



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:18 PM UTC

PDB ID : 7D1U / pdb_00007d1u
EMDB ID : EMD-30548
Title : Cryo-EM Structure of PSII at 2.08 angstrom resolution
Authors : Kato, K.; Miyazaki, N.; Hamaguchi, T.; Nakajima, Y.; Akita, F.; Yonekura, K.; Shen, J.R.
Deposited on : 2020-09-15
Resolution : 2.08 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:

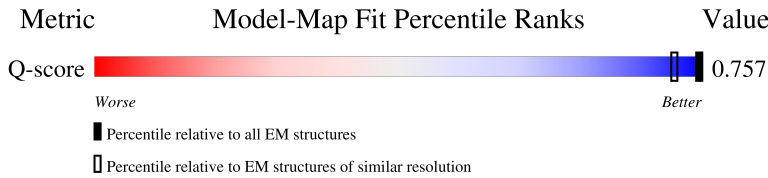
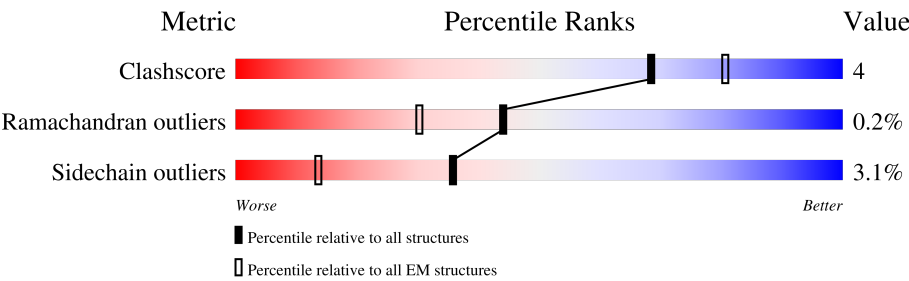
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.08 Å.

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



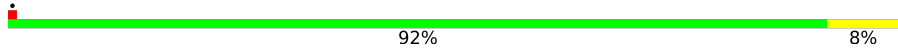
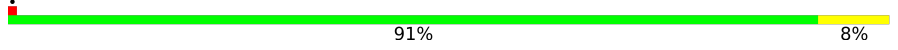
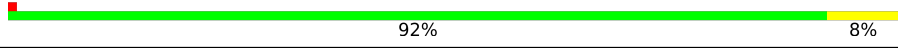
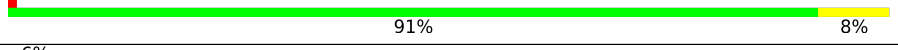
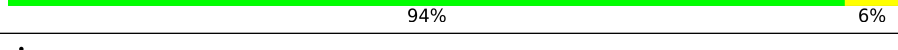
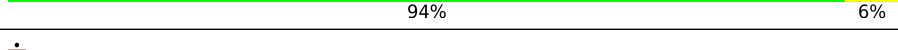
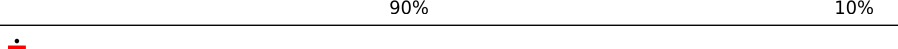
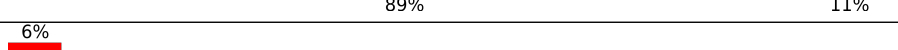
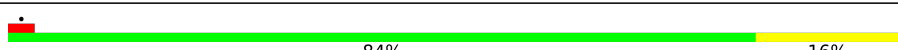
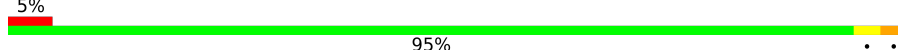
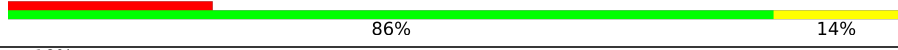
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1976 (1.58 - 2.58)

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	93% 7%
1	a	334	93% 7%
2	B	505	91% 8% .
2	b	505	92% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	451	
3	c	451	
4	D	342	
4	d	342	
5	E	81	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
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	A	408	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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	D	401	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	a	405	X	-	-	-
24	CLA	a	408	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	-	-	-
24	CLA	b	613	X	-	-	-
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	d	401	X	-	-	-
24	CLA	d	403	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	404	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 52655 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	0	0
			2620	1716	431	458	15		
1	a	334	Total	C	N	O	S	0	0
			2620	1716	431	458	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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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			

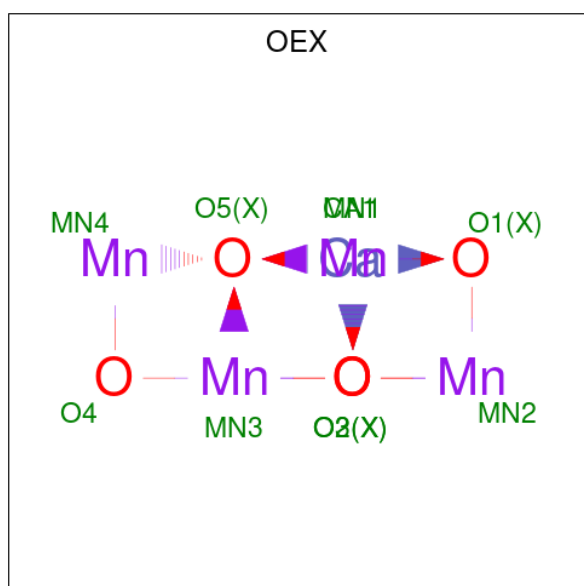
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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	

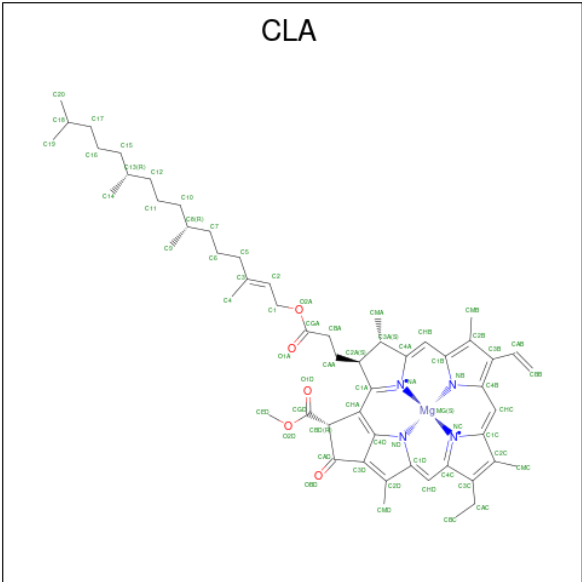
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

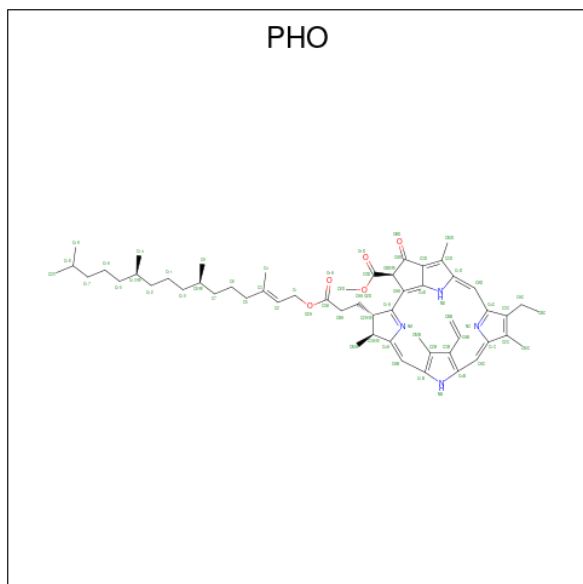
Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total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

Continued on next page...

Continued from previous page...

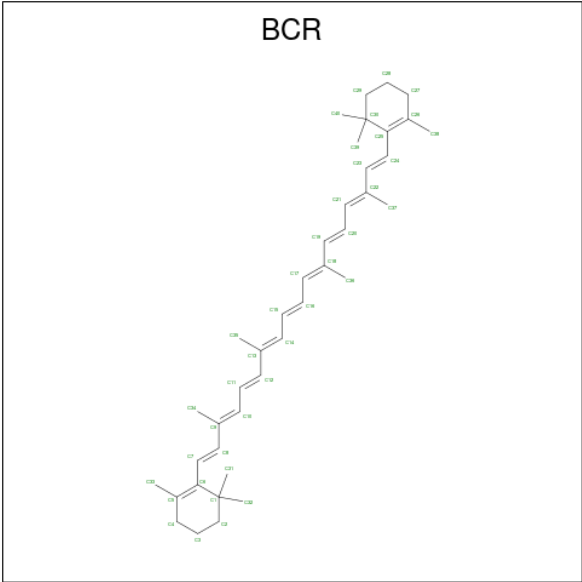
Mol	Chain	Residues	Atoms					AltConf
24	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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



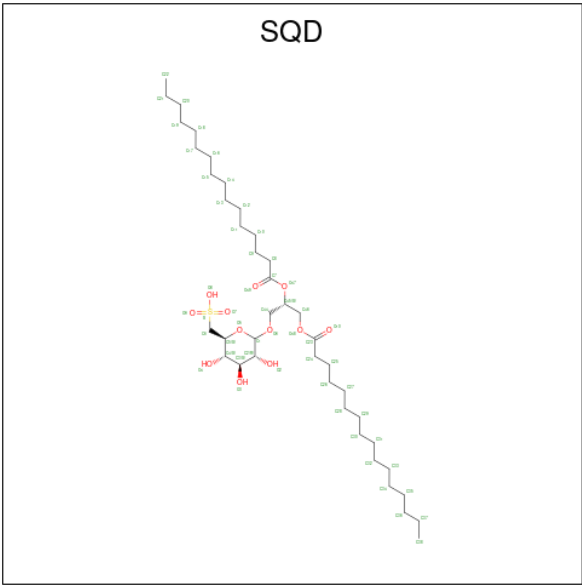
Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	B	1	Total	C	0
			40	40	
26	C	1	Total	C	0
			40	40	
26	C	1	Total	C	0
			40	40	
26	C	1	Total	C	0
			40	40	
26	D	1	Total	C	0
			40	40	
26	T	1	Total	C	0
			40	40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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
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	y	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).



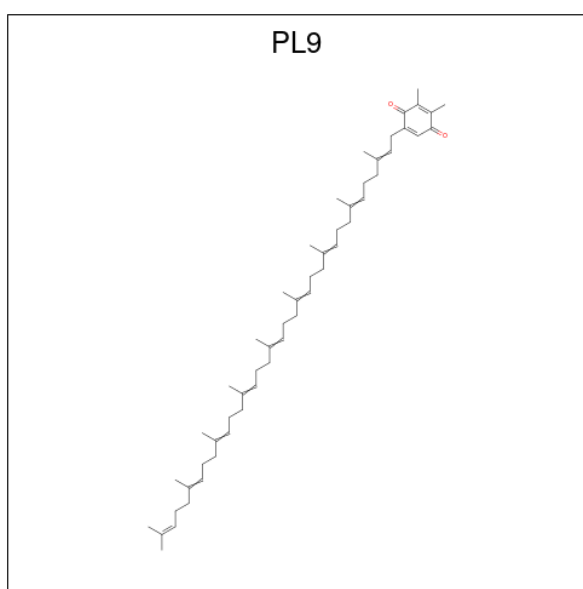
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	S	0
			54	41	12	1	
27	A	1	Total	C	O	S	0
			54	41	12	1	
27	D	1	Total	C	O	S	0
			45	32	12	1	
27	L	1	Total	C	O	S	0
			54	41	12	1	
27	a	1	Total	C	O	S	0
			54	41	12	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
27	a	1	Total	C	O	S	0
			54	41	12	1	
27	d	1	Total	C	O	S	0
			45	32	12	1	
27	l	1	Total	C	O	S	0
			54	41	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:).

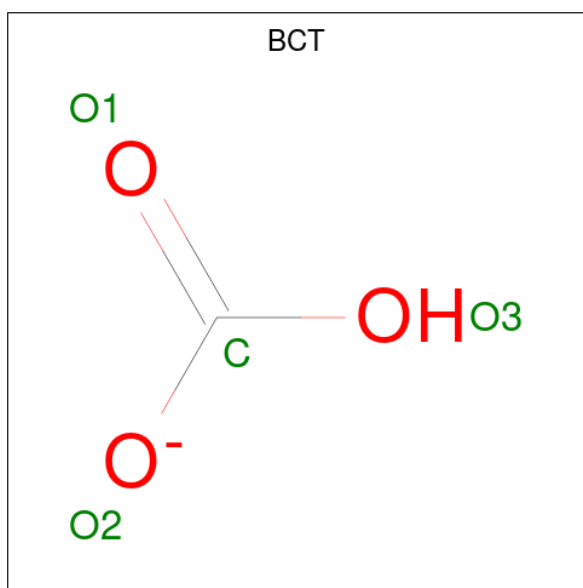
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O		0
			36	31	5		

Continued on next page...

Continued from previous page...

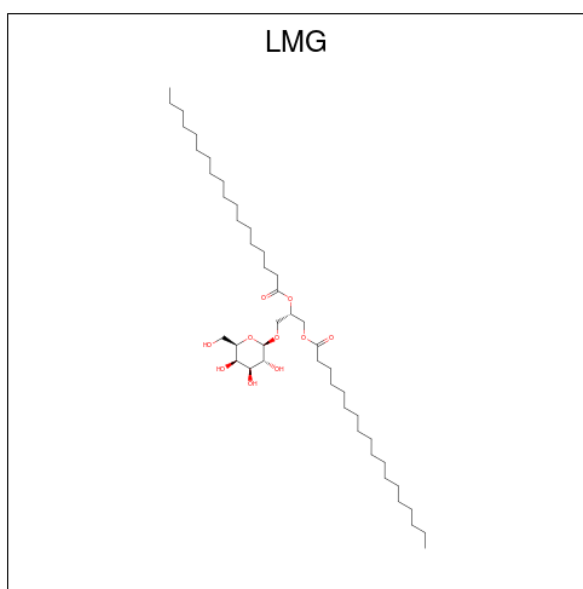
Mol	Chain	Residues	Atoms			AltConf
29	B	6	Total	C	O	0
			85	80	5	
29	C	1	Total	C		0
			10	10		
29	D	1	Total	C	O	0
			40	35	5	
29	E	1	Total	C		0
			10	10		
29	I	2	Total	C		0
			17	17		
29	J	1	Total	C		0
			10	10		
29	K	1	Total	C	O	0
			34	29	5	
29	M	1	Total	C		0
			10	10		
29	T	2	Total	C		0
			26	26		
29	X	1	Total	C		0
			10	10		
29	a	1	Total	C	O	0
			36	31	5	
29	b	6	Total	C	O	0
			85	80	5	
29	c	1	Total	C		0
			10	10		
29	d	1	Total	C	O	0
			40	35	5	
29	e	1	Total	C		0
			10	10		
29	i	2	Total	C		0
			17	17		
29	j	1	Total	C		0
			10	10		
29	k	1	Total	C	O	0
			34	29	5	
29	m	1	Total	C		0
			10	10		
29	t	2	Total	C		0
			26	26		
29	x	1	Total	C		0
			10	10		

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



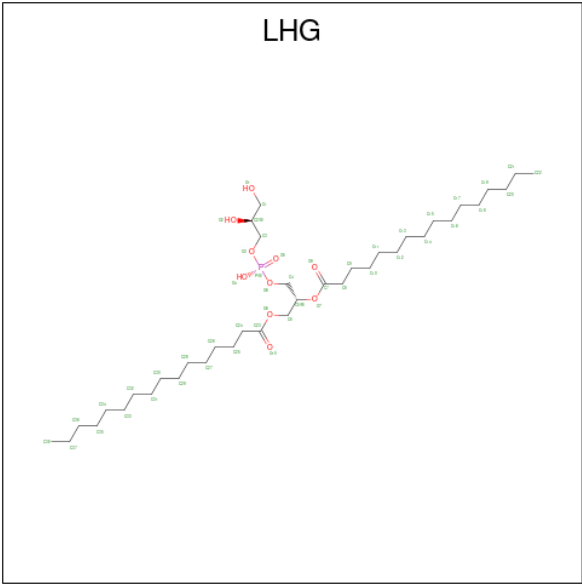
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			4	1	3	
30	a	1	Total	C	O	0
			4	1	3	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



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

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



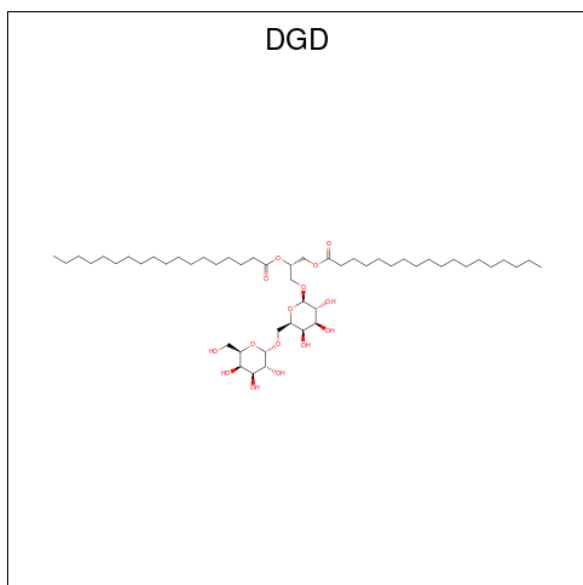
Mol	Chain	Residues	Atoms				AltConf
32	B	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

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

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



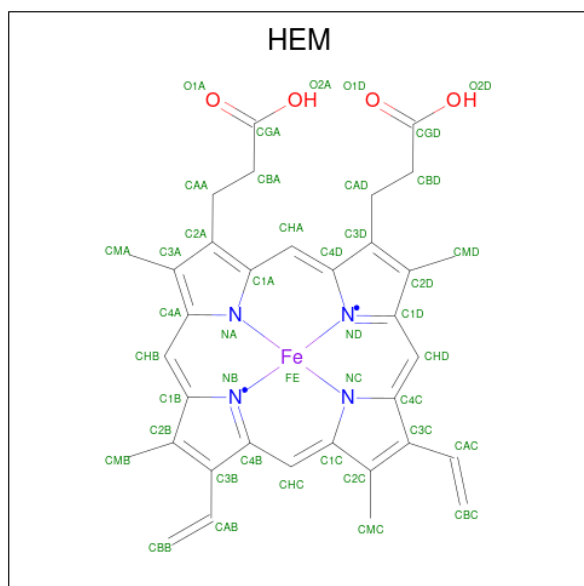
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			62	47	15	
33	C	1	Total	C	O	0
			62	47	15	

Continued on next page...

Continued from previous page...

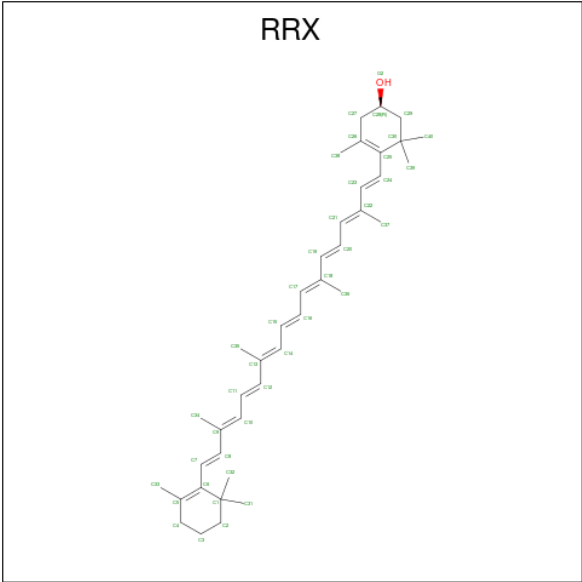
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total 62	C 47	O 15	0
33	H	1	Total 62	C 47	O 15	0
33	c	1	Total 62	C 47	O 15	0
33	c	1	Total 62	C 47	O 15	0
33	c	1	Total 62	C 47	O 15	0
33	h	1	Total 62	C 47	O 15	0

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



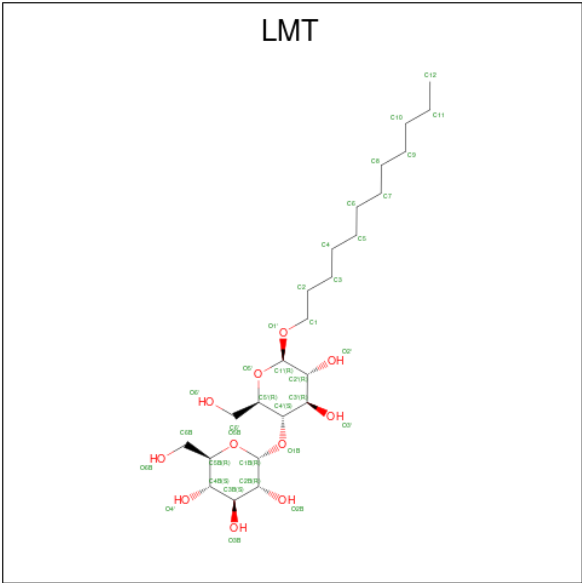
Mol	Chain	Residues	Atoms					AltConf
34	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
34	e	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



Mol	Chain	Residues	Atoms			AltConf
35	H	1	Total	C	O	0
			41	40	1	
35	h	1	Total	C	O	0
			41	40	1	

- Molecule 36 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
36	I	1	Total	C	O	0
			35	24	11	
36	J	1	Total	C	O	0
			24	18	6	

Continued on next page...

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

- | Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 37 | J | 1 | Total
1 | Mg
1 | 0 |
| 37 | j | 1 | Total
1 | Mg
1 | 0 |

- # HEC

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



WORLD WIDE
PDB
PROTEIN DATA BANK

Continued from previous page...

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	142	Total	O	0
			142	142	
39	B	252	Total	O	0
			252	252	
39	C	184	Total	O	0
			184	184	
39	D	145	Total	O	0
			145	145	
39	E	21	Total	O	0
			21	21	
39	F	2	Total	O	0
			2	2	
39	H	34	Total	O	0
			34	34	
39	I	13	Total	O	0
			13	13	
39	J	5	Total	O	0
			5	5	
39	K	3	Total	O	0
			3	3	
39	L	15	Total	O	0
			15	15	
39	M	6	Total	O	0
			6	6	
39	O	104	Total	O	0
			104	104	
39	T	9	Total	O	0
			9	9	
39	U	56	Total	O	0
			56	56	
39	V	63	Total	O	0
			63	63	
39	X	6	Total	O	0
			6	6	
39	a	141	Total	O	0
			141	141	

Continued on next page...

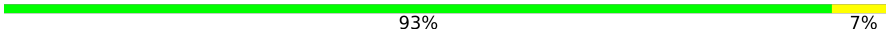
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
39	b	253	Total 253	O 253	0
39	c	184	Total 184	O 184	0
39	d	145	Total 145	O 145	0
39	e	21	Total 21	O 21	0
39	f	2	Total 2	O 2	0
39	h	34	Total 34	O 34	0
39	i	13	Total 13	O 13	0
39	j	5	Total 5	O 5	0
39	k	3	Total 3	O 3	0
39	l	15	Total 15	O 15	0
39	m	6	Total 6	O 6	0
39	o	105	Total 105	O 105	0
39	t	9	Total 9	O 9	0
39	u	56	Total 56	O 56	0
39	v	63	Total 63	O 63	0
39	x	6	Total 6	O 6	0

3 Residue-property plots [i](#)

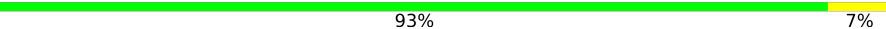
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

Chain A:  93% 7%



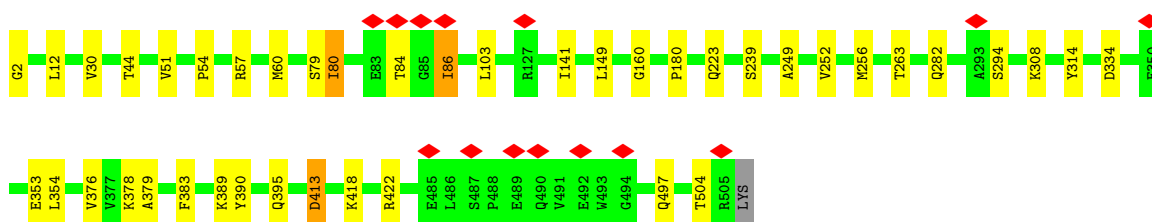
- Molecule 1: Photosystem II protein D1

Chain a:  93% 7%



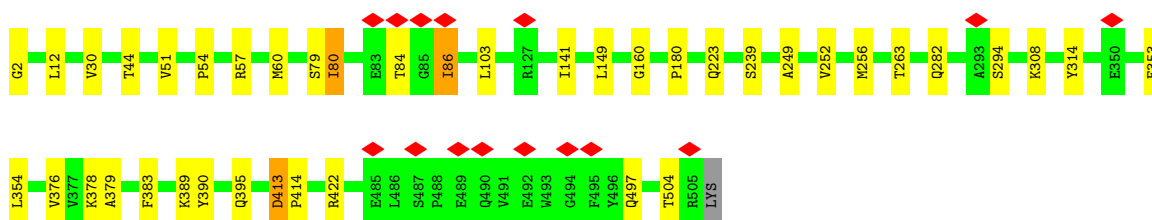
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  91% 8% .

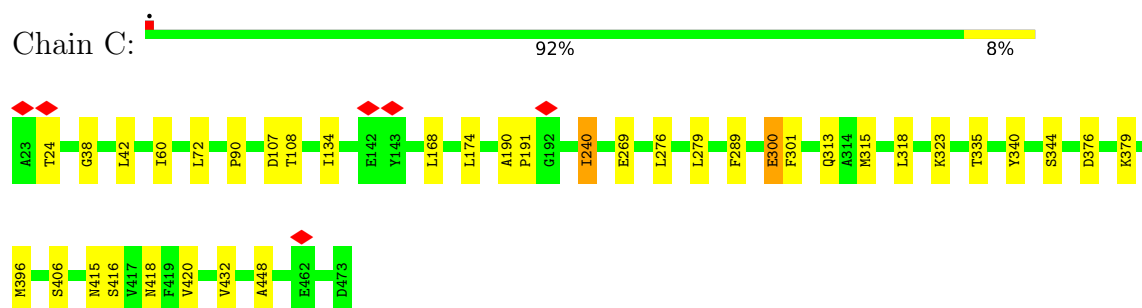


- Molecule 2: Photosystem II CP47 reaction center protein

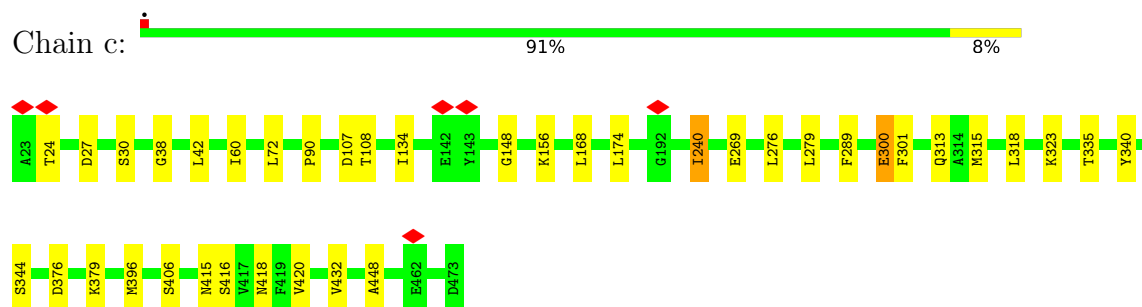
Chain b:  92% 8% .



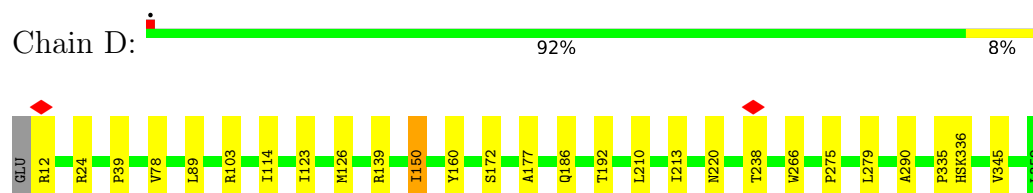
- Molecule 3: Photosystem II CP43 reaction center protein



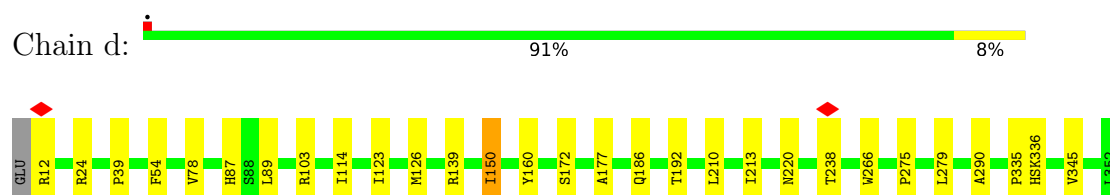
- Molecule 3: Photosystem II CP43 reaction center protein



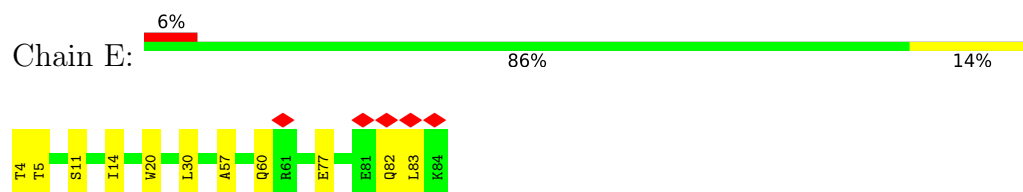
- Molecule 4: Photosystem II D2 protein



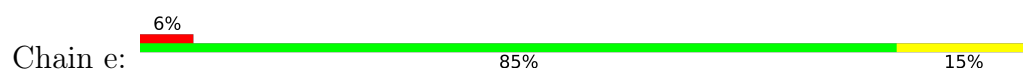
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



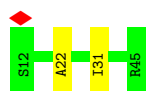
- Molecule 5: Cytochrome b559 subunit alpha





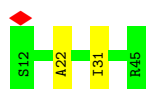
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 94% 6%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 94% 6%



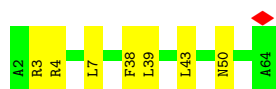
- Molecule 7: Photosystem II reaction center protein H

Chain H: 90% 10%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 89% 11%



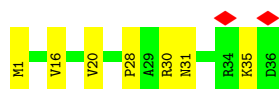
- Molecule 8: Photosystem II reaction center protein I

Chain I: 6% 81% 19%

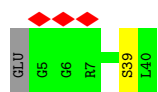


- Molecule 8: Photosystem II reaction center protein I

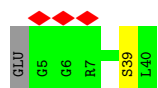
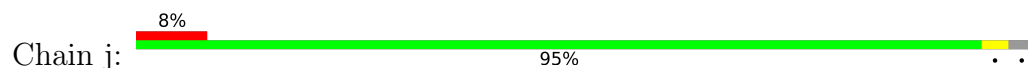
Chain i: 6% 81% 19%



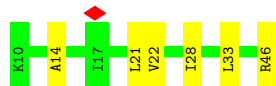
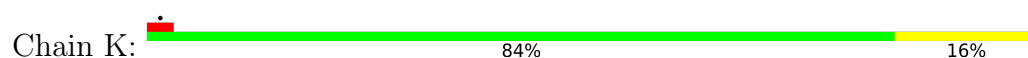
- Molecule 9: Photosystem II reaction center protein J



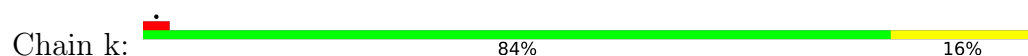
- Molecule 9: Photosystem II reaction center protein J



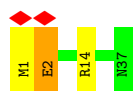
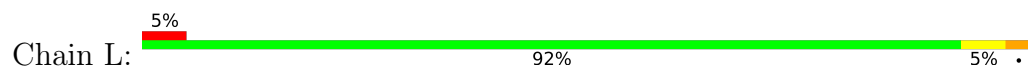
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K



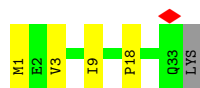
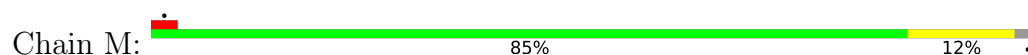
- Molecule 11: Photosystem II reaction center protein L



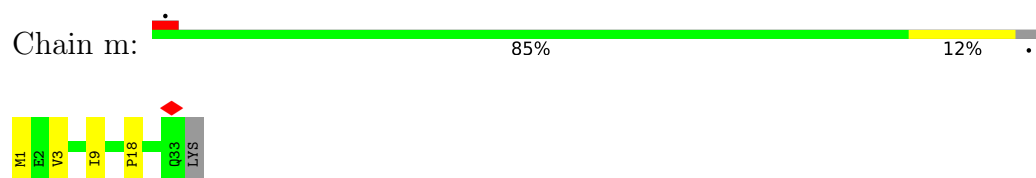
- Molecule 11: Photosystem II reaction center protein L



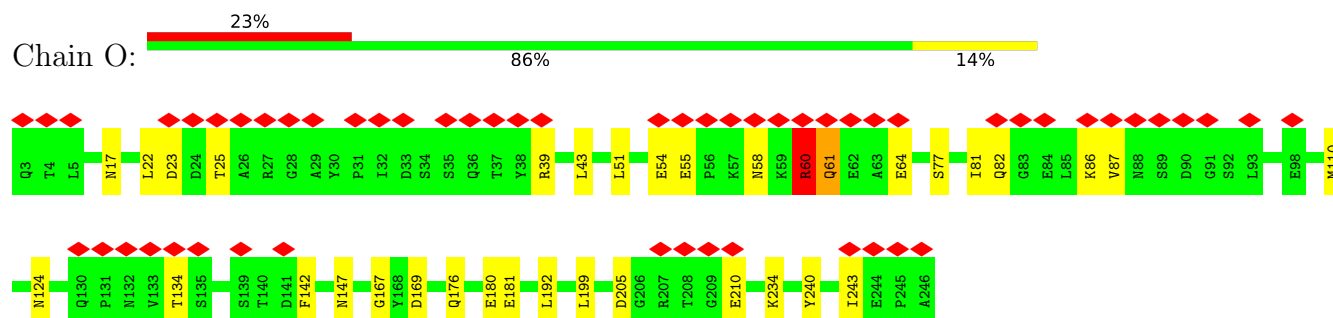
- Molecule 12: Photosystem II reaction center protein M



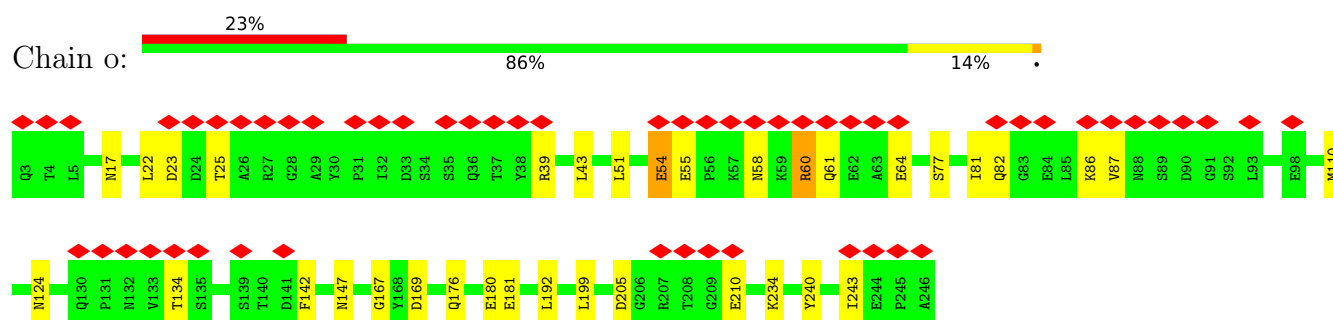
- Molecule 12: Photosystem II reaction center protein M



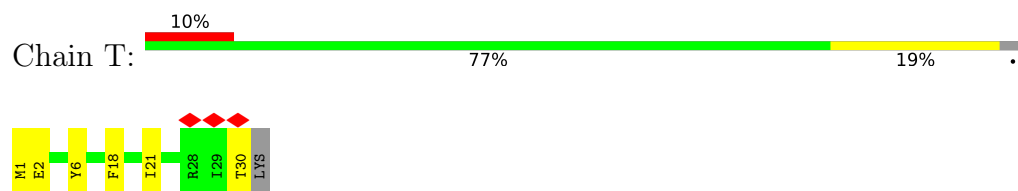
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



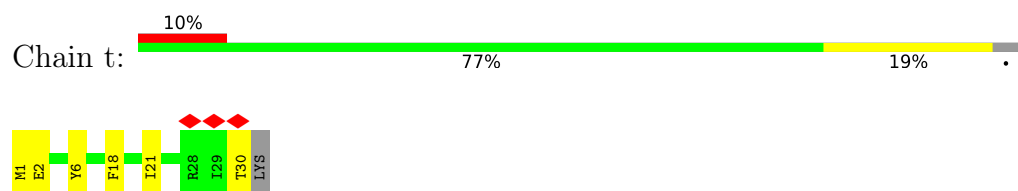
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



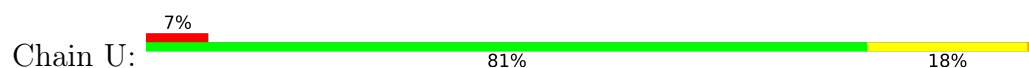
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

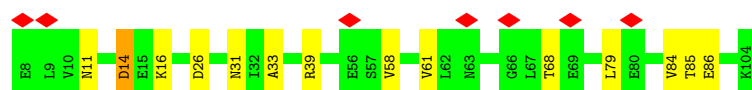
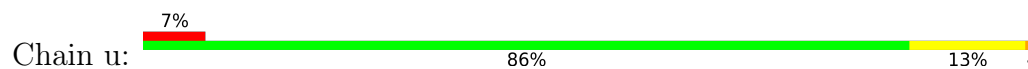


- Molecule 15: Photosystem II 12 kDa extrinsic protein

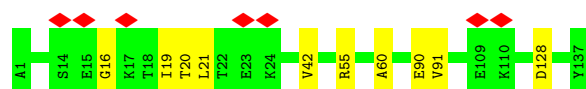




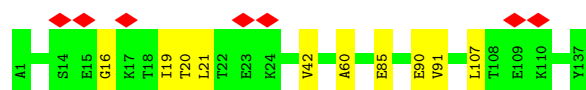
- Molecule 15: Photosystem II 12 kDa extrinsic protein



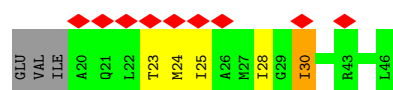
- Molecule 16: Cytochrome c-550



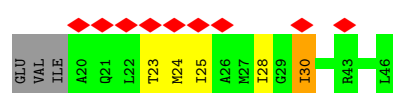
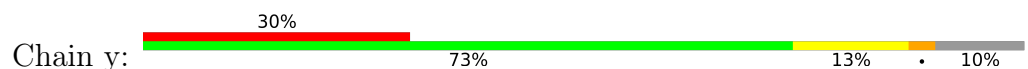
- Molecule 16: Cytochrome c-550



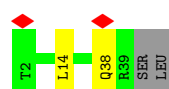
- Molecule 17: Photosystem II reaction center protein Ycf12



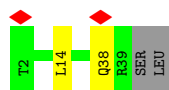
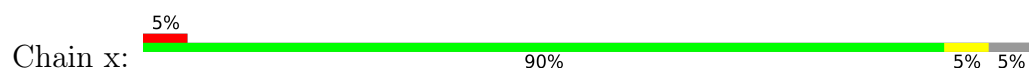
- Molecule 17: Photosystem II reaction center protein Ycf12



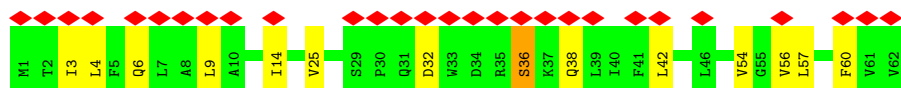
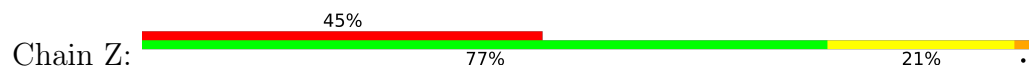
- Molecule 18: Photosystem II reaction center protein X



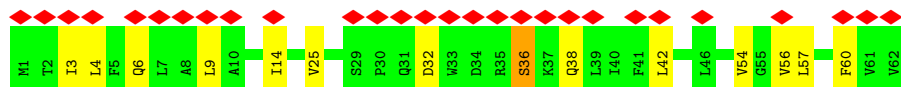
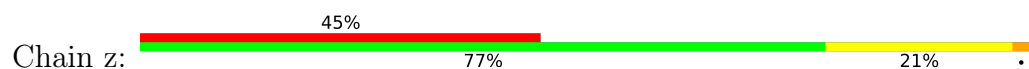
- Molecule 18: Photosystem II reaction center protein X



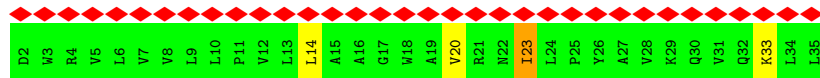
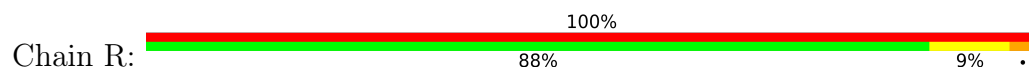
- Molecule 19: Photosystem II reaction center protein Z



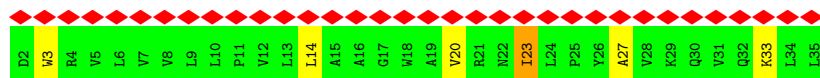
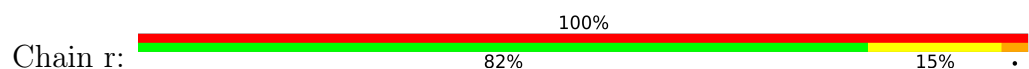
- Molecule 19: Photosystem II reaction center protein Z



- 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	0.057	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	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: RRX, UNL, LHG, PHO, PL9, HSK, DGD, HEC, OEX, HEM, FME, CLA, LMG, CL, FE2, MG, LMT, BCR, SQD, BCT

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	0.39	0/2705	0.60	0/3689
1	a	0.39	0/2705	0.60	0/3689
2	B	0.37	0/4109	0.55	0/5600
2	b	0.37	0/4109	0.55	0/5600
3	C	0.36	0/3599	0.54	0/4900
3	c	0.36	0/3599	0.54	0/4900
4	D	0.39	0/2800	0.59	0/3814
4	d	0.39	0/2800	0.59	0/3814
5	E	0.34	0/680	0.59	0/928
5	e	0.35	0/680	0.59	0/928
6	F	0.35	0/284	0.51	0/387
6	f	0.35	0/284	0.51	0/387
7	H	0.38	0/511	0.55	0/697
7	h	0.38	0/511	0.55	0/697
8	I	0.34	0/293	0.59	0/396
8	i	0.34	0/293	0.59	0/396
9	J	0.29	0/263	0.54	0/356
9	j	0.29	0/263	0.54	0/356
10	K	0.36	0/303	0.64	0/416
10	k	0.36	0/303	0.64	0/416
11	L	0.37	0/311	0.57	0/422
11	l	0.37	0/311	0.57	0/422
12	M	0.40	0/253	0.62	0/346
12	m	0.39	0/253	0.61	0/346
13	O	0.33	0/1905	0.57	0/2583
13	o	0.33	0/1905	0.57	0/2583
14	T	0.36	0/257	0.63	0/349
14	t	0.36	0/257	0.63	0/349
15	U	0.33	0/785	0.55	0/1064
15	u	0.33	0/785	0.55	0/1064
16	V	0.35	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.35	0/1085	0.53	0/1473
17	Y	0.31	0/201	0.58	0/268
17	y	0.31	0/201	0.57	0/268
18	X	0.29	0/284	0.51	0/384
18	x	0.29	0/284	0.51	0/384
19	Z	0.28	0/490	0.55	0/669
19	z	0.28	0/490	0.55	0/669
20	R	0.29	0/279	0.60	0/383
20	r	0.29	0/279	0.59	0/383
All	All	0.36	0/42794	0.57	0/58248

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
4	d	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	335	PRO	Mainchain
4	d	335	PRO	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2620	0	2517	18	0
1	a	2620	0	2517	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3969	0	3828	29	0
2	b	3969	0	3828	29	0
3	C	3486	0	3407	26	0
3	c	3486	0	3407	26	0
4	D	2718	0	2620	18	0
4	d	2718	0	2620	20	0
5	E	661	0	648	4	0
5	e	661	0	648	5	0
6	F	275	0	282	2	0
6	f	275	0	282	2	0
7	H	498	0	518	2	0
7	h	498	0	518	3	0
8	I	296	0	311	5	0
8	i	296	0	311	5	0
9	J	257	0	268	1	0
9	j	257	0	268	1	0
10	K	293	0	305	5	0
10	k	293	0	305	5	0
11	L	304	0	316	3	0
11	l	304	0	316	2	0
12	M	260	0	275	2	0
12	m	260	0	275	2	0
13	O	1874	0	1846	13	0
13	o	1874	0	1846	13	0
14	T	258	0	261	4	0
14	t	258	0	261	4	0
15	U	774	0	773	10	0
15	u	774	0	773	6	0
16	V	1064	0	1073	3	0
16	v	1064	0	1073	4	0
17	Y	200	0	226	4	0
17	y	200	0	226	4	0
18	X	281	0	312	2	0
18	x	281	0	312	2	0
19	Z	479	0	516	4	0
19	z	479	0	516	4	0
20	R	273	0	305	1	0
20	r	273	0	305	3	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	2	0	0	0	0
23	a	2	0	0	0	0
24	A	195	0	216	5	0
24	B	1040	0	1152	16	0
24	C	845	0	936	23	0
24	D	195	0	216	4	0
24	a	195	0	216	5	0
24	b	1040	0	1152	19	0
24	c	845	0	936	24	0
24	d	195	0	216	4	0
25	A	64	0	74	0	0
25	D	64	0	74	1	0
25	a	64	0	74	0	0
25	d	64	0	74	2	0
26	A	40	0	56	1	0
26	B	160	0	224	8	0
26	C	120	0	168	6	0
26	D	40	0	56	0	0
26	T	40	0	56	1	0
26	Y	40	0	56	1	0
26	a	40	0	56	1	0
26	b	120	0	168	1	0
26	c	120	0	168	4	0
26	d	40	0	56	0	0
26	y	40	0	56	0	0
27	A	108	0	154	2	0
27	D	45	0	56	0	0
27	L	54	0	77	1	0
27	a	108	0	154	3	0
27	d	45	0	56	0	0
27	l	54	0	77	1	0
28	A	55	0	80	2	0
28	D	55	0	80	2	0
28	a	55	0	80	2	0
28	d	55	0	80	1	0
29	A	36	0	0	0	0
29	B	85	0	0	0	0
29	C	10	0	0	0	0
29	D	40	0	0	0	0
29	E	10	0	0	0	0
29	I	17	0	0	0	0
29	J	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	34	0	0	0	0
29	M	10	0	0	0	0
29	T	26	0	0	0	0
29	X	10	0	0	0	0
29	a	36	0	0	0	0
29	b	85	0	0	0	0
29	c	10	0	0	0	0
29	d	40	0	0	0	0
29	e	10	0	0	0	0
29	i	17	0	0	0	0
29	j	10	0	0	0	0
29	k	34	0	0	0	0
29	m	10	0	0	0	0
29	t	26	0	0	0	0
29	x	10	0	0	0	0
30	A	4	0	0	0	0
30	a	4	0	0	0	0
31	B	51	0	72	2	0
31	C	153	0	216	5	0
31	D	51	0	72	1	0
31	b	51	0	72	2	0
31	c	153	0	216	5	0
31	d	51	0	72	1	0
32	B	49	0	74	2	0
32	D	144	0	213	3	0
32	E	49	0	74	1	0
32	b	49	0	74	2	0
32	d	144	0	213	3	0
32	e	49	0	74	1	0
33	C	186	0	242	6	0
33	H	62	0	82	1	0
33	c	186	0	242	6	0
33	h	62	0	82	2	0
34	E	43	0	30	3	0
34	e	43	0	30	3	0
35	H	41	0	56	7	0
35	h	41	0	56	9	0
36	I	35	0	44	2	0
36	J	24	0	35	1	0
36	M	35	0	43	0	0
36	Z	35	0	44	0	0
36	i	35	0	44	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	j	24	0	35	1	0
36	m	35	0	43	0	0
36	z	35	0	44	0	0
37	J	1	0	0	0	0
37	j	1	0	0	0	0
38	V	43	0	30	0	0
38	v	43	0	30	0	0
39	A	142	0	0	3	0
39	B	252	0	0	5	0
39	C	184	0	0	2	0
39	D	145	0	0	2	0
39	E	21	0	0	0	0
39	F	2	0	0	0	0
39	H	34	0	0	0	0
39	I	13	0	0	1	0
39	J	5	0	0	0	0
39	K	3	0	0	1	0
39	L	15	0	0	0	0
39	M	6	0	0	0	0
39	O	104	0	0	0	0
39	T	9	0	0	0	0
39	U	56	0	0	1	0
39	V	63	0	0	0	0
39	X	6	0	0	0	0
39	a	141	0	0	3	0
39	b	253	0	0	5	0
39	c	184	0	0	2	0
39	d	145	0	0	2	0
39	e	21	0	0	0	0
39	f	2	0	0	0	0
39	h	34	0	0	0	0
39	i	13	0	0	1	0
39	j	5	0	0	0	0
39	k	3	0	0	1	0
39	l	15	0	0	0	0
39	m	6	0	0	0	0
39	o	105	0	0	0	0
39	t	9	0	0	0	0
39	u	56	0	0	0	0
39	v	63	0	0	1	0
39	x	6	0	0	0	0
All	All	52655	0	51218	380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 380 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:h:101:RRX:H55	35:h:101:RRX:H46	1.73	0.70
1:a:341:LEU:H	3:c:313:GLN:HE22	1.38	0.70
24:c:504:CLA:H193	24:c:511:CLA:HAB	1.75	0.69
35:H:101:RRX:H55	35:H:101:RRX:H46	1.73	0.69
24:C:504:CLA:H193	24:C:511:CLA:HAB	1.75	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	326 (98%)	5 (2%)	1 (0%)	36	36
1	a	332/334 (99%)	326 (98%)	5 (2%)	1 (0%)	36	36
2	B	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
2	b	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
3	C	449/451 (100%)	439 (98%)	9 (2%)	1 (0%)	43	44
3	c	449/451 (100%)	439 (98%)	9 (2%)	1 (0%)	43	44
4	D	338/342 (99%)	329 (97%)	9 (3%)	0	100	100
4	d	338/342 (99%)	329 (97%)	9 (3%)	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
9	j	34/37 (92%)	32 (94%)	2 (6%)	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%)	229 (95%)	11 (4%)	2 (1%)	16	12
13	o	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	16	12
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%)	92 (97%)	3 (3%)	0	100	100
15	u	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	18	14
16	v	135/137 (98%)	130 (96%)	4 (3%)	1 (1%)	18	14
17	Y	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
17	y	25/30 (83%)	24 (96%)	1 (4%)	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%)	56 (93%)	4 (7%)	0	100	100
19	z	60/62 (97%)	56 (93%)	4 (7%)	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	5230/5332 (98%)	5102 (98%)	118 (2%)	10 (0%)	44	44

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	58	ASN
3	c	416	SER
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	269/269 (100%)	268 (100%)	1 (0%)	84	89
1	a	269/269 (100%)	268 (100%)	1 (0%)	84	89
2	B	402/403 (100%)	394 (98%)	8 (2%)	48	54
2	b	402/403 (100%)	394 (98%)	8 (2%)	48	54
3	C	352/352 (100%)	346 (98%)	6 (2%)	53	60
3	c	352/352 (100%)	346 (98%)	6 (2%)	53	60
4	D	275/276 (100%)	272 (99%)	3 (1%)	65	73
4	d	275/276 (100%)	272 (99%)	3 (1%)	65	73
5	E	72/72 (100%)	67 (93%)	5 (7%)	14	11
5	e	72/72 (100%)	67 (93%)	5 (7%)	14	11
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%)	49 (92%)	4 (8%)	12	9
7	h	53/53 (100%)	49 (92%)	4 (8%)	12	9
8	I	32/32 (100%)	31 (97%)	1 (3%)	35	38
8	i	32/32 (100%)	31 (97%)	1 (3%)	35	38
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	35
10	k	30/30 (100%)	29 (97%)	1 (3%)	33	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	40
11	l	35/35 (100%)	34 (97%)	1 (3%)	37	40
12	M	29/30 (97%)	28 (97%)	1 (3%)	32	34
12	m	29/30 (97%)	28 (97%)	1 (3%)	32	34
13	O	207/207 (100%)	193 (93%)	14 (7%)	14	11
13	o	207/207 (100%)	193 (93%)	14 (7%)	14	11
14	T	26/27 (96%)	25 (96%)	1 (4%)	29	30
14	t	26/27 (96%)	25 (96%)	1 (4%)	29	30
15	U	84/84 (100%)	80 (95%)	4 (5%)	23	22
15	u	84/84 (100%)	80 (95%)	4 (5%)	23	22
16	V	117/117 (100%)	113 (97%)	4 (3%)	32	34
16	v	117/117 (100%)	113 (97%)	4 (3%)	32	34
17	Y	20/23 (87%)	18 (90%)	2 (10%)	7	4
17	y	20/23 (87%)	18 (90%)	2 (10%)	7	4
18	X	31/33 (94%)	31 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	44 (85%)	8 (15%)	2	1
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	1
20	R	29/29 (100%)	26 (90%)	3 (10%)	7	4
20	r	29/29 (100%)	26 (90%)	3 (10%)	7	4
All	All	4334/4354 (100%)	4200 (97%)	134 (3%)	36	38

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	u	68	THR
16	v	21	LEU
19	z	56	VAL
15	U	68	THR
15	U	61	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
16	V	34	GLN
15	u	31	ASN
2	b	331	ASN
13	o	196	GLN
16	v	25	GLN

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$
14	FME	t	1	14	8,9,10	1.00	0	8,9,11	1.43	2 (25%)
14	FME	T	1	14	8,9,10	1.01	0	8,9,11	1.43	2 (25%)
8	FME	i	1	8	8,9,10	0.86	0	8,9,11	1.17	1 (12%)
8	FME	I	1	8	8,9,10	0.88	0	8,9,11	1.17	1 (12%)
4	HSK	D	336	4	10,11,12	1.88	2 (20%)	5,14,16	1.03	0
4	HSK	d	336	4	10,11,12	1.89	2 (20%)	5,14,16	1.03	0
12	FME	M	1	12	8,9,10	1.06	1 (12%)	8,9,11	0.91	0
12	FME	m	1	12	8,9,10	1.05	1 (12%)	8,9,11	0.90	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
14	FME	t	1	14	-	3/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
4	HSK	D	336	4	-	1/5/6/8	0/1/1/1
4	HSK	d	336	4	-	1/5/6/8	0/1/1/1
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	HSK	OM-ND1	-4.05	1.30	1.38
4	D	336	HSK	OM-ND1	-4.01	1.31	1.38
4	D	336	HSK	CD2-CG	3.32	1.41	1.36
4	d	336	HSK	CD2-CG	3.32	1.41	1.36
12	M	1	FME	CA-N	-2.09	1.43	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	2.87	115.04	109.50
14	T	1	FME	C-CA-N	2.86	115.01	109.50
8	I	1	FME	C-CA-N	2.24	113.83	109.50
8	i	1	FME	C-CA-N	2.22	113.78	109.50
14	T	1	FME	CB-CA-N	2.18	114.48	110.52

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	336	HSK	O-C-CA-CB
12	M	1	FME	CB-CA-N-CN
4	d	336	HSK	O-C-CA-CB
12	m	1	FME	CB-CA-N-CN
14	T	1	FME	N-CA-CB-CG

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
24	CLA	C	514	3	69,73,73	2.03	19 (27%)	82,113,113	2.74	36 (43%)
31	LMG	C	520	-	51,51,55	1.01	5 (9%)	59,59,63	1.42	7 (11%)
34	HEM	E	103	5,6	50,50,50	1.51	9 (18%)	67,82,82	1.38	9 (13%)
32	LHG	b	627	-	48,48,48	0.79	1 (2%)	51,54,54	1.23	5 (9%)
21	OEX	a	401	1,3,39	0,15,15	-	-	-	-	-
30	BCT	a	414	22	3,3,3	1.22	0	2,3,3	4.52	2 (100%)
36	LMT	j	102	-	24,24,36	1.08	2 (8%)	29,29,47	1.15	2 (6%)
24	CLA	b	614	2	69,73,73	1.83	19 (27%)	82,113,113	2.56	35 (42%)
26	BCR	T	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.31	8 (14%)
35	RRX	H	101	-	42,42,42	1.93	10 (23%)	56,58,58	2.02	16 (28%)
24	CLA	B	603	2	69,73,73	1.93	18 (26%)	82,113,113	2.63	31 (37%)
24	CLA	B	616	2	69,73,73	1.89	18 (26%)	82,113,113	2.64	31 (37%)
32	LHG	D	409	-	48,48,48	0.87	3 (6%)	51,54,54	1.18	6 (11%)
31	LMG	D	411	37	51,51,55	0.97	6 (11%)	59,59,63	1.34	8 (13%)
24	CLA	B	611	2	69,73,73	1.90	18 (26%)	82,113,113	2.44	26 (31%)
26	BCR	d	405	-	41,41,41	1.15	3 (7%)	56,56,56	1.17	7 (12%)
32	LHG	d	408	-	48,48,48	0.82	1 (2%)	51,54,54	1.33	6 (11%)
33	DGD	C	517	-	63,63,67	1.18	7 (11%)	77,77,81	1.37	7 (9%)
31	LMG	c	522	-	51,51,55	0.89	4 (7%)	59,59,63	1.46	7 (11%)
33	DGD	c	518	-	63,63,67	1.22	8 (12%)	77,77,81	1.38	9 (11%)
32	LHG	D	408	-	48,48,48	0.82	1 (2%)	51,54,54	1.33	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	613	2	69,73,73	1.90	18 (26%)	82,113,113	2.44	26 (31%)
36	LMT	i	102	-	36,36,36	1.29	5 (13%)	47,47,47	1.27	3 (6%)
27	SQD	A	412	-	52,54,54	0.95	4 (7%)	62,65,65	1.67	11 (17%)
24	CLA	c	511	3	69,73,73	1.96	18 (26%)	82,113,113	2.56	29 (35%)
31	LMG	c	520	-	51,51,55	1.01	5 (9%)	59,59,63	1.42	7 (11%)
28	PL9	A	411	-	55,55,55	1.48	9 (16%)	68,69,69	1.50	12 (17%)
24	CLA	c	509	3	69,73,73	1.92	19 (27%)	82,113,113	2.59	26 (31%)
33	DGD	H	102	-	63,63,67	1.08	4 (6%)	77,77,81	1.16	5 (6%)
26	BCR	C	516	-	41,41,41	1.03	2 (4%)	56,56,56	1.19	5 (8%)
32	LHG	d	409	-	48,48,48	0.87	3 (6%)	51,54,54	1.18	6 (11%)
24	CLA	B	610	39	69,73,73	1.95	21 (30%)	82,113,113	2.56	31 (37%)
24	CLA	C	507	3	69,73,73	1.95	17 (24%)	82,113,113	2.53	32 (39%)
21	OEX	A	401	1,3,39	0,15,15	-	-	-	-	-
31	LMG	c	501	-	51,51,55	0.95	3 (5%)	59,59,63	1.35	6 (10%)
24	CLA	c	512	3	69,73,73	1.93	21 (30%)	82,113,113	2.63	30 (36%)
26	BCR	Y	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.23	8 (14%)
33	DGD	h	102	-	63,63,67	1.08	4 (6%)	77,77,81	1.16	5 (6%)
24	CLA	A	408	1	69,73,73	1.92	19 (27%)	82,113,113	2.62	33 (40%)
30	BCT	A	414	22	3,3,3	1.22	0	2,3,3	4.51	2 (100%)
33	DGD	c	517	-	63,63,67	1.18	7 (11%)	77,77,81	1.37	7 (9%)
24	CLA	C	508	39	69,73,73	1.90	19 (27%)	82,113,113	2.67	30 (36%)
24	CLA	b	606	2	69,73,73	1.89	19 (27%)	82,113,113	2.55	35 (42%)
24	CLA	B	606	2	69,73,73	1.94	20 (28%)	82,113,113	2.68	32 (39%)
24	CLA	C	509	3	69,73,73	1.92	19 (27%)	82,113,113	2.59	26 (31%)
24	CLA	B	608	2	69,73,73	1.93	21 (30%)	82,113,113	2.41	32 (39%)
26	BCR	B	618	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	6 (10%)
24	CLA	B	609	2	69,73,73	1.95	16 (23%)	82,113,113	2.63	33 (40%)
24	CLA	b	605	2	69,73,73	1.93	18 (26%)	82,113,113	2.63	31 (37%)
31	LMG	b	622	-	51,51,55	0.92	2 (3%)	59,59,63	1.28	7 (11%)
33	DGD	c	519	-	63,63,67	1.15	8 (12%)	77,77,81	1.26	6 (7%)
24	CLA	A	406	39	69,73,73	2.00	19 (27%)	82,113,113	2.60	30 (36%)
26	BCR	b	619	-	41,41,41	1.01	2 (4%)	56,56,56	1.13	4 (7%)
24	CLA	B	615	2	69,73,73	1.90	19 (27%)	82,113,113	2.56	30 (36%)
24	CLA	D	401	39	69,73,73	2.03	20 (28%)	82,113,113	2.66	32 (39%)
24	CLA	C	513	3	69,73,73	1.93	20 (28%)	82,113,113	2.55	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	a	405	1	69,73,73	1.95	22 (31%)	82,113,113	2.48	28 (34%)
24	CLA	B	607	39	69,73,73	1.91	17 (24%)	82,113,113	2.65	32 (39%)
24	CLA	c	510	3	69,73,73	1.98	19 (27%)	82,113,113	2.67	34 (41%)
27	SQD	d	407	-	43,45,54	1.10	5 (11%)	53,56,65	1.91	12 (22%)
24	CLA	C	506	3	69,73,73	1.92	23 (33%)	82,113,113	2.54	27 (32%)
38	HEC	V	201	16	46,50,50	1.92	7 (15%)	58,82,82	1.30	4 (6%)
26	BCR	B	617	-	41,41,41	1.01	2 (4%)	56,56,56	1.13	4 (7%)
24	CLA	B	613	2	69,73,73	1.93	21 (30%)	82,113,113	2.64	29 (35%)
36	LMT	Z	101	-	36,36,36	1.16	6 (16%)	47,47,47	1.02	3 (6%)
24	CLA	C	512	3	69,73,73	1.93	21 (30%)	82,113,113	2.63	31 (37%)
36	LMT	m	102	-	36,36,36	1.26	6 (16%)	47,47,47	0.96	1 (2%)
26	BCR	A	409	-	41,41,41	1.07	3 (7%)	56,56,56	1.28	6 (10%)
31	LMG	C	501	-	51,51,55	0.95	3 (5%)	59,59,63	1.35	6 (10%)
24	CLA	B	605	2	69,73,73	1.86	18 (26%)	82,113,113	2.65	30 (36%)
28	PL9	d	406	-	55,55,55	1.41	7 (12%)	68,69,69	1.47	12 (17%)
31	LMG	B	620	-	51,51,55	0.92	2 (3%)	59,59,63	1.28	7 (11%)
24	CLA	b	611	2	69,73,73	1.95	16 (23%)	82,113,113	2.63	33 (40%)
24	CLA	b	604	2	69,73,73	1.97	19 (27%)	82,113,113	2.73	31 (37%)
27	SQD	a	412	-	52,54,54	0.95	4 (7%)	62,65,65	1.67	12 (19%)
26	BCR	a	409	-	41,41,41	1.07	3 (7%)	56,56,56	1.28	6 (10%)
25	PHO	A	407	-	58,69,69	2.20	9 (15%)	55,99,99	1.53	8 (14%)
24	CLA	C	511	3	69,73,73	1.96	18 (26%)	82,113,113	2.56	29 (35%)
32	LHG	e	101	-	48,48,48	0.69	1 (2%)	51,54,54	1.22	6 (11%)
24	CLA	c	507	3	69,73,73	1.95	17 (24%)	82,113,113	2.53	32 (39%)
36	LMT	I	102	-	36,36,36	1.29	5 (13%)	47,47,47	1.27	3 (6%)
24	CLA	A	405	1	69,73,73	1.95	22 (31%)	82,113,113	2.49	28 (34%)
24	CLA	B	614	2	69,73,73	1.93	18 (26%)	82,113,113	2.56	31 (37%)
26	BCR	b	621	-	41,41,41	1.08	2 (4%)	56,56,56	1.09	2 (3%)
24	CLA	b	608	2	69,73,73	1.94	20 (28%)	82,113,113	2.68	31 (37%)
26	BCR	b	620	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	7 (12%)
36	LMT	J	102	-	24,24,36	1.08	2 (8%)	29,29,47	1.15	1 (3%)
35	RRX	h	101	-	42,42,42	1.93	10 (23%)	56,58,58	2.02	16 (28%)
26	BCR	c	521	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
24	CLA	B	612	2	69,73,73	1.83	19 (27%)	82,113,113	2.56	35 (42%)
27	SQD	D	407	-	43,45,54	1.10	5 (11%)	53,56,65	1.92	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	618	2	69,73,73	1.89	18 (26%)	82,113,113	2.64	31 (37%)
24	CLA	d	403	4	69,73,73	1.86	20 (28%)	82,113,113	2.51	34 (41%)
24	CLA	d	404	4	69,73,73	1.97	21 (30%)	82,113,113	2.74	32 (39%)
24	CLA	c	514	3	69,73,73	2.02	19 (27%)	82,113,113	2.74	36 (43%)
26	BCR	B	627	-	41,41,41	0.98	2 (4%)	56,56,56	1.31	8 (14%)
24	CLA	D	403	4	69,73,73	1.86	19 (27%)	82,113,113	2.51	34 (41%)
24	CLA	c	502	3	69,73,73	1.90	19 (27%)	82,113,113	2.59	26 (31%)
24	CLA	c	506	3	69,73,73	1.92	22 (31%)	82,113,113	2.54	28 (34%)
25	PHO	a	407	-	58,69,69	2.20	9 (15%)	55,99,99	1.53	8 (14%)
24	CLA	b	617	2	69,73,73	1.90	19 (27%)	82,113,113	2.56	30 (36%)
36	LMT	z	101	-	36,36,36	1.16	6 (16%)	47,47,47	1.01	3 (6%)
24	CLA	C	503	3	69,73,73	1.91	19 (27%)	82,113,113	2.51	27 (32%)
24	CLA	b	616	2	69,73,73	1.93	18 (26%)	82,113,113	2.56	31 (37%)
26	BCR	B	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.09	2 (3%)
27	SQD	L	101	-	52,54,54	0.92	5 (9%)	62,65,65	1.99	11 (17%)
24	CLA	d	401	39	69,73,73	2.03	20 (28%)	82,113,113	2.66	32 (39%)
24	CLA	b	603	39	69,73,73	1.99	21 (30%)	82,113,113	2.65	29 (35%)
24	CLA	b	610	2	69,73,73	1.93	21 (30%)	82,113,113	2.41	32 (39%)
24	CLA	b	607	2	69,73,73	1.87	18 (26%)	82,113,113	2.65	30 (36%)
24	CLA	c	513	3	69,73,73	1.93	20 (28%)	82,113,113	2.55	29 (35%)
24	CLA	C	510	3	69,73,73	1.97	19 (27%)	82,113,113	2.67	34 (41%)
26	BCR	y	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.23	8 (14%)
28	PL9	D	406	-	55,55,55	1.40	7 (12%)	68,69,69	1.47	11 (16%)
24	CLA	C	504	3	69,73,73	1.99	23 (33%)	82,113,113	2.59	27 (32%)
24	CLA	C	502	3	69,73,73	1.90	19 (27%)	82,113,113	2.58	26 (31%)
24	CLA	c	508	39	69,73,73	1.90	19 (27%)	82,113,113	2.67	30 (36%)
24	CLA	D	404	4	69,73,73	1.97	21 (30%)	82,113,113	2.74	32 (39%)
27	SQD	l	101	-	52,54,54	0.92	5 (9%)	62,65,65	1.99	11 (17%)
27	SQD	a	410	-	52,54,54	0.95	6 (11%)	62,65,65	1.88	10 (16%)
24	CLA	b	609	39	69,73,73	1.91	17 (24%)	82,113,113	2.65	32 (39%)
26	BCR	C	515	-	41,41,41	1.10	3 (7%)	56,56,56	1.30	6 (10%)
24	CLA	a	408	1	69,73,73	1.93	19 (27%)	82,113,113	2.62	33 (40%)
24	CLA	c	503	3	69,73,73	1.91	19 (27%)	82,113,113	2.51	27 (32%)
27	SQD	A	410	-	52,54,54	0.95	6 (11%)	62,65,65	1.87	10 (16%)
31	LMG	d	411	37	51,51,55	0.97	6 (11%)	59,59,63	1.34	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	505	39	69,73,73	1.96	20 (28%)	82,113,113	2.72	33 (40%)
36	LMT	M	101	-	36,36,36	1.26	6 (16%)	47,47,47	0.96	2 (4%)
24	CLA	b	615	2	69,73,73	1.93	21 (30%)	82,113,113	2.64	28 (34%)
24	CLA	B	601	39	69,73,73	1.99	21 (30%)	82,113,113	2.65	29 (35%)
24	CLA	B	602	2	69,73,73	1.98	19 (27%)	82,113,113	2.73	31 (37%)
32	LHG	d	410	-	45,45,48	0.79	2 (4%)	48,51,54	1.16	5 (10%)
31	LMG	C	522	-	51,51,55	0.89	4 (7%)	59,59,63	1.46	7 (11%)
24	CLA	B	604	2	69,73,73	1.89	19 (27%)	82,113,113	2.55	35 (42%)
24	CLA	b	612	39	69,73,73	1.92	22 (31%)	82,113,113	2.64	30 (36%)
24	CLA	c	504	3	69,73,73	1.99	23 (33%)	82,113,113	2.59	27 (32%)
32	LHG	D	410	-	45,45,48	0.79	2 (4%)	48,51,54	1.16	5 (10%)
32	LHG	B	625	-	48,48,48	0.78	1 (2%)	51,54,54	1.23	5 (9%)
34	HEM	e	103	5,6	50,50,50	1.51	10 (20%)	67,82,82	1.39	9 (13%)
26	BCR	D	405	-	41,41,41	1.15	3 (7%)	56,56,56	1.17	7 (12%)
26	BCR	c	515	-	41,41,41	1.11	3 (7%)	56,56,56	1.30	6 (10%)
33	DGD	C	519	-	63,63,67	1.15	8 (12%)	77,77,81	1.26	6 (7%)
25	PHO	d	402	-	58,69,69	2.13	9 (15%)	55,99,99	1.65	10 (18%)
24	CLA	c	505	39	69,73,73	1.96	19 (27%)	82,113,113	2.71	33 (40%)
24	CLA	a	406	39	69,73,73	2.00	20 (28%)	82,113,113	2.60	31 (37%)
28	PL9	a	411	-	55,55,55	1.47	9 (16%)	68,69,69	1.50	12 (17%)
26	BCR	C	521	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	5 (8%)
26	BCR	c	516	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	5 (8%)
38	HEC	v	201	16	46,50,50	1.91	7 (15%)	58,82,82	1.30	4 (6%)
33	DGD	C	518	-	63,63,67	1.22	8 (12%)	77,77,81	1.38	9 (11%)
25	PHO	D	402	-	58,69,69	2.14	9 (15%)	55,99,99	1.64	11 (20%)
32	LHG	E	101	-	48,48,48	0.69	1 (2%)	51,54,54	1.22	6 (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
24	CLA	C	514	3	-	11/39/115/115	-
31	LMG	C	520	-	-	22/46/66/70	0/1/1/1
34	HEM	E	103	5,6	-	3/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	b	627	-	-	18/53/53/53	-
36	LMT	j	102	-	-	5/15/35/61	0/1/1/2
24	CLA	b	614	2	1/1/15/20	6/39/115/115	-
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2
35	RRX	H	101	-	-	1/29/65/65	0/2/2/2
24	CLA	B	603	2	1/1/15/20	10/39/115/115	-
24	CLA	B	616	2	1/1/15/20	11/39/115/115	-
32	LHG	D	409	-	-	17/53/53/53	-
31	LMG	D	411	37	-	16/46/66/70	0/1/1/1
24	CLA	B	611	2	1/1/15/20	6/39/115/115	-
26	BCR	d	405	-	-	4/29/63/63	0/2/2/2
32	LHG	d	408	-	-	12/53/53/53	-
33	DGD	C	517	-	-	17/51/91/95	0/2/2/2
31	LMG	c	522	-	-	25/46/66/70	0/1/1/1
33	DGD	c	518	-	-	23/51/91/95	0/2/2/2
32	LHG	D	408	-	-	12/53/53/53	-
24	CLA	b	613	2	1/1/15/20	6/39/115/115	-
36	LMT	i	102	-	-	10/21/61/61	0/2/2/2
27	SQD	A	412	-	-	19/49/69/69	0/1/1/1
24	CLA	c	511	3	1/1/15/20	6/39/115/115	-
31	LMG	c	520	-	-	22/46/66/70	0/1/1/1
28	PL9	A	411	-	-	13/53/73/73	0/1/1/1
24	CLA	c	509	3	1/1/15/20	1/39/115/115	-
33	DGD	H	102	-	-	14/51/91/95	0/2/2/2
26	BCR	C	516	-	-	8/29/63/63	0/2/2/2
32	LHG	d	409	-	-	17/53/53/53	-
24	CLA	B	610	39	1/1/15/20	8/39/115/115	-
24	CLA	C	507	3	1/1/15/20	13/39/115/115	-
31	LMG	c	501	-	-	21/46/66/70	0/1/1/1
24	CLA	c	512	3	1/1/15/20	5/39/115/115	-
26	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
33	DGD	h	102	-	-	14/51/91/95	0/2/2/2
24	CLA	A	408	1	1/1/15/20	14/39/115/115	-
33	DGD	c	517	-	-	17/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	508	39	1/1/15/20	10/39/115/115	-
24	CLA	b	606	2	1/1/15/20	5/39/115/115	-
24	CLA	B	606	2	1/1/15/20	3/39/115/115	-
24	CLA	C	509	3	1/1/15/20	1/39/115/115	-
24	CLA	B	608	2	-	2/39/115/115	-
26	BCR	B	618	-	-	3/29/63/63	0/2/2/2
24	CLA	B	609	2	1/1/15/20	4/39/115/115	-
24	CLA	b	605	2	1/1/15/20	10/39/115/115	-
31	LMG	b	622	-	-	18/46/66/70	0/1/1/1
33	DGD	c	519	-	-	16/51/91/95	0/2/2/2
24	CLA	A	406	39	-	8/39/115/115	-
26	BCR	b	619	-	-	7/29/63/63	0/2/2/2
24	CLA	B	615	2	1/1/15/20	5/39/115/115	-
24	CLA	D	401	39	1/1/15/20	6/39/115/115	-
24	CLA	C	513	3	1/1/15/20	10/39/115/115	-
24	CLA	a	405	1	1/1/15/20	5/39/115/115	-
24	CLA	B	607	39	1/1/15/20	4/39/115/115	-
24	CLA	c	510	3	1/1/15/20	5/39/115/115	-
27	SQD	d	407	-	-	17/40/60/69	0/1/1/1
24	CLA	C	506	3	1/1/15/20	5/39/115/115	-
38	HEC	V	201	16	-	6/14/54/54	-
26	BCR	B	617	-	-	7/29/63/63	0/2/2/2
24	CLA	B	613	2	1/1/15/20	8/39/115/115	-
36	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
24	CLA	C	512	3	1/1/15/20	5/39/115/115	-
36	LMT	m	102	-	-	4/21/61/61	0/2/2/2
26	BCR	A	409	-	-	7/29/63/63	0/2/2/2
31	LMG	C	501	-	-	21/46/66/70	0/1/1/1
24	CLA	B	605	2	1/1/15/20	8/39/115/115	-
28	PL9	d	406	-	-	10/53/73/73	0/1/1/1
31	LMG	B	620	-	-	18/46/66/70	0/1/1/1
24	CLA	b	611	2	1/1/15/20	4/39/115/115	-
24	CLA	b	604	2	1/1/15/20	3/39/115/115	-
27	SQD	a	412	-	-	19/49/69/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	a	409	-	-	7/29/63/63	0/2/2/2
25	PHO	A	407	-	-	2/37/103/103	0/5/6/6
24	CLA	C	511	3	1/1/15/20	6/39/115/115	-
32	LHG	e	101	-	-	24/53/53/53	-
24	CLA	c	507	3	1/1/15/20	13/39/115/115	-
36	LMT	I	102	-	-	10/21/61/61	0/2/2/2
24	CLA	A	405	1	1/1/15/20	5/39/115/115	-
24	CLA	B	614	2	1/1/15/20	11/39/115/115	-
26	BCR	b	621	-	-	10/29/63/63	0/2/2/2
24	CLA	b	608	2	1/1/15/20	3/39/115/115	-
26	BCR	b	620	-	-	3/29/63/63	0/2/2/2
36	LMT	J	102	-	-	5/15/35/61	0/1/1/2
35	RRX	h	101	-	-	1/29/65/65	0/2/2/2
26	BCR	c	521	-	-	7/29/63/63	0/2/2/2
24	CLA	B	612	2	1/1/15/20	6/39/115/115	-
27	SQD	D	407	-	-	17/40/60/69	0/1/1/1
24	CLA	b	618	2	1/1/15/20	11/39/115/115	-
24	CLA	d	403	4	1/1/15/20	4/39/115/115	-
24	CLA	d	404	4	1/1/15/20	11/39/115/115	-
24	CLA	c	514	3	-	11/39/115/115	-
26	BCR	B	627	-	-	8/29/63/63	0/2/2/2
24	CLA	D	403	4	1/1/15/20	4/39/115/115	-
24	CLA	c	502	3	1/1/15/20	4/39/115/115	-
24	CLA	c	506	3	1/1/15/20	5/39/115/115	-
25	PHO	a	407	-	-	2/37/103/103	0/5/6/6
24	CLA	b	617	2	1/1/15/20	5/39/115/115	-
36	LMT	z	101	-	-	11/21/61/61	0/2/2/2
24	CLA	b	616	2	1/1/15/20	11/39/115/115	-
24	CLA	C	503	3	-	8/39/115/115	-
26	BCR	B	619	-	-	10/29/63/63	0/2/2/2
27	SQD	L	101	-	-	23/49/69/69	0/1/1/1
24	CLA	d	401	39	1/1/15/20	6/39/115/115	-
24	CLA	b	603	39	1/1/15/20	10/39/115/115	-
24	CLA	b	610	2	-	2/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	607	2	1/1/15/20	8/39/115/115	-
24	CLA	c	513	3	1/1/15/20	10/39/115/115	-
24	CLA	C	510	3	1/1/15/20	5/39/115/115	-
26	BCR	y	101	-	-	5/29/63/63	0/2/2/2
28	PL9	D	406	-	-	10/53/73/73	0/1/1/1
24	CLA	C	504	3	1/1/15/20	6/39/115/115	-
24	CLA	C	502	3	1/1/15/20	4/39/115/115	-
24	CLA	c	508	39	1/1/15/20	10/39/115/115	-
24	CLA	D	404	4	1/1/15/20	11/39/115/115	-
27	SQD	l	101	-	-	23/49/69/69	0/1/1/1
27	SQD	a	410	-	-	21/49/69/69	0/1/1/1
24	CLA	b	609	39	1/1/15/20	4/39/115/115	-
26	BCR	C	515	-	-	7/29/63/63	0/2/2/2
24	CLA	a	408	1	1/1/15/20	14/39/115/115	-
24	CLA	c	503	3	-	8/39/115/115	-
27	SQD	A	410	-	-	21/49/69/69	0/1/1/1
31	LMG	d	411	37	-	16/46/66/70	0/1/1/1
24	CLA	C	505	39	1/1/15/20	6/39/115/115	-
36	LMT	M	101	-	-	4/21/61/61	0/2/2/2
24	CLA	b	615	2	1/1/15/20	8/39/115/115	-
24	CLA	B	601	39	1/1/15/20	10/39/115/115	-
24	CLA	B	602	2	1/1/15/20	3/39/115/115	-
32	LHG	d	410	-	-	15/50/50/53	-
31	LMG	C	522	-	-	25/46/66/70	0/1/1/1
24	CLA	B	604	2	1/1/15/20	5/39/115/115	-
24	CLA	b	612	39	-	8/39/115/115	-
24	CLA	c	504	3	1/1/15/20	6/39/115/115	-
32	LHG	D	410	-	-	15/50/50/53	-
32	LHG	B	625	-	-	18/53/53/53	-
34	HEM	e	103	5,6	-	3/14/54/54	-
26	BCR	D	405	-	-	4/29/63/63	0/2/2/2
26	BCR	c	515	-	-	7/29/63/63	0/2/2/2
33	DGD	C	519	-	-	16/51/91/95	0/2/2/2
25	PHO	d	402	-	-	3/37/103/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	505	39	1/1/15/20	6/39/115/115	-
24	CLA	a	406	39	-	8/39/115/115	-
28	PL9	a	411	-	-	13/53/73/73	0/1/1/1
26	BCR	C	521	-	-	7/29/63/63	0/2/2/2
26	BCR	c	516	-	-	8/29/63/63	0/2/2/2
38	HEC	v	201	16	-	6/14/54/54	-
33	DGD	C	518	-	-	23/51/91/95	0/2/2/2
25	PHO	D	402	-	-	3/37/103/103	0/5/6/6
32	LHG	E	101	-	-	24/53/53/53	-

The worst 5 of 1716 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	407	PHO	C1B-C2B	10.00	1.50	1.39
25	a	407	PHO	C1B-C2B	10.00	1.50	1.39
25	D	402	PHO	C1B-C2B	9.23	1.49	1.39
25	d	402	PHO	C1B-C2B	9.21	1.49	1.39
25	A	407	PHO	C3B-C4B	9.04	1.50	1.41

The worst 5 of 2693 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	C1D-ND-C4D	-10.23	99.14	106.31
24	D	404	CLA	C1D-ND-C4D	-10.15	99.19	106.31
24	C	512	CLA	C1D-ND-C4D	-9.96	99.32	106.31
24	c	512	CLA	C1D-ND-C4D	-9.96	99.32	106.31
24	B	613	CLA	C1D-ND-C4D	-9.95	99.33	106.31

5 of 61 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	408	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND

5 of 1428 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	603	CLA	C2-C3-C5-C6
24	B	603	CLA	C4-C3-C5-C6
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	B	616	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

110 monomers are involved in 185 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	514	CLA	1	0
31	C	520	LMG	2	0
34	E	103	HEM	3	0
32	b	627	LHG	2	0
36	j	102	LMT	1	0
24	b	614	CLA	2	0
26	T	101	BCR	1	0
35	H	101	RRX	7	0
24	B	616	CLA	1	0
32	D	409	LHG	2	0
31	D	411	LMG	1	0
24	B	611	CLA	1	0
31	c	522	LMG	3	0
33	c	518	DGD	3	0
24	b	613	CLA	2	0
36	i	102	LMT	2	0
27	A	412	SQD	1	0
24	c	511	CLA	3	0
31	c	520	LMG	2	0
28	A	411	PL9	2	0
24	c	509	CLA	3	0
33	H	102	DGD	1	0
26	C	516	BCR	1	0
32	d	409	LHG	2	0
24	c	512	CLA	3	0
26	Y	101	BCR	1	0
33	h	102	DGD	2	0
24	A	408	CLA	3	0
24	C	508	CLA	4	0
24	b	606	CLA	2	0
24	C	509	CLA	3	0
24	B	608	CLA	1	0
26	B	618	BCR	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	609	CLA	2	0
31	b	622	LMG	2	0
33	c	519	DGD	3	0
24	A	406	CLA	2	0
24	B	615	CLA	3	0
24	D	401	CLA	1	0
24	B	607	CLA	1	0
24	c	510	CLA	2	0
24	C	506	CLA	4	0
26	B	617	BCR	1	0
24	B	613	CLA	1	0
24	C	512	CLA	3	0
26	A	409	BCR	1	0
24	B	605	CLA	2	0
28	d	406	PL9	1	0
31	B	620	LMG	2	0
24	b	611	CLA	2	0
24	b	604	CLA	1	0
27	a	412	SQD	1	0
26	a	409	BCR	1	0
24	C	511	CLA	3	0
32	e	101	LHG	1	0
36	I	102	LMT	2	0
24	B	614	CLA	1	0
26	b	620	BCR	1	0
36	J	102	LMT	1	0
35	h	101	RRX	9	0
24	B	612	CLA	3	0
24	b	618	CLA	2	0
24	d	403	CLA	2	0
24	d	404	CLA	1	0
24	c	514	CLA	2	0
26	B	627	BCR	3	0
24	D	403	CLA	2	0
24	c	502	CLA	2	0
24	c	506	CLA	4	0
24	b	617	CLA	3	0
24	C	503	CLA	1	0
24	b	616	CLA	1	0
27	L	101	SQD	1	0
24	d	401	CLA	1	0
24	b	603	CLA	1	0

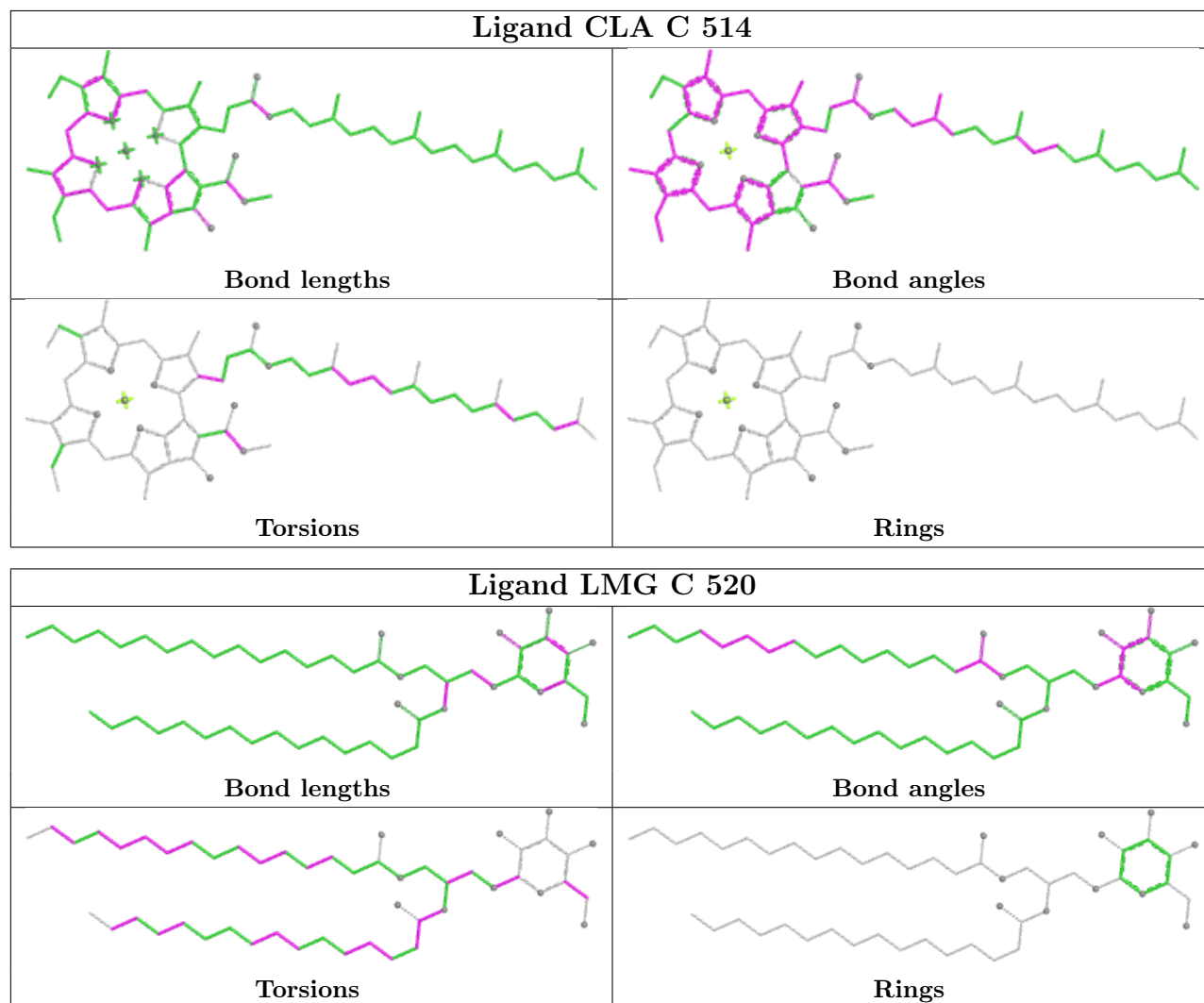
Continued on next page...

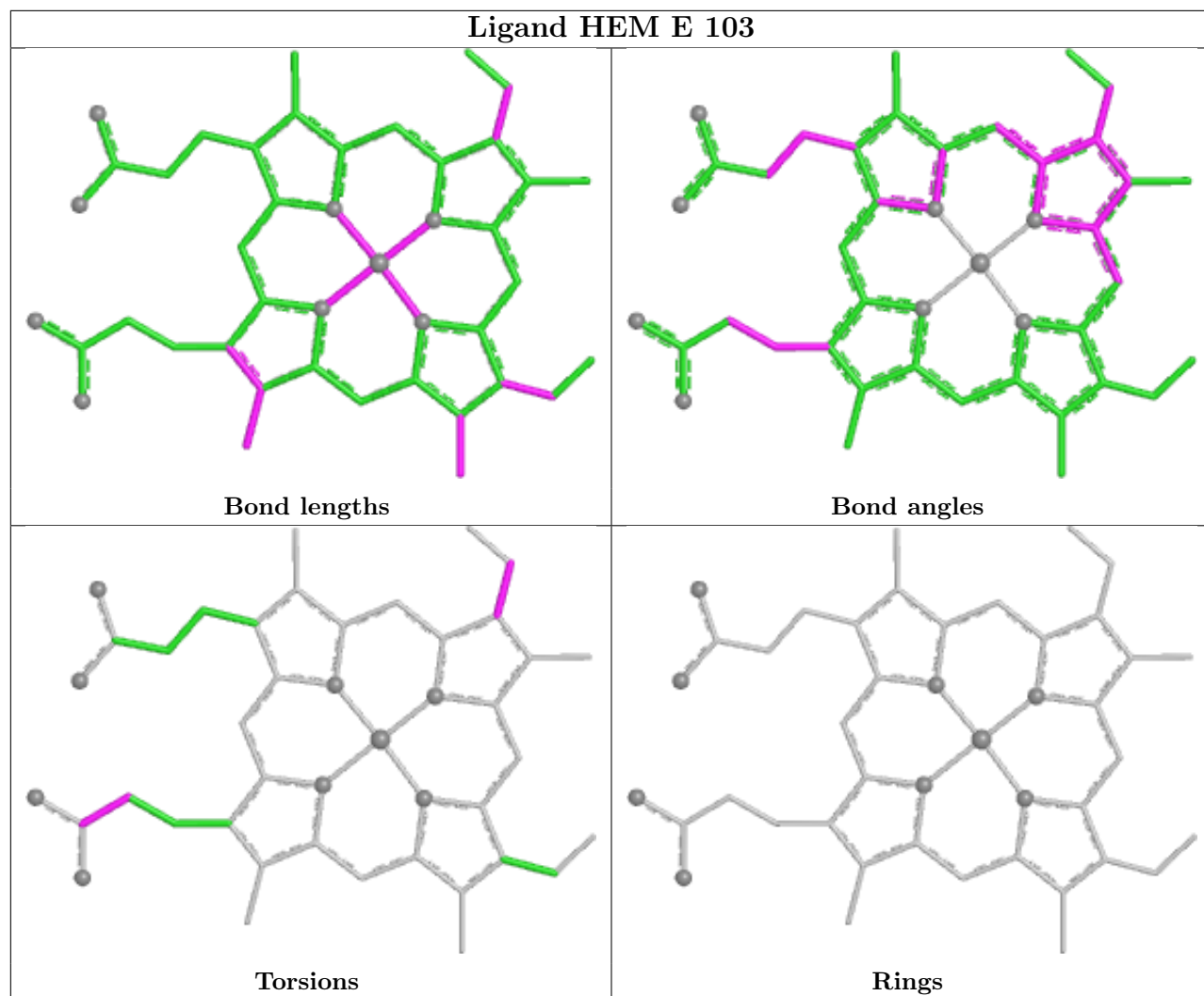
Continued from previous page...

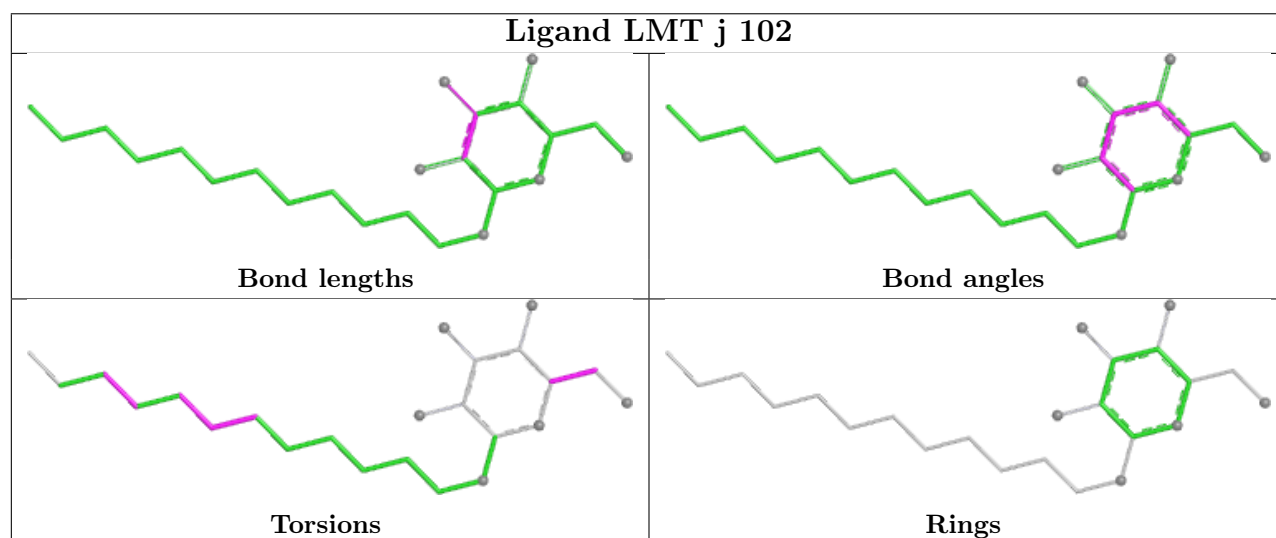
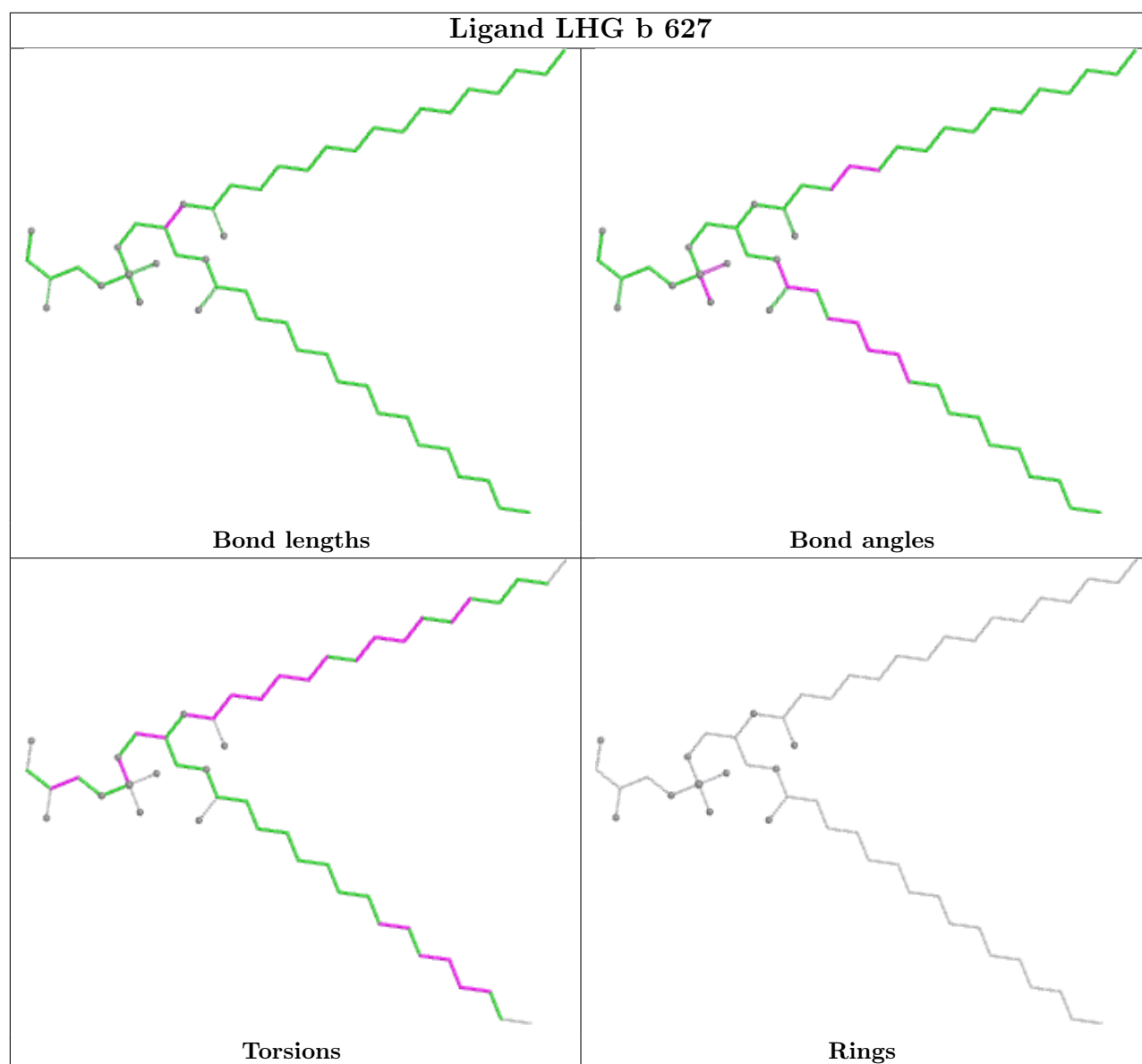
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	610	CLA	1	0
24	b	607	CLA	2	0
24	C	510	CLA	2	0
28	D	406	PL9	2	0
24	C	504	CLA	3	0
24	C	502	CLA	2	0
24	c	508	CLA	4	0
24	D	404	CLA	1	0
27	l	101	SQD	1	0
27	a	410	SQD	2	0
24	b	609	CLA	1	0
26	C	515	BCR	3	0
24	a	408	CLA	3	0
24	c	503	CLA	1	0
27	A	410	SQD	1	0
31	d	411	LMG	1	0
24	C	505	CLA	2	0
32	d	410	LHG	1	0
31	C	522	LMG	3	0
24	B	604	CLA	1	0
24	c	504	CLA	3	0
32	D	410	LHG	1	0
32	B	625	LHG	2	0
34	e	103	HEM	3	0
26	c	515	BCR	2	0
33	C	519	DGD	3	0
25	d	402	PHO	2	0
24	c	505	CLA	2	0
24	a	406	CLA	2	0
28	a	411	PL9	2	0
26	C	521	BCR	2	0
26	c	516	BCR	2	0
33	C	518	DGD	3	0
25	D	402	PHO	1	0
32	E	101	LHG	1	0

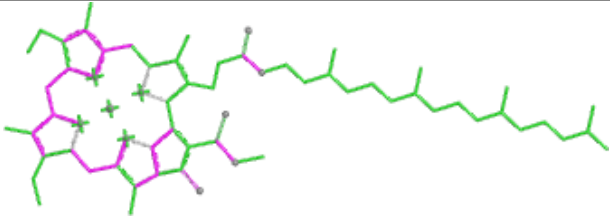
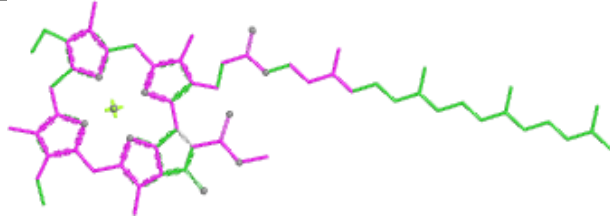
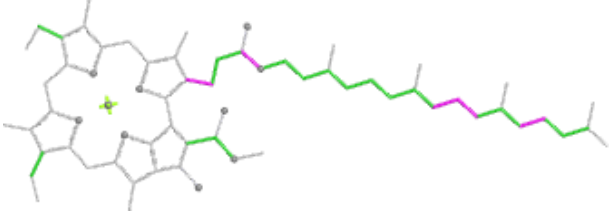
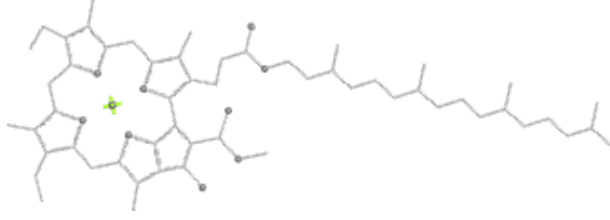
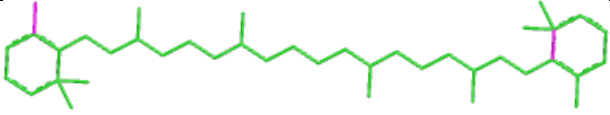
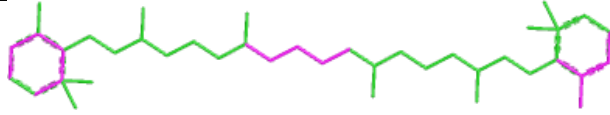
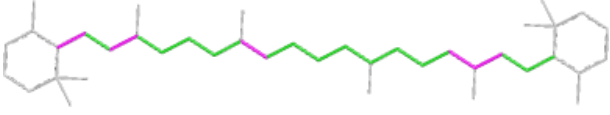
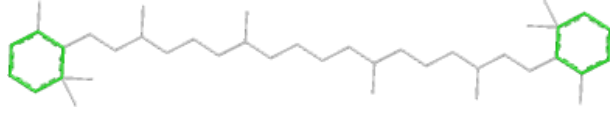
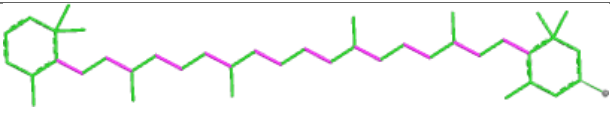
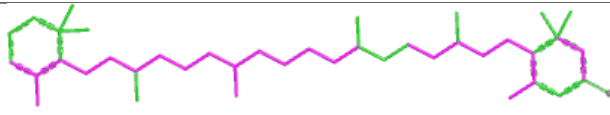
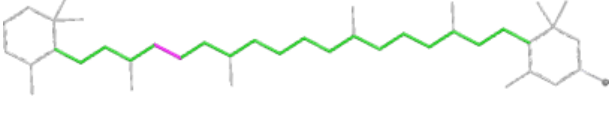
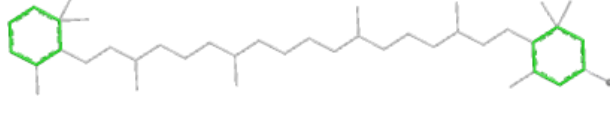
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

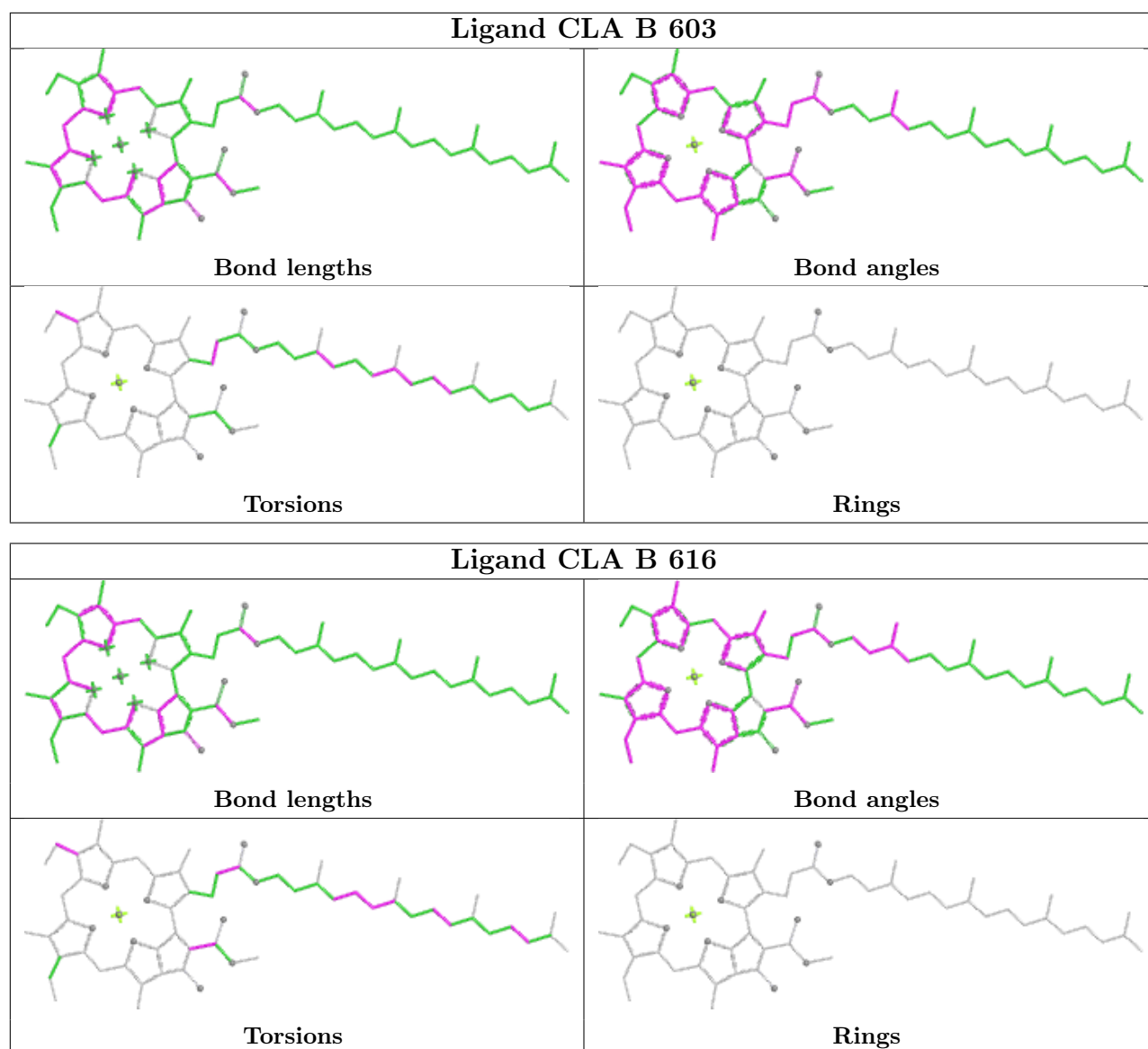
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

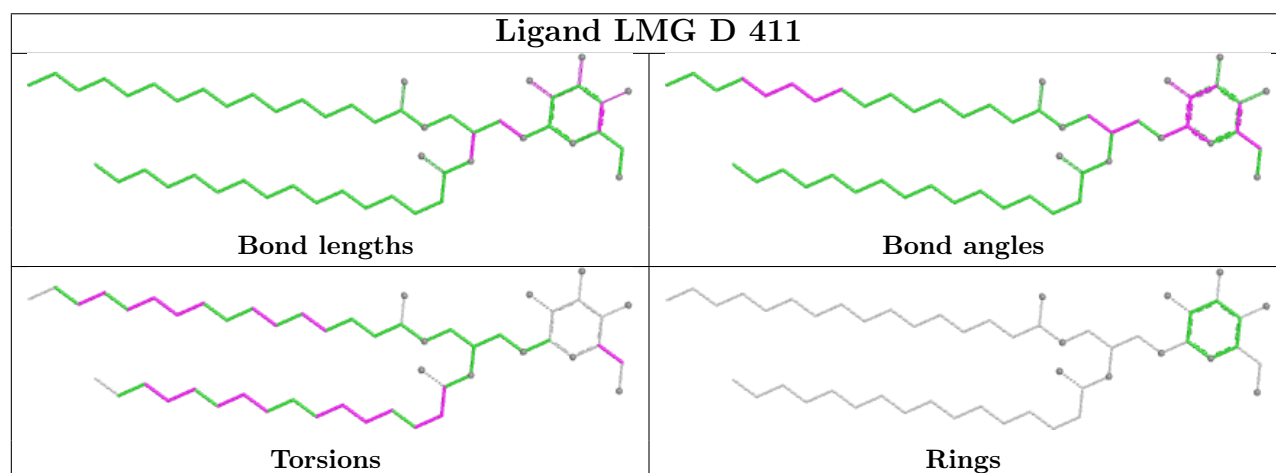
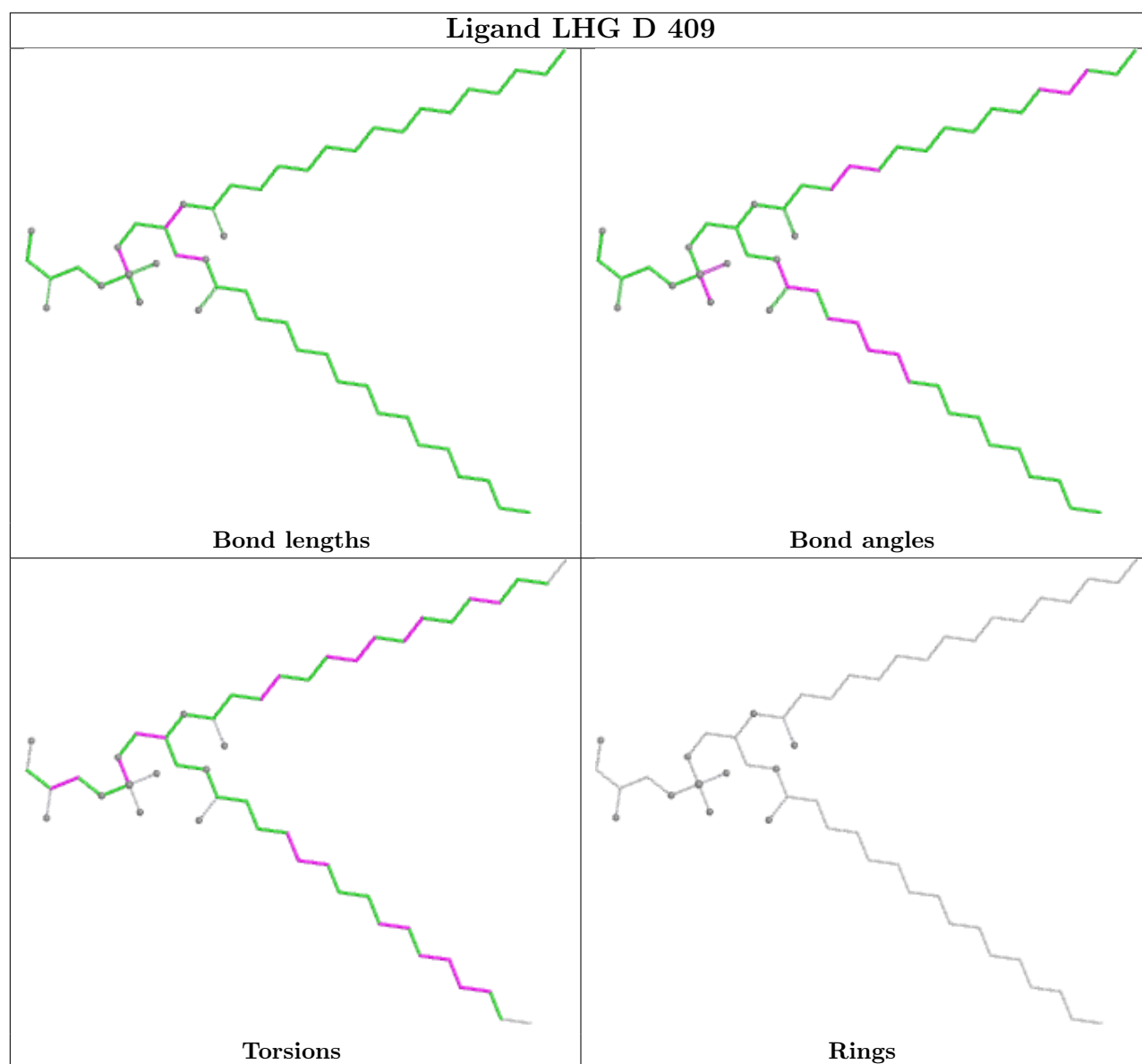


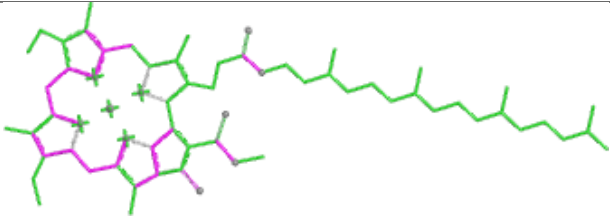
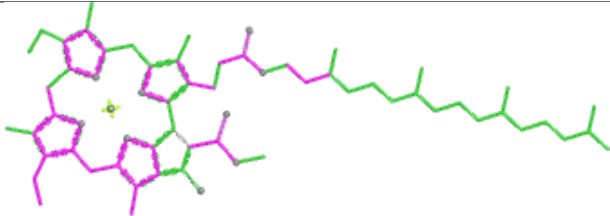
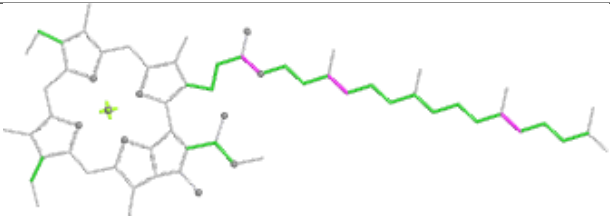
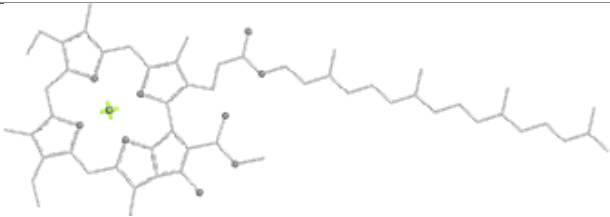
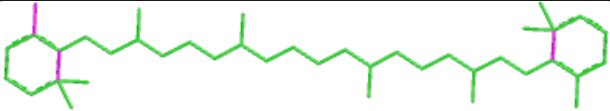
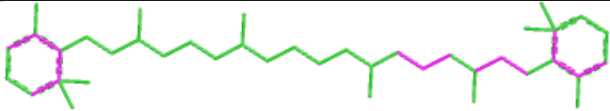
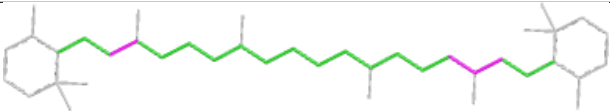
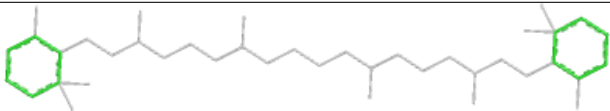


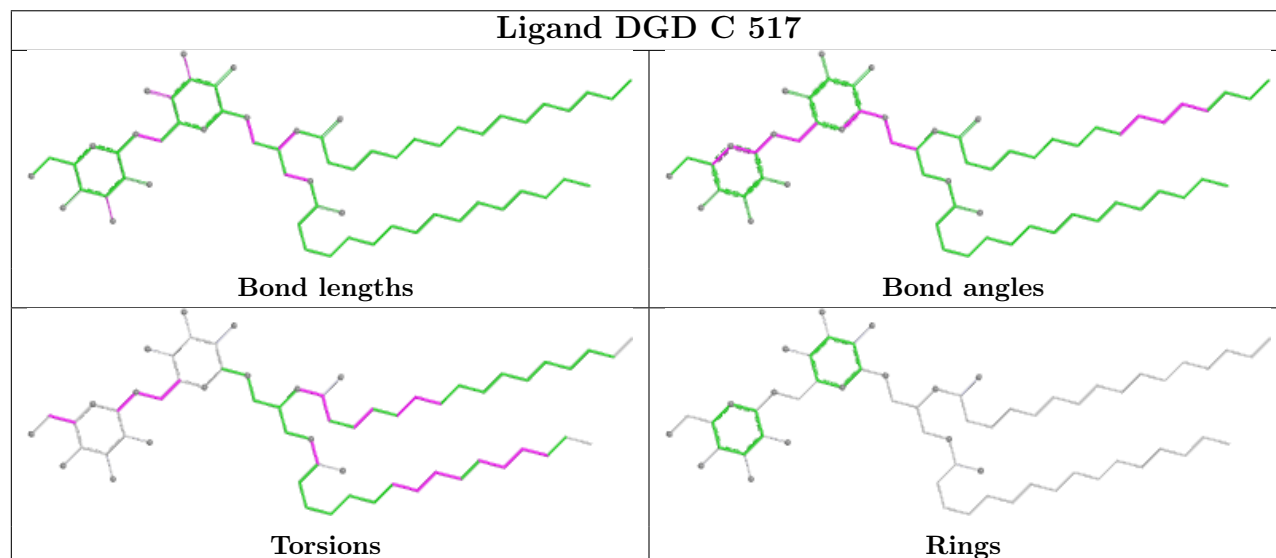
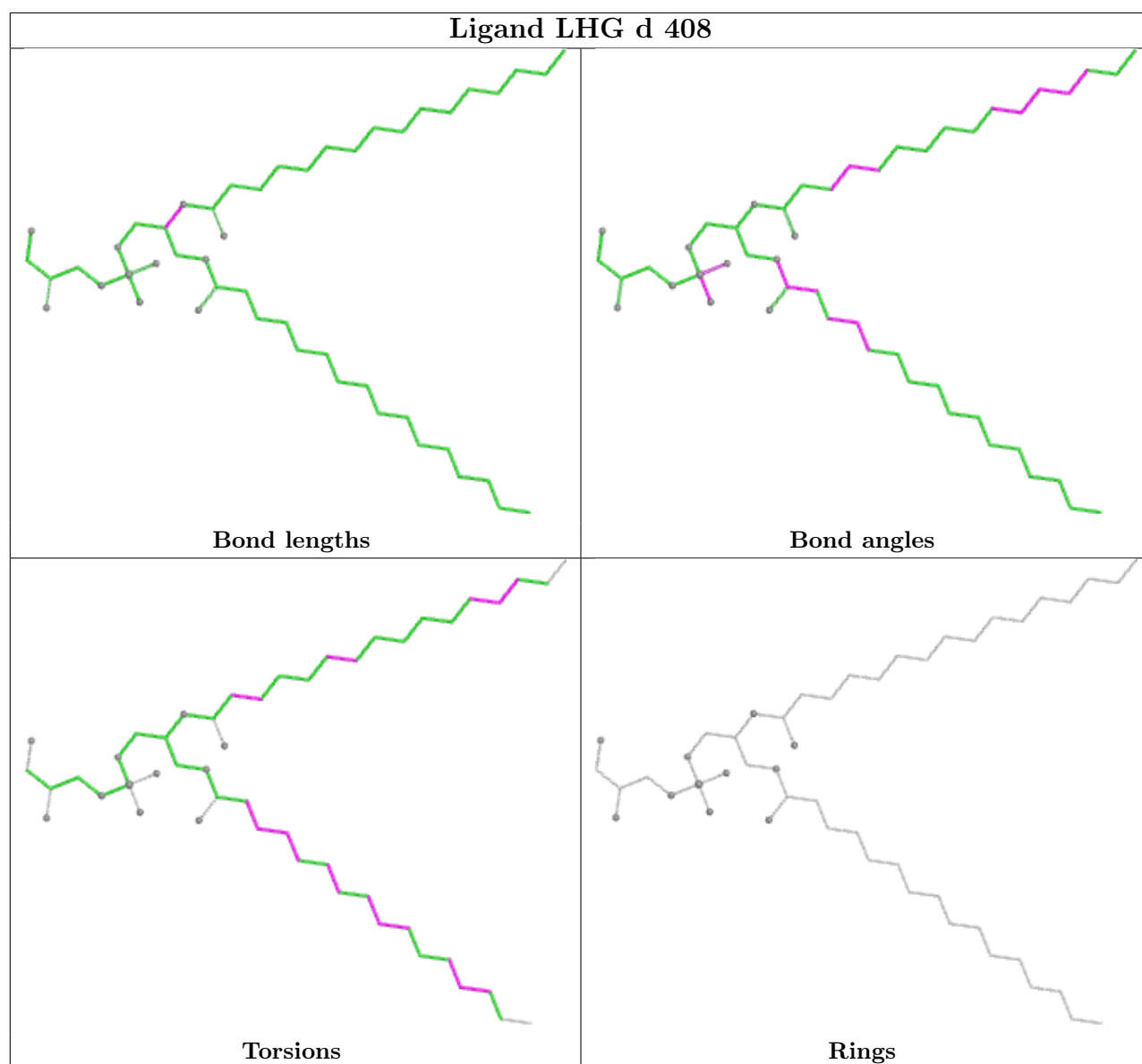


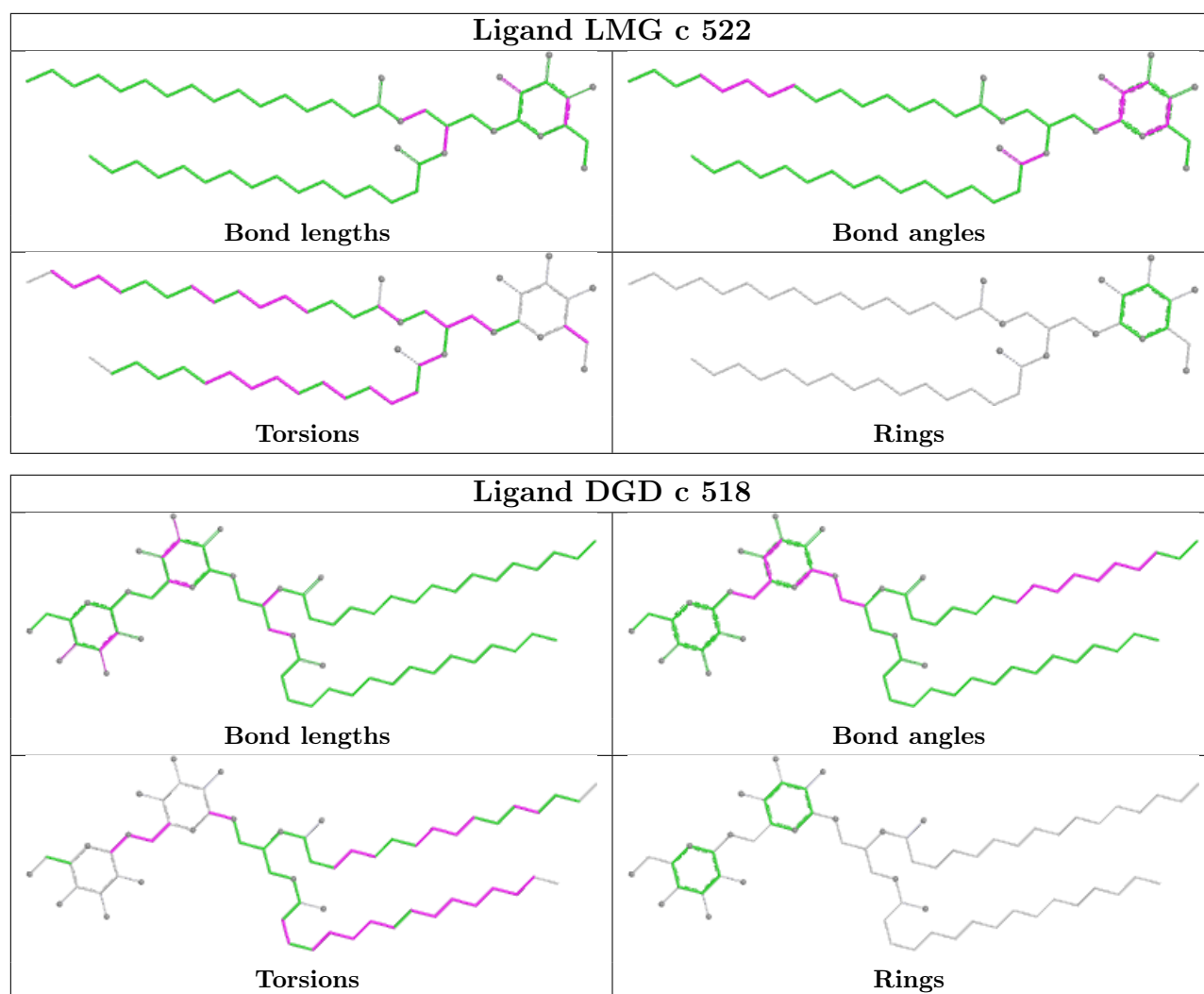
Ligand CLA b 614	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand RRX H 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

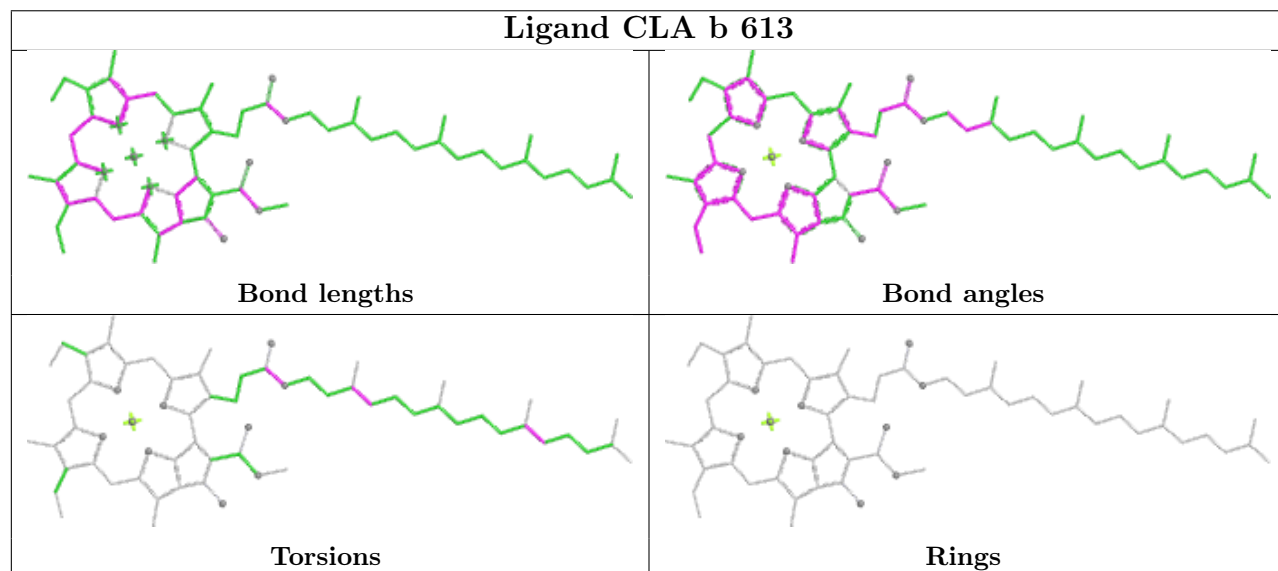
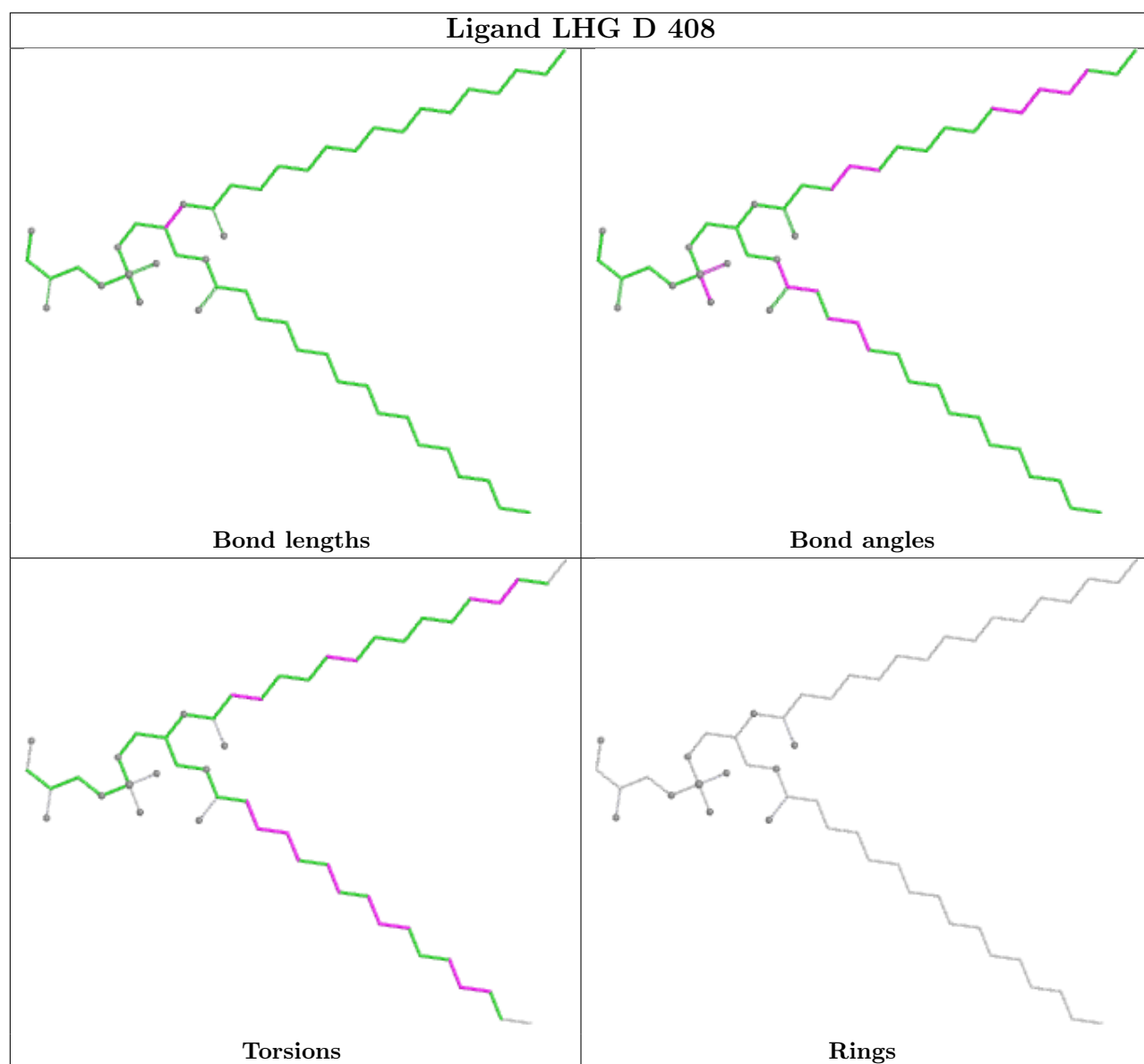


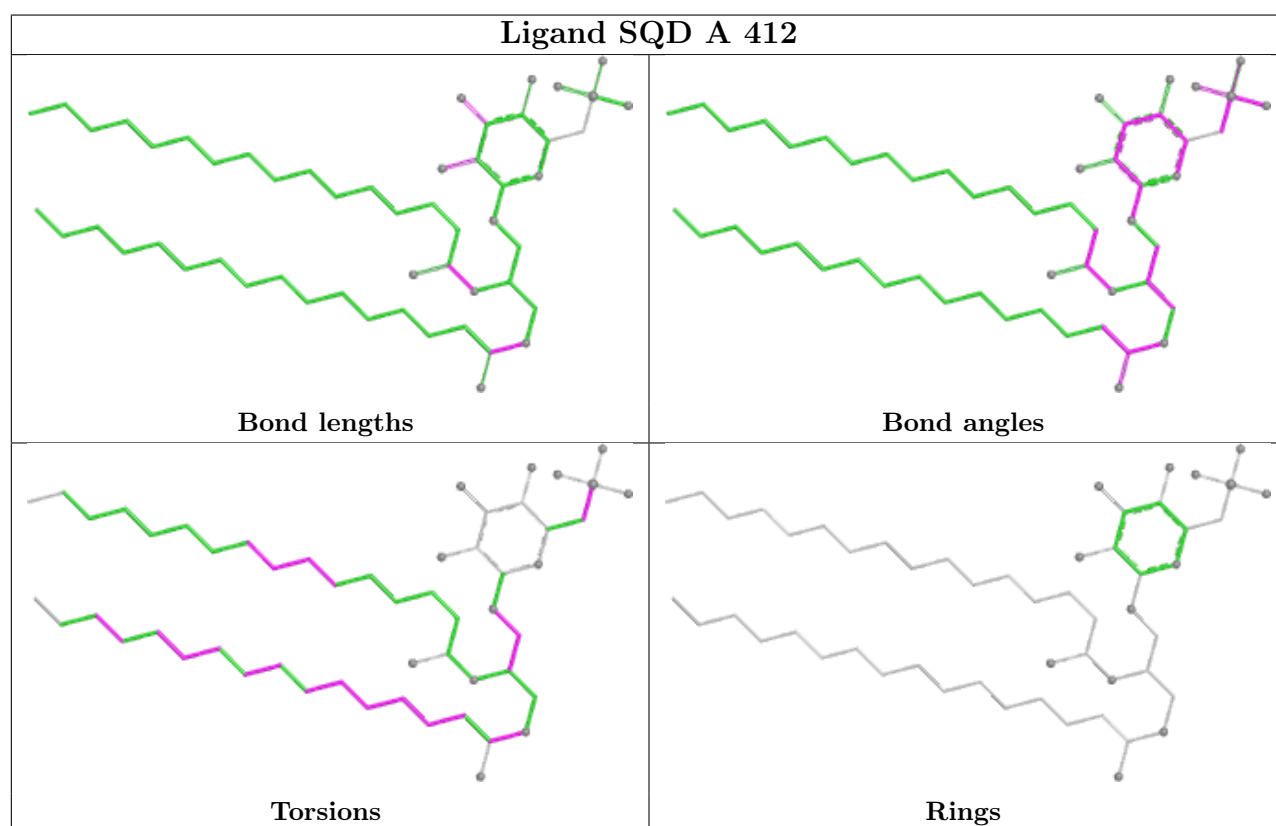
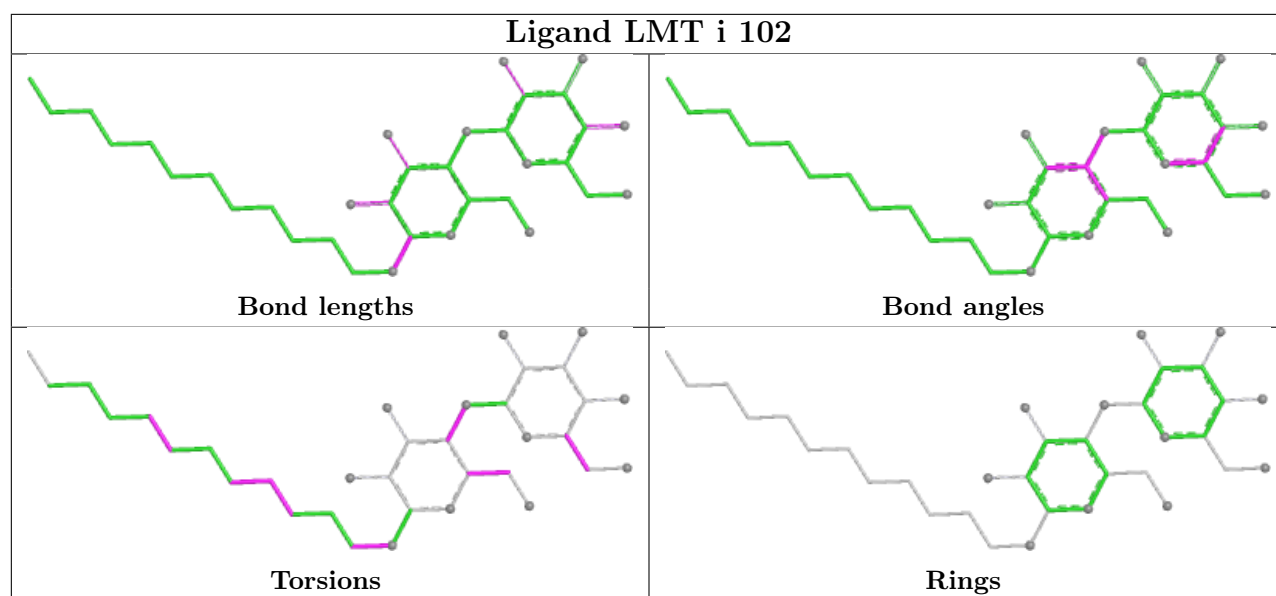


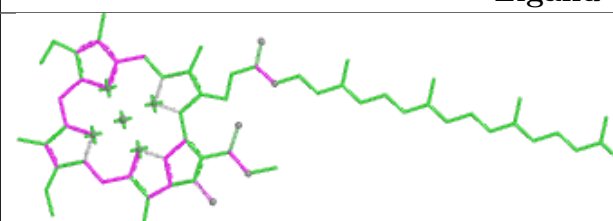
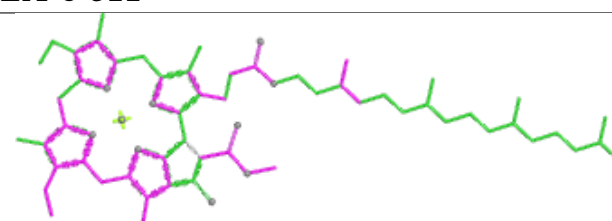
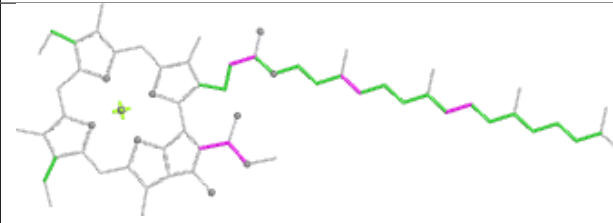
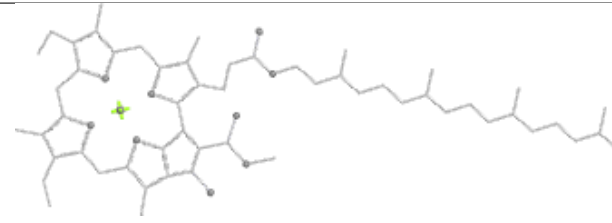
Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

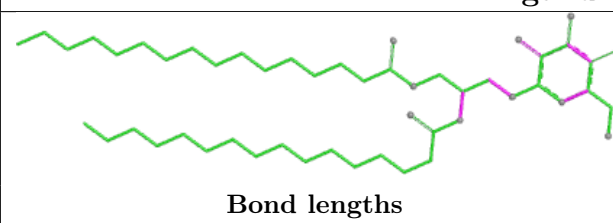
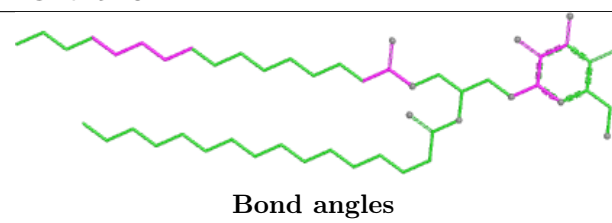
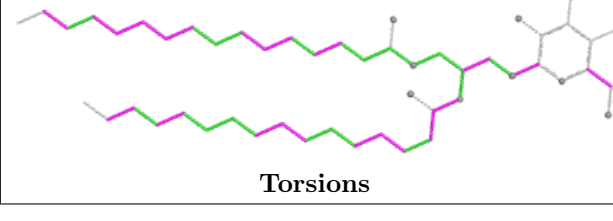
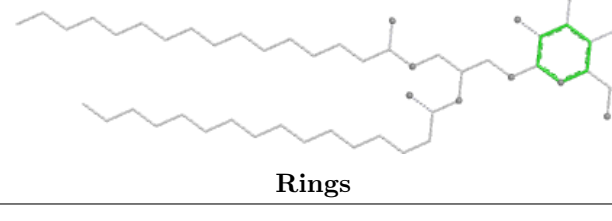


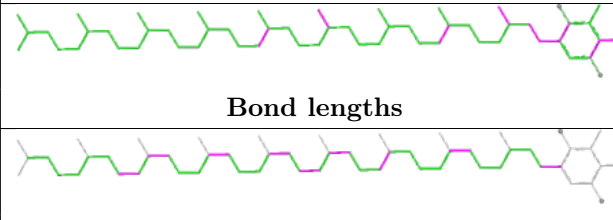
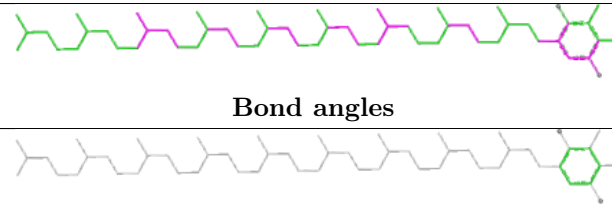


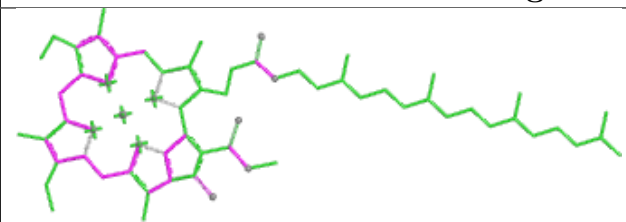
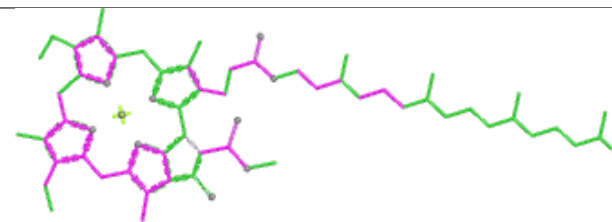
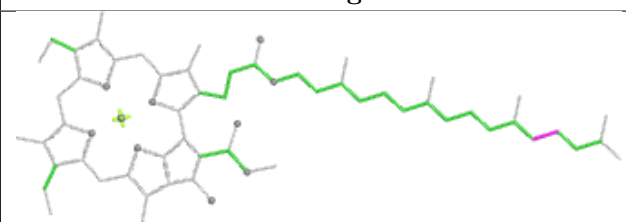
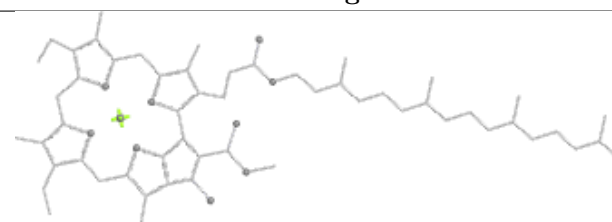


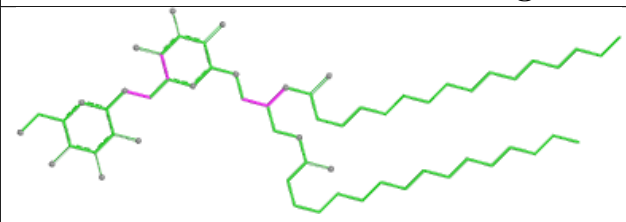
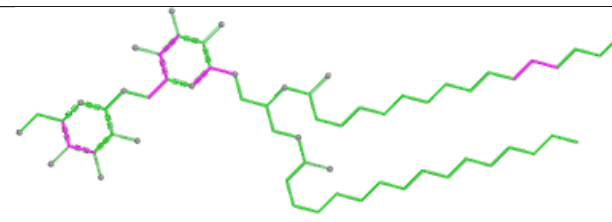
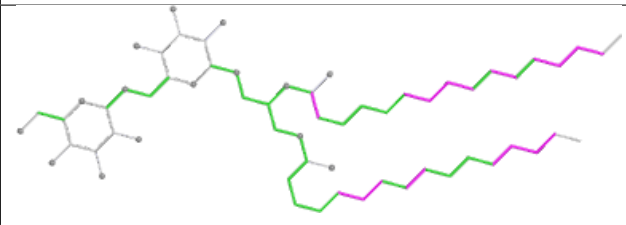
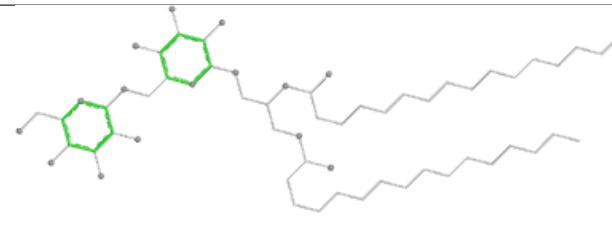


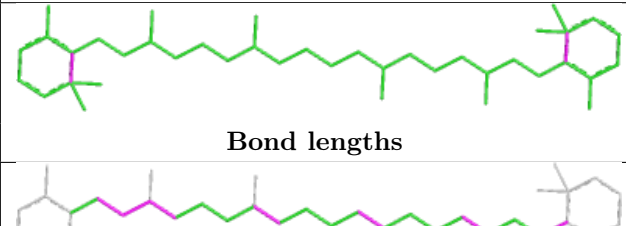
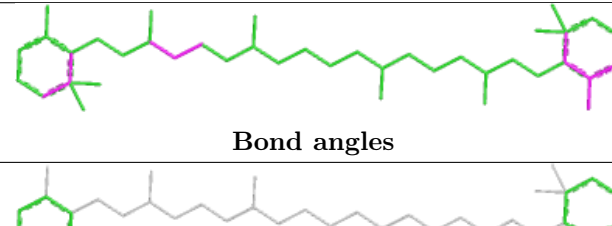
Ligand CLA c 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

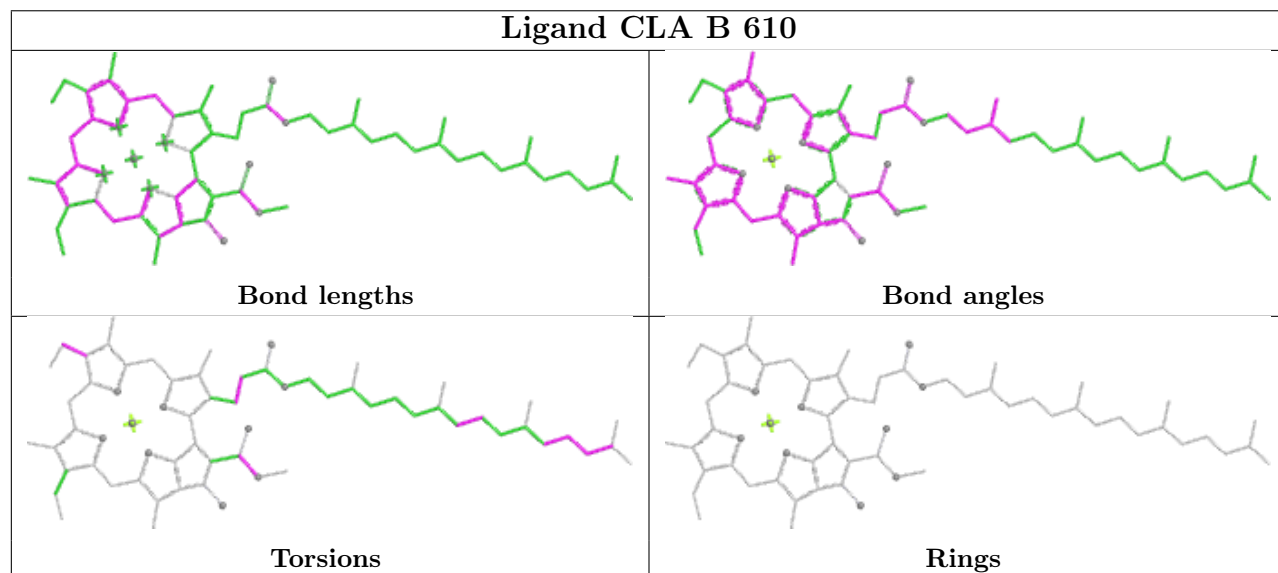
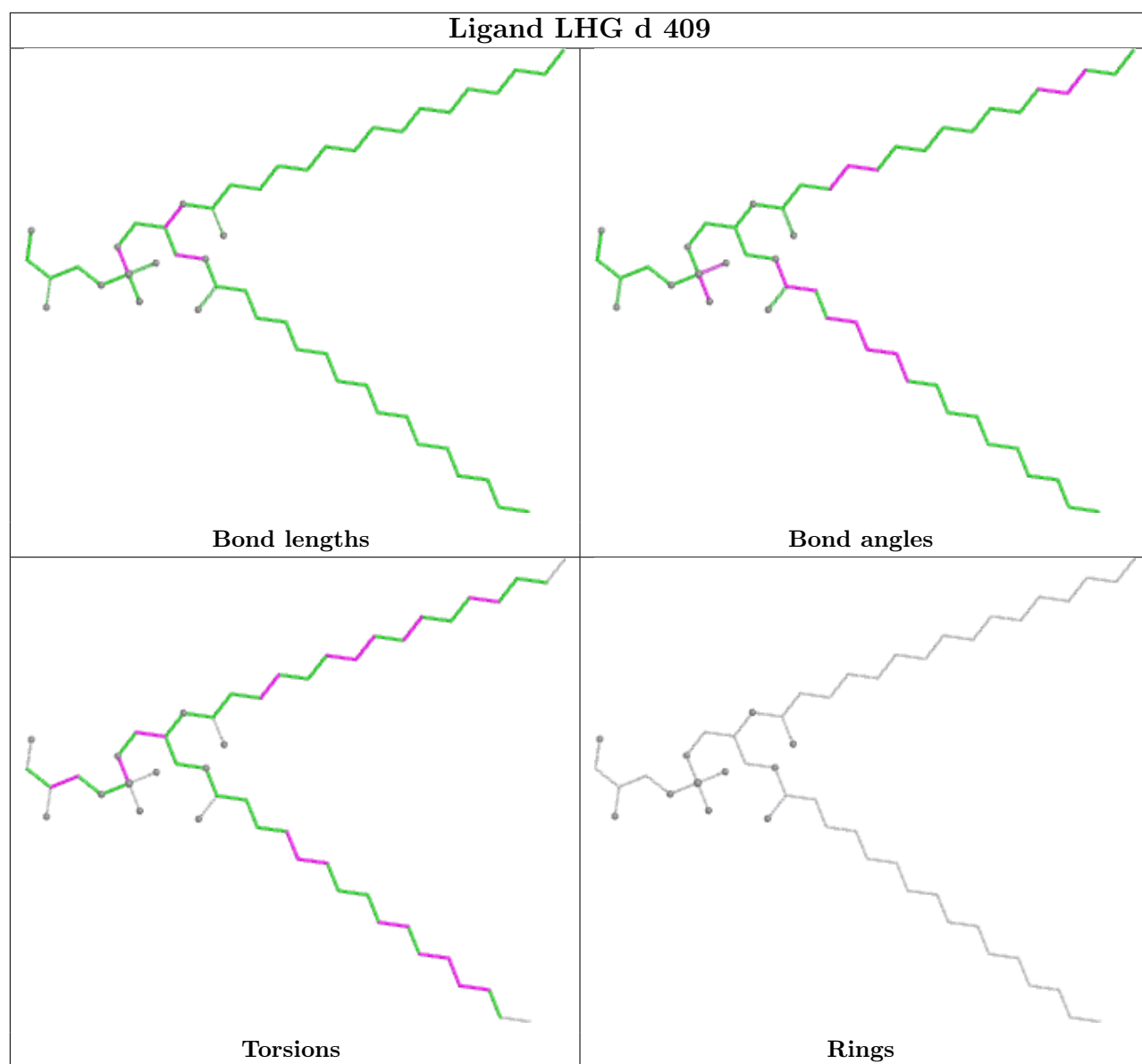
Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

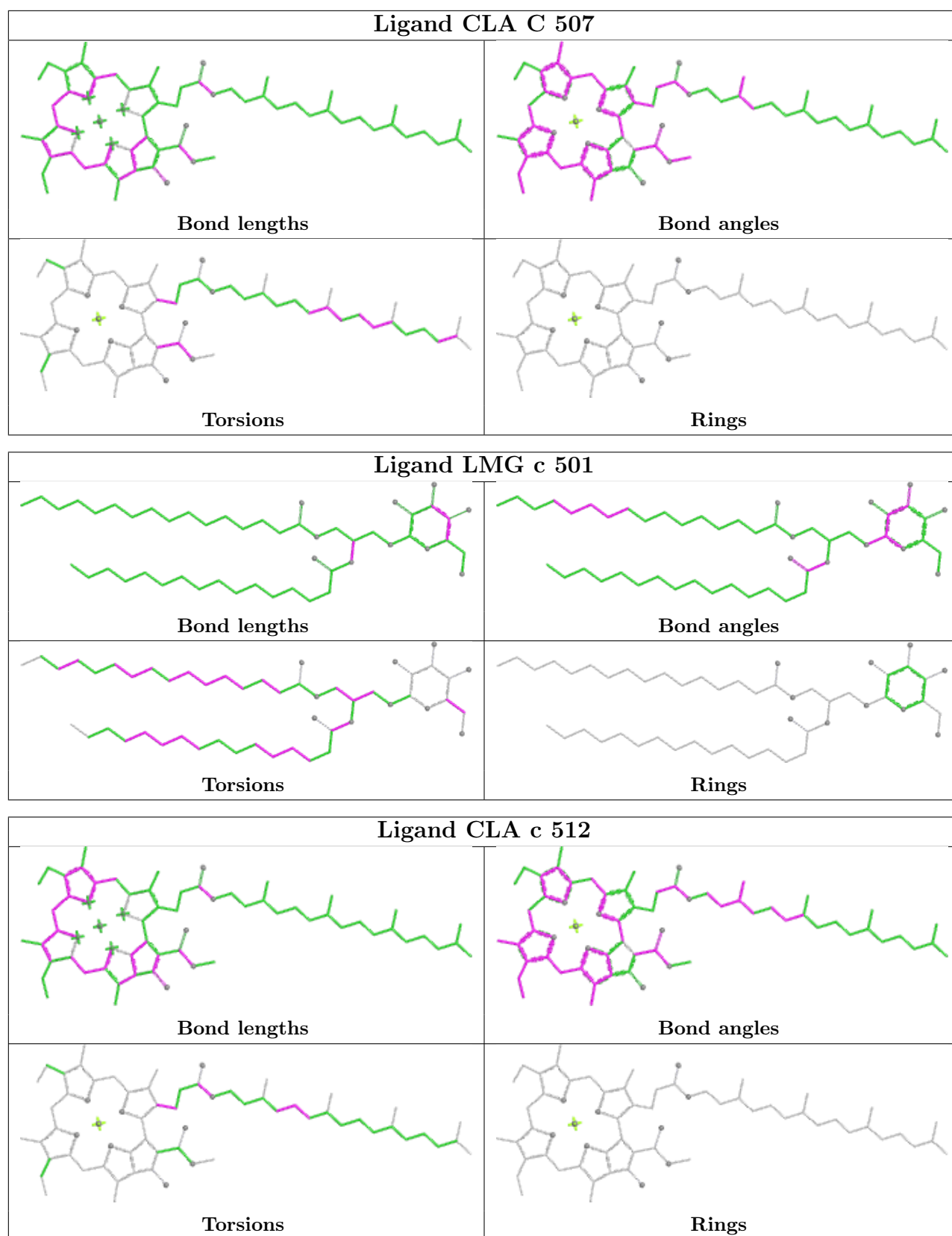
Ligand PL9 A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

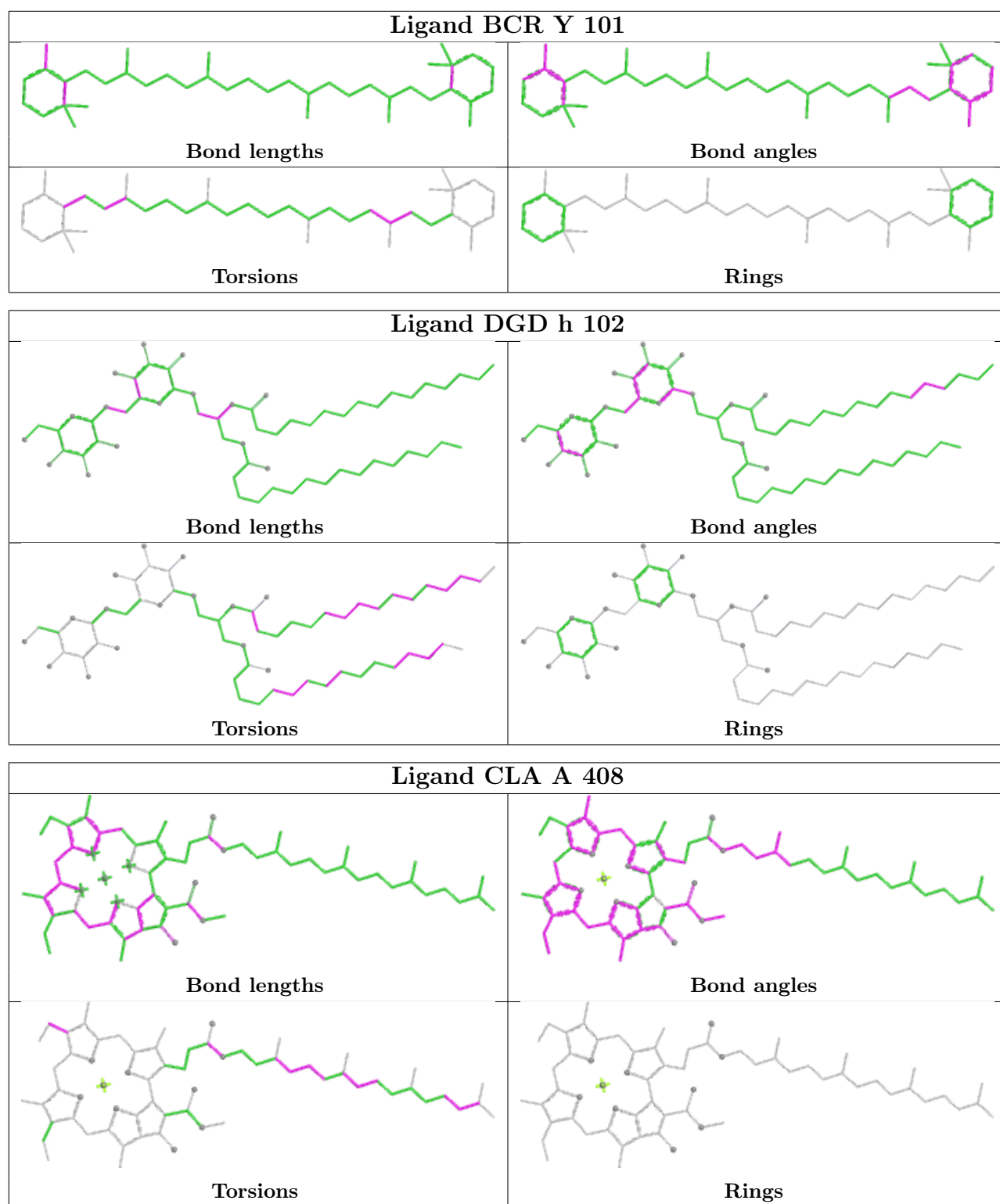
Ligand CLA c 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

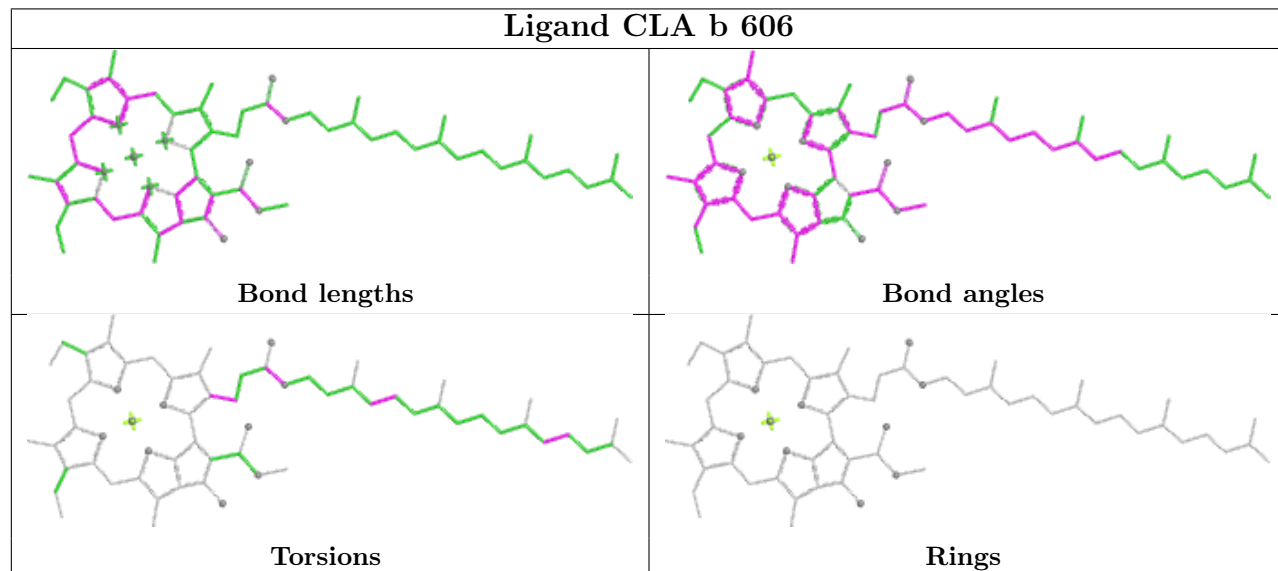
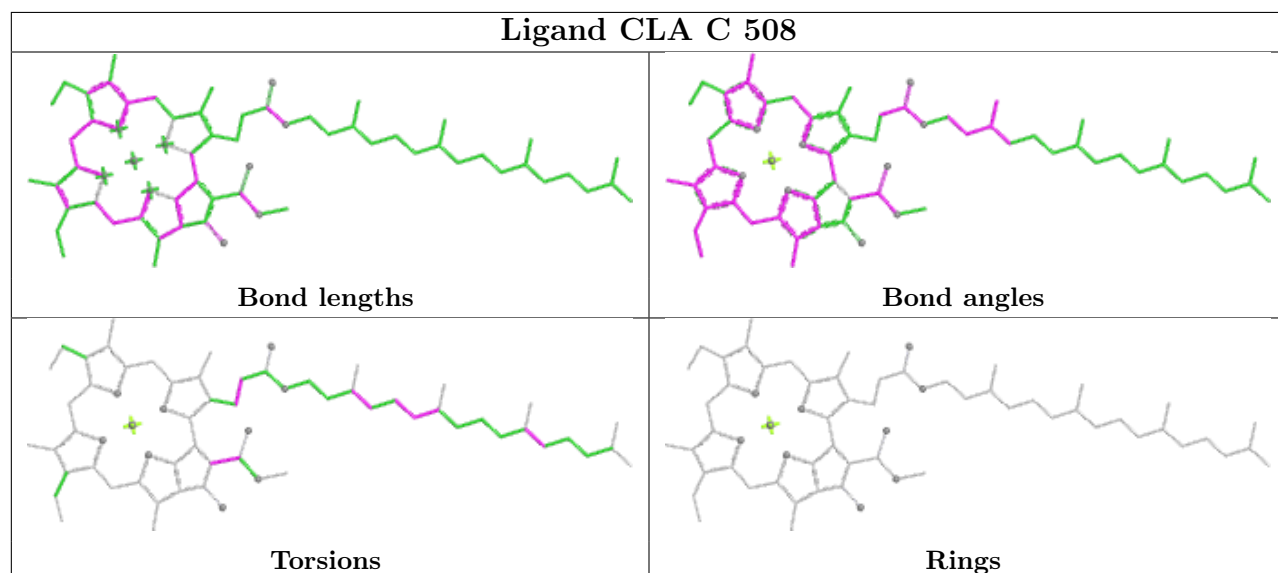
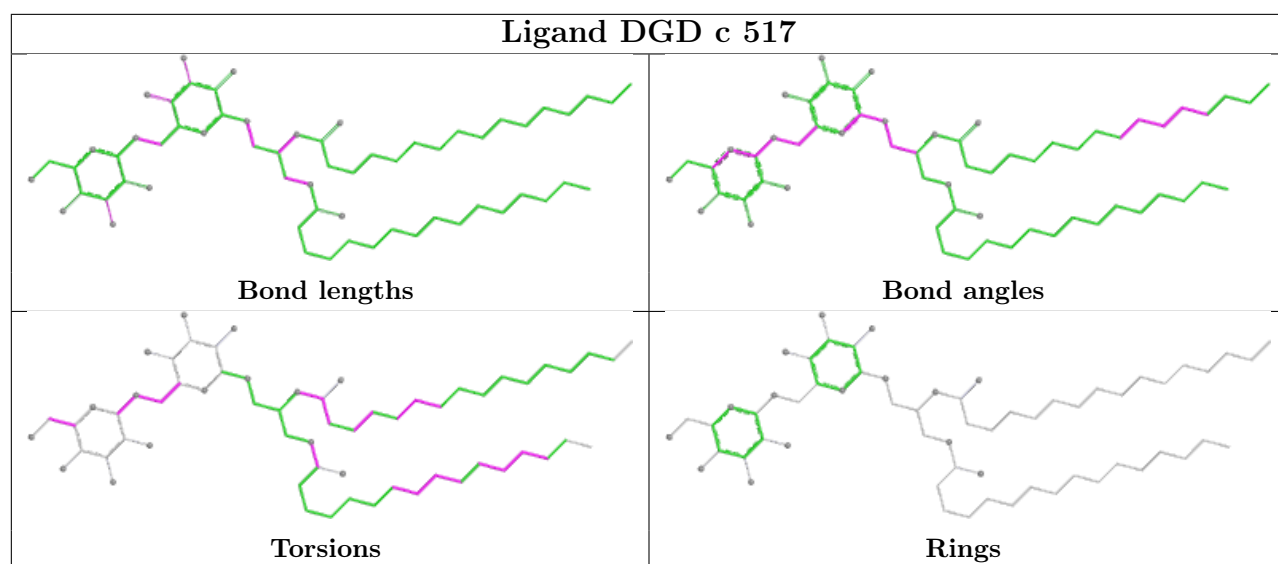
Ligand DGD H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

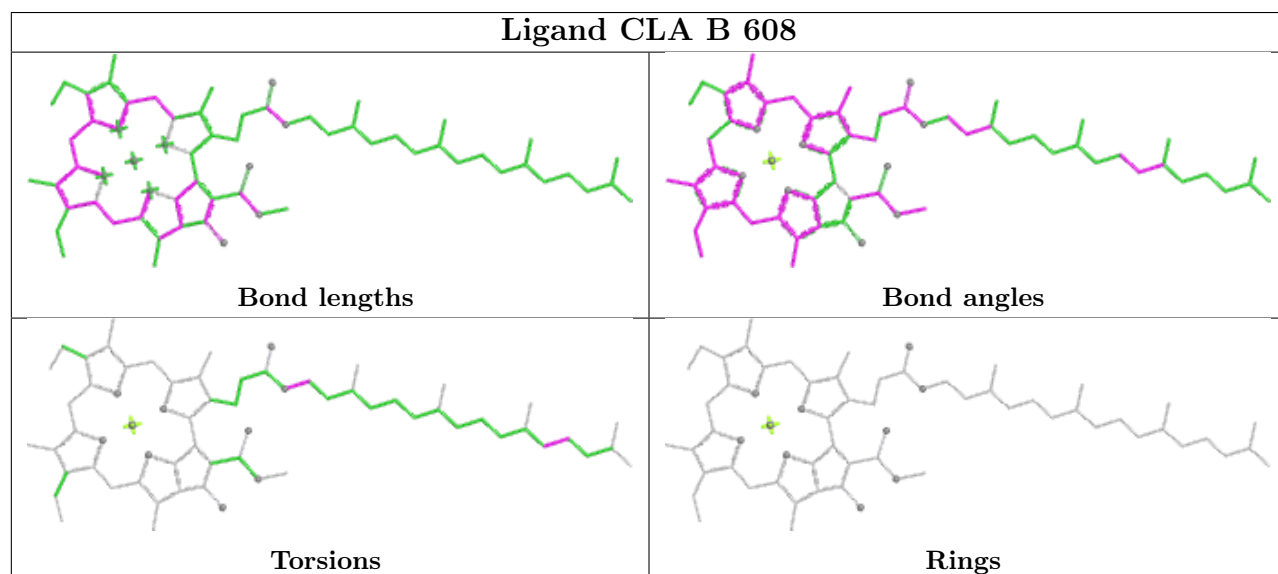
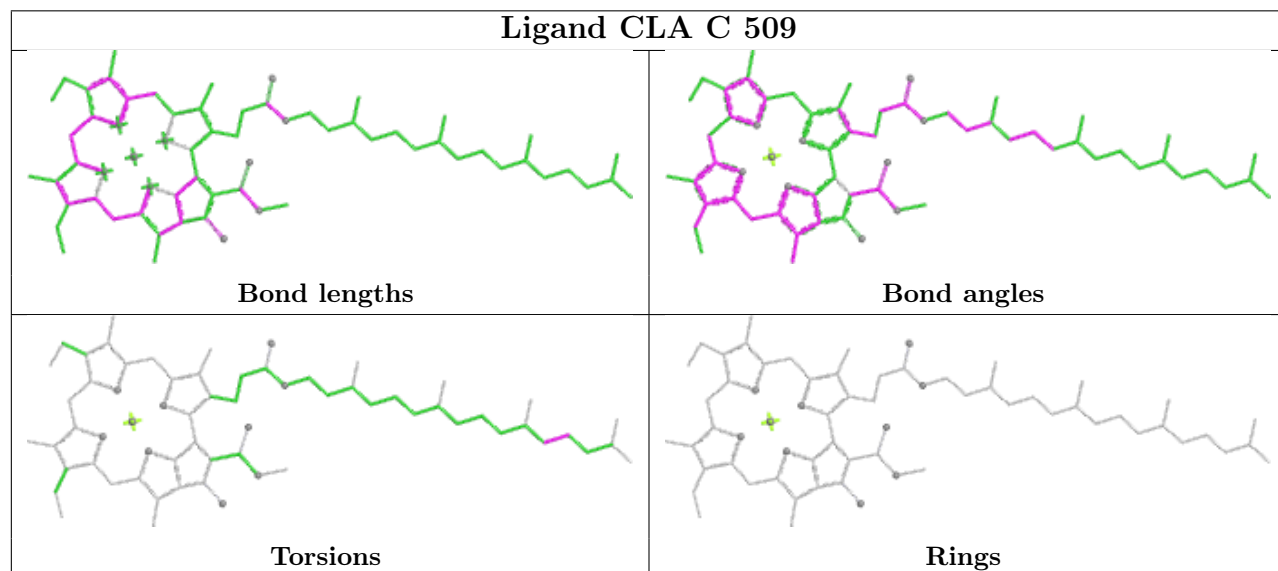
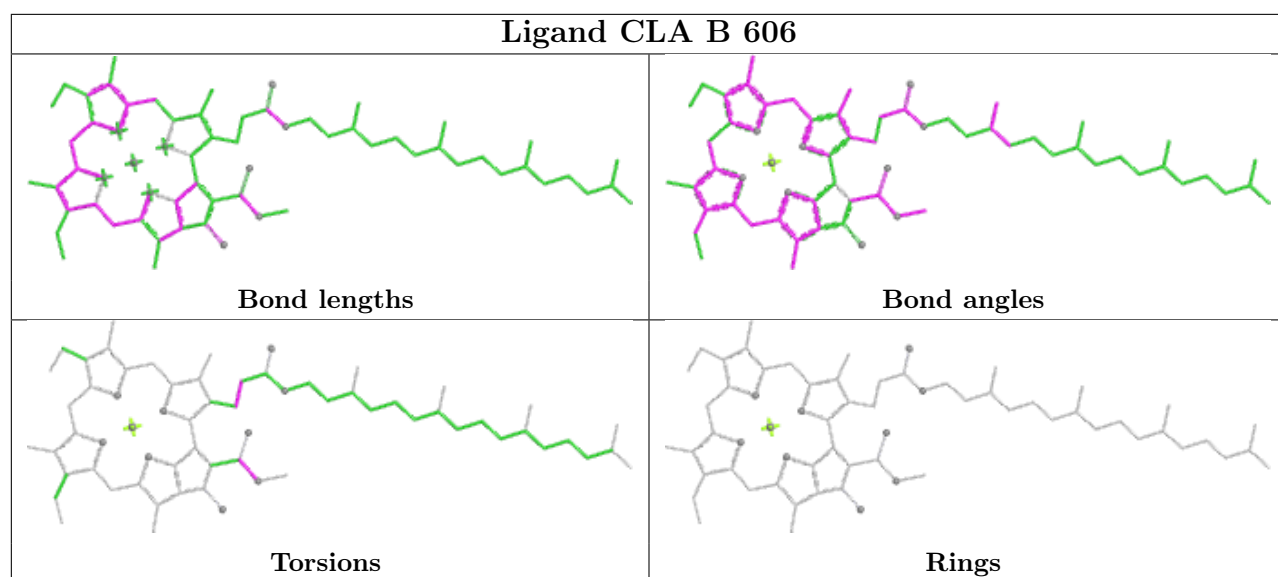
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

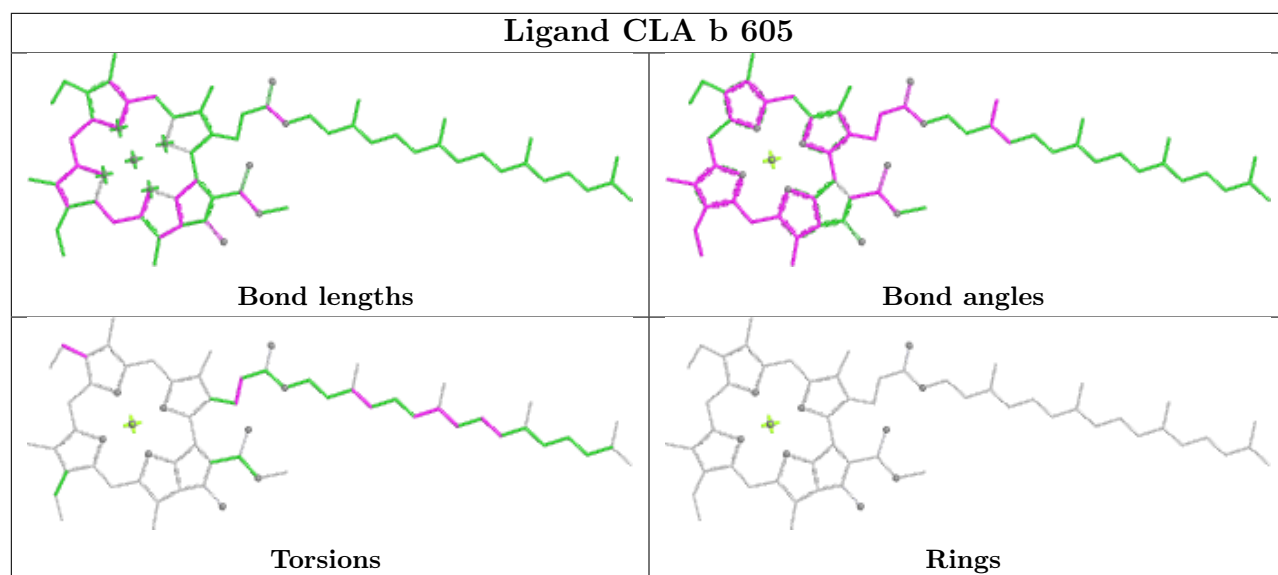
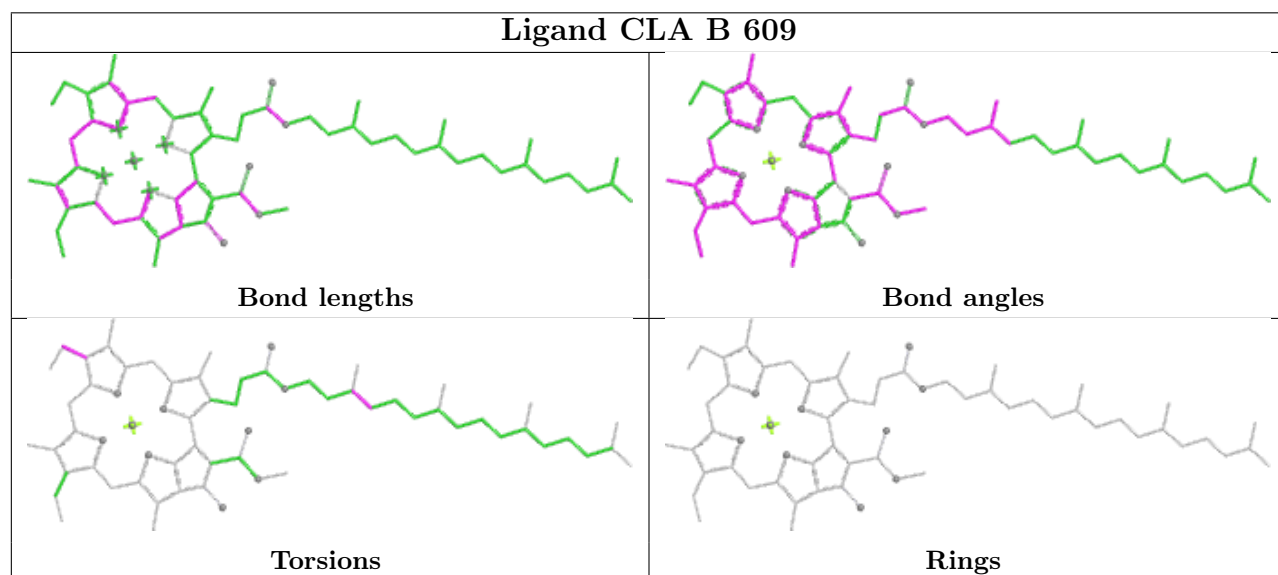
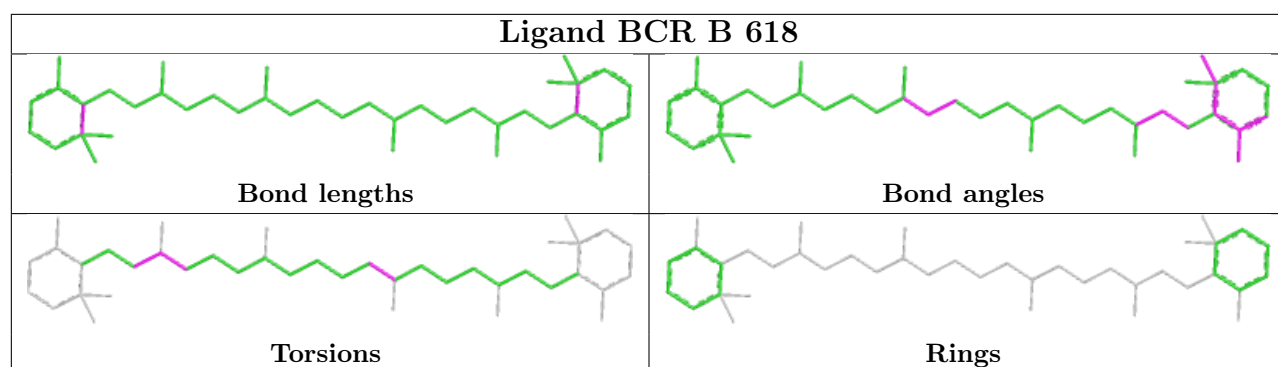


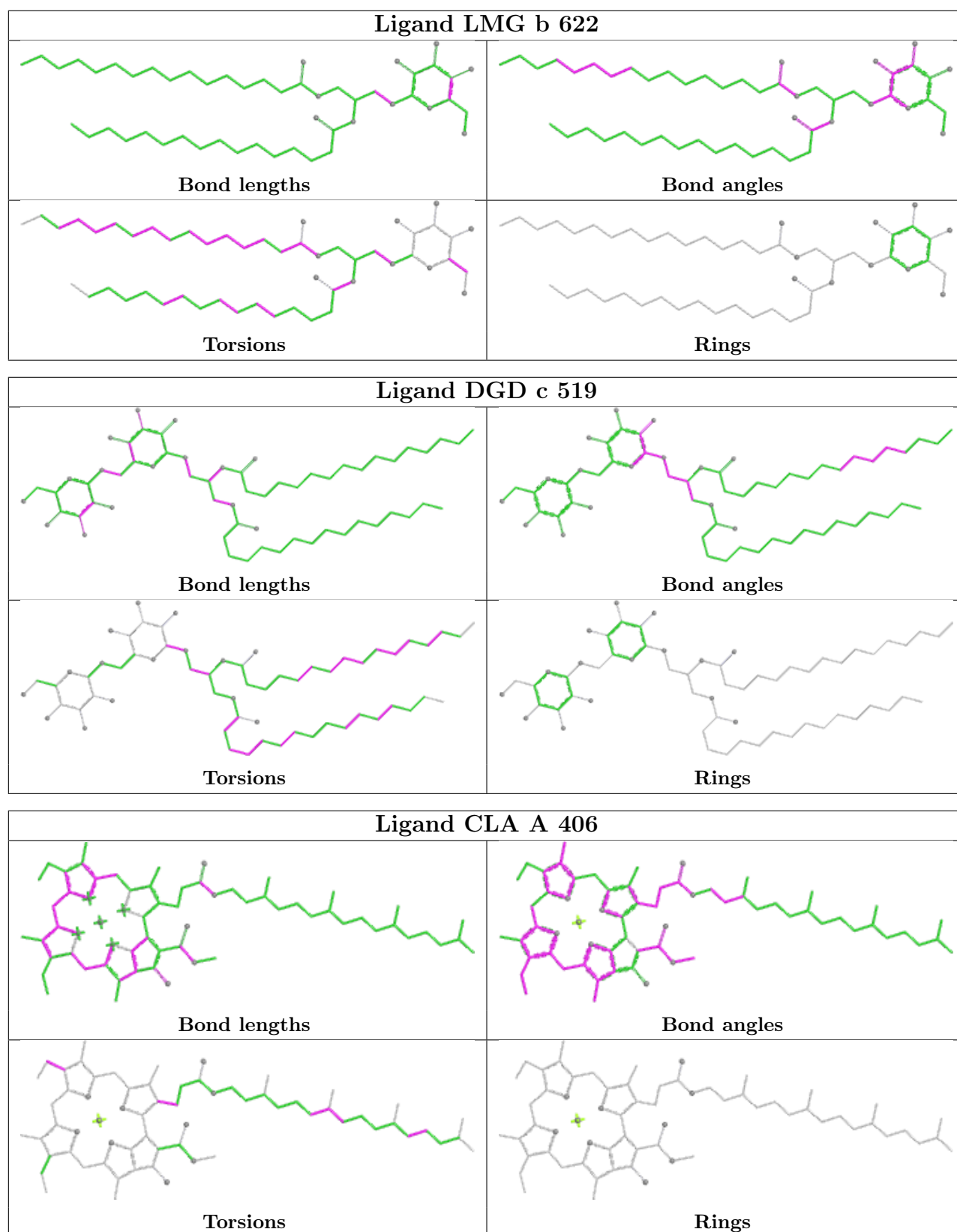


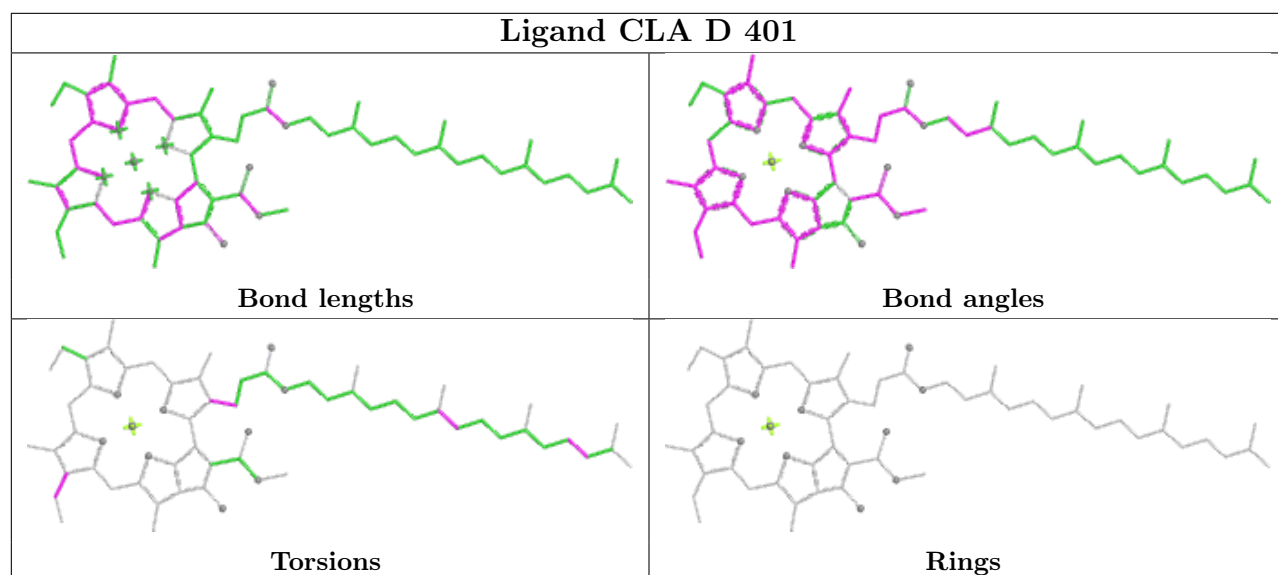
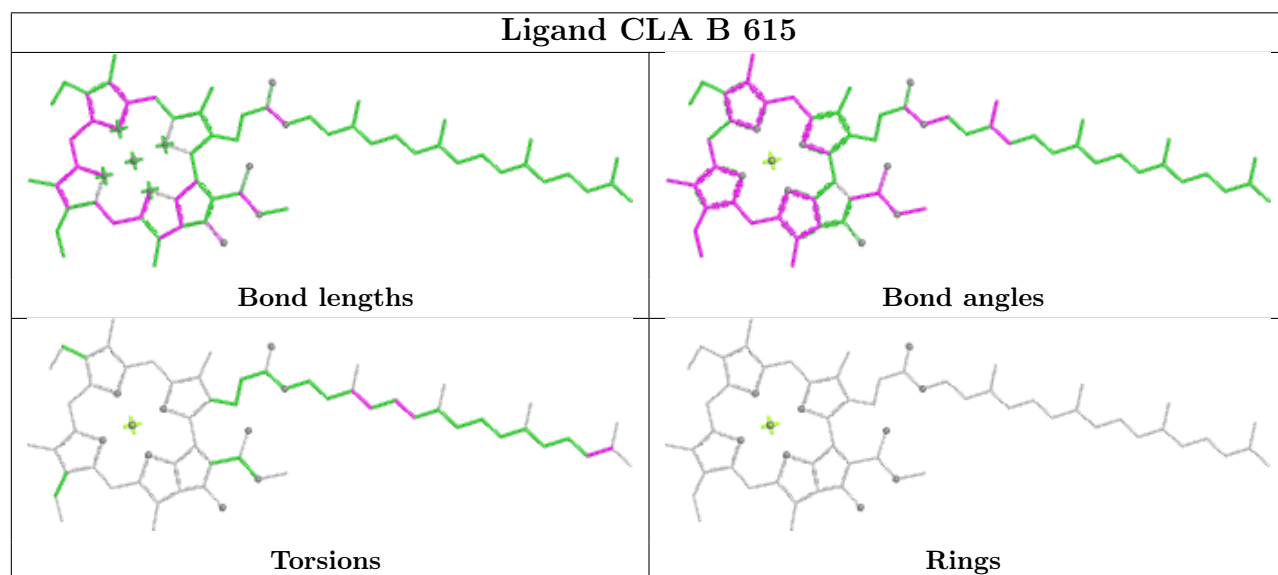
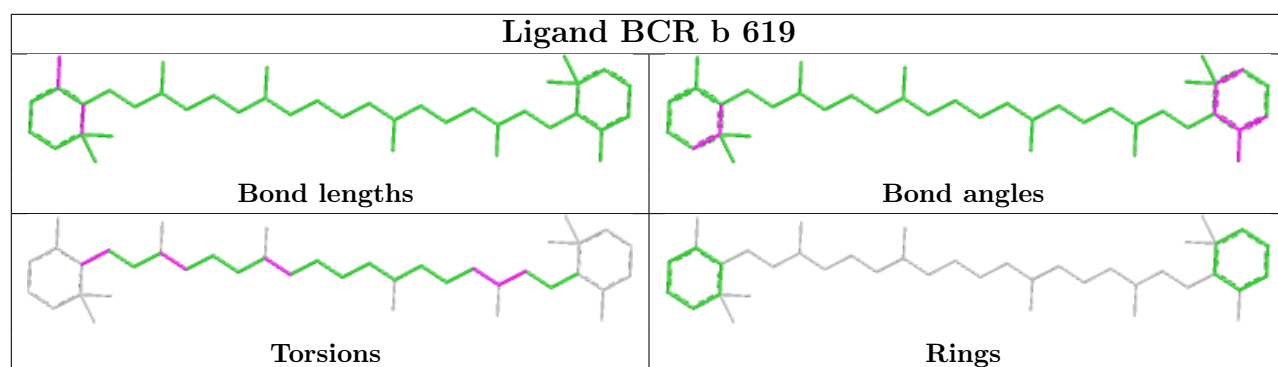


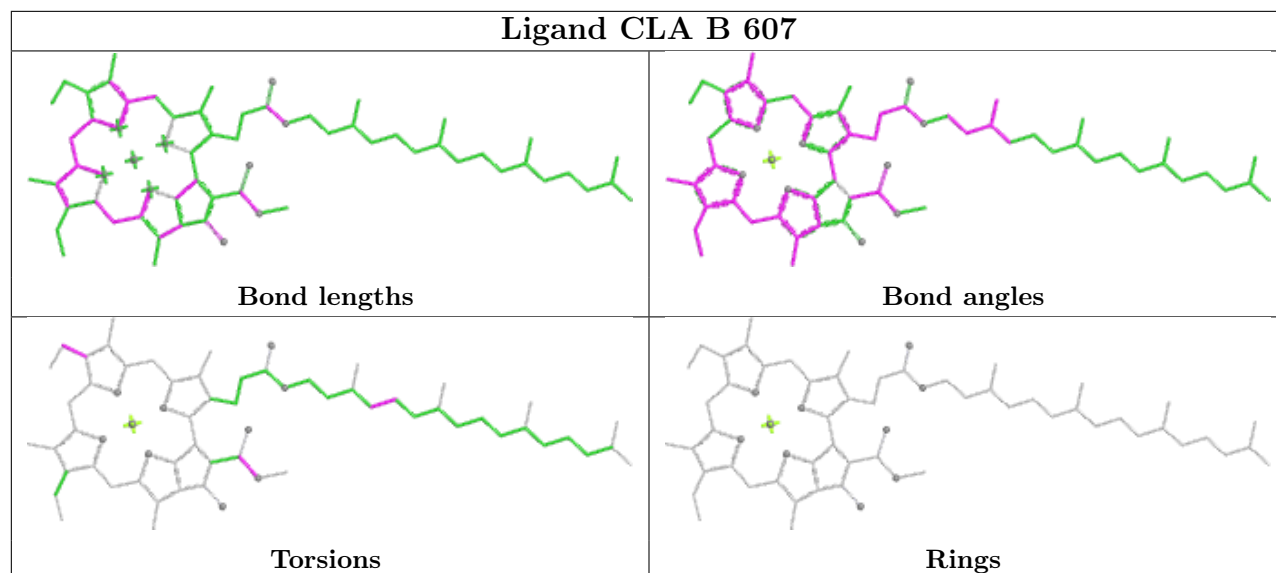
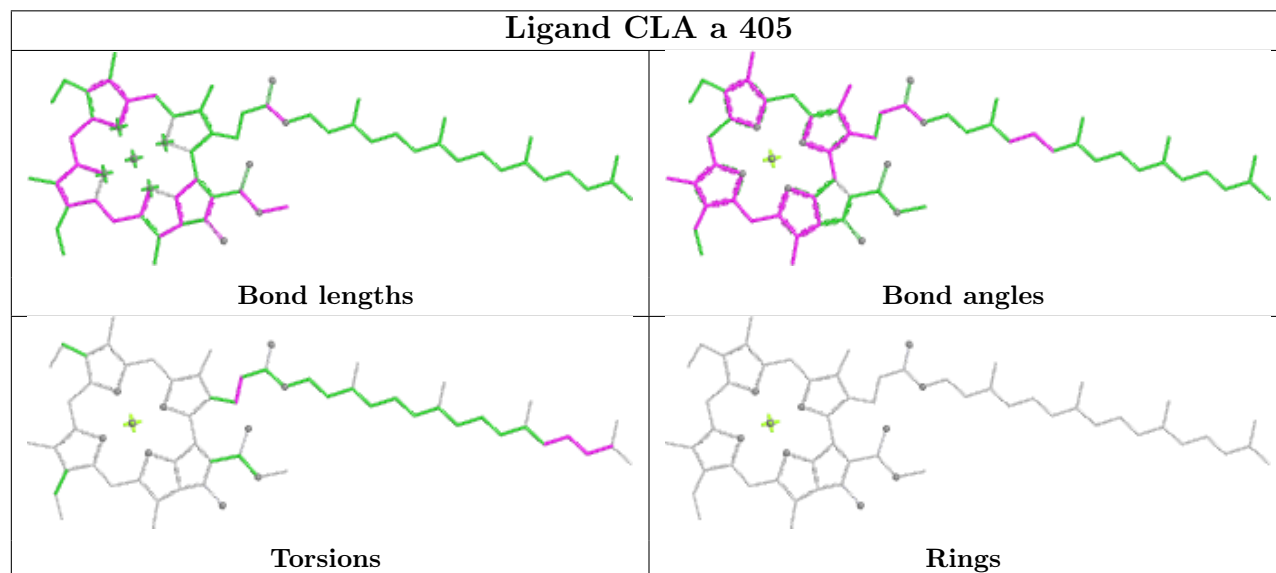
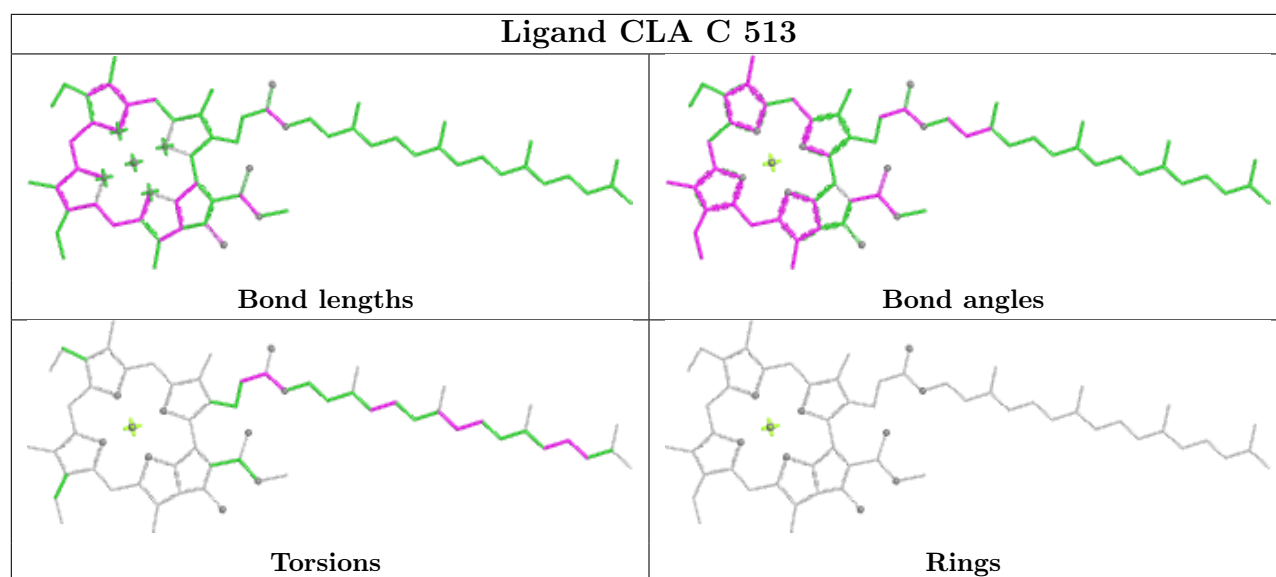


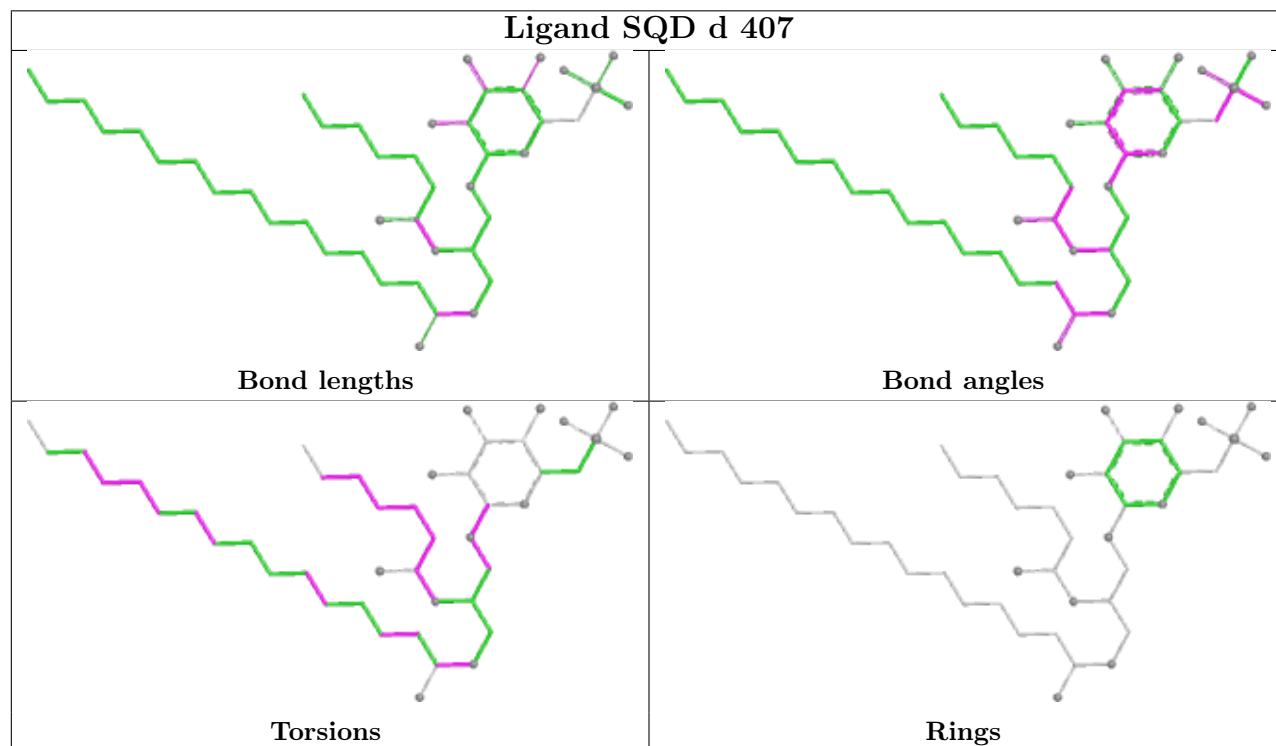
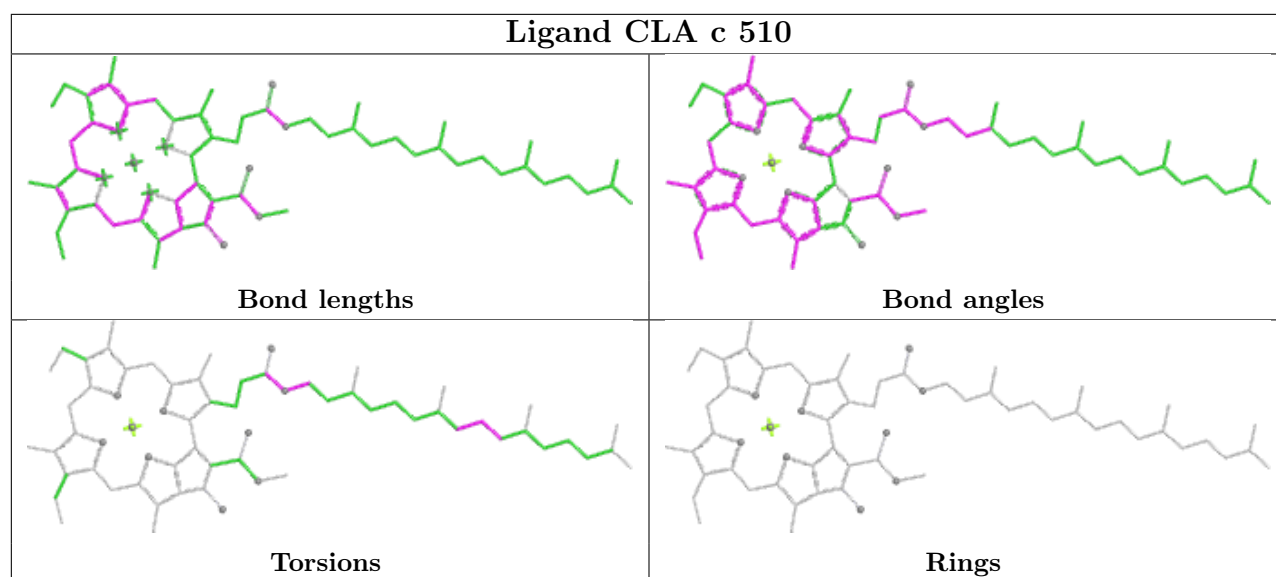


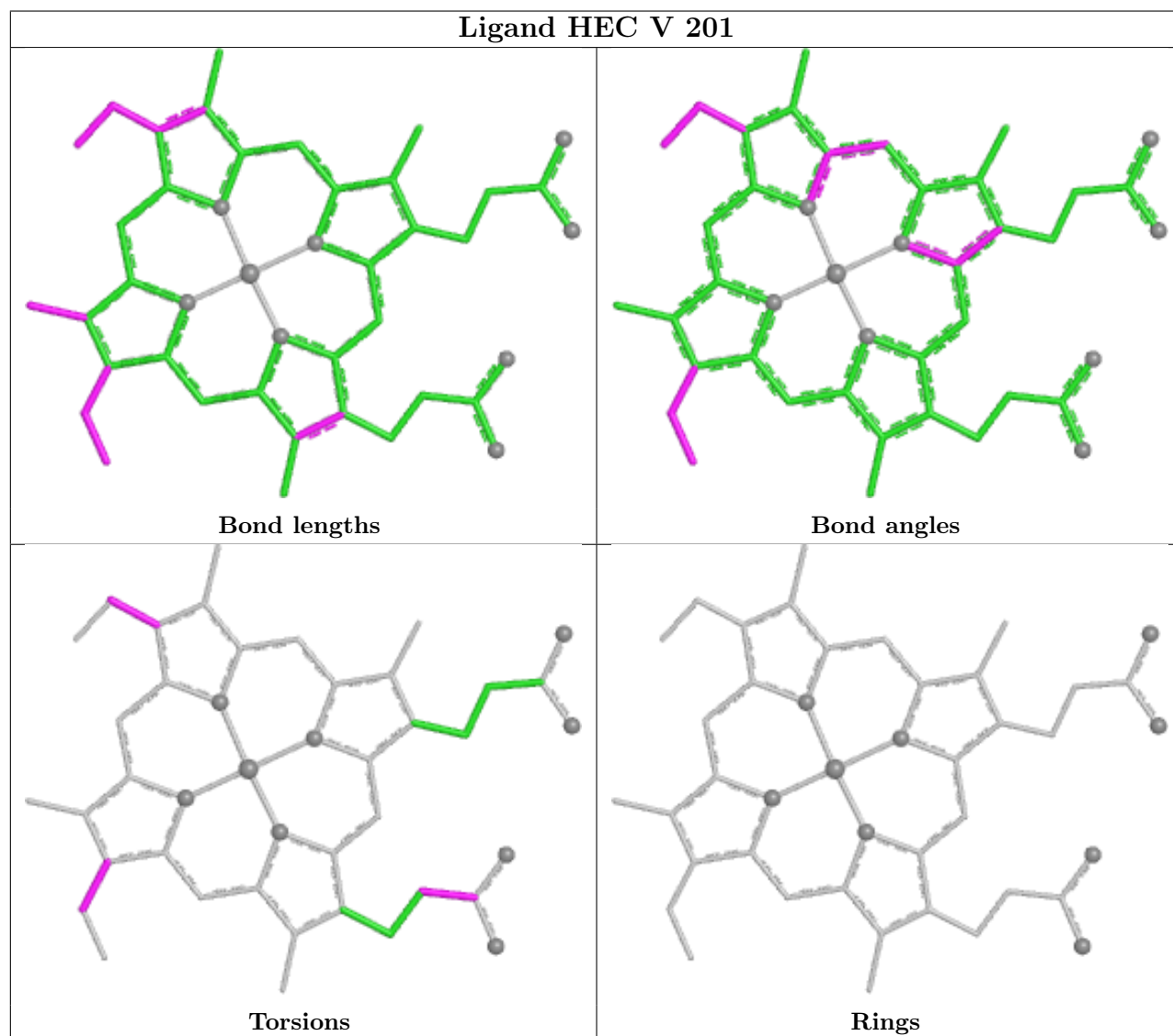
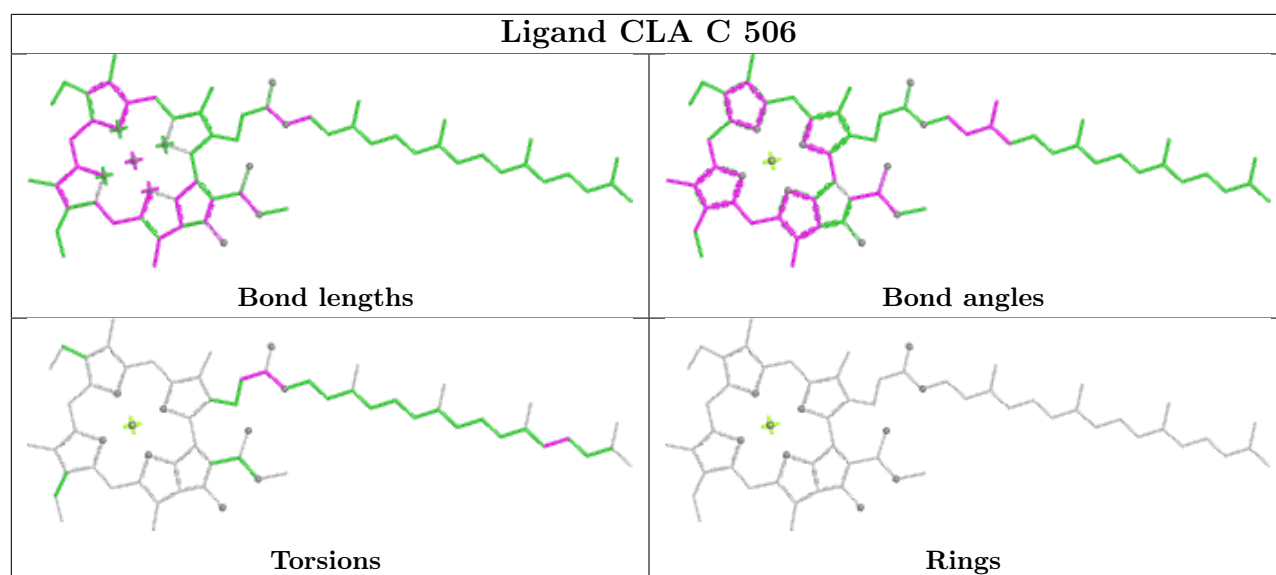


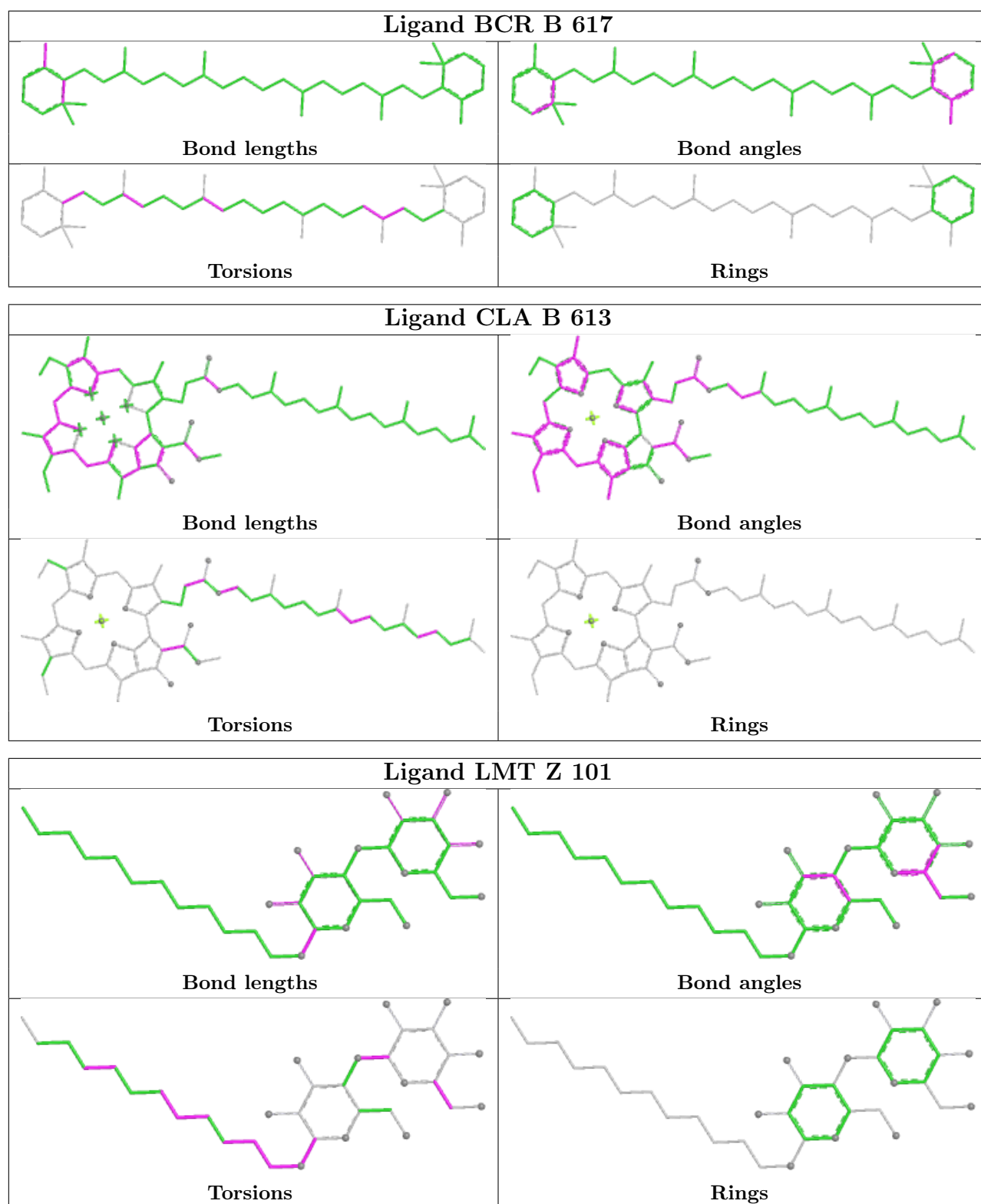


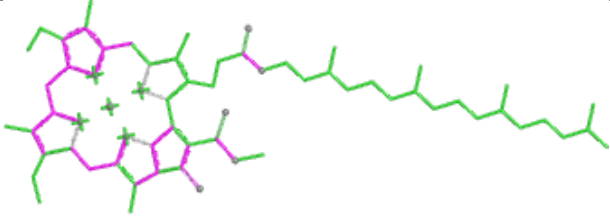
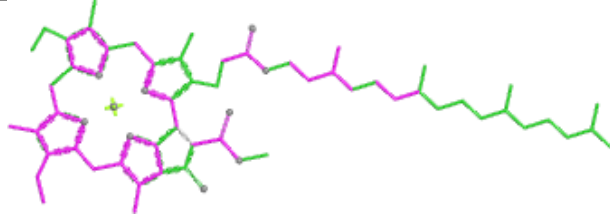
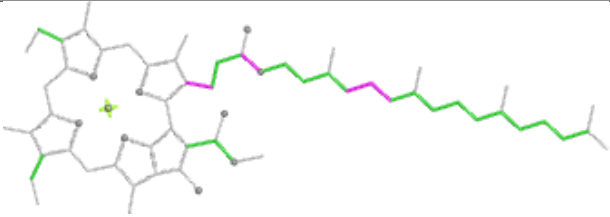
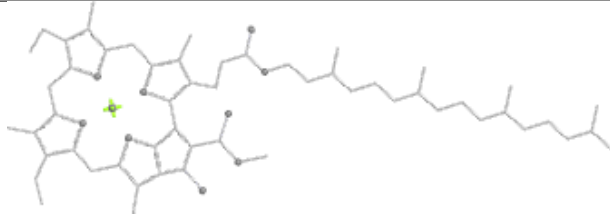
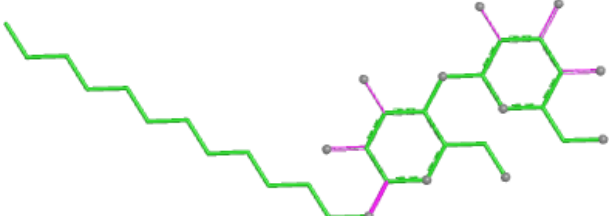
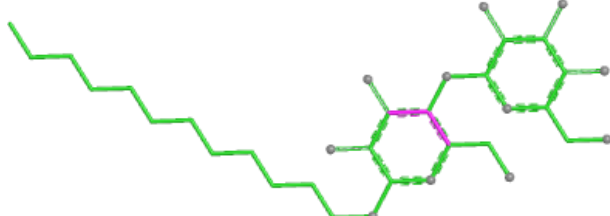
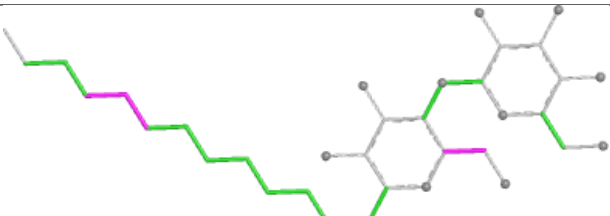
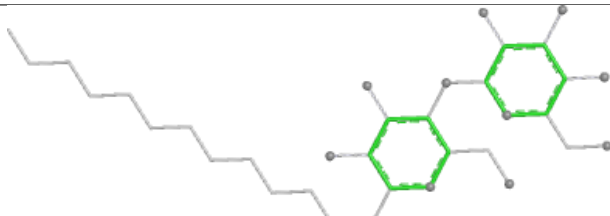
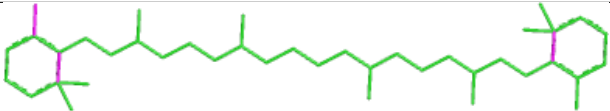
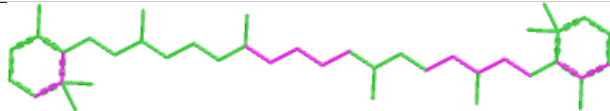
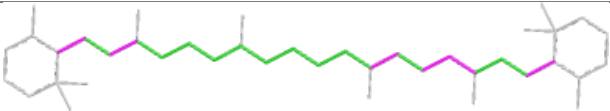
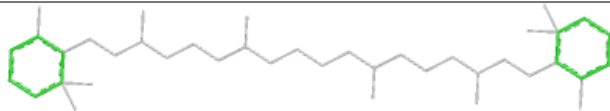


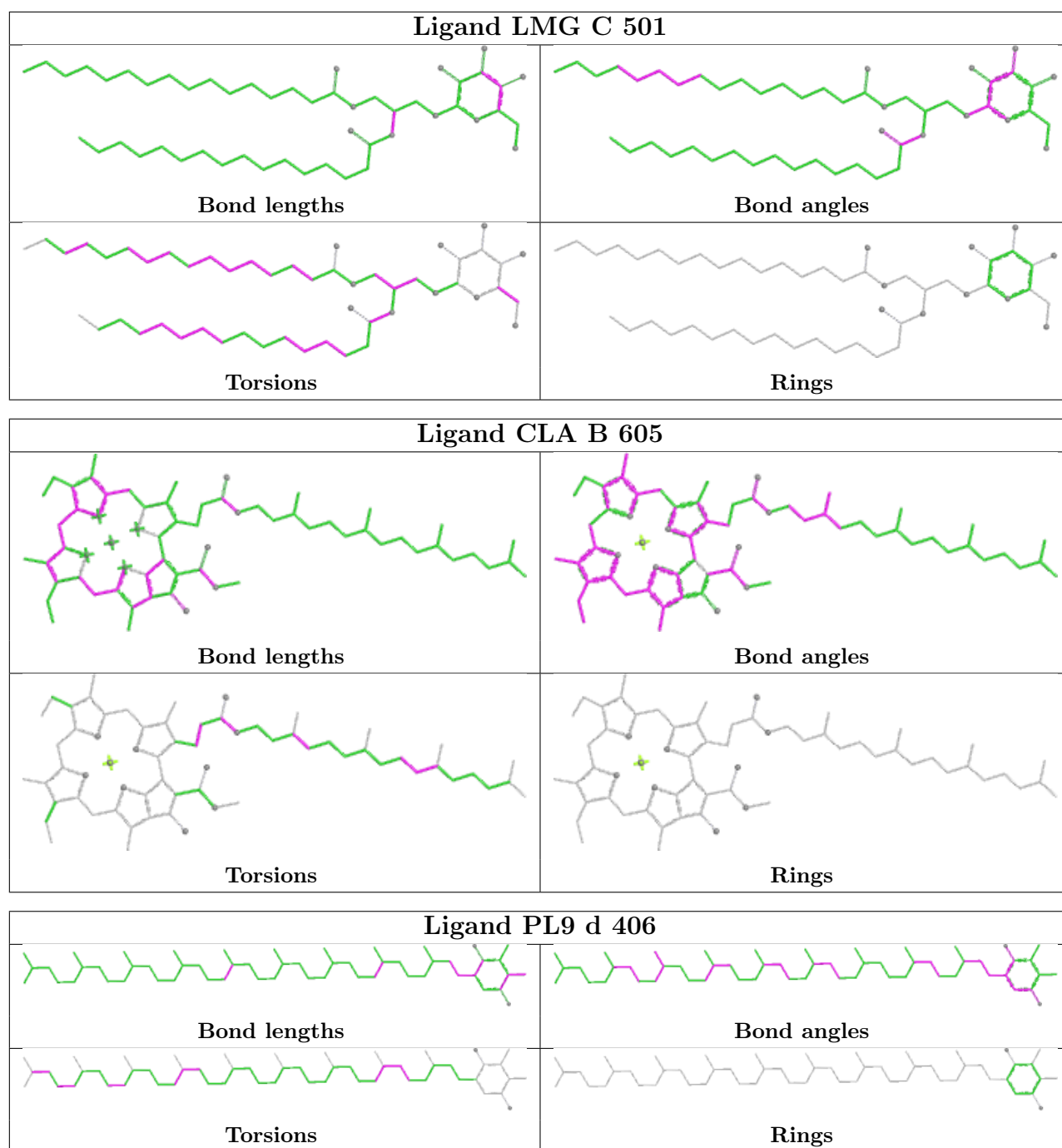


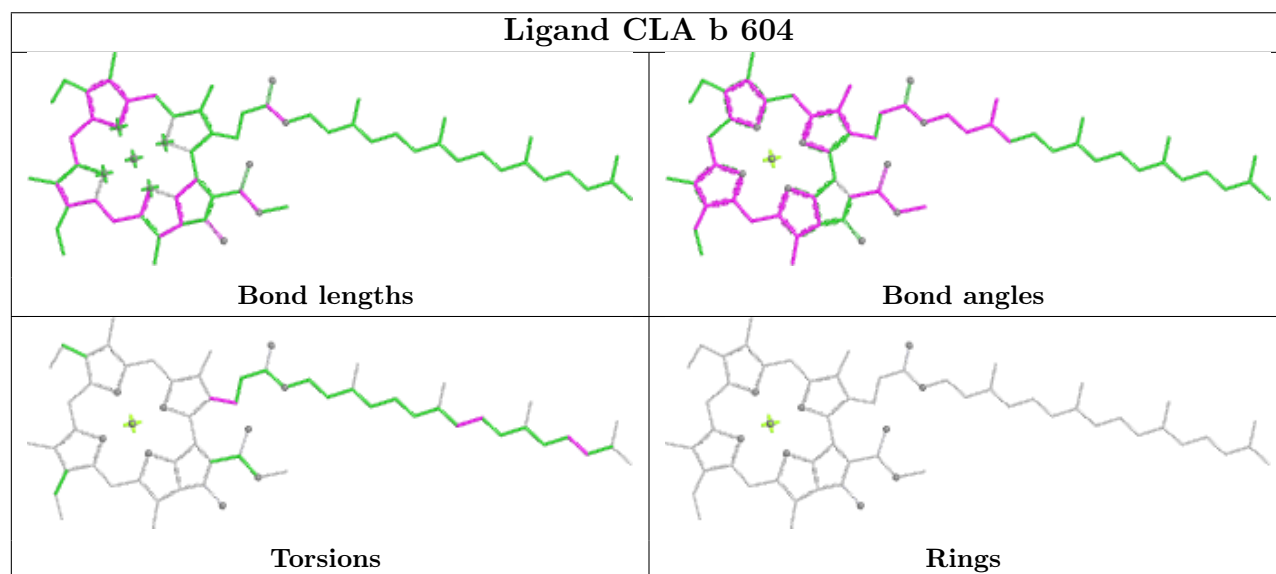
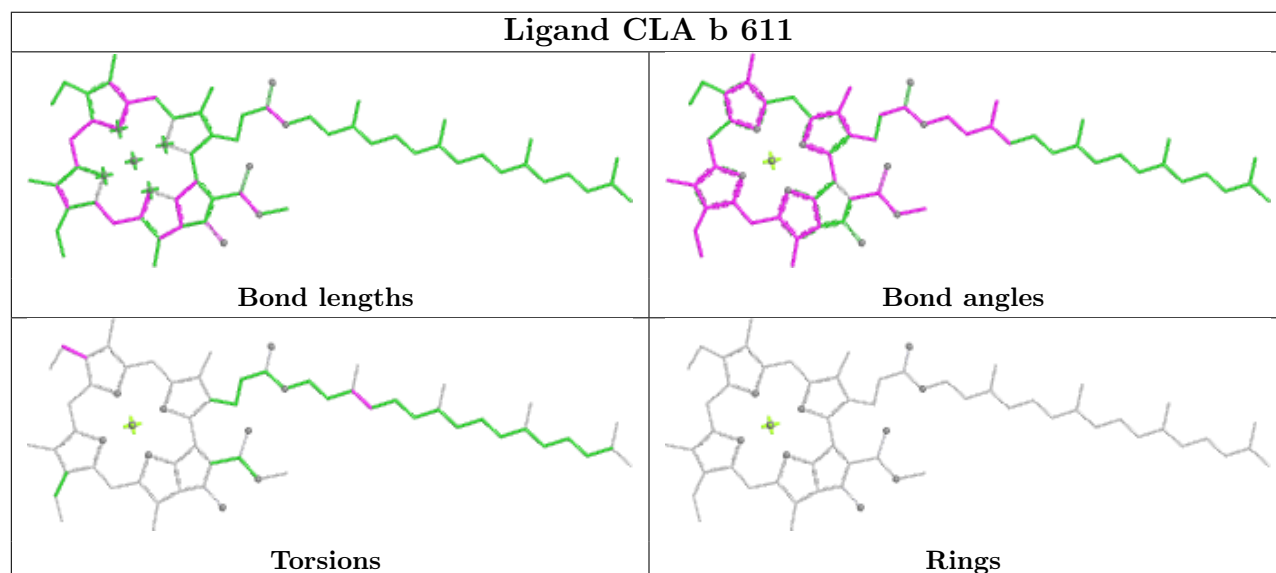
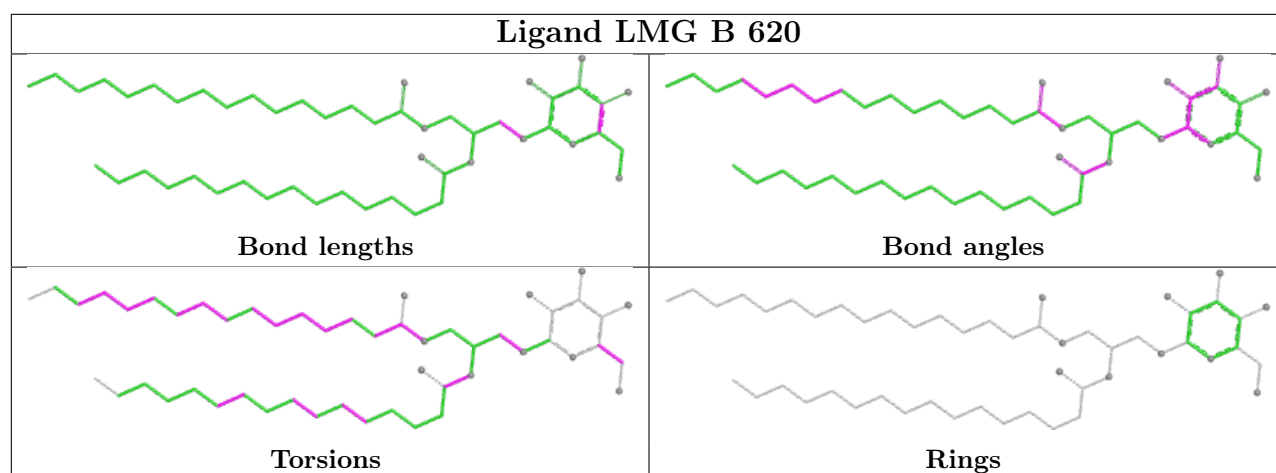


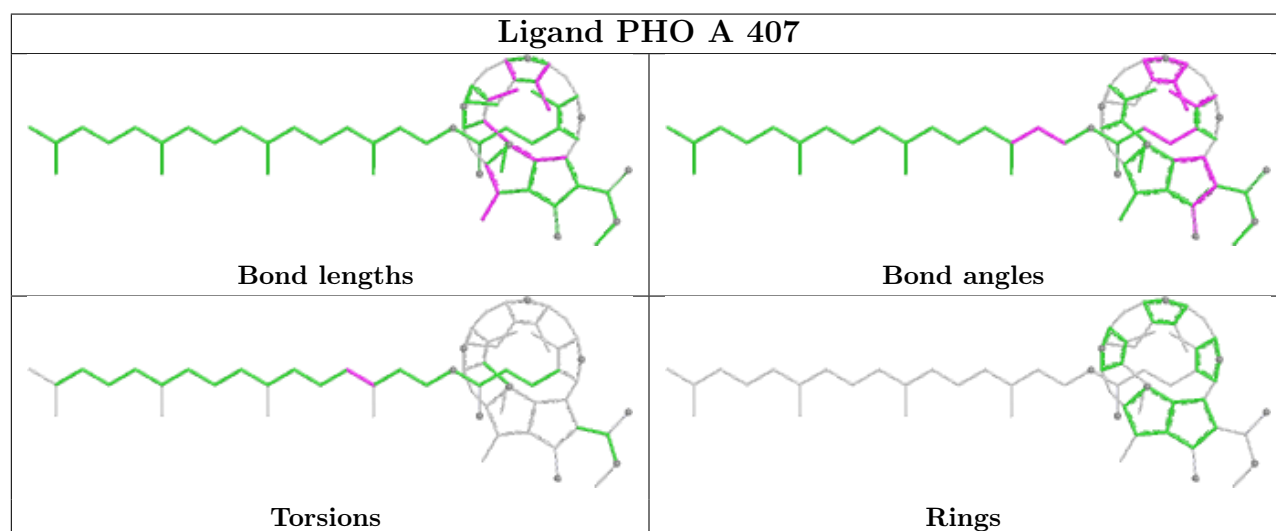
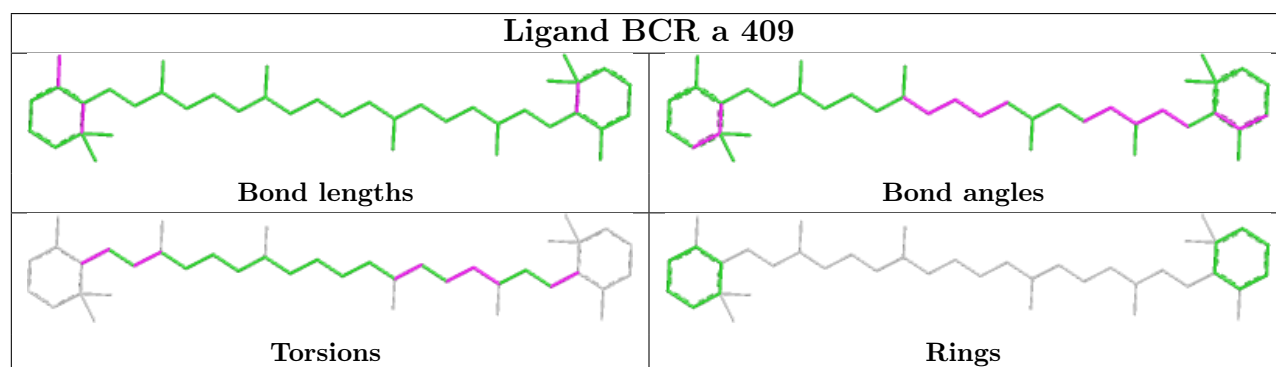
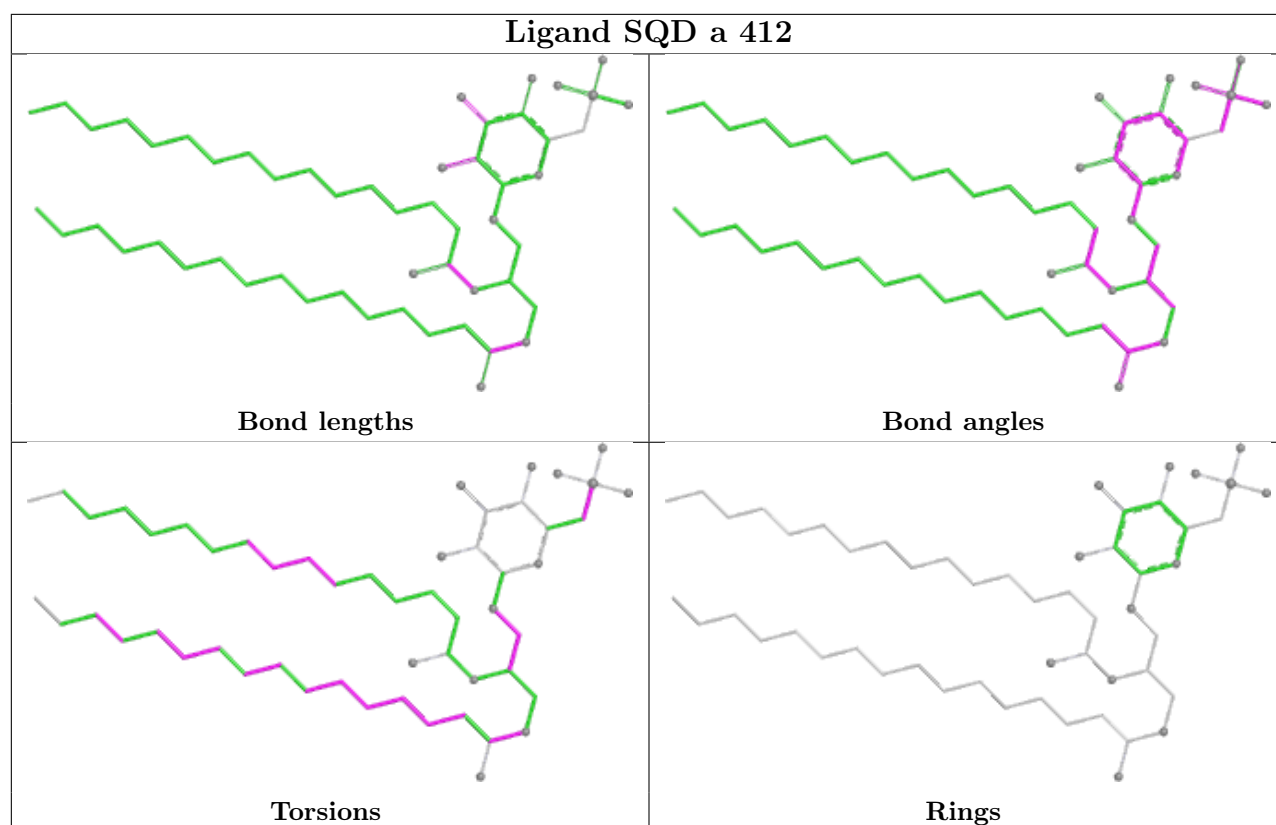


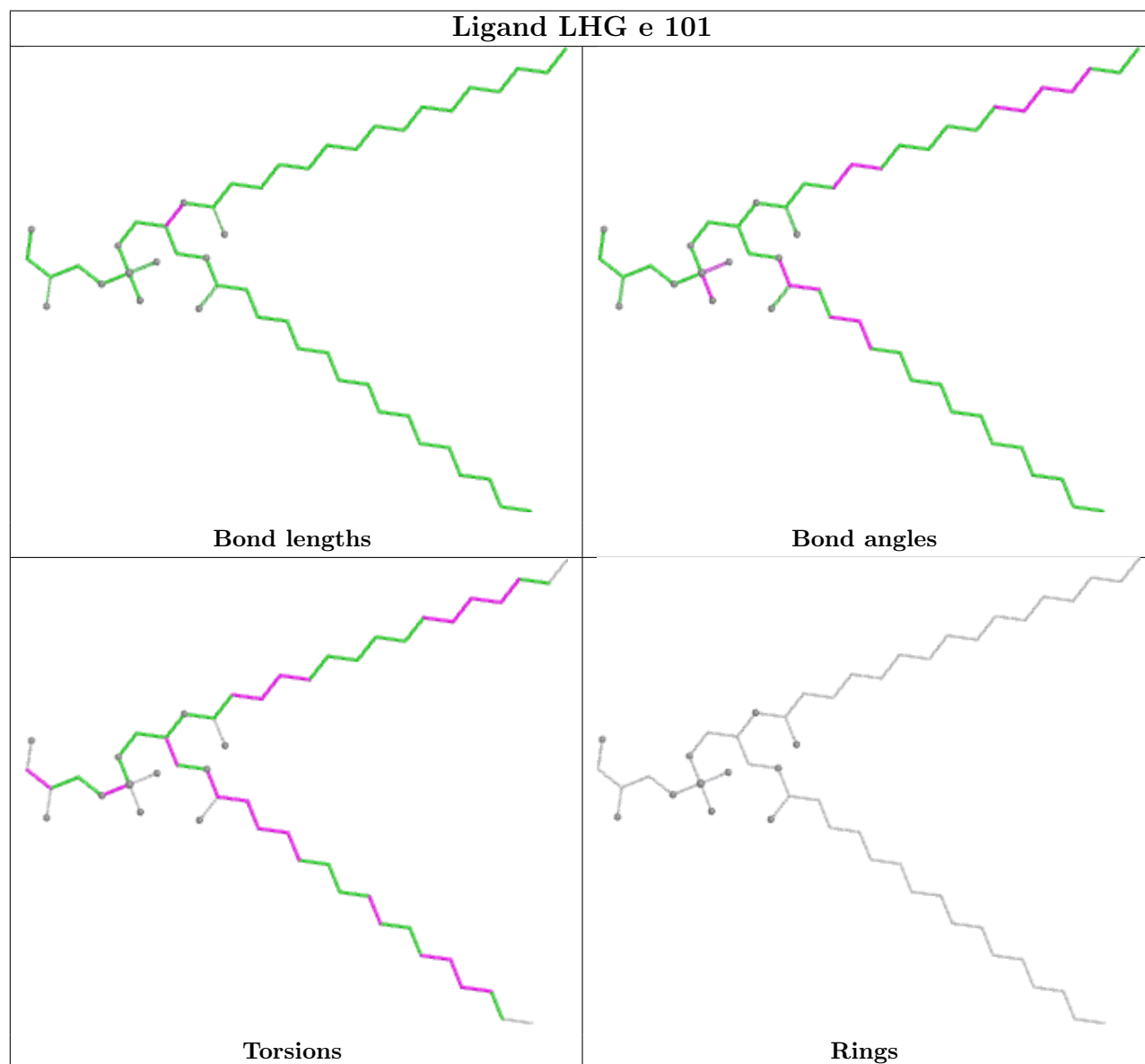
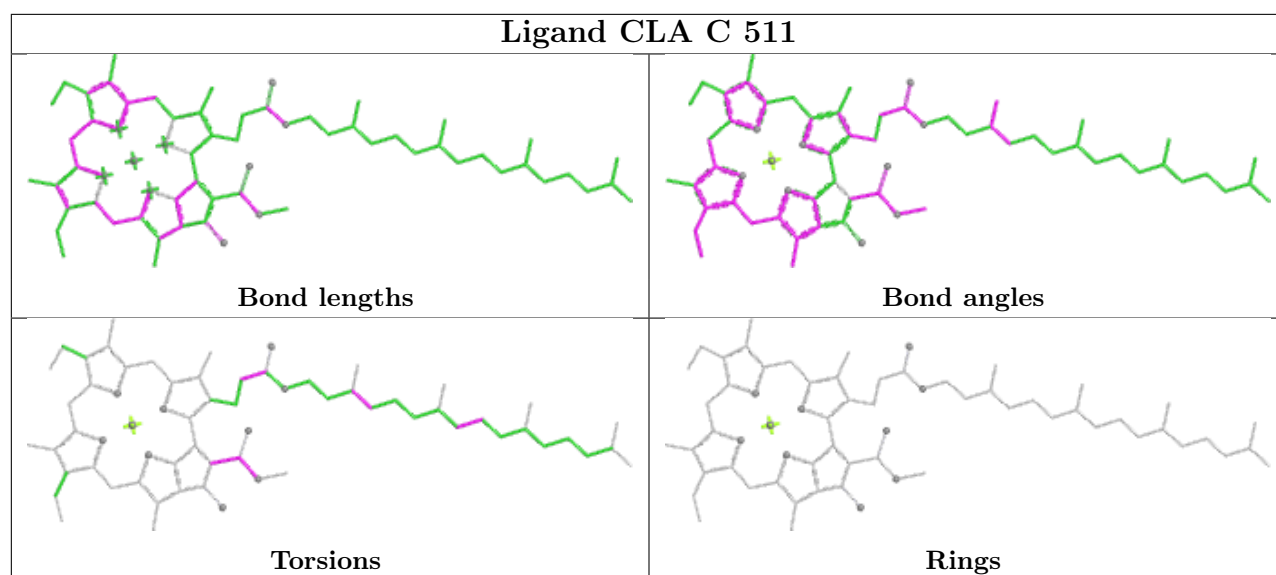


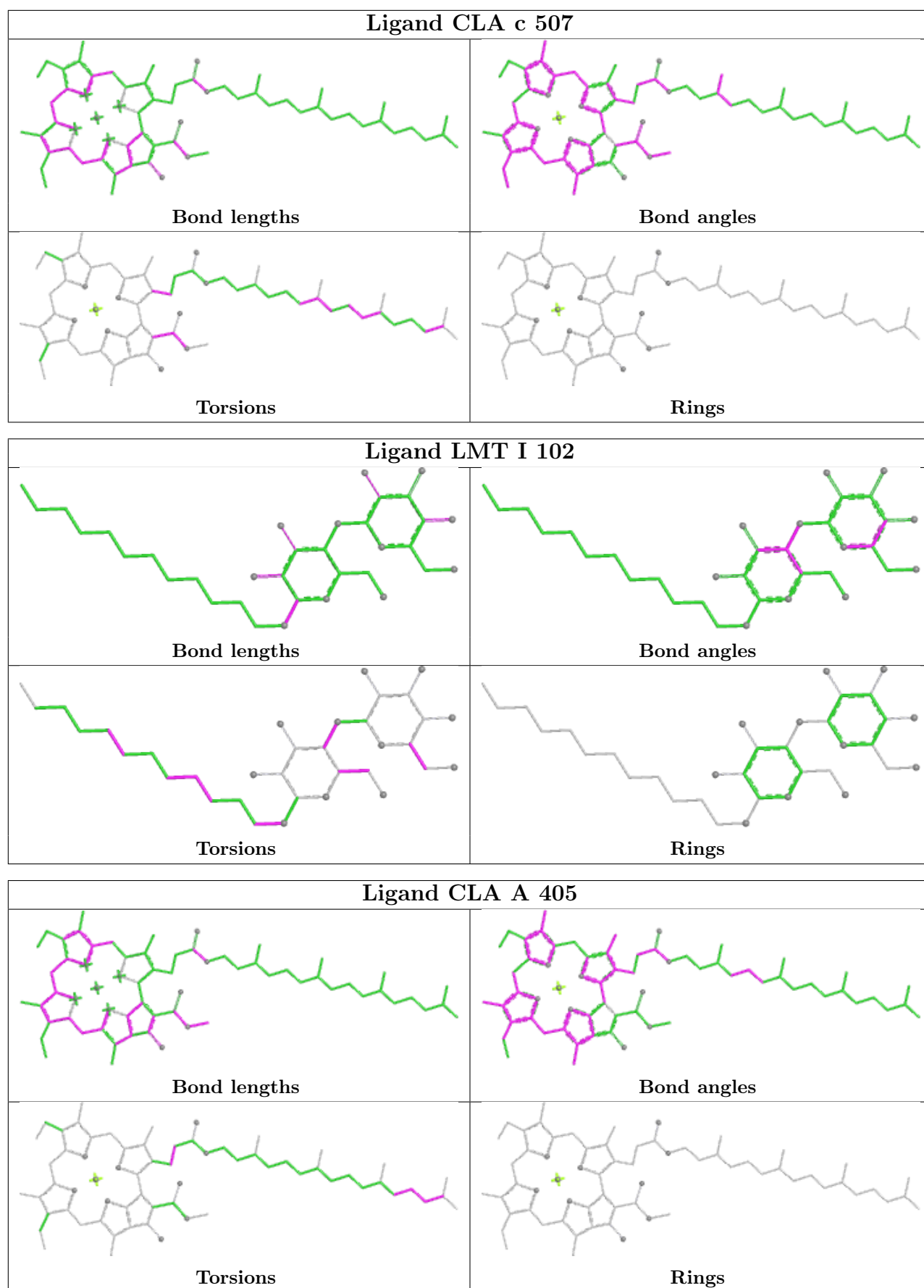
Ligand CLA C 512	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT m 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

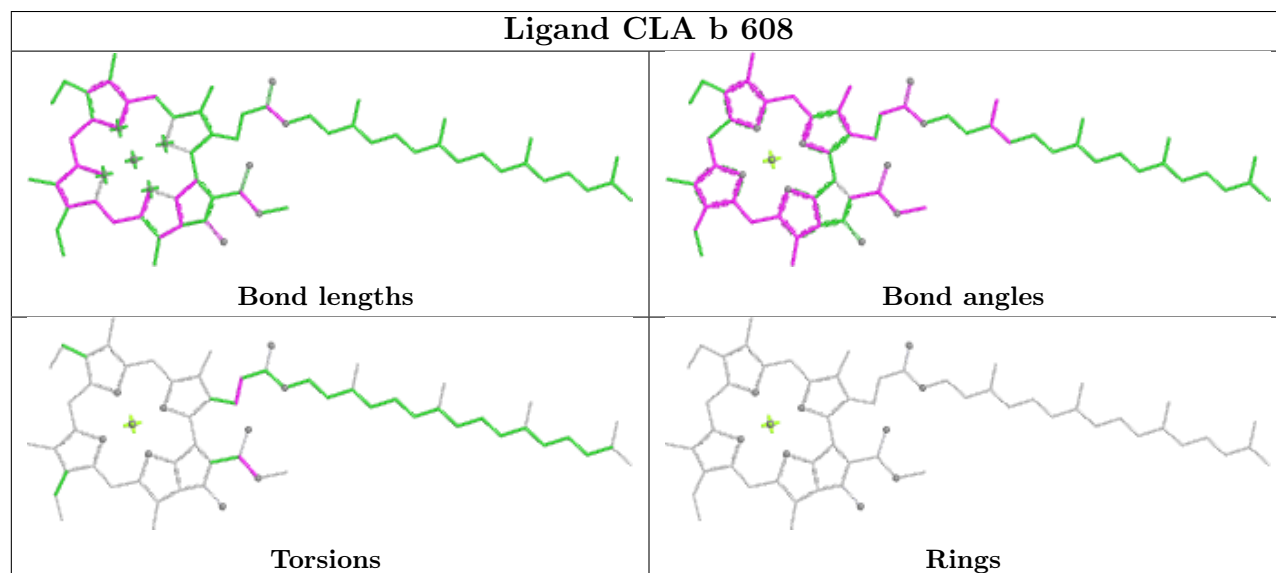
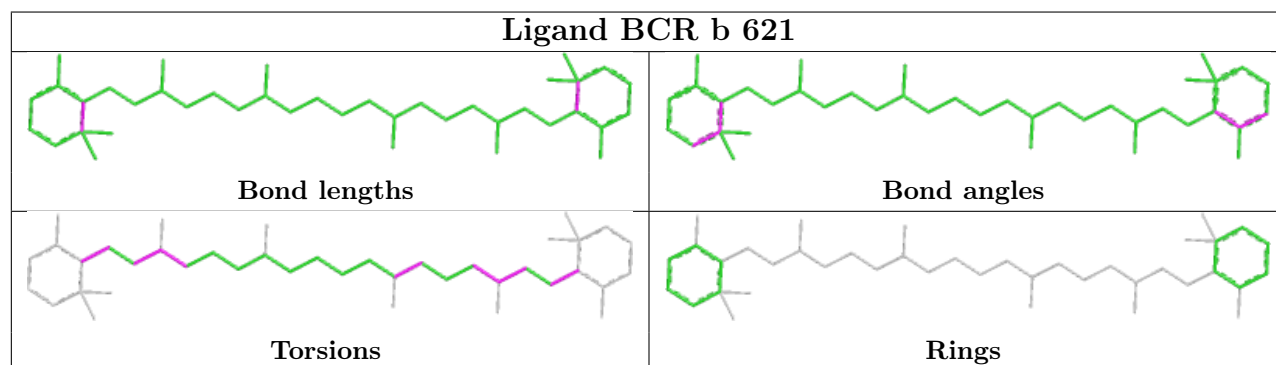
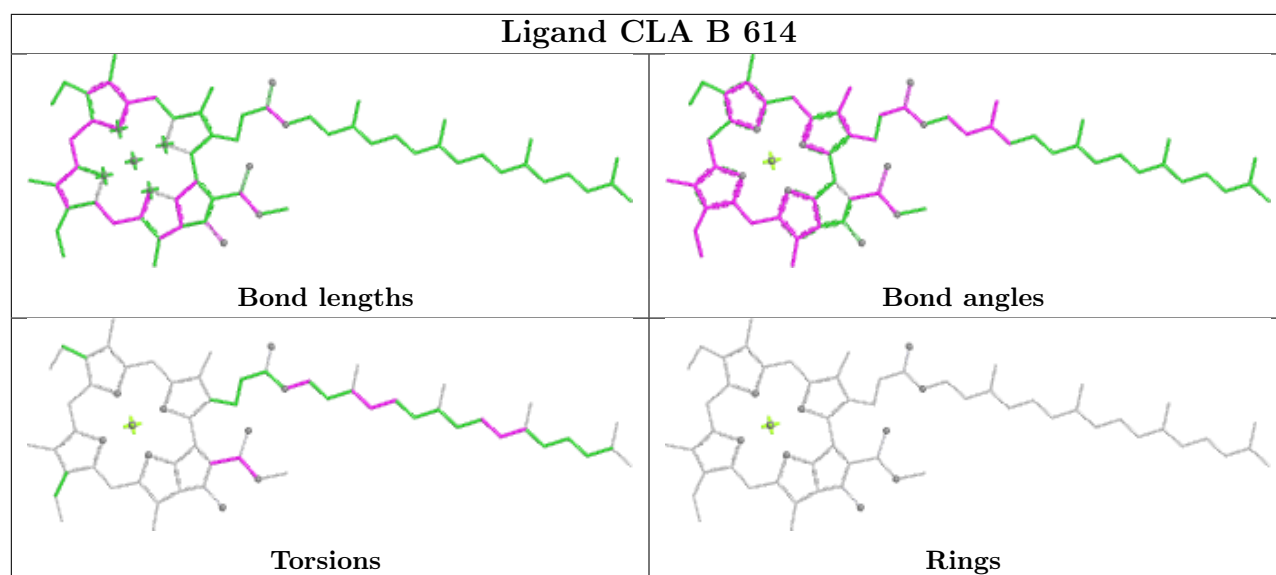


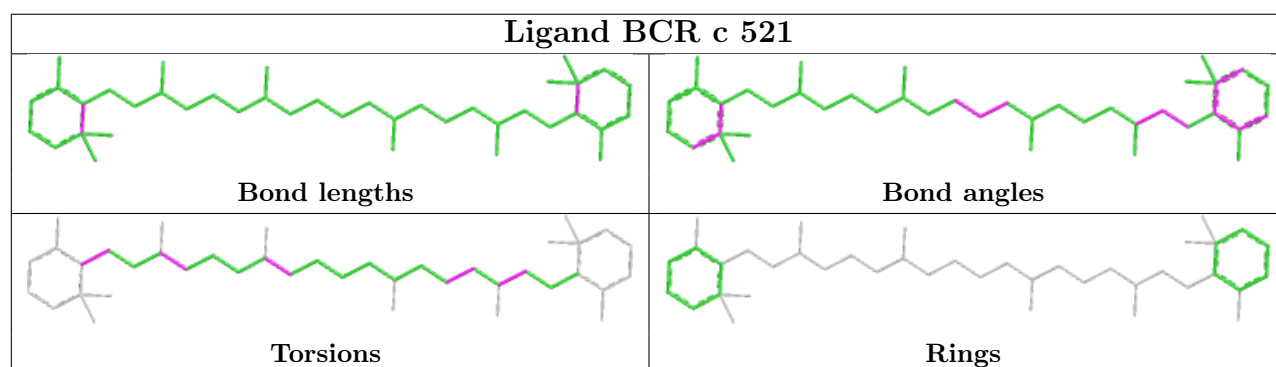
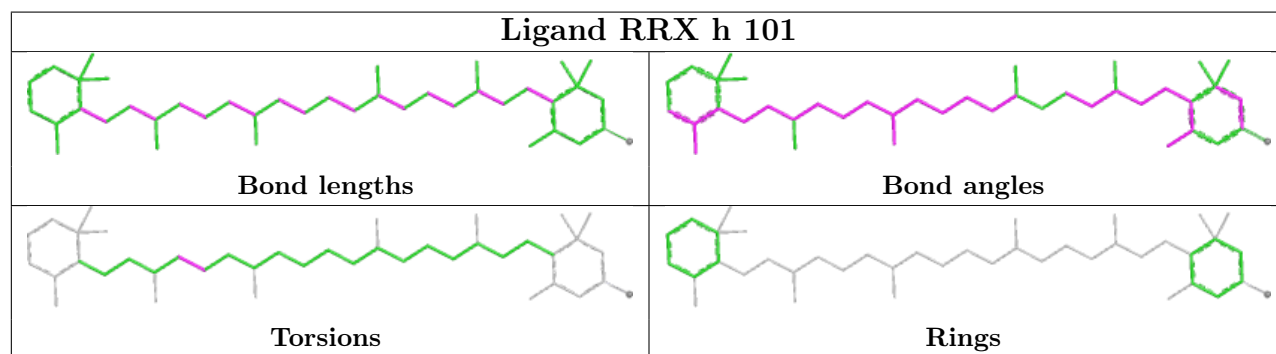
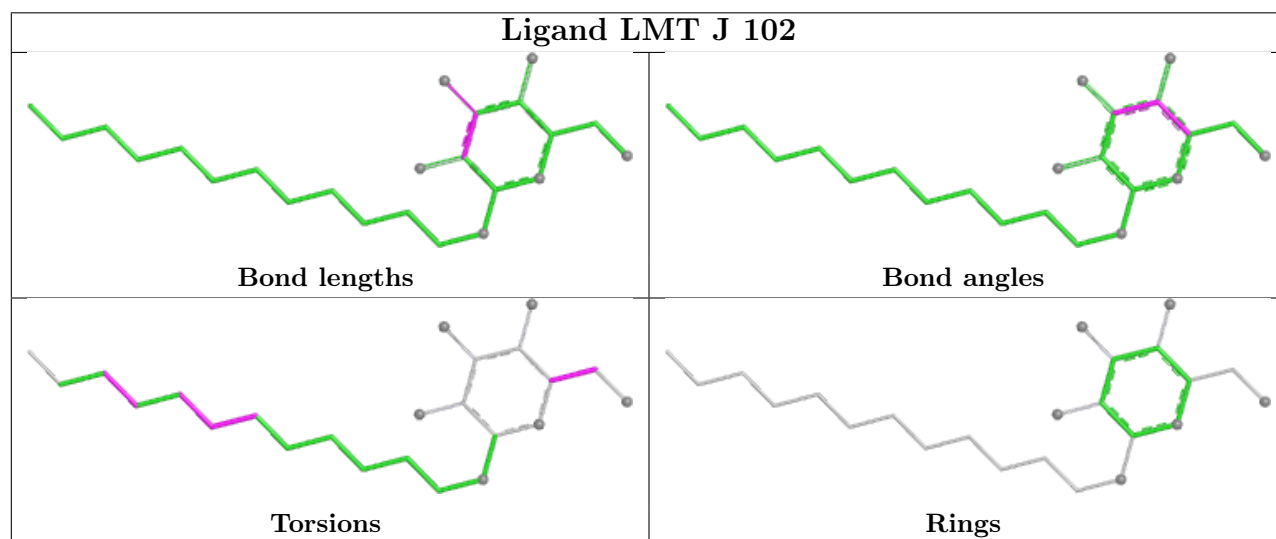
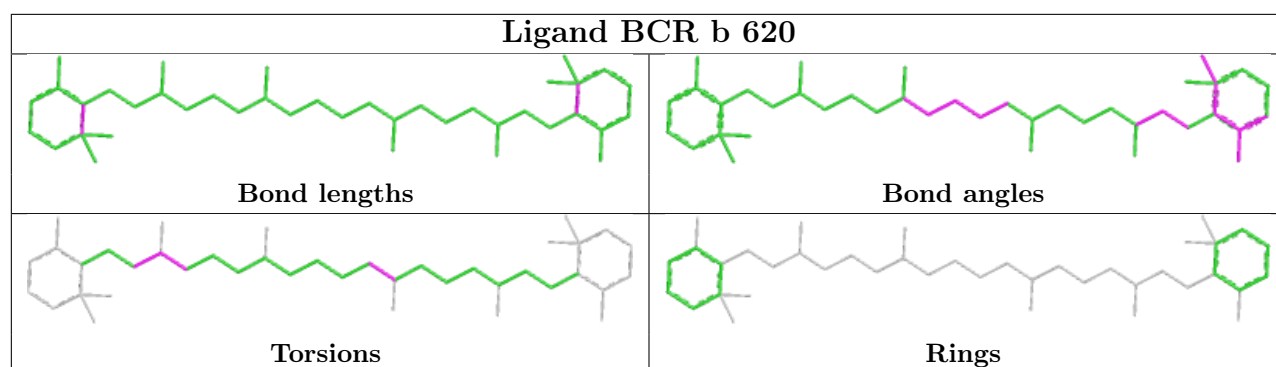


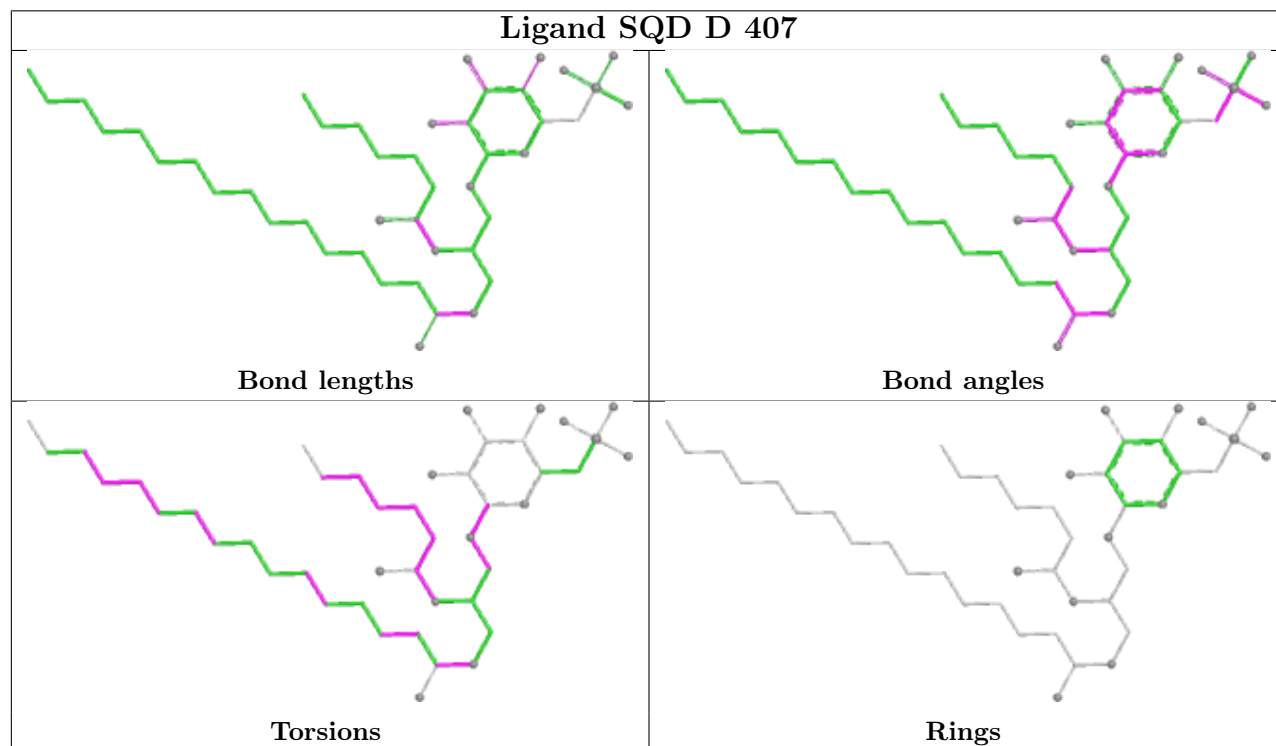
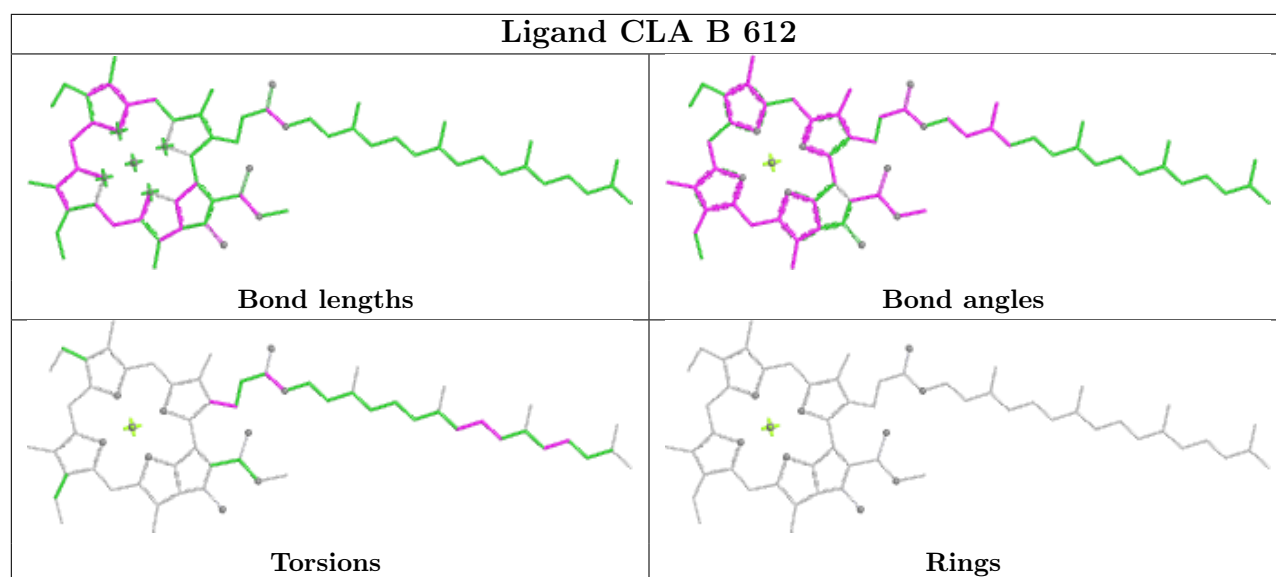


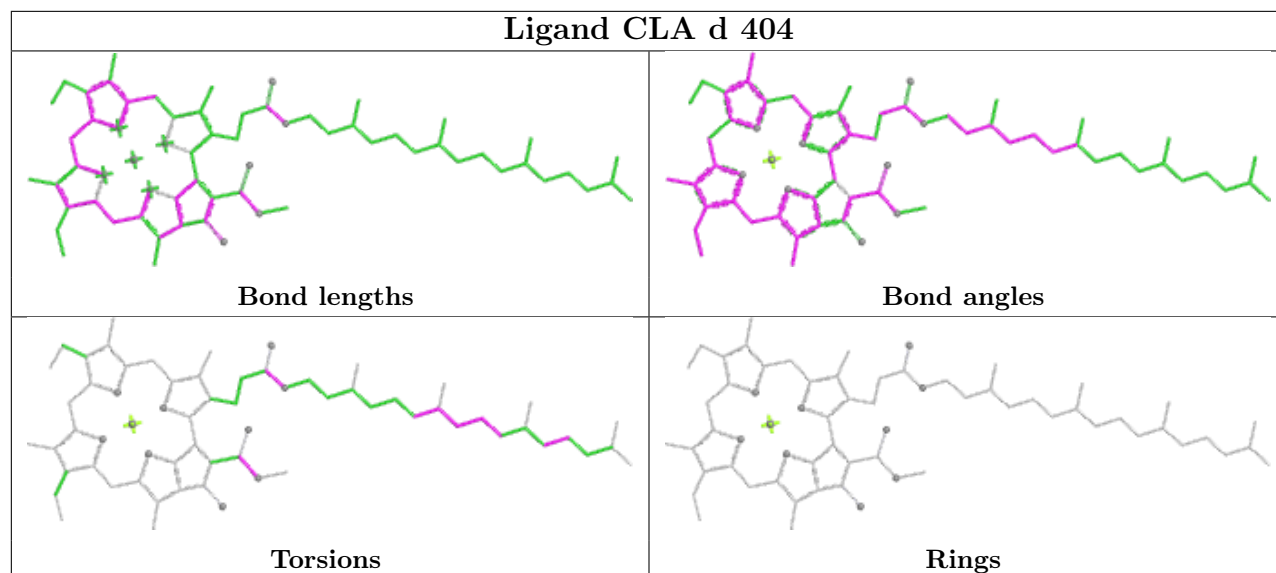
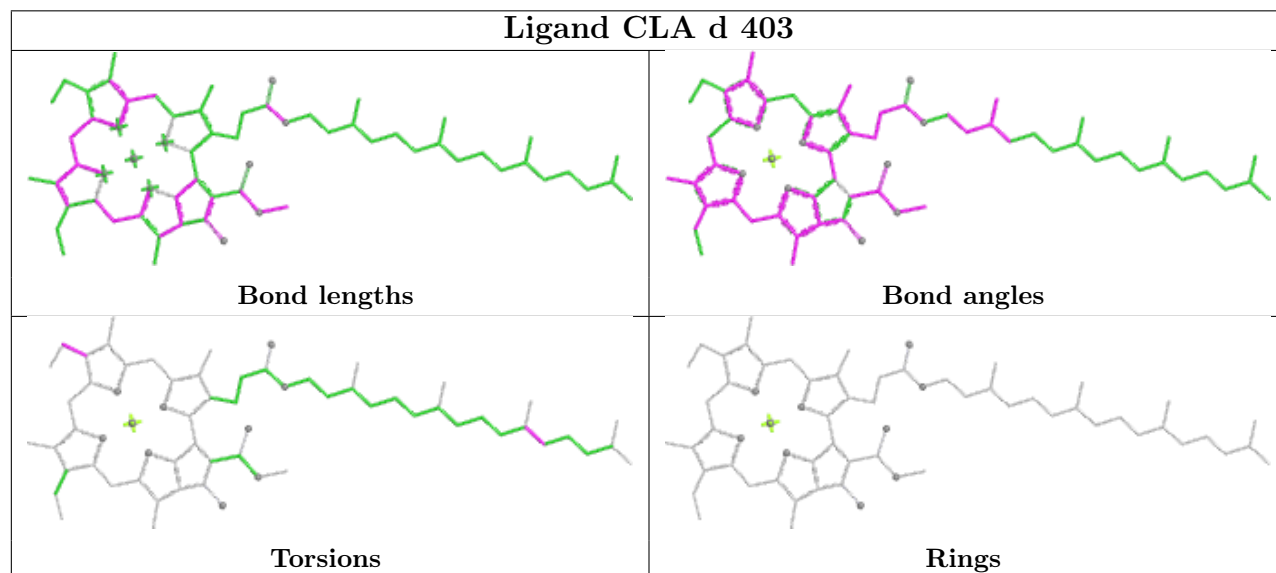
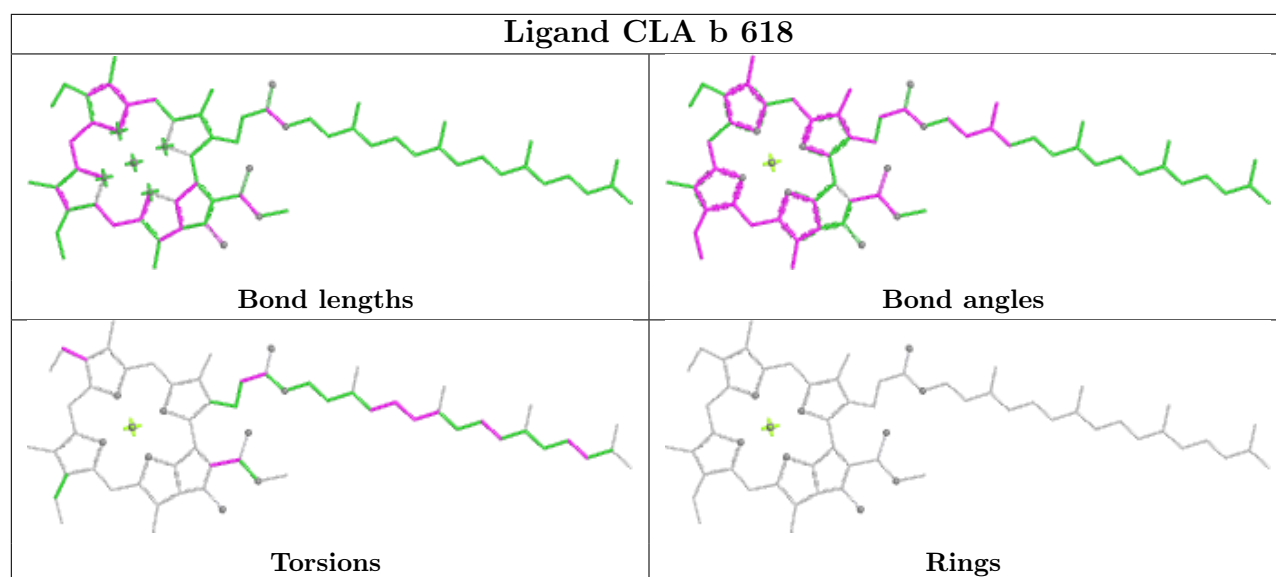


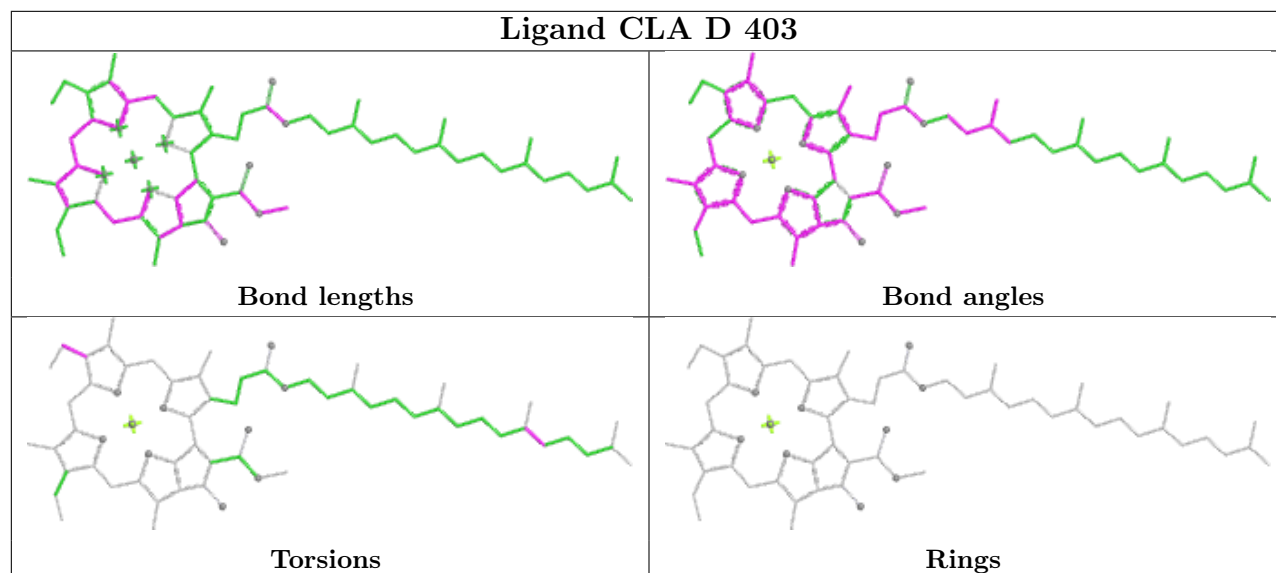
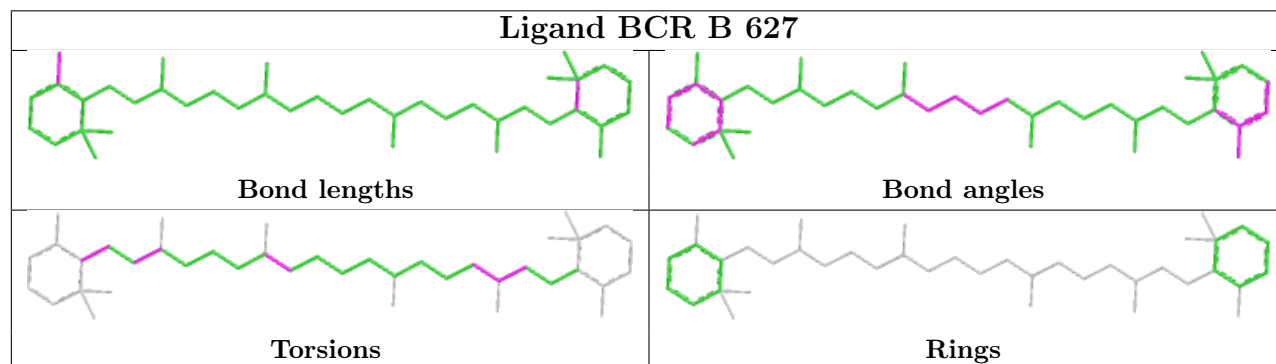
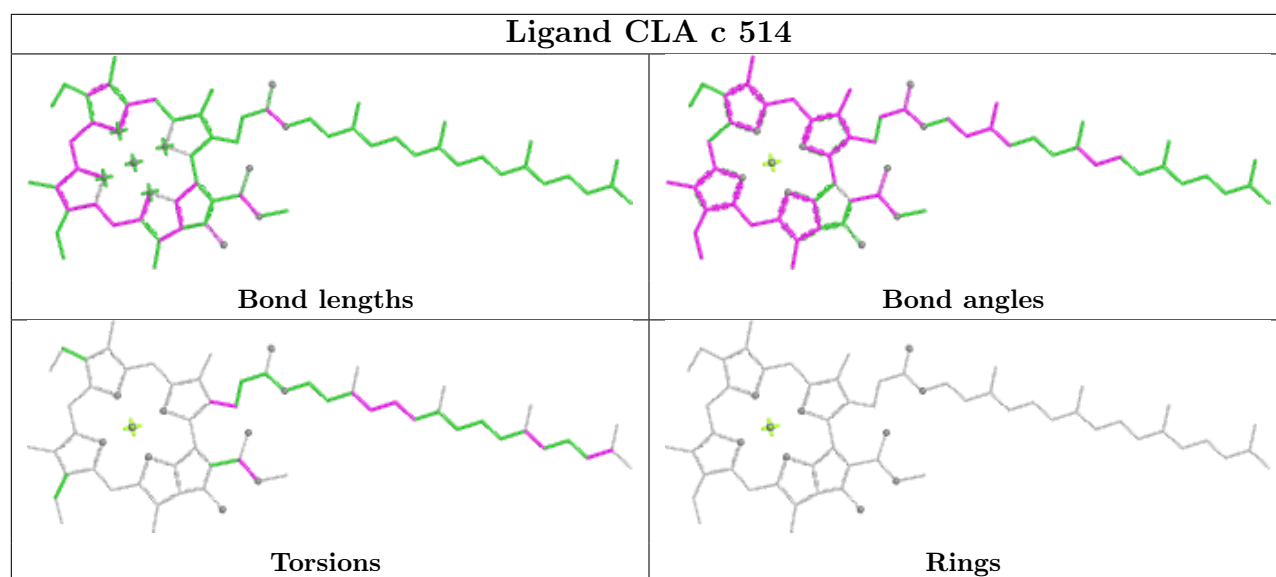


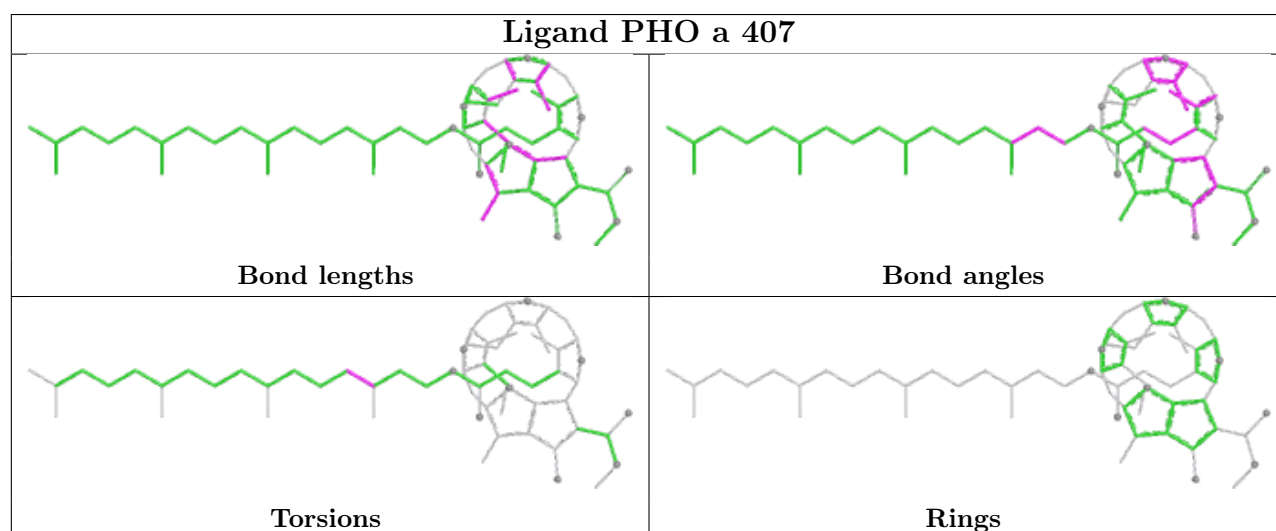
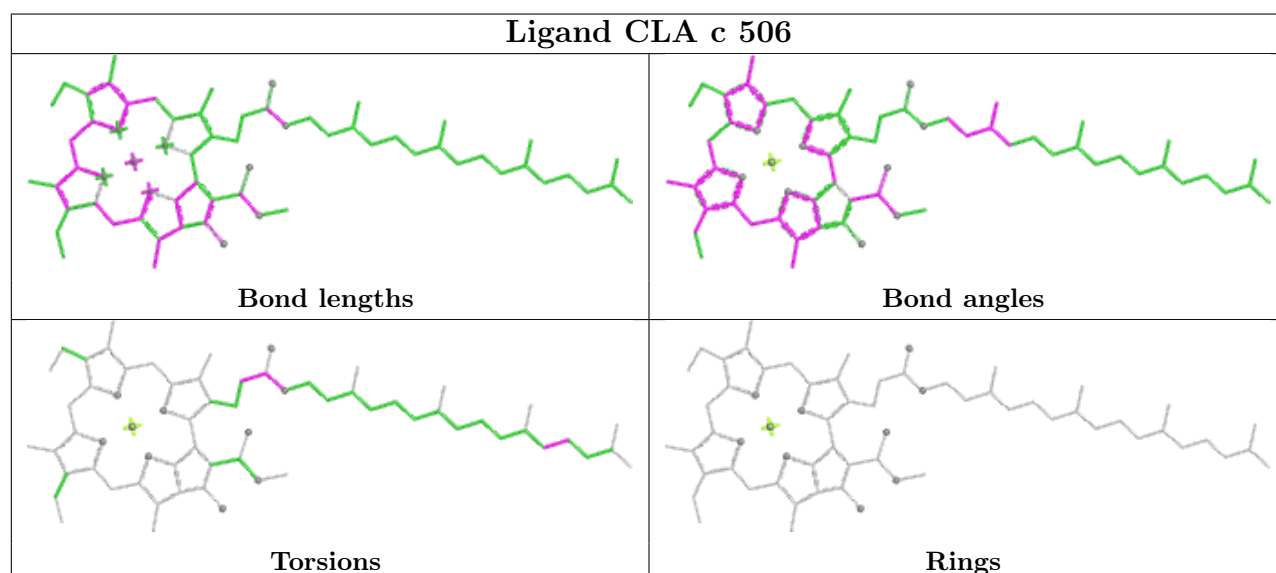
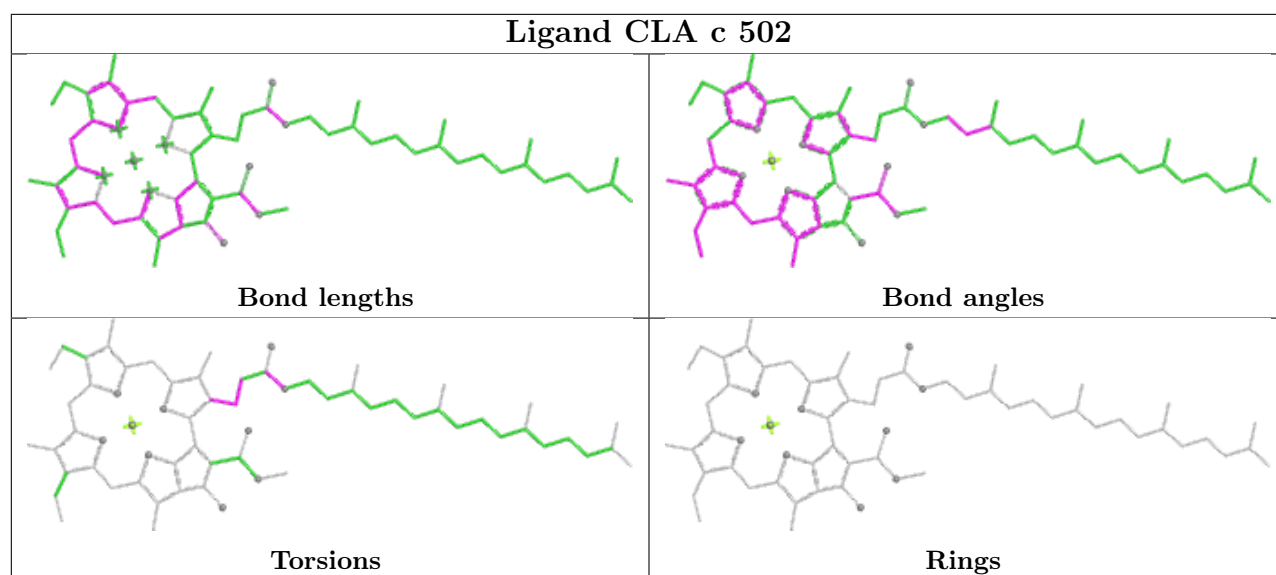


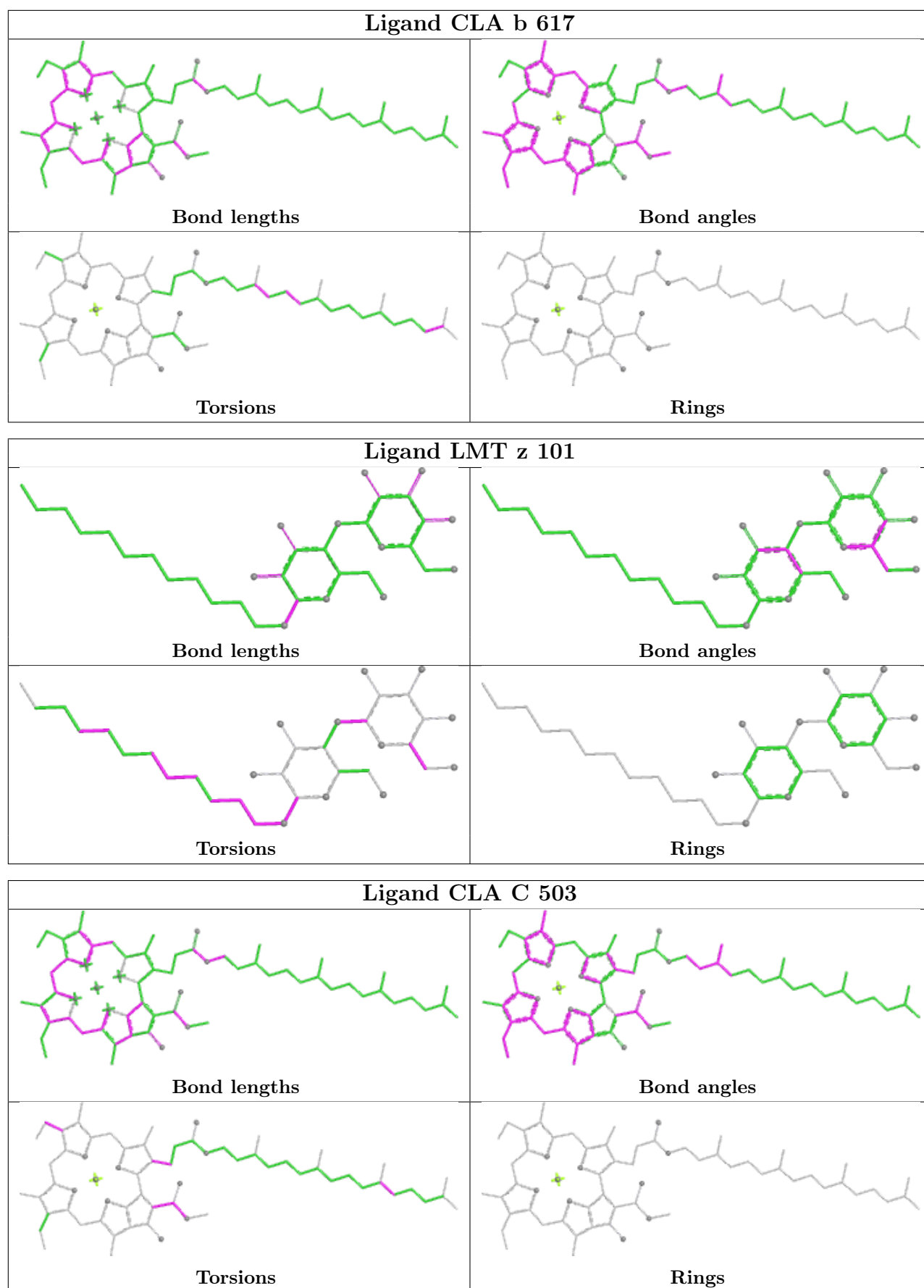


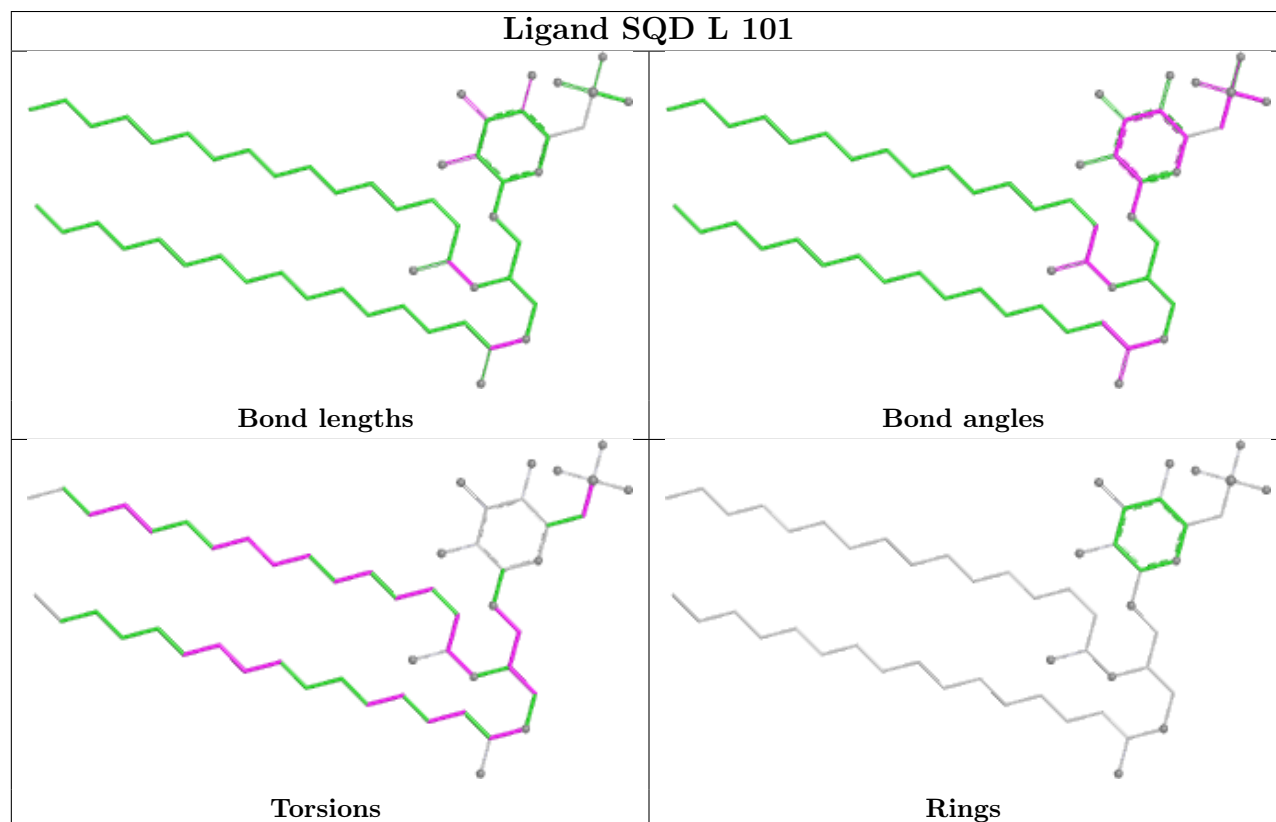
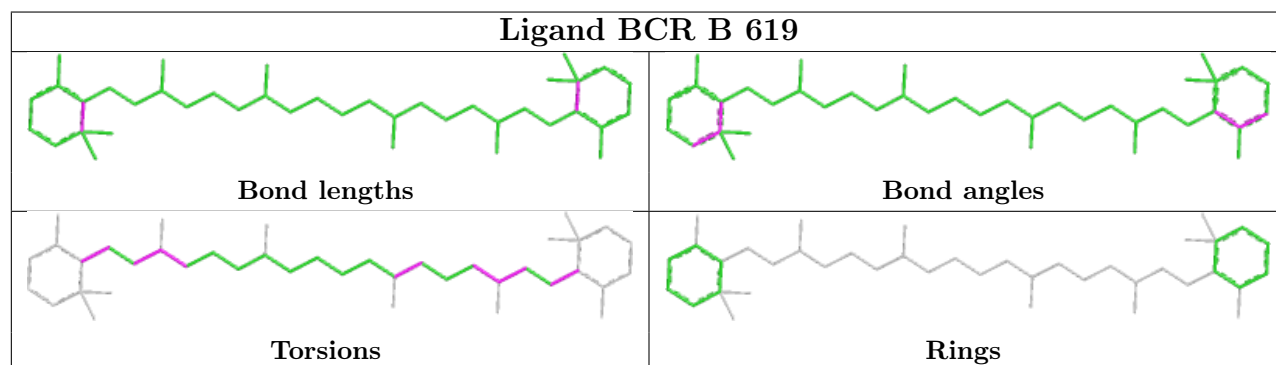
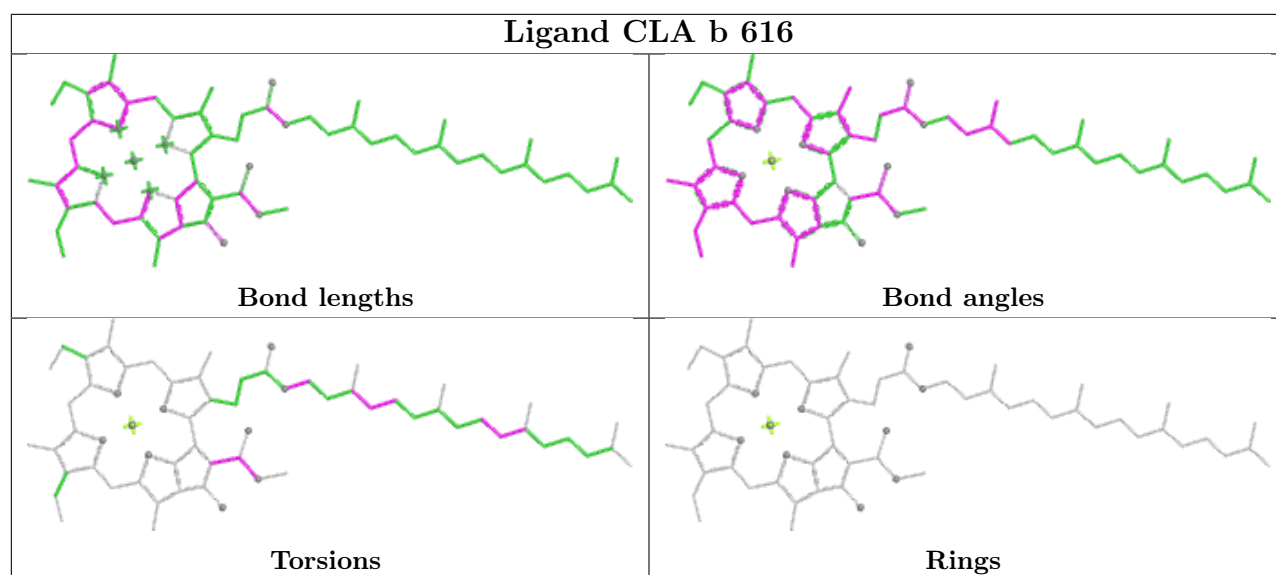


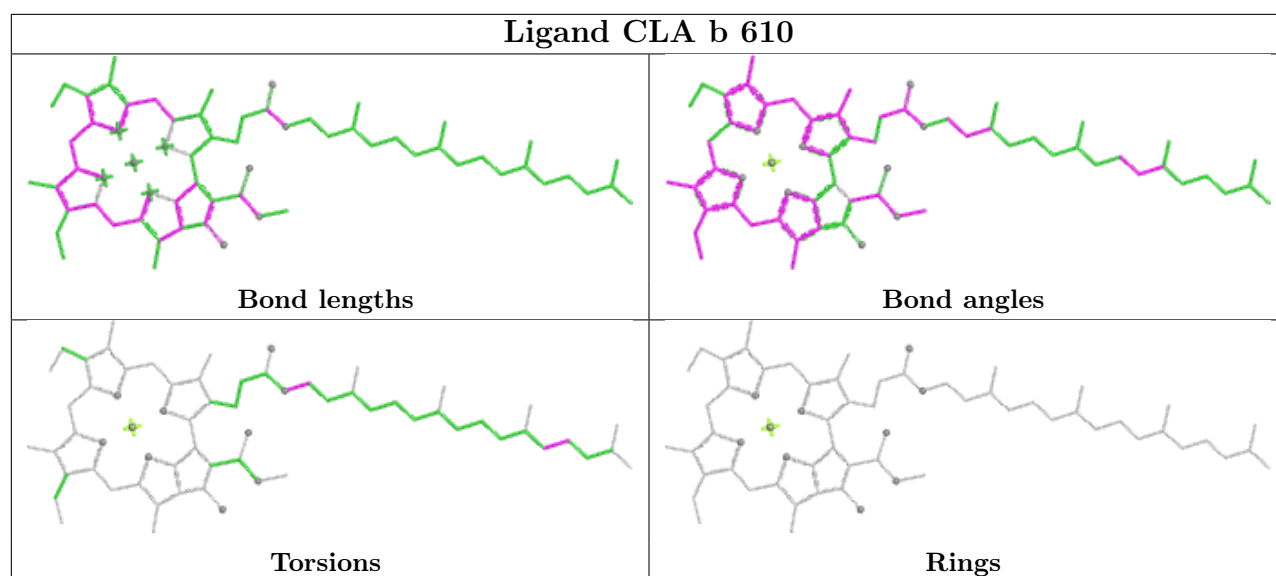
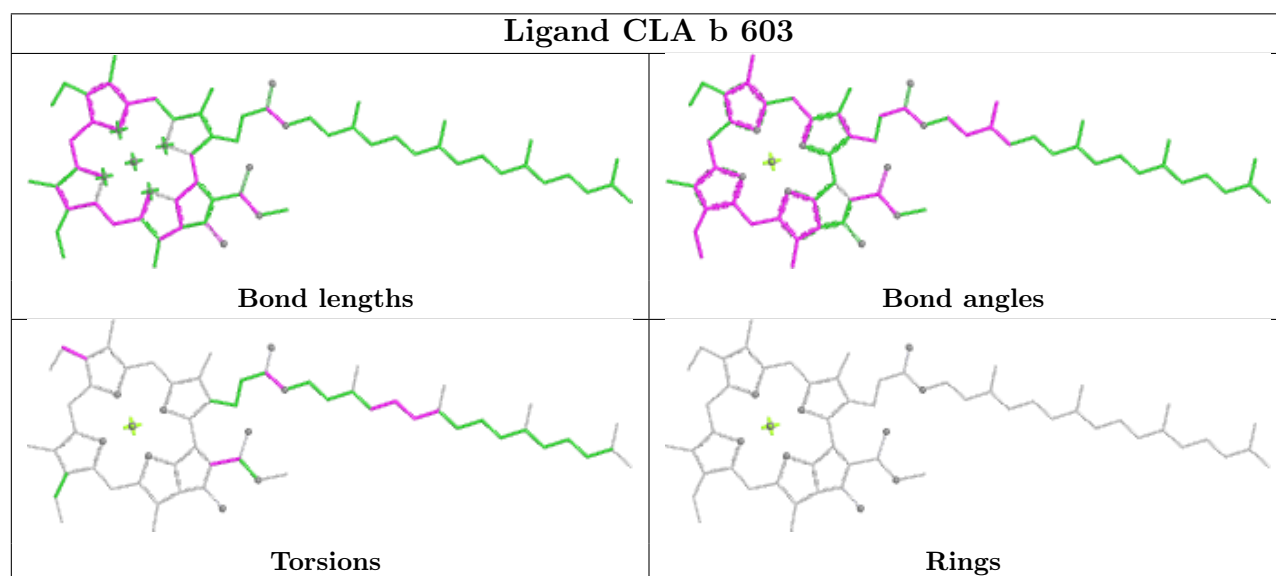
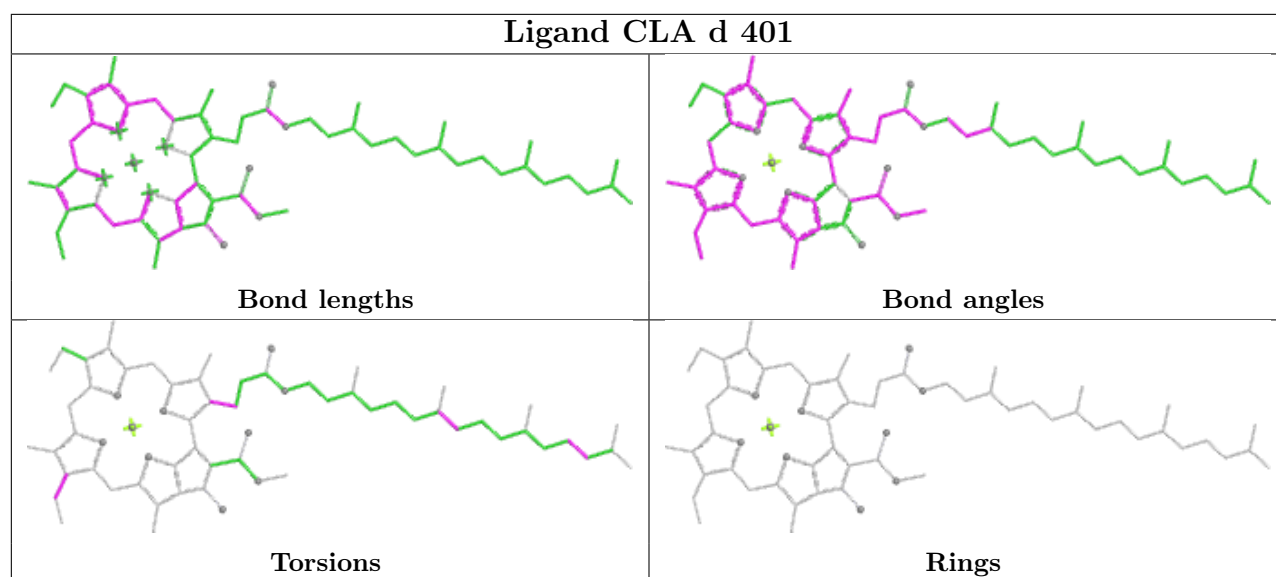


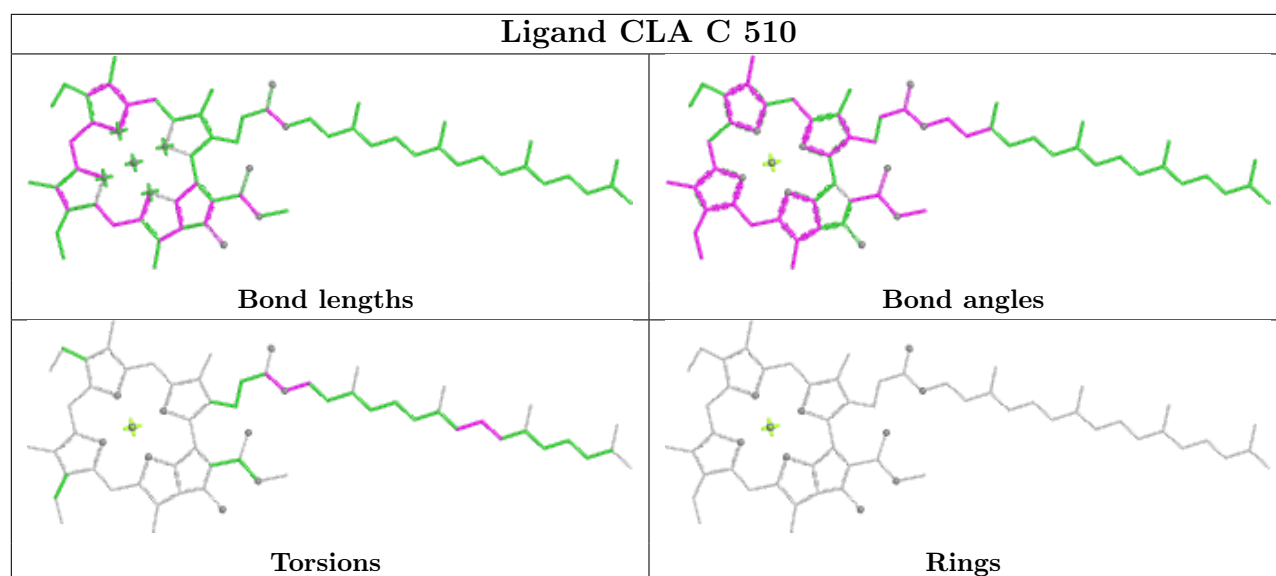
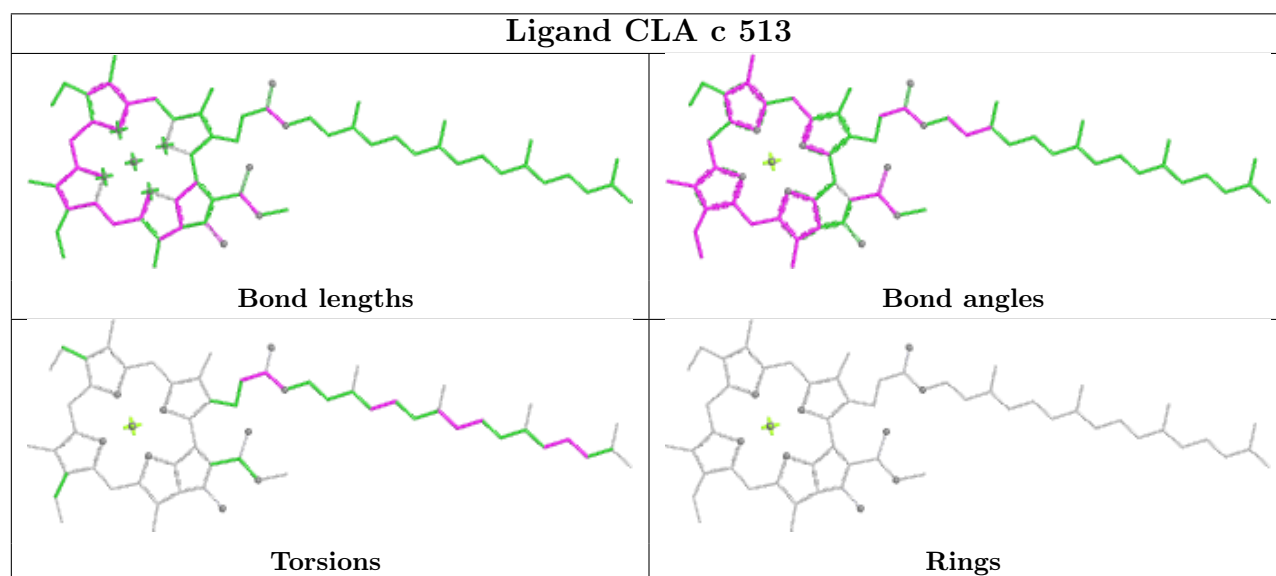
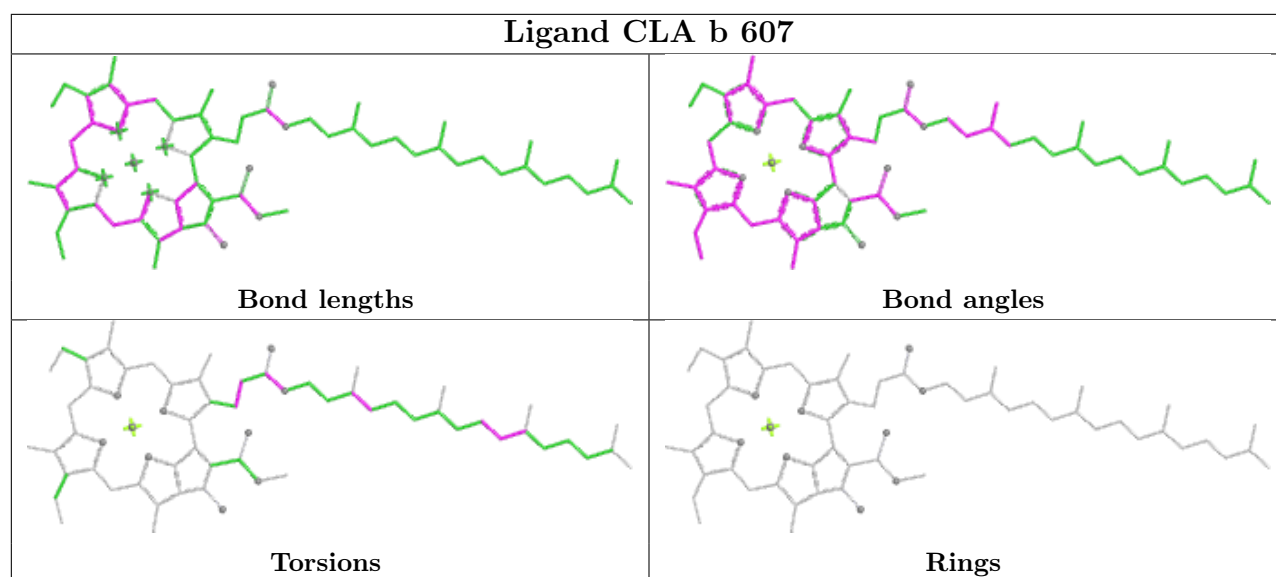


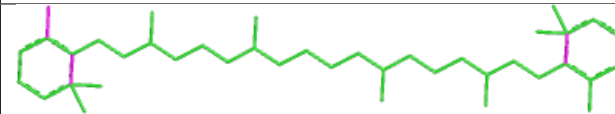
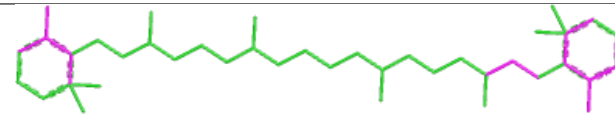
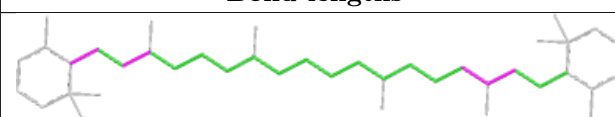
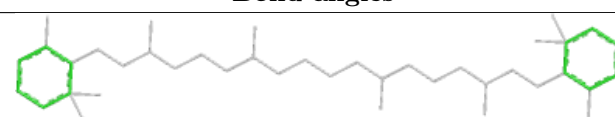


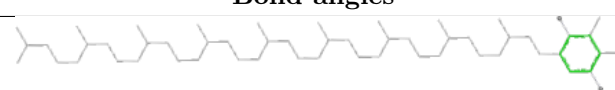


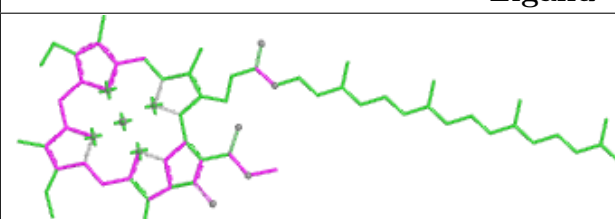
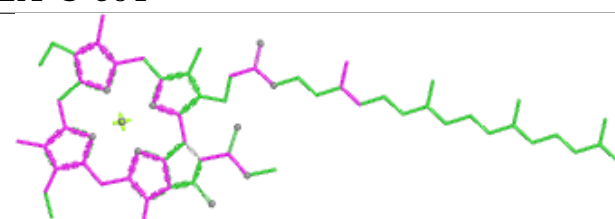
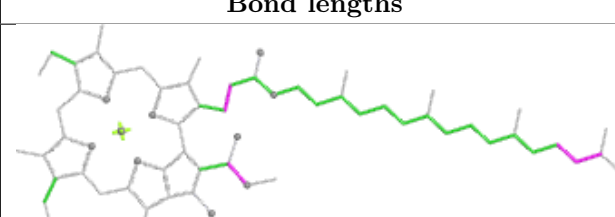
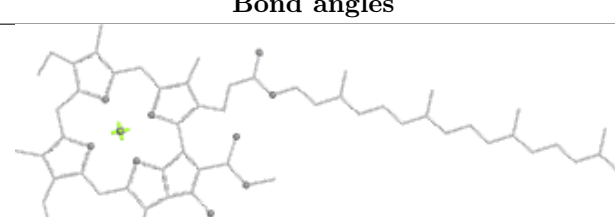


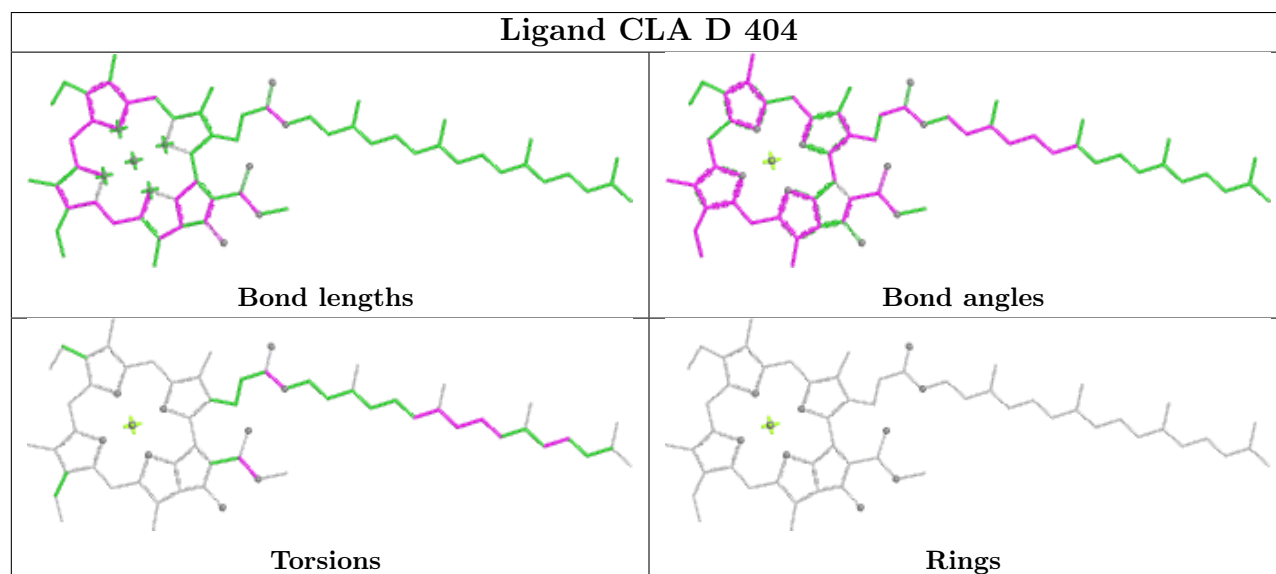
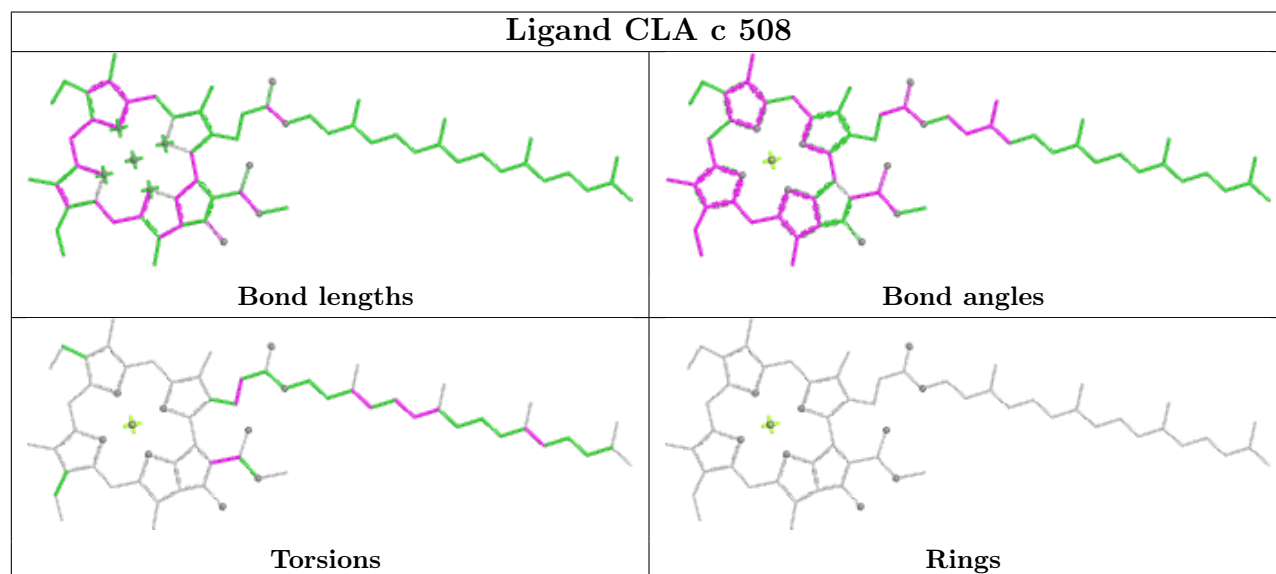
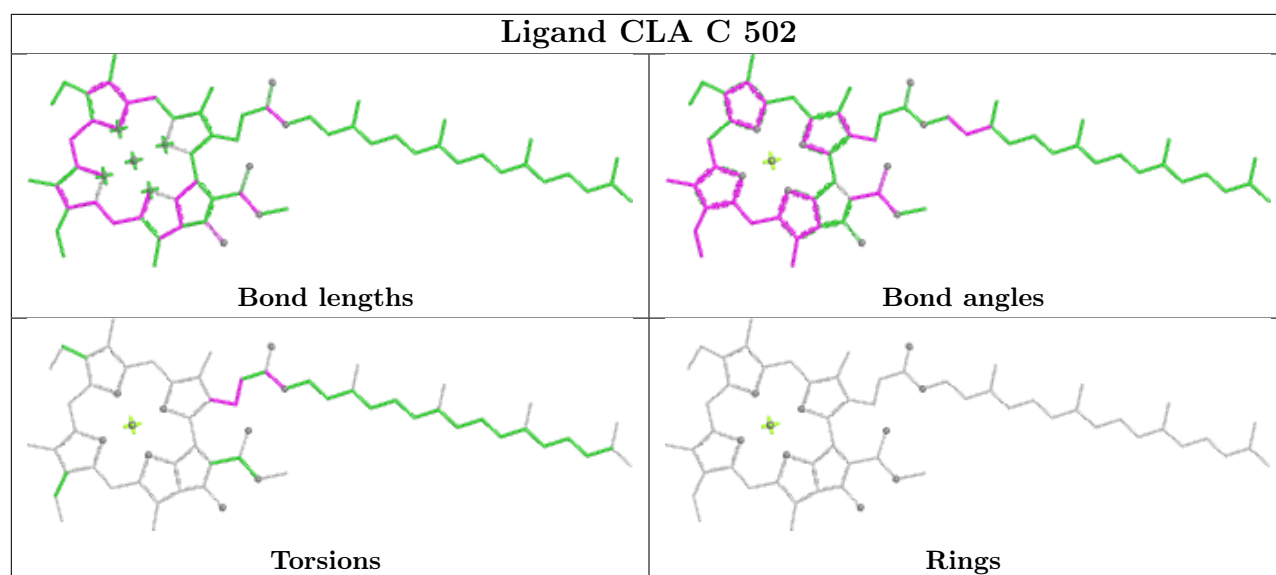


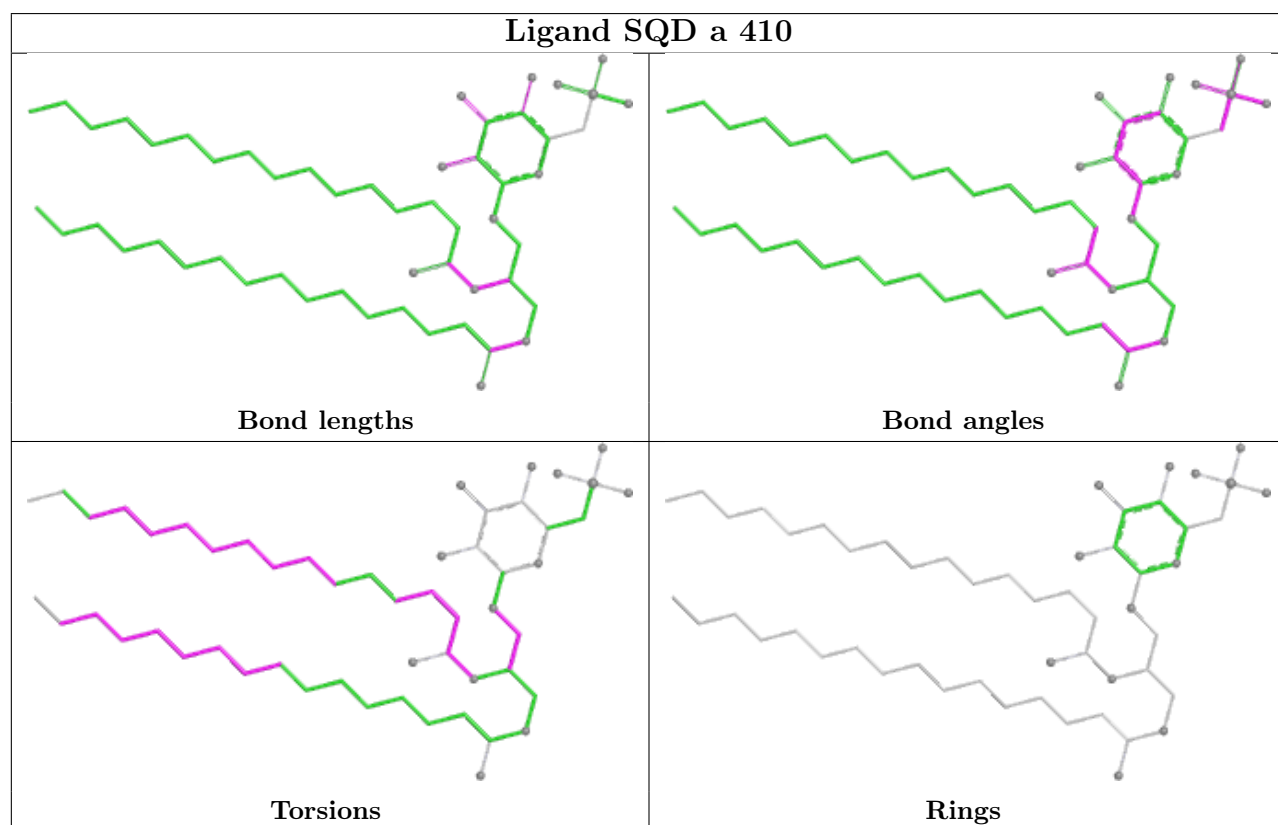
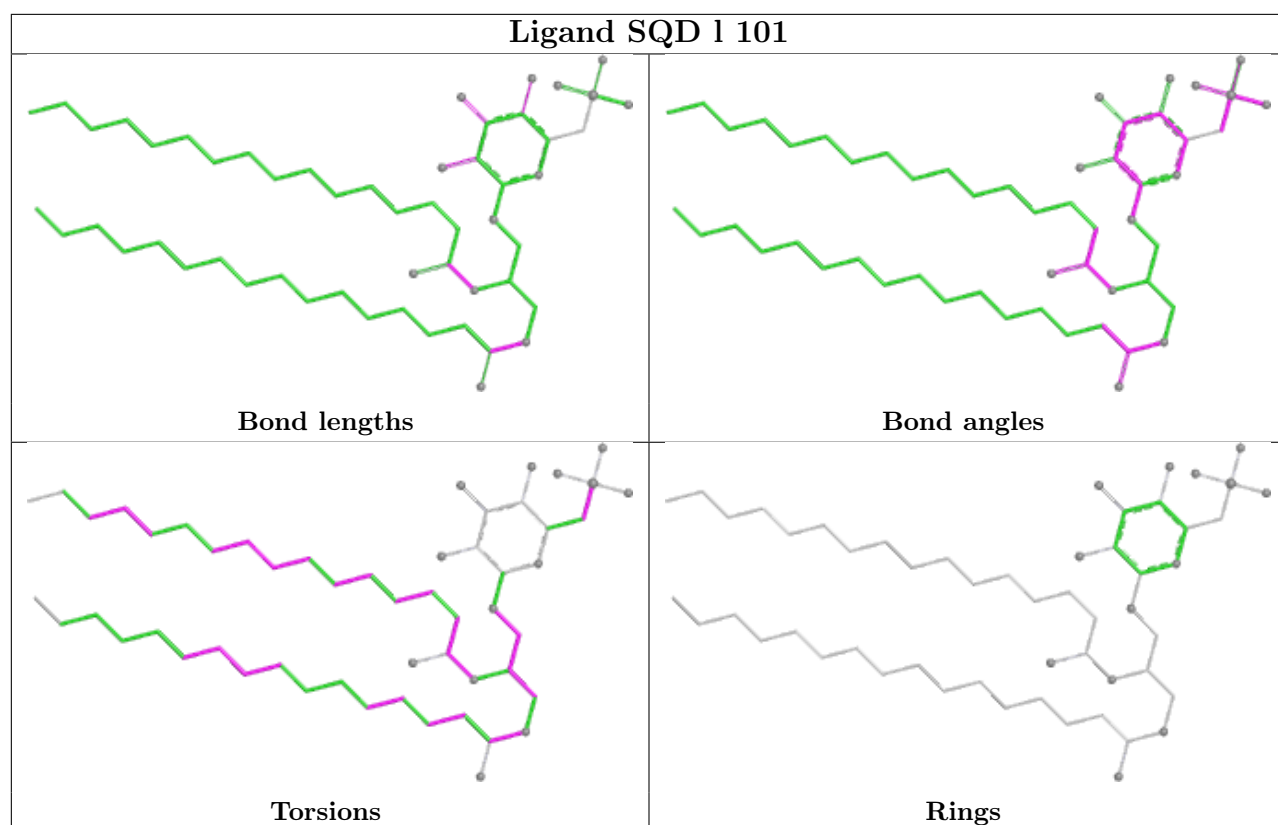


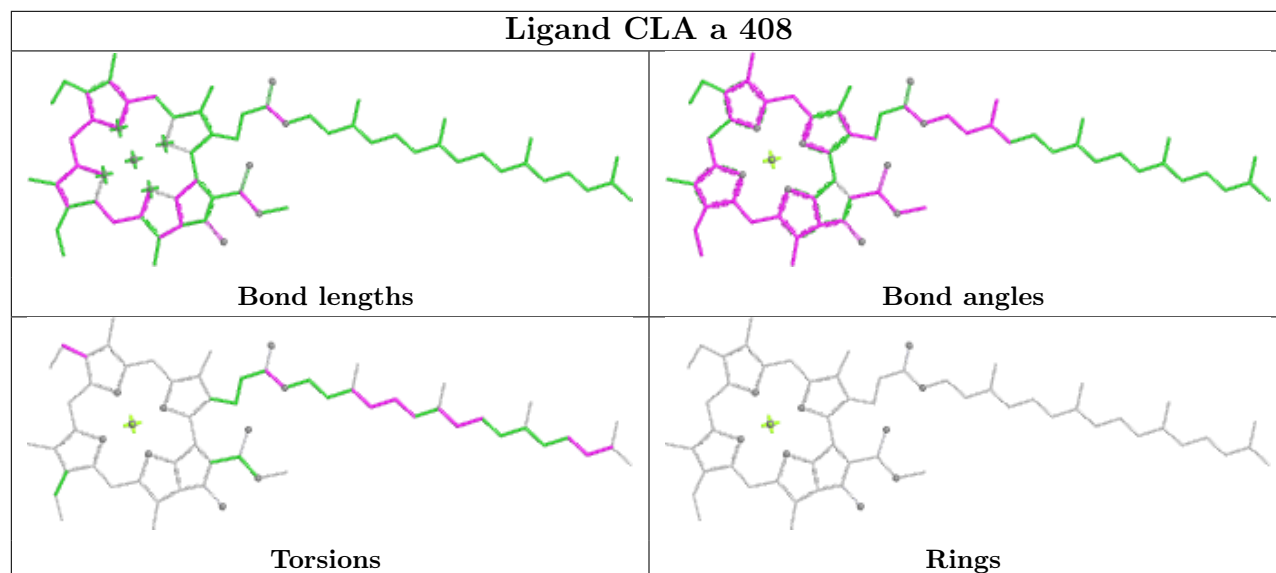
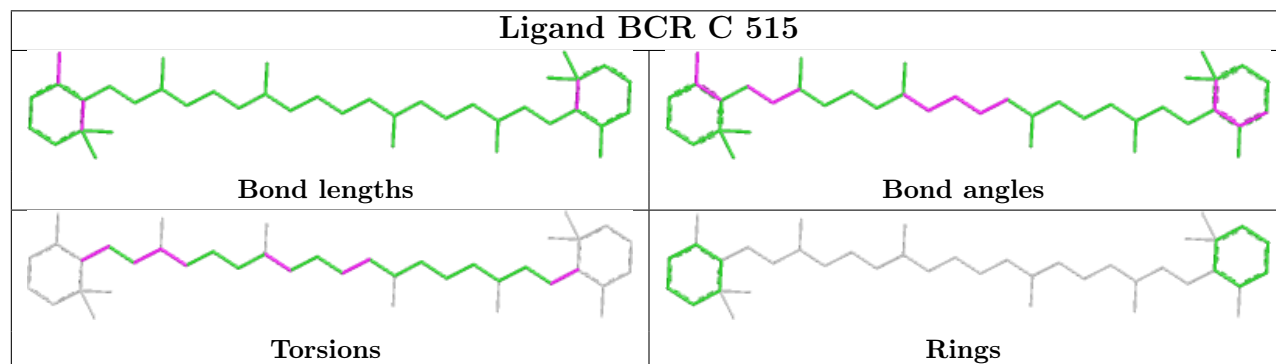
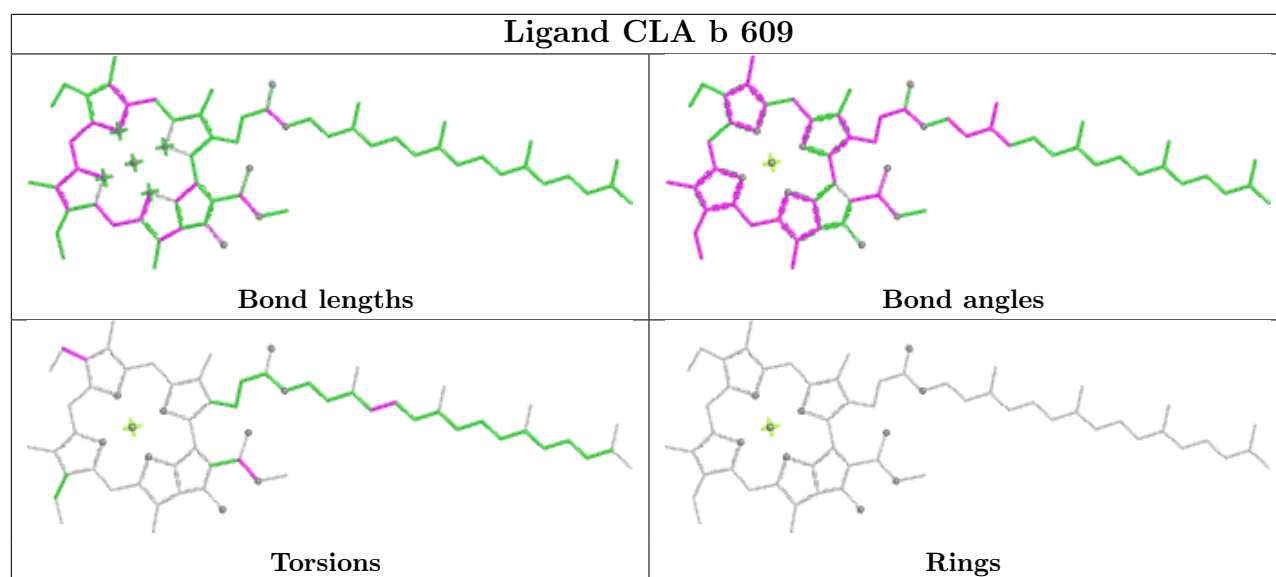
Ligand BCR y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

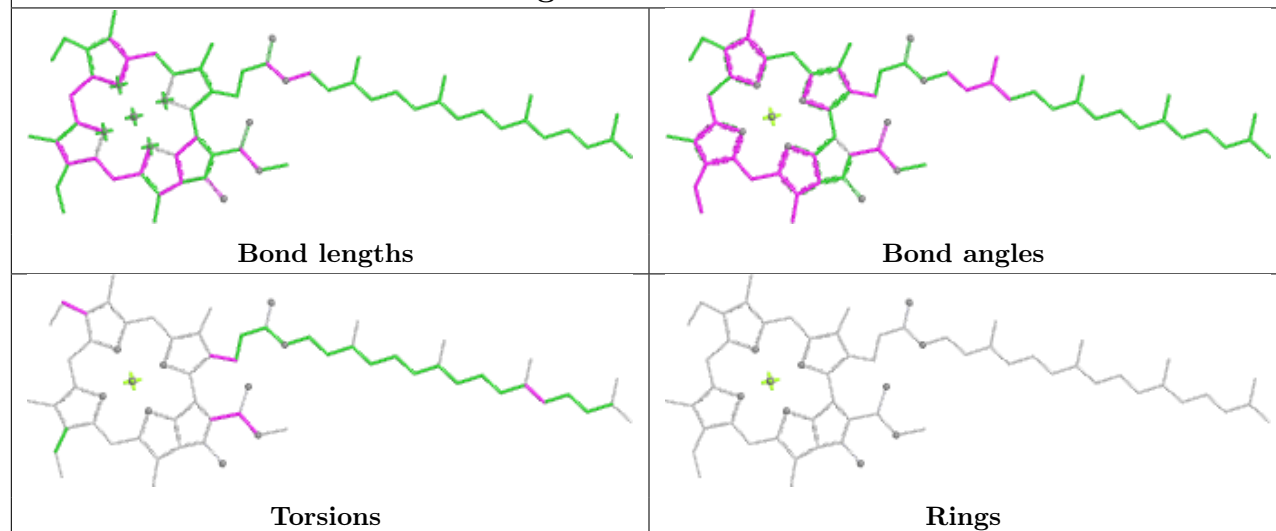
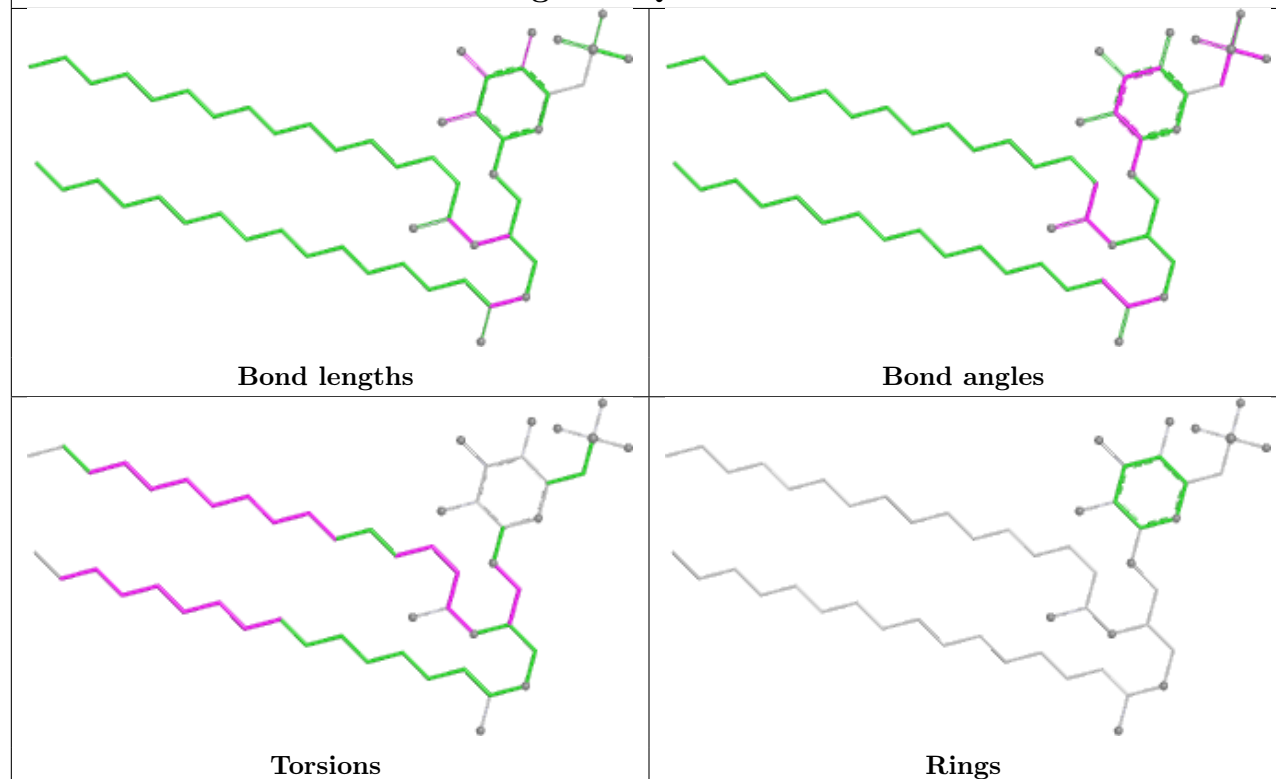
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

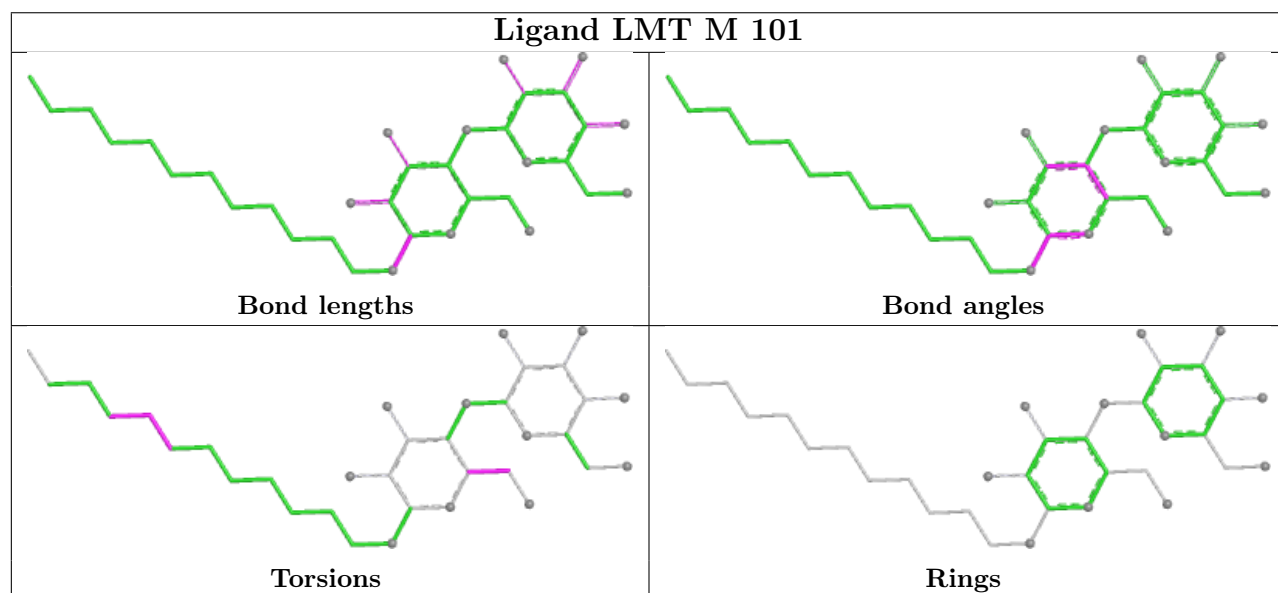
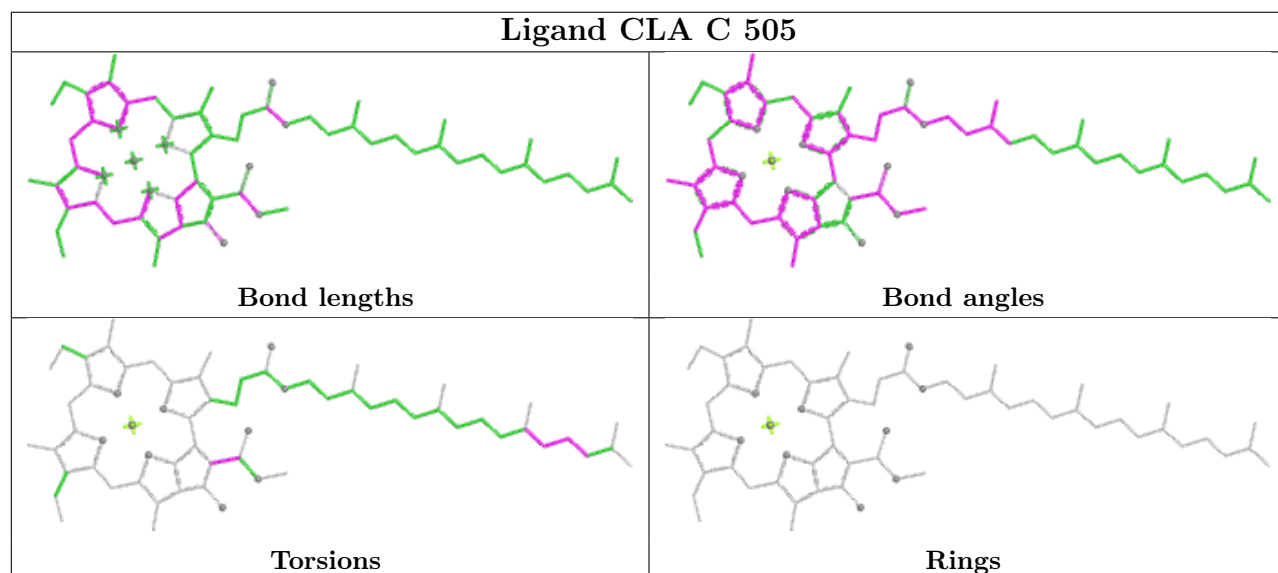
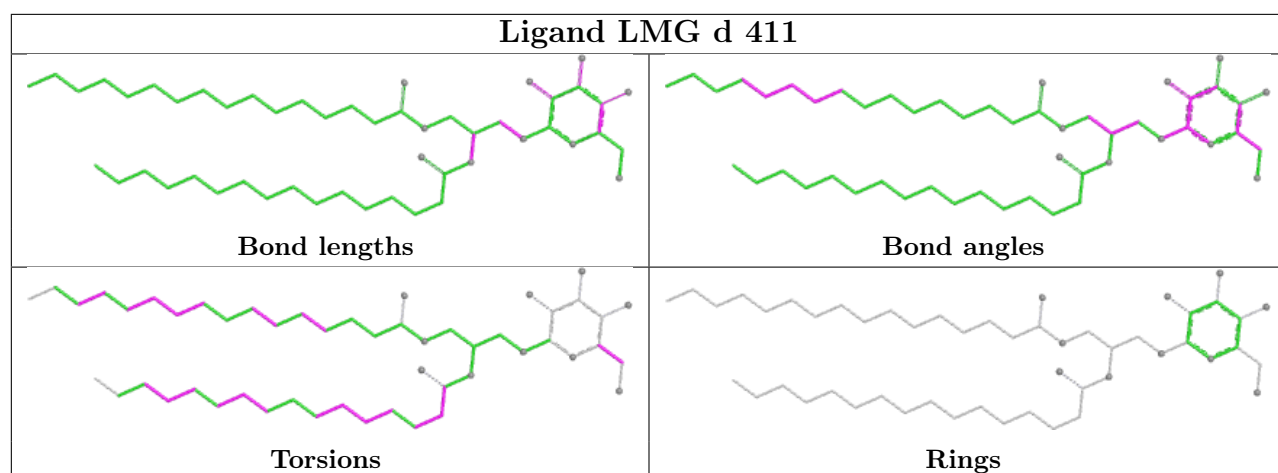
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

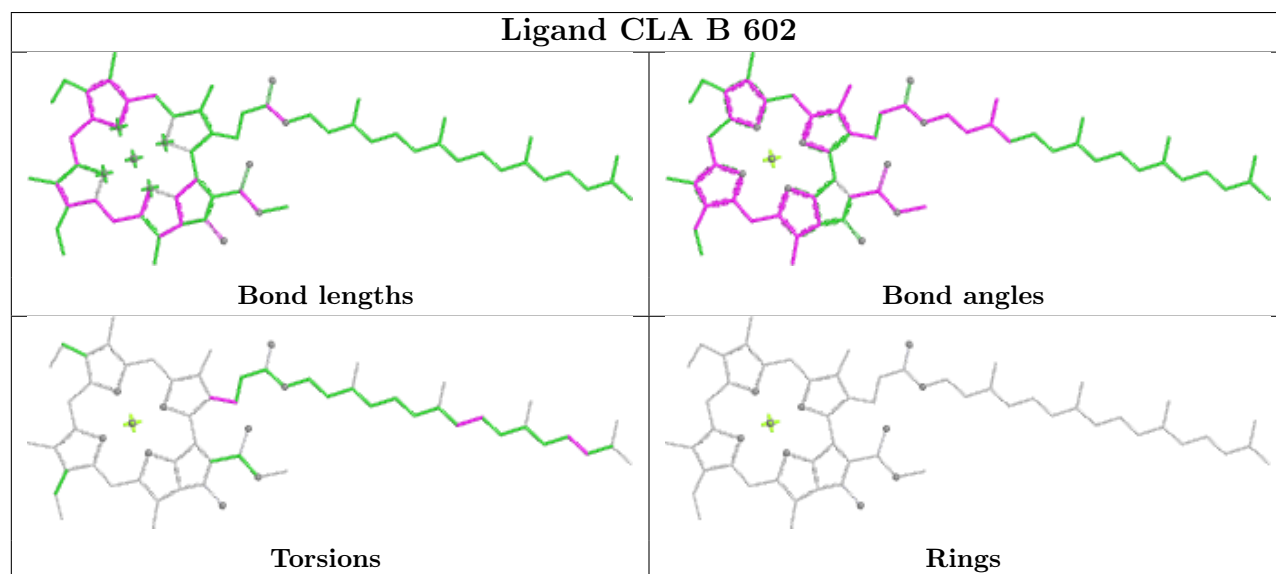
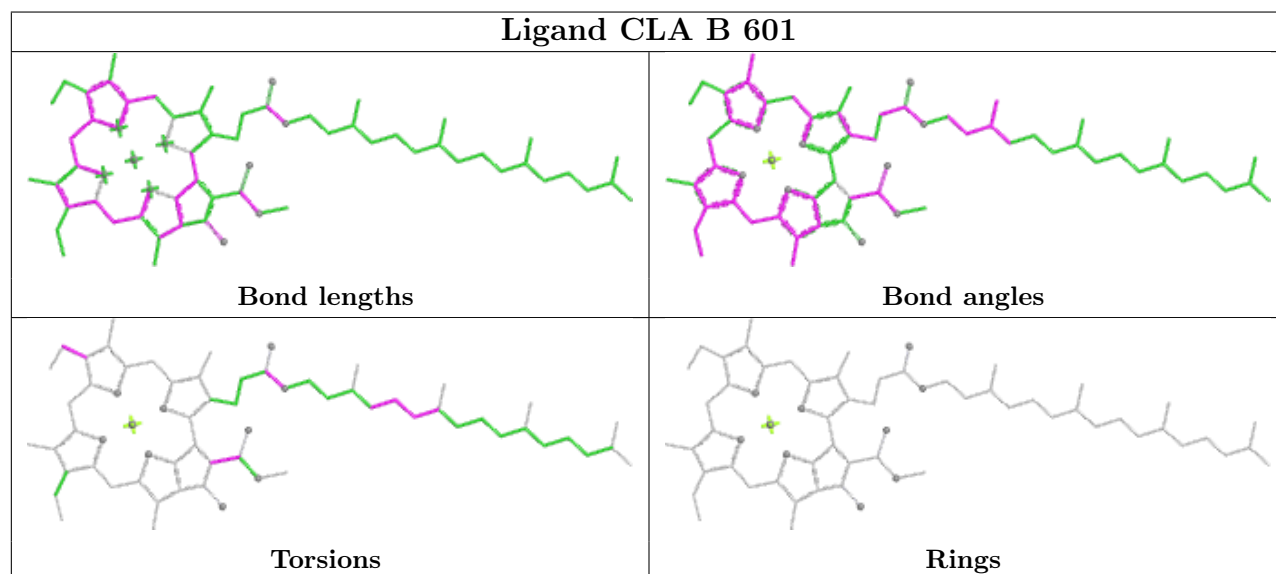
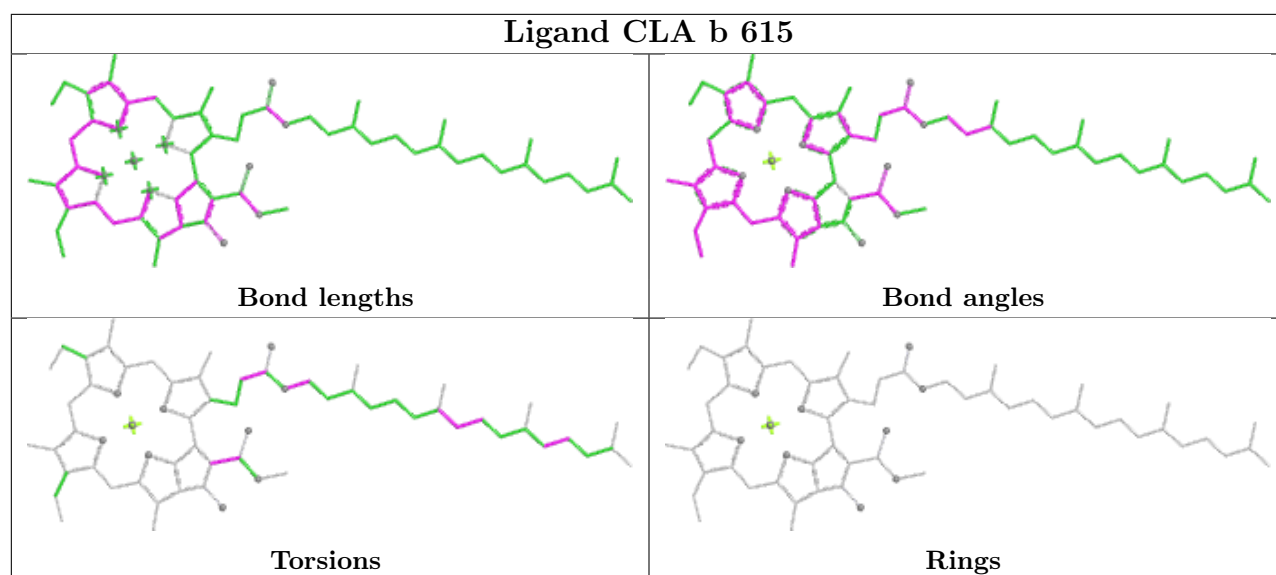


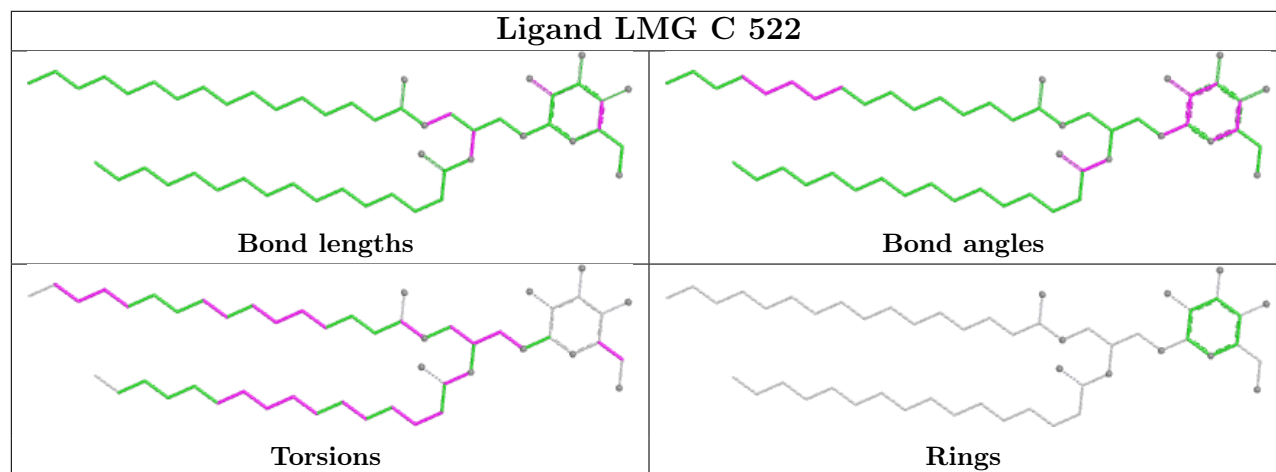
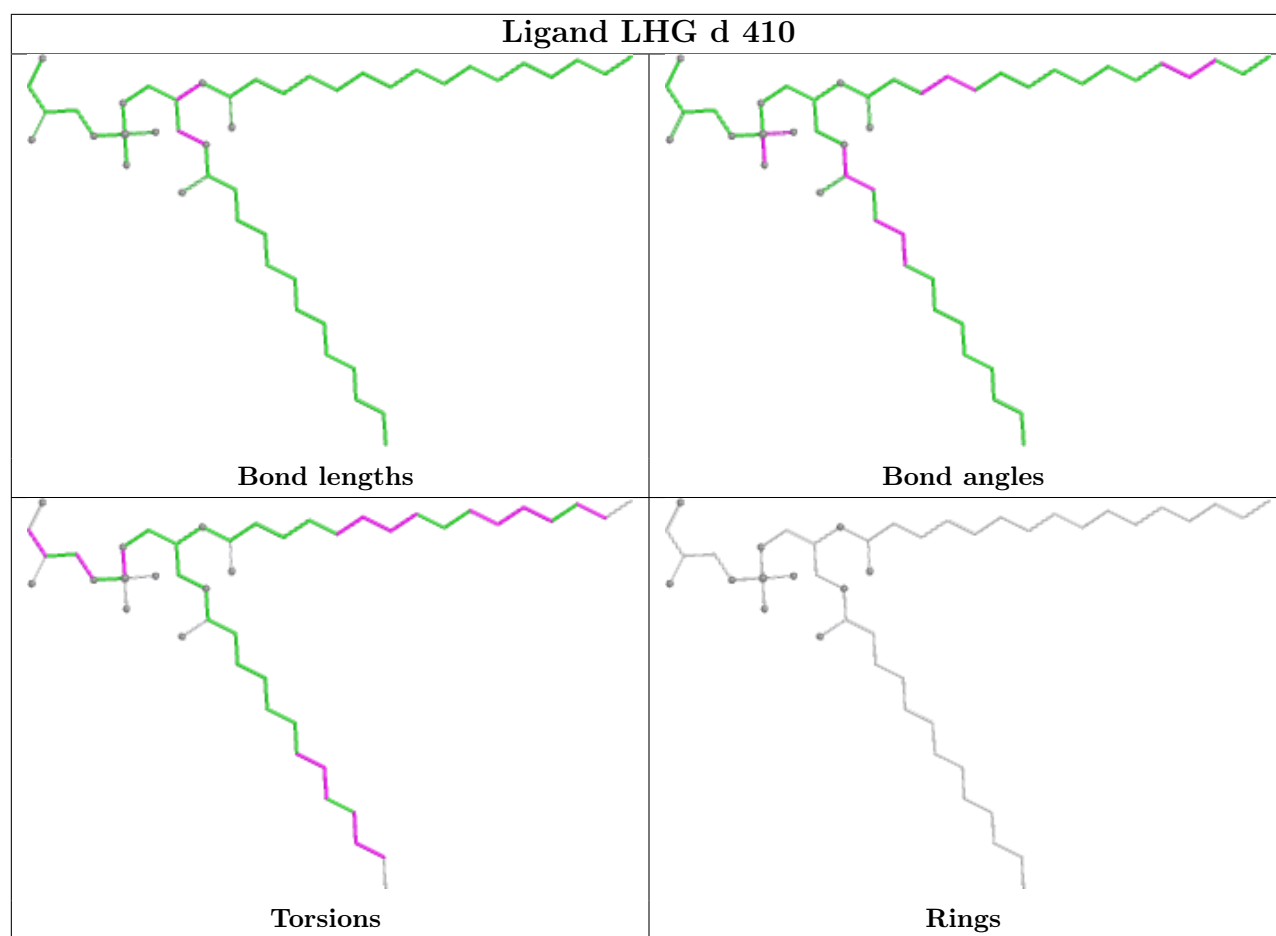


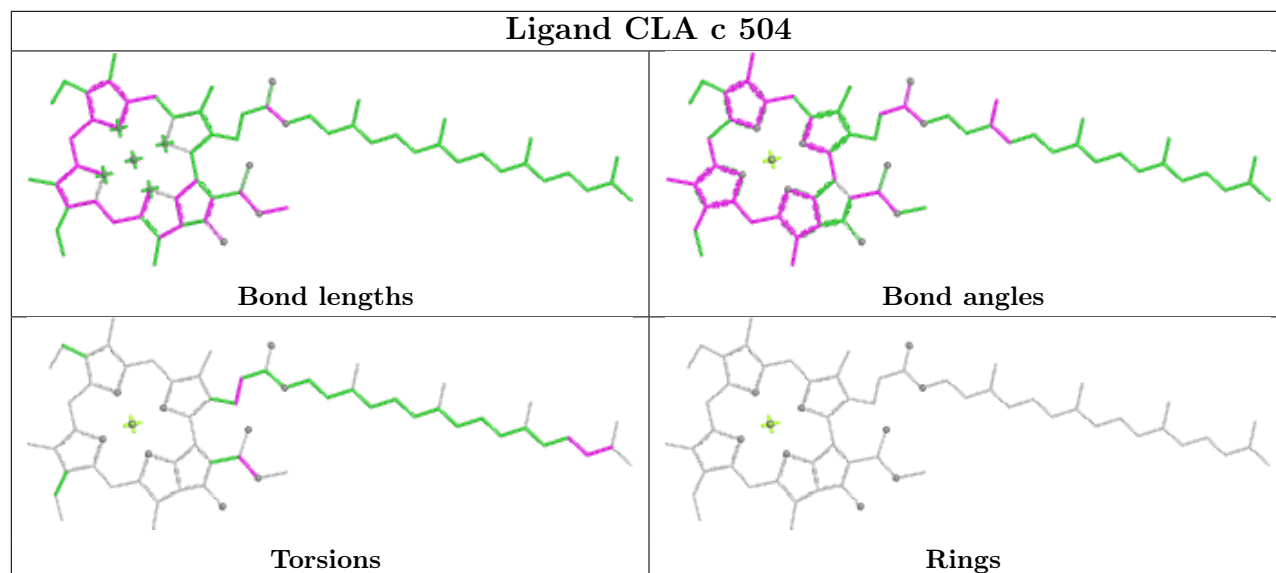
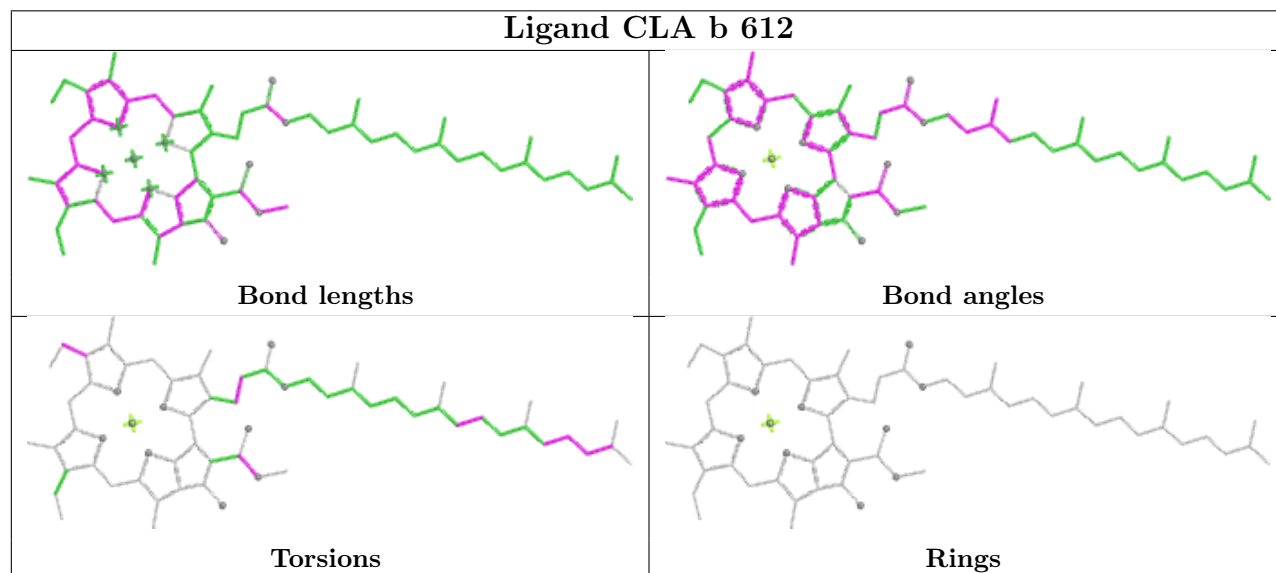
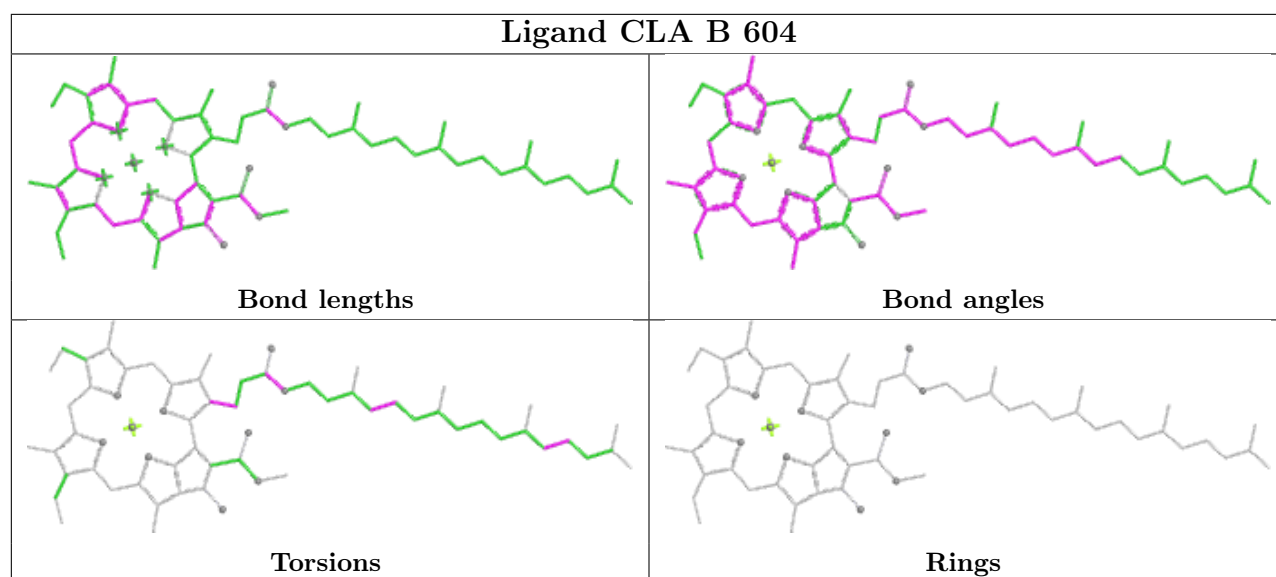


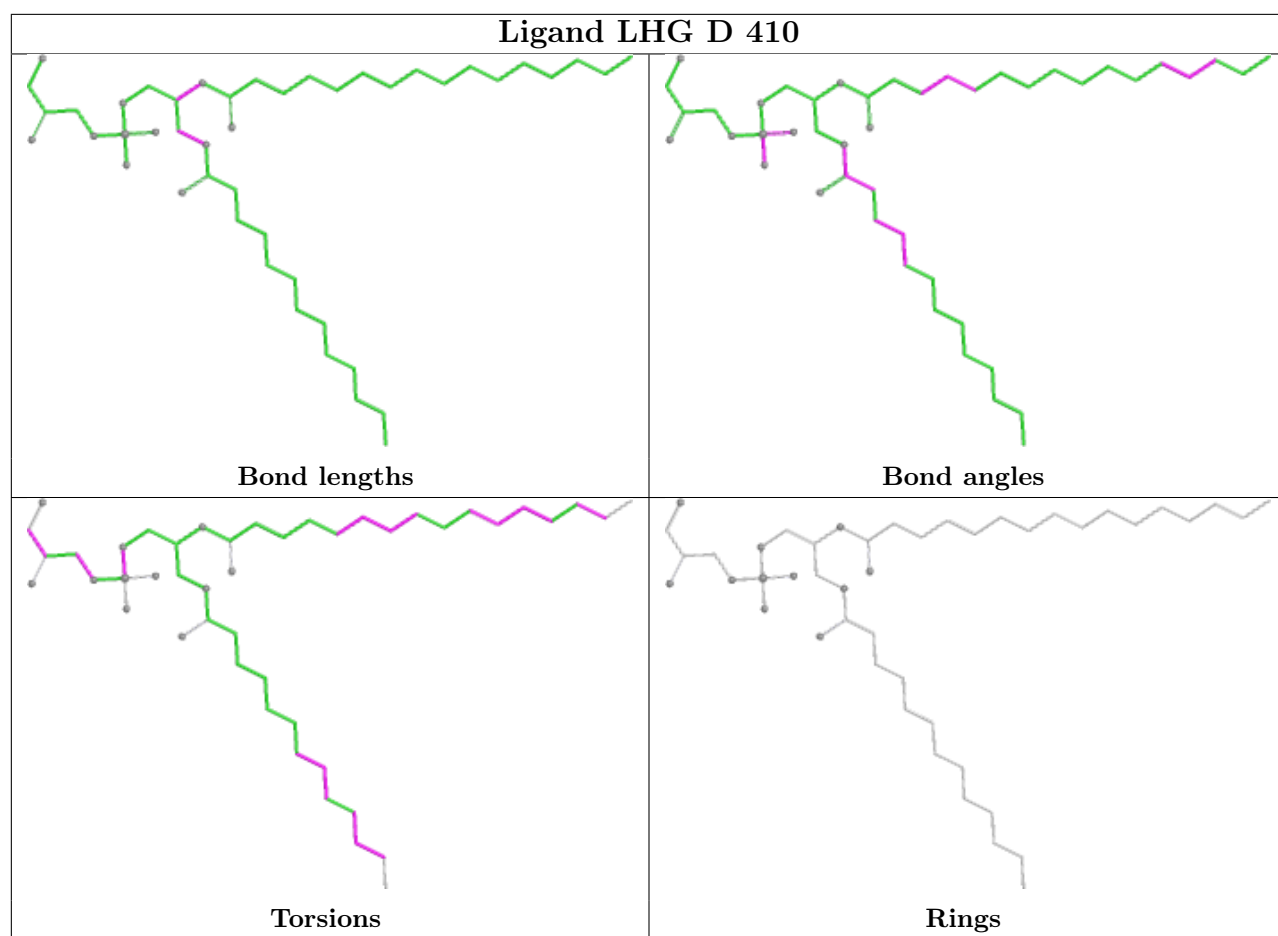
Ligand CLA c 503**Ligand SQD A 410**

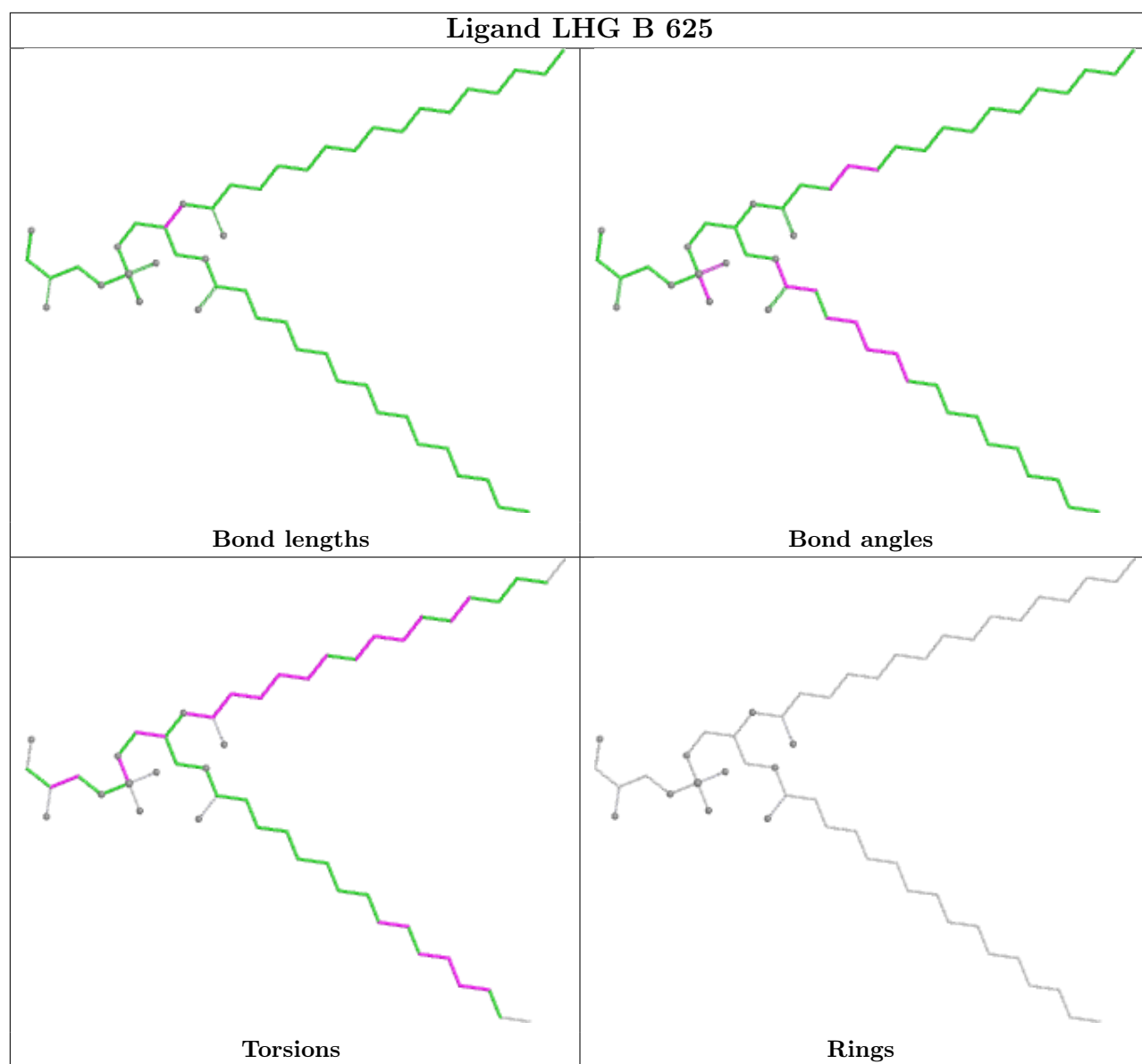




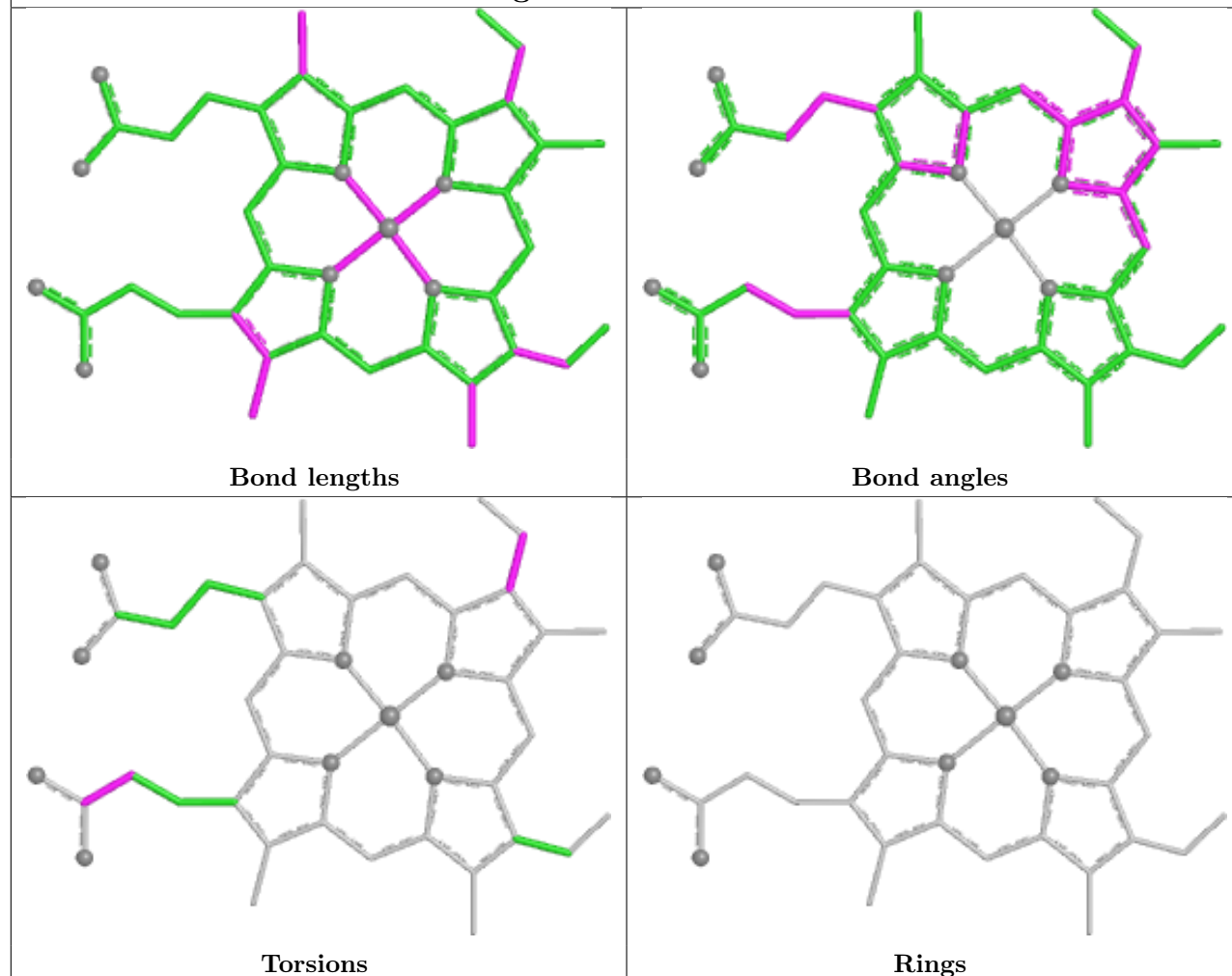




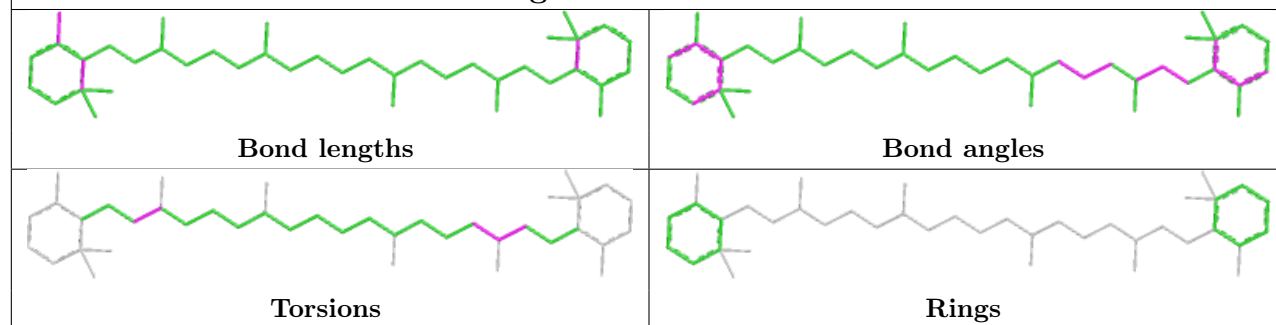


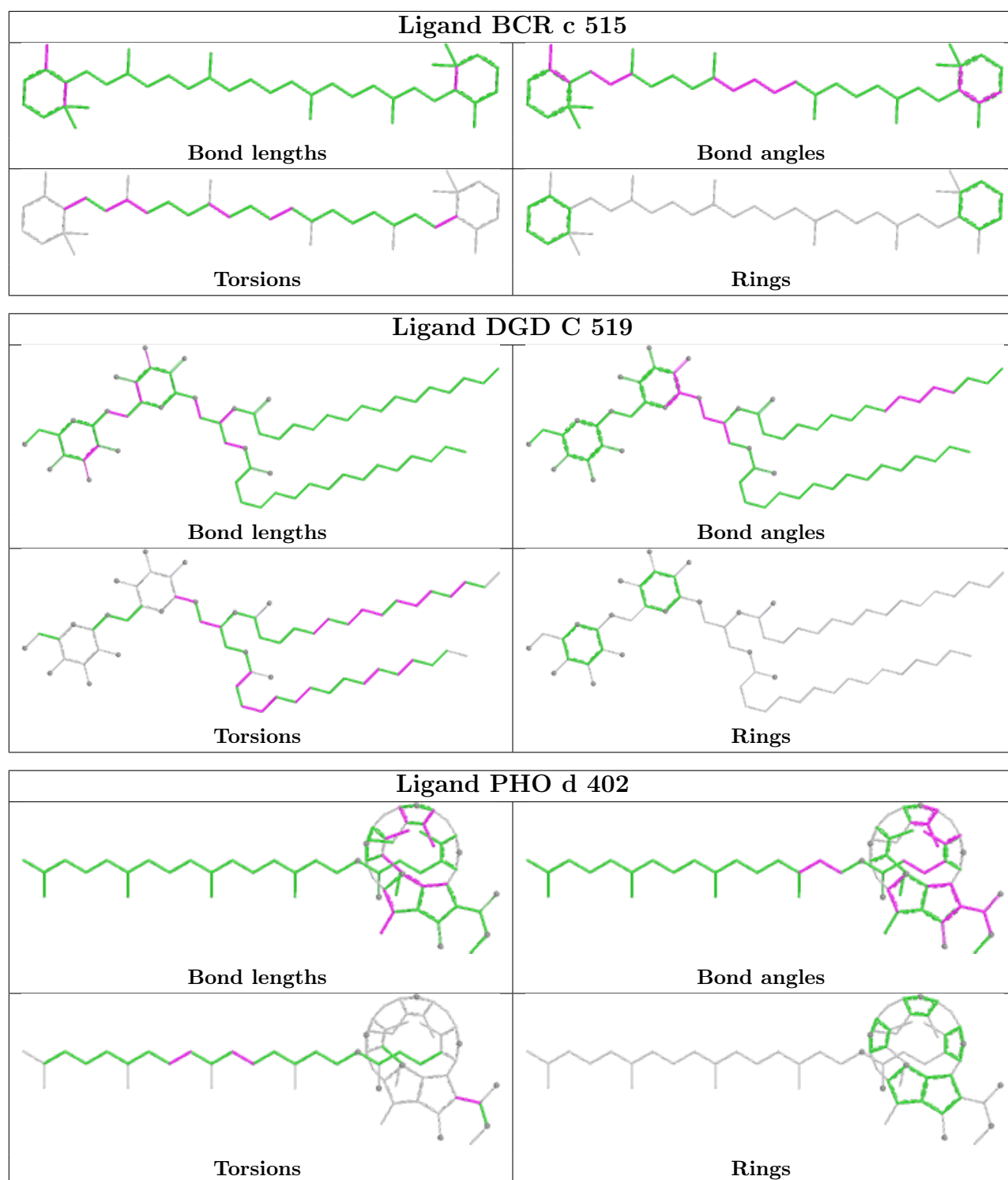


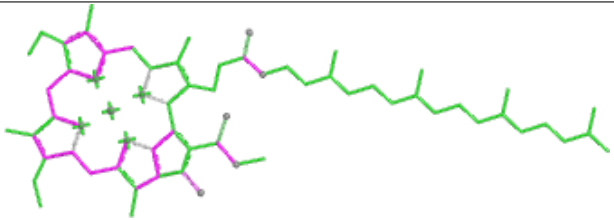
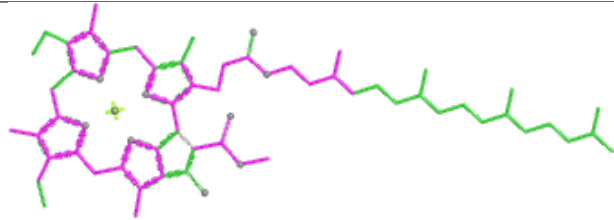
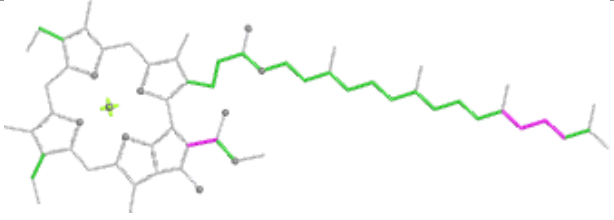
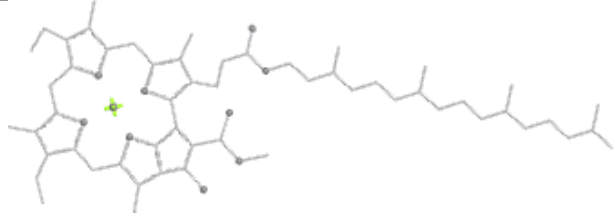
Ligand HEM e 103

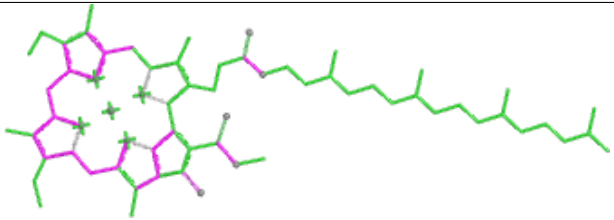
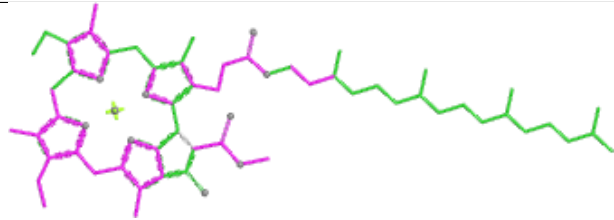
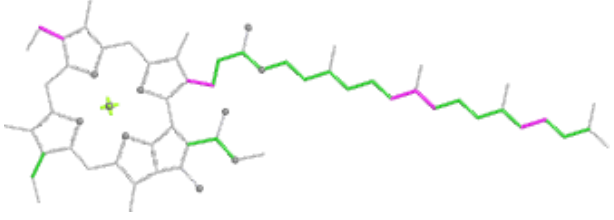
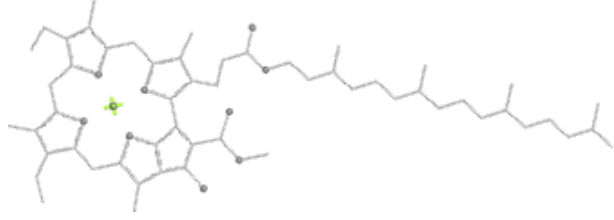


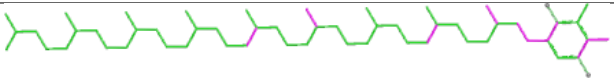
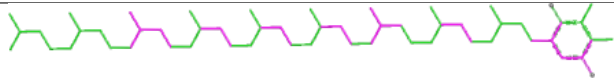
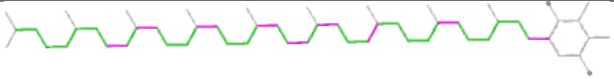
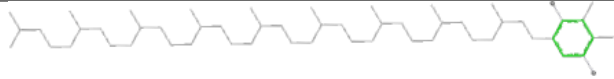
Ligand BCR D 405

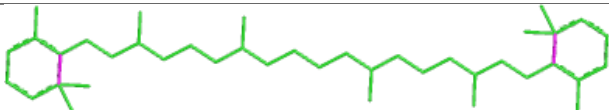
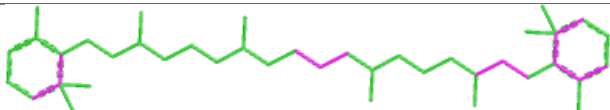
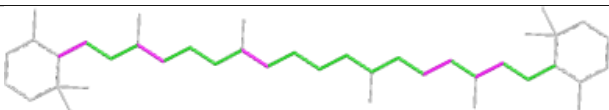
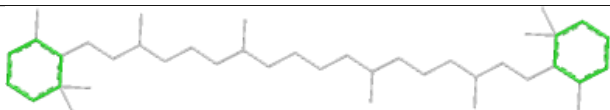


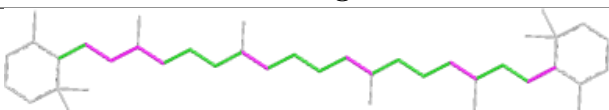
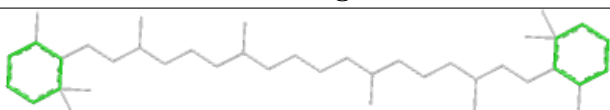


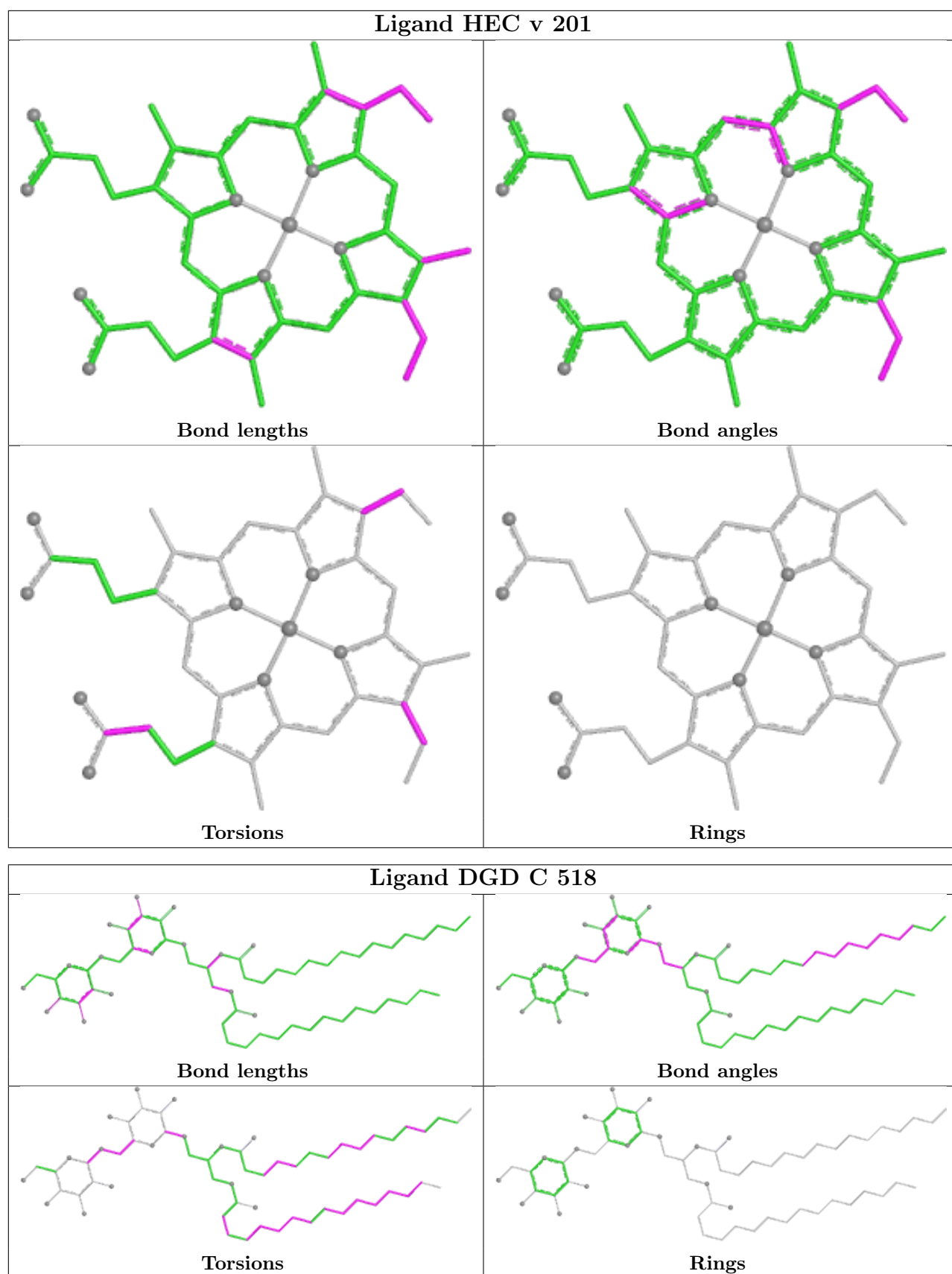
Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

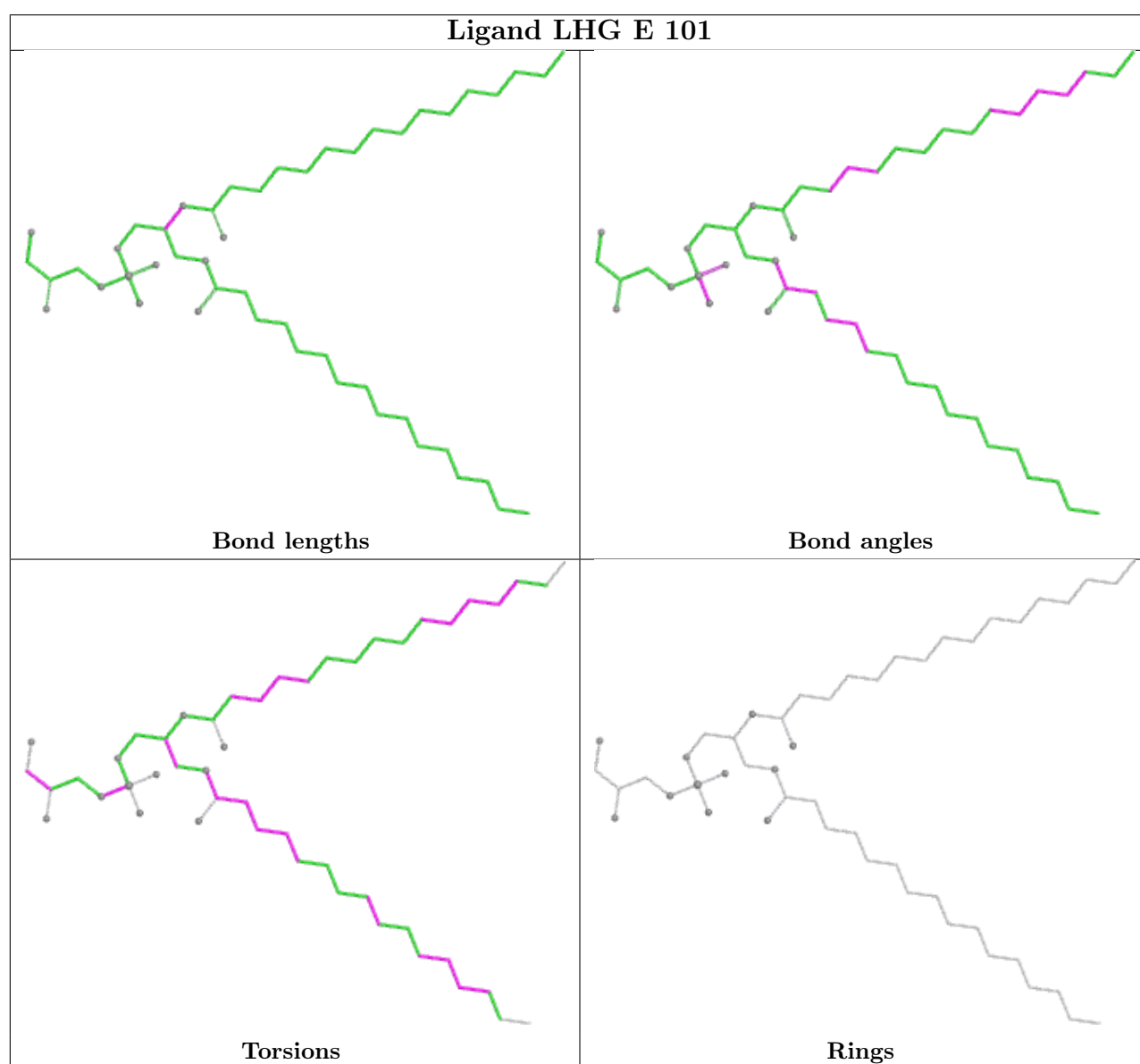
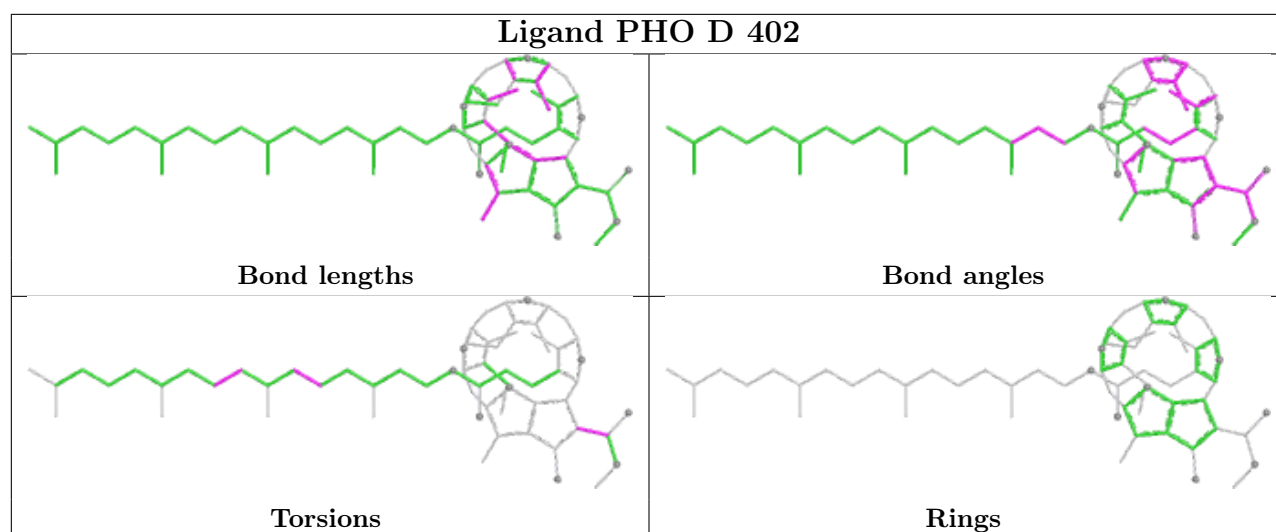
Ligand CLA a 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 a 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 521	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR c 516	
	Bond lengths
	Bond angles
	Torsions
	Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

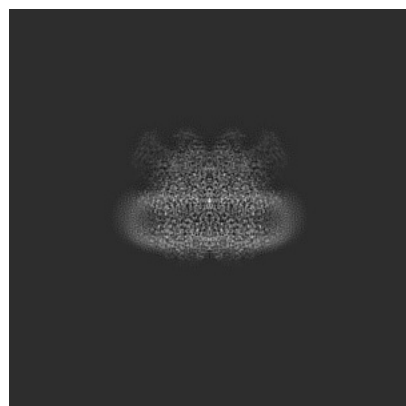
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30548. These allow visual inspection of the internal detail of the map and identification of artifacts.

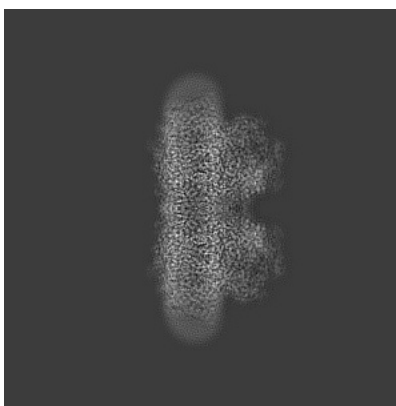
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

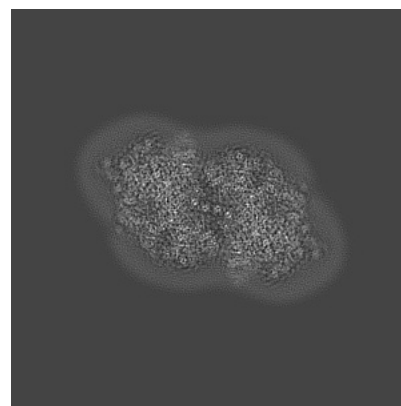
6.1.1 Primary map



X

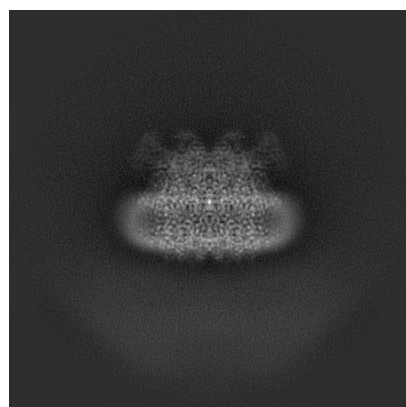


Y

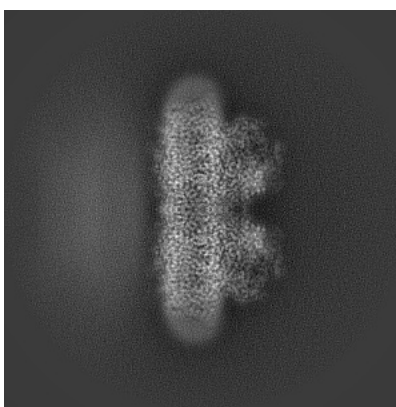


Z

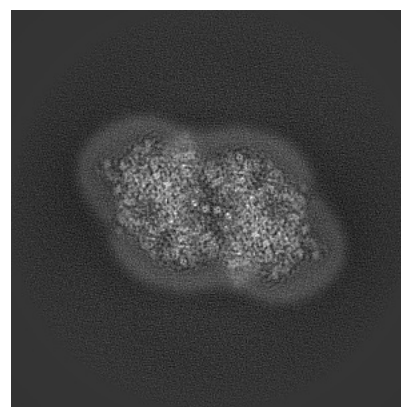
6.1.2 Raw map



X



Y

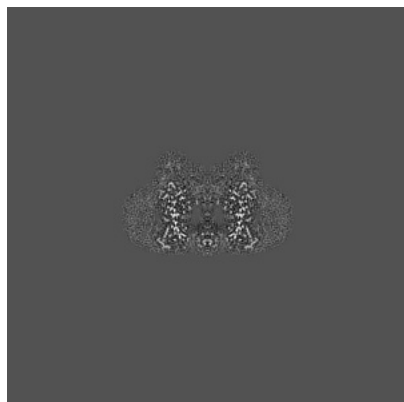


Z

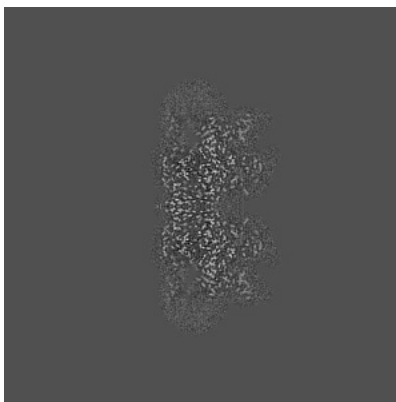
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

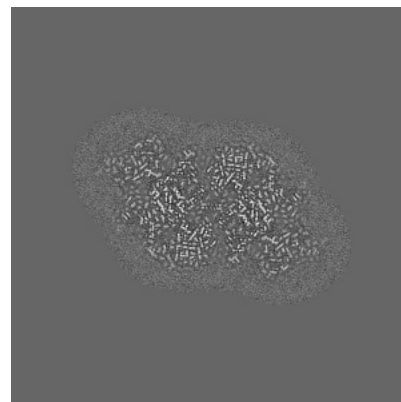
6.2.1 Primary map



X Index: 200

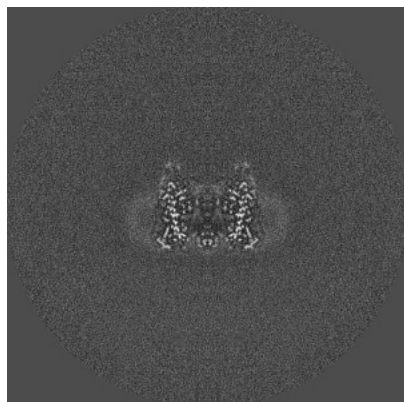


Y Index: 200

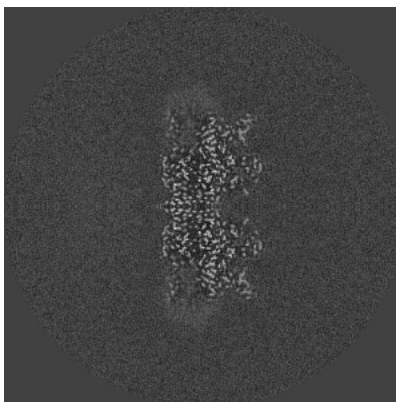


Z Index: 200

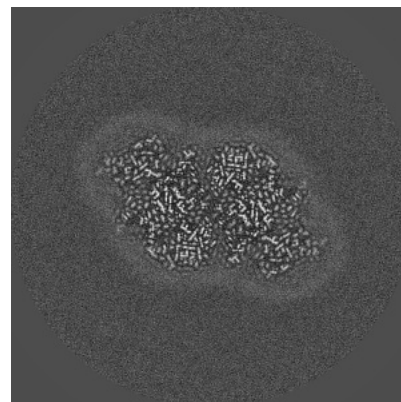
6.2.2 Raw map



X Index: 200



Y Index: 200

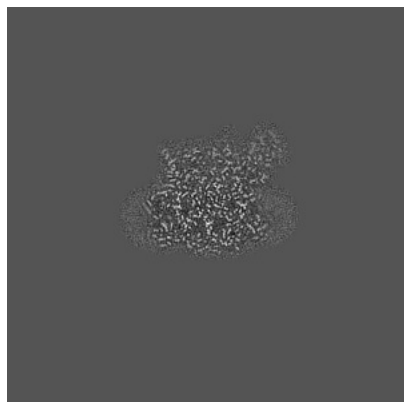


Z Index: 200

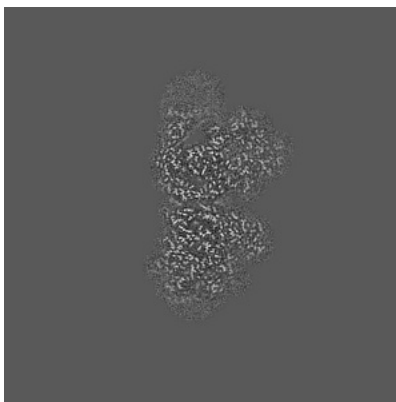
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

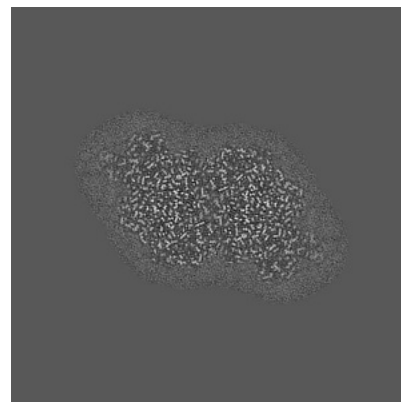
6.3.1 Primary map



X Index: 167

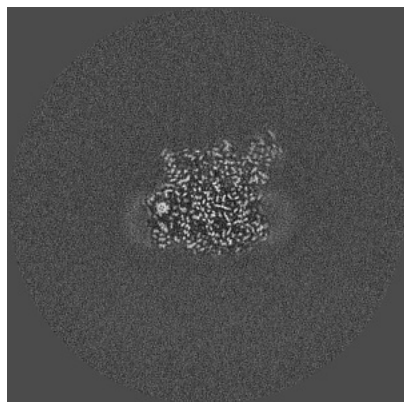


Y Index: 182

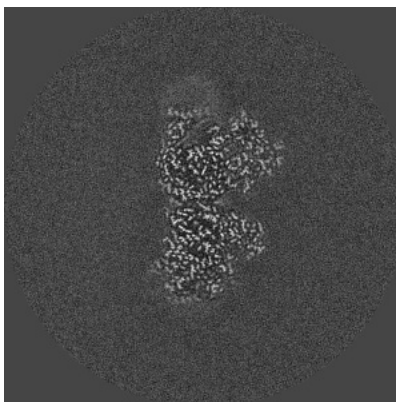


Z Index: 209

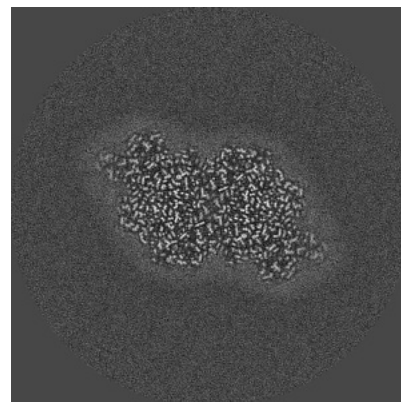
6.3.2 Raw map



X Index: 166



Y Index: 182

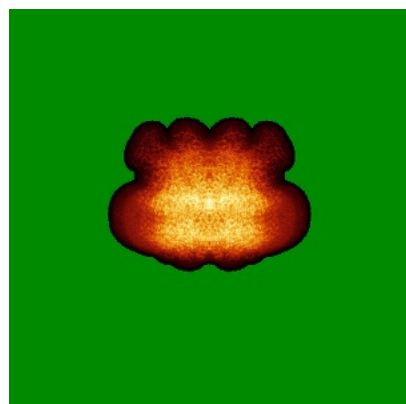


Z Index: 209

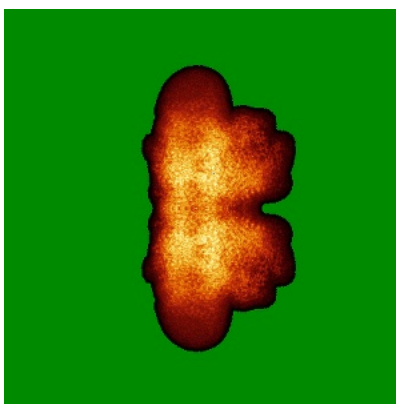
The images above show the largest variance slices of the map in three orthogonal directions.

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

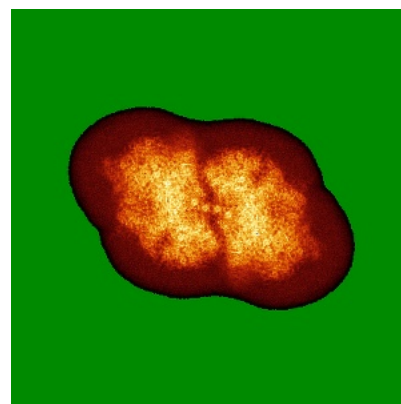
6.4.1 Primary map



X

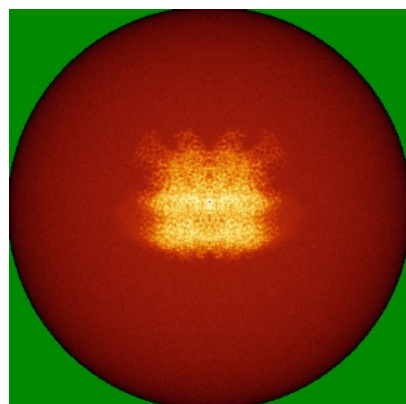


Y

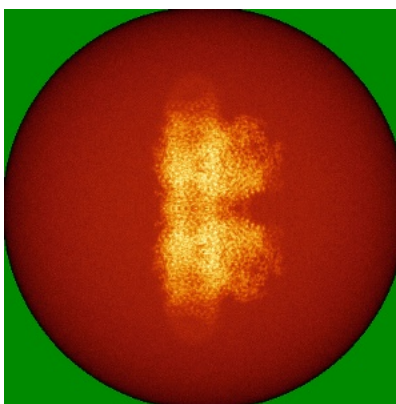


Z

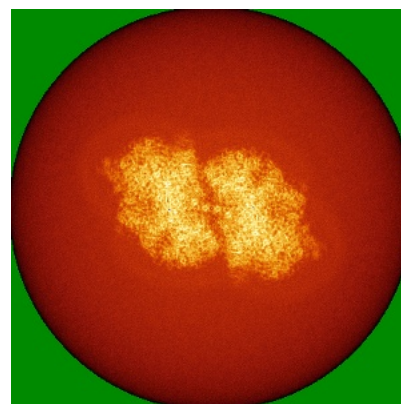
6.4.2 Raw map



X



Y

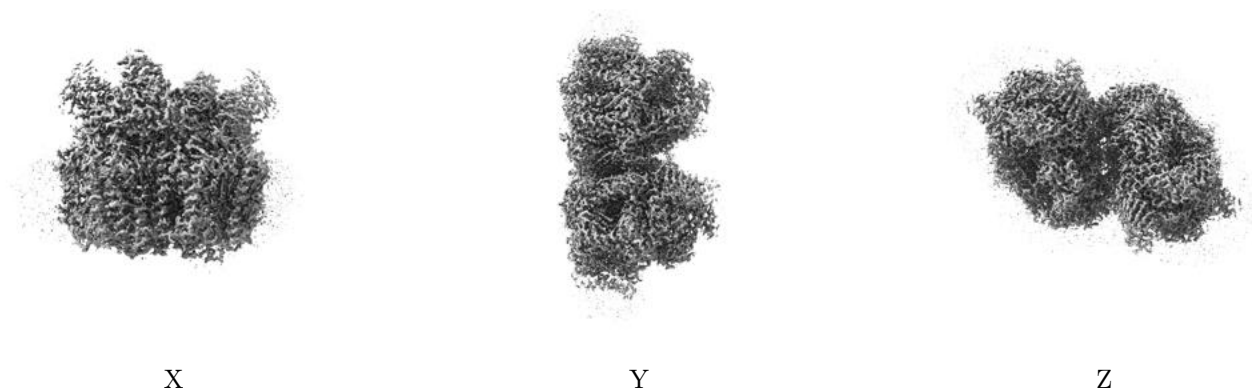


Z

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.

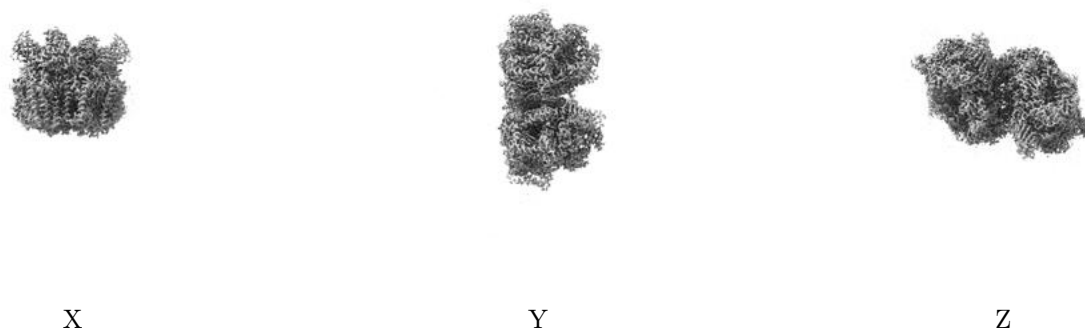
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

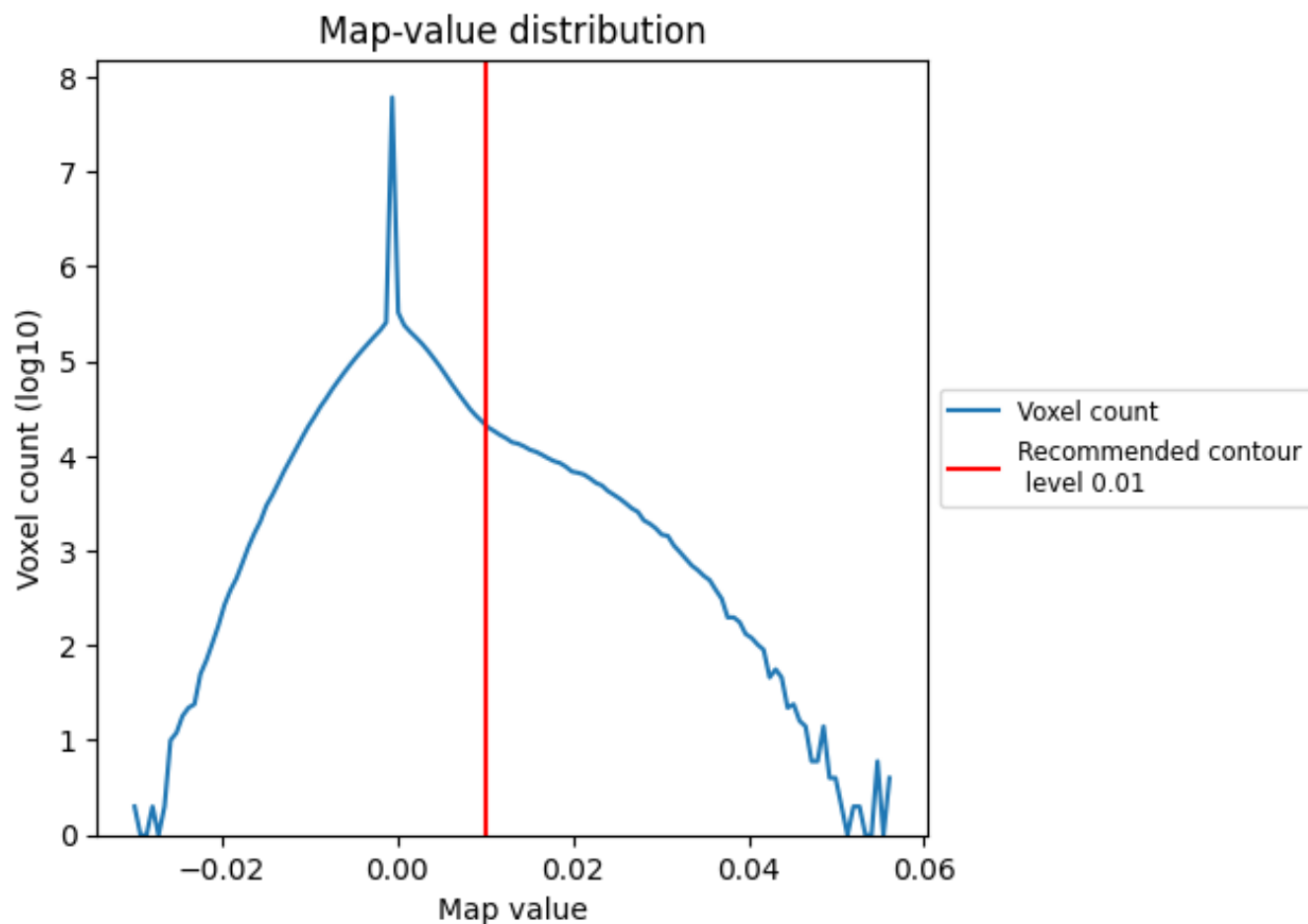
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

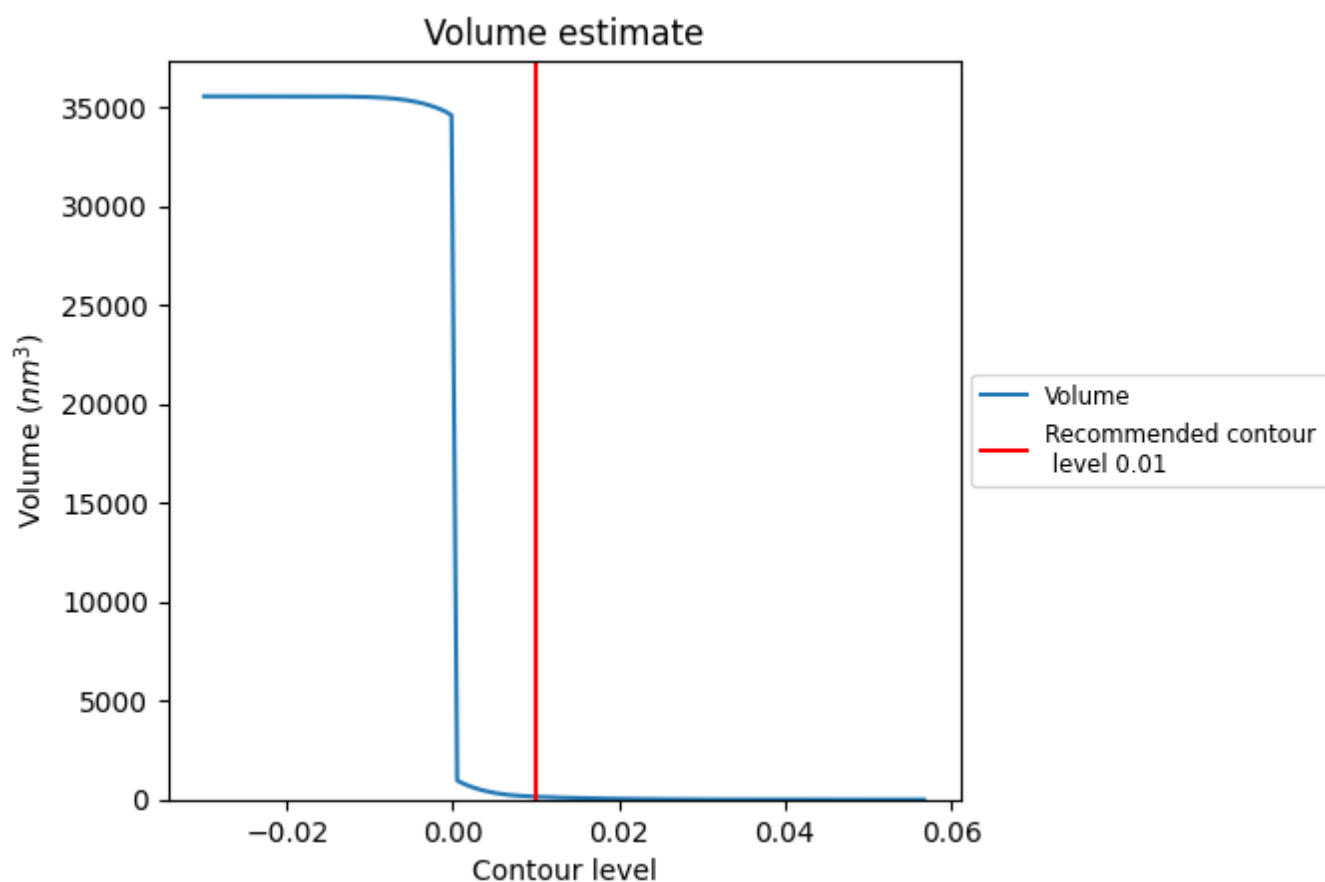
This section contains the results of statistical analysis of the map.

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.

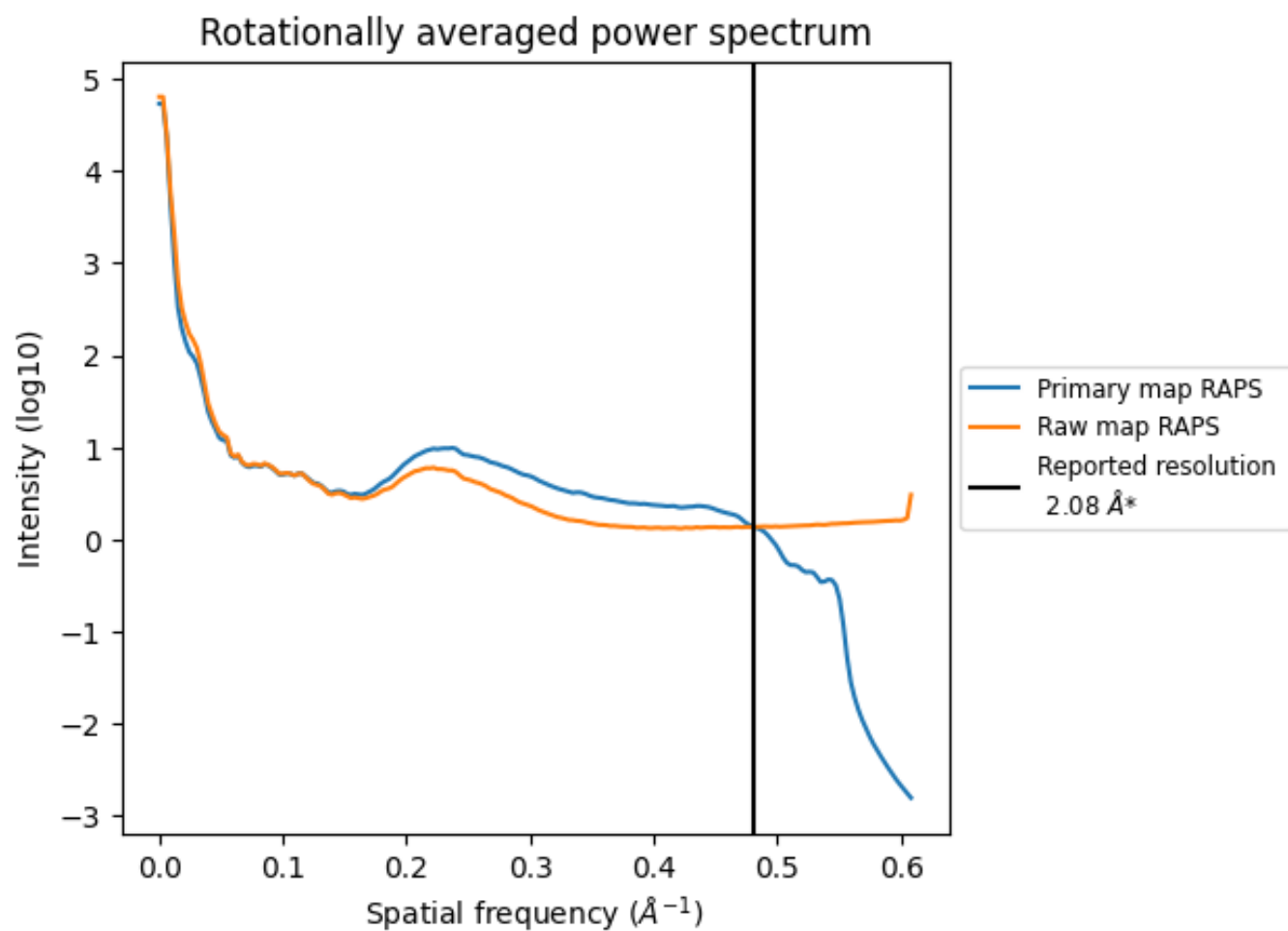
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm³; this corresponds to an approximate mass of 130 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 ⓘ

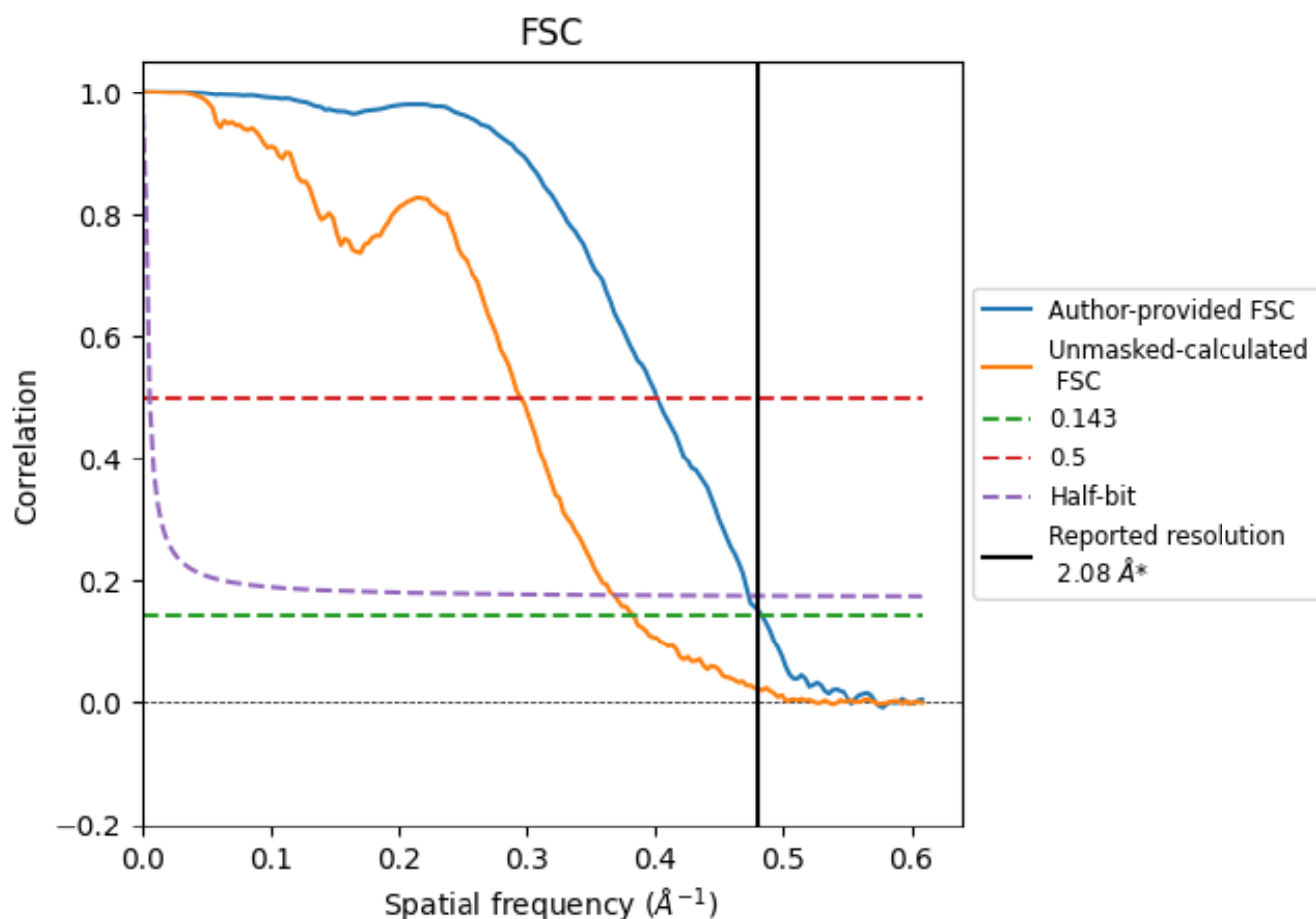


*Reported resolution corresponds to spatial frequency of $0.481 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.481 Å⁻¹

8.2 Resolution estimates [i](#)

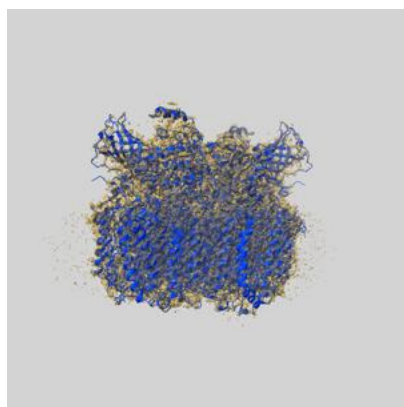
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.07	2.49	2.11
Unmasked-calculated*	2.61	3.39	2.72

*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 2.61 differs from the reported value 2.08 by more than 10 %

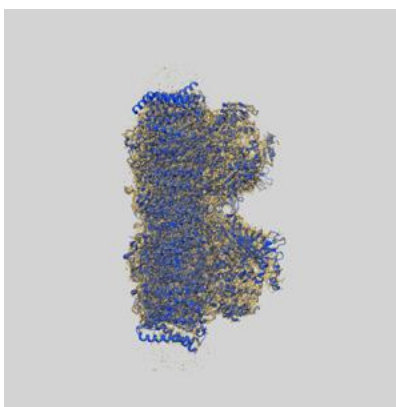
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30548 and PDB model 7D1U. Per-residue inclusion information can be found in [section 3](#) on [page 29](#).

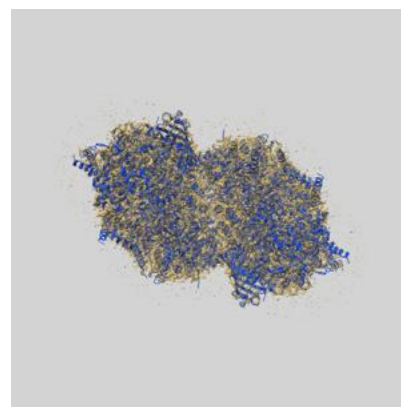
9.1 Map-model overlay [i](#)



X



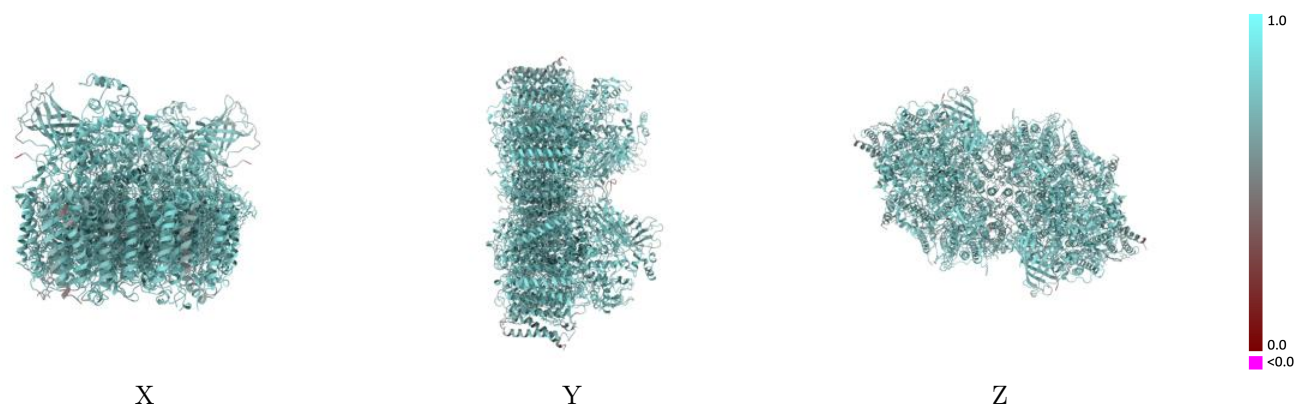
Y



Z

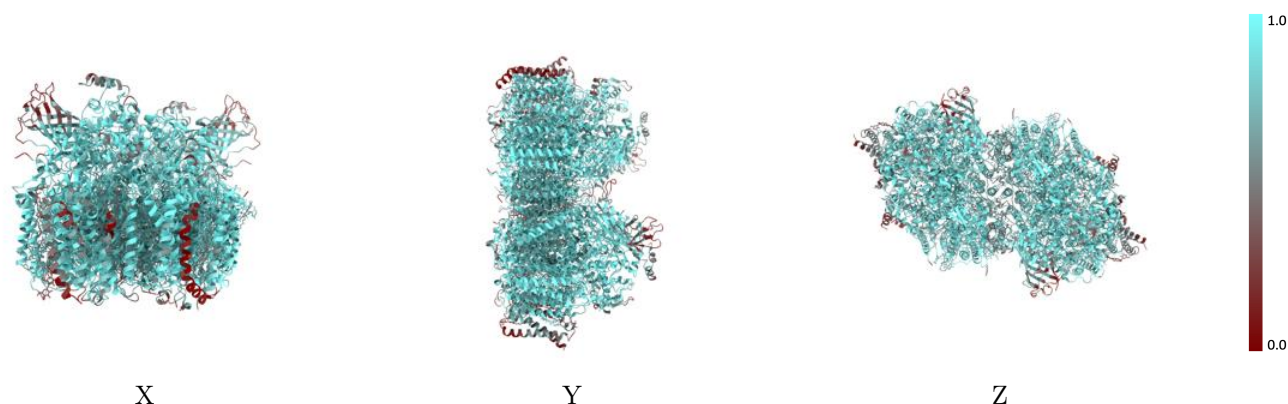
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



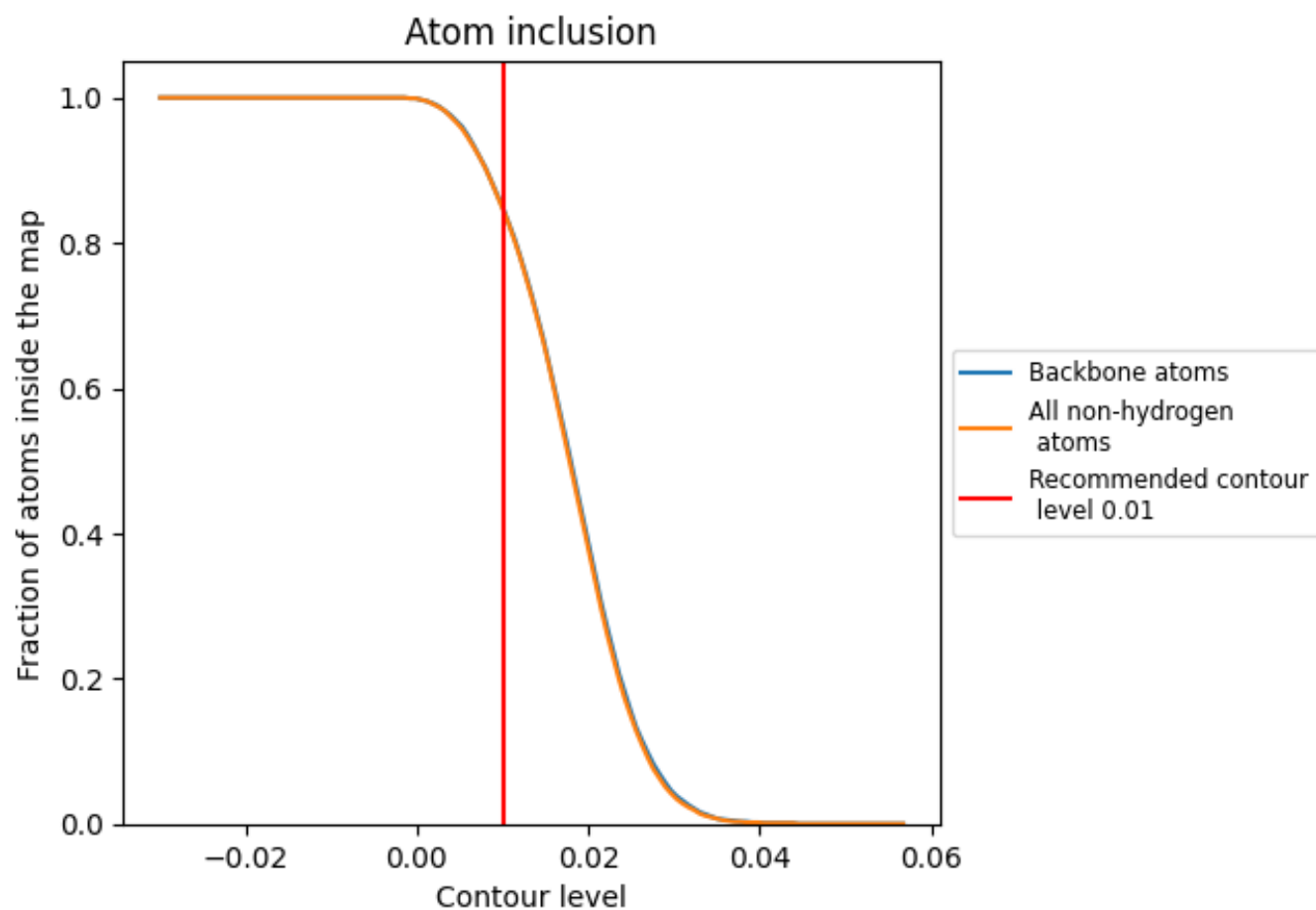
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.7570
A	 0.9260	 0.7880
B	 0.9070	 0.7750
C	 0.8830	 0.7580
D	 0.9350	 0.7890
E	 0.7720	 0.7350
F	 0.8770	 0.7660
H	 0.9050	 0.7620
I	 0.8190	 0.7350
J	 0.7980	 0.7450
K	 0.7680	 0.7150
L	 0.8380	 0.7630
M	 0.8520	 0.7760
O	 0.6800	 0.7040
R	 0.0940	 0.5780
T	 0.8750	 0.7760
U	 0.7700	 0.7360
V	 0.8080	 0.7400
X	 0.8030	 0.7360
Y	 0.5980	 0.6790
Z	 0.4130	 0.6240
a	 0.9260	 0.7880
b	 0.9060	 0.7750
c	 0.8830	 0.7580
d	 0.9350	 0.7890
e	 0.7720	 0.7360
f	 0.8770	 0.7650
h	 0.9050	 0.7610
i	 0.8190	 0.7390
j	 0.7980	 0.7420
k	 0.7680	 0.7160
l	 0.8380	 0.7690
m	 0.8490	 0.7750
o	 0.6800	 0.7040
r	 0.0940	 0.5770



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
t	 0.8600	 0.7780
u	 0.7700	 0.7390
v	 0.8080	 0.7410
x	 0.8030	 0.7380
y	 0.5980	 0.6750
z	 0.4110	 0.6210