



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 01:32 PM UTC

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

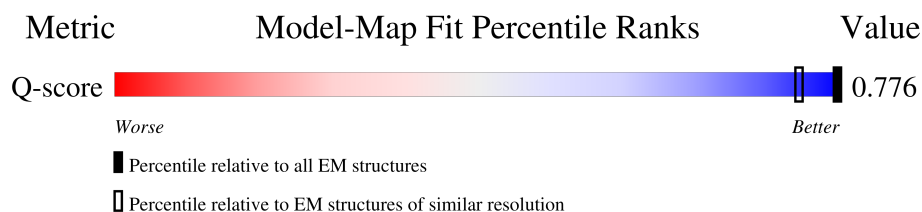
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	1316 (1.45 - 2.45)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

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
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			

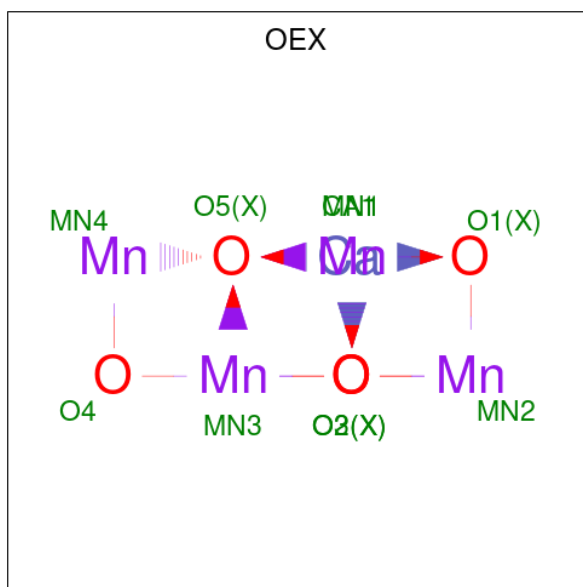
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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	

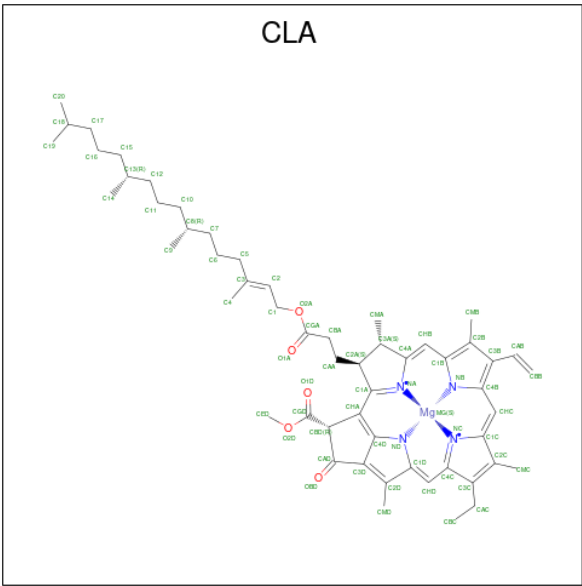
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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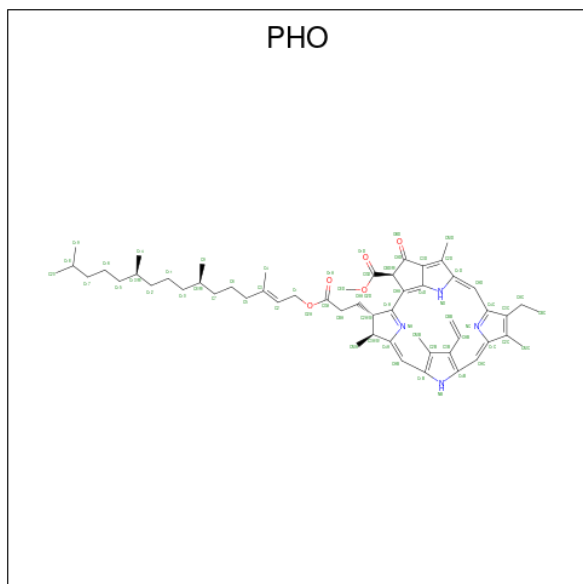
Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total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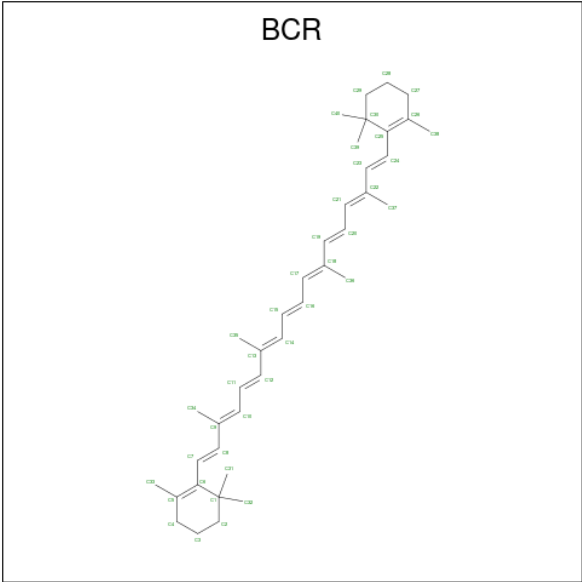
Mol	Chain	Residues	Atoms					AltConf
24	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- 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: $C_{40}H_{56}$).



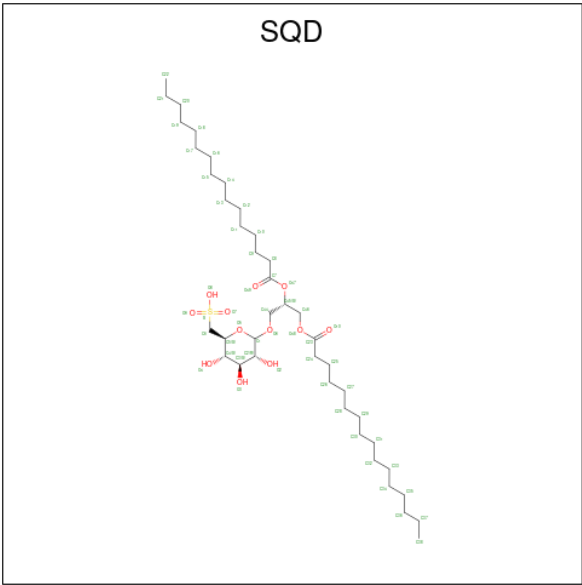
Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	C	1	Total	C	0
			40	40	
26	C	1	Total	C	0
			40	40	
26	C	1	Total	C	0
			40	40	
26	D	1	Total	C	0
			40	40	
26	J	1	Total	C	0
			40	40	
26	T	1	Total	C	0
			40	40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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



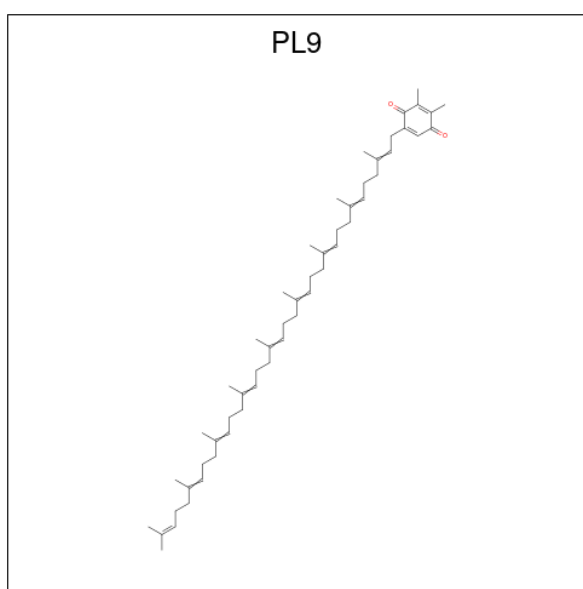
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	S	0
			54	41	12	1	
27	A	1	Total	C	O	S	0
			54	41	12	1	
27	B	1	Total	C	O	S	0
			54	41	12	1	
27	F	1	Total	C	O	S	0
			45	32	12	1	
27	L	1	Total	C	O	S	0
			54	41	12	1	

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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:).

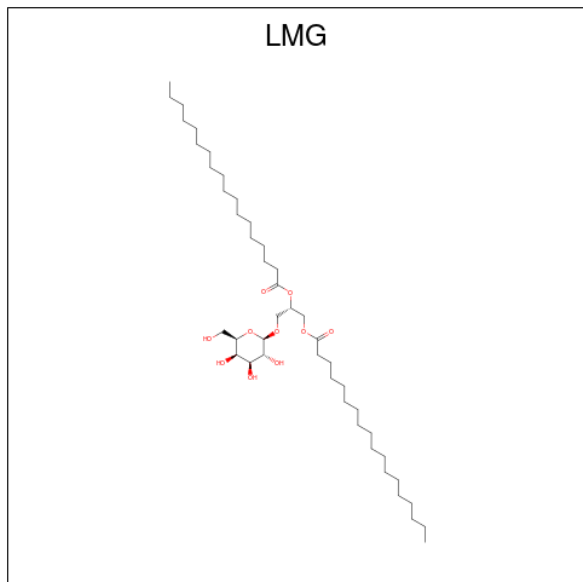
Mol	Chain	Residues	Atoms				AltConf
29	A	2	Total	C	O		0
			59	49	10		

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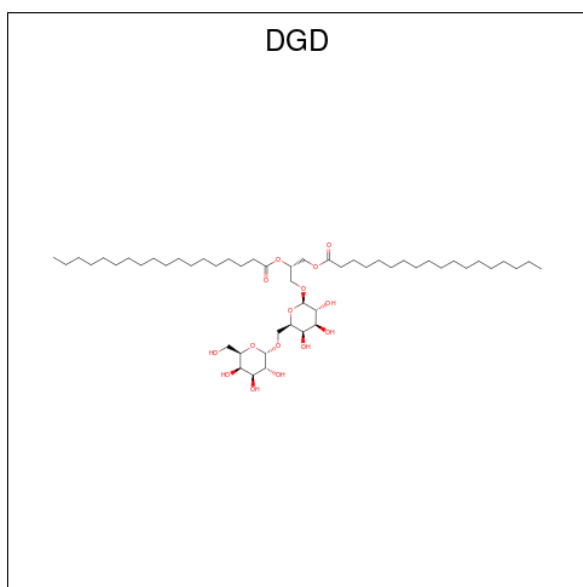
Mol	Chain	Residues	Atoms	AltConf
29	B	5	Total C 56 56	0
29	C	1	Total C 10 10	0
29	D	2	Total C O 56 51 5	0
29	E	1	Total C 10 10	0
29	I	2	Total C 17 17	0
29	J	1	Total C 10 10	0
29	K	1	Total C O 34 29 5	0
29	M	1	Total C 10 10	0
29	T	1	Total C 16 16	0
29	X	1	Total C 10 10	0
29	a	2	Total C O 59 49 10	0
29	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: $C_{45}H_{86}O_{10}$).



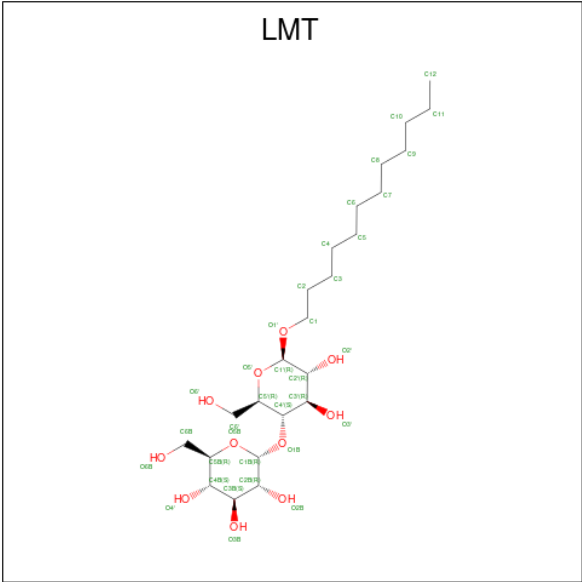
Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	C	1	Total	C	O	0
			51	41	10	
30	D	1	Total	C	O	0
			51	41	10	
30	b	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			51	41	10	
30	c	1	Total	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: $C_{51}H_{96}O_{15}$).



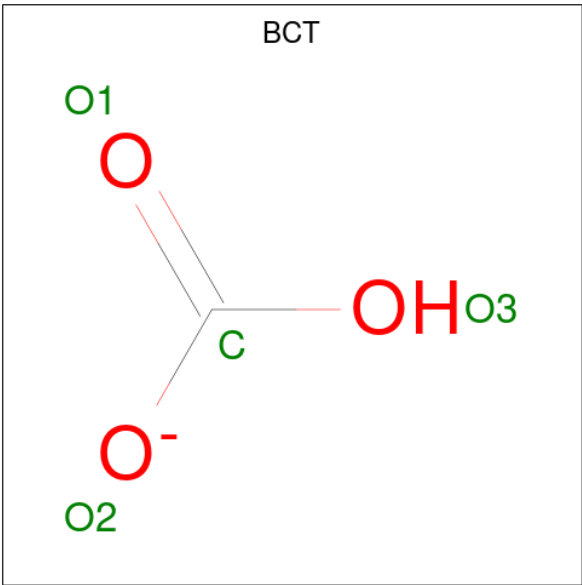
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	H	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			62	47	15	
31	c	1	Total	C	O	0
			62	47	15	
31	h	1	Total	C	O	0
			62	47	15	

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



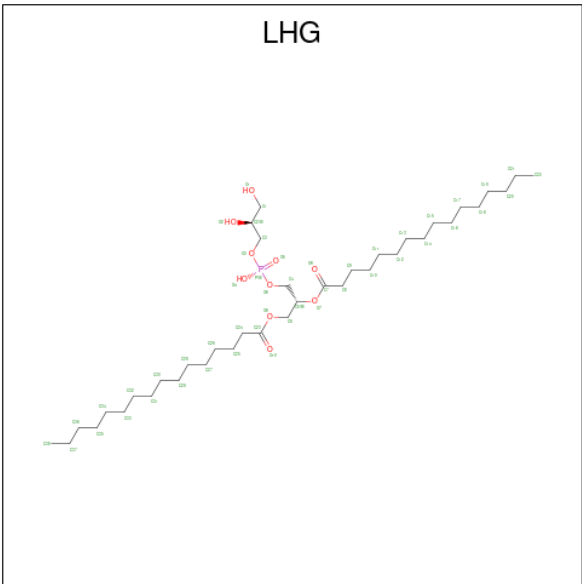
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			35	24	11	
32	J	1	Total	C	O	0
			24	18	6	
32	M	1	Total	C	O	0
			35	24	11	
32	Z	1	Total	C	O	0
			35	24	11	
32	c	1	Total	C	O	0
			35	24	11	
32	j	1	Total	C	O	0
			24	18	6	
32	m	1	Total	C	O	0
			35	24	11	
32	z	1	Total	C	O	0
			35	24	11	

- 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

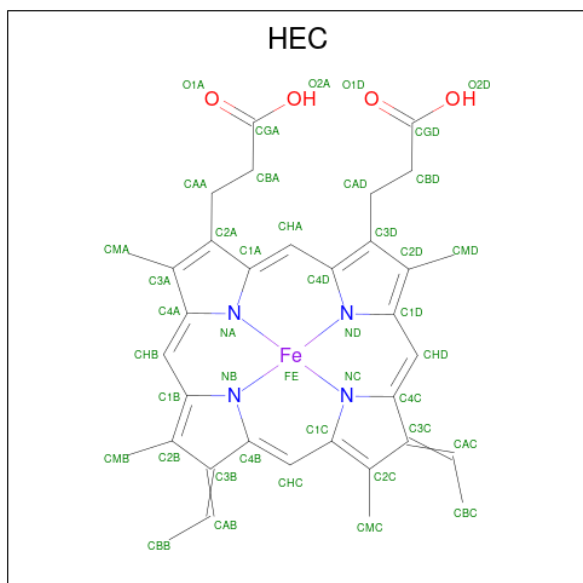
- # HEM

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

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

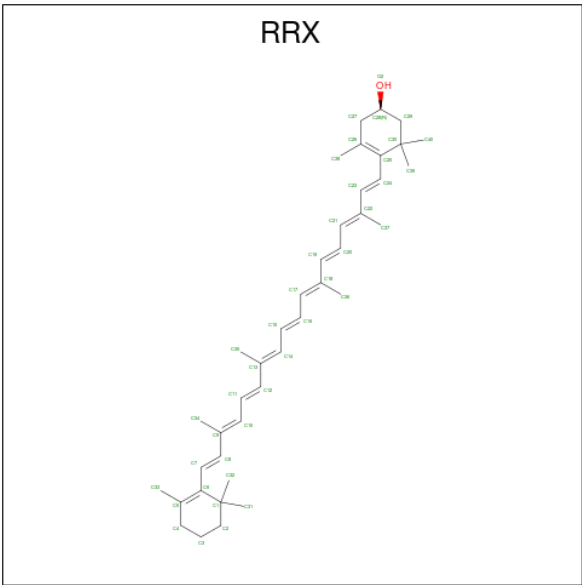
Mol	Chain	Residues	Atoms		AltConf
36	J	1	Total	Mg	0
			1	1	
36	j	1	Total	Mg	0
			1	1	

- Molecule 37 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



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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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

MolProbity failed to run properly - this section is therefore empty.

3 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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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	$\# Z > 2$
8	FME	I	1	8	8,9,10	1.02	0	8,9,11	1.11	1 (12%)
14	FME	t	1	14	8,9,10	0.95	0	8,9,11	1.62	2 (25%)
14	FME	T	1	14	8,9,10	0.94	0	8,9,11	1.62	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HSK	D	336	4	10,11,12	1.78	2 (20%)	5,14,16	1.24	1 (20%)
8	FME	i	1	8	8,9,10	1.02	0	8,9,11	1.11	1 (12%)
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	1.02	1 (12%)
12	FME	M	1	12	8,9,10	0.97	0	8,9,11	1.02	1 (12%)
4	HSK	d	336	4	10,11,12	1.80	2 (20%)	5,14,16	1.19	0

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	HSK	OM-ND1	-4.57	1.29	1.38
4	D	336	HSK	OM-ND1	-4.52	1.30	1.38
4	d	336	HSK	CD2-CG	2.33	1.39	1.36
4	D	336	HSK	CD2-CG	2.25	1.39	1.36

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CB-CA-N	3.11	116.19	110.52
14	T	1	FME	CB-CA-N	3.10	116.17	110.52
14	t	1	FME	C-CA-N	2.58	114.47	109.50
14	T	1	FME	C-CA-N	2.56	114.44	109.50
12	M	1	FME	CB-CA-N	2.47	115.02	110.52

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 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	$\# Z > 2$
27	SQD	B	620	-	52,54,54	0.92	5 (9%)	62,65,65	2.19	11 (17%)
25	PHO	D	402	-	58,69,69	2.09	9 (15%)	55,99,99	1.76	11 (20%)
24	CLA	B	605	2	69,73,73	1.85	19 (27%)	82,113,113	2.66	34 (41%)
24	CLA	B	615	2	69,73,73	1.83	19 (27%)	82,113,113	2.57	30 (36%)
30	LMG	D	411	36	51,51,55	1.06	6 (11%)	59,59,63	1.32	7 (11%)
30	LMG	C	520	-	51,51,55	0.95	4 (7%)	59,59,63	1.36	7 (11%)
25	PHO	A	407	-	58,69,69	2.32	14 (24%)	55,99,99	1.68	4 (7%)
30	LMG	d	411	36	51,51,55	1.06	6 (11%)	59,59,63	1.32	7 (11%)
27	SQD	A	410	-	52,54,54	1.06	6 (11%)	62,65,65	1.85	8 (12%)
38	RRX	X	101	-	42,42,42	1.86	9 (21%)	56,58,58	2.05	17 (30%)
28	PL9	D	407	-	55,55,55	1.92	11 (20%)	68,69,69	1.53	14 (20%)
34	LHG	d	408	-	48,48,48	0.88	1 (2%)	51,54,54	1.24	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	507	3	69,73,73	1.89	18 (26%)	82,113,113	2.59	32 (39%)
24	CLA	a	408	1	69,73,73	1.88	16 (23%)	82,113,113	2.73	31 (37%)
28	PL9	d	407	-	55,55,55	1.91	11 (20%)	68,69,69	1.54	14 (20%)
24	CLA	c	502	3	69,73,73	1.86	18 (26%)	82,113,113	2.61	31 (37%)
24	CLA	C	509	3	69,73,73	1.86	17 (24%)	82,113,113	2.63	31 (37%)
38	RRX	x	101	-	42,42,42	1.86	9 (21%)	56,58,58	2.05	17 (30%)
30	LMG	B	621	-	51,51,55	1.05	3 (5%)	59,59,63	1.30	6 (10%)
31	DGD	C	519	-	63,63,67	1.20	7 (11%)	77,77,81	1.31	8 (10%)
24	CLA	B	610	39	69,73,73	1.85	19 (27%)	82,113,113	2.47	29 (35%)
26	BCR	b	620	-	41,41,41	1.12	3 (7%)	56,56,56	1.26	7 (12%)
30	LMG	C	501	-	51,51,55	1.21	6 (11%)	59,59,63	1.38	7 (11%)
24	CLA	d	401	39	69,73,73	1.97	18 (26%)	82,113,113	2.70	31 (37%)
24	CLA	c	512	3	69,73,73	1.91	20 (28%)	82,113,113	2.71	30 (36%)
21	OEX	A	401	3,1,39	0,15,15	-	-	-	-	-
30	LMG	c	501	-	51,51,55	1.21	6 (11%)	59,59,63	1.38	7 (11%)
26	BCR	b	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	3 (5%)
26	BCR	B	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.08	4 (7%)
32	LMT	z	101	-	36,36,36	1.26	6 (16%)	47,47,47	1.14	5 (10%)
24	CLA	b	609	39	69,73,73	1.85	18 (26%)	82,113,113	2.62	28 (34%)
24	CLA	C	513	3	69,73,73	1.83	18 (26%)	82,113,113	2.72	34 (41%)
24	CLA	B	604	2	69,73,73	1.90	22 (31%)	82,113,113	2.57	32 (39%)
24	CLA	b	608	2	69,73,73	1.95	21 (30%)	82,113,113	2.69	33 (40%)
30	LMG	c	520	-	51,51,55	0.95	4 (7%)	59,59,63	1.36	7 (11%)
26	BCR	c	522	-	41,41,41	1.02	2 (4%)	56,56,56	1.19	6 (10%)
24	CLA	B	609	2	69,73,73	1.84	17 (24%)	82,113,113	2.67	35 (42%)
35	HEM	E	103	5,6	50,50,50	1.54	6 (12%)	67,82,82	1.36	9 (13%)
31	DGD	H	101	-	63,63,67	1.27	6 (9%)	77,77,81	1.27	9 (11%)
24	CLA	A	408	1	69,73,73	1.88	16 (23%)	82,113,113	2.73	31 (37%)
34	LHG	D	409	-	48,48,48	0.88	1 (2%)	51,54,54	1.13	3 (5%)
24	CLA	B	614	2	69,73,73	1.83	20 (28%)	82,113,113	2.72	32 (39%)
24	CLA	B	606	2	69,73,73	1.95	21 (30%)	82,113,113	2.69	33 (40%)
24	CLA	C	506	3	69,73,73	1.87	22 (31%)	82,113,113	2.47	28 (34%)
34	LHG	d	409	-	48,48,48	0.88	1 (2%)	51,54,54	1.13	3 (5%)
24	CLA	b	615	2	69,73,73	1.87	19 (27%)	82,113,113	2.49	31 (37%)
33	BCT	D	403	22	3,3,3	1.65	1 (33%)	2,3,3	3.97	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LHG	l	101	-	48,48,48	0.73	1 (2%)	51,54,54	1.14	4 (7%)
24	CLA	A	405	1	69,73,73	1.78	18 (26%)	82,113,113	2.36	25 (30%)
24	CLA	D	405	4	69,73,73	1.91	21 (30%)	82,113,113	2.62	31 (37%)
24	CLA	c	513	3	69,73,73	1.83	18 (26%)	82,113,113	2.72	35 (42%)
24	CLA	d	405	4	69,73,73	1.91	21 (30%)	82,113,113	2.62	30 (36%)
24	CLA	c	506	3	69,73,73	1.87	22 (31%)	82,113,113	2.47	28 (34%)
24	CLA	C	511	3	69,73,73	1.93	18 (26%)	82,113,113	2.54	32 (39%)
27	SQD	a	412	-	52,54,54	0.97	4 (7%)	62,65,65	1.68	10 (16%)
24	CLA	C	508	39	69,73,73	1.87	21 (30%)	82,113,113	2.67	30 (36%)
32	LMT	C	521	-	36,36,36	1.28	4 (11%)	47,47,47	1.31	4 (8%)
24	CLA	C	512	3	69,73,73	1.91	20 (28%)	82,113,113	2.71	30 (36%)
24	CLA	D	401	39	69,73,73	1.97	18 (26%)	82,113,113	2.70	31 (37%)
24	CLA	b	603	39	69,73,73	1.96	21 (30%)	82,113,113	2.56	30 (36%)
26	BCR	D	406	-	41,41,41	1.19	3 (7%)	56,56,56	1.43	9 (16%)
24	CLA	C	503	3	69,73,73	1.89	17 (24%)	82,113,113	2.50	26 (31%)
24	CLA	b	618	2	69,73,73	1.85	17 (24%)	82,113,113	2.63	35 (42%)
24	CLA	b	605	2	69,73,73	1.87	18 (26%)	82,113,113	2.56	33 (40%)
24	CLA	c	508	39	69,73,73	1.87	21 (30%)	82,113,113	2.67	30 (36%)
25	PHO	d	402	-	58,69,69	2.09	9 (15%)	55,99,99	1.76	11 (20%)
24	CLA	b	607	2	69,73,73	1.85	19 (27%)	82,113,113	2.66	34 (41%)
26	BCR	A	409	-	41,41,41	1.02	3 (7%)	56,56,56	1.28	8 (14%)
24	CLA	b	617	2	69,73,73	1.83	19 (27%)	82,113,113	2.57	30 (36%)
26	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.19	4 (7%)
30	LMG	c	523	-	51,51,55	0.85	2 (3%)	59,59,63	1.36	8 (13%)
24	CLA	B	603	2	69,73,73	1.87	18 (26%)	82,113,113	2.56	33 (40%)
32	LMT	Z	101	-	36,36,36	1.26	6 (16%)	47,47,47	1.13	5 (10%)
34	LHG	e	101	-	48,48,48	0.73	1 (2%)	51,54,54	1.29	7 (13%)
26	BCR	j	104	-	41,41,41	1.16	3 (7%)	56,56,56	1.15	4 (7%)
26	BCR	c	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.18	4 (7%)
24	CLA	C	507	3	69,73,73	1.89	18 (26%)	82,113,113	2.59	32 (39%)
26	BCR	B	617	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	3 (5%)
30	LMG	C	523	-	51,51,55	0.85	2 (3%)	59,59,63	1.36	8 (13%)
26	BCR	J	104	-	41,41,41	1.16	3 (7%)	56,56,56	1.16	4 (7%)
26	BCR	B	618	-	41,41,41	1.12	3 (7%)	56,56,56	1.26	7 (12%)
34	LHG	E	101	-	48,48,48	0.73	1 (2%)	51,54,54	1.28	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMT	M	101	-	36,36,36	1.37	4 (11%)	47,47,47	1.03	1 (2%)
31	DGD	c	517	-	63,63,67	1.12	5 (7%)	77,77,81	1.42	11 (14%)
24	CLA	C	505	39	69,73,73	1.86	18 (26%)	82,113,113	2.57	33 (40%)
24	CLA	B	602	2	69,73,73	1.85	17 (24%)	82,113,113	2.74	30 (36%)
24	CLA	B	611	2	69,73,73	1.76	18 (26%)	82,113,113	2.57	31 (37%)
26	BCR	C	515	-	41,41,41	1.13	4 (9%)	56,56,56	1.44	10 (17%)
31	DGD	C	518	-	63,63,67	1.54	13 (20%)	77,77,81	1.44	10 (12%)
24	CLA	c	503	3	69,73,73	1.89	17 (24%)	82,113,113	2.50	26 (31%)
34	LHG	L	101	-	48,48,48	0.72	1 (2%)	51,54,54	1.14	4 (7%)
26	BCR	d	406	-	41,41,41	1.19	3 (7%)	56,56,56	1.43	9 (16%)
24	CLA	c	509	3	69,73,73	1.86	17 (24%)	82,113,113	2.64	31 (37%)
26	BCR	c	515	-	41,41,41	1.13	4 (9%)	56,56,56	1.44	10 (17%)
27	SQD	A	412	-	52,54,54	0.97	4 (7%)	62,65,65	1.67	10 (16%)
31	DGD	h	101	-	63,63,67	1.27	6 (9%)	77,77,81	1.27	9 (11%)
32	LMT	J	102	-	24,24,36	0.99	1 (4%)	29,29,47	1.51	3 (10%)
24	CLA	C	504	3	69,73,73	1.84	21 (30%)	82,113,113	2.58	25 (30%)
24	CLA	b	611	2	69,73,73	1.85	17 (24%)	82,113,113	2.67	35 (42%)
26	BCR	T	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.30	7 (12%)
24	CLA	B	612	2	69,73,73	1.83	17 (24%)	82,113,113	2.54	30 (36%)
24	CLA	B	607	39	69,73,73	1.86	18 (26%)	82,113,113	2.62	28 (34%)
27	SQD	f	101	-	43,45,54	1.10	5 (11%)	53,56,65	2.13	14 (26%)
31	DGD	c	519	-	63,63,67	1.20	7 (11%)	77,77,81	1.31	8 (10%)
24	CLA	c	504	3	69,73,73	1.84	21 (30%)	82,113,113	2.58	25 (30%)
24	CLA	B	613	2	69,73,73	1.87	19 (27%)	82,113,113	2.50	31 (37%)
26	BCR	C	522	-	41,41,41	1.02	2 (4%)	56,56,56	1.19	6 (10%)
24	CLA	b	612	39	69,73,73	1.84	20 (28%)	82,113,113	2.48	29 (35%)
34	LHG	D	410	-	45,45,48	0.81	1 (2%)	48,51,54	1.19	4 (8%)
24	CLA	D	404	4	69,73,73	1.81	20 (28%)	82,113,113	2.55	26 (31%)
34	LHG	d	410	-	45,45,48	0.81	1 (2%)	48,51,54	1.19	4 (8%)
24	CLA	a	405	1	69,73,73	1.78	19 (27%)	82,113,113	2.36	25 (30%)
24	CLA	c	514	3	69,73,73	1.98	20 (28%)	82,113,113	2.71	34 (41%)
26	BCR	b	621	-	41,41,41	1.13	2 (4%)	56,56,56	1.08	4 (7%)
31	DGD	C	517	-	63,63,67	1.12	5 (7%)	77,77,81	1.42	11 (14%)
28	PL9	a	411	-	55,55,55	1.52	9 (16%)	68,69,69	1.53	11 (16%)
32	LMT	j	102	-	24,24,36	0.99	1 (4%)	29,29,47	1.51	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	OEX	a	401	3,1,39	0,15,15	-	-	-		
24	CLA	b	610	2	69,73,73	1.89	20 (28%)	82,113,113	2.41	29 (35%)
24	CLA	b	613	2	69,73,73	1.77	18 (26%)	82,113,113	2.57	31 (37%)
24	CLA	C	510	3	69,73,73	1.93	18 (26%)	82,113,113	2.55	33 (40%)
24	CLA	C	514	3	69,73,73	1.97	20 (28%)	82,113,113	2.71	34 (41%)
24	CLA	B	601	39	69,73,73	1.96	21 (30%)	82,113,113	2.56	30 (36%)
24	CLA	c	505	39	69,73,73	1.86	18 (26%)	82,113,113	2.58	33 (40%)
24	CLA	c	511	3	69,73,73	1.93	18 (26%)	82,113,113	2.54	32 (39%)
26	BCR	t	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.29	7 (12%)
27	SQD	F	101	-	43,45,54	1.10	5 (11%)	53,56,65	2.13	14 (26%)
24	CLA	C	502	3	69,73,73	1.86	18 (26%)	82,113,113	2.61	29 (35%)
26	BCR	a	409	-	41,41,41	1.01	3 (7%)	56,56,56	1.28	8 (14%)
34	LHG	D	408	-	48,48,48	0.88	1 (2%)	51,54,54	1.24	8 (15%)
24	CLA	B	608	2	69,73,73	1.89	19 (27%)	82,113,113	2.41	29 (35%)
24	CLA	b	614	2	69,73,73	1.83	17 (24%)	82,113,113	2.54	30 (36%)
37	HEC	v	201	16	46,50,50	2.01	8 (17%)	58,82,82	1.38	5 (8%)
30	LMG	b	622	-	51,51,55	1.05	3 (5%)	59,59,63	1.30	6 (10%)
32	LMT	c	521	-	36,36,36	1.28	4 (11%)	47,47,47	1.31	4 (8%)
24	CLA	b	616	2	69,73,73	1.82	20 (28%)	82,113,113	2.72	32 (39%)
31	DGD	c	518	-	63,63,67	1.54	13 (20%)	77,77,81	1.44	10 (12%)
37	HEC	V	201	16	46,50,50	2.01	9 (19%)	58,82,82	1.38	5 (8%)
27	SQD	a	410	-	52,54,54	1.06	6 (11%)	62,65,65	1.86	9 (14%)
33	BCT	d	403	22	3,3,3	1.64	1 (33%)	2,3,3	3.96	2 (100%)
25	PHO	a	407	-	58,69,69	2.32	14 (24%)	55,99,99	1.68	4 (7%)
24	CLA	d	404	4	69,73,73	1.81	20 (28%)	82,113,113	2.56	26 (31%)
24	CLA	A	406	39	69,73,73	1.90	21 (30%)	82,113,113	2.39	30 (36%)
24	CLA	b	606	2	69,73,73	1.90	22 (31%)	82,113,113	2.57	32 (39%)
24	CLA	a	406	39	69,73,73	1.90	20 (28%)	82,113,113	2.38	30 (36%)
32	LMT	m	102	-	36,36,36	1.36	4 (11%)	47,47,47	1.03	1 (2%)
27	SQD	L	102	-	52,54,54	0.92	5 (9%)	62,65,65	2.19	11 (17%)
24	CLA	B	616	2	69,73,73	1.85	17 (24%)	82,113,113	2.63	35 (42%)
35	HEM	e	103	5,6	50,50,50	1.54	6 (12%)	67,82,82	1.36	9 (13%)
24	CLA	b	604	2	69,73,73	1.85	17 (24%)	82,113,113	2.74	31 (37%)
24	CLA	c	510	3	69,73,73	1.94	18 (26%)	82,113,113	2.55	33 (40%)
28	PL9	A	411	-	55,55,55	1.52	9 (16%)	68,69,69	1.53	11 (16%)

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
27	SQD	B	620	-	-	25/49/69/69	0/1/1/1
25	PHO	D	402	-	-	3/37/103/103	0/5/6/6
24	CLA	B	605	2	1/1/15/20	5/39/115/115	-
24	CLA	B	615	2	1/1/15/20	14/39/115/115	-
30	LMG	D	411	36	-	16/46/66/70	0/1/1/1
30	LMG	C	520	-	-	21/46/66/70	0/1/1/1
25	PHO	A	407	-	-	5/37/103/103	0/5/6/6
30	LMG	d	411	36	-	16/46/66/70	0/1/1/1
27	SQD	A	410	-	-	12/49/69/69	0/1/1/1
38	RRX	X	101	-	-	3/29/65/65	0/2/2/2
28	PL9	D	407	-	-	10/53/73/73	0/1/1/1
34	LHG	d	408	-	-	15/53/53/53	-
24	CLA	c	507	3	1/1/15/20	6/39/115/115	-
24	CLA	a	408	1	-	13/39/115/115	-
28	PL9	d	407	-	-	10/53/73/73	0/1/1/1
24	CLA	c	502	3	1/1/15/20	4/39/115/115	-
24	CLA	C	509	3	1/1/15/20	4/39/115/115	-
38	RRX	x	101	-	-	3/29/65/65	0/2/2/2
30	LMG	B	621	-	-	15/46/66/70	0/1/1/1
31	DGD	C	519	-	-	13/51/91/95	0/2/2/2
24	CLA	B	610	39	1/1/15/20	4/39/115/115	-
26	BCR	b	620	-	-	3/29/63/63	0/2/2/2
30	LMG	C	501	-	-	27/46/66/70	0/1/1/1
24	CLA	d	401	39	1/1/15/20	5/39/115/115	-
24	CLA	c	512	3	1/1/15/20	11/39/115/115	-
30	LMG	c	501	-	-	27/46/66/70	0/1/1/1
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
26	BCR	B	619	-	-	10/29/63/63	0/2/2/2
32	LMT	z	101	-	-	13/21/61/61	0/2/2/2
24	CLA	b	609	39	1/1/15/20	8/39/115/115	-
24	CLA	C	513	3	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	604	2	1/1/15/20	6/39/115/115	-
24	CLA	b	608	2	1/1/15/20	3/39/115/115	-
30	LMG	c	520	-	-	21/46/66/70	0/1/1/1
26	BCR	c	522	-	-	10/29/63/63	0/2/2/2
24	CLA	B	609	2	1/1/15/20	4/39/115/115	-
35	HEM	E	103	5,6	-	1/14/54/54	-
31	DGD	H	101	-	-	11/51/91/95	0/2/2/2
24	CLA	A	408	1	-	13/39/115/115	-
34	LHG	D	409	-	-	19/53/53/53	-
24	CLA	B	614	2	1/1/15/20	14/39/115/115	-
24	CLA	B	606	2	1/1/15/20	3/39/115/115	-
24	CLA	C	506	3	1/1/15/20	8/39/115/115	-
34	LHG	d	409	-	-	19/53/53/53	-
24	CLA	b	615	2	1/1/15/20	6/39/115/115	-
34	LHG	l	101	-	-	16/53/53/53	-
24	CLA	A	405	1	1/1/15/20	5/39/115/115	-
24	CLA	D	405	4	-	11/39/115/115	-
24	CLA	c	513	3	1/1/15/20	12/39/115/115	-
24	CLA	d	405	4	-	11/39/115/115	-
24	CLA	c	506	3	1/1/15/20	8/39/115/115	-
24	CLA	C	511	3	1/1/15/20	5/39/115/115	-
27	SQD	a	412	-	-	19/49/69/69	0/1/1/1
24	CLA	C	508	39	1/1/15/20	10/39/115/115	-
32	LMT	C	521	-	-	10/21/61/61	0/2/2/2
24	CLA	C	512	3	1/1/15/20	11/39/115/115	-
24	CLA	D	401	39	1/1/15/20	5/39/115/115	-
24	CLA	b	603	39	1/1/15/20	12/39/115/115	-
26	BCR	D	406	-	-	5/29/63/63	0/2/2/2
24	CLA	b	618	2	1/1/15/20	9/39/115/115	-
24	CLA	C	503	3	-	9/39/115/115	-
24	CLA	b	605	2	1/1/15/20	7/39/115/115	-
24	CLA	c	508	39	1/1/15/20	10/39/115/115	-
25	PHO	d	402	-	-	3/37/103/103	0/5/6/6
24	CLA	b	607	2	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	A	409	-	-	7/29/63/63	0/2/2/2
24	CLA	b	617	2	1/1/15/20	14/39/115/115	-
26	BCR	C	516	-	-	7/29/63/63	0/2/2/2
30	LMG	c	523	-	-	27/46/66/70	0/1/1/1
24	CLA	B	603	2	1/1/15/20	7/39/115/115	-
32	LMT	Z	101	-	-	13/21/61/61	0/2/2/2
34	LHG	e	101	-	-	24/53/53/53	-
26	BCR	j	104	-	-	11/29/63/63	0/2/2/2
26	BCR	c	516	-	-	7/29/63/63	0/2/2/2
24	CLA	C	507	3	1/1/15/20	6/39/115/115	-
26	BCR	B	617	-	-	4/29/63/63	0/2/2/2
30	LMG	C	523	-	-	27/46/66/70	0/1/1/1
26	BCR	J	104	-	-	11/29/63/63	0/2/2/2
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
34	LHG	E	101	-	-	24/53/53/53	-
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
31	DGD	c	517	-	-	13/51/91/95	0/2/2/2
24	CLA	C	505	39	1/1/15/20	5/39/115/115	-
24	CLA	B	602	2	1/1/15/20	5/39/115/115	-
24	CLA	B	611	2	1/1/15/20	2/39/115/115	-
26	BCR	C	515	-	-	11/29/63/63	0/2/2/2
31	DGD	C	518	-	-	25/51/91/95	0/2/2/2
24	CLA	c	503	3	-	9/39/115/115	-
34	LHG	L	101	-	-	16/53/53/53	-
26	BCR	d	406	-	-	5/29/63/63	0/2/2/2
24	CLA	c	509	3	1/1/15/20	4/39/115/115	-
26	BCR	c	515	-	-	11/29/63/63	0/2/2/2
27	SQD	A	412	-	-	19/49/69/69	0/1/1/1
31	DGD	h	101	-	-	11/51/91/95	0/2/2/2
32	LMT	J	102	-	-	4/15/35/61	0/1/1/2
24	CLA	C	504	3	1/1/15/20	9/39/115/115	-
24	CLA	b	611	2	1/1/15/20	4/39/115/115	-
26	BCR	T	101	-	-	10/29/63/63	0/2/2/2
24	CLA	B	612	2	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	607	39	1/1/15/20	8/39/115/115	-
27	SQD	f	101	-	-	12/40/60/69	0/1/1/1
31	DGD	c	519	-	-	13/51/91/95	0/2/2/2
24	CLA	c	504	3	1/1/15/20	9/39/115/115	-
24	CLA	B	613	2	1/1/15/20	6/39/115/115	-
26	BCR	C	522	-	-	10/29/63/63	0/2/2/2
24	CLA	b	612	39	1/1/15/20	4/39/115/115	-
34	LHG	D	410	-	-	15/50/50/53	-
24	CLA	D	404	4	1/1/15/20	2/39/115/115	-
34	LHG	d	410	-	-	15/50/50/53	-
24	CLA	a	405	1	1/1/15/20	5/39/115/115	-
24	CLA	c	514	3	1/1/15/20	10/39/115/115	-
26	BCR	b	621	-	-	10/29/63/63	0/2/2/2
31	DGD	C	517	-	-	13/51/91/95	0/2/2/2
28	PL9	a	411	-	-	19/53/73/73	0/1/1/1
32	LMT	j	102	-	-	4/15/35/61	0/1/1/2
24	CLA	b	610	2	-	2/39/115/115	-
24	CLA	b	613	2	1/1/15/20	2/39/115/115	-
24	CLA	C	510	3	1/1/15/20	12/39/115/115	-
24	CLA	C	514	3	1/1/15/20	10/39/115/115	-
24	CLA	B	601	39	1/1/15/20	12/39/115/115	-
24	CLA	c	505	39	1/1/15/20	5/39/115/115	-
24	CLA	c	511	3	1/1/15/20	5/39/115/115	-
26	BCR	t	102	-	-	10/29/63/63	0/2/2/2
27	SQD	F	101	-	-	12/40/60/69	0/1/1/1
24	CLA	C	502	3	1/1/15/20	4/39/115/115	-
26	BCR	a	409	-	-	7/29/63/63	0/2/2/2
34	LHG	D	408	-	-	15/53/53/53	-
24	CLA	B	608	2	-	2/39/115/115	-
24	CLA	b	614	2	1/1/15/20	5/39/115/115	-
37	HEC	v	201	16	-	6/14/54/54	-
30	LMG	b	622	-	-	15/46/66/70	0/1/1/1
32	LMT	c	521	-	-	10/21/61/61	0/2/2/2
24	CLA	b	616	2	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	c	518	-	-	25/51/91/95	0/2/2/2
37	HEC	V	201	16	-	6/14/54/54	-
27	SQD	a	410	-	-	12/49/69/69	0/1/1/1
25	PHO	a	407	-	-	5/37/103/103	0/5/6/6
24	CLA	d	404	4	1/1/15/20	2/39/115/115	-
24	CLA	A	406	39	-	8/39/115/115	-
24	CLA	b	606	2	1/1/15/20	6/39/115/115	-
24	CLA	a	406	39	-	8/39/115/115	-
32	LMT	m	102	-	-	4/21/61/61	0/2/2/2
27	SQD	L	102	-	-	25/49/69/69	0/1/1/1
24	CLA	B	616	2	1/1/15/20	9/39/115/115	-
35	HEM	e	103	5,6	-	1/14/54/54	-
24	CLA	b	604	2	1/1/15/20	5/39/115/115	-
24	CLA	c	510	3	1/1/15/20	12/39/115/115	-
28	PL9	A	411	-	-	19/53/73/73	0/1/1/1

The worst 5 of 1691 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	407	PHO	C1B-C2B	10.25	1.50	1.39
25	a	407	PHO	C1B-C2B	10.25	1.50	1.39
25	A	407	PHO	C3B-C4B	9.12	1.50	1.41
25	a	407	PHO	C3B-C4B	9.12	1.50	1.41
25	D	402	PHO	C3B-C4B	9.09	1.50	1.41

The worst 5 of 2730 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	102	SQD	O6-C1-C2	10.89	124.81	108.27
27	B	620	SQD	O6-C1-C2	10.89	124.81	108.27
24	B	614	CLA	C1D-ND-C4D	-10.10	99.23	106.31
24	b	616	CLA	C1D-ND-C4D	-10.10	99.23	106.31
24	D	401	CLA	C1D-ND-C4D	-9.99	99.30	106.31

5 of 60 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	B	601	CLA	ND

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

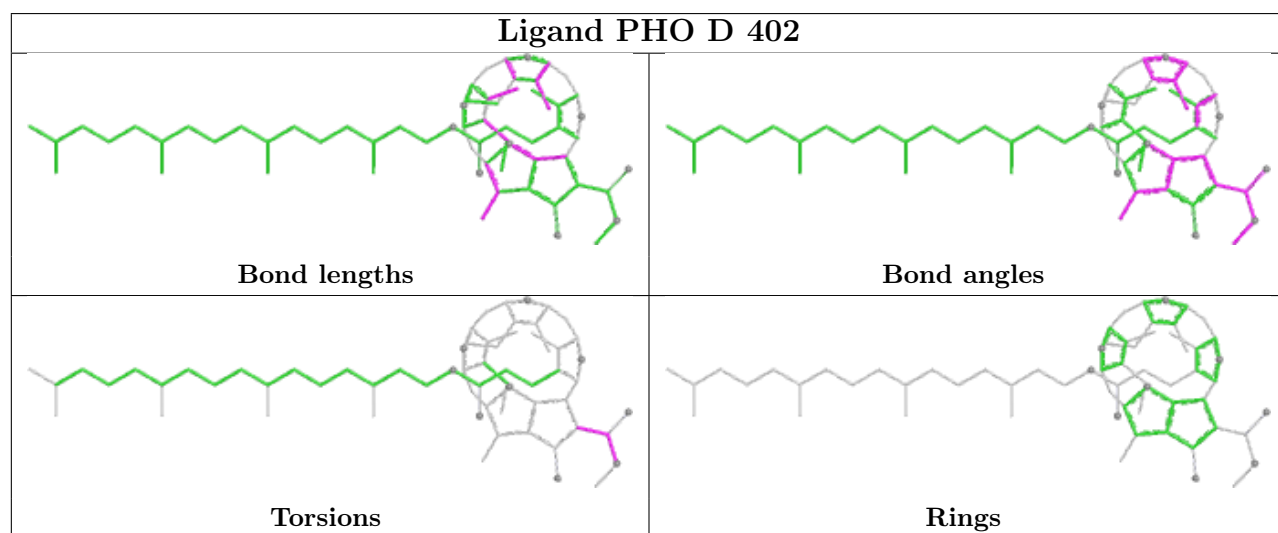
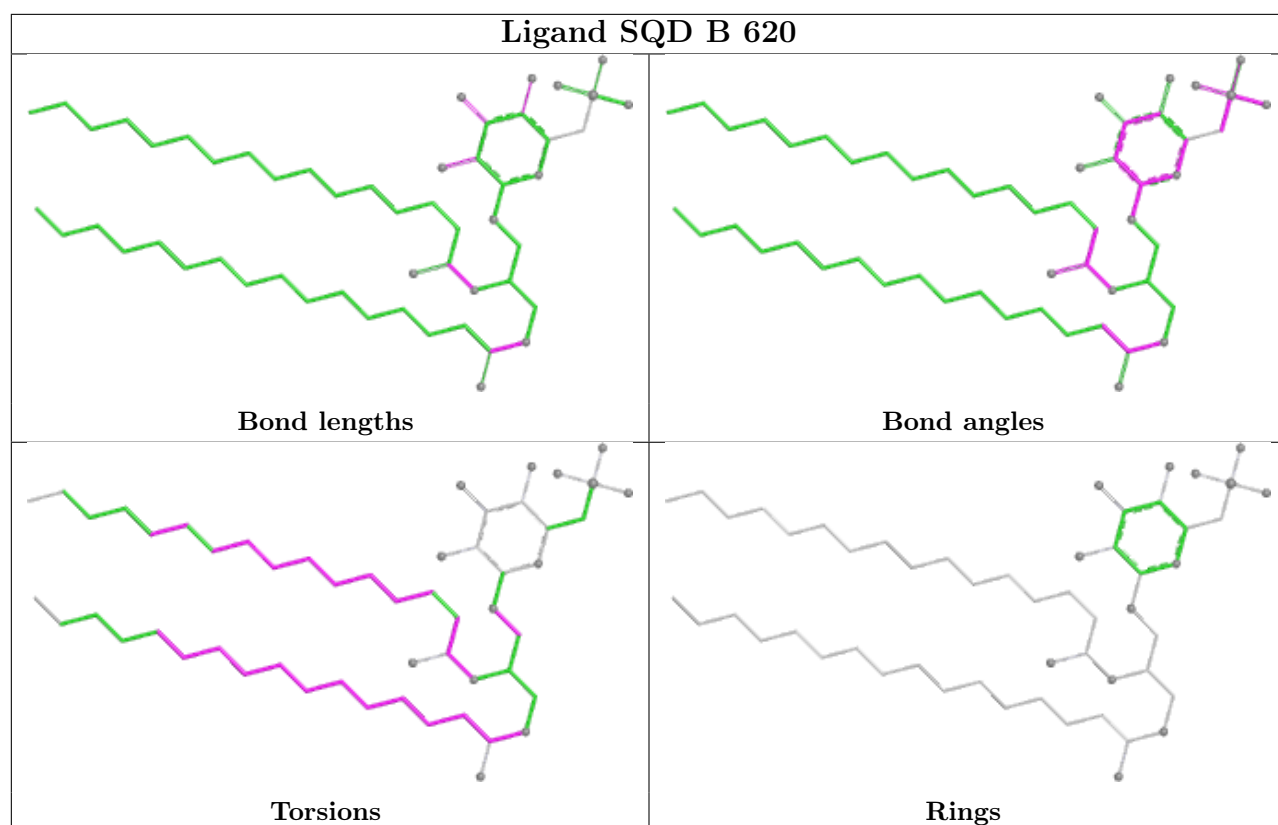
5 of 1472 torsion outliers are listed below:

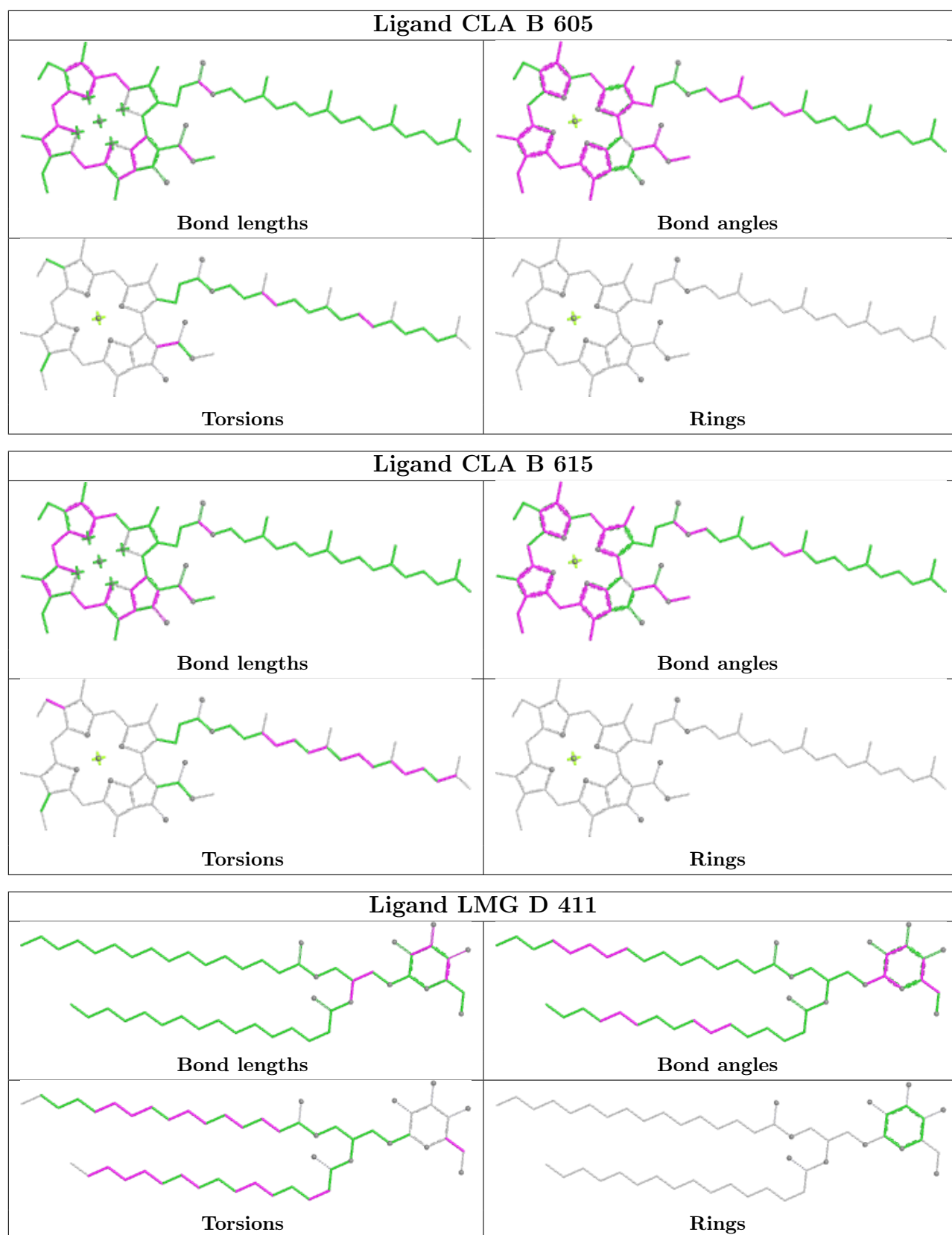
Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C14-C13-C15-C16
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2B-C3B-CAB-CBB
24	B	615	CLA	C4B-C3B-CAB-CBB

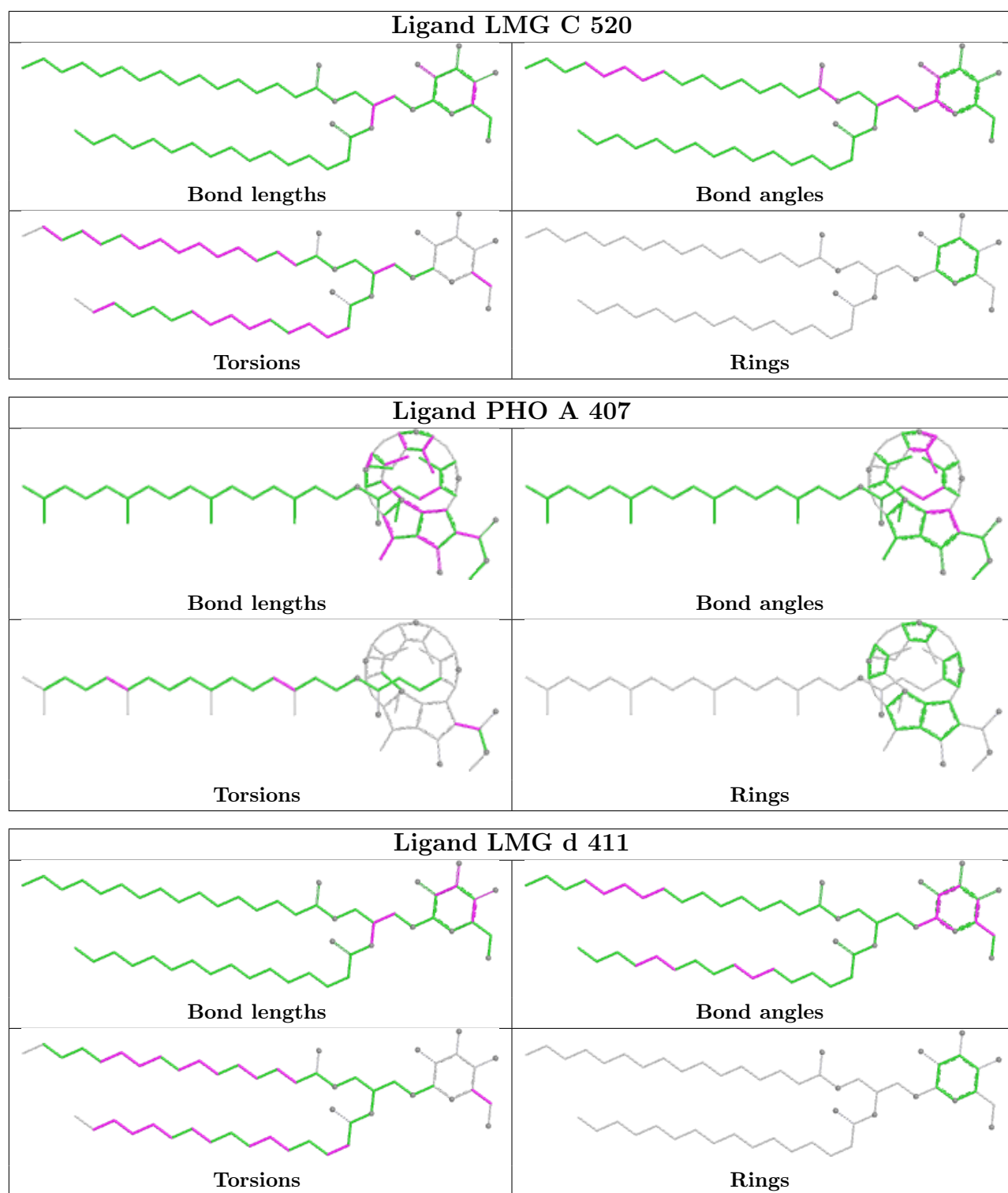
There are no ring outliers.

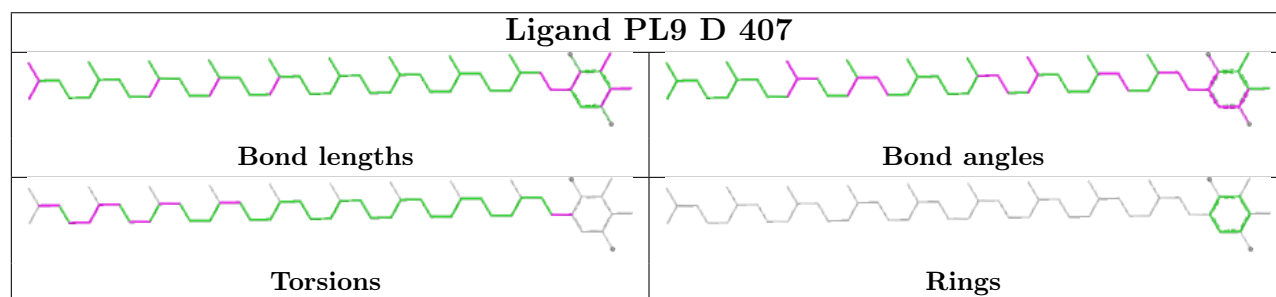
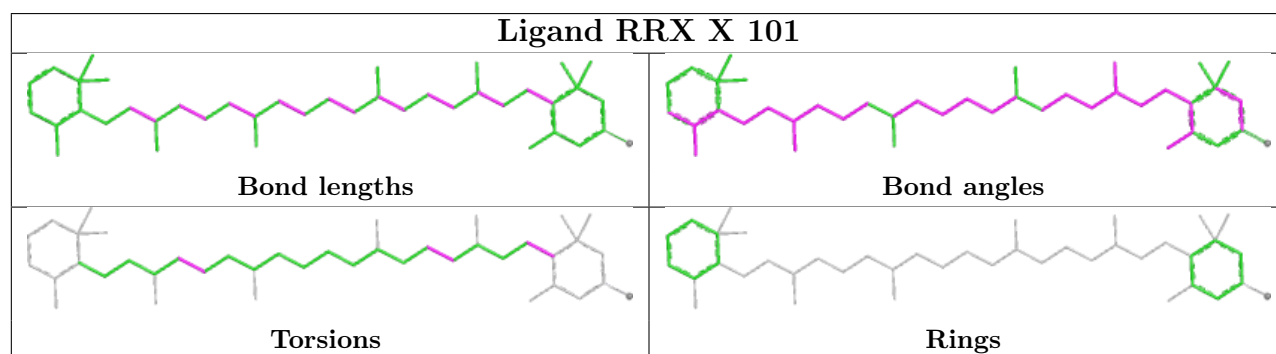
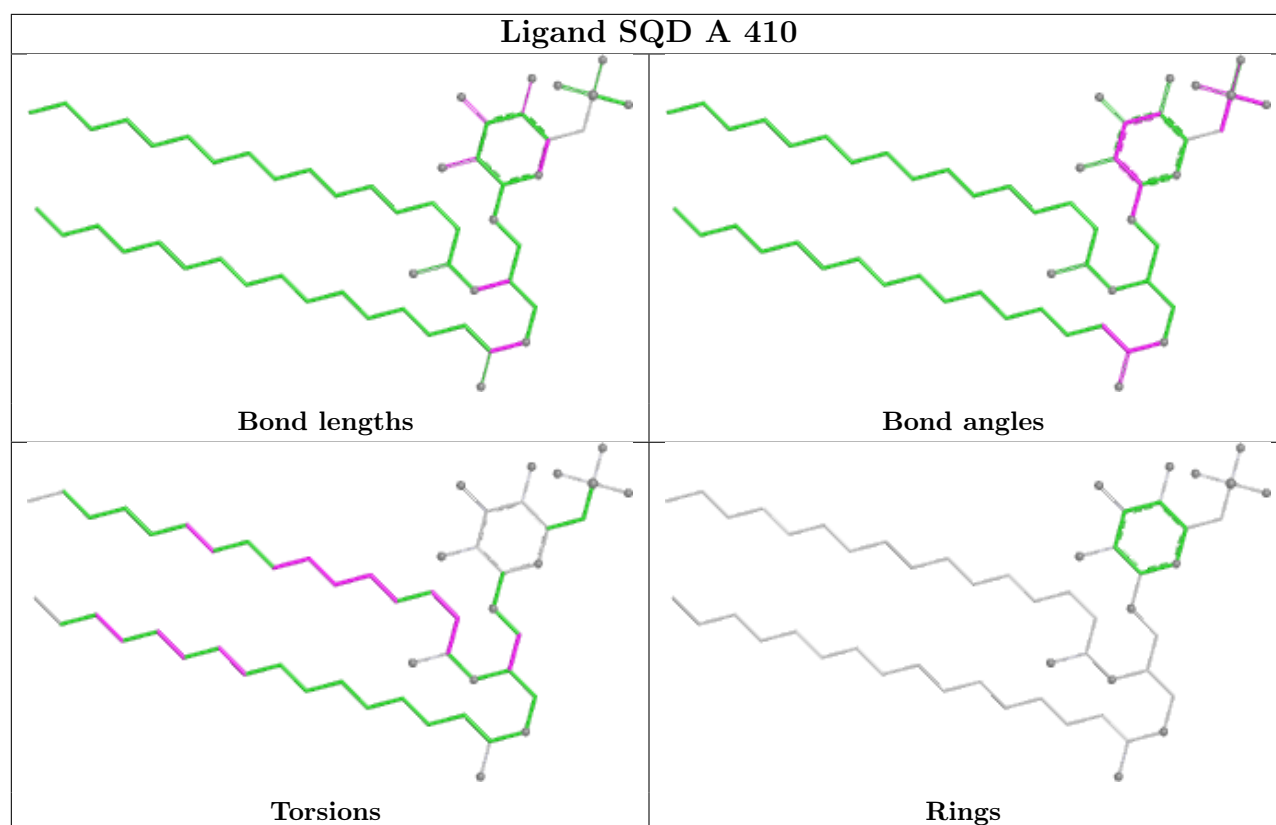
No monomer is involved in short contacts.

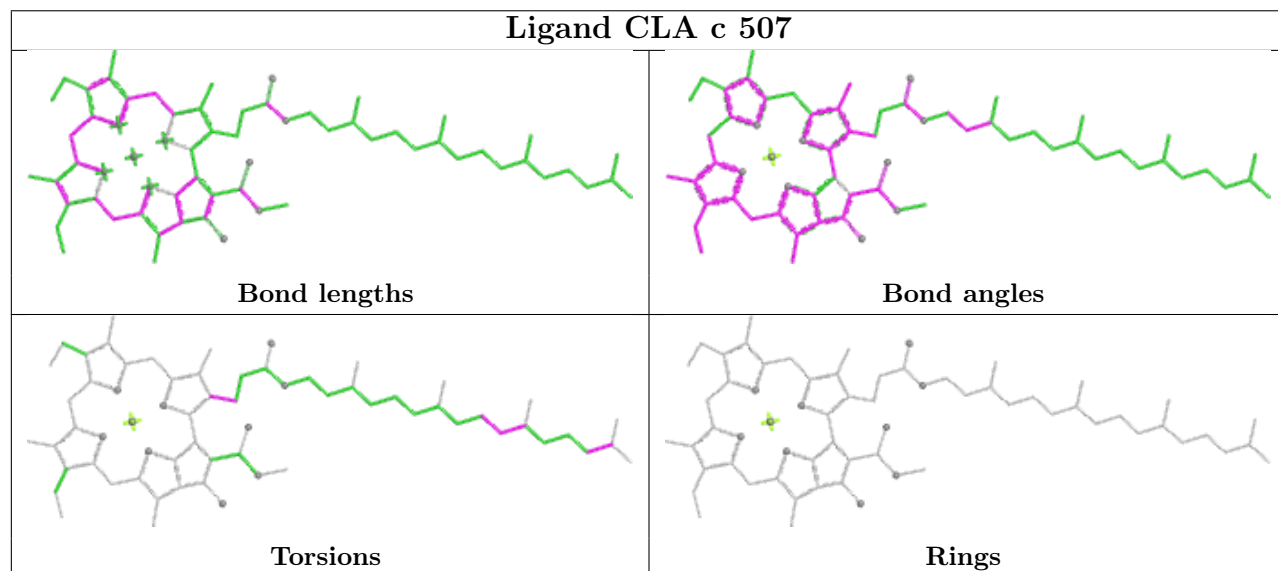
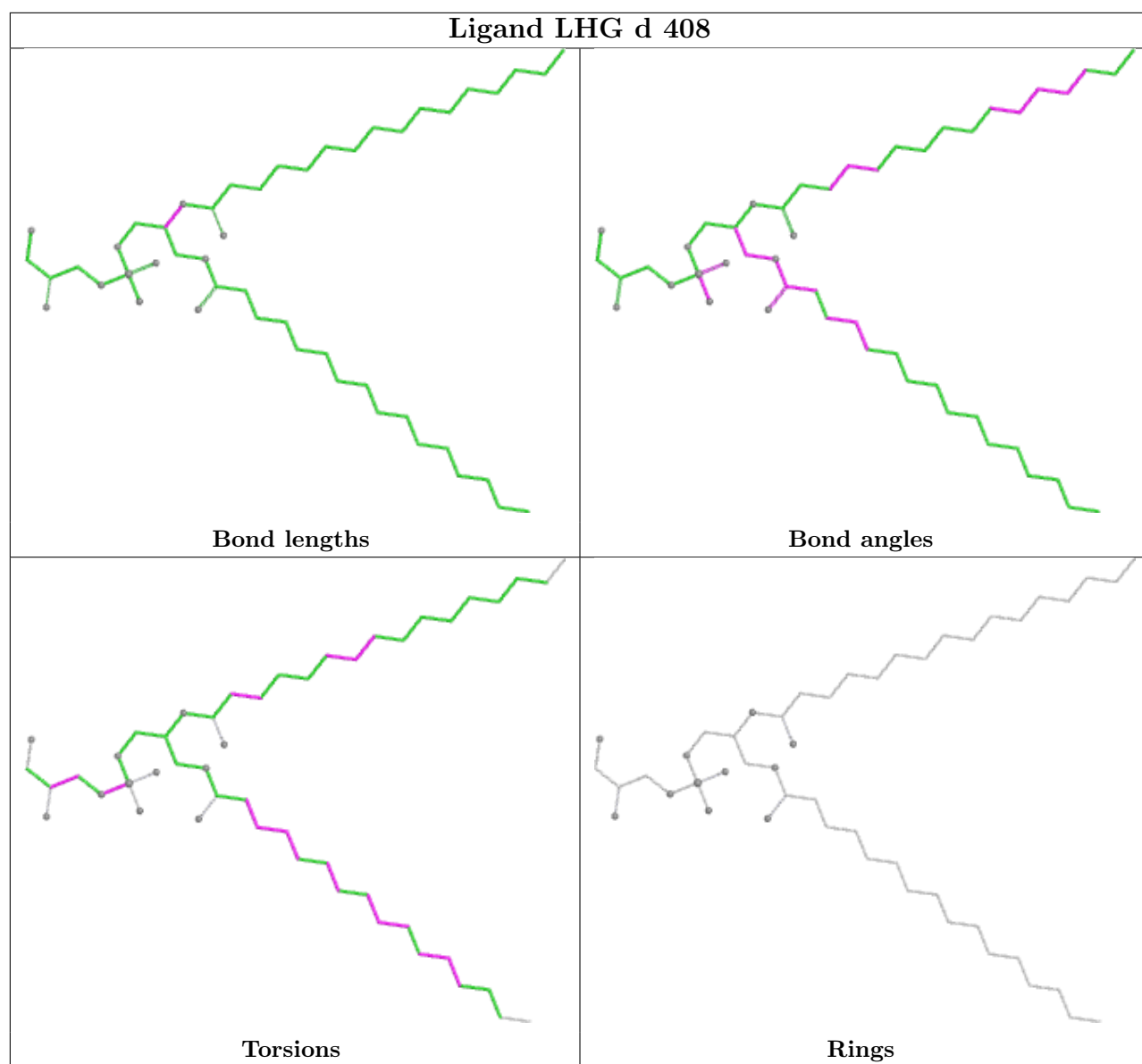
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

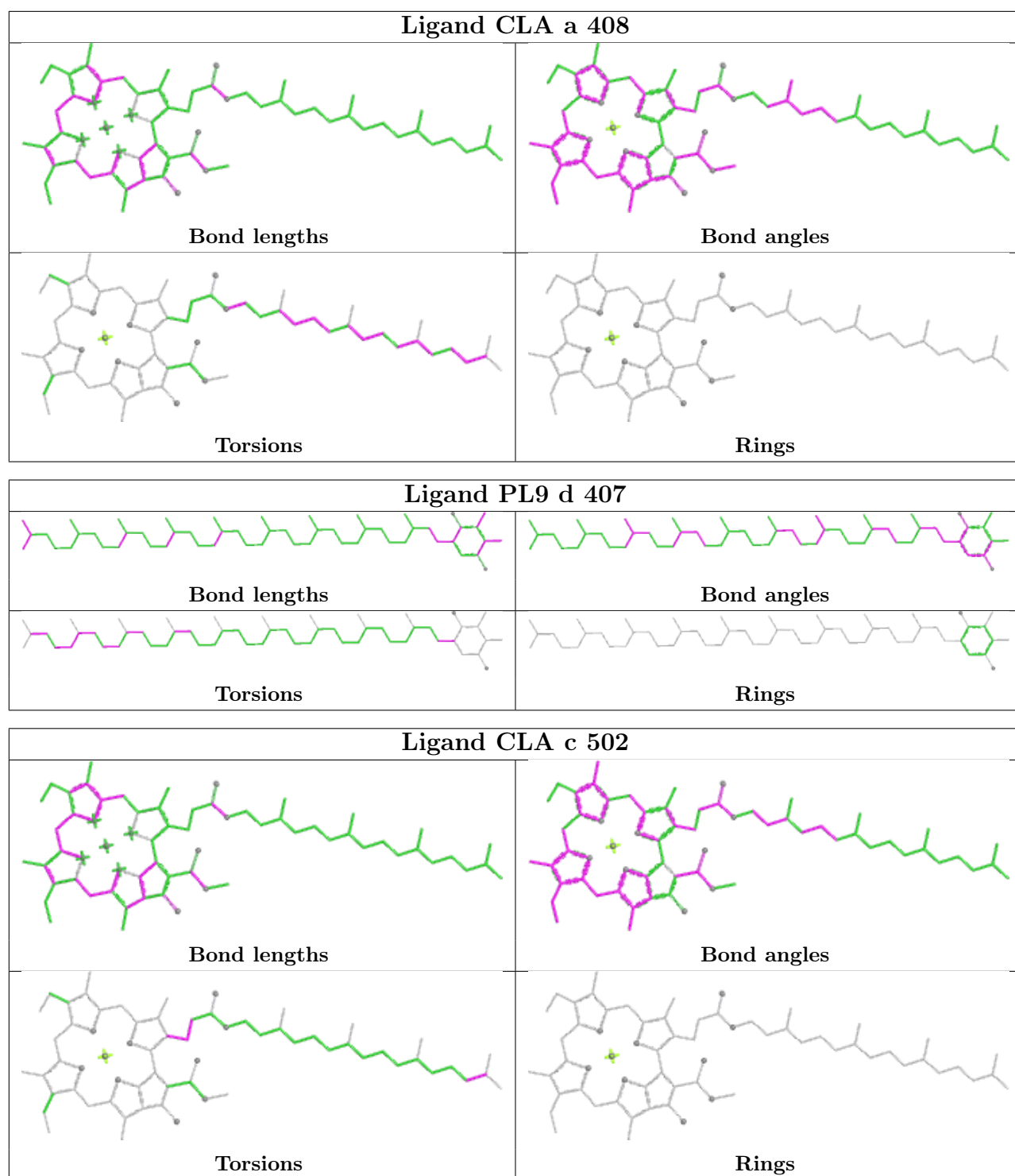


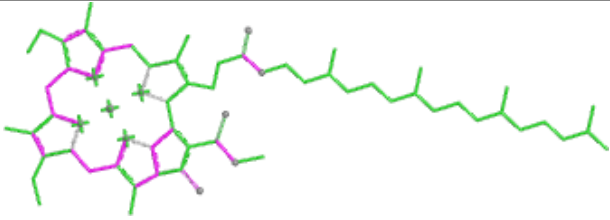
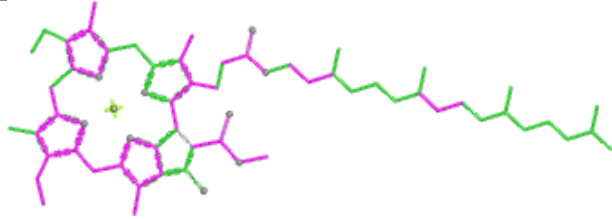
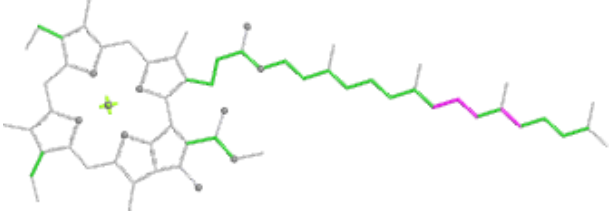
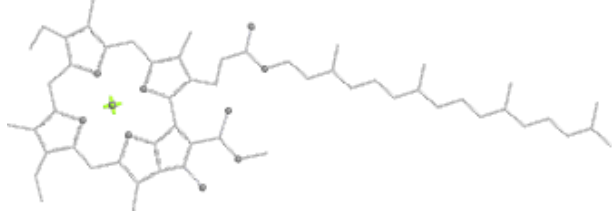
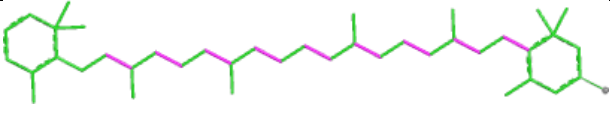
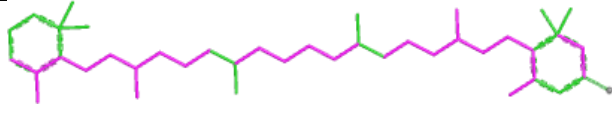
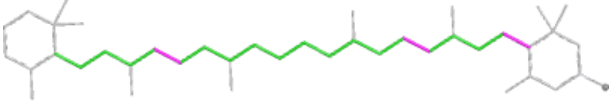
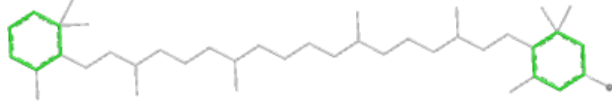
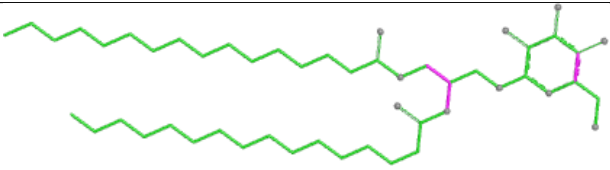
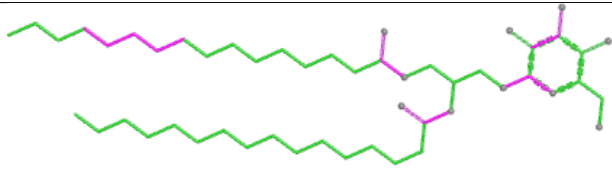
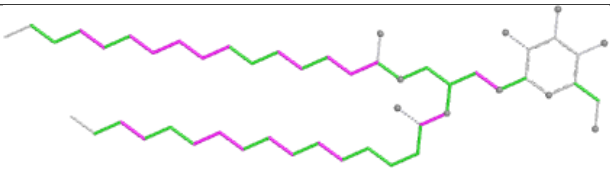
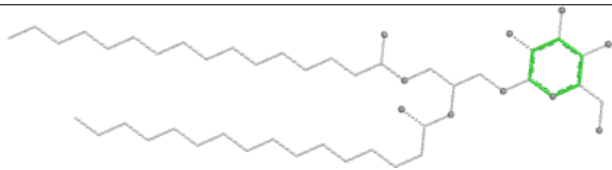


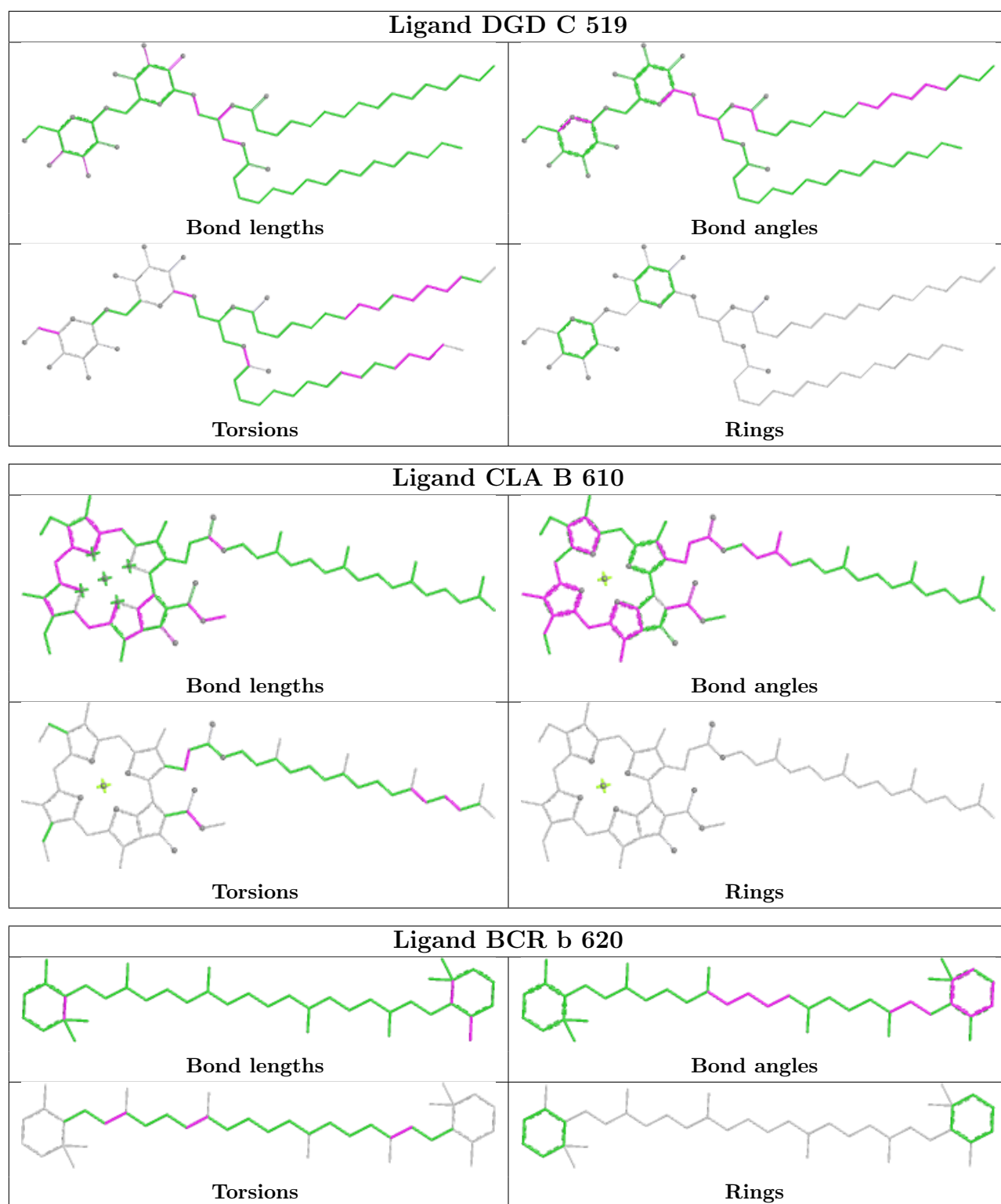


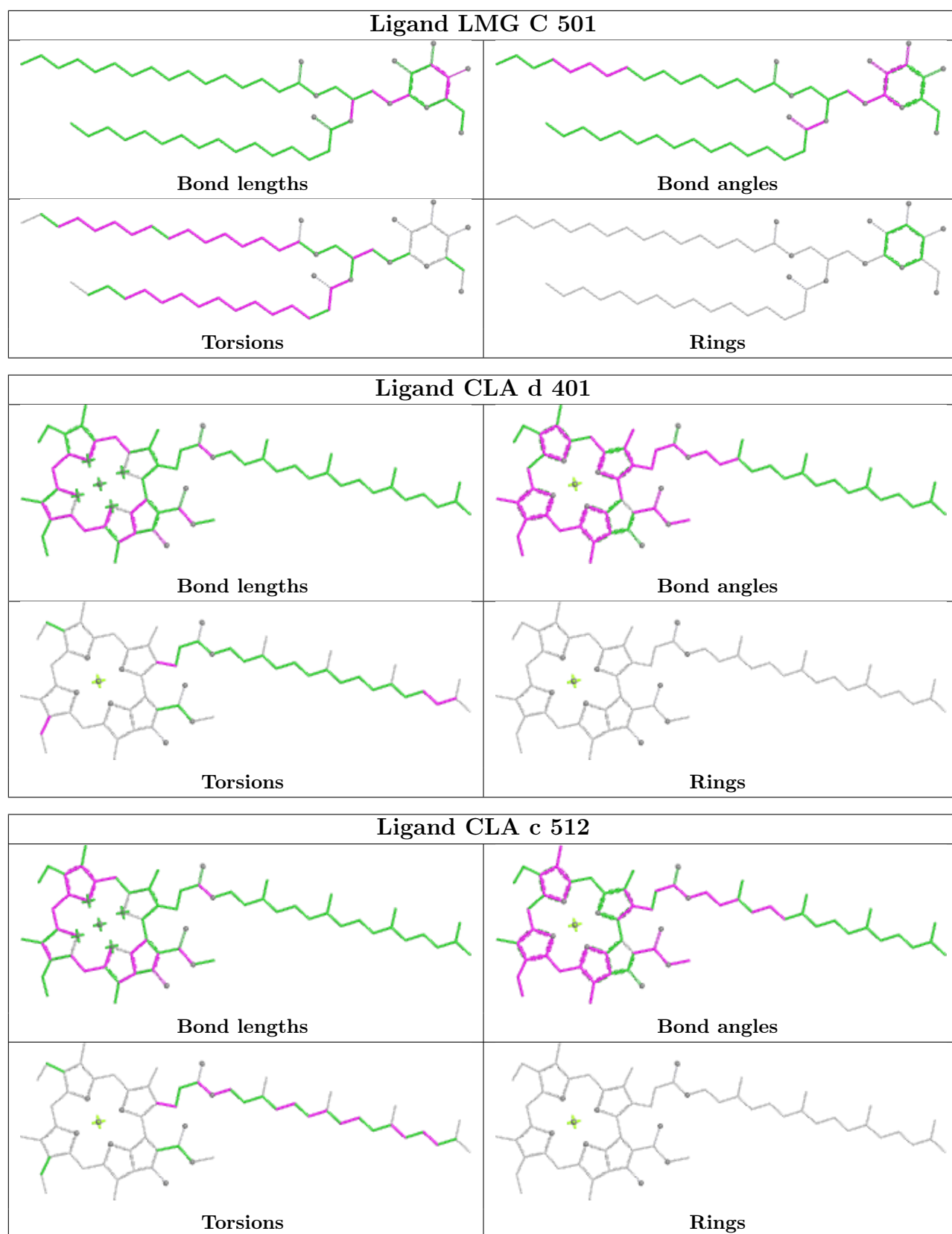


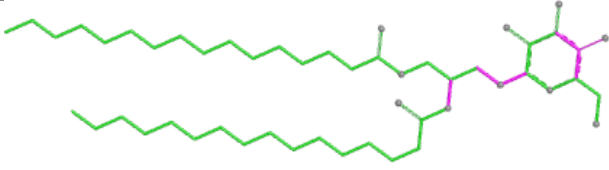
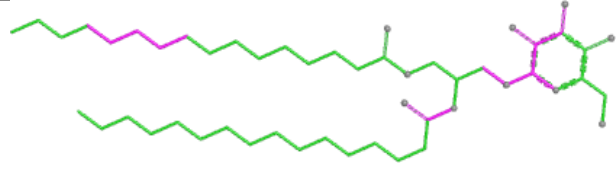
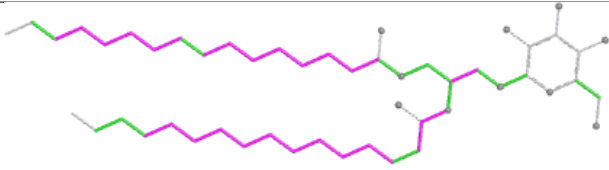
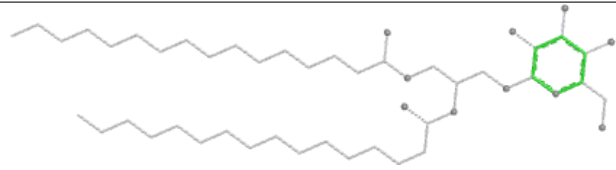


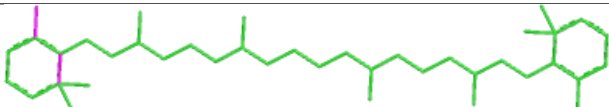
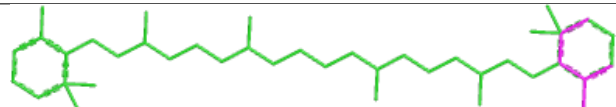
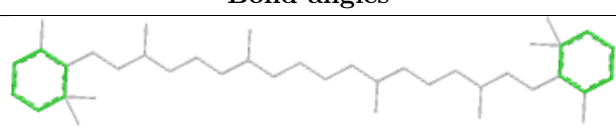


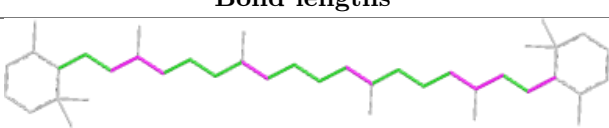
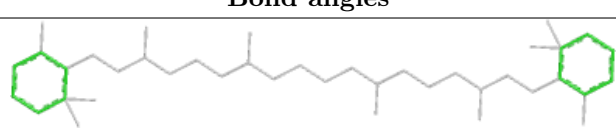
Ligand CLA C 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand RRX x 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG B 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

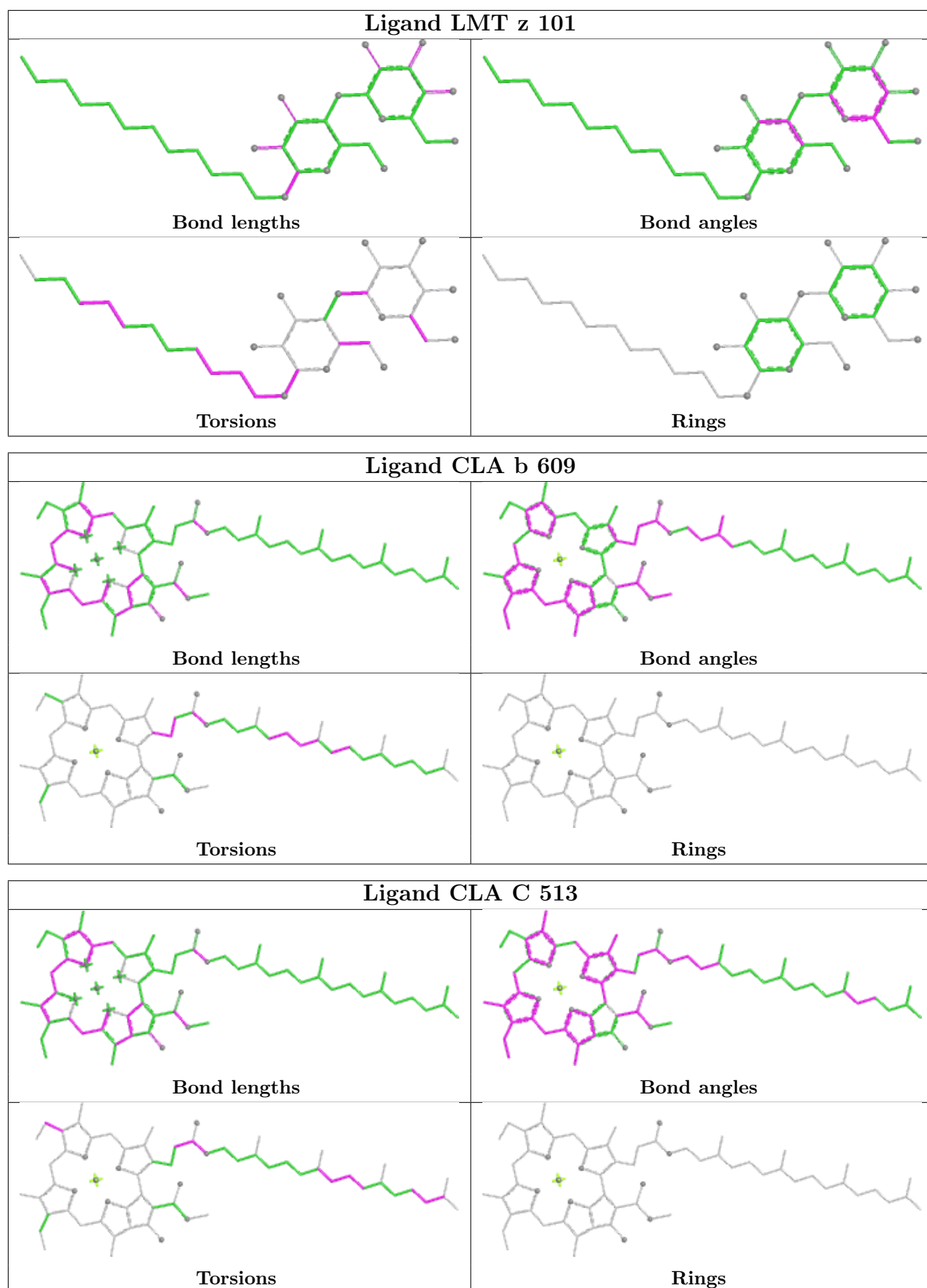


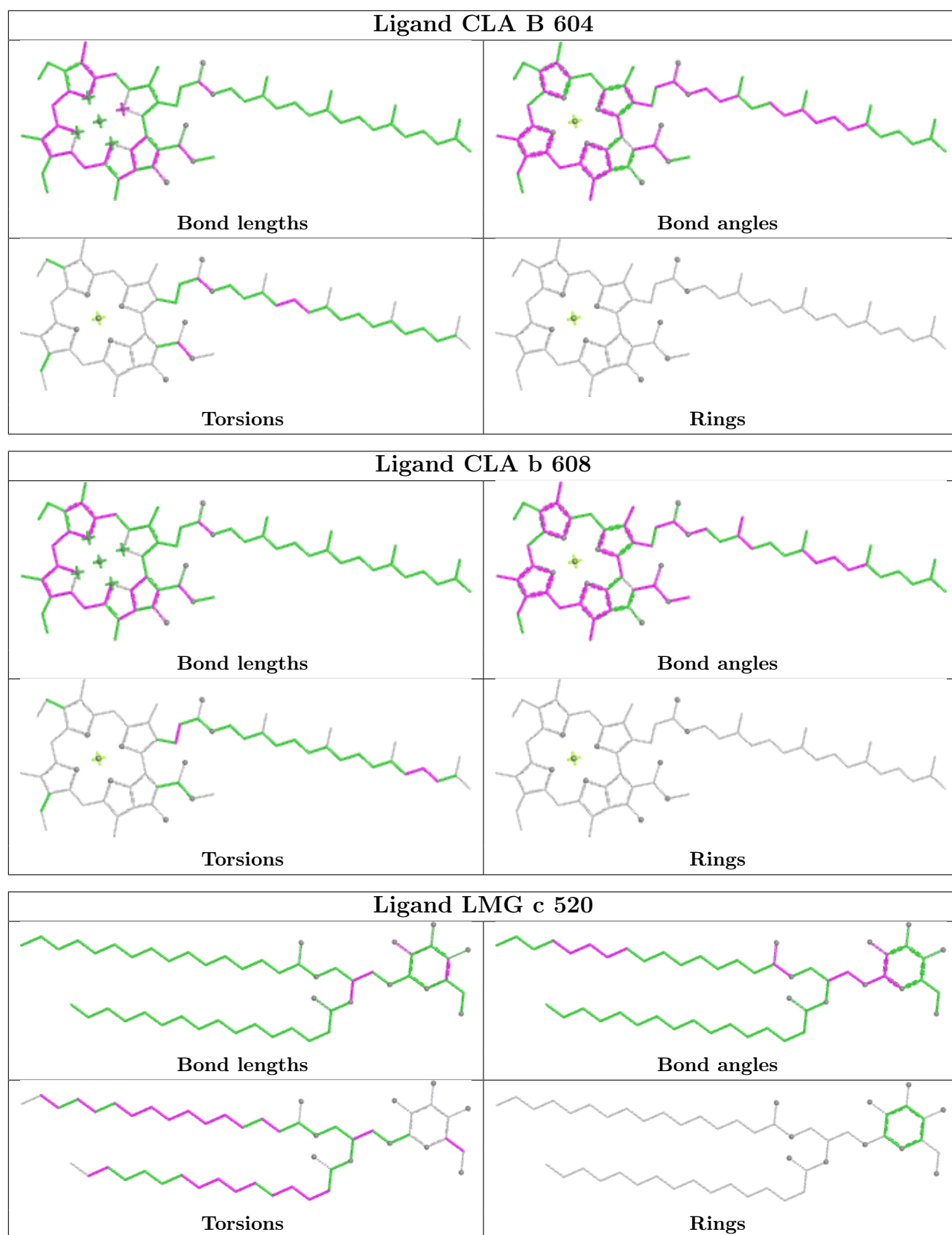


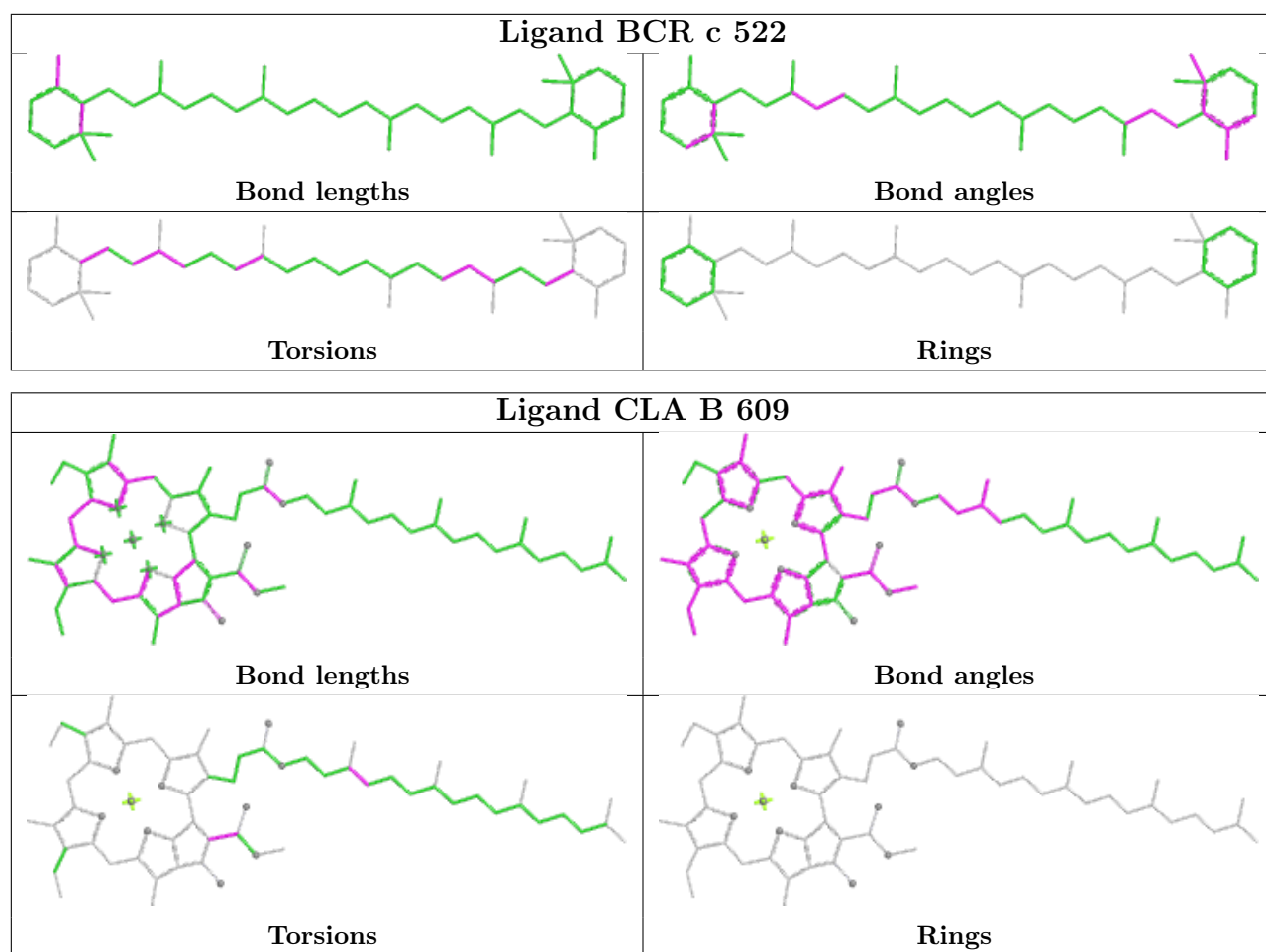
Ligand LMG c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

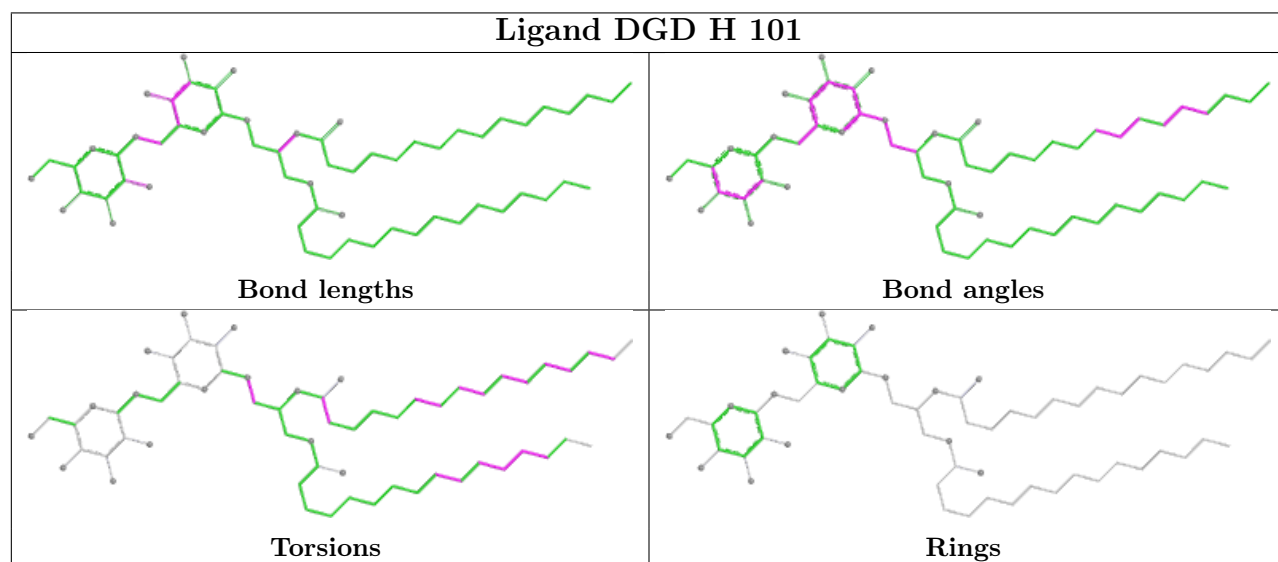
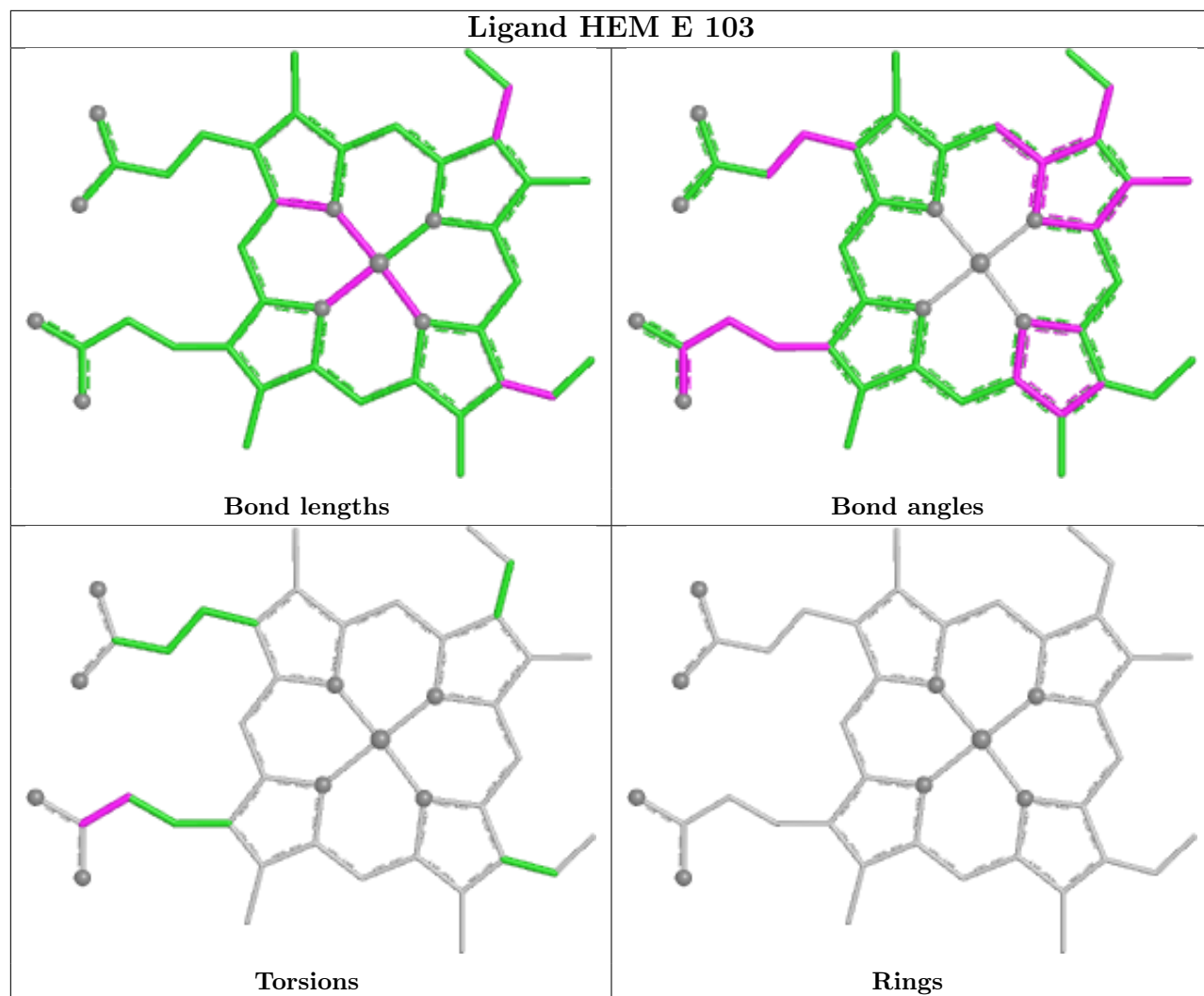
Ligand BCR b 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

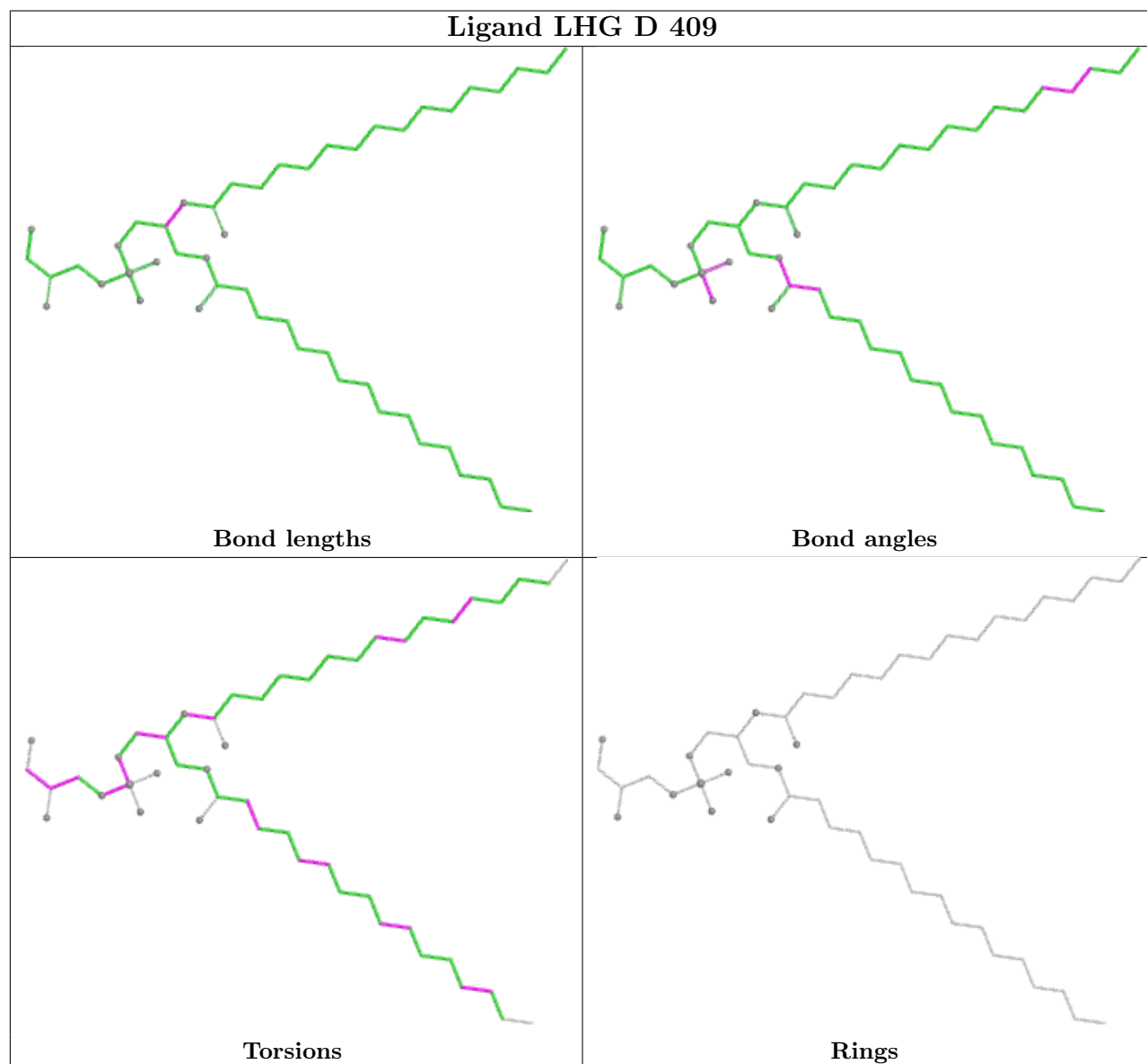
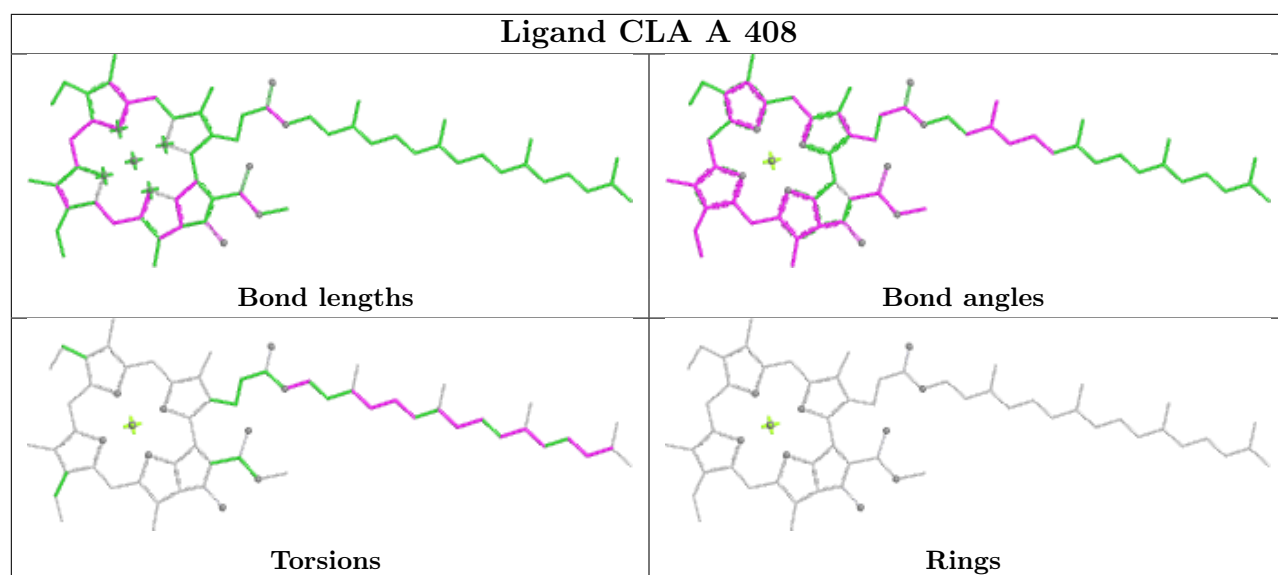
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

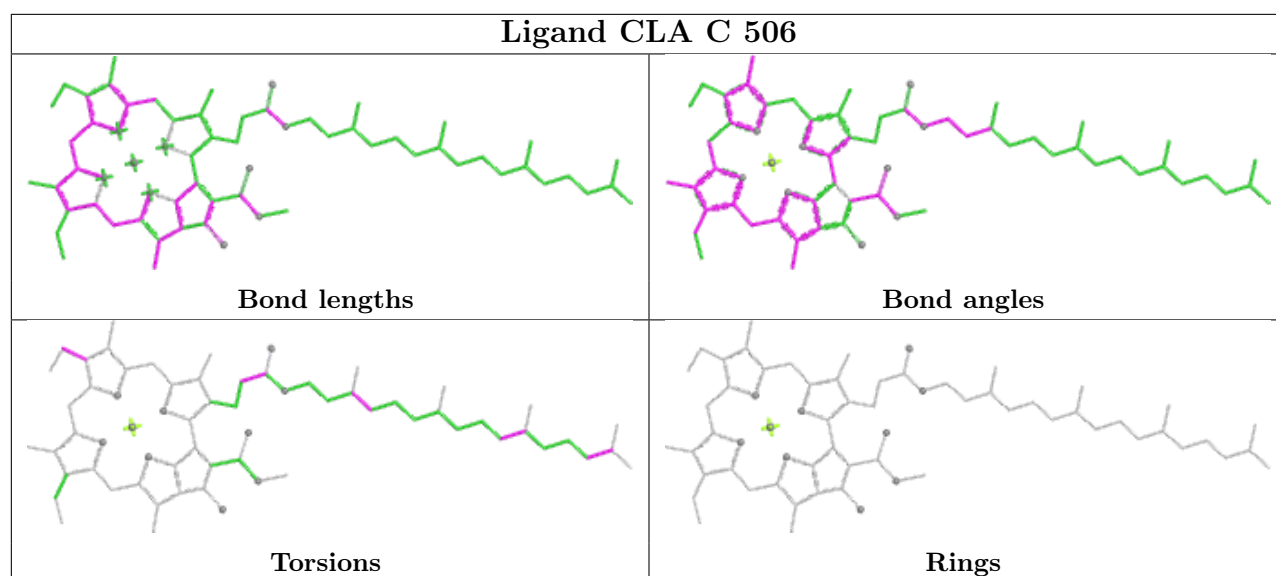
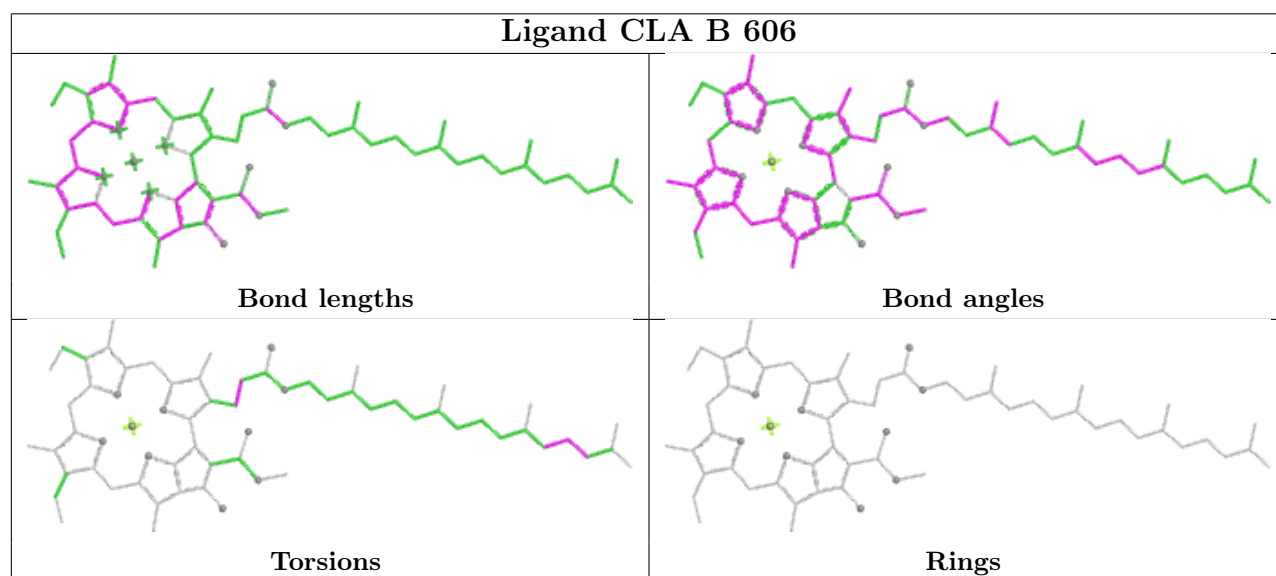
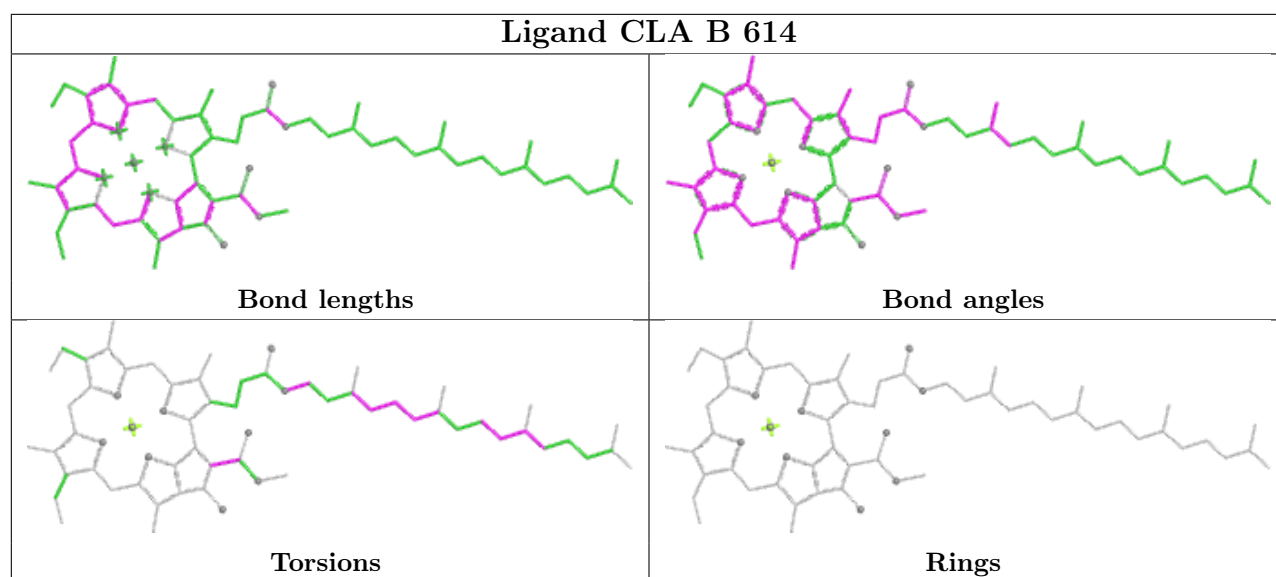


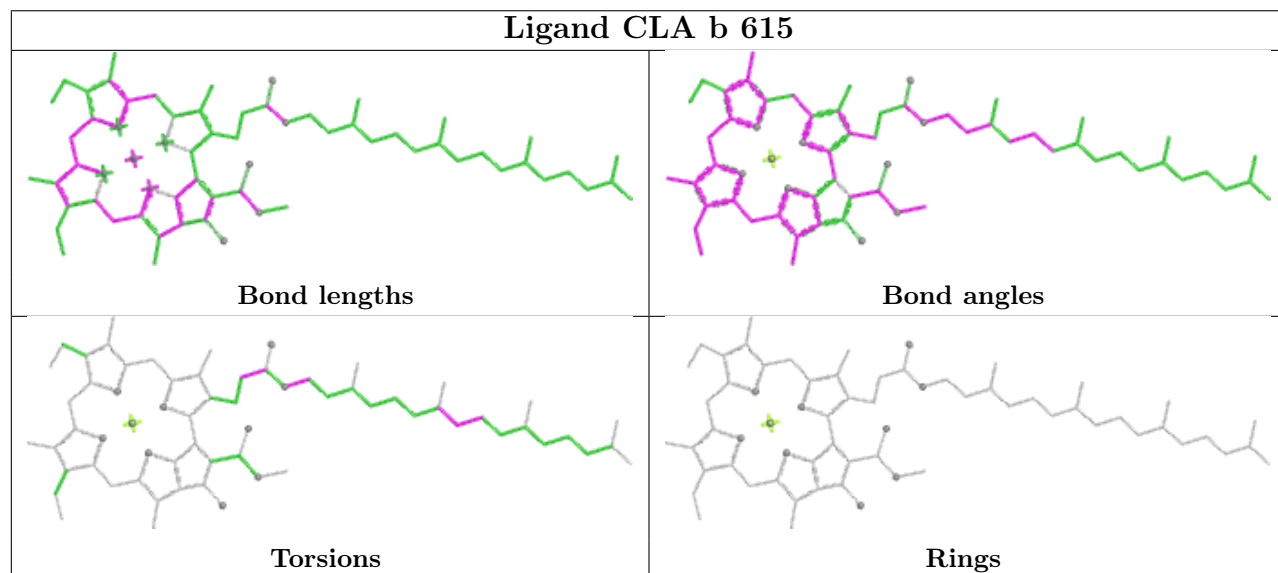
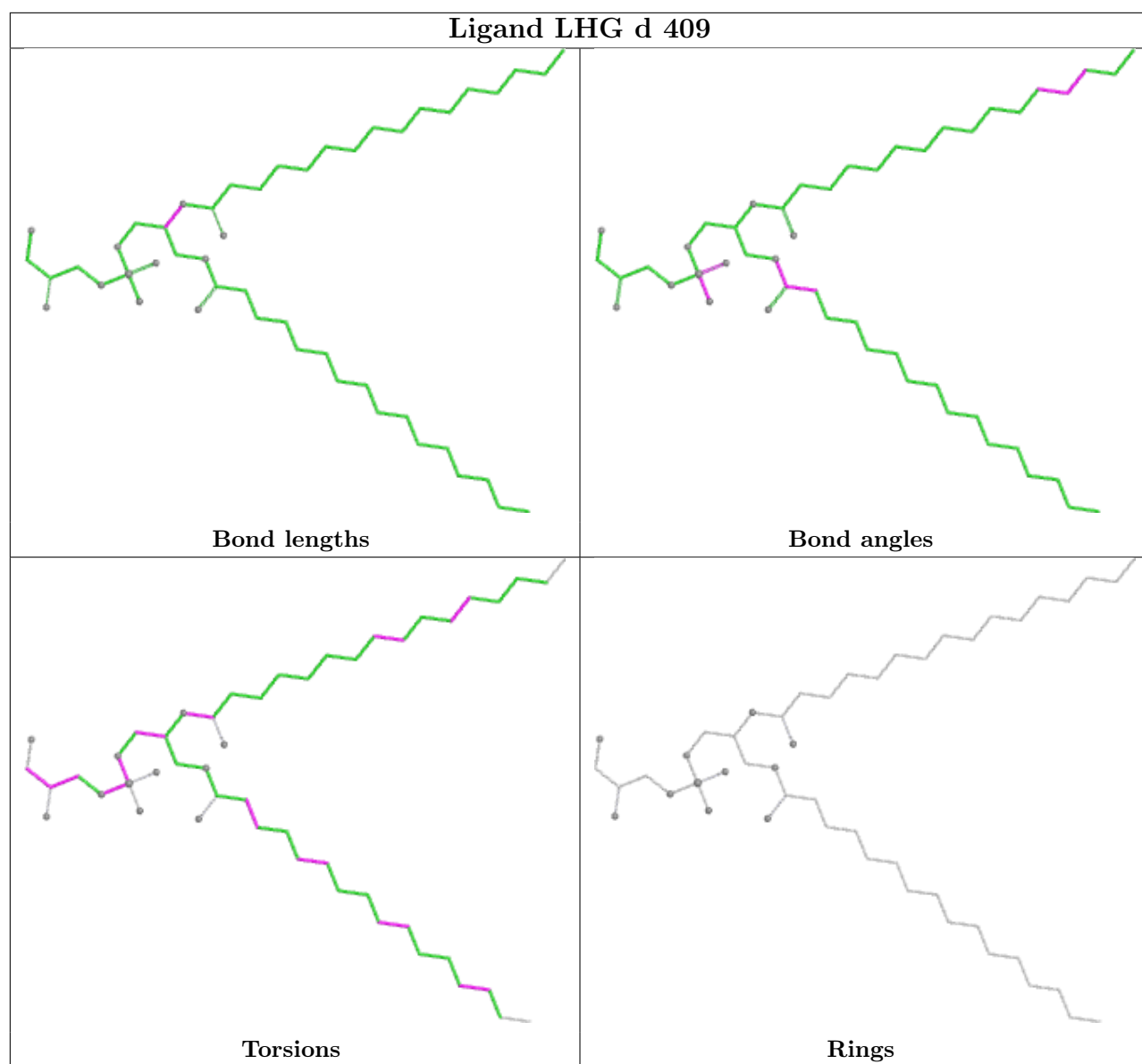


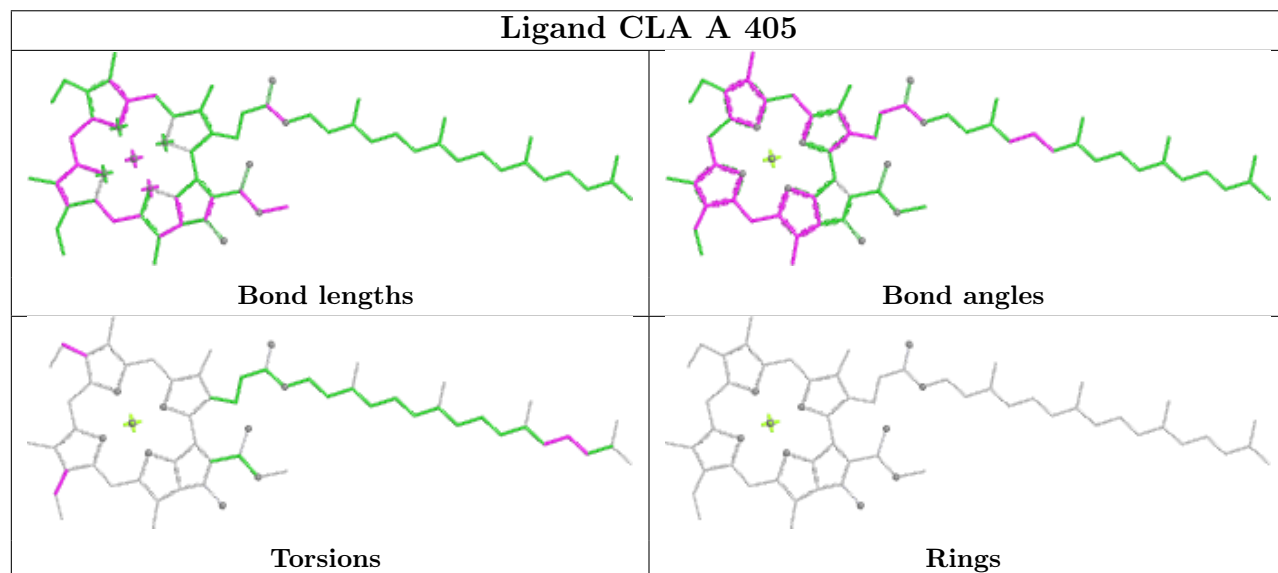
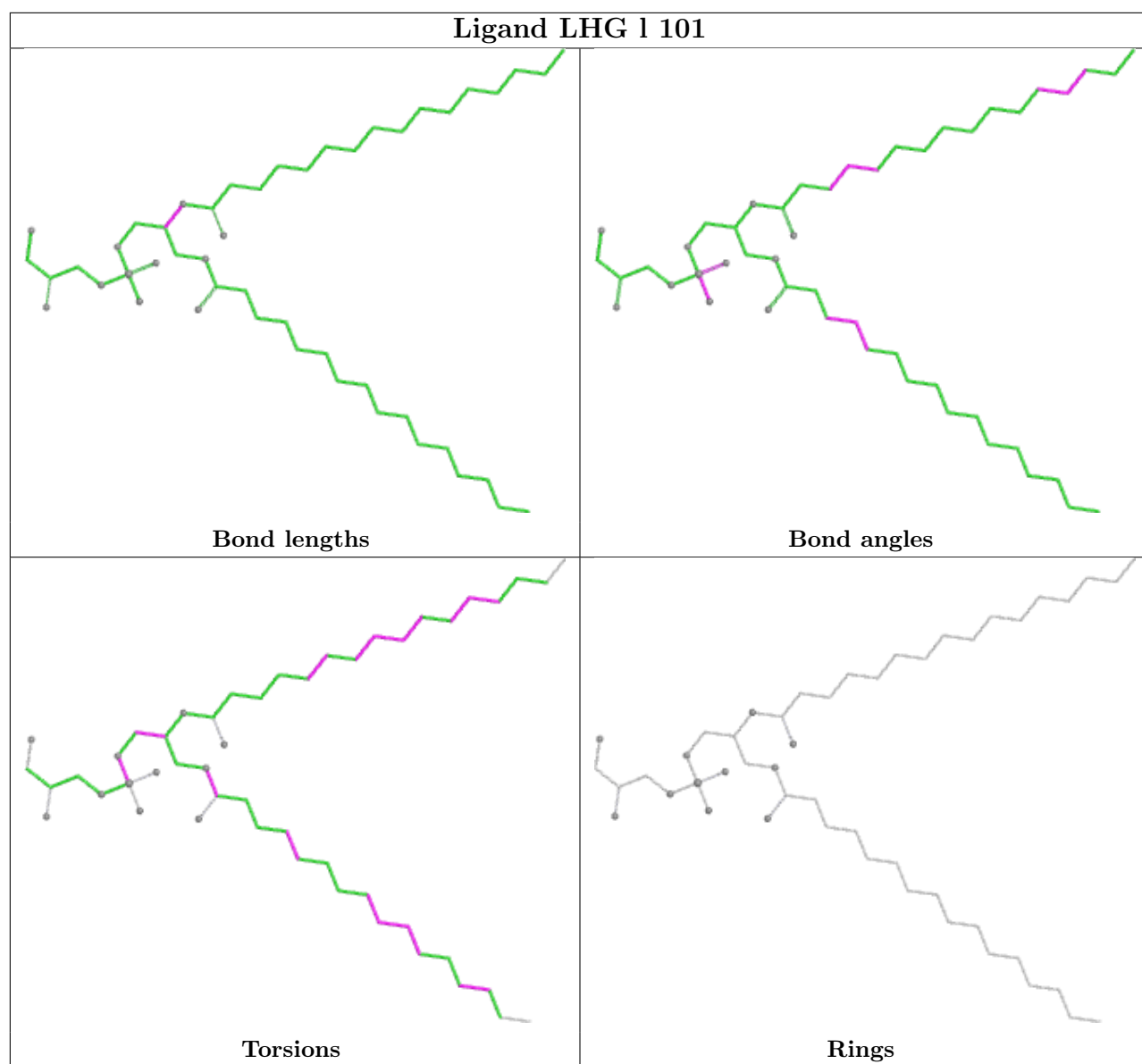


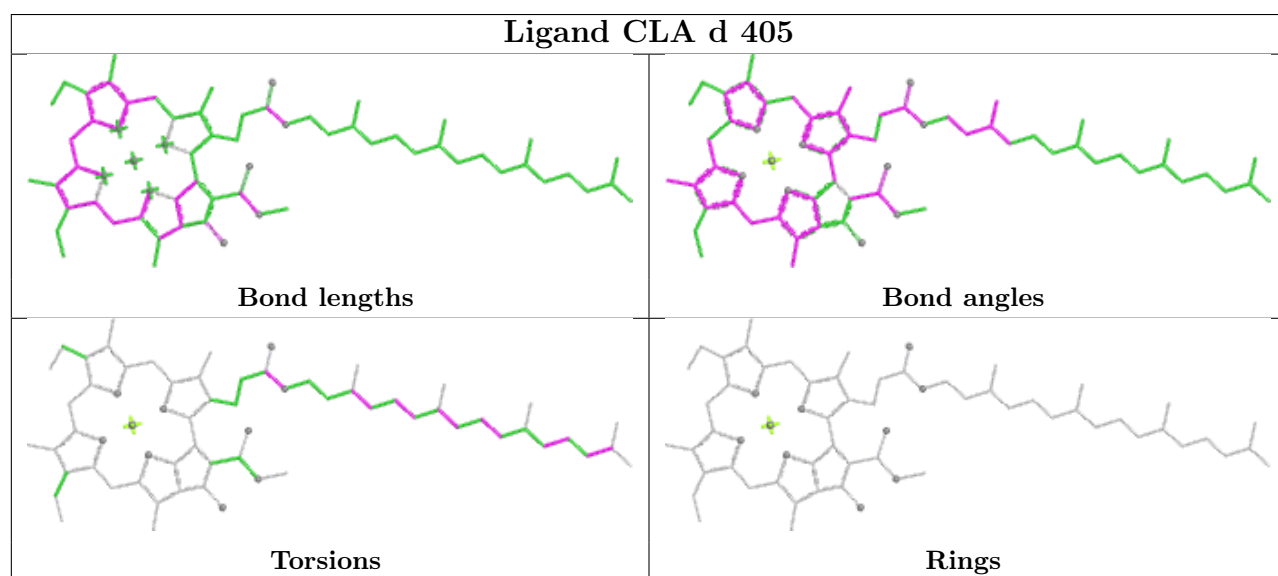
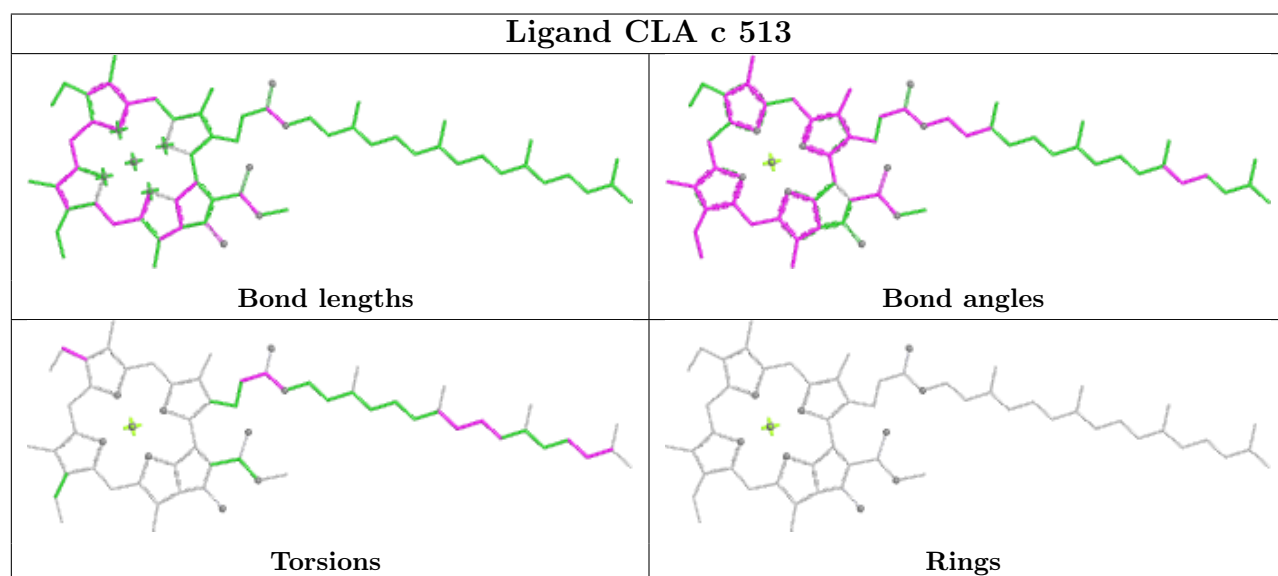
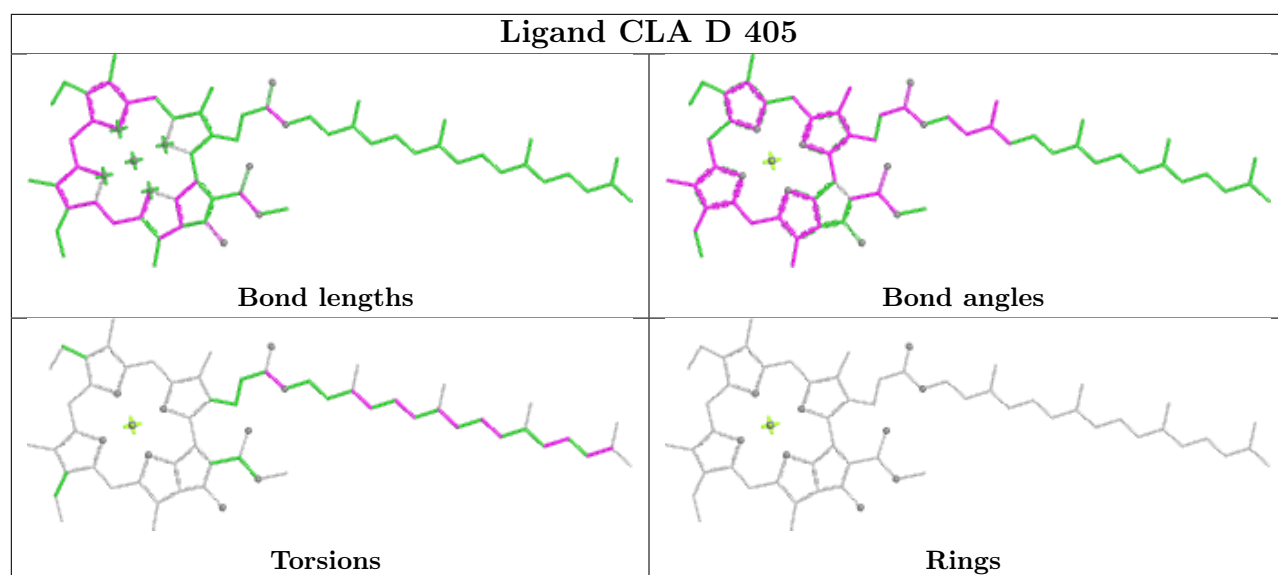


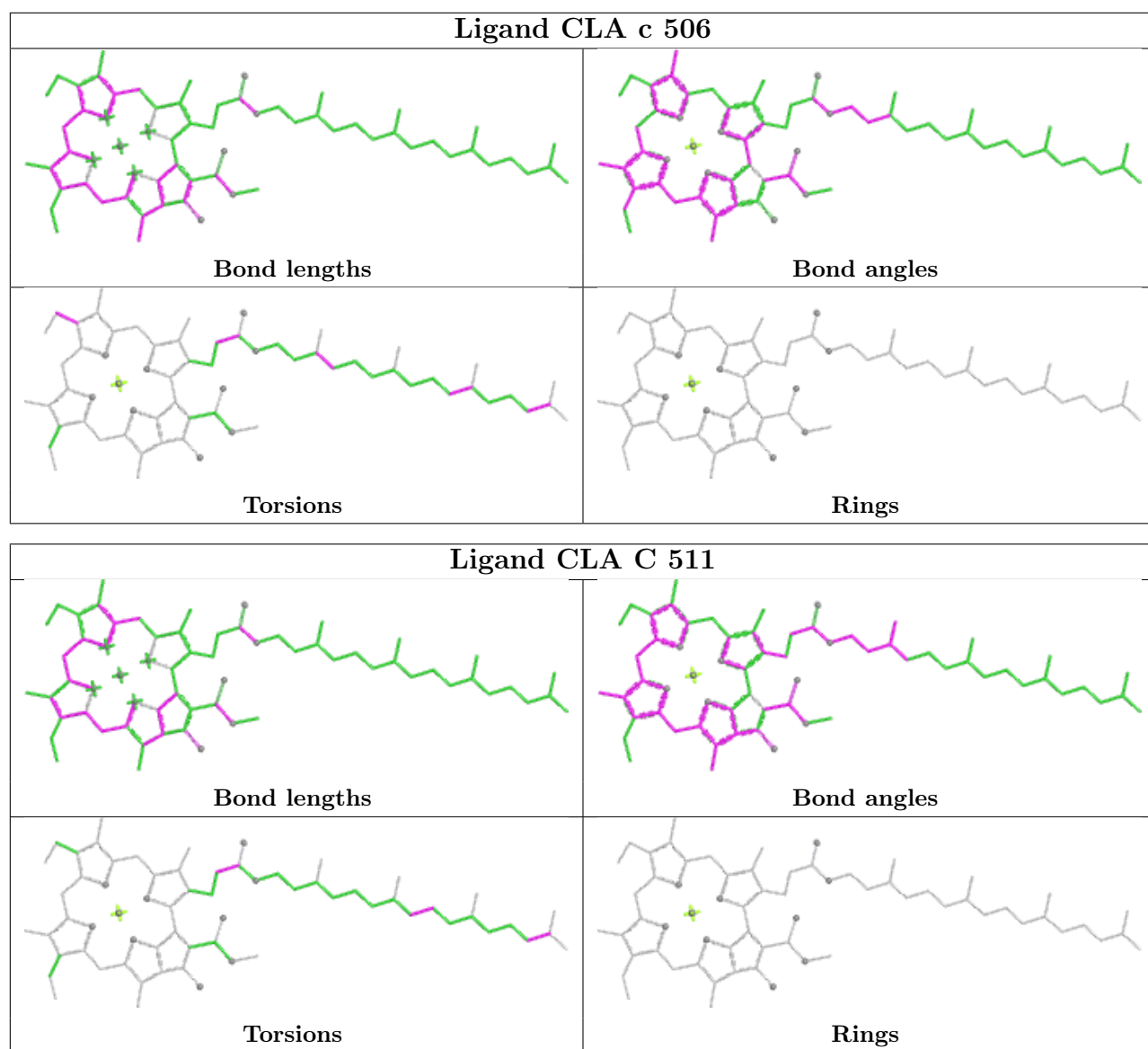


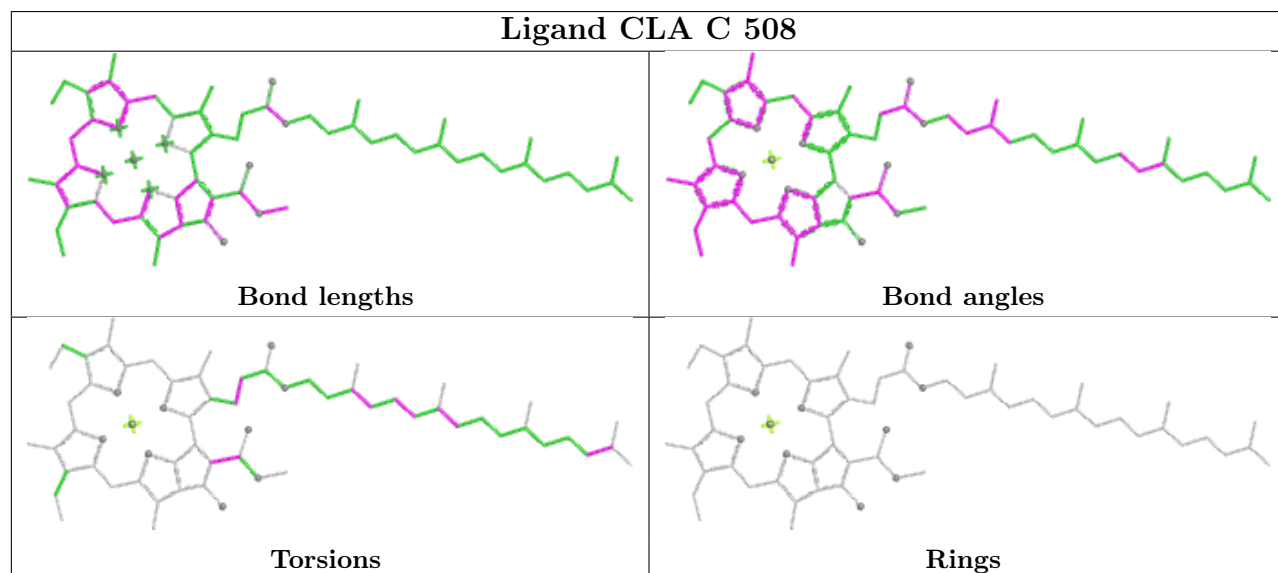
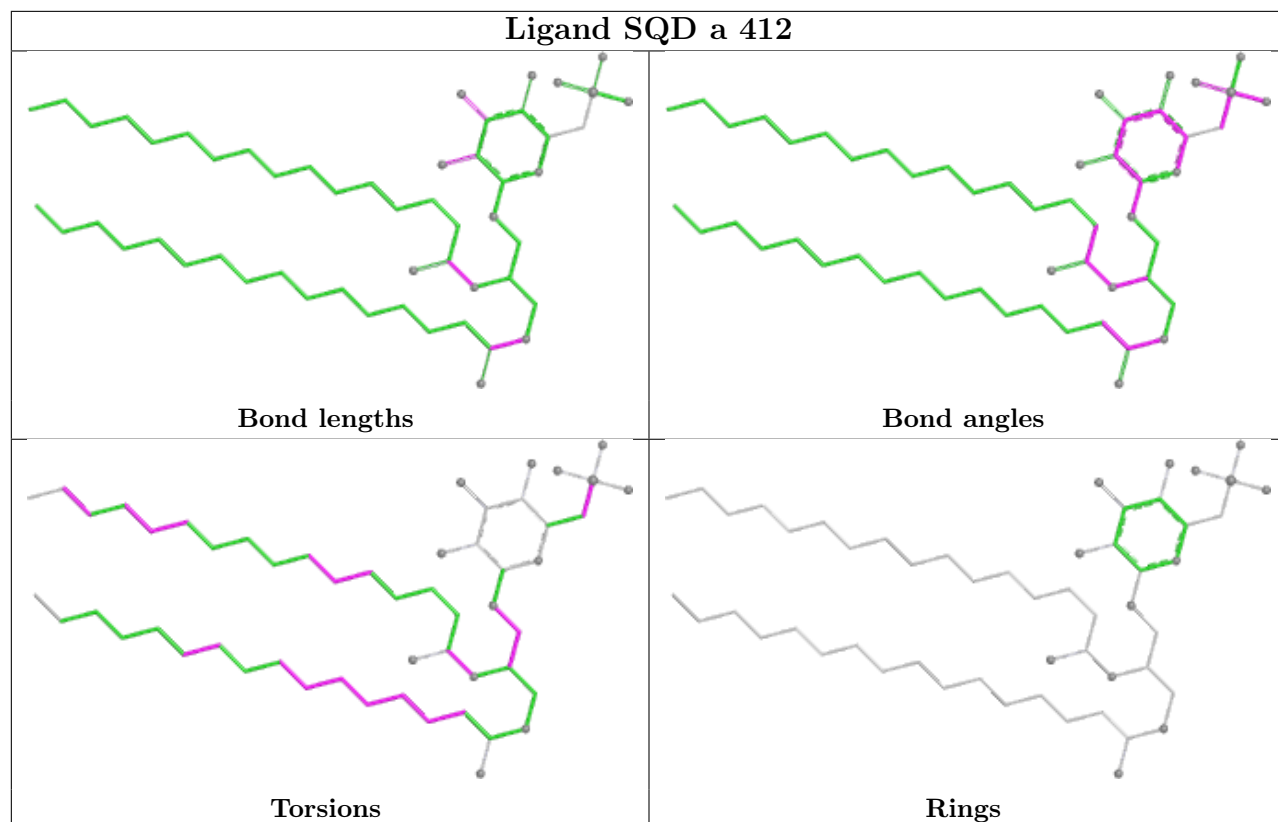


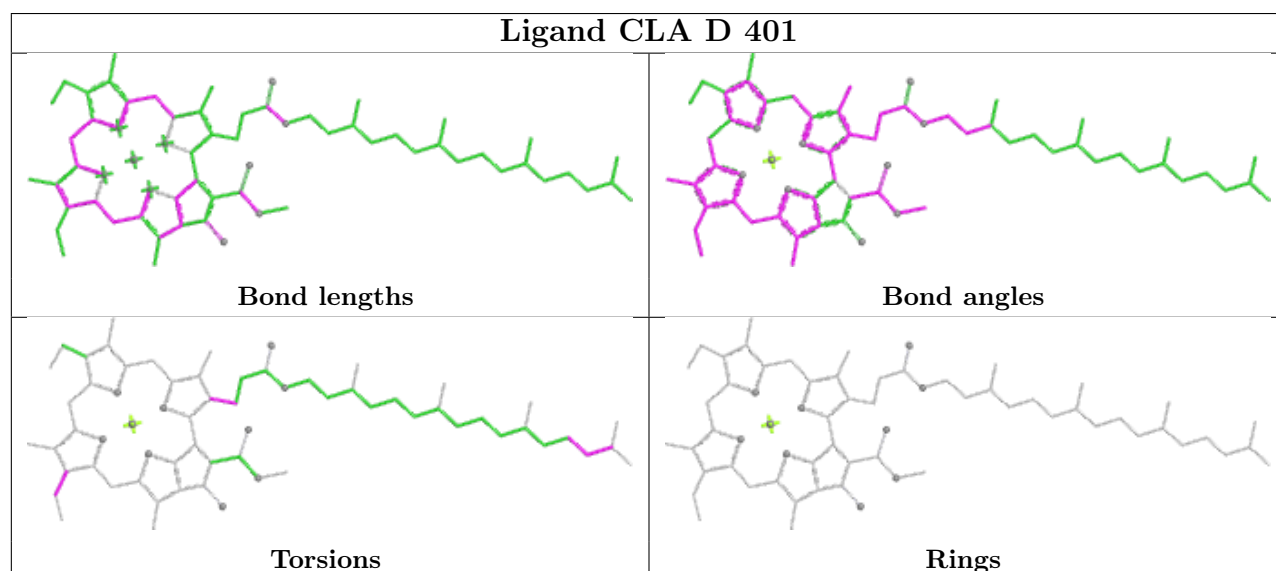
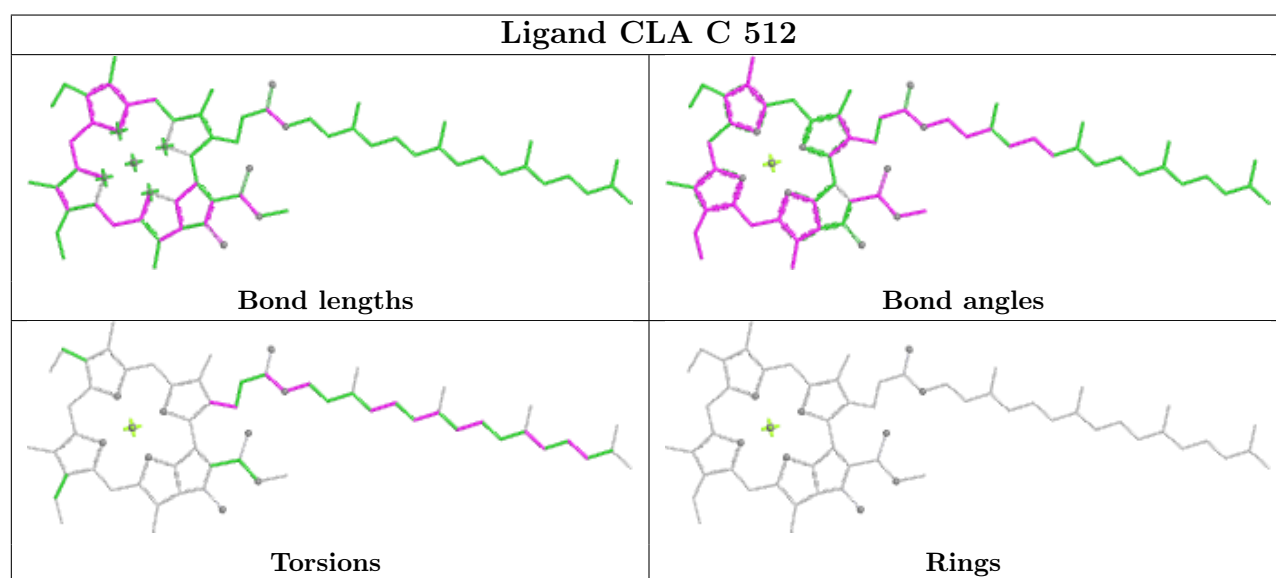
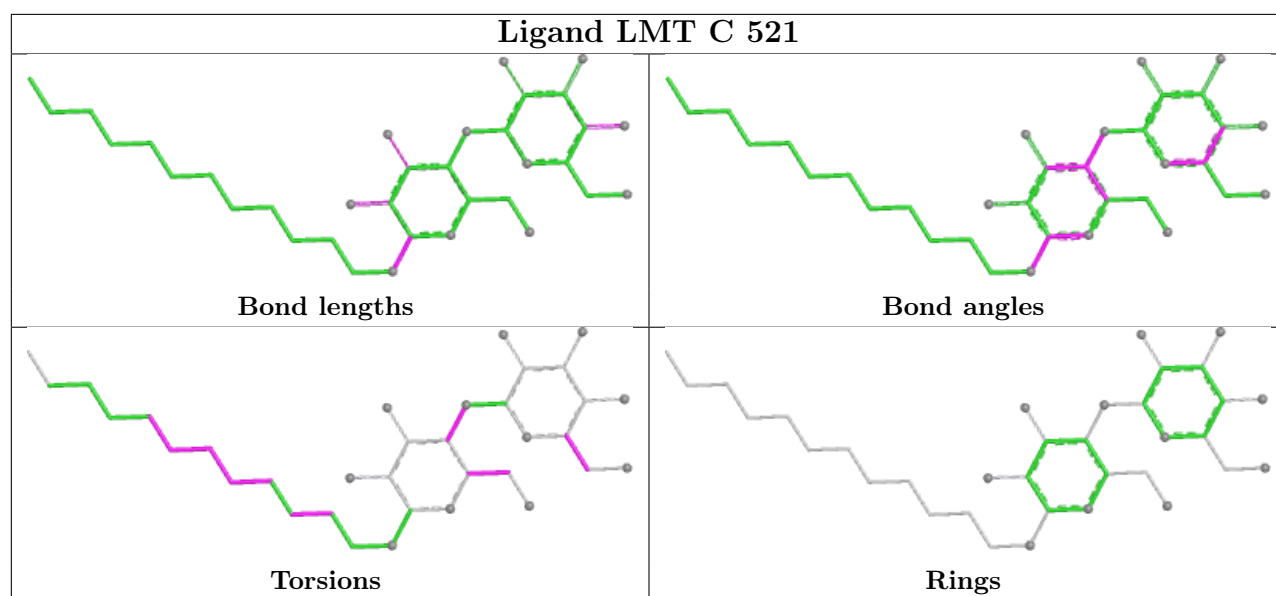


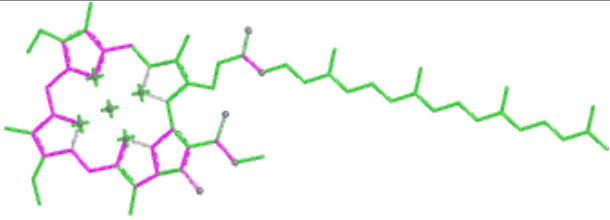
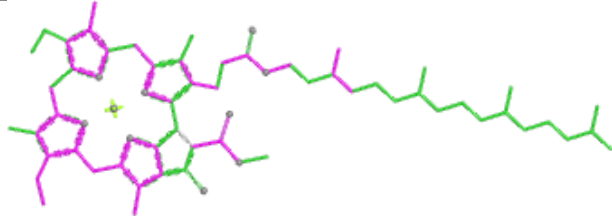
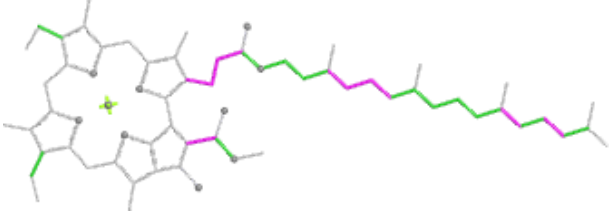
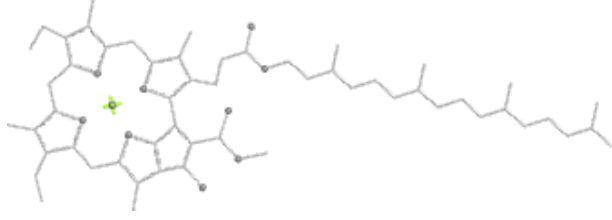
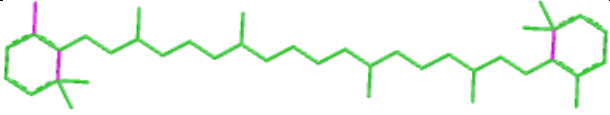
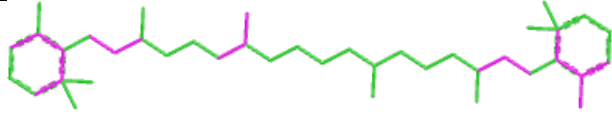
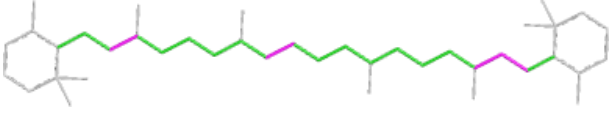
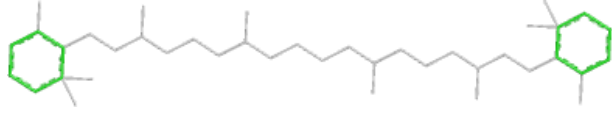
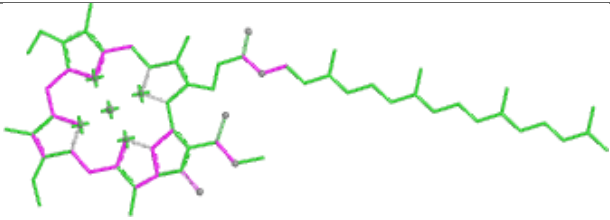
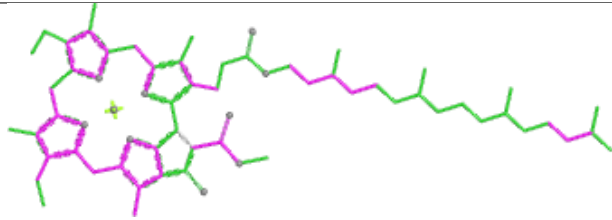
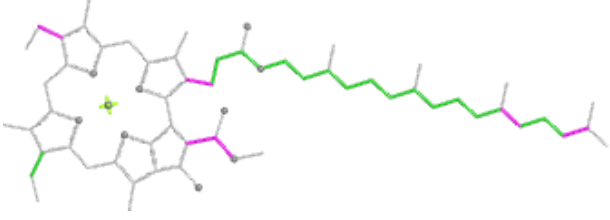
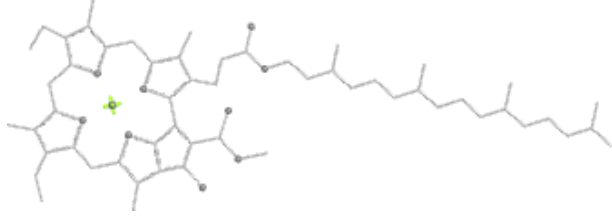


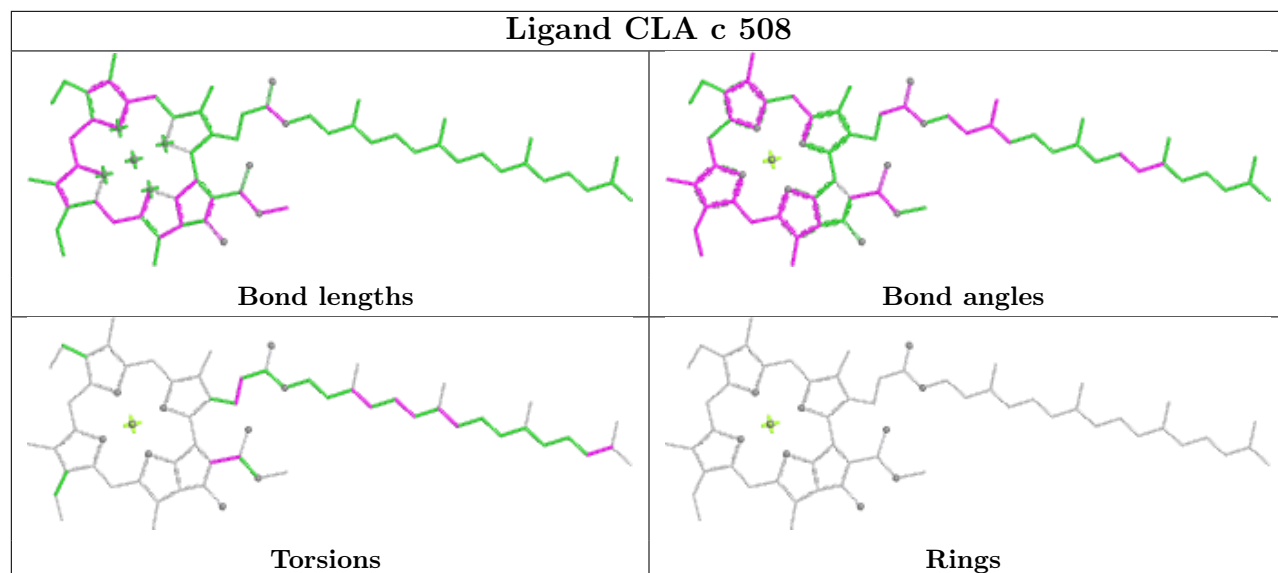
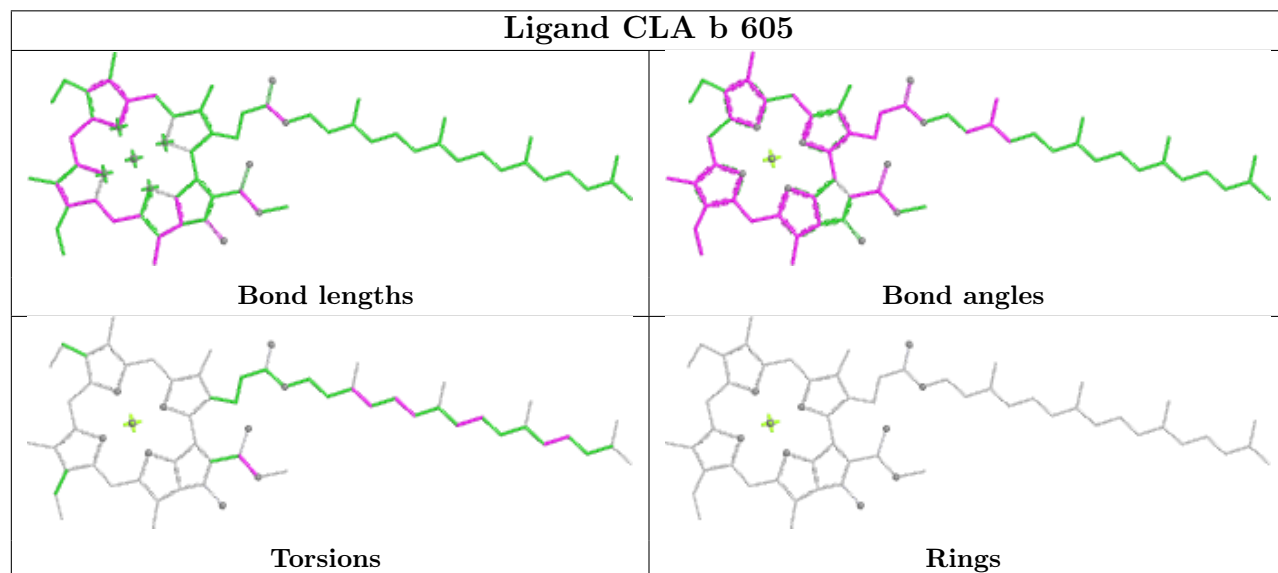
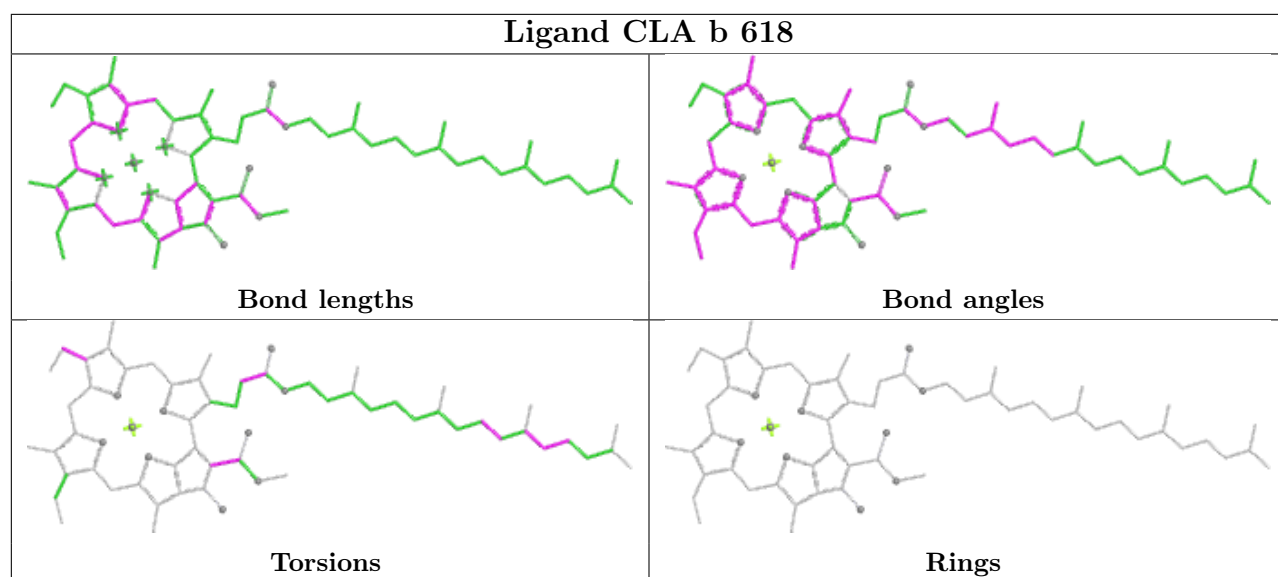


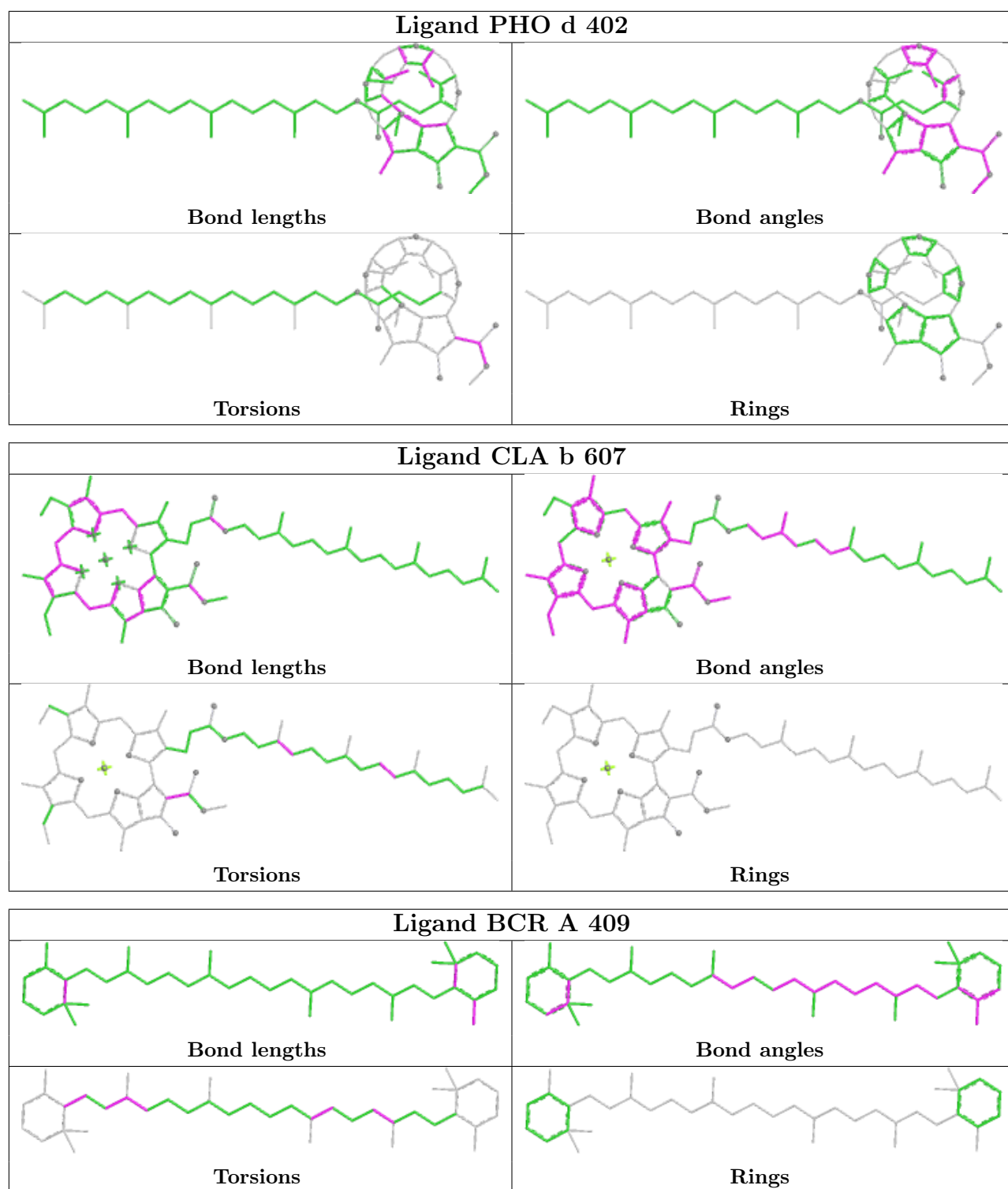


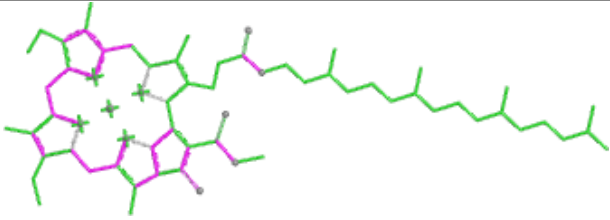
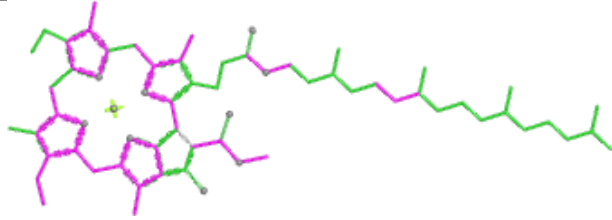
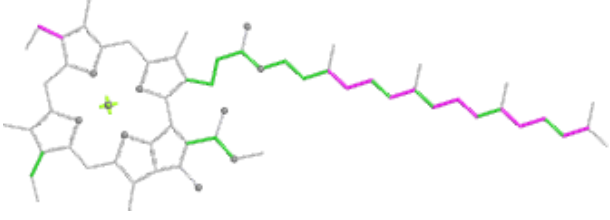
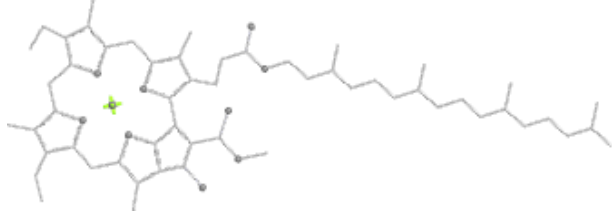
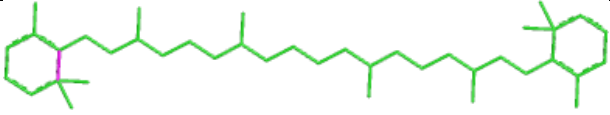
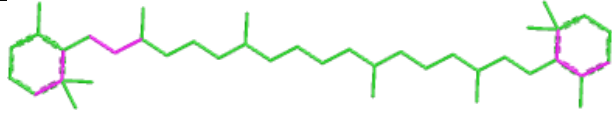
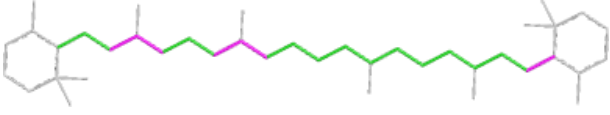
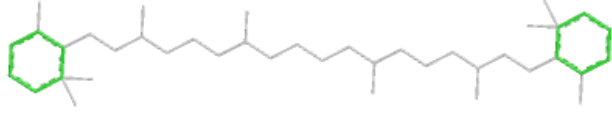
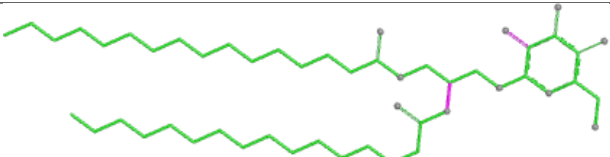
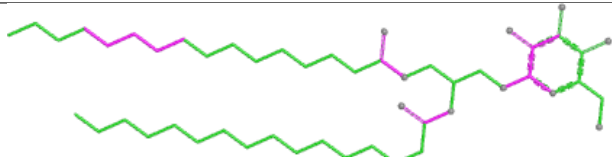
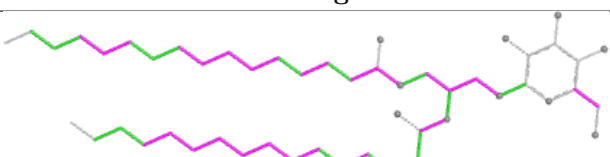
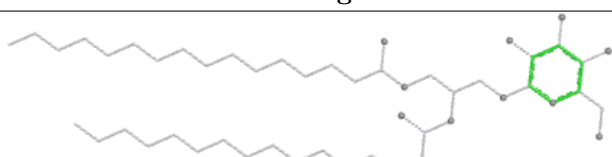


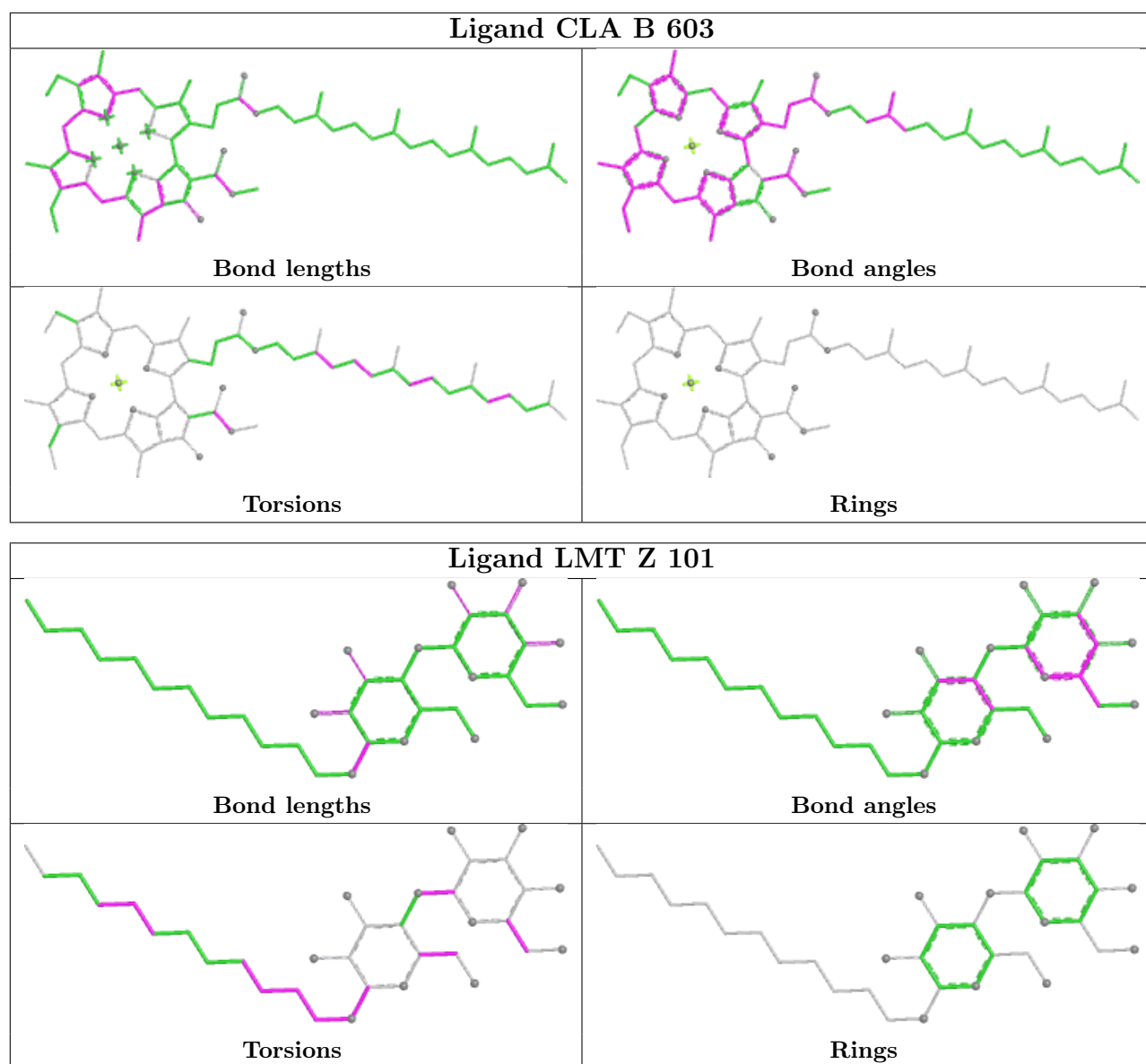


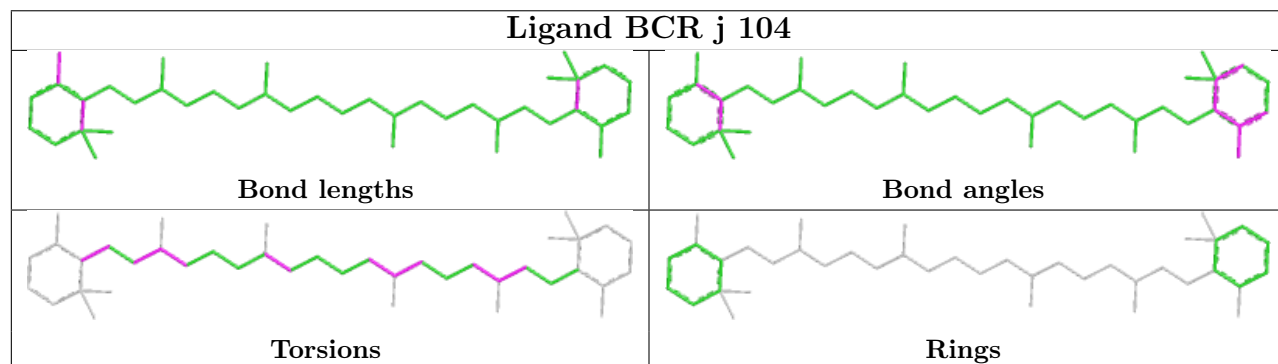
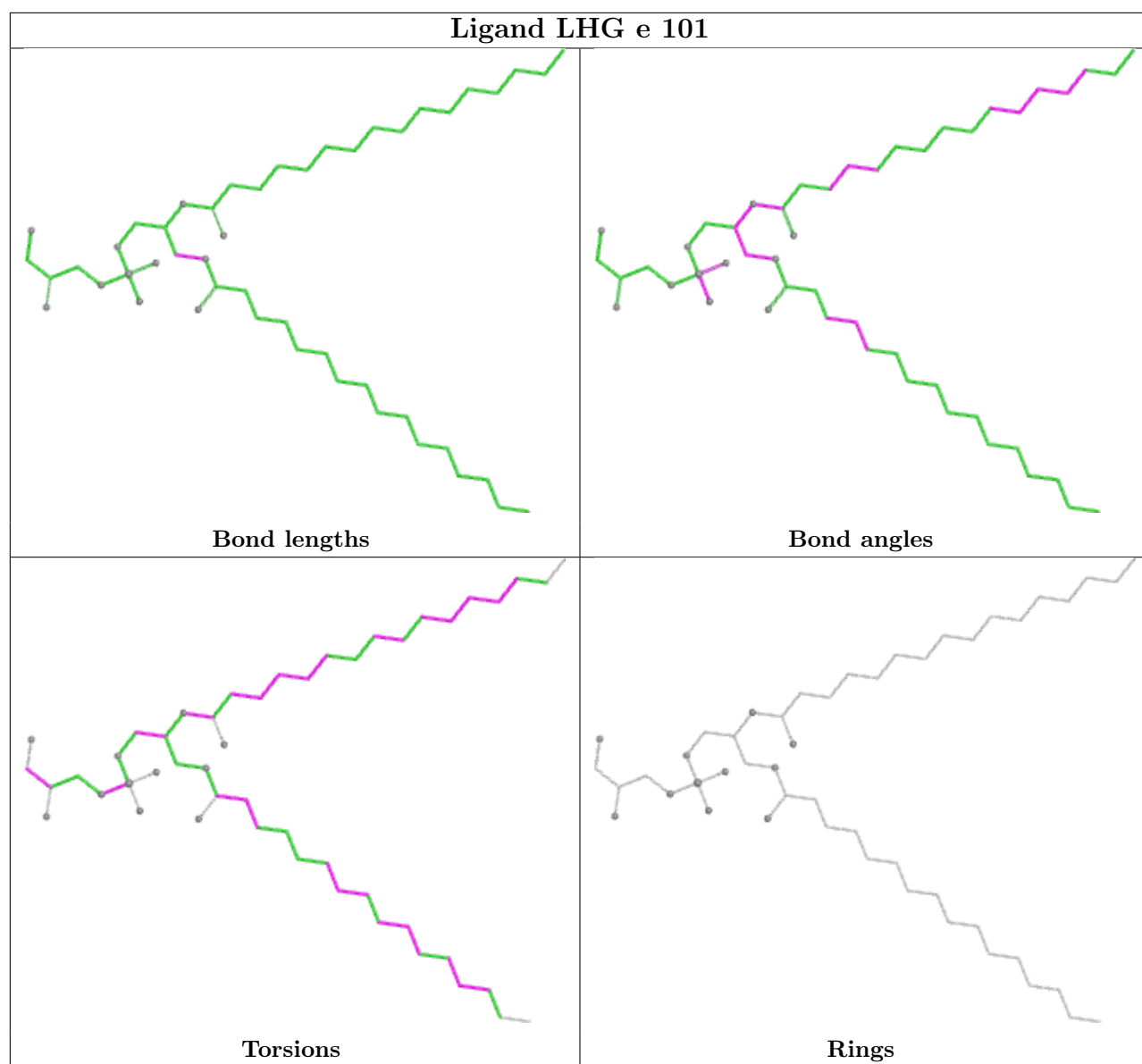
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

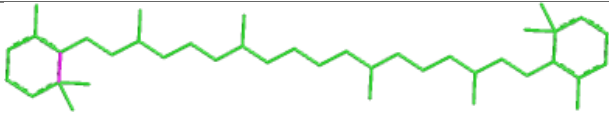
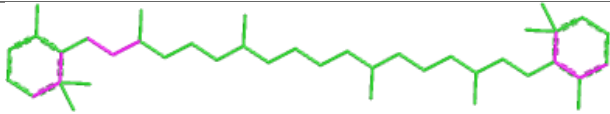
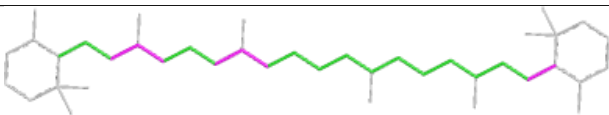
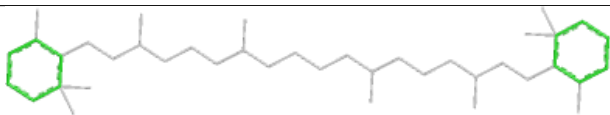


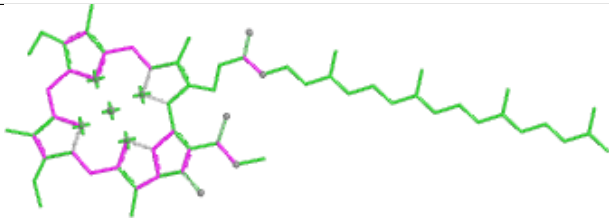
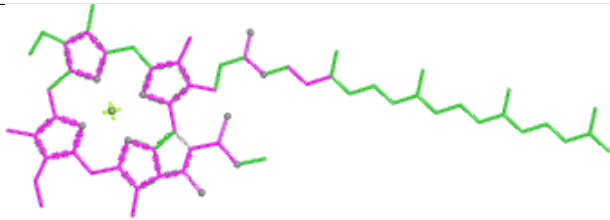
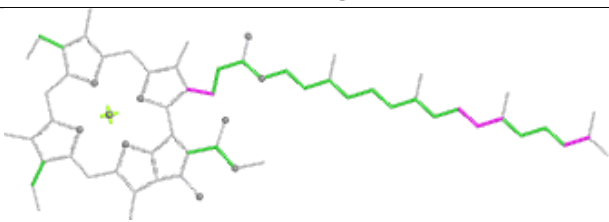
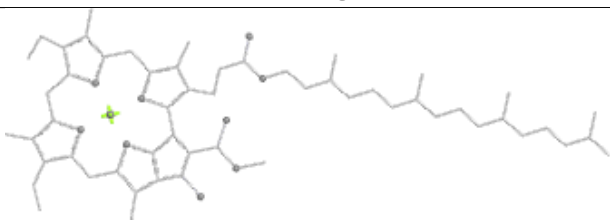


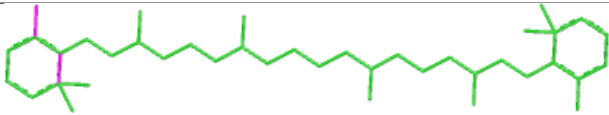
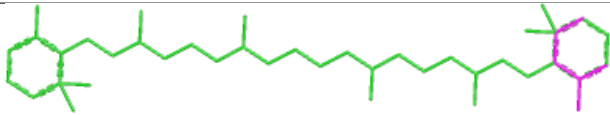
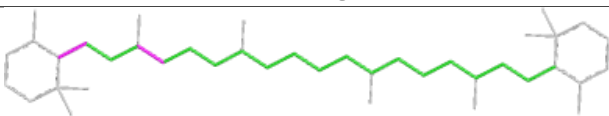
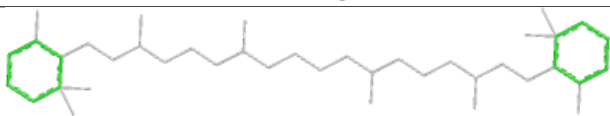
Ligand CLA b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 516	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 523	
 Bond lengths	 Bond angles
 Torsions	 Rings

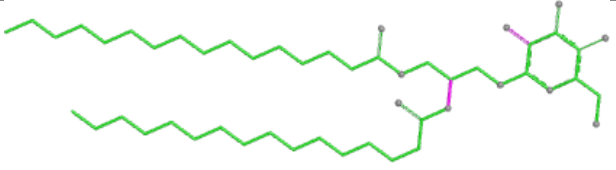
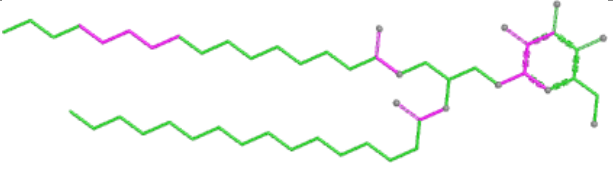
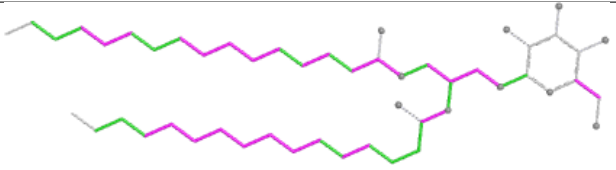
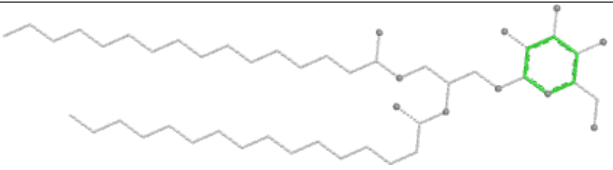
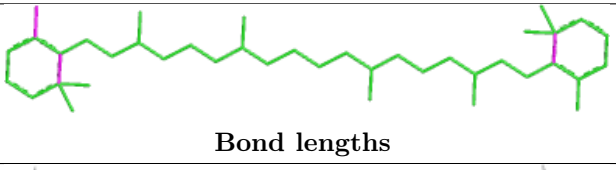
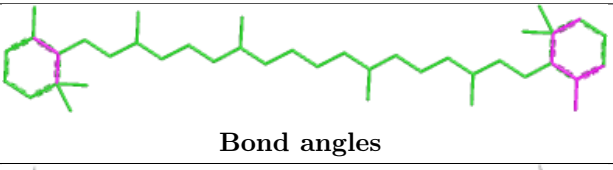
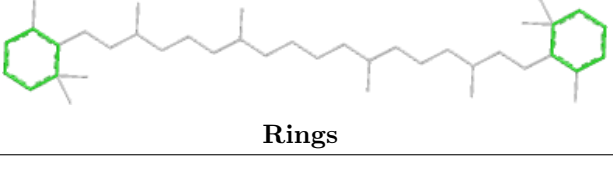
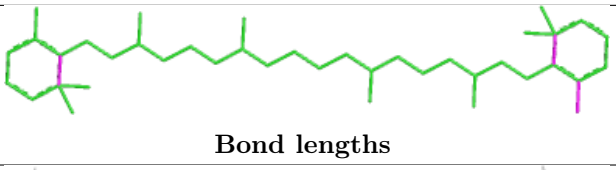
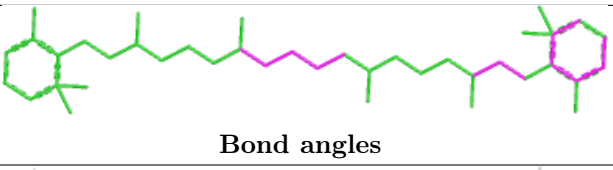
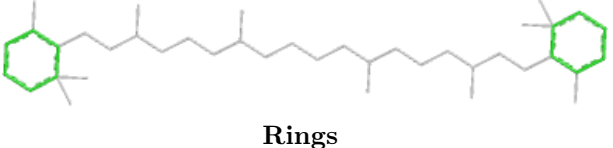


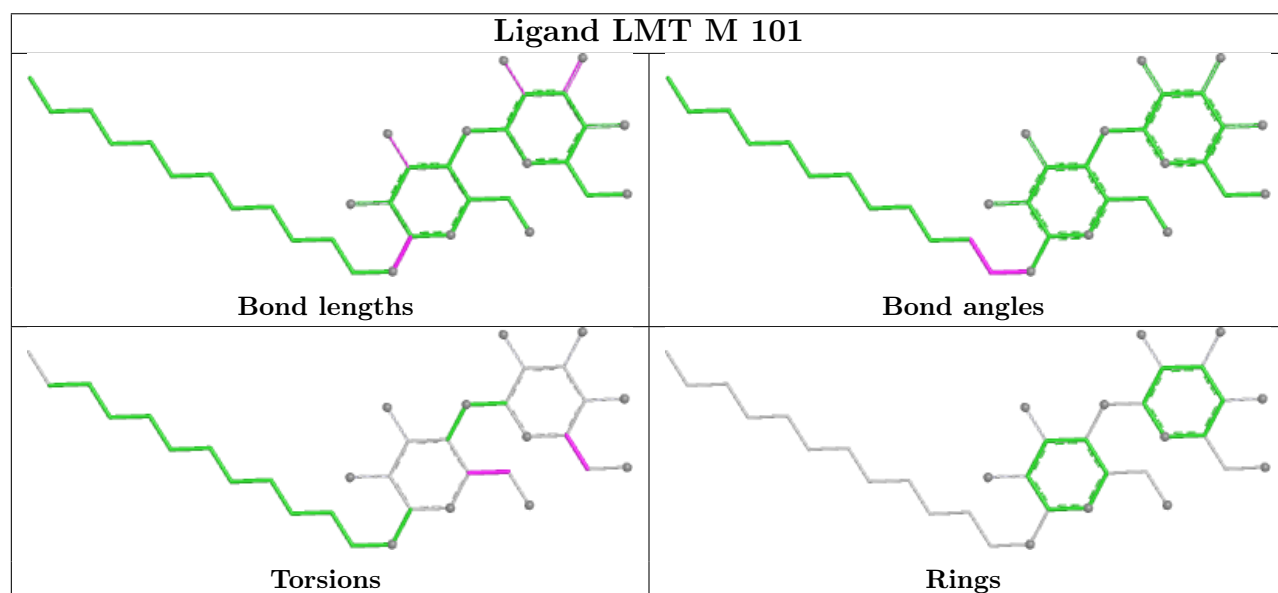
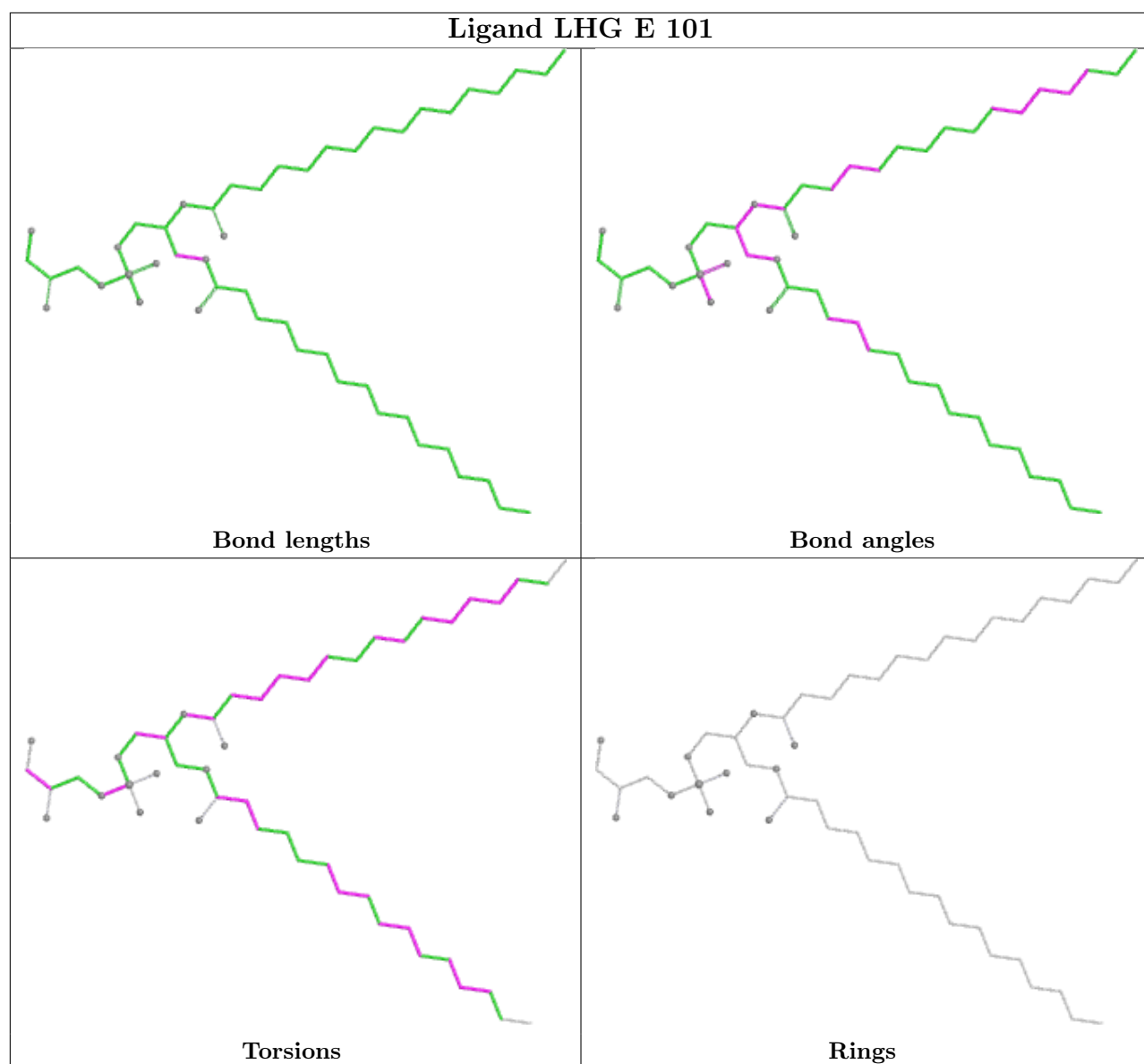


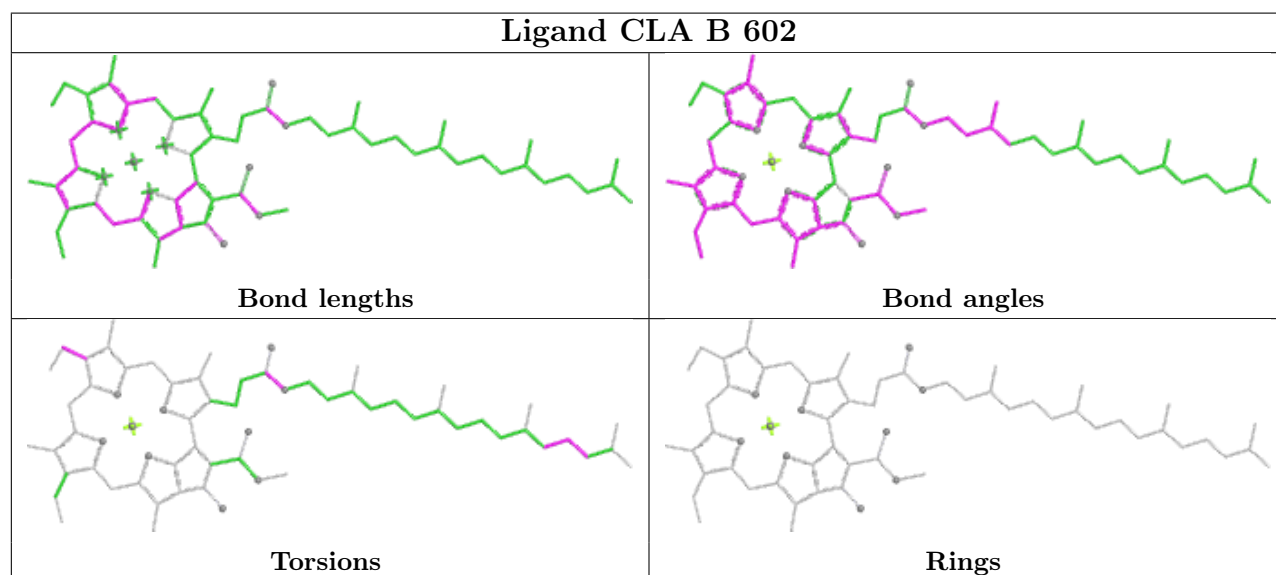
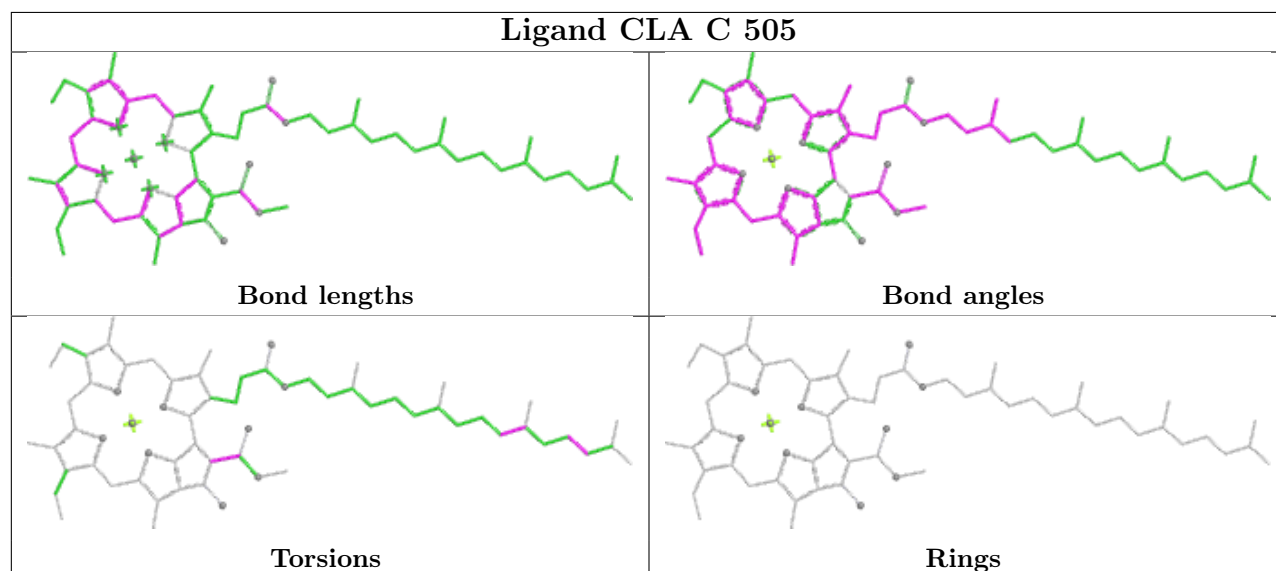
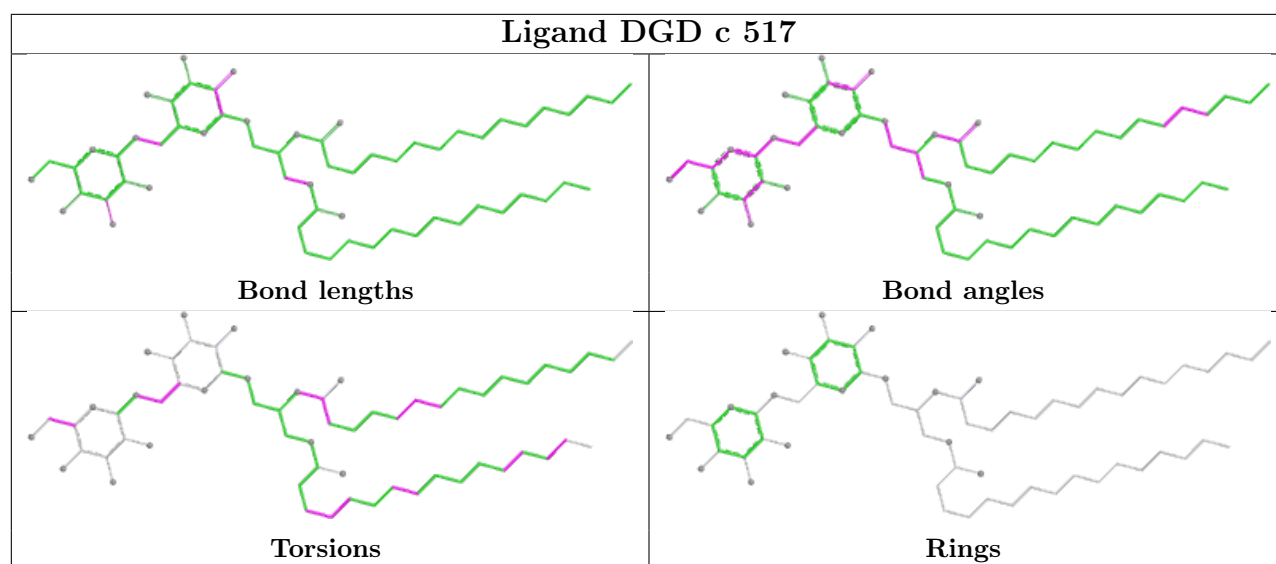
Ligand BCR c 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

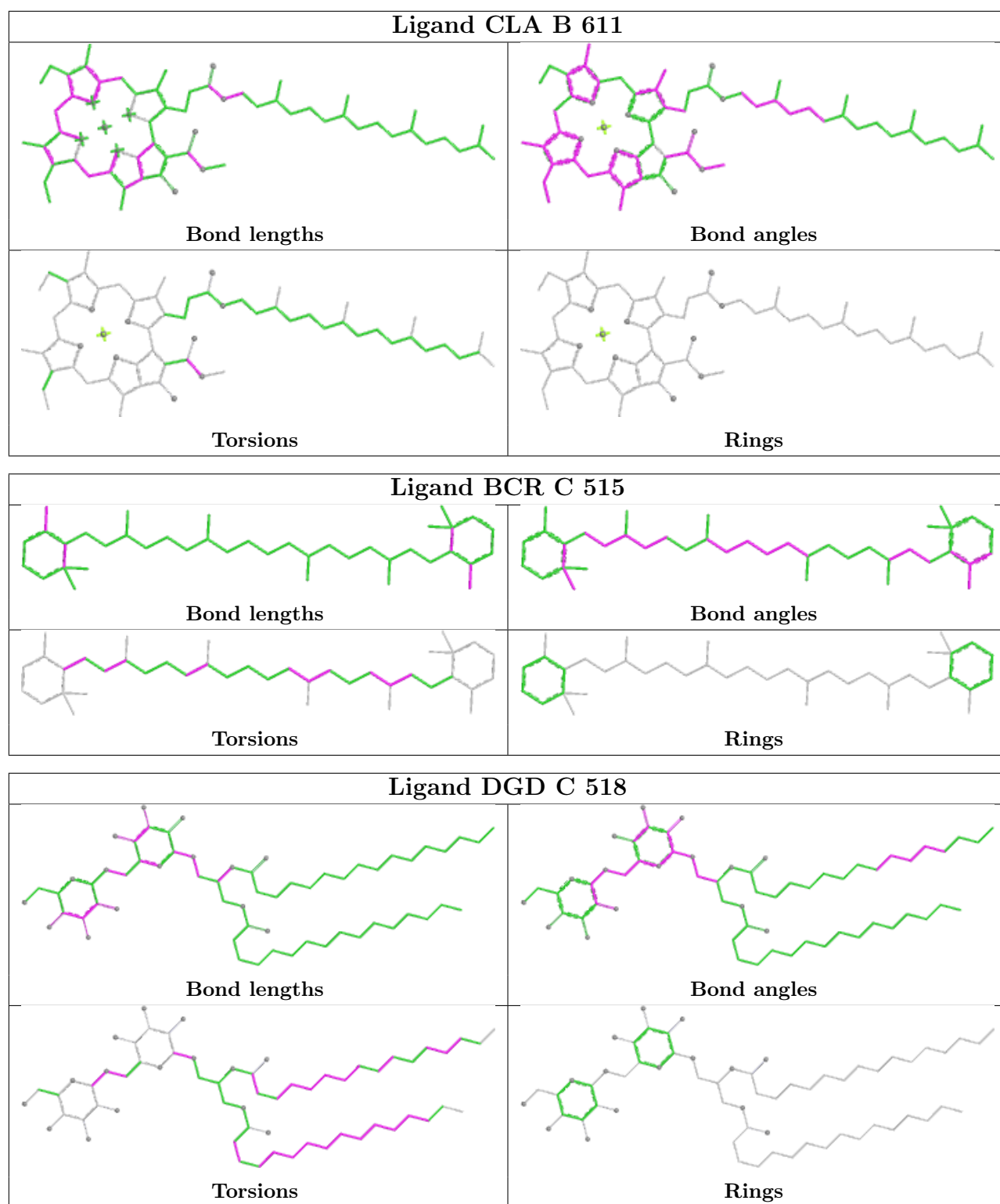
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

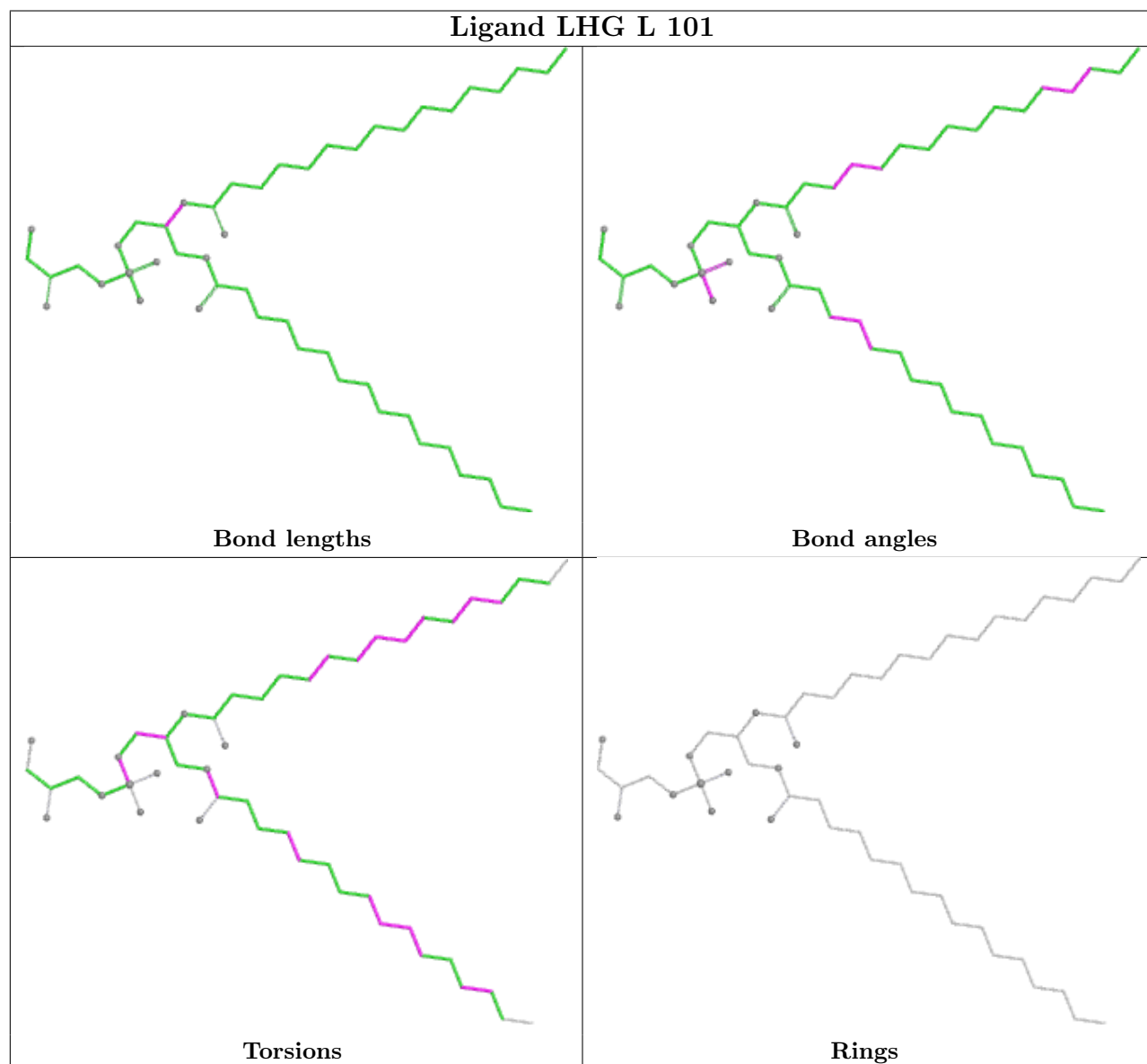
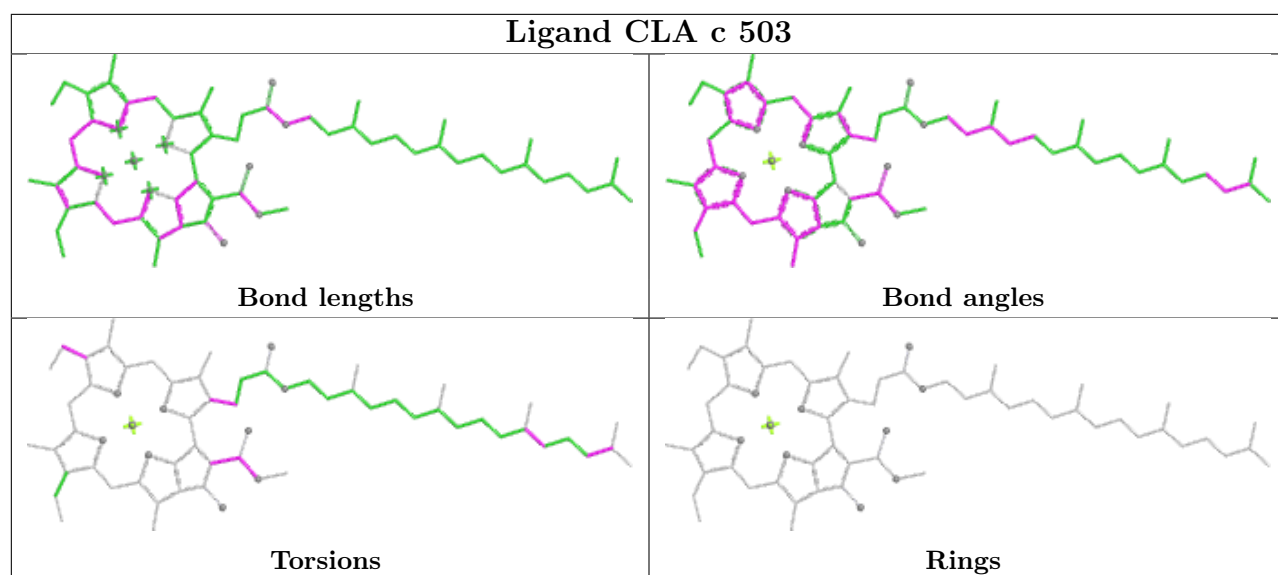
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

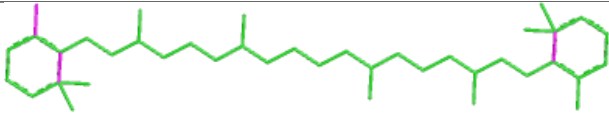
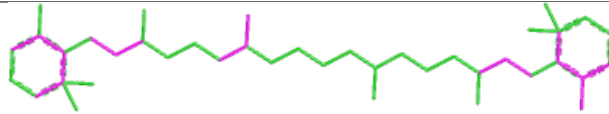
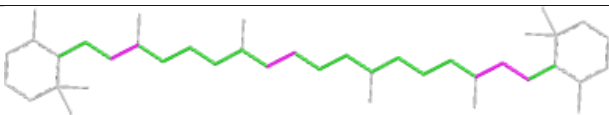
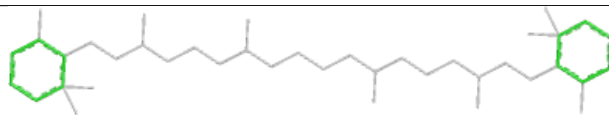
Ligand LMG C 523	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR J 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

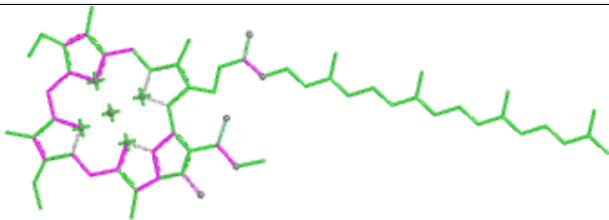
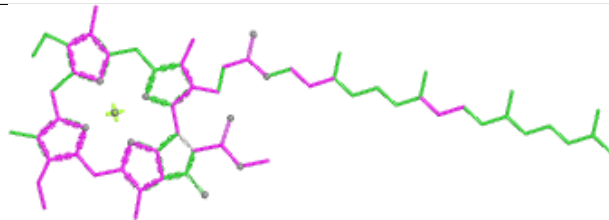
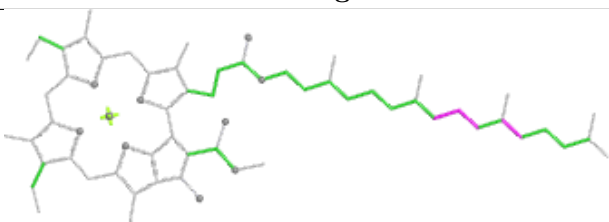
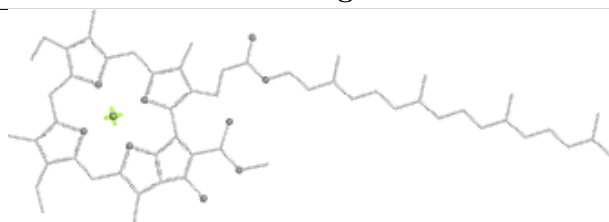


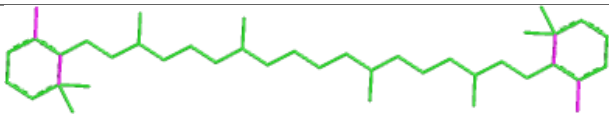
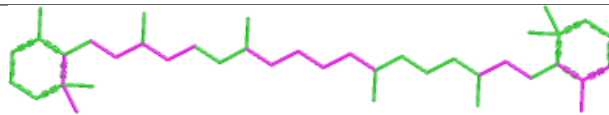
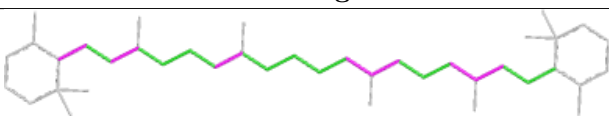
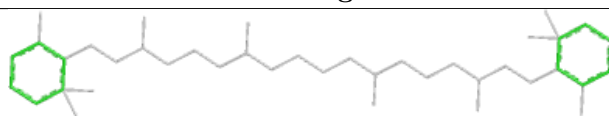


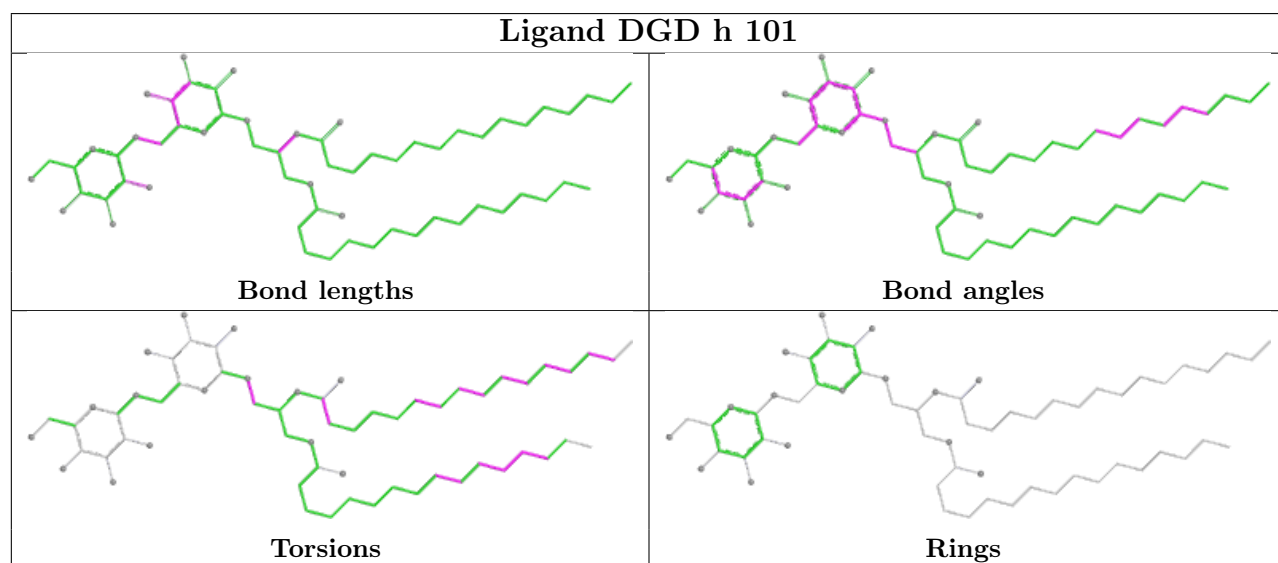
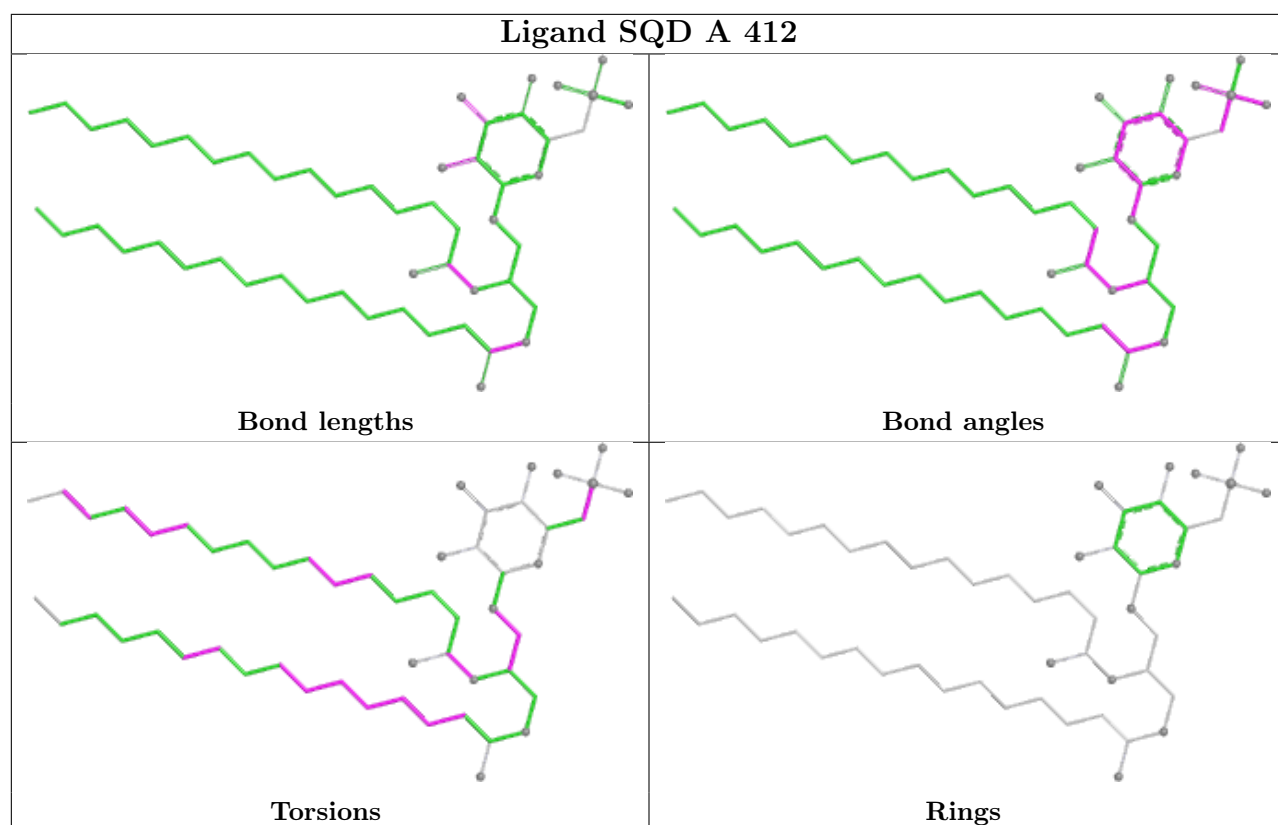


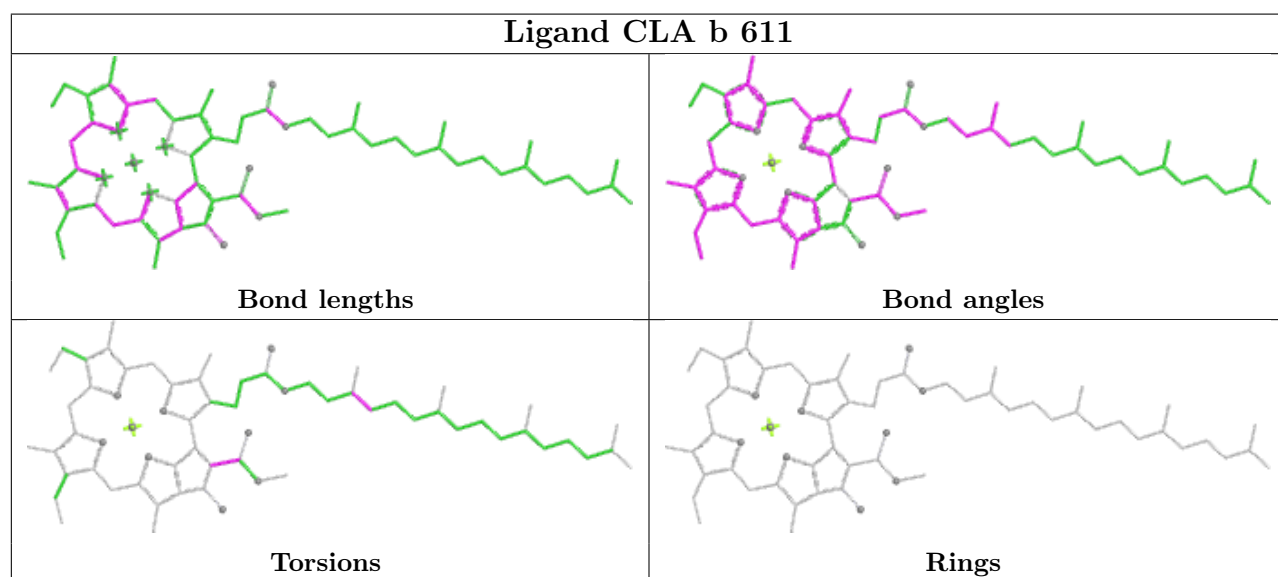
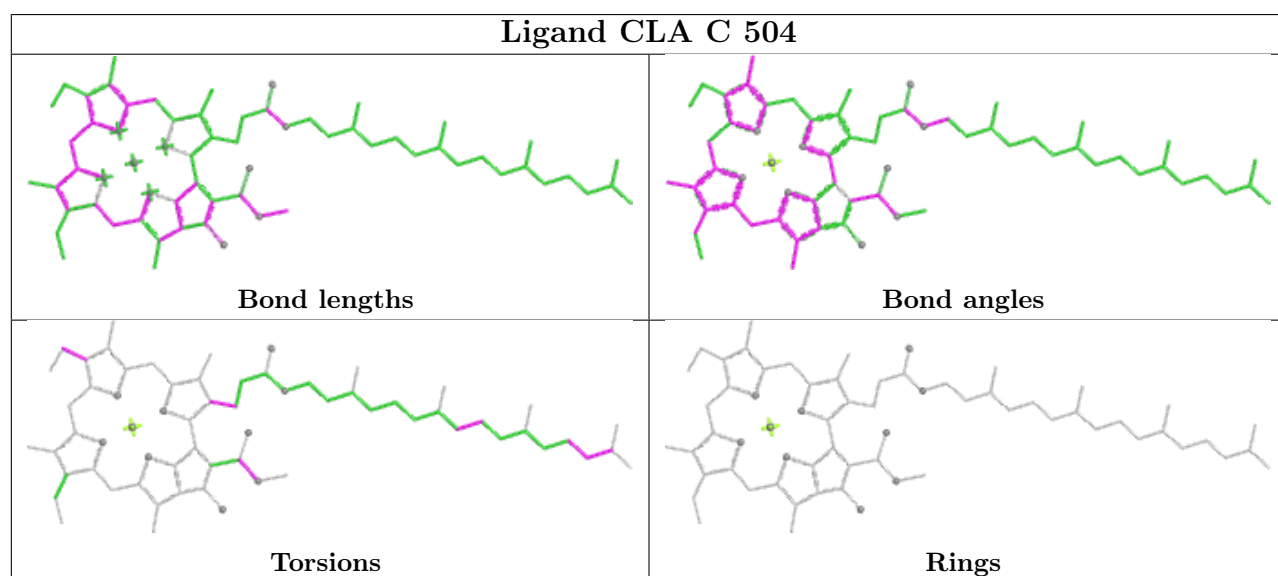
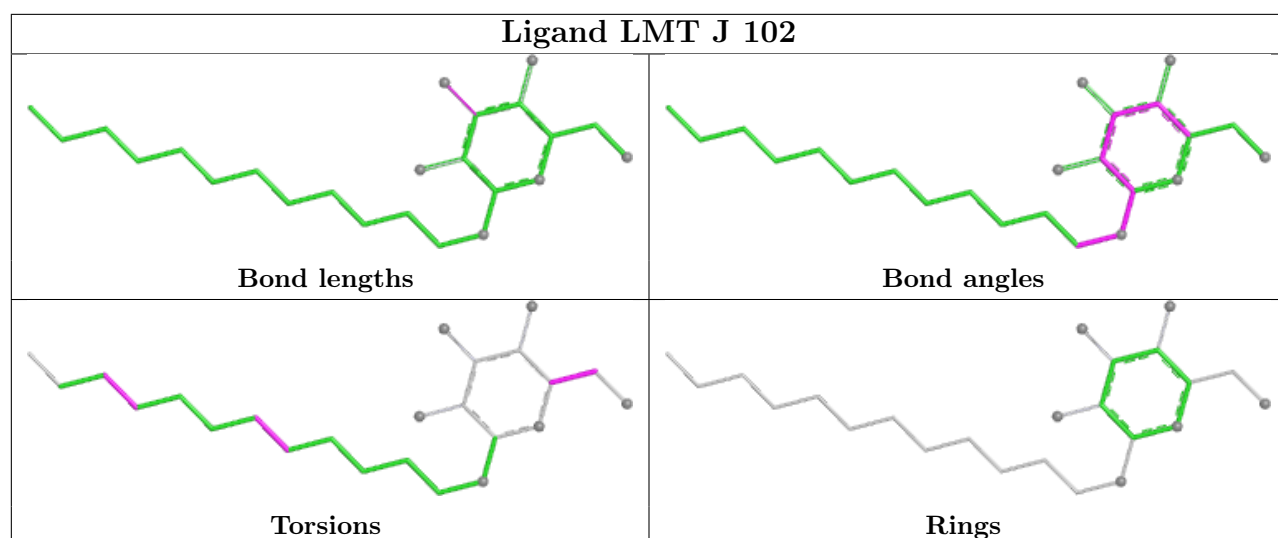


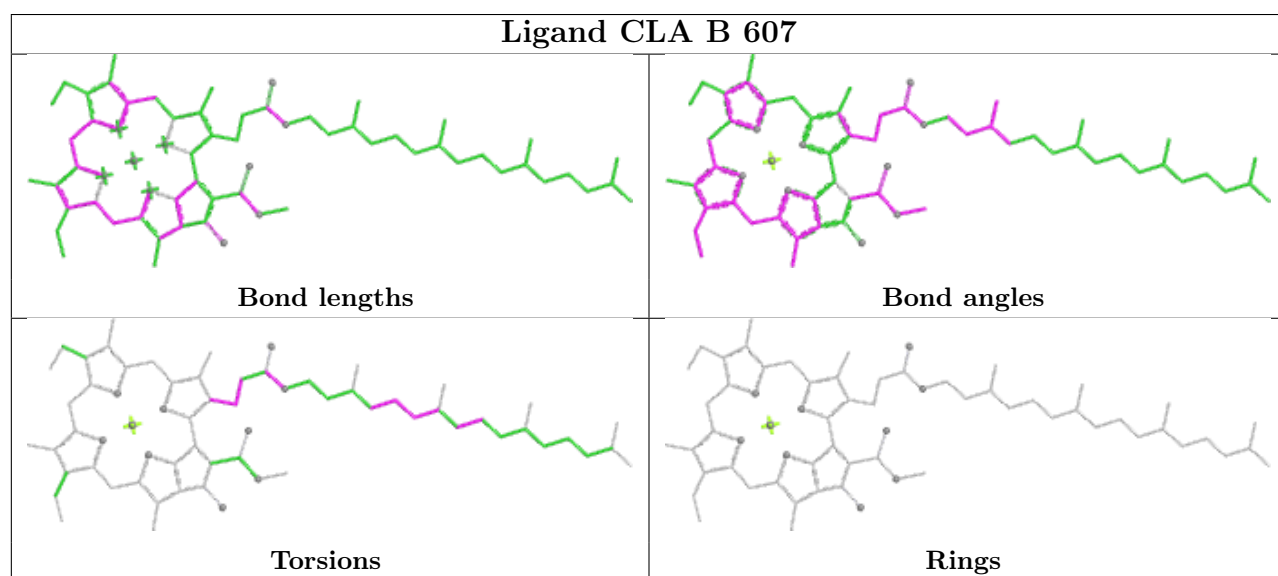
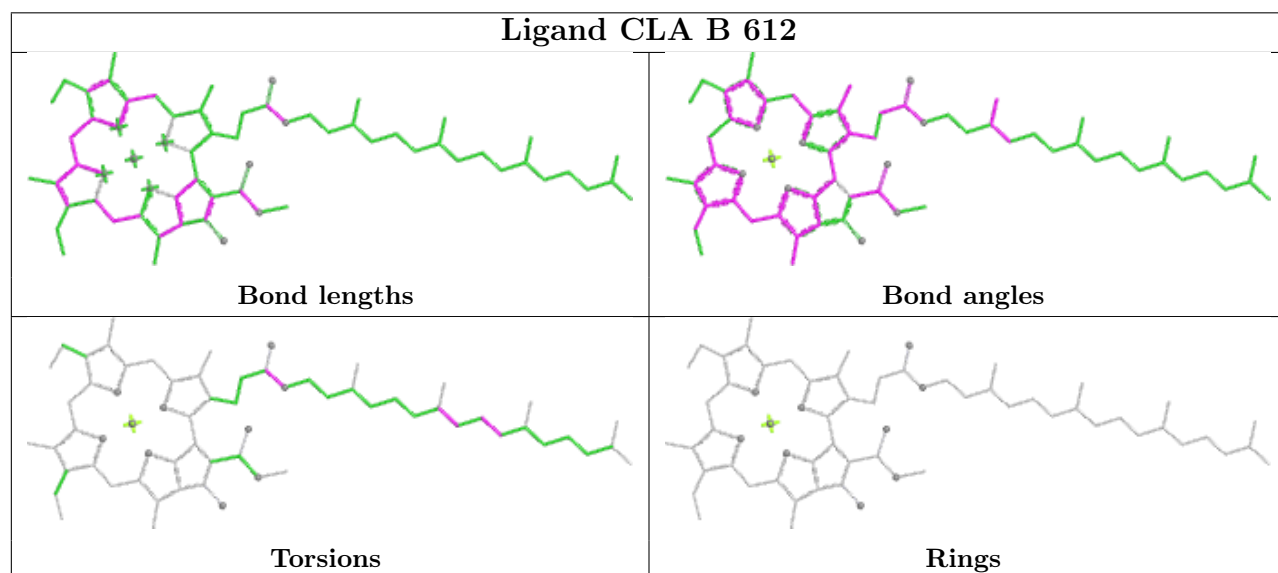
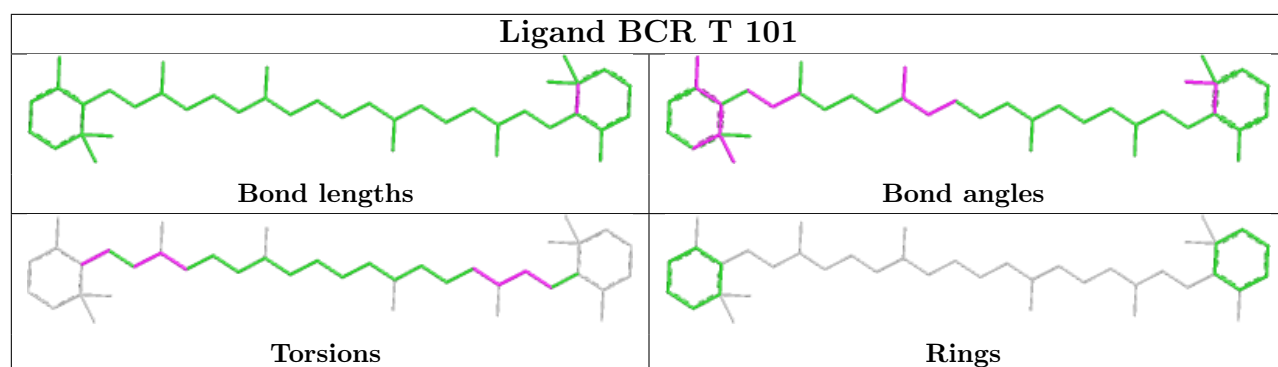
Ligand BCR d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

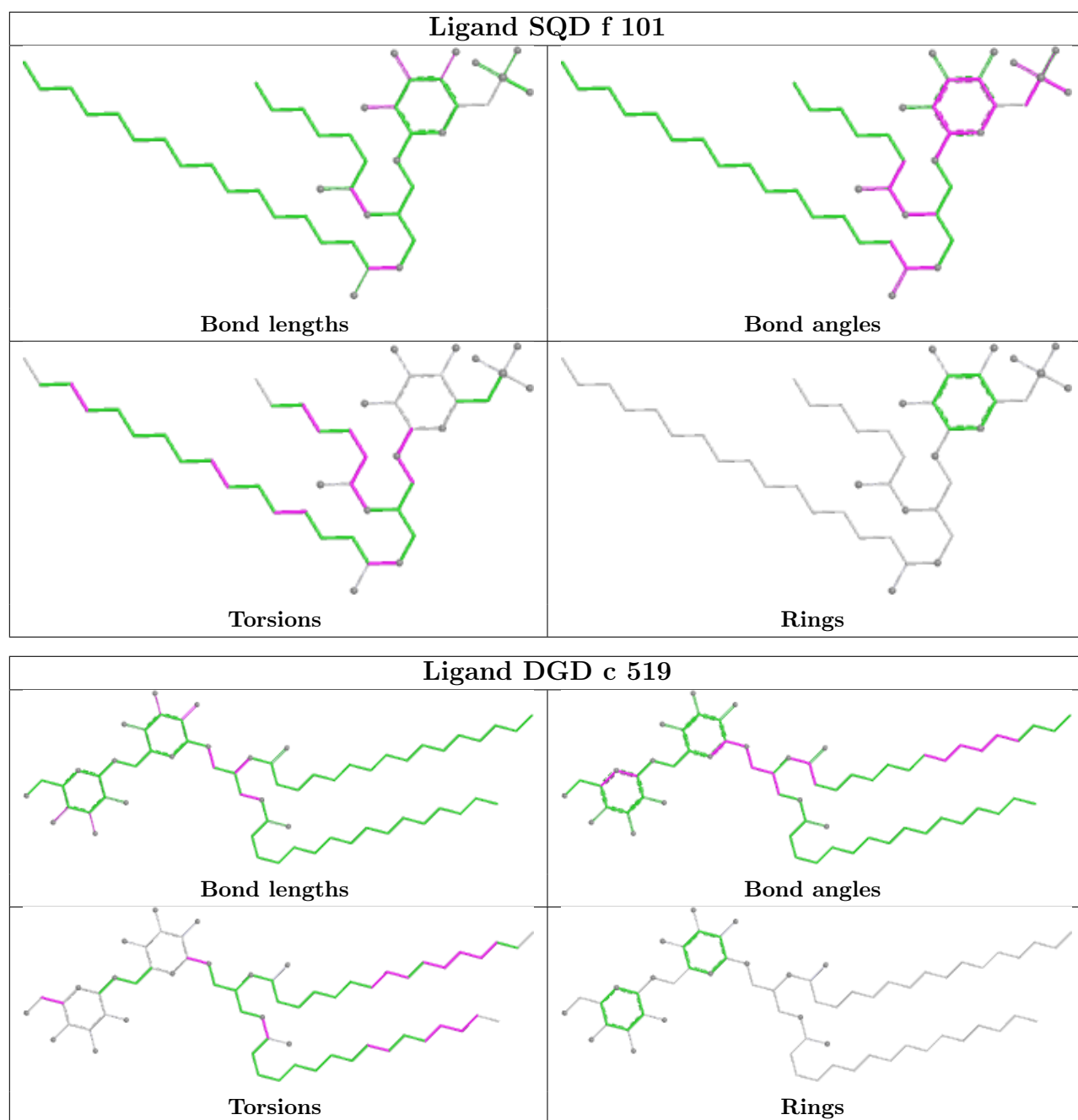
Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

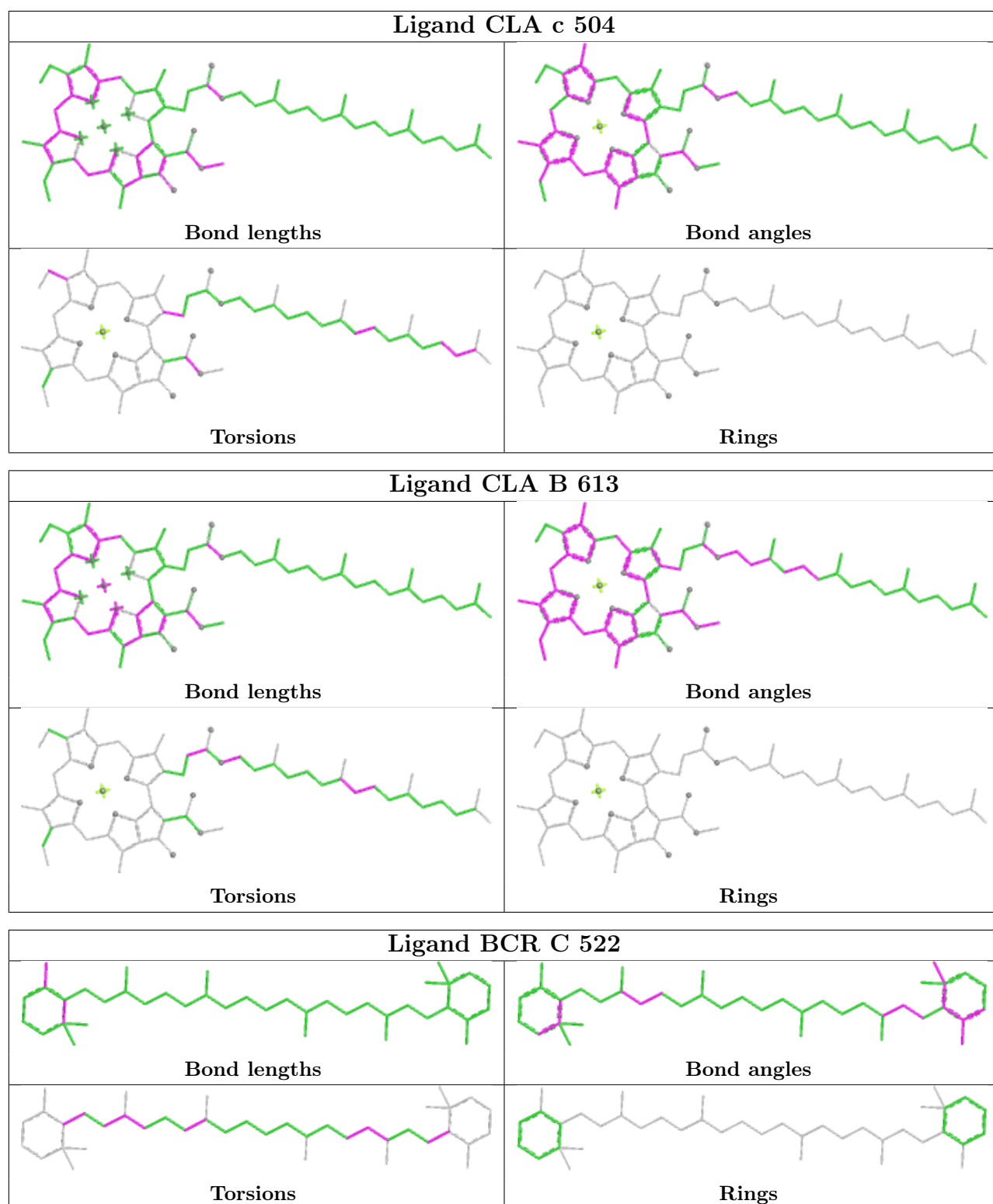
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

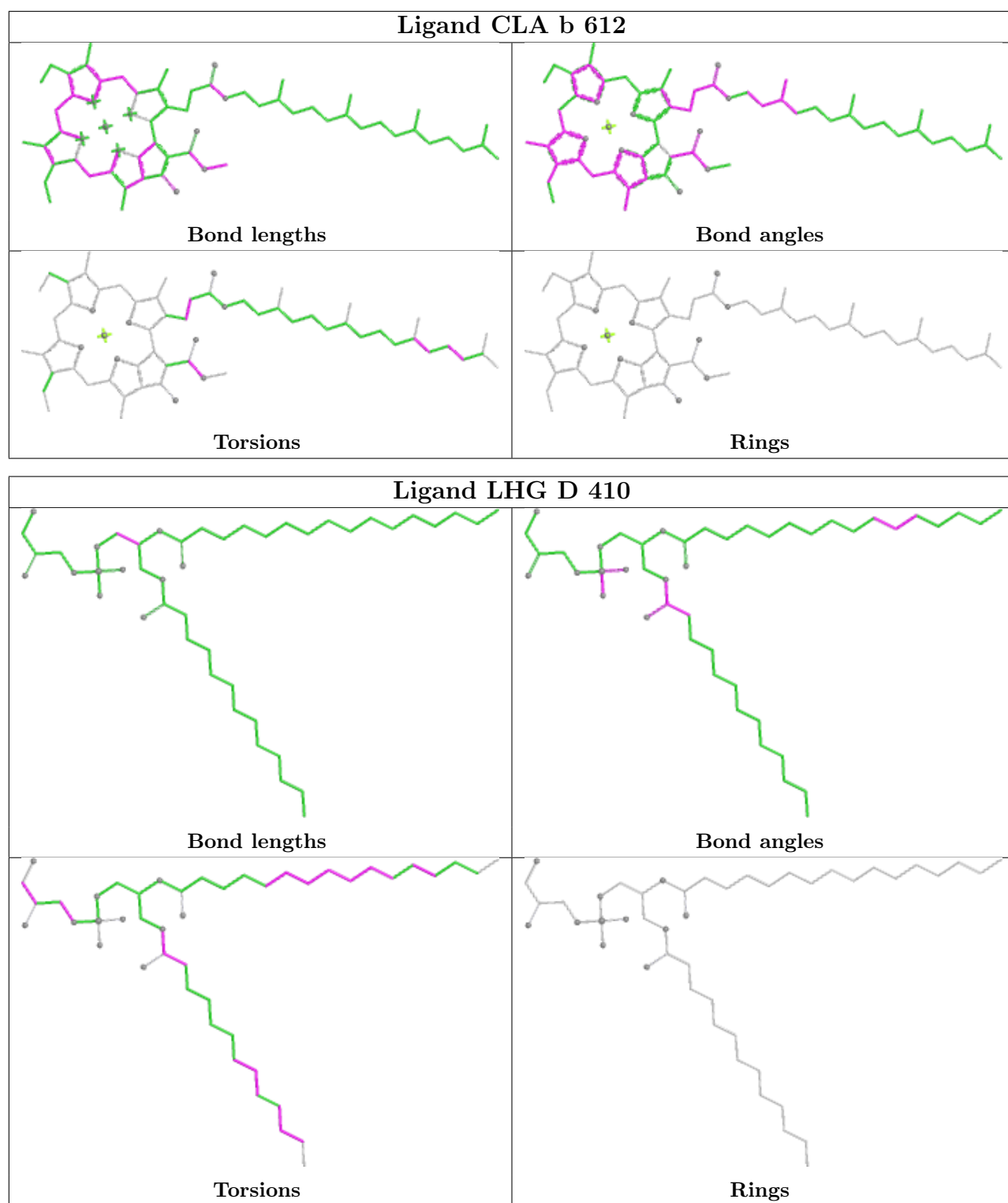


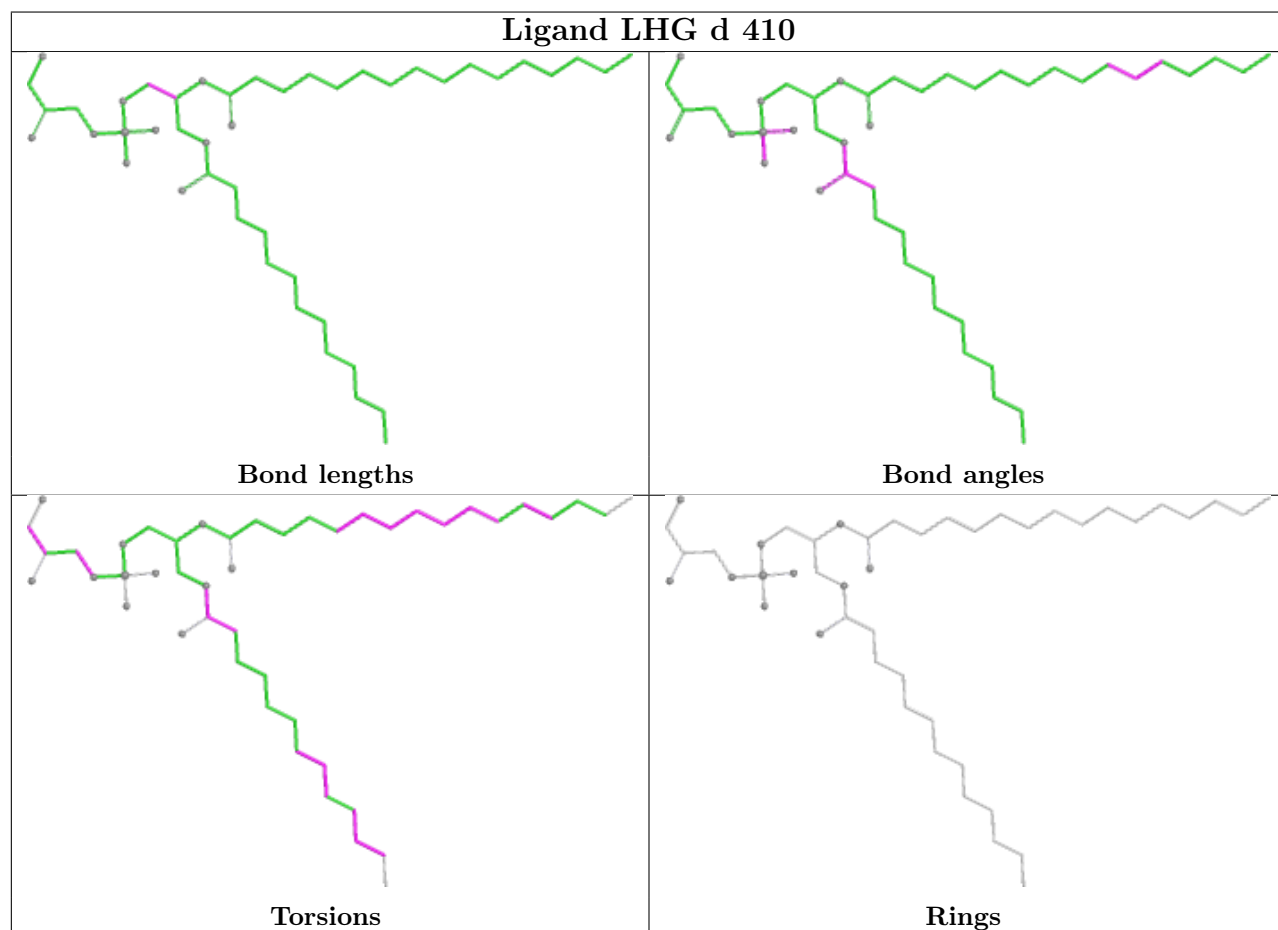
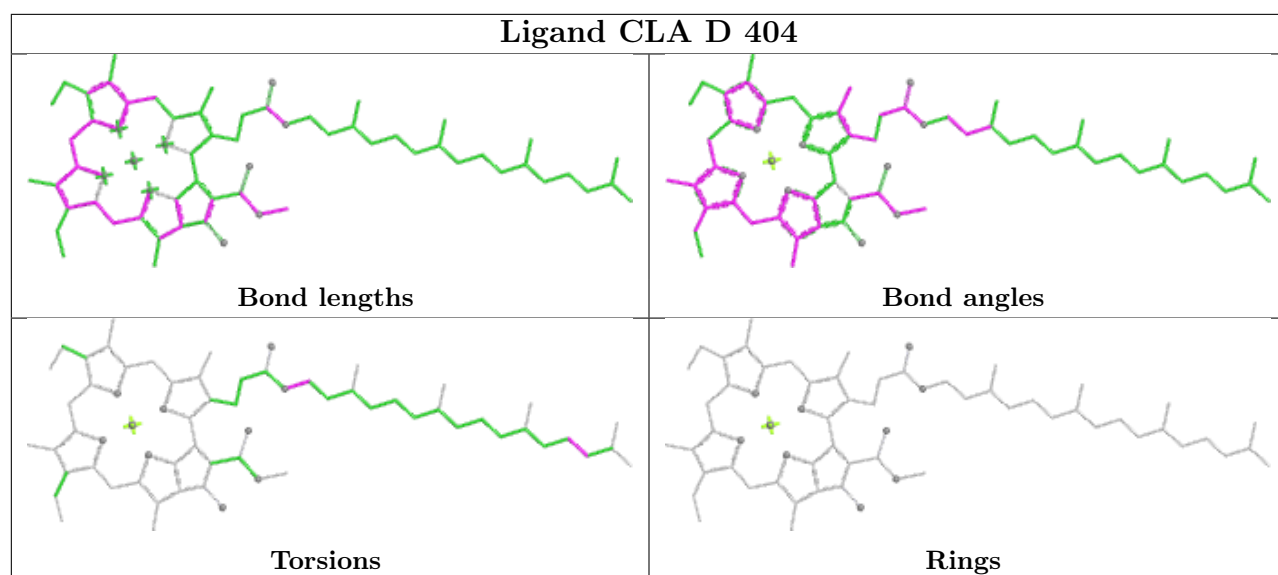


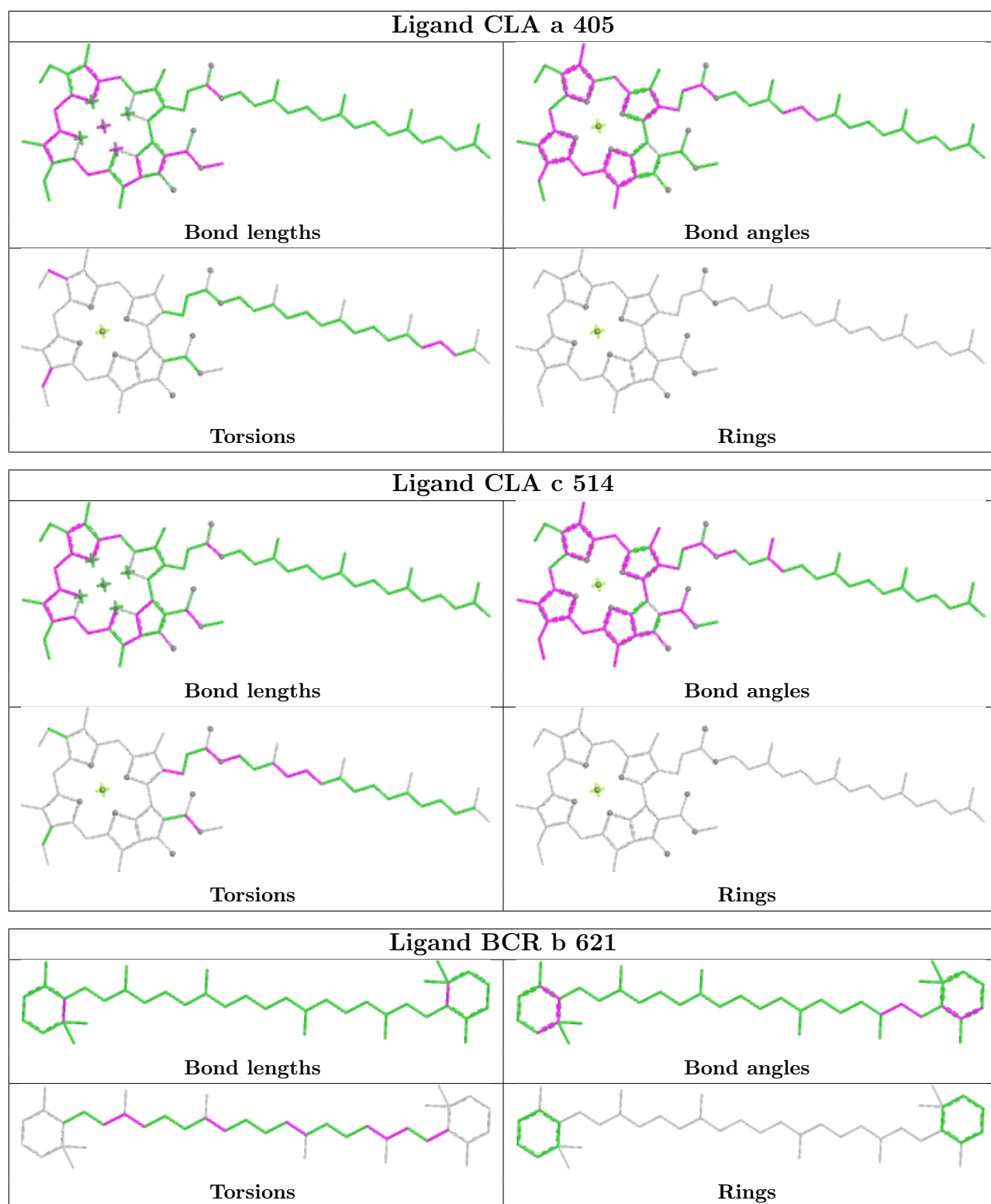


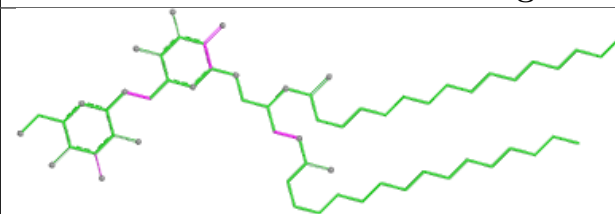
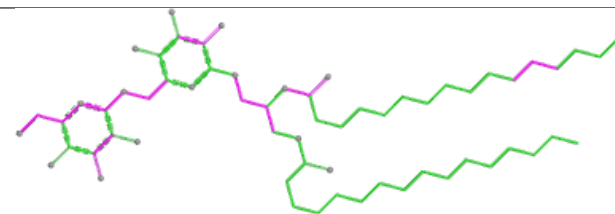
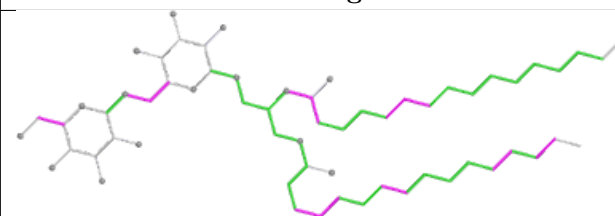
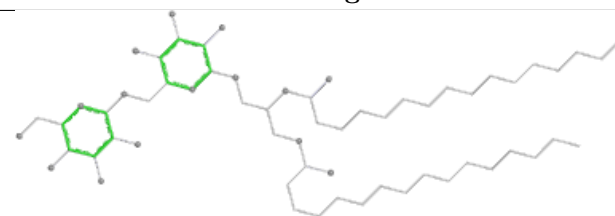


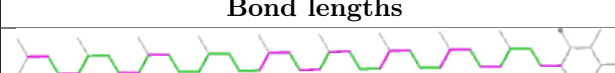
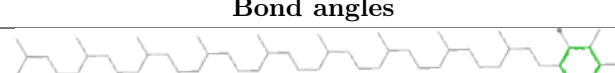


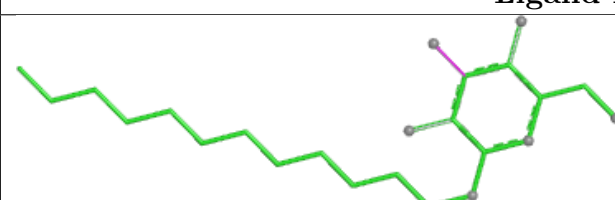
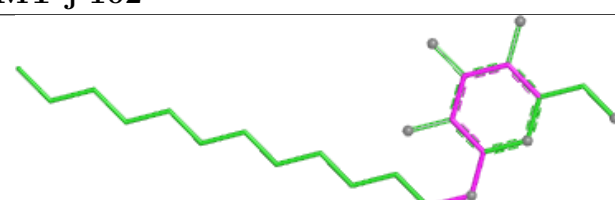
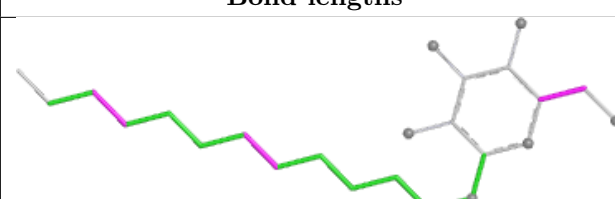
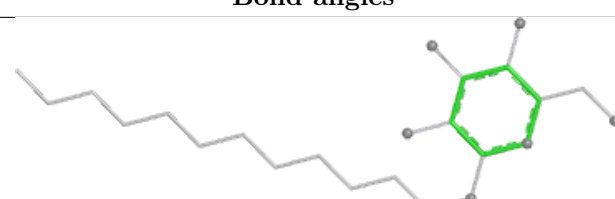


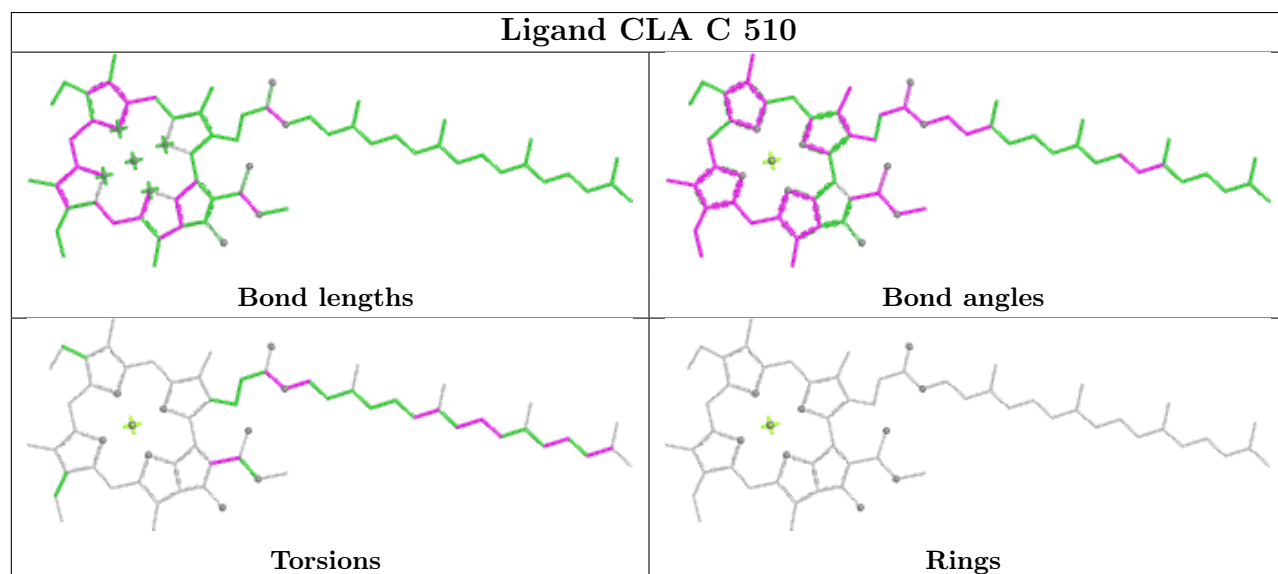
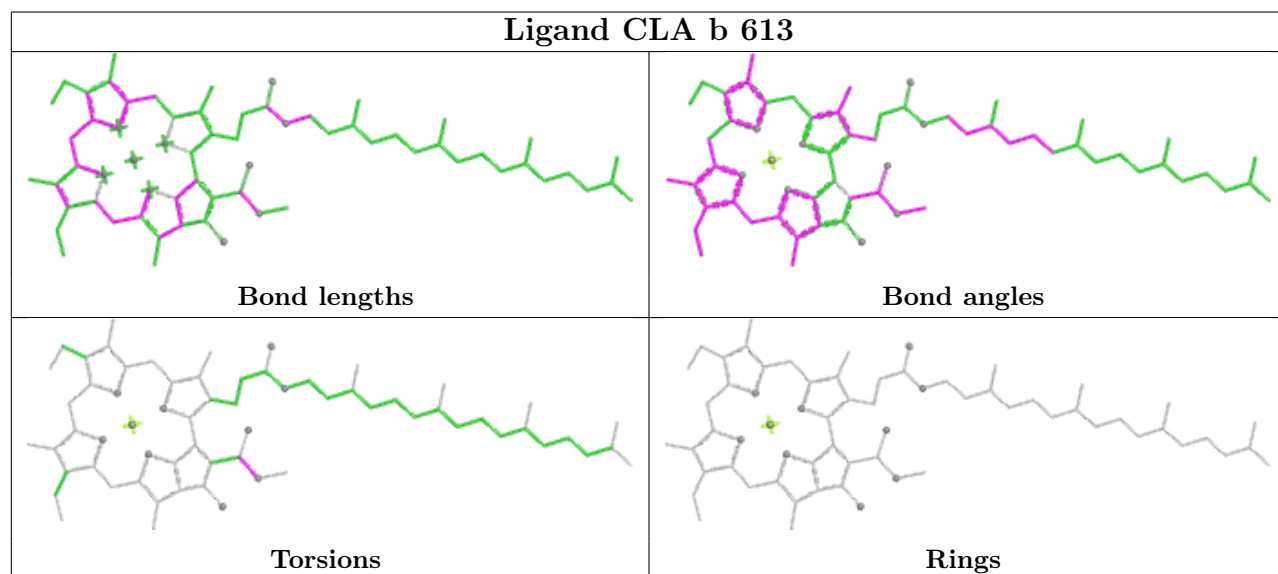
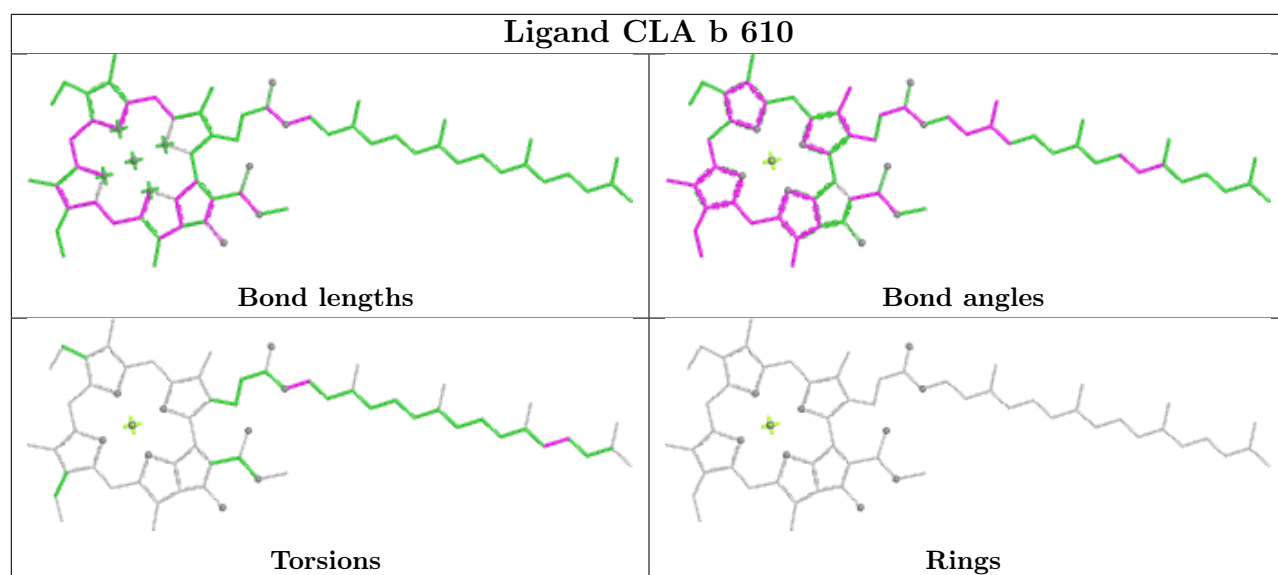


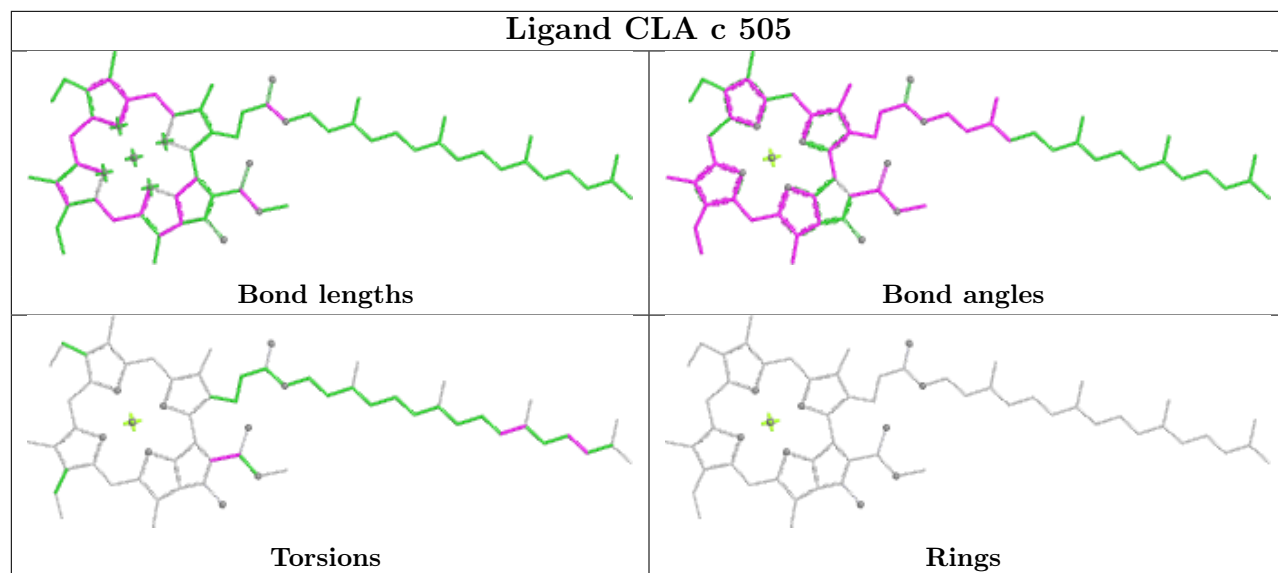
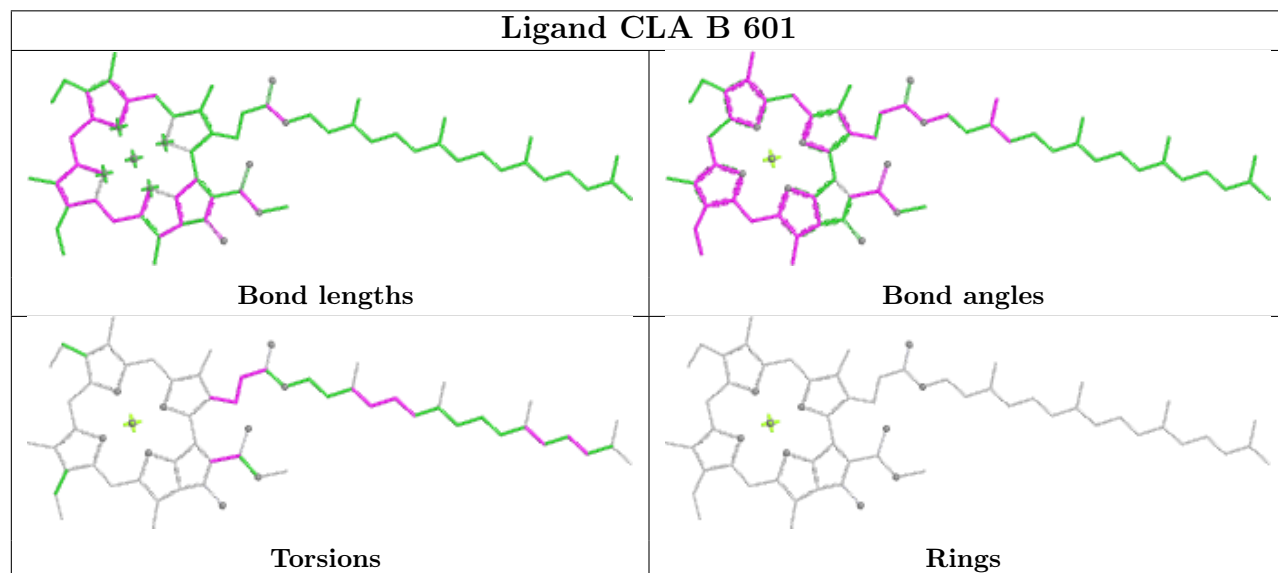
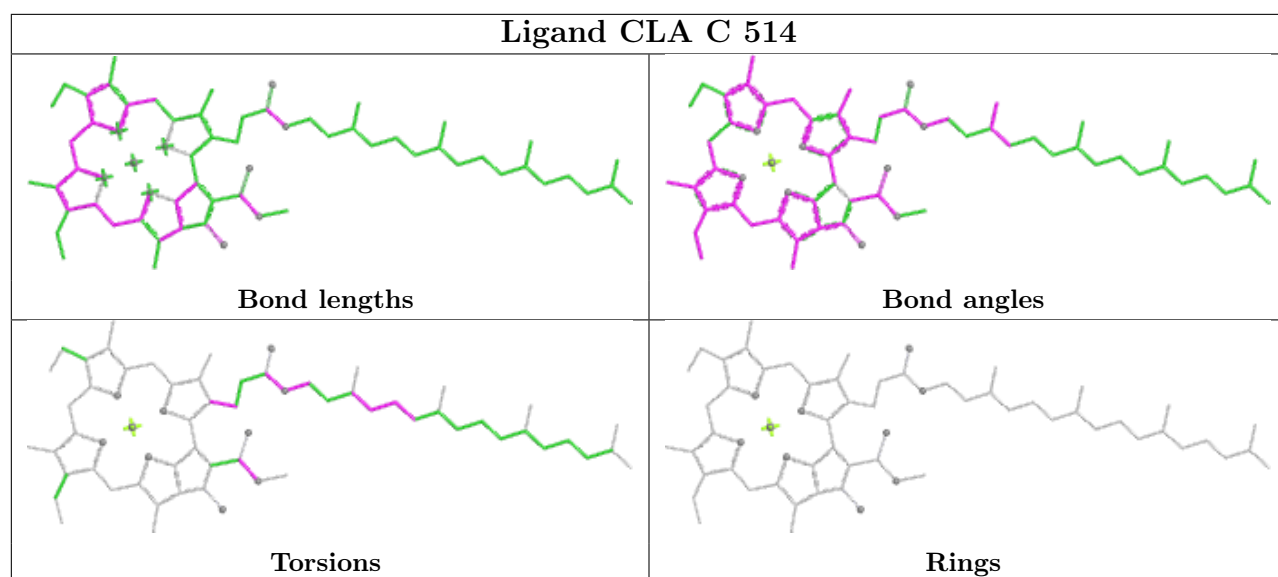


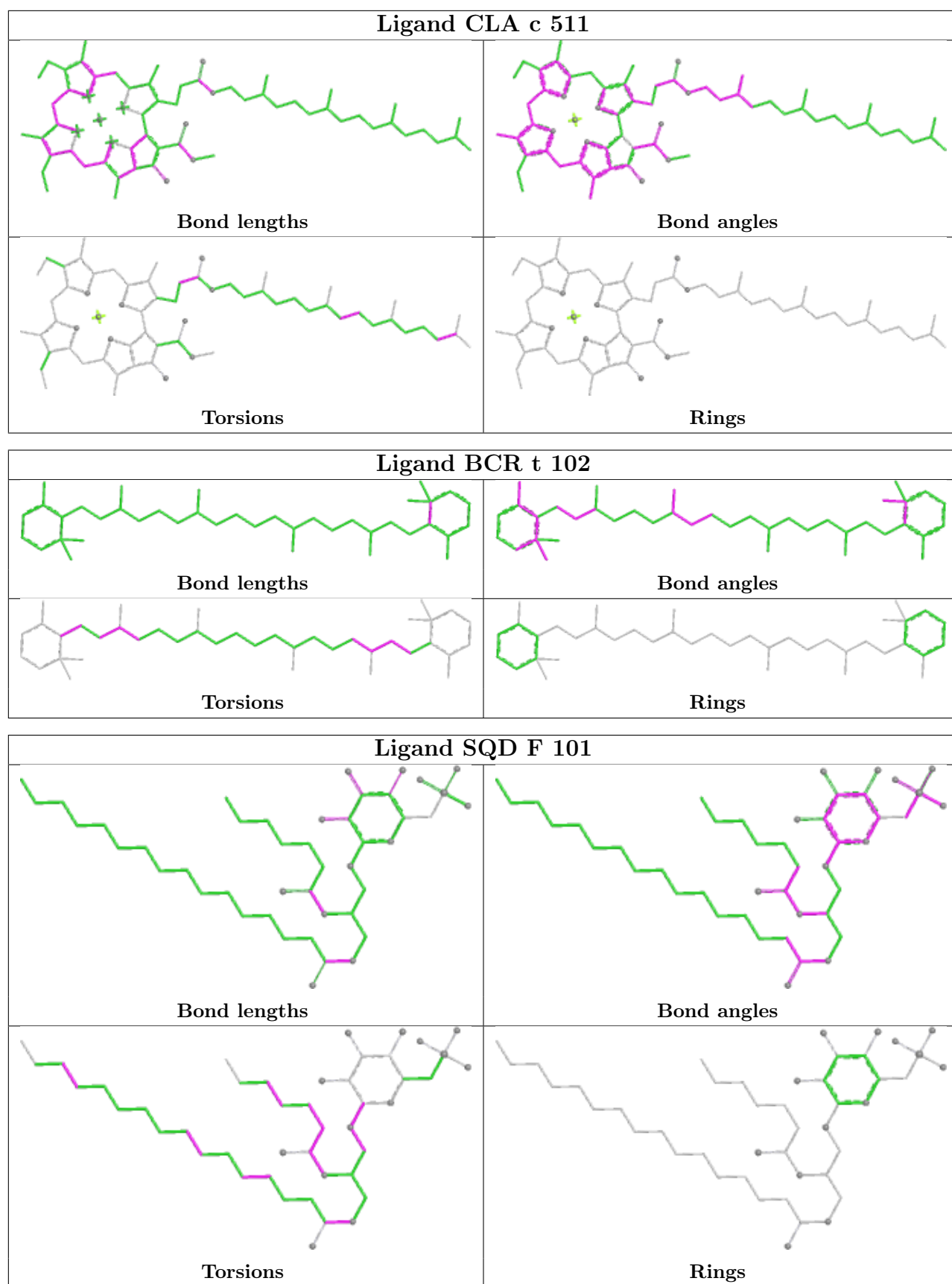
Ligand DGD C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

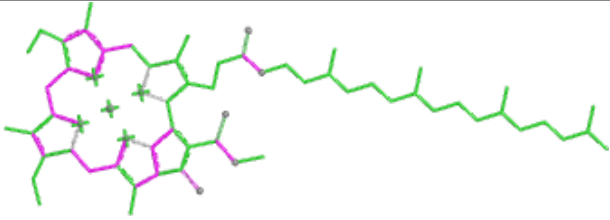
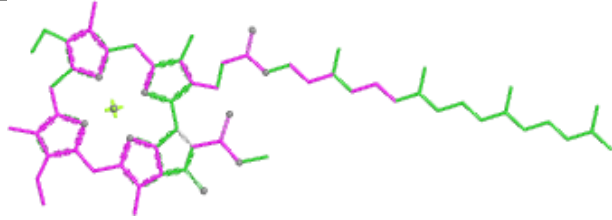
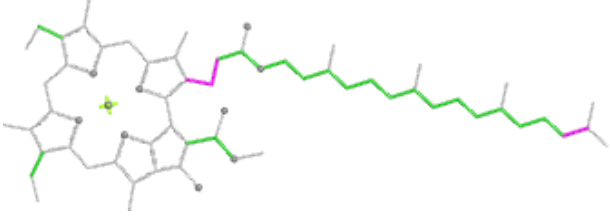
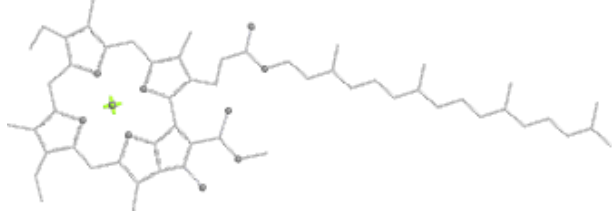
Ligand PL9 a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

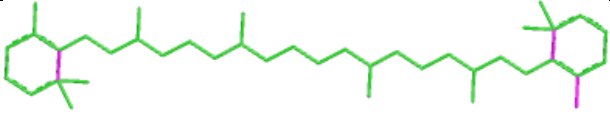
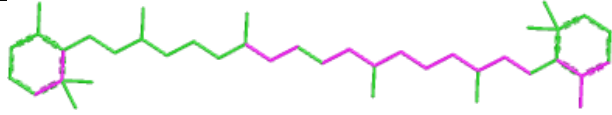
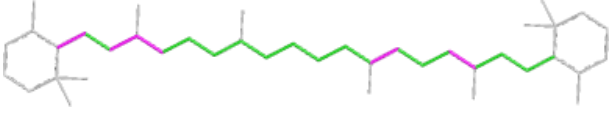
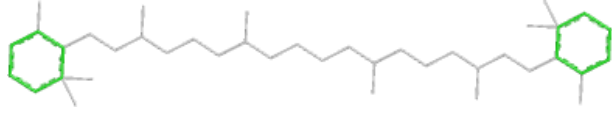
Ligand LMT j 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

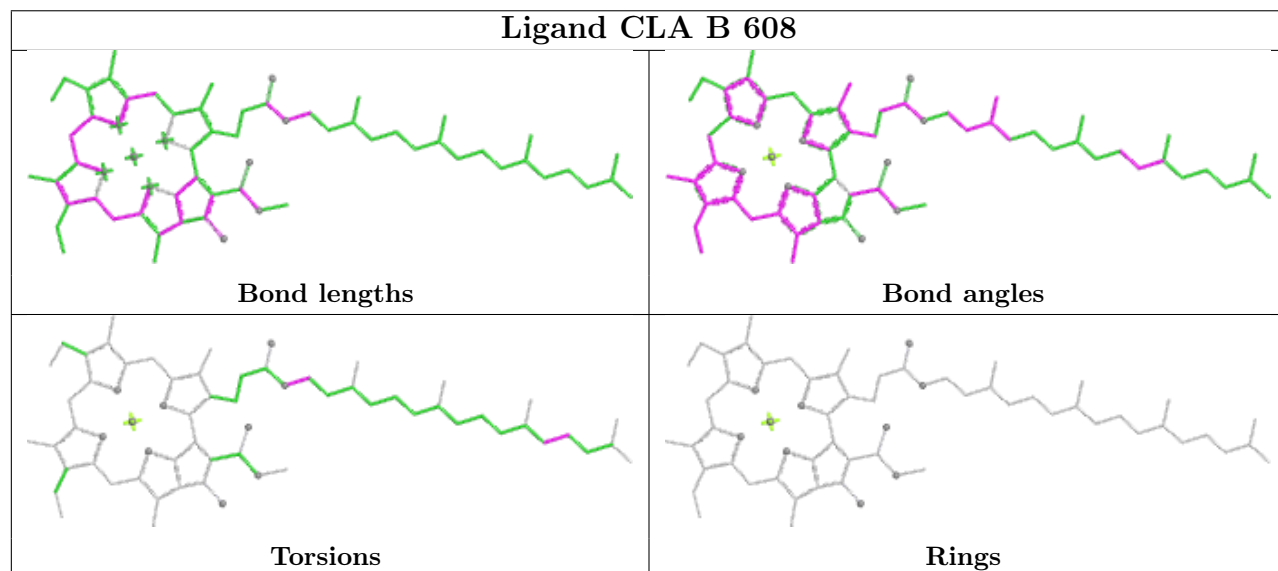
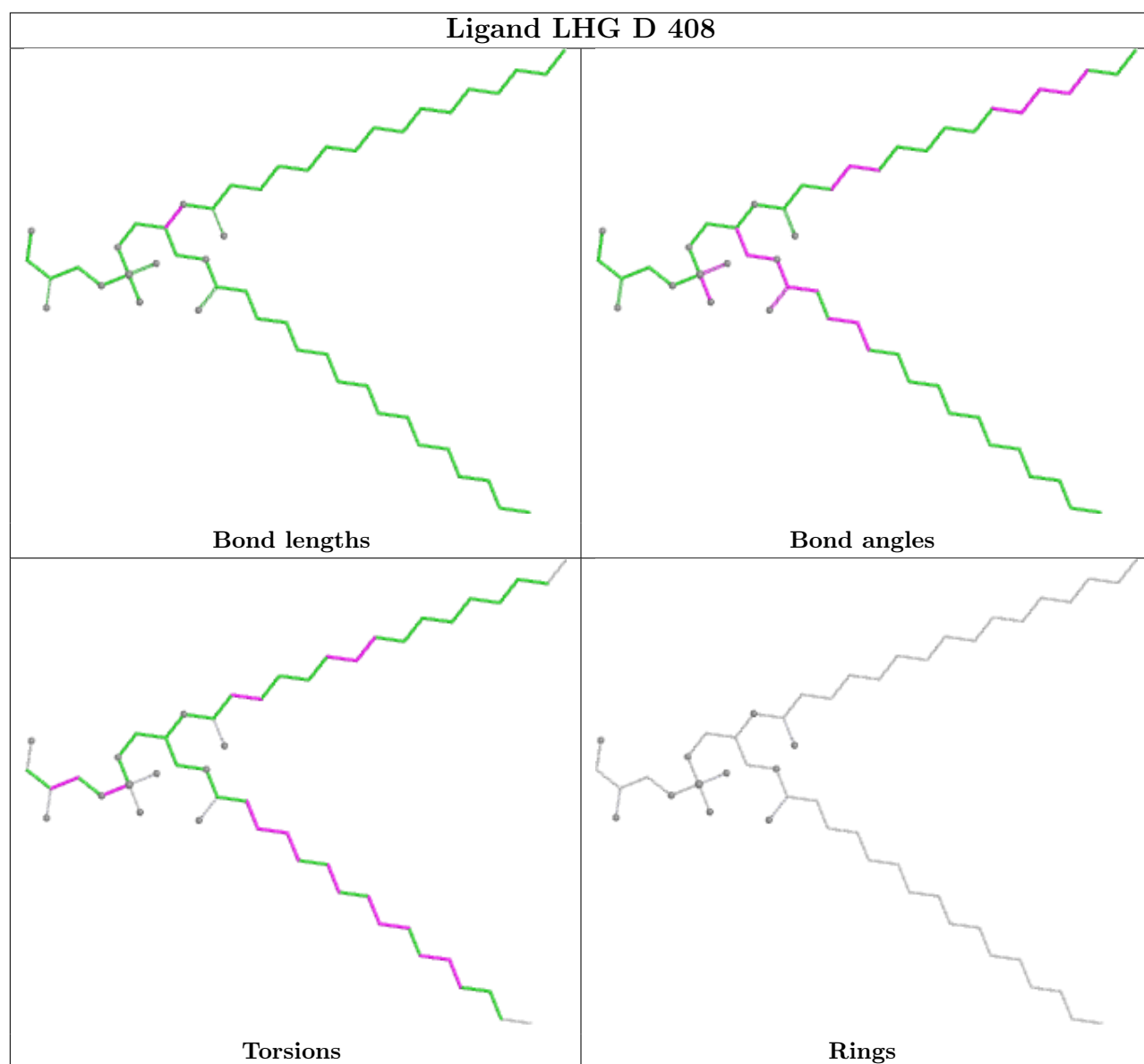


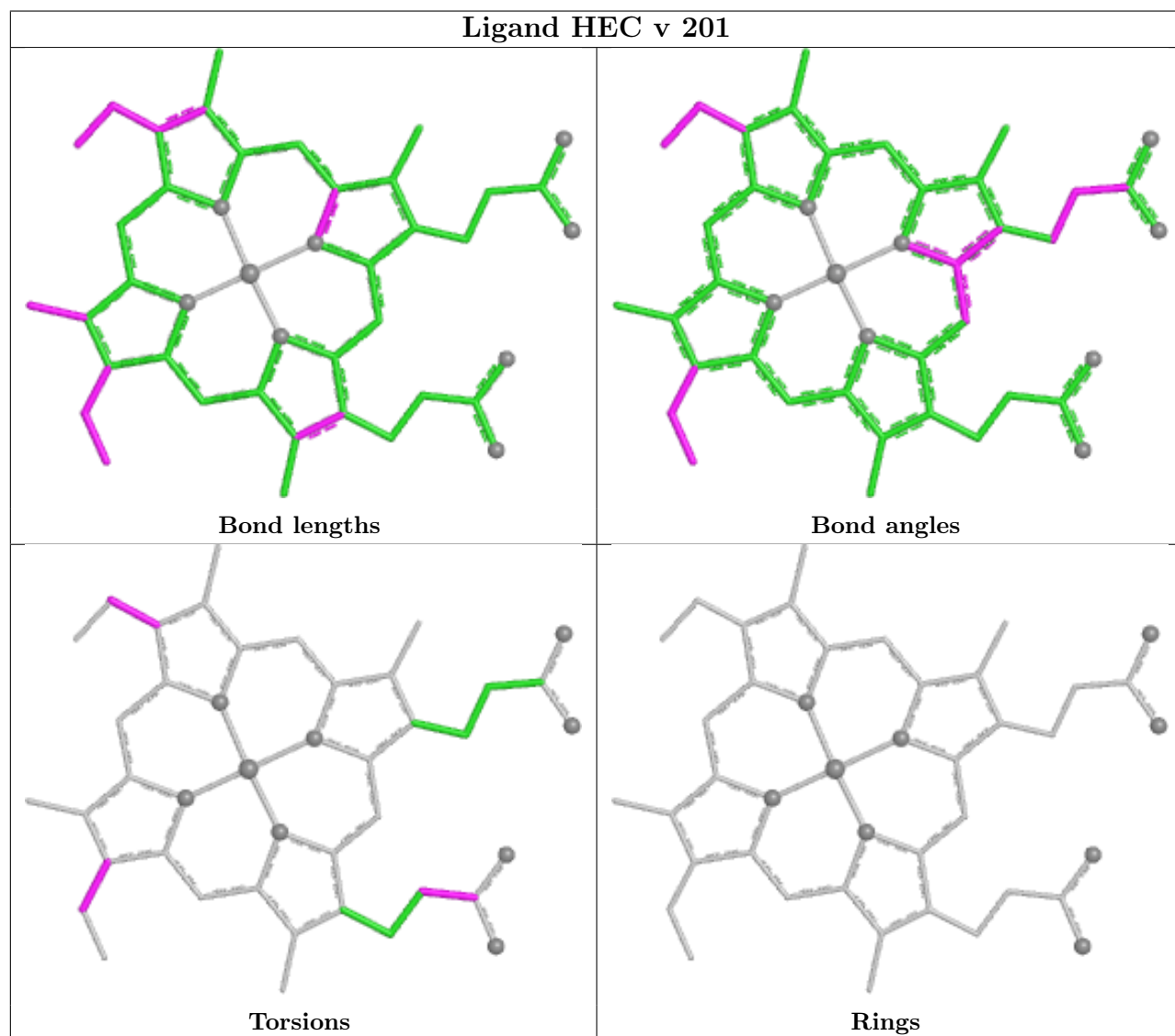
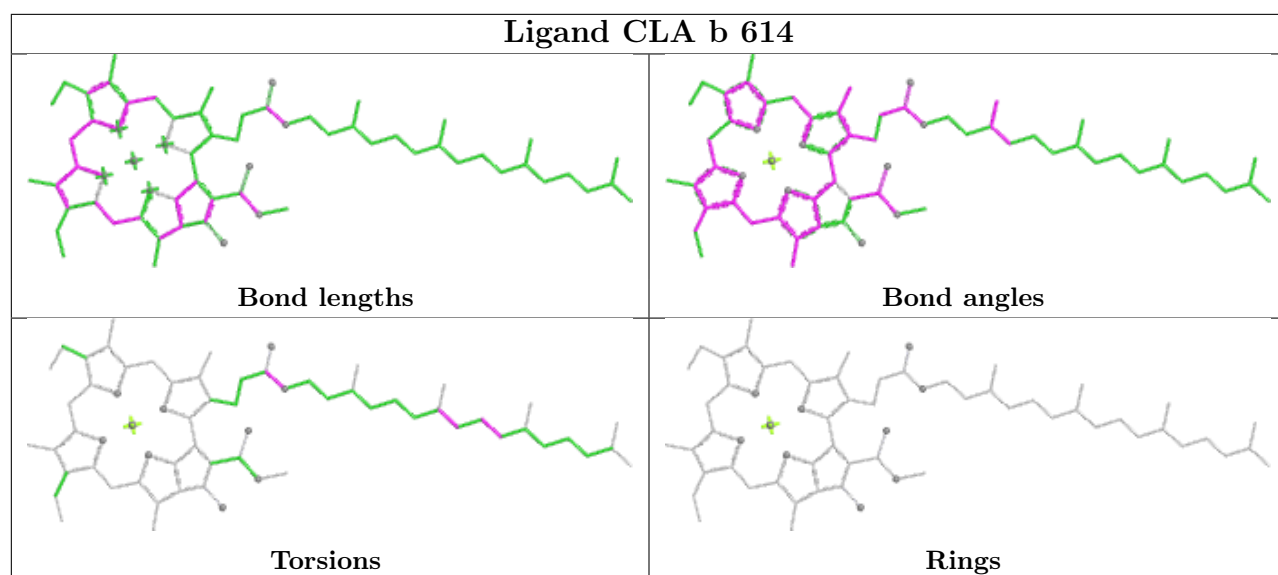


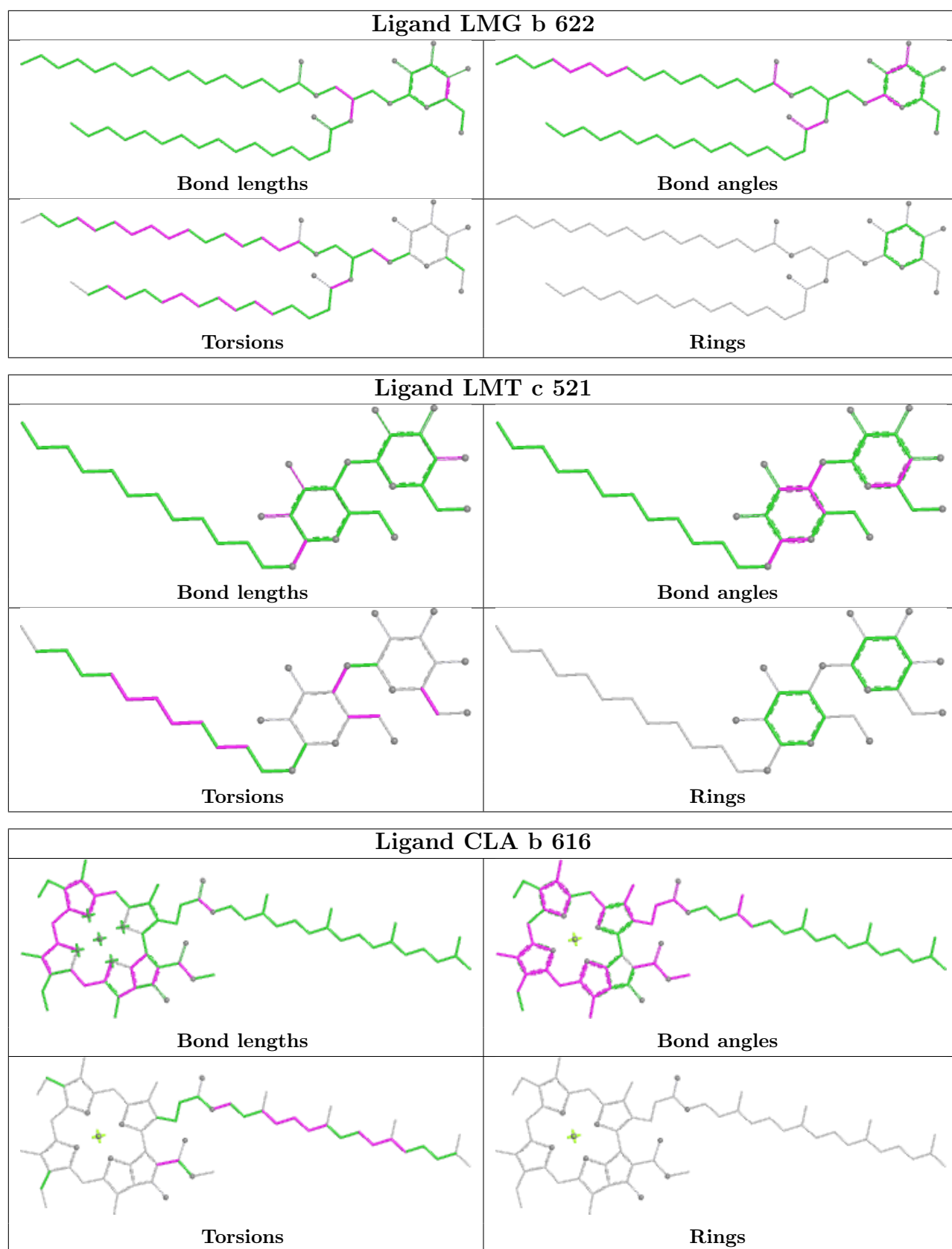


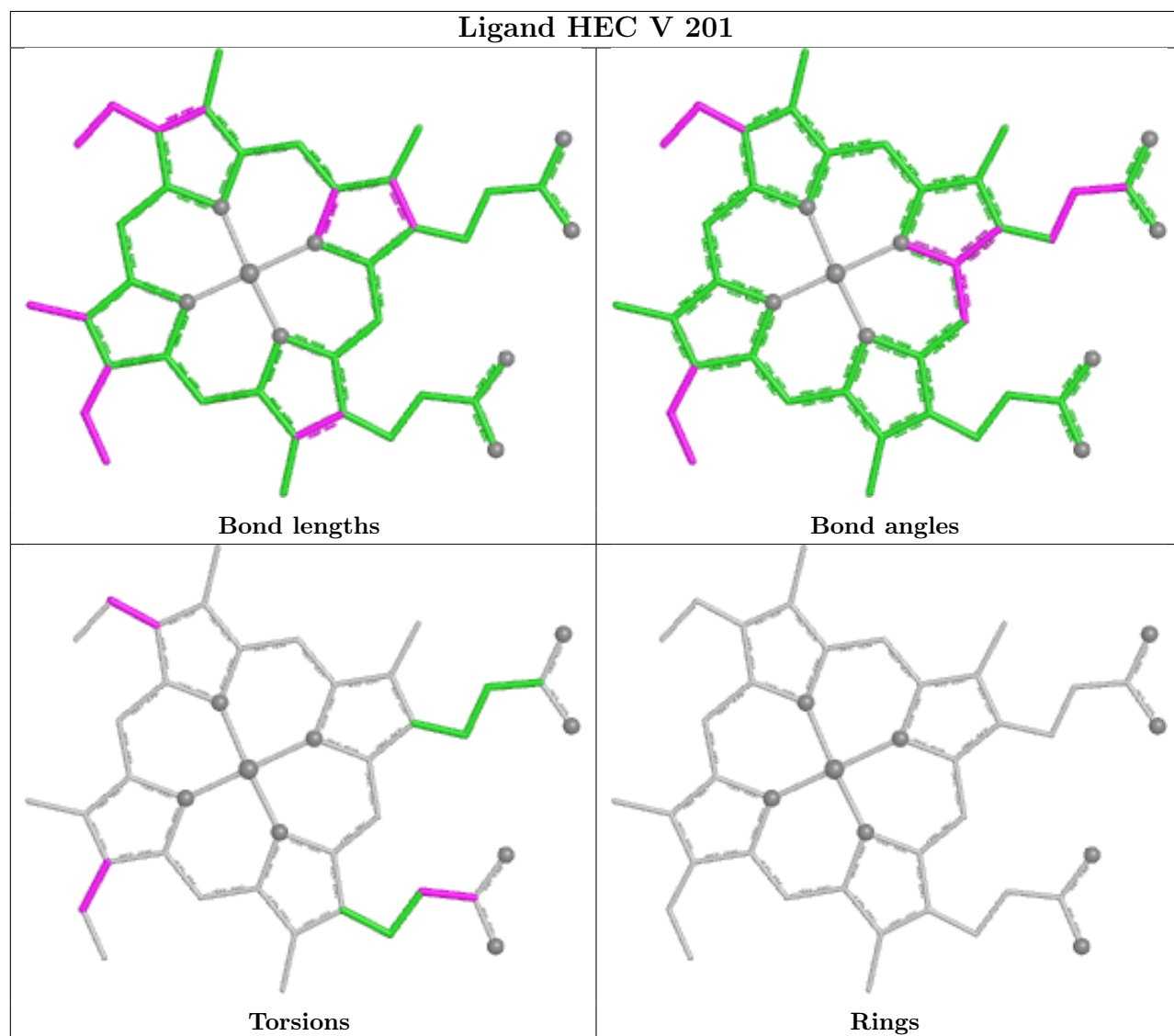
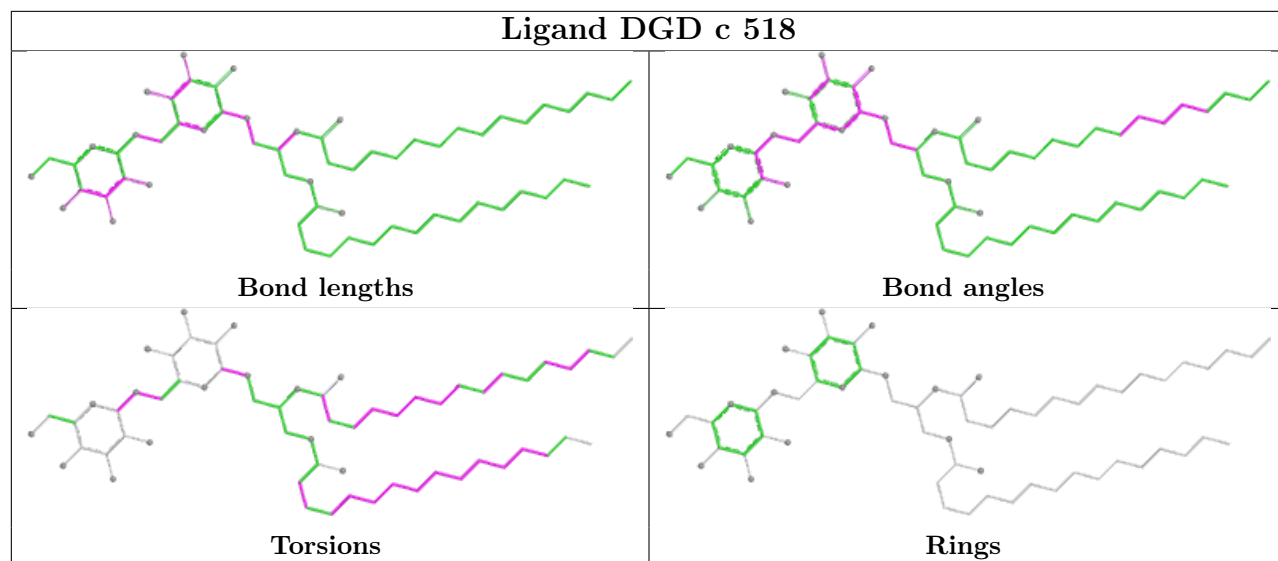
Ligand CLA C 502			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

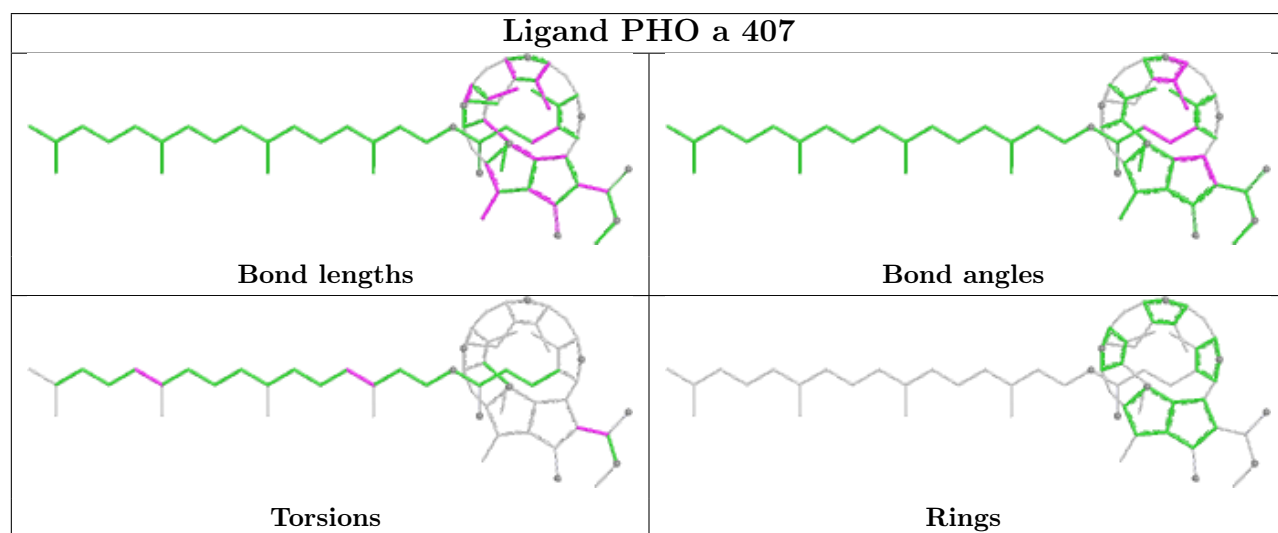
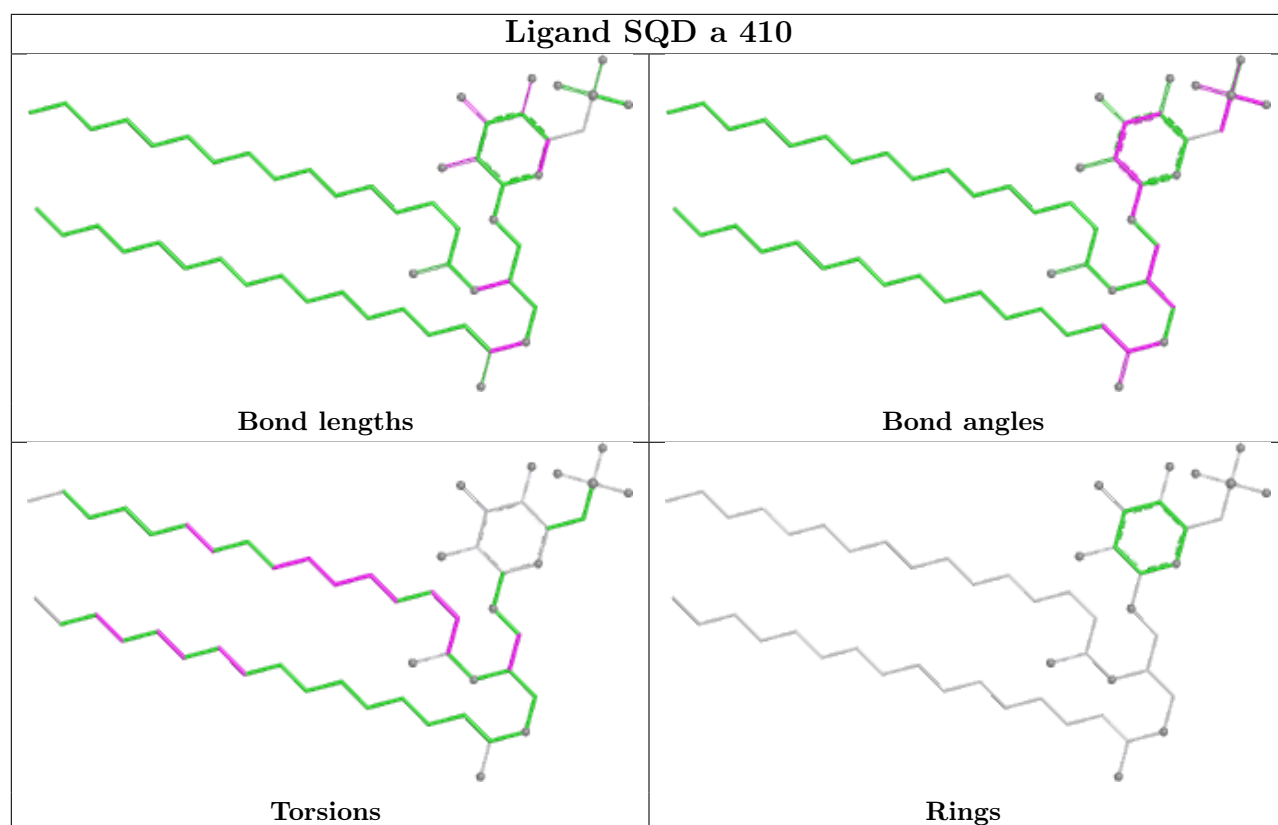
Ligand BCR a 409			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

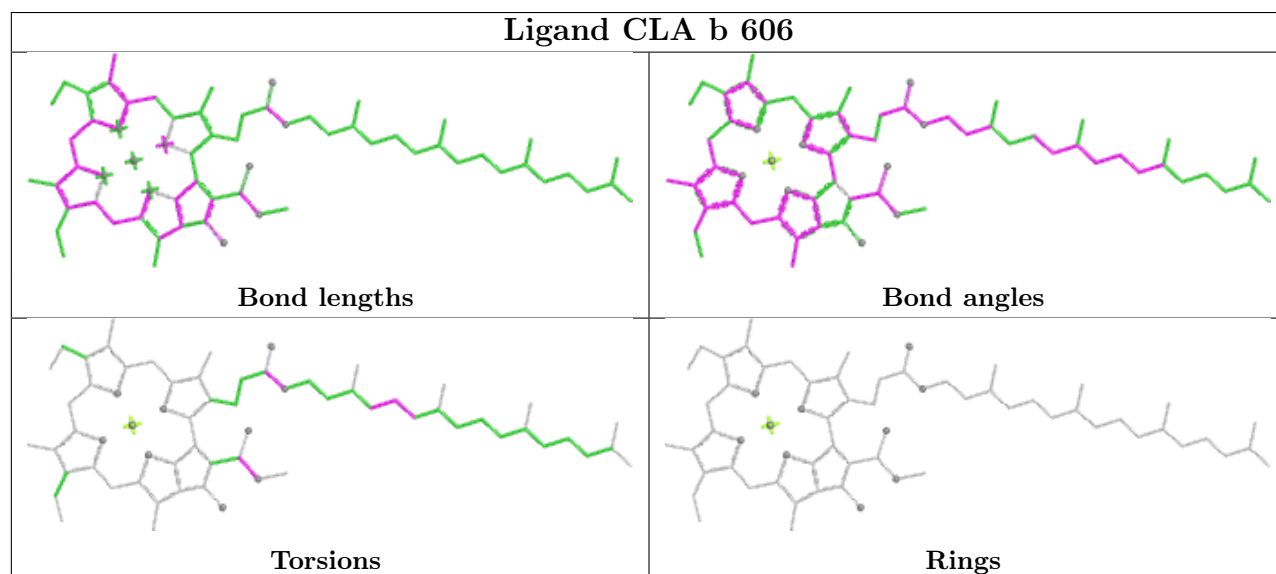
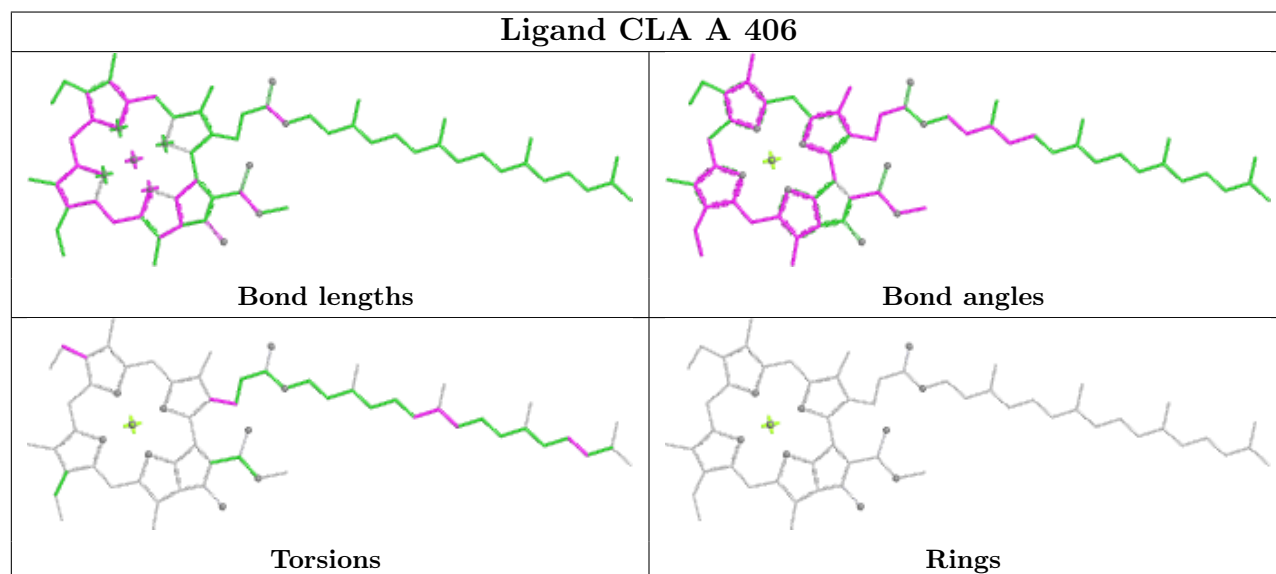
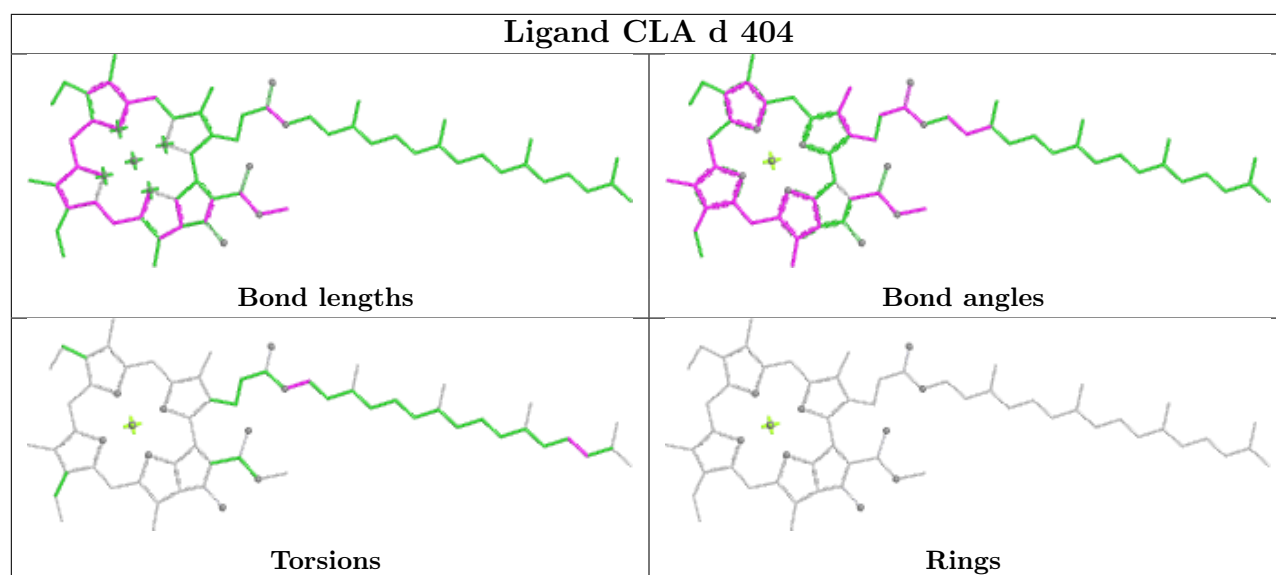


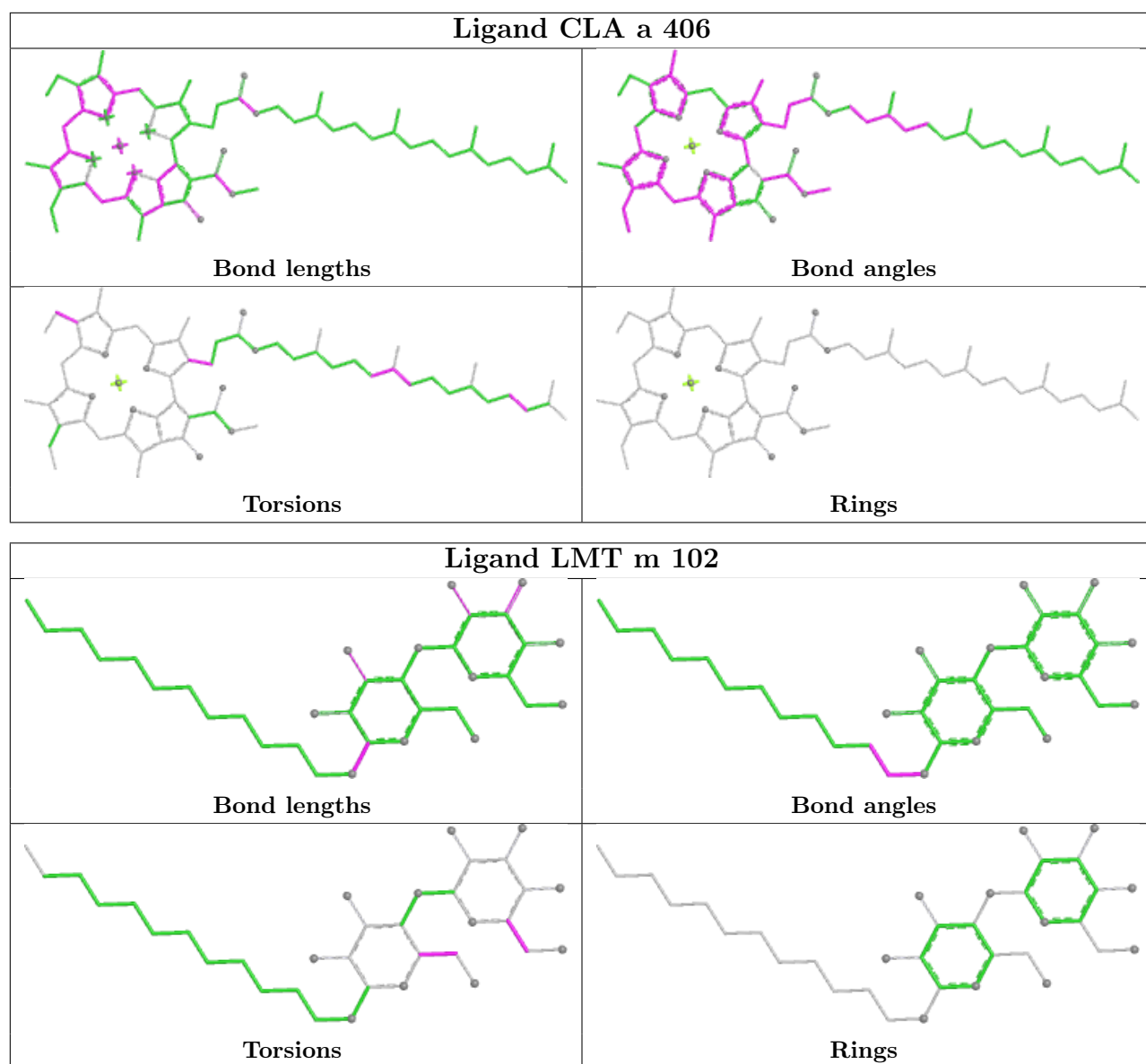


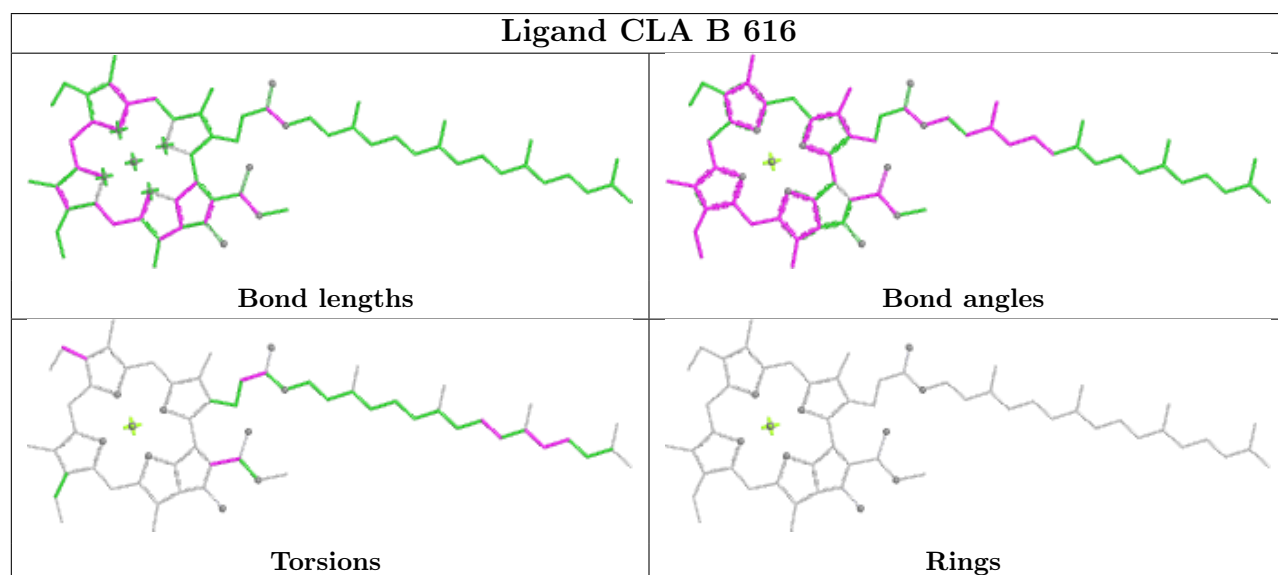
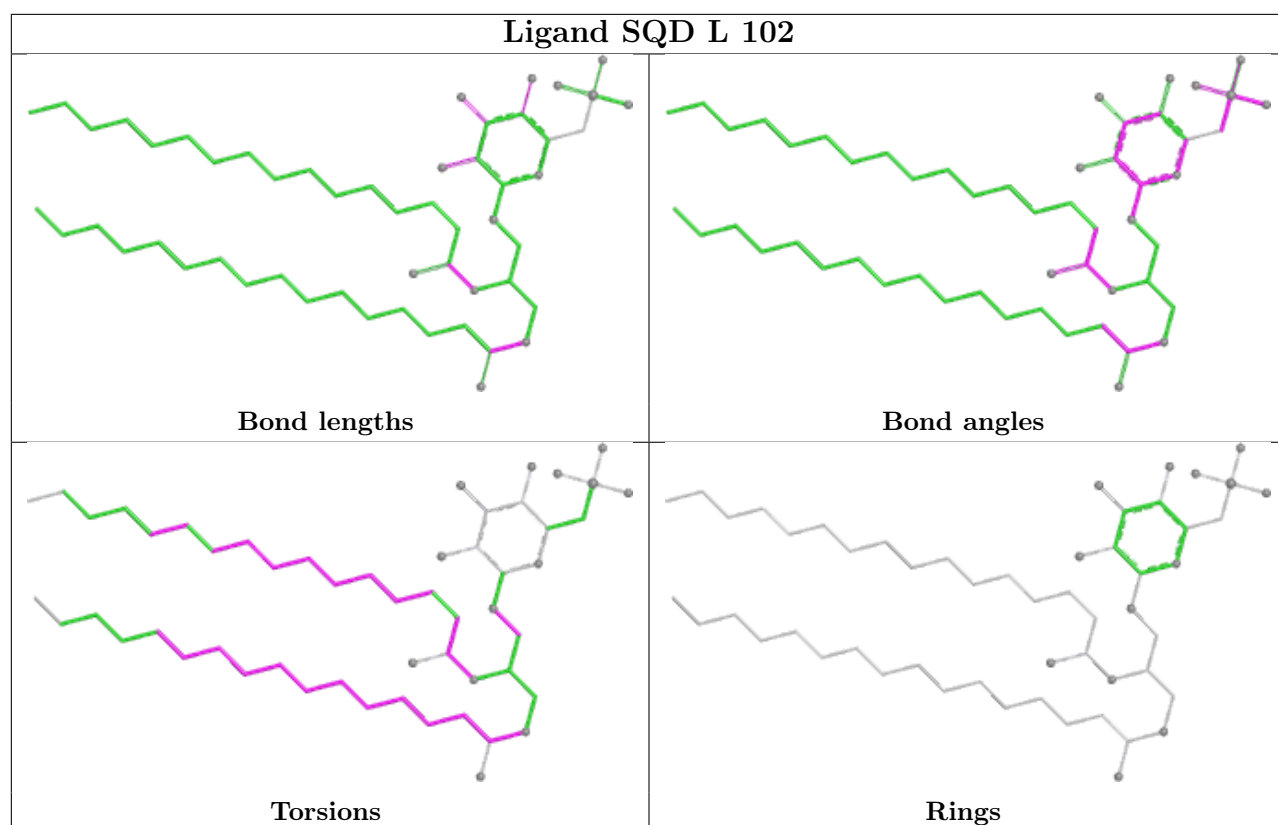




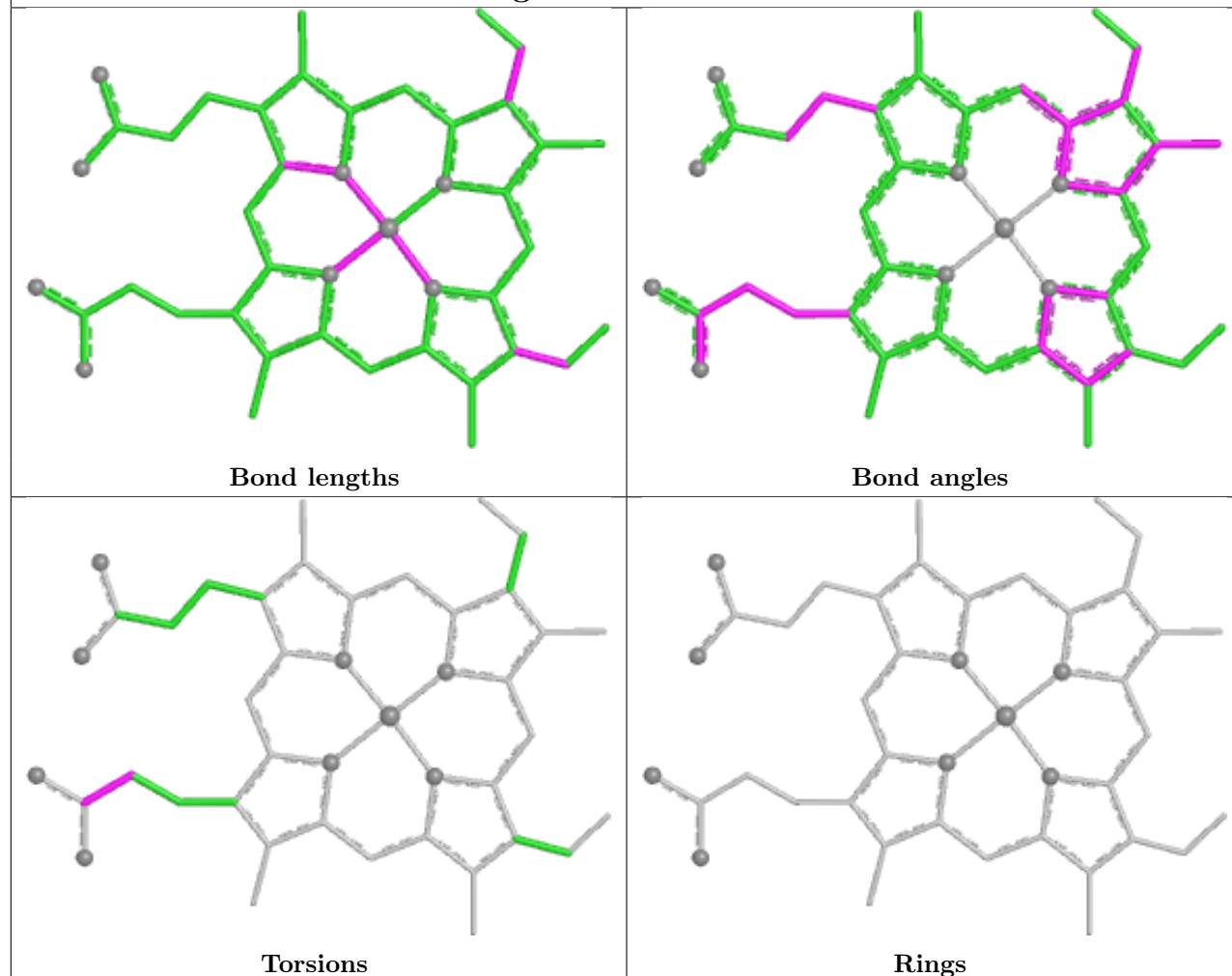




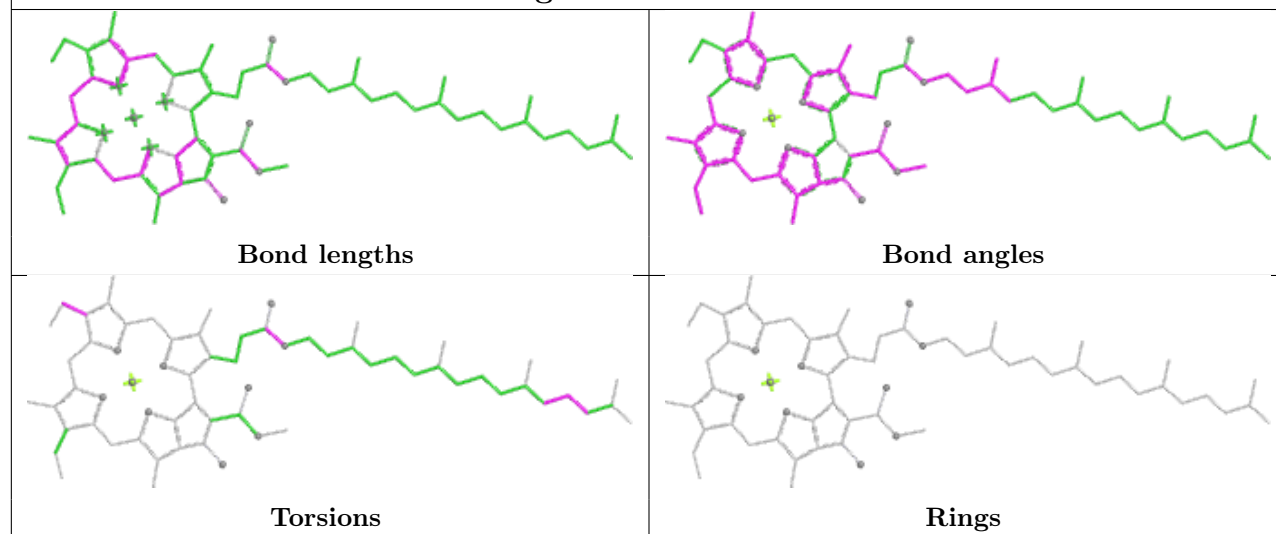


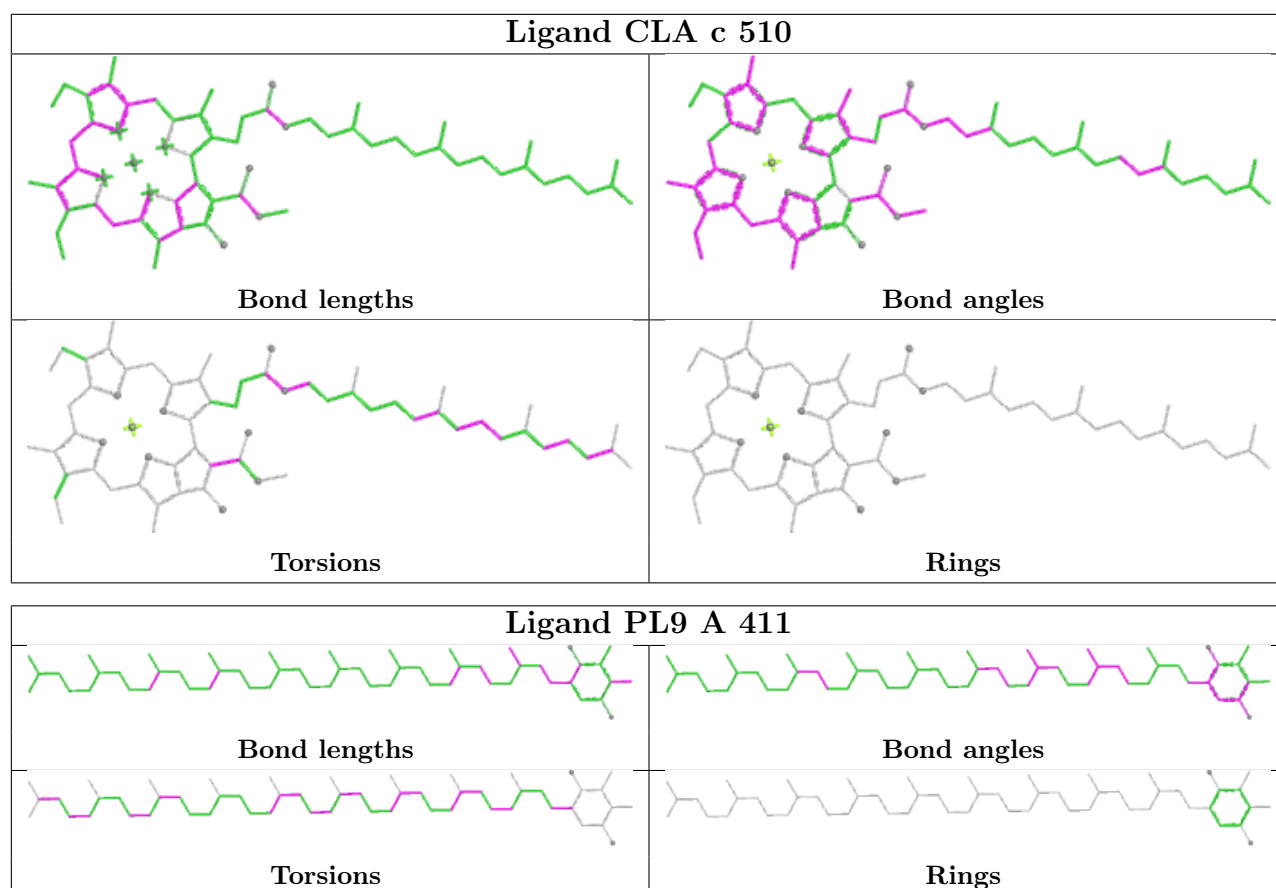


Ligand HEM e 103



Ligand CLA b 604





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

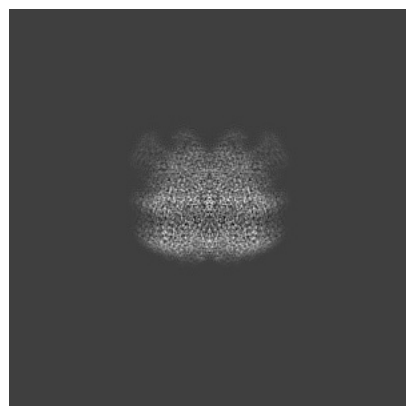
5 Map visualisation [i](#)

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.

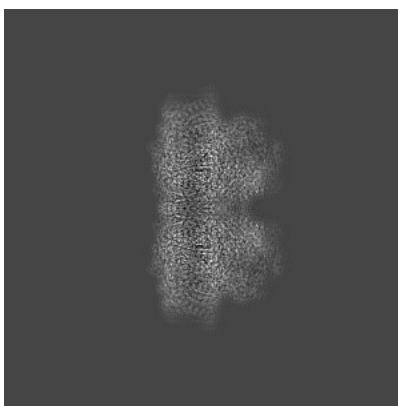
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

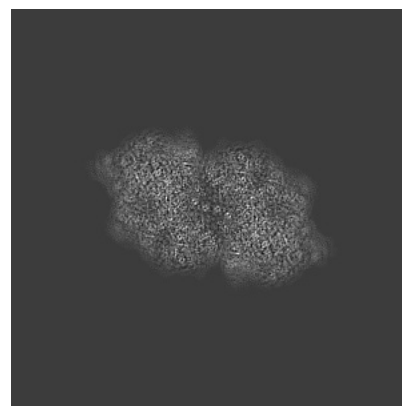
5.1.1 Primary map



X

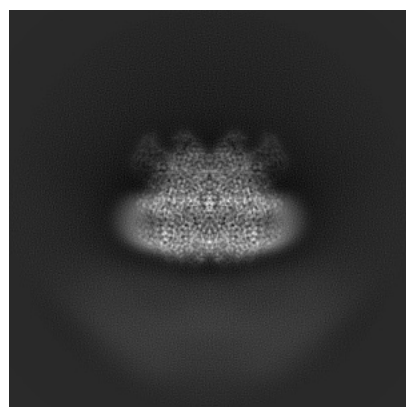


Y

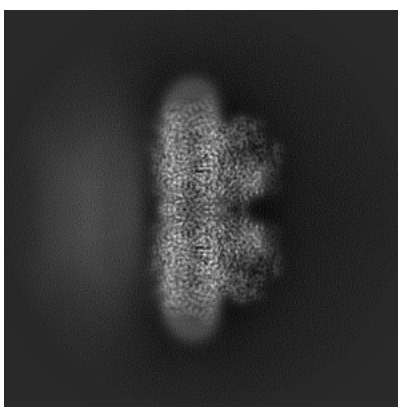


Z

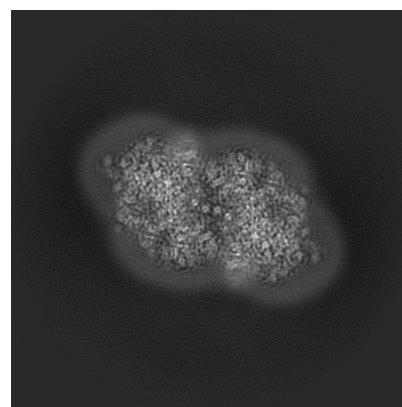
5.1.2 Raw map



X



Y

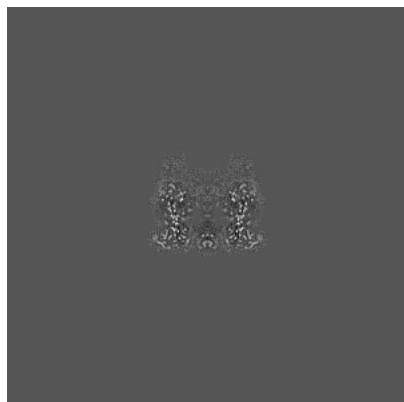


Z

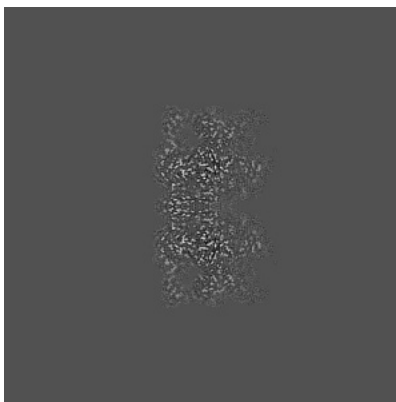
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

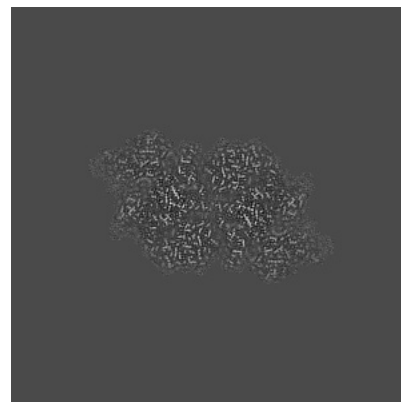
5.2.1 Primary map



X Index: 200

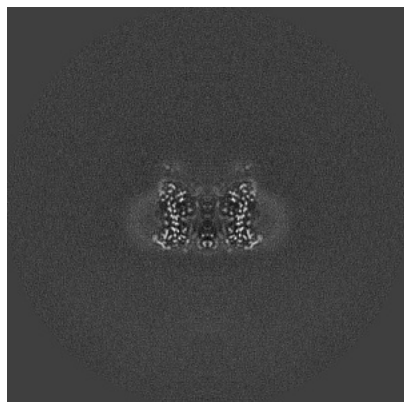


Y Index: 200

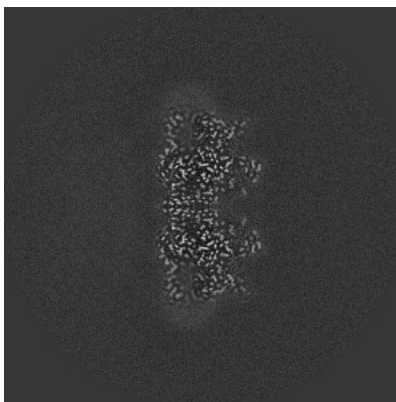


Z Index: 200

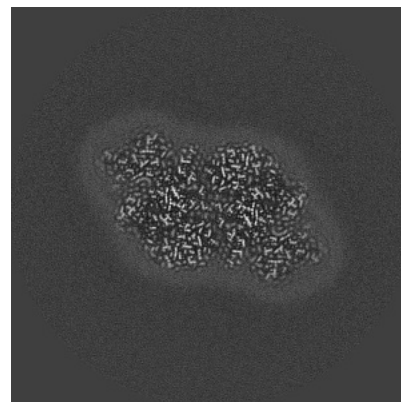
5.2.2 Raw map



X Index: 200



Y Index: 200

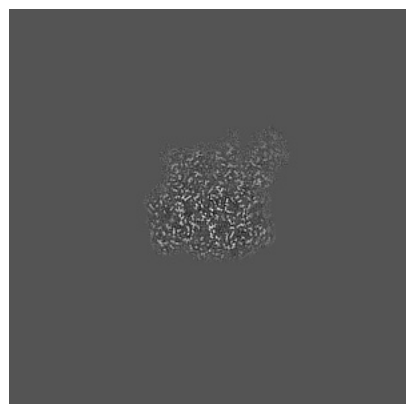


Z Index: 200

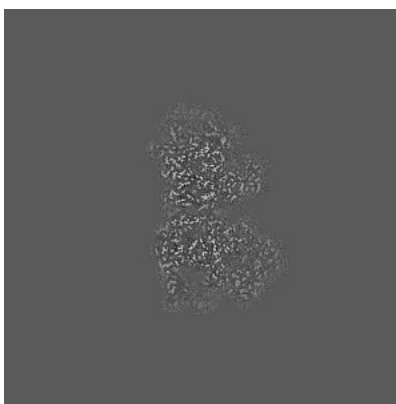
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

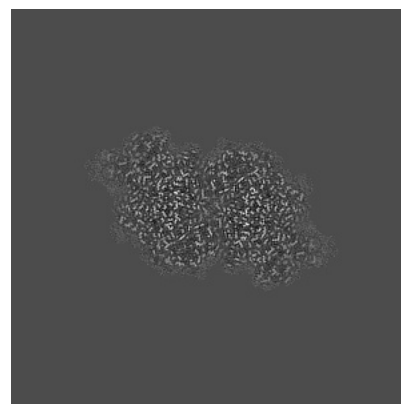
5.3.1 Primary map



X Index: 167

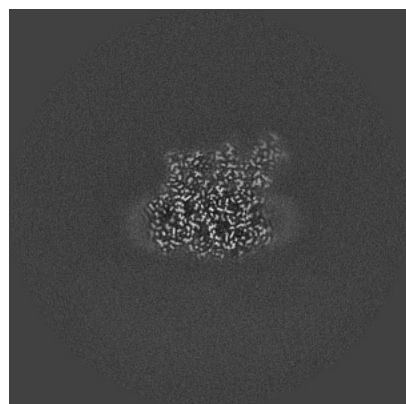


Y Index: 218

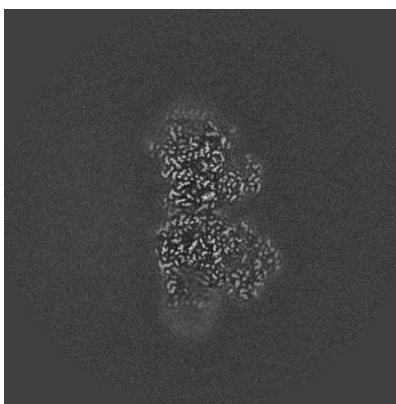


Z Index: 207

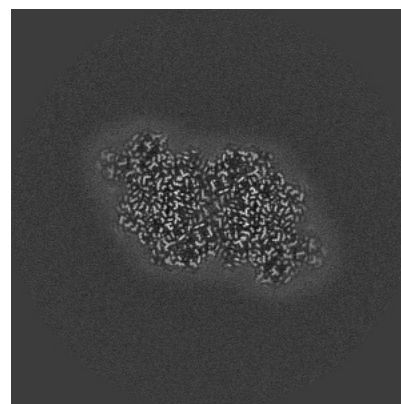
5.3.2 Raw map



X Index: 167



Y Index: 218

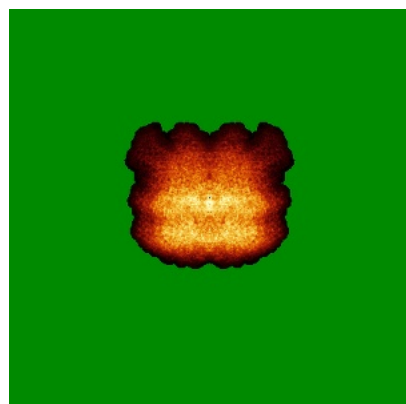


Z Index: 207

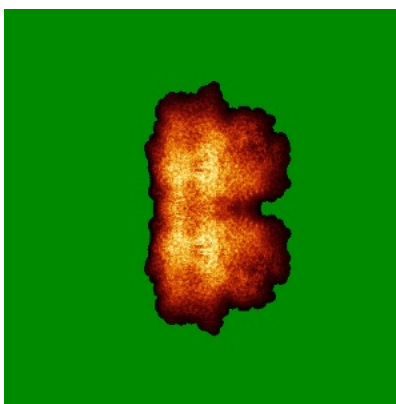
The images above show the largest variance slices of the map in three orthogonal directions.

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

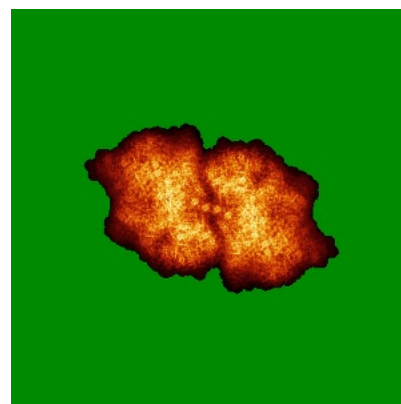
5.4.1 Primary map



X

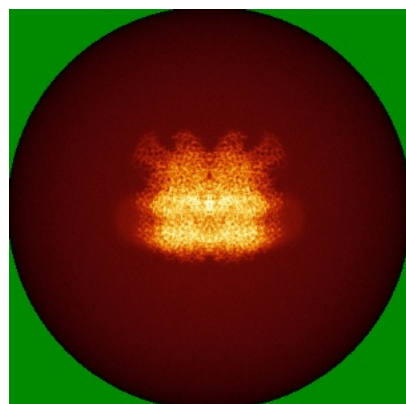


Y

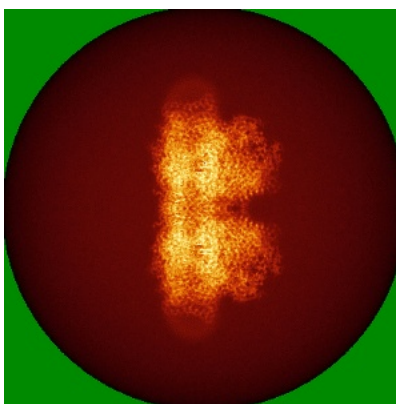


Z

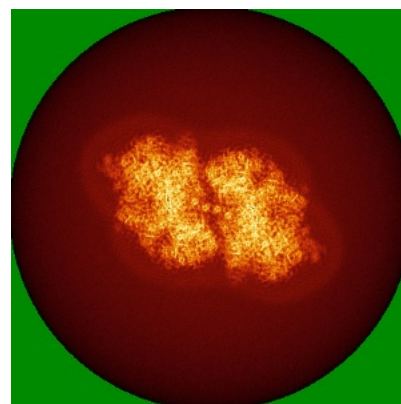
5.4.2 Raw map



X



Y

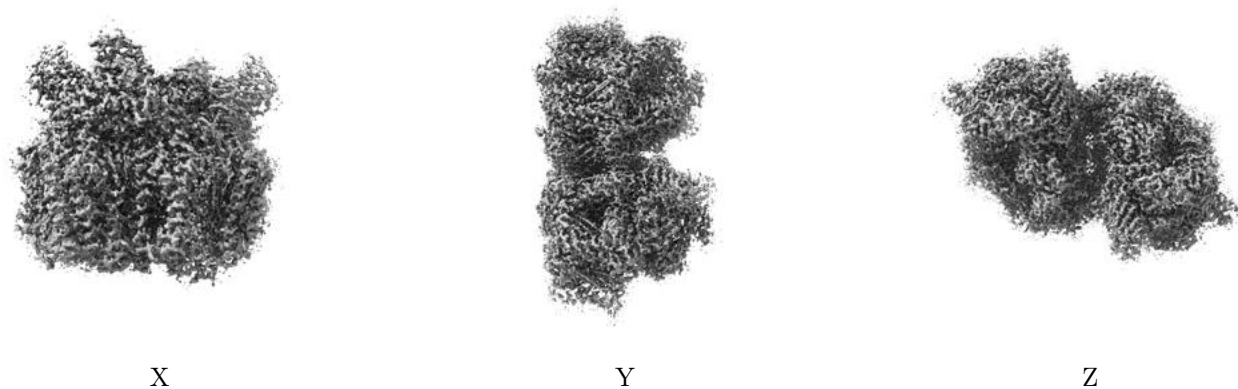


Z

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.

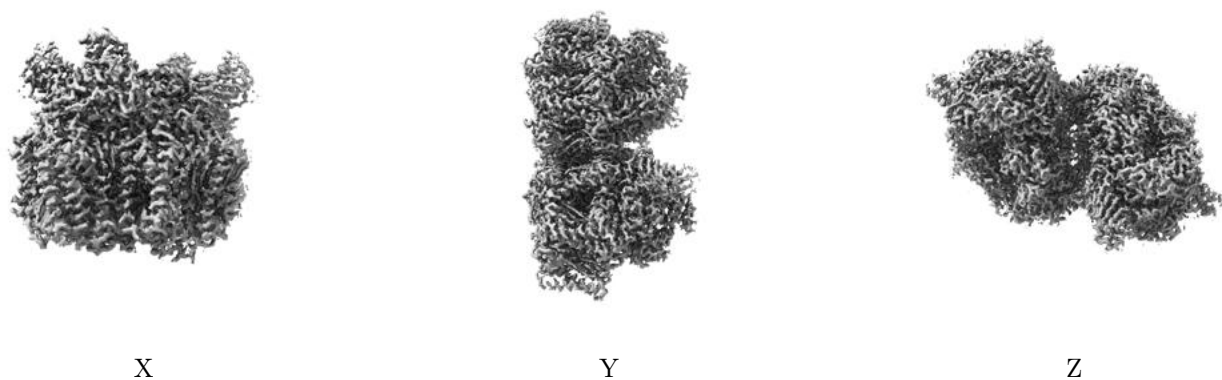
5.5 Orthogonal surface views [i](#)

5.5.1 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.

5.5.2 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.

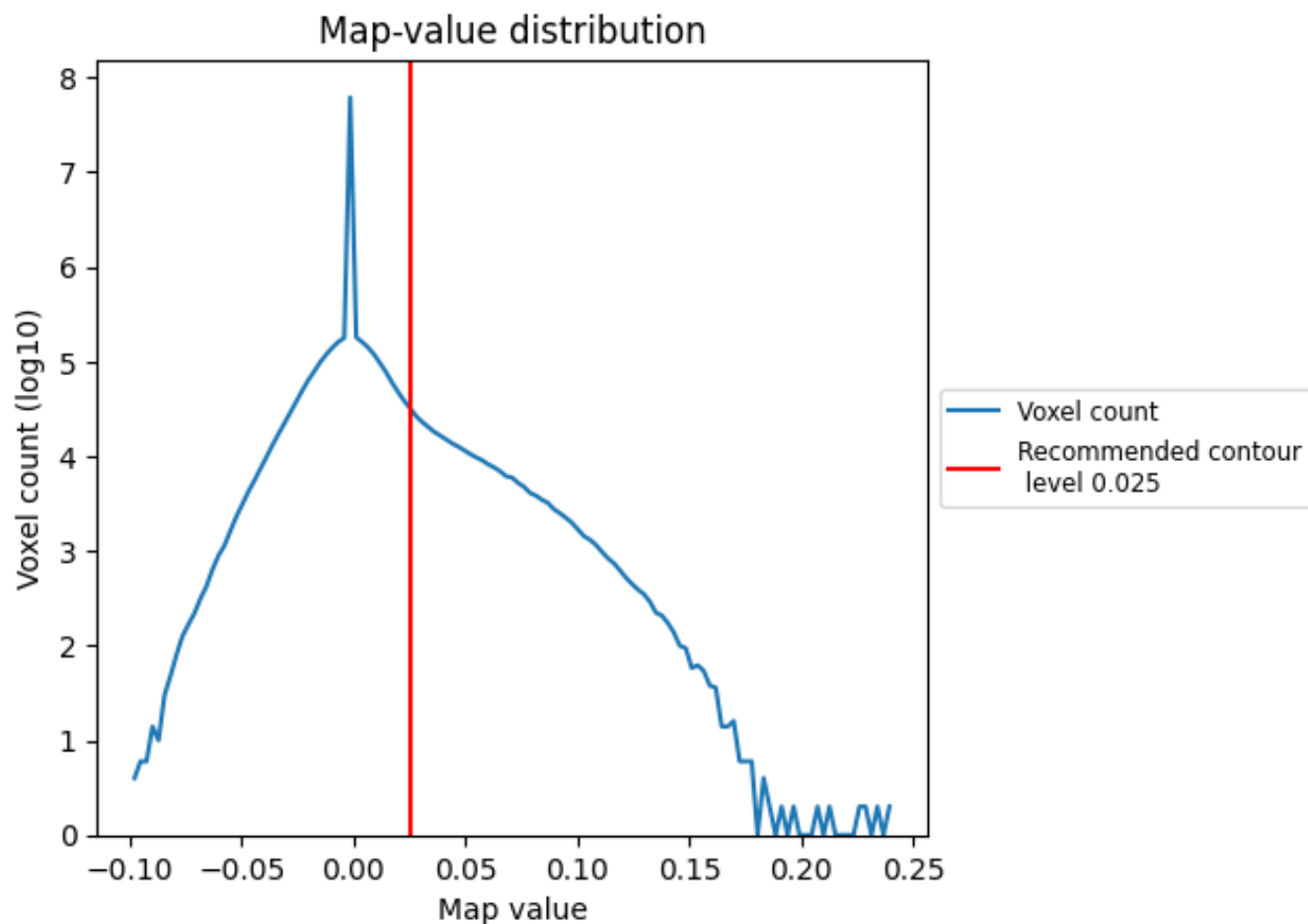
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

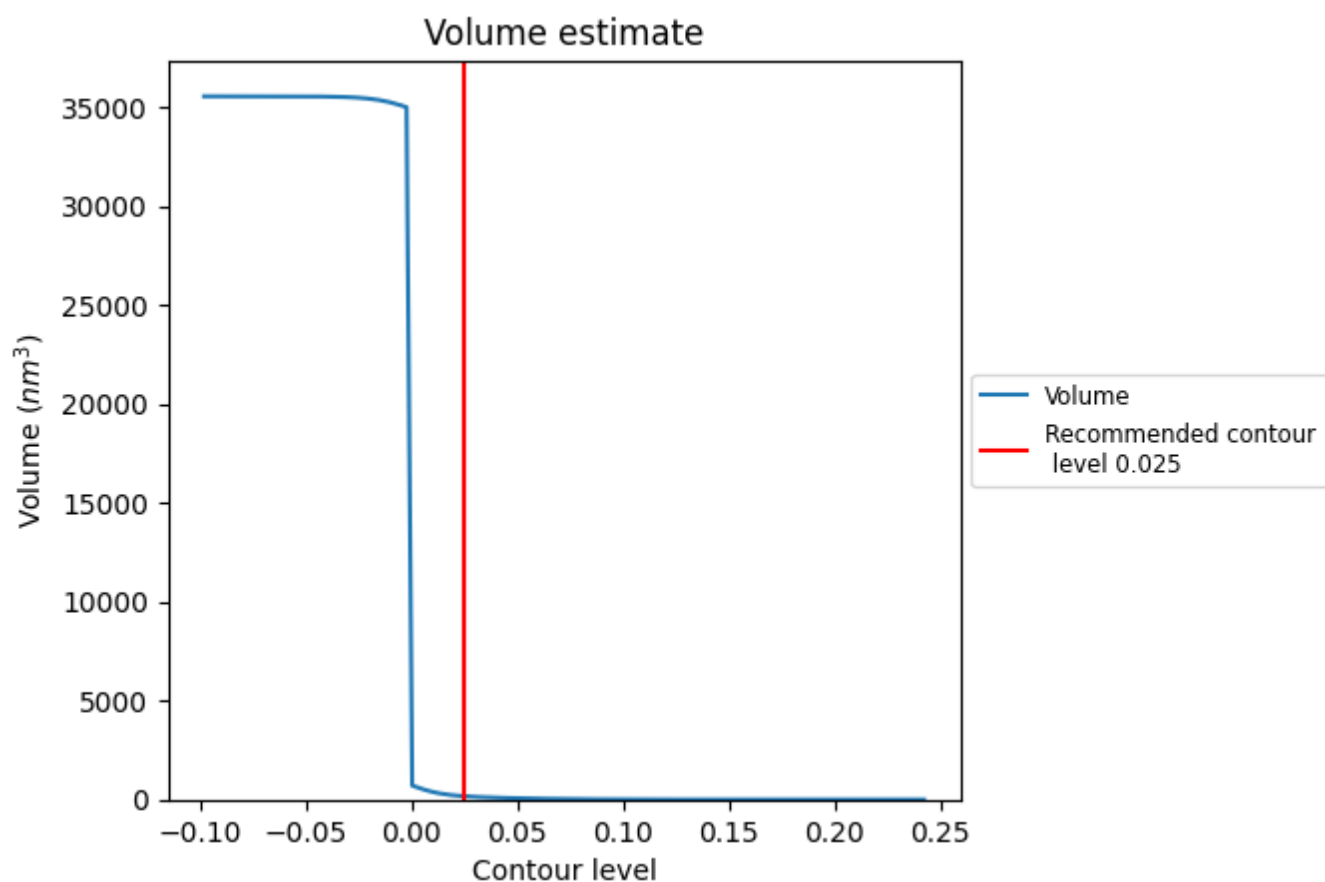
This section contains the results of statistical analysis of the map.

6.1 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.

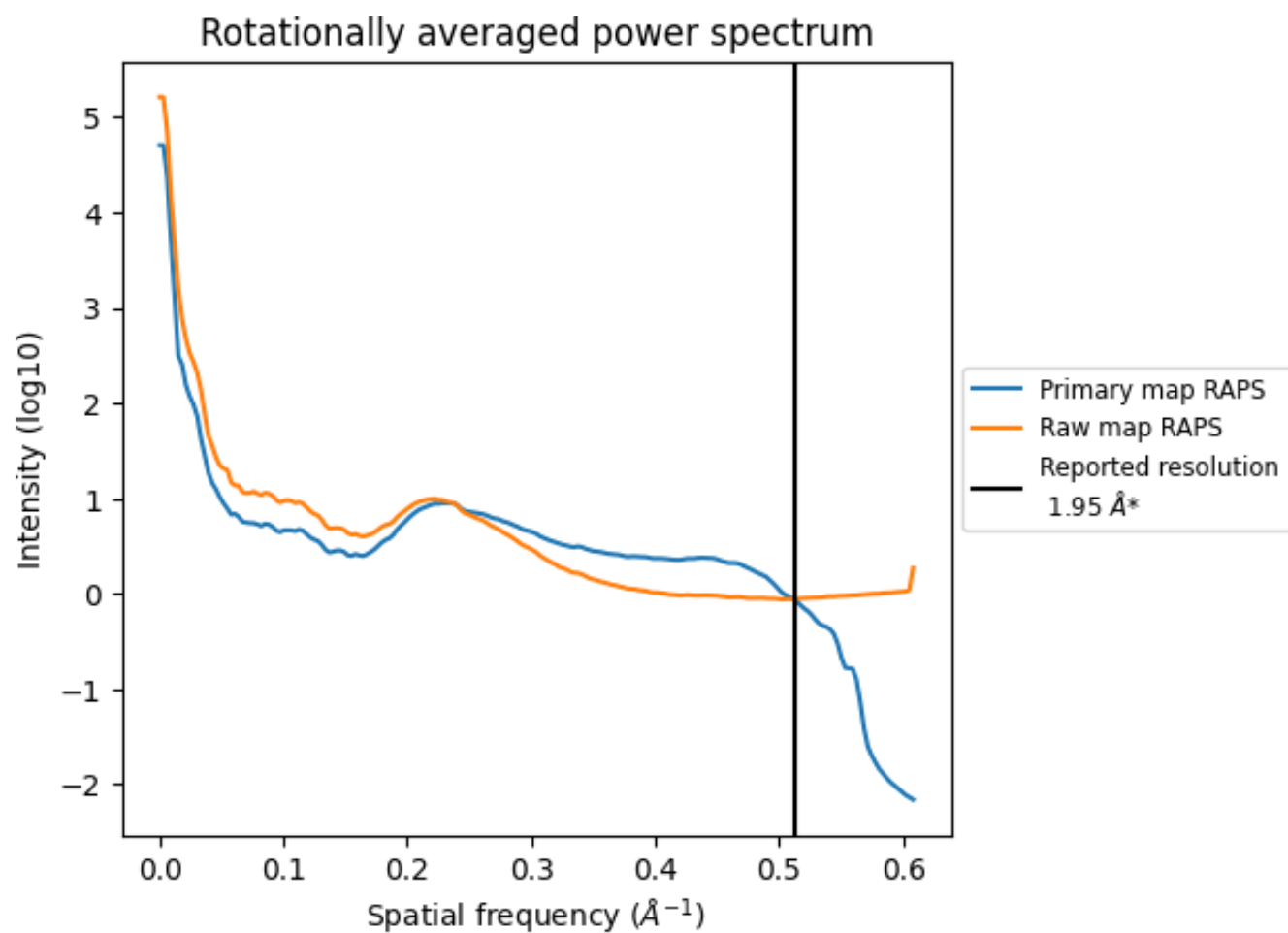
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 169 nm³; 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.

6.3 Rotationally averaged power spectrum ⓘ

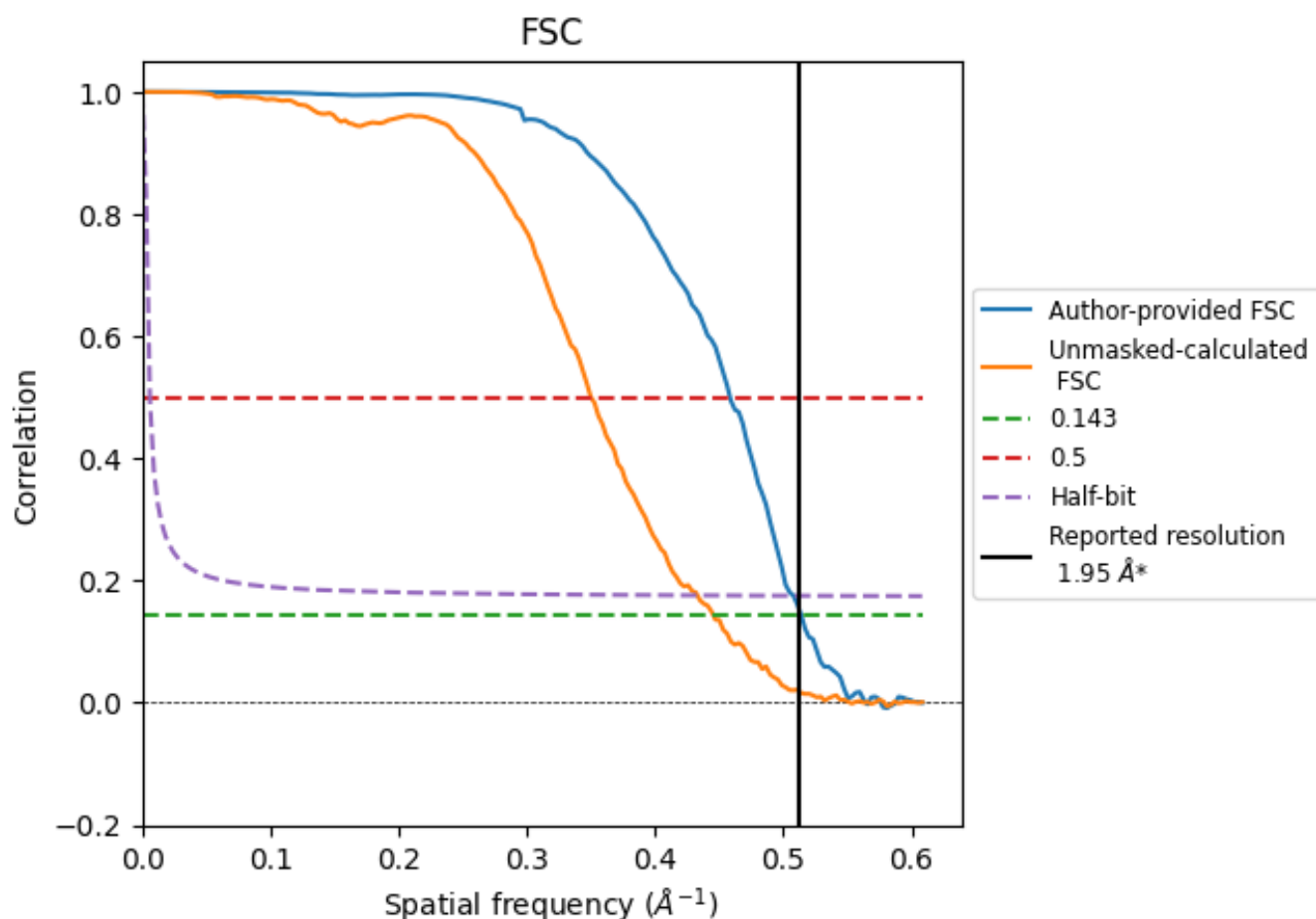


*Reported resolution corresponds to spatial frequency of 0.513 Å⁻¹

7 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.

7.1 FSC [i](#)



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

7.2 Resolution estimates [i](#)

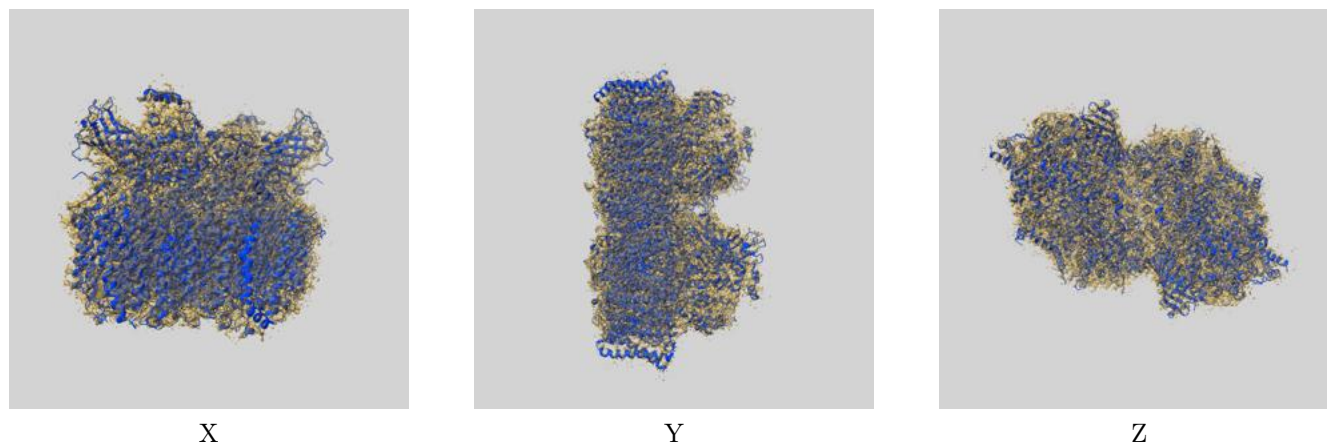
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.95	-	-
Author-provided FSC curve	1.95	2.18	1.97
Unmasked-calculated*	2.24	2.86	2.31

*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 %

8 Map-model fit [i](#)

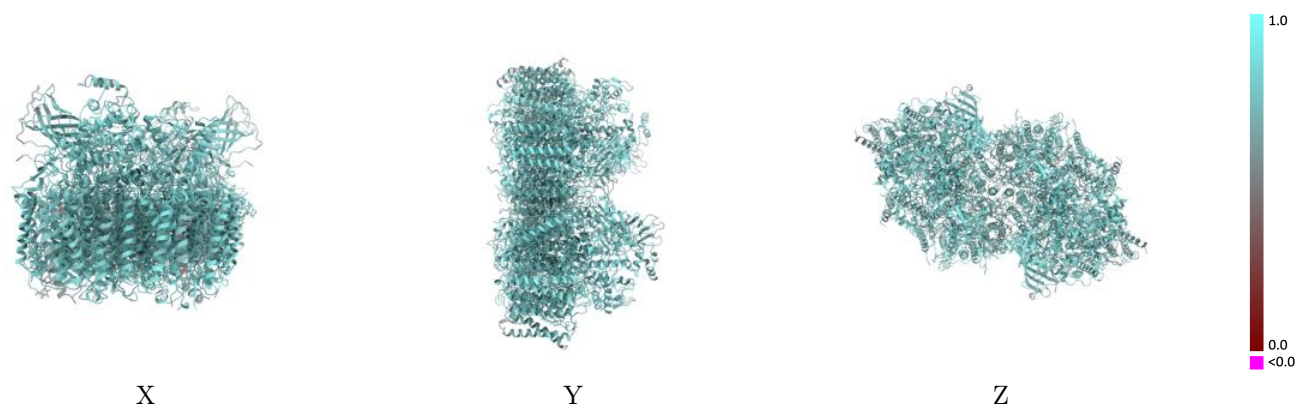
This section contains information regarding the fit between EMDB map EMD-30547 and PDB model 7D1T. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



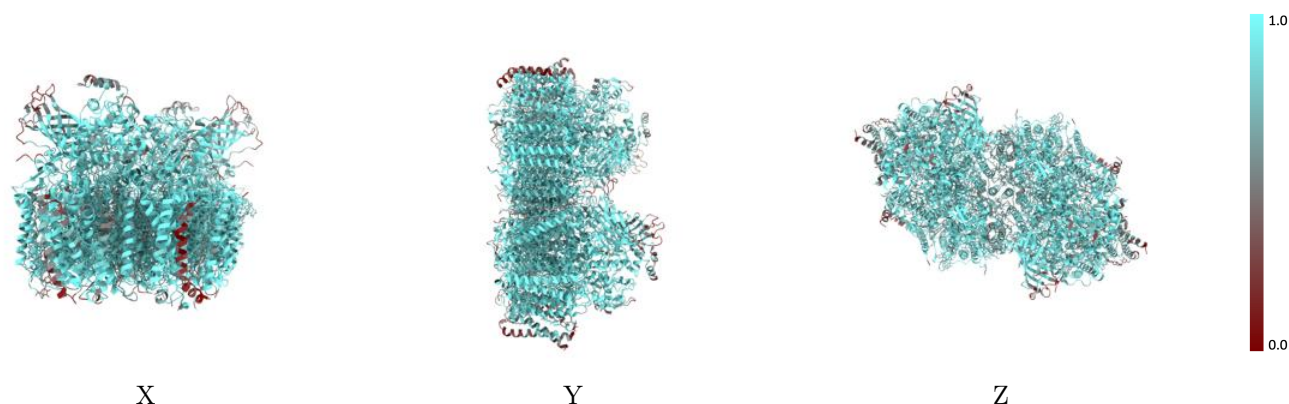
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



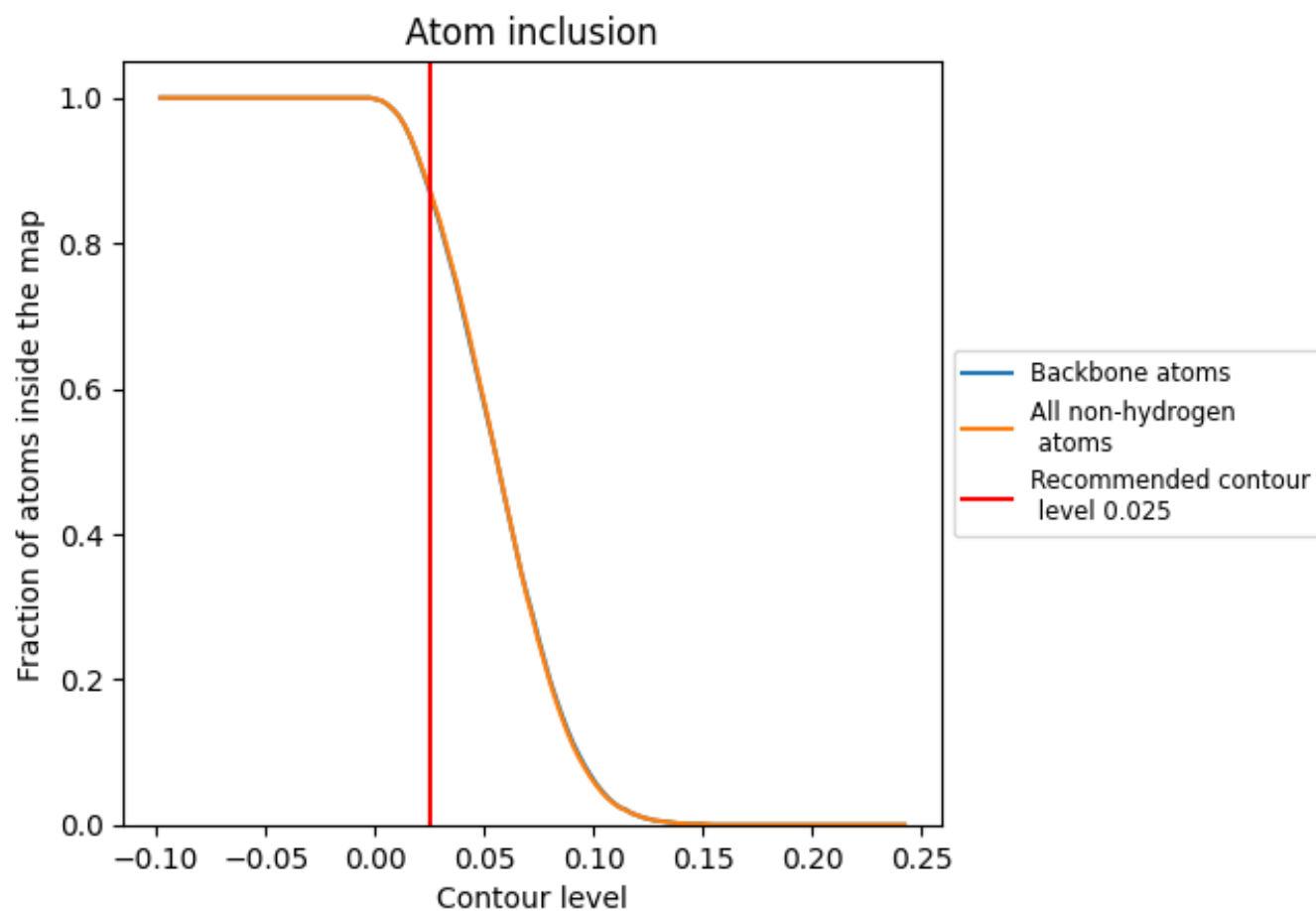
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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).

8.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 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