



## wwPDB EM Validation Summary Report ⓘ

Jun 7, 2026 – 07:54 am BST

PDB ID : 9T5U / pdb\_00009t5u  
EMDB ID : EMD-55594  
Title : Chlorophyll f-containing monomeric far-red Photosystem II from Calothrix sp. NIES-3974  
Authors : Leong, H.F.; Consoli, G.; Murray, J.W.; Fantuzzi, A.; Rutherford, A.W.  
Deposited on : 2025-11-06  
Resolution : 2.33 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

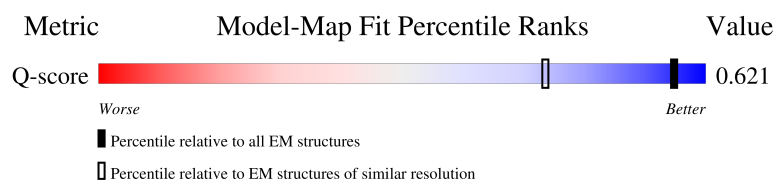
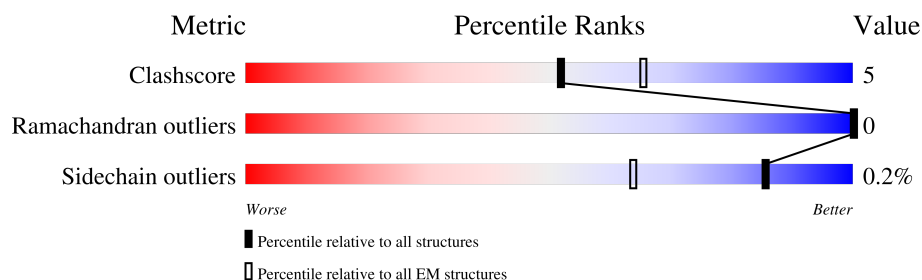
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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


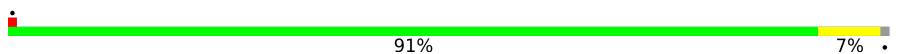

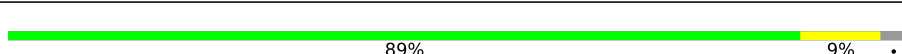
The reported resolution of this entry is 2.33 Å.

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.



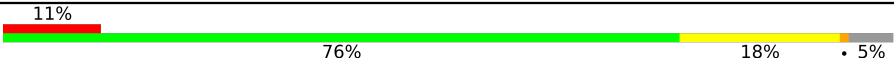

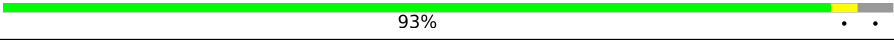
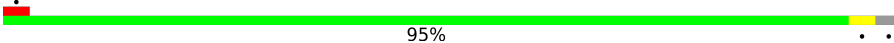


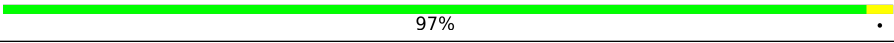



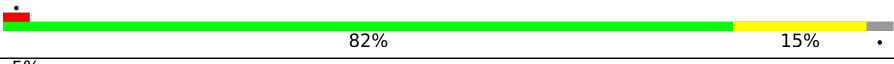


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4434 ( 1.83 - 2.83 )

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

Mol	Chain	Length	Quality of chain
1	A	363	
2	B	510	
3	C	465	
4	D	352	

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Mol	Chain	Length	Quality of chain
5	E	82	
6	F	46	
7	H	67	
8	I	38	
9	J	39	
10	K	45	
11	L	39	
12	M	39	
13	R	41	
14	T	34	
15	X	39	
16	Y	40	
17	Z	62	

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
22	CL7	A	406	X	-	-	-
29	F6C	B	614	X	-	-	-
29	F6C	C	507	X	-	-	-

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 21449 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 PsbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2620	1720	425	457	18		

- Molecule 2 is a protein called PsbB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	0	0
			3977	2606	667	691	13		

- Molecule 3 is a protein called PsbC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3453	2262	587	595	9		

- Molecule 4 is a protein called PsbD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	342	Total	C	N	O	S	0	0
			2756	1835	445	465	11		

- Molecule 5 is a protein called PsbE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	78	Total	C	N	O		0	0
			629	411	103	115			

- Molecule 6 is a protein called PsbF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	33	Total	C	N	O	S	0	0
			269	184	44	40	1		

- Molecule 7 is a protein called PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	64	Total	C	N	O	S	0	0
			516	343	85	85	3		

- Molecule 8 is a protein called PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			300	203	49	47	1		

- Molecule 9 is a protein called PsbJ.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	36	Total	C	N	O	0	0
			256	173	40	43		

- Molecule 10 is a protein called PsbK.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			304	213	44	47		

- Molecule 11 is a protein called PsbL.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	39	Total	C	N	O	S	0	0
			322	213	51	57	1		

- Molecule 12 is a protein called PsbM.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	33	Total	C	N	O	S	0	0
			260	175	38	46	1		

- Molecule 13 is a protein called PsbY.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	R	33	Total	C	N	O	0	0
			238	161	38	39		

- Molecule 14 is a protein called PsbT.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	29	Total	C	N	O	S	0	0
			235	162	35	37	1		

- Molecule 15 is a protein called PsbX.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	38	Total	C	N	O	S	0	0
			303	204	47	51	1		

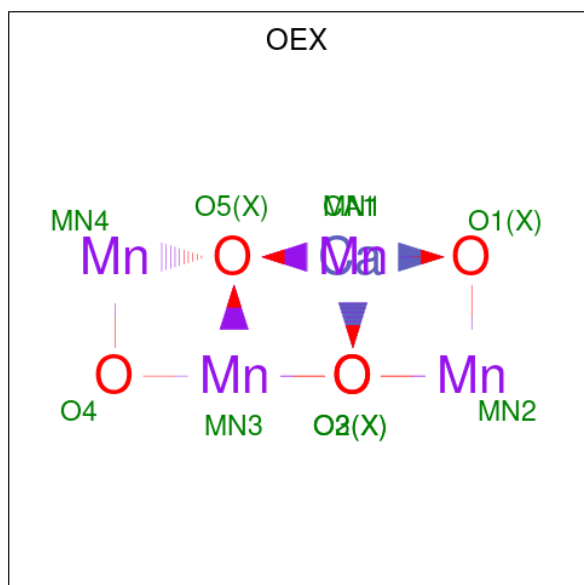
- Molecule 16 is a protein called Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	32	Total	C	N	O	S	0	0
			242	163	38	40	1		

- Molecule 17 is a protein called PsbZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	61	Total	C	N	O	S	0	0
			470	326	69	73	2		

- Molecule 18 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

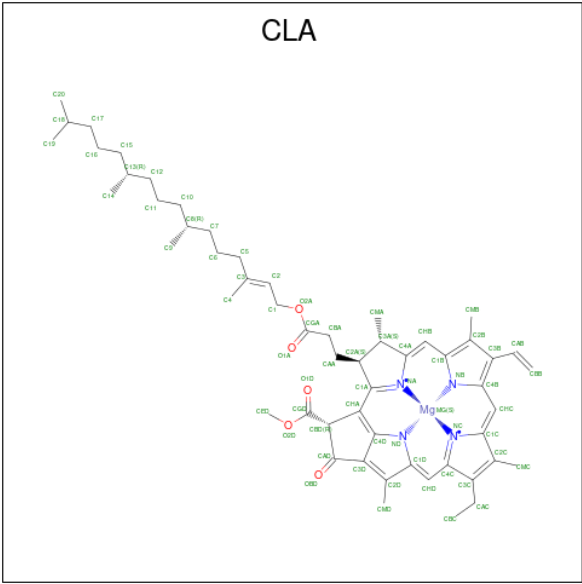
- Molecule 19 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Fe	0
			1	1	

- Molecule 20 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Cl	0
			1	1	

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

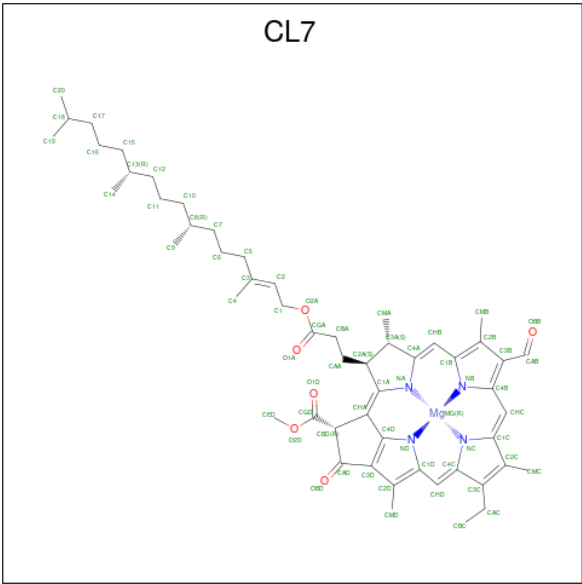
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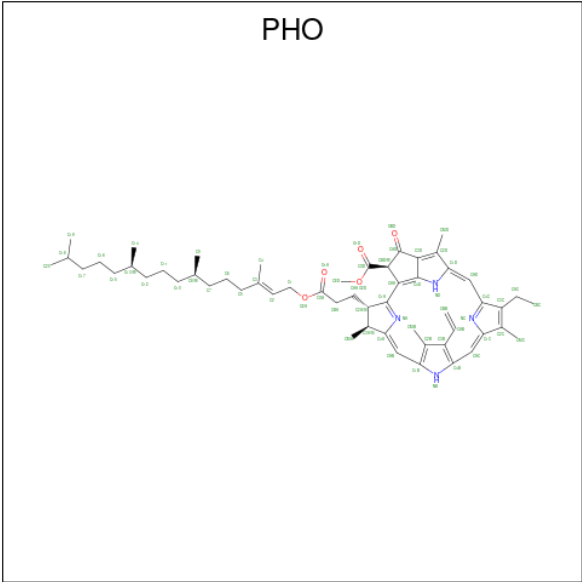
Mol	Chain	Residues	Atoms					AltConf
21	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 22 is CHLOROPHYLL D (CCD ID: CL7) (formula: C<sub>54</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



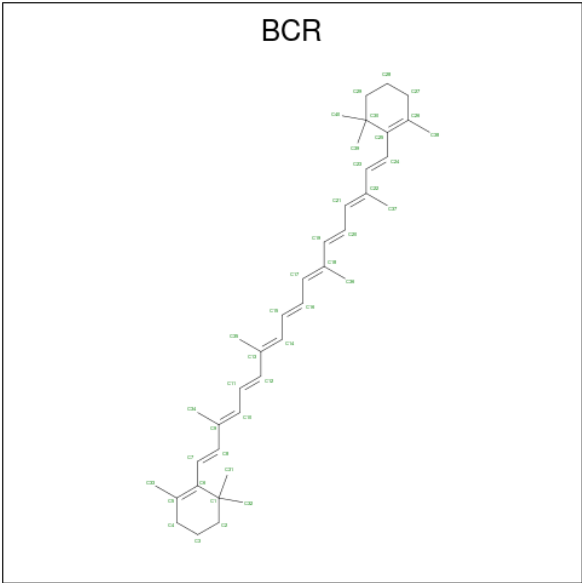
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



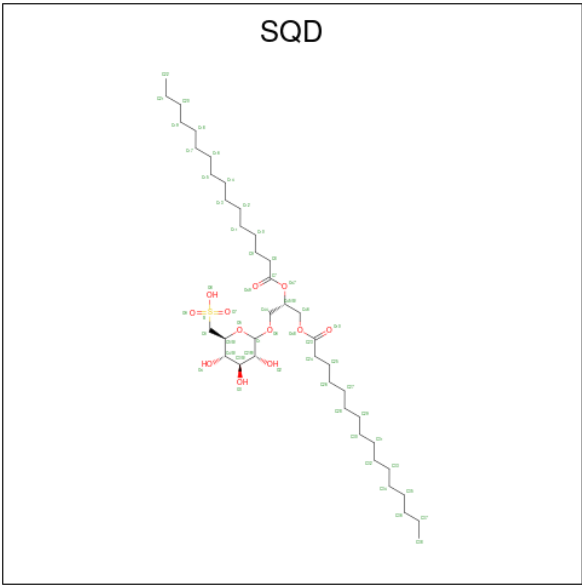
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	

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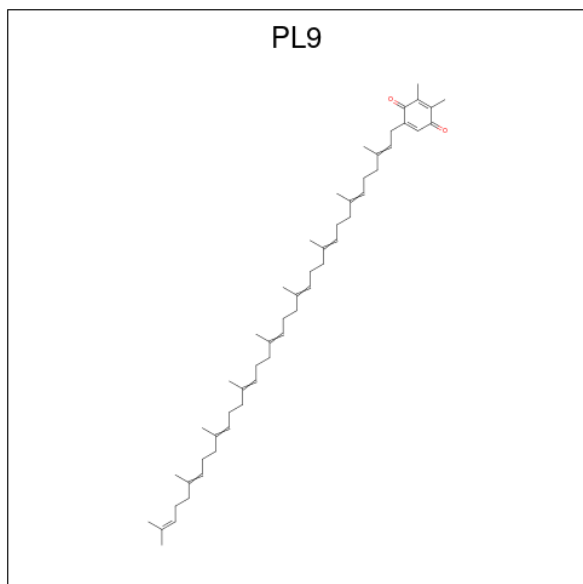
Mol	Chain	Residues	Atoms		AltConf
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	
24	C	1	Total	C	0
			40	40	
24	C	1	Total	C	0
			40	40	
24	D	1	Total	C	0
			40	40	
24	K	1	Total	C	0
			40	40	
24	K	1	Total	C	0
			40	40	

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



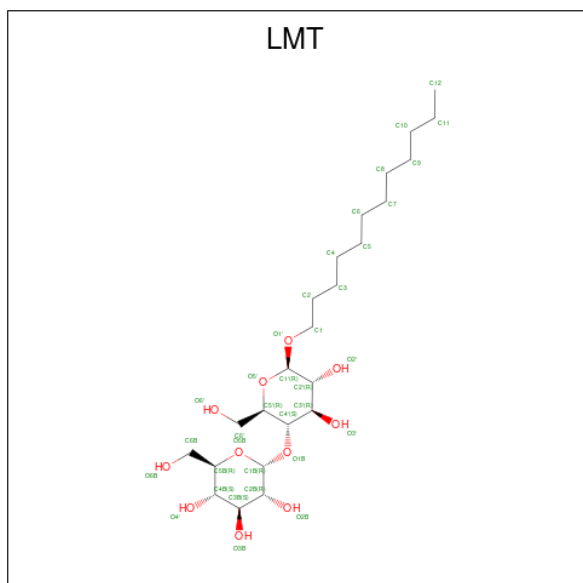
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	S	0
			54	41	12	1	
25	D	1	Total	C	O	S	0
			45	32	12	1	
25	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 26 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:  $C_{53}H_{80}O_2$ ).



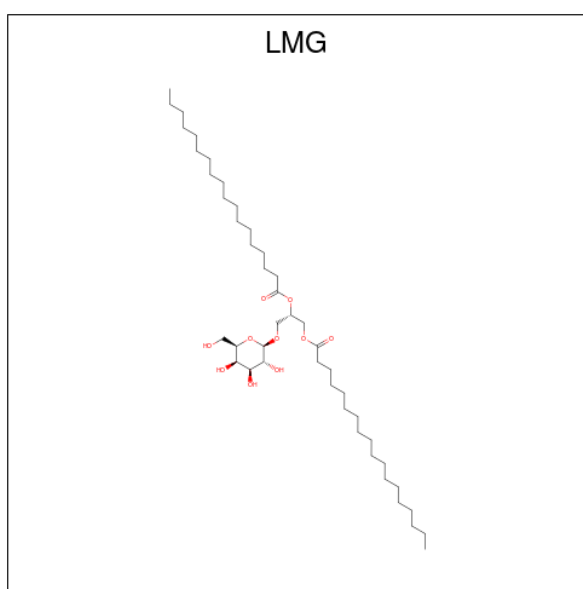
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			55	53	2	
26	D	1	Total	C	O	0
			55	53	2	

- Molecule 27 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



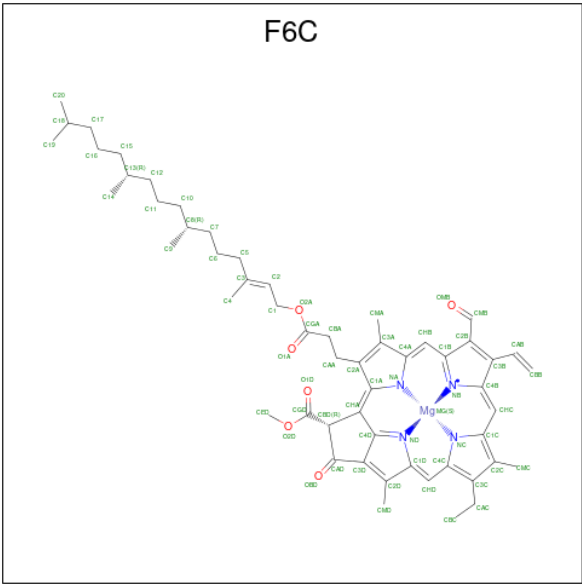
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			35	24	11	
27	F	1	Total	C	O	0
			35	24	11	
27	Z	1	Total	C	O	0
			35	24	11	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



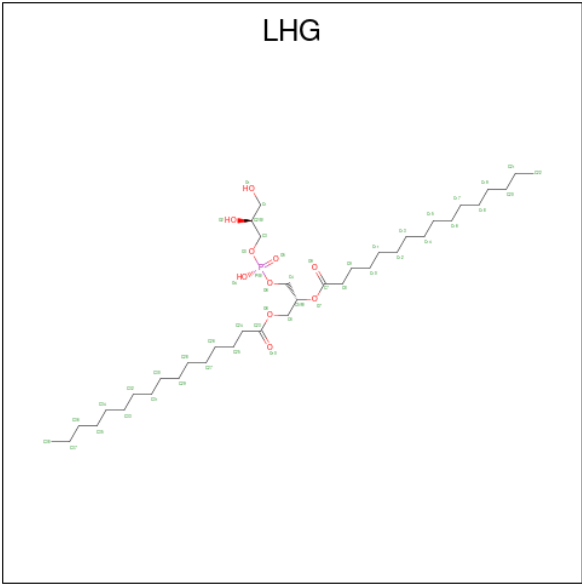
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			41	31	10	
28	B	1	Total	C	O	0
			51	41	10	
28	B	1	Total	C	O	0
			46	36	10	
28	C	1	Total	C	O	0
			51	41	10	
28	D	1	Total	C	O	0
			47	37	10	
28	D	1	Total	C	O	0
			51	41	10	
28	D	1	Total	C	O	0
			44	34	10	

- Molecule 29 is Chlorophyll F (CCD ID: F6C) (formula: C<sub>55</sub>H<sub>68</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



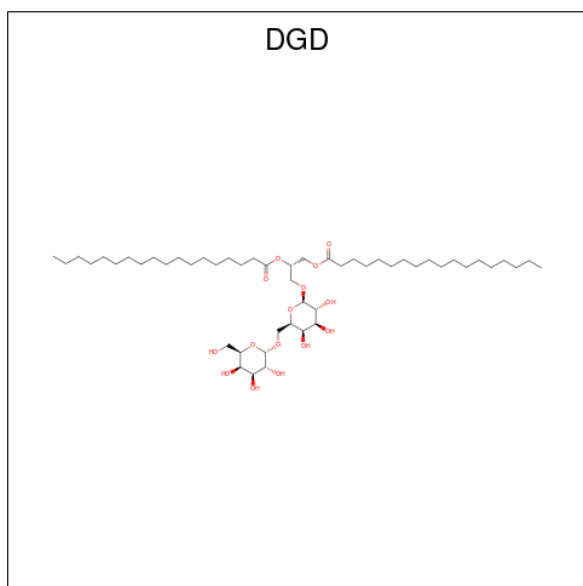
Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
29	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
30	B	1	Total	C	O	P	0
			45	34	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			46	35	10	1	
30	E	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	

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



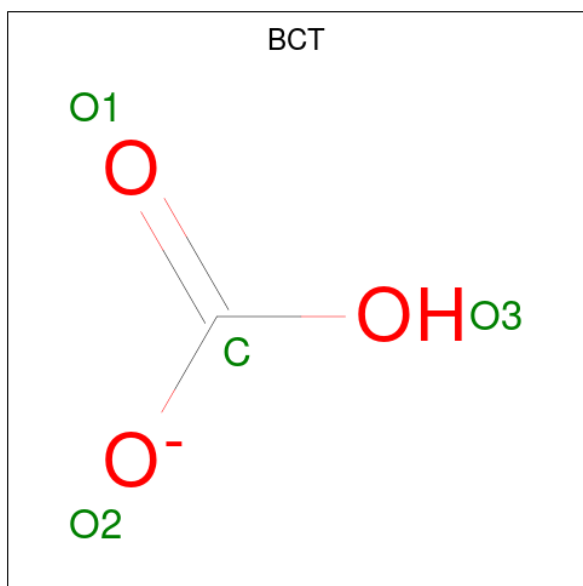
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	D	1	Total	C	O	0
			53	42	11	

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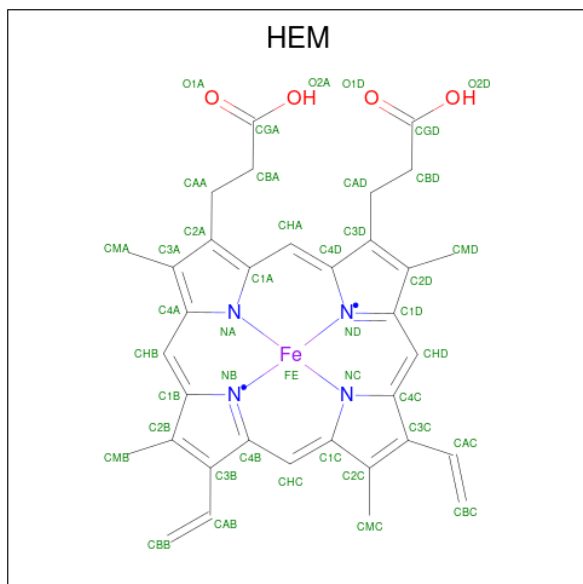
Mol	Chain	Residues	Atoms			AltConf
31	H	1	Total	C	O	0
			62	47	15	

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).





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

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	A	3	Total	O	0
			3	3	
34	A	14	Total	O	0
			14	14	
34	A	1	Total	O	0
			1	1	
34	A	7	Total	O	0
			7	7	
34	A	1	Total	O	0
			1	1	
34	A	1	Total	O	0
			1	1	
34	A	1	Total	O	0
			1	1	
34	B	25	Total	O	0
			25	25	
34	B	1	Total	O	0
			1	1	
34	B	1	Total	O	0
			1	1	
34	C	1	Total	O	0
			1	1	
34	C	2	Total	O	0
			2	2	
34	C	19	Total	O	0
			19	19	
34	C	1	Total	O	0
			1	1	
34	D	1	Total	O	0
			1	1	
34	D	17	Total	O	0
			17	17	
34	D	6	Total	O	0
			6	6	
34	D	4	Total	O	0
			4	4	
34	D	1	Total	O	0
			1	1	

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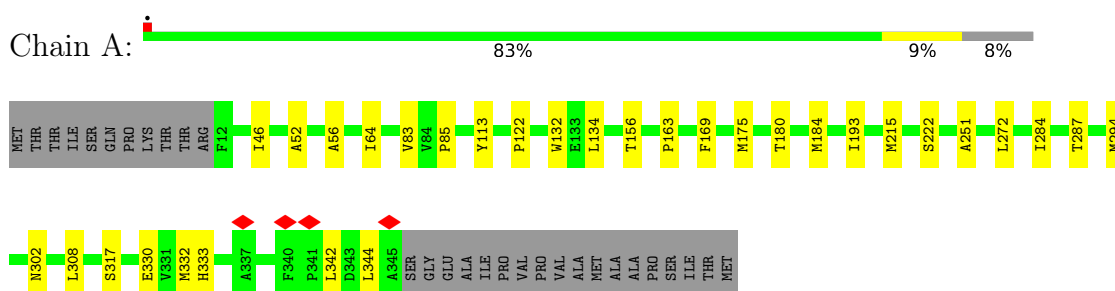
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Mol	Chain	Residues	Atoms		AltConf
34	D	1	Total 1	O 1	0
34	H	1	Total 1	O 1	0
34	I	1	Total 1	O 1	0
34	L	1	Total 1	O 1	0
34	X	2	Total 2	O 2	0
34	G	1	Total 1	O 1	0
34	G	1	Total 1	O 1	0
34	G	1	Total 1	O 1	0
34	G	1	Total 1	O 1	0

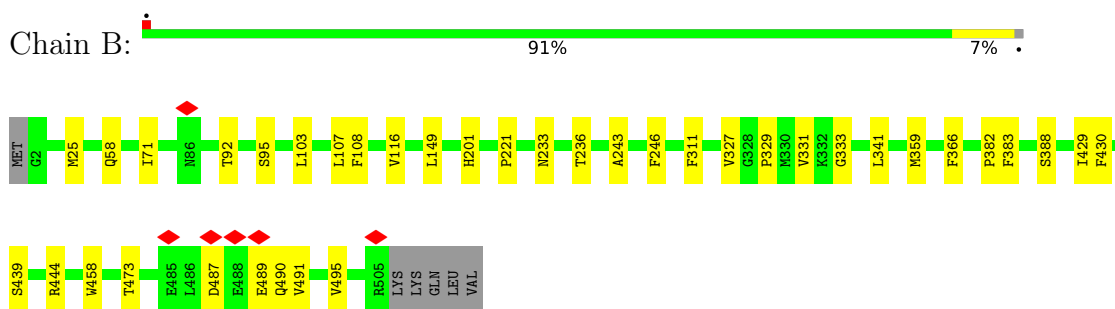
### 3 Residue-property plots [i](#)

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.

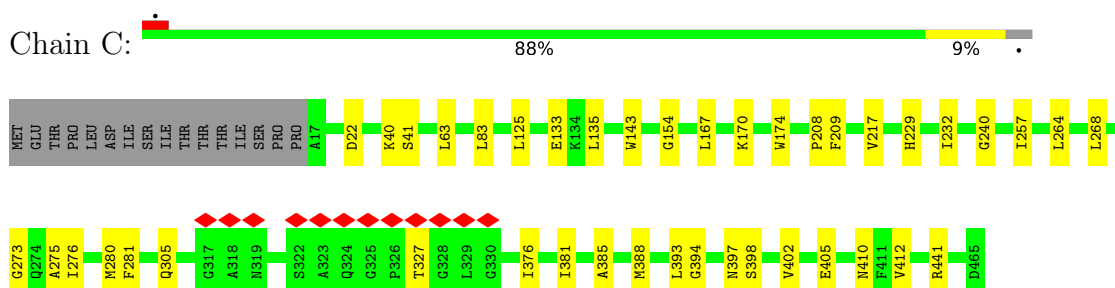
#### • Molecule 1: PsbA



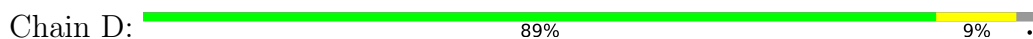
#### • Molecule 2: PsbB

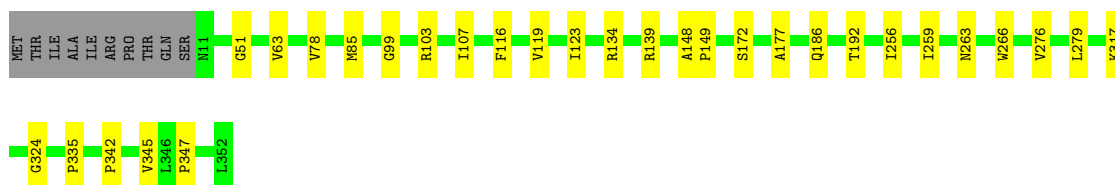


#### • Molecule 3: PsbC

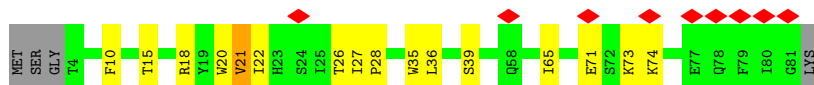
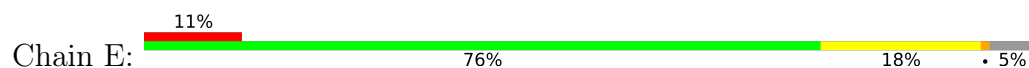


#### • Molecule 4: PsbD





- Molecule 5: PsbE



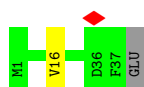
- Molecule 6: PsbF



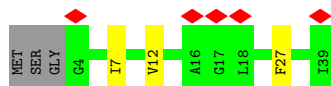
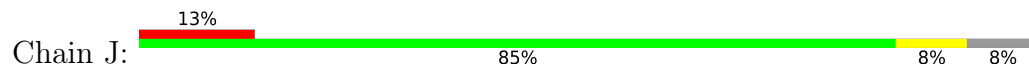
- Molecule 7: PsbH



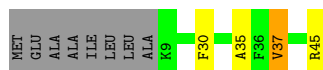
- Molecule 8: PsbI



- Molecule 9: PsbJ



- Molecule 10: PsbK



- Molecule 11: PsbL

Chain L:  97% .



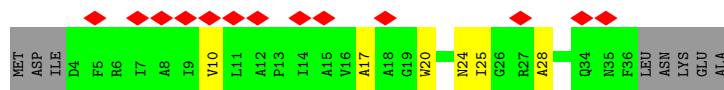
• Molecule 12: PsbM

Chain M:  72% 13% 15%




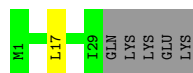
• Molecule 13: PsbY

Chain R:  32% 66% 15% 20%




• Molecule 14: PsbT

Chain T:  82% . 15%



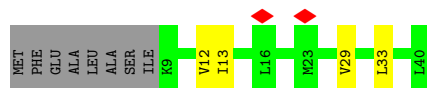
• Molecule 15: PsbX

Chain X:  82% 15% .



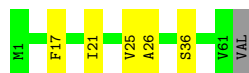
• Molecule 16: Ycf12

Chain Y:  5% 70% 10% 20%



• Molecule 17: PsbZ

Chain Z:  90% 8% .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.284	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	496.2, 496.2, 496.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, OEX, SQD, HEM, FE2, LHG, LMG, FME, DGD, PHO, BCT, F6C, LMT, BCR, CLA, CL, CL7

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	0.16	0/2707	0.29	0/3694
2	B	0.15	0/4111	0.26	0/5604
3	C	0.14	0/3564	0.27	0/4855
4	D	0.16	0/2858	0.28	0/3894
5	E	0.11	0/648	0.26	0/885
6	F	0.14	0/278	0.28	0/379
7	H	0.14	0/528	0.27	0/716
8	I	0.14	0/298	0.27	0/404
9	J	0.08	0/262	0.25	0/356
10	K	0.15	0/315	0.27	0/431
11	L	0.14	0/320	0.25	0/434
12	M	0.13	0/254	0.24	0/347
13	R	0.09	0/243	0.20	0/334
14	T	0.13	0/231	0.21	0/314
15	X	0.12	0/301	0.27	0/413
16	Y	0.08	0/244	0.20	0/328
17	Z	0.10	0/483	0.20	0/663
All	All	0.15	0/17645	0.27	0/24051

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2515	26	0
2	B	3977	0	3847	30	0
3	C	3453	0	3386	31	0
4	D	2756	0	2632	25	0
5	E	629	0	601	12	0
6	F	269	0	277	6	0
7	H	516	0	540	2	0
8	I	300	0	308	1	0
9	J	256	0	266	3	0
10	K	304	0	314	4	0
11	L	322	0	324	1	0
12	M	260	0	276	3	0
13	R	238	0	238	5	0
14	T	235	0	248	1	0
15	X	303	0	317	5	0
16	Y	242	0	271	3	0
17	Z	470	0	506	4	0
18	A	10	0	0	0	0
19	A	1	0	0	0	0
20	A	1	0	0	1	0
21	A	195	0	216	7	0
21	B	927	0	981	37	0
21	C	780	0	864	38	0
21	D	130	0	144	6	0
22	A	65	0	70	1	0
23	A	128	0	148	3	0
24	A	40	0	56	0	0
24	B	160	0	224	7	0
24	C	80	0	112	4	0
24	D	40	0	56	1	0
24	K	80	0	112	6	0
25	A	54	0	78	4	0
25	D	45	0	57	3	0
25	L	54	0	78	0	0
26	A	55	0	80	7	0
26	D	55	0	80	1	0
27	A	35	0	46	0	0
27	B	35	0	46	2	0
27	F	35	0	46	0	0
27	Z	35	0	46	0	0
28	A	41	0	52	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	97	0	134	3	0
28	C	51	0	72	3	0
28	D	142	0	197	5	0
29	B	66	0	0	0	0
29	C	61	0	0	0	0
30	B	45	0	63	2	0
30	D	193	0	287	5	0
30	E	49	0	74	2	0
30	L	49	0	74	1	0
31	C	186	0	246	13	0
31	D	53	0	71	0	0
31	H	62	0	82	3	0
32	D	4	0	0	0	0
33	F	43	0	30	3	0
34	A	28	0	0	0	0
34	B	27	0	0	0	0
34	C	23	0	0	0	0
34	D	30	0	0	0	0
34	G	4	0	0	0	0
34	H	1	0	0	0	0
34	I	1	0	0	0	0
34	L	1	0	0	0	0
34	X	2	0	0	0	0
All	All	21449	0	21788	234	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 5.

The worst 5 of 234 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)
33:F:101:HEM:HBC2	33:F:101:HEM:HHD	1.67	0.76
1:A:308:LEU:HB2	6:F:46:ARG:HD2	1.68	0.75
21:B:603:CLA:H161	31:H:102:DGD:HAW2	1.69	0.73
1:A:251:ALA:HA	2:B:491:VAL:HG11	1.70	0.73
23:A:409:PHO:HBC3	4:D:279:LEU:HD22	1.73	0.70

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/363 (92%)	322 (97%)	10 (3%)	0	100	100
2	B	502/510 (98%)	498 (99%)	4 (1%)	0	100	100
3	C	447/465 (96%)	438 (98%)	9 (2%)	0	100	100
4	D	340/352 (97%)	335 (98%)	5 (2%)	0	100	100
5	E	76/82 (93%)	76 (100%)	0	0	100	100
6	F	31/46 (67%)	31 (100%)	0	0	100	100
7	H	62/67 (92%)	62 (100%)	0	0	100	100
8	I	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	34/39 (87%)	32 (94%)	2 (6%)	0	100	100
10	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
11	L	37/39 (95%)	37 (100%)	0	0	100	100
12	M	31/39 (80%)	30 (97%)	1 (3%)	0	100	100
13	R	31/41 (76%)	31 (100%)	0	0	100	100
14	T	27/34 (79%)	27 (100%)	0	0	100	100
15	X	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
16	Y	30/40 (75%)	30 (100%)	0	0	100	100
17	Z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
All	All	2145/2301 (93%)	2109 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/296 (91%)	270 (100%)	0	100	100
2	B	406/412 (98%)	406 (100%)	0	100	100
3	C	340/360 (94%)	340 (100%)	0	100	100
4	D	278/288 (96%)	278 (100%)	0	100	100
5	E	66/72 (92%)	65 (98%)	1 (2%)	57	69
6	F	27/40 (68%)	26 (96%)	1 (4%)	30	39
7	H	56/58 (97%)	56 (100%)	0	100	100
8	I	31/32 (97%)	31 (100%)	0	100	100
9	J	24/26 (92%)	24 (100%)	0	100	100
10	K	32/37 (86%)	31 (97%)	1 (3%)	35	45
11	L	36/36 (100%)	36 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
13	R	21/30 (70%)	21 (100%)	0	100	100
14	T	23/28 (82%)	23 (100%)	0	100	100
15	X	33/34 (97%)	33 (100%)	0	100	100
16	Y	26/33 (79%)	26 (100%)	0	100	100
17	Z	50/51 (98%)	50 (100%)	0	100	100
All	All	1748/1866 (94%)	1745 (100%)	3 (0%)	85	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	21	VAL
6	F	32	VAL
10	K	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
13	R	24	ASN
10	K	39	GLN
3	C	397	ASN
3	C	253	HIS

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Mol	Chain	Res	Type
4	D	186	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	$\# Z  > 2$
15	FME	X	1	15	8,9,10	0.37	0	7,9,11	0.85	0
14	FME	T	1	14	8,9,10	0.36	0	7,9,11	0.85	0
8	FME	I	1	8	8,9,10	0.36	0	7,9,11	0.79	0
11	FME	L	1	11	8,9,10	0.36	0	7,9,11	0.96	0
12	FME	M	1	12	8,9,10	0.36	0	7,9,11	0.83	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
15	FME	X	1	15	-	2/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
11	FME	L	1	11	-	5/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	CB-CA-N-CN
11	L	1	FME	N-CA-CB-CG
11	L	1	FME	O-C-CA-CB
14	T	1	FME	N-CA-CB-CG
14	T	1	FME	C-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 80 ligands modelled in this entry, 2 are monoatomic - leaving 78 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	$\# Z  > 2$
30	LHG	B	1006	-	44,44,48	0.53	0	47,50,54	0.51	0
21	CLA	B	602	34	51,55,73	1.38	7 (13%)	61,91,113	1.18	5 (8%)
32	BCT	D	401	19	2,3,3	0.88	0	2,3,3	3.23	2 (100%)
24	BCR	B	618	-	41,41,41	0.32	0	56,56,56	0.64	1 (1%)
18	OEX	A	401	1,3	0,15,15	-	-	-	-	-
24	BCR	C	514	-	41,41,41	0.30	0	56,56,56	0.47	0
24	BCR	B	627	-	41,41,41	0.32	0	56,56,56	0.88	1 (1%)
24	BCR	K	102	-	41,41,41	0.31	0	56,56,56	0.76	0
21	CLA	B	611	34	69,73,73	1.16	6 (8%)	83,113,113	1.00	4 (4%)
21	CLA	B	617	2	49,53,73	1.40	7 (14%)	59,89,113	1.09	5 (8%)
29	F6C	C	507	34	67,69,74	1.75	11 (16%)	75,108,114	2.14	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CLA	C	503	3	69,73,73	1.20	7 (10%)	83,113,113	0.98	5 (6%)
25	SQD	A	412	-	53,54,54	1.53	7 (13%)	62,65,65	1.38	6 (9%)
25	SQD	D	407	-	44,45,54	1.61	7 (15%)	53,56,65	1.45	6 (11%)
23	PHO	A	408	-	58,69,69	1.99	11 (18%)	56,99,99	1.53	6 (10%)
28	LMG	C	519	-	51,51,55	0.52	0	59,59,63	0.62	0
21	CLA	B	608	34	69,73,73	1.17	6 (8%)	83,113,113	0.92	4 (4%)
21	CLA	B	605	2	69,73,73	1.20	8 (11%)	83,113,113	0.95	4 (4%)
30	LHG	D	409	-	48,48,48	0.51	0	51,54,54	0.49	0
21	CLA	D	403	4	69,73,73	1.17	7 (10%)	83,113,113	0.95	4 (4%)
28	LMG	D	630	-	44,44,55	0.52	0	52,52,63	0.64	0
30	LHG	D	408	-	48,48,48	0.51	0	51,54,54	0.49	0
24	BCR	C	515	-	41,41,41	0.31	0	56,56,56	0.64	0
21	CLA	C	502	3	69,73,73	1.19	7 (10%)	83,113,113	0.95	5 (6%)
23	PHO	A	409	-	58,69,69	1.99	10 (17%)	56,99,99	1.55	7 (12%)
21	CLA	B	609	2	69,73,73	1.18	8 (11%)	83,113,113	0.93	4 (4%)
21	CLA	B	616	2	69,73,73	1.21	7 (10%)	83,113,113	1.00	4 (4%)
31	DGD	D	406	-	53,53,67	0.51	0	60,61,81	0.60	0
24	BCR	A	411	-	41,41,41	0.30	0	56,56,56	0.49	0
21	CLA	A	405	1	69,73,73	1.17	7 (10%)	83,113,113	0.92	4 (4%)
21	CLA	C	506	3	69,73,73	1.17	7 (10%)	83,113,113	0.95	4 (4%)
28	LMG	D	628	-	47,47,55	0.51	0	55,55,63	0.62	0
26	PL9	D	405	-	55,55,55	1.22	4 (7%)	68,69,69	1.55	12 (17%)
31	DGD	C	517	-	63,63,67	0.56	0	77,77,81	0.68	0
21	CLA	C	513	3	69,73,73	1.15	6 (8%)	83,113,113	0.97	4 (4%)
21	CLA	B	615	2	69,73,73	1.16	6 (8%)	83,113,113	0.94	4 (4%)
33	HEM	F	101	5,6	50,50,50	1.40	6 (12%)	66,82,82	1.23	5 (7%)
21	CLA	D	402	4	69,73,73	1.17	6 (8%)	83,113,113	0.92	4 (4%)
28	LMG	B	622	-	51,51,55	0.51	0	59,59,63	0.62	0
21	CLA	B	610	2	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
30	LHG	D	410	-	45,45,48	0.53	0	48,51,54	0.48	0
26	PL9	A	414	-	55,55,55	1.04	4 (7%)	68,69,69	1.52	13 (19%)
21	CLA	C	509	3	69,73,73	1.17	7 (10%)	83,113,113	0.96	5 (6%)
21	CLA	C	501	3	69,73,73	1.17	6 (8%)	83,113,113	0.98	5 (6%)
27	LMT	A	419	-	36,36,36	0.56	0	47,47,47	0.68	0
21	CLA	B	604	2	69,73,73	1.16	7 (10%)	83,113,113	0.90	3 (3%)
21	CLA	C	508	3	69,73,73	1.18	7 (10%)	83,113,113	0.93	5 (6%)
27	LMT	B	1008	-	36,36,36	0.58	0	47,47,47	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMT	Z	102	-	36,36,36	0.53	0	47,47,47	0.72	0
28	LMG	B	1007	-	46,46,55	0.53	0	54,54,63	0.63	0
27	LMT	F	102	-	36,36,36	0.54	0	47,47,47	0.68	0
30	LHG	L	101	-	48,48,48	0.51	0	51,54,54	0.51	0
24	BCR	B	619	-	41,41,41	0.31	0	56,56,56	0.72	1 (1%)
31	DGD	C	516	-	63,63,67	0.59	0	77,77,81	0.69	2 (2%)
28	LMG	A	413	-	41,41,55	0.53	0	49,49,63	0.64	0
31	DGD	C	518	-	63,63,67	0.56	0	77,77,81	0.64	0
24	BCR	K	101	-	41,41,41	0.32	0	56,56,56	0.93	2 (3%)
21	CLA	B	612	2	69,73,73	1.18	7 (10%)	83,113,113	0.97	5 (6%)
29	F6C	B	614	2	72,74,74	1.67	10 (13%)	81,114,114	2.04	16 (19%)
30	LHG	D	629	-	48,48,48	0.49	0	51,54,54	0.63	1 (1%)
25	SQD	L	103	-	53,54,54	1.54	8 (15%)	62,65,65	1.39	6 (9%)
21	CLA	C	512	3	69,73,73	1.16	7 (10%)	83,113,113	0.93	4 (4%)
30	LHG	E	101	-	48,48,48	0.51	0	51,54,54	0.48	0
21	CLA	A	407	34	69,73,73	1.15	6 (8%)	83,113,113	0.95	4 (4%)
21	CLA	B	603	2	69,73,73	1.16	7 (10%)	83,113,113	0.94	4 (4%)
21	CLA	B	607	2	59,63,73	1.28	6 (10%)	71,101,113	0.99	4 (5%)
21	CLA	A	410	1	69,73,73	1.16	6 (8%)	83,113,113	0.96	4 (4%)
21	CLA	C	505	3	69,73,73	1.19	8 (11%)	83,113,113	0.94	4 (4%)
21	CLA	B	606	2	69,73,73	1.19	7 (10%)	83,113,113	0.99	4 (4%)
31	DGD	H	102	-	63,63,67	0.57	0	77,77,81	0.76	0
21	CLA	C	511	3	69,73,73	1.19	8 (11%)	83,113,113	0.95	4 (4%)
21	CLA	B	613	2	69,73,73	1.18	8 (11%)	83,113,113	0.93	4 (4%)
28	LMG	D	411	-	51,51,55	0.53	0	59,59,63	0.63	0
21	CLA	C	510	3	69,73,73	1.18	7 (10%)	83,113,113	0.94	4 (4%)
24	BCR	B	620	-	41,41,41	0.31	0	56,56,56	0.59	0
22	CL7	A	406	34	71,73,73	1.14	5 (7%)	80,113,113	0.84	3 (3%)
24	BCR	D	404	-	41,41,41	0.32	0	56,56,56	0.87	3 (5%)
21	CLA	C	504	34	69,73,73	1.16	6 (8%)	83,113,113	0.96	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	C	501	3	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	C	509	3	-	3/39/115/115	-
30	LHG	B	1006	-	-	10/49/49/53	-
21	CLA	B	602	34	-	6/18/94/115	-
21	CLA	D	403	4	-	6/39/115/115	-
27	LMT	A	419	-	-	6/21/61/61	0/2/2/2
21	CLA	C	512	3	-	4/39/115/115	-
28	LMG	D	630	-	-	7/39/59/70	0/1/1/1
30	LHG	E	101	-	-	20/53/53/53	-
21	CLA	B	604	2	-	1/39/115/115	-
24	BCR	B	618	-	-	4/29/63/63	0/2/2/2
30	LHG	D	408	-	-	16/53/53/53	-
21	CLA	C	508	3	-	3/39/115/115	-
21	CLA	A	407	34	-	3/39/115/115	-
24	BCR	C	515	-	-	1/29/63/63	0/2/2/2
27	LMT	B	1008	-	-	6/21/61/61	0/2/2/2
21	CLA	C	502	3	-	7/39/115/115	-
23	PHO	A	409	-	-	6/37/103/103	0/5/6/6
27	LMT	Z	102	-	-	5/21/61/61	0/2/2/2
21	CLA	B	609	2	-	0/39/115/115	-
24	BCR	C	514	-	-	2/29/63/63	0/2/2/2
21	CLA	B	616	2	-	1/39/115/115	-
28	LMG	B	1007	-	-	13/41/61/70	0/1/1/1
27	LMT	F	102	-	-	6/21/61/61	0/2/2/2
31	DGD	D	406	-	-	8/47/68/95	0/1/1/2
24	BCR	A	411	-	-	2/29/63/63	0/2/2/2
21	CLA	A	405	1	-	1/39/115/115	-
21	CLA	C	506	3	-	6/39/115/115	-
24	BCR	B	627	-	-	5/29/63/63	0/2/2/2
21	CLA	B	603	2	-	2/39/115/115	-
26	PL9	D	405	-	-	5/53/73/73	0/1/1/1
24	BCR	K	102	-	-	3/29/63/63	0/2/2/2
21	CLA	B	607	2	-	5/27/103/115	-
21	CLA	B	611	34	-	1/39/115/115	-
21	CLA	C	513	3	-	10/39/115/115	-
28	LMG	D	628	-	-	13/42/62/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	D	629	-	-	18/53/53/53	-
21	CLA	B	617	2	-	0/15/91/115	-
30	LHG	L	101	-	-	10/53/53/53	-
31	DGD	C	517	-	-	12/51/91/95	0/2/2/2
21	CLA	A	410	1	-	2/39/115/115	-
21	CLA	C	505	3	-	7/39/115/115	-
29	F6C	C	507	34	1/1/9/16	6/35/91/97	-
21	CLA	B	615	2	-	7/39/115/115	-
21	CLA	C	503	3	-	2/39/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
25	SQD	A	412	-	-	27/49/69/69	0/1/1/1
25	SQD	D	407	-	-	22/40/60/69	0/1/1/1
31	DGD	C	516	-	-	15/51/91/95	0/2/2/2
23	PHO	A	408	-	-	7/37/103/103	0/5/6/6
28	LMG	A	413	-	-	9/36/56/70	0/1/1/1
33	HEM	F	101	5,6	-	2/14/54/54	-
21	CLA	B	606	2	-	4/39/115/115	-
28	LMG	C	519	-	-	8/46/66/70	0/1/1/1
21	CLA	B	608	34	-	4/39/115/115	-
21	CLA	D	402	4	-	3/39/115/115	-
31	DGD	C	518	-	-	4/51/91/95	0/2/2/2
31	DGD	H	102	-	-	17/51/91/95	0/2/2/2
21	CLA	B	605	2	-	7/39/115/115	-
28	LMG	B	622	-	-	12/46/66/70	0/1/1/1
21	CLA	B	610	2	-	1/39/115/115	-
21	CLA	C	511	3	-	1/39/115/115	-
24	BCR	K	101	-	-	9/29/63/63	0/2/2/2
30	LHG	D	410	-	-	9/50/50/53	-
21	CLA	B	613	2	-	2/39/115/115	-
30	LHG	D	409	-	-	10/53/53/53	-
28	LMG	D	411	-	-	11/46/66/70	0/1/1/1
21	CLA	B	612	2	-	2/39/115/115	-
21	CLA	C	510	3	-	5/39/115/115	-
24	BCR	B	620	-	-	2/29/63/63	0/2/2/2
22	CL7	A	406	34	2/2/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PL9	A	414	-	-	23/53/73/73	0/1/1/1
29	F6C	B	614	2	1/1/10/16	13/41/97/97	-
24	BCR	D	404	-	-	11/29/63/63	0/2/2/2
21	CLA	C	504	34	-	3/39/115/115	-
25	SQD	L	103	-	-	27/49/69/69	0/1/1/1

The worst 5 of 302 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	PHO	C1B-C2B	9.05	1.49	1.39
23	A	409	PHO	C1B-C2B	9.03	1.49	1.39
29	C	507	F6C	C2A-C3A	8.61	1.55	1.36
29	B	614	F6C	C2A-C3A	8.53	1.54	1.36
23	A	409	PHO	C3B-C4B	7.51	1.50	1.41

The worst 5 of 245 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	507	F6C	CAA-C2A-C3A	-9.37	110.42	127.88
29	B	614	F6C	CAA-C2A-C3A	-8.61	111.85	127.88
23	A	409	PHO	C4D-CHA-CBD	-7.14	105.29	108.52
29	C	507	F6C	CMA-C3A-C4A	-7.12	112.17	124.71
29	B	614	F6C	CMA-C3A-C4A	-7.11	112.19	124.71

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	406	CL7	NC
22	A	406	CL7	NA
29	B	614	F6C	NA
29	C	507	F6C	NA

5 of 538 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	407	CLA	CHA-CBD-CGD-O1D
21	A	407	CLA	CHA-CBD-CGD-O2D
21	B	602	CLA	CBA-CGA-O2A-C1
21	B	602	CLA	O1A-CGA-O2A-C1
21	B	602	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

66 monomers are involved in 148 short contacts:

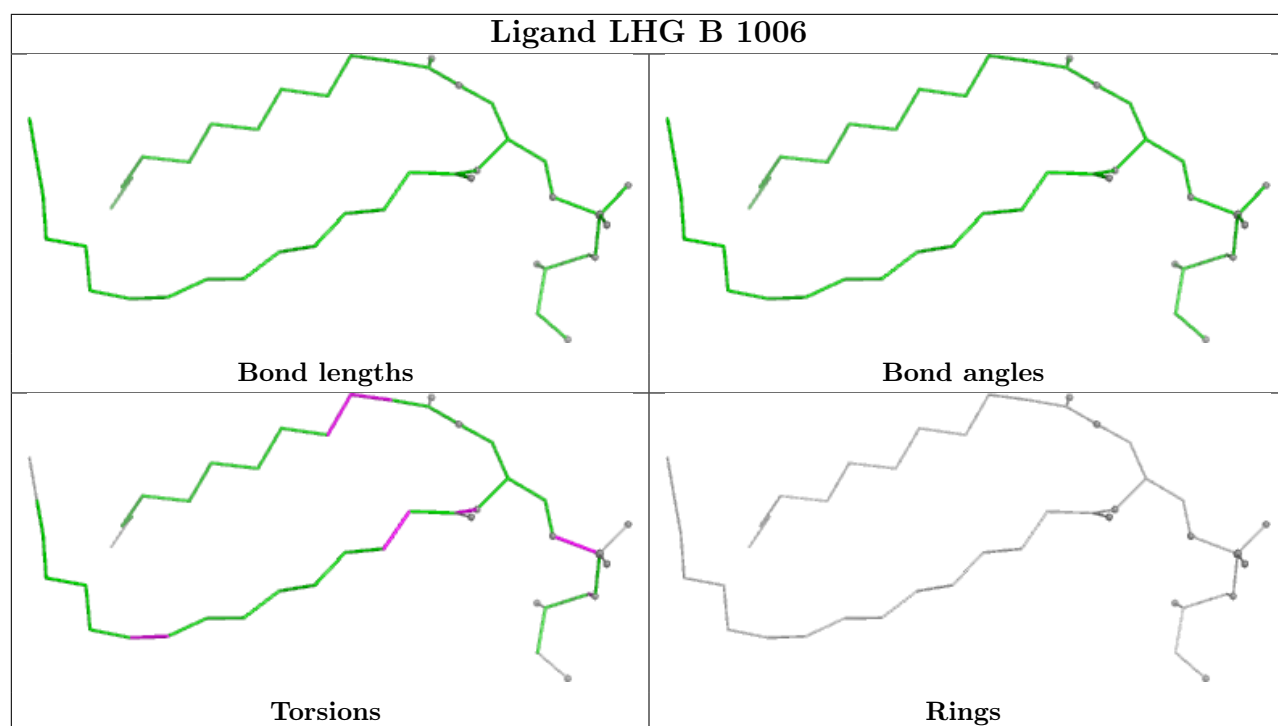
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	B	1006	LHG	2	0
21	B	602	CLA	3	0
24	B	618	BCR	1	0
24	C	514	BCR	1	0
24	B	627	BCR	3	0
24	K	102	BCR	2	0
21	B	611	CLA	2	0
21	B	617	CLA	1	0
21	C	503	CLA	7	0
25	A	412	SQD	4	0
25	D	407	SQD	3	0
23	A	408	PHO	2	0
28	C	519	LMG	3	0
21	B	608	CLA	1	0
21	B	605	CLA	6	0
30	D	409	LHG	3	0
21	D	403	CLA	3	0
28	D	630	LMG	2	0
24	C	515	BCR	3	0
21	C	502	CLA	6	0
23	A	409	PHO	1	0
21	B	609	CLA	1	0
21	B	616	CLA	4	0
21	A	405	CLA	2	0
21	C	506	CLA	4	0
28	D	628	LMG	1	0
26	D	405	PL9	1	0
31	C	517	DGD	4	0
21	C	513	CLA	3	0
21	B	615	CLA	3	0
33	F	101	HEM	3	0
21	D	402	CLA	3	0
28	B	622	LMG	1	0
21	B	610	CLA	2	0
30	D	410	LHG	2	0
26	A	414	PL9	7	0
21	C	509	CLA	2	0
21	C	501	CLA	5	0
21	B	604	CLA	2	0
21	C	508	CLA	1	0

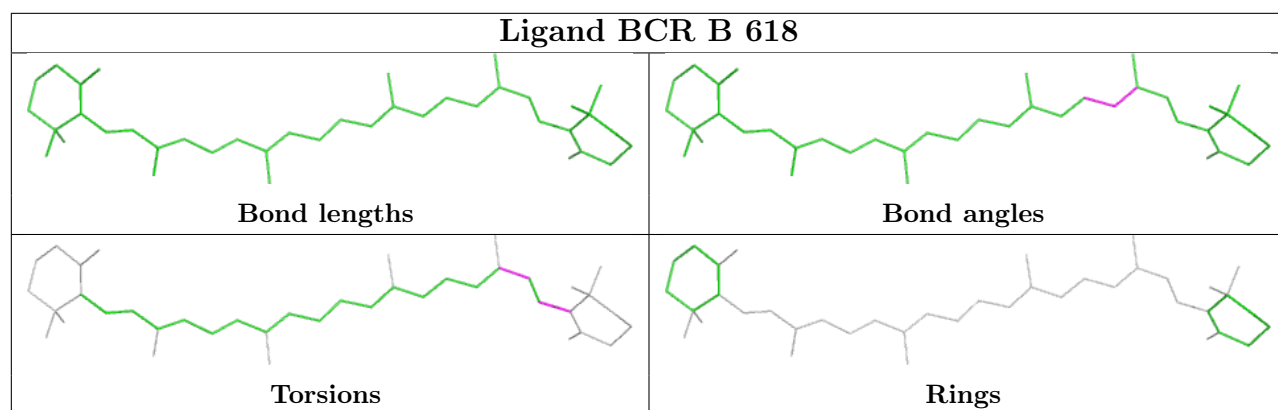
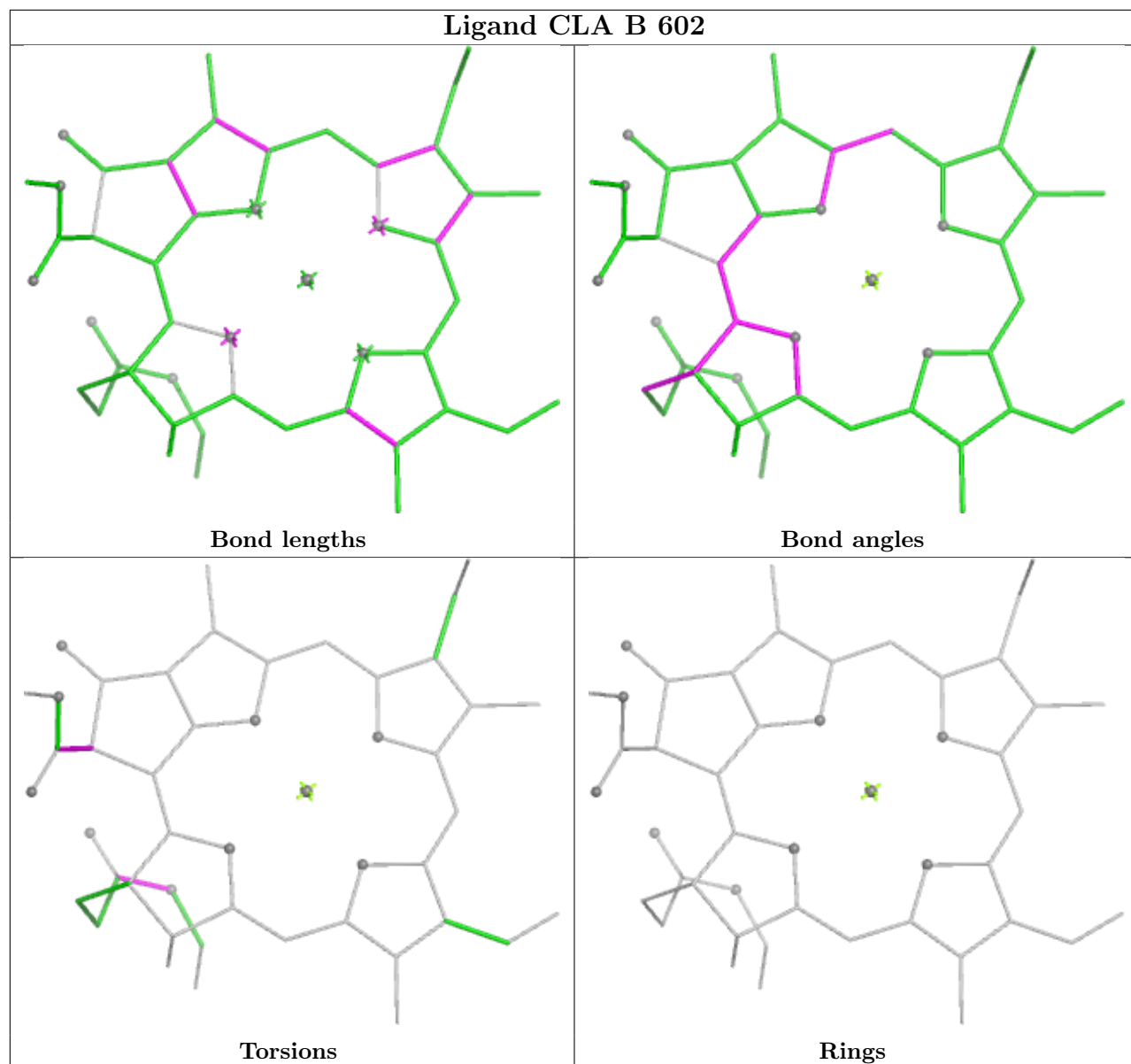
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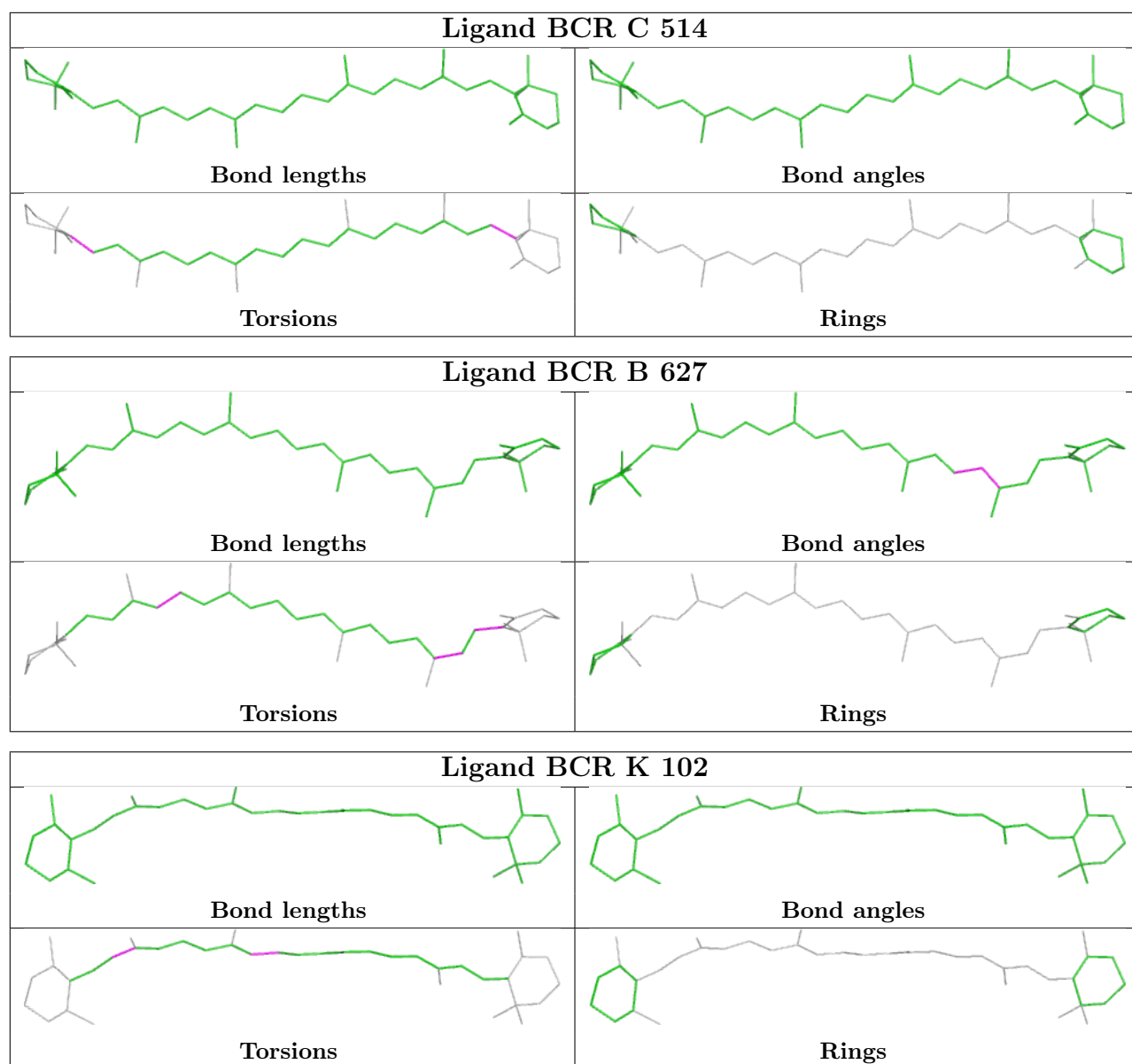
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	1008	LMT	2	0
28	B	1007	LMG	2	0
30	L	101	LHG	1	0
24	B	619	BCR	1	0
31	C	516	DGD	6	0
28	A	413	LMG	4	0
31	C	518	DGD	3	0
24	K	101	BCR	4	0
21	B	612	CLA	1	0
21	C	512	CLA	4	0
30	E	101	LHG	2	0
21	A	407	CLA	1	0
21	B	603	CLA	5	0
21	B	607	CLA	3	0
21	A	410	CLA	4	0
21	C	505	CLA	5	0
21	B	606	CLA	4	0
31	H	102	DGD	3	0
21	C	511	CLA	3	0
21	B	613	CLA	2	0
28	D	411	LMG	2	0
21	C	510	CLA	2	0
24	B	620	BCR	2	0
22	A	406	CL7	1	0
24	D	404	BCR	1	0
21	C	504	CLA	2	0

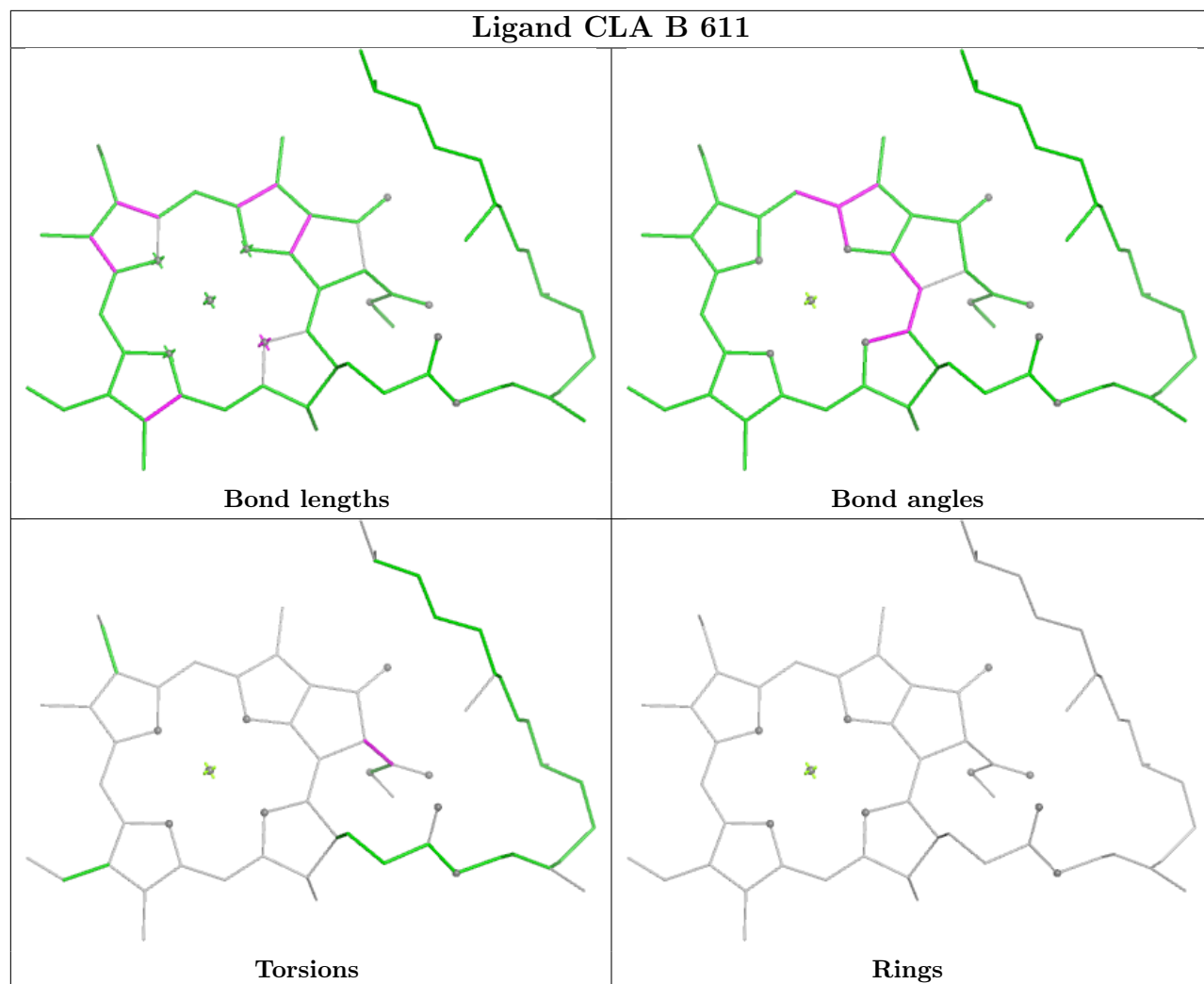
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



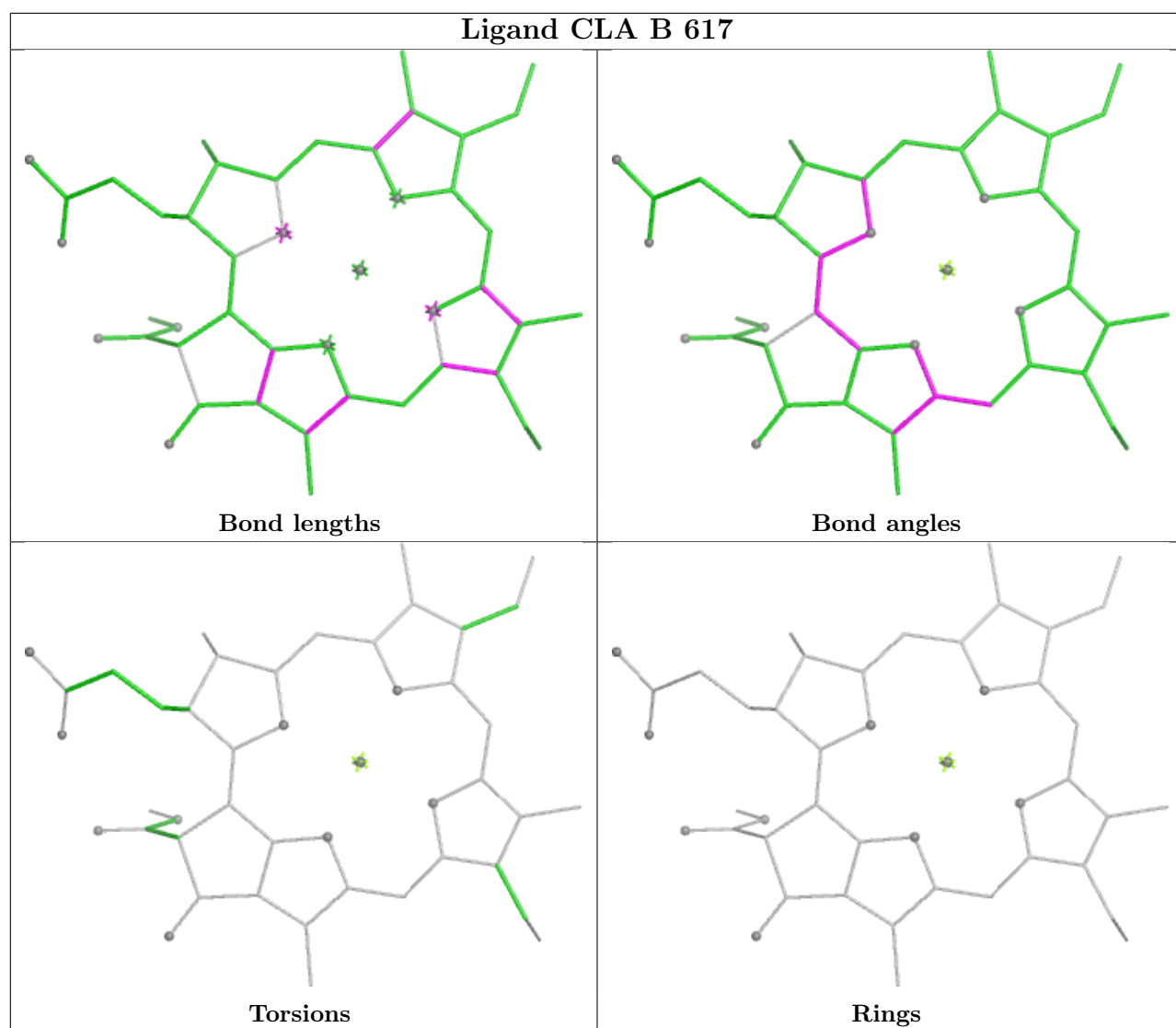


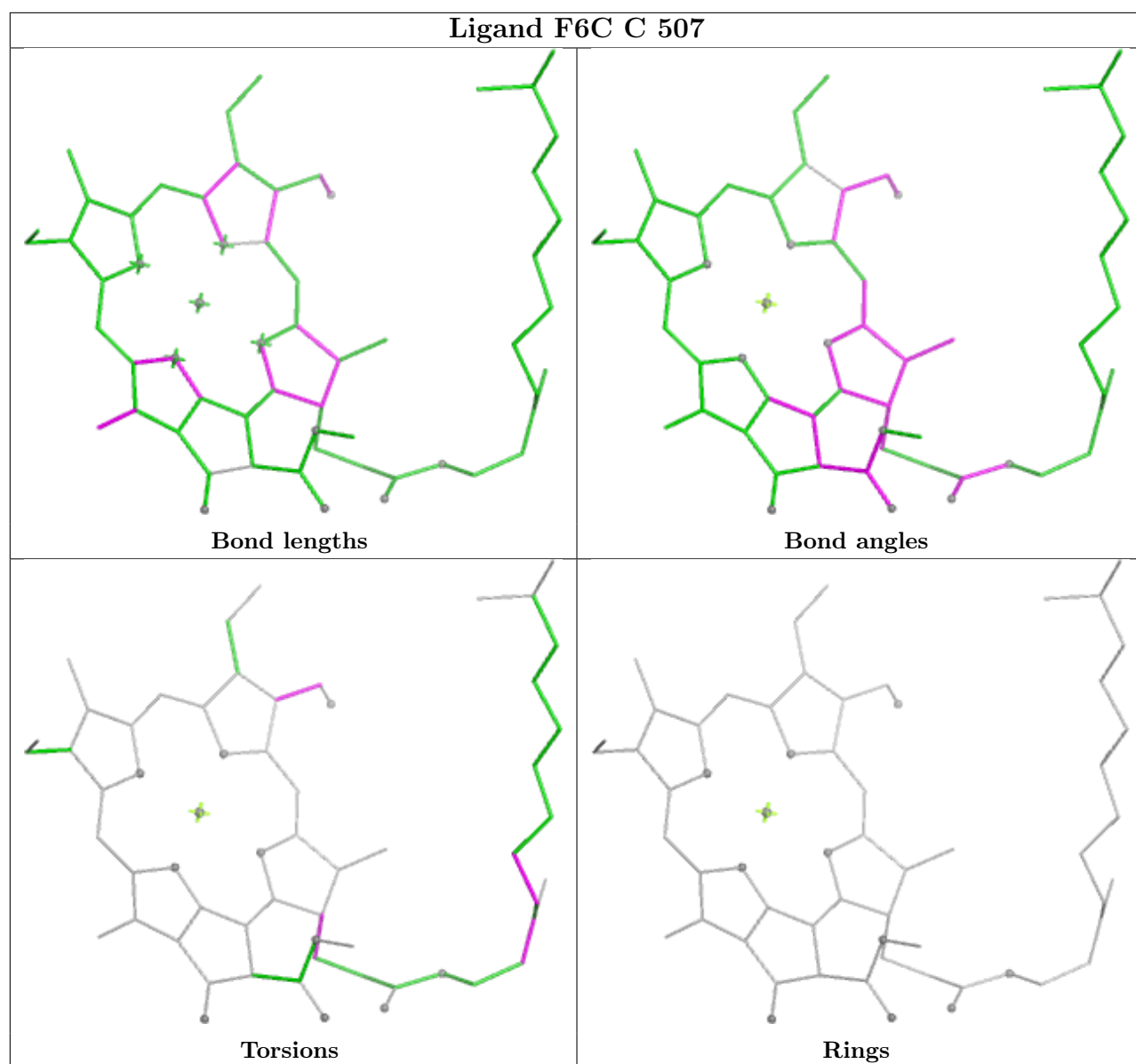


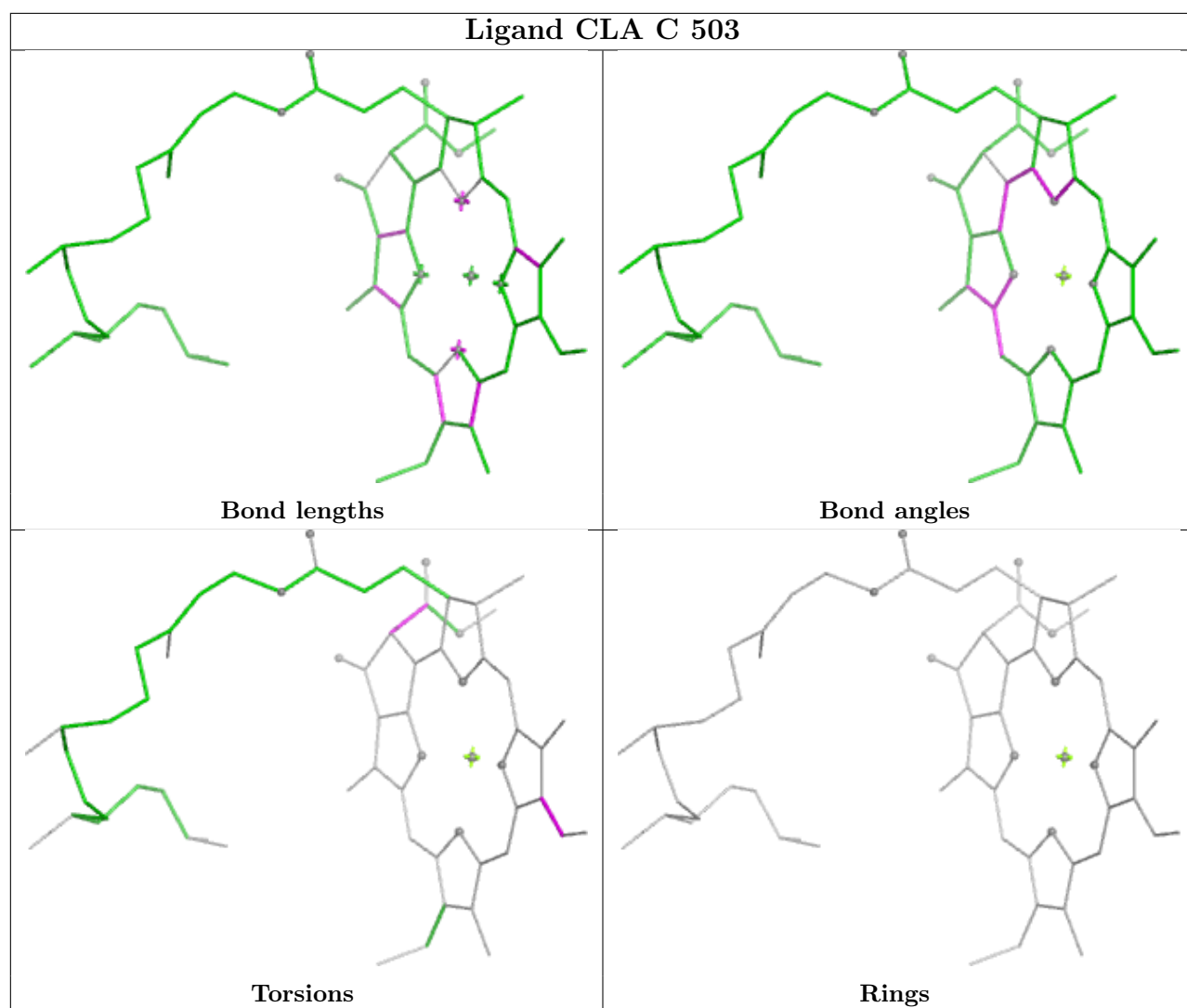
## Ligand CLA B 611

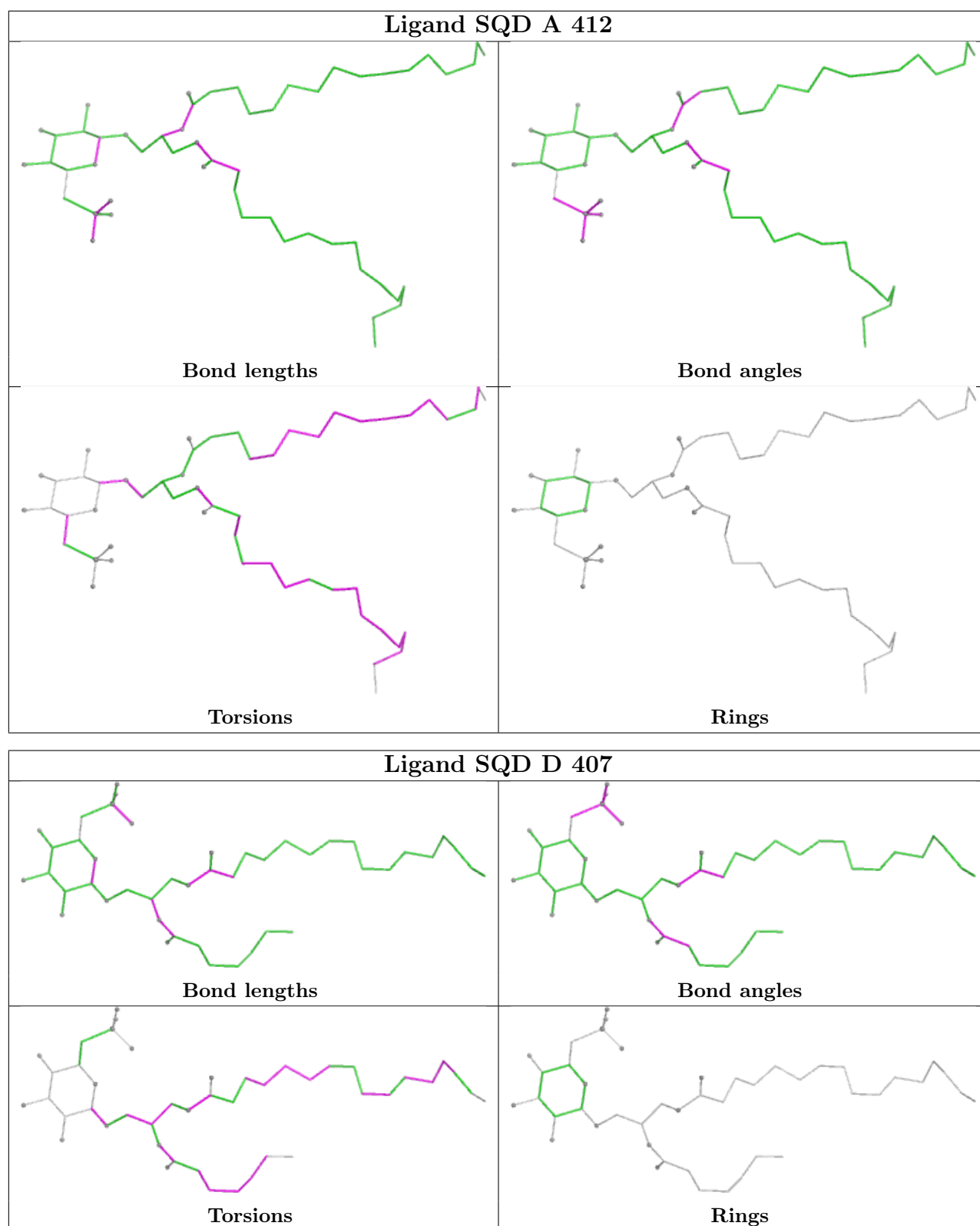


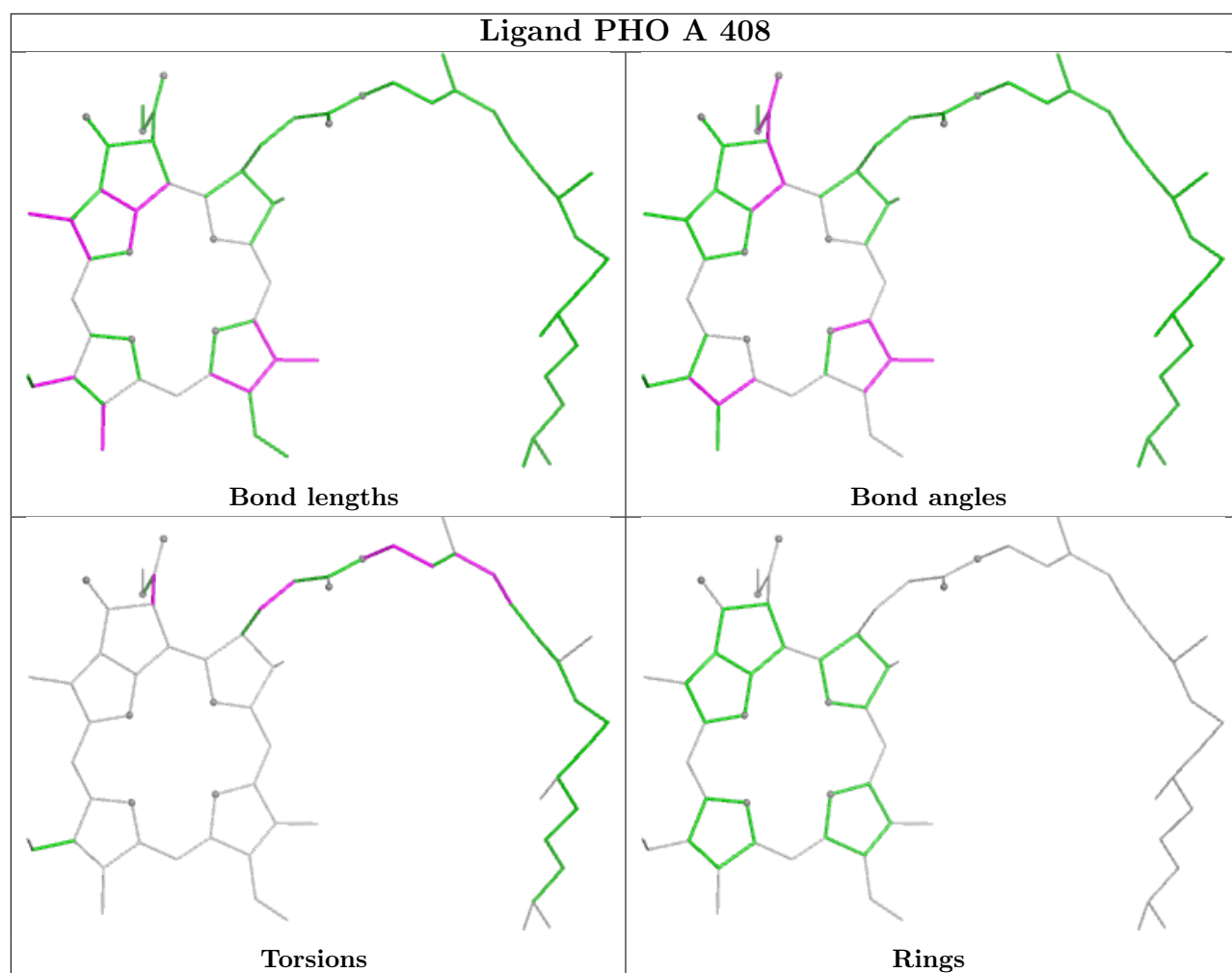


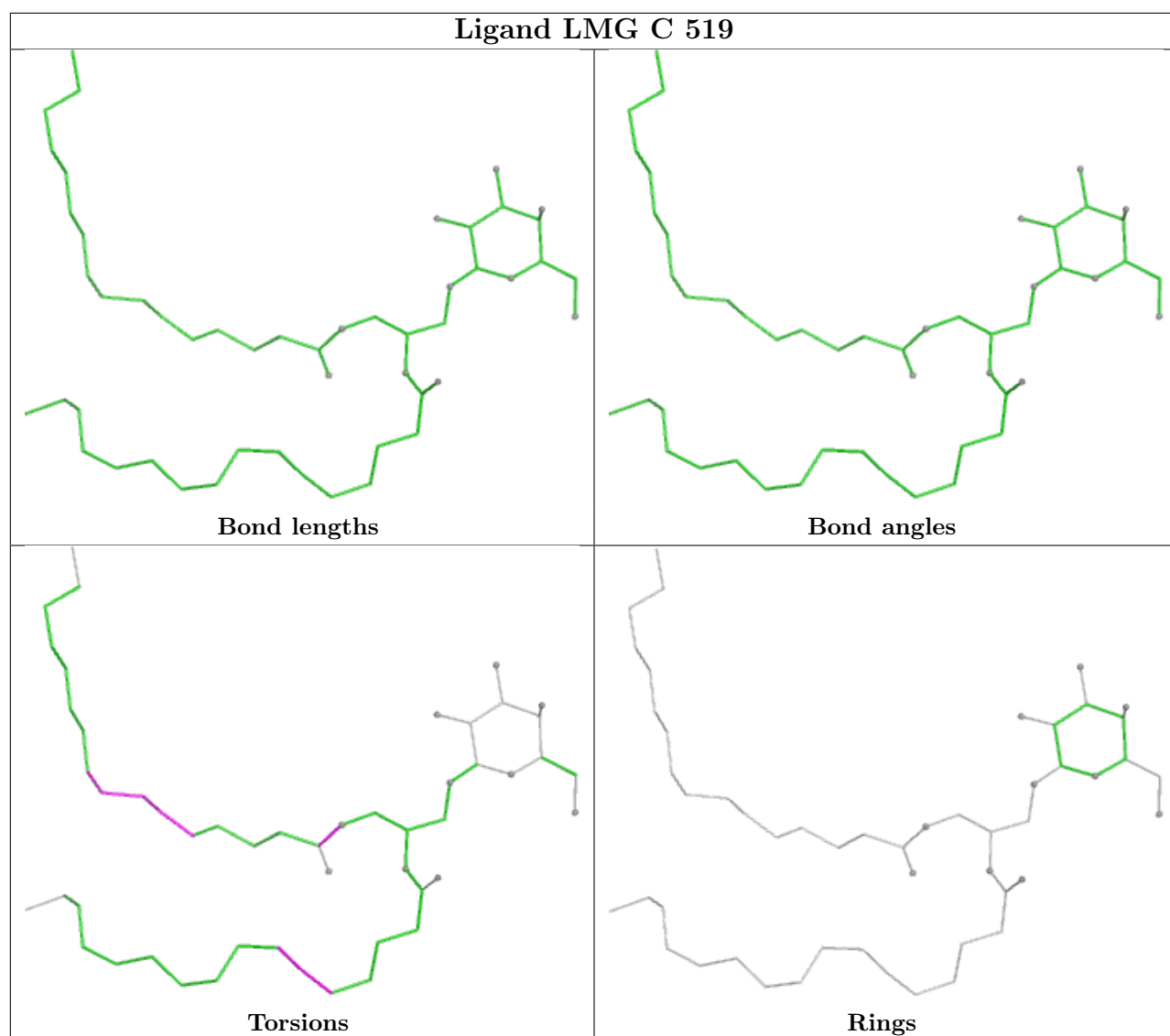


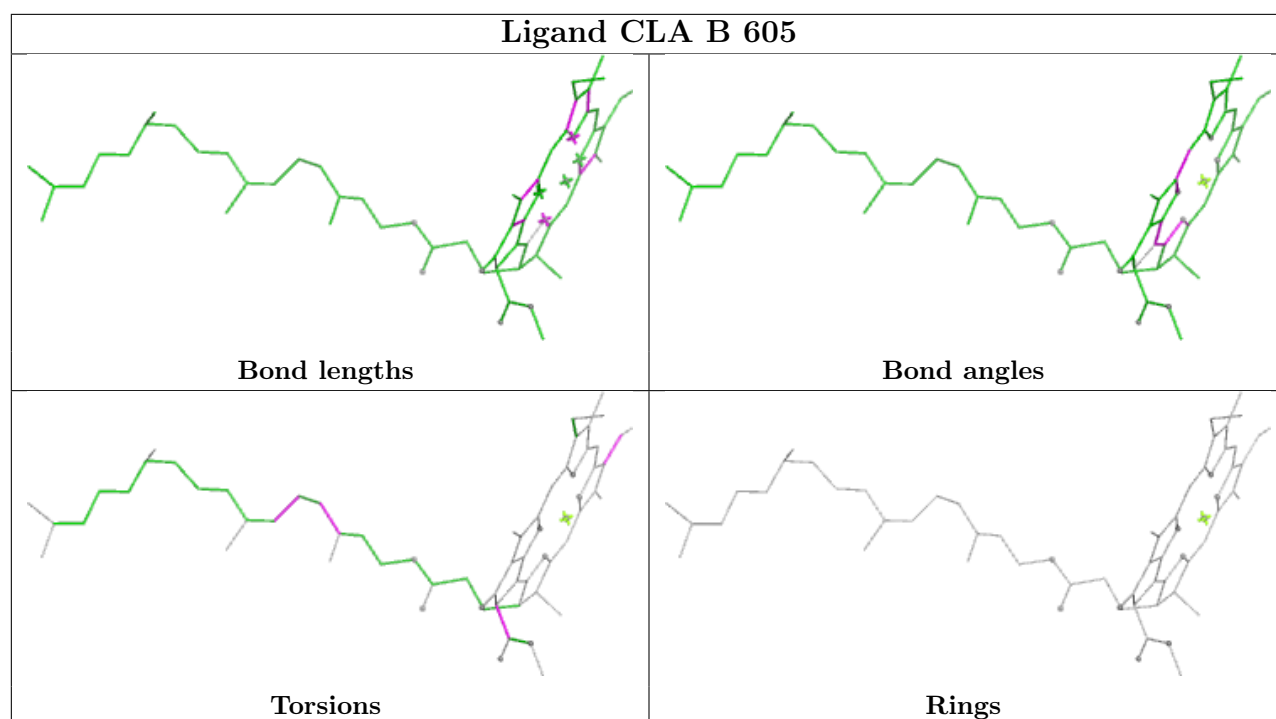
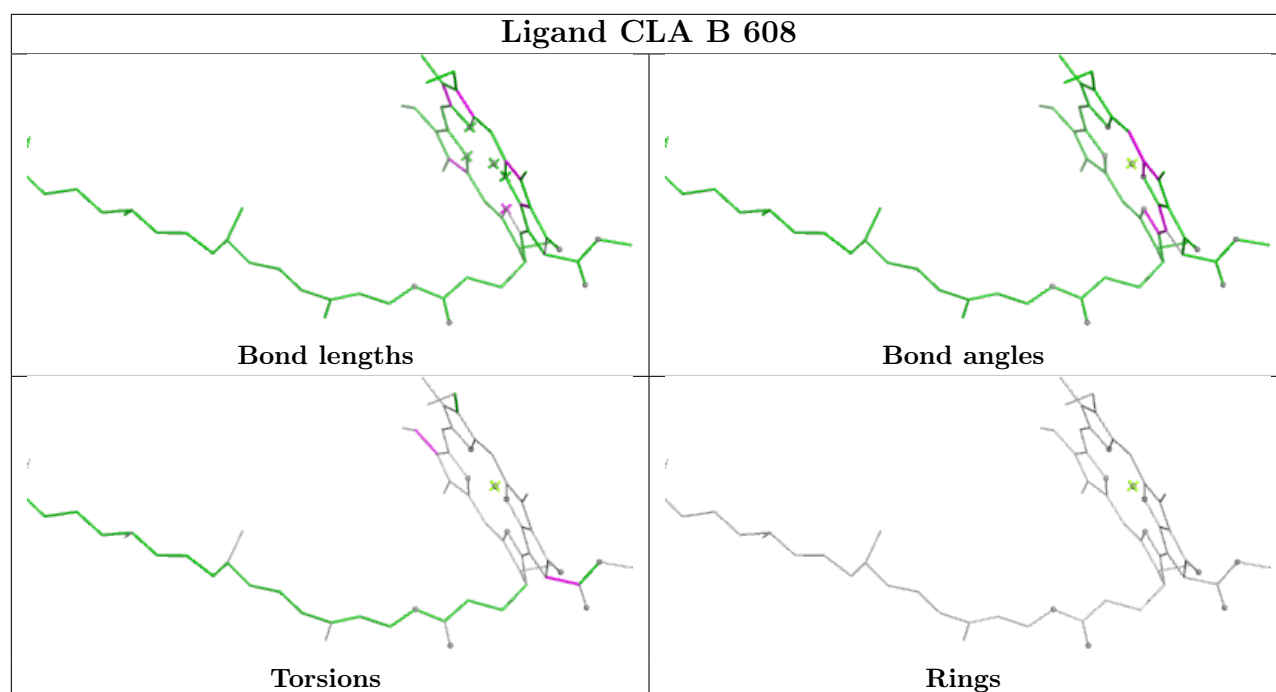


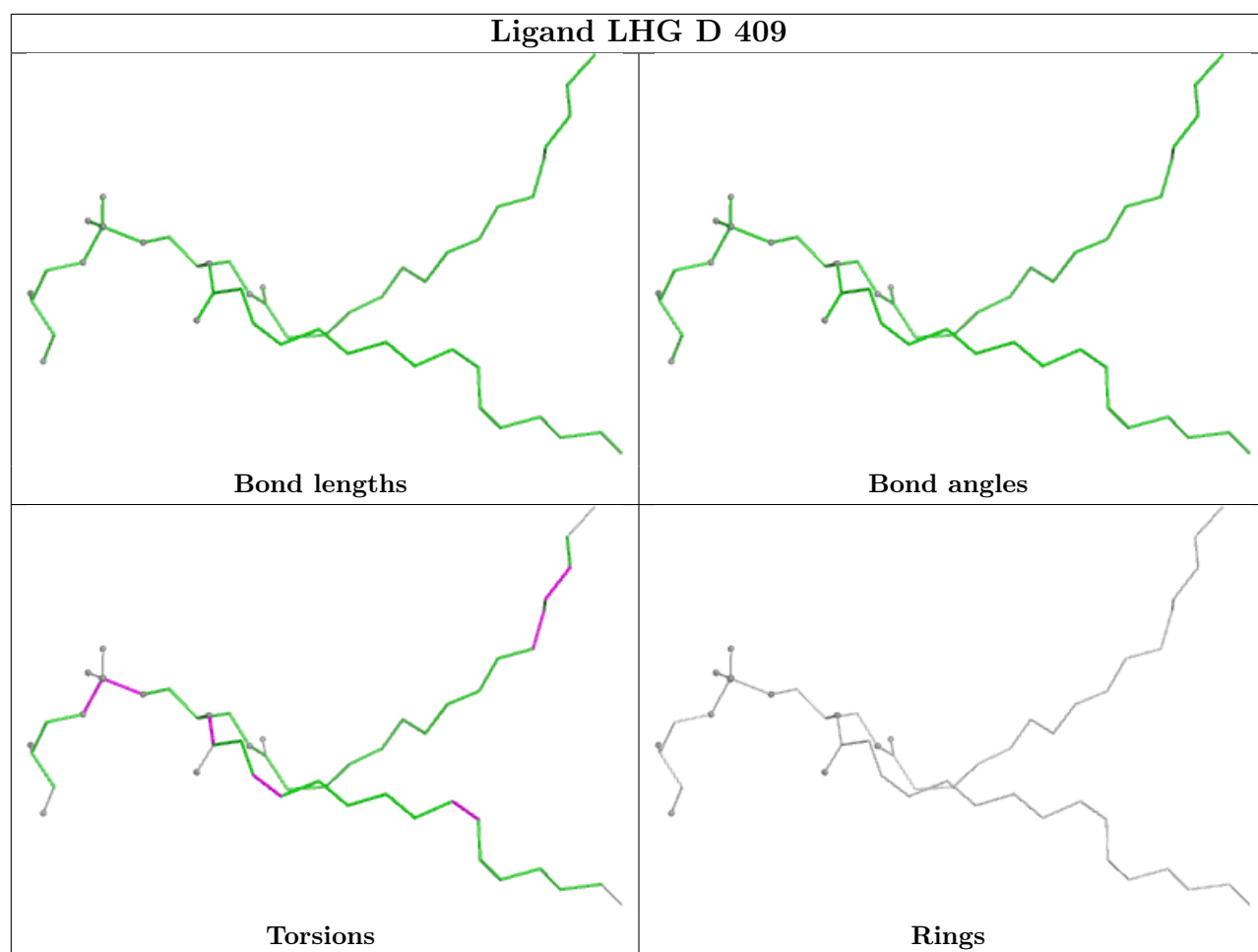




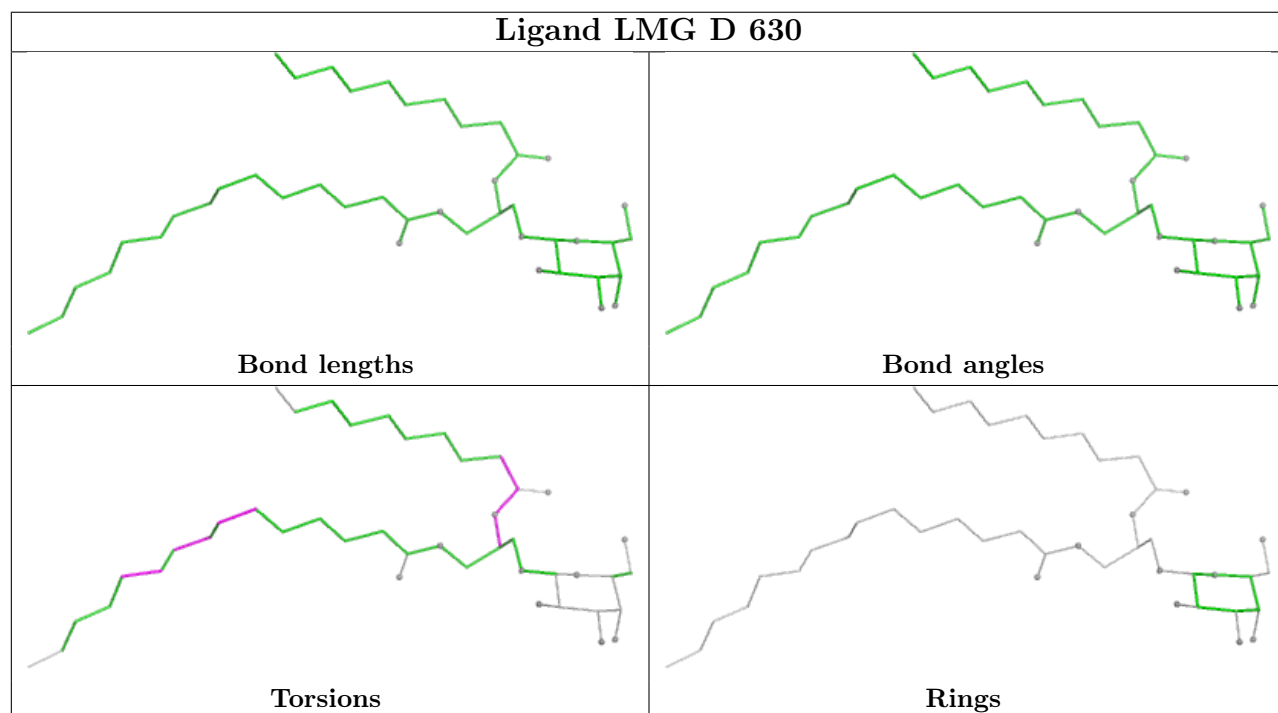
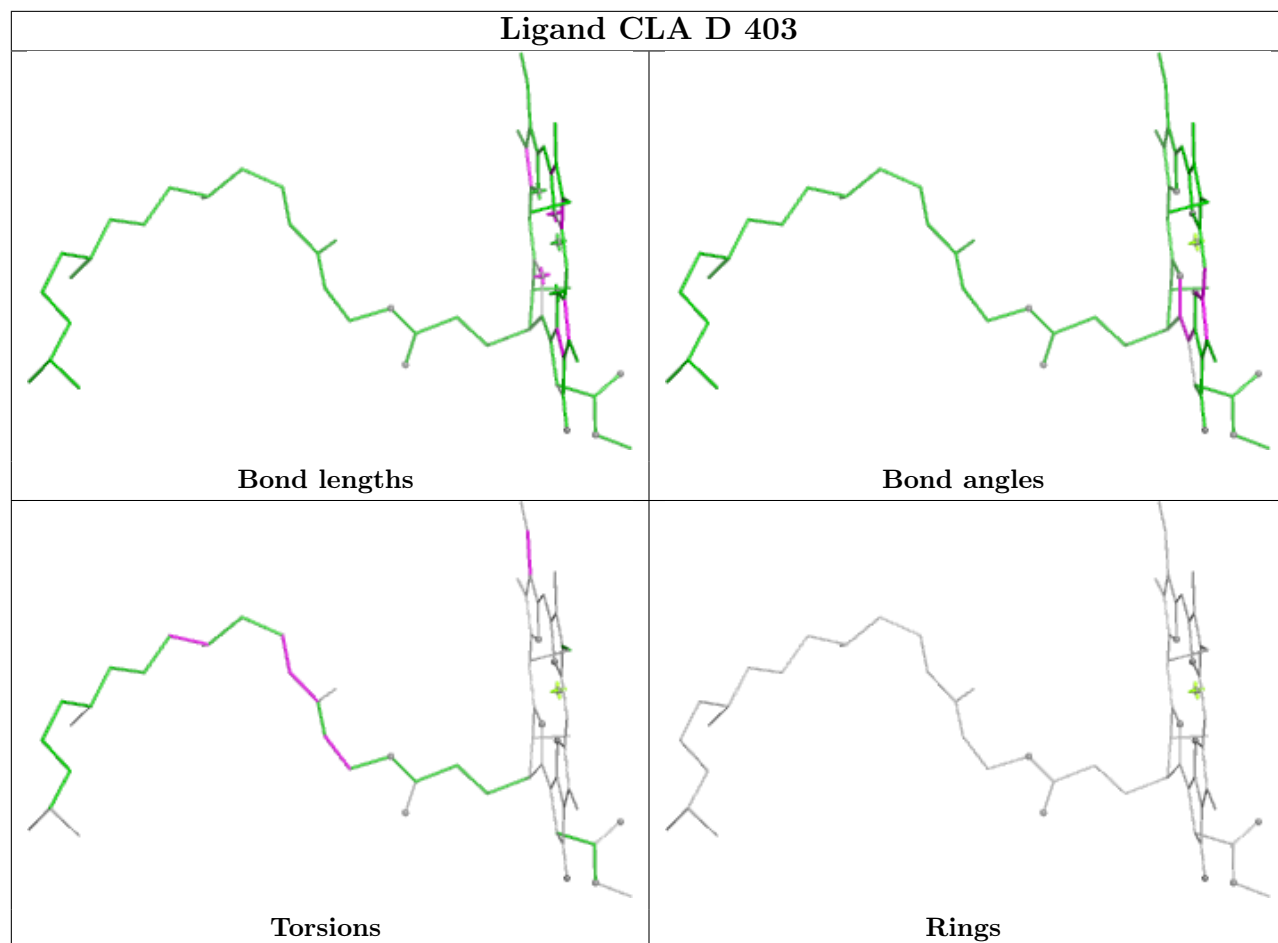


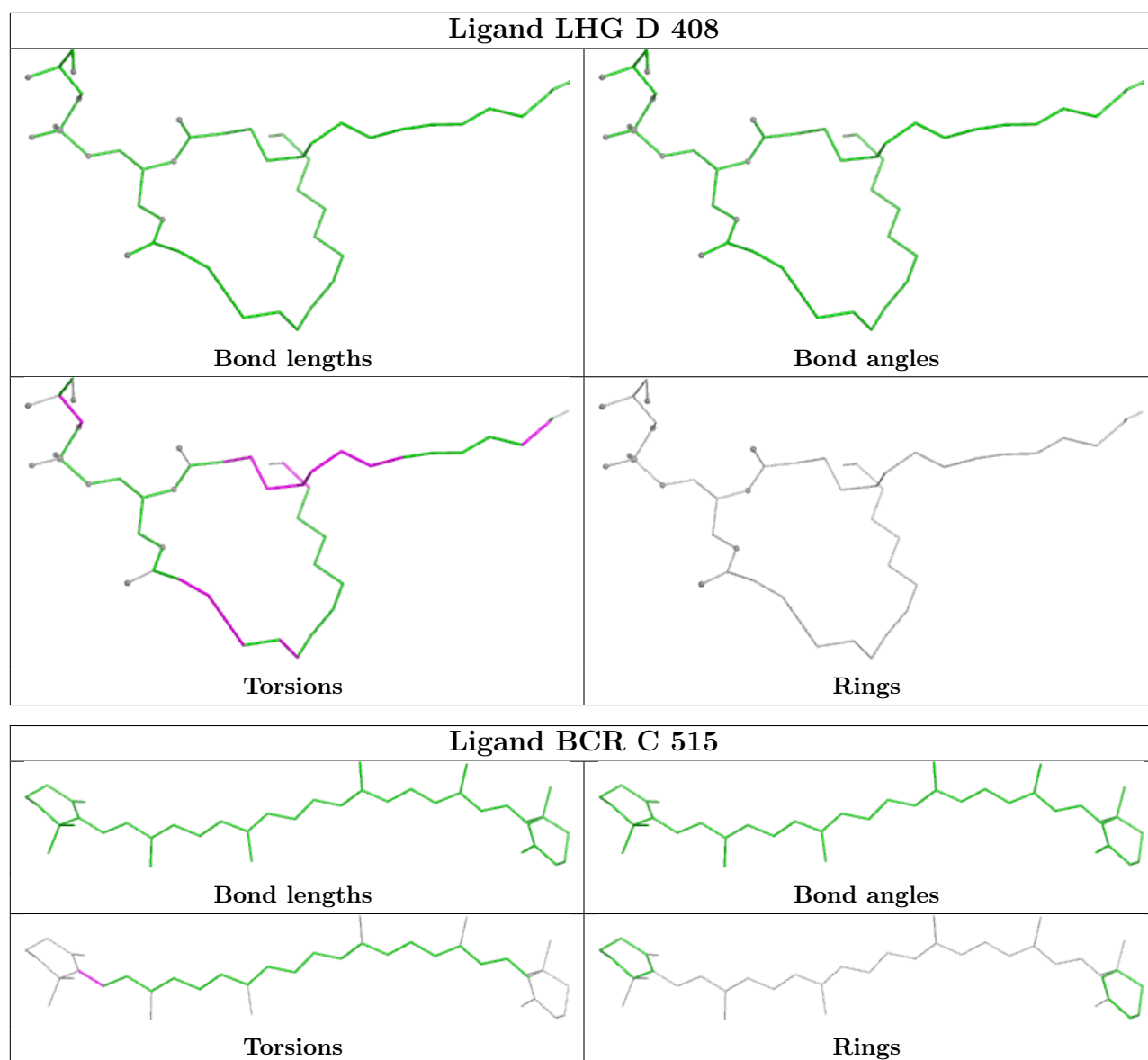


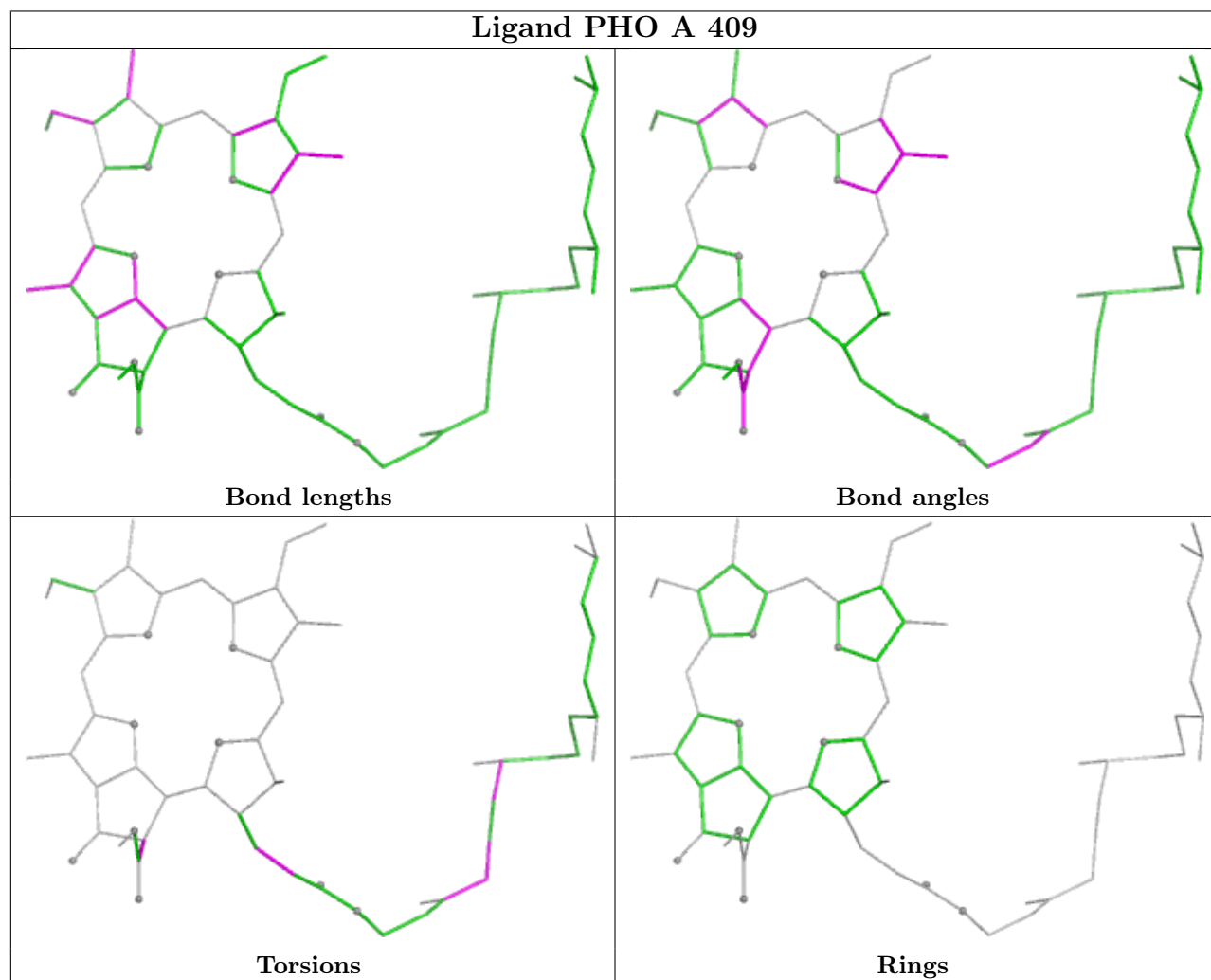
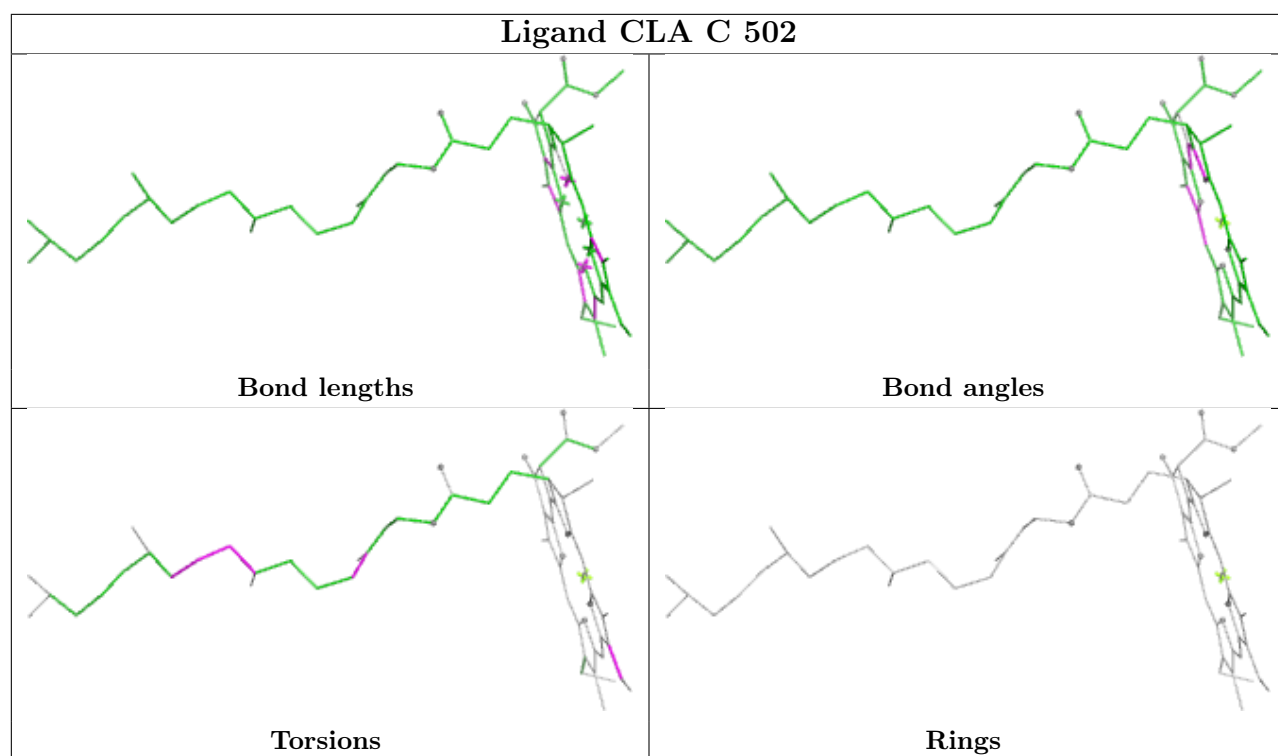


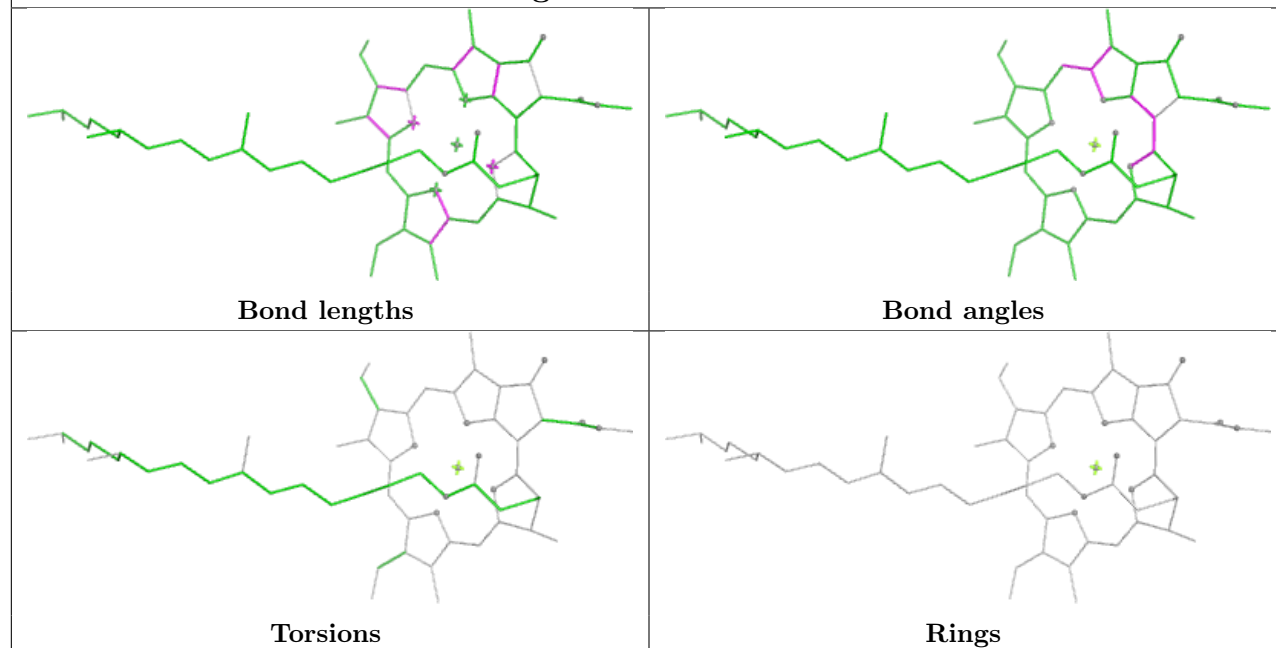
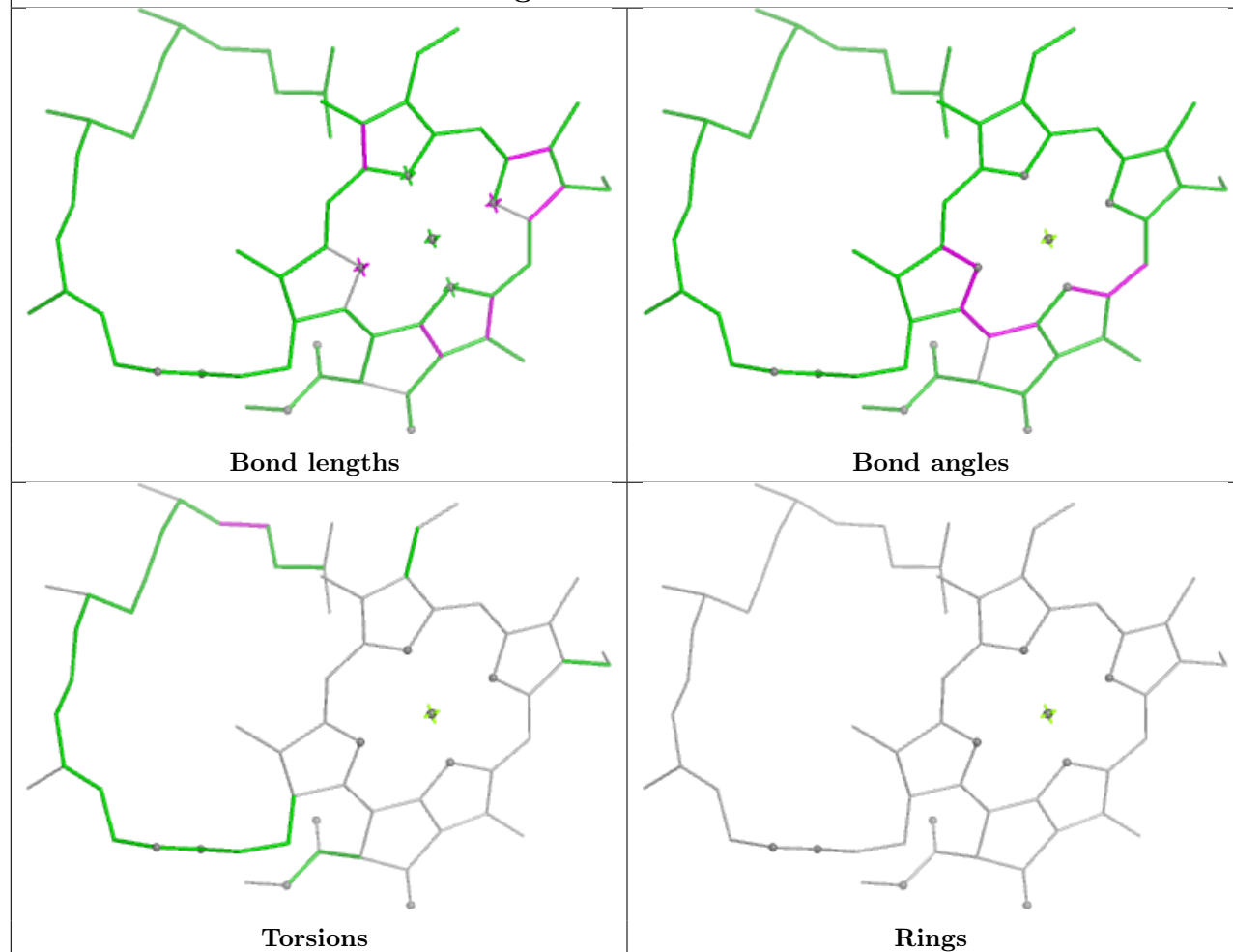


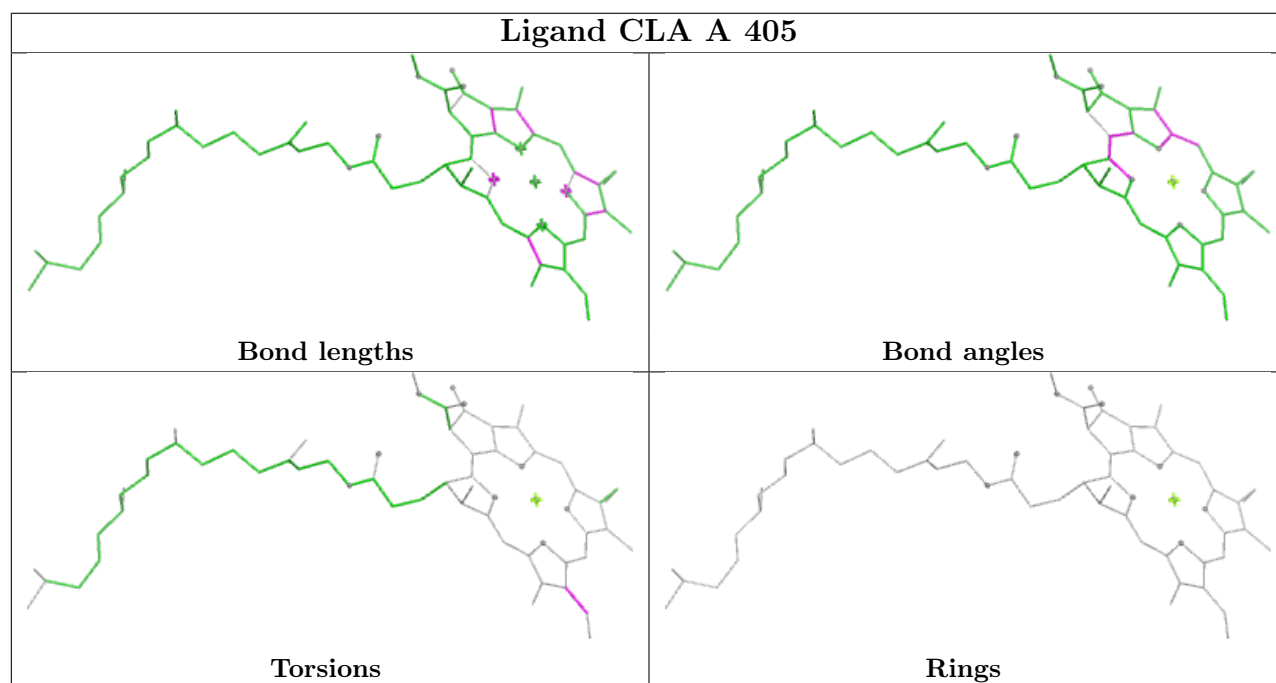
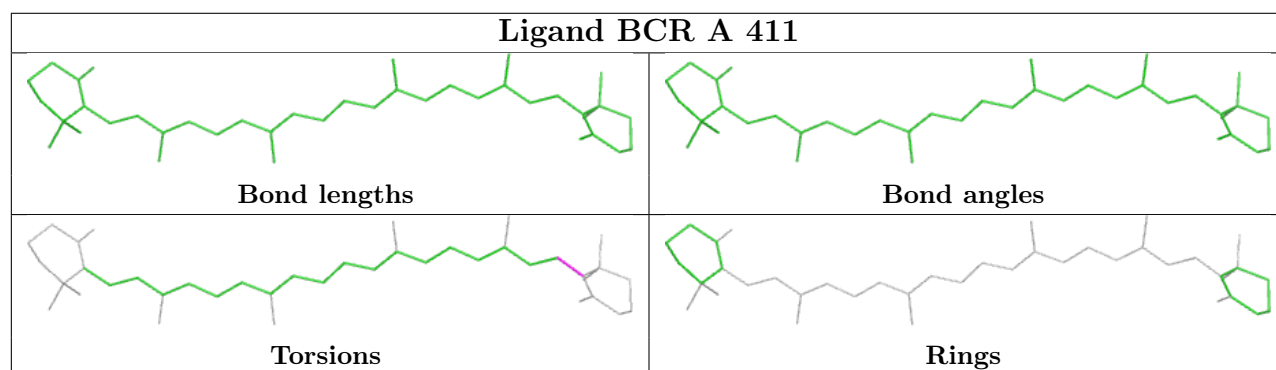
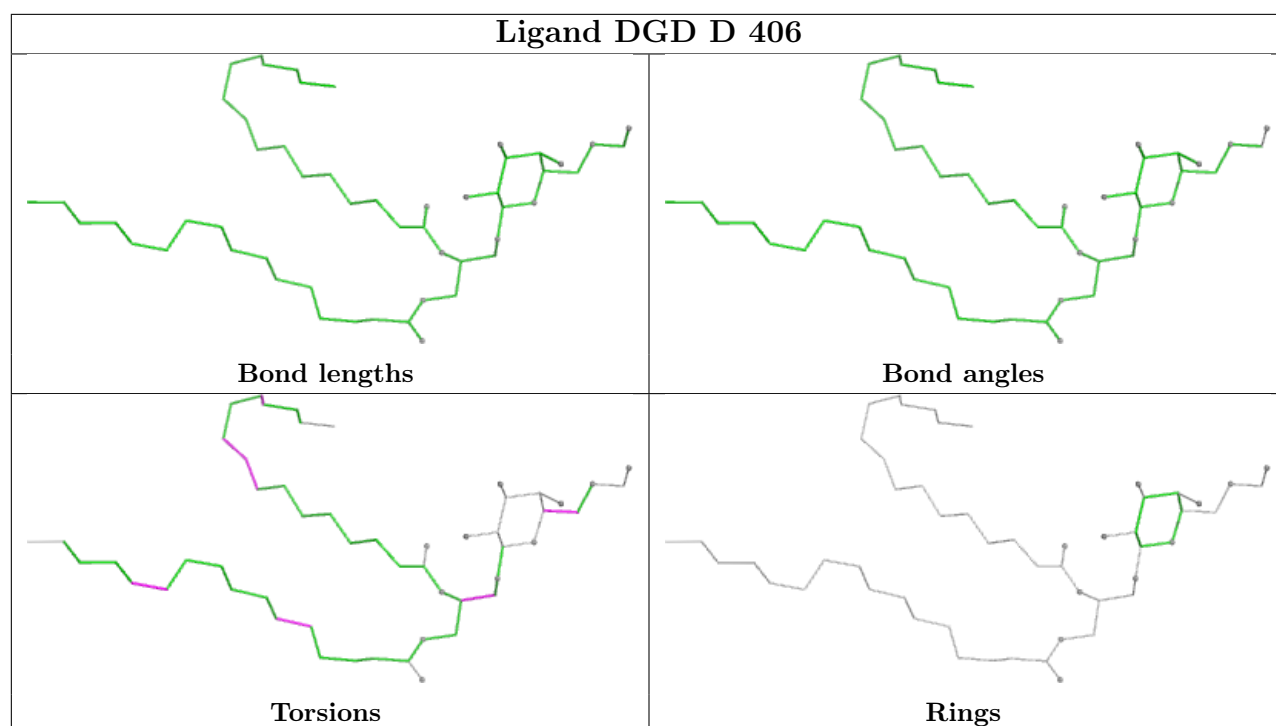


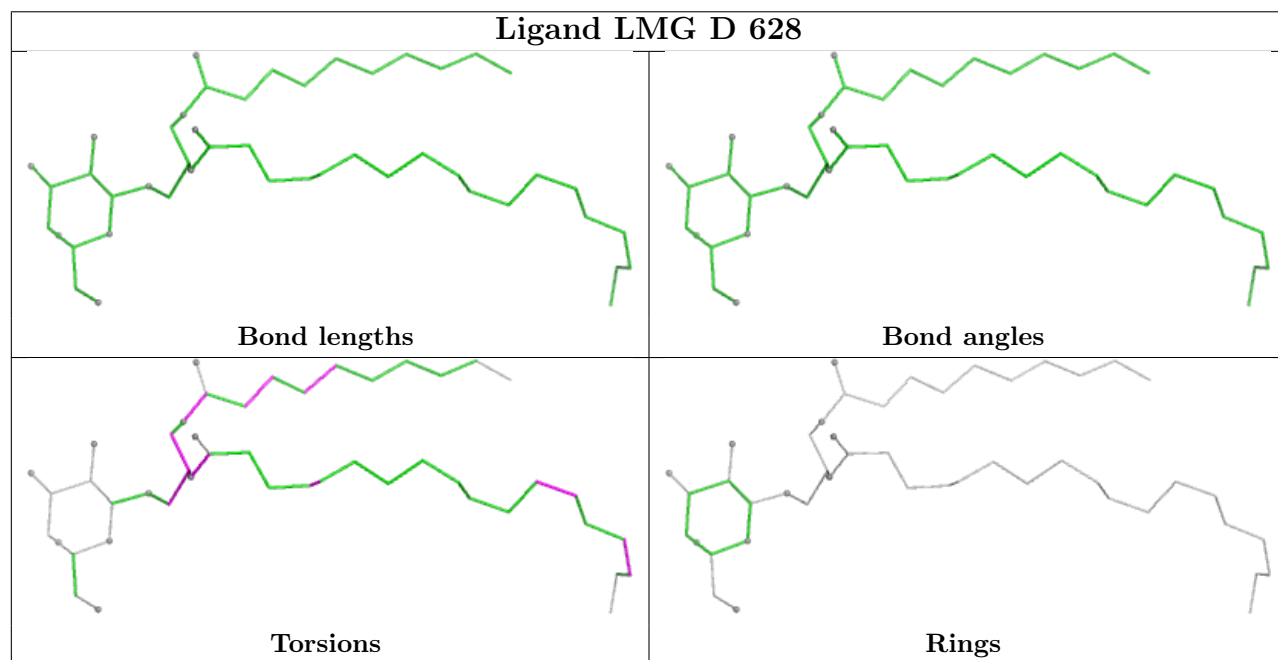
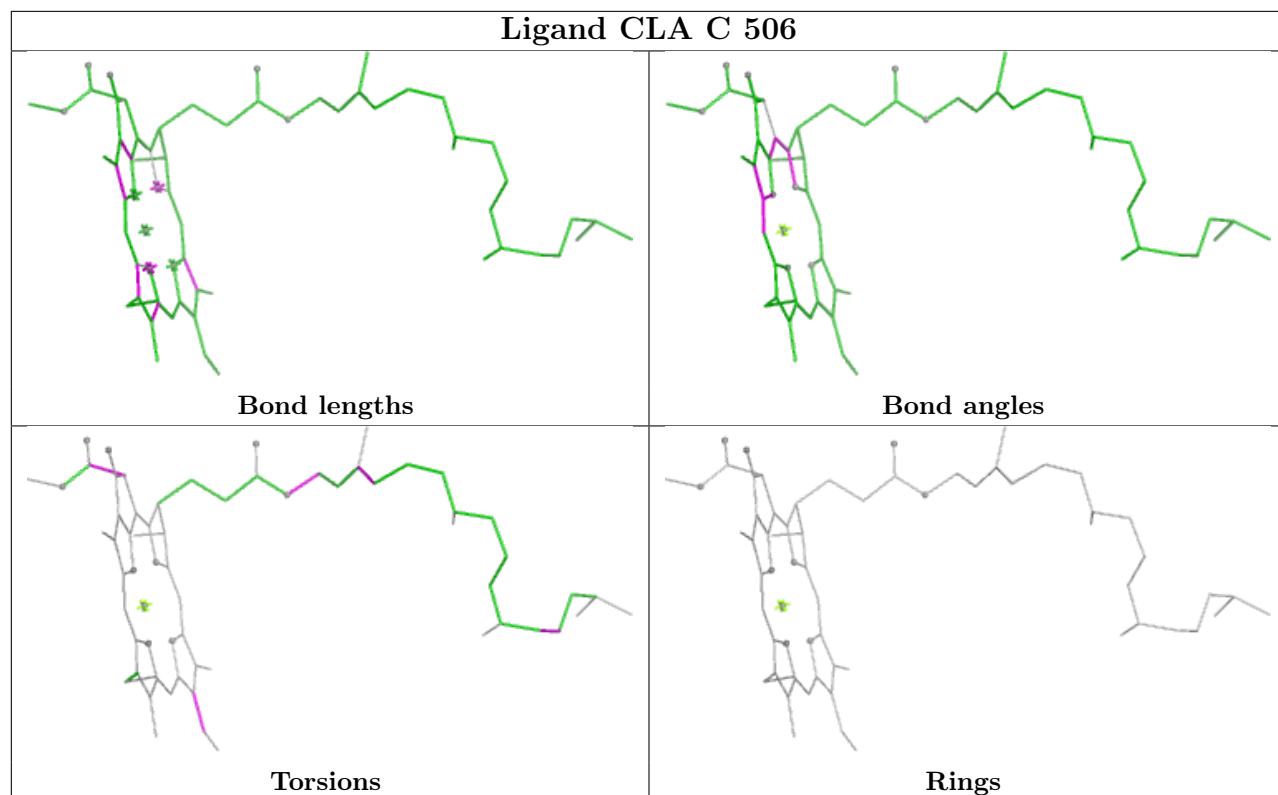


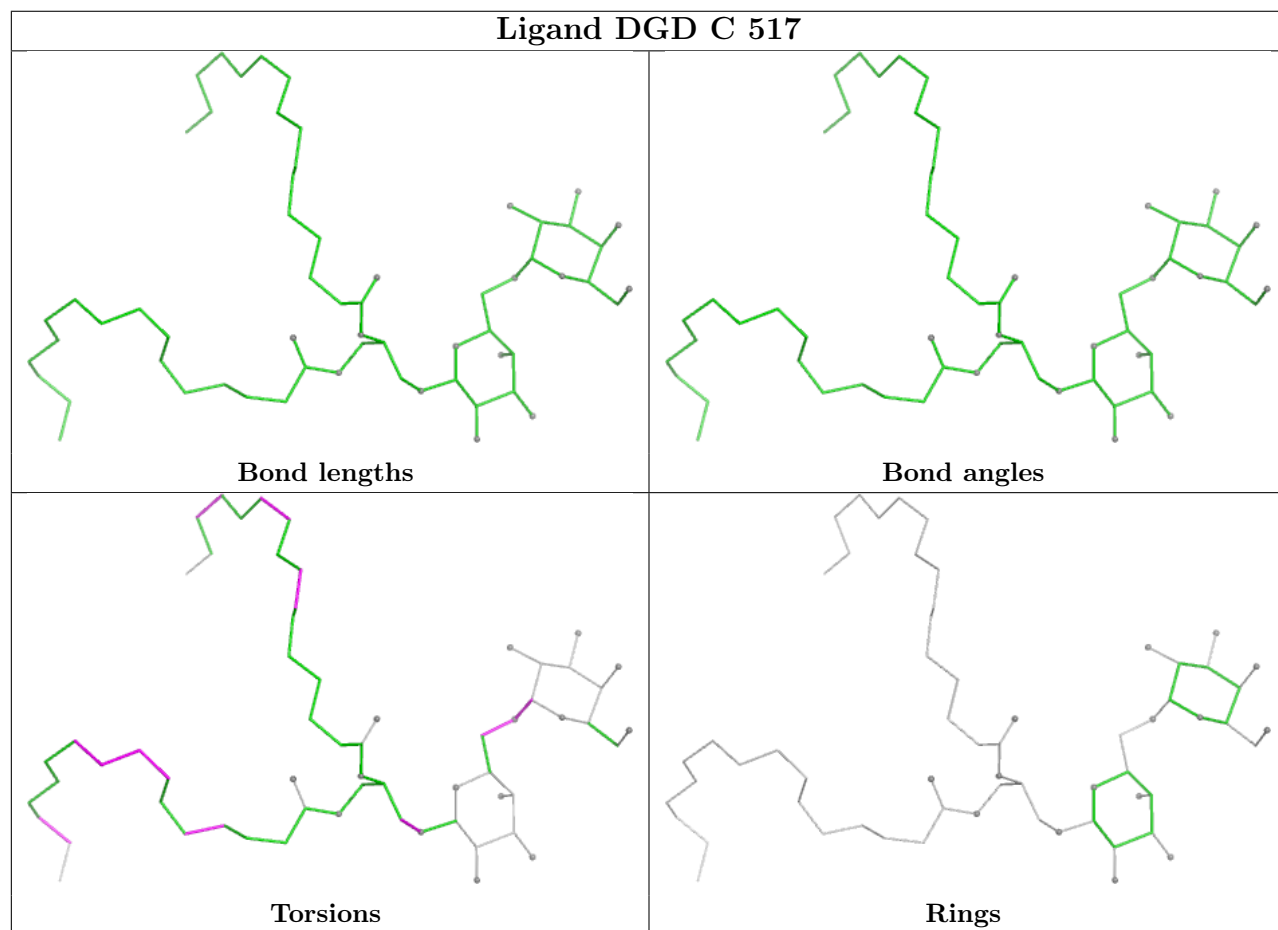
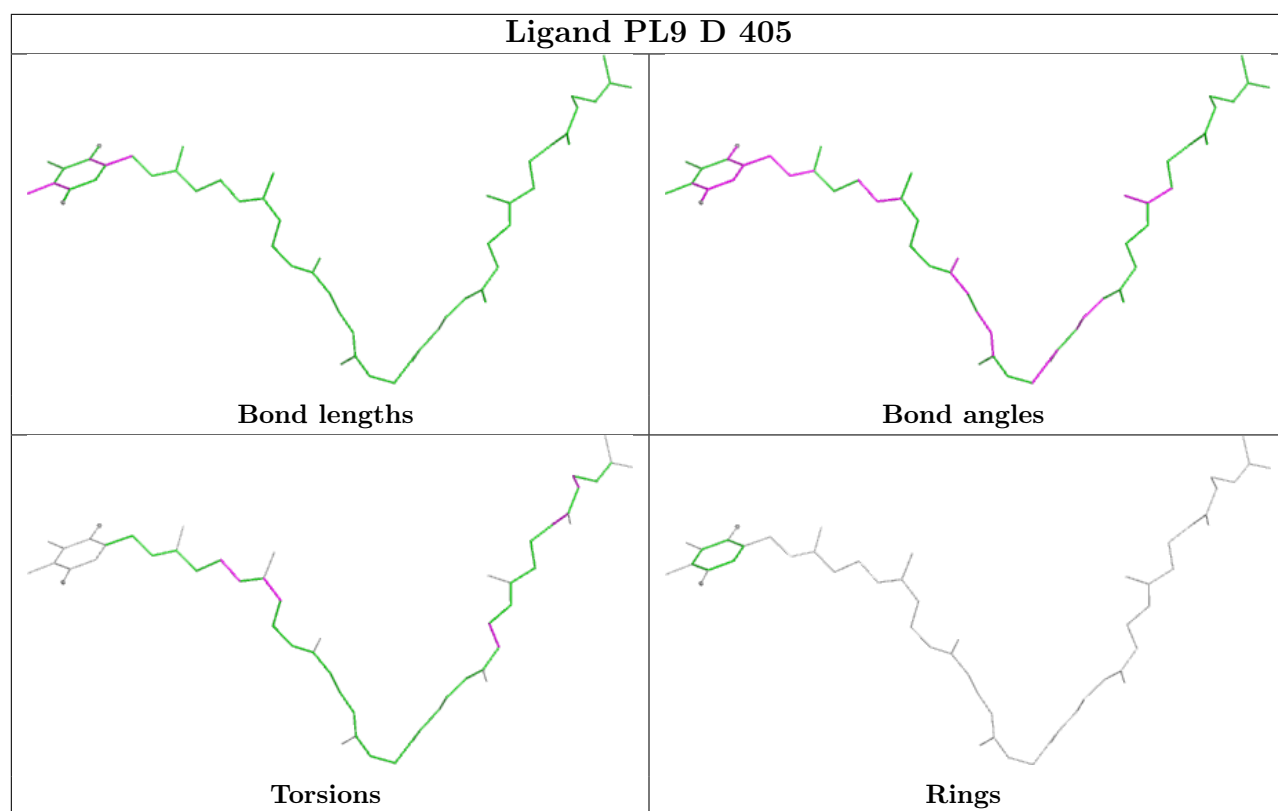


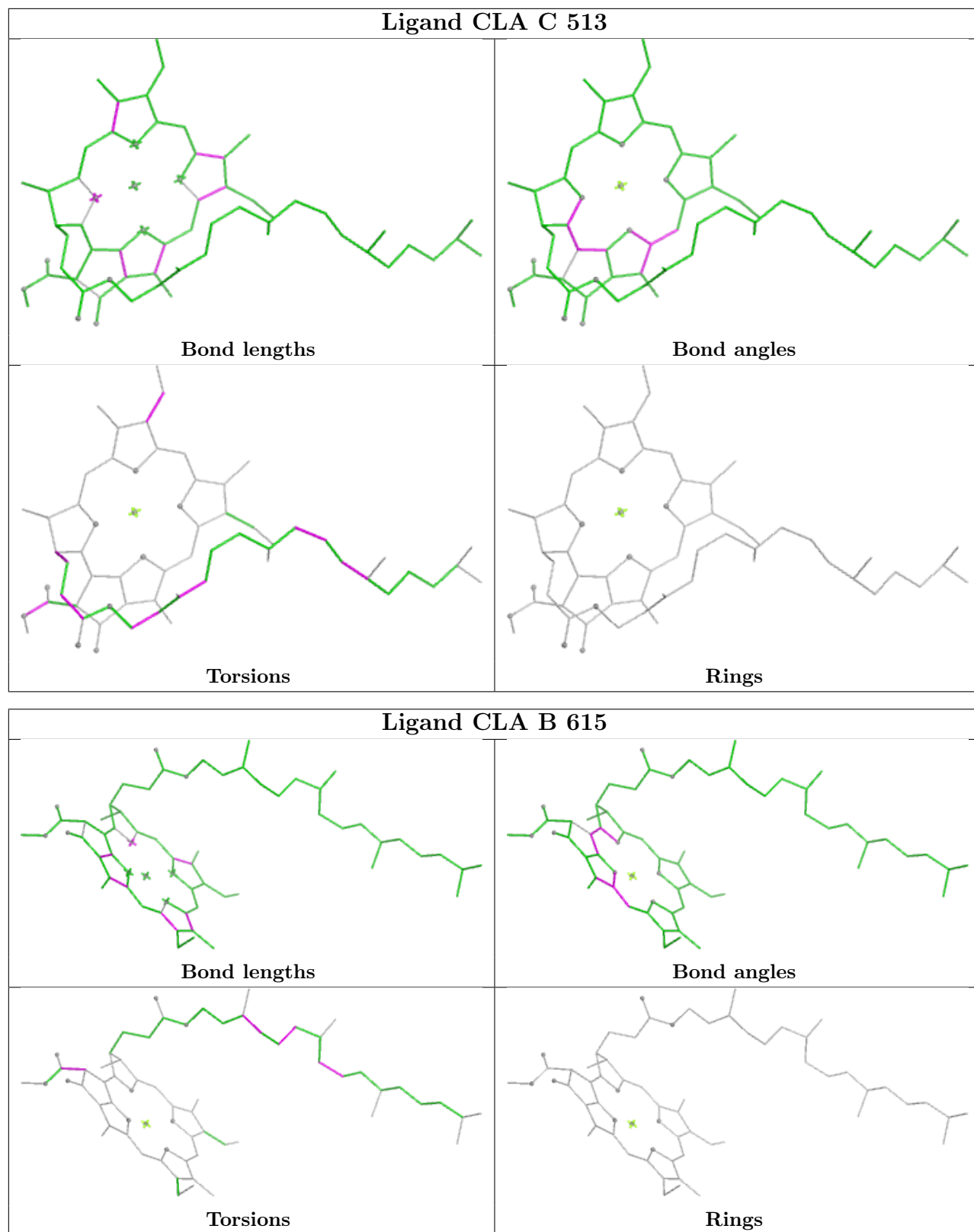


**Ligand CLA B 609****Ligand CLA B 616**

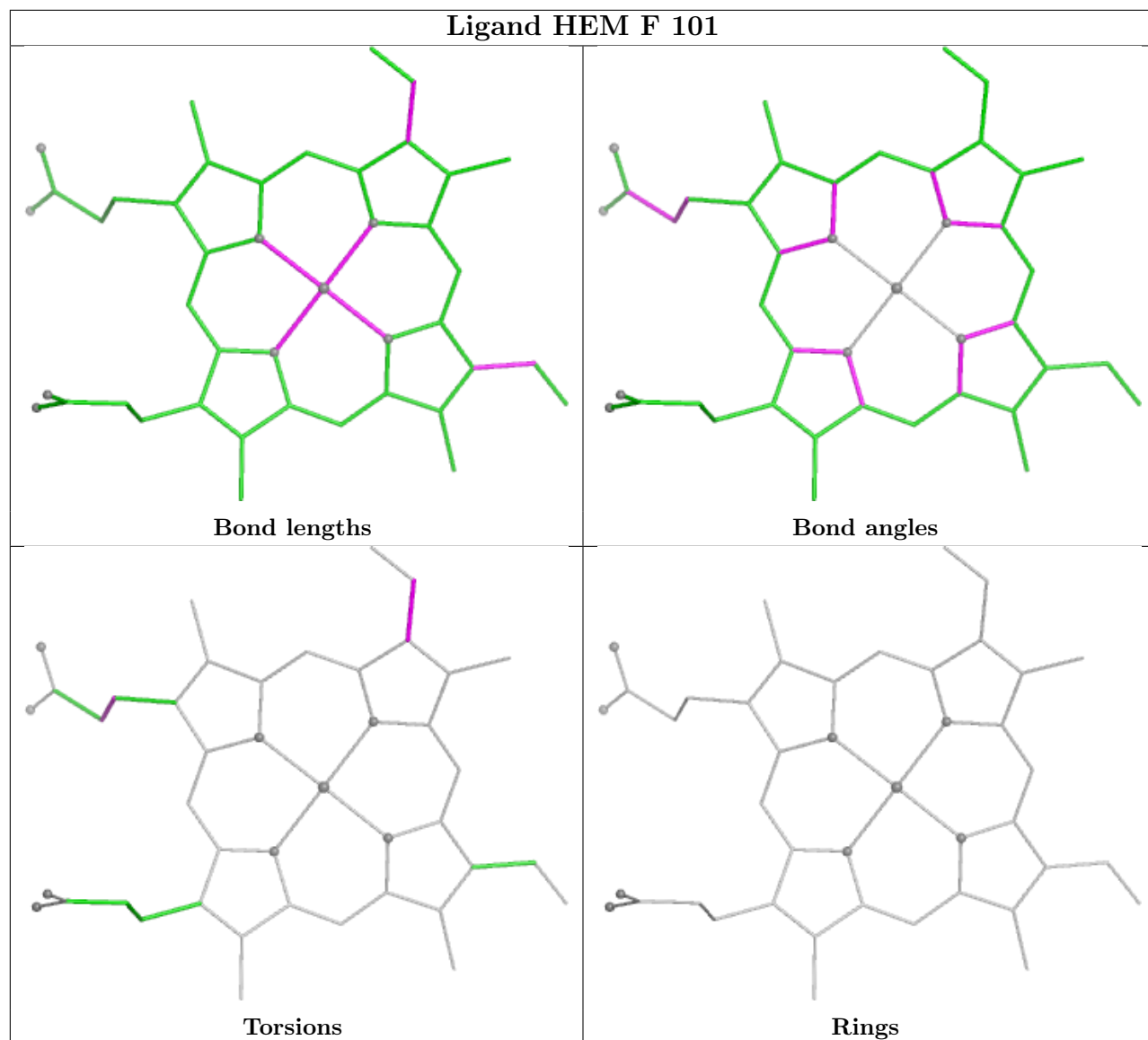


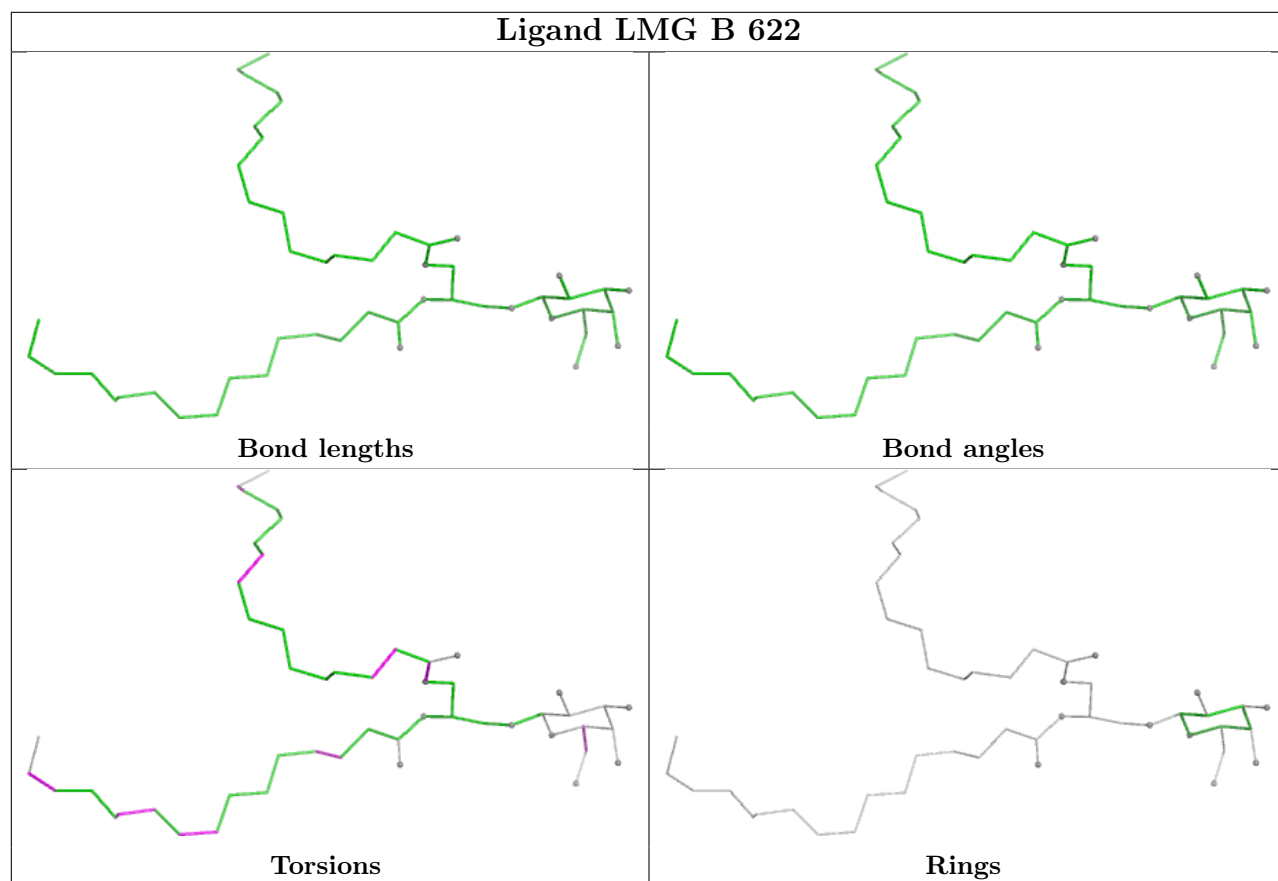
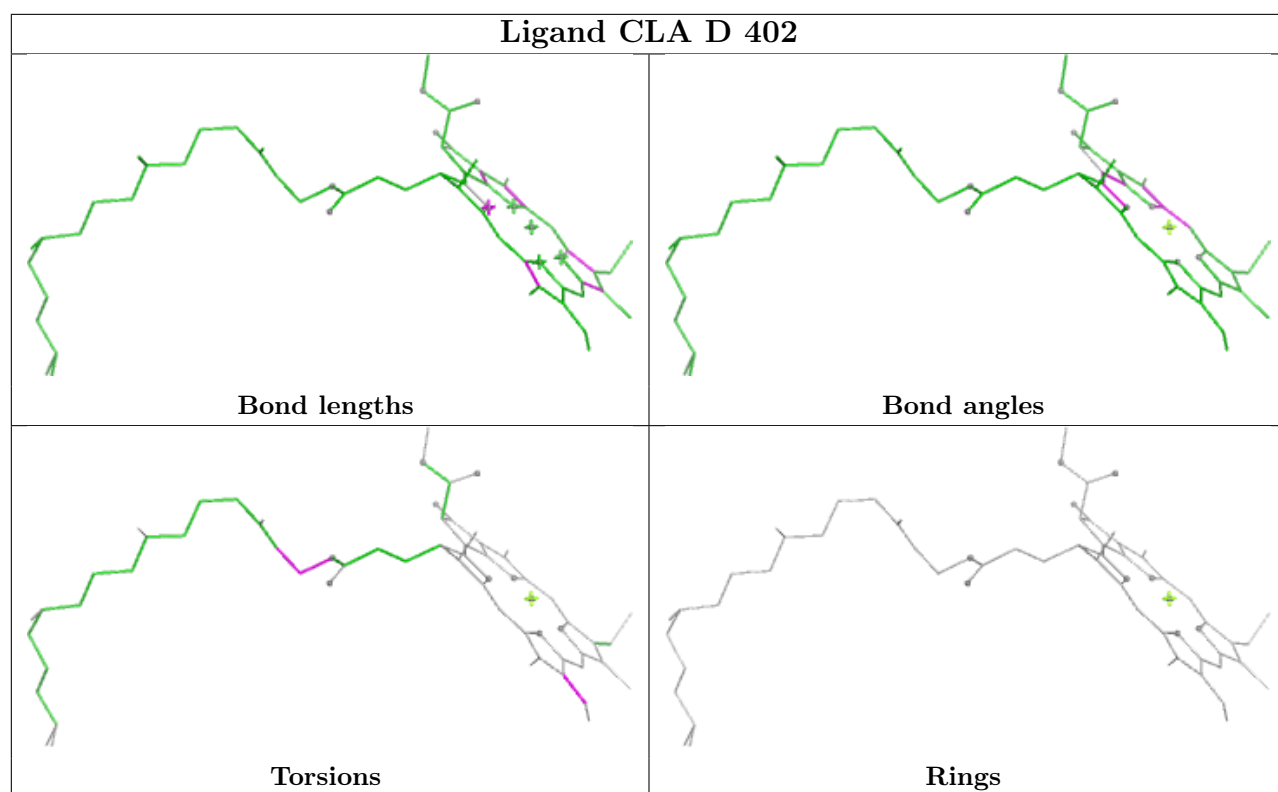


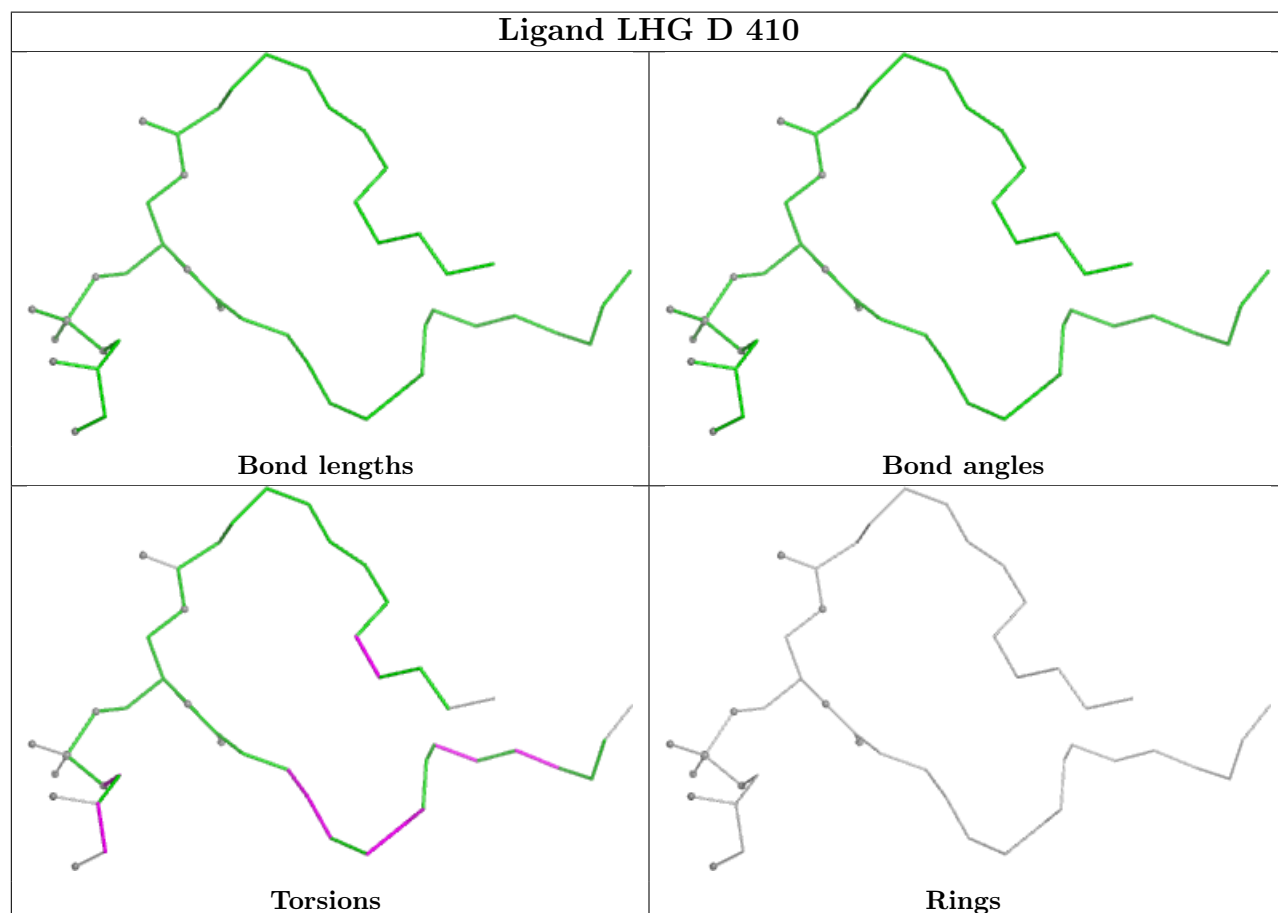
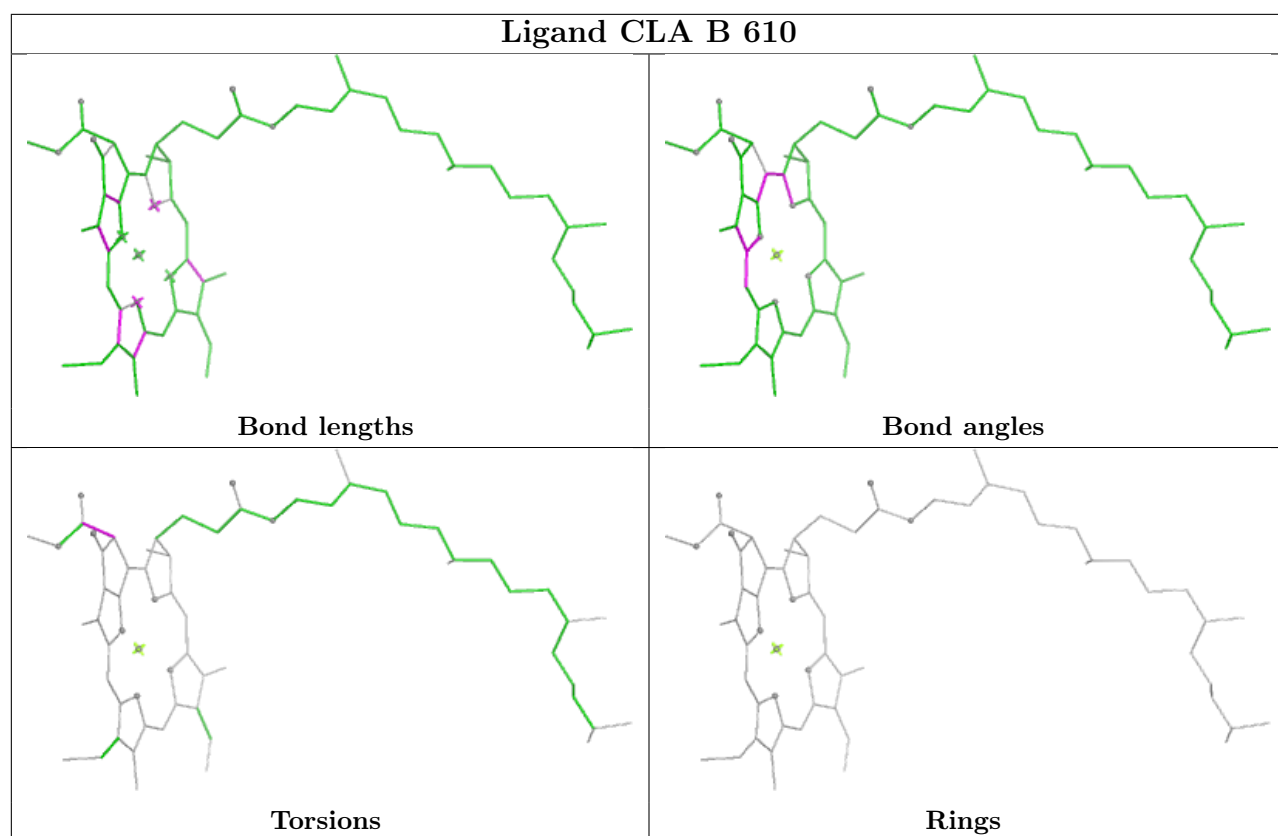


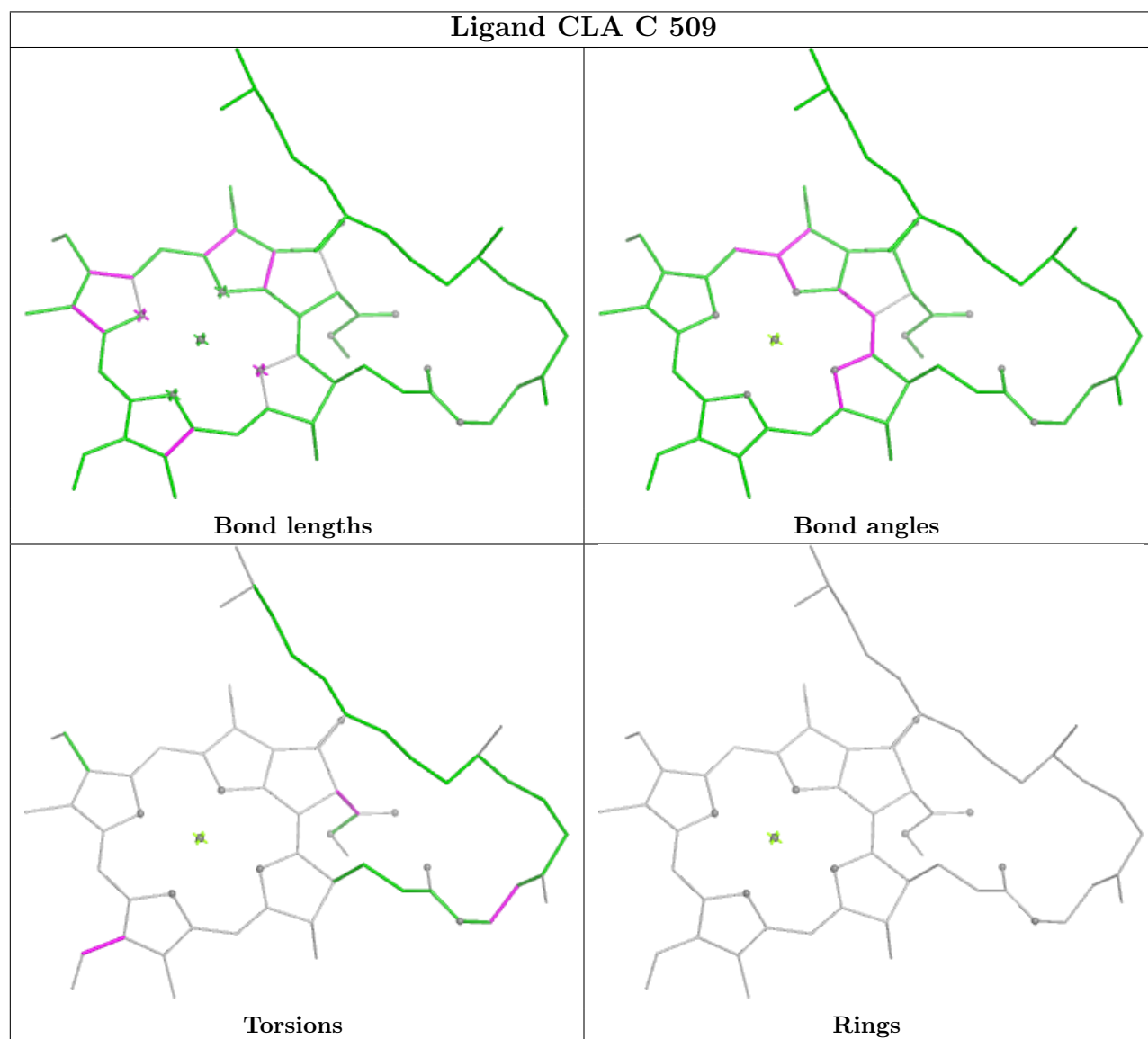
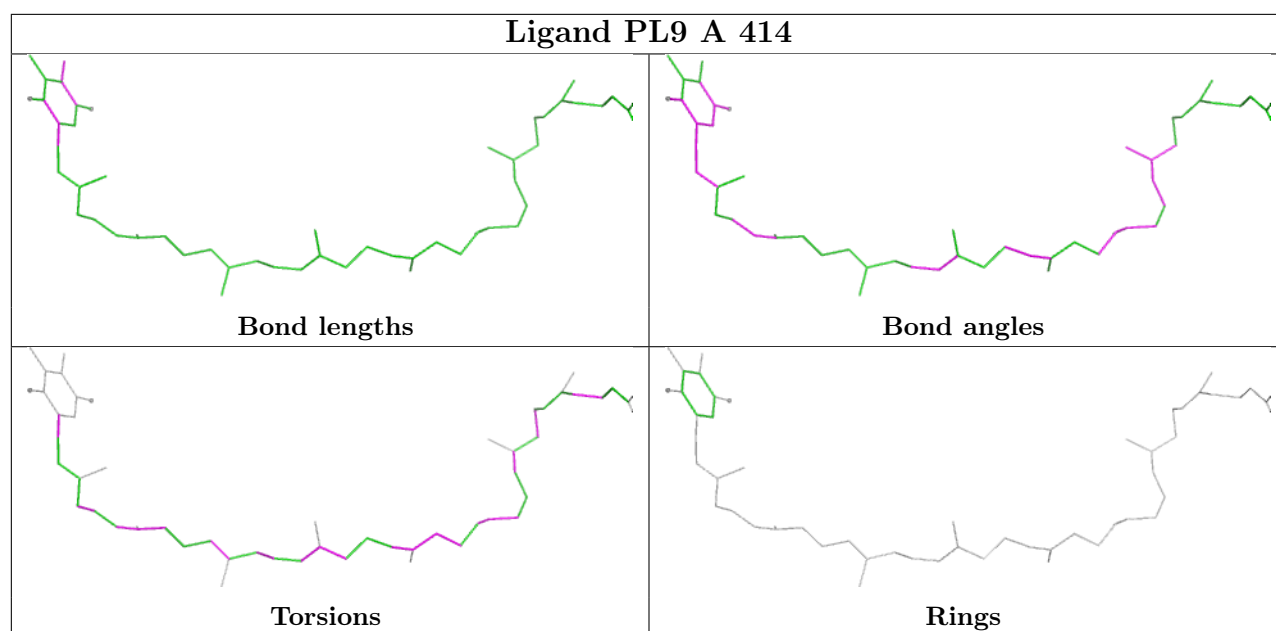


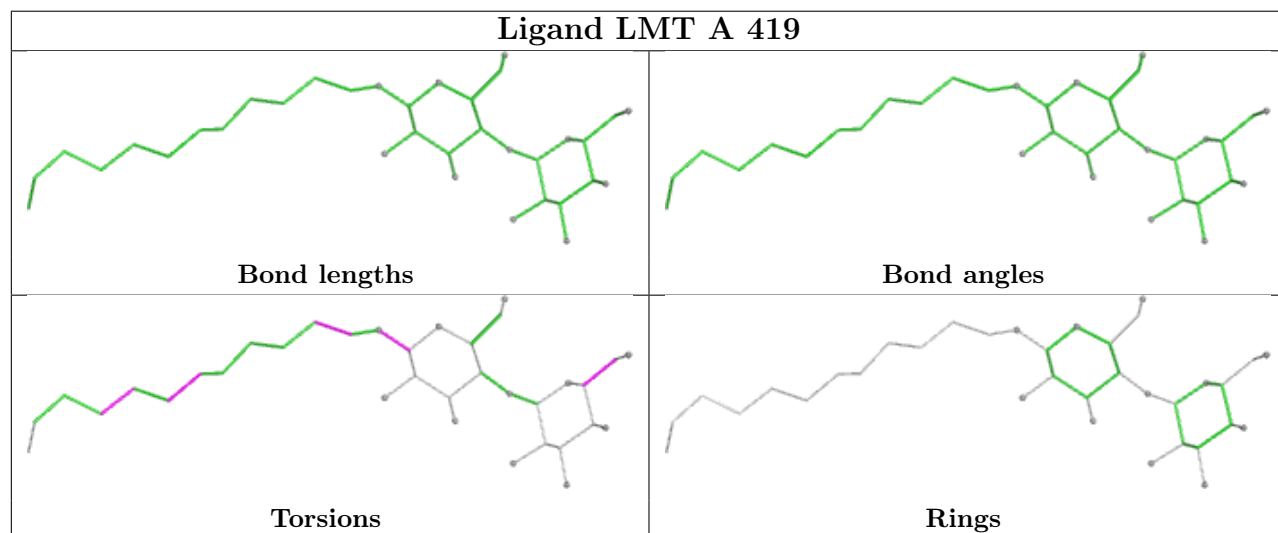
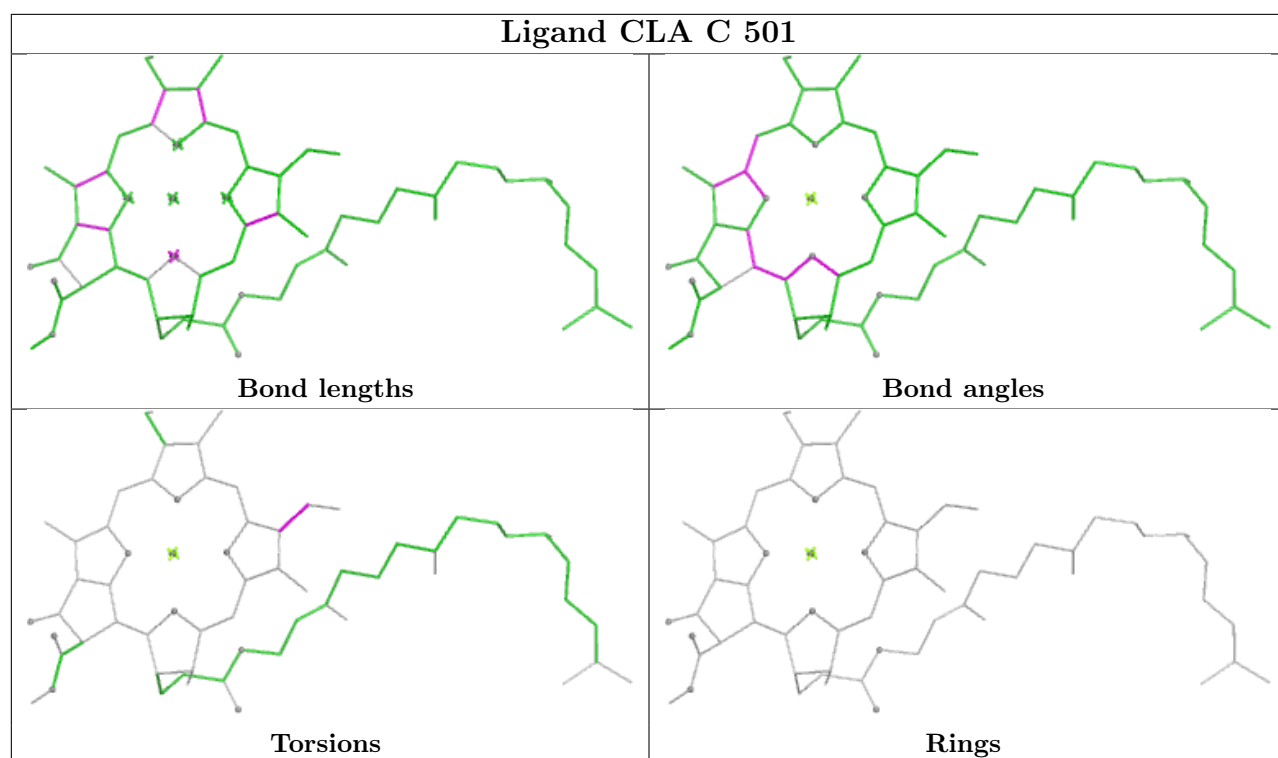


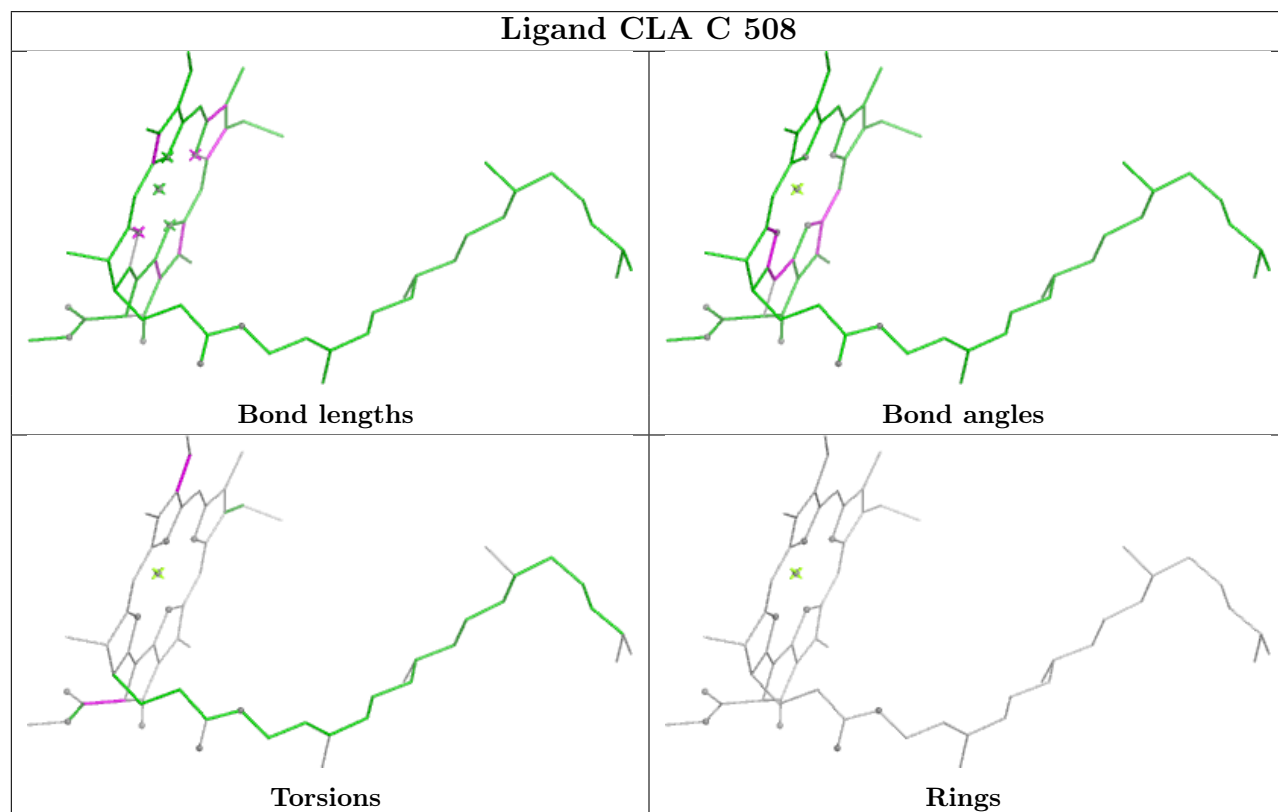
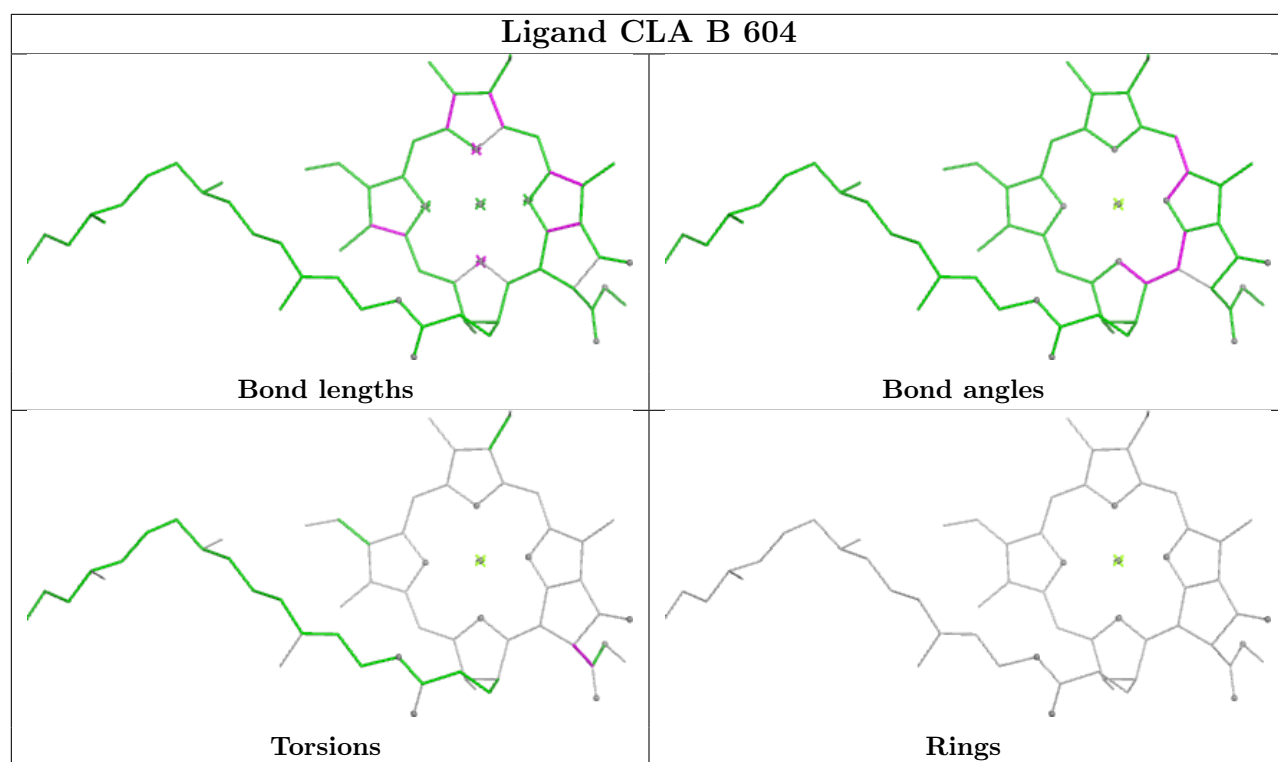


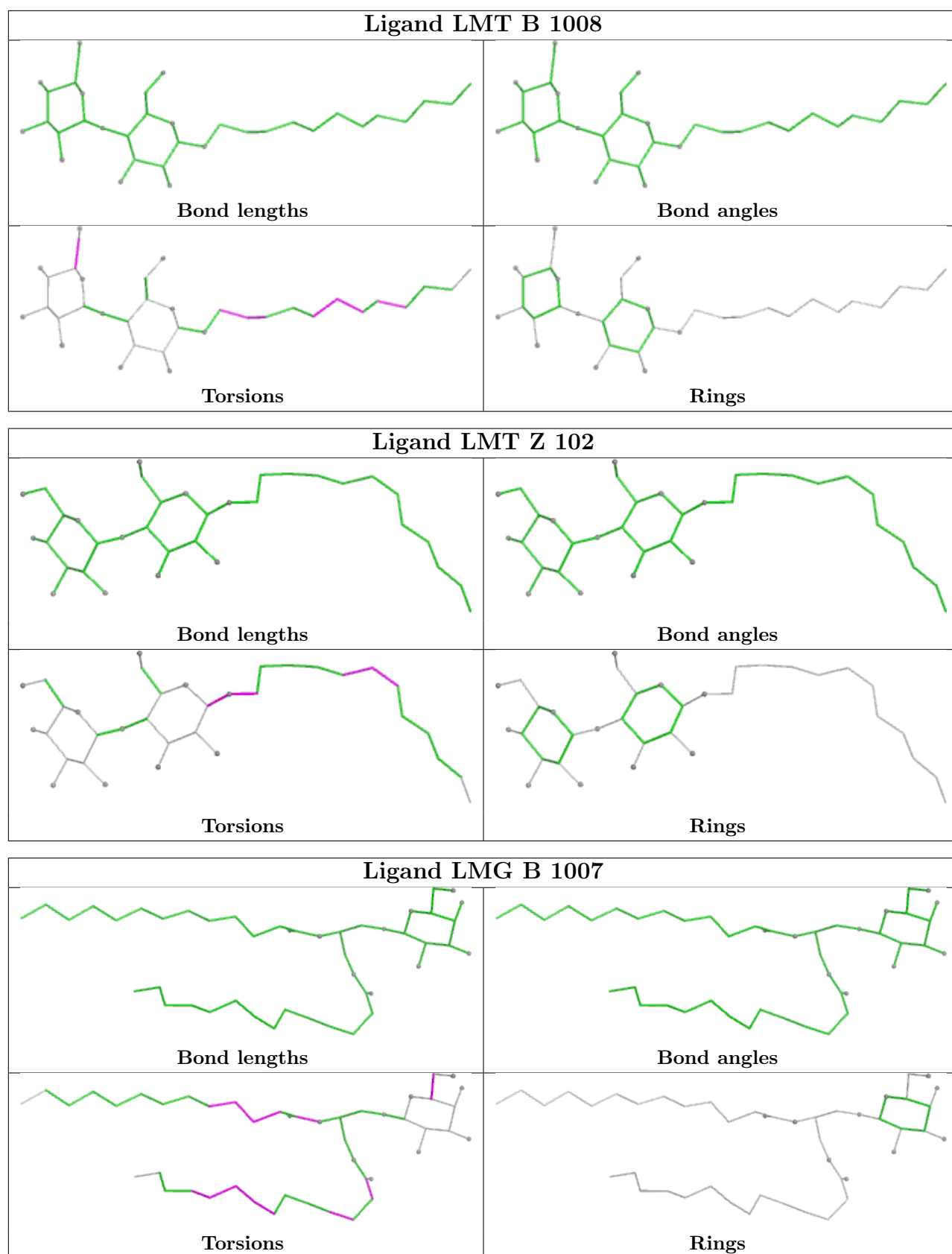


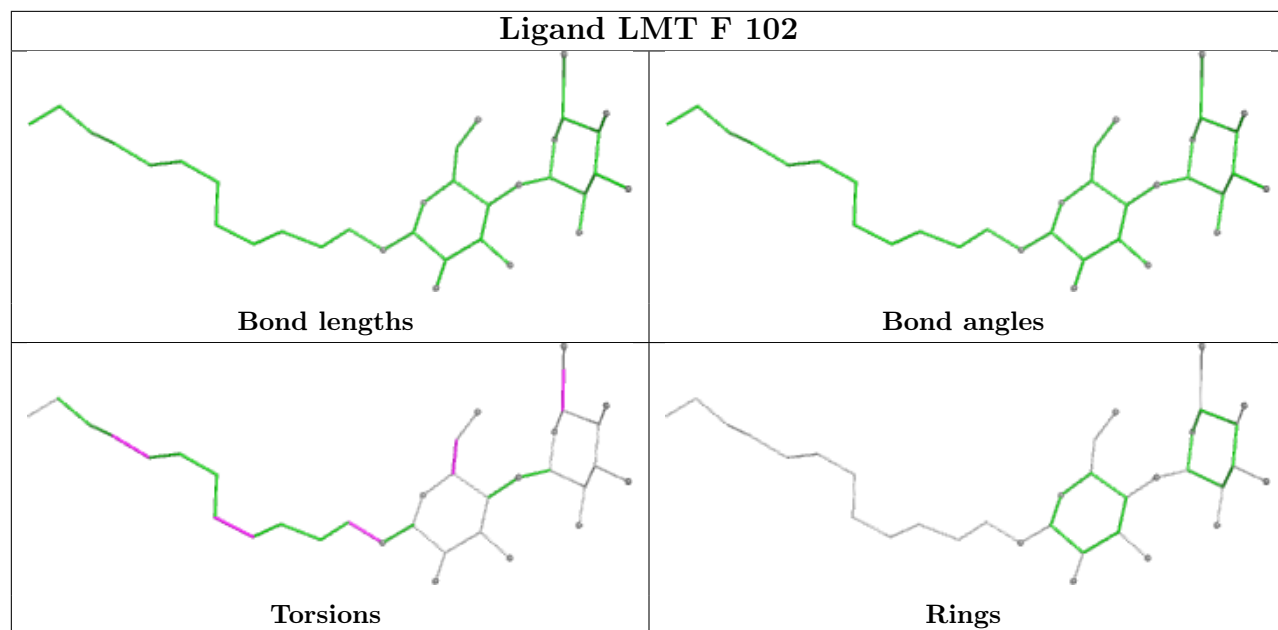




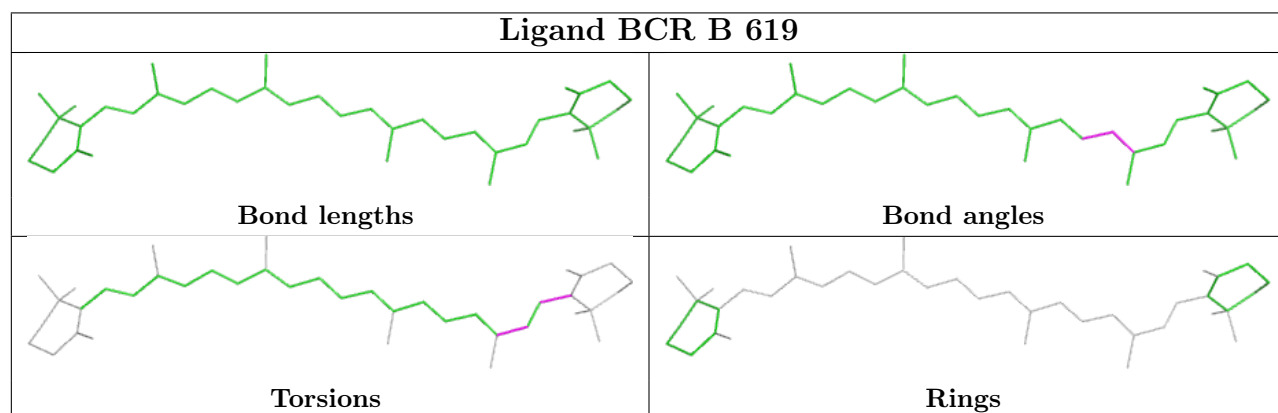
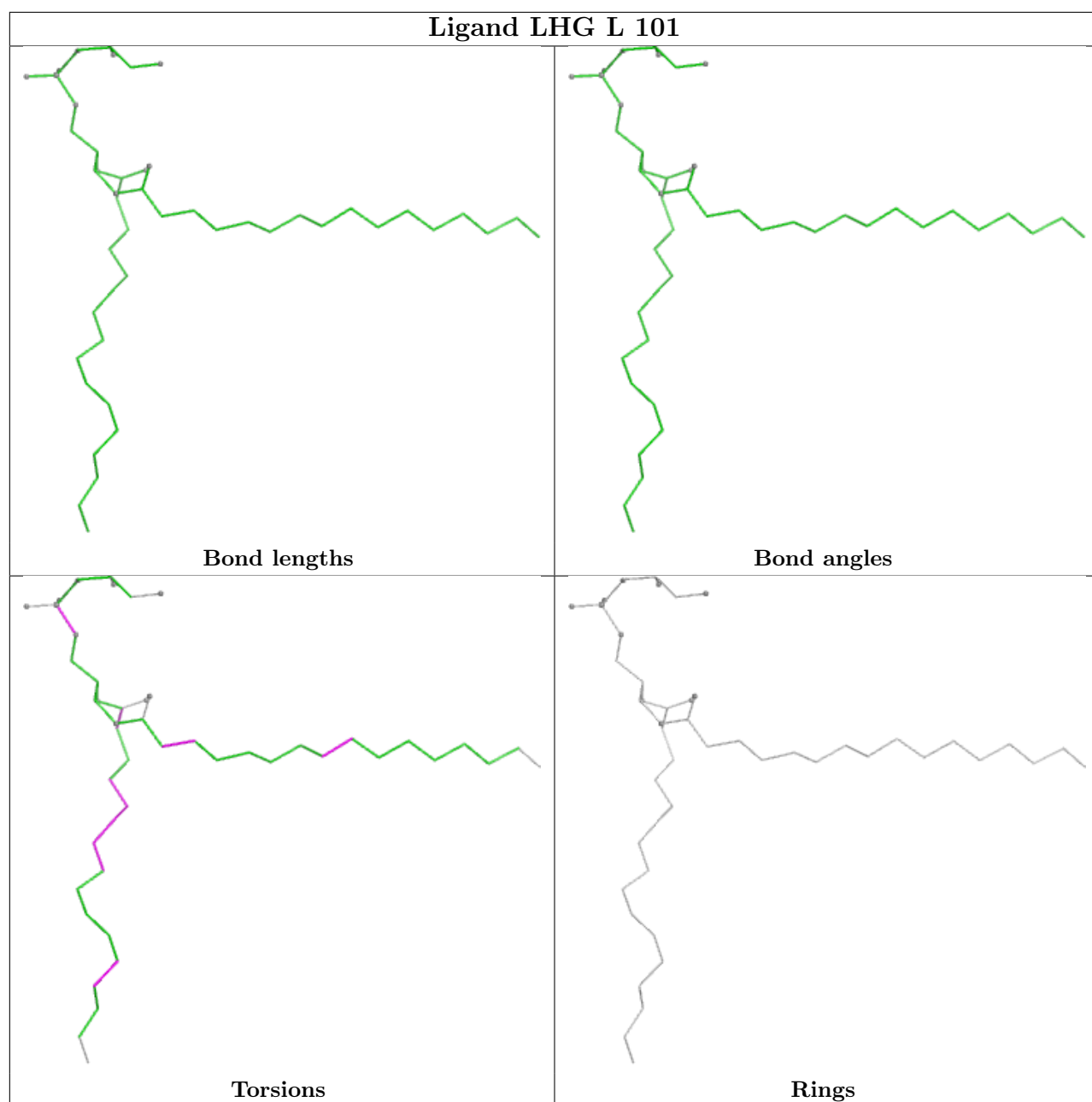


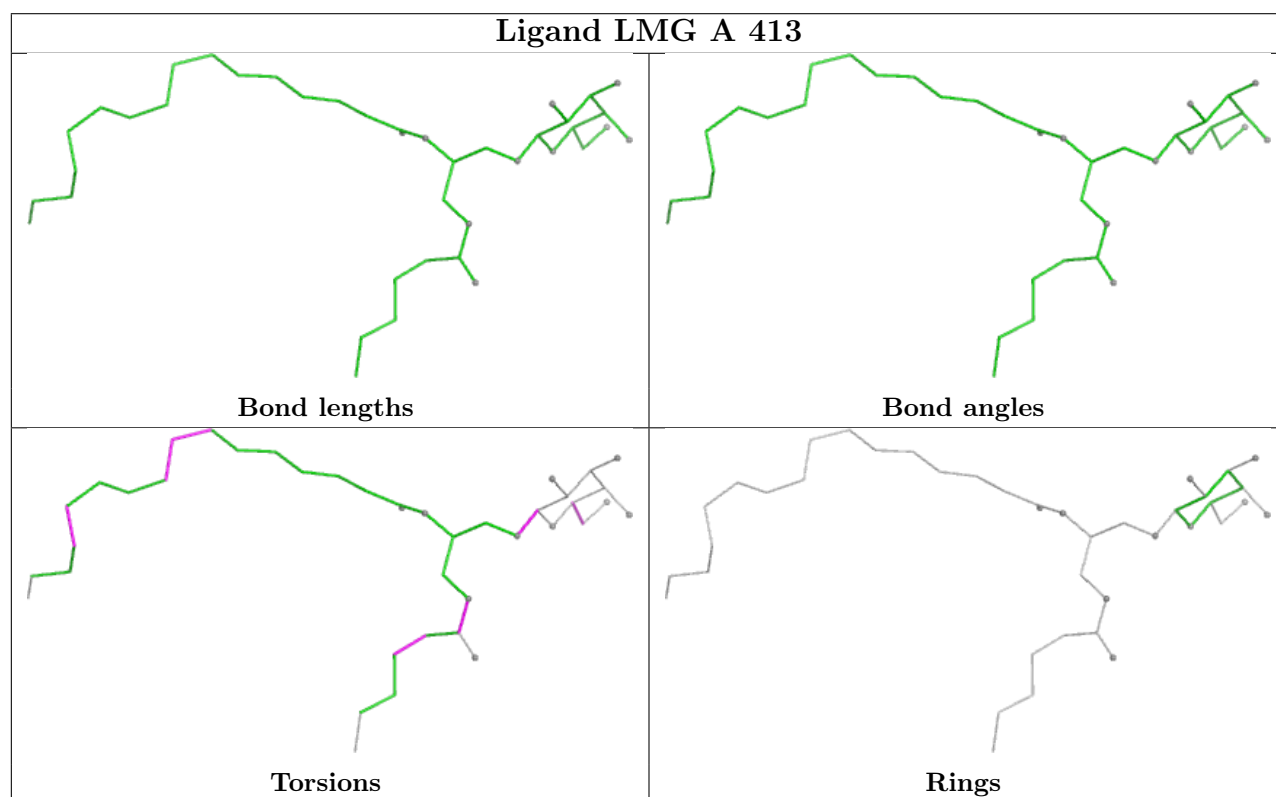
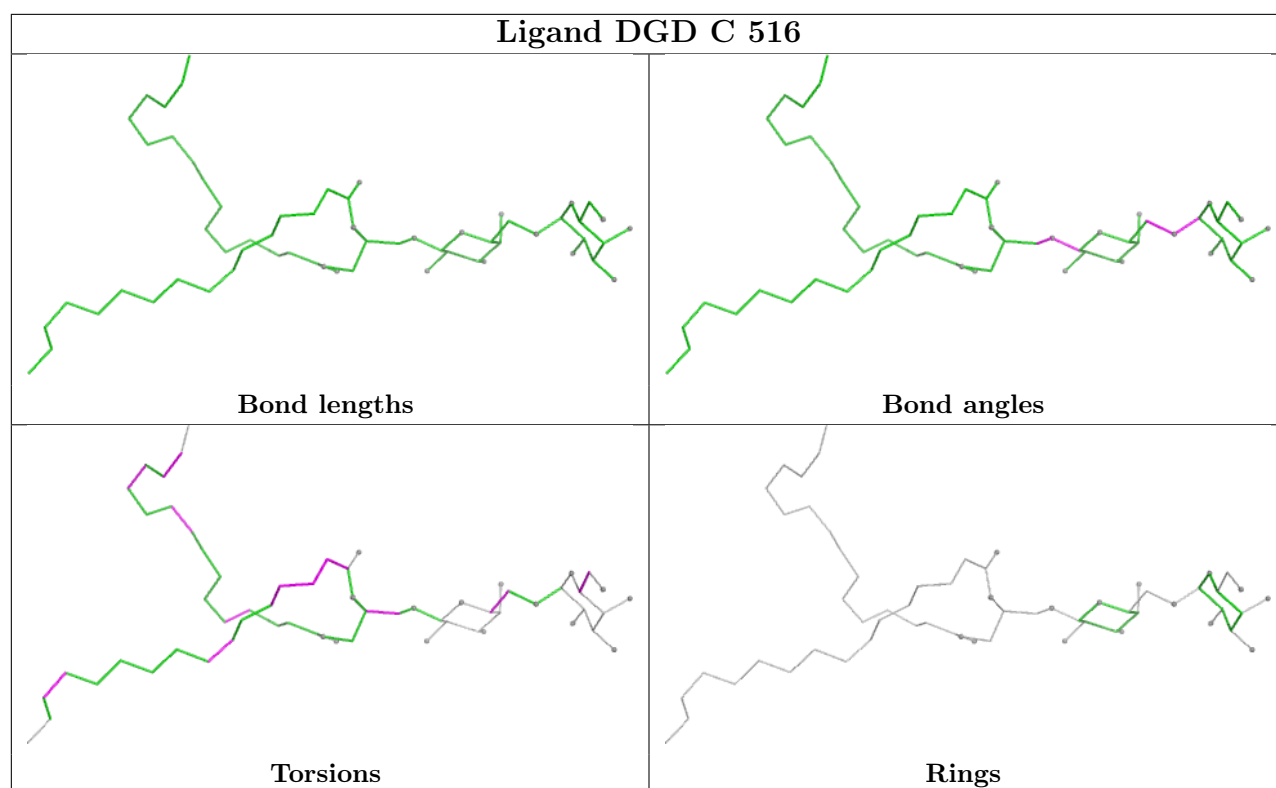


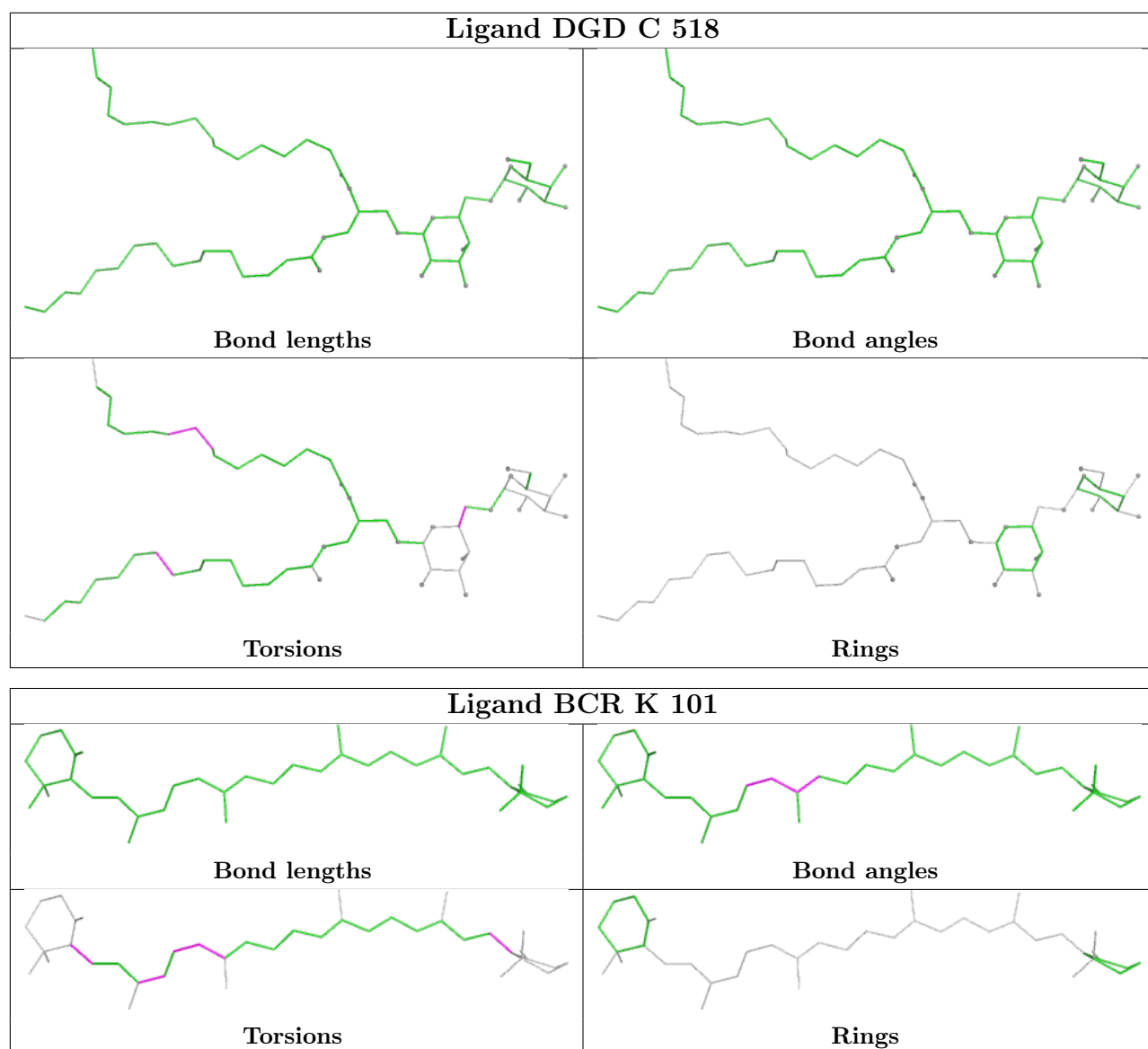


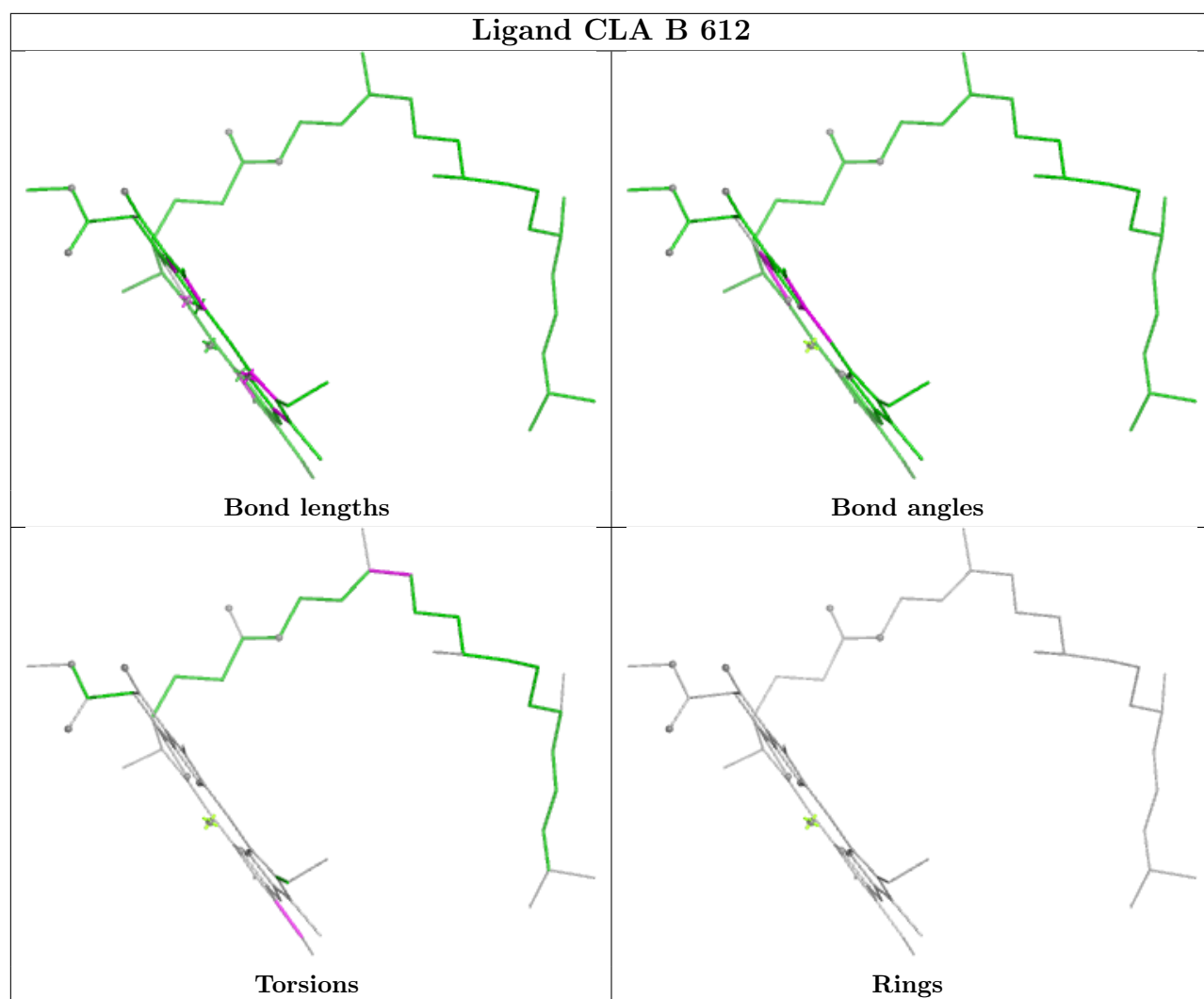


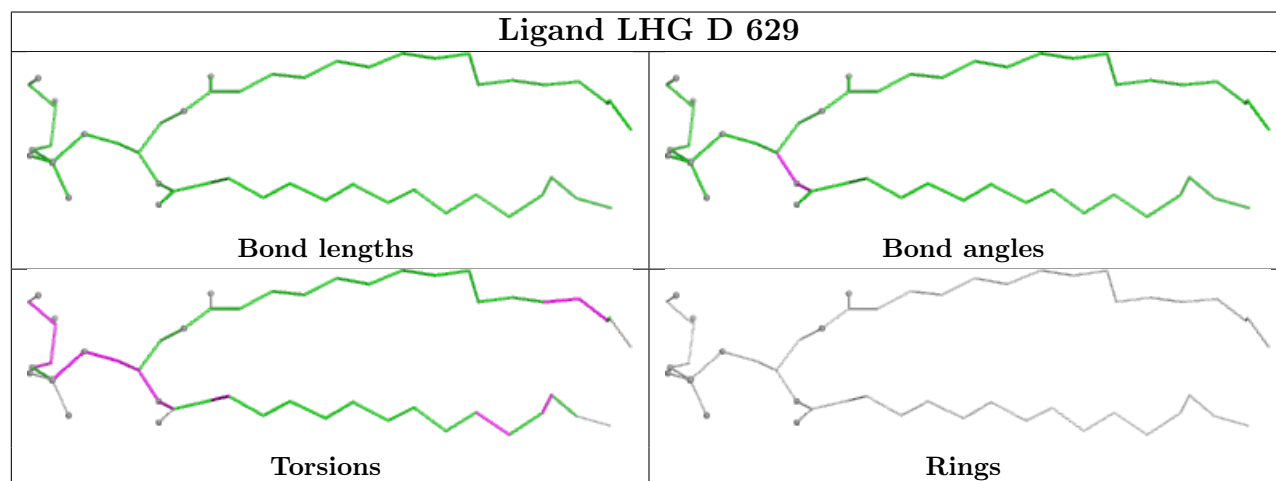
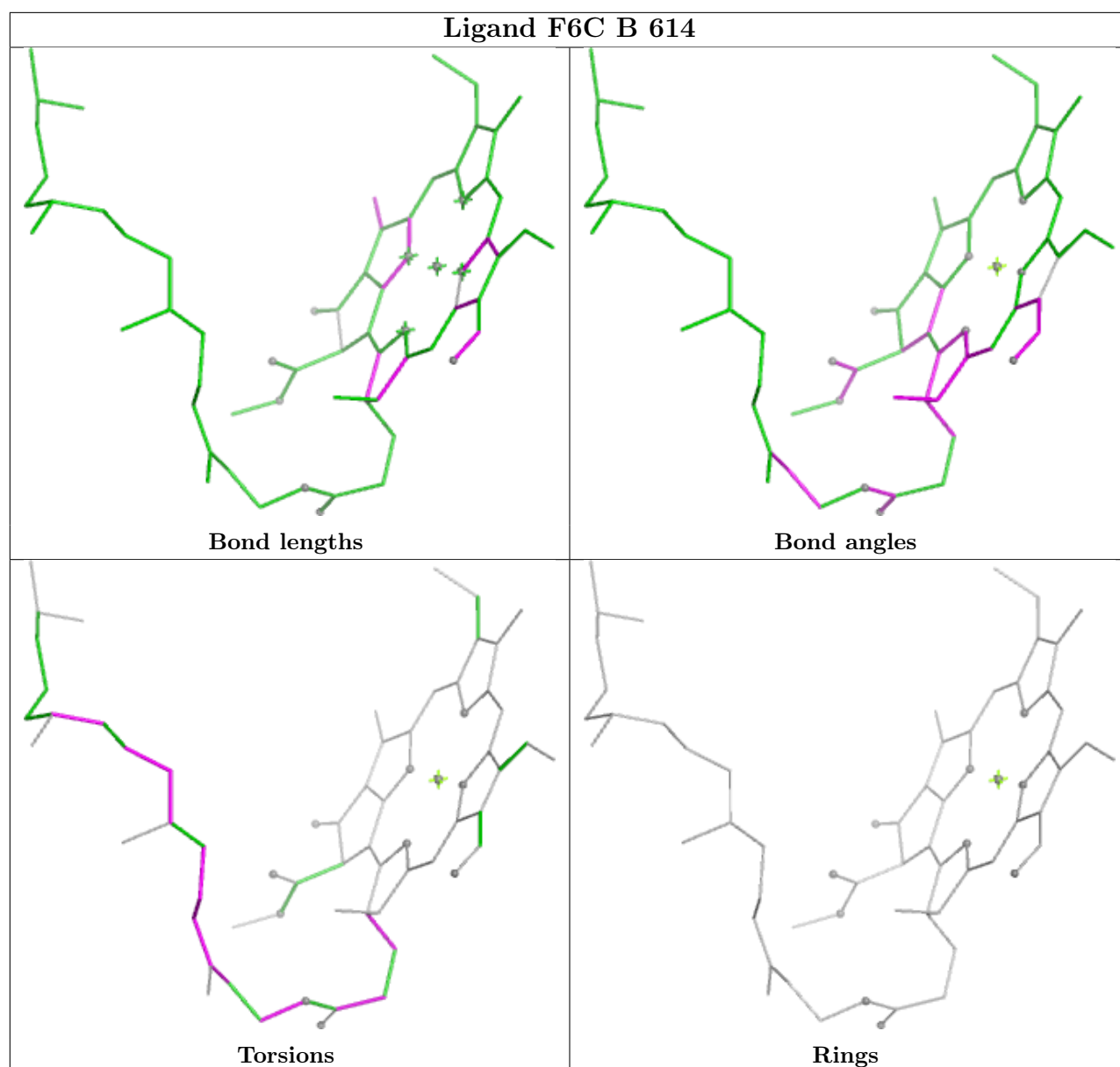


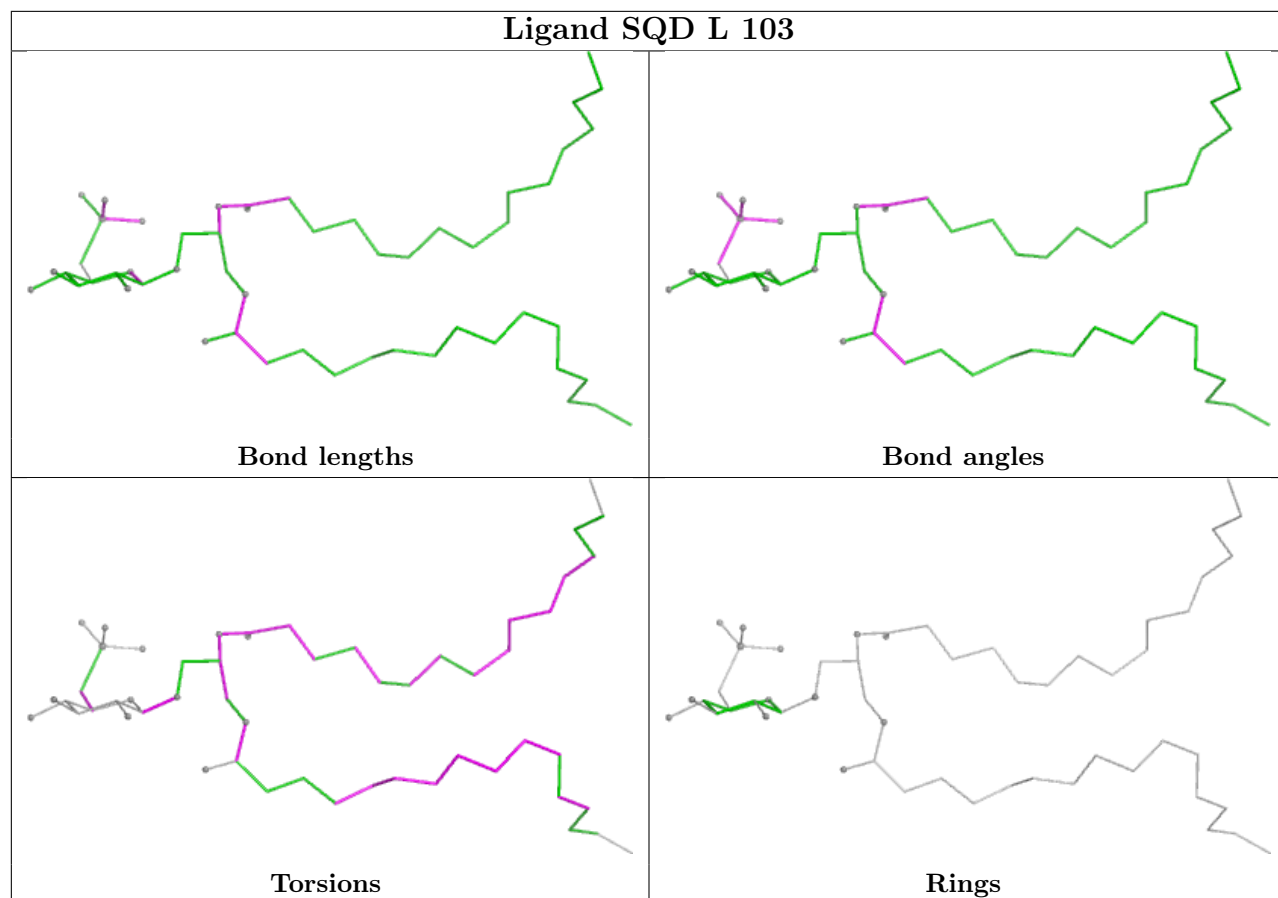


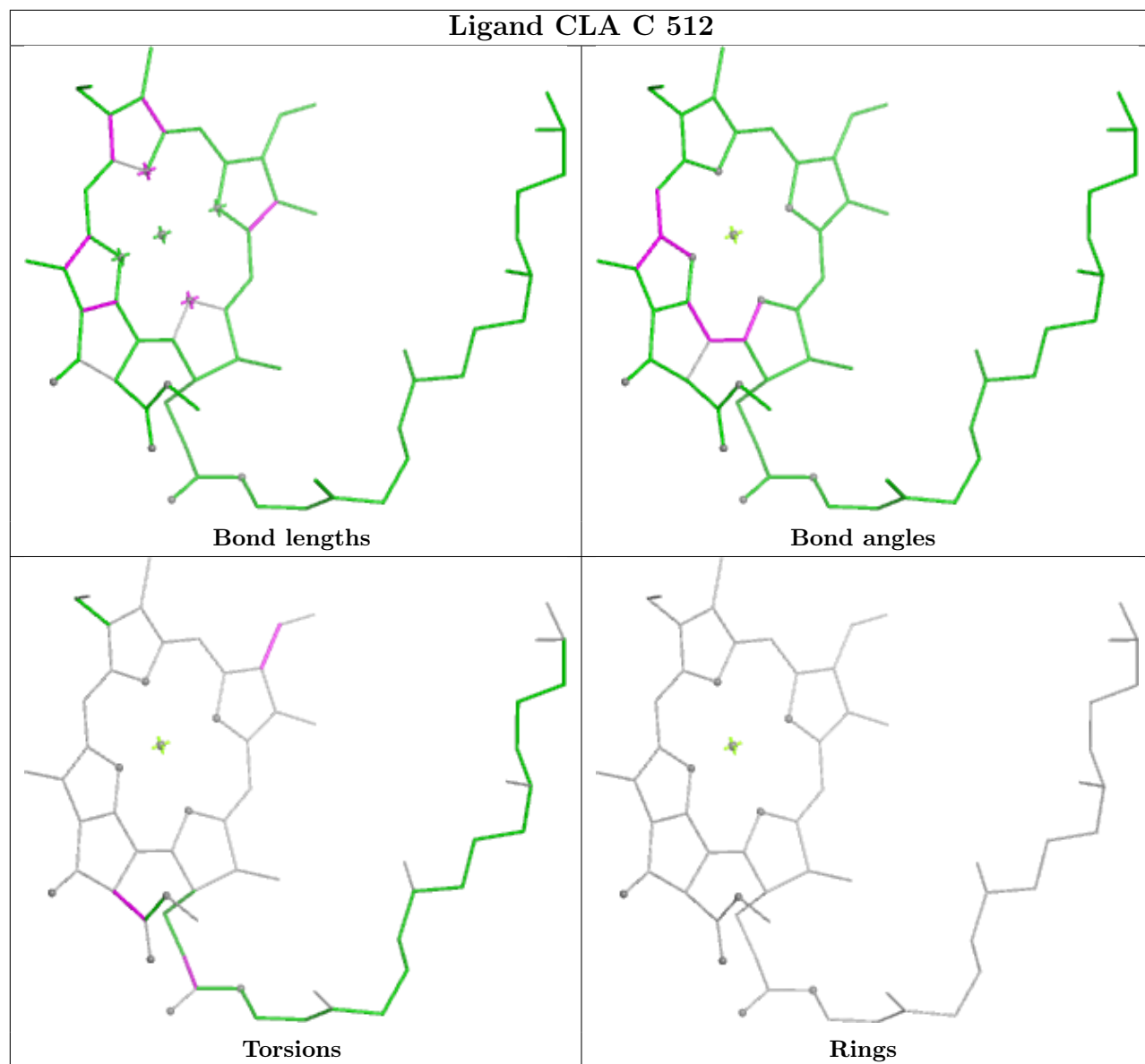


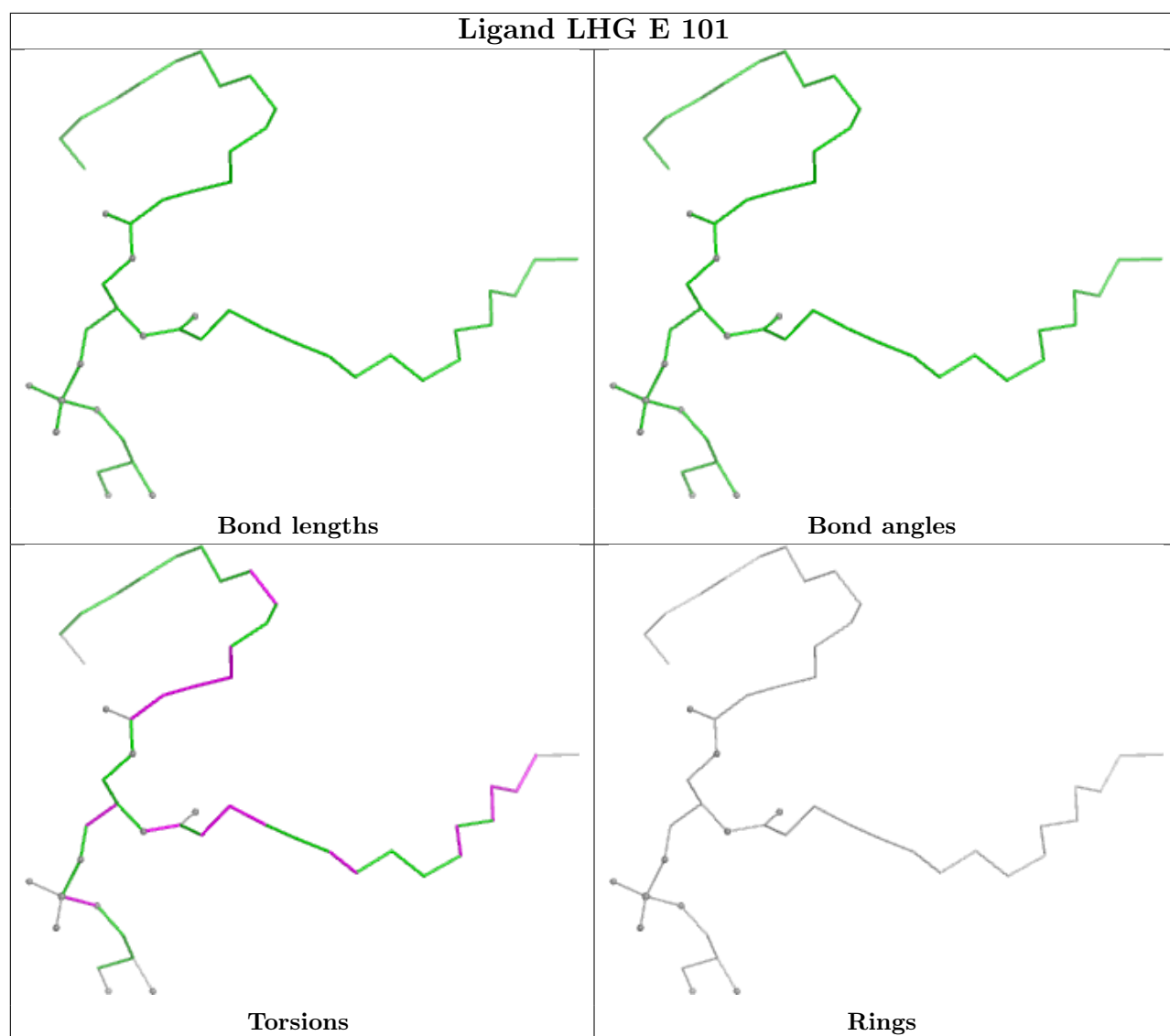




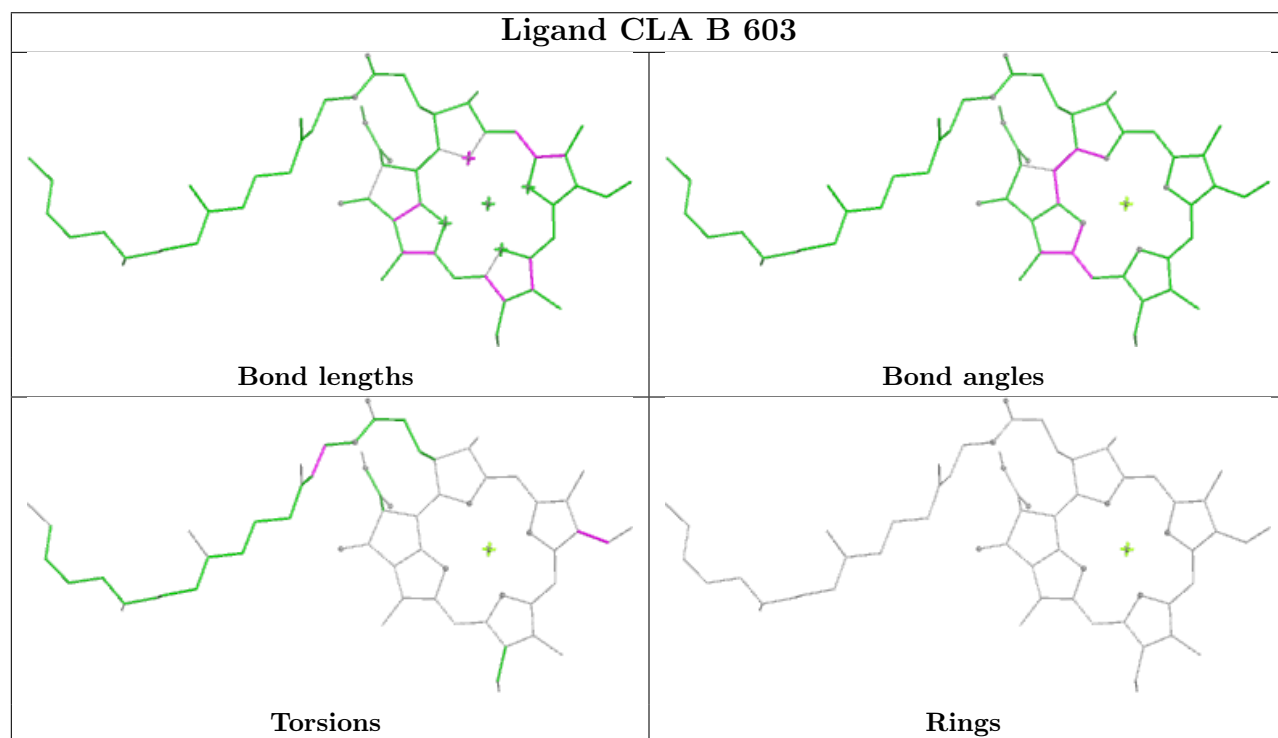
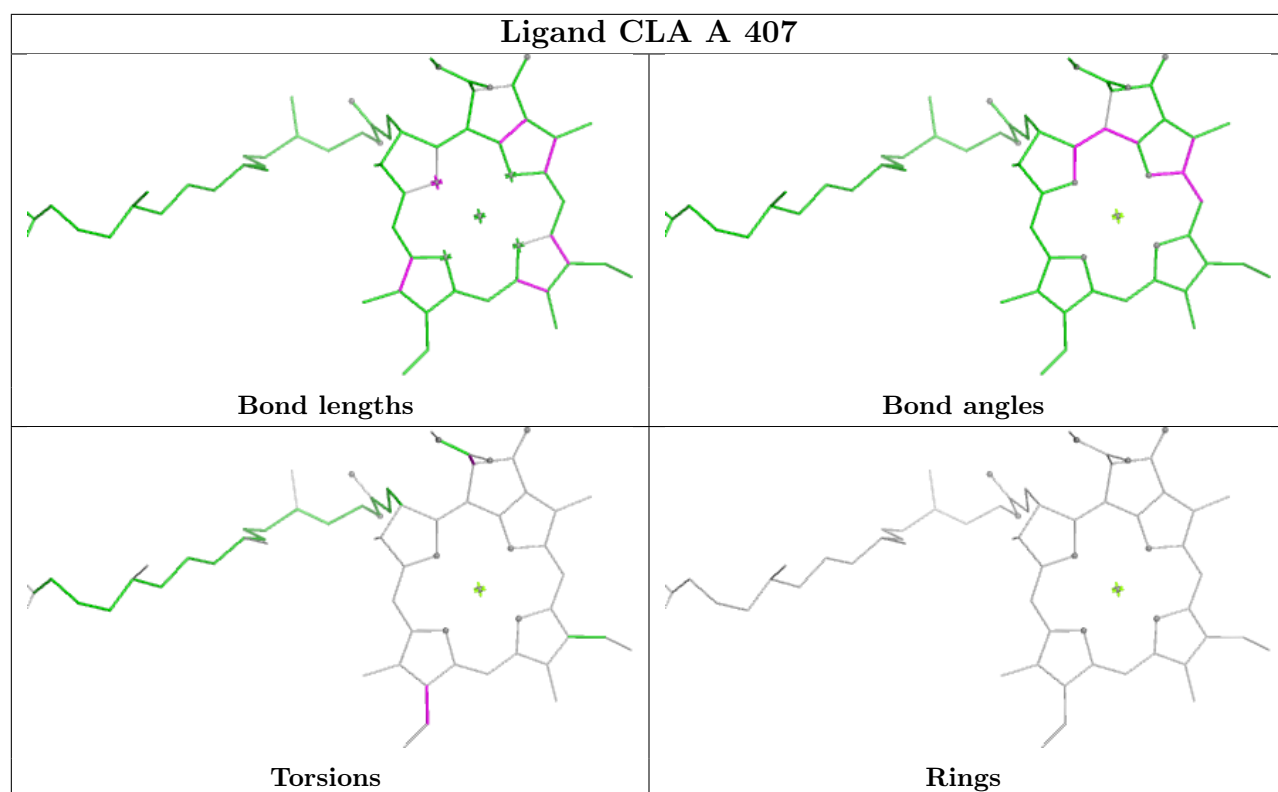


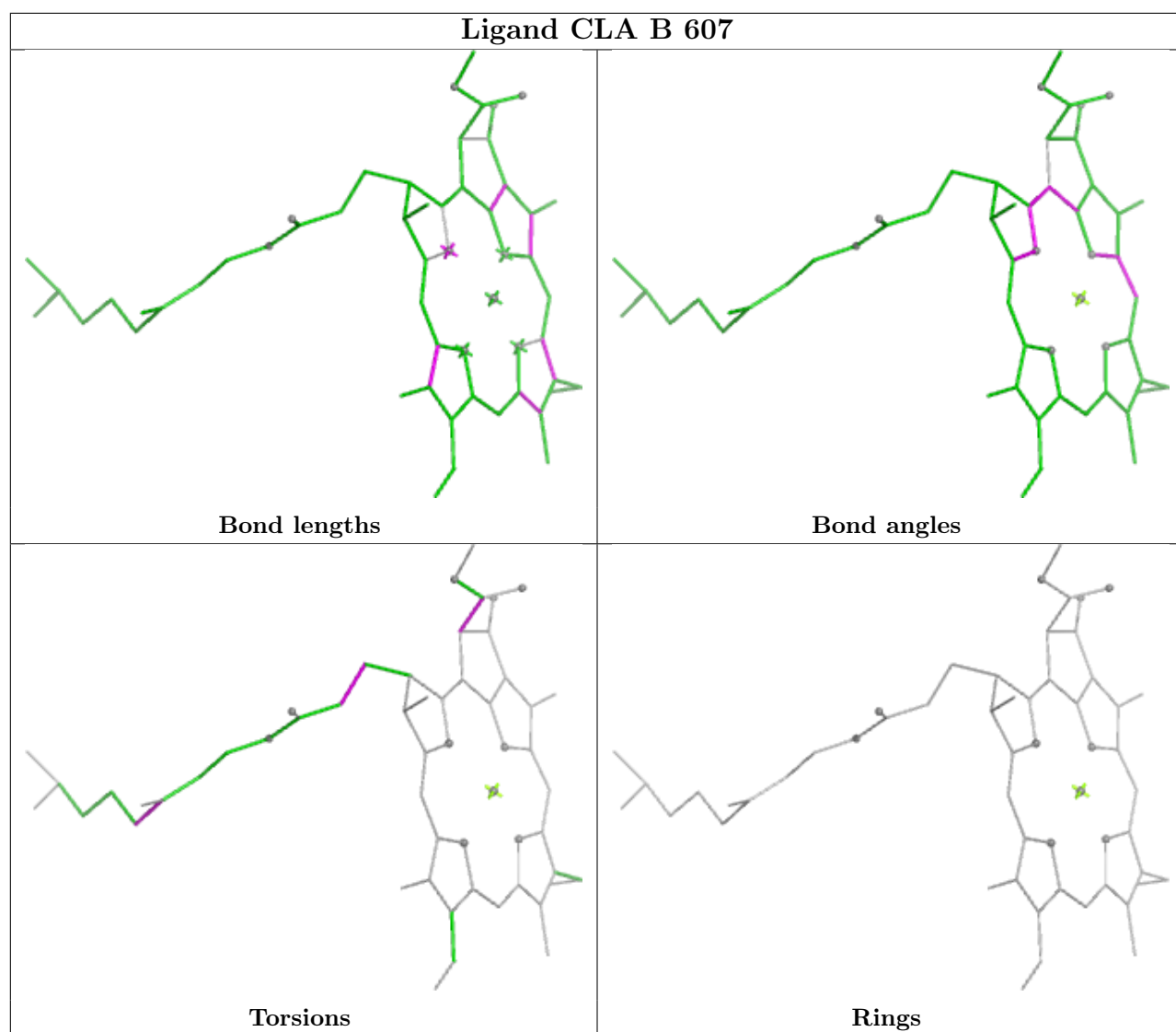


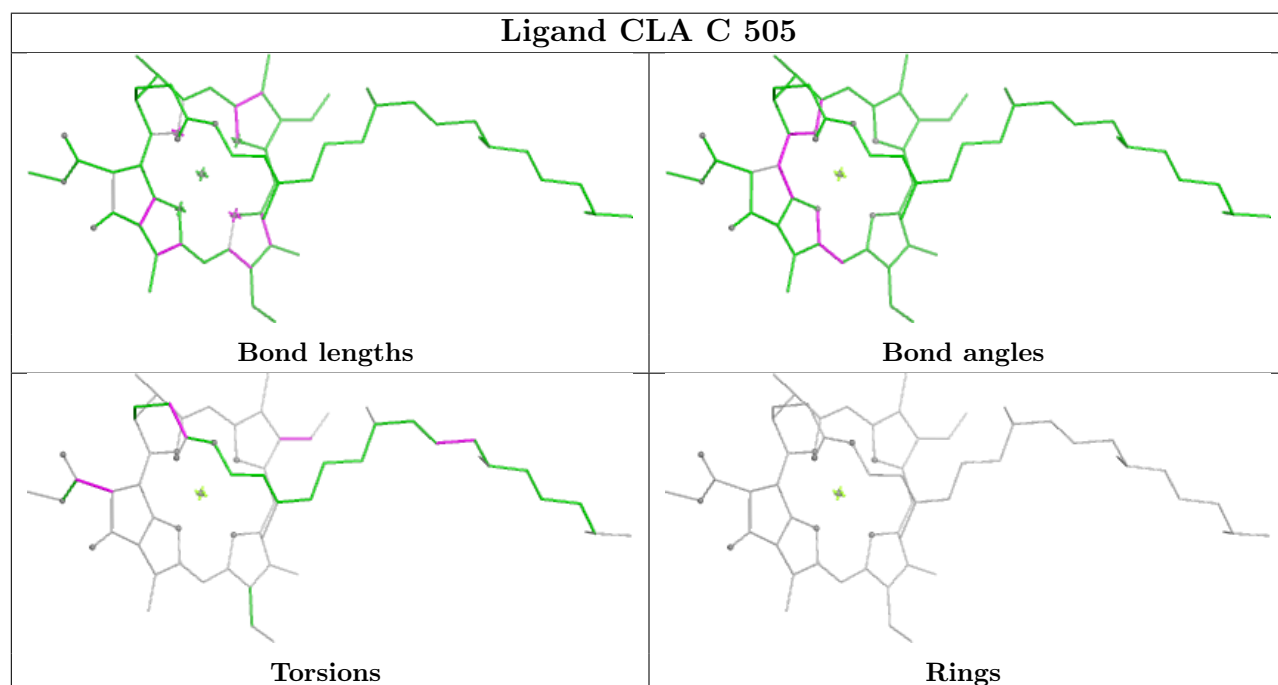
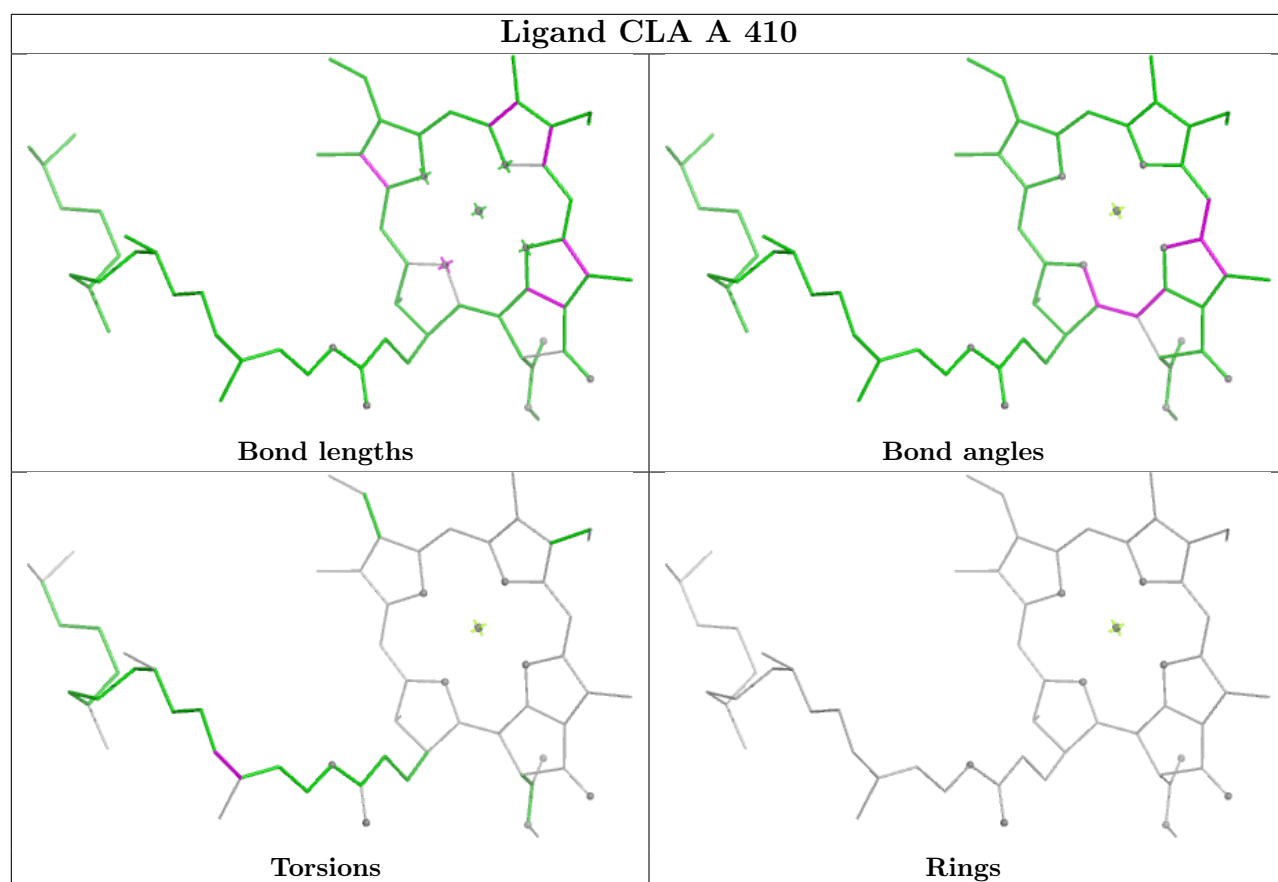


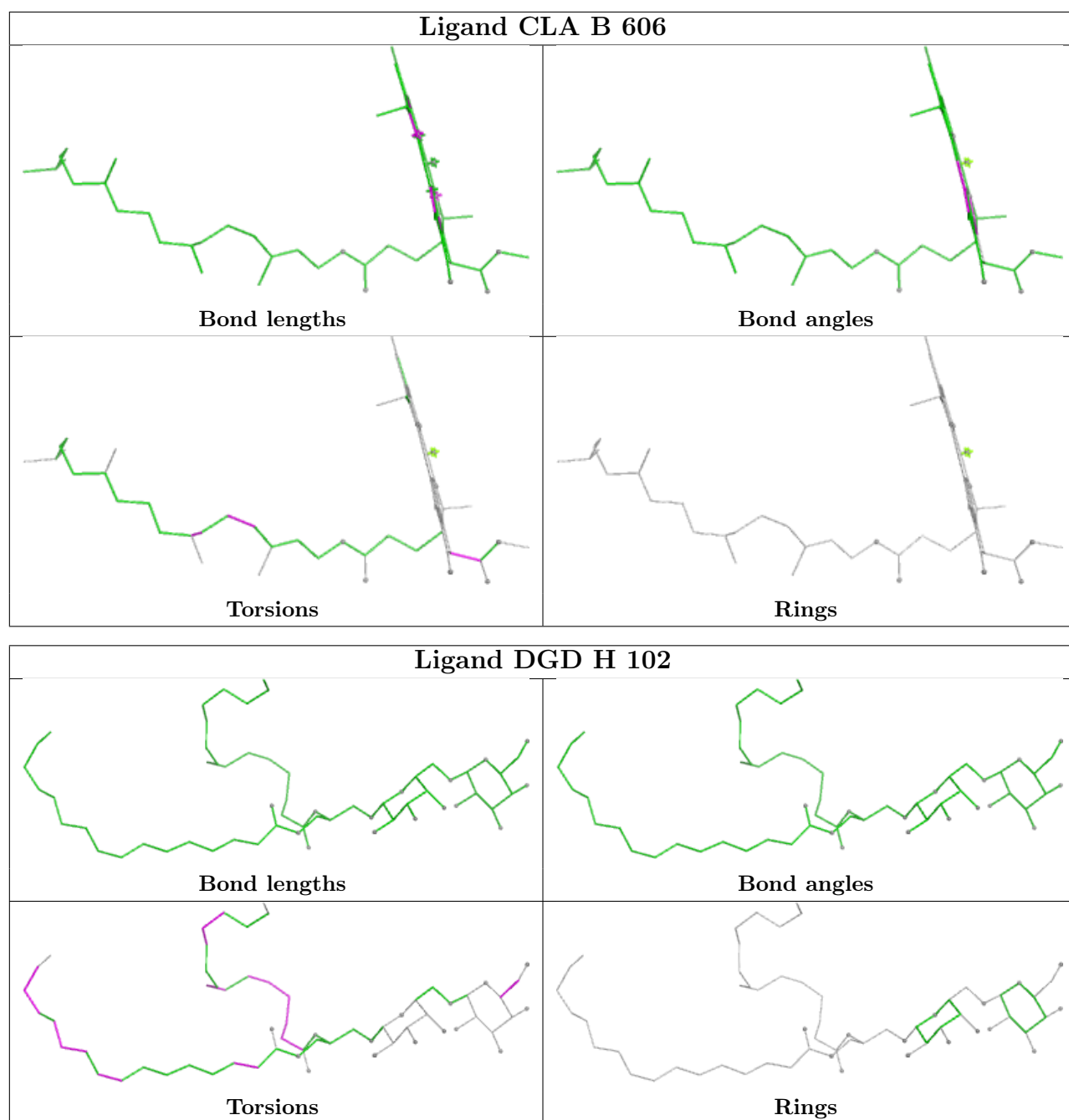


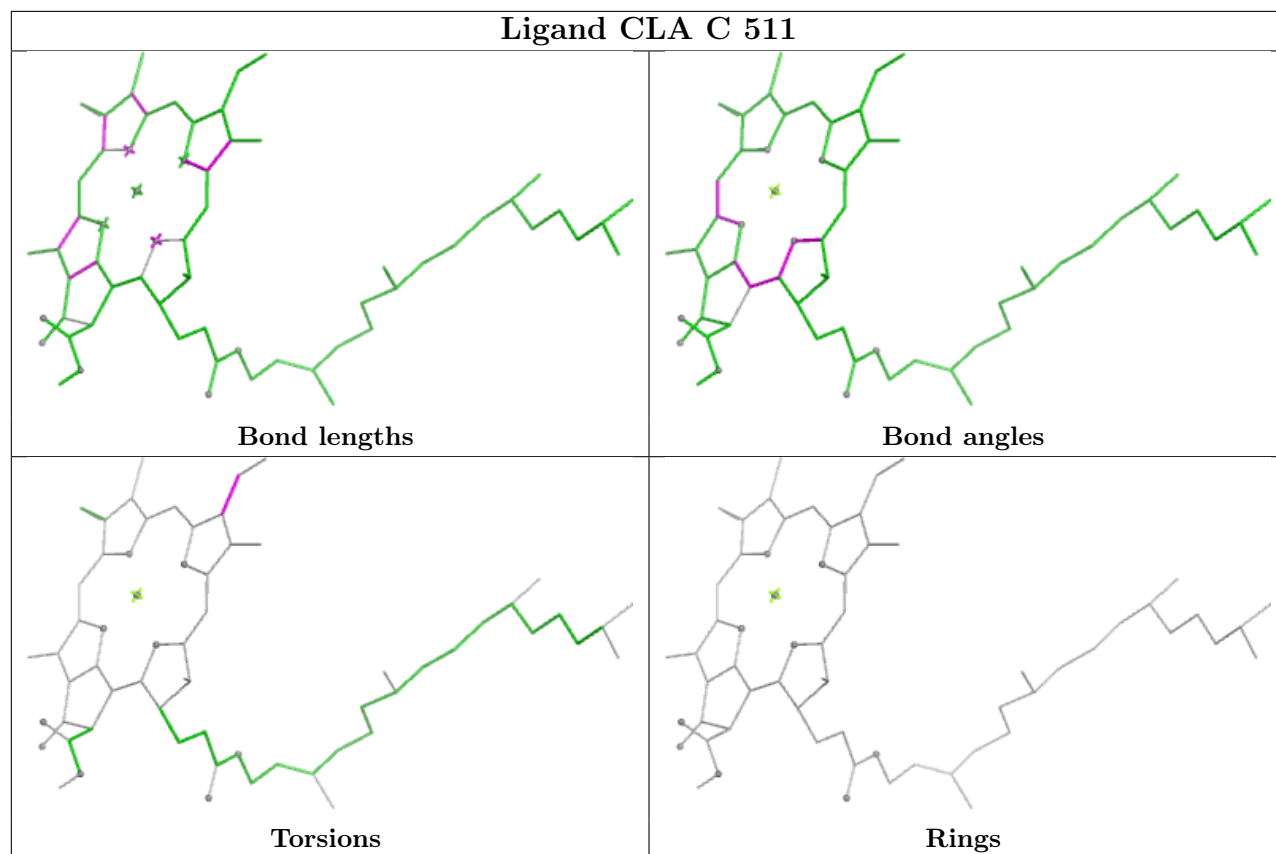
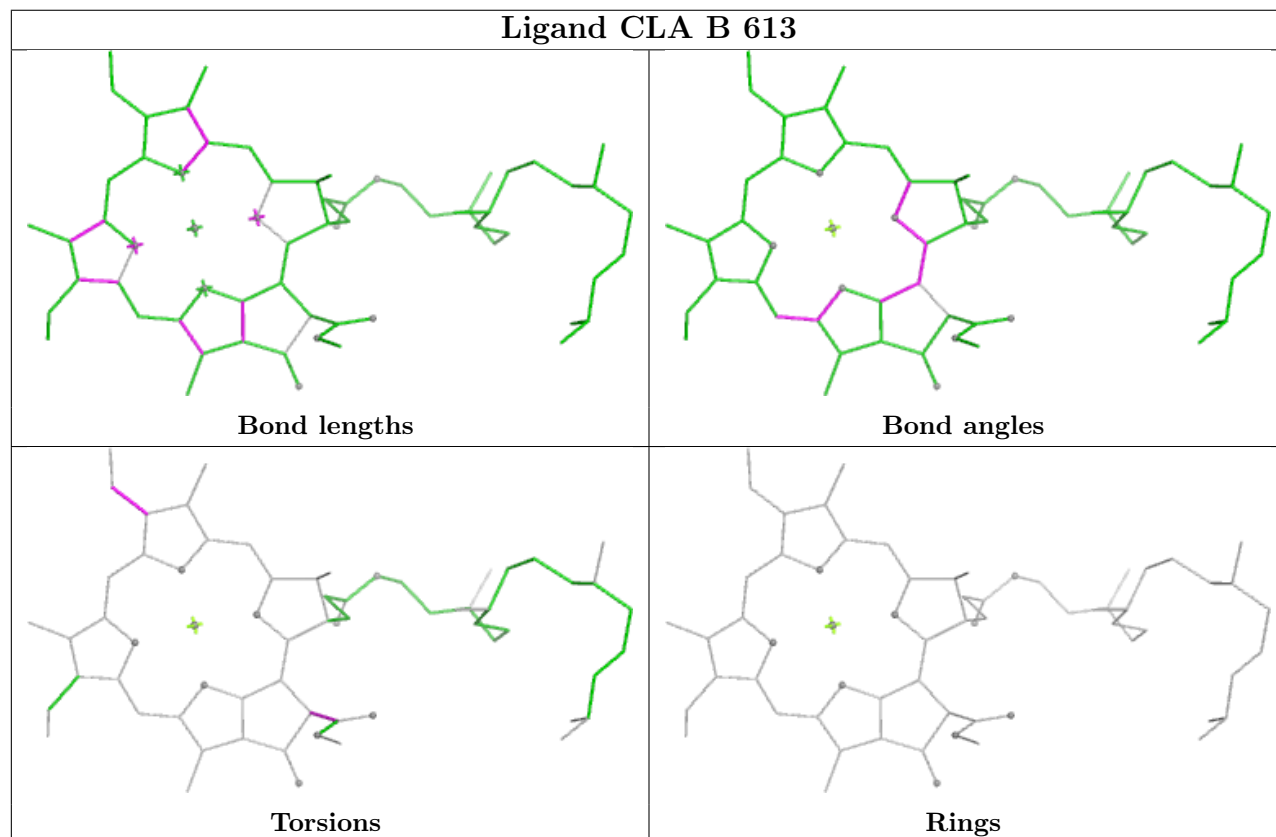


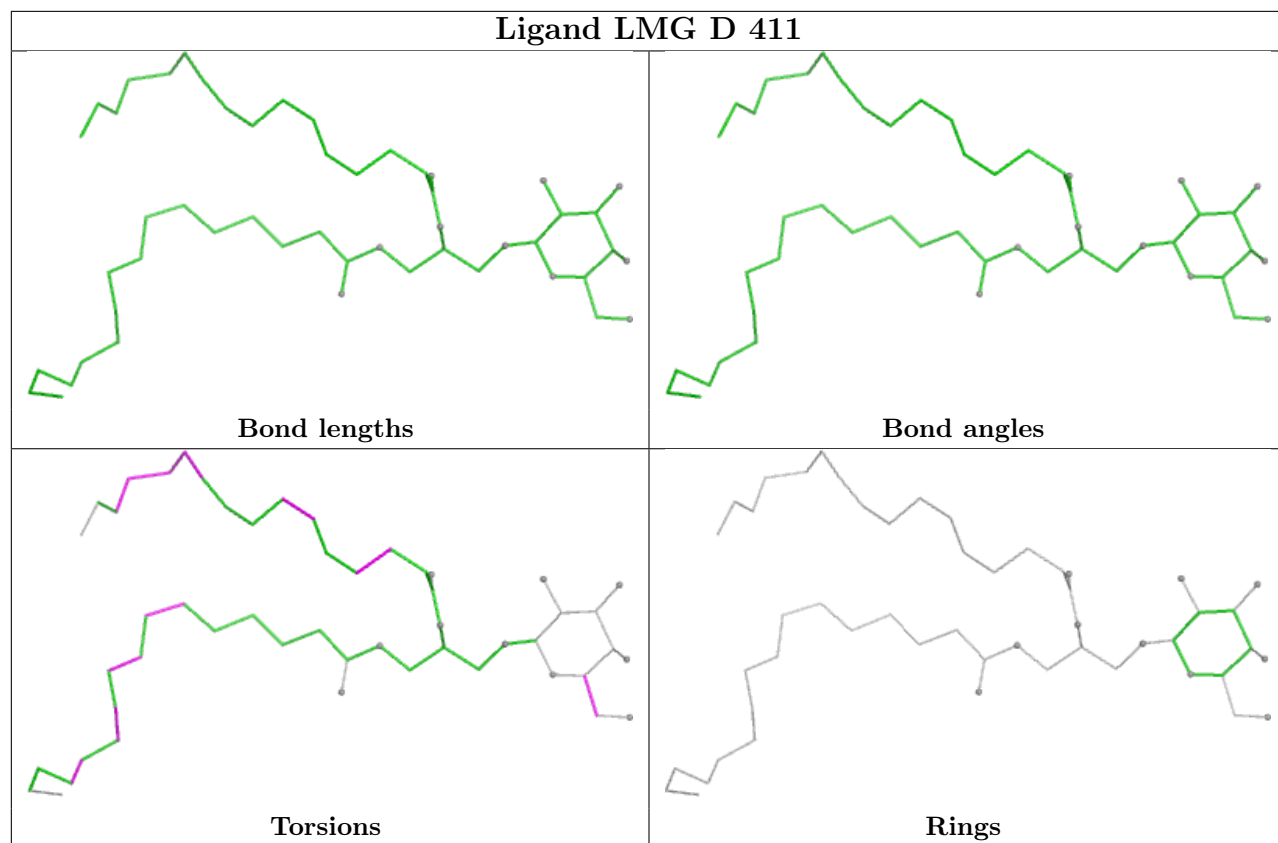


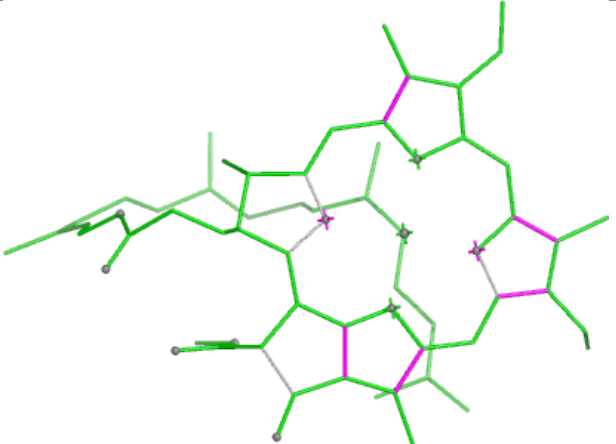
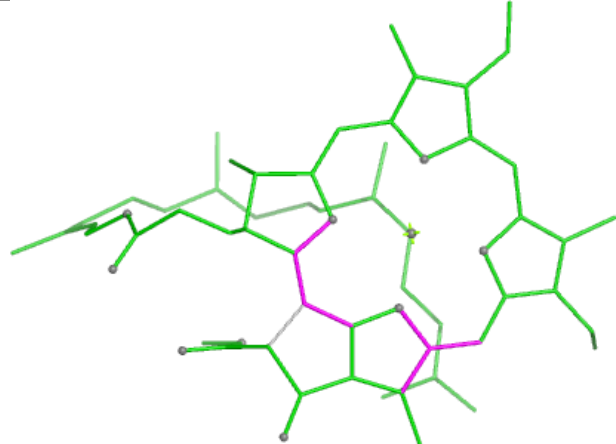
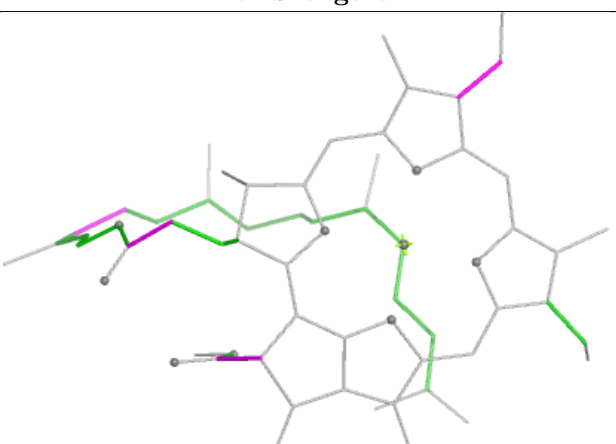
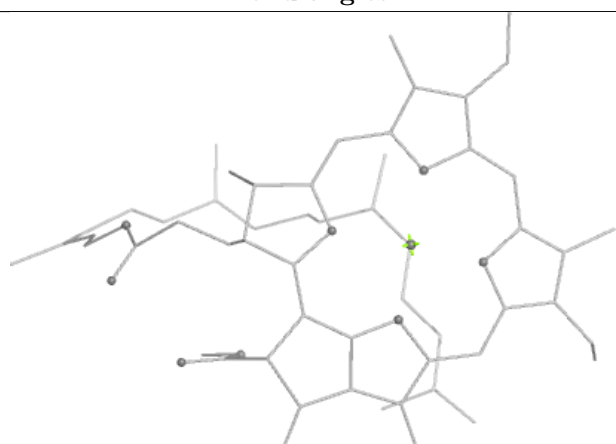



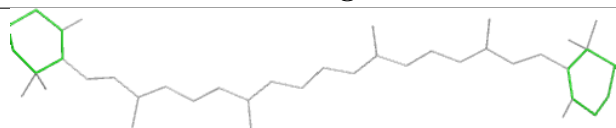


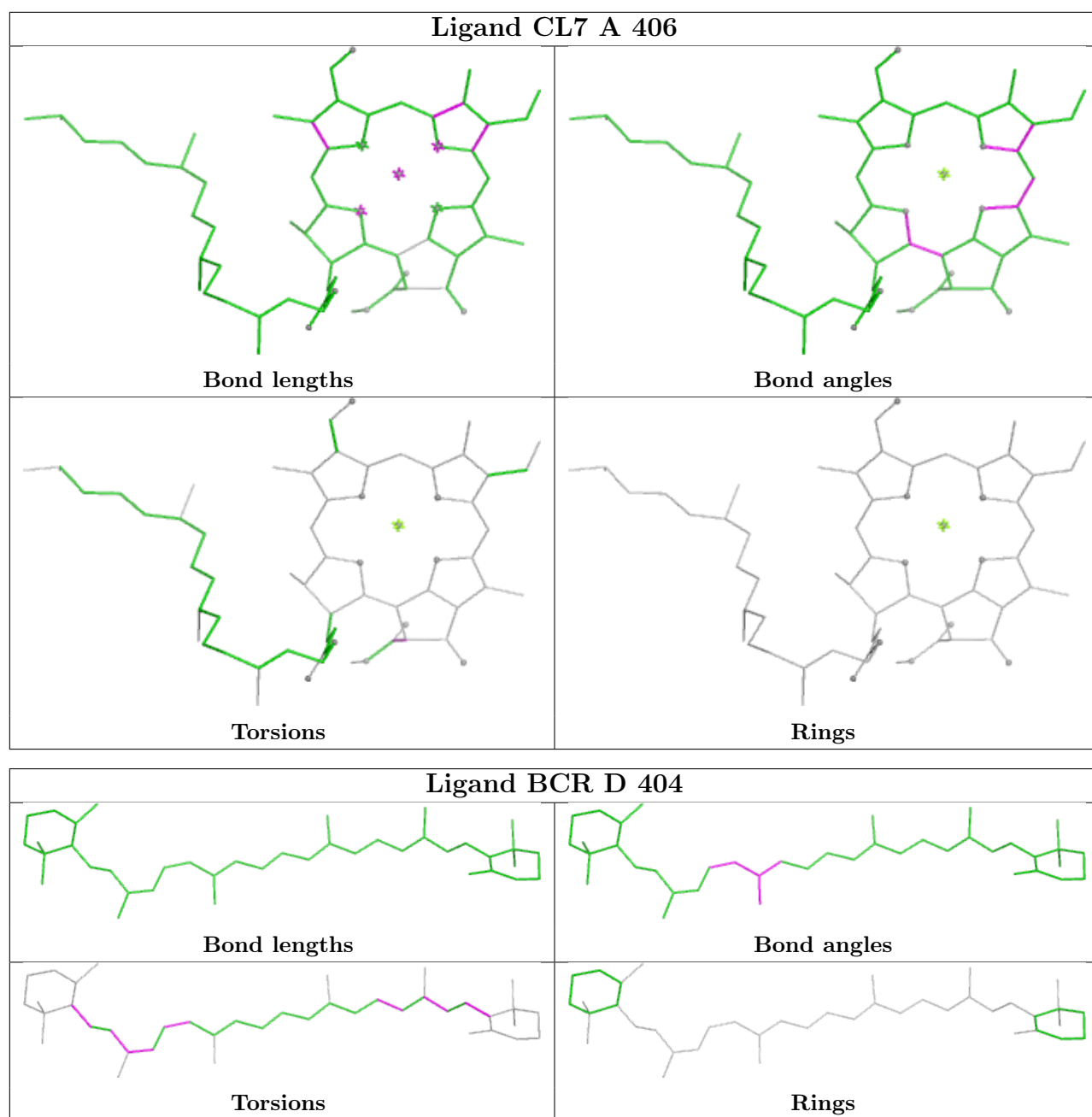




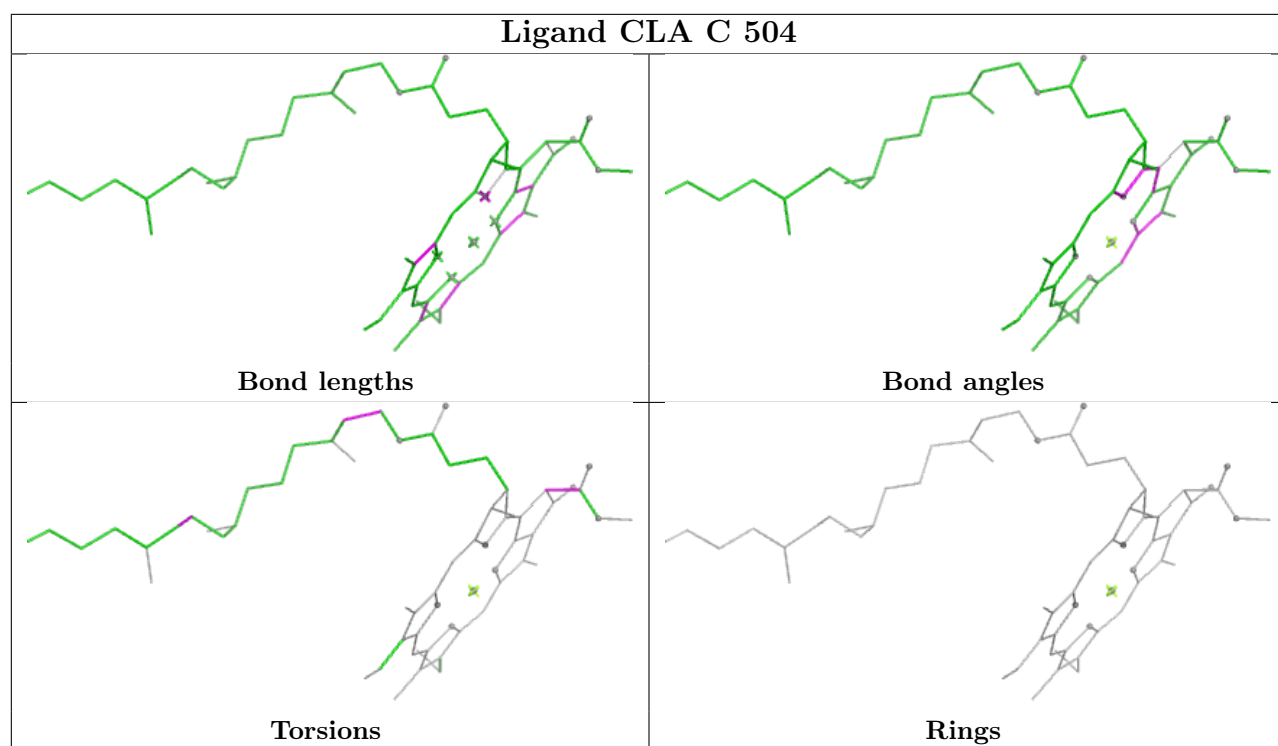
**Ligand CLA C 511****Ligand CLA B 613**



Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 620	
	
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.

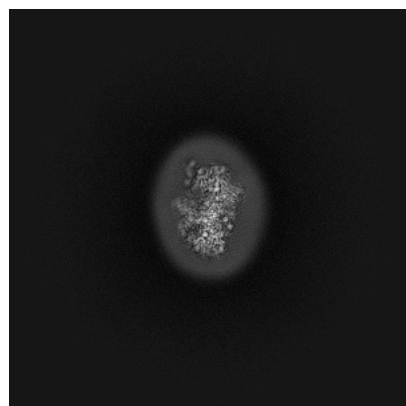
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55594. These allow visual inspection of the internal detail of the map and identification of artifacts.

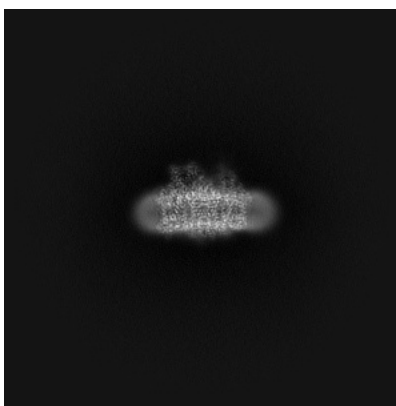
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

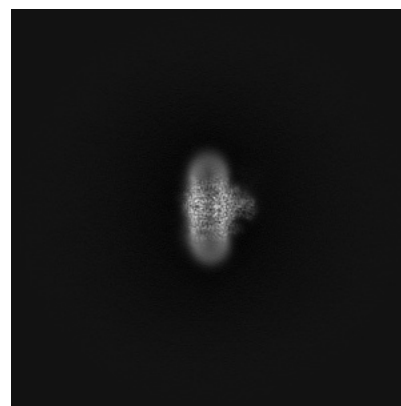
#### 6.1.1 Primary map



X

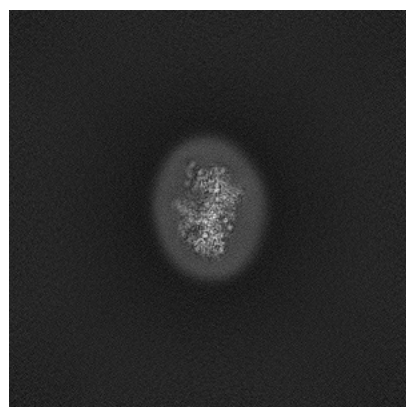


Y

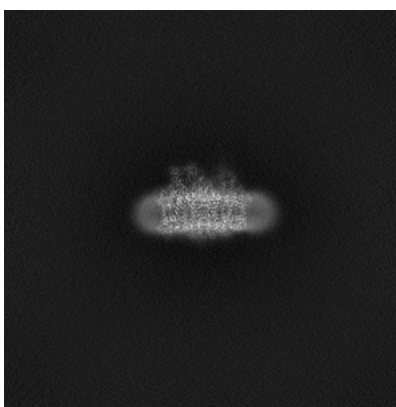


Z

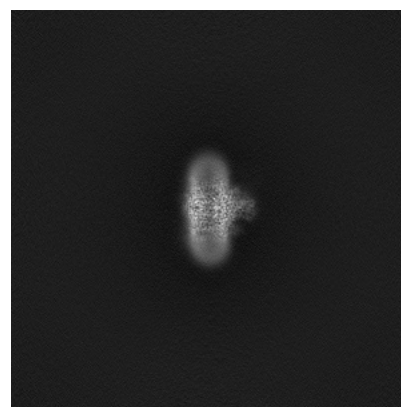
#### 6.1.2 Raw map



X



Y

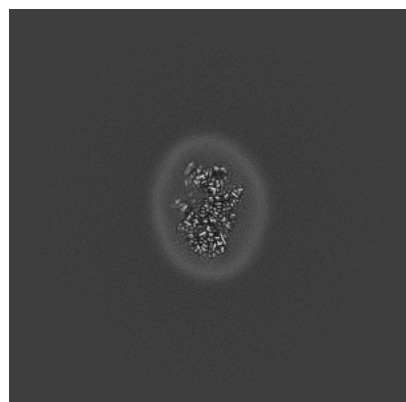


Z

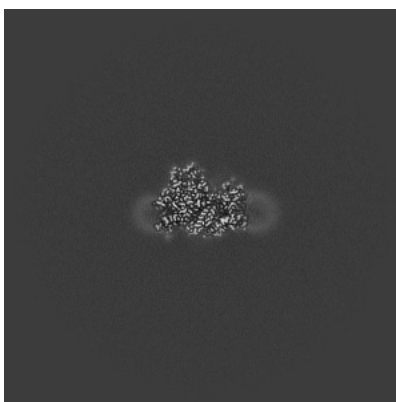
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

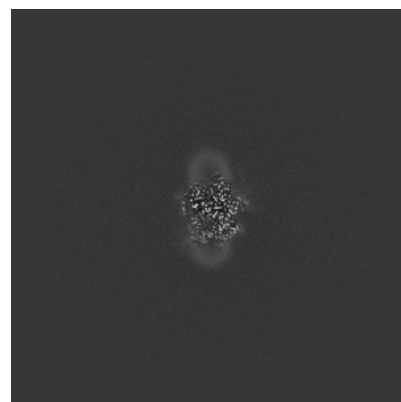
### 6.2.1 Primary map



X Index: 300

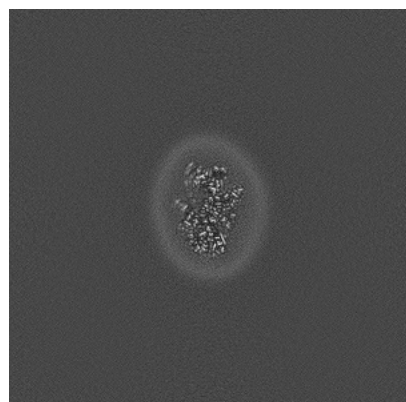


Y Index: 300

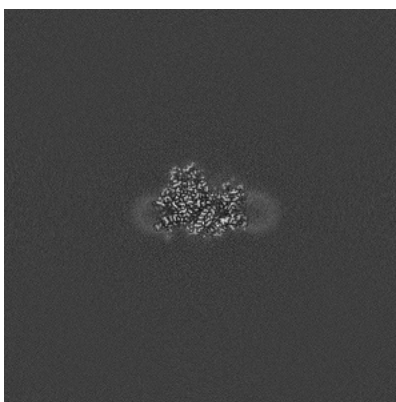


Z Index: 300

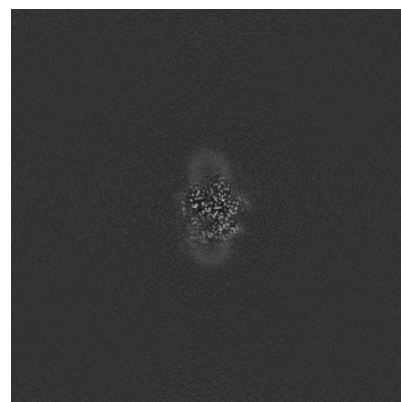
### 6.2.2 Raw map



X Index: 300



Y Index: 300

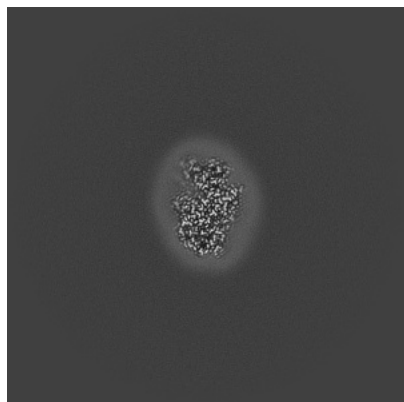


Z Index: 300

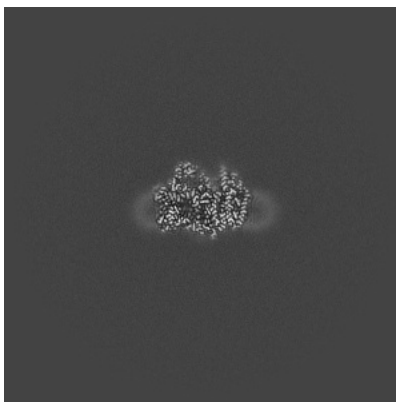
The images above show central slices of the map in three orthogonal directions.

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

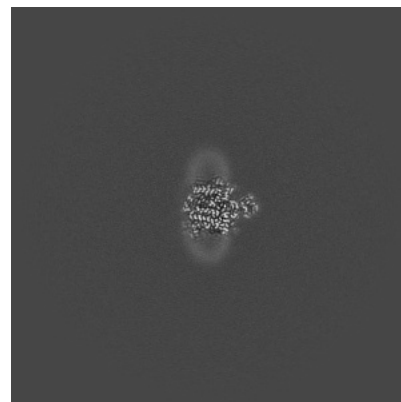
### 6.3.1 Primary map



X Index: 315

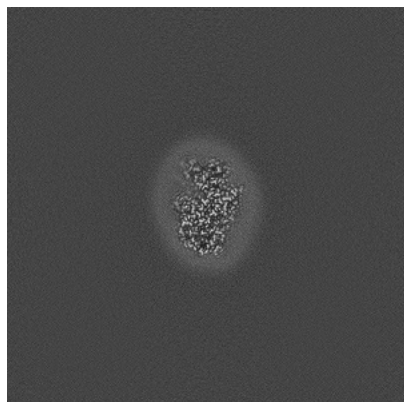


Y Index: 312

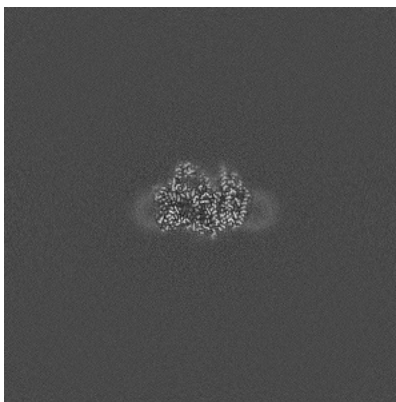


Z Index: 283

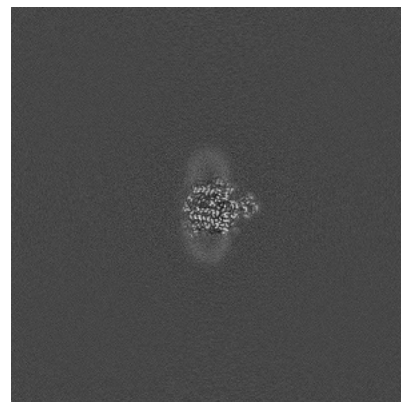
### 6.3.2 Raw map



X Index: 315



Y Index: 312

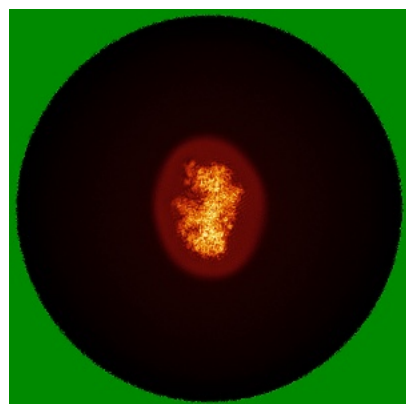


Z Index: 283

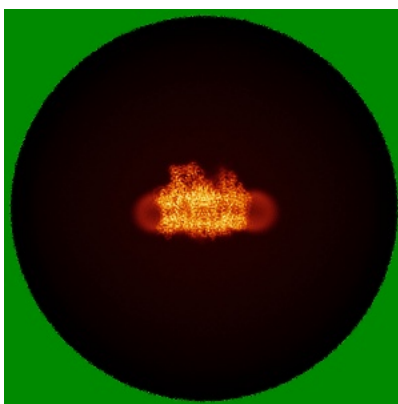
The images above show the largest variance slices of the map in three orthogonal directions.

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

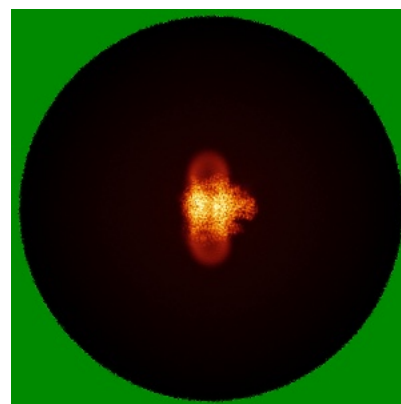
### 6.4.1 Primary map



X

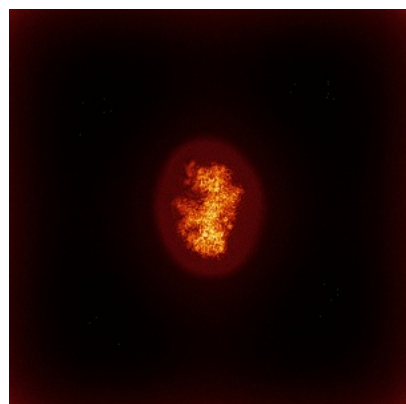


Y

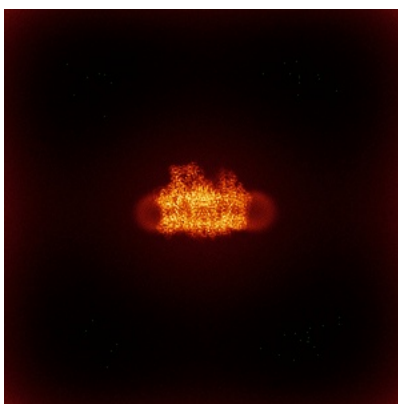


Z

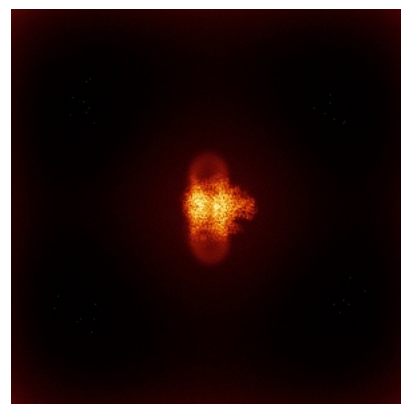
### 6.4.2 Raw map



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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

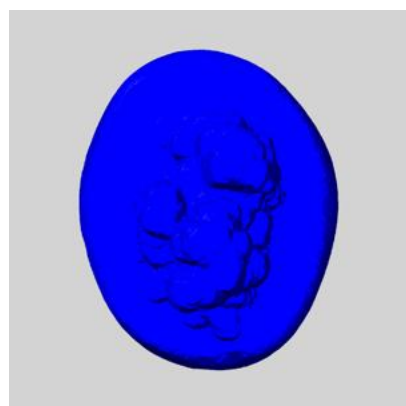
## 6.6 Mask visualisation [i](#)

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

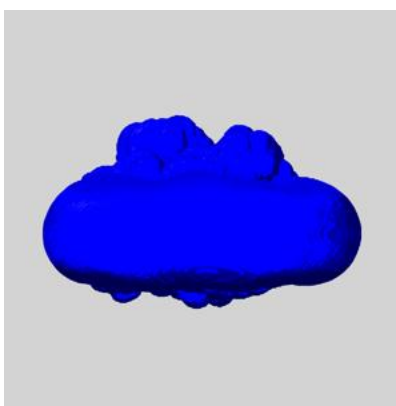
A mask typically either:

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

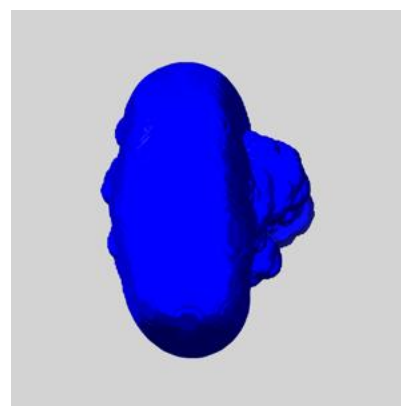
### 6.6.1 emd\_55594\_msk\_1.map [i](#)



X



Y



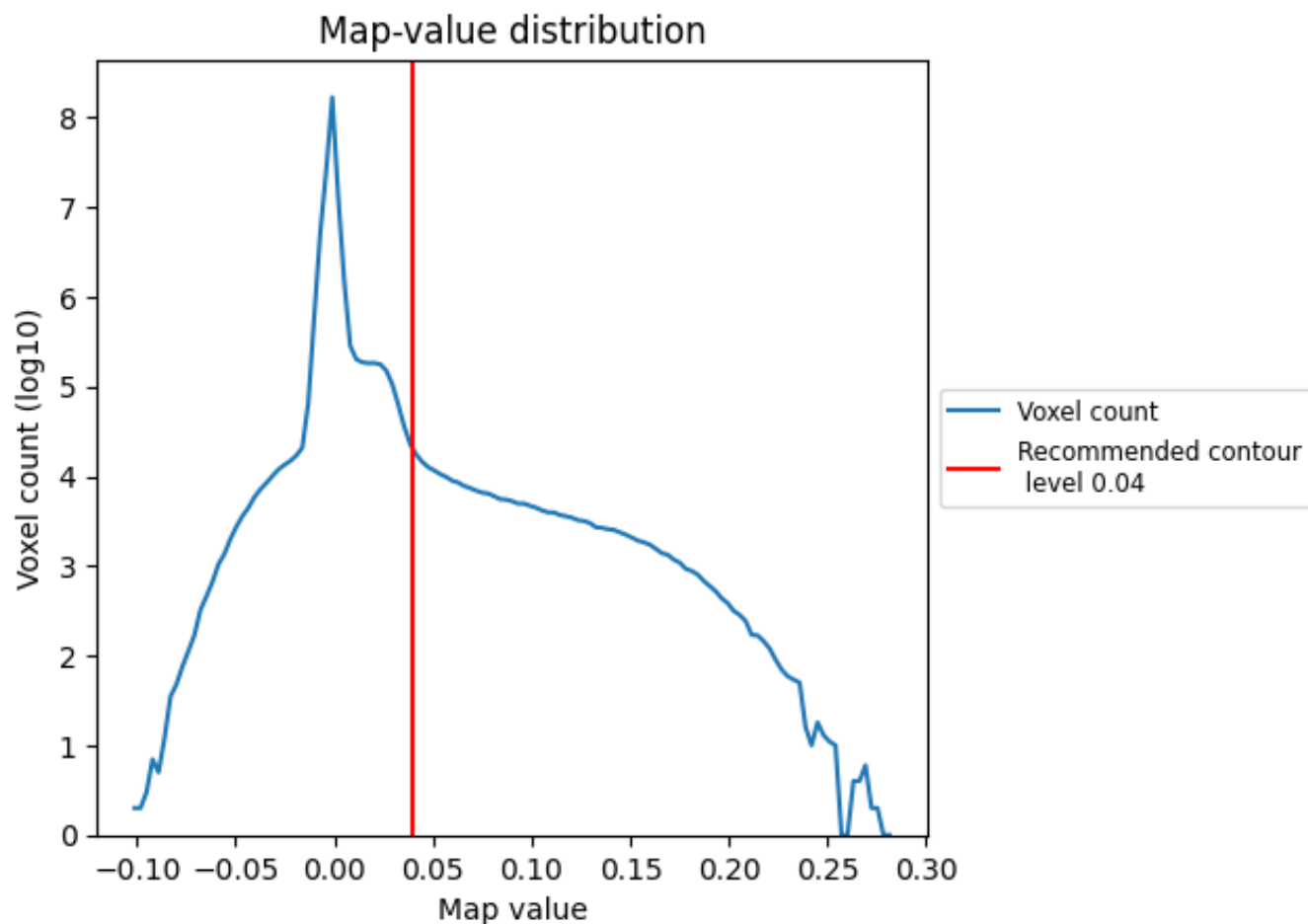
Z



## 7 Map analysis [i](#)

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

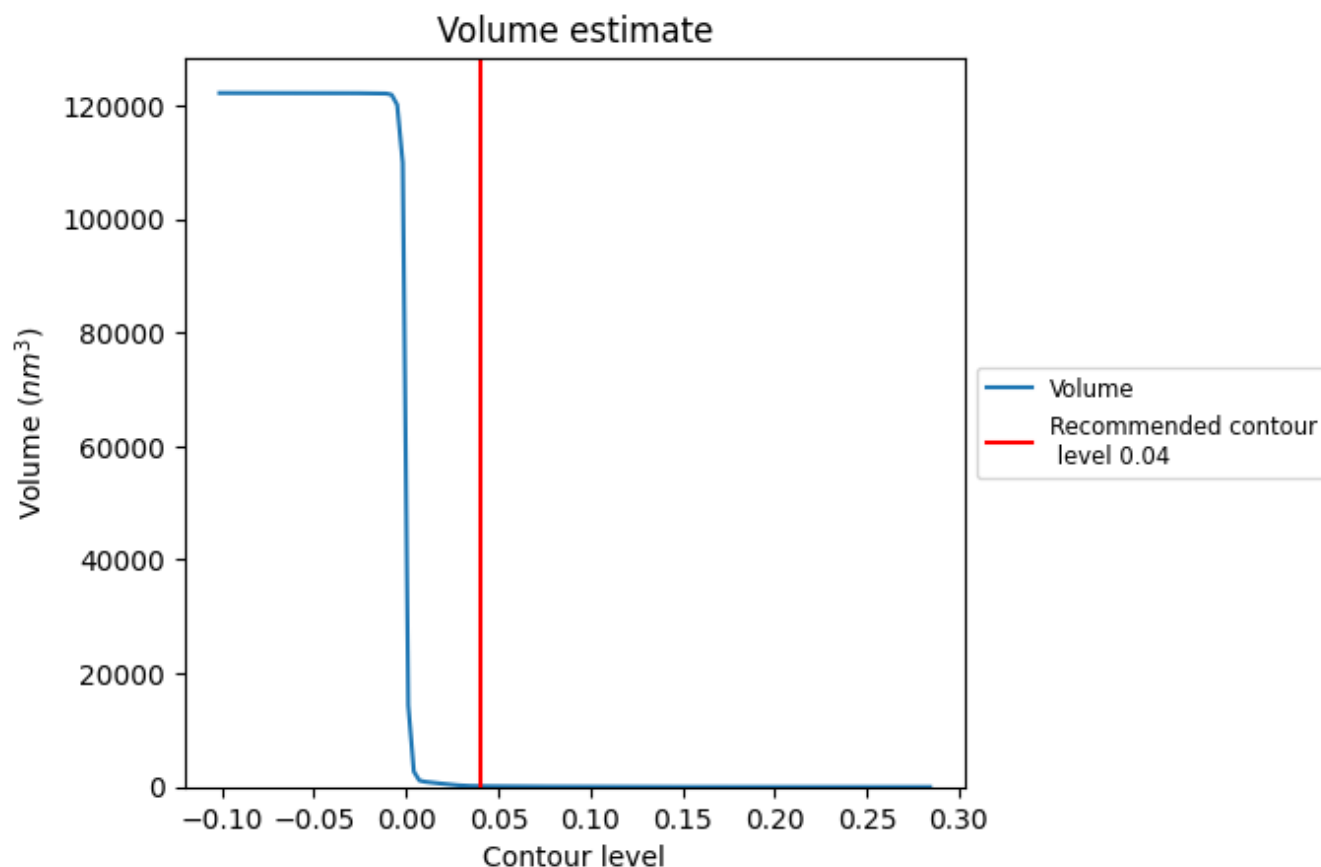
### 7.1 Map-value distribution [i](#)



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



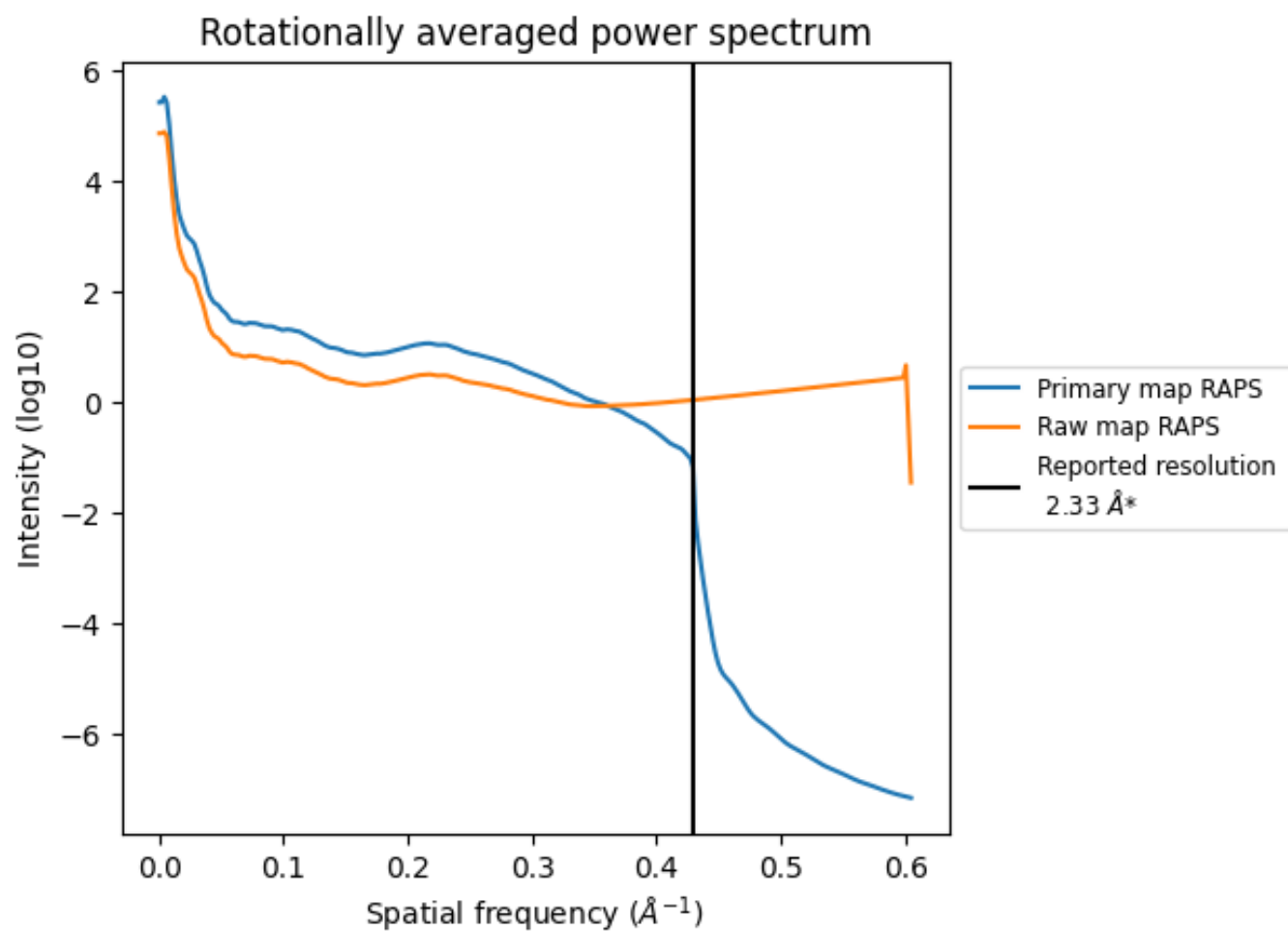
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm<sup>3</sup>; this corresponds to an approximate mass of 128 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 ⓘ

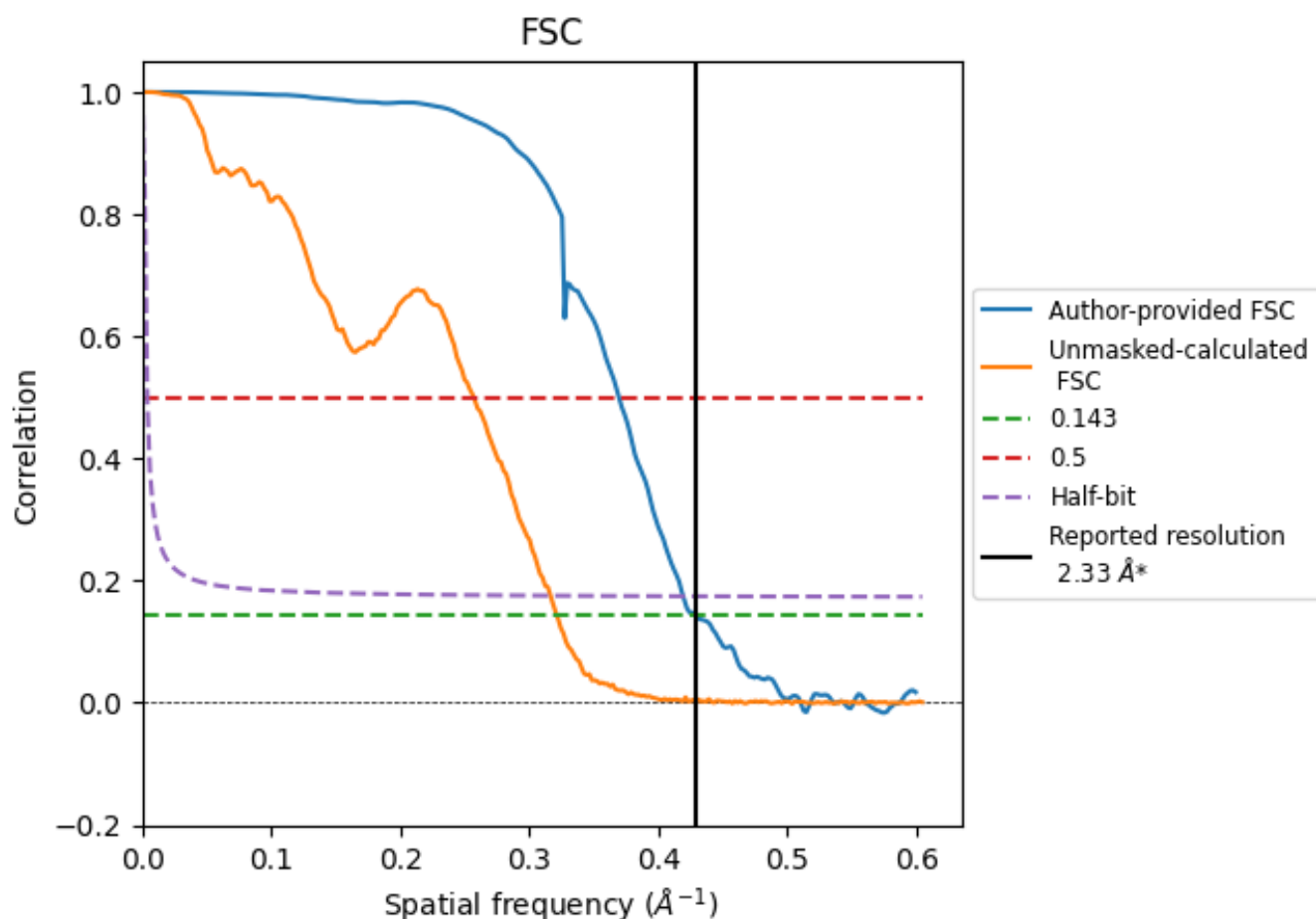


\*Reported resolution corresponds to spatial frequency of 0.429  $\text{\AA}^{-1}$

## 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 0.429 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

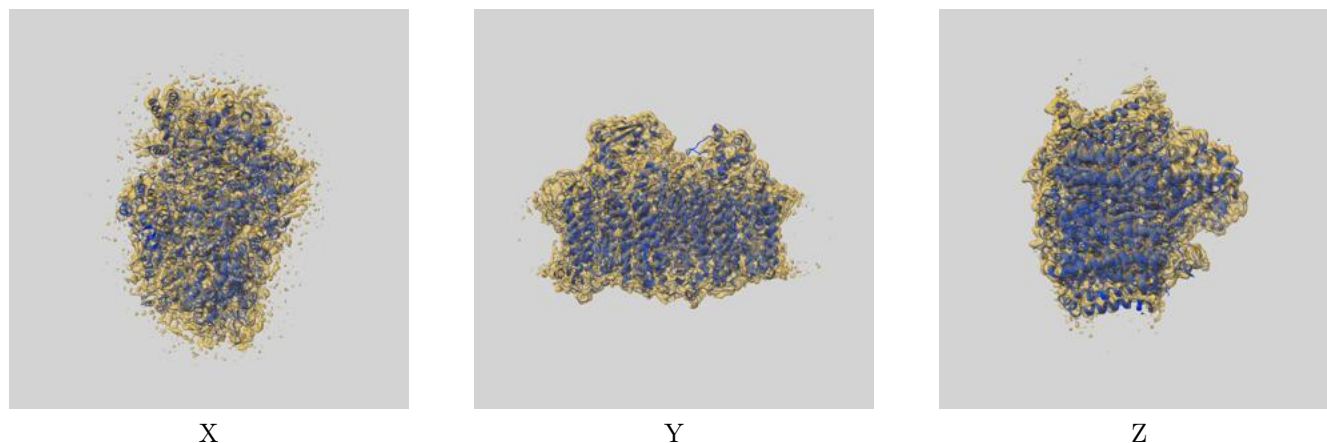
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.33	2.71	2.38
Unmasked-calculated*	3.11	3.89	3.16

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.33 by more than 10 %

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

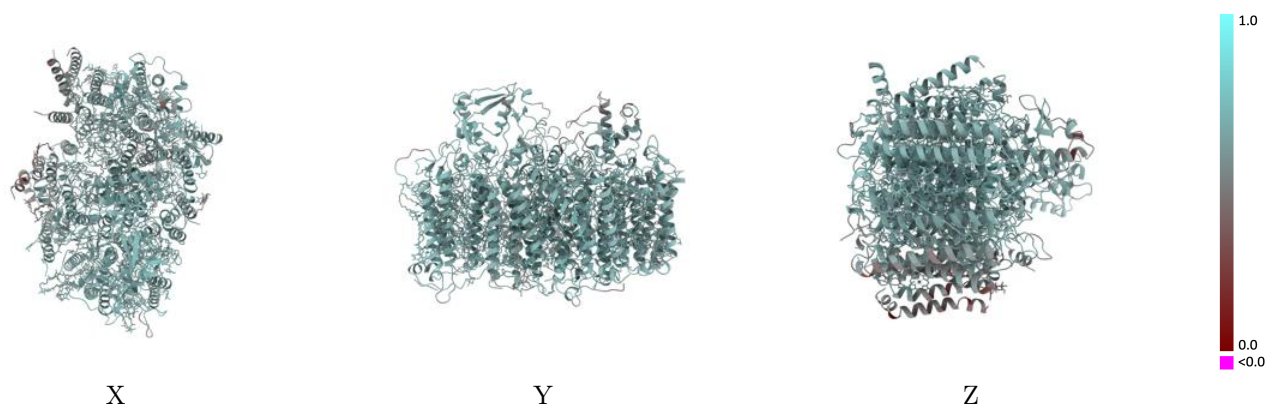
This section contains information regarding the fit between EMDB map EMD-55594 and PDB model 9T5U. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

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



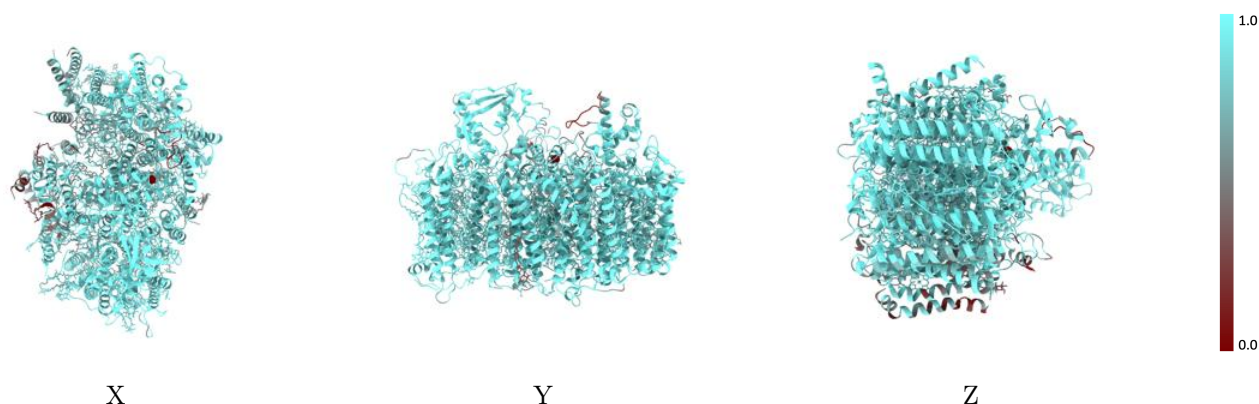
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



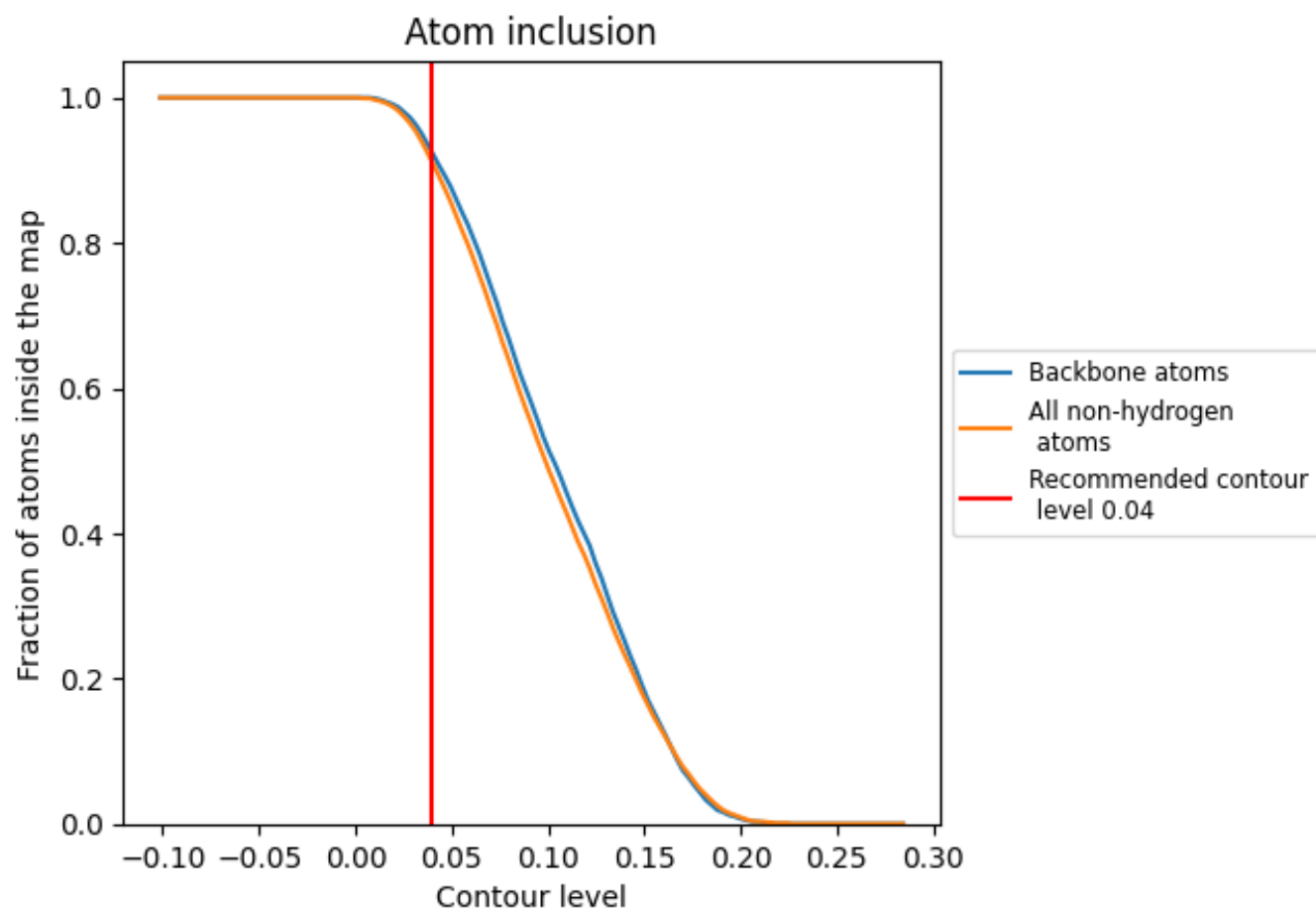
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9110	<div></div> 0.6210
A	<div></div> 0.9400	<div></div> 0.6390
B	<div></div> 0.9500	<div></div> 0.6420
C	<div></div> 0.9130	<div></div> 0.6220
D	<div></div> 0.9410	<div></div> 0.6430
E	<div></div> 0.7550	<div></div> 0.5550
F	<div></div> 0.8160	<div></div> 0.5220
H	<div></div> 0.9680	<div></div> 0.6320
I	<div></div> 0.9560	<div></div> 0.6050
J	<div></div> 0.6570	<div></div> 0.5800
K	<div></div> 0.8920	<div></div> 0.5920
L	<div></div> 0.8690	<div></div> 0.6200
M	<div></div> 0.9260	<div></div> 0.6160
R	<div></div> 0.4890	<div></div> 0.4310
T	<div></div> 0.9260	<div></div> 0.6160
X	<div></div> 0.8830	<div></div> 0.5930
Y	<div></div> 0.7130	<div></div> 0.5080
Z	<div></div> 0.7760	<div></div> 0.5070

1.0

0.0

<0.0