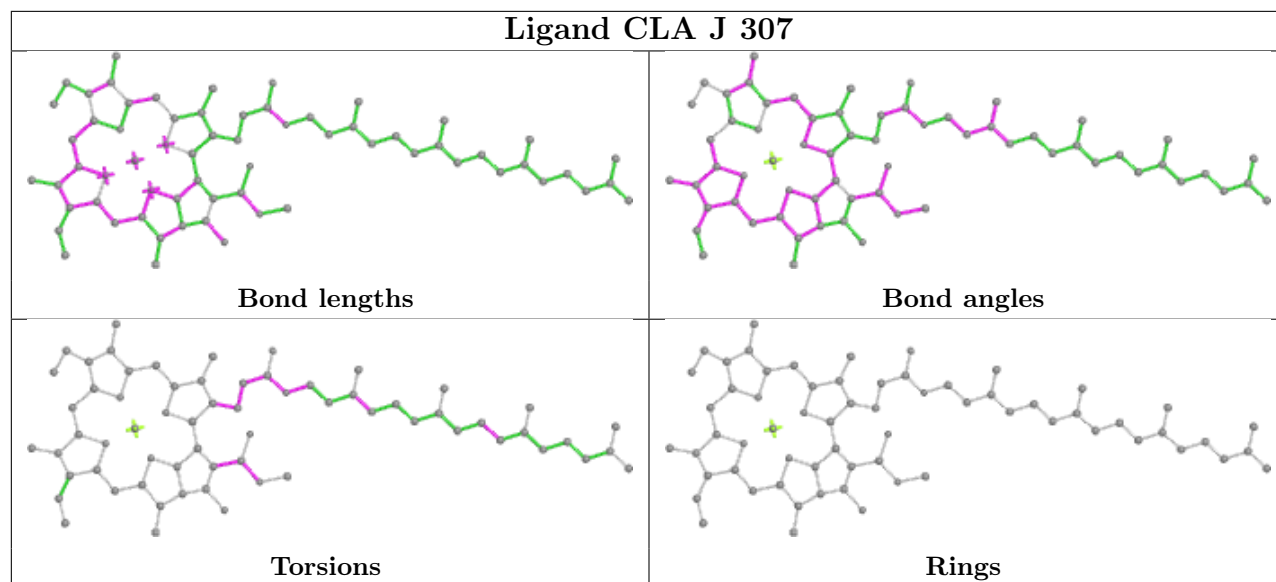
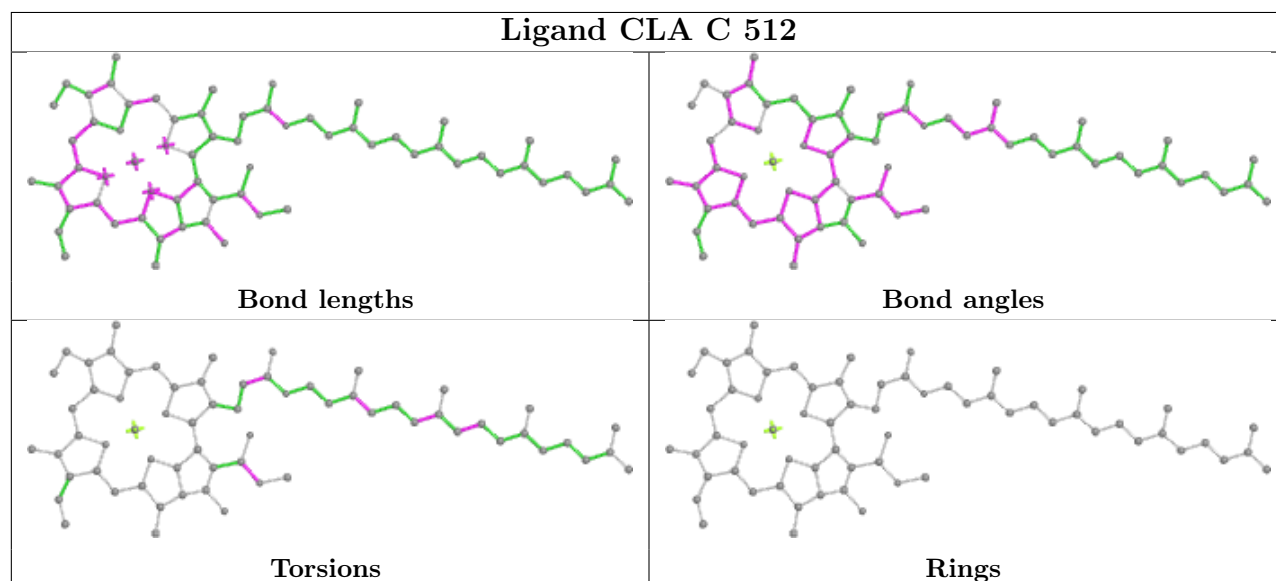


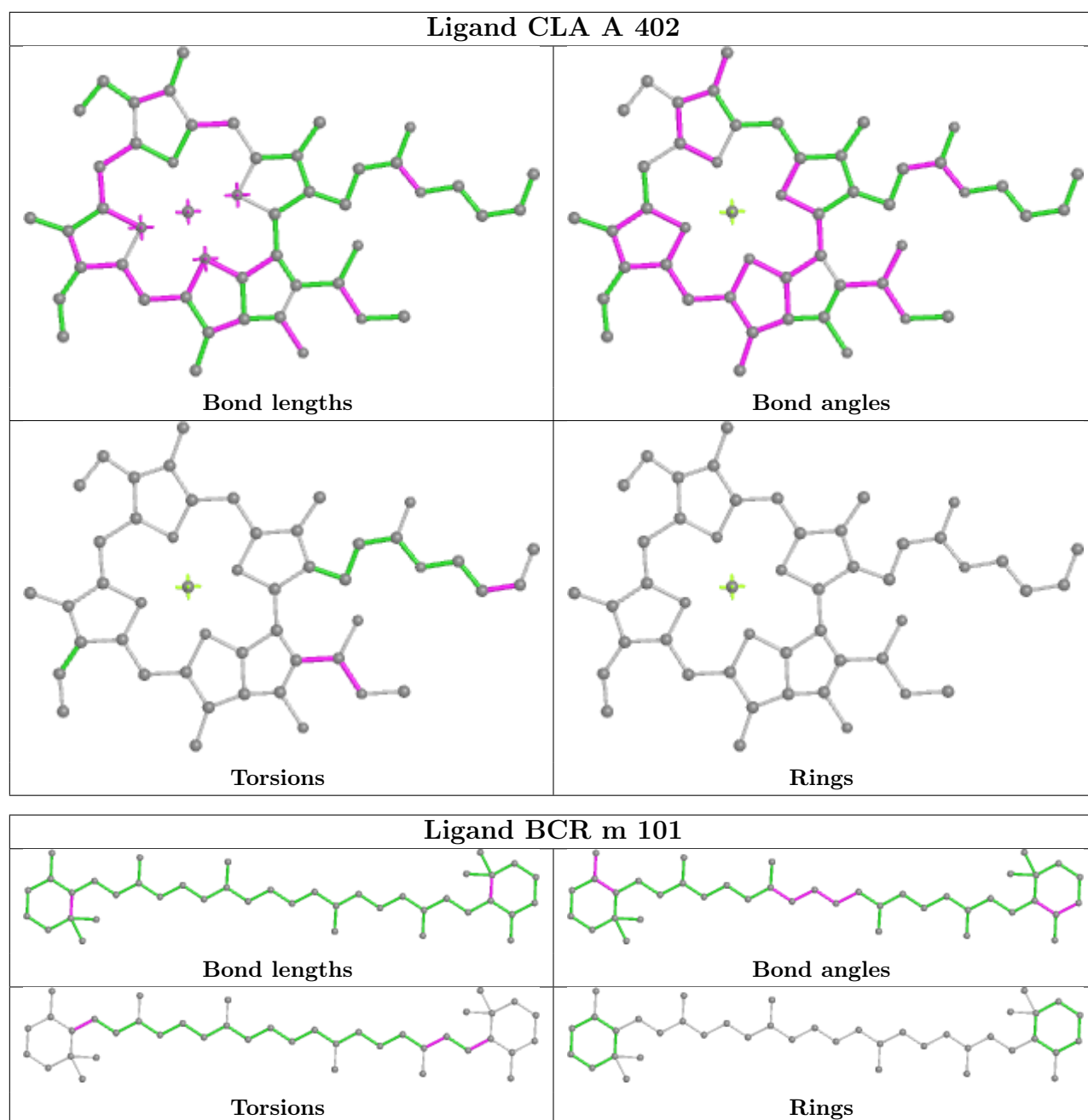
## Ligand LMG f 102



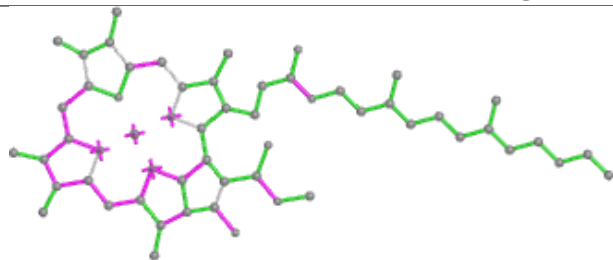
## Ligand CLA 2 302



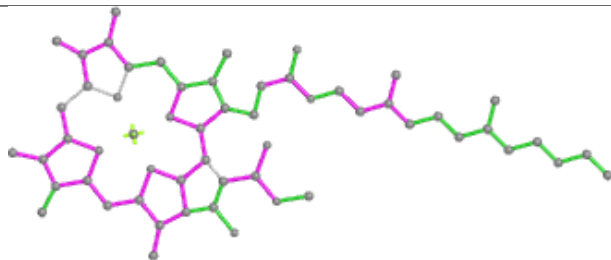
**Ligand CLA J 307****Ligand CLA C 512**



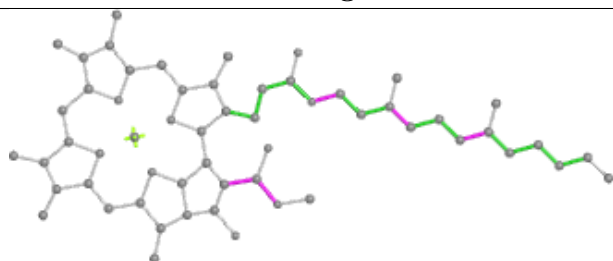
## Ligand CLA d 405



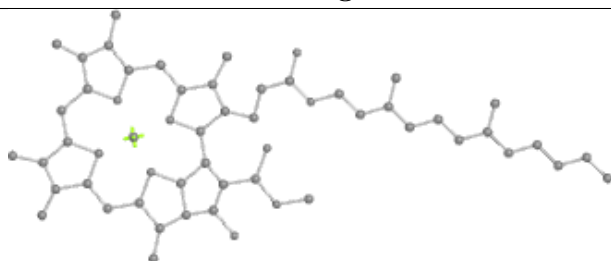
Bond lengths



Bond angles

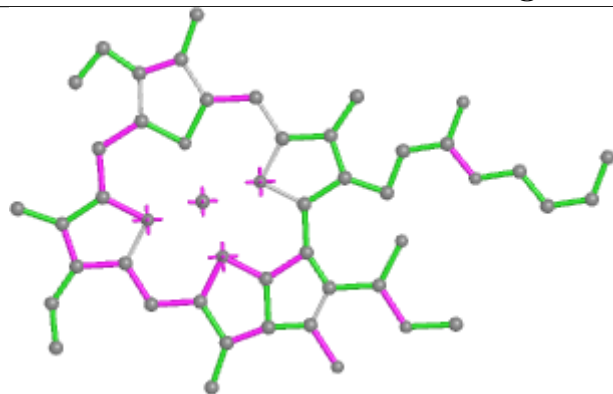


Torsions

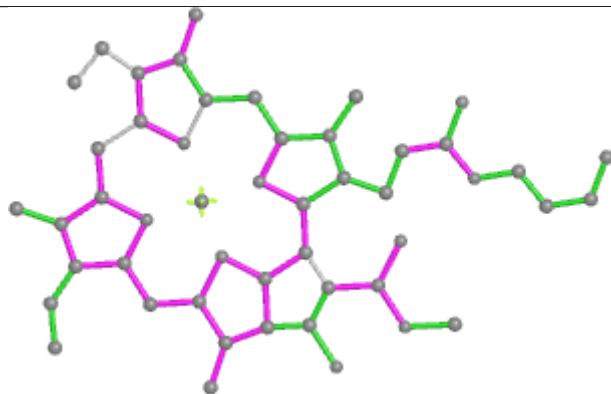


Rings

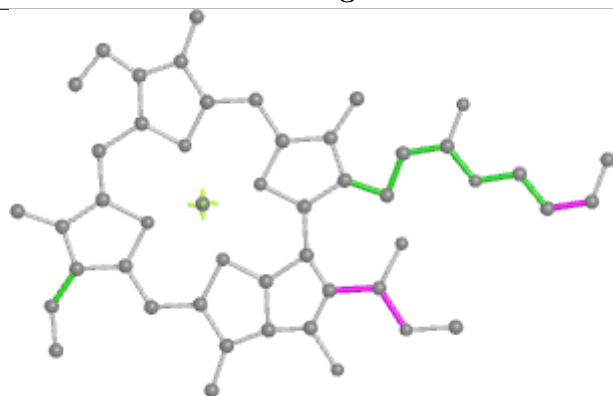
## Ligand CLA a 403



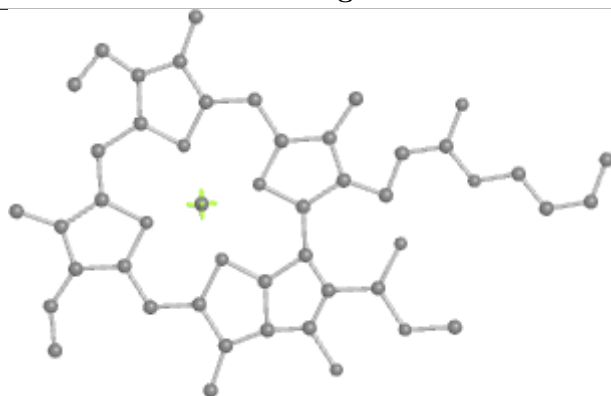
Bond lengths



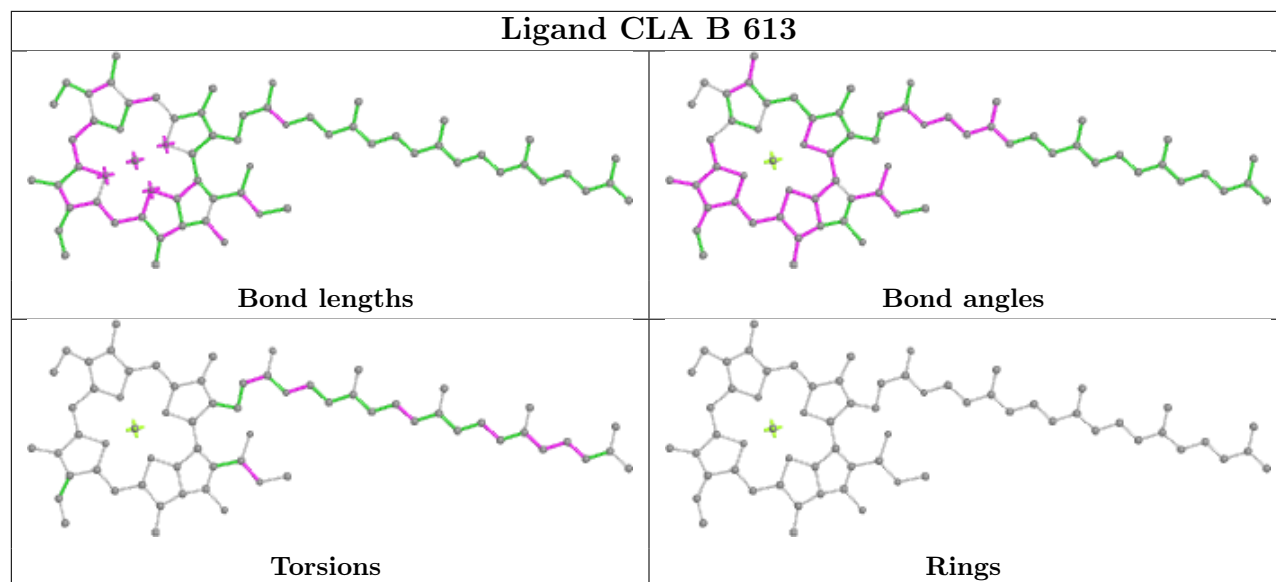
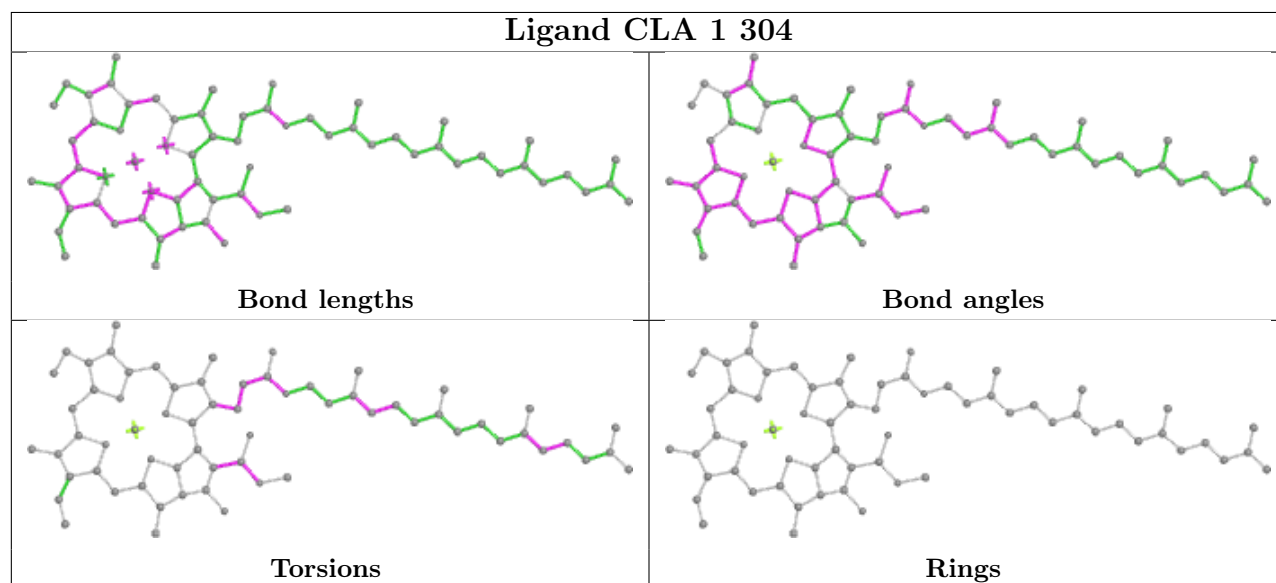
Bond angles



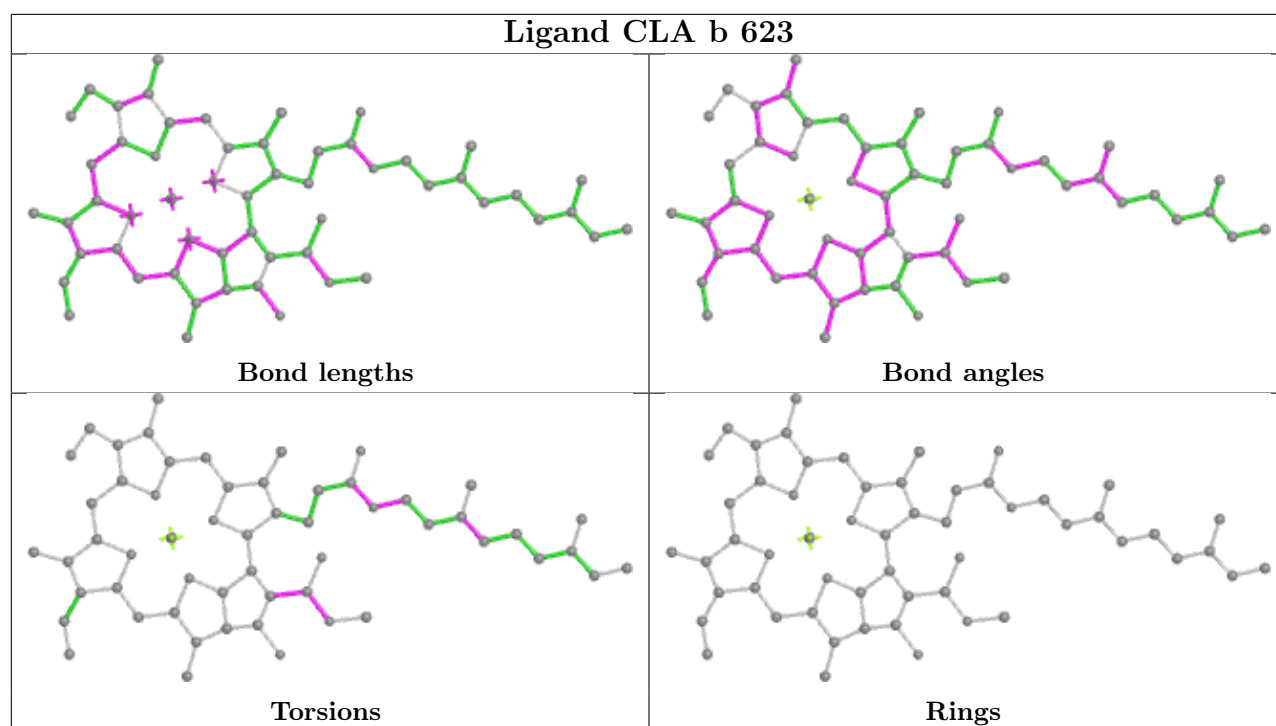
Torsions



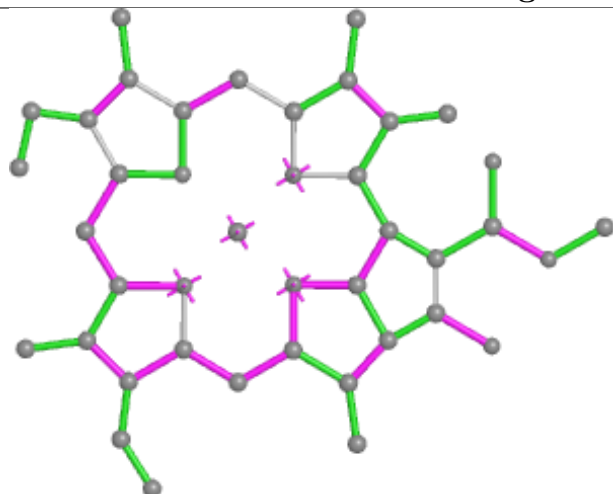
Rings

**Ligand CLA B 613****Ligand CLA 1 304**

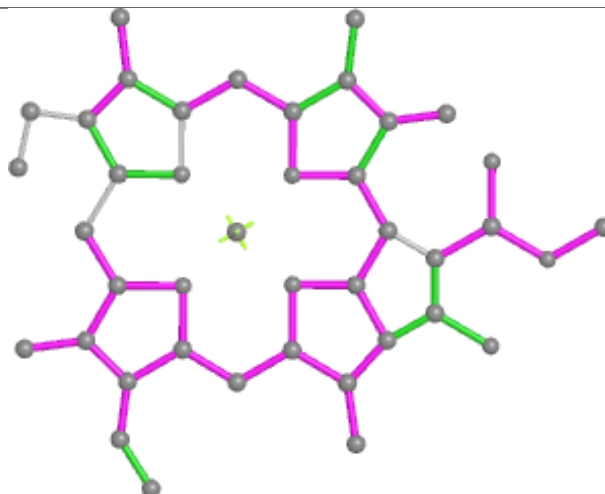




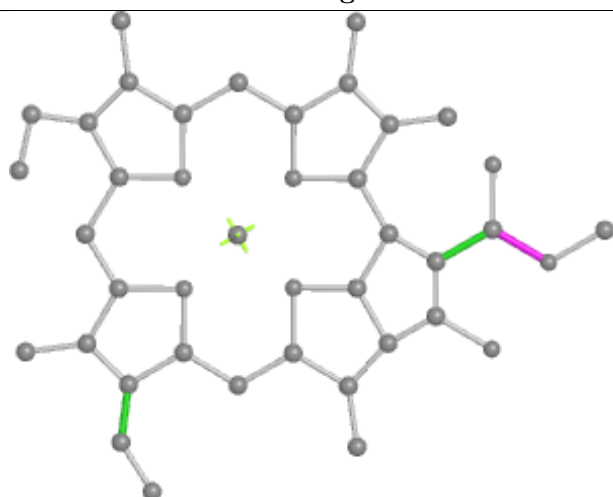
## Ligand CLA 5 305



Bond lengths



Bond angles

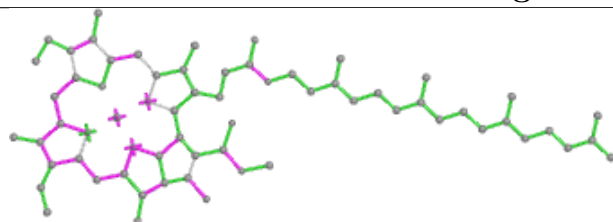


Torsions

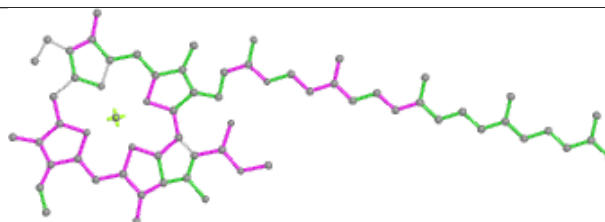


Rings

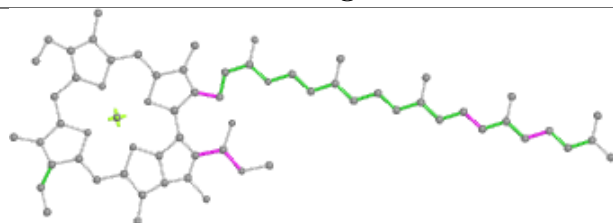
## Ligand CLA G 300



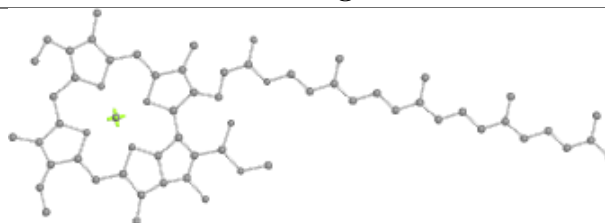
Bond lengths



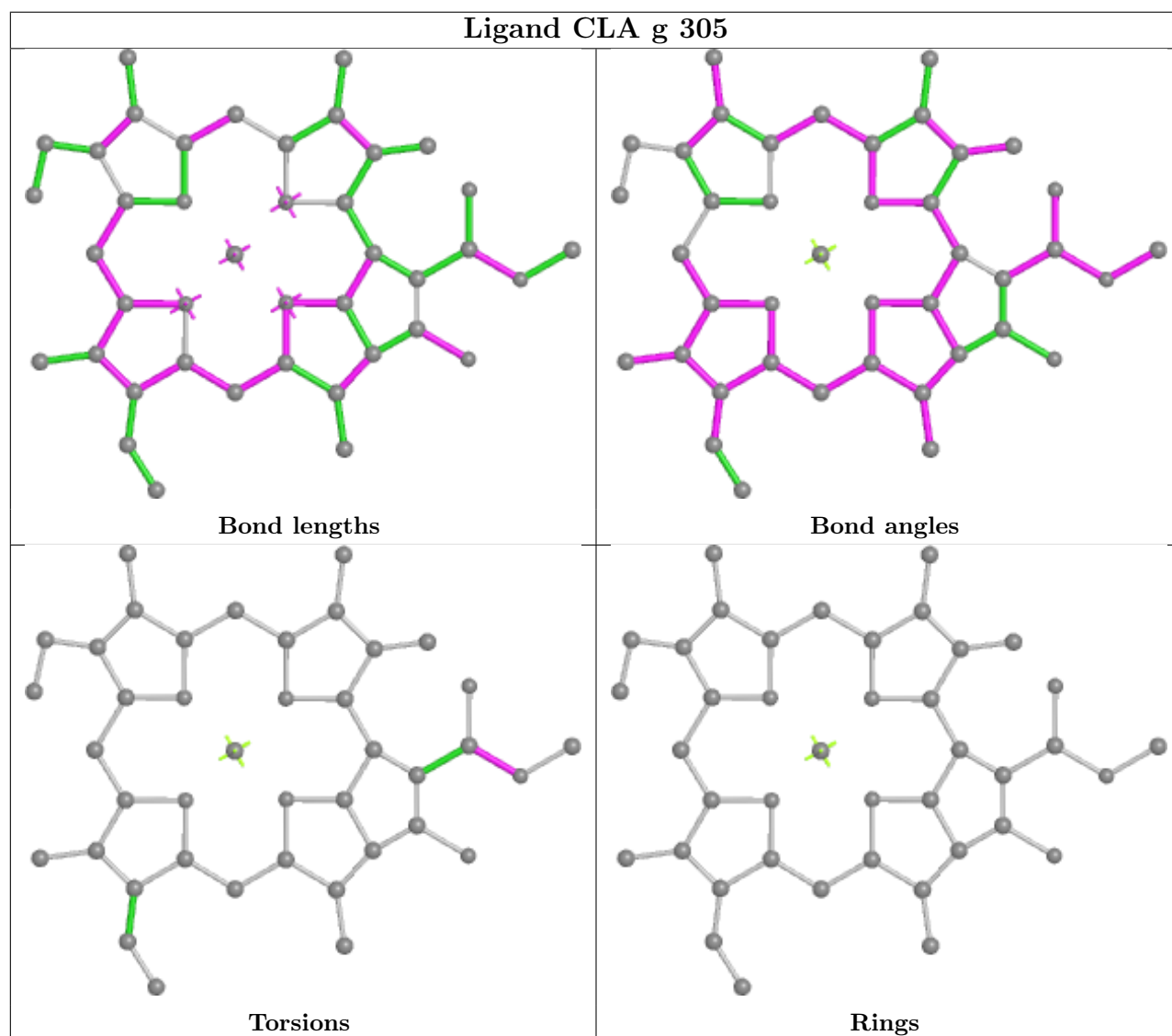
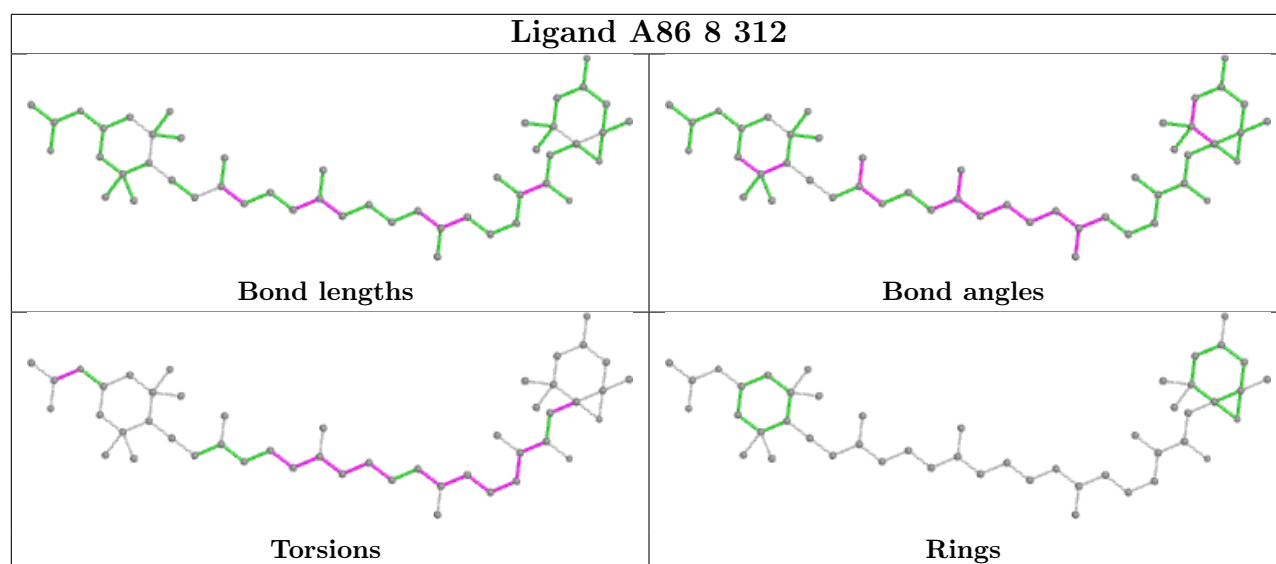
Bond angles



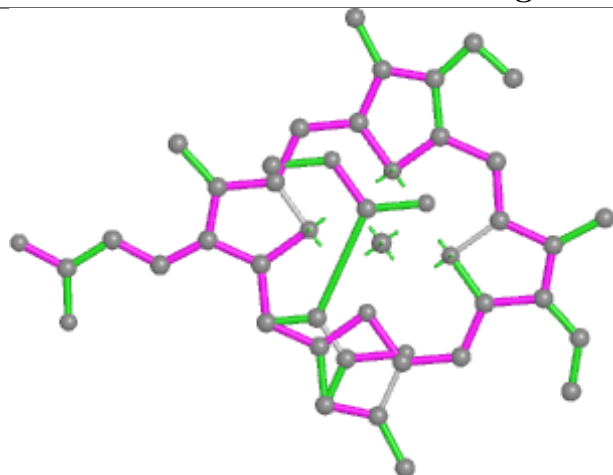
Torsions



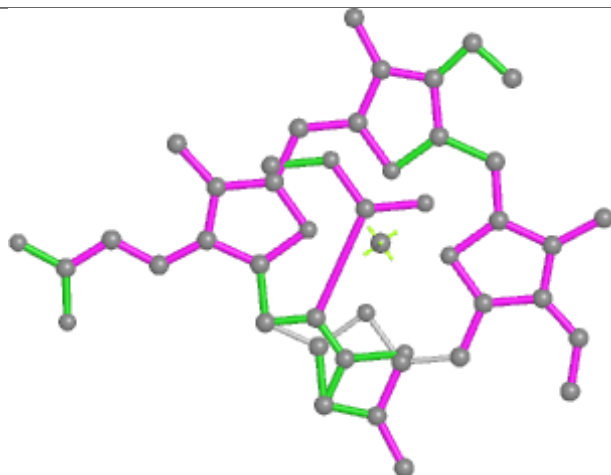
Rings



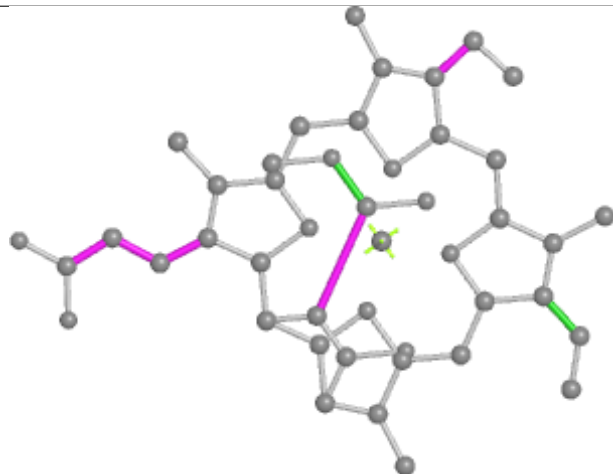
## Ligand KC1 G 309



Bond lengths



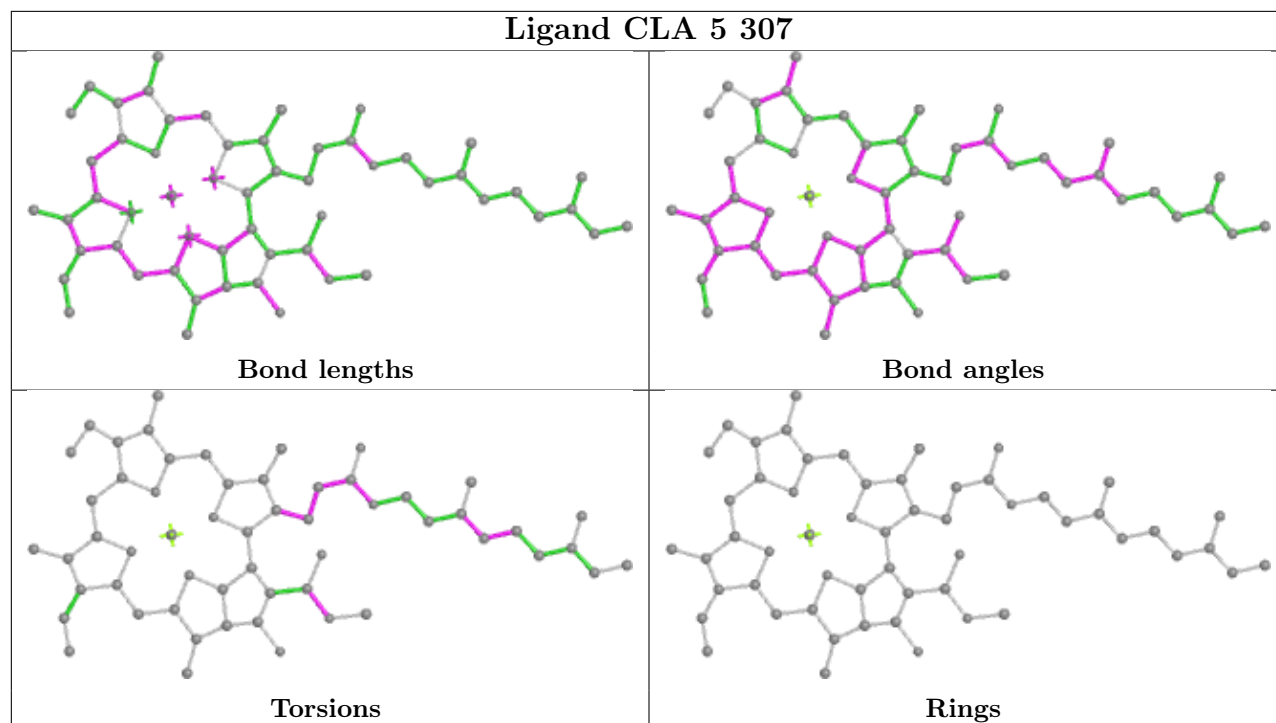
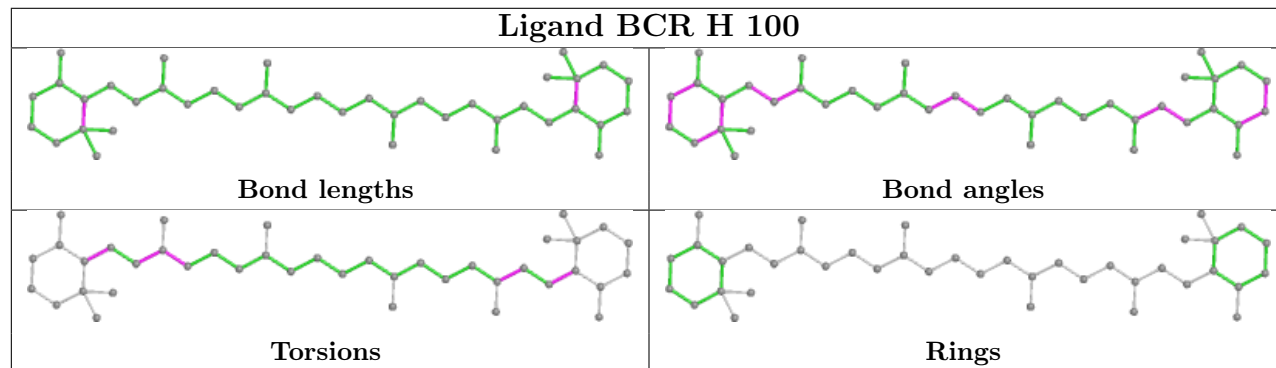
Bond angles

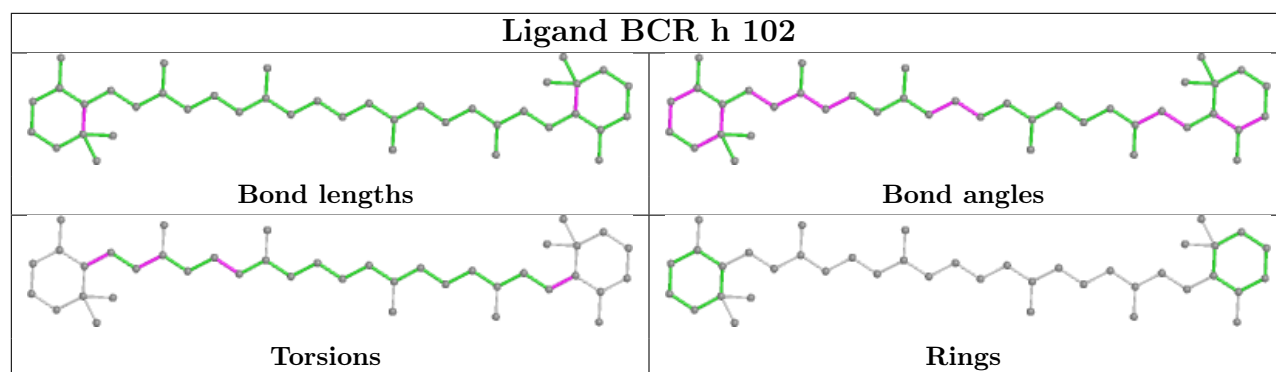
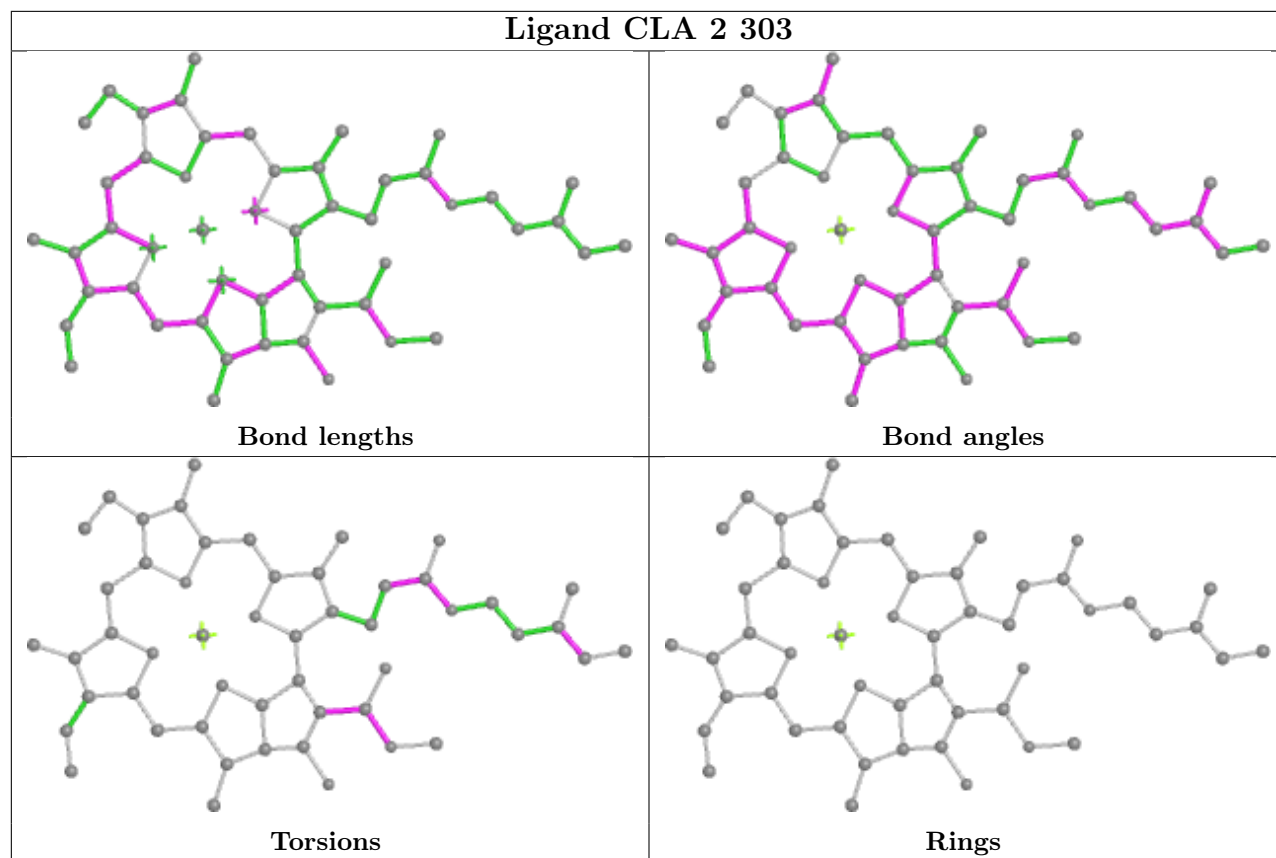


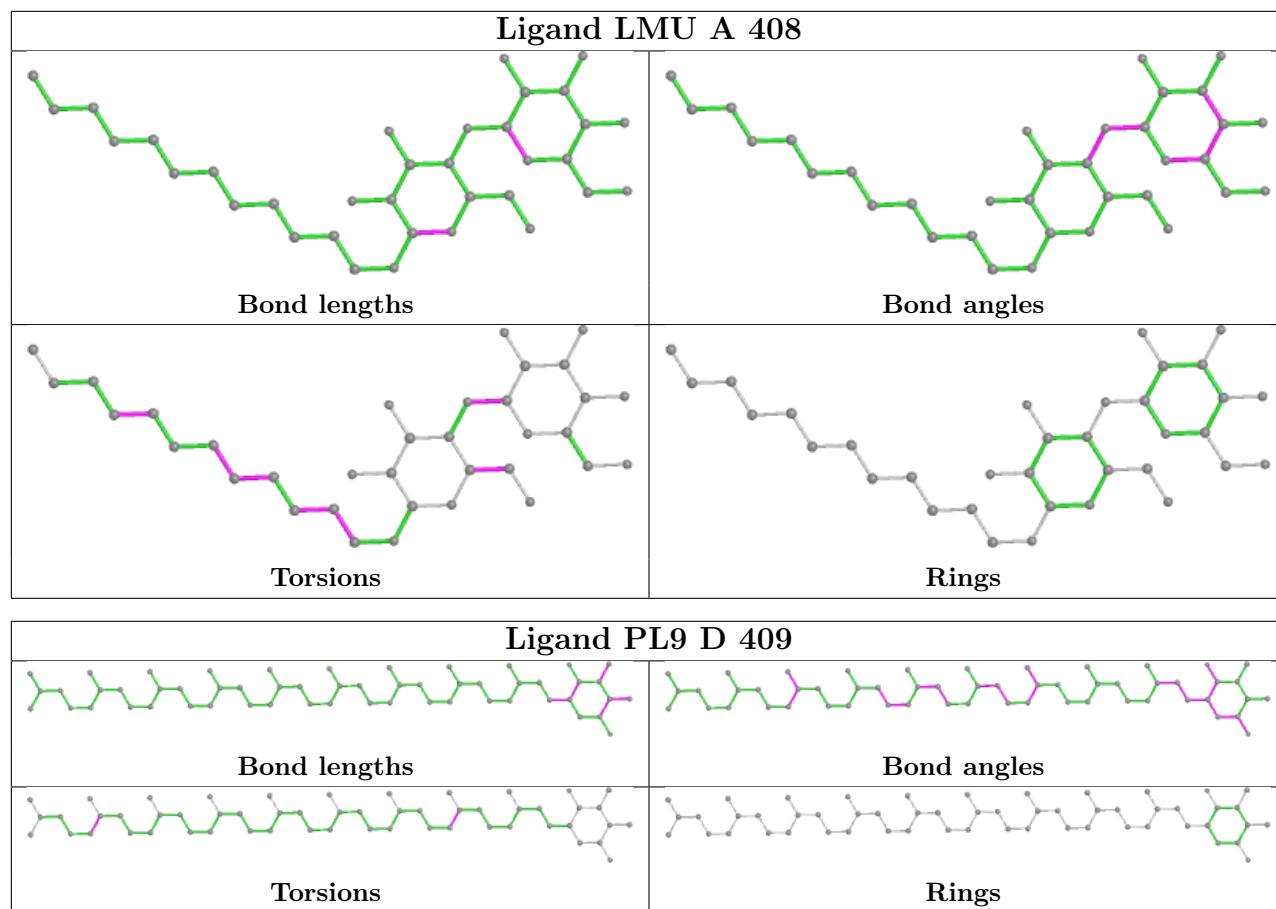
Torsions



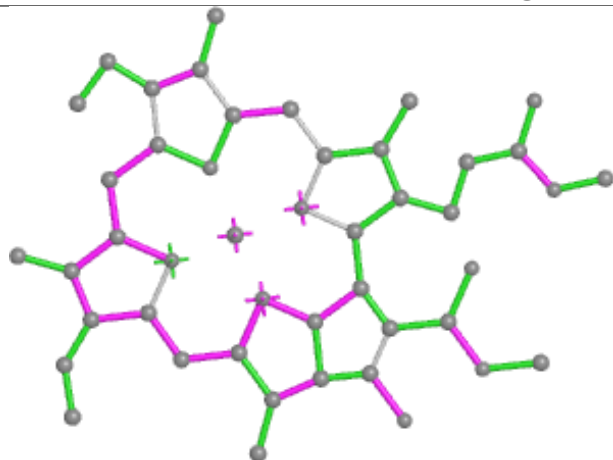
Rings

**Ligand CLA 5 307****Ligand BCR H 100**

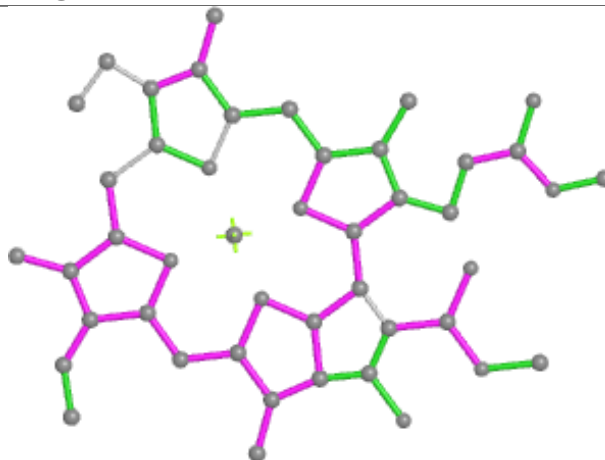




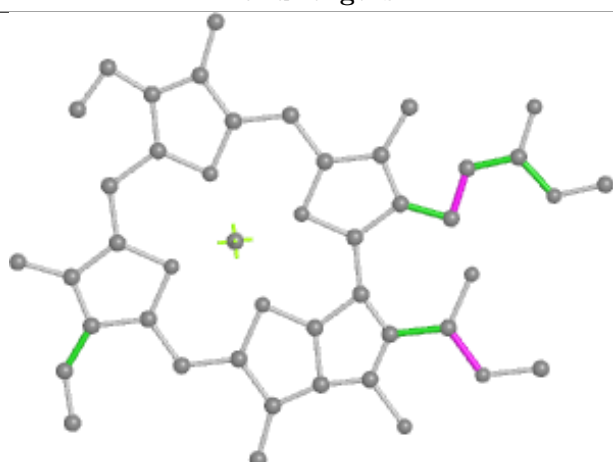
## Ligand CLA g 307



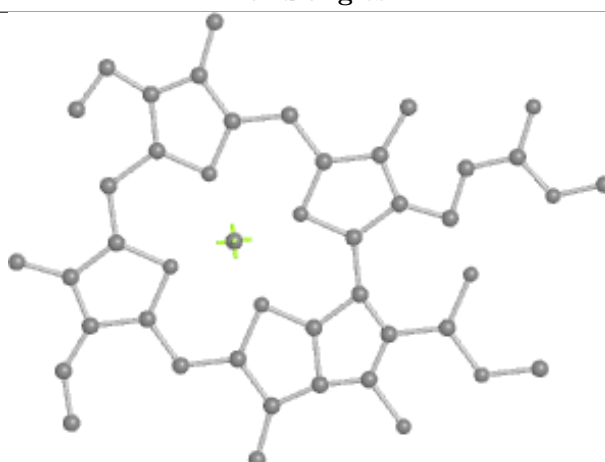
Bond lengths



Bond angles



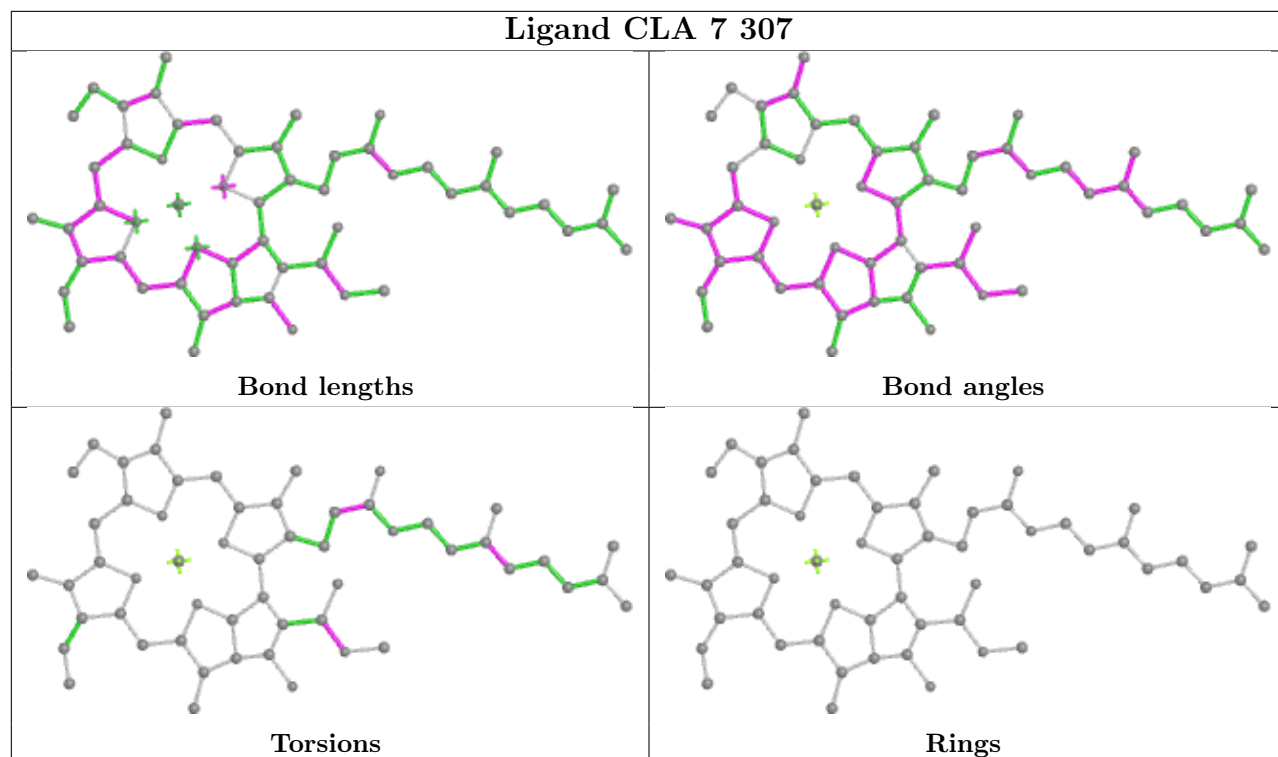
Torsions



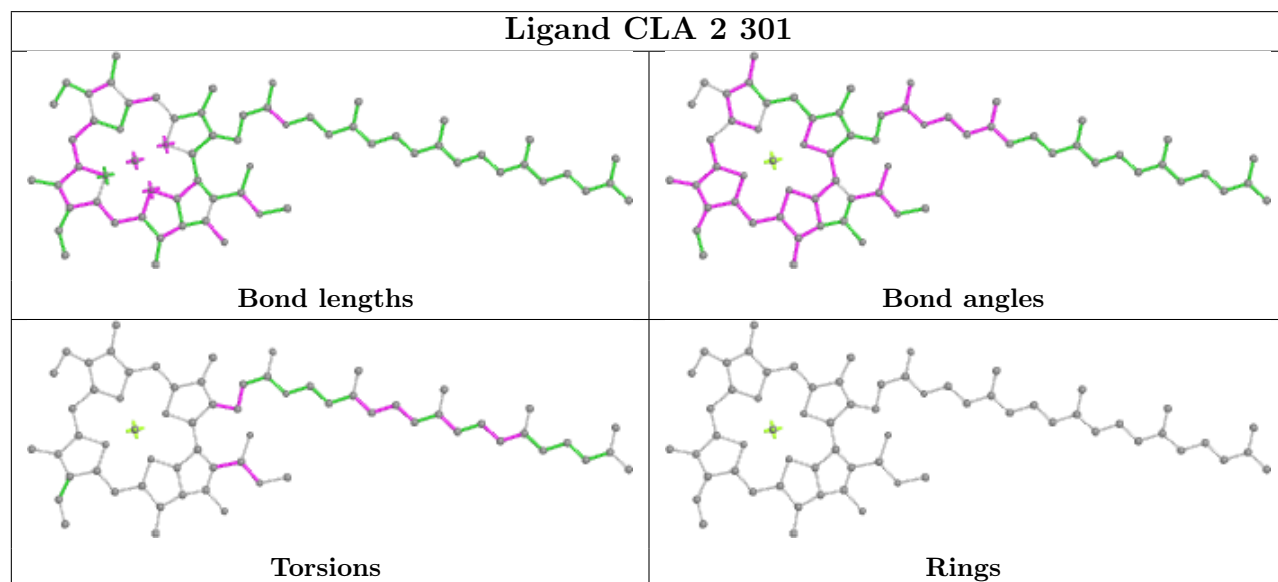
Rings



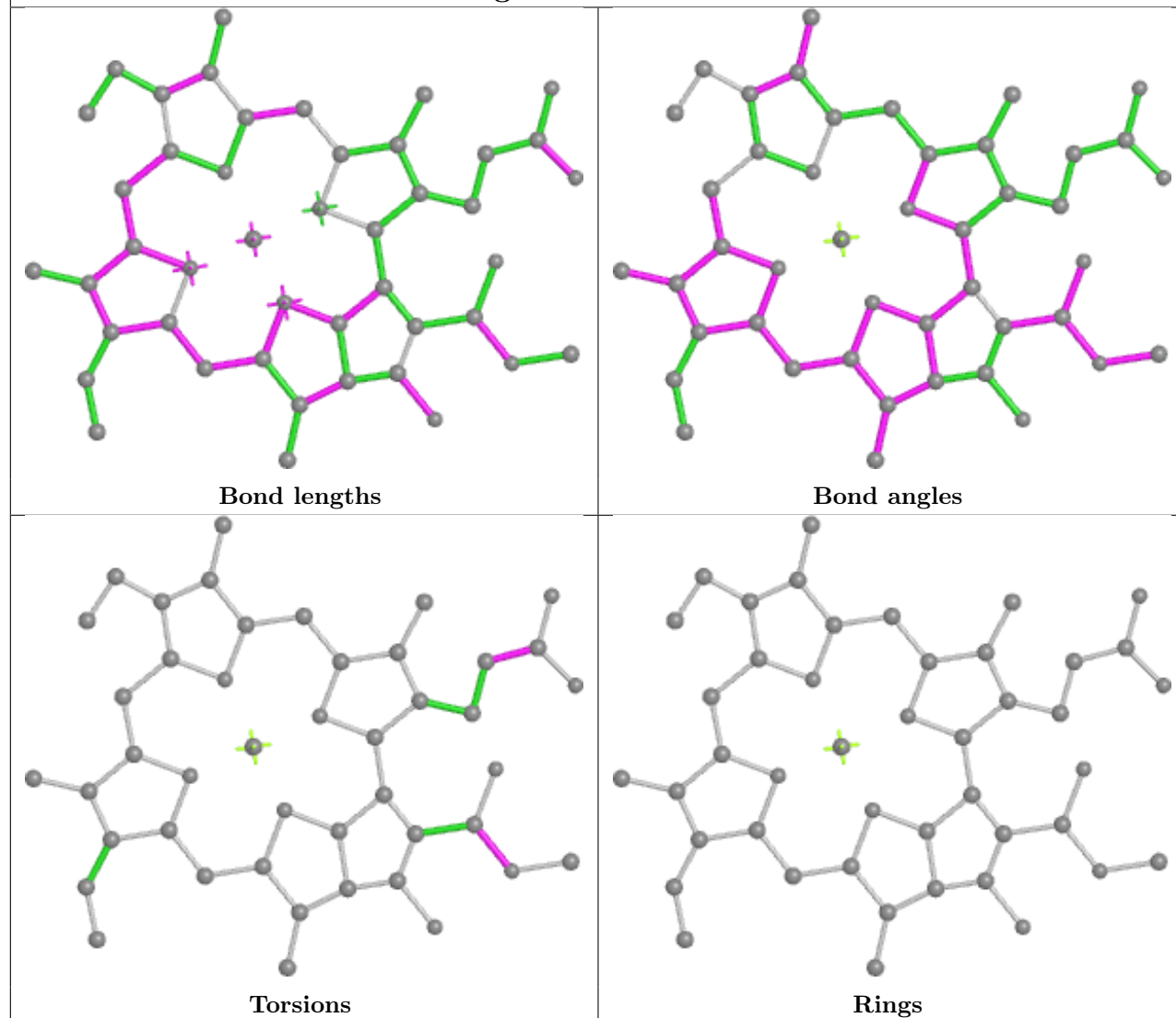
## Ligand CLA 7 307



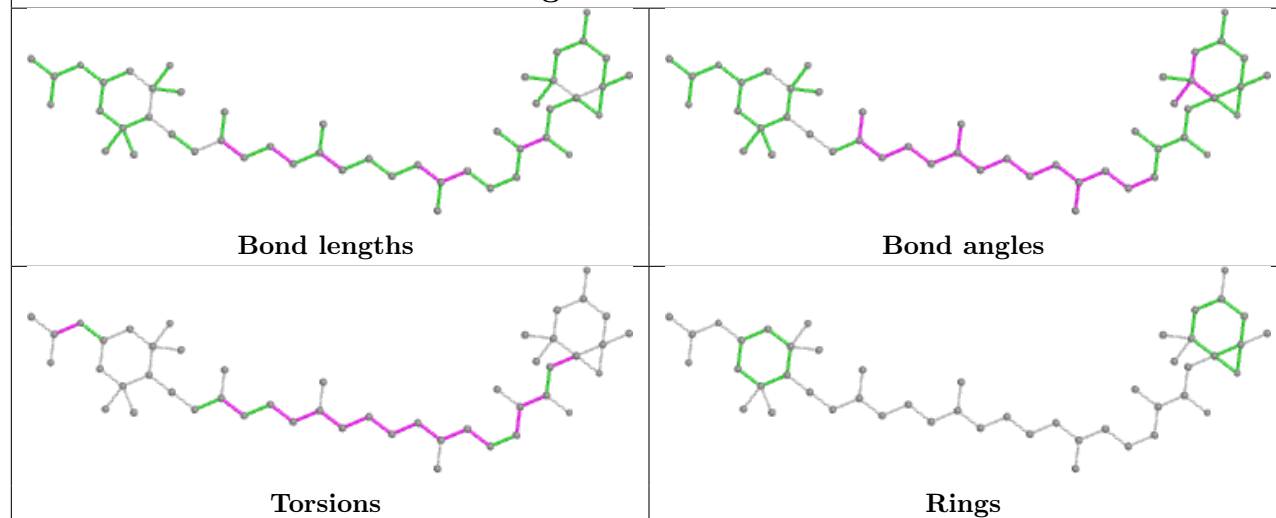
## Ligand CLA 2 301

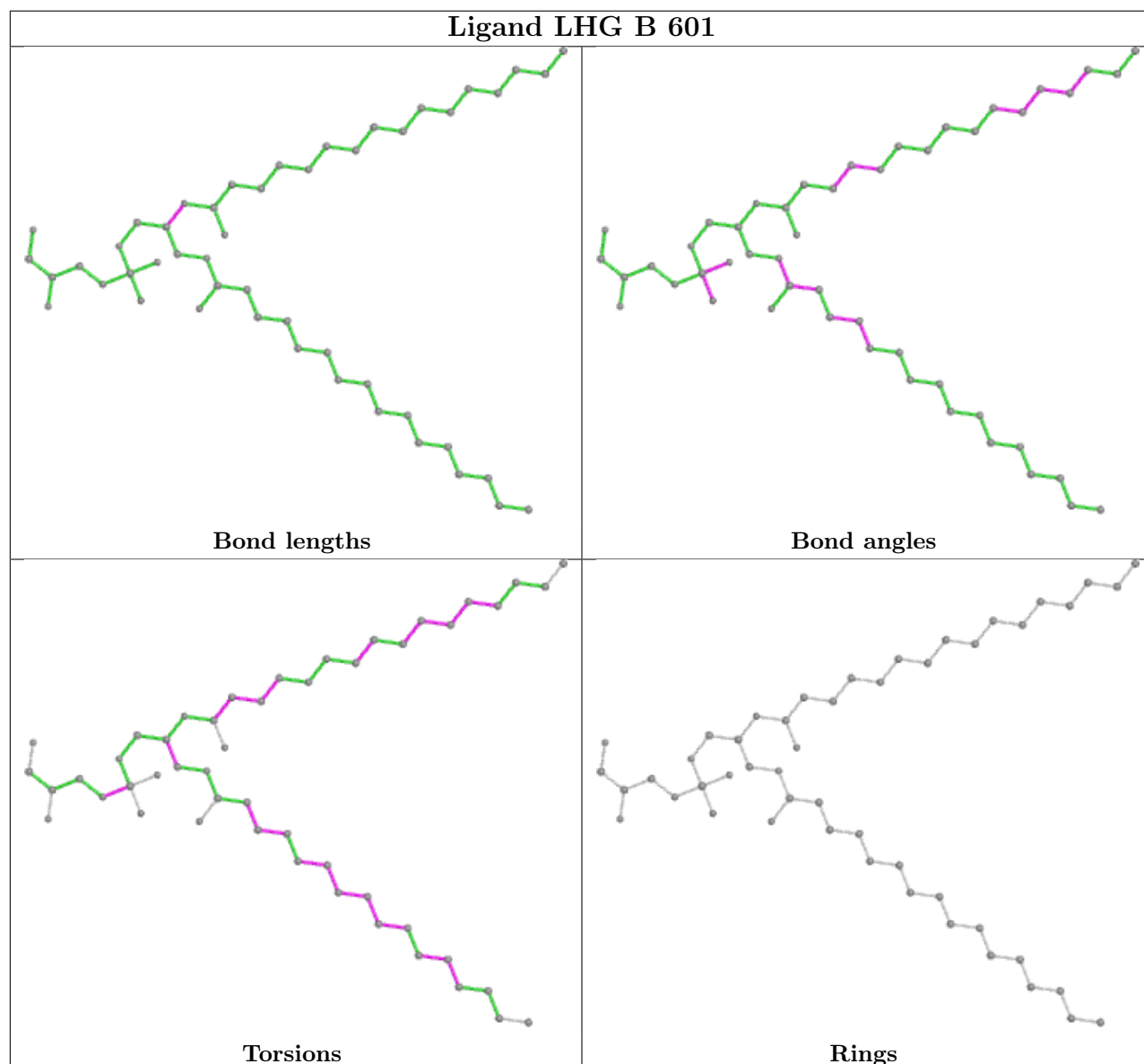
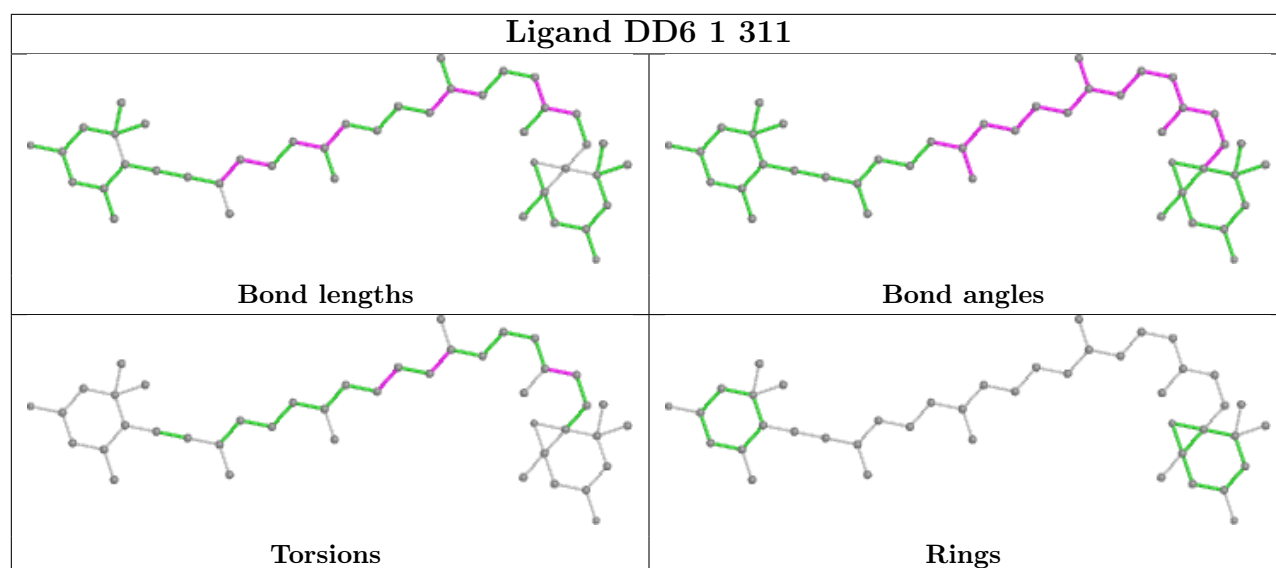


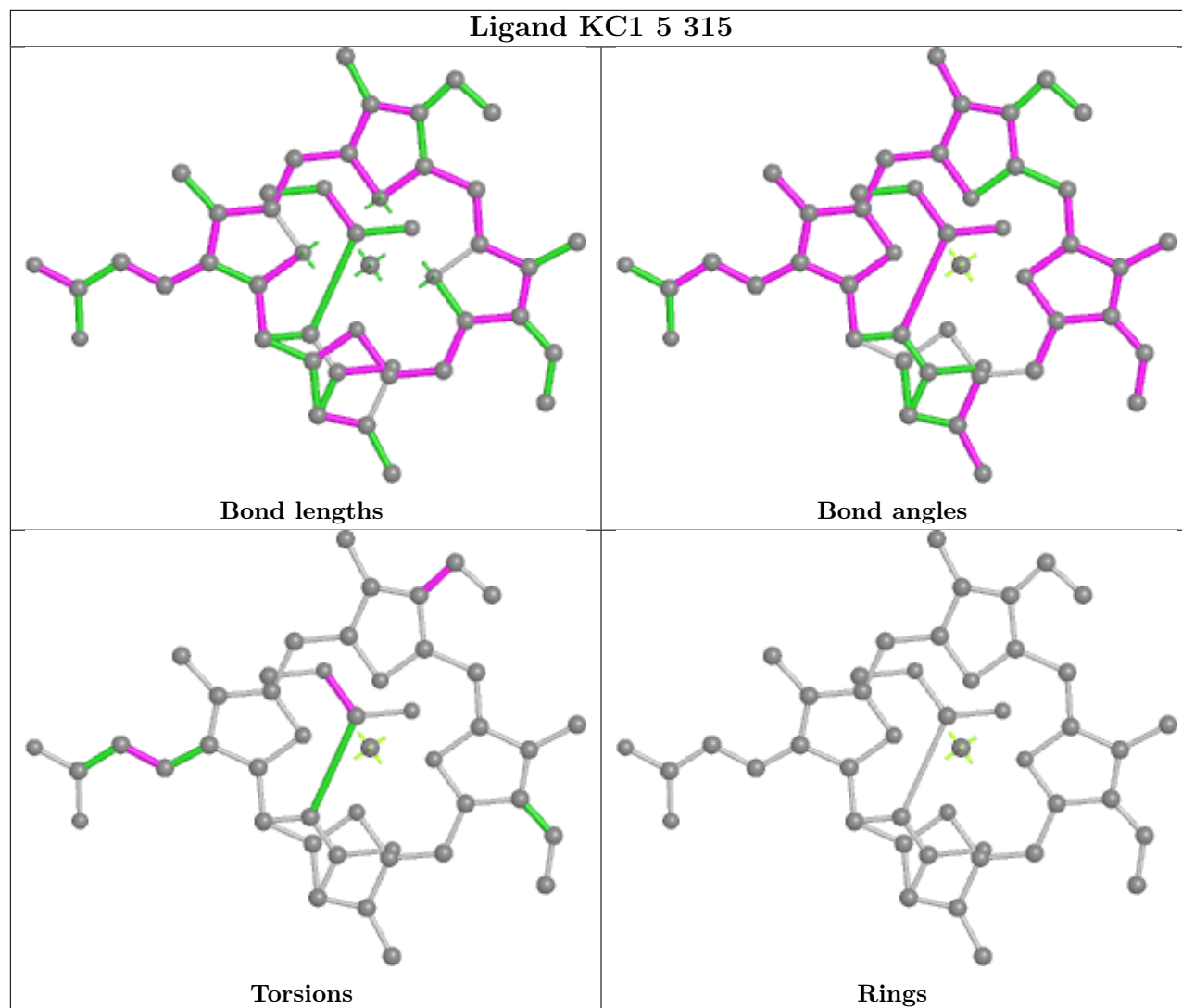
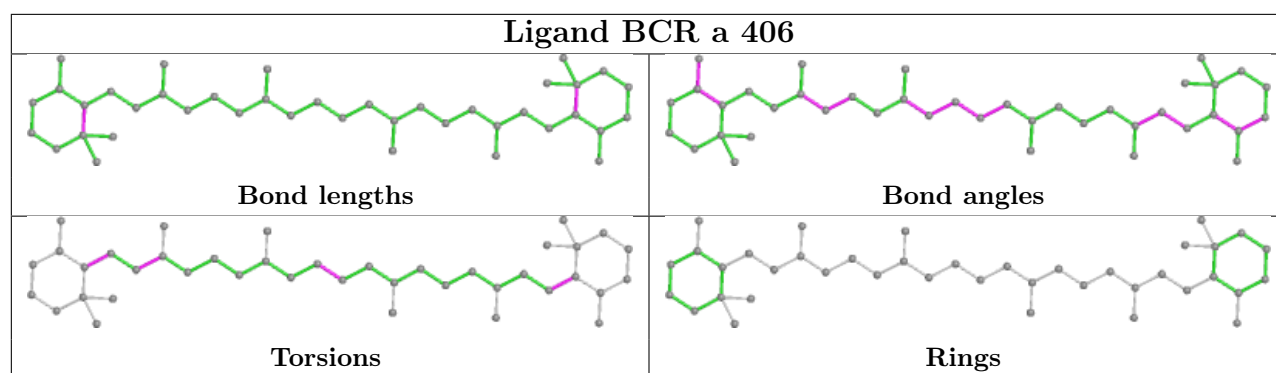
## Ligand CLA 6 305

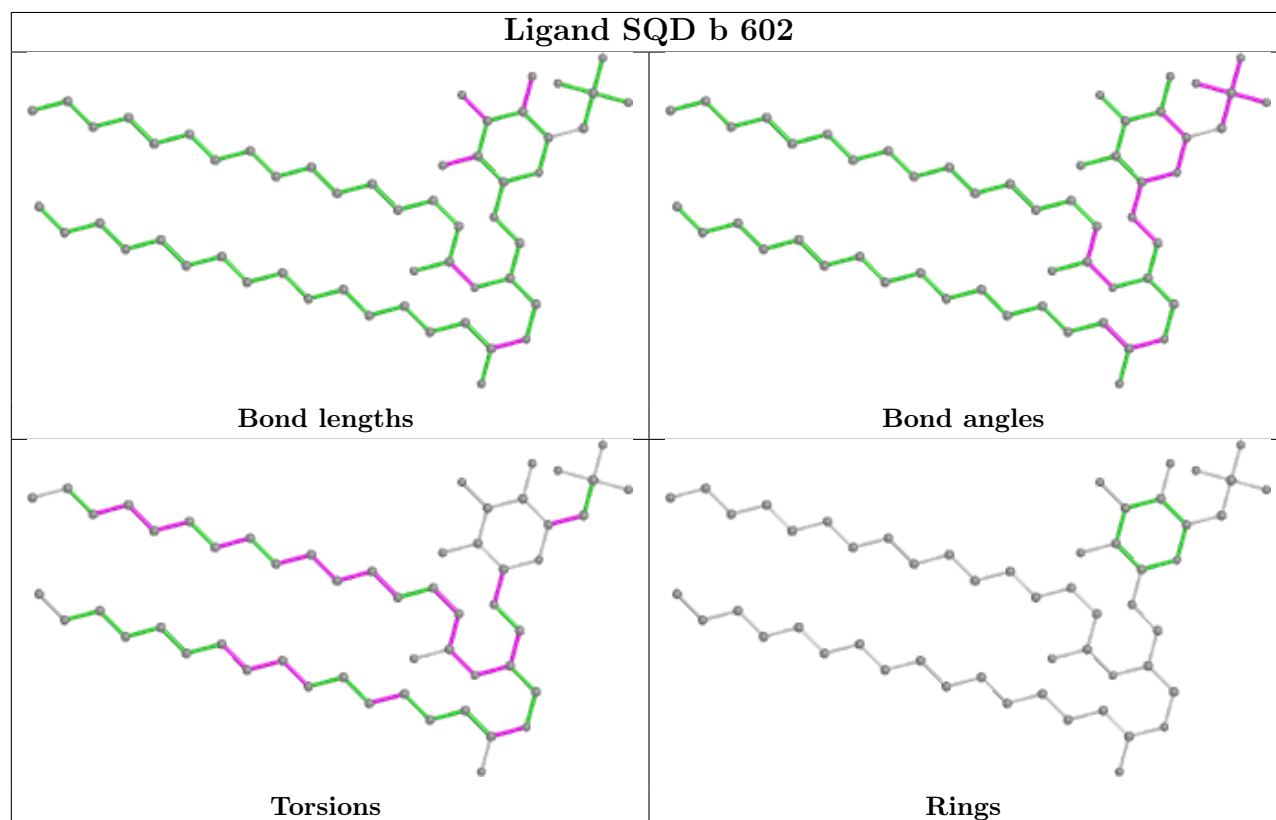
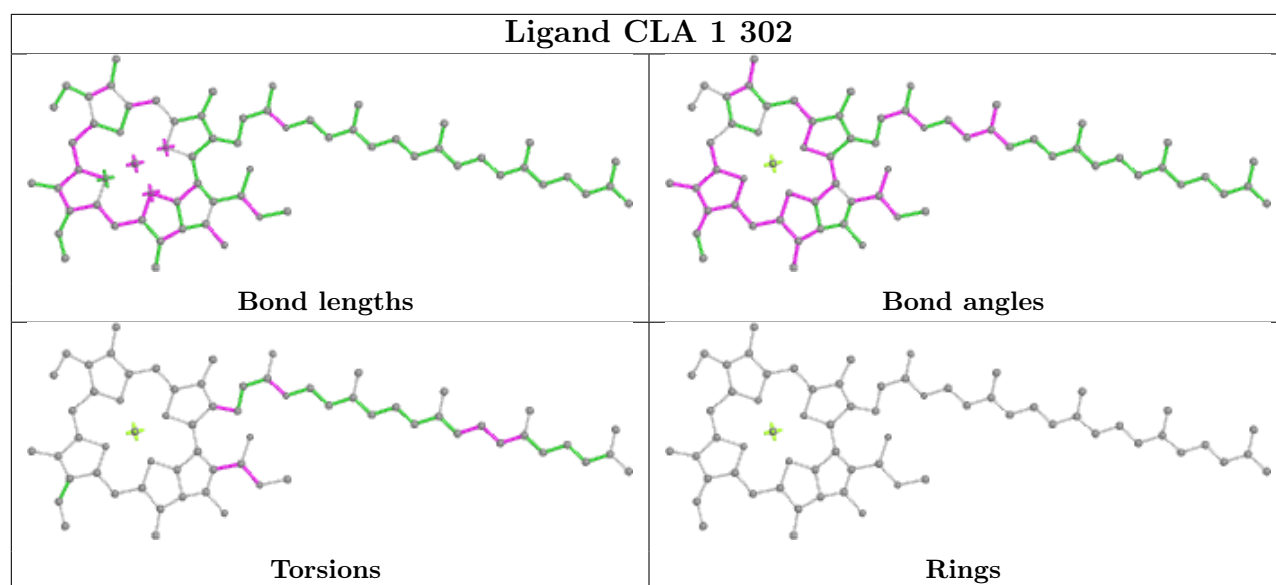


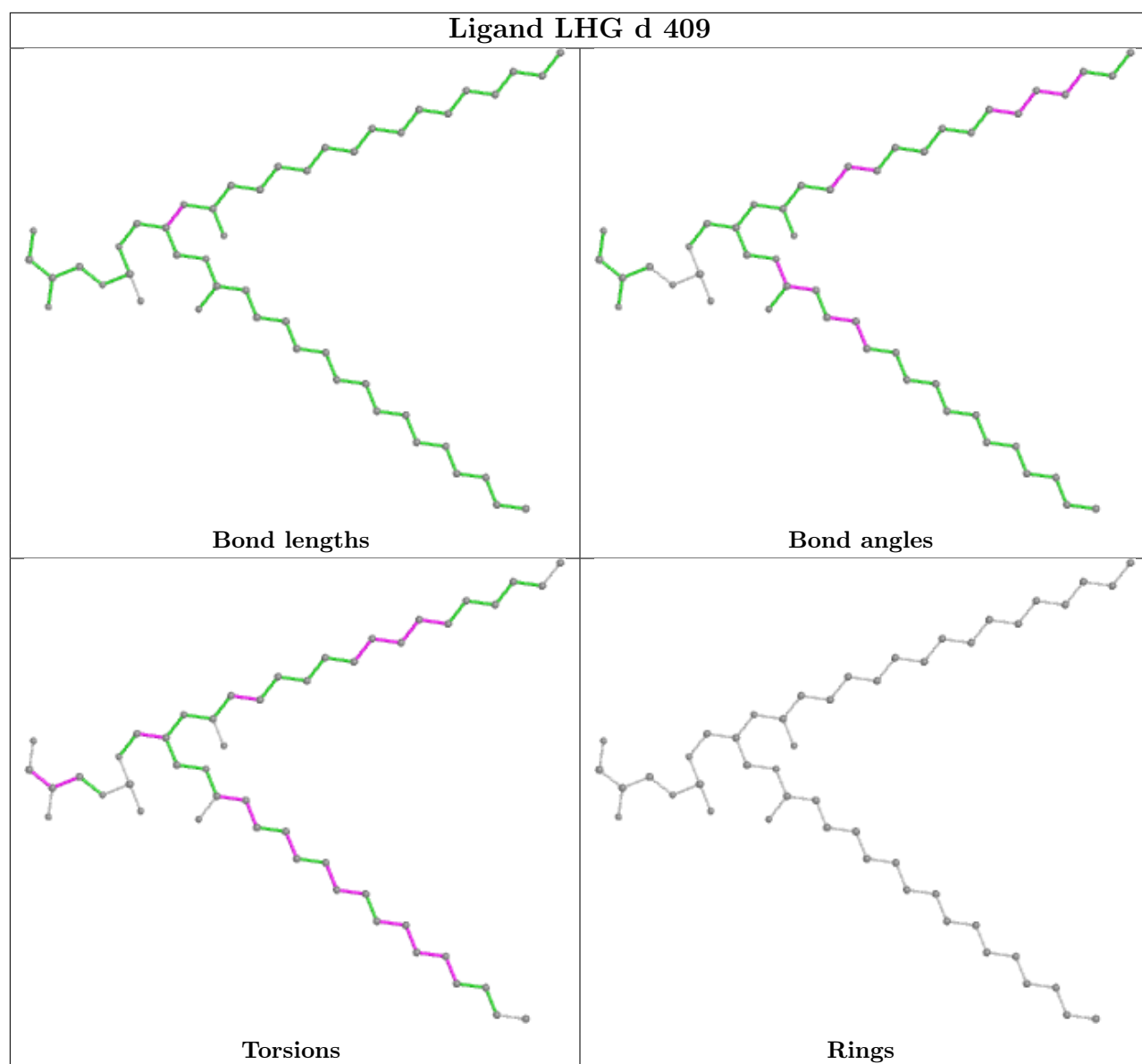
## Ligand A86 8 308



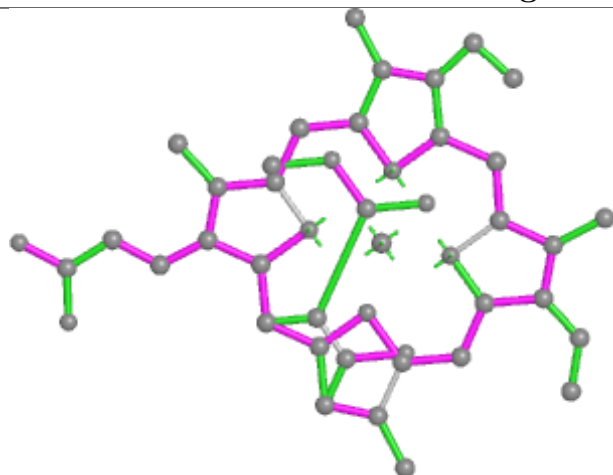




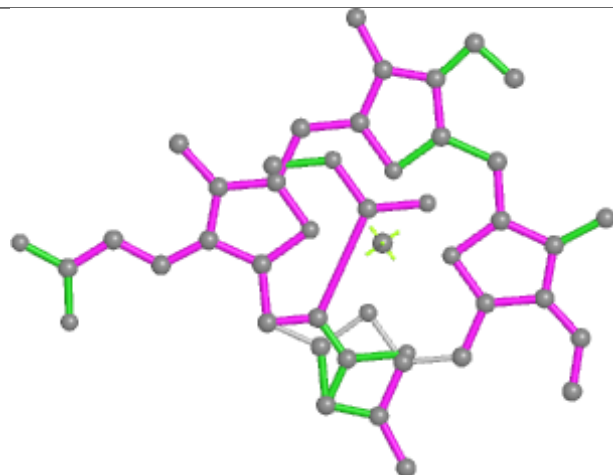




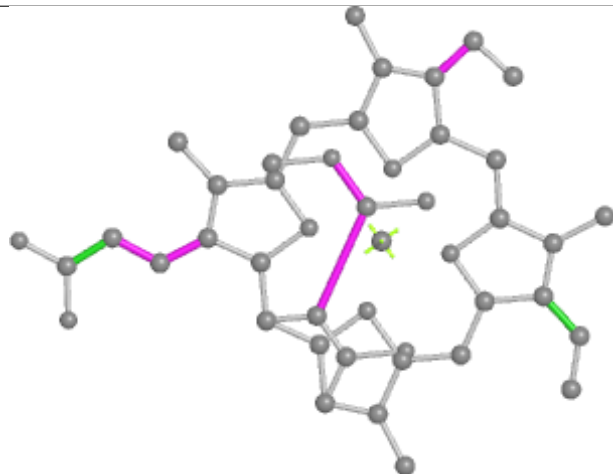
## Ligand KC1 J 311



Bond lengths



Bond angles

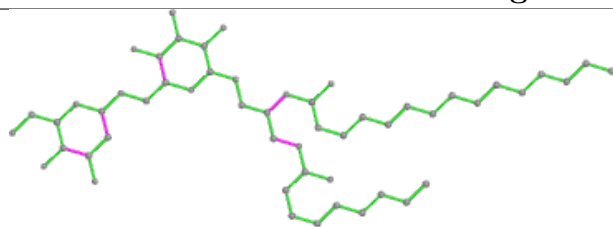


Torsions

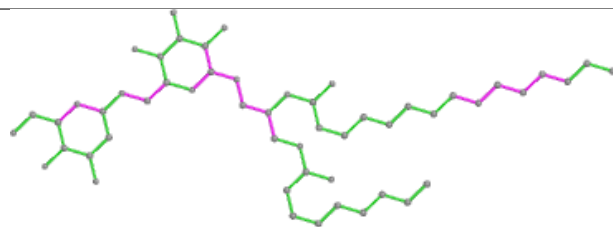


Rings

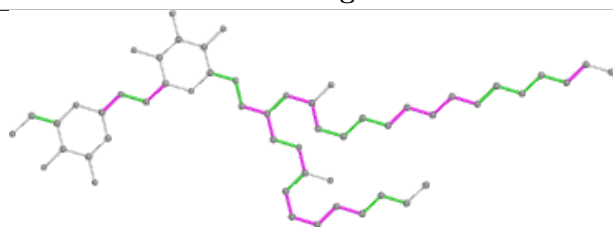
## Ligand DGD B 624



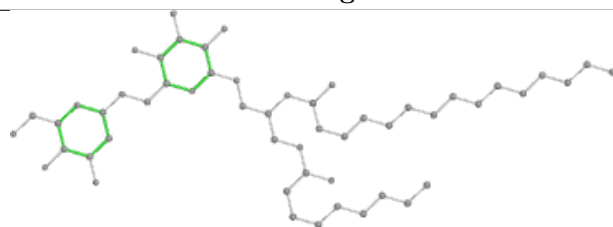
Bond lengths



Bond angles

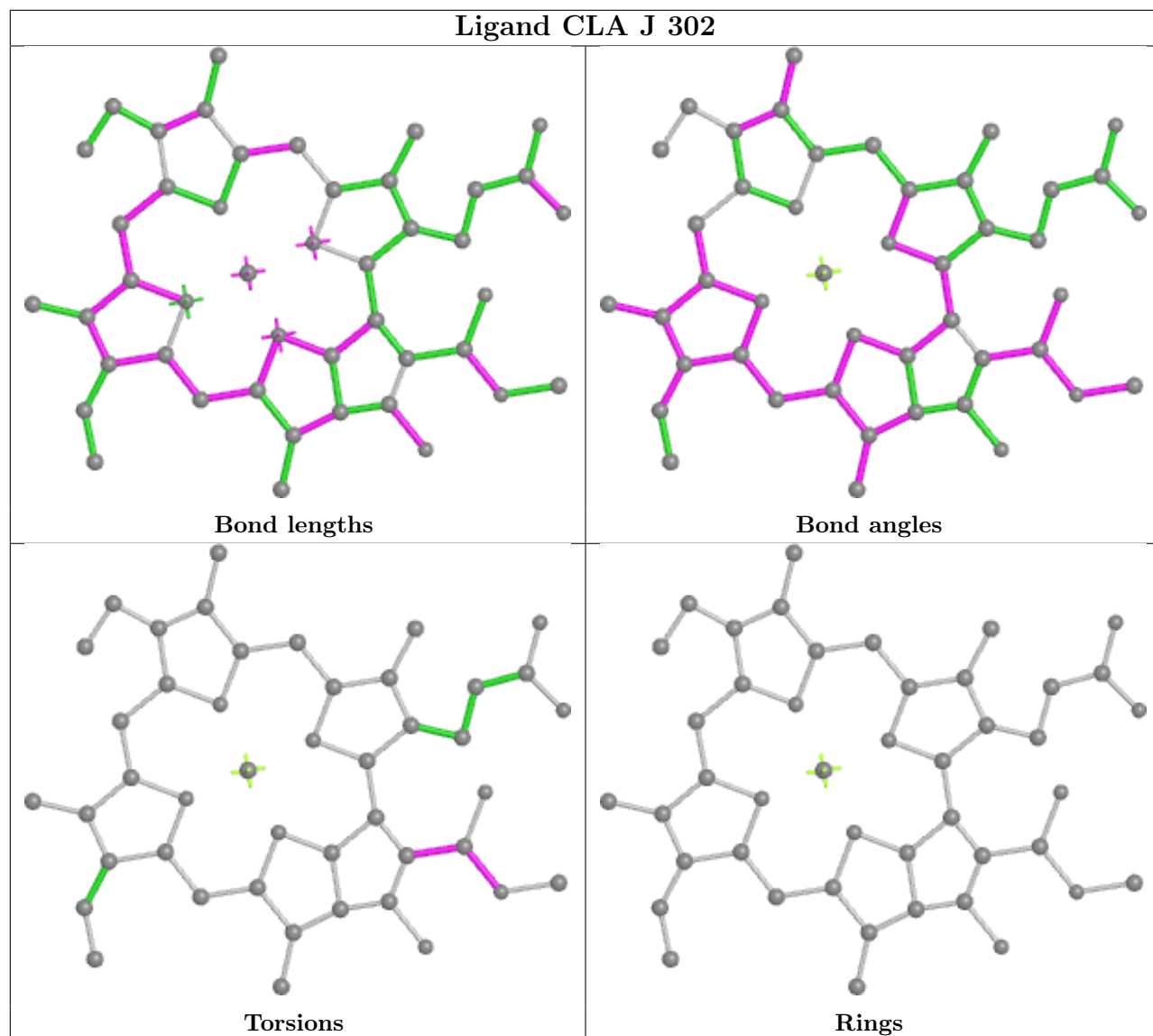


Torsions



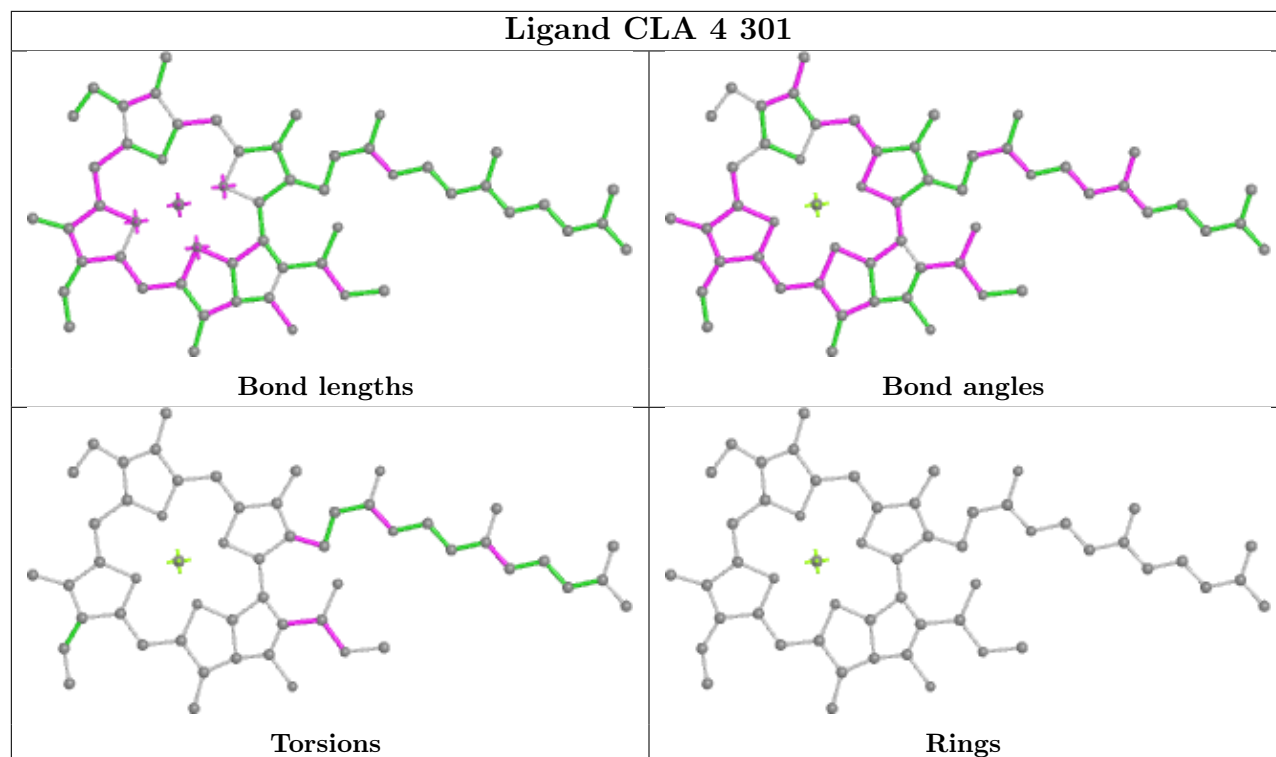
Rings

## Ligand CLA J 302

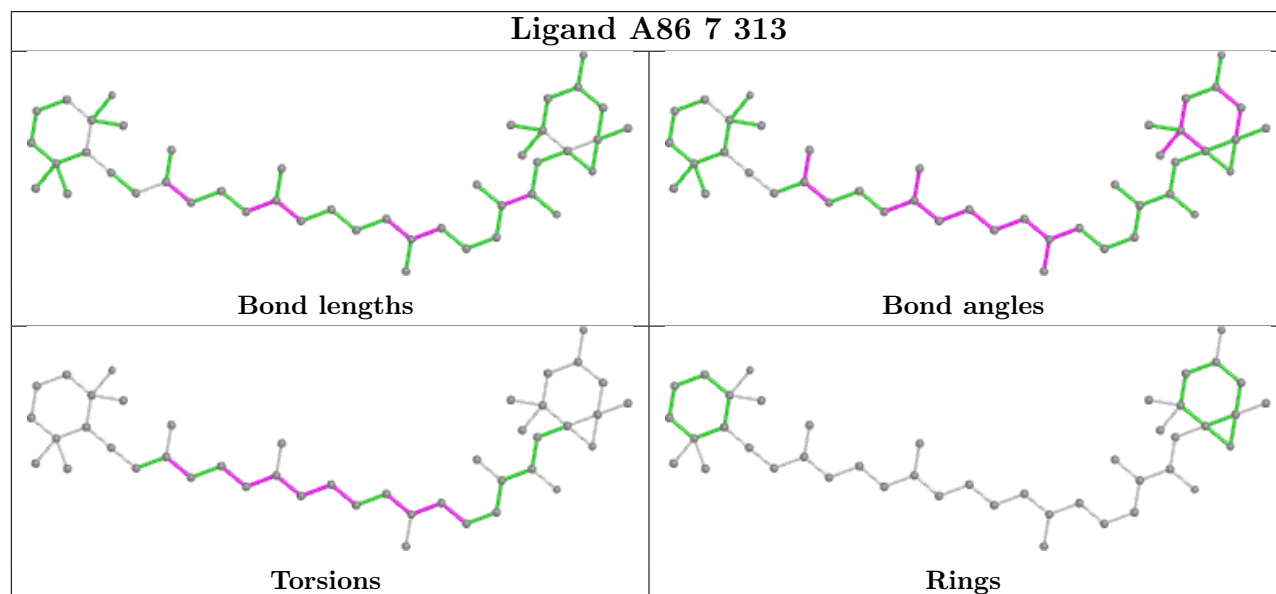


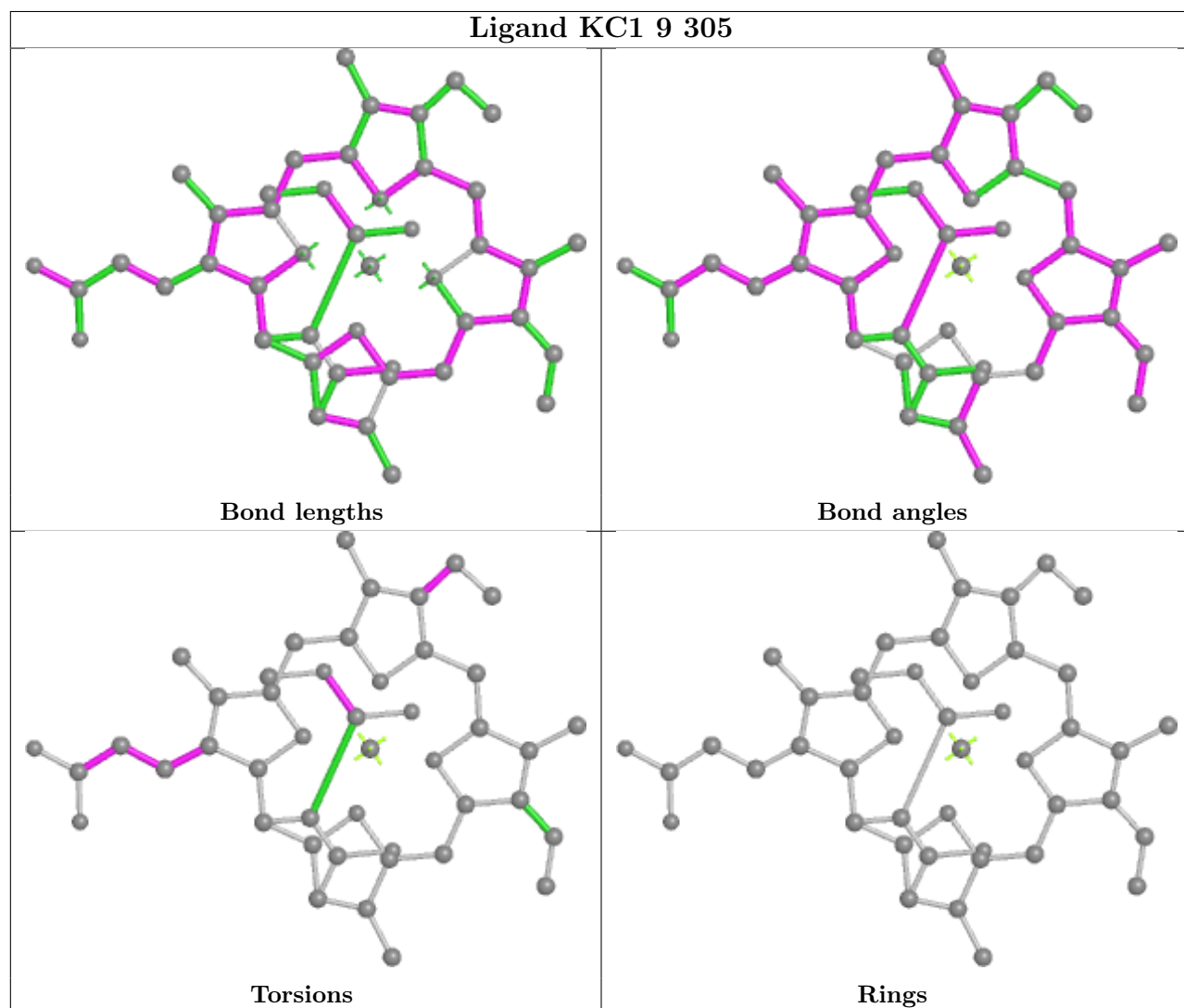
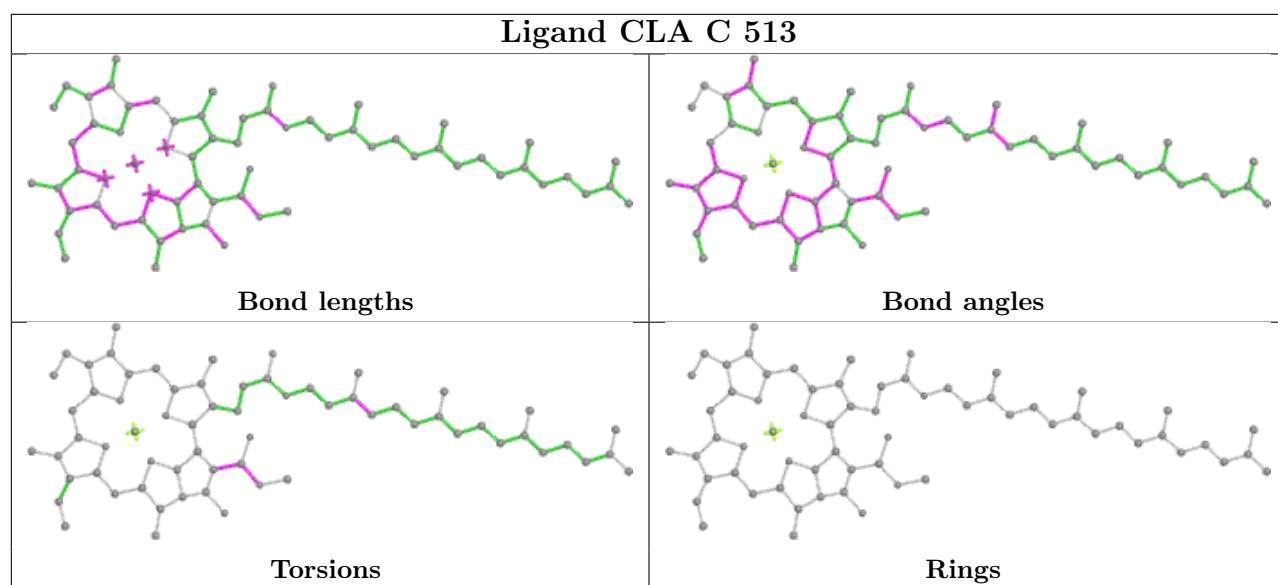


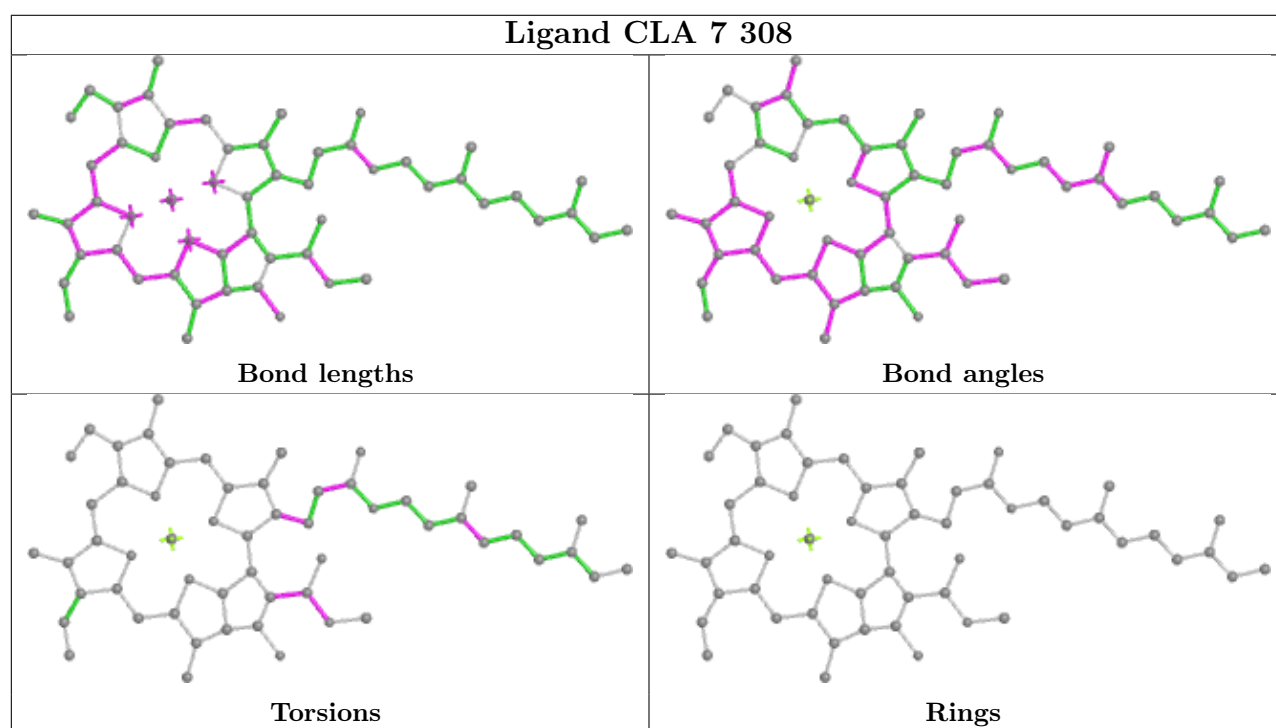
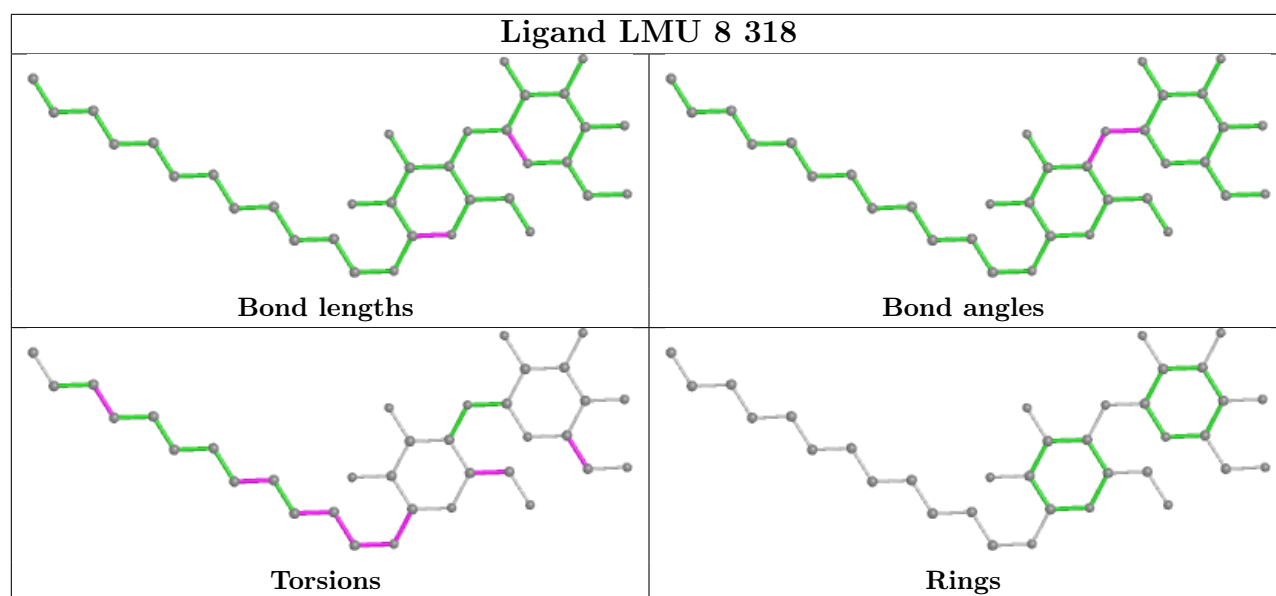
## Ligand CLA 4 301



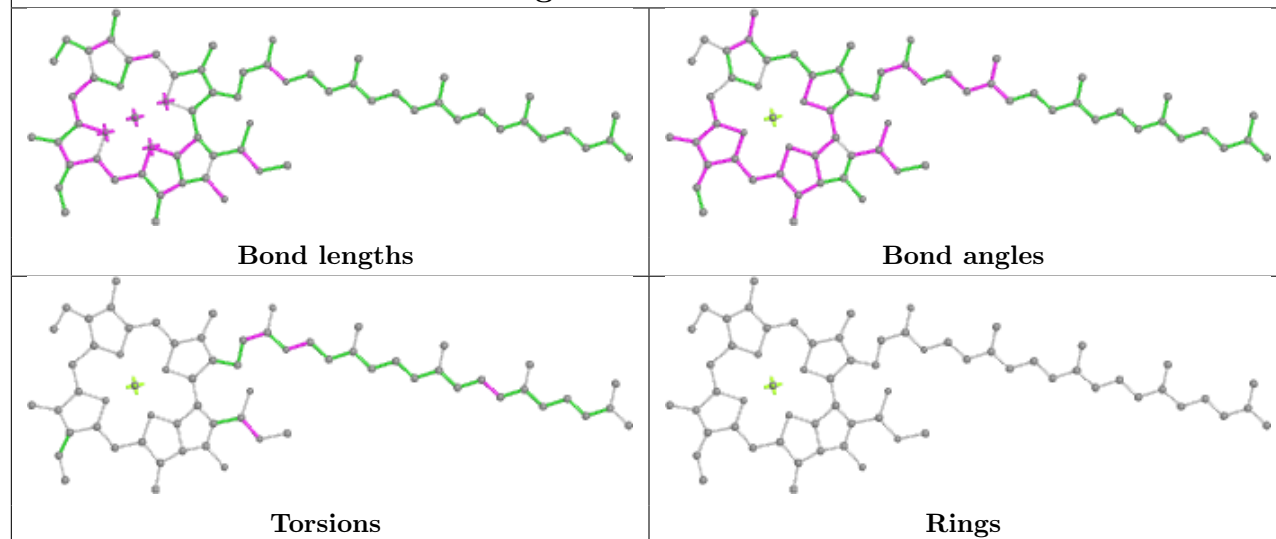
## Ligand A86 7 313



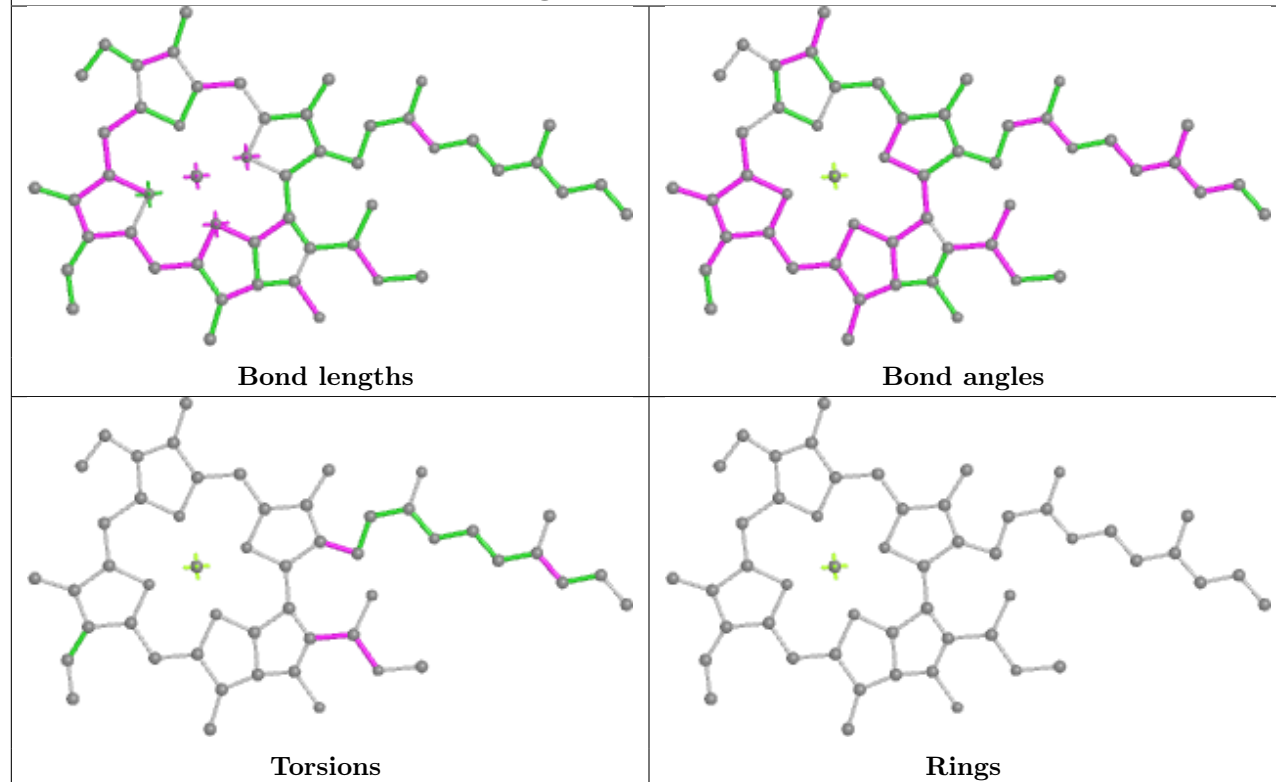




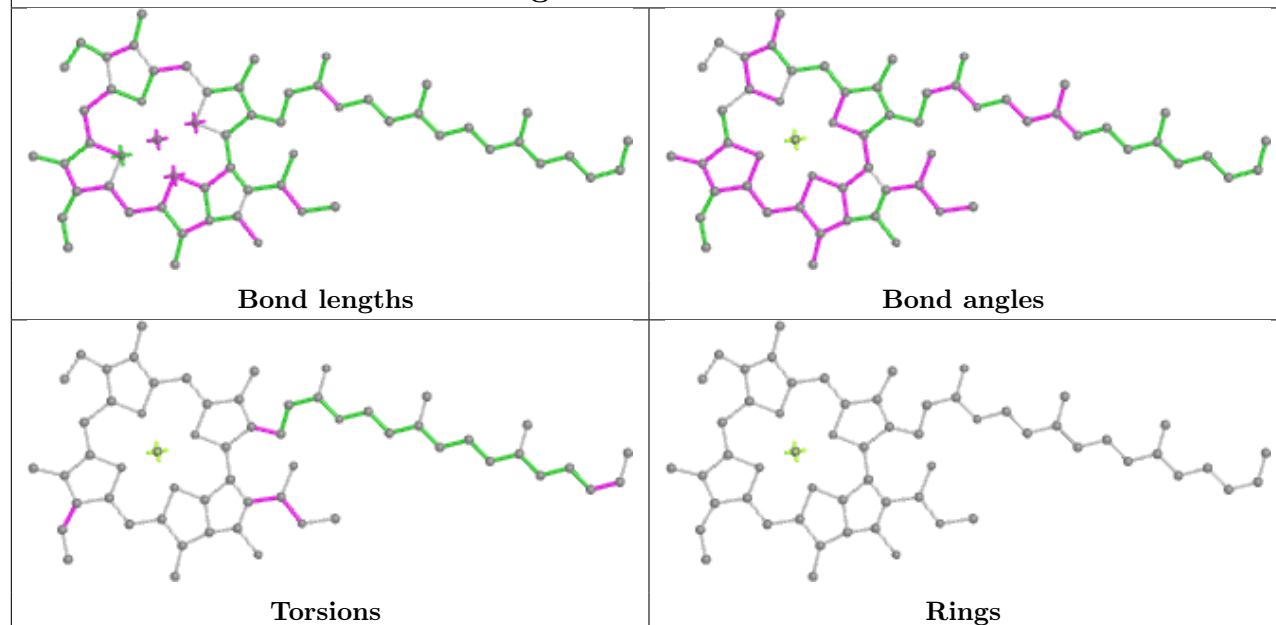
## Ligand CLA b 614



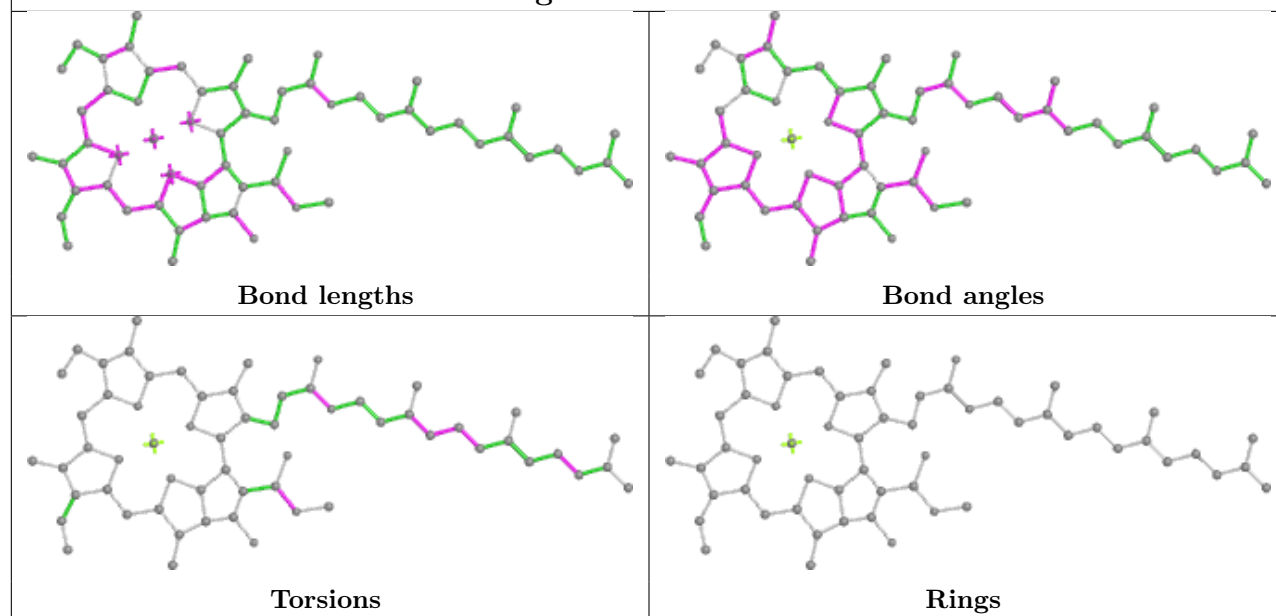
## Ligand CLA J 300

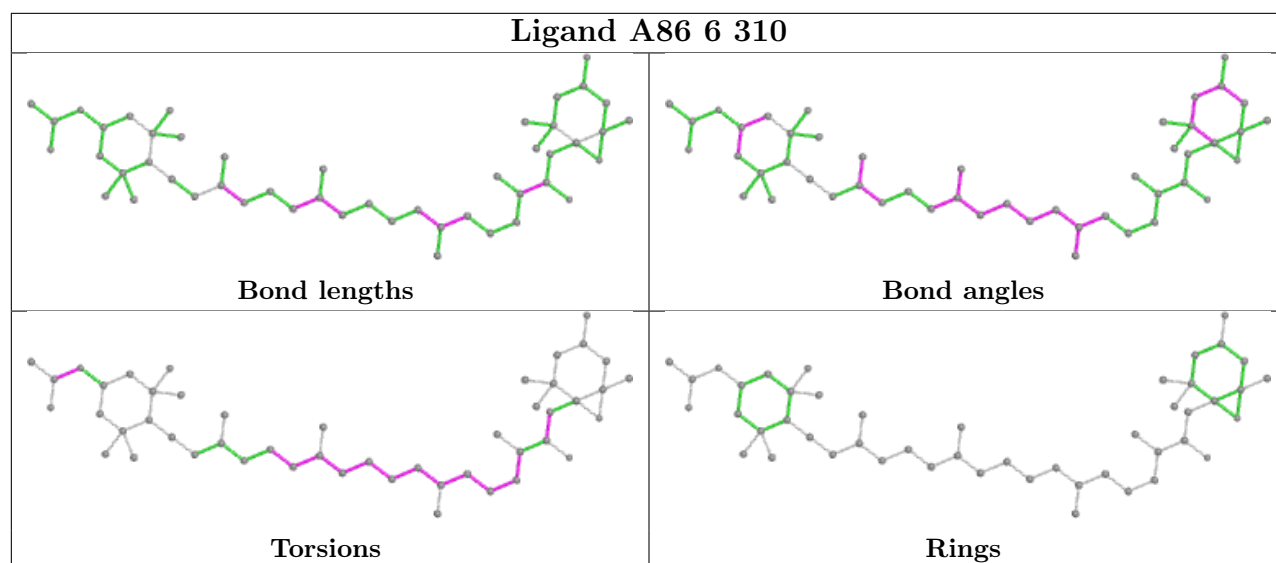
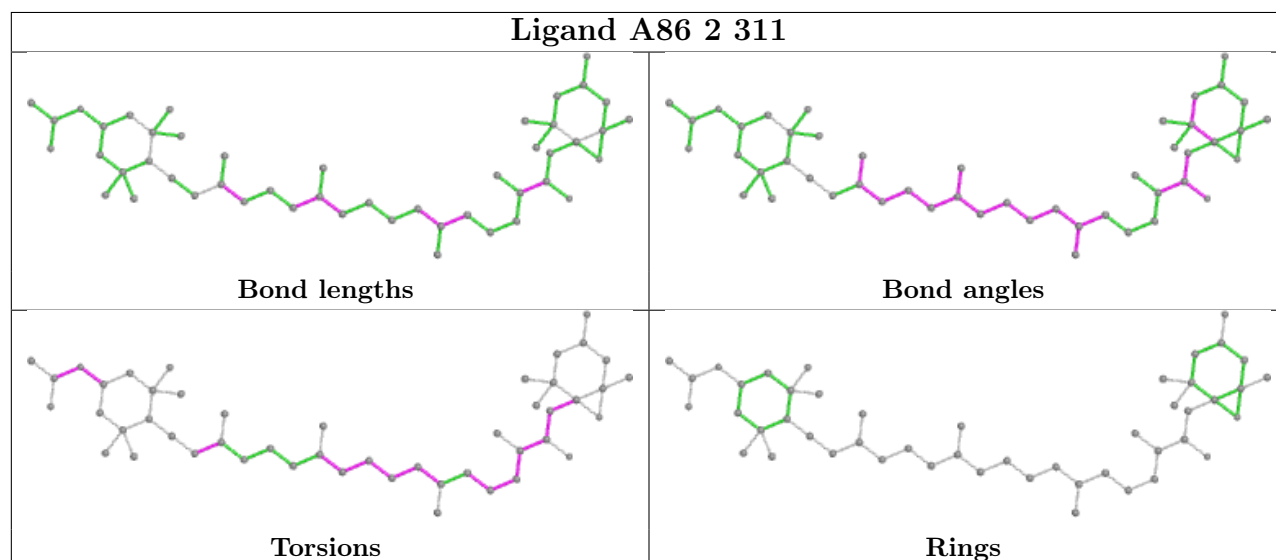
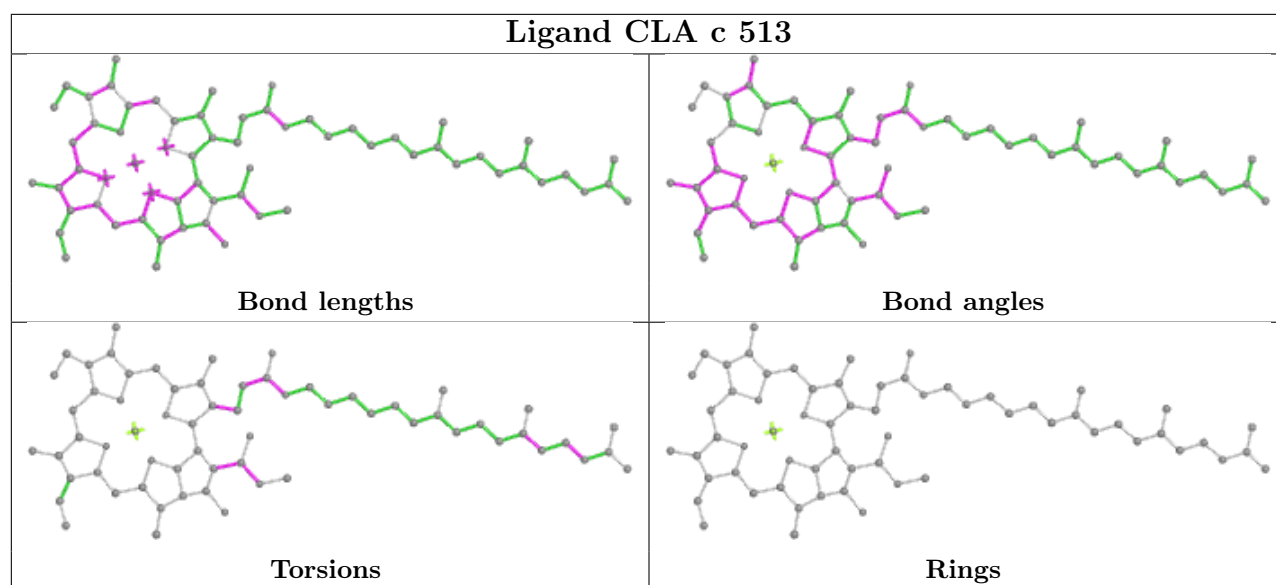


## Ligand CLA D 404

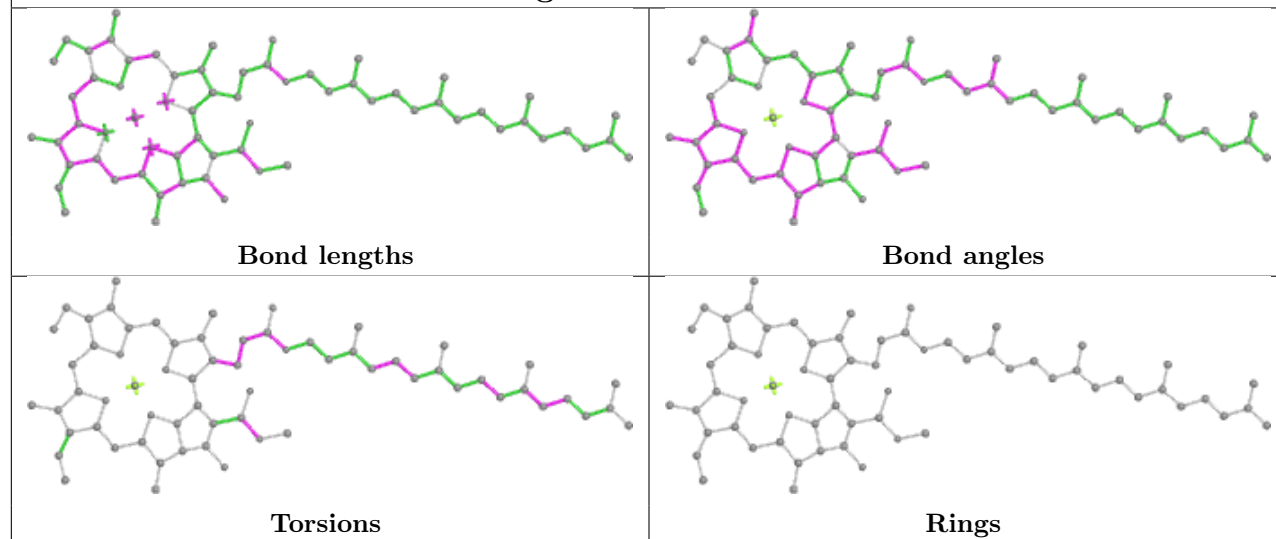


## Ligand CLA d 406

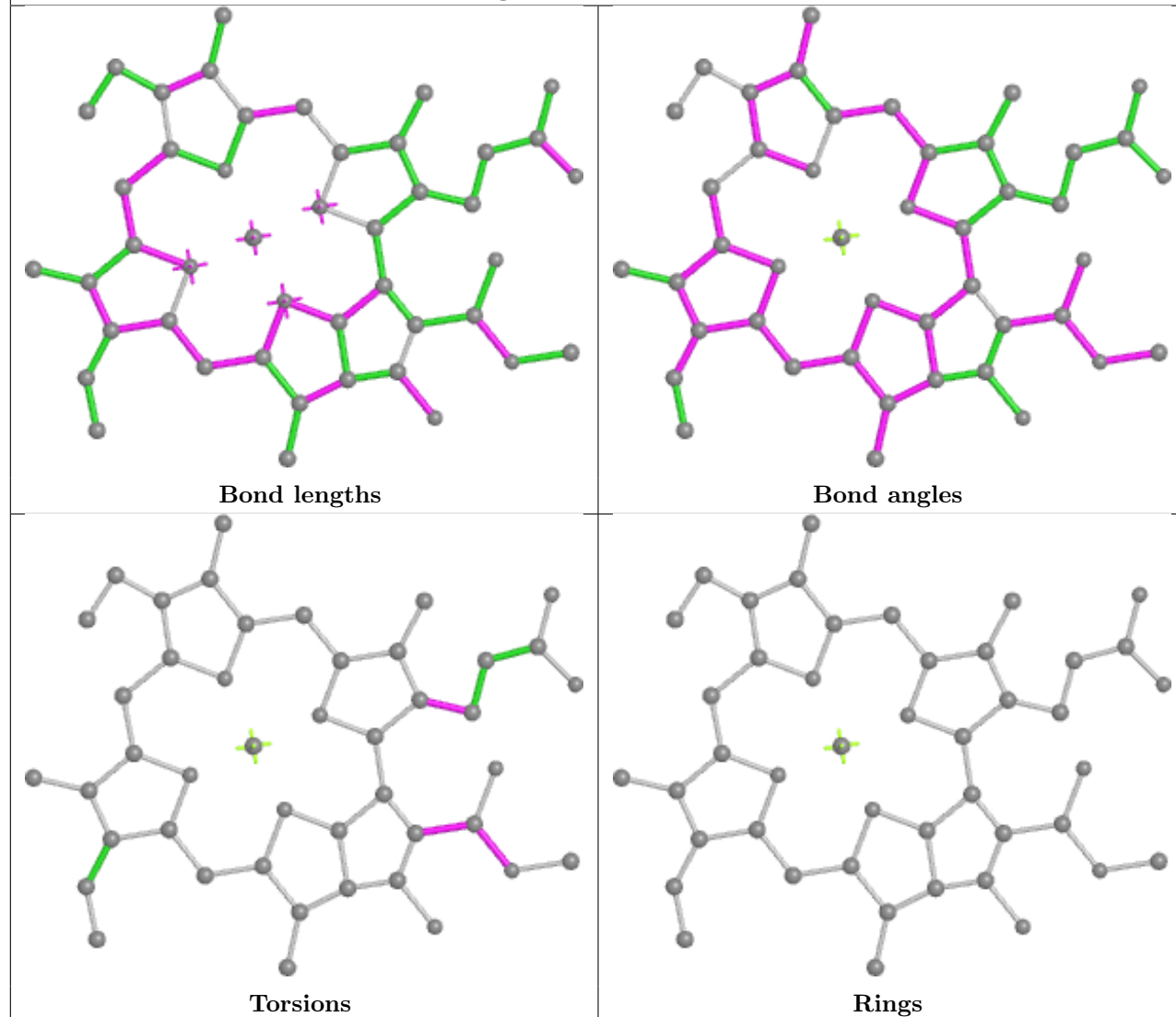


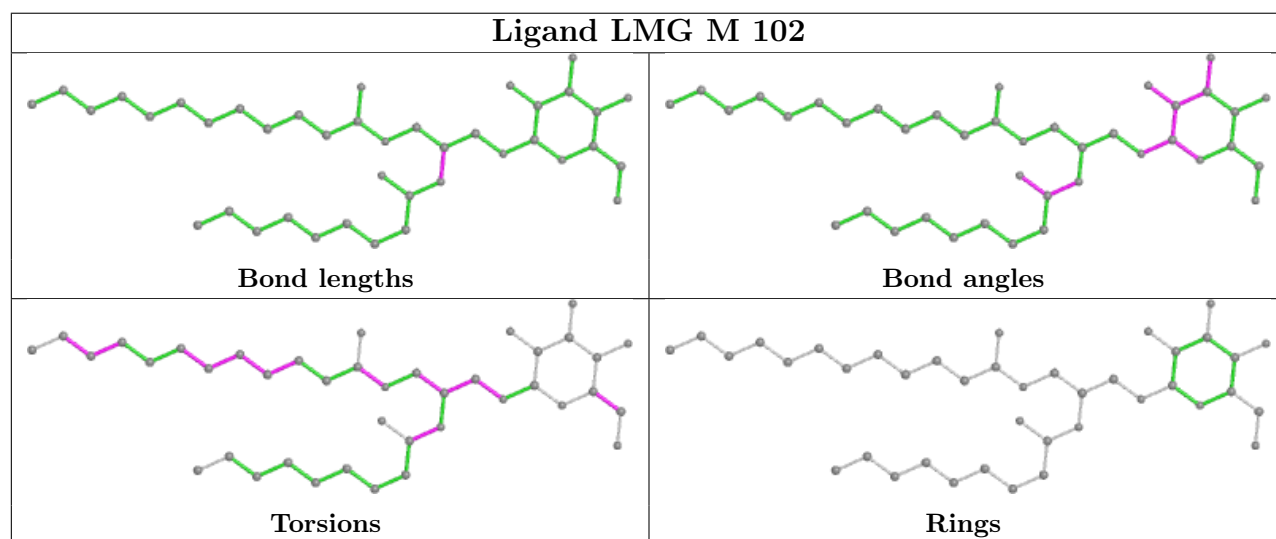
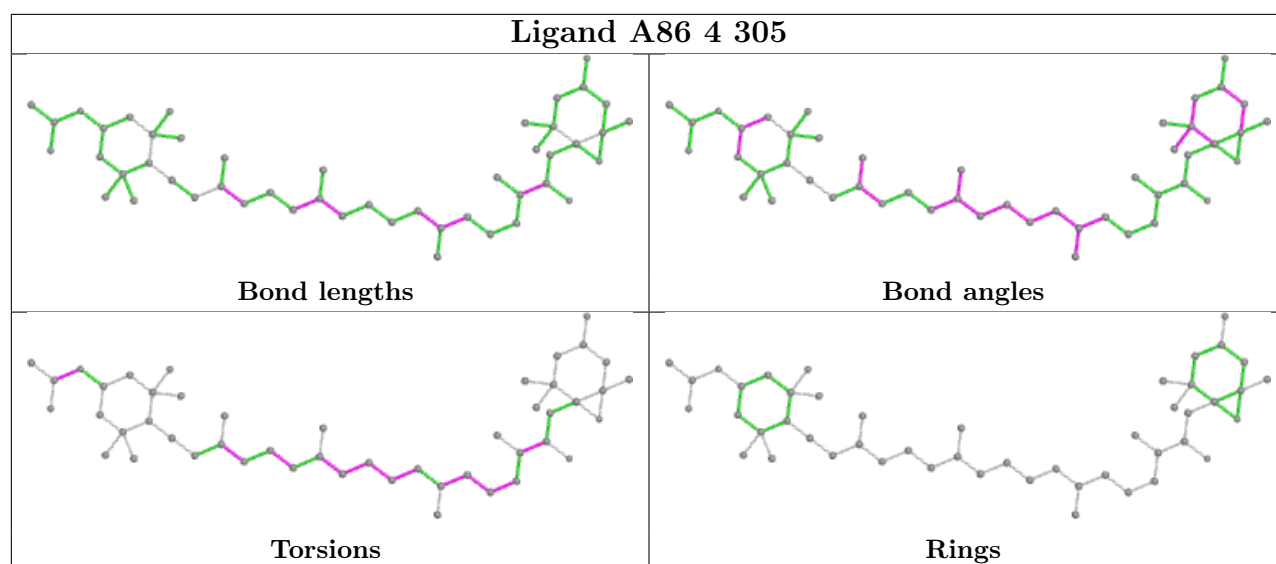


## Ligand CLA 7 303



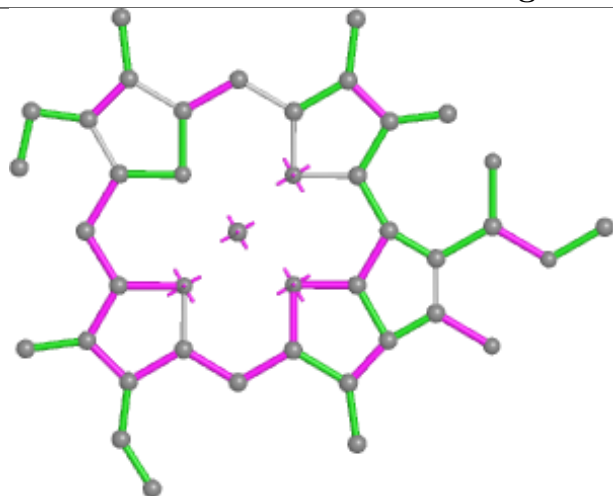
## Ligand CLA c 507



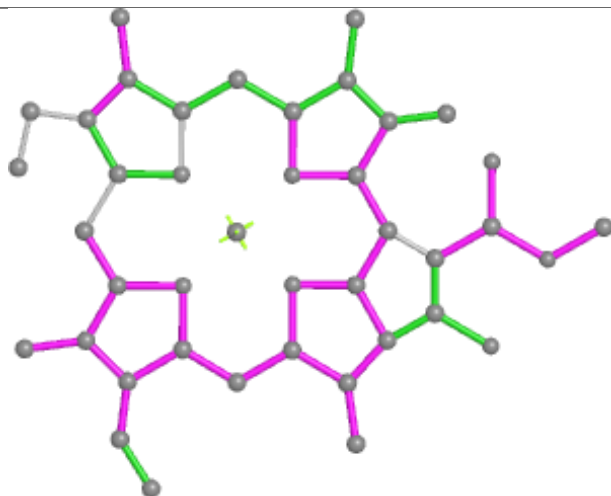




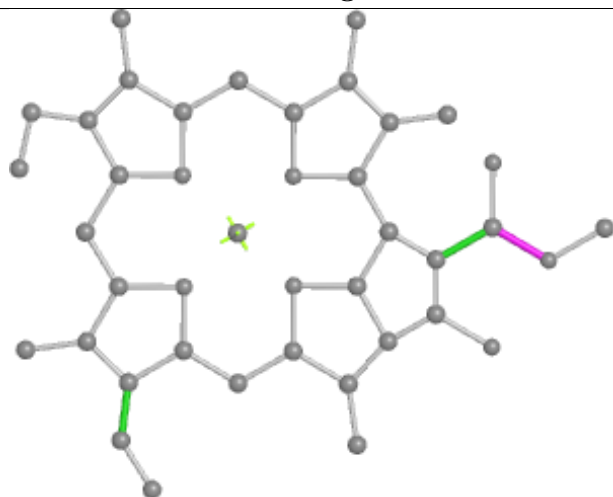
## Ligand CLA 1 306



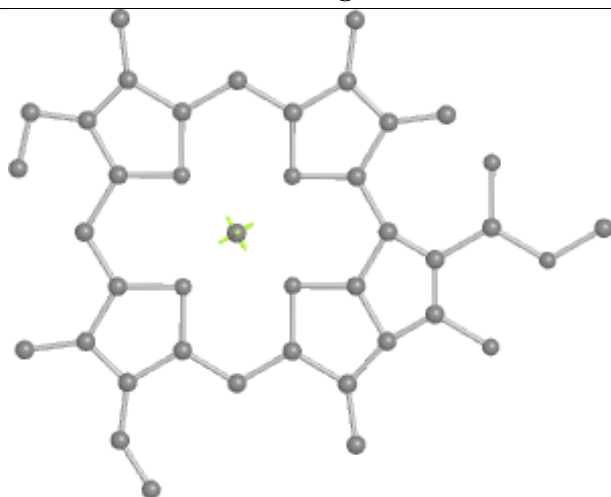
Bond lengths



Bond angles

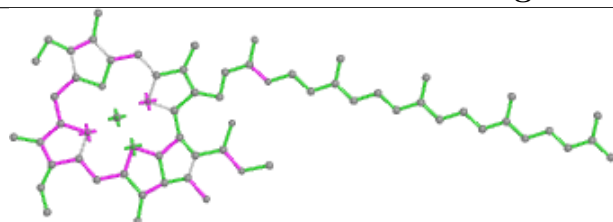


Torsions

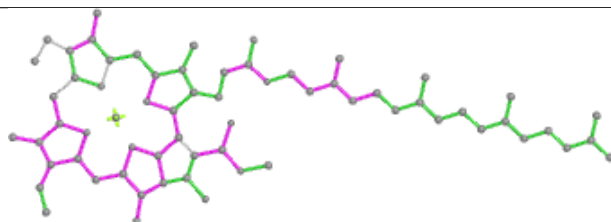


Rings

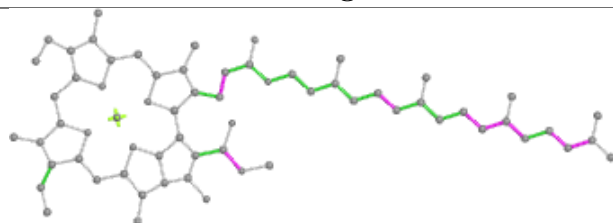
## Ligand CLA B 607



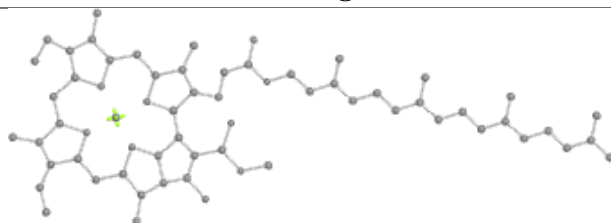
Bond lengths



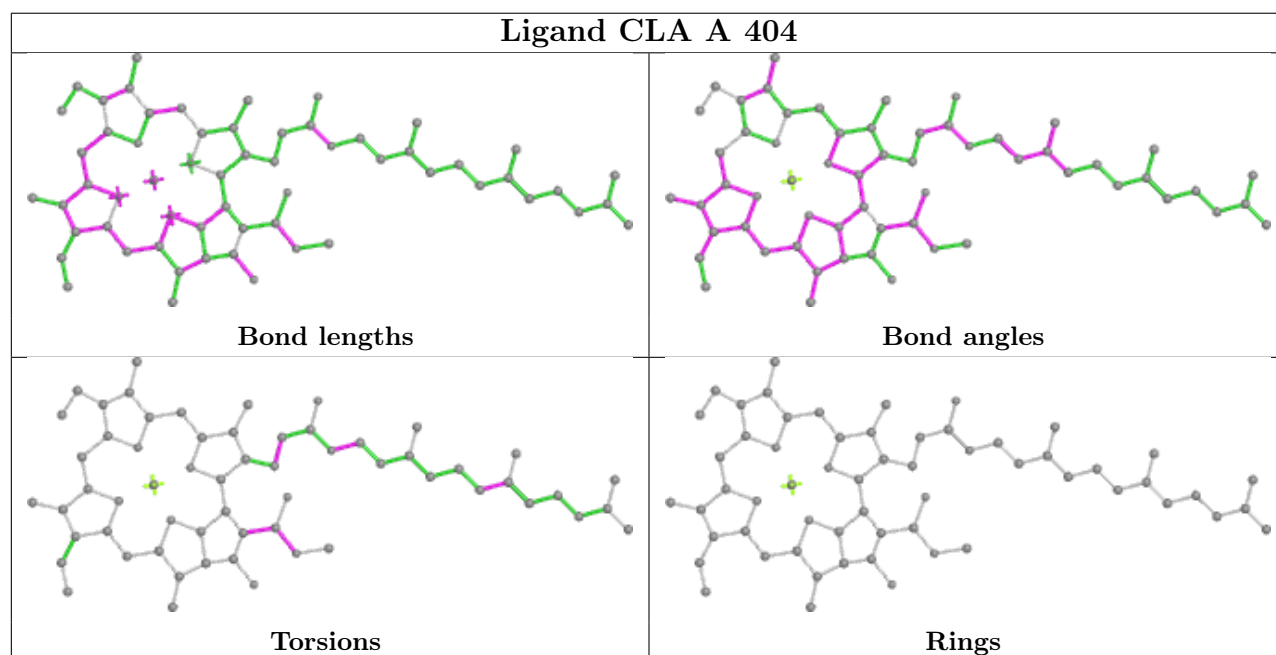
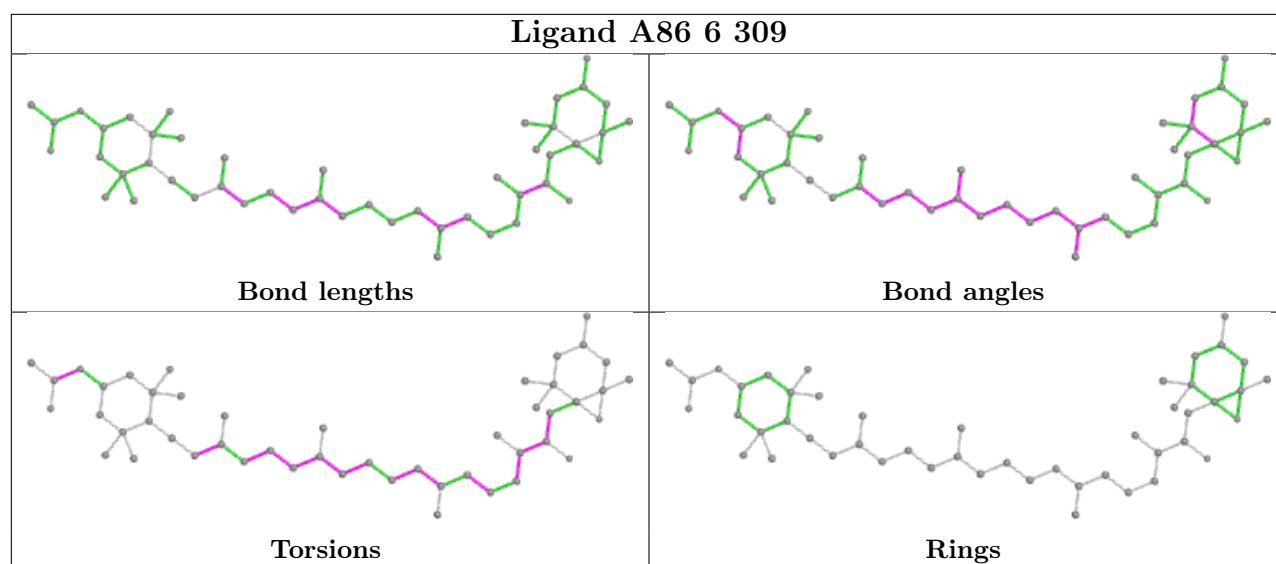
Bond angles

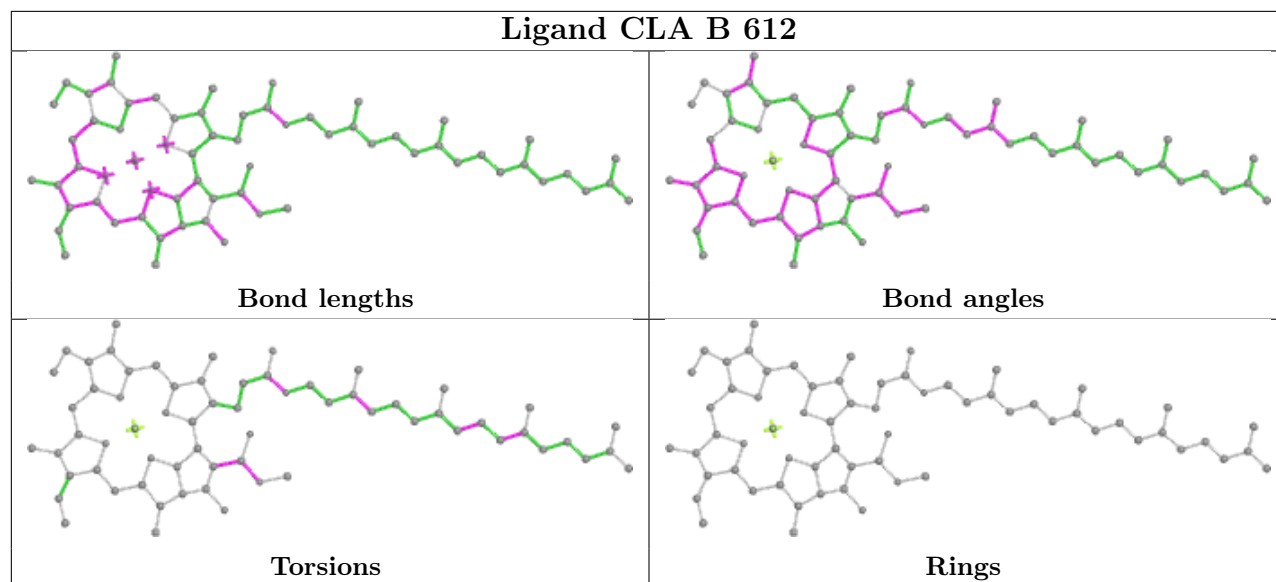
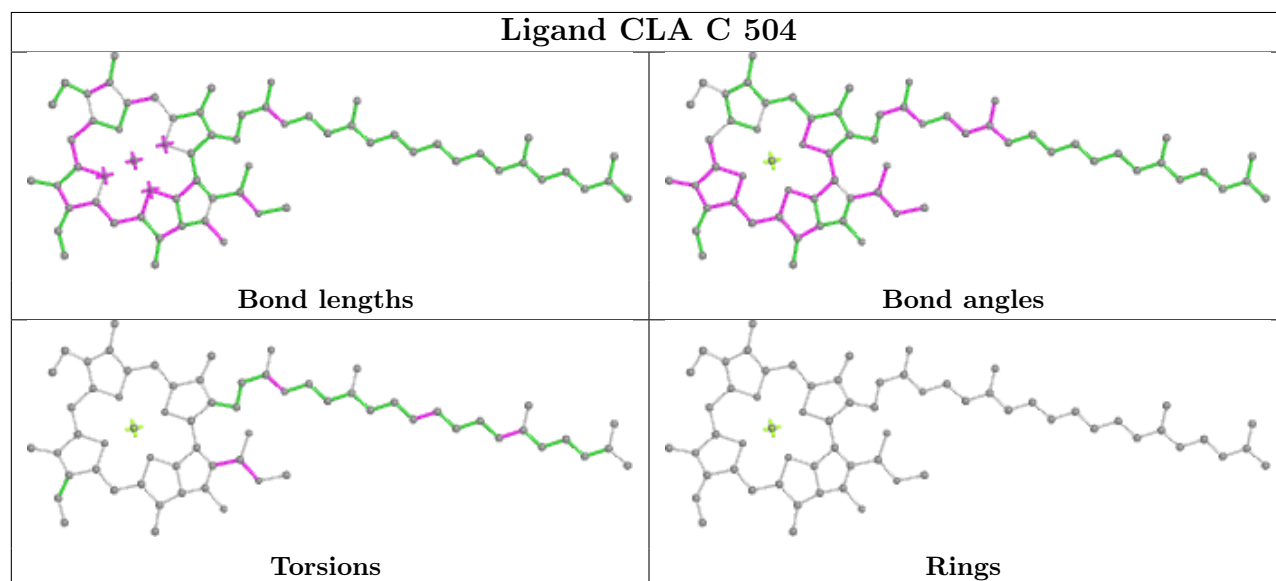


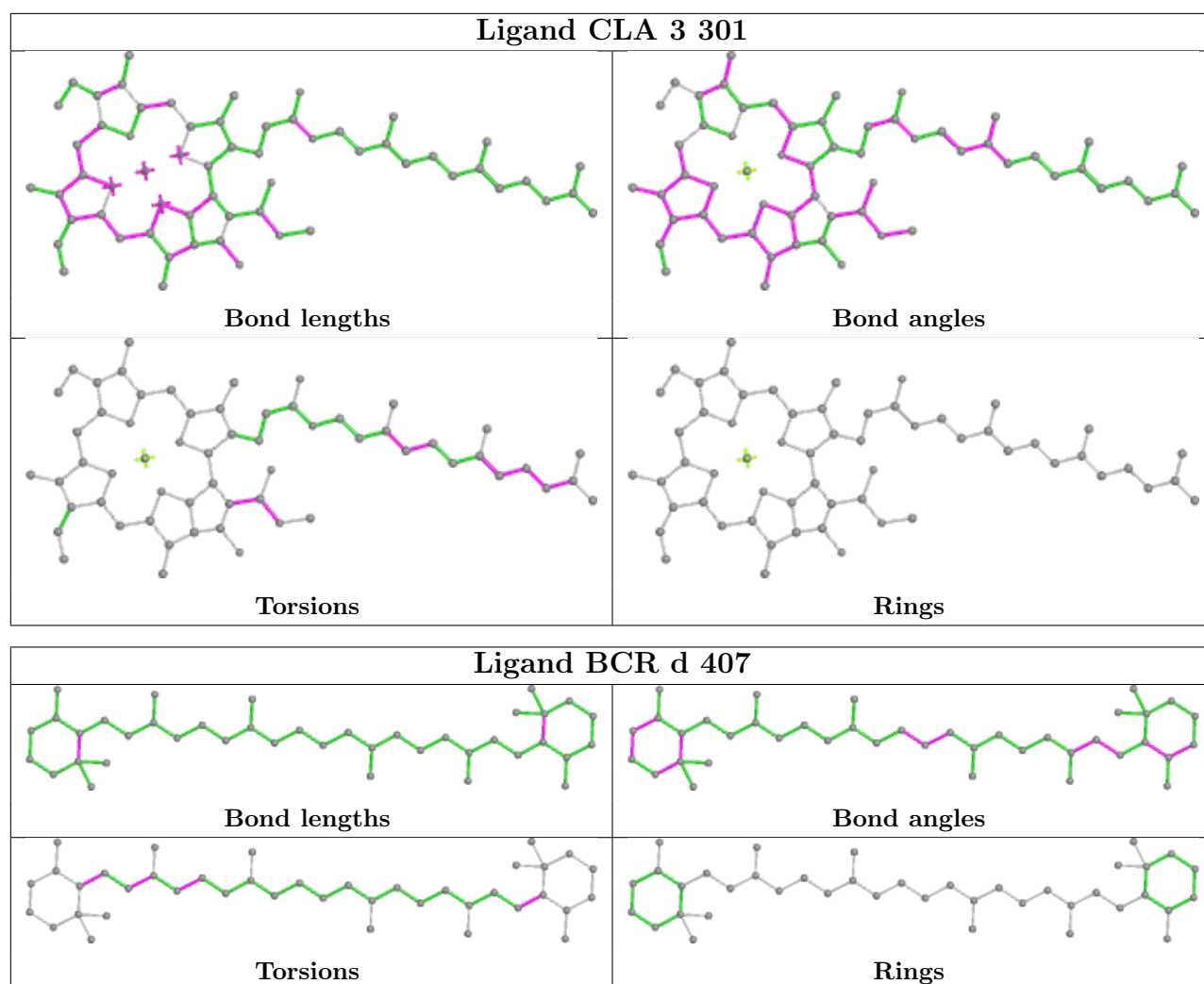
Torsions

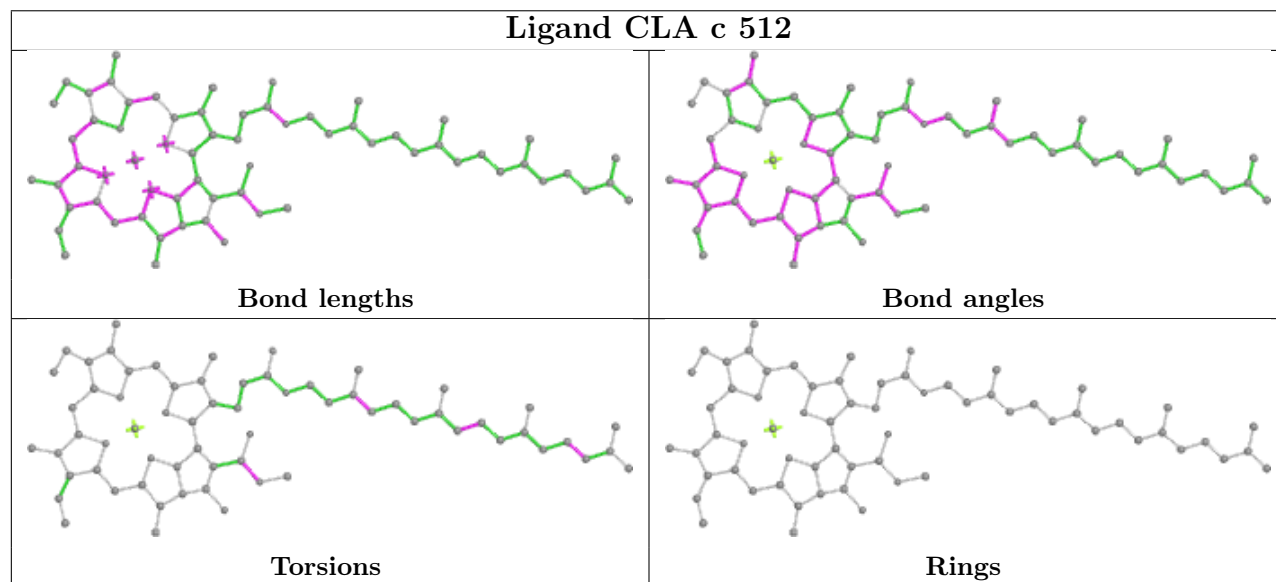
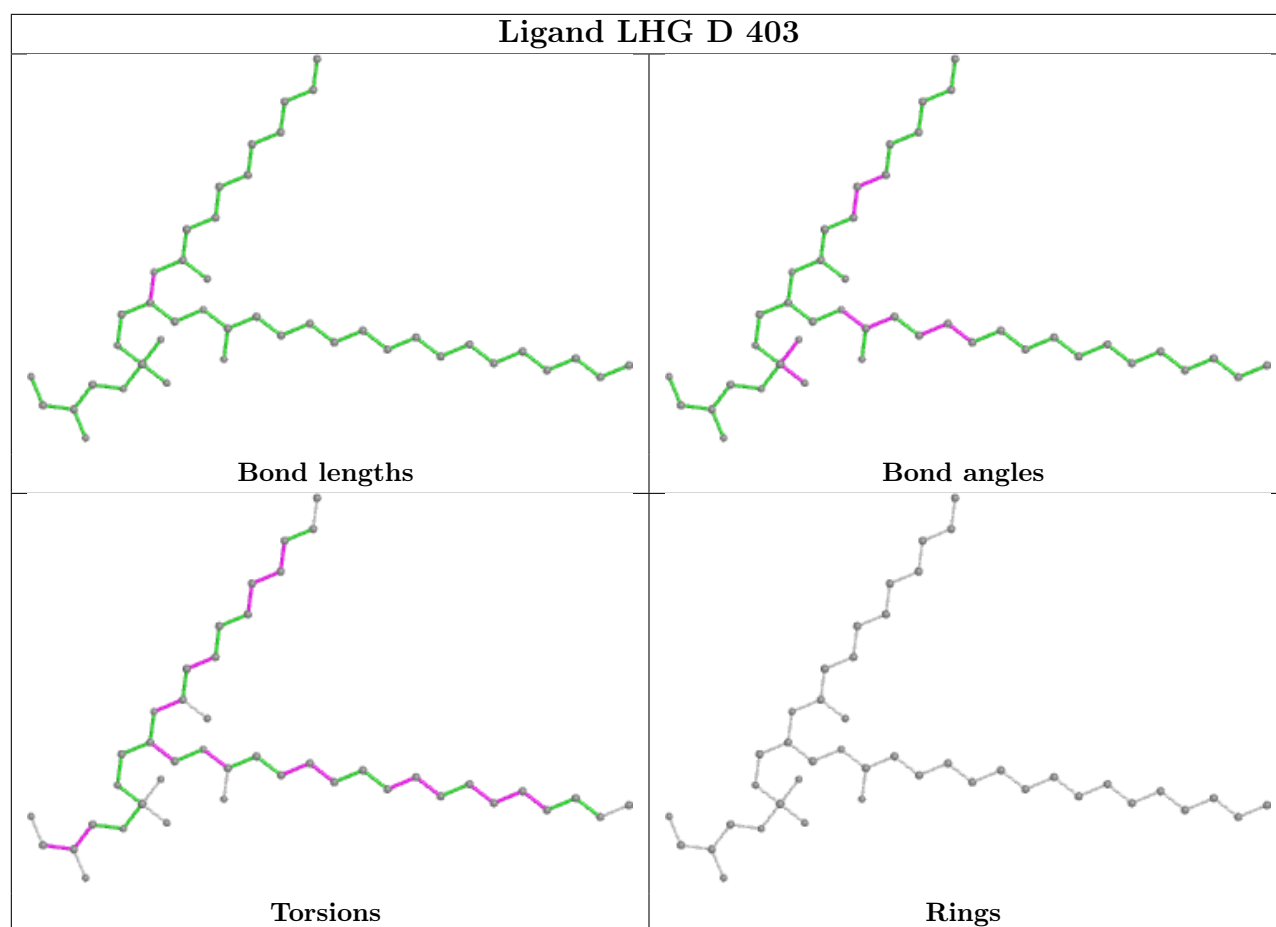


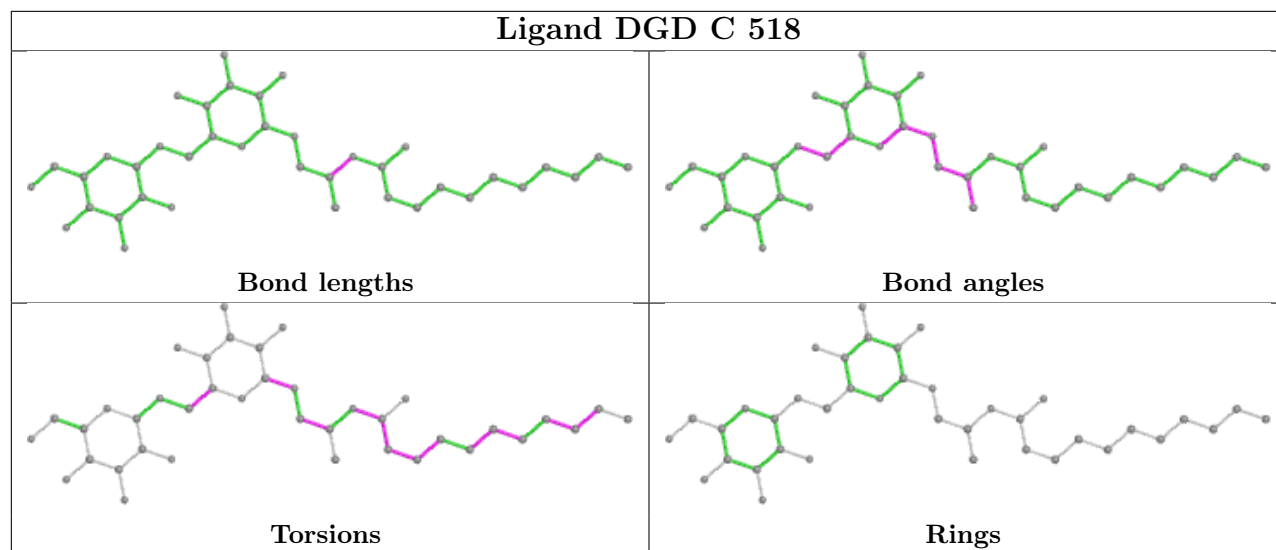
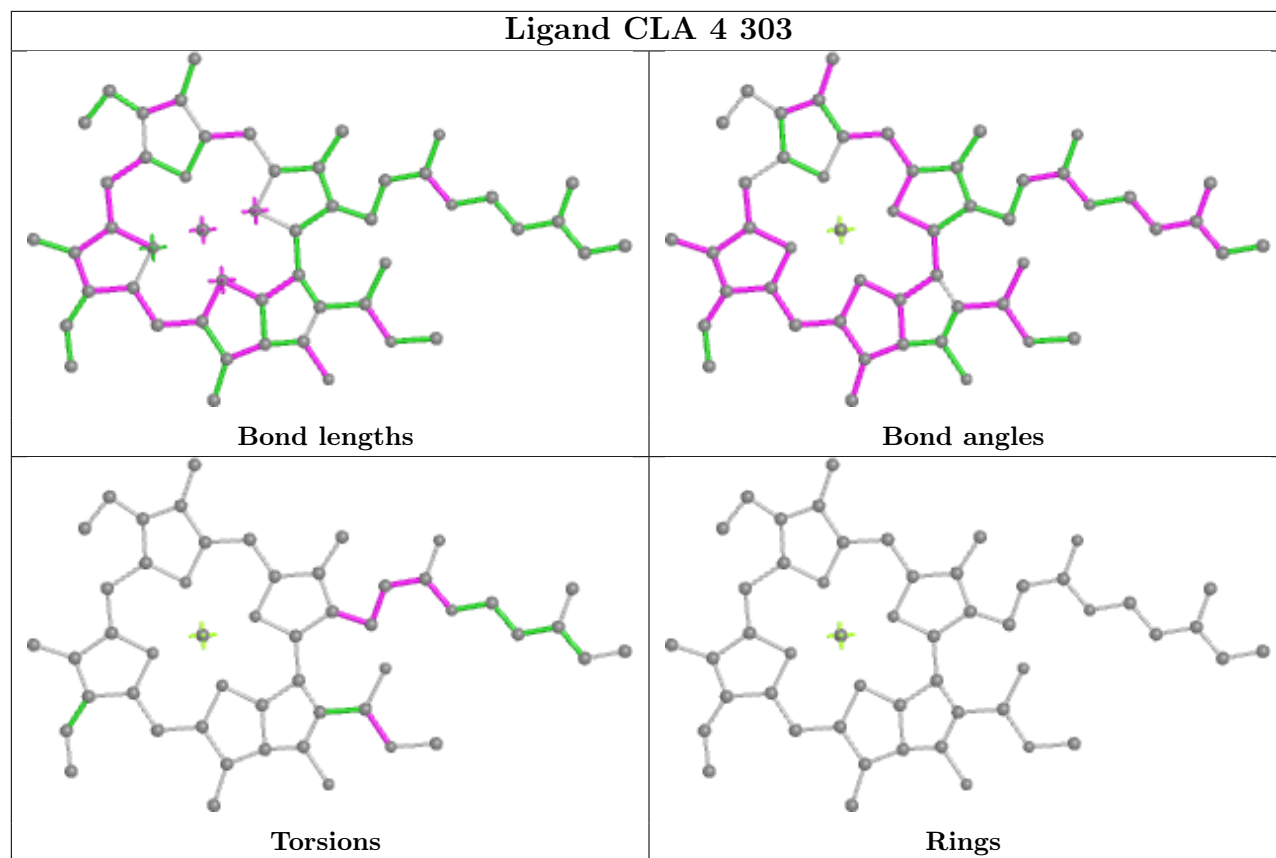
Rings



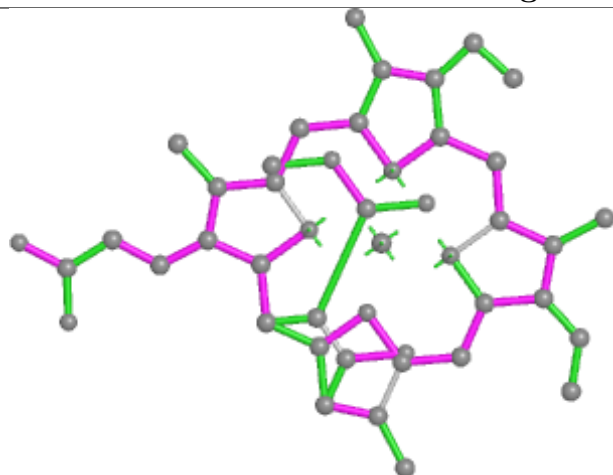
**Ligand CLA B 612****Ligand CLA C 504**



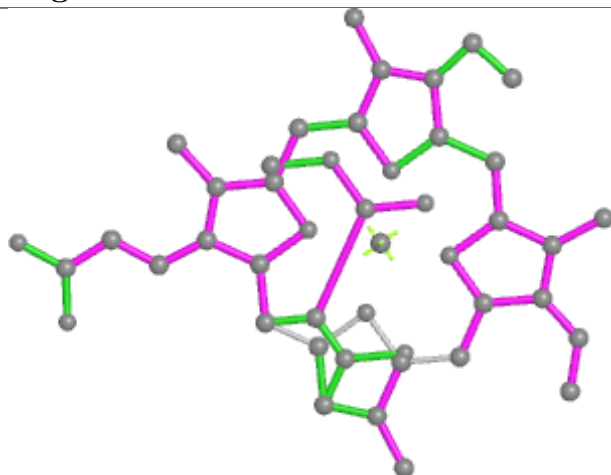




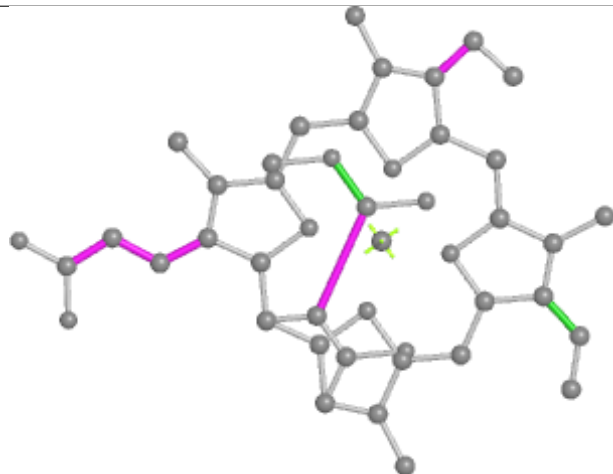
## Ligand KC1 g 314



Bond lengths



Bond angles

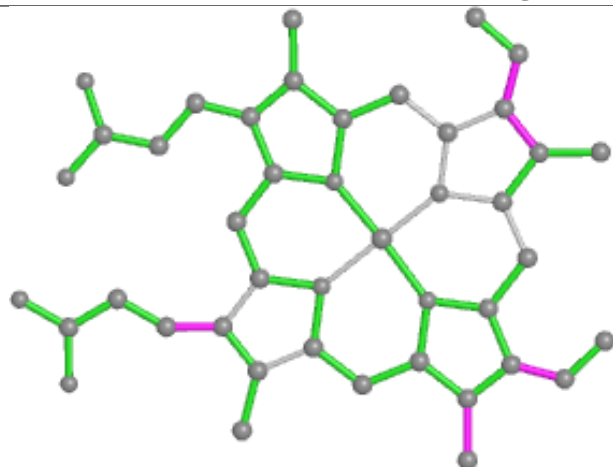


Torsions

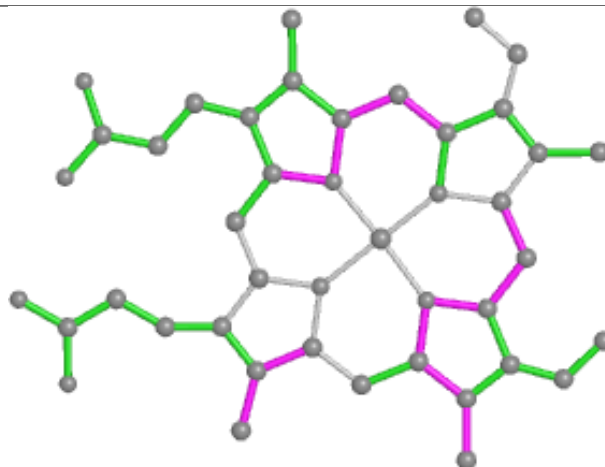


Rings

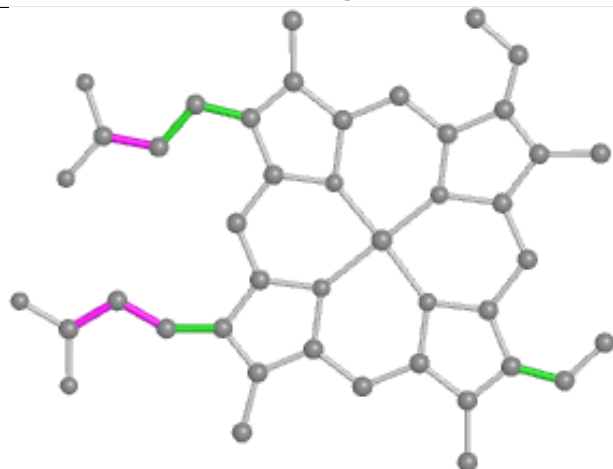
## Ligand HEM f 101



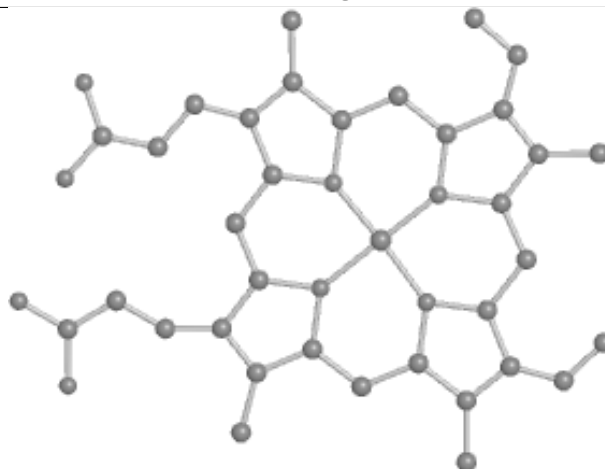
Bond lengths



Bond angles

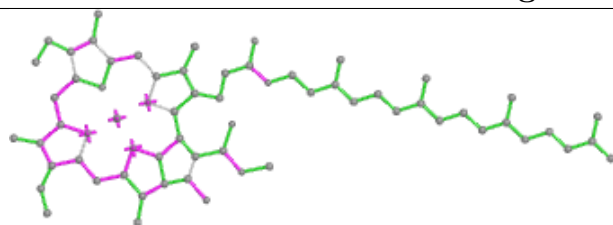


Torsions

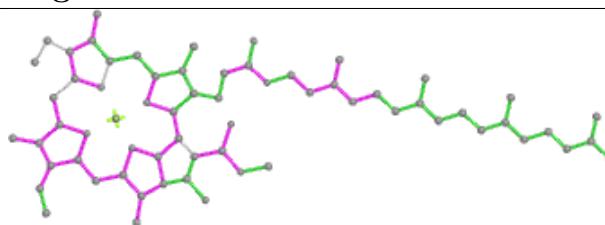


Rings

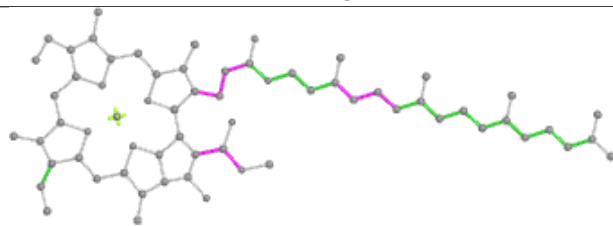
## Ligand CLA g 302



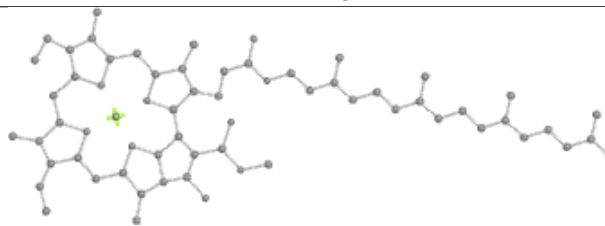
Bond lengths



Bond angles



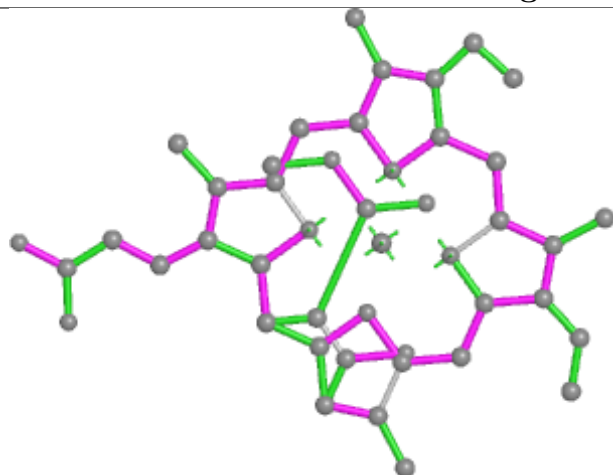
Torsions



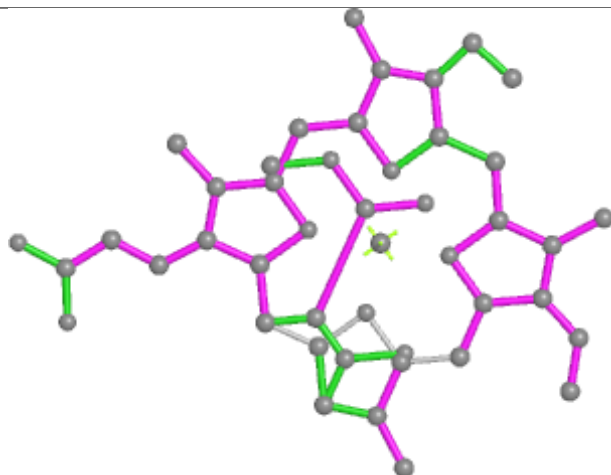
Rings



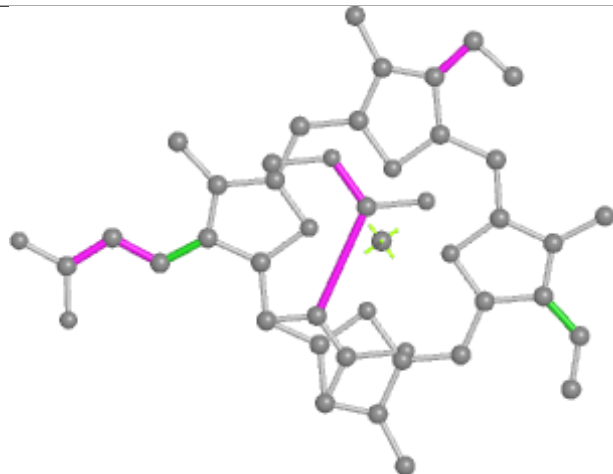
## Ligand KC1 4 307



Bond lengths



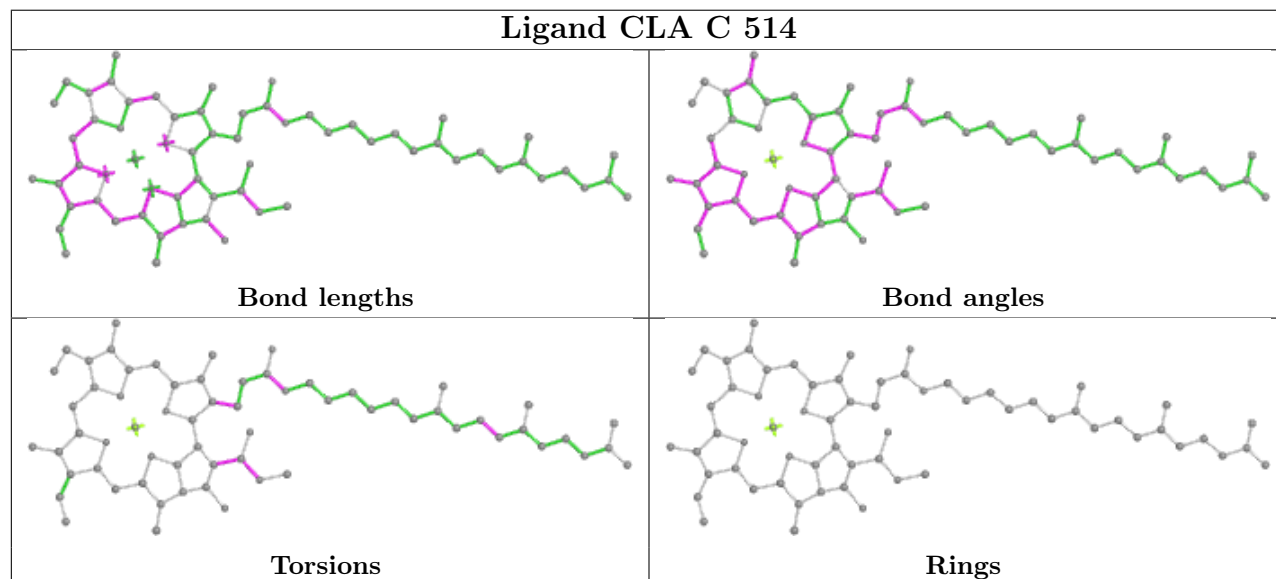
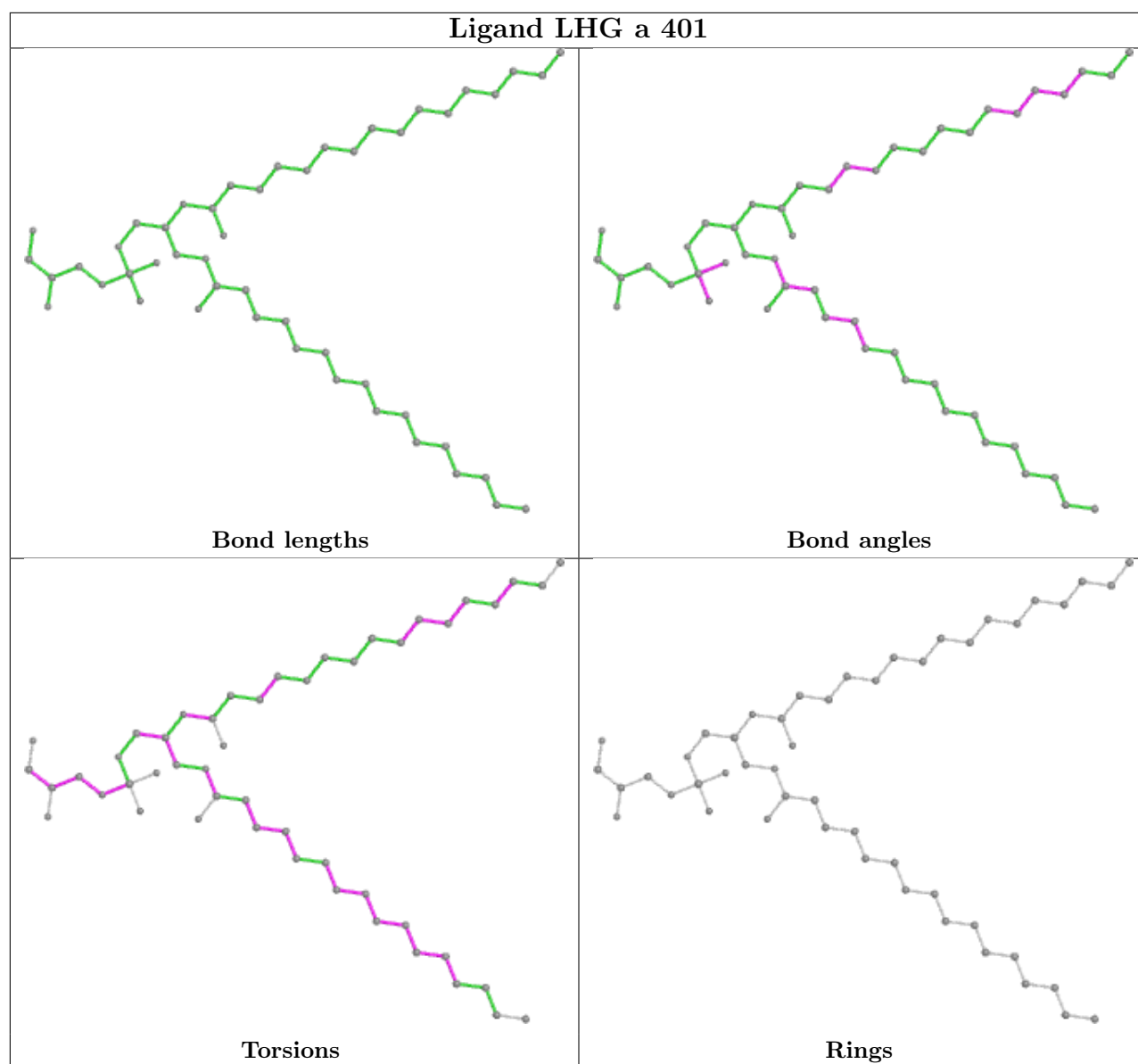
Bond angles



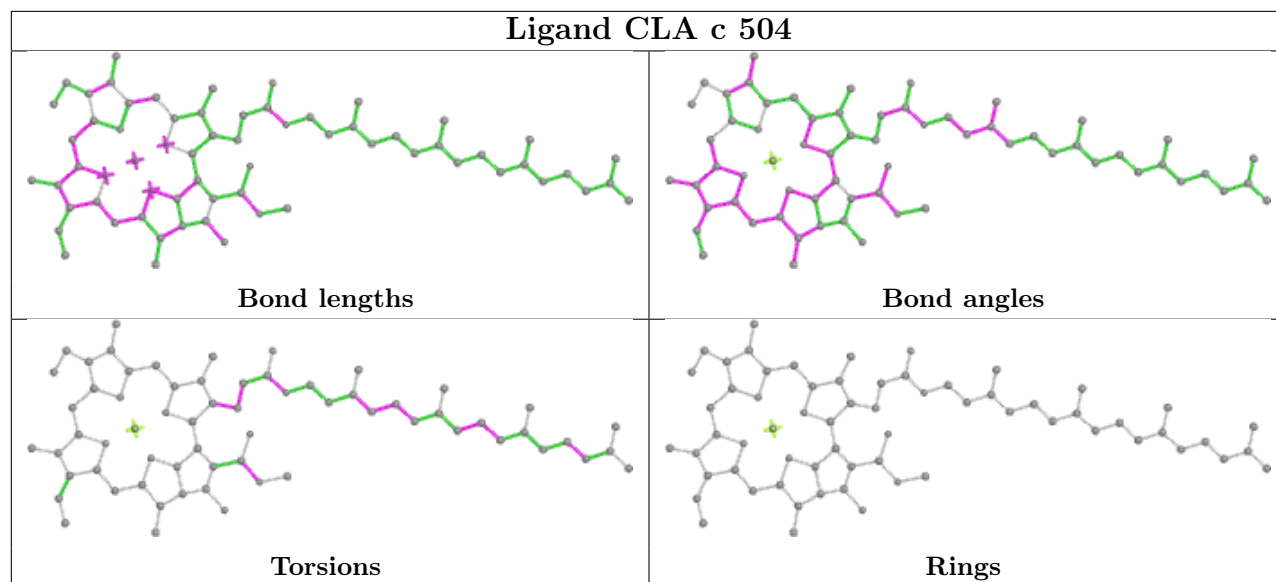
Torsions



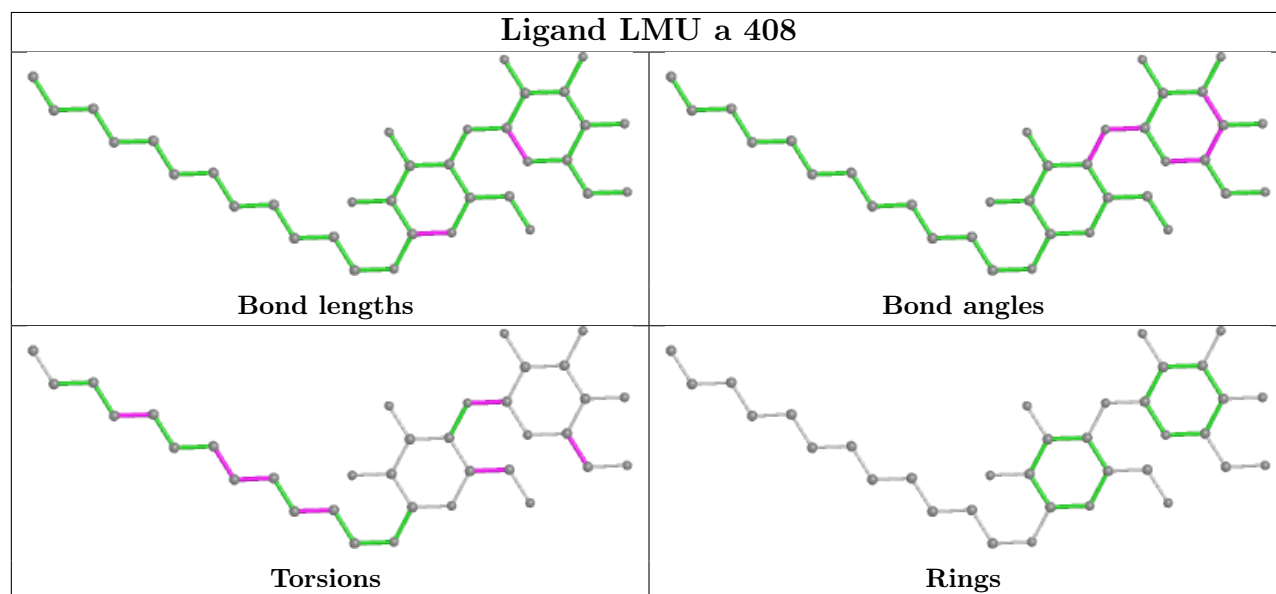
Rings



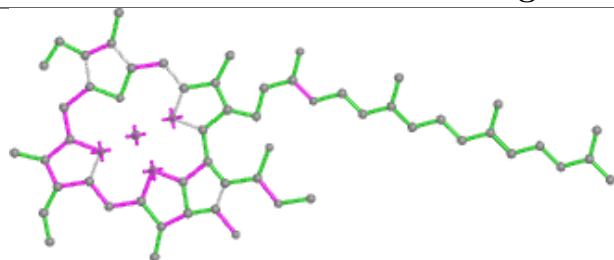
## Ligand CLA c 504



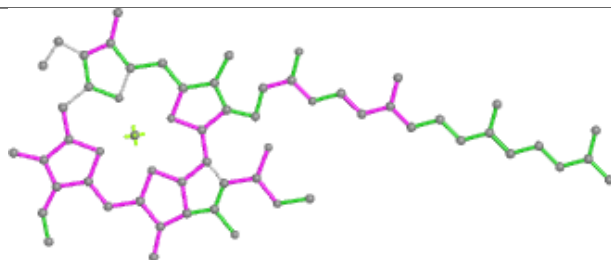
## Ligand LMU a 408



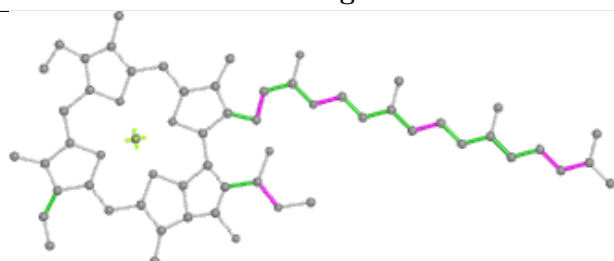
## Ligand CLA a 405



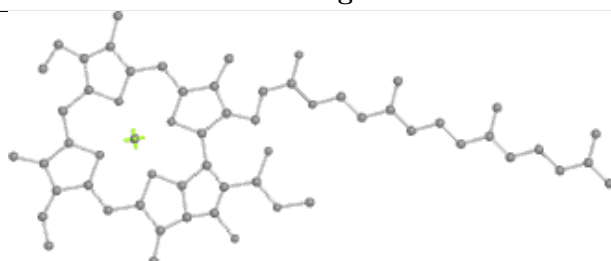
Bond lengths



Bond angles

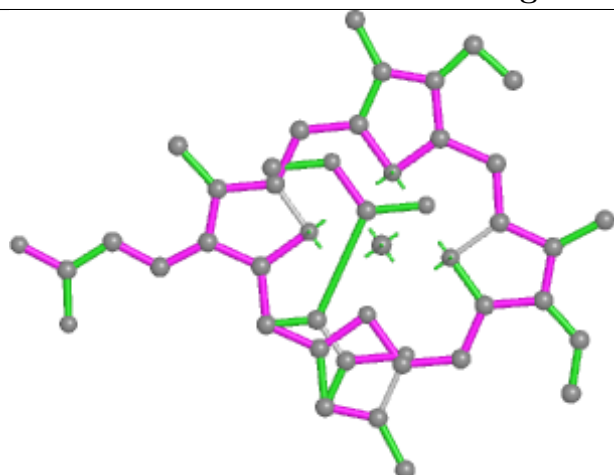


Torsions

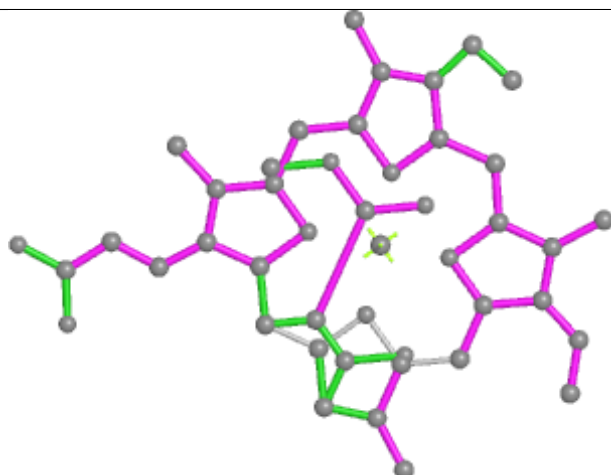


Rings

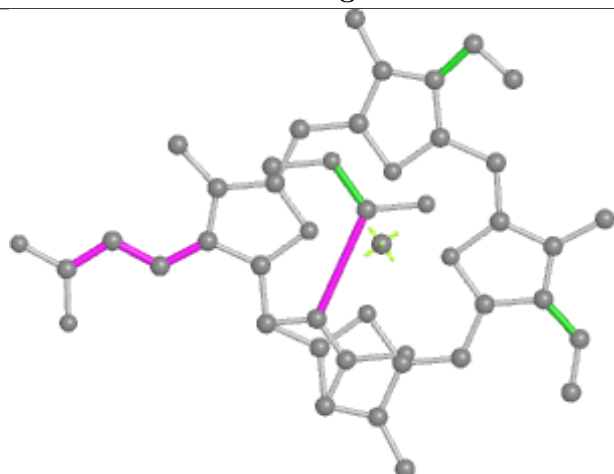
## Ligand KC1 4 308



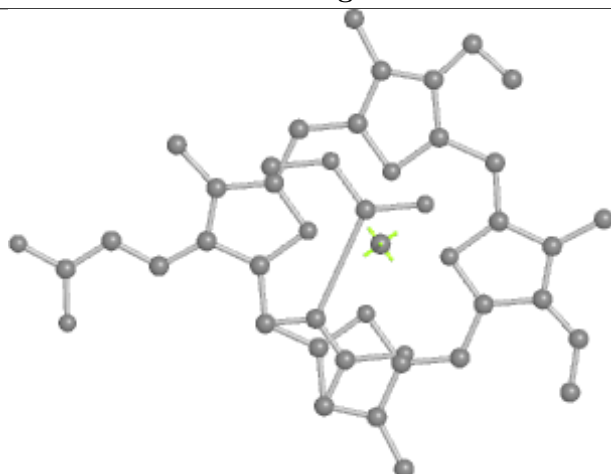
Bond lengths



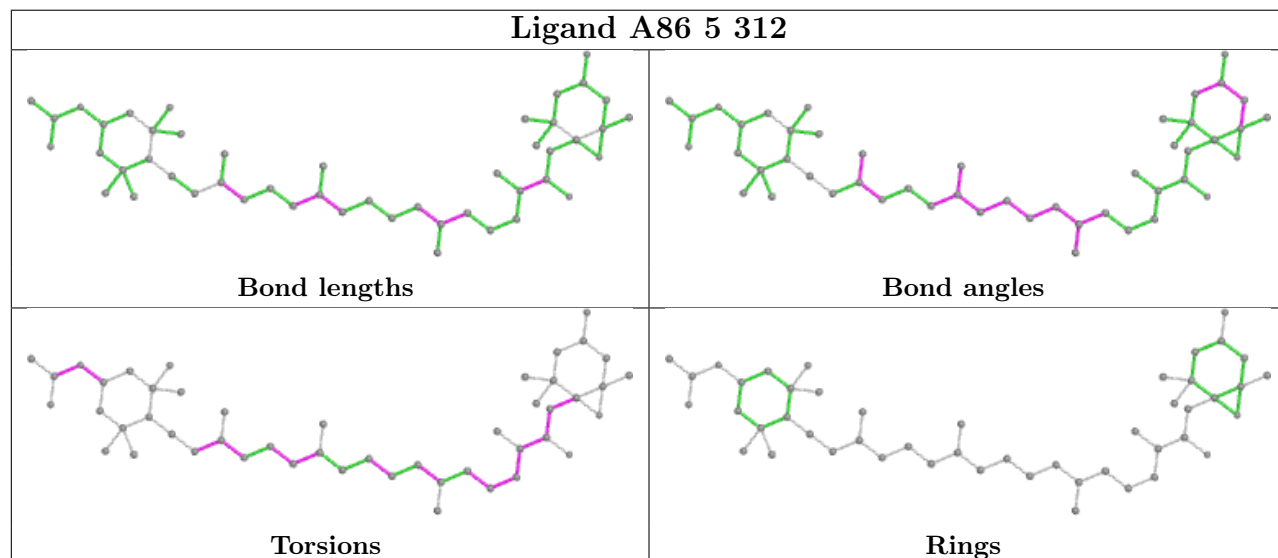
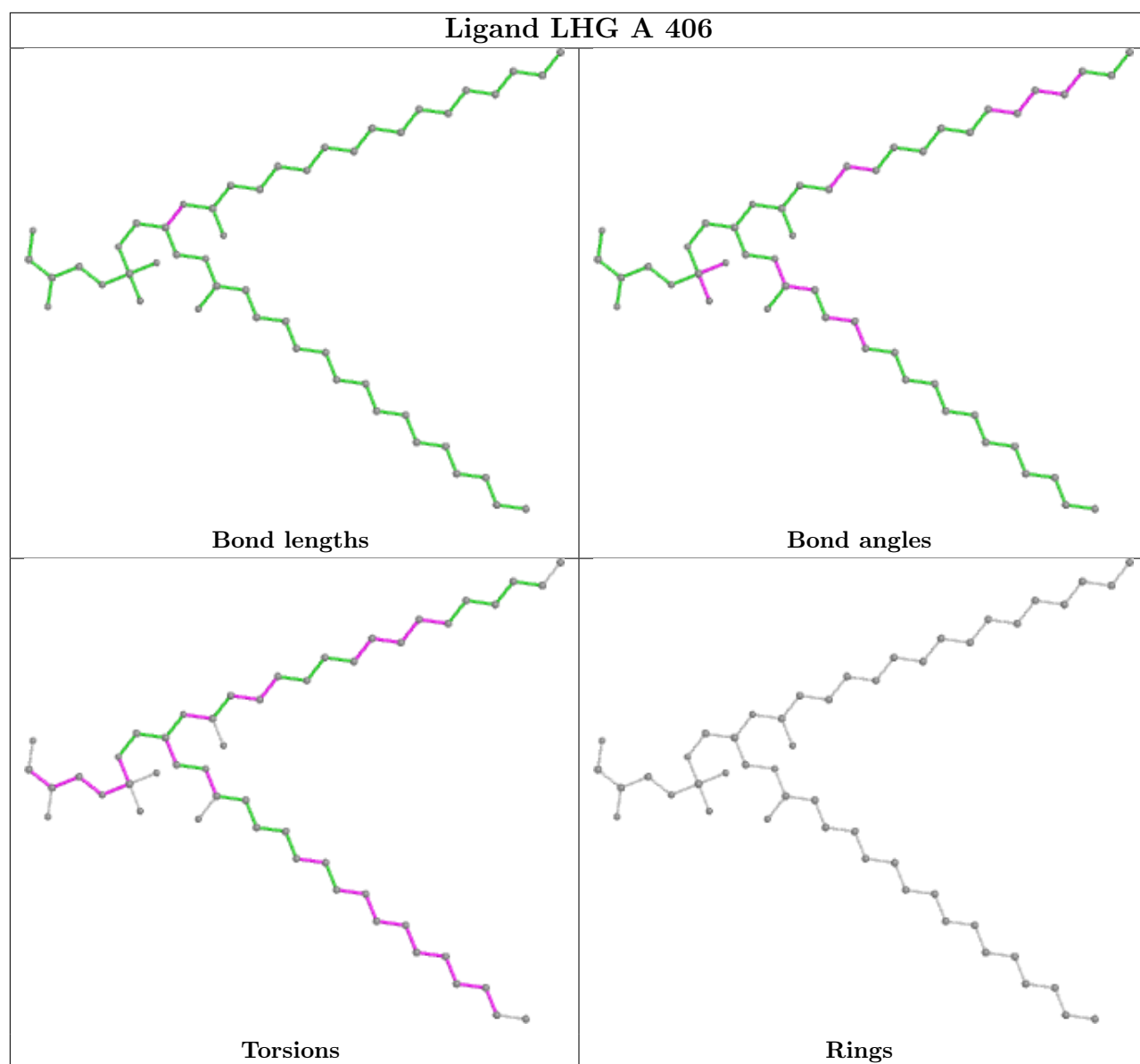
Bond angles

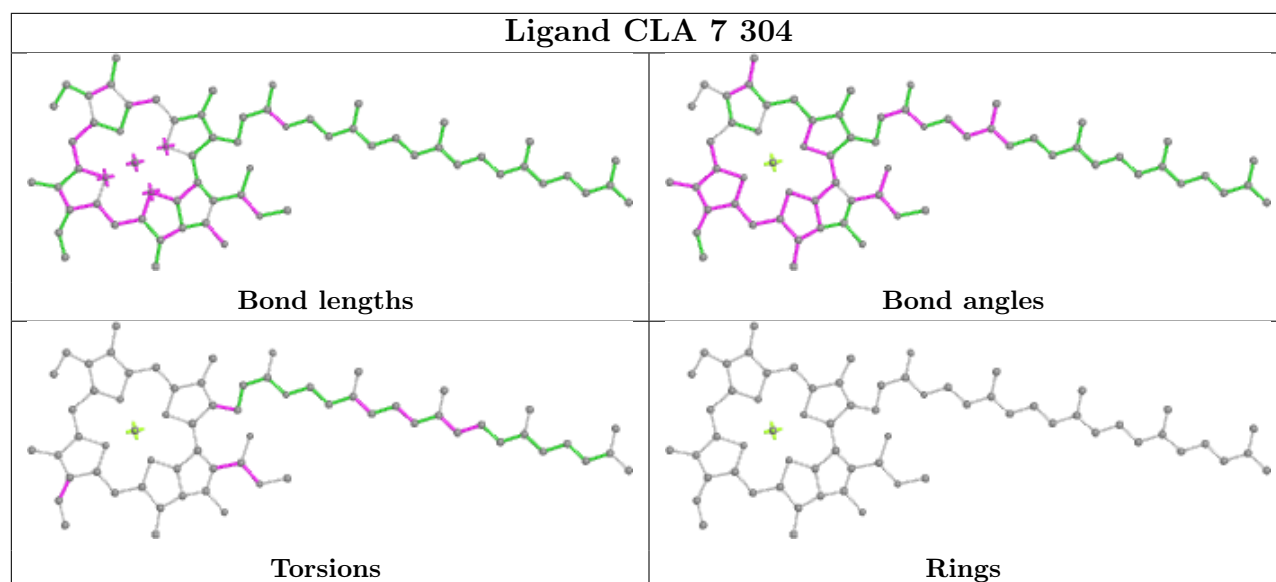
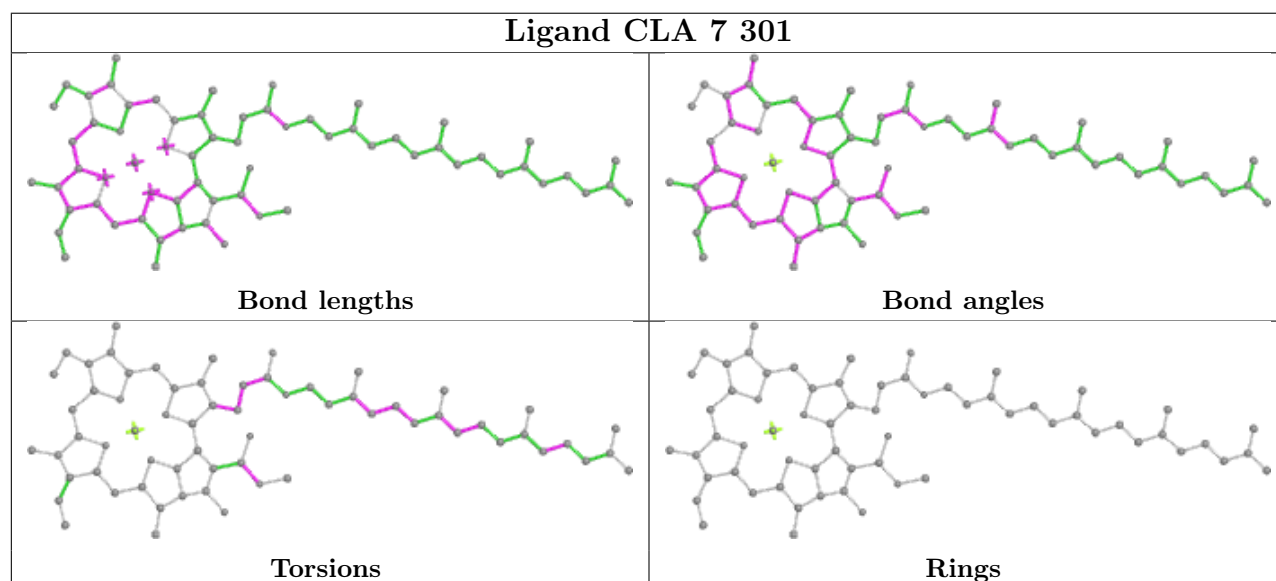
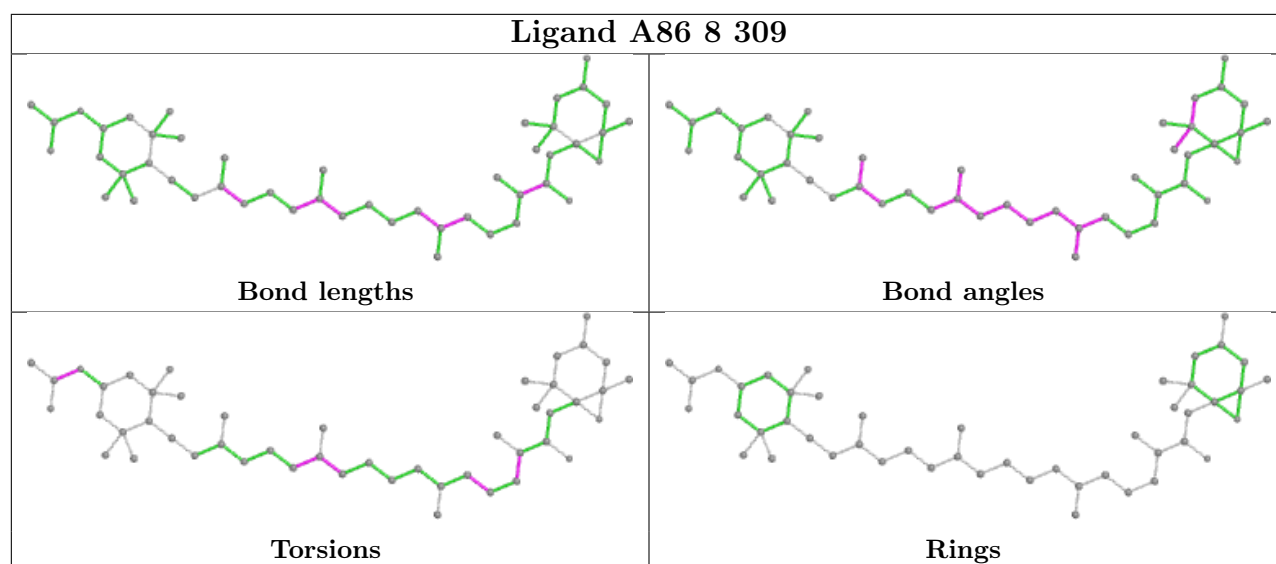


Torsions

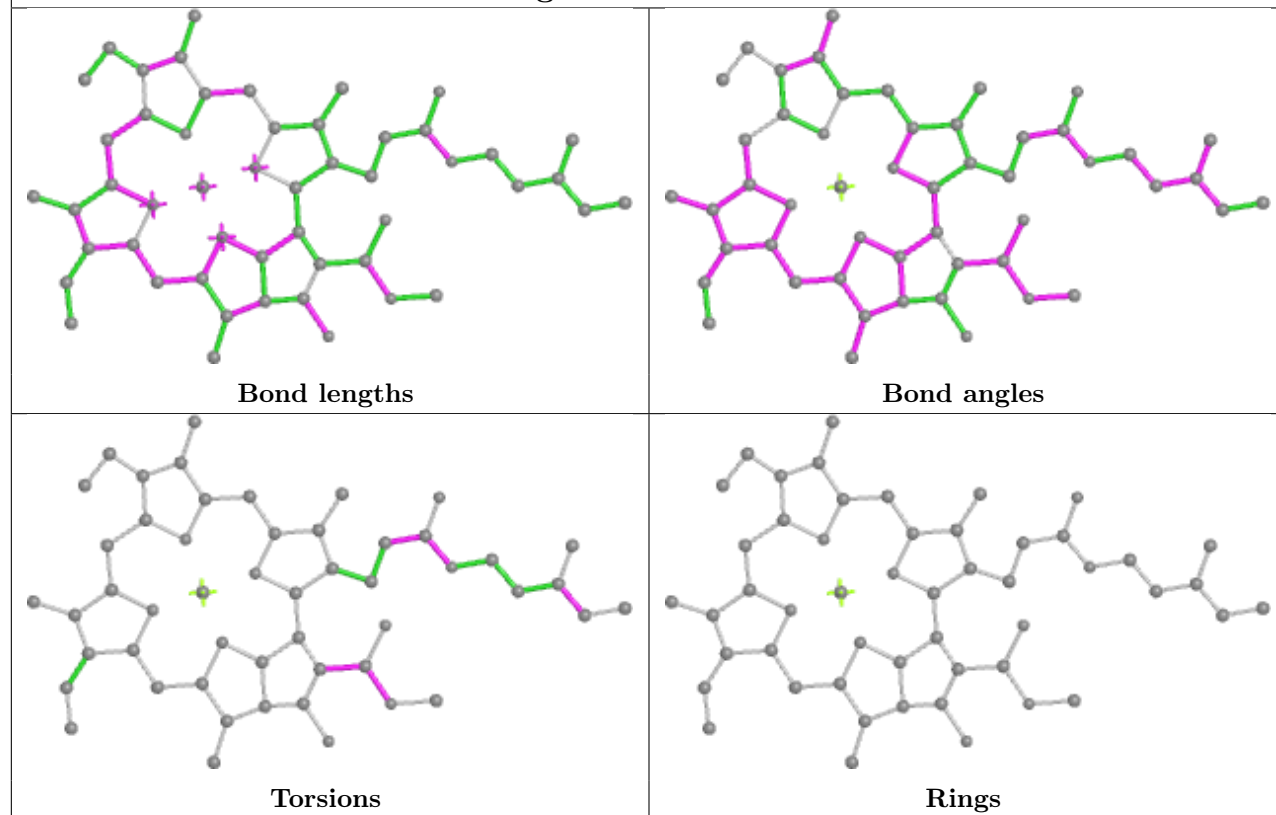


Rings

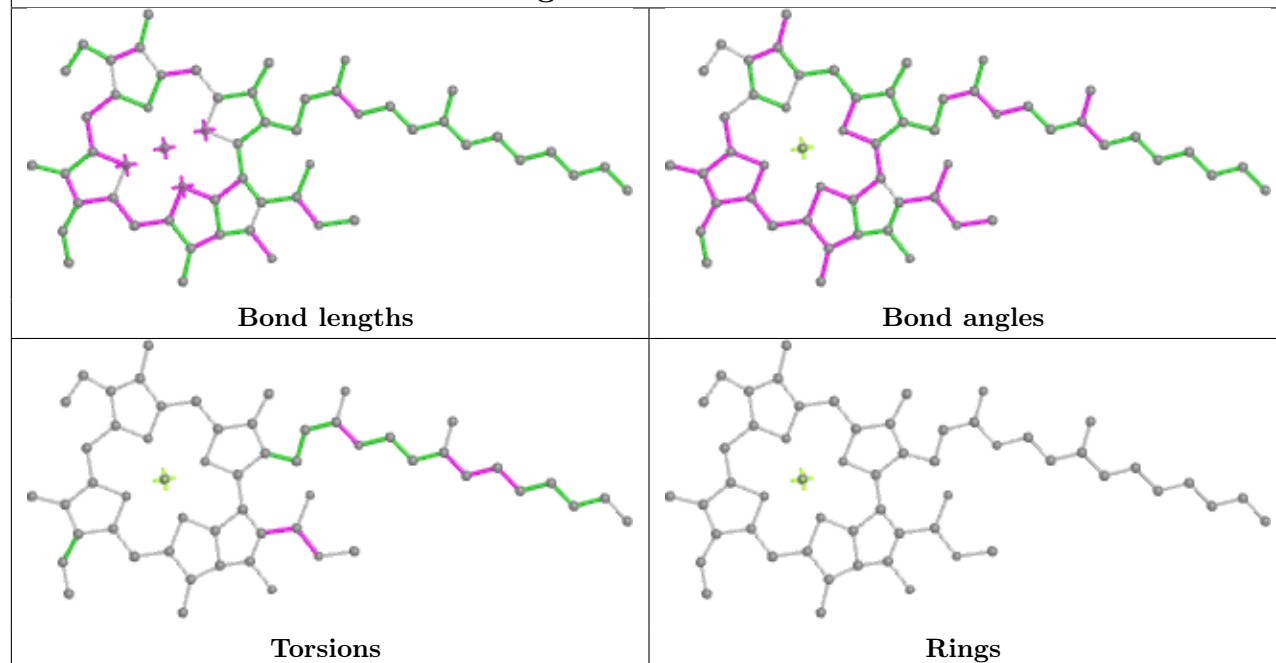


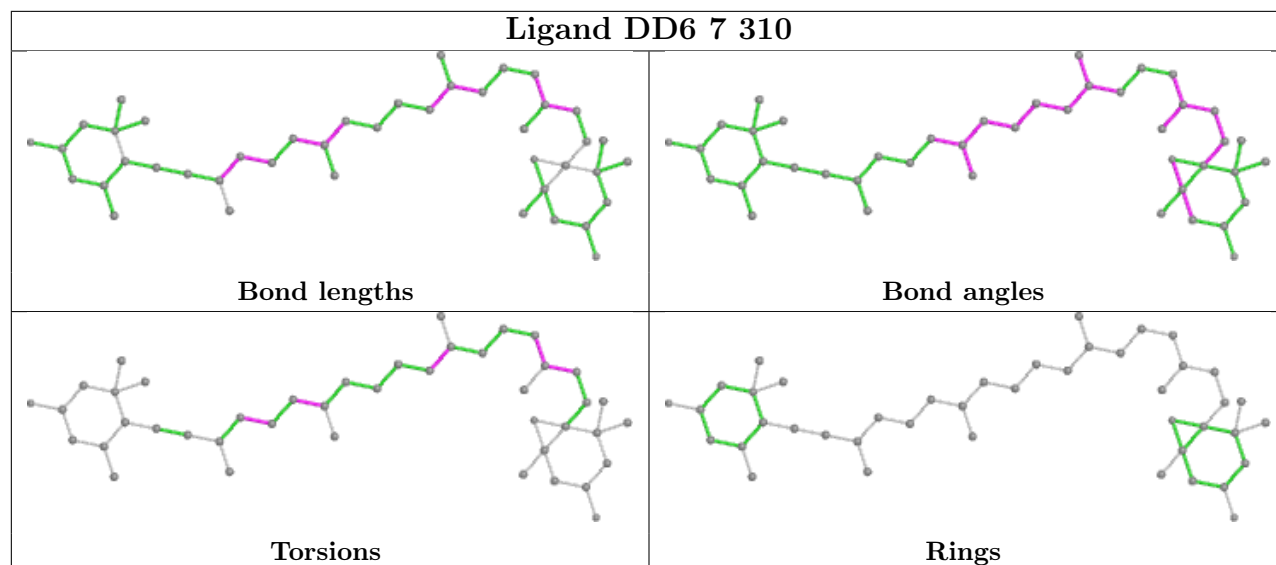
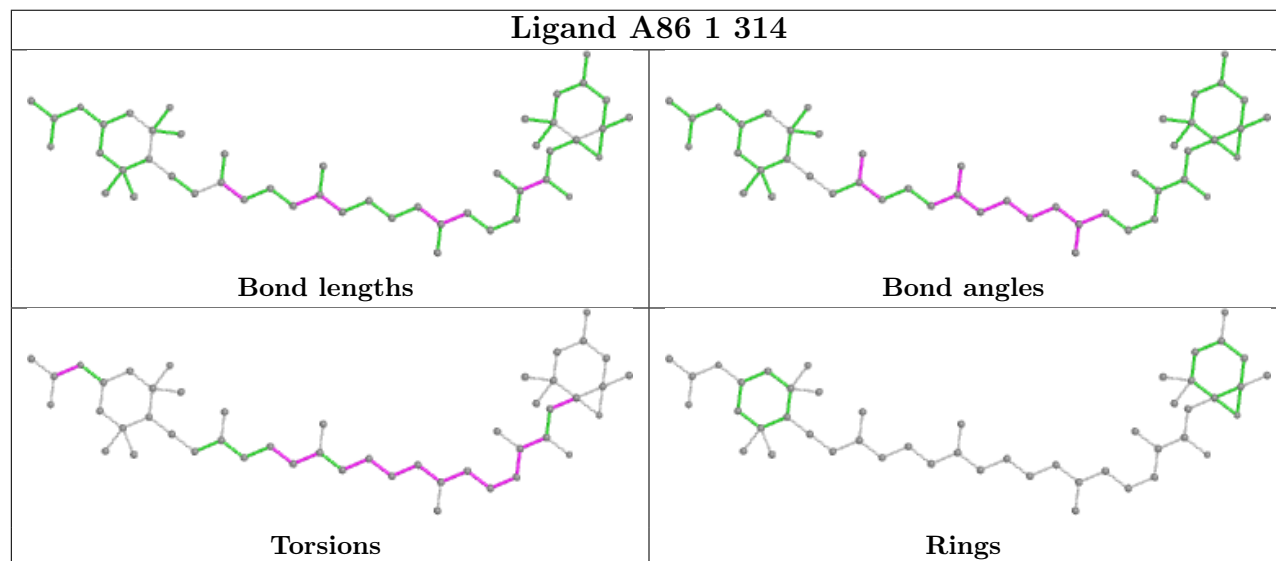


## Ligand CLA 1 305



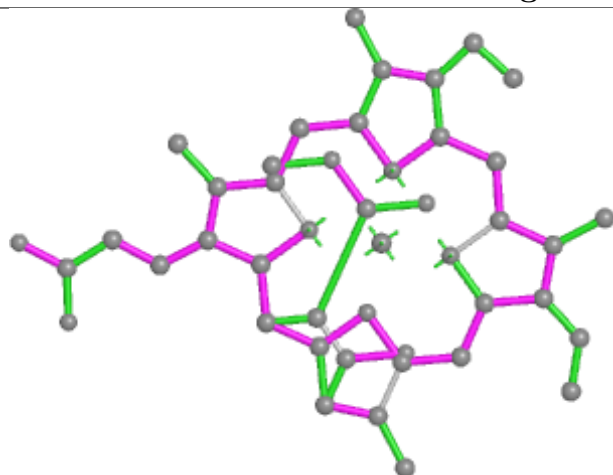
## Ligand CLA c 505



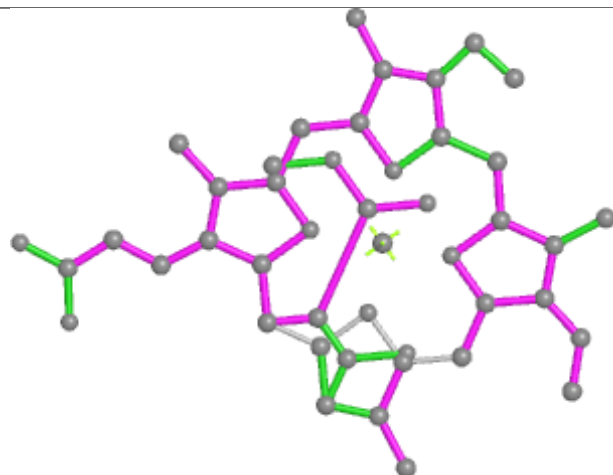
**Ligand DD6 7 310****Ligand A86 1 314**



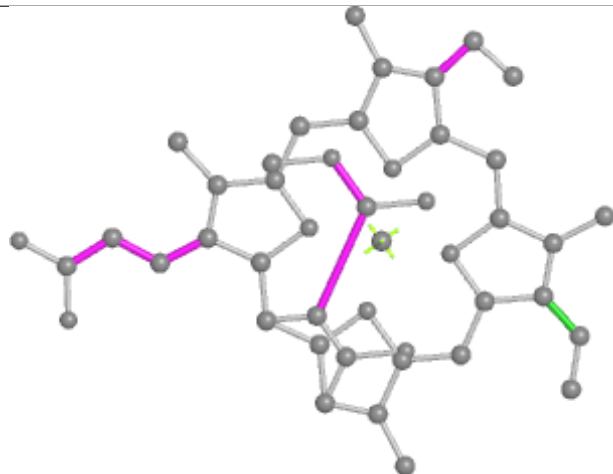
## Ligand KC1 6 311



Bond lengths



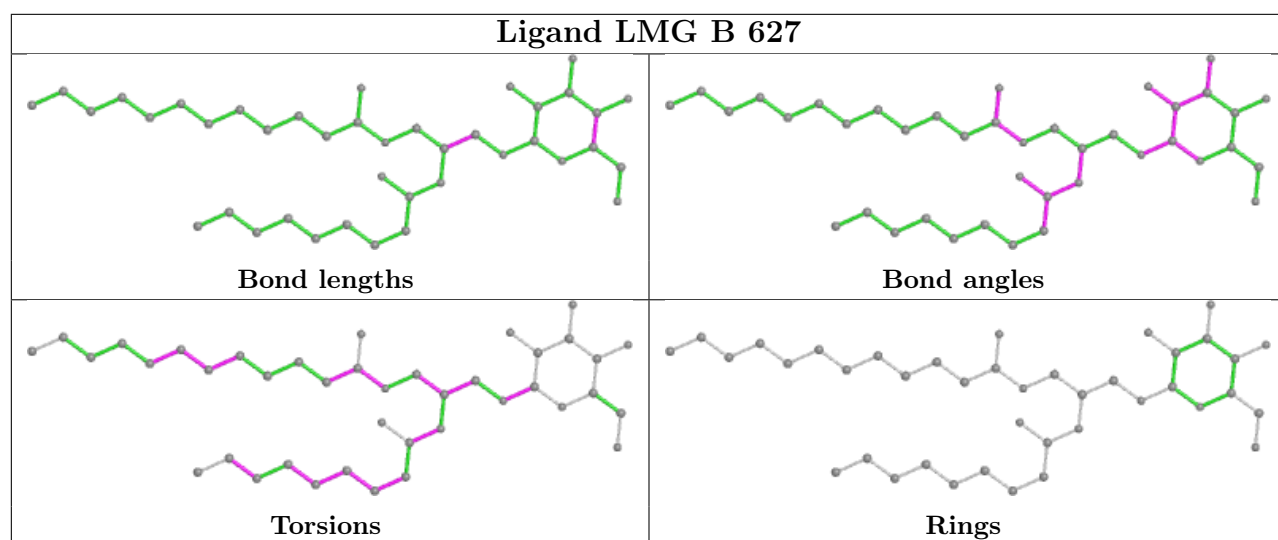
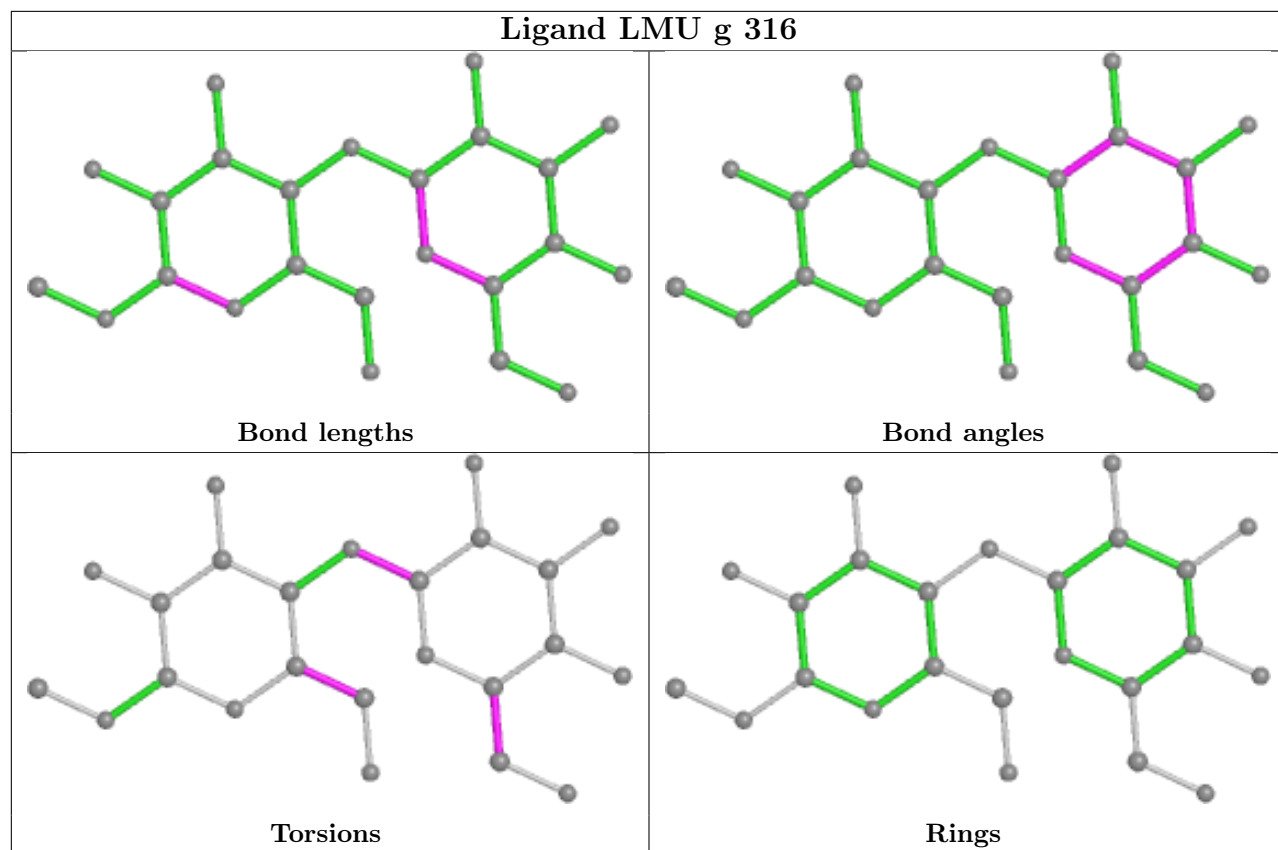
Bond angles

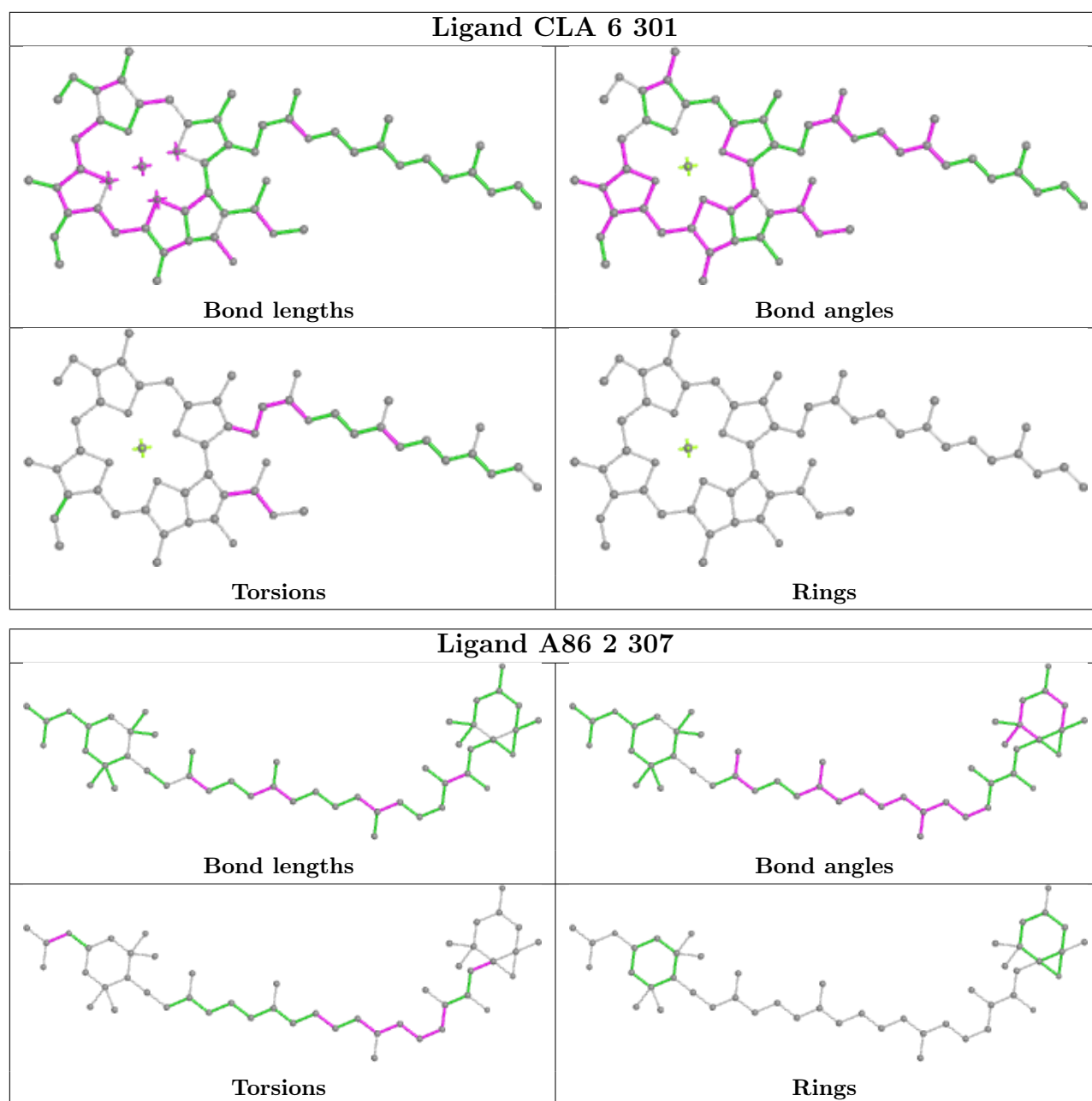


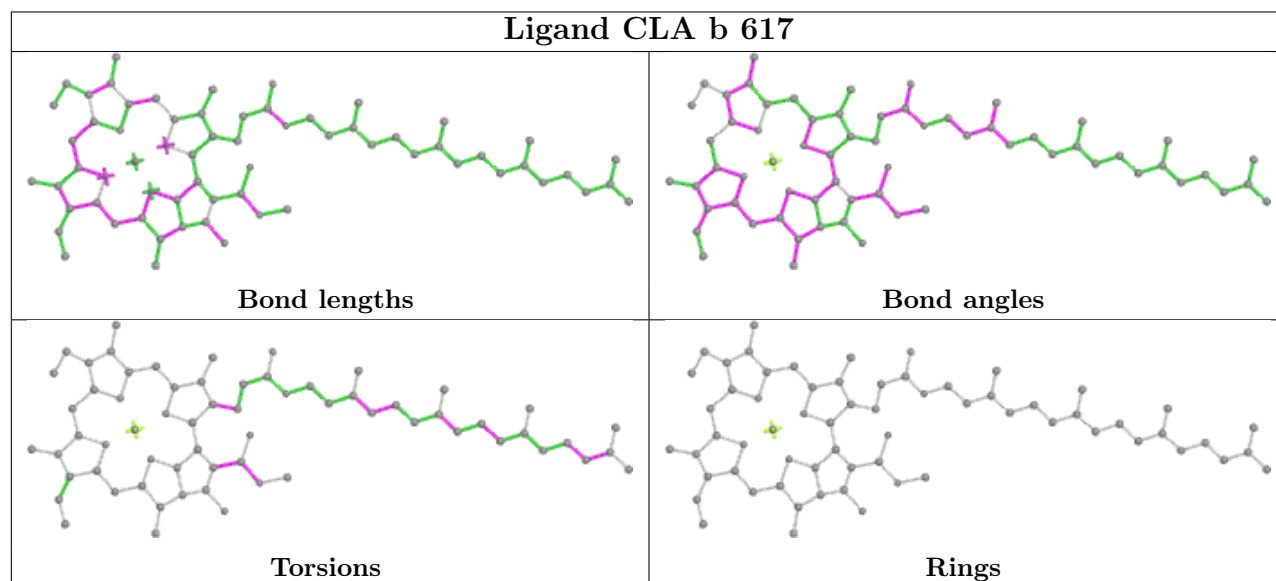
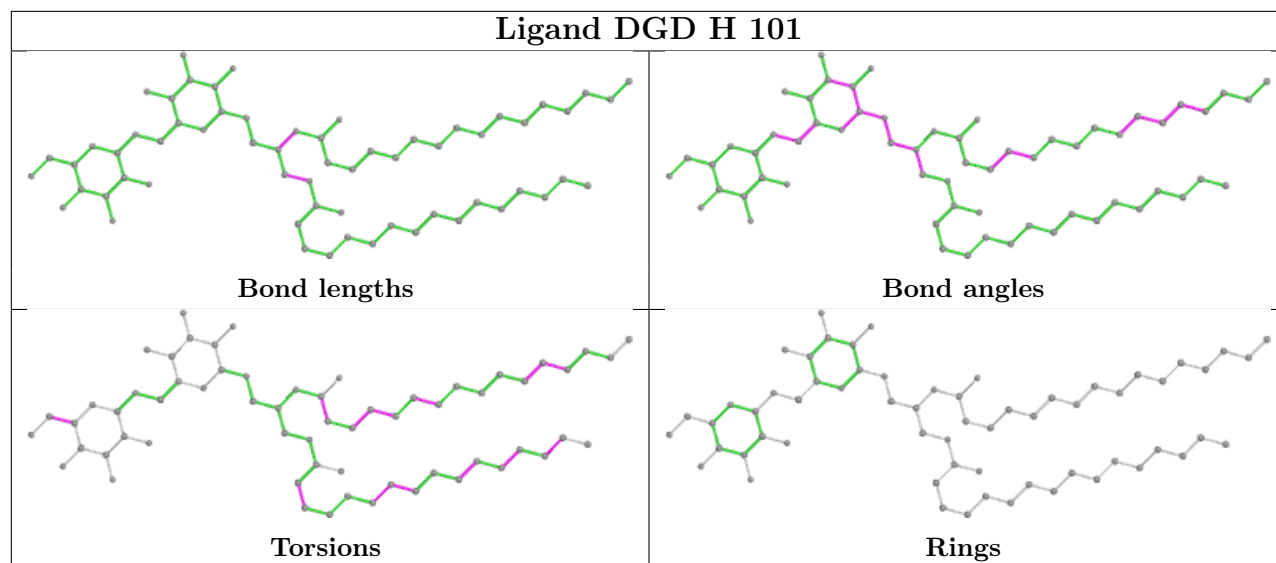
Torsions



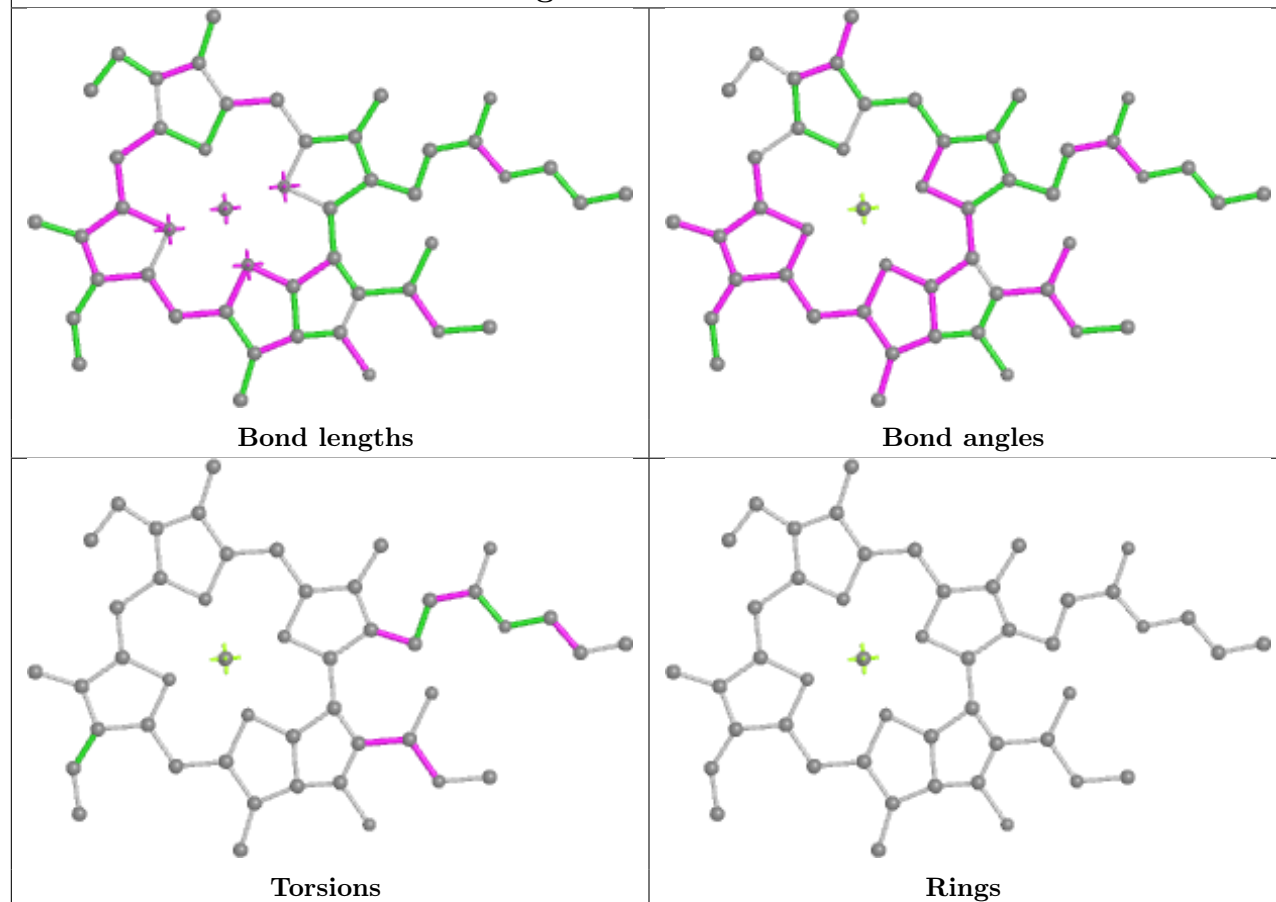
Rings



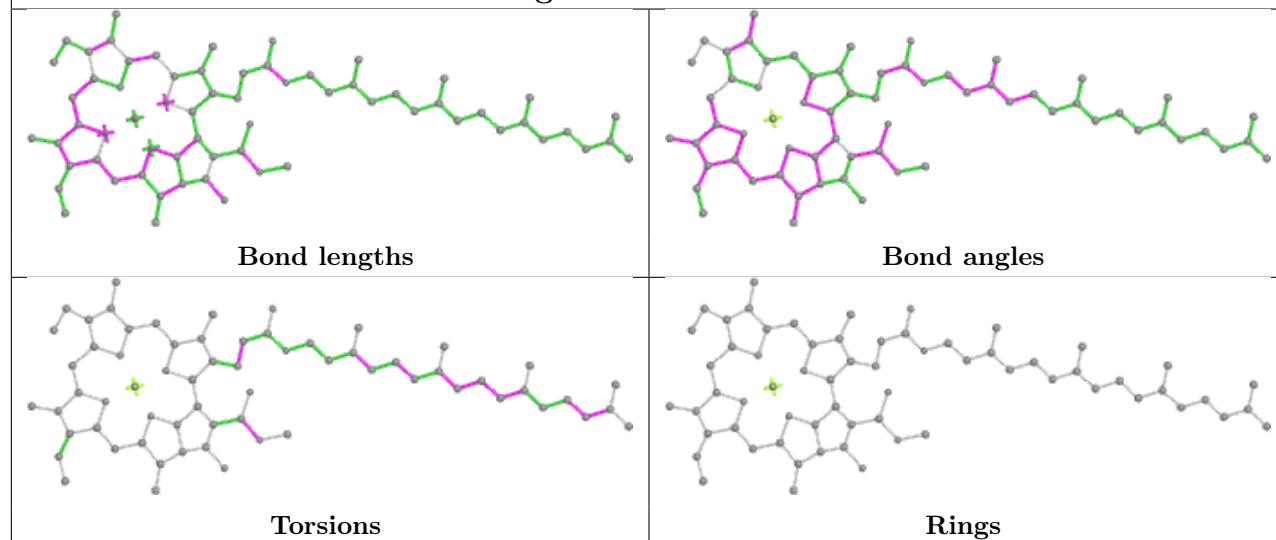




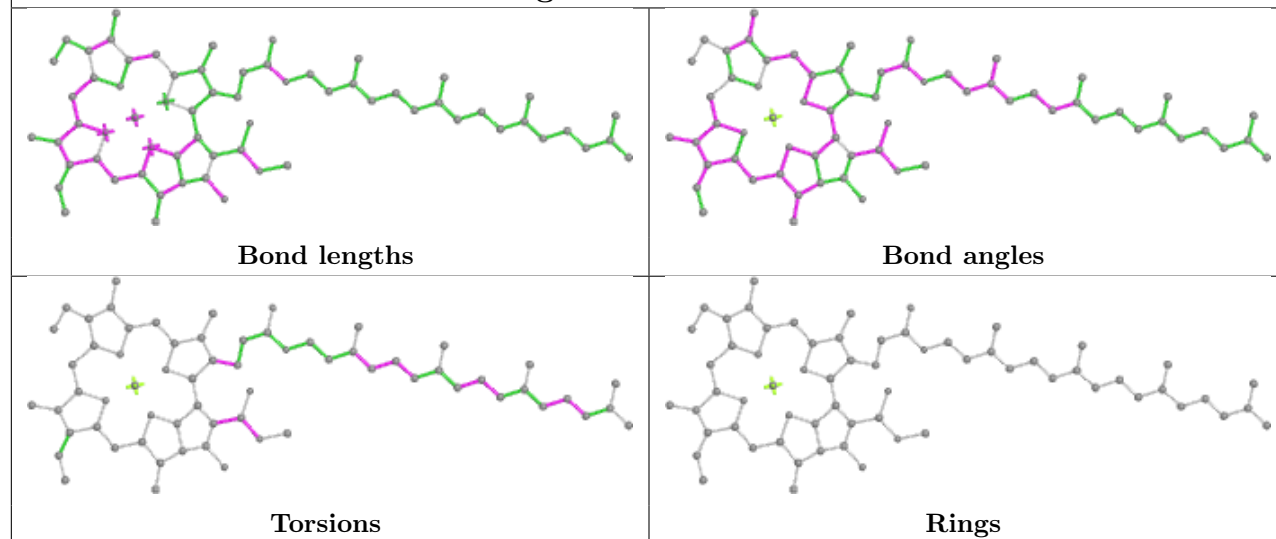
## Ligand CLA 5 304



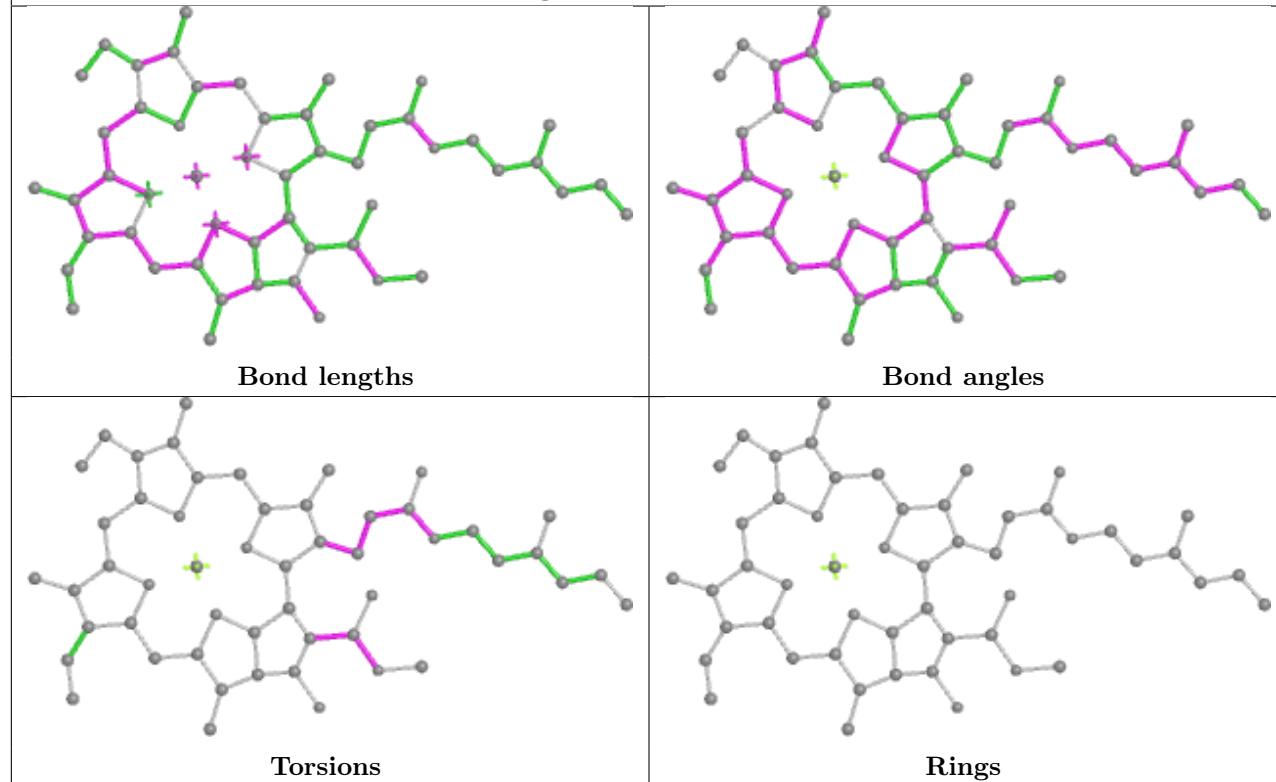
## Ligand CLA b 608

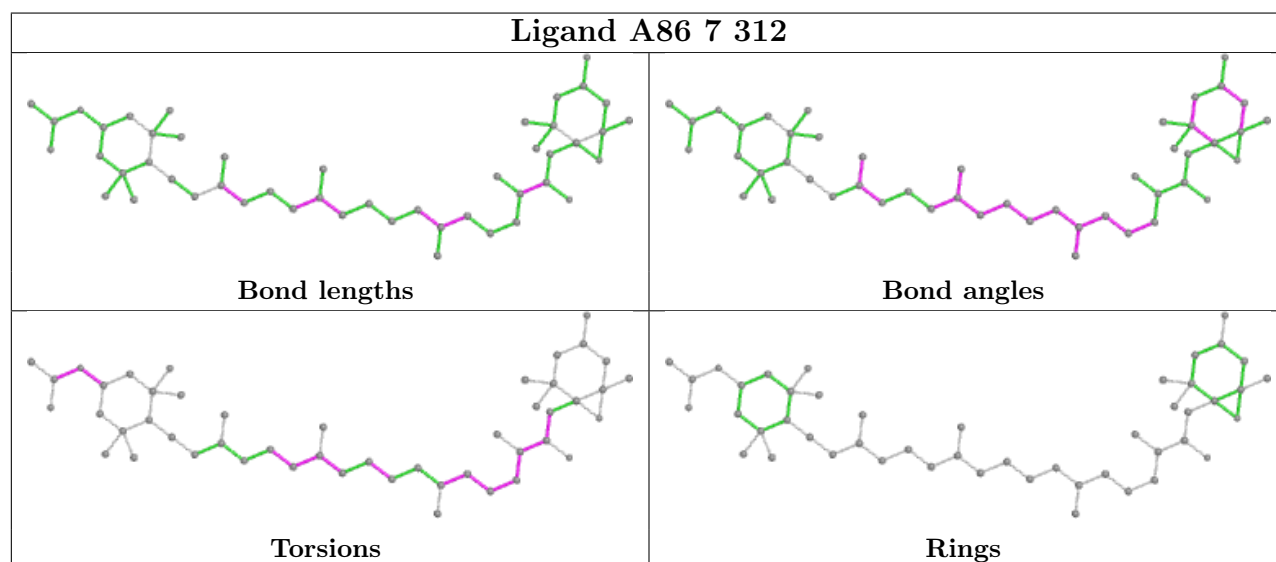
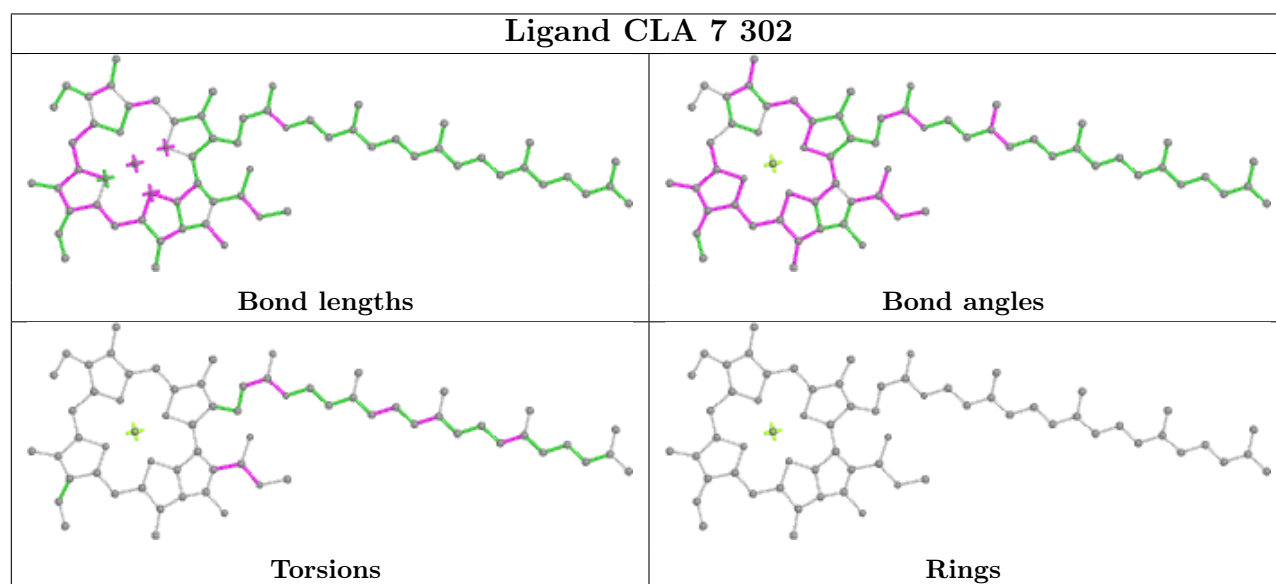
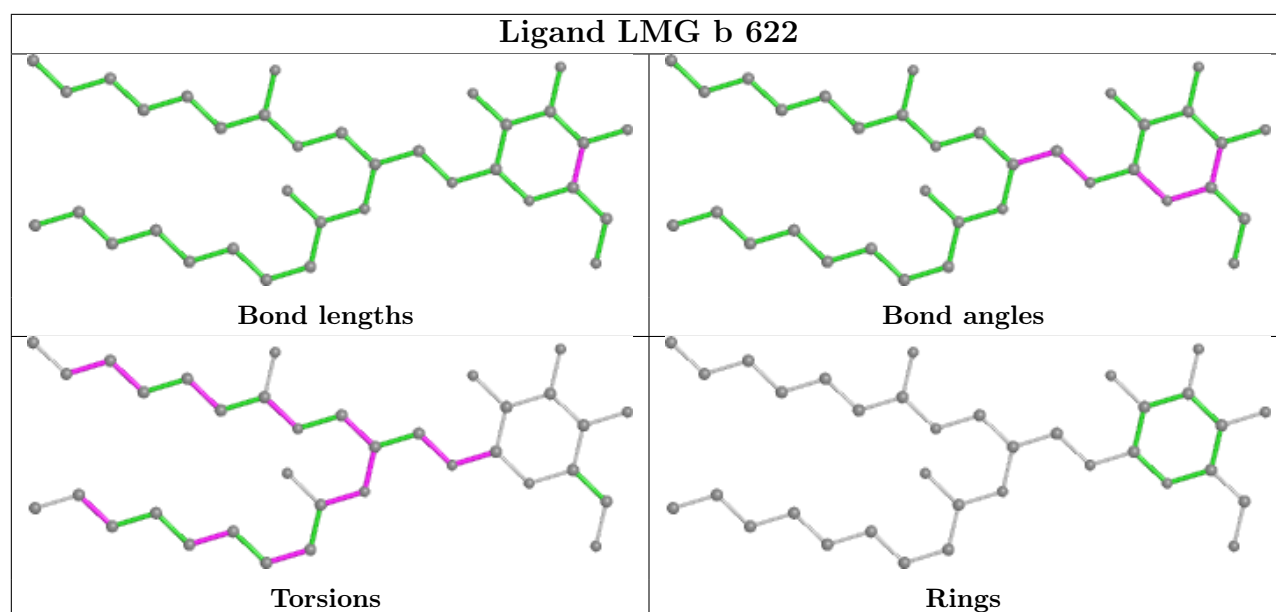


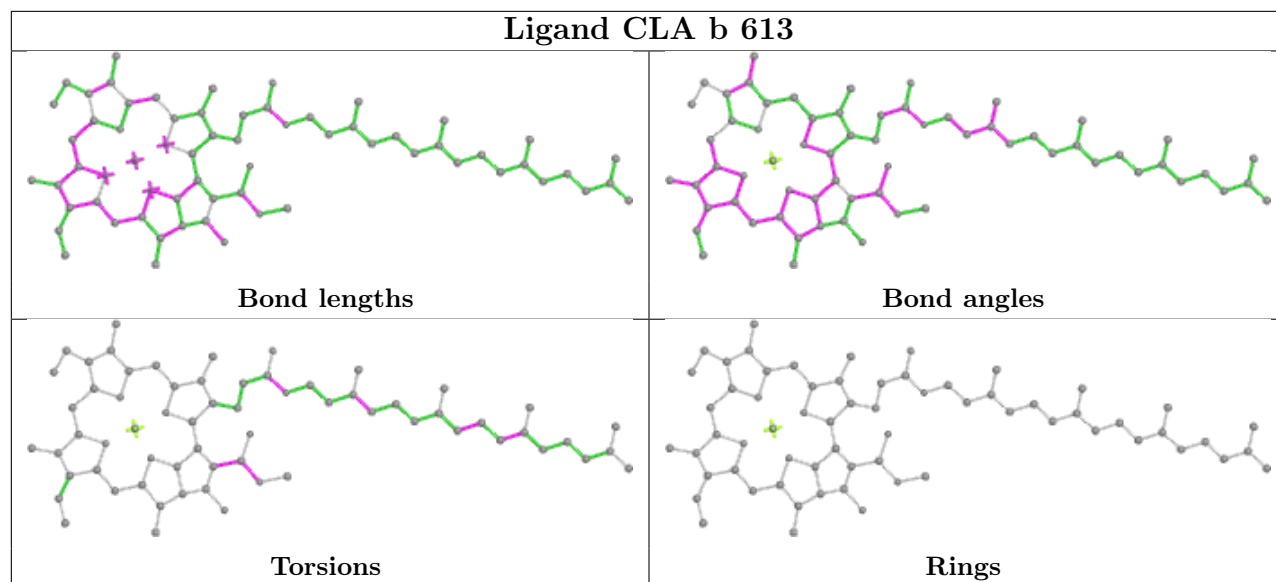
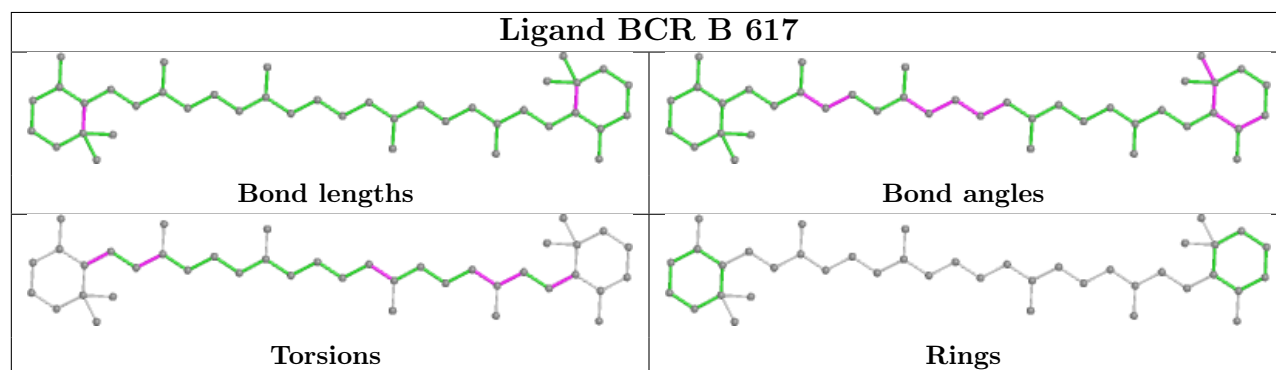
## Ligand CLA 4 300



## Ligand CLA 5 303

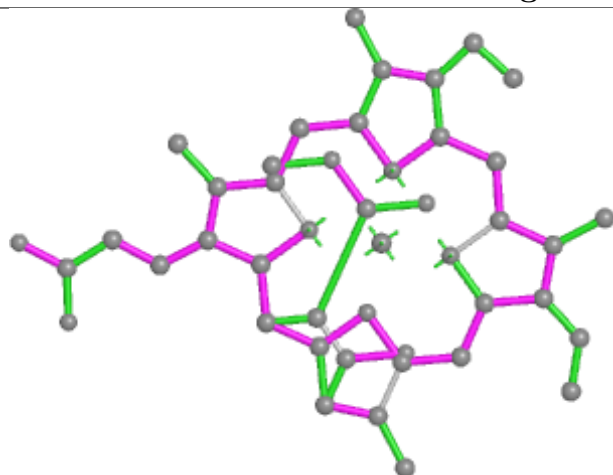




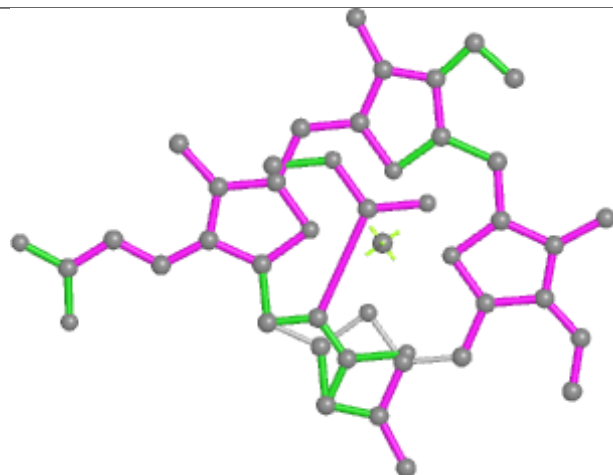
**Ligand CLA b 613****Ligand BCR B 617**



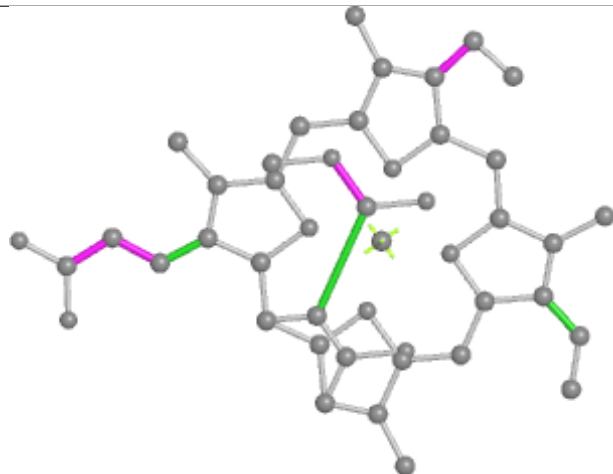
## Ligand KC1 7 315



Bond lengths



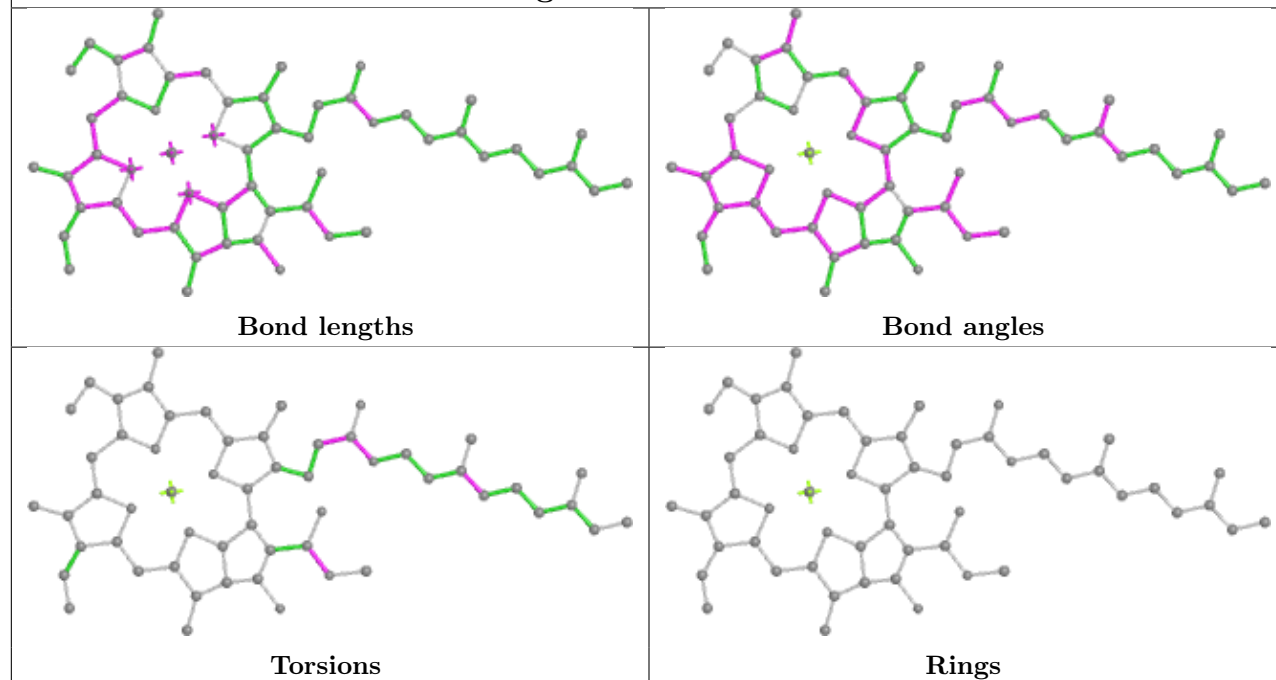
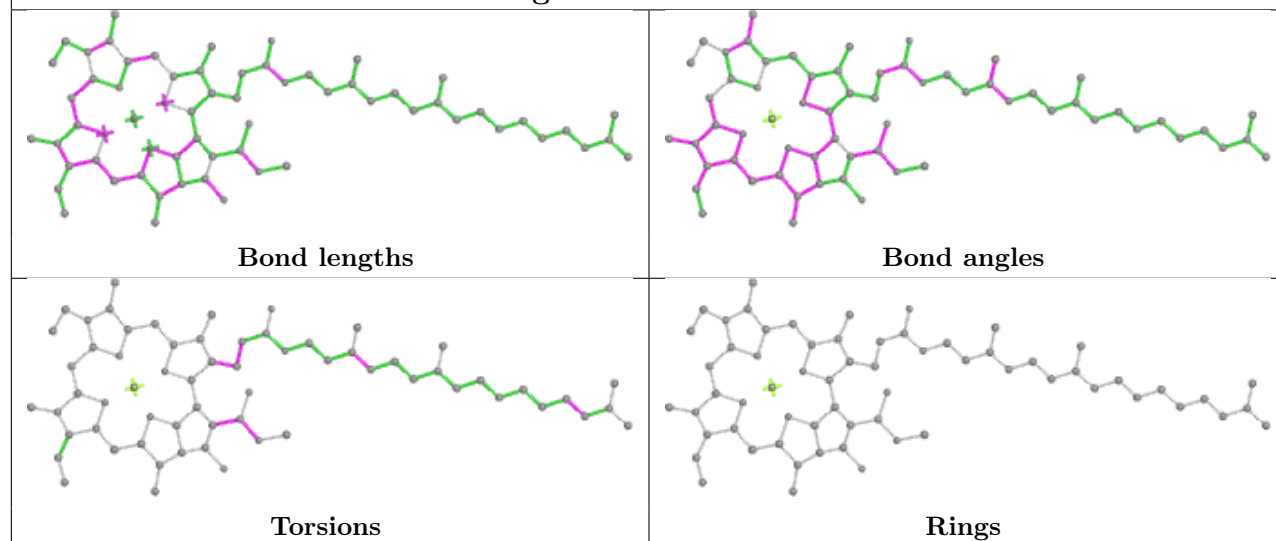
Bond angles



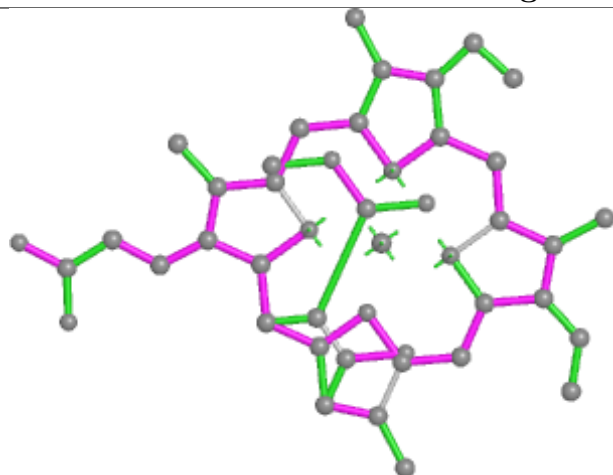
Torsions



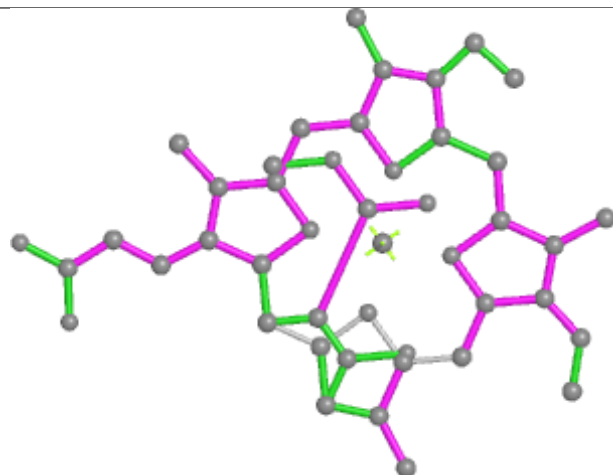
Rings

**Ligand CLA 1 309****Ligand CLA B 604**

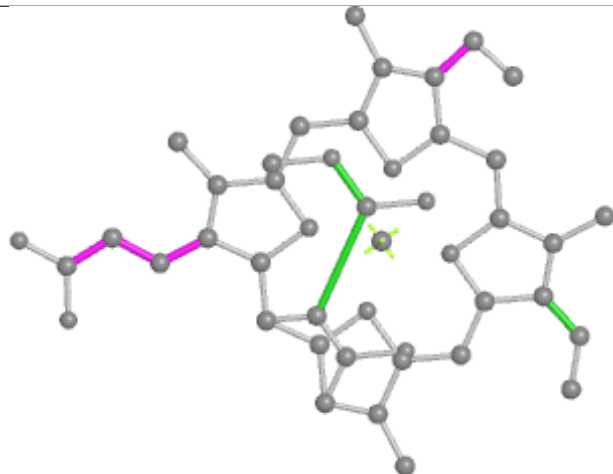
## Ligand KC1 2 314



Bond lengths



Bond angles

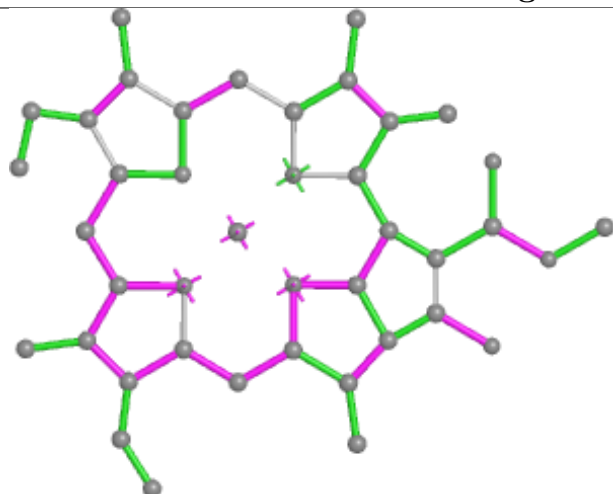


Torsions

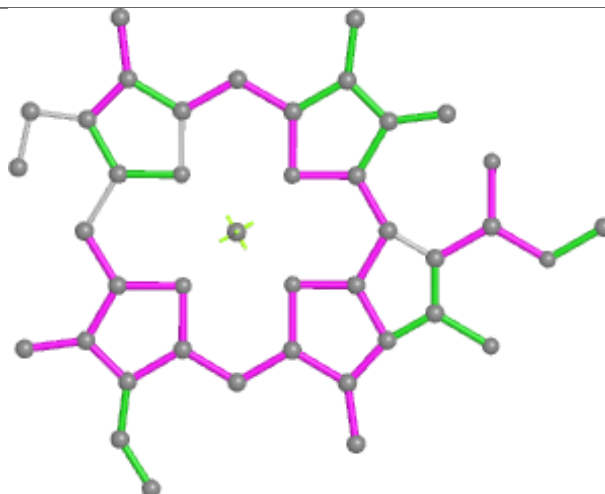


Rings

## Ligand CLA 7 305



Bond lengths



Bond angles

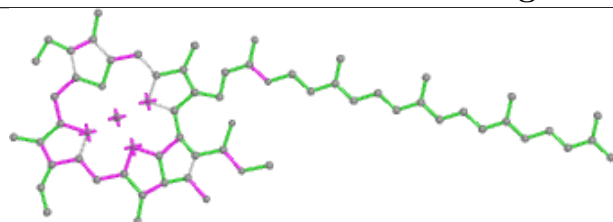


Torsions

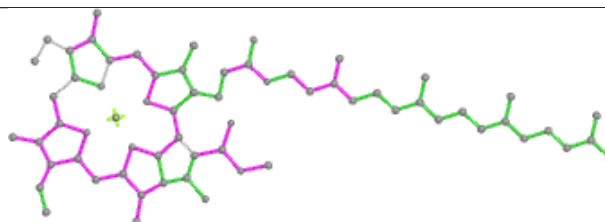


Rings

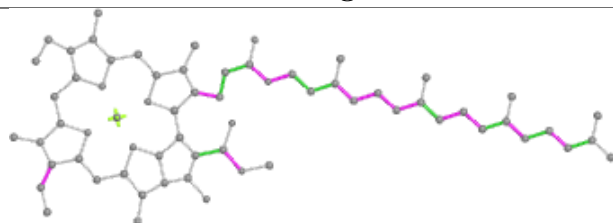
## Ligand CLA 4 304



Bond lengths



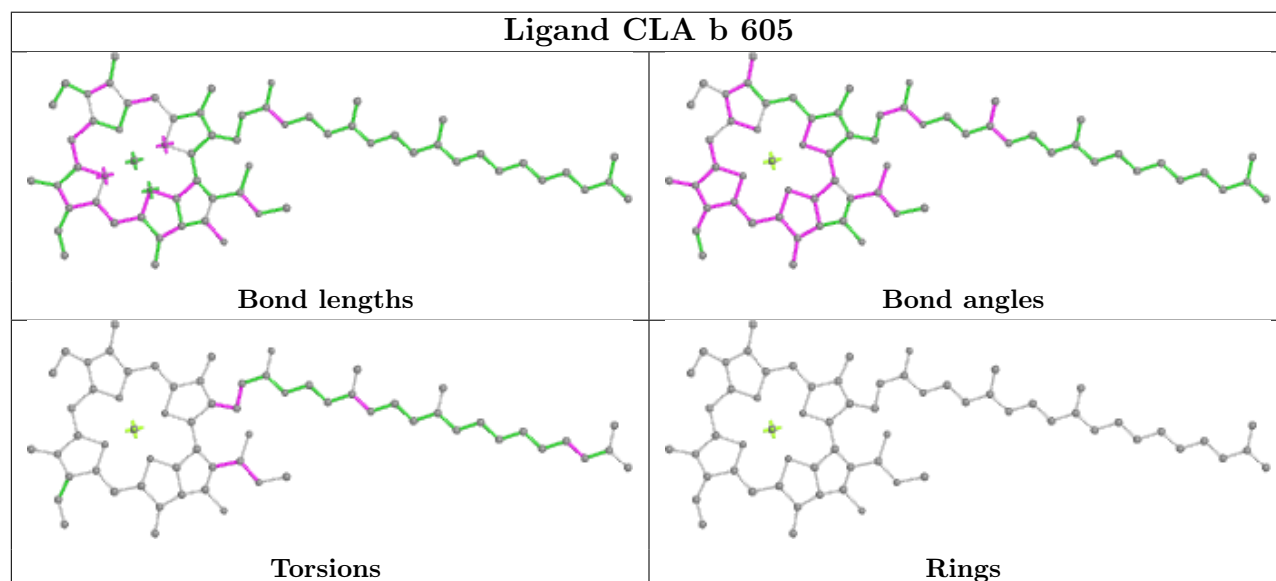
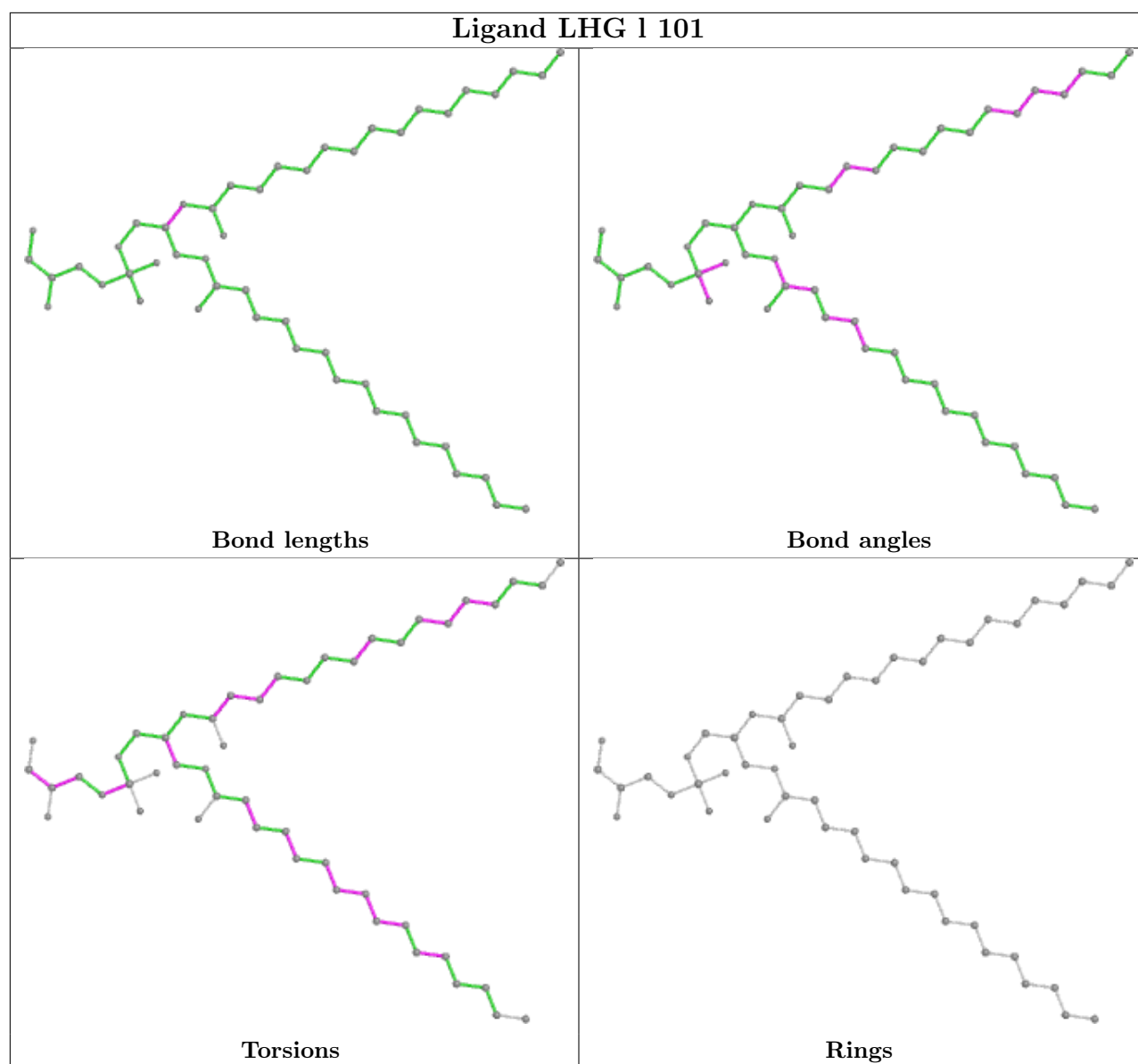
Bond angles

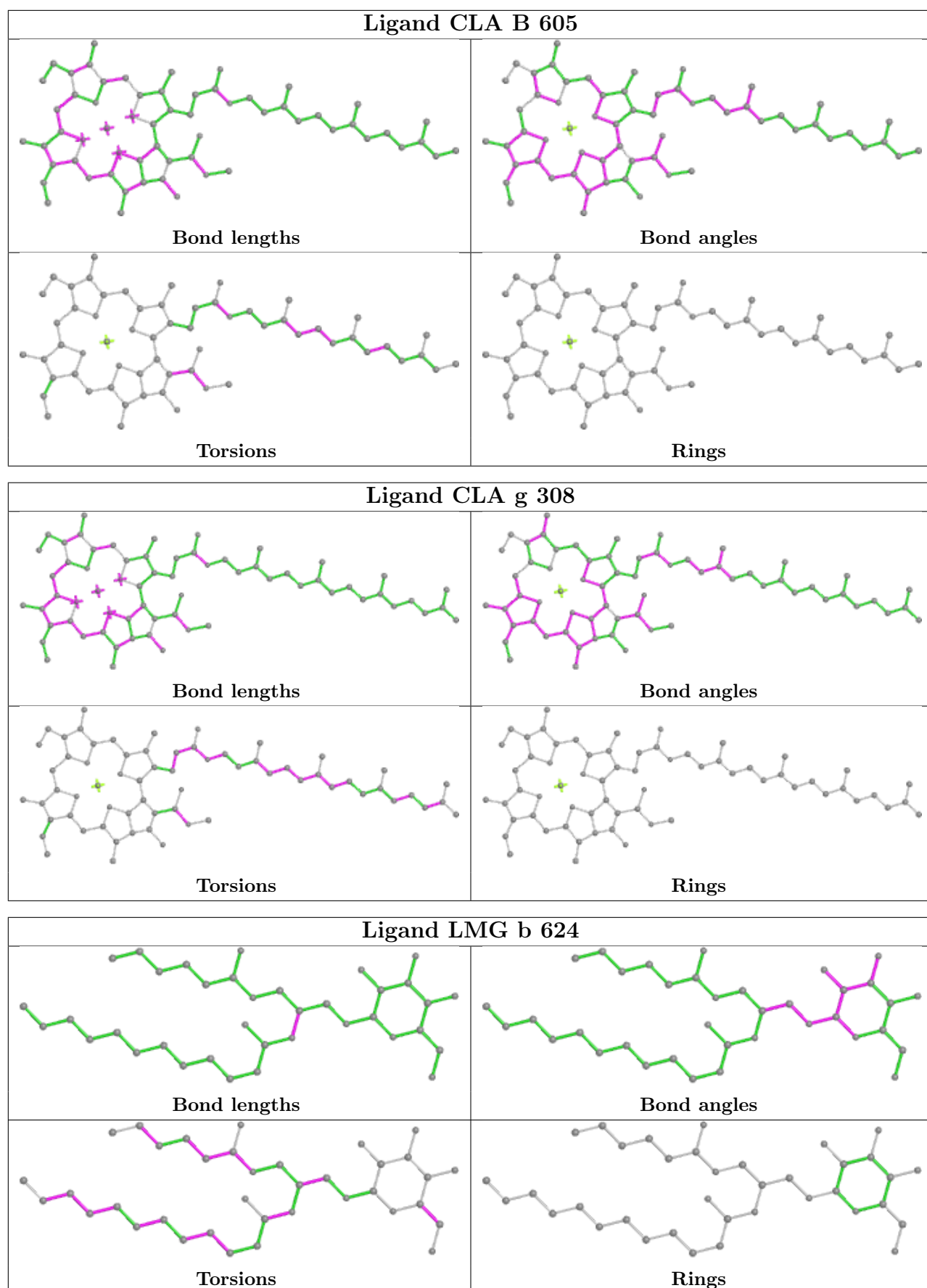


Torsions

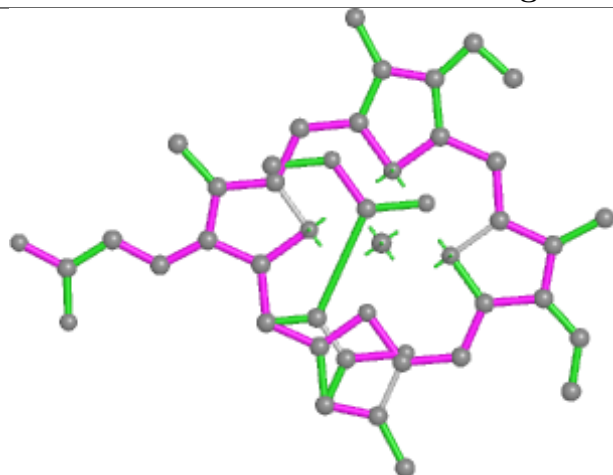


Rings

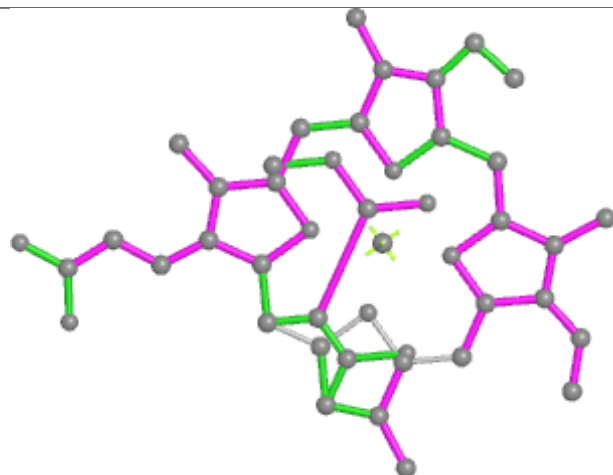




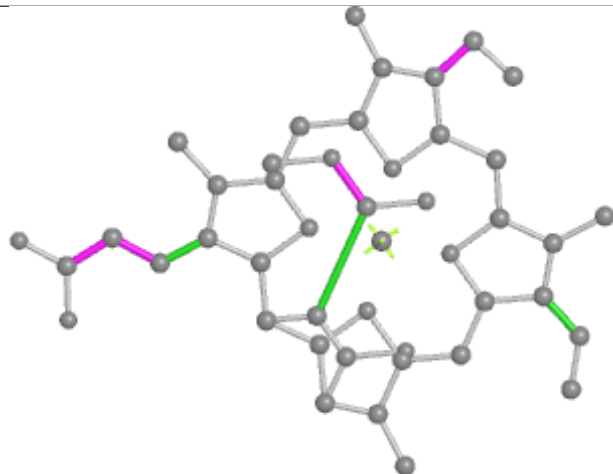
## Ligand KC1 1 316



Bond lengths



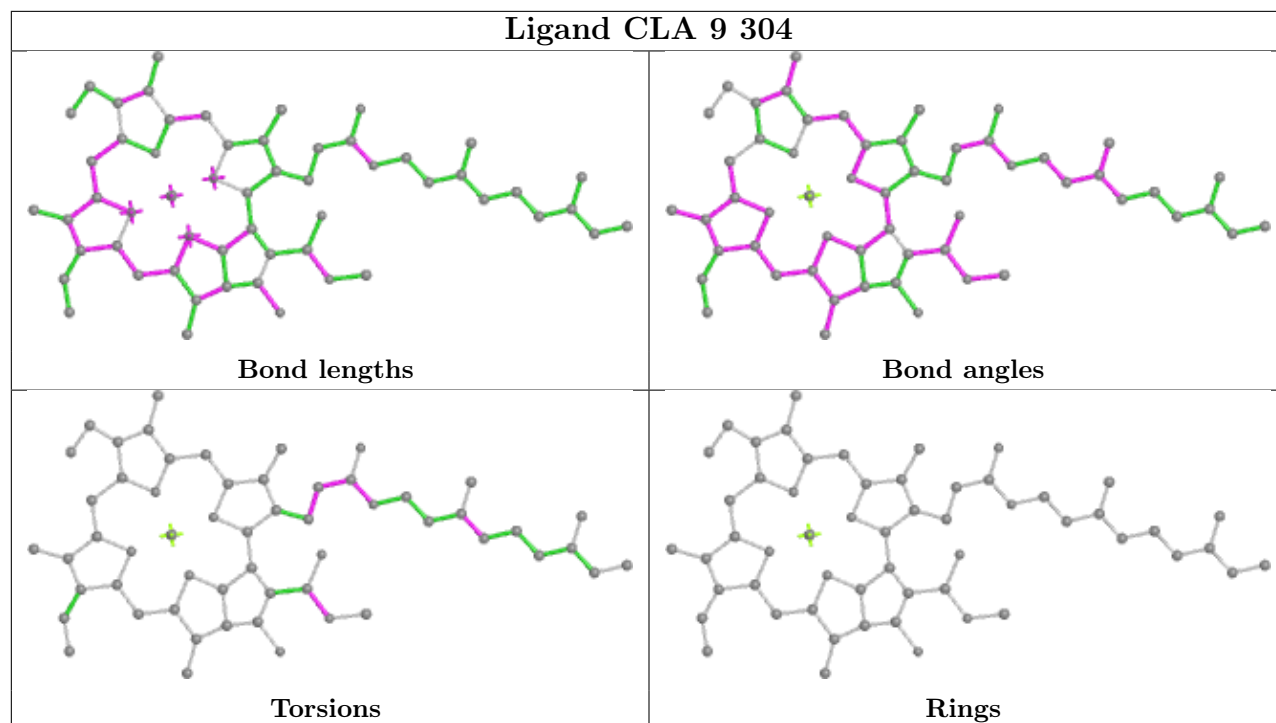
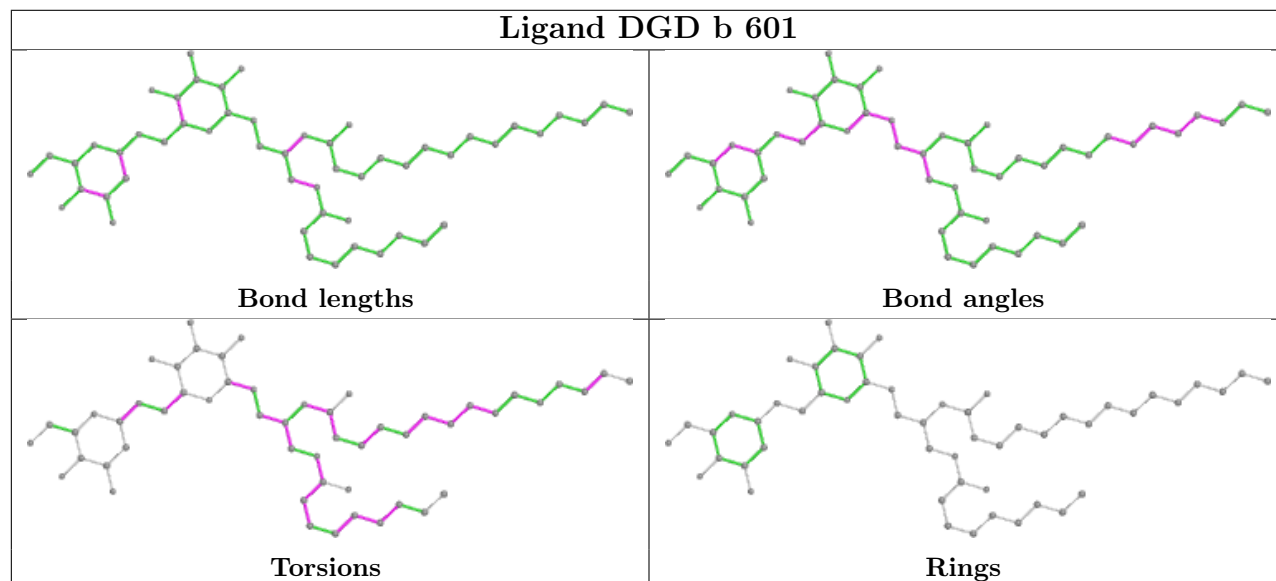
Bond angles



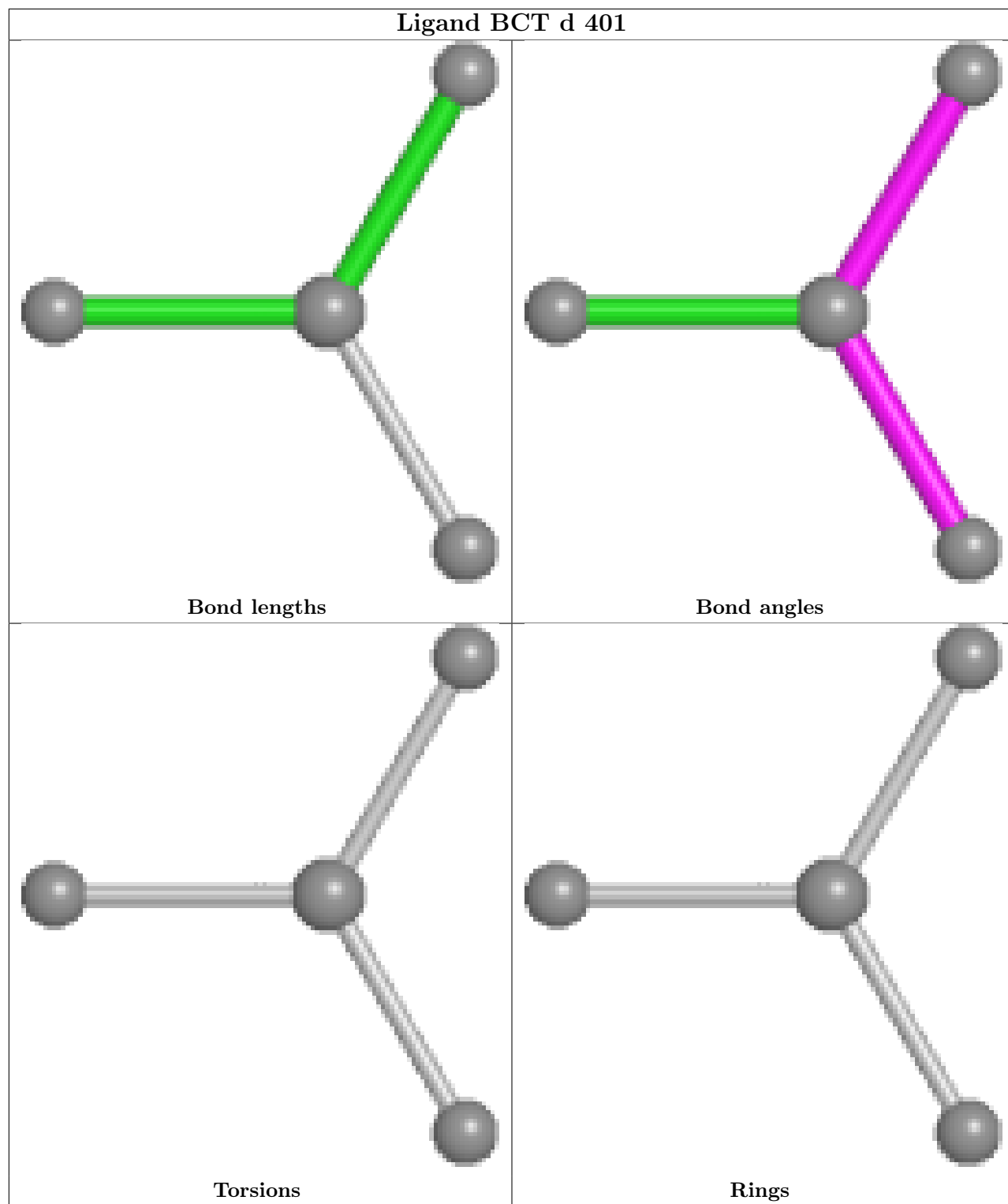
Torsions



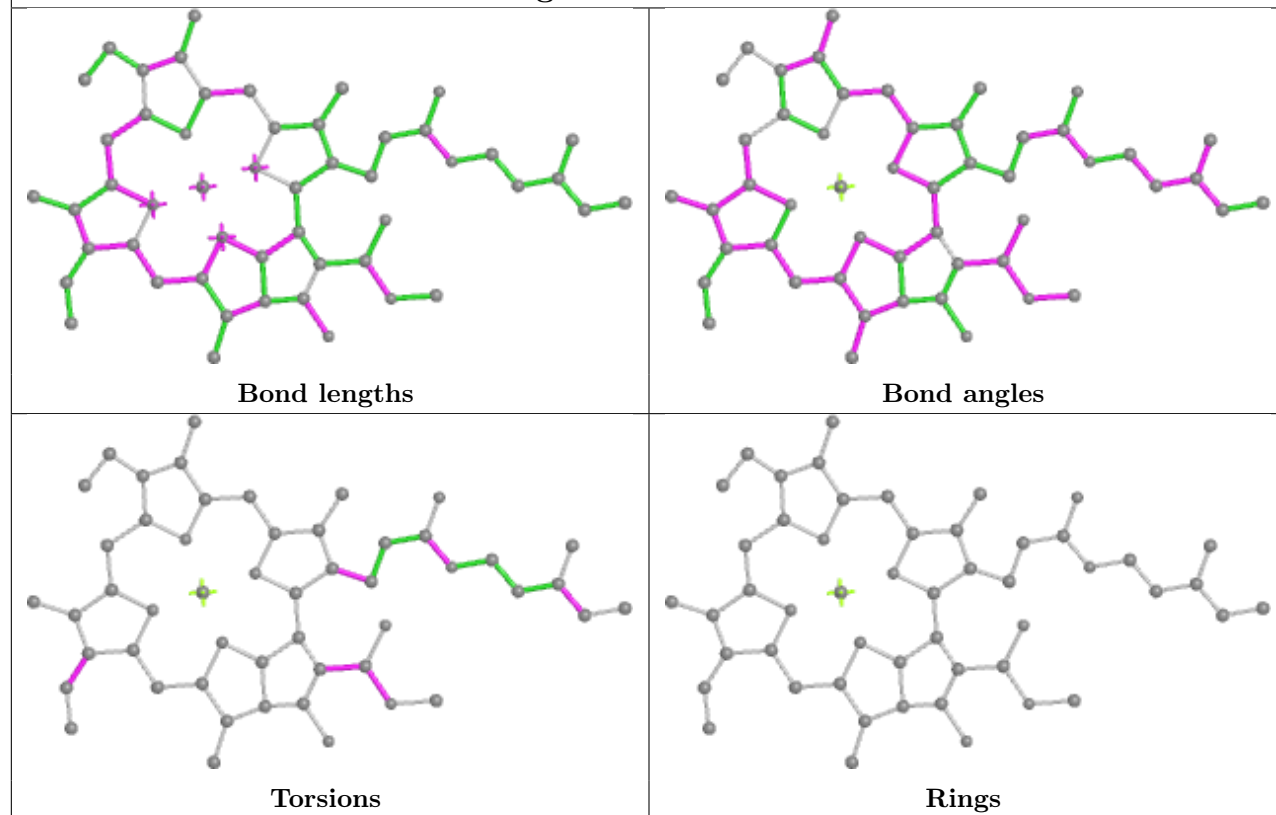
Rings

**Ligand CLA 9 304****Ligand DGD b 601**

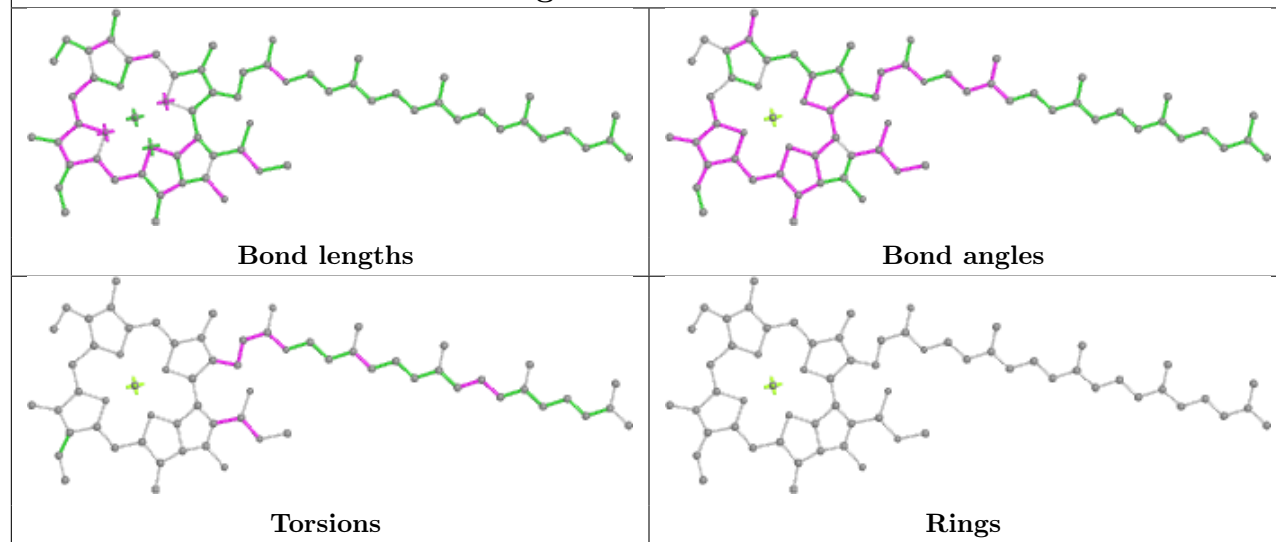


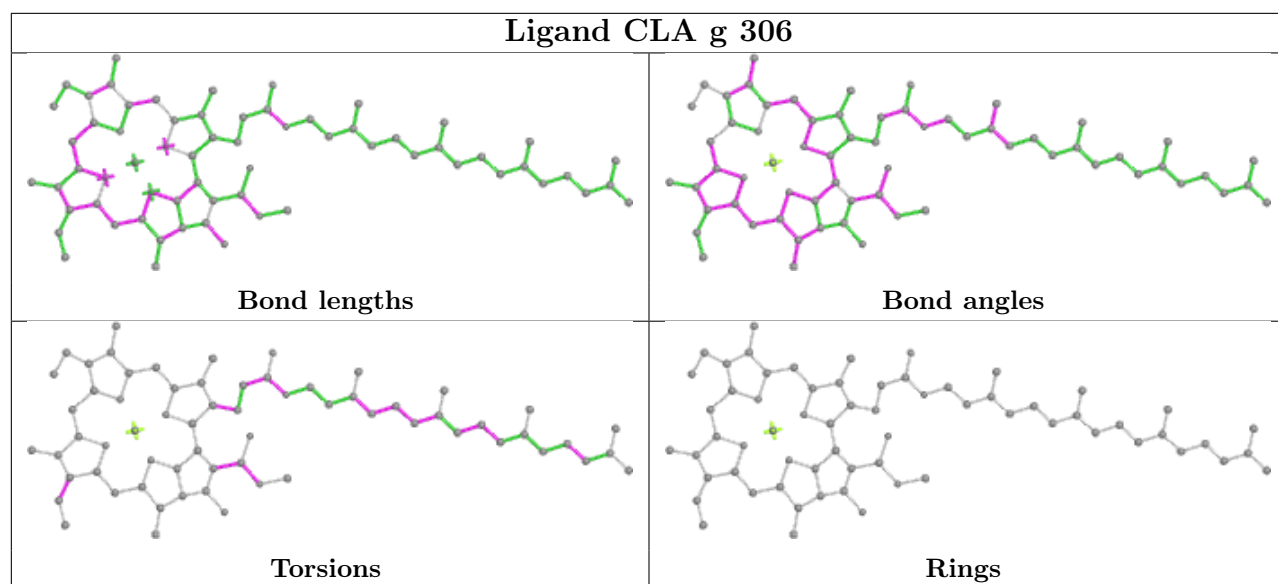
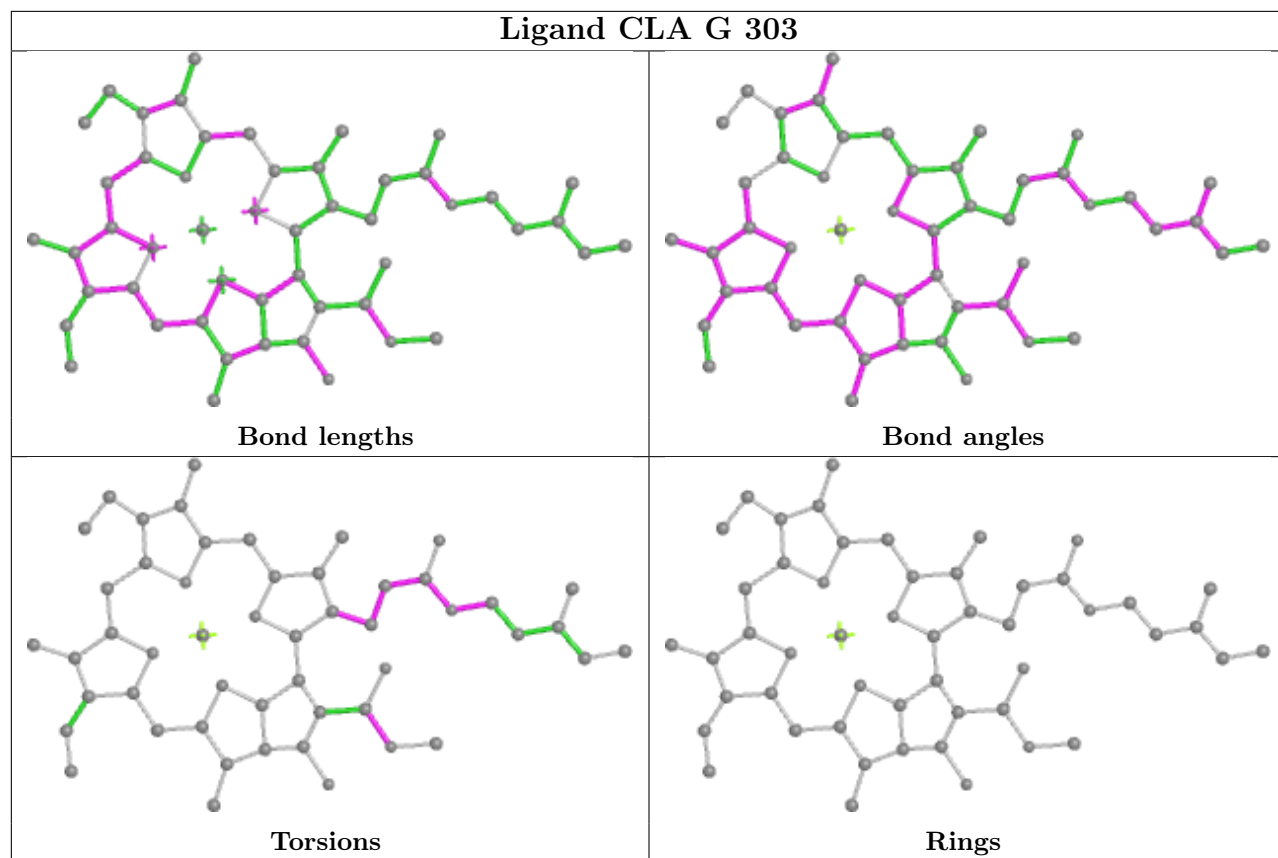


## Ligand CLA 9 303

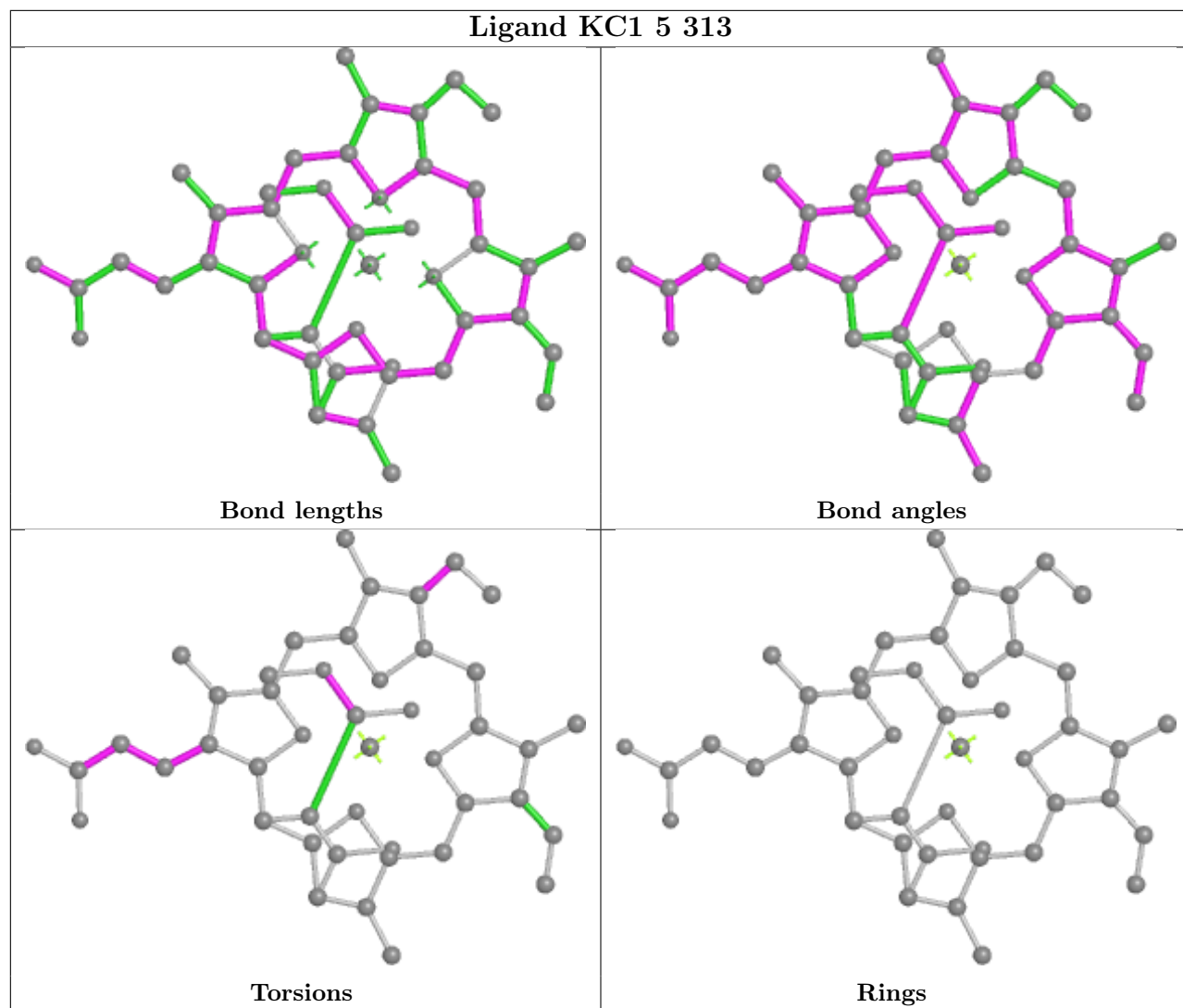


## Ligand CLA 6 307

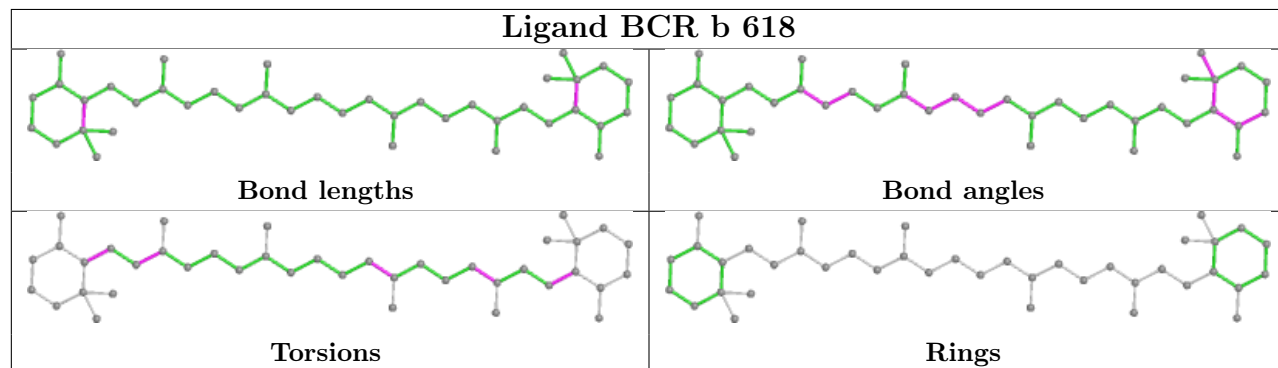


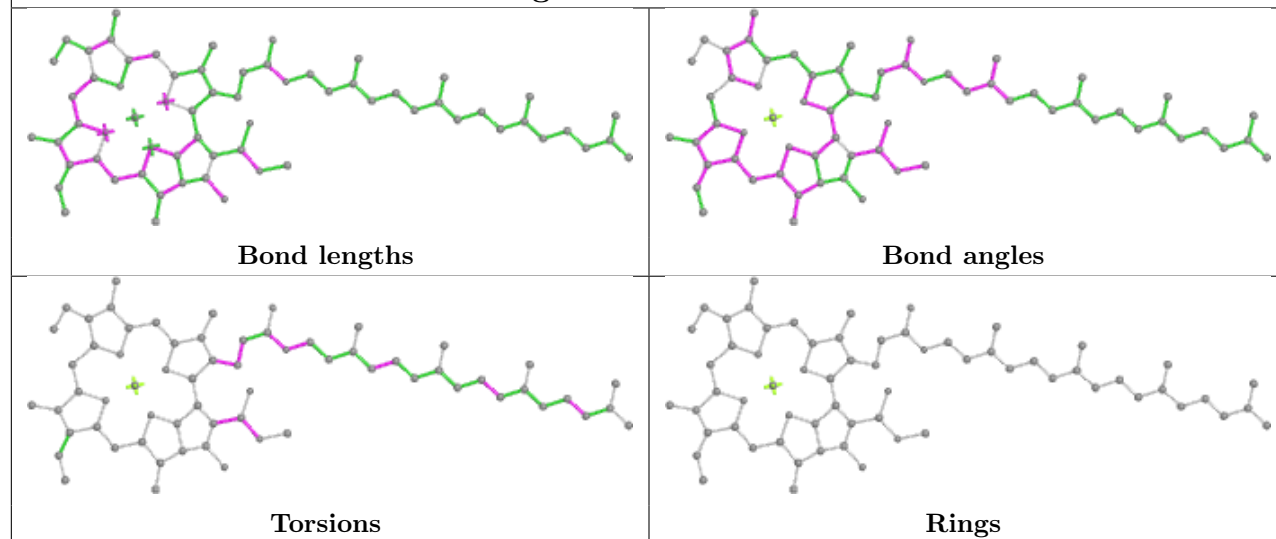
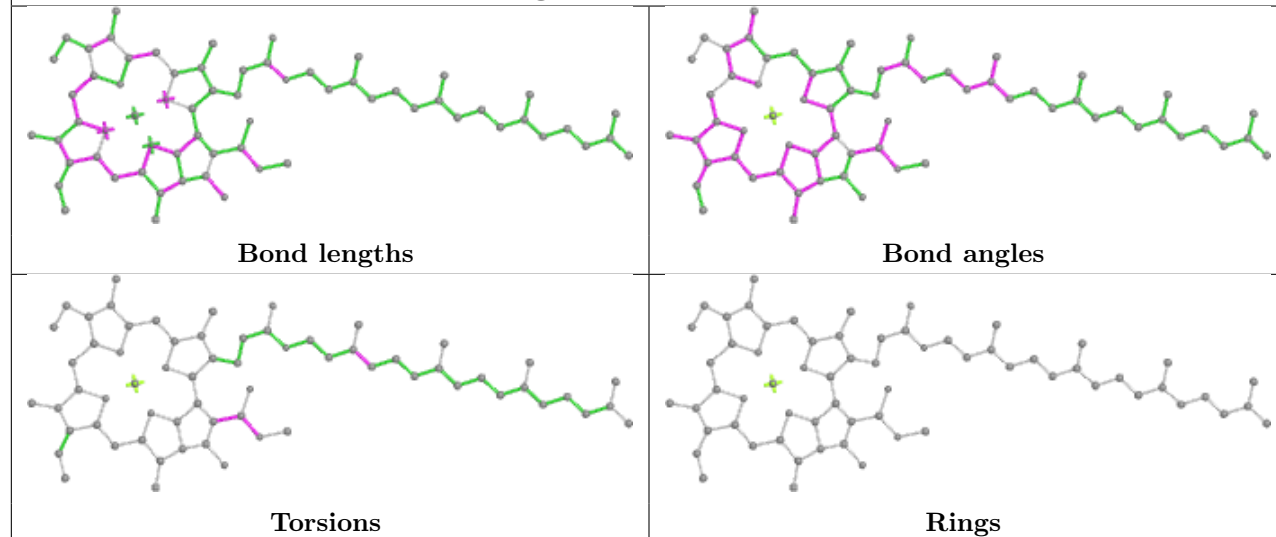
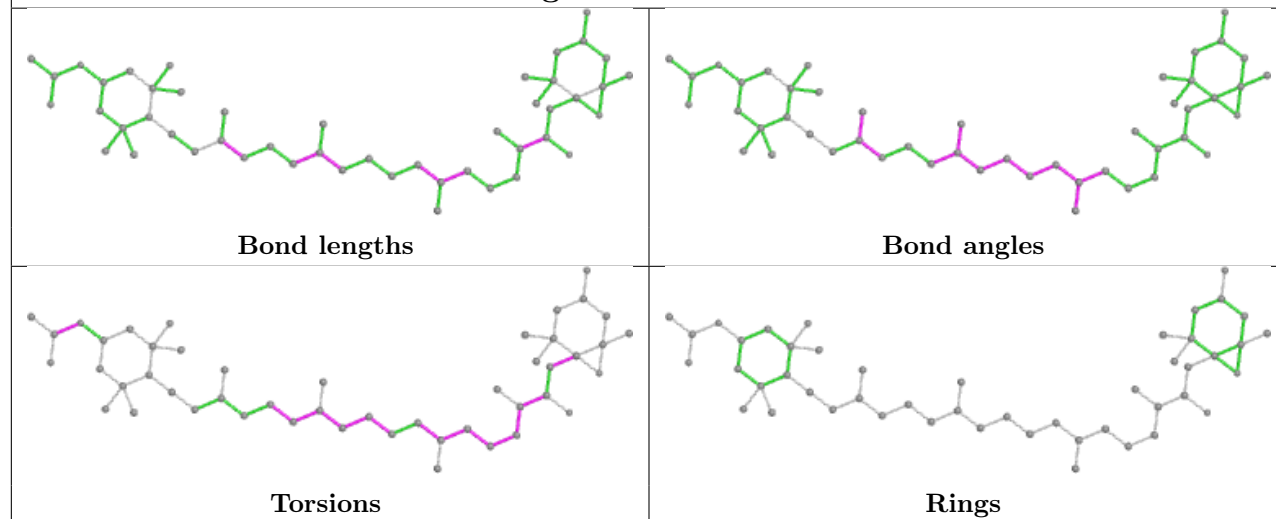


## Ligand KC1 5 313

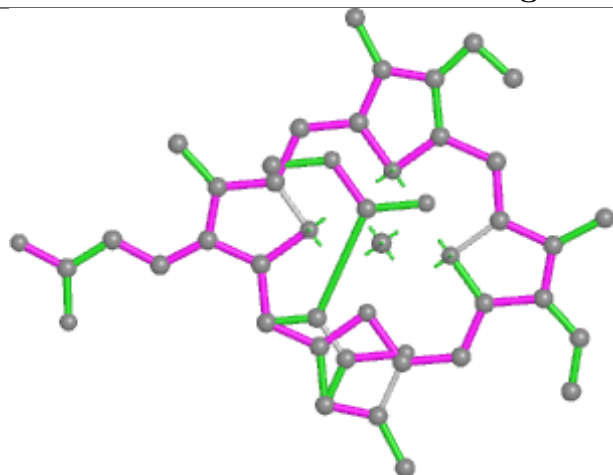


## Ligand BCR b 618

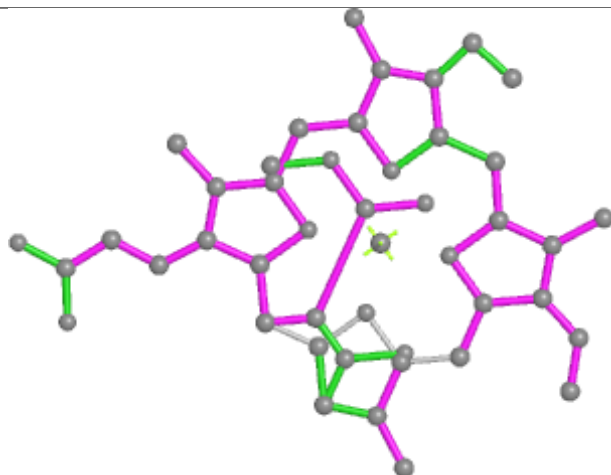


**Ligand CLA B 616****Ligand CLA B 609****Ligand A86 1 313**

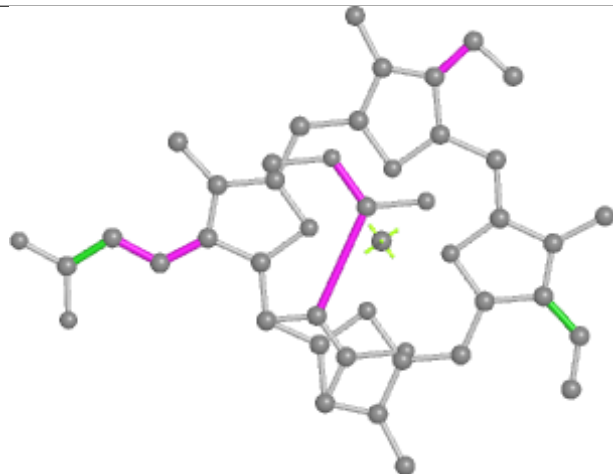
## Ligand KC1 2 313



Bond lengths



Bond angles

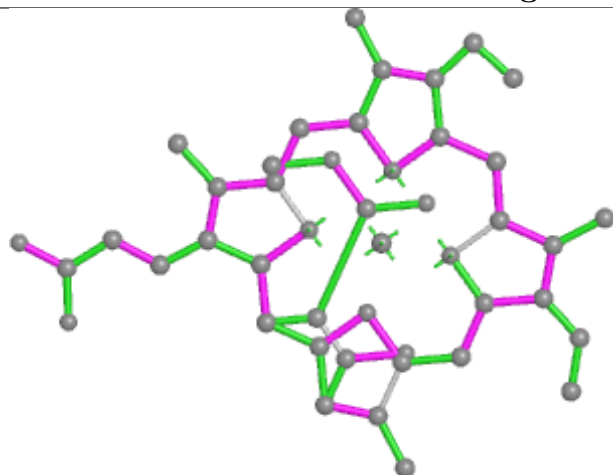


Torsions

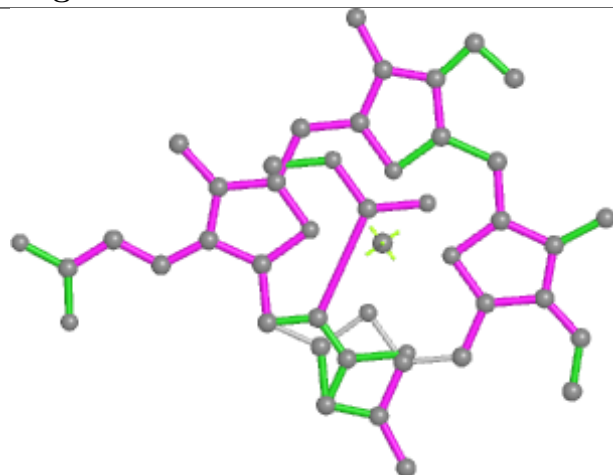


Rings

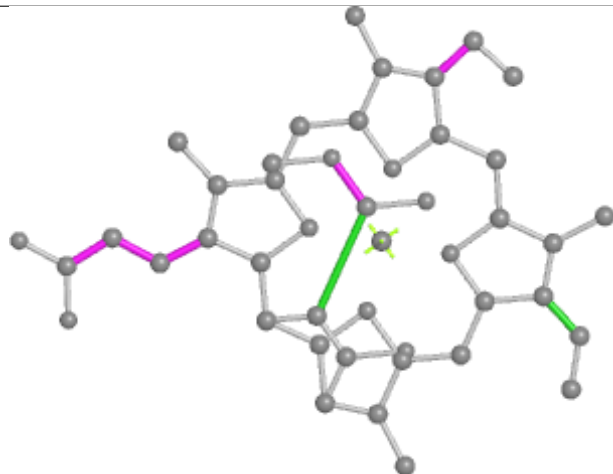
## Ligand KC1 g 313



Bond lengths



Bond angles

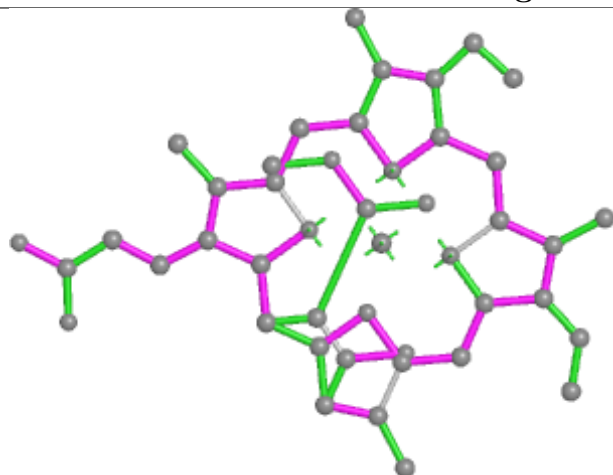


Torsions

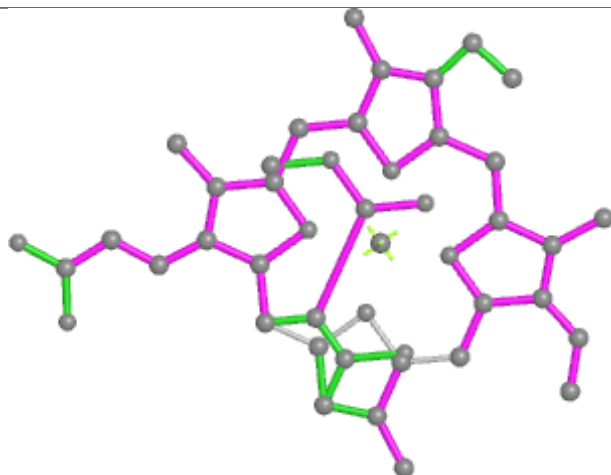


Rings

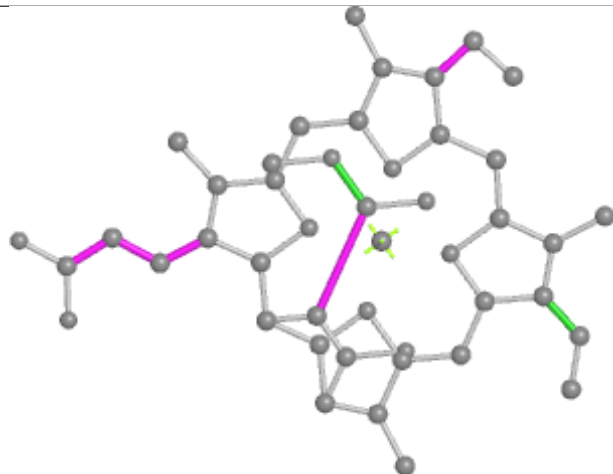
## Ligand KC1 G 307



Bond lengths



Bond angles



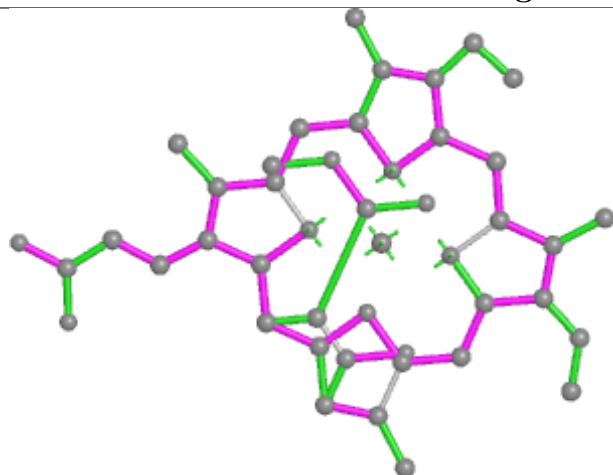
Torsions



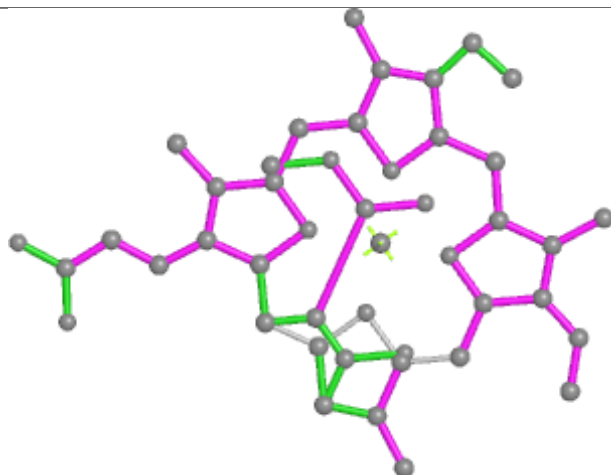
Rings



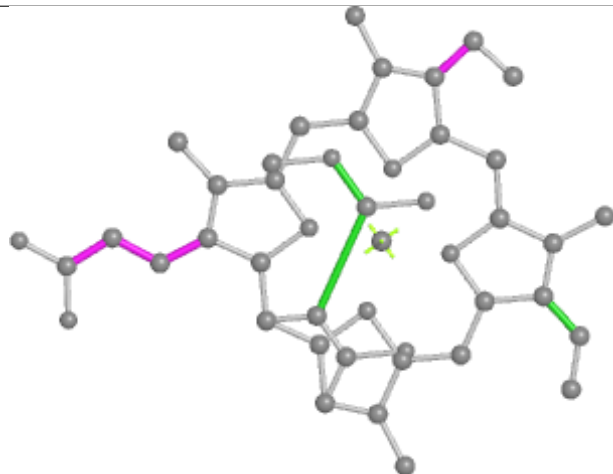
## Ligand KC1 G 308



Bond lengths



Bond angles

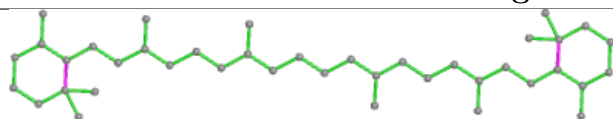


Torsions

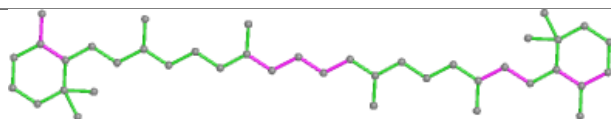


Rings

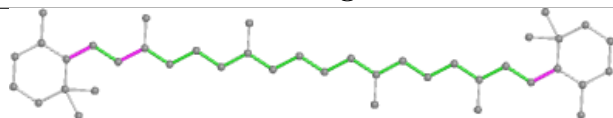
## Ligand BCR A 405



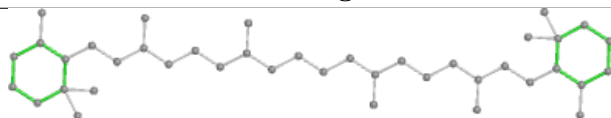
Bond lengths



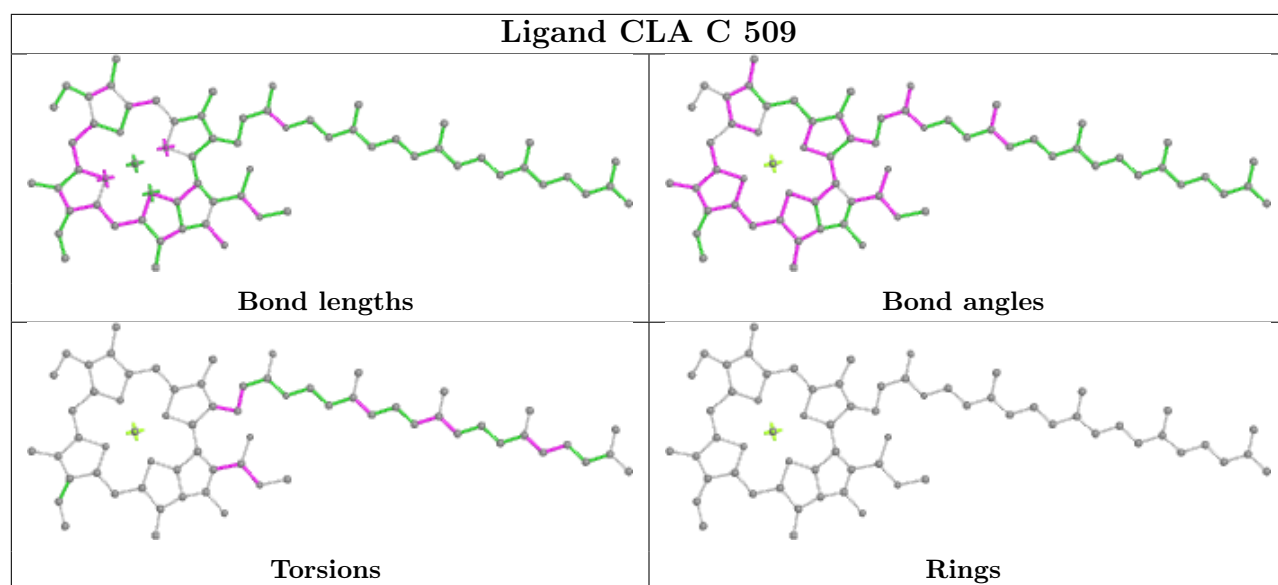
Bond angles

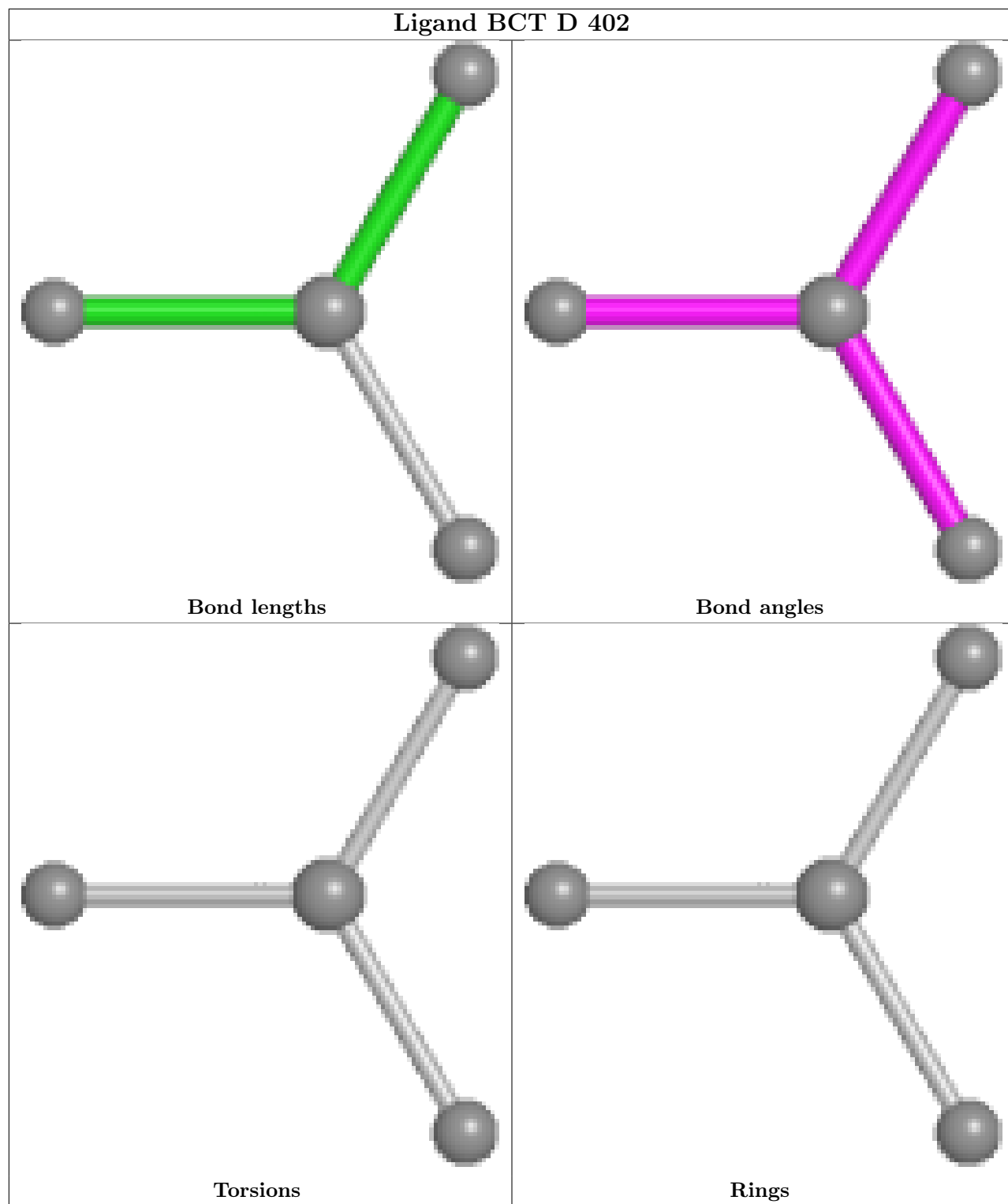


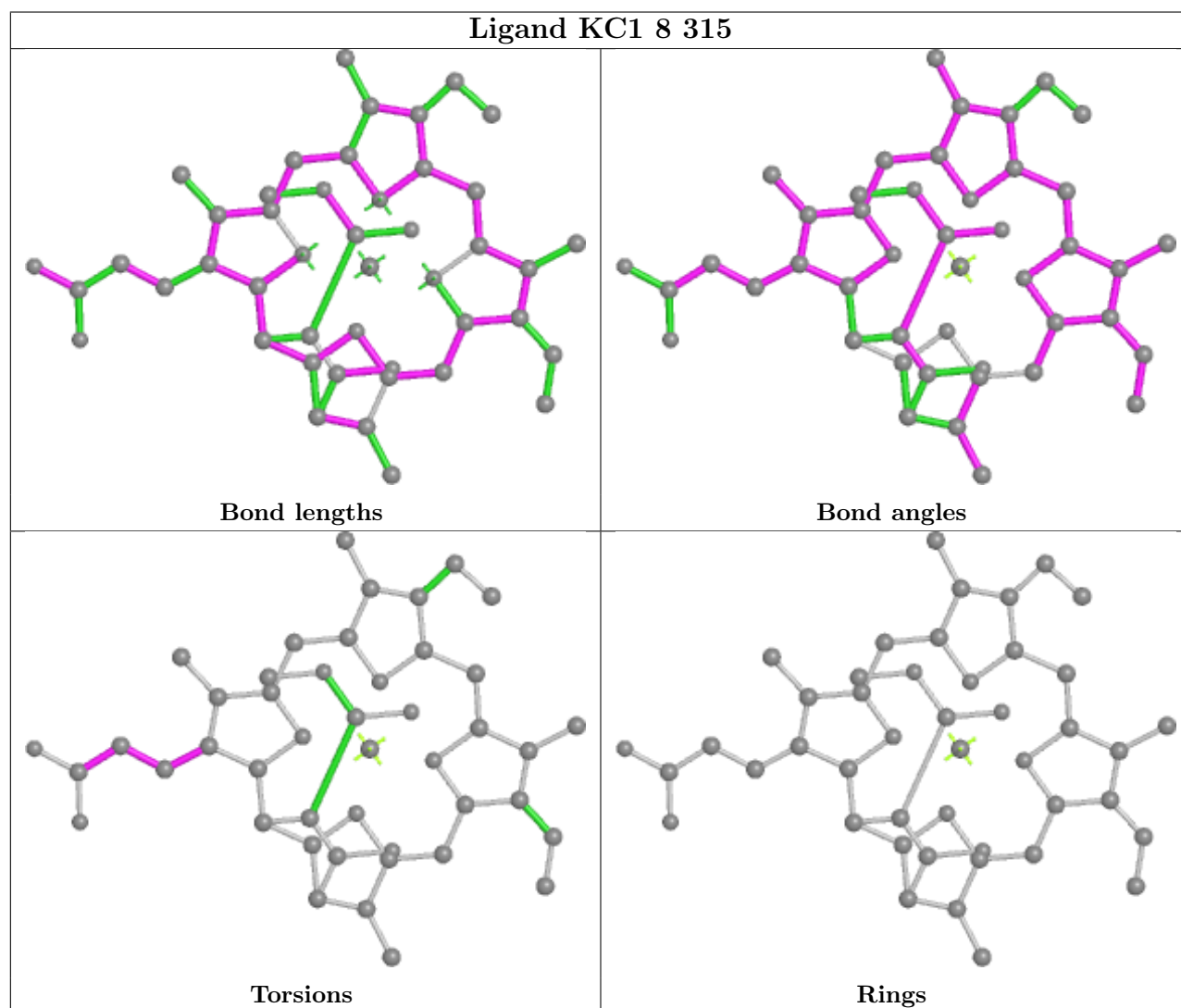
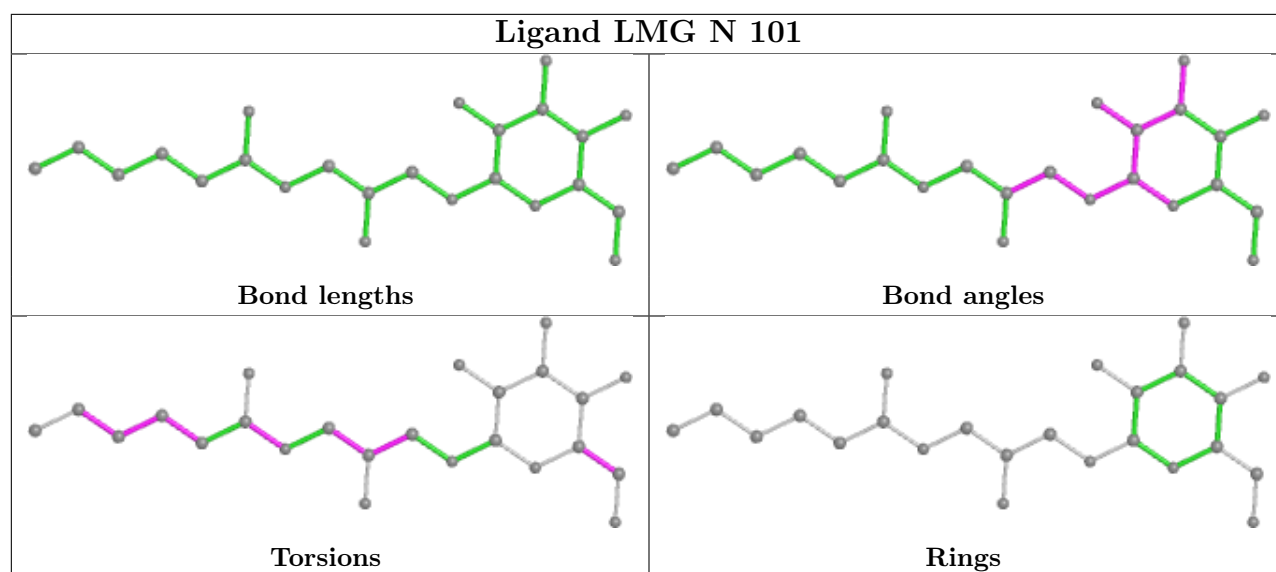
Torsions



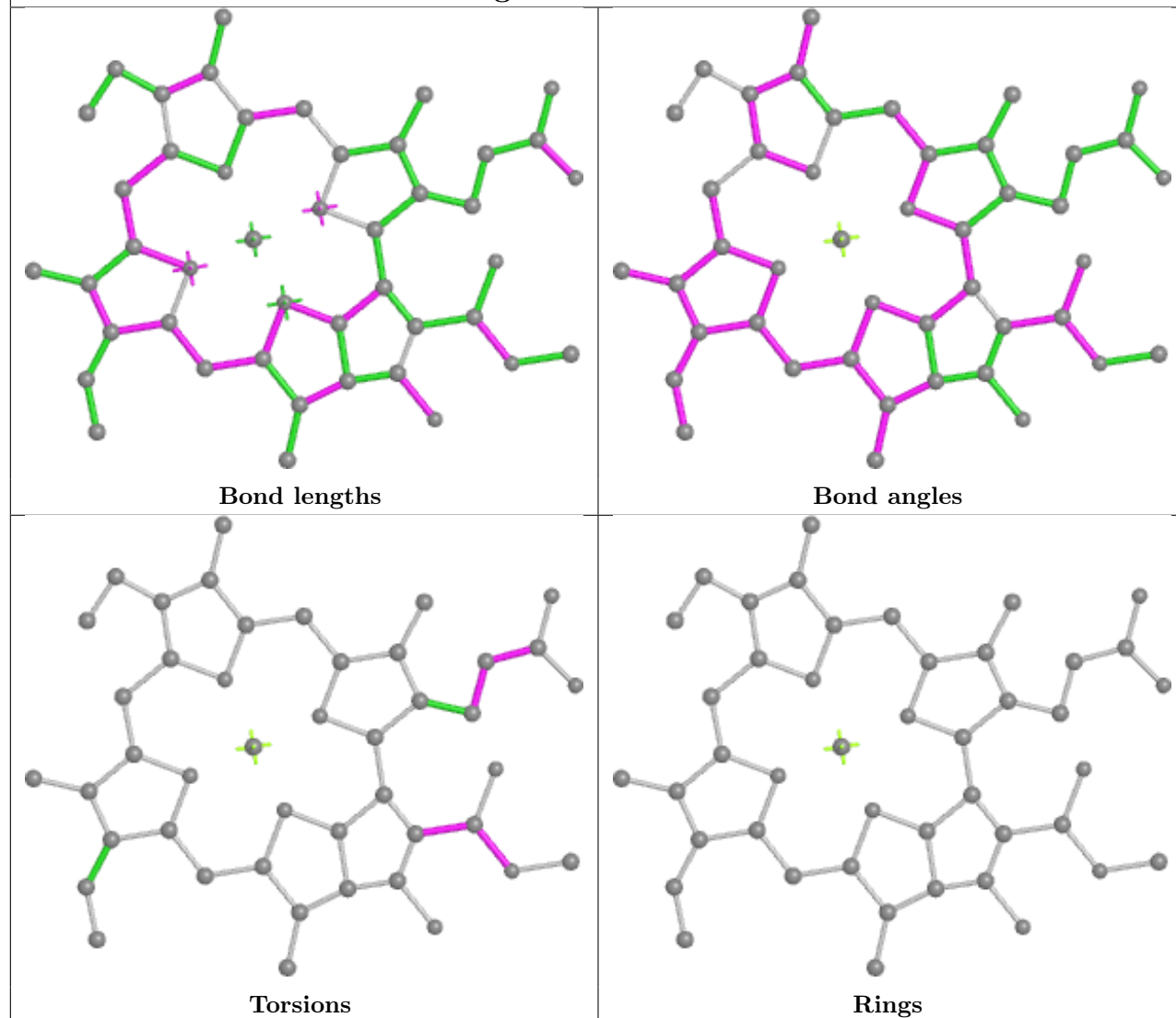
Rings



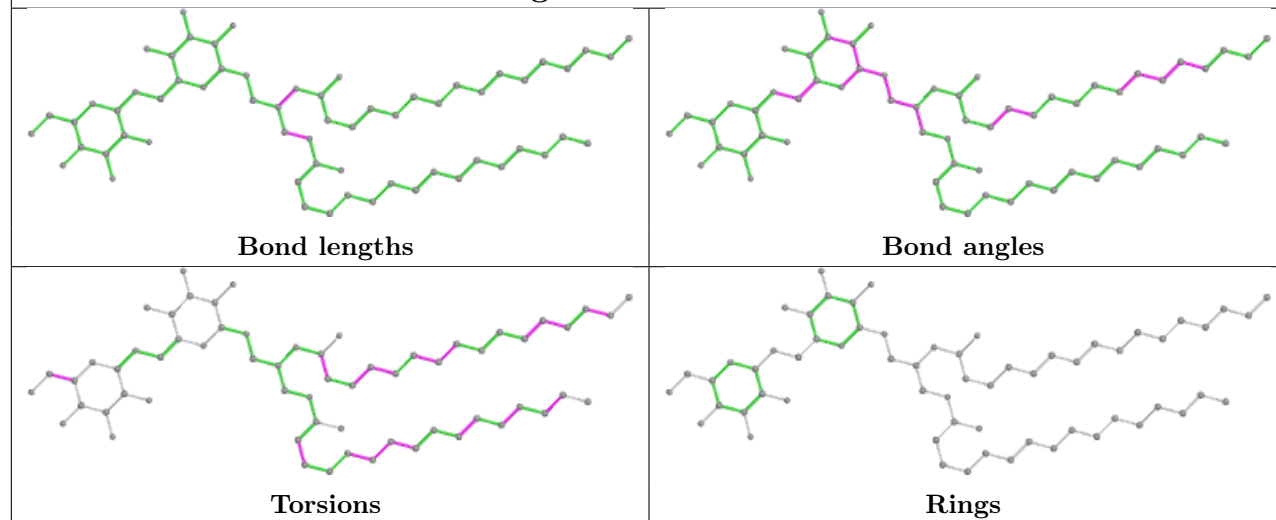


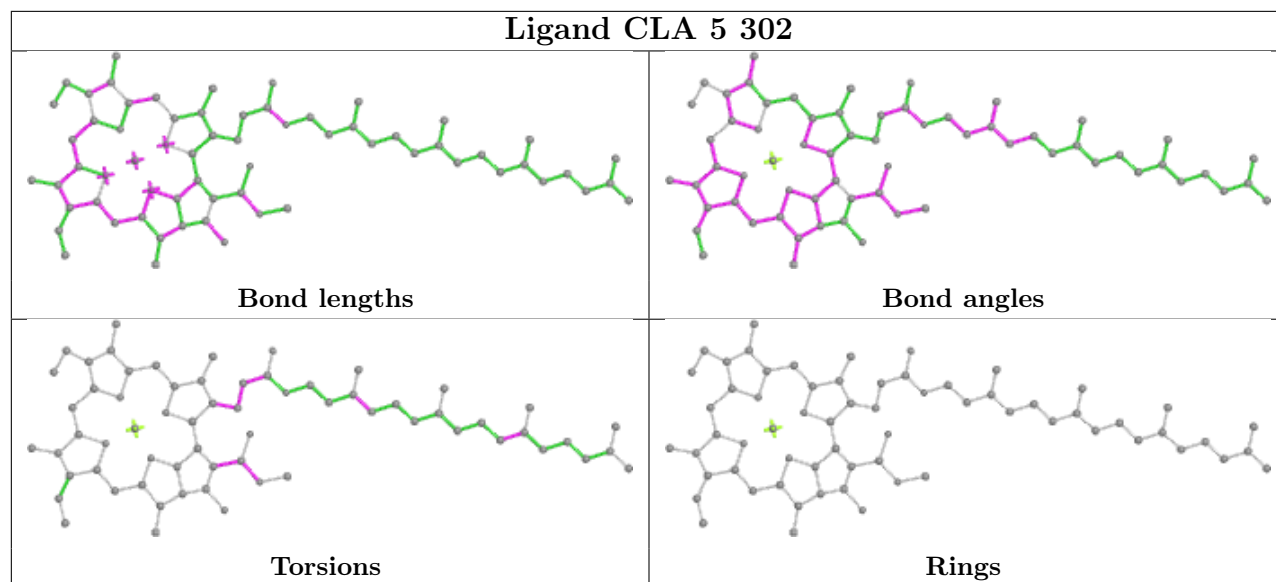
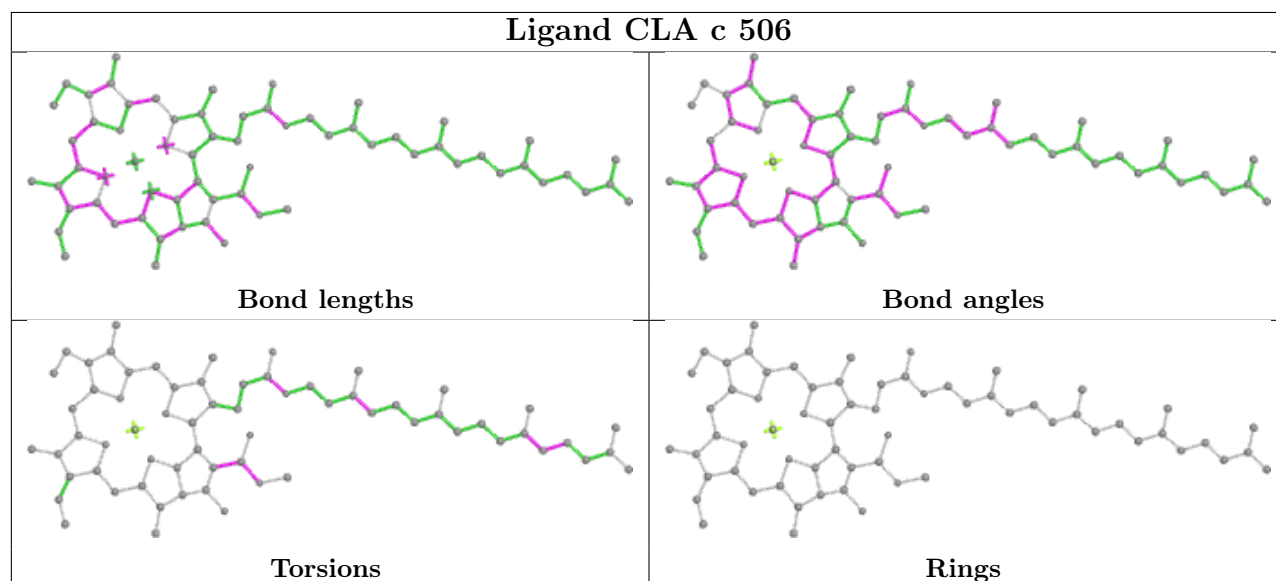
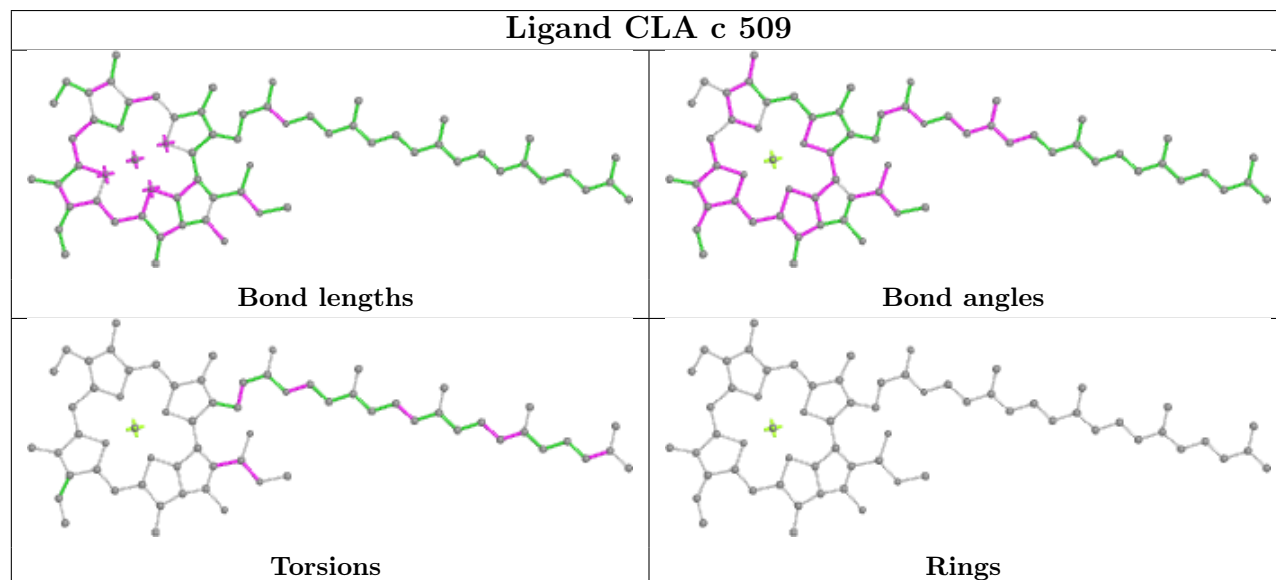


## Ligand CLA 2 306

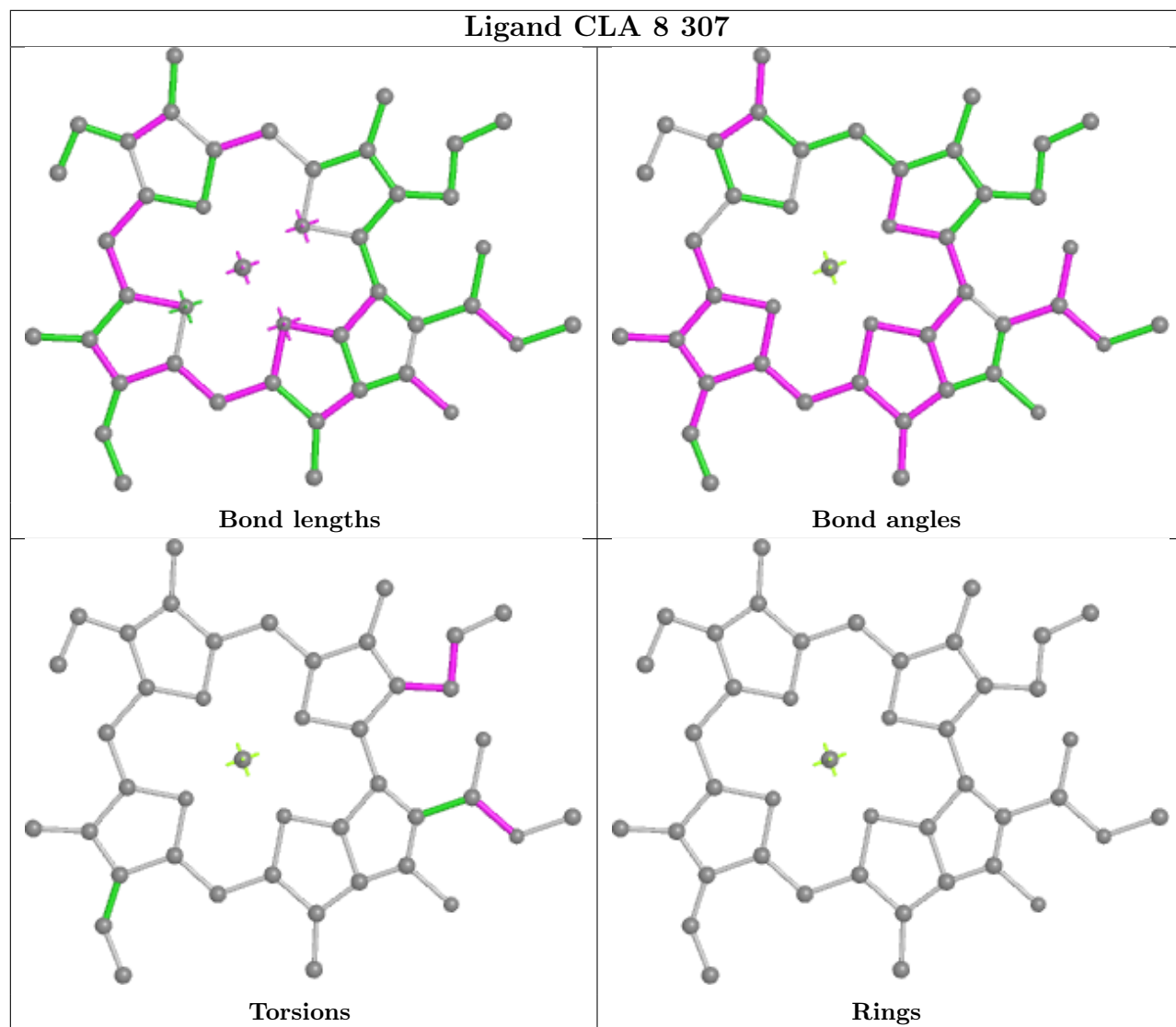


## Ligand DGD h 103

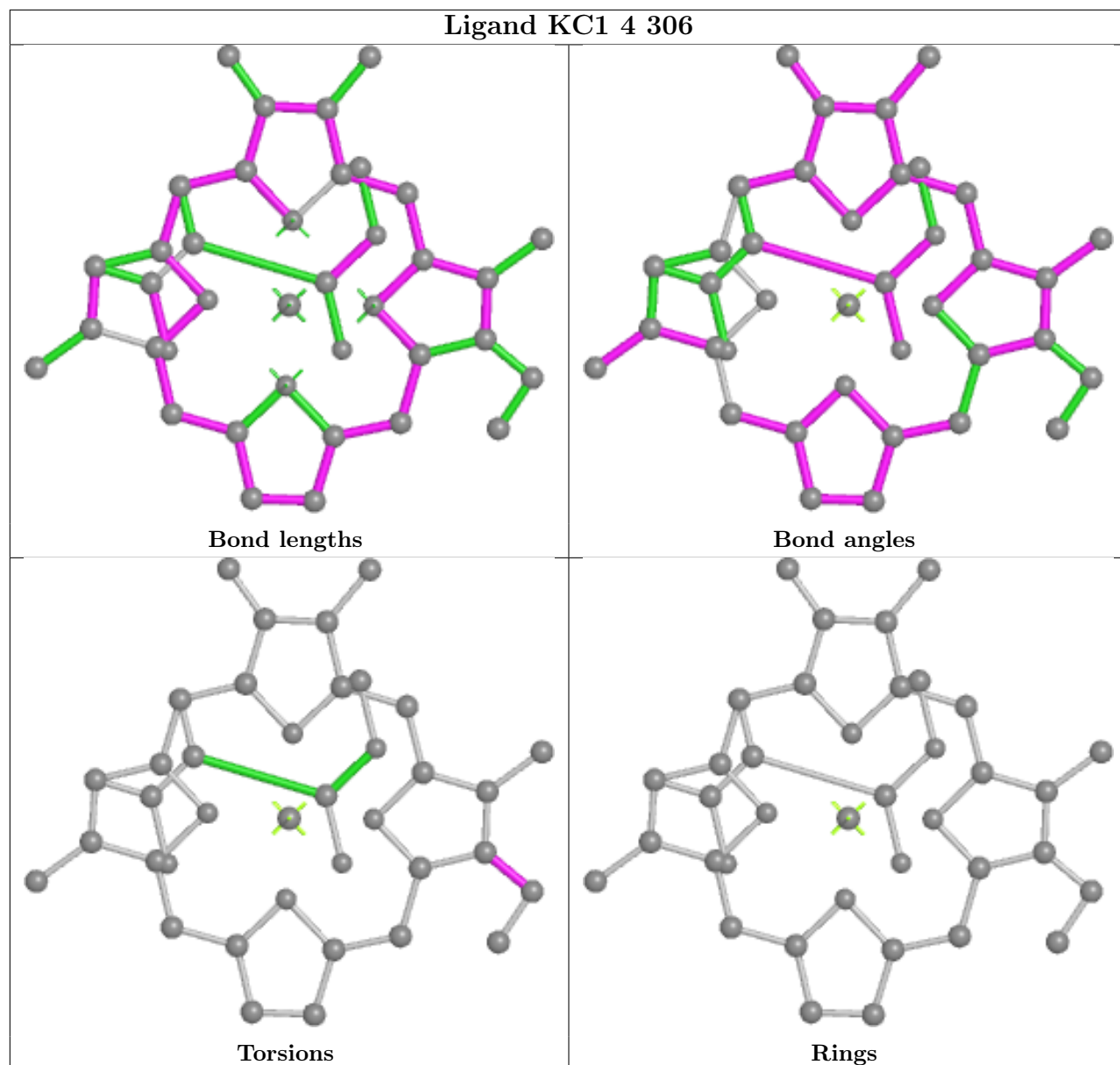


**Ligand CLA 5 302****Ligand CLA c 506****Ligand CLA c 509**

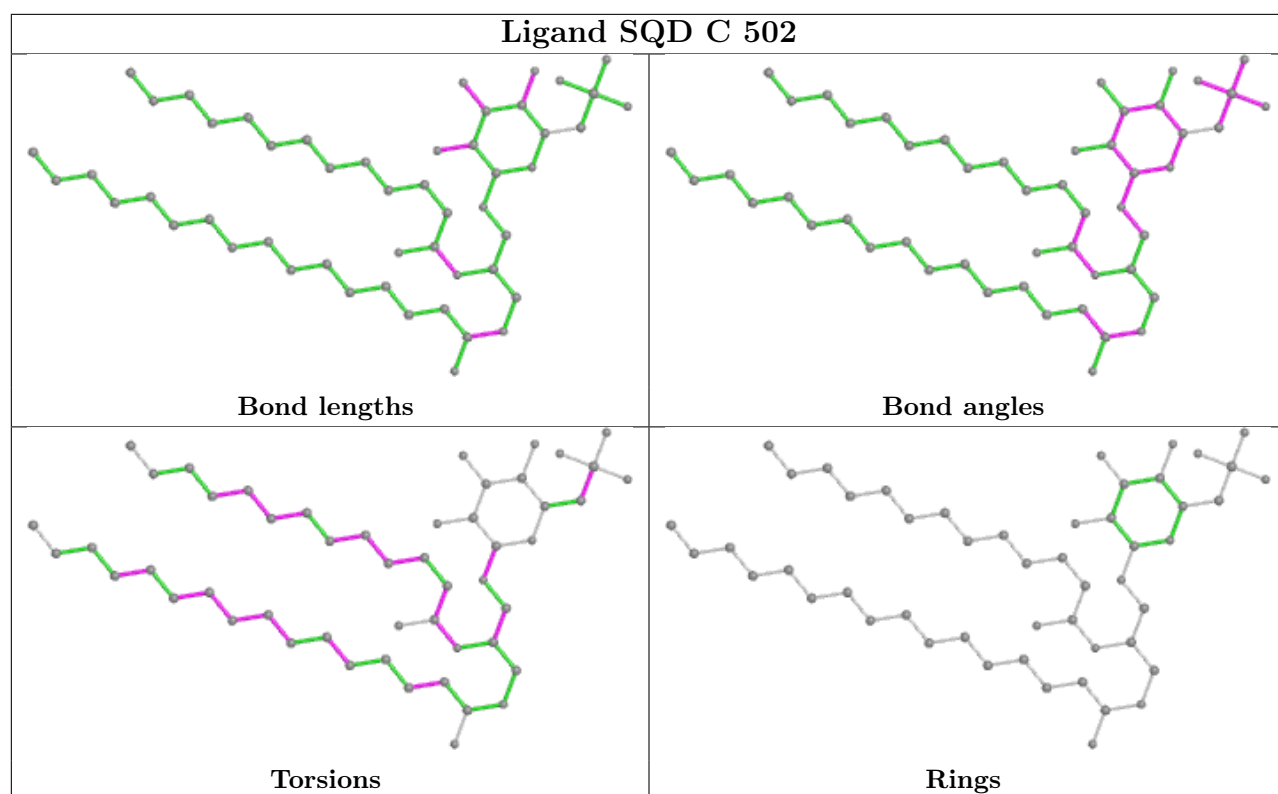
## Ligand CLA 8 307



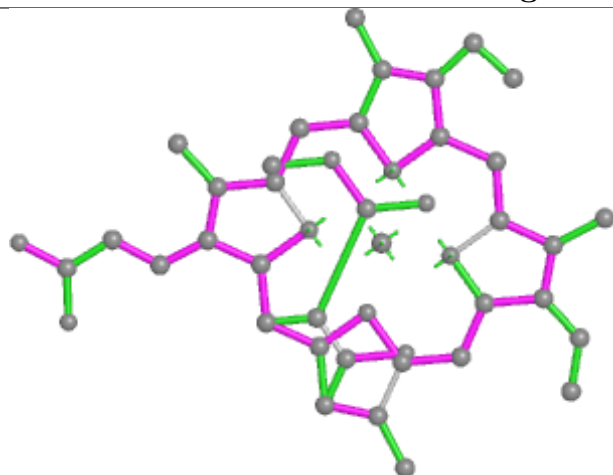
## Ligand KC1 4 306



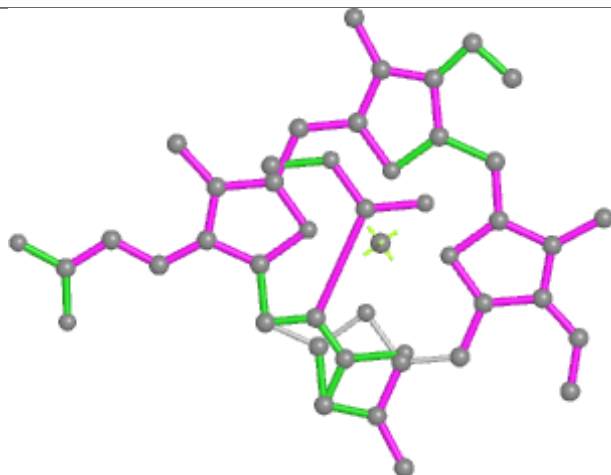




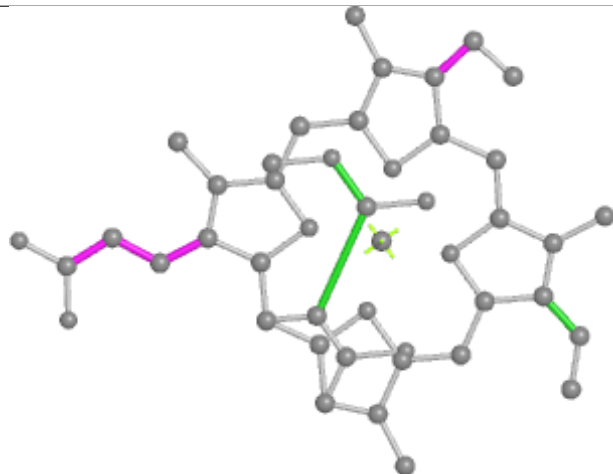
## Ligand KC1 9 306



Bond lengths



Bond angles

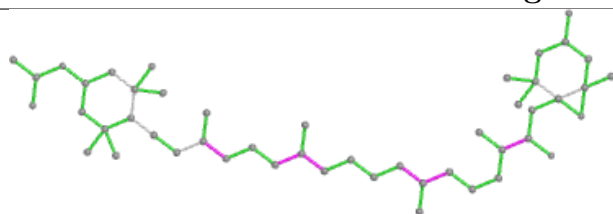


Torsions

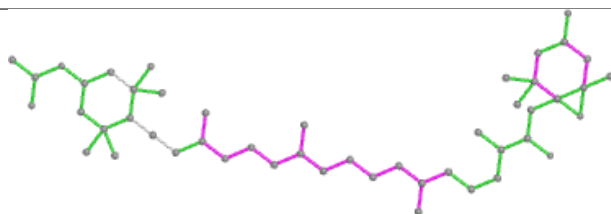


Rings

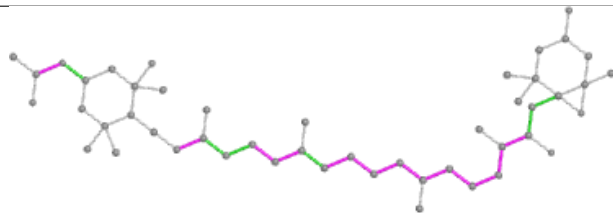
## Ligand A86 2 309



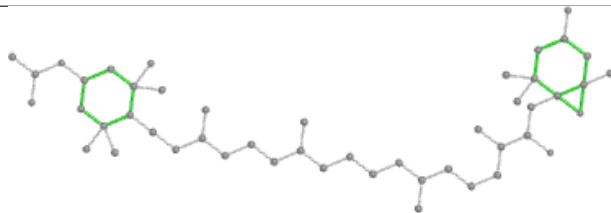
Bond lengths



Bond angles

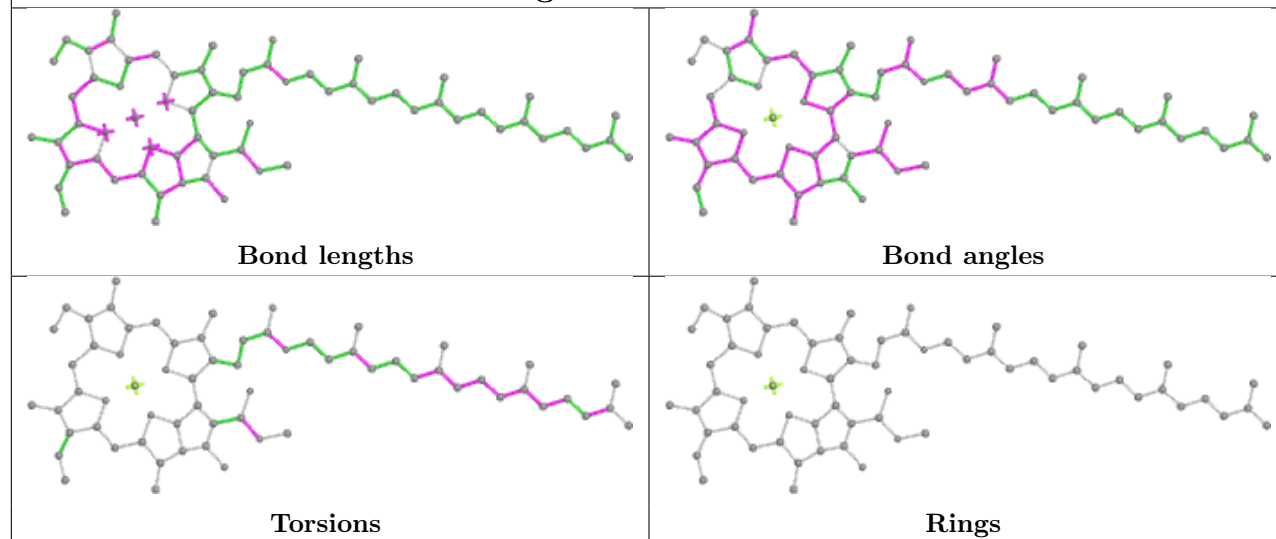


Torsions

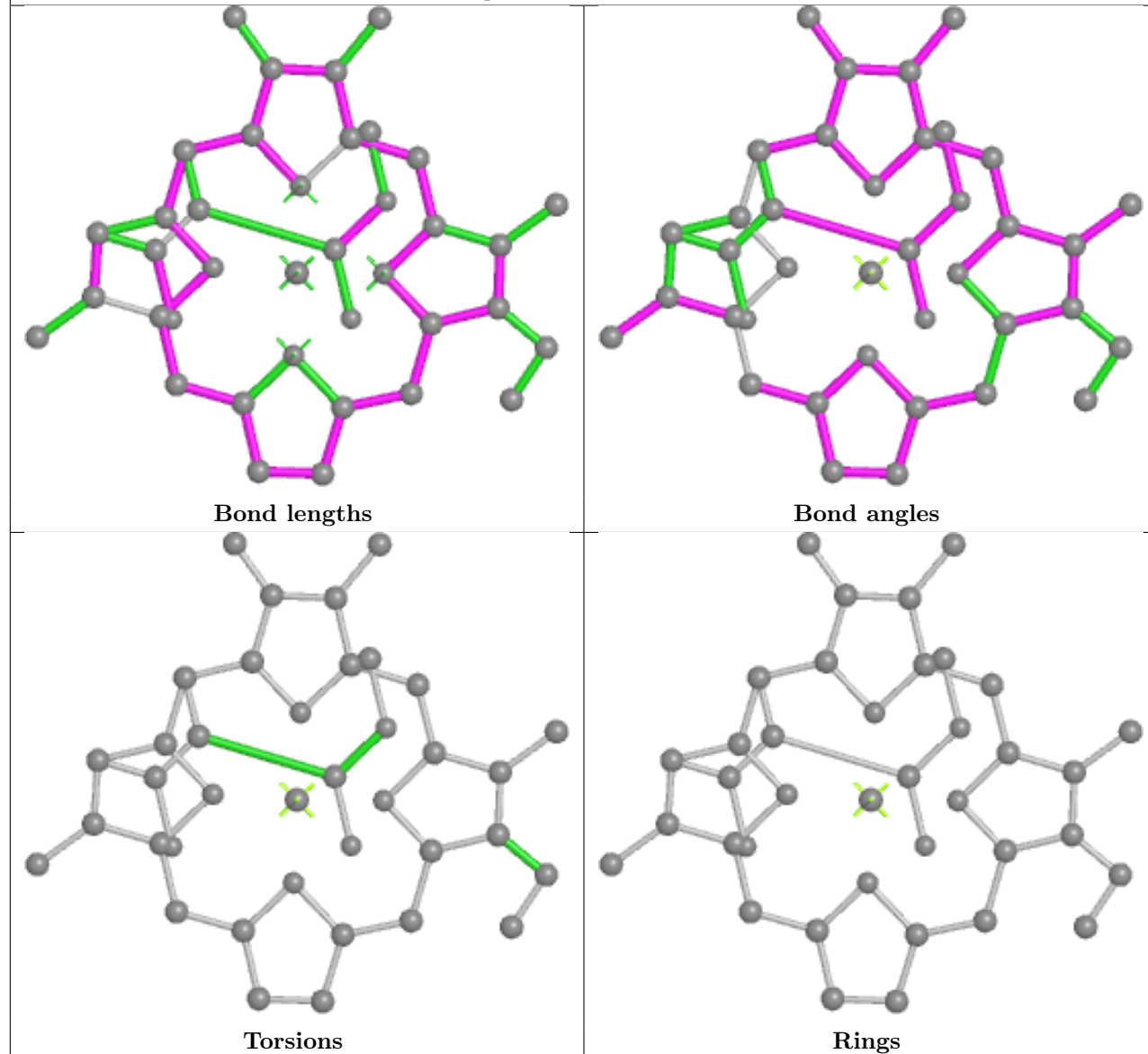


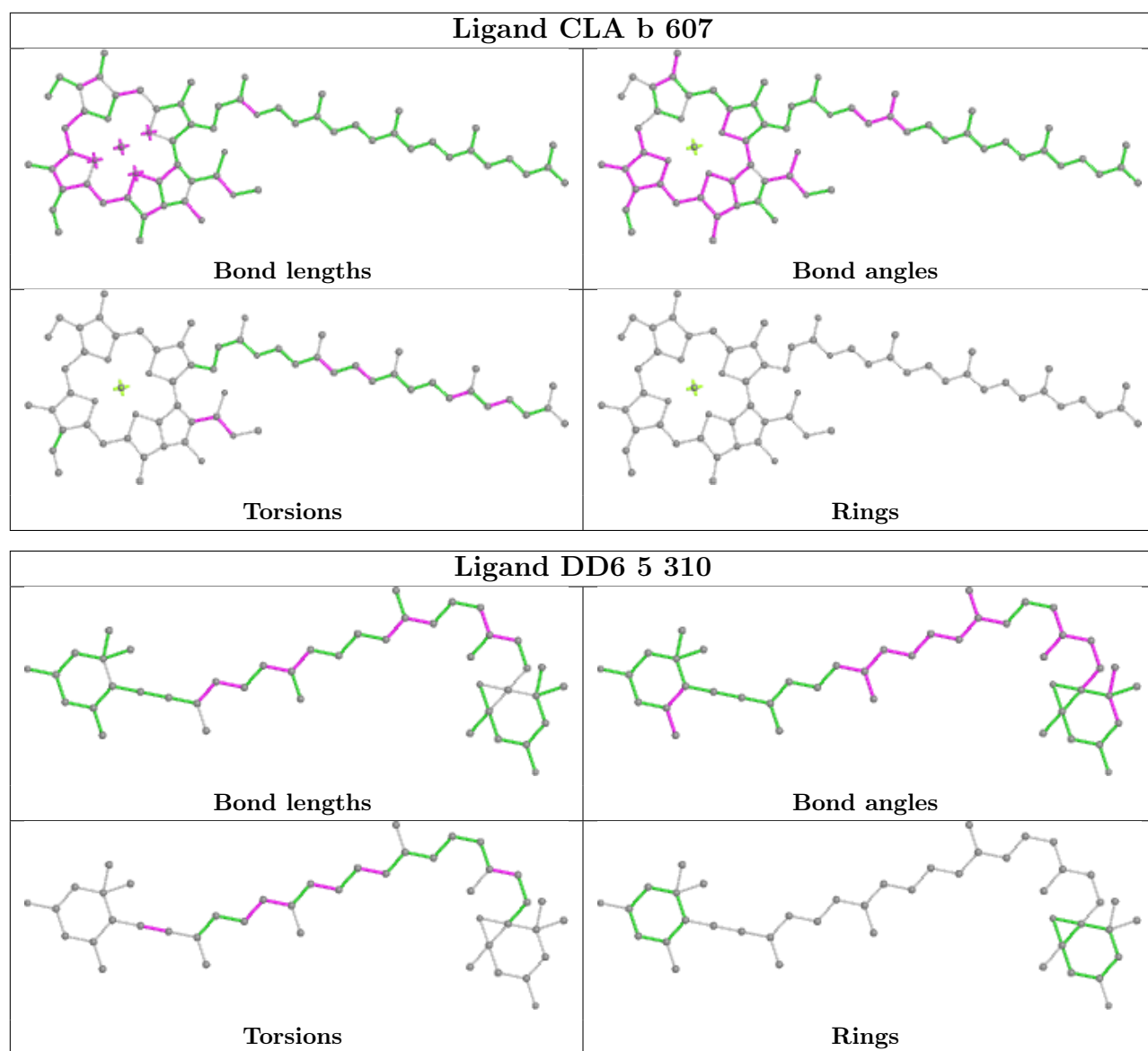
Rings

## Ligand CLA 5 309

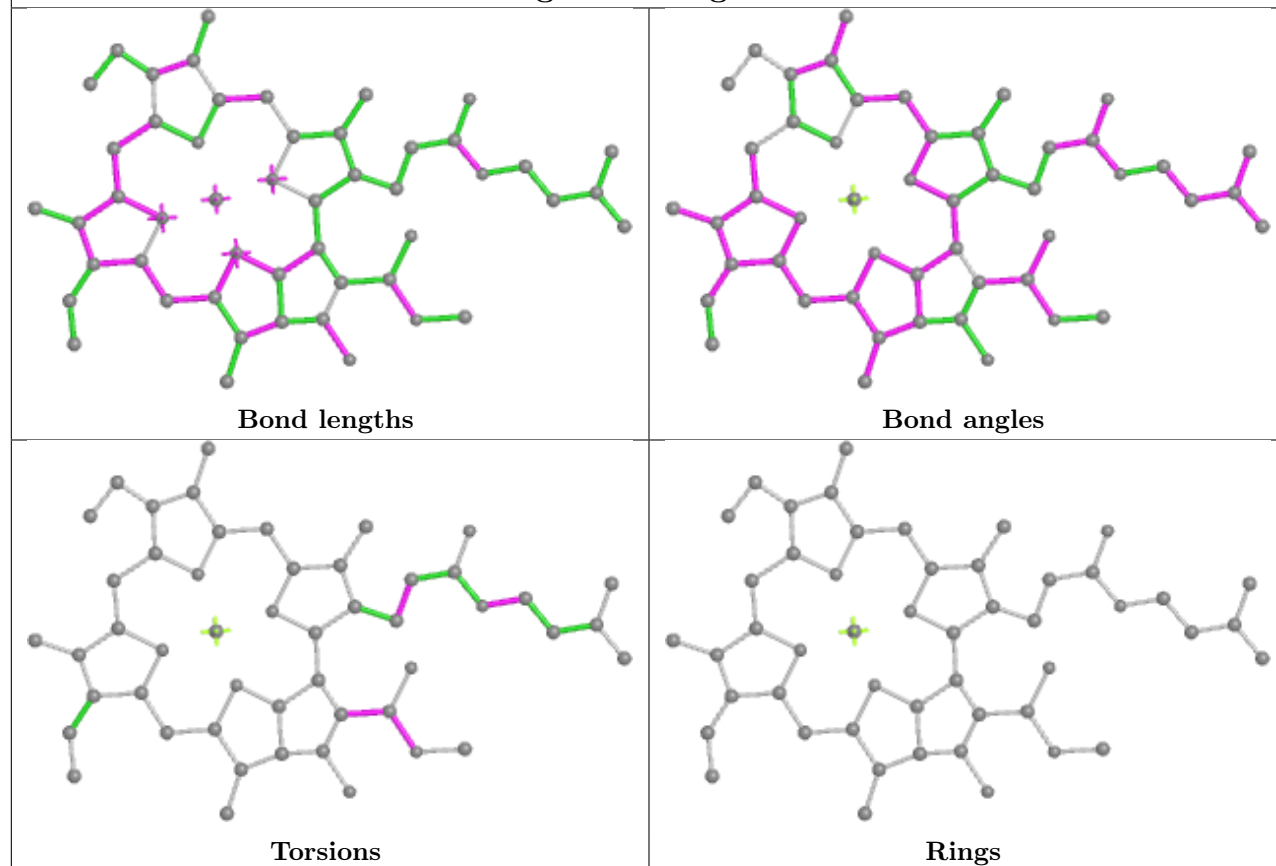


## Ligand KC1 G 306

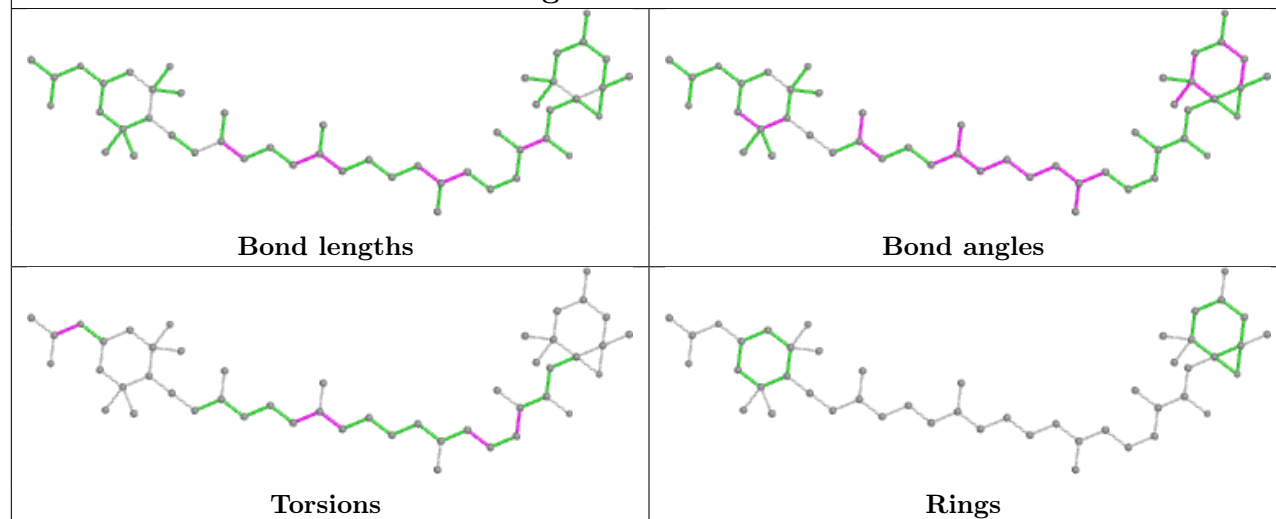




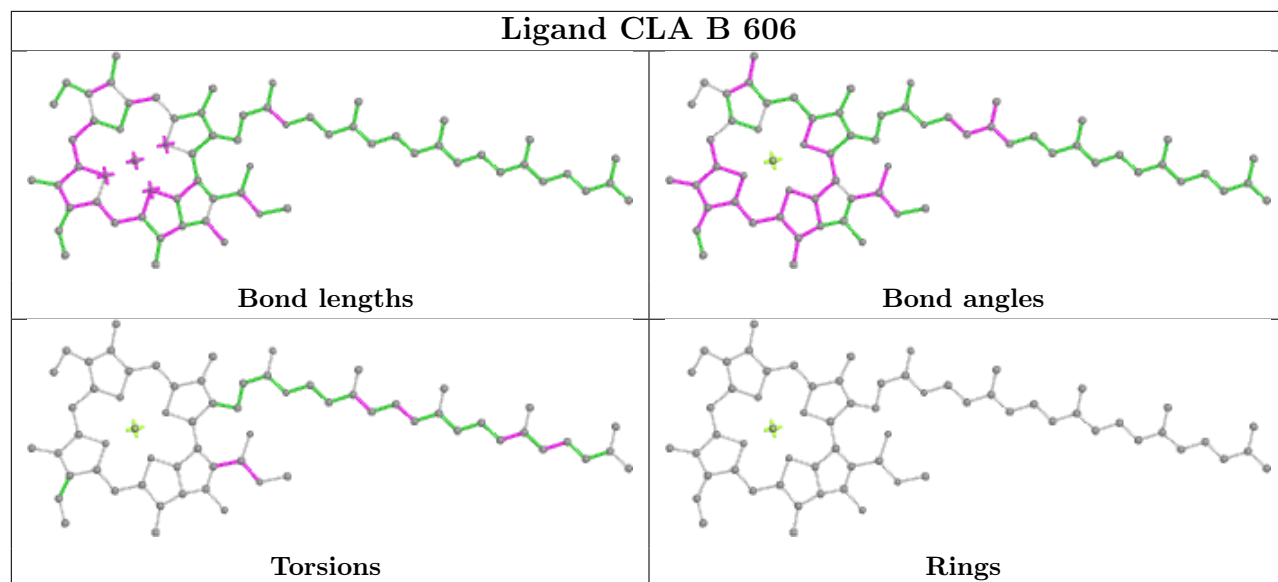
## Ligand CLA g 309



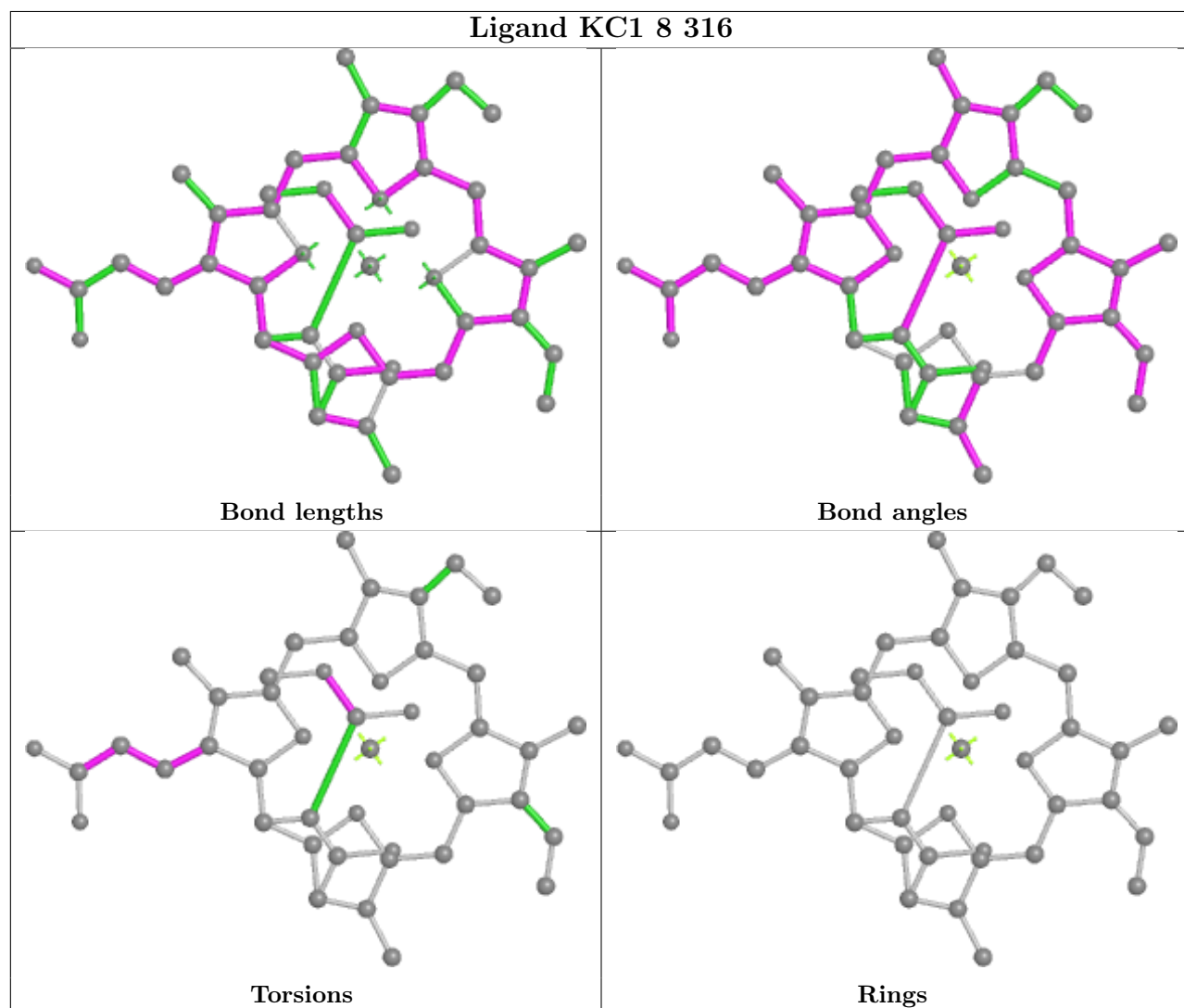
## Ligand A86 2 308



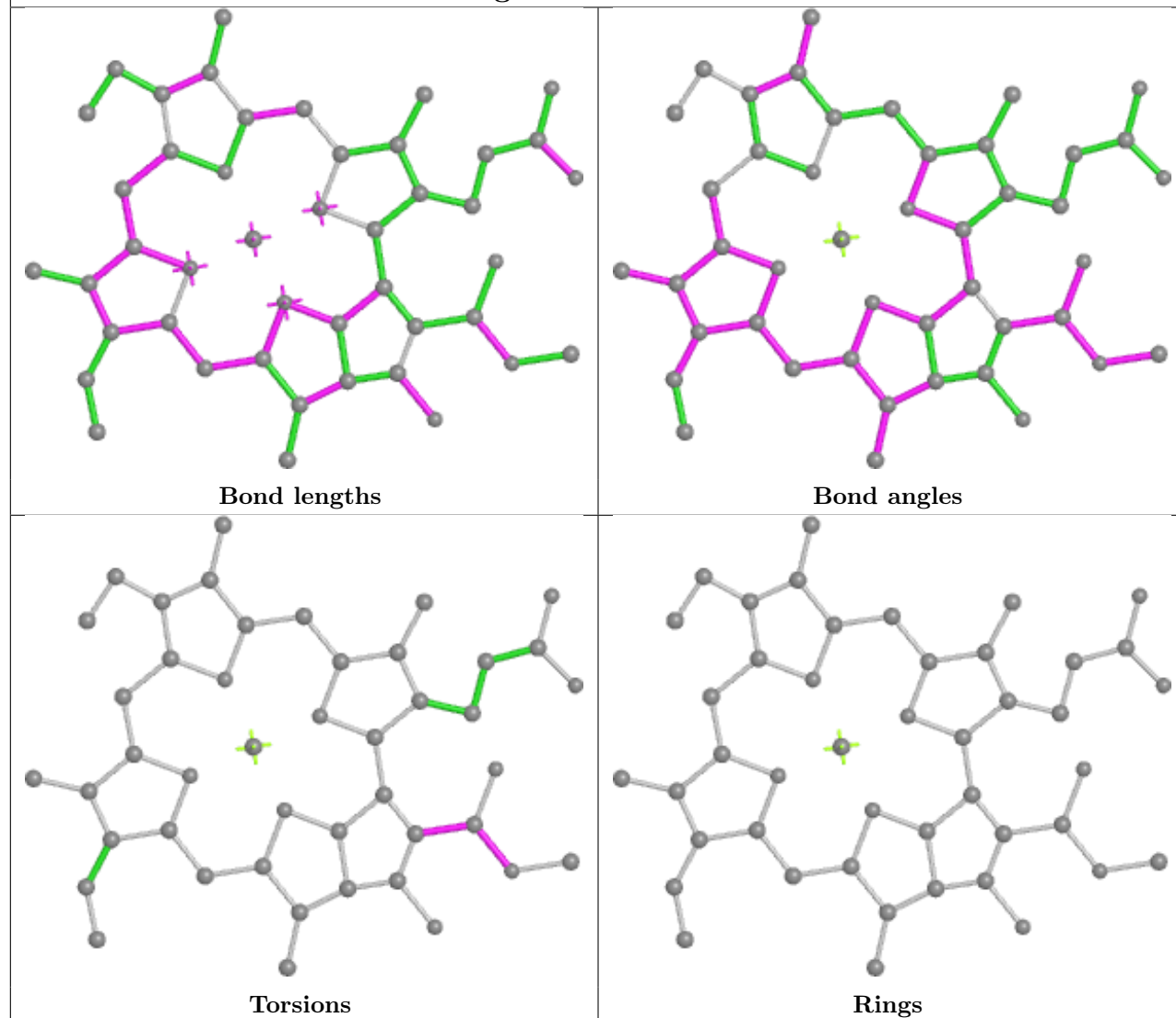
## Ligand CLA B 606



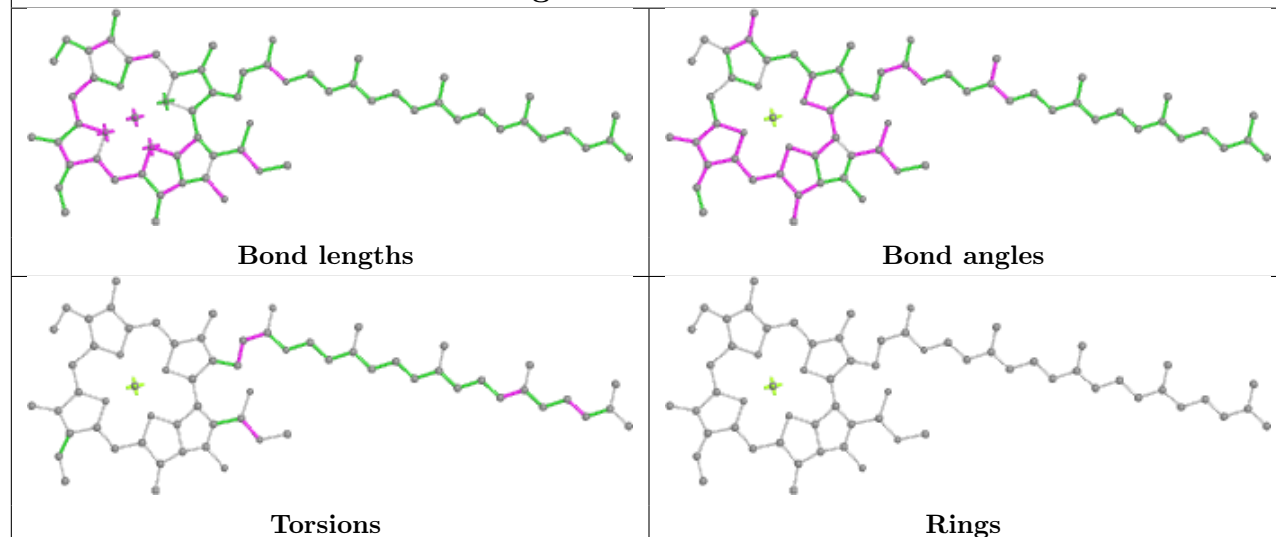
## Ligand KC1 8 316

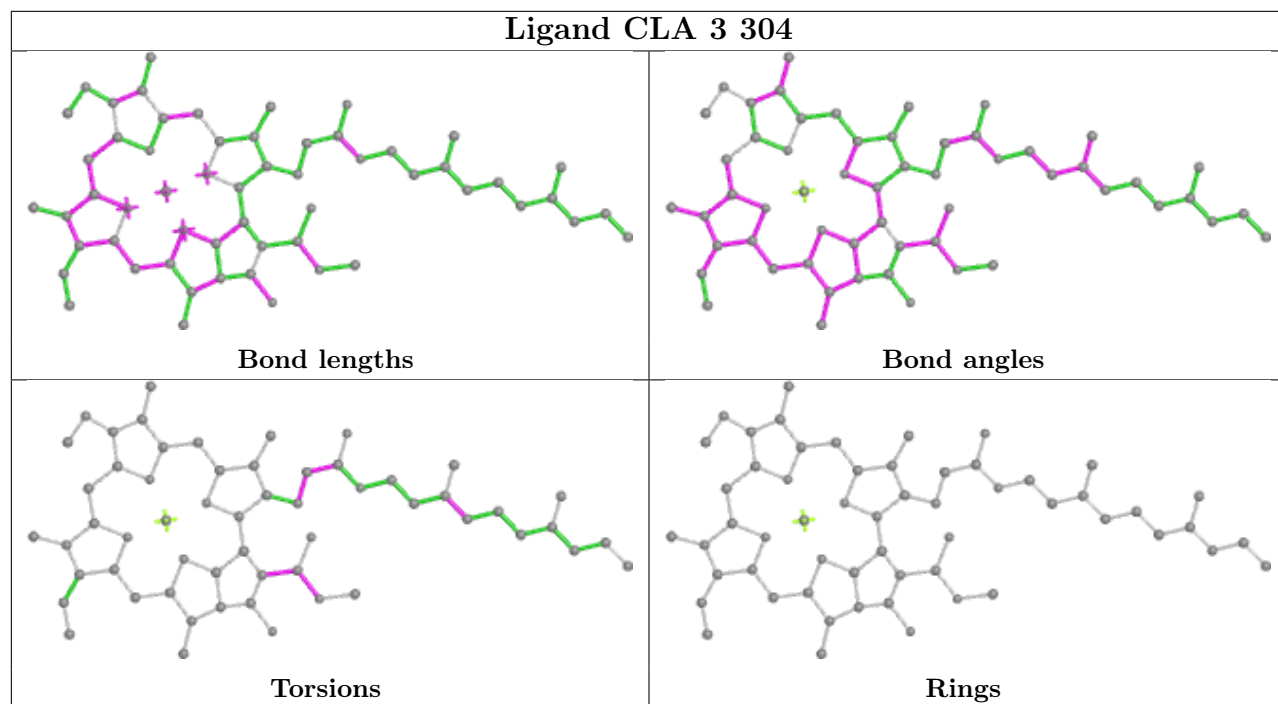


## Ligand CLA 6 302



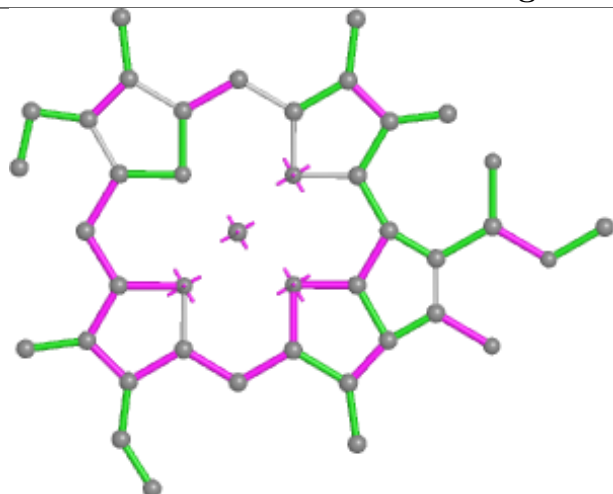
## Ligand CLA B 610



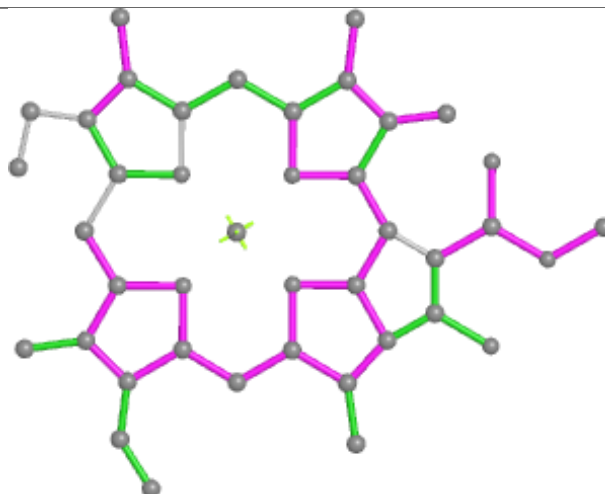




## Ligand CLA 8 305



Bond lengths



Bond angles

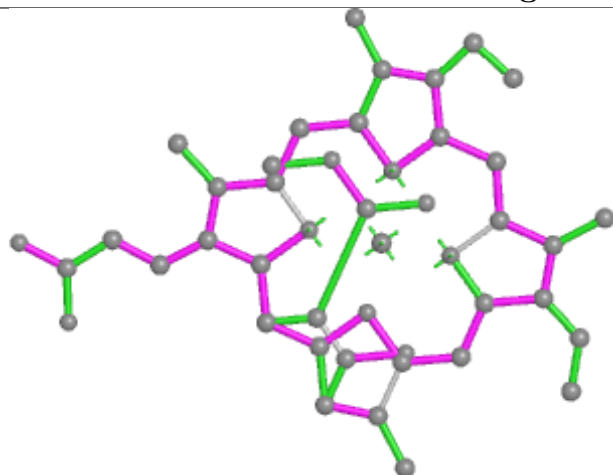


Torsions

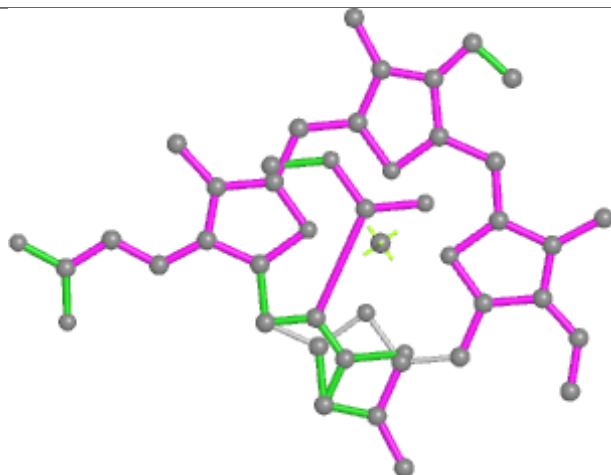


Rings

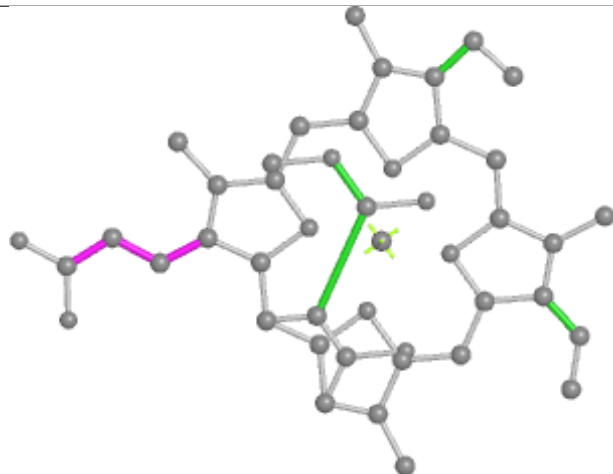
## Ligand KC1 J 312



Bond lengths



Bond angles

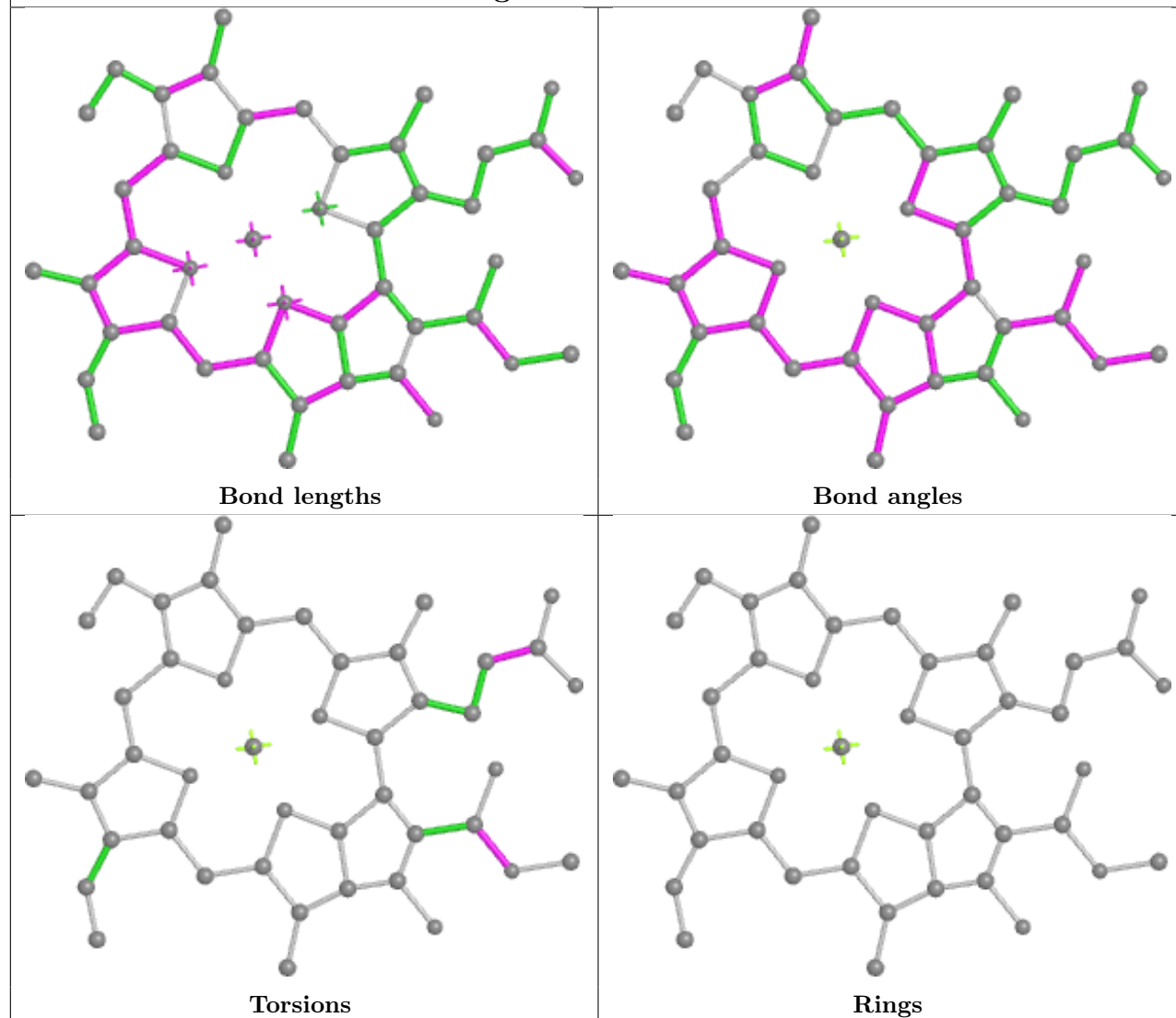


Torsions

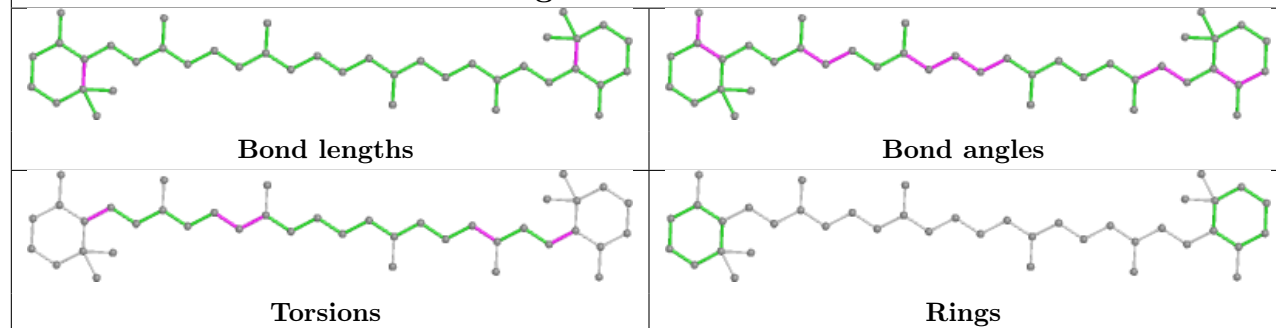


Rings

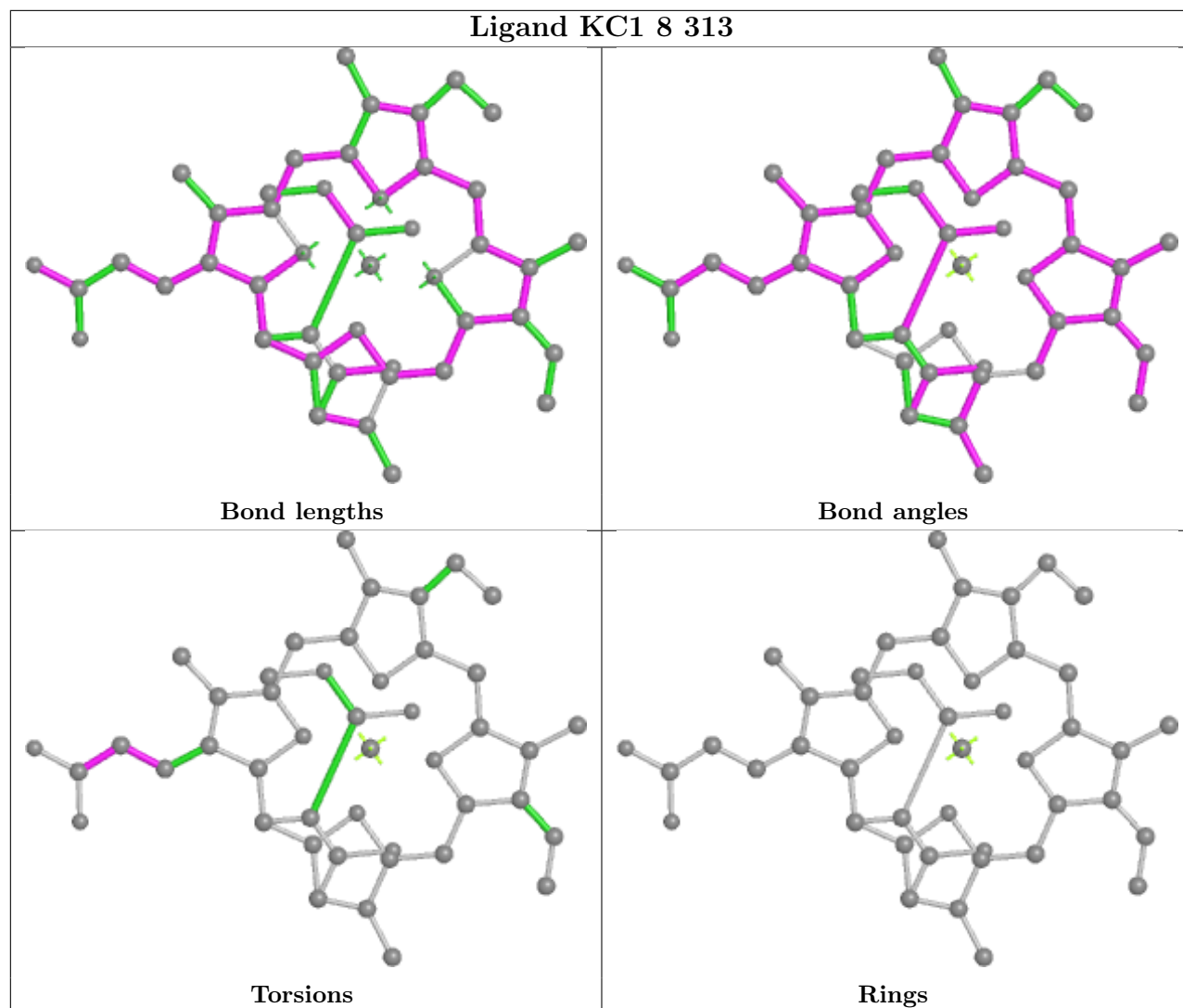
## Ligand CLA J 305



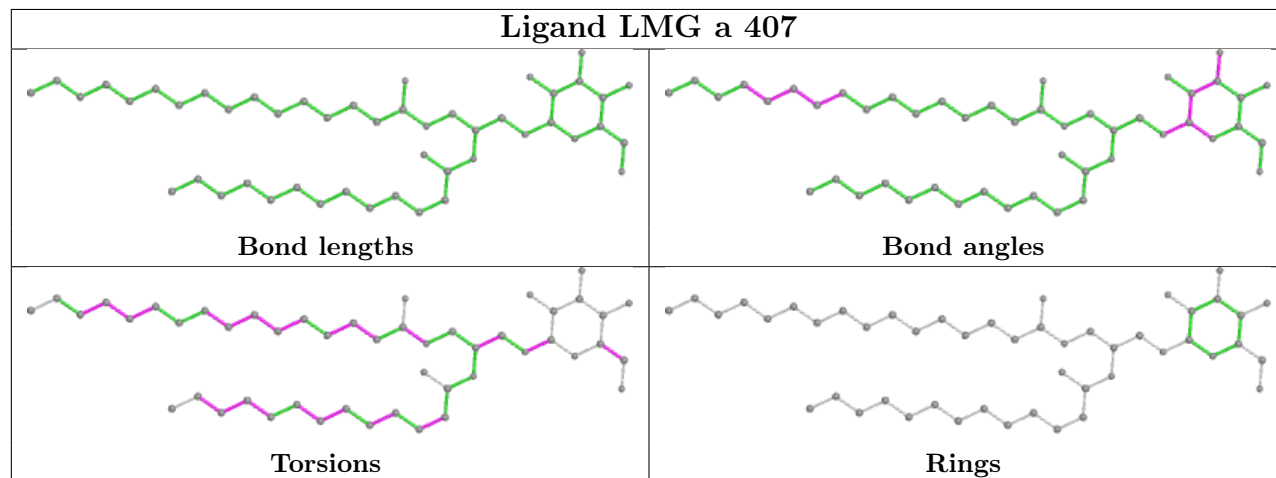
## Ligand BCR c 501

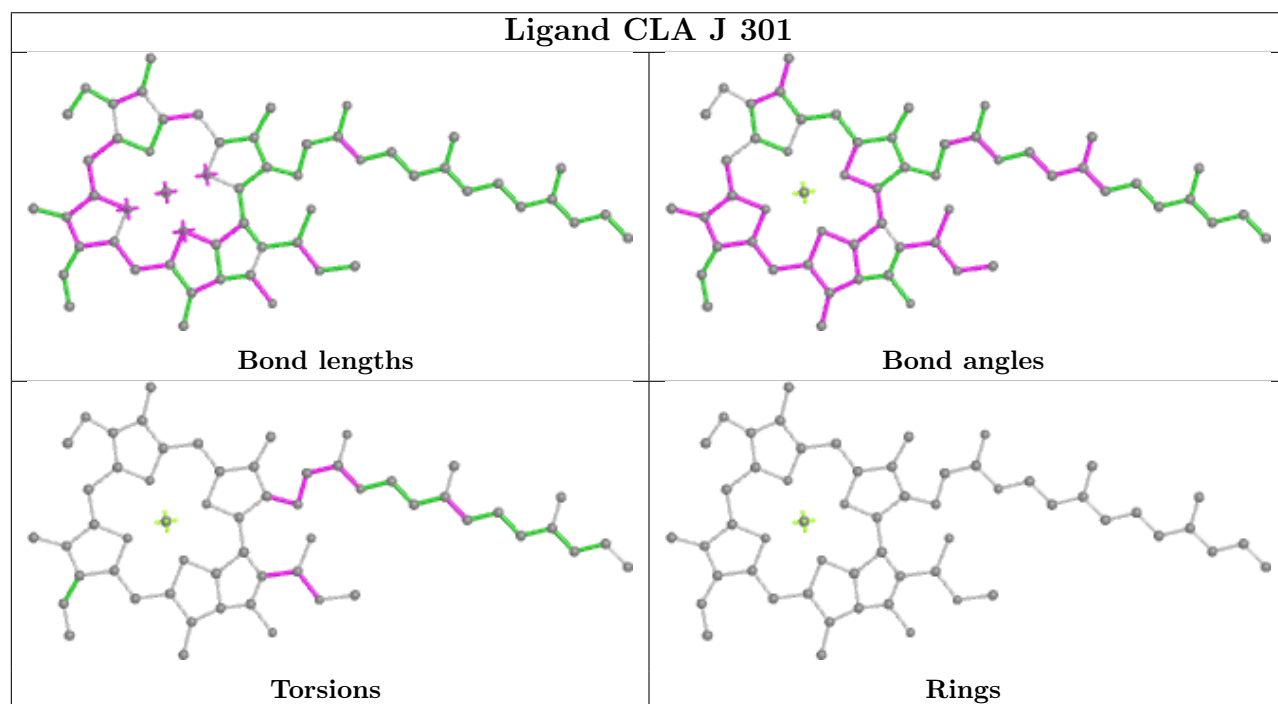
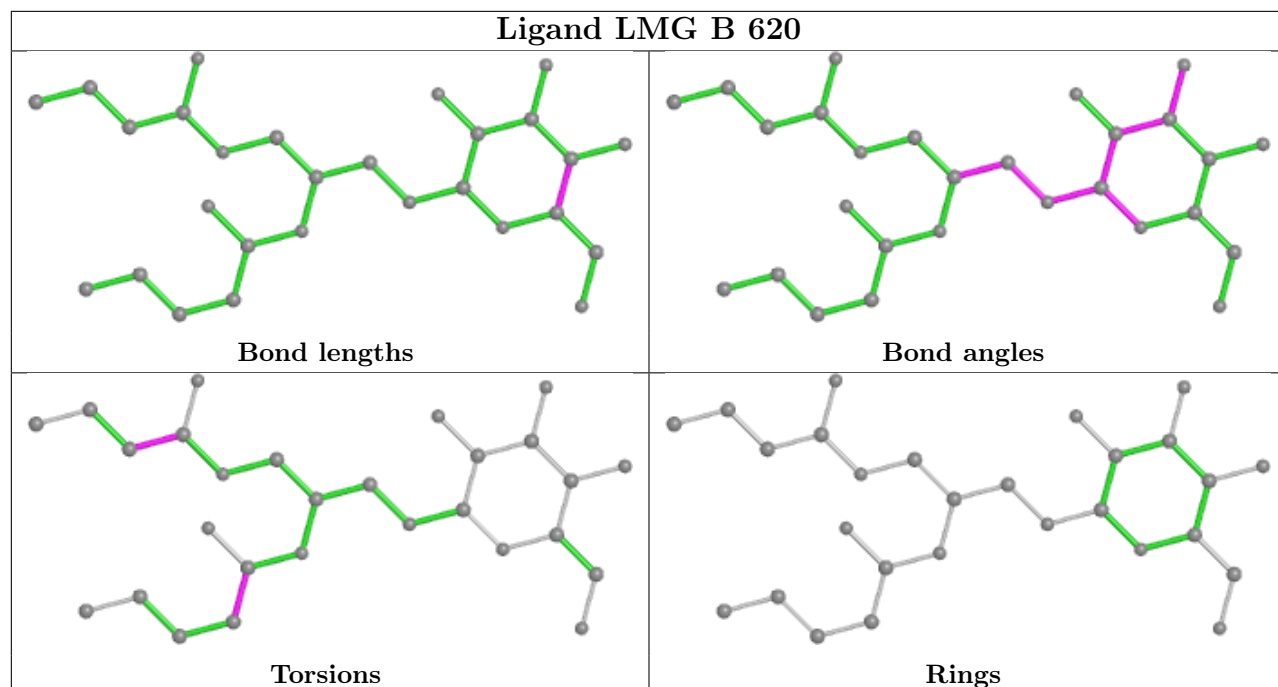


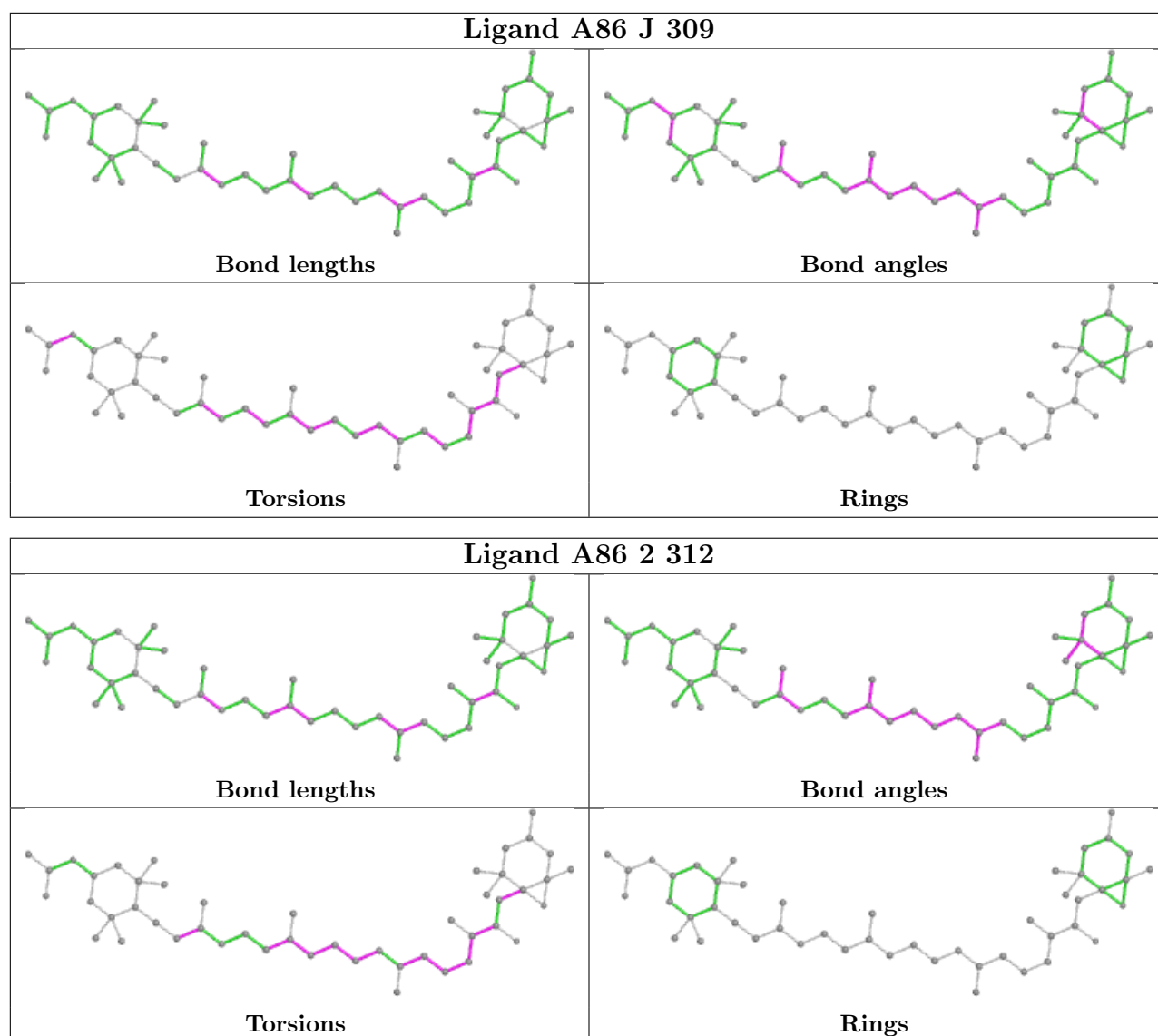
## Ligand KC1 8 313



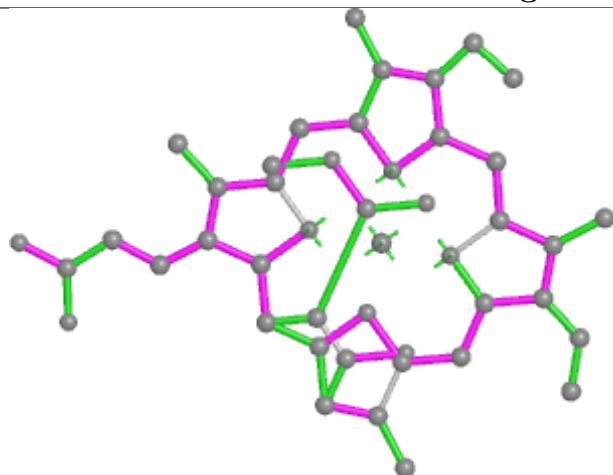
## Ligand LMG a 407



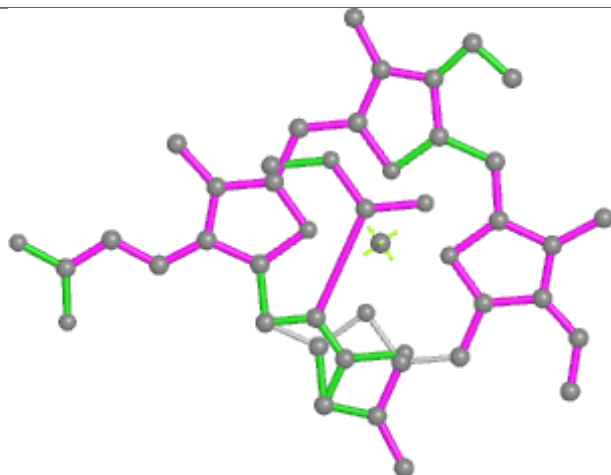




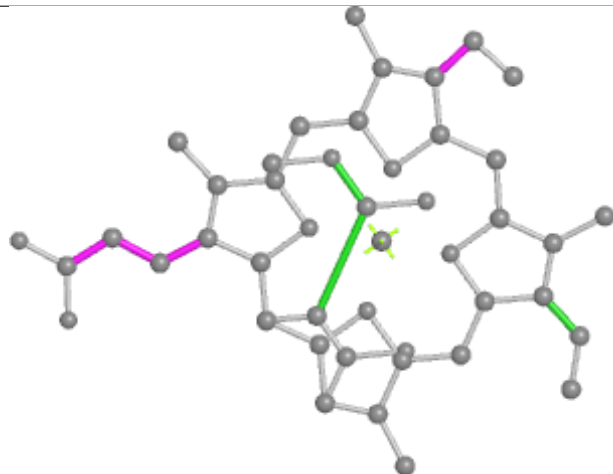
## Ligand KC1 7 314



Bond lengths



Bond angles

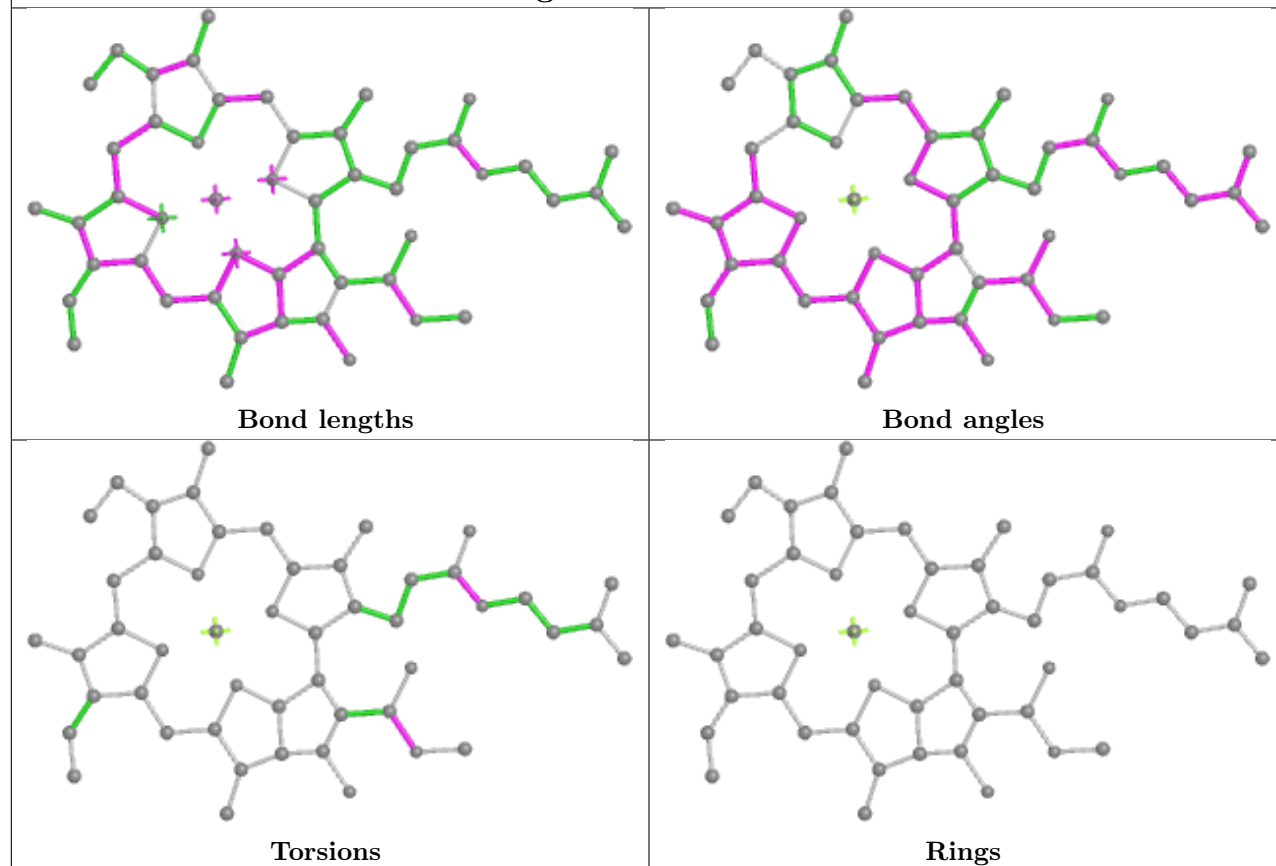


Torsions

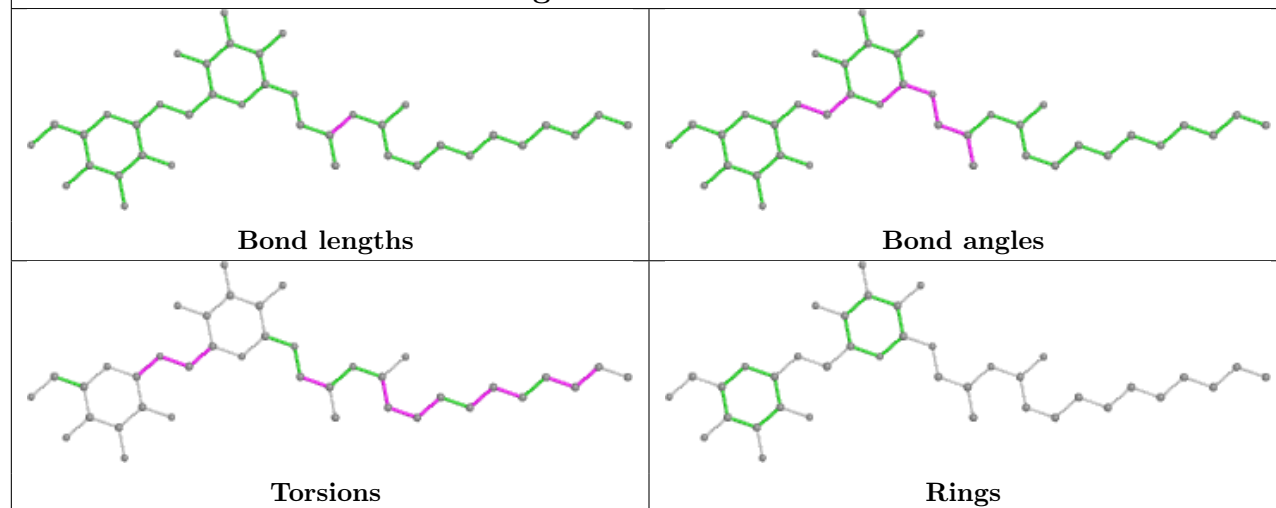


Rings

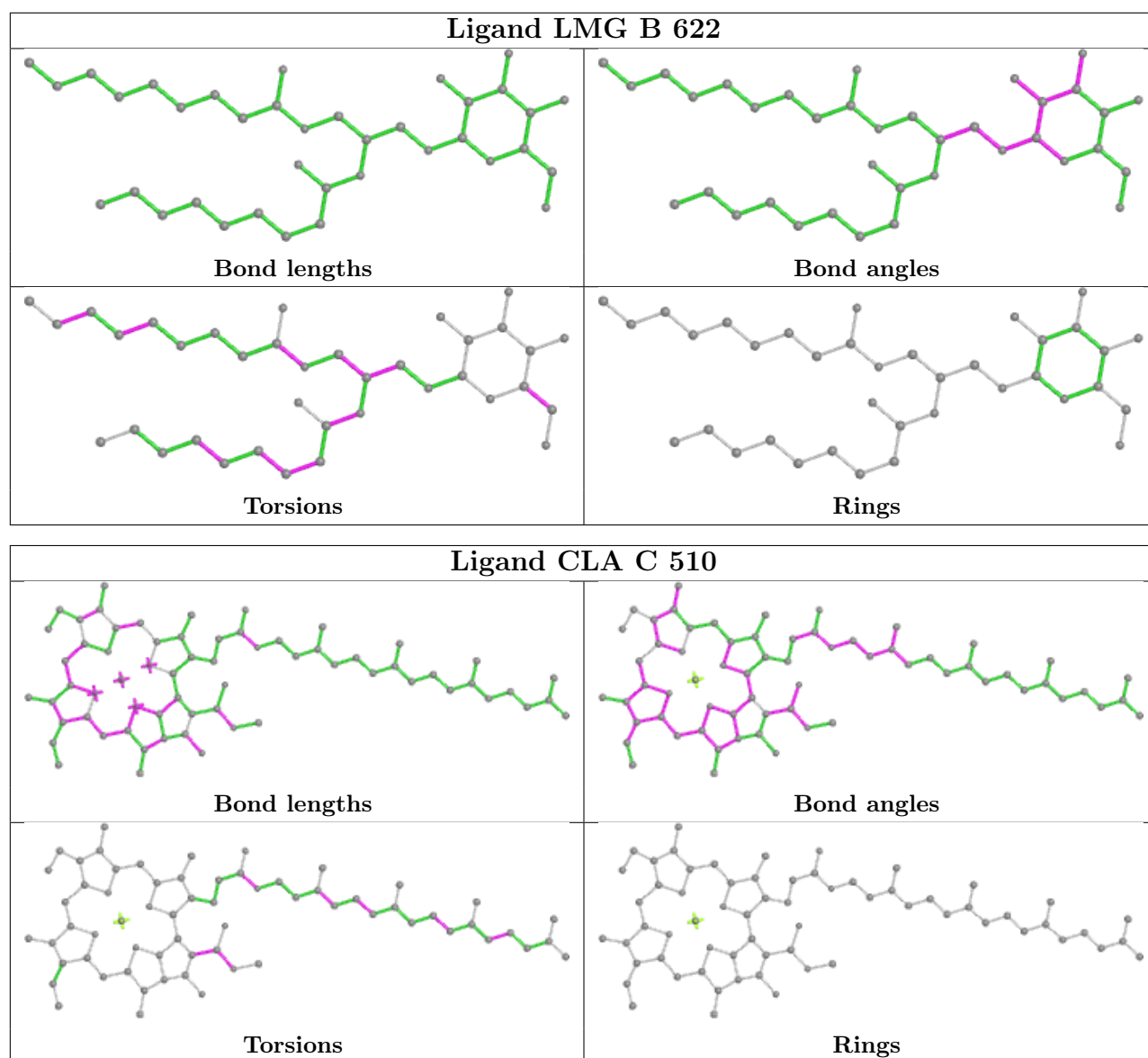
## Ligand CLA 8 303



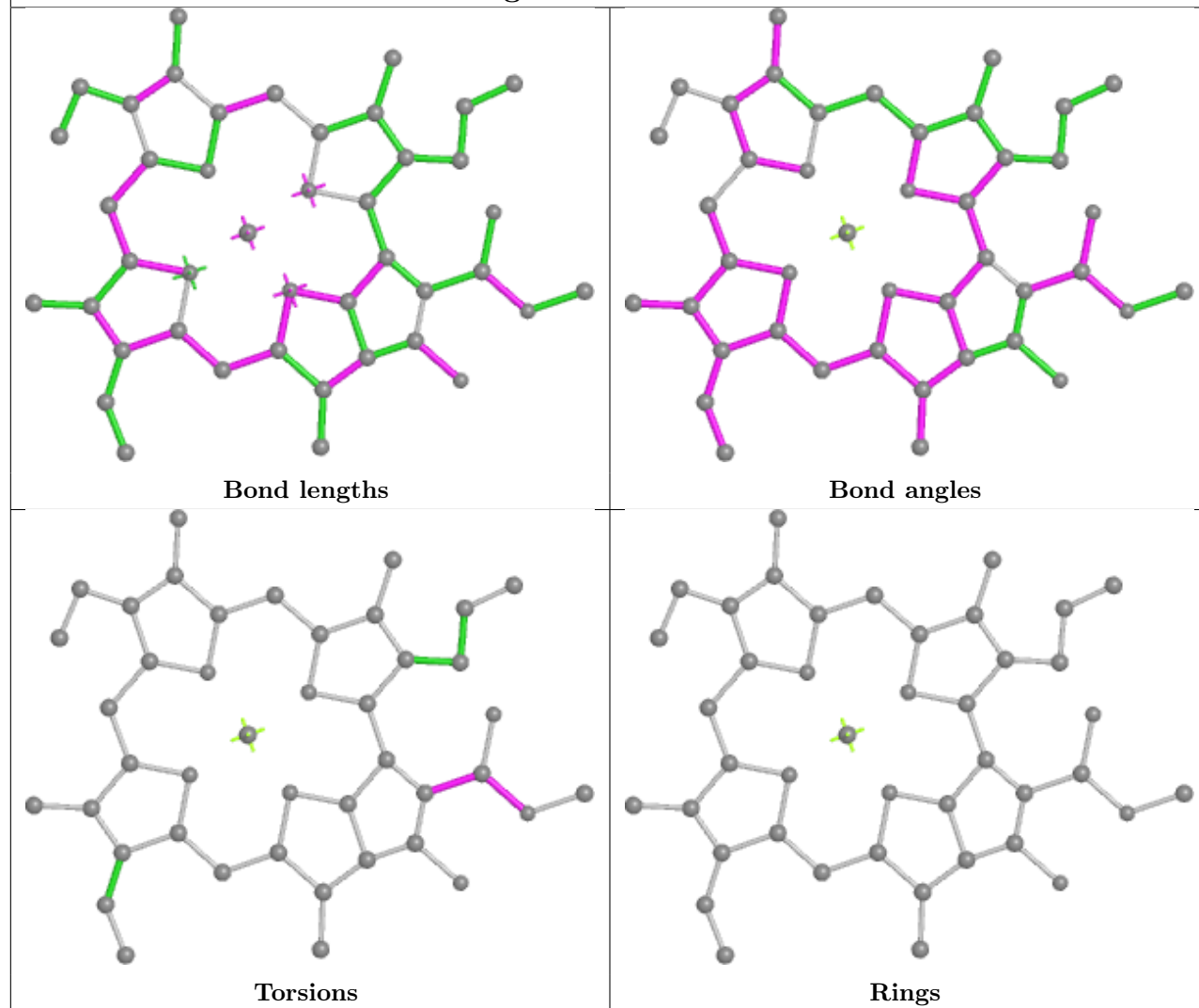
## Ligand DGD c 517



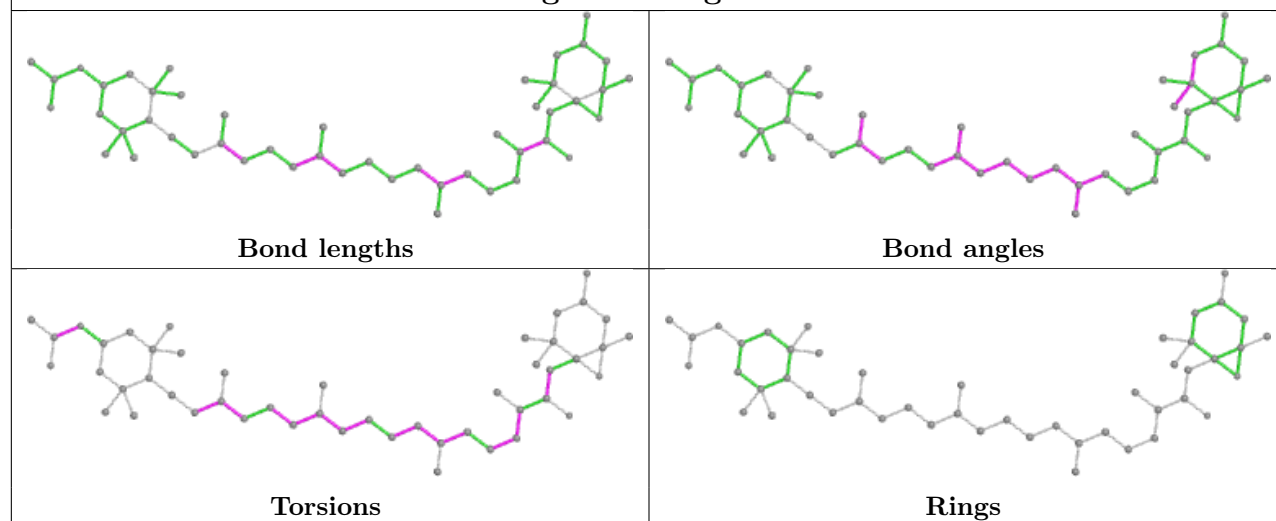




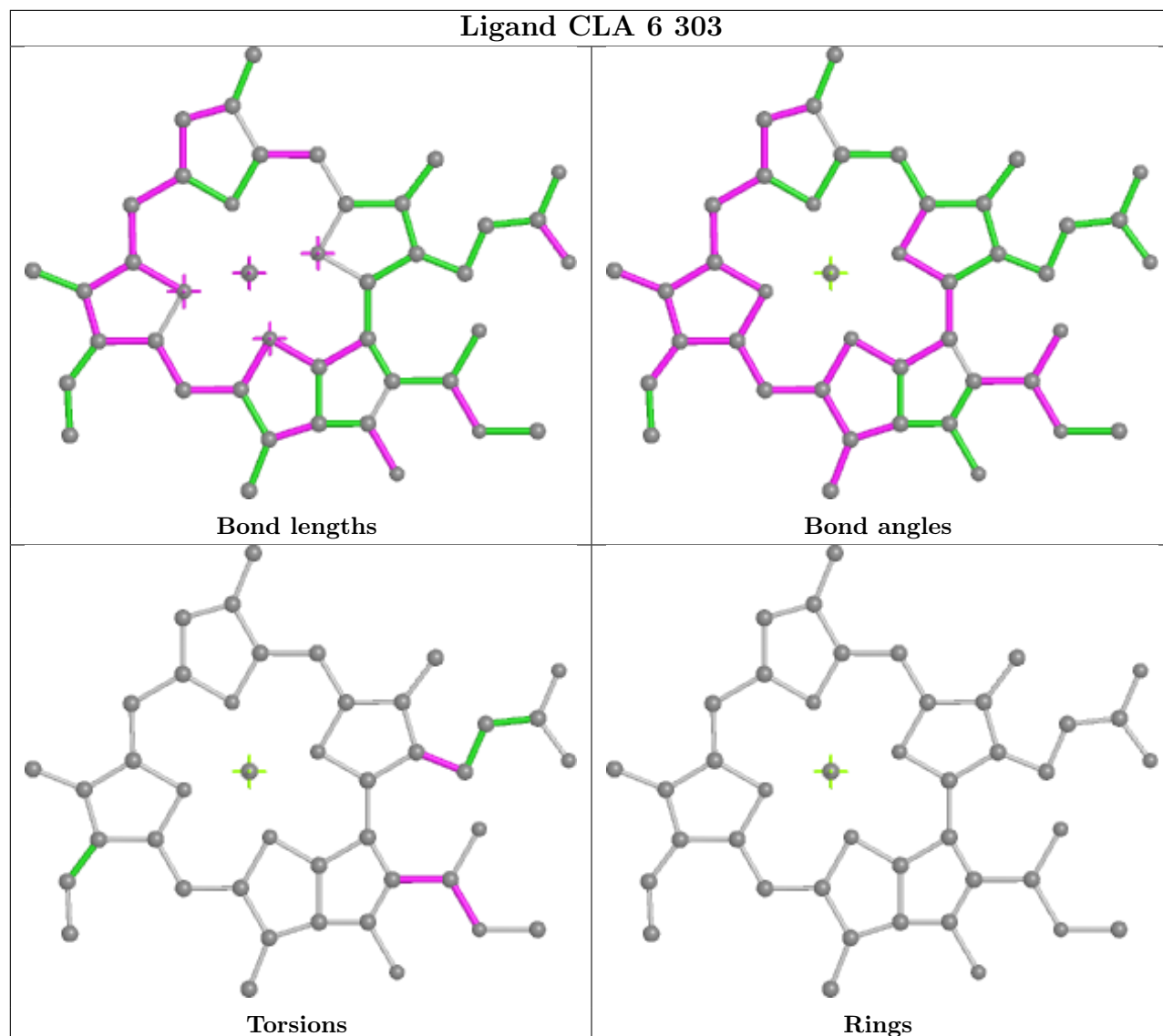
## Ligand CLA 6 304



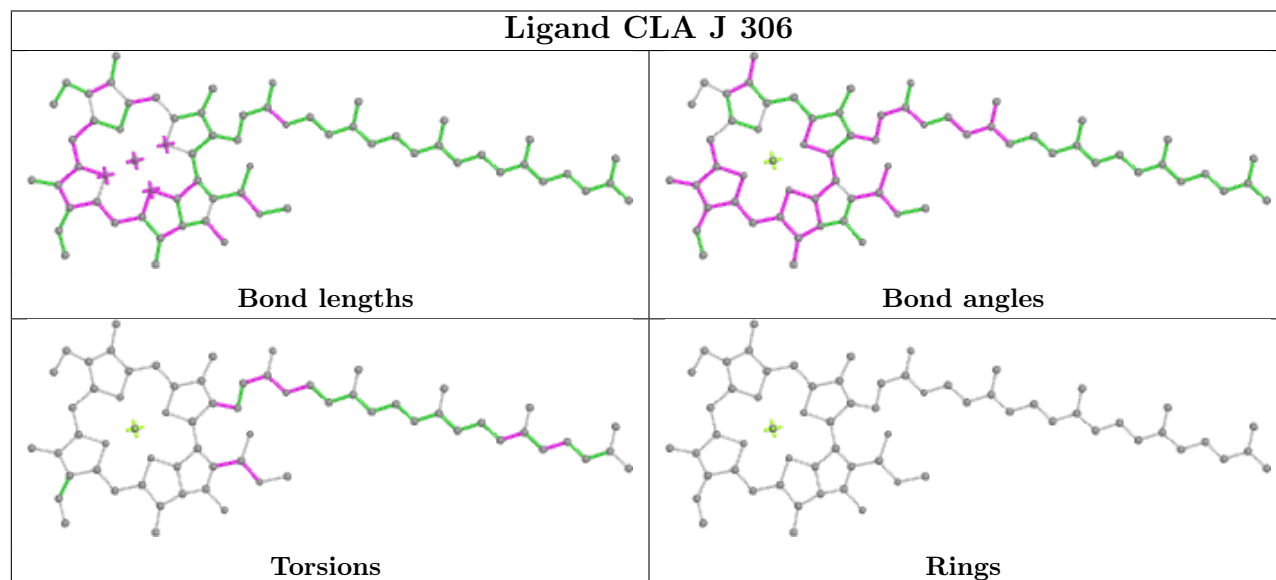
## Ligand A86 g 311



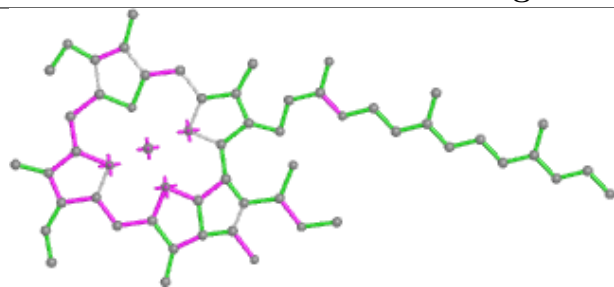
## Ligand CLA 6 303



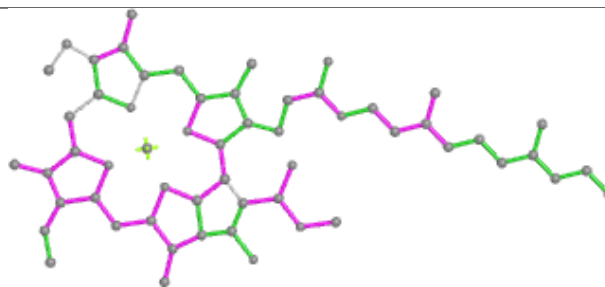
## Ligand CLA J 306



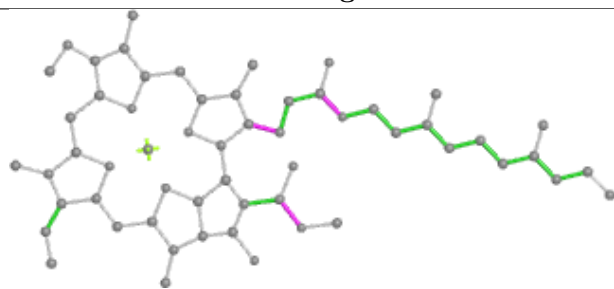
## Ligand CLA G 301



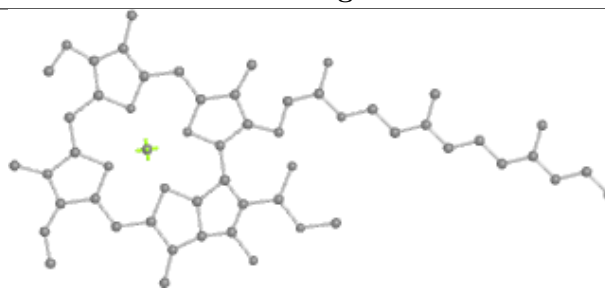
Bond lengths



Bond angles

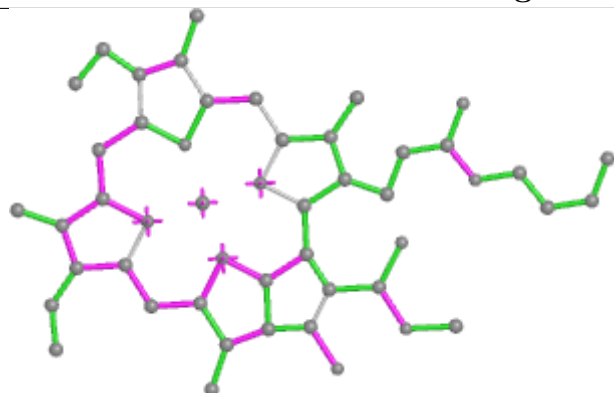


Torsions

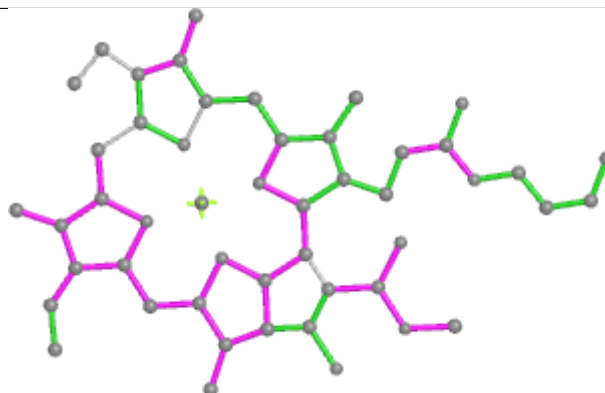


Rings

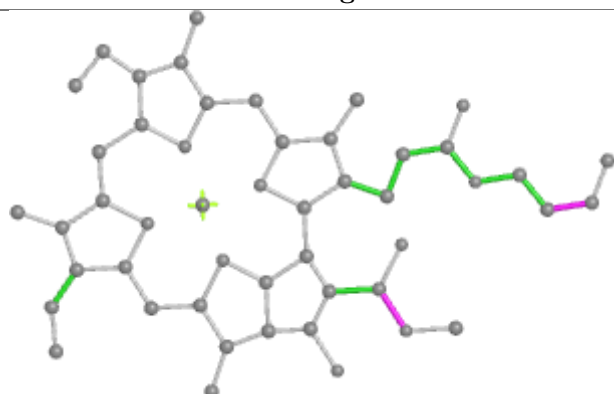
## Ligand CLA C 515



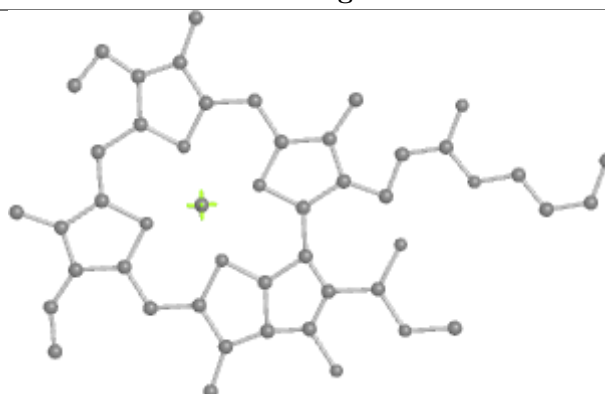
Bond lengths



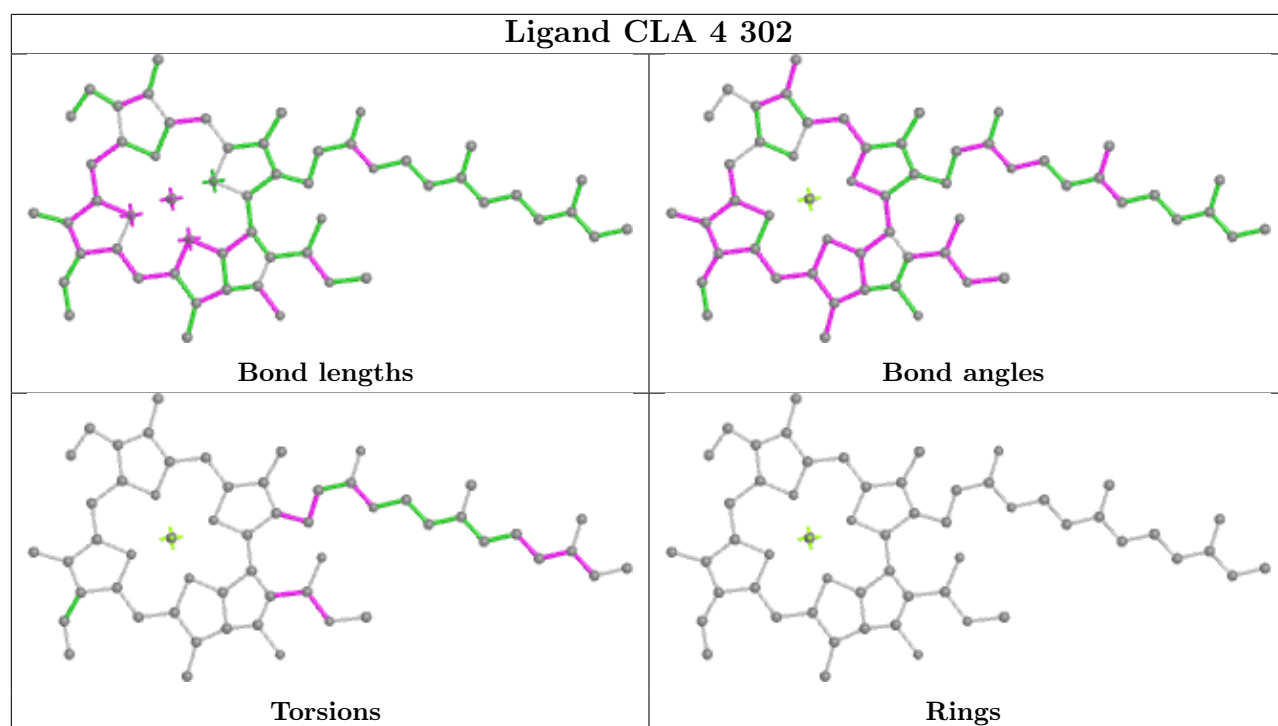
Bond angles



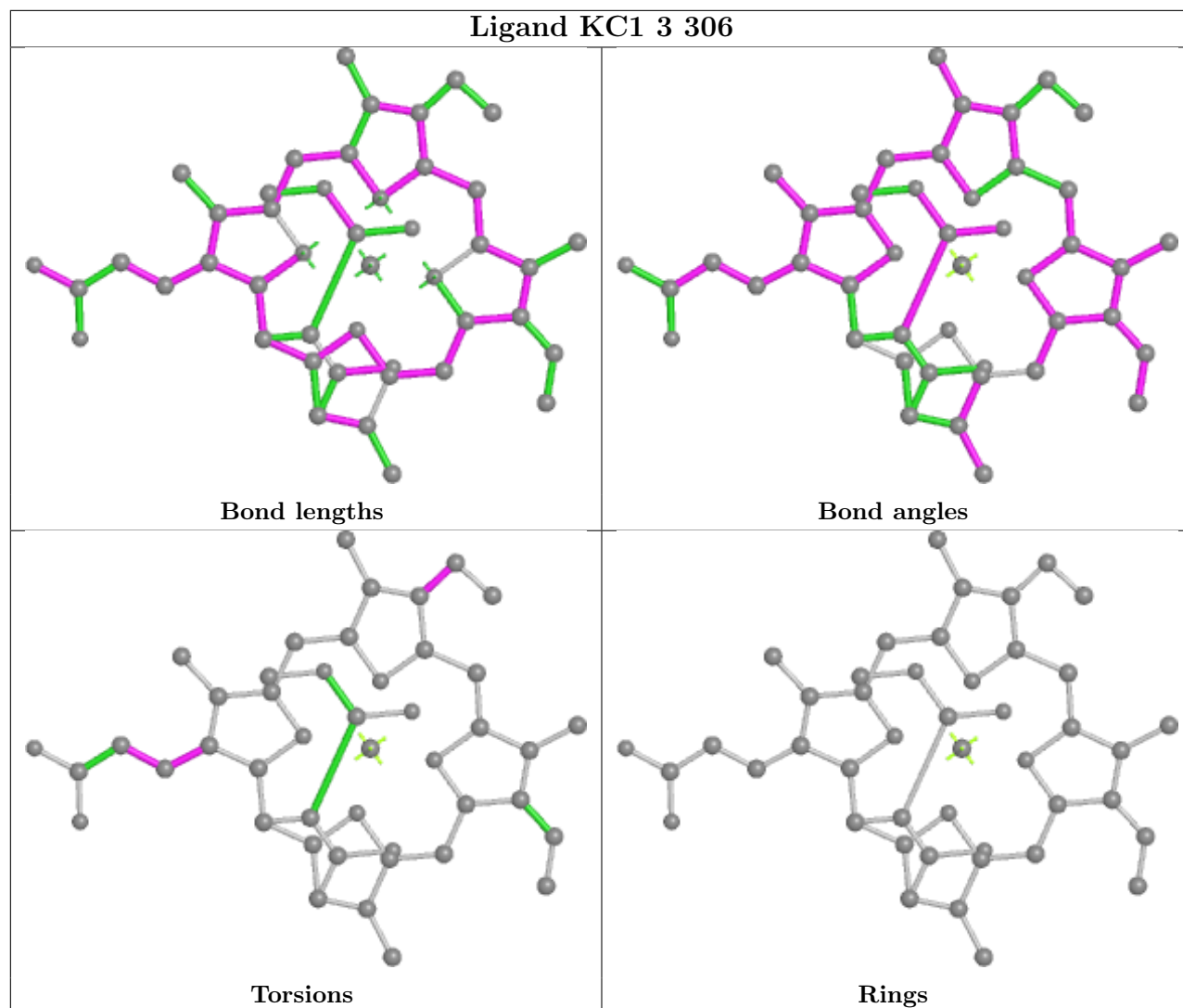
Torsions



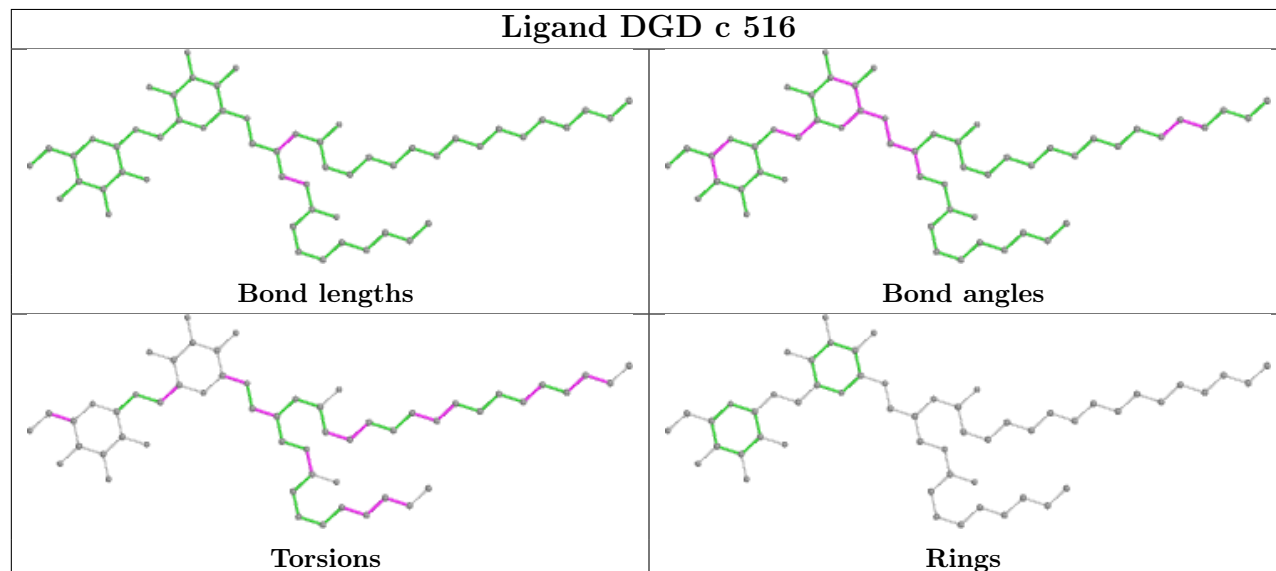
Rings

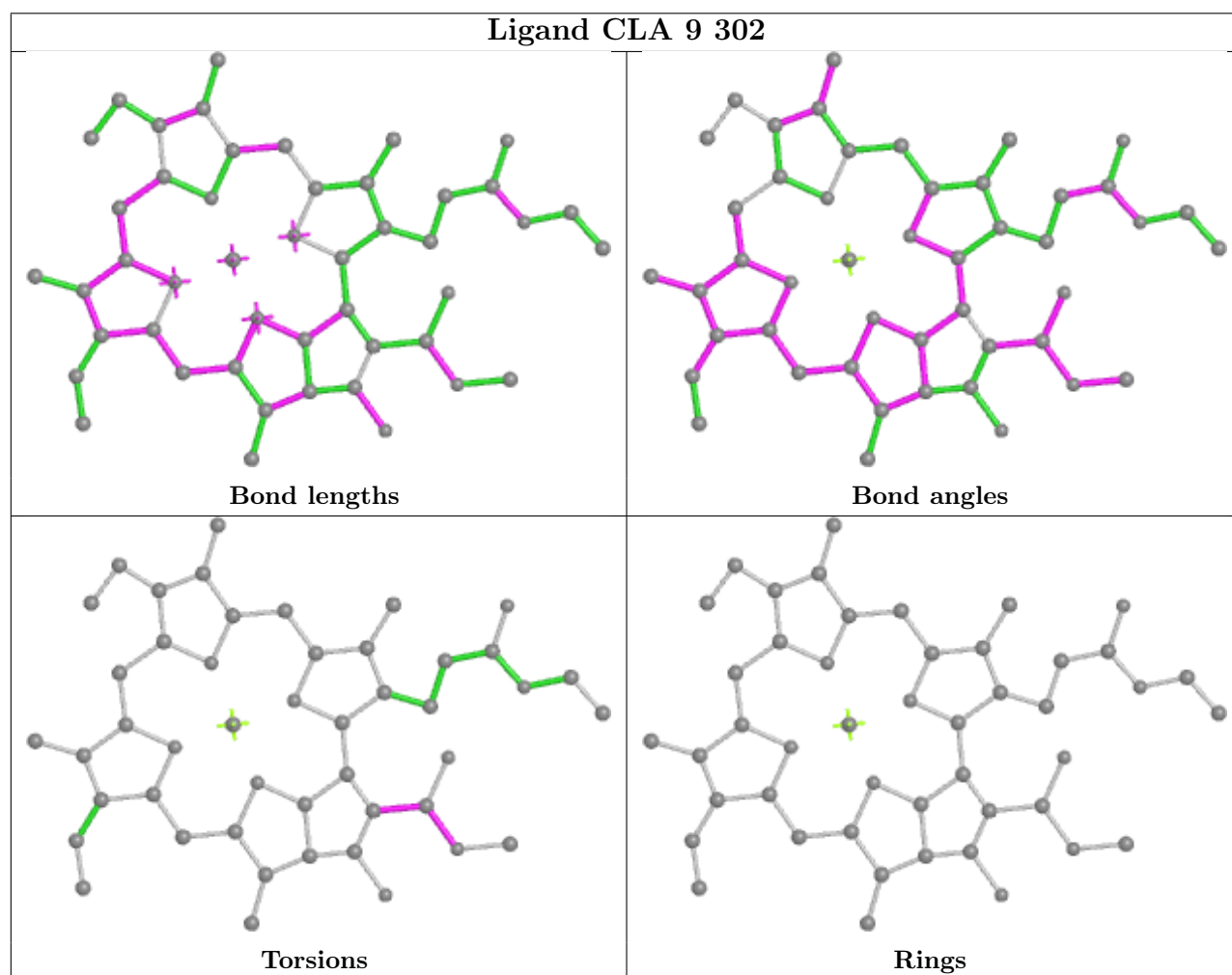
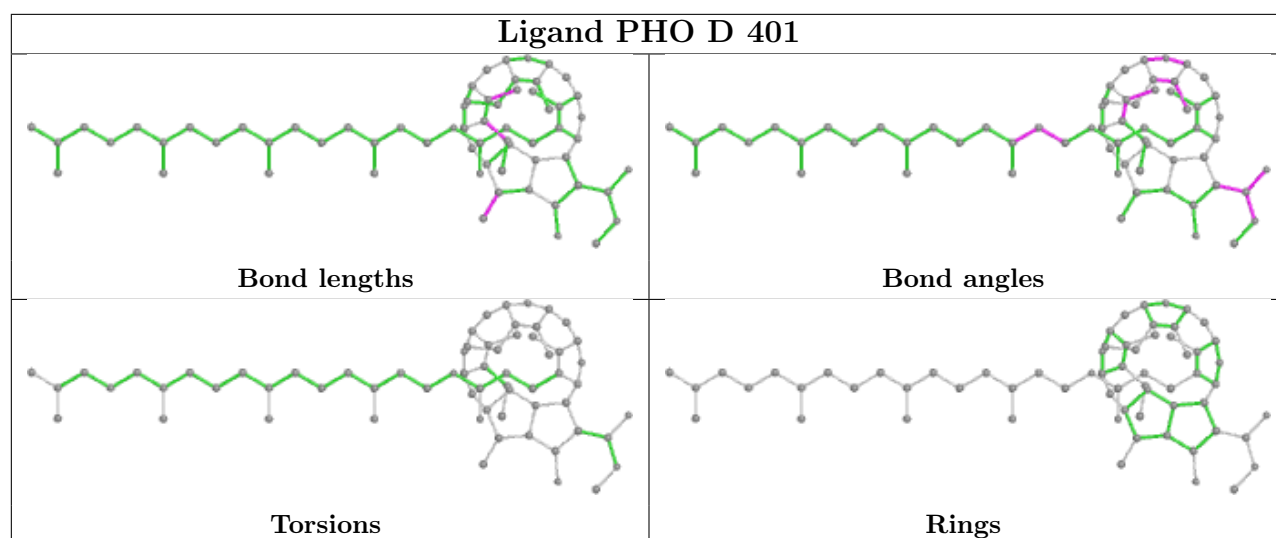


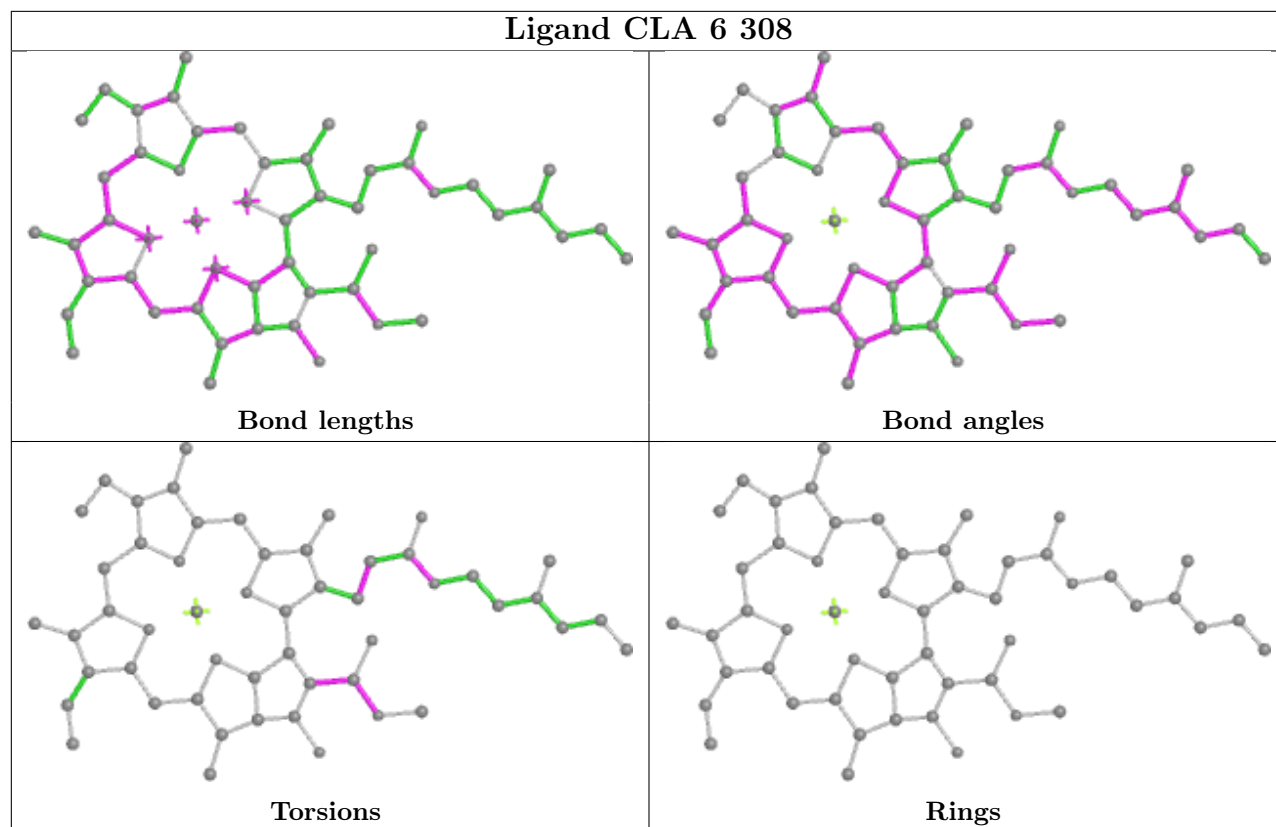
## Ligand KC1 3 306



## Ligand DGD c 516

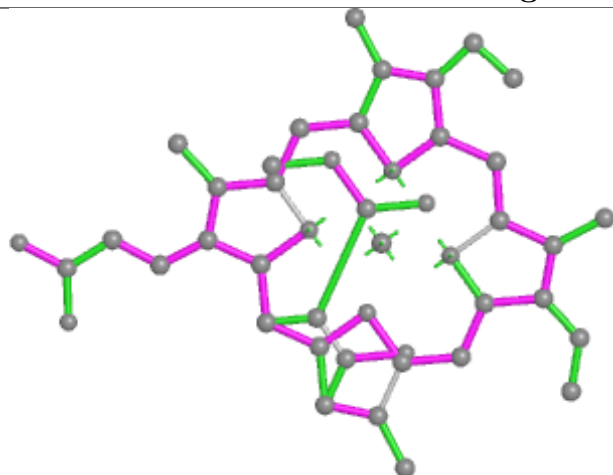




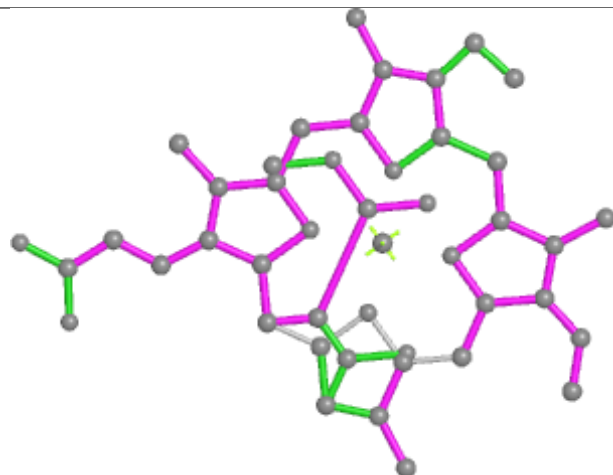




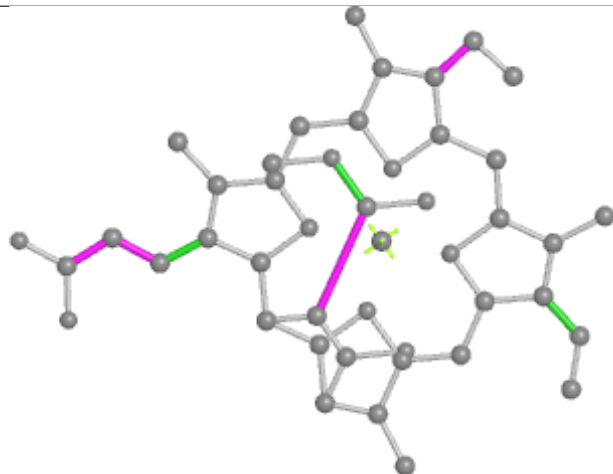
## Ligand KC1 6 313



Bond lengths



Bond angles

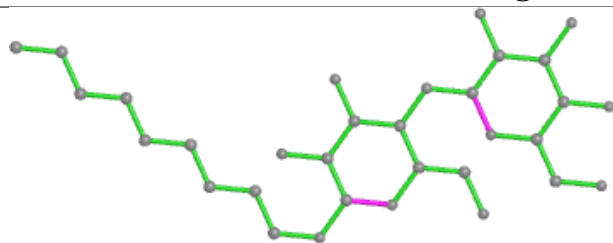


Torsions

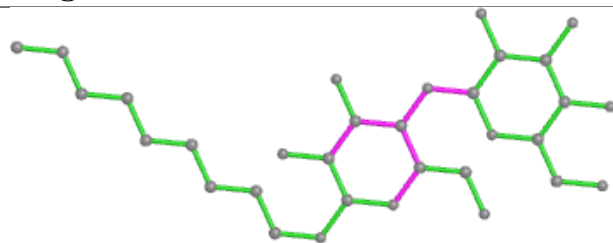


Rings

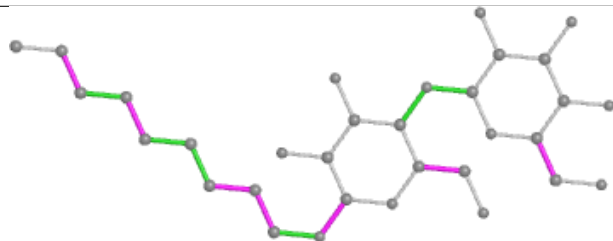
## Ligand LMU g 301



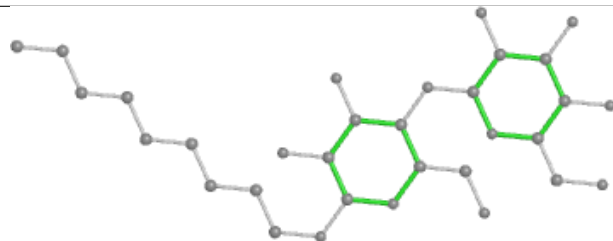
Bond lengths



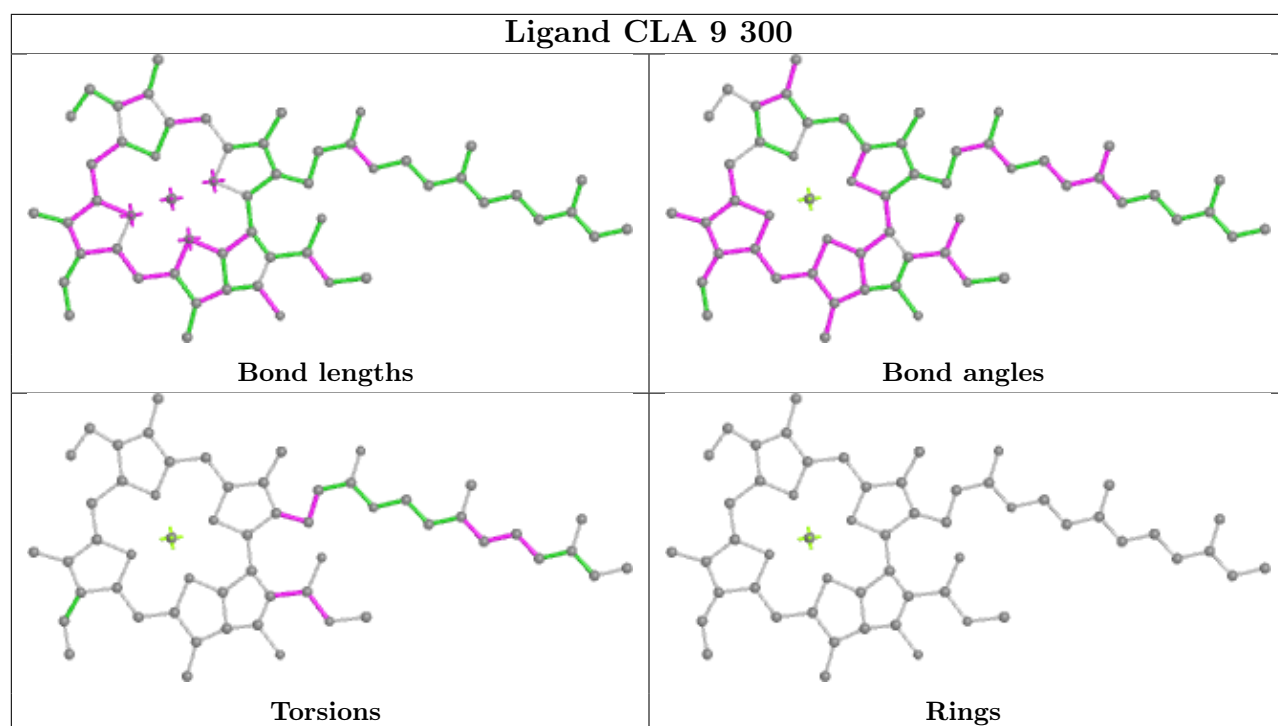
Bond angles



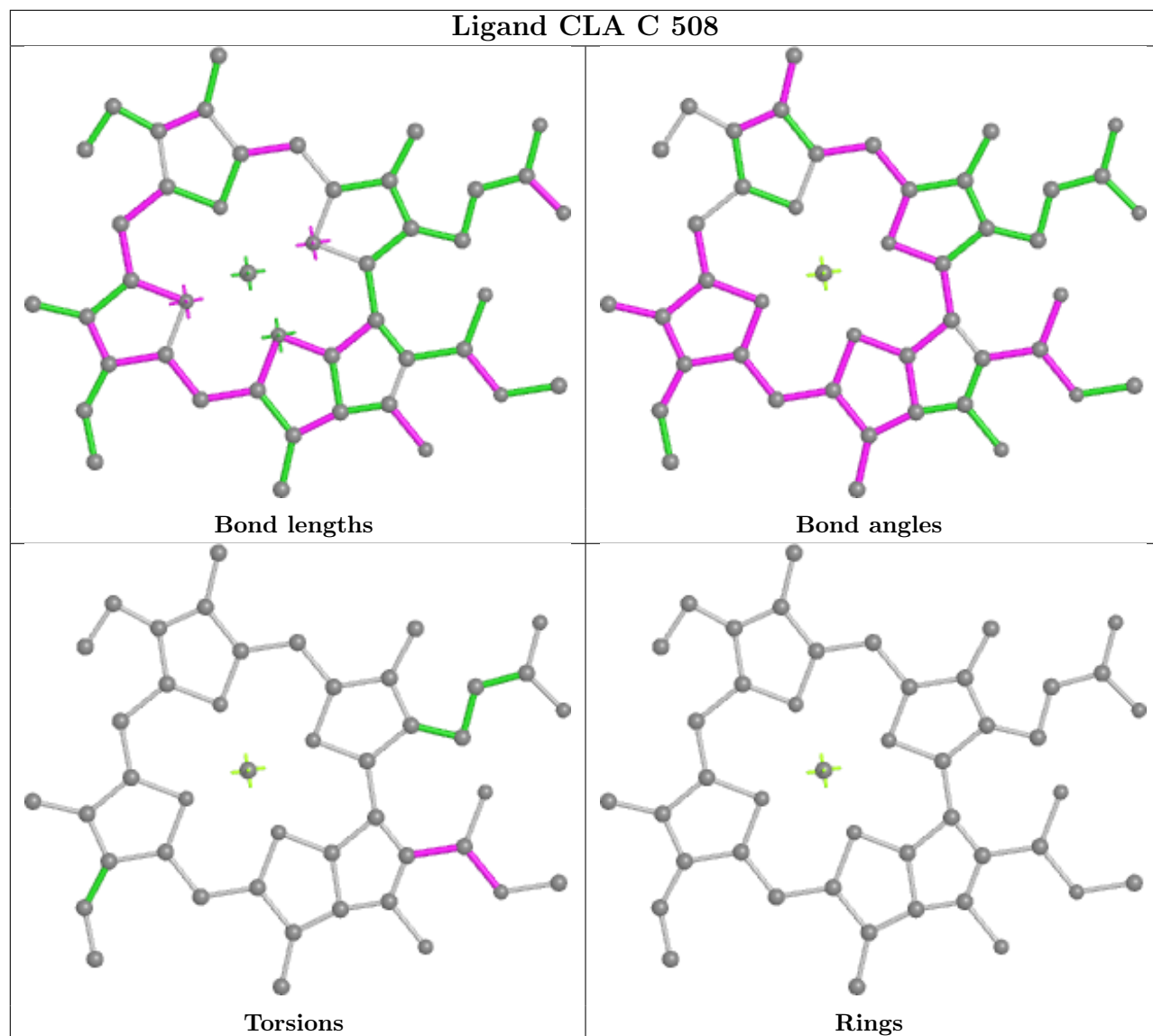
Torsions



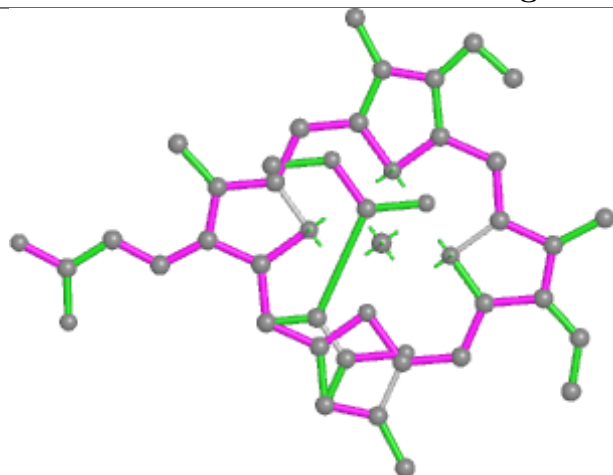
Rings



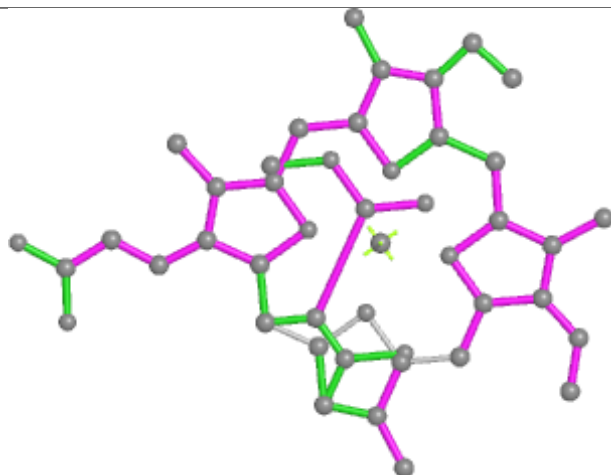
## Ligand CLA C 508



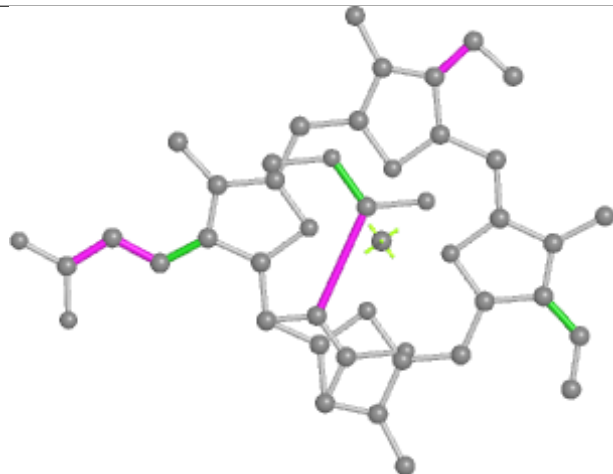
## Ligand KC1 8 314



Bond lengths



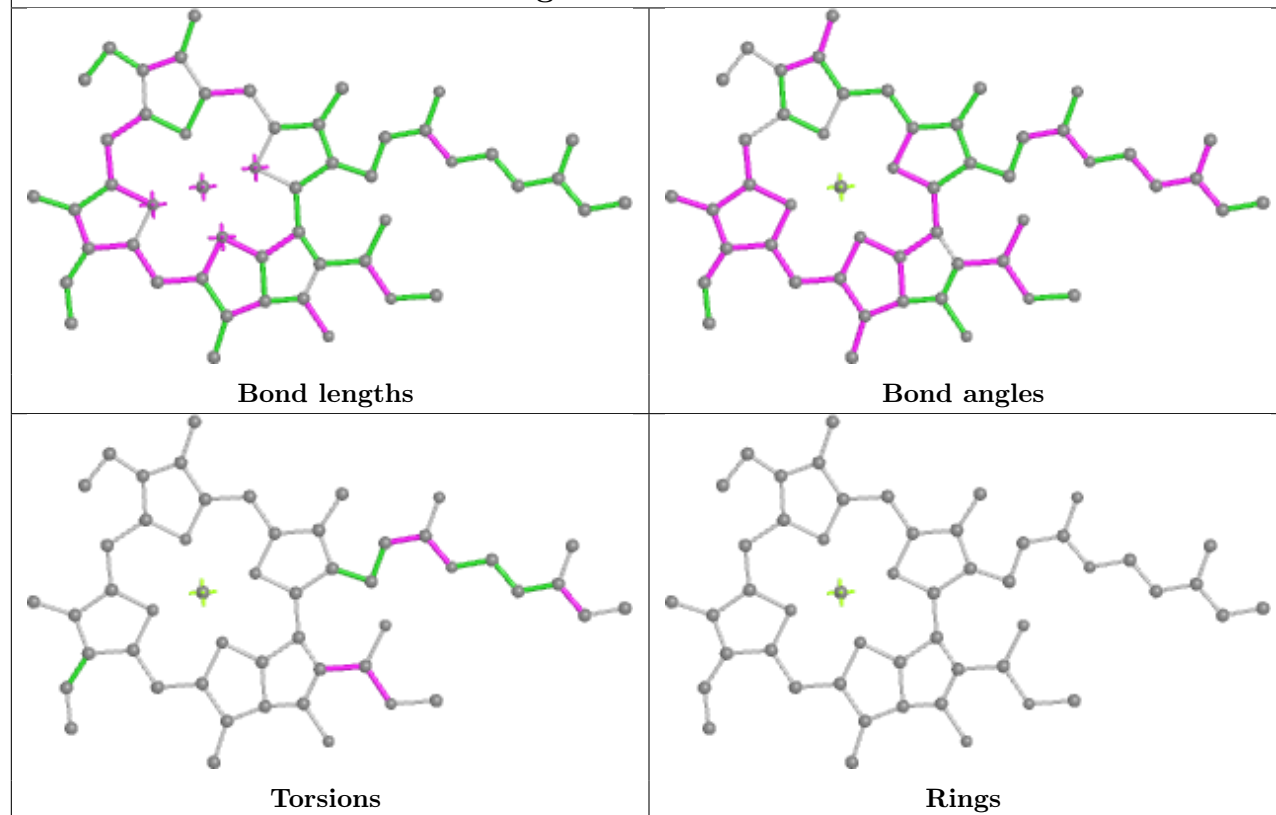
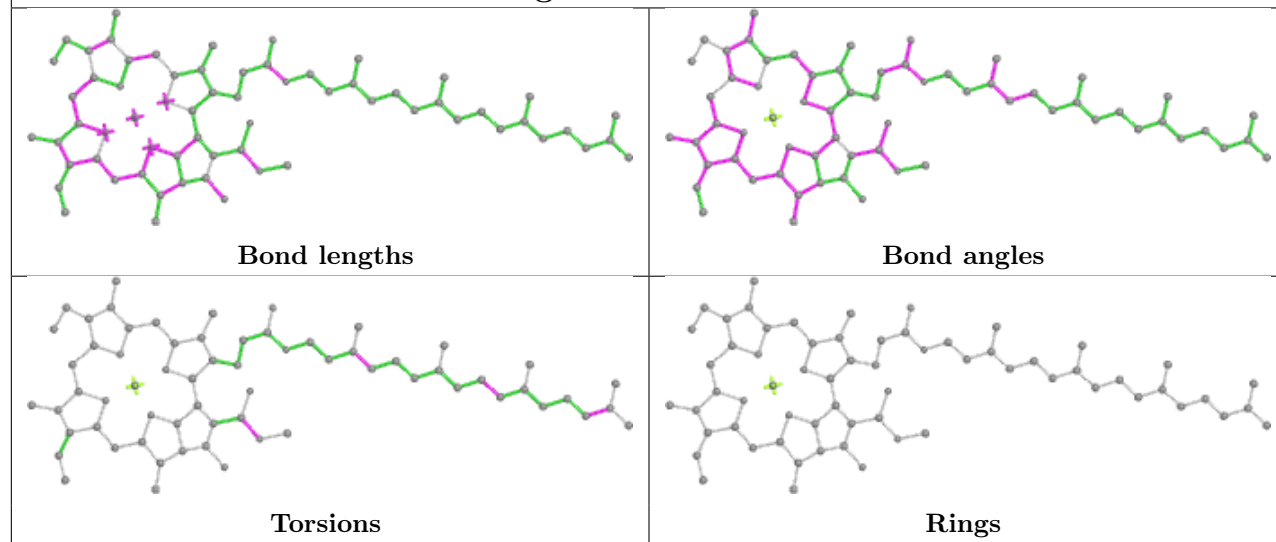
Bond angles

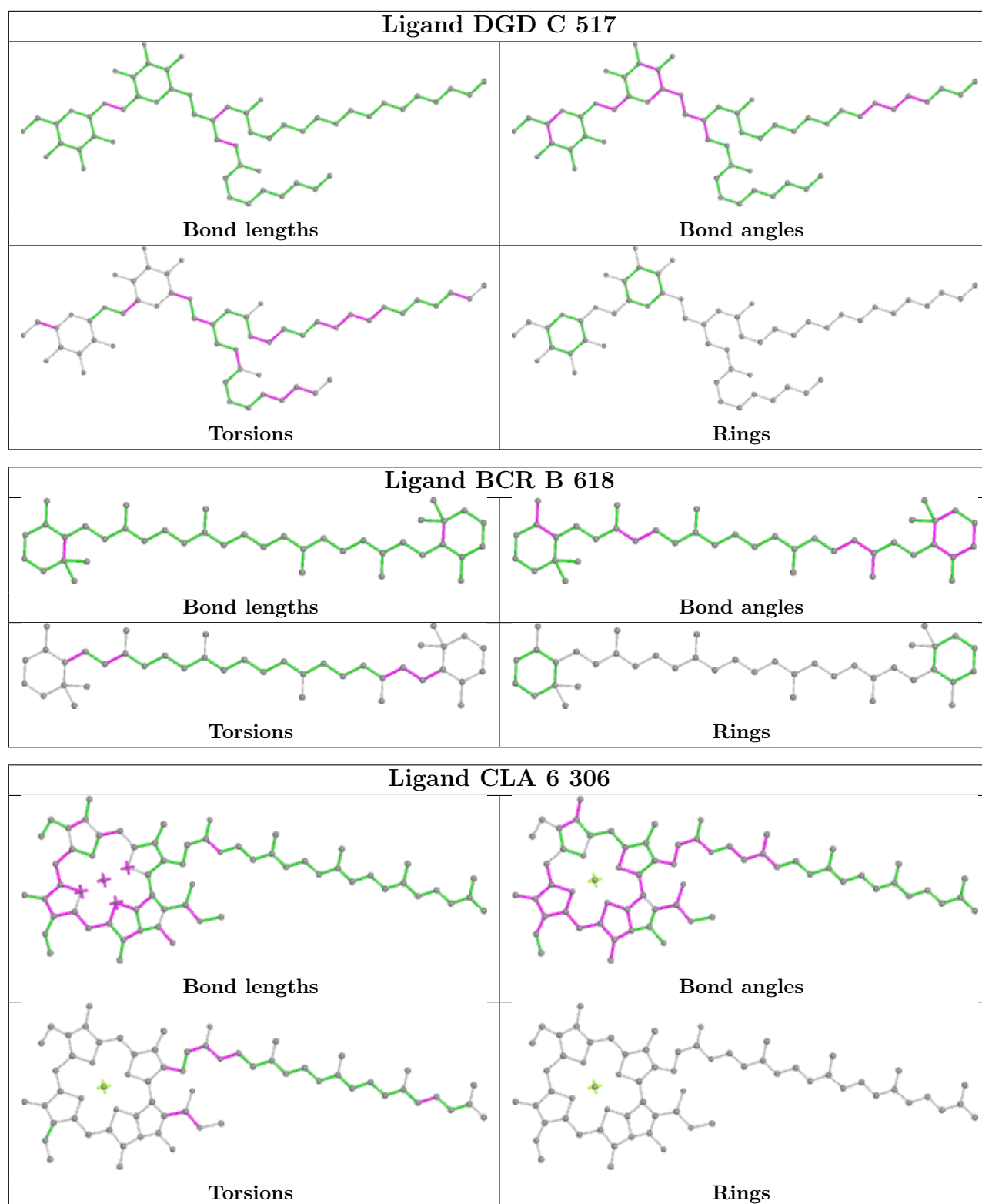


Torsions

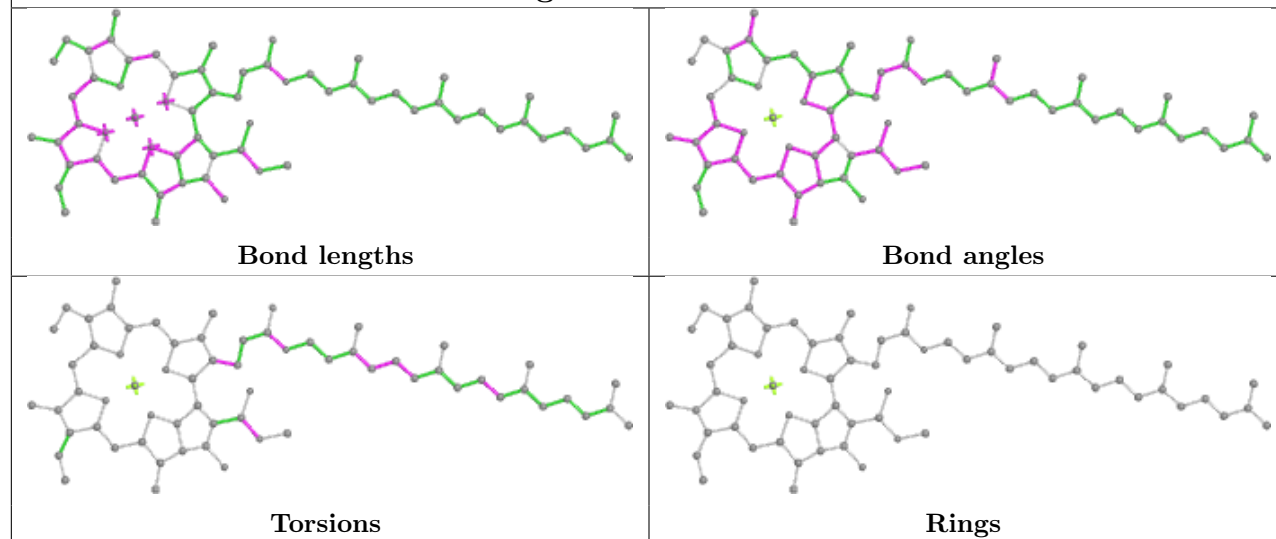


Rings

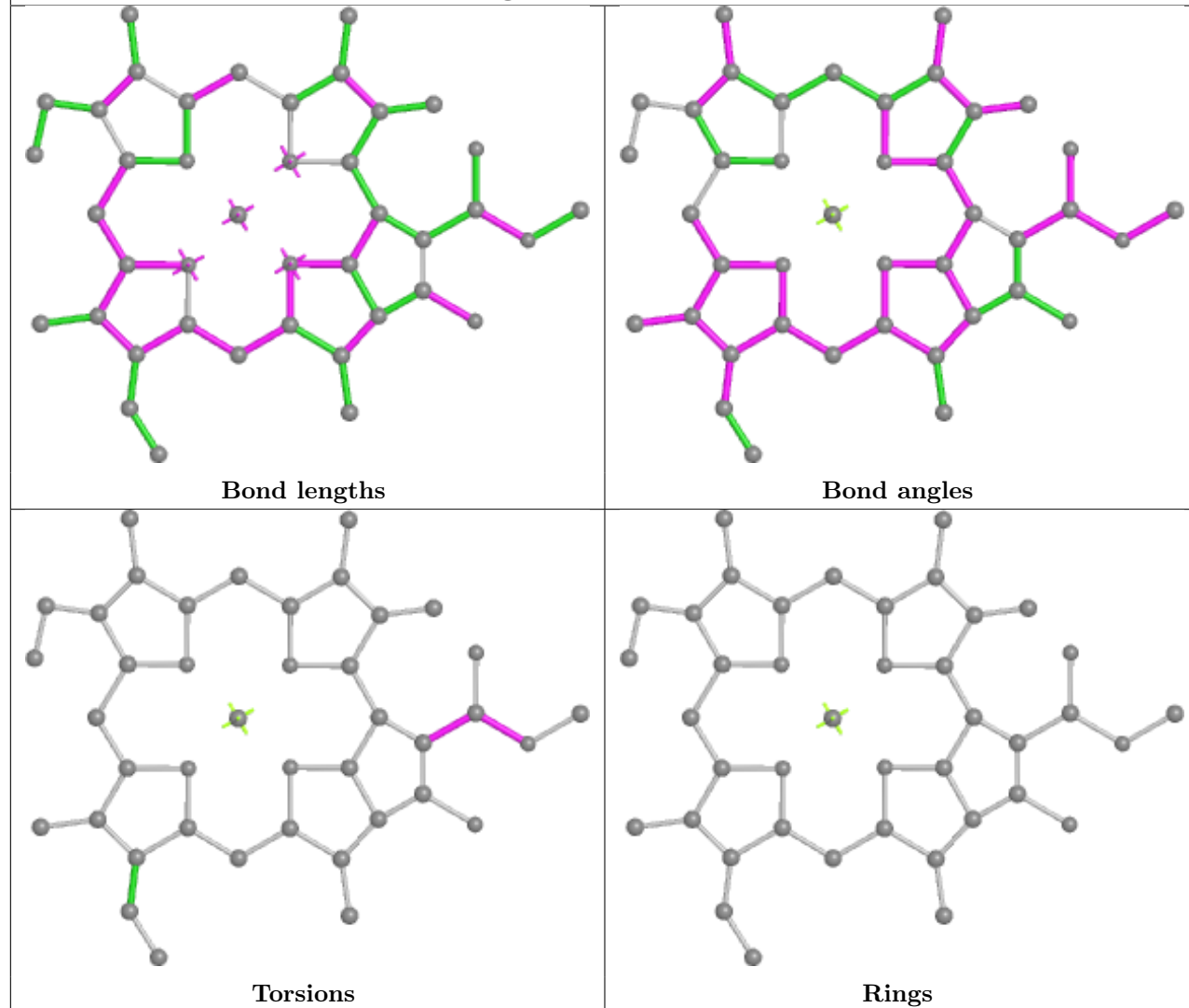
**Ligand CLA 8 304****Ligand CLA b 616**

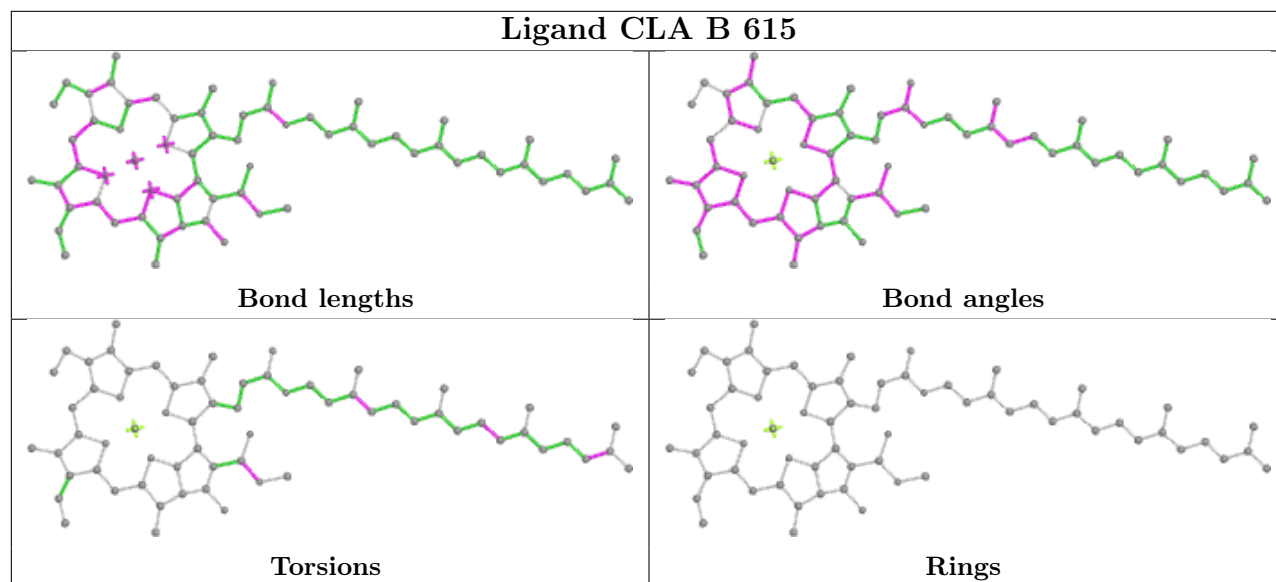
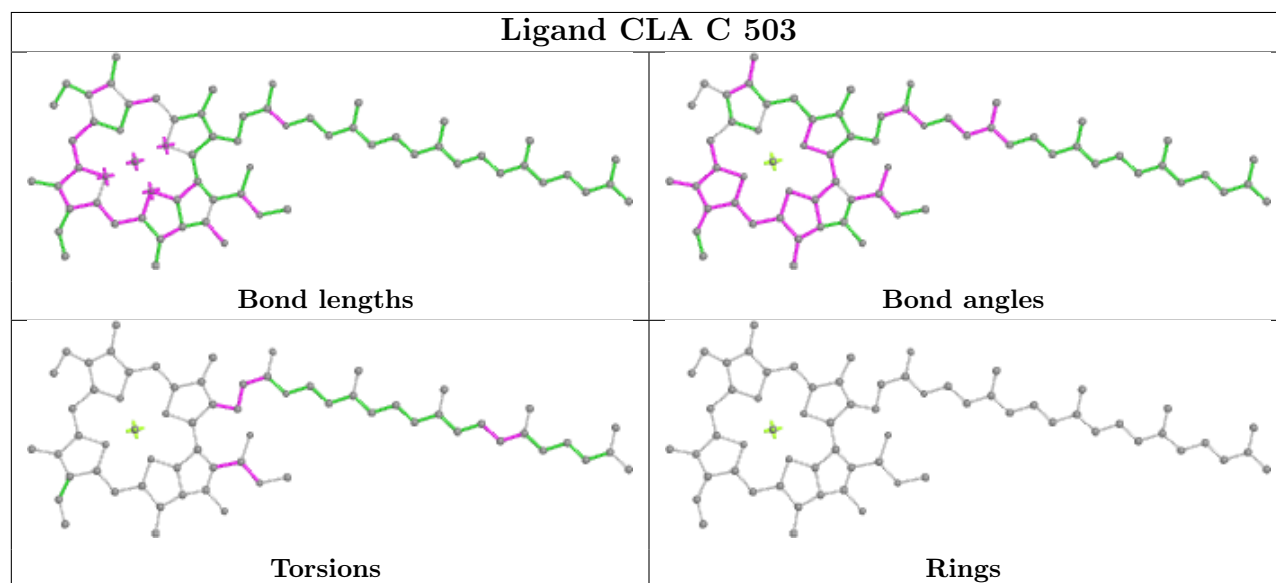


## Ligand CLA 5 308



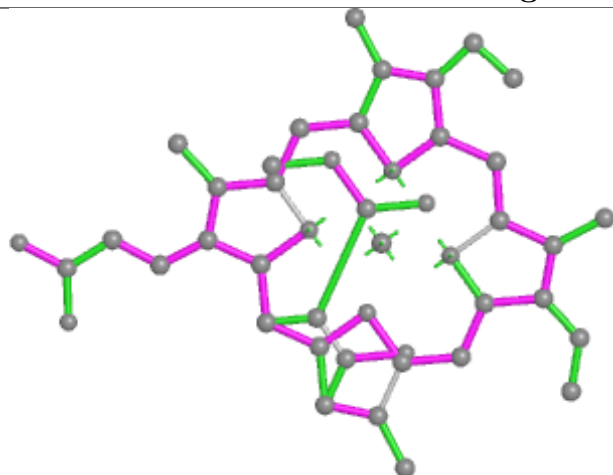
## Ligand CLA 1 307



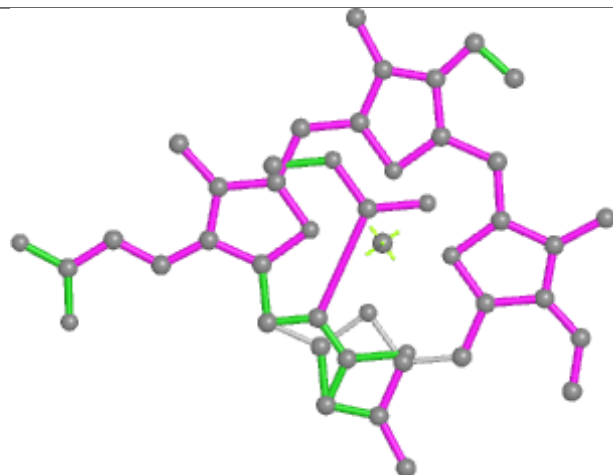
**Ligand CLA B 615****Ligand CLA C 503**



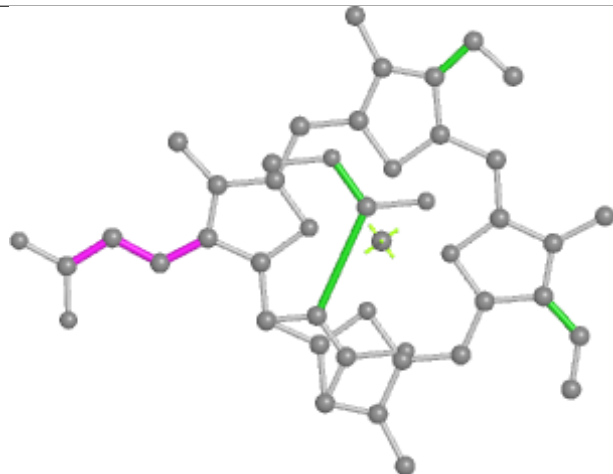
## Ligand KC1 6 312



Bond lengths



Bond angles

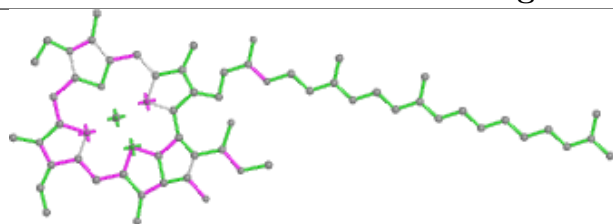


Torsions

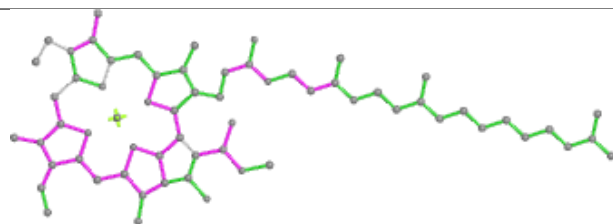


Rings

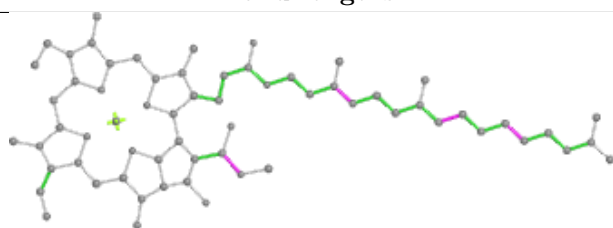
## Ligand CLA b 612



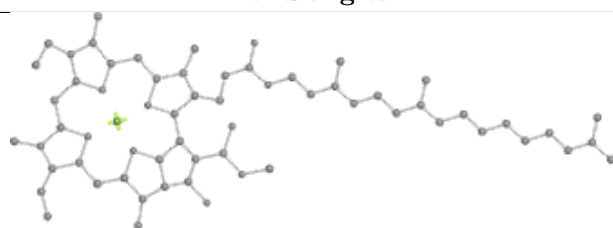
Bond lengths



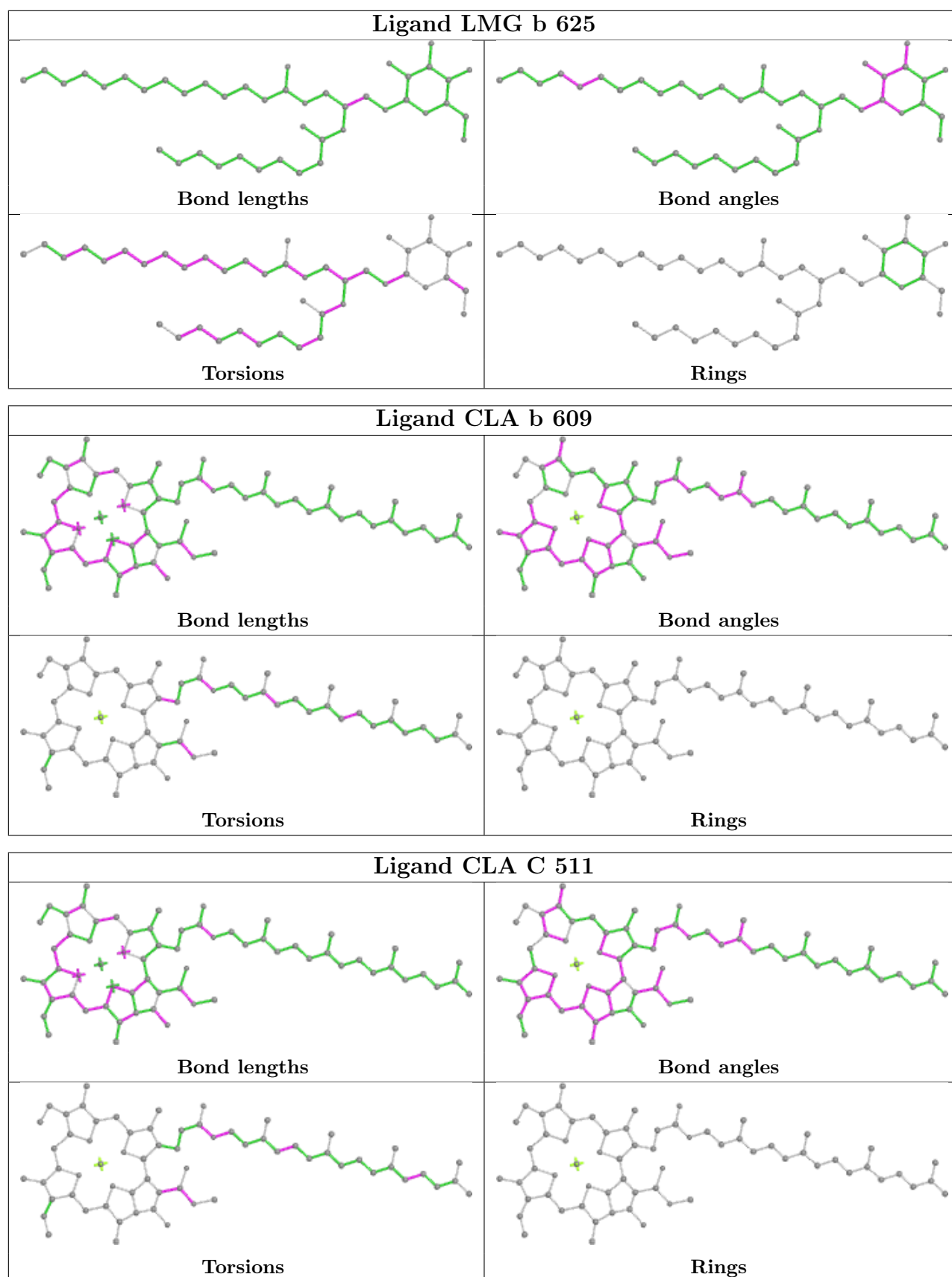
Bond angles



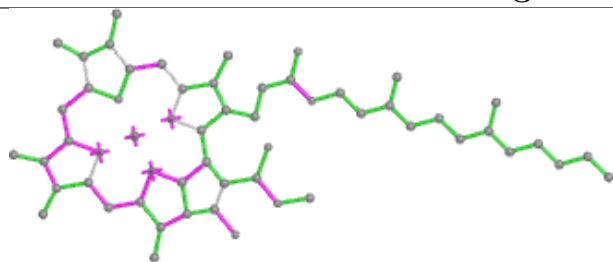
Torsions



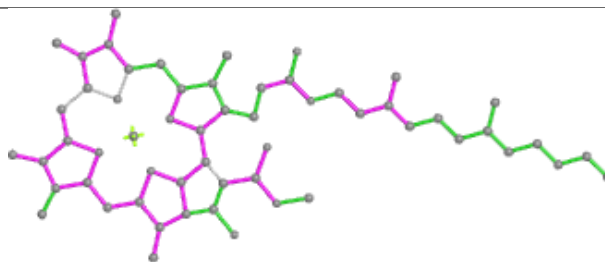
Rings



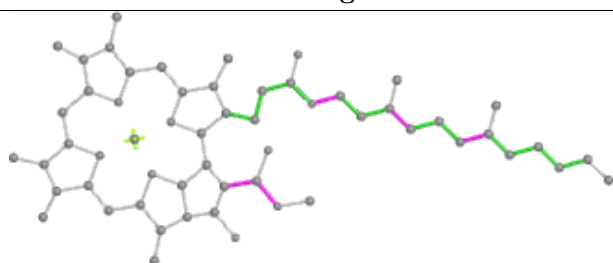
## Ligand CLA D 406



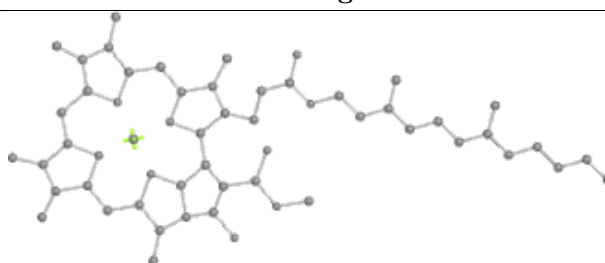
Bond lengths



Bond angles

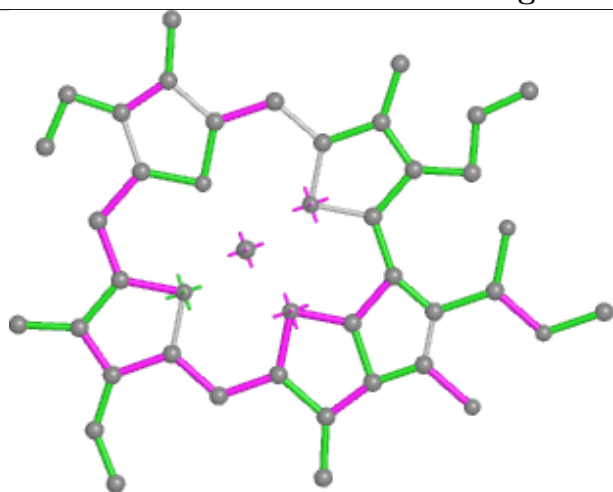


Torsions

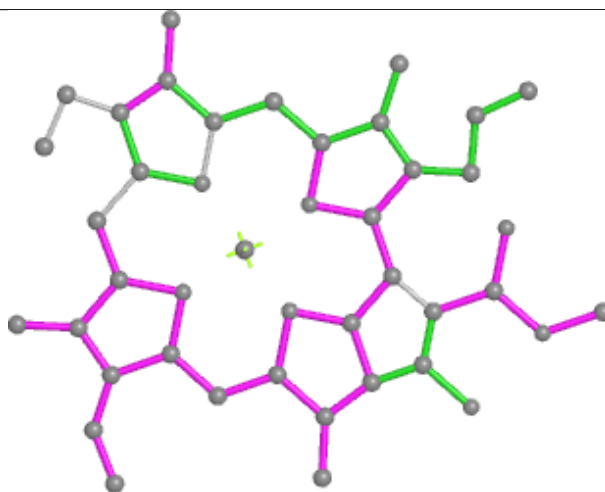


Rings

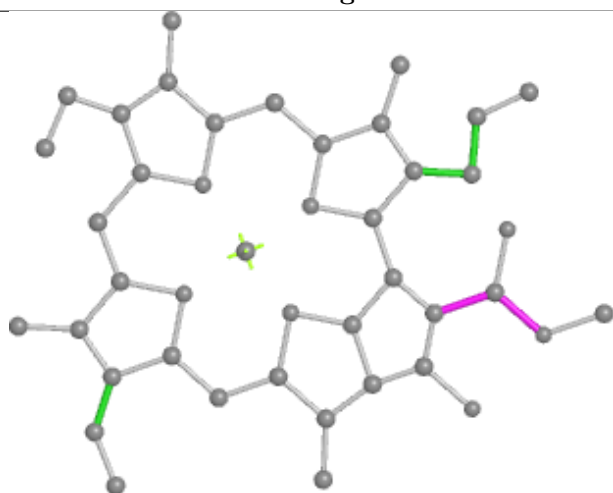
## Ligand CLA J 304



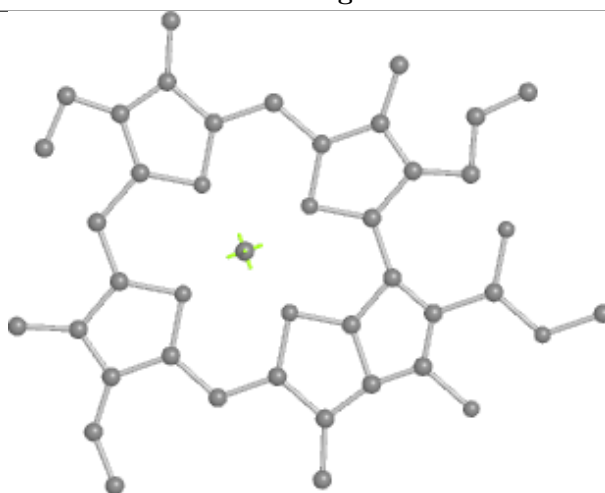
Bond lengths



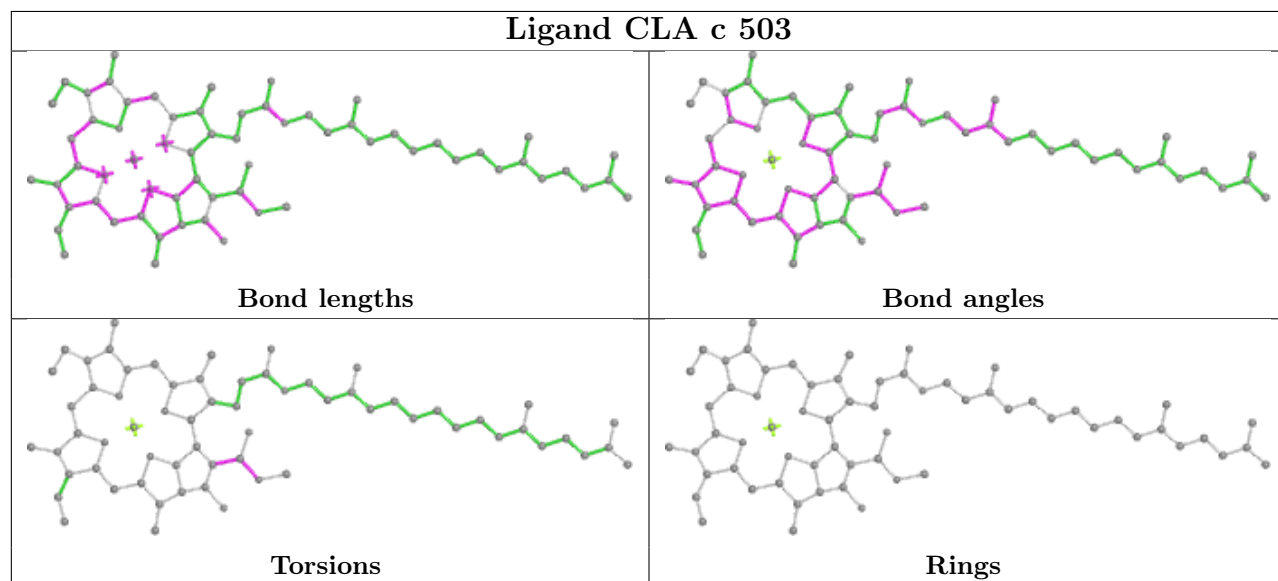
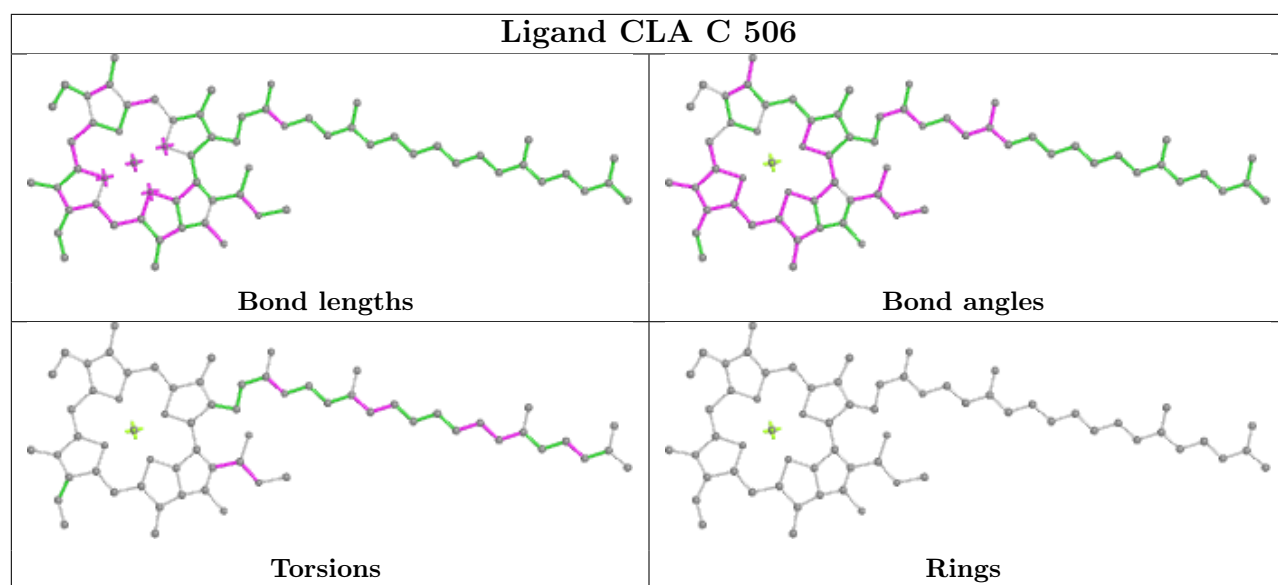
Bond angles



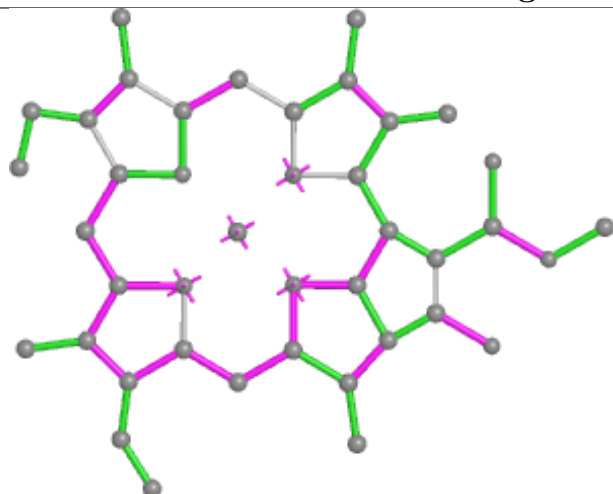
Torsions



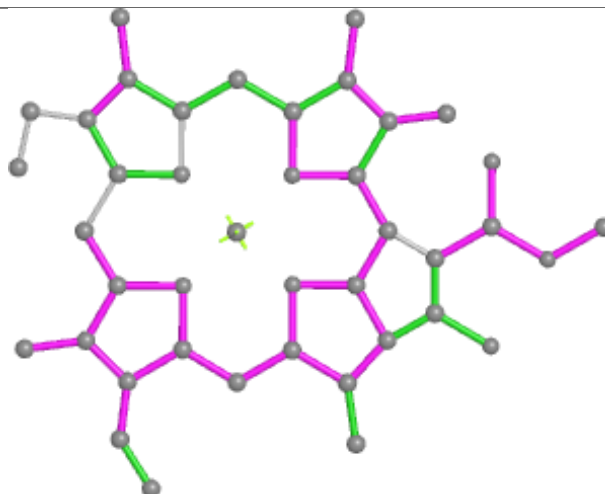
Rings



## Ligand CLA 7 306



Bond lengths



Bond angles

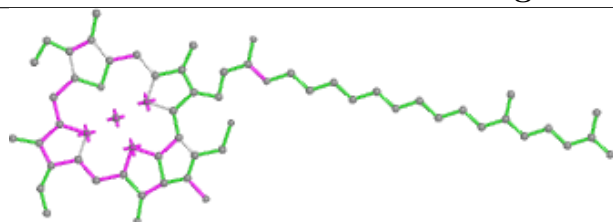


Torsions

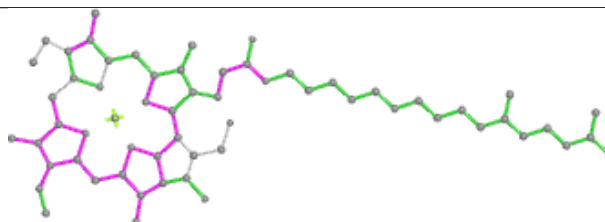


Rings

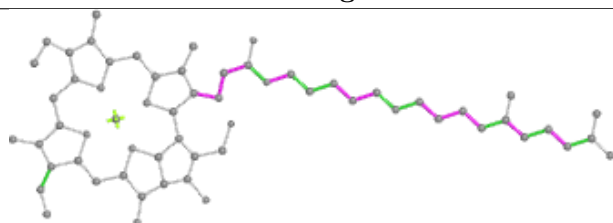
## Ligand CLA B 603



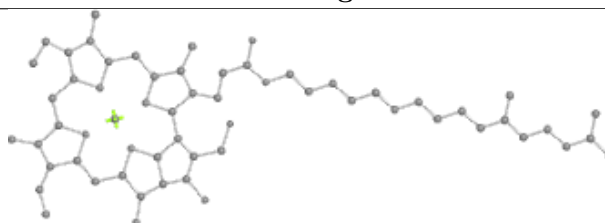
Bond lengths



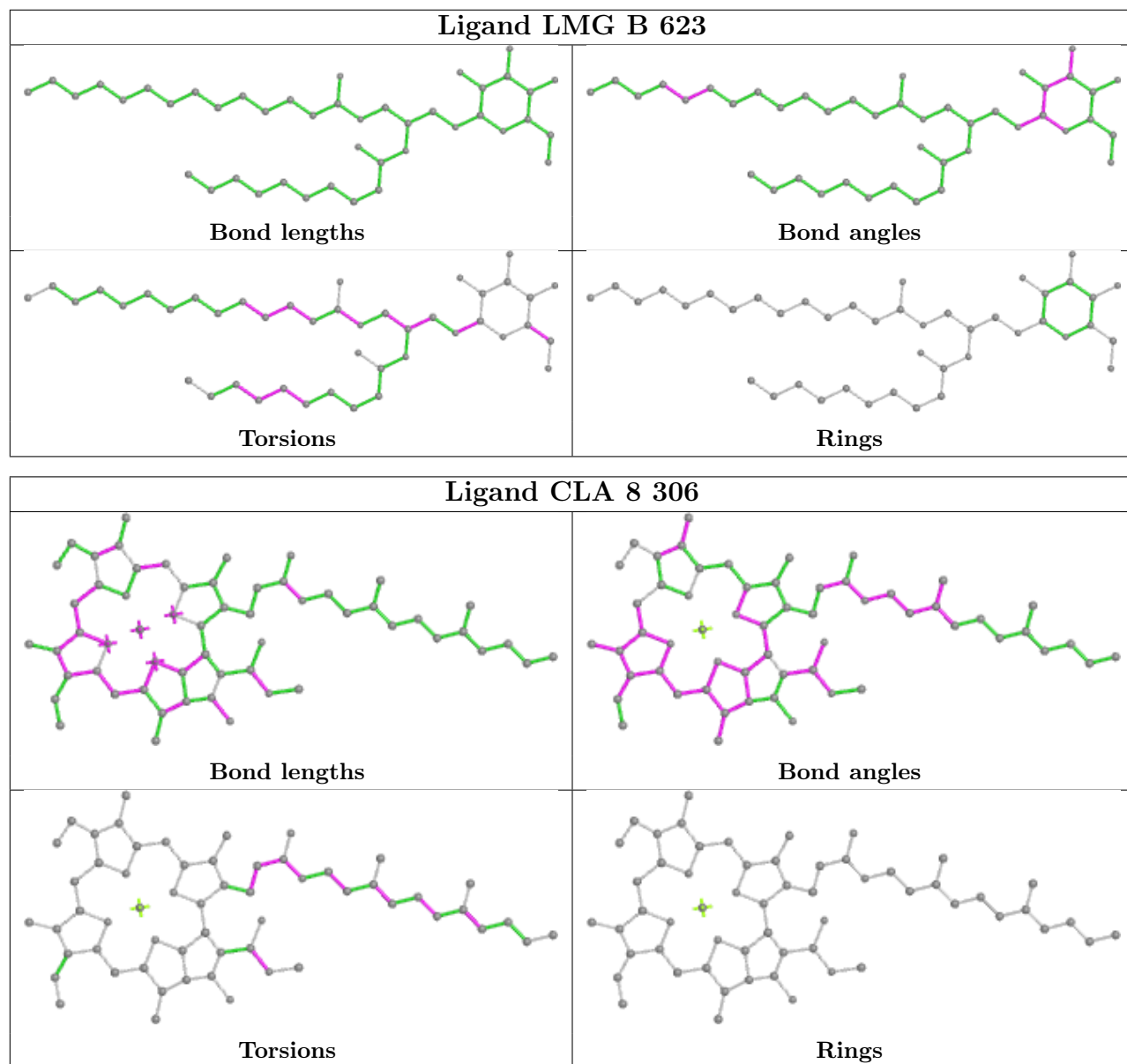
Bond angles

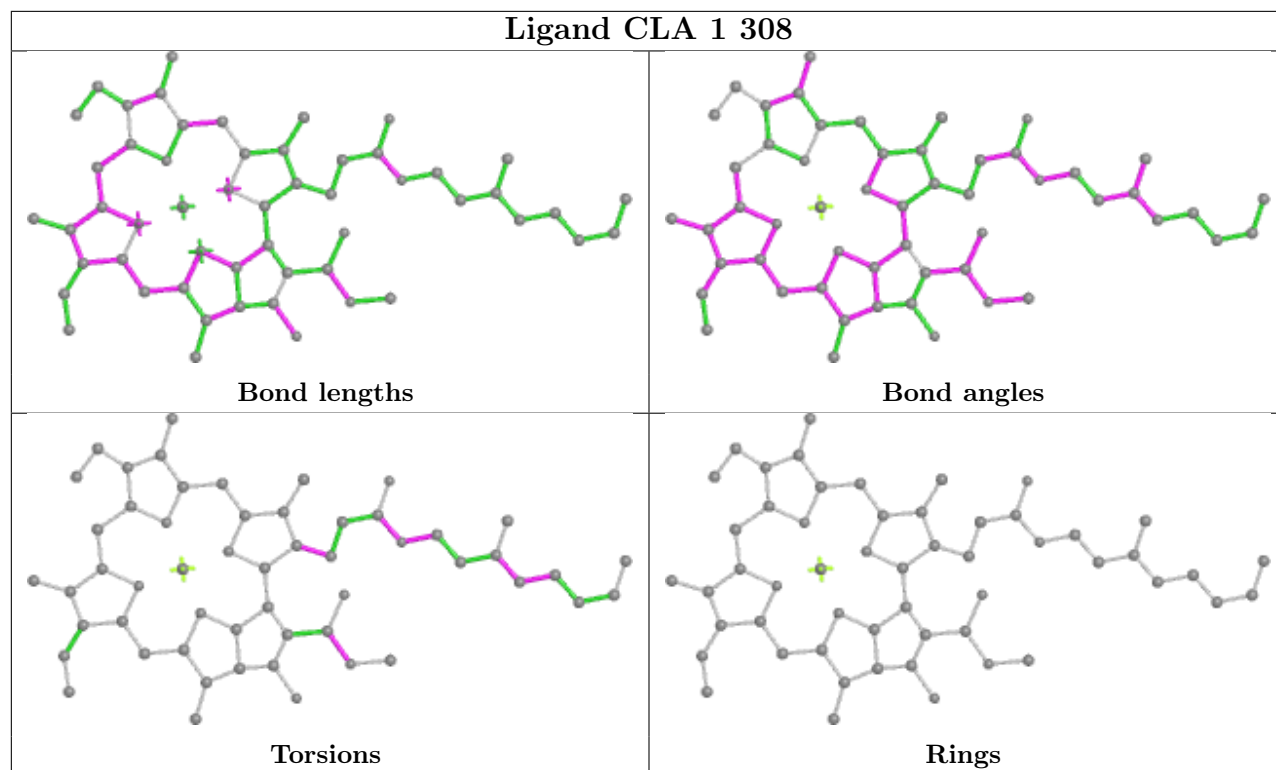
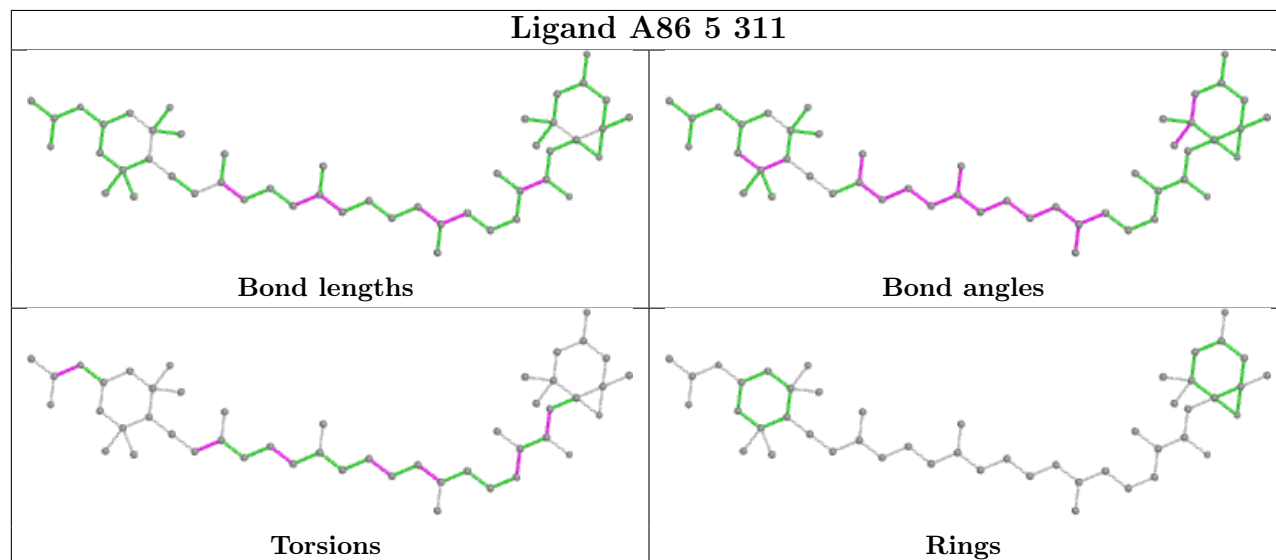


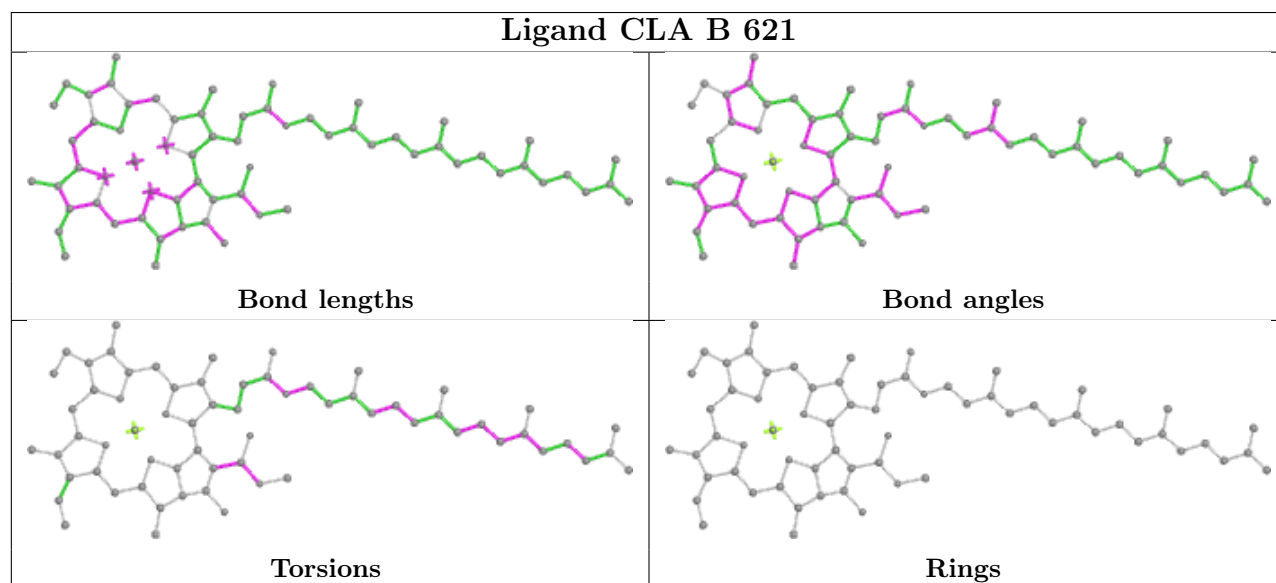
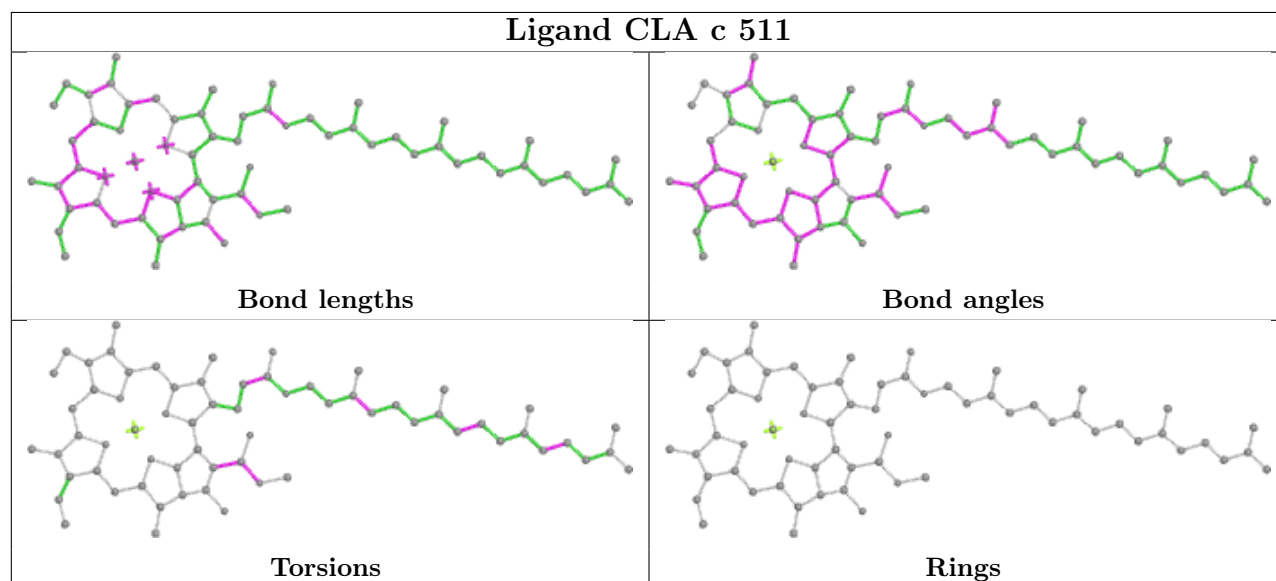
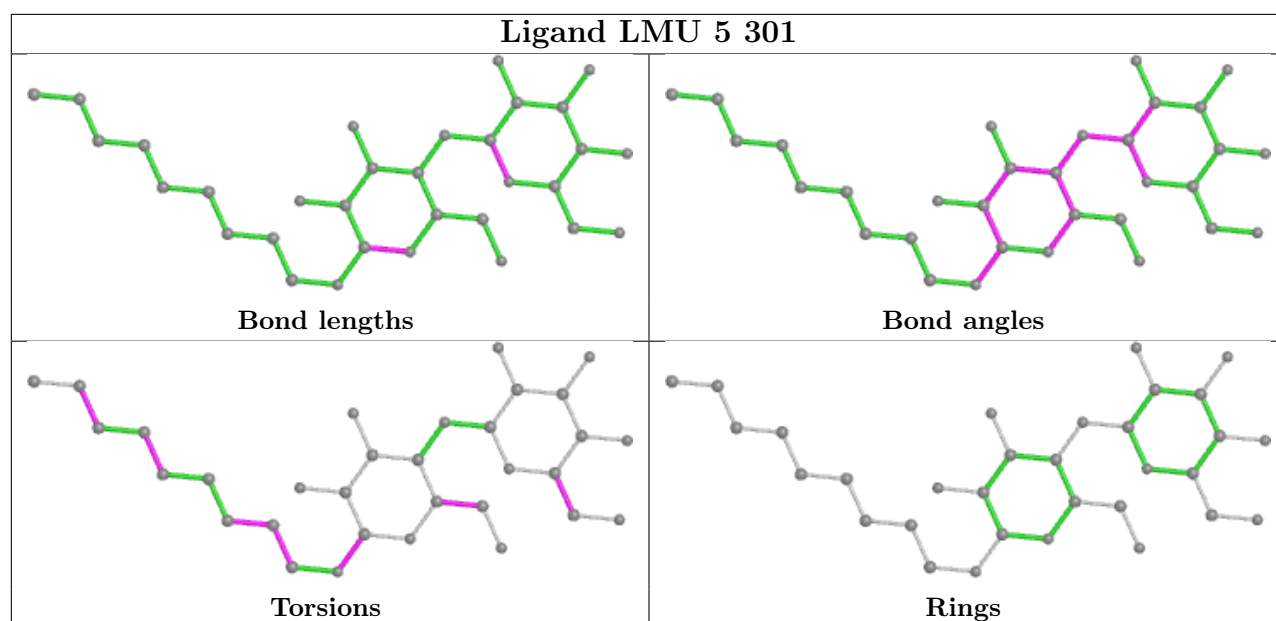
Torsions



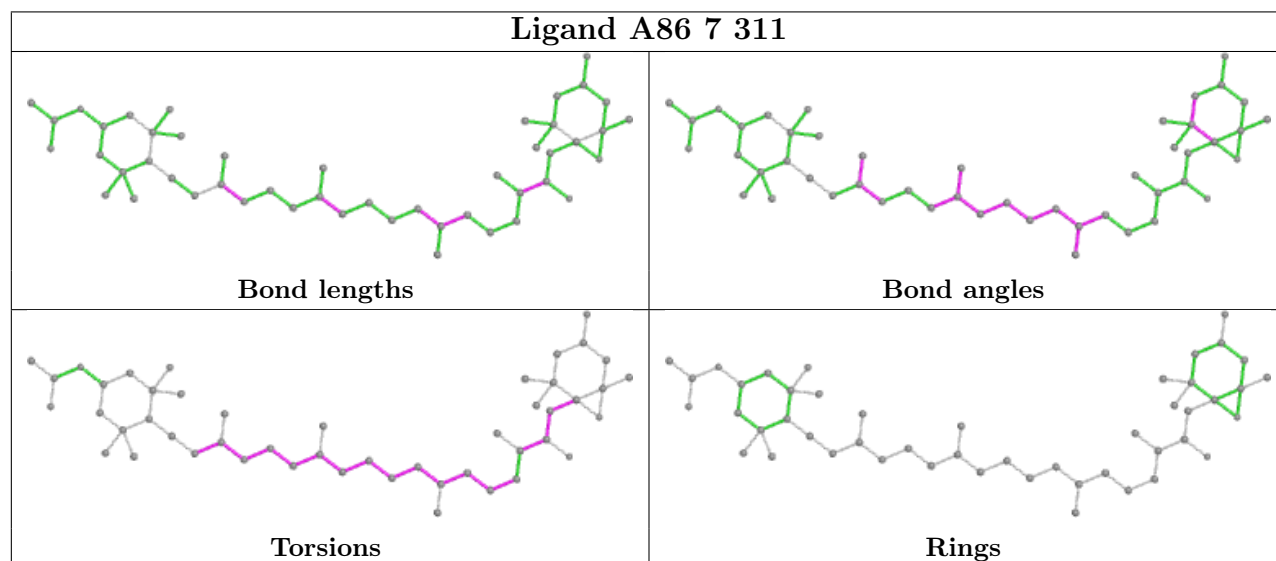
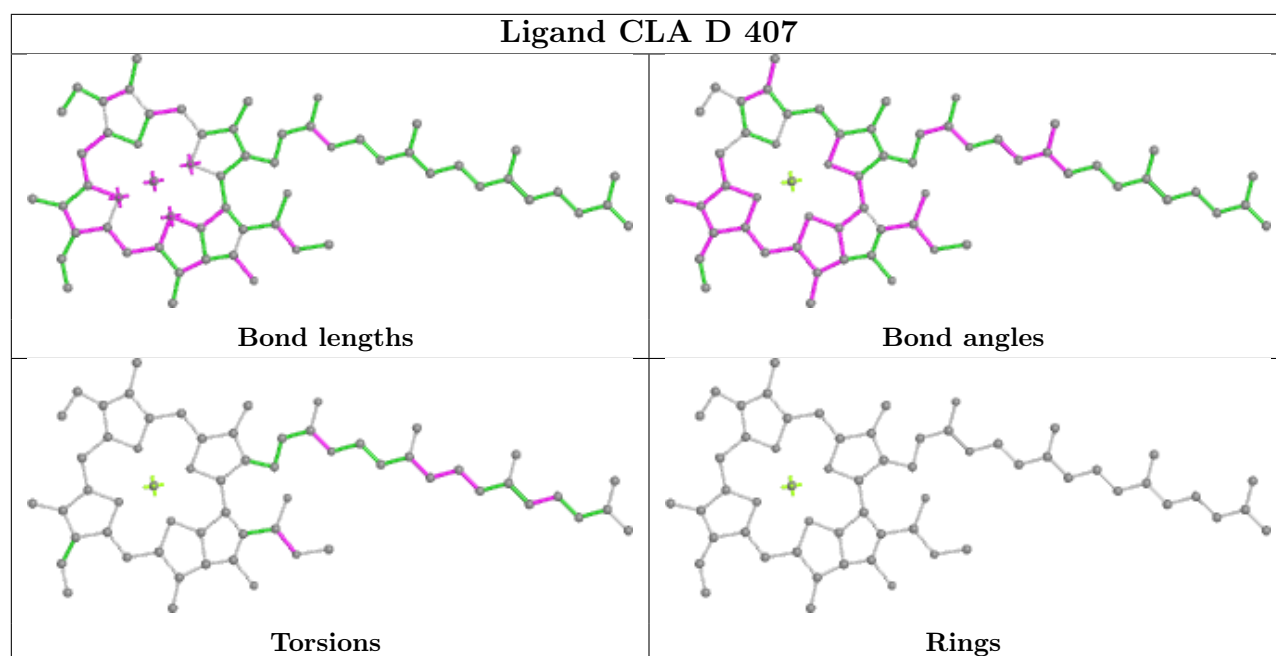
Rings



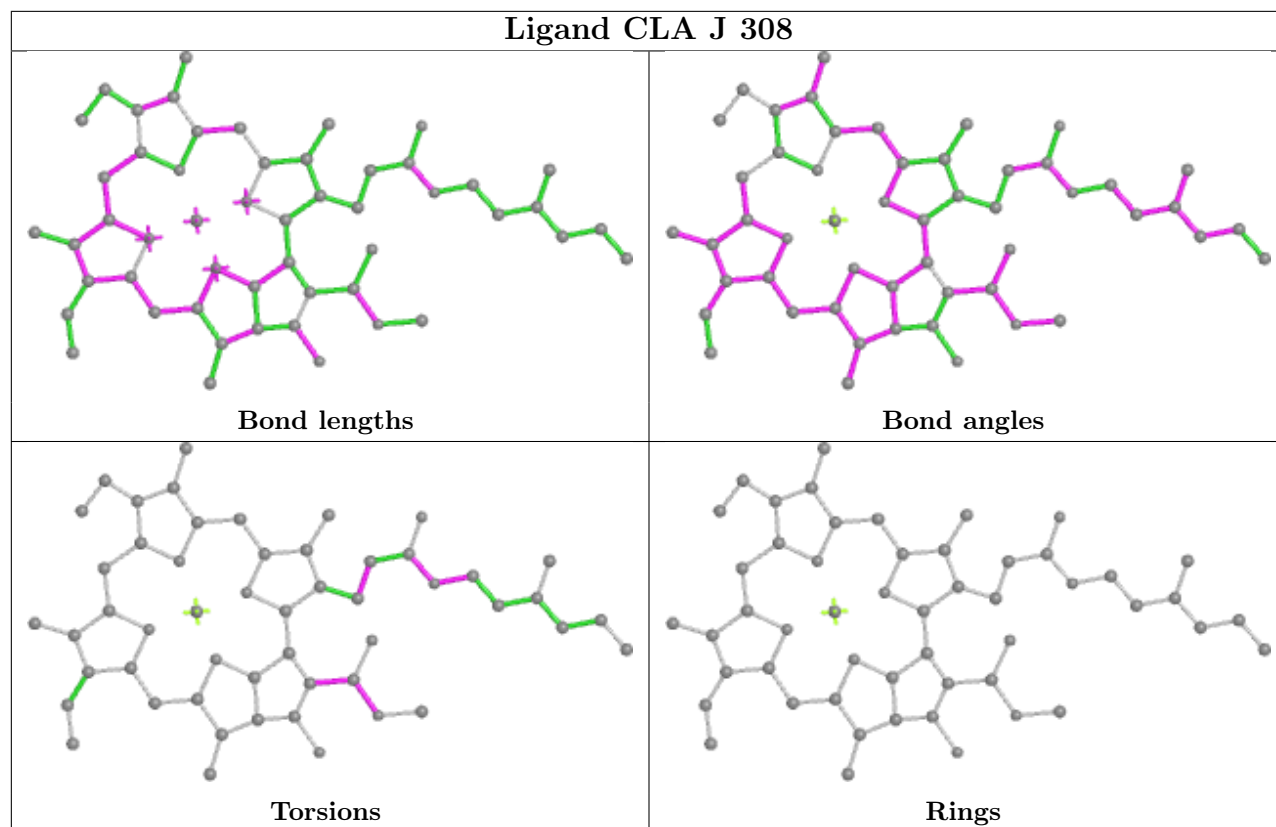
**Ligand CLA 1 308****Ligand A86 5 311**



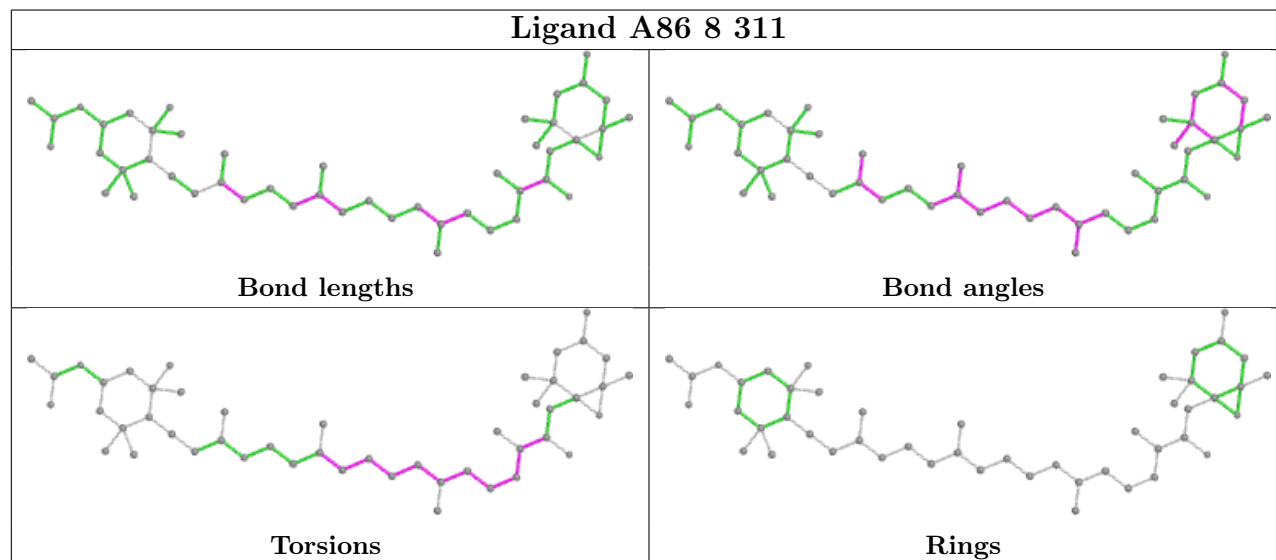




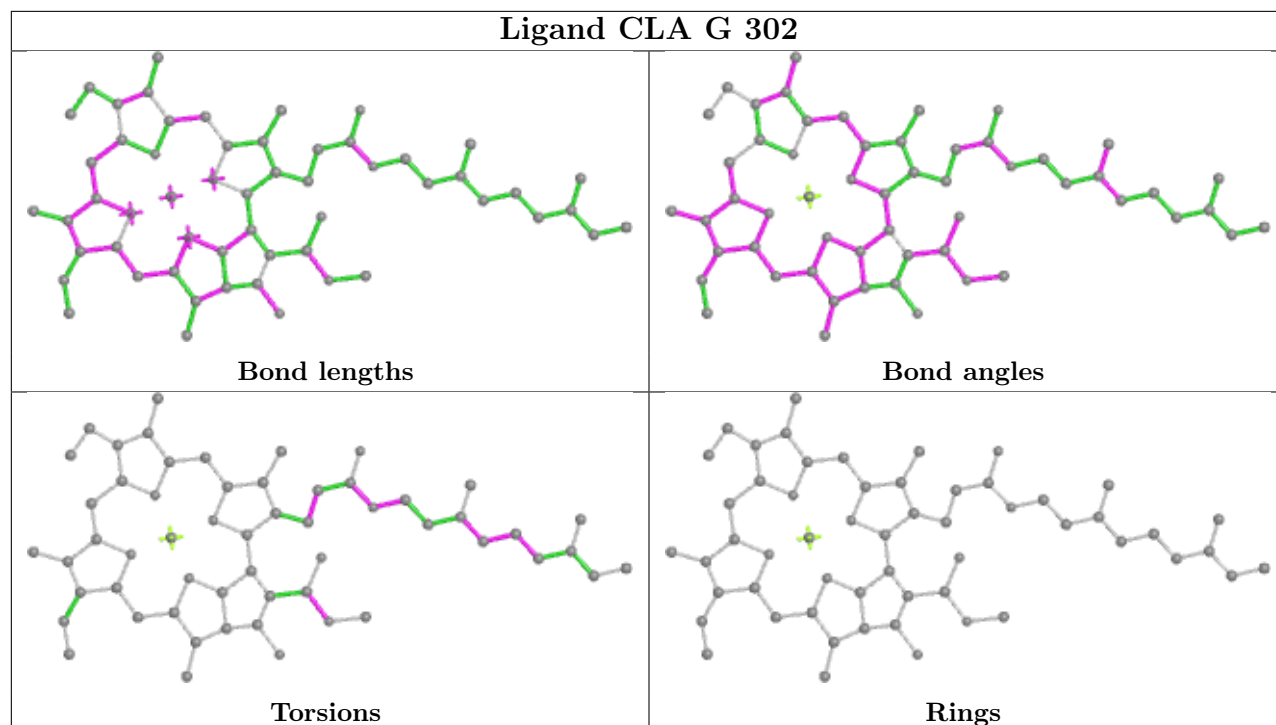
## Ligand CLA J 308



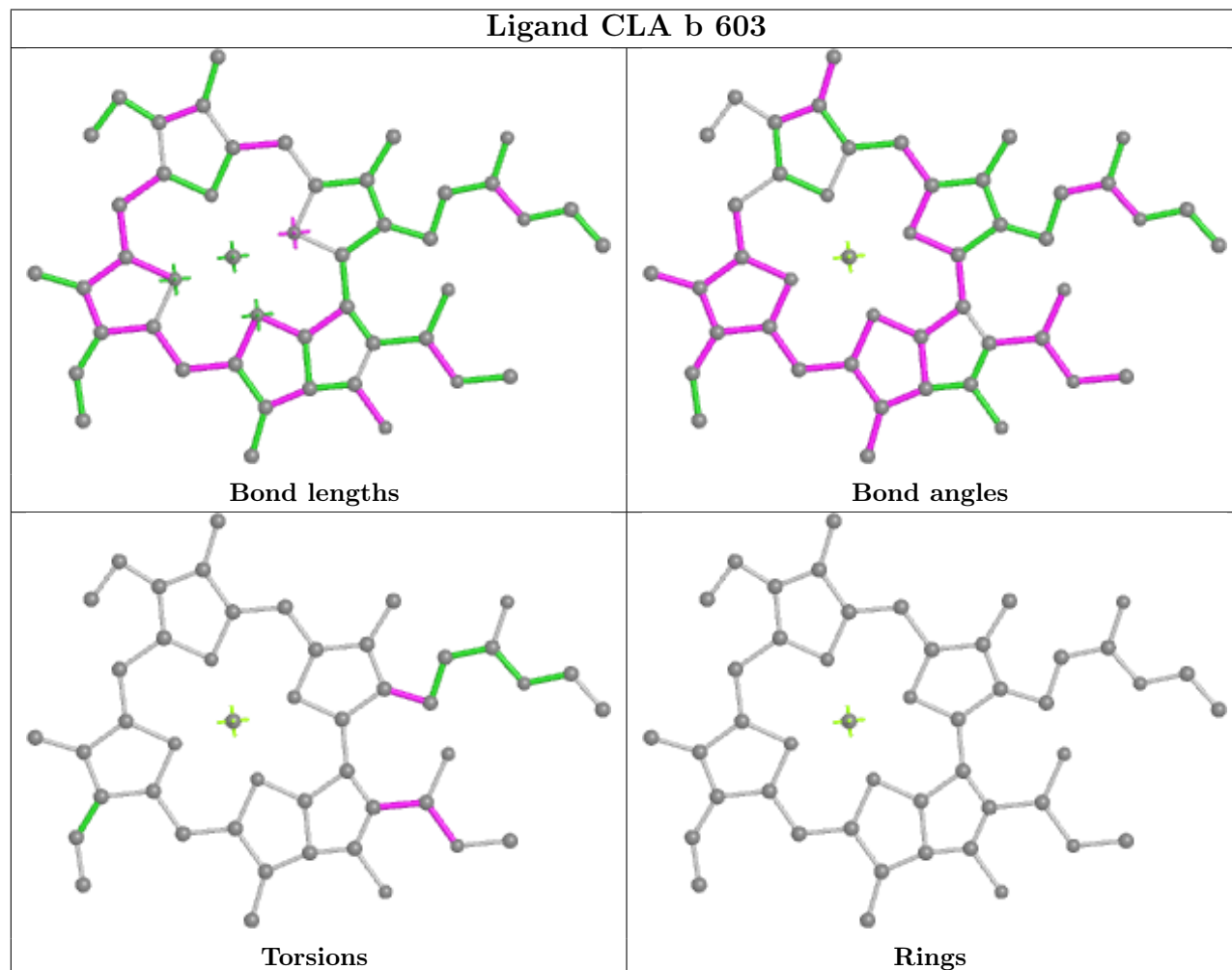
## Ligand A86 8 311

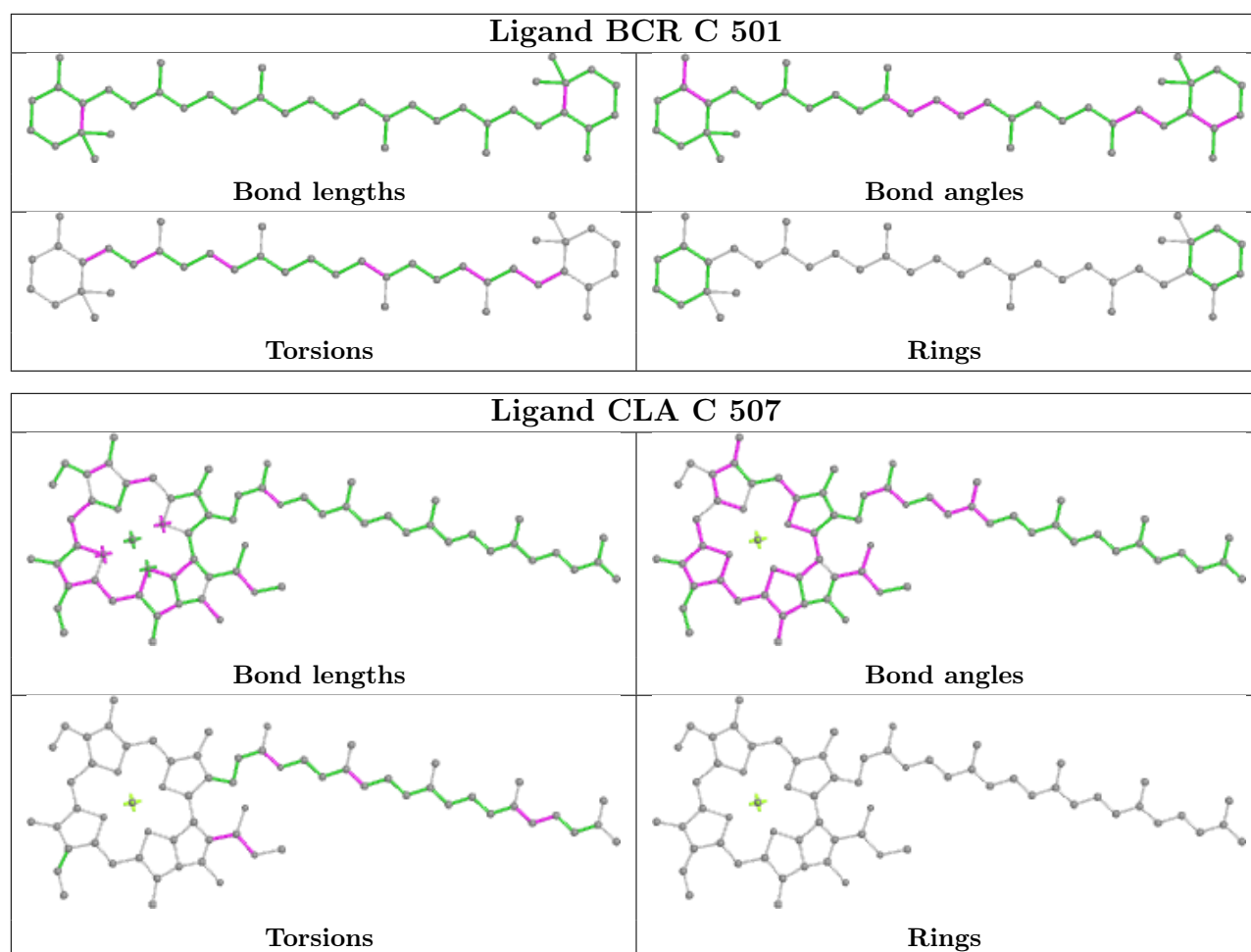


## Ligand CLA G 302



## Ligand CLA b 603





## 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.

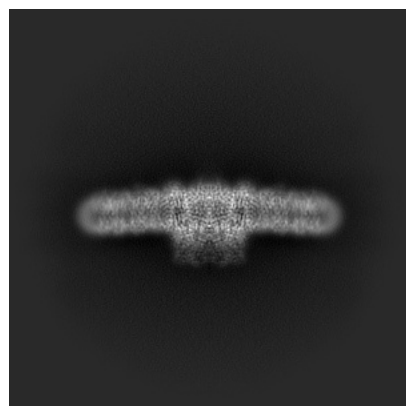
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62499. These allow visual inspection of the internal detail of the map and identification of artifacts.

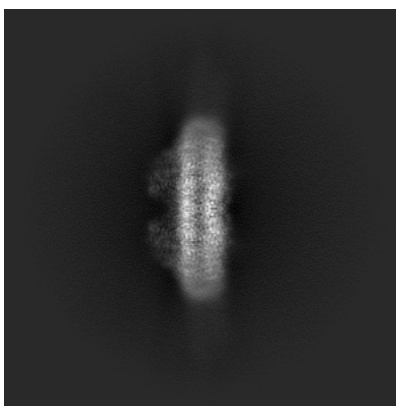
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

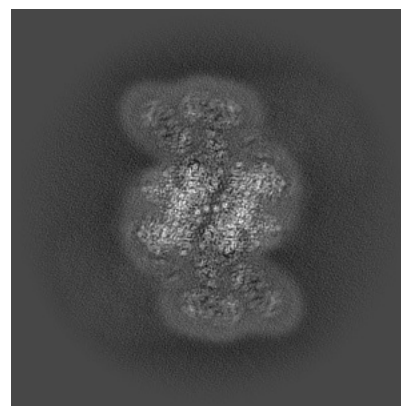
#### 6.1.1 Primary map



X

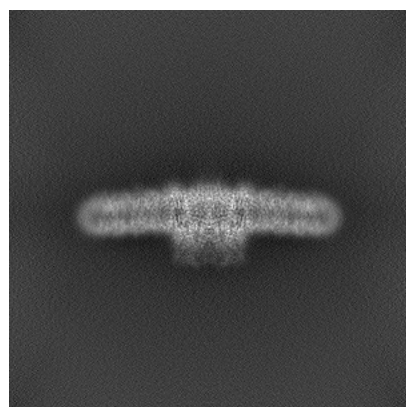


Y

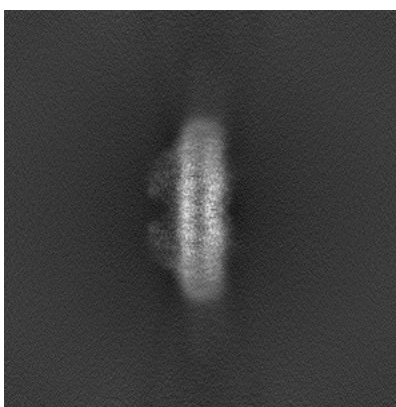


Z

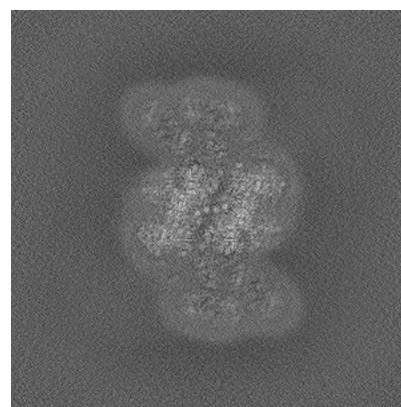
#### 6.1.2 Raw map



X



Y

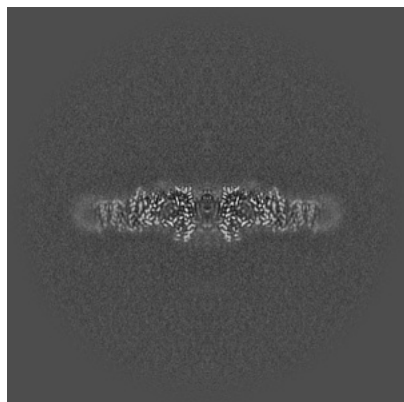


Z

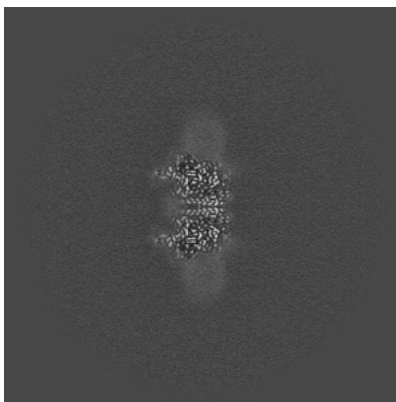
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

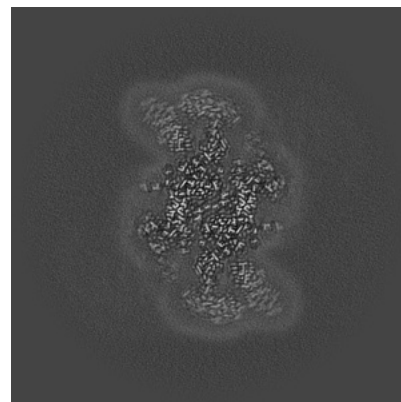
### 6.2.1 Primary map



X Index: 300

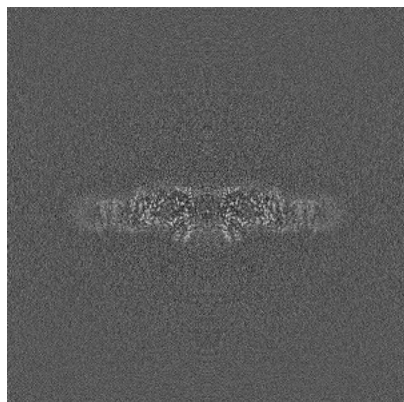


Y Index: 300

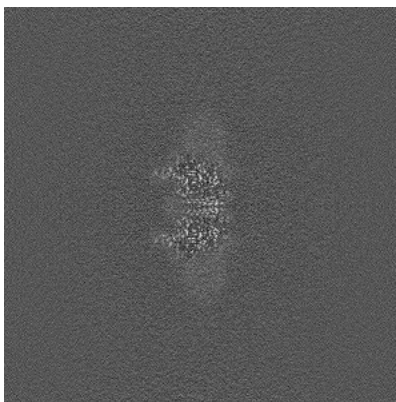


Z Index: 300

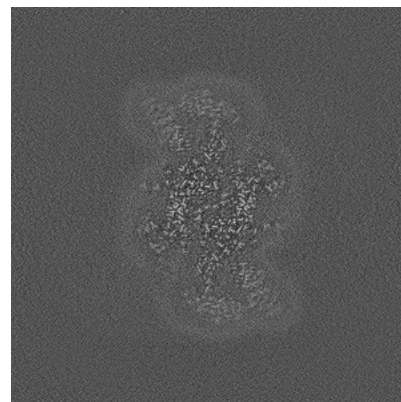
### 6.2.2 Raw map



X Index: 300



Y Index: 300



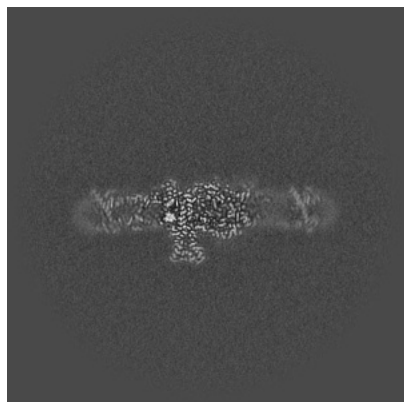
Z Index: 300

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

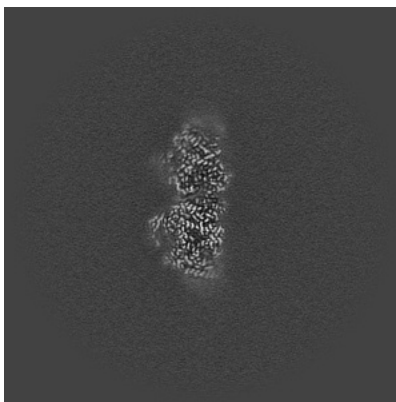


## 6.3 Largest variance slices [i](#)

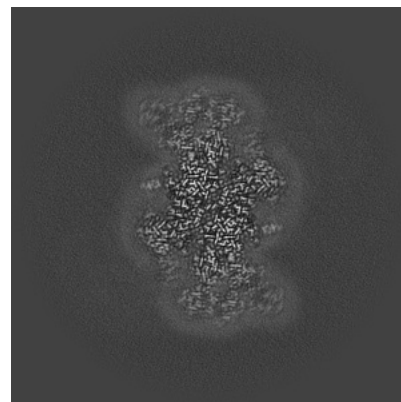
### 6.3.1 Primary map



X Index: 332

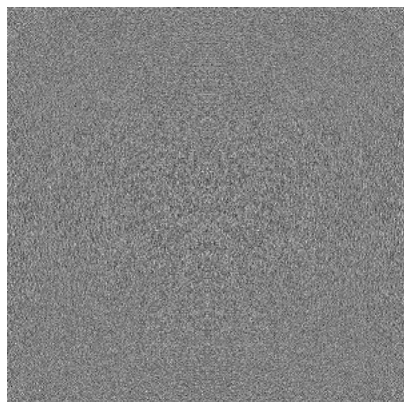


Y Index: 328

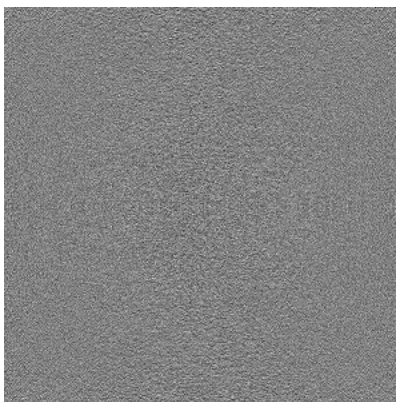


Z Index: 308

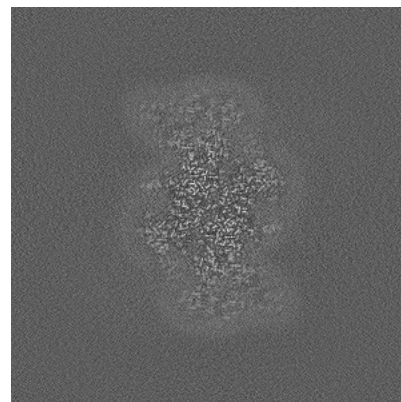
### 6.3.2 Raw map



X Index: 0



Y Index: 0

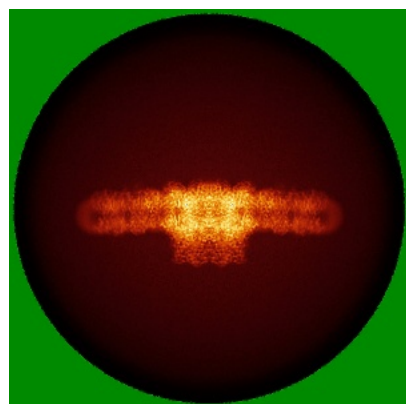


Z Index: 308

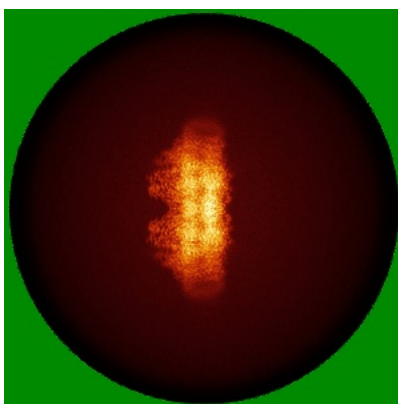
The images above show the largest variance slices of the map in three orthogonal directions.

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

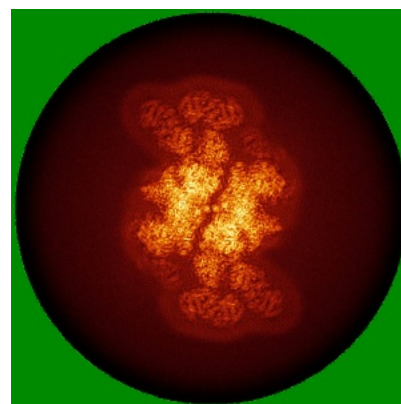
### 6.4.1 Primary map



X

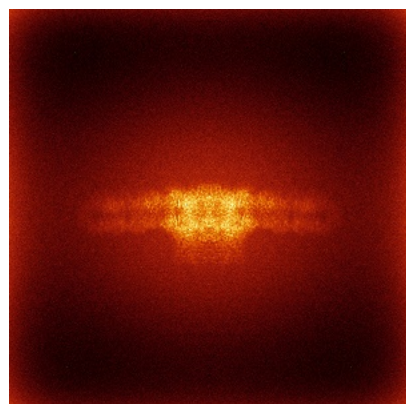


Y

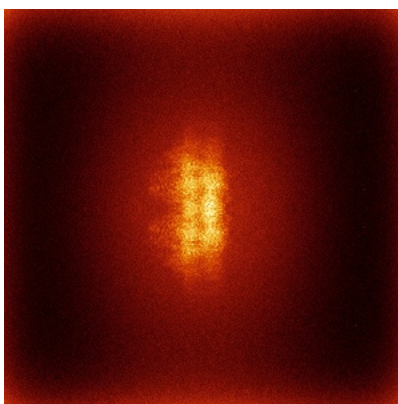


Z

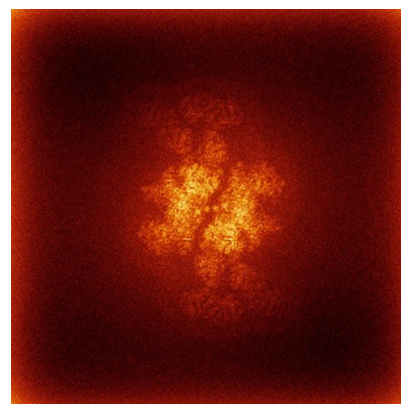
### 6.4.2 Raw map



X



Y



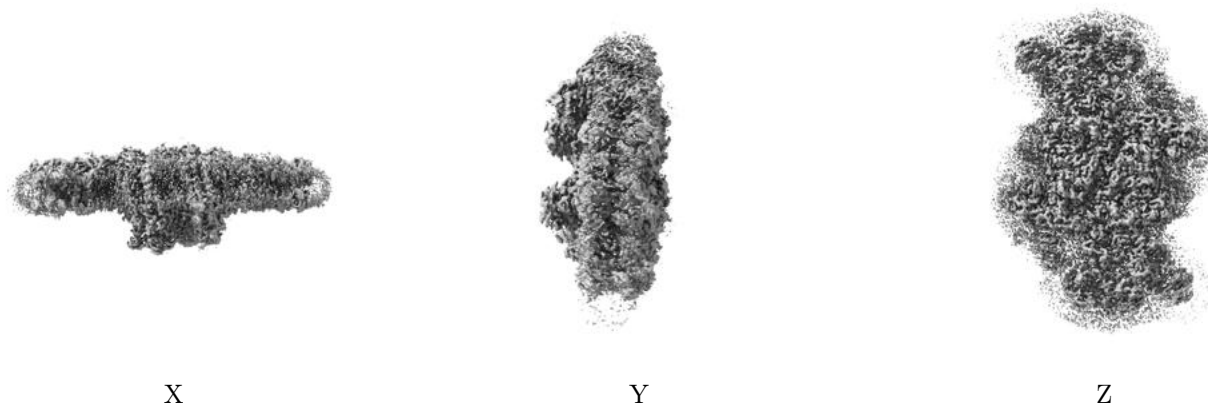
Z

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.



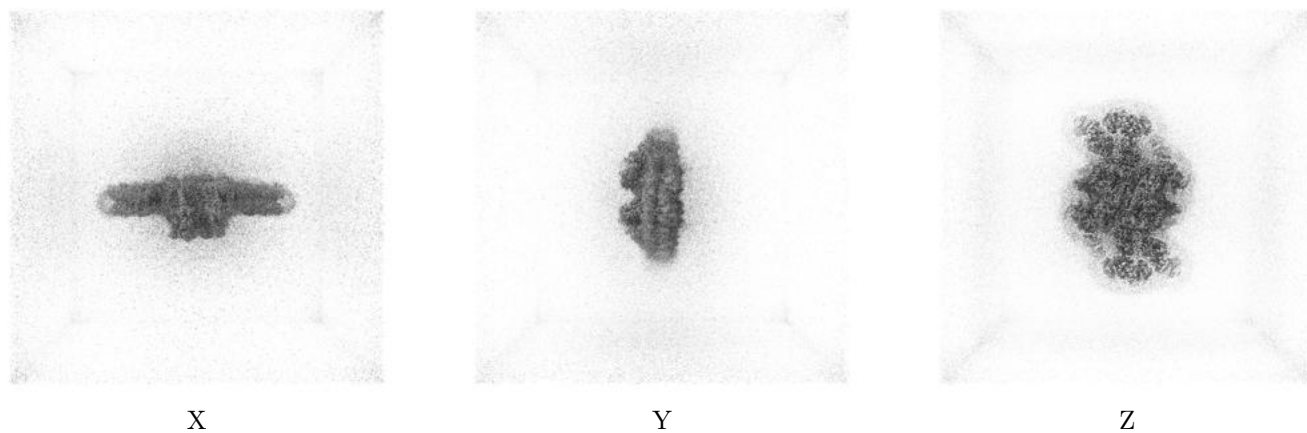
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

### 6.6.1 emd\_62499\_msk\_1.map [i](#)



X



Y

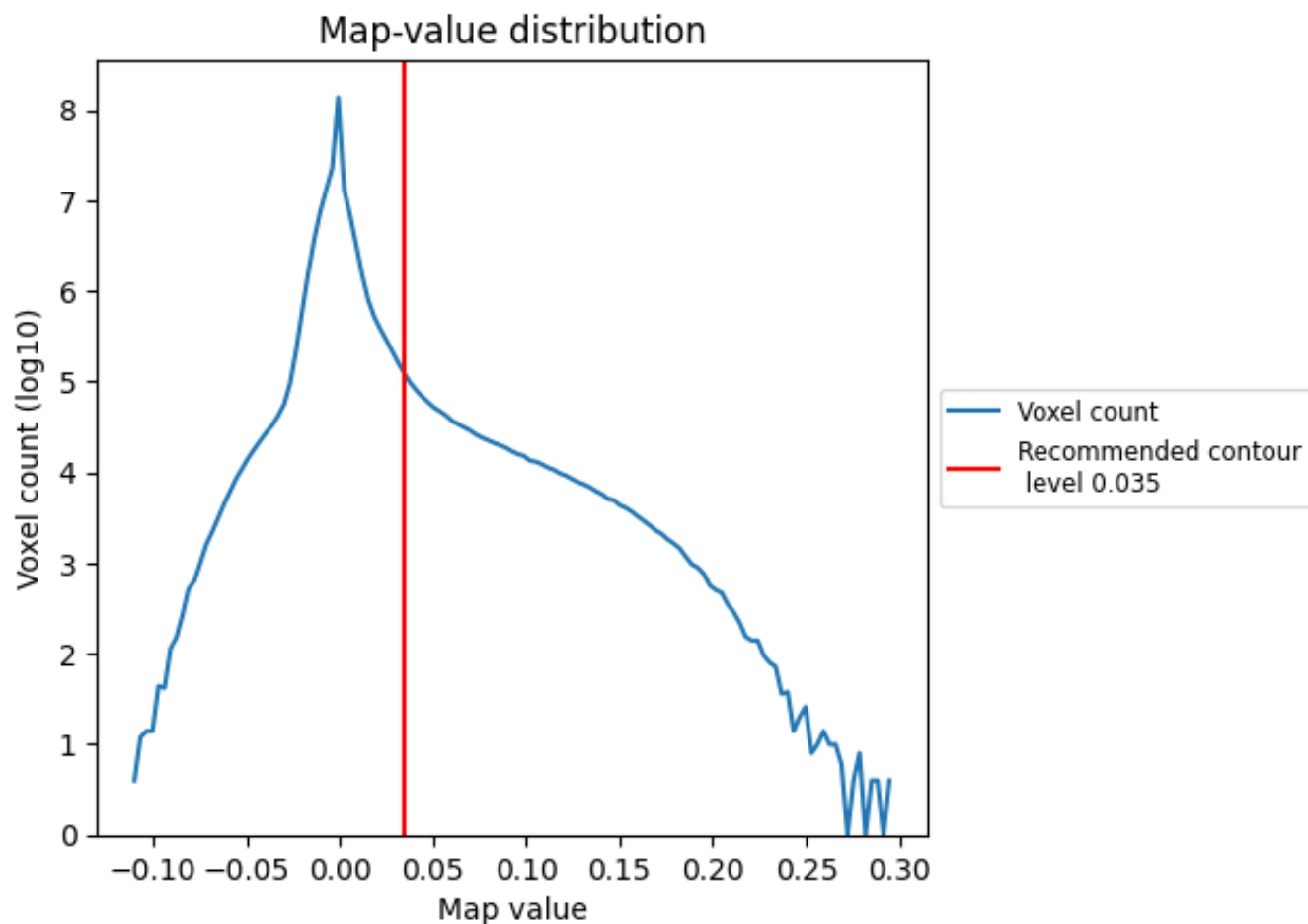


Z

## 7 Map analysis [i](#)

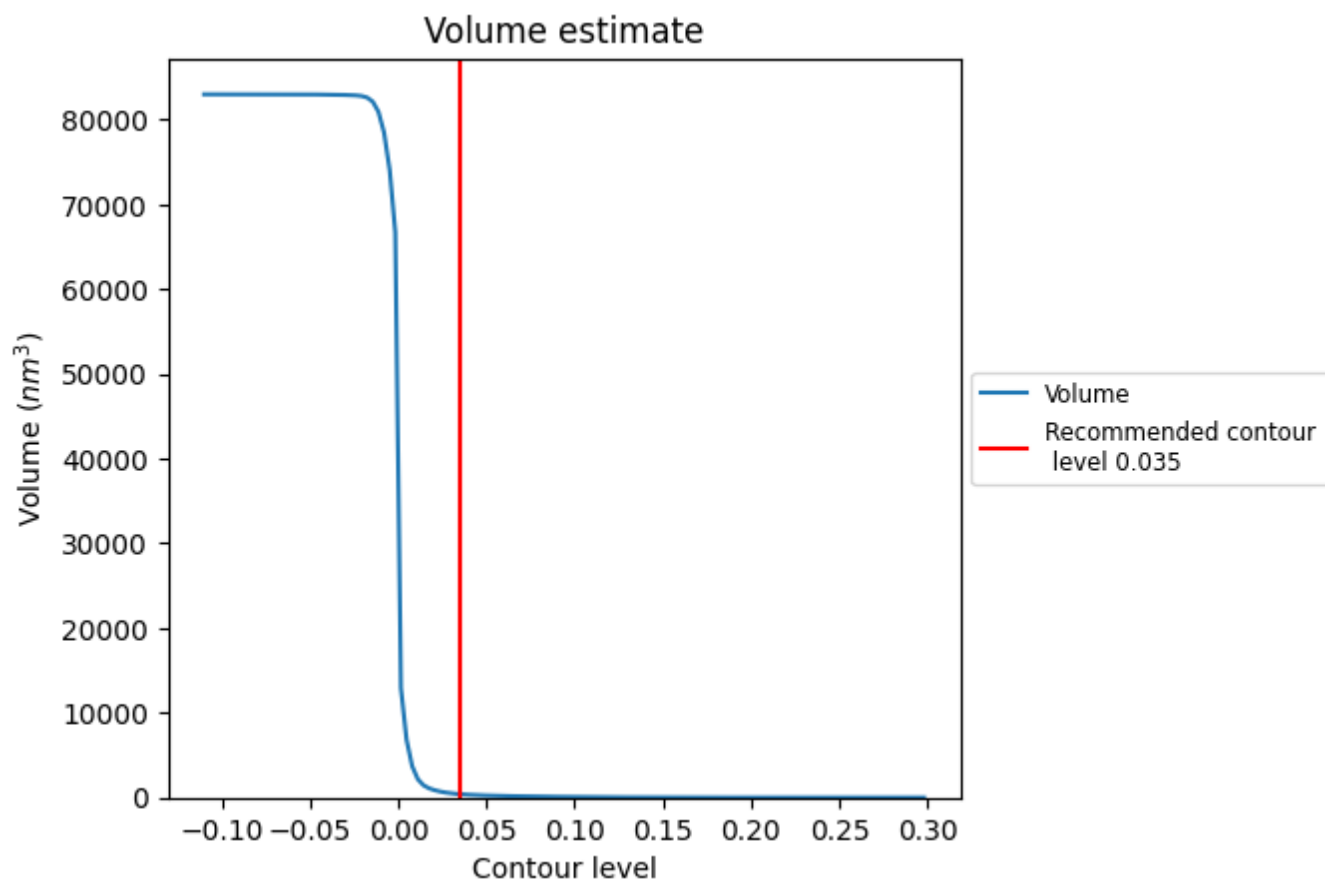
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

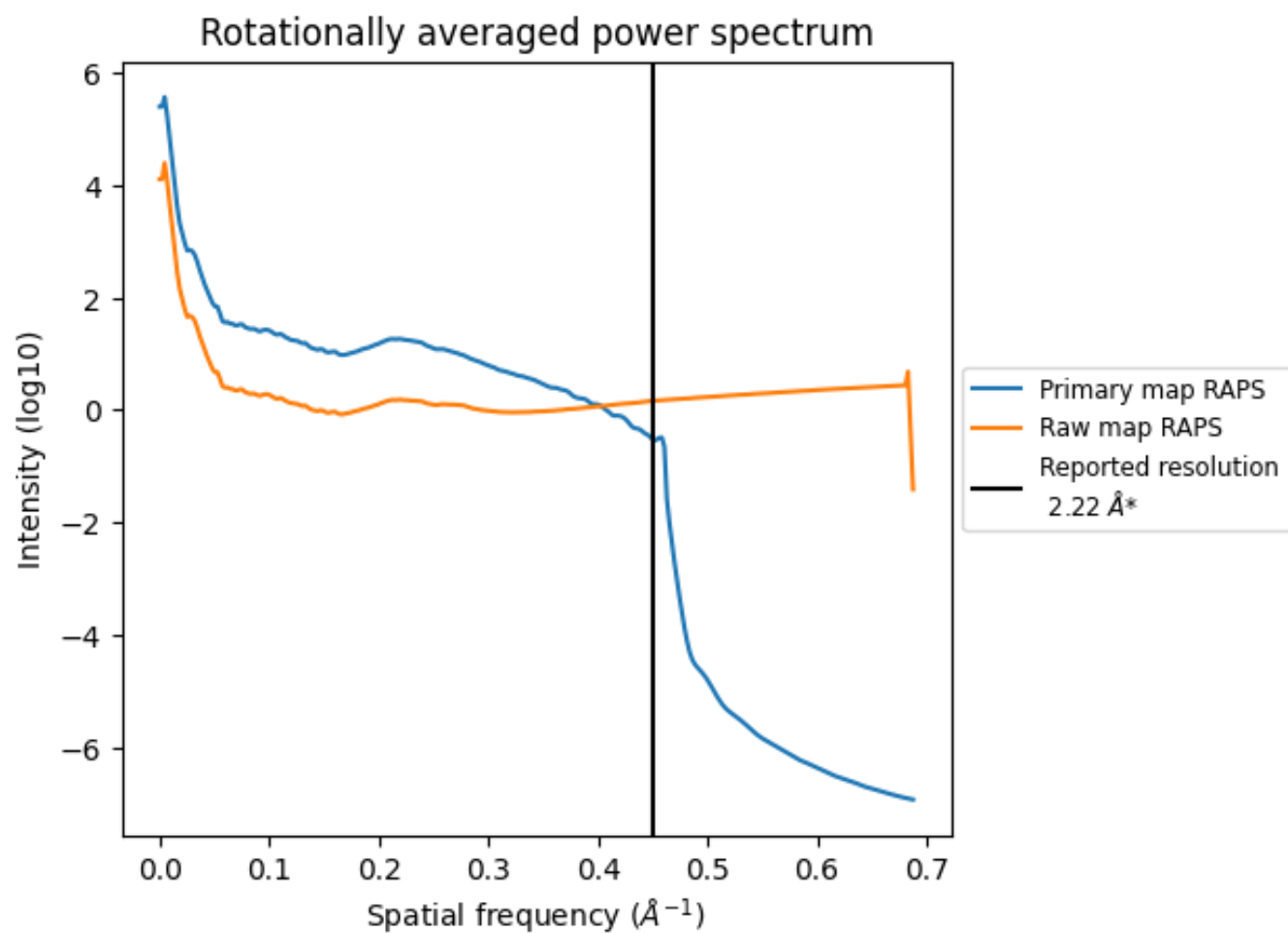
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 402  $\text{nm}^3$ ; this corresponds to an approximate mass of 363 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 ⓘ

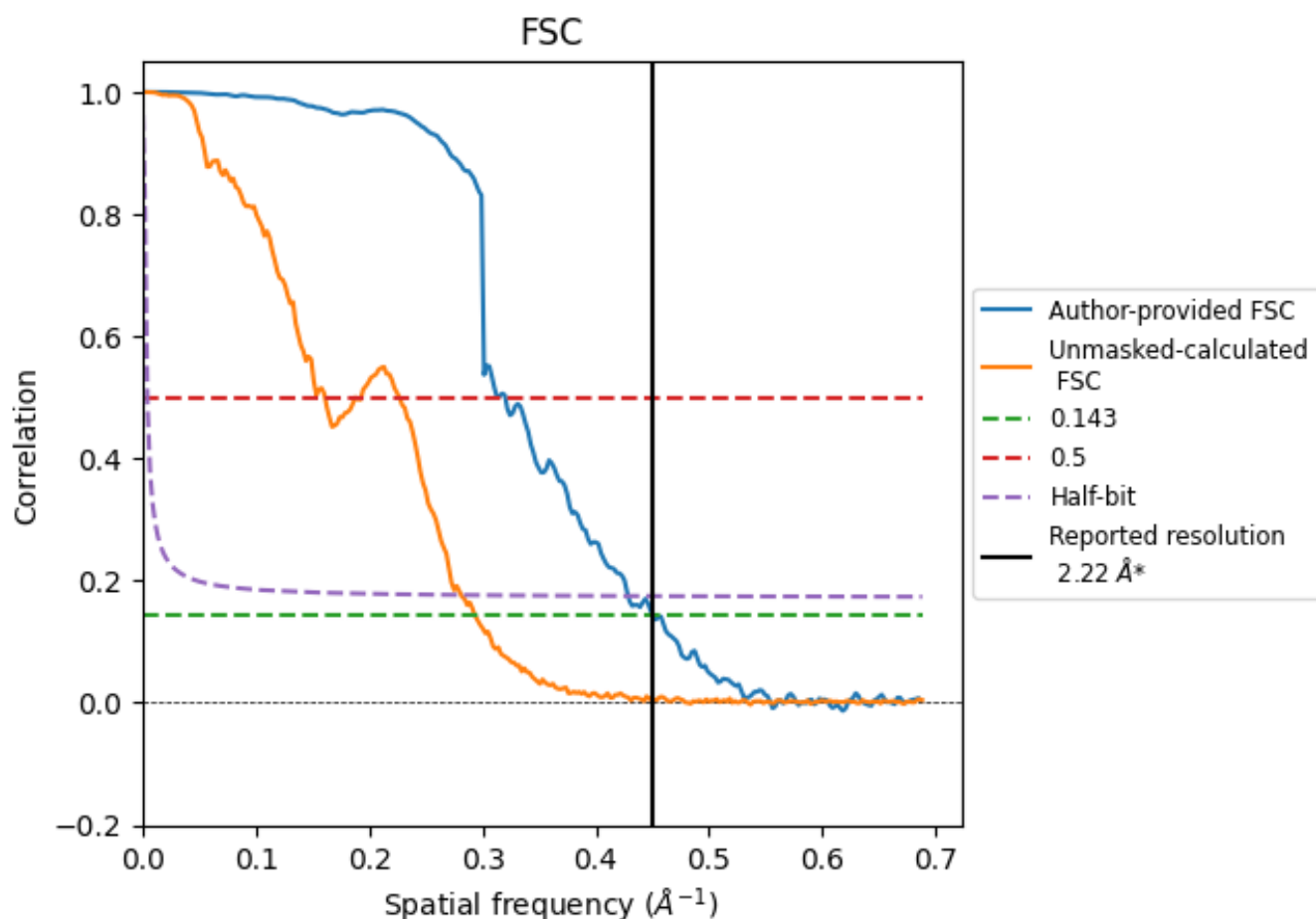


\*Reported resolution corresponds to spatial frequency of 0.450  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.450  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

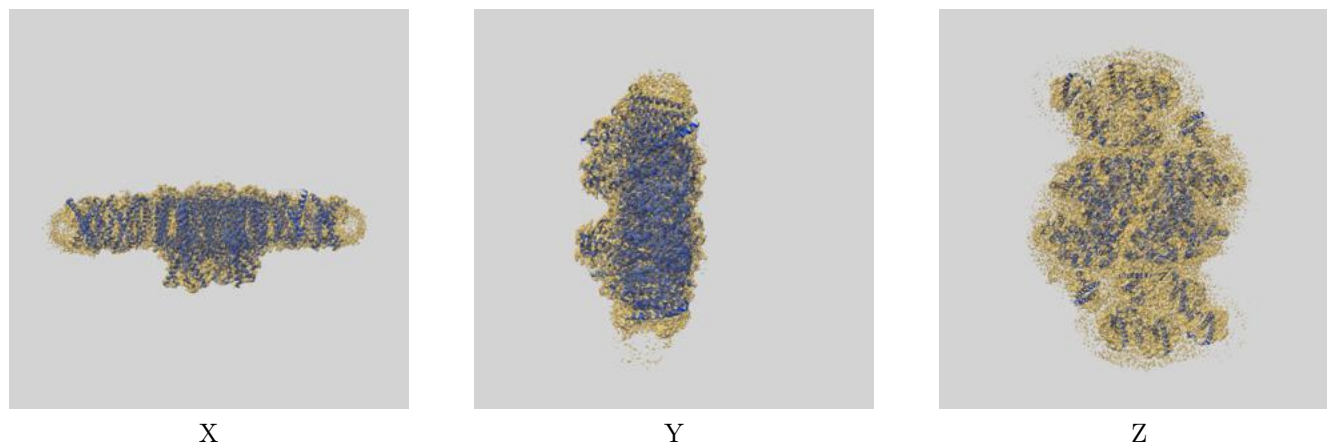
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.22	-	-
Author-provided FSC curve	2.22	3.12	2.33
Unmasked-calculated*	3.41	6.21	3.56

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.41 differs from the reported value 2.22 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62499 and PDB model 9KQB. Per-residue inclusion information can be found in section [3](#) on page [36](#).

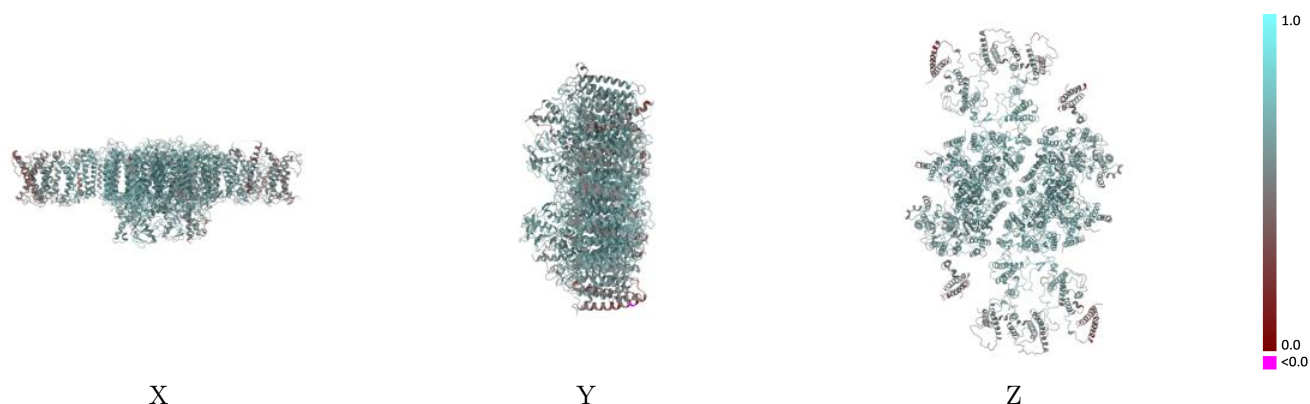
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

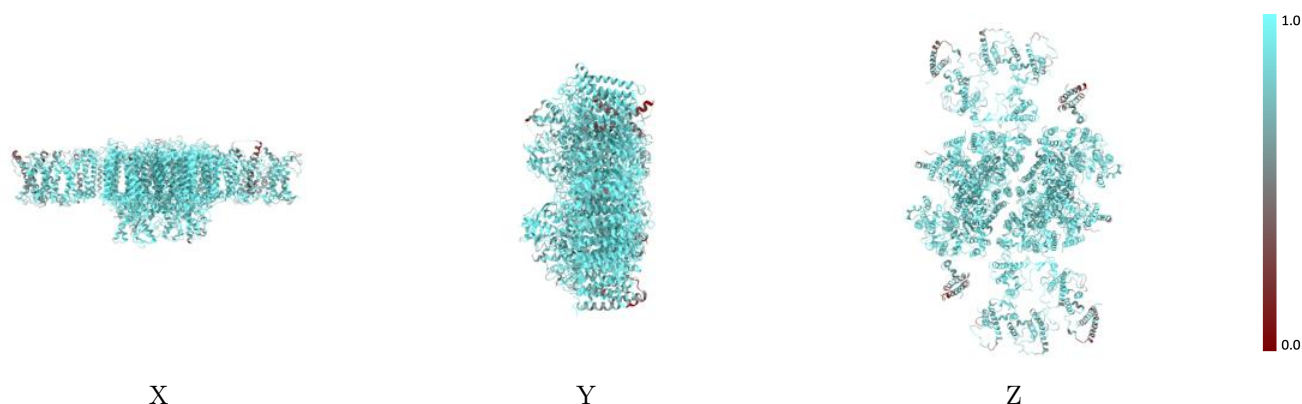


## 9.2 Q-score mapped to coordinate model [i](#)



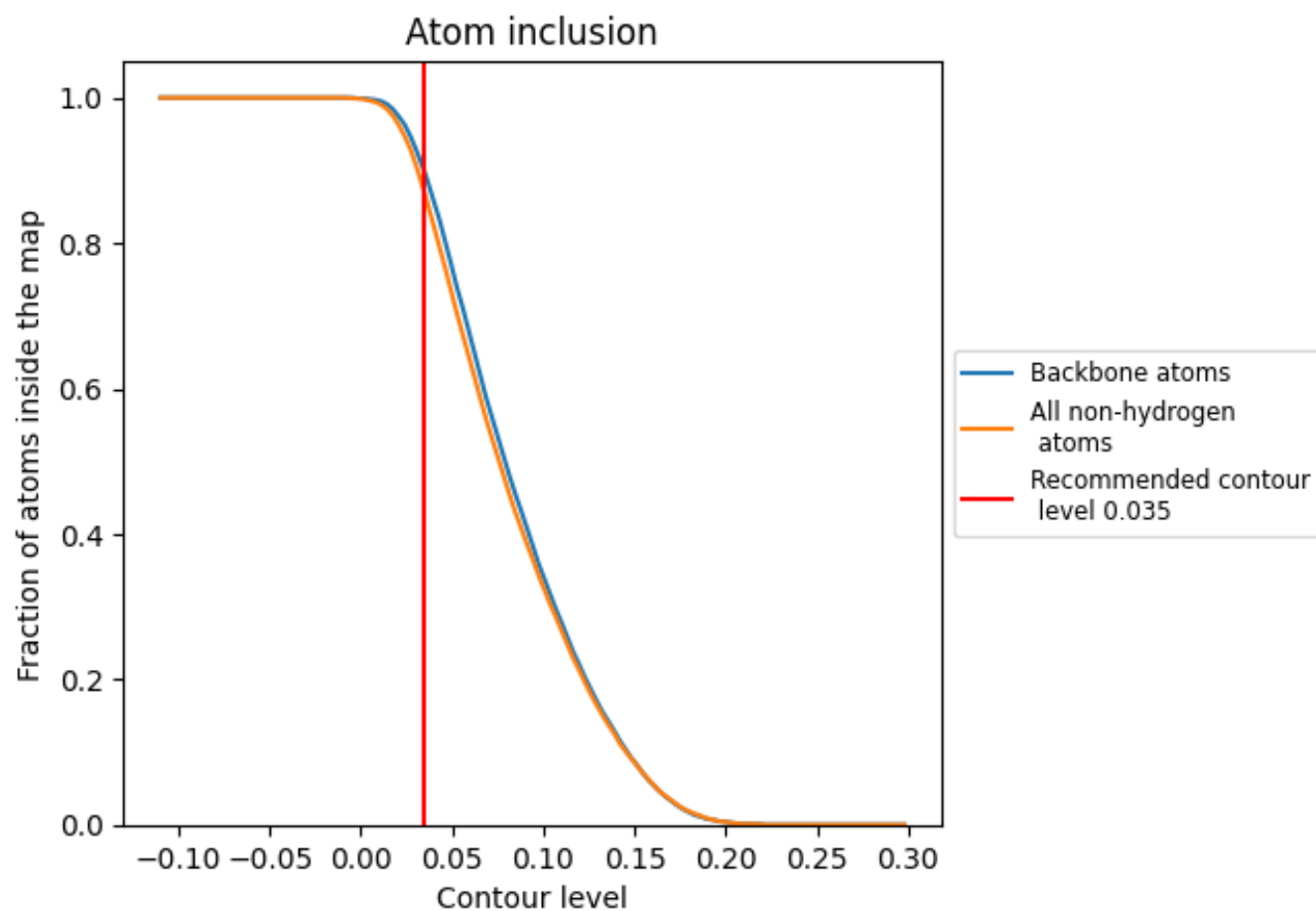
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.5890
1	 0.8120	 0.5590
2	 0.9190	 0.6140
3	 0.5640	 0.4510
4	 0.6030	 0.3970
5	 0.7310	 0.4840
6	 0.7480	 0.4860
7	 0.8190	 0.5580
8	 0.9180	 0.6110
9	 0.5510	 0.4530
A	 0.9370	 0.6400
B	 0.9510	 0.6520
C	 0.8820	 0.5840
D	 0.9510	 0.6650
E	 0.8340	 0.5730
F	 0.8420	 0.5610
G	 0.6060	 0.3930
H	 0.9820	 0.6700
I	 0.9520	 0.6410
J	 0.7550	 0.4840
K	 0.7990	 0.5050
L	 0.9370	 0.6450
M	 0.9260	 0.6350
N	 0.9160	 0.6200
T	 0.9530	 0.6600
W	 0.8900	 0.5810
X	 0.9350	 0.6080
a	 0.9340	 0.6440
b	 0.9530	 0.6530
c	 0.8870	 0.5870
d	 0.9750	 0.6730
e	 0.8440	 0.5730
f	 0.8090	 0.5570
g	 0.7280	 0.4800
h	 0.9460	 0.6490



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Chain	Atom inclusion	Q-score
i	 0.9420	 0.6340
k	 0.8100	 0.5140
l	 0.9640	 0.6710
m	 0.9420	 0.6450
n	 0.9300	 0.6330
t	 0.9450	 0.6540
w	 0.8950	 0.5800
x	 0.9460	 0.6130