



wwPDB EM Validation Summary Report ⓘ

Aug 13, 2026 – 12:13 AM JST

PDB ID : 9L5V / pdb_00009l5v
EMDB ID : EMD-62846
Title : cryo-EM structure of PSII-ACPII from Rhodomonas sp. NIES-2332
Authors : Yonehara, N.; Akita, F.; Shen, J.R.
Deposited on : 2024-12-23
Resolution : 2.17 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

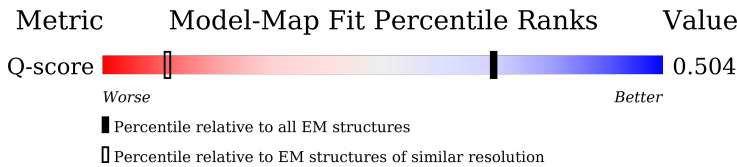
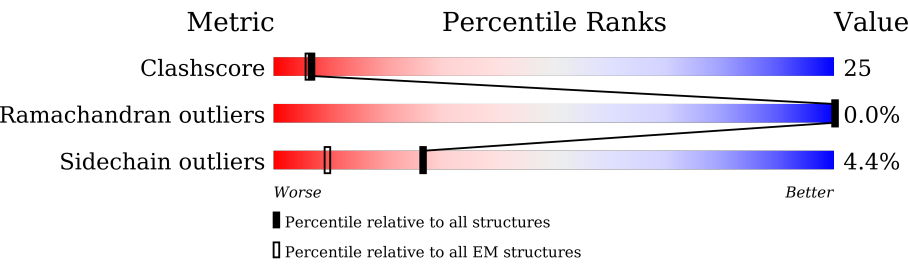
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.17 Å.

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



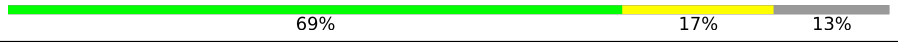
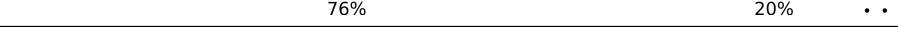
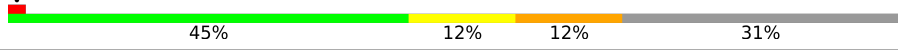
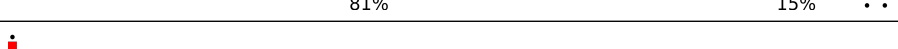
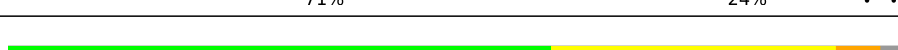
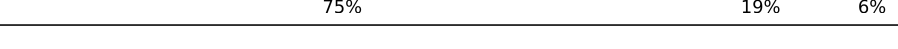
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2651 (1.67 - 2.67)

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

Mol	Chain	Length	Quality of chain
1	A	374	60%20%19%
1	a	374	63%18%17%
2	B	508	65%26%5%
2	b	508	70%22%5%

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Mol	Chain	Length	Quality of chain
3	C	486	
3	c	486	
4	D	351	
4	d	351	
5	E	84	
5	e	84	
6	F	42	
6	f	42	
7	H	67	
7	h	67	
8	I	38	
8	i	38	
9	K	45	
9	k	45	
10	L	38	
10	l	38	
11	M	118	
11	m	118	
12	T	32	
12	t	32	
13	W	121	
13	w	121	
14	X	39	
14	x	39	
15	Y	34	

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Mol	Chain	Length	Quality of chain
15	y	34	
16	Z	62	
16	z	62	
17	1	234	
17	N	234	
18	2	215	
18	O	215	
19	3	182	
19	P	182	
20	4	200	
20	Q	200	
21	5	228	
21	R	228	
22	6	174	
22	S	174	
23	G	292	
24	g	292	

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
26	CLA	1	606	-	-	X	-
26	CLA	2	301	-	-	X	-
26	CLA	2	311	-	-	X	-
26	CLA	2	319	-	-	X	-
26	CLA	3	307	-	-	X	-
26	CLA	4	301	-	-	X	-
26	CLA	4	303	-	-	X	-
26	CLA	4	306	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	5	605	-	-	X	-
26	CLA	5	611	-	-	X	-
26	CLA	6	609	-	-	X	-
26	CLA	N	601	-	-	X	-
26	CLA	N	606	-	-	X	-
26	CLA	N	614	-	-	X	-
26	CLA	O	601	-	-	X	-
26	CLA	R	306	-	-	X	-
28	WVN	3	313	-	-	X	-
28	WVN	C	516	-	X	-	-
34	LHG	1	620	-	-	X	-
34	LHG	2	321	-	-	X	-
34	LHG	N	621	-	-	X	-
38	KC2	N	612	-	-	X	-
38	KC2	Q	310	-	-	X	-
39	II0	3	310	-	-	X	-
39	II0	3	311	-	-	X	-
39	II0	4	320	-	-	X	-
40	IHT	1	619	-	X	-	-
40	IHT	2	317	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 69223 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	303	Total	C	N	O	S	1	0
			2377	1562	393	410	12		
1	a	311	Total	C	N	O	S	0	0
			2438	1603	401	422	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	482	Total	C	N	O	S	1	0
			3797	2479	650	656	12		
2	b	481	Total	C	N	O	S	0	0
			3782	2471	645	654	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	424	Total	C	N	O	S	1	0
			3331	2188	559	573	11		
3	c	421	Total	C	N	O	S	0	0
			3299	2164	555	569	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	1	0
			2713	1792	445	464	12		
4	d	341	Total	C	N	O	S	0	0
			2705	1788	443	462	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			525	345	85	95		
5	e	64	Total	C	N	O	0	0
			525	345	85	95		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	29	Total	C	N	O	S	0	0
			235	159	40	35	1		
6	f	30	Total	C	N	O	S	0	0
			246	168	41	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			508	337	81	88	2		
7	h	65	Total	C	N	O	S	0	0
			508	337	81	88	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			284	188	46	49	1		
8	i	35	Total	C	N	O	S	0	0
			284	188	46	49	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			296	209	44	43		
9	k	37	Total	C	N	O	0	0
			296	209	44	43		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	37	Total	C	N	O	0	0
			301	204	47	50		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	37	Total	C	N	O	0	0
			301	204	47	50		

- Molecule 11 is a protein called Photosystem II protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	36	Total	C	N	O	0	0
			271	181	42	48		
11	m	36	Total	C	N	O	0	0
			271	181	42	48		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	30	Total	C	N	O	S	0	0
			244	169	36	38	1		
12	t	30	Total	C	N	O	S	0	0
			244	169	36	38	1		

- Molecule 13 is a protein called Photosystem II protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	W	45	Total	C	N	O	0	0
			361	233	58	70		
13	w	45	Total	C	N	O	0	0
			361	233	58	70		

- Molecule 14 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	34	Total	C	N	O	S	0	0
			249	167	36	45	1		
14	x	34	Total	C	N	O	S	0	0
			249	167	36	45	1		

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Y	28	Total	C	N	O	0	0
			209	140	36	33		
15	y	28	Total	C	N	O	0	0
			209	140	36	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	61	Total	C	N	O	S	0	0
			451	305	67	76	3		
16	z	61	Total	C	N	O	S	0	0
			460	314	67	76	3		

- Molecule 17 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1	192	Total	C	N	O	S	0	0
			1477	944	262	263	8		
17	N	192	Total	C	N	O	S	0	0
			1477	944	262	263	8		

- Molecule 18 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	172	Total	C	N	O	S	0	0
			1377	910	225	239	3		
18	O	172	Total	C	N	O	S	0	0
			1377	910	225	239	3		

- Molecule 19 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	180	Total	C	N	O	S	0	0
			1388	898	232	249	9		
19	P	180	Total	C	N	O	S	0	0
			1388	898	232	249	9		

- Molecule 20 is a protein called ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	160	Total	C	N	O	S	0	0
			1226	787	210	219	10		
20	Q	160	Total	C	N	O	S	0	0
			1226	787	210	219	10		

- Molecule 21 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	189	Total	C	N	O	S	0	0
			1481	972	242	264	3		
21	R	189	Total	C	N	O	S	0	0
			1481	972	242	264	3		

- Molecule 22 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6	173	Total	C	N	O	S	0	0
			1327	856	227	236	8		
22	S	173	Total	C	N	O	S	0	0
			1327	856	227	236	8		

- Molecule 23 is a protein called Psb-gama_linker.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	G	96	Total	C	N	O	0	0
			755	503	120	132		

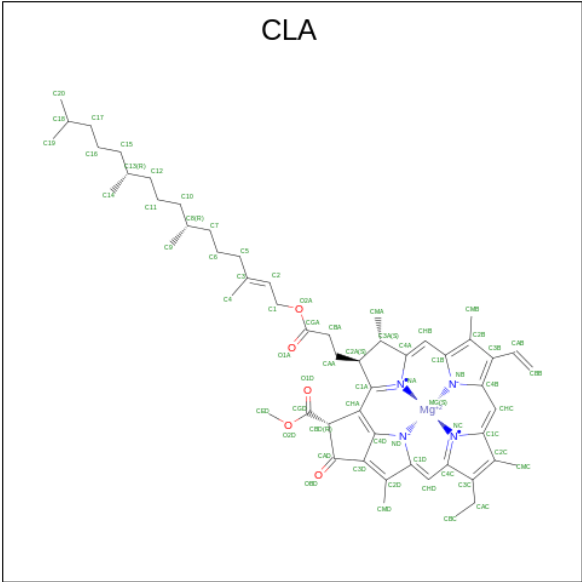
- Molecule 24 is a protein called Psb-gama_linker.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	95	Total	C	N	O	S	0	0
			747	499	118	129	1		

- Molecule 25 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	Fe	0
			1	1	
25	a	1	Total	Fe	0
			1	1	

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	1	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	1	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	1	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	1	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	N	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	N	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	N	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	N	1	Total 46	C 36	Mg 1	N 4	O 5	0
26	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	N	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	2	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	2	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	3	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 63	C 53	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	4	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	4	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
26	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	O	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	O	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	P	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	P	1	Total 63	C 53	Mg 1	N 4	O 5	0
26	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	P	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	P	1	Total 53	C 43	Mg 1	N 4	O 5	0

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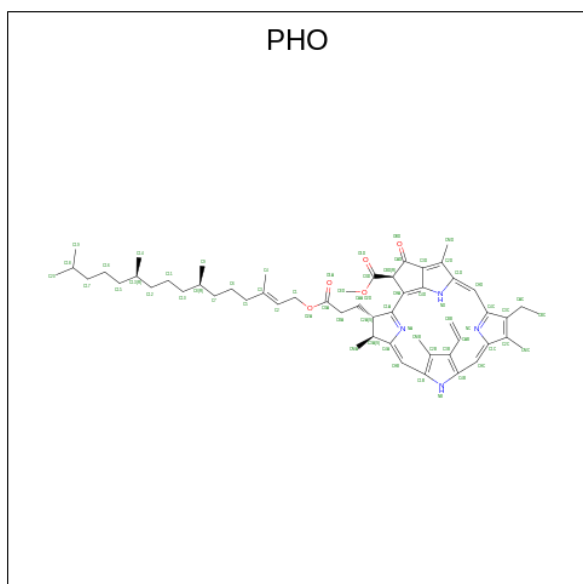
Mol	Chain	Residues	Atoms					AltConf
26	P	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	Q	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	Q	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	R	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 55	C 45	Mg 1	N 4	O 5	0

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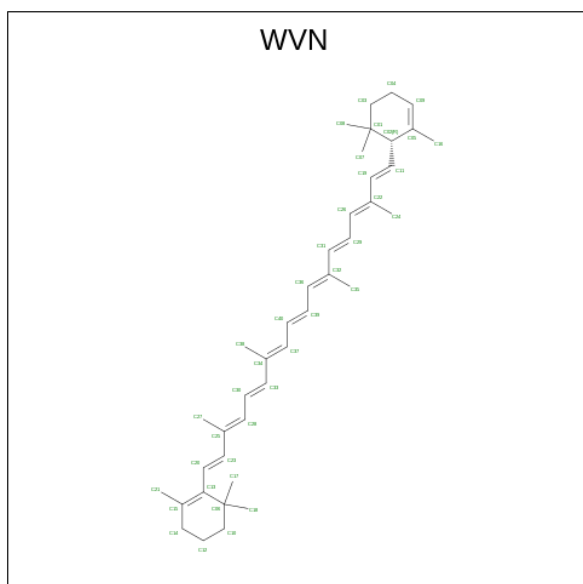
Mol	Chain	Residues	Atoms					AltConf
26	R	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (CCD ID: WVN) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



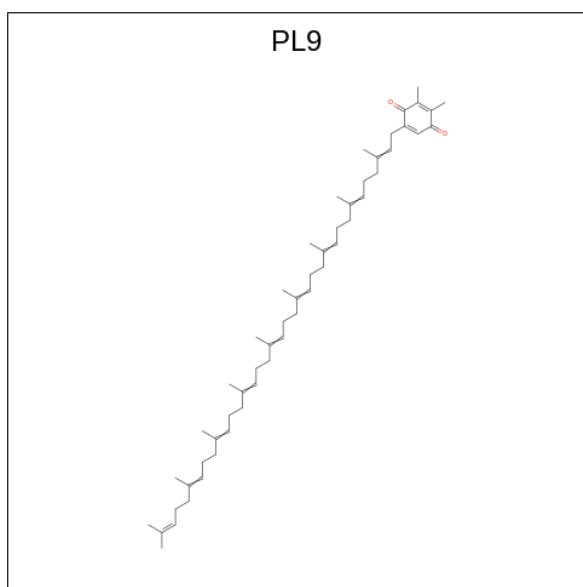
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	C	1	Total	C	0
			40	40	
28	C	1	Total	C	0
			40	40	
28	D	1	Total	C	0
			40	40	

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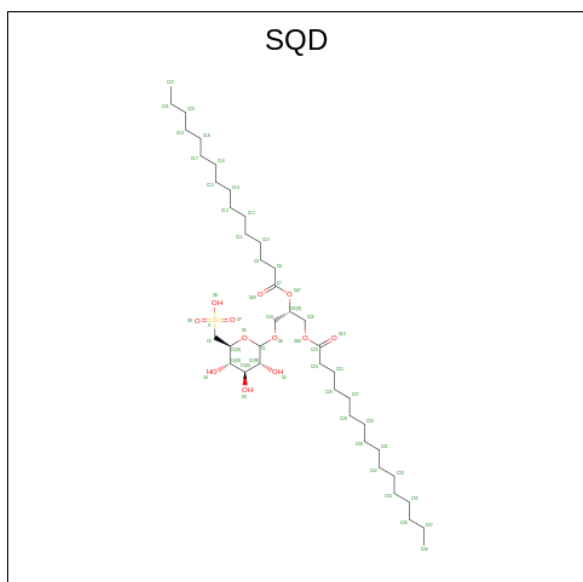
Mol	Chain	Residues	Atoms	AltConf
28	H	1	Total C 40 40	0
28	Y	1	Total C 40 40	0
28	Z	1	Total C 40 40	0
28	a	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	d	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	x	1	Total C 40 40	0
28	3	1	Total C 40 40	0
28	5	1	Total C 40 40	0
28	P	1	Total C 40 40	0
28	S	1	Total C 40 40	0

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			33	31	2	
29	d	1	Total	C	O	0
			55	53	2	

- Molecule 30 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
30	A	1	Total	C	O	S	0
			40	27	12	1	
30	D	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			40	27	12	1	
30	c	1	Total	C	O	S	0
			45	32	12	1	

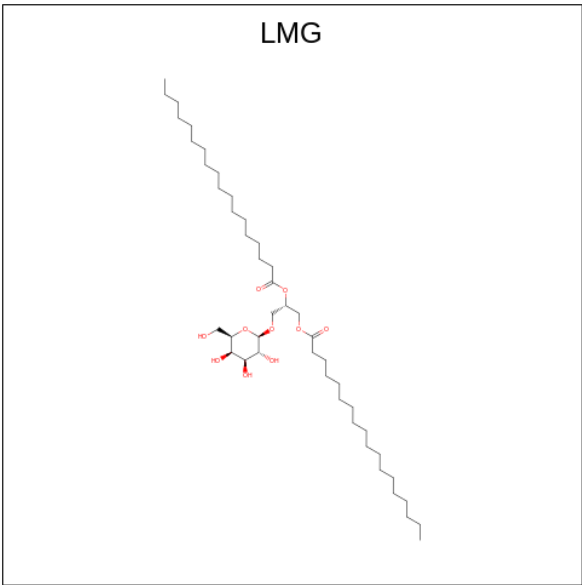
- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	Cl	0
			1	1	
31	a	1	Total	Cl	0
			1	1	
31	c	1	Total	Cl	0
			1	1	

- Molecule 32 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
32	A	2	Total	Mn	0
			2	2	
32	a	2	Total	Mn	0
			2	2	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



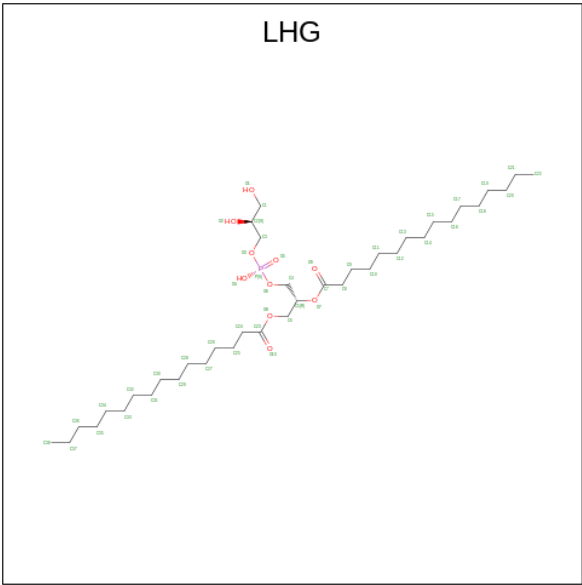
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			48	38	10	
33	B	1	Total	C	O	0
			51	41	10	
33	C	1	Total	C	O	0
			47	37	10	
33	C	1	Total	C	O	0
			31	21	10	
33	D	1	Total	C	O	0
			40	30	10	
33	D	1	Total	C	O	0
			37	27	10	
33	D	1	Total	C	O	0
			46	36	10	
33	M	1	Total	C	O	0
			40	30	10	
33	a	1	Total	C	O	0
			48	38	10	
33	b	1	Total	C	O	0
			51	41	10	
33	c	1	Total	C	O	0
			51	41	10	
33	c	1	Total	C	O	0
			31	21	10	
33	d	1	Total	C	O	0
			40	30	10	
33	d	1	Total	C	O	0
			37	27	10	

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Mol	Chain	Residues	Atoms			AltConf
33	d	1	Total	C	O	0
			46	36	10	
33	m	1	Total	C	O	0
			40	30	10	
33	2	1	Total	C	O	0
			40	30	10	
33	4	1	Total	C	O	0
			43	33	10	
33	5	1	Total	C	O	0
			40	30	10	
33	O	1	Total	C	O	0
			40	30	10	
33	Q	1	Total	C	O	0
			43	33	10	
33	R	1	Total	C	O	0
			40	30	10	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



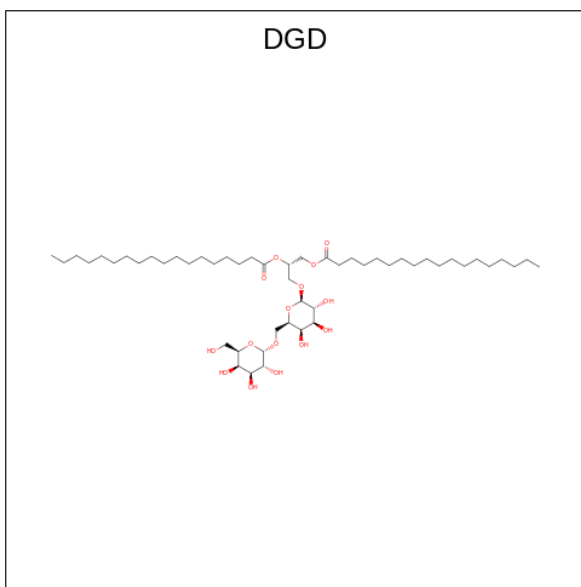
Mol	Chain	Residues	Atoms				AltConf
34	C	1	Total	C	O	P	0
			42	31	10	1	
34	C	1	Total	C	O	P	0
			40	29	10	1	
34	D	1	Total	C	O	P	0
			43	32	10	1	

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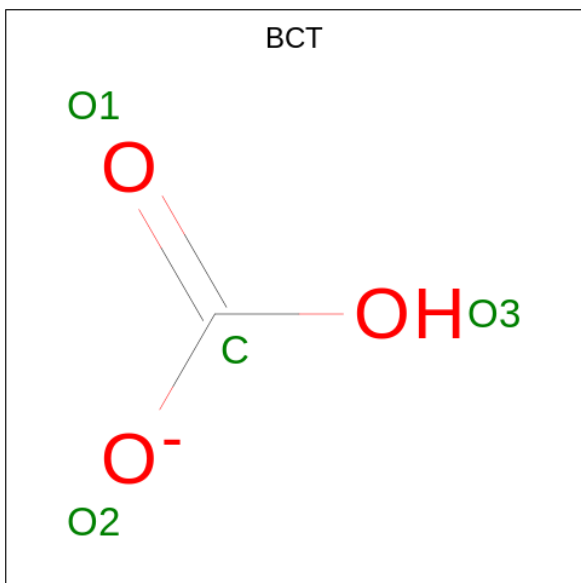
Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total	C	O	P	0
			49	38	10	1	
34	L	1	Total	C	O	P	0
			49	38	10	1	
34	Z	1	Total	C	O	P	0
			25	14	10	1	
34	a	1	Total	C	O	P	0
			42	31	10	1	
34	b	1	Total	C	O	P	0
			43	32	10	1	
34	c	1	Total	C	O	P	0
			40	29	10	1	
34	d	1	Total	C	O	P	0
			49	38	10	1	
34	l	1	Total	C	O	P	0
			49	38	10	1	
34	z	1	Total	C	O	P	0
			25	14	10	1	
34	1	1	Total	C	O	P	0
			46	35	10	1	
34	N	1	Total	C	O	P	0
			46	35	10	1	
34	2	1	Total	C	O	P	0
			49	38	10	1	
34	5	1	Total	C	O	P	0
			40	29	10	1	
34	G	1	Total	C	O	P	0
			49	38	10	1	
34	R	1	Total	C	O	P	0
			40	29	10	1	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



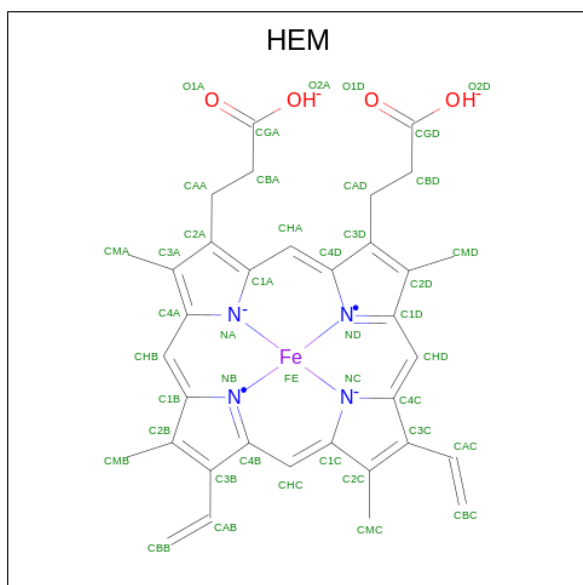
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			54	39	15	
35	H	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			54	39	15	
35	h	1	Total	C	O	0
			62	47	15	

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



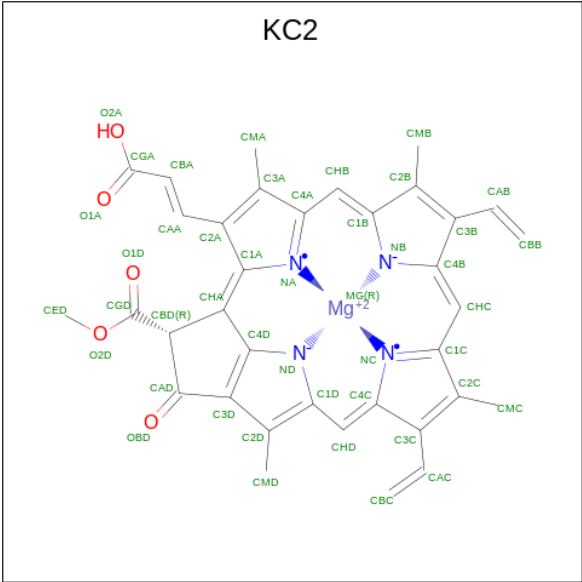
Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total 4	C 1	O 3	0
36	d	1	Total 4	C 1	O 3	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
37	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
37	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 38 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



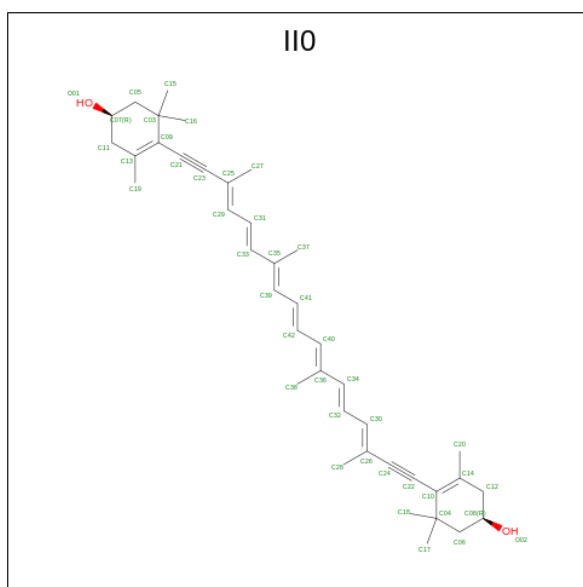
Mol	Chain	Residues	Atoms					AltConf
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
38	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total	C	O	0
			42	40	2	
39	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total 42	C 40	O 2	0
39	1	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	3	1	Total 42	C 40	O 2	0
39	3	1	Total 42	C 40	O 2	0
39	3	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	5	1	Total 42	C 40	O 2	0

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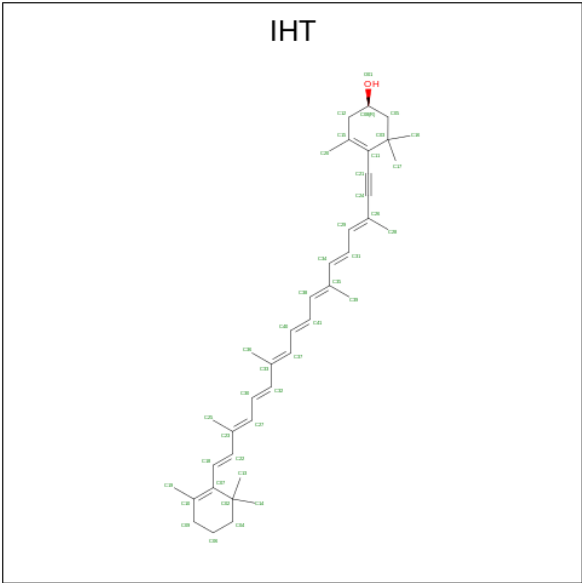
Mol	Chain	Residues	Atoms			AltConf
39	5	1	Total 42	C 40	O 2	0
39	5	1	Total 42	C 40	O 2	0
39	6	1	Total 42	C 40	O 2	0
39	6	1	Total 42	C 40	O 2	0
39	6	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	P	1	Total 42	C 40	O 2	0
39	P	1	Total 42	C 40	O 2	0
39	P	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
39	S	1	Total	C	O	0
			42	40	2	
39	S	1	Total	C	O	0
			42	40	2	

- Molecule 40 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	O	0
			41	40	1	
40	N	1	Total	C	O	0
			41	40	1	
40	2	1	Total	C	O	0
			41	40	1	
40	4	1	Total	C	O	0
			41	40	1	
40	5	1	Total	C	O	0
			41	40	1	
40	O	1	Total	C	O	0
			41	40	1	
40	Q	1	Total	C	O	0
			41	40	1	
40	R	1	Total	C	O	0
			41	40	1	

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	A	52	Total 52	O 52	0
41	B	117	Total 117	O 117	0
41	C	52	Total 52	O 52	0
41	D	70	Total 70	O 70	0
41	E	8	Total 8	O 8	0
41	F	2	Total 2	O 2	0
41	H	14	Total 14	O 14	0
41	I	1	Total 1	O 1	0
41	K	4	Total 4	O 4	0
41	L	7	Total 7	O 7	0
41	M	1	Total 1	O 1	0
41	T	4	Total 4	O 4	0
41	W	2	Total 2	O 2	0
41	X	3	Total 3	O 3	0
41	a	48	Total 48	O 48	0
41	b	125	Total 125	O 125	0
41	c	52	Total 52	O 52	0
41	d	71	Total 71	O 71	0
41	e	9	Total 9	O 9	0
41	h	14	Total 14	O 14	0
41	i	1	Total 1	O 1	0

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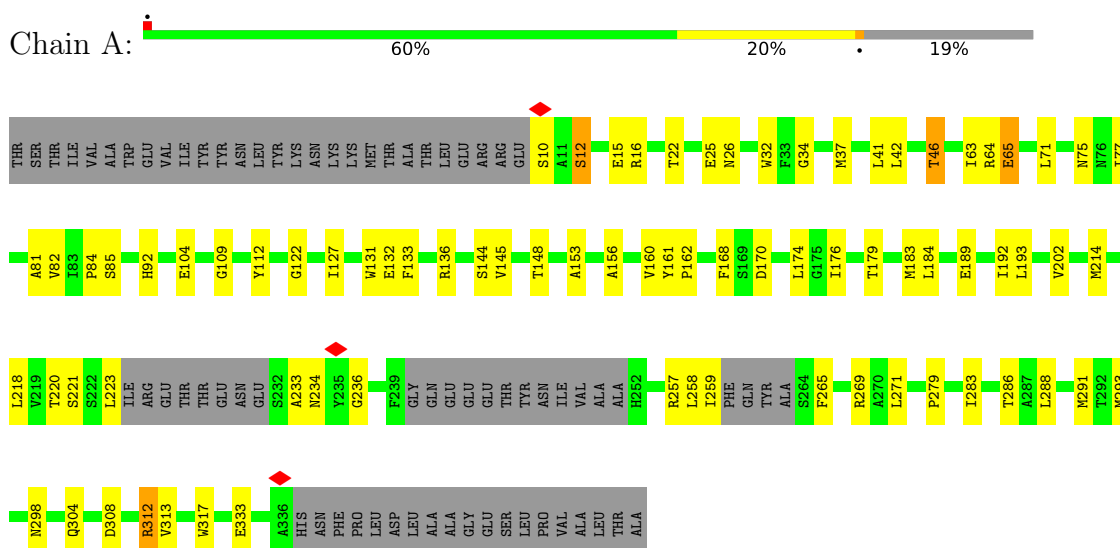
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
41	k	3	Total 3	O 3	0
41	l	5	Total 5	O 5	0
41	m	4	Total 4	O 4	0
41	t	5	Total 5	O 5	0
41	w	1	Total 1	O 1	0
41	x	1	Total 1	O 1	0

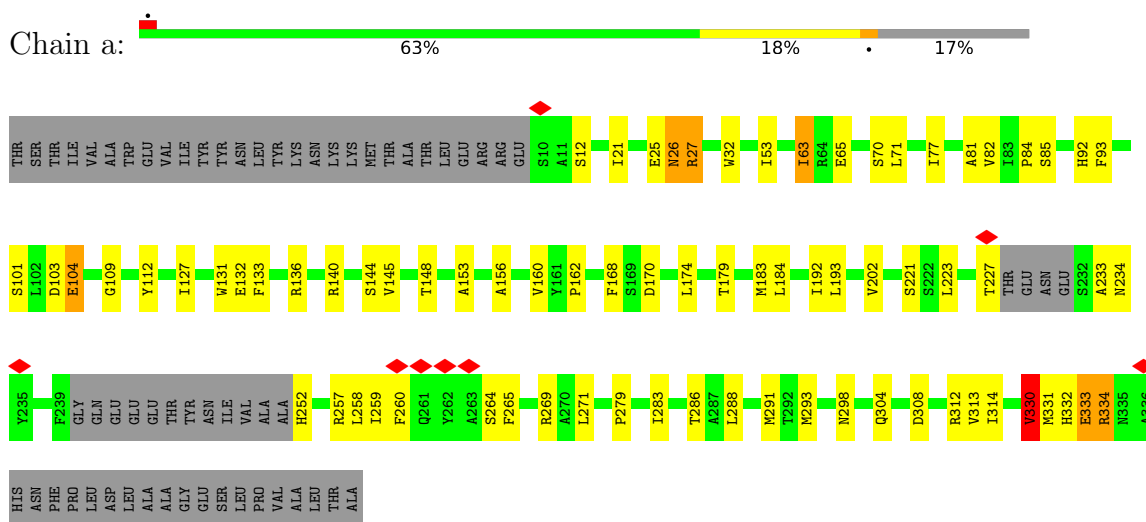
3 Residue-property plots

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

- Molecule 1: Photosystem II protein D1

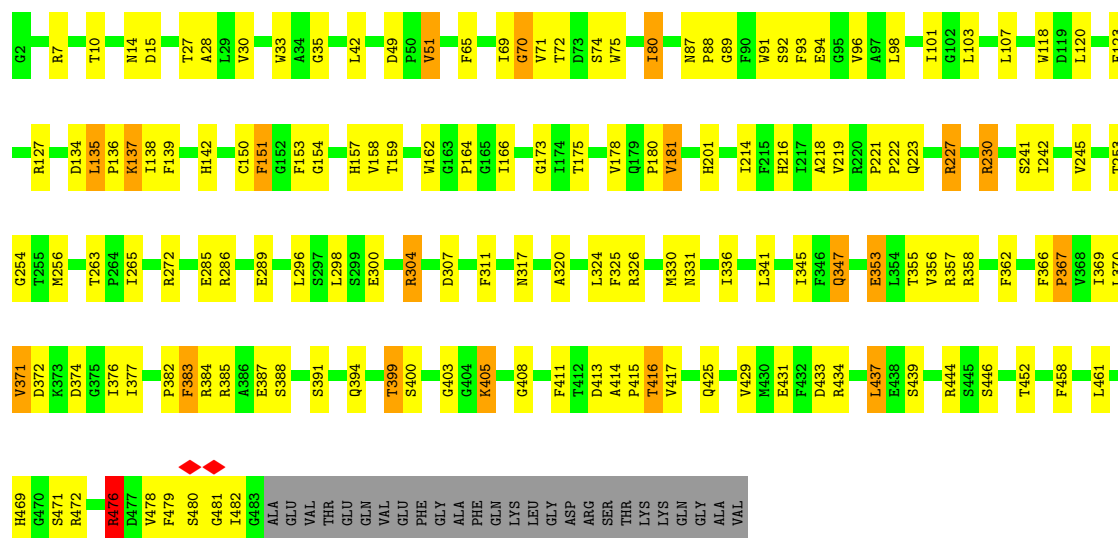


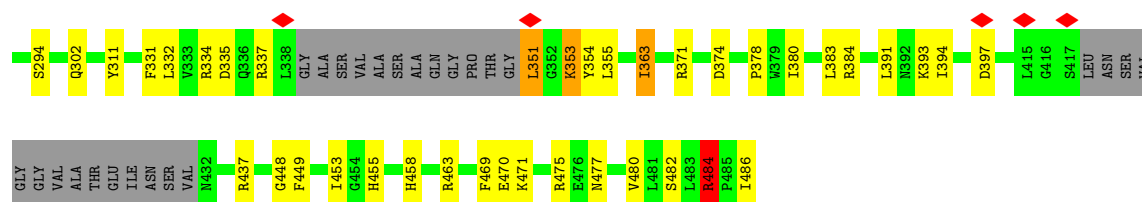
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

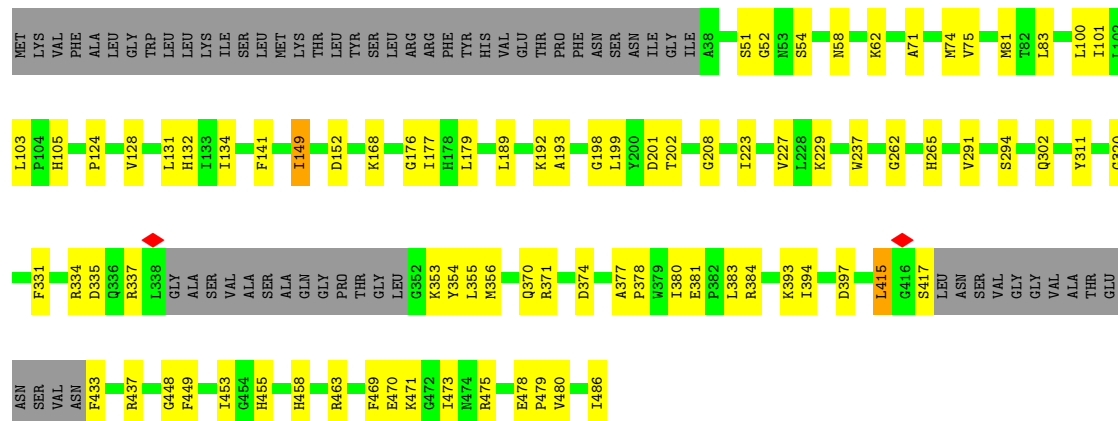
Chain B:  65% 26% 5%





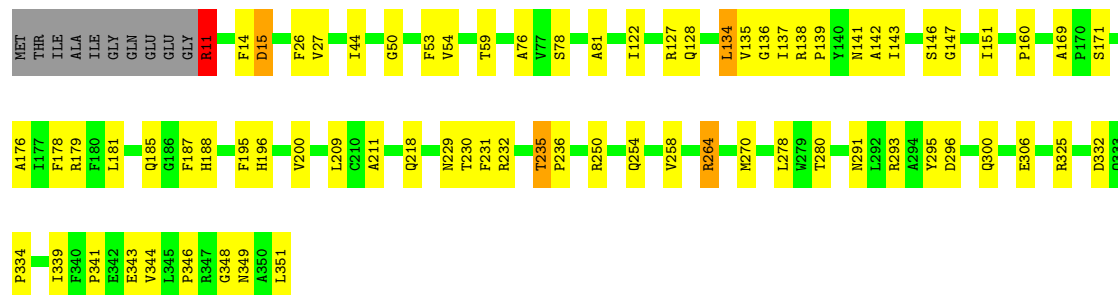
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 69% 17% 13%



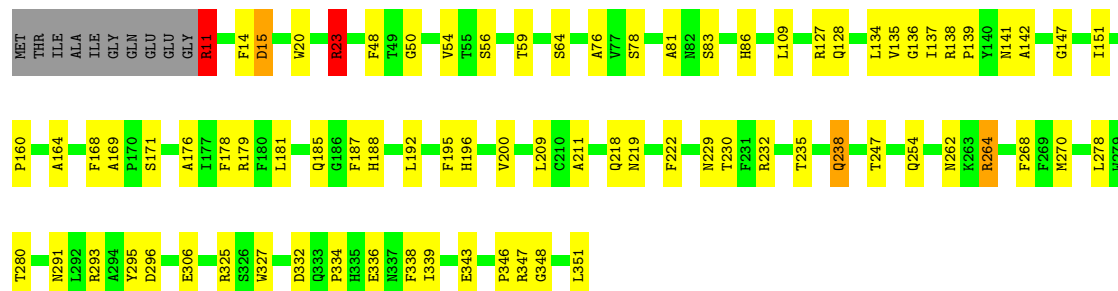
• Molecule 4: Photosystem II D2 protein

Chain D: 76% 20% ..

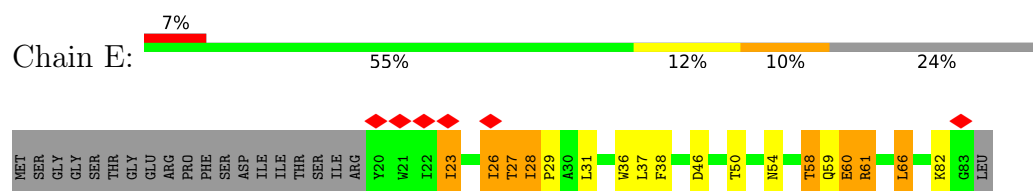


• Molecule 4: Photosystem II D2 protein

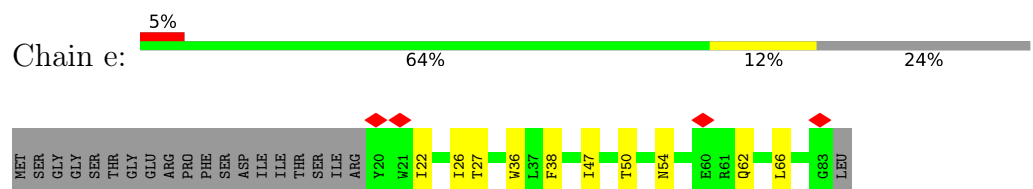
Chain d: 74% 21% ..



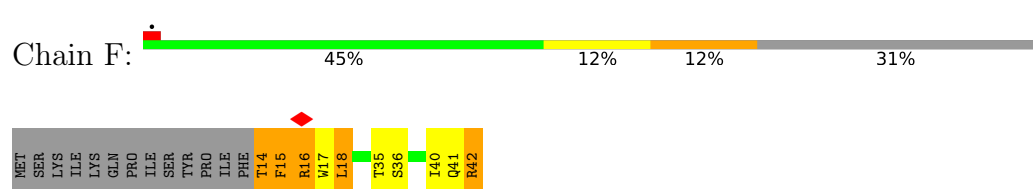
- Molecule 5: Cytochrome b559 subunit alpha



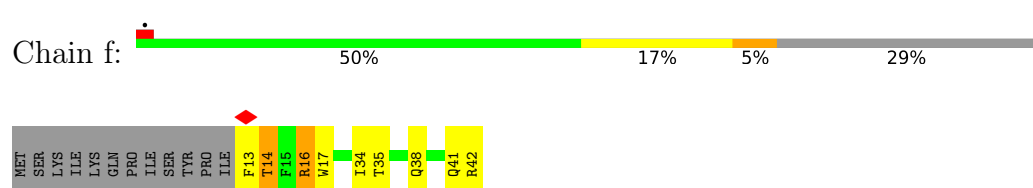
- Molecule 5: Cytochrome b559 subunit alpha



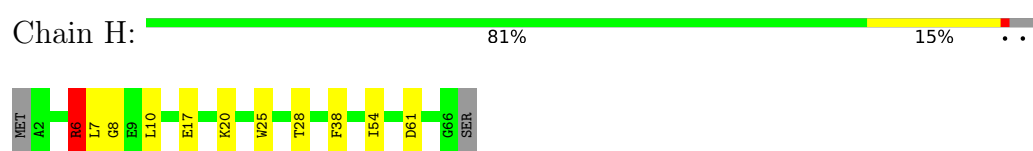
- Molecule 6: Cytochrome b559 subunit beta



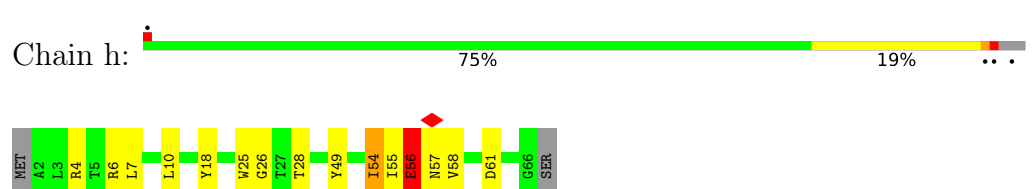
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I





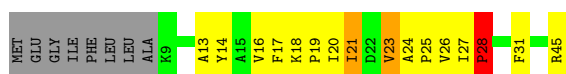
- Molecule 8: Photosystem II reaction center protein I

Chain i: 76% 13% 8%



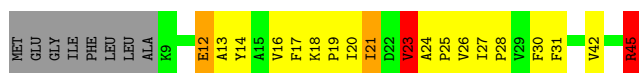
- Molecule 9: Photosystem II reaction center protein K

Chain K: 47% 29% 18%



- Molecule 9: Photosystem II reaction center protein K

Chain k: 40% 33% 18%



- Molecule 10: Photosystem II reaction center protein L

Chain L: 71% 24% 5%



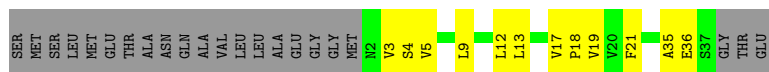
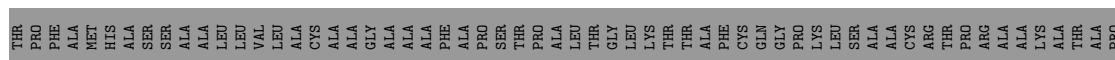
- Molecule 10: Photosystem II reaction center protein L

Chain l: 61% 32% 5%



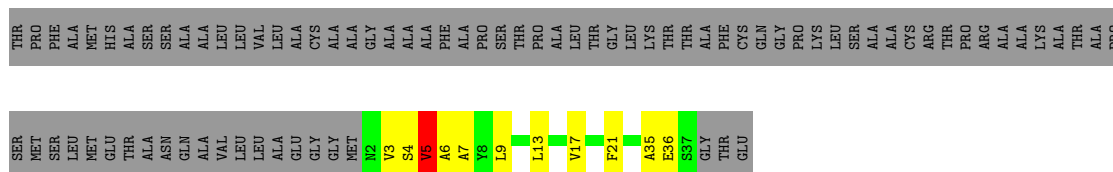
- Molecule 11: Photosystem II protein M

Chain M: 20% 10% 69%



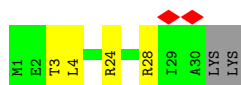
- Molecule 11: Photosystem II protein M

Chain m:  21% 8% 69%



• Molecule 12: Photosystem II reaction center protein T

Chain T:  6% 81% 12% 6%



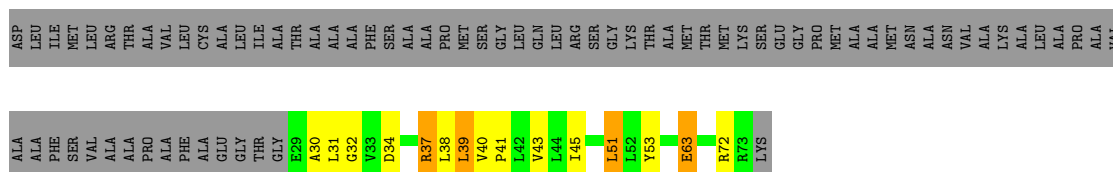
• Molecule 12: Photosystem II reaction center protein T

Chain t:  6% 75% 19% 6%



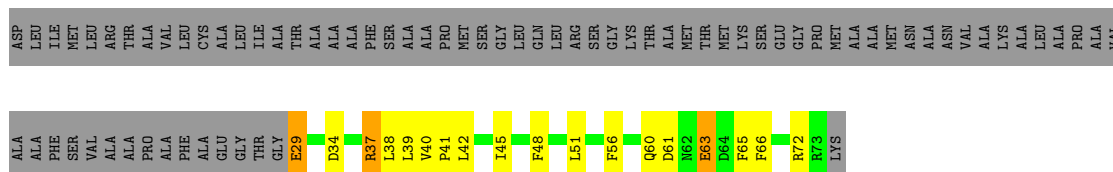
• Molecule 13: Photosystem II protein W

Chain W:  25% 9% 63%



• Molecule 13: Photosystem II protein W

Chain w:  22% 12% 63%



• Molecule 14: Photosystem II reaction center X protein

Chain X:  69% 10% 8% 13%



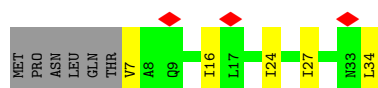
• Molecule 14: Photosystem II reaction center X protein

Chain x:  64% 15% 8% 13%



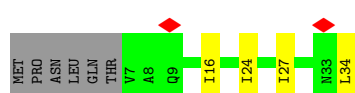
- Molecule 15: Photosystem II reaction center protein Psb30

Chain Y:  9% 68% 15% 18%



- Molecule 15: Photosystem II reaction center protein Psb30

Chain y:  6% 71% 12% 18%



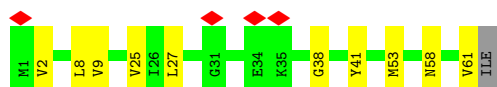
- Molecule 16: Photosystem II reaction center protein Z

Chain Z:  56% 31% 11% .



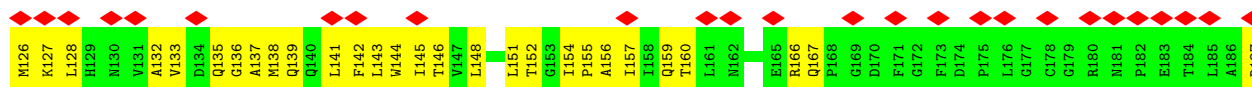
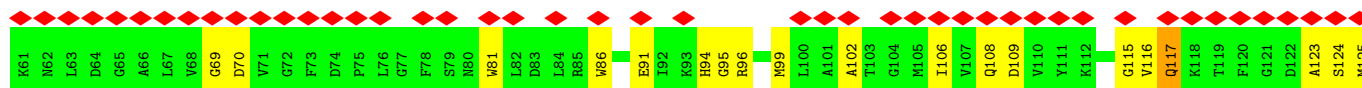
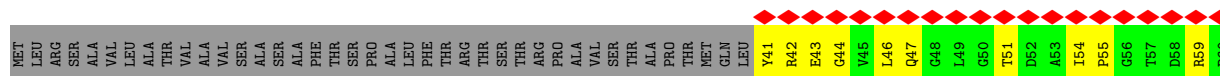
- Molecule 16: Photosystem II reaction center protein Z

Chain z:  6% 82% 16% .



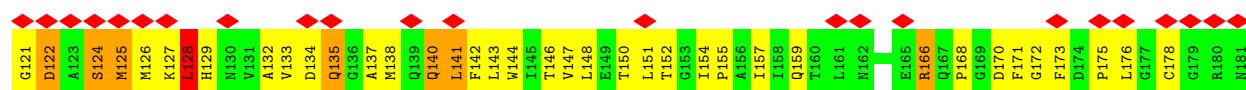
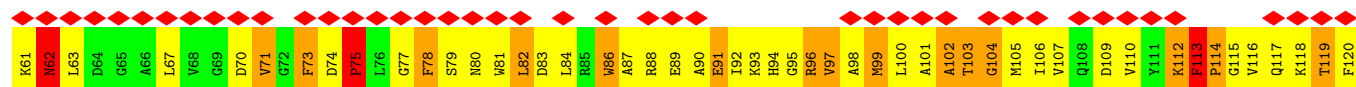
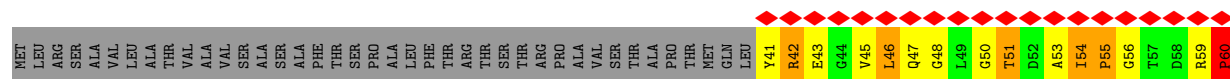
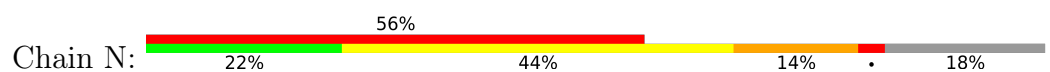
- Molecule 17: ACPH-1

Chain 1:  55% 45% 37% 18%

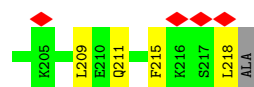
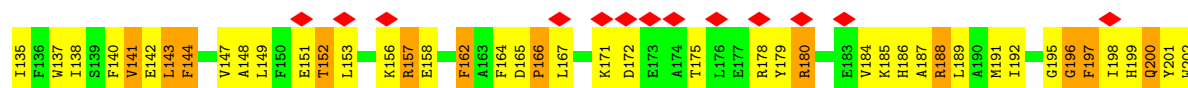
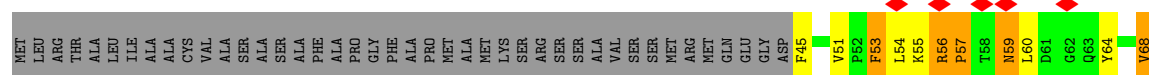




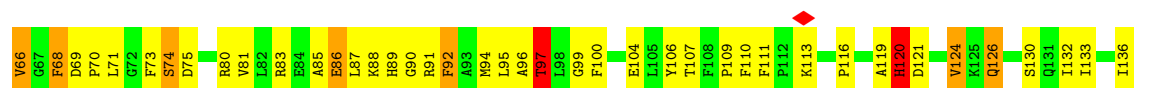
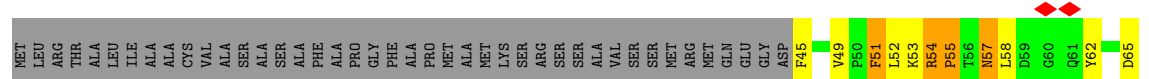
• Molecule 17: ACPII-1

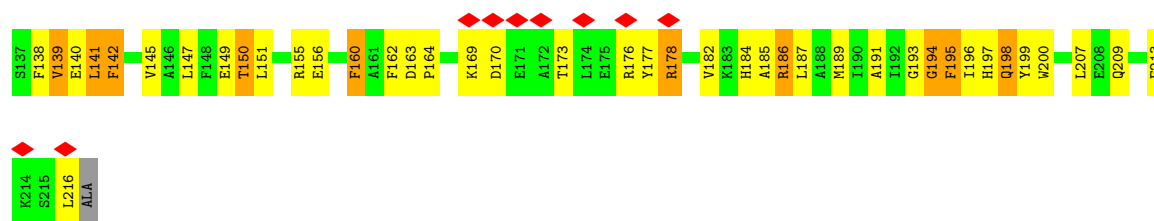


• Molecule 18: ACPII-2

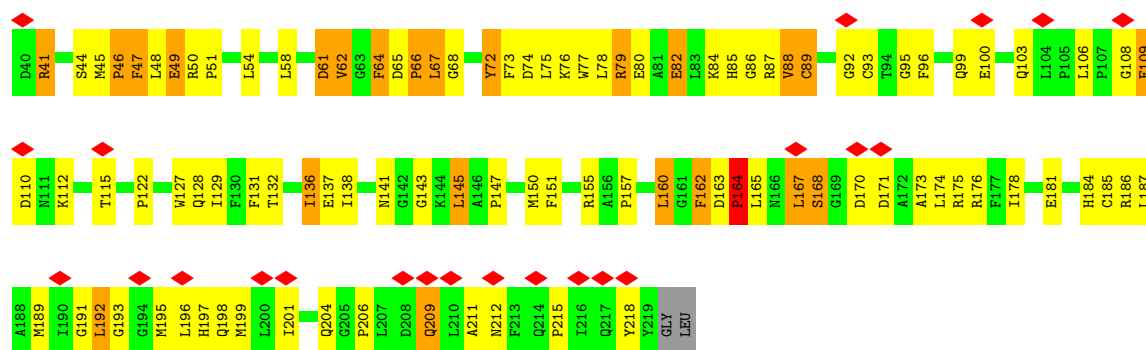
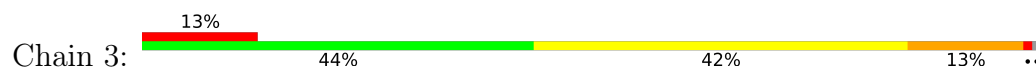


• Molecule 18: ACPII-2

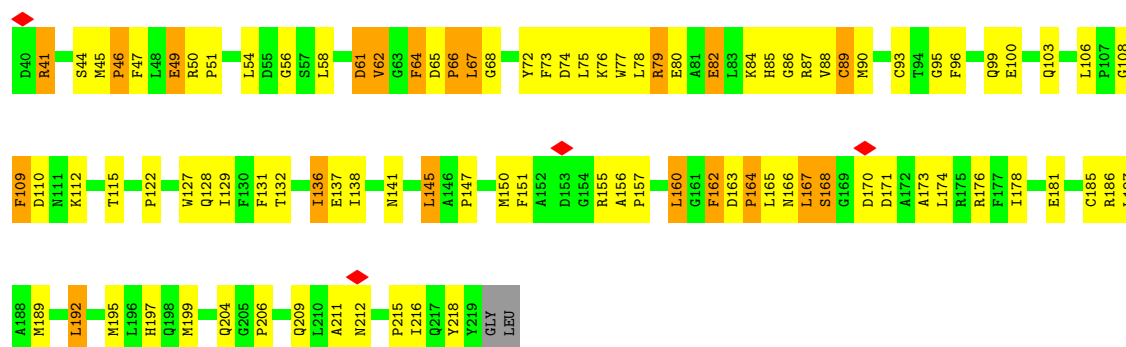




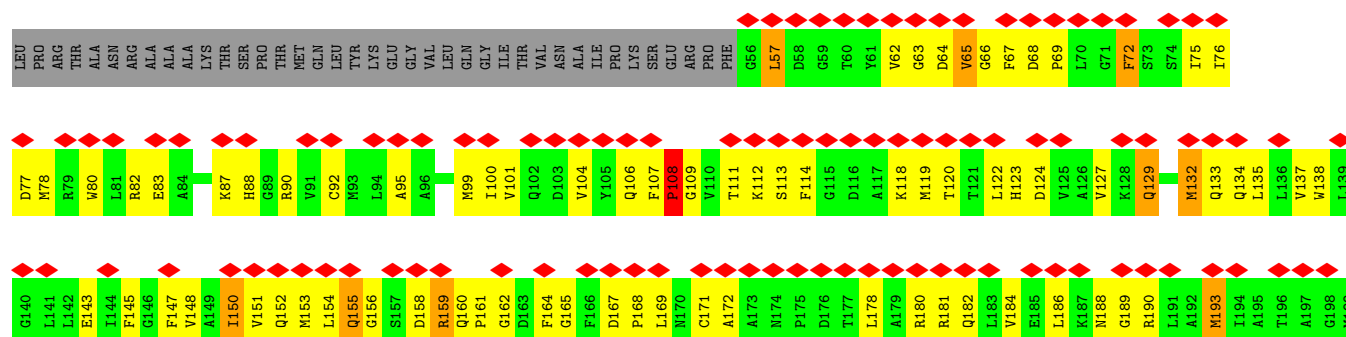
• Molecule 19: ACPII-3



• Molecule 19: ACPII-3

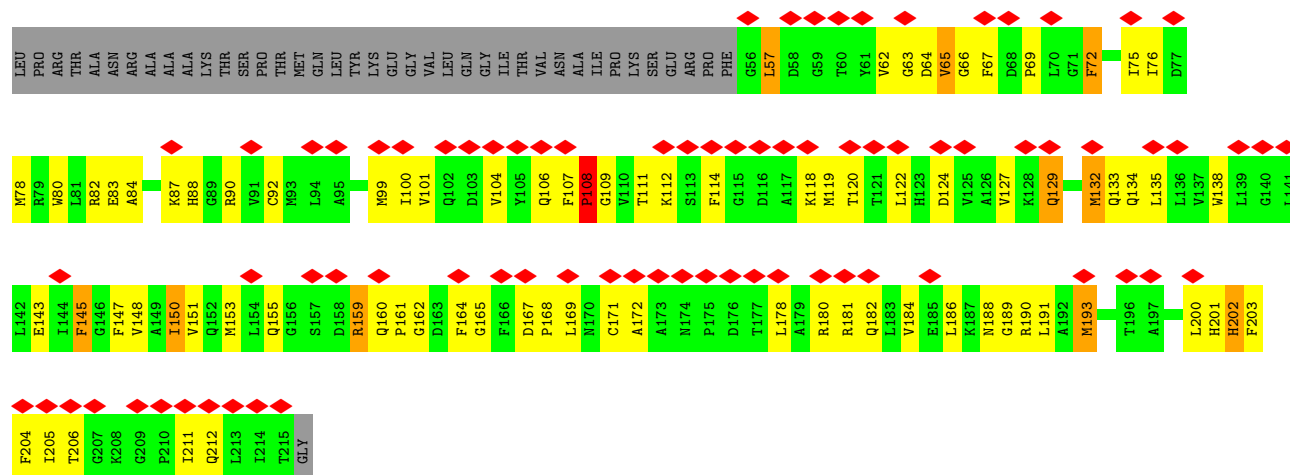
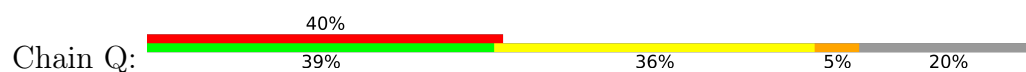


• Molecule 20: ACPII-4

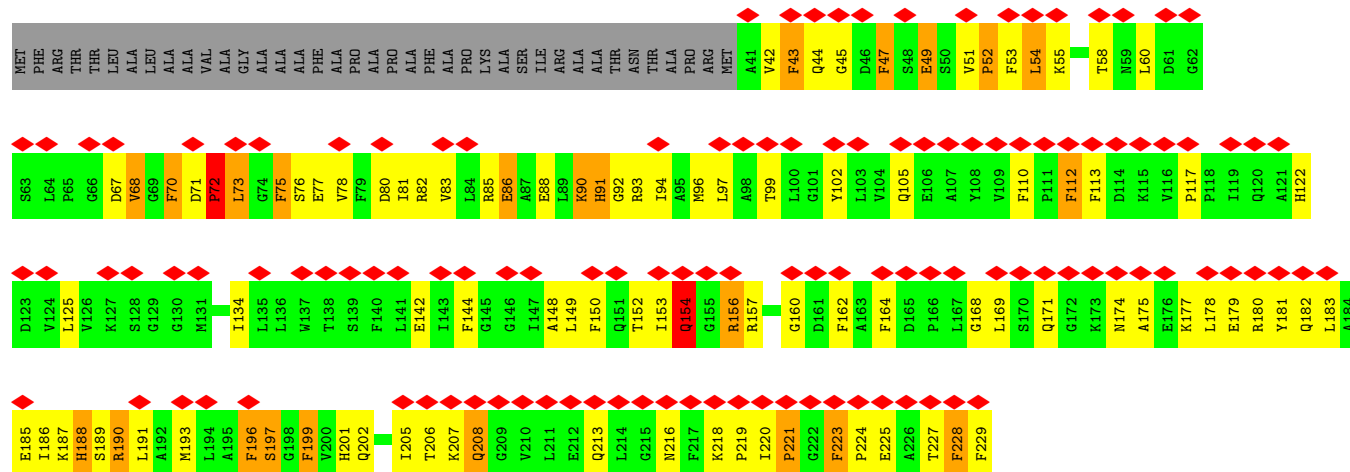




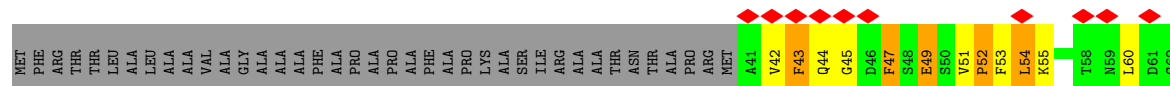
• Molecule 20: ACPII-4

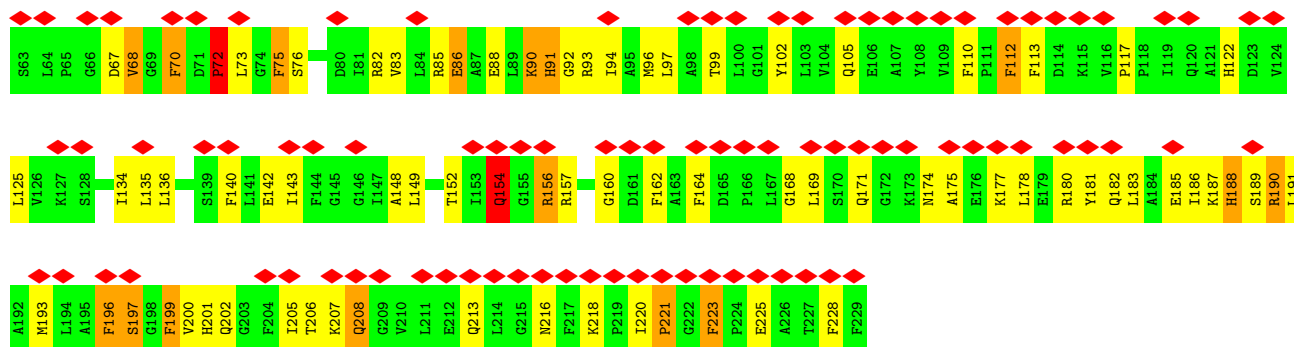


• Molecule 21: ACPII-5

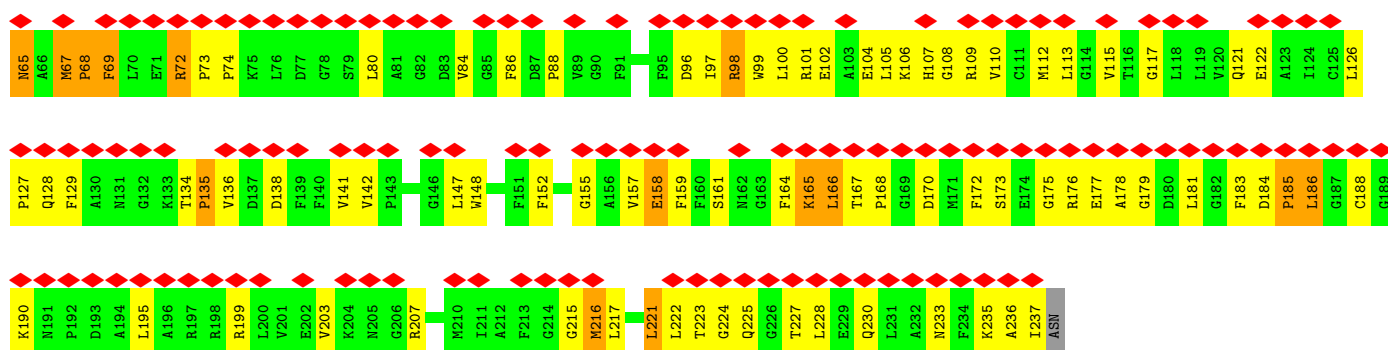
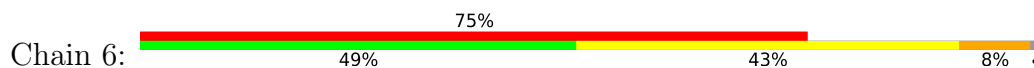


• Molecule 21: ACPII-5

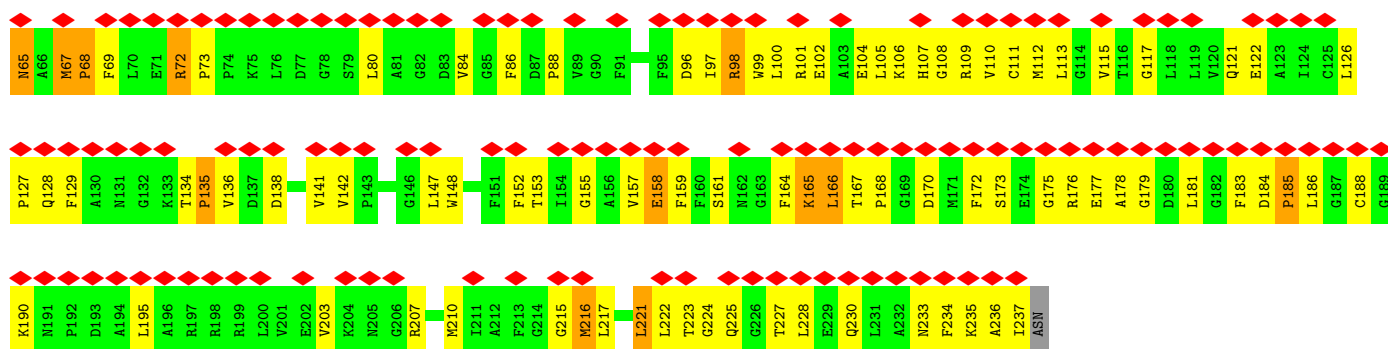




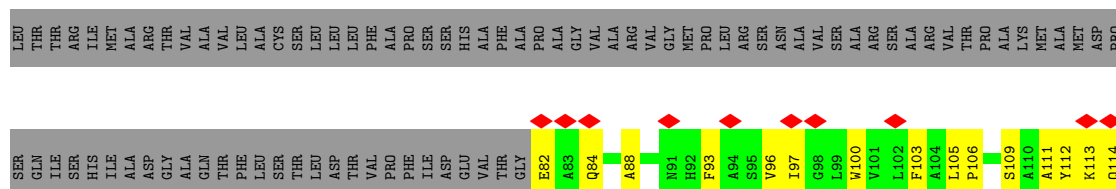
• Molecule 22: ACPH-6

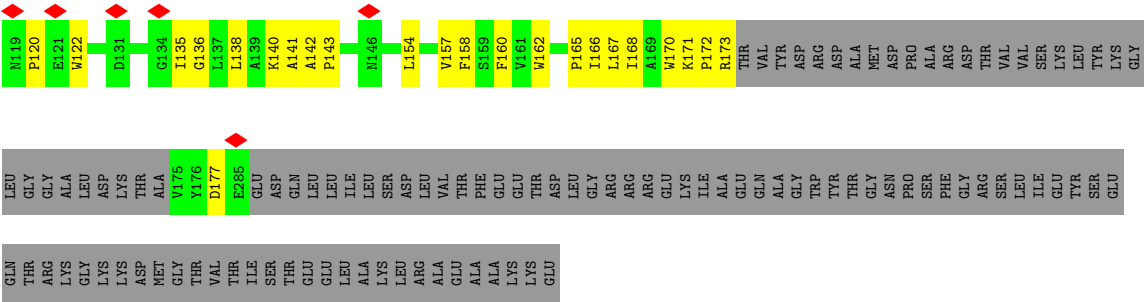


• Molecule 22: ACPH-6

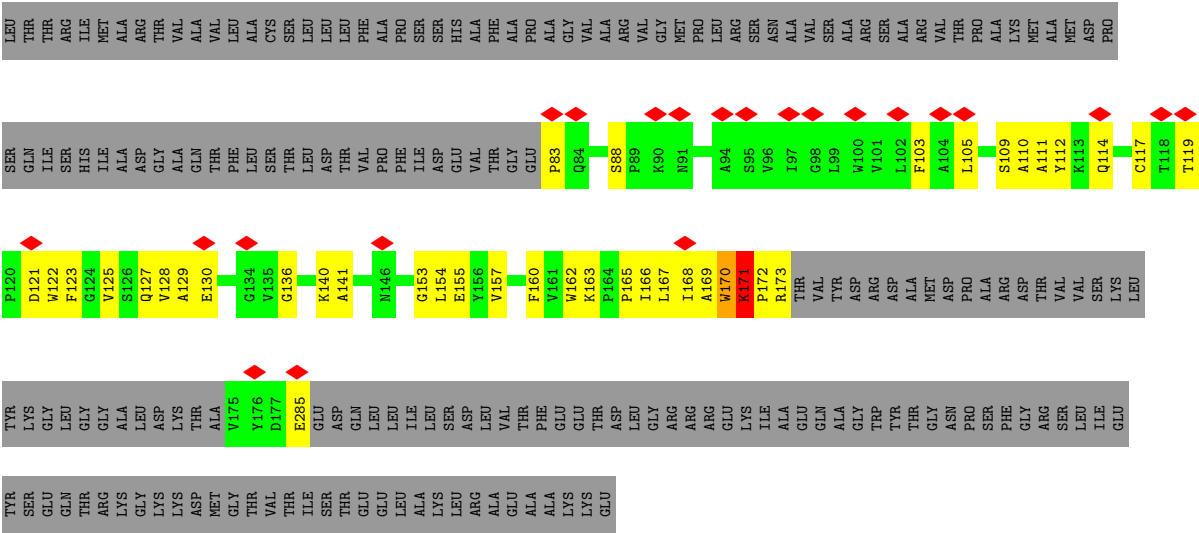


• Molecule 23: Psh-gama_linker





● Molecule 24: Psb-gama_linker



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28657	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)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, IHT, DGD, LHG, WVN, KC2, FE2, PL9, BCT, PHO, II0, HEM, SQD, MN, CL, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	1/2452 (0.0%)	0.54	0/3339
1	a	0.37	0/2516	0.57	3/3428 (0.1%)
2	B	0.62	0/3927	0.94	11/5349 (0.2%)
2	b	0.44	0/3912	0.64	3/5330 (0.1%)
3	C	0.39	0/3442	0.54	1/4692 (0.0%)
3	c	0.29	0/3409	0.51	2/4647 (0.0%)
4	D	0.32	0/2806	0.48	0/3823
4	d	0.35	0/2798	0.53	0/3812
5	E	0.74	0/541	0.92	1/738 (0.1%)
5	e	0.35	0/541	0.49	0/738
6	F	0.75	0/242	1.04	0/328
6	f	0.65	0/254	0.87	0/344
7	H	0.38	0/519	0.61	0/707
7	h	0.48	0/519	0.73	1/707 (0.1%)
8	I	0.25	0/290	0.46	0/392
8	i	0.28	0/290	0.47	0/392
9	K	0.63	0/307	0.98	1/421 (0.2%)
9	k	0.75	0/307	1.07	1/421 (0.2%)
10	L	0.37	0/311	0.60	0/424
10	l	0.58	0/311	0.96	2/424 (0.5%)
11	M	0.65	0/275	0.93	0/375
11	m	0.55	0/275	0.93	2/375 (0.5%)
12	T	0.41	0/251	0.54	0/341
12	t	0.21	0/251	0.43	0/341
13	W	0.71	0/368	1.22	1/501 (0.2%)
13	w	0.77	0/368	1.33	2/501 (0.4%)
14	X	0.72	0/253	1.05	0/345
14	x	0.85	0/253	1.32	2/345 (0.6%)
15	Y	0.32	0/210	0.54	0/285
15	y	0.10	0/210	0.25	0/285
16	Z	0.77	0/460	1.12	2/628 (0.3%)
16	z	0.19	0/470	0.33	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1	0.26	0/1510	0.57	0/2046
17	N	1.11	3/1510 (0.2%)	2.08	65/2046 (3.2%)
18	2	1.10	2/1416 (0.1%)	1.89	40/1915 (2.1%)
18	O	1.11	2/1416 (0.1%)	1.89	40/1915 (2.1%)
19	3	1.15	2/1424 (0.1%)	1.91	42/1925 (2.2%)
19	P	1.15	2/1424 (0.1%)	1.91	42/1925 (2.2%)
20	4	0.99	0/1251	1.95	30/1690 (1.8%)
20	Q	0.99	0/1251	1.95	29/1690 (1.7%)
21	5	1.08	1/1522 (0.1%)	1.99	54/2059 (2.6%)
21	R	1.08	1/1522 (0.1%)	1.99	53/2059 (2.6%)
22	6	0.90	0/1359	1.68	25/1836 (1.4%)
22	S	0.90	0/1359	1.68	25/1836 (1.4%)
23	G	0.92	0/784	1.14	1/1072 (0.1%)
24	g	0.31	0/777	0.52	2/1064 (0.2%)
All	All	0.70	14/51863 (0.0%)	1.19	483/70497 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	a	0	3
2	B	0	8
2	b	0	6
3	C	0	2
4	D	0	3
4	d	0	3
5	E	0	1
6	F	0	2
7	H	0	1
9	k	0	1
12	T	0	1
13	W	0	1
13	w	0	1
17	N	0	4
18	2	0	2
18	O	0	2
20	4	0	2
20	Q	0	2
23	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	g	0	1
All	All	0	50

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	44	SER	CA-CB	-6.26	1.43	1.53
19	3	44	SER	CA-CB	-6.26	1.43	1.53
1	A	10	SER	C-N	6.08	1.41	1.33
19	3	168	SER	CA-CB	-5.75	1.45	1.53
19	P	168	SER	CA-CB	-5.74	1.45	1.53

The worst 5 of 483 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	89	CYS	CB-CA-C	16.52	137.68	110.09
19	P	89	CYS	CB-CA-C	16.50	137.65	110.09
17	N	42	ARG	N-CA-C	-13.48	96.58	111.14
17	N	55	PRO	N-CA-C	-12.72	90.53	111.26
17	N	226	ASN	N-CA-C	-11.86	100.40	112.97

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ARG	Sidechain
1	A	312[B]	ARG	Mainchain
1	A	64	ARG	Sidechain
2	B	151	PHE	Mainchain
2	B	227	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2377	0	2304	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	2438	0	2361	73	0
2	B	3797	0	3683	136	0
2	b	3782	0	3668	115	0
3	C	3331	0	3256	89	0
3	c	3299	0	3224	81	0
4	D	2713	0	2607	83	0
4	d	2705	0	2602	98	0
5	E	525	0	510	16	0
5	e	525	0	510	7	0
6	F	235	0	241	17	0
6	f	246	0	250	5	0
7	H	508	0	529	15	0
7	h	508	0	529	23	0
8	I	284	0	295	8	0
8	i	284	0	295	6	0
9	K	296	0	312	24	0
9	k	296	0	312	12	0
10	L	301	0	301	9	0
10	l	301	0	301	10	0
11	M	271	0	287	12	0
11	m	271	0	287	7	0
12	T	244	0	256	3	0
12	t	244	0	256	5	0
13	W	361	0	346	20	0
13	w	361	0	346	11	0
14	X	249	0	269	16	0
14	x	249	0	269	13	0
15	Y	209	0	243	4	0
15	y	209	0	243	3	0
16	Z	451	0	483	15	0
16	z	460	0	499	10	0
17	1	1477	0	1487	145	0
17	N	1477	0	1489	305	0
18	2	1377	0	1365	230	0
18	O	1377	0	1365	121	0
19	3	1388	0	1370	156	0
19	P	1388	0	1370	89	0
20	4	1226	0	1234	225	0
20	Q	1226	0	1234	116	0
21	5	1481	0	1466	136	0
21	R	1481	0	1466	83	0
22	6	1327	0	1311	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	S	1327	0	1311	80	0
23	G	755	0	724	43	0
24	g	747	0	720	157	0
25	A	1	0	0	0	0
25	a	1	0	0	0	0
26	1	510	0	428	66	0
26	2	678	0	647	174	0
26	3	473	0	471	91	0
26	4	534	0	488	147	0
26	5	620	0	589	101	0
26	6	525	0	510	52	0
26	A	174	0	170	13	0
26	B	1014	0	1092	50	0
26	C	827	0	894	32	0
26	D	190	0	203	11	0
26	G	110	0	105	8	0
26	N	509	0	426	135	0
26	O	633	0	614	105	0
26	P	570	0	547	56	0
26	Q	482	0	445	61	0
26	R	620	0	589	69	0
26	S	525	0	510	36	0
26	a	174	0	170	17	0
26	b	1014	0	1092	54	0
26	c	828	0	896	29	0
26	d	191	0	205	13	0
26	g	110	0	104	25	0
27	A	64	0	74	2	0
27	D	64	0	74	5	0
27	a	64	0	74	2	0
27	d	64	0	74	5	0
28	3	40	0	0	21	0
28	5	40	0	0	0	0
28	A	40	0	0	0	0
28	B	120	0	0	6	0
28	C	80	0	0	2	0
28	D	40	0	0	0	0
28	H	40	0	0	1	0
28	P	40	0	0	3	0
28	S	40	0	0	0	0
28	Y	40	0	0	0	0
28	Z	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	40	0	0	0	0
28	b	120	0	0	1	0
28	c	120	0	0	0	0
28	d	40	0	0	0	0
28	k	40	0	0	0	0
28	x	40	0	0	0	0
29	A	33	0	42	6	0
29	D	55	0	80	3	0
29	a	33	0	42	0	0
29	d	55	0	80	3	0
30	A	40	0	44	1	0
30	D	54	0	78	2	0
30	a	40	0	44	0	0
30	c	45	0	57	1	0
31	A	1	0	0	0	0
31	a	1	0	0	0	0
31	c	1	0	0	0	0
32	A	2	0	0	0	0
32	a	2	0	0	0	0
33	2	40	0	50	5	0
33	4	43	0	56	5	0
33	5	40	0	50	20	0
33	A	48	0	66	1	0
33	B	51	0	72	2	0
33	C	78	0	96	3	0
33	D	123	0	156	5	0
33	M	40	0	50	1	0
33	O	40	0	50	5	0
33	Q	43	0	56	2	0
33	R	40	0	50	9	0
33	a	48	0	66	3	0
33	b	51	0	72	1	0
33	c	82	0	104	8	0
33	d	123	0	156	6	0
33	m	40	0	50	2	0
34	1	46	0	65	48	0
34	2	49	0	74	23	0
34	5	40	0	53	8	0
34	C	82	0	107	3	0
34	D	92	0	133	12	0
34	G	49	0	74	11	0
34	L	49	0	74	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	N	46	0	65	26	0
34	R	40	0	53	12	0
34	Z	25	0	20	0	0
34	a	42	0	57	0	0
34	b	43	0	59	2	0
34	c	40	0	50	1	0
34	d	49	0	74	5	0
34	l	49	0	74	5	0
34	z	25	0	20	0	0
35	C	54	0	66	1	0
35	H	62	0	82	4	0
35	c	54	0	66	2	0
35	h	62	0	82	6	0
36	D	4	0	0	0	0
36	d	4	0	0	0	0
37	F	43	0	30	2	0
37	f	43	0	30	1	0
38	1	180	0	0	5	0
38	2	45	0	0	7	0
38	3	45	0	0	1	0
38	4	135	0	0	27	0
38	5	45	0	0	3	0
38	6	45	0	0	0	0
38	N	180	0	0	39	0
38	O	45	0	0	7	0
38	P	45	0	0	1	0
38	Q	135	0	0	28	0
38	R	45	0	0	3	0
38	S	45	0	0	0	0
39	1	168	0	0	1	0
39	2	210	0	0	33	0
39	3	126	0	0	60	0
39	4	210	0	0	48	0
39	5	126	0	0	7	0
39	6	126	0	0	1	0
39	N	210	0	0	39	0
39	O	168	0	0	28	0
39	P	126	0	0	13	0
39	Q	210	0	0	26	0
39	R	168	0	0	7	0
39	S	84	0	0	11	0
40	1	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2	41	0	0	21	0
40	4	41	0	0	5	0
40	5	41	0	0	1	0
40	N	41	0	0	16	0
40	O	41	0	0	9	0
40	Q	41	0	0	4	0
40	R	41	0	0	4	0
41	A	52	0	0	6	0
41	B	117	0	0	20	0
41	C	52	0	0	8	0
41	D	70	0	0	12	0
41	E	8	0	0	2	0
41	F	2	0	0	6	0
41	H	14	0	0	1	0
41	I	1	0	0	0	0
41	K	4	0	0	4	0
41	L	7	0	0	4	0
41	M	1	0	0	0	0
41	T	4	0	0	2	0
41	W	2	0	0	0	0
41	X	3	0	0	1	0
41	a	48	0	0	8	0
41	b	125	0	0	36	0
41	c	52	0	0	8	0
41	d	71	0	0	16	0
41	e	9	0	0	5	0
41	h	14	0	0	4	0
41	i	1	0	0	0	0
41	k	3	0	0	1	0
41	l	5	0	0	2	0
41	m	4	0	0	0	0
41	t	5	0	0	1	0
41	w	1	0	0	1	0
41	x	1	0	0	1	0
All	All	69223	0	64352	3265	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 25.

The worst 5 of 3265 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)
19:3:196:LEU:HD11	28:3:313:WVN:C16	1.12	1.58
26:N:606:CLA:CBB	34:N:621:LHG:H172	1.37	1.54
26:5:605:CLA:HBB1	26:6:609:CLA:C6	1.41	1.49
1:a:331:MET:HE3	4:d:347:ARG:C	1.36	1.46
17:1:145:ILE:CD1	34:1:620:LHG:H221	1.49	1.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/374 (79%)	291 (98%)	5 (2%)	0	100	100
1	a	305/374 (82%)	299 (98%)	6 (2%)	0	100	100
2	B	481/508 (95%)	472 (98%)	9 (2%)	0	100	100
2	b	479/508 (94%)	472 (98%)	7 (2%)	0	100	100
3	C	419/486 (86%)	415 (99%)	4 (1%)	0	100	100
3	c	415/486 (85%)	406 (98%)	9 (2%)	0	100	100
4	D	340/351 (97%)	332 (98%)	8 (2%)	0	100	100
4	d	339/351 (97%)	331 (98%)	8 (2%)	0	100	100
5	E	62/84 (74%)	57 (92%)	5 (8%)	0	100	100
5	e	62/84 (74%)	62 (100%)	0	0	100	100
6	F	27/42 (64%)	26 (96%)	1 (4%)	0	100	100
6	f	28/42 (67%)	28 (100%)	0	0	100	100
7	H	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
7	h	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
9	k	35/45 (78%)	35 (100%)	0	0	100	100
10	L	35/38 (92%)	35 (100%)	0	0	100	100
10	l	35/38 (92%)	35 (100%)	0	0	100	100
11	M	34/118 (29%)	33 (97%)	1 (3%)	0	100	100
11	m	34/118 (29%)	32 (94%)	2 (6%)	0	100	100
12	T	28/32 (88%)	28 (100%)	0	0	100	100
12	t	28/32 (88%)	28 (100%)	0	0	100	100
13	W	43/121 (36%)	43 (100%)	0	0	100	100
13	w	43/121 (36%)	43 (100%)	0	0	100	100
14	X	32/39 (82%)	32 (100%)	0	0	100	100
14	x	32/39 (82%)	32 (100%)	0	0	100	100
15	Y	26/34 (76%)	25 (96%)	1 (4%)	0	100	100
15	y	26/34 (76%)	26 (100%)	0	0	100	100
16	Z	59/62 (95%)	56 (95%)	2 (3%)	1 (2%)	7	4
16	z	59/62 (95%)	59 (100%)	0	0	100	100
17	1	190/234 (81%)	181 (95%)	8 (4%)	1 (0%)	24	25
17	N	190/234 (81%)	182 (96%)	8 (4%)	0	100	100
18	2	170/215 (79%)	168 (99%)	2 (1%)	0	100	100
18	O	170/215 (79%)	168 (99%)	2 (1%)	0	100	100
19	3	178/182 (98%)	176 (99%)	2 (1%)	0	100	100
19	P	178/182 (98%)	176 (99%)	2 (1%)	0	100	100
20	4	158/200 (79%)	157 (99%)	1 (1%)	0	100	100
20	Q	158/200 (79%)	157 (99%)	1 (1%)	0	100	100
21	5	187/228 (82%)	185 (99%)	2 (1%)	0	100	100
21	R	187/228 (82%)	185 (99%)	2 (1%)	0	100	100
22	6	171/174 (98%)	166 (97%)	5 (3%)	0	100	100
22	S	171/174 (98%)	166 (97%)	5 (3%)	0	100	100
23	G	92/292 (32%)	88 (96%)	4 (4%)	0	100	100
24	g	91/292 (31%)	87 (96%)	4 (4%)	0	100	100
All	All	6320/7928 (80%)	6191 (98%)	127 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Z	33	TRP
17	1	116	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/305 (81%)	240 (98%)	6 (2%)	43	55
1	a	252/305 (83%)	243 (96%)	9 (4%)	31	39
2	B	384/403 (95%)	356 (93%)	28 (7%)	13	13
2	b	383/403 (95%)	362 (94%)	21 (6%)	19	22
3	C	337/387 (87%)	319 (95%)	18 (5%)	20	23
3	c	334/387 (86%)	328 (98%)	6 (2%)	51	65
4	D	274/280 (98%)	268 (98%)	6 (2%)	45	58
4	d	273/280 (98%)	266 (97%)	7 (3%)	40	51
5	E	56/73 (77%)	47 (84%)	9 (16%)	2	2
5	e	56/73 (77%)	54 (96%)	2 (4%)	31	39
6	F	24/37 (65%)	21 (88%)	3 (12%)	4	3
6	f	25/37 (68%)	22 (88%)	3 (12%)	5	4
7	H	55/57 (96%)	53 (96%)	2 (4%)	31	39
7	h	55/57 (96%)	53 (96%)	2 (4%)	31	39
8	I	33/36 (92%)	31 (94%)	2 (6%)	17	18
8	i	33/36 (92%)	30 (91%)	3 (9%)	9	8
9	K	30/36 (83%)	25 (83%)	5 (17%)	2	1
9	k	30/36 (83%)	23 (77%)	7 (23%)	1	0
10	L	34/35 (97%)	32 (94%)	2 (6%)	18	19
10	l	34/35 (97%)	31 (91%)	3 (9%)	9	9
11	M	29/83 (35%)	25 (86%)	4 (14%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	m	29/83 (35%)	26 (90%)	3 (10%)	7	6
12	T	26/28 (93%)	25 (96%)	1 (4%)	29	37
12	t	26/28 (93%)	26 (100%)	0	100	100
13	W	39/88 (44%)	34 (87%)	5 (13%)	4	3
13	w	39/88 (44%)	32 (82%)	7 (18%)	2	1
14	X	29/34 (85%)	26 (90%)	3 (10%)	7	6
14	x	29/34 (85%)	28 (97%)	1 (3%)	32	41
15	Y	23/29 (79%)	22 (96%)	1 (4%)	26	32
15	y	23/29 (79%)	23 (100%)	0	100	100
16	Z	49/52 (94%)	40 (82%)	9 (18%)	1	1
16	z	51/52 (98%)	51 (100%)	0	100	100
17	1	154/188 (82%)	152 (99%)	2 (1%)	61	74
17	N	154/188 (82%)	147 (96%)	7 (4%)	24	30
18	2	141/171 (82%)	139 (99%)	2 (1%)	59	72
18	O	141/171 (82%)	139 (99%)	2 (1%)	59	72
19	3	143/144 (99%)	138 (96%)	5 (4%)	32	40
19	P	143/144 (99%)	138 (96%)	5 (4%)	32	40
20	4	129/161 (80%)	126 (98%)	3 (2%)	44	56
20	Q	129/161 (80%)	126 (98%)	3 (2%)	44	56
21	5	155/179 (87%)	151 (97%)	4 (3%)	40	51
21	R	155/179 (87%)	151 (97%)	4 (3%)	40	51
22	6	136/137 (99%)	130 (96%)	6 (4%)	25	31
22	S	136/137 (99%)	130 (96%)	6 (4%)	25	31
23	G	75/233 (32%)	73 (97%)	2 (3%)	39	50
24	g	76/235 (32%)	74 (97%)	2 (3%)	40	51
All	All	5207/6354 (82%)	4976 (96%)	231 (4%)	27	31

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	85	VAL
21	R	154	GLN
4	d	83	SER

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Mol	Chain	Res	Type
21	R	44	GLN
21	5	154	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
22	6	128	GLN
18	O	198	GLN
21	R	151	GLN
1	a	310	GLN
1	a	296	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 363 ligands modelled in this entry, 9 are monoatomic - leaving 354 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
39	II0	O	614	-	39,43,43	2.51	10 (25%)	50,60,60	3.32	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	c	515	3	57,61,73	1.38	5 (8%)	68,98,113	1.24	6 (8%)
33	LMG	2	318	-	40,40,55	1.06	2 (5%)	48,48,63	1.01	2 (4%)
28	WVN	B	618	-	40,41,41	5.11	16 (40%)	50,56,56	7.22	31 (62%)
28	WVN	a	406	-	40,41,41	1.95	14 (35%)	50,56,56	2.30	19 (38%)
26	CLA	2	319	19	49,53,73	1.50	6 (12%)	59,89,113	1.24	4 (6%)
38	KC2	N	612	17	49,53,53	2.92	20 (40%)	62,89,89	4.05	35 (56%)
26	CLA	O	606	18	64,68,73	1.32	6 (9%)	77,107,113	1.08	6 (7%)
26	CLA	a	402	1	69,73,73	1.27	6 (8%)	83,113,113	1.13	7 (8%)
39	II0	6	611	-	39,43,43	2.51	11 (28%)	50,60,60	3.36	16 (32%)
38	KC2	1	611	17	49,53,53	1.56	9 (18%)	62,89,89	1.01	1 (1%)
26	CLA	O	609	-	64,68,73	1.32	7 (10%)	77,107,113	1.21	5 (6%)
39	II0	4	314	-	39,43,43	2.54	11 (28%)	50,60,60	3.28	17 (34%)
26	CLA	G	401	-	69,73,73	1.23	7 (10%)	83,113,113	1.13	5 (6%)
26	CLA	N	613	-	52,56,73	1.45	6 (11%)	62,92,113	1.35	6 (9%)
26	CLA	5	611	21	59,63,73	1.36	7 (11%)	71,101,113	1.38	5 (7%)
26	CLA	D	408	4	64,68,73	1.31	6 (9%)	77,107,113	1.20	5 (6%)
39	II0	P	613	-	39,43,43	6.02	21 (53%)	50,60,60	6.83	26 (52%)
28	WVN	H	101	-	40,41,41	5.11	15 (37%)	50,56,56	6.97	32 (64%)
26	CLA	6	606	22	61,65,73	1.33	6 (9%)	73,103,113	1.25	7 (9%)
26	CLA	P	609	19	57,61,73	1.39	7 (12%)	68,98,113	1.31	8 (11%)
36	BCT	d	401	25	2,3,3	1.22	0	2,3,3	4.20	1 (50%)
26	CLA	2	304	18	69,73,73	1.25	7 (10%)	83,113,113	1.17	5 (6%)
28	WVN	B	619	-	40,41,41	1.86	14 (35%)	50,56,56	2.36	15 (30%)
26	CLA	5	609	-	69,73,73	1.27	7 (10%)	83,113,113	1.12	3 (3%)
34	LHG	1	620	-	45,45,48	0.98	2 (4%)	48,51,54	1.00	3 (6%)
38	KC2	O	610	18	49,53,53	2.82	20 (40%)	62,89,89	4.05	33 (53%)
26	CLA	4	307	20	47,51,73	1.53	6 (12%)	56,86,113	1.21	5 (8%)
26	CLA	6	607	34	59,63,73	1.35	6 (10%)	71,101,113	1.19	5 (7%)
33	LMG	D	411	-	37,37,55	1.08	2 (5%)	45,45,63	1.03	3 (6%)
26	CLA	c	508	3	69,73,73	1.27	7 (10%)	83,113,113	1.19	8 (9%)
26	CLA	5	604	21	64,68,73	1.32	6 (9%)	77,107,113	1.16	5 (6%)
34	LHG	2	321	26	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
39	II0	5	614	-	39,43,43	2.51	11 (28%)	50,60,60	3.32	17 (34%)
26	CLA	1	609	17	64,68,73	1.30	9 (14%)	77,107,113	1.29	6 (7%)
28	WVN	B	617	-	40,41,41	5.07	15 (37%)	50,56,56	7.24	31 (62%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PL9	a	407	-	33,33,55	1.22	3 (9%)	41,42,69	1.58	9 (21%)
38	KC2	6	608	22	49,53,53	2.83	20 (40%)	62,89,89	4.17	36 (58%)
26	CLA	C	506	-	69,73,73	1.25	7 (10%)	83,113,113	1.19	9 (10%)
26	CLA	5	605	21	69,73,73	1.27	6 (8%)	83,113,113	1.14	4 (4%)
26	CLA	S	607	34	59,63,73	1.35	6 (10%)	71,101,113	1.18	5 (7%)
26	CLA	5	607	21	69,73,73	1.25	8 (11%)	83,113,113	1.25	8 (9%)
26	CLA	B	606	-	69,73,73	1.26	7 (10%)	83,113,113	1.17	8 (9%)
26	CLA	N	601	-	49,53,73	1.51	6 (12%)	59,89,113	1.32	3 (5%)
26	CLA	1	606	17	54,58,73	1.41	8 (14%)	65,95,113	1.45	5 (7%)
29	PL9	D	409	-	55,55,55	1.05	4 (7%)	68,69,69	1.50	11 (16%)
26	CLA	6	602	22	69,73,73	1.25	6 (8%)	83,113,113	1.19	5 (6%)
26	CLA	6	605	22	59,63,73	1.35	6 (10%)	71,101,113	1.33	6 (8%)
26	CLA	4	303	20	69,73,73	1.28	6 (8%)	83,113,113	1.21	9 (10%)
34	LHG	Z	102	-	24,24,48	1.34	2 (8%)	27,30,54	1.14	2 (7%)
39	II0	N	617	-	39,43,43	2.58	10 (25%)	50,60,60	3.33	19 (38%)
26	CLA	2	303	18	69,73,73	1.29	8 (11%)	83,113,113	1.16	6 (7%)
26	CLA	b	613	2	69,73,73	1.26	6 (8%)	83,113,113	1.17	5 (6%)
26	CLA	3	303	19	67,71,73	1.25	7 (10%)	80,110,113	1.26	6 (7%)
38	KC2	P	605	19	49,53,53	2.85	20 (40%)	62,89,89	4.07	36 (58%)
38	KC2	1	605	-	49,53,53	1.56	8 (16%)	62,89,89	0.95	2 (3%)
26	CLA	N	606	17	54,58,73	1.40	6 (11%)	65,95,113	1.26	9 (13%)
26	CLA	D	404	41	69,73,73	1.25	5 (7%)	83,113,113	1.14	6 (7%)
34	LHG	C	518	-	39,39,48	1.03	2 (5%)	42,45,54	1.10	3 (7%)
26	CLA	4	308	20	60,64,73	1.34	8 (13%)	72,102,113	1.29	4 (5%)
26	CLA	6	610	22	69,73,73	1.24	7 (10%)	83,113,113	1.21	5 (6%)
26	CLA	P	602	19	66,70,73	1.28	6 (9%)	79,109,113	1.23	6 (7%)
39	II0	R	314	-	39,43,43	2.51	11 (28%)	50,60,60	3.34	17 (34%)
26	CLA	3	302	19	69,73,73	1.27	7 (10%)	83,113,113	1.17	7 (8%)
38	KC2	4	311	20	49,53,53	2.86	20 (40%)	62,89,89	4.09	34 (54%)
28	WVN	3	313	-	40,41,41	5.19	17 (42%)	50,56,56	6.84	30 (60%)
26	CLA	N	614	17	51,55,73	1.45	6 (11%)	61,91,113	1.29	5 (8%)
26	CLA	c	510	3	69,73,73	1.26	6 (8%)	83,113,113	1.17	8 (9%)
36	BCT	D	402	25	2,3,3	1.22	0	2,3,3	4.18	1 (50%)
33	LMG	d	404	-	40,40,55	1.05	2 (5%)	48,48,63	1.03	3 (6%)
26	CLA	d	406	4	65,69,73	1.29	6 (9%)	78,108,113	1.18	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	0.86	3 (3%)
34	LHG	c	520	-	39,39,48	1.04	2 (5%)	42,45,54	1.12	2 (4%)
26	CLA	C	508	41	69,73,73	1.26	6 (8%)	83,113,113	1.23	6 (7%)
39	II0	2	320	-	39,43,43	0.30	0	50,60,60	1.03	5 (10%)
26	CLA	b	616	-	69,73,73	1.25	7 (10%)	83,113,113	1.15	5 (6%)
39	II0	O	618	-	39,43,43	0.34	0	50,60,60	0.46	0
26	CLA	3	309	19	49,53,73	1.46	7 (14%)	59,89,113	1.36	7 (11%)
26	CLA	G	402	23	49,53,73	1.48	6 (12%)	59,89,113	1.26	4 (6%)
34	LHG	N	621	-	45,45,48	0.98	2 (4%)	48,51,54	0.99	3 (6%)
26	CLA	2	311	18	64,68,73	1.29	7 (10%)	77,107,113	1.19	4 (5%)
34	LHG	R	319	26	39,39,48	1.03	2 (5%)	42,45,54	1.04	2 (4%)
26	CLA	B	610	41	69,73,73	1.27	6 (8%)	83,113,113	1.13	5 (6%)
26	CLA	P	610	19	59,63,73	1.35	7 (11%)	71,101,113	1.24	6 (8%)
26	CLA	4	301	34	56,60,73	1.38	5 (8%)	67,97,113	1.21	6 (8%)
28	WVN	S	613	-	40,41,41	1.89	14 (35%)	50,56,56	1.88	12 (24%)
33	LMG	b	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.00	3 (5%)
26	CLA	B	614	2	64,68,73	1.30	7 (10%)	77,107,113	1.13	7 (9%)
26	CLA	R	304	21	56,60,73	1.40	8 (14%)	67,97,113	1.38	7 (10%)
26	CLA	1	603	17	56,60,73	1.40	9 (16%)	67,97,113	1.38	6 (8%)
40	IHT	O	616	-	40,42,42	2.11	11 (27%)	53,58,58	2.71	19 (35%)
28	WVN	c	516	-	40,41,41	1.89	14 (35%)	50,56,56	2.15	15 (30%)
26	CLA	Q	305	20	59,63,73	1.37	7 (11%)	71,101,113	1.20	7 (9%)
39	II0	S	612	-	39,43,43	2.51	12 (30%)	50,60,60	3.32	16 (32%)
40	IHT	Q	317	-	40,42,42	2.13	11 (27%)	53,58,58	2.79	23 (43%)
39	II0	2	313	-	39,43,43	2.52	12 (30%)	50,60,60	3.33	16 (32%)
26	CLA	S	604	22	69,73,73	1.23	7 (10%)	83,113,113	1.22	6 (7%)
26	CLA	1	607	17	47,51,73	1.51	10 (21%)	56,86,113	1.44	8 (14%)
26	CLA	4	306	20	59,63,73	1.37	7 (11%)	71,101,113	1.20	8 (11%)
39	II0	3	312	-	39,43,43	5.96	19 (48%)	50,60,60	6.91	27 (54%)
26	CLA	Q	312	20	47,51,73	1.50	7 (14%)	56,86,113	1.27	6 (10%)
26	CLA	O	611	18	64,68,73	1.30	7 (10%)	77,107,113	1.20	5 (6%)
33	LMG	D	406	-	40,40,55	1.06	2 (5%)	48,48,63	1.03	2 (4%)
26	CLA	6	603	22	59,63,73	1.35	8 (13%)	71,101,113	1.34	6 (8%)
38	KC2	1	612	17	49,53,53	1.56	8 (16%)	62,89,89	1.06	3 (4%)
26	CLA	S	602	22	69,73,73	1.25	6 (8%)	83,113,113	1.19	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	5	602	21	59,63,73	1.36	7 (11%)	71,101,113	1.24	7 (9%)
26	CLA	2	309	-	64,68,73	1.32	7 (10%)	77,107,113	1.20	5 (6%)
26	CLA	S	610	22	69,73,73	1.24	7 (10%)	83,113,113	1.21	5 (6%)
26	CLA	d	405	-	69,73,73	1.27	7 (10%)	83,113,113	1.13	4 (4%)
34	LHG	C	501	-	41,41,48	1.03	2 (4%)	44,47,54	0.98	2 (4%)
26	CLA	O	602	18	69,73,73	1.26	6 (8%)	83,113,113	1.22	8 (9%)
39	II0	1	616	-	39,43,43	6.03	20 (51%)	50,60,60	7.06	30 (60%)
26	CLA	B	603	2	69,73,73	1.26	7 (10%)	83,113,113	1.13	6 (7%)
26	CLA	b	604	2	63,67,73	1.33	7 (11%)	75,105,113	1.29	6 (8%)
26	CLA	1	604	17	63,67,73	1.30	9 (14%)	75,105,113	1.38	7 (9%)
26	CLA	c	509	41	69,73,73	1.25	6 (8%)	83,113,113	1.23	5 (6%)
26	CLA	c	503	3	69,73,73	1.26	7 (10%)	83,113,113	1.15	5 (6%)
40	IHT	5	616	-	40,42,42	2.00	10 (25%)	53,58,58	2.96	25 (47%)
37	HEM	F	101	6,5	50,50,50	1.59	9 (18%)	66,82,82	1.63	12 (18%)
35	DGD	c	519	-	55,55,67	0.93	2 (3%)	69,69,81	0.97	3 (4%)
26	CLA	O	601	18	53,57,73	1.43	5 (9%)	62,93,113	1.33	5 (8%)
34	LHG	G	403	26	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
39	II0	N	618	-	39,43,43	2.58	12 (30%)	50,60,60	3.45	18 (36%)
38	KC2	N	605	17	49,53,53	2.86	20 (40%)	62,89,89	4.06	34 (54%)
26	CLA	R	302	21	59,63,73	1.37	6 (10%)	71,101,113	1.23	5 (7%)
26	CLA	N	603	17	55,59,73	1.41	8 (14%)	66,96,113	1.26	5 (7%)
39	II0	O	615	-	39,43,43	6.05	21 (53%)	50,60,60	6.82	28 (56%)
26	CLA	6	604	22	69,73,73	1.23	7 (10%)	83,113,113	1.22	6 (7%)
38	KC2	R	311	-	49,53,53	2.85	20 (40%)	62,89,89	4.04	36 (58%)
26	CLA	a	405	1	64,68,73	1.30	7 (10%)	77,107,113	1.18	4 (5%)
26	CLA	b	611	2	69,73,73	1.26	7 (10%)	83,113,113	1.14	8 (9%)
26	CLA	P	601	19	49,53,73	1.51	6 (12%)	59,89,113	1.25	4 (6%)
26	CLA	c	512	3	69,73,73	1.27	7 (10%)	83,113,113	1.22	7 (8%)
26	CLA	2	308	18	69,73,73	1.28	6 (8%)	83,113,113	1.18	4 (4%)
39	II0	3	310	-	39,43,43	6.07	20 (51%)	50,60,60	6.84	27 (54%)
26	CLA	B	611	2	69,73,73	1.26	6 (8%)	83,113,113	1.14	8 (9%)
26	CLA	b	609	2	69,73,73	1.27	5 (7%)	83,113,113	1.17	7 (8%)
28	WVN	P	615	-	40,41,41	1.86	14 (35%)	50,56,56	2.34	19 (38%)
40	IHT	1	619	-	40,42,42	5.66	20 (50%)	53,58,58	6.94	32 (60%)
40	IHT	N	619	-	40,42,42	2.10	10 (25%)	53,58,58	2.84	22 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	KC2	3	304	19	49,53,53	2.85	20 (40%)	62,89,89	4.08	36 (58%)
39	II0	6	612	-	39,43,43	2.52	12 (30%)	50,60,60	3.32	16 (32%)
26	CLA	B	607	41	69,73,73	1.25	6 (8%)	83,113,113	1.12	7 (8%)
39	II0	R	318	-	39,43,43	2.67	10 (25%)	50,60,60	3.42	22 (44%)
26	CLA	2	305	18	55,59,73	2.32	17 (30%)	66,96,113	4.45	29 (43%)
26	CLA	b	602	2	69,73,73	1.26	6 (8%)	83,113,113	1.23	9 (10%)
26	CLA	N	607	-	47,51,73	1.52	7 (14%)	56,86,113	1.19	5 (8%)
26	CLA	Q	308	20	55,59,73	1.41	7 (12%)	66,96,113	1.29	8 (12%)
40	IHT	R	317	-	40,42,42	2.00	10 (25%)	53,58,58	2.97	24 (45%)
34	LHG	z	101	-	24,24,48	1.33	2 (8%)	27,30,54	1.14	2 (7%)
30	SQD	A	408	-	39,40,54	1.35	4 (10%)	48,51,65	1.12	6 (12%)
26	CLA	b	607	41	69,73,73	1.25	6 (8%)	83,113,113	1.15	7 (8%)
26	CLA	2	302	18	69,73,73	1.26	6 (8%)	83,113,113	1.22	8 (9%)
26	CLA	C	513	3	69,73,73	1.27	7 (10%)	83,113,113	1.20	5 (6%)
27	PHO	A	404	-	58,69,69	2.06	10 (17%)	56,99,99	1.53	7 (12%)
28	WVN	b	617	-	40,41,41	1.86	14 (35%)	50,56,56	2.56	15 (30%)
28	WVN	5	617	-	40,41,41	1.89	14 (35%)	50,56,56	1.89	12 (24%)
26	CLA	c	511	3	69,73,73	1.26	7 (10%)	83,113,113	1.24	5 (6%)
26	CLA	4	304	20	65,69,73	1.28	6 (9%)	78,108,113	1.17	6 (7%)
26	CLA	P	604	19	67,71,73	1.26	7 (10%)	80,110,113	1.25	6 (7%)
26	CLA	4	309	20	55,59,73	1.41	6 (10%)	66,96,113	1.29	9 (13%)
26	CLA	R	312	21	59,63,73	1.36	7 (11%)	71,101,113	1.37	5 (7%)
26	CLA	B	613	2	69,73,73	1.26	7 (10%)	83,113,113	1.15	5 (6%)
33	LMG	c	521	-	51,51,55	0.91	2 (3%)	59,59,63	0.99	3 (5%)
38	KC2	4	305	-	49,53,53	2.87	20 (40%)	62,89,89	4.03	36 (58%)
26	CLA	A	403	41	53,57,73	1.44	7 (13%)	62,93,113	1.24	4 (6%)
28	WVN	k	101	-	40,41,41	1.86	14 (35%)	50,56,56	2.49	16 (32%)
26	CLA	b	608	2	69,73,73	1.26	7 (10%)	83,113,113	1.14	7 (8%)
33	LMG	O	617	-	40,40,55	1.06	2 (5%)	48,48,63	1.01	2 (4%)
26	CLA	B	601	41	54,58,73	1.44	6 (11%)	65,95,113	1.33	6 (9%)
34	LHG	D	410	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
26	CLA	c	505	3	69,73,73	1.27	5 (7%)	83,113,113	1.10	3 (3%)
26	CLA	3	306	19	69,73,73	1.26	6 (8%)	83,113,113	1.17	4 (4%)
33	LMG	d	411	-	46,46,55	0.99	2 (4%)	54,54,63	1.03	3 (5%)
26	CLA	1	613	-	52,56,73	1.46	7 (13%)	62,92,113	1.41	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	616	2	69,73,73	1.26	7 (10%)	83,113,113	1.16	5 (6%)
26	CLA	g	402	24	49,53,73	1.46	7 (14%)	59,89,113	1.52	7 (11%)
26	CLA	R	303	21	59,63,73	1.35	8 (13%)	71,101,113	1.23	7 (9%)
26	CLA	c	506	41	64,68,73	1.30	5 (7%)	77,107,113	1.19	7 (9%)
33	LMG	A	412	-	48,48,55	0.96	2 (4%)	56,56,63	1.09	4 (7%)
26	CLA	N	608	-	50,54,73	1.21	7 (14%)	60,90,113	1.55	8 (13%)
39	II0	2	316	-	39,43,43	6.05	21 (53%)	50,60,60	6.81	28 (56%)
26	CLA	R	307	21	47,51,73	1.49	6 (12%)	56,86,113	1.33	6 (10%)
26	CLA	S	605	22	59,63,73	1.35	6 (10%)	71,101,113	1.34	6 (8%)
39	II0	3	311	-	39,43,43	6.03	21 (53%)	50,60,60	6.84	26 (52%)
26	CLA	4	313	20	47,51,73	1.50	7 (14%)	56,86,113	1.27	6 (10%)
28	WVN	Z	101	-	40,41,41	1.93	14 (35%)	50,56,56	2.25	16 (32%)
38	KC2	Q	309	-	49,53,53	2.85	20 (40%)	62,89,89	4.11	36 (58%)
39	II0	4	317	-	39,43,43	2.60	12 (30%)	50,60,60	3.32	20 (40%)
39	II0	Q	313	-	39,43,43	2.54	11 (28%)	50,60,60	3.28	17 (34%)
26	CLA	C	512	3	69,73,73	1.28	6 (8%)	83,113,113	1.20	5 (6%)
26	CLA	R	310	-	69,73,73	1.27	7 (10%)	83,113,113	1.12	3 (3%)
26	CLA	O	612	18	49,53,73	1.47	7 (14%)	59,89,113	1.29	6 (10%)
26	CLA	S	609	22	57,61,73	1.35	6 (10%)	68,98,113	1.24	7 (10%)
33	LMG	m	101	-	40,40,55	1.03	2 (5%)	48,48,63	1.08	4 (8%)
26	CLA	O	605	-	55,59,73	1.41	7 (12%)	66,96,113	1.25	8 (12%)
39	II0	Q	314	-	39,43,43	2.54	12 (30%)	50,60,60	3.32	17 (34%)
38	KC2	S	608	22	49,53,53	2.82	20 (40%)	62,89,89	4.17	36 (58%)
39	II0	S	611	-	39,43,43	2.51	11 (28%)	50,60,60	3.37	16 (32%)
38	KC2	Q	310	20	49,53,53	2.85	20 (40%)	62,89,89	4.09	35 (56%)
26	CLA	1	614	17	51,55,73	1.53	7 (13%)	61,91,113	1.53	10 (16%)
26	CLA	R	308	21	69,73,73	1.25	8 (11%)	83,113,113	1.25	8 (9%)
40	IHT	4	318	-	40,42,42	2.13	11 (27%)	53,58,58	2.80	23 (43%)
26	CLA	5	606	21	47,51,73	1.48	7 (14%)	56,86,113	1.32	6 (10%)
39	II0	Q	315	-	39,43,43	2.56	11 (28%)	50,60,60	3.36	20 (40%)
34	LHG	D	403	-	42,42,48	1.00	2 (4%)	45,48,54	1.06	3 (6%)
39	II0	1	617	-	39,43,43	6.08	21 (53%)	50,60,60	7.02	28 (56%)
39	II0	R	316	-	39,43,43	2.54	11 (28%)	50,60,60	3.31	15 (30%)
26	CLA	C	510	3	69,73,73	1.25	7 (10%)	83,113,113	1.22	6 (7%)
26	CLA	O	608	18	69,73,73	1.27	6 (8%)	83,113,113	1.18	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	P	603	19	69,73,73	1.27	7 (10%)	83,113,113	1.17	8 (9%)
26	CLA	5	603	21	56,60,73	1.40	8 (14%)	67,97,113	1.39	7 (10%)
26	CLA	4	302	20	69,73,73	1.24	6 (8%)	83,113,113	1.19	4 (4%)
26	CLA	b	612	2	69,73,73	1.24	8 (11%)	83,113,113	1.31	8 (9%)
26	CLA	2	307	18	52,56,73	1.45	6 (11%)	62,92,113	1.22	6 (9%)
26	CLA	b	605	2	69,73,73	1.27	6 (8%)	83,113,113	1.19	6 (7%)
26	CLA	C	507	3	69,73,73	1.26	8 (11%)	83,113,113	1.19	8 (9%)
29	PL9	A	407	-	33,33,55	1.21	3 (9%)	41,42,69	1.57	9 (21%)
30	SQD	c	501	-	44,45,54	1.29	4 (9%)	53,56,65	1.20	6 (11%)
28	WVN	D	412	-	40,41,41	1.88	14 (35%)	50,56,56	2.13	15 (30%)
27	PHO	D	405	-	58,69,69	2.06	10 (17%)	56,99,99	1.51	8 (14%)
26	CLA	4	312	20	47,51,73	1.48	6 (12%)	56,86,113	1.31	6 (10%)
33	LMG	R	301	-	40,40,55	1.04	2 (5%)	48,48,63	1.01	3 (6%)
33	LMG	M	101	-	40,40,55	1.04	2 (5%)	48,48,63	1.08	4 (8%)
26	CLA	B	605	2	69,73,73	1.26	7 (10%)	83,113,113	1.18	7 (8%)
38	KC2	1	610	-	49,53,53	1.57	9 (18%)	62,89,89	1.00	2 (3%)
26	CLA	N	609	17	64,68,73	1.31	7 (10%)	77,107,113	1.21	5 (6%)
33	LMG	d	409	-	37,37,55	1.08	2 (5%)	45,45,63	1.03	3 (6%)
26	CLA	3	308	-	59,63,73	1.14	6 (10%)	71,101,113	1.66	11 (15%)
26	CLA	B	615	2	69,73,73	1.25	6 (8%)	83,113,113	1.23	3 (3%)
26	CLA	O	604	18	69,73,73	1.26	7 (10%)	83,113,113	1.16	5 (6%)
26	CLA	Q	302	20	69,73,73	1.29	8 (11%)	83,113,113	1.21	9 (10%)
34	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
27	PHO	a	404	-	58,69,69	2.07	10 (17%)	56,99,99	1.51	7 (12%)
26	CLA	3	305	19	69,73,73	1.25	6 (8%)	83,113,113	1.19	7 (8%)
26	CLA	B	609	2	69,73,73	1.27	7 (10%)	83,113,113	1.17	7 (8%)
38	KC2	5	610	-	49,53,53	2.85	20 (40%)	62,89,89	4.05	37 (59%)
28	WVN	c	517	-	40,41,41	1.85	14 (35%)	50,56,56	1.85	13 (26%)
26	CLA	O	607	18	52,56,73	1.45	7 (13%)	62,92,113	1.23	6 (9%)
26	CLA	Q	311	20	47,51,73	1.48	6 (12%)	56,86,113	1.31	6 (10%)
38	KC2	4	310	-	49,53,53	2.85	20 (40%)	62,89,89	4.11	36 (58%)
39	II0	2	314	-	39,43,43	2.50	11 (28%)	50,60,60	3.33	17 (34%)
26	CLA	N	604	17	63,67,73	1.32	7 (11%)	75,105,113	1.19	4 (5%)
28	WVN	b	619	-	40,41,41	1.86	14 (35%)	50,56,56	2.32	14 (28%)
33	LMG	C	520	-	31,31,55	1.20	2 (6%)	39,39,63	1.08	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	d	402	41	69,73,73	1.26	5 (7%)	83,113,113	1.16	4 (4%)
34	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
26	CLA	c	504	3	69,73,73	1.26	8 (11%)	83,113,113	1.17	4 (4%)
39	II0	4	315	-	39,43,43	2.55	11 (28%)	50,60,60	3.32	17 (34%)
26	CLA	6	601	22	59,63,73	1.37	7 (11%)	71,101,113	1.19	4 (5%)
33	LMG	c	522	-	31,31,55	1.19	2 (6%)	39,39,63	1.09	3 (7%)
28	WVN	C	515	-	40,41,41	1.85	14 (35%)	50,56,56	1.95	13 (26%)
39	II0	2	315	-	39,43,43	2.58	12 (30%)	50,60,60	3.29	18 (36%)
26	CLA	c	513	3	69,73,73	1.27	6 (8%)	83,113,113	1.20	5 (6%)
26	CLA	b	614	2	64,68,73	1.31	6 (9%)	77,107,113	1.13	7 (9%)
26	CLA	N	602	17	64,68,73	1.30	6 (9%)	77,107,113	1.22	7 (9%)
28	WVN	C	516	-	40,41,41	5.18	17 (42%)	50,56,56	7.09	32 (64%)
26	CLA	B	604	2	63,67,73	1.31	7 (11%)	75,105,113	1.27	5 (6%)
39	II0	Q	319	-	39,43,43	2.56	10 (25%)	50,60,60	3.34	17 (34%)
26	CLA	1	601	-	49,53,73	1.49	7 (14%)	59,89,113	1.43	4 (6%)
35	DGD	C	517	-	55,55,67	0.92	2 (3%)	69,69,81	0.97	3 (4%)
39	II0	4	316	-	39,43,43	2.56	11 (28%)	50,60,60	3.37	20 (40%)
39	II0	N	615	-	39,43,43	2.54	10 (25%)	50,60,60	3.37	16 (32%)
33	LMG	B	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	3 (5%)
37	HEM	f	101	6,5	50,50,50	1.59	9 (18%)	66,82,82	1.66	12 (18%)
26	CLA	S	601	22	59,63,73	1.36	7 (11%)	71,101,113	1.19	4 (5%)
28	WVN	c	518	-	40,41,41	1.86	14 (35%)	50,56,56	2.32	14 (28%)
26	CLA	5	608	21	63,67,73	1.32	6 (9%)	75,105,113	1.20	4 (5%)
26	CLA	B	612	2	69,73,73	1.23	7 (10%)	83,113,113	1.31	9 (10%)
34	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
26	CLA	B	602	2	69,73,73	1.26	7 (10%)	83,113,113	1.23	9 (10%)
26	CLA	3	307	19	57,61,73	1.40	6 (10%)	68,98,113	1.32	6 (8%)
26	CLA	g	401	-	69,73,73	1.28	6 (8%)	83,113,113	1.17	8 (9%)
26	CLA	1	602	17	64,68,73	1.31	8 (12%)	77,107,113	1.31	7 (9%)
26	CLA	5	601	21	59,63,73	1.37	6 (10%)	71,101,113	1.23	5 (7%)
34	LHG	a	409	-	41,41,48	1.02	2 (4%)	44,47,54	0.97	2 (4%)
26	CLA	P	607	19	69,73,73	1.26	6 (8%)	83,113,113	1.17	4 (4%)
26	CLA	C	511	3	69,73,73	1.25	7 (10%)	83,113,113	1.21	7 (8%)
26	CLA	B	608	2	69,73,73	1.24	7 (10%)	83,113,113	1.13	7 (8%)
26	CLA	P	608	34	56,60,73	1.39	5 (8%)	67,97,113	1.21	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	c	507	-	69,73,73	1.25	7 (10%)	83,113,113	1.18	7 (8%)
39	II0	5	615	-	39,43,43	2.53	11 (28%)	50,60,60	3.31	15 (30%)
28	WVN	b	618	-	40,41,41	1.87	14 (35%)	50,56,56	2.54	17 (34%)
33	LMG	4	319	-	43,43,55	1.05	2 (4%)	51,51,63	0.89	2 (3%)
26	CLA	3	301	19	66,70,73	1.28	6 (9%)	79,109,113	1.23	6 (7%)
39	II0	1	615	-	39,43,43	6.00	21 (53%)	50,60,60	7.01	28 (56%)
26	CLA	D	407	-	69,73,73	1.27	7 (10%)	83,113,113	1.15	4 (4%)
35	DGD	h	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	3 (3%)
26	CLA	b	610	41	69,73,73	1.28	6 (8%)	83,113,113	1.13	5 (6%)
26	CLA	b	615	2	69,73,73	1.26	5 (7%)	83,113,113	1.23	3 (3%)
26	CLA	b	606	-	69,73,73	1.26	6 (8%)	83,113,113	1.16	7 (8%)
33	LMG	D	413	-	46,46,55	0.99	2 (4%)	54,54,63	1.02	3 (5%)
30	SQD	a	408	-	39,40,54	1.36	4 (10%)	48,51,65	1.12	6 (12%)
34	LHG	b	621	-	42,42,48	1.00	2 (4%)	45,48,54	1.08	3 (6%)
26	CLA	Q	306	20	47,51,73	1.54	6 (12%)	56,86,113	1.21	5 (8%)
26	CLA	A	402	1	69,73,73	1.26	7 (10%)	83,113,113	1.14	7 (8%)
26	CLA	O	603	18	69,73,73	1.29	6 (8%)	83,113,113	1.16	6 (7%)
26	CLA	c	514	3	69,73,73	1.25	6 (8%)	83,113,113	1.18	5 (6%)
33	LMG	5	619	-	40,40,55	1.05	2 (5%)	48,48,63	1.01	3 (6%)
26	CLA	6	609	22	57,61,73	1.35	6 (10%)	68,98,113	1.24	7 (10%)
26	CLA	R	309	21	63,67,73	1.32	6 (9%)	75,105,113	1.20	5 (6%)
38	KC2	N	610	-	49,53,53	2.86	20 (40%)	62,89,89	4.02	36 (58%)
26	CLA	Q	303	20	65,69,73	1.28	6 (9%)	78,108,113	1.17	5 (6%)
26	CLA	R	306	21	69,73,73	1.28	6 (8%)	83,113,113	1.14	4 (4%)
28	WVN	A	406	-	40,41,41	1.88	14 (35%)	50,56,56	2.34	15 (30%)
26	CLA	2	301	18	53,57,73	1.43	6 (11%)	62,93,113	1.34	5 (8%)
26	CLA	C	509	3	69,73,73	1.26	8 (11%)	83,113,113	1.17	8 (9%)
26	CLA	C	503	3	69,73,73	1.25	8 (11%)	83,113,113	1.18	4 (4%)
26	CLA	a	403	41	53,57,73	1.44	7 (13%)	62,93,113	1.24	5 (8%)
40	IHT	2	317	-	40,42,42	5.65	19 (47%)	53,58,58	7.04	31 (58%)
39	II0	P	612	-	39,43,43	2.53	11 (28%)	50,60,60	3.34	15 (30%)
26	CLA	Q	307	20	60,64,73	1.34	8 (13%)	72,102,113	1.29	4 (5%)
26	CLA	b	603	2	69,73,73	1.26	7 (10%)	83,113,113	1.10	6 (7%)
26	CLA	1	608	17	50,54,73	1.46	8 (16%)	60,90,113	1.37	4 (6%)
26	CLA	C	504	3	69,73,73	1.27	6 (8%)	83,113,113	1.11	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	II0	N	616	-	39,43,43	2.50	11 (28%)	50,60,60	3.32	17 (34%)
29	PL9	d	407	-	55,55,55	1.05	3 (5%)	68,69,69	1.52	11 (16%)
33	LMG	C	519	-	47,47,55	0.97	2 (4%)	55,55,63	1.18	4 (7%)
26	CLA	P	606	19	69,73,73	1.26	6 (8%)	83,113,113	1.18	7 (8%)
26	CLA	R	305	21	64,68,73	1.31	7 (10%)	77,107,113	1.16	6 (7%)
26	CLA	R	313	21	50,54,73	1.46	6 (12%)	60,90,113	1.25	6 (10%)
38	KC2	Q	304	-	49,53,53	2.86	20 (40%)	62,89,89	4.03	36 (58%)
39	II0	O	613	-	39,43,43	2.53	12 (30%)	50,60,60	3.33	16 (32%)
26	CLA	S	606	22	61,65,73	1.33	6 (9%)	73,103,113	1.26	6 (8%)
28	WVN	Y	101	-	40,41,41	1.90	14 (35%)	50,56,56	2.26	12 (24%)
33	LMG	a	413	-	48,48,55	0.97	2 (4%)	56,56,63	1.12	4 (7%)
39	II0	6	613	-	39,43,43	2.67	10 (25%)	50,60,60	3.42	22 (44%)
26	CLA	b	601	41	54,58,73	1.42	6 (11%)	65,95,113	1.32	6 (9%)
39	II0	N	620	-	39,43,43	2.58	12 (30%)	50,60,60	3.29	18 (36%)
39	II0	4	320	-	39,43,43	2.56	10 (25%)	50,60,60	3.34	17 (34%)
39	II0	1	618	-	39,43,43	6.08	21 (53%)	50,60,60	6.81	28 (56%)
33	LMG	Q	318	-	43,43,55	1.05	2 (4%)	51,51,63	0.89	2 (3%)
39	II0	R	315	-	39,43,43	2.52	11 (28%)	50,60,60	3.32	17 (34%)
26	CLA	2	306	18	64,68,73	1.31	6 (9%)	77,107,113	1.07	6 (7%)
28	WVN	x	101	-	40,41,41	1.87	14 (35%)	50,56,56	2.46	13 (26%)
27	PHO	d	403	-	58,69,69	2.06	10 (17%)	56,99,99	1.52	8 (14%)
26	CLA	P	611	19	49,53,73	1.45	7 (14%)	59,89,113	1.35	7 (11%)
28	WVN	d	410	-	40,41,41	1.89	14 (35%)	50,56,56	2.21	16 (32%)
26	CLA	Q	301	20	69,73,73	1.25	6 (8%)	83,113,113	1.19	4 (4%)
30	SQD	D	401	-	53,54,54	1.17	4 (7%)	62,65,65	1.15	6 (9%)
38	KC2	2	310	18	49,53,53	2.83	20 (40%)	62,89,89	4.06	33 (53%)
26	CLA	5	612	21	50,54,73	1.48	7 (14%)	60,90,113	1.25	7 (11%)
34	LHG	5	618	26	39,39,48	1.03	2 (5%)	42,45,54	1.04	2 (4%)
26	CLA	2	312	18	49,53,73	1.47	7 (14%)	59,89,113	1.29	6 (10%)
39	II0	5	613	-	39,43,43	2.52	11 (28%)	50,60,60	3.34	17 (34%)
39	II0	Q	316	-	39,43,43	2.60	12 (30%)	50,60,60	3.32	20 (40%)
26	CLA	A	405	1	64,68,73	1.30	5 (7%)	77,107,113	1.20	6 (7%)
26	CLA	C	505	41	64,68,73	1.31	7 (10%)	77,107,113	1.16	7 (9%)
26	CLA	C	502	3	69,73,73	1.27	6 (8%)	83,113,113	1.13	4 (4%)
38	KC2	N	611	17	49,53,53	2.83	20 (40%)	62,89,89	4.13	34 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	II0	P	614	-	39,43,43	2.54	11 (28%)	50,60,60	3.31	16 (32%)
26	CLA	C	514	3	56,60,73	1.39	7 (12%)	67,97,113	1.22	6 (8%)
26	CLA	S	603	22	59,63,73	1.35	7 (11%)	71,101,113	1.34	7 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	II0	O	614	-	-	1/21/67/67	0/2/2/2
26	CLA	c	515	3	-	11/25/101/115	-
33	LMG	2	318	-	-	2/35/55/70	0/1/1/1
28	WVN	B	618	-	-	17/29/63/63	0/2/2/2
28	WVN	a	406	-	-	9/29/63/63	0/2/2/2
26	CLA	2	319	19	-	4/15/91/115	-
38	KC2	N	612	17	-	10/15/71/71	-
26	CLA	O	606	18	-	15/33/109/115	-
26	CLA	a	402	1	-	10/39/115/115	-
39	II0	6	611	-	-	6/21/67/67	0/2/2/2
38	KC2	1	611	17	-	8/15/71/71	-
26	CLA	O	609	-	-	17/33/109/115	-
39	II0	4	314	-	-	2/21/67/67	0/2/2/2
26	CLA	G	401	-	-	21/39/115/115	-
26	CLA	N	613	-	-	6/19/95/115	-
26	CLA	5	611	21	-	16/27/103/115	-
26	CLA	D	408	4	-	13/33/109/115	-
39	II0	P	613	-	-	12/21/67/67	0/2/2/2
28	WVN	H	101	-	-	15/29/63/63	0/2/2/2
26	CLA	6	606	22	-	11/30/106/115	-
26	CLA	P	609	19	-	7/25/101/115	-
26	CLA	2	304	18	-	12/39/115/115	-
28	WVN	B	619	-	-	10/29/63/63	0/2/2/2
26	CLA	5	609	-	-	17/39/115/115	-
34	LHG	1	620	-	-	9/50/50/53	-
38	KC2	O	610	18	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	4	307	20	-	3/13/89/115	-
26	CLA	6	607	34	-	13/27/103/115	-
33	LMG	D	411	-	-	2/32/52/70	0/1/1/1
26	CLA	c	508	3	-	7/39/115/115	-
26	CLA	5	604	21	-	11/33/109/115	-
34	LHG	2	321	26	-	19/53/53/53	-
39	II0	5	614	-	-	1/21/67/67	0/2/2/2
26	CLA	1	609	17	-	15/33/109/115	-
28	WVN	B	617	-	-	15/29/63/63	0/2/2/2
29	PL9	a	407	-	-	10/27/47/73	0/1/1/1
38	KC2	6	608	22	-	5/15/71/71	-
26	CLA	C	506	-	-	13/39/115/115	-
26	CLA	5	605	21	-	16/39/115/115	-
26	CLA	S	607	34	-	13/27/103/115	-
26	CLA	5	607	21	-	12/39/115/115	-
26	CLA	B	606	-	-	14/39/115/115	-
26	CLA	N	601	-	-	9/15/91/115	-
26	CLA	1	606	17	-	10/21/97/115	-
29	PL9	D	409	-	-	7/53/73/73	0/1/1/1
26	CLA	6	602	22	-	17/39/115/115	-
26	CLA	6	605	22	-	14/27/103/115	-
26	CLA	4	303	20	-	16/39/115/115	-
34	LHG	Z	102	-	-	8/29/29/53	-
39	II0	N	617	-	-	3/21/67/67	0/2/2/2
26	CLA	2	303	18	-	8/39/115/115	-
26	CLA	b	613	2	-	18/39/115/115	-
26	CLA	3	303	19	-	8/37/113/115	-
38	KC2	P	605	19	-	9/15/71/71	-
38	KC2	1	605	-	-	12/15/71/71	-
26	CLA	N	606	17	-	8/21/97/115	-
26	CLA	D	404	41	-	10/39/115/115	-
34	LHG	C	518	-	-	16/44/44/53	-
26	CLA	4	308	20	-	11/29/105/115	-
26	CLA	6	610	22	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	P	602	19	-	15/36/112/115	-
39	II0	R	314	-	-	0/21/67/67	0/2/2/2
26	CLA	3	302	19	-	16/39/115/115	-
38	KC2	4	311	20	-	3/15/71/71	-
28	WVN	3	313	-	-	16/29/63/63	0/2/2/2
26	CLA	N	614	17	-	12/18/94/115	-
26	CLA	c	510	3	-	12/39/115/115	-
33	LMG	d	404	-	-	9/35/55/70	0/1/1/1
26	CLA	d	406	4	-	16/35/111/115	-
35	DGD	H	102	-	-	14/51/91/95	0/2/2/2
34	LHG	c	520	-	-	13/44/44/53	-
26	CLA	C	508	41	-	8/39/115/115	-
39	II0	2	320	-	-	3/21/67/67	0/2/2/2
26	CLA	b	616	-	-	15/39/115/115	-
39	II0	O	618	-	-	1/21/67/67	0/2/2/2
26	CLA	3	309	19	-	8/15/91/115	-
26	CLA	G	402	23	-	6/15/91/115	-
34	LHG	N	621	-	-	12/50/50/53	-
26	CLA	2	311	18	-	10/33/109/115	-
34	LHG	R	319	26	-	12/44/44/53	-
26	CLA	B	610	41	-	11/39/115/115	-
26	CLA	P	610	19	-	11/27/103/115	-
26	CLA	4	301	34	-	8/24/100/115	-
28	WVN	S	613	-	-	9/29/63/63	0/2/2/2
33	LMG	b	620	-	-	6/46/66/70	0/1/1/1
26	CLA	B	614	2	-	11/33/109/115	-
26	CLA	R	304	21	-	11/24/100/115	-
26	CLA	1	603	17	-	7/24/100/115	-
40	IHT	O	616	-	-	6/25/65/65	0/2/2/2
28	WVN	c	516	-	-	10/29/63/63	0/2/2/2
26	CLA	Q	305	20	-	11/27/103/115	-
39	II0	S	612	-	-	1/21/67/67	0/2/2/2
40	IHT	Q	317	-	-	10/25/65/65	0/2/2/2
39	II0	2	313	-	-	1/21/67/67	0/2/2/2
26	CLA	S	604	22	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	1	607	17	-	7/13/89/115	-
26	CLA	4	306	20	-	11/27/103/115	-
39	II0	3	312	-	-	10/21/67/67	0/2/2/2
26	CLA	Q	312	20	-	4/13/89/115	-
26	CLA	O	611	18	-	10/33/109/115	-
33	LMG	D	406	-	-	9/35/55/70	0/1/1/1
26	CLA	6	603	22	-	11/27/103/115	-
38	KC2	1	612	17	-	9/15/71/71	-
26	CLA	S	602	22	-	17/39/115/115	-
26	CLA	5	602	21	-	14/27/103/115	-
26	CLA	2	309	-	-	17/33/109/115	-
26	CLA	S	610	22	-	12/39/115/115	-
26	CLA	d	405	-	-	7/39/115/115	-
34	LHG	C	501	-	-	29/46/46/53	-
26	CLA	O	602	18	-	16/39/115/115	-
39	II0	1	616	-	-	13/21/67/67	0/2/2/2
26	CLA	B	603	2	-	9/39/115/115	-
26	CLA	b	604	2	-	12/32/108/115	-
26	CLA	1	604	17	-	15/32/108/115	-
26	CLA	c	509	41	-	9/39/115/115	-
26	CLA	c	503	3	-	8/39/115/115	-
40	IHT	5	616	-	-	11/25/65/65	0/2/2/2
37	HEM	F	101	6,5	-	8/14/54/54	-
35	DGD	c	519	-	-	8/43/83/95	0/2/2/2
26	CLA	O	601	18	-	9/20/96/115	-
34	LHG	G	403	26	-	19/53/53/53	-
39	II0	N	618	-	-	4/21/67/67	0/2/2/2
38	KC2	N	605	17	-	12/15/71/71	-
26	CLA	R	302	21	-	8/27/103/115	-
26	CLA	N	603	17	-	9/23/99/115	-
39	II0	O	615	-	-	11/21/67/67	0/2/2/2
26	CLA	6	604	22	-	18/39/115/115	-
38	KC2	R	311	-	-	8/15/71/71	-
26	CLA	a	405	1	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	611	2	-	10/39/115/115	-
26	CLA	P	601	19	-	4/15/91/115	-
26	CLA	c	512	3	-	11/39/115/115	-
26	CLA	2	308	18	-	10/39/115/115	-
39	II0	3	310	-	-	10/21/67/67	0/2/2/2
26	CLA	B	611	2	-	10/39/115/115	-
26	CLA	b	609	2	-	8/39/115/115	-
28	WVN	P	615	-	-	8/29/63/63	0/2/2/2
40	IHT	1	619	-	-	15/25/65/65	0/2/2/2
40	IHT	N	619	-	-	7/25/65/65	0/2/2/2
38	KC2	3	304	19	-	9/15/71/71	-
39	II0	6	612	-	-	1/21/67/67	0/2/2/2
26	CLA	B	607	41	-	13/39/115/115	-
39	II0	R	318	-	-	4/21/67/67	0/2/2/2
26	CLA	2	305	18	-	5/23/99/115	-
26	CLA	b	602	2	-	6/39/115/115	-
26	CLA	N	607	-	-	5/13/89/115	-
26	CLA	Q	308	20	-	4/23/99/115	-
40	IHT	R	317	-	-	11/25/65/65	0/2/2/2
34	LHG	z	101	-	-	8/29/29/53	-
30	SQD	A	408	-	-	3/35/55/69	0/1/1/1
26	CLA	b	607	41	-	12/39/115/115	-
26	CLA	2	302	18	-	16/39/115/115	-
26	CLA	C	513	3	-	13/39/115/115	-
27	PHO	A	404	-	-	14/37/103/103	0/5/6/6
28	WVN	b	617	-	-	13/29/63/63	0/2/2/2
28	WVN	5	617	-	-	9/29/63/63	0/2/2/2
26	CLA	c	511	3	-	13/39/115/115	-
26	CLA	4	304	20	-	17/35/111/115	-
26	CLA	P	604	19	-	8/37/113/115	-
26	CLA	4	309	20	-	4/23/99/115	-
26	CLA	R	312	21	-	16/27/103/115	-
26	CLA	B	613	2	-	17/39/115/115	-
33	LMG	c	521	-	-	19/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC2	4	305	-	-	7/15/71/71	-
26	CLA	A	403	41	-	10/20/96/115	-
28	WVN	k	101	-	-	8/29/63/63	0/2/2/2
26	CLA	b	608	2	-	6/39/115/115	-
33	LMG	O	617	-	-	2/35/55/70	0/1/1/1
26	CLA	B	601	41	-	11/21/97/115	-
34	LHG	D	410	-	-	13/53/53/53	-
26	CLA	c	505	3	-	11/39/115/115	-
26	CLA	3	306	19	-	14/39/115/115	-
33	LMG	d	411	-	-	3/41/61/70	0/1/1/1
26	CLA	1	613	-	-	8/19/95/115	-
26	CLA	B	616	2	-	15/39/115/115	-
26	CLA	g	402	24	-	8/15/91/115	-
26	CLA	R	303	21	-	14/27/103/115	-
26	CLA	c	506	41	-	12/33/109/115	-
33	LMG	A	412	-	-	9/43/63/70	0/1/1/1
26	CLA	N	608	-	-	6/17/93/115	-
39	II0	2	316	-	-	11/21/67/67	0/2/2/2
26	CLA	R	307	21	-	4/13/89/115	-
26	CLA	S	605	22	-	14/27/103/115	-
39	II0	3	311	-	-	12/21/67/67	0/2/2/2
26	CLA	4	313	20	-	4/13/89/115	-
28	WVN	Z	101	-	-	10/29/63/63	0/2/2/2
38	KC2	Q	309	-	-	8/15/71/71	-
39	II0	4	317	-	-	5/21/67/67	0/2/2/2
39	II0	Q	313	-	-	2/21/67/67	0/2/2/2
26	CLA	C	512	3	-	13/39/115/115	-
26	CLA	R	310	-	-	17/39/115/115	-
26	CLA	O	612	18	-	10/15/91/115	-
26	CLA	S	609	22	-	5/25/101/115	-
33	LMG	m	101	-	-	6/35/55/70	0/1/1/1
26	CLA	O	605	-	-	8/23/99/115	-
39	II0	Q	314	-	-	0/21/67/67	0/2/2/2
38	KC2	S	608	22	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	II0	S	611	-	-	5/21/67/67	0/2/2/2
38	KC2	Q	310	20	-	3/15/71/71	-
26	CLA	1	614	17	-	10/18/94/115	-
26	CLA	R	308	21	-	12/39/115/115	-
40	IHT	4	318	-	-	10/25/65/65	0/2/2/2
26	CLA	5	606	21	-	4/13/89/115	-
39	II0	Q	315	-	-	1/21/67/67	0/2/2/2
34	LHG	D	403	-	-	12/47/47/53	-
39	II0	1	617	-	-	10/21/67/67	0/2/2/2
39	II0	R	316	-	-	3/21/67/67	0/2/2/2
26	CLA	C	510	3	-	13/39/115/115	-
26	CLA	O	608	18	-	10/39/115/115	-
26	CLA	P	603	19	-	16/39/115/115	-
26	CLA	5	603	21	-	11/24/100/115	-
26	CLA	4	302	20	-	8/39/115/115	-
26	CLA	b	612	2	-	13/39/115/115	-
26	CLA	2	307	18	-	4/19/95/115	-
26	CLA	b	605	2	-	9/39/115/115	-
26	CLA	C	507	3	-	8/39/115/115	-
29	PL9	A	407	-	-	10/27/47/73	0/1/1/1
30	SQD	c	501	-	-	6/40/60/69	0/1/1/1
28	WVN	D	412	-	-	9/29/63/63	0/2/2/2
27	PHO	D	405	-	-	11/37/103/103	0/5/6/6
26	CLA	4	312	20	-	8/13/89/115	-
33	LMG	R	301	-	-	8/35/55/70	0/1/1/1
33	LMG	M	101	-	-	7/35/55/70	0/1/1/1
26	CLA	B	605	2	-	9/39/115/115	-
38	KC2	1	610	-	-	11/15/71/71	-
26	CLA	N	609	17	-	7/33/109/115	-
33	LMG	d	409	-	-	2/32/52/70	0/1/1/1
26	CLA	3	308	-	-	10/27/103/115	-
26	CLA	B	615	2	-	10/39/115/115	-
26	CLA	O	604	18	-	12/39/115/115	-
26	CLA	Q	302	20	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	d	408	-	-	13/53/53/53	-
27	PHO	a	404	-	-	14/37/103/103	0/5/6/6
26	CLA	3	305	19	-	9/39/115/115	-
26	CLA	B	609	2	-	9/39/115/115	-
38	KC2	5	610	-	-	8/15/71/71	-
28	WVN	c	517	-	-	10/29/63/63	0/2/2/2
26	CLA	O	607	18	-	4/19/95/115	-
26	CLA	Q	311	20	-	8/13/89/115	-
38	KC2	4	310	-	-	8/15/71/71	-
39	II0	2	314	-	-	1/21/67/67	0/2/2/2
26	CLA	N	604	17	-	8/32/108/115	-
28	WVN	b	619	-	-	9/29/63/63	0/2/2/2
33	LMG	C	520	-	-	5/26/46/70	0/1/1/1
26	CLA	d	402	41	-	10/39/115/115	-
34	LHG	l	101	-	-	6/53/53/53	-
26	CLA	c	504	3	-	16/39/115/115	-
39	II0	4	315	-	-	0/21/67/67	0/2/2/2
26	CLA	6	601	22	-	10/27/103/115	-
33	LMG	c	522	-	-	5/26/46/70	0/1/1/1
28	WVN	C	515	-	-	10/29/63/63	0/2/2/2
39	II0	2	315	-	-	3/21/67/67	0/2/2/2
26	CLA	c	513	3	-	11/39/115/115	-
26	CLA	b	614	2	-	12/33/109/115	-
26	CLA	N	602	17	-	8/33/109/115	-
28	WVN	C	516	-	-	16/29/63/63	0/2/2/2
26	CLA	B	604	2	-	11/32/108/115	-
39	II0	Q	319	-	-	0/21/67/67	0/2/2/2
26	CLA	1	601	-	-	8/15/91/115	-
35	DGD	C	517	-	-	8/43/83/95	0/2/2/2
39	II0	4	316	-	-	2/21/67/67	0/2/2/2
39	II0	N	615	-	-	4/21/67/67	0/2/2/2
33	LMG	B	620	-	-	7/46/66/70	0/1/1/1
37	HEM	f	101	6,5	-	8/14/54/54	-
26	CLA	S	601	22	-	10/27/103/115	-
28	WVN	c	518	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	5	608	21	-	12/32/108/115	-
26	CLA	B	612	2	-	12/39/115/115	-
34	LHG	L	101	-	-	7/53/53/53	-
26	CLA	B	602	2	-	6/39/115/115	-
26	CLA	3	307	19	-	7/25/101/115	-
26	CLA	g	401	-	-	11/39/115/115	-
26	CLA	1	602	17	-	6/33/109/115	-
26	CLA	5	601	21	-	8/27/103/115	-
34	LHG	a	409	-	-	28/46/46/53	-
26	CLA	P	607	19	-	14/39/115/115	-
26	CLA	C	511	3	-	11/39/115/115	-
26	CLA	B	608	2	-	4/39/115/115	-
26	CLA	P	608	34	-	8/24/100/115	-
26	CLA	c	507	-	-	10/39/115/115	-
39	II0	5	615	-	-	3/21/67/67	0/2/2/2
28	WVN	b	618	-	-	10/29/63/63	0/2/2/2
33	LMG	4	319	-	-	4/38/58/70	0/1/1/1
26	CLA	3	301	19	-	15/36/112/115	-
39	II0	1	615	-	-	14/21/67/67	0/2/2/2
26	CLA	D	407	-	-	7/39/115/115	-
35	DGD	h	101	-	-	14/51/91/95	0/2/2/2
26	CLA	b	610	41	-	11/39/115/115	-
26	CLA	b	615	2	-	9/39/115/115	-
26	CLA	b	606	-	-	12/39/115/115	-
33	LMG	D	413	-	-	3/41/61/70	0/1/1/1
30	SQD	a	408	-	-	4/35/55/69	0/1/1/1
34	LHG	b	621	-	-	20/47/47/53	-
26	CLA	Q	306	20	-	3/13/89/115	-
26	CLA	A	402	1	-	10/39/115/115	-
26	CLA	O	603	18	-	8/39/115/115	-
26	CLA	c	514	3	-	14/39/115/115	-
33	LMG	5	619	-	-	8/35/55/70	0/1/1/1
26	CLA	6	609	22	-	5/25/101/115	-
26	CLA	R	309	21	-	12/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC2	N	610	-	-	4/15/71/71	-
26	CLA	Q	303	20	-	16/35/111/115	-
26	CLA	R	306	21	-	16/39/115/115	-
28	WVN	A	406	-	-	2/29/63/63	0/2/2/2
26	CLA	2	301	18	-	9/20/96/115	-
26	CLA	C	509	3	-	12/39/115/115	-
26	CLA	C	503	3	-	16/39/115/115	-
26	CLA	a	403	41	-	10/20/96/115	-
40	IHT	2	317	-	-	16/25/65/65	0/2/2/2
39	II0	P	612	-	-	2/21/67/67	0/2/2/2
26	CLA	Q	307	20	-	11/29/105/115	-
26	CLA	b	603	2	-	9/39/115/115	-
26	CLA	1	608	17	-	7/17/93/115	-
26	CLA	C	504	3	-	11/39/115/115	-
39	II0	N	616	-	-	1/21/67/67	0/2/2/2
29	PL9	d	407	-	-	8/53/73/73	0/1/1/1
33	LMG	C	519	-	-	20/42/62/70	0/1/1/1
26	CLA	P	606	19	-	9/39/115/115	-
26	CLA	R	305	21	-	11/33/109/115	-
26	CLA	R	313	21	-	7/17/93/115	-
38	KC2	Q	304	-	-	7/15/71/71	-
39	II0	O	613	-	-	2/21/67/67	0/2/2/2
26	CLA	S	606	22	-	11/30/106/115	-
28	WVN	Y	101	-	-	9/29/63/63	0/2/2/2
33	LMG	a	413	-	-	8/43/63/70	0/1/1/1
39	II0	6	613	-	-	4/21/67/67	0/2/2/2
26	CLA	b	601	41	-	11/21/97/115	-
39	II0	N	620	-	-	3/21/67/67	0/2/2/2
39	II0	4	320	-	-	0/21/67/67	0/2/2/2
39	II0	1	618	-	-	14/21/67/67	0/2/2/2
33	LMG	Q	318	-	-	4/38/58/70	0/1/1/1
39	II0	R	315	-	-	1/21/67/67	0/2/2/2
26	CLA	2	306	18	-	15/33/109/115	-
28	WVN	x	101	-	-	11/29/63/63	0/2/2/2
27	PHO	d	403	-	-	12/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	P	611	19	-	8/15/91/115	-
28	WVN	d	410	-	-	12/29/63/63	0/2/2/2
26	CLA	Q	301	20	-	8/39/115/115	-
30	SQD	D	401	-	-	7/49/69/69	0/1/1/1
38	KC2	2	310	18	-	7/15/71/71	-
26	CLA	5	612	21	-	7/17/93/115	-
34	LHG	5	618	26	-	11/44/44/53	-
26	CLA	2	312	18	-	10/15/91/115	-
39	II0	5	613	-	-	0/21/67/67	0/2/2/2
39	II0	Q	316	-	-	5/21/67/67	0/2/2/2
26	CLA	A	405	1	-	10/33/109/115	-
26	CLA	C	505	41	-	12/33/109/115	-
26	CLA	C	502	3	-	7/39/115/115	-
38	KC2	N	611	17	-	4/15/71/71	-
39	II0	P	614	-	-	6/21/67/67	0/2/2/2
26	CLA	C	514	3	-	11/24/100/115	-
26	CLA	S	603	22	-	11/27/103/115	-

The worst 5 of 2895 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	616	II0	C14-C10	18.08	1.55	1.34
39	2	316	II0	C14-C10	17.59	1.54	1.34
39	O	615	II0	C14-C10	17.57	1.54	1.34
40	1	619	IHT	C15-C11	17.56	1.54	1.34
39	1	618	II0	C14-C10	17.39	1.54	1.34

The worst 5 of 3570 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	617	WVN	C20-C23-C25	-27.60	84.52	126.23
28	B	618	WVN	C20-C23-C25	-26.81	85.73	126.23
28	C	516	WVN	C20-C23-C25	-26.79	85.76	126.23
39	3	312	II0	C24-C22-C10	-25.49	110.88	175.43
39	3	310	II0	C23-C21-C09	-25.28	111.43	175.43

There are no chirality outliers.

5 of 3329 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	402	CLA	C2B-C3B-CAB-CBB
26	A	402	CLA	C4B-C3B-CAB-CBB
26	A	403	CLA	C1A-C2A-CAA-CBA
26	A	403	CLA	C3A-C2A-CAA-CBA
26	A	405	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

301 monomers are involved in 1707 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	O	614	II0	6	0
26	c	515	CLA	2	0
33	2	318	LMG	5	0
28	B	618	WVN	3	0
26	2	319	CLA	26	0
38	N	612	KC2	28	0
26	O	606	CLA	4	0
26	a	402	CLA	11	0
39	6	611	II0	1	0
38	1	611	KC2	3	0
26	O	609	CLA	1	0
39	4	314	II0	6	0
26	G	401	CLA	7	0
26	N	613	CLA	3	0
26	5	611	CLA	35	0
26	D	408	CLA	1	0
39	P	613	II0	6	0
28	H	101	WVN	1	0
26	6	606	CLA	4	0
26	P	609	CLA	1	0
26	2	304	CLA	4	0
26	5	609	CLA	2	0
34	1	620	LHG	48	0
38	O	610	KC2	7	0
26	4	307	CLA	8	0
33	D	411	LMG	2	0
26	c	508	CLA	4	0
26	5	604	CLA	4	0
34	2	321	LHG	23	0
39	5	614	II0	1	0
26	1	609	CLA	5	0
28	B	617	WVN	3	0
26	C	506	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	5	605	CLA	31	0
26	S	607	CLA	2	0
26	5	607	CLA	7	0
26	B	606	CLA	4	0
26	N	601	CLA	24	0
26	1	606	CLA	42	0
29	D	409	PL9	3	0
26	6	602	CLA	1	0
26	6	605	CLA	5	0
26	4	303	CLA	36	0
39	N	617	II0	5	0
26	2	303	CLA	19	0
26	b	613	CLA	8	0
26	3	303	CLA	5	0
38	P	605	KC2	1	0
26	N	606	CLA	21	0
26	D	404	CLA	3	0
34	C	518	LHG	3	0
26	4	308	CLA	12	0
26	6	610	CLA	6	0
26	P	602	CLA	8	0
39	R	314	II0	2	0
26	3	302	CLA	9	0
38	4	311	KC2	20	0
28	3	313	WVN	21	0
26	N	614	CLA	26	0
26	c	510	CLA	3	0
33	d	404	LMG	4	0
26	d	406	CLA	1	0
35	H	102	DGD	4	0
34	c	520	LHG	1	0
26	C	508	CLA	3	0
39	2	320	II0	4	0
26	b	616	CLA	2	0
39	O	618	II0	2	0
26	3	309	CLA	2	0
26	G	402	CLA	1	0
34	N	621	LHG	26	0
26	2	311	CLA	47	0
34	R	319	LHG	12	0
26	B	610	CLA	7	0
26	P	610	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	4	301	CLA	31	0
33	b	620	LMG	1	0
26	B	614	CLA	2	0
26	R	304	CLA	1	0
26	1	603	CLA	8	0
40	O	616	IHT	9	0
26	Q	305	CLA	6	0
40	Q	317	IHT	4	0
39	2	313	II0	6	0
26	S	604	CLA	5	0
26	1	607	CLA	2	0
26	4	306	CLA	45	0
39	3	312	II0	8	0
26	O	611	CLA	12	0
33	D	406	LMG	4	0
26	6	603	CLA	2	0
38	1	612	KC2	1	0
26	S	602	CLA	2	0
26	5	602	CLA	6	0
26	2	309	CLA	1	0
26	S	610	CLA	4	0
26	d	405	CLA	8	0
26	O	602	CLA	8	0
26	B	603	CLA	3	0
26	b	604	CLA	3	0
26	1	604	CLA	3	0
26	c	509	CLA	3	0
26	c	503	CLA	2	0
40	5	616	IHT	1	0
37	F	101	HEM	2	0
35	c	519	DGD	2	0
26	O	601	CLA	25	0
34	G	403	LHG	11	0
39	N	618	II0	2	0
38	N	605	KC2	6	0
26	R	302	CLA	6	0
26	N	603	CLA	13	0
39	O	615	II0	8	0
26	6	604	CLA	5	0
38	R	311	KC2	3	0
26	a	405	CLA	3	0
26	b	611	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	601	CLA	10	0
26	c	512	CLA	6	0
26	2	308	CLA	12	0
39	3	310	II0	26	0
26	B	611	CLA	4	0
26	b	609	CLA	4	0
28	P	615	WVN	3	0
40	1	619	IHT	1	0
40	N	619	IHT	16	0
38	3	304	KC2	1	0
26	B	607	CLA	2	0
26	2	305	CLA	14	0
26	b	602	CLA	3	0
26	N	607	CLA	19	0
26	Q	308	CLA	10	0
40	R	317	IHT	4	0
30	A	408	SQD	1	0
26	b	607	CLA	2	0
26	2	302	CLA	10	0
26	C	513	CLA	2	0
27	A	404	PHO	2	0
28	b	617	WVN	1	0
26	4	304	CLA	1	0
26	P	604	CLA	3	0
26	4	309	CLA	8	0
26	R	312	CLA	6	0
26	B	613	CLA	6	0
33	c	521	LMG	6	0
38	4	305	KC2	6	0
26	A	403	CLA	2	0
26	b	608	CLA	1	0
33	O	617	LMG	5	0
26	B	601	CLA	1	0
34	D	410	LHG	5	0
26	c	505	CLA	4	0
26	3	306	CLA	6	0
33	d	411	LMG	2	0
26	B	616	CLA	1	0
26	g	402	CLA	18	0
26	R	303	CLA	9	0
33	A	412	LMG	1	0
26	N	608	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	2	316	II0	5	0
26	S	605	CLA	5	0
39	3	311	II0	26	0
38	Q	309	KC2	12	0
39	4	317	II0	4	0
39	Q	313	II0	7	0
26	C	512	CLA	3	0
26	R	310	CLA	2	0
26	O	612	CLA	3	0
26	S	609	CLA	9	0
33	m	101	LMG	2	0
26	O	605	CLA	13	0
39	Q	314	II0	4	0
39	S	611	II0	11	0
38	Q	310	KC2	21	0
26	1	614	CLA	4	0
26	R	308	CLA	11	0
40	4	318	IHT	5	0
34	D	403	LHG	7	0
39	R	316	II0	4	0
26	O	608	CLA	15	0
26	P	603	CLA	5	0
26	5	603	CLA	1	0
26	4	302	CLA	11	0
26	b	612	CLA	8	0
26	2	307	CLA	13	0
26	b	605	CLA	7	0
26	C	507	CLA	4	0
29	A	407	PL9	6	0
30	c	501	SQD	1	0
27	D	405	PHO	5	0
26	4	312	CLA	10	0
33	R	301	LMG	9	0
33	M	101	LMG	1	0
26	B	605	CLA	8	0
38	1	610	KC2	1	0
26	N	609	CLA	4	0
33	d	409	LMG	2	0
26	3	308	CLA	8	0
26	B	615	CLA	3	0
26	O	604	CLA	2	0
26	Q	302	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	d	408	LHG	5	0
27	a	404	PHO	2	0
26	3	305	CLA	7	0
26	B	609	CLA	5	0
38	5	610	KC2	3	0
26	O	607	CLA	19	0
26	Q	311	CLA	9	0
38	4	310	KC2	12	0
39	2	314	II0	5	0
26	N	604	CLA	16	0
33	C	520	LMG	3	0
26	d	402	CLA	4	0
34	l	101	LHG	5	0
26	c	504	CLA	5	0
39	4	315	II0	9	0
26	6	601	CLA	8	0
33	c	522	LMG	2	0
39	2	315	II0	13	0
26	c	513	CLA	1	0
26	b	614	CLA	3	0
26	N	602	CLA	7	0
28	C	516	WVN	2	0
26	B	604	CLA	3	0
39	Q	319	II0	10	0
35	C	517	DGD	1	0
39	N	615	II0	5	0
33	B	620	LMG	2	0
37	f	101	HEM	1	0
26	S	601	CLA	6	0
26	5	608	CLA	10	0
26	B	612	CLA	7	0
34	L	101	LHG	7	0
26	B	602	CLA	3	0
26	3	307	CLA	43	0
26	g	401	CLA	7	0
26	5	601	CLA	6	0
26	P	607	CLA	3	0
26	C	511	CLA	6	0
26	B	608	CLA	1	0
26	P	608	CLA	5	0
26	c	507	CLA	2	0
39	5	615	II0	4	0

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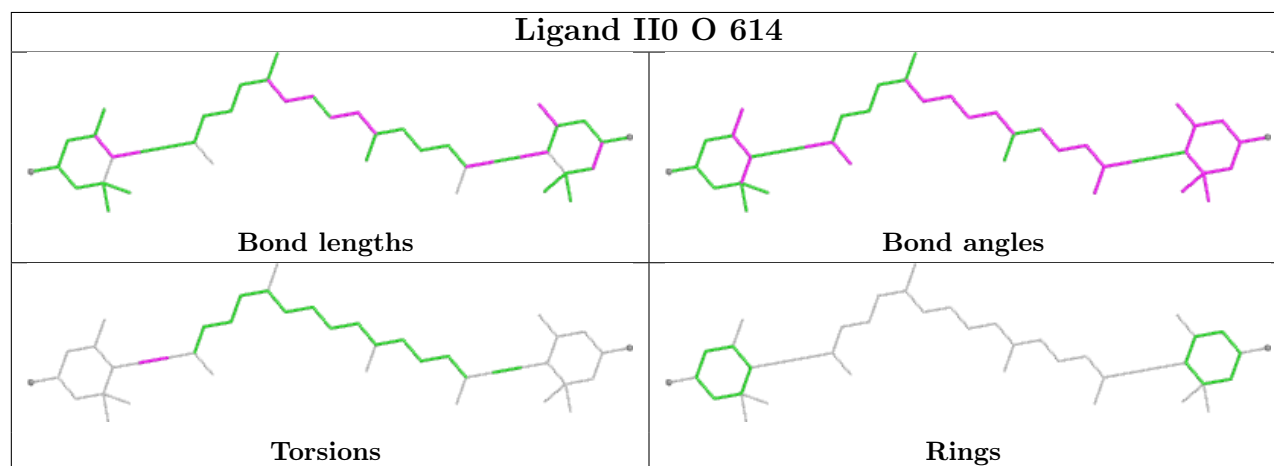
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26	3	301	CLA	12	0
26	D	407	CLA	7	0
35	h	101	DGD	6	0
26	b	610	CLA	5	0
26	b	615	CLA	6	0
26	b	606	CLA	5	0
33	D	413	LMG	1	0
34	b	621	LHG	2	0
26	Q	306	CLA	8	0
26	A	402	CLA	10	0
26	O	603	CLA	15	0
26	c	514	CLA	2	0
33	5	619	LMG	20	0
26	6	609	CLA	24	0
26	R	309	CLA	10	0
38	N	610	KC2	5	0
26	Q	303	CLA	1	0
26	R	306	CLA	21	0
26	2	301	CLA	31	0
26	C	509	CLA	3	0
26	C	503	CLA	4	0
26	a	403	CLA	4	0
40	2	317	IHT	21	0
39	P	612	II0	3	0
26	Q	307	CLA	9	0
26	b	603	CLA	3	0
26	1	608	CLA	5	0
26	C	504	CLA	4	0
39	N	616	II0	16	0
29	d	407	PL9	3	0
26	P	606	CLA	5	0
26	R	305	CLA	4	0
38	Q	304	KC2	6	0
39	O	613	II0	12	0
26	S	606	CLA	4	0
33	a	413	LMG	3	0
26	b	601	CLA	1	0
39	N	620	II0	11	0
39	4	320	II0	29	0
39	1	618	II0	1	0
33	Q	318	LMG	2	0

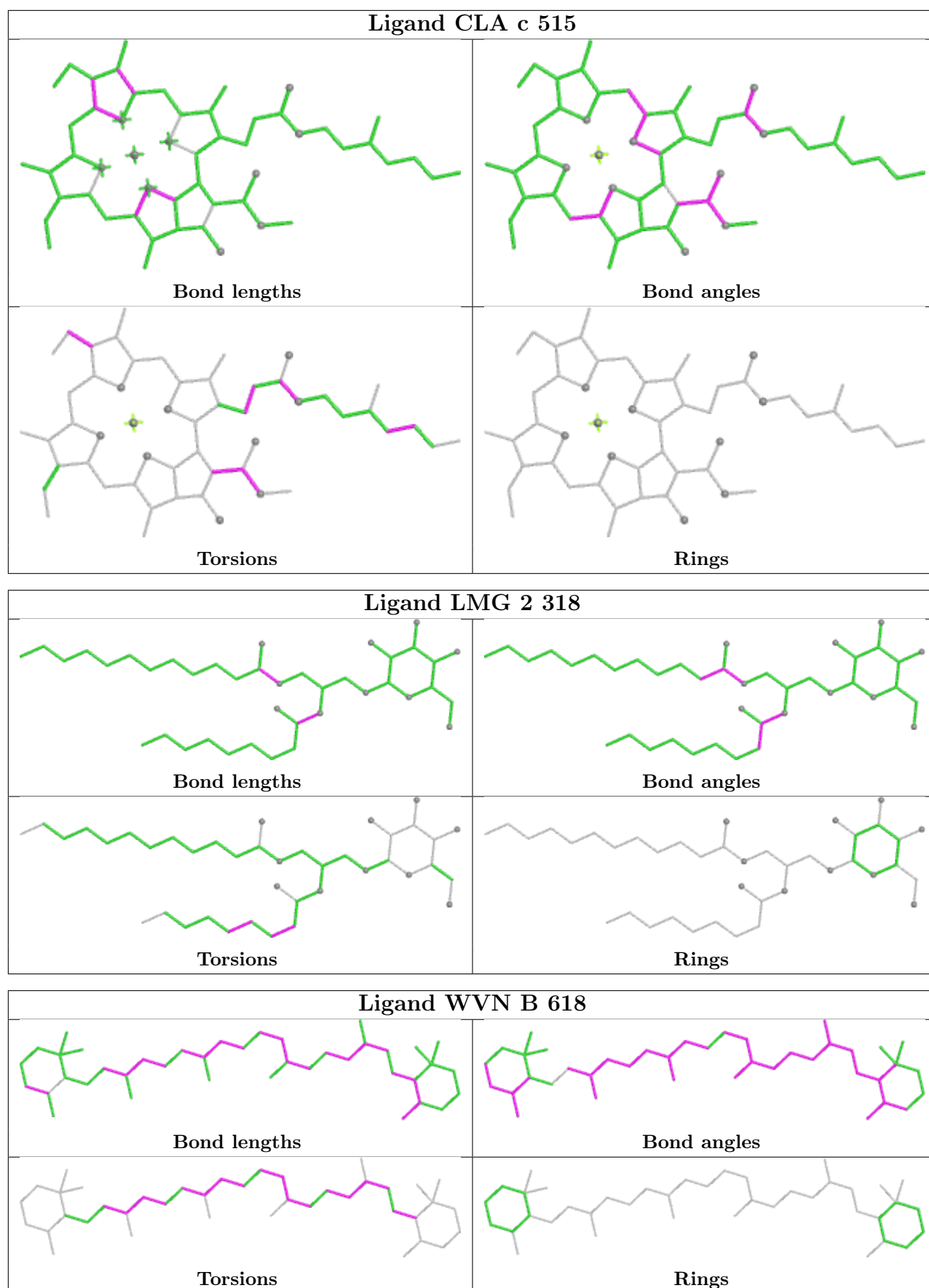
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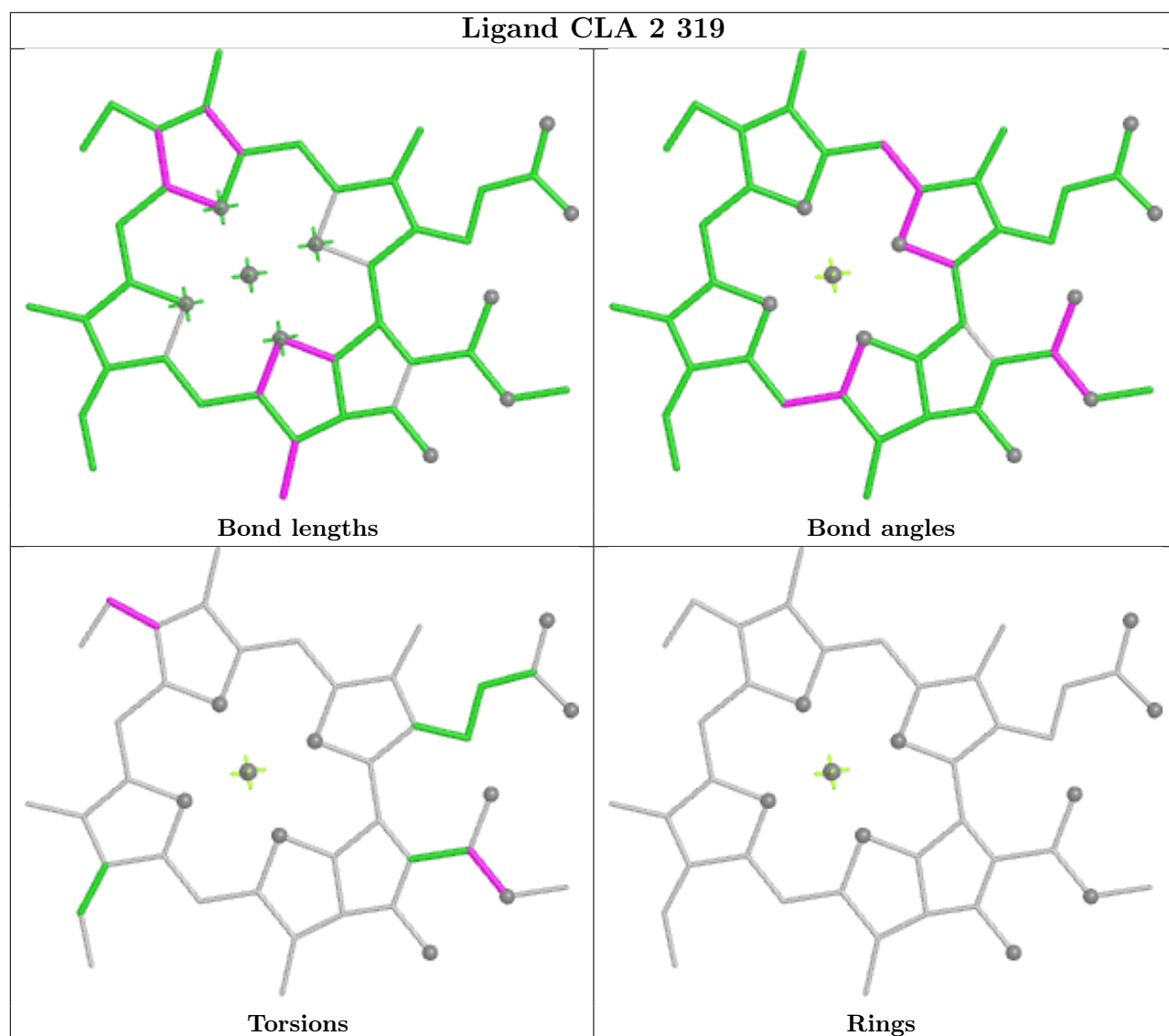
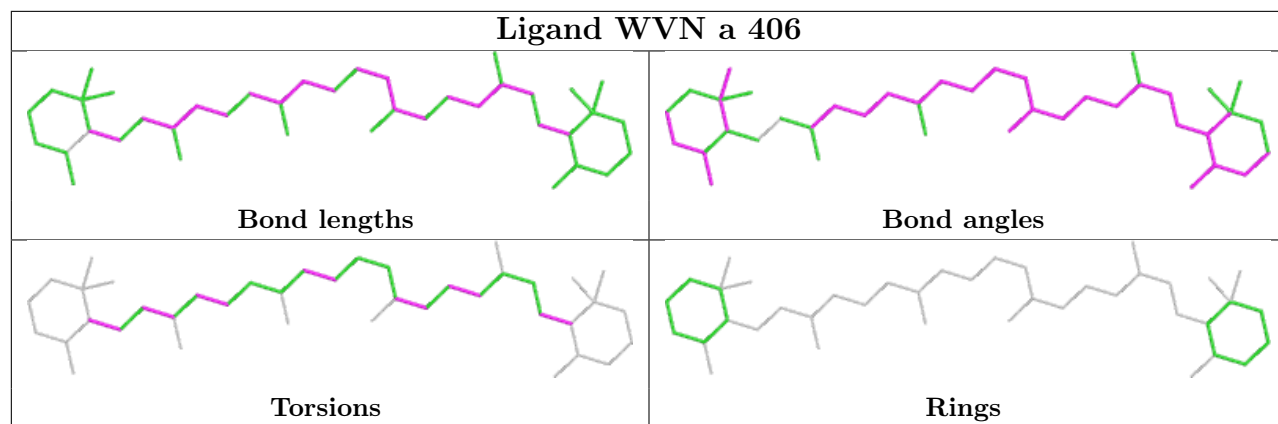
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	R	315	II0	1	0
26	2	306	CLA	4	0
27	d	403	PHO	5	0
26	P	611	CLA	3	0
26	Q	301	CLA	11	0
30	D	401	SQD	2	0
38	2	310	KC2	7	0
34	5	618	LHG	8	0
26	2	312	CLA	6	0
39	5	613	II0	2	0
39	Q	316	II0	5	0
26	A	405	CLA	2	0
26	C	502	CLA	1	0
39	P	614	II0	4	0
26	C	514	CLA	2	0
26	S	603	CLA	2	0

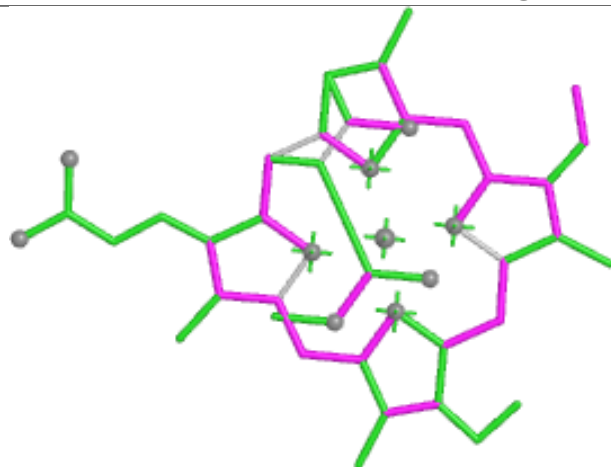
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



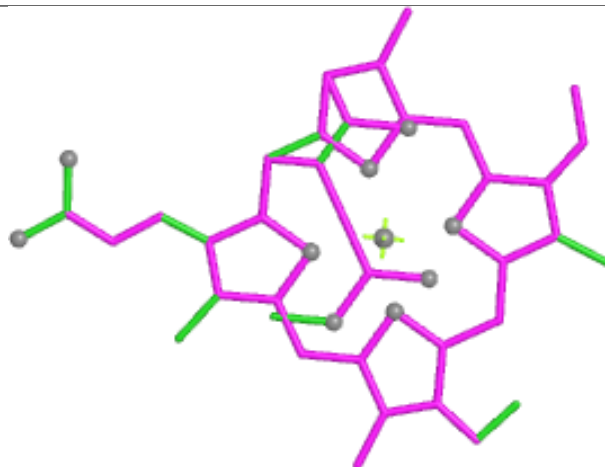




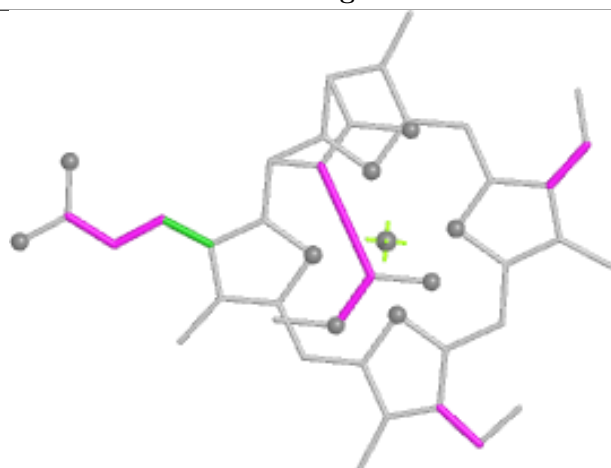
Ligand KC2 N 612



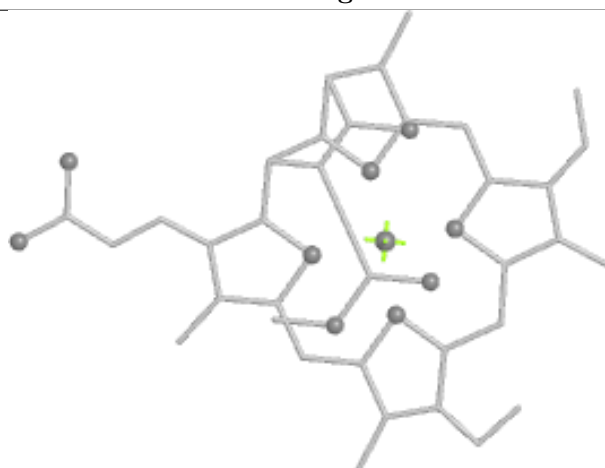
Bond lengths



Bond angles

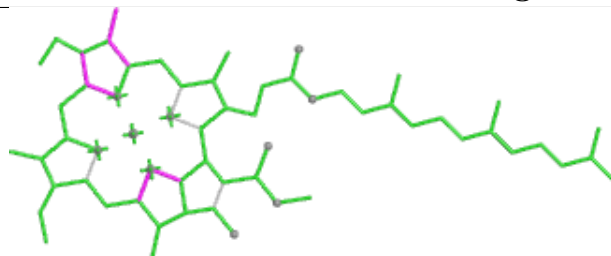


Torsions

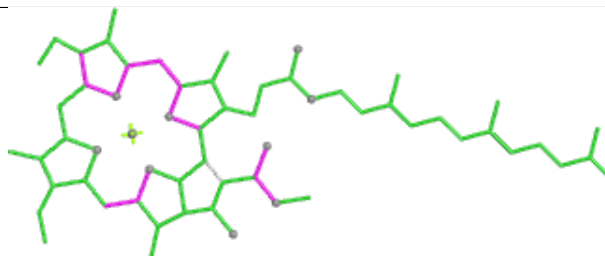


Rings

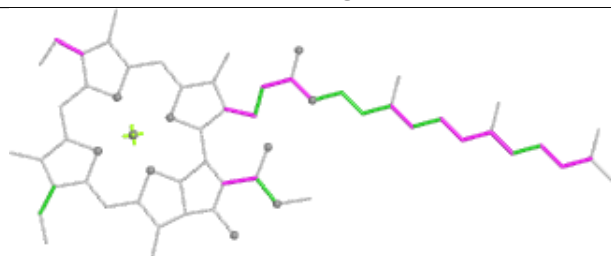
Ligand CLA O 606



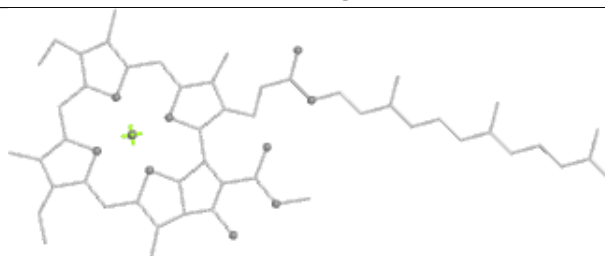
Bond lengths



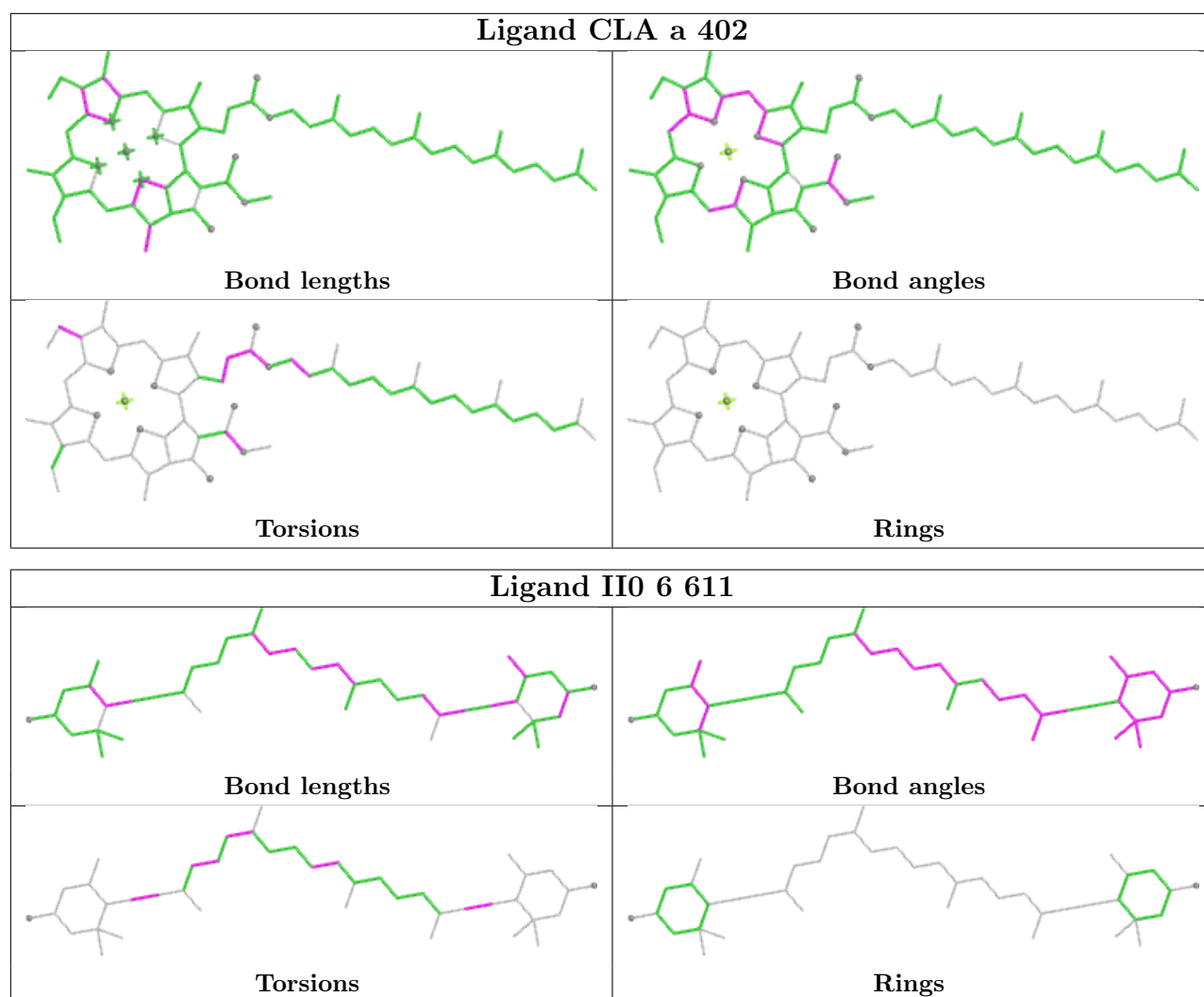
Bond angles



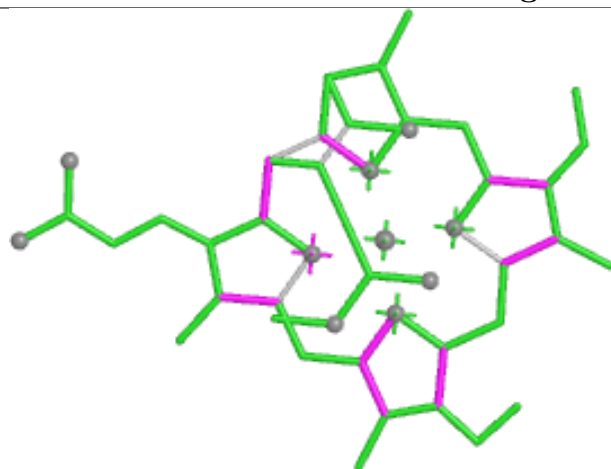
Torsions



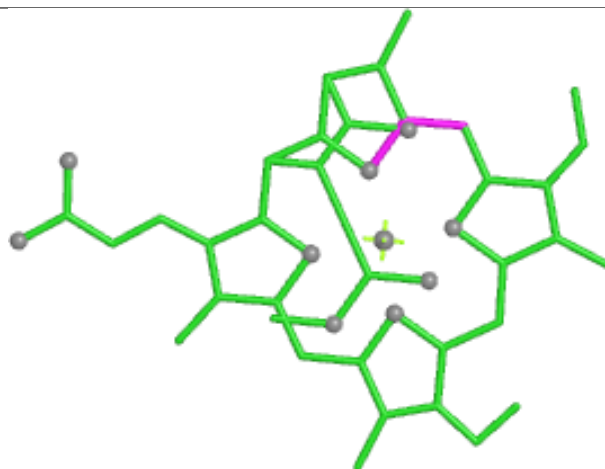
Rings



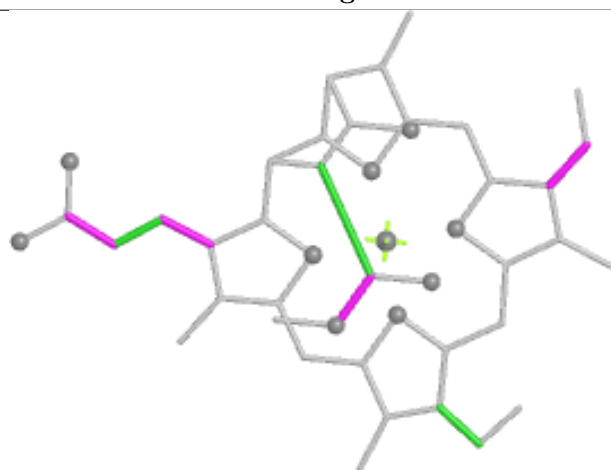
Ligand KC2 1 611



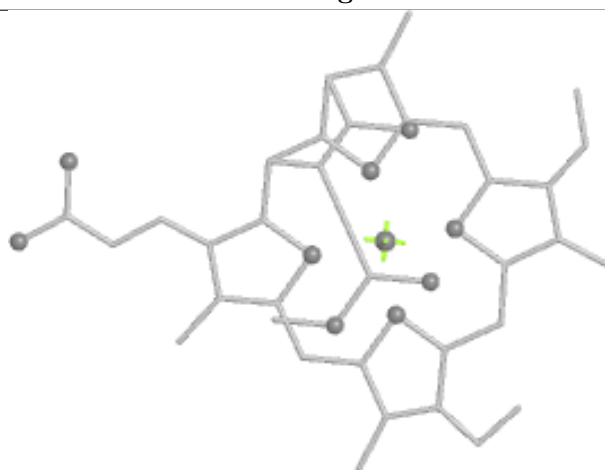
Bond lengths



Bond angles

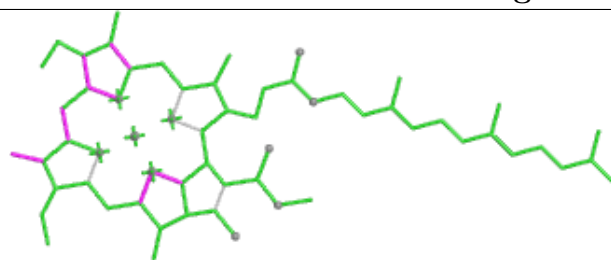


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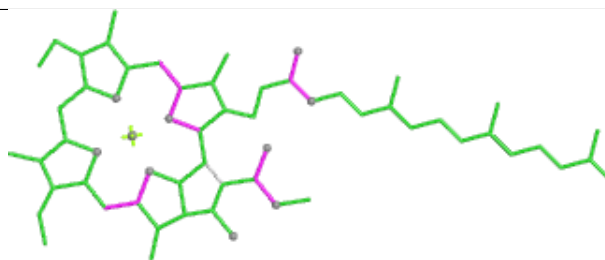


Rings

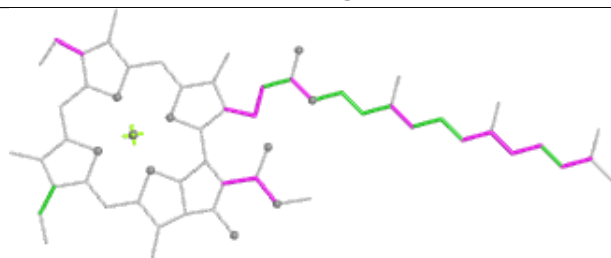
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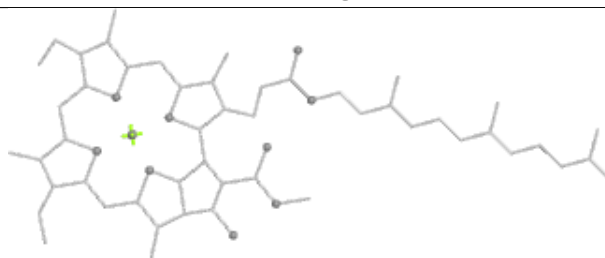
Bond lengths



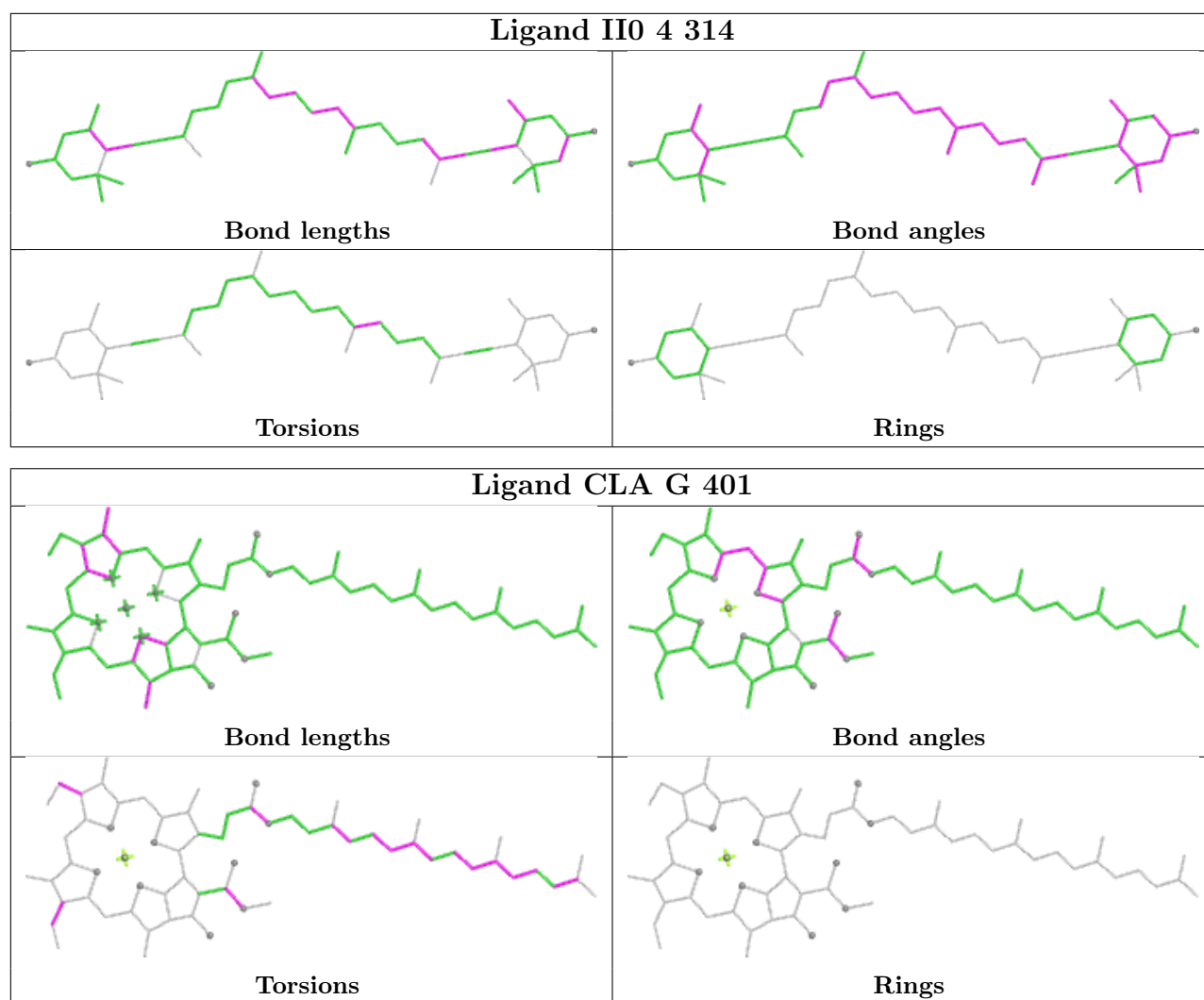
Bond angles



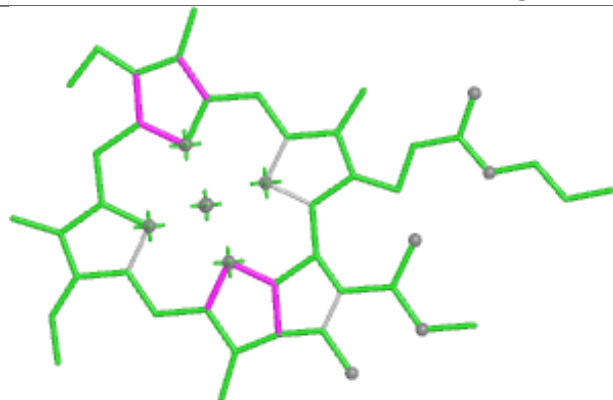
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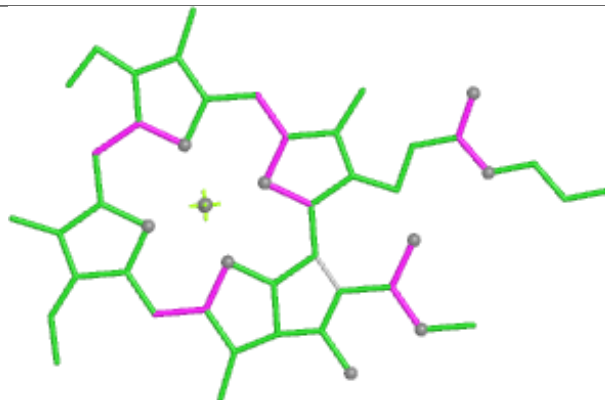
Rings



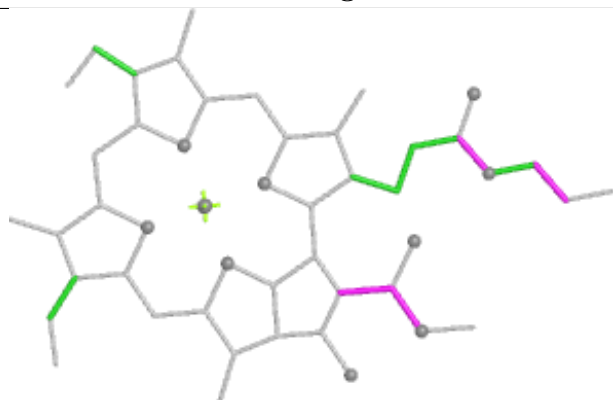
Ligand CLA N 613



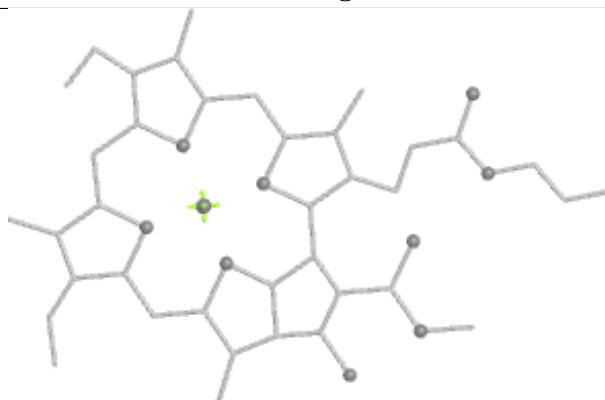
Bond lengths



Bond angles

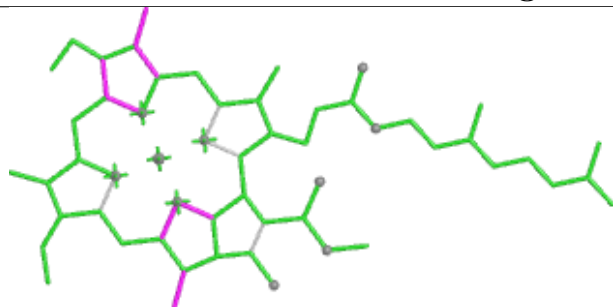


Torsions

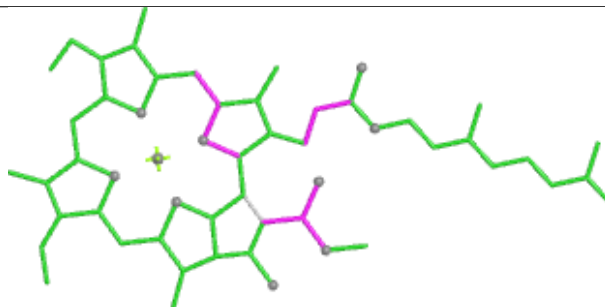


Rings

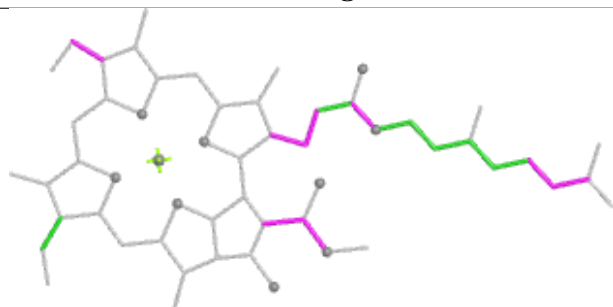
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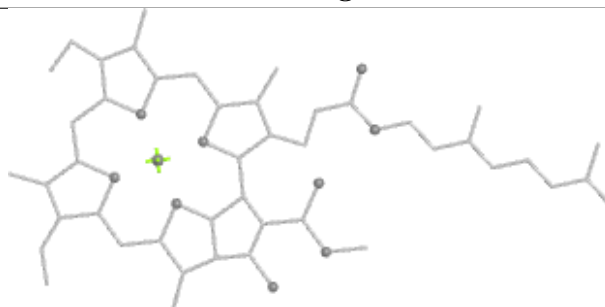
Bond lengths



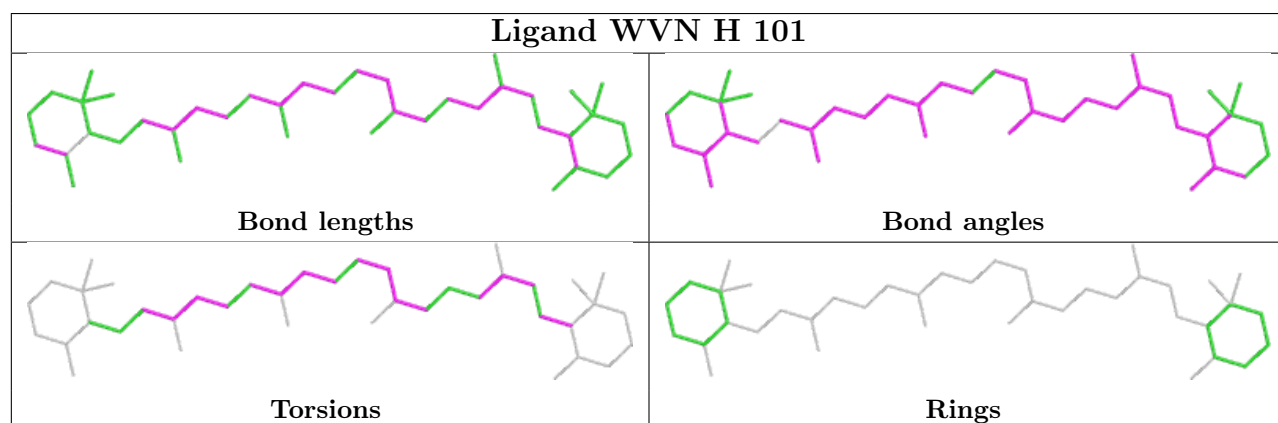
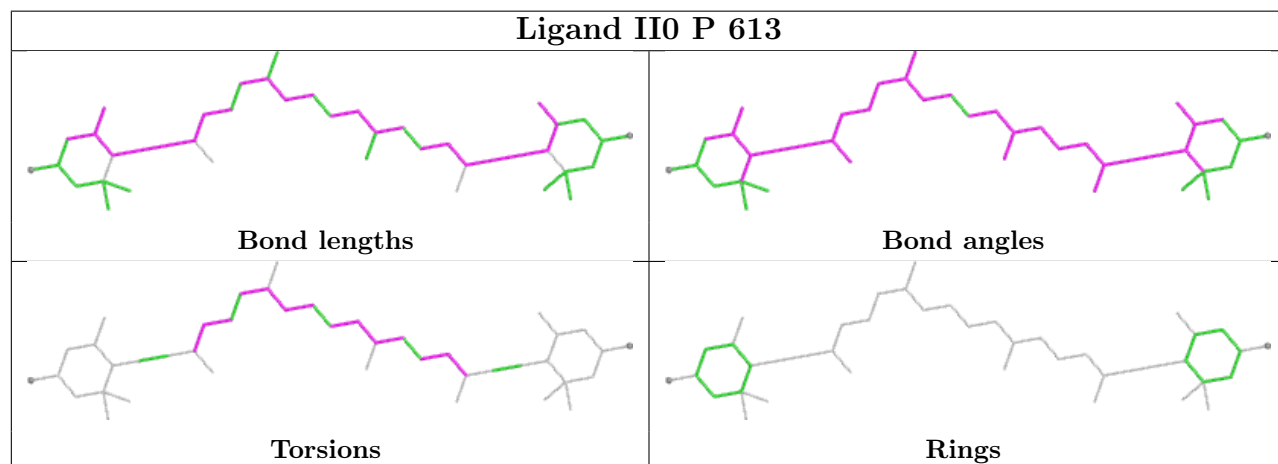
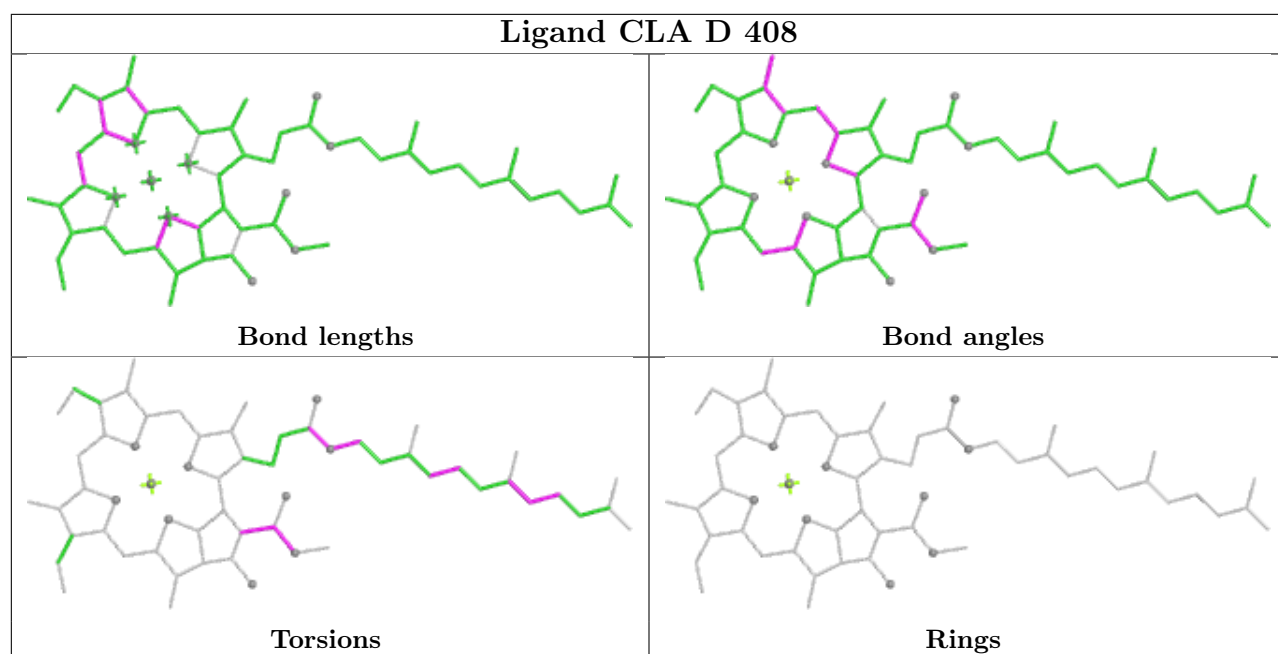
Bond angles

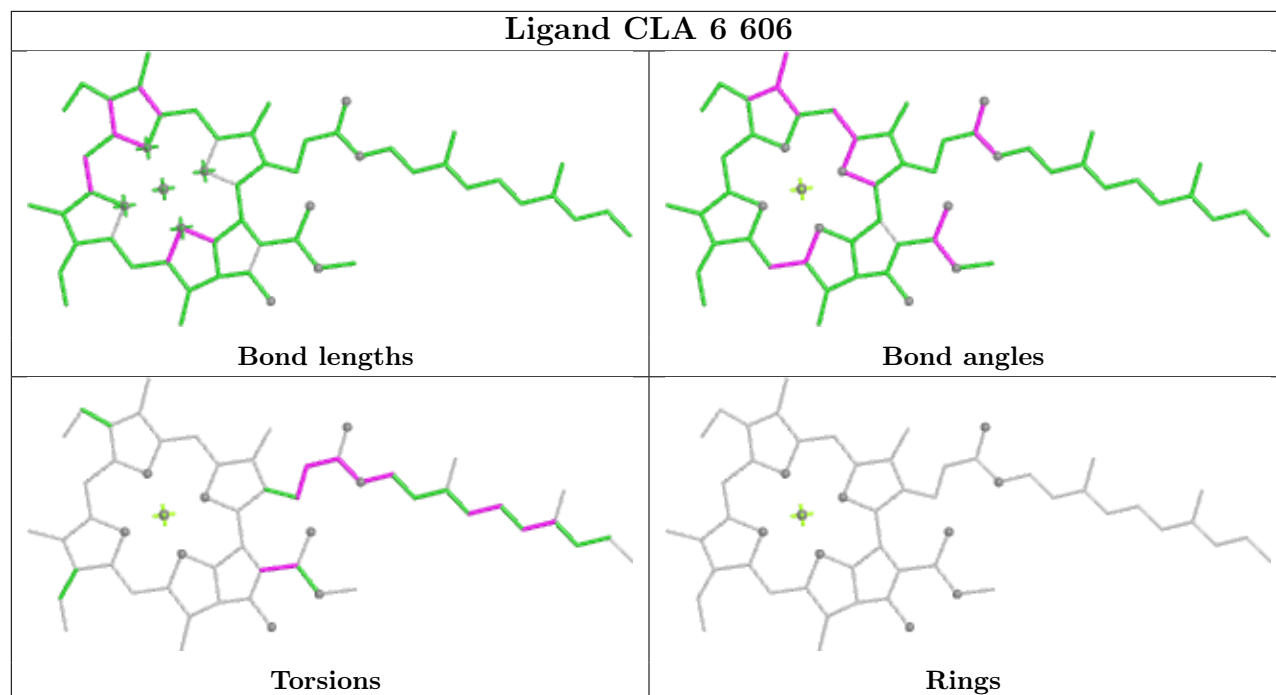
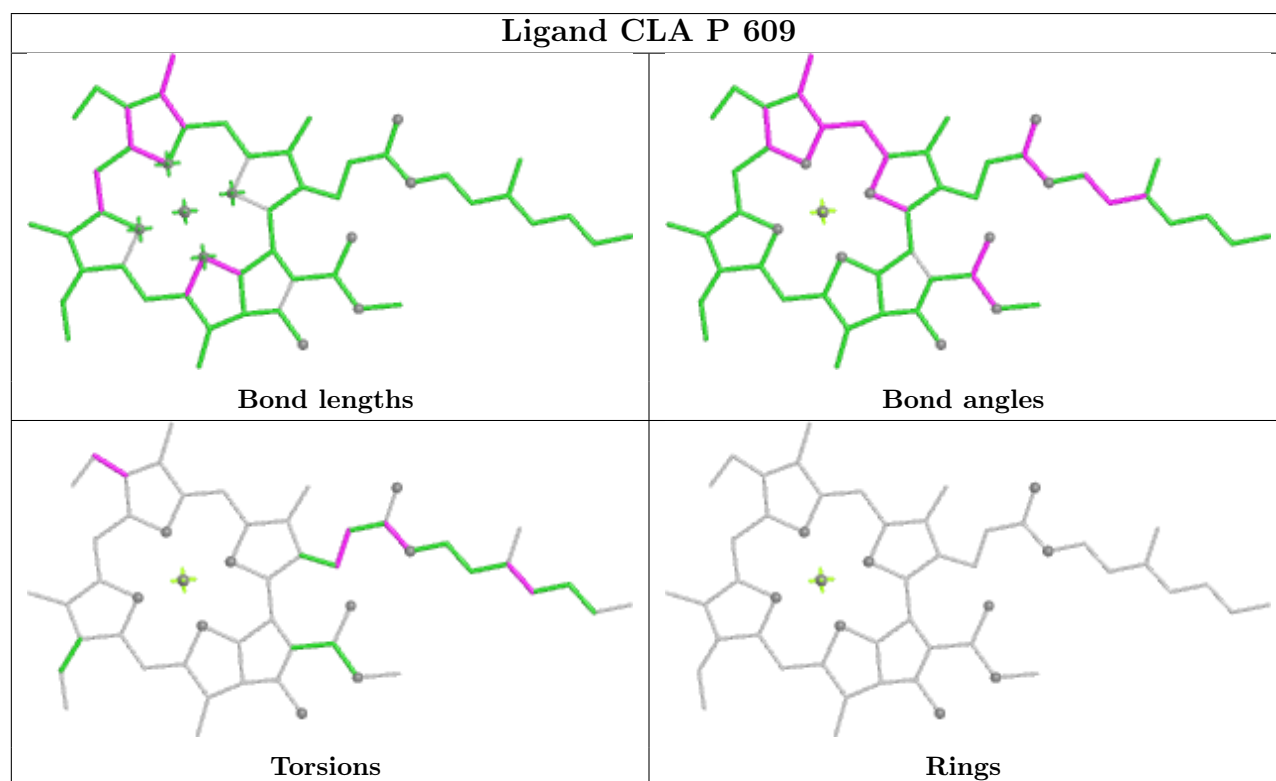


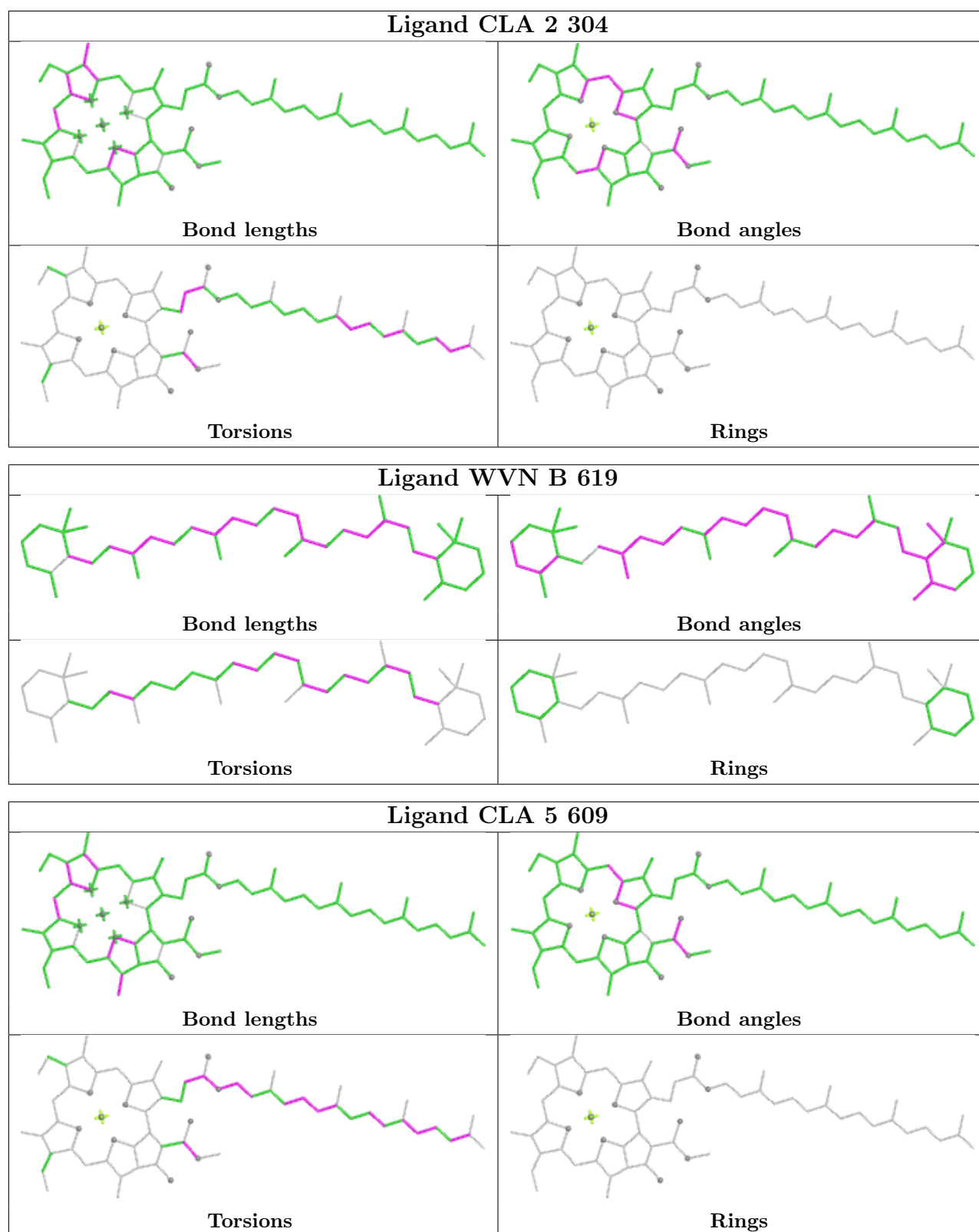
Torsions

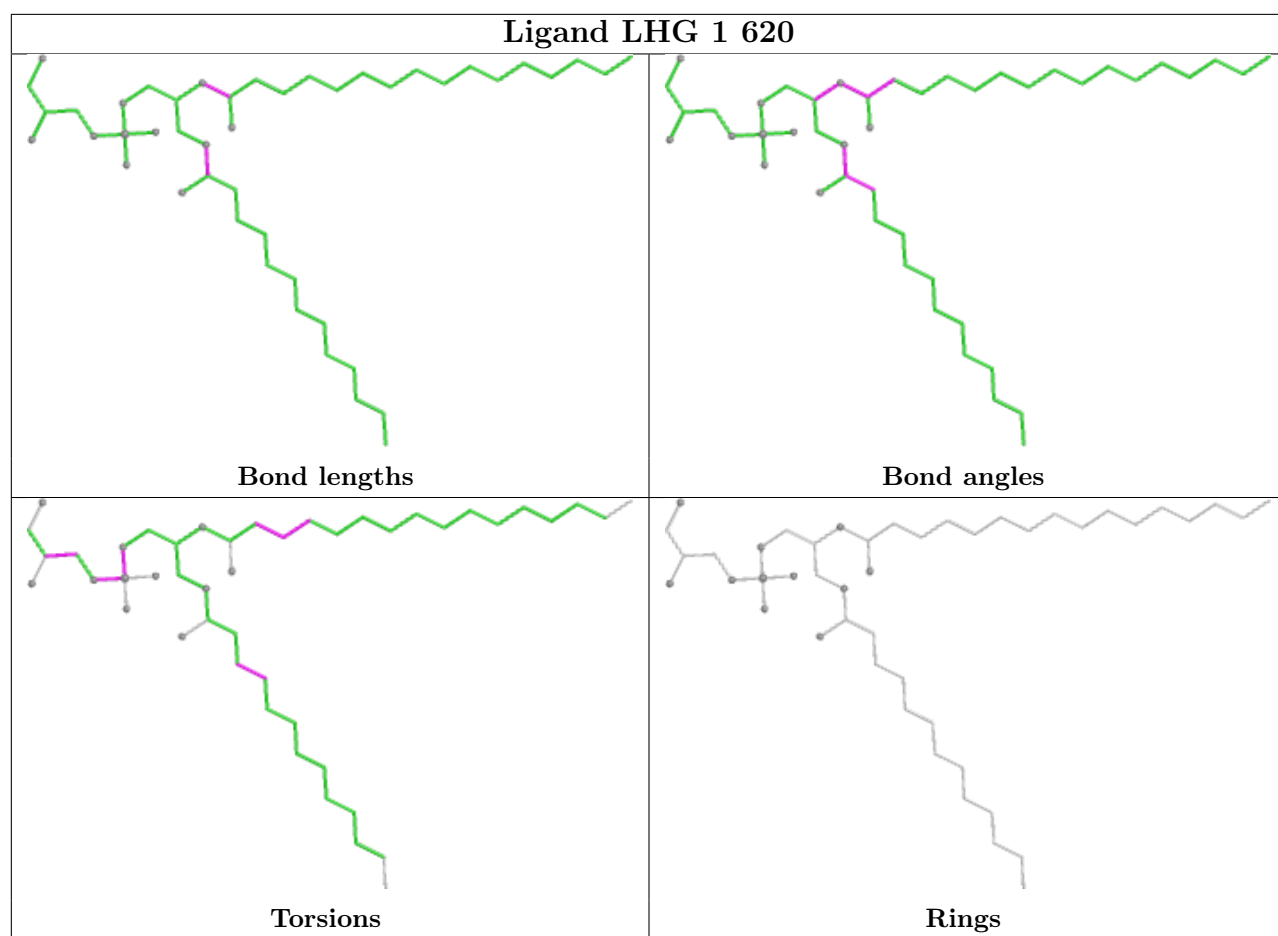


Rings

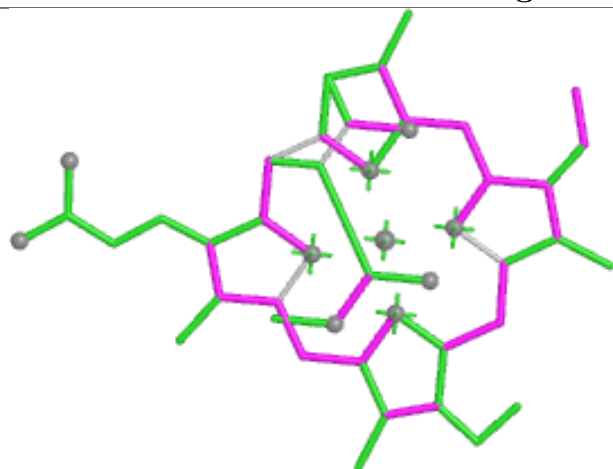


Ligand CLA 6 606**Ligand CLA P 609**

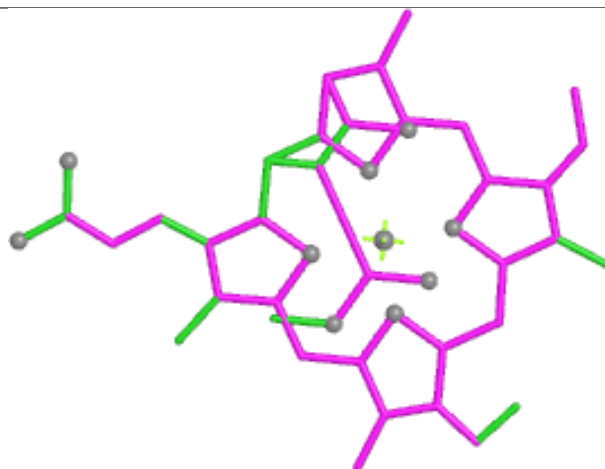




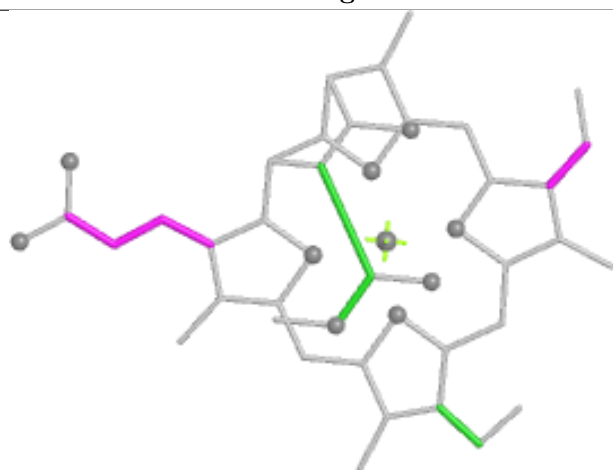
Ligand KC2 O 610



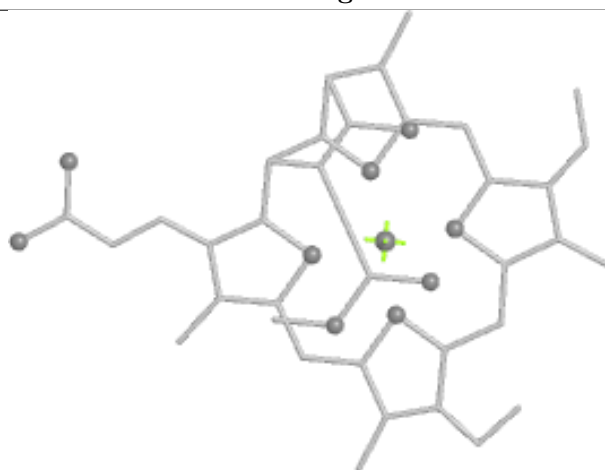
Bond lengths



Bond angles

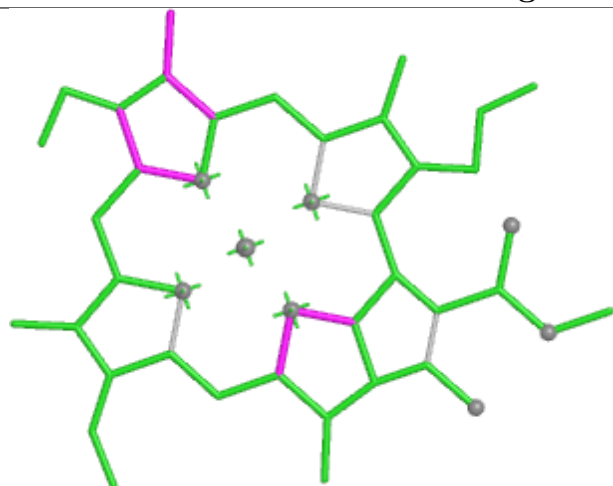


Torsions

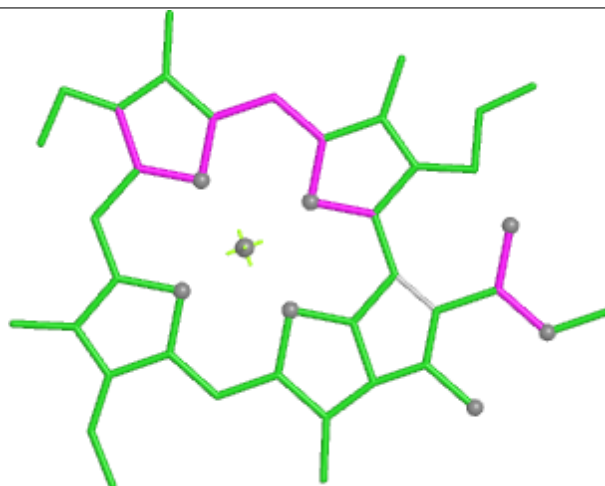


Rings

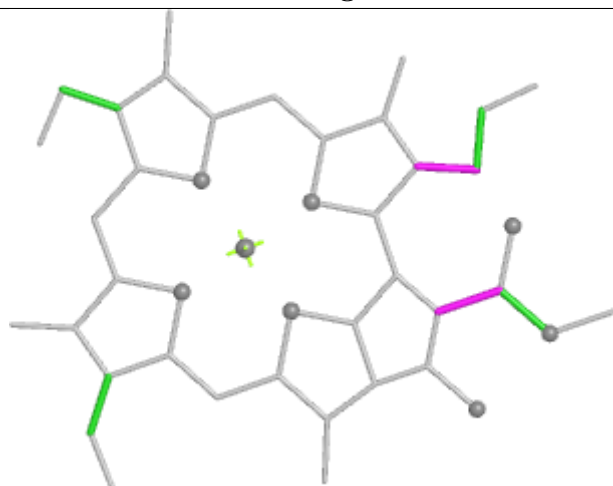
Ligand CLA 4 307



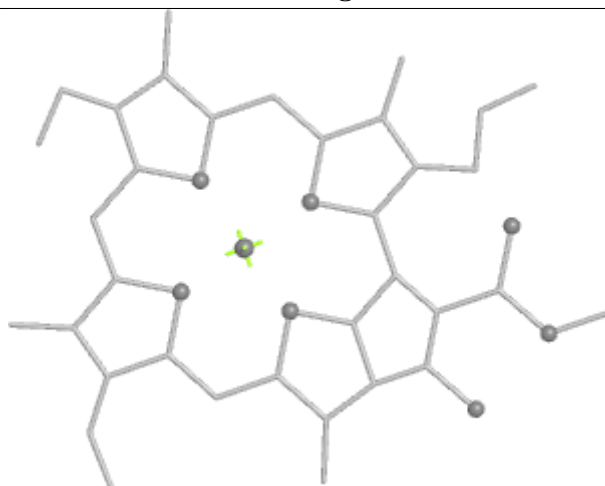
Bond lengths



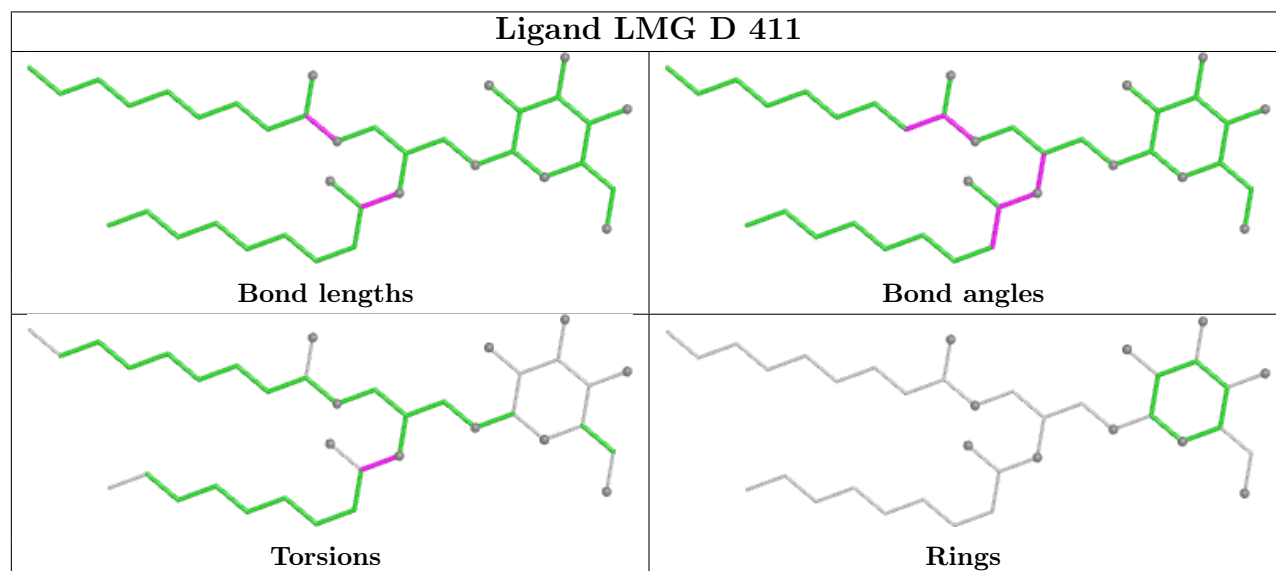
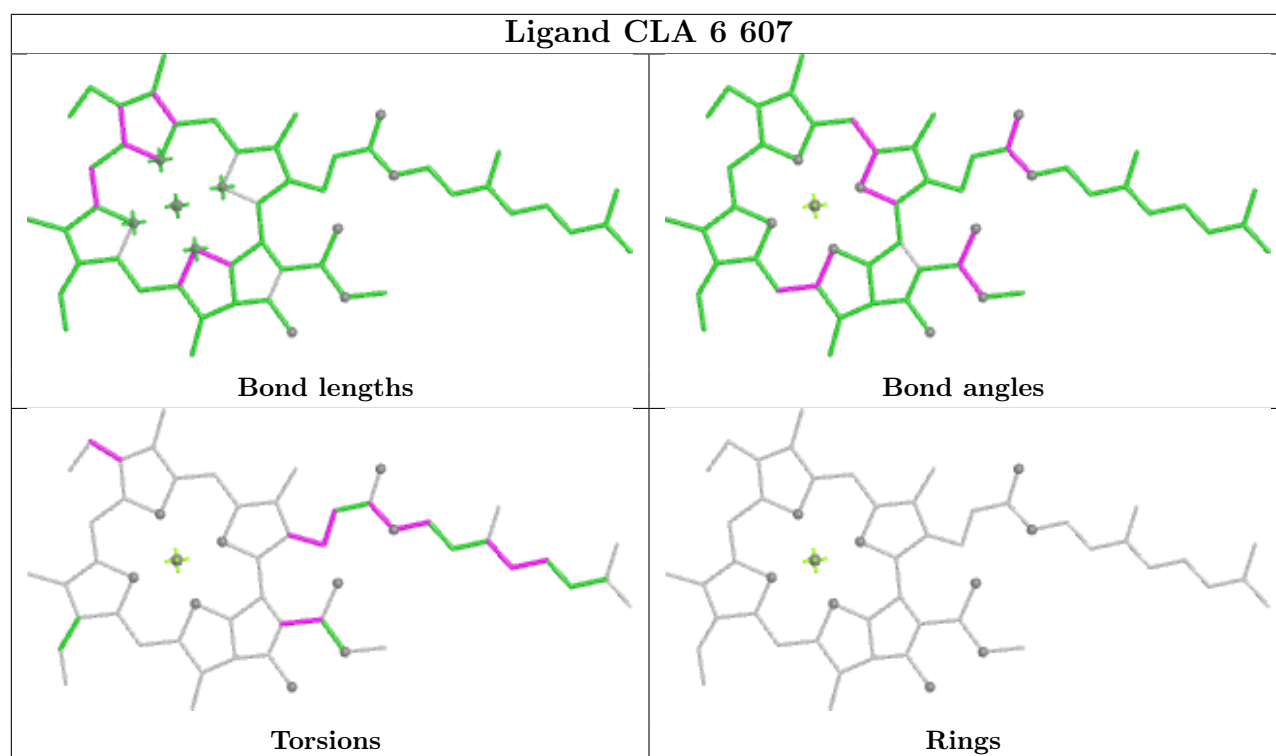
Bond angles

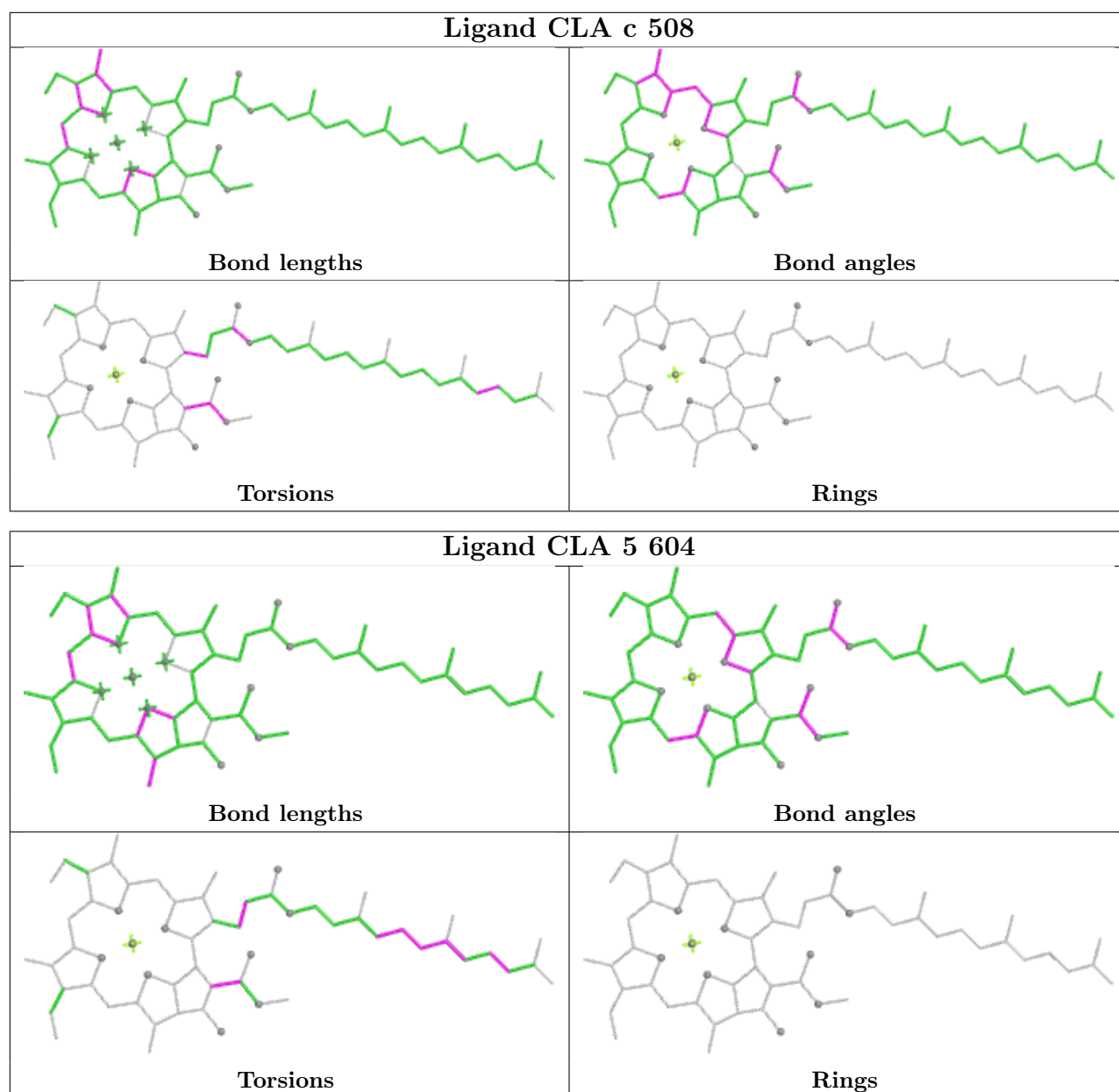


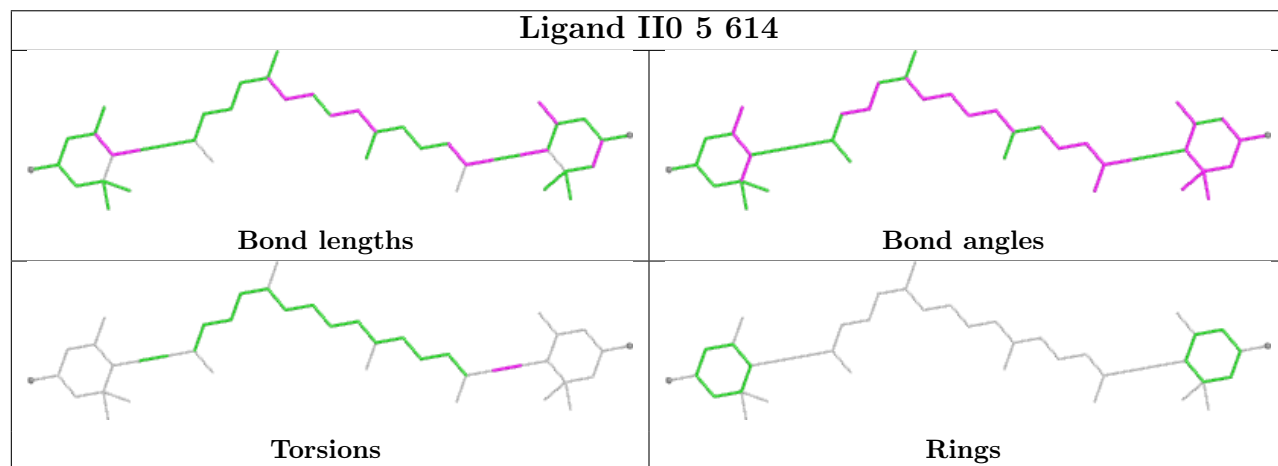
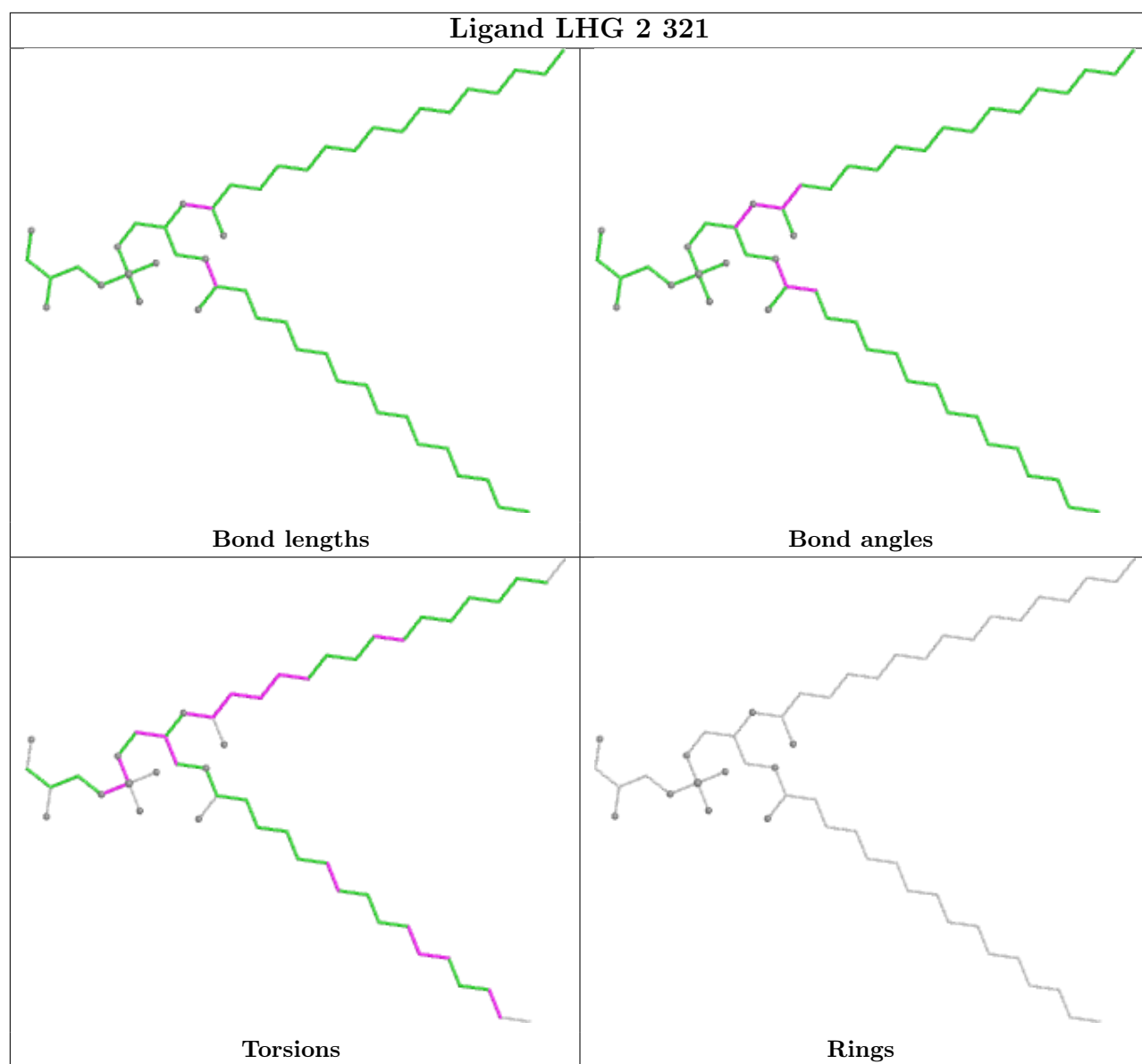
Torsions

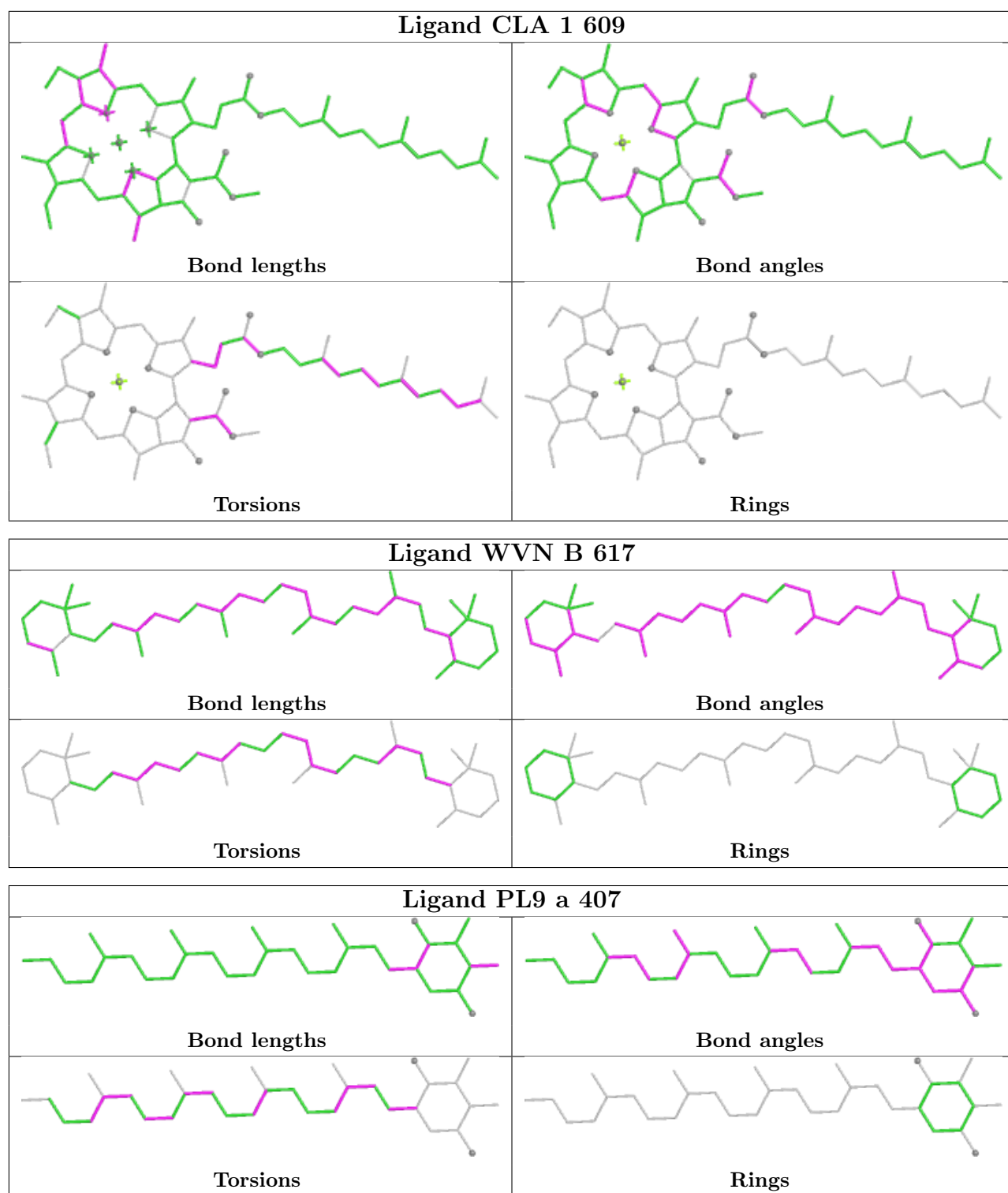


Rings

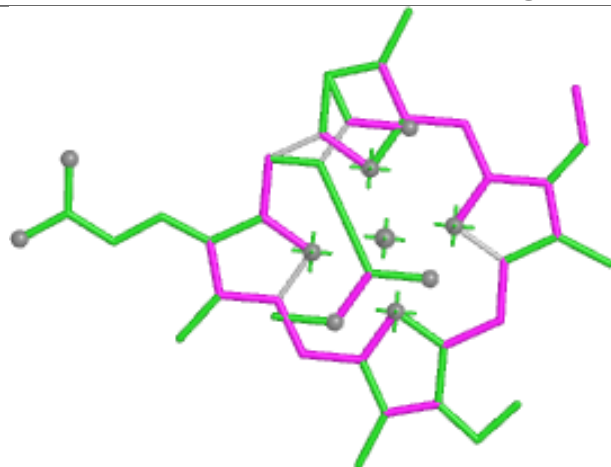




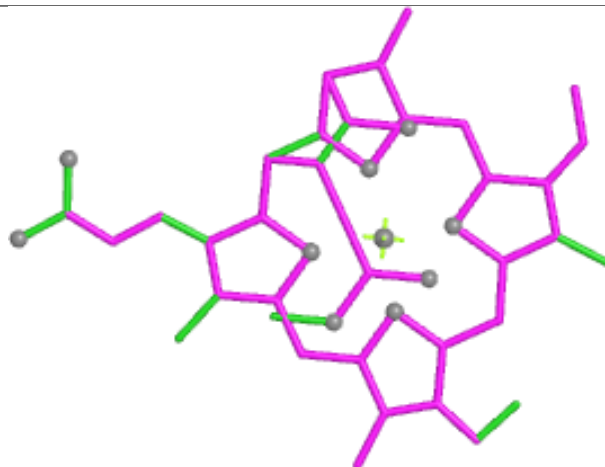




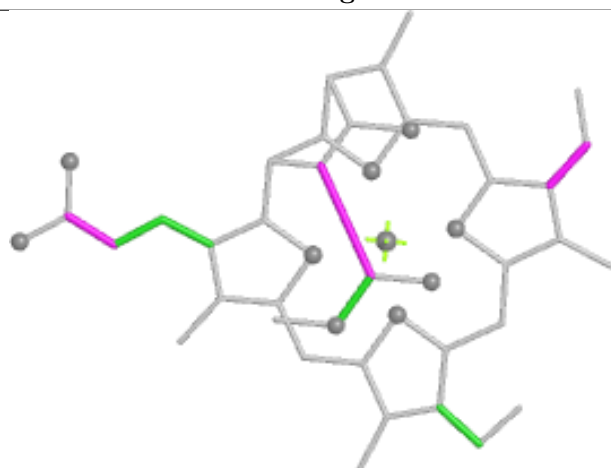
Ligand KC2 6 608



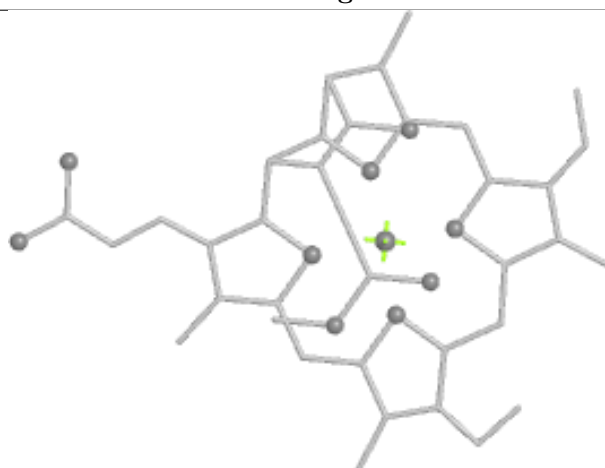
Bond lengths



Bond angles

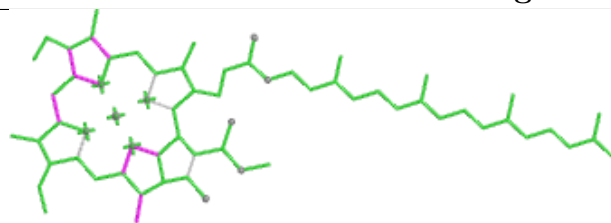


Torsions

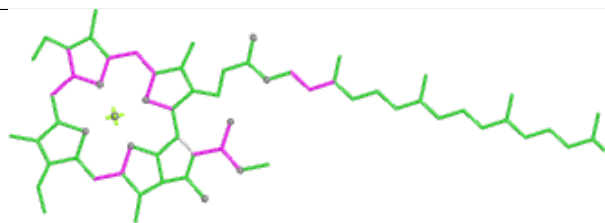


Rings

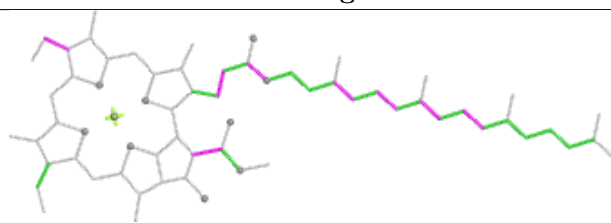
Ligand CLA C 506



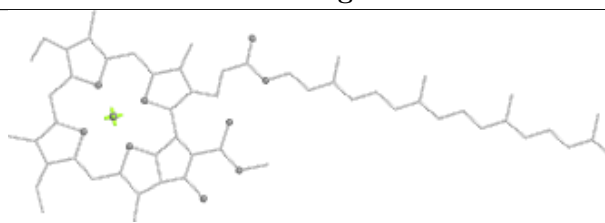
Bond lengths



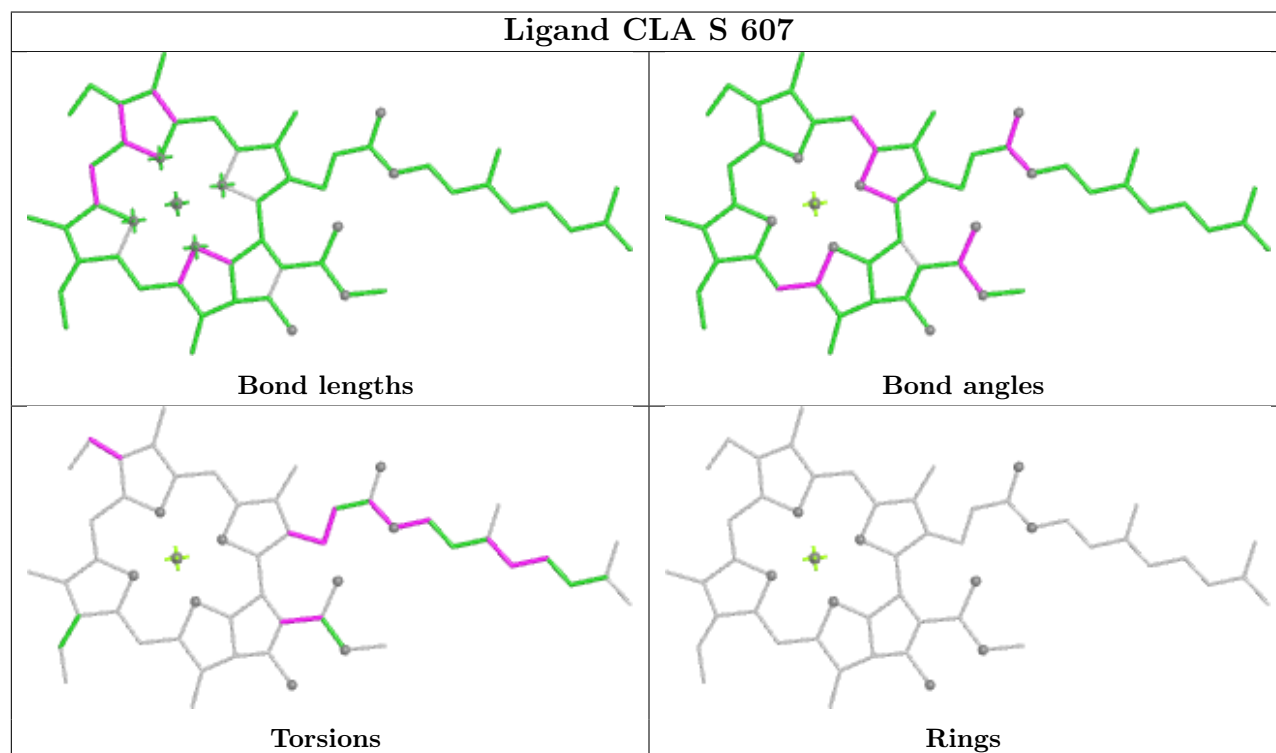
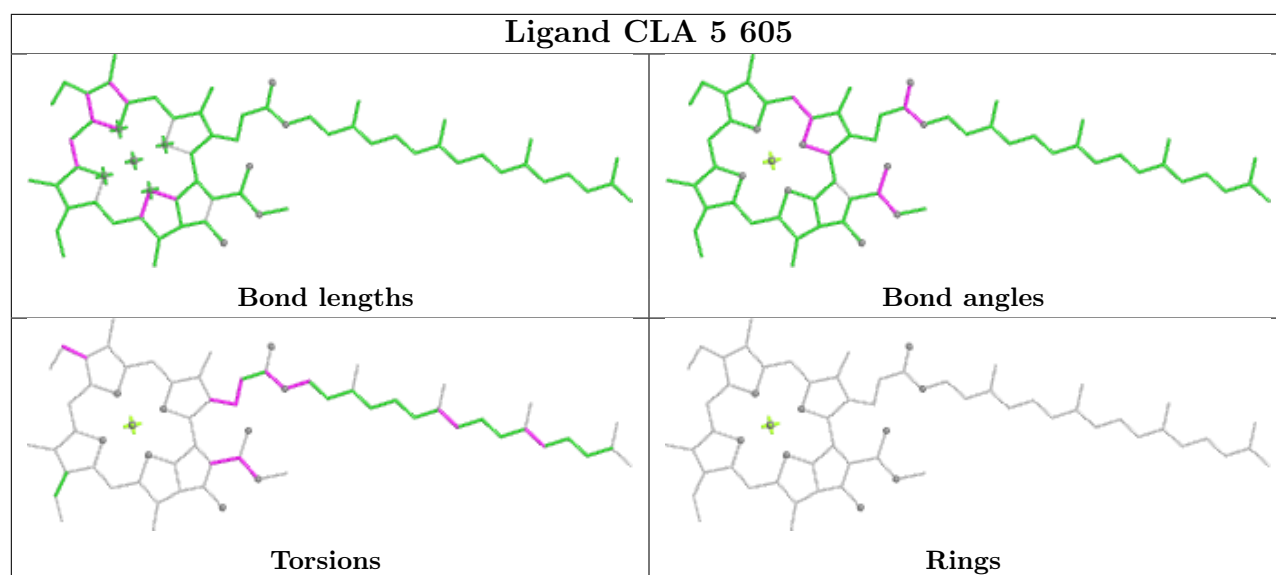
Bond angles

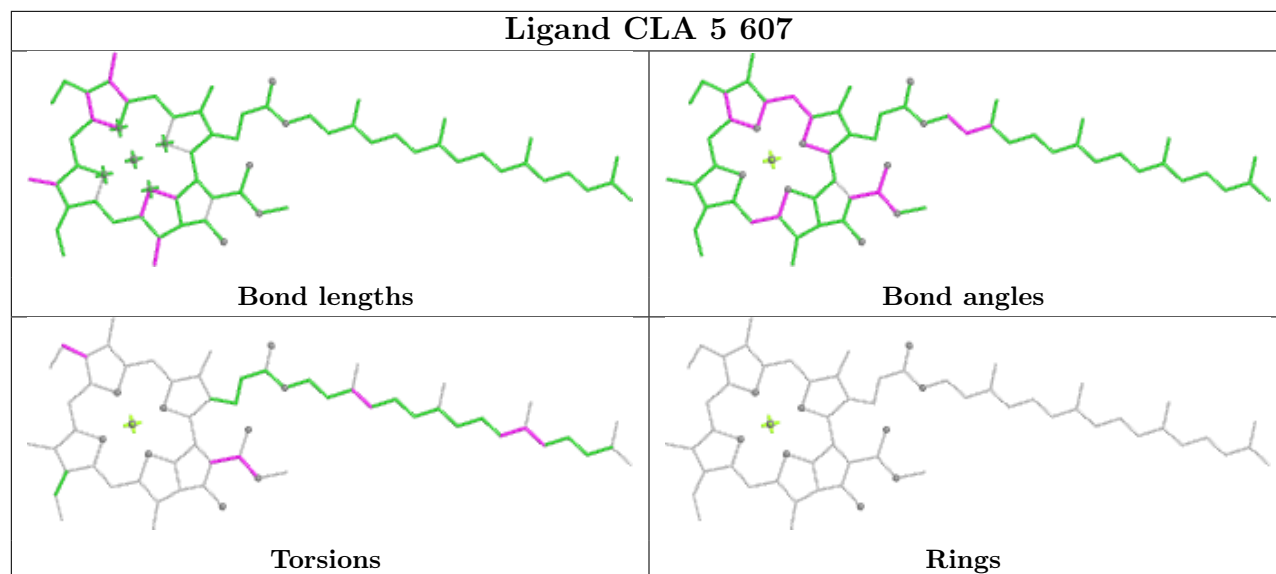
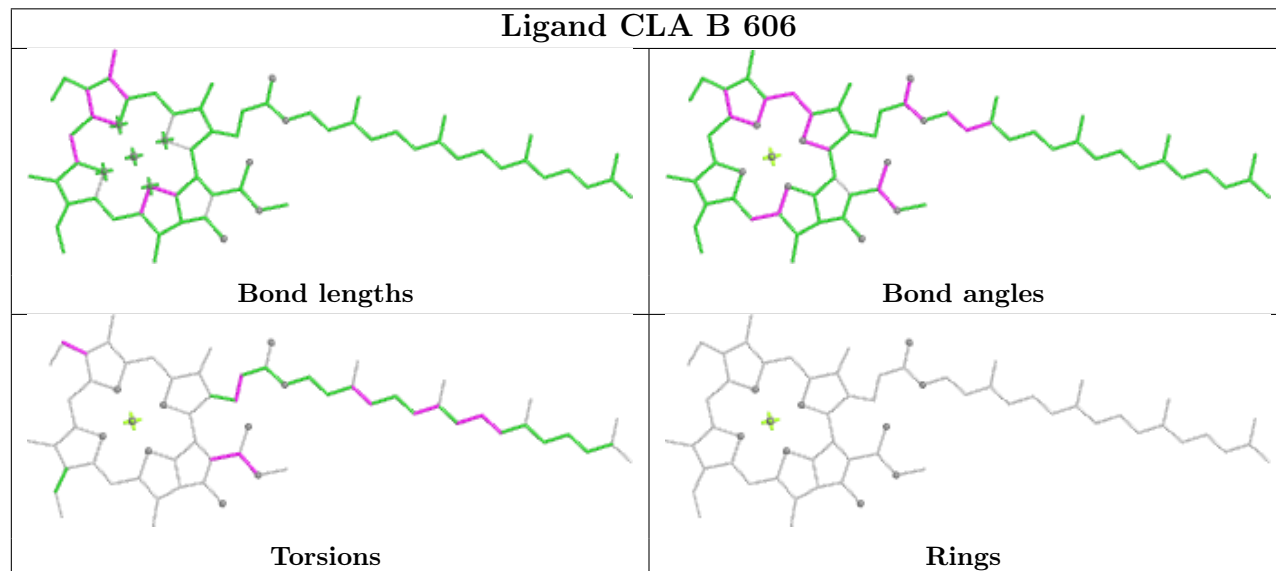


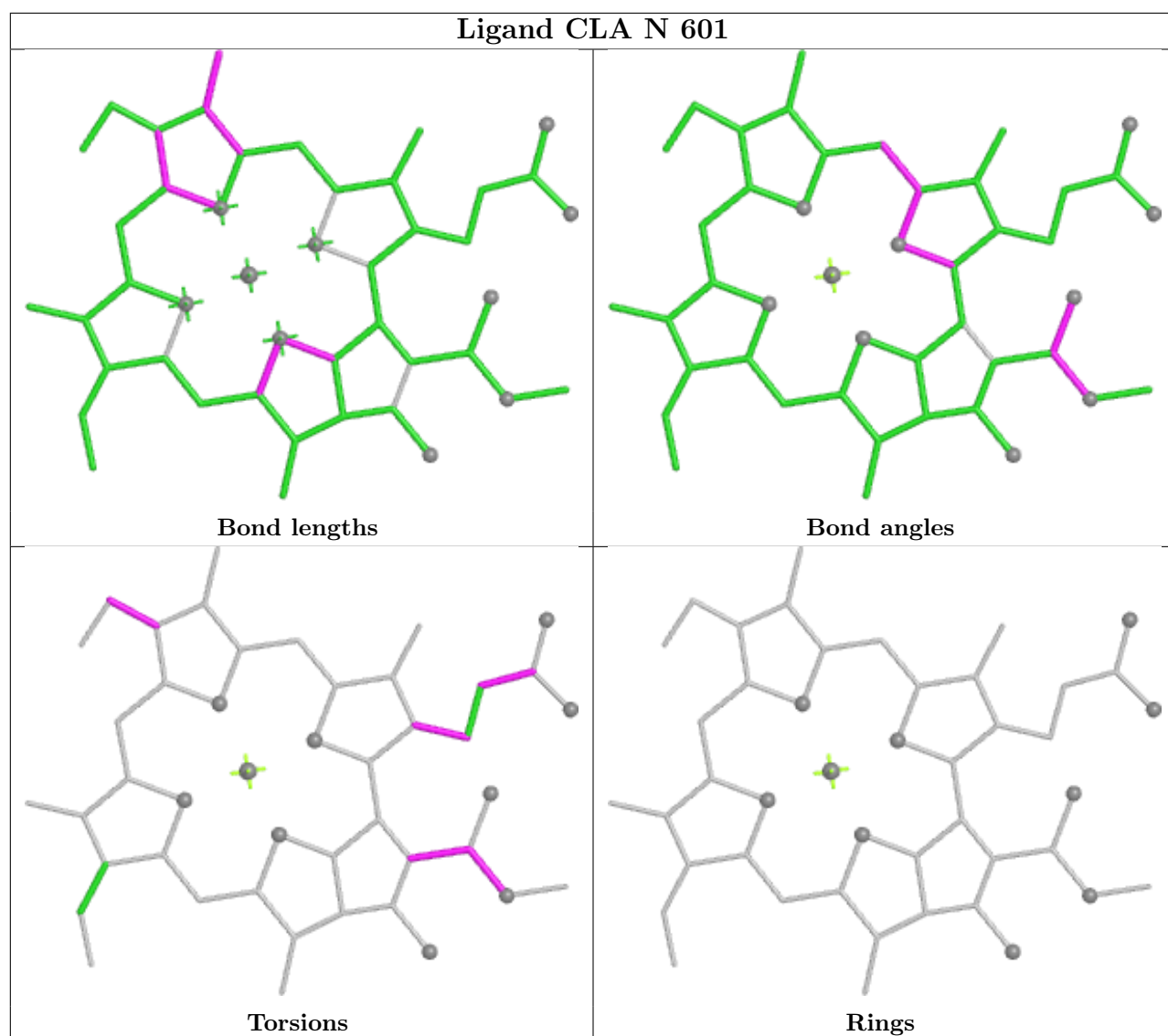
Torsions



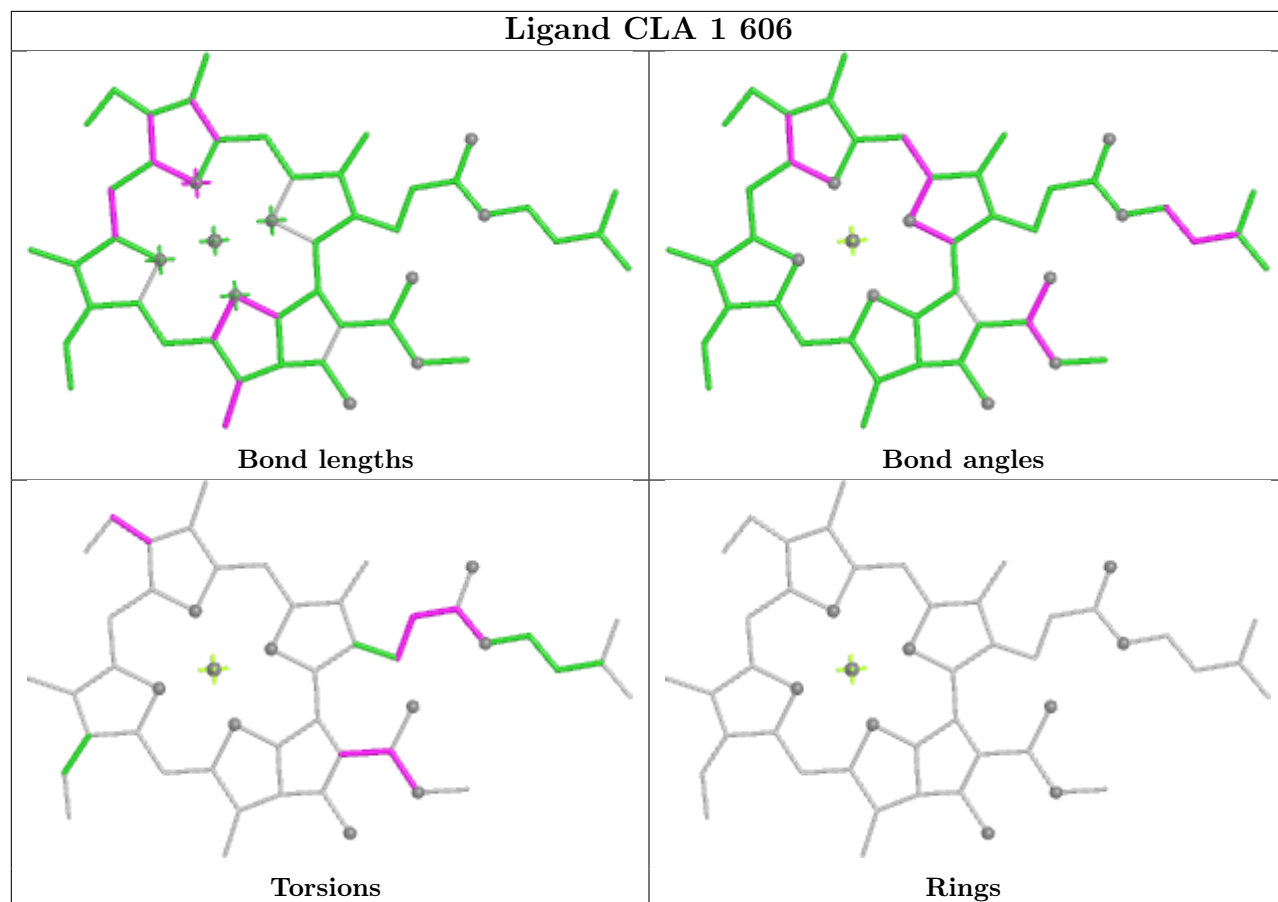
Rings



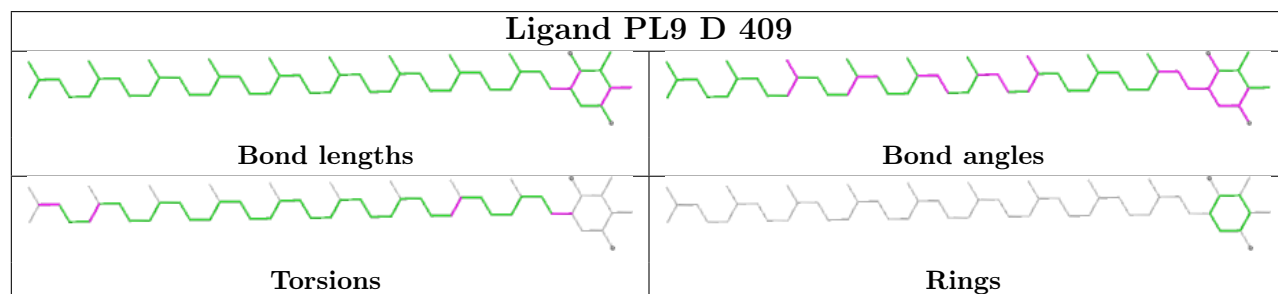
Ligand CLA 5 607**Ligand CLA B 606**



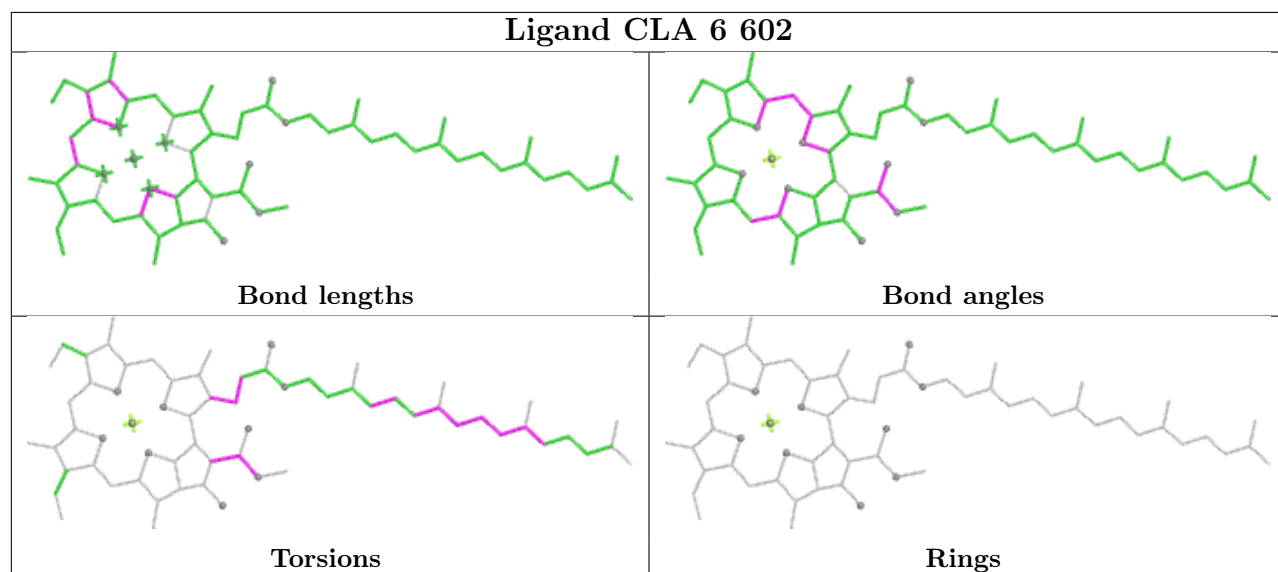
Ligand CLA 1 606

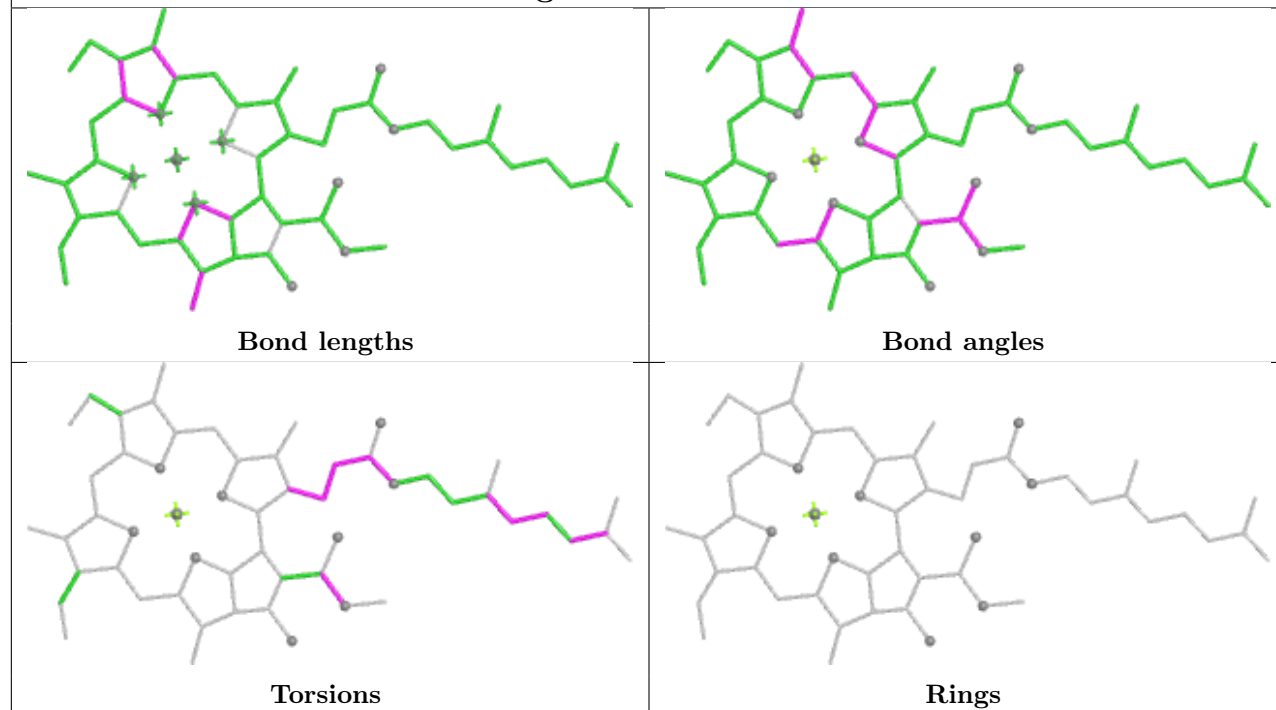
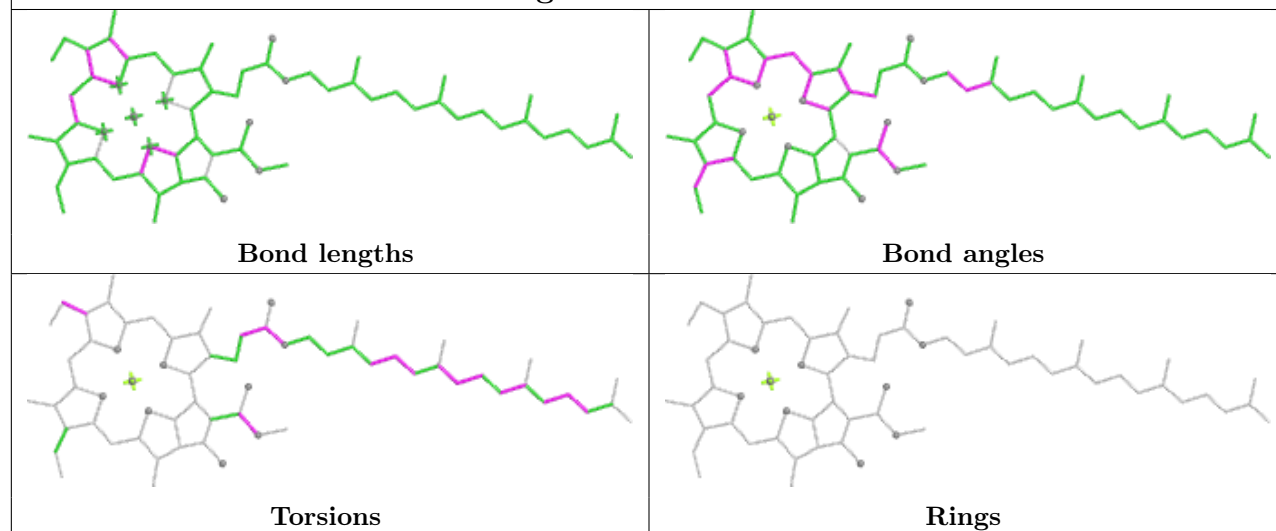


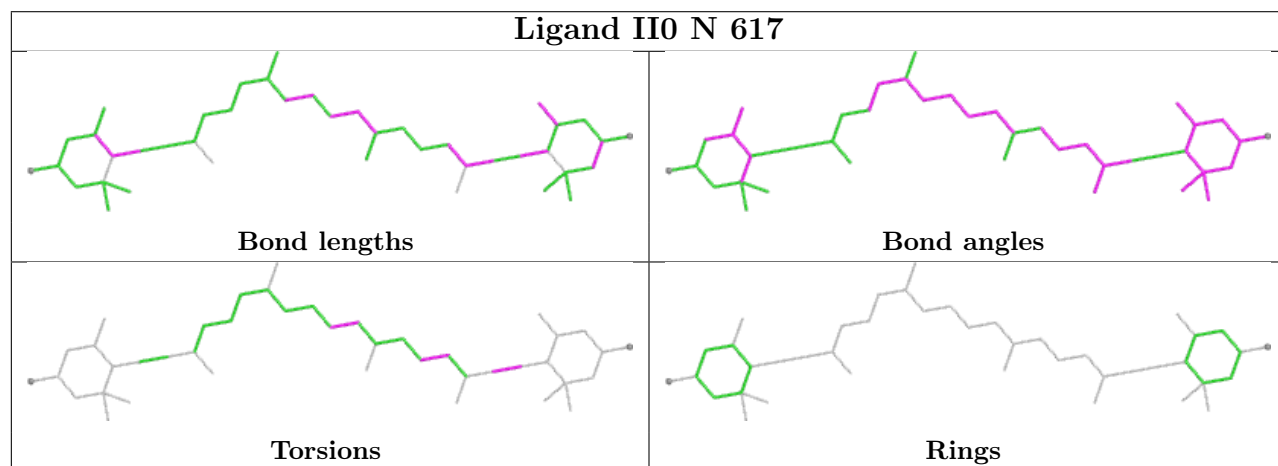
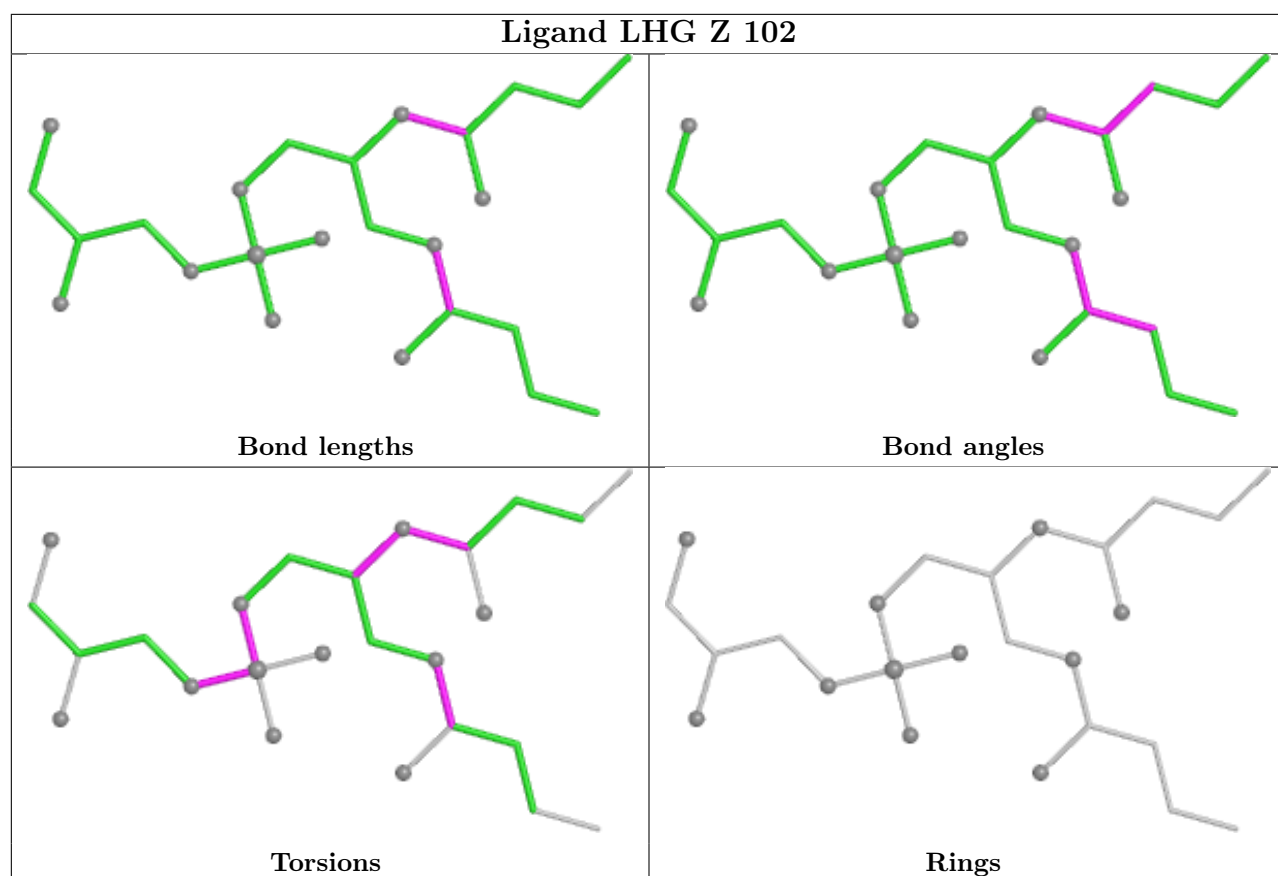
Ligand PL9 D 409

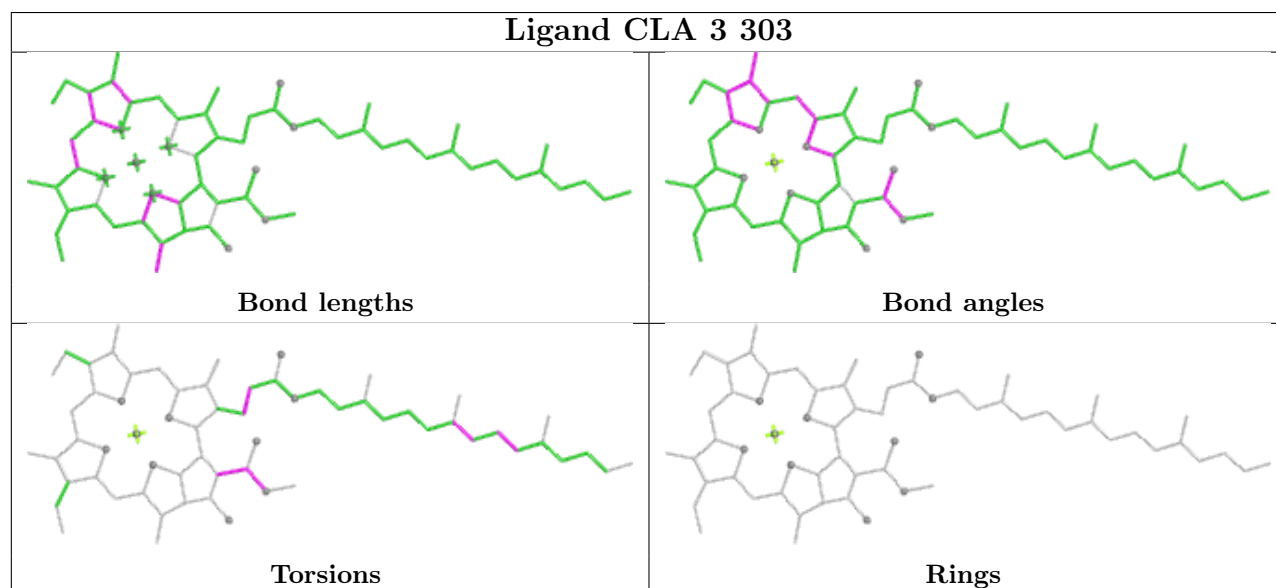
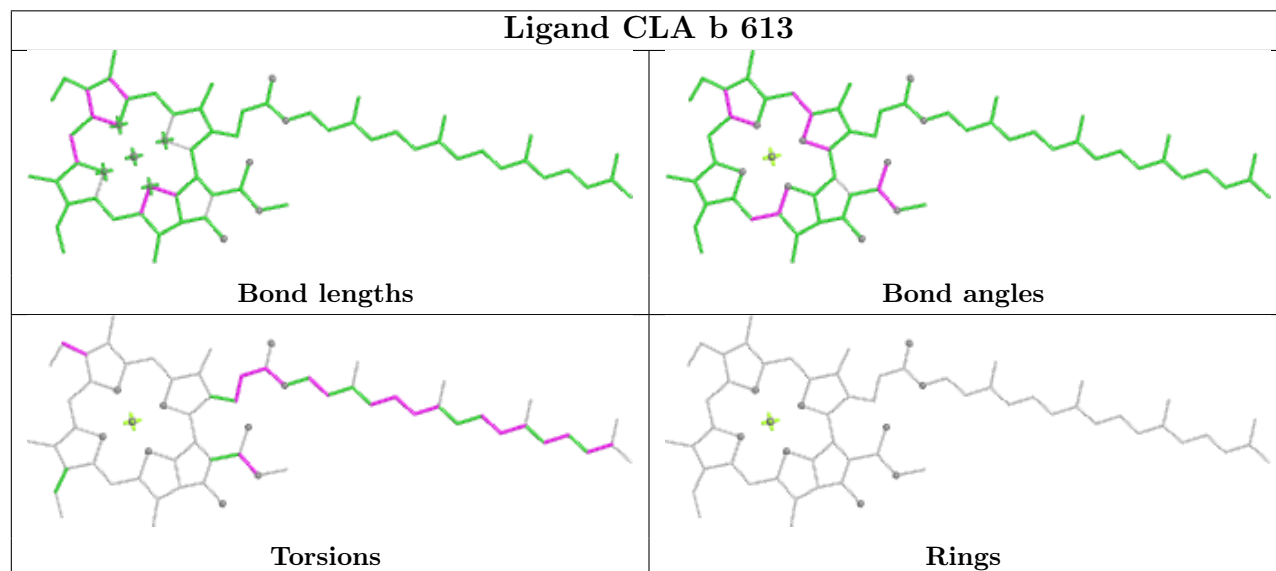
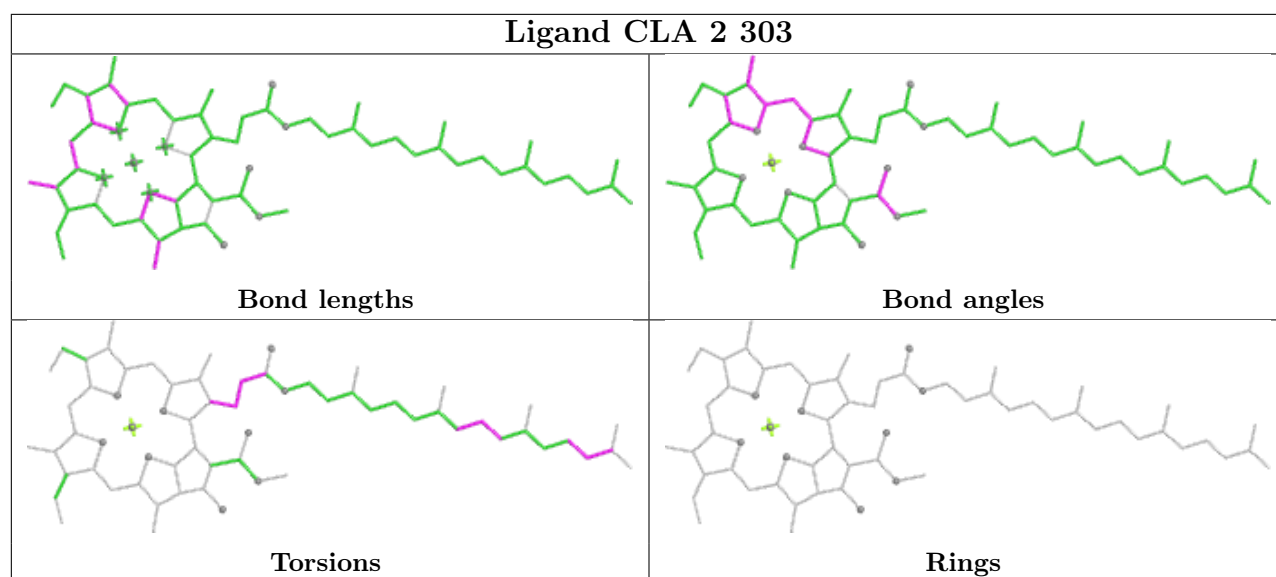


Ligand CLA 6 602

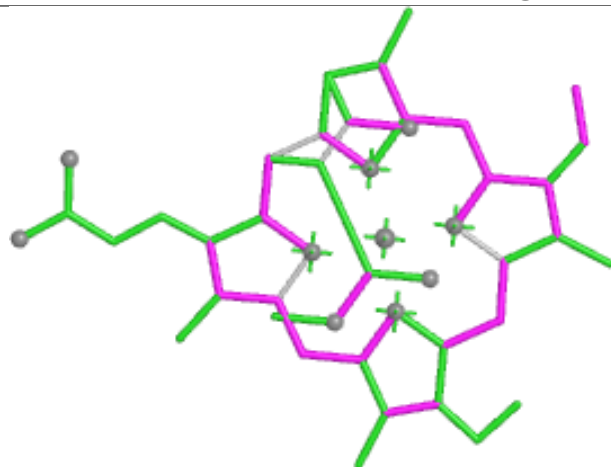


Ligand CLA 6 605**Ligand CLA 4 303**

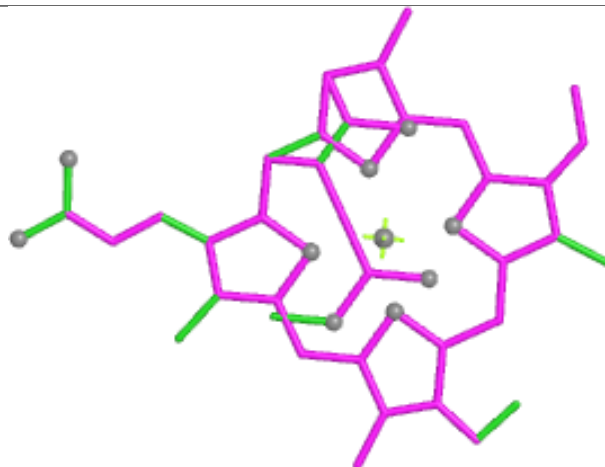




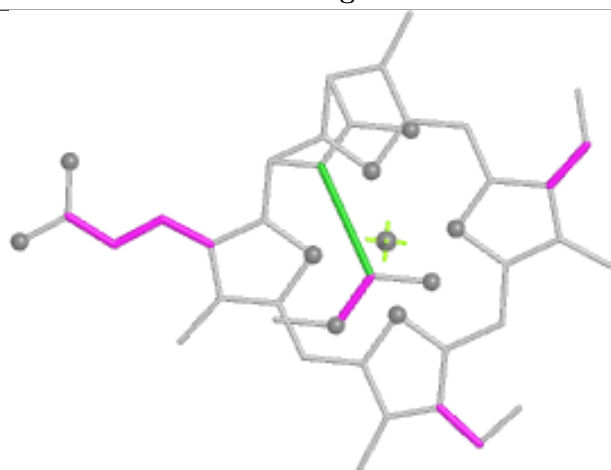
Ligand KC2 P 605



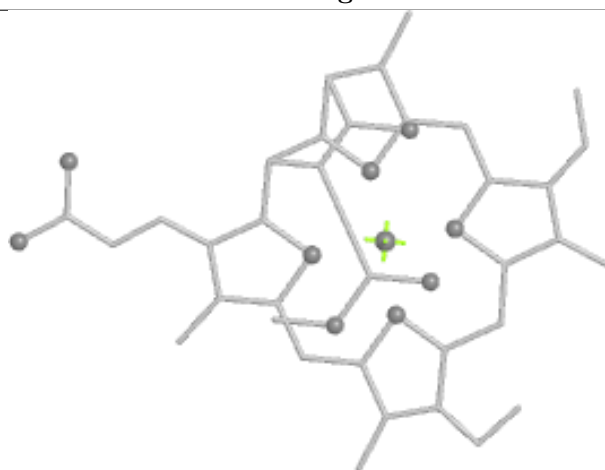
Bond lengths



Bond angles

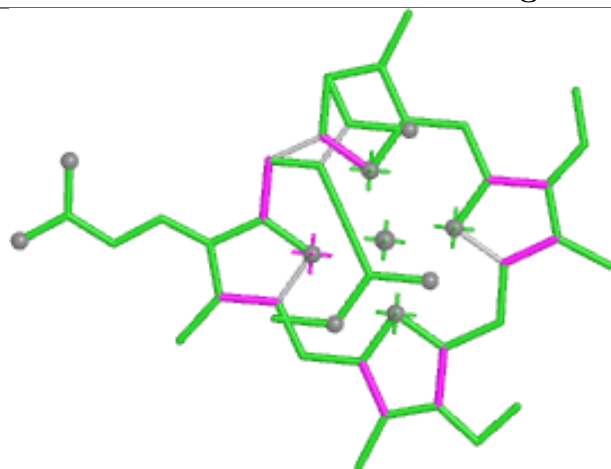


Torsions

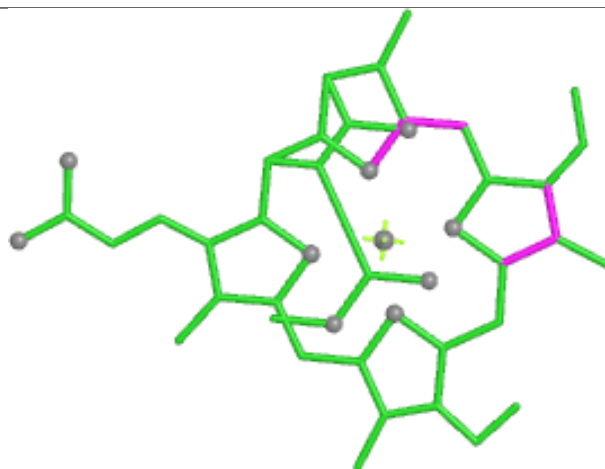


Rings

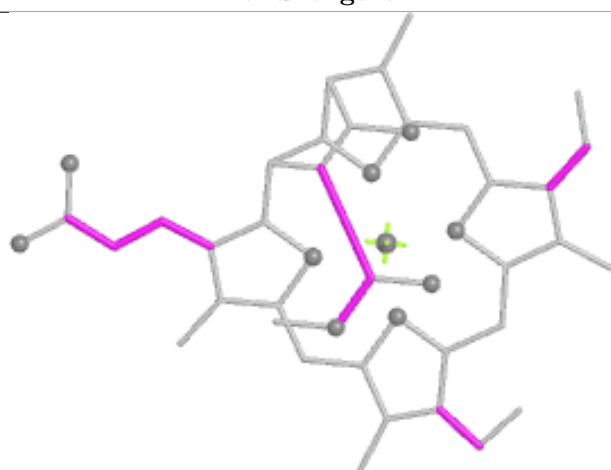
Ligand KC2 1 605



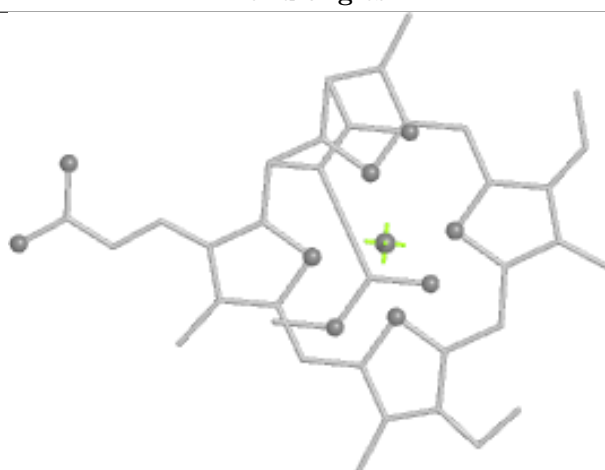
Bond lengths



Bond angles

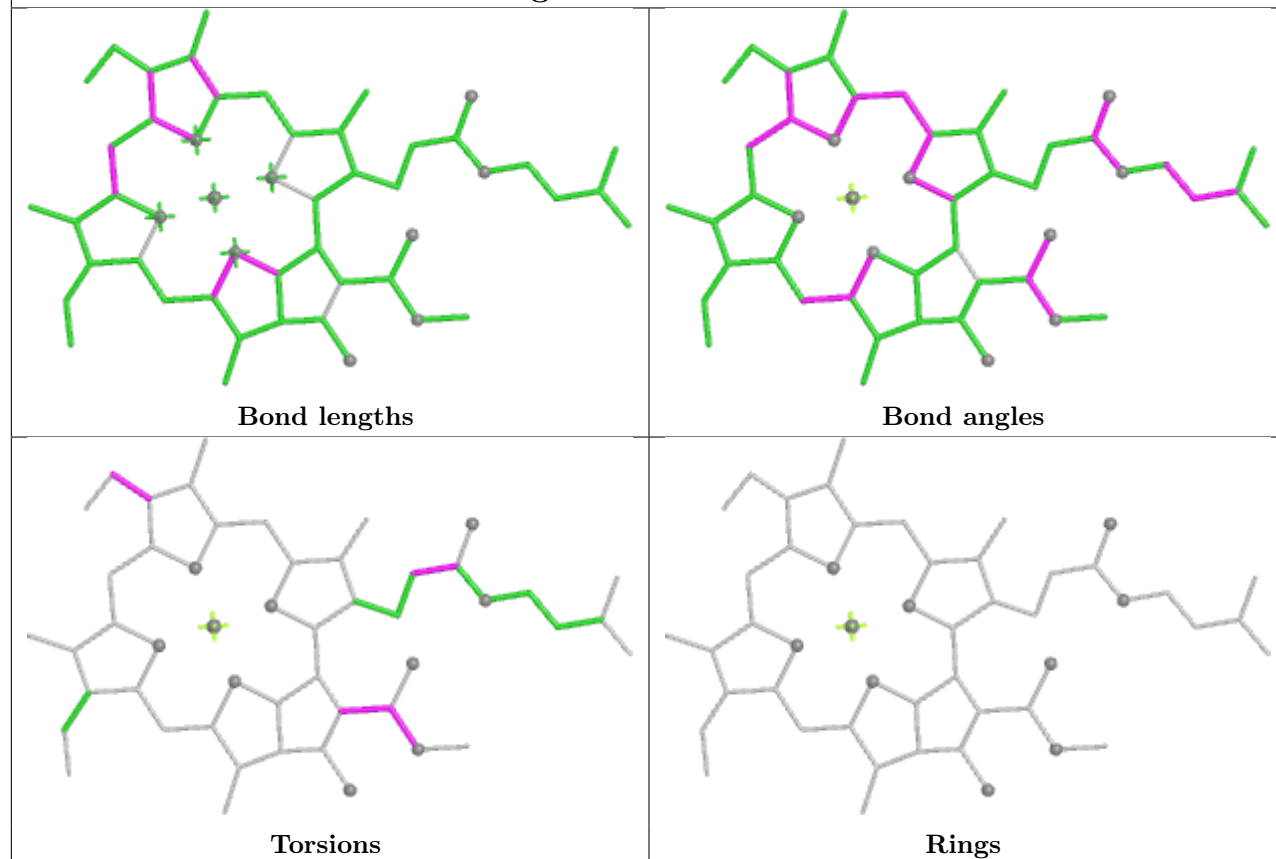


Torsions

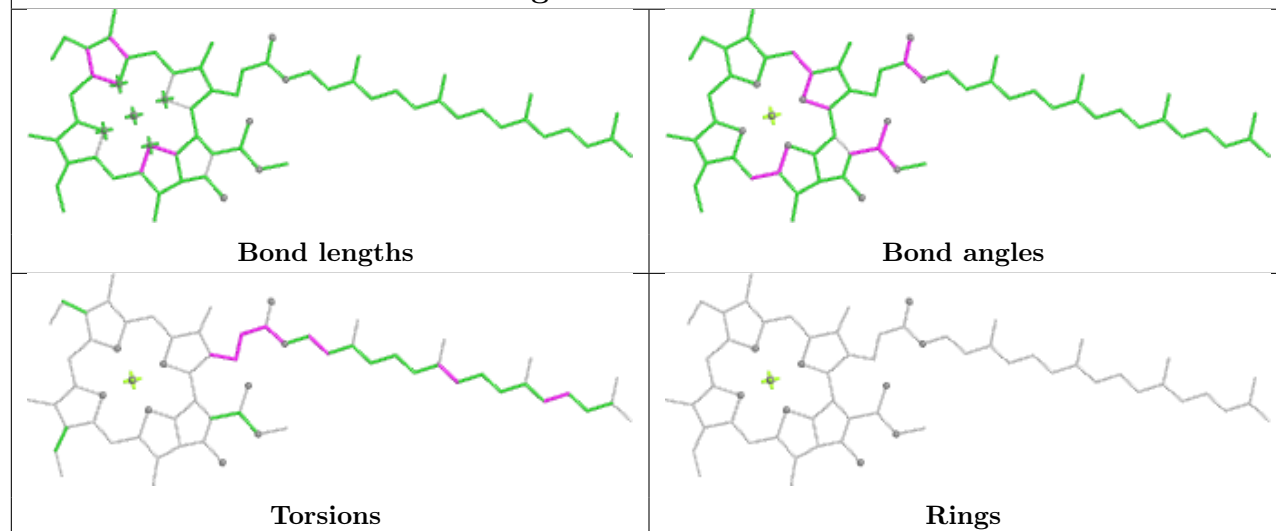


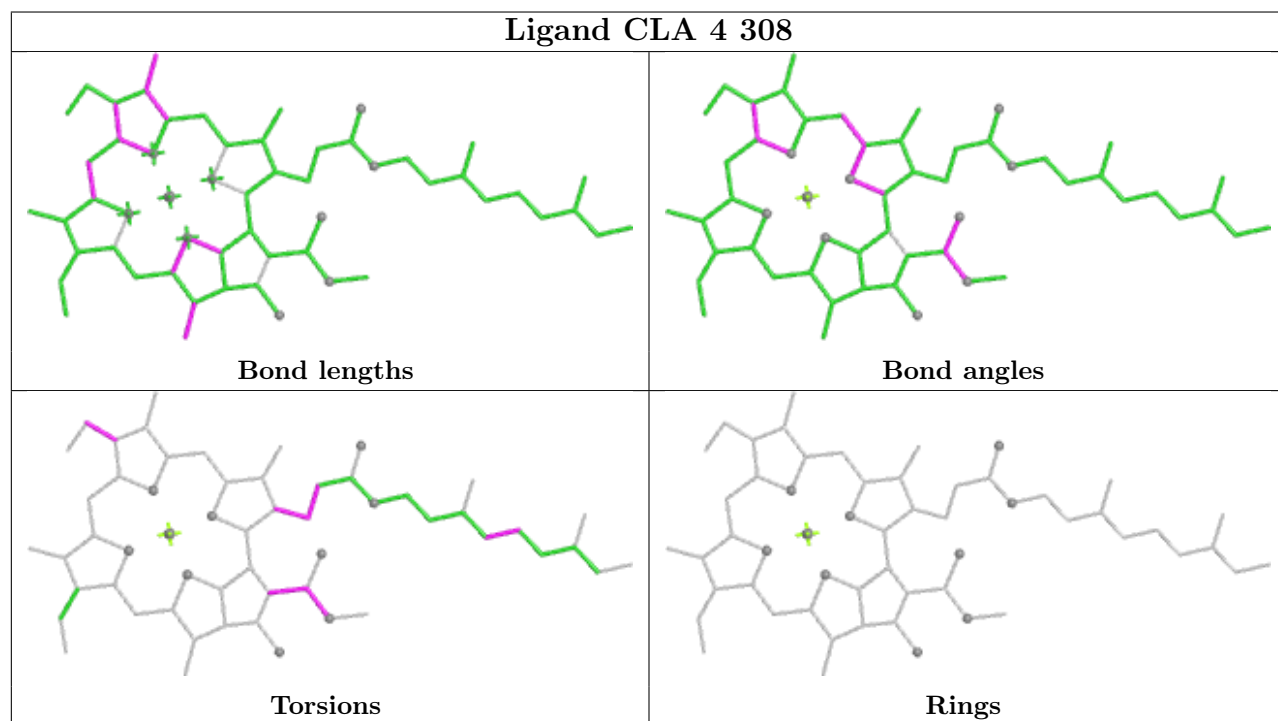
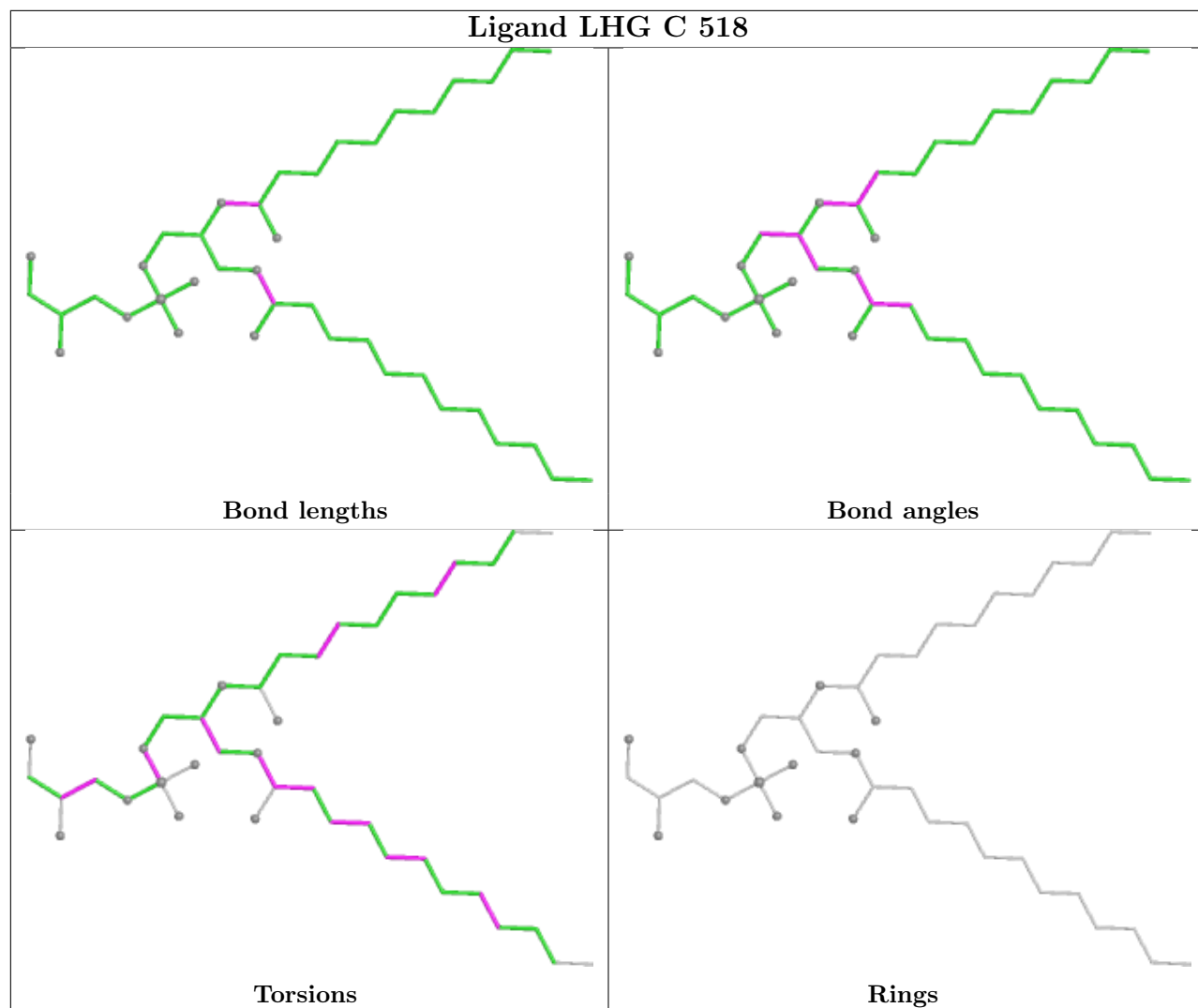
Rings

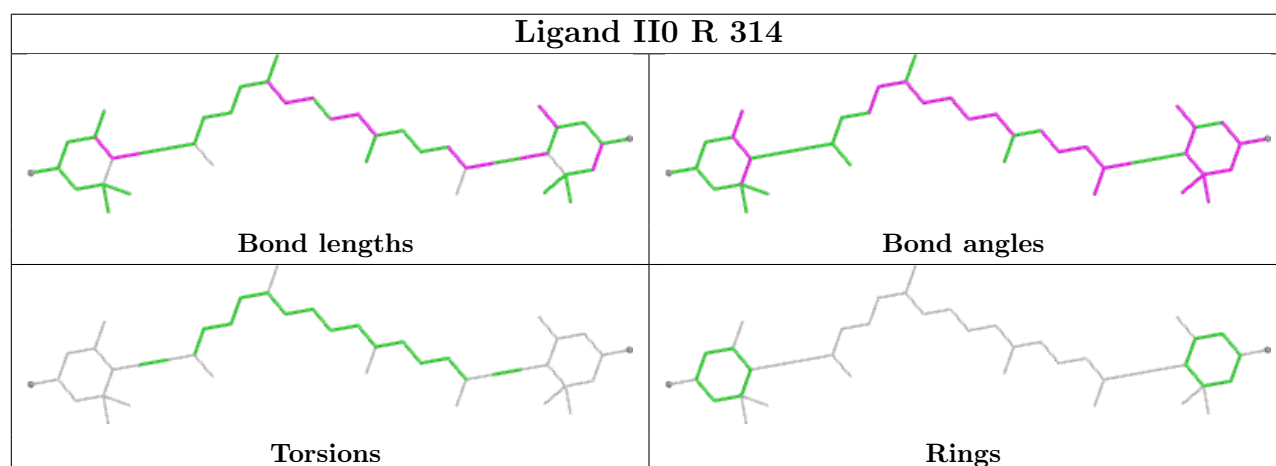
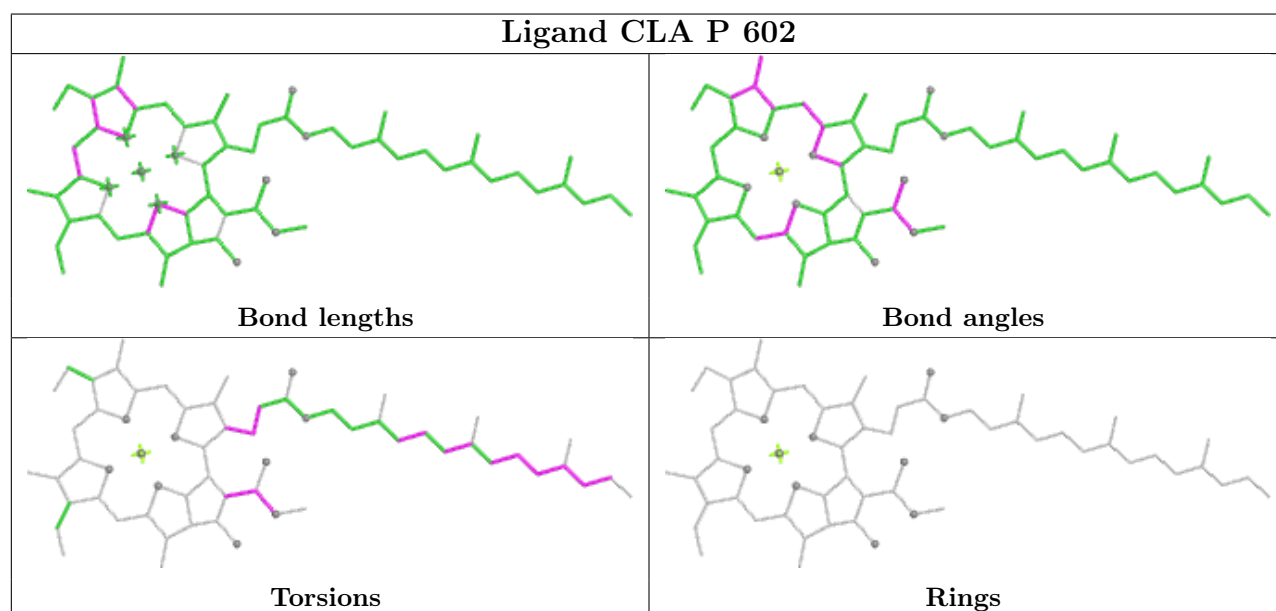
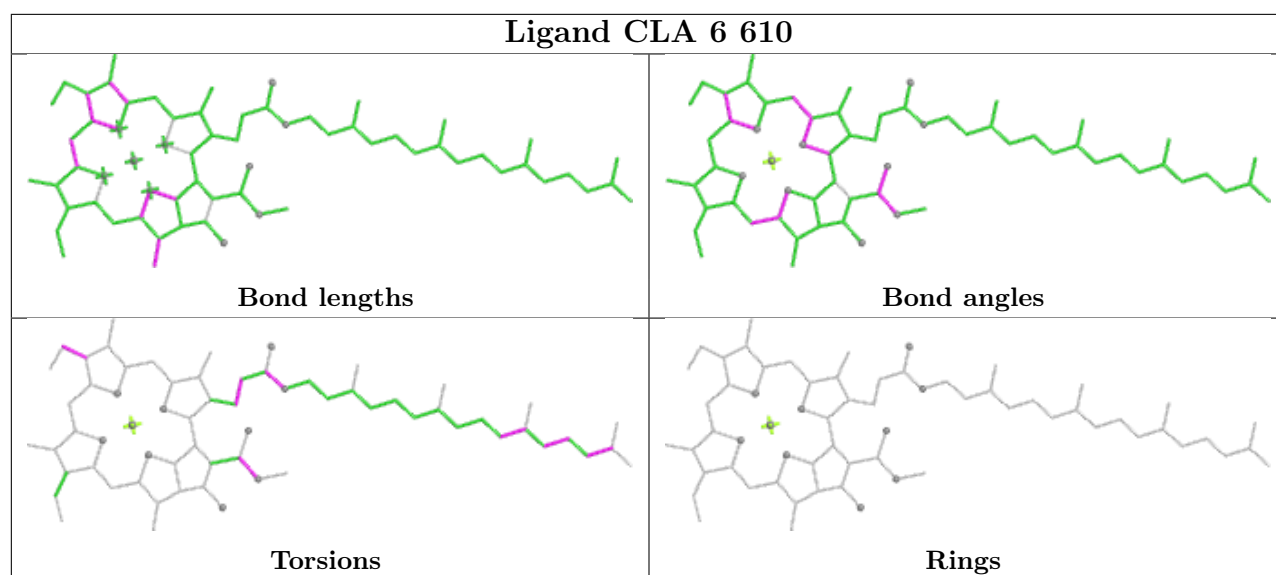
Ligand CLA N 606



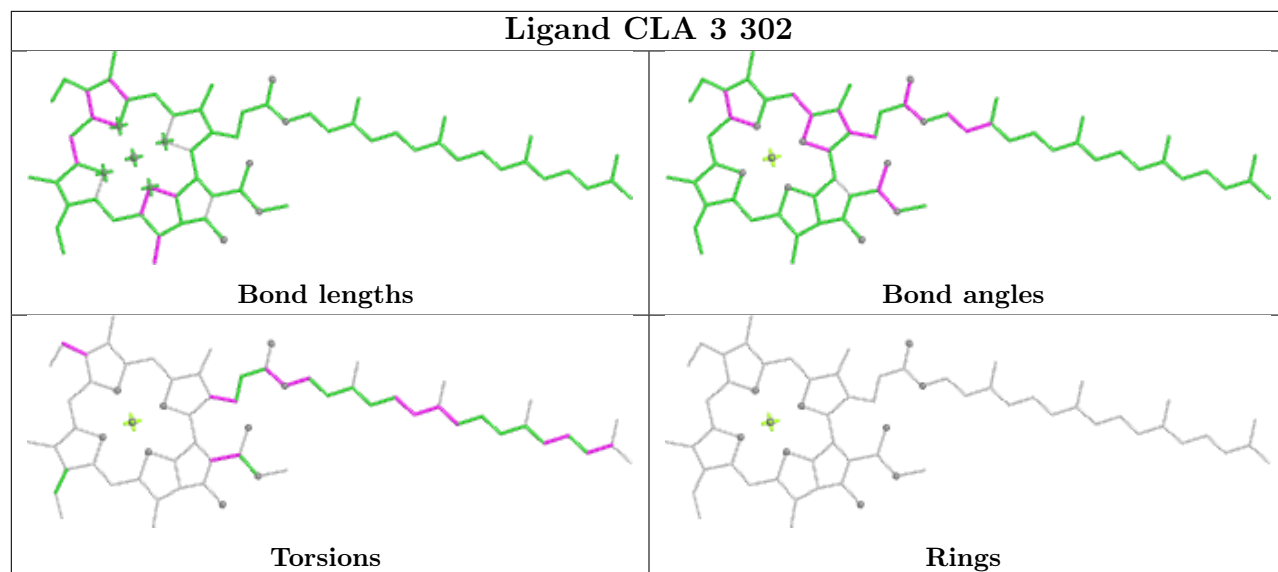
Ligand CLA D 404



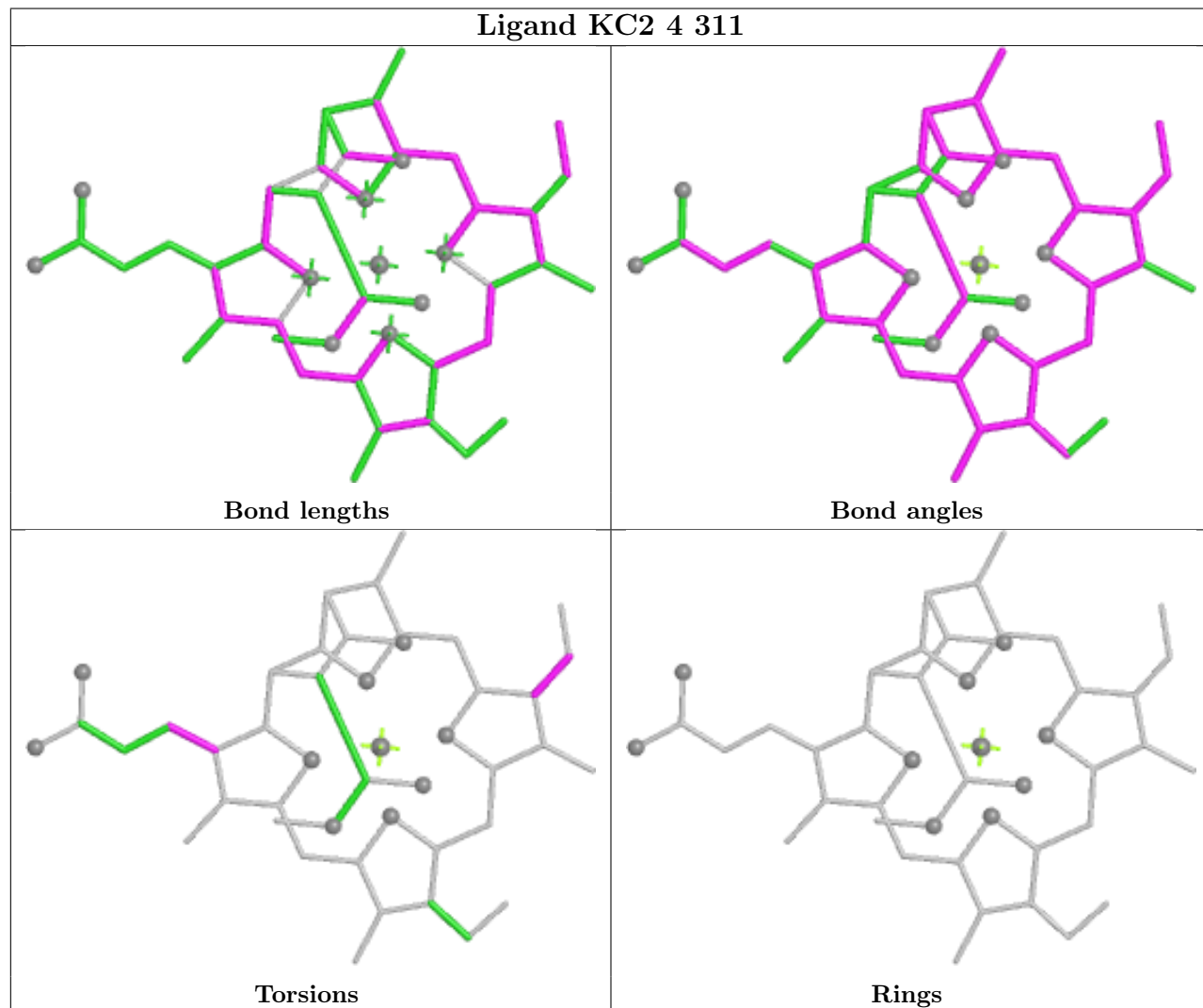


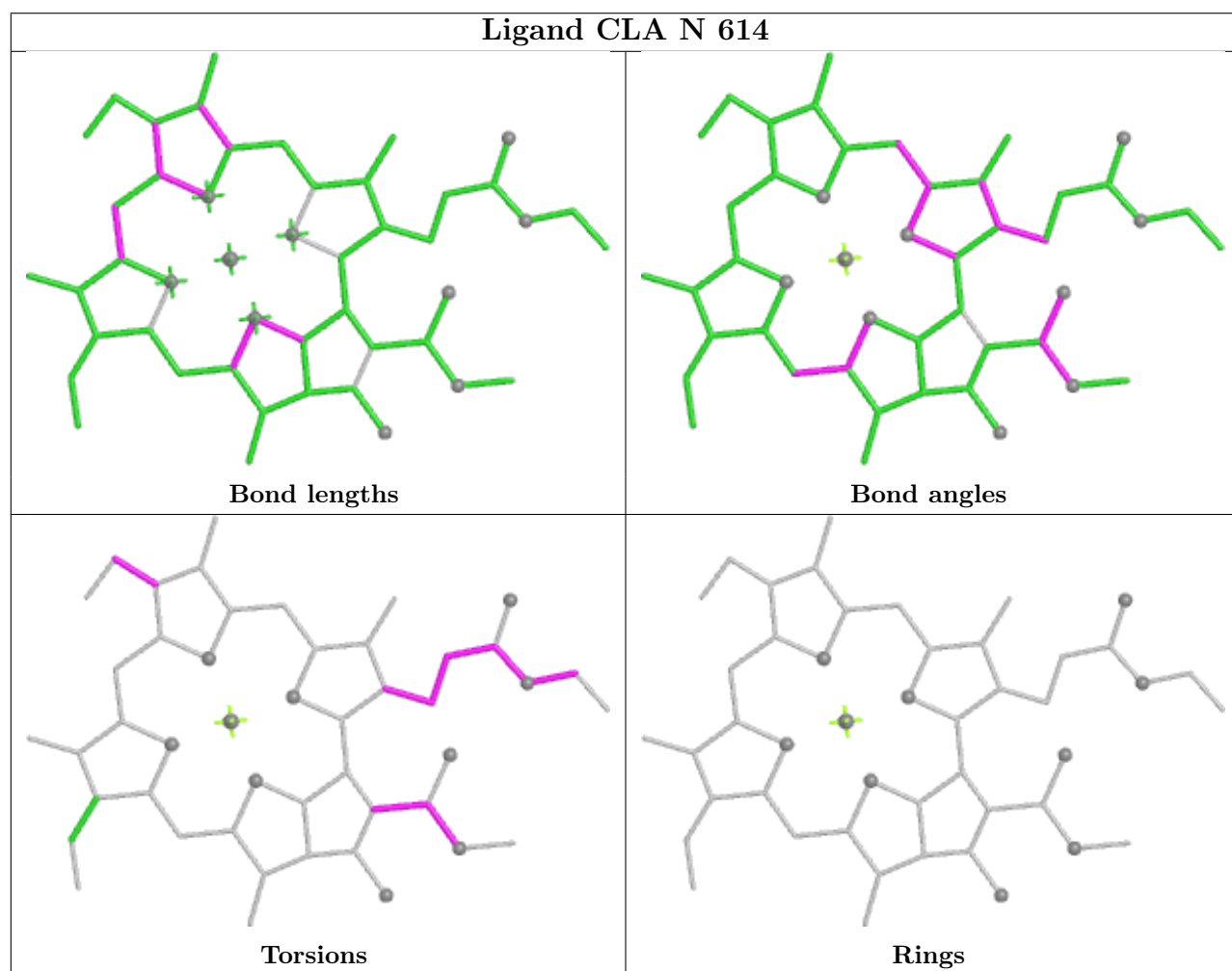
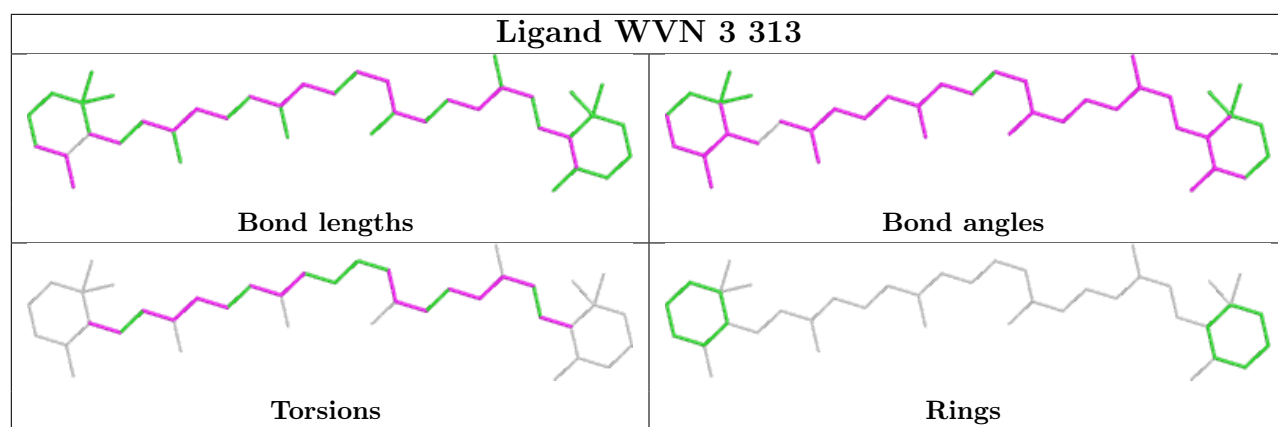


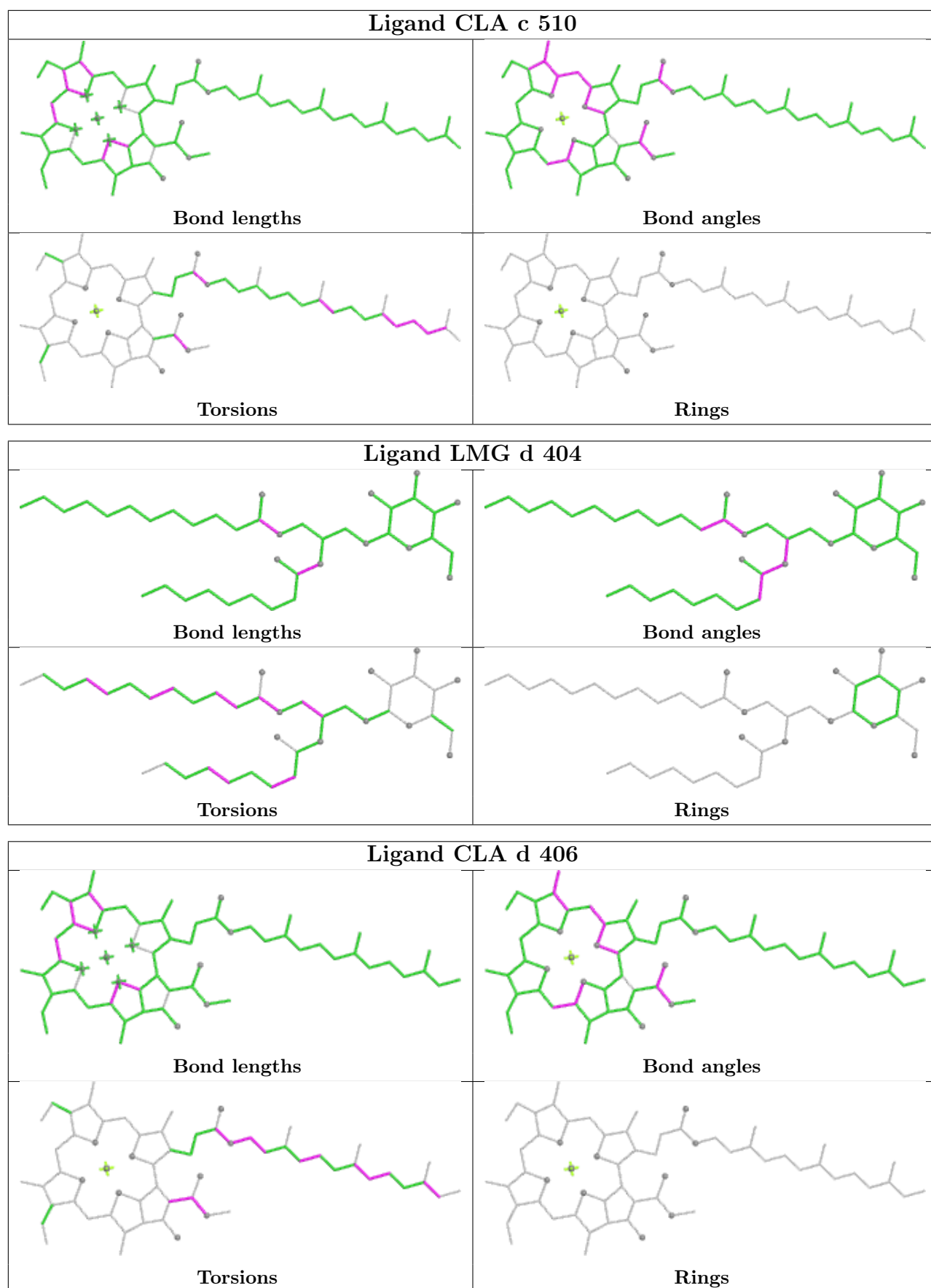
Ligand CLA 3 302

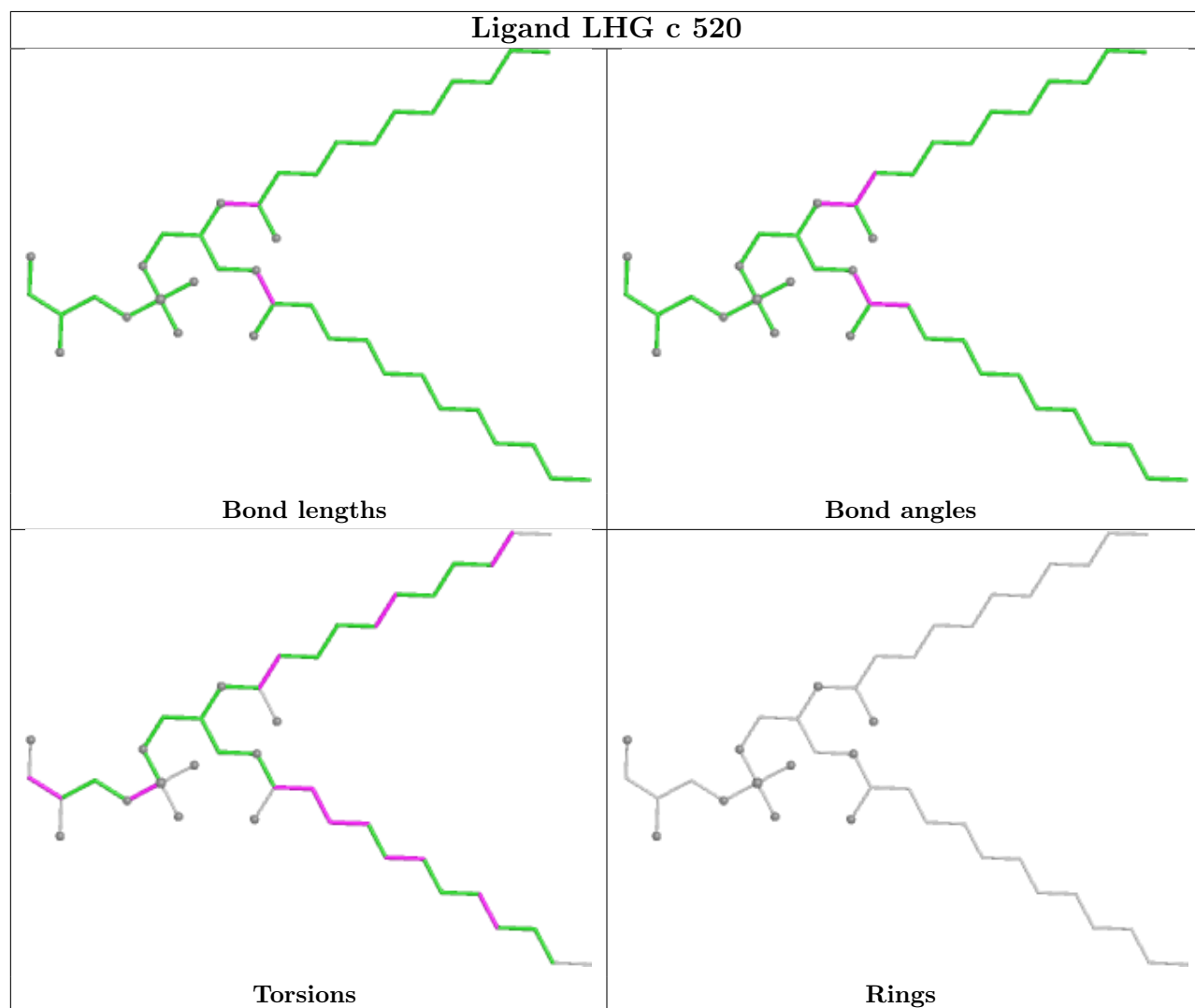
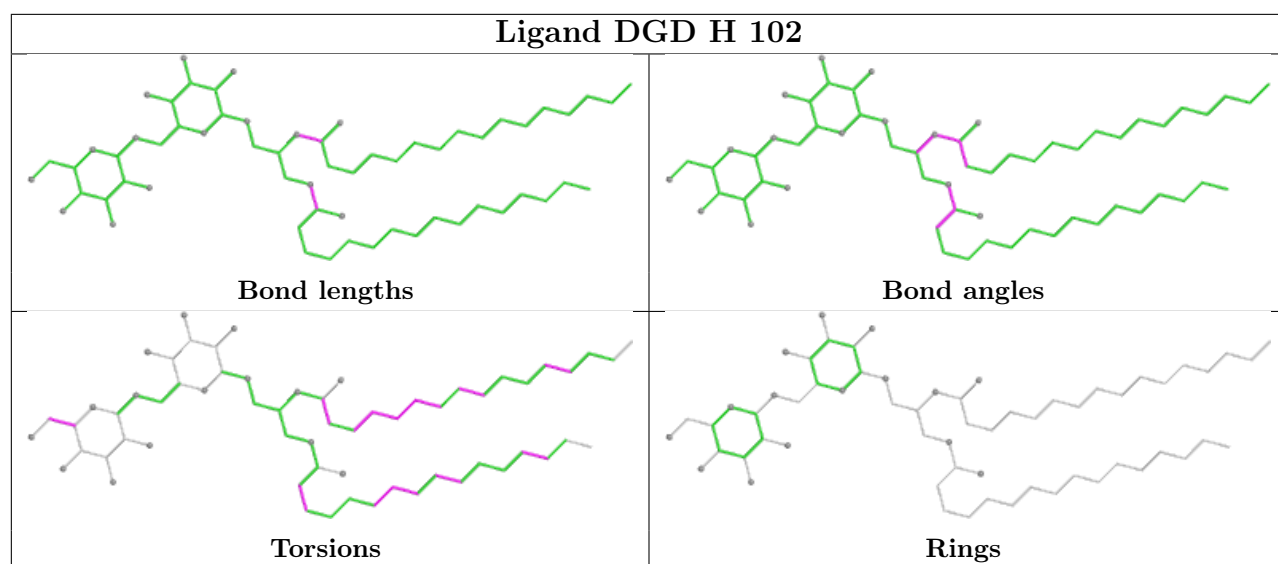


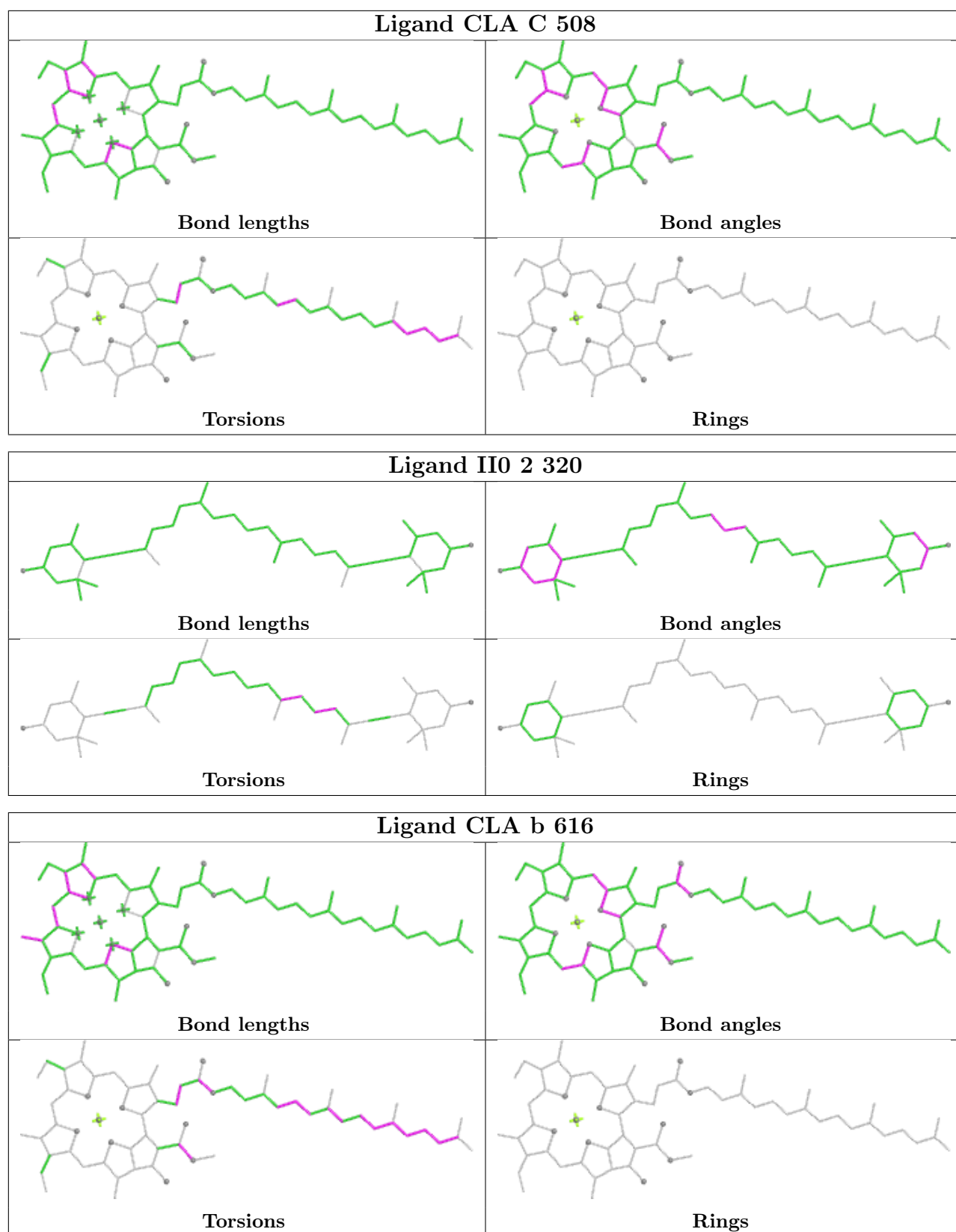
Ligand KC2 4 311



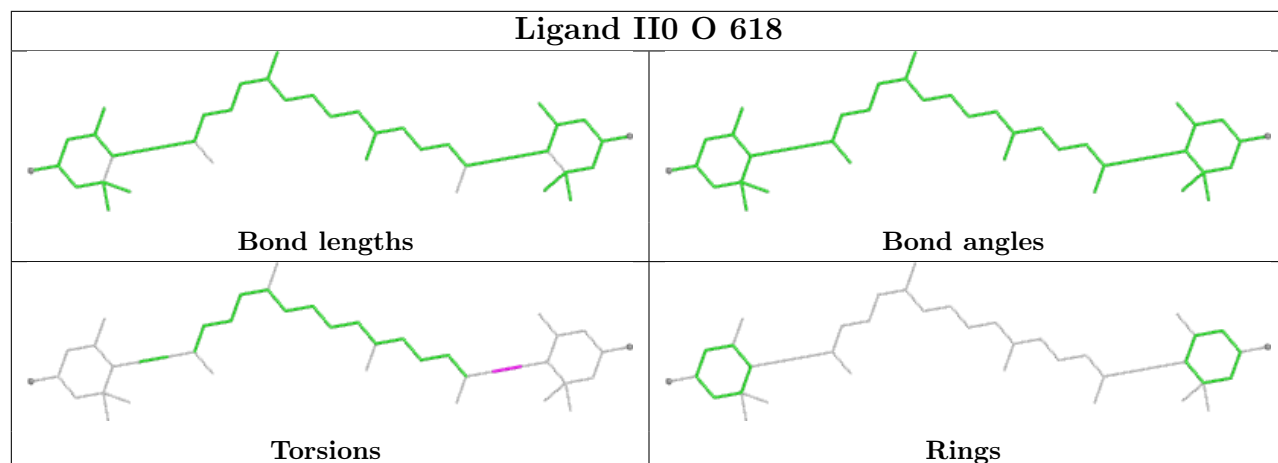




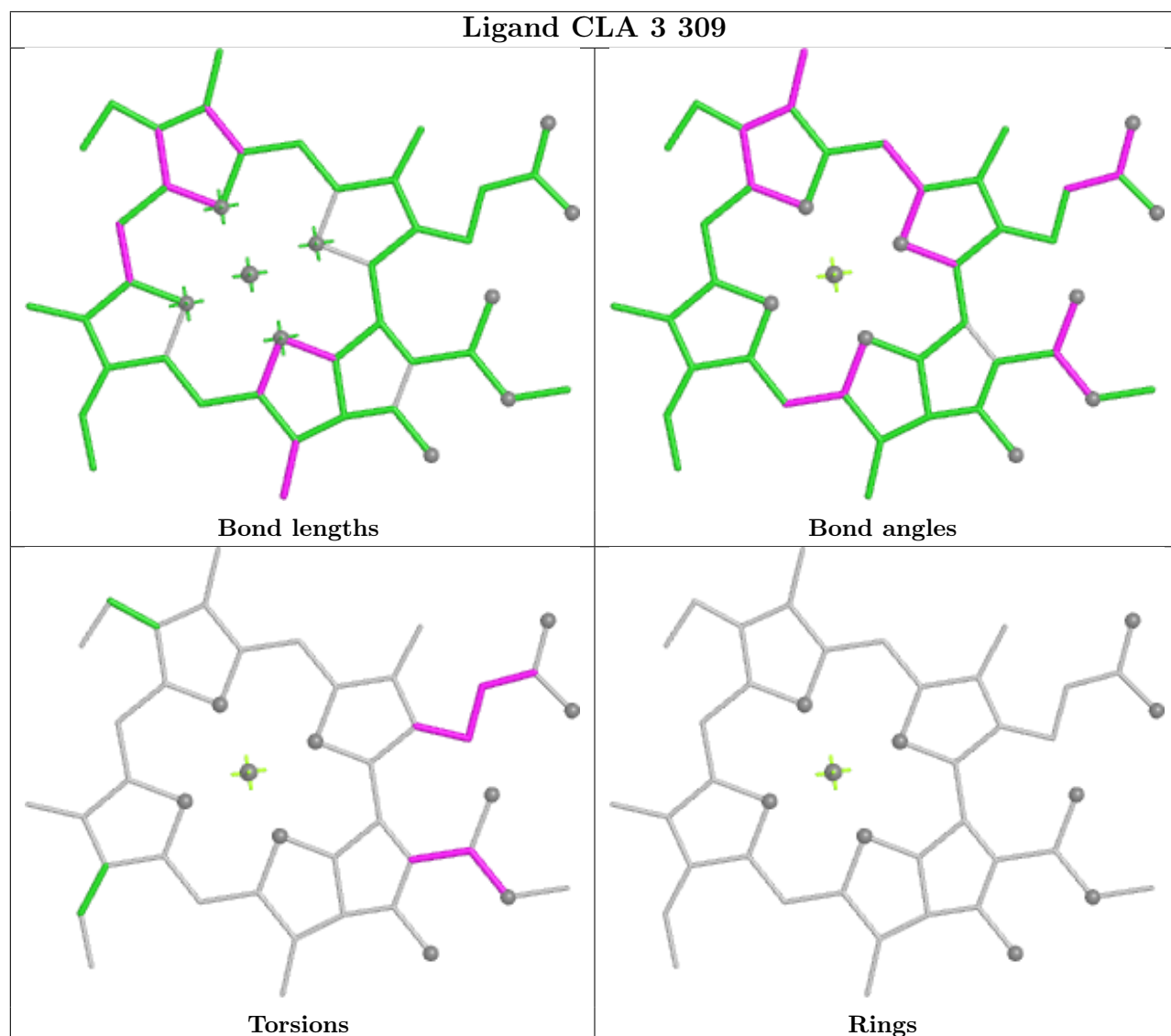


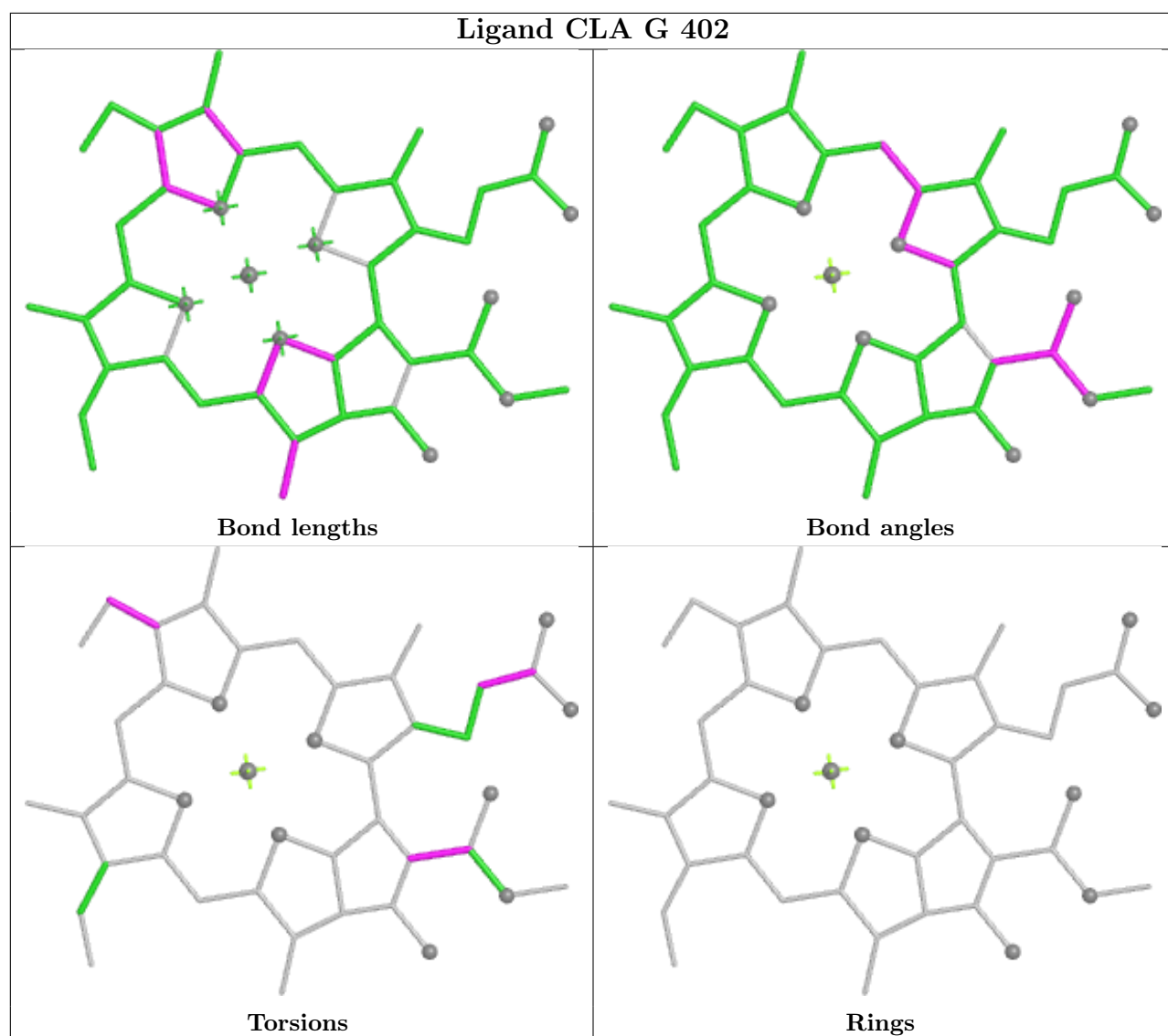


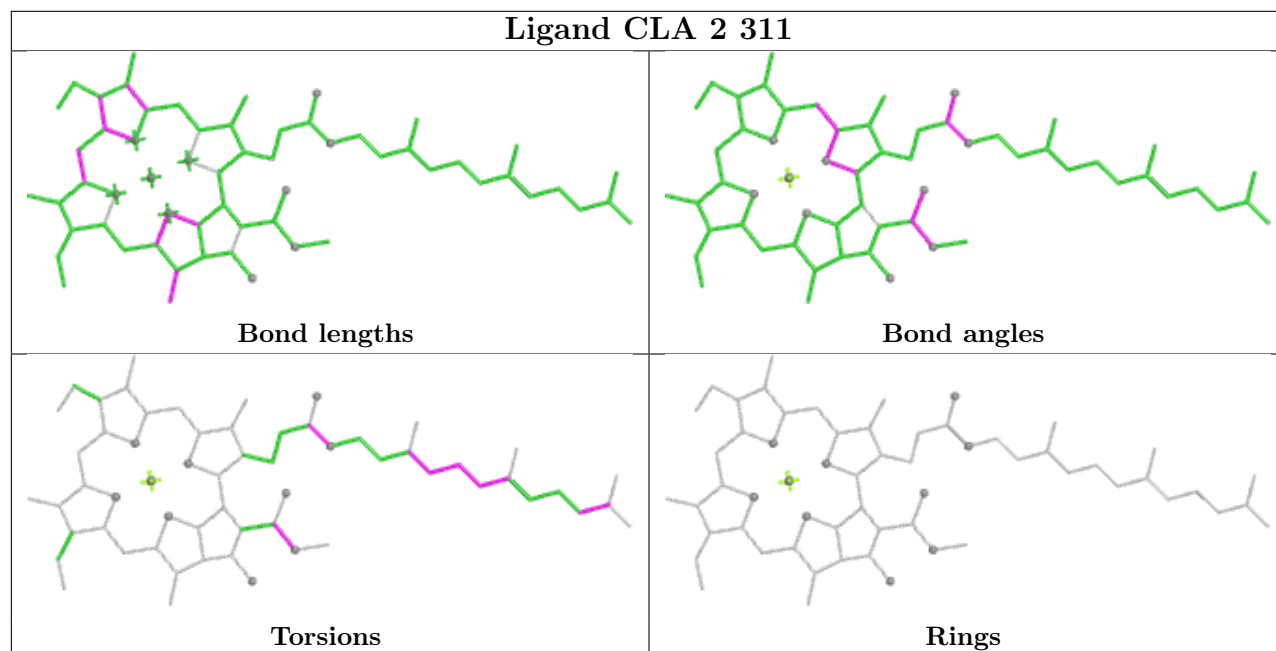
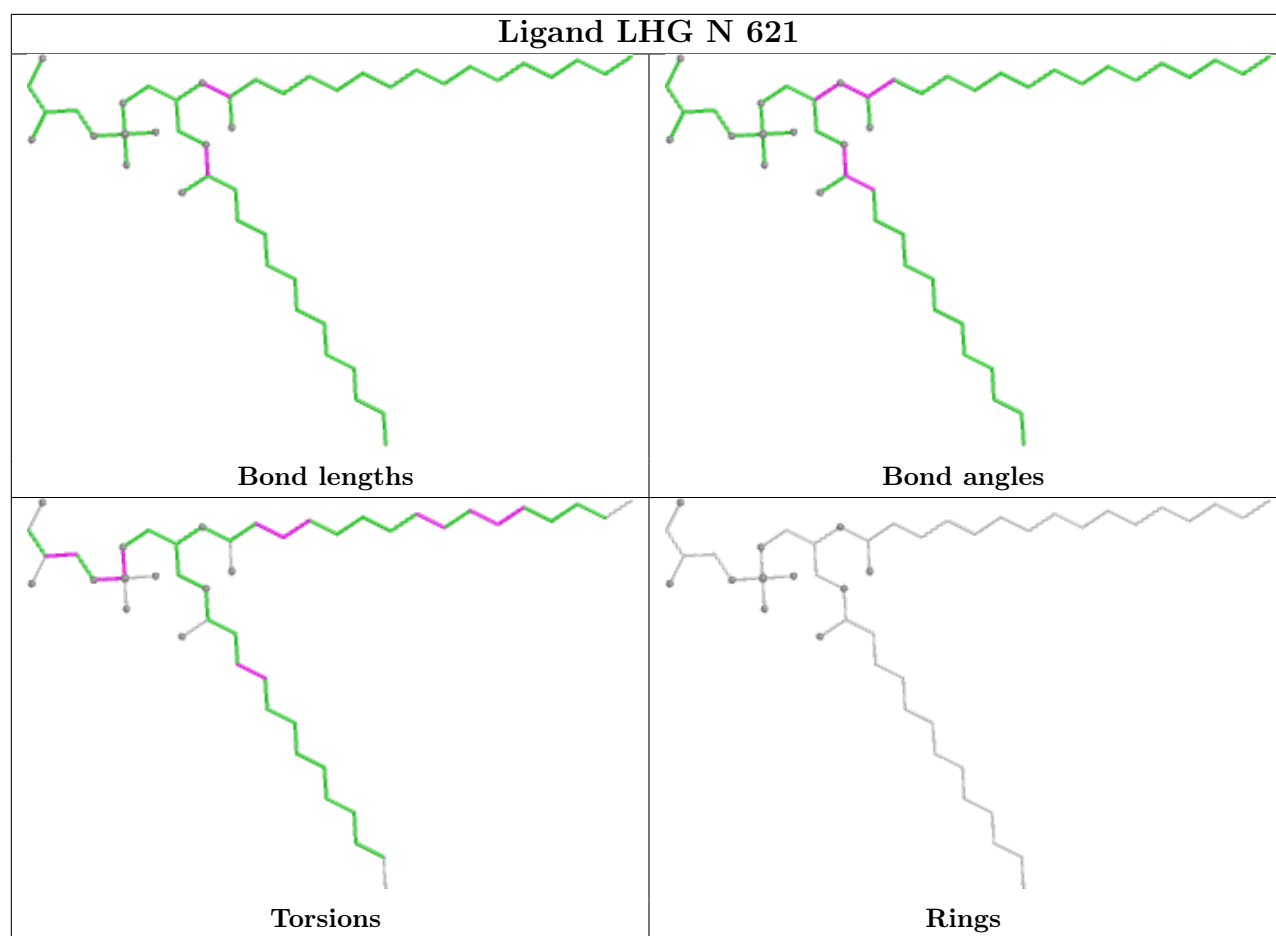
Ligand II0 O 618

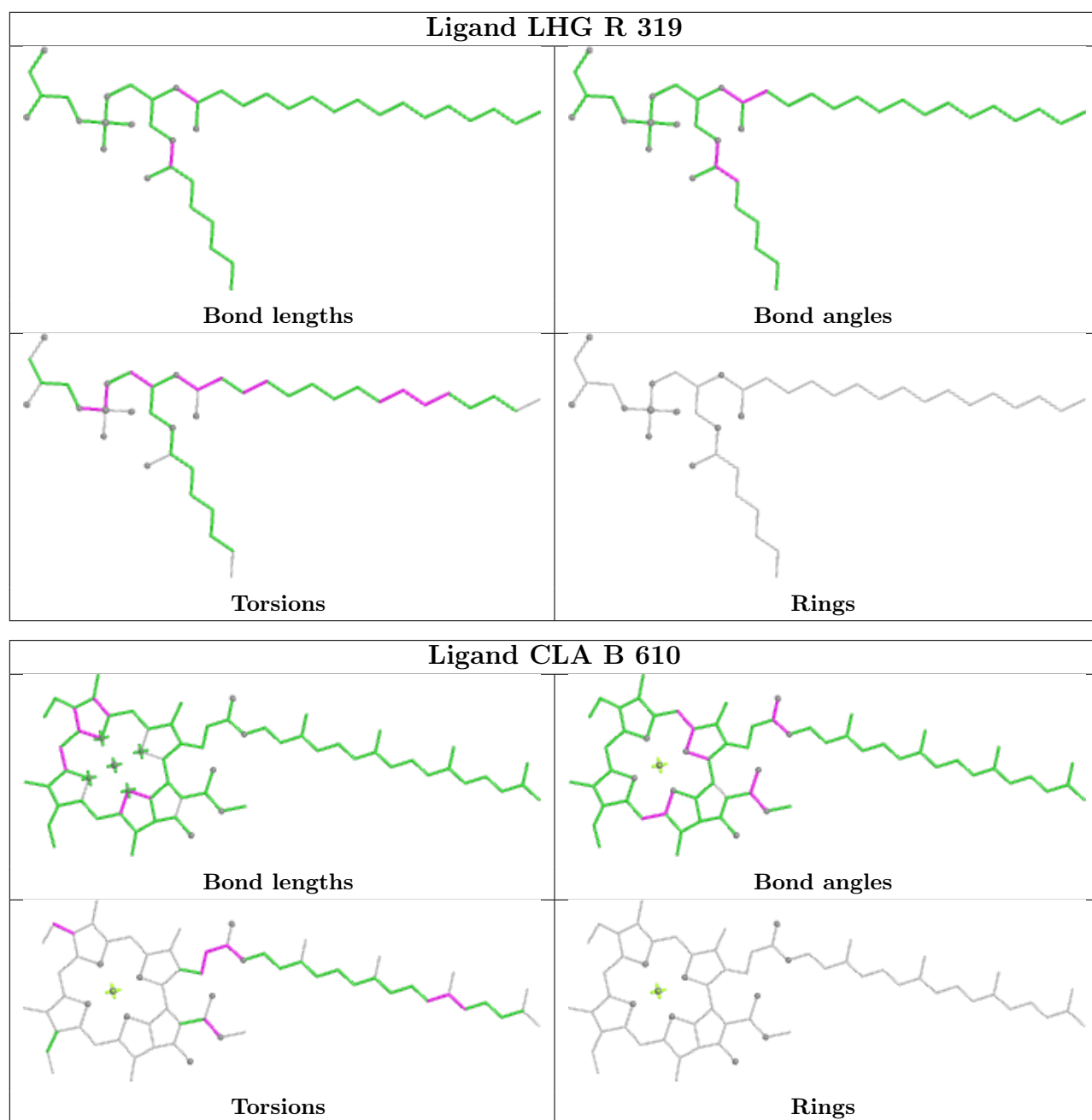


Ligand CLA 3 309

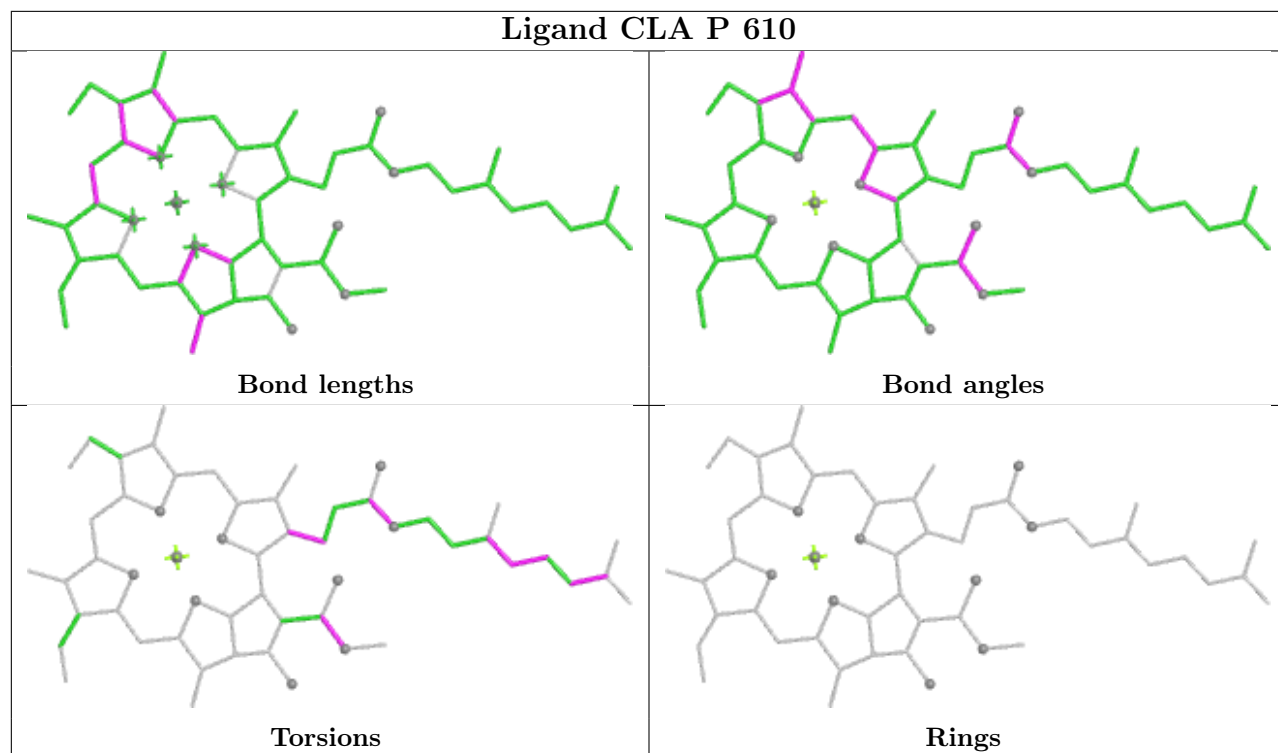




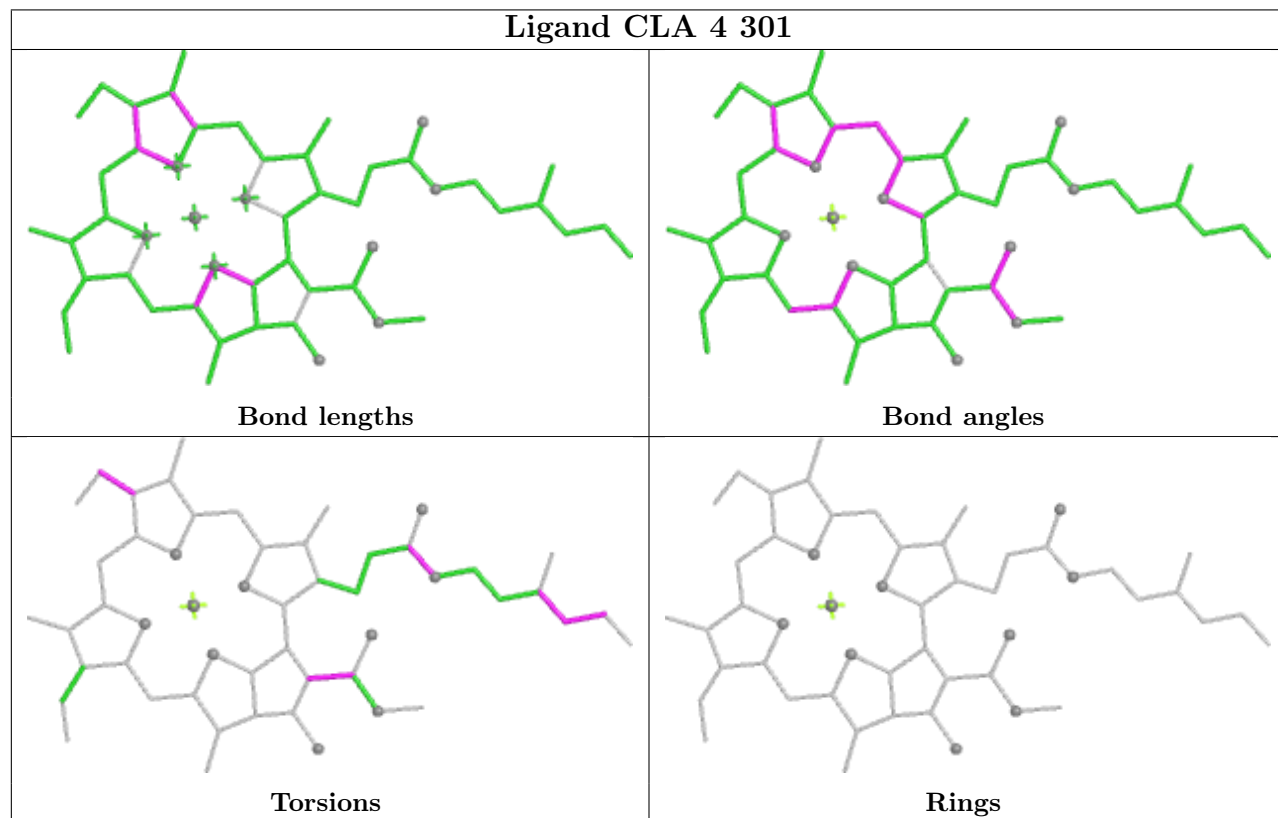


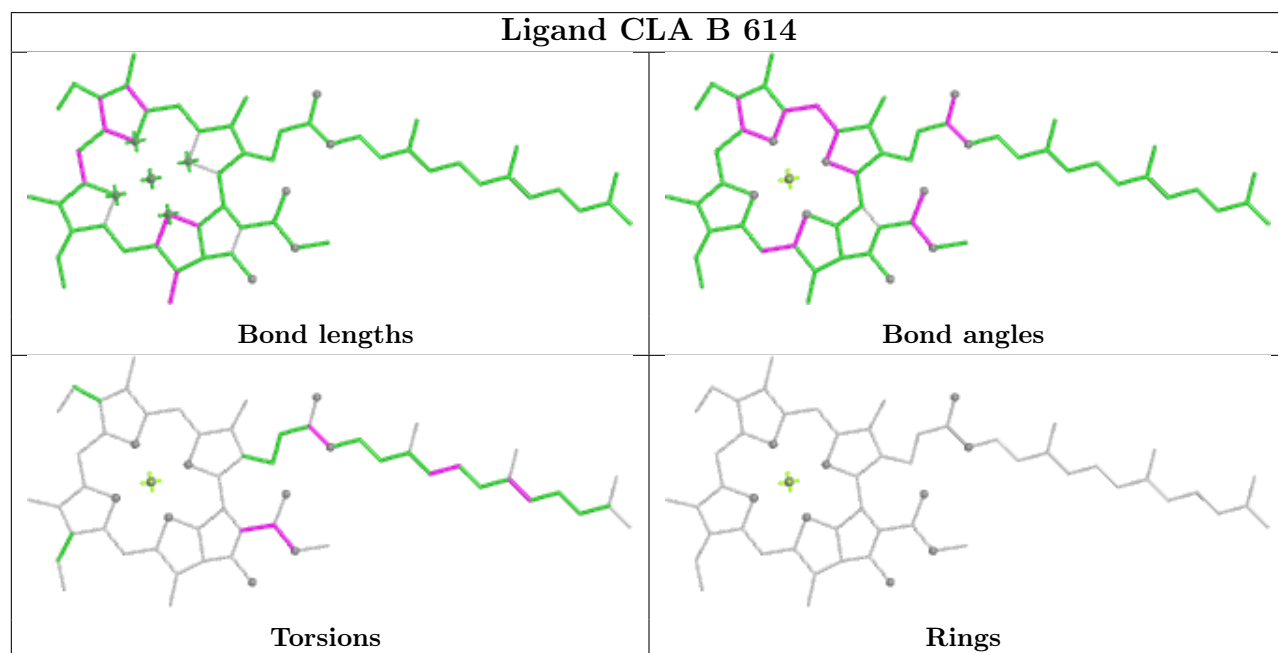
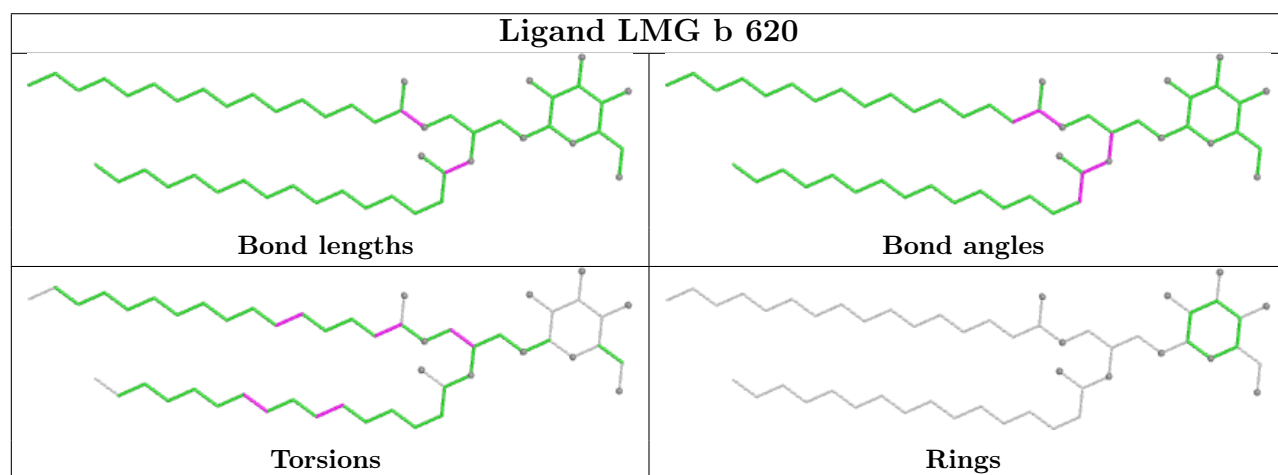
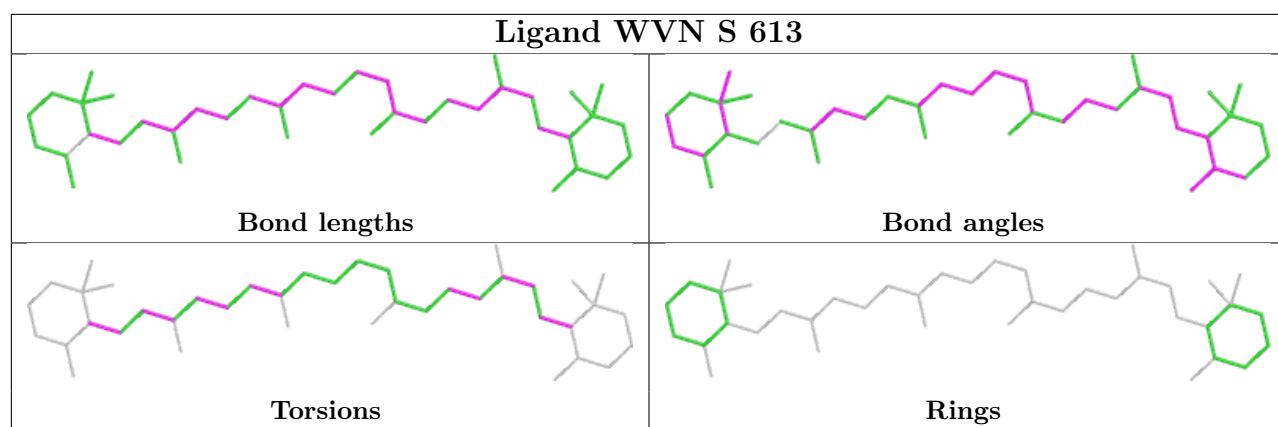


Ligand CLA P 610

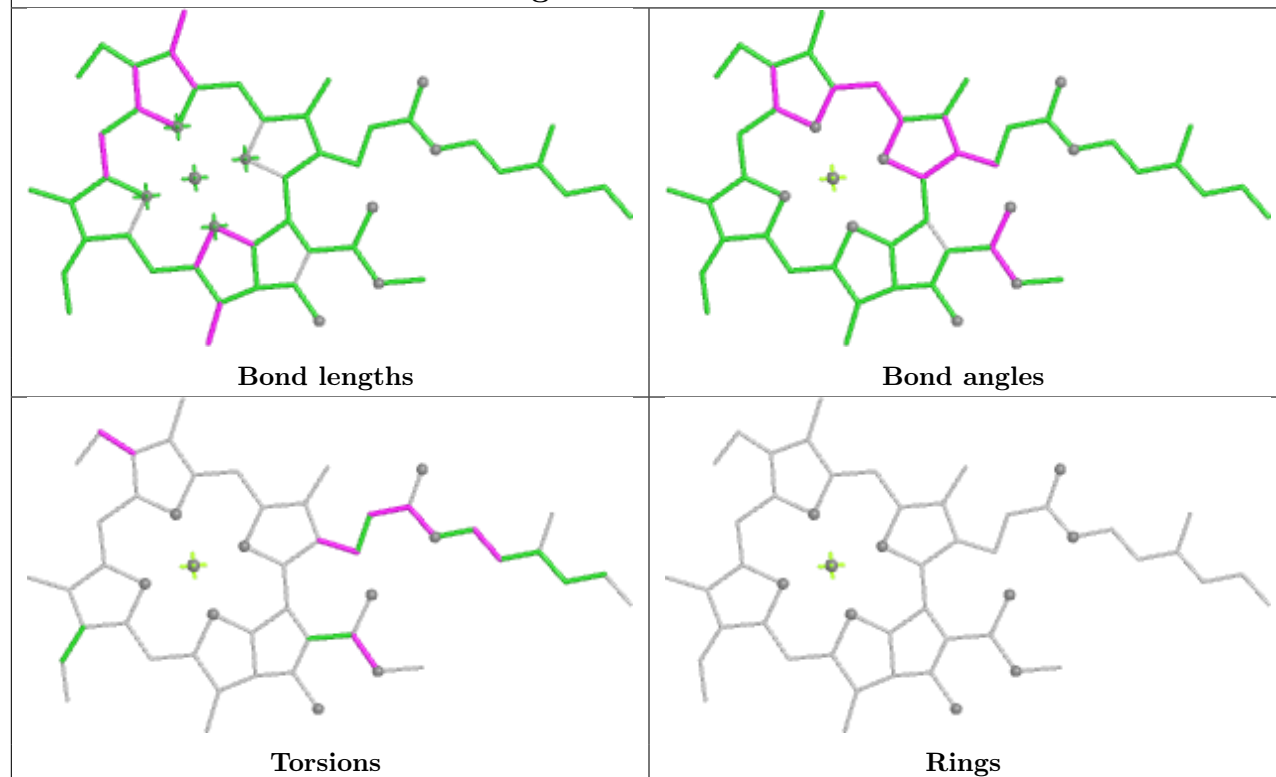


Ligand CLA 4 301

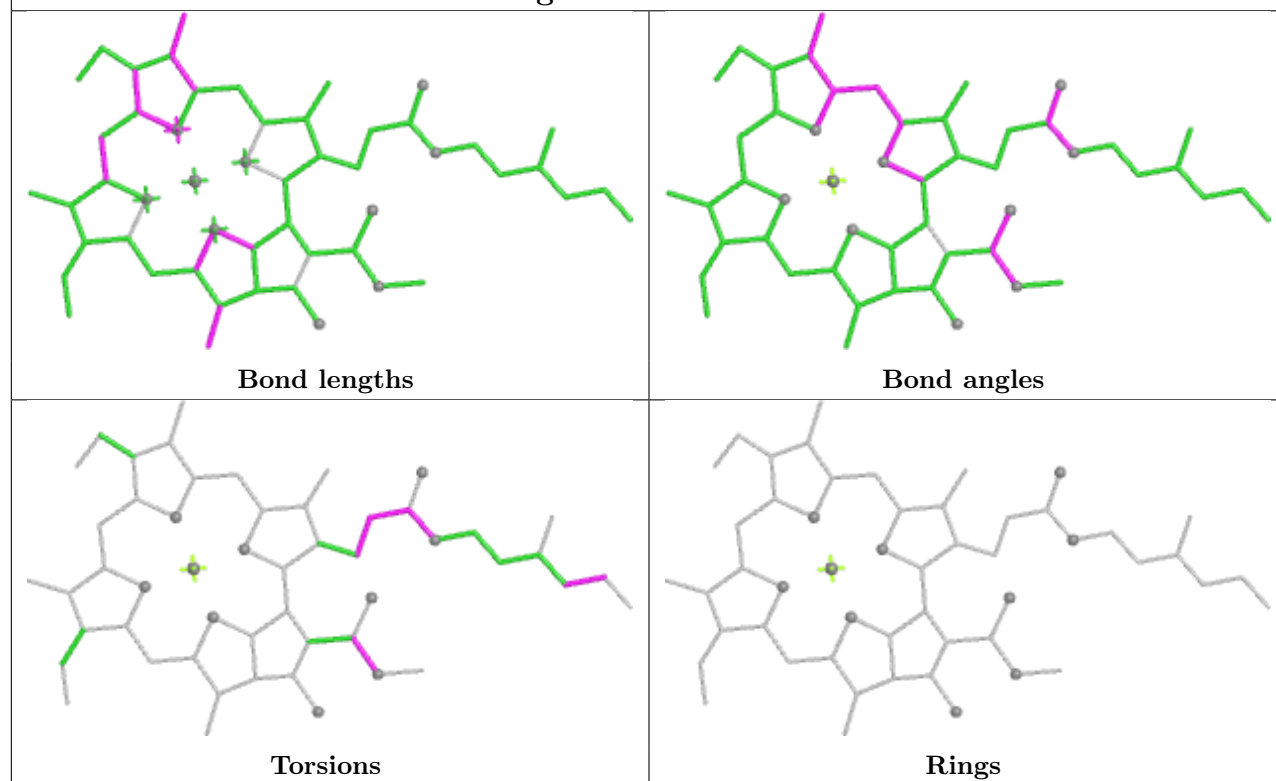


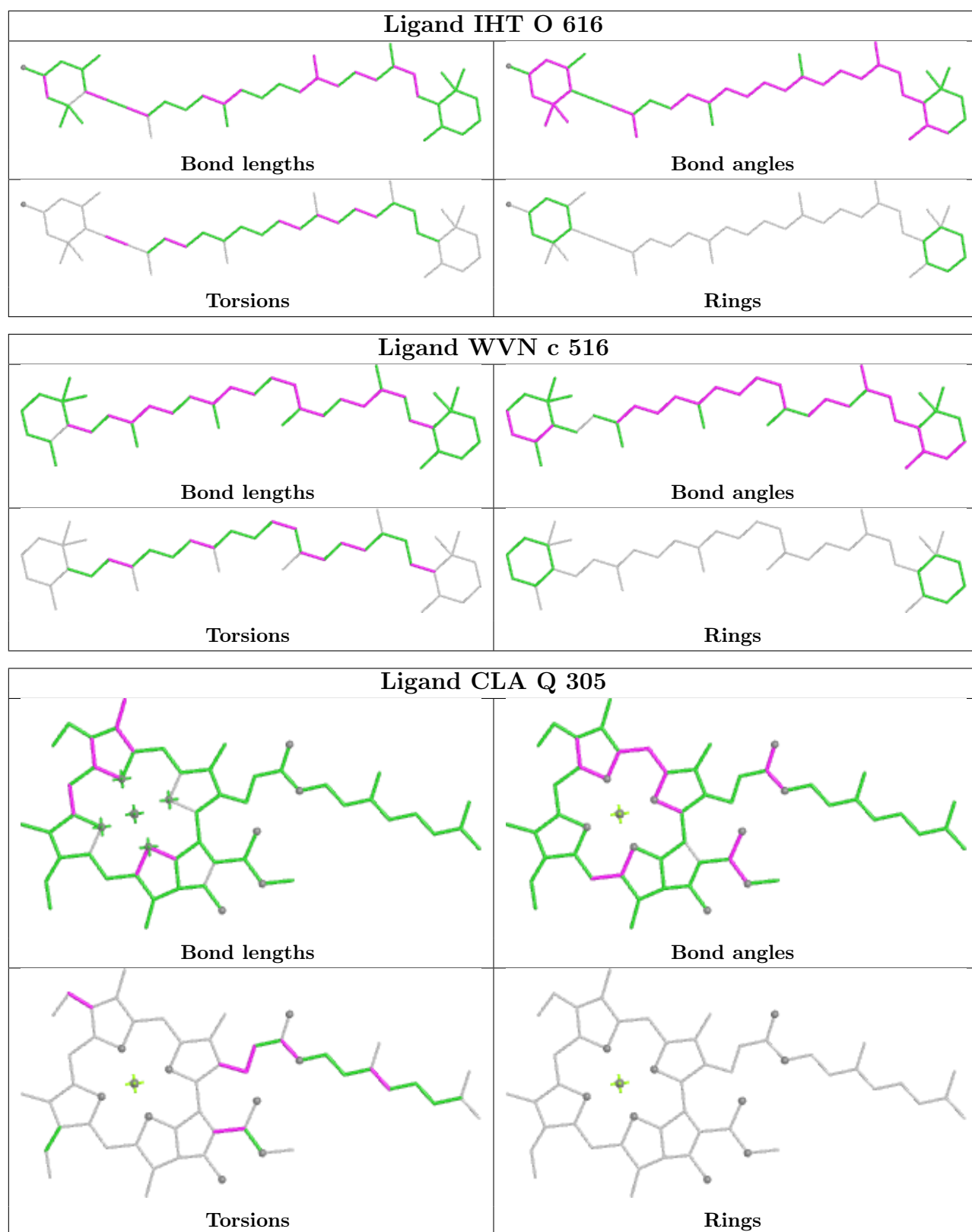


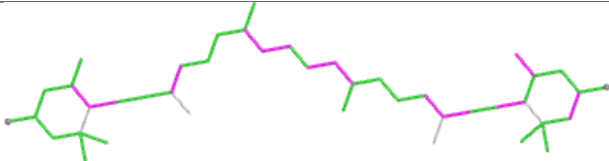
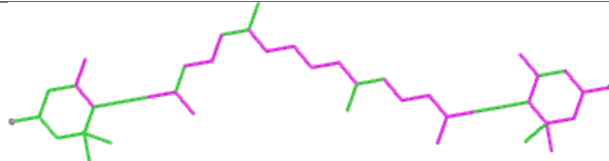
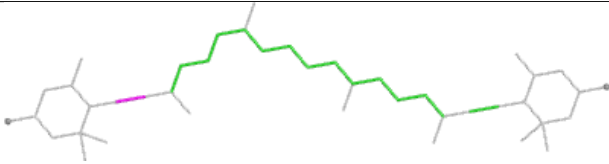
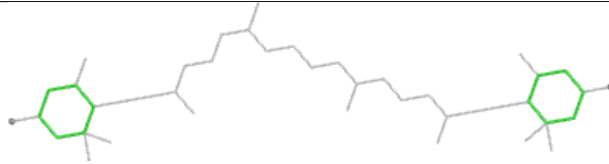
Ligand CLA R 304

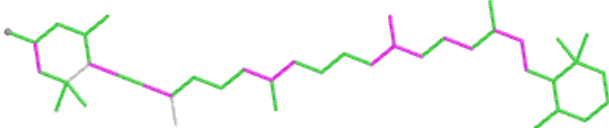
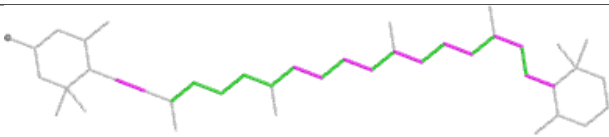
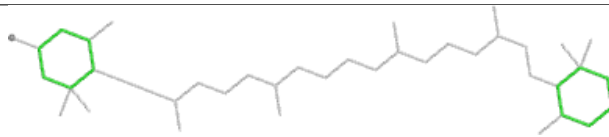


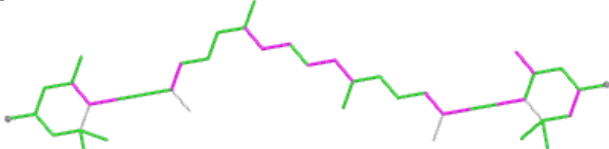
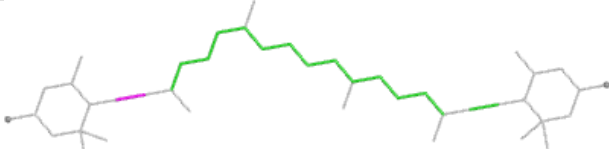
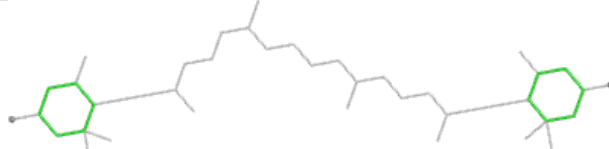
Ligand CLA 1 603

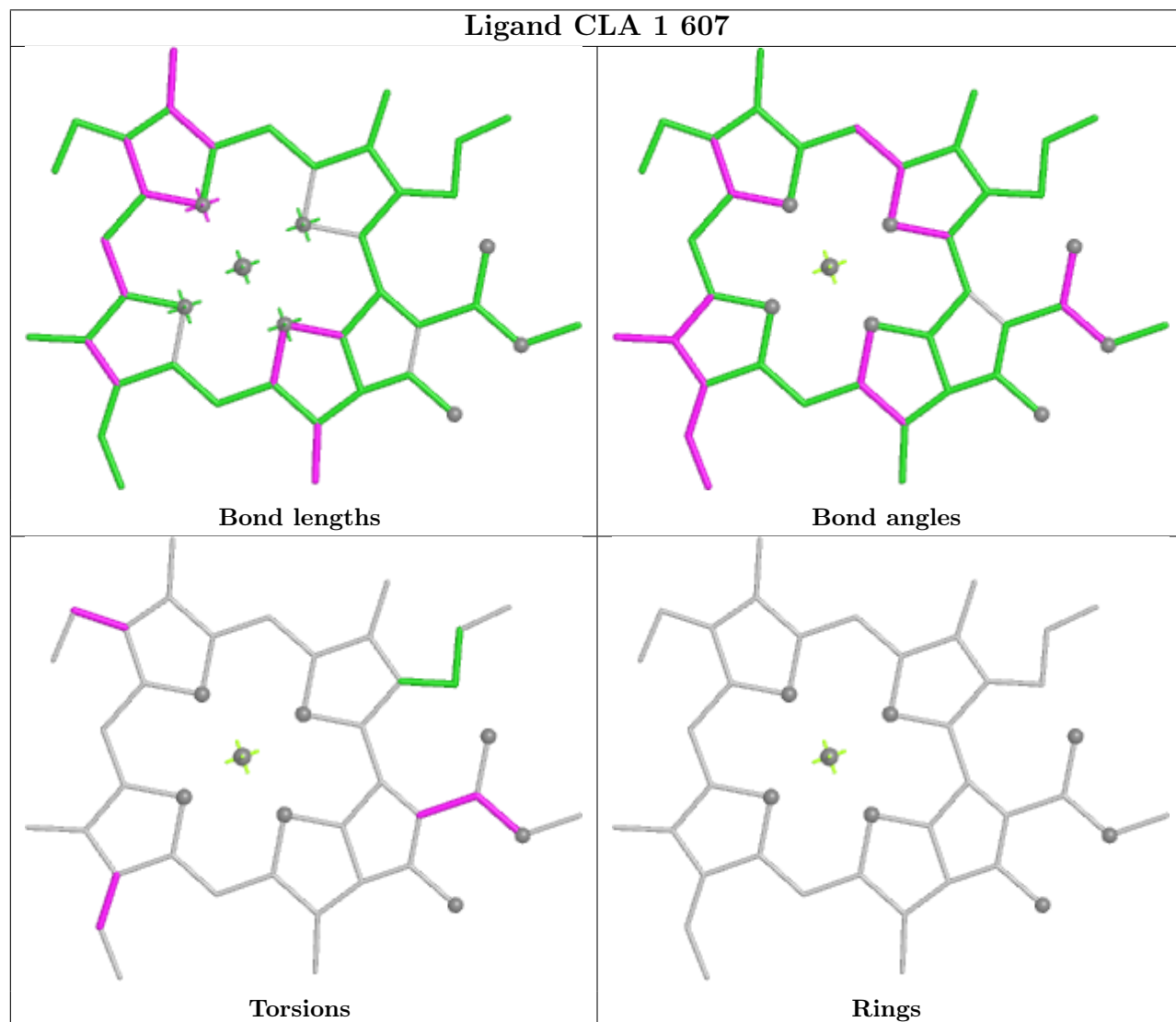
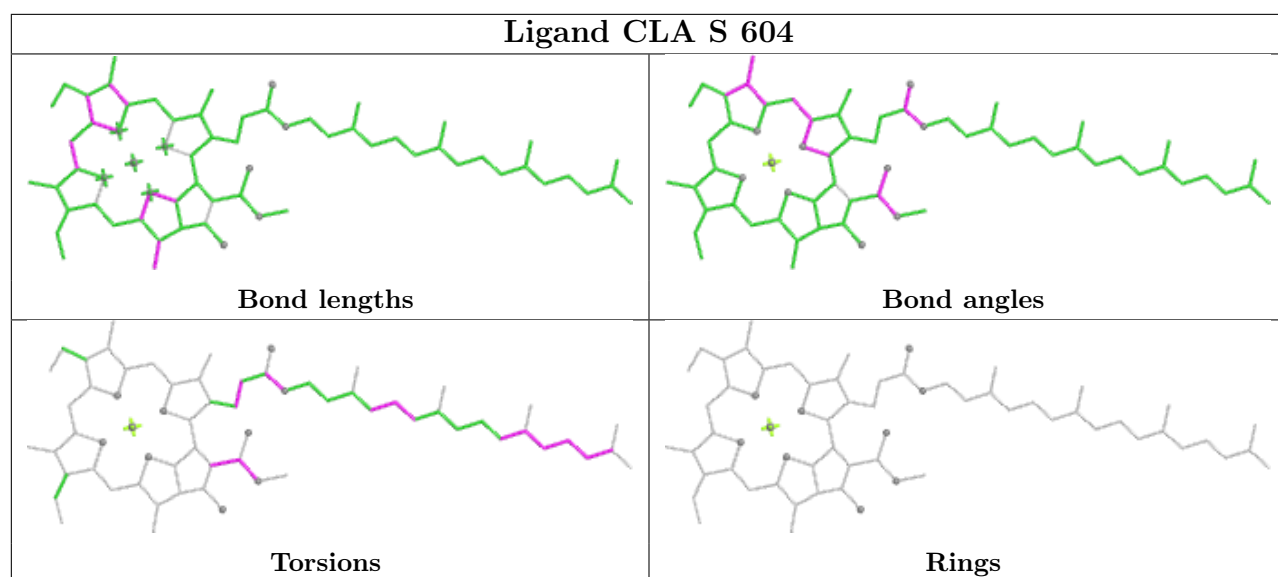


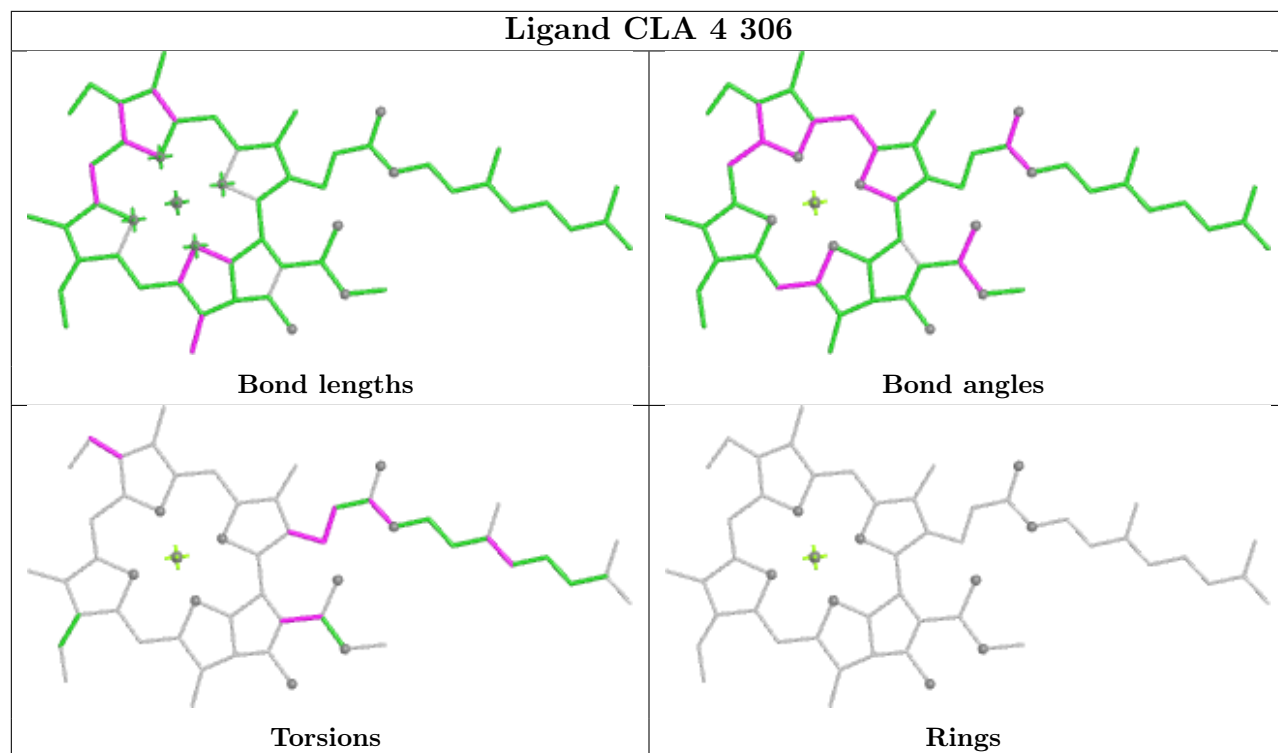
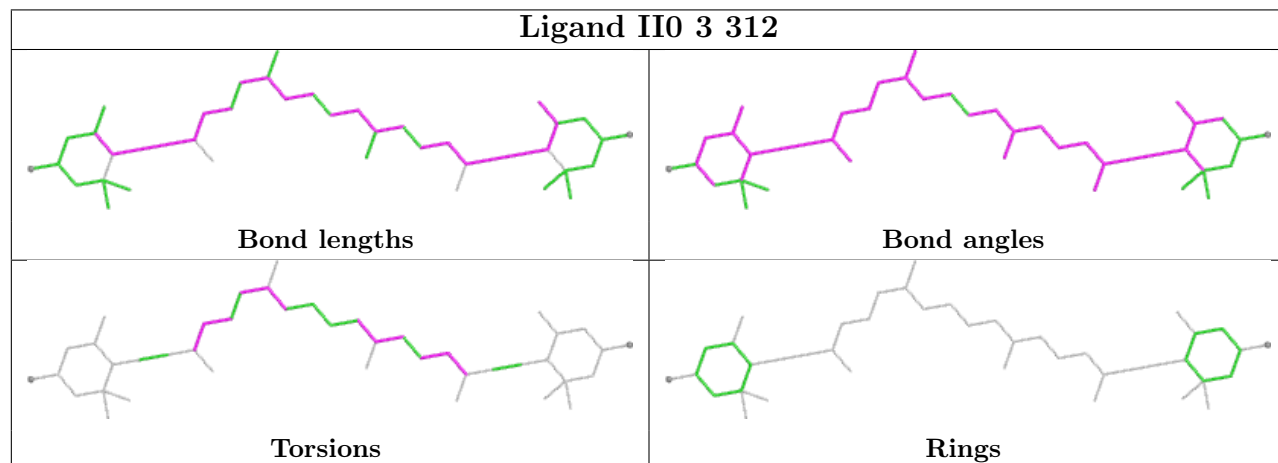


Ligand II0 S 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

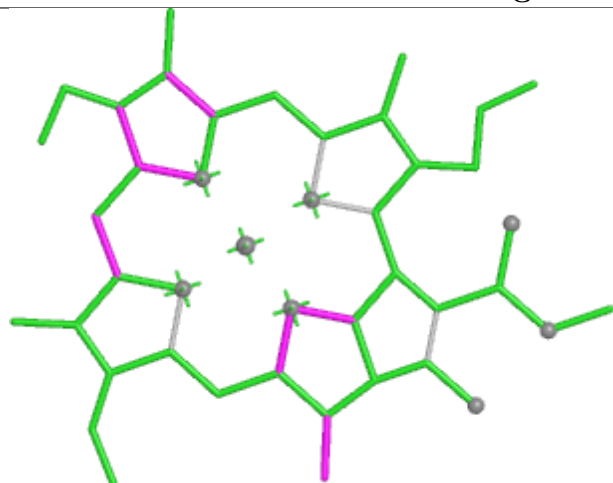
Ligand IHT Q 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 2 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

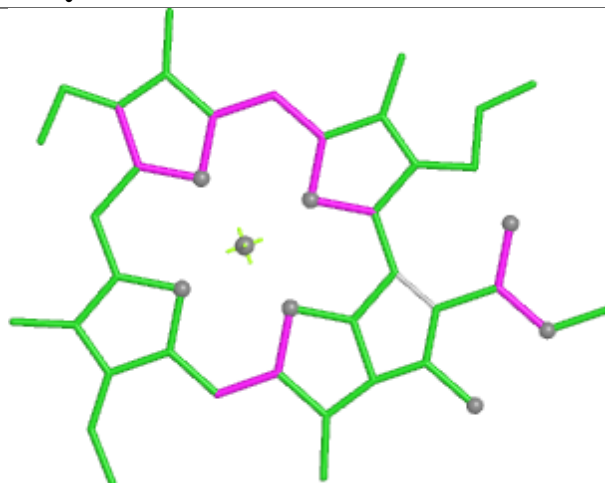


Ligand CLA 4 306**Ligand II0 3 312**

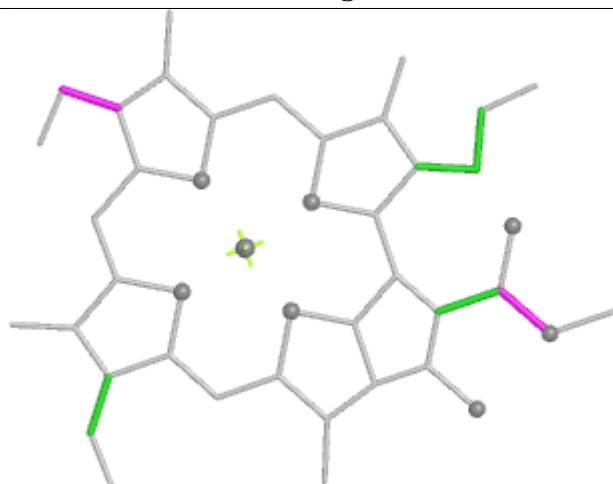
Ligand CLA Q 312



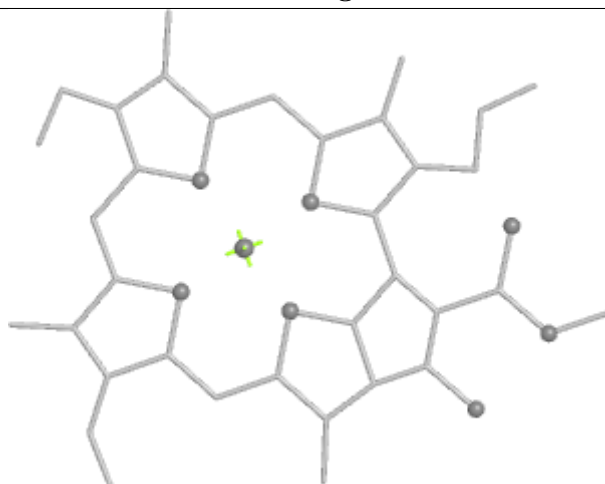
Bond lengths



Bond angles

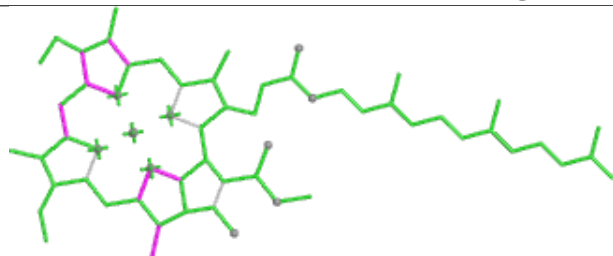


Torsions

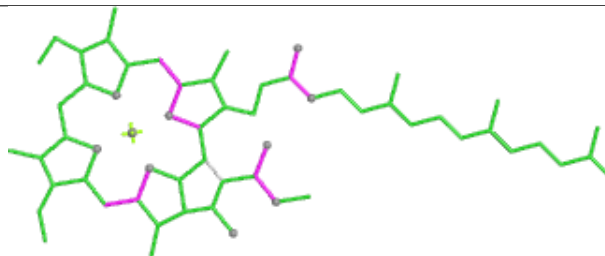


Rings

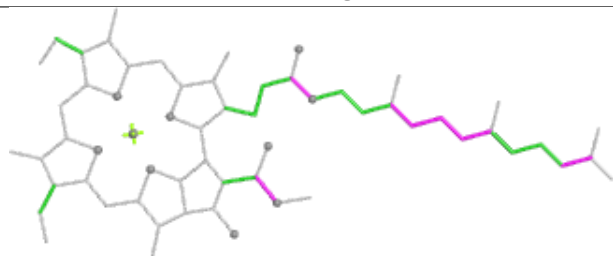
Ligand CLA O 611



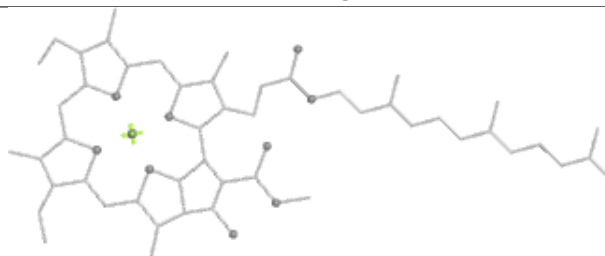
Bond lengths



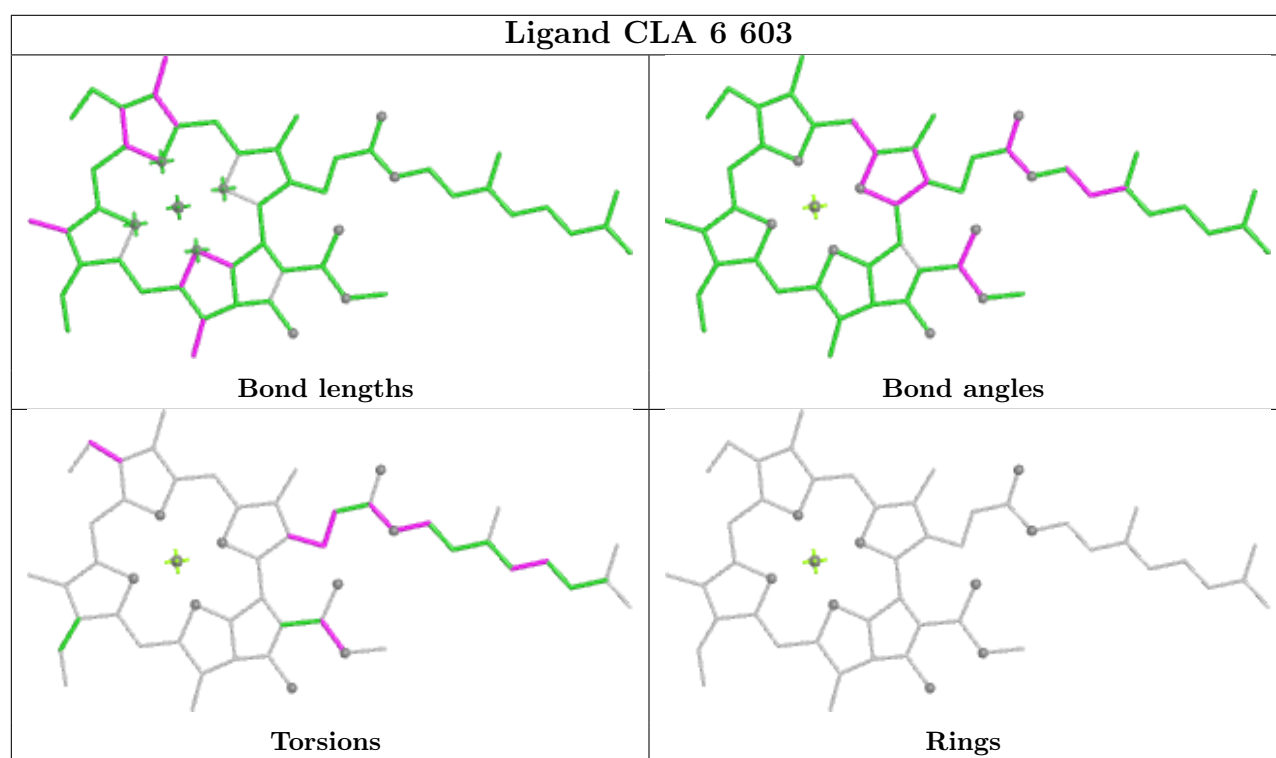
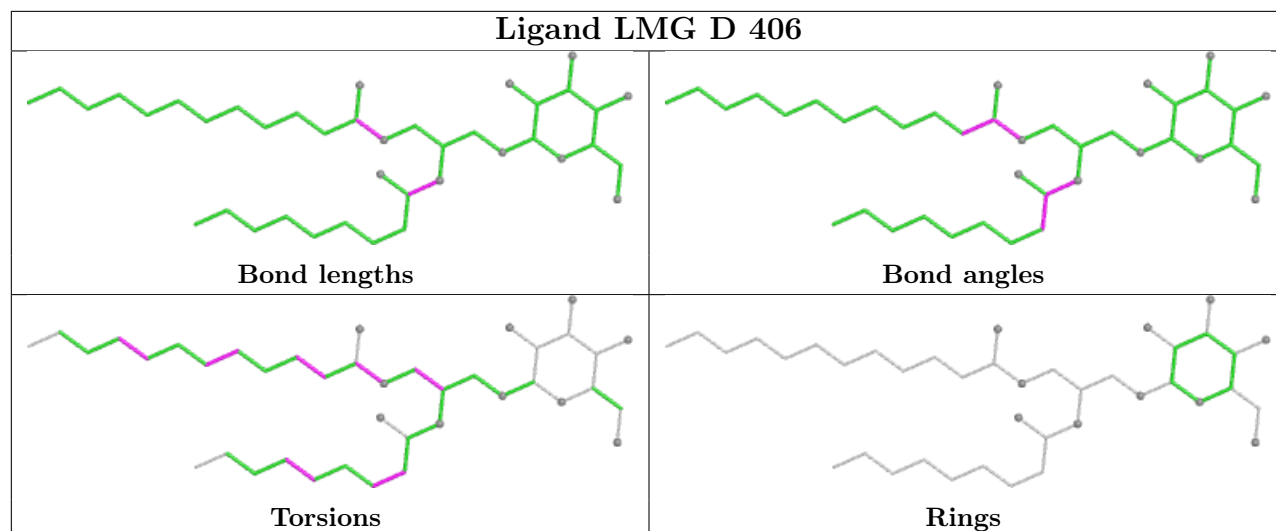
Bond angles



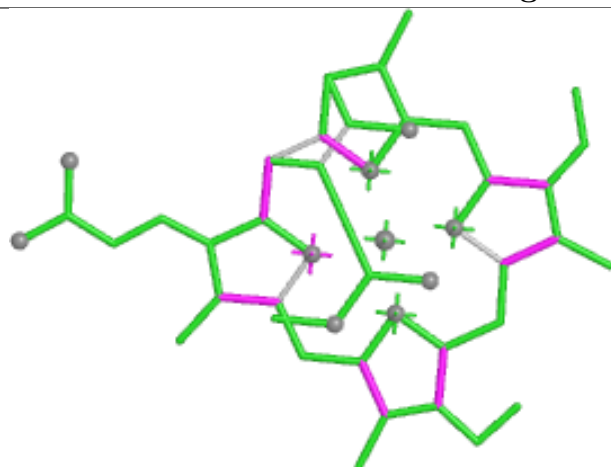
Torsions



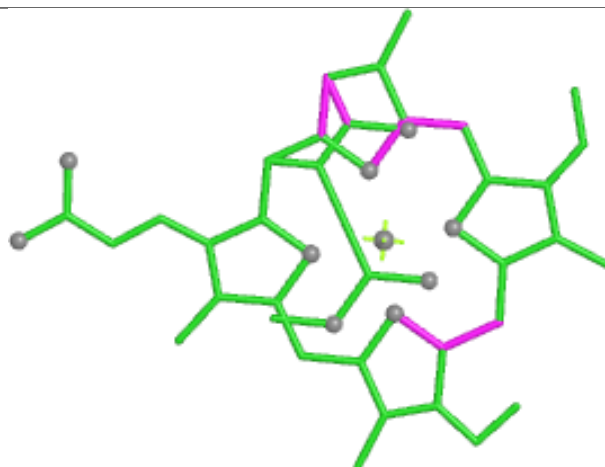
Rings



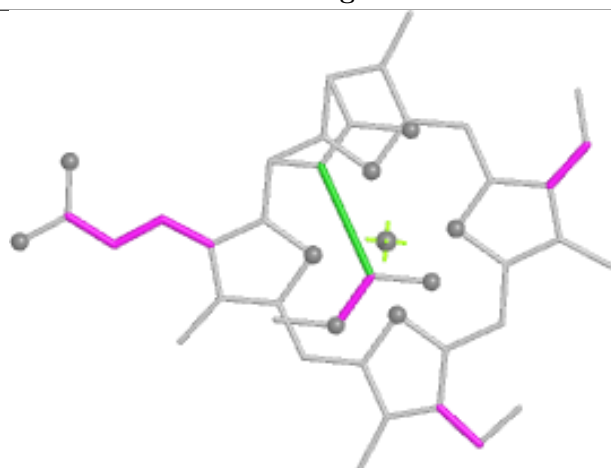
Ligand KC2 1 612



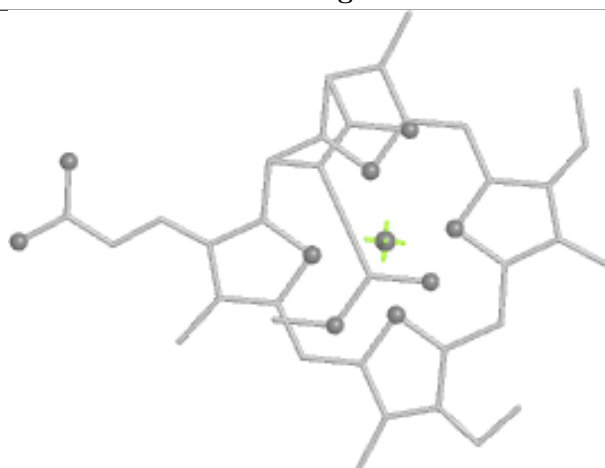
Bond lengths



Bond angles

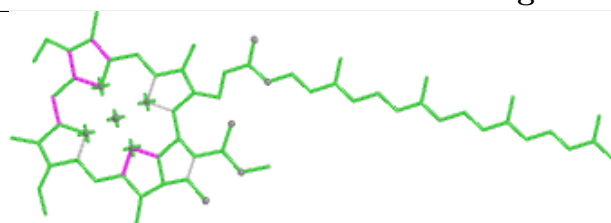


Torsions

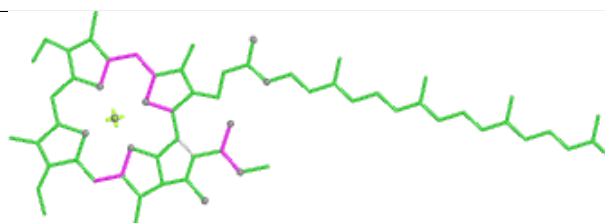


Rings

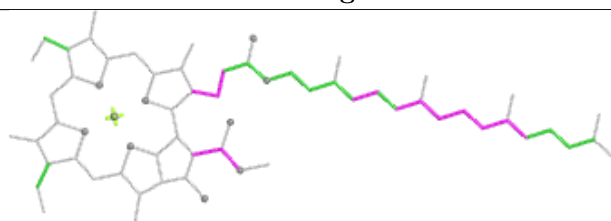
Ligand CLA S 602



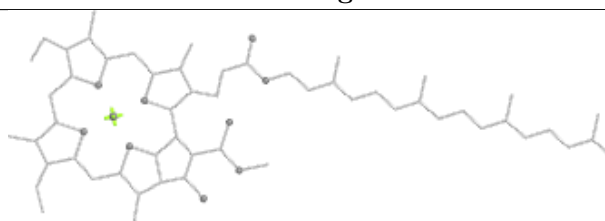
Bond lengths



Bond angles

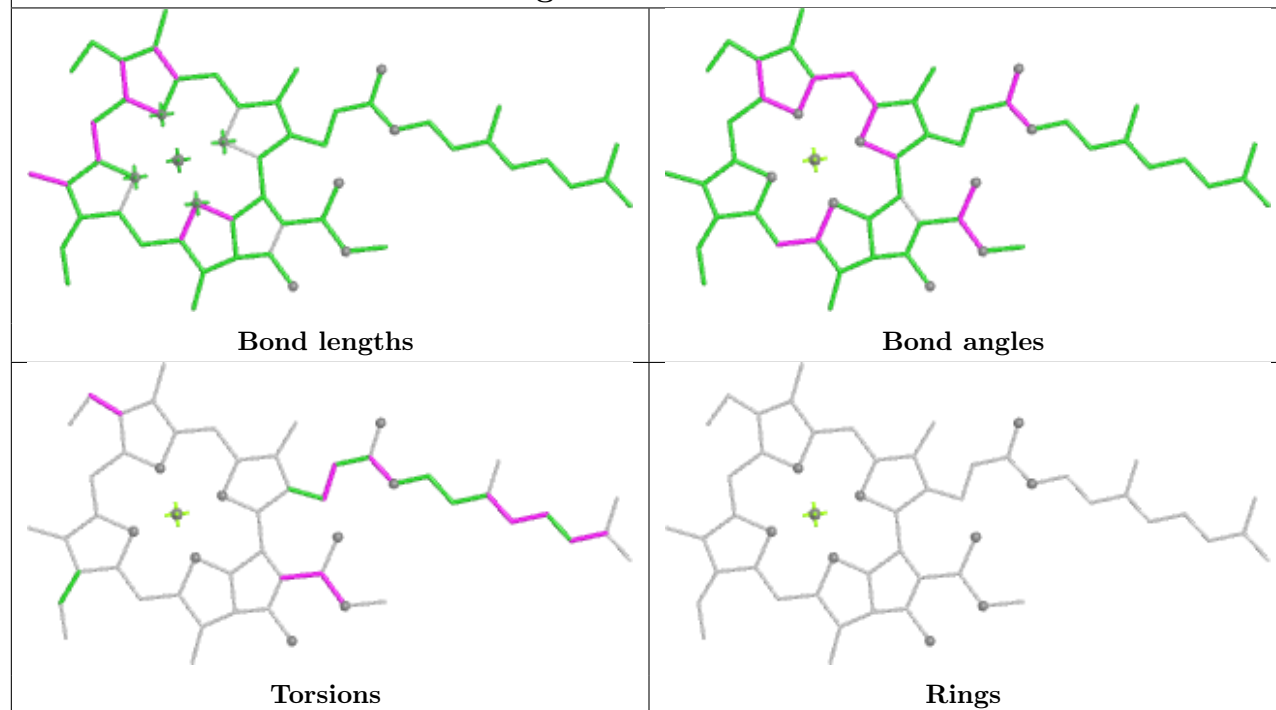


Torsions

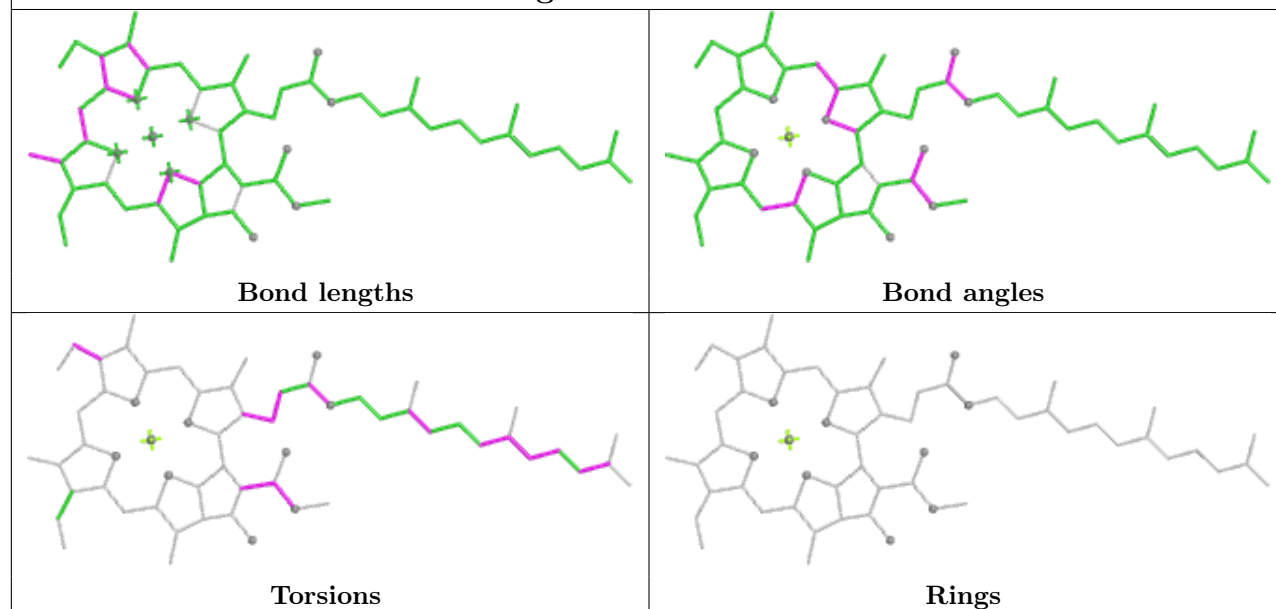


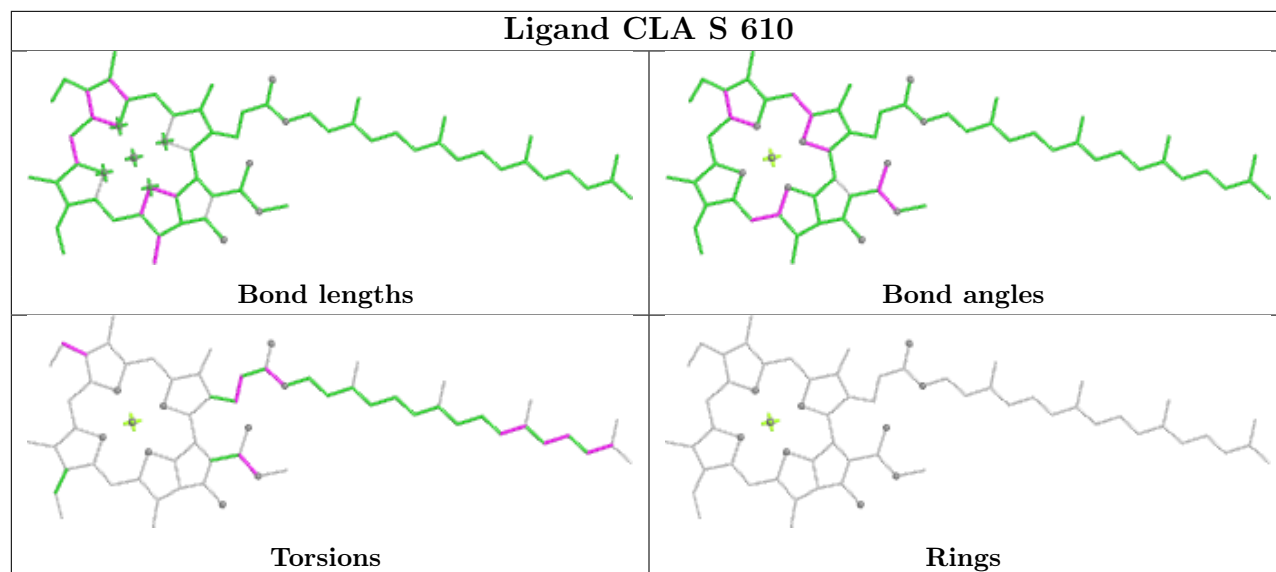
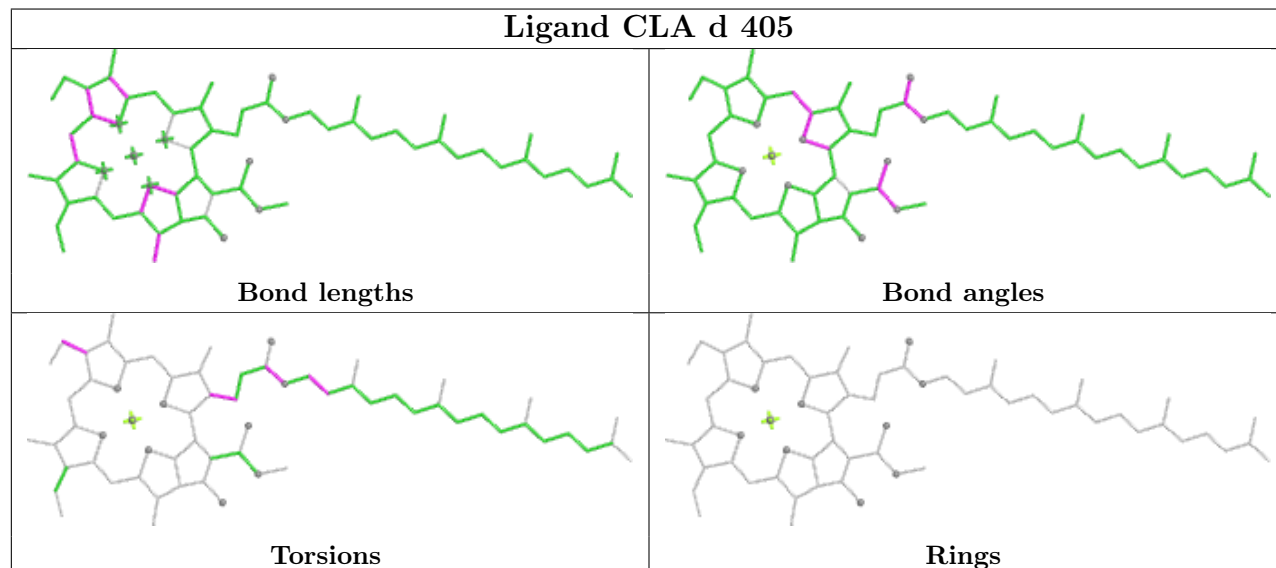
Rings

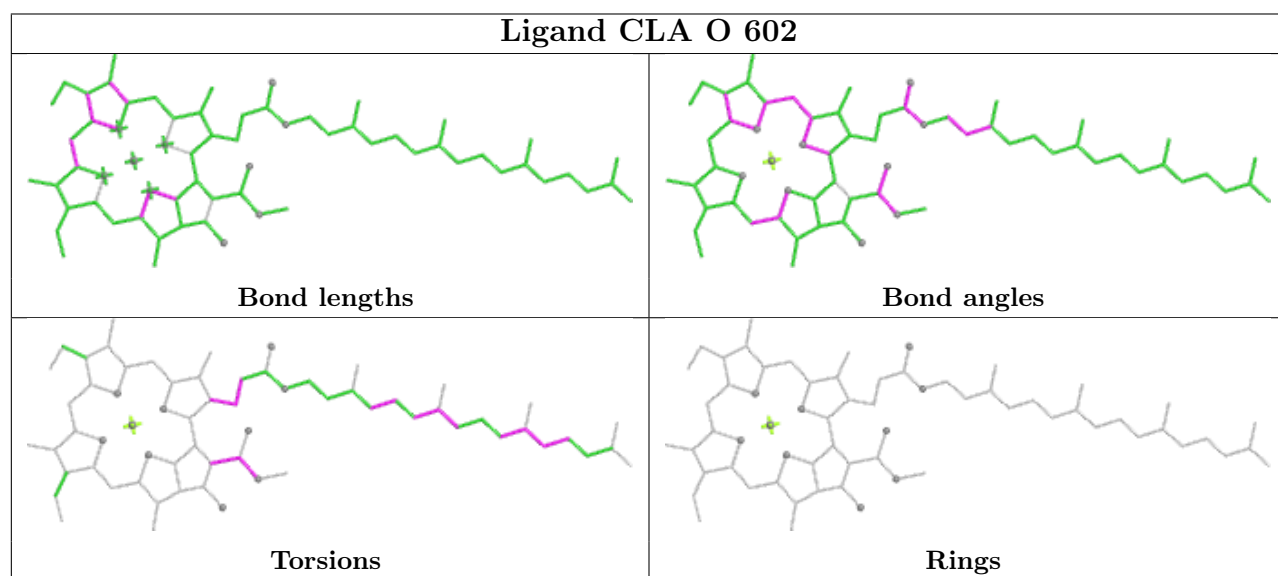
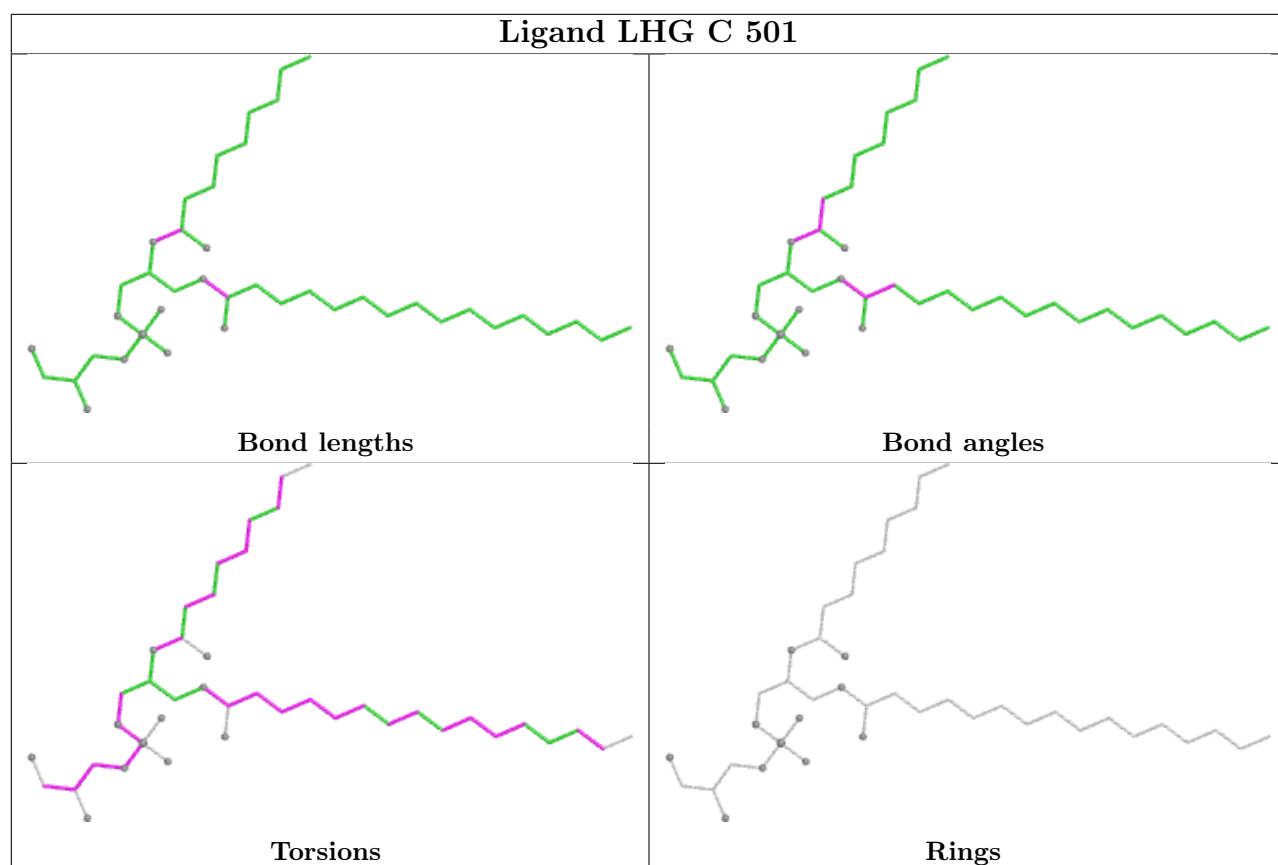
Ligand CLA 5 602

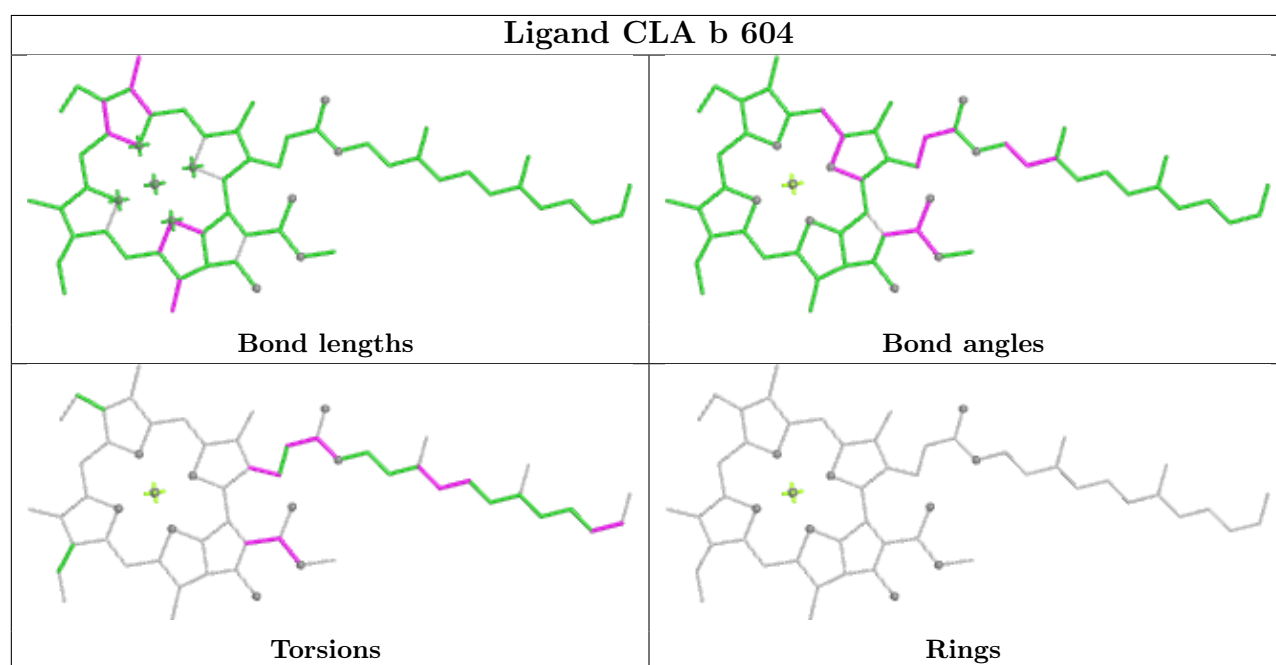
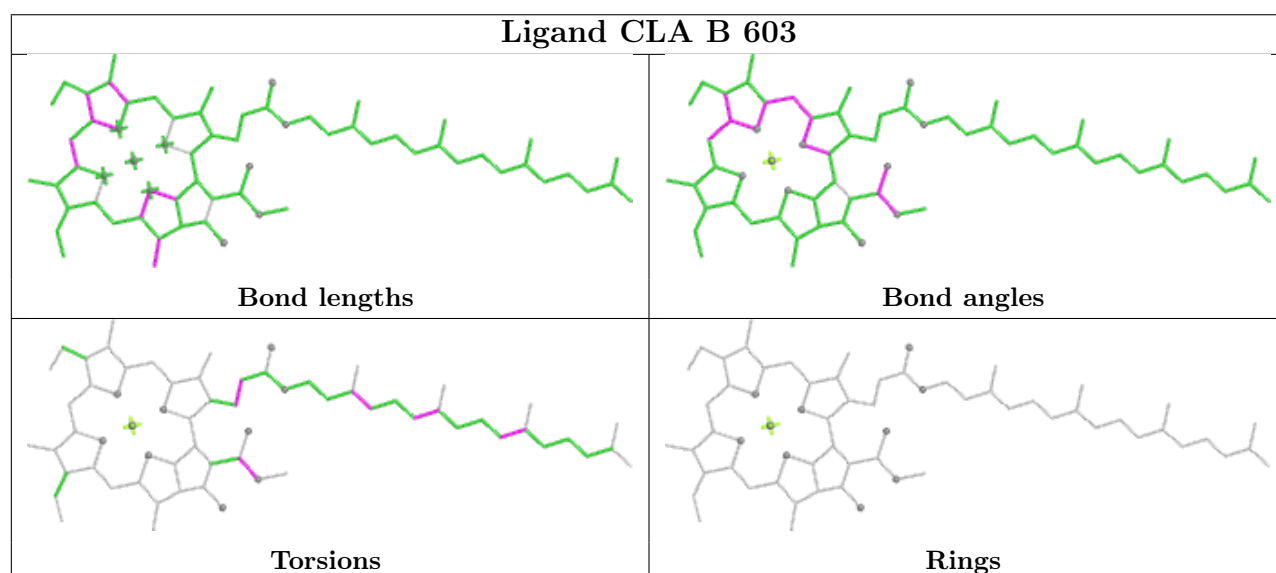
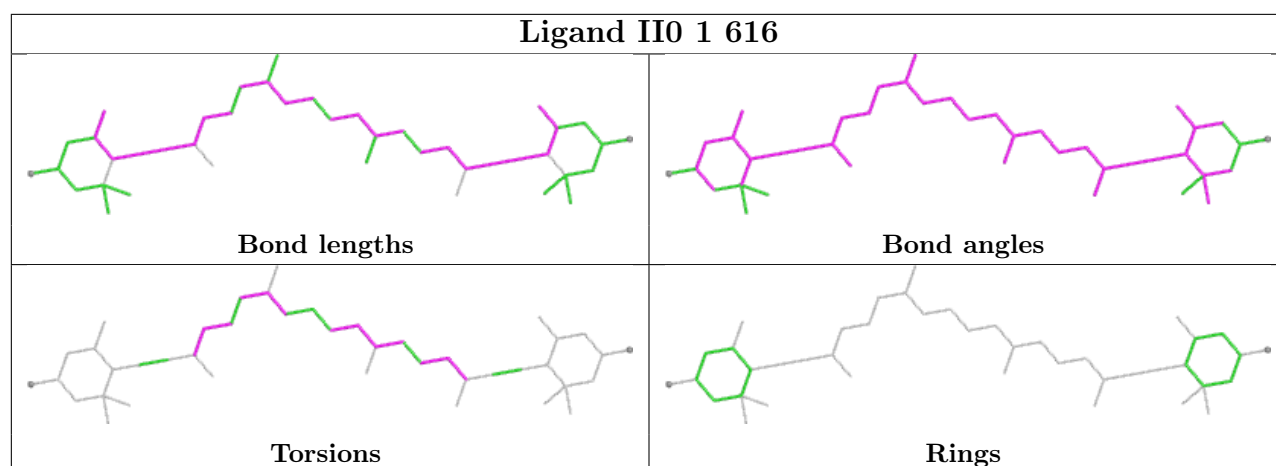


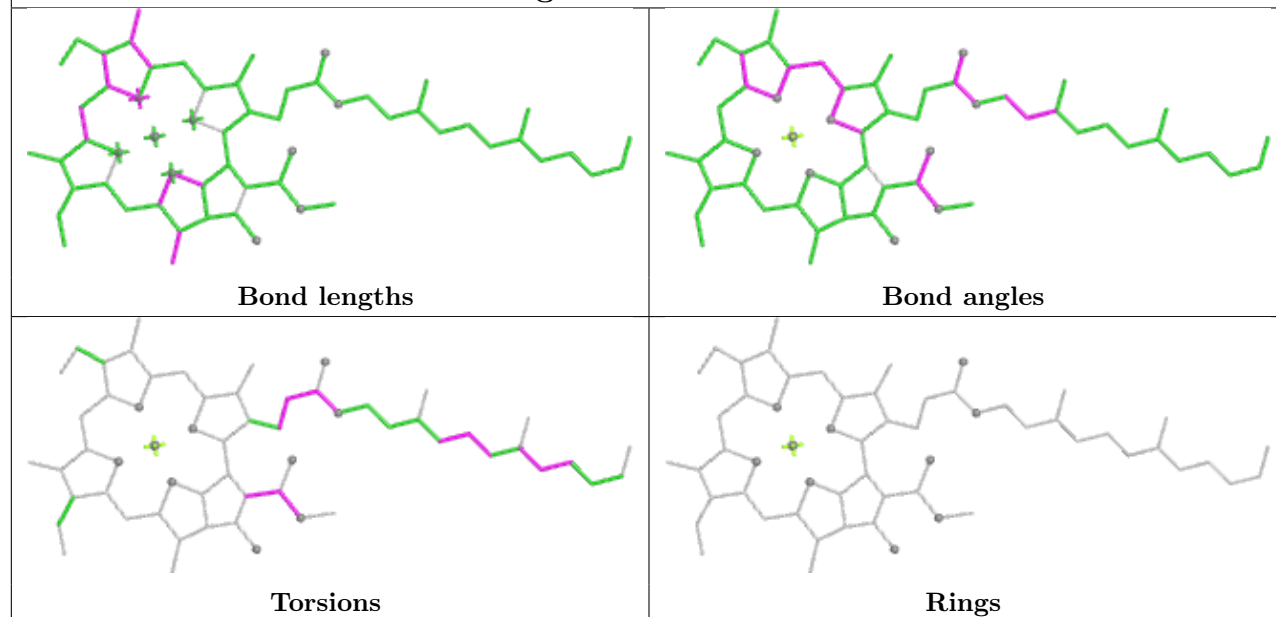
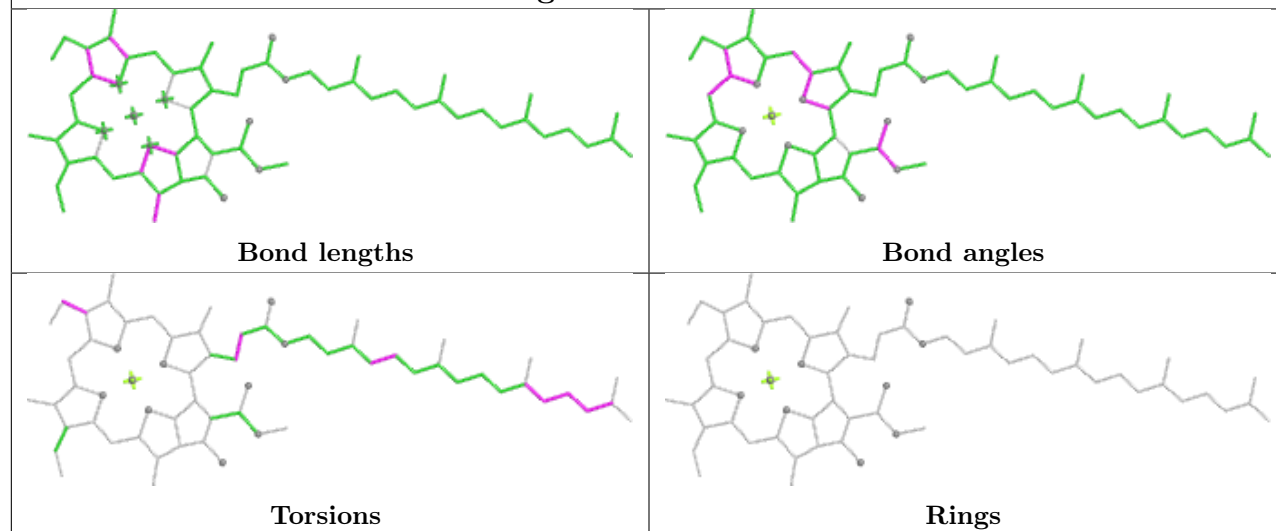
Ligand CLA 2 309

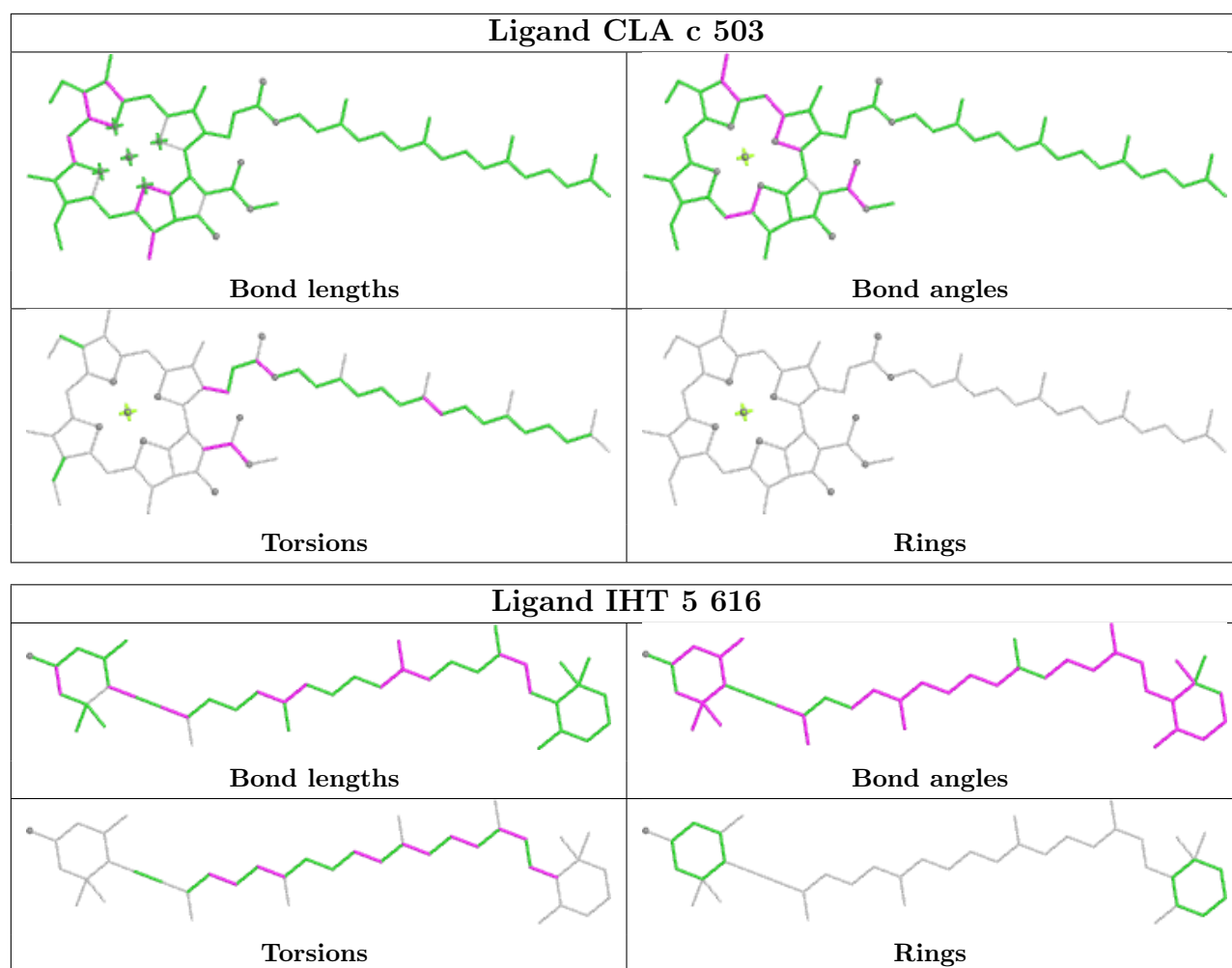


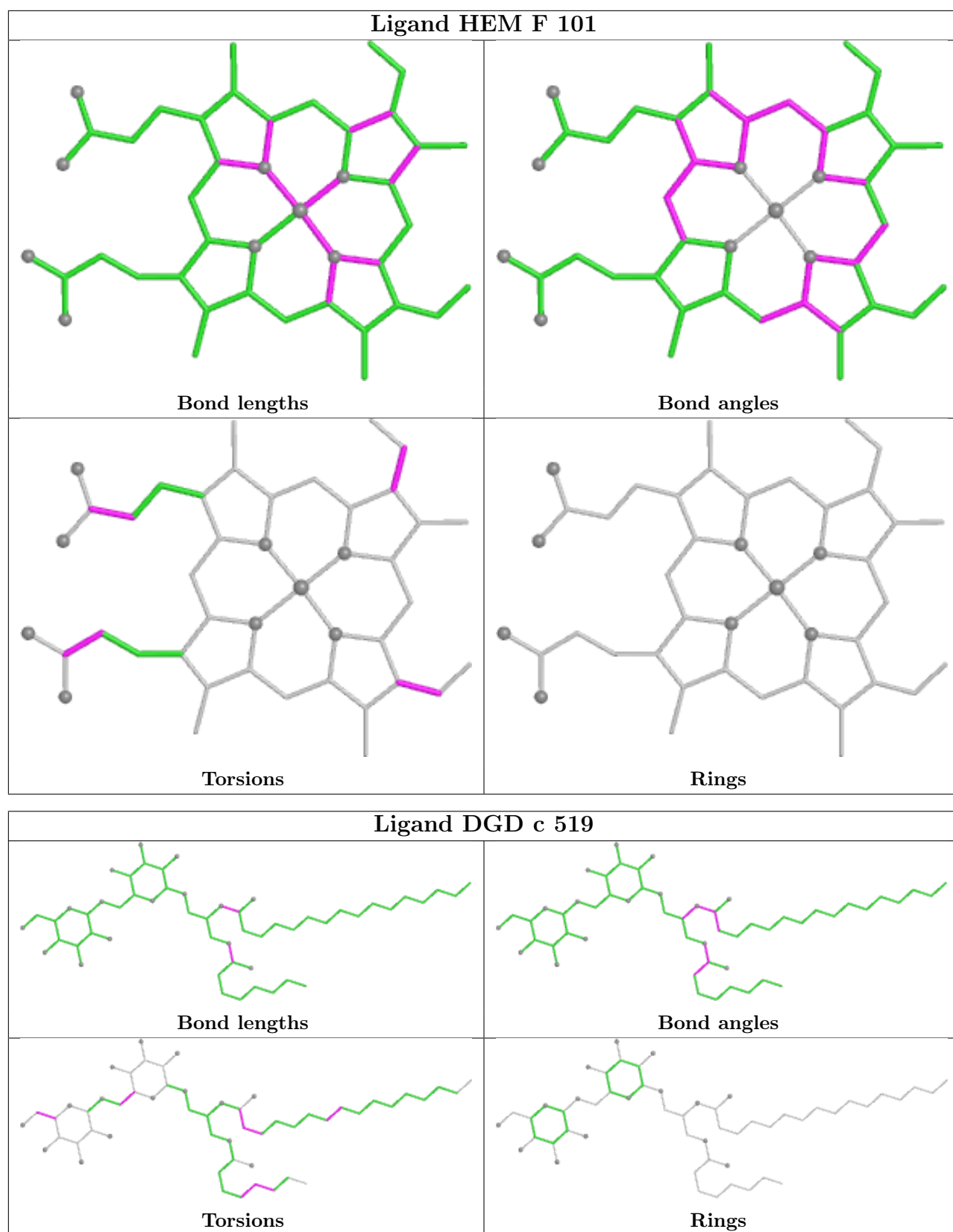
Ligand CLA S 610**Ligand CLA d 405**

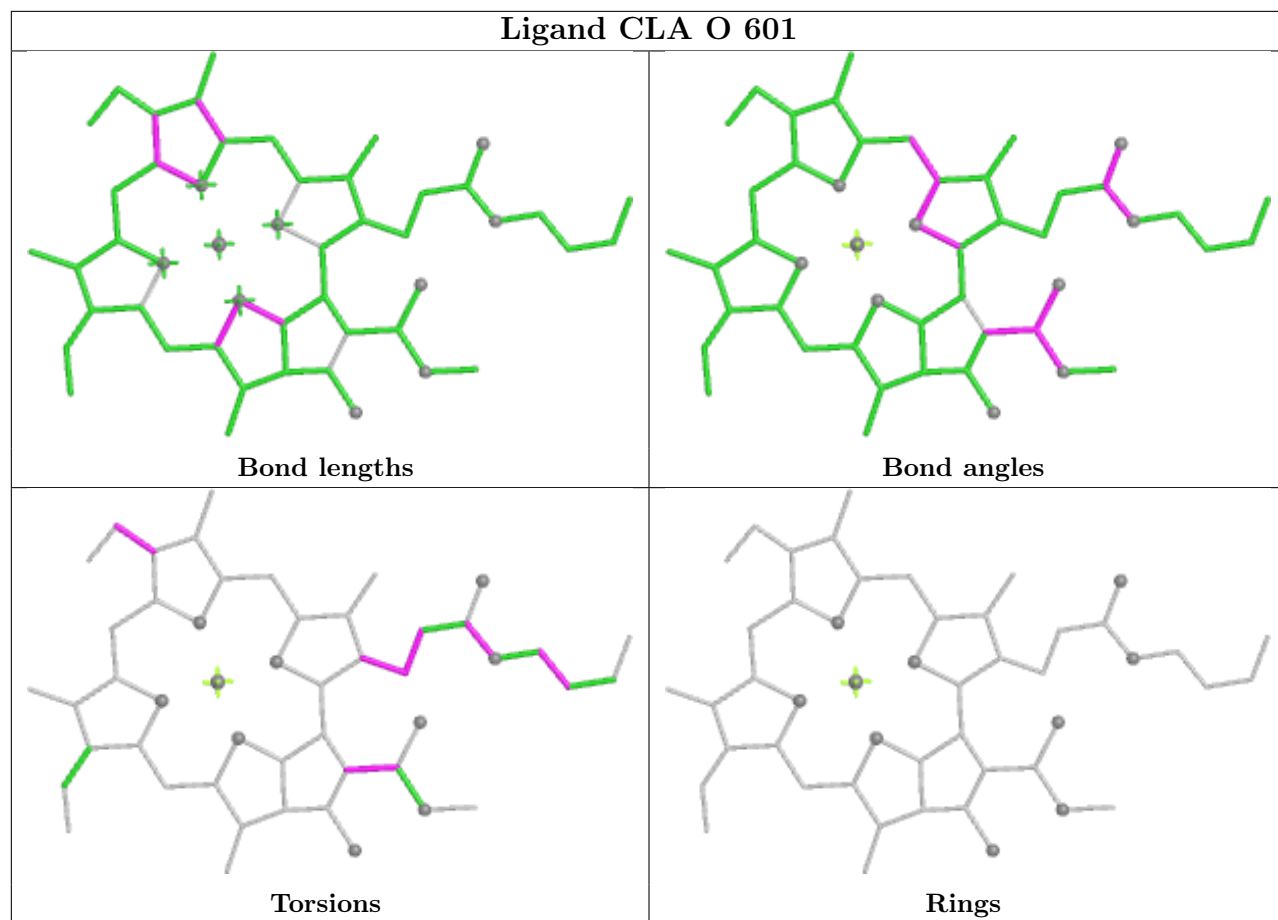


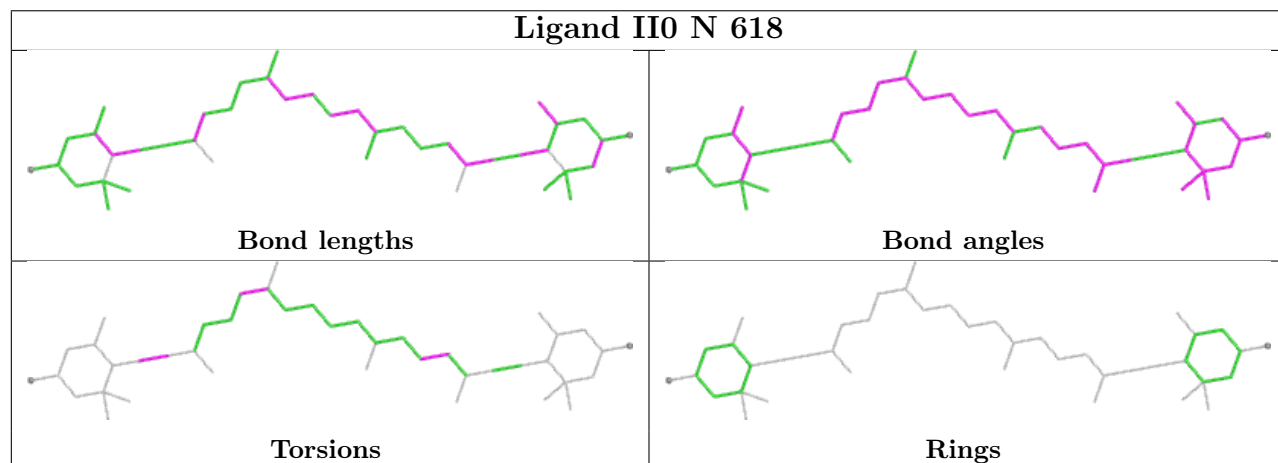
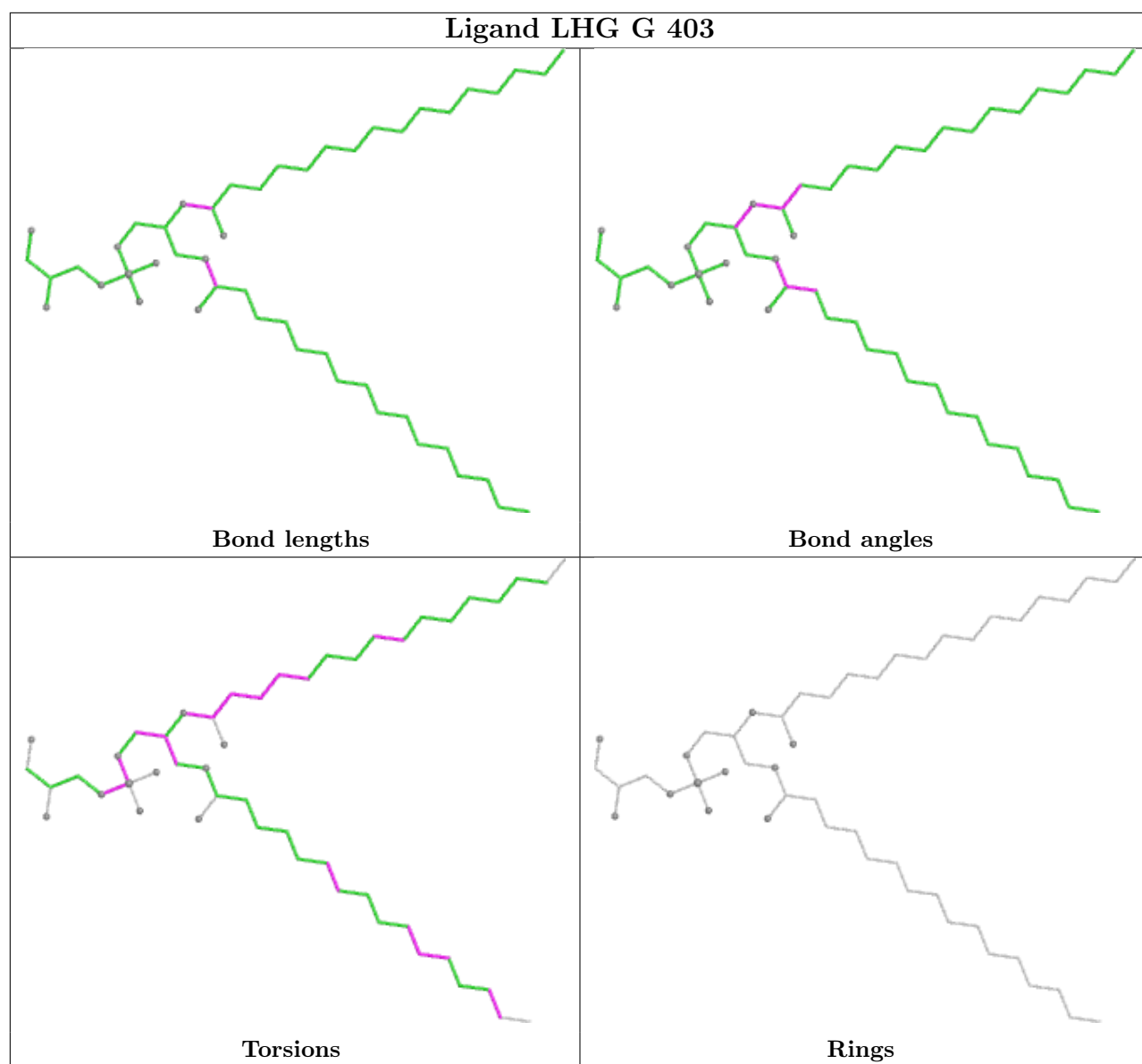


Ligand CLA 1 604**Ligand CLA c 509**

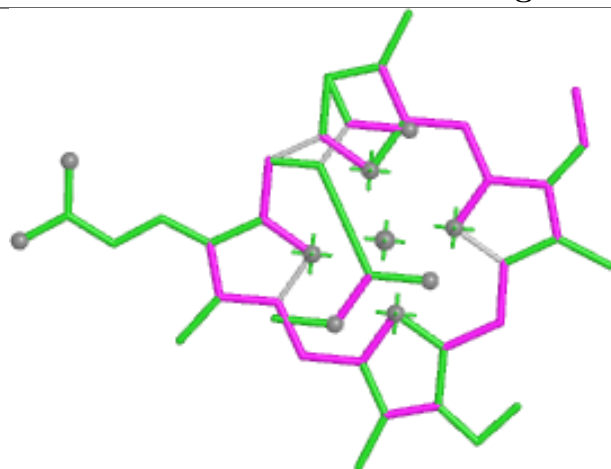




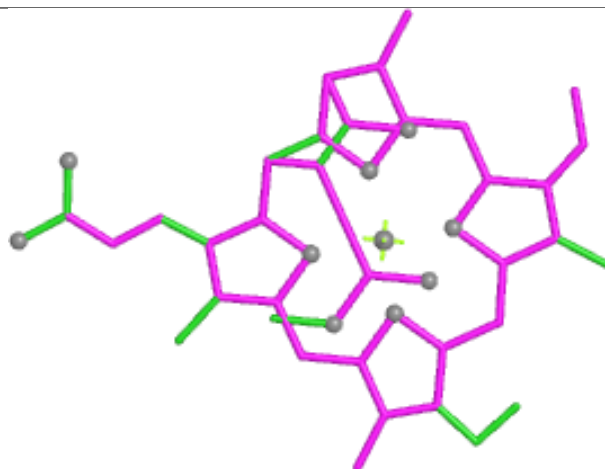




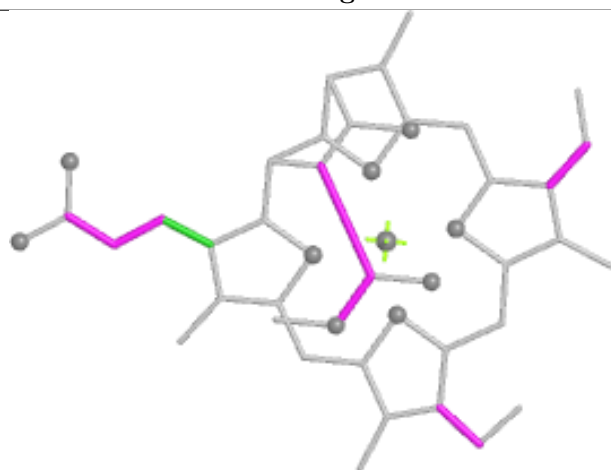
Ligand KC2 N 605



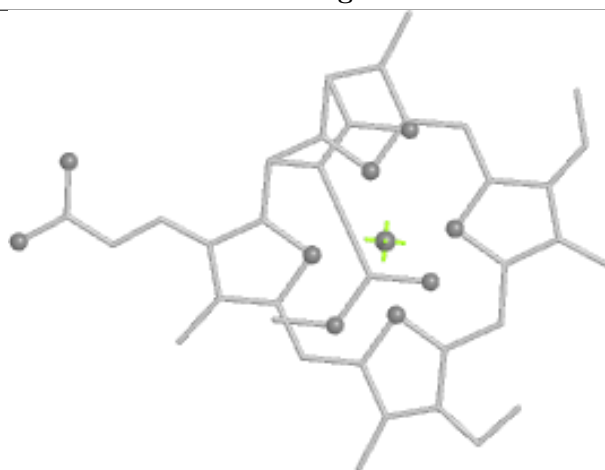
Bond lengths



Bond angles

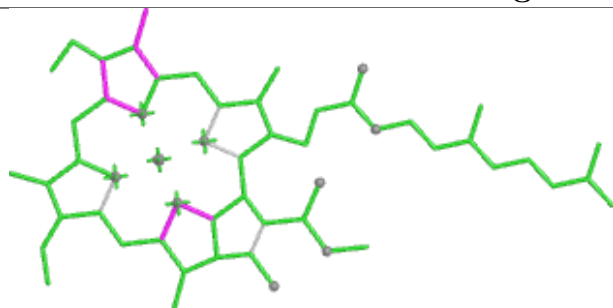


Torsions

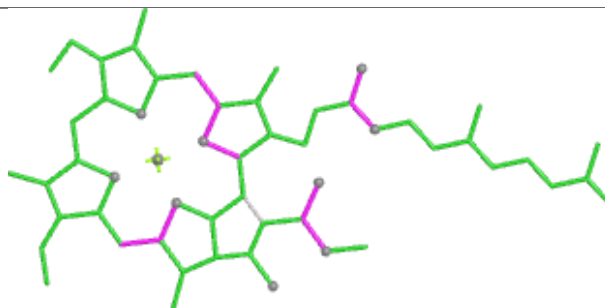


Rings

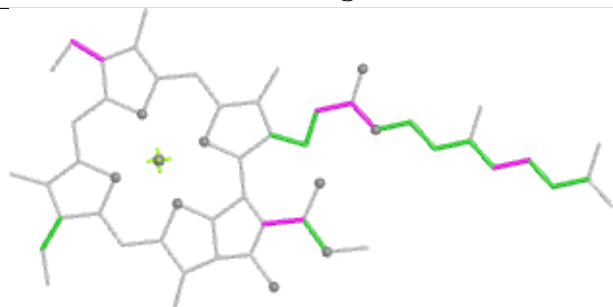
Ligand CLA R 302



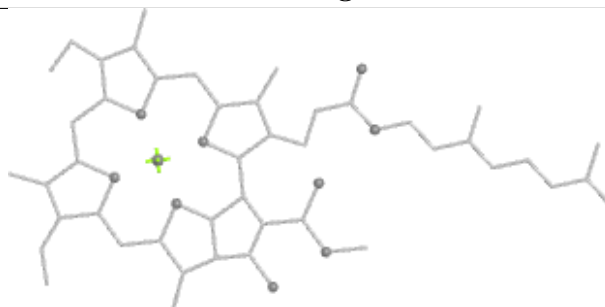
Bond lengths



Bond angles

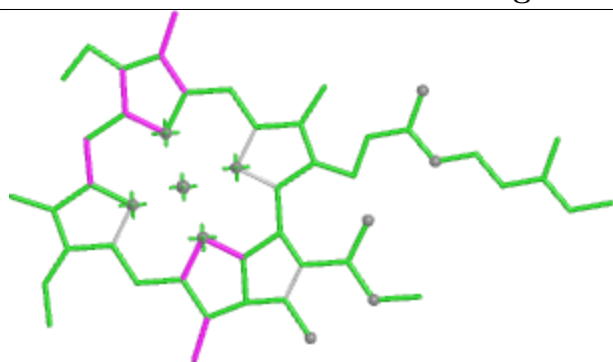


Torsions

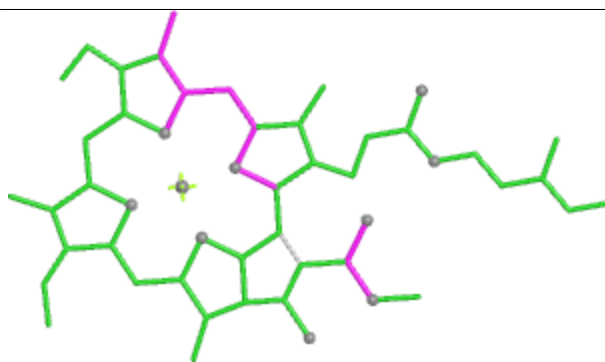


Rings

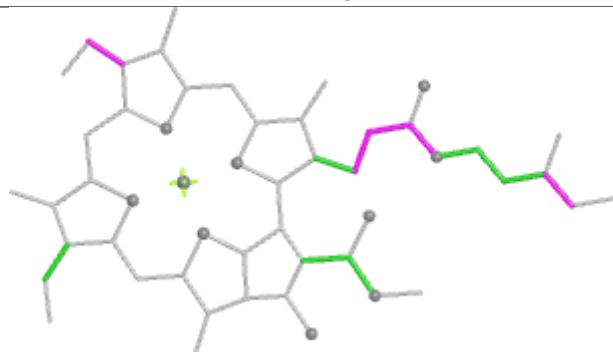
Ligand CLA N 603



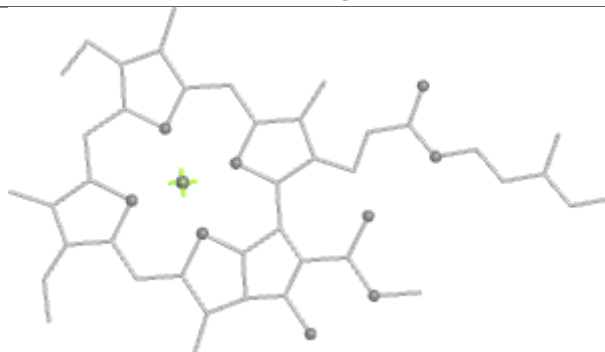
Bond lengths



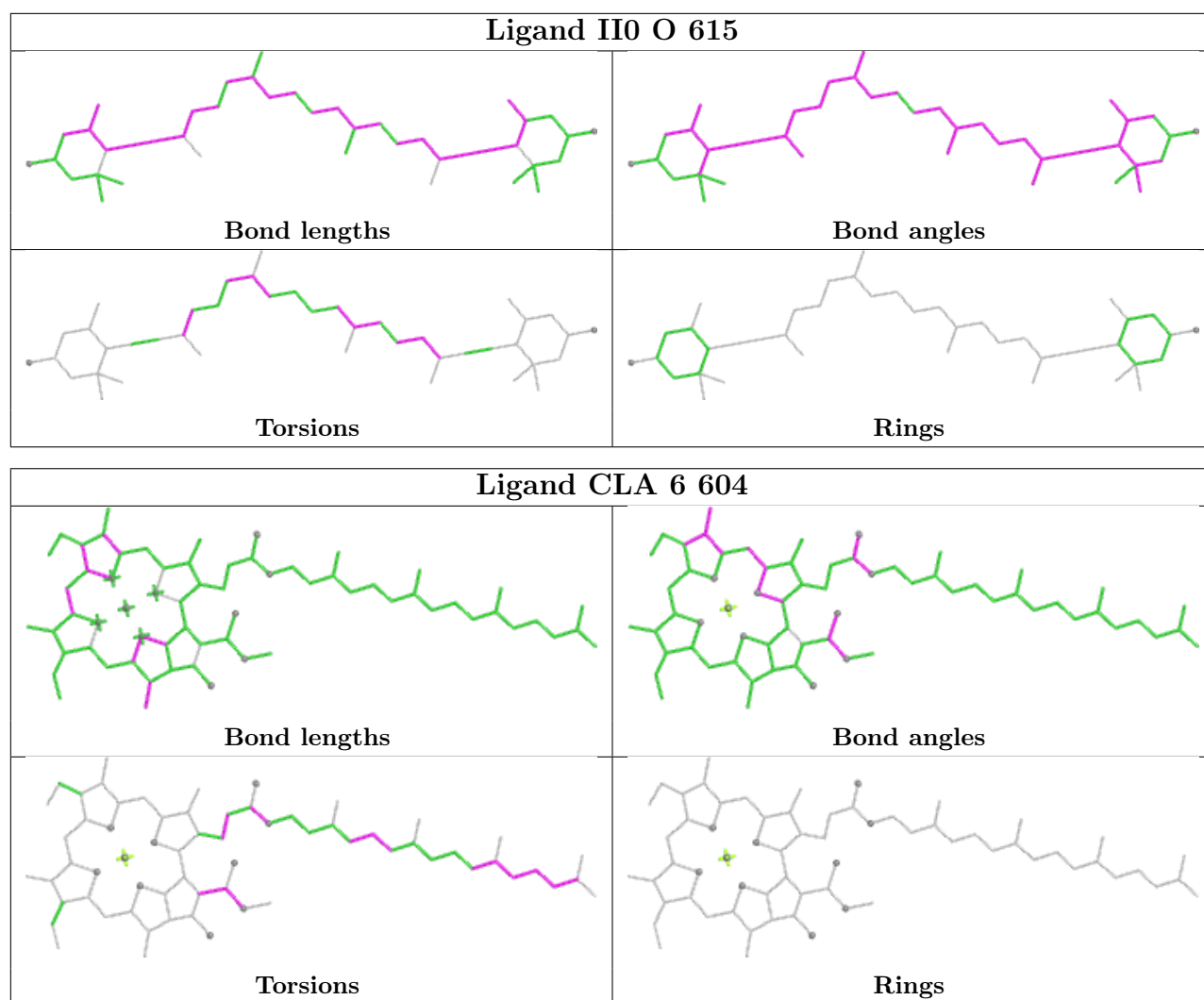
Bond angles



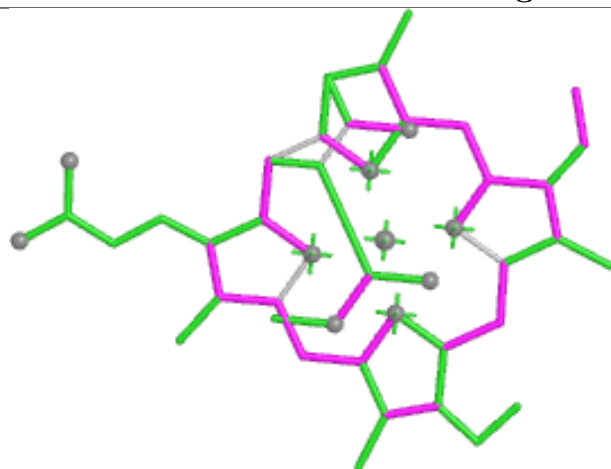
Torsions



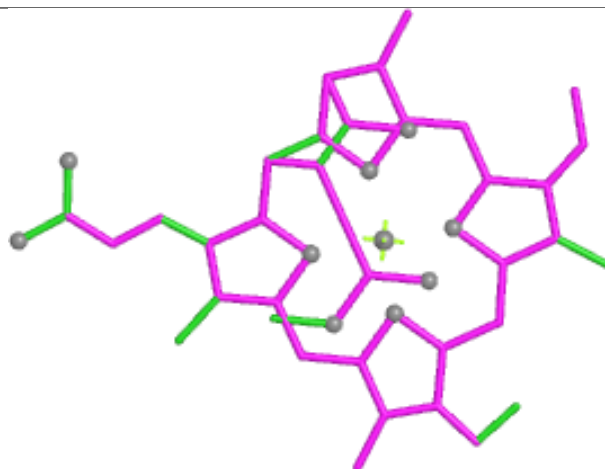
Rings



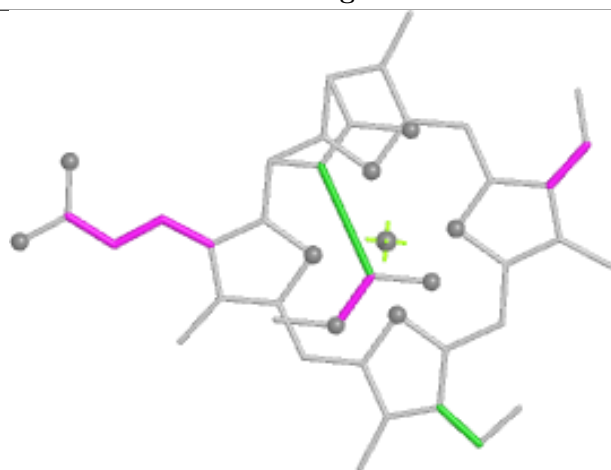
Ligand KC2 R 311



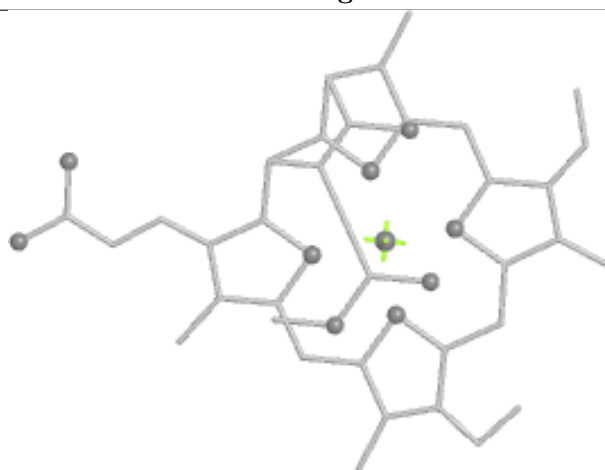
Bond lengths



Bond angles

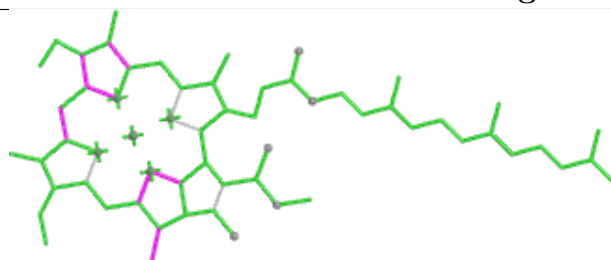


Torsions

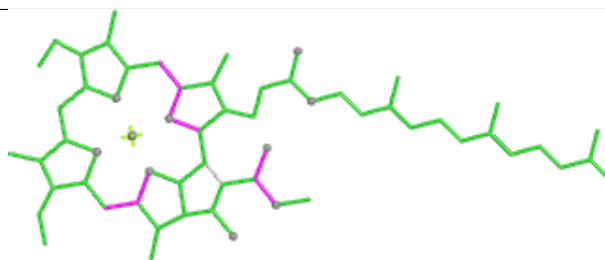


Rings

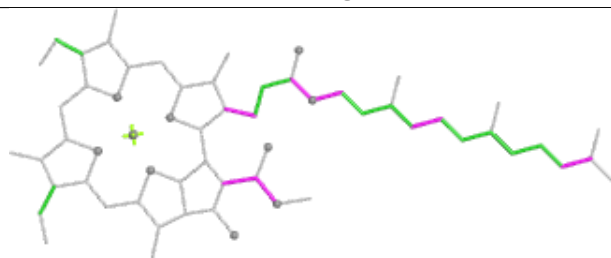
Ligand CLA a 405



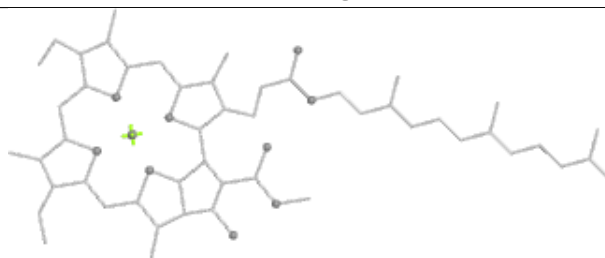
Bond lengths



Bond angles

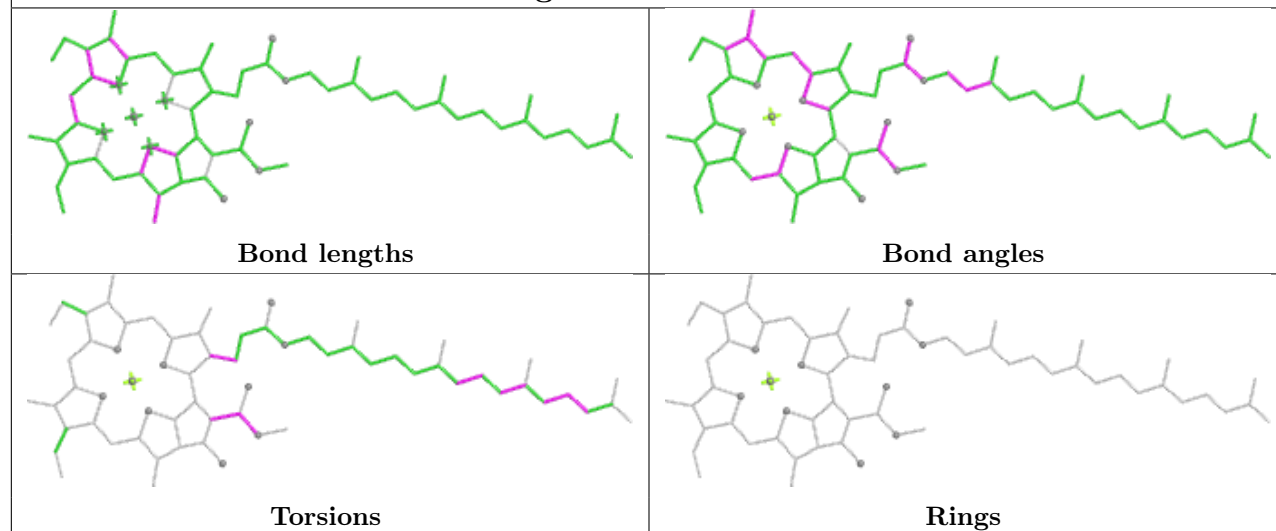


Torsions

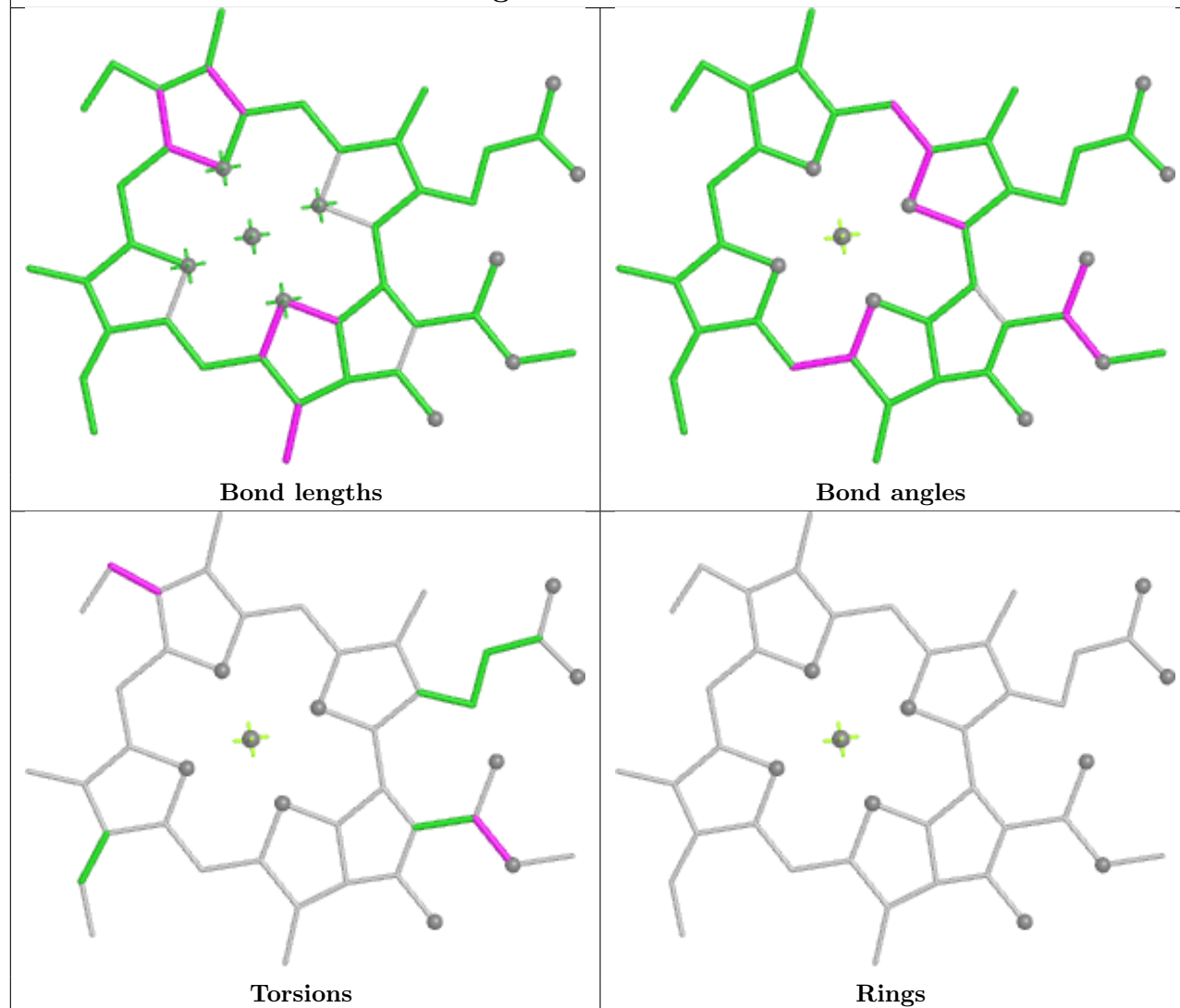


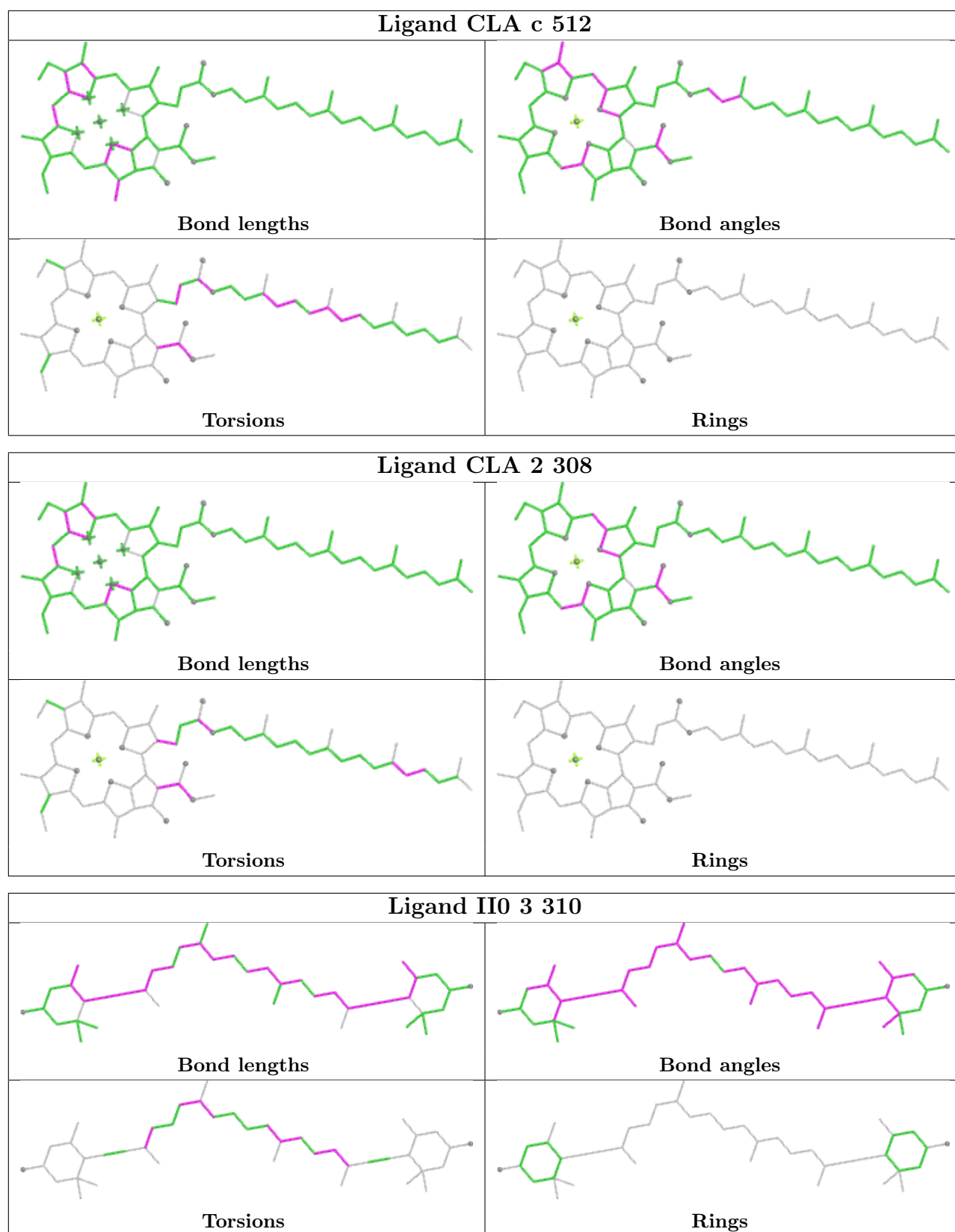
Rings

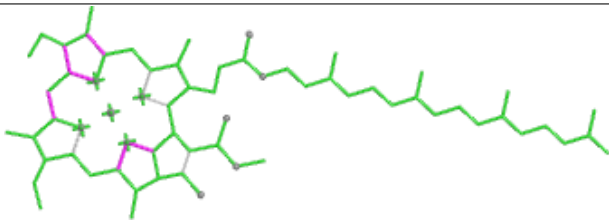
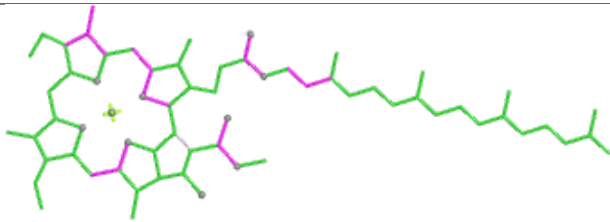
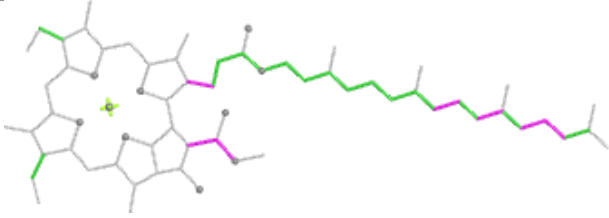
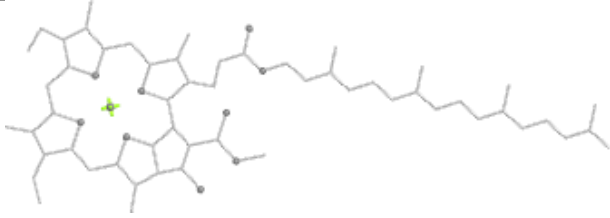
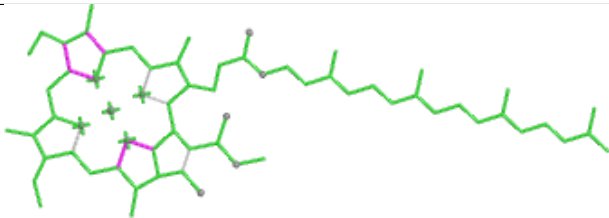
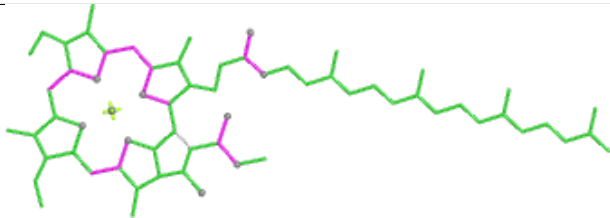
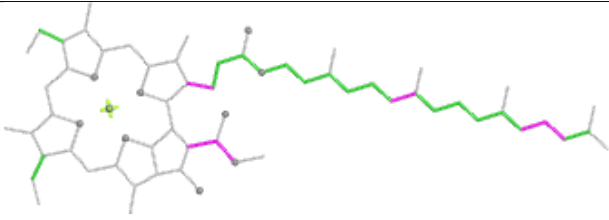
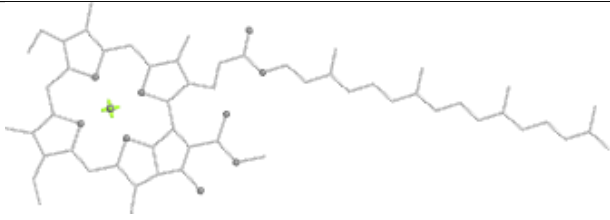
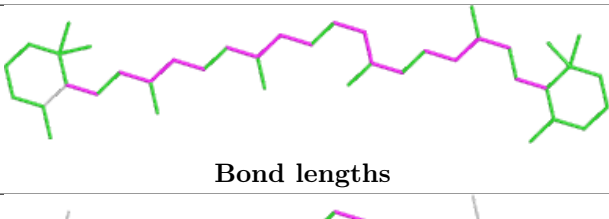
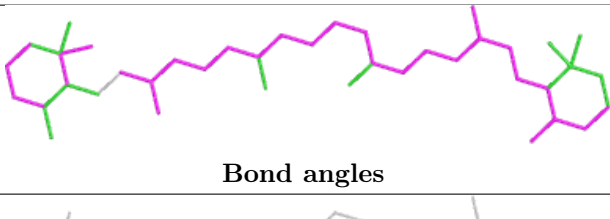
Ligand CLA b 611

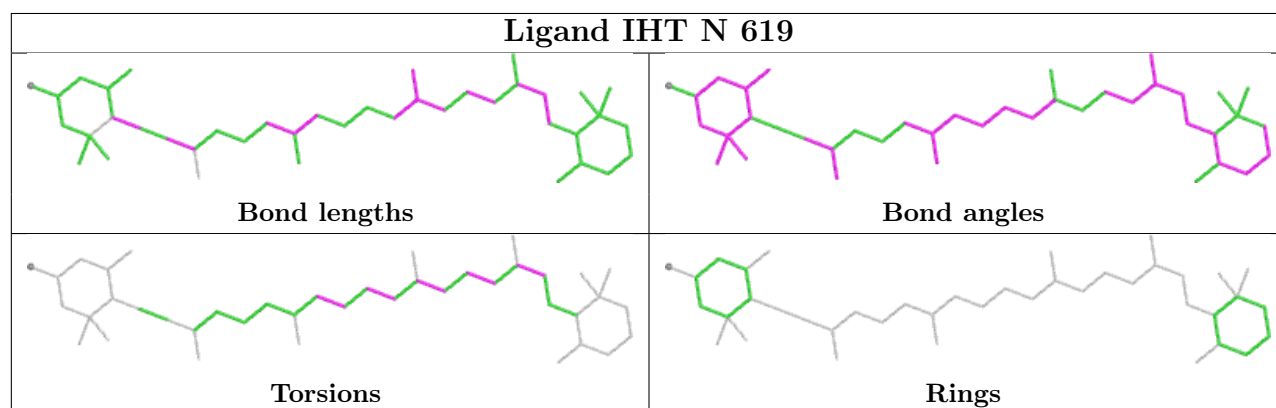
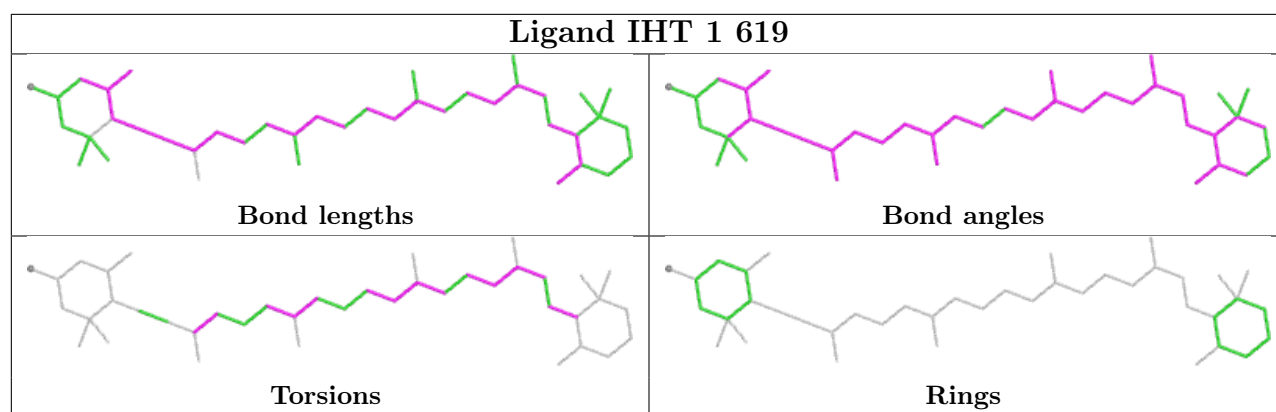


Ligand CLA P 601

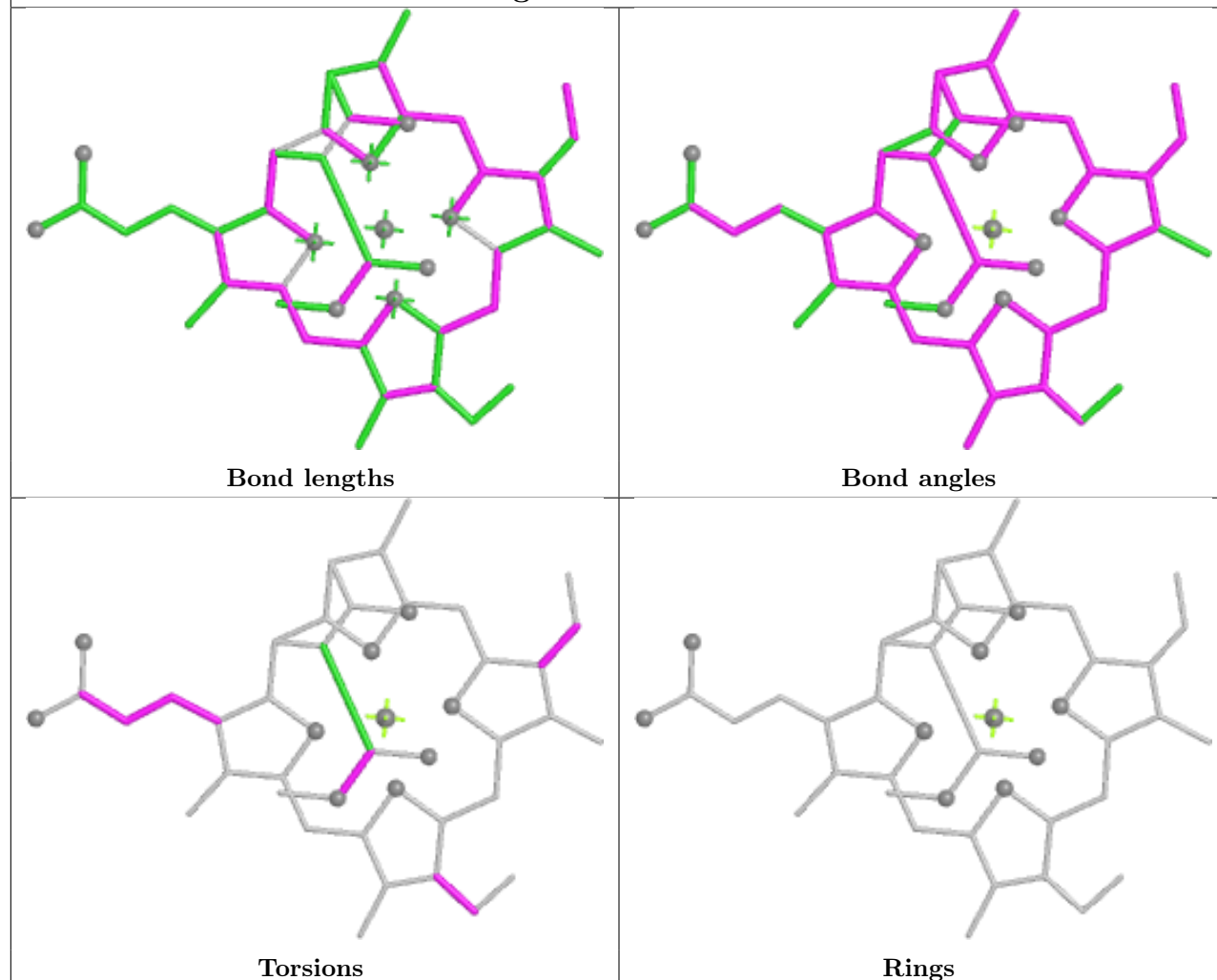




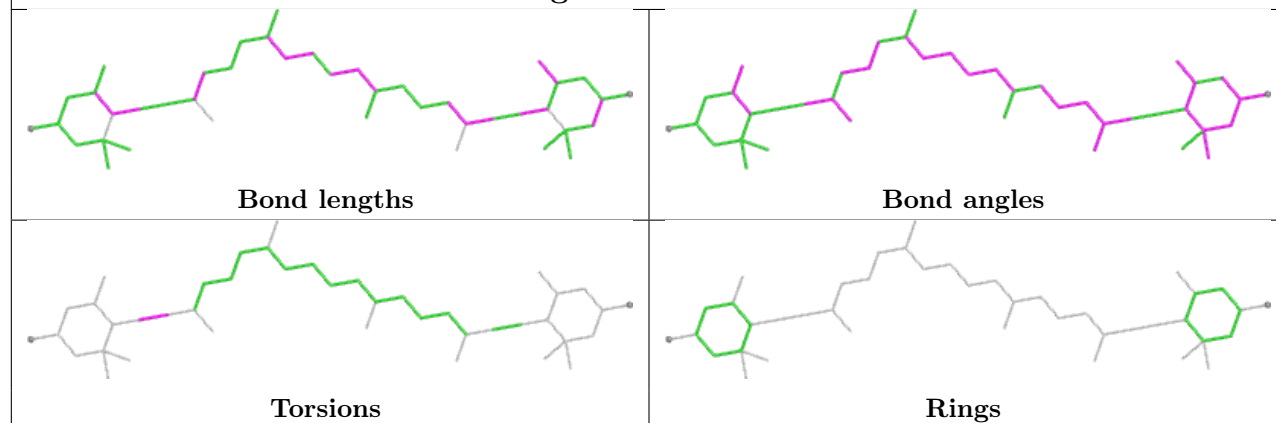
Ligand CLA B 611	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand CLA b 609	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand WVN P 615	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings

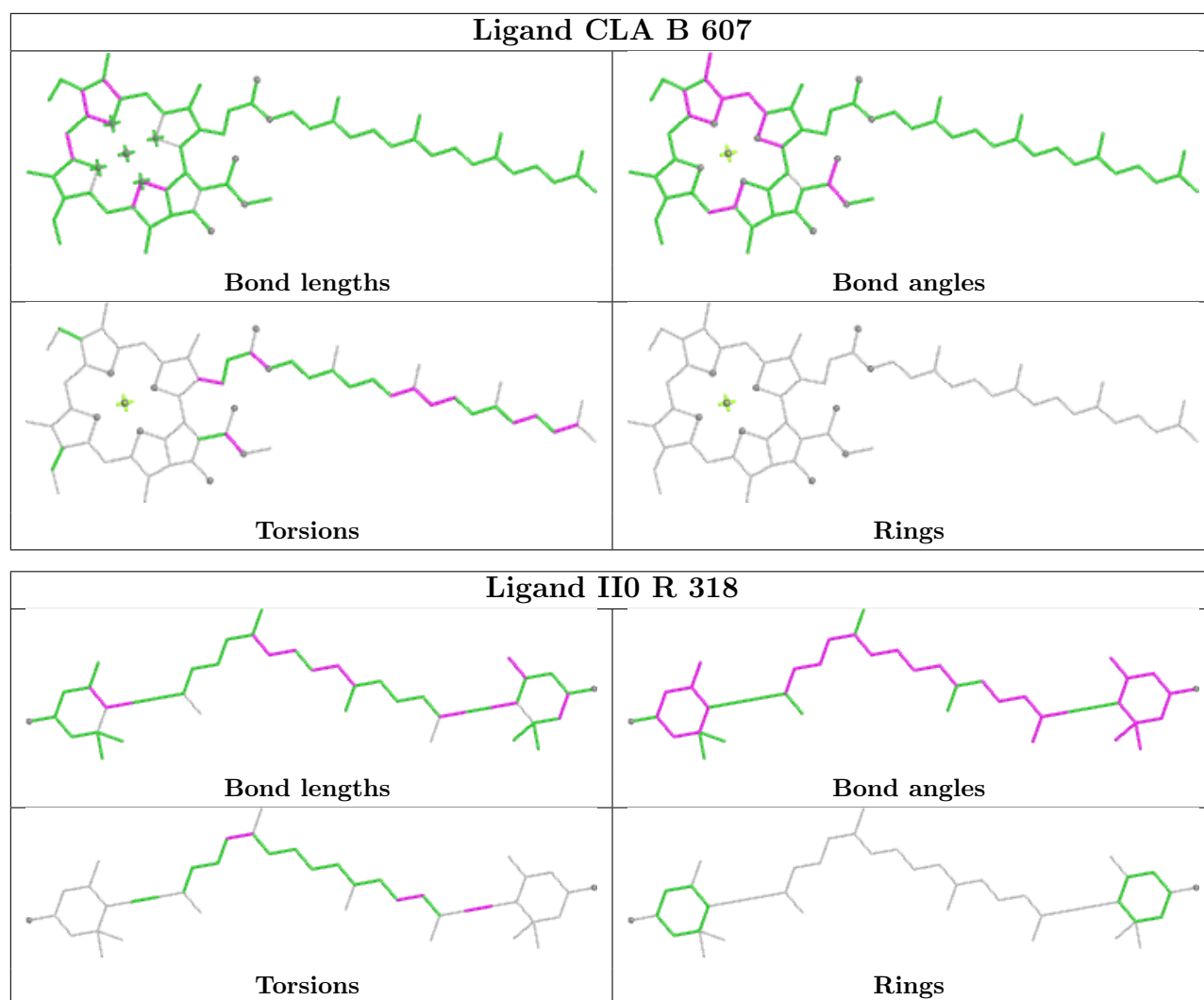


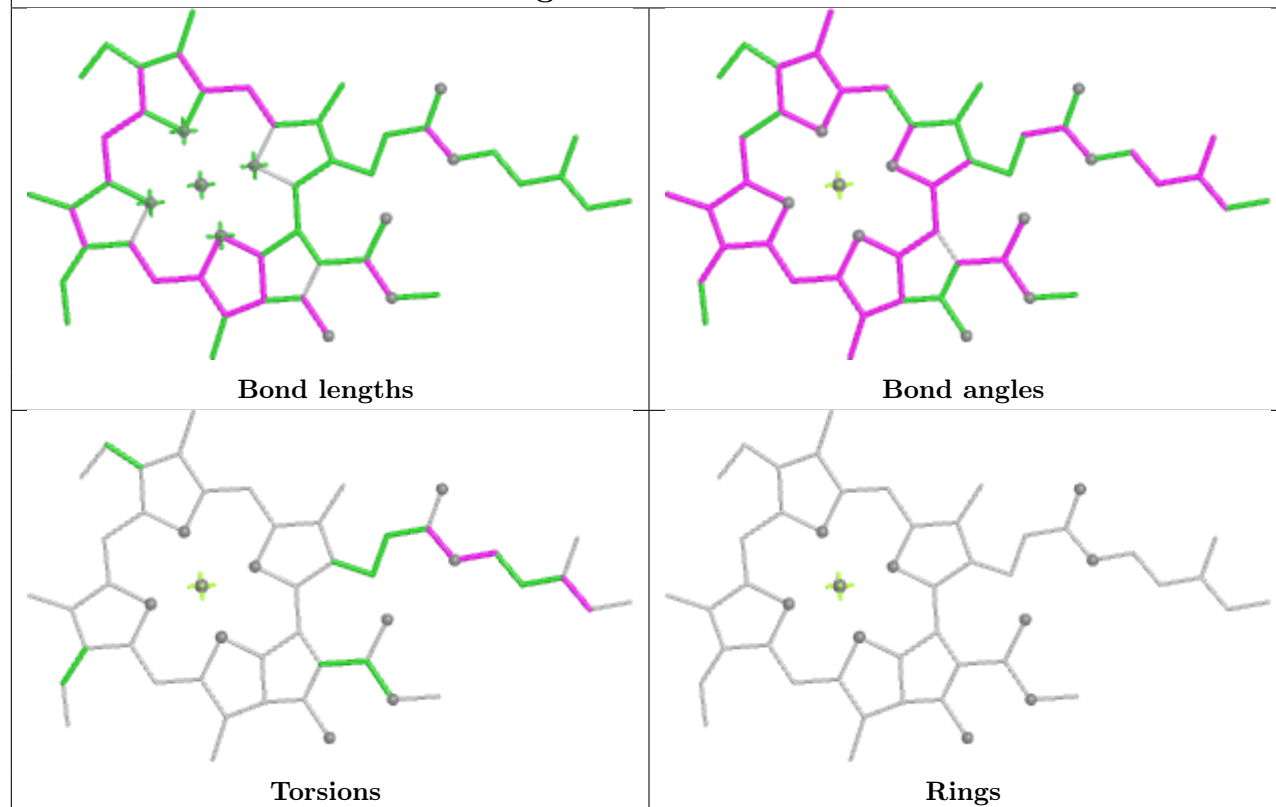
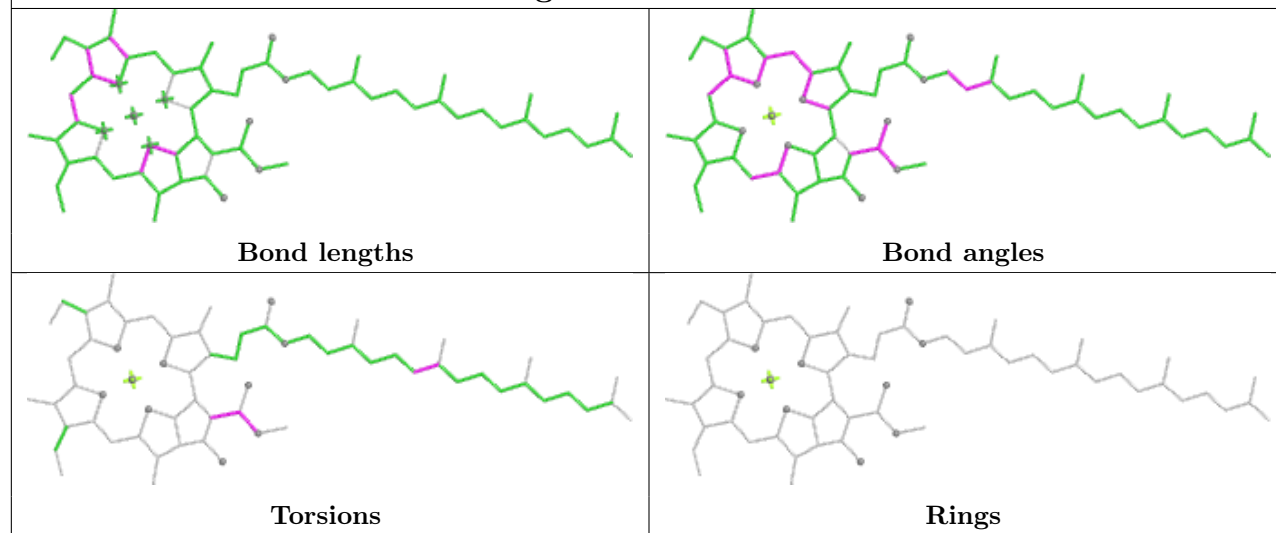
Ligand KC2 3 304



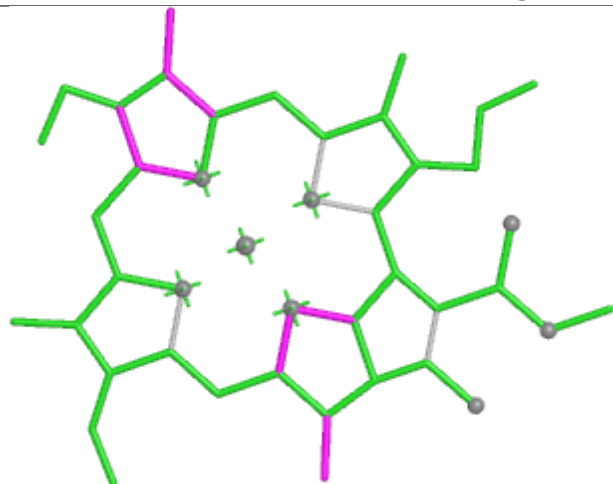
Ligand II0 6 612



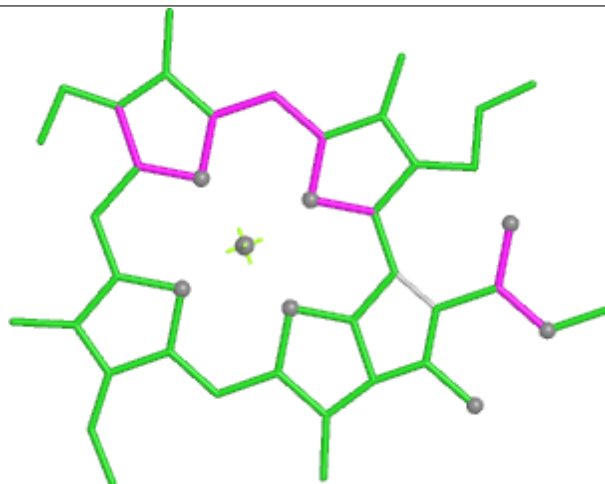


Ligand CLA 2 305**Ligand CLA b 602**

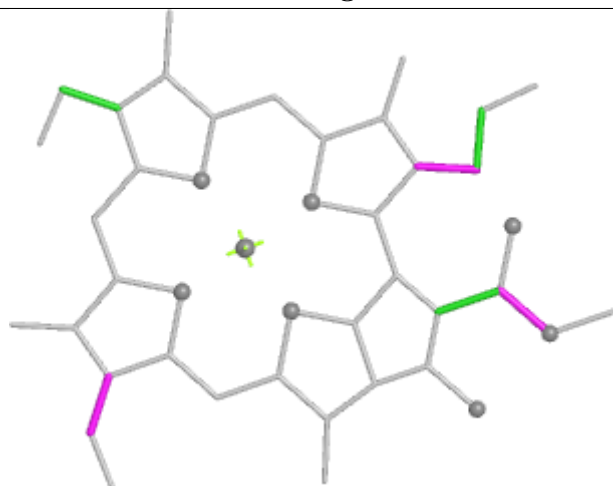
Ligand CLA N 607



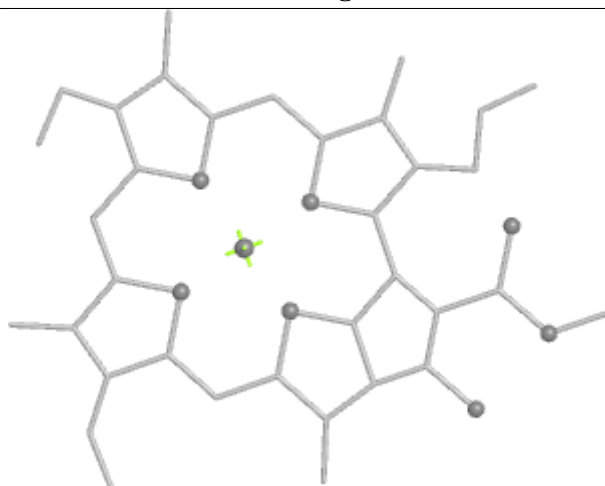
Bond lengths



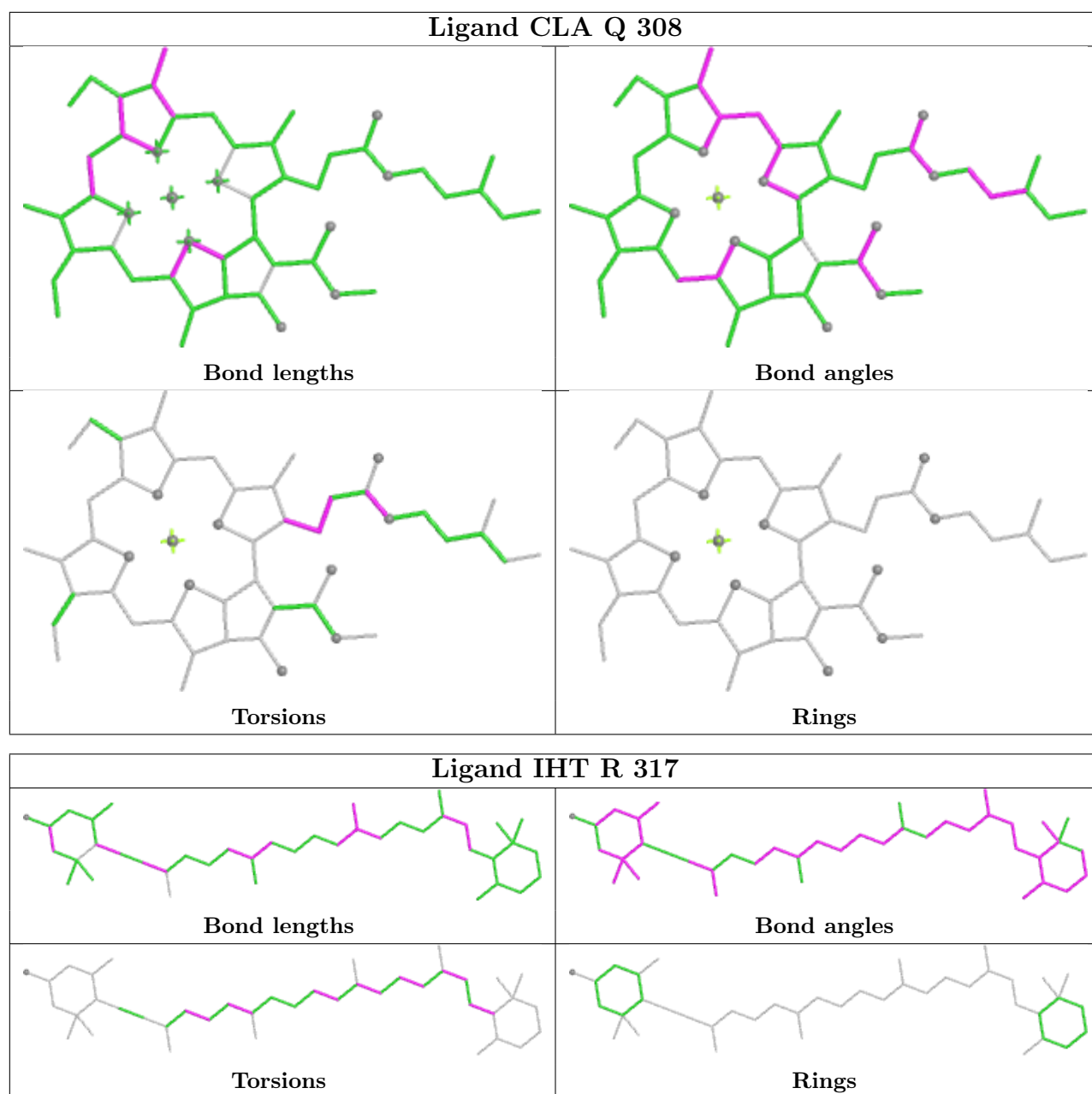
Bond angles

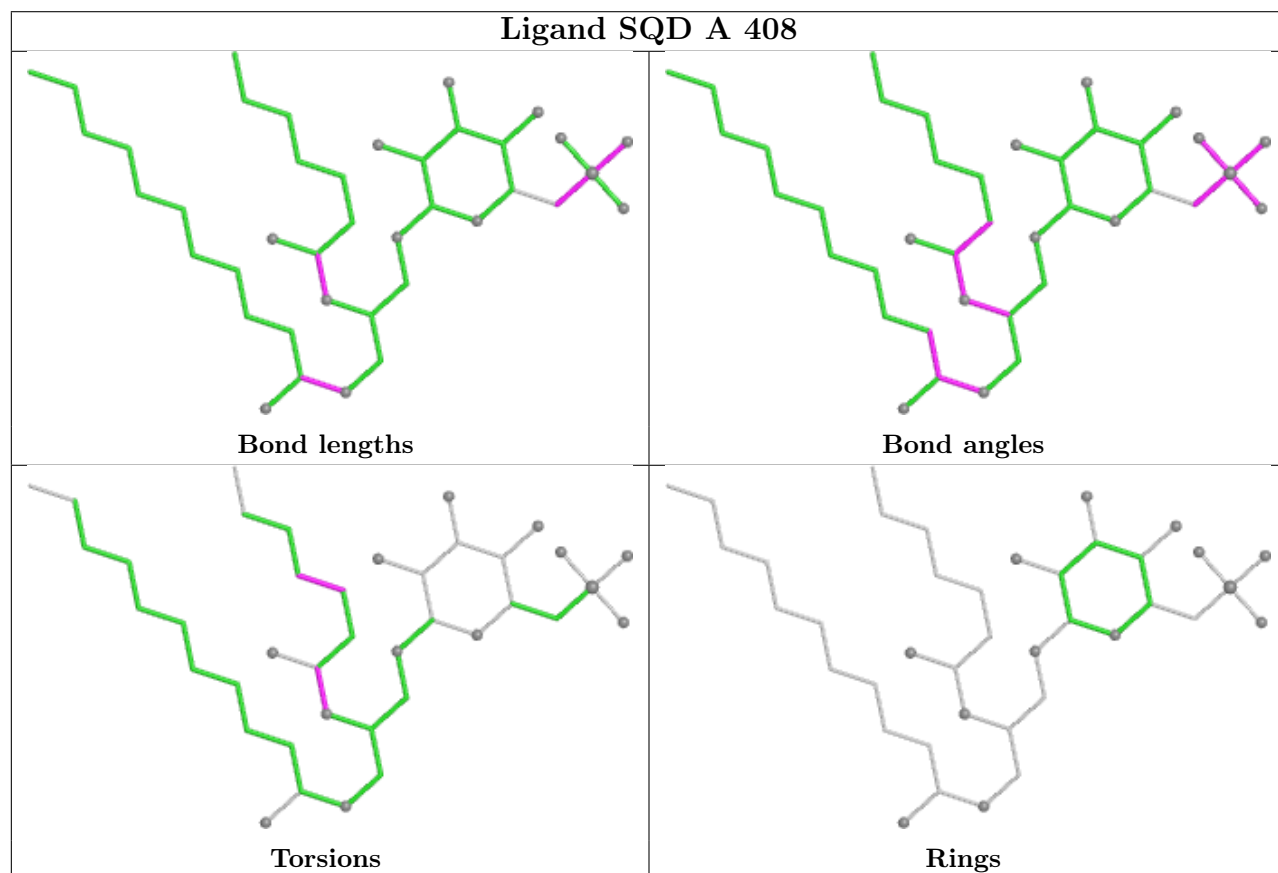
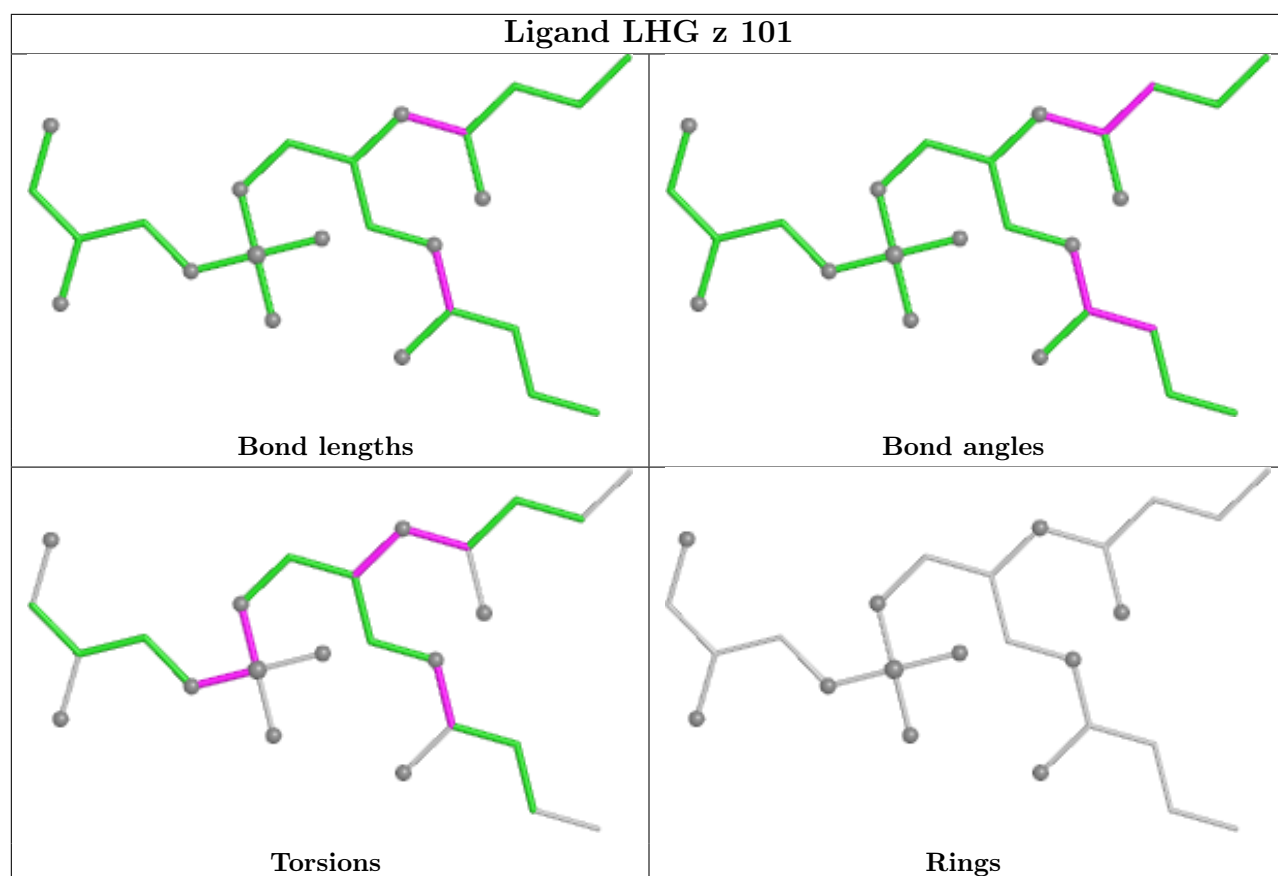


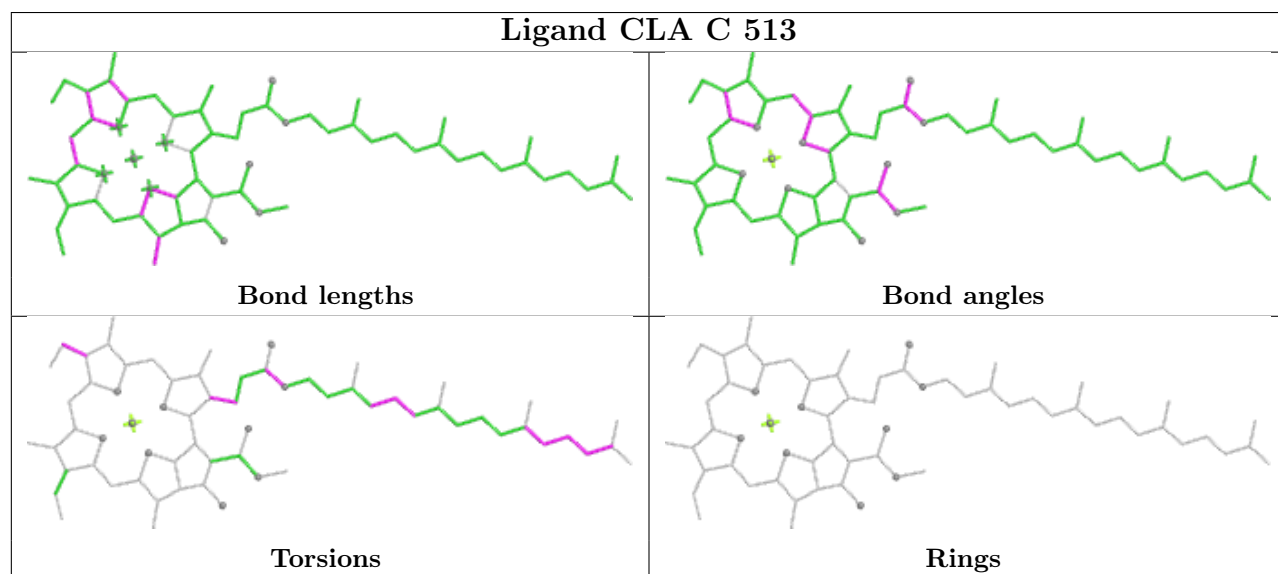
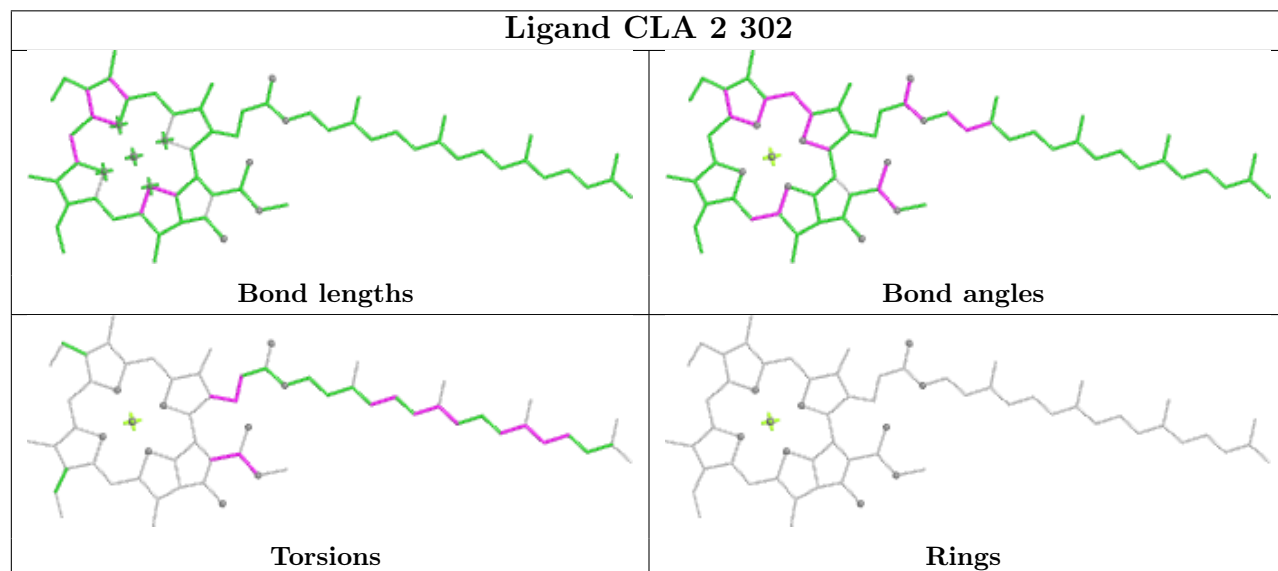
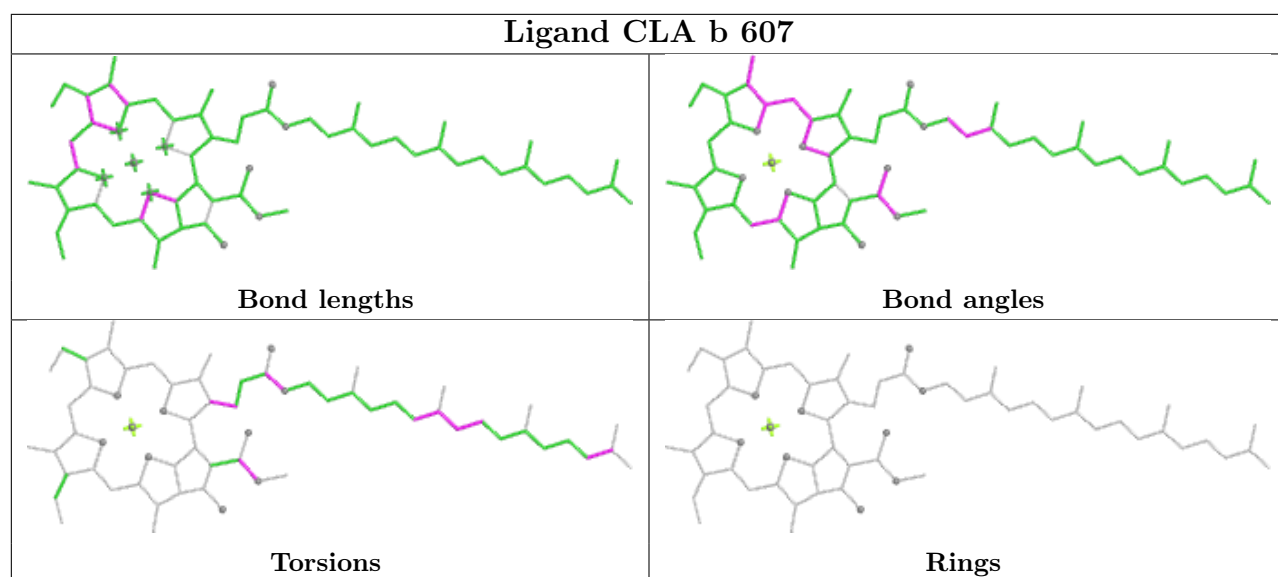
Torsions

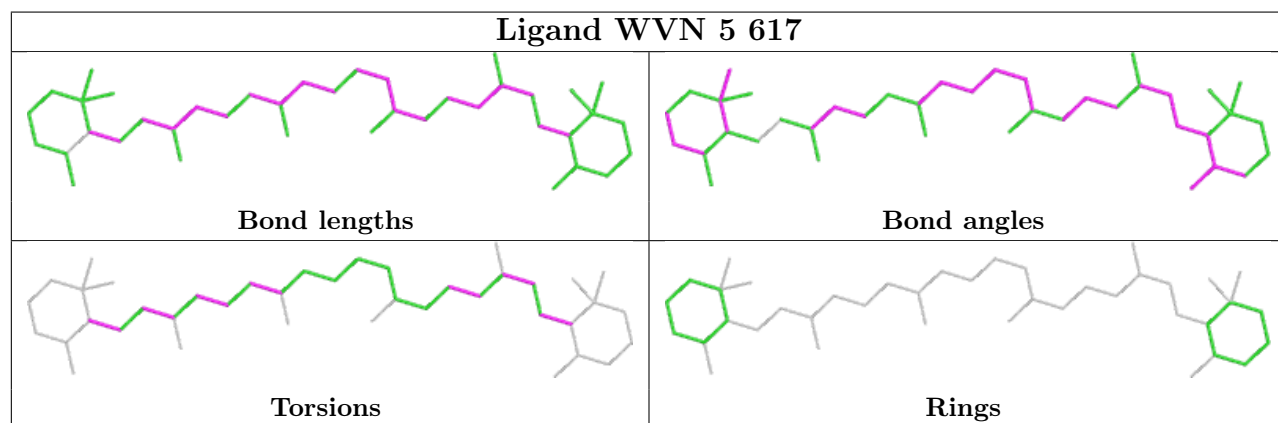
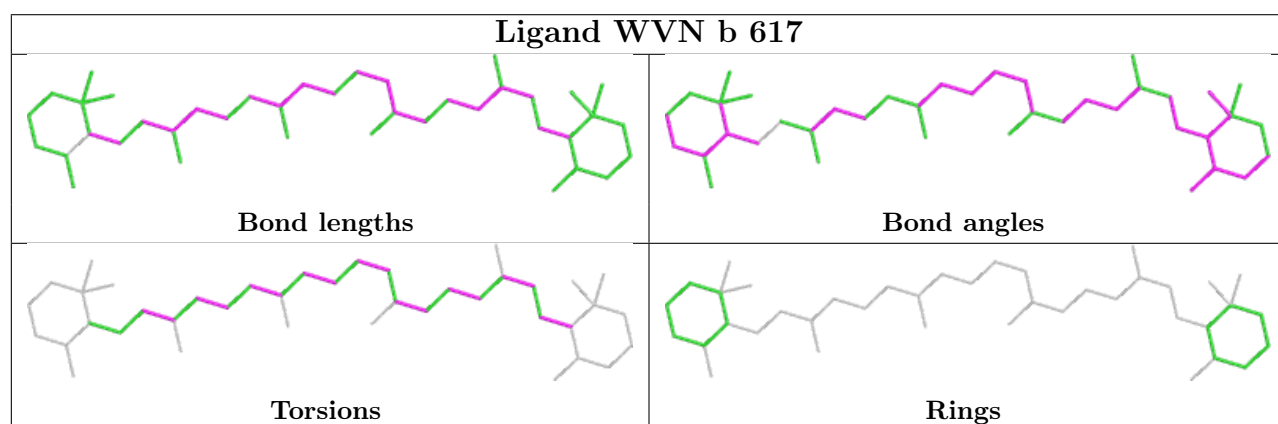
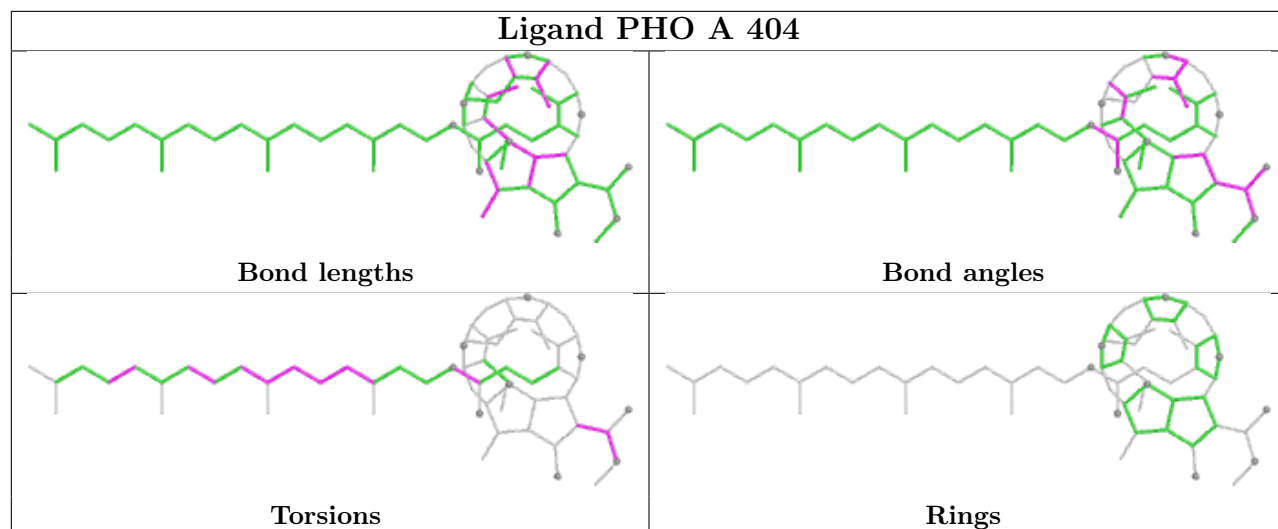


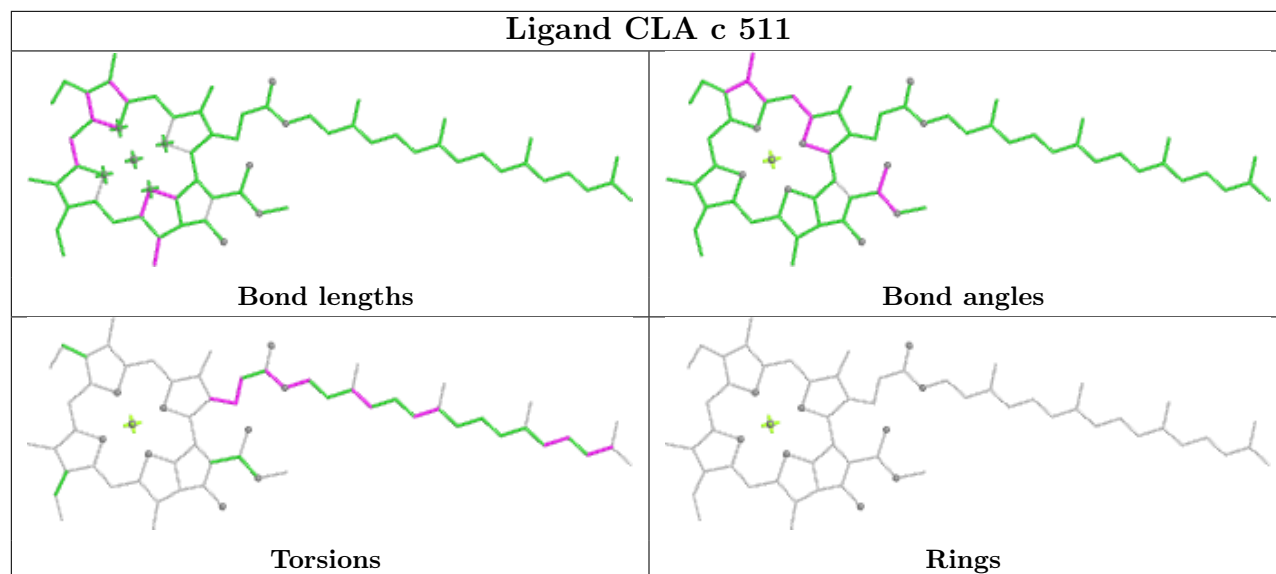
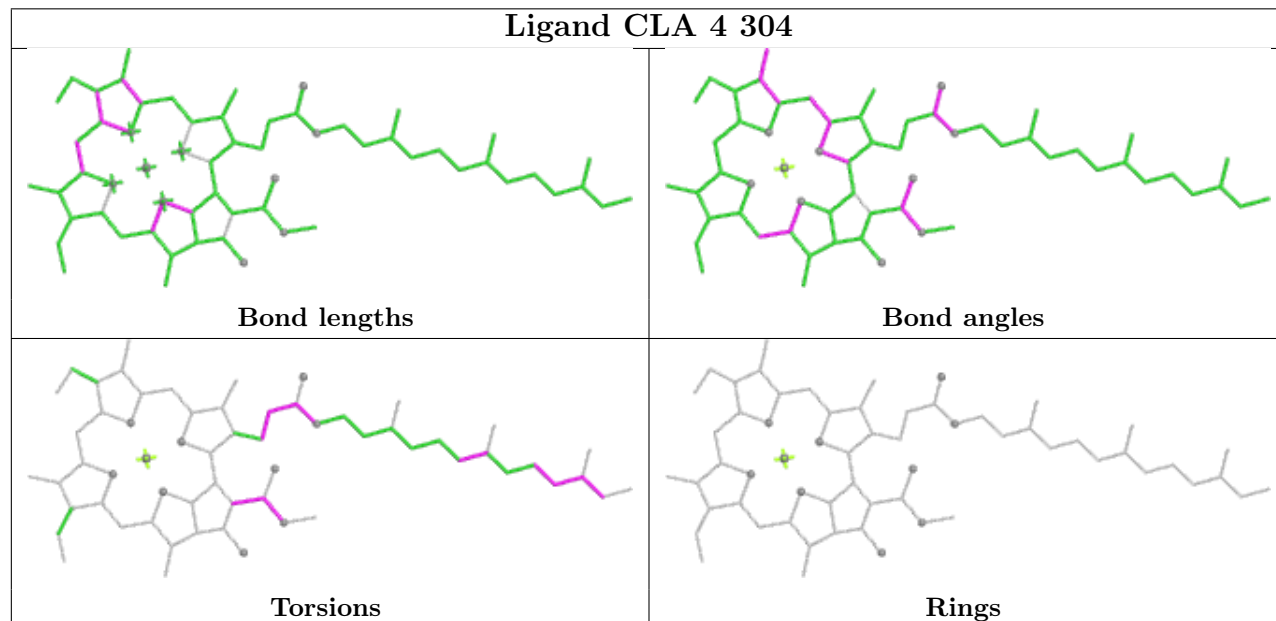
Rings

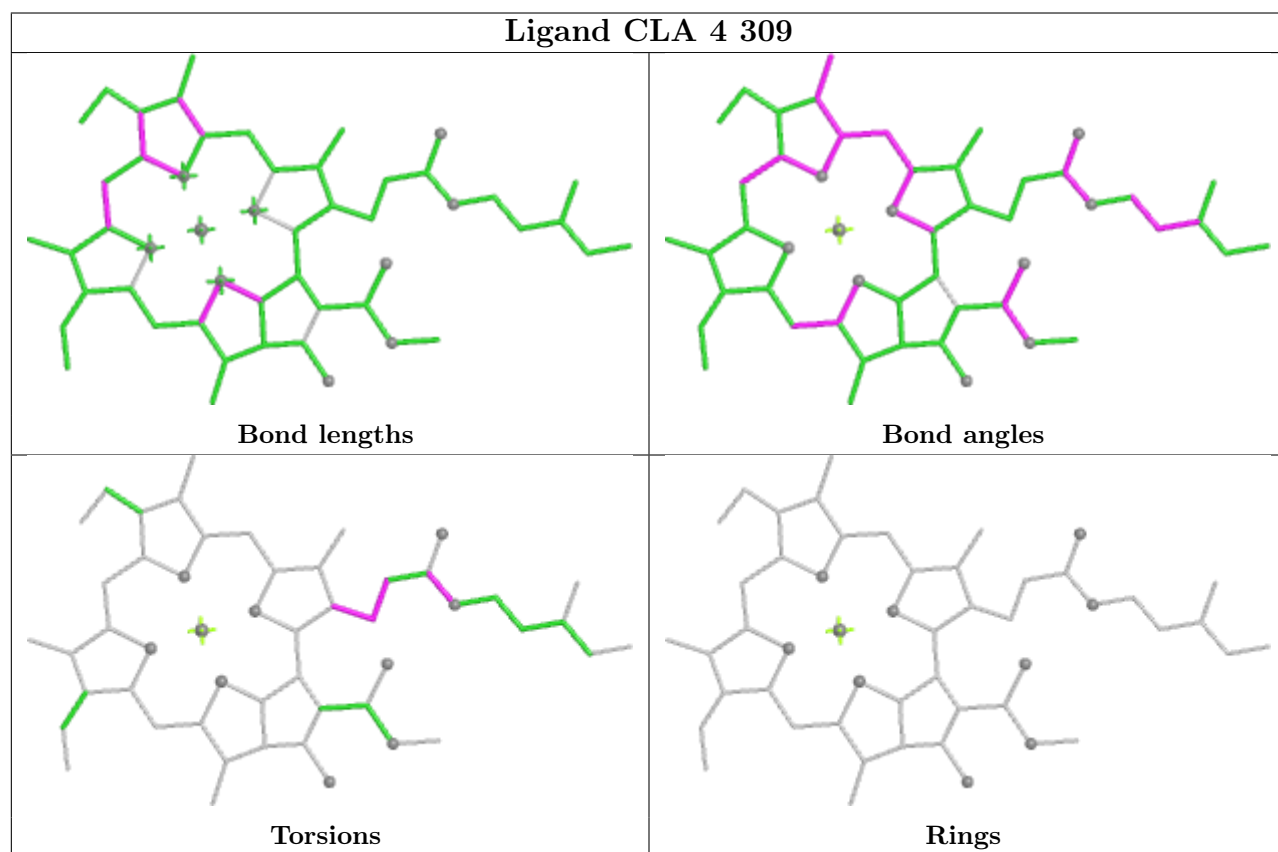
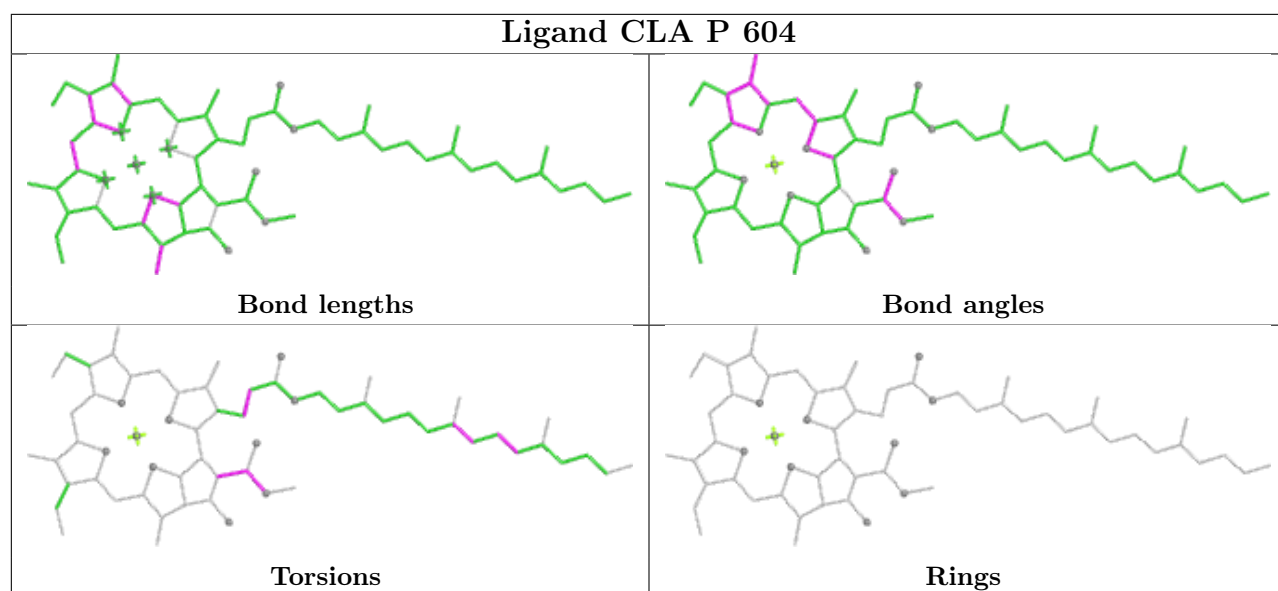


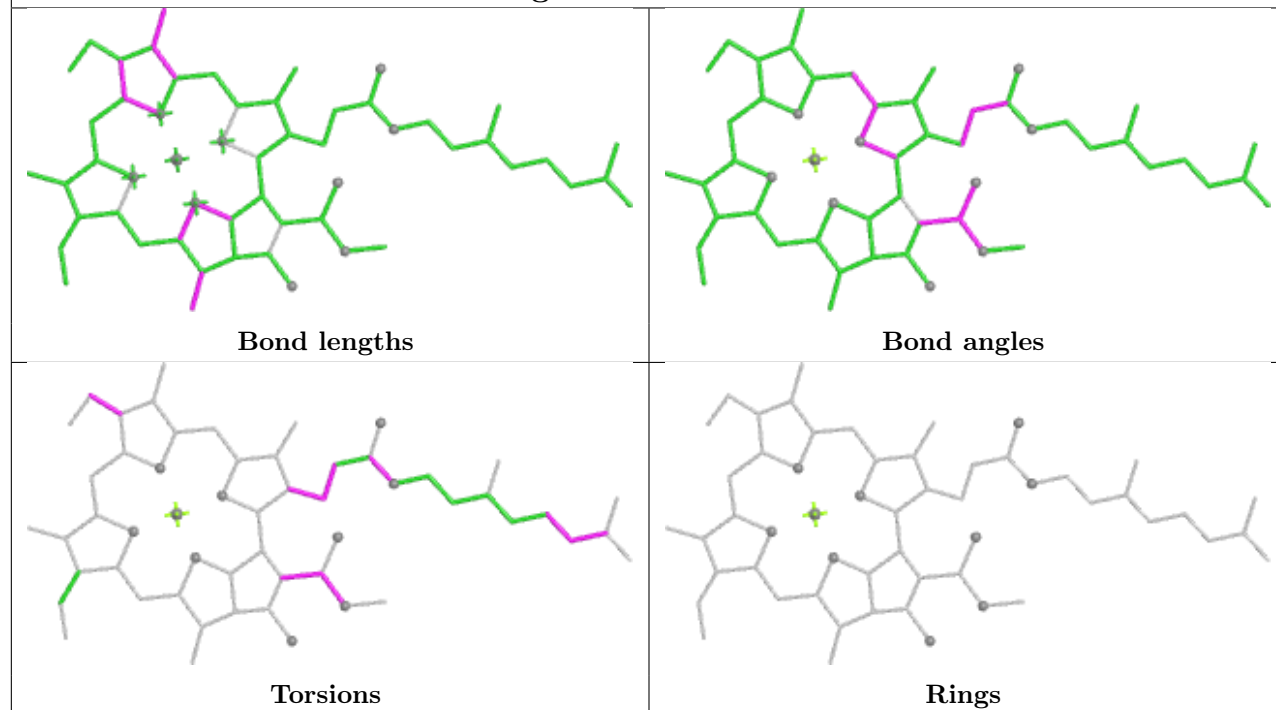
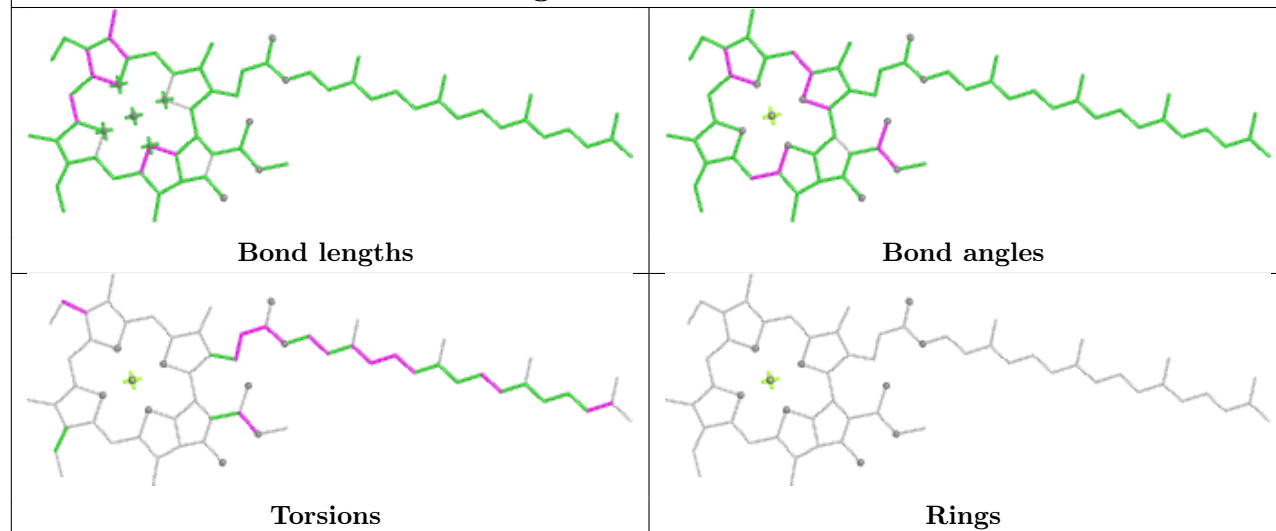


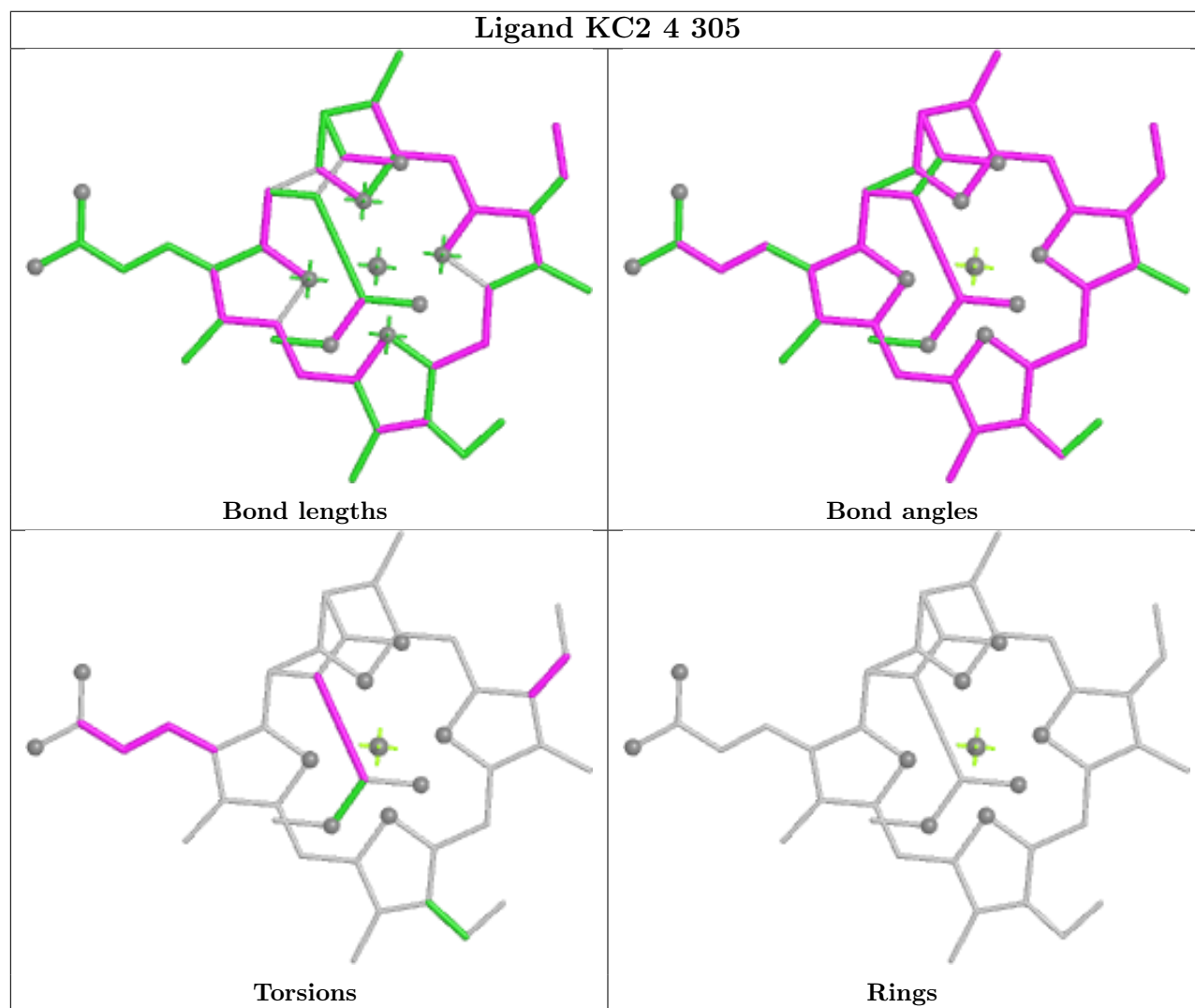
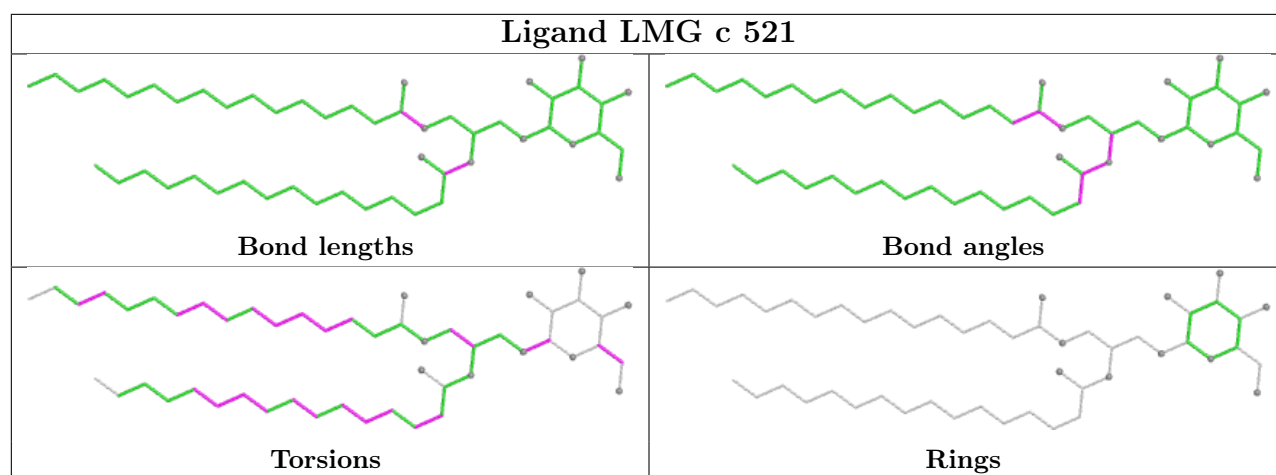




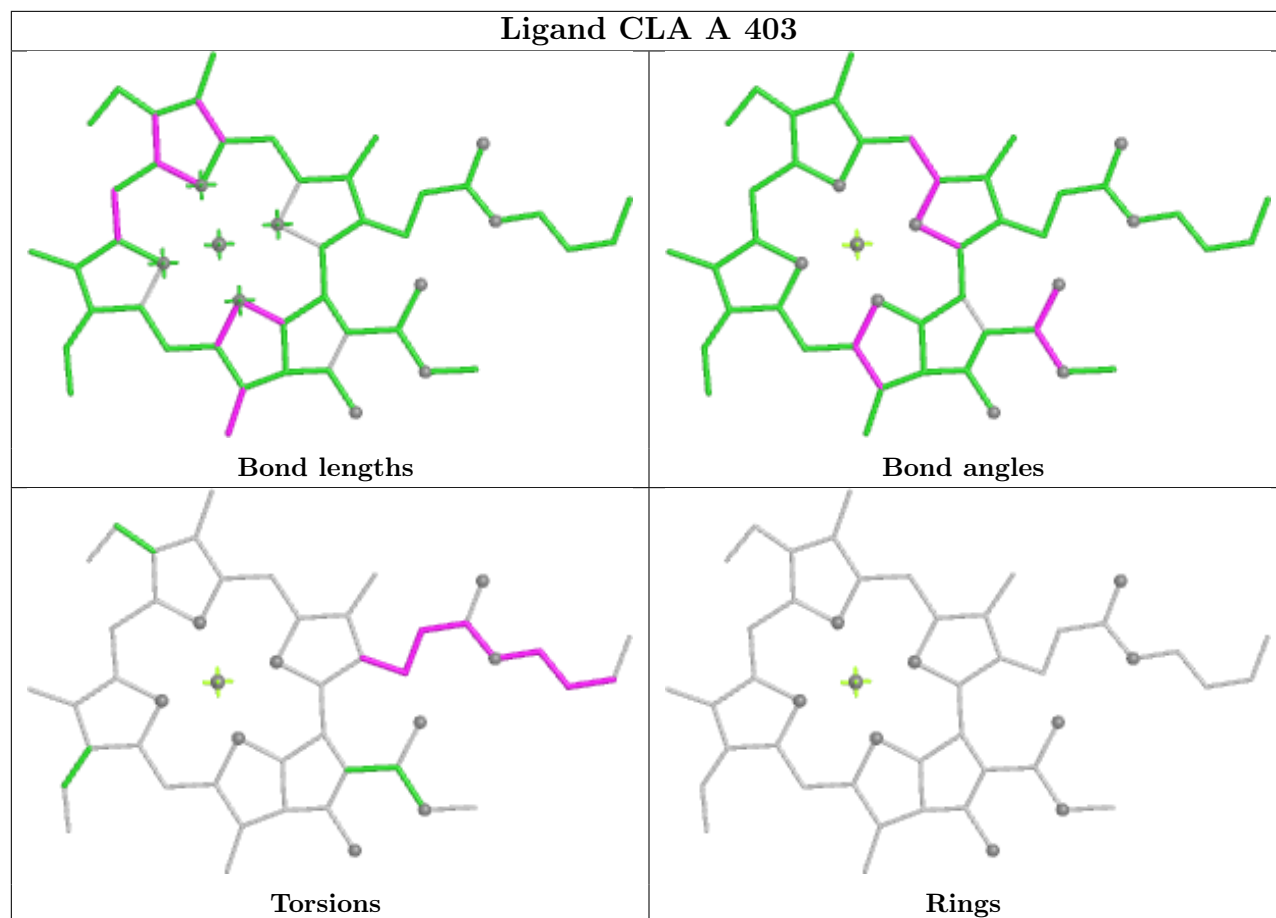
Ligand CLA c 511**Ligand CLA 4 304**



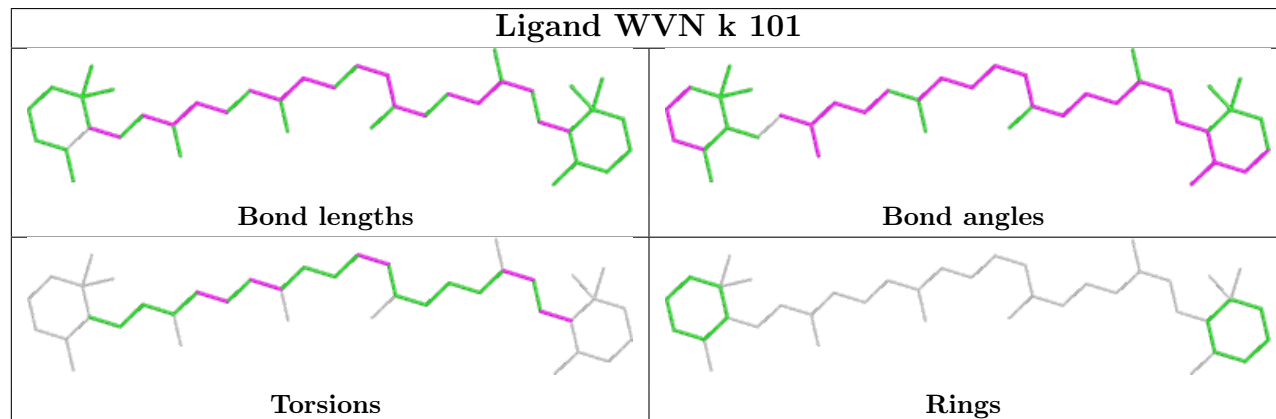
Ligand CLA R 312**Ligand CLA B 613**

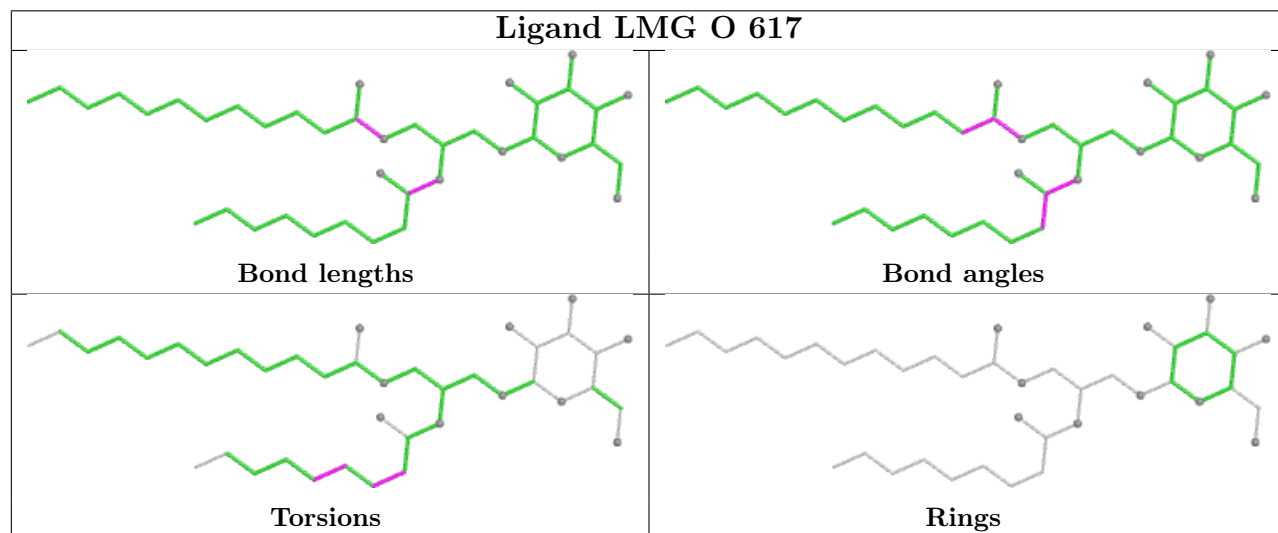
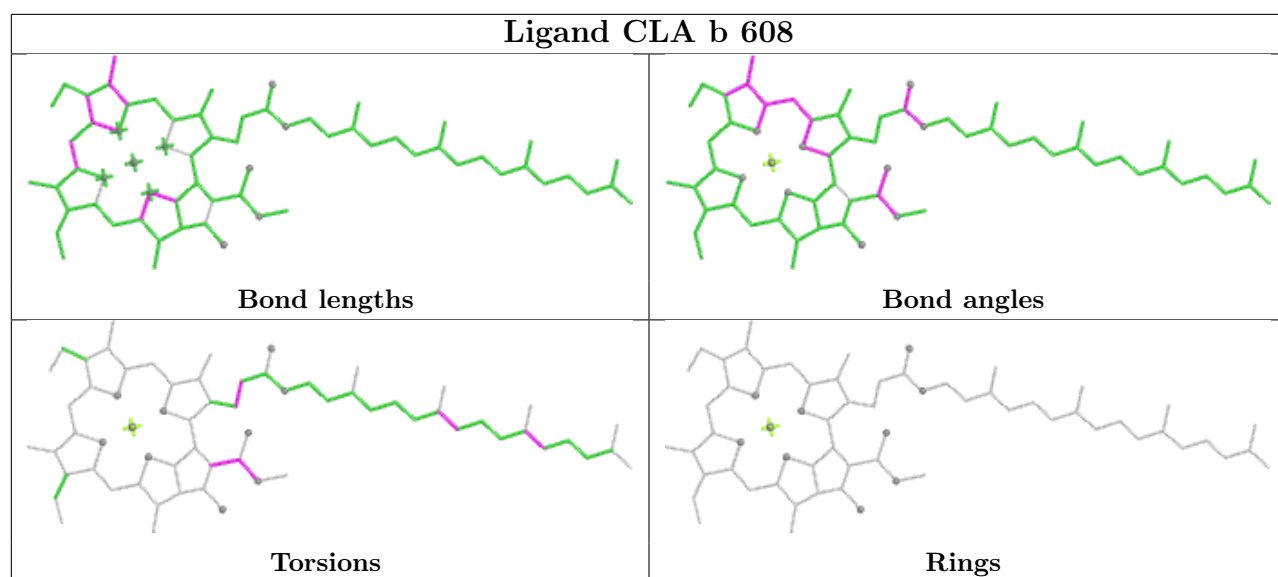


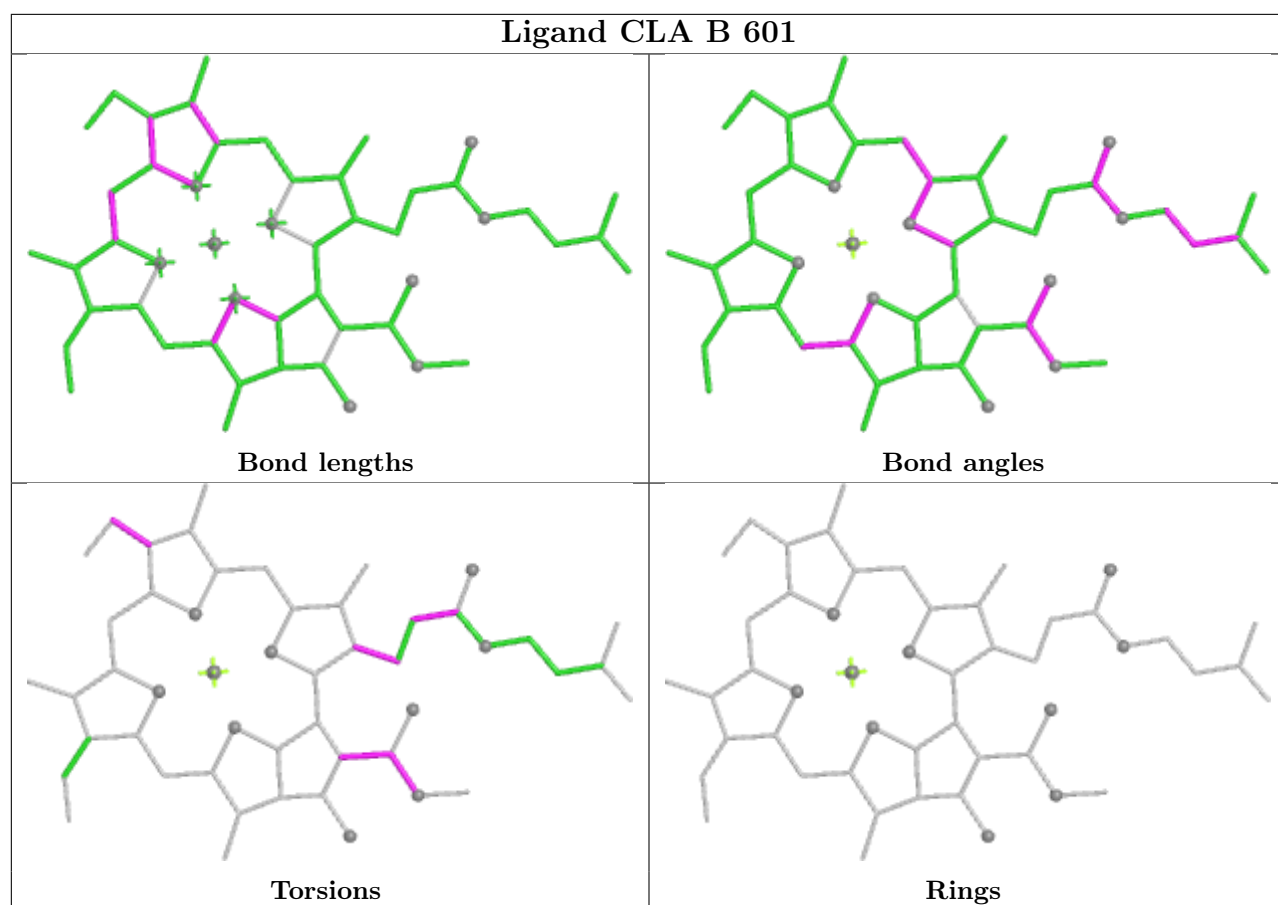
Ligand CLA A 403

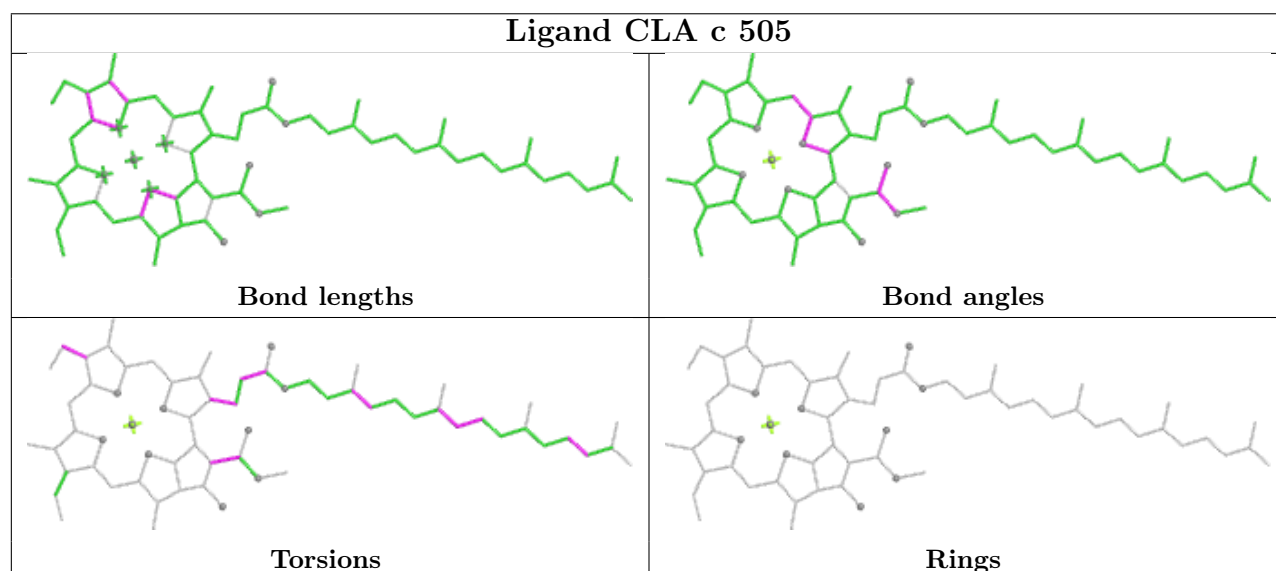
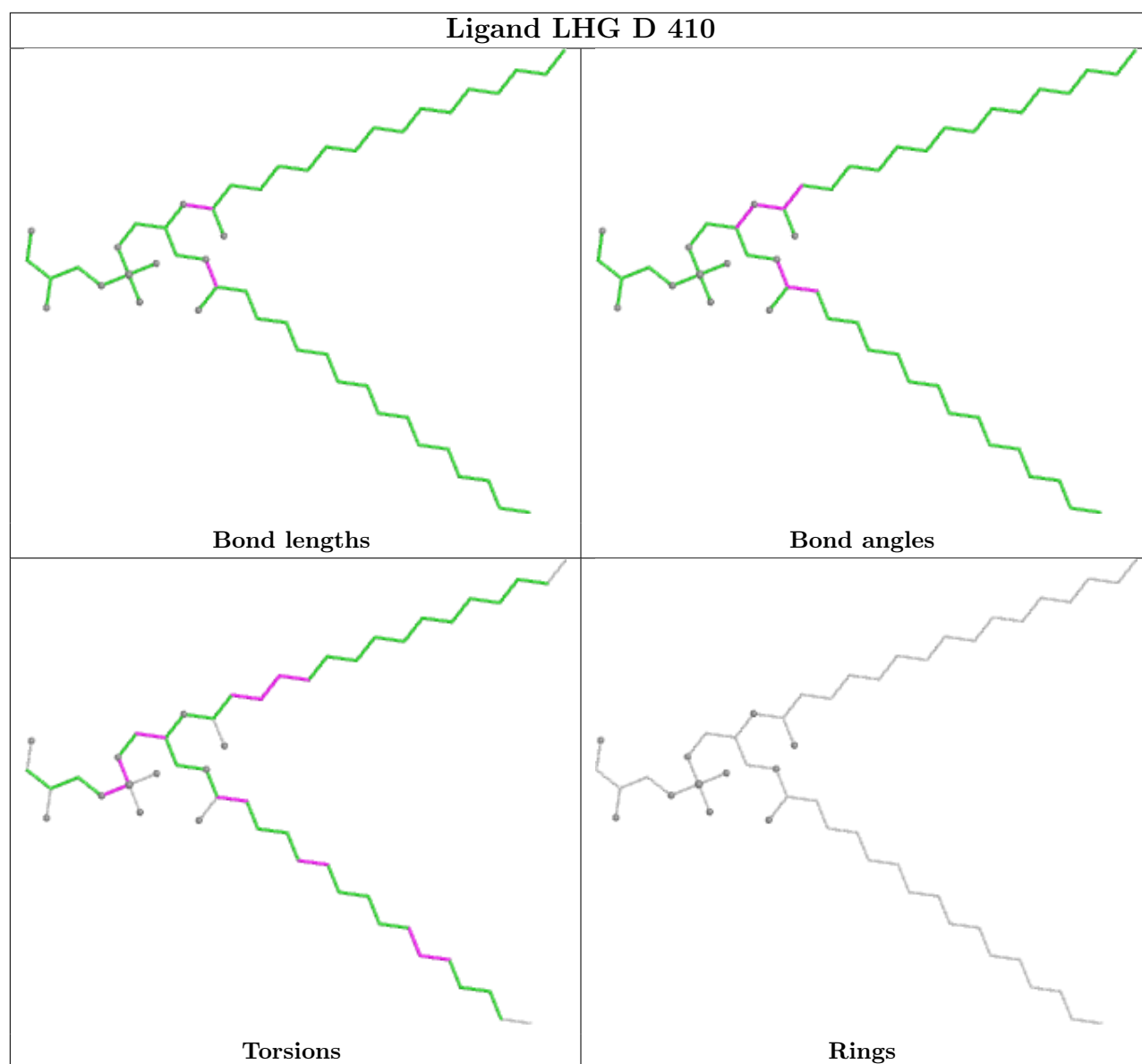


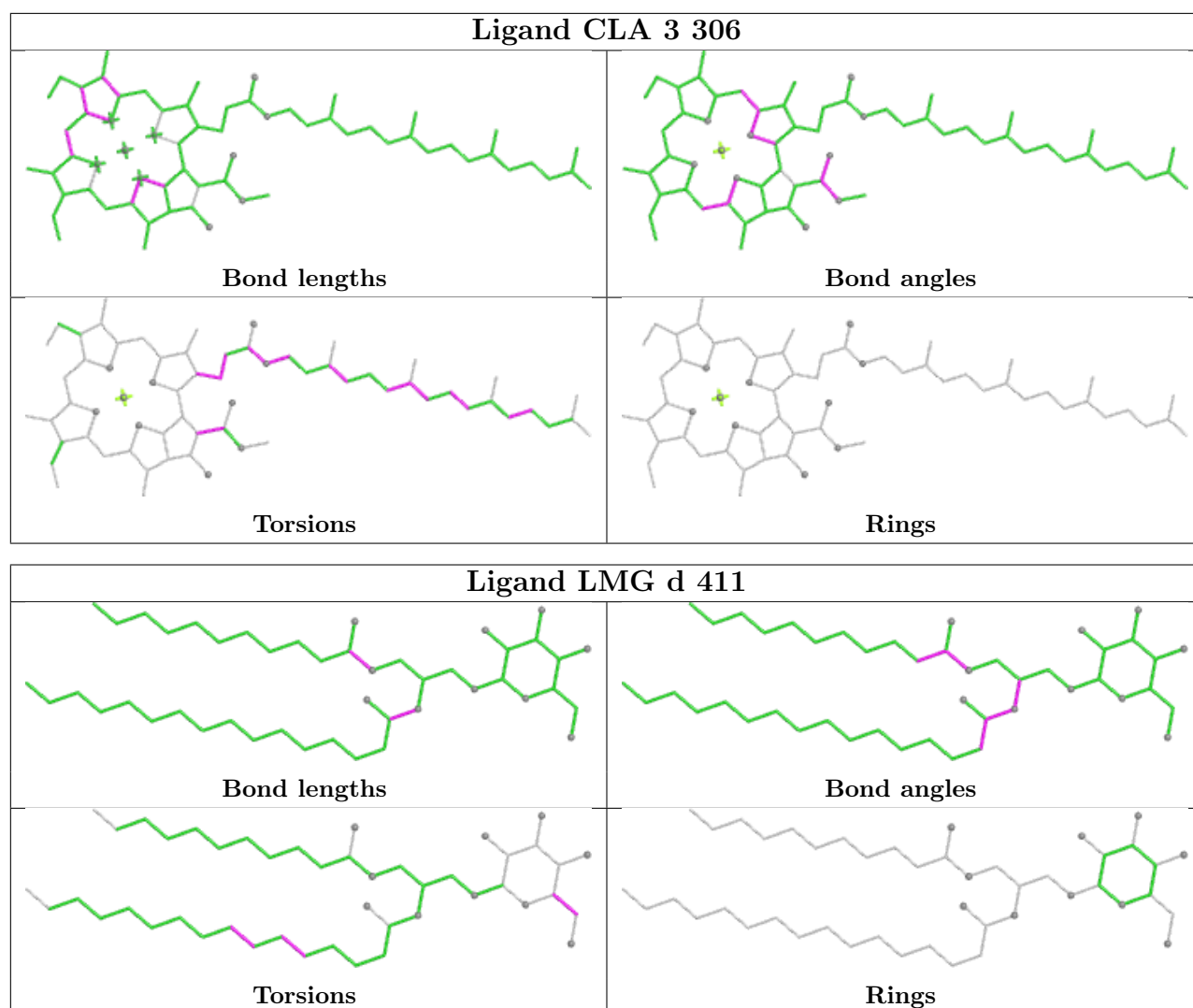
Ligand WVN k 101



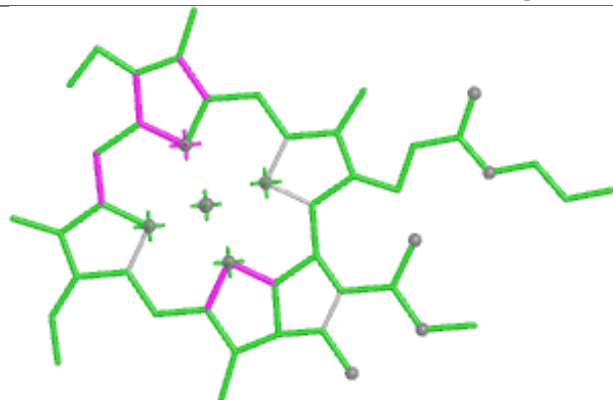




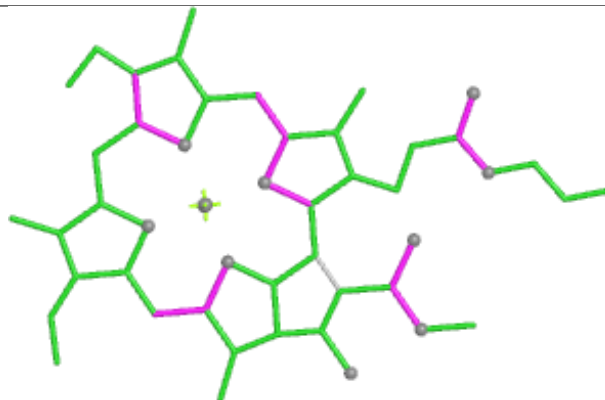




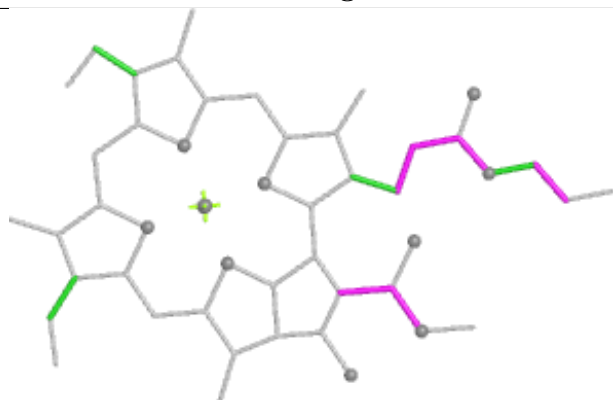
Ligand CLA 1 613



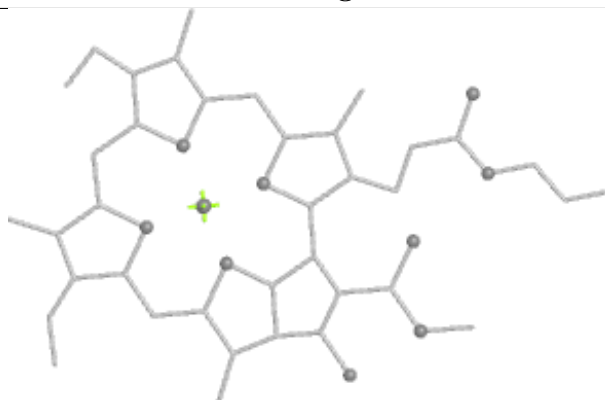
Bond lengths



Bond angles

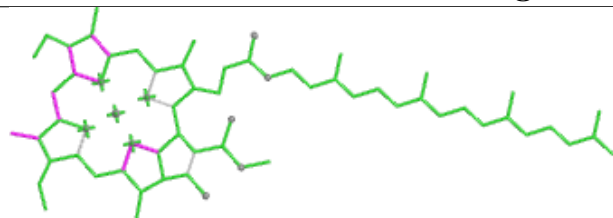


Torsions

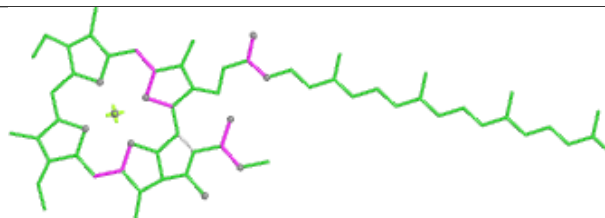


Rings

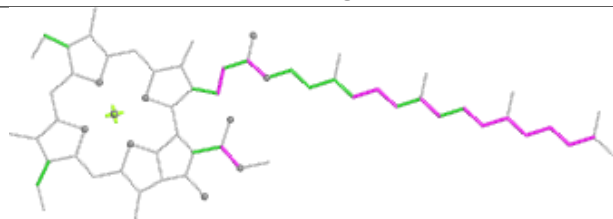
Ligand CLA B 616



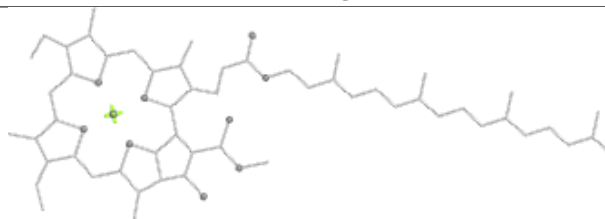
Bond lengths



Bond angles

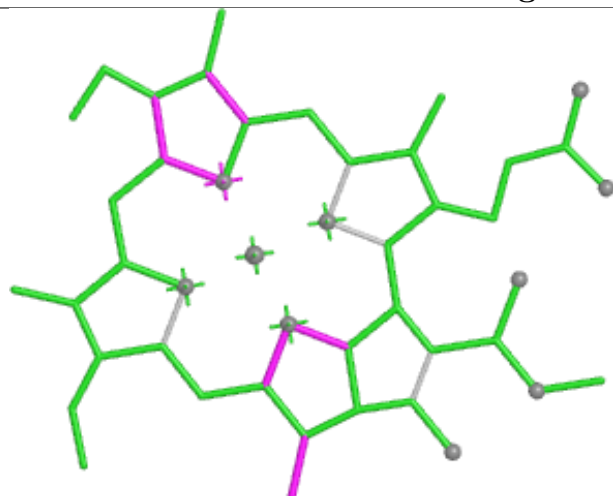


Torsions

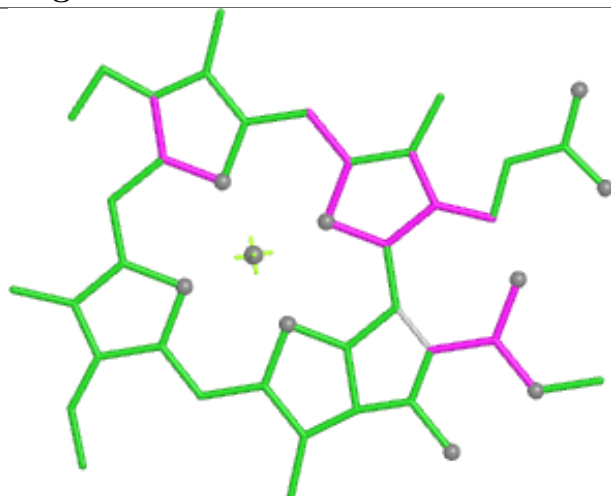


Rings

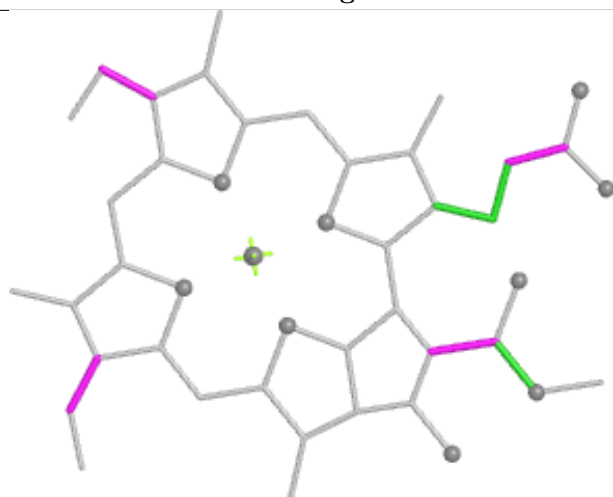
Ligand CLA g 402



Bond lengths



Bond angles

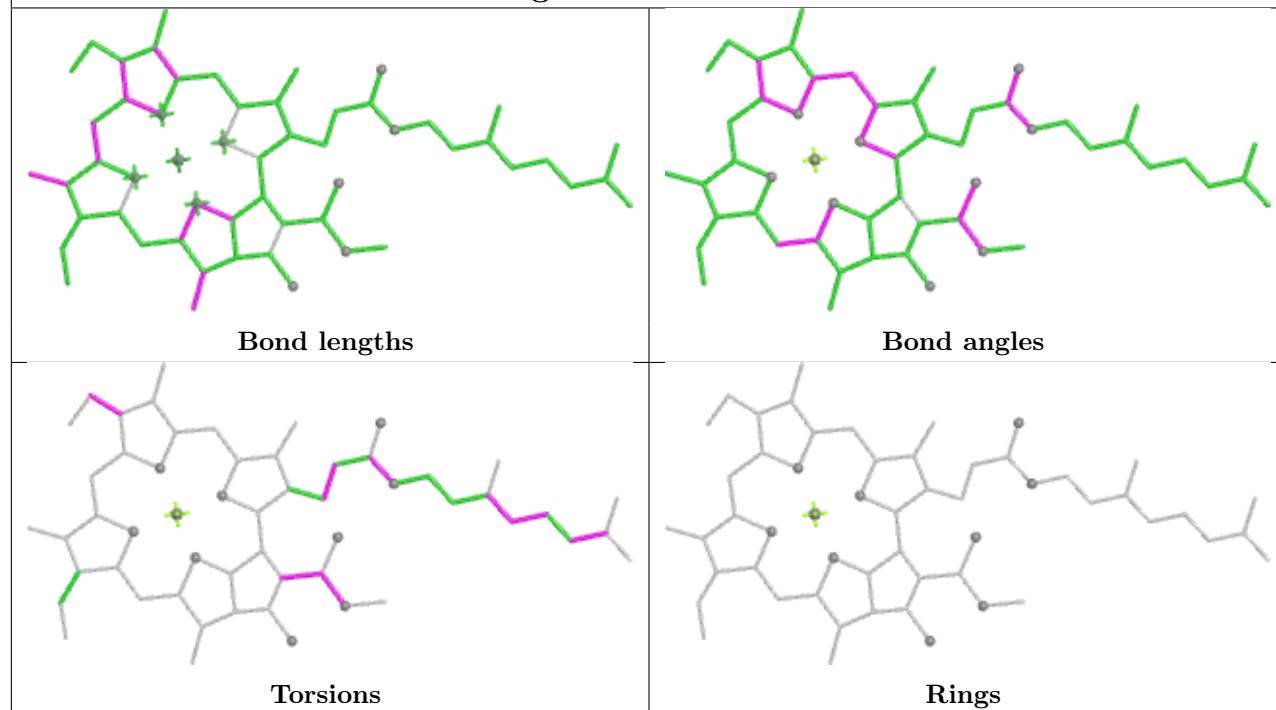


Torsions

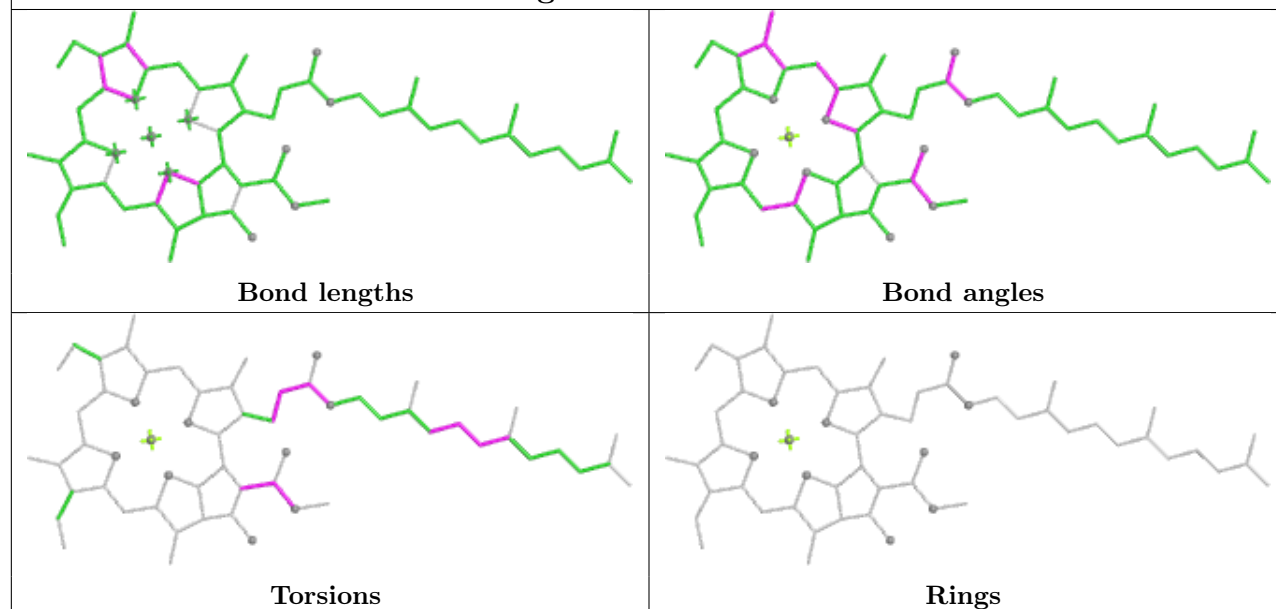


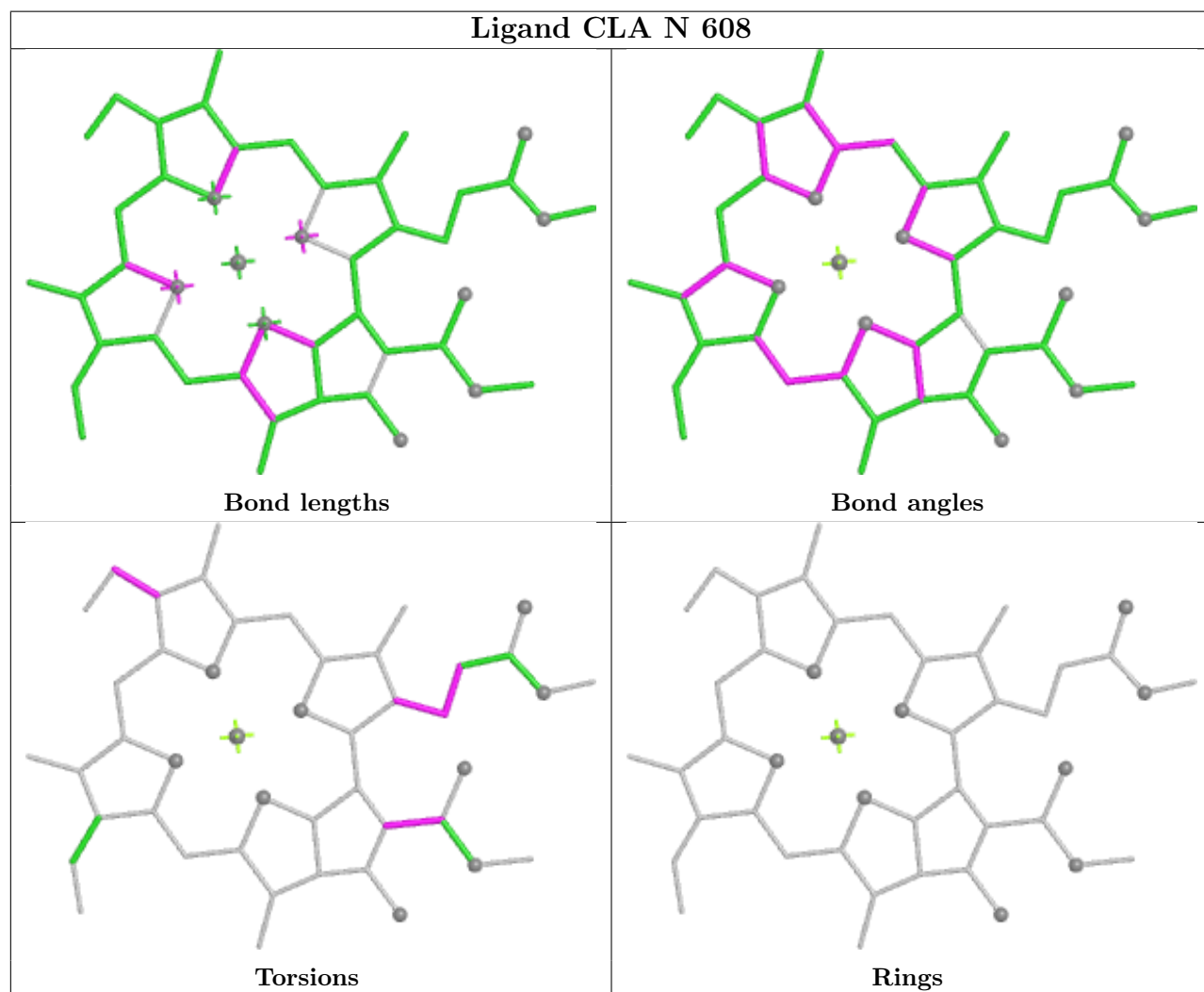
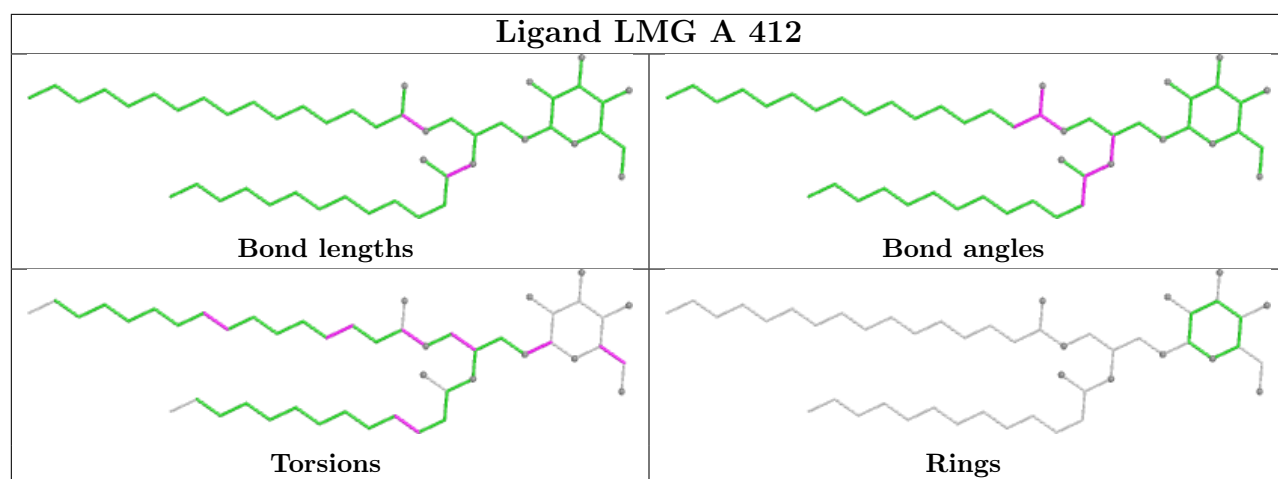
Rings

Ligand CLA R 303

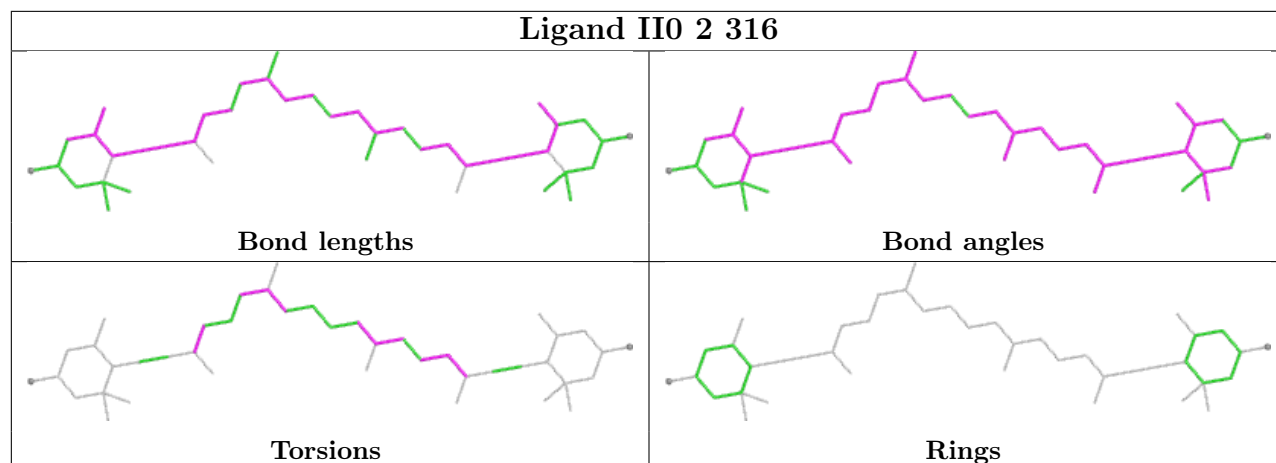


Ligand CLA c 506

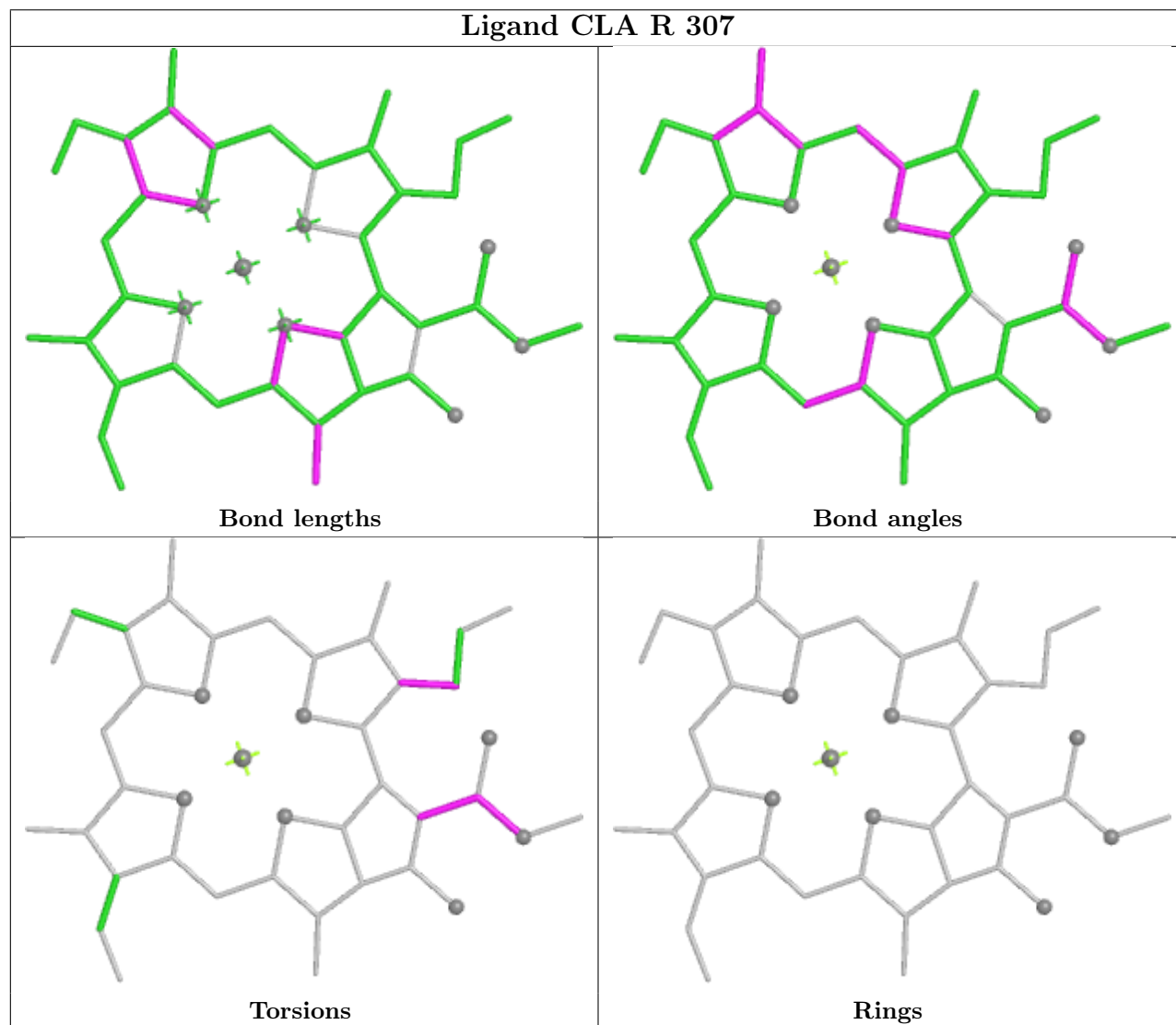


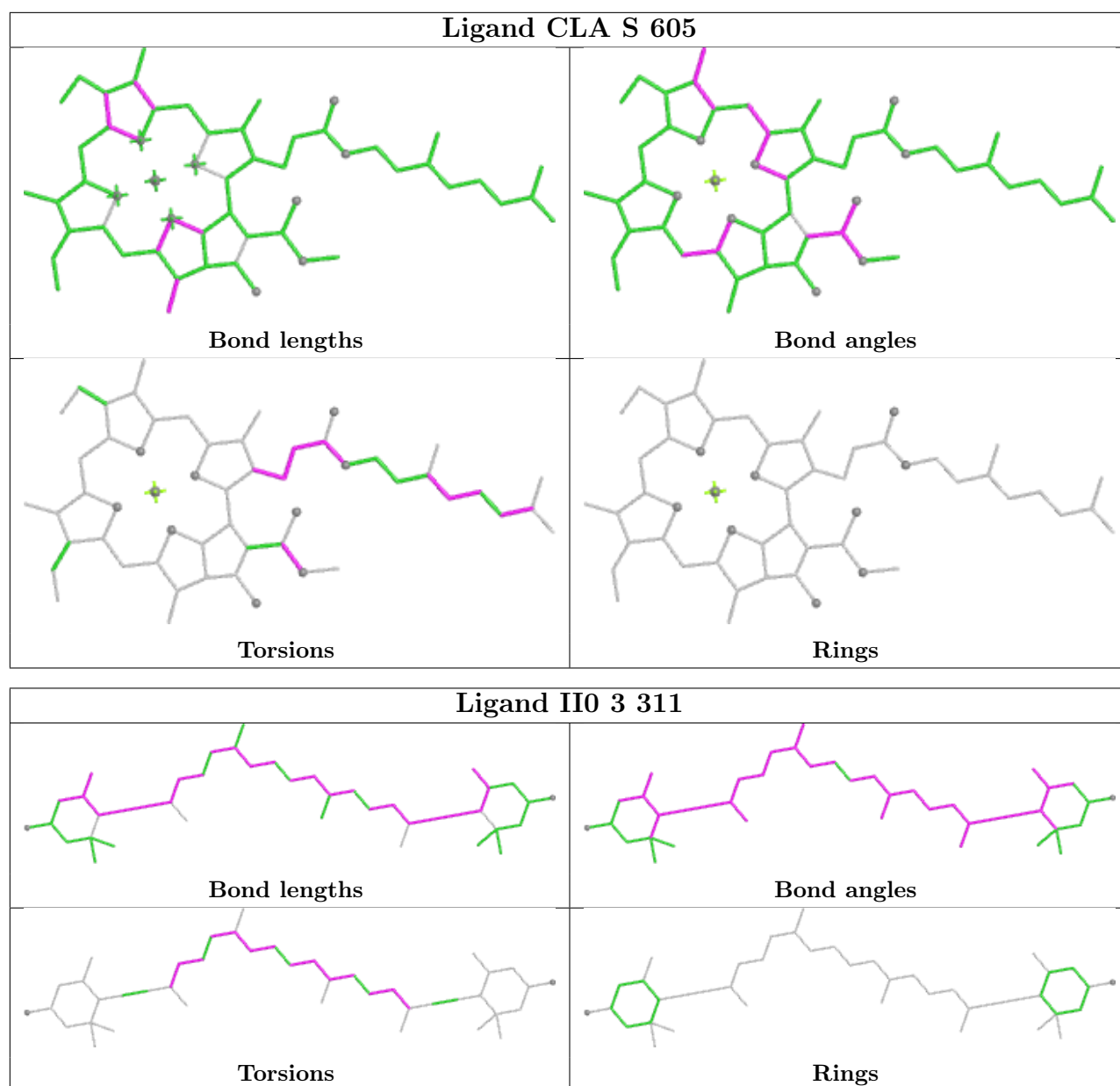


Ligand II0 2 316

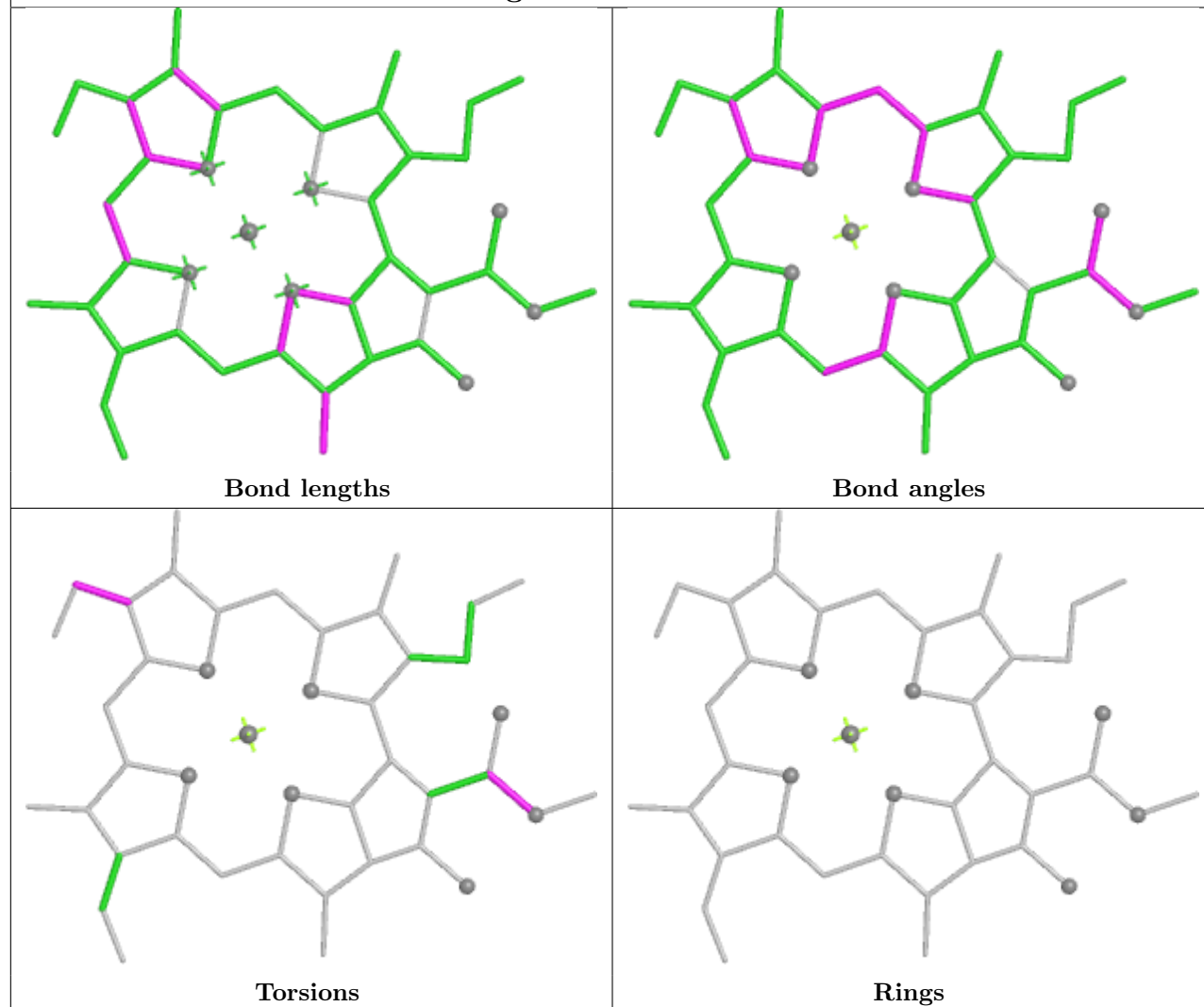


Ligand CLA R 307

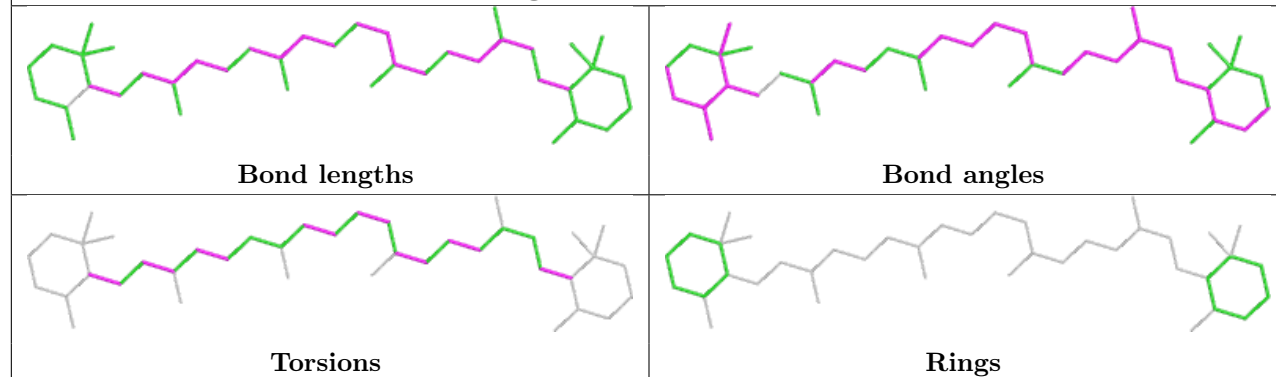




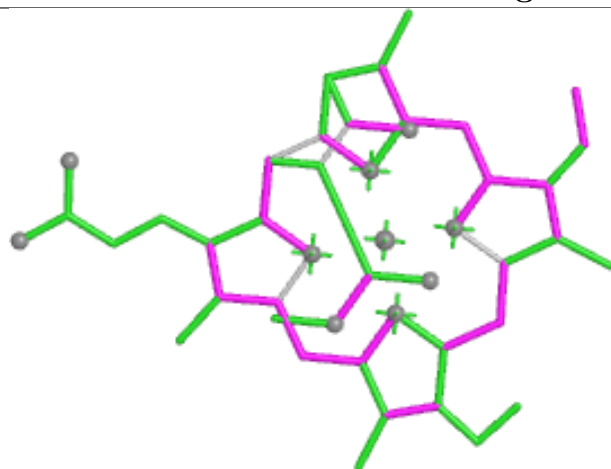
Ligand CLA 4 313



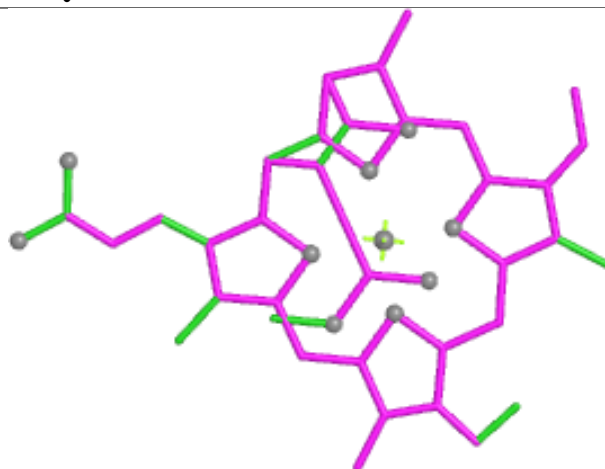
Ligand WVN Z 101



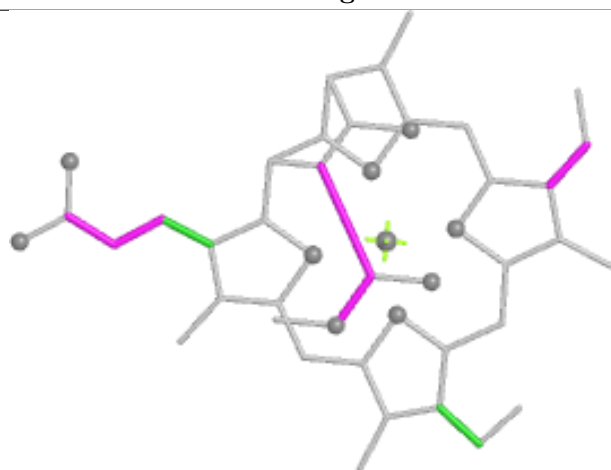
Ligand KC2 Q 309



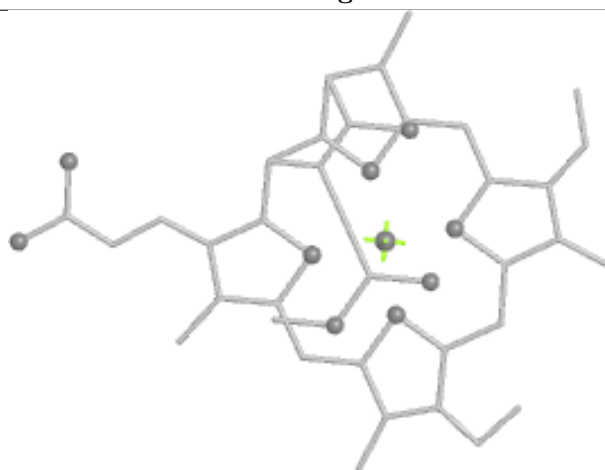
Bond lengths



Bond angles

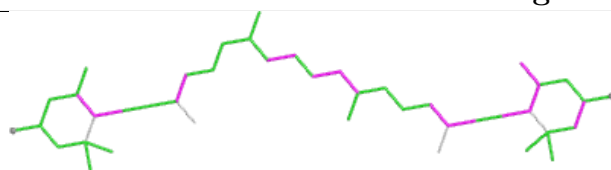


Torsions

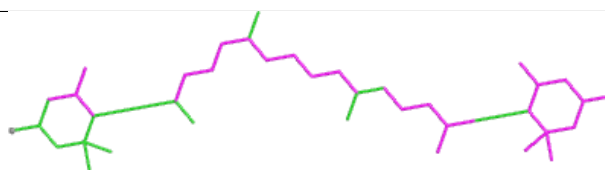


Rings

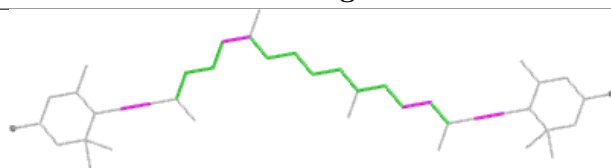
Ligand II0 4 317



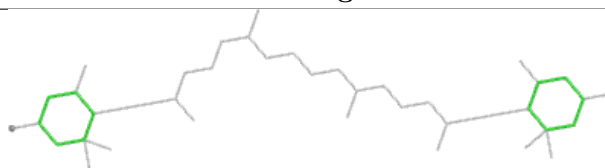
Bond lengths



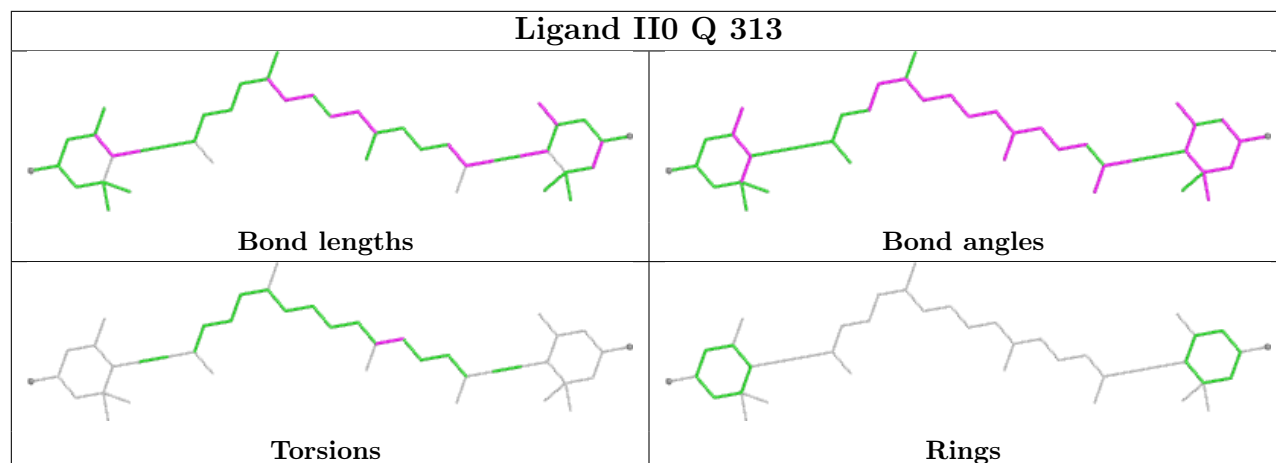
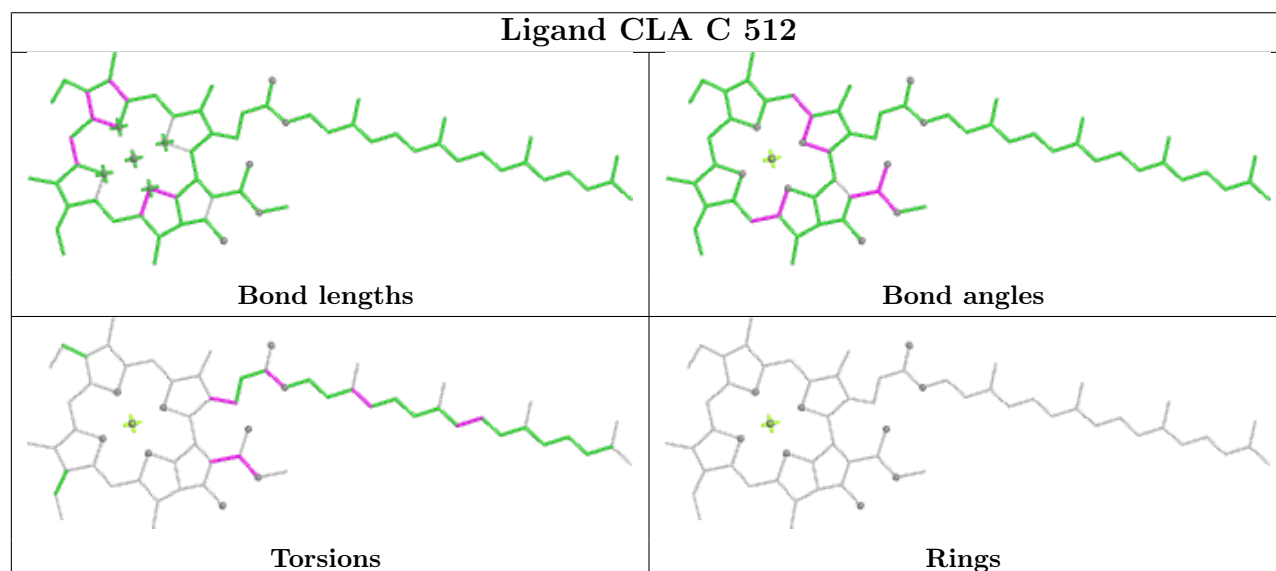
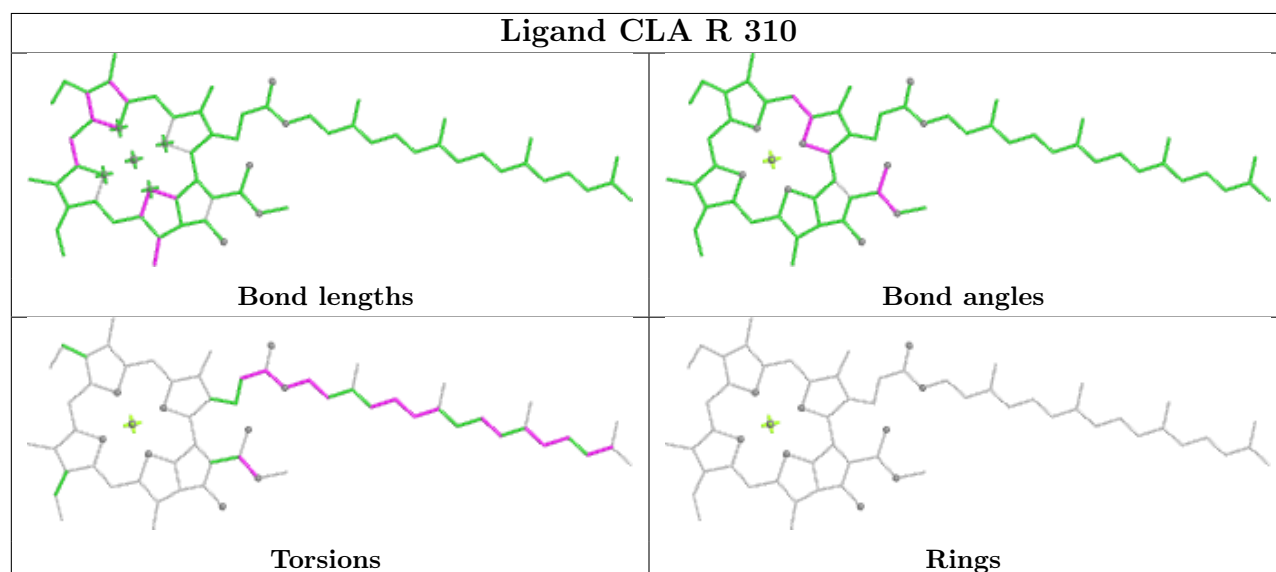
Bond angles

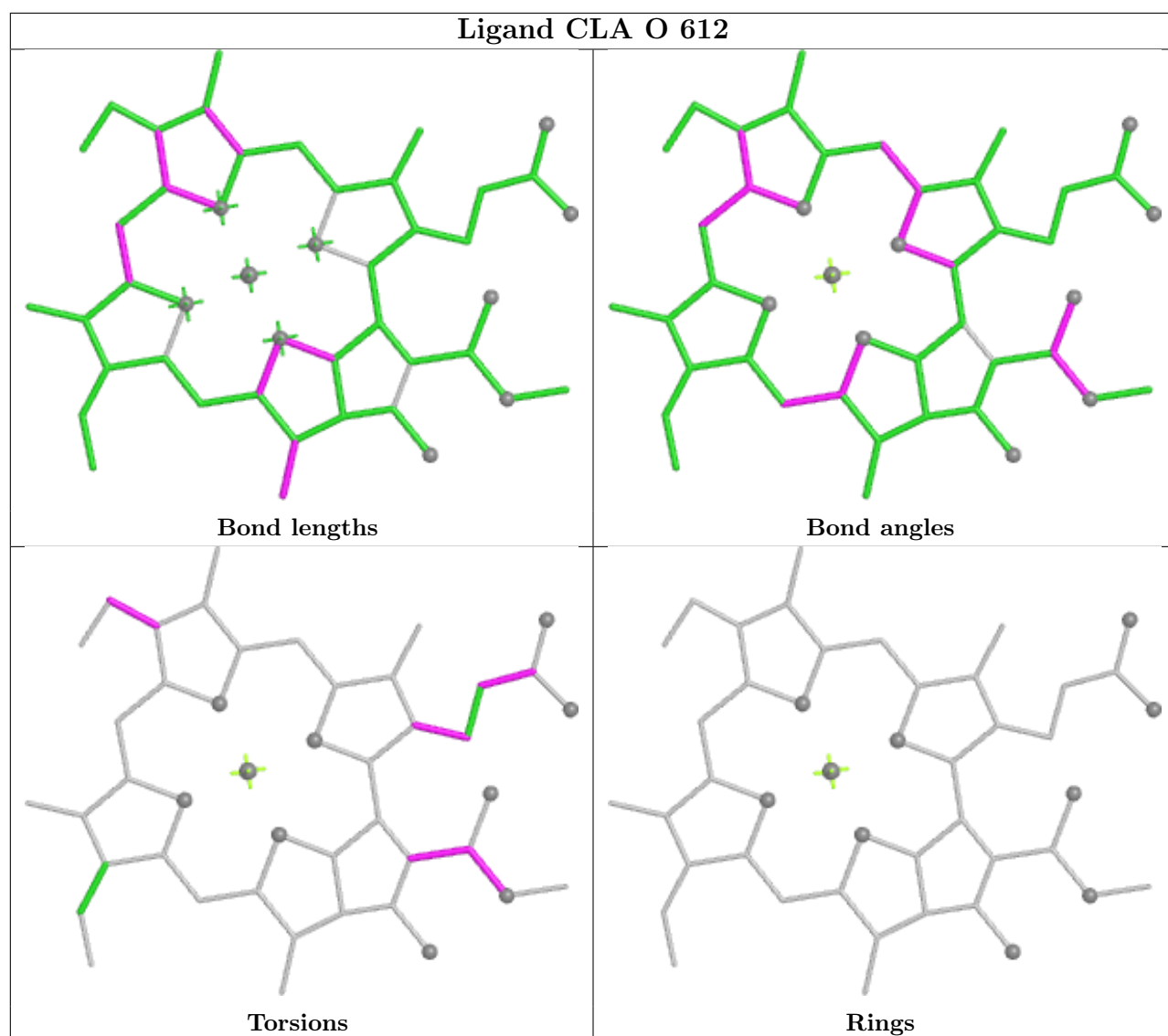


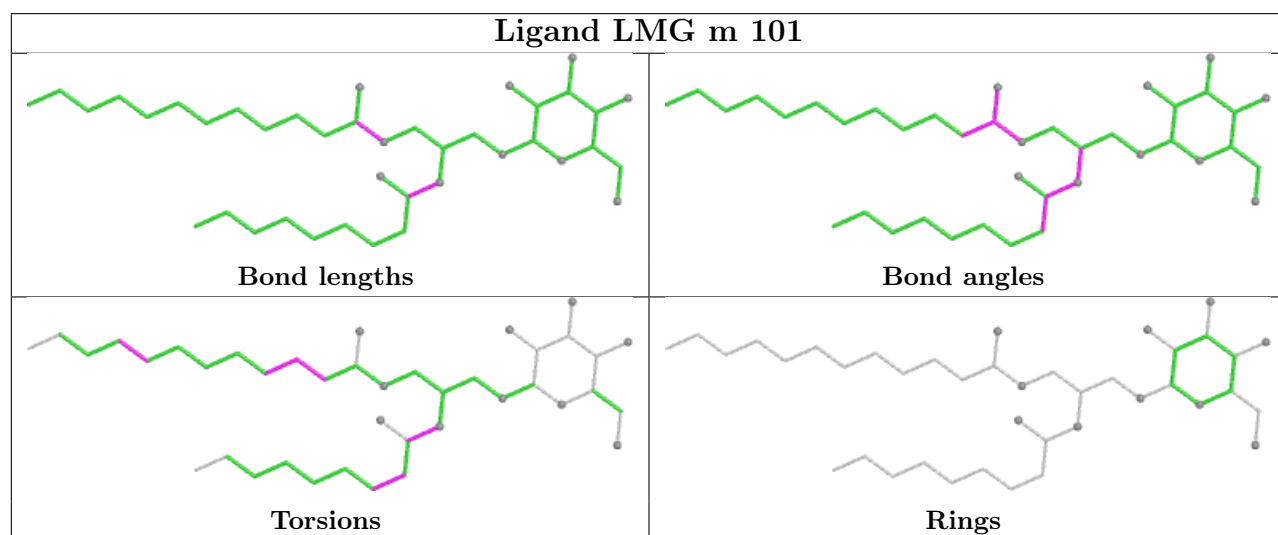
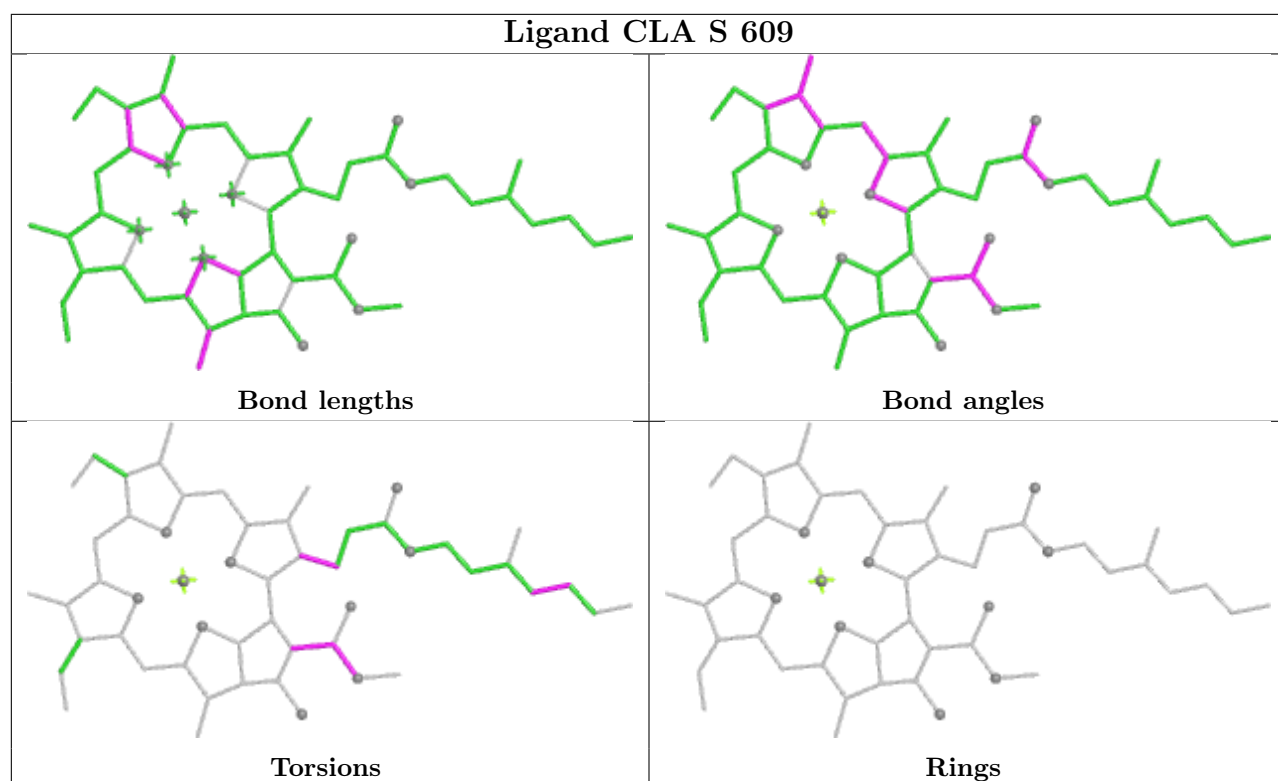
Torsions

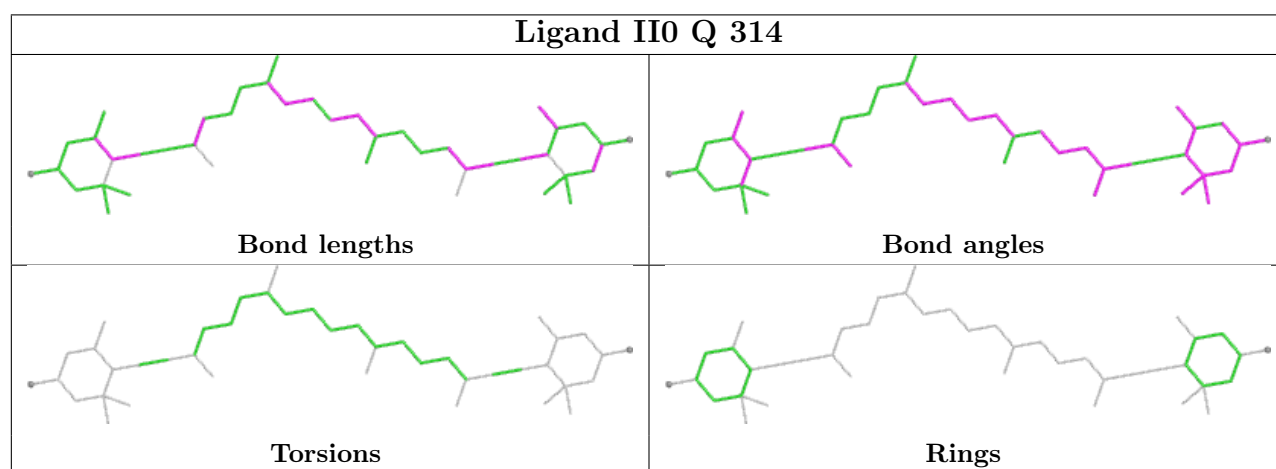
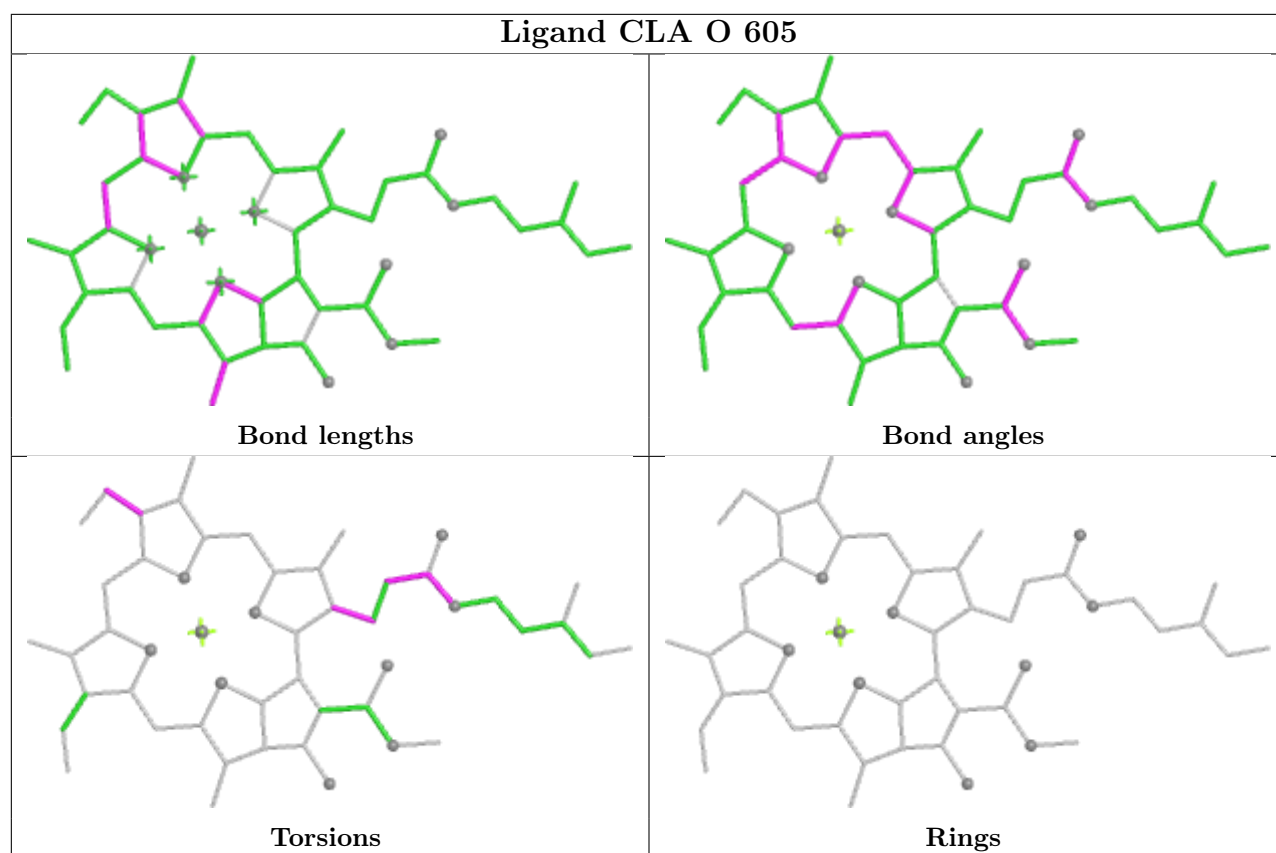


Rings

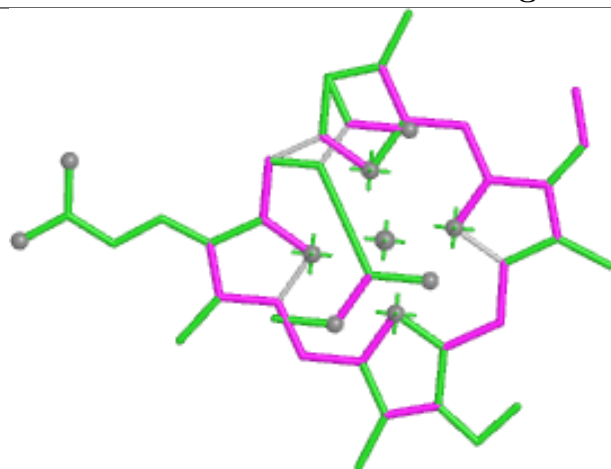
Ligand II0 Q 313**Ligand CLA C 512****Ligand CLA R 310**



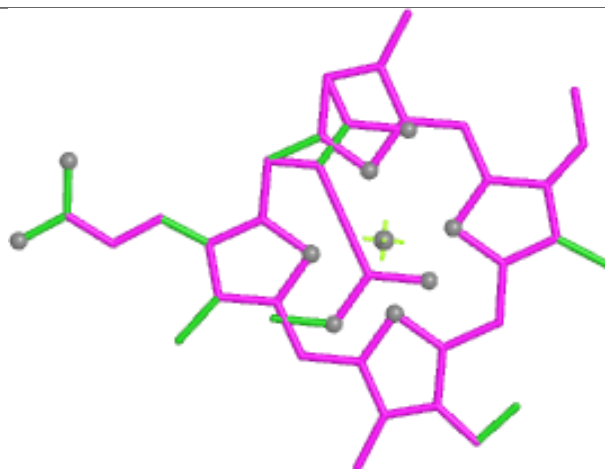




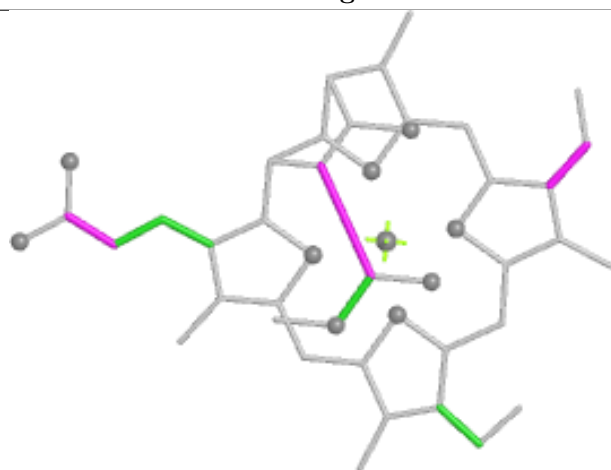
Ligand KC2 S 608



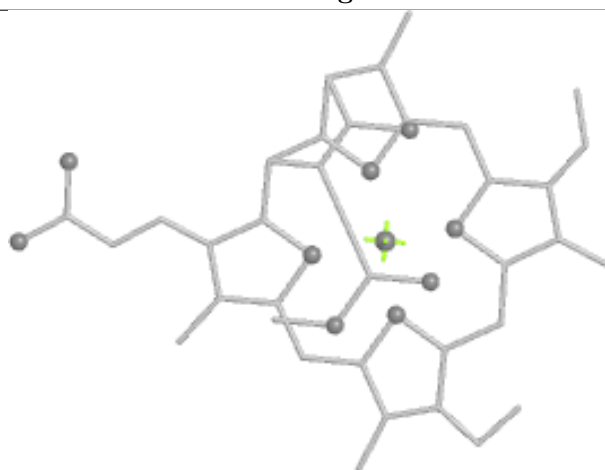
Bond lengths



Bond angles



Torsions

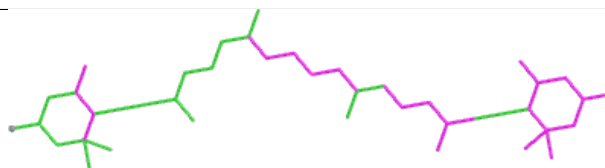


Rings

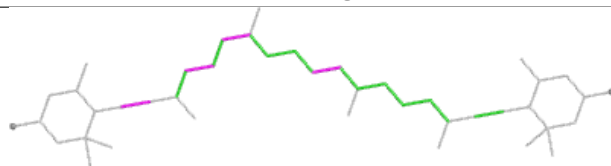
Ligand II0 S 611



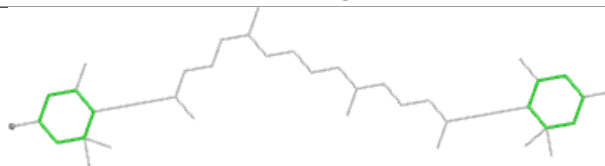
Bond lengths



Bond angles

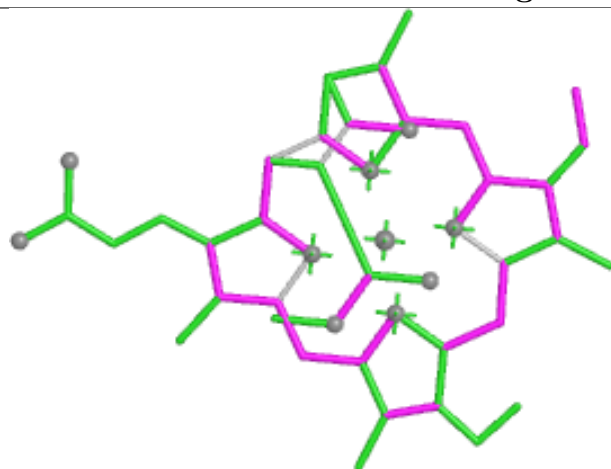


Torsions

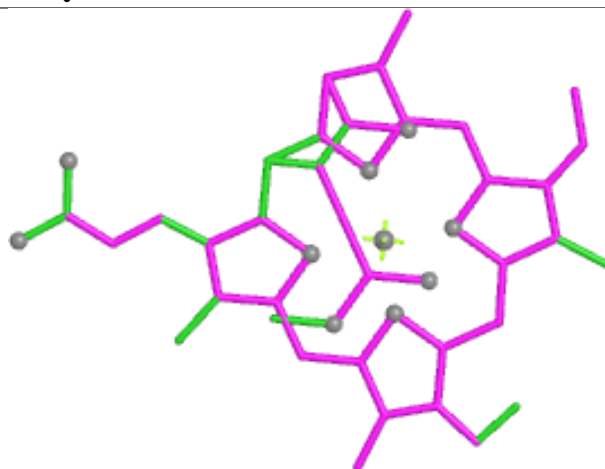


Rings

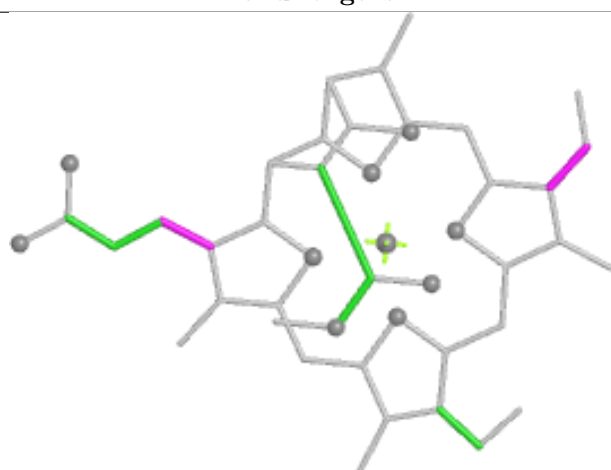
Ligand KC2 Q 310



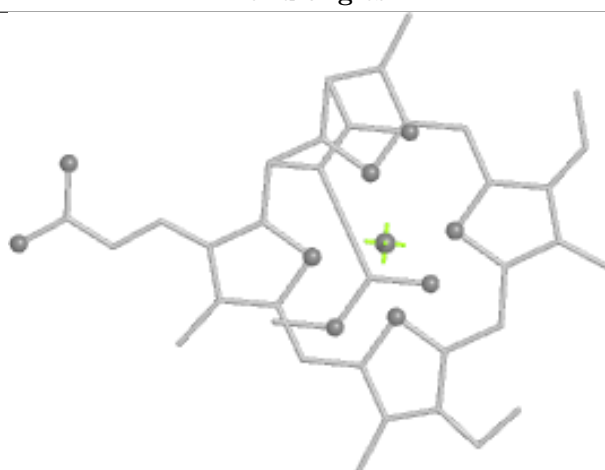
Bond lengths



Bond angles

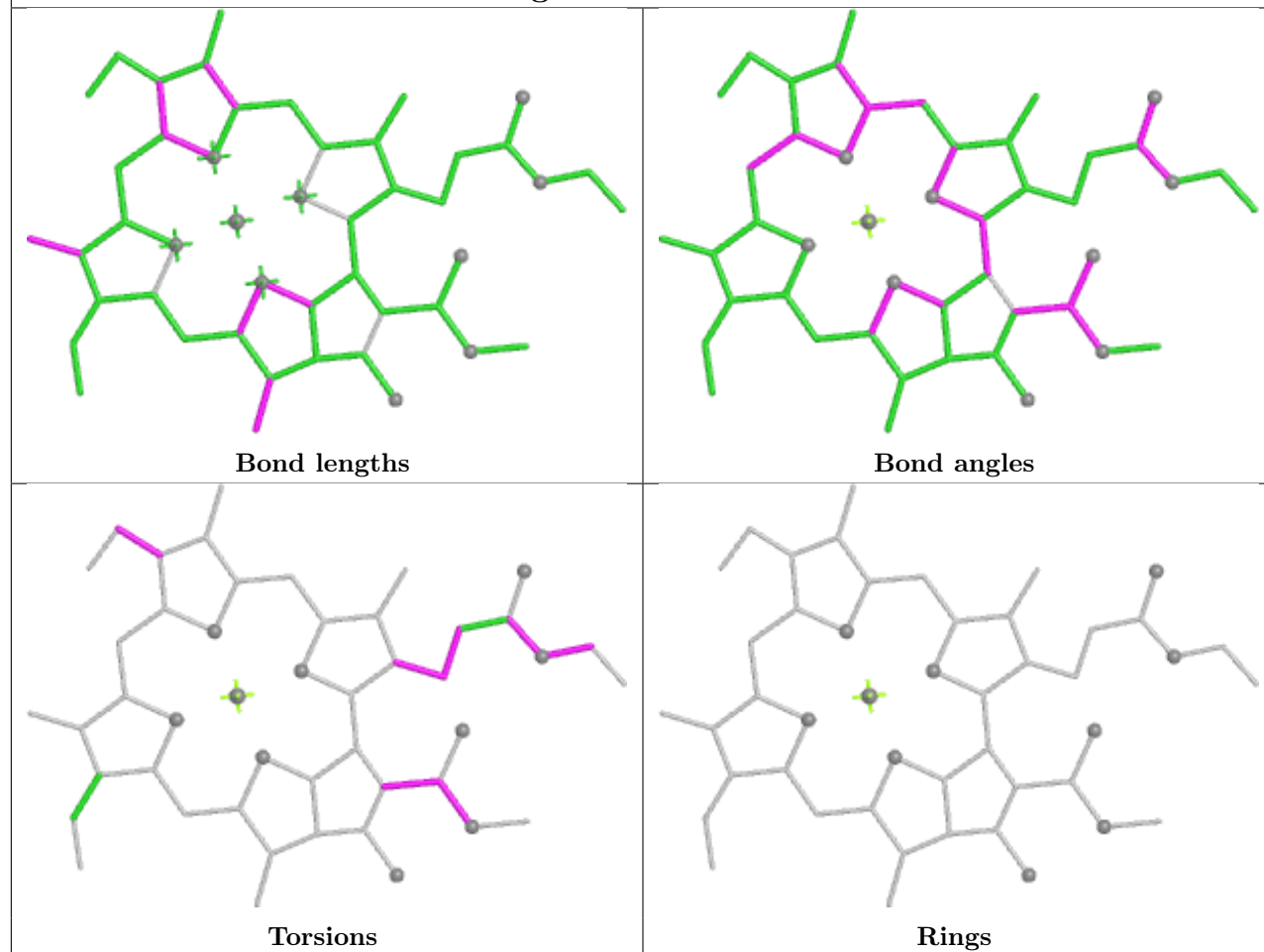


Torsions

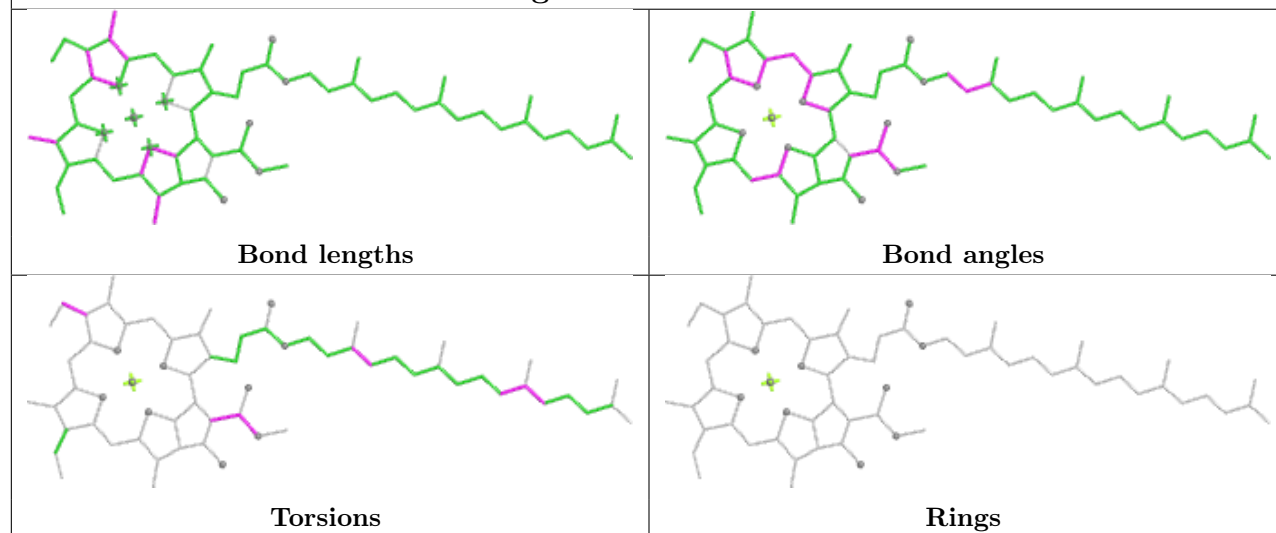


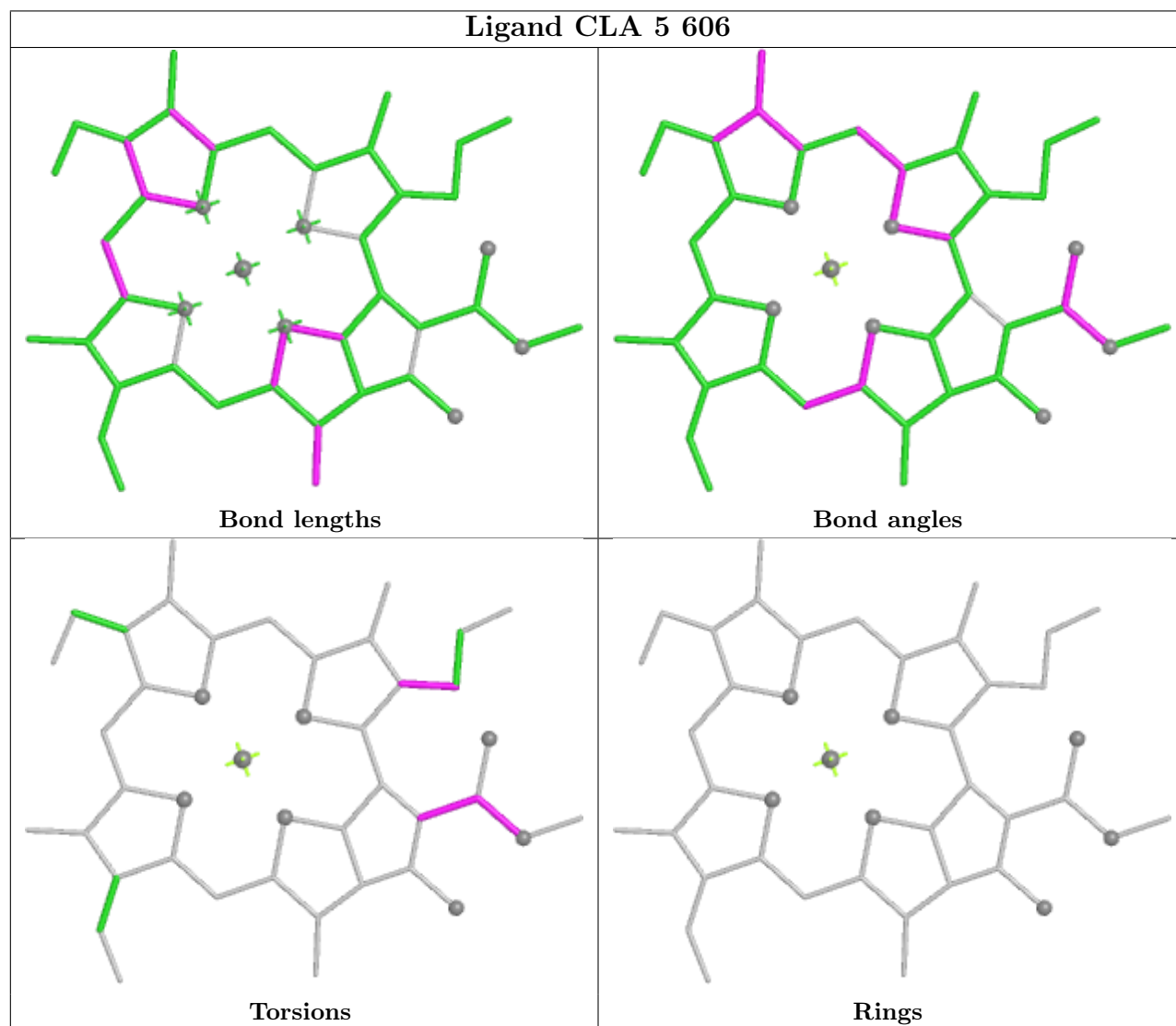
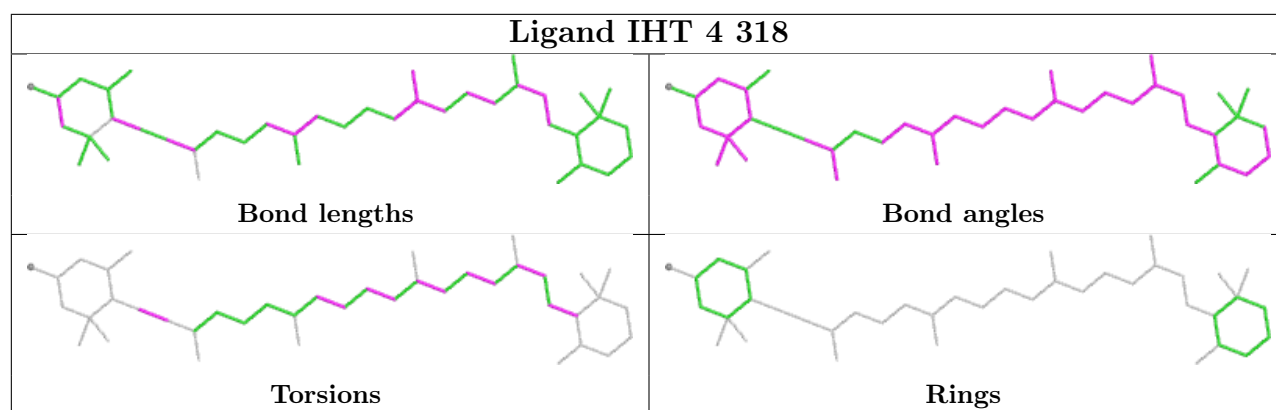
Rings

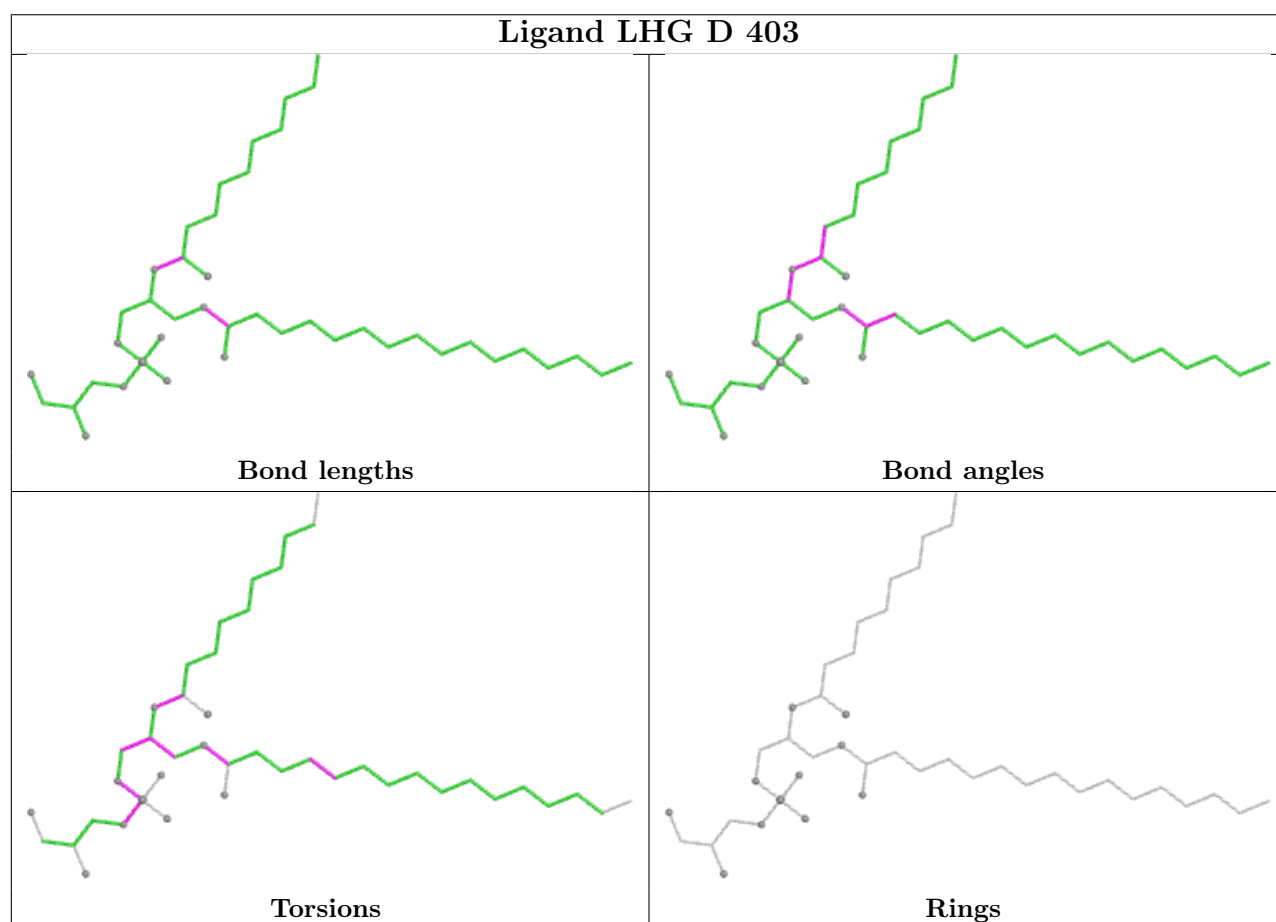
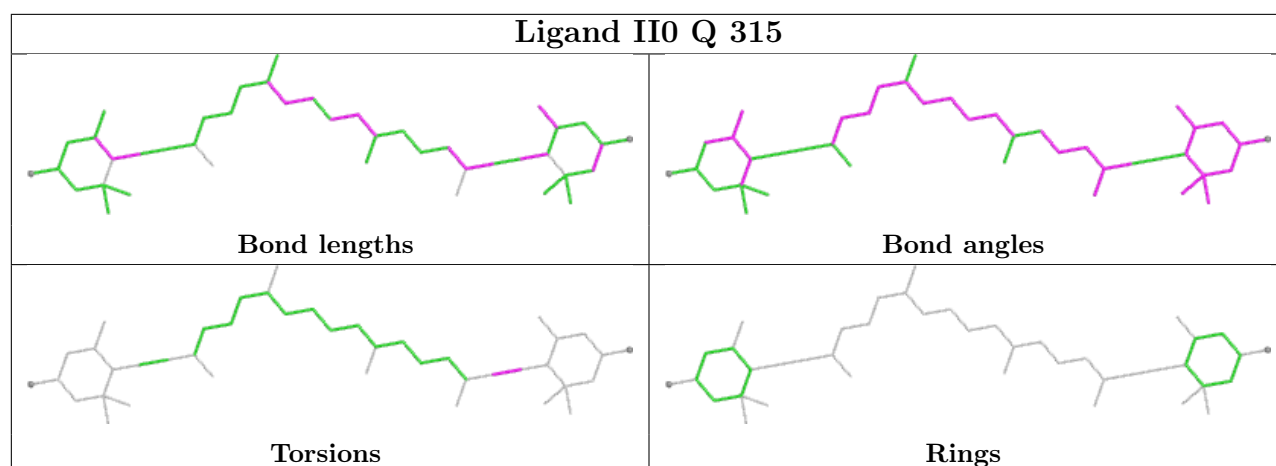
Ligand CLA 1 614

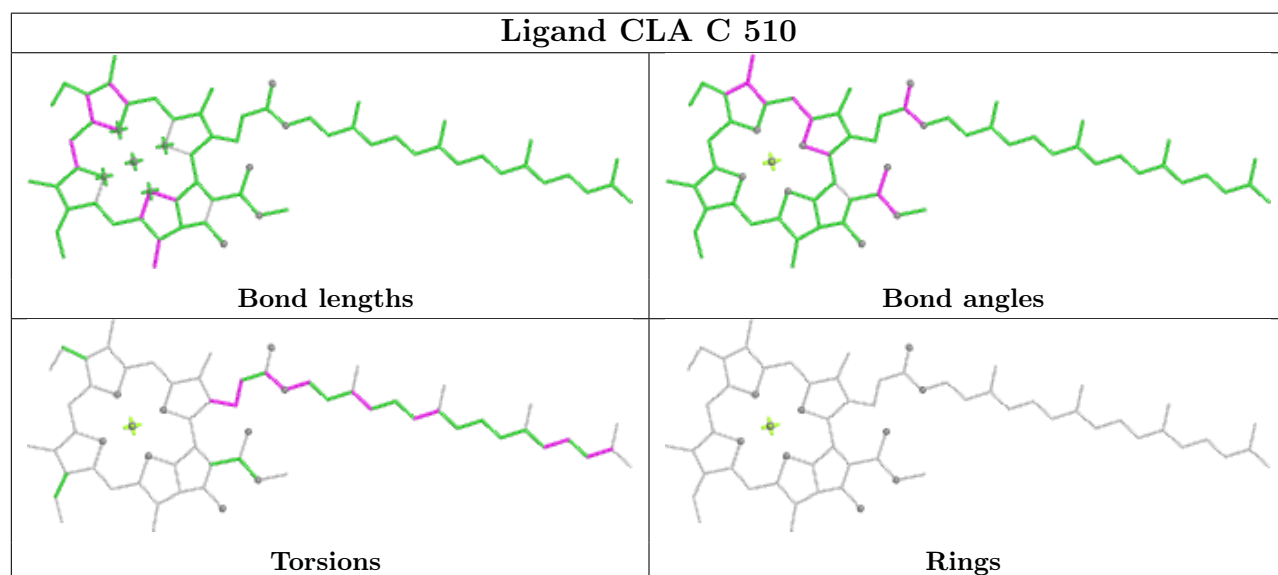
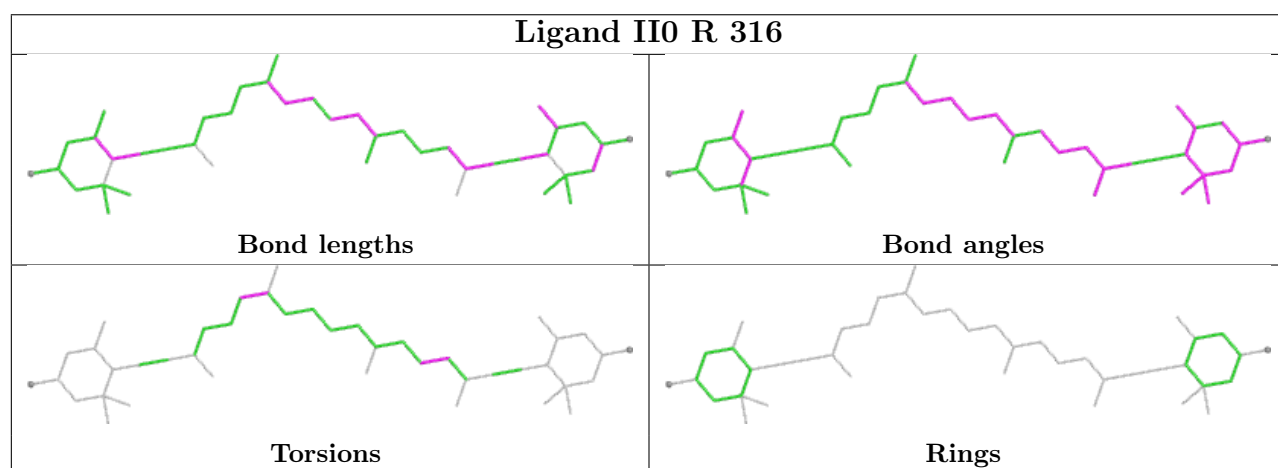
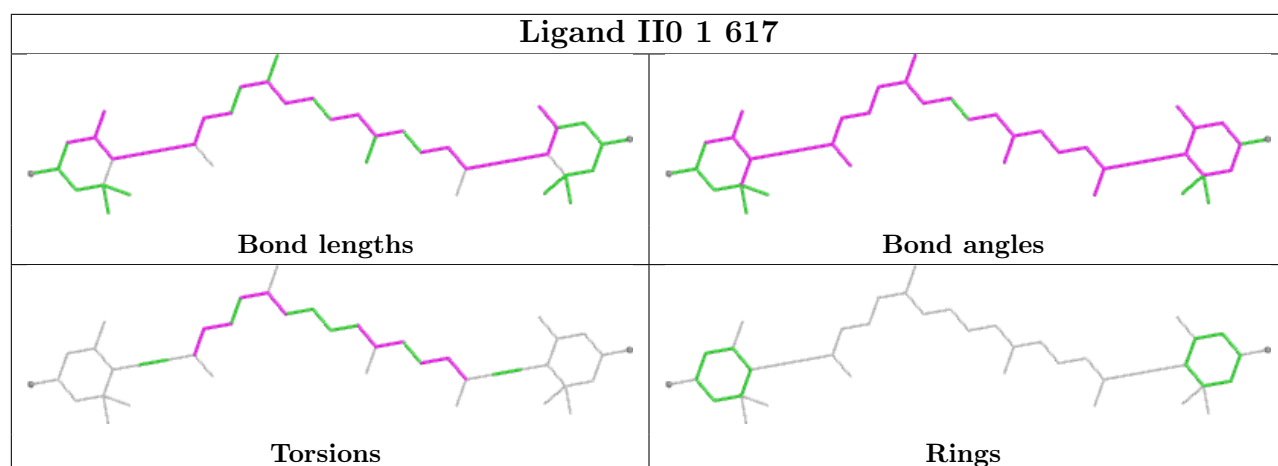


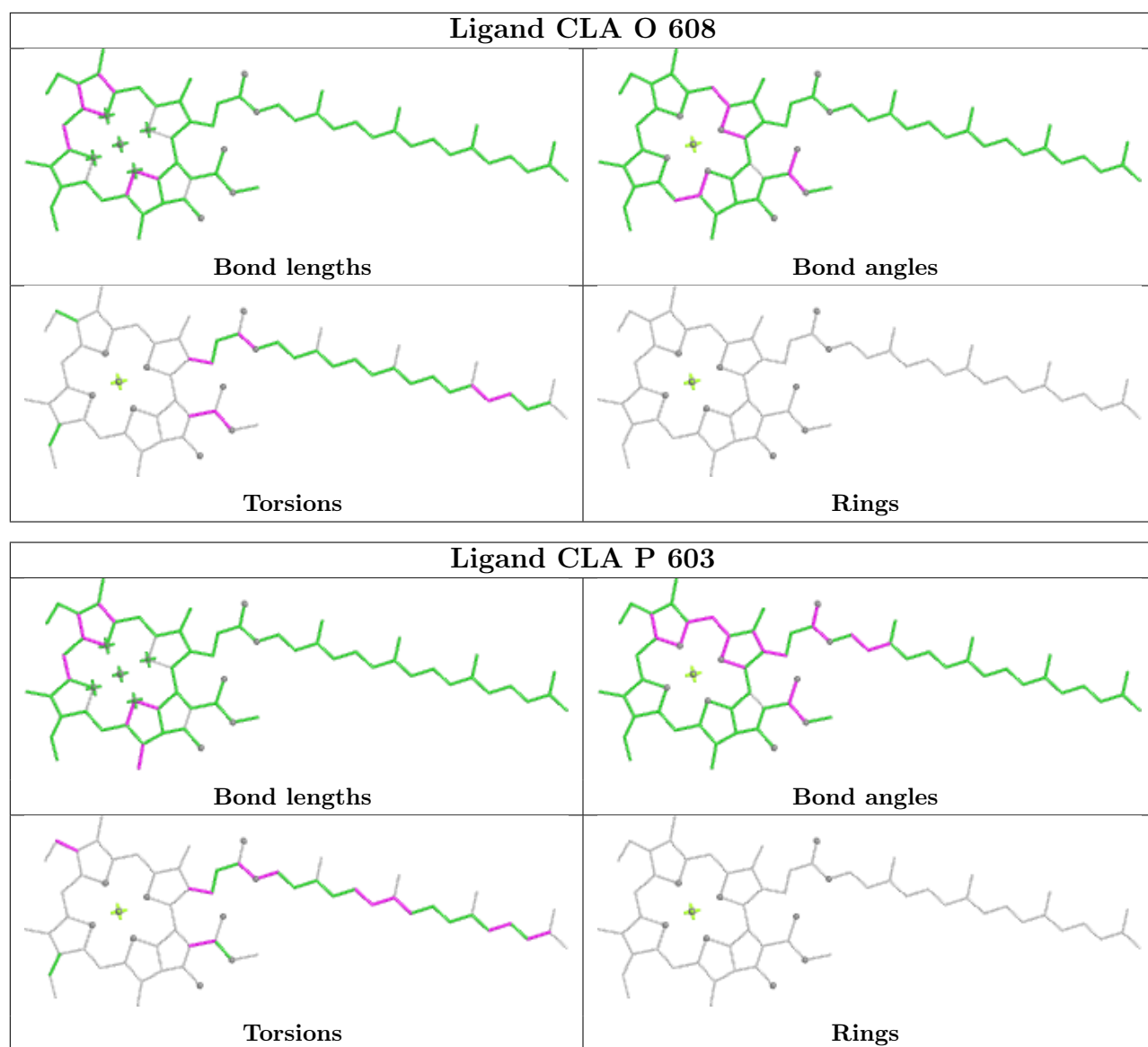
Ligand CLA R 308

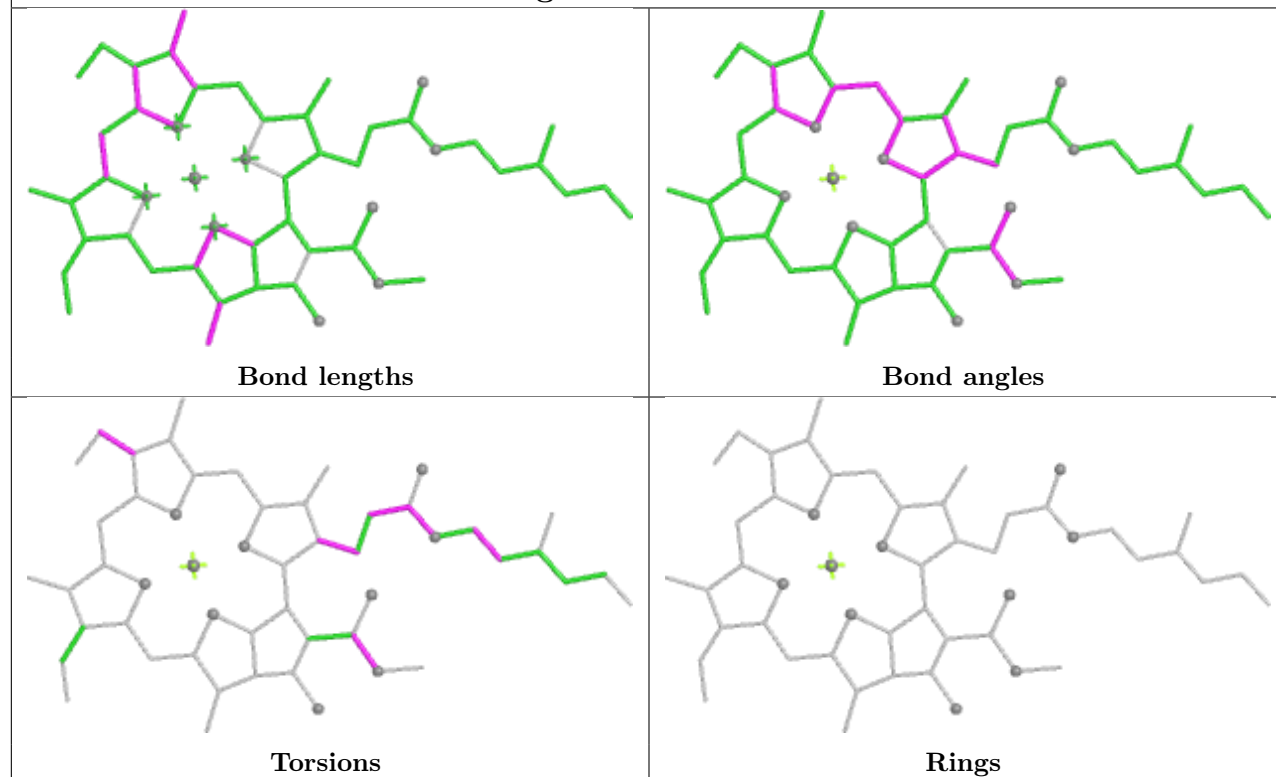
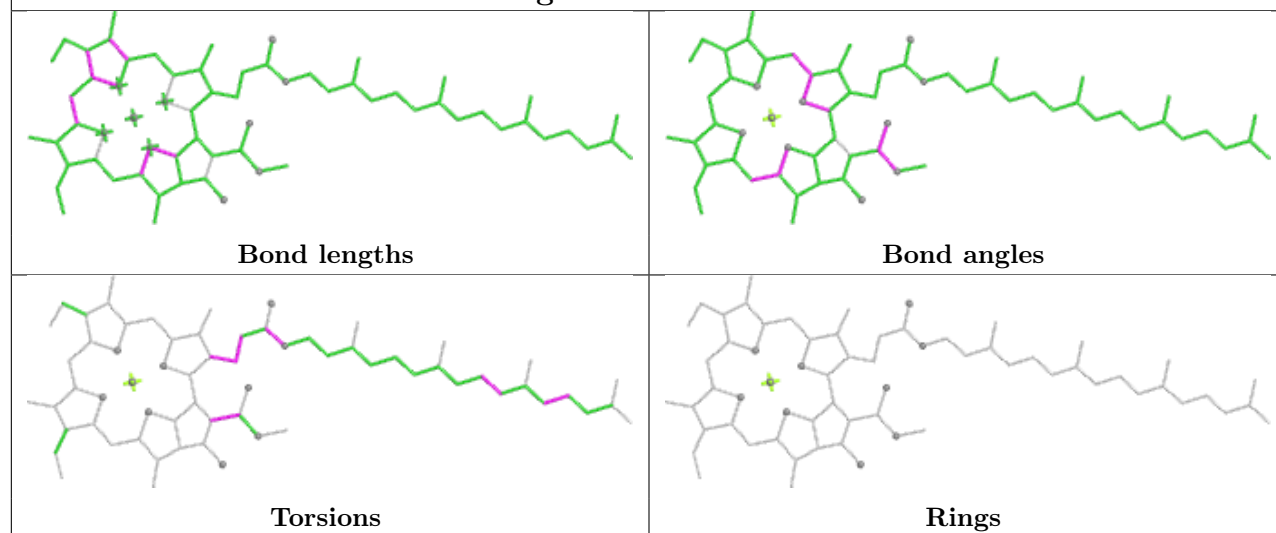




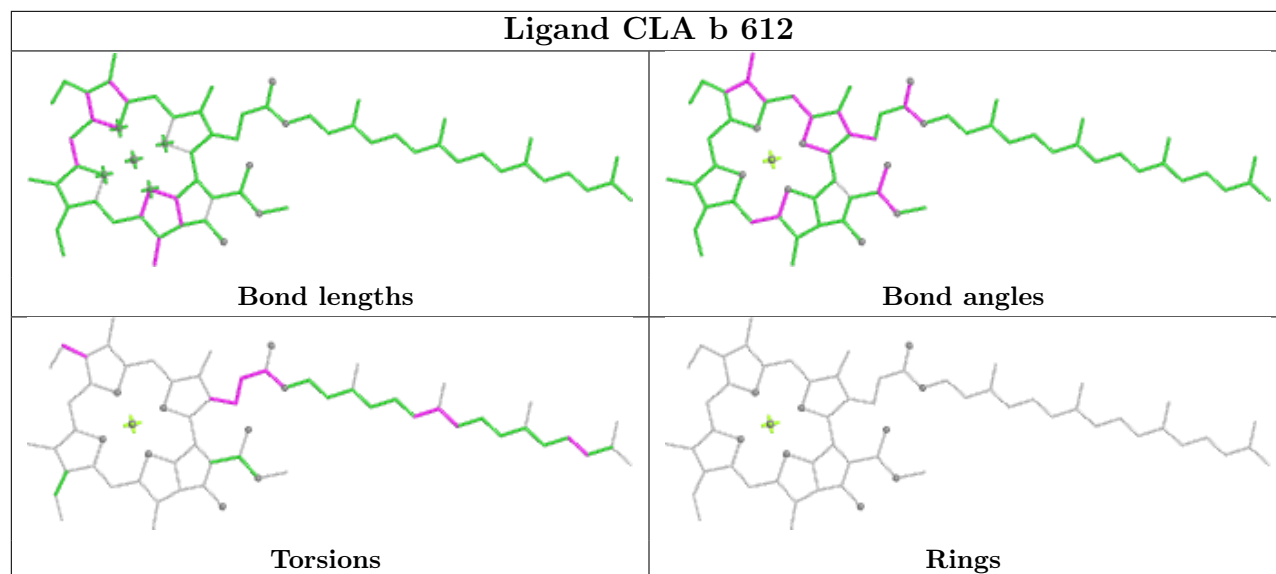




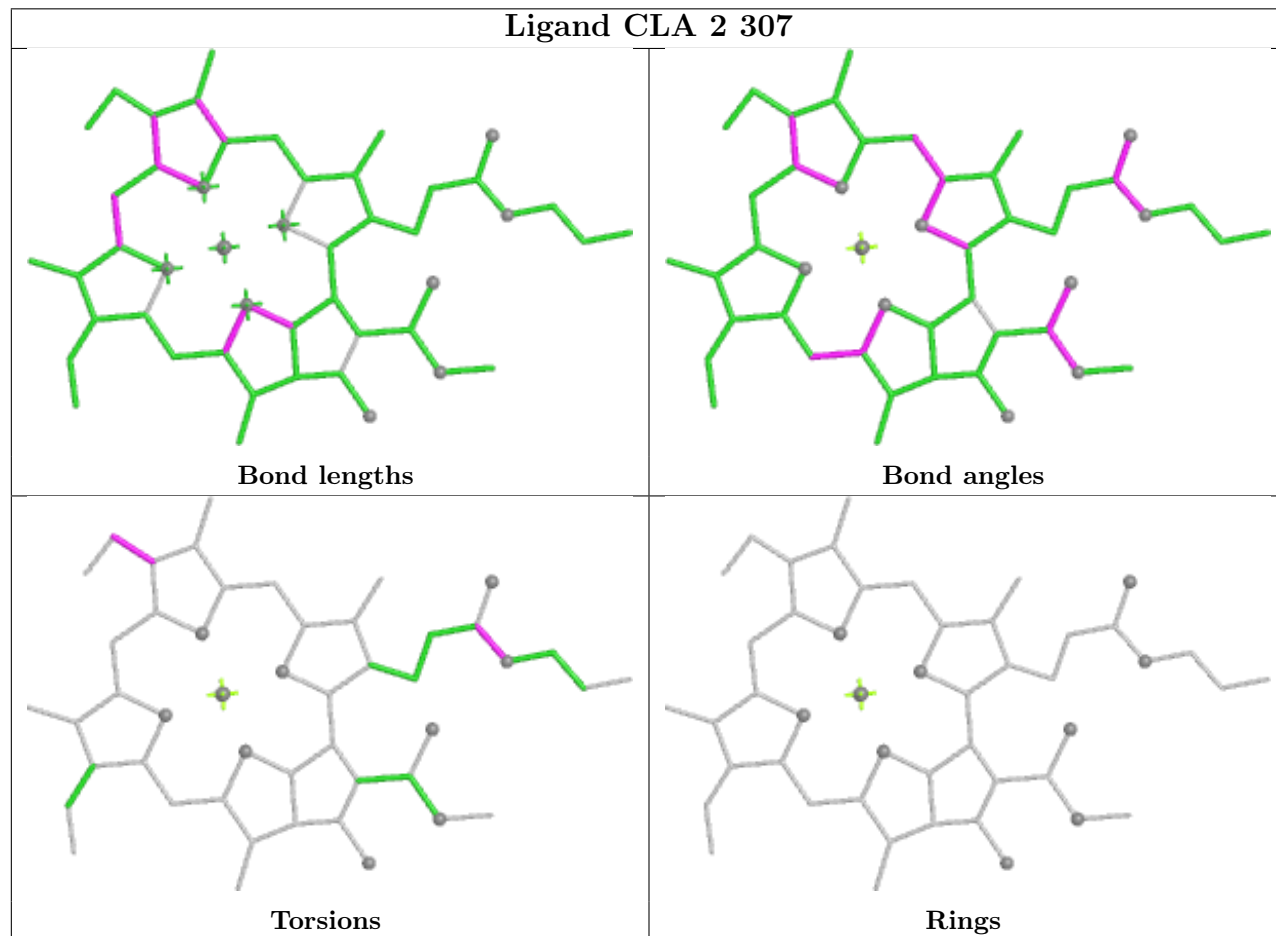


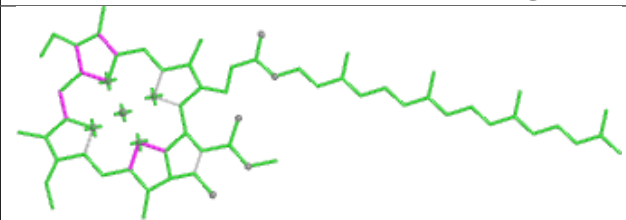
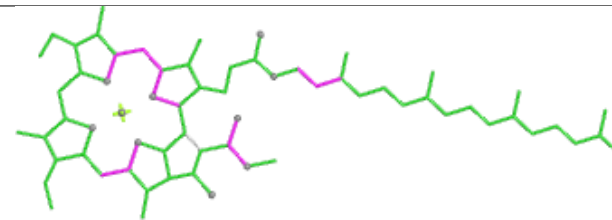
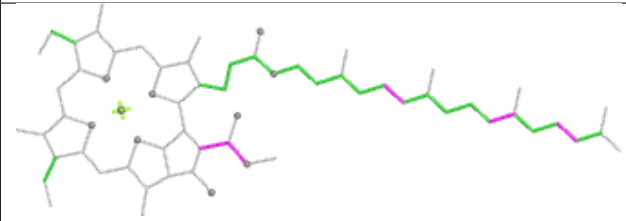
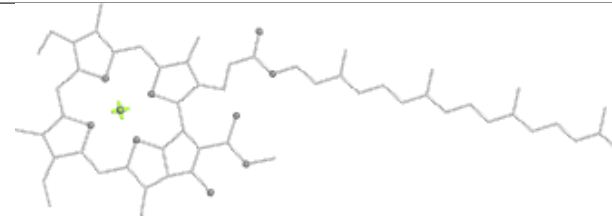
Ligand CLA 5 603**Ligand CLA 4 302**

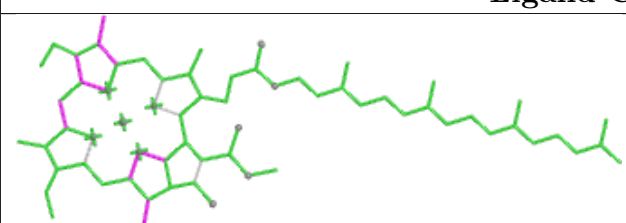
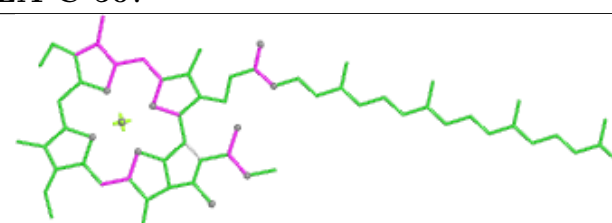
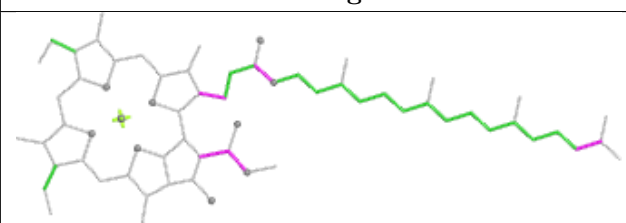
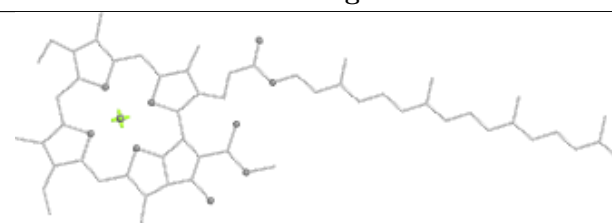
Ligand CLA b 612

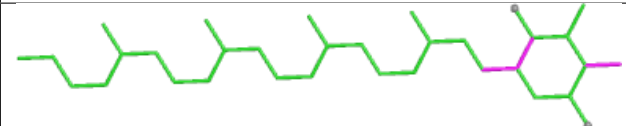
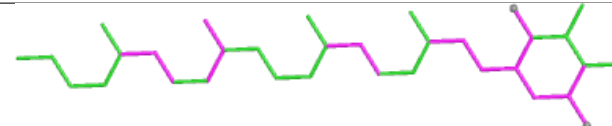
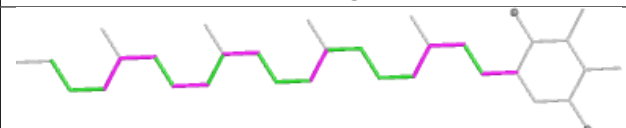
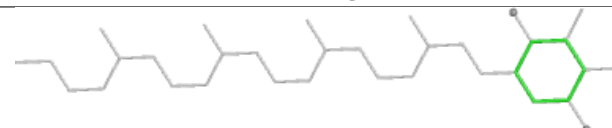


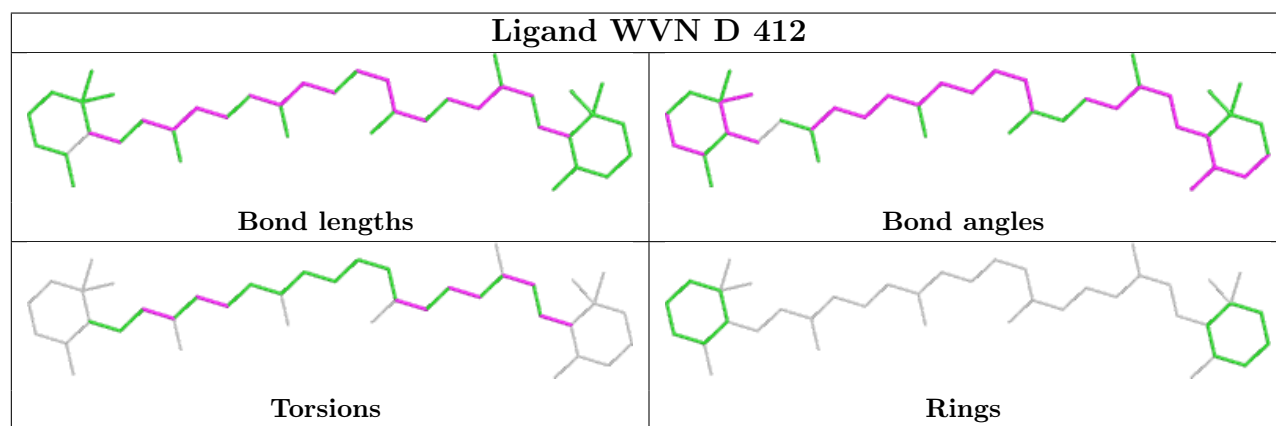
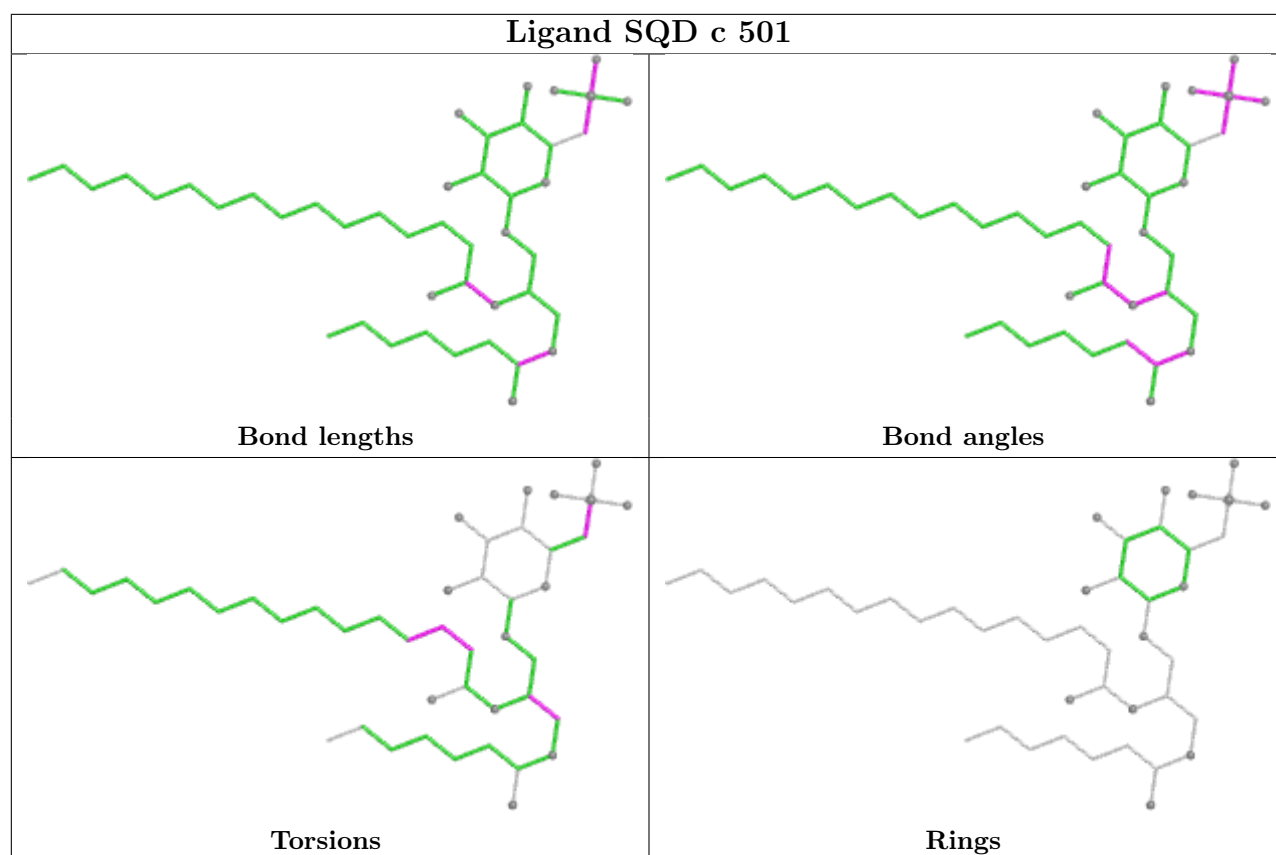
Ligand CLA 2 307

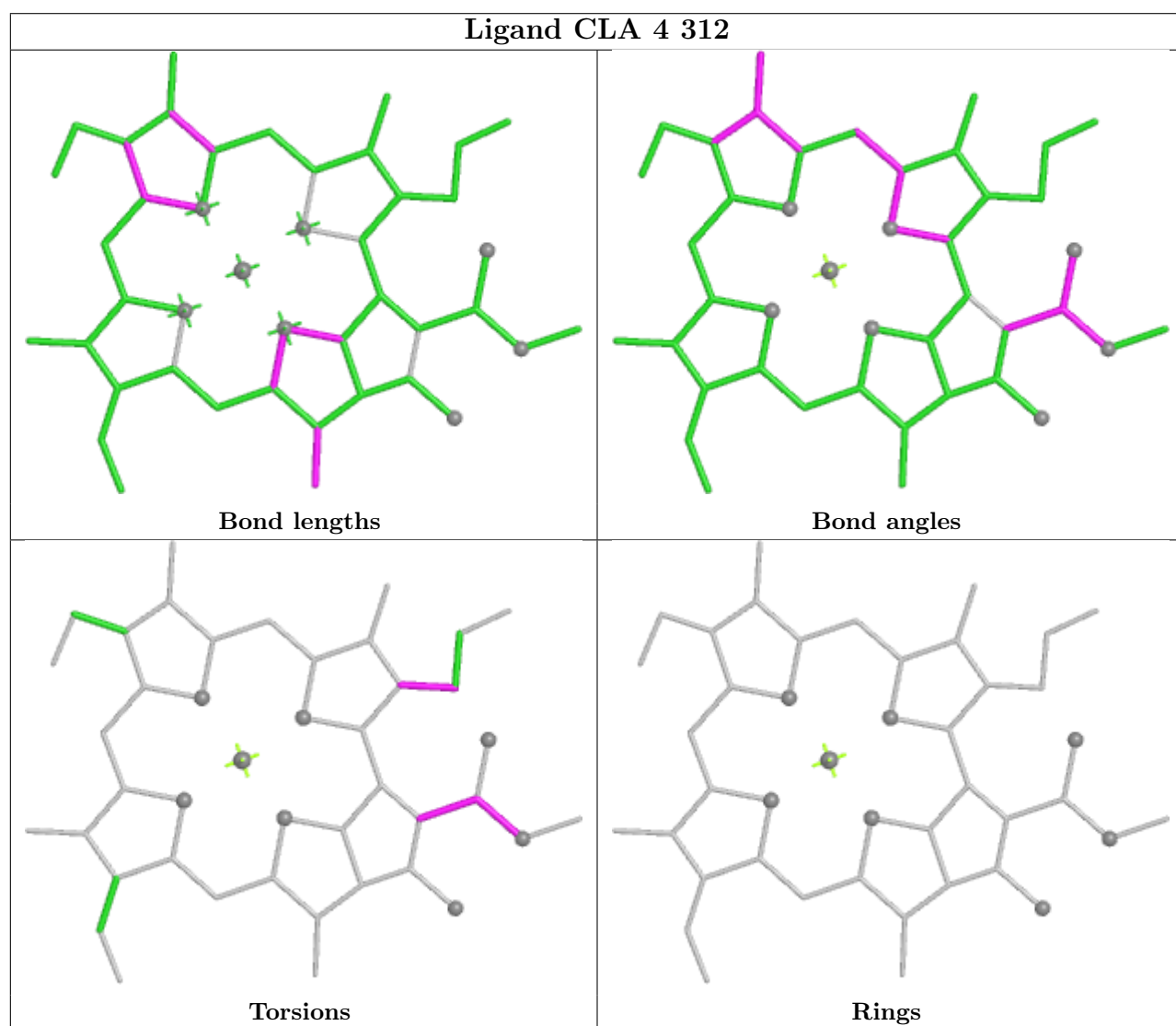
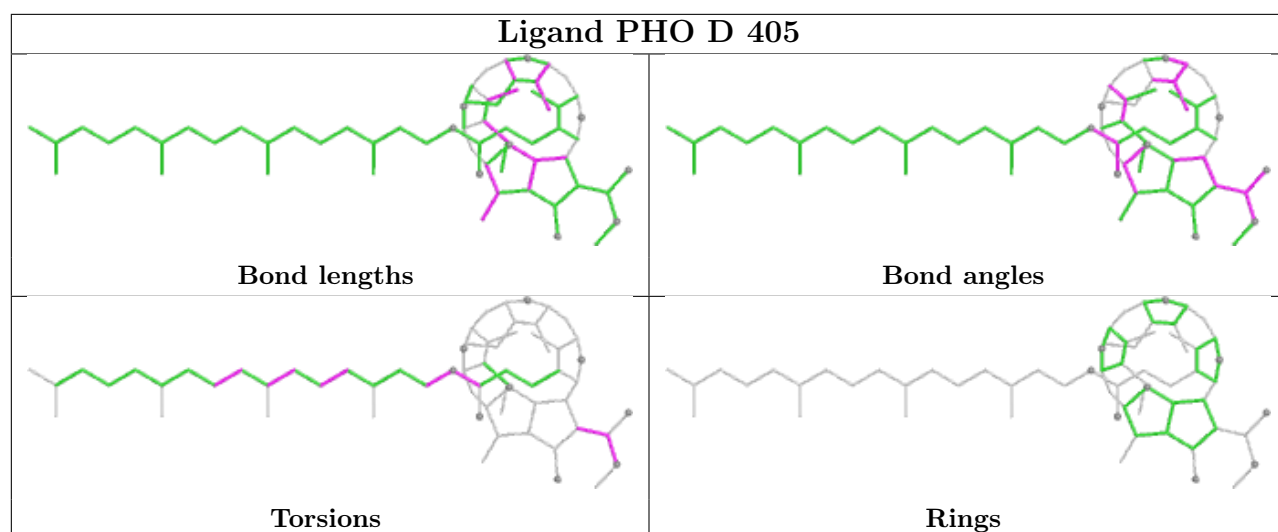


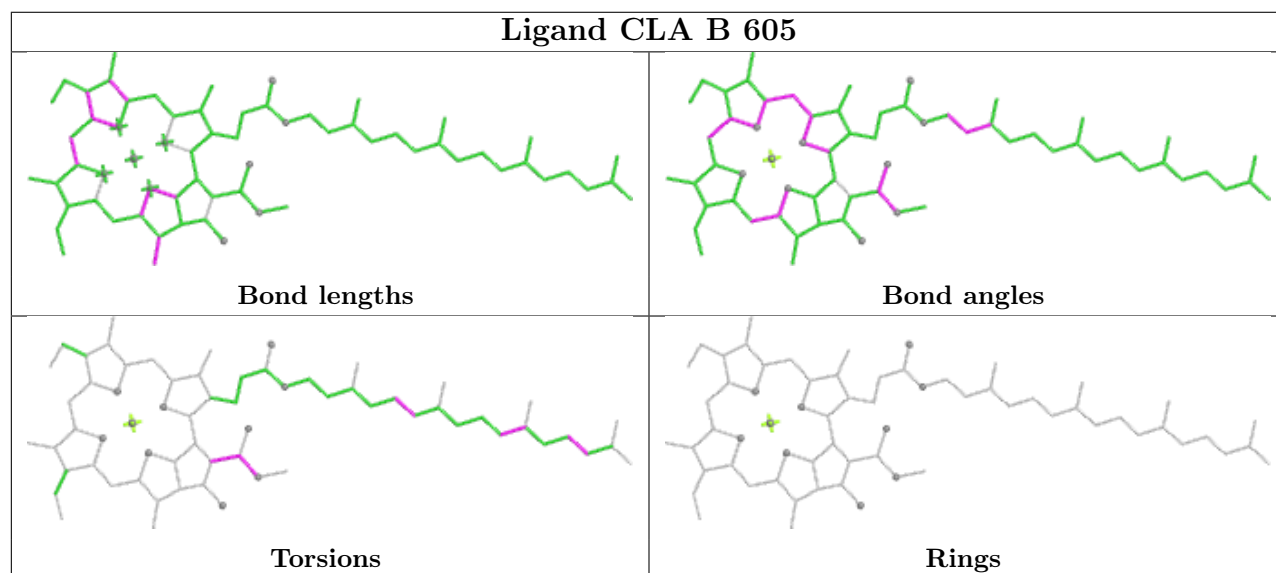
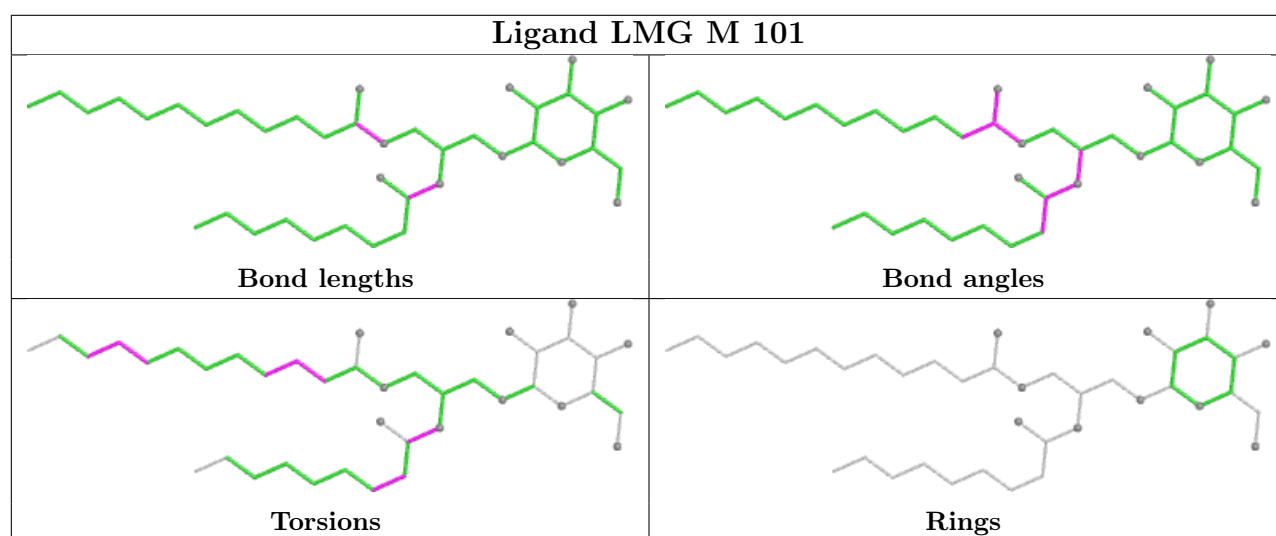
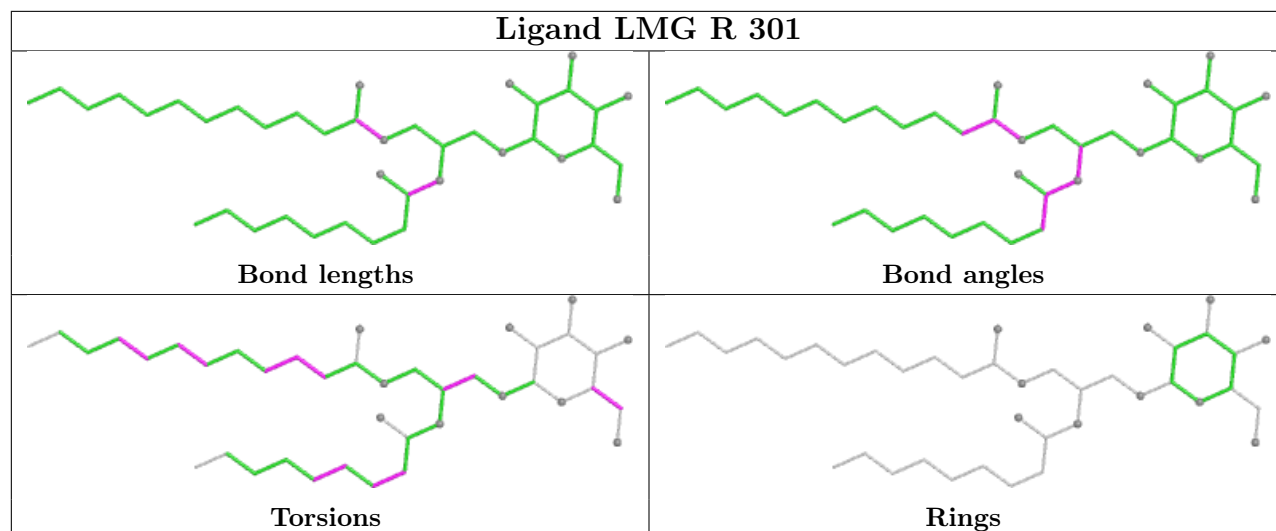
Ligand CLA b 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

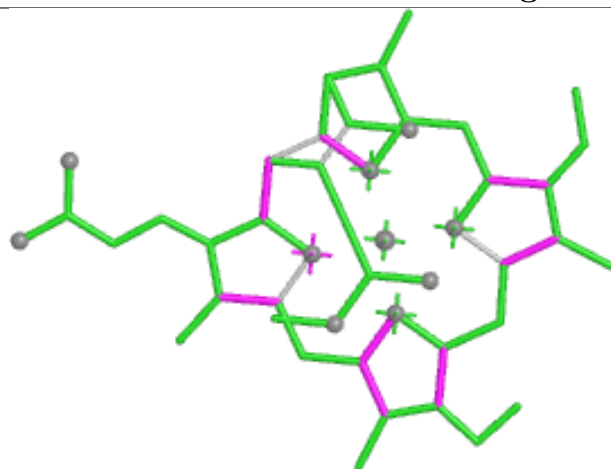
Ligand PL9 A 407	
	
Bond lengths	Bond angles
	
Torsions	Rings



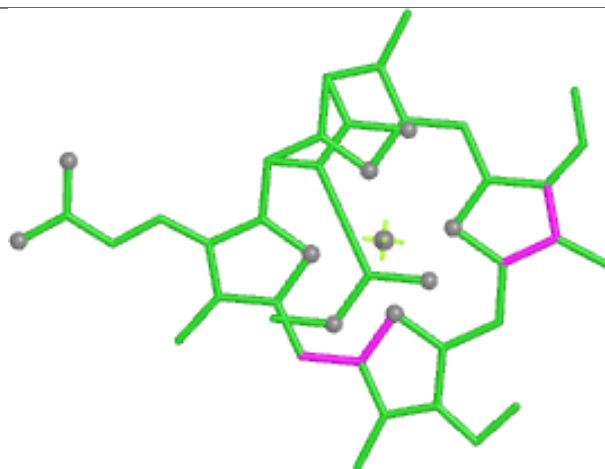




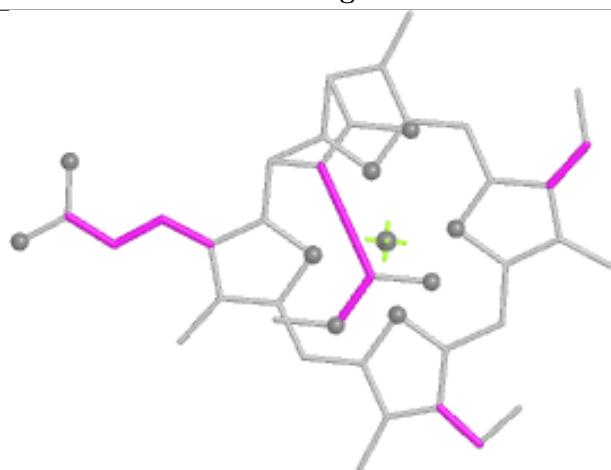
Ligand KC2 1 610



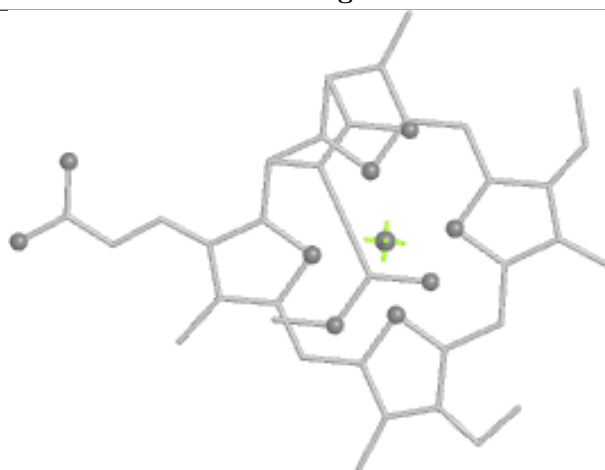
Bond lengths



Bond angles

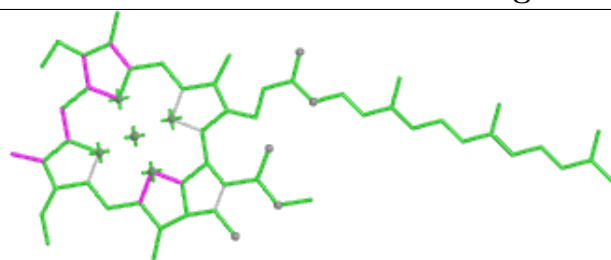


Torsions

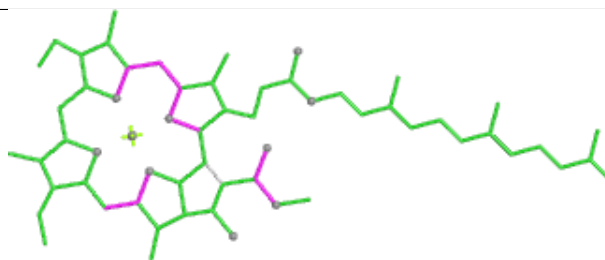


Rings

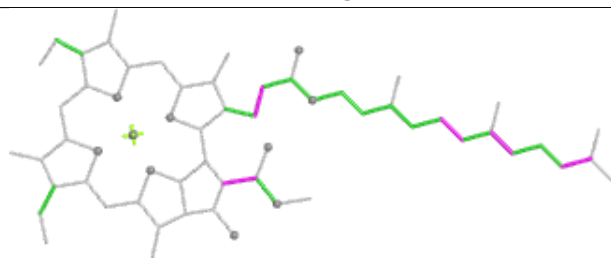
Ligand CLA N 609



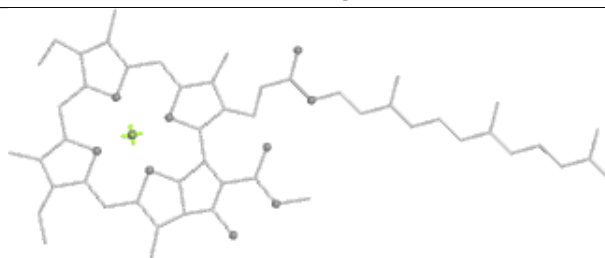
Bond lengths



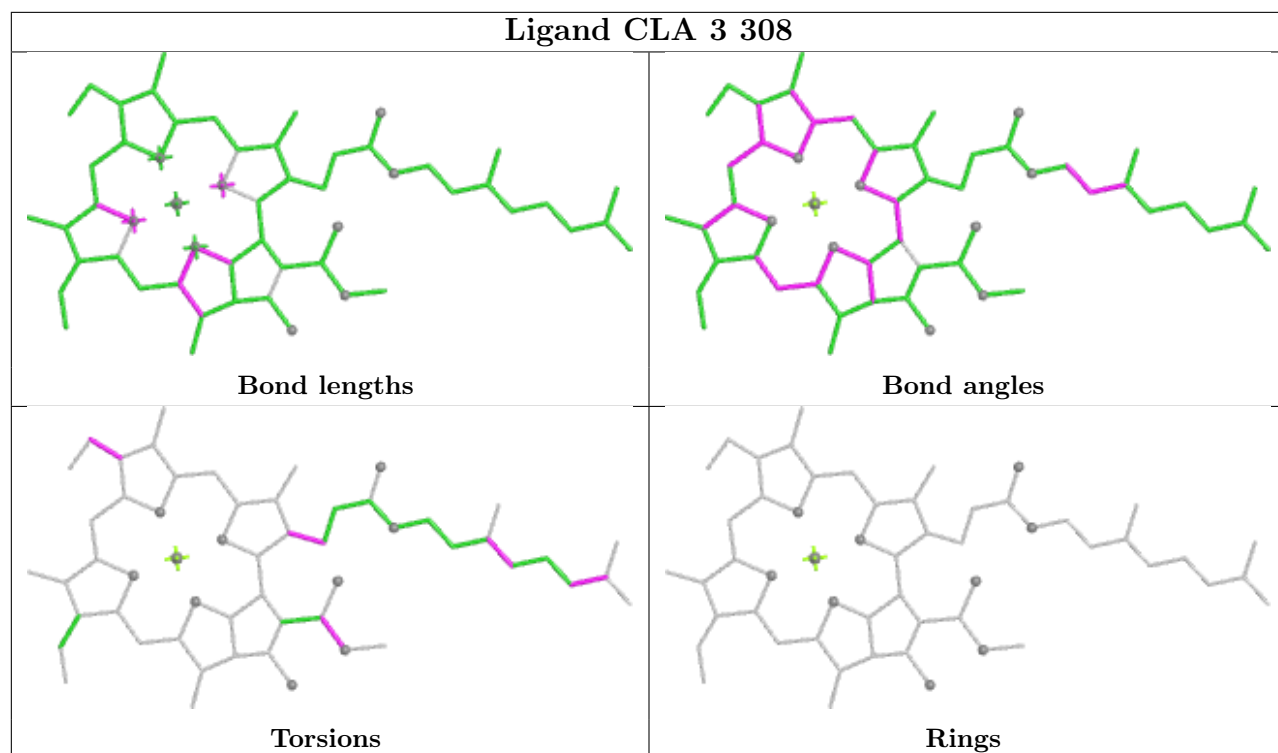
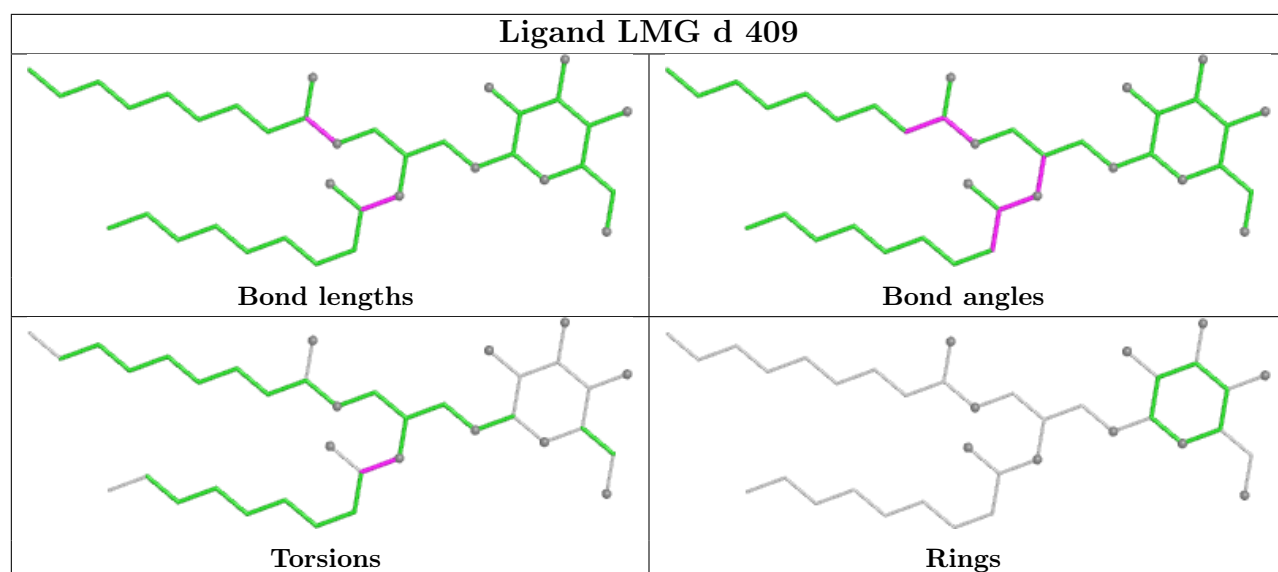
Bond angles

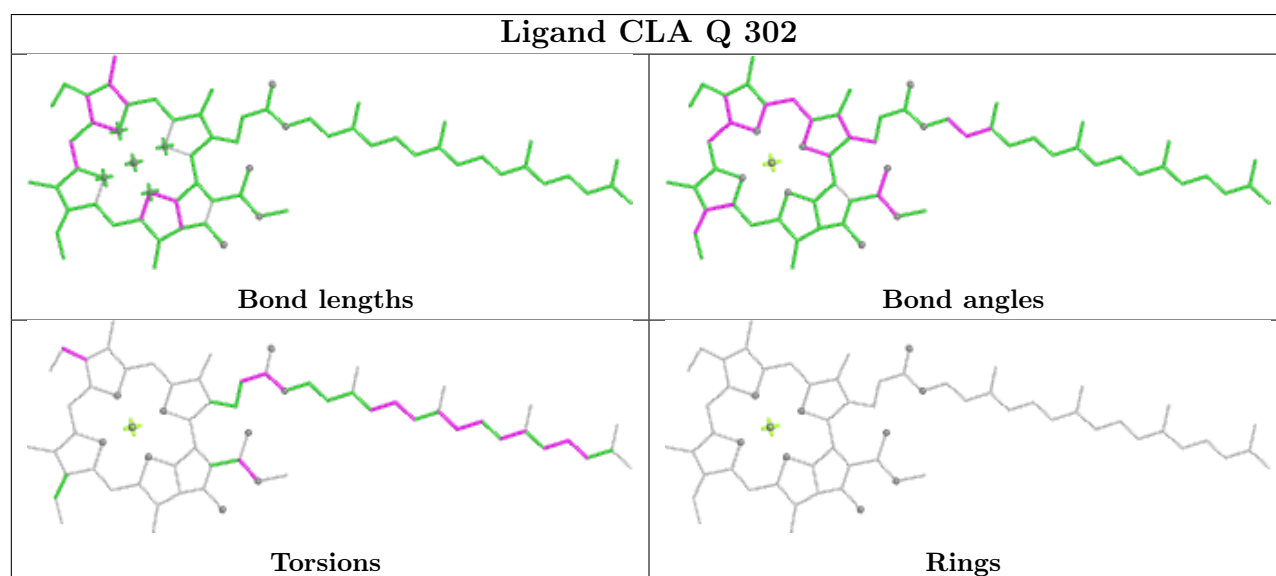
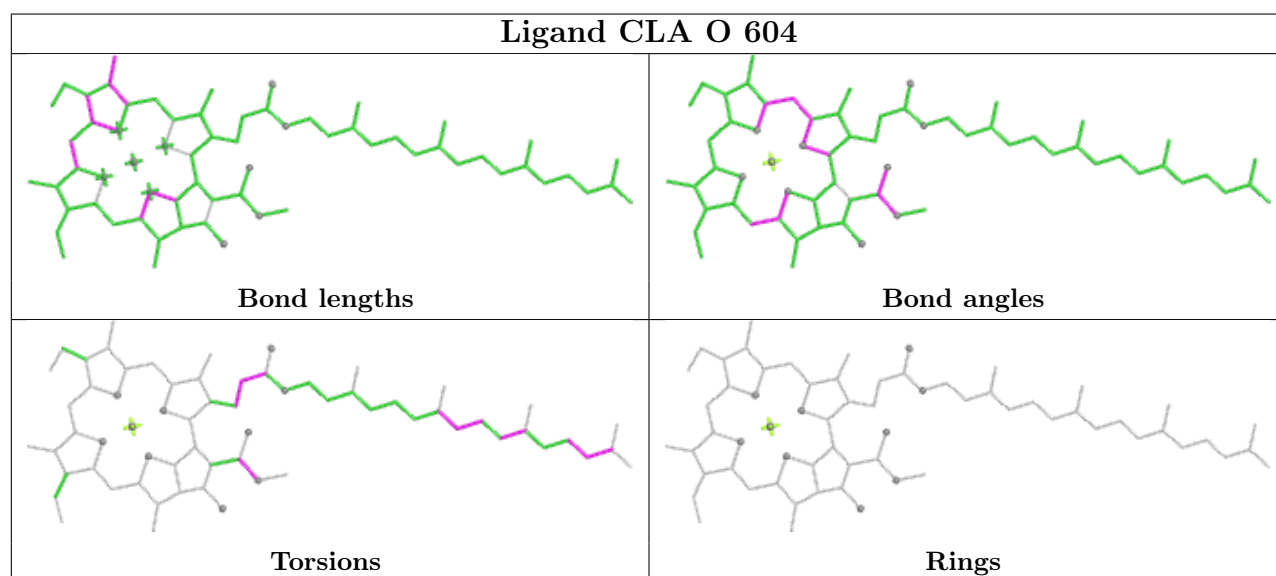
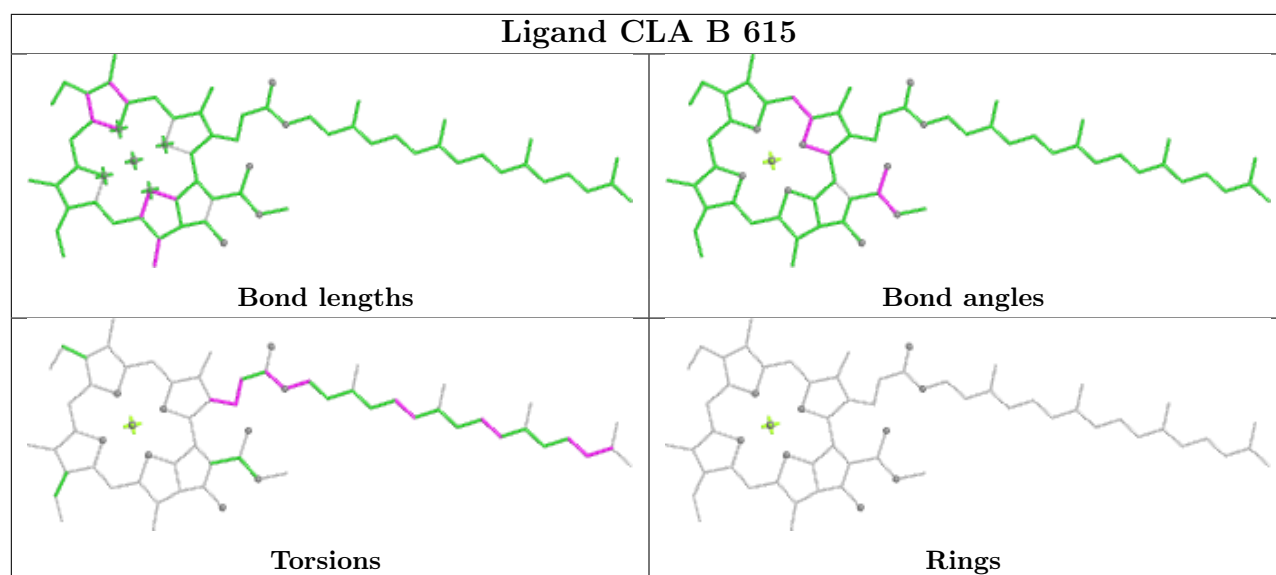


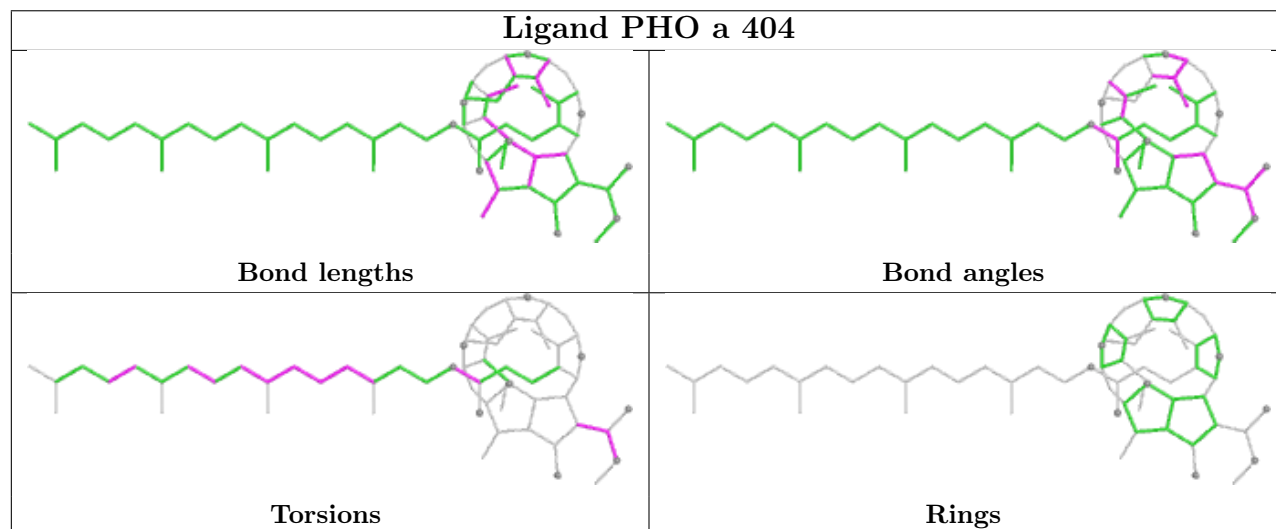
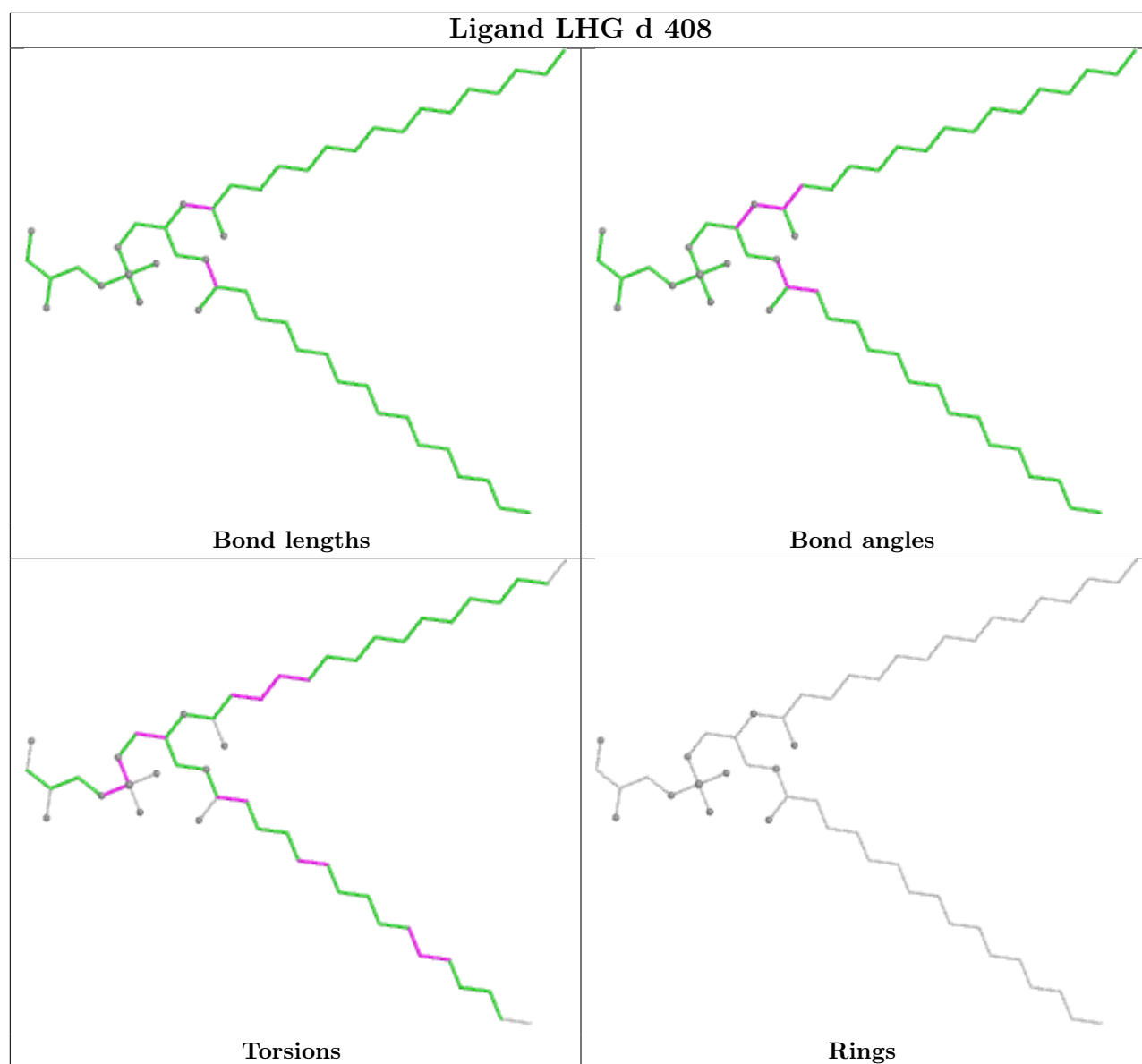
Torsions

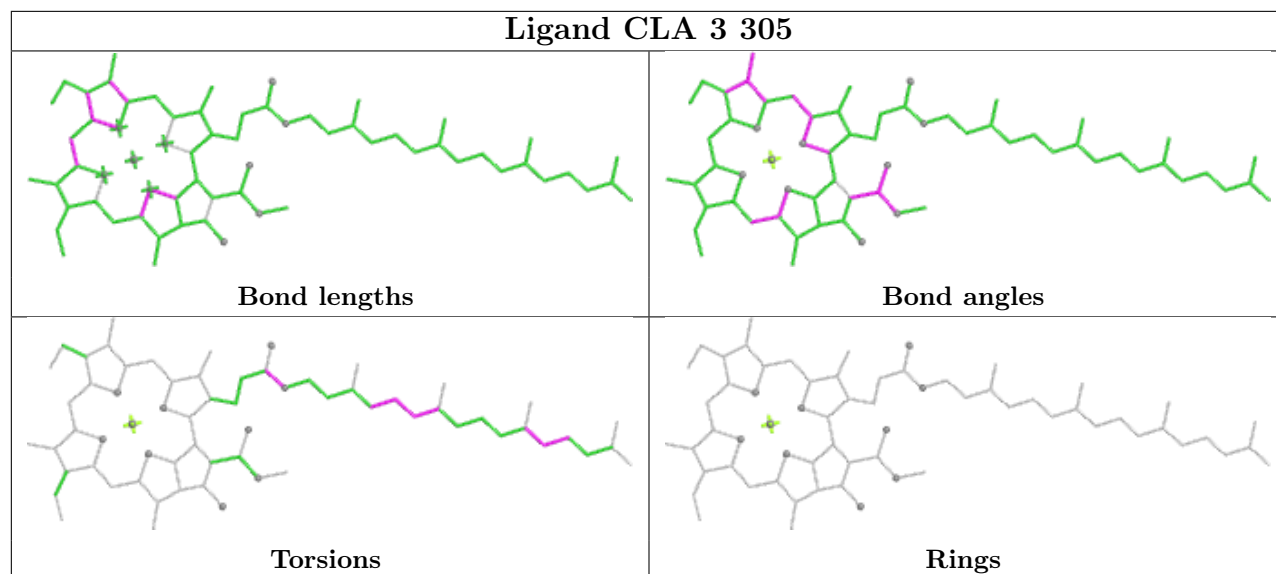
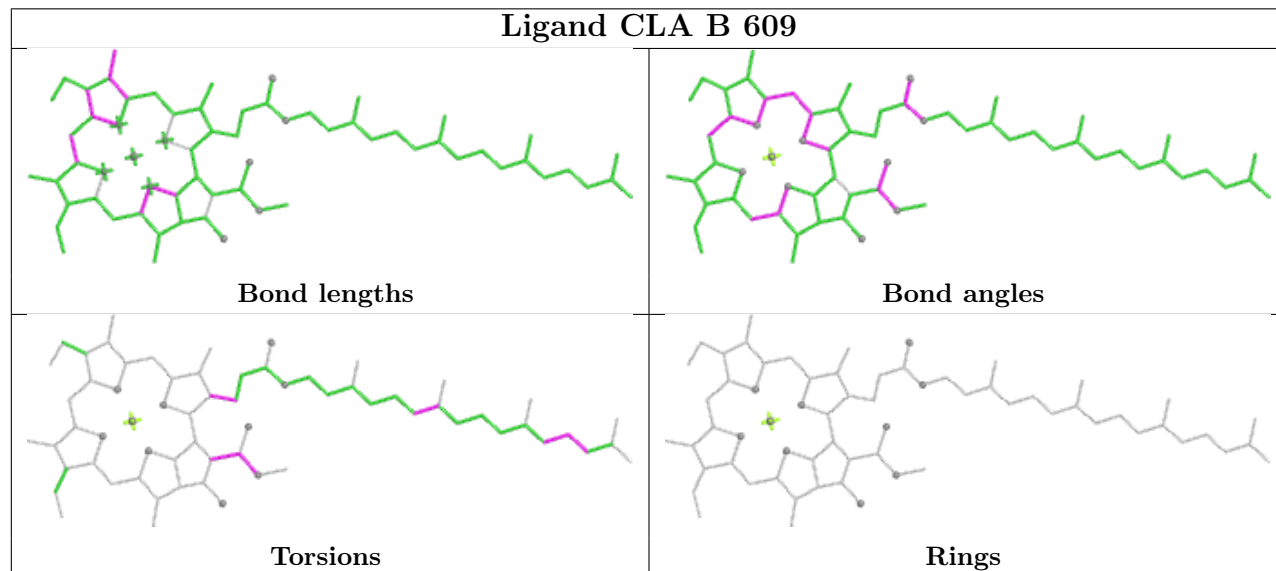


Rings

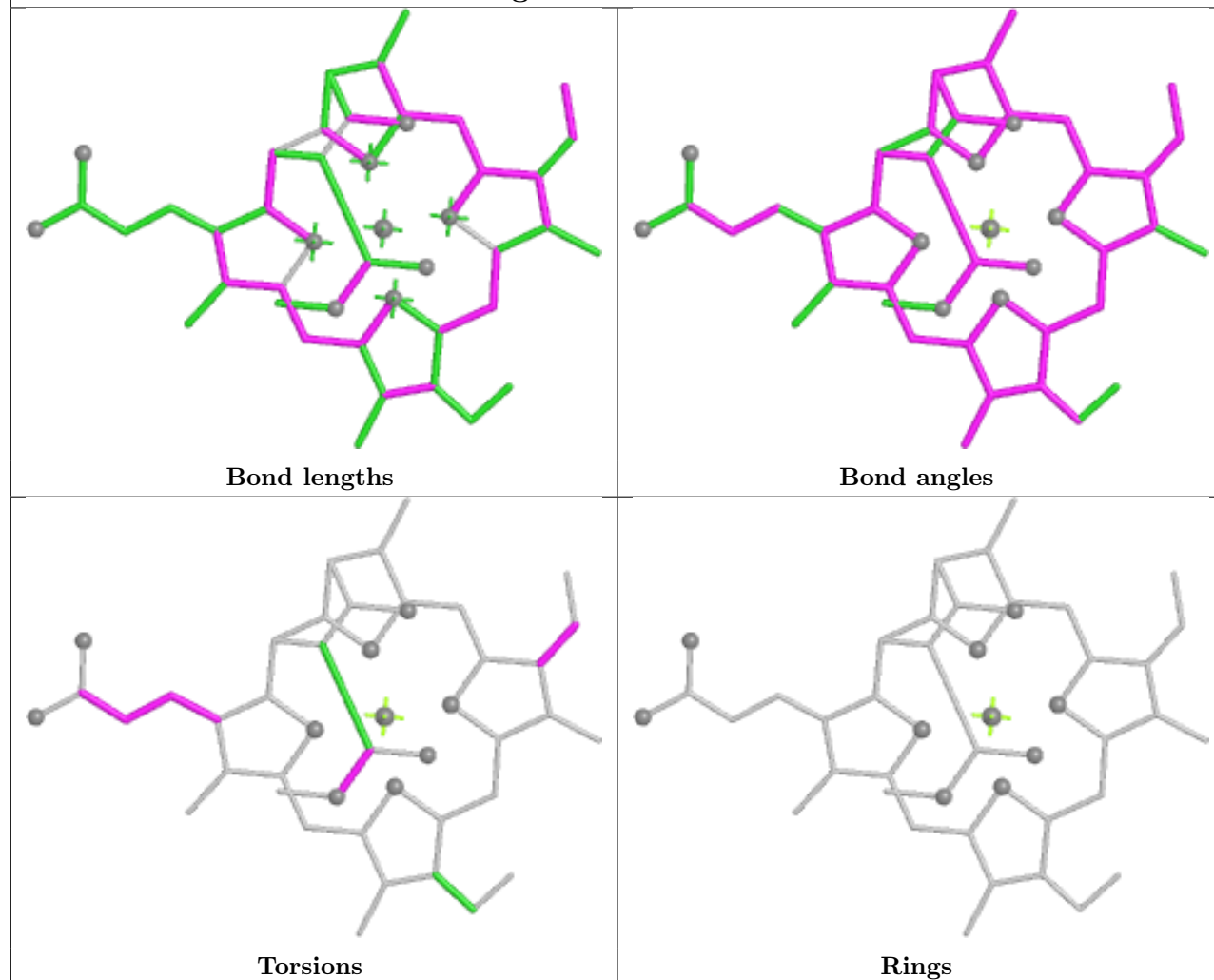




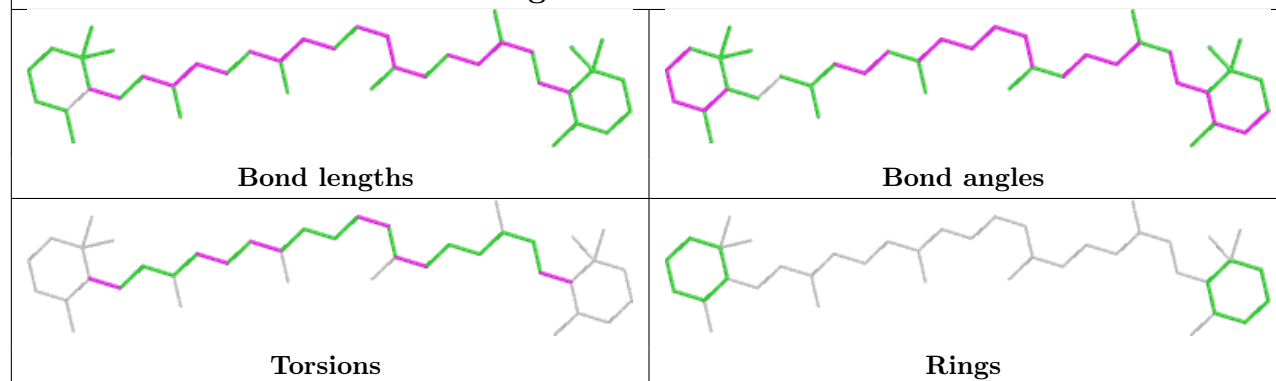


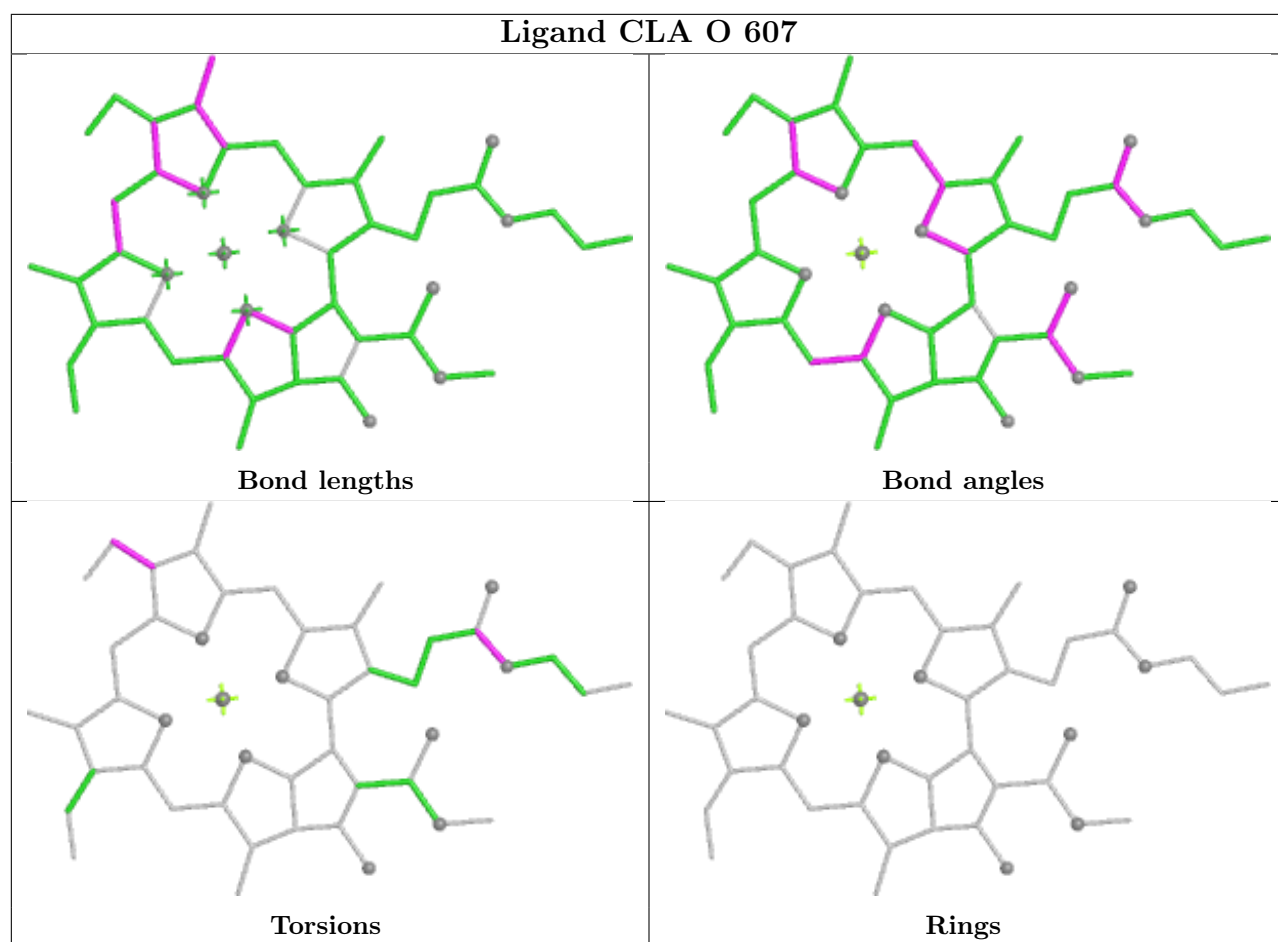
Ligand CLA 3 305**Ligand CLA B 609**

Ligand KC2 5 610

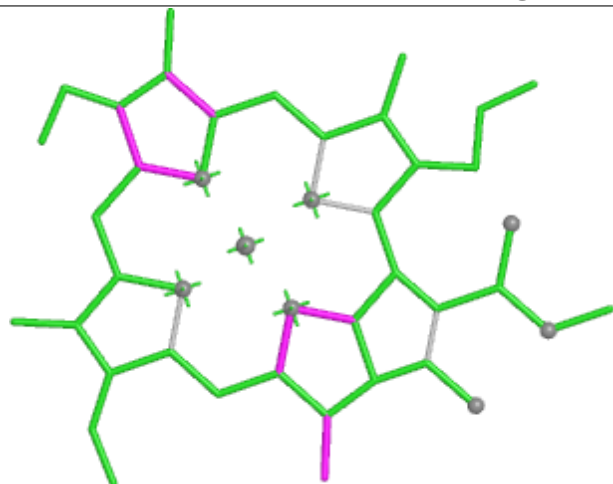


Ligand WVN c 517

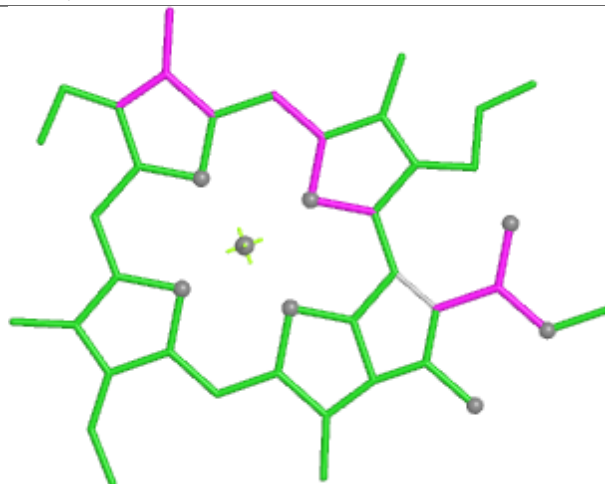




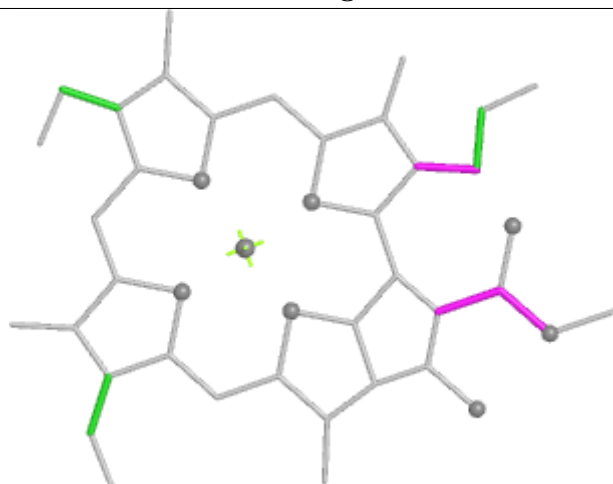
Ligand CLA Q 311



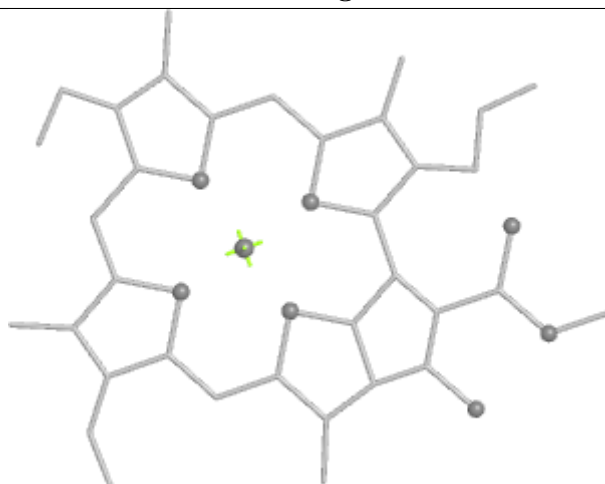
Bond lengths



Bond angles

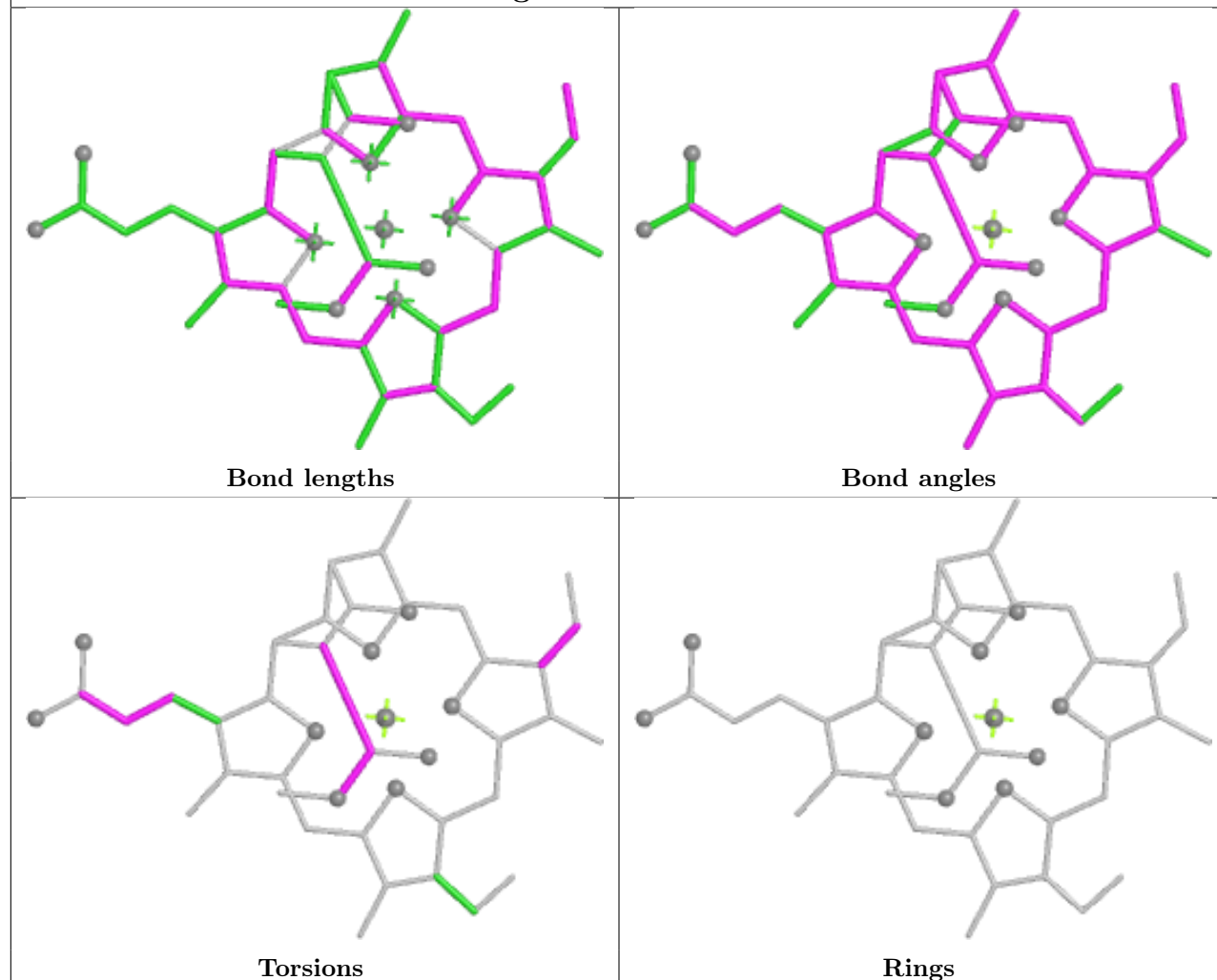


Torsions

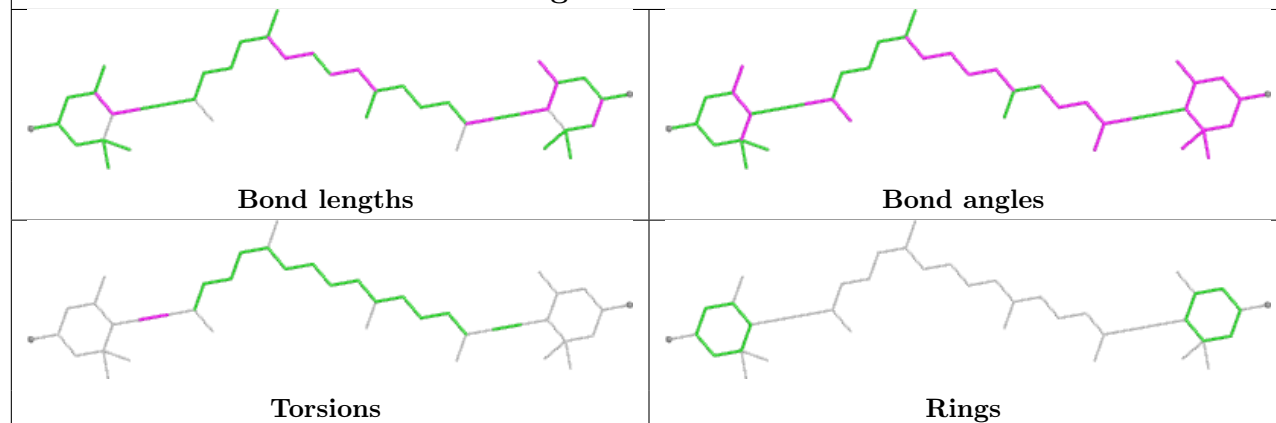


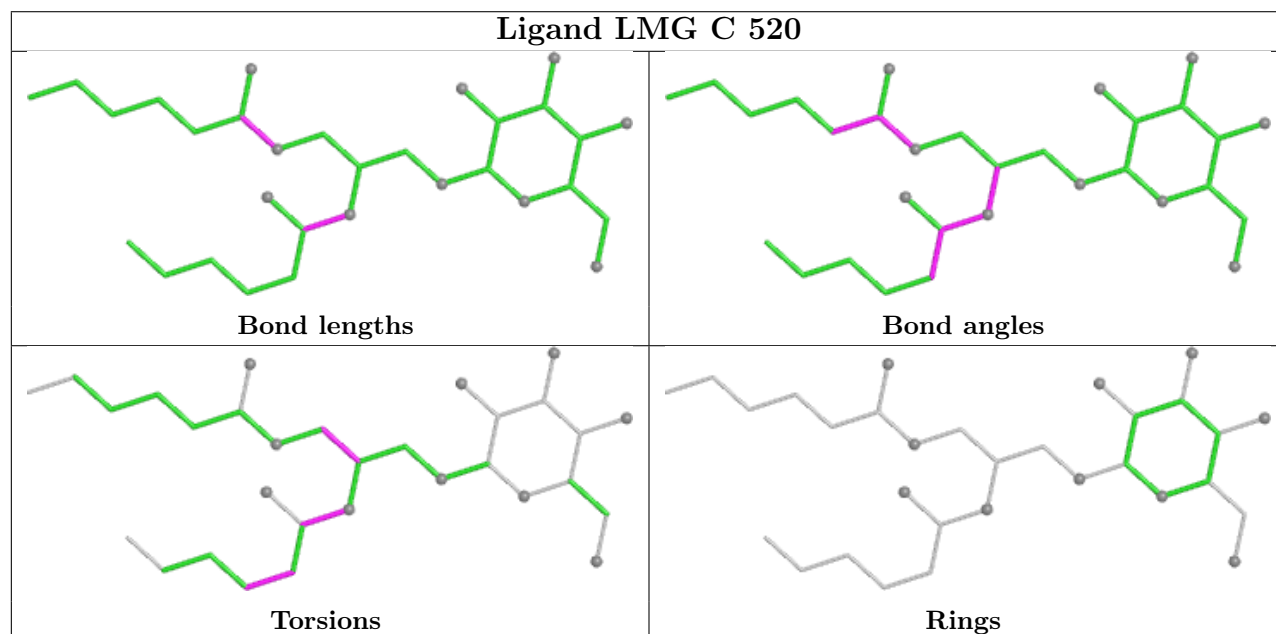
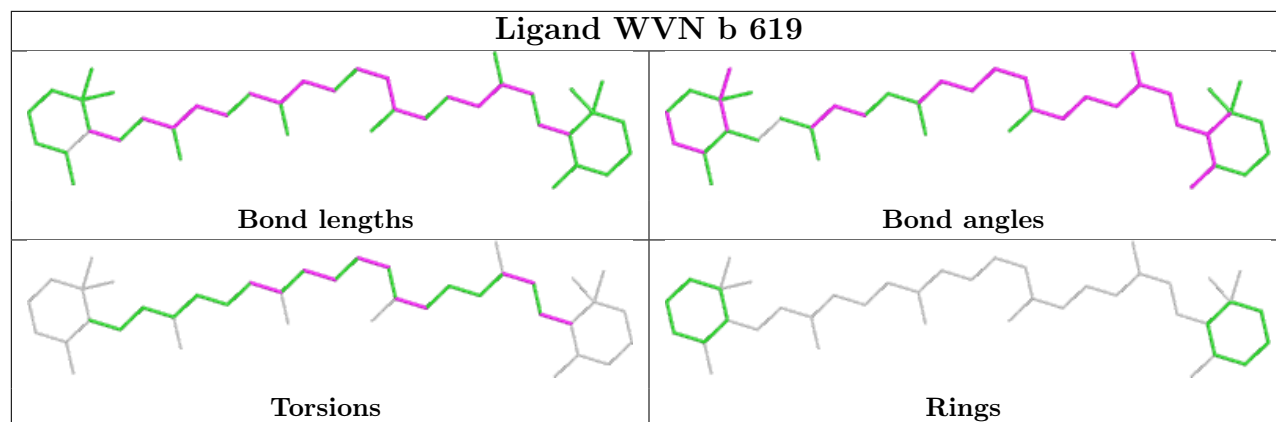
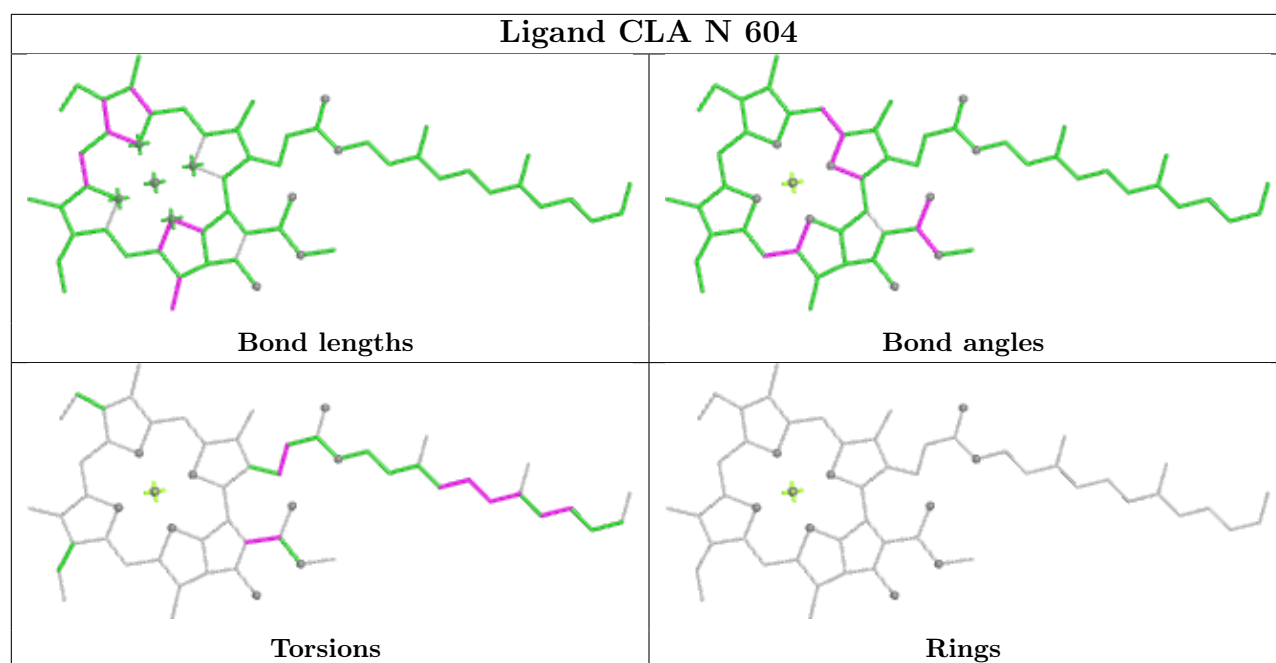
Rings

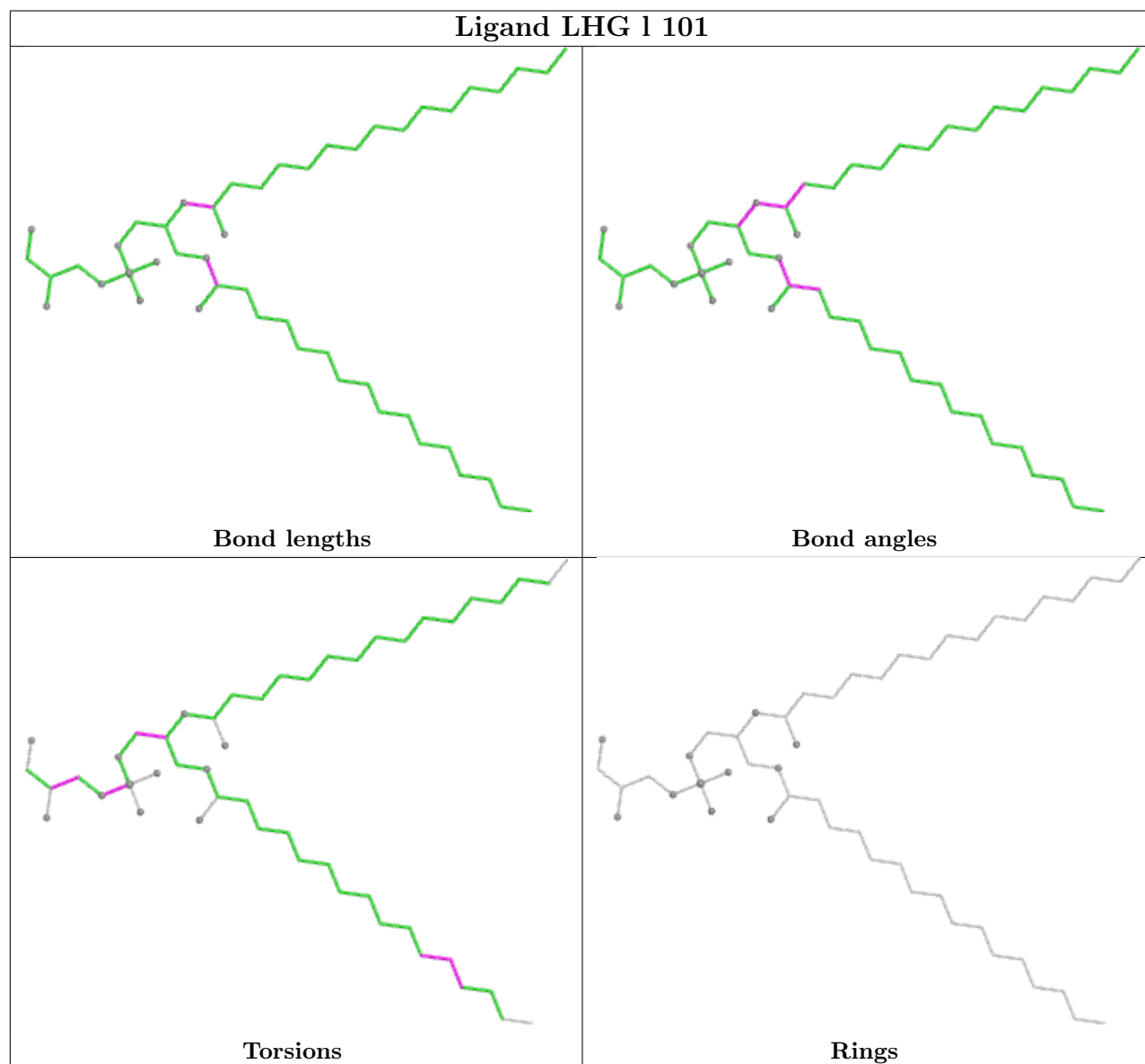
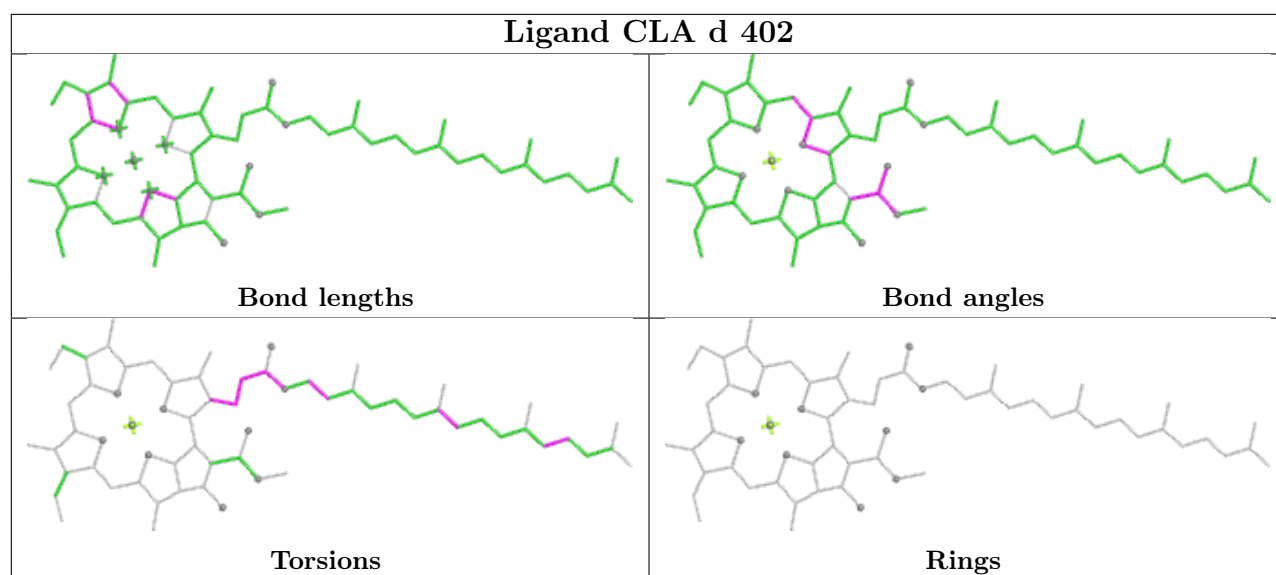
Ligand KC2 4 310

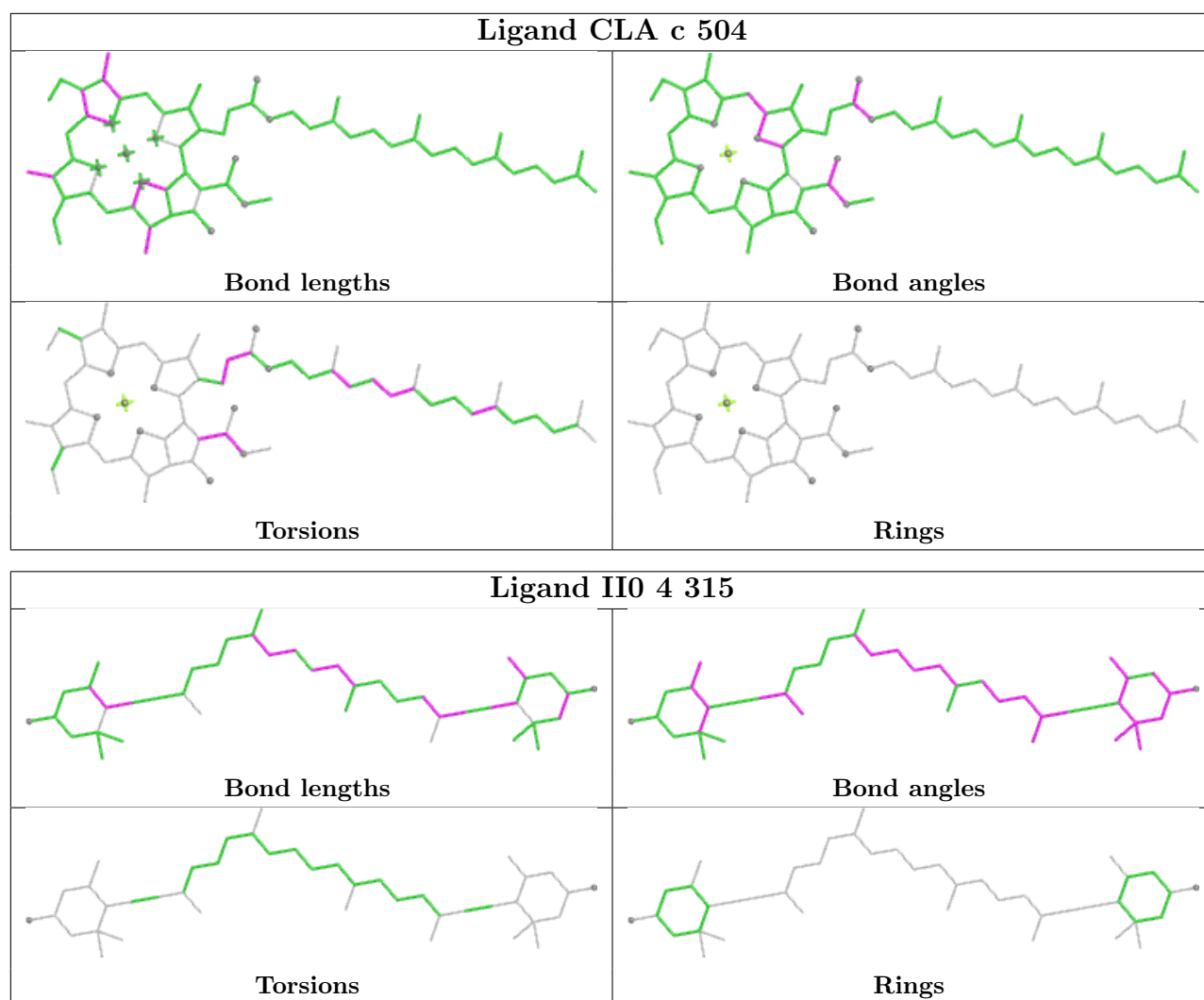


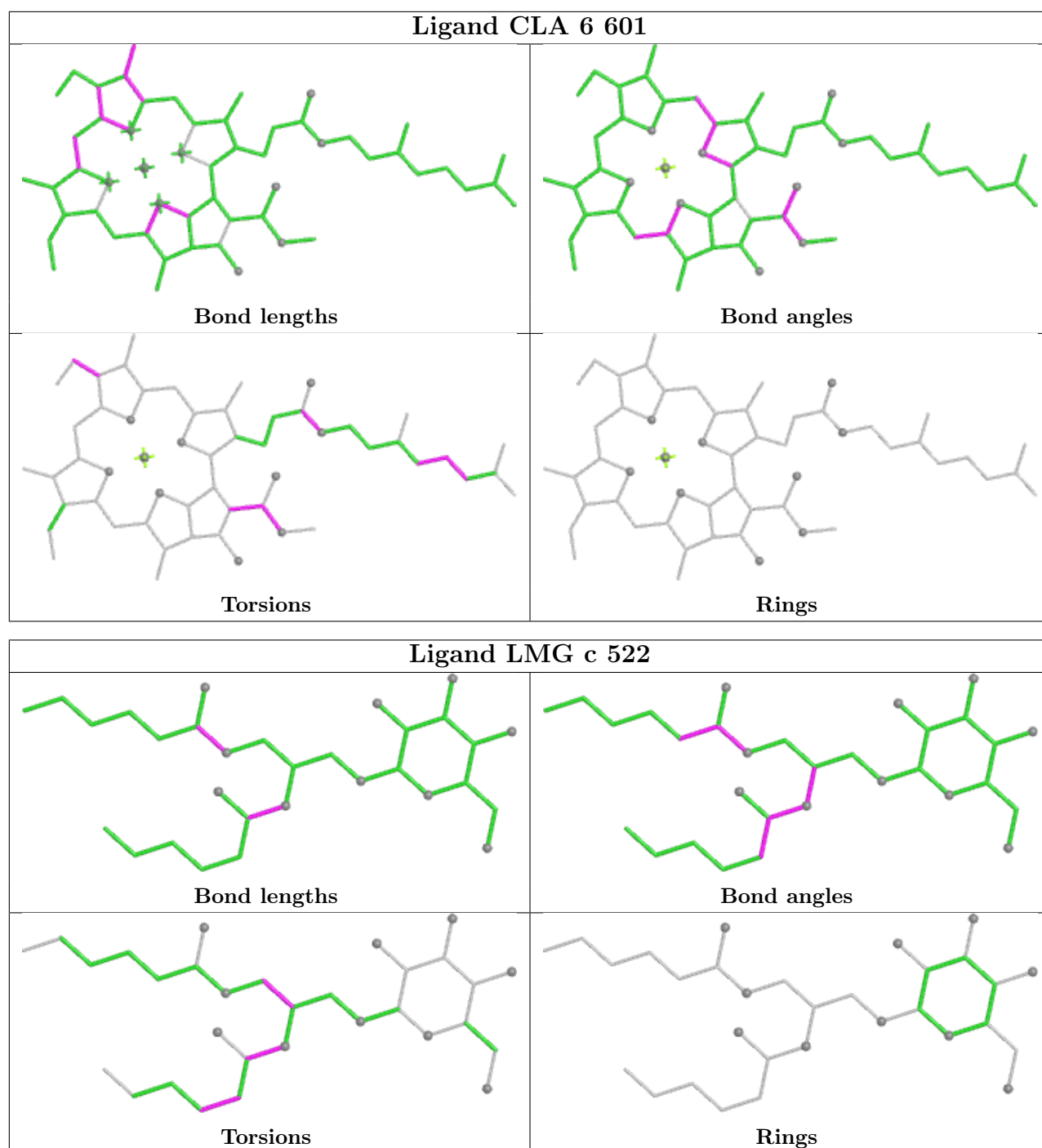
Ligand II0 2 314

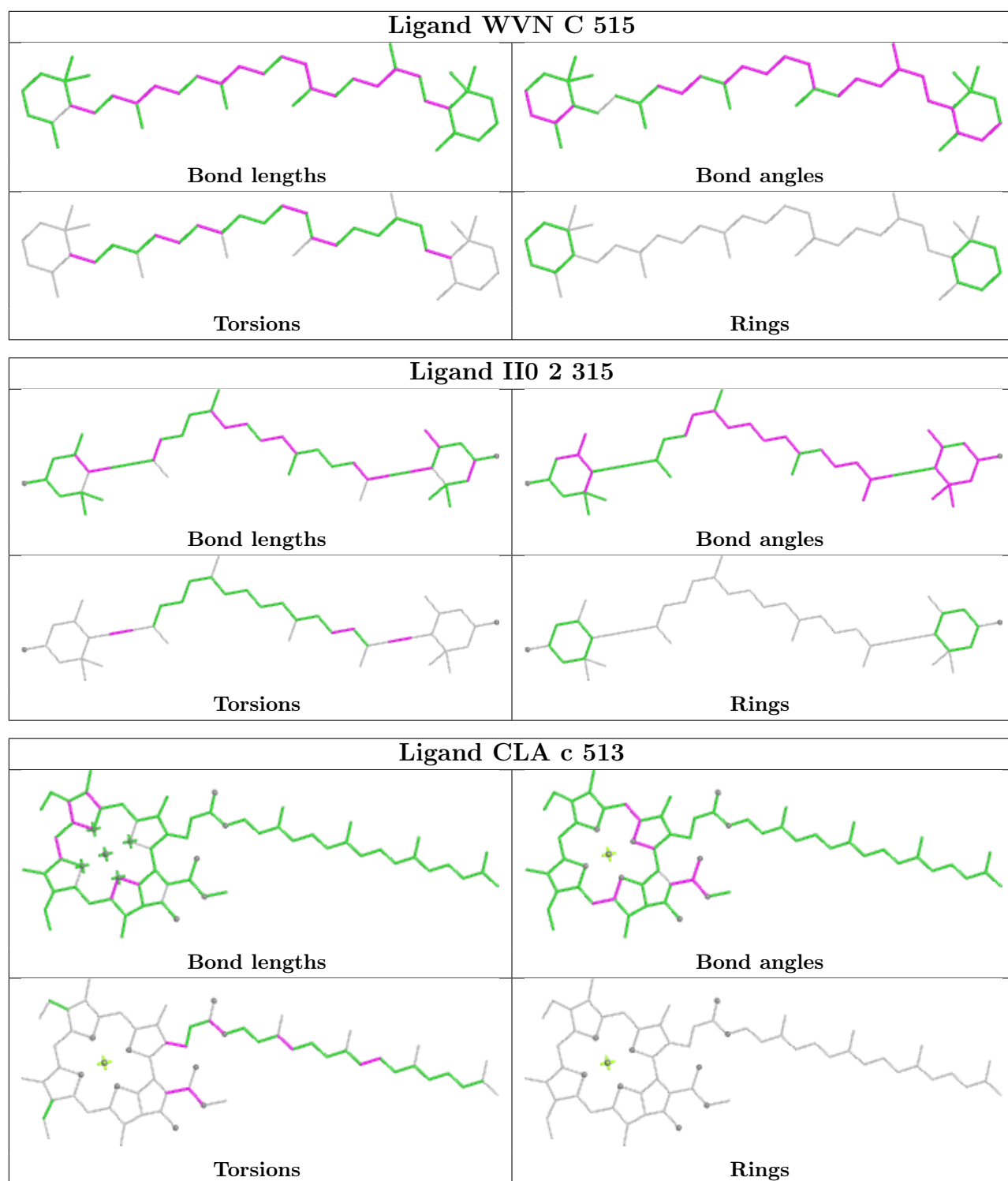


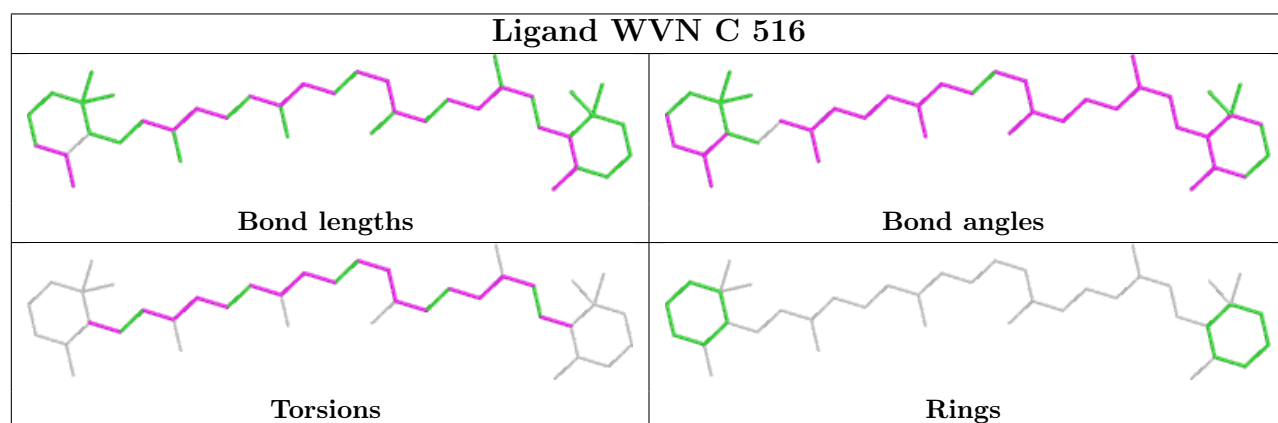
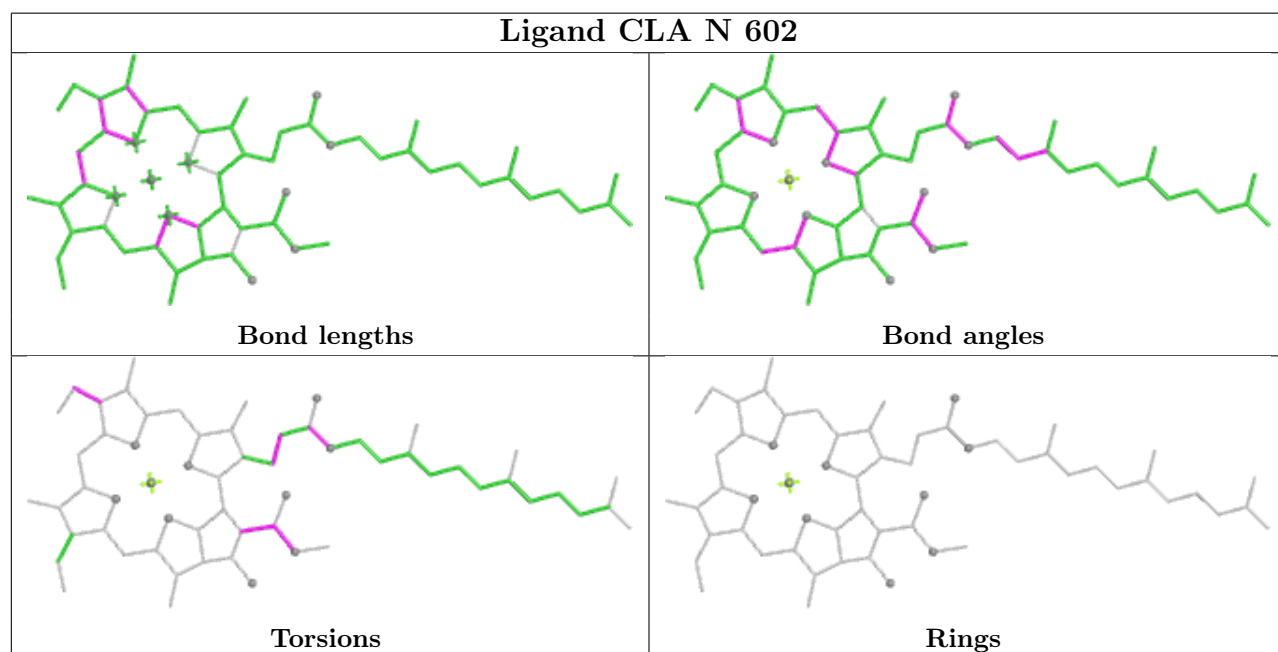
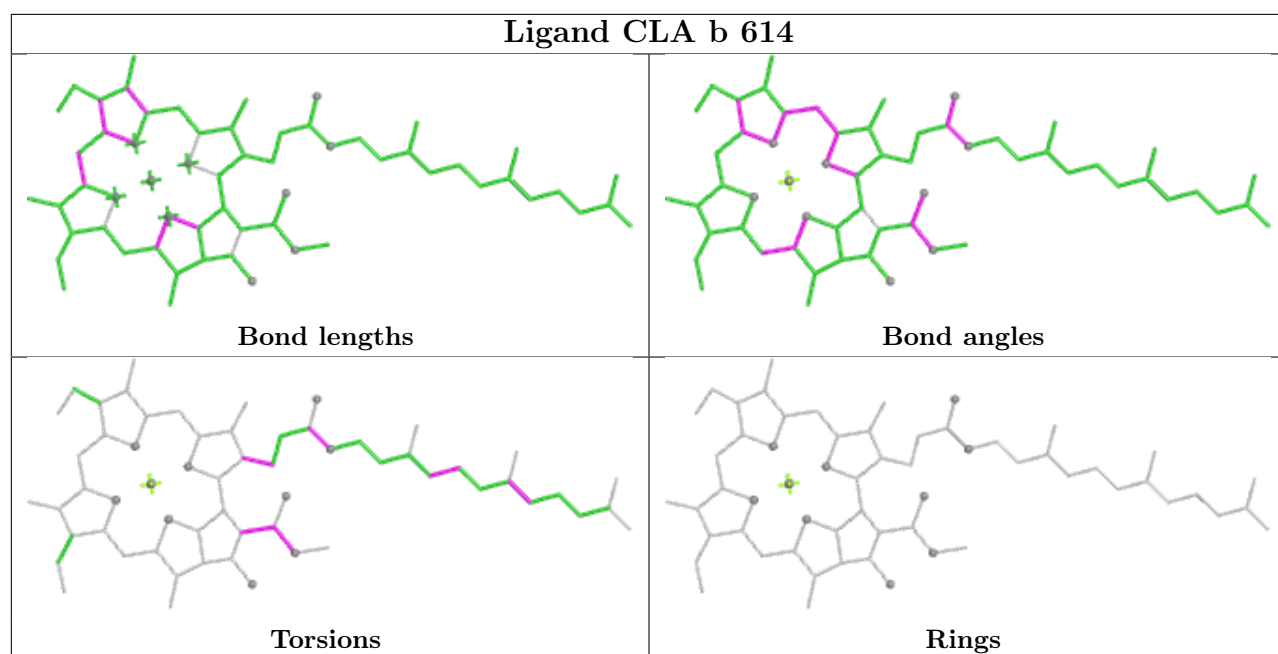


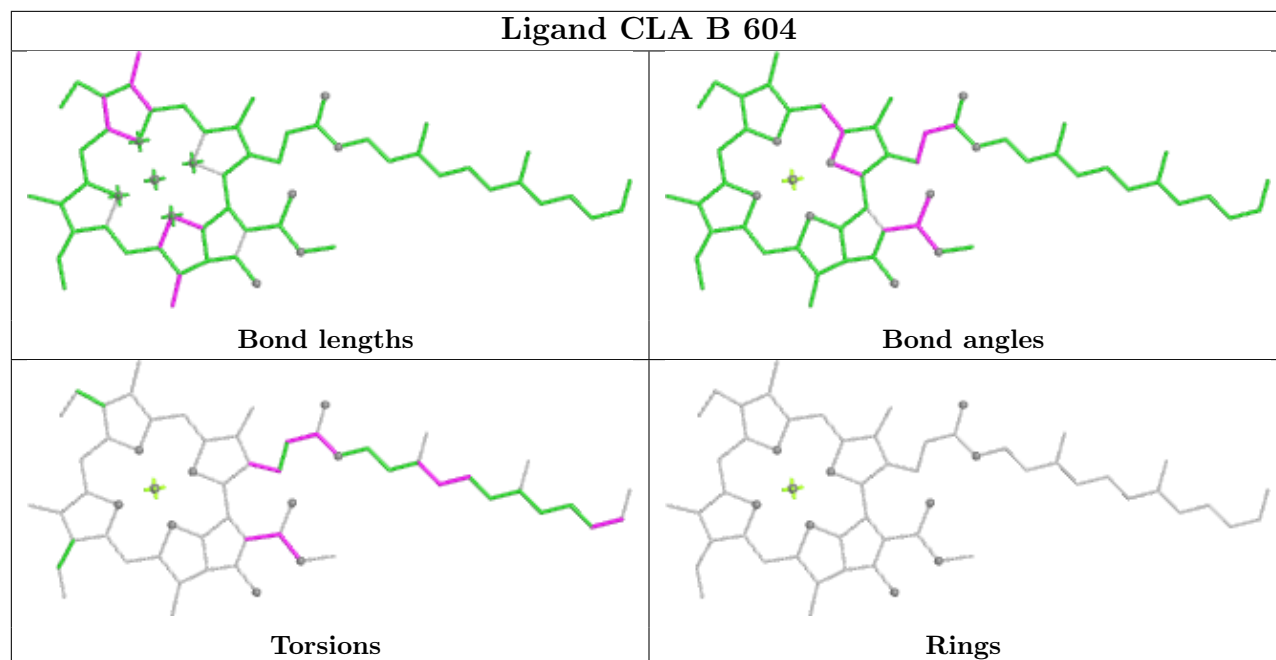
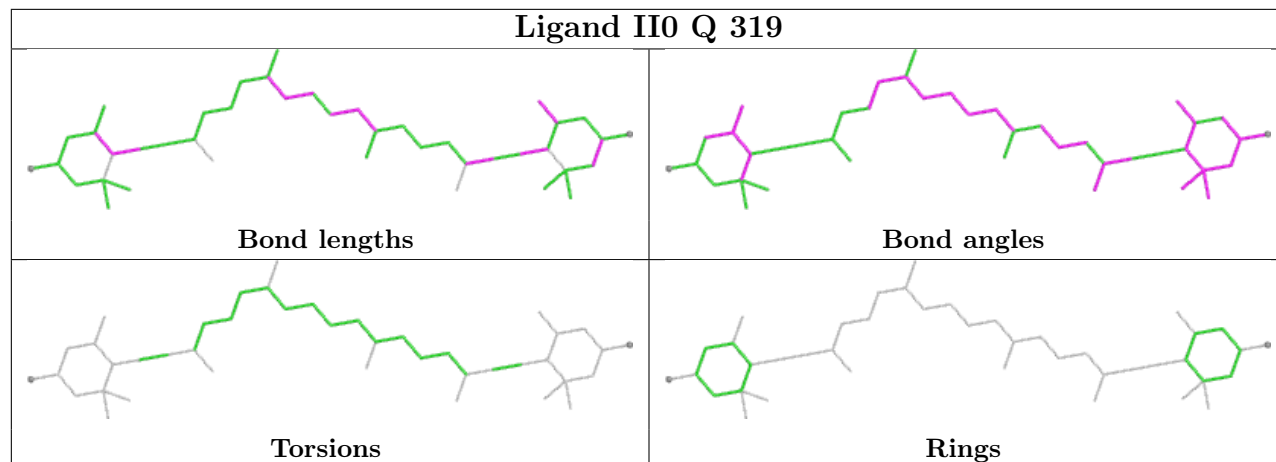




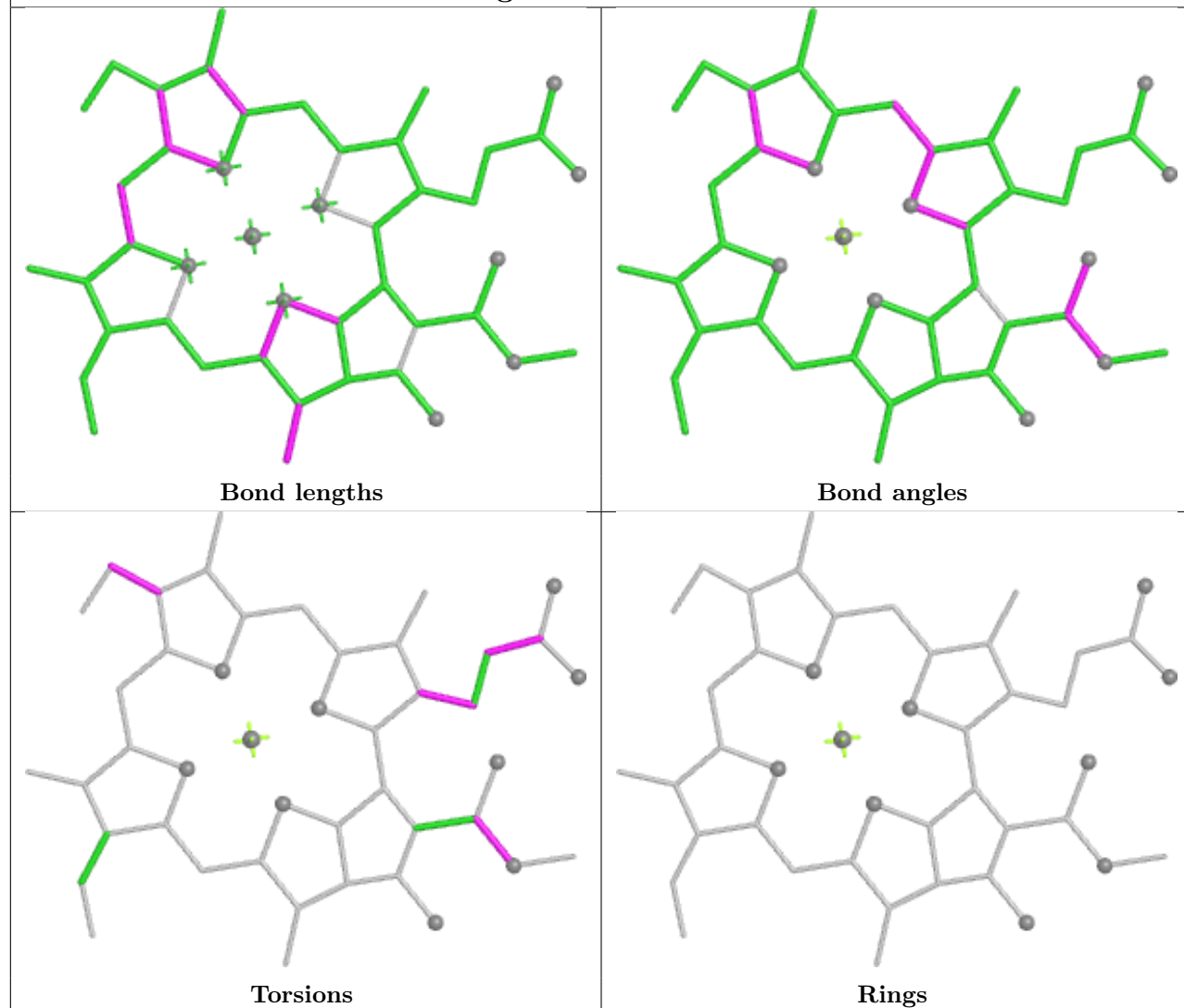




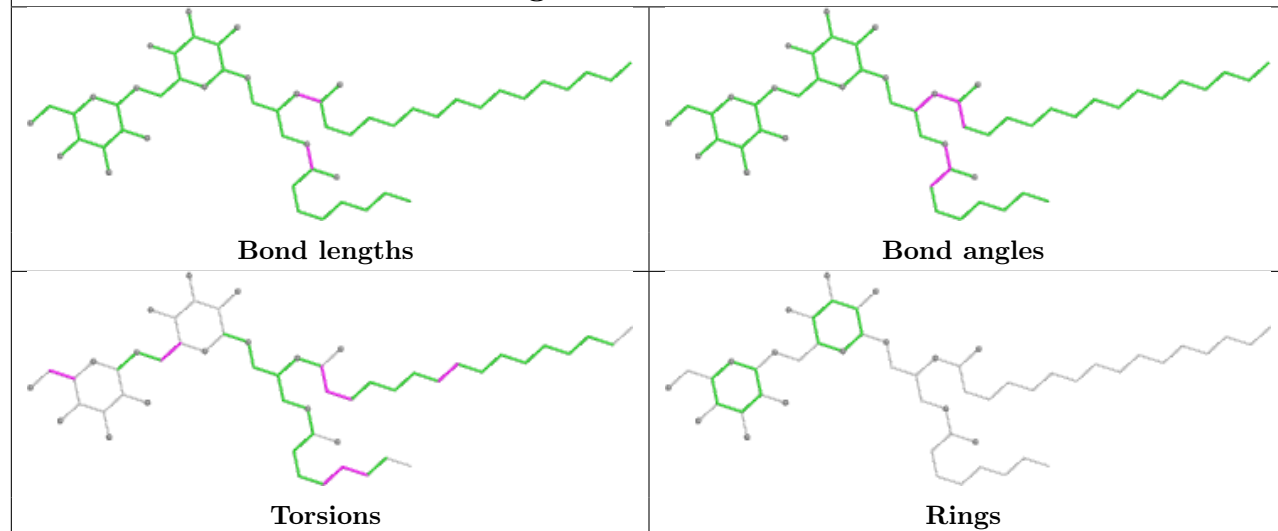


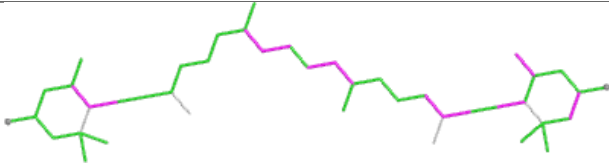
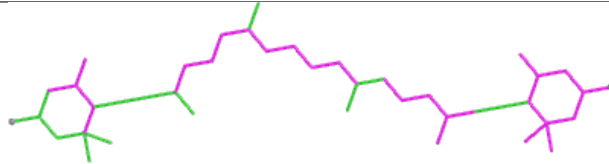
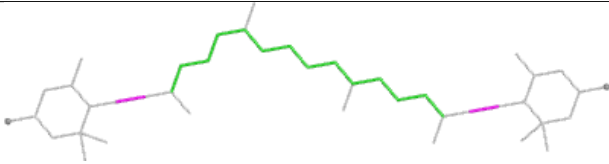
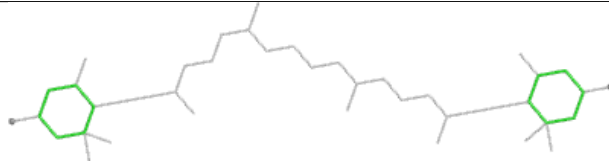
Ligand CLA B 604**Ligand II0 Q 319**

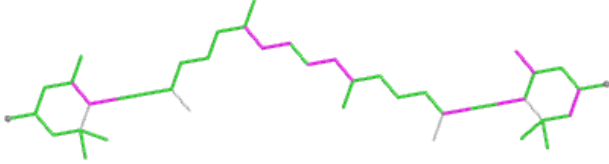
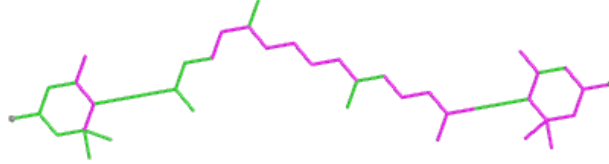
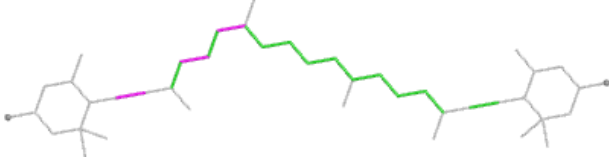
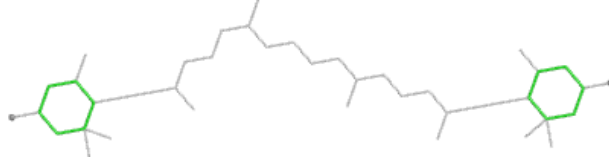
Ligand CLA 1 601

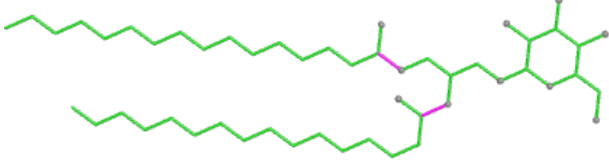
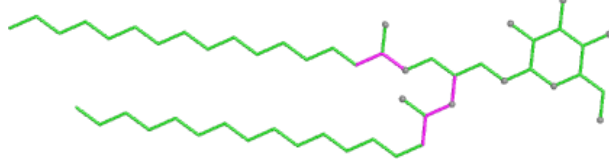
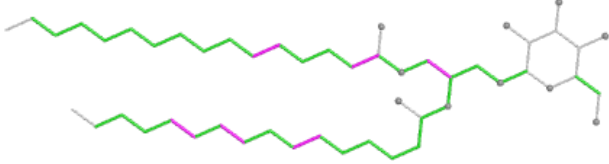
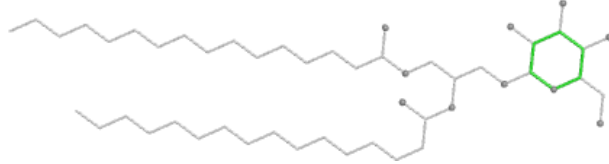


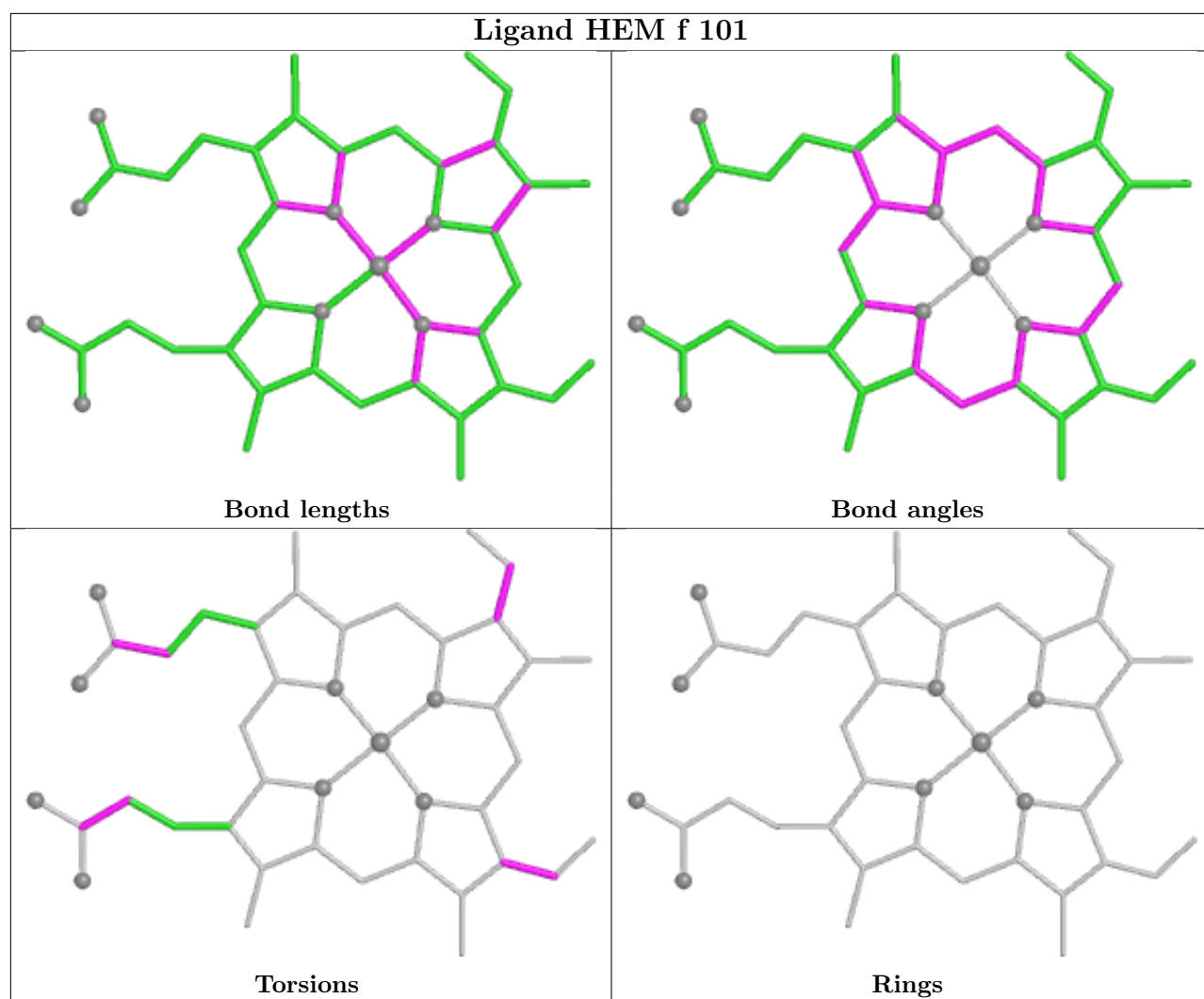
Ligand DGD C 517

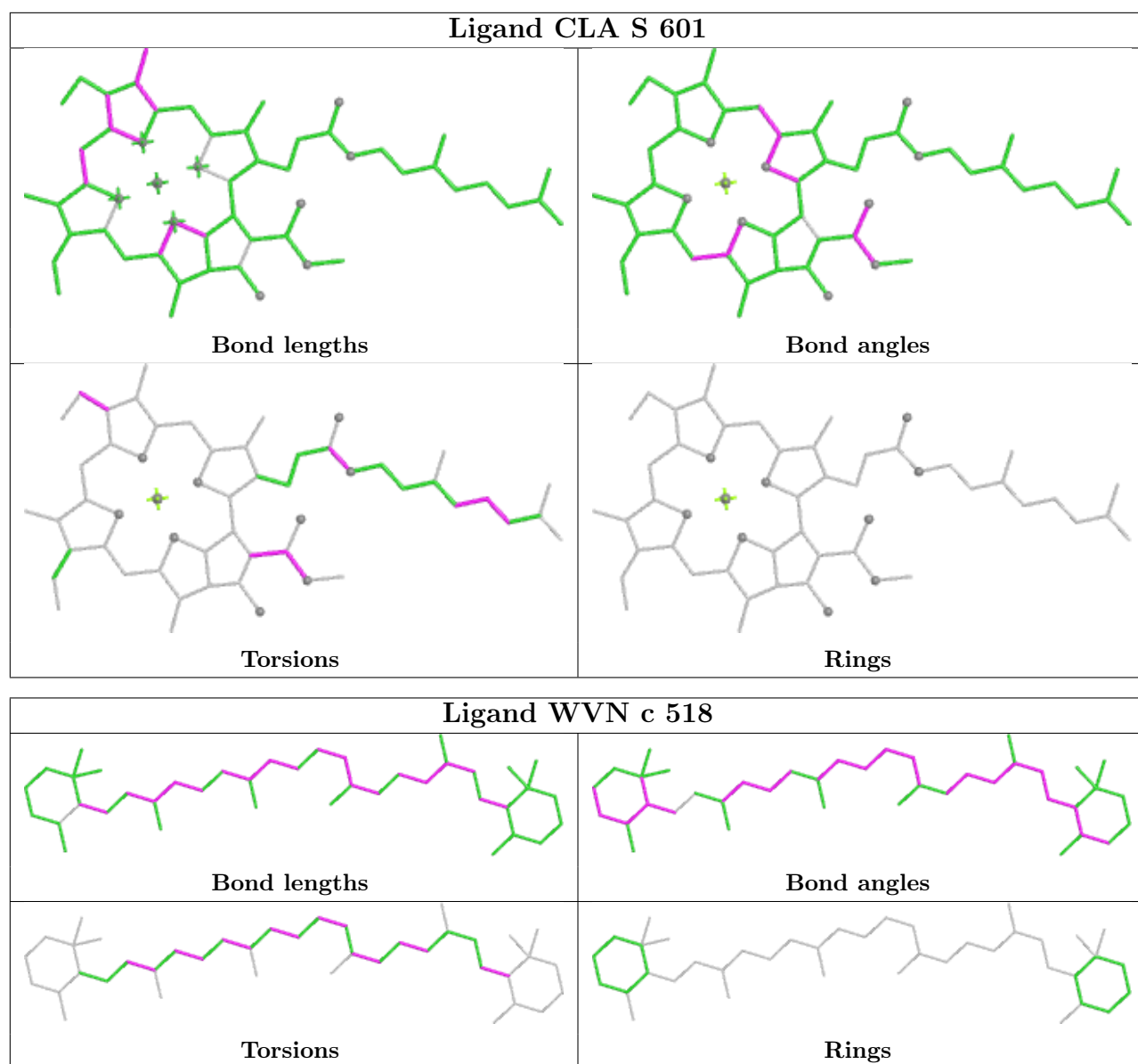


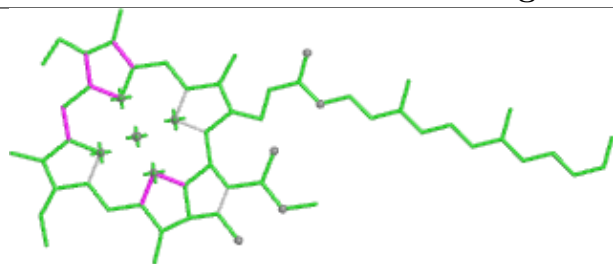
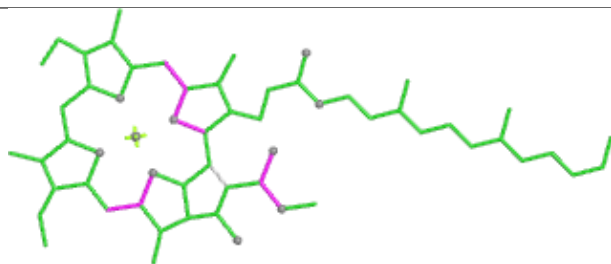
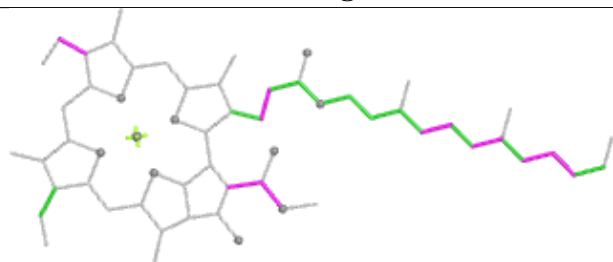
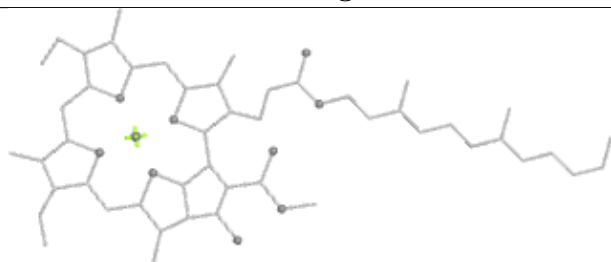
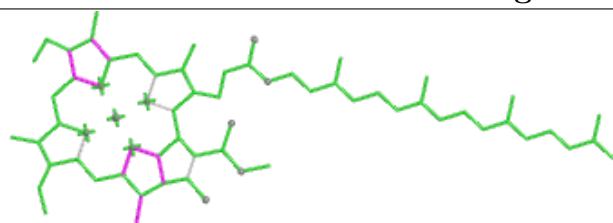
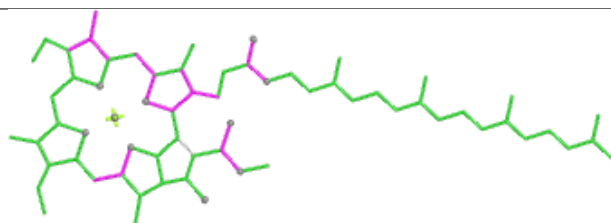
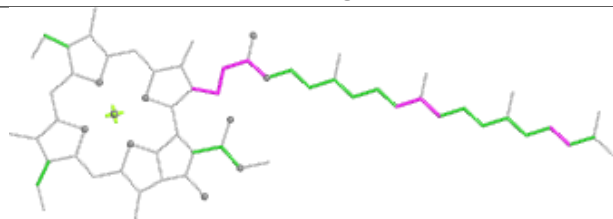
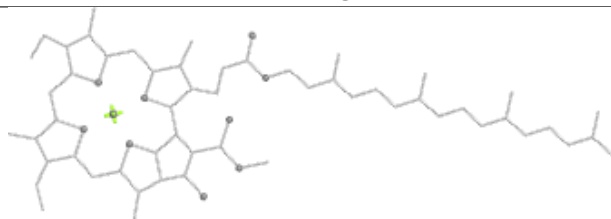
Ligand II0 4 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

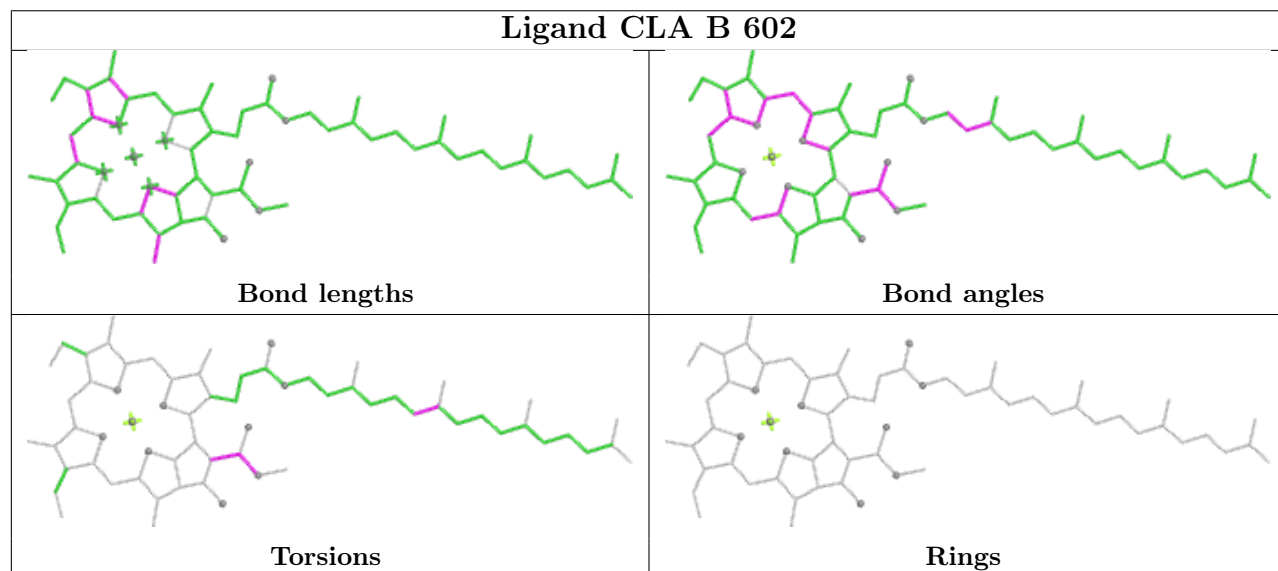
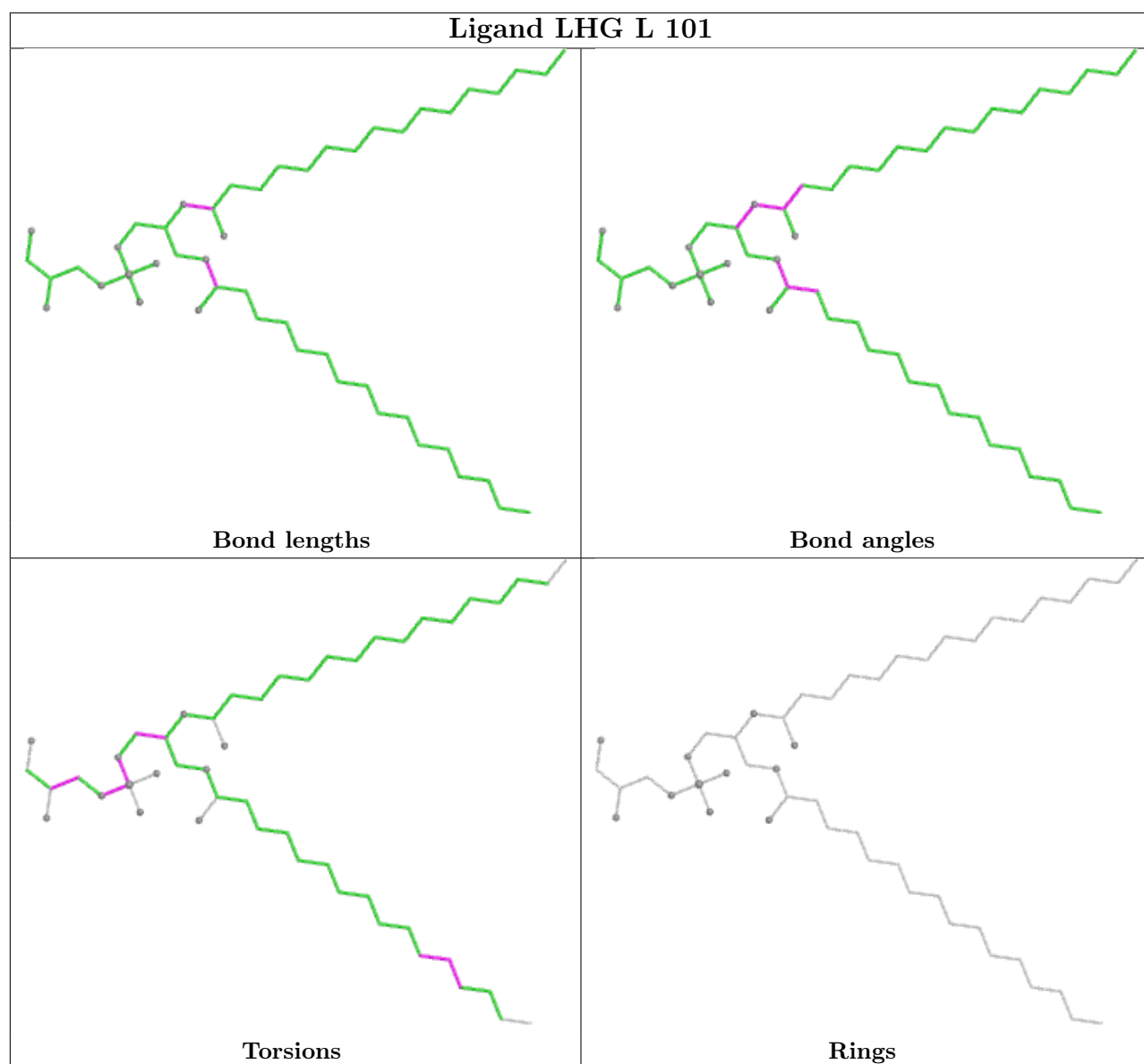
Ligand II0 N 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

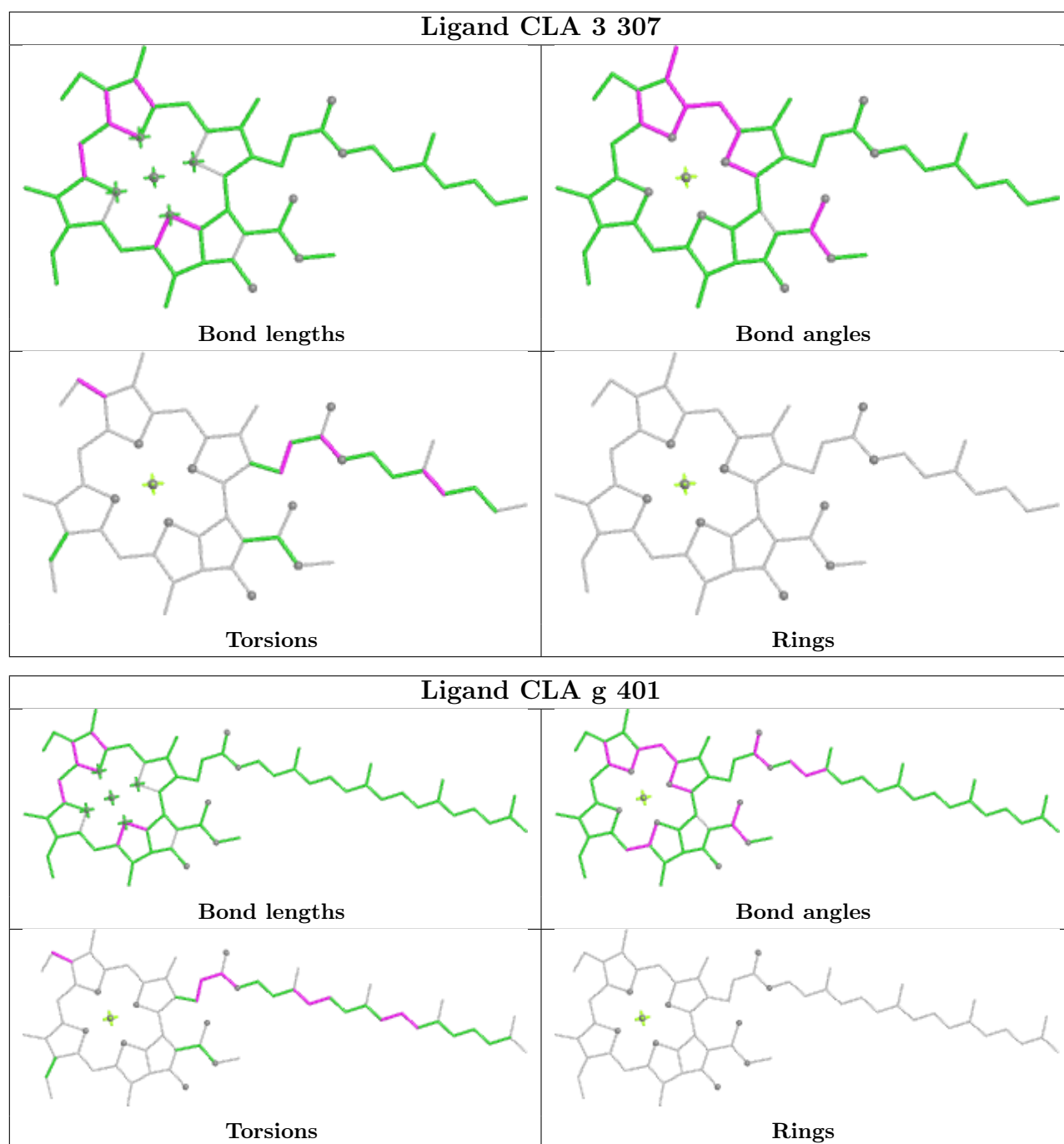
Ligand LMG B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

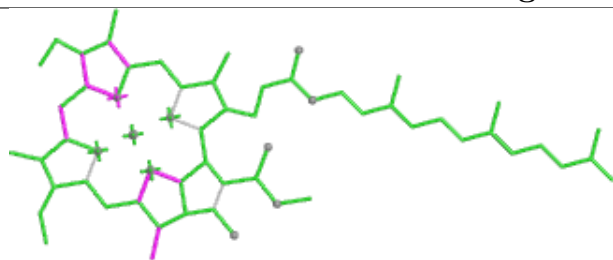
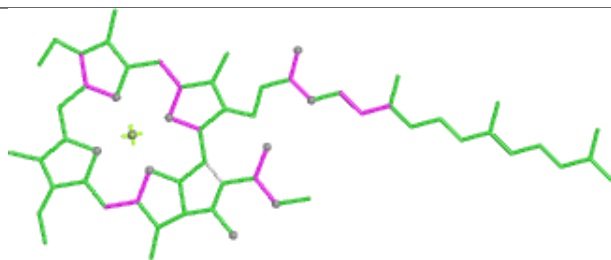
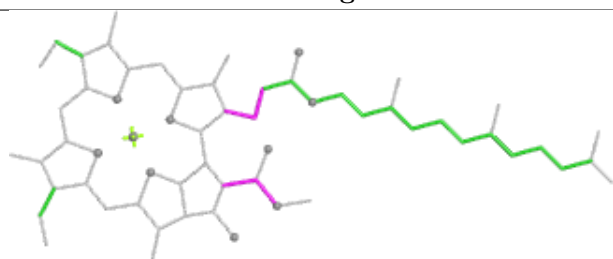
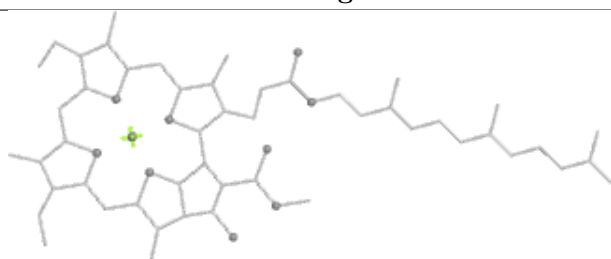
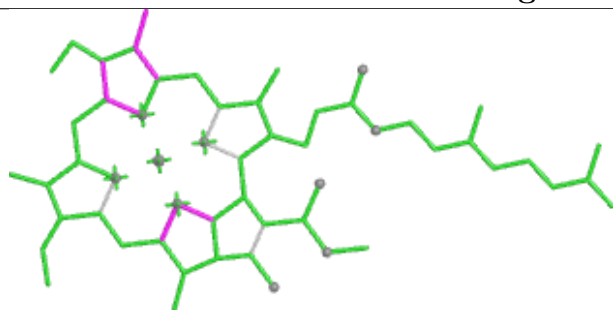
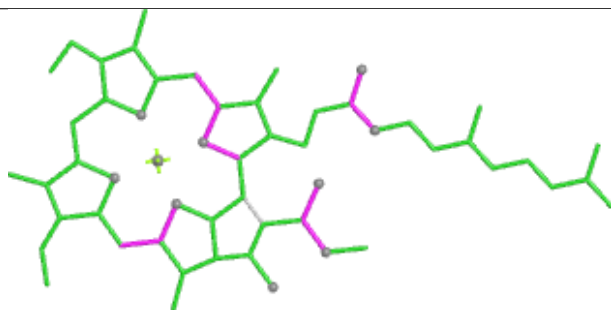
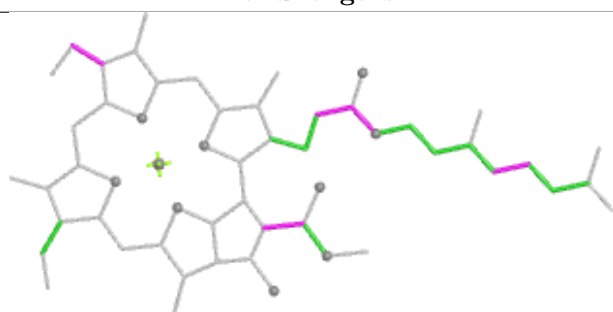
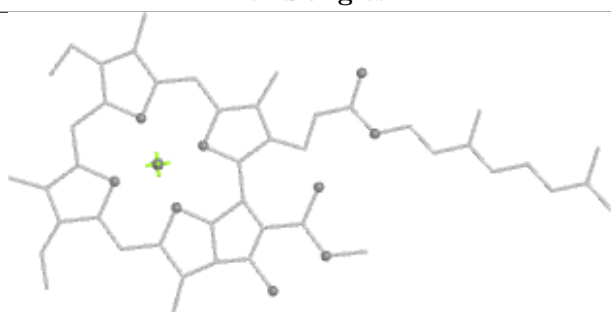


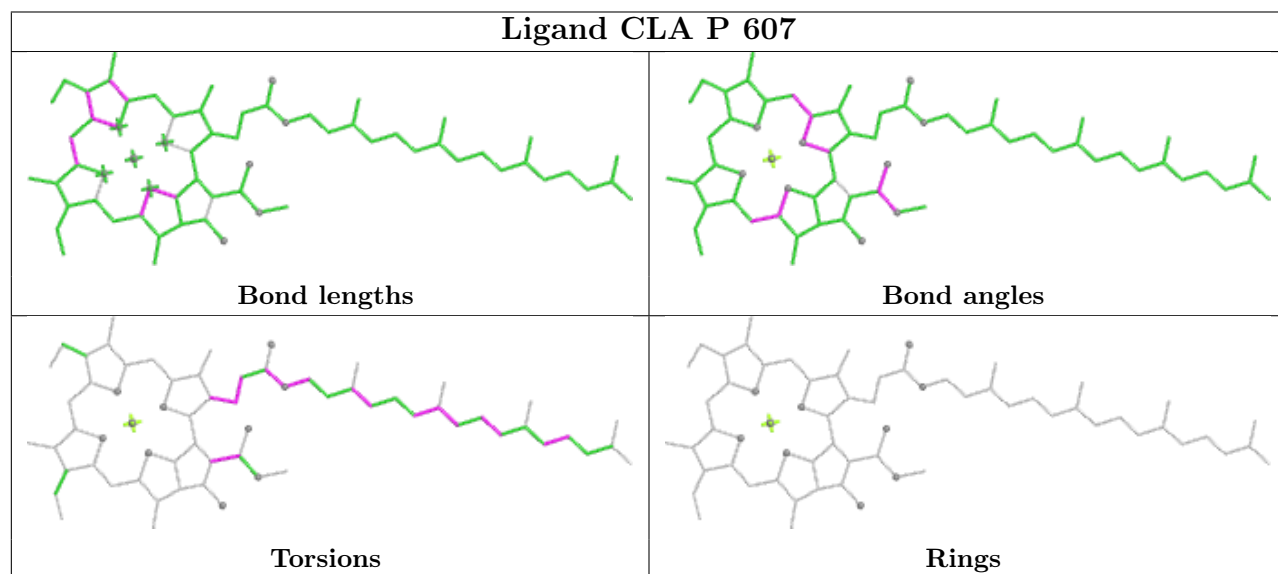
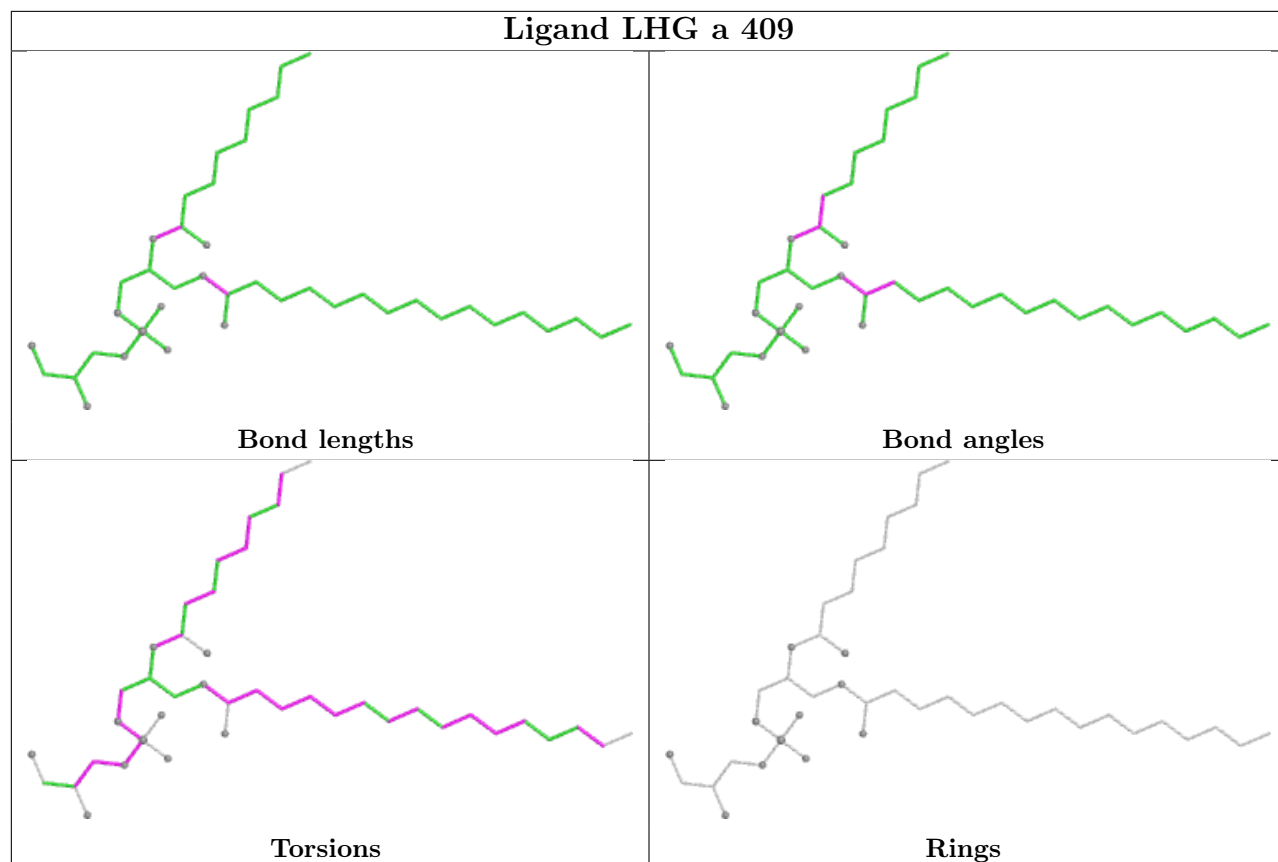


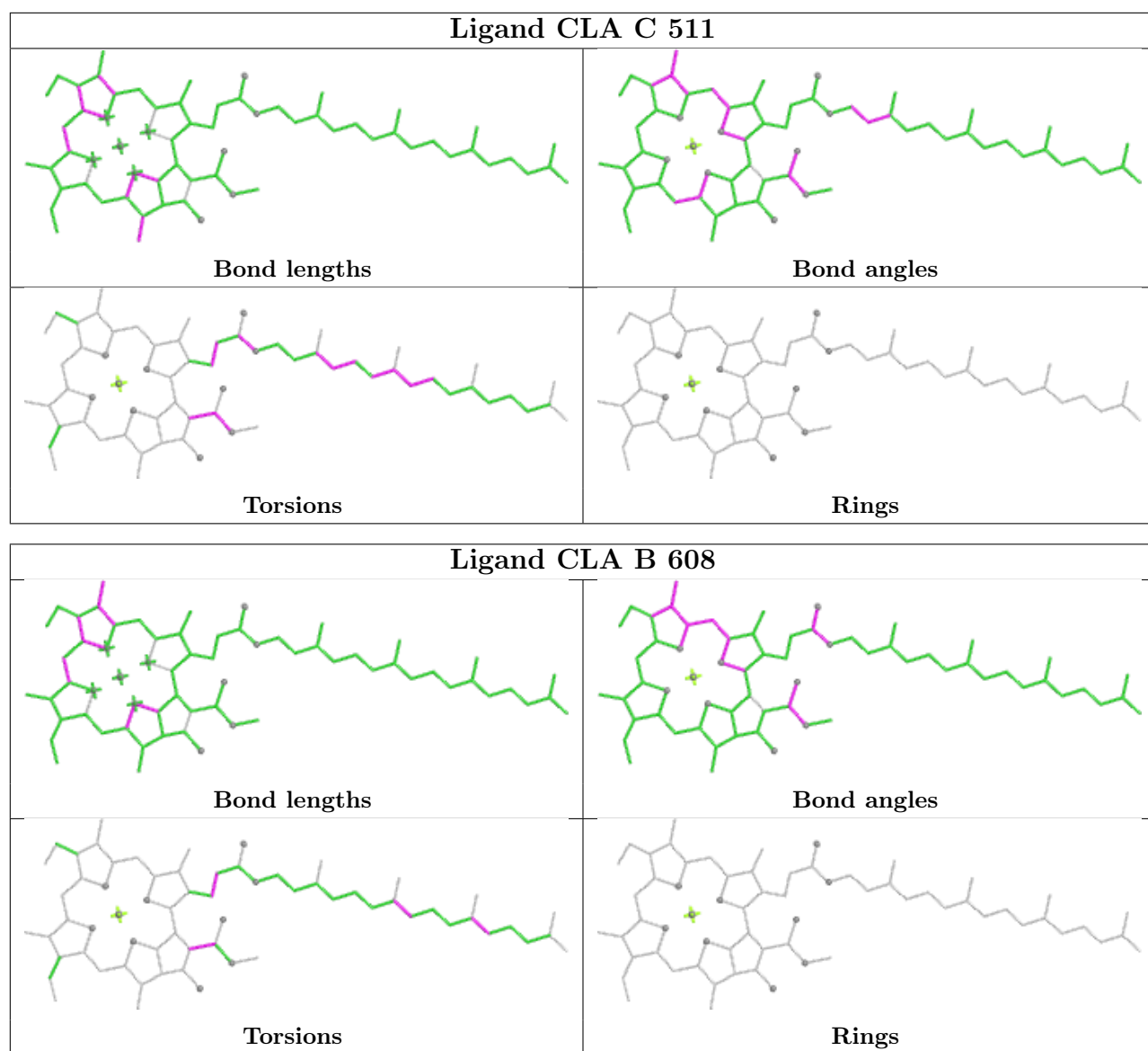
Ligand CLA 5 608**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 612****Bond lengths****Bond angles****Torsions****Rings**

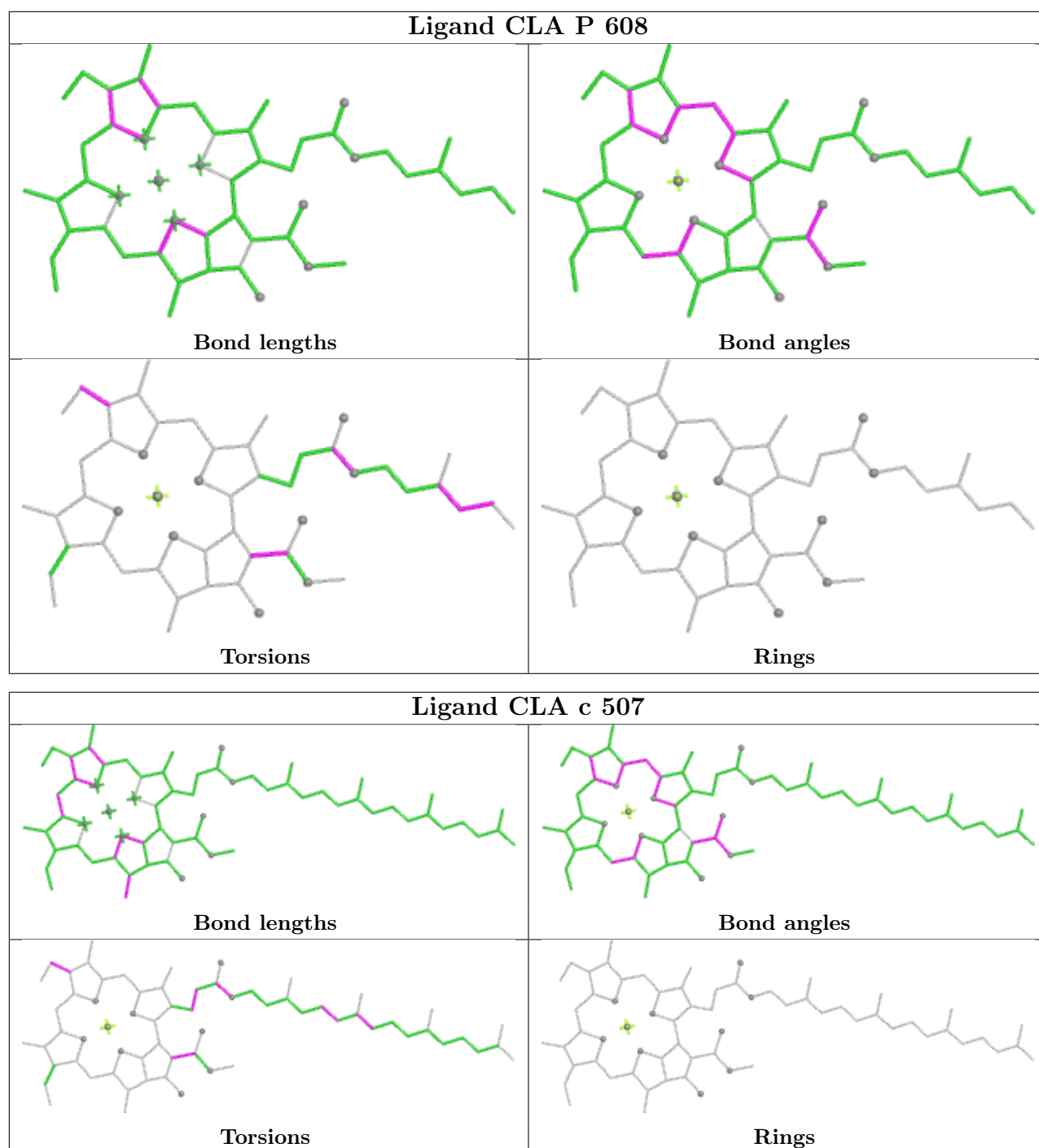


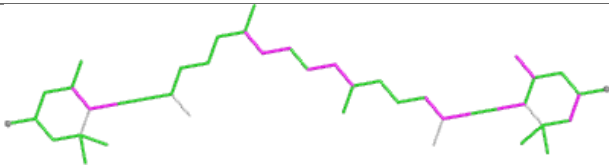
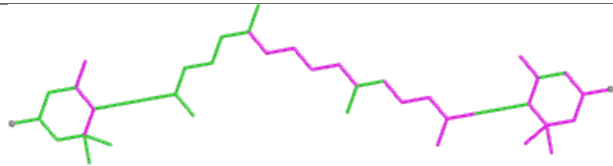
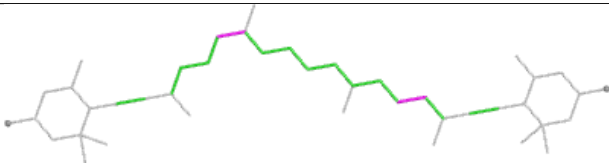
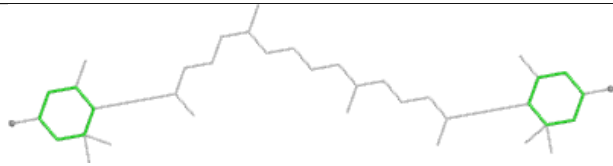


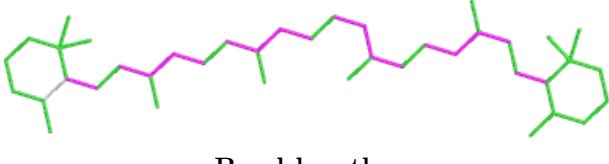
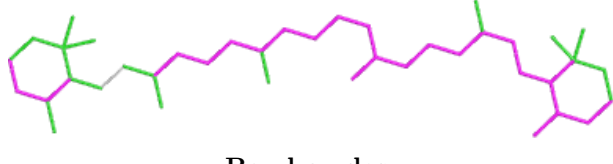
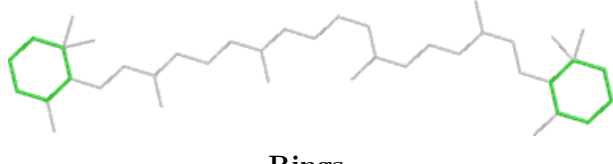
Ligand CLA 1 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 5 601****Bond lengths****Bond angles****Torsions****Rings**

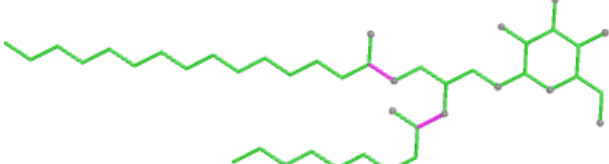
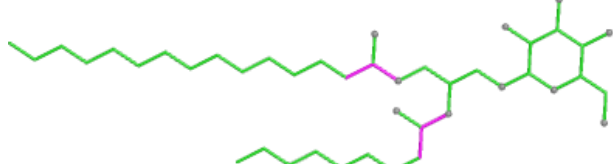
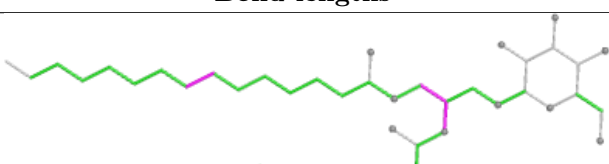
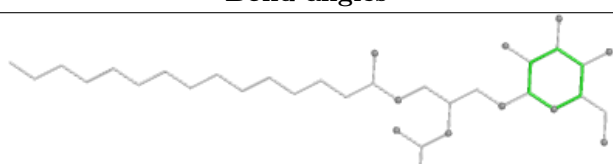


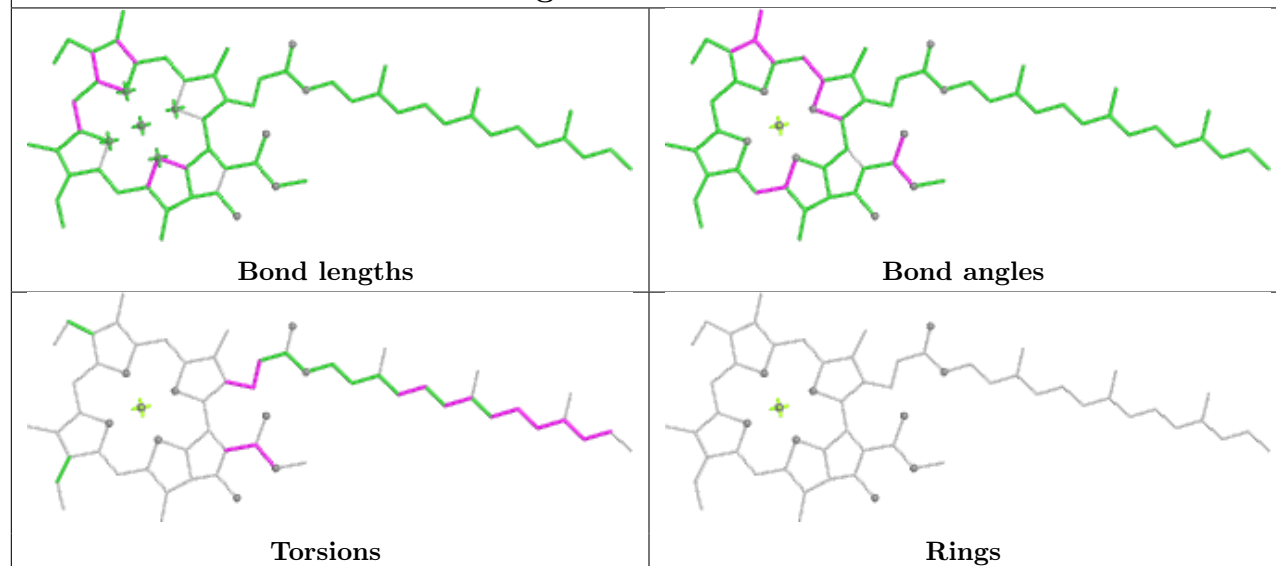
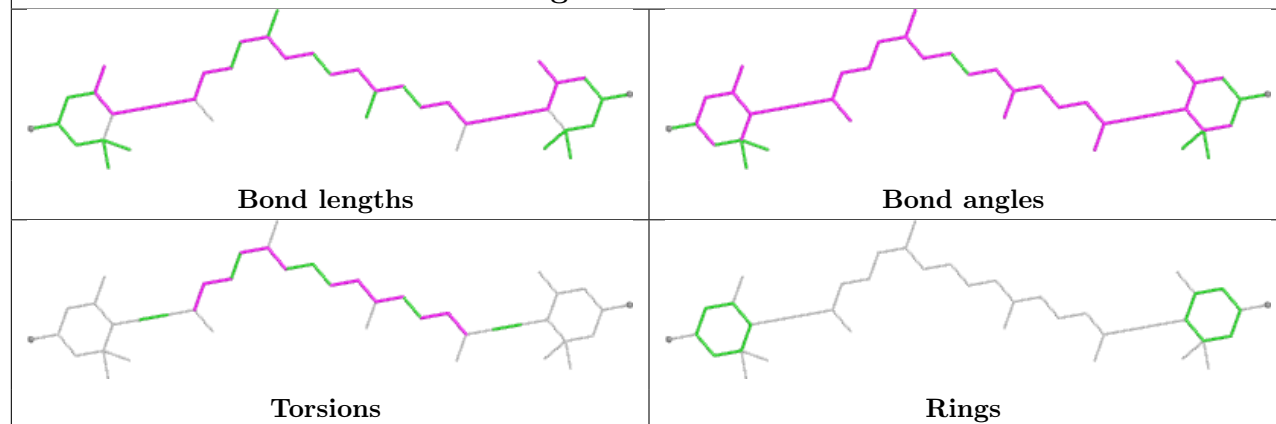
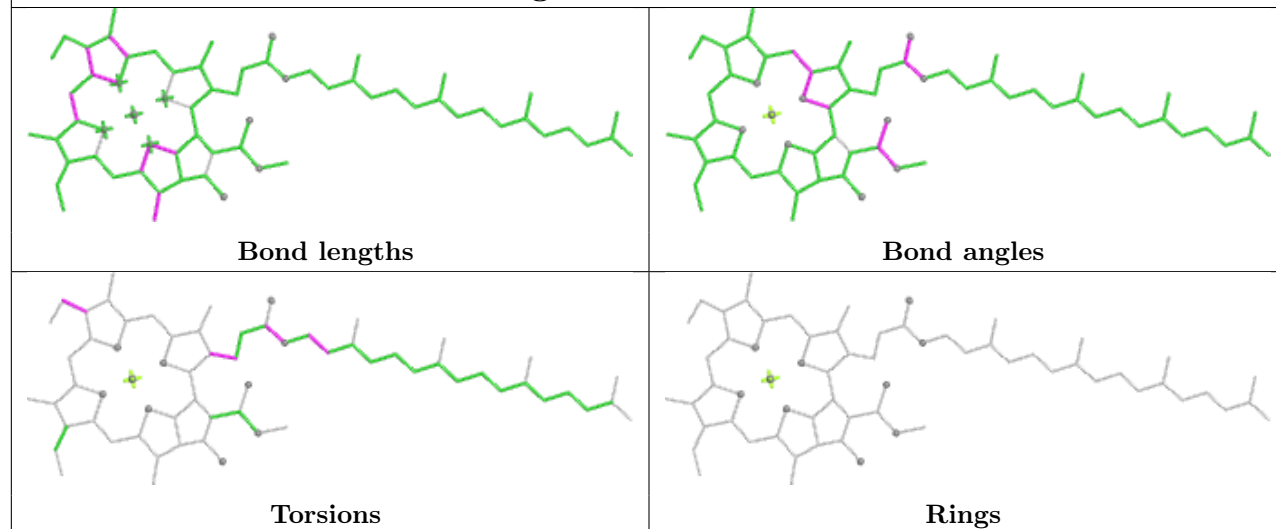


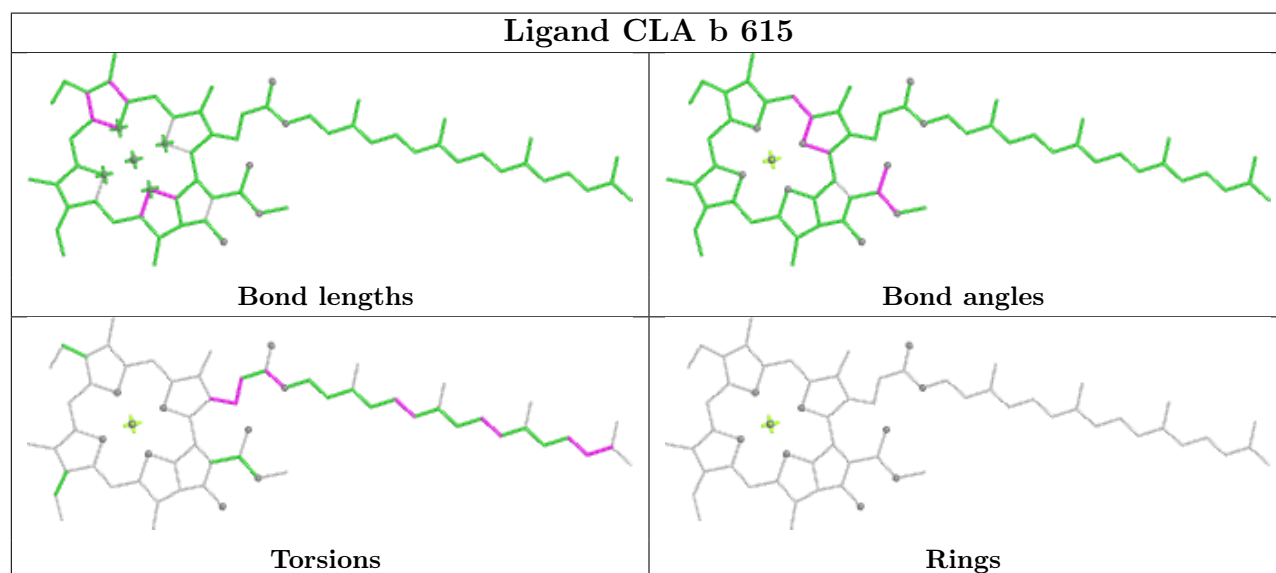
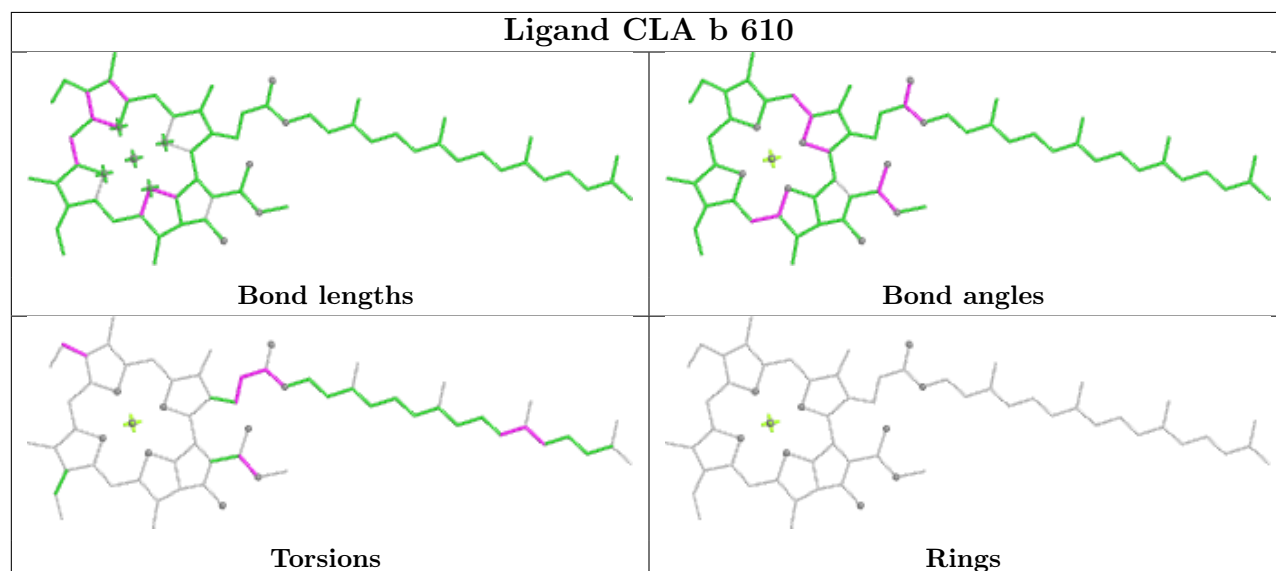
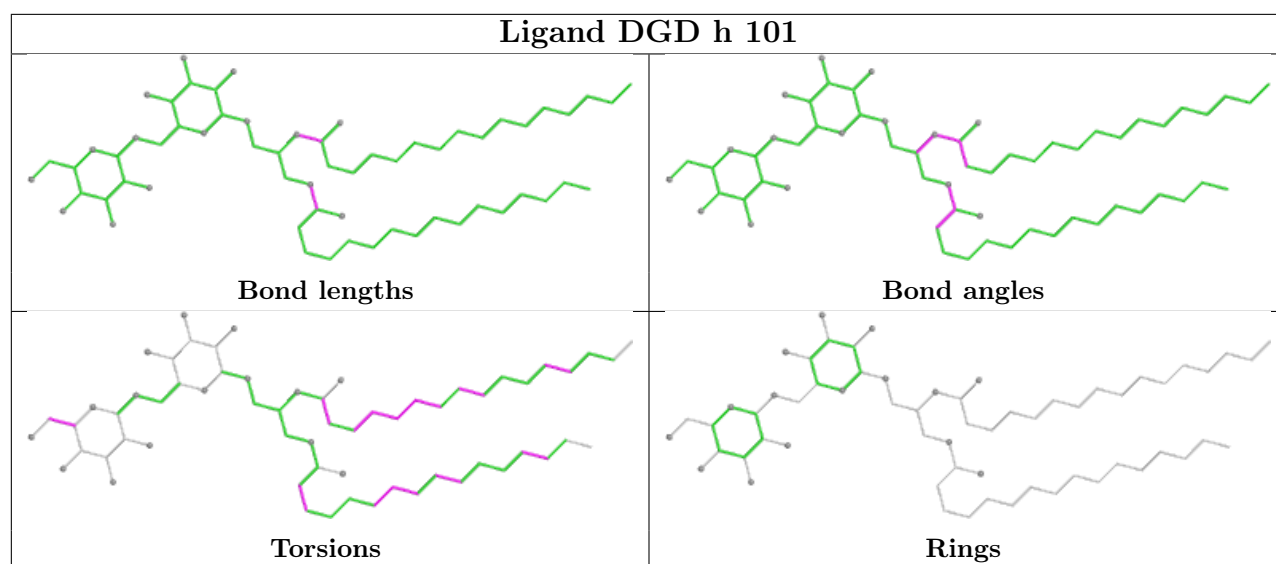


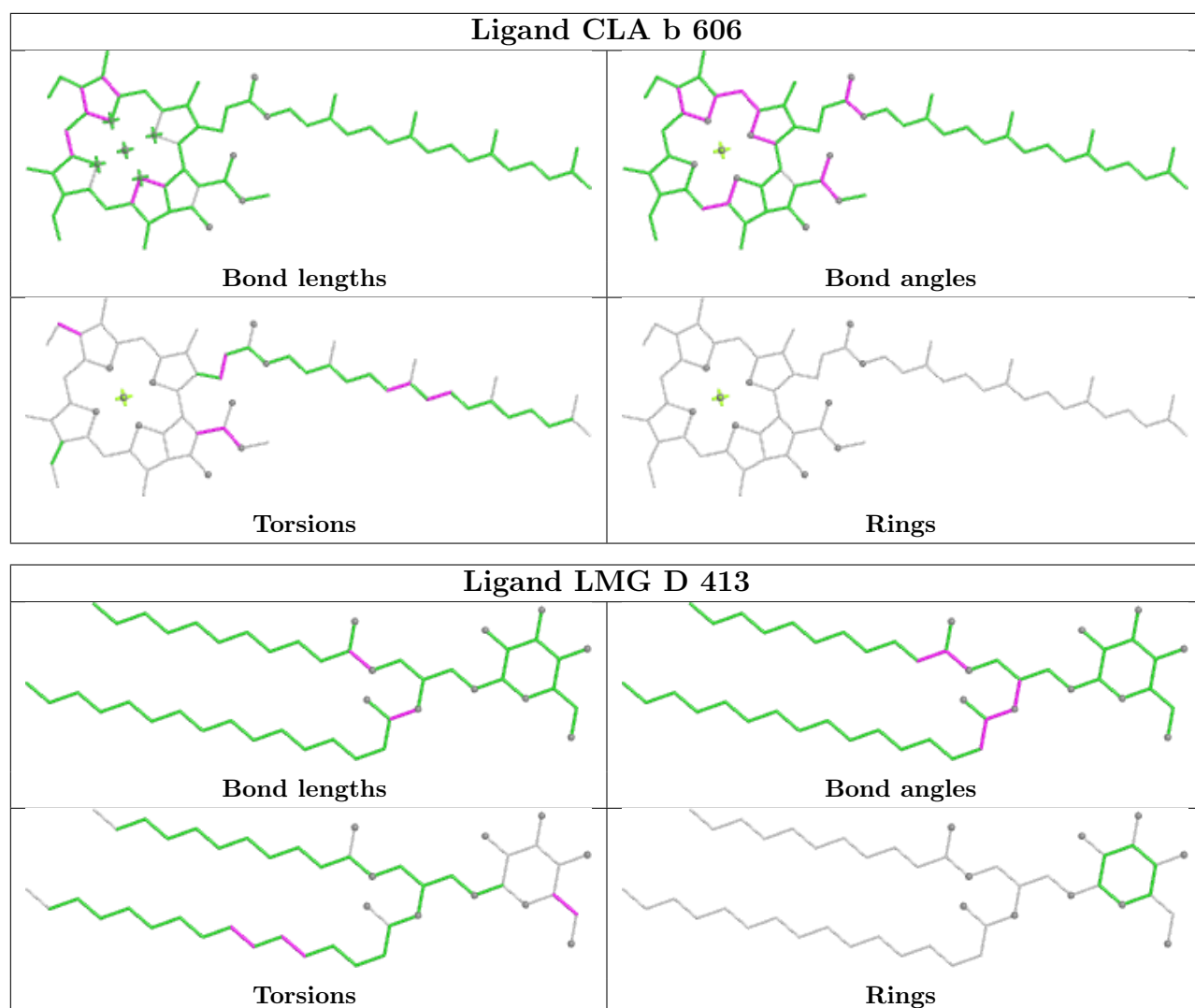
Ligand II0 5 615	
	Bond lengths
	Bond angles
	Torsions
	Rings

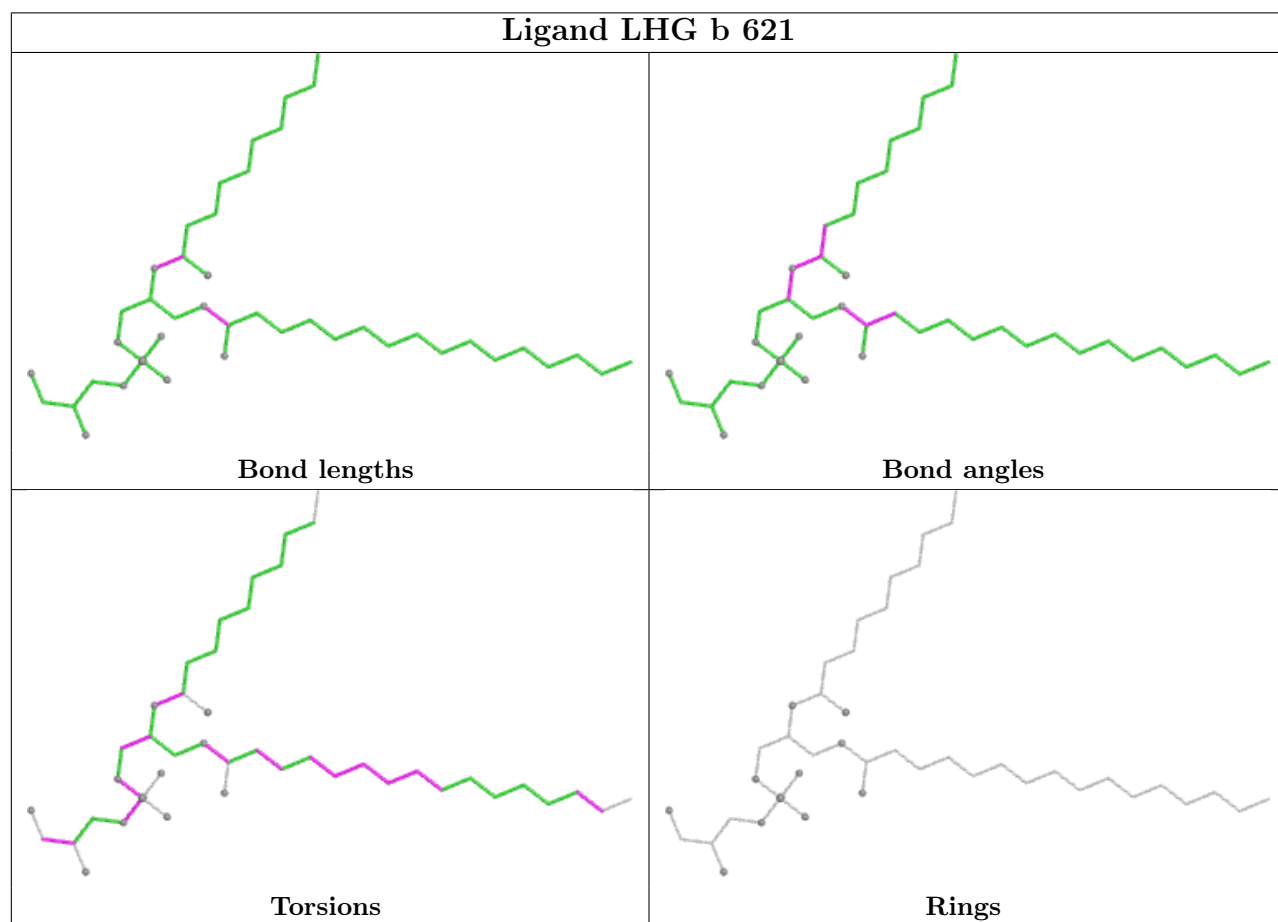
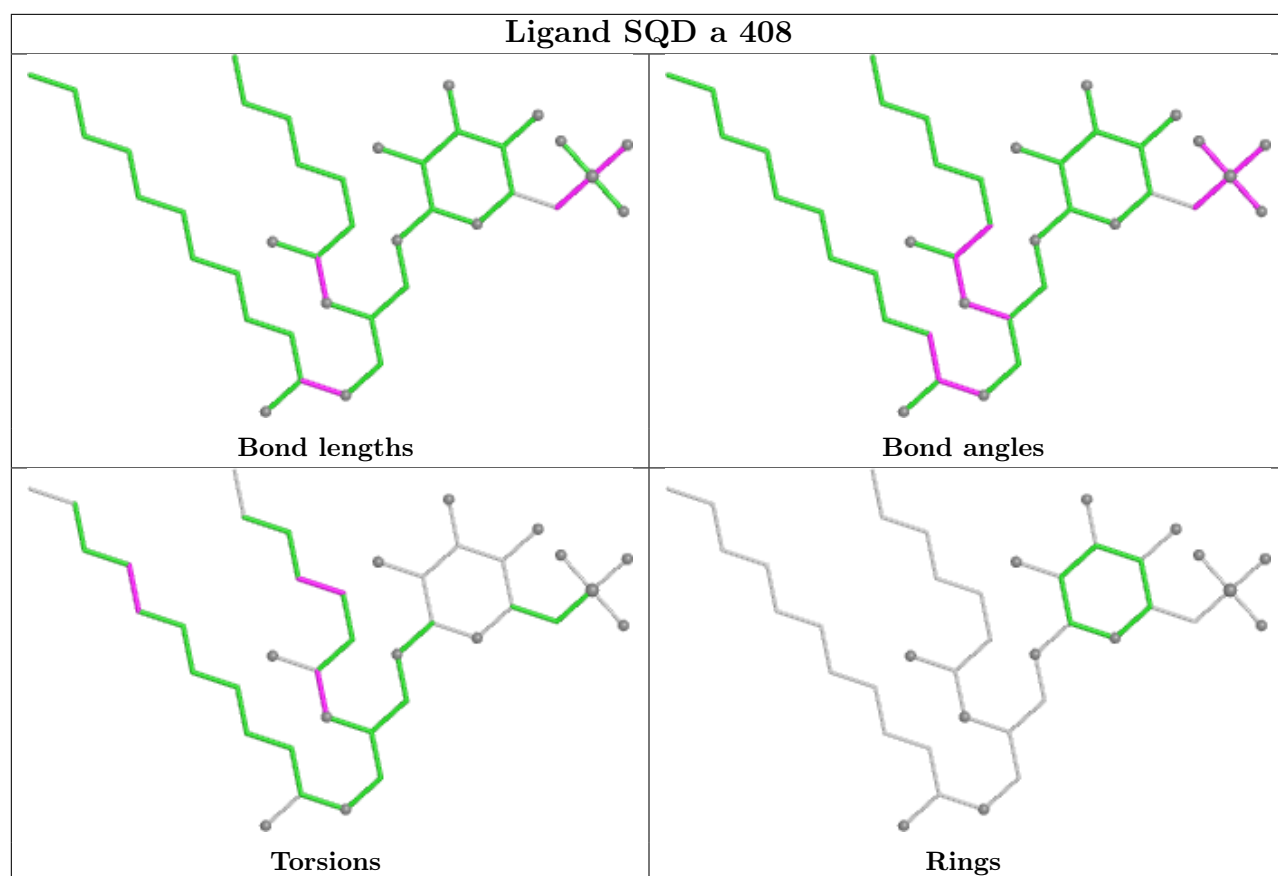
Ligand WVN b 618	
	Bond lengths
	Bond angles
	Torsions
	Rings

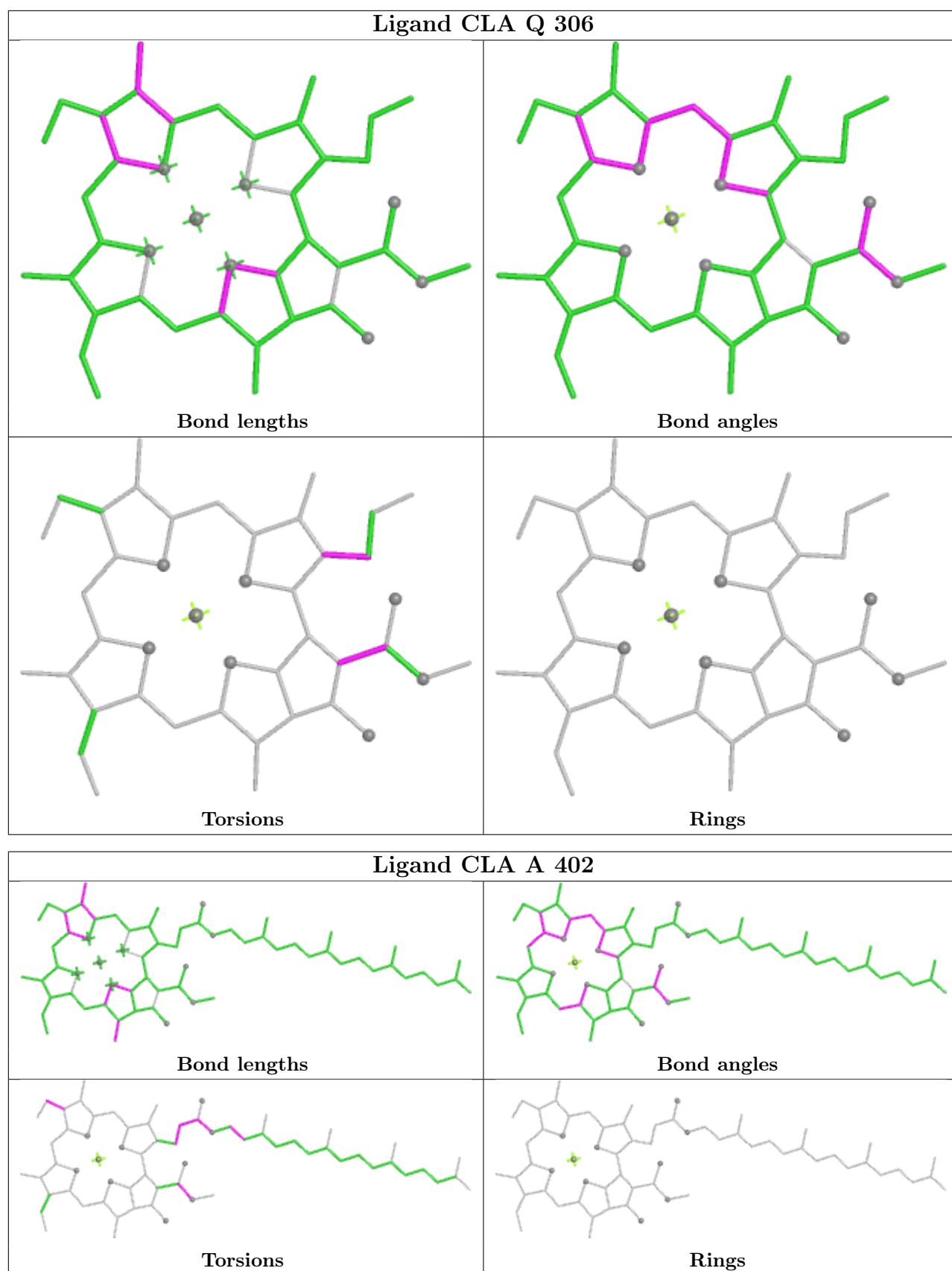
Ligand LMG 4 319	
	Bond lengths
	Bond angles
	Torsions
	Rings

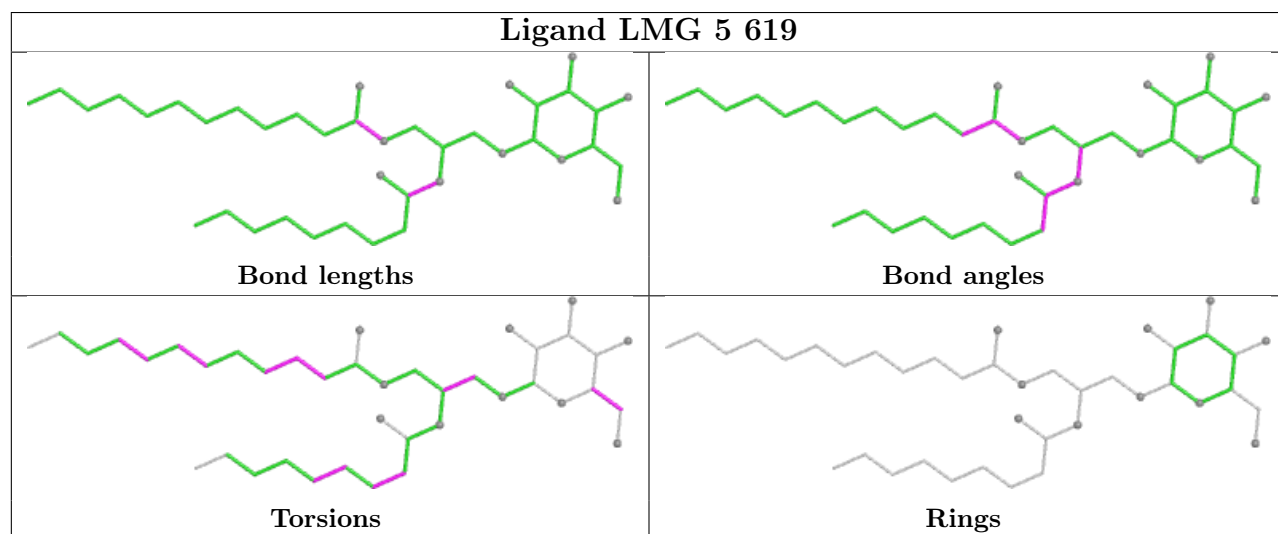
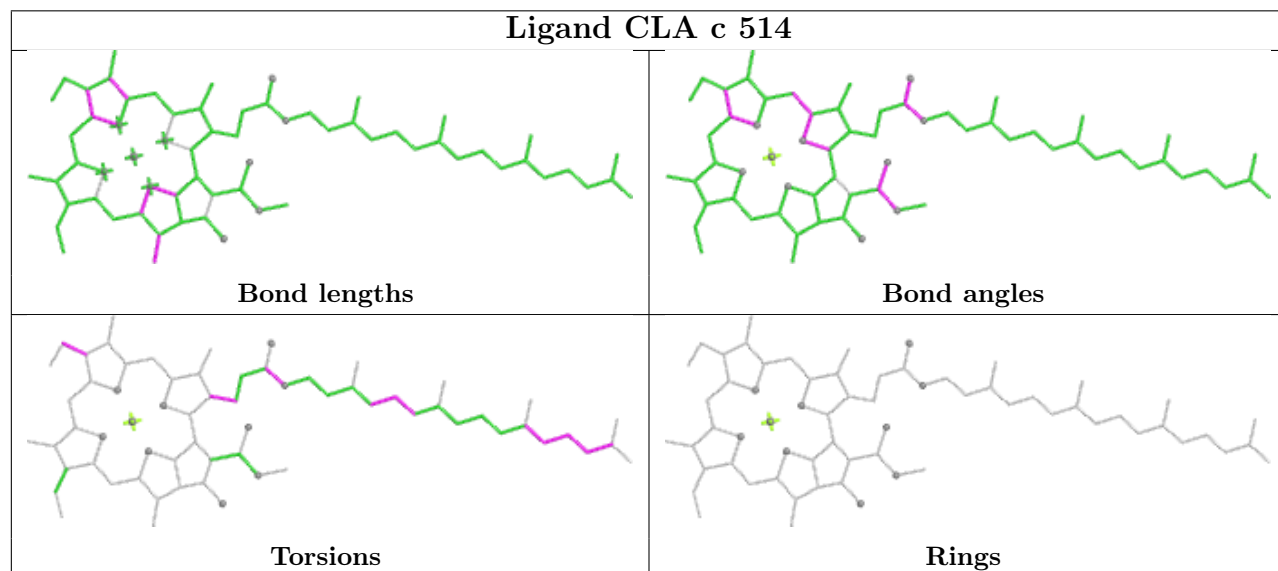
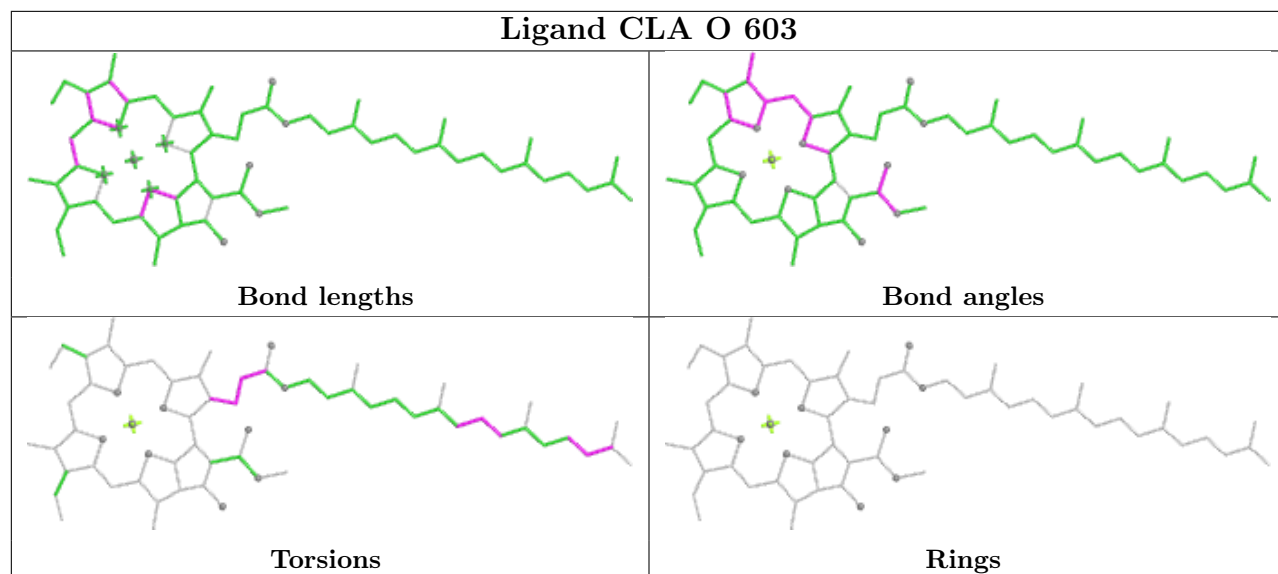
Ligand CLA 3 301**Ligand II0 1 615****Ligand CLA D 407**



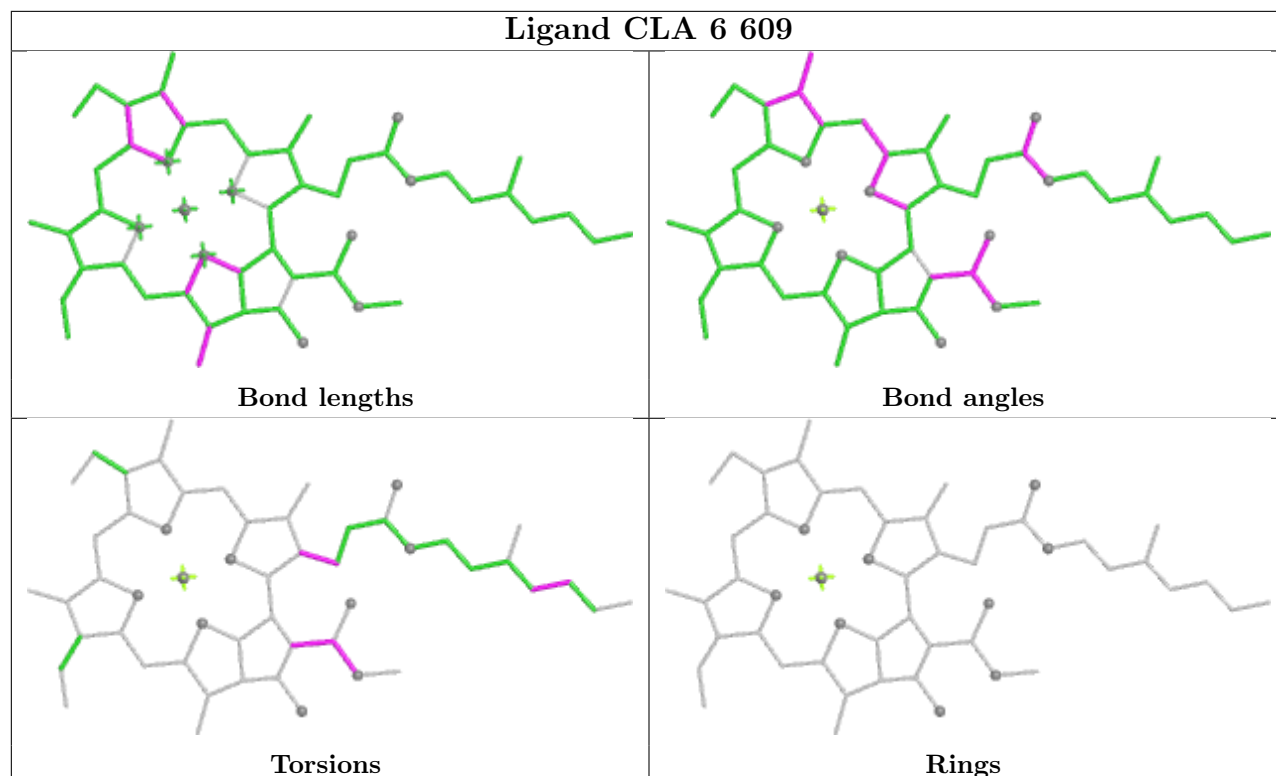




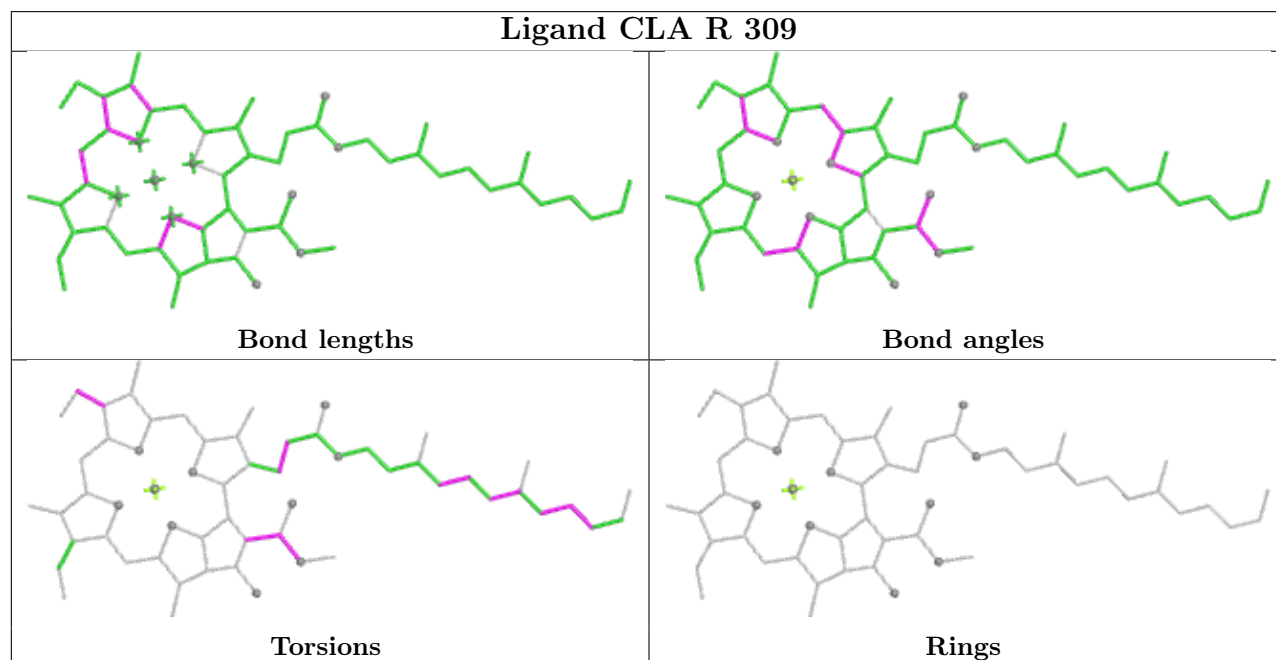




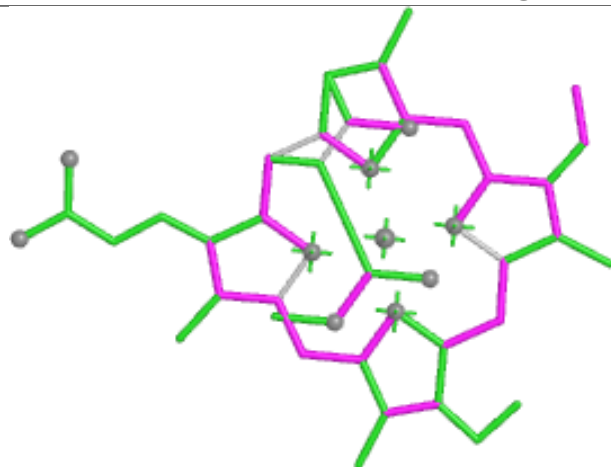
Ligand CLA 6 609



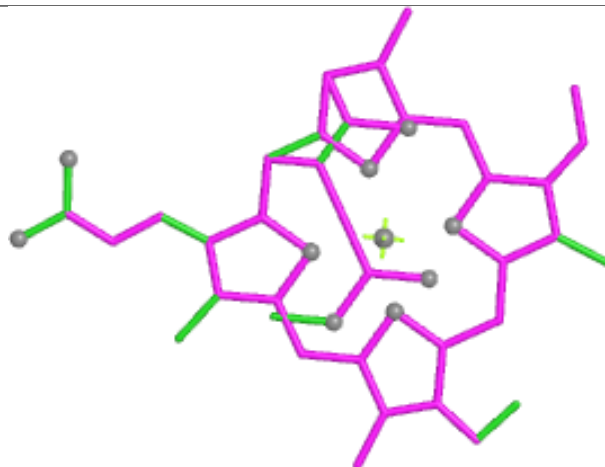
Ligand CLA R 309



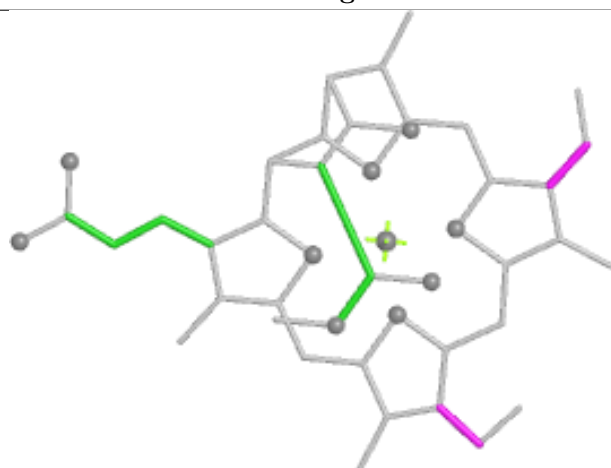
Ligand KC2 N 610



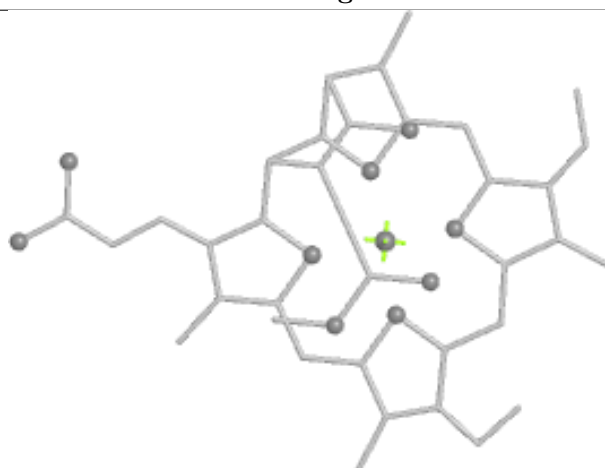
Bond lengths



Bond angles

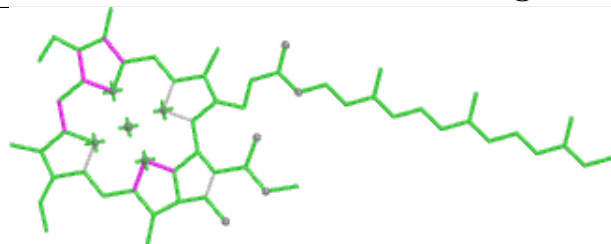


Torsions

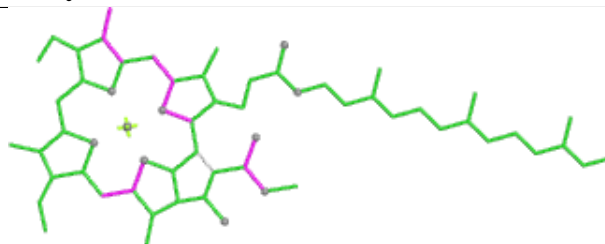


Rings

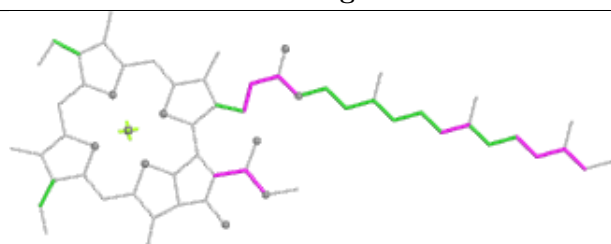
Ligand CLA Q 303



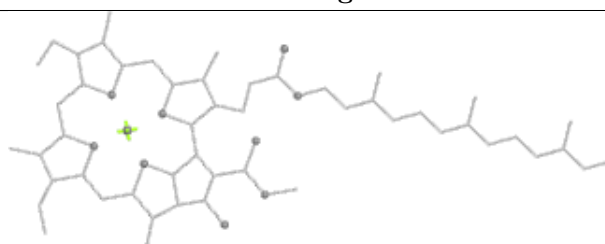
Bond lengths



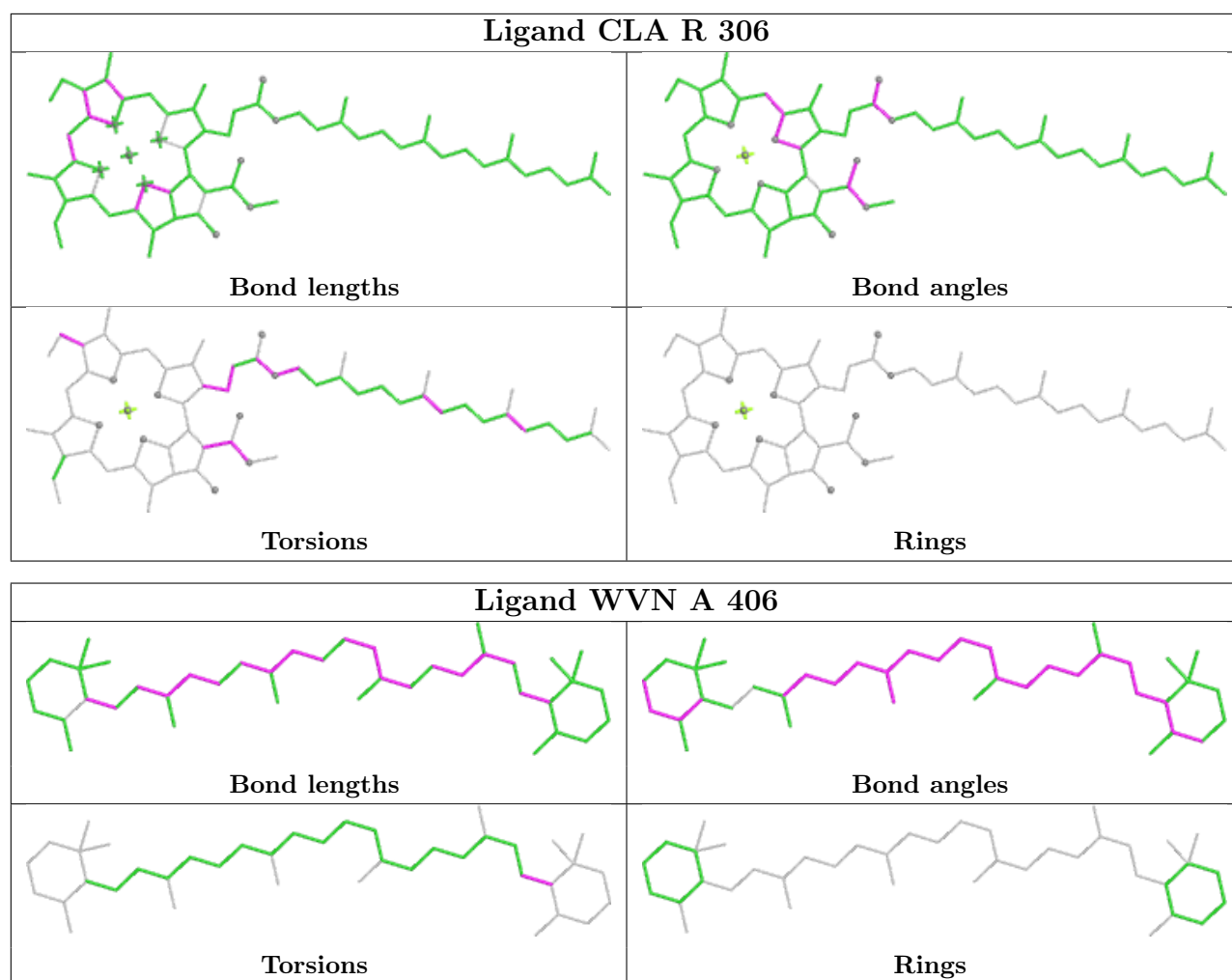
Bond angles



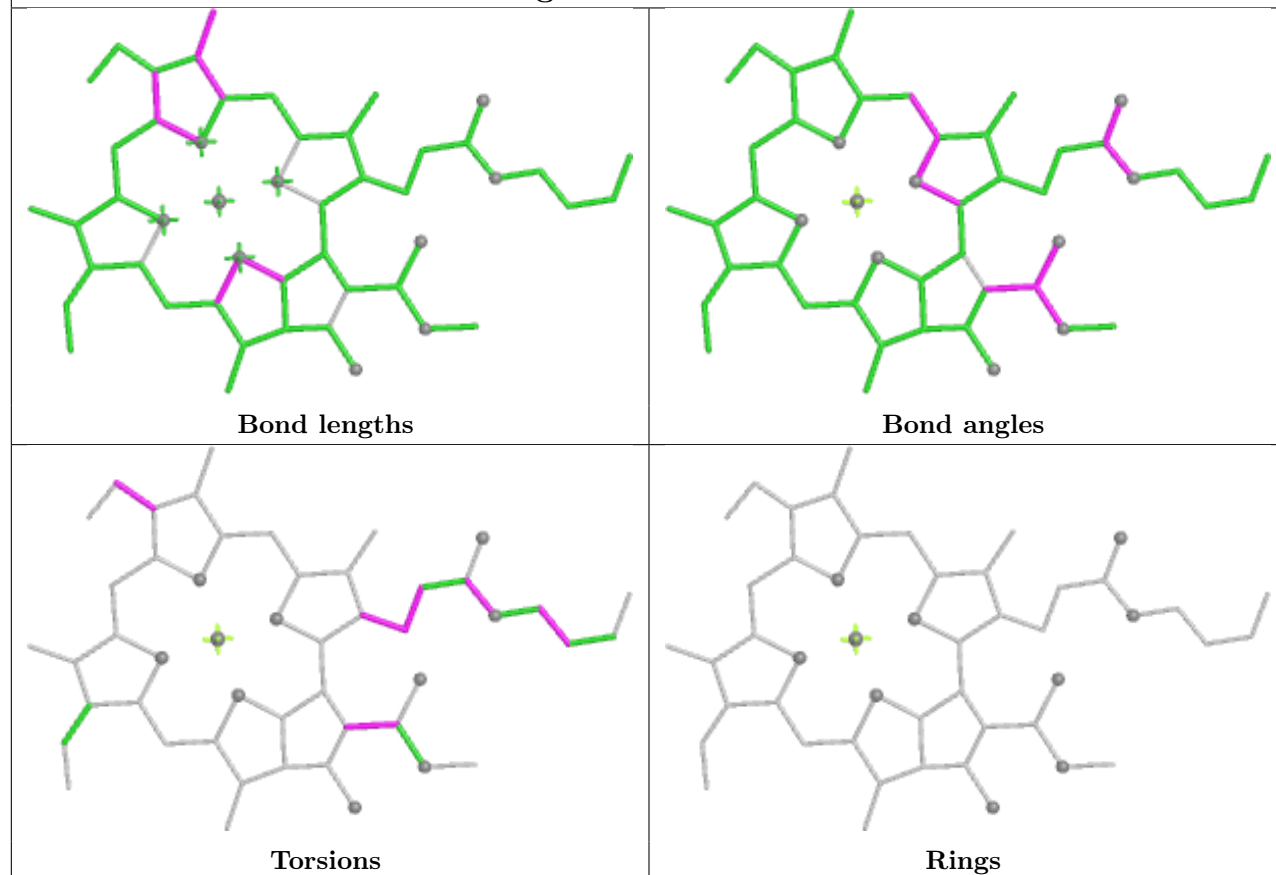
Torsions



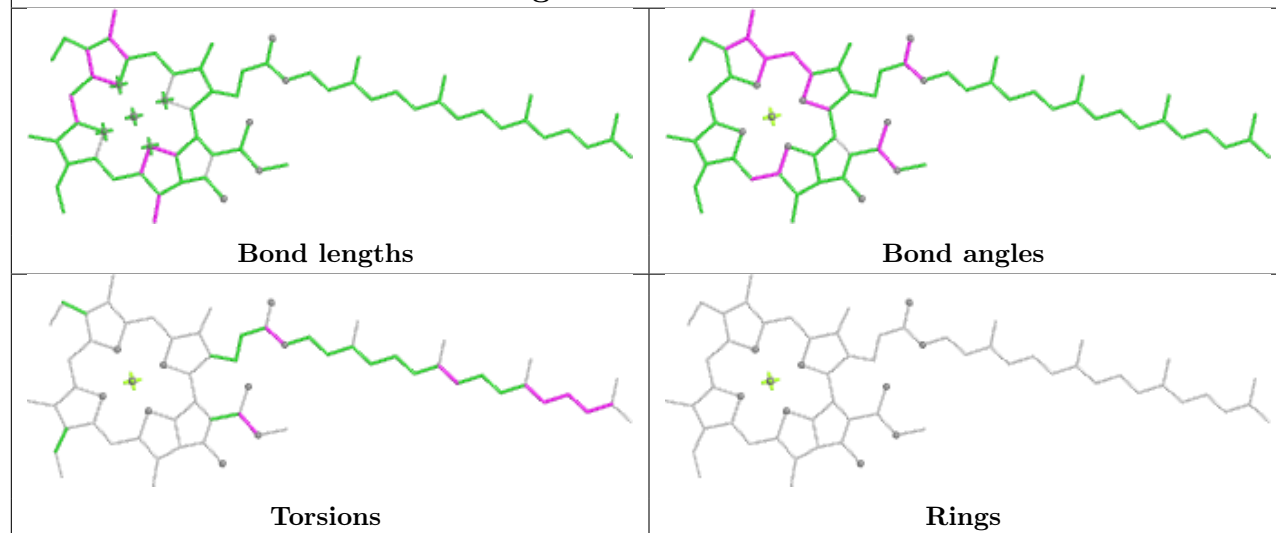
Rings

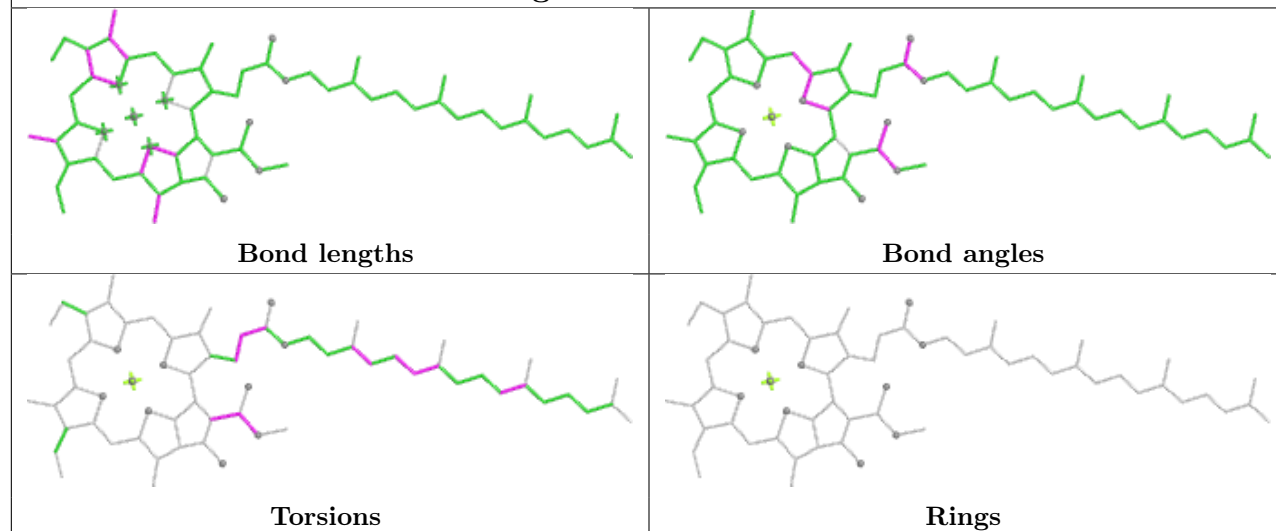
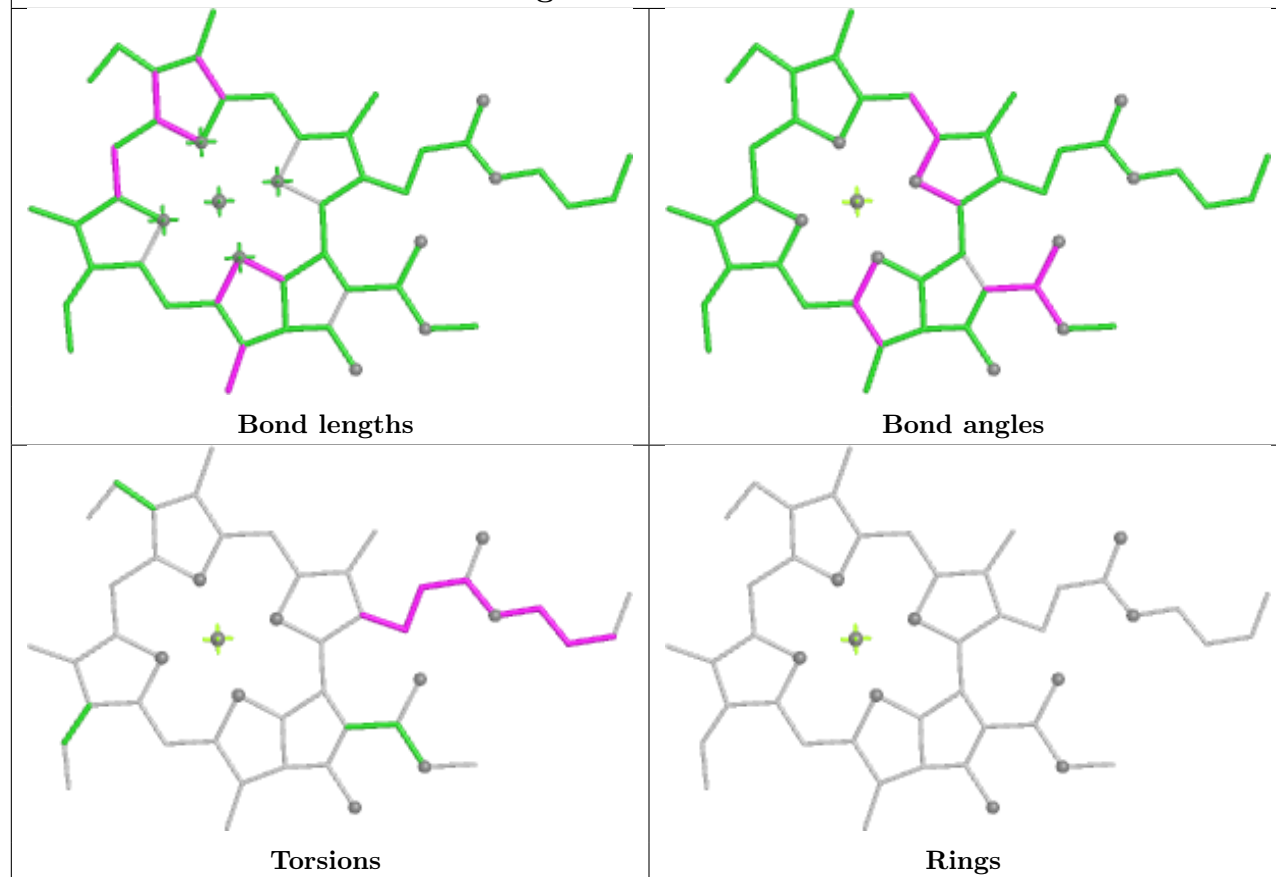


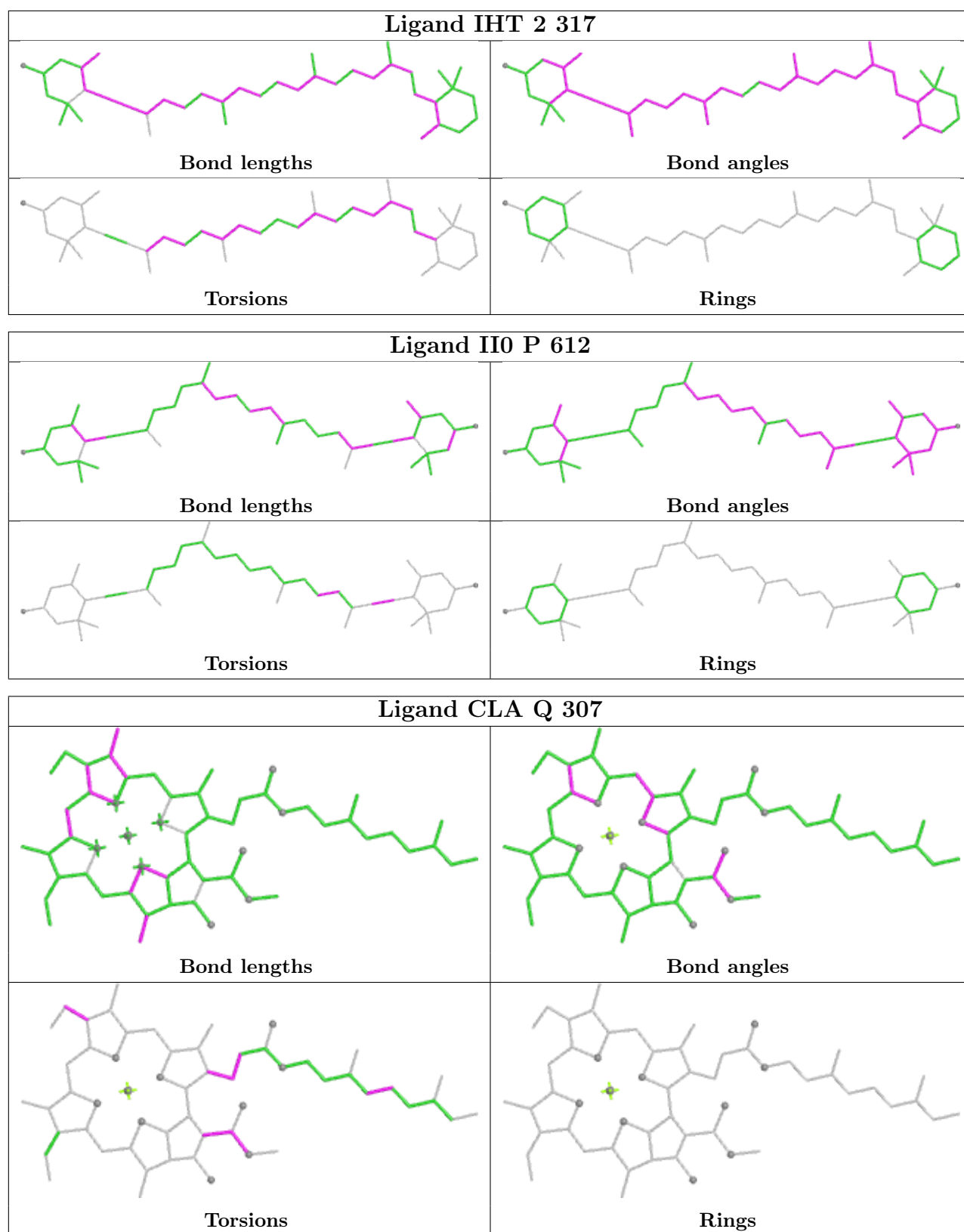
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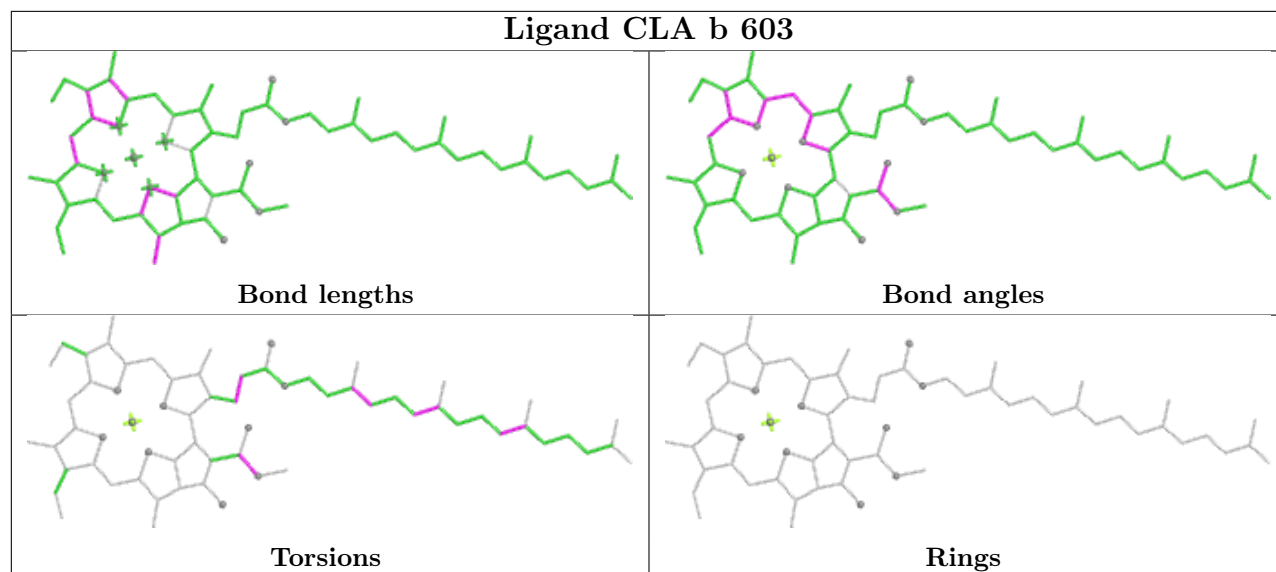
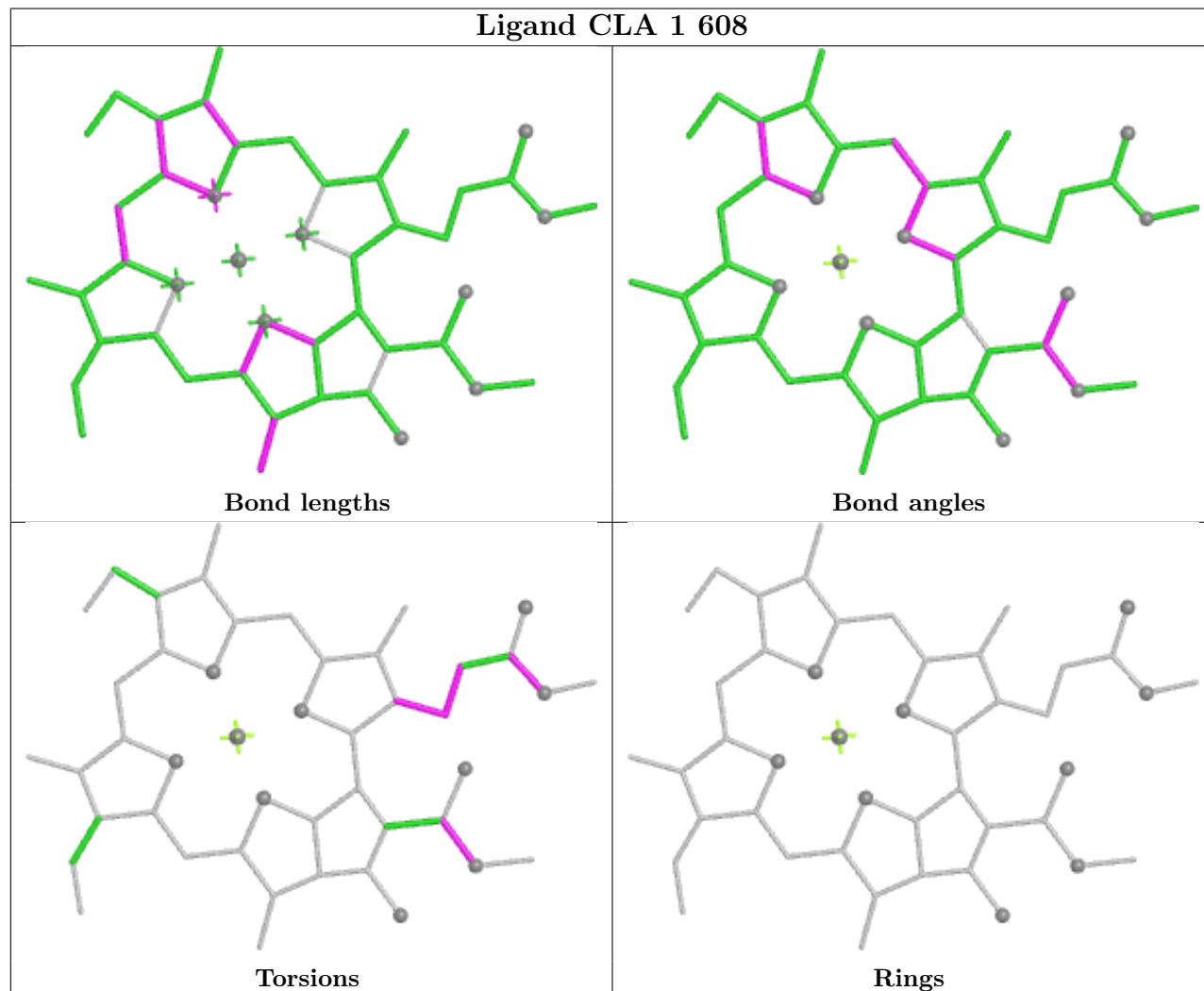


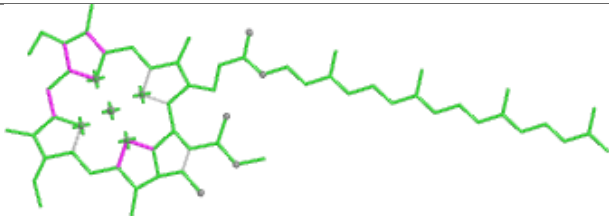
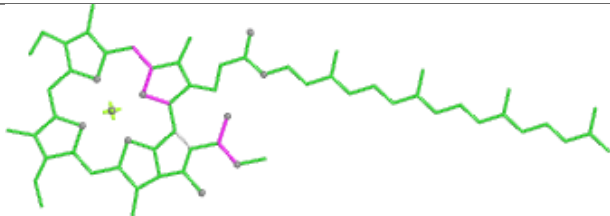
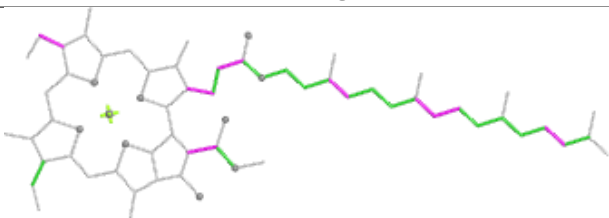
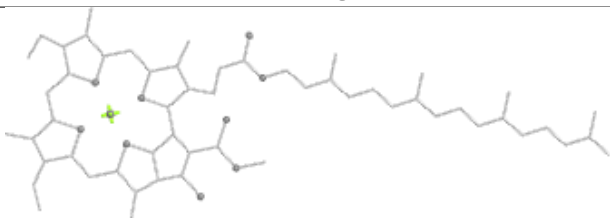
Ligand CLA C 509

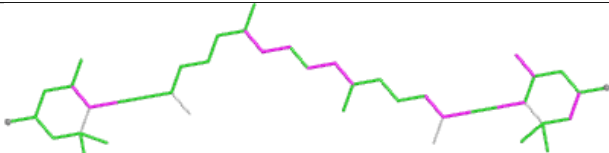
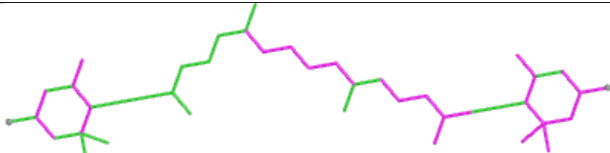
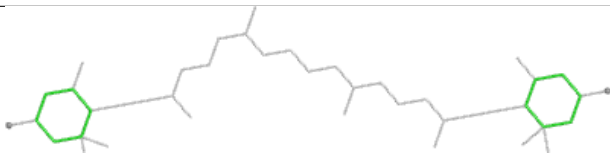


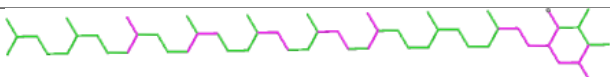
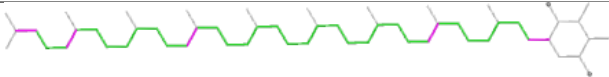
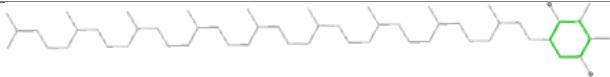
Ligand CLA C 503**Ligand CLA a 403**

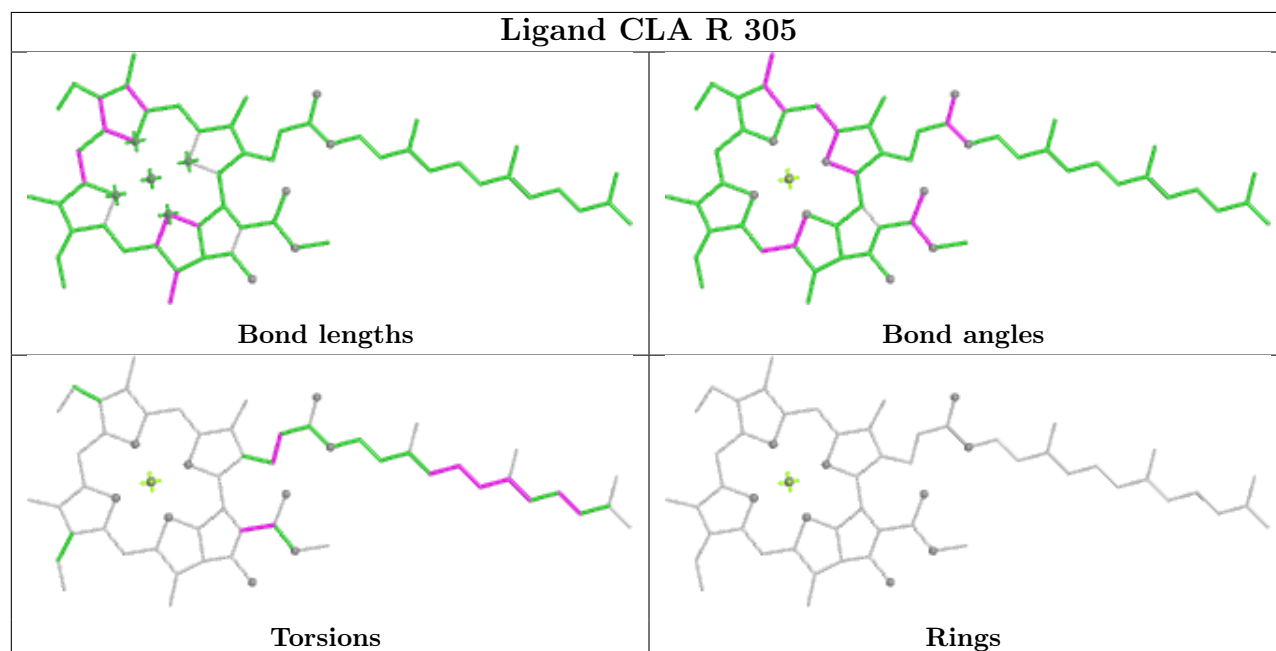
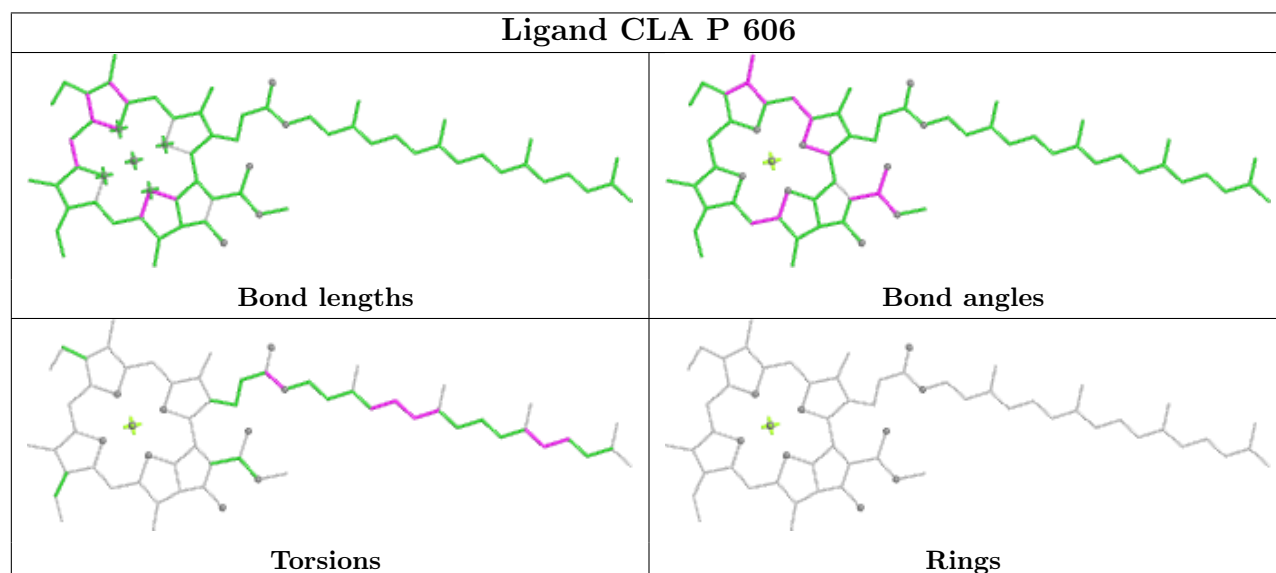
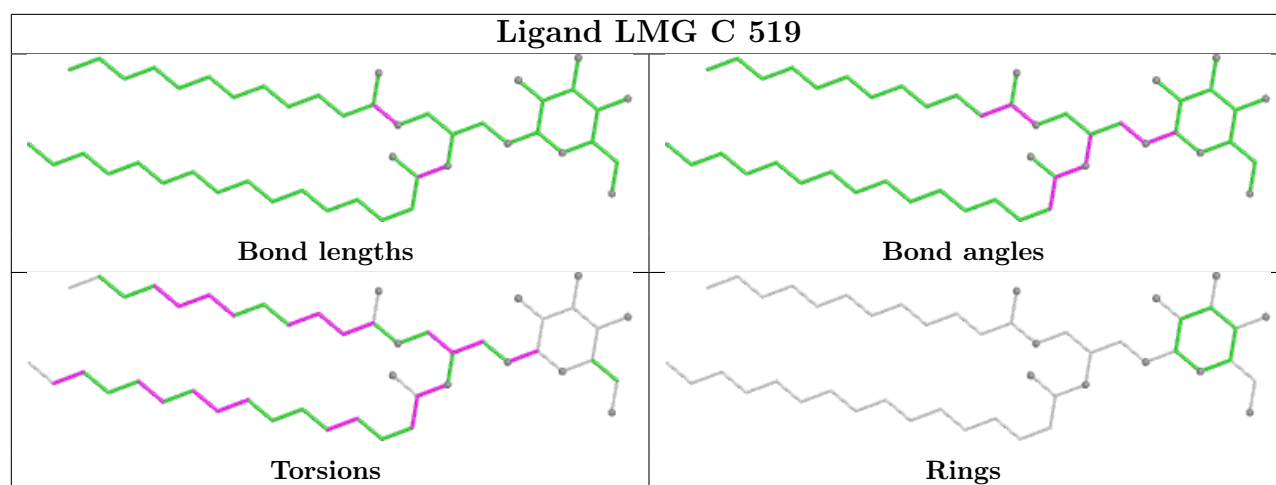


Ligand CLA b 603**Ligand CLA 1 608**

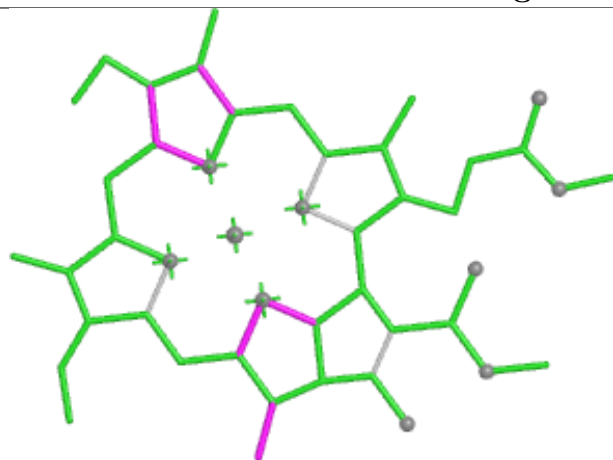
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 N 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

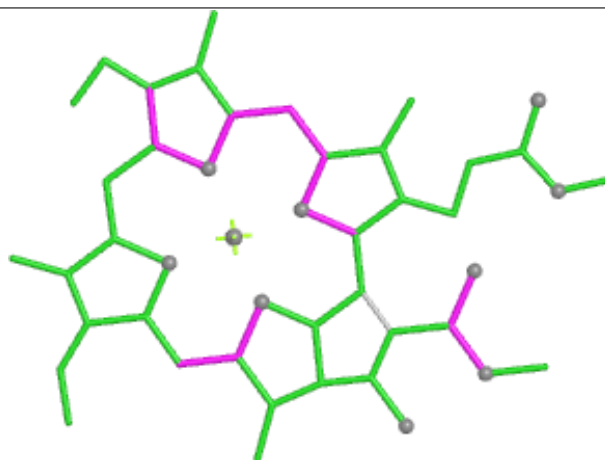
Ligand PL9 d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings



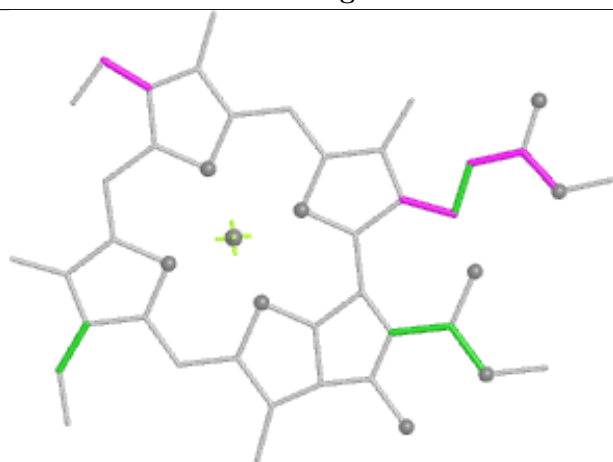
Ligand CLA R 313



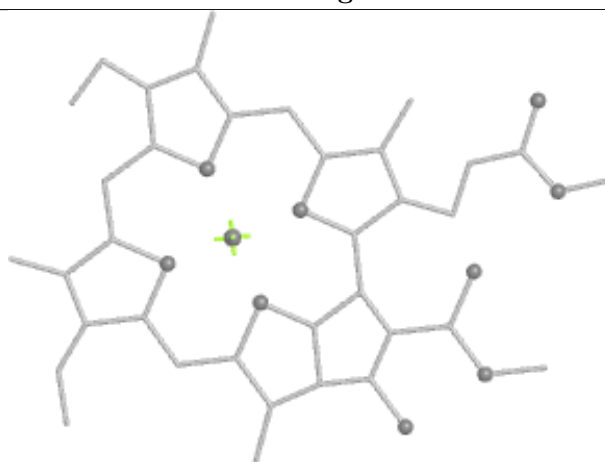
Bond lengths



Bond angles

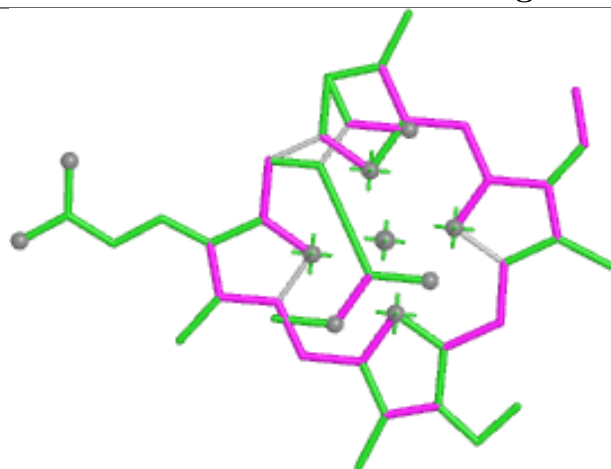


Torsions

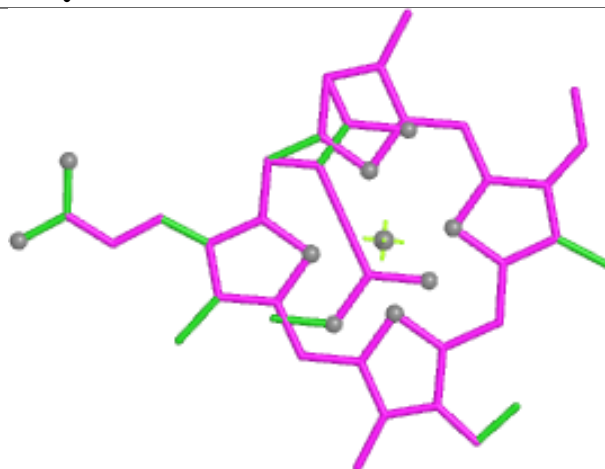


Rings

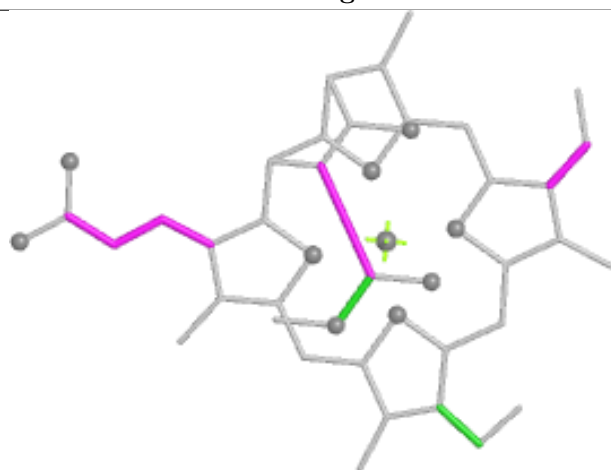
Ligand KC2 Q 304



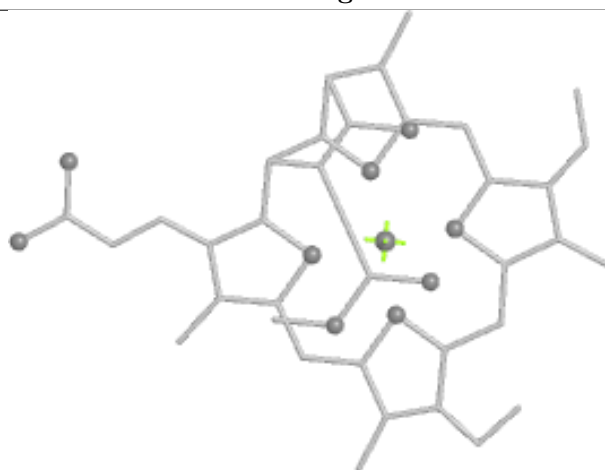
Bond lengths



Bond angles



Torsions

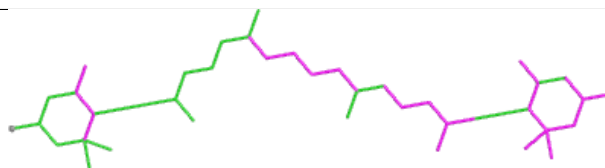


Rings

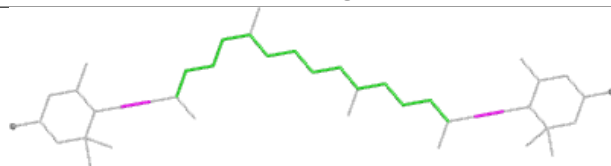
Ligand II0 O 613



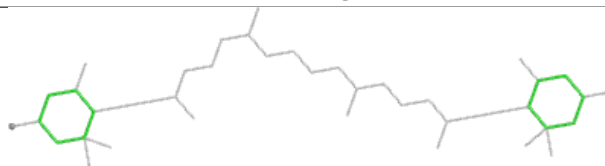
Bond lengths



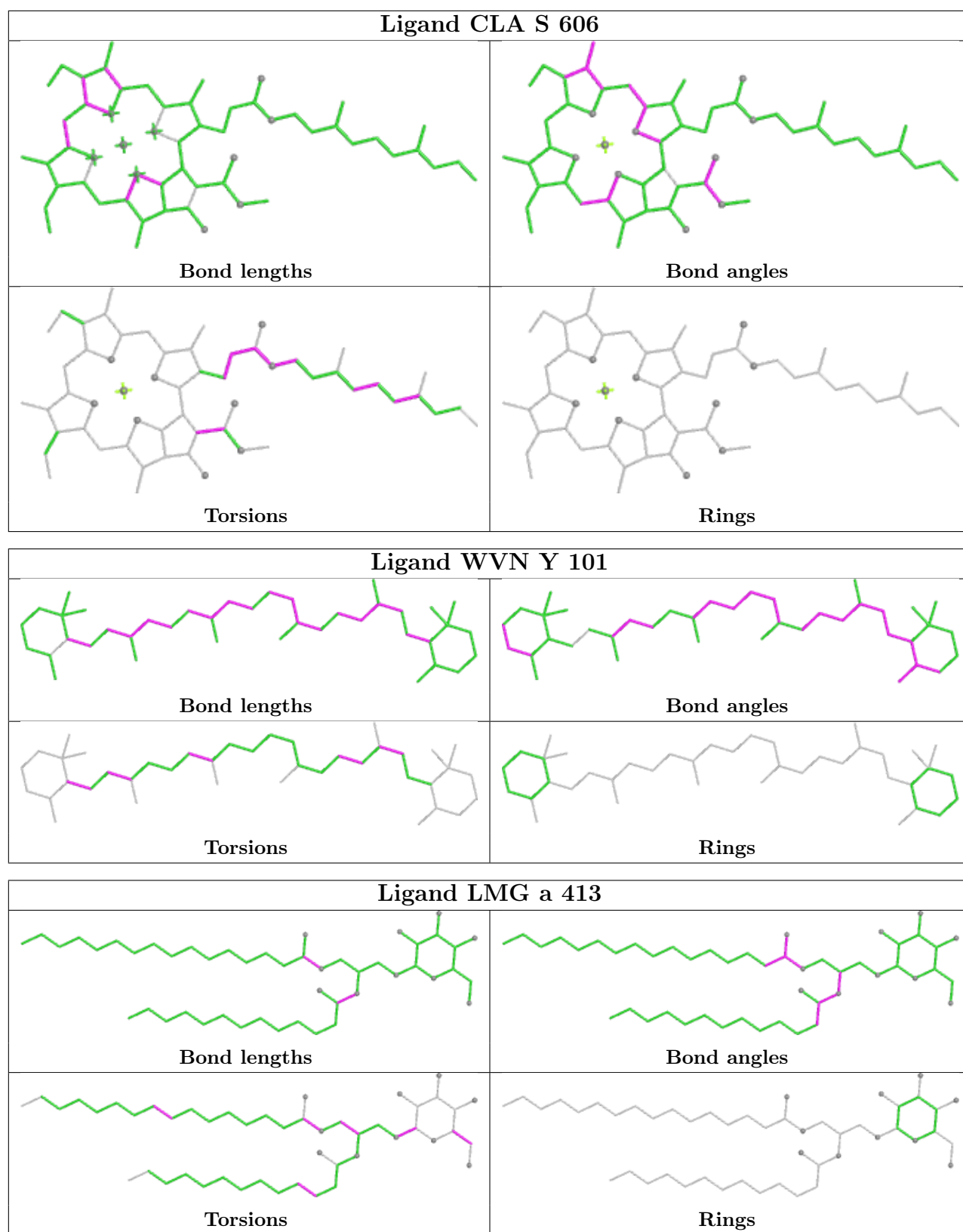
Bond angles

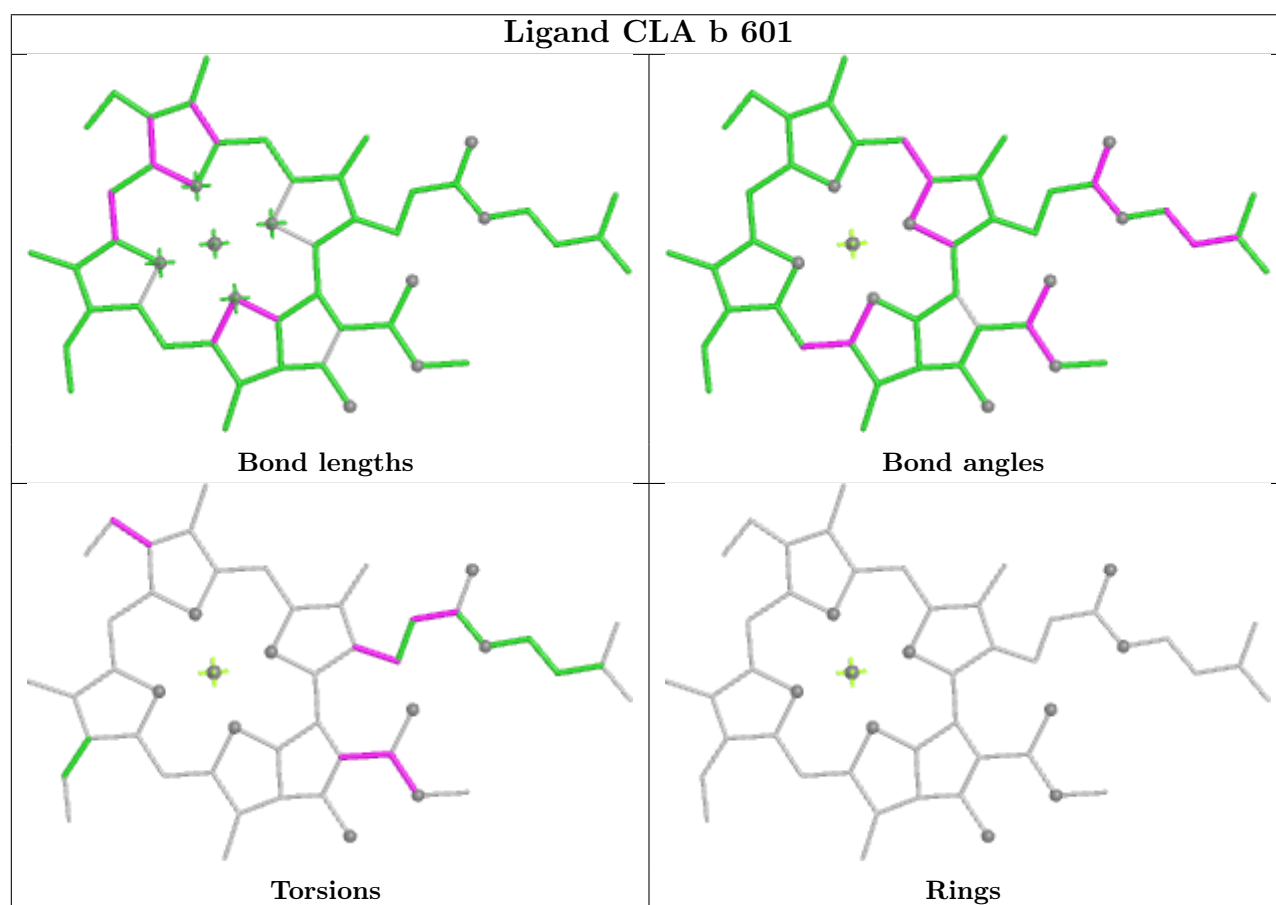
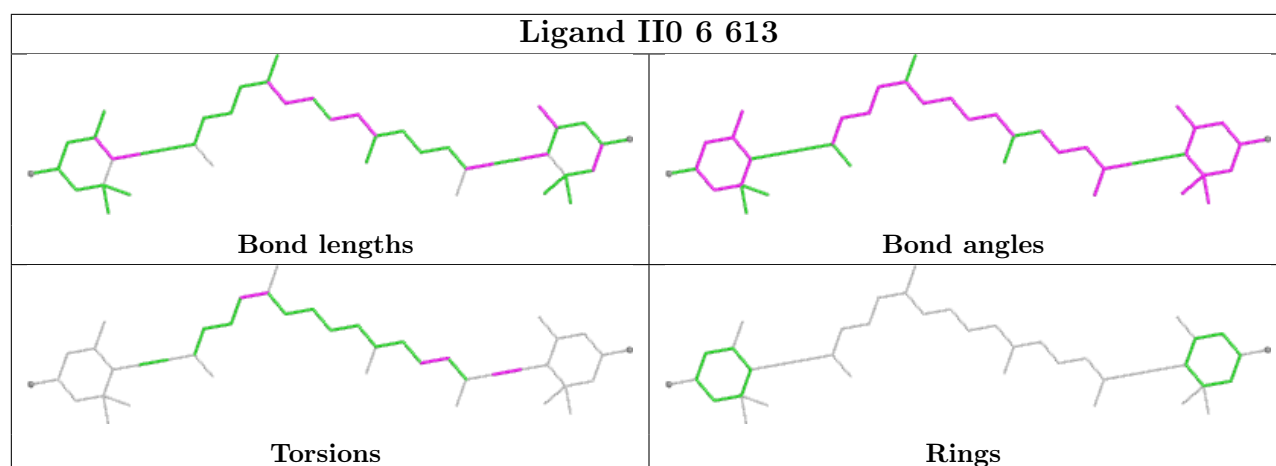


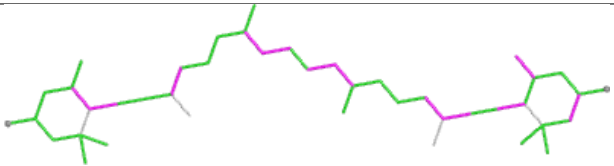
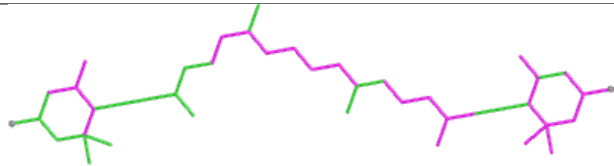
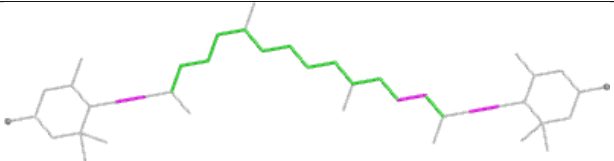
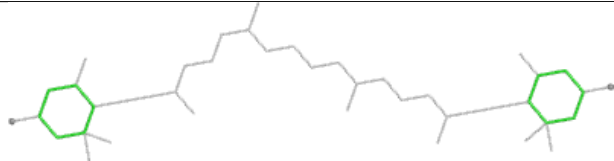
Torsions

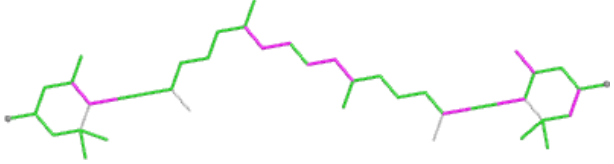
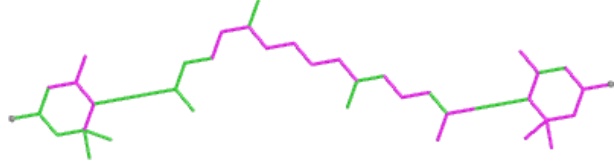
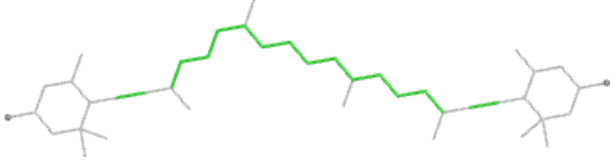
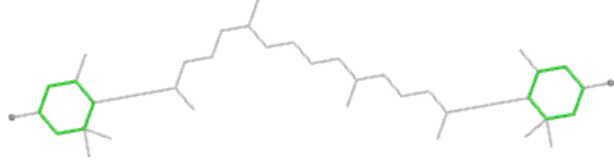


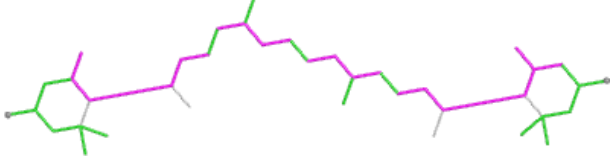
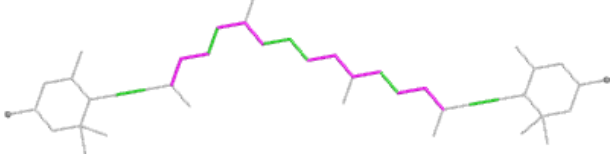
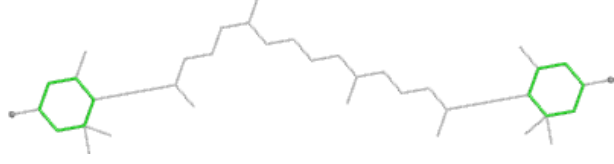
Rings

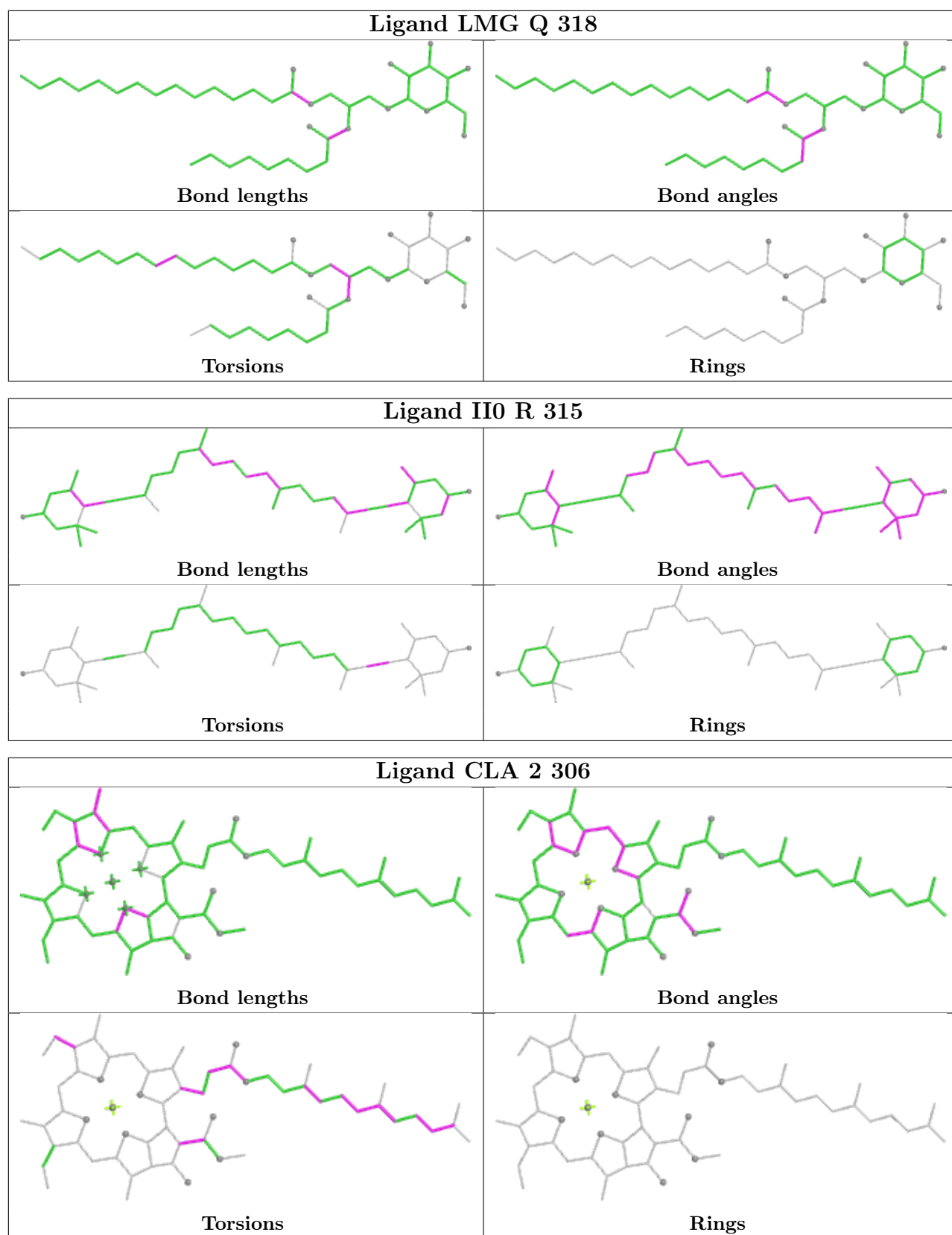


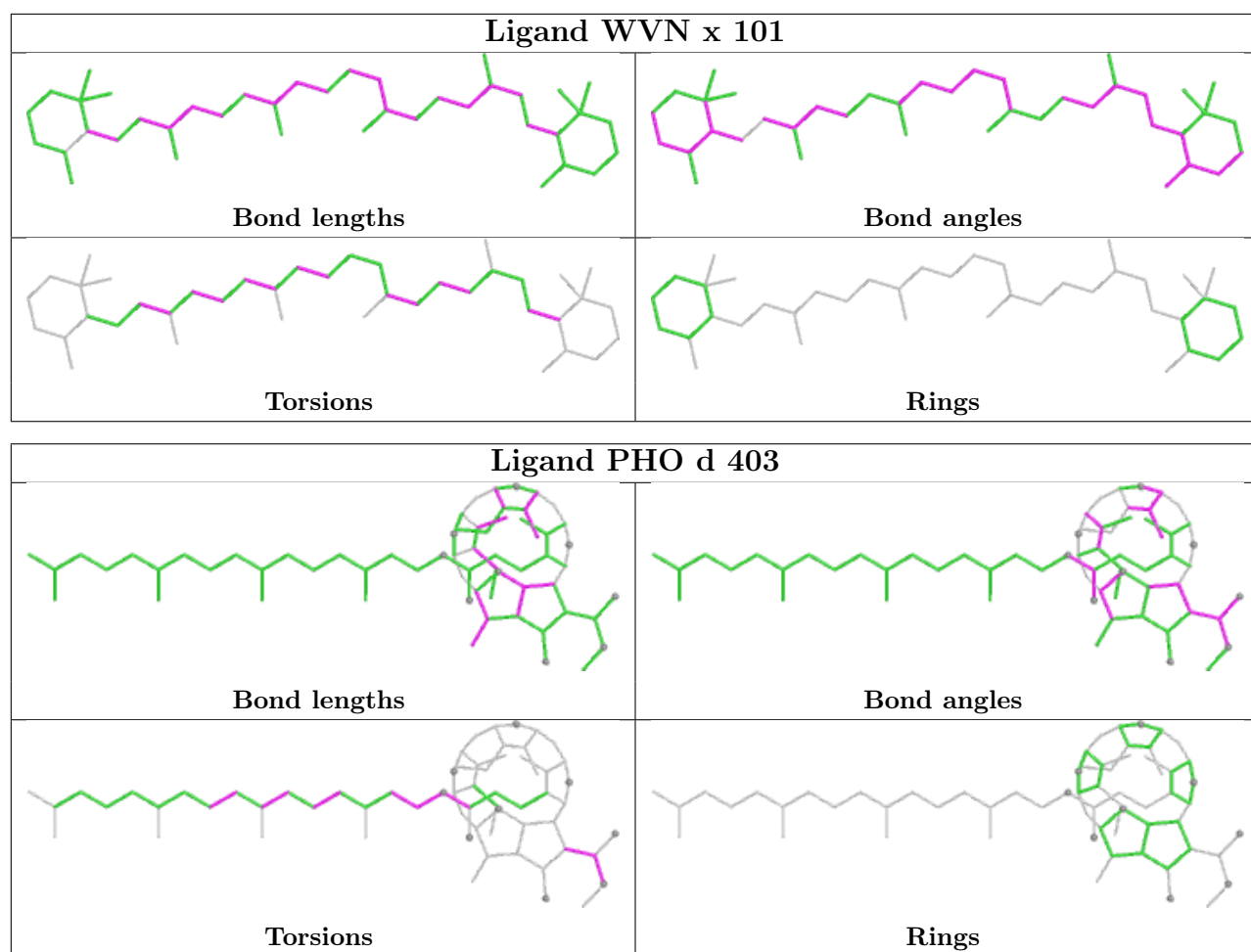


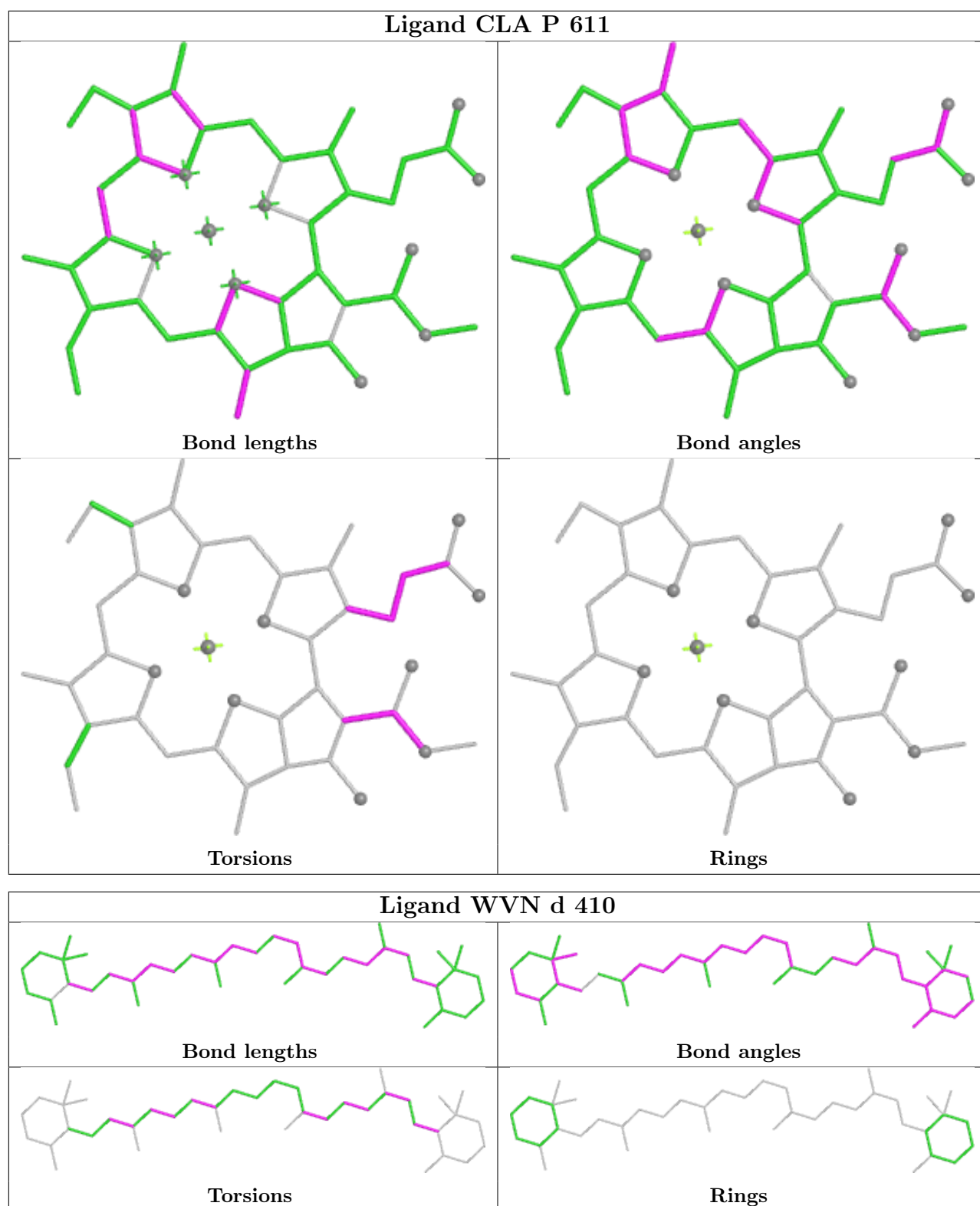
Ligand II0 N 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

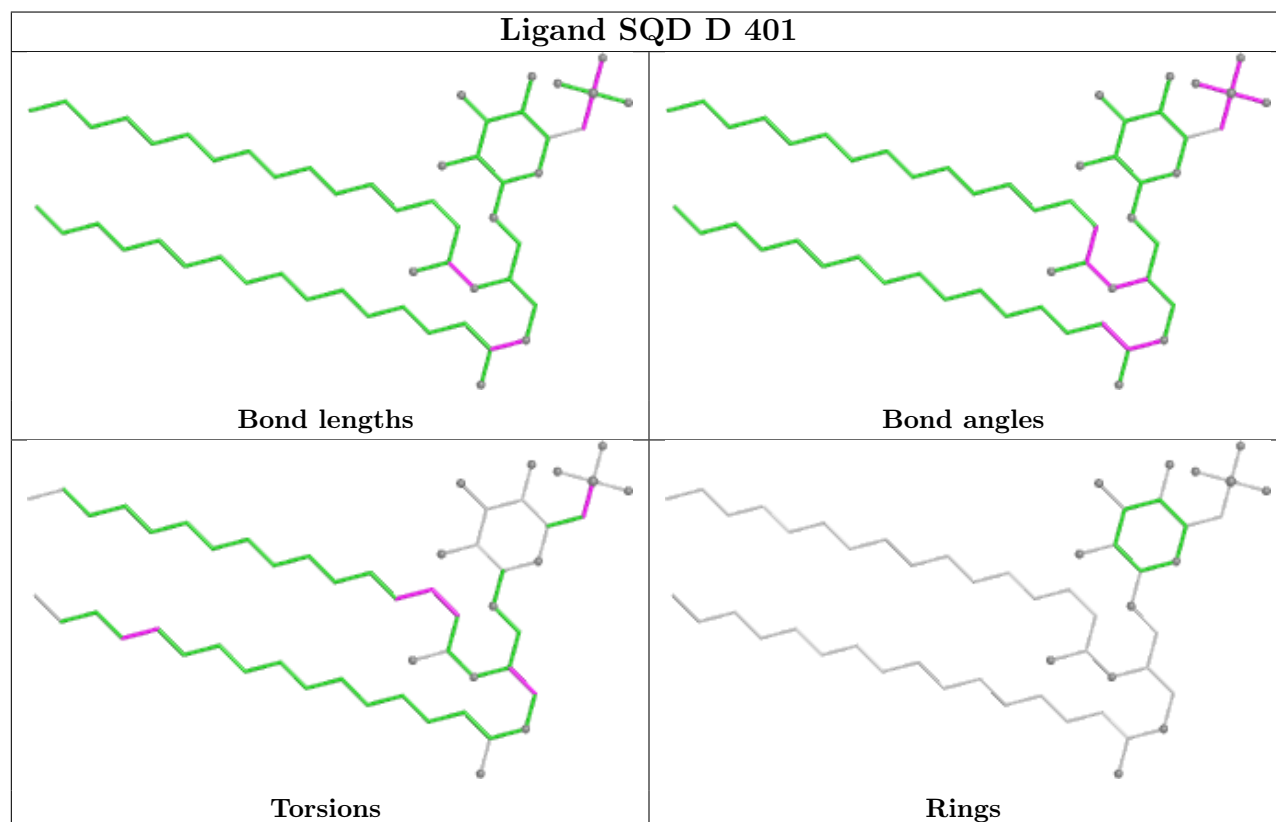
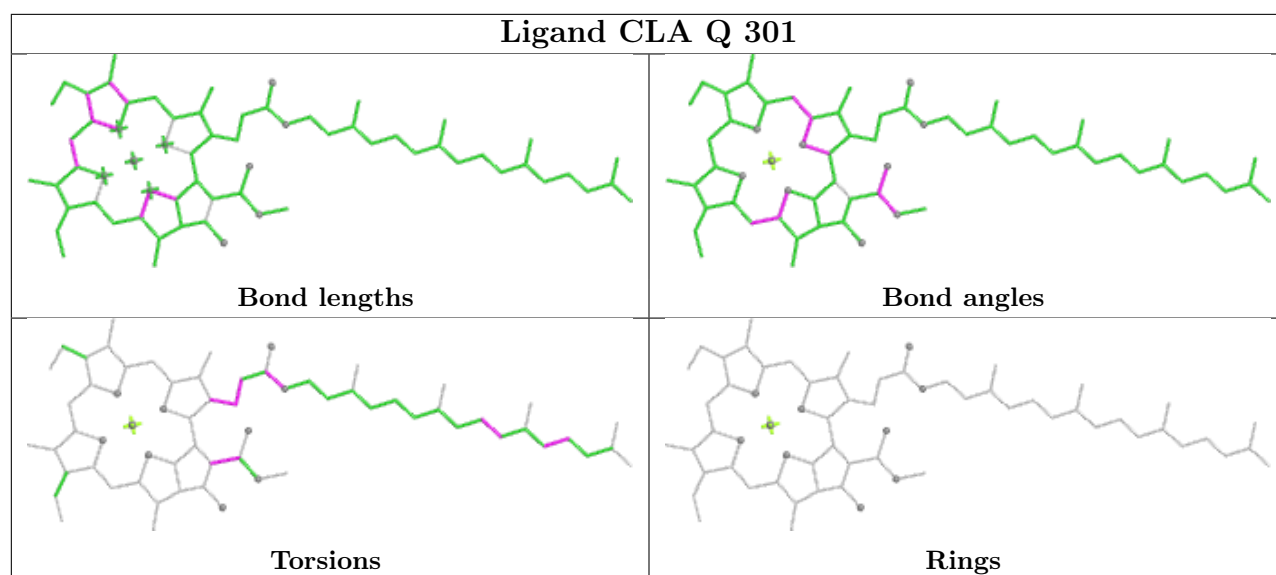
Ligand II0 4 320	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 1 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

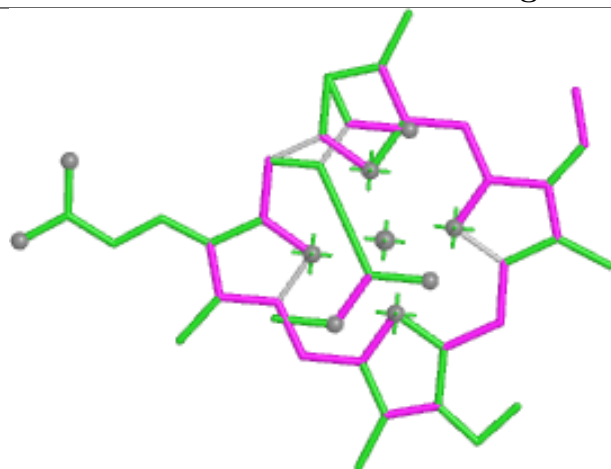




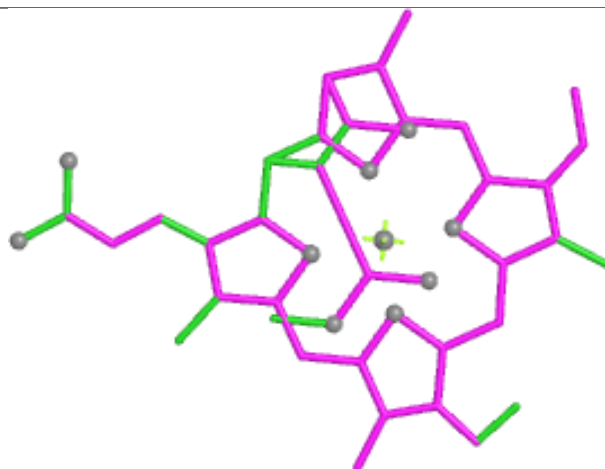




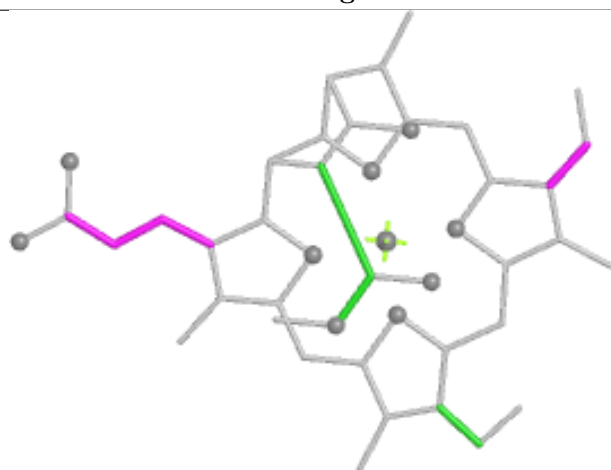
Ligand KC2 2 310



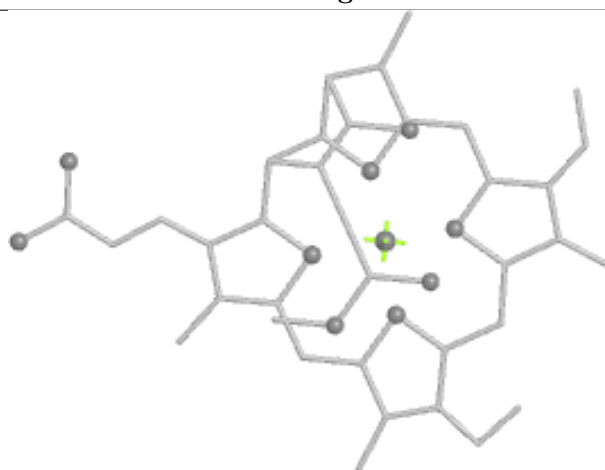
Bond lengths



Bond angles

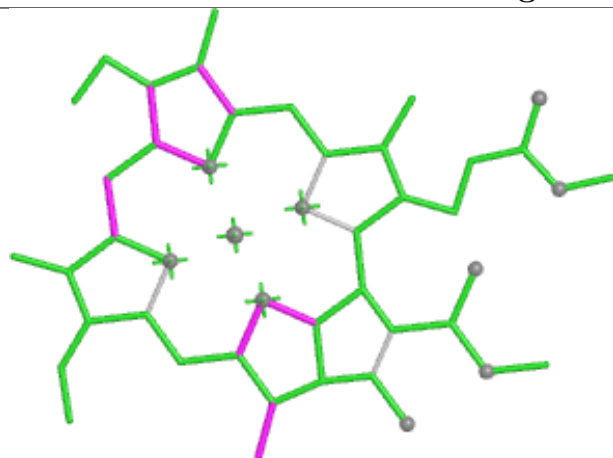


Torsions

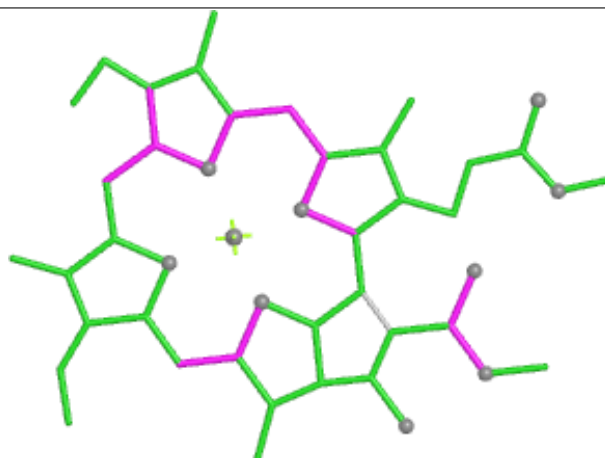


Rings

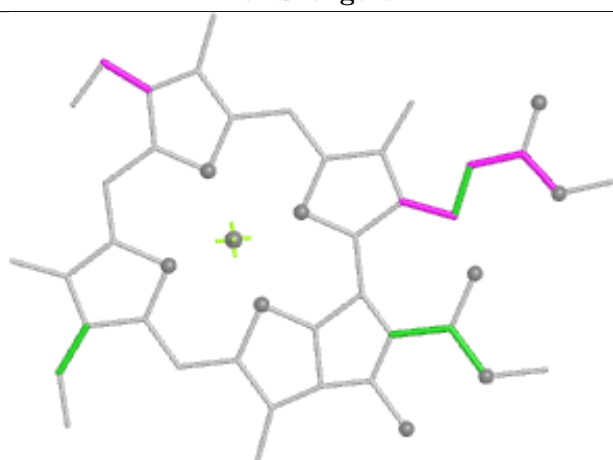
Ligand CLA 5 612



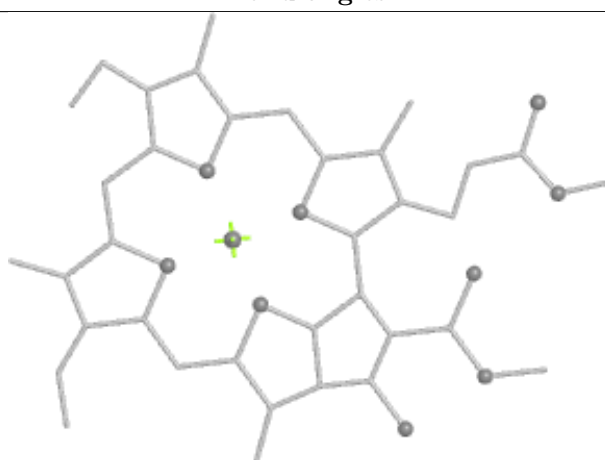
Bond lengths



Bond angles

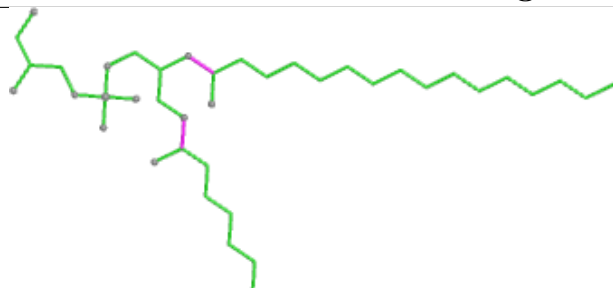


Torsions

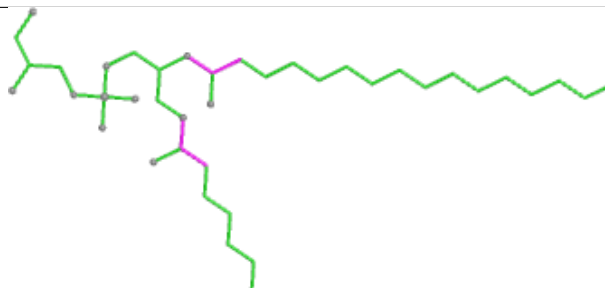


Rings

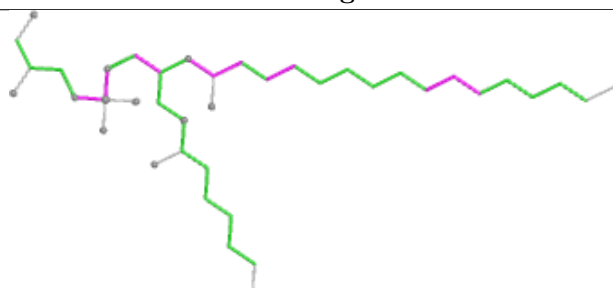
Ligand LHG 5 618



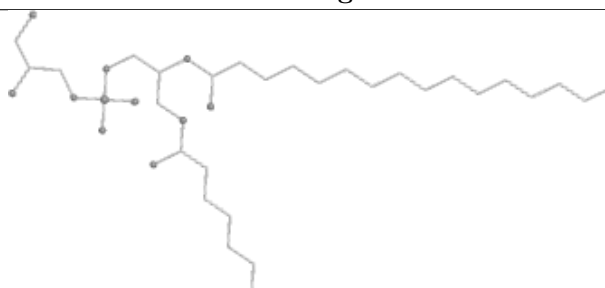
Bond lengths



Bond angles

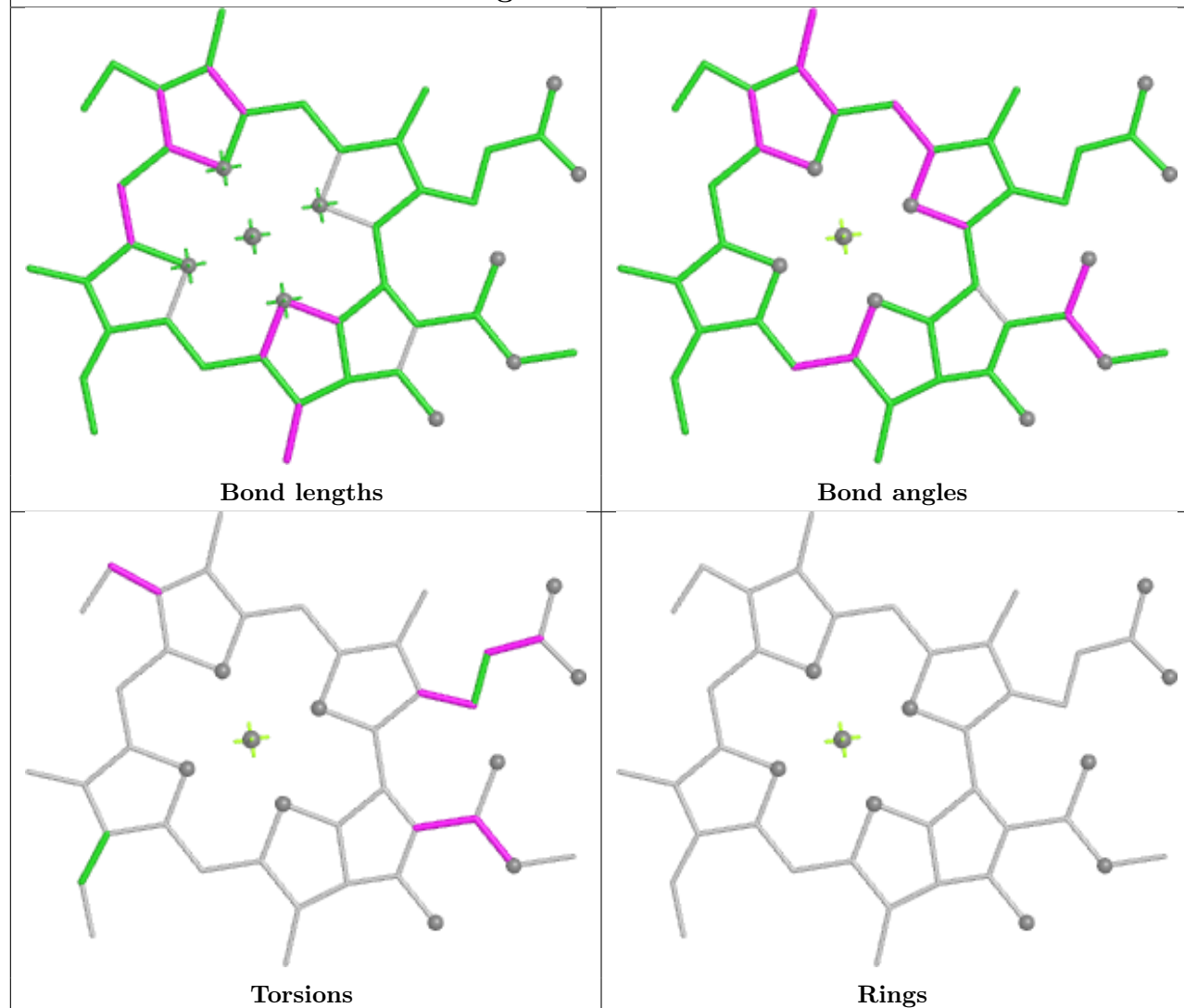


Torsions

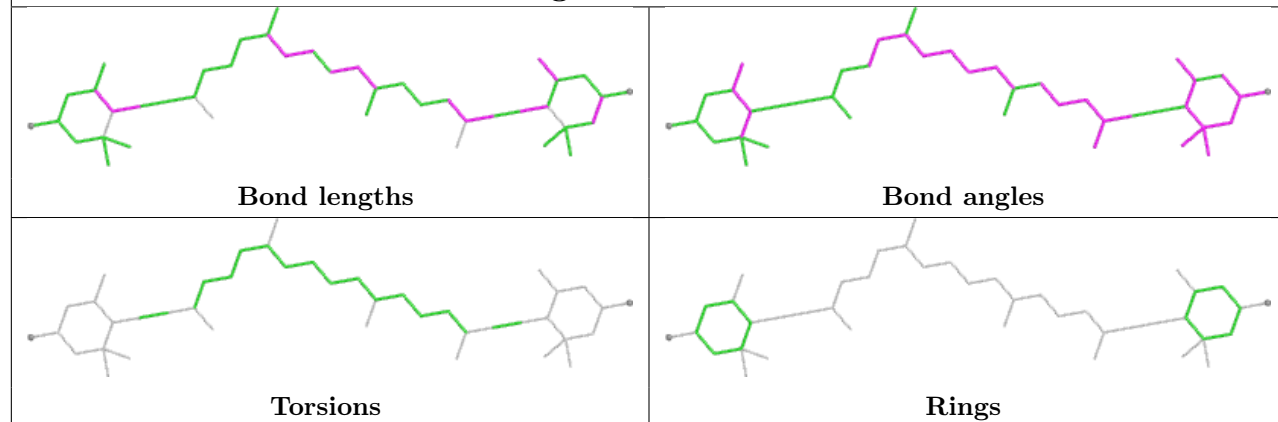


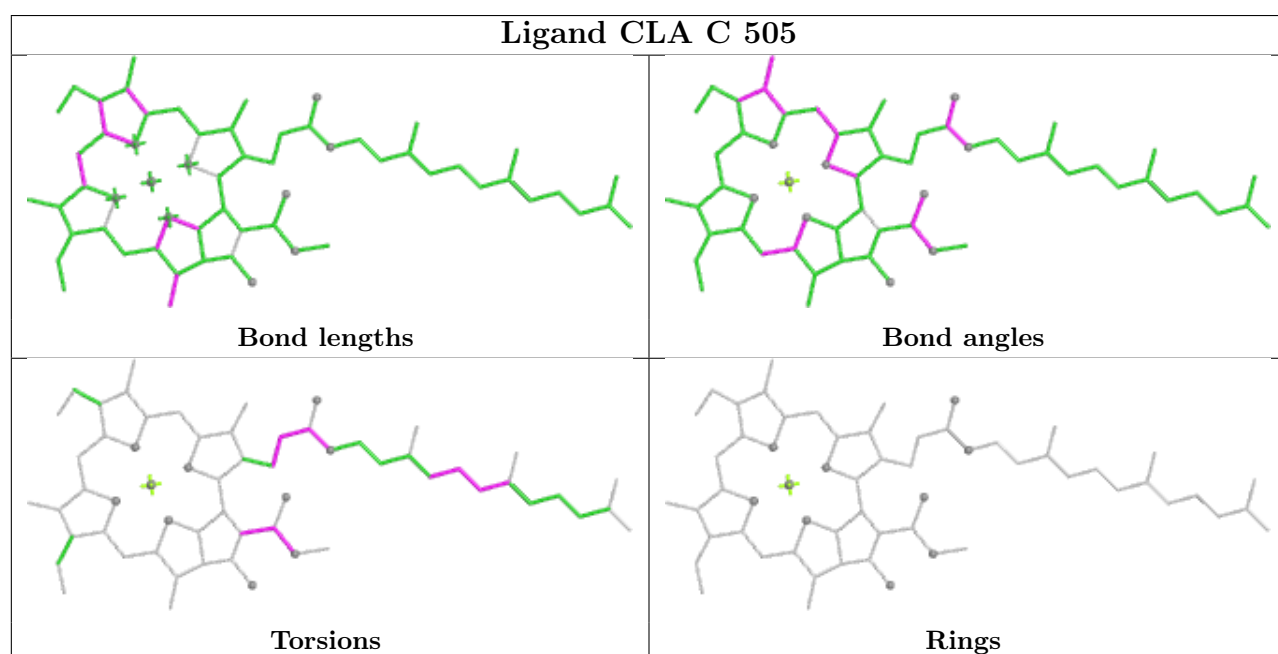
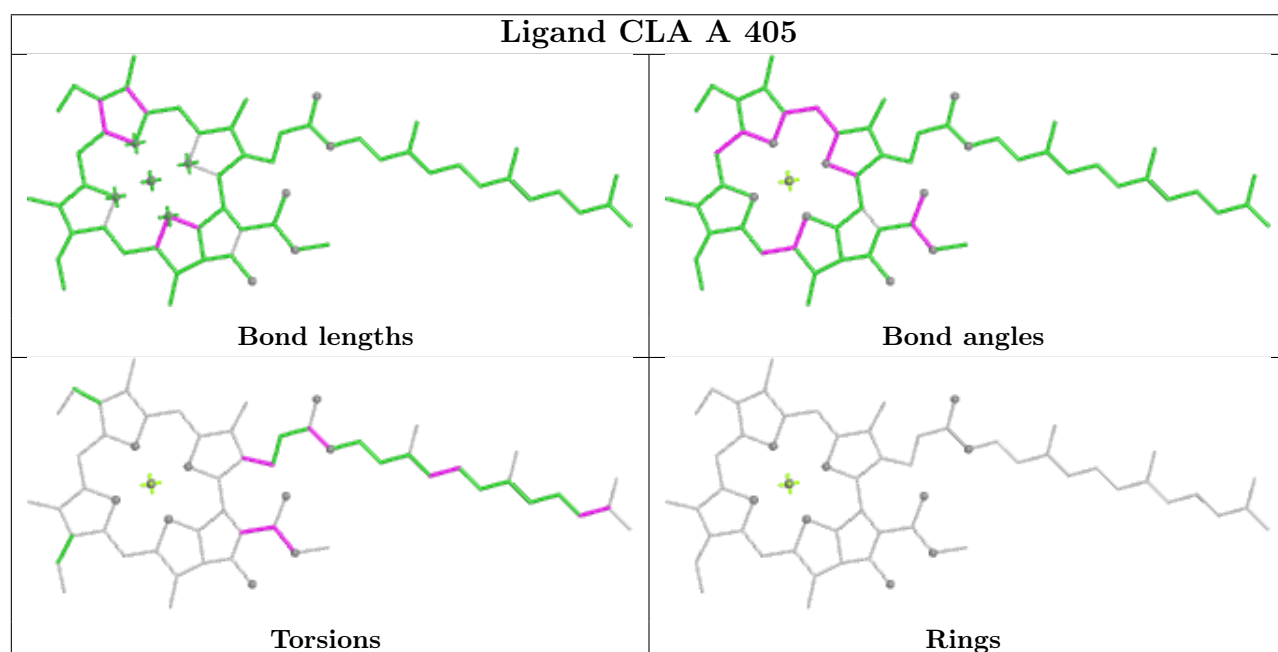
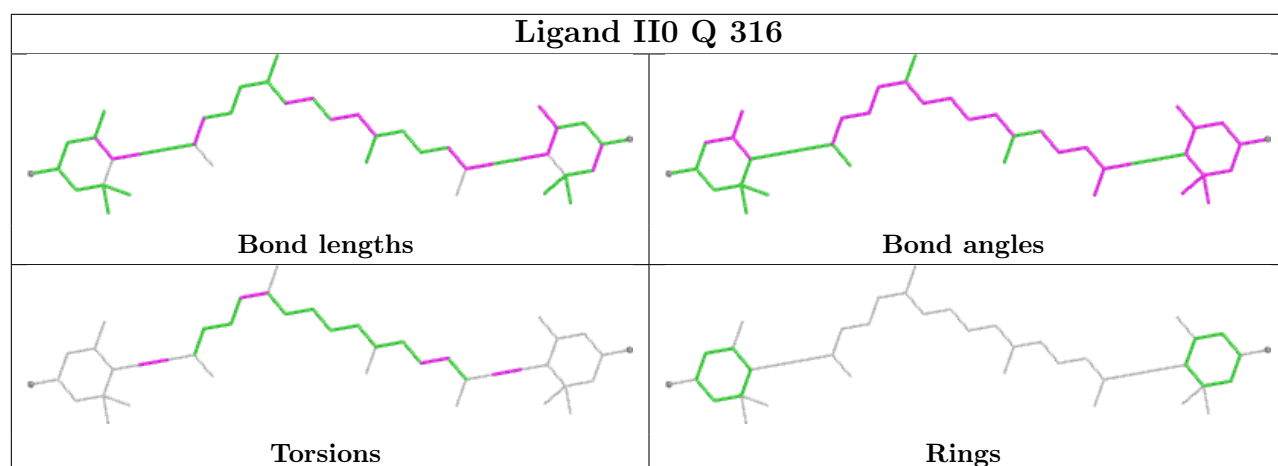
Rings

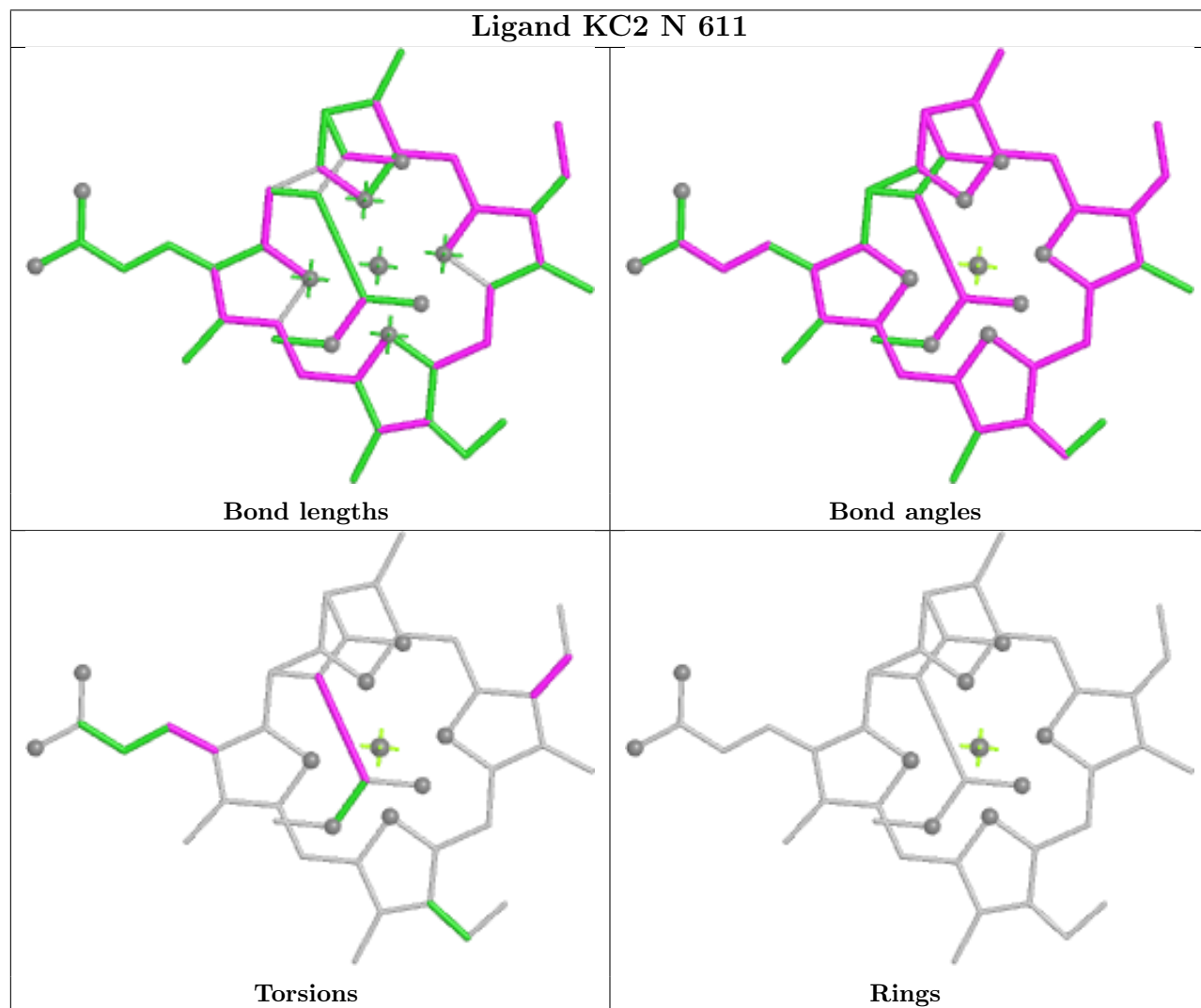
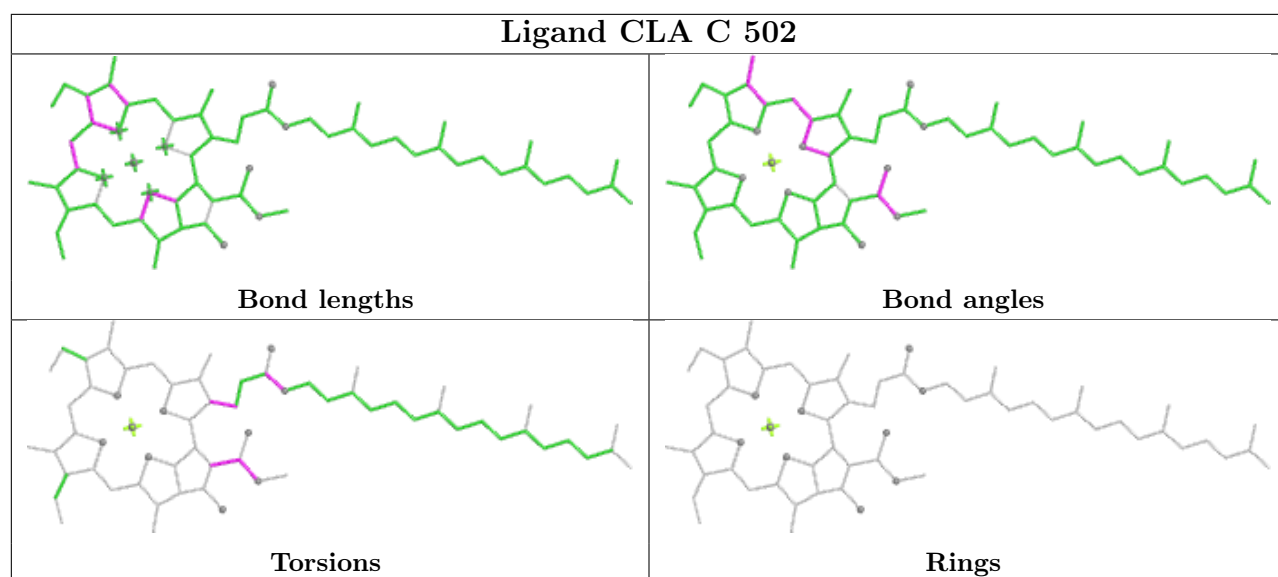
Ligand CLA 2 312

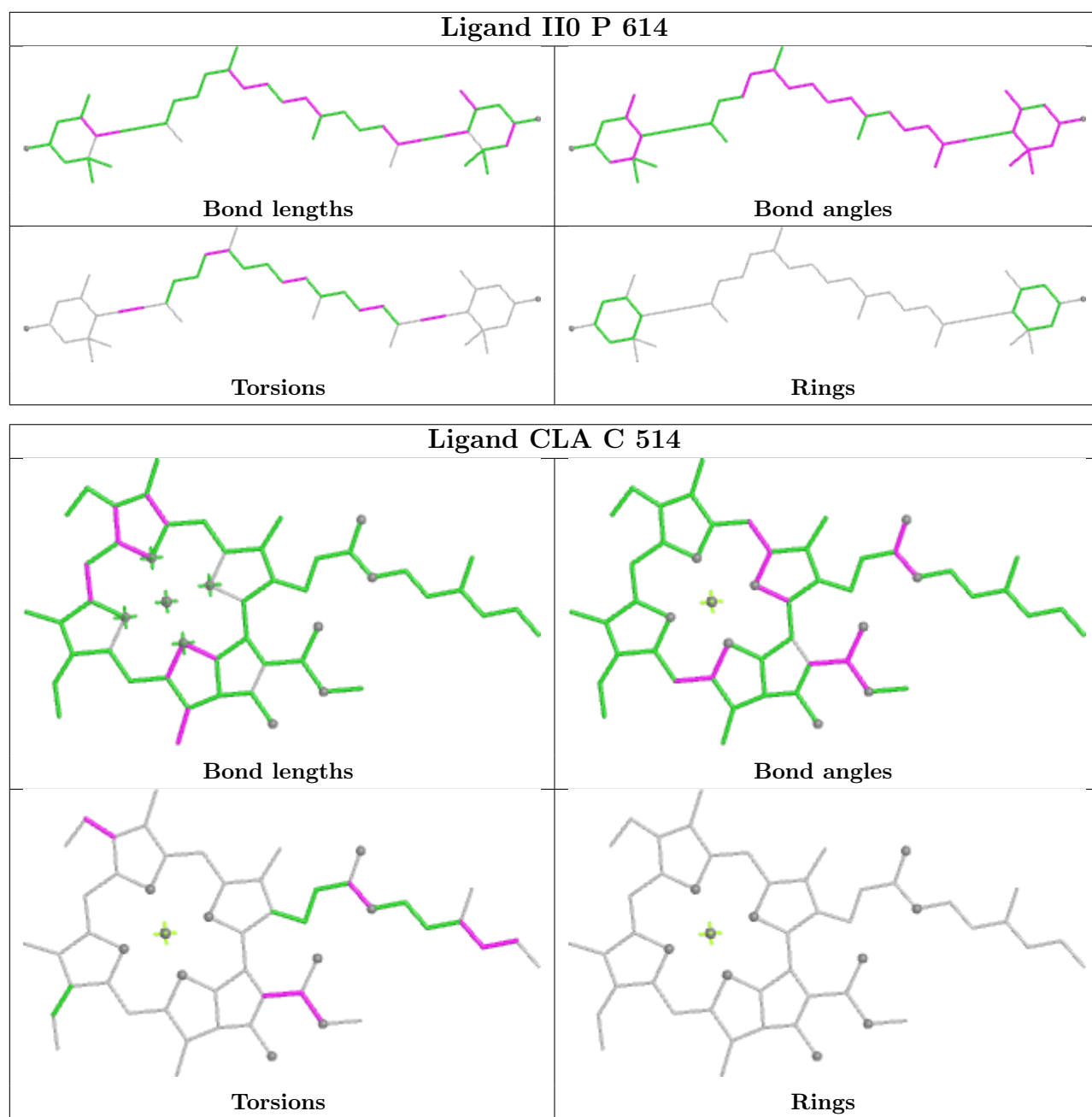


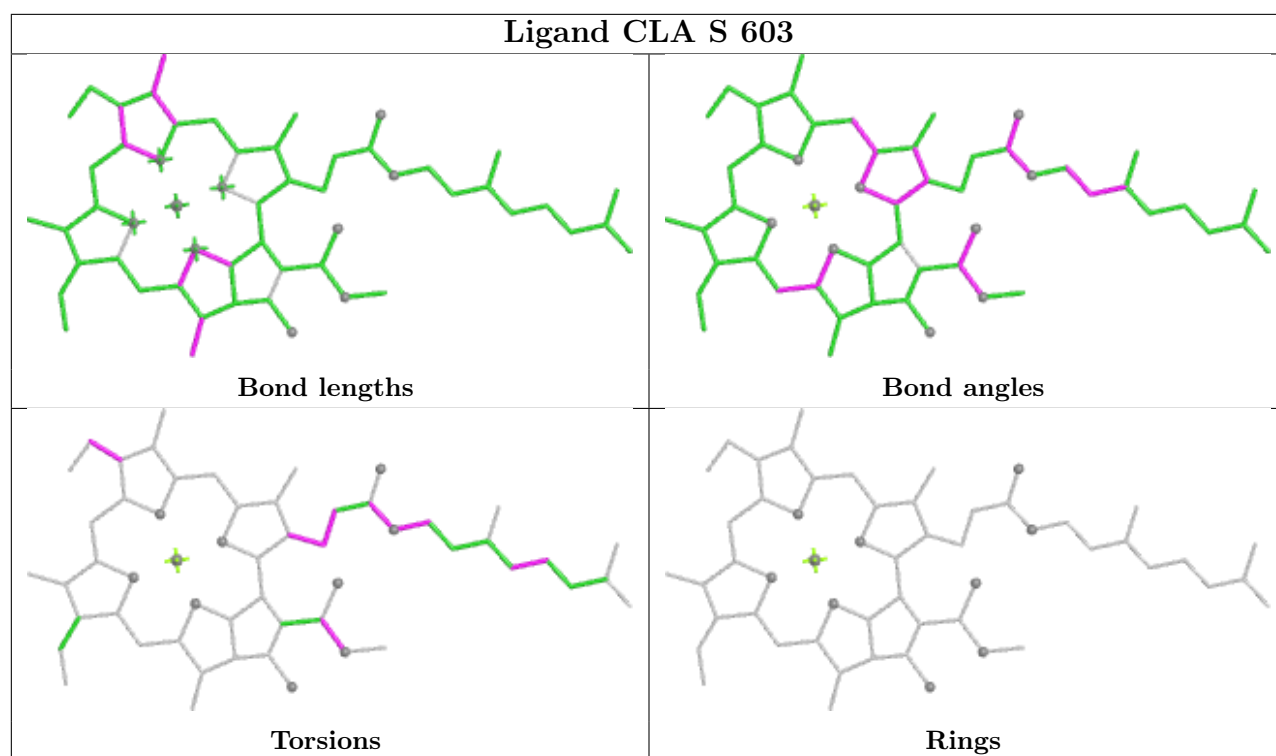
Ligand II0 5 613











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.

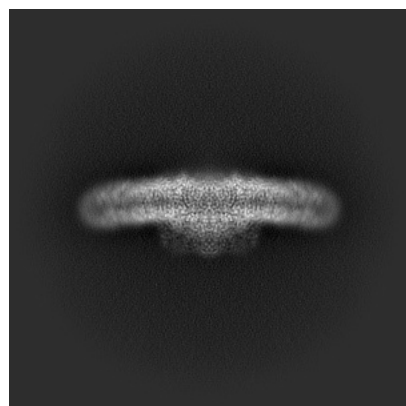
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62846. These allow visual inspection of the internal detail of the map and identification of artifacts.

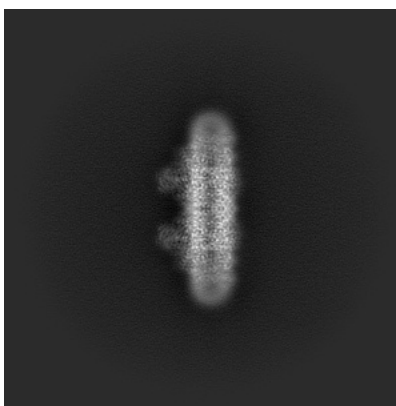
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

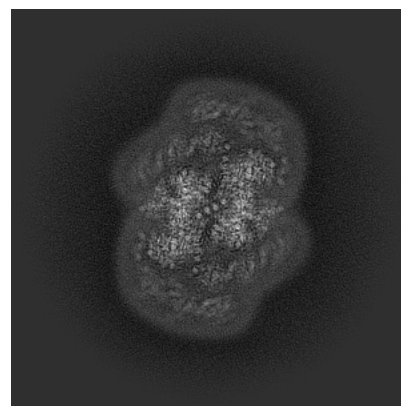
6.1.1 Primary map



X

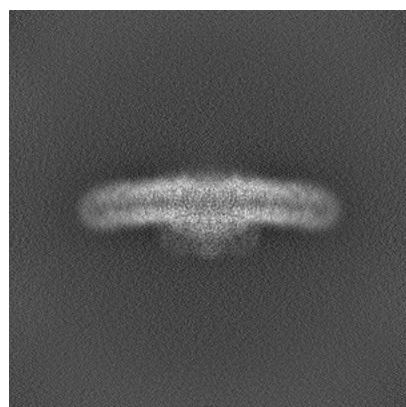


Y

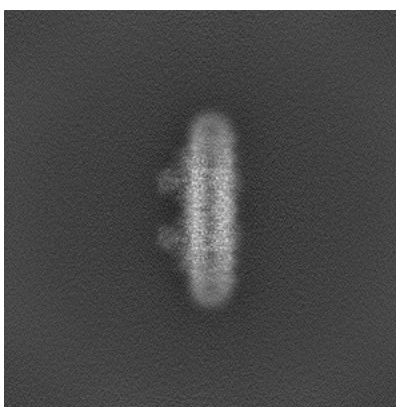


Z

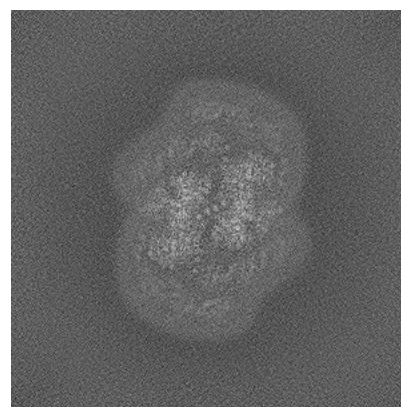
6.1.2 Raw map



X



Y

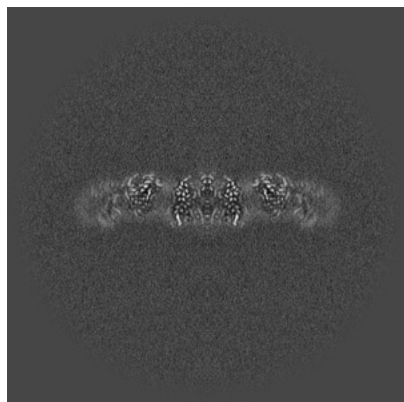


Z

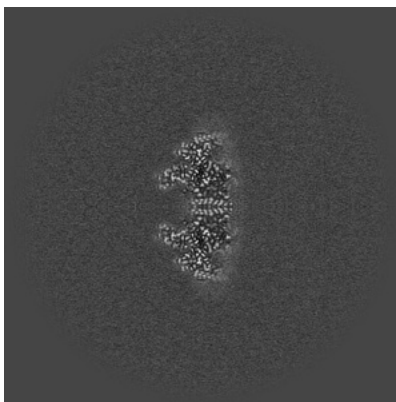
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

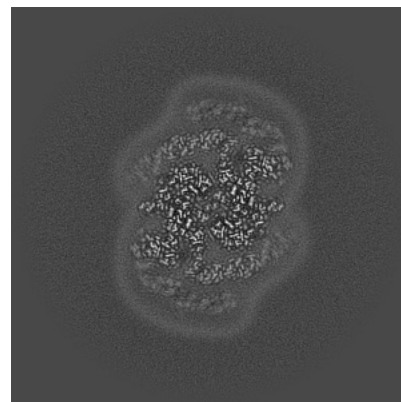
6.2.1 Primary map



X Index: 300

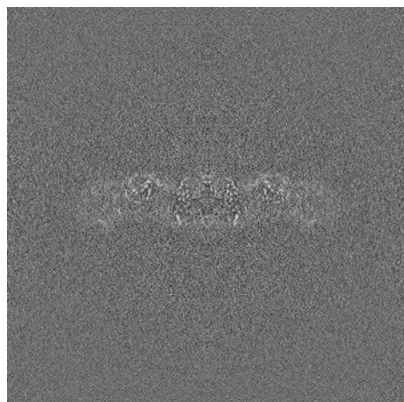


Y Index: 300

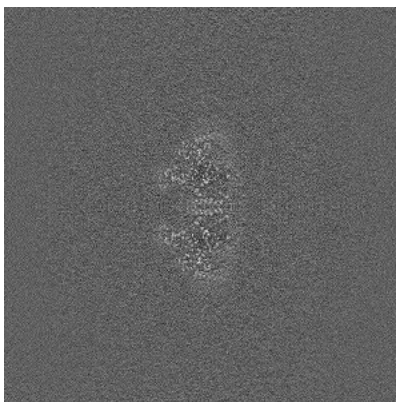


Z Index: 300

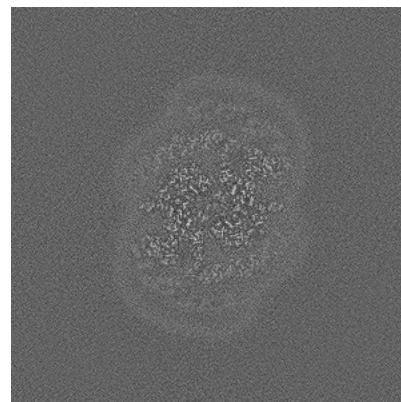
6.2.2 Raw map



X Index: 300



Y Index: 300

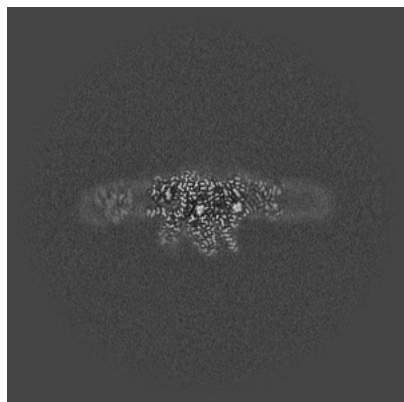


Z Index: 300

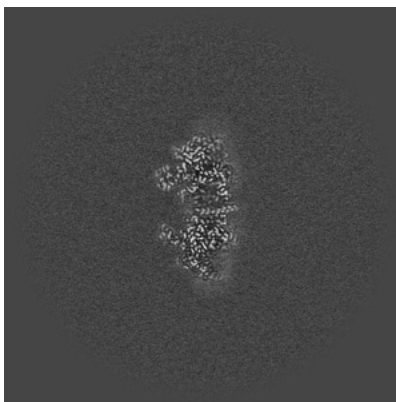
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

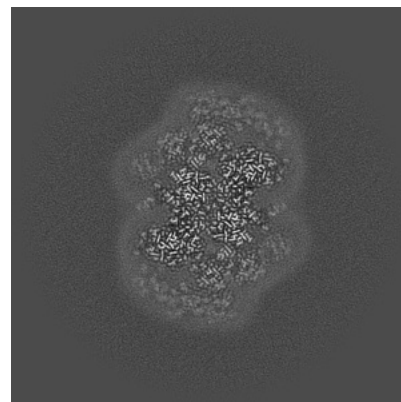
6.3.1 Primary map



X Index: 254

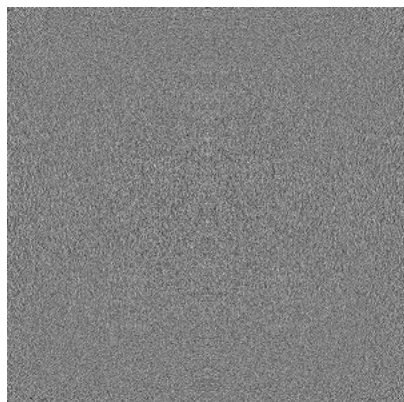


Y Index: 296

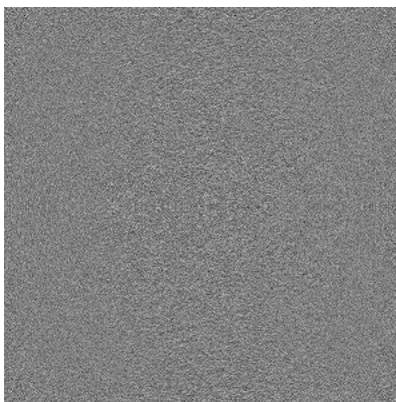


Z Index: 324

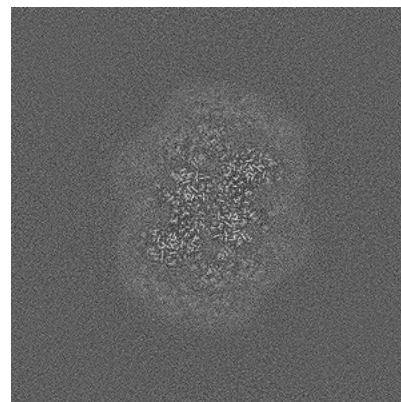
6.3.2 Raw map



X Index: 0



Y Index: 0

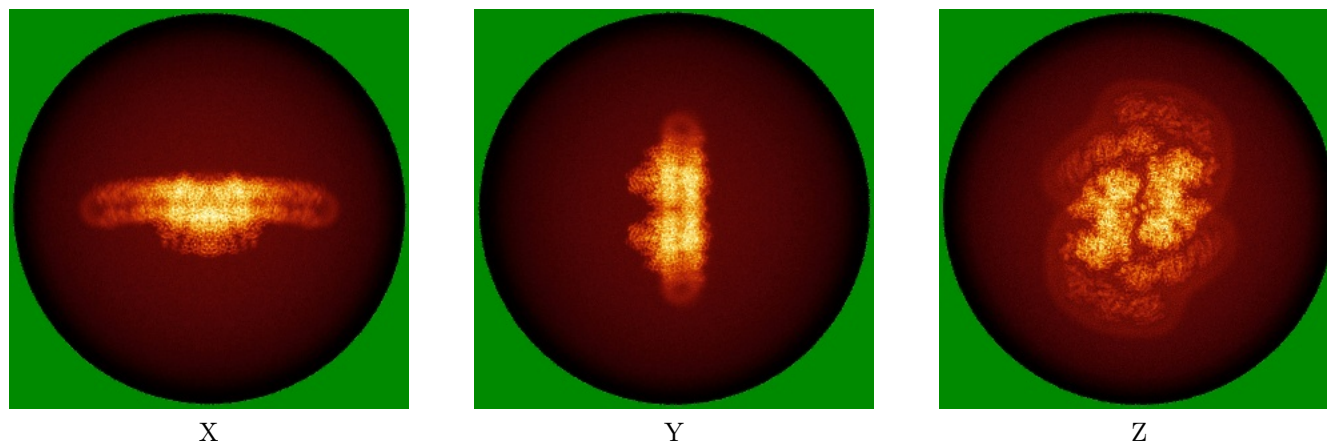


Z Index: 324

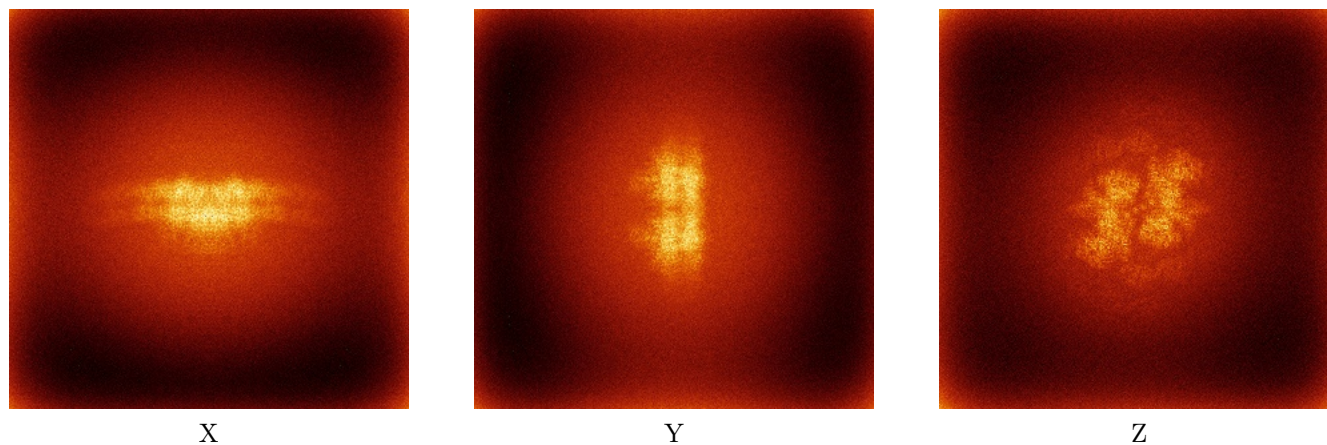
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



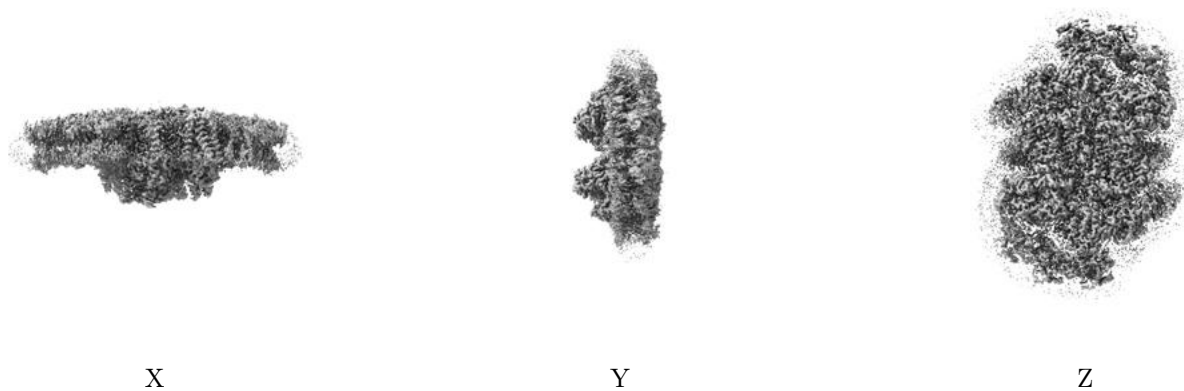
6.4.2 Raw map



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

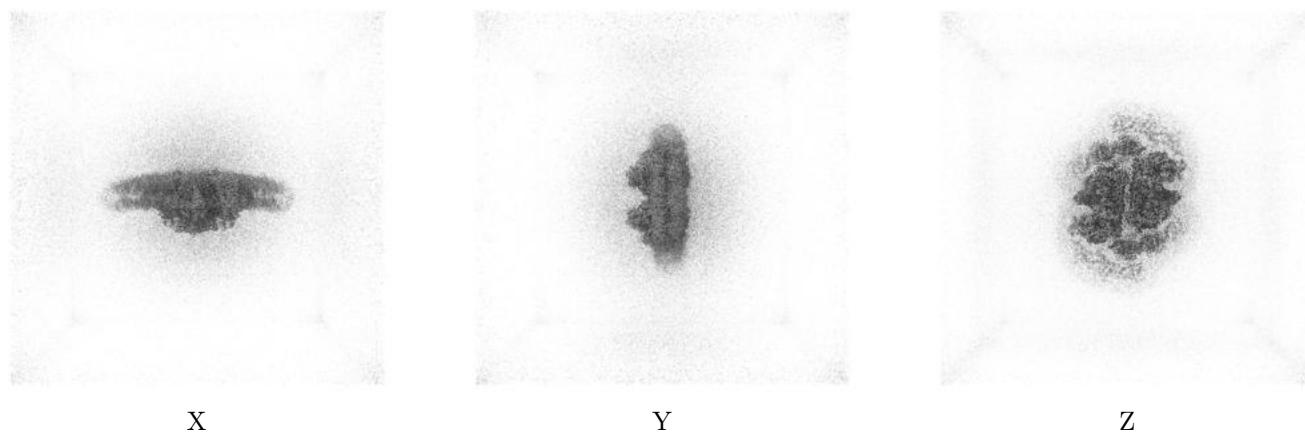
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

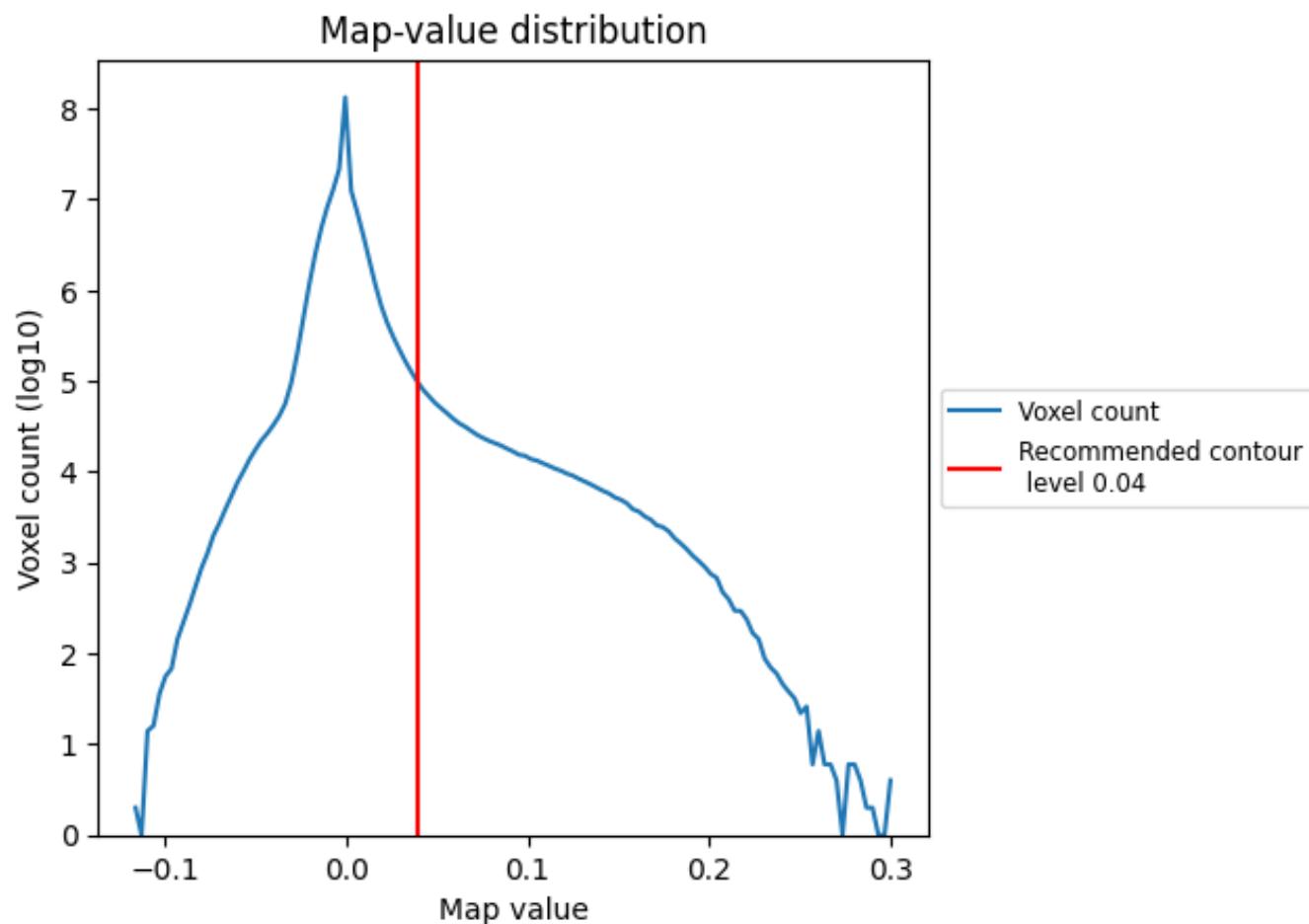
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

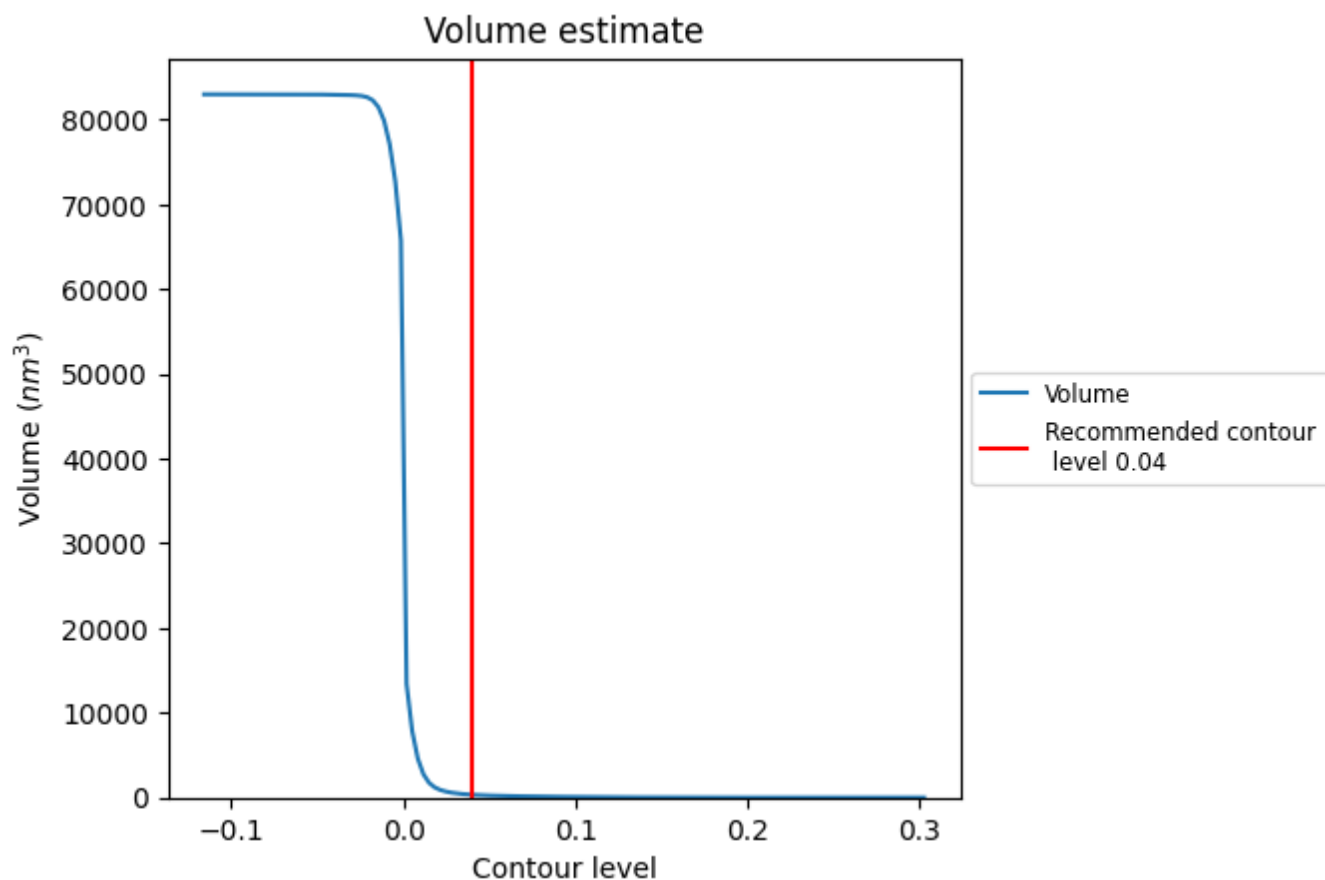
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

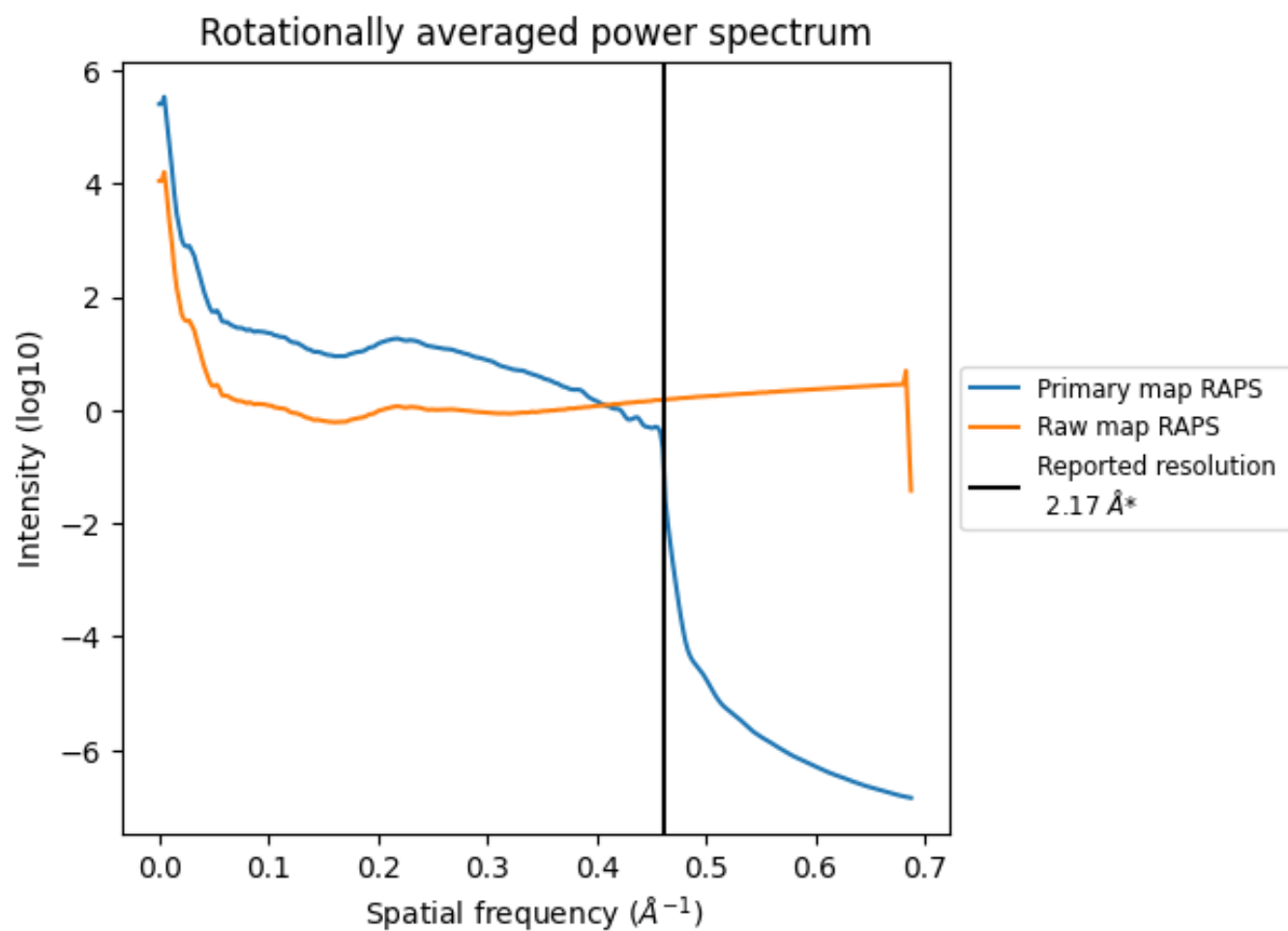
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm^3 ; this corresponds to an approximate mass of 300 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 ⓘ

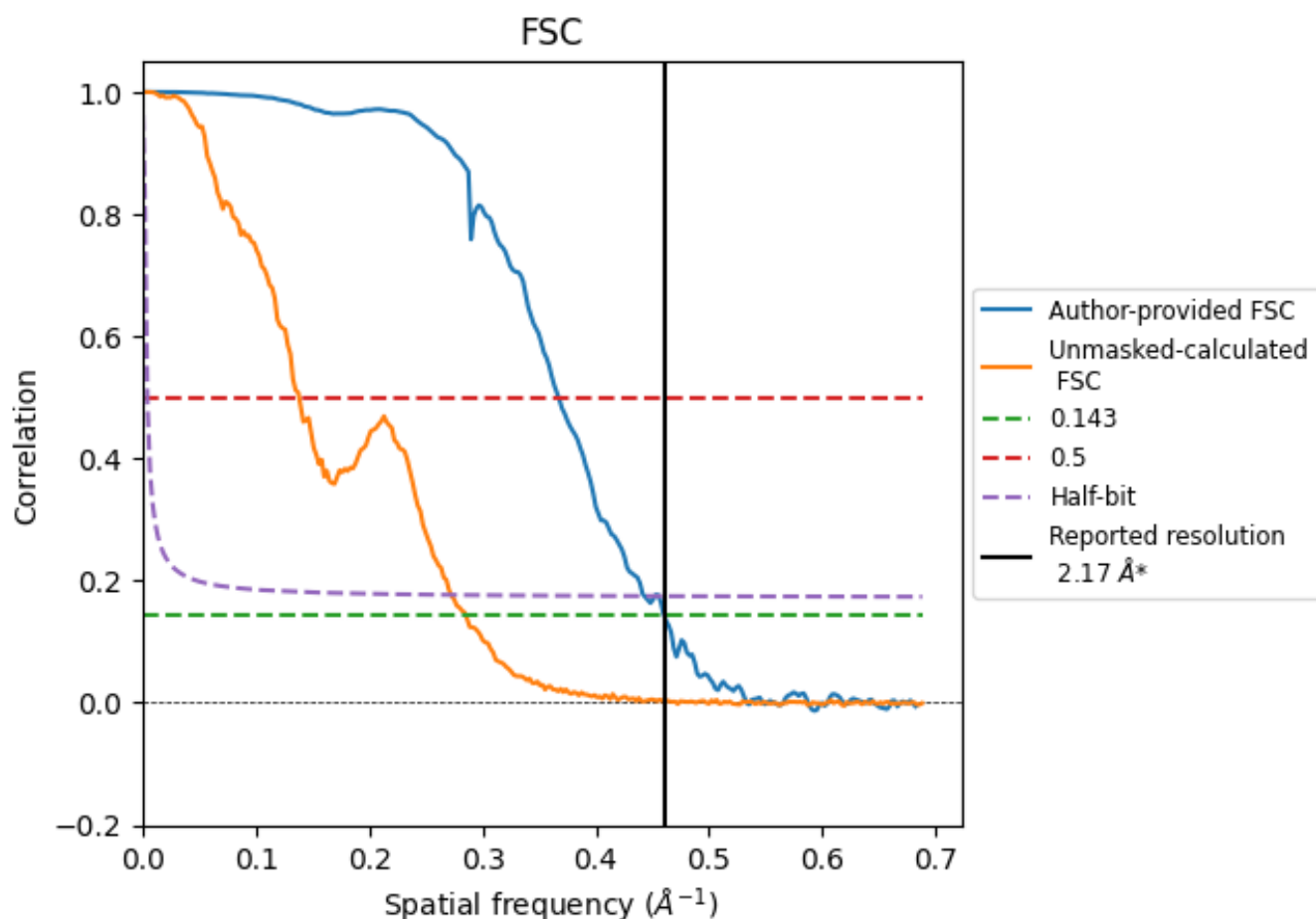


*Reported resolution corresponds to spatial frequency of 0.461 $\text{\AA}^{-1}$

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 $0.461 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

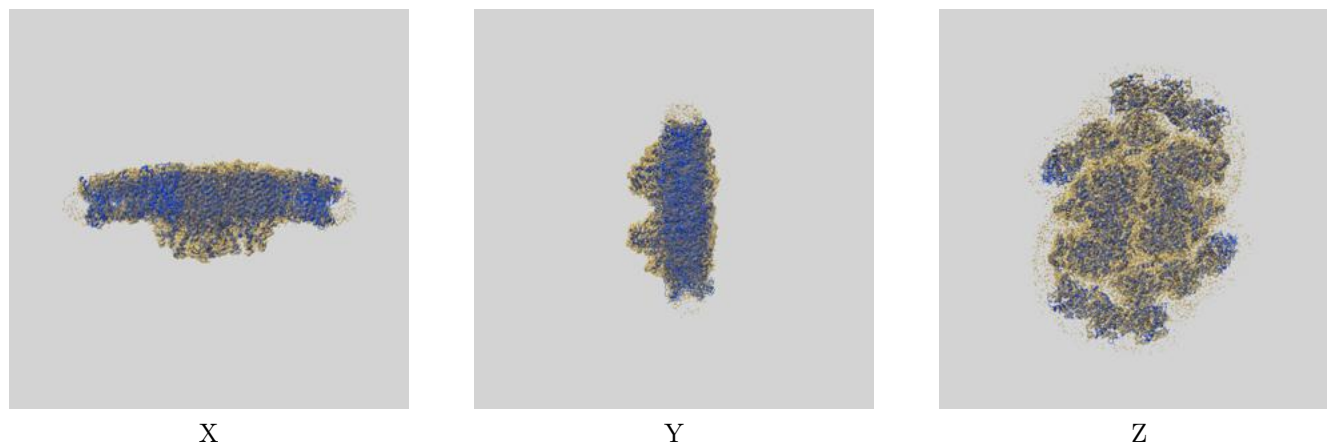
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	2.17	2.72	2.26
Unmasked-calculated*	3.51	7.23	3.67

*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 3.51 differs from the reported value 2.17 by more than 10 %

9 Map-model fit [i](#)

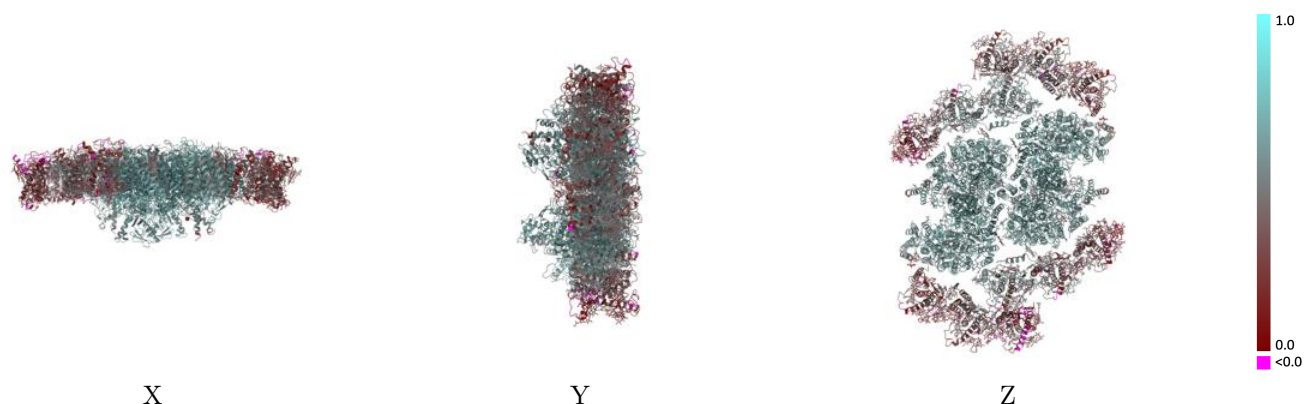
This section contains information regarding the fit between EMDB map EMD-62846 and PDB model 9L5V. Per-residue inclusion information can be found in section [3](#) on page [37](#).

9.1 Map-model overlay [i](#)



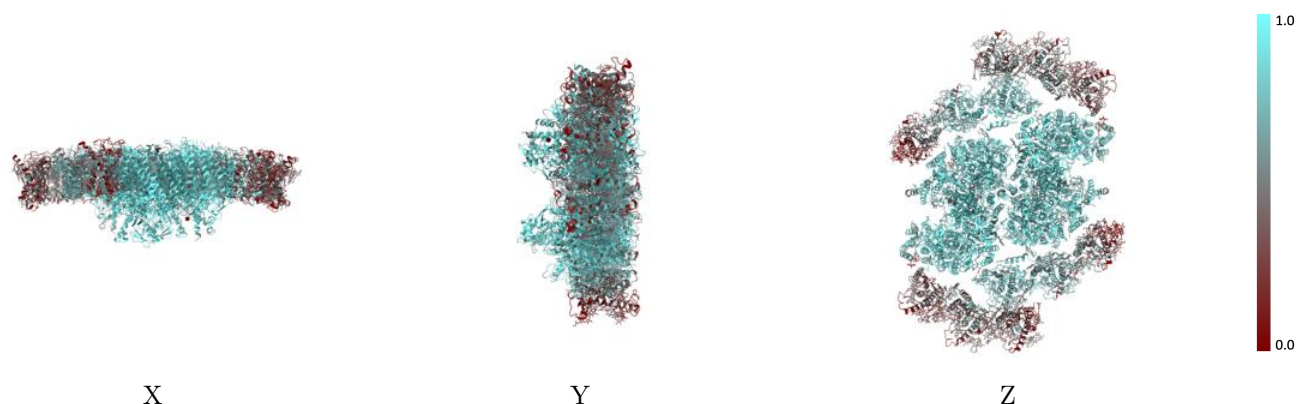
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



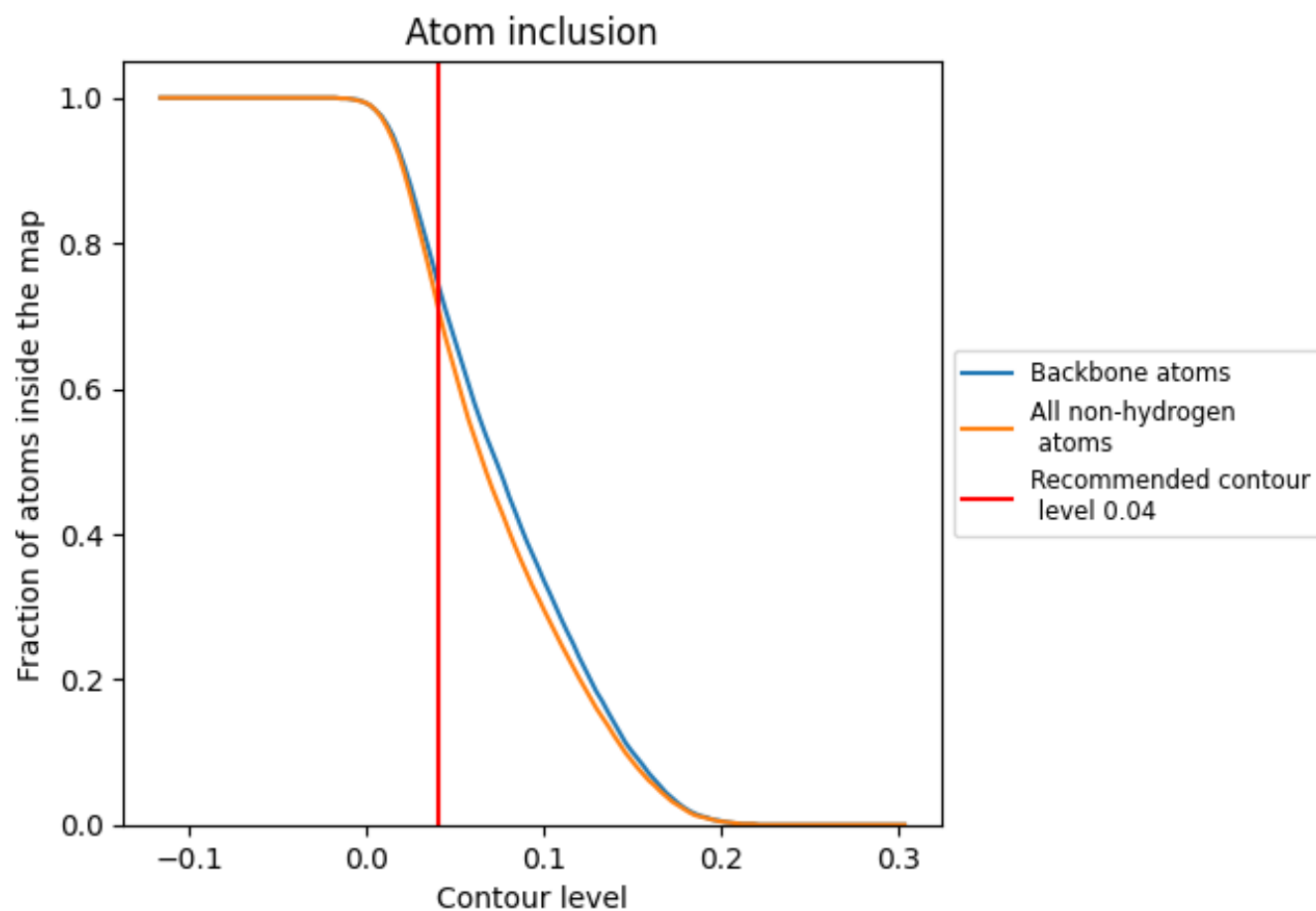
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.5040
1	 0.2870	 0.2650
2	 0.6190	 0.3710
3	 0.7070	 0.4300
4	 0.3100	 0.2220
5	 0.3450	 0.2950
6	 0.2880	 0.2460
A	 0.9230	 0.6450
B	 0.9300	 0.6430
C	 0.8890	 0.6090
D	 0.9250	 0.6420
E	 0.7920	 0.5590
F	 0.7880	 0.5400
G	 0.6010	 0.4290
H	 0.9420	 0.6420
I	 0.9710	 0.6660
K	 0.8900	 0.6090
L	 0.9480	 0.6420
M	 0.8310	 0.6070
N	 0.2850	 0.2380
O	 0.7210	 0.4800
P	 0.7860	 0.5300
Q	 0.4000	 0.3430
R	 0.3820	 0.3370
S	 0.2910	 0.2520
T	 0.8830	 0.6370
W	 0.9120	 0.6400
X	 0.8830	 0.6240
Y	 0.6410	 0.5270
Z	 0.6820	 0.5240
a	 0.9040	 0.6330
b	 0.9240	 0.6350
c	 0.8840	 0.6080
d	 0.9310	 0.6470
e	 0.7980	 0.5510



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Chain	Atom inclusion	Q-score
f	 0.7860	 0.5430
g	 0.5930	 0.3990
h	 0.9230	 0.6210
i	 0.9790	 0.6720
k	 0.8550	 0.6000
l	 0.9650	 0.6580
m	 0.8250	 0.6040
t	 0.8910	 0.6410
w	 0.9290	 0.6520
x	 0.8750	 0.6250
y	 0.6540	 0.5320
z	 0.6410	 0.4730