



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 07:06 PM JST

PDB ID : 7D1T / pdb_00007d1t
EMDB ID : EMD-30547
Title : Cryo-EM Structure of PSII at 1.95 angstrom resolution
Authors : Kato, K.; Miyazaki, N.; Hamaguchi, T.; Nakajima, Y.; Akita, F.; Yonekura, K.; Shen, J.R.
Deposited on : 2020-09-15
Resolution : 1.95 Å(reported)
Based on initial model : 3WU2

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:

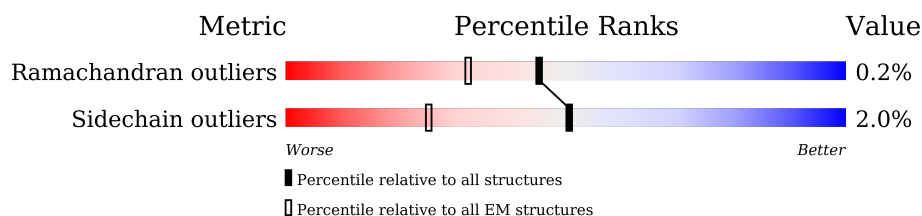
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance

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

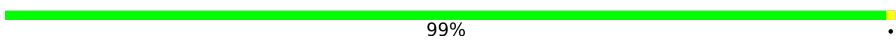
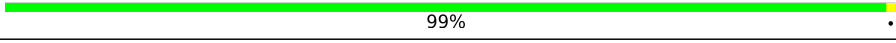
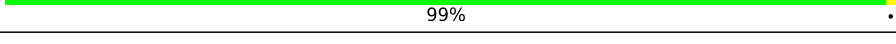
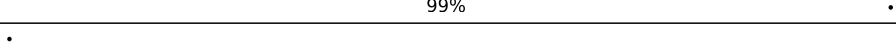
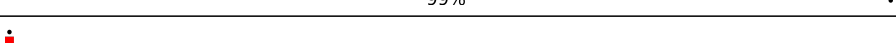




The reported resolution of this entry is 1.95 Å.

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.



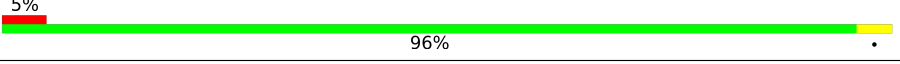
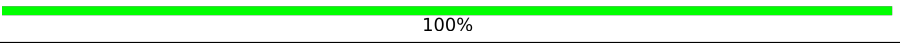
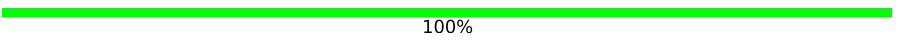
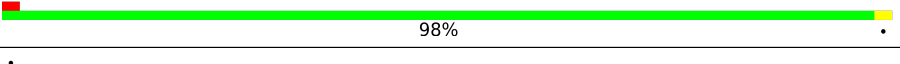
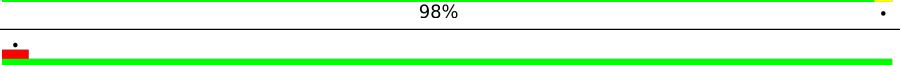
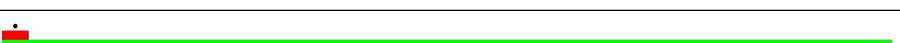
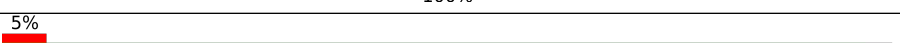
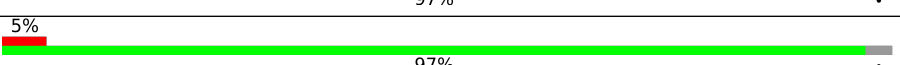
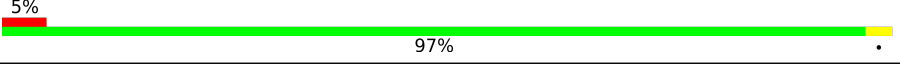
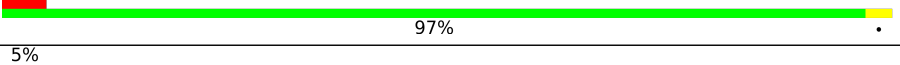
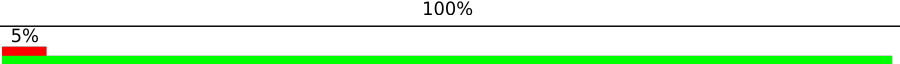

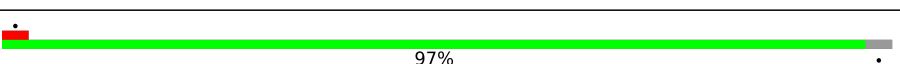
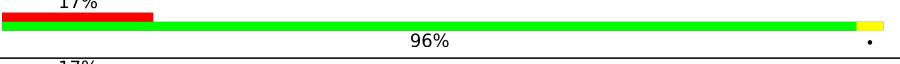
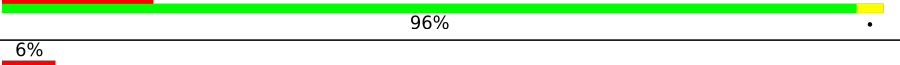

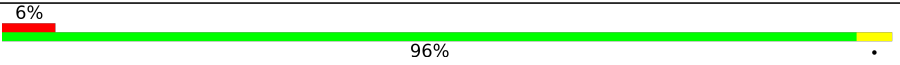
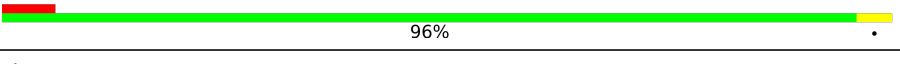
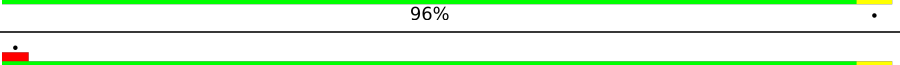
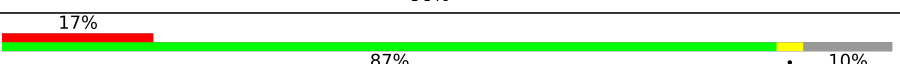




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	334	 99% .
1	a	334	 99% .
2	B	505	 99% .
2	b	505	 99% .
3	C	451	 99% .
3	c	451	 99% .
4	D	342	 98% .
4	d	342	 98% .
5	E	81	 5% 96% .


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Mol	Chain	Length	Quality of chain
5	e	81	
6	F	34	
6	f	34	
7	H	63	
7	h	63	
8	I	36	
8	i	36	
9	J	37	
9	j	37	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	244	
13	o	244	
14	T	31	
14	t	31	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	

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Mol	Chain	Length	Quality of chain
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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
24	CLA	A	405	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	514	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	405	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	611	X	-	-	-
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24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	404	X	-	-	-
33	BCT	D	403	-	X	-	-
33	BCT	d	403	-	X	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 52994 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	334	Total	C	N	O	S	2	0
			2634	1725	433	461	15		
1	a	334	Total	C	N	O	S	2	0
			2634	1725	433	461	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	0	0
			3969	2605	661	690	13		
2	b	504	Total	C	N	O	S	0	0
			3969	2605	661	690	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3486	2281	584	608	13		
3	c	451	Total	C	N	O	S	0	0
			3486	2281	584	608	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2718	1800	444	462	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	341	Total	C	N	O	S	0	0
			2718	1800	444	462	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	81	Total	C	N	O		0	0
			661	432	107	122			
5	e	81	Total	C	N	O		0	0
			661	432	107	122			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	34	Total	C	N	O	S	0	0
			275	187	45	42	1		
6	f	34	Total	C	N	O	S	0	0
			275	187	45	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	63	Total	C	N	O	S	0	0
			498	333	80	83	2		
7	h	63	Total	C	N	O	S	0	0
			498	333	80	83	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	36	Total	C	N	O	S	0	0
			296	200	46	49	1		
8	i	36	Total	C	N	O	S	0	0
			296	200	46	49	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	36	Total	C	N	O	S	0	0
			257	174	40	42	1		
9	j	36	Total	C	N	O	S	0	0
			257	174	40	42	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			293	204	43	46		
10	k	37	Total	C	N	O	0	0
			293	204	43	46		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	UNP P19054

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	37	Total	C	N	O	S	0	0
			304	202	48	53	1		
11	l	37	Total	C	N	O	S	0	0
			304	202	48	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	33	Total	C	N	O	S	0	0
			260	173	38	48	1		
12	m	33	Total	C	N	O	S	0	0
			260	173	38	48	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	244	Total	C	N	O	S	0	0
			1874	1170	317	383	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	o	244	Total	C	N	O	S	0	0
			1874	1170	317	383	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total	C	N	O	S	0	0
			258	181	36	39	2		
14	t	30	Total	C	N	O	S	0	0
			258	181	36	39	2		

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	97	Total	C	N	O	S	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	S	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	137	Total	C	N	O	S	0	0
			1064	675	177	208	4		
16	v	137	Total	C	N	O	S	0	0
			1064	675	177	208	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0
			200	131	35	31	3		
17	y	27	Total	C	N	O	S	0	0
			200	131	35	31	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	38	Total	C	N	O	S	0	0
			281	188	45	48			
18	x	38	Total	C	N	O	S	0	0
			281	188	45	48			

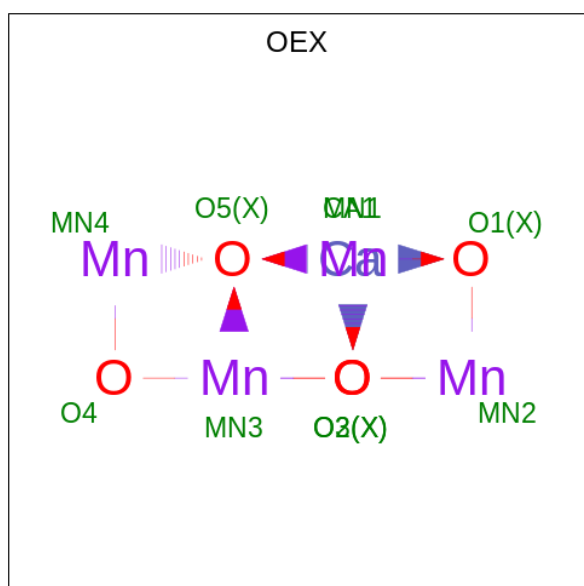
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0
			479	328	72	77	2		
19	z	62	Total	C	N	O	S	0	0
			479	328	72	77	2		

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	34	Total	C	N	O	0	0
			273	186	47	40		
20	r	34	Total	C	N	O	0	0
			273	186	47	40		

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

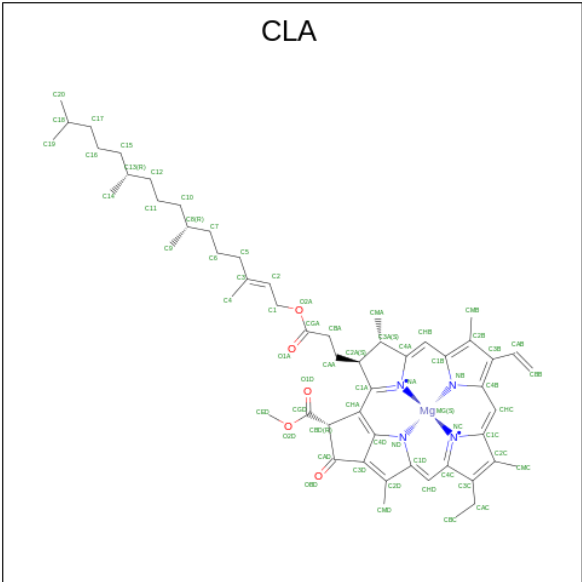
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Cl	0
			2	2	
23	a	2	Total	Cl	0
			2	2	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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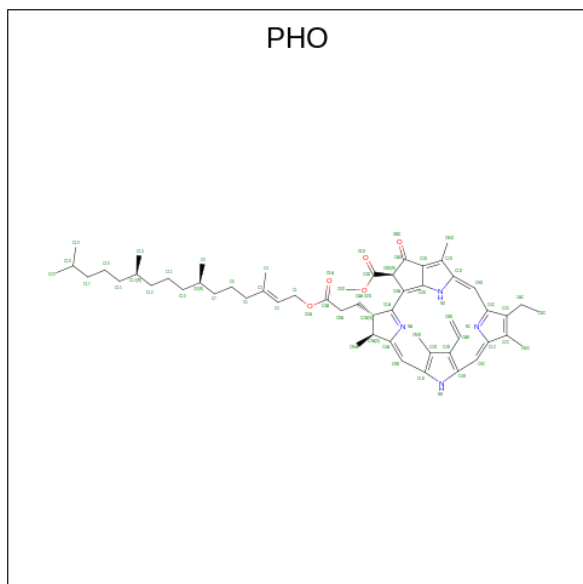
Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0

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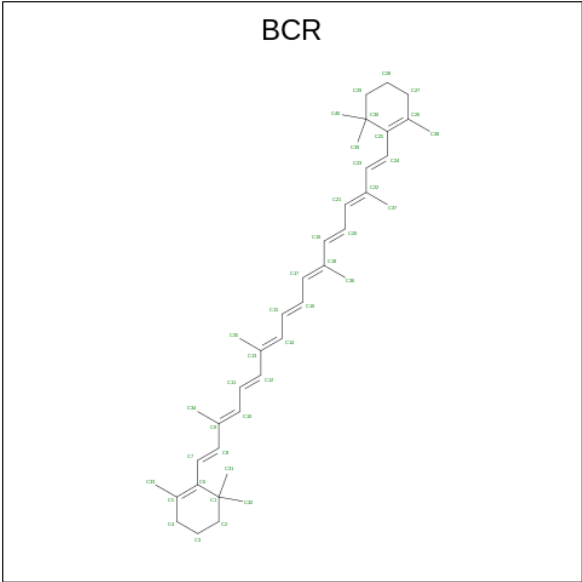
Mol	Chain	Residues	Atoms					AltConf
24	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



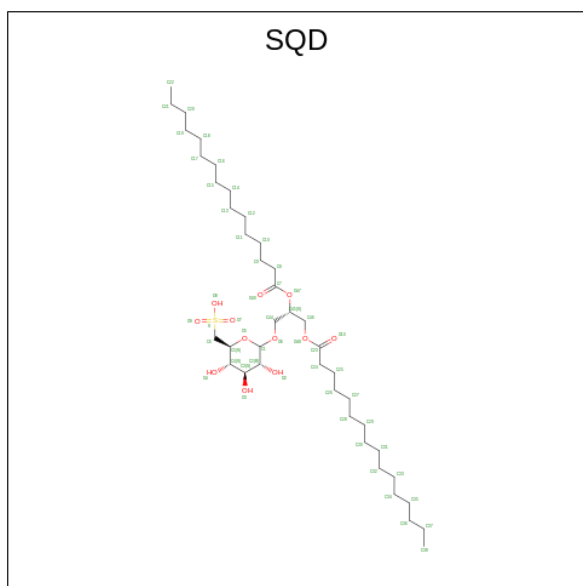
Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	C	1	Total	C	0
			40	40	
26	C	1	Total	C	0
			40	40	
26	C	1	Total	C	0
			40	40	
26	D	1	Total	C	0
			40	40	
26	J	1	Total	C	0
			40	40	
26	T	1	Total	C	0
			40	40	
26	a	1	Total	C	0
			40	40	
26	b	1	Total	C	0
			40	40	
26	b	1	Total	C	0
			40	40	
26	b	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
26	c	1	Total C 40 40	0
26	c	1	Total C 40 40	0
26	c	1	Total C 40 40	0
26	d	1	Total C 40 40	0
26	j	1	Total C 40 40	0
26	t	1	Total C 40 40	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



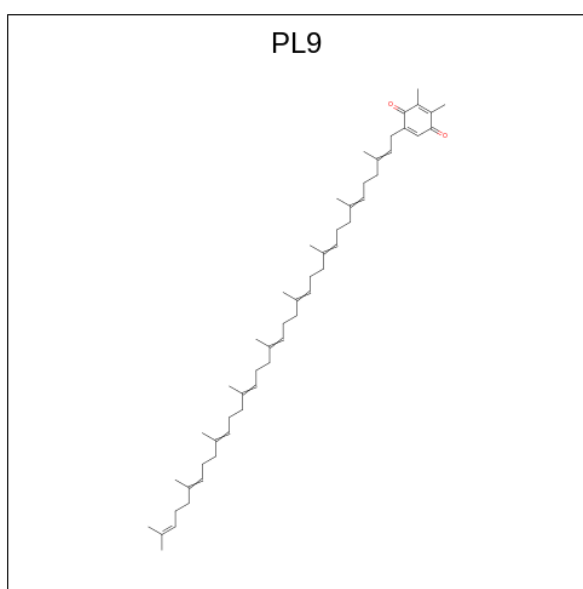
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C O S 54 41 12 1	0
27	A	1	Total C O S 54 41 12 1	0
27	B	1	Total C O S 54 41 12 1	0
27	F	1	Total C O S 45 32 12 1	0
27	L	1	Total C O S 54 41 12 1	0

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Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	C	O	S	0
			54	41	12	1	
27	a	1	Total	C	O	S	0
			54	41	12	1	
27	f	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

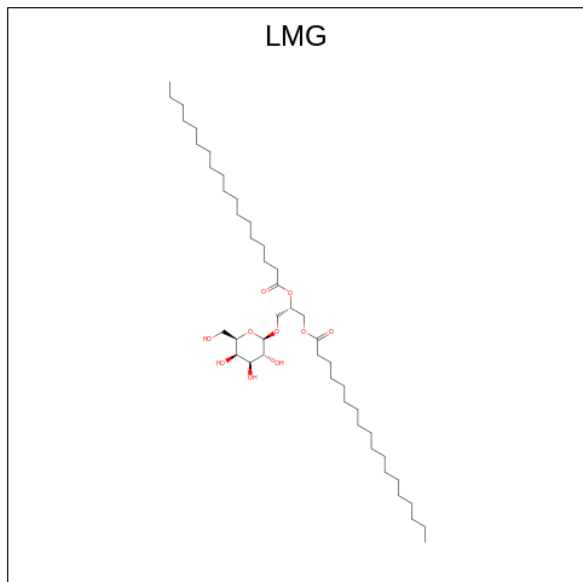
Mol	Chain	Residues	Atoms				AltConf
29	A	2	Total	C	O		0
			59	49	10		

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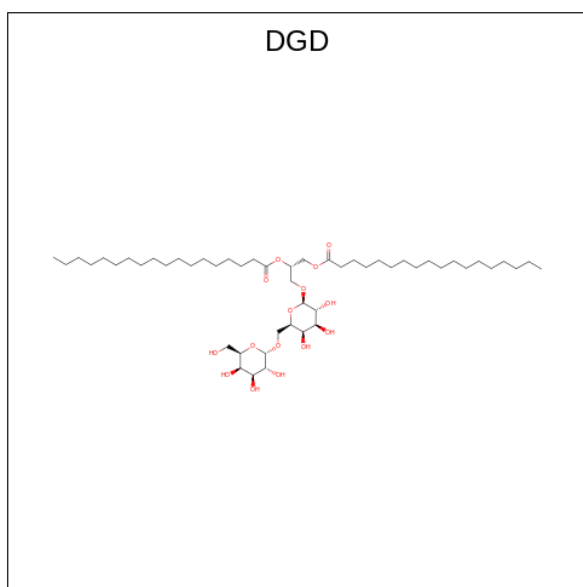
Mol	Chain	Residues	Atoms	AltConf
29	B	5	Total C 56 56	0
29	C	1	Total C 10 10	0
29	D	2	Total C O 56 51 5	0
29	E	1	Total C 10 10	0
29	I	2	Total C 17 17	0
29	J	1	Total C 10 10	0
29	K	1	Total C O 34 29 5	0
29	M	1	Total C 10 10	0
29	T	1	Total C 16 16	0
29	X	1	Total C 10 10	0
29	a	2	Total C O 59 49 10	0
29	b	5	Total C 56 56	0
29	c	1	Total C 10 10	0
29	d	2	Total C O 56 51 5	0
29	e	1	Total C 10 10	0
29	i	2	Total C 17 17	0
29	j	1	Total C 10 10	0
29	k	1	Total C O 34 29 5	0
29	m	1	Total C 10 10	0
29	t	1	Total C 16 16	0
29	x	1	Total C 10 10	0

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



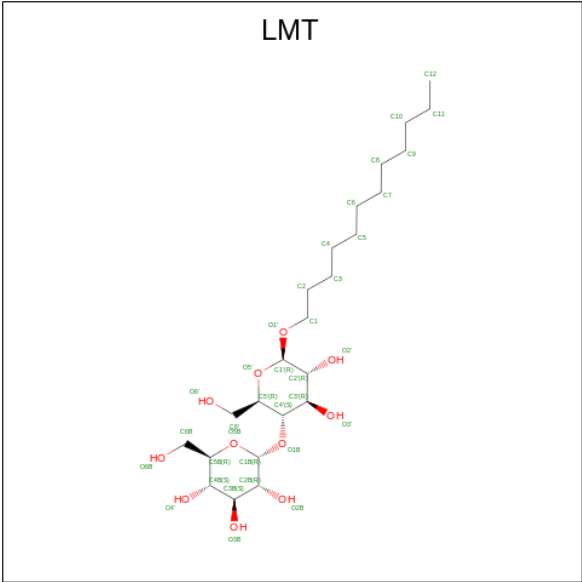
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	D	1	Total	C	O	0
			51	41	10	
30	b	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			51	41	10	
30	d	1	Total	C	O	0
			51	41	10	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



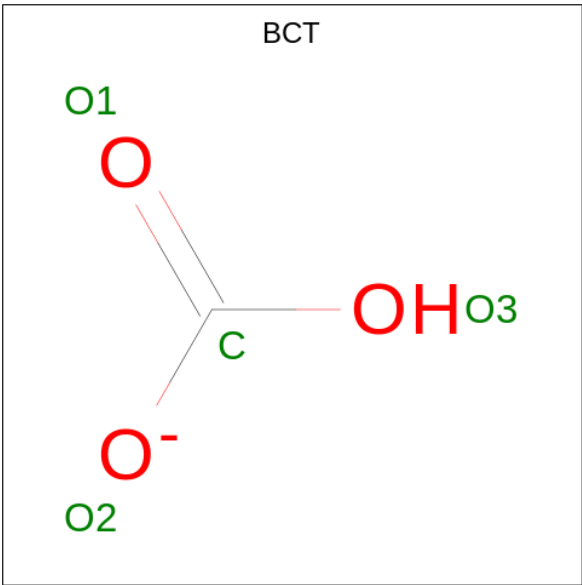
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	H	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			62	47	15	
31	h	1	Total	C	O	0
			62	47	15	

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



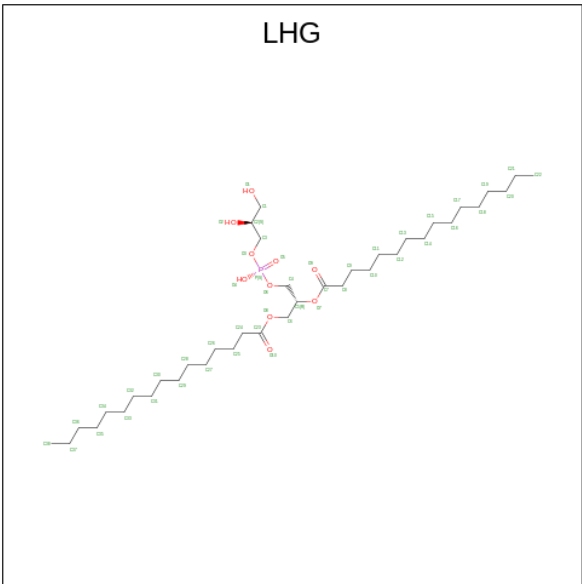
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			35	24	11	
32	J	1	Total	C	O	0
			24	18	6	
32	M	1	Total	C	O	0
			35	24	11	
32	Z	1	Total	C	O	0
			35	24	11	
32	c	1	Total	C	O	0
			35	24	11	
32	j	1	Total	C	O	0
			24	18	6	
32	m	1	Total	C	O	0
			35	24	11	
32	z	1	Total	C	O	0
			35	24	11	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total 49	C 38	O 10	P 1	0
34	D	1	Total 46	C 35	O 10	P 1	0
34	E	1	Total 49	C 38	O 10	P 1	0
34	L	1	Total 49	C 38	O 10	P 1	0
34	d	1	Total 49	C 38	O 10	P 1	0
34	d	1	Total 49	C 38	O 10	P 1	0
34	d	1	Total 46	C 35	O 10	P 1	0
34	e	1	Total 49	C 38	O 10	P 1	0
34	l	1	Total 49	C 38	O 10	P 1	0

- # HEM

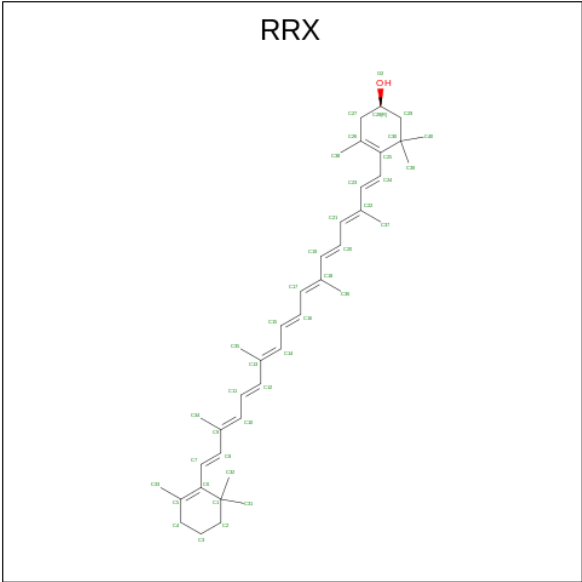
Mol	Chain	Residues	Atoms					AltConf
35	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
35	e	1	Total 43	C 34	Fe 1	N 4	O 4	0

- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 36 | J | 1 | Total Mg
1 1 | 0 |
| 36 | j | 1 | Total Mg
1 1 | 0 |

-
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various side chains and a central hydroxyl group (OH). The atoms are labeled with codes: O1A, O2A, O1D, O2D for the carboxylate groups; CAA, CBA, CAD, CBD for the side chains; CMA, C3A, C4A, C3B, C4B, C3C, C4C, C3D, C4D for the ring carbons; and C1A, C1B, C1C, C1D for the bridgehead carbons. The central iron atom is labeled FE, and the central hydroxyl group is labeled OH.

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

- 



Mol	Chain	Residues	Atoms			AltConf
38	X	1	Total	C	O	0
			41	40	1	
38	x	1	Total	C	O	0
			41	40	1	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	152	Total	O	0
			152	152	
39	B	298	Total	O	0
			298	298	
39	C	220	Total	O	0
			220	220	
39	D	154	Total	O	0
			154	154	
39	E	26	Total	O	0
			26	26	
39	F	5	Total	O	0
			5	5	
39	H	38	Total	O	0
			38	38	
39	I	13	Total	O	0
			13	13	
39	J	11	Total	O	0
			11	11	
39	K	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
39	L	19	Total 19	O 19	0
39	M	8	Total 8	O 8	0
39	O	114	Total 114	O 114	0
39	T	9	Total 9	O 9	0
39	U	64	Total 64	O 64	0
39	V	78	Total 78	O 78	0
39	Y	2	Total 2	O 2	0
39	X	8	Total 8	O 8	0
39	a	152	Total 152	O 152	0
39	b	292	Total 292	O 292	0
39	c	220	Total 220	O 220	0
39	d	154	Total 154	O 154	0
39	e	26	Total 26	O 26	0
39	f	5	Total 5	O 5	0
39	h	38	Total 38	O 38	0
39	i	13	Total 13	O 13	0
39	j	11	Total 11	O 11	0
39	k	3	Total 3	O 3	0
39	l	13	Total 13	O 13	0
39	m	8	Total 8	O 8	0
39	o	114	Total 114	O 114	0

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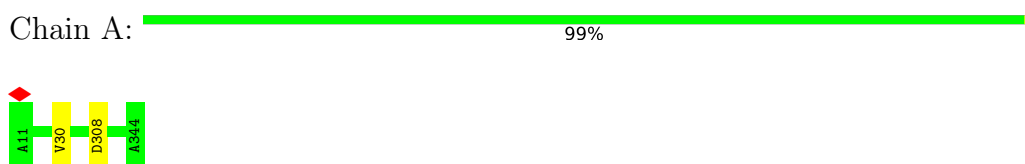
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Mol	Chain	Residues	Atoms		AltConf
39	t	9	Total 9	O 9	0
39	u	64	Total 64	O 64	0
39	v	78	Total 78	O 78	0
39	y	2	Total 2	O 2	0
39	x	8	Total 8	O 8	0

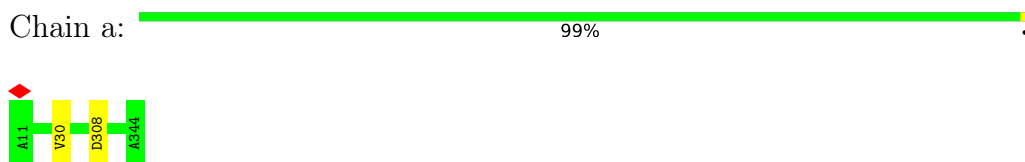
3 Residue-property plots [i](#)

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

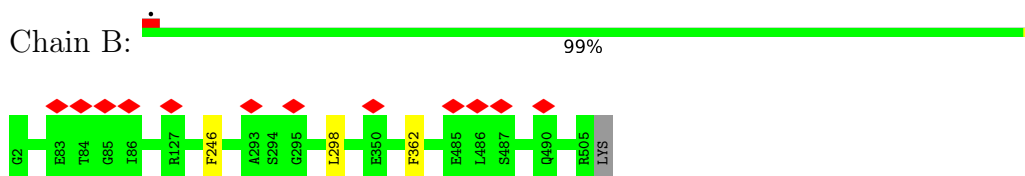
- Molecule 1: Photosystem II protein D1



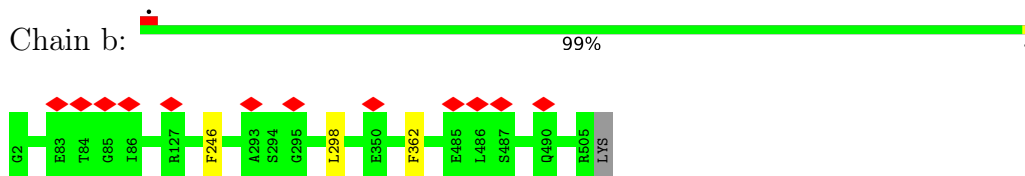
- Molecule 1: Photosystem II protein D1



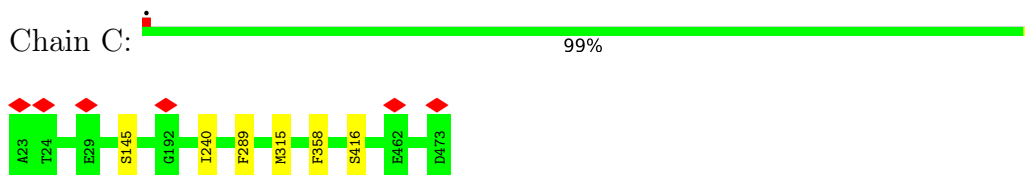
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein

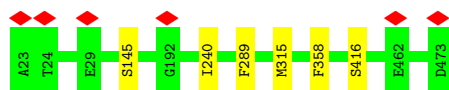


- Molecule 3: Photosystem II CP43 reaction center protein



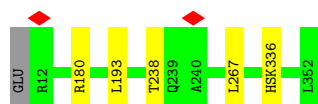
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  99%



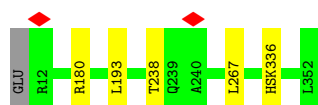
- Molecule 4: Photosystem II D2 protein

Chain D:  98%



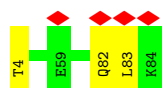
- Molecule 4: Photosystem II D2 protein

Chain d:  98%



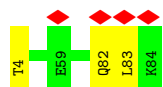
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  96%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  96%



- Molecule 6: Cytochrome b559 subunit beta

Chain F:  100%

There are no outlier residues recorded for this chain.

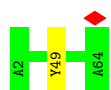
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  100%

There are no outlier residues recorded for this chain.

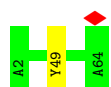
- Molecule 7: Photosystem II reaction center protein H

Chain H:  98%



- Molecule 7: Photosystem II reaction center protein H

Chain h:  98%



- Molecule 8: Photosystem II reaction center protein I

Chain I:  100%



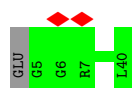
- Molecule 8: Photosystem II reaction center protein I

Chain i:  100%




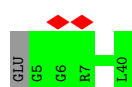
- Molecule 9: Photosystem II reaction center protein J

Chain J:  5% 97%



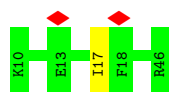
- Molecule 9: Photosystem II reaction center protein J

Chain j:  5% 97%

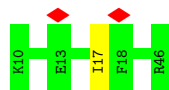


- Molecule 10: Photosystem II reaction center protein K

Chain K:  5% 97%



- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



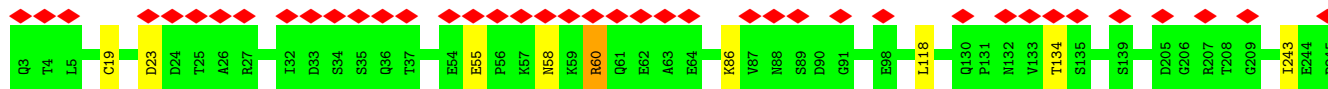
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M



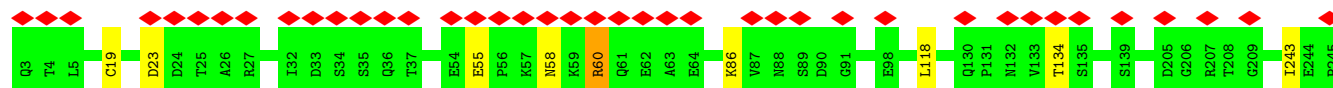
- Molecule 13: Photosystem II manganese-stabilizing polypeptide





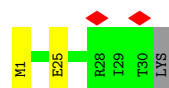
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 17% 96%



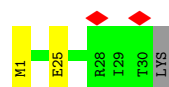
- Molecule 14: Photosystem II reaction center protein T

Chain T: 6% 90% 6%



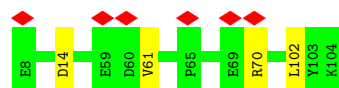
- Molecule 14: Photosystem II reaction center protein T

Chain t: 6% 90% 6%



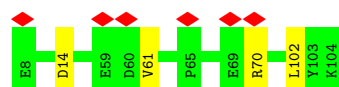
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 6% 96%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 6% 96%



- Molecule 16: Cytochrome c-550

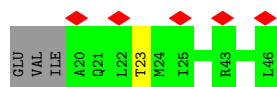
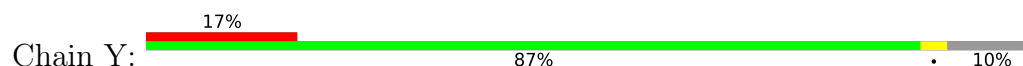
Chain V: 6% 96%



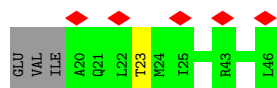
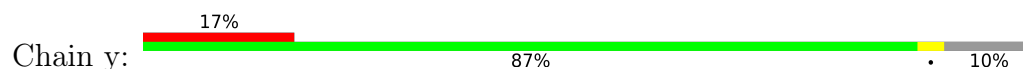
- Molecule 16: Cytochrome c-550



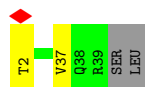
- Molecule 17: Photosystem II reaction center protein Ycf12



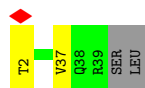
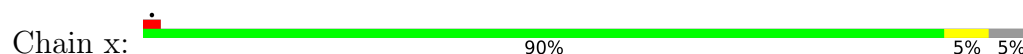
- Molecule 17: Photosystem II reaction center protein Ycf12



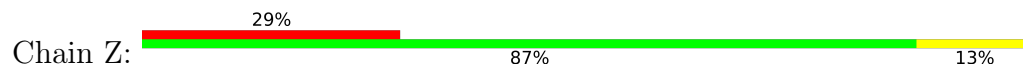
- Molecule 18: Photosystem II reaction center protein X



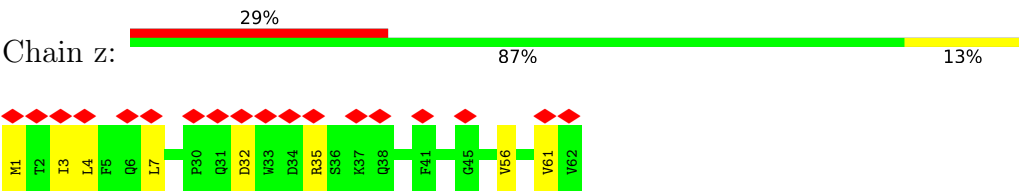
- Molecule 18: Photosystem II reaction center protein X



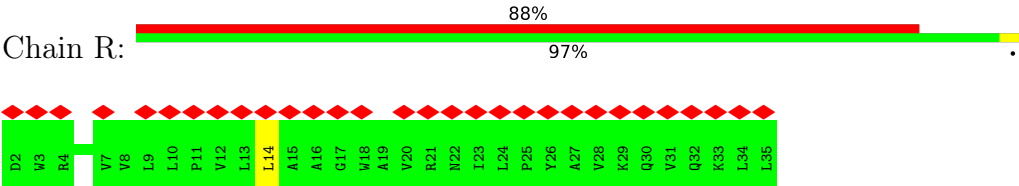
- Molecule 19: Photosystem II reaction center protein Z



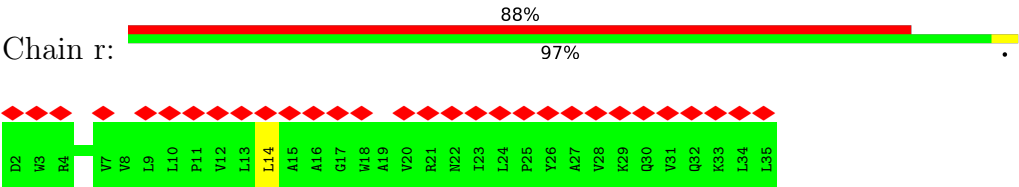
- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	174099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	83	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.242	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	328.80002, 328.80002, 328.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, UNL, SQD, LMT, HSK, BCT, MG, PL9, CLA, HEC, CL, HEM, BCR, RRX, LMG, PHO, DGD, LHG, OEX, FME

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	0.53	0/2718	0.66	1/3704 (0.0%)
1	a	0.53	0/2718	0.66	1/3704 (0.0%)
2	B	0.52	0/4109	0.62	0/5600
2	b	0.52	0/4109	0.62	0/5600
3	C	0.52	1/3599 (0.0%)	0.61	0/4900
3	c	0.52	1/3599 (0.0%)	0.61	0/4900
4	D	0.55	1/2800 (0.0%)	0.66	1/3814 (0.0%)
4	d	0.55	1/2800 (0.0%)	0.66	1/3814 (0.0%)
5	E	0.46	0/680	0.60	0/928
5	e	0.46	0/680	0.60	0/928
6	F	0.48	0/284	0.57	0/387
6	f	0.47	0/284	0.57	0/387
7	H	0.51	0/511	0.64	0/697
7	h	0.51	0/511	0.64	0/697
8	I	0.48	0/293	0.58	0/396
8	i	0.48	0/293	0.58	0/396
9	J	0.42	0/263	0.60	0/356
9	j	0.42	0/263	0.60	0/356
10	K	0.51	0/303	0.70	0/416
10	k	0.51	0/303	0.70	0/416
11	L	0.49	0/311	0.60	0/422
11	l	0.49	0/311	0.60	0/422
12	M	0.52	0/253	0.66	0/346
12	m	0.52	0/253	0.66	0/346
13	O	0.45	0/1905	0.68	0/2583
13	o	0.45	0/1905	0.68	0/2583
14	T	0.47	0/257	0.58	0/349
14	t	0.47	0/257	0.58	0/349
15	U	0.46	0/785	0.66	0/1064
15	u	0.46	0/785	0.66	0/1064
16	V	0.45	0/1085	0.60	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.45	0/1085	0.61	0/1473
17	Y	0.34	0/201	0.61	0/268
17	y	0.34	0/201	0.61	0/268
18	X	0.39	0/284	0.56	0/384
18	x	0.39	0/284	0.56	0/384
19	Z	0.43	0/490	0.58	0/669
19	z	0.42	0/490	0.58	0/669
20	R	0.38	0/279	0.71	0/383
20	r	0.38	0/279	0.71	0/383
All	All	0.50	4/42820 (0.0%)	0.63	4/58278 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	358	PHE	CD2-CE2	-5.64	1.27	1.39
4	D	193	LEU	C-N	-5.64	1.21	1.34
3	c	358	PHE	CD2-CE2	-5.64	1.27	1.39
4	d	193	LEU	C-N	-5.64	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ASP	CB-CG-OD1	5.74	123.47	118.30
1	a	308	ASP	CB-CG-OD1	5.74	123.47	118.30
4	D	267	LEU	CB-CG-CD2	5.13	119.72	111.00
4	d	267	LEU	CB-CG-CD2	5.13	119.72	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	37	29
1	a	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	37	29
2	B	502/505 (99%)	495 (99%)	7 (1%)	0	100	100
2	b	502/505 (99%)	495 (99%)	7 (1%)	0	100	100
3	C	449/451 (100%)	443 (99%)	5 (1%)	1 (0%)	44	37
3	c	449/451 (100%)	443 (99%)	5 (1%)	1 (0%)	44	37
4	D	338/342 (99%)	332 (98%)	6 (2%)	0	100	100
4	d	338/342 (99%)	332 (98%)	6 (2%)	0	100	100
5	E	79/81 (98%)	79 (100%)	0	0	100	100
5	e	79/81 (98%)	79 (100%)	0	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
7	h	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
9	J	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
9	j	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	31/34 (91%)	31 (100%)	0	0	100	100
12	m	31/34 (91%)	31 (100%)	0	0	100	100
13	O	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	16	8
13	o	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	16	8
14	T	28/31 (90%)	28 (100%)	0	0	100	100
14	t	28/31 (90%)	28 (100%)	0	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	u	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
16	V	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	19	10
16	v	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	19	10
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
17	y	25/30 (83%)	25 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	32 (100%)	0	0	100	100
20	r	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5232/5332 (98%)	5120 (98%)	102 (2%)	10 (0%)	45	37

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER
13	O	58	ASN
13	o	58	ASN
13	O	60	ARG

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	270/269 (100%)	270 (100%)	0	100	100
1	a	270/269 (100%)	270 (100%)	0	100	100
2	B	402/403 (100%)	399 (99%)	3 (1%)	81	81
2	b	402/403 (100%)	399 (99%)	3 (1%)	81	81
3	C	352/352 (100%)	348 (99%)	4 (1%)	70	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	352/352 (100%)	348 (99%)	4 (1%)	70	68
4	D	275/276 (100%)	273 (99%)	2 (1%)	81	81
4	d	275/276 (100%)	273 (99%)	2 (1%)	81	81
5	E	72/72 (100%)	69 (96%)	3 (4%)	25	15
5	e	72/72 (100%)	69 (96%)	3 (4%)	25	15
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	28/28 (100%)	28 (100%)	0	100	100
7	H	53/53 (100%)	52 (98%)	1 (2%)	52	47
7	h	53/53 (100%)	52 (98%)	1 (2%)	52	47
8	I	32/32 (100%)	32 (100%)	0	100	100
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	24/25 (96%)	24 (100%)	0	100	100
9	j	24/25 (96%)	24 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	23
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	23
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	29/30 (97%)	29 (100%)	0	100	100
12	m	29/30 (97%)	29 (100%)	0	100	100
13	O	207/207 (100%)	199 (96%)	8 (4%)	27	17
13	o	207/207 (100%)	199 (96%)	8 (4%)	27	17
14	T	26/27 (96%)	25 (96%)	1 (4%)	28	18
14	t	26/27 (96%)	25 (96%)	1 (4%)	28	18
15	U	84/84 (100%)	80 (95%)	4 (5%)	21	10
15	u	84/84 (100%)	80 (95%)	4 (5%)	21	10
16	V	117/117 (100%)	113 (97%)	4 (3%)	32	22
16	v	117/117 (100%)	113 (97%)	4 (3%)	32	22
17	Y	20/23 (87%)	19 (95%)	1 (5%)	20	10
17	y	20/23 (87%)	19 (95%)	1 (5%)	20	10
18	X	31/33 (94%)	29 (94%)	2 (6%)	14	5
18	x	31/33 (94%)	29 (94%)	2 (6%)	14	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Z	52/52 (100%)	44 (85%)	8 (15%)	2	0
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	0
20	R	29/29 (100%)	28 (97%)	1 (3%)	32	22
20	r	29/29 (100%)	28 (97%)	1 (3%)	32	22
All	All	4336/4354 (100%)	4250 (98%)	86 (2%)	50	44

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	19	CYS
16	v	21	LEU
13	o	55	GLU
14	t	25	GLU
18	x	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	331	ASN
3	c	415	ASN
15	u	31	ASN
3	c	313	GLN
7	h	50	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HSK	d	336	4	7,11,12	1.34	1 (14%)	3,14,16	1.54	0
4	HSK	D	336	4	7,11,12	1.31	1 (14%)	3,14,16	1.30	0
8	FME	I	1	8	8,9,10	1.02	0	7,9,11	0.86	0
14	FME	T	1	14	8,9,10	0.94	0	7,9,11	1.31	1 (14%)
12	FME	M	1	12	8,9,10	0.93	0	7,9,11	0.61	0
8	FME	i	1	8	8,9,10	1.02	0	7,9,11	0.86	0
12	FME	m	1	12	8,9,10	0.93	0	7,9,11	0.61	0
14	FME	t	1	14	8,9,10	0.95	0	7,9,11	1.31	1 (14%)

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
4	HSK	d	336	4	-	0/5/6/8	0/1/1/1
4	HSK	D	336	4	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	HSK	CE1-ND1	2.70	1.40	1.36
4	D	336	HSK	CE1-ND1	2.54	1.39	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	2.62	114.47	109.73
14	T	1	FME	C-CA-N	2.61	114.44	109.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	N-CA-CB-CG
12	m	1	FME	N-CA-CB-CG
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 196 ligands modelled in this entry, 8 are monoatomic and 36 are unknown - leaving 152 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	$\# Z > 2$
34	LHG	D	409	-	48,48,48	0.84	1 (2%)	51,54,54	1.11	3 (5%)
26	BCR	J	104	-	41,41,41	1.16	3 (7%)	56,56,56	1.13	3 (5%)
30	LMG	C	523	-	51,51,55	0.86	2 (3%)	59,59,63	1.36	8 (13%)
24	CLA	a	405	-	65,73,73	1.80	15 (23%)	76,113,113	2.45	23 (30%)
24	CLA	b	616	-	65,73,73	1.85	15 (23%)	76,113,113	2.78	28 (36%)
30	LMG	b	622	-	51,51,55	1.05	3 (5%)	59,59,63	1.29	6 (10%)
24	CLA	B	605	-	65,73,73	1.86	17 (26%)	76,113,113	2.76	29 (38%)
24	CLA	B	608	-	65,73,73	1.88	17 (26%)	76,113,113	2.49	27 (35%)
28	PL9	D	407	-	55,55,55	1.90	11 (20%)	68,69,69	1.56	16 (23%)
24	CLA	C	507	-	65,73,73	1.93	15 (23%)	76,113,113	2.69	30 (39%)
24	CLA	B	615	-	65,73,73	1.84	15 (23%)	76,113,113	2.64	27 (35%)
28	PL9	a	411	-	55,55,55	1.53	8 (14%)	68,69,69	1.55	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	509	-	65,73,73	1.90	16 (24%)	76,113,113	2.81	30 (39%)
24	CLA	c	511	-	65,73,73	1.95	17 (26%)	76,113,113	2.60	27 (35%)
24	CLA	c	508	39	65,73,73	1.91	17 (26%)	76,113,113	2.73	27 (35%)
24	CLA	b	604	-	65,73,73	1.85	16 (24%)	76,113,113	2.82	27 (35%)
24	CLA	b	605	-	65,73,73	1.93	16 (24%)	76,113,113	2.66	31 (40%)
26	BCR	B	618	-	41,41,41	1.10	3 (7%)	56,56,56	1.24	7 (12%)
26	BCR	b	621	-	41,41,41	1.11	2 (4%)	56,56,56	1.06	4 (7%)
26	BCR	c	522	-	41,41,41	1.02	1 (2%)	56,56,56	1.16	6 (10%)
32	LMT	C	521	-	36,36,36	1.31	5 (13%)	47,47,47	1.28	3 (6%)
27	SQD	f	101	-	44,45,54	1.10	5 (11%)	53,56,65	2.18	11 (20%)
33	BCT	d	403	22	2,3,3	1.84	1 (50%)	2,3,3	3.92	2 (100%)
24	CLA	B	601	39	65,73,73	1.94	19 (29%)	76,113,113	2.60	25 (32%)
24	CLA	C	509	-	65,73,73	1.89	16 (24%)	76,113,113	2.80	30 (39%)
34	LHG	D	410	-	45,45,48	0.80	1 (2%)	48,51,54	1.17	4 (8%)
32	LMT	j	102	-	24,24,36	1.01	2 (8%)	29,29,47	1.51	3 (10%)
24	CLA	C	504	-	65,73,73	1.84	18 (27%)	76,113,113	2.67	22 (28%)
24	CLA	d	404	-	65,73,73	1.82	17 (26%)	76,113,113	2.67	24 (31%)
26	BCR	c	515	-	41,41,41	1.16	3 (7%)	56,56,56	1.42	9 (16%)
24	CLA	b	609	39	65,73,73	1.87	16 (24%)	76,113,113	2.70	26 (34%)
24	CLA	B	609	-	65,73,73	1.82	15 (23%)	76,113,113	2.77	32 (42%)
24	CLA	D	405	-	65,73,73	1.94	18 (27%)	76,113,113	2.68	29 (38%)
24	CLA	B	611	-	65,73,73	1.80	14 (21%)	76,113,113	2.70	28 (36%)
24	CLA	c	504	-	65,73,73	1.84	18 (27%)	76,113,113	2.67	22 (28%)
30	LMG	C	520	-	51,51,55	0.95	4 (7%)	59,59,63	1.36	7 (11%)
24	CLA	c	512	3	65,73,73	1.92	15 (23%)	76,113,113	2.75	26 (34%)
24	CLA	b	615	-	65,73,73	1.87	18 (27%)	76,113,113	2.61	27 (35%)
34	LHG	l	101	-	48,48,48	0.70	0	51,54,54	1.12	4 (7%)
34	LHG	e	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.26	7 (13%)
26	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.27	7 (12%)
26	BCR	C	515	-	41,41,41	1.16	3 (7%)	56,56,56	1.42	9 (16%)
24	CLA	b	611	-	65,73,73	1.83	15 (23%)	76,113,113	2.77	32 (42%)
26	BCR	j	104	-	41,41,41	1.16	3 (7%)	56,56,56	1.13	3 (5%)
27	SQD	B	620	-	53,54,54	0.92	5 (9%)	62,65,65	2.23	11 (17%)
25	PHO	A	407	-	51,69,69	1.15	6 (11%)	47,99,99	1.22	3 (6%)
24	CLA	C	508	39	65,73,73	1.91	17 (26%)	76,113,113	2.73	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	b	620	-	41,41,41	1.10	3 (7%)	56,56,56	1.24	7 (12%)
26	BCR	d	406	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	7 (12%)
26	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.17	5 (8%)
32	LMT	Z	101	-	36,36,36	1.30	6 (16%)	47,47,47	1.13	5 (10%)
27	SQD	A	410	-	53,54,54	1.05	6 (11%)	62,65,65	1.88	8 (12%)
24	CLA	C	505	39	65,73,73	1.89	15 (23%)	76,113,113	2.62	32 (42%)
27	SQD	a	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	11 (17%)
24	CLA	B	612	-	65,73,73	1.88	15 (23%)	76,113,113	2.61	29 (38%)
24	CLA	B	616	-	65,73,73	1.85	14 (21%)	76,113,113	2.65	32 (42%)
24	CLA	b	618	-	65,73,73	1.85	14 (21%)	76,113,113	2.65	31 (40%)
24	CLA	c	507	-	65,73,73	1.93	15 (23%)	76,113,113	2.69	30 (39%)
30	LMG	B	621	-	51,51,55	1.05	3 (5%)	59,59,63	1.29	6 (10%)
24	CLA	b	610	-	65,73,73	1.89	17 (26%)	76,113,113	2.49	27 (35%)
24	CLA	B	610	39	65,73,73	1.87	17 (26%)	76,113,113	2.55	27 (35%)
27	SQD	F	101	-	44,45,54	1.10	5 (11%)	53,56,65	2.18	11 (20%)
24	CLA	c	513	-	65,73,73	1.84	15 (23%)	76,113,113	2.85	30 (39%)
24	CLA	c	505	39	65,73,73	1.89	15 (23%)	76,113,113	2.62	32 (42%)
24	CLA	D	401	39	65,73,73	1.99	16 (24%)	76,113,113	2.86	29 (38%)
33	BCT	D	403	22	2,3,3	1.85	1 (50%)	2,3,3	3.93	2 (100%)
24	CLA	A	408	-	65,73,73	1.88	14 (21%)	76,113,113	2.87	29 (38%)
24	CLA	a	408	-	65,73,73	1.88	14 (21%)	76,113,113	2.87	29 (38%)
24	CLA	A	405	-	65,73,73	1.80	15 (23%)	76,113,113	2.45	23 (30%)
24	CLA	b	614	-	65,73,73	1.88	16 (24%)	76,113,113	2.62	29 (38%)
38	RRX	X	101	-	42,42,42	1.89	11 (26%)	57,58,58	2.00	16 (28%)
24	CLA	B	614	-	65,73,73	1.85	15 (23%)	76,113,113	2.78	28 (36%)
34	LHG	D	408	-	48,48,48	0.85	1 (2%)	51,54,54	1.23	8 (15%)
24	CLA	B	613	-	65,73,73	1.87	18 (27%)	76,113,113	2.61	27 (35%)
24	CLA	c	506	-	65,73,73	1.84	19 (29%)	76,113,113	2.47	25 (32%)
27	SQD	L	102	-	53,54,54	0.92	5 (9%)	62,65,65	2.23	11 (17%)
28	PL9	d	407	-	55,55,55	1.90	11 (20%)	68,69,69	1.56	16 (23%)
26	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.06	4 (7%)
24	CLA	C	510	-	65,73,73	1.97	16 (24%)	76,113,113	2.64	31 (40%)
24	CLA	c	503	-	65,73,73	1.93	17 (26%)	76,113,113	2.57	24 (31%)
35	HEM	e	103	5,6	41,50,50	1.45	4 (9%)	45,82,82	1.65	9 (20%)
24	CLA	a	406	39	65,73,73	1.87	17 (26%)	76,113,113	2.42	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	A	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	11 (17%)
32	LMT	m	102	-	36,36,36	1.38	6 (16%)	47,47,47	1.02	1 (2%)
26	BCR	a	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.27	7 (12%)
34	LHG	d	410	-	45,45,48	0.80	1 (2%)	48,51,54	1.17	4 (8%)
24	CLA	B	603	-	65,73,73	1.94	17 (26%)	76,113,113	2.66	31 (40%)
24	CLA	C	503	-	65,73,73	1.92	17 (26%)	76,113,113	2.57	24 (31%)
24	CLA	c	514	-	65,73,73	2.02	18 (27%)	76,113,113	2.76	30 (39%)
24	CLA	b	612	39	65,73,73	1.86	17 (26%)	76,113,113	2.57	27 (35%)
34	LHG	d	409	-	48,48,48	0.84	1 (2%)	51,54,54	1.11	3 (5%)
24	CLA	B	602	-	65,73,73	1.85	17 (26%)	76,113,113	2.82	26 (34%)
24	CLA	b	617	-	65,73,73	1.84	15 (23%)	76,113,113	2.64	27 (35%)
24	CLA	d	405	-	65,73,73	1.94	18 (27%)	76,113,113	2.68	28 (36%)
31	DGD	H	101	-	63,63,67	1.27	7 (11%)	77,77,81	1.27	9 (11%)
26	BCR	C	522	-	41,41,41	1.02	1 (2%)	56,56,56	1.16	6 (10%)
26	BCR	c	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.17	5 (8%)
30	LMG	c	523	-	51,51,55	0.85	2 (3%)	59,59,63	1.36	8 (13%)
31	DGD	c	518	-	63,63,67	1.55	13 (20%)	77,77,81	1.44	11 (14%)
21	OEX	A	401	3,39,1	0,15,15	-	-	-	-	-
24	CLA	C	506	-	65,73,73	1.84	19 (29%)	76,113,113	2.47	25 (32%)
32	LMT	J	102	-	24,24,36	1.01	1 (4%)	29,29,47	1.52	3 (10%)
24	CLA	C	502	-	65,73,73	1.91	17 (26%)	76,113,113	2.70	27 (35%)
24	CLA	c	510	-	65,73,73	1.98	16 (24%)	76,113,113	2.64	31 (40%)
27	SQD	a	410	-	53,54,54	1.05	6 (11%)	62,65,65	1.88	8 (12%)
31	DGD	C	519	-	63,63,67	1.20	7 (11%)	77,77,81	1.31	8 (10%)
25	PHO	a	407	-	51,69,69	1.15	6 (11%)	47,99,99	1.22	3 (6%)
32	LMT	z	101	-	36,36,36	1.30	6 (16%)	47,47,47	1.13	5 (10%)
24	CLA	B	604	-	65,73,73	1.87	20 (30%)	76,113,113	2.66	31 (40%)
24	CLA	b	606	-	65,73,73	1.87	20 (30%)	76,113,113	2.66	31 (40%)
32	LMT	c	521	-	36,36,36	1.32	5 (13%)	47,47,47	1.28	3 (6%)
28	PL9	A	411	-	55,55,55	1.53	8 (14%)	68,69,69	1.56	13 (19%)
30	LMG	C	501	-	51,51,55	1.18	6 (11%)	59,59,63	1.38	8 (13%)
30	LMG	d	411	36	51,51,55	1.07	7 (13%)	59,59,63	1.32	7 (11%)
24	CLA	c	502	-	65,73,73	1.90	17 (26%)	76,113,113	2.70	28 (36%)
24	CLA	C	511	-	65,73,73	1.95	17 (26%)	76,113,113	2.60	27 (35%)
24	CLA	B	606	-	65,73,73	2.00	18 (27%)	76,113,113	2.80	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LHG	L	101	-	48,48,48	0.70	0	51,54,54	1.12	4 (7%)
24	CLA	b	603	39	65,73,73	1.95	19 (29%)	76,113,113	2.61	25 (32%)
35	HEM	E	103	5,6	41,50,50	1.45	4 (9%)	45,82,82	1.65	9 (20%)
24	CLA	b	607	-	65,73,73	1.86	17 (26%)	76,113,113	2.76	29 (38%)
37	HEC	v	201	16	32,50,50	2.14	5 (15%)	24,82,82	1.95	8 (33%)
37	HEC	V	201	16	32,50,50	2.13	5 (15%)	24,82,82	1.95	8 (33%)
24	CLA	C	513	-	65,73,73	1.85	15 (23%)	76,113,113	2.85	30 (39%)
26	BCR	B	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	3 (5%)
32	LMT	M	101	-	36,36,36	1.38	6 (16%)	47,47,47	1.02	1 (2%)
34	LHG	d	408	-	48,48,48	0.85	1 (2%)	51,54,54	1.23	8 (15%)
24	CLA	D	404	-	65,73,73	1.82	17 (26%)	76,113,113	2.67	24 (31%)
25	PHO	d	402	-	51,69,69	1.04	3 (5%)	47,99,99	1.51	8 (17%)
24	CLA	A	406	39	65,73,73	1.87	17 (26%)	76,113,113	2.42	26 (34%)
24	CLA	b	613	-	65,73,73	1.80	14 (21%)	76,113,113	2.70	28 (36%)
26	BCR	A	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.27	7 (12%)
24	CLA	b	608	-	65,73,73	2.00	18 (27%)	76,113,113	2.81	30 (39%)
26	BCR	b	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	3 (5%)
34	LHG	E	101	-	48,48,48	0.71	1 (2%)	51,54,54	1.26	7 (13%)
38	RRX	x	101	-	42,42,42	1.89	11 (26%)	57,58,58	2.01	16 (28%)
31	DGD	c	519	-	63,63,67	1.20	7 (11%)	77,77,81	1.31	8 (10%)
30	LMG	D	411	36	51,51,55	1.07	7 (13%)	59,59,63	1.32	7 (11%)
31	DGD	c	517	-	63,63,67	1.13	7 (11%)	77,77,81	1.44	11 (14%)
31	DGD	C	518	-	63,63,67	1.55	13 (20%)	77,77,81	1.44	11 (14%)
30	LMG	c	501	-	51,51,55	1.18	6 (11%)	59,59,63	1.38	8 (13%)
24	CLA	B	607	39	65,73,73	1.87	16 (24%)	76,113,113	2.70	26 (34%)
30	LMG	c	520	-	51,51,55	0.95	4 (7%)	59,59,63	1.36	7 (11%)
26	BCR	D	406	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	7 (12%)
24	CLA	C	512	3	65,73,73	1.92	15 (23%)	76,113,113	2.75	26 (34%)
31	DGD	C	517	-	63,63,67	1.13	7 (11%)	77,77,81	1.44	11 (14%)
26	BCR	t	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.27	7 (12%)
25	PHO	D	402	-	51,69,69	1.04	3 (5%)	47,99,99	1.51	8 (17%)
24	CLA	d	401	39	65,73,73	1.99	16 (24%)	76,113,113	2.86	29 (38%)
24	CLA	C	514	-	65,73,73	2.01	18 (27%)	76,113,113	2.75	30 (39%)
21	OEX	a	401	3,39,1	0,15,15	-	-	-	-	-
31	DGD	h	101	-	63,63,67	1.28	7 (11%)	77,77,81	1.28	9 (11%)

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
34	LHG	D	409	-	-	19/53/53/53	-
26	BCR	J	104	-	-	11/29/63/63	0/2/2/2
30	LMG	C	523	-	-	27/46/66/70	0/1/1/1
24	CLA	a	405	-	1/1/15/20	4/37/115/115	-
24	CLA	b	616	-	1/1/15/20	16/37/115/115	-
30	LMG	b	622	-	-	13/46/66/70	0/1/1/1
24	CLA	B	605	-	1/1/15/20	7/37/115/115	-
24	CLA	B	608	-	-	2/37/115/115	-
28	PL9	D	407	-	-	10/53/73/73	0/1/1/1
24	CLA	C	507	-	1/1/15/20	9/37/115/115	-
24	CLA	B	615	-	1/1/15/20	12/37/115/115	-
28	PL9	a	411	-	-	18/53/73/73	0/1/1/1
24	CLA	c	509	-	1/1/15/20	6/37/115/115	-
24	CLA	c	511	-	1/1/15/20	6/37/115/115	-
24	CLA	c	508	39	1/1/15/20	10/37/115/115	-
24	CLA	b	604	-	1/1/15/20	3/37/115/115	-
24	CLA	b	605	-	1/1/15/20	9/37/115/115	-
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
26	BCR	b	621	-	-	12/29/63/63	0/2/2/2
26	BCR	c	522	-	-	12/29/63/63	0/2/2/2
32	LMT	C	521	-	-	10/21/61/61	0/2/2/2
27	SQD	f	101	-	-	12/40/60/69	0/1/1/1
24	CLA	B	601	39	1/1/15/20	13/37/115/115	-
24	CLA	C	509	-	1/1/15/20	6/37/115/115	-
34	LHG	D	410	-	-	15/50/50/53	-
32	LMT	j	102	-	-	4/15/35/61	0/1/1/2
24	CLA	C	504	-	1/1/15/20	8/37/115/115	-
24	CLA	d	404	-	1/1/15/20	2/37/115/115	-
26	BCR	c	515	-	-	11/29/63/63	0/2/2/2
24	CLA	b	609	39	1/1/15/20	9/37/115/115	-
24	CLA	B	609	-	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	405	-	-	11/37/115/115	-
24	CLA	B	611	-	1/1/15/20	2/37/115/115	-
24	CLA	c	504	-	1/1/15/20	8/37/115/115	-
30	LMG	C	520	-	-	21/46/66/70	0/1/1/1
24	CLA	c	512	3	1/1/15/20	12/37/115/115	-
24	CLA	b	615	-	1/1/15/20	7/37/115/115	-
34	LHG	l	101	-	-	17/53/53/53	-
34	LHG	e	101	-	-	25/53/53/53	-
26	BCR	T	101	-	-	10/29/63/63	0/2/2/2
26	BCR	C	515	-	-	11/29/63/63	0/2/2/2
24	CLA	b	611	-	1/1/15/20	3/37/115/115	-
26	BCR	j	104	-	-	11/29/63/63	0/2/2/2
27	SQD	B	620	-	-	26/49/69/69	0/1/1/1
25	PHO	A	407	-	-	5/37/103/103	0/5/6/6
24	CLA	C	508	39	1/1/15/20	10/37/115/115	-
26	BCR	b	620	-	-	5/29/63/63	0/2/2/2
26	BCR	d	406	-	-	5/29/63/63	0/2/2/2
26	BCR	C	516	-	-	9/29/63/63	0/2/2/2
32	LMT	Z	101	-	-	13/21/61/61	0/2/2/2
27	SQD	A	410	-	-	12/49/69/69	0/1/1/1
24	CLA	C	505	39	1/1/15/20	6/37/115/115	-
27	SQD	a	412	-	-	19/49/69/69	0/1/1/1
24	CLA	B	612	-	1/1/15/20	6/37/115/115	-
24	CLA	B	616	-	1/1/15/20	6/37/115/115	-
24	CLA	b	618	-	1/1/15/20	6/37/115/115	-
24	CLA	c	507	-	1/1/15/20	9/37/115/115	-
30	LMG	B	621	-	-	13/46/66/70	0/1/1/1
24	CLA	b	610	-	-	2/37/115/115	-
24	CLA	B	610	39	1/1/15/20	5/37/115/115	-
27	SQD	F	101	-	-	12/40/60/69	0/1/1/1
24	CLA	c	513	-	1/1/15/20	12/37/115/115	-
24	CLA	c	505	39	1/1/15/20	6/37/115/115	-
24	CLA	D	401	39	1/1/15/20	7/37/115/115	-
24	CLA	a	408	-	-	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	405	-	1/1/15/20	4/37/115/115	-
24	CLA	b	614	-	1/1/15/20	6/37/115/115	-
38	RRX	X	101	-	-	3/29/65/65	0/2/2/2
24	CLA	B	614	-	1/1/15/20	16/37/115/115	-
34	LHG	D	408	-	-	16/53/53/53	-
24	CLA	B	613	-	1/1/15/20	7/37/115/115	-
24	CLA	c	506	-	1/1/15/20	7/37/115/115	-
27	SQD	L	102	-	-	26/49/69/69	0/1/1/1
28	PL9	d	407	-	-	10/53/73/73	0/1/1/1
26	BCR	B	619	-	-	12/29/63/63	0/2/2/2
24	CLA	C	510	-	1/1/15/20	11/37/115/115	-
24	CLA	c	503	-	-	10/37/115/115	-
35	HEM	e	103	5,6	-	2/12/54/54	-
24	CLA	a	406	39	-	9/37/115/115	-
27	SQD	A	412	-	-	19/49/69/69	0/1/1/1
32	LMT	m	102	-	-	4/21/61/61	0/2/2/2
26	BCR	a	409	-	-	9/29/63/63	0/2/2/2
34	LHG	d	410	-	-	15/50/50/53	-
24	CLA	B	603	-	1/1/15/20	9/37/115/115	-
24	CLA	C	503	-	-	10/37/115/115	-
24	CLA	c	514	-	1/1/15/20	10/37/115/115	-
24	CLA	b	612	39	1/1/15/20	5/37/115/115	-
34	LHG	d	409	-	-	19/53/53/53	-
24	CLA	B	602	-	1/1/15/20	3/37/115/115	-
24	CLA	b	617	-	1/1/15/20	12/37/115/115	-
24	CLA	d	405	-	-	11/37/115/115	-
31	DGD	H	101	-	-	10/51/91/95	0/2/2/2
26	BCR	C	522	-	-	12/29/63/63	0/2/2/2
26	BCR	c	516	-	-	9/29/63/63	0/2/2/2
30	LMG	c	523	-	-	27/46/66/70	0/1/1/1
31	DGD	c	518	-	-	26/51/91/95	0/2/2/2
24	CLA	C	506	-	1/1/15/20	7/37/115/115	-
32	LMT	J	102	-	-	4/15/35/61	0/1/1/2
24	CLA	C	502	-	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	510	-	1/1/15/20	11/37/115/115	-
27	SQD	a	410	-	-	12/49/69/69	0/1/1/1
31	DGD	C	519	-	-	14/51/91/95	0/2/2/2
25	PHO	a	407	-	-	5/37/103/103	0/5/6/6
32	LMT	z	101	-	-	13/21/61/61	0/2/2/2
24	CLA	B	604	-	1/1/15/20	9/37/115/115	-
24	CLA	b	606	-	1/1/15/20	9/37/115/115	-
32	LMT	c	521	-	-	10/21/61/61	0/2/2/2
28	PL9	A	411	-	-	18/53/73/73	0/1/1/1
30	LMG	C	501	-	-	29/46/66/70	0/1/1/1
30	LMG	d	411	36	-	16/46/66/70	0/1/1/1
24	CLA	c	502	-	1/1/15/20	4/37/115/115	-
24	CLA	C	511	-	1/1/15/20	6/37/115/115	-
24	CLA	B	606	-	1/1/15/20	5/37/115/115	-
34	LHG	L	101	-	-	17/53/53/53	-
24	CLA	b	603	39	1/1/15/20	13/37/115/115	-
35	HEM	E	103	5,6	-	1/12/54/54	-
24	CLA	b	607	-	1/1/15/20	7/37/115/115	-
37	HEC	v	201	16	-	2/10/54/54	-
37	HEC	V	201	16	-	2/10/54/54	-
24	CLA	C	513	-	1/1/15/20	12/37/115/115	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
34	LHG	d	408	-	-	16/53/53/53	-
24	CLA	D	404	-	1/1/15/20	2/37/115/115	-
25	PHO	d	402	-	-	3/37/103/103	0/5/6/6
24	CLA	A	406	39	-	9/37/115/115	-
24	CLA	b	613	-	1/1/15/20	2/37/115/115	-
26	BCR	A	409	-	-	9/29/63/63	0/2/2/2
24	CLA	b	608	-	1/1/15/20	5/37/115/115	-
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
34	LHG	E	101	-	-	25/53/53/53	-
38	RRX	x	101	-	-	3/29/65/65	0/2/2/2
31	DGD	c	519	-	-	14/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMG	D	411	36	-	16/46/66/70	0/1/1/1
31	DGD	c	517	-	-	12/51/91/95	0/2/2/2
31	DGD	C	518	-	-	26/51/91/95	0/2/2/2
30	LMG	c	501	-	-	29/46/66/70	0/1/1/1
24	CLA	B	607	39	1/1/15/20	9/37/115/115	-
30	LMG	c	520	-	-	21/46/66/70	0/1/1/1
26	BCR	D	406	-	-	5/29/63/63	0/2/2/2
24	CLA	C	512	3	1/1/15/20	12/37/115/115	-
31	DGD	C	517	-	-	12/51/91/95	0/2/2/2
26	BCR	t	102	-	-	10/29/63/63	0/2/2/2
25	PHO	D	402	-	-	3/37/103/103	0/5/6/6
24	CLA	d	401	39	1/1/15/20	7/37/115/115	-
24	CLA	C	514	-	1/1/15/20	10/37/115/115	-
24	CLA	A	408	-	-	13/37/115/115	-
31	DGD	h	101	-	-	10/51/91/95	0/2/2/2

The worst 5 of 1488 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	407	PL9	C3-C4	-7.64	1.36	1.49
28	d	407	PL9	C3-C4	-7.64	1.36	1.49
37	V	201	HEC	C2B-C3B	-6.92	1.33	1.40
37	v	201	HEC	C2B-C3B	-6.92	1.33	1.40
24	B	603	CLA	C3B-C2B	6.47	1.49	1.40

The worst 5 of 2526 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	102	SQD	O6-C1-C2	10.58	124.81	108.30
27	B	620	SQD	O6-C1-C2	10.57	124.81	108.30
24	C	513	CLA	C2D-C1D-ND	10.29	117.69	110.10
24	c	513	CLA	C2D-C1D-ND	10.29	117.69	110.10
24	B	614	CLA	C1D-ND-C4D	-10.01	99.23	106.33

5 of 60 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND

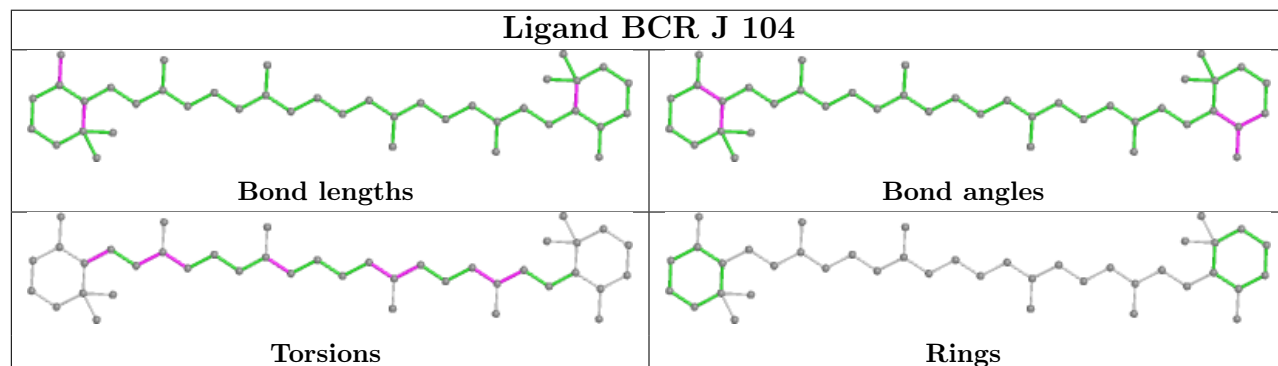
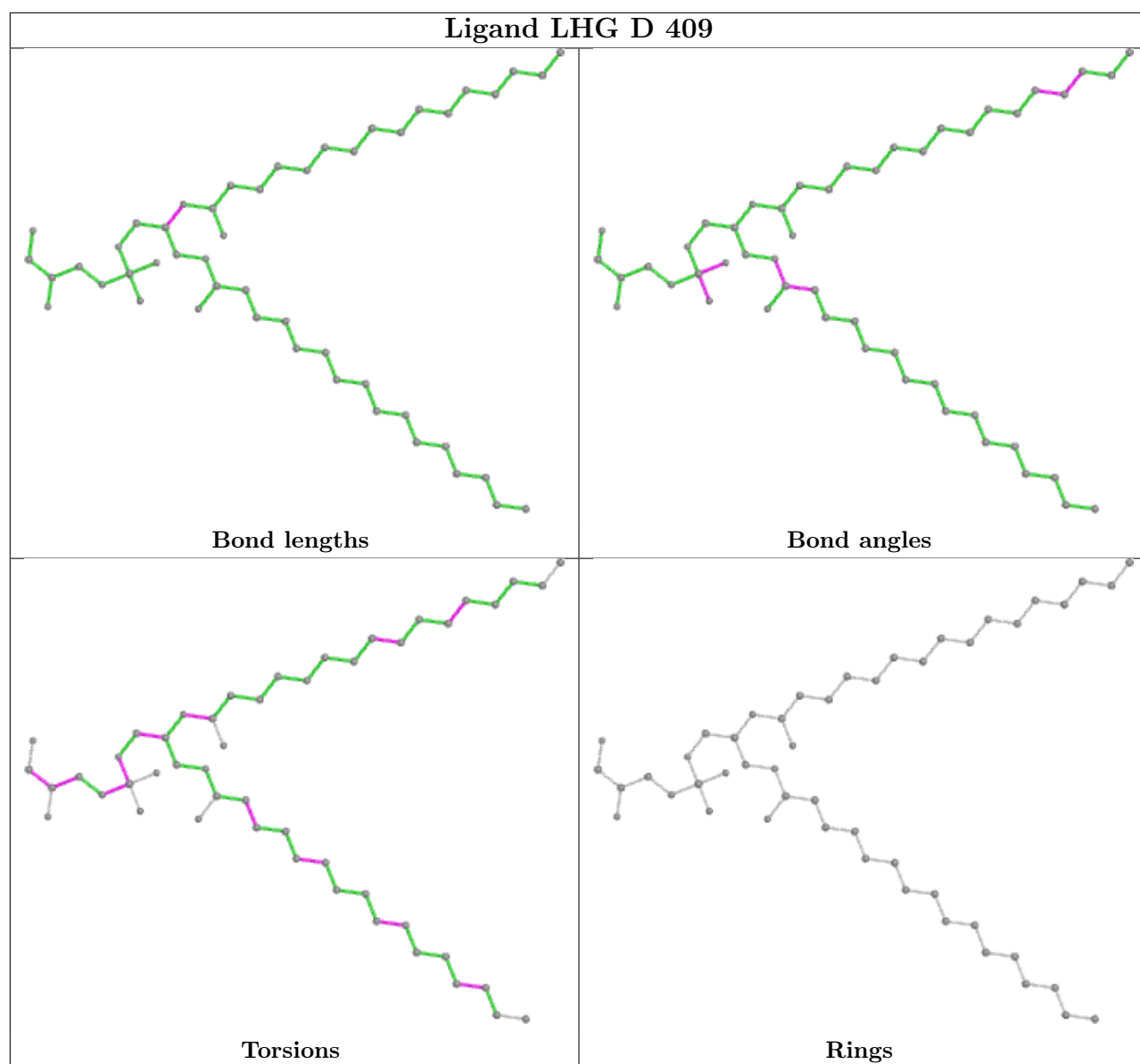
5 of 1523 torsion outliers are listed below:

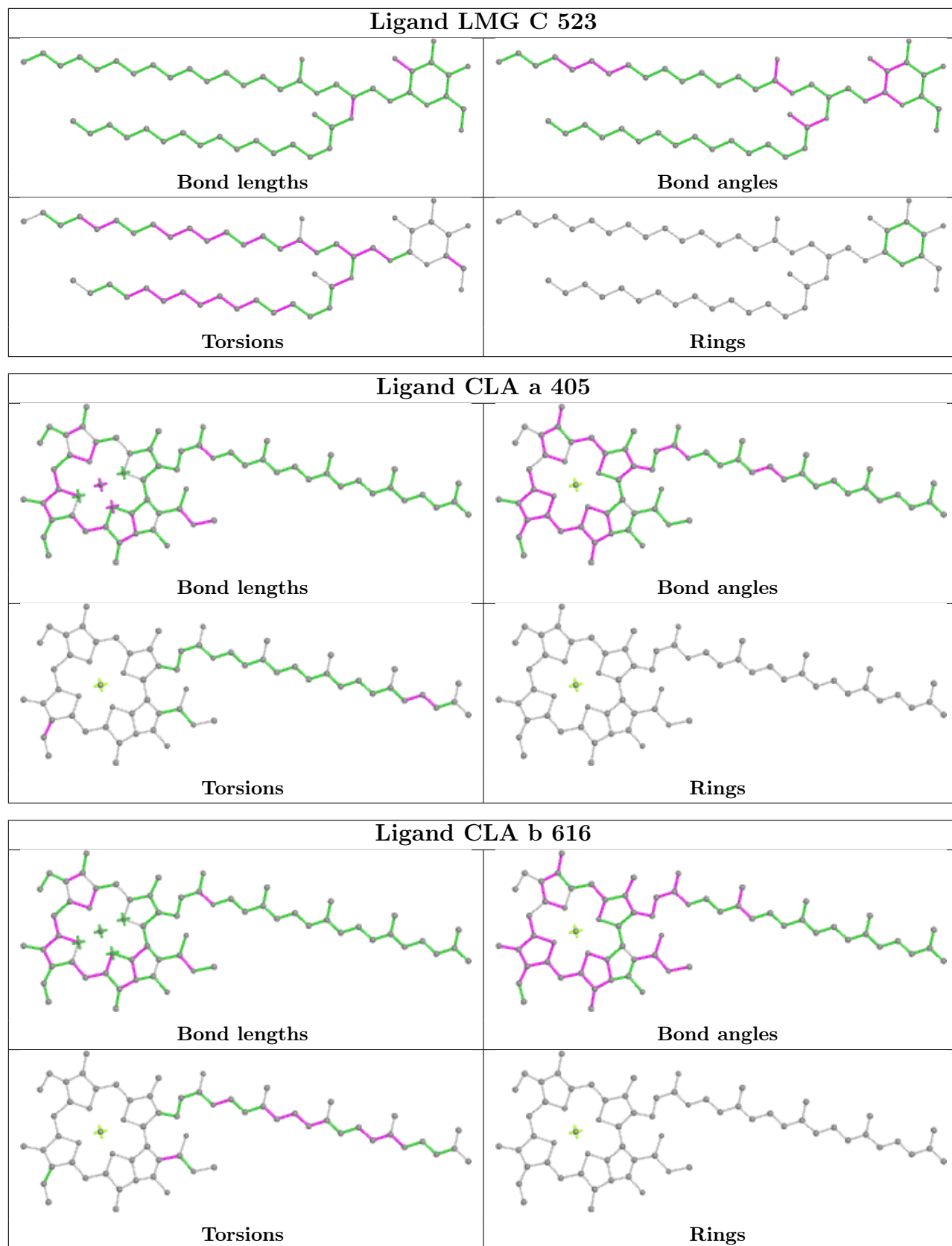
Mol	Chain	Res	Type	Atoms
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	601	CLA	C14-C13-C15-C16
24	B	603	CLA	C2-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6

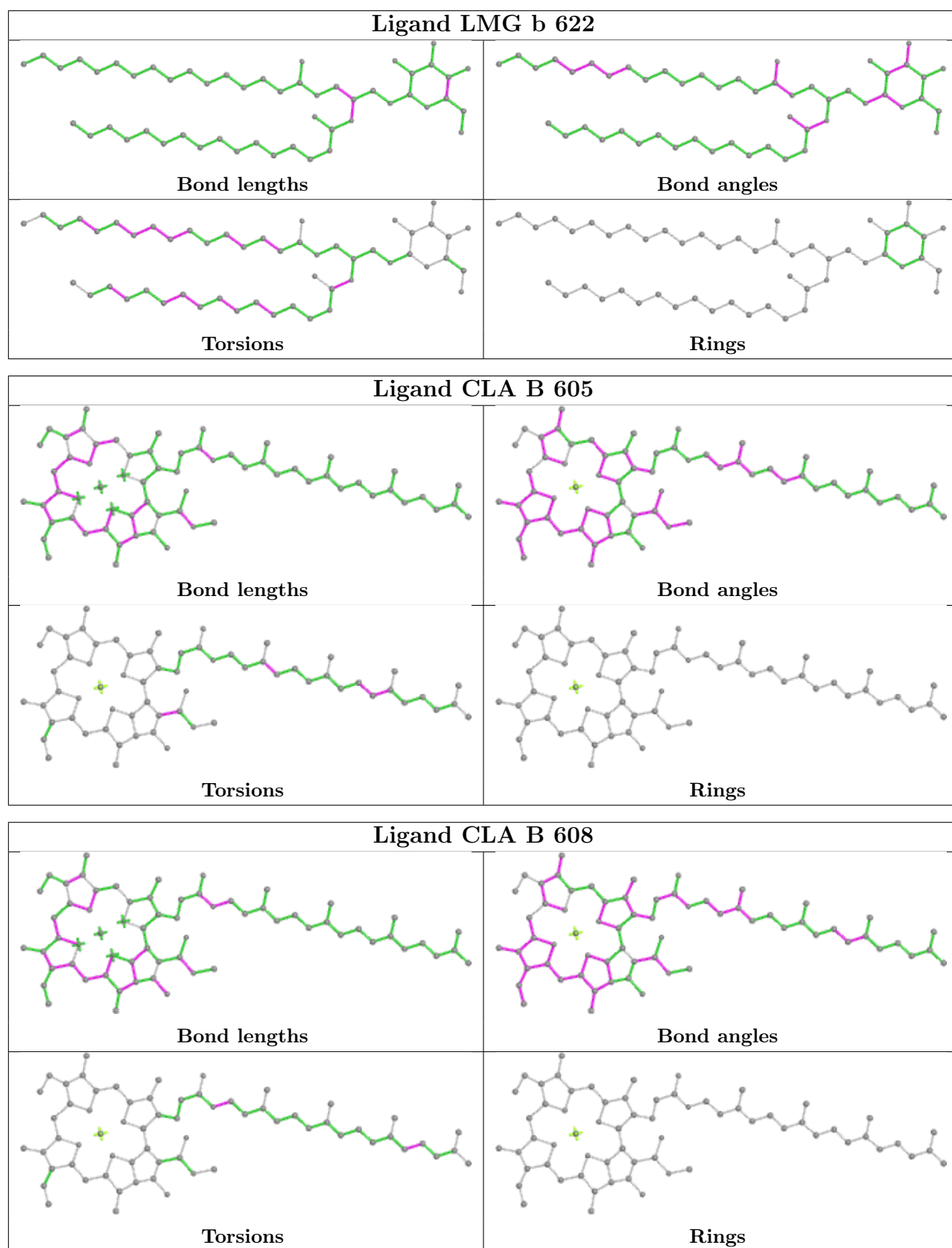
There are no ring outliers.

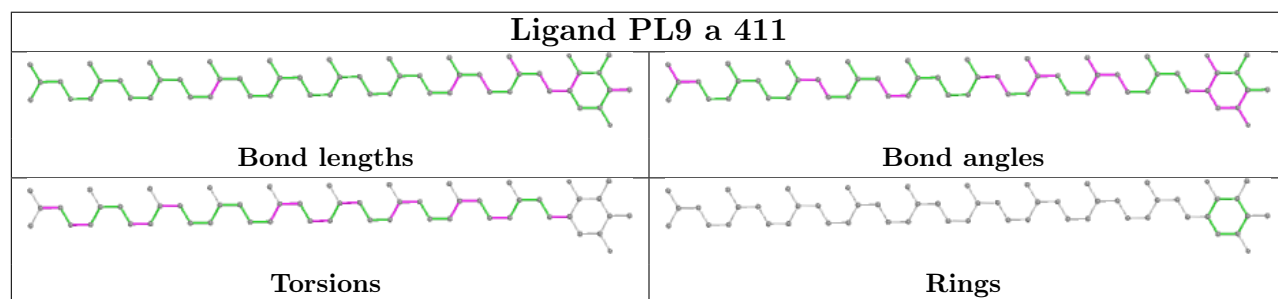
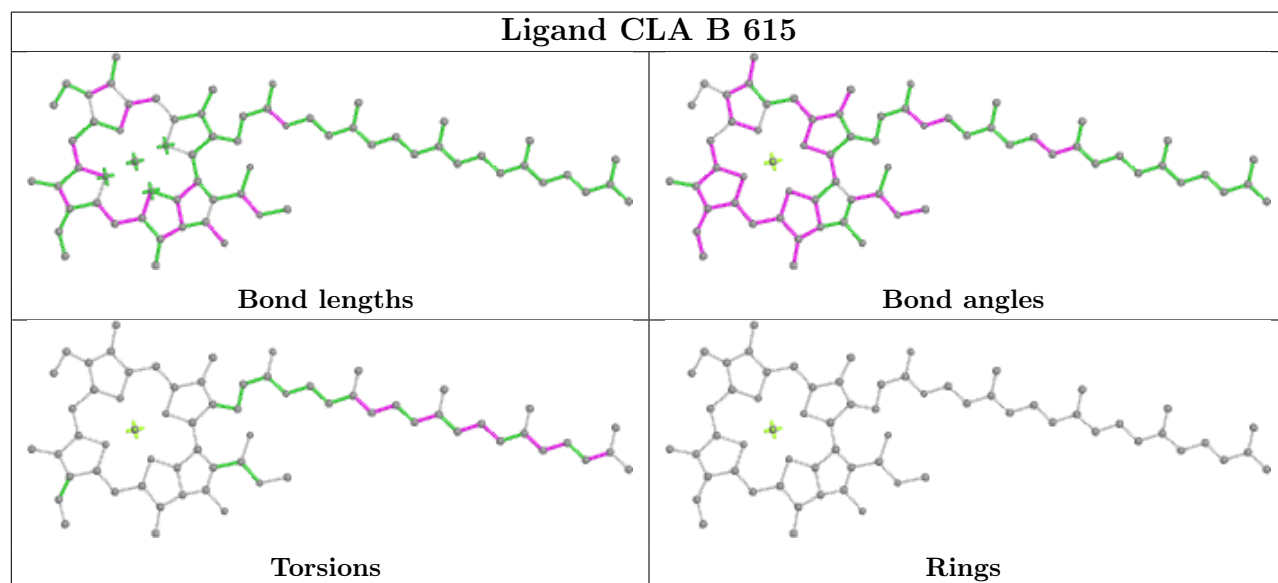
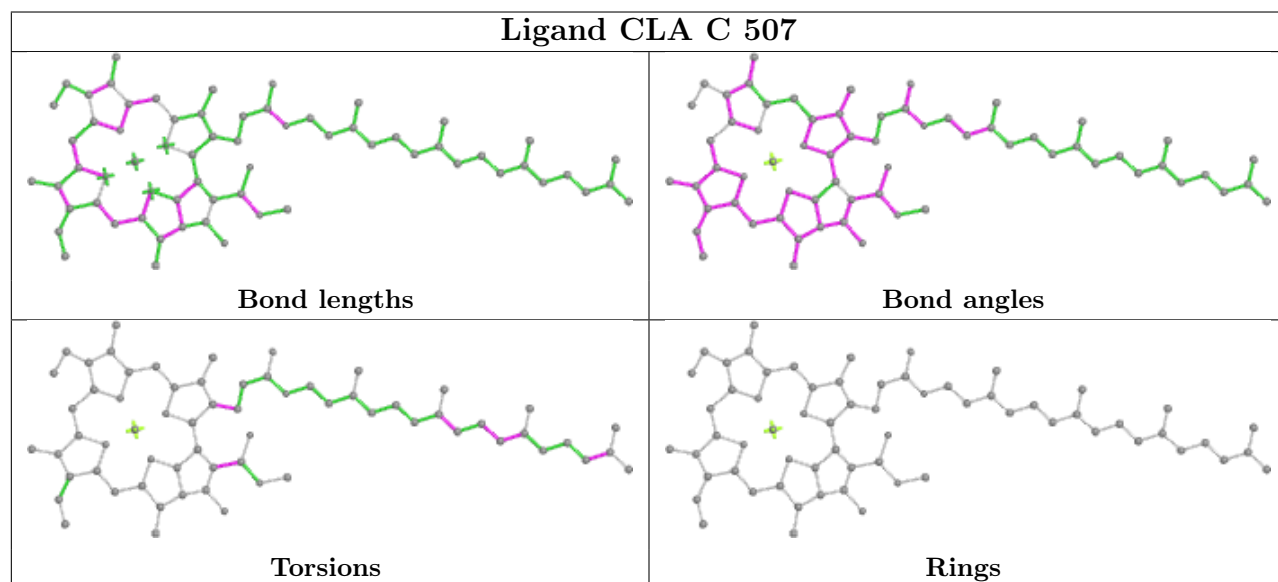
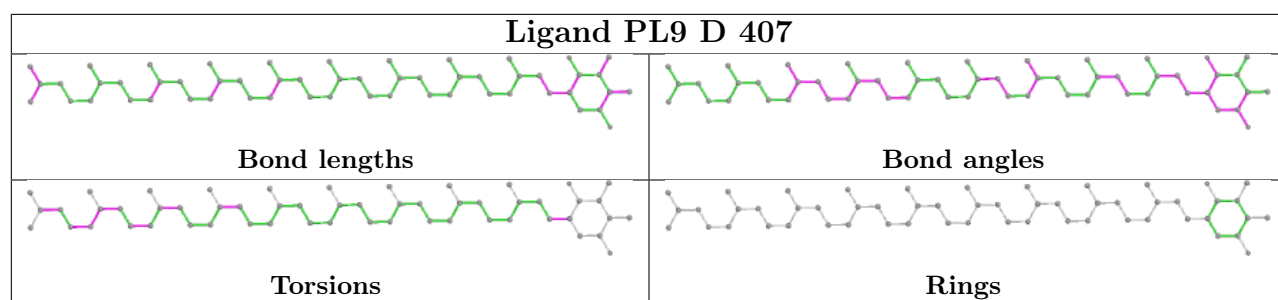
No monomer is involved in short contacts.

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

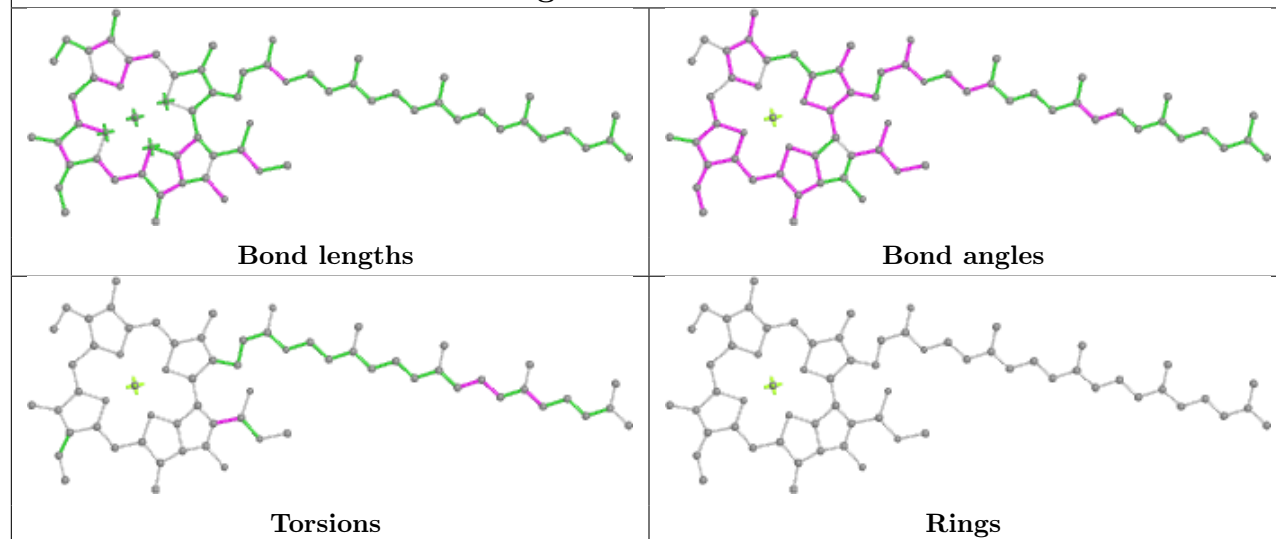




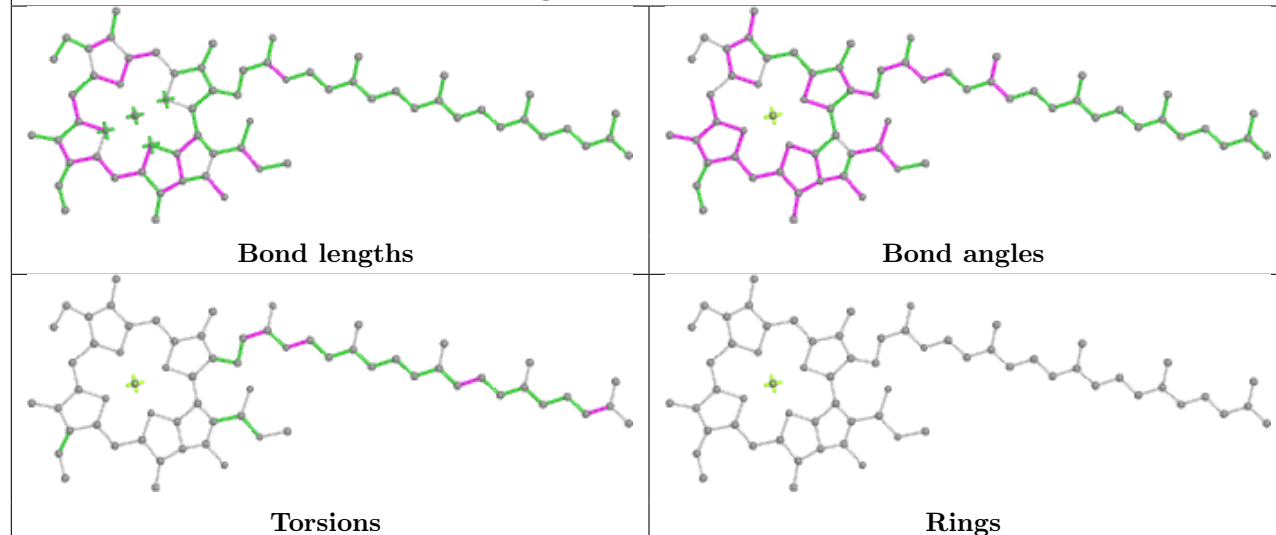




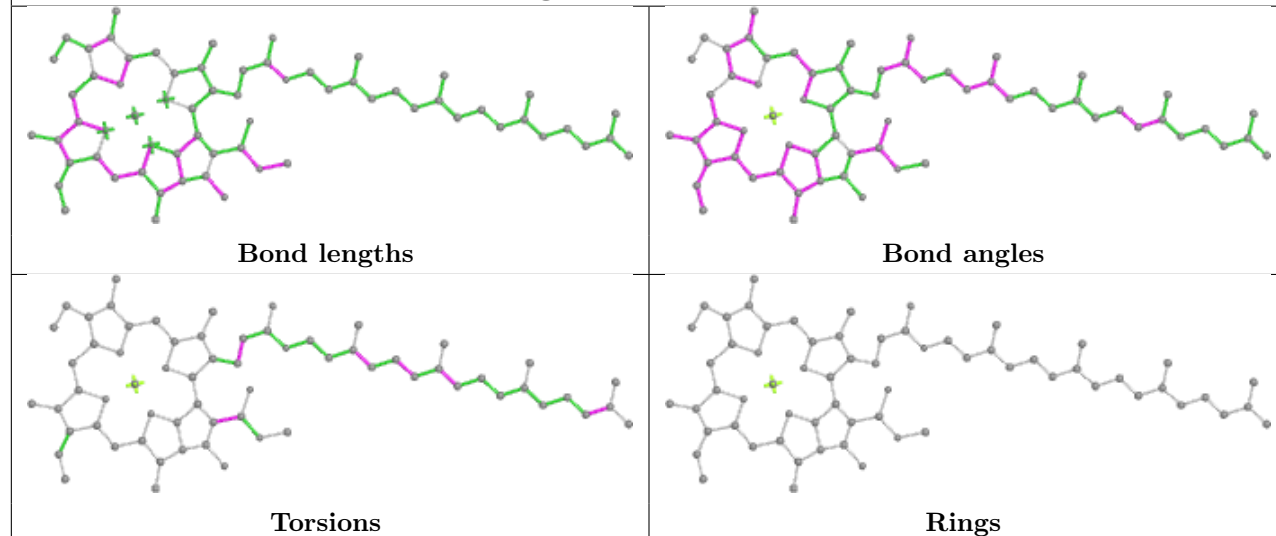
Ligand CLA c 509



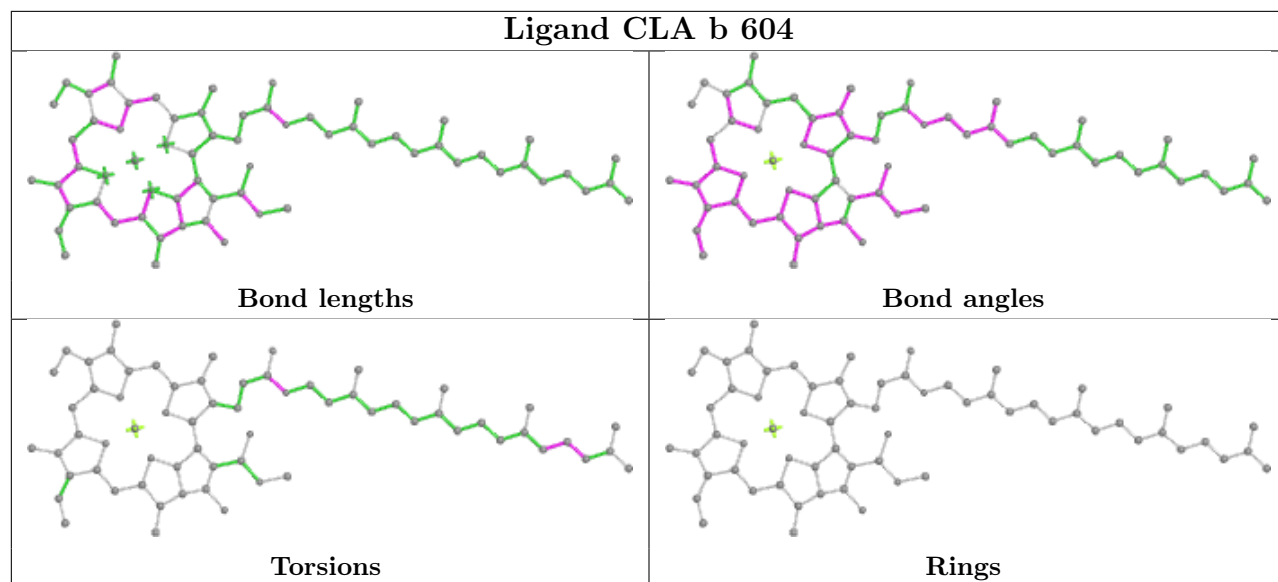
Ligand CLA c 511



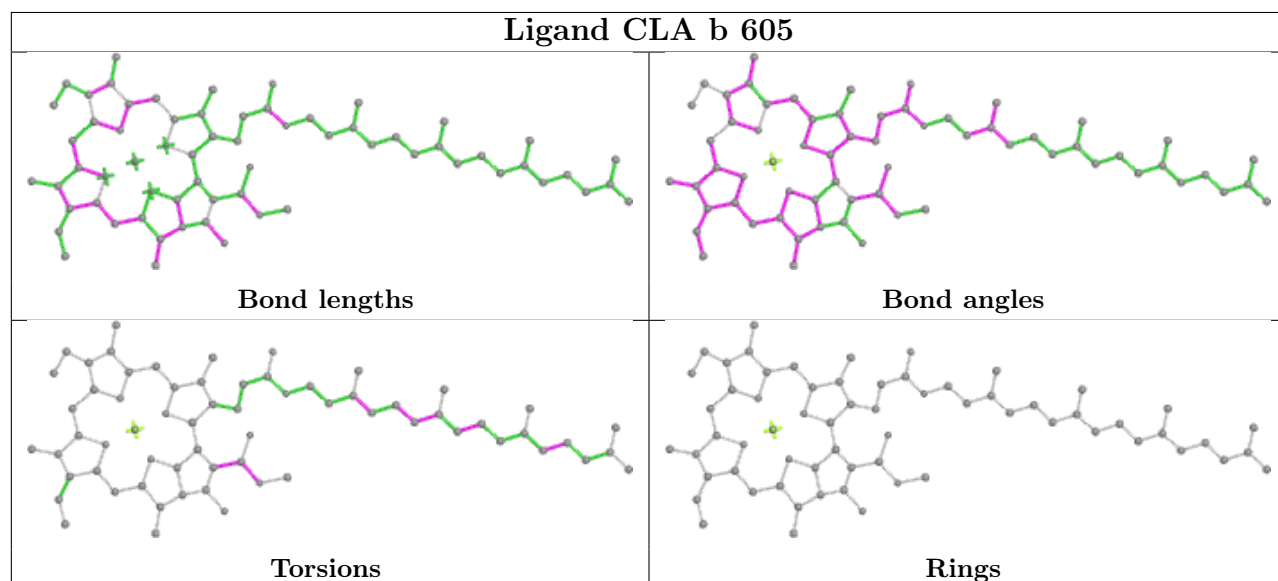
Ligand CLA c 508



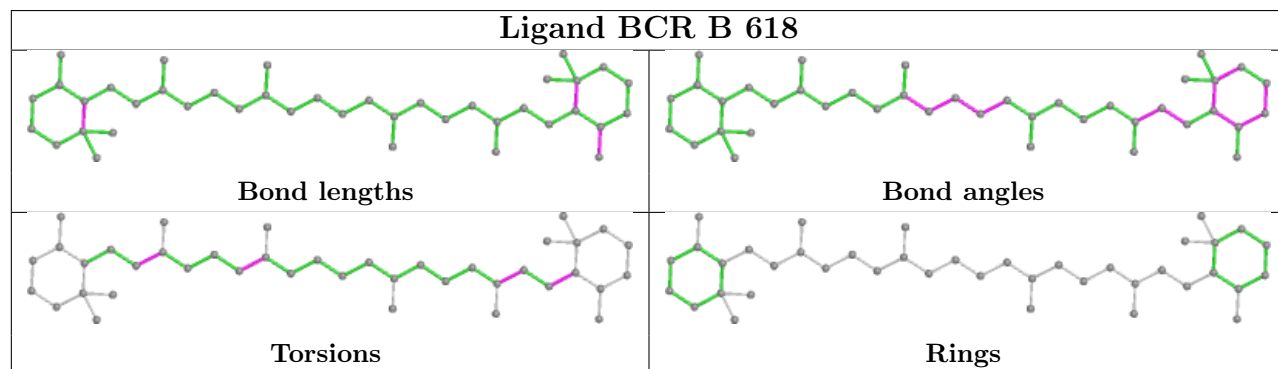
Ligand CLA b 604

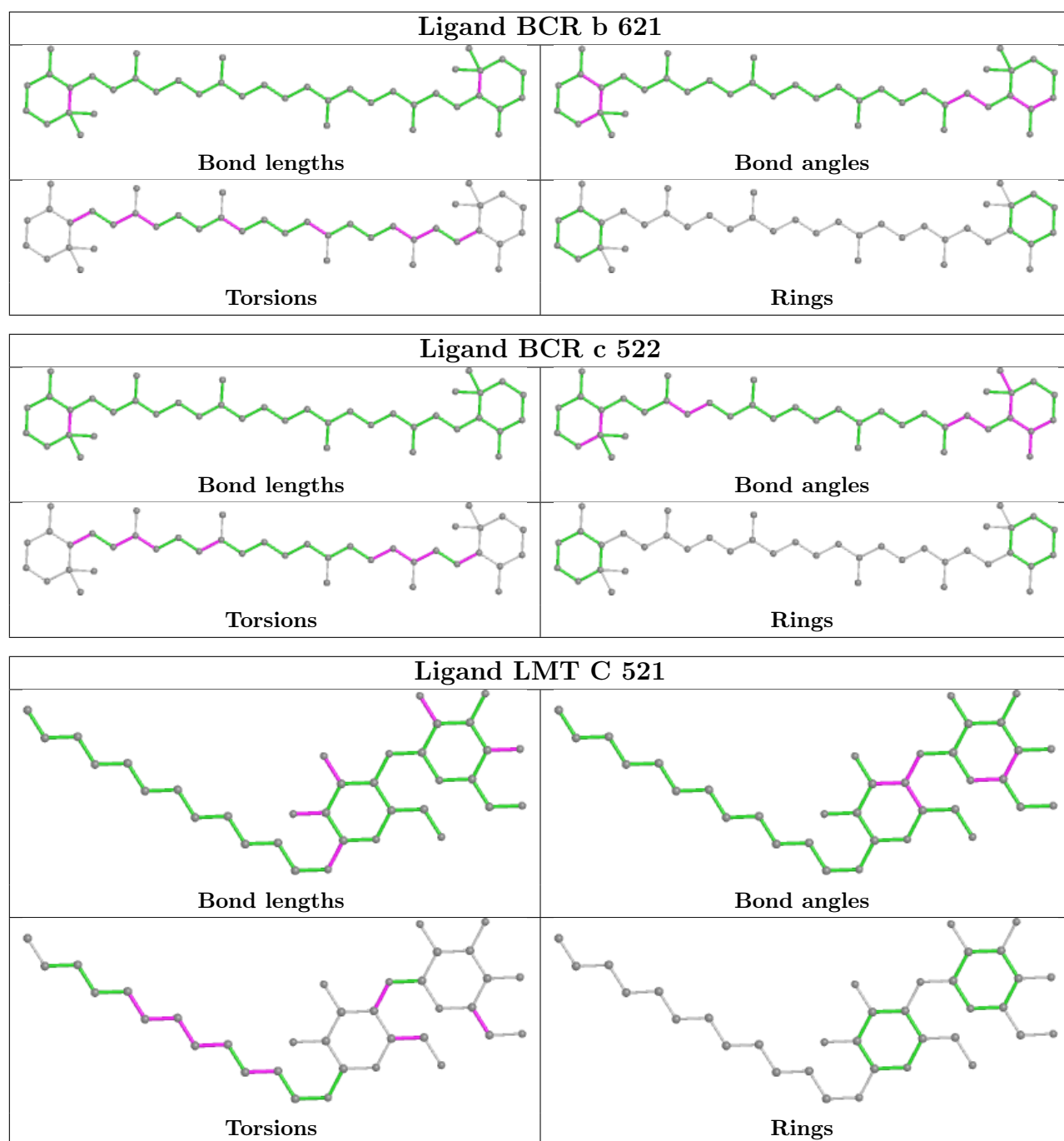


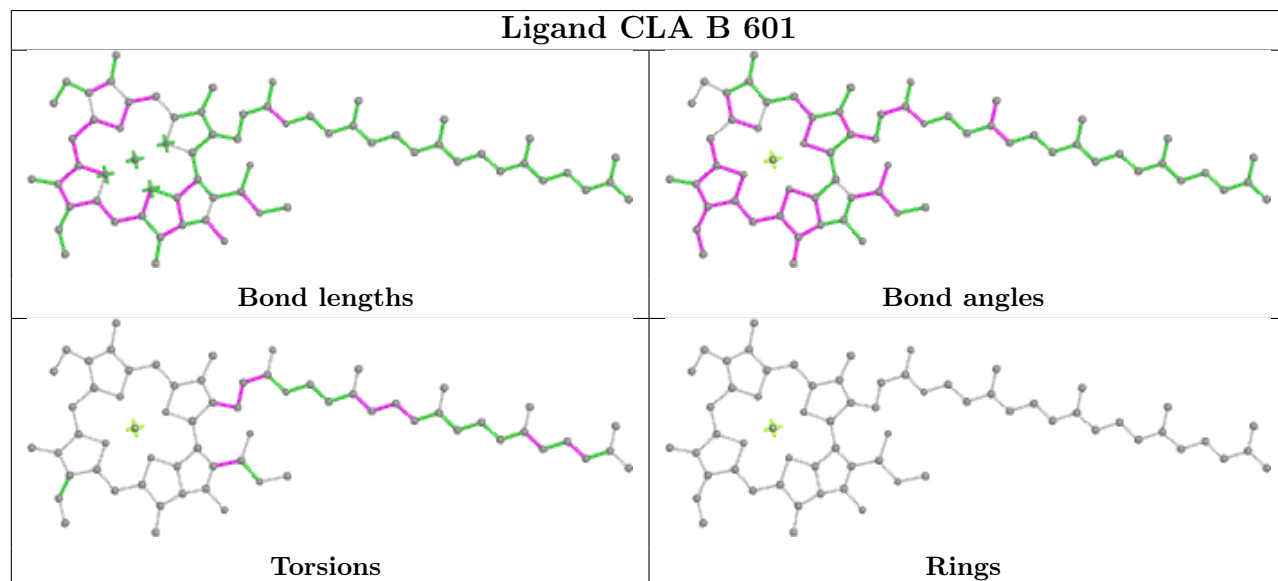
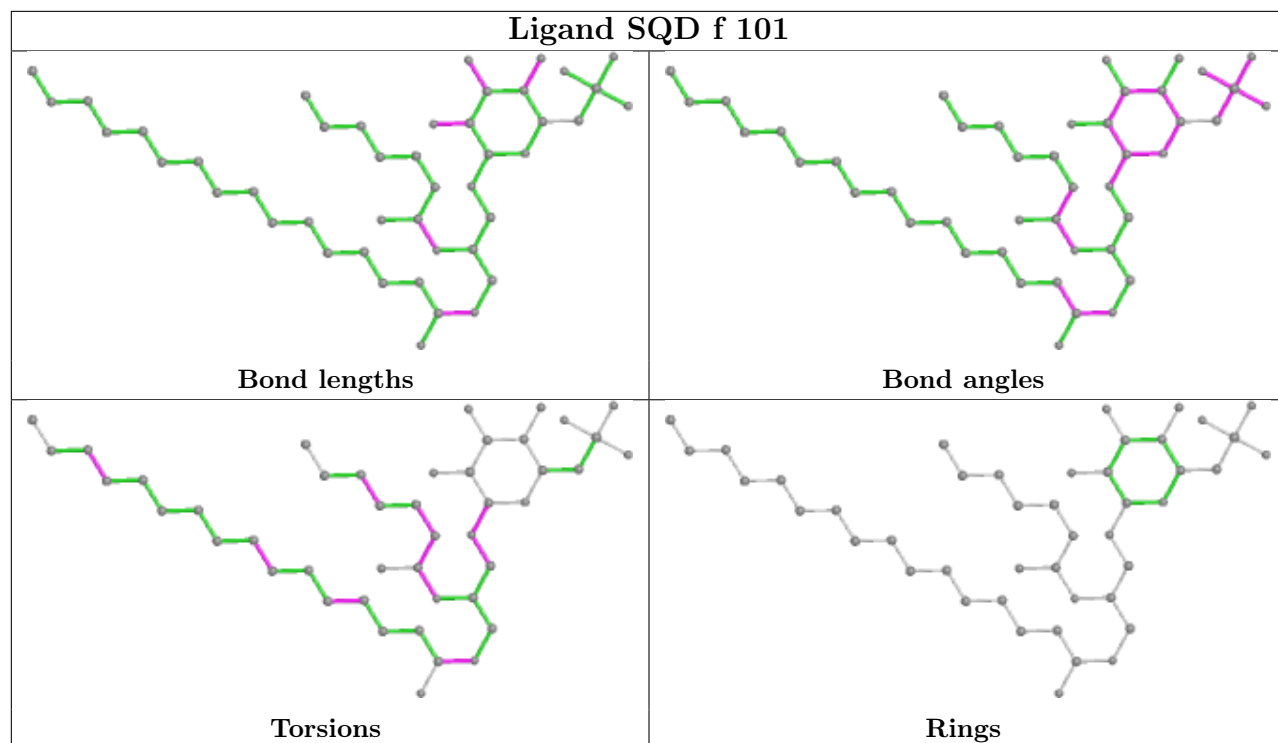
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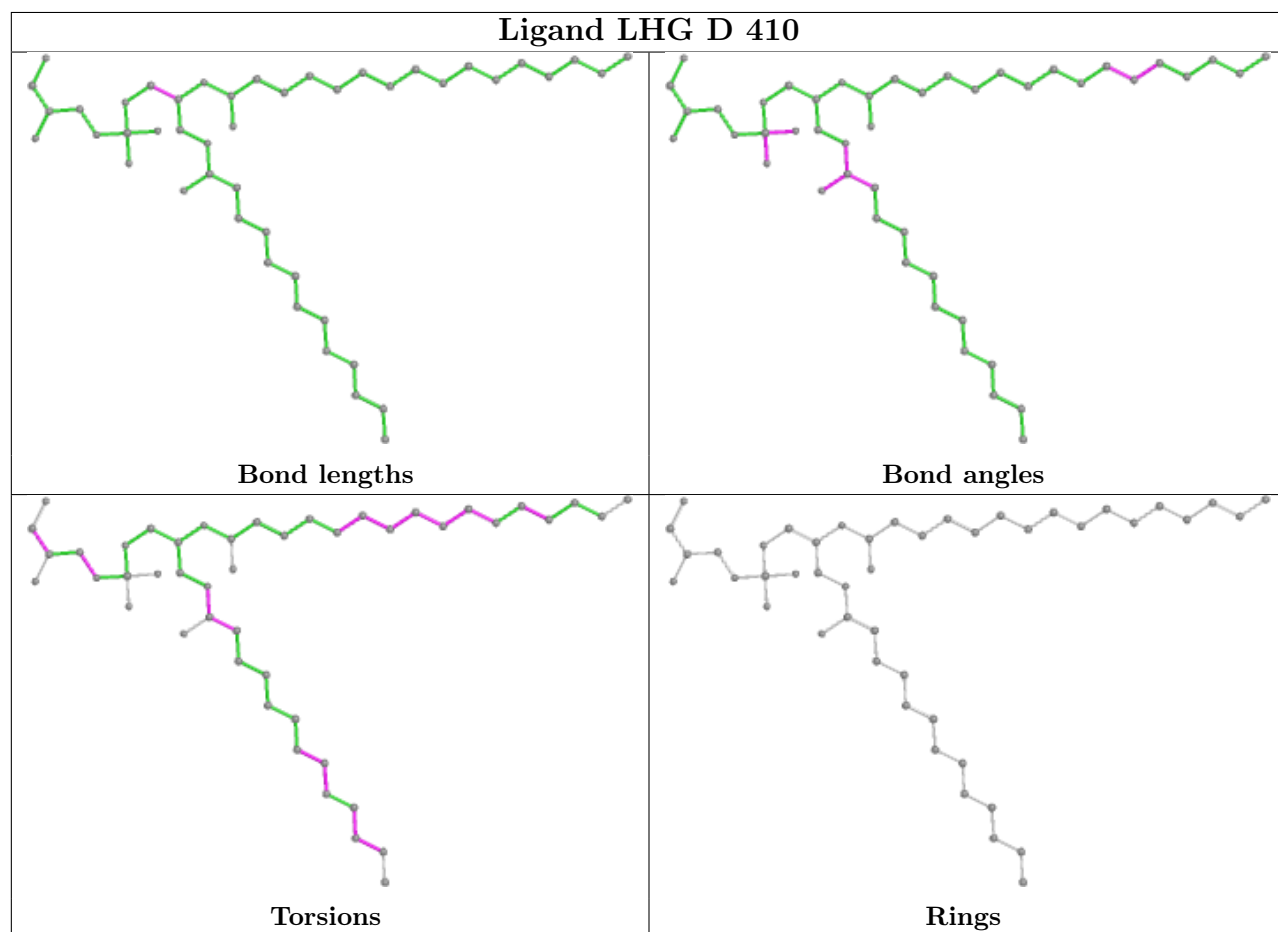
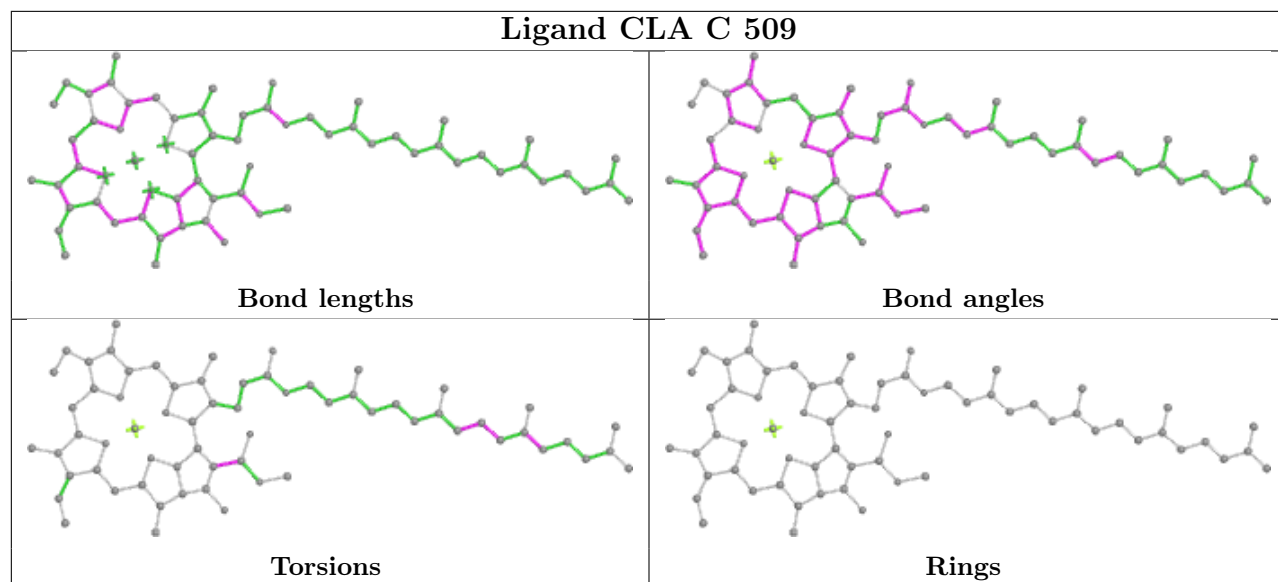


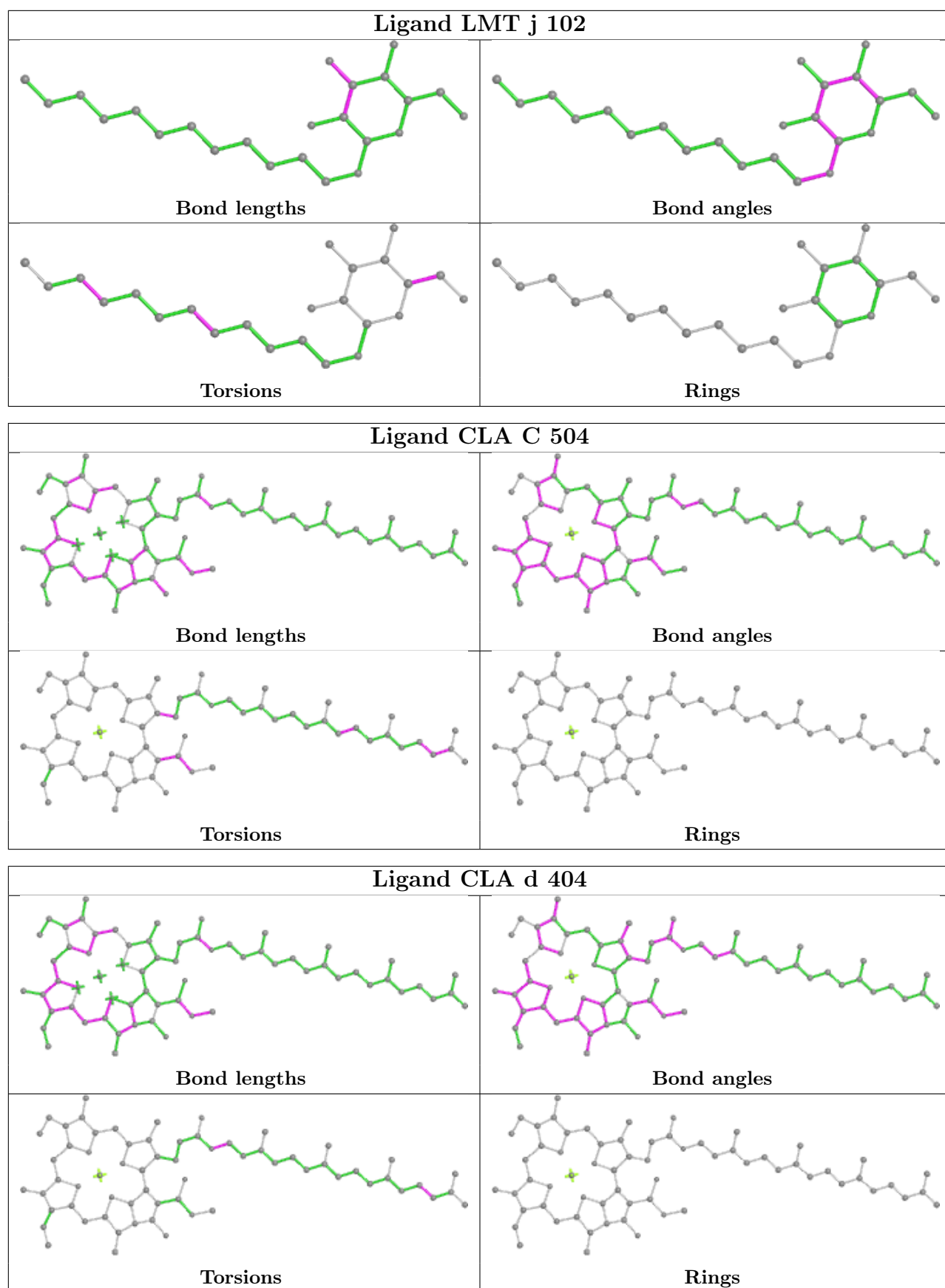
Ligand BCR B 618

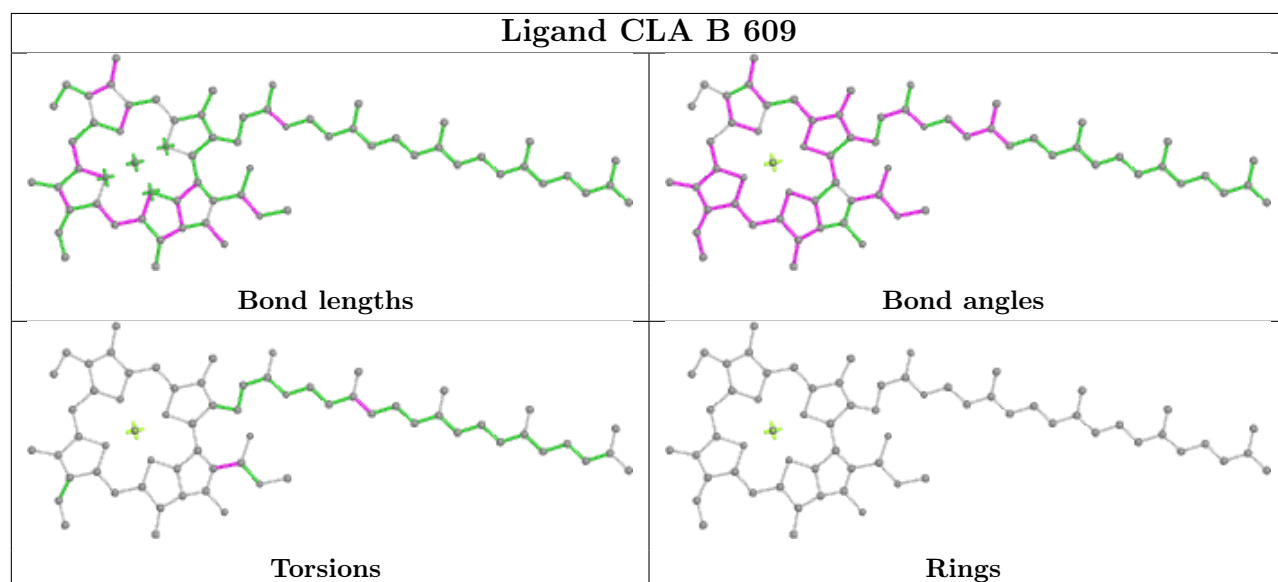
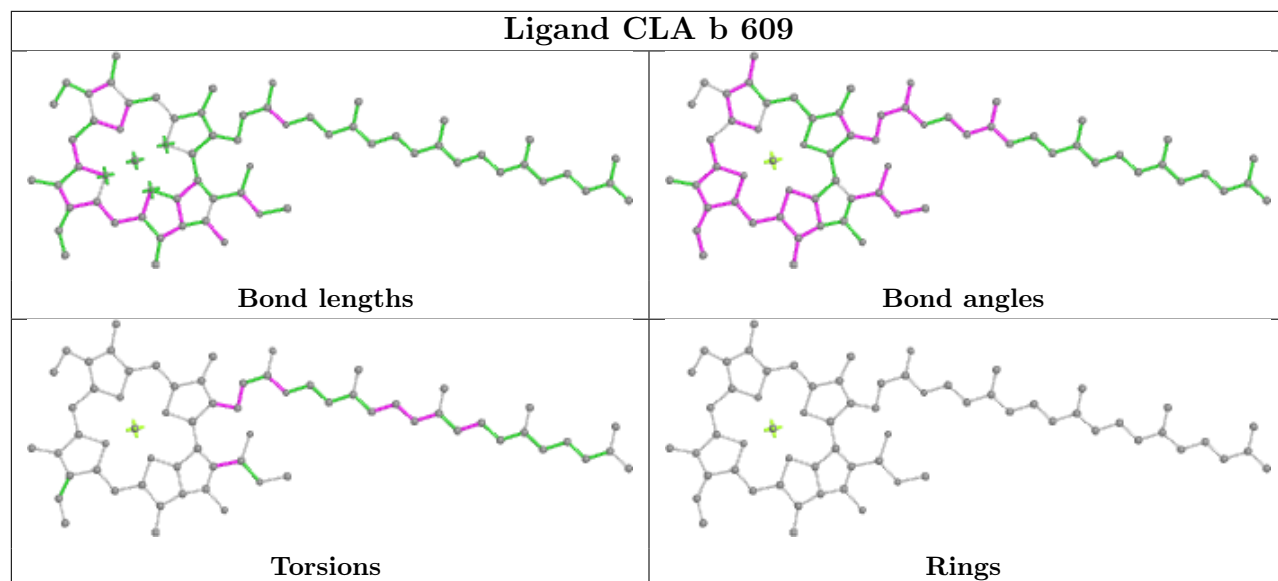
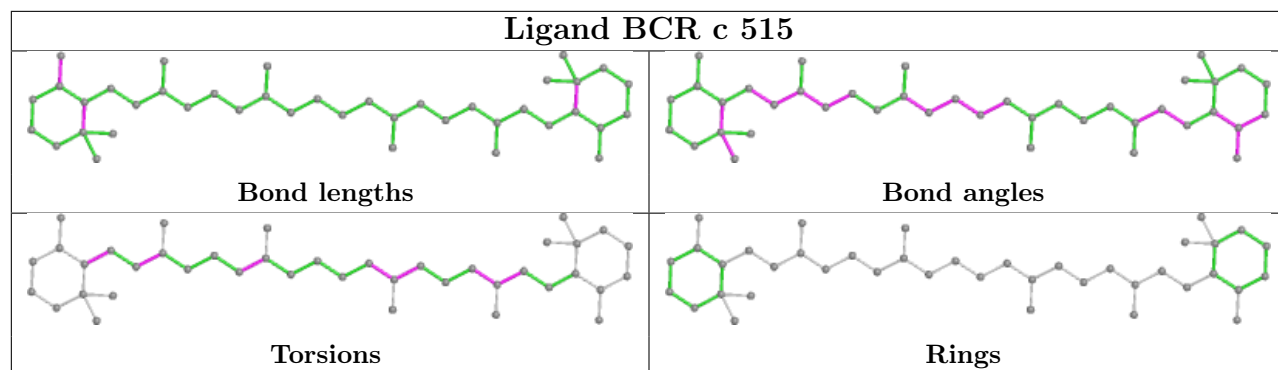


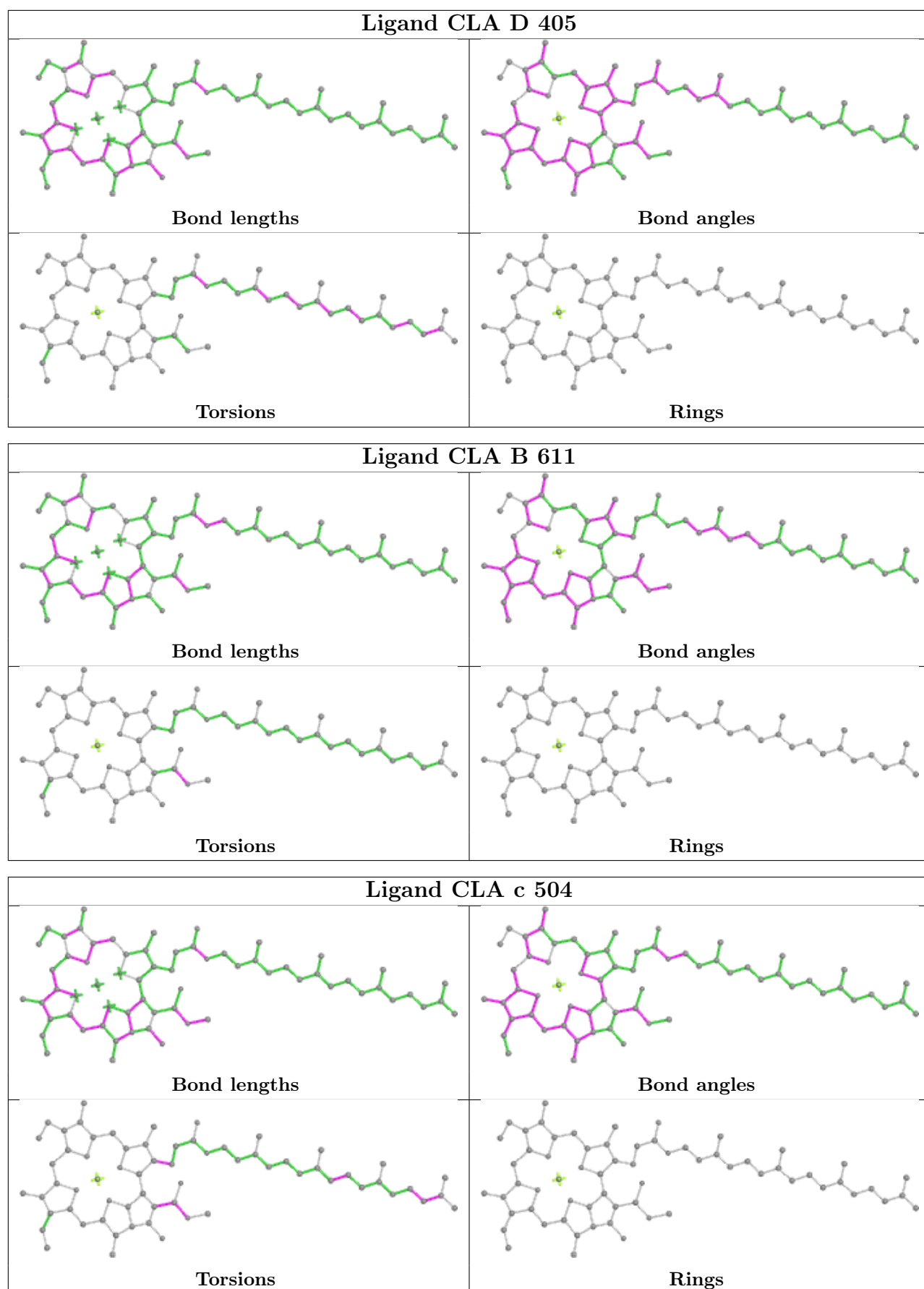


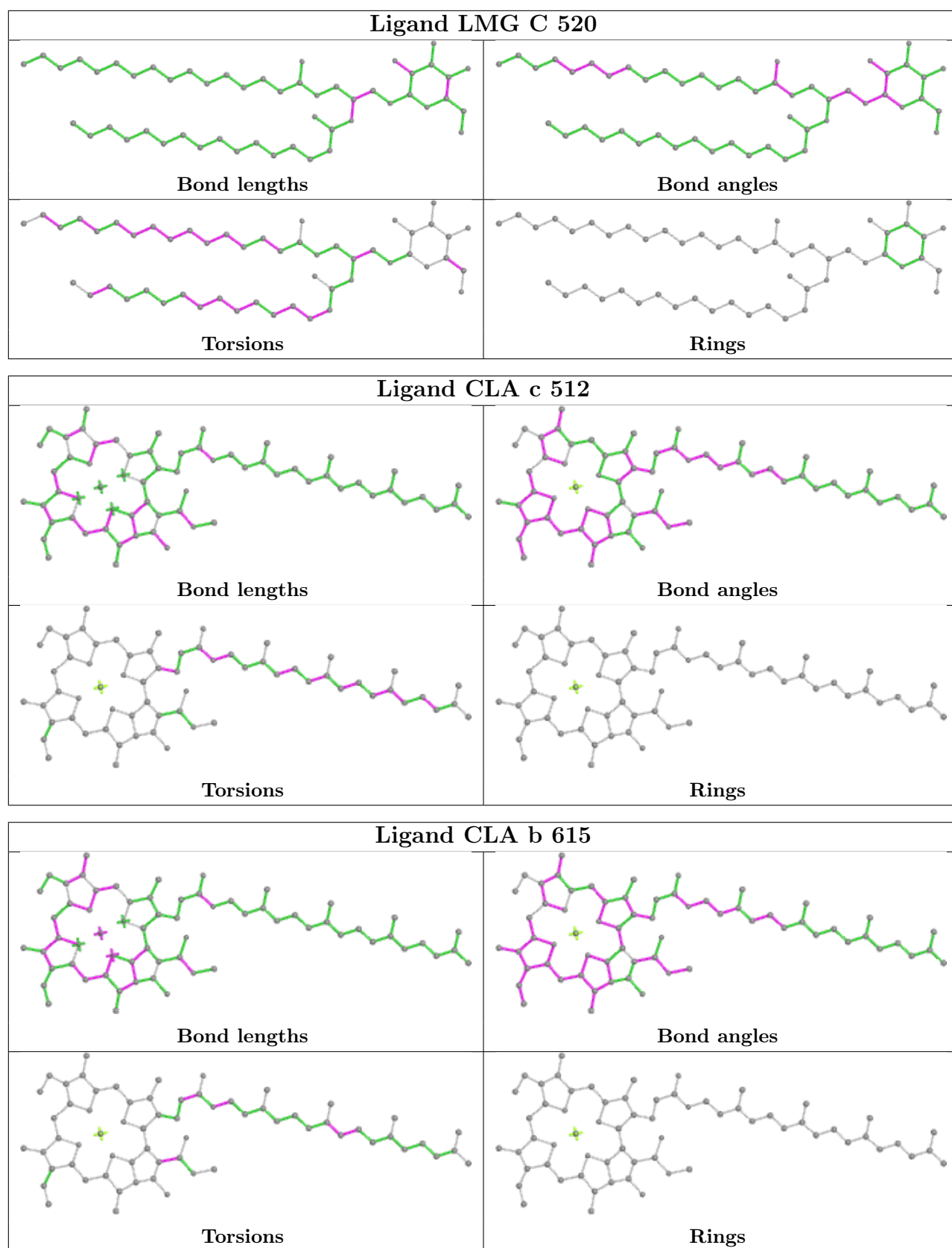


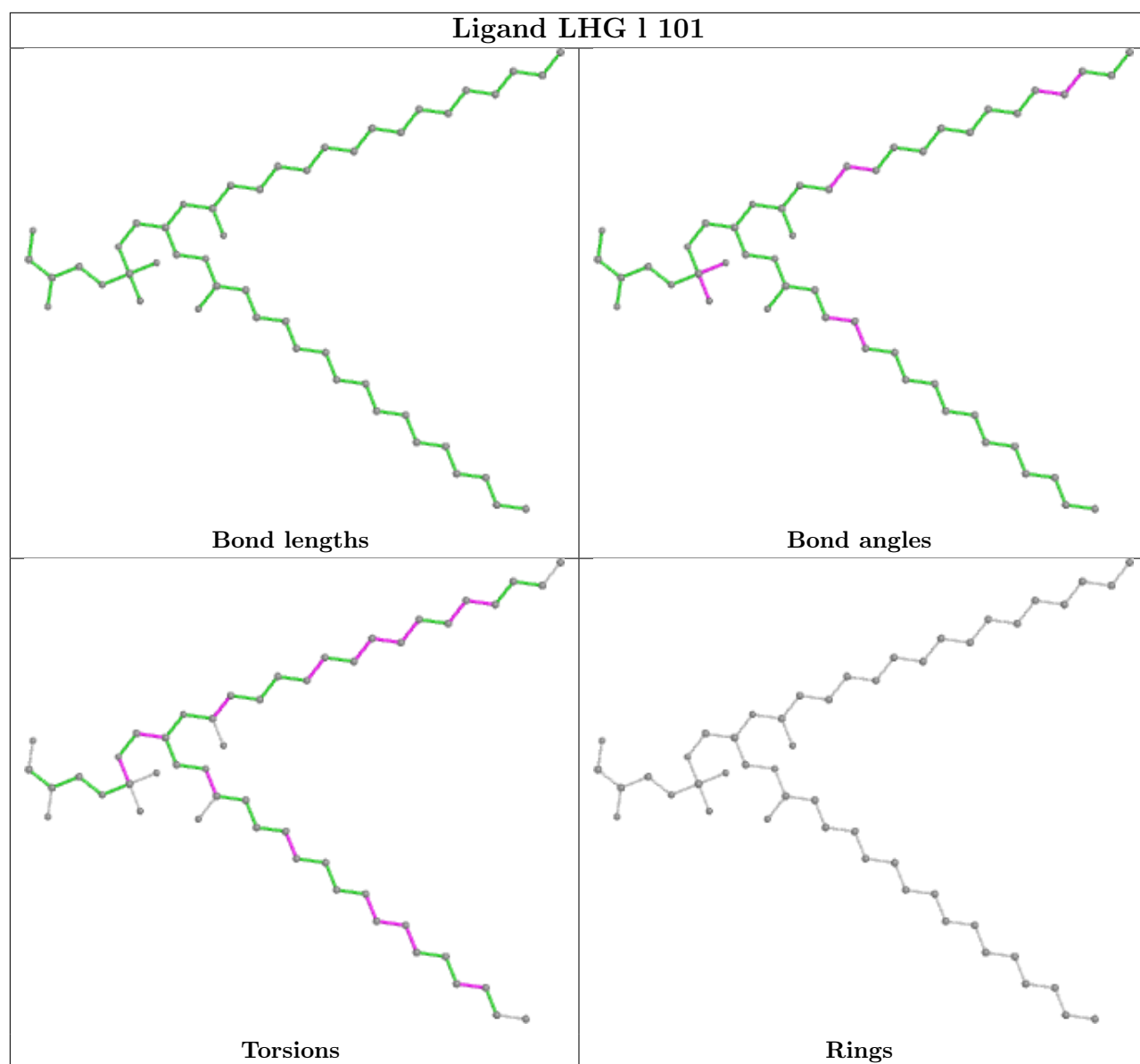


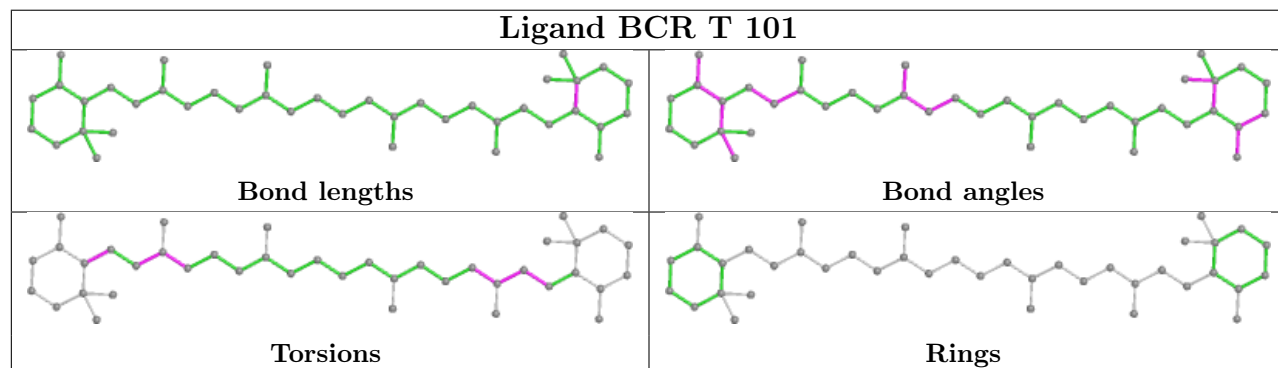
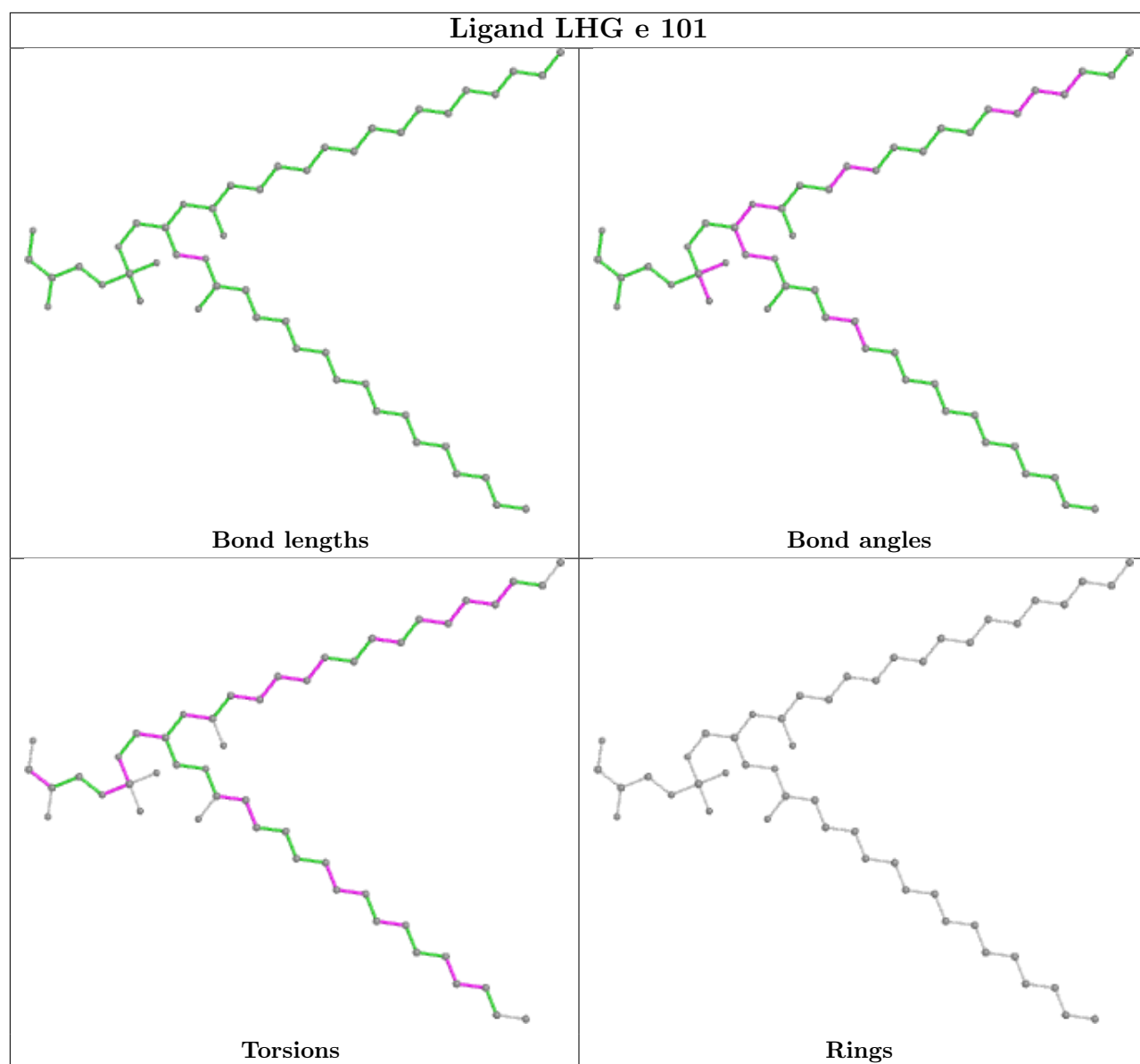


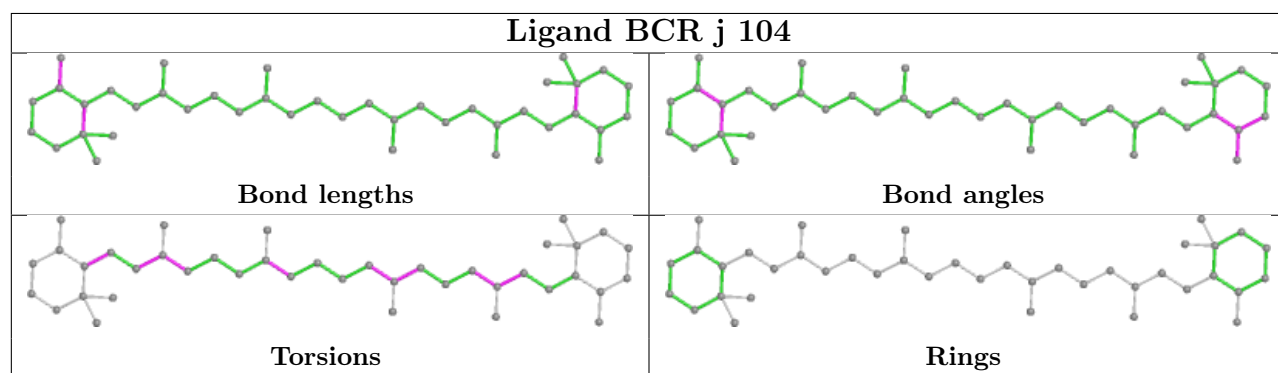
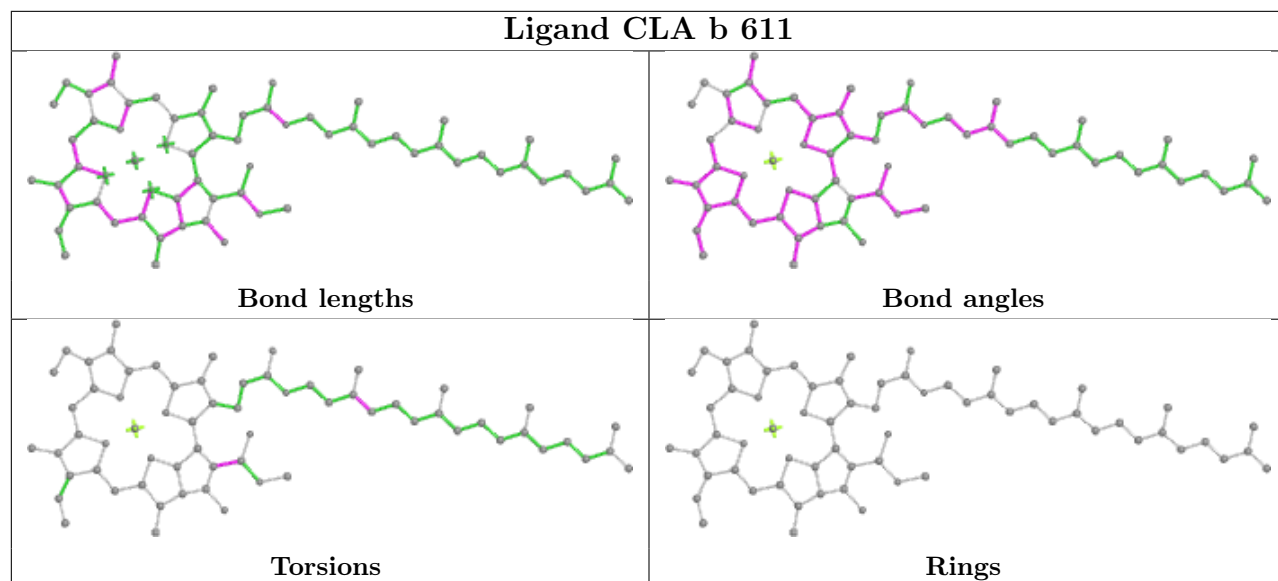
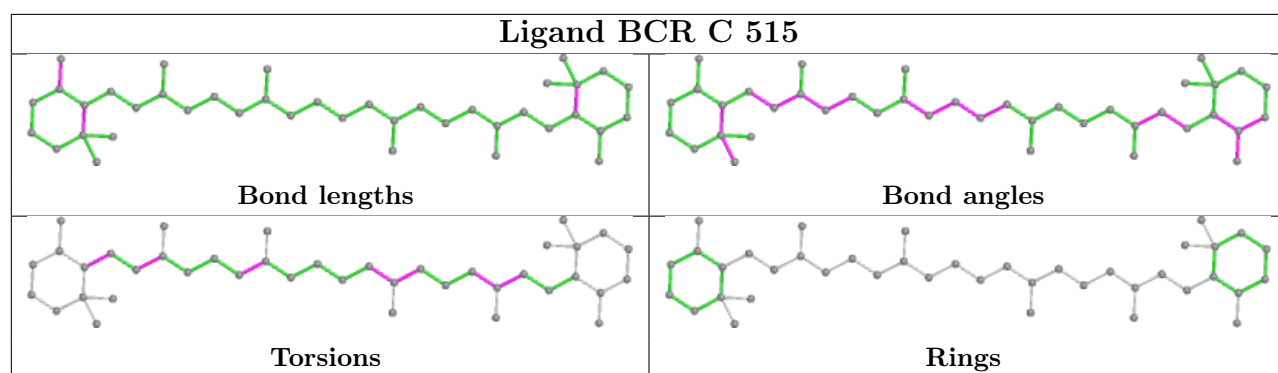


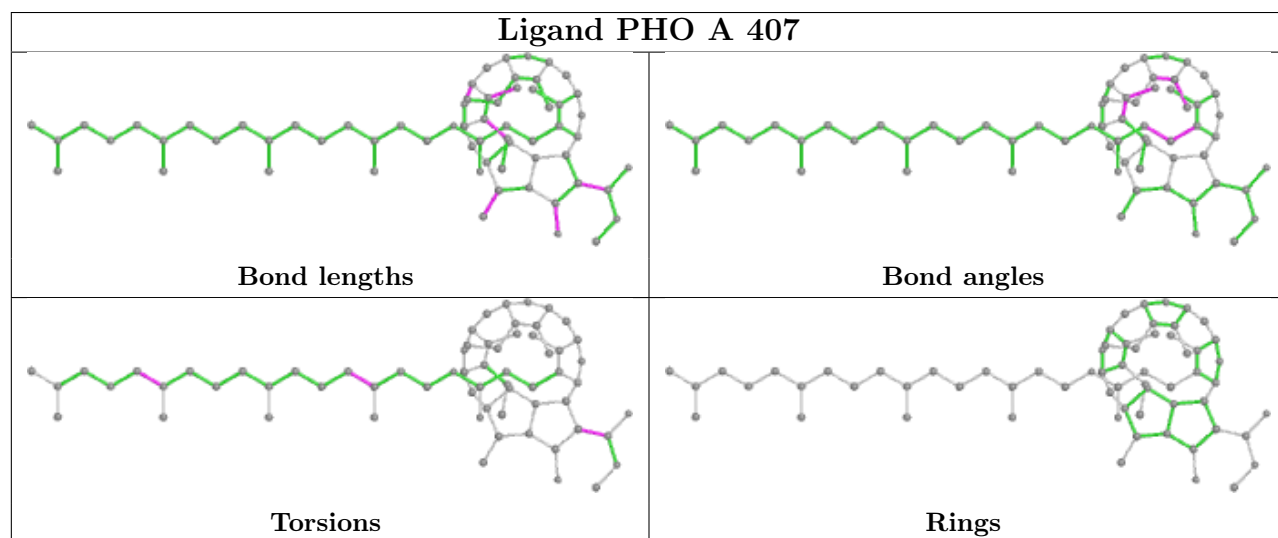
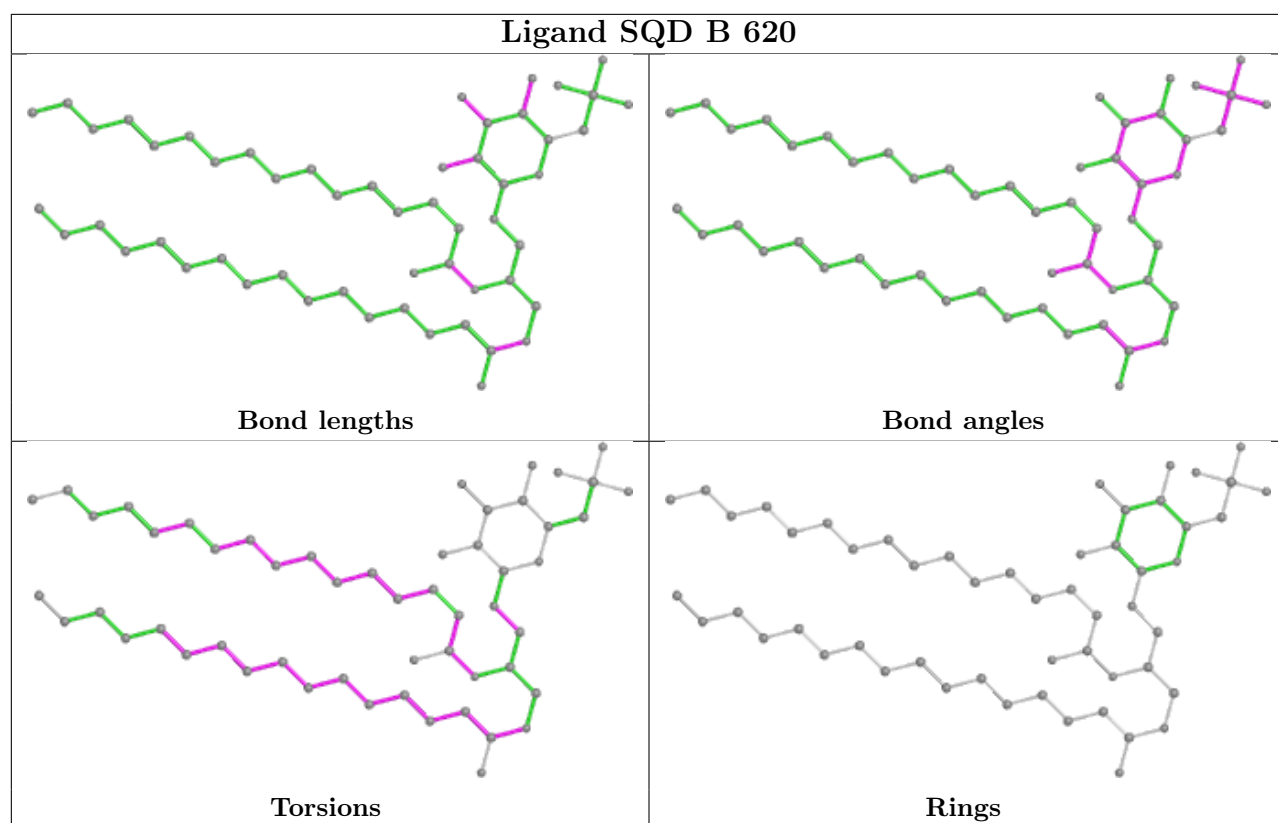


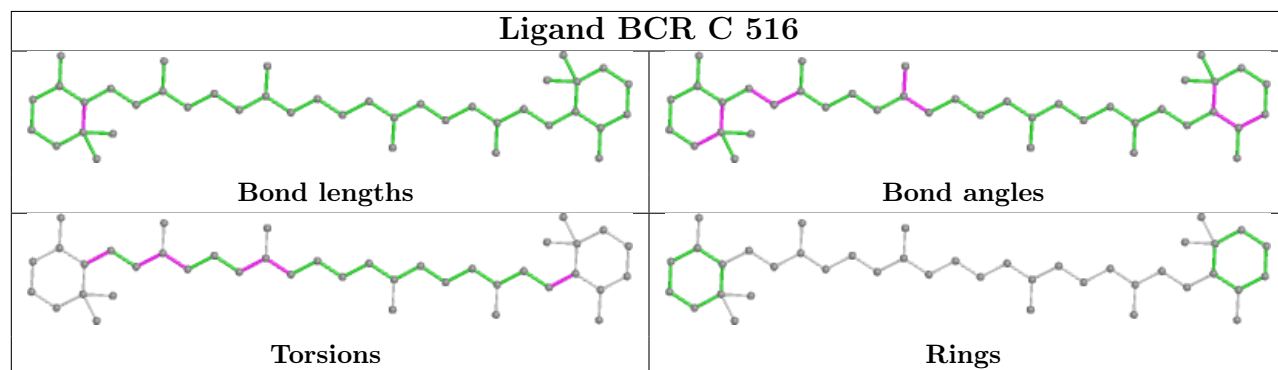
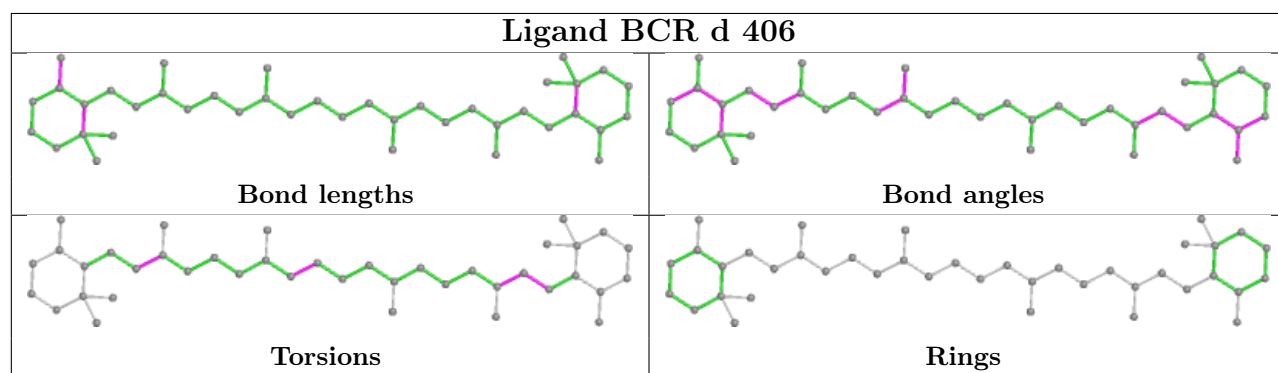
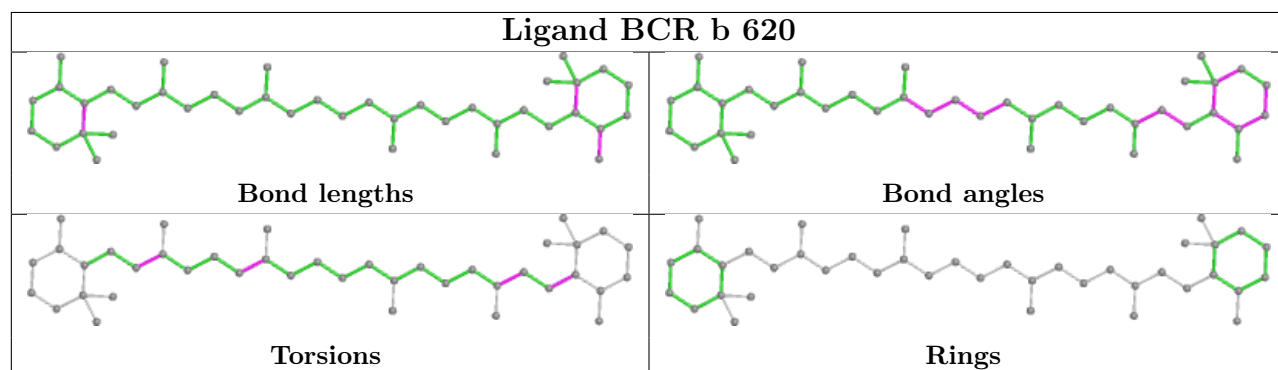
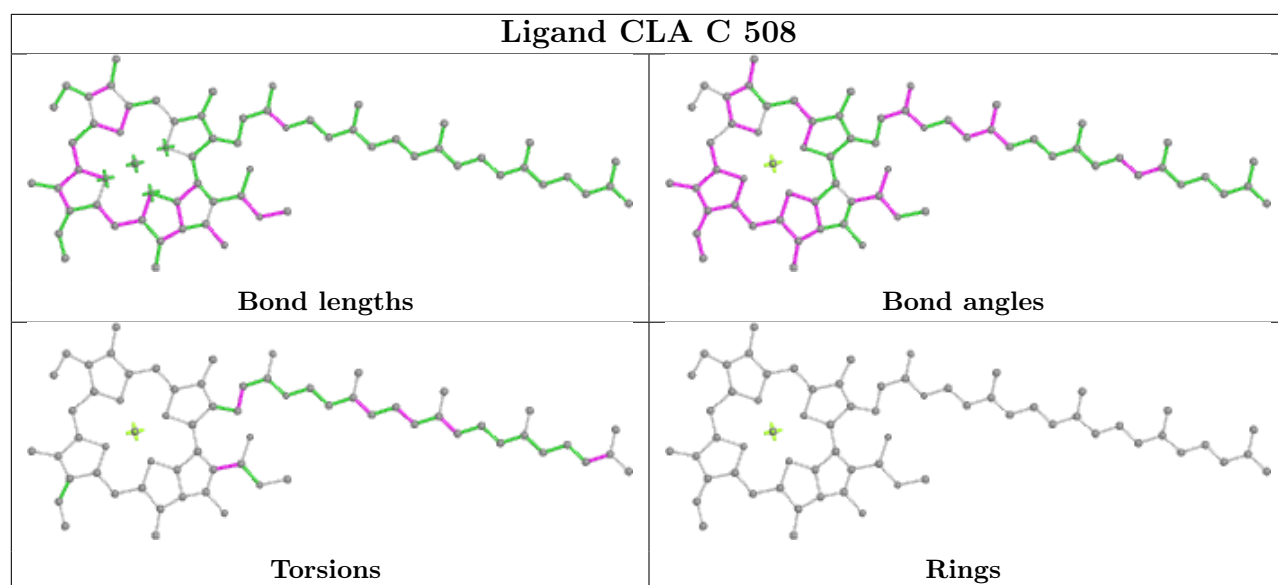


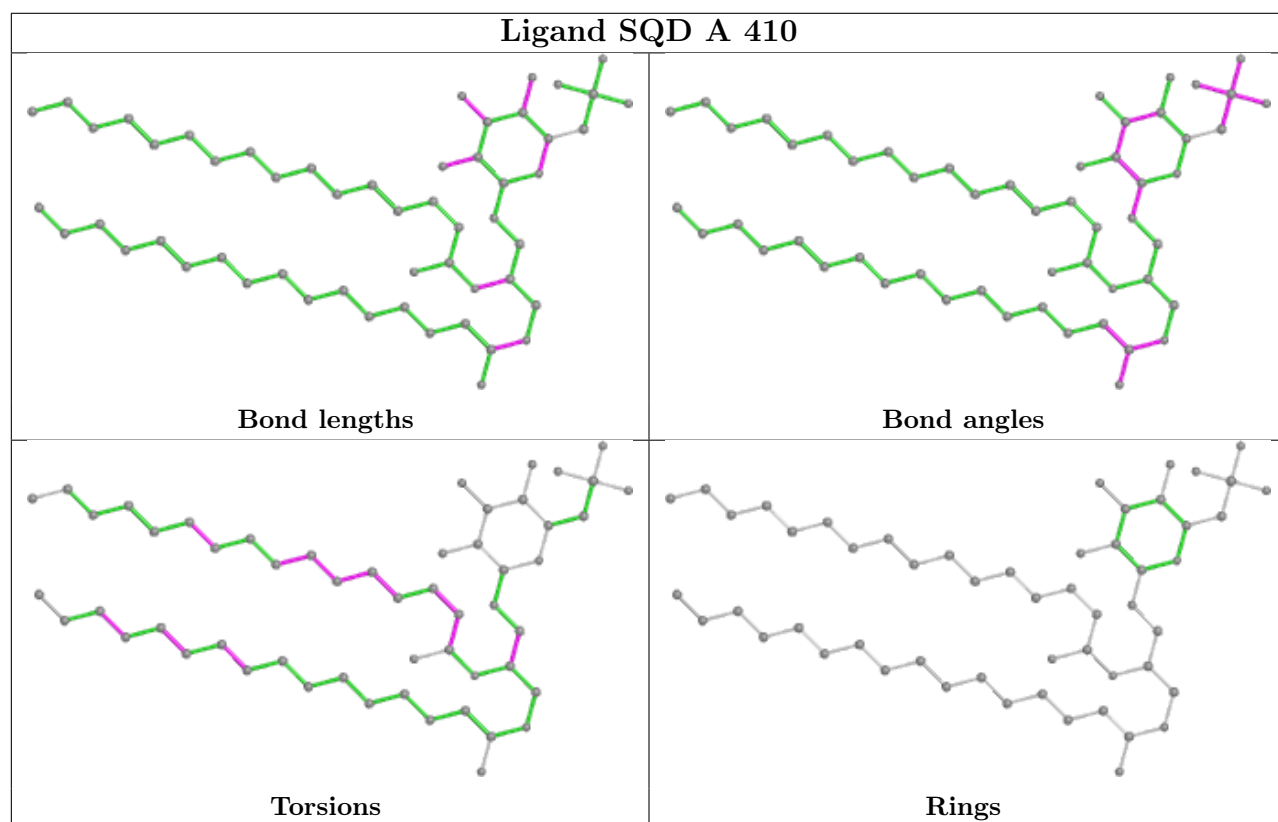
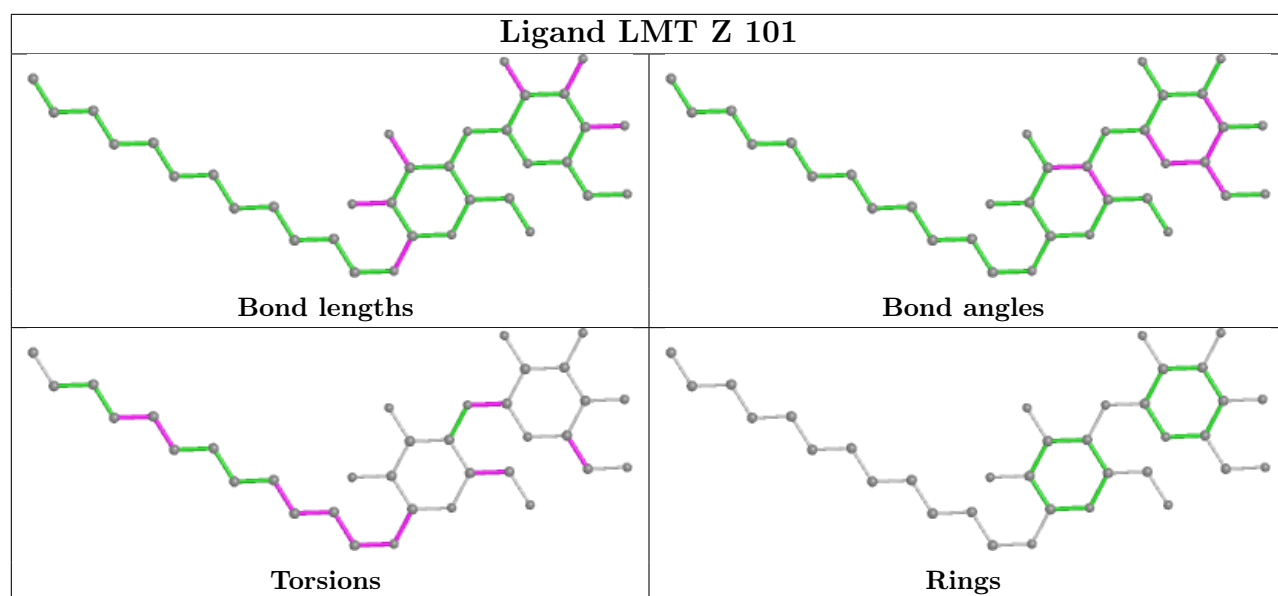


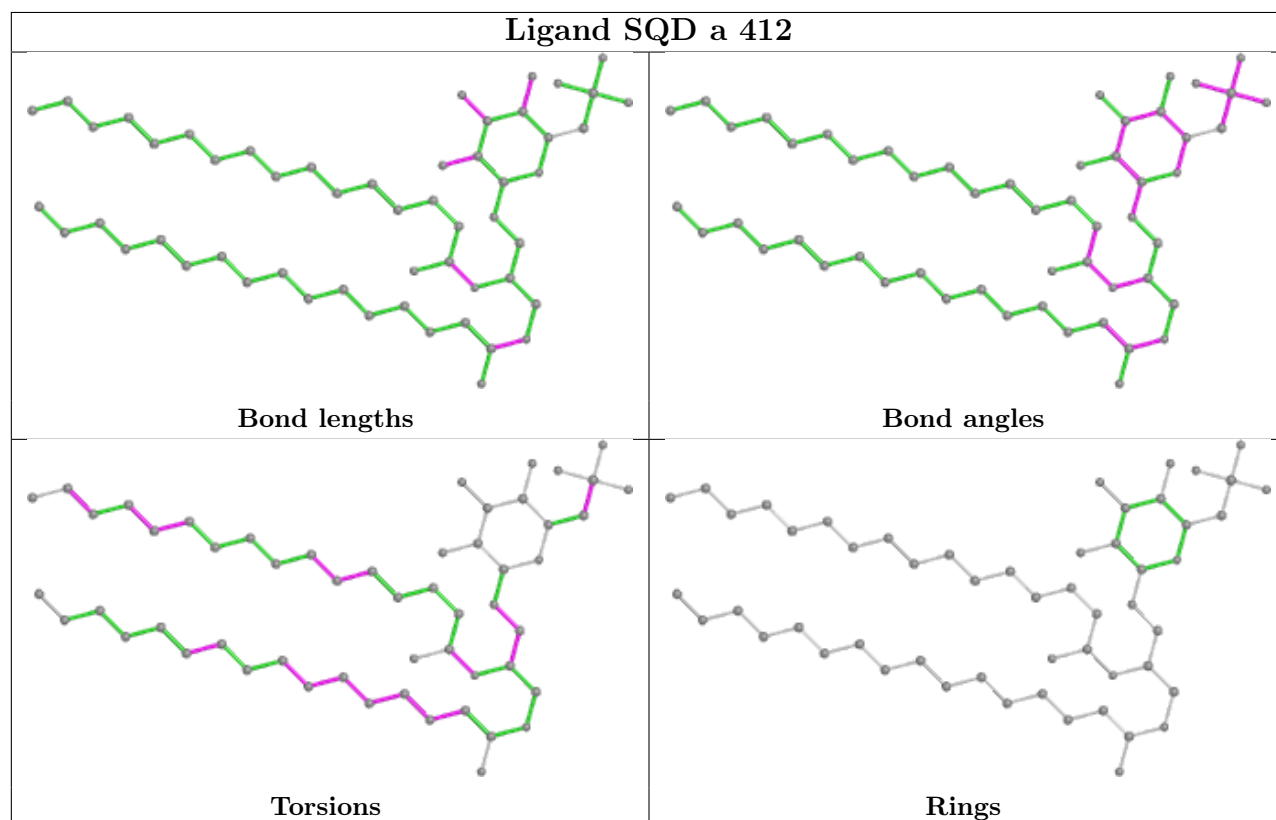
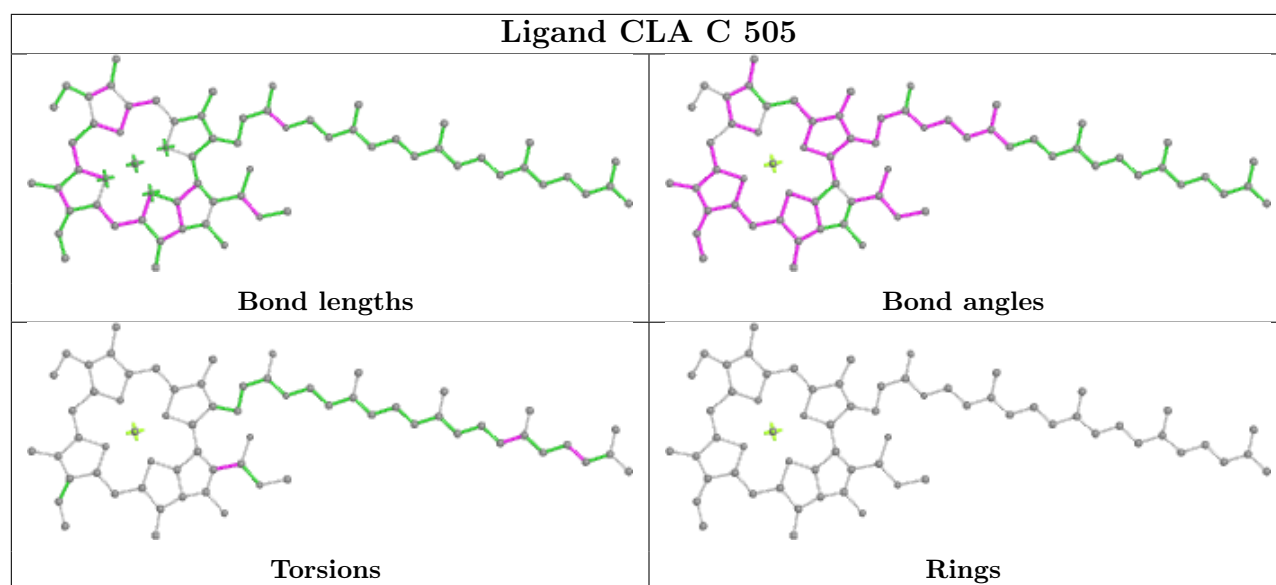


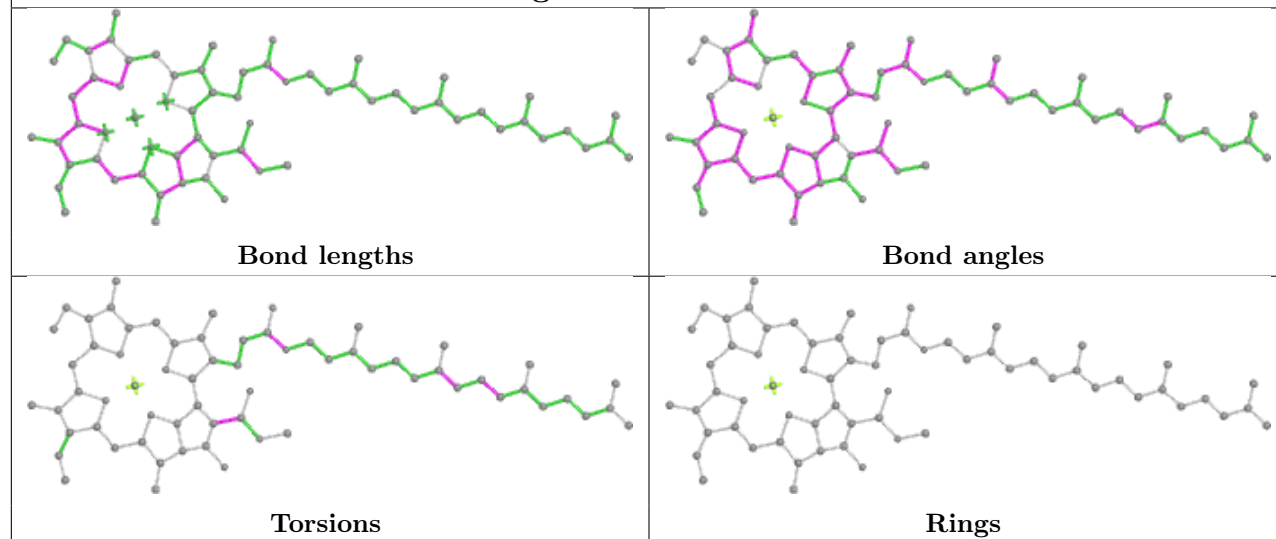
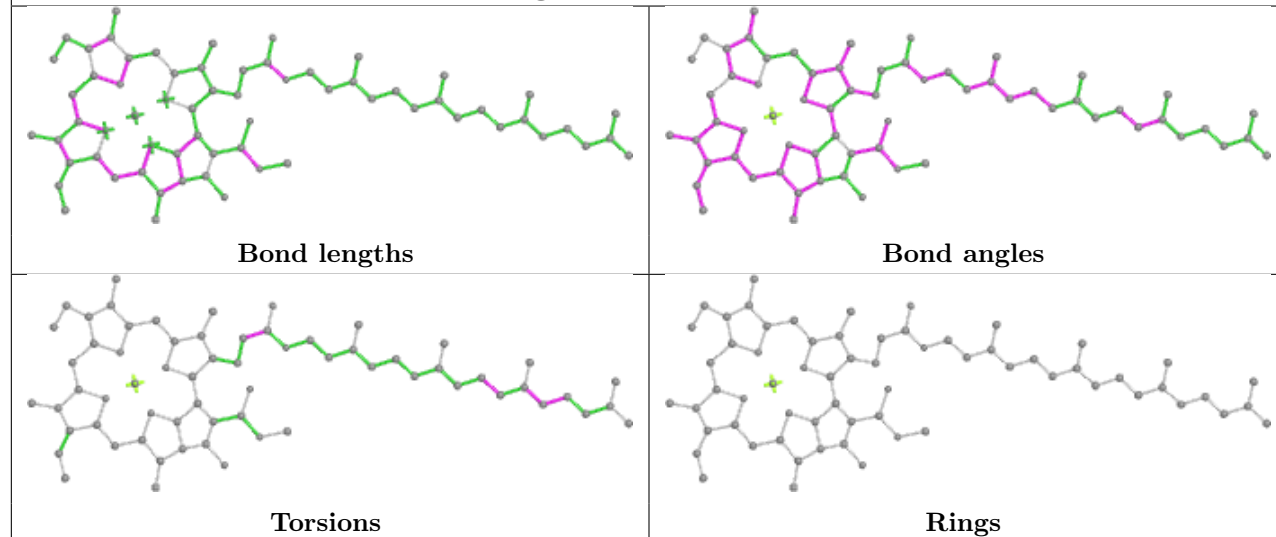
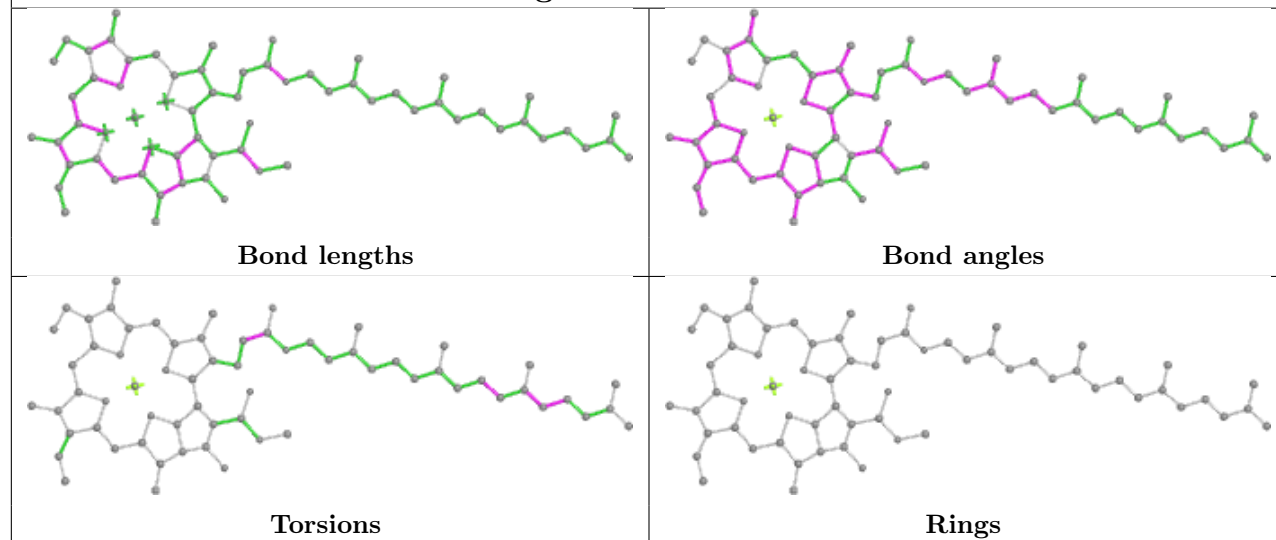




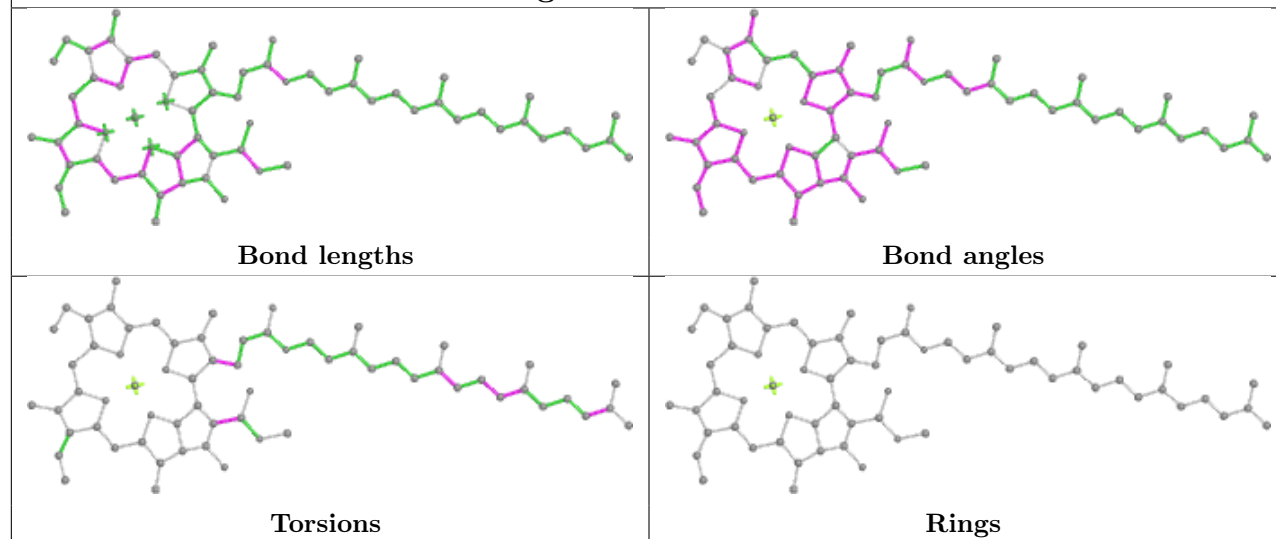




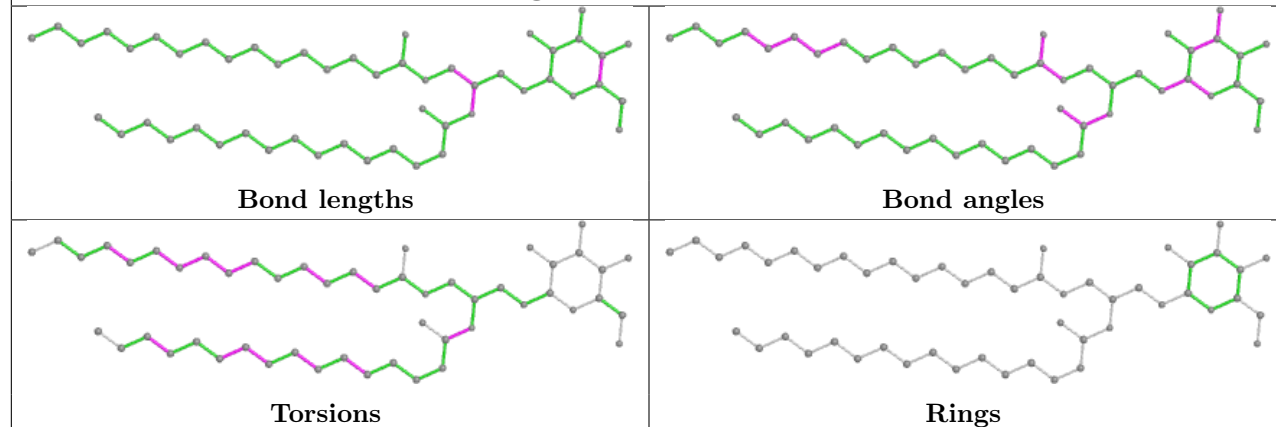


Ligand CLA B 612**Ligand CLA B 616****Ligand CLA b 618**

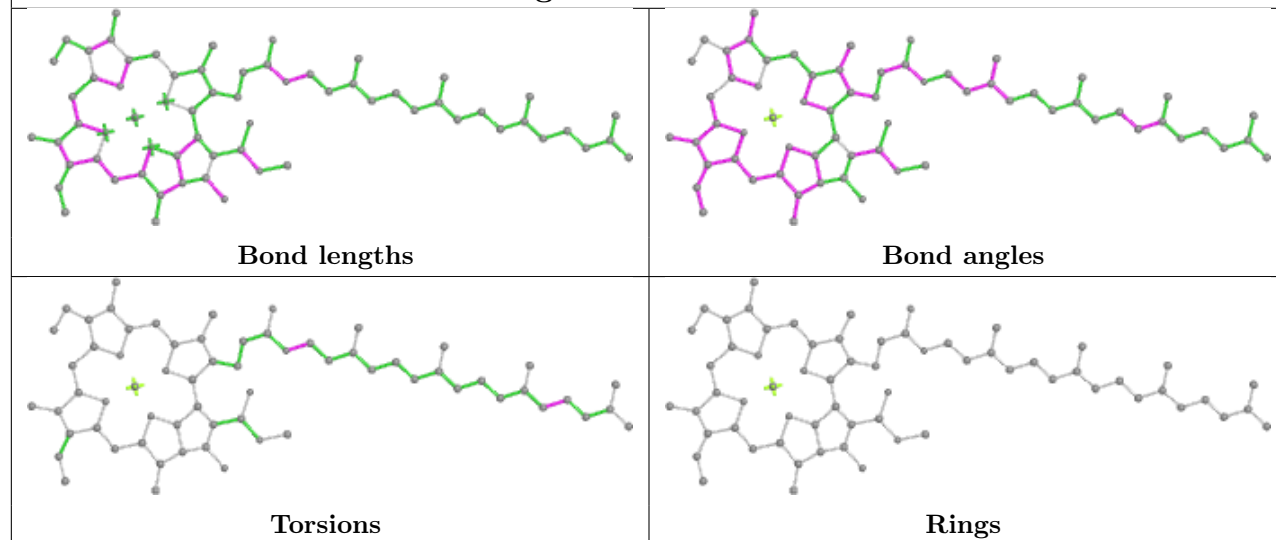
Ligand CLA c 507

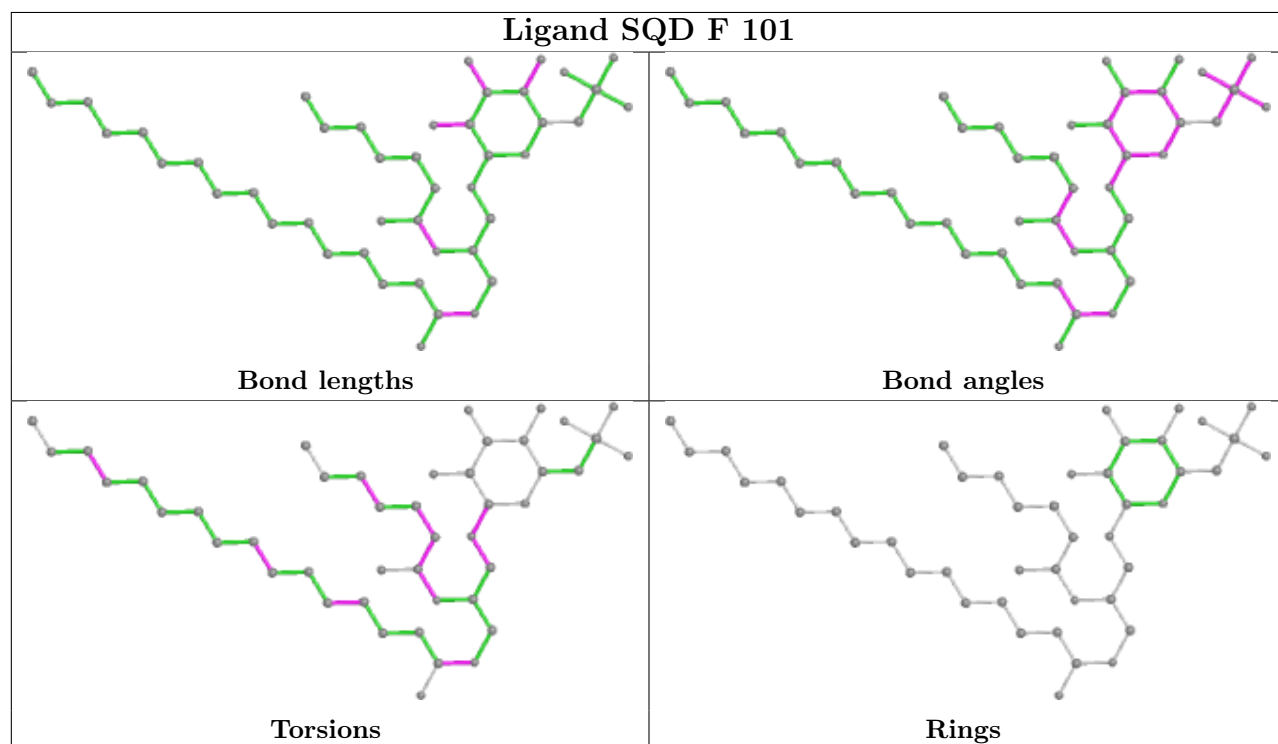
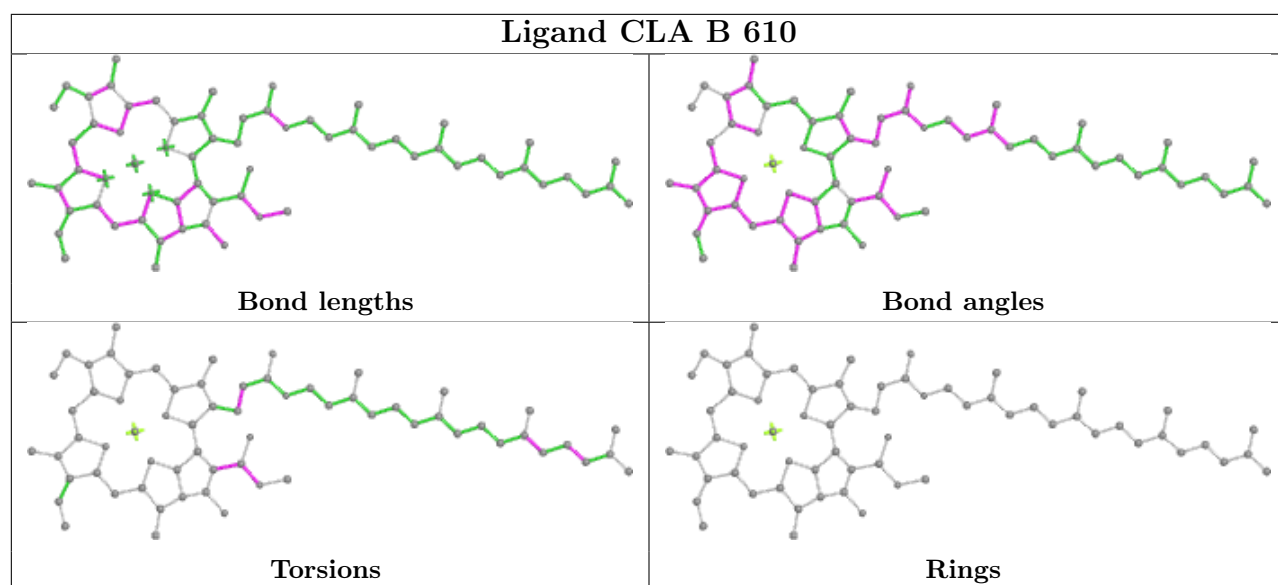


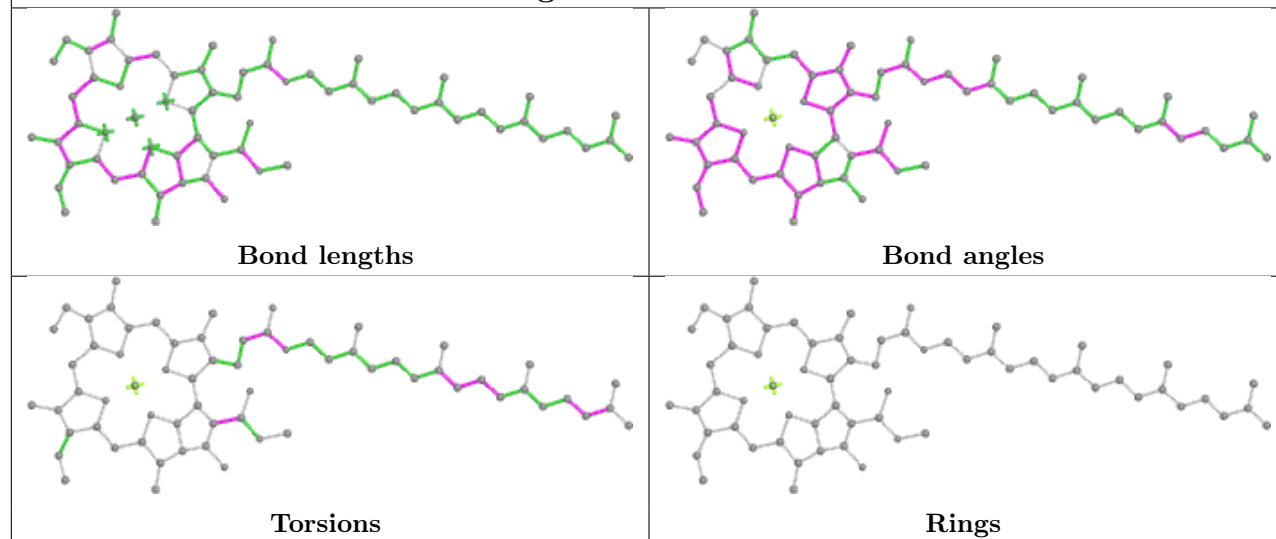
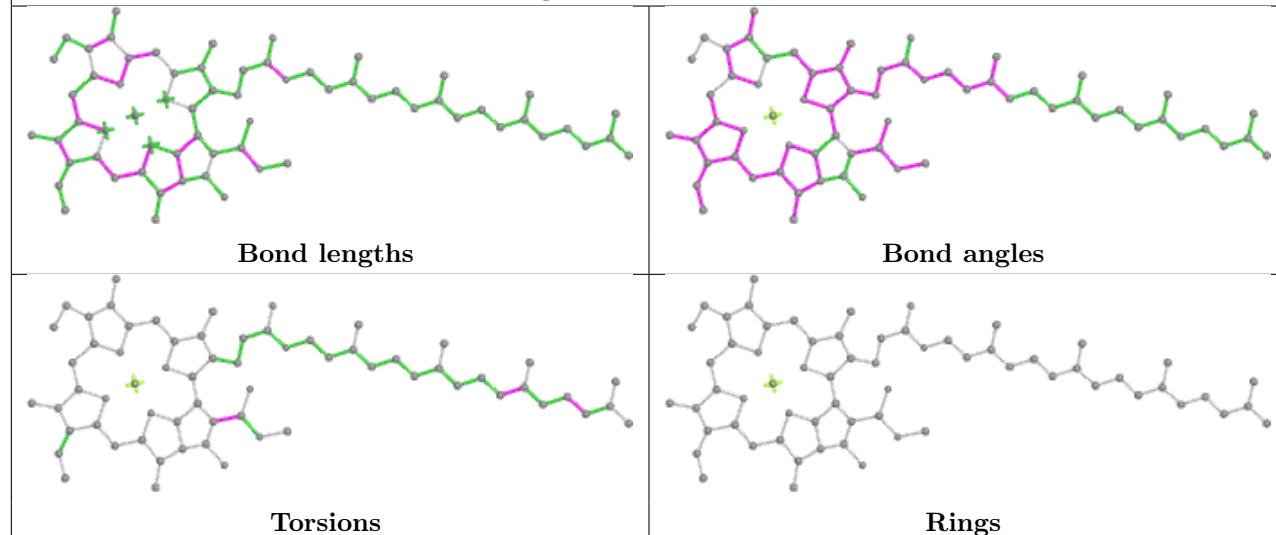
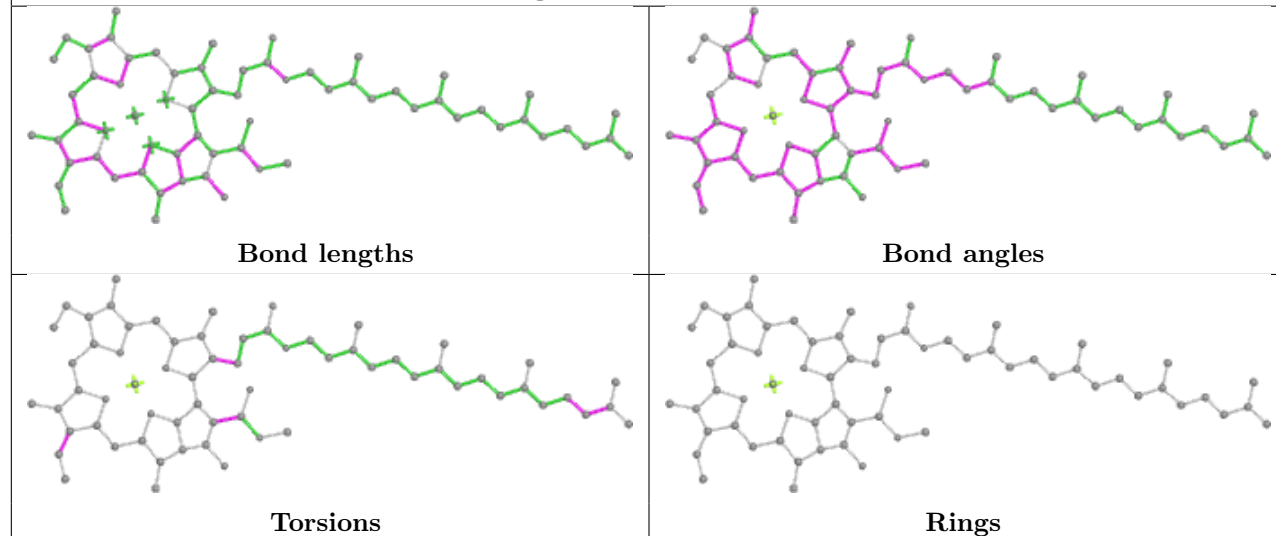
Ligand LMG B 621

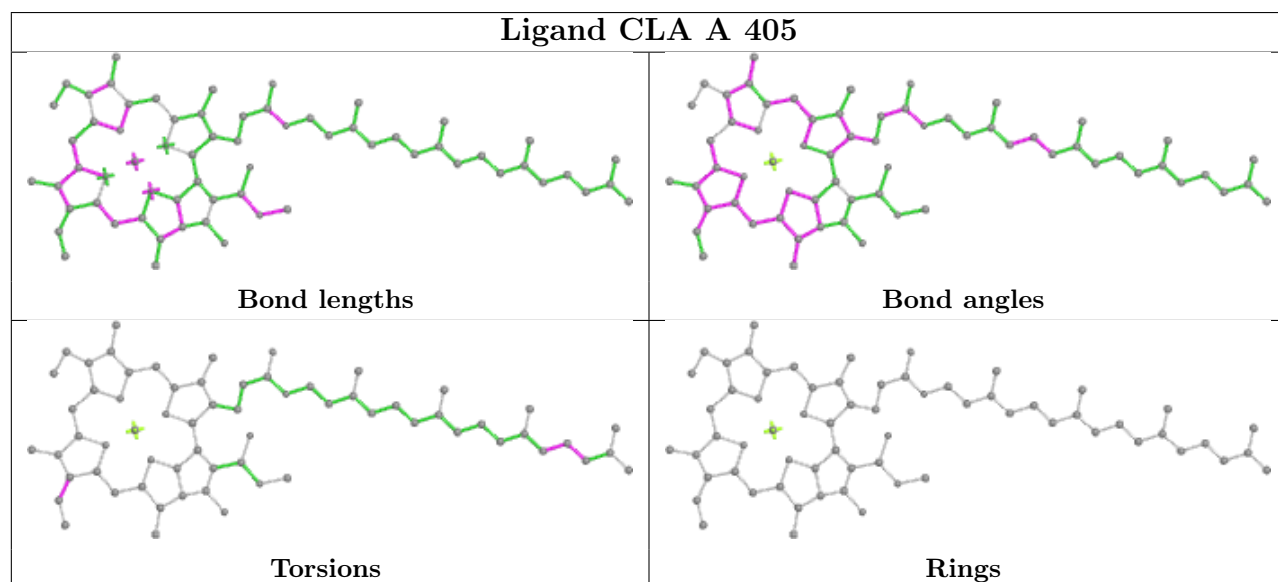
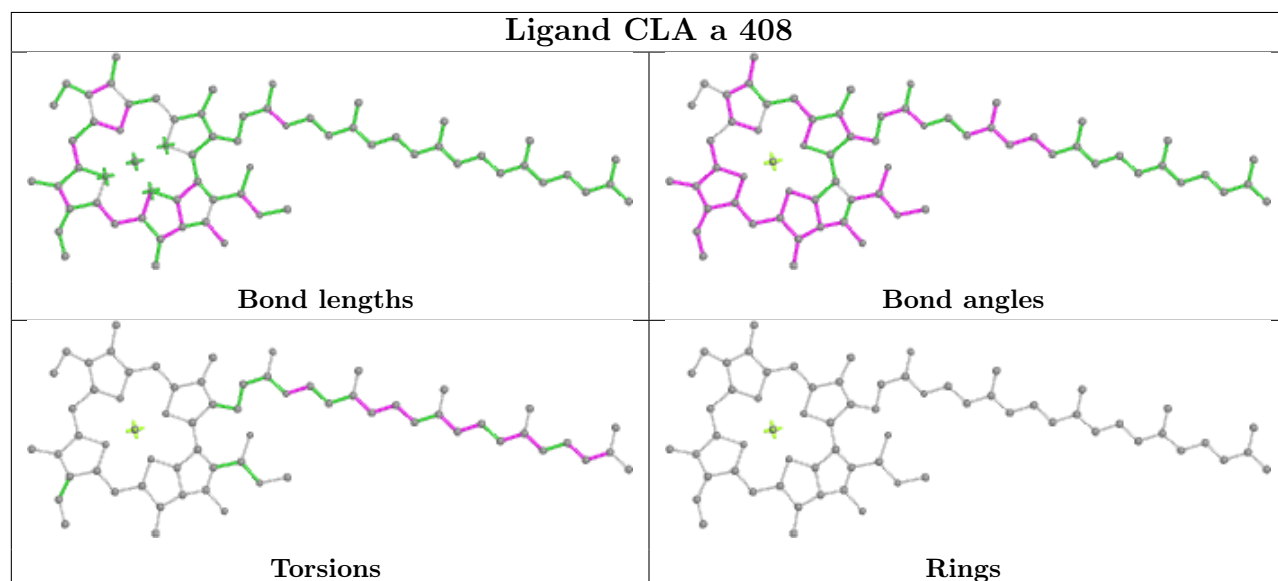
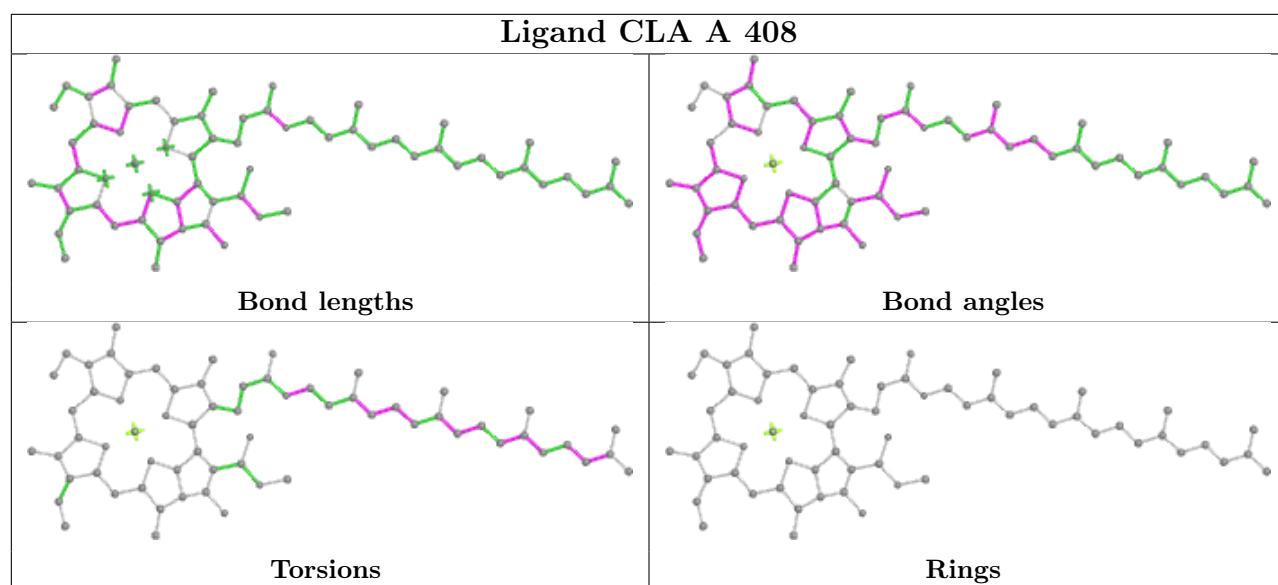


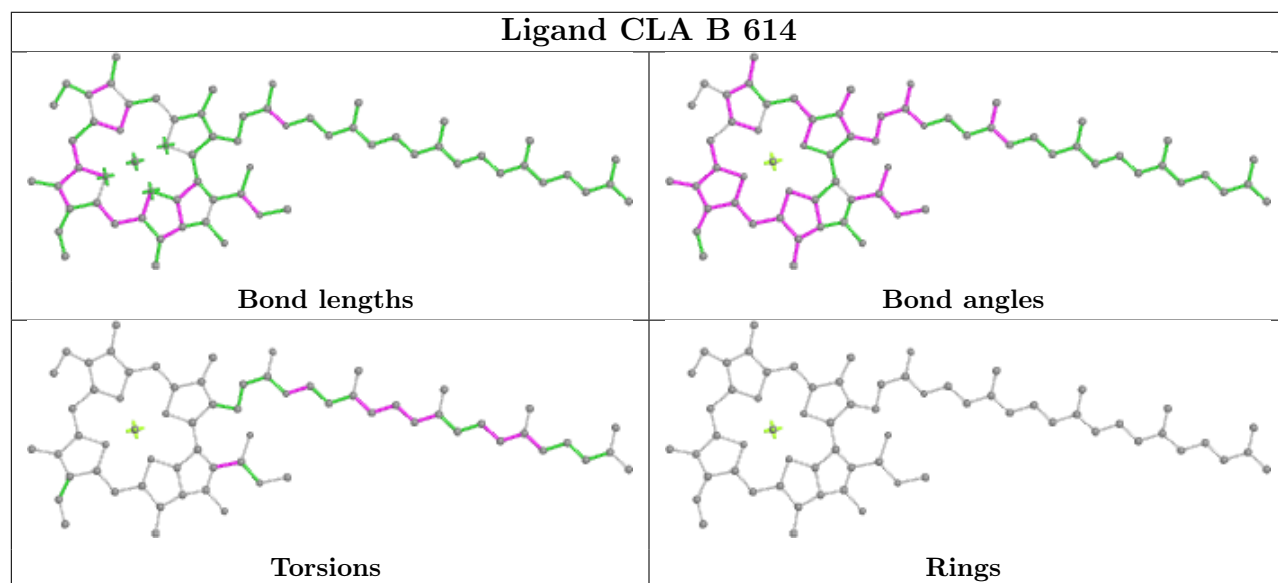
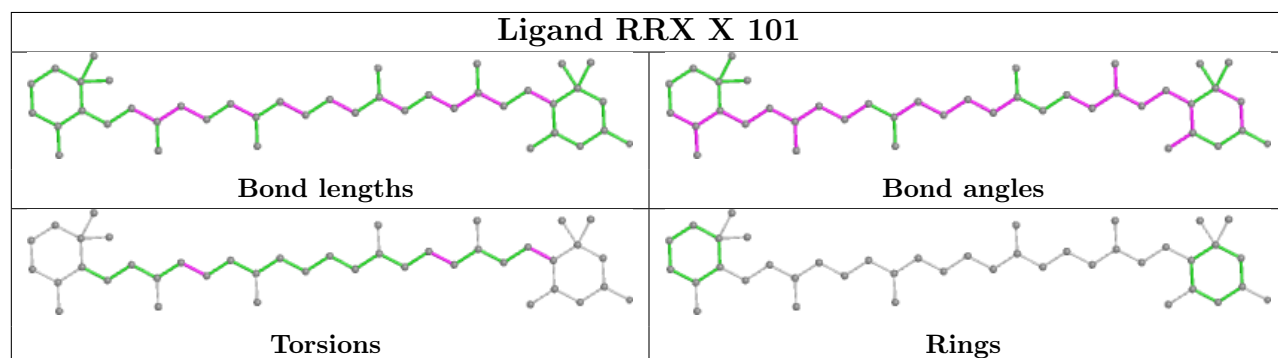
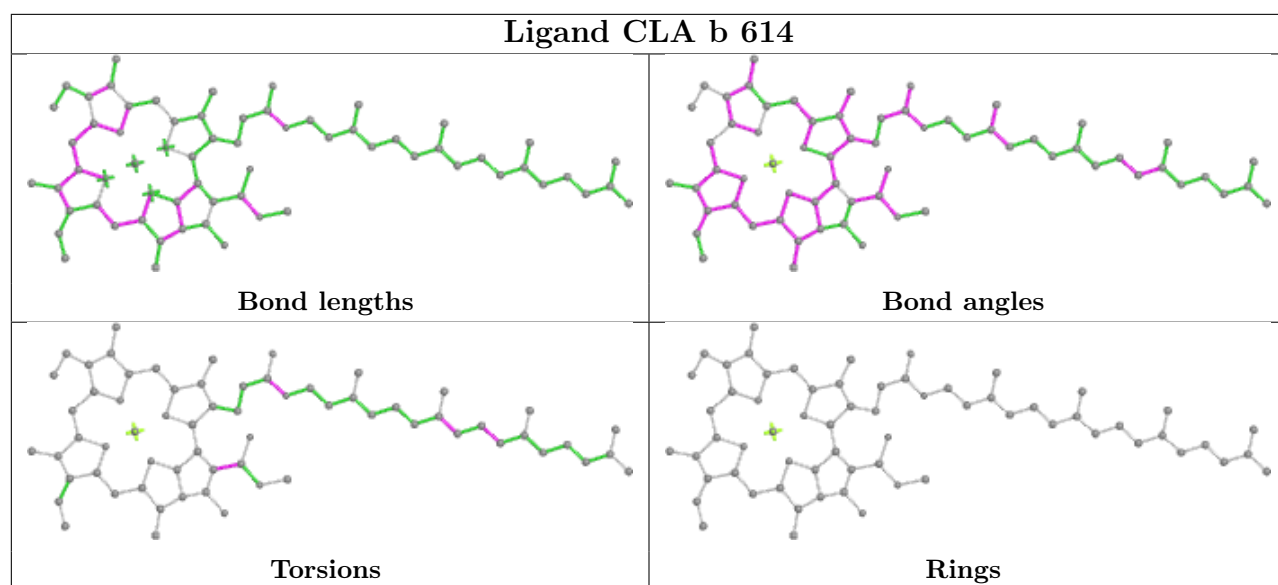
Ligand CLA b 610

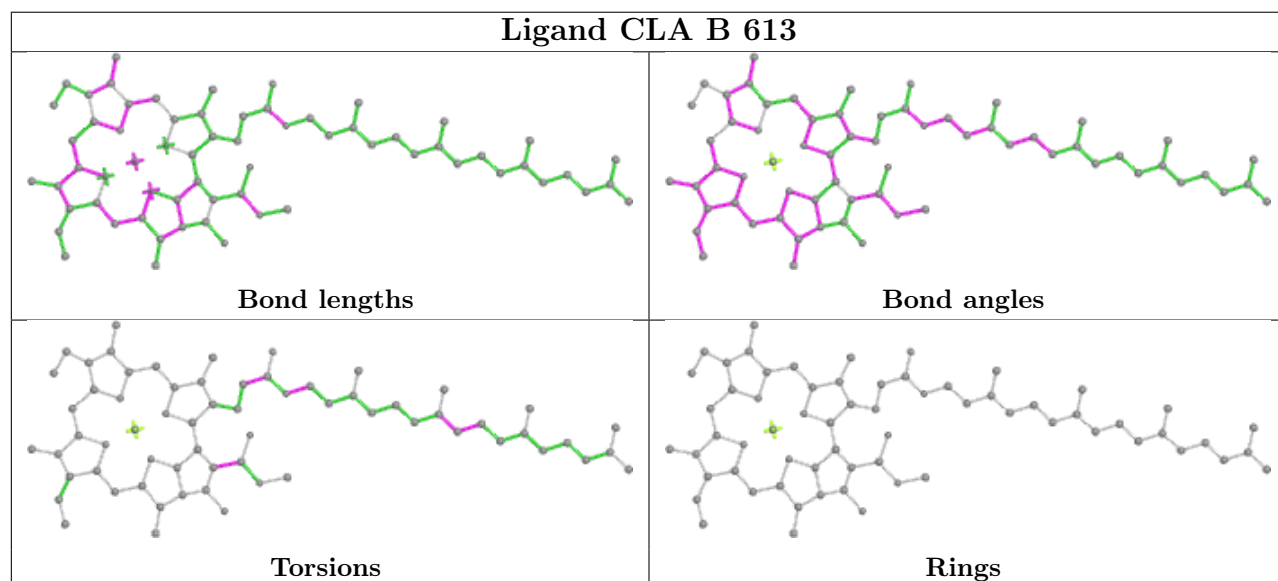
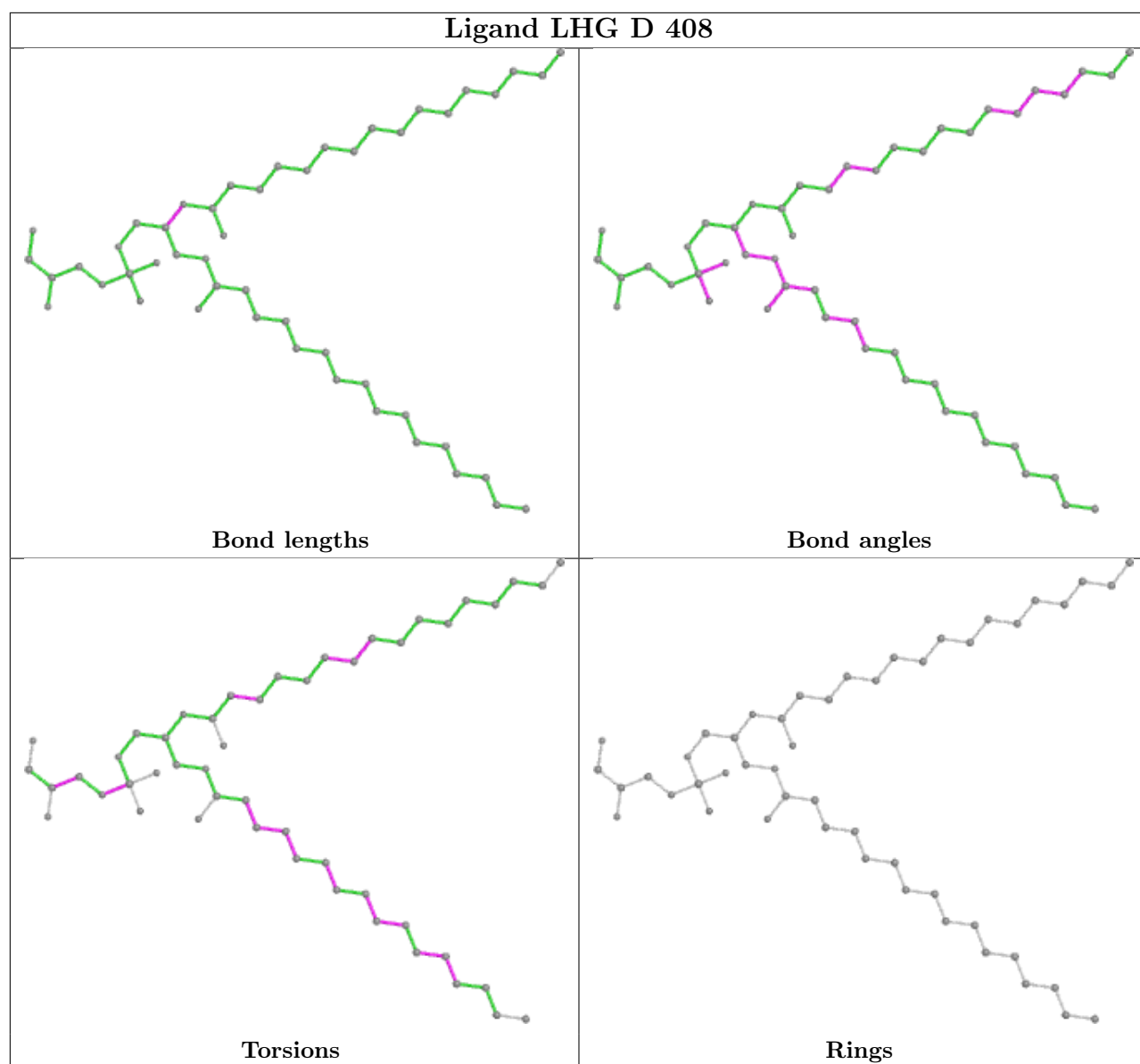


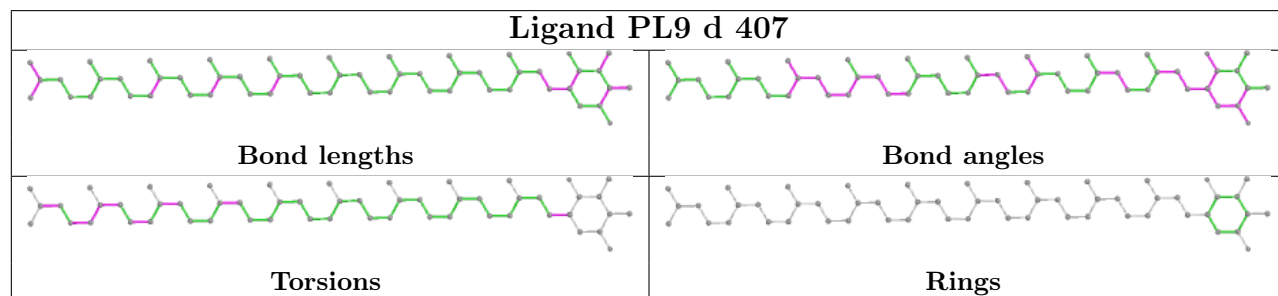
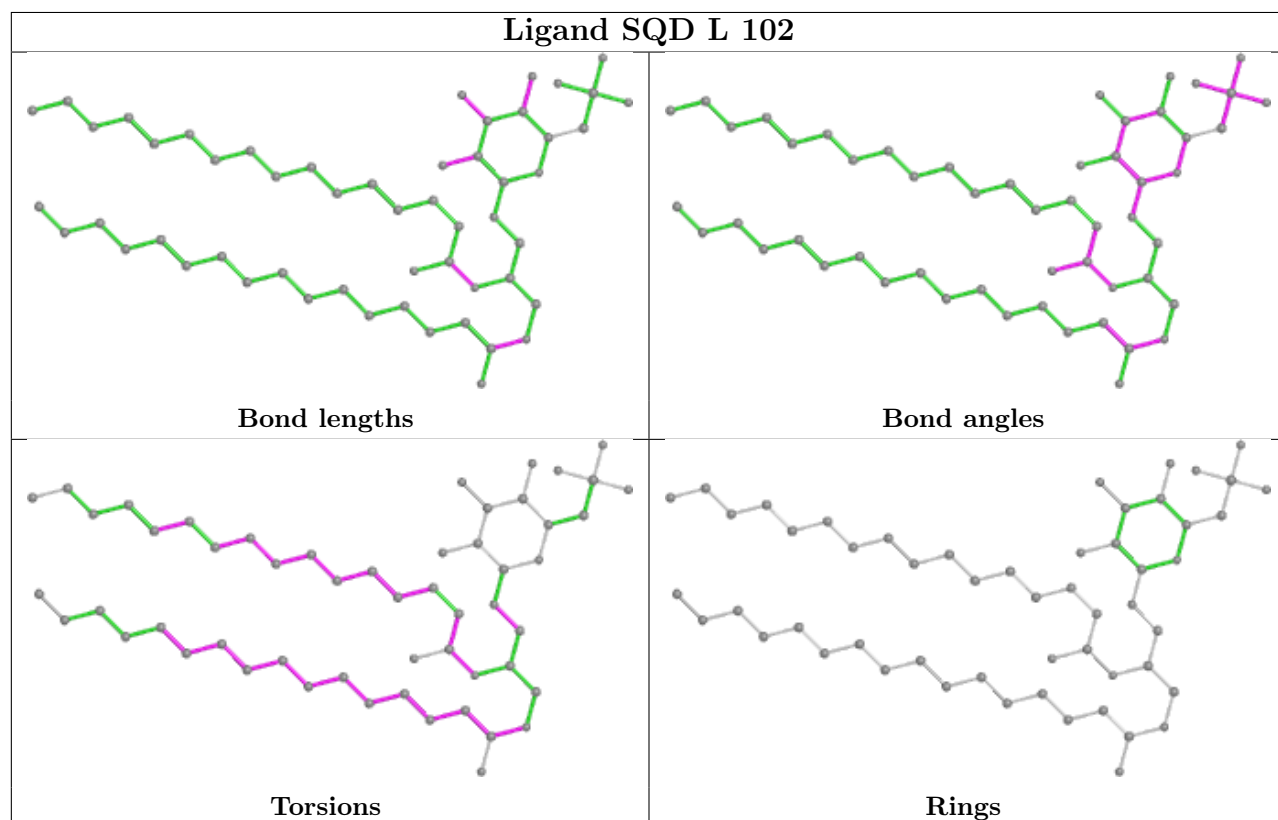
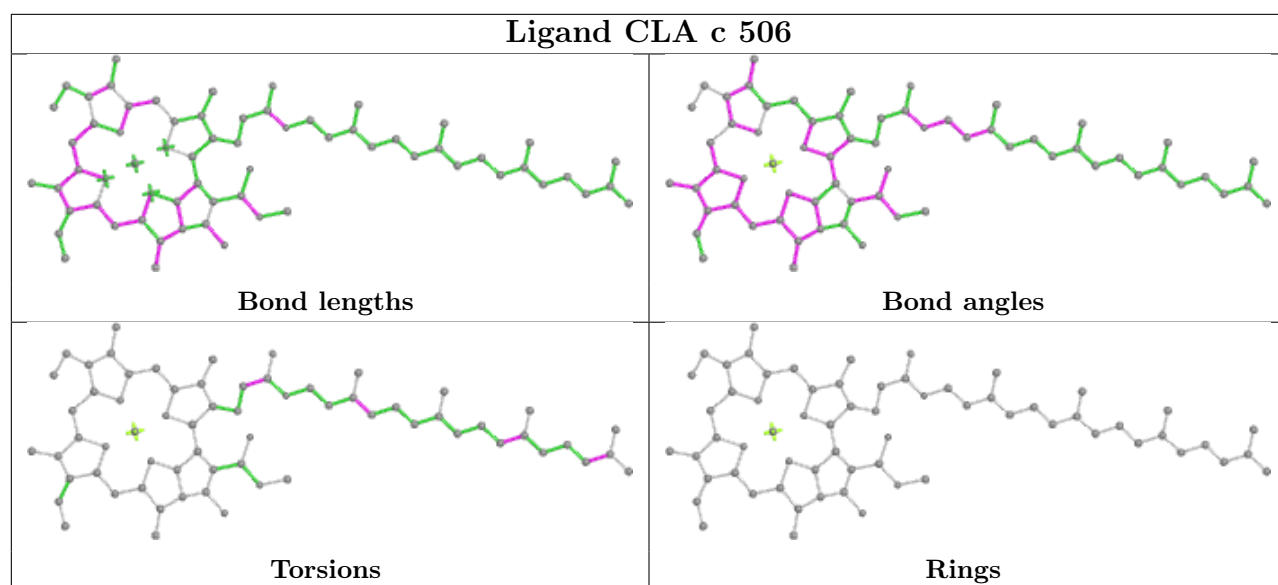


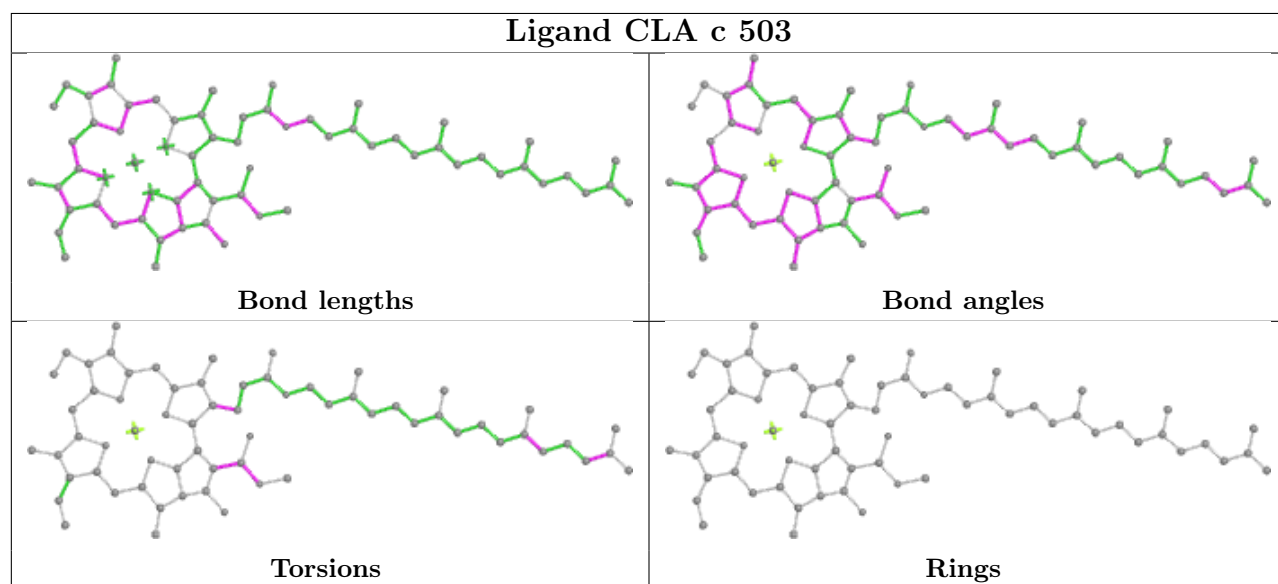
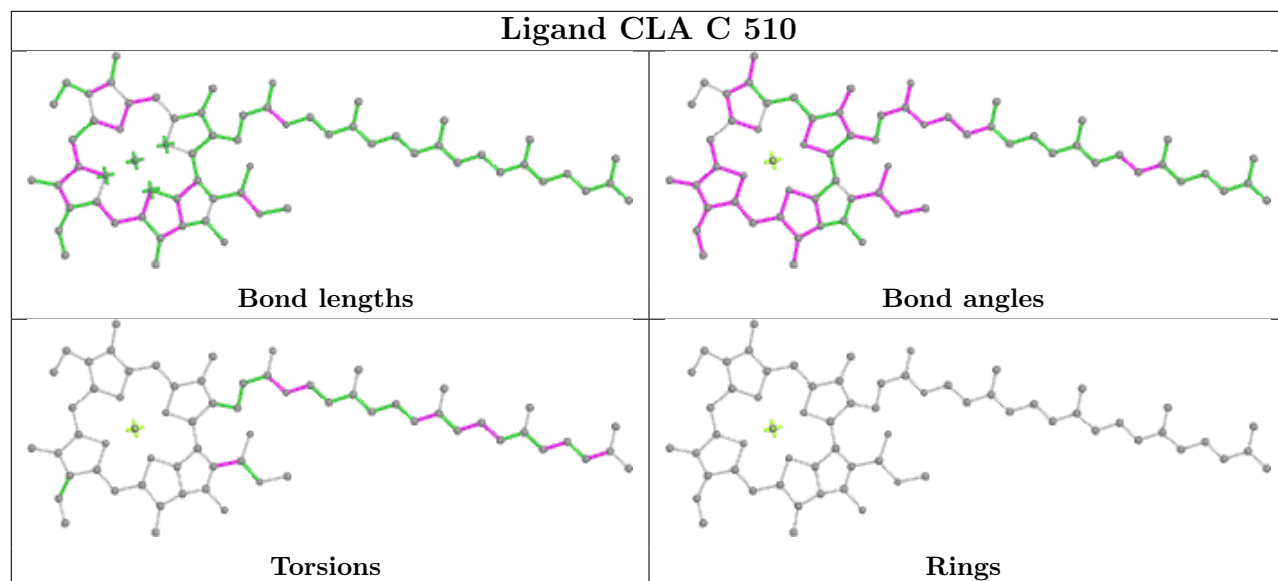
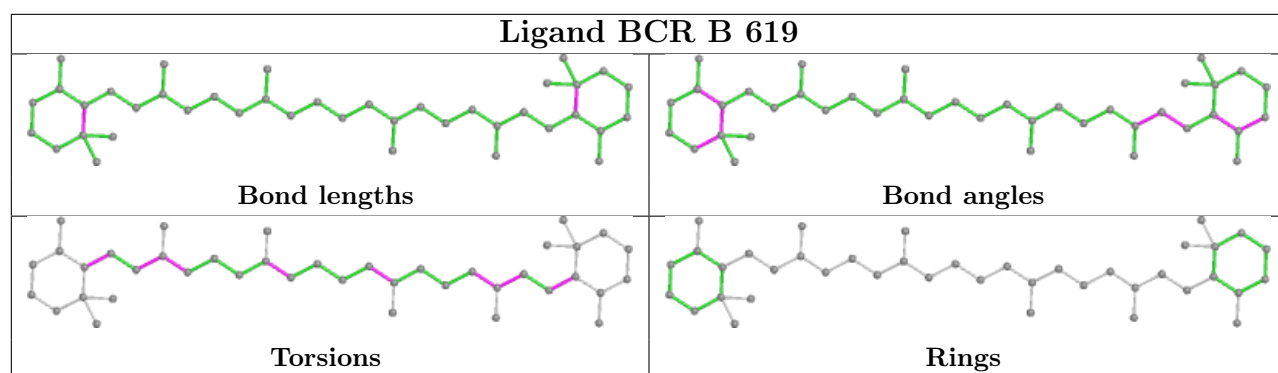
Ligand CLA c 513**Ligand CLA c 505****Ligand CLA D 401**

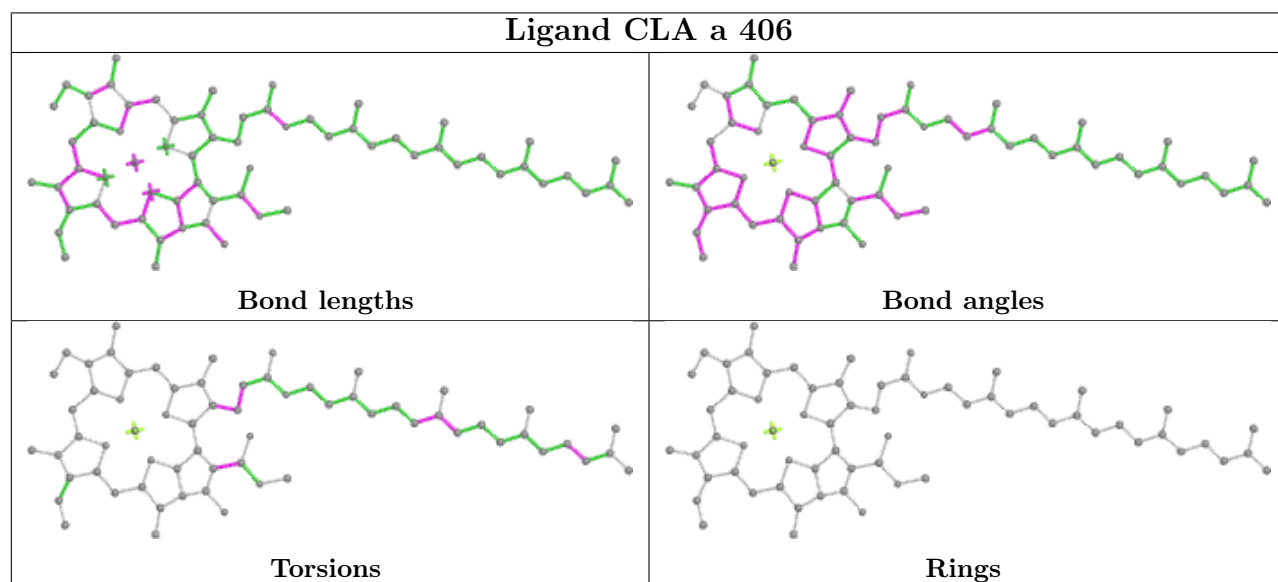
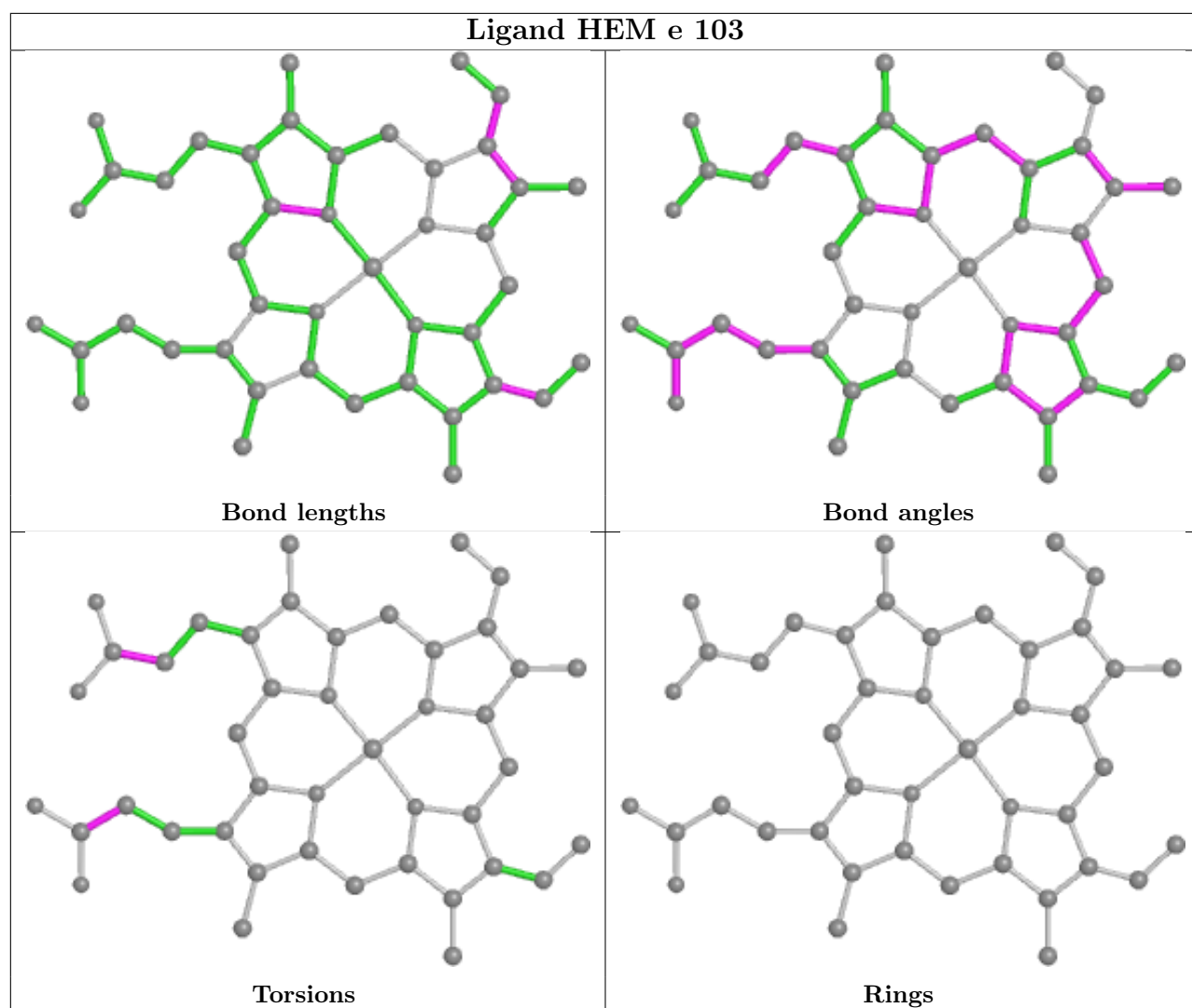


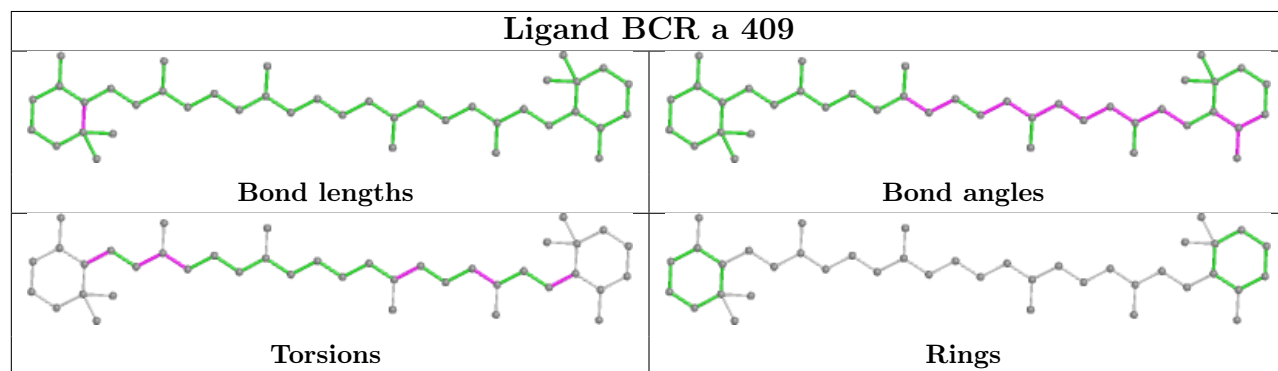
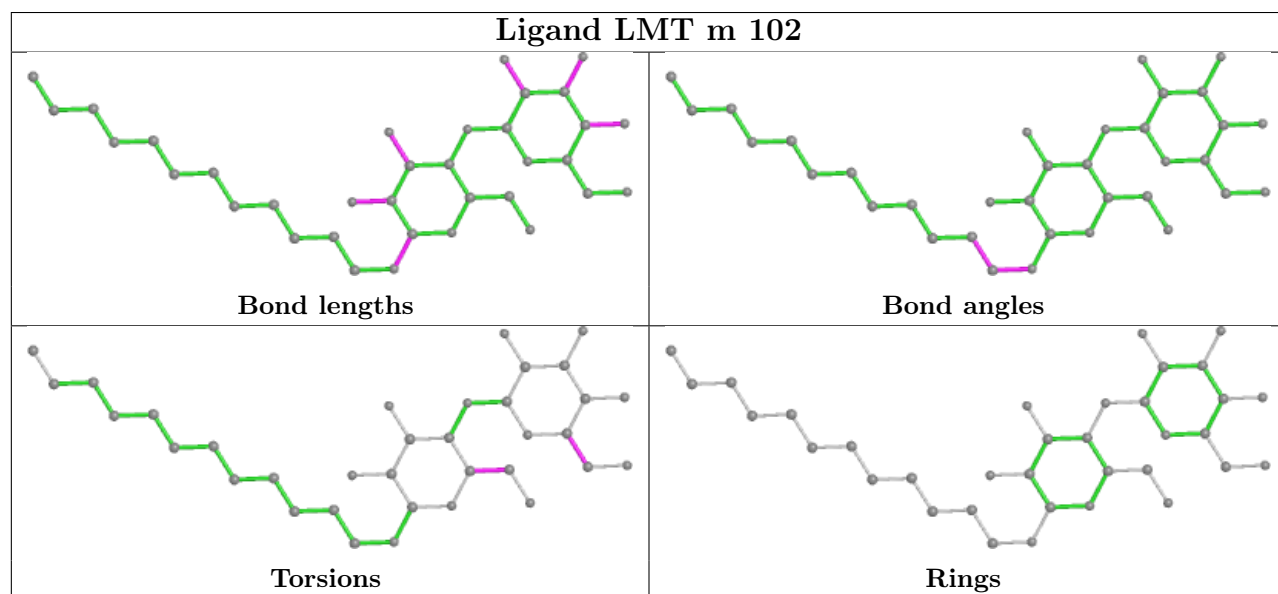
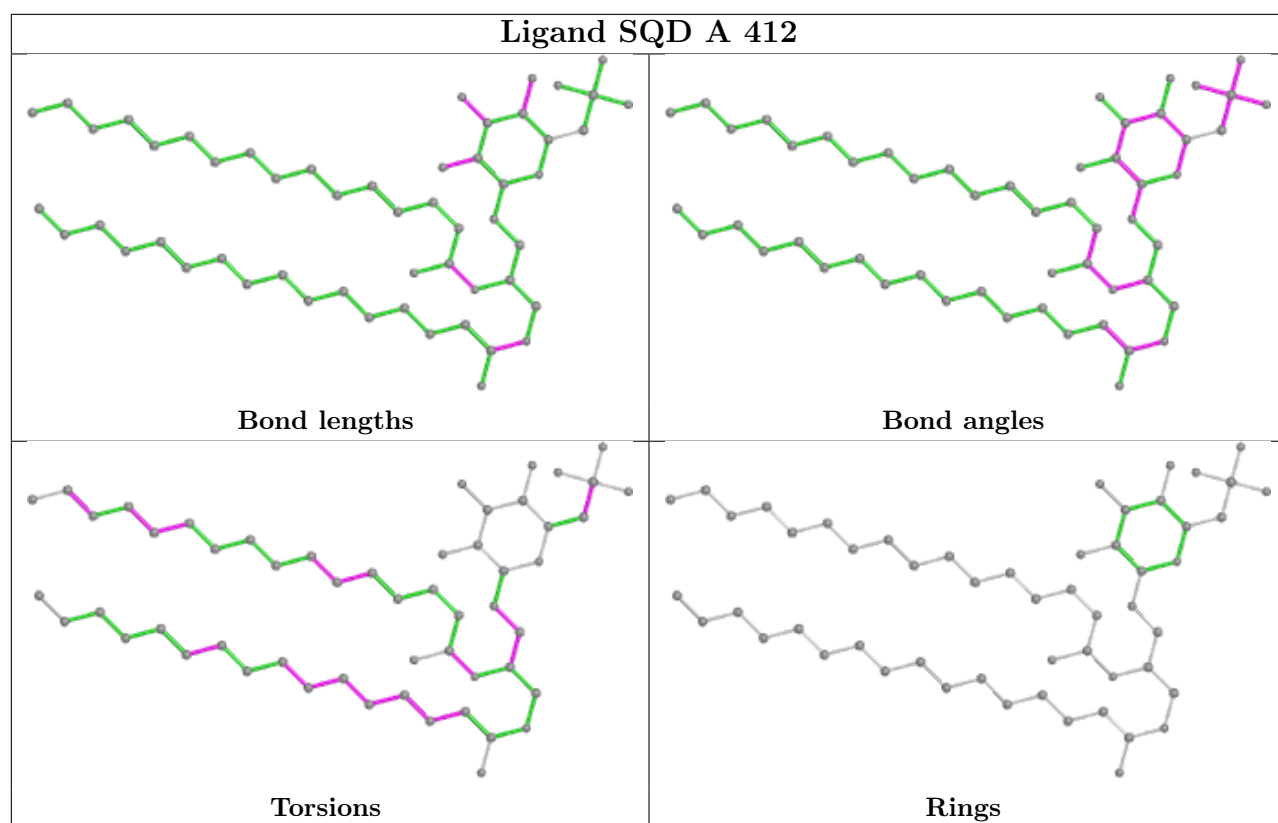


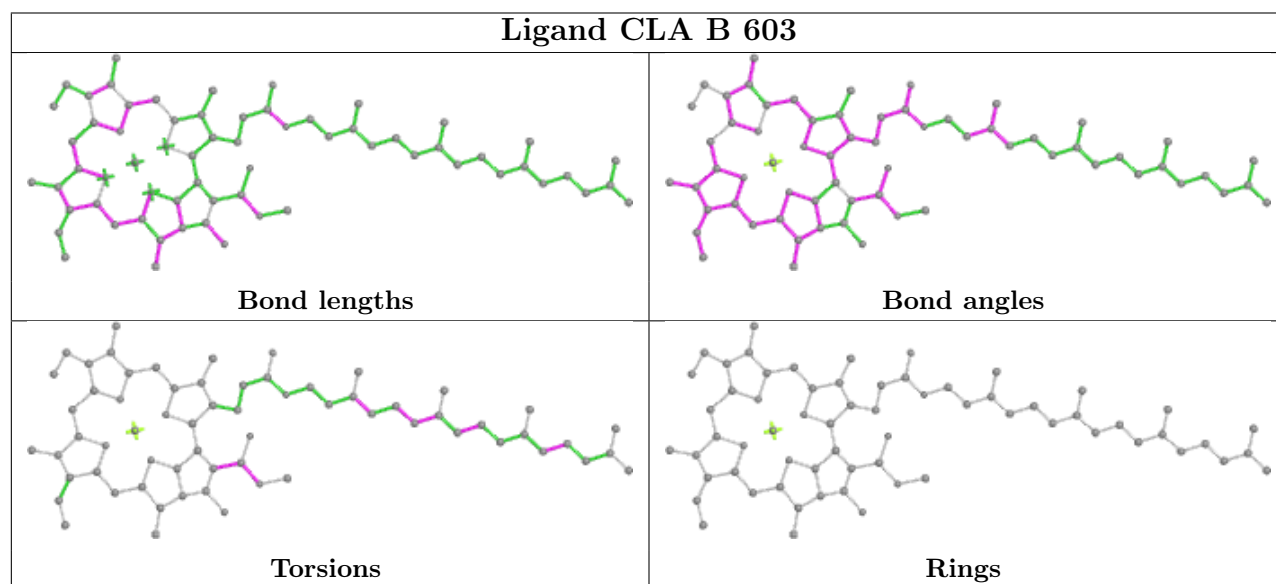
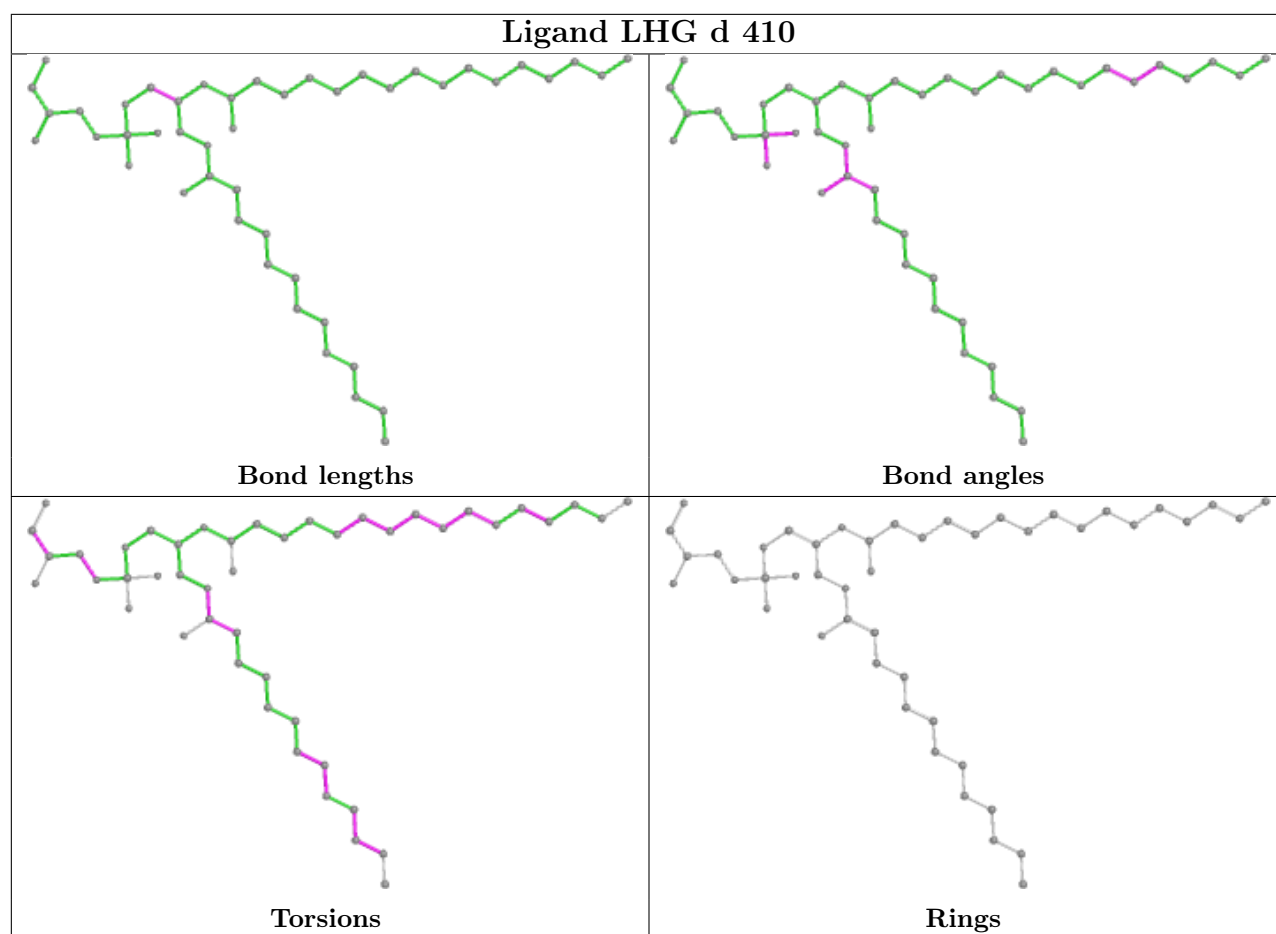


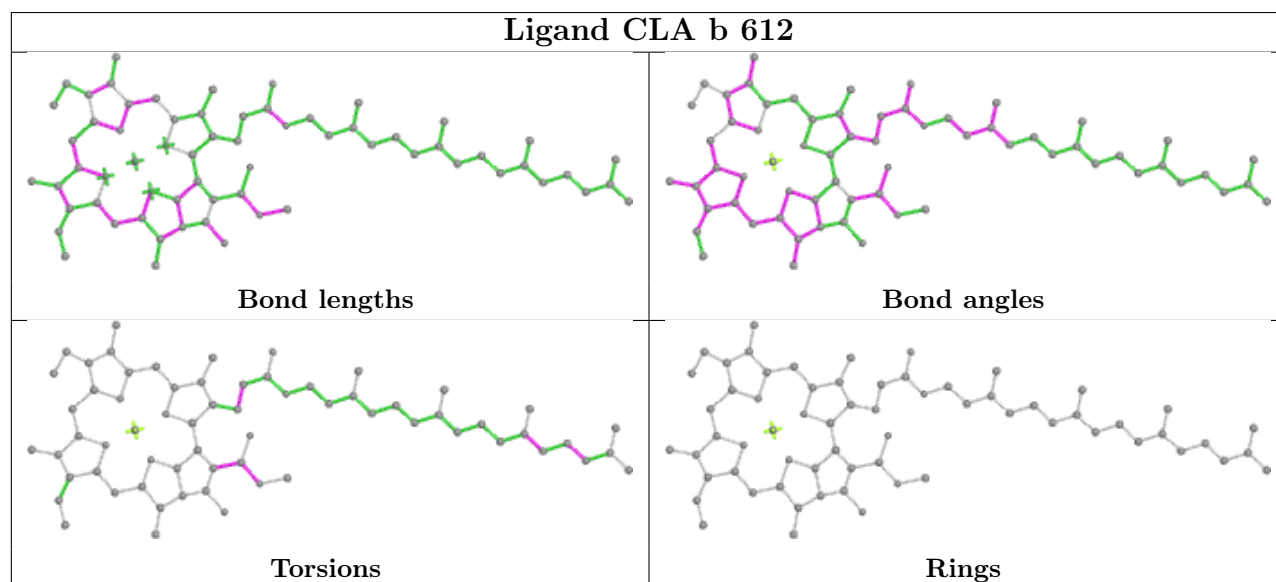
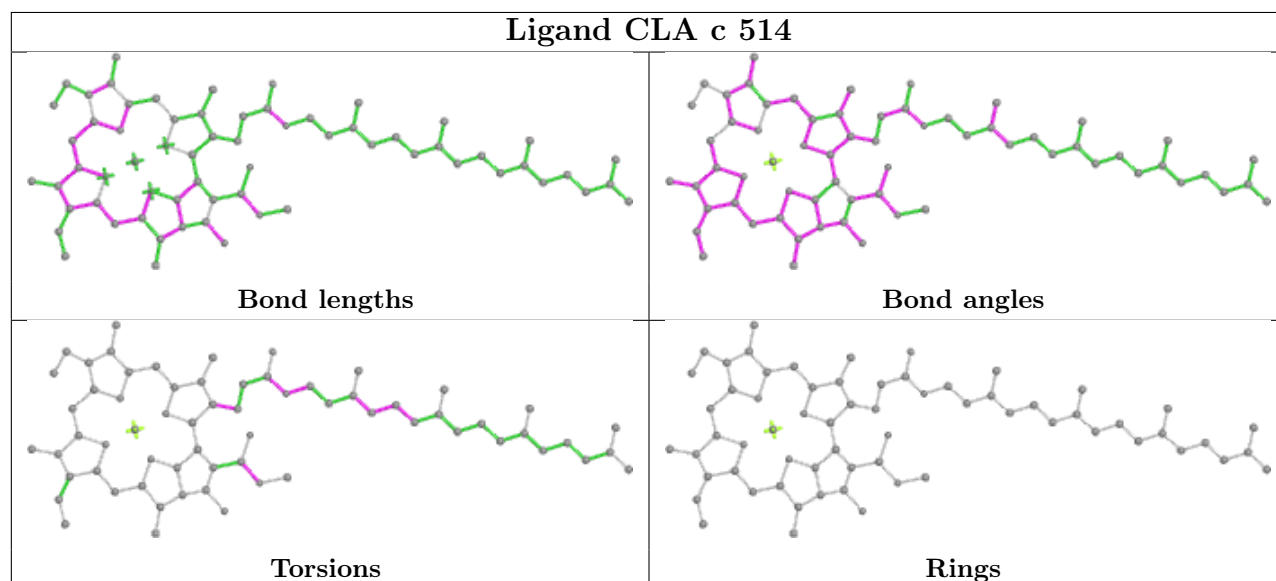
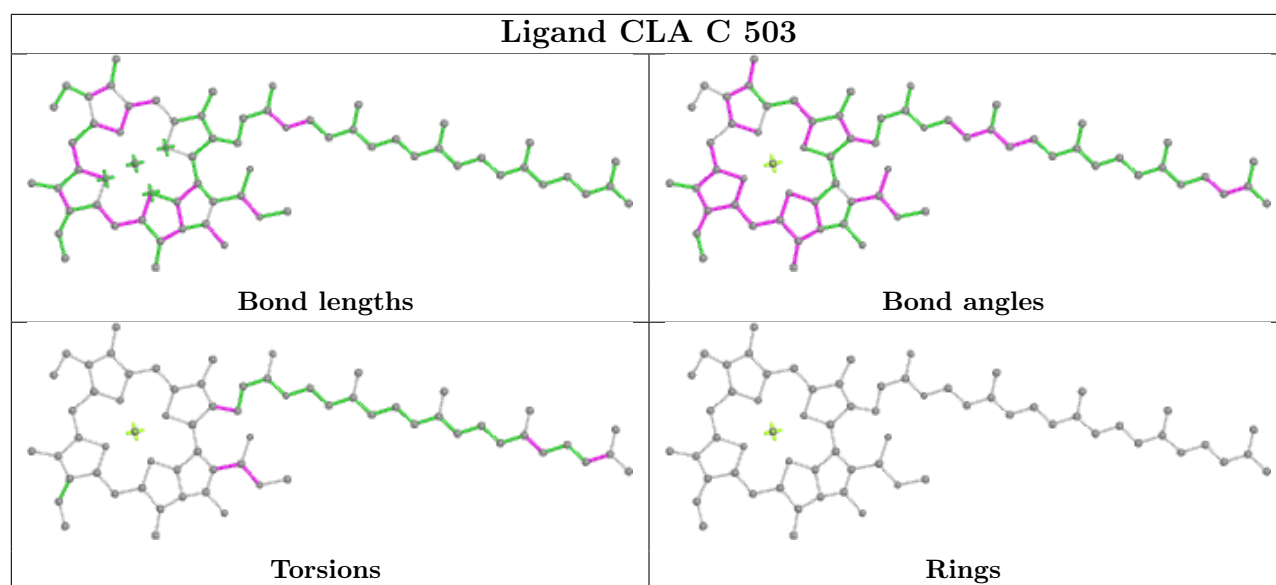


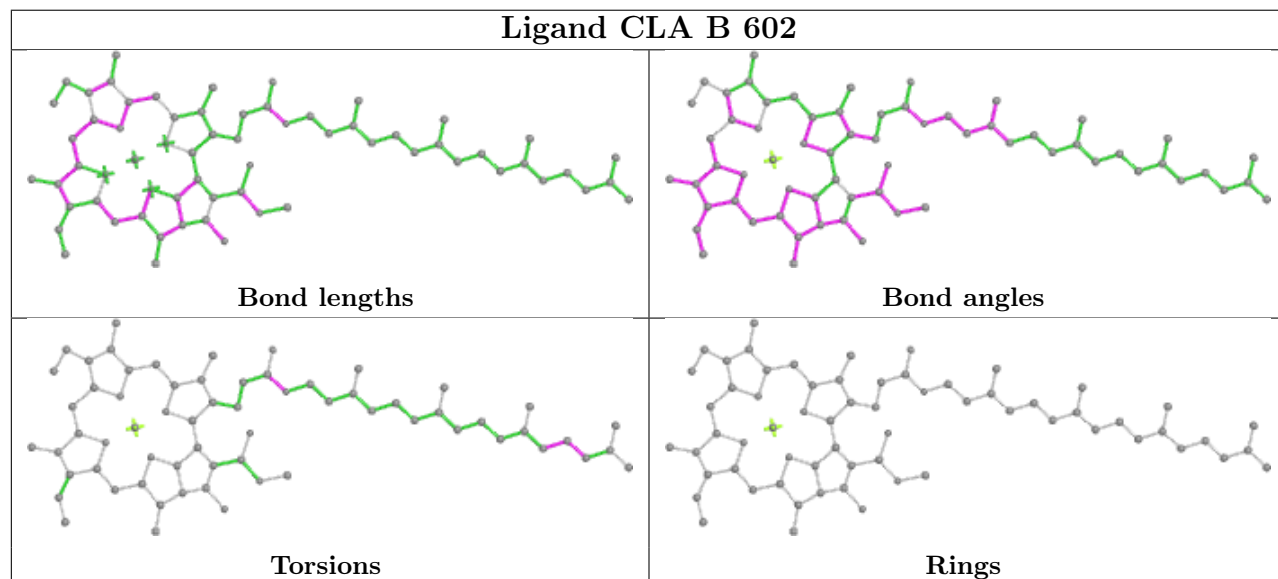
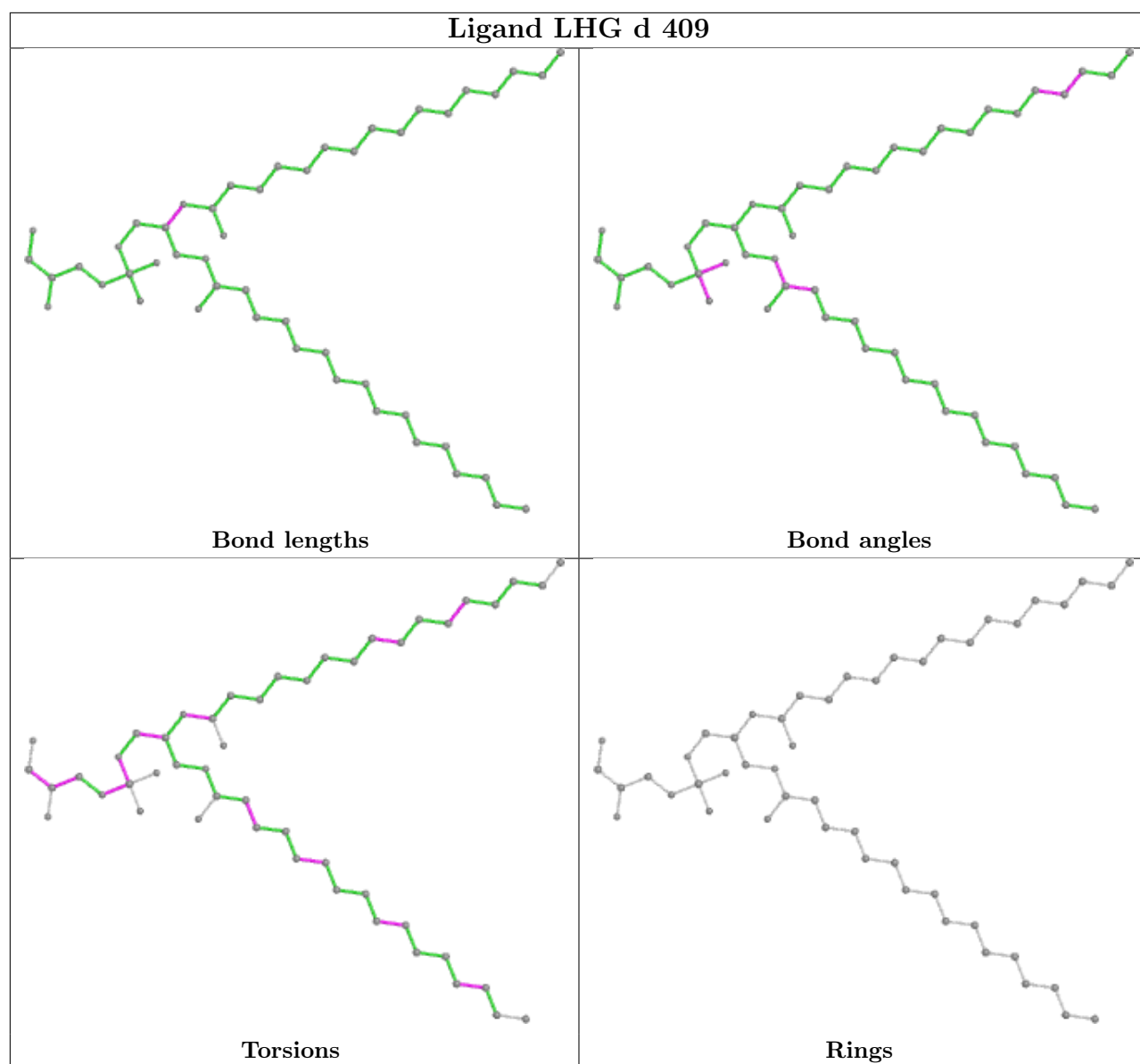




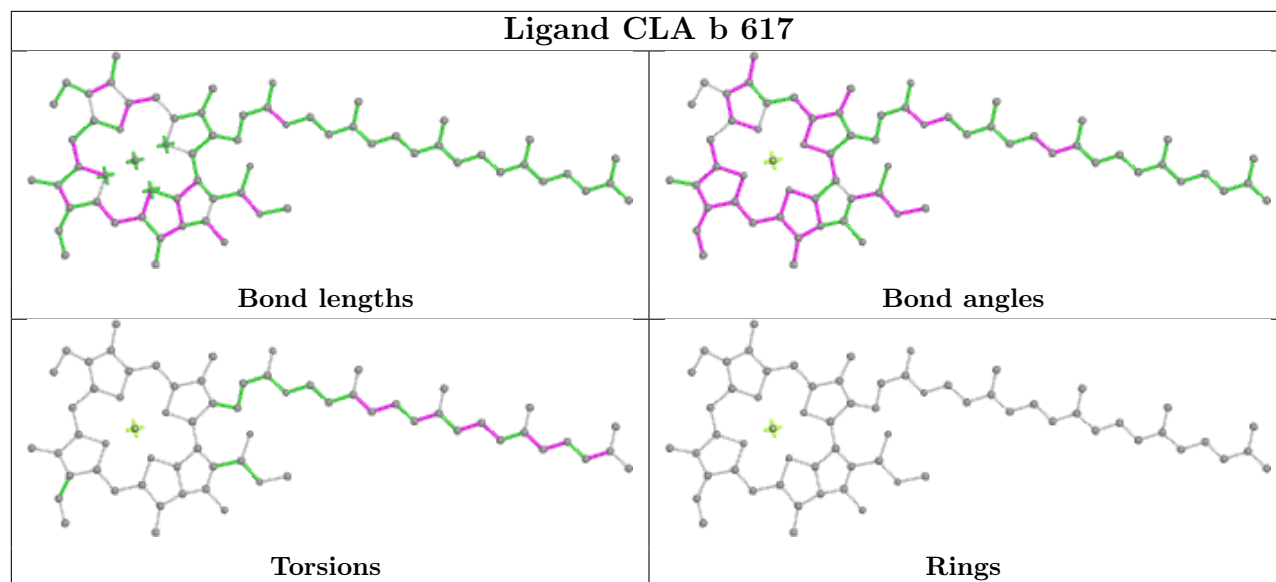




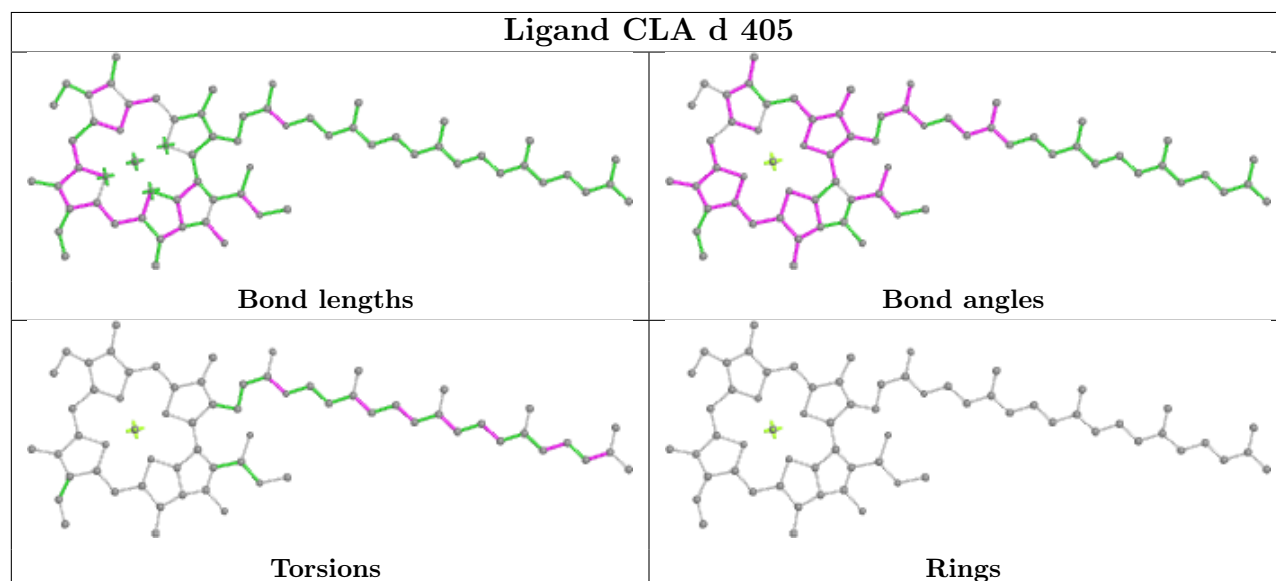




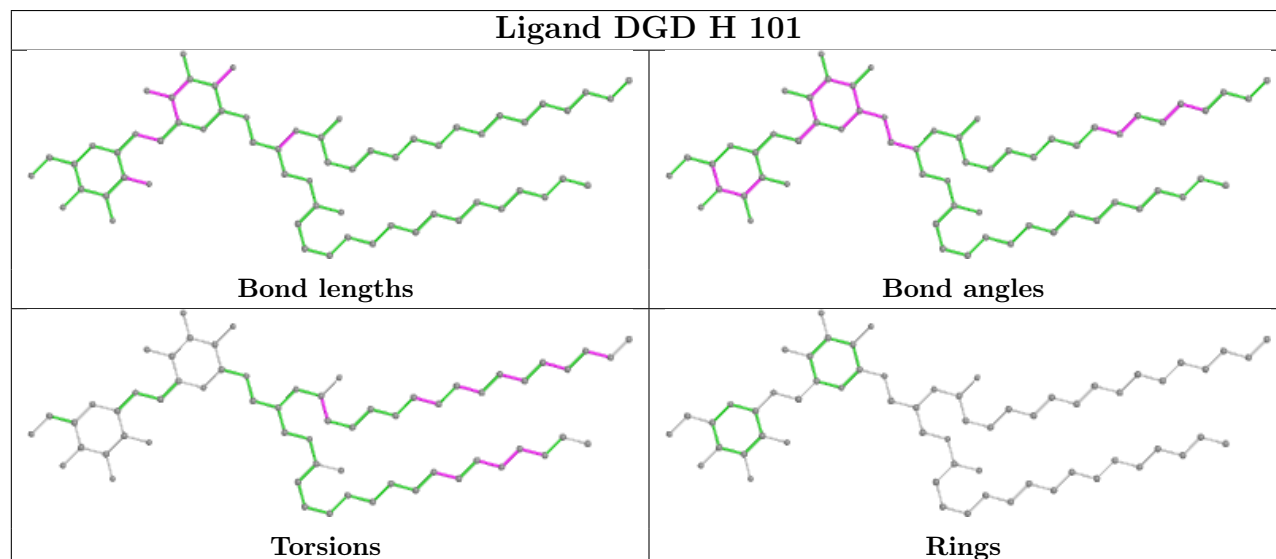
Ligand CLA b 617

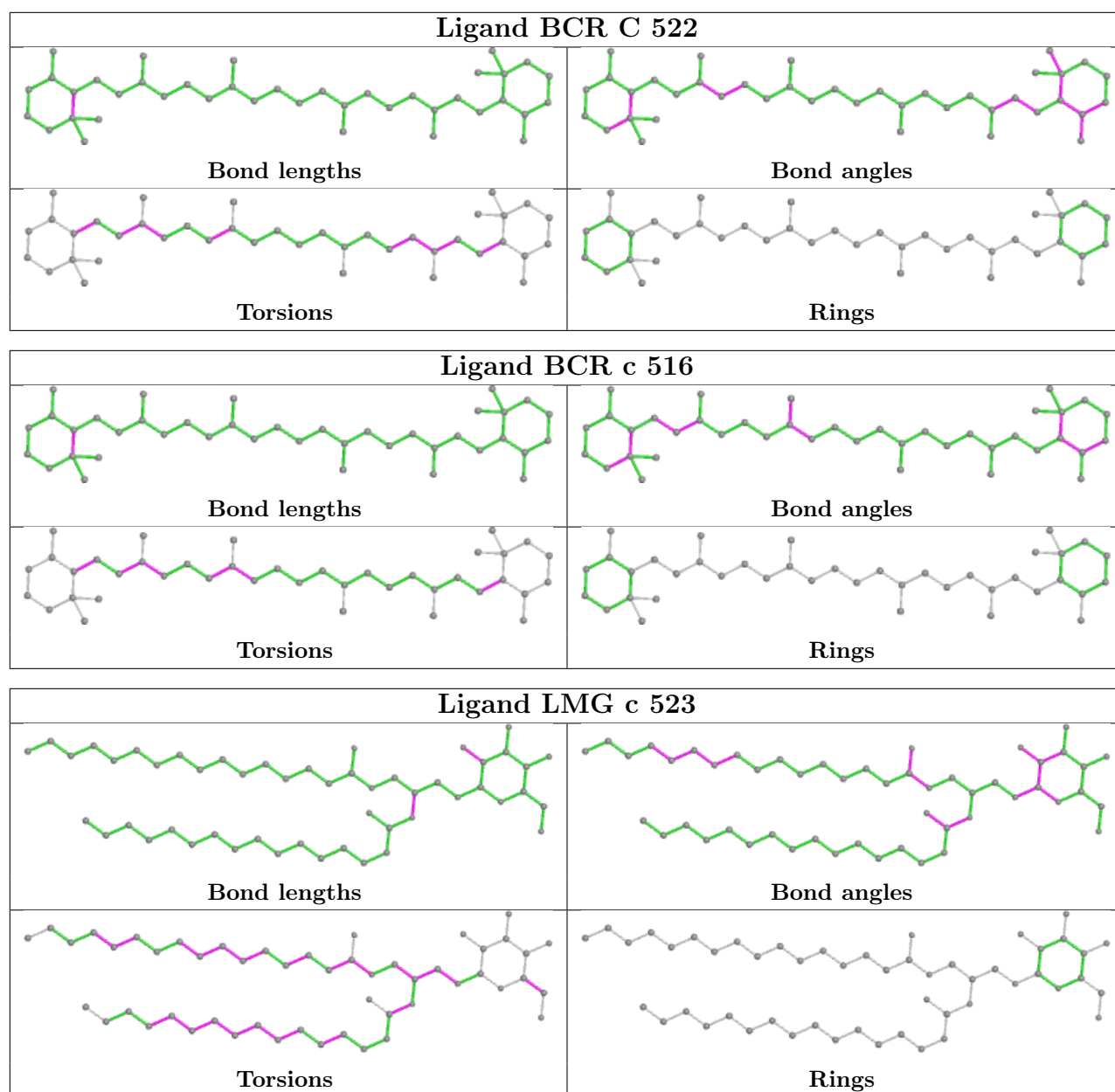


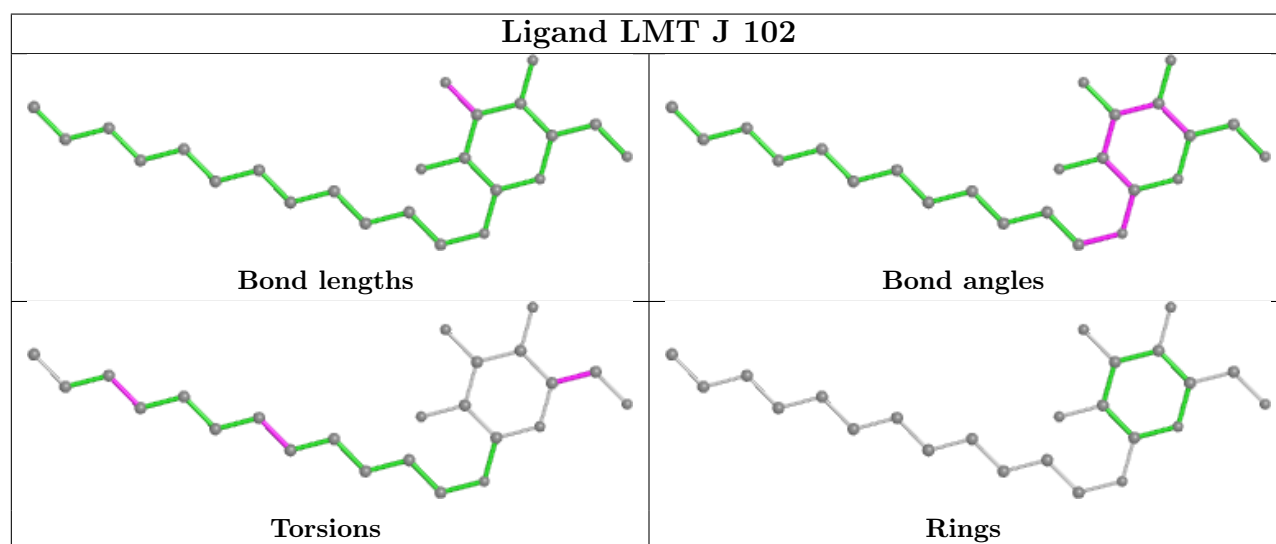
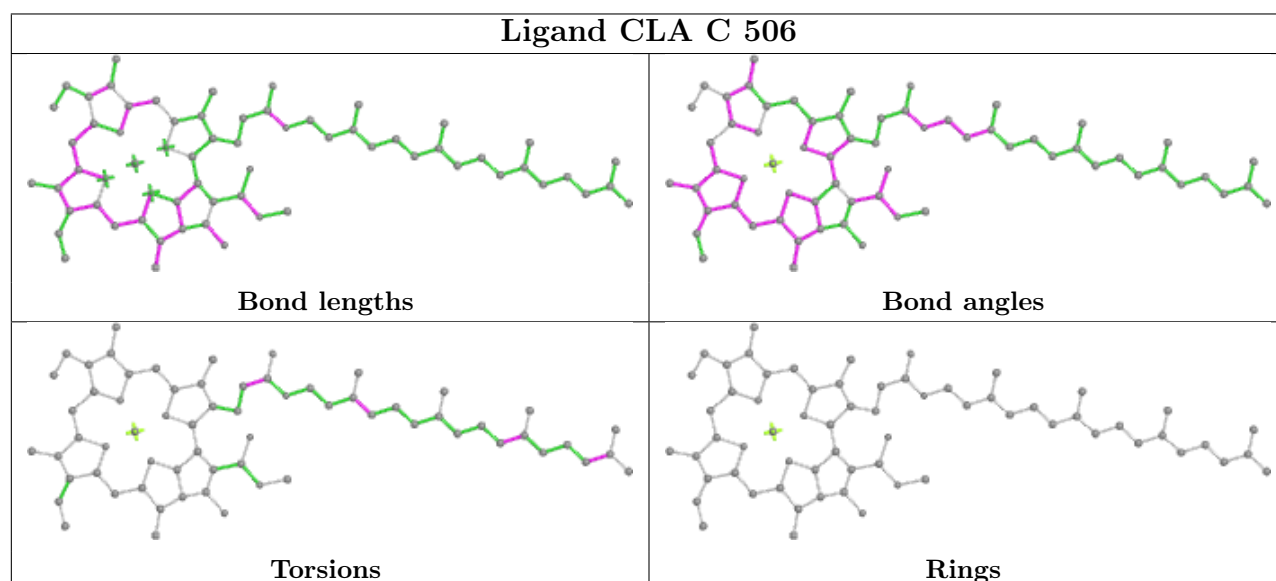
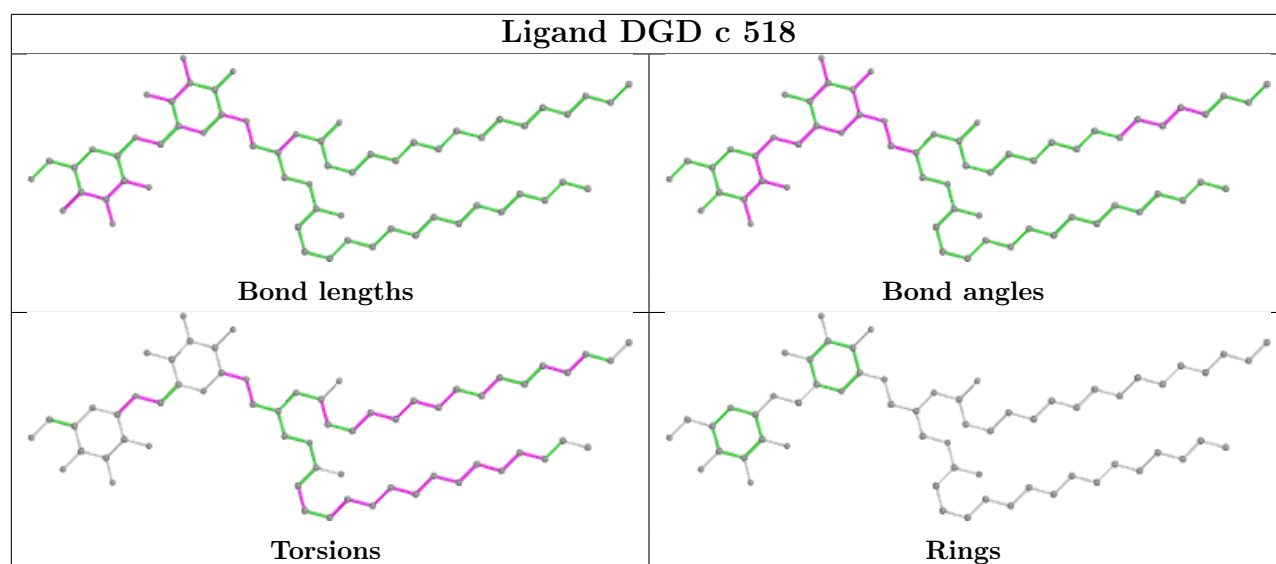
Ligand CLA d 405

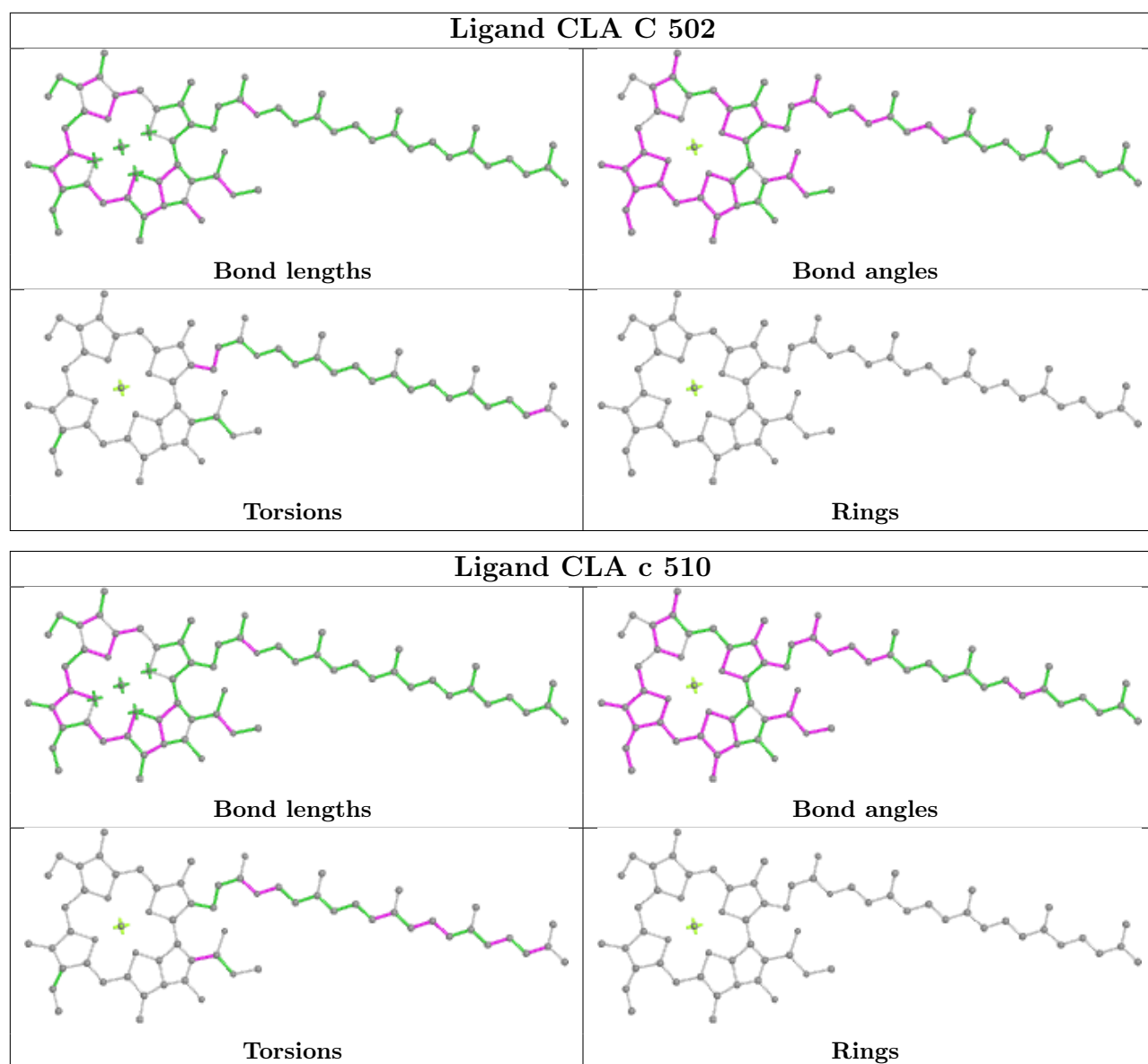


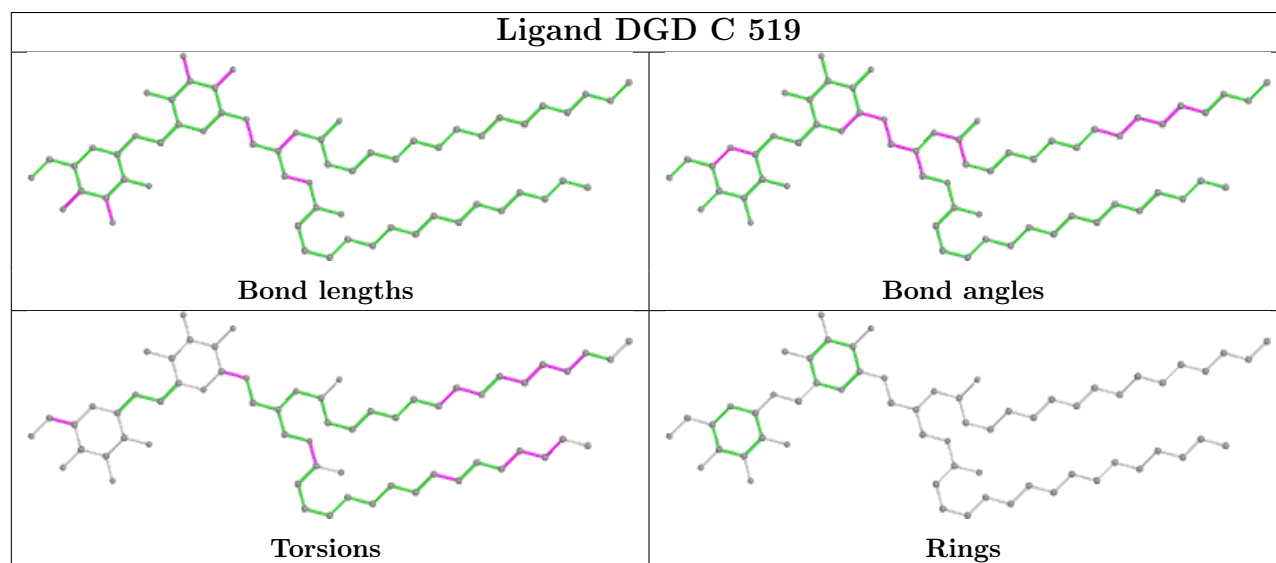
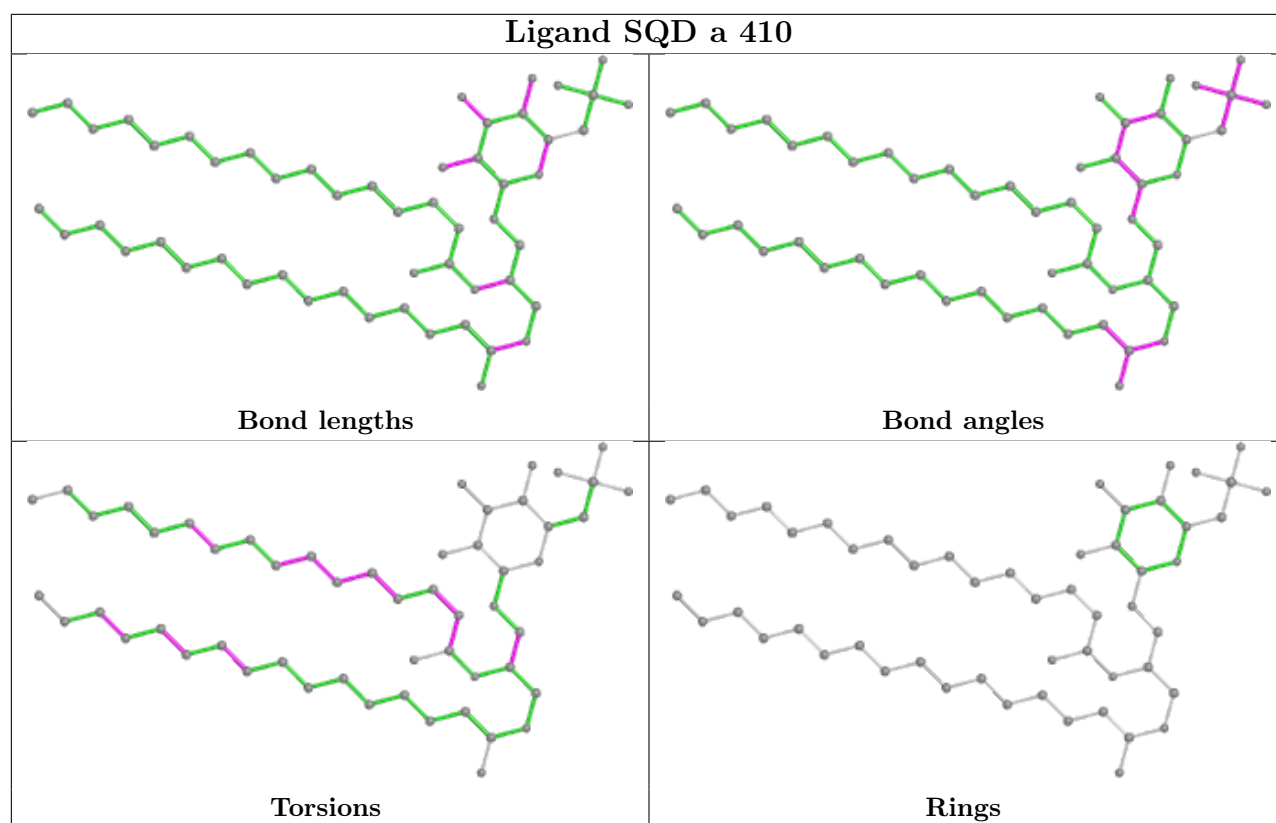
Ligand DGD H 101

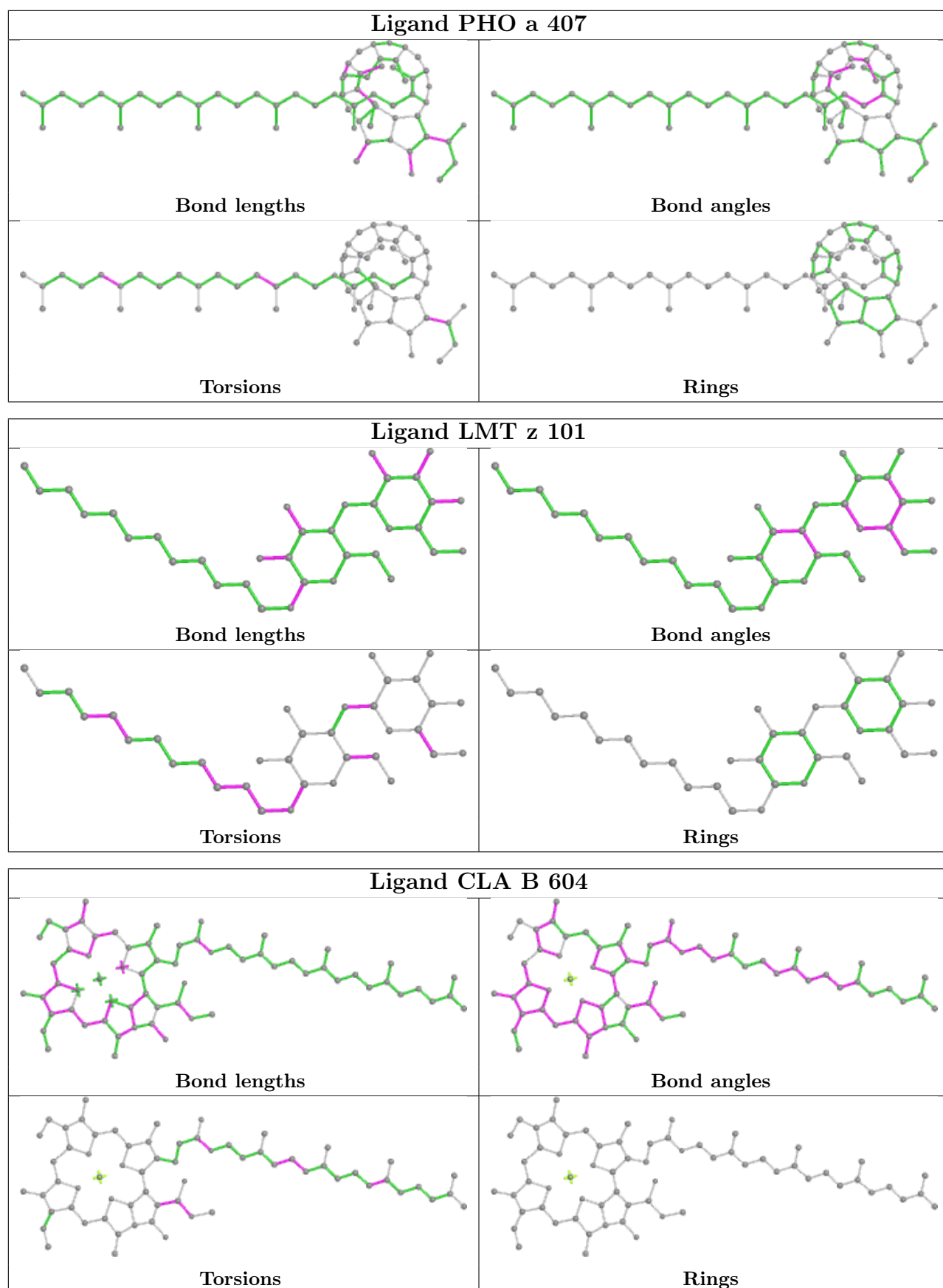


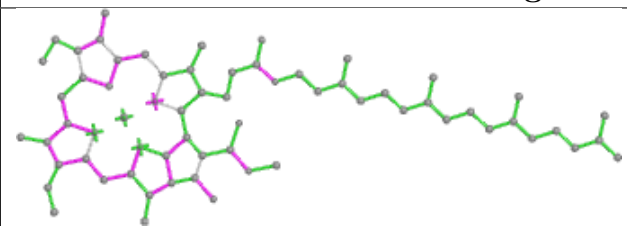
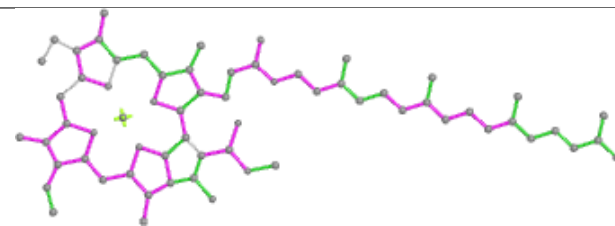
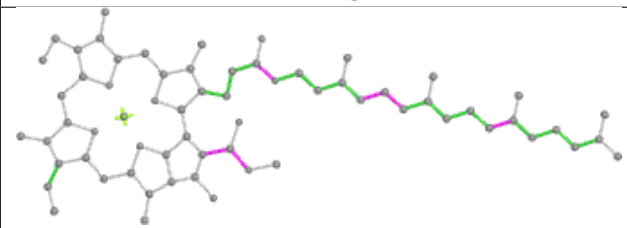
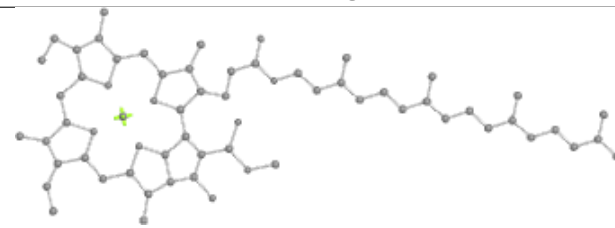


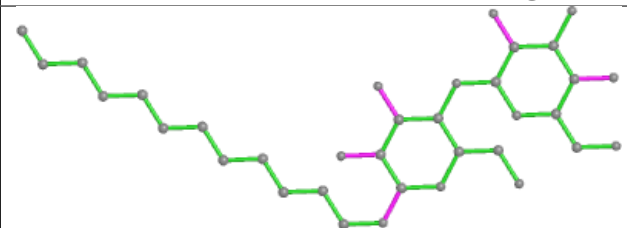
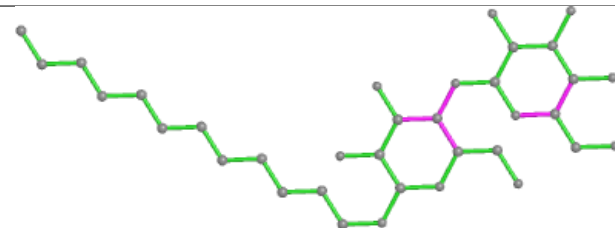
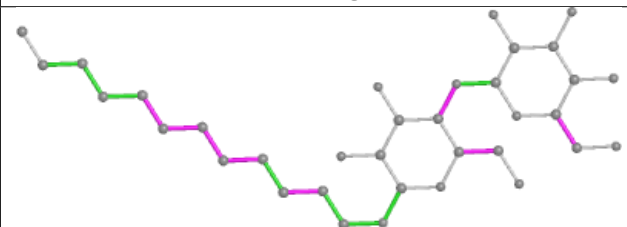
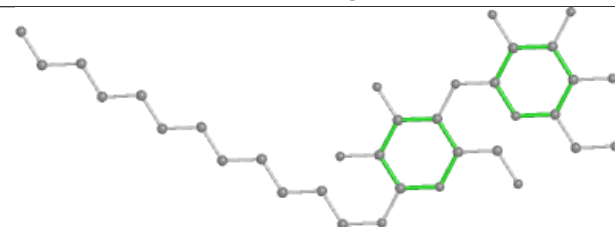


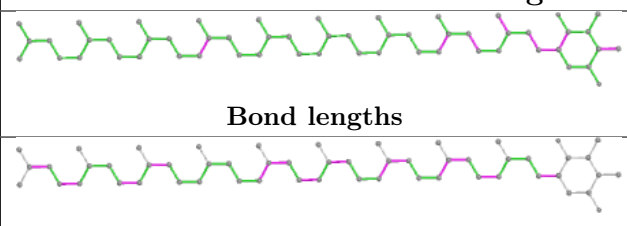
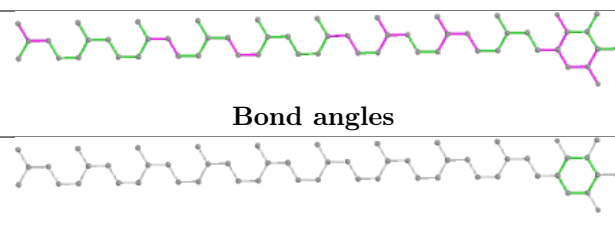
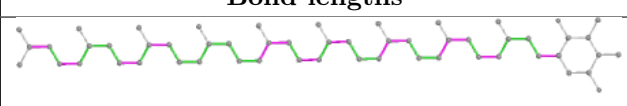
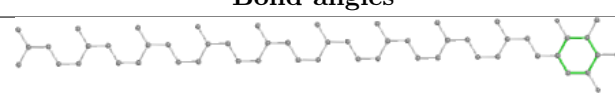


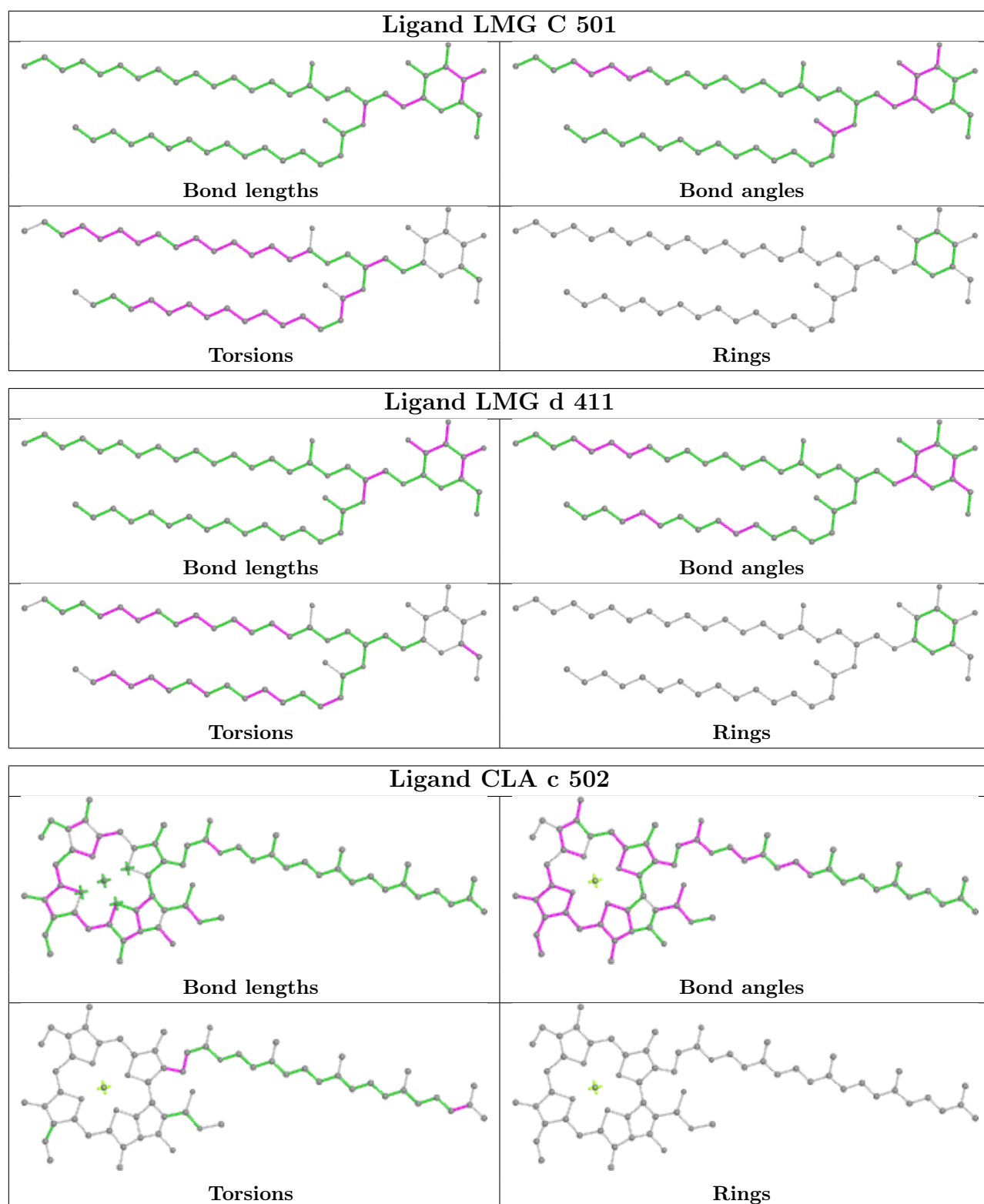


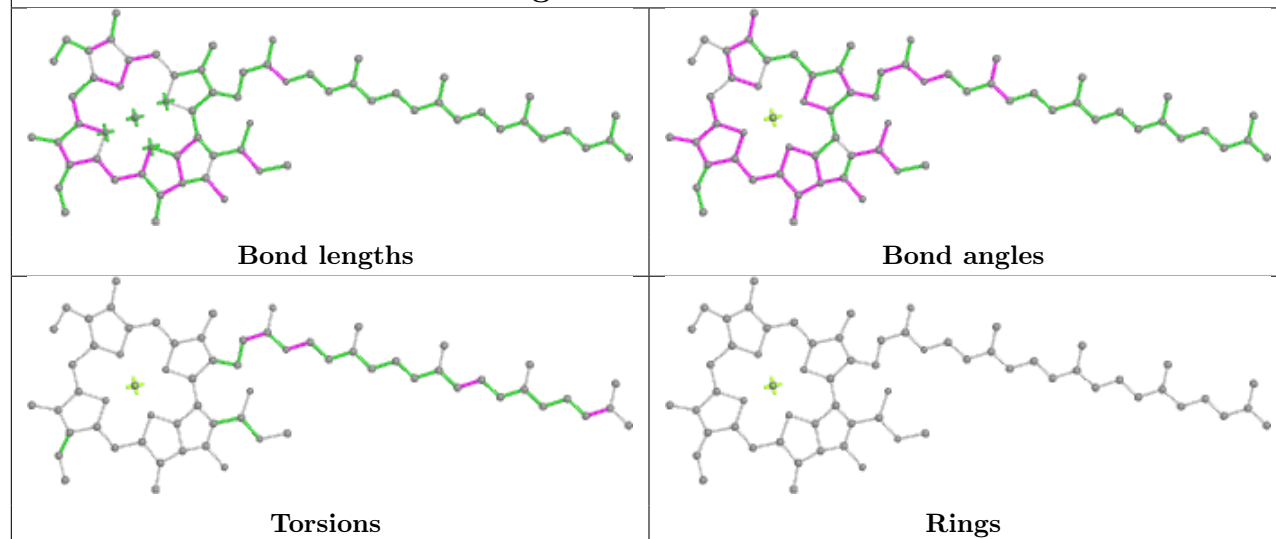
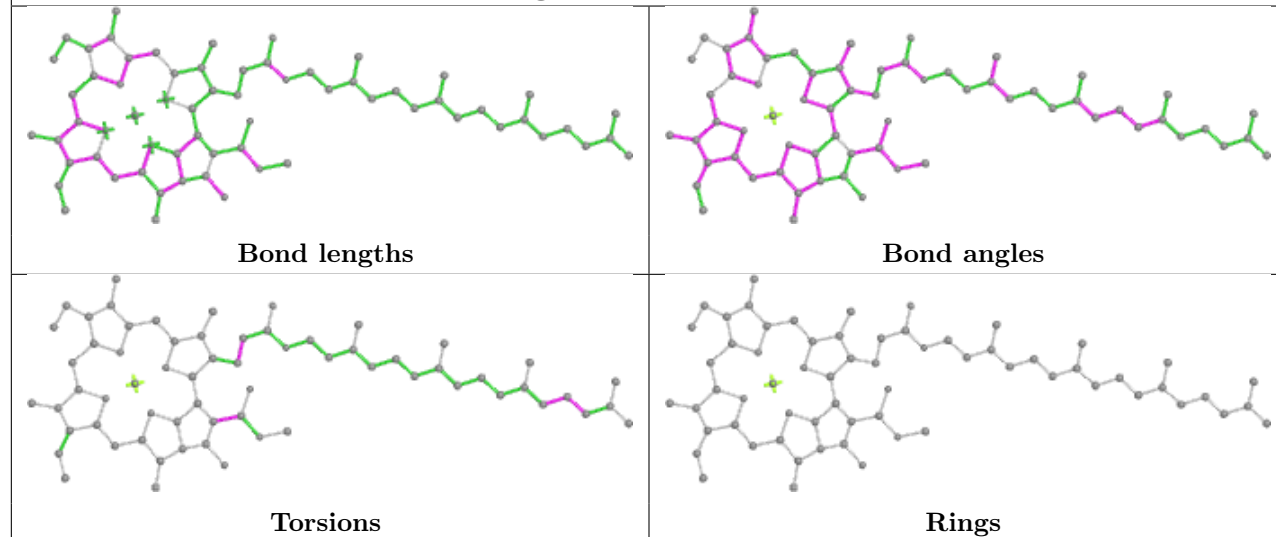


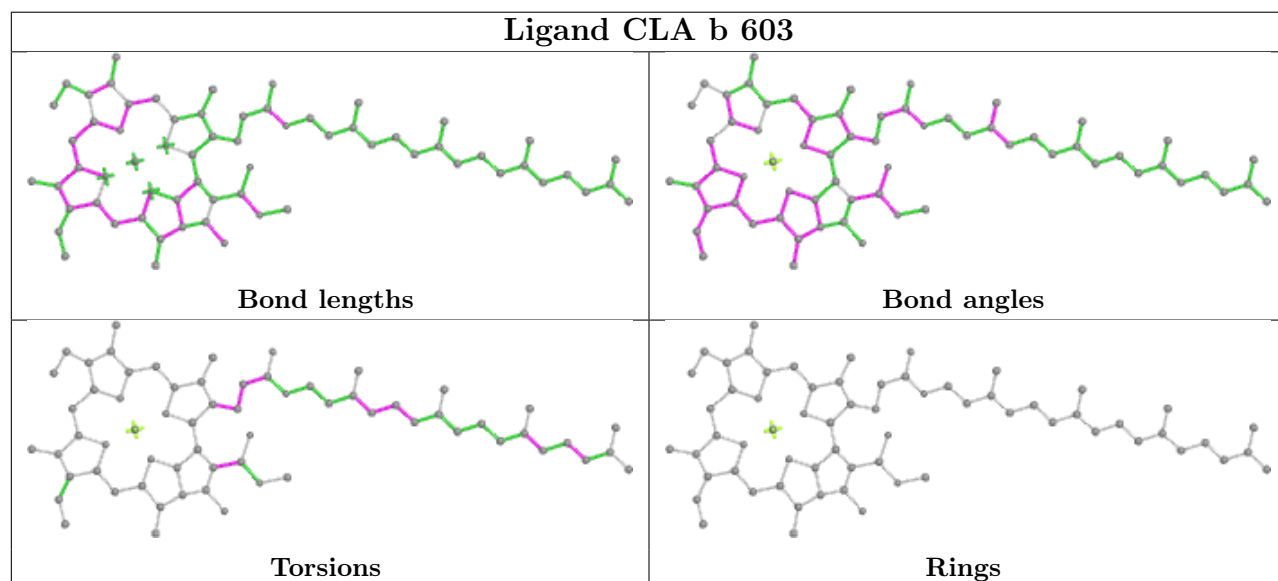
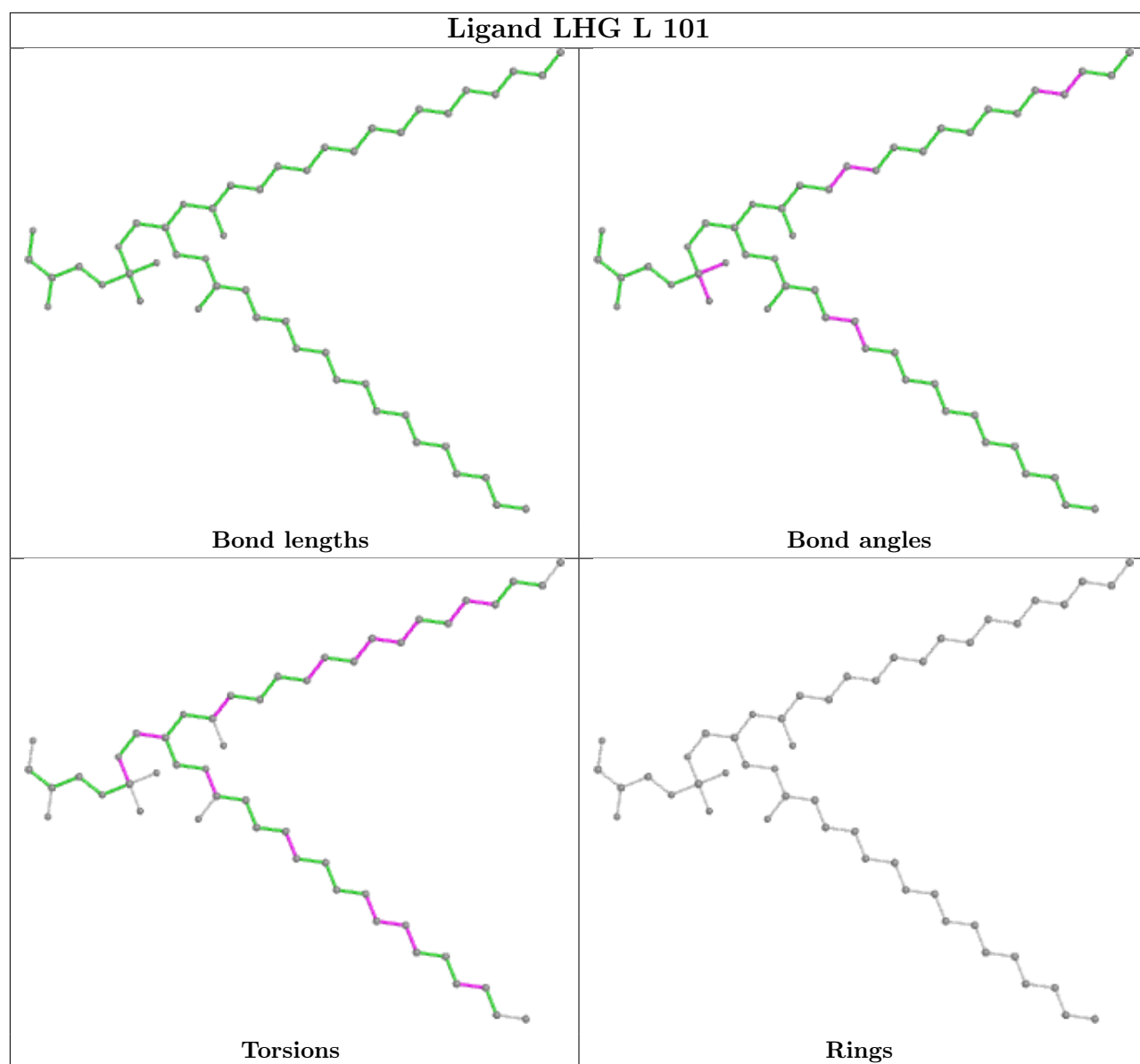
Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

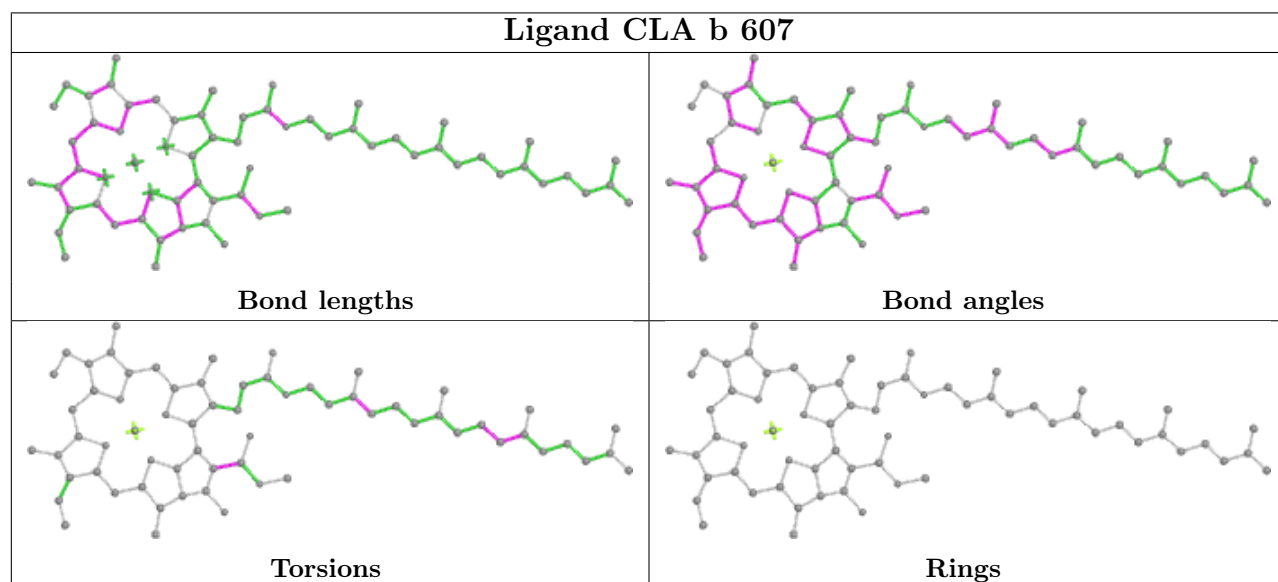
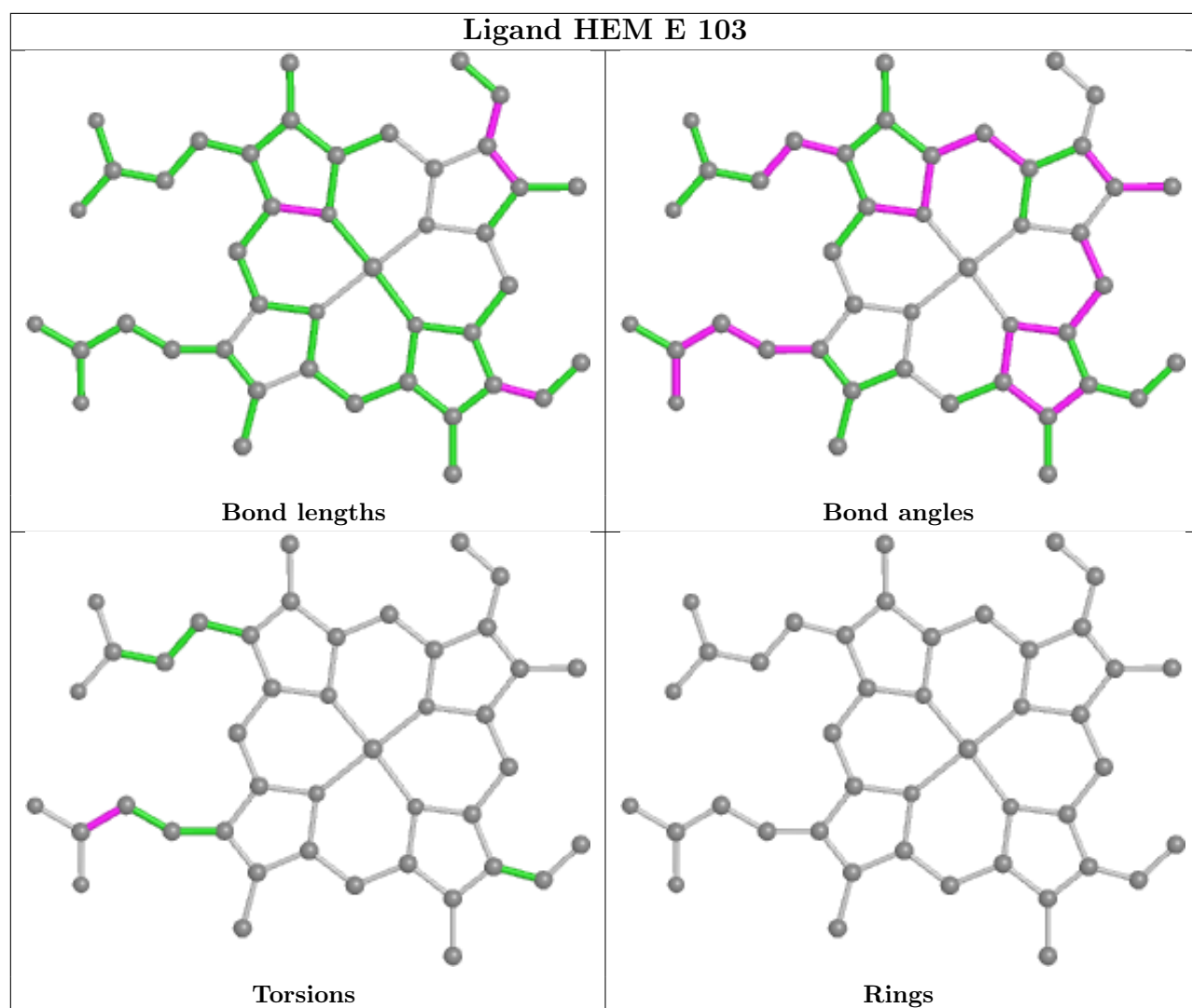
Ligand LMT c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

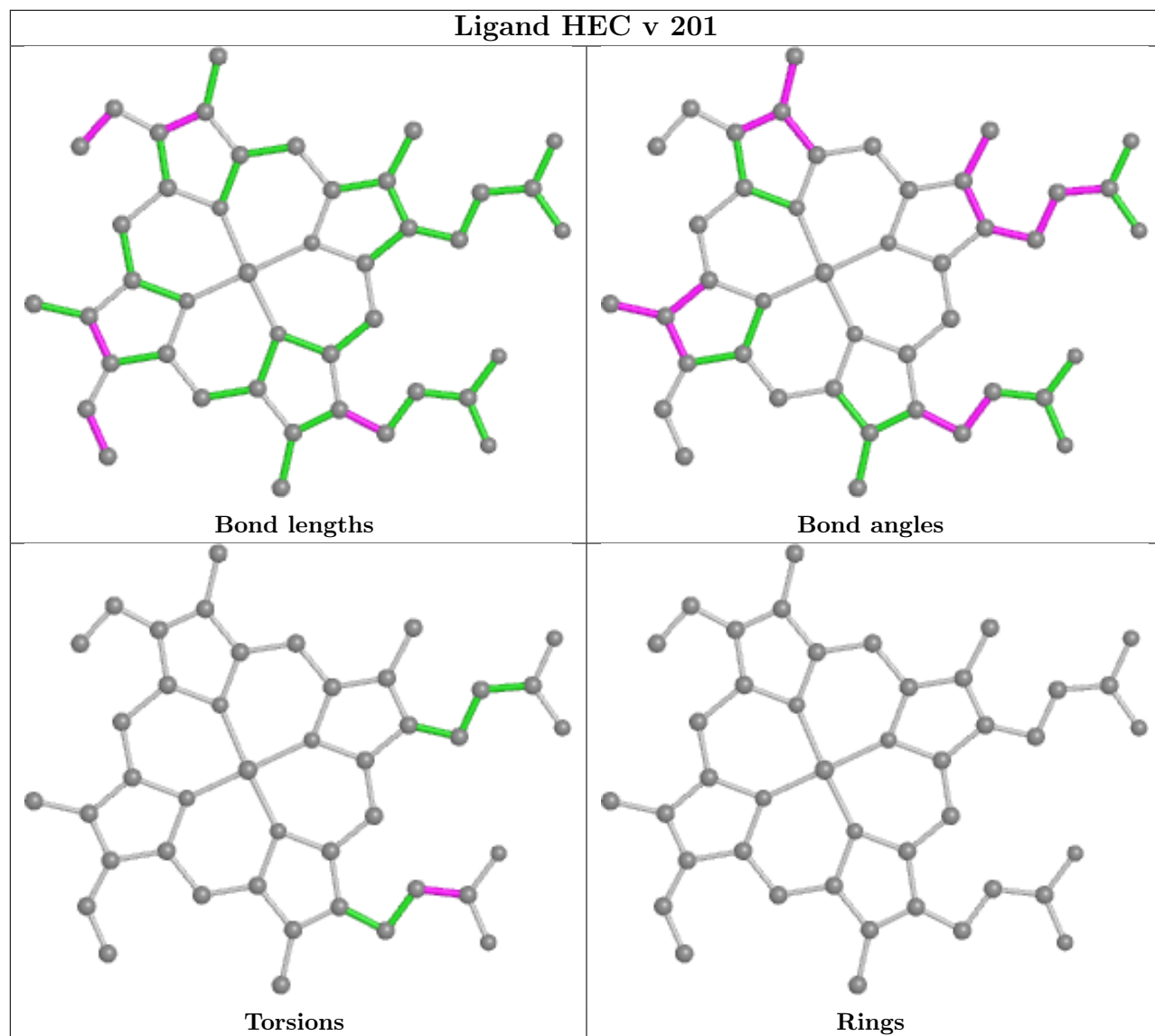


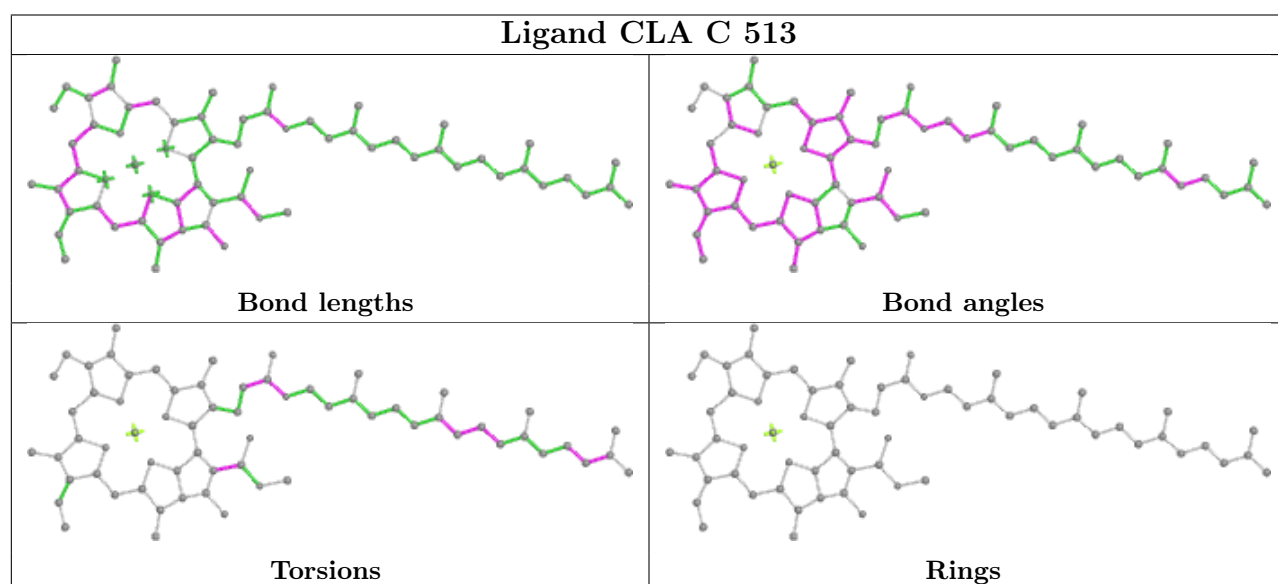
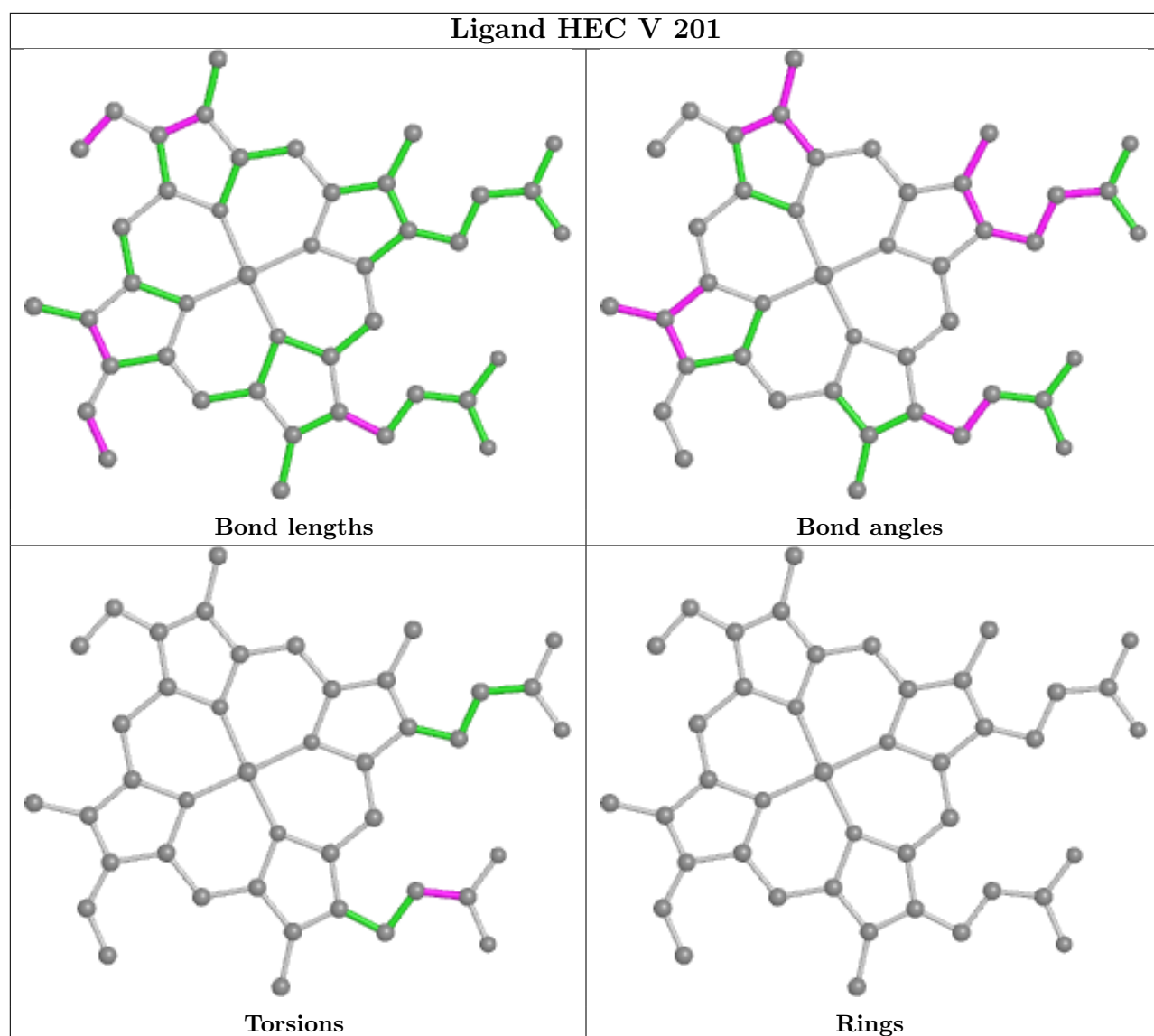
Ligand CLA C 511**Ligand CLA B 606**

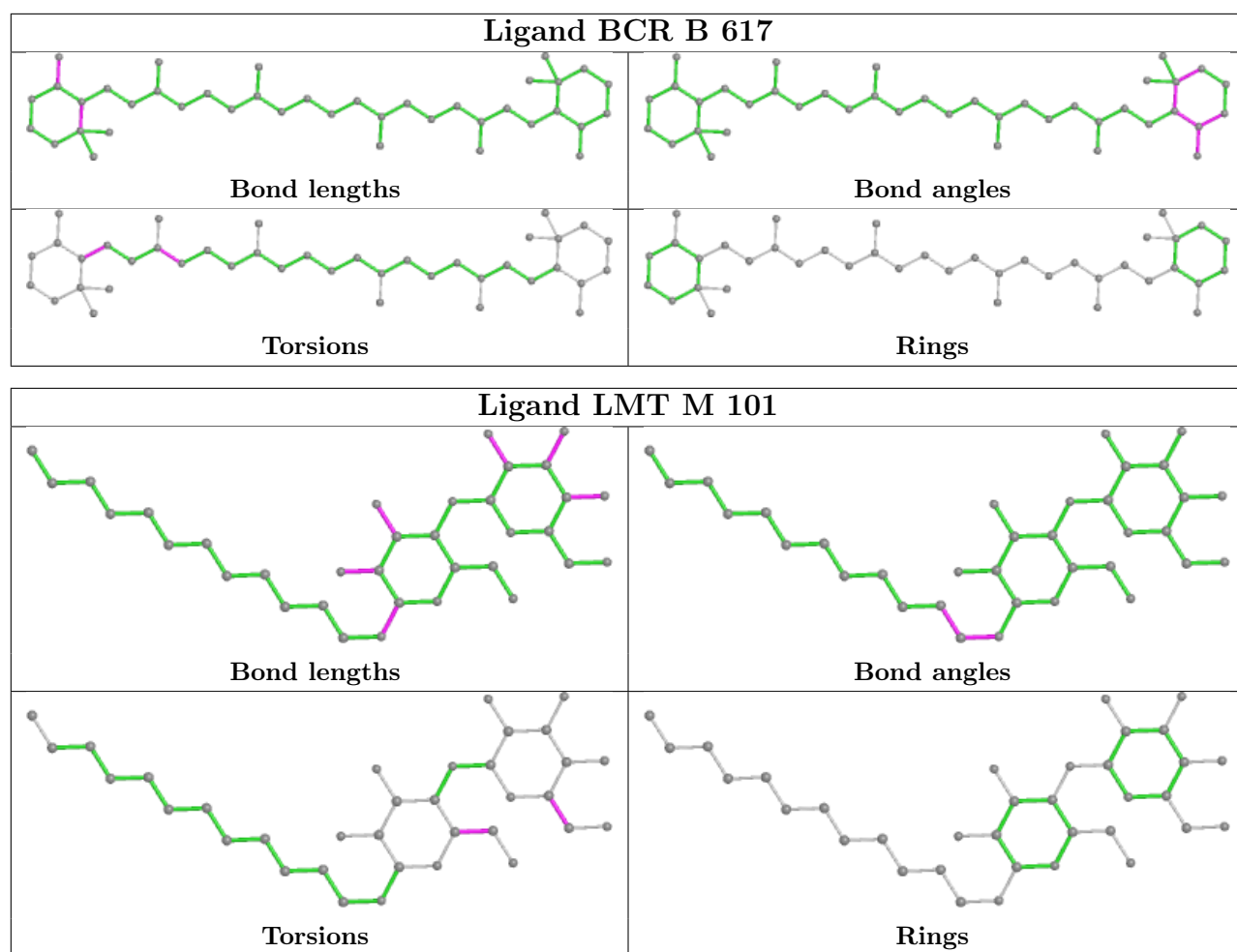


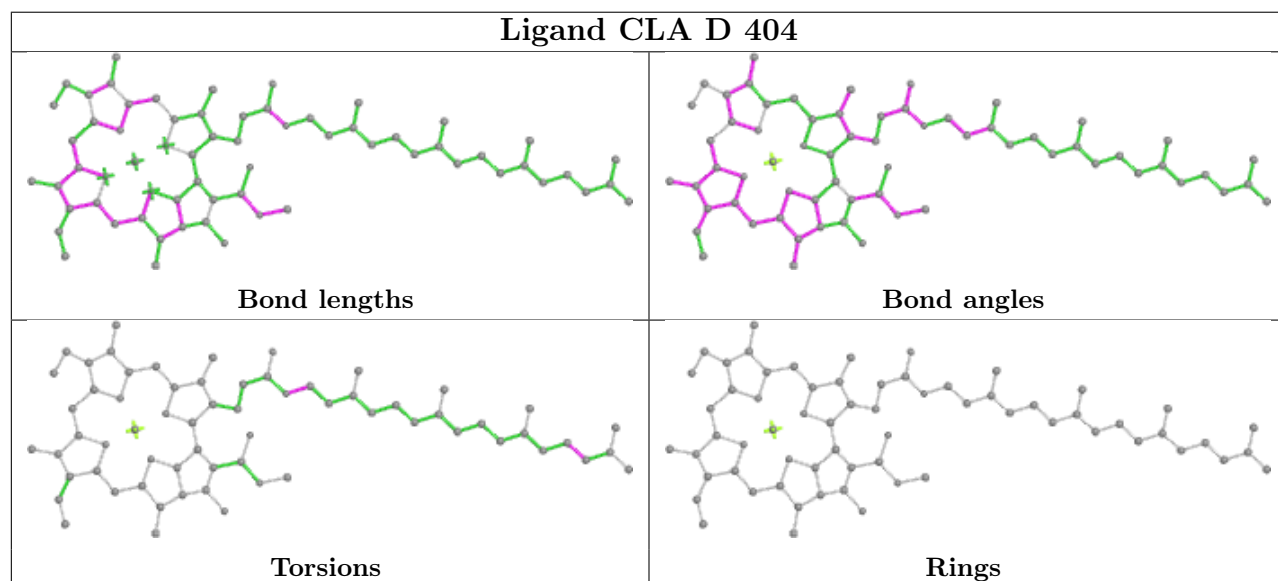
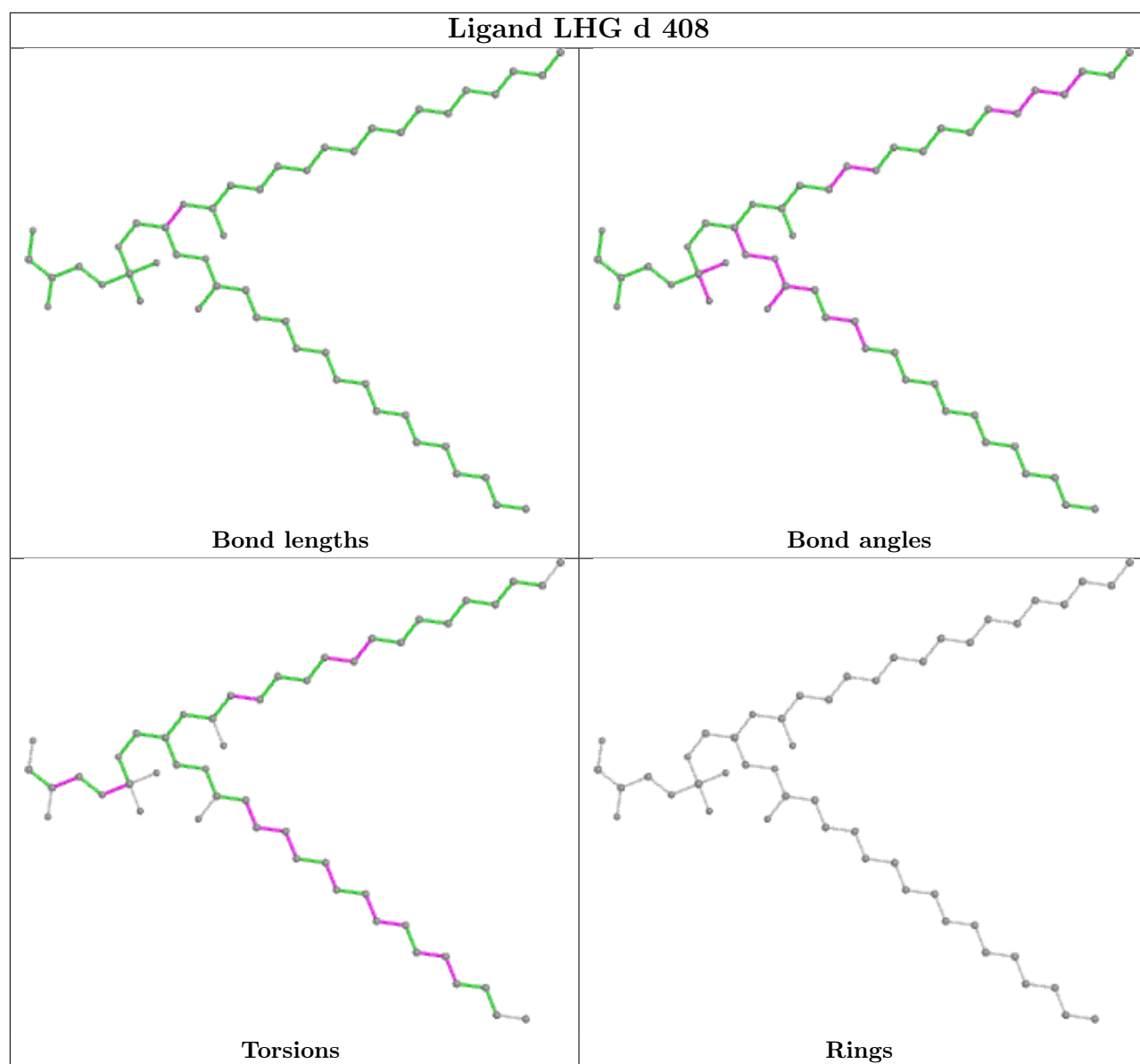


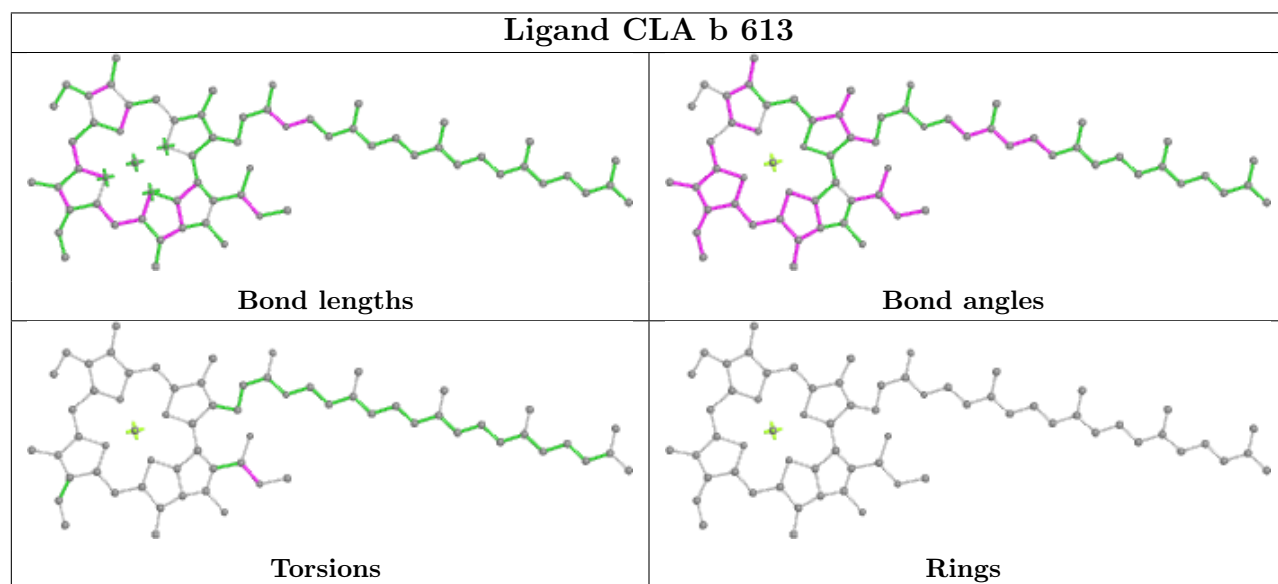
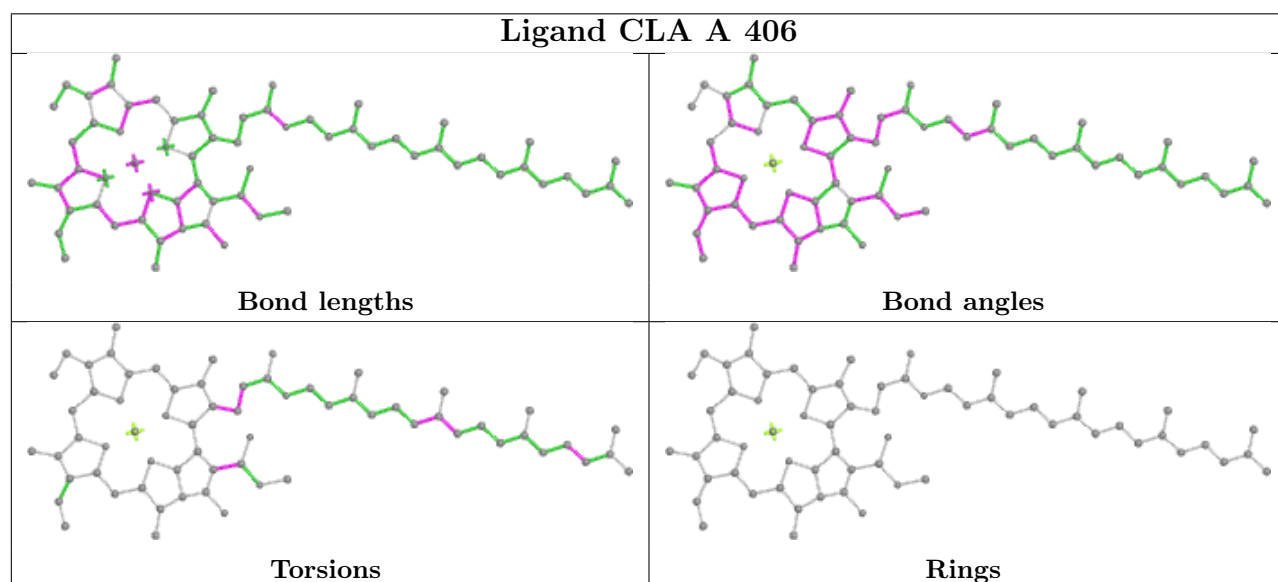
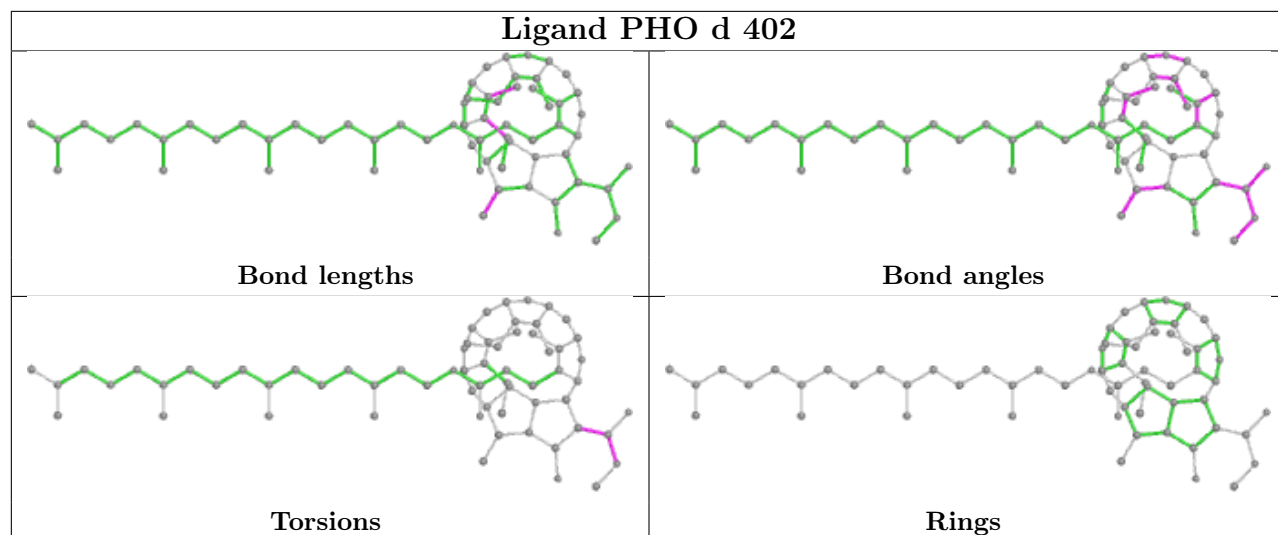
Ligand HEC v 201

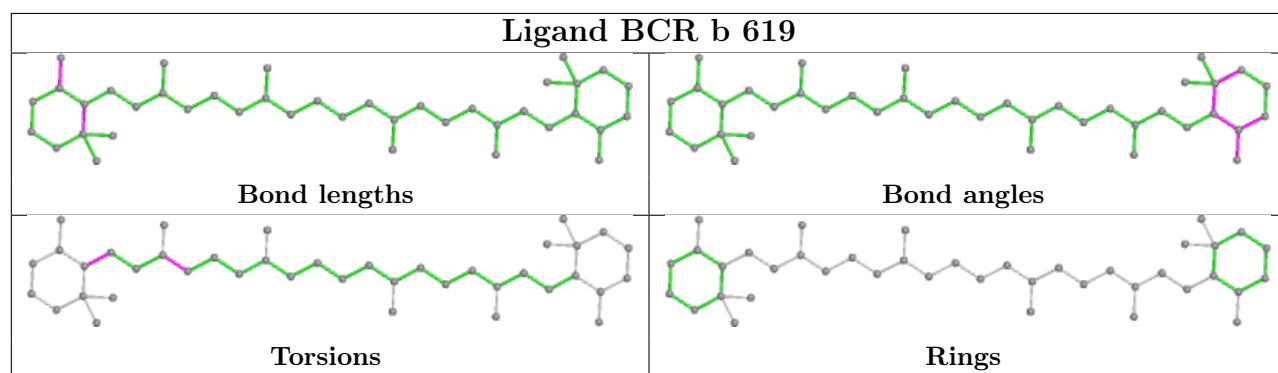
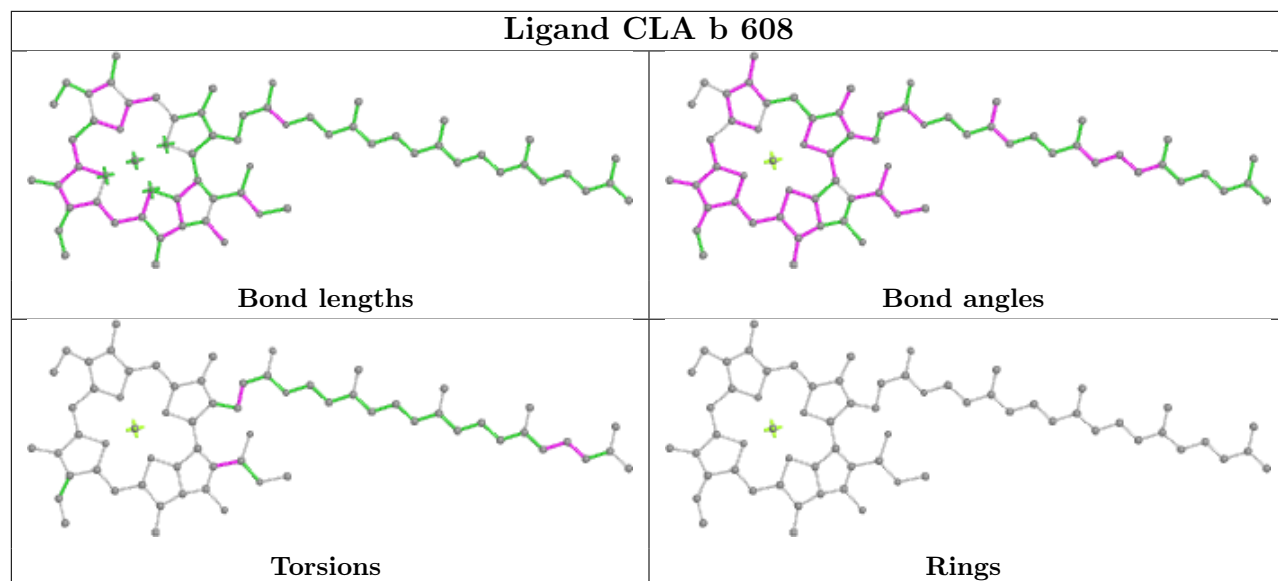
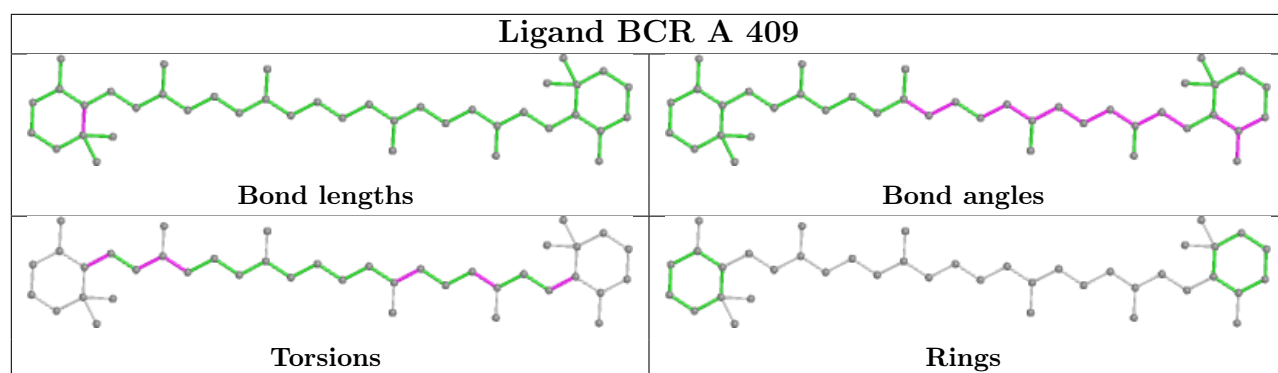


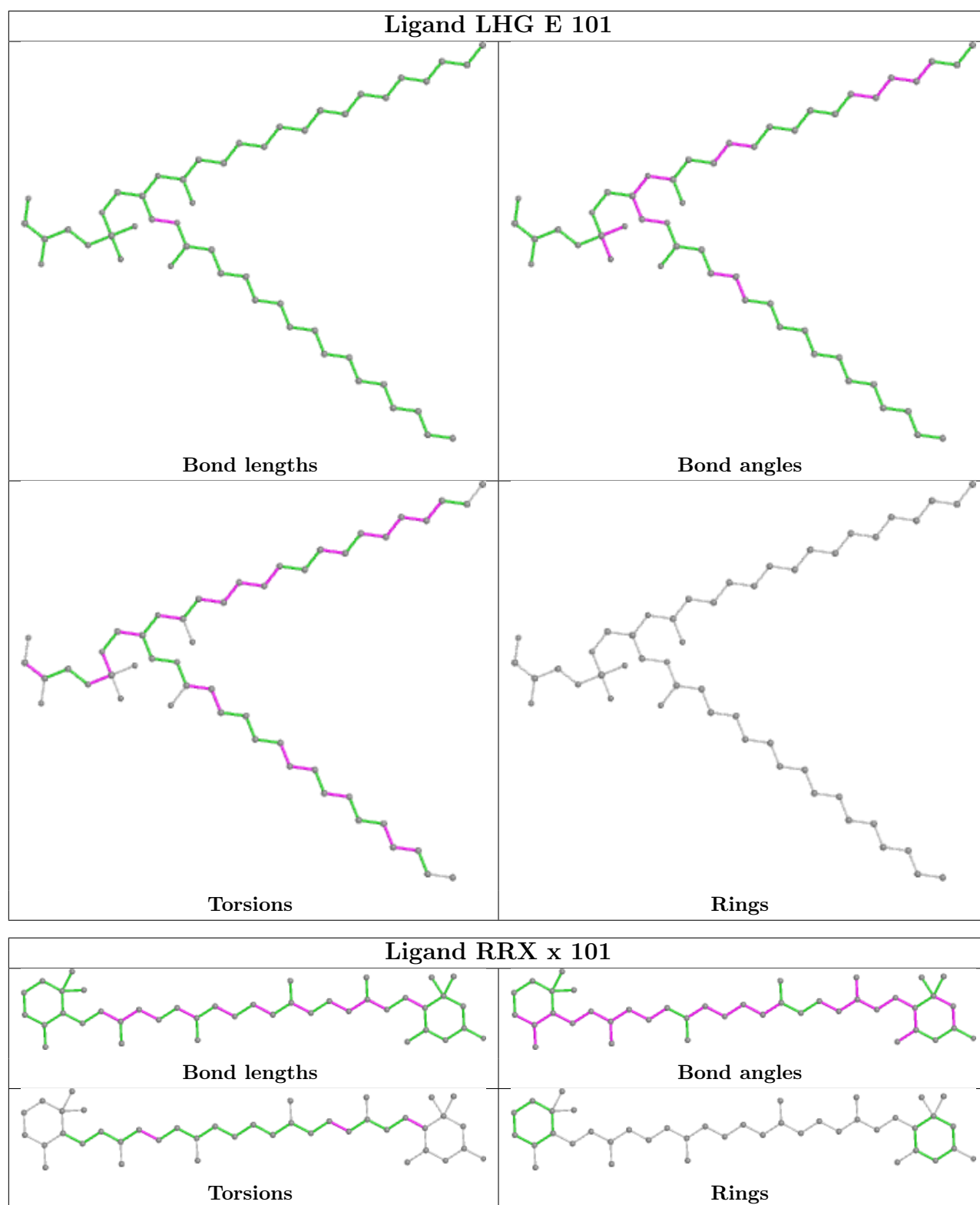


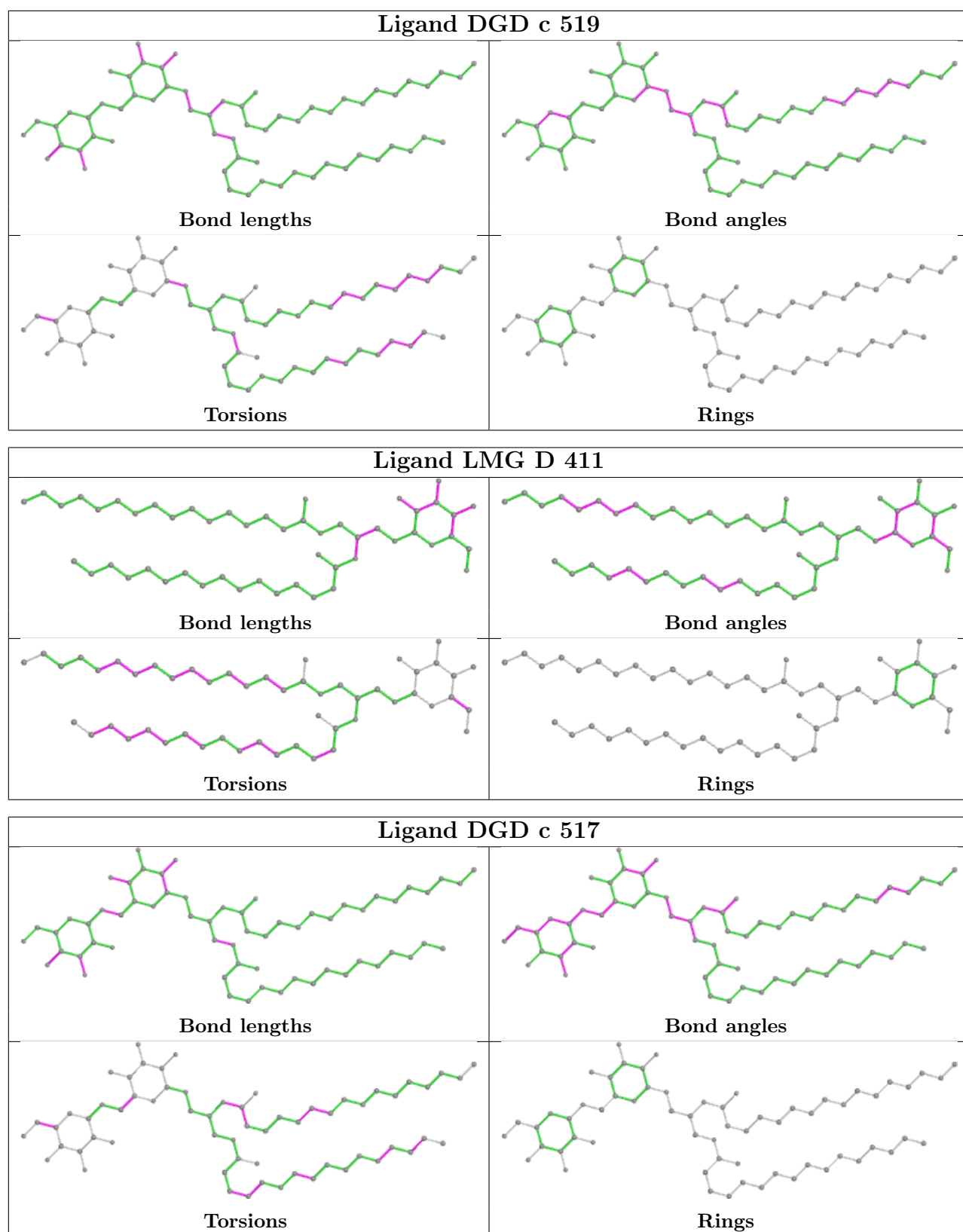


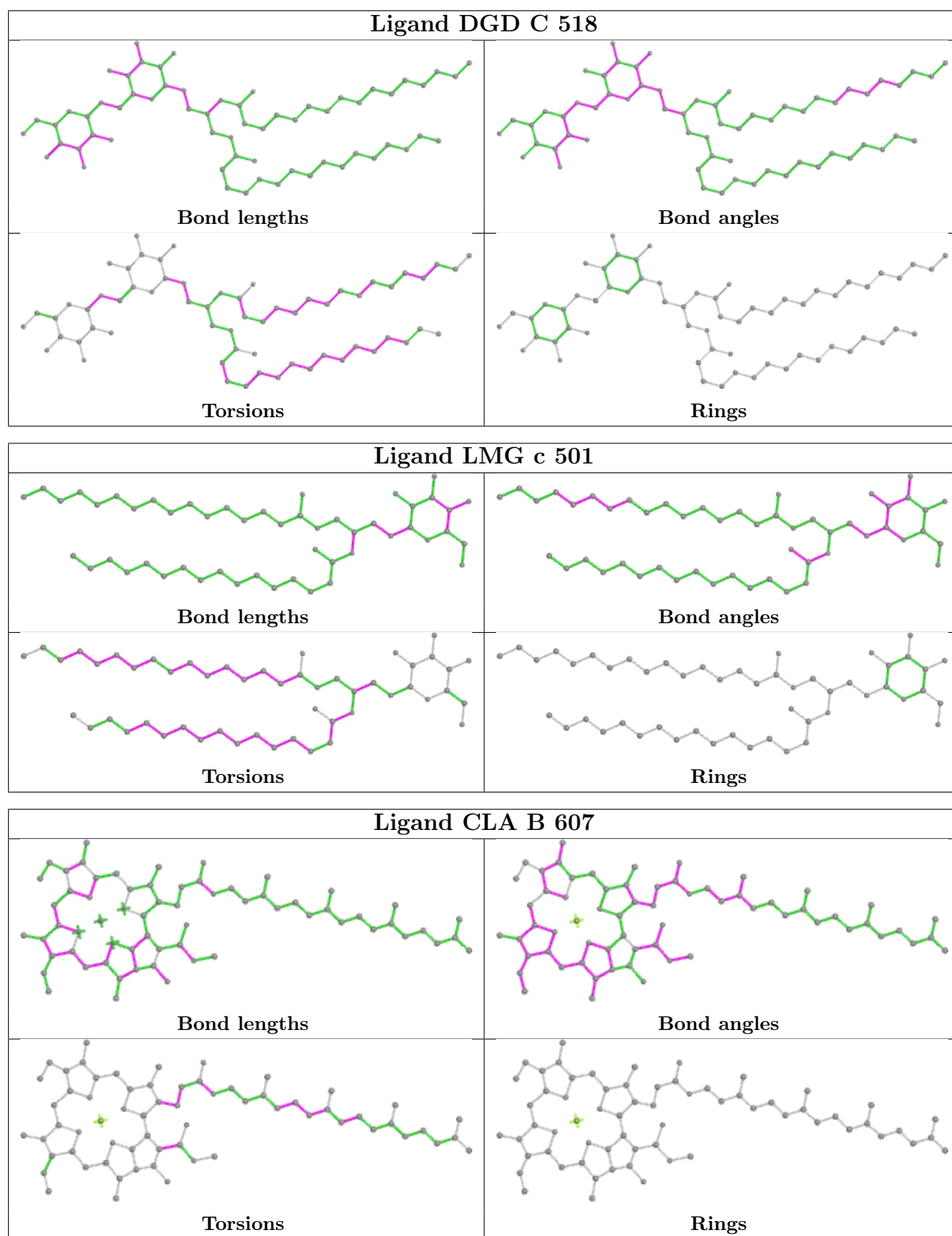


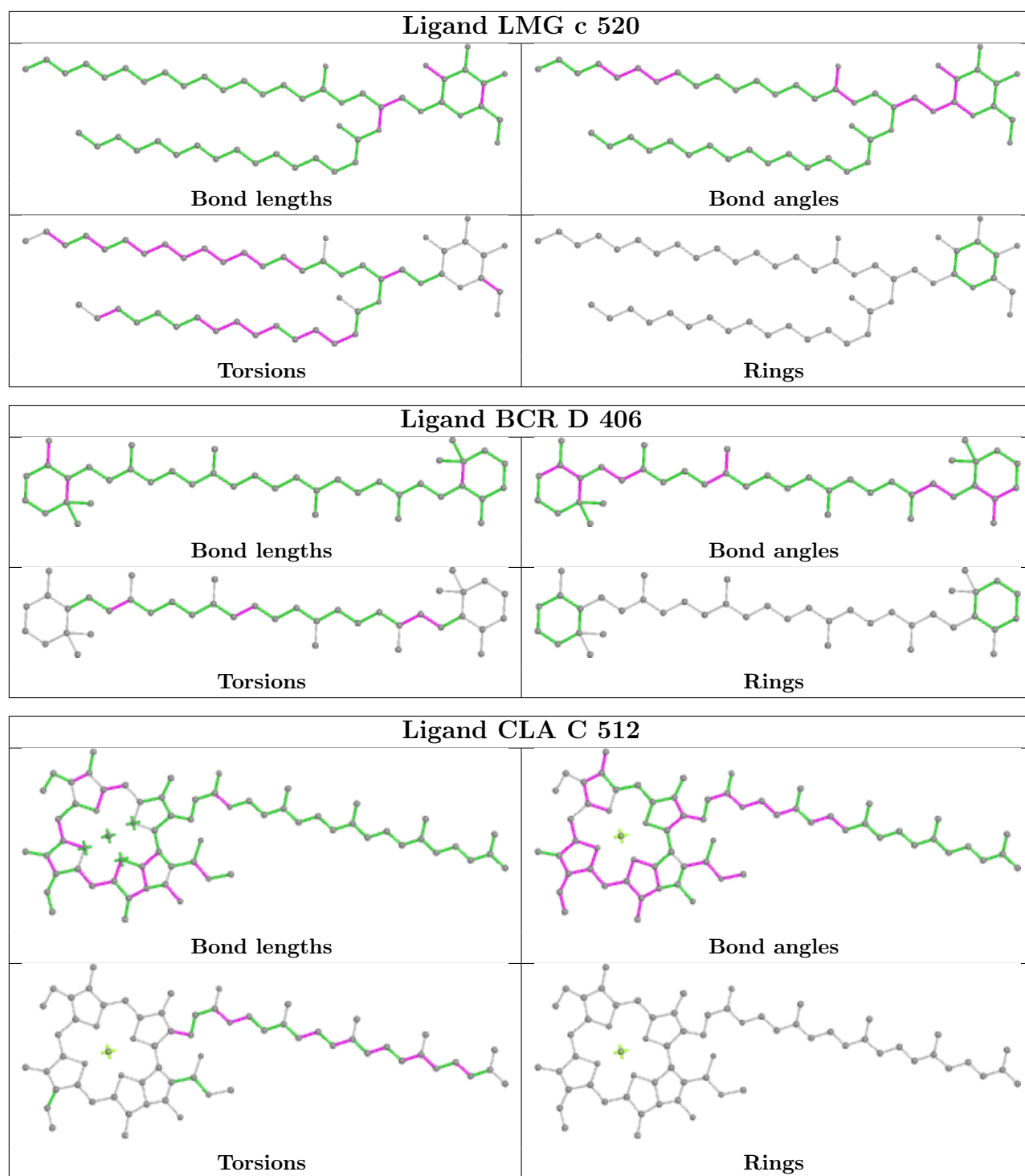


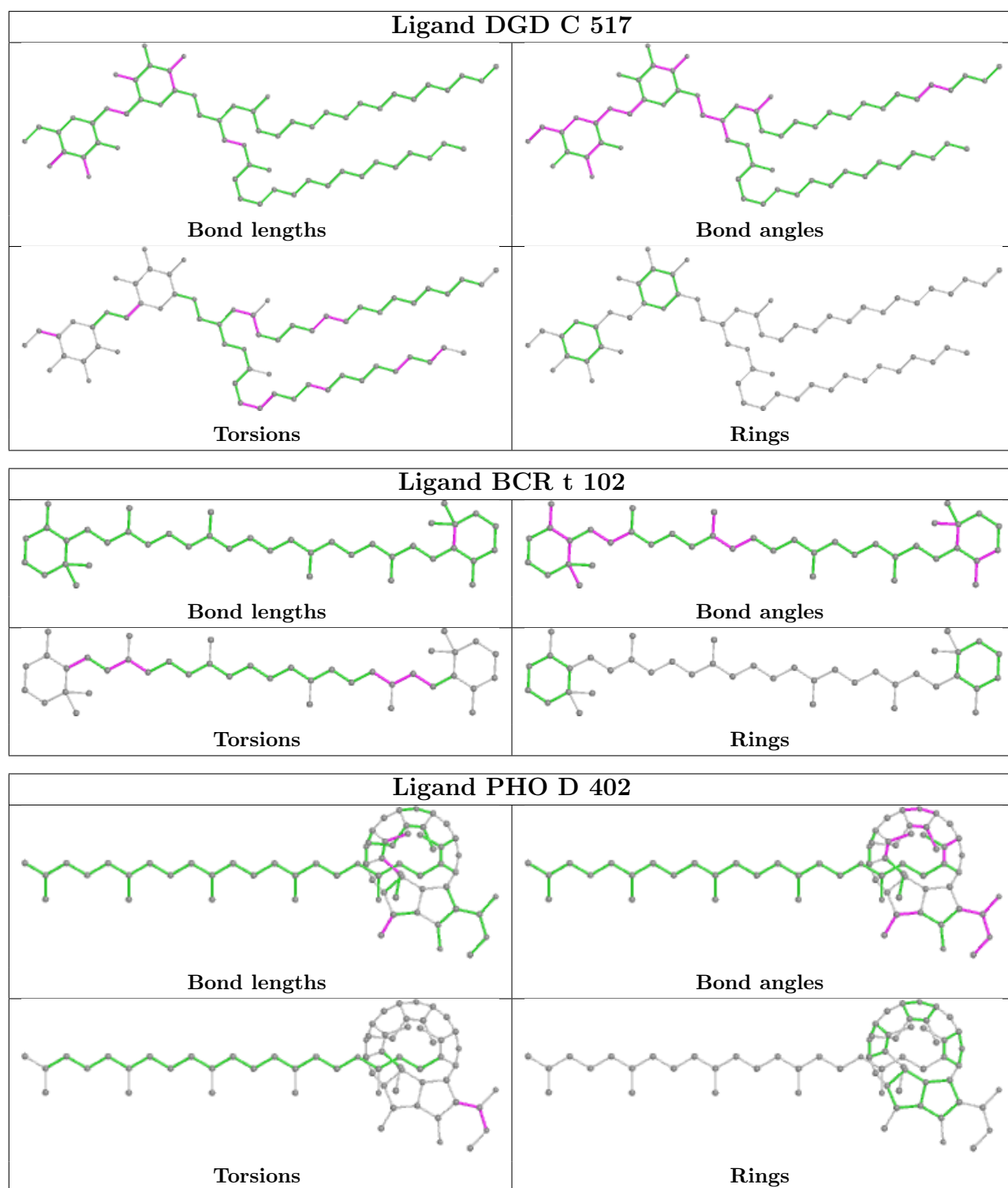




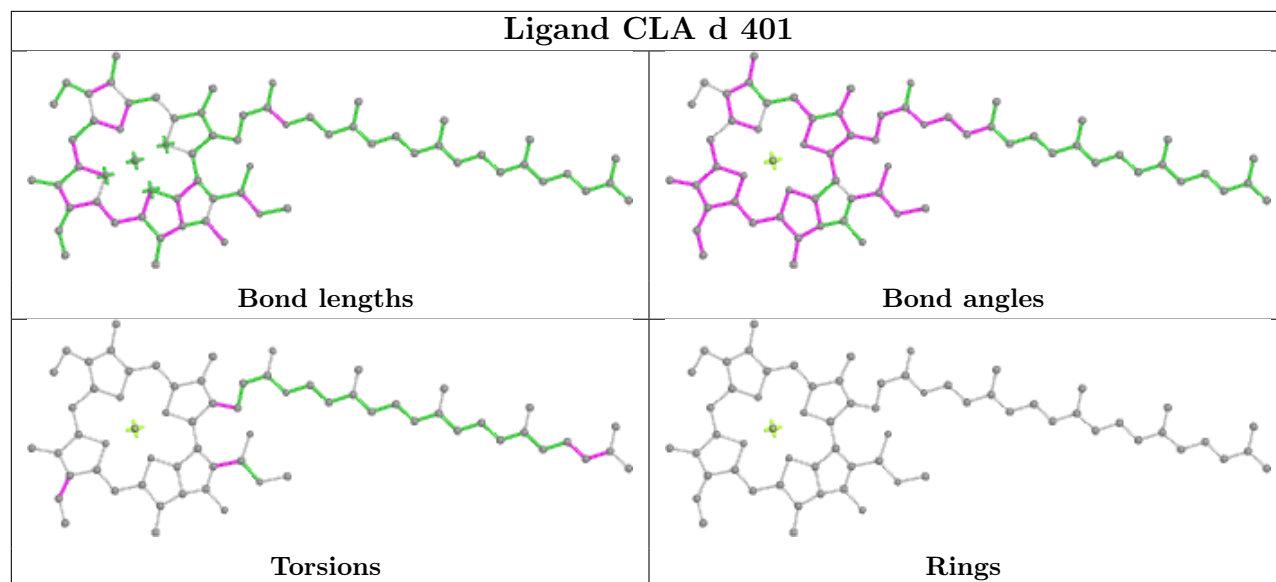




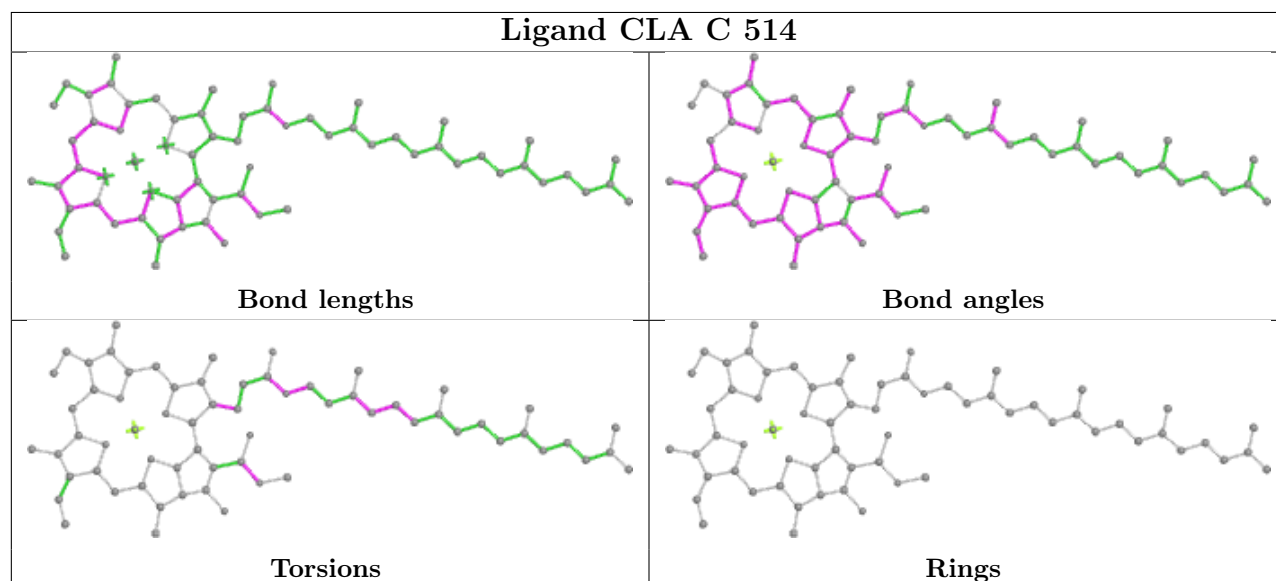




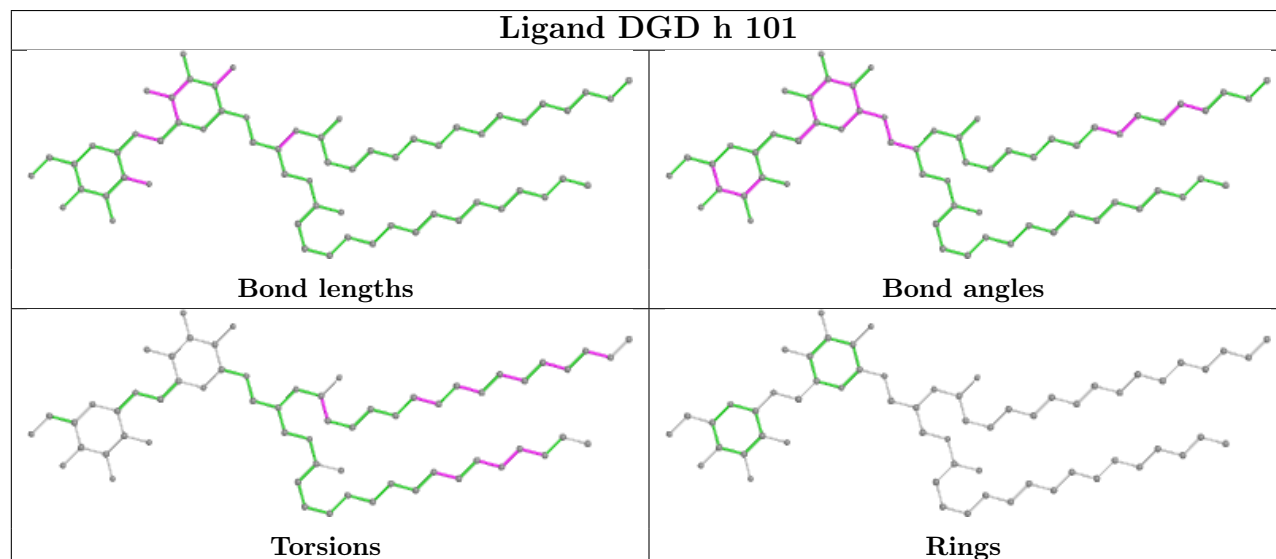
Ligand CLA d 401



Ligand CLA C 514



Ligand DGD h 101



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.

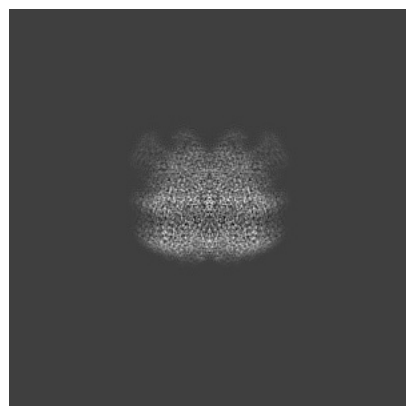
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30547. These allow visual inspection of the internal detail of the map and identification of artifacts.

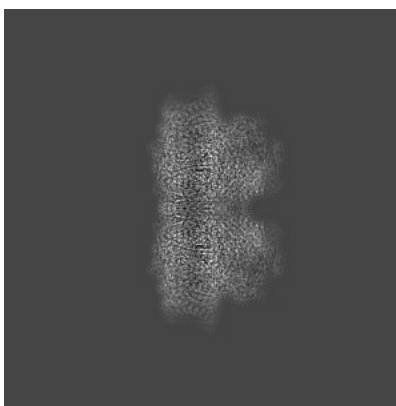
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

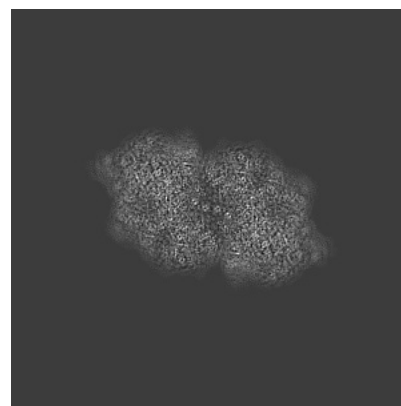
6.1.1 Primary map



X

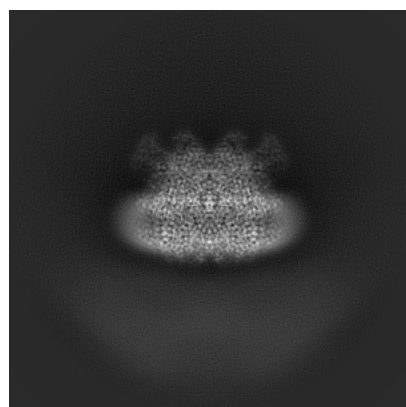


Y

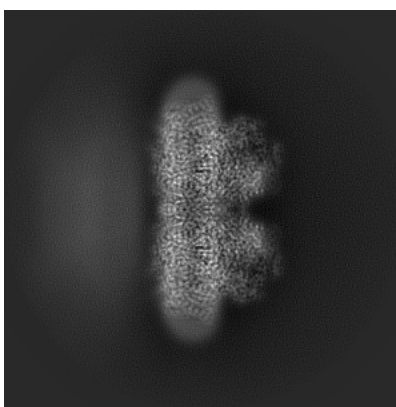


Z

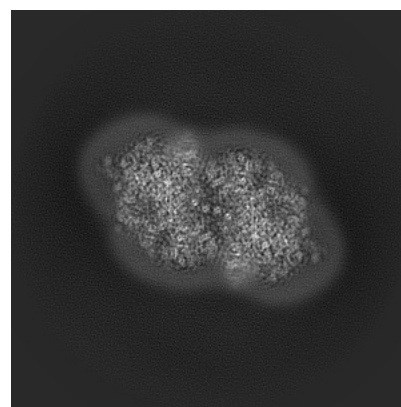
6.1.2 Raw map



X



Y

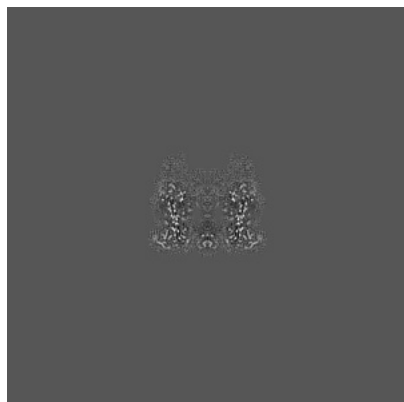


Z

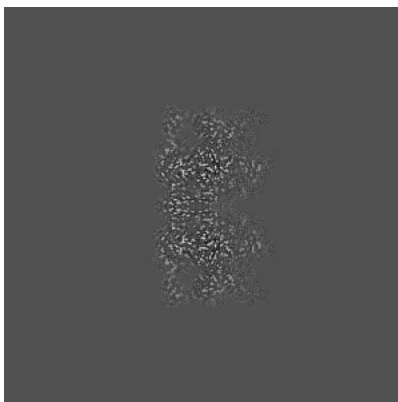
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

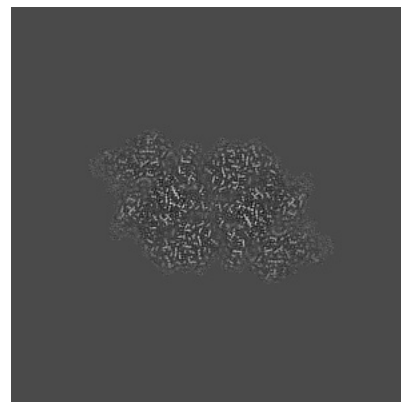
6.2.1 Primary map



X Index: 200

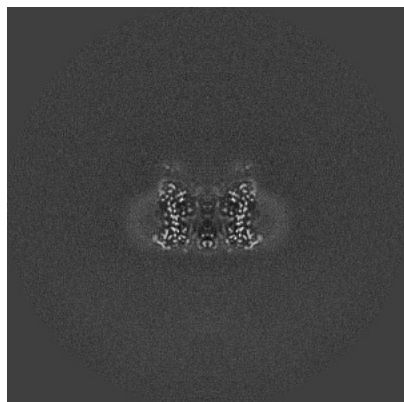


Y Index: 200

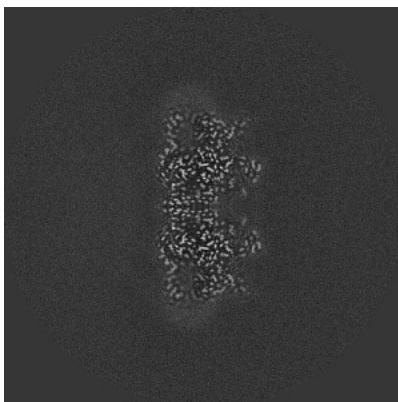


Z Index: 200

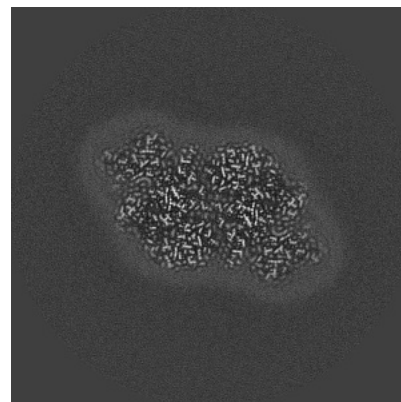
6.2.2 Raw map



X Index: 200



Y Index: 200

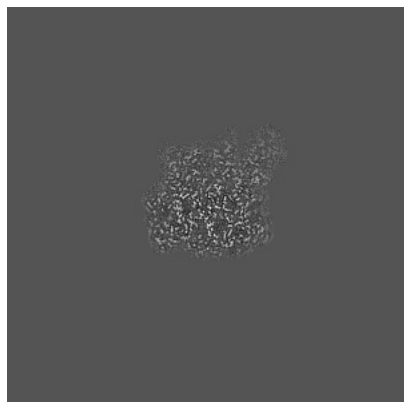


Z Index: 200

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

6.3 Largest variance slices [i](#)

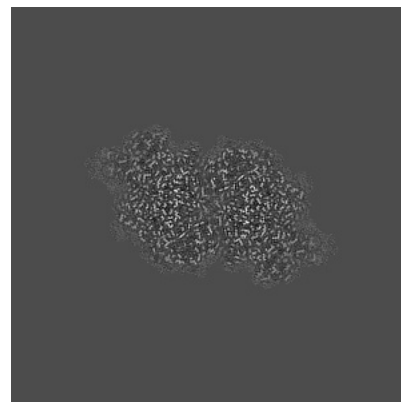
6.3.1 Primary map



X Index: 167

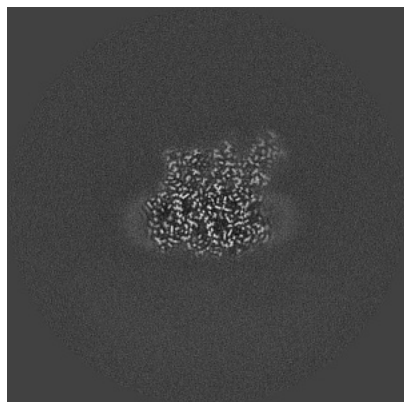


Y Index: 218

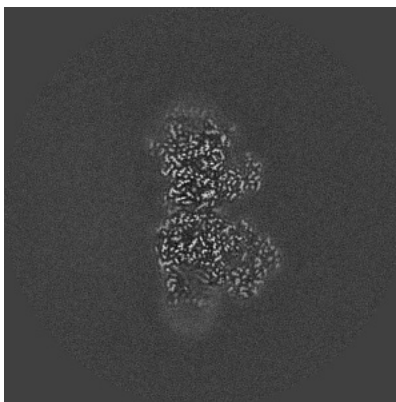


Z Index: 207

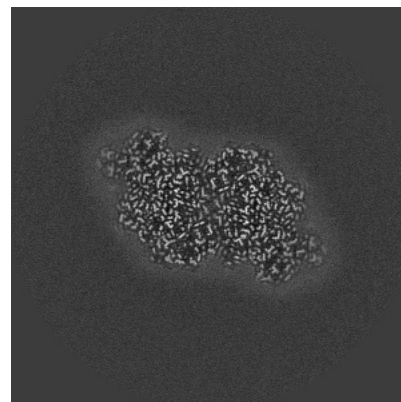
6.3.2 Raw map



X Index: 167



Y Index: 218

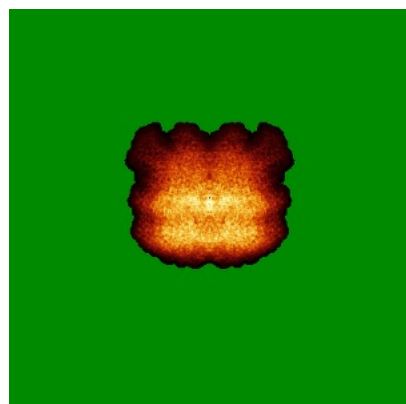


Z Index: 207

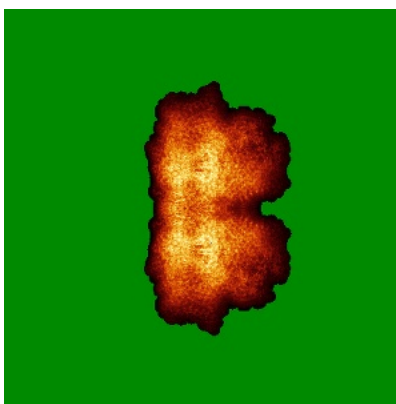
The images above show the largest variance slices of the map in three orthogonal directions.

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

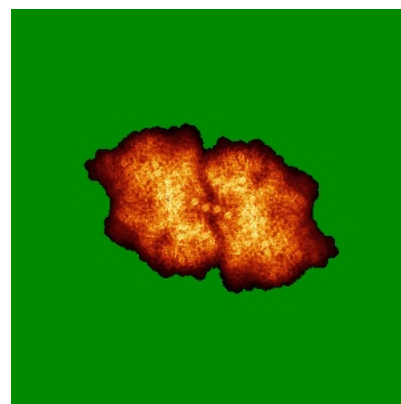
6.4.1 Primary map



X

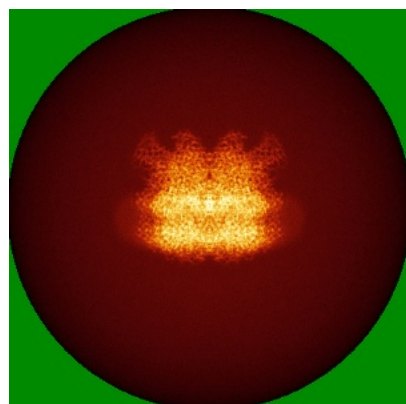


Y

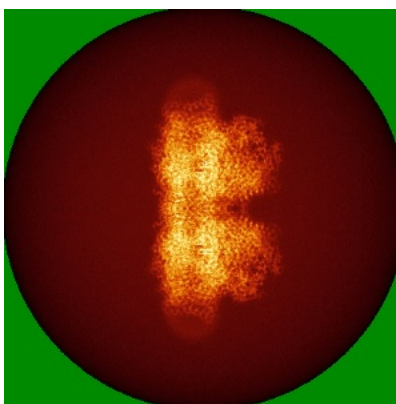


Z

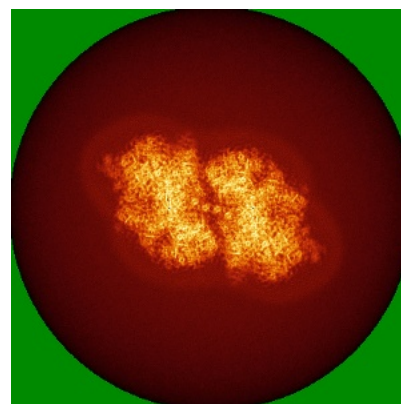
6.4.2 Raw map



X



Y

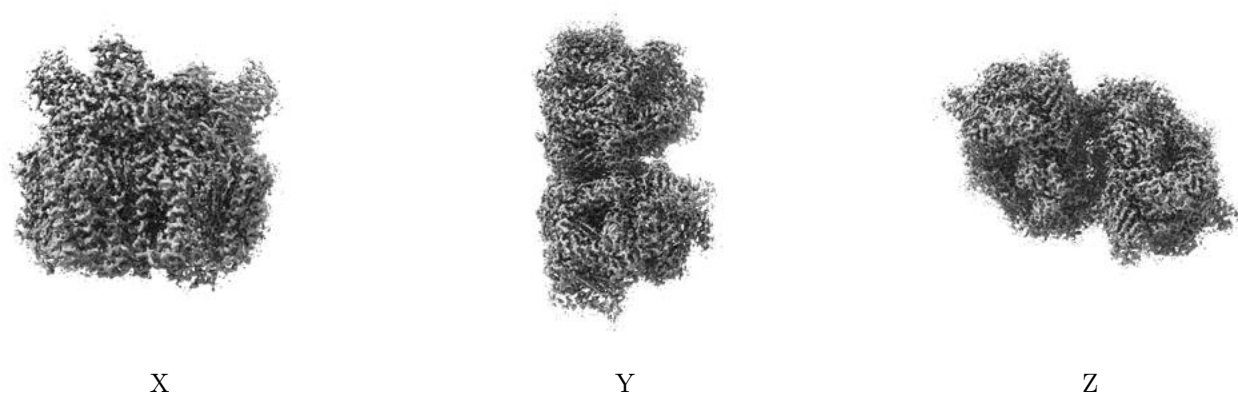


Z

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

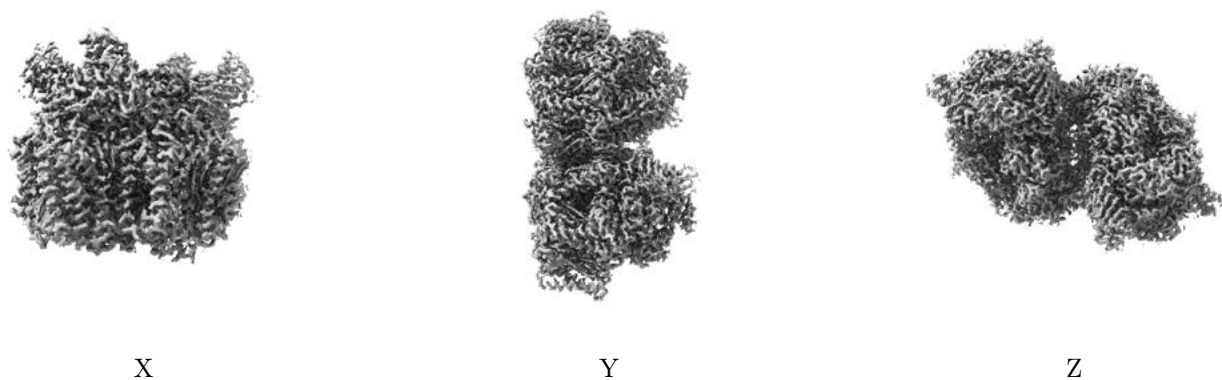
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

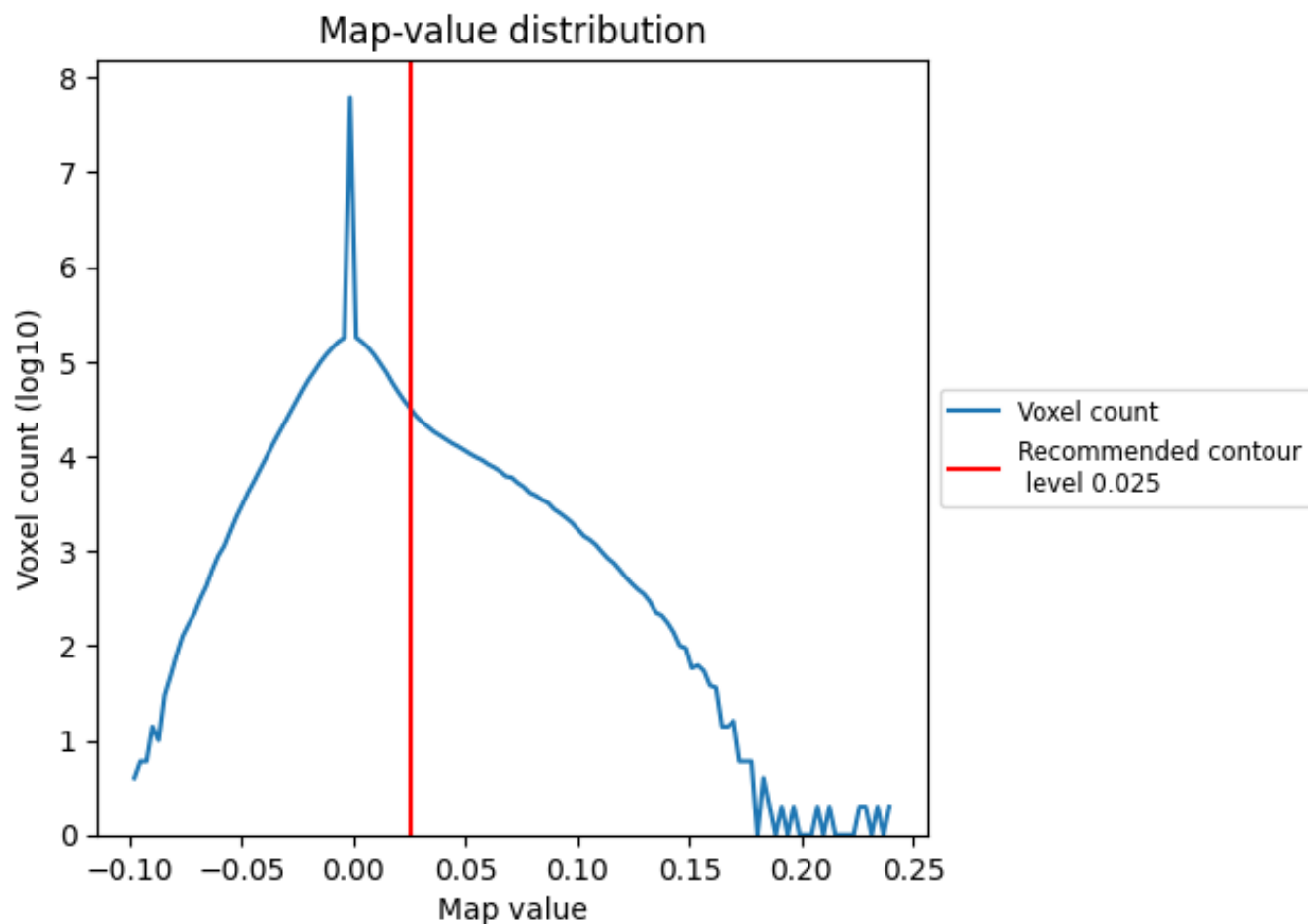
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

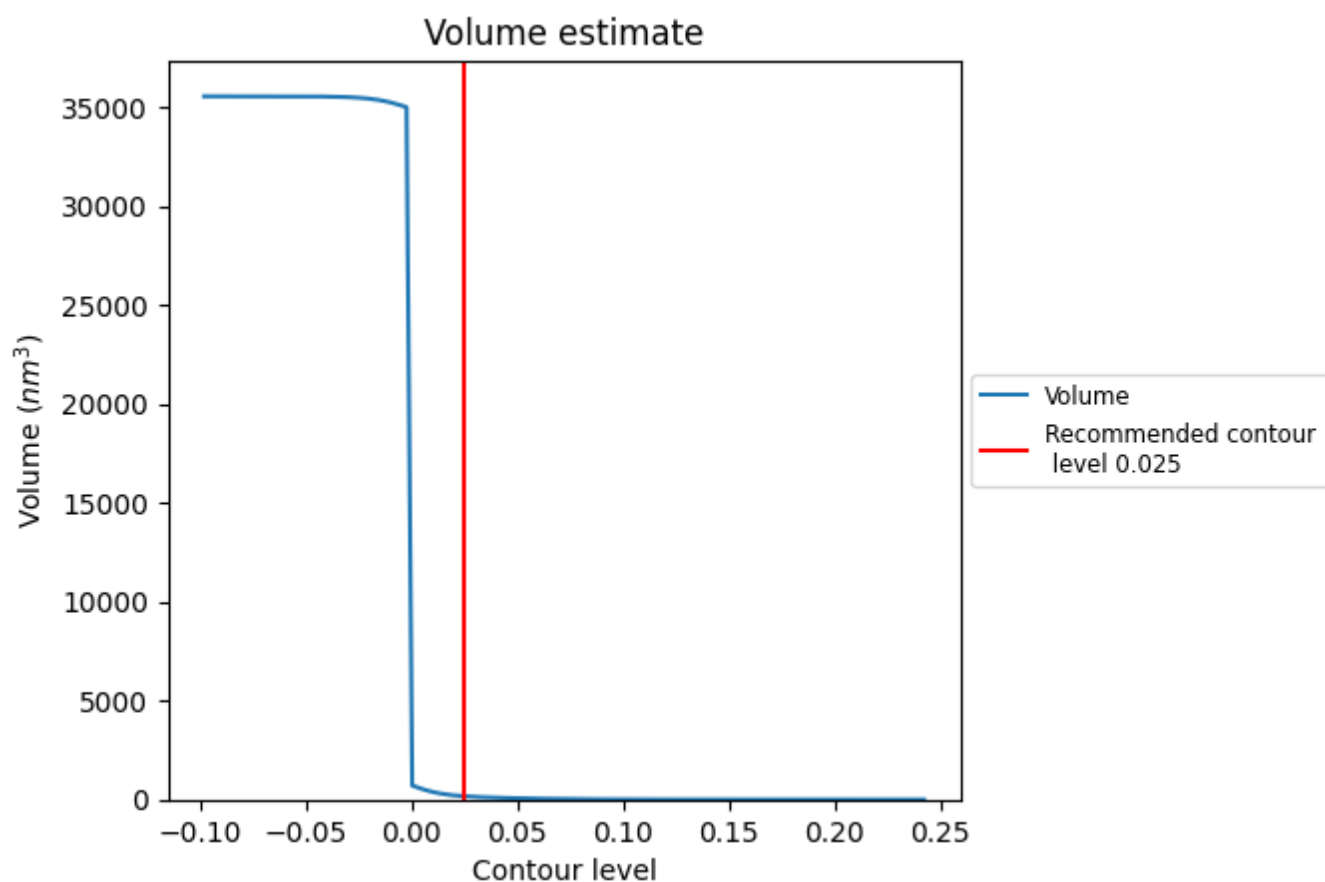
This section contains the results of statistical analysis of the map.

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.

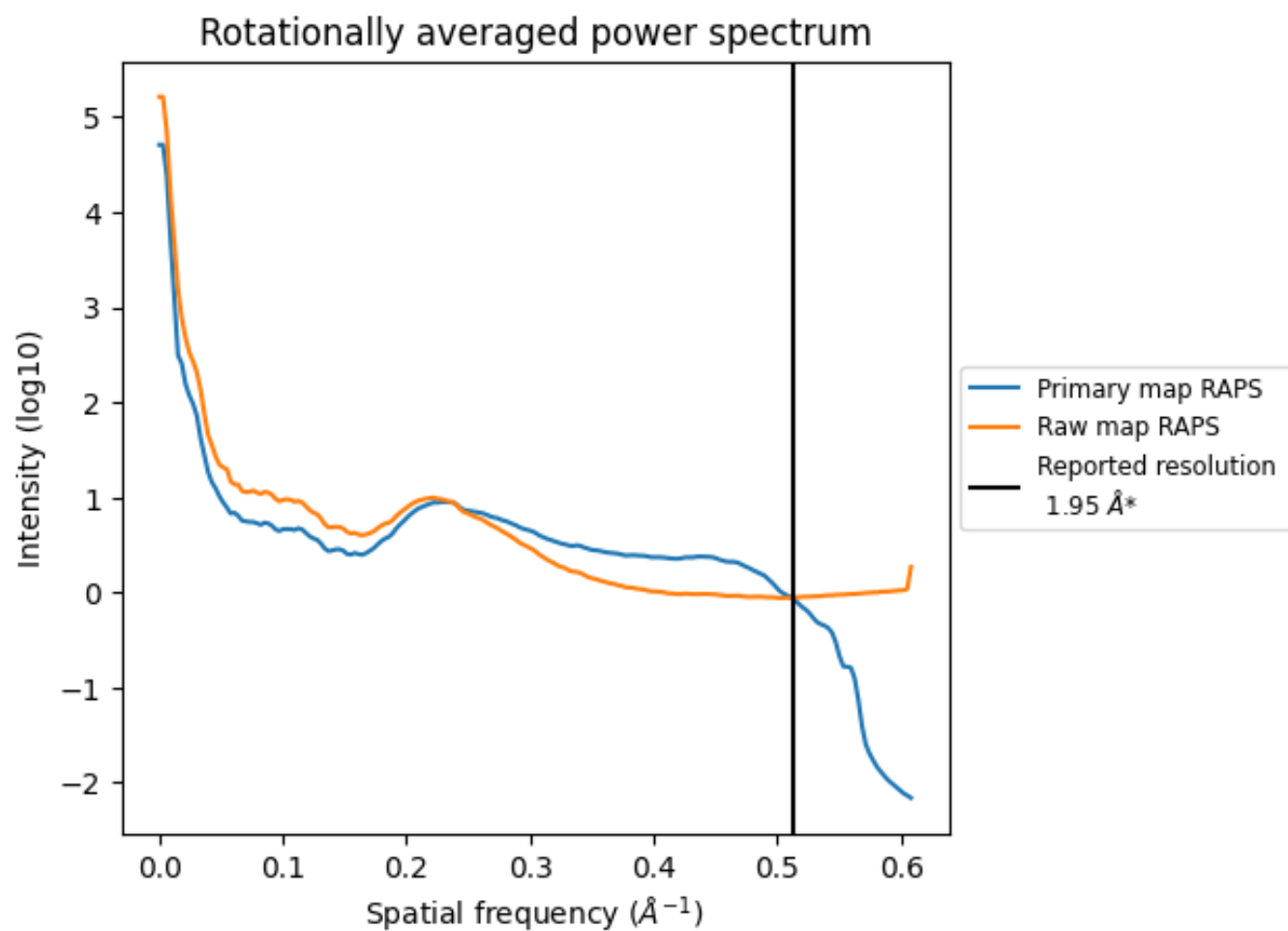
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm^3 ; this corresponds to an approximate mass of 152 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 ⓘ

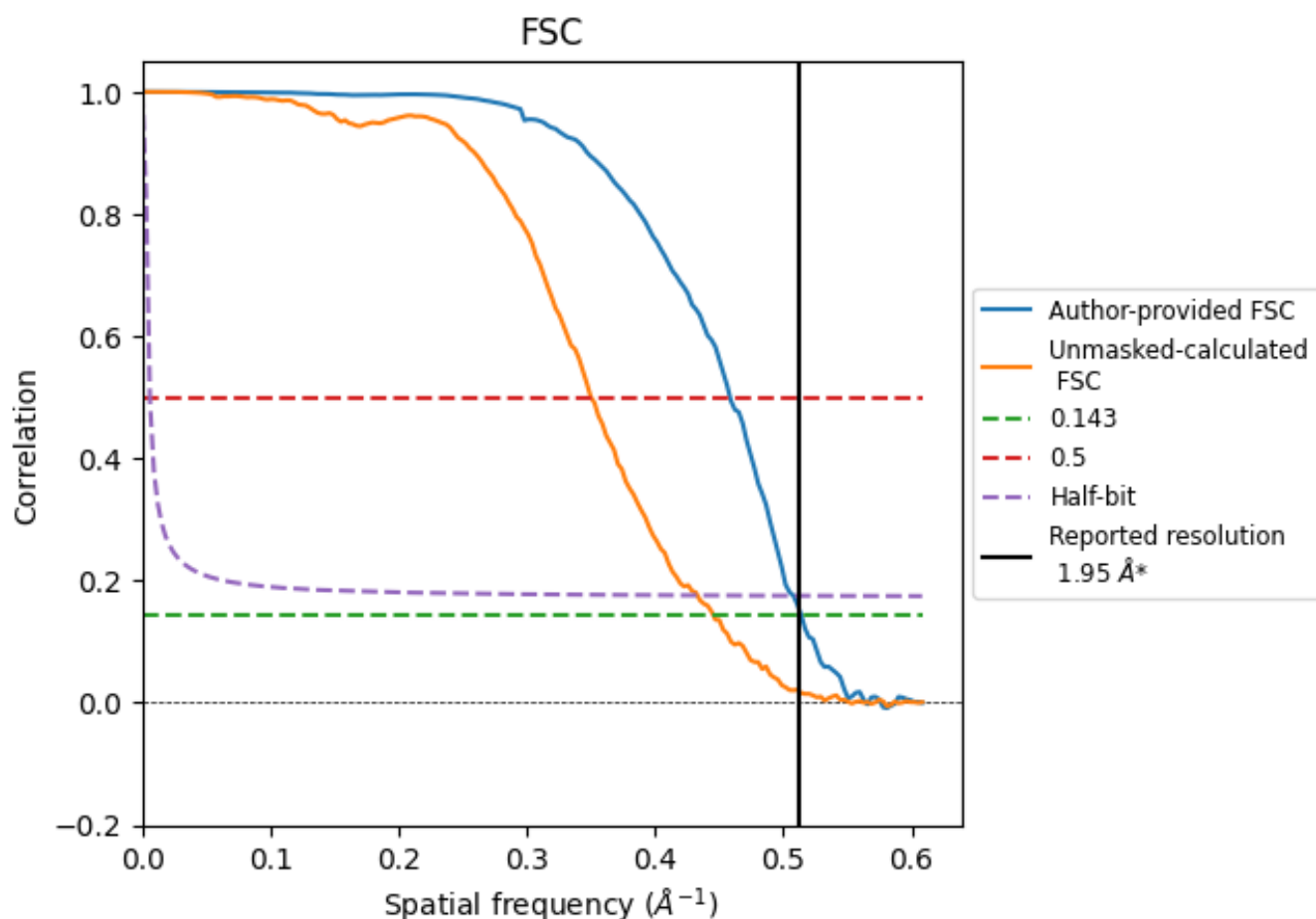


*Reported resolution corresponds to spatial frequency of 0.513 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.513 \AA^{-1}

8.2 Resolution estimates [i](#)

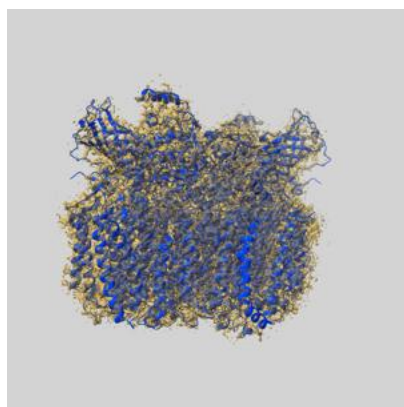
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.95	-	-
Author-provided FSC curve	1.95	2.18	1.97
Unmasked-calculated*	2.24	2.86	2.31

*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 2.24 differs from the reported value 1.95 by more than 10 %

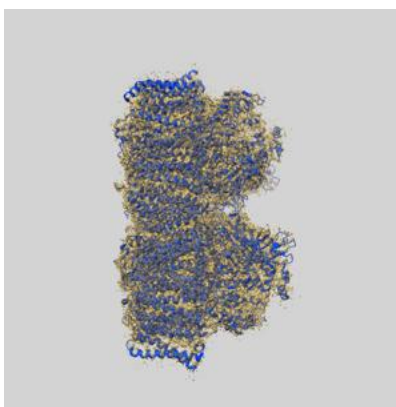
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30547 and PDB model 7D1T. Per-residue inclusion information can be found in [section 3](#) on [page 29](#).

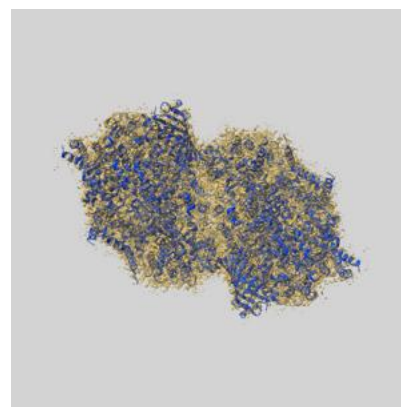
9.1 Map-model overlay [i](#)



X



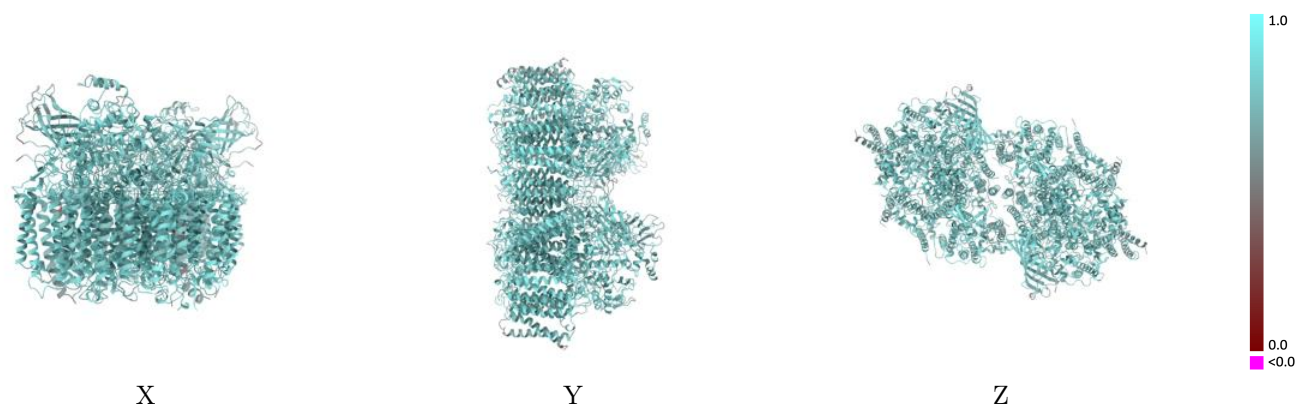
Y



Z

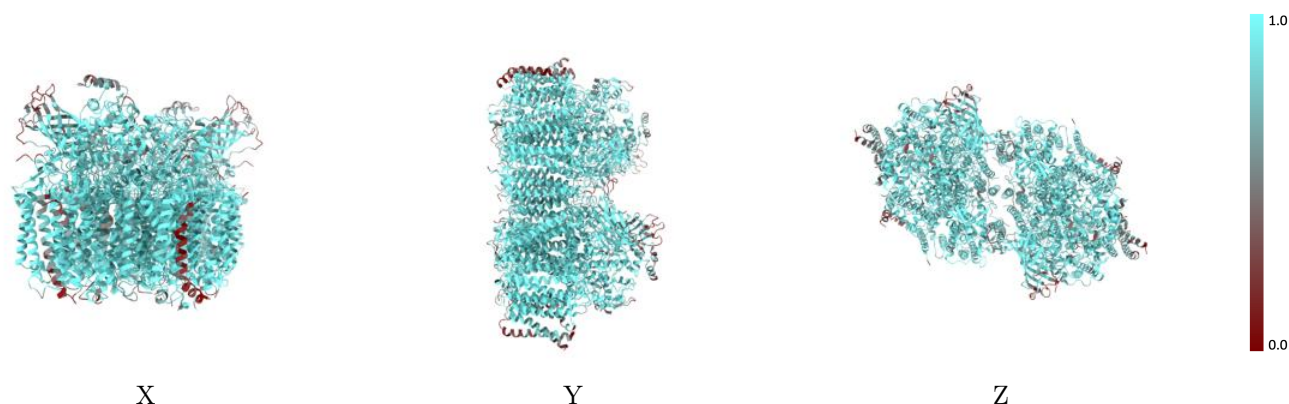
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



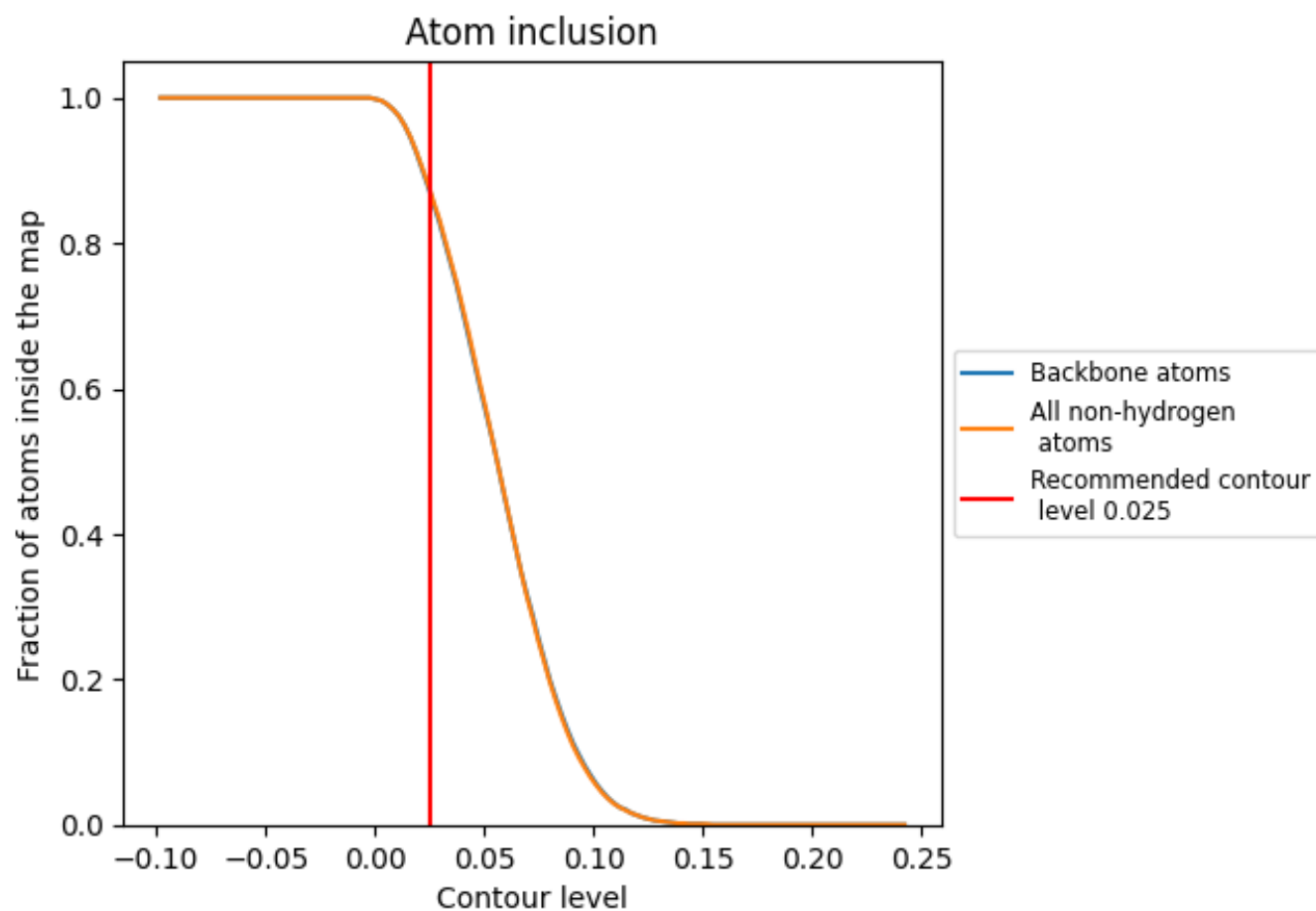
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 88% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8750	 0.7760
A	 0.9330	 0.8060
B	 0.9180	 0.7910
C	 0.9010	 0.7770
D	 0.9450	 0.8080
E	 0.8350	 0.7550
F	 0.8600	 0.7660
H	 0.9200	 0.7810
I	 0.8990	 0.7730
J	 0.8410	 0.7630
K	 0.8080	 0.7400
L	 0.8830	 0.7850
M	 0.8750	 0.7860
O	 0.7410	 0.7210
R	 0.1990	 0.6150
T	 0.9000	 0.7970
U	 0.7840	 0.7400
V	 0.8660	 0.7580
X	 0.8730	 0.7610
Y	 0.6680	 0.6940
Z	 0.5480	 0.6450
a	 0.9330	 0.8070
b	 0.9220	 0.7920
c	 0.9010	 0.7780
d	 0.9450	 0.8080
e	 0.8350	 0.7550
f	 0.8600	 0.7660
h	 0.9200	 0.7820
i	 0.8990	 0.7780
j	 0.8410	 0.7630
k	 0.8080	 0.7410
l	 0.9280	 0.8030
m	 0.8750	 0.7870
o	 0.7410	 0.7210
r	 0.1990	 0.6080



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Chain	Atom inclusion	Q-score
t	 0.9000	 0.7970
u	 0.7840	 0.7410
v	 0.8660	 0.7610
x	 0.8730	 0.7590
y	 0.6680	 0.6900
z	 0.5480	 0.6410