



Full wwPDB EM Validation Report ⓘ

Jul 25, 2026 – 08:12 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, 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) : 2.50

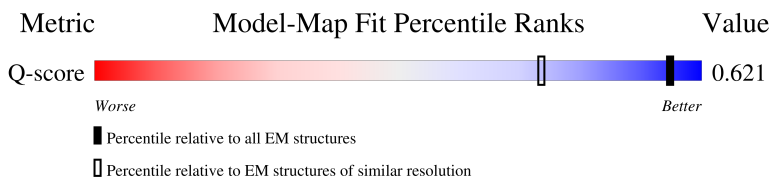
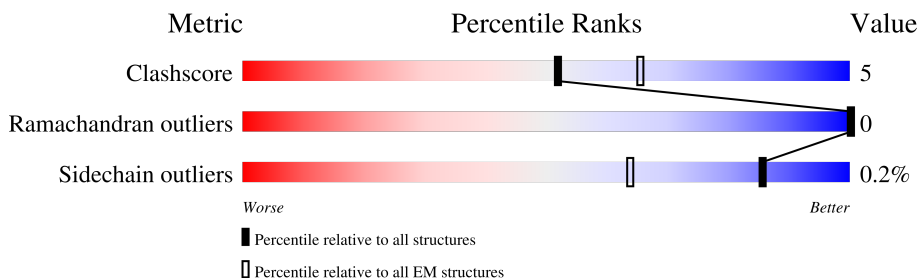
1 Overall quality at a glance

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.



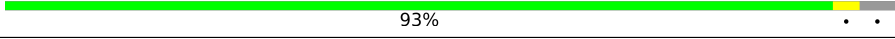
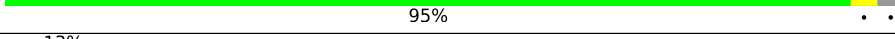
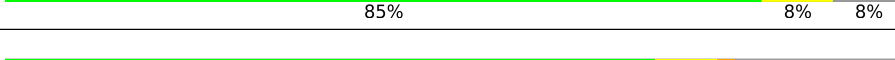
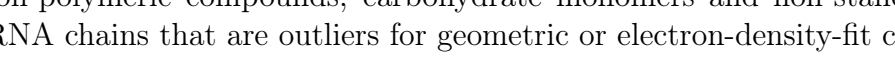
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4434 (1.83 - 2.83)

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 ≥ 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	

Continued on next page...

Continued from previous page...

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		

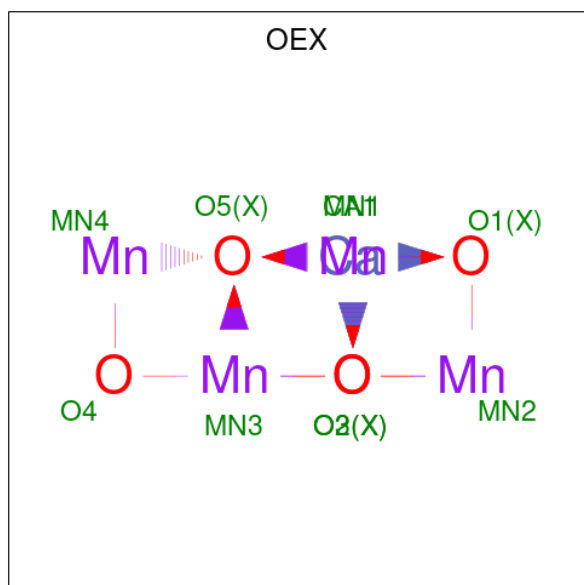
- Molecule 16 is a protein called Ycf12.

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: CaMn_4O_5).



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

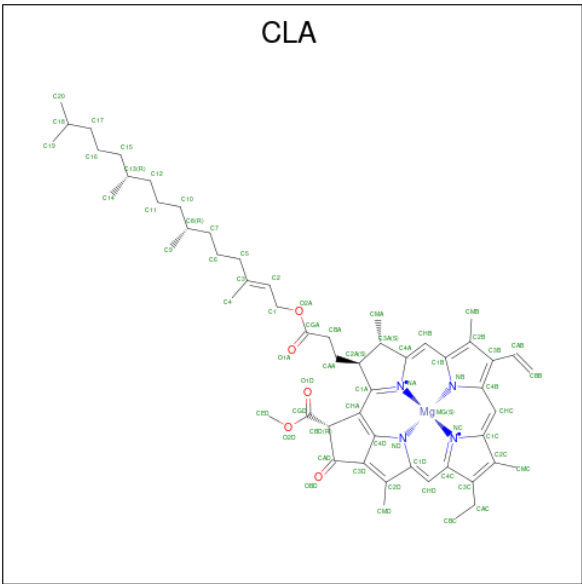
- Molecule 19 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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: C₅₅H₇₂MgN₄O₅).



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	

Continued on next page...

Continued from previous page...

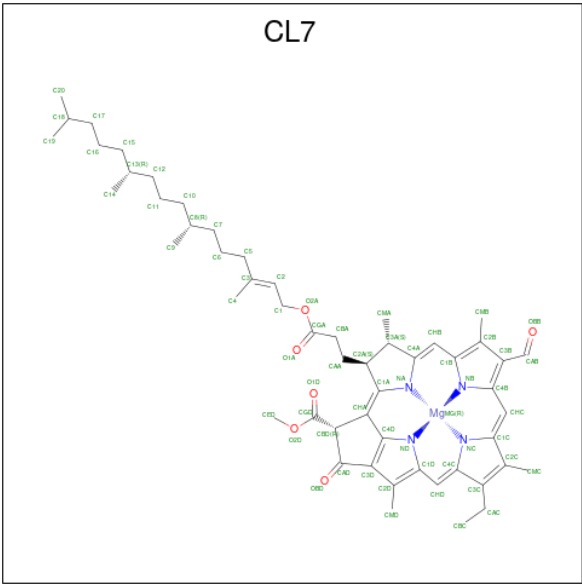
Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total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

Continued on next page...

Continued from previous page...

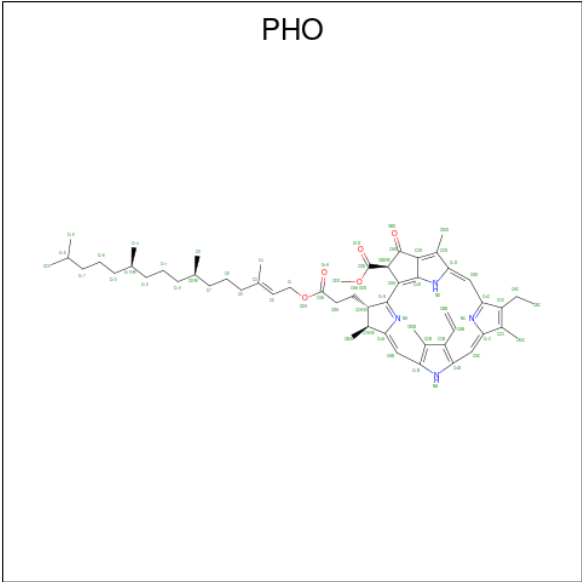
Mol	Chain	Residues	Atoms					AltConf
21	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 22 is CHLOROPHYLL D (CCD ID: CL7) (formula: C₅₄H₇₀MgN₄O₆).



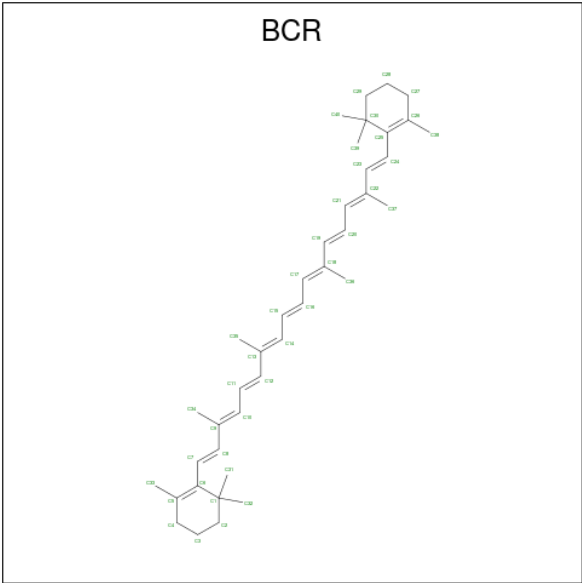
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



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: C₄₀H₅₆).



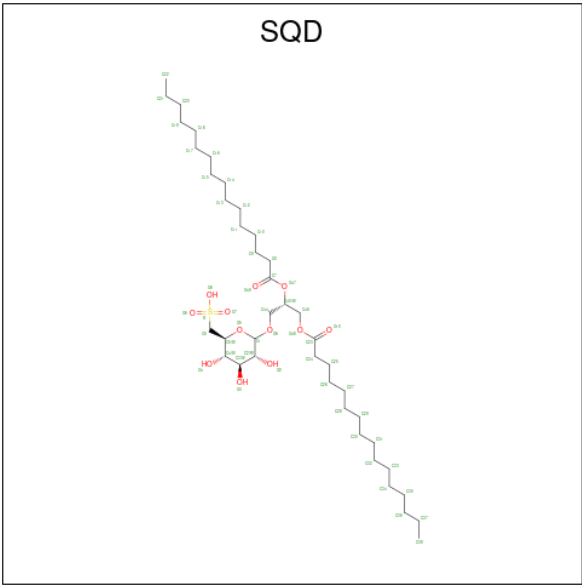
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	C	0
			40	40	
24	B	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

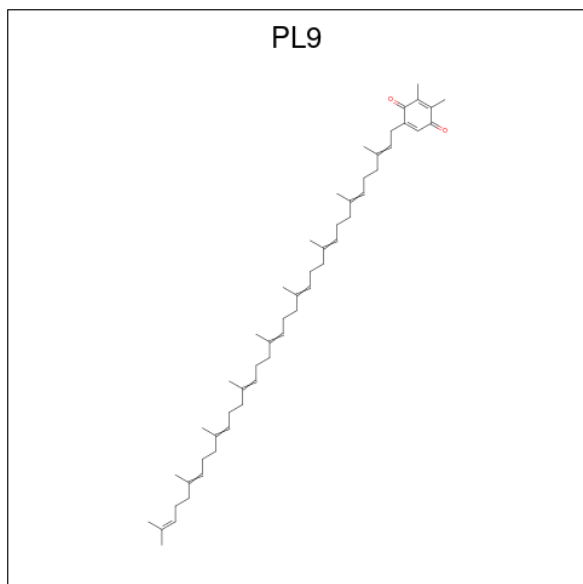
Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	C	1	Total C 40 40	0
24	C	1	Total C 40 40	0
24	D	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	K	1	Total C 40 40	0

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



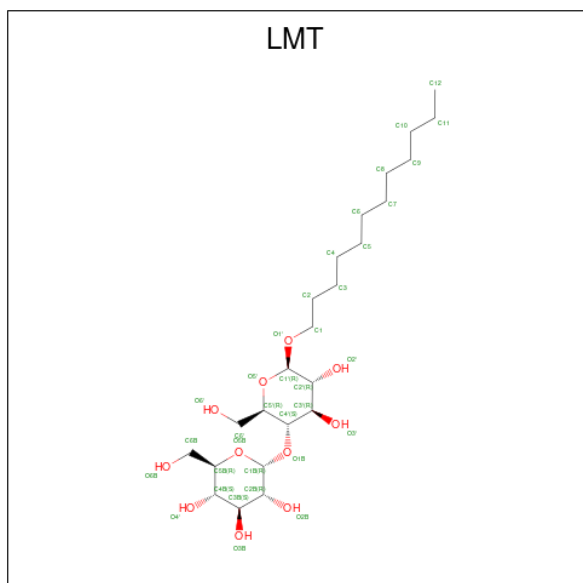
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C O S 54 41 12 1	0
25	D	1	Total C O S 45 32 12 1	0
25	L	1	Total C O S 54 41 12 1	0

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



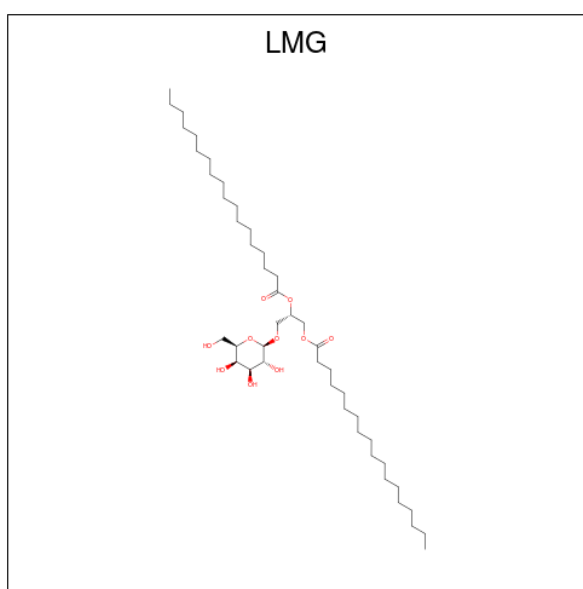
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			55	53	2	
26	D	1	Total	C	O	0
			55	53	2	

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



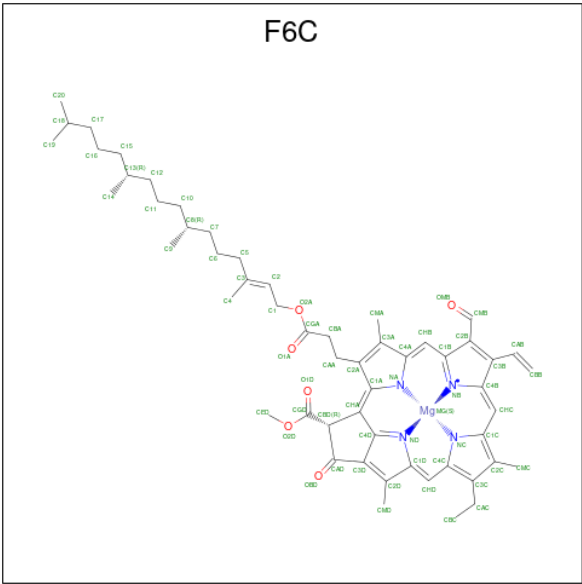
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			35	24	11	
27	F	1	Total	C	O	0
			35	24	11	
27	Z	1	Total	C	O	0
			35	24	11	

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



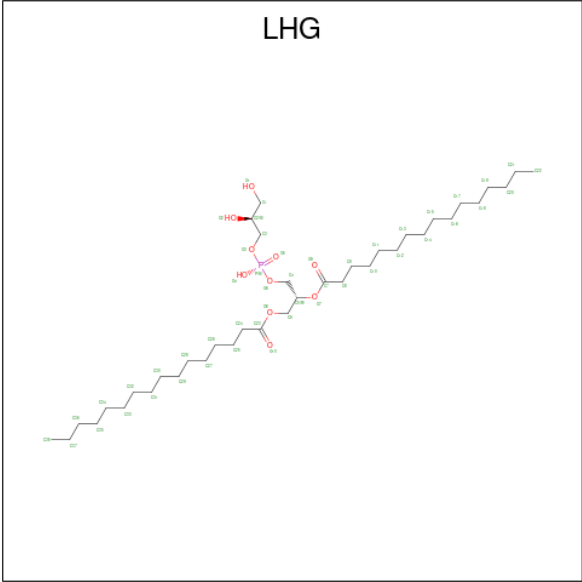
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			41	31	10	
28	B	1	Total	C	O	0
			51	41	10	
28	B	1	Total	C	O	0
			46	36	10	
28	C	1	Total	C	O	0
			51	41	10	
28	D	1	Total	C	O	0
			47	37	10	
28	D	1	Total	C	O	0
			51	41	10	
28	D	1	Total	C	O	0
			44	34	10	

- Molecule 29 is Chlorophyll F (CCD ID: F6C) (formula: C₅₅H₆₈MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



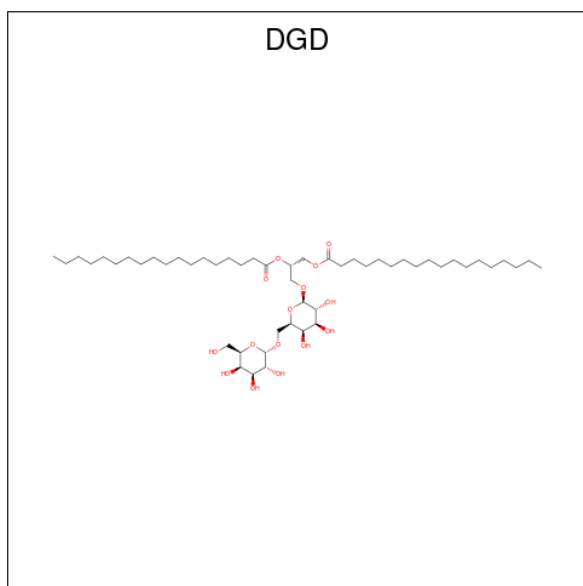
Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
29	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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: $C_{51}H_{96}O_{15}$).



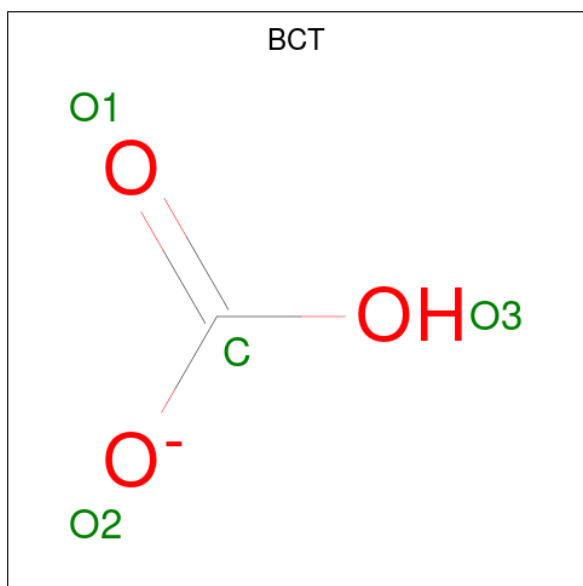
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			62	47	15	
31	D	1	Total	C	O	0
			53	42	11	

Continued on next page...

Continued from previous page...

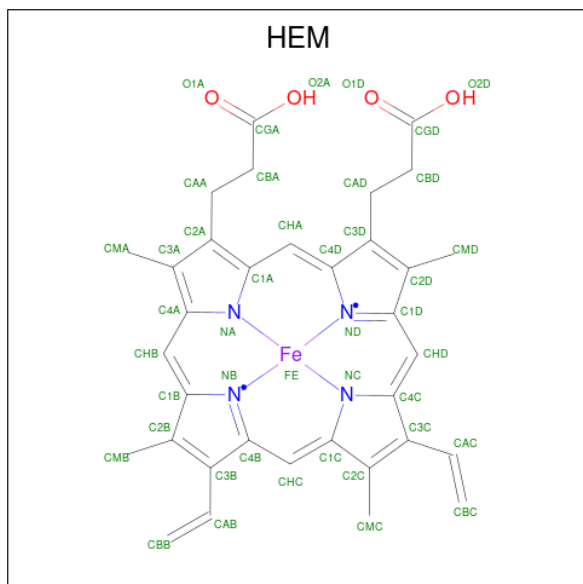
Mol	Chain	Residues	Atoms			AltConf
31	H	1	Total	C	O	0
			62	47	15	

- Molecule 32 is BICARBONATE ION (CCD ID: BCT) (formula: 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	

Continued on next page...

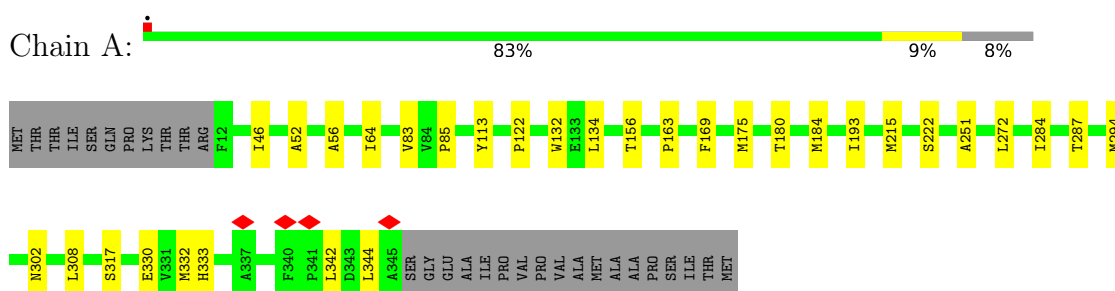
Continued from previous page...

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

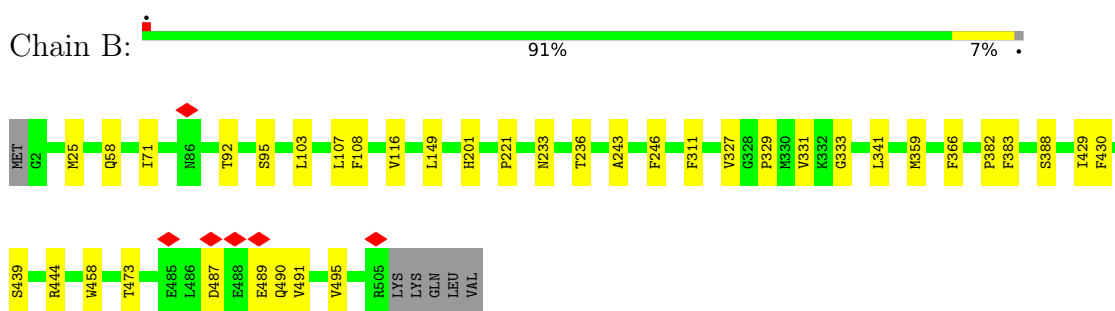
3 Residue-property plots [i](#)

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.

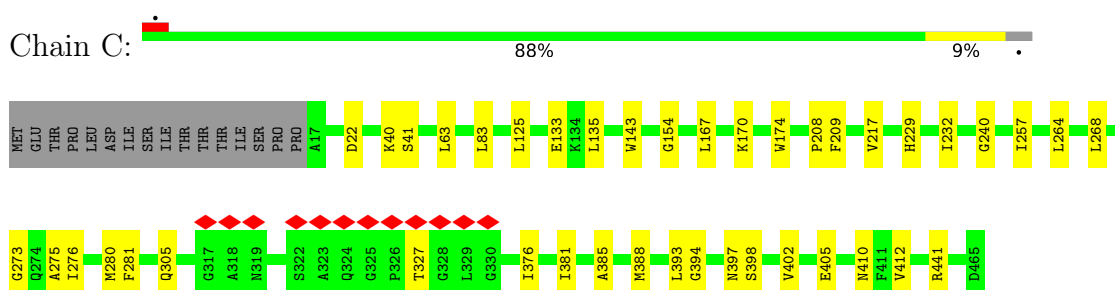
• Molecule 1: PsbA



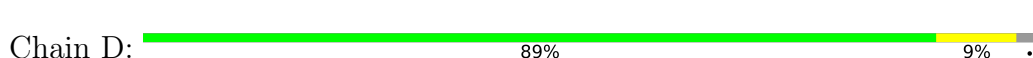
• Molecule 2: PsbB

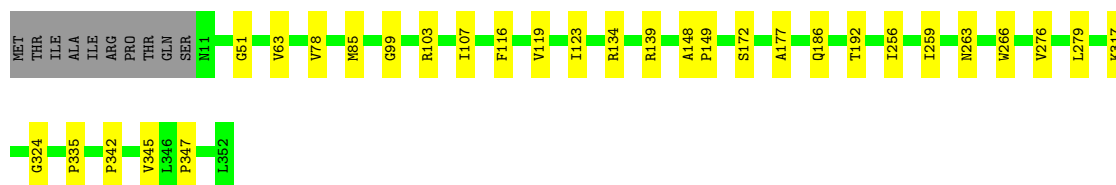


• Molecule 3: PsbC

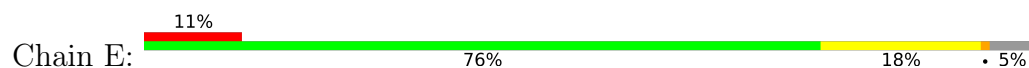


• Molecule 4: PsbD





- Molecule 5: PsbE



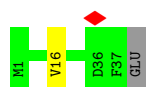
- Molecule 6: PsbF



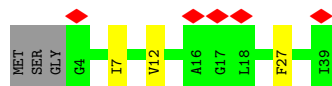
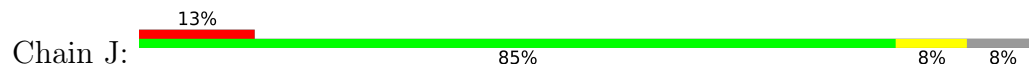
- Molecule 7: PsbH



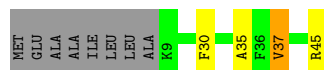
- Molecule 8: PsbI



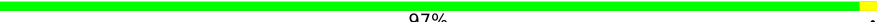
- Molecule 9: PsbJ

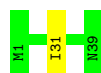


- Molecule 10: PsbK



- Molecule 11: PsbL

Chain L:  97% .



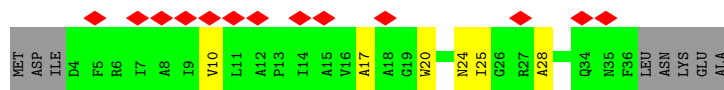
• Molecule 12: PsbM

Chain M:  72% 13% 15%



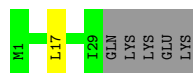
• Molecule 13: PsbY

Chain R:  32% 66% 15% 20%



• Molecule 14: PsbT

Chain T:  82% . 15%



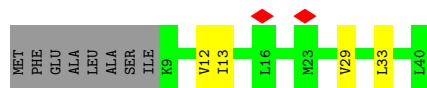
• Molecule 15: PsbX

Chain X:  82% 15% .



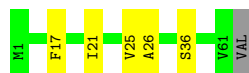
• Molecule 16: Ycf12

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: FME, SQD, OEX, PHO, LMT, LMG, CL7, F6C, CL, BCR, LHG, DGD, BCT, HEM, CLA, FE2, PL9

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

Continued on next page...

Continued from previous page...

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.

All (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
4:D:192:THR:HG23	21:D:402:CLA:HBC2	1.73	0.70
4:D:186:GLN:HB2	21:D:402:CLA:HBC1	1.73	0.69
24:D:404:BCR:H21C	24:D:404:BCR:H361	1.74	0.69
16:Y:29:VAL:HG22	17:Z:21:ILE:HG23	1.75	0.69
21:B:605:CLA:H42	21:B:606:CLA:H2	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:HG2	26:A:414:PL9:H102	1.77	0.67
21:B:602:CLA:HHC	21:B:602:CLA:HBB1	1.77	0.67
21:B:611:CLA:HHC	21:B:611:CLA:HBB1	1.77	0.66
21:B:616:CLA:HHC	21:B:616:CLA:HBB1	1.77	0.66
21:B:610:CLA:HHC	21:B:610:CLA:HBB1	1.79	0.64
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.80	0.64
21:B:606:CLA:HHC	21:B:606:CLA:HBB1	1.77	0.64
3:C:275:ALA:HB2	21:C:502:CLA:HBC3	1.79	0.64
5:E:71:GLU:HB3	5:E:74:LYS:HE2	1.81	0.63
3:C:170:LYS:HA	3:C:174:TRP:HB2	1.80	0.63
1:A:193:ILE:HG13	1:A:294:MET:HE1	1.81	0.63
4:D:259:ILE:HD13	30:D:409:LHG:H262	1.84	0.59
5:E:10:PHE:H	30:E:101:LHG:HC32	1.67	0.59
21:A:410:CLA:H102	8:I:16:VAL:HG11	1.83	0.58
3:C:394:GLY:HA3	3:C:412:VAL:HG22	1.85	0.58
6:F:25:HIS:NE2	33:F:101:HEM:C1B	2.71	0.58
3:C:273:GLY:HA3	21:C:501:CLA:H143	1.86	0.58
5:E:26:THR:HG23	13:R:17:ALA:HB1	1.86	0.57
4:D:324:GLY:HA2	4:D:347:PRO:HG2	1.84	0.57
21:B:605:CLA:H152	30:B:1006:LHG:H192	1.87	0.56
13:R:20:TRP:NE1	13:R:24:ASN:HD21	2.04	0.56
21:C:504:CLA:H121	31:C:517:DGD:HBF2	1.88	0.56
1:A:134:LEU:HD23	4:D:256:ILE:HG12	1.87	0.55
10:K:35:ALA:HB2	24:K:102:BCR:H391	1.86	0.55
12:M:12:LEU:O	12:M:16:LEU:HB2	2.07	0.55
16:Y:12:VAL:HG13	16:Y:13:ILE:HD12	1.87	0.55
3:C:402:VAL:HG22	3:C:405:GLU:HG2	1.88	0.55
1:A:330:GLU:HA	1:A:333:HIS:HD2	1.72	0.55
28:D:630:LMG:H141	28:D:630:LMG:H291	1.88	0.54
2:B:382:PRO:HG3	2:B:388:SER:HB3	1.88	0.54
4:D:134:ARG:HG2	28:D:628:LMG:HC1	1.88	0.54
33:F:101:HEM:HBB2	33:F:101:HEM:HMB2	1.88	0.54
27:B:1008:LMT:H122	30:L:101:LHG:H371	1.88	0.54
25:D:407:SQD:H462	15:X:30:ILE:HD11	1.88	0.54
2:B:116:VAL:HG21	24:B:620:BCR:H292	1.90	0.54
2:B:71:ILE:HD13	21:B:607:CLA:HED1	1.90	0.53
3:C:376:ILE:HG21	3:C:381:ILE:HG23	1.89	0.53
1:A:83:VAL:HB	1:A:175:MET:HB2	1.90	0.53
21:A:410:CLA:H152	21:C:505:CLA:H192	1.91	0.53
15:X:18:ILE:HG23	15:X:19:VAL:HG23	1.89	0.53
21:A:410:CLA:HMB1	21:A:410:CLA:HBB1	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:604:CLA:HBB1	21:B:604:CLA:HMB1	1.91	0.52
21:B:612:CLA:HBB1	21:B:612:CLA:HMB3	1.92	0.52
1:A:317:SER:HA	4:D:63:VAL:HG13	1.92	0.52
21:C:506:CLA:H12	24:C:515:BCR:H323	1.92	0.52
21:C:509:CLA:HBB1	21:C:509:CLA:HMB1	1.92	0.52
1:A:222:SER:HA	4:D:139:ARG:HB2	1.91	0.51
31:C:517:DGD:HB22	28:C:519:LMG:H291	1.92	0.51
2:B:333:GLY:O	2:B:439:SER:HB3	2.10	0.51
21:B:605:CLA:HBB1	21:B:605:CLA:HMB1	1.93	0.51
1:A:163:PRO:HB3	1:A:169:PHE:HA	1.92	0.51
21:B:605:CLA:HBA2	21:B:613:CLA:H152	1.93	0.51
1:A:287:THR:HG23	21:A:405:CLA:HED3	1.93	0.51
21:C:502:CLA:H121	21:C:512:CLA:H2	1.93	0.51
2:B:327:VAL:HG11	28:B:622:LMG:H302	1.93	0.51
21:C:506:CLA:HMB3	21:C:506:CLA:HBB1	1.93	0.51
21:D:402:CLA:HMB1	21:D:402:CLA:HBB1	1.93	0.51
21:B:608:CLA:HMB1	21:B:608:CLA:HBB1	1.94	0.50
3:C:385:ALA:HA	3:C:388:MET:HG2	1.93	0.50
21:C:508:CLA:HMB3	21:C:508:CLA:HBB1	1.94	0.50
21:B:613:CLA:HBB1	21:B:613:CLA:HMB1	1.93	0.50
21:C:512:CLA:HMB3	21:C:512:CLA:HBB1	1.94	0.50
21:B:609:CLA:HBB1	21:B:609:CLA:HMB3	1.93	0.50
1:A:122:PRO:HD3	28:A:413:LMG:H172	1.93	0.50
21:D:403:CLA:HMB1	21:D:403:CLA:HBB1	1.93	0.50
24:B:627:BCR:H401	28:B:1007:LMG:H311	1.92	0.50
21:C:511:CLA:HBB1	21:C:511:CLA:HMB3	1.93	0.50
5:E:15:THR:HG23	9:J:7:ILE:O	2.11	0.50
21:A:405:CLA:HBB1	21:A:405:CLA:HMB1	1.94	0.50
4:D:103:ARG:HD3	5:E:73:LYS:HA	1.94	0.50
21:C:504:CLA:HBB1	21:C:504:CLA:HMB1	1.94	0.49
21:C:513:CLA:HBB1	21:C:513:CLA:HMB3	1.92	0.49
21:C:502:CLA:HMB1	21:C:502:CLA:HBB1	1.94	0.49
21:C:510:CLA:HMB1	21:C:510:CLA:HBB1	1.93	0.49
5:E:35:TRP:CD1	5:E:39:SER:HG	2.31	0.49
30:D:409:LHG:H291	14:T:17:LEU:HD22	1.95	0.49
2:B:489:GLU:HB3	2:B:495:VAL:HG11	1.94	0.49
21:B:603:CLA:HBB1	21:B:603:CLA:HMB1	1.94	0.49
21:A:407:CLA:HBB1	21:A:407:CLA:HMB1	1.94	0.49
25:A:412:SQD:H321	25:A:412:SQD:H352	1.50	0.48
28:A:413:LMG:H241	31:C:516:DGD:HBH2	1.94	0.48
21:B:615:CLA:HBB1	21:B:615:CLA:HMB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:THR:HB	2:B:473:THR:HG21	1.94	0.48
21:C:503:CLA:HBB1	21:C:503:CLA:HMB3	1.94	0.48
5:E:36:LEU:HB3	13:R:10:VAL:HG22	1.95	0.48
21:B:607:CLA:HBB1	21:B:607:CLA:HMB3	1.95	0.48
2:B:233:ASN:O	2:B:236:THR:HG22	2.14	0.48
21:C:501:CLA:HBB1	21:C:501:CLA:HMB3	1.94	0.48
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.48	0.48
21:C:505:CLA:HBB1	21:C:505:CLA:HMB3	1.95	0.48
21:C:506:CLA:H41	21:C:506:CLA:H62	1.65	0.48
3:C:125:LEU:HD22	21:C:511:CLA:H172	1.95	0.48
20:A:403:CL:CL	4:D:317:LYS:HE2	2.50	0.47
26:A:414:PL9:H271	30:E:101:LHG:H223	1.96	0.47
3:C:217:VAL:HG13	3:C:281:PHE:HA	1.95	0.47
16:Y:33:LEU:HD21	17:Z:25:VAL:HA	1.96	0.47
1:A:180:THR:O	1:A:184:MET:HG3	2.13	0.47
2:B:221:PRO:HA	21:B:610:CLA:HED3	1.96	0.47
21:C:501:CLA:C4D	21:C:503:CLA:H2	2.45	0.47
21:B:602:CLA:HBA2	21:B:602:CLA:H11	1.34	0.47
1:A:302:ASN:H	3:C:397:ASN:HD21	1.61	0.47
4:D:263:ASN:HB3	4:D:266:TRP:HB3	1.96	0.47
21:B:615:CLA:HBA2	27:B:1008:LMT:H32	1.96	0.47
31:H:102:DGD:HB62	31:H:102:DGD:HB91	1.77	0.47
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.50	0.47
21:B:606:CLA:H92	21:B:606:CLA:H52	1.97	0.47
31:C:518:DGD:HAF2	28:D:411:LMG:H202	1.96	0.47
6:F:24:VAL:HG23	6:F:25:HIS:ND1	2.29	0.46
2:B:329:PRO:HB2	2:B:331:VAL:HG22	1.97	0.46
28:B:1007:LMG:H162	28:B:1007:LMG:H402	1.98	0.46
30:D:410:LHG:H152	30:D:410:LHG:H321	1.98	0.46
1:A:272:LEU:HD11	26:A:414:PL9:C4	2.46	0.46
24:K:101:BCR:H322	17:Z:17:PHE:HD2	1.81	0.46
2:B:25:MET:HE1	2:B:108:PHE:HD1	1.81	0.46
5:E:22:ILE:HG12	13:R:24:ASN:HD22	1.81	0.46
2:B:58:GLN:C	2:B:329:PRO:HB3	2.41	0.46
21:B:617:CLA:HBB1	21:B:617:CLA:HMB3	1.97	0.46
1:A:85:PRO:HA	1:A:113:TYR:CG	2.51	0.46
23:A:408:PHO:H2	23:A:408:PHO:H61	1.72	0.46
26:A:414:PL9:H301	26:A:414:PL9:H321	1.59	0.45
21:C:512:CLA:H143	24:C:514:BCR:H23C	1.98	0.45
13:R:25:ILE:HG23	13:R:28:ALA:HB3	1.98	0.45
21:C:501:CLA:C3D	21:C:503:CLA:H2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:C:517:DGD:HA82	28:C:519:LMG:H352	1.98	0.45
21:A:410:CLA:H203	21:C:506:CLA:H101	1.97	0.45
2:B:201:HIS:HB2	21:B:603:CLA:CHB	2.47	0.44
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.52	0.44
3:C:41:SER:HB2	3:C:135:LEU:H	1.82	0.44
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.99	0.44
1:A:132:TRP:CH2	21:C:505:CLA:HAA2	2.53	0.44
3:C:280:MET:HG3	31:C:516:DGD:HB32	1.99	0.44
10:K:37:VAL:HG23	24:K:101:BCR:H20C	2.00	0.44
1:A:52:ALA:HA	1:A:56:ALA:HB2	2.00	0.44
4:D:85:MET:HE3	4:D:107:ILE:HB	2.00	0.44
4:D:99:GLY:HA3	28:D:630:LMG:H111	1.98	0.44
30:D:410:LHG:H341	30:D:410:LHG:H151	1.98	0.44
1:A:46:ILE:HD11	23:A:408:PHO:H51	2.00	0.44
21:C:512:CLA:H142	21:C:513:CLA:H93	2.00	0.44
25:D:407:SQD:H441	6:F:17:PHE:O	2.17	0.44
3:C:273:GLY:O	3:C:276:ILE:HG22	2.18	0.43
21:D:403:CLA:H61	21:D:403:CLA:H41	1.62	0.43
26:D:405:PL9:H411	11:L:31:ILE:HG21	2.00	0.43
28:D:411:LMG:H112	9:J:27:PHE:HB3	2.00	0.43
26:A:414:PL9:H512	25:D:407:SQD:H331	1.99	0.43
21:C:502:CLA:H62	21:C:502:CLA:H41	1.87	0.43
4:D:123:ILE:HD11	31:H:102:DGD:HAE1	2.00	0.43
3:C:229:HIS:HA	3:C:232:ILE:HG22	2.00	0.43
21:C:502:CLA:HBD	21:C:503:CLA:H43	2.00	0.43
6:F:29:VAL:HB	6:F:30:PRO:HD3	2.00	0.43
21:C:505:CLA:HBC2	24:C:515:BCR:H341	2.01	0.43
31:C:517:DGD:HA61	31:C:517:DGD:HA92	1.81	0.43
21:B:615:CLA:H121	21:B:615:CLA:H91	1.99	0.43
6:F:28:ALA:O	6:F:32:VAL:HG22	2.19	0.43
1:A:344:LEU:HA	3:C:393:LEU:HD11	2.01	0.43
3:C:398:SER:HA	3:C:412:VAL:HG23	2.01	0.43
28:A:413:LMG:HC8	3:C:208:PRO:HB3	2.00	0.43
2:B:201:HIS:HB2	21:B:603:CLA:C1B	2.49	0.43
21:C:505:CLA:H61	21:C:505:CLA:H2	1.82	0.43
28:A:413:LMG:H182	31:C:516:DGD:HA91	2.00	0.42
24:B:620:BCR:H331	30:B:1006:LHG:H222	2.01	0.42
2:B:383:PHE:CD2	4:D:347:PRO:HA	2.54	0.42
26:A:414:PL9:H271	26:A:414:PL9:H251	1.75	0.42
2:B:107:LEU:HD21	21:B:616:CLA:H43	2.01	0.42
31:C:516:DGD:HB72	31:C:516:DGD:HA72	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:HB2	3:C:305:GLN:NE2	2.35	0.42
21:B:616:CLA:H172	21:B:616:CLA:H121	2.00	0.42
21:C:510:CLA:H2	21:C:510:CLA:H61	1.58	0.42
2:B:103:LEU:HD21	21:B:606:CLA:HMC2	2.01	0.42
2:B:341:LEU:HD12	2:B:429:ILE:HG22	2.01	0.42
24:B:627:BCR:H371	15:X:9:LEU:HD21	2.00	0.42
3:C:264:LEU:O	3:C:268:LEU:HG	2.19	0.42
21:C:502:CLA:HBA2	21:C:503:CLA:H171	2.01	0.42
2:B:329:PRO:O	2:B:444:ARG:HD3	2.19	0.42
3:C:125:LEU:HD21	21:C:511:CLA:H152	2.01	0.42
3:C:154:GLY:HA2	3:C:240:GLY:HA2	2.01	0.42
21:C:513:CLA:H61	21:C:513:CLA:H41	1.79	0.42
2:B:359:MET:HG3	2:B:366:PHE:HB2	2.00	0.42
24:K:101:BCR:H392	24:K:101:BCR:H24C	1.75	0.42
17:Z:26:ALA:HB1	17:Z:36:SER:HB3	2.02	0.42
26:A:414:PL9:H171	26:A:414:PL9:H151	1.88	0.41
5:E:18:ARG:O	5:E:21:VAL:HG12	2.20	0.41
2:B:201:HIS:HE2	21:B:604:CLA:C2B	2.33	0.41
24:B:619:BCR:H11C	24:B:619:BCR:H341	1.89	0.41
3:C:22:ASP:HB3	10:K:45:ARG:HD2	2.02	0.41
1:A:156:THR:HG21	31:C:516:DGD:HBW2	2.02	0.41
3:C:209:PHE:HD1	31:C:516:DGD:HB21	1.85	0.41
3:C:410:ASN:HB2	31:C:518:DGD:HE2	2.03	0.41
1:A:284:ILE:HA	1:A:287:THR:HG22	2.01	0.41
12:M:17:VAL:HB	12:M:18:PRO:HD3	2.02	0.41
21:B:603:CLA:H41	7:H:46:LEU:HA	2.03	0.41
3:C:40:LYS:HD3	3:C:133:GLU:HG2	2.03	0.41
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.02	0.41
21:B:602:CLA:HBB2	24:B:627:BCR:H351	2.03	0.41
21:B:611:CLA:H122	21:B:616:CLA:HAA1	2.02	0.41
1:A:332:MET:CG	4:D:324:GLY:HA3	2.51	0.41
2:B:458:TRP:HB3	21:B:605:CLA:HBC2	2.02	0.41
3:C:83:LEU:HD13	21:C:503:CLA:HED3	2.02	0.41
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.41
25:A:412:SQD:H341	25:A:412:SQD:H372	1.84	0.41
2:B:149:LEU:HD21	21:B:605:CLA:H91	2.03	0.41
2:B:487:ASP:O	2:B:490:GLN:HG2	2.20	0.41
3:C:63:LEU:HD22	21:C:503:CLA:HED2	2.03	0.41
3:C:257:ILE:HG13	3:C:441:ARG:HD2	2.03	0.41
28:C:519:LMG:H221	10:K:30:PHE:HE1	1.86	0.41
4:D:335:PRO:HB2	5:E:65:ILE:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:342:PRO:O	4:D:345:VAL:HG22	2.21	0.41
21:D:403:CLA:H111	15:X:12:LEU:HB3	2.03	0.41
5:E:20:TRP:HZ2	9:J:12:VAL:HG13	1.86	0.41
24:K:102:BCR:H24C	24:K:102:BCR:H371	1.73	0.41
1:A:64:ILE:HD12	3:C:327:THR:HG21	2.03	0.41
24:B:618:BCR:H11C	24:B:618:BCR:H341	1.91	0.41
3:C:167:LEU:HD22	21:C:501:CLA:C2D	2.51	0.41
24:C:515:BCR:H24C	24:C:515:BCR:H371	1.90	0.41
22:A:406:CL7:H92C	30:D:409:LHG:H172	2.03	0.40
1:A:332:MET:HG3	4:D:324:GLY:HA3	2.03	0.40
25:A:412:SQD:H221	31:C:518:DGD:HAF1	2.03	0.40
2:B:92:THR:H	2:B:95:SER:HB2	1.86	0.40
4:D:116:PHE:O	4:D:119:VAL:HG12	2.21	0.40
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.03	0.40
7:H:53:ILE:HD11	15:X:8:PHE:CG	2.56	0.40
12:M:25:LEU:HD23	12:M:25:LEU:HA	1.91	0.40
2:B:103:LEU:HD22	21:B:607:CLA:H51	2.03	0.40
3:C:143:TRP:CZ3	21:C:509:CLA:H202	2.57	0.40
25:A:412:SQD:H383	24:K:101:BCR:H393	2.04	0.40

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	332/363 (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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	274	GLN
2	B	343	HIS
2	B	409	GLN
3	C	253	HIS
3	C	397	ASN
4	D	186	GLN
10	K	39	GLN
13	R	24	ASN

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

All (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
11	L	1	FME	CB-CG-SD-CE
14	T	1	FME	CB-CG-SD-CE
11	L	1	FME	CA-CB-CG-SD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	X	1	FME	CB-CG-SD-CE
11	L	1	FME	C-CA-CB-CG
12	M	1	FME	N-CA-CB-CG
15	X	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	D	409	-	48,48,48	0.51	0	51,54,54	0.49	0
21	CLA	B	605	2	69,73,73	1.20	8 (11%)	83,113,113	0.95	4 (4%)
28	LMG	D	411	-	51,51,55	0.53	0	59,59,63	0.63	0
21	CLA	B	617	2	49,53,73	1.40	7 (14%)	59,89,113	1.09	5 (8%)
24	BCR	K	102	-	41,41,41	0.31	0	56,56,56	0.76	0
21	CLA	D	402	4	69,73,73	1.17	6 (8%)	83,113,113	0.92	4 (4%)
25	SQD	D	407	-	44,45,54	1.61	7 (15%)	53,56,65	1.45	6 (11%)
21	CLA	D	403	4	69,73,73	1.17	7 (10%)	83,113,113	0.95	4 (4%)
31	DGD	C	516	-	63,63,67	0.59	0	77,77,81	0.69	2 (2%)
21	CLA	B	613	2	69,73,73	1.18	8 (11%)	83,113,113	0.93	4 (4%)
28	LMG	B	1007	-	46,46,55	0.53	0	54,54,63	0.63	0
21	CLA	B	615	2	69,73,73	1.16	6 (8%)	83,113,113	0.94	4 (4%)
21	CLA	A	405	1	69,73,73	1.17	7 (10%)	83,113,113	0.92	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	D	408	-	48,48,48	0.51	0	51,54,54	0.49	0
30	LHG	D	629	-	48,48,48	0.49	0	51,54,54	0.63	1 (1%)
33	HEM	F	101	5,6	50,50,50	1.40	6 (12%)	66,82,82	1.23	5 (7%)
21	CLA	C	505	3	69,73,73	1.19	8 (11%)	83,113,113	0.94	4 (4%)
29	F6C	B	614	2	72,74,74	1.67	10 (13%)	81,114,114	2.04	16 (19%)
24	BCR	B	619	-	41,41,41	0.31	0	56,56,56	0.72	1 (1%)
28	LMG	D	630	-	44,44,55	0.52	0	52,52,63	0.64	0
24	BCR	D	404	-	41,41,41	0.32	0	56,56,56	0.87	3 (5%)
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	B	603	2	69,73,73	1.16	7 (10%)	83,113,113	0.94	4 (4%)
24	BCR	B	618	-	41,41,41	0.32	0	56,56,56	0.64	1 (1%)
21	CLA	C	504	34	69,73,73	1.16	6 (8%)	83,113,113	0.96	5 (6%)
26	PL9	D	405	-	55,55,55	1.22	4 (7%)	68,69,69	1.55	12 (17%)
25	SQD	A	412	-	53,54,54	1.53	7 (13%)	62,65,65	1.38	6 (9%)
24	BCR	B	620	-	41,41,41	0.31	0	56,56,56	0.59	0
21	CLA	C	511	3	69,73,73	1.19	8 (11%)	83,113,113	0.95	4 (4%)
30	LHG	B	1006	-	44,44,48	0.53	0	47,50,54	0.51	0
24	BCR	K	101	-	41,41,41	0.32	0	56,56,56	0.93	2 (3%)
28	LMG	C	519	-	51,51,55	0.52	0	59,59,63	0.62	0
21	CLA	B	604	2	69,73,73	1.16	7 (10%)	83,113,113	0.90	3 (3%)
28	LMG	A	413	-	41,41,55	0.53	0	49,49,63	0.64	0
21	CLA	A	410	1	69,73,73	1.16	6 (8%)	83,113,113	0.96	4 (4%)
29	F6C	C	507	34	67,69,74	1.75	11 (16%)	75,108,114	2.14	16 (21%)
21	CLA	B	611	34	69,73,73	1.16	6 (8%)	83,113,113	1.00	4 (4%)
21	CLA	B	610	2	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
32	BCT	D	401	19	2,3,3	0.88	0	2,3,3	3.23	2 (100%)
21	CLA	C	502	3	69,73,73	1.19	7 (10%)	83,113,113	0.95	5 (6%)
26	PL9	A	414	-	55,55,55	1.04	4 (7%)	68,69,69	1.52	13 (19%)
30	LHG	L	101	-	48,48,48	0.51	0	51,54,54	0.51	0
21	CLA	B	609	2	69,73,73	1.18	8 (11%)	83,113,113	0.93	4 (4%)
24	BCR	C	515	-	41,41,41	0.31	0	56,56,56	0.64	0
22	CL7	A	406	34	71,73,73	1.14	5 (7%)	80,113,113	0.84	3 (3%)
24	BCR	A	411	-	41,41,41	0.30	0	56,56,56	0.49	0
21	CLA	B	606	2	69,73,73	1.19	7 (10%)	83,113,113	0.99	4 (4%)
21	CLA	A	407	34	69,73,73	1.15	6 (8%)	83,113,113	0.95	4 (4%)
28	LMG	B	622	-	51,51,55	0.51	0	59,59,63	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMT	B	1008	-	36,36,36	0.58	0	47,47,47	0.70	0
23	PHO	A	409	-	58,69,69	1.99	10 (17%)	56,99,99	1.55	7 (12%)
21	CLA	B	616	2	69,73,73	1.21	7 (10%)	83,113,113	1.00	4 (4%)
21	CLA	B	607	2	59,63,73	1.28	6 (10%)	71,101,113	0.99	4 (5%)
28	LMG	D	628	-	47,47,55	0.51	0	55,55,63	0.62	0
21	CLA	C	503	3	69,73,73	1.20	7 (10%)	83,113,113	0.98	5 (6%)
23	PHO	A	408	-	58,69,69	1.99	11 (18%)	56,99,99	1.53	6 (10%)
21	CLA	C	508	3	69,73,73	1.18	7 (10%)	83,113,113	0.93	5 (6%)
31	DGD	C	518	-	63,63,67	0.56	0	77,77,81	0.64	0
21	CLA	B	612	2	69,73,73	1.18	7 (10%)	83,113,113	0.97	5 (6%)
21	CLA	C	506	3	69,73,73	1.17	7 (10%)	83,113,113	0.95	4 (4%)
21	CLA	B	602	34	51,55,73	1.38	7 (13%)	61,91,113	1.18	5 (8%)
21	CLA	C	513	3	69,73,73	1.15	6 (8%)	83,113,113	0.97	4 (4%)
25	SQD	L	103	-	53,54,54	1.54	8 (15%)	62,65,65	1.39	6 (9%)
24	BCR	B	627	-	41,41,41	0.32	0	56,56,56	0.88	1 (1%)
27	LMT	A	419	-	36,36,36	0.56	0	47,47,47	0.68	0
31	DGD	D	406	-	53,53,67	0.51	0	60,61,81	0.60	0
27	LMT	F	102	-	36,36,36	0.54	0	47,47,47	0.68	0
31	DGD	C	517	-	63,63,67	0.56	0	77,77,81	0.68	0
30	LHG	D	410	-	45,45,48	0.53	0	48,51,54	0.48	0
31	DGD	H	102	-	63,63,67	0.57	0	77,77,81	0.76	0
27	LMT	Z	102	-	36,36,36	0.53	0	47,47,47	0.72	0
21	CLA	C	501	3	69,73,73	1.17	6 (8%)	83,113,113	0.98	5 (6%)
18	OEX	A	401	3,1	0,15,15	-	-	-	-	-
24	BCR	C	514	-	41,41,41	0.30	0	56,56,56	0.47	0
21	CLA	B	608	34	69,73,73	1.17	6 (8%)	83,113,113	0.92	4 (4%)
21	CLA	C	510	3	69,73,73	1.18	7 (10%)	83,113,113	0.94	4 (4%)
21	CLA	C	509	3	69,73,73	1.17	7 (10%)	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
30	LHG	D	409	-	-	10/53/53/53	-
24	BCR	D	404	-	-	11/29/63/63	0/2/2/2
21	CLA	C	503	3	-	2/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	C	502	3	-	7/39/115/115	-
21	CLA	B	605	2	-	7/39/115/115	-
21	CLA	C	508	3	-	3/39/115/115	-
23	PHO	A	408	-	-	7/37/103/103	0/5/6/6
26	PL9	A	414	-	-	23/53/73/73	0/1/1/1
31	DGD	C	518	-	-	4/51/91/95	0/2/2/2
28	LMG	D	411	-	-	11/46/66/70	0/1/1/1
21	CLA	B	612	2	-	2/39/115/115	-
21	CLA	B	617	2	-	0/15/91/115	-
21	CLA	B	602	34	-	6/18/94/115	-
21	CLA	C	506	3	-	6/39/115/115	-
21	CLA	C	512	3	-	4/39/115/115	-
21	CLA	C	513	3	-	10/39/115/115	-
21	CLA	B	603	2	-	2/39/115/115	-
24	BCR	B	618	-	-	4/29/63/63	0/2/2/2
24	BCR	K	102	-	-	3/29/63/63	0/2/2/2
25	SQD	L	103	-	-	27/49/69/69	0/1/1/1
21	CLA	C	504	34	-	3/39/115/115	-
21	CLA	D	402	4	-	3/39/115/115	-
26	PL9	D	405	-	-	5/53/73/73	0/1/1/1
24	BCR	B	627	-	-	5/29/63/63	0/2/2/2
30	LHG	E	101	-	-	20/53/53/53	-
30	LHG	L	101	-	-	10/53/53/53	-
25	SQD	A	412	-	-	27/49/69/69	0/1/1/1
25	SQD	D	407	-	-	22/40/60/69	0/1/1/1
21	CLA	D	403	4	-	6/39/115/115	-
31	DGD	C	516	-	-	15/51/91/95	0/2/2/2
21	CLA	B	613	2	-	2/39/115/115	-
24	BCR	B	620	-	-	2/29/63/63	0/2/2/2
21	CLA	C	511	3	-	1/39/115/115	-
21	CLA	B	609	2	-	0/39/115/115	-
27	LMT	A	419	-	-	6/21/61/61	0/2/2/2
30	LHG	B	1006	-	-	10/49/49/53	-
24	BCR	K	101	-	-	9/29/63/63	0/2/2/2
27	LMT	F	102	-	-	6/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	C	519	-	-	8/46/66/70	0/1/1/1
21	CLA	B	604	2	-	1/39/115/115	-
21	CLA	B	615	2	-	7/39/115/115	-
28	LMG	B	1007	-	-	13/41/61/70	0/1/1/1
24	BCR	C	515	-	-	1/29/63/63	0/2/2/2
21	CLA	A	405	1	-	1/39/115/115	-
30	LHG	D	410	-	-	9/50/50/53	-
22	CL7	A	406	34	2/2/15/20	2/39/115/115	-
31	DGD	C	517	-	-	12/51/91/95	0/2/2/2
28	LMG	A	413	-	-	9/36/56/70	0/1/1/1
31	DGD	D	406	-	-	8/47/68/95	0/1/1/2
24	BCR	A	411	-	-	2/29/63/63	0/2/2/2
31	DGD	H	102	-	-	17/51/91/95	0/2/2/2
30	LHG	D	408	-	-	16/53/53/53	-
27	LMT	Z	102	-	-	5/21/61/61	0/2/2/2
30	LHG	D	629	-	-	18/53/53/53	-
21	CLA	B	606	2	-	4/39/115/115	-
21	CLA	C	501	3	-	1/39/115/115	-
21	CLA	A	407	34	-	3/39/115/115	-
33	HEM	F	101	5,6	-	2/14/54/54	-
21	CLA	A	410	1	-	2/39/115/115	-
29	F6C	C	507	34	1/1/9/16	6/35/91/97	-
21	CLA	C	505	3	-	7/39/115/115	-
24	BCR	C	514	-	-	2/29/63/63	0/2/2/2
28	LMG	B	622	-	-	12/46/66/70	0/1/1/1
29	F6C	B	614	2	1/1/10/16	13/41/97/97	-
21	CLA	B	611	34	-	1/39/115/115	-
21	CLA	B	608	34	-	4/39/115/115	-
23	PHO	A	409	-	-	6/37/103/103	0/5/6/6
27	LMT	B	1008	-	-	6/21/61/61	0/2/2/2
21	CLA	C	510	3	-	5/39/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
21	CLA	B	616	2	-	1/39/115/115	-
21	CLA	B	610	2	-	1/39/115/115	-
21	CLA	C	509	3	-	3/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	D	630	-	-	7/39/59/70	0/1/1/1
21	CLA	B	607	2	-	5/27/103/115	-
28	LMG	D	628	-	-	13/42/62/70	0/1/1/1

All (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
23	A	408	PHO	C3B-C4B	7.28	1.49	1.41
22	A	406	CL7	C1C-C2C	-4.69	1.36	1.45
25	D	407	SQD	O48-C23	4.68	1.47	1.33
25	L	103	SQD	O48-C23	4.61	1.46	1.33
25	A	412	SQD	O48-C23	4.59	1.46	1.33
21	D	402	CLA	C4C-C3C	-4.57	1.37	1.45
21	B	613	CLA	C4C-C3C	-4.54	1.37	1.45
21	B	606	CLA	C4C-C3C	-4.53	1.37	1.45
21	C	501	CLA	C4C-C3C	-4.53	1.37	1.45
21	B	612	CLA	C4C-C3C	-4.52	1.37	1.45
21	C	508	CLA	C4C-C3C	-4.52	1.37	1.45
21	B	608	CLA	C4C-C3C	-4.50	1.37	1.45
21	A	410	CLA	C4C-C3C	-4.48	1.37	1.45
21	B	610	CLA	C4C-C3C	-4.47	1.37	1.45
21	C	504	CLA	C4C-C3C	-4.47	1.37	1.45
21	B	604	CLA	C4C-C3C	-4.46	1.37	1.45
21	B	607	CLA	C4C-C3C	-4.46	1.37	1.45
21	B	615	CLA	C4C-C3C	-4.46	1.37	1.45
21	C	511	CLA	C4C-C3C	-4.46	1.37	1.45
21	D	403	CLA	C4C-C3C	-4.46	1.37	1.45
21	C	512	CLA	C4C-C3C	-4.45	1.37	1.45
22	A	406	CL7	C4C-C3C	-4.45	1.37	1.45
21	B	603	CLA	C4C-C3C	-4.45	1.37	1.45
21	B	616	CLA	C4C-C3C	-4.45	1.37	1.45
21	B	609	CLA	C4C-C3C	-4.44	1.37	1.45
21	C	503	CLA	C4C-C3C	-4.44	1.37	1.45
21	C	510	CLA	C4C-C3C	-4.44	1.37	1.45
21	C	505	CLA	C4C-C3C	-4.44	1.37	1.45
21	A	405	CLA	C4C-C3C	-4.43	1.37	1.45
21	C	509	CLA	C4C-C3C	-4.43	1.37	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	513	CLA	C4C-C3C	-4.43	1.37	1.45
21	C	502	CLA	C1C-C2C	-4.43	1.36	1.44
21	B	607	CLA	C1C-C2C	-4.42	1.36	1.44
21	C	506	CLA	C4C-C3C	-4.42	1.37	1.45
21	B	611	CLA	C4C-C3C	-4.42	1.37	1.45
21	B	617	CLA	C1C-C2C	-4.41	1.36	1.44
21	B	605	CLA	C1C-C2C	-4.39	1.36	1.44
21	A	407	CLA	C4C-C3C	-4.39	1.37	1.45
21	B	617	CLA	C4C-C3C	-4.39	1.37	1.45
21	B	602	CLA	C4C-C3C	-4.38	1.37	1.45
21	C	501	CLA	C1C-C2C	-4.37	1.36	1.44
21	B	608	CLA	C1C-C2C	-4.36	1.36	1.44
21	B	609	CLA	C1C-C2C	-4.35	1.36	1.44
21	C	503	CLA	C1C-C2C	-4.35	1.36	1.44
21	B	604	CLA	C1C-C2C	-4.35	1.36	1.44
21	B	616	CLA	C1C-C2C	-4.35	1.36	1.44
21	B	612	CLA	C1C-C2C	-4.34	1.36	1.44
21	C	502	CLA	C4C-C3C	-4.34	1.37	1.45
21	B	605	CLA	C4C-C3C	-4.34	1.37	1.45
21	A	407	CLA	C1C-C2C	-4.34	1.36	1.44
29	B	614	F6C	OMB-CMB	-4.34	1.12	1.22
21	A	405	CLA	C1C-C2C	-4.34	1.36	1.44
21	C	504	CLA	C1C-C2C	-4.34	1.36	1.44
21	C	506	CLA	C1C-C2C	-4.34	1.36	1.44
21	C	511	CLA	C1C-C2C	-4.33	1.36	1.44
21	C	508	CLA	C1C-C2C	-4.33	1.36	1.44
21	B	615	CLA	C1C-C2C	-4.32	1.36	1.44
21	B	602	CLA	C1C-C2C	-4.32	1.36	1.44
21	B	611	CLA	C1C-C2C	-4.32	1.36	1.44
21	C	509	CLA	C1C-C2C	-4.32	1.36	1.44
21	B	610	CLA	C1C-C2C	-4.31	1.36	1.44
21	C	510	CLA	C1C-C2C	-4.31	1.36	1.44
21	D	403	CLA	C1C-C2C	-4.30	1.36	1.44
21	C	505	CLA	C1C-C2C	-4.30	1.36	1.44
21	D	402	CLA	C1C-C2C	-4.30	1.36	1.44
21	A	410	CLA	C1C-C2C	-4.29	1.36	1.44
21	B	603	CLA	C1C-C2C	-4.29	1.36	1.44
21	B	606	CLA	C1C-C2C	-4.28	1.36	1.44
21	B	613	CLA	C1C-C2C	-4.27	1.36	1.44
21	C	512	CLA	C1C-C2C	-4.26	1.36	1.44
29	C	507	F6C	OMB-CMB	-4.26	1.12	1.22
21	C	513	CLA	C1C-C2C	-4.24	1.36	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	406	CL7	MG-NA	4.15	2.14	2.05
26	D	405	PL9	C7-C3	-4.15	1.47	1.51
29	B	614	F6C	C4A-C3A	4.03	1.53	1.45
21	C	503	CLA	MG-NA	4.02	2.15	2.06
21	B	616	CLA	MG-NA	3.99	2.15	2.06
29	C	507	F6C	C4A-C3A	3.99	1.53	1.45
21	B	605	CLA	MG-NA	3.93	2.15	2.06
21	C	511	CLA	MG-NA	3.88	2.15	2.06
21	C	505	CLA	MG-NA	3.86	2.15	2.06
21	B	602	CLA	MG-NA	3.84	2.15	2.06
21	B	606	CLA	MG-NA	3.84	2.15	2.06
23	A	409	PHO	C1D-C2D	3.78	1.43	1.39
23	A	408	PHO	C1D-C2D	3.76	1.43	1.39
21	C	502	CLA	MG-NA	3.71	2.15	2.06
21	B	617	CLA	MG-NA	3.69	2.15	2.06
21	B	607	CLA	MG-NA	3.68	2.15	2.06
21	B	612	CLA	MG-NA	3.68	2.15	2.06
21	C	508	CLA	MG-NA	3.67	2.15	2.06
21	B	610	CLA	MG-NA	3.64	2.14	2.06
21	B	609	CLA	MG-NA	3.62	2.14	2.06
21	C	510	CLA	MG-NA	3.59	2.14	2.06
21	C	506	CLA	MG-NA	3.57	2.14	2.06
21	C	509	CLA	MG-NA	3.57	2.14	2.06
26	D	405	PL9	C3-C4	-3.57	1.43	1.49
21	D	403	CLA	MG-NA	3.54	2.14	2.06
21	B	608	CLA	MG-NA	3.53	2.14	2.06
29	C	507	F6C	C1A-C2A	3.52	1.53	1.45
21	B	613	CLA	MG-NA	3.51	2.14	2.06
21	C	501	CLA	MG-NA	3.50	2.14	2.06
21	C	512	CLA	MG-NA	3.50	2.14	2.06
25	D	407	SQD	O47-C45	-3.49	1.37	1.46
21	D	402	CLA	MG-NA	3.48	2.14	2.06
25	A	412	SQD	O47-C45	-3.47	1.37	1.46
21	C	504	CLA	MG-NA	3.43	2.14	2.06
21	A	410	CLA	MG-NA	3.43	2.14	2.06
21	B	604	CLA	MG-NA	3.42	2.14	2.06
21	B	615	CLA	MG-NA	3.41	2.14	2.06
25	L	103	SQD	O47-C45	-3.40	1.38	1.46
21	B	603	CLA	MG-NA	3.39	2.14	2.06
21	A	405	CLA	MG-NA	3.39	2.14	2.06
26	A	414	PL9	C7-C3	-3.37	1.47	1.51
25	L	103	SQD	O5-C1	3.36	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	407	CLA	MG-NA	3.34	2.14	2.06
21	B	611	CLA	MG-NA	3.33	2.14	2.06
25	L	103	SQD	O47-C7	3.32	1.43	1.34
23	A	409	PHO	C4D-CHA	3.32	1.44	1.39
25	A	412	SQD	O5-C1	3.32	1.50	1.41
33	F	101	HEM	FE-NB	3.32	2.05	1.94
29	B	614	F6C	C1A-C2A	3.30	1.52	1.45
23	A	408	PHO	C4D-CHA	3.28	1.44	1.39
25	D	407	SQD	O5-C1	3.28	1.50	1.41
25	A	412	SQD	O47-C7	3.28	1.43	1.34
25	D	407	SQD	O47-C7	3.25	1.43	1.34
33	F	101	HEM	FE-ND	3.25	2.04	1.94
21	C	513	CLA	MG-NA	3.24	2.14	2.06
33	F	101	HEM	FE-NC	3.12	2.05	1.95
25	D	407	SQD	C24-C23	3.06	1.59	1.50
25	L	103	SQD	C24-C23	3.02	1.59	1.50
25	A	412	SQD	C24-C23	2.99	1.59	1.50
29	C	507	F6C	C1D-ND	2.99	1.42	1.37
33	F	101	HEM	CAB-C3B	2.97	1.55	1.47
29	B	614	F6C	C1D-ND	2.93	1.42	1.37
33	F	101	HEM	CAC-C3C	2.88	1.55	1.47
26	A	414	PL9	C3-C4	-2.83	1.44	1.49
33	F	101	HEM	FE-NA	2.72	2.04	1.95
23	A	409	PHO	CMC-C2C	-2.58	1.46	1.50
26	D	405	PL9	C6-C1	-2.57	1.44	1.48
21	A	407	CLA	C3D-C4D	-2.55	1.38	1.44
21	B	616	CLA	C3D-C4D	-2.55	1.38	1.44
23	A	408	PHO	CMC-C2C	-2.54	1.46	1.50
21	B	603	CLA	C3D-C4D	-2.54	1.38	1.44
21	A	405	CLA	C3D-C4D	-2.54	1.38	1.44
21	B	604	CLA	C3D-C4D	-2.54	1.38	1.44
21	D	402	CLA	C3D-C4D	-2.53	1.38	1.44
21	B	609	CLA	C3D-C4D	-2.53	1.38	1.44
21	B	615	CLA	C3D-C4D	-2.52	1.38	1.44
21	A	410	CLA	C3D-C4D	-2.52	1.38	1.44
21	B	611	CLA	C3D-C4D	-2.52	1.38	1.44
21	C	510	CLA	C3D-C4D	-2.52	1.38	1.44
29	B	614	F6C	C4B-NB	2.52	1.41	1.37
21	C	508	CLA	C3D-C4D	-2.52	1.38	1.44
21	B	613	CLA	C3D-C4D	-2.51	1.38	1.44
21	B	612	CLA	C3D-C4D	-2.51	1.38	1.44
21	B	607	CLA	C3D-C4D	-2.50	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	512	CLA	C3D-C4D	-2.50	1.38	1.44
21	C	513	CLA	C3D-C4D	-2.50	1.38	1.44
21	B	608	CLA	C3D-C4D	-2.50	1.38	1.44
21	D	403	CLA	C3D-C4D	-2.50	1.38	1.44
21	B	606	CLA	C3D-C4D	-2.49	1.38	1.44
21	B	617	CLA	C3D-C4D	-2.49	1.38	1.44
21	B	605	CLA	C3D-C4D	-2.49	1.38	1.44
21	C	504	CLA	C3D-C4D	-2.49	1.38	1.44
21	C	509	CLA	C3D-C4D	-2.49	1.38	1.44
21	C	502	CLA	C3D-C4D	-2.48	1.38	1.44
21	C	505	CLA	C3D-C4D	-2.48	1.38	1.44
21	C	506	CLA	C3D-C4D	-2.48	1.38	1.44
21	C	501	CLA	C3D-C4D	-2.47	1.38	1.44
21	B	613	CLA	C1D-C2D	-2.47	1.40	1.45
29	C	507	F6C	C4B-NB	2.46	1.41	1.37
21	B	610	CLA	C3D-C4D	-2.46	1.38	1.44
21	C	511	CLA	C3D-C4D	-2.45	1.38	1.44
23	A	409	PHO	CMD-C2D	-2.45	1.46	1.51
23	A	408	PHO	CMD-C2D	-2.45	1.46	1.51
21	C	503	CLA	C3D-C4D	-2.44	1.38	1.44
23	A	408	PHO	CMB-C2B	-2.44	1.46	1.51
21	B	605	CLA	MG-NC	2.42	2.12	2.06
21	B	602	CLA	C3D-C4D	-2.41	1.38	1.44
21	C	505	CLA	C1D-C2D	-2.39	1.40	1.45
21	B	605	CLA	C1D-C2D	-2.37	1.40	1.45
23	A	409	PHO	C4D-ND	-2.36	1.35	1.38
23	A	409	PHO	CMB-C2B	-2.36	1.46	1.51
21	C	505	CLA	MG-NC	2.36	2.11	2.06
23	A	408	PHO	C4D-ND	-2.36	1.35	1.38
22	A	406	CL7	MG-NC	2.34	2.10	2.05
21	B	611	CLA	C1B-C2B	-2.32	1.37	1.43
21	B	610	CLA	C1B-C2B	-2.32	1.37	1.43
23	A	408	PHO	CAC-C3C	-2.32	1.47	1.51
21	B	616	CLA	MG-NC	2.31	2.11	2.06
21	C	503	CLA	MG-NC	2.31	2.11	2.06
21	B	616	CLA	C1D-C2D	-2.31	1.40	1.45
21	B	604	CLA	C1D-C2D	-2.31	1.40	1.45
21	D	402	CLA	C1D-C2D	-2.30	1.40	1.45
26	A	414	PL9	C53-C6	-2.30	1.45	1.50
21	B	607	CLA	C1D-C2D	-2.30	1.40	1.45
21	C	511	CLA	C1D-C2D	-2.30	1.40	1.45
21	C	502	CLA	MG-NC	2.29	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	405	PL9	C53-C6	-2.29	1.46	1.50
21	B	608	CLA	C1D-C2D	-2.29	1.40	1.45
21	B	609	CLA	C1D-C2D	-2.28	1.40	1.45
21	B	606	CLA	C1B-C2B	-2.28	1.37	1.43
21	B	616	CLA	C1B-C2B	-2.27	1.37	1.43
21	B	602	CLA	C1B-C2B	-2.26	1.37	1.43
21	C	509	CLA	C1D-C2D	-2.25	1.40	1.45
21	A	405	CLA	C1D-C2D	-2.25	1.40	1.45
21	B	606	CLA	C1D-C2D	-2.25	1.40	1.45
29	C	507	F6C	C4D-ND	-2.25	1.33	1.37
21	C	502	CLA	C1D-C2D	-2.25	1.40	1.45
21	C	511	CLA	MG-NC	2.24	2.11	2.06
22	A	406	CL7	C1B-C2B	-2.24	1.38	1.43
21	B	602	CLA	C1D-C2D	-2.24	1.40	1.45
29	C	507	F6C	C2B-C1B	2.24	1.49	1.44
21	C	503	CLA	C1D-C2D	-2.24	1.40	1.45
21	C	508	CLA	C1D-C2D	-2.23	1.40	1.45
26	A	414	PL9	C6-C1	-2.23	1.44	1.48
21	B	612	CLA	C1D-C2D	-2.23	1.40	1.45
21	B	609	CLA	C1B-C2B	-2.22	1.38	1.43
29	B	614	F6C	C4D-ND	-2.22	1.33	1.37
21	C	512	CLA	C1D-C2D	-2.22	1.40	1.45
29	B	614	F6C	C2B-C1B	2.22	1.49	1.44
25	L	103	SQD	O9-S	2.21	1.51	1.45
21	B	617	CLA	C1D-C2D	-2.21	1.41	1.45
21	B	615	CLA	C1D-C2D	-2.21	1.41	1.45
23	A	409	PHO	CAC-C3C	-2.21	1.47	1.51
25	A	412	SQD	O9-S	2.20	1.51	1.45
23	A	408	PHO	C3D-C4D	2.20	1.44	1.41
21	B	617	CLA	MG-NC	2.19	2.11	2.06
21	C	501	CLA	C1D-C2D	-2.19	1.41	1.45
21	B	612	CLA	C1B-C2B	-2.19	1.38	1.43
21	A	410	CLA	C1D-C2D	-2.18	1.41	1.45
21	C	510	CLA	MG-NC	2.18	2.11	2.06
21	A	410	CLA	C1B-C2B	-2.18	1.38	1.43
21	C	510	CLA	C1D-C2D	-2.18	1.41	1.45
21	B	610	CLA	C1D-C2D	-2.17	1.41	1.45
21	D	403	CLA	C1B-C2B	-2.17	1.38	1.43
21	B	603	CLA	C1D-C2D	-2.17	1.41	1.45
21	C	504	CLA	C1D-C2D	-2.17	1.41	1.45
21	B	613	CLA	C1B-C2B	-2.16	1.38	1.43
21	C	506	CLA	MG-NC	2.16	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	508	CLA	C1B-C2B	-2.16	1.38	1.43
21	A	407	CLA	C1B-C2B	-2.16	1.38	1.43
21	B	615	CLA	C1B-C2B	-2.16	1.38	1.43
29	C	507	F6C	C1A-NA	2.15	1.40	1.37
21	C	509	CLA	C1B-C2B	-2.15	1.38	1.43
21	B	612	CLA	MG-NC	2.15	2.11	2.06
23	A	409	PHO	C3D-C4D	2.15	1.44	1.41
25	D	407	SQD	O9-S	2.15	1.51	1.45
25	L	103	SQD	O7-S	2.15	1.51	1.45
21	B	602	CLA	MG-NC	2.15	2.11	2.06
21	B	603	CLA	C1B-C2B	-2.14	1.38	1.43
21	C	513	CLA	C1D-C2D	-2.14	1.41	1.45
21	C	513	CLA	C1B-C2B	-2.14	1.38	1.43
21	C	504	CLA	C1B-C2B	-2.14	1.38	1.43
21	C	508	CLA	MG-NC	2.14	2.11	2.06
21	C	506	CLA	C1B-C2B	-2.13	1.38	1.43
21	B	606	CLA	MG-NC	2.13	2.11	2.06
21	C	512	CLA	C1B-C2B	-2.13	1.38	1.43
21	C	510	CLA	C1B-C2B	-2.13	1.38	1.43
21	C	506	CLA	C1D-C2D	-2.13	1.41	1.45
21	B	607	CLA	C1B-C2B	-2.13	1.38	1.43
21	B	604	CLA	MG-NC	2.12	2.11	2.06
21	D	402	CLA	C1B-C2B	-2.12	1.38	1.43
21	B	608	CLA	C1B-C2B	-2.12	1.38	1.43
21	A	405	CLA	C1B-C2B	-2.12	1.38	1.43
25	A	412	SQD	O7-S	2.12	1.51	1.45
21	D	403	CLA	C1D-C2D	-2.11	1.41	1.45
21	C	503	CLA	C1B-C2B	-2.11	1.38	1.43
21	B	604	CLA	C1B-C2B	-2.11	1.38	1.43
21	C	501	CLA	C1B-C2B	-2.11	1.38	1.43
21	C	511	CLA	C1B-C2B	-2.11	1.38	1.43
21	B	605	CLA	C1B-C2B	-2.11	1.38	1.43
21	A	407	CLA	C1D-C2D	-2.11	1.41	1.45
29	B	614	F6C	C3B-C4B	2.10	1.49	1.44
21	C	512	CLA	MG-NC	2.10	2.11	2.06
21	B	611	CLA	C1D-C2D	-2.10	1.41	1.45
21	C	505	CLA	C1B-C2B	-2.10	1.38	1.43
21	B	617	CLA	C1B-C2B	-2.10	1.38	1.43
29	C	507	F6C	CMD-C2D	-2.09	1.46	1.50
29	B	614	F6C	CMD-C2D	-2.08	1.46	1.50
21	B	605	CLA	C1B-NB	-2.08	1.35	1.37
21	D	403	CLA	MG-NC	2.08	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	610	CLA	MG-NC	2.06	2.11	2.06
25	D	407	SQD	O7-S	2.05	1.51	1.45
21	C	502	CLA	C1B-C2B	-2.05	1.38	1.43
21	B	609	CLA	C1B-NB	-2.05	1.35	1.37
21	B	609	CLA	MG-NC	2.04	2.11	2.06
21	A	405	CLA	MG-NC	2.04	2.11	2.06
21	B	613	CLA	MG-NC	2.03	2.11	2.06
25	L	103	SQD	C8-C7	2.03	1.56	1.50
23	A	408	PHO	C3B-C2B	-2.03	1.37	1.40
29	C	507	F6C	C3B-C4B	2.02	1.48	1.44
21	C	511	CLA	C1B-NB	-2.02	1.35	1.37
21	B	613	CLA	C1B-NB	-2.01	1.35	1.37
21	C	509	CLA	MG-NC	2.01	2.11	2.06
21	B	603	CLA	CHB-C1B	2.01	1.43	1.39
21	C	505	CLA	C1B-NB	-2.00	1.35	1.37

All (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
23	A	408	PHO	C4D-CHA-CBD	-6.95	105.38	108.52
29	B	614	F6C	CAA-C2A-C1A	-6.68	109.72	128.11
29	C	507	F6C	CAA-C2A-C1A	-6.04	111.48	128.11
29	B	614	F6C	CMA-C3A-C2A	-5.23	111.92	126.12
29	C	507	F6C	CMA-C3A-C2A	-5.06	112.38	126.12
26	A	414	PL9	C7-C3-C4	5.03	120.97	116.88
26	D	405	PL9	C7-C3-C4	5.00	120.94	116.88
29	C	507	F6C	C4A-NA-C1A	4.64	109.63	106.33
29	B	614	F6C	C4A-NA-C1A	4.26	109.36	106.33
25	L	103	SQD	O47-C7-C8	4.19	120.53	111.50
25	D	407	SQD	O9-S-C6	4.10	111.81	106.94
25	L	103	SQD	O9-S-C6	4.07	111.78	106.94
25	D	407	SQD	O47-C7-C8	4.06	120.26	111.50
25	A	412	SQD	O47-C7-C8	4.04	120.21	111.50
25	A	412	SQD	O9-S-C6	4.03	111.73	106.94
32	D	401	BCT	O2-C-O1	4.02	129.99	119.55
21	A	407	CLA	CHD-C1D-ND	-3.96	120.81	124.45
21	B	611	CLA	CHD-C1D-ND	-3.96	120.82	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	103	SQD	O7-S-C6	3.93	111.61	106.94
21	B	610	CLA	C4D-CHA-C1A	3.89	125.98	121.25
21	B	610	CLA	CHD-C1D-ND	-3.88	120.89	124.45
21	C	506	CLA	C4D-CHA-C1A	3.88	125.97	121.25
21	D	403	CLA	CHD-C1D-ND	-3.88	120.89	124.45
21	C	502	CLA	C4D-CHA-C1A	3.87	125.96	121.25
21	B	612	CLA	C4D-CHA-C1A	3.86	125.95	121.25
21	A	407	CLA	C4D-CHA-C1A	3.83	125.90	121.25
21	C	513	CLA	CHD-C1D-ND	-3.82	120.94	124.45
25	D	407	SQD	O9-S-O7	-3.81	100.75	113.95
21	D	402	CLA	CHD-C1D-ND	-3.80	120.96	124.45
21	A	410	CLA	CHD-C1D-ND	-3.79	120.97	124.45
21	B	603	CLA	CHD-C1D-ND	-3.79	120.97	124.45
21	C	504	CLA	CHD-C1D-ND	-3.77	120.99	124.45
29	B	614	F6C	C1A-C2A-C3A	-3.77	103.00	106.97
21	C	501	CLA	C4D-CHA-C1A	3.77	125.83	121.25
21	C	501	CLA	CHD-C1D-ND	-3.75	121.00	124.45
21	B	617	CLA	C4D-CHA-C1A	3.75	125.81	121.25
21	C	508	CLA	C4D-CHA-C1A	3.75	125.81	121.25
21	C	503	CLA	C4D-CHA-C1A	3.73	125.79	121.25
21	B	611	CLA	C4D-CHA-C1A	3.73	125.79	121.25
21	C	506	CLA	CHD-C1D-ND	-3.73	121.03	124.45
21	D	403	CLA	C4D-CHA-C1A	3.72	125.78	121.25
21	A	410	CLA	C4D-CHA-C1A	3.71	125.77	121.25
21	B	612	CLA	CHD-C1D-ND	-3.71	121.05	124.45
21	B	603	CLA	C4D-CHA-C1A	3.70	125.76	121.25
21	B	606	CLA	C4D-CHA-C1A	3.70	125.75	121.25
25	A	412	SQD	O9-S-O7	-3.70	101.15	113.95
21	C	512	CLA	CHD-C1D-ND	-3.69	121.07	124.45
25	L	103	SQD	O9-S-O7	-3.69	101.19	113.95
23	A	408	PHO	C2B-C1B-NB	-3.67	106.99	109.53
21	D	402	CLA	C4D-CHA-C1A	3.67	125.72	121.25
21	C	504	CLA	C4D-CHA-C1A	3.65	125.69	121.25
21	B	606	CLA	CHD-C1D-ND	-3.62	121.13	124.45
21	C	509	CLA	C4D-CHA-C1A	3.62	125.65	121.25
21	C	508	CLA	CHD-C1D-ND	-3.61	121.14	124.45
21	B	616	CLA	C4D-CHA-C1A	3.60	125.64	121.25
21	A	405	CLA	CHD-C1D-ND	-3.58	121.16	124.45
21	B	609	CLA	C4D-CHA-C1A	3.58	125.61	121.25
21	C	510	CLA	CHD-C1D-ND	-3.58	121.16	124.45
21	C	509	CLA	CHD-C1D-ND	-3.58	121.17	124.45
21	C	512	CLA	C4D-CHA-C1A	3.57	125.59	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	608	CLA	C4D-CHA-C1A	3.55	125.57	121.25
21	C	511	CLA	C4D-CHA-C1A	3.54	125.56	121.25
21	B	615	CLA	CHD-C1D-ND	-3.54	121.20	124.45
21	B	613	CLA	C4D-CHA-C1A	3.53	125.54	121.25
21	B	609	CLA	CHD-C1D-ND	-3.51	121.23	124.45
21	A	405	CLA	C4D-CHA-C1A	3.50	125.51	121.25
21	B	608	CLA	CHD-C1D-ND	-3.48	121.26	124.45
21	C	503	CLA	CHD-C1D-ND	-3.47	121.26	124.45
29	C	507	F6C	CHB-C4A-NA	3.47	127.64	124.45
25	D	407	SQD	O7-S-C6	3.46	111.06	106.94
23	A	409	PHO	CMB-C2B-C3B	3.46	131.15	124.68
21	C	510	CLA	C4D-CHA-C1A	3.46	125.46	121.25
21	B	602	CLA	C4D-CHA-C1A	3.44	125.44	121.25
24	B	627	BCR	C20-C21-C22	-3.44	122.40	127.31
21	B	617	CLA	CHD-C1D-ND	-3.43	121.30	124.45
26	D	405	PL9	C7-C3-C2	-3.43	118.79	123.30
21	C	505	CLA	C4D-CHA-C1A	3.42	125.42	121.25
21	B	607	CLA	C4D-CHA-C1A	3.42	125.41	121.25
25	A	412	SQD	O7-S-C6	3.41	111.00	106.94
21	B	607	CLA	CHD-C1D-ND	-3.41	121.32	124.45
29	B	614	F6C	CHB-C4A-NA	3.41	127.58	124.45
21	C	511	CLA	CHD-C1D-ND	-3.36	121.36	124.45
21	C	502	CLA	CHD-C1D-ND	-3.36	121.37	124.45
21	B	604	CLA	C4D-CHA-C1A	3.36	125.33	121.25
21	B	605	CLA	C4D-CHA-C1A	3.34	125.31	121.25
23	A	409	PHO	C2B-C1B-NB	-3.33	107.22	109.53
21	B	602	CLA	CHD-C1D-ND	-3.33	121.39	124.45
21	B	604	CLA	CHD-C1D-ND	-3.33	121.39	124.45
29	C	507	F6C	O2D-CGD-O1D	-3.33	117.34	123.84
21	B	615	CLA	C4D-CHA-C1A	3.30	125.27	121.25
26	A	414	PL9	C7-C3-C2	-3.27	119.00	123.30
22	A	406	CL7	CHD-C1D-ND	-3.25	120.81	124.26
21	B	616	CLA	CHD-C1D-ND	-3.20	121.52	124.45
21	B	613	CLA	CHD-C1D-ND	-3.19	121.53	124.45
21	C	513	CLA	C4D-CHA-C1A	3.18	125.11	121.25
29	C	507	F6C	C1A-C2A-C3A	-3.17	103.63	106.97
21	C	505	CLA	CHD-C1D-ND	-3.12	121.59	124.45
25	A	412	SQD	O8-S-C6	3.11	110.70	105.74
23	A	409	PHO	O1D-CGD-CBD	3.09	129.88	124.74
21	B	605	CLA	CHD-C1D-ND	-3.03	121.67	124.45
26	D	405	PL9	C7-C8-C9	-3.01	121.78	126.79
24	D	404	BCR	C20-C19-C18	2.94	134.69	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	PHO	O2D-CGD-O1D	-2.94	118.08	123.84
26	D	405	PL9	C40-C39-C41	2.94	120.22	115.27
29	B	614	F6C	O2D-CGD-O1D	-2.91	118.15	123.84
30	D	629	LHG	C5-O7-C7	2.90	124.93	117.79
26	A	414	PL9	C22-C23-C24	-2.86	120.78	127.66
29	B	614	F6C	C4A-C3A-C2A	-2.83	102.81	106.94
26	A	414	PL9	C7-C8-C9	-2.83	122.08	126.79
25	D	407	SQD	O8-S-C6	2.80	110.20	105.74
21	B	602	CLA	CHA-C1A-NA	-2.79	120.00	126.40
21	B	605	CLA	CHA-C1A-NA	-2.77	120.05	126.40
23	A	409	PHO	O2D-CGD-O1D	-2.77	118.43	123.84
21	C	505	CLA	CHA-C1A-NA	-2.77	120.06	126.40
21	C	503	CLA	CHA-C1A-NA	-2.77	120.06	126.40
21	B	602	CLA	C4A-NA-C1A	2.76	107.95	106.71
21	B	605	CLA	C4A-NA-C1A	2.76	107.95	106.71
23	A	408	PHO	CMB-C2B-C3B	2.76	129.83	124.68
21	C	511	CLA	C4A-NA-C1A	2.75	107.94	106.71
23	A	408	PHO	O1D-CGD-CBD	2.74	129.31	124.74
21	C	503	CLA	C4A-NA-C1A	2.74	107.94	106.71
21	C	511	CLA	CHA-C1A-NA	-2.73	120.14	126.40
26	A	414	PL9	C27-C28-C29	-2.73	121.09	127.66
21	B	616	CLA	CHA-C1A-NA	-2.73	120.15	126.40
33	F	101	HEM	C4C-NC-C1C	2.72	108.01	105.35
29	C	507	F6C	C3A-C4A-NA	2.72	112.11	110.10
21	B	610	CLA	CHA-C1A-NA	-2.71	120.19	126.40
24	D	404	BCR	C36-C18-C19	2.71	122.35	118.08
25	L	103	SQD	O8-S-C6	2.70	110.05	105.74
21	C	502	CLA	CHA-C1A-NA	-2.67	120.28	126.40
24	B	619	BCR	C11-C10-C9	-2.67	123.50	127.31
21	B	609	CLA	CHA-C1A-NA	-2.66	120.31	126.40
25	L	103	SQD	O48-C23-C24	2.65	120.23	111.91
21	B	607	CLA	CHA-C1A-NA	-2.65	120.34	126.40
21	C	510	CLA	CHA-C1A-NA	-2.65	120.34	126.40
21	B	612	CLA	CHA-C1A-NA	-2.64	120.35	126.40
21	B	606	CLA	CHA-C1A-NA	-2.64	120.36	126.40
21	B	613	CLA	CHA-C1A-NA	-2.64	120.36	126.40
21	C	508	CLA	CHA-C1A-NA	-2.63	120.37	126.40
25	A	412	SQD	O48-C23-C24	2.63	120.16	111.91
21	C	501	CLA	CHA-C1A-NA	-2.63	120.38	126.40
21	C	506	CLA	CHA-C1A-NA	-2.62	120.39	126.40
21	B	608	CLA	CHA-C1A-NA	-2.62	120.39	126.40
21	C	509	CLA	CHA-C1A-NA	-2.62	120.40	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	505	CLA	C4A-NA-C1A	2.62	107.88	106.71
21	D	402	CLA	CHA-C1A-NA	-2.62	120.41	126.40
21	B	617	CLA	CHA-C1A-NA	-2.61	120.42	126.40
21	C	504	CLA	CHA-C1A-NA	-2.61	120.42	126.40
21	D	403	CLA	CHA-C1A-NA	-2.61	120.43	126.40
23	A	408	PHO	C1C-C2C-C3C	-2.60	106.45	108.61
25	D	407	SQD	O48-C23-C24	2.60	120.07	111.91
21	C	513	CLA	CHA-C1A-NA	-2.59	120.46	126.40
21	A	410	CLA	CHA-C1A-NA	-2.59	120.47	126.40
21	B	615	CLA	CHA-C1A-NA	-2.59	120.47	126.40
21	B	604	CLA	CHA-C1A-NA	-2.58	120.49	126.40
21	A	407	CLA	CHA-C1A-NA	-2.57	120.50	126.40
33	F	101	HEM	C4D-ND-C1D	2.57	107.73	105.07
26	D	405	PL9	C27-C28-C29	-2.56	121.50	127.66
21	C	512	CLA	CHA-C1A-NA	-2.56	120.54	126.40
21	B	603	CLA	CHA-C1A-NA	-2.55	120.55	126.40
21	A	405	CLA	CHA-C1A-NA	-2.55	120.56	126.40
26	D	405	PL9	C22-C23-C24	-2.55	121.53	127.66
24	K	101	BCR	C20-C19-C18	2.54	133.56	126.42
21	B	611	CLA	CHA-C1A-NA	-2.53	120.61	126.40
21	B	616	CLA	C4A-NA-C1A	2.51	107.83	106.71
33	F	101	HEM	C4A-NA-C1A	2.51	107.80	105.35
29	C	507	F6C	CHB-C4A-C3A	-2.49	120.25	125.48
29	C	507	F6C	OMB-CMB-C2B	-2.48	120.07	125.69
21	C	502	CLA	C4A-NA-C1A	2.48	107.82	106.71
26	A	414	PL9	C40-C39-C41	2.48	119.44	115.27
21	C	501	CLA	C4A-NA-C1A	2.45	107.81	106.71
33	F	101	HEM	C1B-NB-C4B	2.45	107.60	105.07
26	A	414	PL9	C36-C34-C33	-2.44	116.17	121.12
29	C	507	F6C	CBD-CHA-C4D	-2.43	105.81	108.54
26	D	405	PL9	C20-C19-C21	2.42	119.35	115.27
29	C	507	F6C	C4A-C3A-C2A	-2.41	103.42	106.94
29	B	614	F6C	OMB-CMB-C2B	-2.38	120.30	125.69
24	D	404	BCR	C19-C18-C17	-2.38	115.29	118.94
24	B	618	BCR	C11-C10-C9	-2.34	123.97	127.31
21	C	509	CLA	C4A-NA-C1A	2.33	107.75	106.71
22	A	406	CL7	CHA-C1A-NA	-2.32	120.48	125.98
23	A	409	PHO	C1C-C2C-C3C	-2.32	106.68	108.61
29	C	507	F6C	O2A-CGA-O1A	-2.31	117.76	123.59
29	B	614	F6C	CHB-C4A-C3A	-2.30	120.66	125.48
26	D	405	PL9	O1-C4-C3	-2.27	118.22	120.72
21	A	407	CLA	CHD-C1D-C2D	2.27	130.23	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	613	CLA	C4A-NA-C1A	2.26	107.72	106.71
29	B	614	F6C	C3A-C4A-NA	2.24	111.76	110.10
21	B	611	CLA	CHD-C1D-C2D	2.24	130.18	125.48
23	A	409	PHO	C1-C2-C3	-2.20	122.24	126.04
21	B	602	CLA	CAA-C2A-C1A	2.19	119.17	111.97
21	D	403	CLA	CHD-C1D-C2D	2.19	130.08	125.48
24	K	101	BCR	C19-C18-C17	-2.17	115.61	118.94
21	C	513	CLA	CHD-C1D-C2D	2.17	130.03	125.48
21	B	603	CLA	CHD-C1D-C2D	2.17	130.03	125.48
26	D	405	PL9	O2-C1-C2	-2.16	116.82	121.78
21	A	410	CLA	CHD-C1D-C2D	2.16	130.01	125.48
21	B	607	CLA	C4A-NA-C1A	2.16	107.68	106.71
21	C	504	CLA	CHD-C1D-C2D	2.16	130.01	125.48
32	D	401	BCT	O3-C-O1	-2.15	113.96	119.55
21	B	610	CLA	CHD-C1D-C2D	2.15	129.99	125.48
21	C	506	CLA	CHD-C1D-C2D	2.15	129.99	125.48
29	B	614	F6C	CMB-C2B-C1B	-2.15	122.75	128.26
26	A	414	PL9	O2-C1-C6	2.15	124.31	120.59
26	D	405	PL9	O2-C1-C6	2.13	124.29	120.59
22	A	406	CL7	C3C-C4C-NC	-2.13	108.63	110.18
26	A	414	PL9	C37-C38-C39	-2.13	122.53	127.66
33	F	101	HEM	CAD-CBD-CGD	-2.13	109.02	113.60
29	B	614	F6C	CBD-CHA-C4D	-2.13	106.14	108.54
26	A	414	PL9	O2-C1-C2	-2.12	116.92	121.78
21	C	501	CLA	CHD-C1D-C2D	2.12	129.92	125.48
21	C	510	CLA	CHD-C1D-C2D	2.12	129.92	125.48
29	C	507	F6C	CMB-C2B-C1B	-2.11	122.84	128.26
26	D	405	PL9	C31-C32-C33	-2.11	104.94	111.88
26	A	414	PL9	C12-C13-C14	-2.11	122.58	127.66
26	A	414	PL9	O1-C4-C3	-2.11	118.40	120.72
21	C	508	CLA	C4A-NA-C1A	2.10	107.65	106.71
21	B	612	CLA	CHD-C1D-C2D	2.09	129.87	125.48
21	C	509	CLA	CHD-C1D-C2D	2.08	129.85	125.48
21	C	504	CLA	C4A-NA-C1A	2.08	107.64	106.71
21	C	512	CLA	CHD-C1D-C2D	2.08	129.84	125.48
29	B	614	F6C	O2A-CGA-O1A	-2.08	118.35	123.59
31	C	516	DGD	C6D-O5D-C1E	2.07	117.79	113.74
26	D	405	PL9	C12-C13-C14	-2.07	122.67	127.66
29	B	614	F6C	C1-C2-C3	-2.07	122.47	126.04
21	D	402	CLA	CHD-C1D-C2D	2.07	129.81	125.48
21	B	609	CLA	CHD-C1D-C2D	2.07	129.81	125.48
21	B	612	CLA	C4A-NA-C1A	2.06	107.63	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	405	CLA	CHD-C1D-C2D	2.06	129.80	125.48
21	C	508	CLA	CHD-C1D-C2D	2.06	129.79	125.48
21	B	606	CLA	CHD-C1D-C2D	2.04	129.76	125.48
31	C	516	DGD	C3G-O3G-C1D	2.04	117.72	113.74
21	B	615	CLA	CHD-C1D-C2D	2.04	129.75	125.48
26	A	414	PL9	C32-C33-C34	-2.03	122.78	127.66
21	B	617	CLA	C4A-NA-C1A	2.02	107.62	106.71
21	C	502	CLA	CHD-C1D-C2D	2.01	129.70	125.48
21	B	617	CLA	CHD-C1D-C2D	2.01	129.70	125.48
29	C	507	F6C	O2D-CGD-CBD	2.01	114.84	111.27
21	C	503	CLA	CHD-C1D-C2D	2.01	129.69	125.48
21	B	608	CLA	CHD-C1D-C2D	2.00	129.68	125.48

All (4) chirality outliers are listed below:

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

All (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
21	B	602	CLA	CHA-CBD-CGD-O2D
21	B	602	CLA	CAD-CBD-CGD-O1D
21	B	602	CLA	CAD-CBD-CGD-O2D
21	B	607	CLA	CHA-CBD-CGD-O1D
21	B	607	CLA	CHA-CBD-CGD-O2D
21	B	615	CLA	CHA-CBD-CGD-O1D
21	B	615	CLA	CHA-CBD-CGD-O2D
21	B	615	CLA	CAD-CBD-CGD-O1D
21	B	615	CLA	CAD-CBD-CGD-O2D
21	C	506	CLA	C2-C3-C5-C6
21	C	506	CLA	C4-C3-C5-C6
21	C	508	CLA	CHA-CBD-CGD-O1D
21	C	508	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	C	513	CLA	C1A-C2A-CAA-CBA
21	C	513	CLA	CBD-CGD-O2D-CED
21	C	513	CLA	O1D-CGD-O2D-CED
22	A	406	CL7	CHA-CBD-CGD-O2D
22	A	406	CL7	CHA-CBD-CGD-O1D
24	B	618	BCR	C7-C8-C9-C10
24	B	619	BCR	C7-C8-C9-C10
24	B	627	BCR	C21-C22-C23-C24
24	B	627	BCR	C37-C22-C23-C24
24	B	627	BCR	C23-C24-C25-C26
24	D	404	BCR	C1-C6-C7-C8
24	D	404	BCR	C7-C8-C9-C10
24	D	404	BCR	C7-C8-C9-C34
24	K	101	BCR	C17-C18-C19-C20
24	K	101	BCR	C36-C18-C19-C20
24	K	101	BCR	C23-C24-C25-C30
24	K	102	BCR	C7-C8-C9-C10
24	K	102	BCR	C7-C8-C9-C34
25	A	412	SQD	O5-C1-O6-C44
25	A	412	SQD	O5-C5-C6-S
25	D	407	SQD	O5-C1-O6-C44
25	L	103	SQD	C2-C1-O6-C44
25	L	103	SQD	O5-C1-O6-C44
25	L	103	SQD	O49-C7-O47-C45
25	L	103	SQD	O5-C5-C6-S
26	A	414	PL9	C9-C11-C12-C13
26	A	414	PL9	C12-C13-C14-C16
26	A	414	PL9	C22-C23-C24-C26
26	A	414	PL9	C27-C28-C29-C30
26	A	414	PL9	C28-C29-C31-C32
26	A	414	PL9	C32-C33-C34-C35
26	A	414	PL9	C37-C38-C39-C40
26	A	414	PL9	C37-C38-C39-C41
26	D	405	PL9	C42-C43-C44-C46
27	A	419	LMT	C2'-C1'-O1'-C1
27	A	419	LMT	O5'-C1'-O1'-C1
27	F	102	LMT	C2-C1-O1'-C1'
27	Z	102	LMT	C2'-C1'-O1'-C1
27	Z	102	LMT	O5'-C1'-O1'-C1
28	A	413	LMG	C2-C1-O1-C7
28	A	413	LMG	O6-C1-O1-C7
28	D	628	LMG	O9-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	B	614	F6C	C1A-C2A-CAA-CBA
29	C	507	F6C	C1A-C2A-CAA-CBA
29	C	507	F6C	C1B-C2B-CMB-OMB
29	C	507	F6C	C3B-C2B-CMB-OMB
29	C	507	F6C	C1-C2-C3-C4
29	C	507	F6C	C1-C2-C3-C5
30	B	1006	LHG	C4-O6-P-O5
30	D	629	LHG	C4-O6-P-O4
30	D	629	LHG	C8-C7-O7-C5
30	D	409	LHG	C3-O3-P-O4
30	E	101	LHG	C3-O3-P-O4
31	D	406	DGD	O2G-C2G-C3G-O3G
25	D	407	SQD	O10-C23-O48-C46
28	A	413	LMG	O10-C28-O8-C9
23	A	409	PHO	C3-C5-C6-C7
29	C	507	F6C	C3-C5-C6-C7
28	A	413	LMG	C29-C28-O8-C9
25	L	103	SQD	C8-C7-O47-C45
28	D	628	LMG	C11-C10-O7-C8
29	B	614	F6C	C4-C3-C5-C6
25	D	407	SQD	C24-C23-O48-C46
30	D	629	LHG	O9-C7-O7-C5
26	A	414	PL9	C27-C28-C29-C31
26	A	414	PL9	C32-C33-C34-C36
28	D	628	LMG	O10-C28-O8-C9
28	D	628	LMG	C29-C28-O8-C9
25	L	103	SQD	C31-C32-C33-C34
21	D	403	CLA	C4-C3-C5-C6
21	D	403	CLA	C2-C3-C5-C6
29	B	614	F6C	C2-C3-C5-C6
25	A	412	SQD	C24-C23-O48-C46
30	D	629	LHG	C1-C2-C3-O3
25	A	412	SQD	O10-C23-O48-C46
25	D	407	SQD	O47-C45-C46-O48
29	B	614	F6C	C11-C12-C13-C14
28	D	411	LMG	C32-C33-C34-C35
21	B	607	CLA	C2A-CAA-CBA-CGA
24	D	404	BCR	C37-C22-C23-C24
30	B	1006	LHG	C8-C7-O7-C5
28	C	519	LMG	C31-C32-C33-C34
29	B	614	F6C	C8-C10-C11-C12
31	C	516	DGD	C1B-C2B-C3B-C4B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	A	412	SQD	C9-C10-C11-C12
25	A	412	SQD	C23-C24-C25-C26
30	D	629	LHG	C7-C8-C9-C10
29	B	614	F6C	C5-C6-C7-C8
30	D	629	LHG	O2-C2-C3-O3
27	A	419	LMT	O1'-C1-C2-C3
25	A	412	SQD	C32-C33-C34-C35
28	D	630	LMG	C11-C10-O7-C8
31	C	517	DGD	CCB-CDB-CEB-CFB
21	C	504	CLA	C10-C11-C12-C13
30	B	1006	LHG	C4-O6-P-O3
30	D	629	LHG	C4-O6-P-O3
30	D	409	LHG	C3-O3-P-O6
28	B	622	LMG	C28-C29-C30-C31
28	C	519	LMG	C29-C28-O8-C9
27	B	1008	LMT	O5B-C5B-C6B-O6B
27	F	102	LMT	O5'-C5'-C6'-O6'
28	D	630	LMG	O9-C10-O7-C8
30	B	1006	LHG	O9-C7-O7-C5
31	C	517	DGD	C3A-C4A-C5A-C6A
25	D	407	SQD	C8-C7-O47-C45
28	A	413	LMG	C20-C21-C22-C23
28	D	411	LMG	C38-C39-C40-C41
30	D	408	LHG	C27-C28-C29-C30
31	H	102	DGD	C2B-C3B-C4B-C5B
31	H	102	DGD	CAB-CBB-CCB-CDB
28	C	519	LMG	C13-C14-C15-C16
25	D	407	SQD	O49-C7-O47-C45
25	A	412	SQD	C27-C28-C29-C30
27	B	1008	LMT	C4-C5-C6-C7
30	L	101	LHG	C29-C30-C31-C32
30	E	101	LHG	C11-C12-C13-C14
31	H	102	DGD	C4B-C5B-C6B-C7B
31	C	517	DGD	C2E-C1E-O5D-C6D
27	B	1008	LMT	C5-C6-C7-C8
28	B	1007	LMG	C34-C35-C36-C37
28	D	411	LMG	C21-C22-C23-C24
25	D	407	SQD	C9-C10-C11-C12
25	D	407	SQD	C33-C34-C35-C36
25	L	103	SQD	C25-C26-C27-C28
29	B	614	F6C	C11-C10-C8-C9
30	E	101	LHG	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	618	BCR	C7-C8-C9-C34
24	B	619	BCR	C7-C8-C9-C34
30	D	629	LHG	O1-C1-C2-C3
30	D	410	LHG	O1-C1-C2-C3
25	D	407	SQD	C11-C10-C9-C8
25	L	103	SQD	C9-C10-C11-C12
28	B	622	LMG	C19-C20-C21-C22
30	L	101	LHG	C11-C12-C13-C14
25	A	412	SQD	C26-C27-C28-C29
25	D	407	SQD	C32-C33-C34-C35
25	L	103	SQD	C33-C34-C35-C36
28	D	628	LMG	C30-C31-C32-C33
31	C	517	DGD	O6E-C1E-O5D-C6D
30	D	410	LHG	C12-C13-C14-C15
25	D	407	SQD	C25-C26-C27-C28
30	D	408	LHG	C25-C26-C27-C28
25	L	103	SQD	C11-C12-C13-C14
30	E	101	LHG	C28-C29-C30-C31
21	C	509	CLA	O2A-C1-C2-C3
26	D	405	PL9	C13-C14-C16-C17
25	A	412	SQD	C29-C30-C31-C32
28	C	519	LMG	O10-C28-O8-C9
30	D	409	LHG	C34-C35-C36-C37
25	A	412	SQD	C13-C14-C15-C16
28	D	411	LMG	C19-C20-C21-C22
24	A	411	BCR	C23-C24-C25-C26
24	B	618	BCR	C1-C6-C7-C8
24	B	618	BCR	C5-C6-C7-C8
24	B	619	BCR	C1-C6-C7-C8
24	B	619	BCR	C5-C6-C7-C8
24	B	627	BCR	C23-C24-C25-C30
24	D	404	BCR	C5-C6-C7-C8
24	D	404	BCR	C23-C24-C25-C26
24	K	101	BCR	C5-C6-C7-C8
24	K	101	BCR	C23-C24-C25-C26
28	A	413	LMG	C15-C16-C17-C18
31	D	406	DGD	C8B-C9B-CAB-CBB
30	E	101	LHG	C8-C7-O7-C5
28	B	622	LMG	C11-C12-C13-C14
31	C	516	DGD	CDA-CEA-CFA-CGA
28	D	630	LMG	C34-C35-C36-C37
25	A	412	SQD	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	B	1008	LMT	C7-C8-C9-C10
31	H	102	DGD	C3B-C4B-C5B-C6B
30	E	101	LHG	O9-C7-O7-C5
28	D	628	LMG	C28-C29-C30-C31
31	H	102	DGD	C1B-C2B-C3B-C4B
25	L	103	SQD	C24-C23-O48-C46
28	B	1007	LMG	C29-C30-C31-C32
28	B	1007	LMG	C10-C11-C12-C13
26	A	414	PL9	C12-C13-C14-C15
28	D	630	LMG	C32-C33-C34-C35
26	D	405	PL9	C44-C46-C47-C48
31	D	406	DGD	C4A-C5A-C6A-C7A
25	A	412	SQD	C33-C34-C35-C36
33	F	101	HEM	C4C-C3C-CAC-CBC
30	D	408	LHG	C23-C24-C25-C26
31	C	517	DGD	C6B-C7B-C8B-C9B
27	F	102	LMT	O5B-C5B-C6B-O6B
31	C	516	DGD	O6E-C5E-C6E-O5E
25	A	412	SQD	C16-C17-C18-C19
30	L	101	LHG	C10-C11-C12-C13
30	D	408	LHG	C7-C8-C9-C10
26	A	414	PL9	C4-C3-C7-C8
28	D	411	LMG	C36-C37-C38-C39
28	B	1007	LMG	O6-C5-C6-O5
25	L	103	SQD	C15-C16-C17-C18
25	L	103	SQD	O10-C23-O48-C46
25	L	103	SQD	C30-C31-C32-C33
31	C	516	DGD	C3A-C4A-C5A-C6A
30	E	101	LHG	C3-O3-P-O6
30	L	101	LHG	C4-O6-P-O3
25	A	412	SQD	C30-C31-C32-C33
30	D	629	LHG	C18-C19-C20-C21
30	D	410	LHG	C11-C10-C9-C8
30	L	101	LHG	C23-C24-C25-C26
27	A	419	LMT	O5B-C5B-C6B-O6B
28	D	411	LMG	C18-C19-C20-C21
30	D	410	LHG	C30-C31-C32-C33
25	A	412	SQD	C25-C26-C27-C28
28	B	622	LMG	C16-C17-C18-C19
25	A	412	SQD	C17-C18-C19-C20
31	C	517	DGD	C7A-C8A-C9A-CAA
31	H	102	DGD	CAA-CBA-CCA-CDA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	411	LMG	O6-C5-C6-O5
25	D	407	SQD	C44-C45-C46-O48
28	D	628	LMG	C20-C21-C22-C23
31	C	517	DGD	C2G-C3G-O3G-C1D
31	C	517	DGD	C5D-C6D-O5D-C1E
27	B	1008	LMT	O1'-C1-C2-C3
28	A	413	LMG	O6-C5-C6-O5
28	C	519	LMG	C34-C35-C36-C37
30	D	629	LHG	C4-C5-O7-C7
30	E	101	LHG	C19-C20-C21-C22
25	D	407	SQD	C27-C28-C29-C30
30	D	629	LHG	C34-C35-C36-C37
30	B	1006	LHG	C7-C8-C9-C10
31	C	518	DGD	C8B-C9B-CAB-CBB
25	L	103	SQD	C29-C30-C31-C32
28	B	1007	LMG	C35-C36-C37-C38
31	D	406	DGD	O6D-C5D-C6D-O5D
30	B	1006	LHG	C23-C24-C25-C26
21	C	505	CLA	C10-C11-C12-C13
30	D	408	LHG	C35-C36-C37-C38
25	D	407	SQD	C30-C31-C32-C33
28	C	519	LMG	C14-C15-C16-C17
27	Z	102	LMT	C2-C1-O1'-C1'
31	H	102	DGD	CCA-CDA-CEA-CFA
25	D	407	SQD	O6-C44-C45-C46
31	C	516	DGD	C1G-C2G-C3G-O3G
31	D	406	DGD	C1G-C2G-C3G-O3G
30	E	101	LHG	C18-C19-C20-C21
27	B	1008	LMT	C1-C2-C3-C4
25	L	103	SQD	C27-C28-C29-C30
23	A	409	PHO	C4-C3-C5-C6
28	D	411	LMG	C34-C35-C36-C37
21	C	510	CLA	C3-C5-C6-C7
27	A	419	LMT	C7-C8-C9-C10
31	H	102	DGD	CDA-CEA-CFA-CGA
30	D	408	LHG	C1-C2-C3-O3
25	A	412	SQD	C31-C32-C33-C34
25	D	407	SQD	C10-C11-C12-C13
21	D	402	CLA	C2-C1-O2A-CGA
30	B	1006	LHG	C14-C15-C16-C17
30	D	408	LHG	C2-C3-O3-P
24	C	514	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	K	101	BCR	C1-C6-C7-C8
28	B	1007	LMG	C33-C34-C35-C36
31	H	102	DGD	CBB-CCB-CDB-CEB
24	D	404	BCR	C21-C22-C23-C24
25	L	103	SQD	C26-C27-C28-C29
28	B	622	LMG	C18-C19-C20-C21
31	H	102	DGD	C6B-C7B-C8B-C9B
31	C	516	DGD	C8A-C9A-CAA-CBA
30	D	629	LHG	O6-C4-C5-C6
28	C	519	LMG	C32-C33-C34-C35
30	D	408	LHG	C13-C14-C15-C16
21	B	606	CLA	C6-C7-C8-C10
30	D	408	LHG	C11-C10-C9-C8
25	A	412	SQD	C11-C12-C13-C14
21	C	510	CLA	CAD-CBD-CGD-O2D
28	D	630	LMG	C7-C8-O7-C10
26	A	414	PL9	C22-C23-C24-C25
30	D	408	LHG	C12-C13-C14-C15
26	A	414	PL9	C29-C31-C32-C33
28	D	628	LMG	O1-C7-C8-C9
30	D	629	LHG	C2-C3-O3-P
30	D	410	LHG	C2-C3-O3-P
27	F	102	LMT	C3-C4-C5-C6
30	D	629	LHG	O6-C4-C5-O7
31	C	516	DGD	O2G-C1B-C2B-C3B
28	D	411	LMG	C14-C15-C16-C17
31	C	516	DGD	C2B-C3B-C4B-C5B
23	A	408	PHO	C2A-CAA-CBA-CGA
21	B	605	CLA	CHA-CBD-CGD-O1D
21	B	605	CLA	CHA-CBD-CGD-O2D
21	B	608	CLA	CHA-CBD-CGD-O1D
21	B	608	CLA	CHA-CBD-CGD-O2D
21	C	505	CLA	CHA-CBD-CGD-O1D
31	C	516	DGD	O2G-C2G-C3G-O3G
31	C	517	DGD	C6A-C7A-C8A-C9A
28	B	1007	LMG	C11-C12-C13-C14
25	L	103	SQD	C14-C15-C16-C17
30	D	409	LHG	O9-C7-O7-C5
25	D	407	SQD	C26-C27-C28-C29
31	C	517	DGD	C8A-C9A-CAA-CBA
21	C	506	CLA	C13-C15-C16-C17
25	A	412	SQD	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	620	BCR	C37-C22-C23-C24
28	D	628	LMG	C23-C24-C25-C26
31	H	102	DGD	C7B-C8B-C9B-CAB
30	D	409	LHG	C8-C7-O7-C5
26	A	414	PL9	C17-C18-C19-C21
21	B	615	CLA	C8-C10-C11-C12
30	D	629	LHG	C5-C4-O6-P
30	B	1006	LHG	C4-O6-P-O4
30	D	409	LHG	C4-O6-P-O4
30	L	101	LHG	C17-C18-C19-C20
30	D	629	LHG	C16-C17-C18-C19
30	D	408	LHG	C11-C12-C13-C14
21	B	605	CLA	CAD-CBD-CGD-O1D
21	B	608	CLA	CAD-CBD-CGD-O1D
21	C	505	CLA	CAD-CBD-CGD-O1D
25	A	412	SQD	C19-C20-C21-C22
21	C	502	CLA	C11-C10-C8-C7
29	B	614	F6C	C11-C12-C13-C15
30	D	408	LHG	C10-C11-C12-C13
31	H	102	DGD	C4E-C5E-C6E-O5E
28	D	630	LMG	O7-C10-C11-C12
28	B	622	LMG	C35-C36-C37-C38
31	H	102	DGD	C1A-C2A-C3A-C4A
28	B	622	LMG	C4-C5-C6-O5
21	B	606	CLA	C3-C5-C6-C7
28	D	411	LMG	C11-C12-C13-C14
25	D	407	SQD	O6-C44-C45-O47
25	L	103	SQD	O47-C45-C46-O48
28	D	628	LMG	O1-C7-C8-O7
21	D	403	CLA	C3-C5-C6-C7
26	A	414	PL9	C44-C46-C47-C48
24	D	404	BCR	C18-C19-C20-C21
24	K	101	BCR	C18-C19-C20-C21
24	B	627	BCR	C9-C10-C11-C12
30	E	101	LHG	C25-C26-C27-C28
30	E	101	LHG	C15-C16-C17-C18
21	C	506	CLA	C2-C1-O2A-CGA
23	A	408	PHO	C2-C1-O2A-CGA
28	A	413	LMG	C28-C29-C30-C31
30	E	101	LHG	O6-C4-C5-O7
30	D	629	LHG	C33-C34-C35-C36
25	D	407	SQD	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	A	408	PHO	C4-C3-C5-C6
24	A	411	BCR	C23-C24-C25-C30
24	C	514	BCR	C23-C24-C25-C26
28	B	1007	LMG	C36-C37-C38-C39
28	B	622	LMG	C29-C28-O8-C9
25	D	407	SQD	C24-C25-C26-C27
27	F	102	LMT	C4'-C5'-C6'-O6'
30	L	101	LHG	C12-C13-C14-C15
26	A	414	PL9	C33-C34-C36-C37
30	D	410	LHG	C17-C18-C19-C20
25	L	103	SQD	C16-C17-C18-C19
28	D	411	LMG	C20-C21-C22-C23
30	E	101	LHG	C17-C18-C19-C20
28	C	519	LMG	C33-C34-C35-C36
30	B	1006	LHG	C2-C3-O3-P
30	D	629	LHG	O1-C1-C2-O2
26	A	414	PL9	C13-C14-C16-C17
25	L	103	SQD	C17-C18-C19-C20
28	B	622	LMG	O6-C5-C6-O5
28	B	622	LMG	O10-C28-O8-C9
25	A	412	SQD	C12-C13-C14-C15
25	L	103	SQD	C28-C29-C30-C31
30	E	101	LHG	C24-C25-C26-C27
26	A	414	PL9	C39-C41-C42-C43
31	C	516	DGD	O6D-C5D-C6D-O5D
21	B	615	CLA	C5-C6-C7-C8
25	L	103	SQD	C13-C14-C15-C16
28	D	630	LMG	C36-C37-C38-C39
21	C	502	CLA	C4-C3-C5-C6
26	A	414	PL9	C30-C29-C31-C32
31	C	516	DGD	C4D-C5D-C6D-O5D
23	A	408	PHO	C2-C3-C5-C6
25	A	412	SQD	C15-C16-C17-C18
21	C	513	CLA	C3A-C2A-CAA-CBA
28	D	628	LMG	C12-C13-C14-C15
21	C	513	CLA	CAA-CBA-CGA-O2A
33	F	101	HEM	C3D-CAD-CBD-CGD
21	B	616	CLA	C13-C15-C16-C17
31	C	518	DGD	C7A-C8A-C9A-CAA
24	D	404	BCR	C20-C21-C22-C37
24	K	101	BCR	C20-C21-C22-C37
21	D	403	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	A	413	LMG	C16-C17-C18-C19
31	C	516	DGD	CCB-CDB-CEB-CFB
25	L	103	SQD	C46-C45-O47-C7
28	D	628	LMG	C9-C8-O7-C10
30	L	101	LHG	C9-C10-C11-C12
31	C	518	DGD	C7B-C8B-C9B-CAB
30	D	410	LHG	C11-C12-C13-C14
28	B	1007	LMG	C12-C13-C14-C15
21	C	513	CLA	C8-C10-C11-C12
29	B	614	F6C	C3-C5-C6-C7
28	B	1007	LMG	O9-C10-O7-C8
24	D	404	BCR	C20-C21-C22-C23
24	K	101	BCR	C20-C21-C22-C23
31	C	516	DGD	C3B-C4B-C5B-C6B
31	H	102	DGD	O6E-C5E-C6E-O5E
31	H	102	DGD	C9A-CAA-CBA-CCA
28	B	622	LMG	C40-C41-C42-C43
21	A	410	CLA	C4-C3-C5-C6
29	B	614	F6C	C2-C1-O2A-CGA
21	C	513	CLA	C11-C12-C13-C14
26	A	414	PL9	C2-C3-C7-C8
30	D	410	LHG	C9-C10-C11-C12
27	Z	102	LMT	C5-C6-C7-C8
24	D	404	BCR	C9-C10-C11-C12
24	B	620	BCR	C21-C22-C23-C24
23	A	409	PHO	C2-C3-C5-C6
25	A	412	SQD	C45-C44-O6-C1
31	H	102	DGD	C7A-C8A-C9A-CAA
21	B	607	CLA	C4-C3-C5-C6
21	C	513	CLA	C4-C3-C5-C6
31	C	518	DGD	O6D-C5D-C6D-O5D
31	D	406	DGD	CBB-CCB-CDB-CEB
29	B	614	F6C	C1-C2-C3-C4
28	B	1007	LMG	O8-C28-C29-C30
26	A	414	PL9	C23-C24-C26-C27
21	C	510	CLA	CAA-CBA-CGA-O2A
21	B	606	CLA	C6-C7-C8-C9
21	C	502	CLA	C11-C10-C8-C9
23	A	409	PHO	C6-C7-C8-C9
25	A	412	SQD	C14-C15-C16-C17
21	B	604	CLA	CAD-CBD-CGD-O2D
21	B	610	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	611	CLA	CAD-CBD-CGD-O2D
21	B	613	CLA	CAD-CBD-CGD-O2D
21	C	506	CLA	CAD-CBD-CGD-O2D
27	F	102	LMT	C7-C8-C9-C10
30	D	409	LHG	C32-C33-C34-C35
21	B	605	CLA	C4-C3-C5-C6
30	D	410	LHG	C15-C16-C17-C18
21	A	410	CLA	C2-C3-C5-C6
21	B	605	CLA	C2-C3-C5-C6
29	B	614	F6C	CAA-CBA-CGA-O2A
21	C	502	CLA	C10-C11-C12-C13
28	D	628	LMG	C7-C8-C9-O8
30	B	1006	LHG	C24-C25-C26-C27
30	D	408	LHG	C9-C10-C11-C12
31	D	406	DGD	CAA-CBA-CCA-CDA
31	D	406	DGD	C7B-C8B-C9B-CAB
27	A	419	LMT	C5-C6-C7-C8
21	B	603	CLA	O2A-C1-C2-C3
21	C	504	CLA	O2A-C1-C2-C3
21	C	513	CLA	O2A-C1-C2-C3
21	D	402	CLA	O2A-C1-C2-C3
23	A	408	PHO	O2A-C1-C2-C3
30	D	409	LHG	C14-C15-C16-C17
23	A	408	PHO	C3-C5-C6-C7
30	D	409	LHG	C11-C10-C9-C8
31	C	517	DGD	CDA-CEA-CFA-CGA
21	B	606	CLA	CHA-CBD-CGD-O2D
21	C	503	CLA	CHA-CBD-CGD-O2D
21	C	505	CLA	CHA-CBD-CGD-O2D
21	C	509	CLA	CHA-CBD-CGD-O2D
21	C	512	CLA	CHA-CBD-CGD-O2D
31	C	517	DGD	C9B-CAB-CBB-CCB
25	D	407	SQD	C34-C35-C36-C37
30	D	408	LHG	C24-C25-C26-C27
30	E	101	LHG	C23-C24-C25-C26
23	A	408	PHO	CHA-CBD-CGD-O1D
23	A	409	PHO	CHA-CBD-CGD-O1D
21	B	607	CLA	C2-C3-C5-C6
21	C	512	CLA	CAA-CBA-CGA-O2A
26	A	414	PL9	C19-C21-C22-C23
26	D	405	PL9	C34-C36-C37-C38
31	C	516	DGD	C6B-C7B-C8B-C9B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	A	405	CLA	C2B-C3B-CAB-CBB
21	A	407	CLA	C2B-C3B-CAB-CBB
21	B	603	CLA	C2B-C3B-CAB-CBB
21	B	605	CLA	C2B-C3B-CAB-CBB
21	B	608	CLA	C2B-C3B-CAB-CBB
21	B	612	CLA	C2B-C3B-CAB-CBB
21	B	613	CLA	C2B-C3B-CAB-CBB
21	C	501	CLA	C2B-C3B-CAB-CBB
21	C	502	CLA	C2B-C3B-CAB-CBB
21	C	503	CLA	C2B-C3B-CAB-CBB
21	C	505	CLA	C2B-C3B-CAB-CBB
21	C	506	CLA	C2B-C3B-CAB-CBB
21	C	508	CLA	C2B-C3B-CAB-CBB
21	C	509	CLA	C2B-C3B-CAB-CBB
21	C	510	CLA	C2B-C3B-CAB-CBB
21	C	511	CLA	C2B-C3B-CAB-CBB
21	C	512	CLA	C2B-C3B-CAB-CBB
21	C	513	CLA	C2B-C3B-CAB-CBB
21	D	402	CLA	C2B-C3B-CAB-CBB
21	D	403	CLA	C2B-C3B-CAB-CBB
25	A	412	SQD	C4-C5-C6-S
28	B	1007	LMG	C11-C10-O7-C8
26	D	405	PL9	C11-C12-C13-C14
25	A	412	SQD	C34-C35-C36-C37
21	B	612	CLA	C2-C3-C5-C6
25	L	103	SQD	C7-C8-C9-C10
29	B	614	F6C	CAA-CBA-CGA-O1A
30	E	101	LHG	C11-C10-C9-C8
21	C	510	CLA	CAA-CBA-CGA-O1A
28	B	1007	LMG	O10-C28-C29-C30
25	L	103	SQD	C44-C45-C46-O48
30	D	408	LHG	O2-C2-C3-O3
21	C	512	CLA	CAA-CBA-CGA-O1A
21	C	502	CLA	C2-C3-C5-C6
25	D	407	SQD	C2-C1-O6-C44
30	D	409	LHG	C4-O6-P-O5
30	E	101	LHG	C3-O3-P-O5
30	E	101	LHG	O6-C4-C5-C6
28	B	622	LMG	C22-C23-C24-C25
24	C	515	BCR	C5-C6-C7-C8
31	C	516	DGD	CBA-CCA-CDA-CEA
21	B	615	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	C	504	CLA	CAD-CBD-CGD-O1D
21	C	502	CLA	C8-C10-C11-C12
30	E	101	LHG	O8-C23-C24-C25
30	L	101	LHG	O7-C7-C8-C9
21	D	403	CLA	C11-C10-C8-C7
21	C	505	CLA	CAA-CBA-CGA-O2A
31	H	102	DGD	O2G-C1B-C2B-C3B
30	D	408	LHG	C18-C19-C20-C21
30	L	101	LHG	O9-C7-C8-C9
24	K	102	BCR	C13-C14-C15-C16
21	C	505	CLA	CAA-CBA-CGA-O1A
21	B	605	CLA	C5-C6-C7-C8
30	E	101	LHG	O10-C23-C24-C25
23	A	409	PHO	C2A-CAA-CBA-CGA
27	Z	102	LMT	C4-C5-C6-C7
25	L	103	SQD	O47-C7-C8-C9

There are no ring outliers.

66 monomers are involved in 148 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	D	409	LHG	3	0
21	B	605	CLA	6	0
28	D	411	LMG	2	0
21	B	617	CLA	1	0
24	K	102	BCR	2	0
21	D	402	CLA	3	0
25	D	407	SQD	3	0
21	D	403	CLA	3	0
31	C	516	DGD	6	0
21	B	613	CLA	2	0
28	B	1007	LMG	2	0
21	B	615	CLA	3	0
21	A	405	CLA	2	0
33	F	101	HEM	3	0
21	C	505	CLA	5	0
24	B	619	BCR	1	0
28	D	630	LMG	2	0
24	D	404	BCR	1	0
21	C	512	CLA	4	0
30	E	101	LHG	2	0
21	B	603	CLA	5	0

Continued on next page...

Continued from previous page...

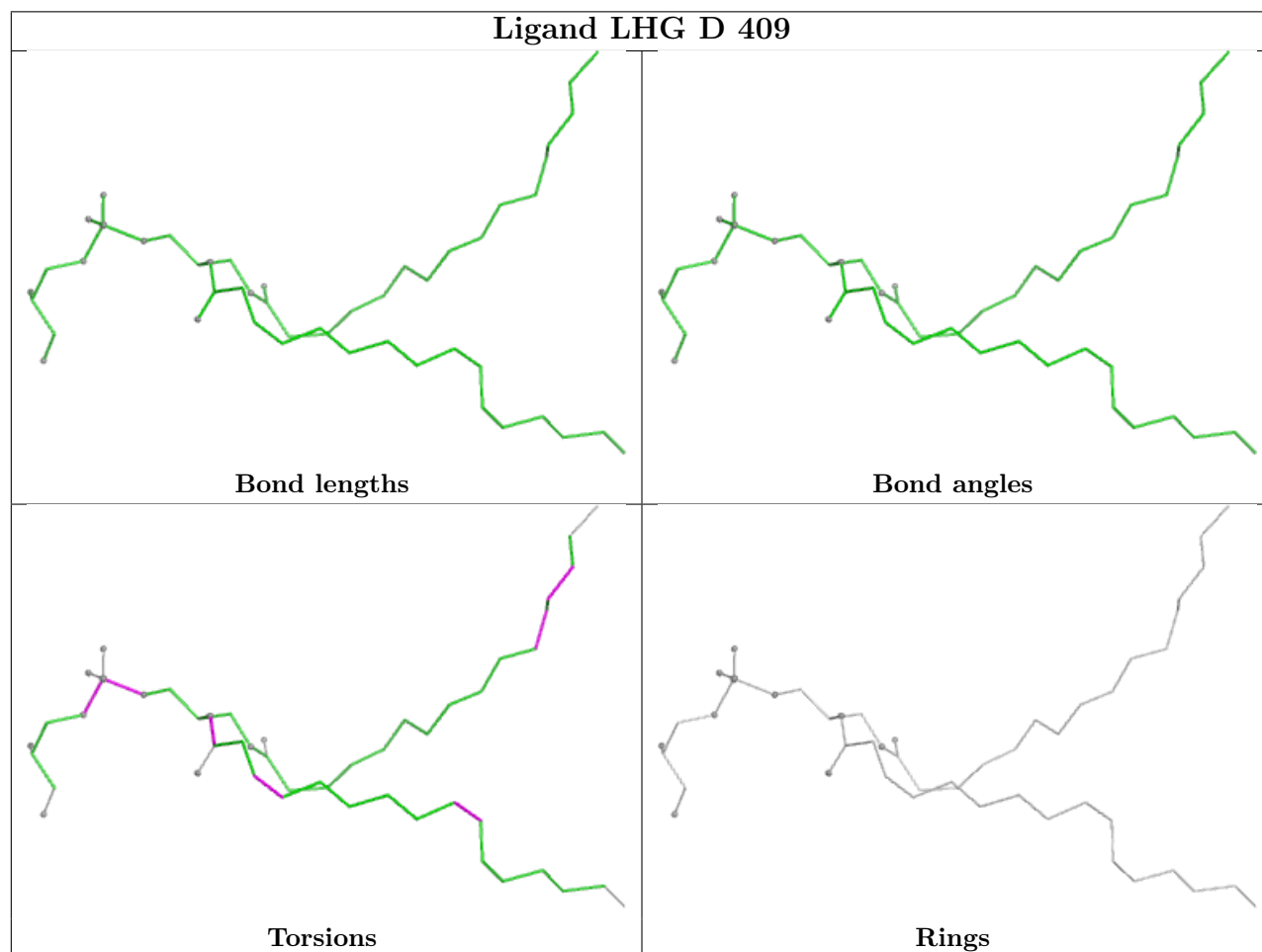
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	618	BCR	1	0
21	C	504	CLA	2	0
26	D	405	PL9	1	0
25	A	412	SQD	4	0
24	B	620	BCR	2	0
21	C	511	CLA	3	0
30	B	1006	LHG	2	0
24	K	101	BCR	4	0
28	C	519	LMG	3	0
21	B	604	CLA	2	0
28	A	413	LMG	4	0
21	A	410	CLA	4	0
21	B	611	CLA	2	0
21	B	610	CLA	2	0
21	C	502	CLA	6	0
26	A	414	PL9	7	0
30	L	101	LHG	1	0
21	B	609	CLA	1	0
24	C	515	BCR	3	0
22	A	406	CL7	1	0
21	B	606	CLA	4	0
21	A	407	CLA	1	0
28	B	622	LMG	1	0
27	B	1008	LMT	2	0
23	A	409	PHO	1	0
21	B	616	CLA	4	0
21	B	607	CLA	3	0
28	D	628	LMG	1	0
21	C	503	CLA	7	0
23	A	408	PHO	2	0
21	C	508	CLA	1	0
31	C	518	DGD	3	0
21	B	612	CLA	1	0
21	C	506	CLA	4	0
21	B	602	CLA	3	0
21	C	513	CLA	3	0
24	B	627	BCR	3	0
31	C	517	DGD	4	0
30	D	410	LHG	2	0
31	H	102	DGD	3	0
21	C	501	CLA	5	0
24	C	514	BCR	1	0

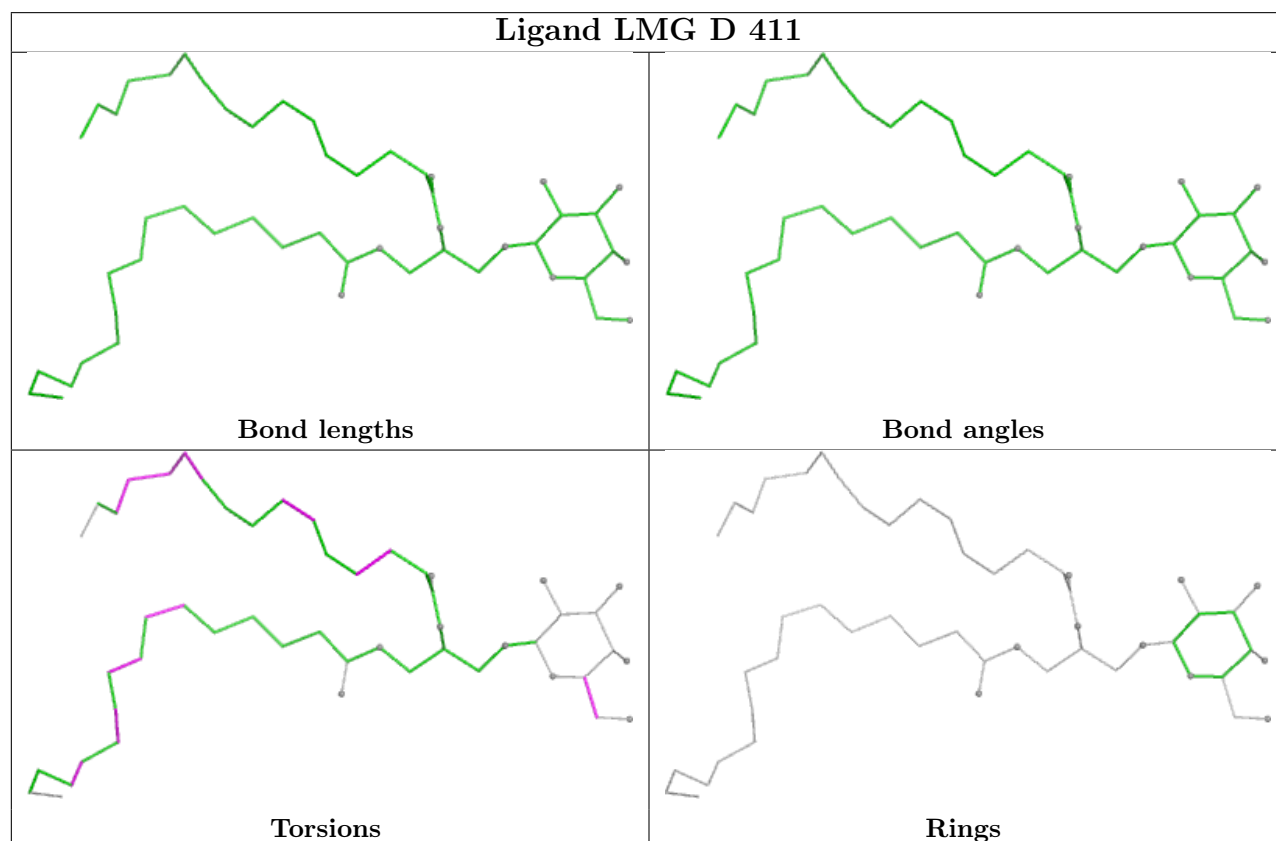
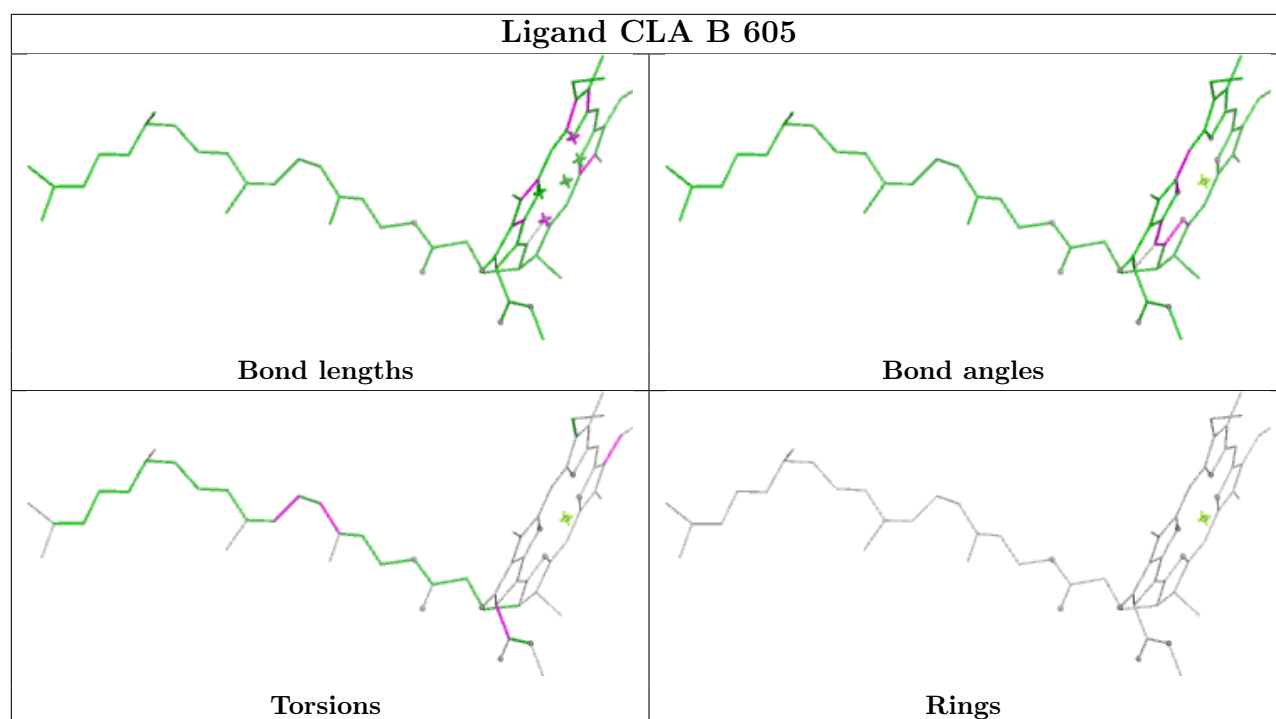
Continued on next page...

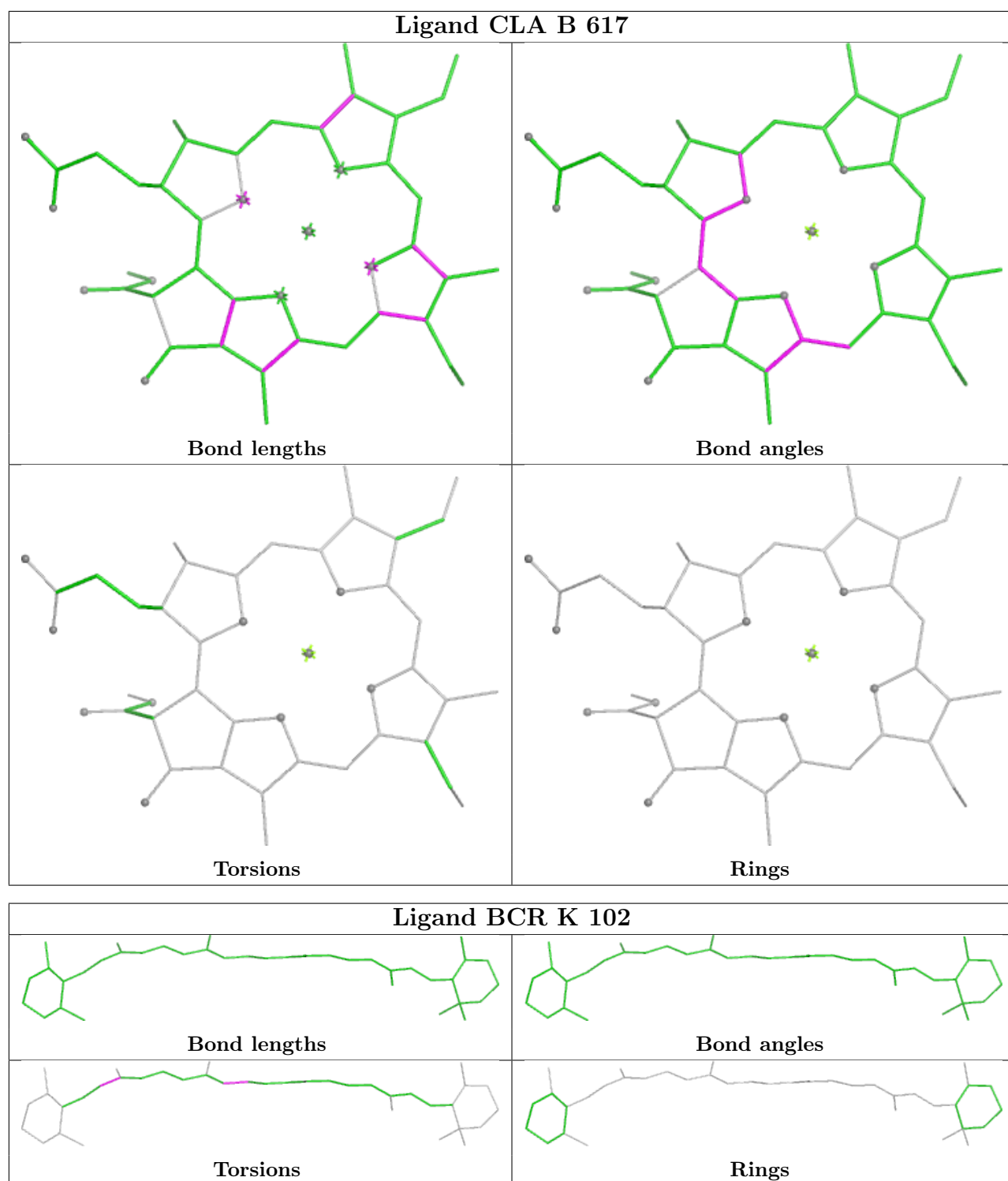
Continued from previous page...

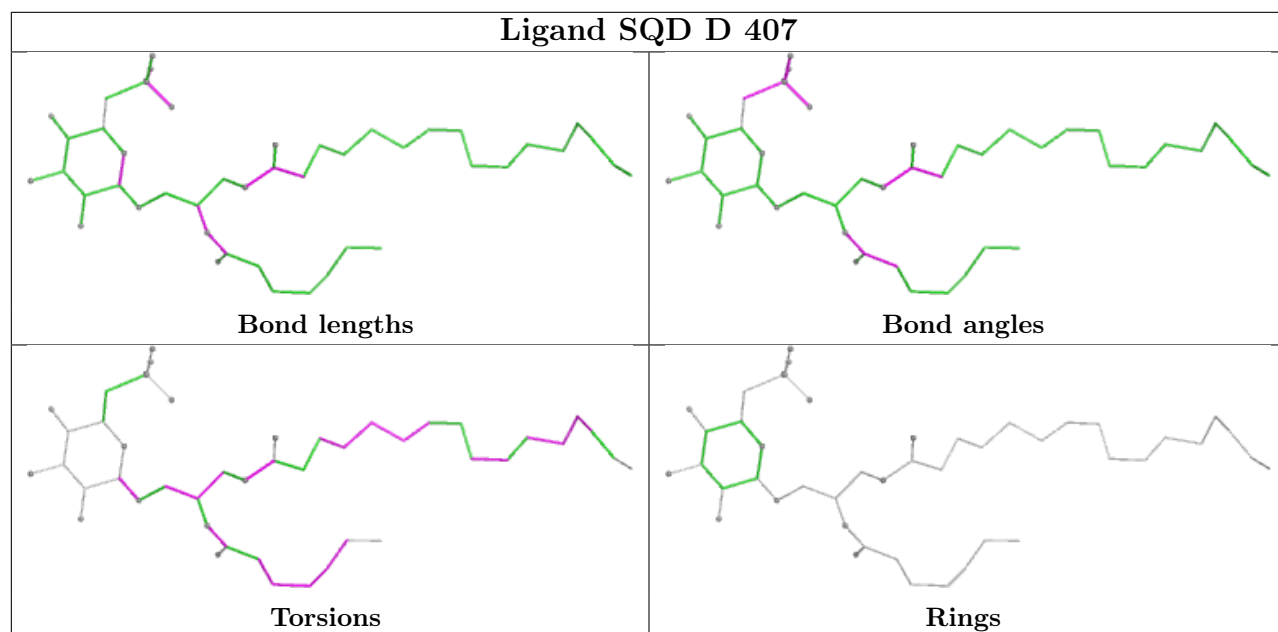
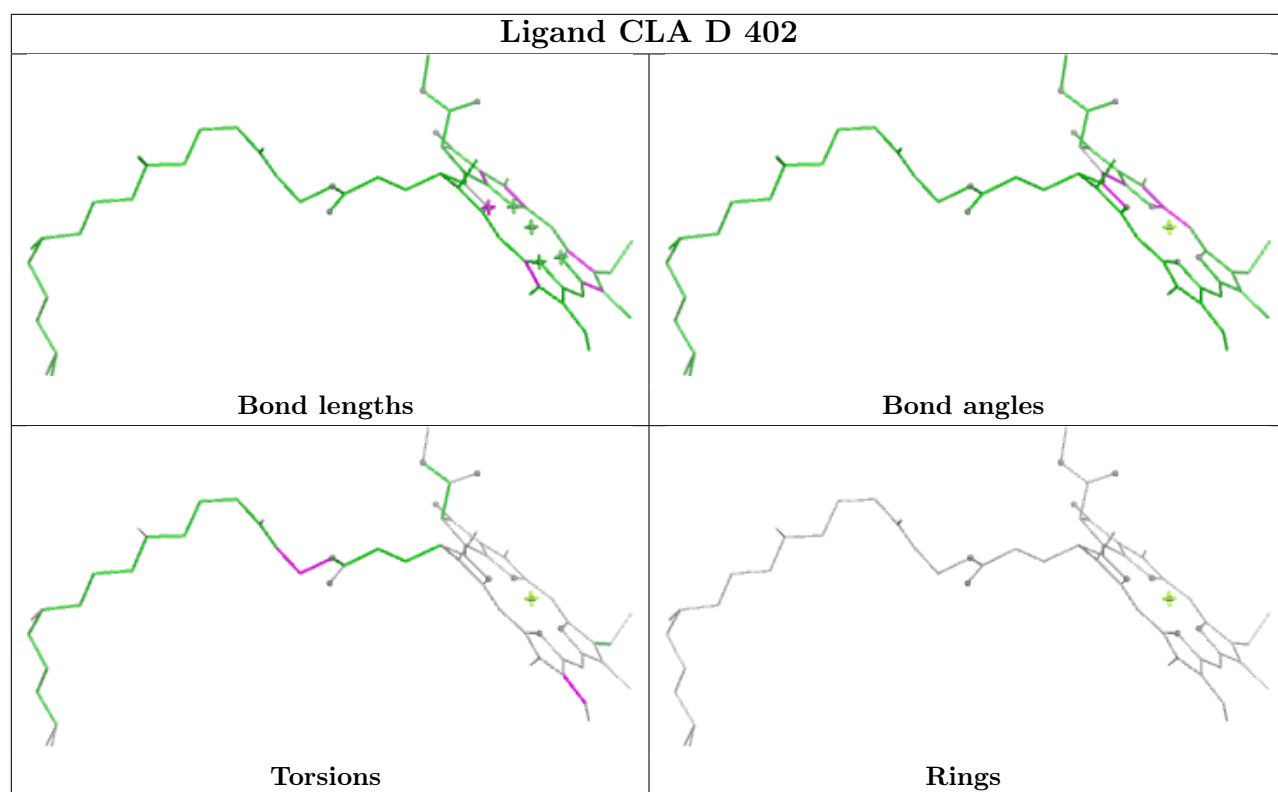
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	608	CLA	1	0
21	C	510	CLA	2	0
21	C	509	CLA	2	0

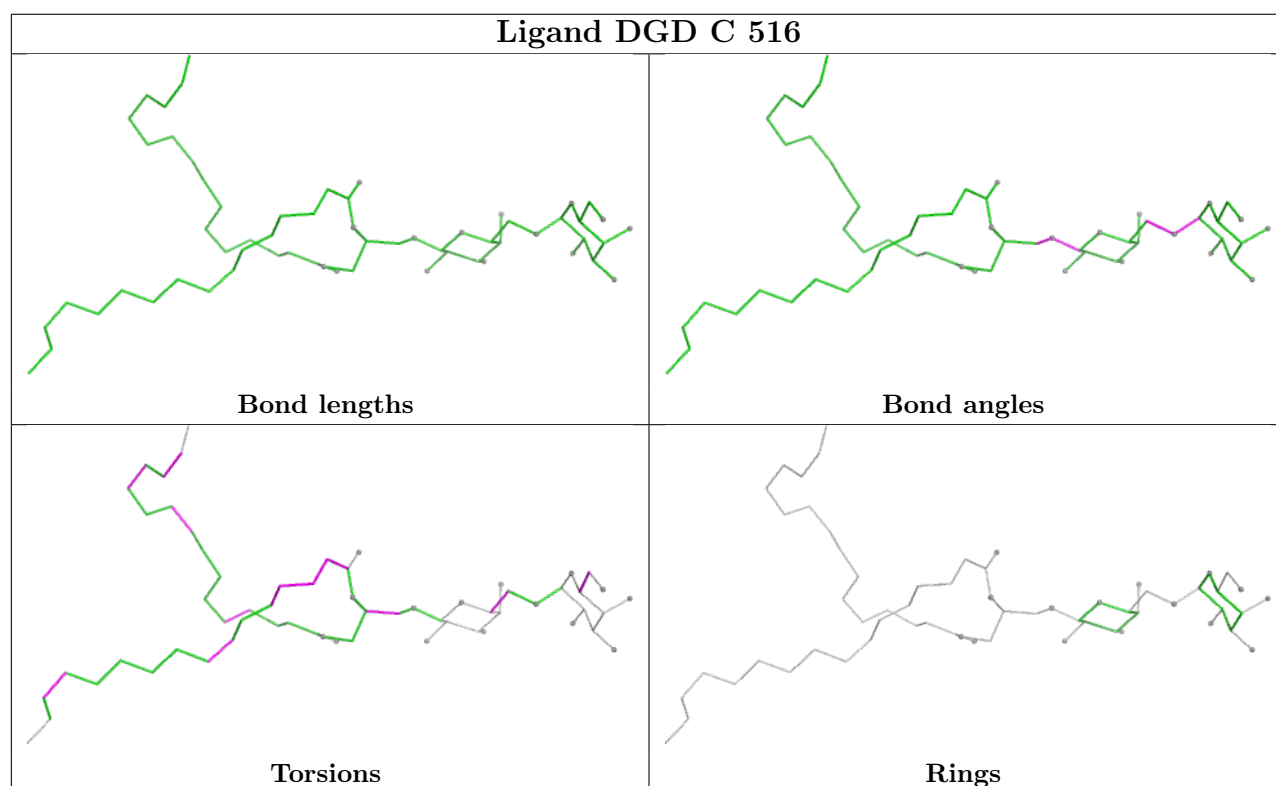
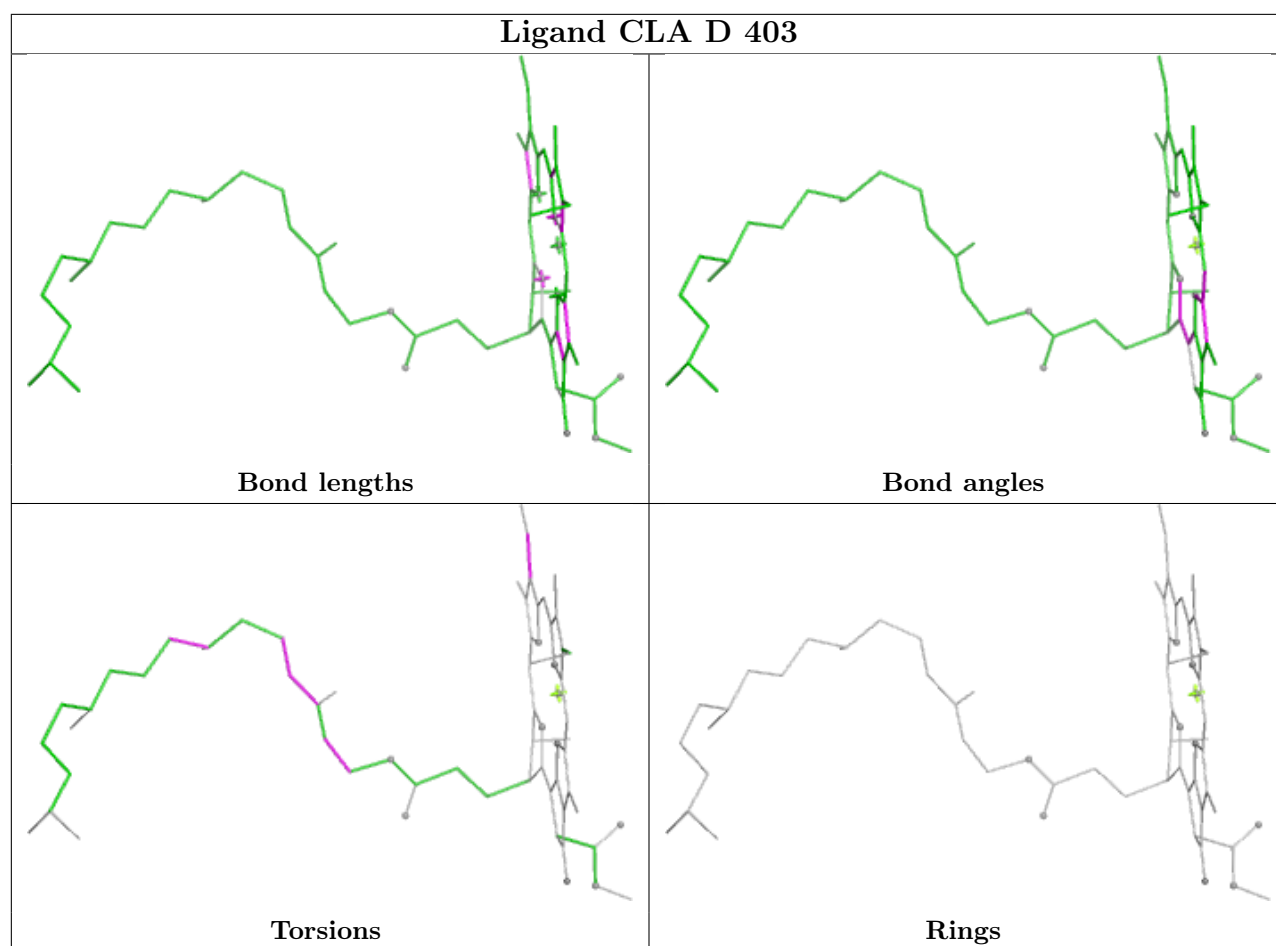
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

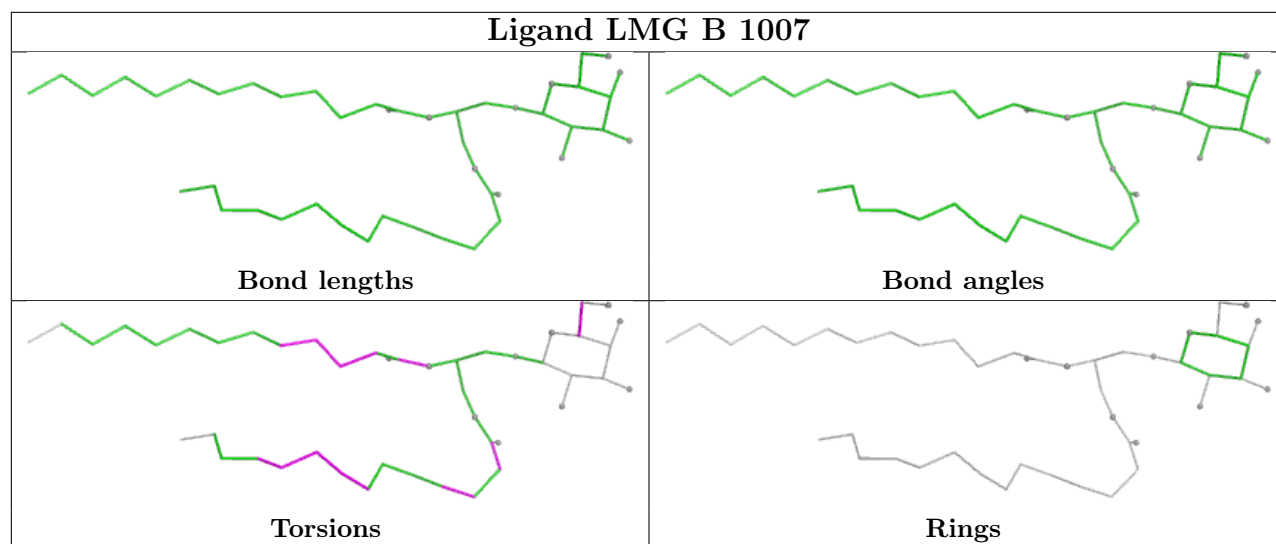
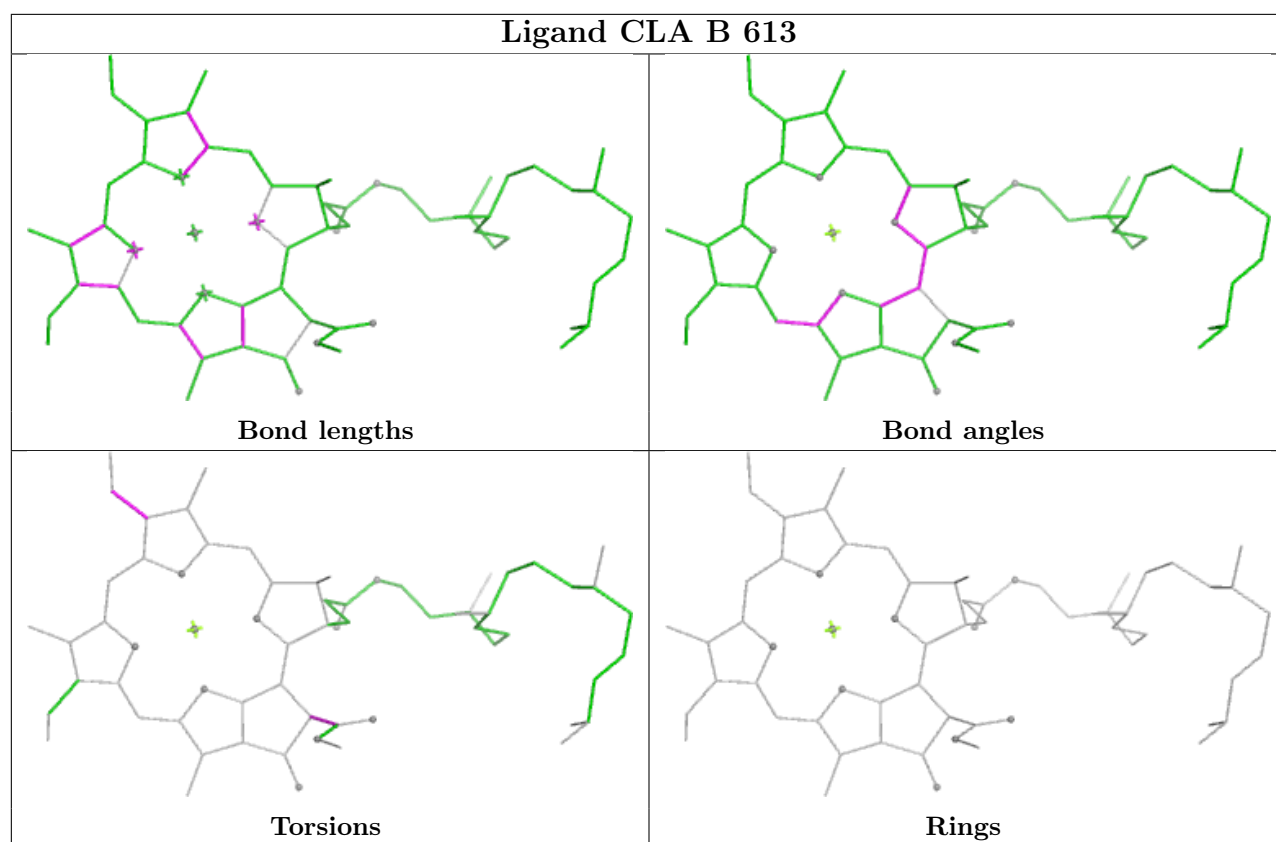


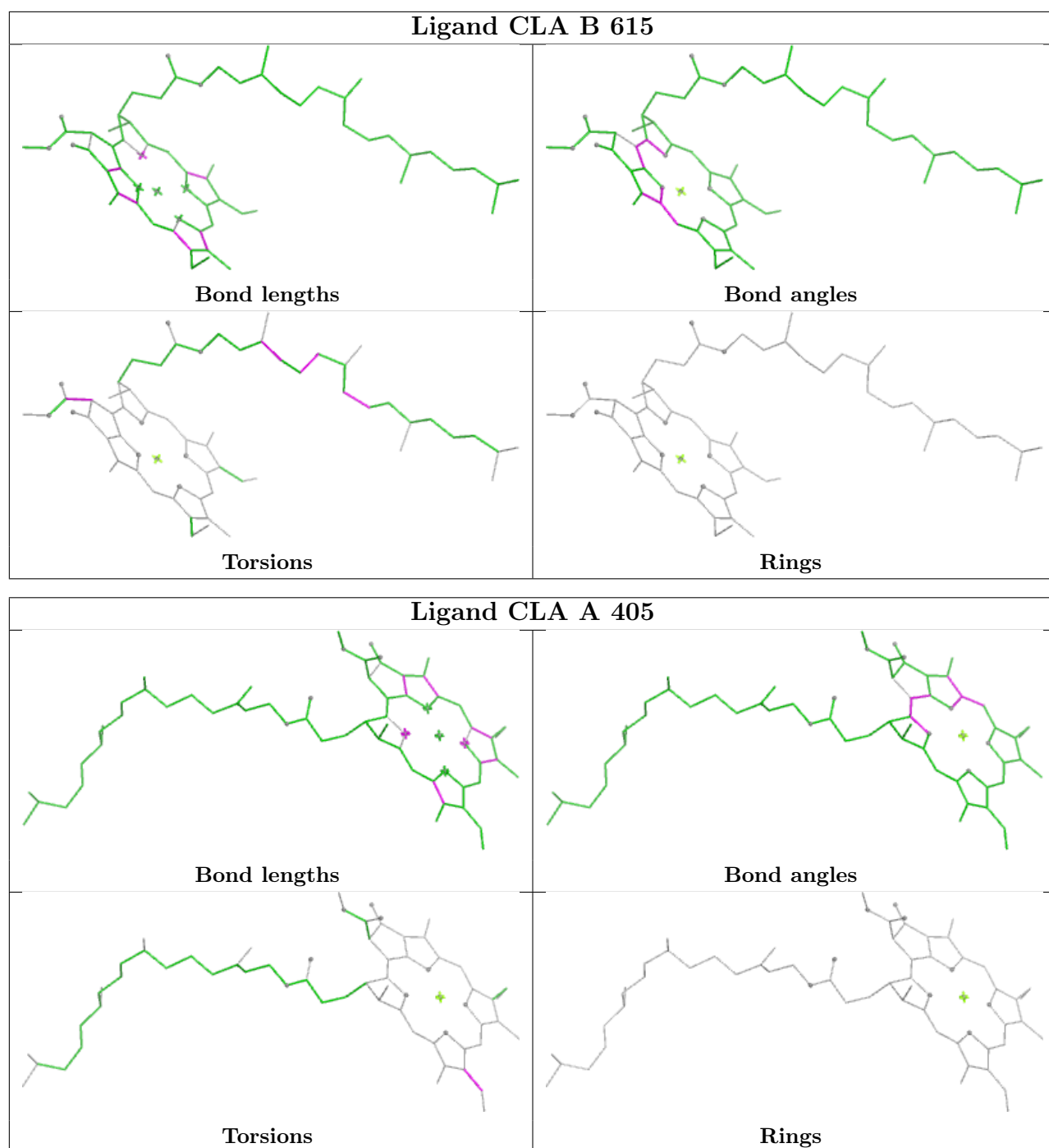


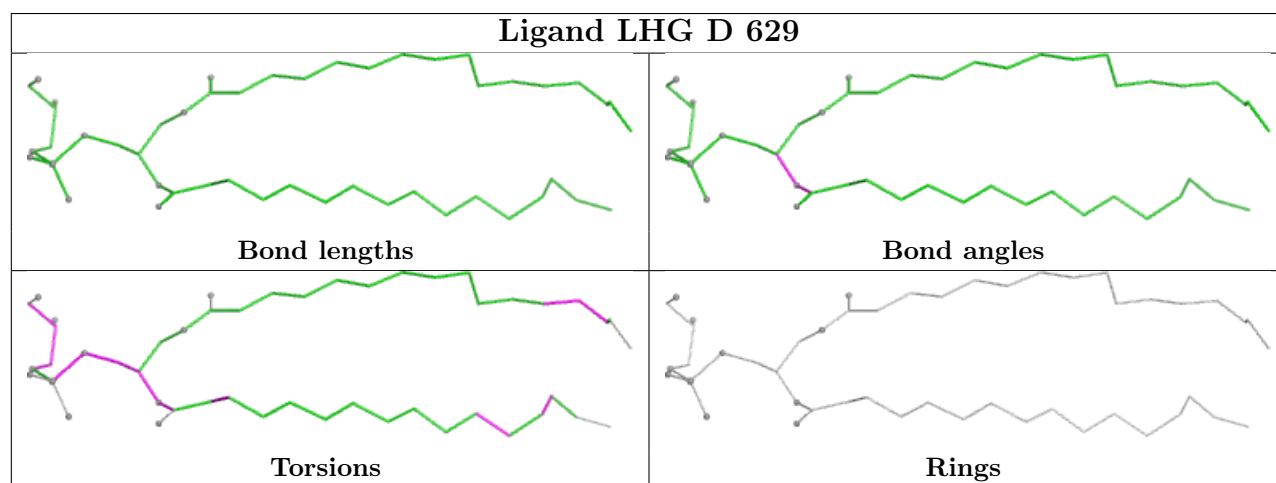
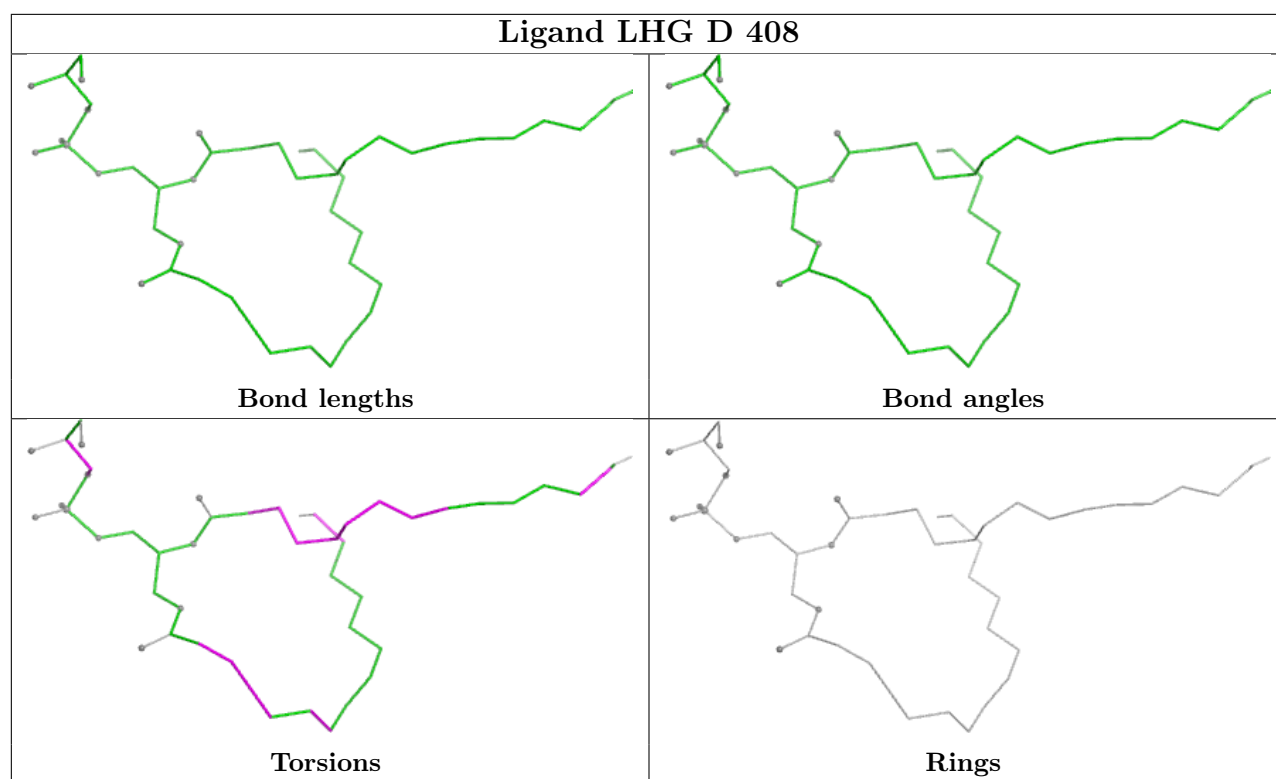


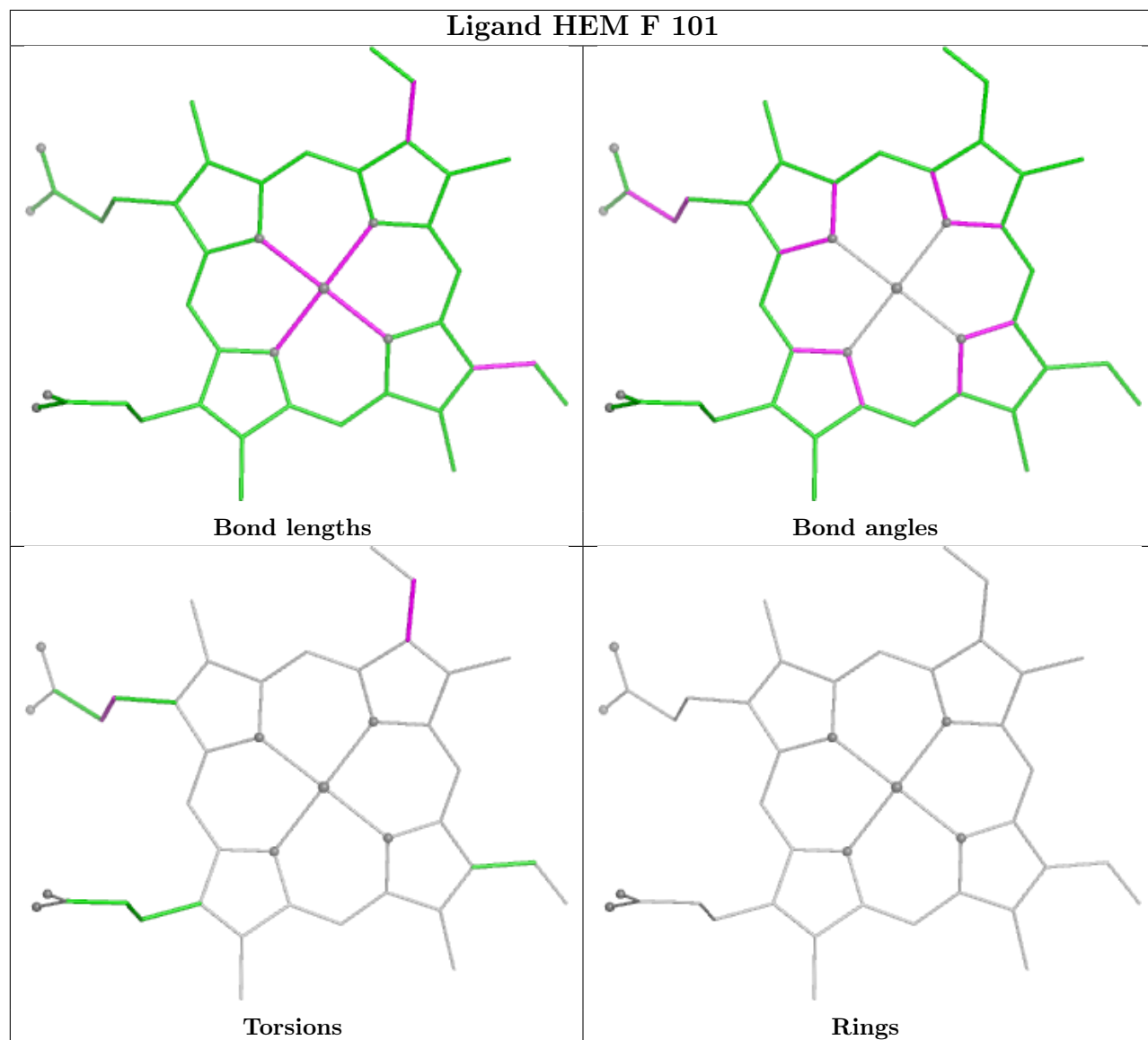


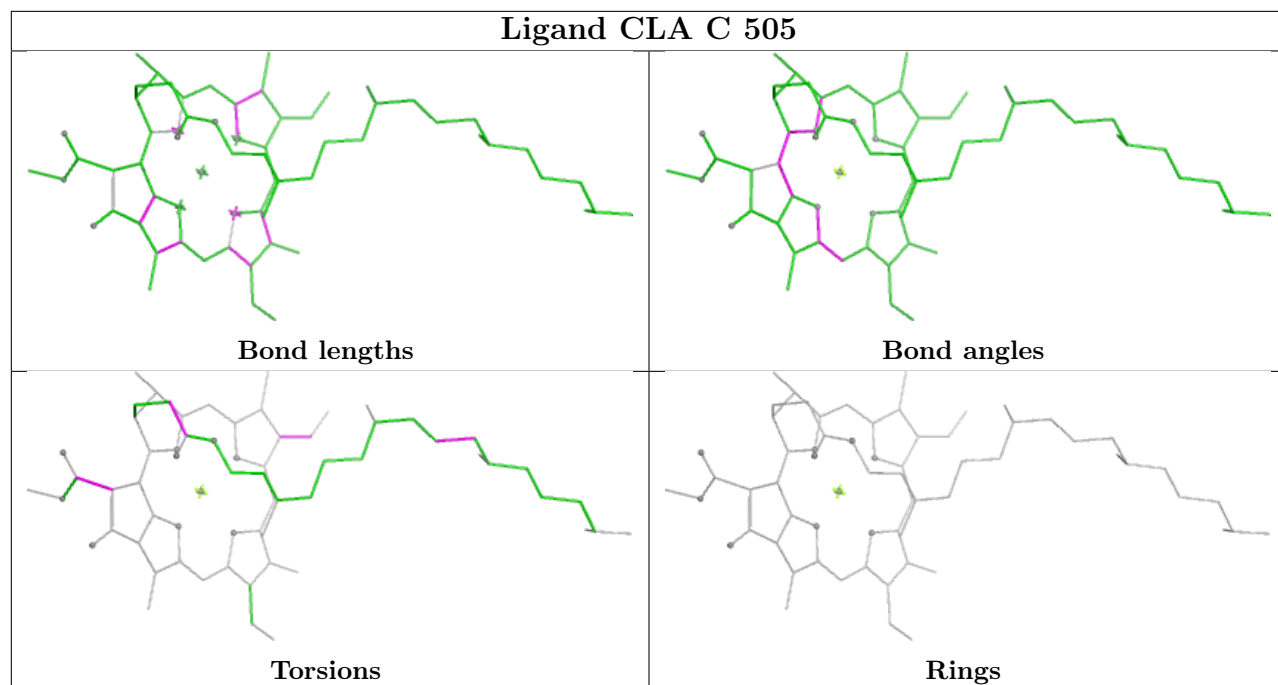


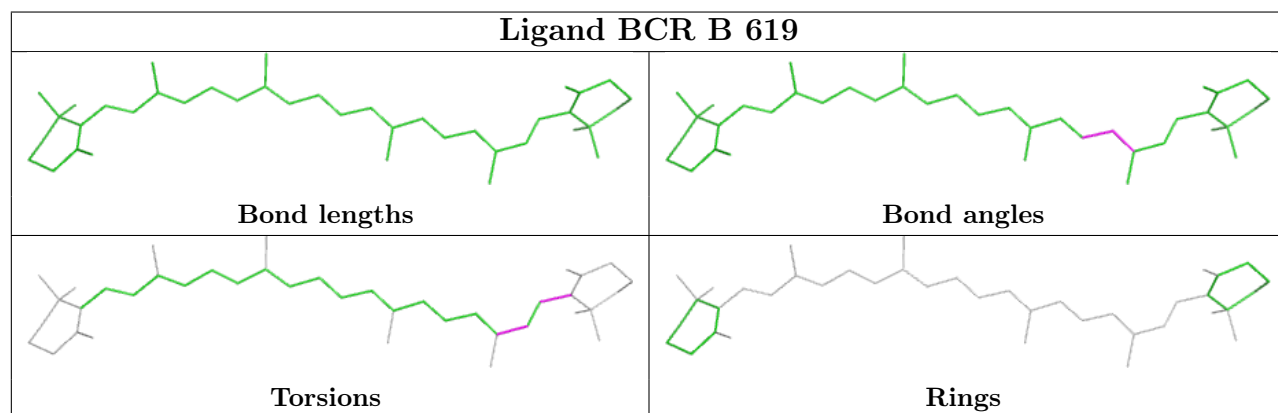
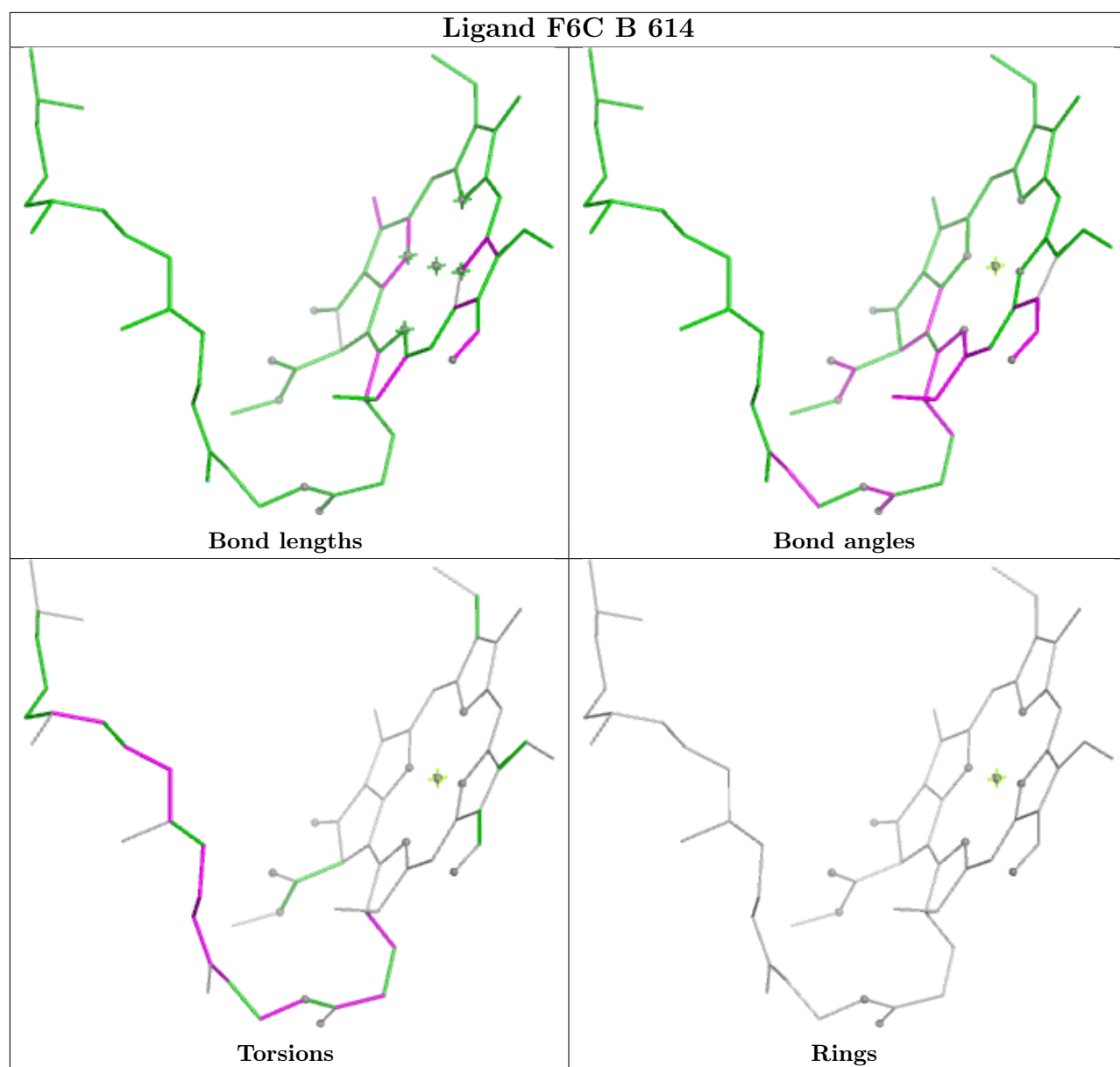


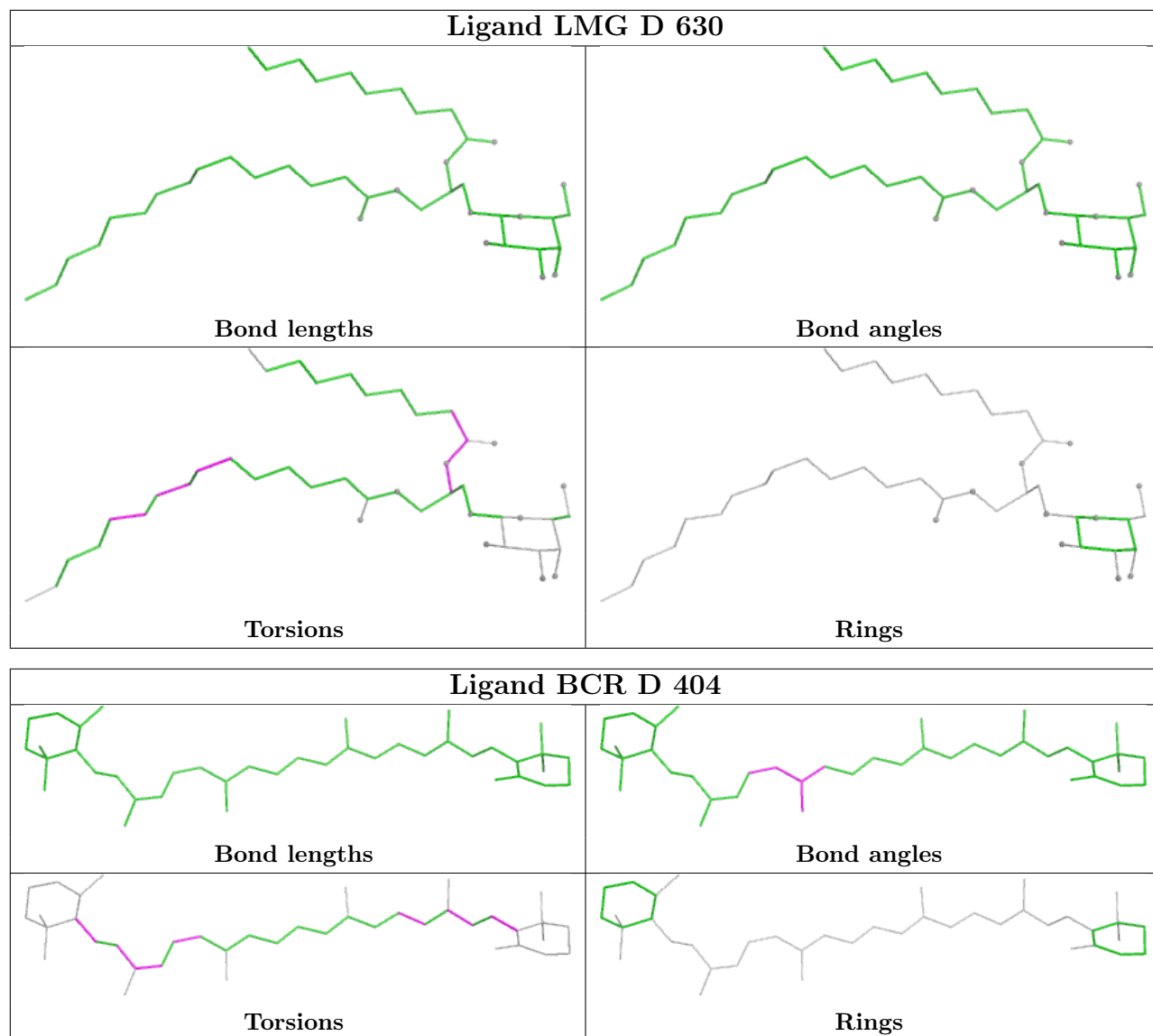


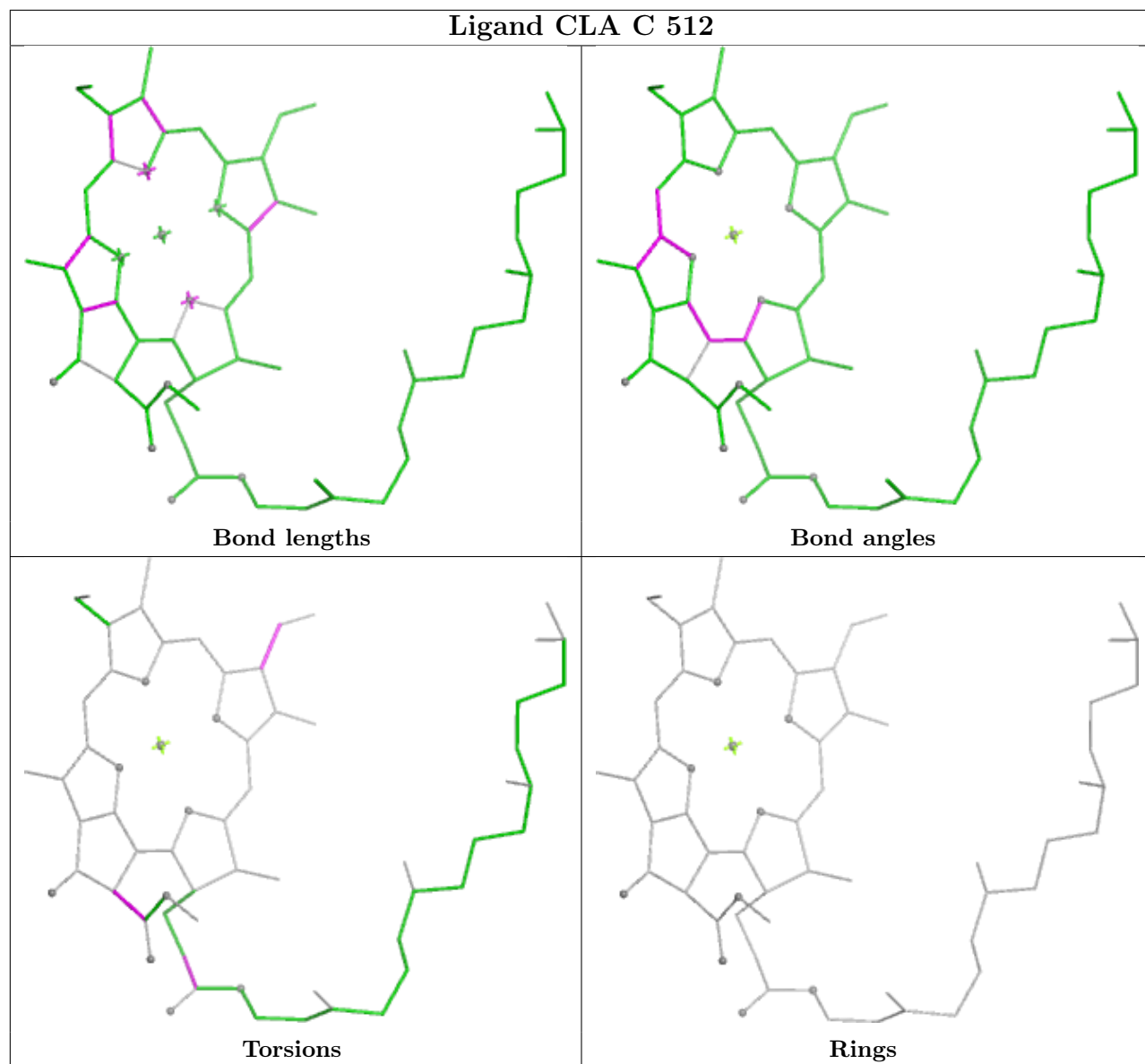


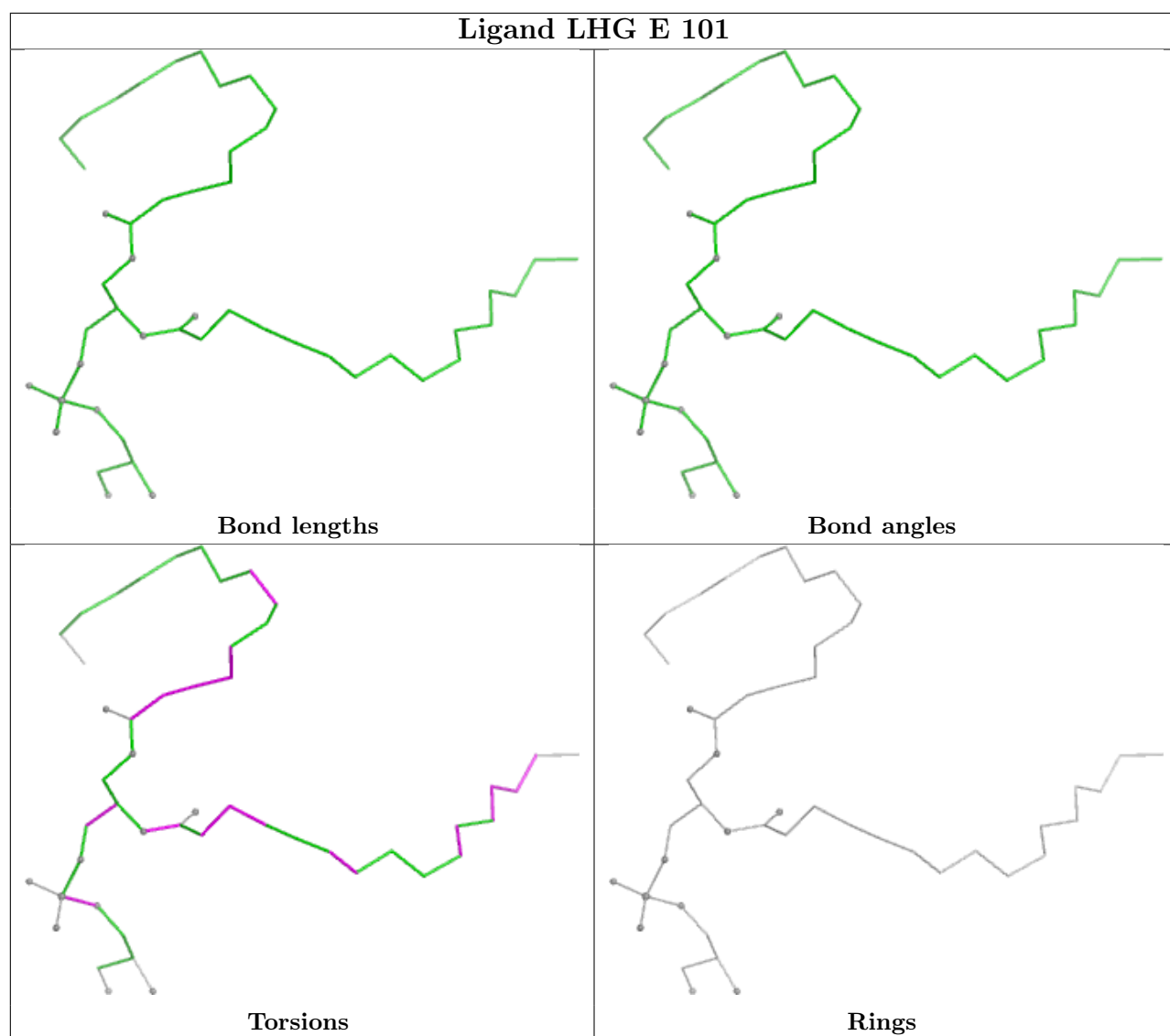


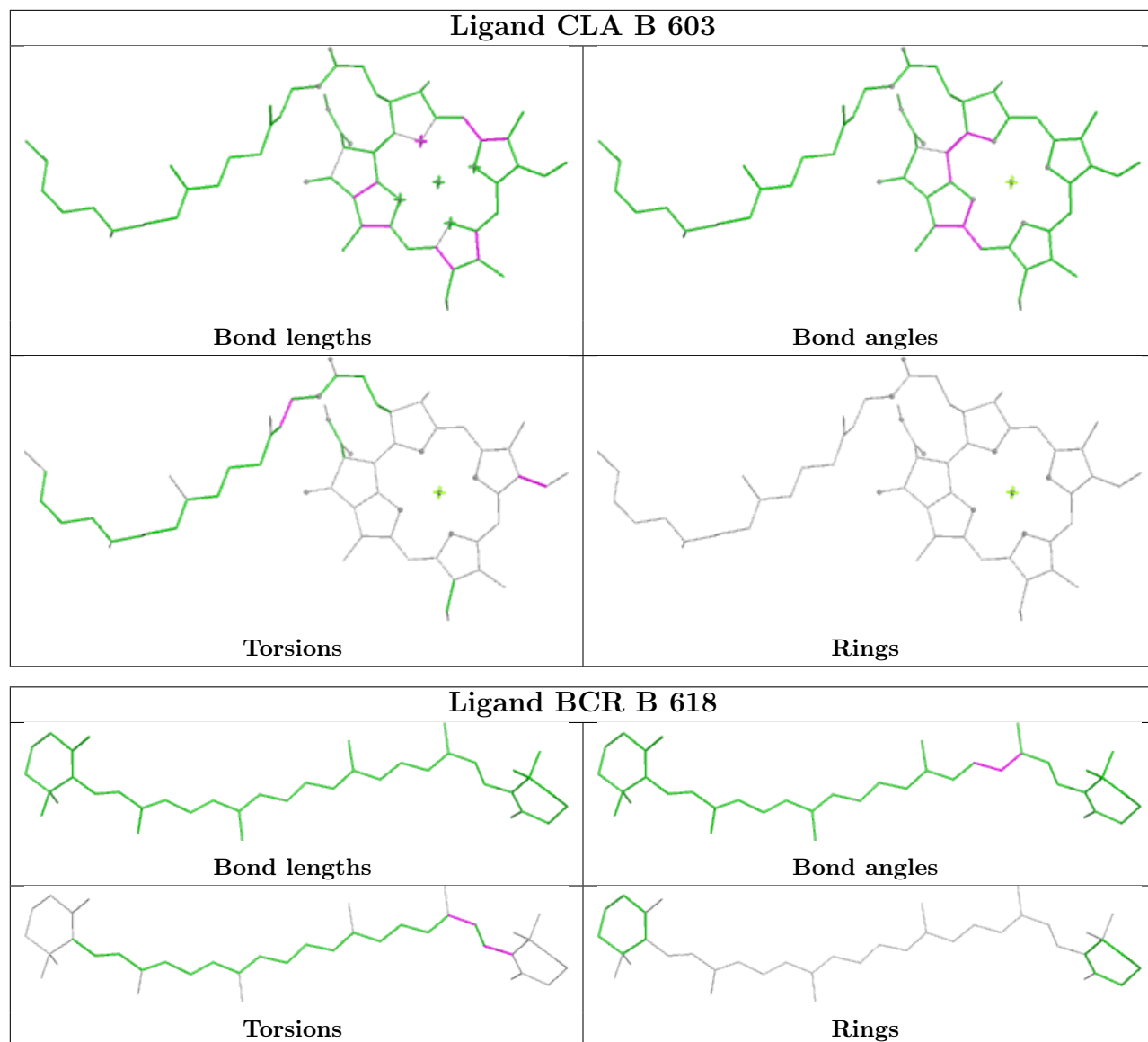


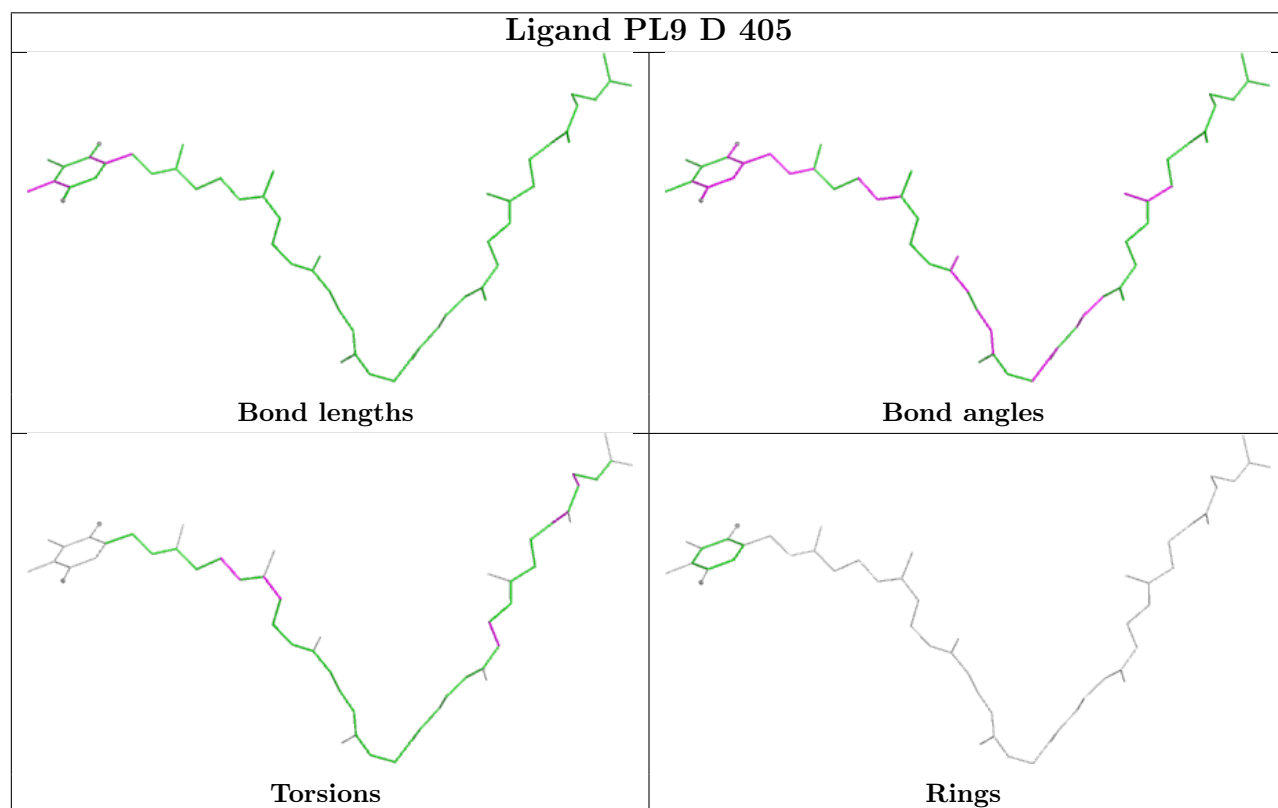
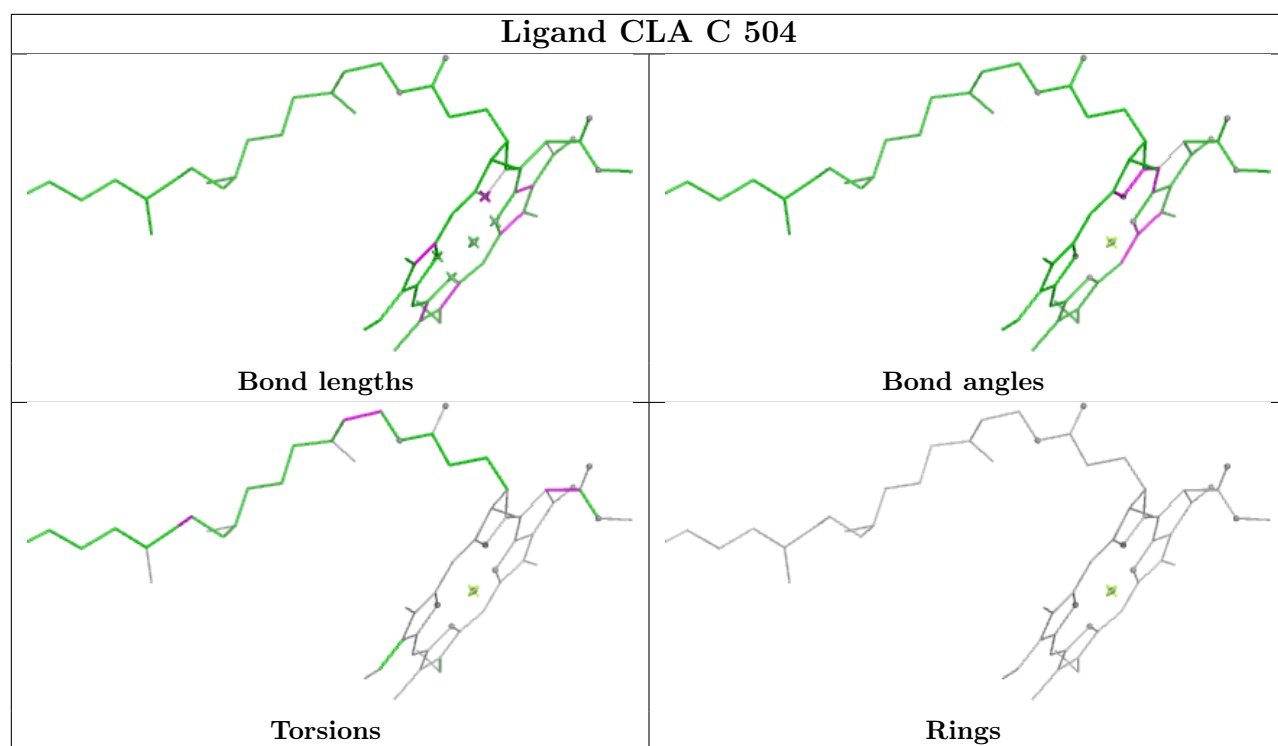


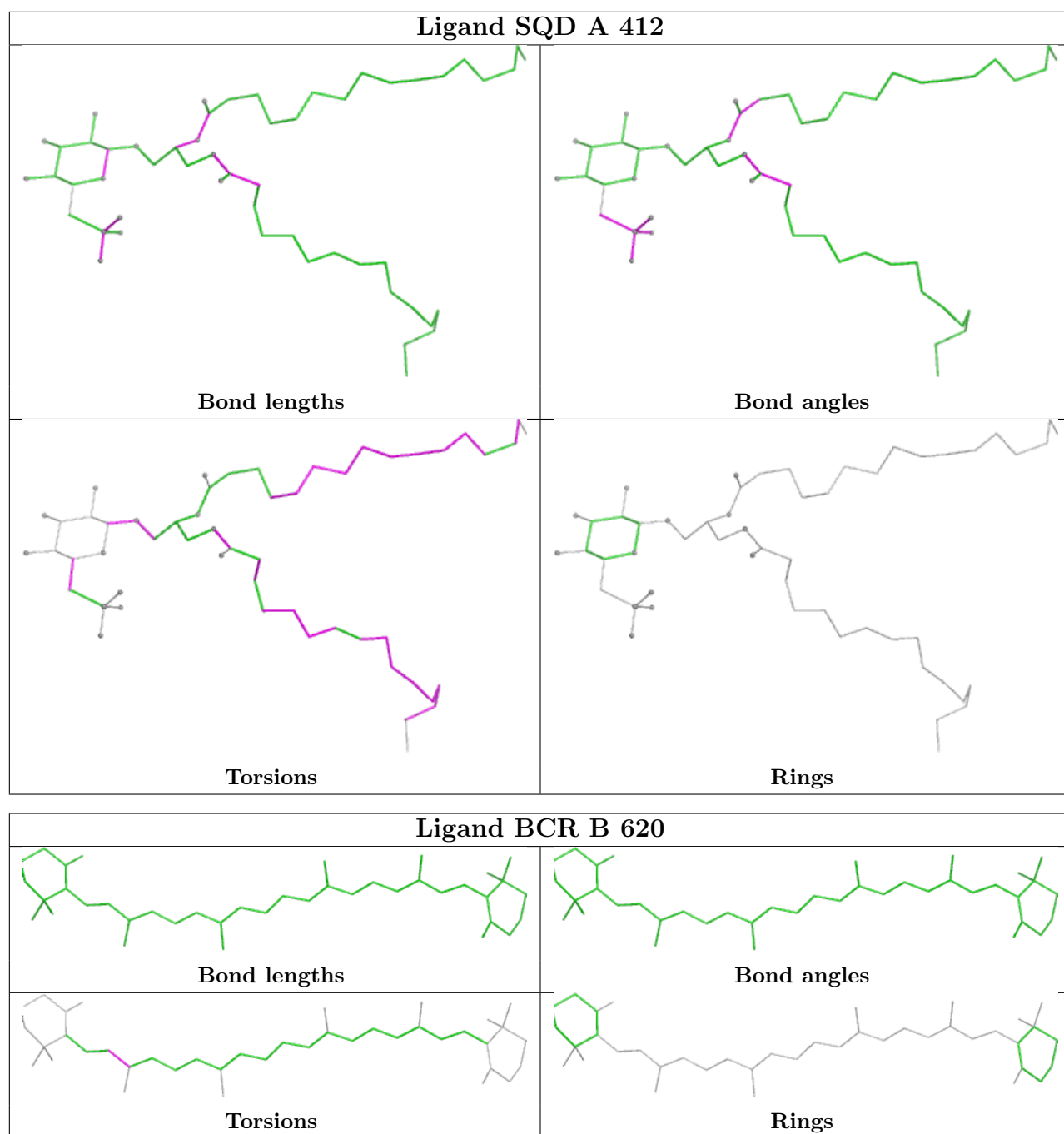


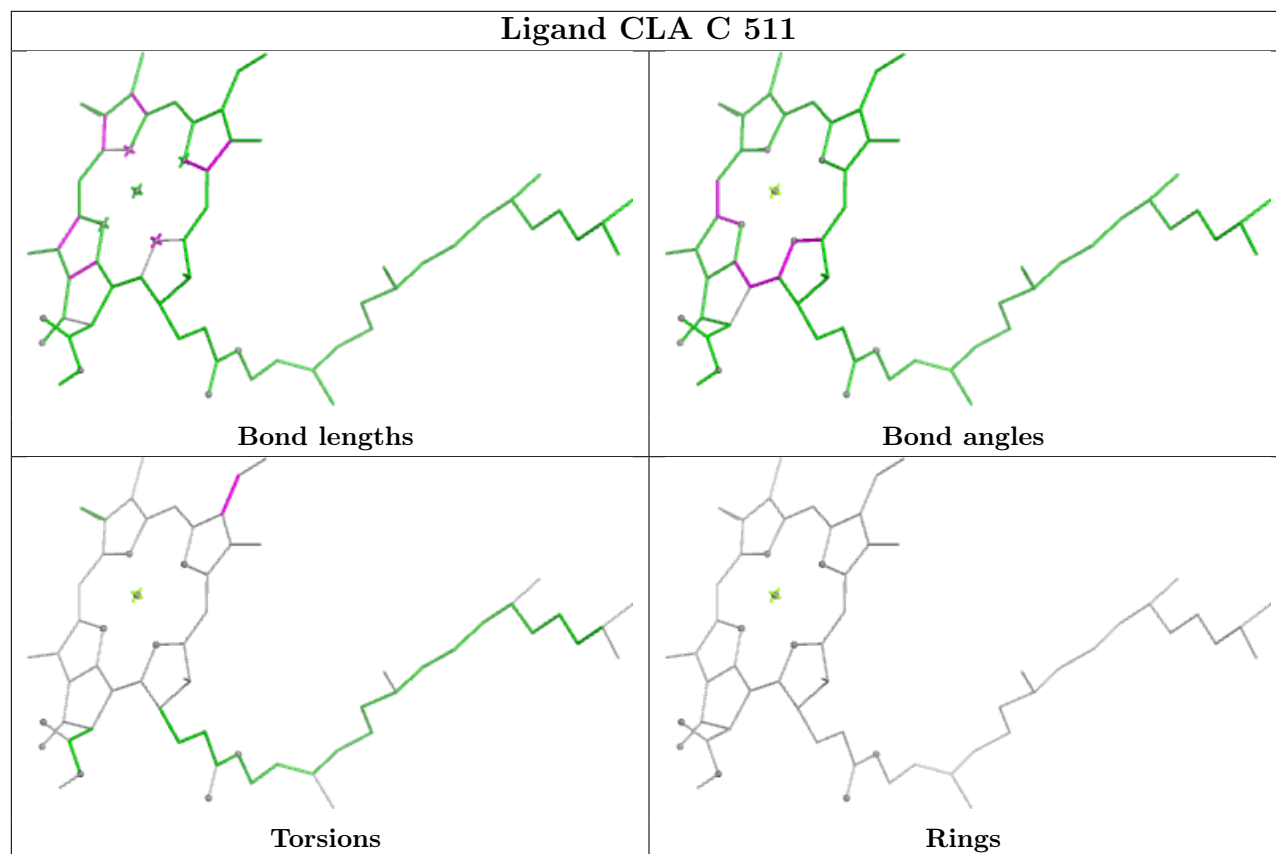
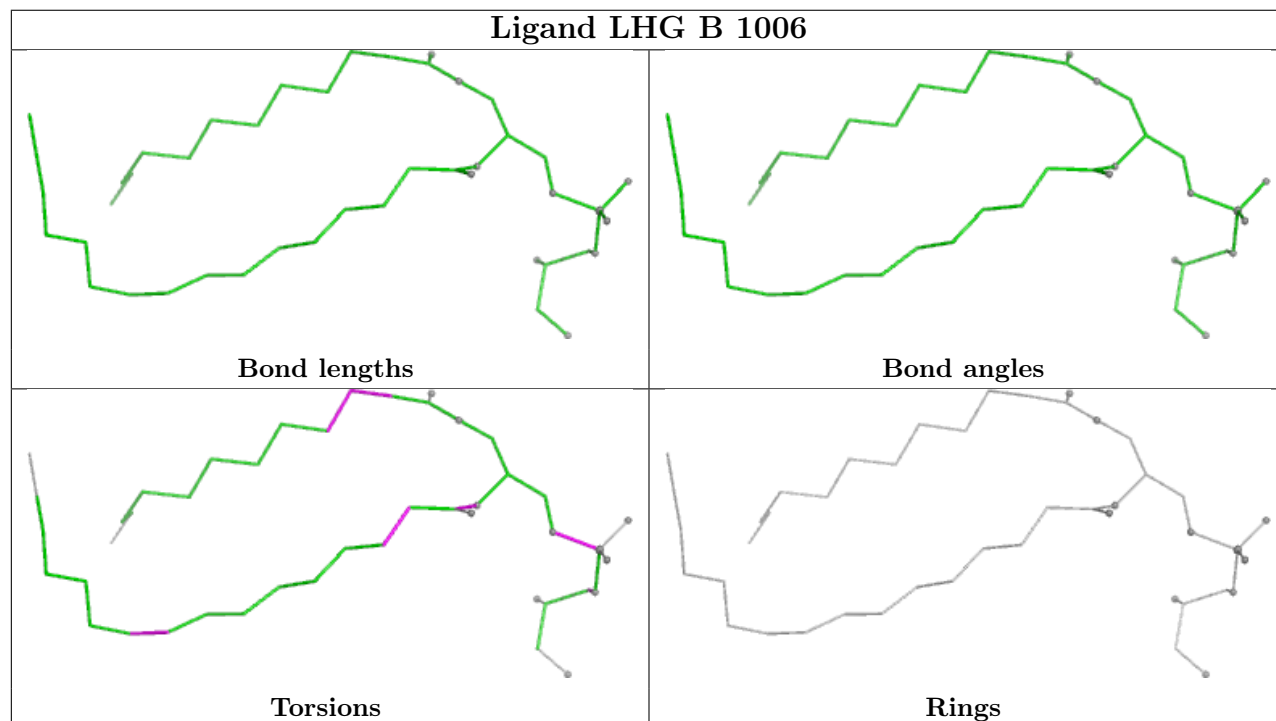


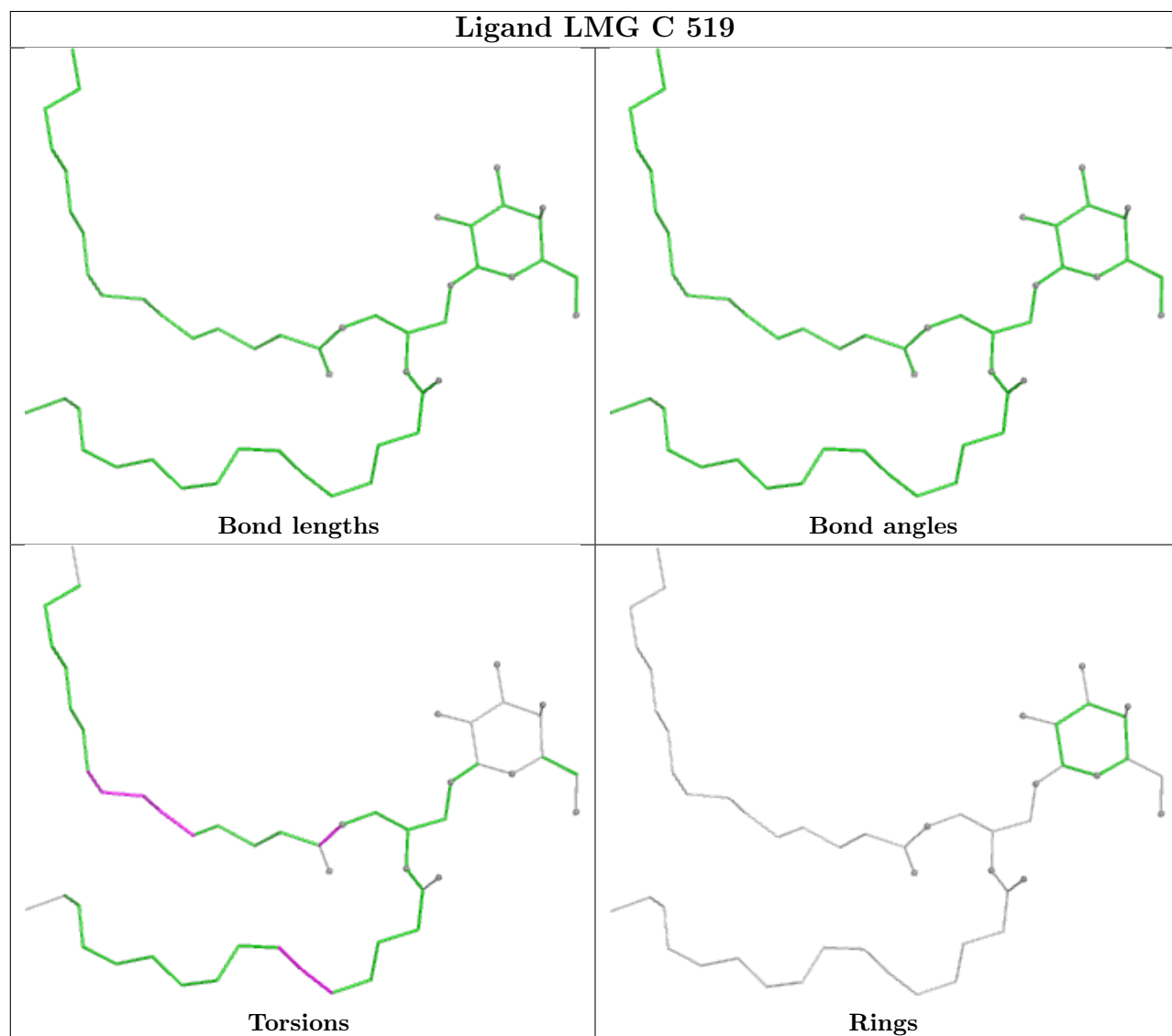
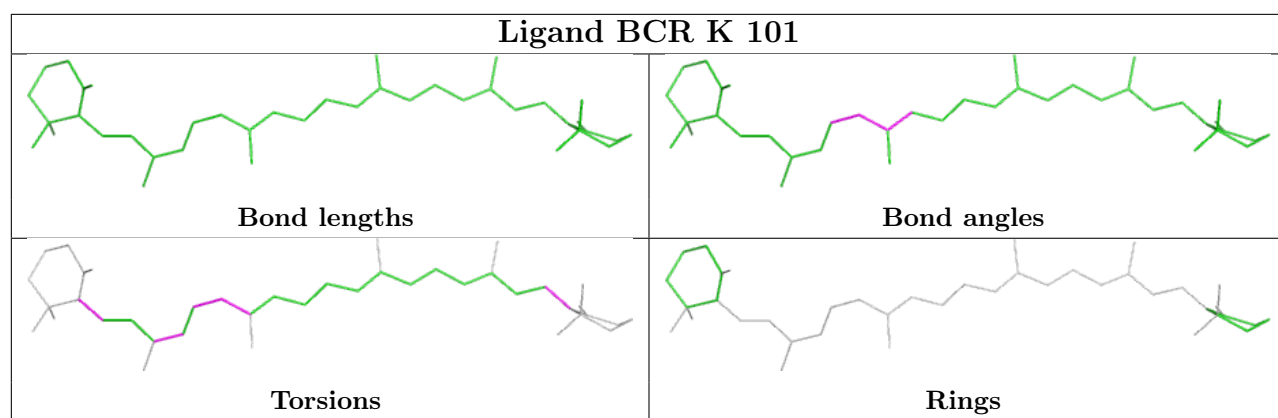


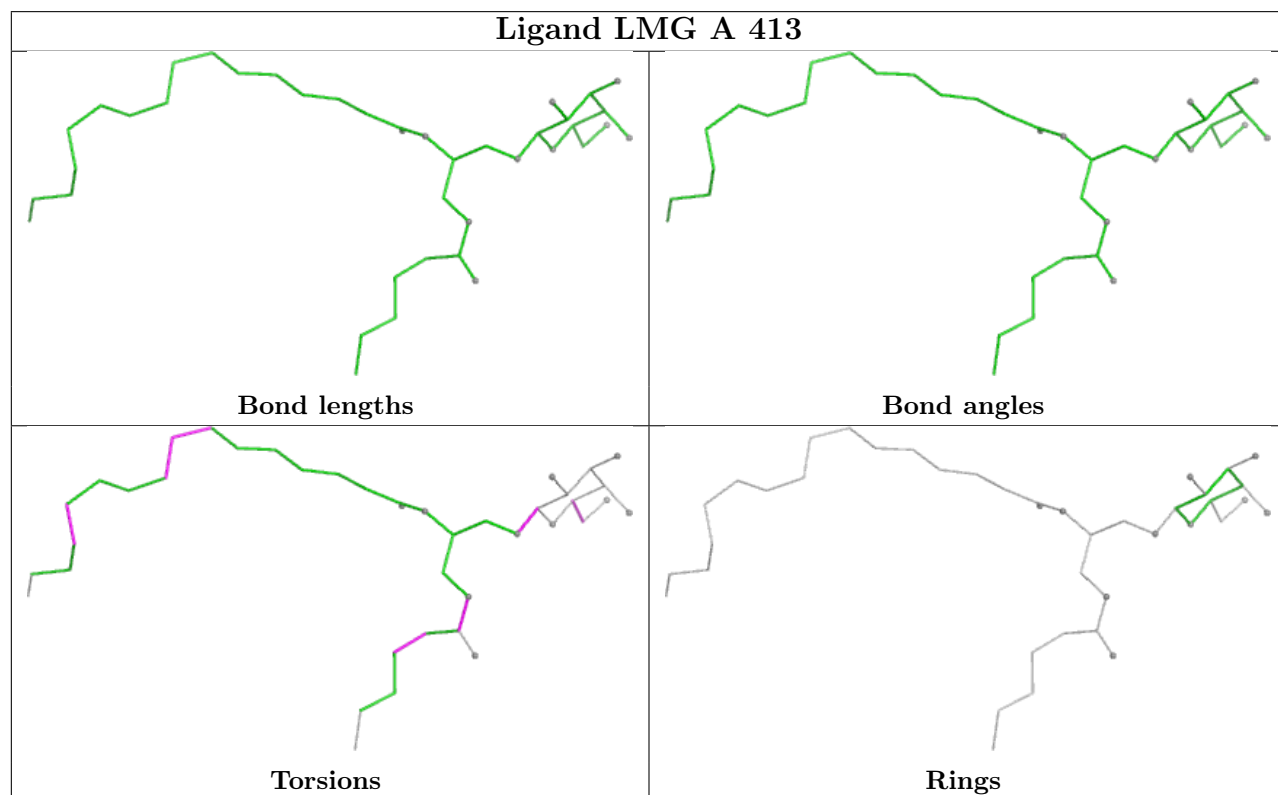
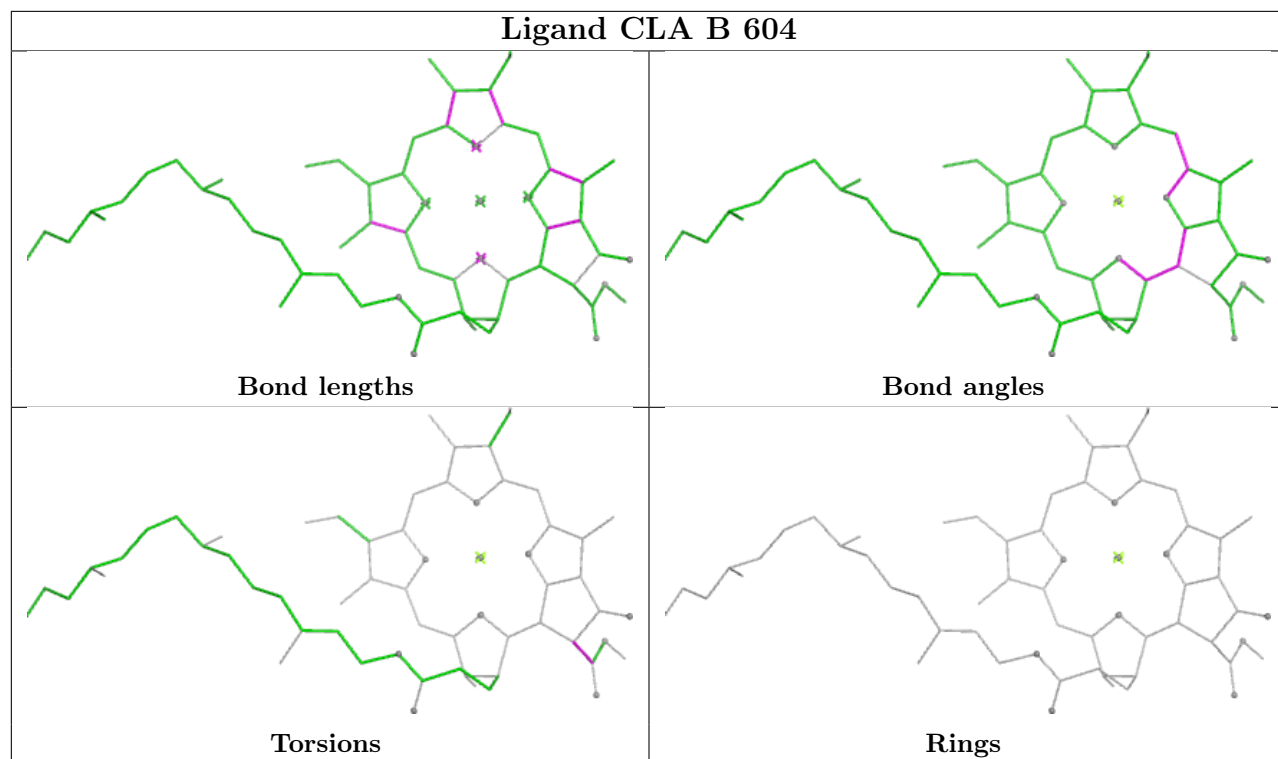


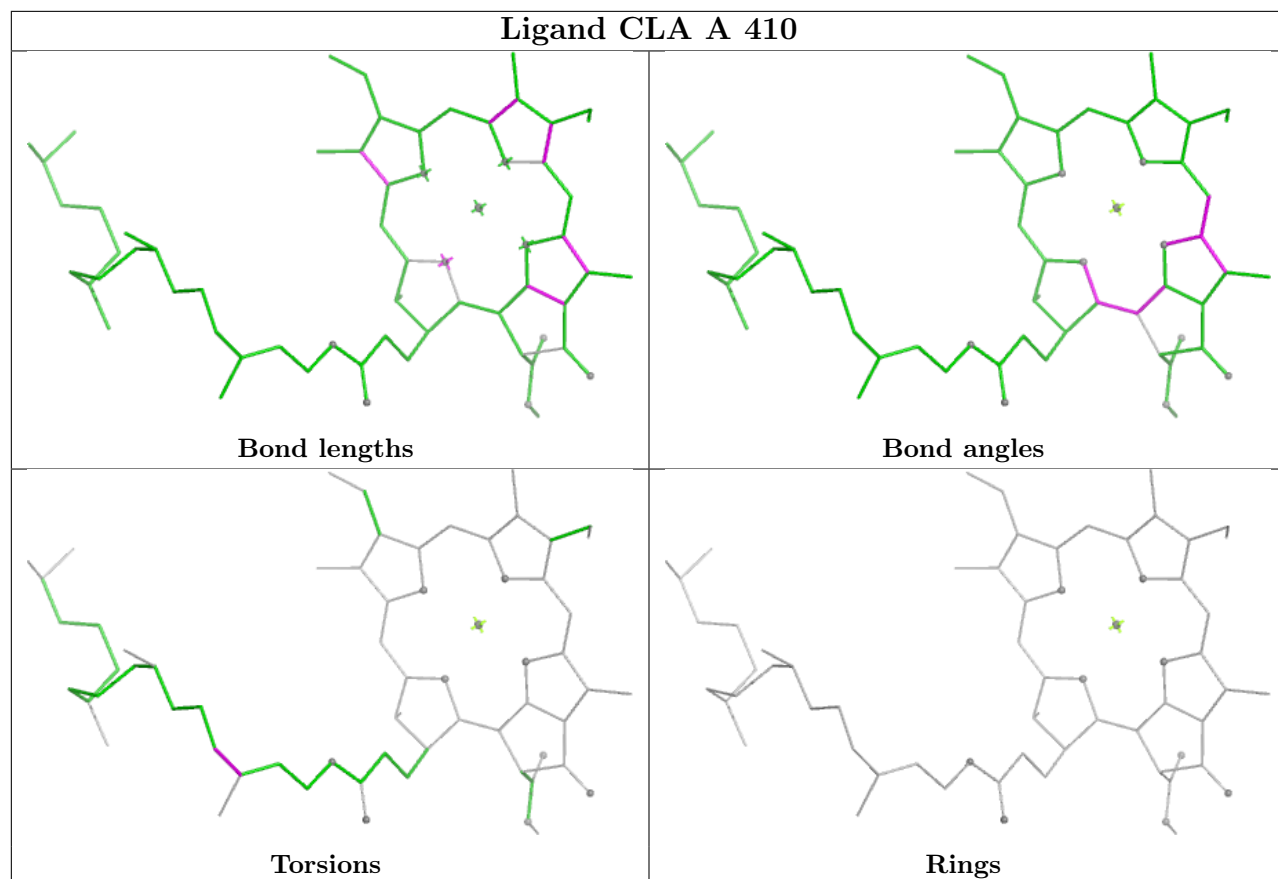


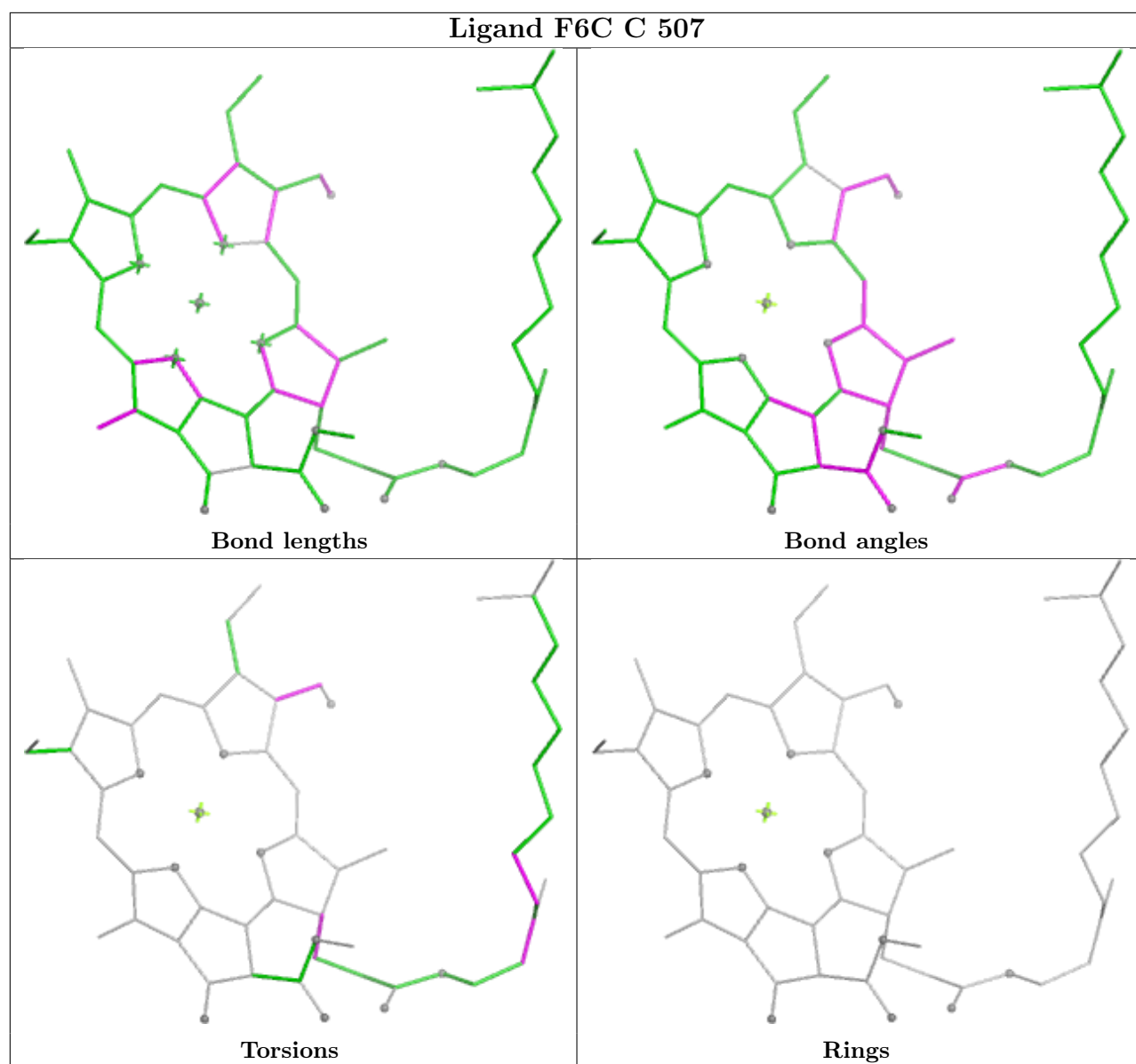


Ligand CLA C 511**Ligand LHG B 1006**

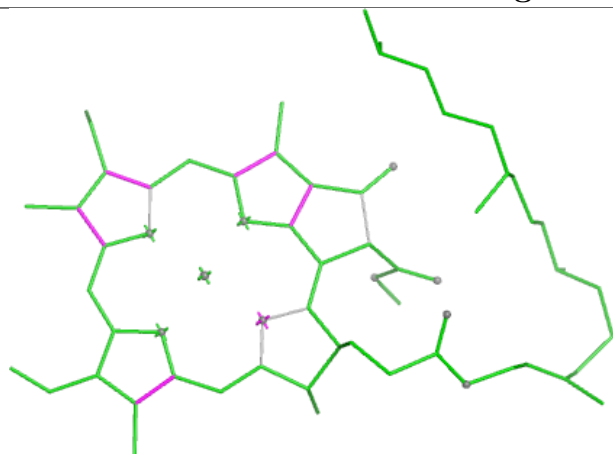




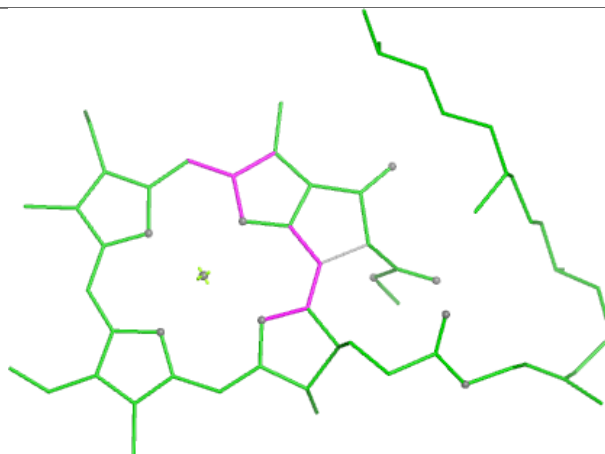




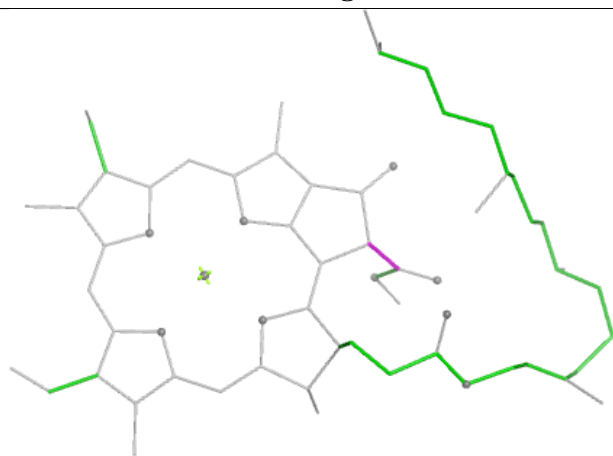
Ligand CLA B 611



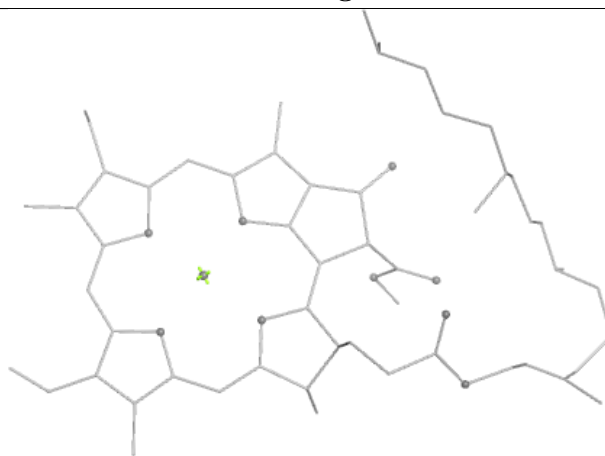
Bond lengths



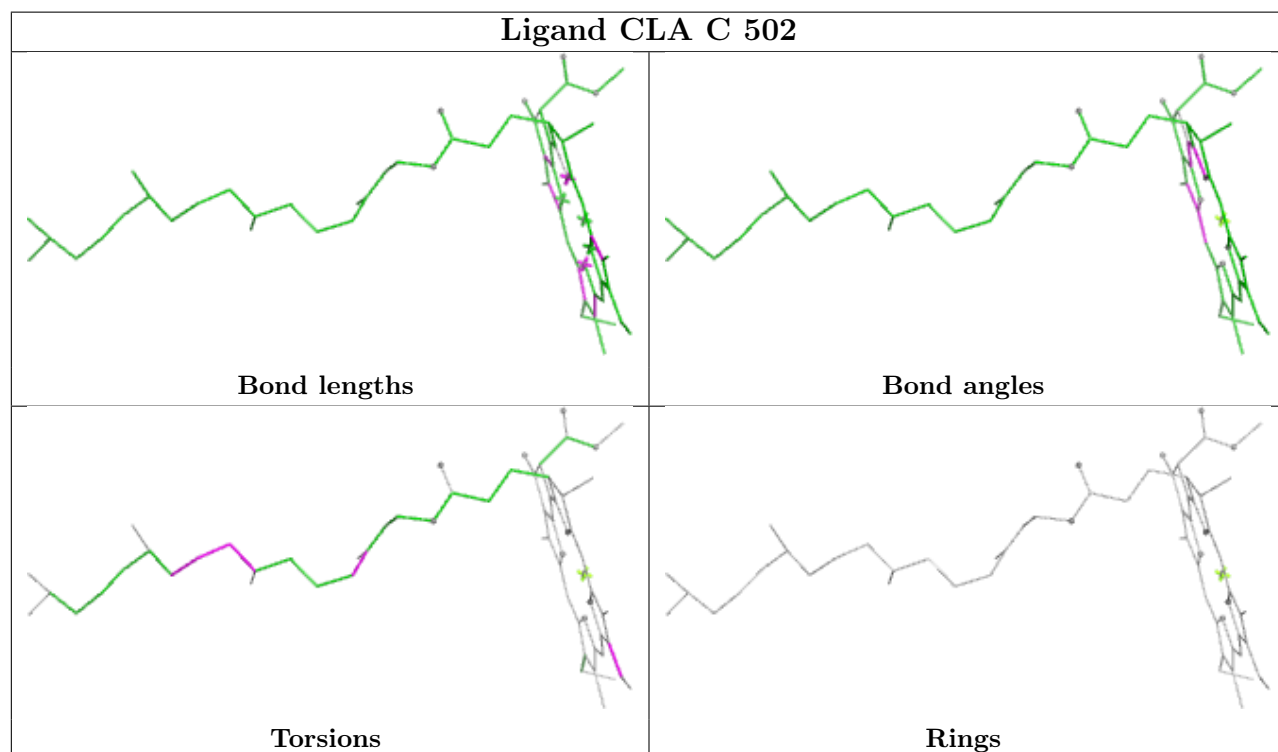
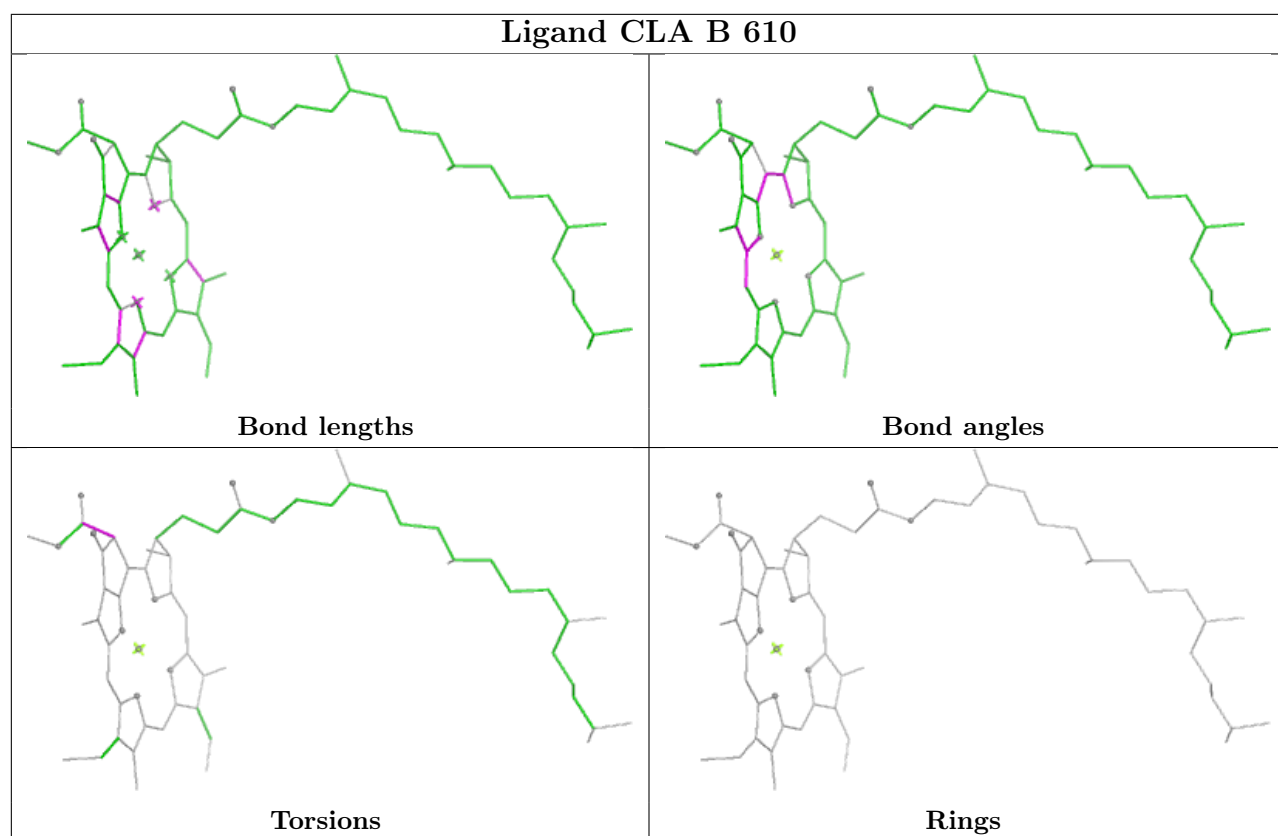
Bond angles

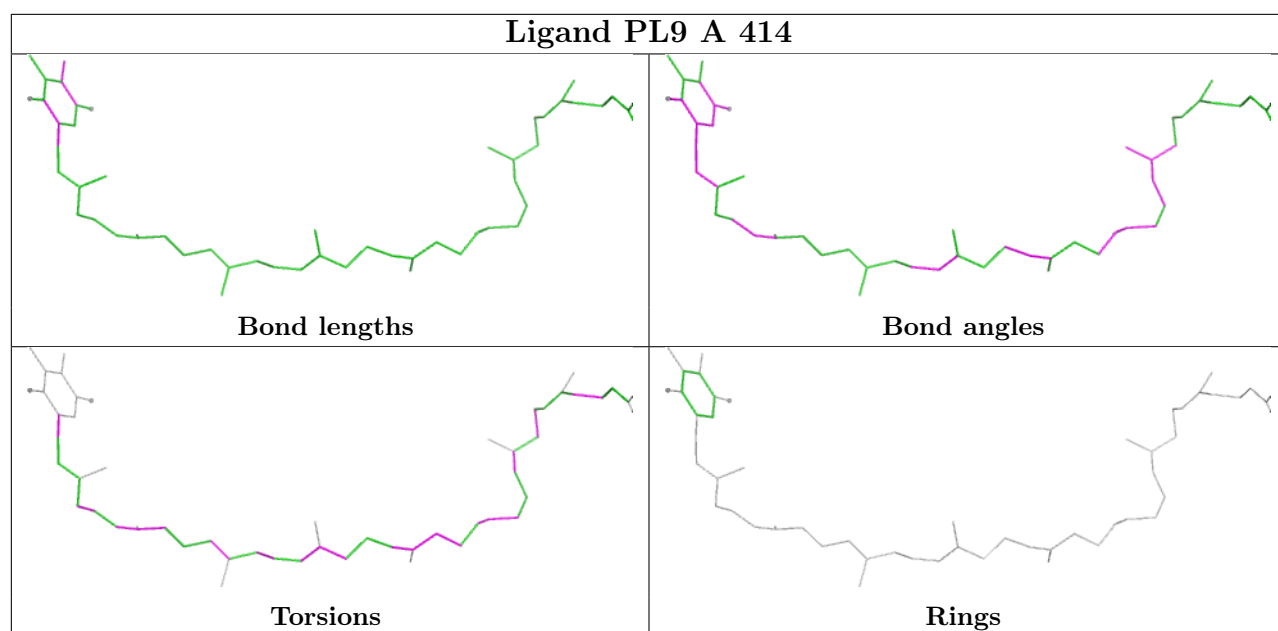


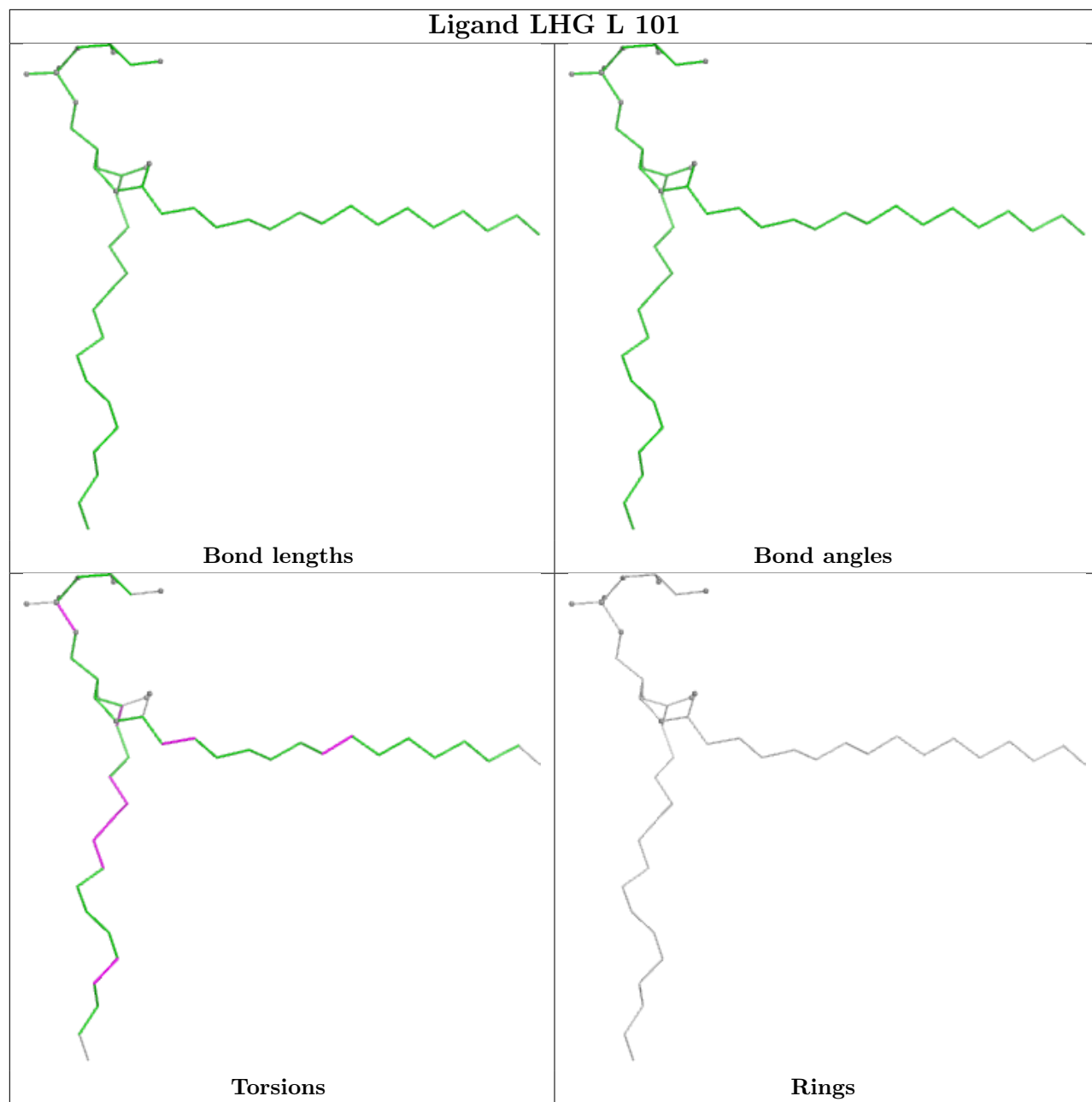
Torsions

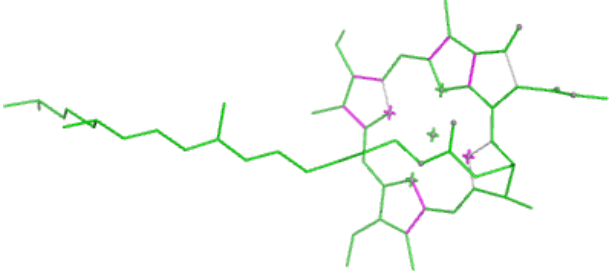
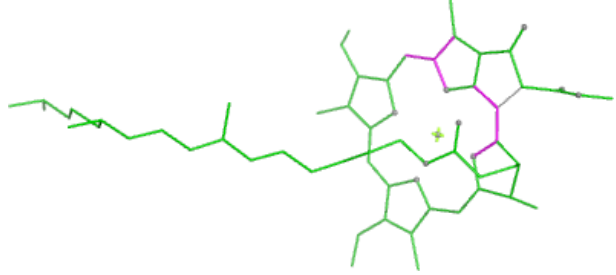
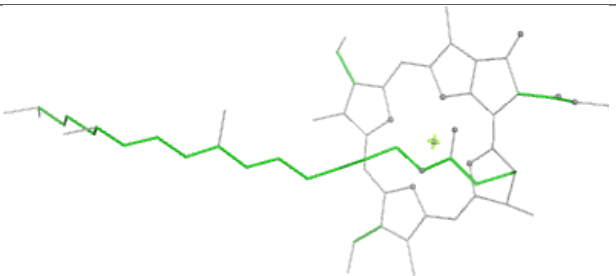
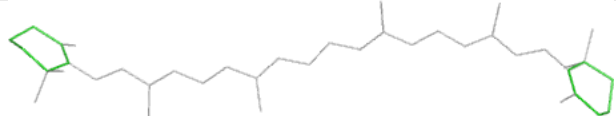


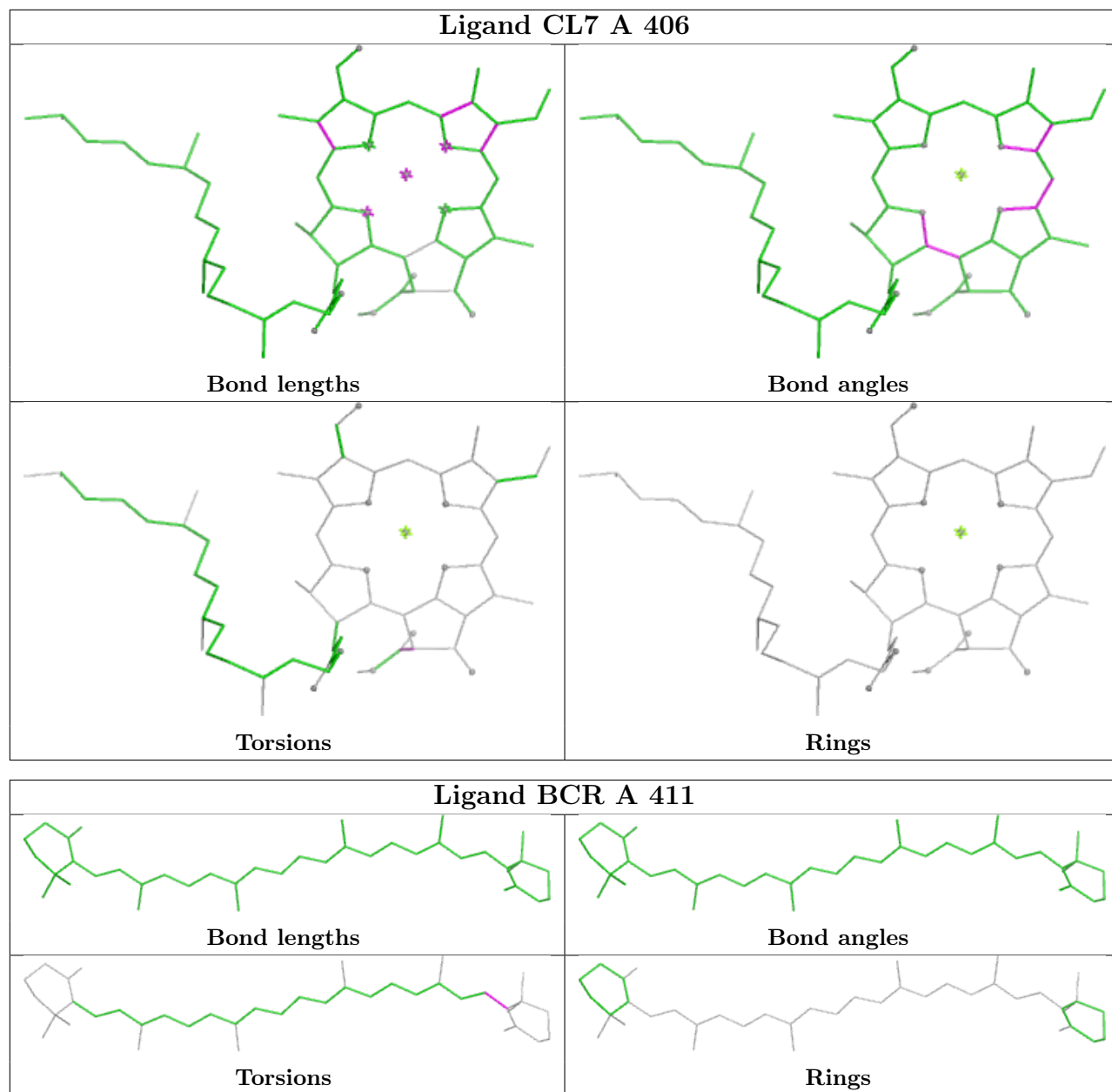
Rings

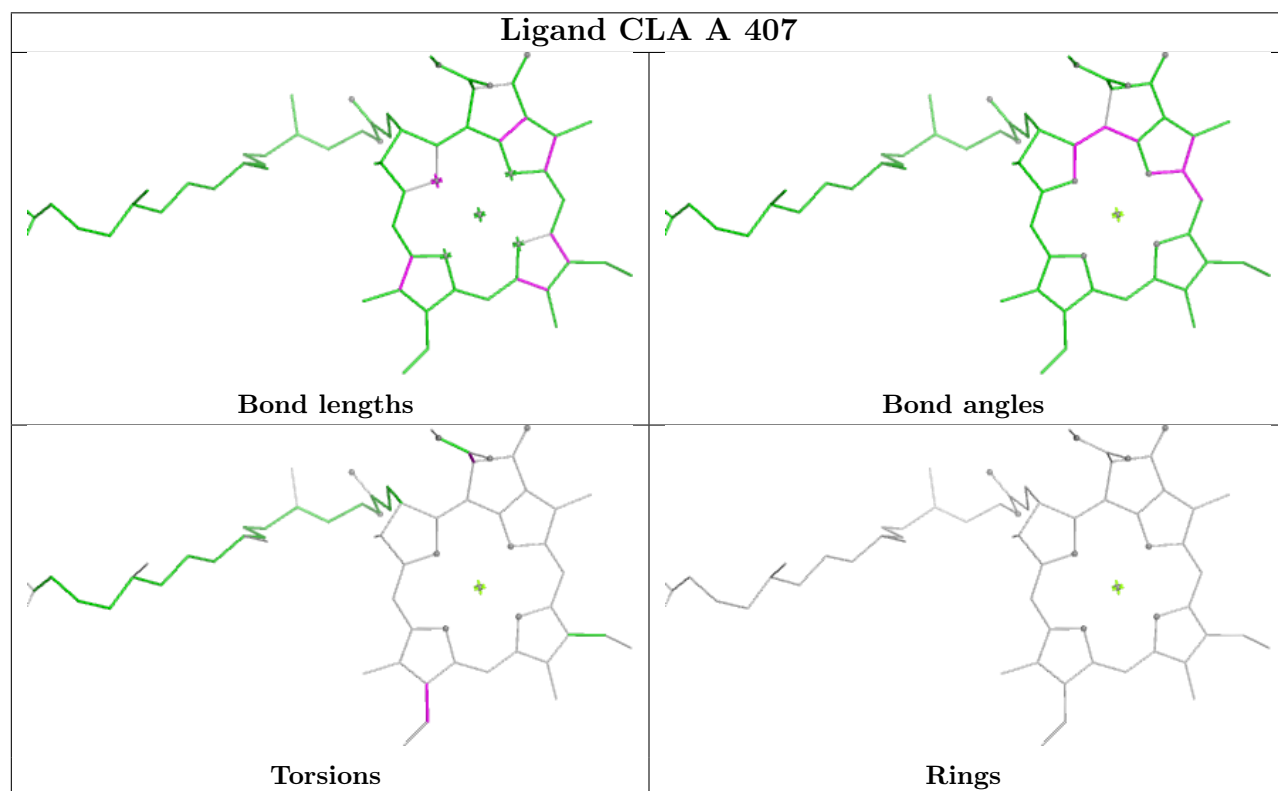
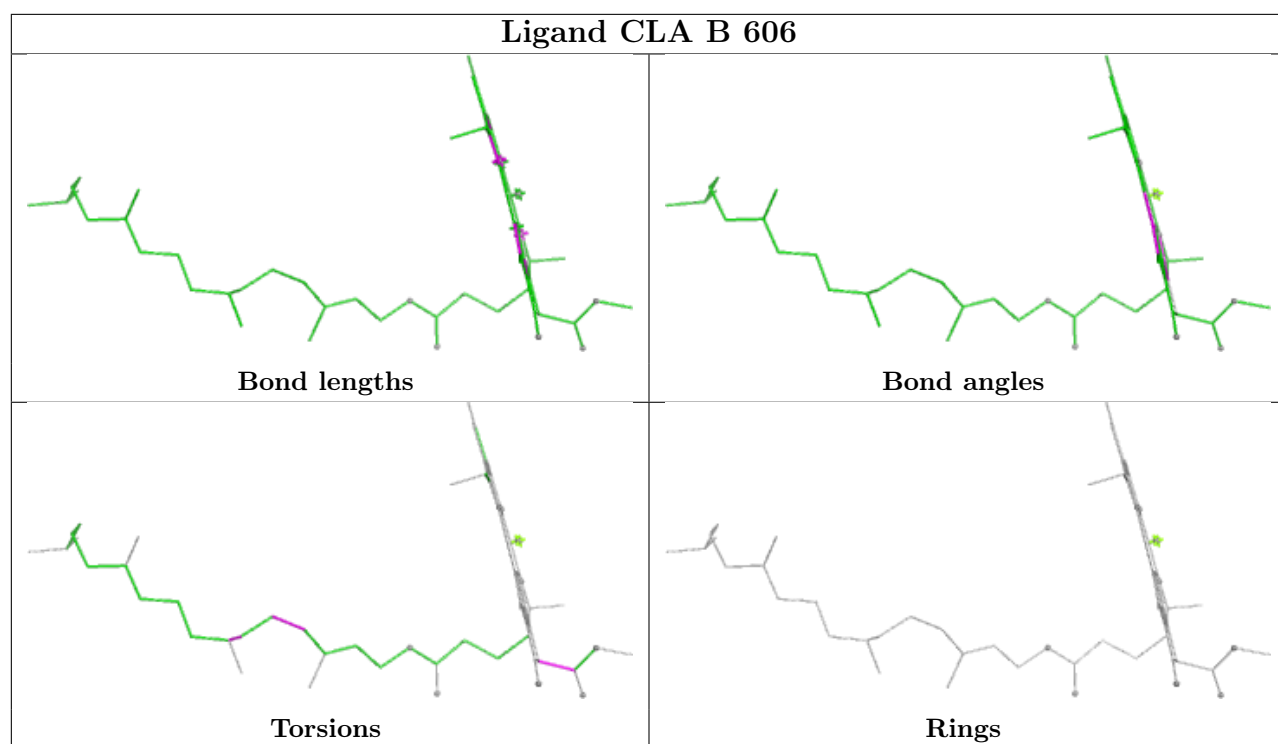


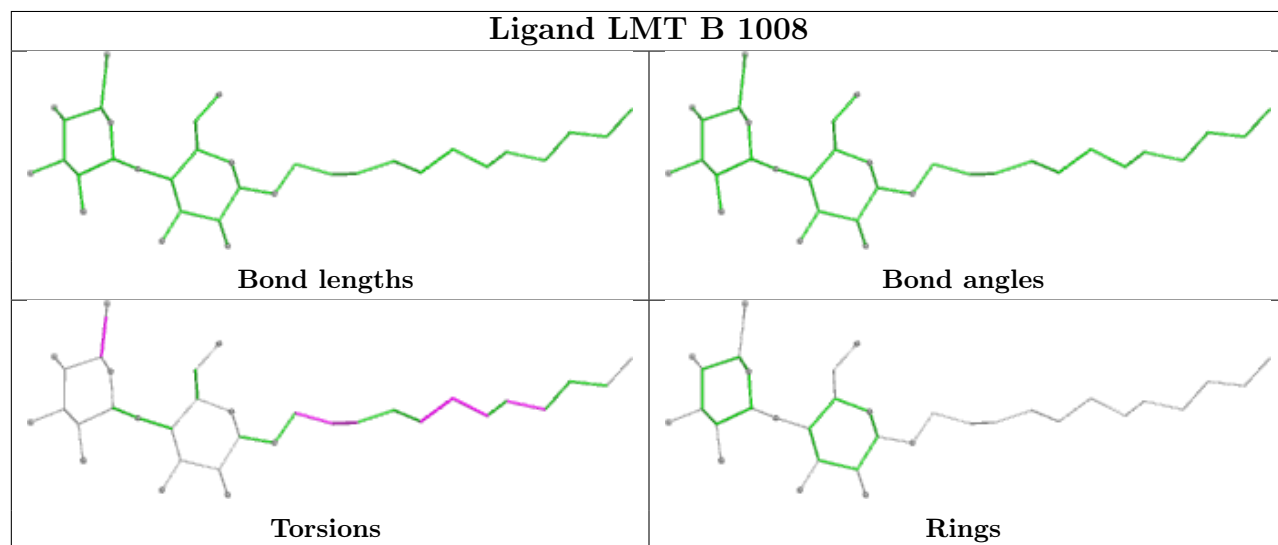
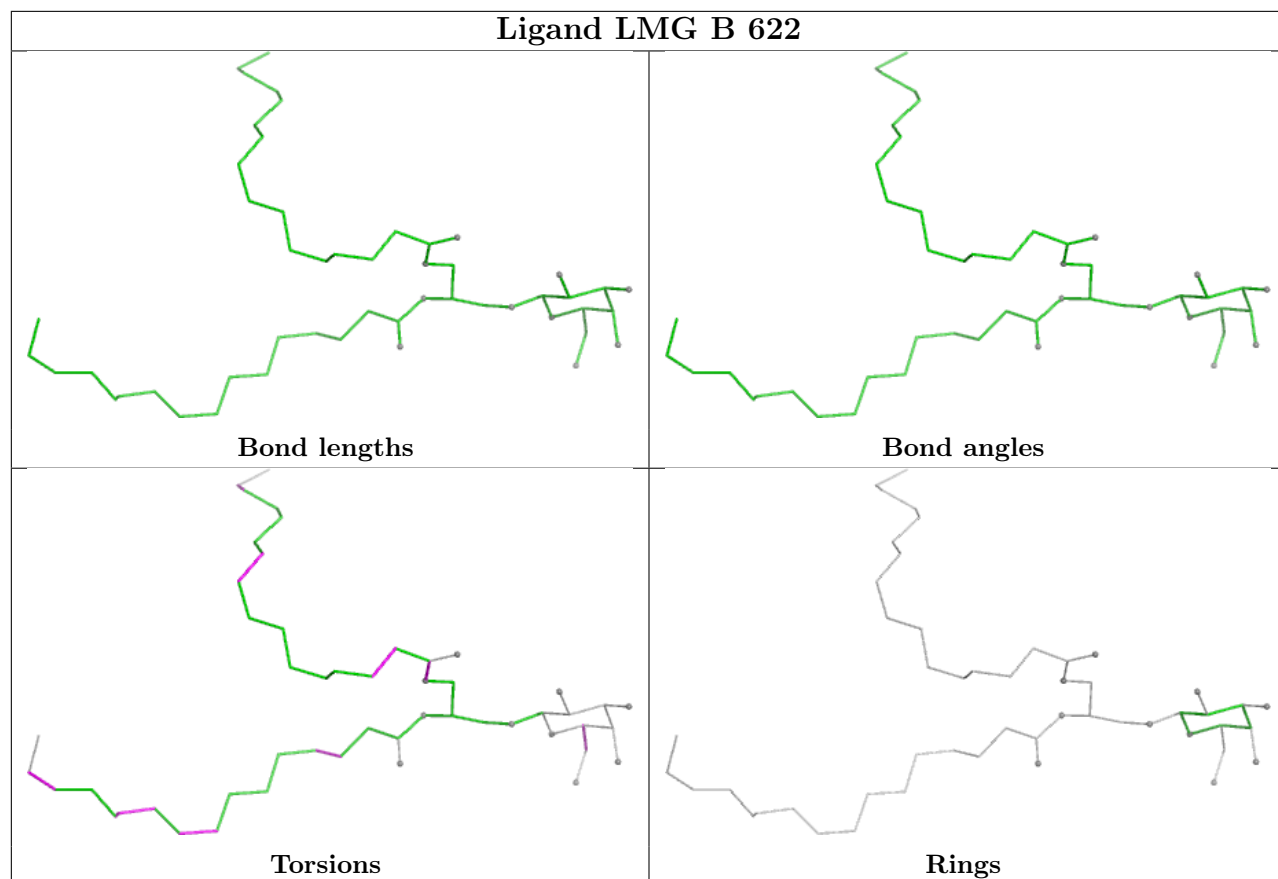


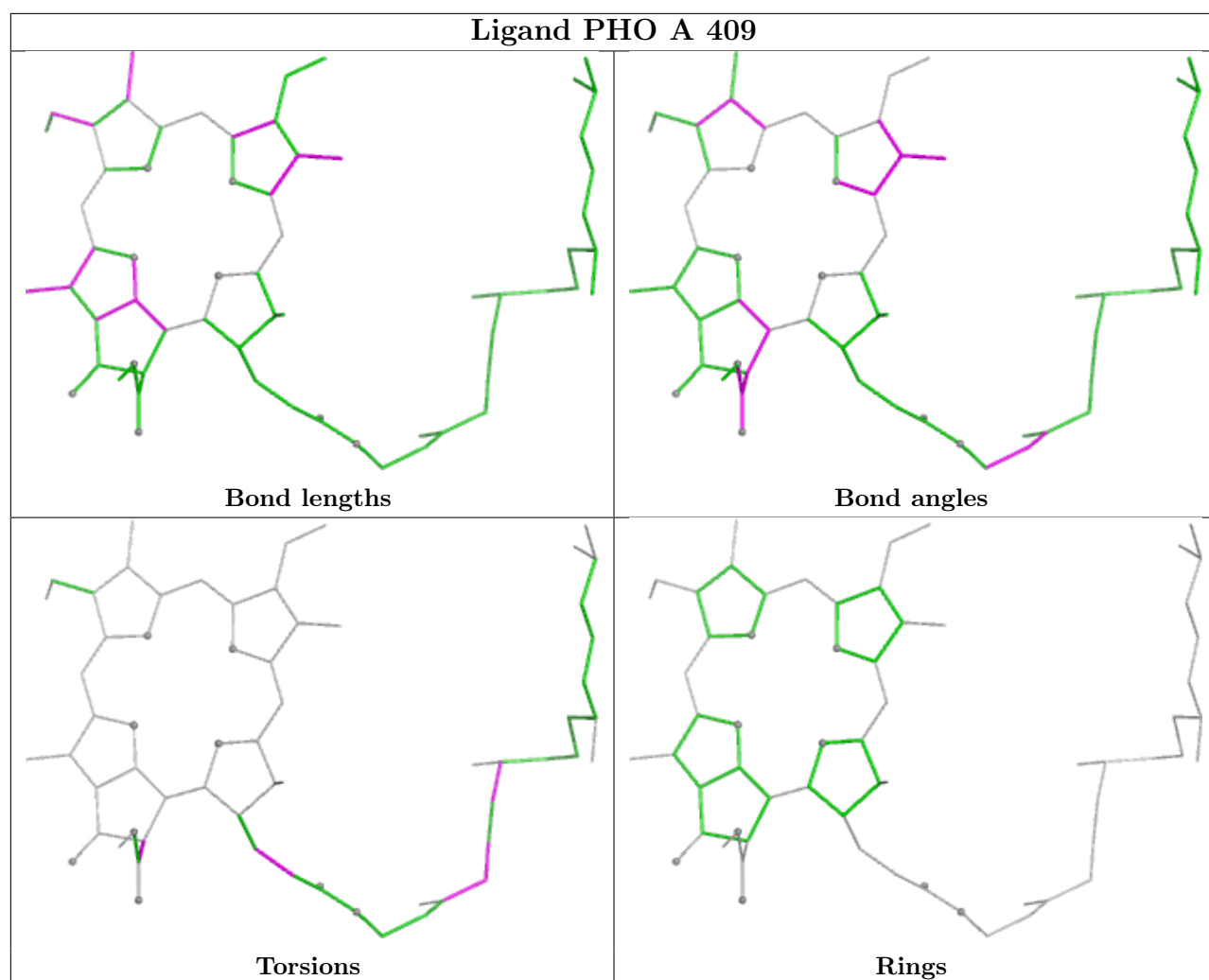


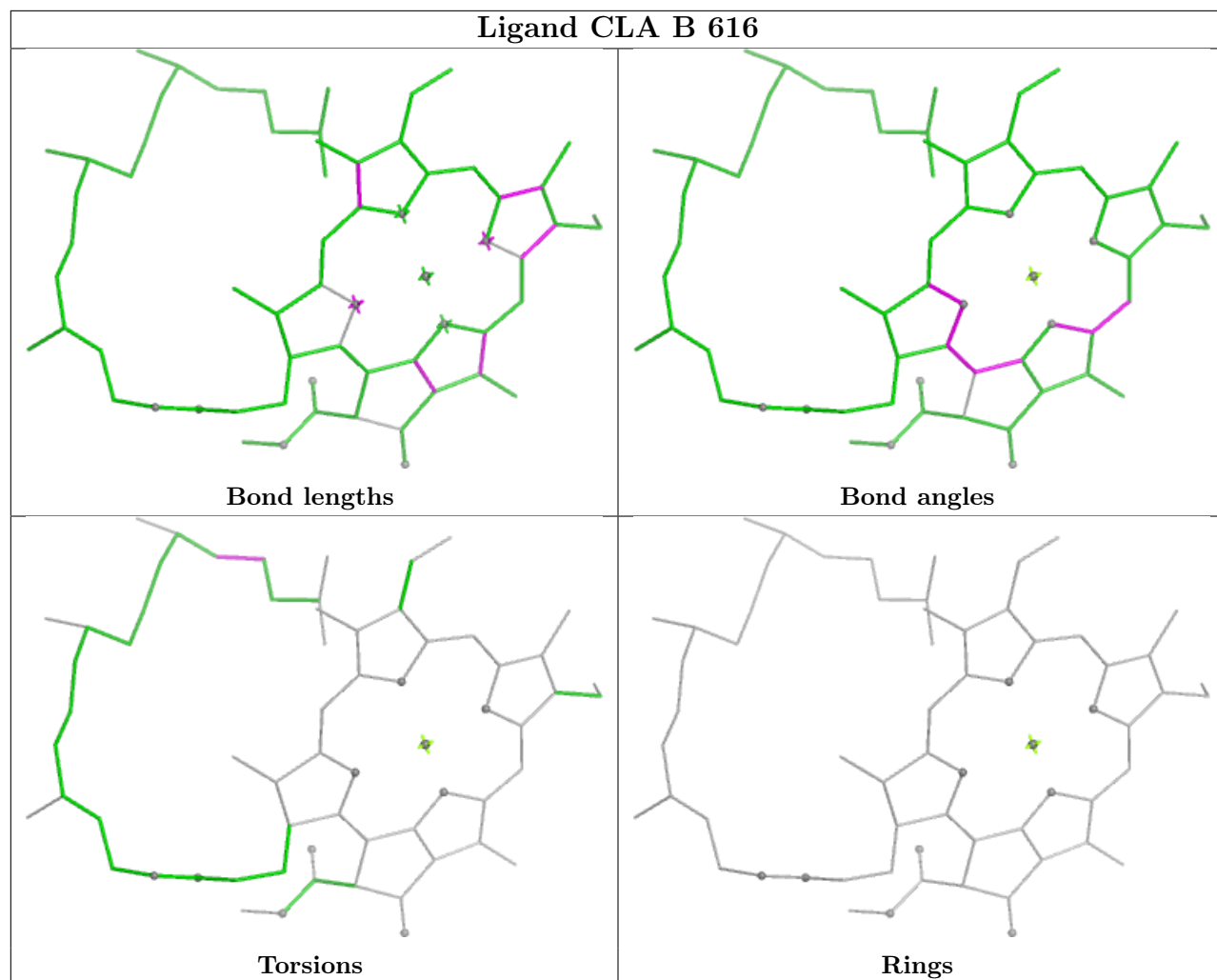
Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

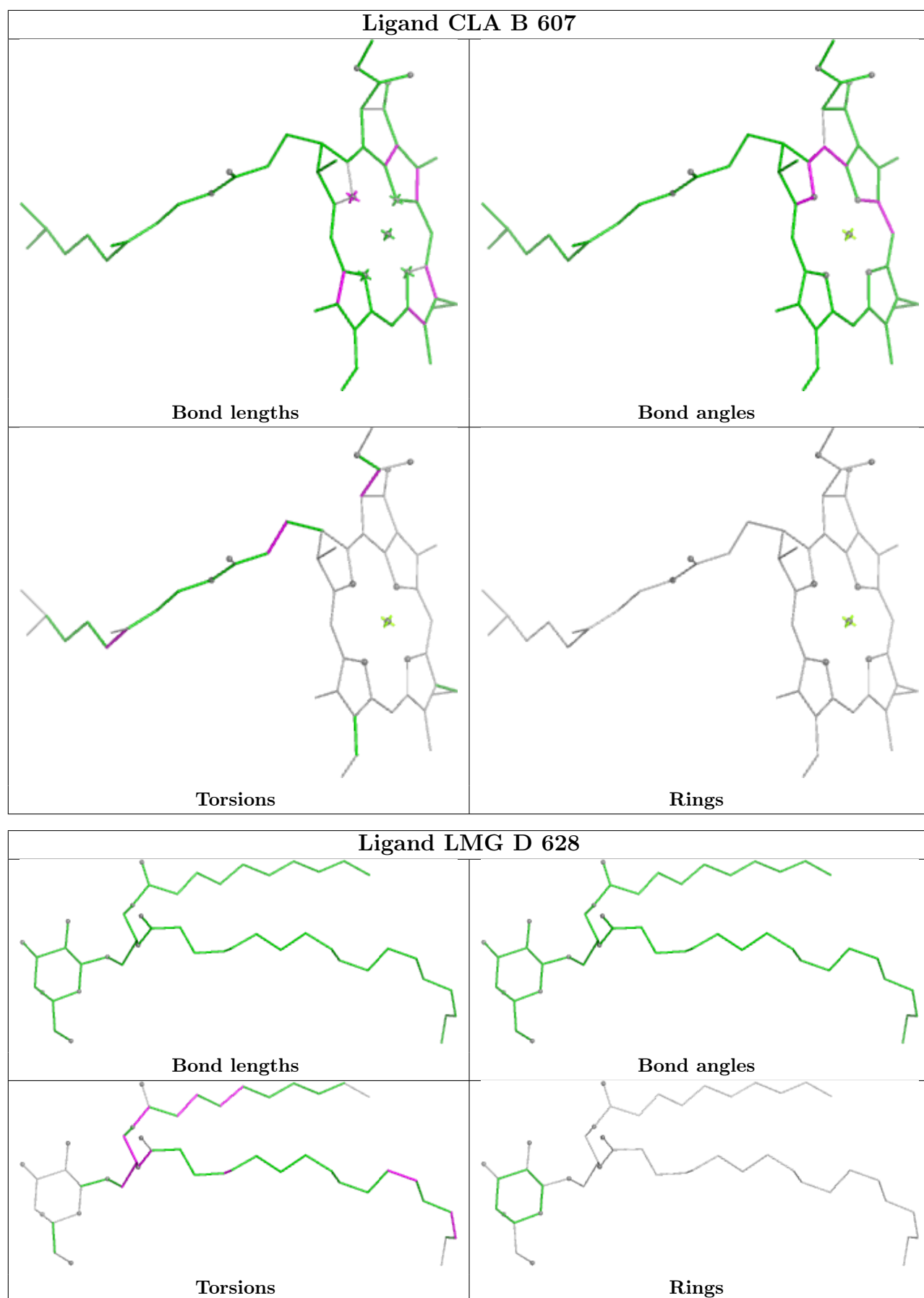


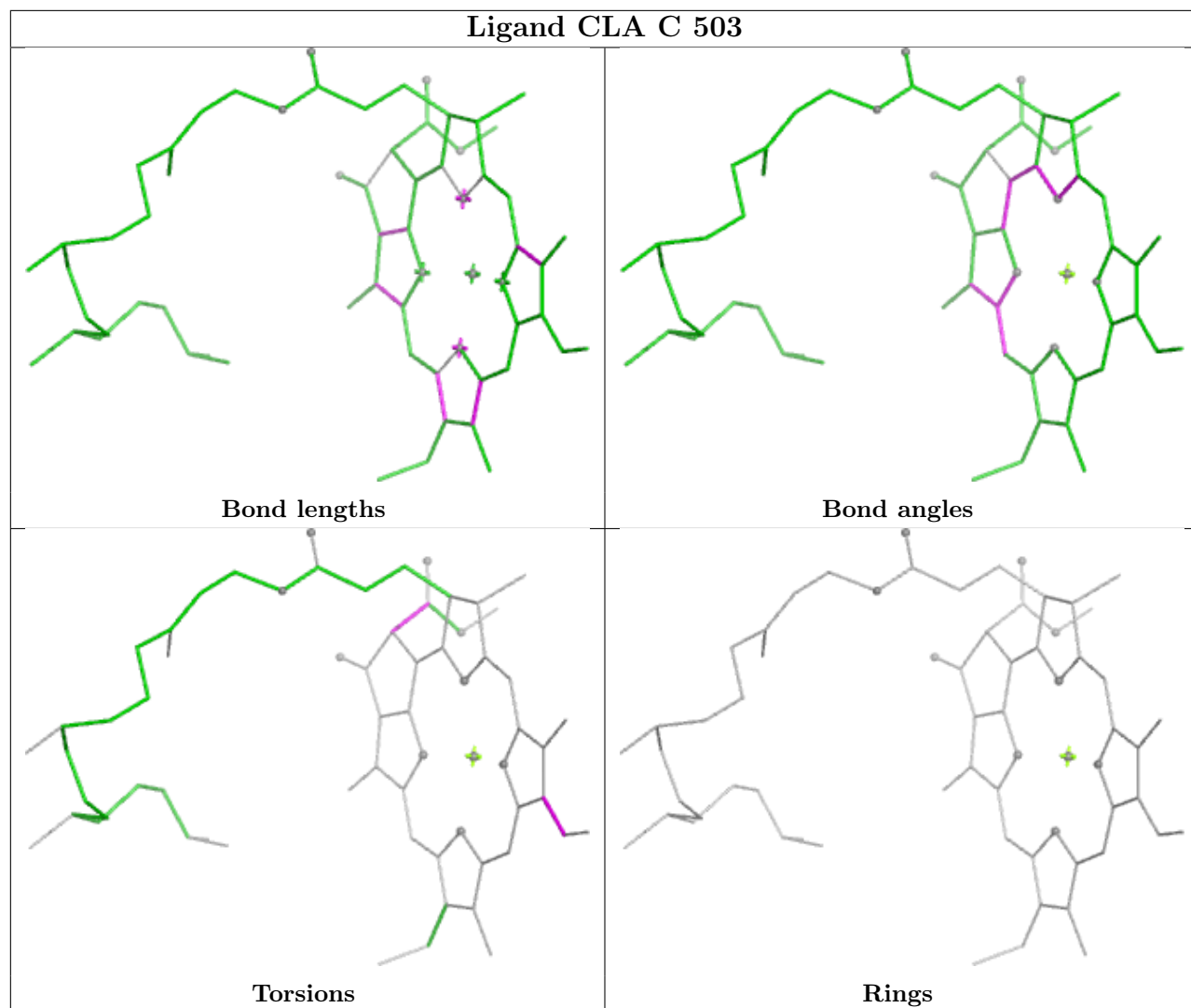


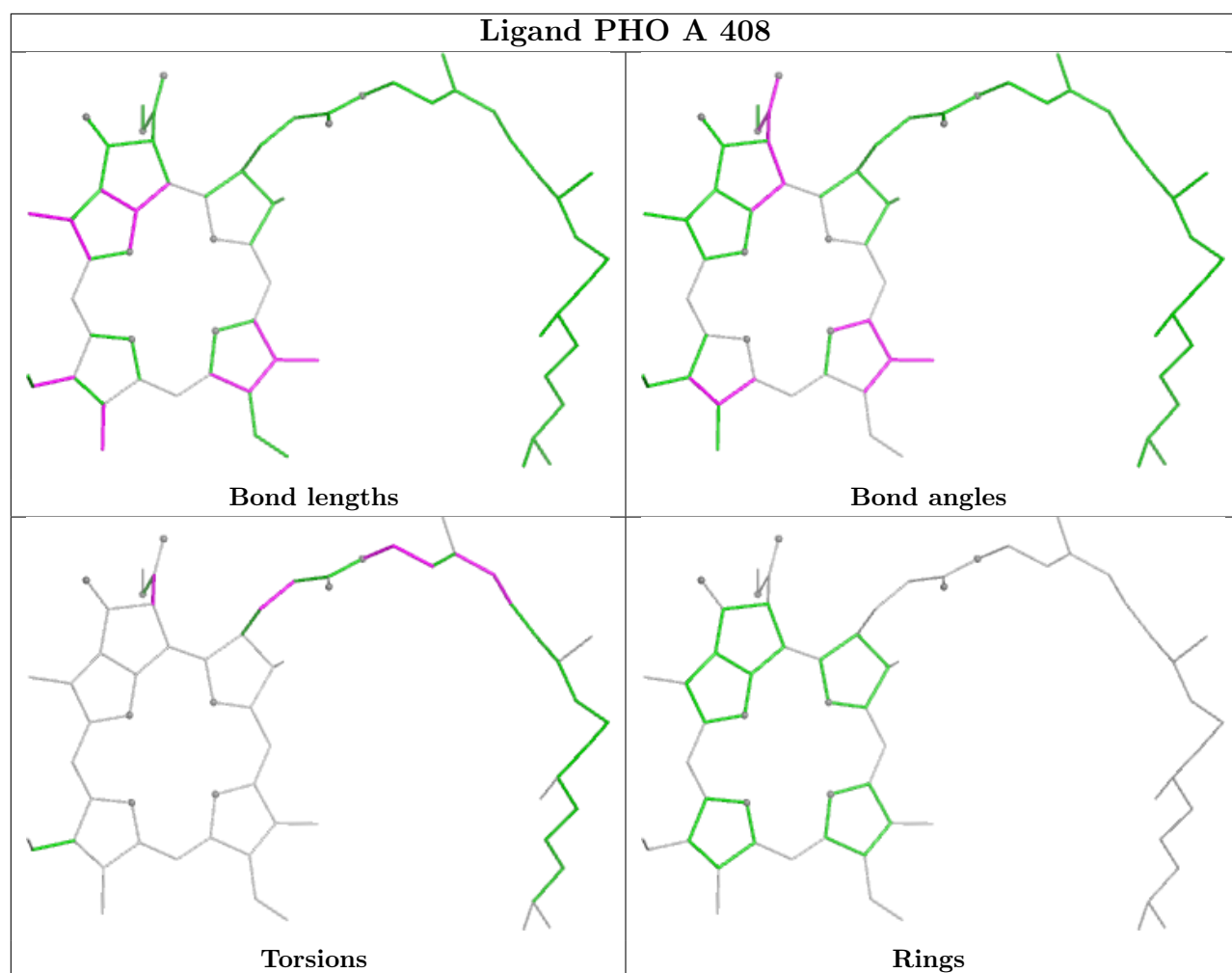


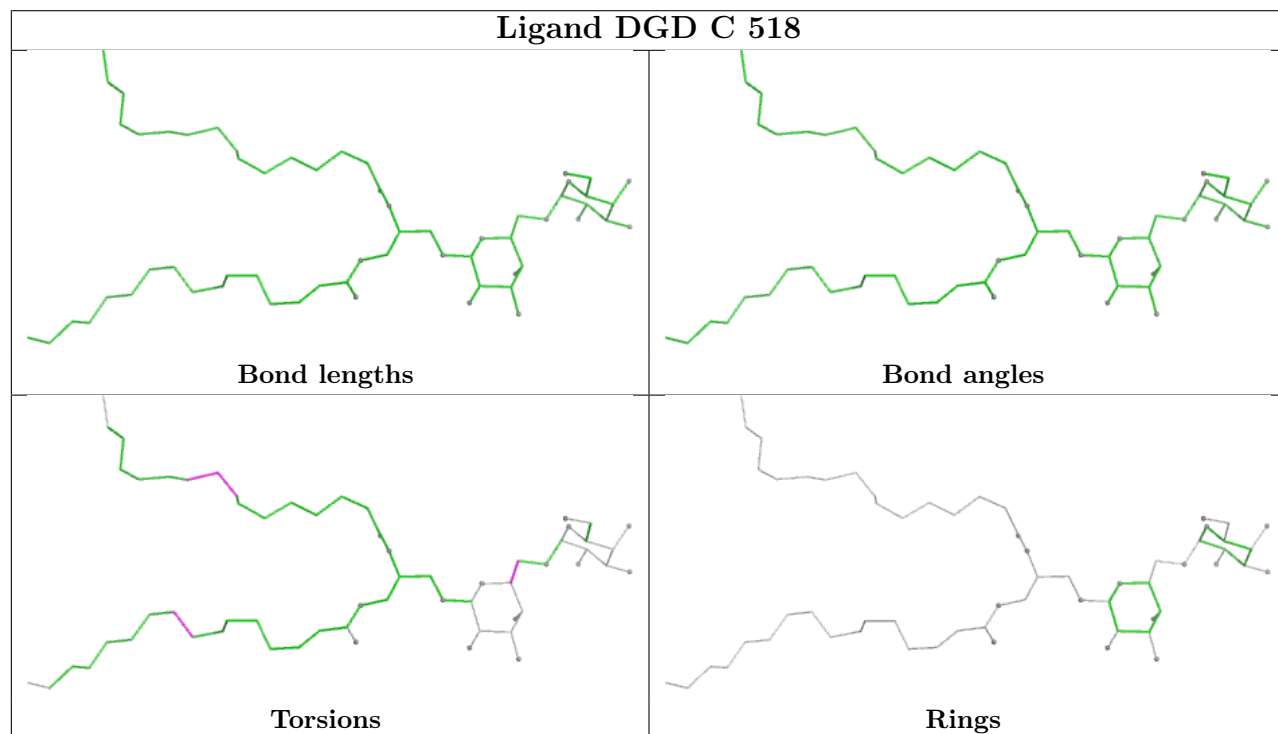
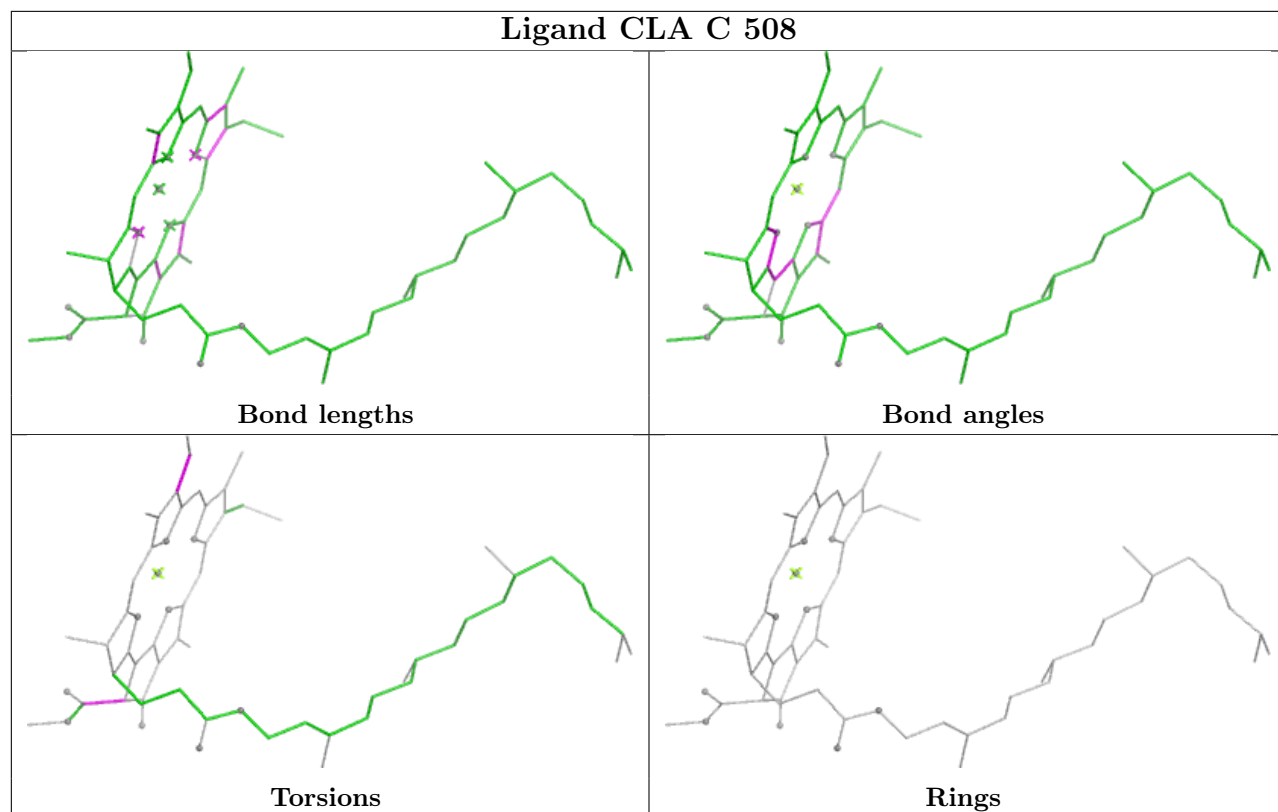


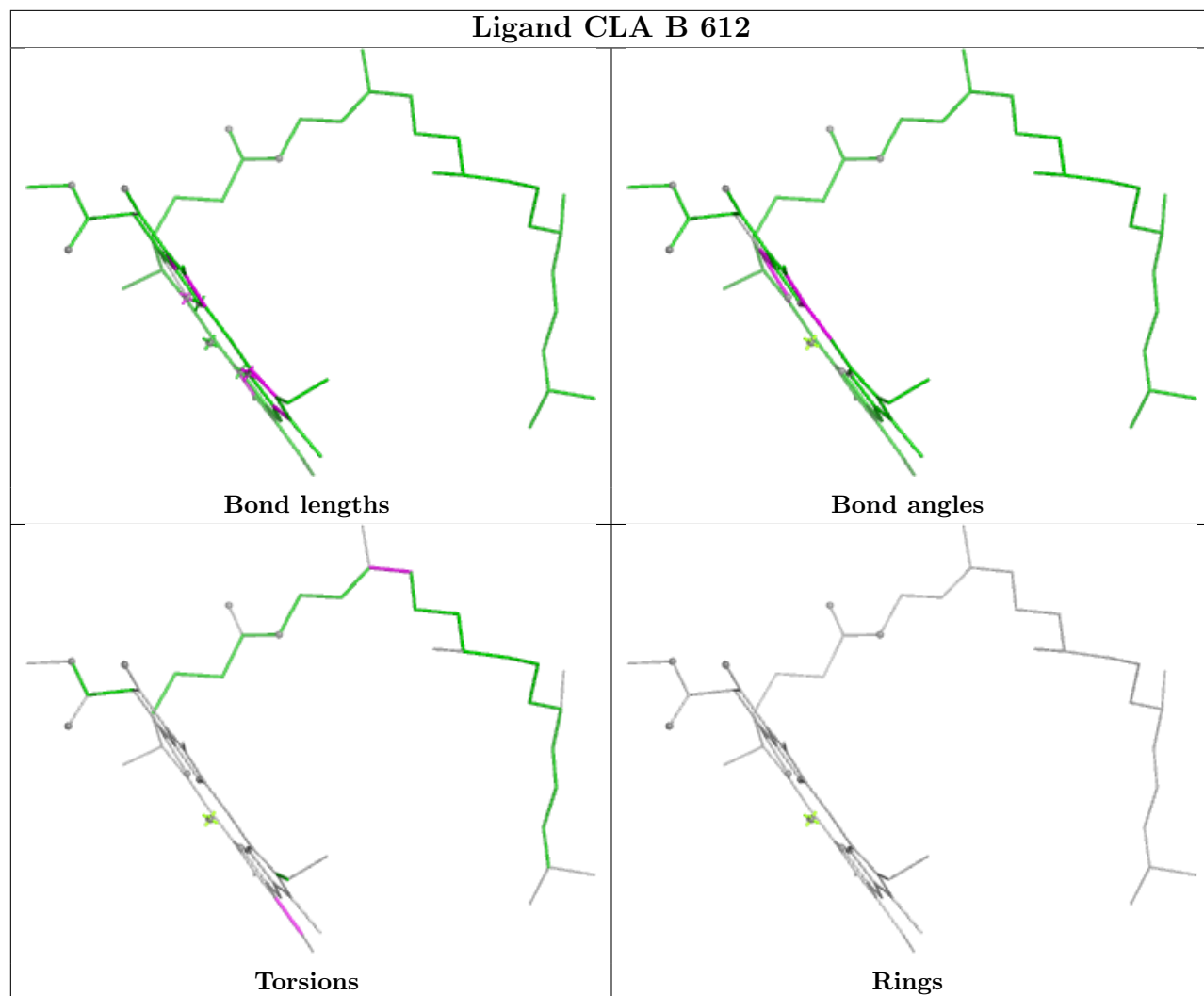


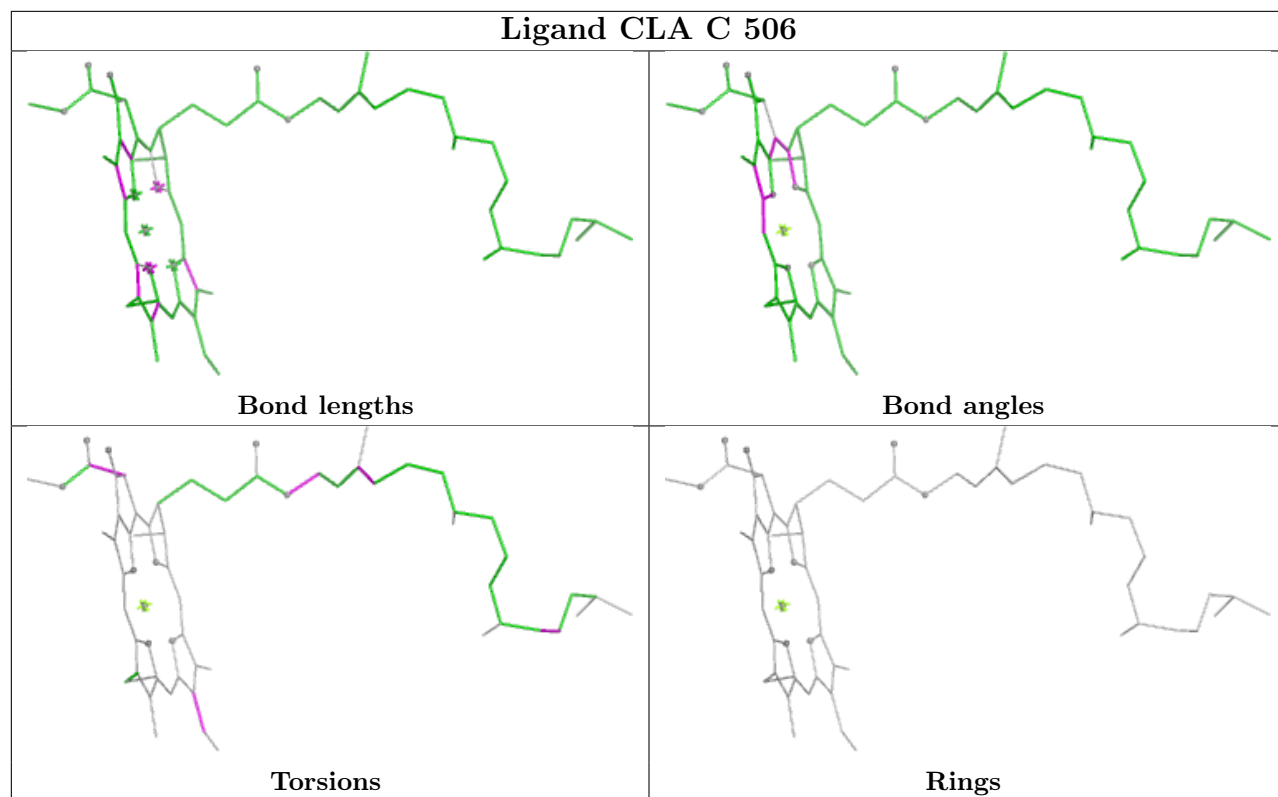


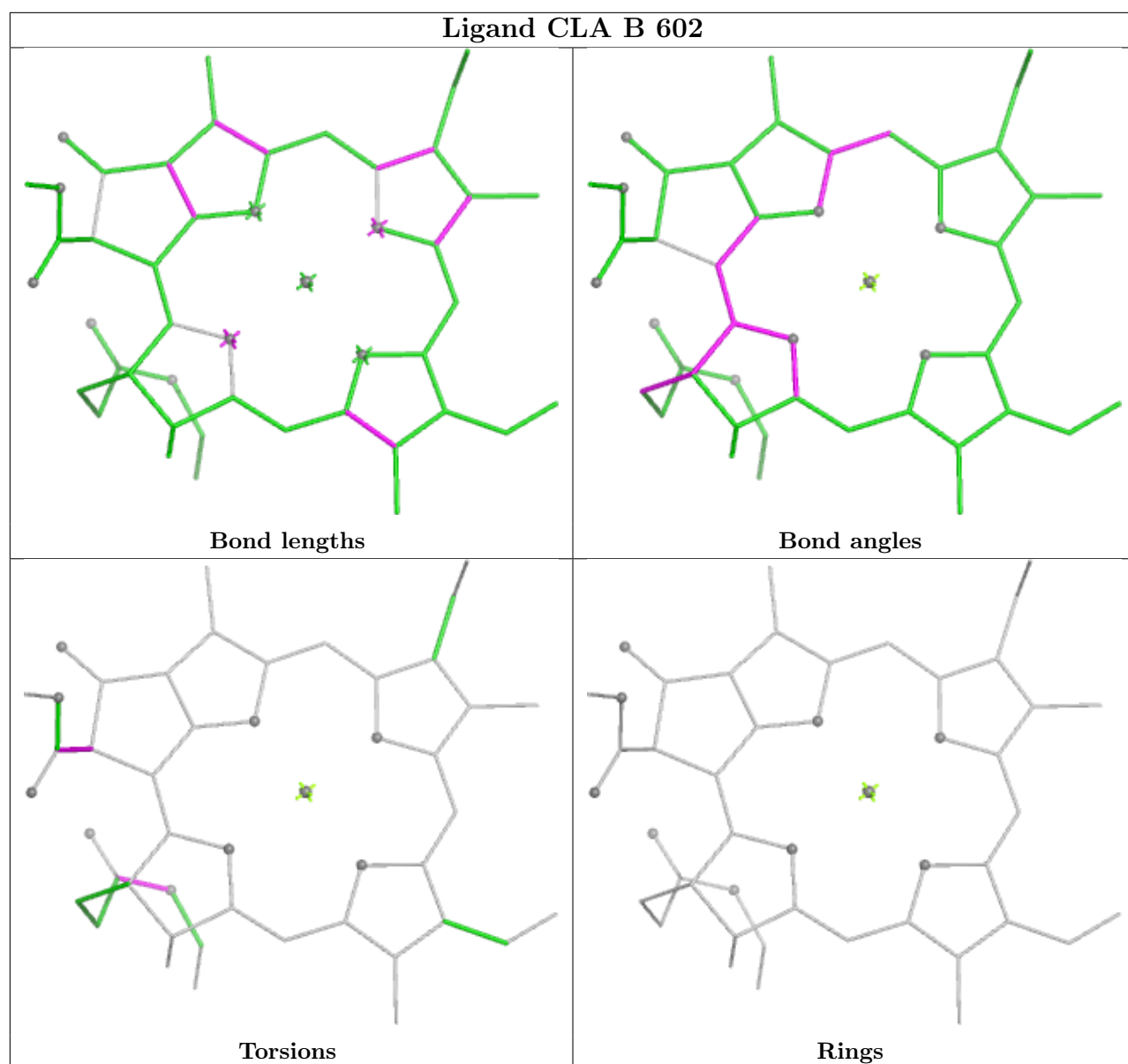




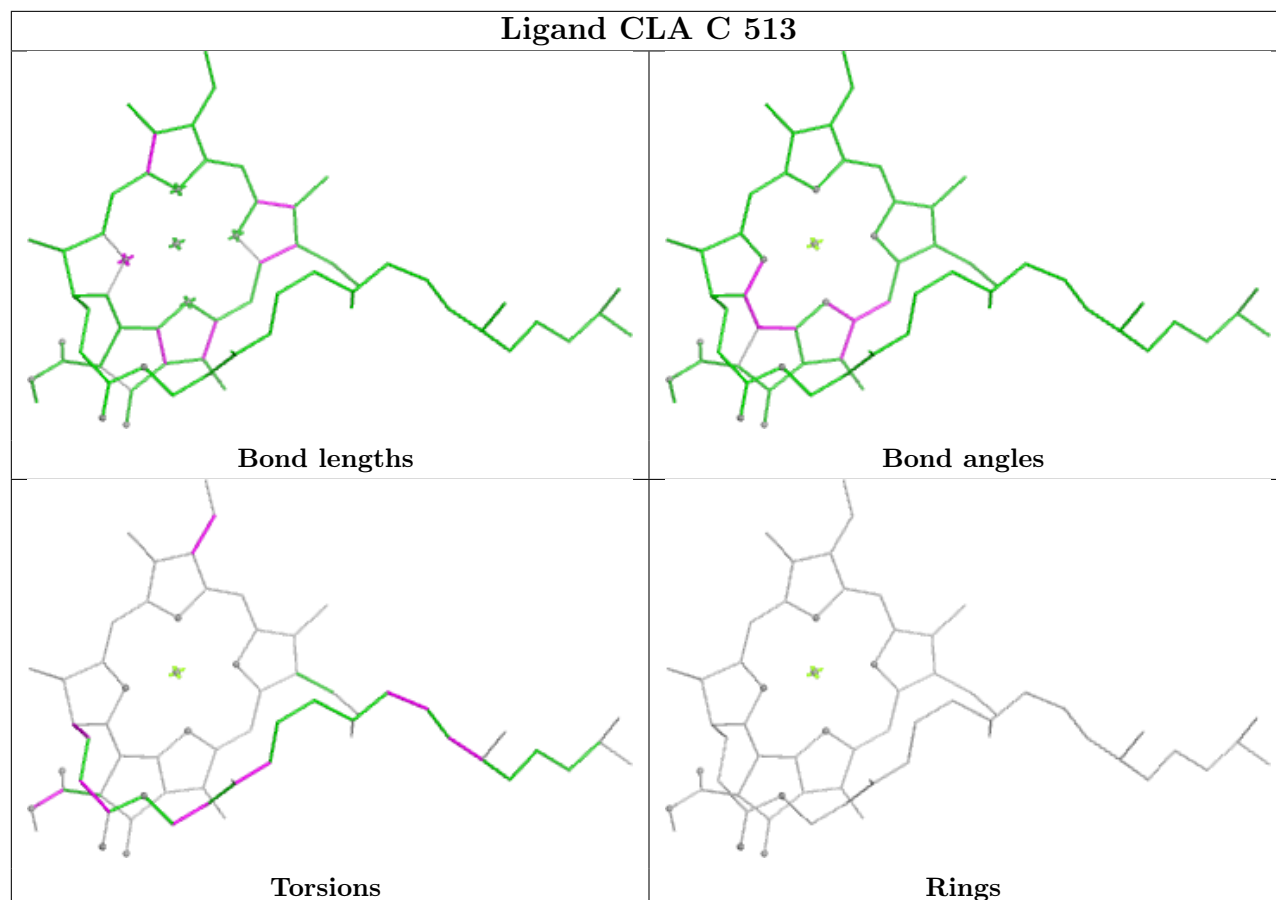




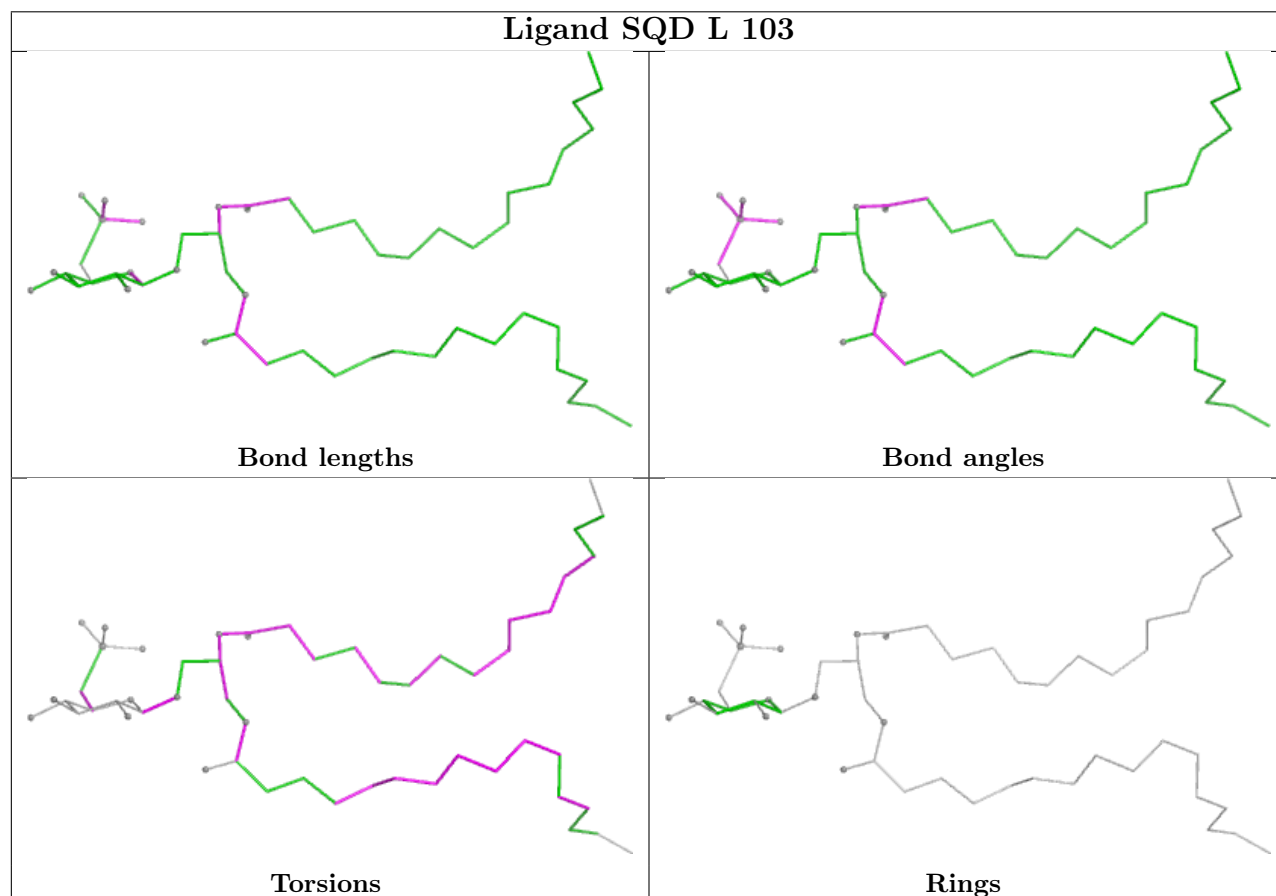


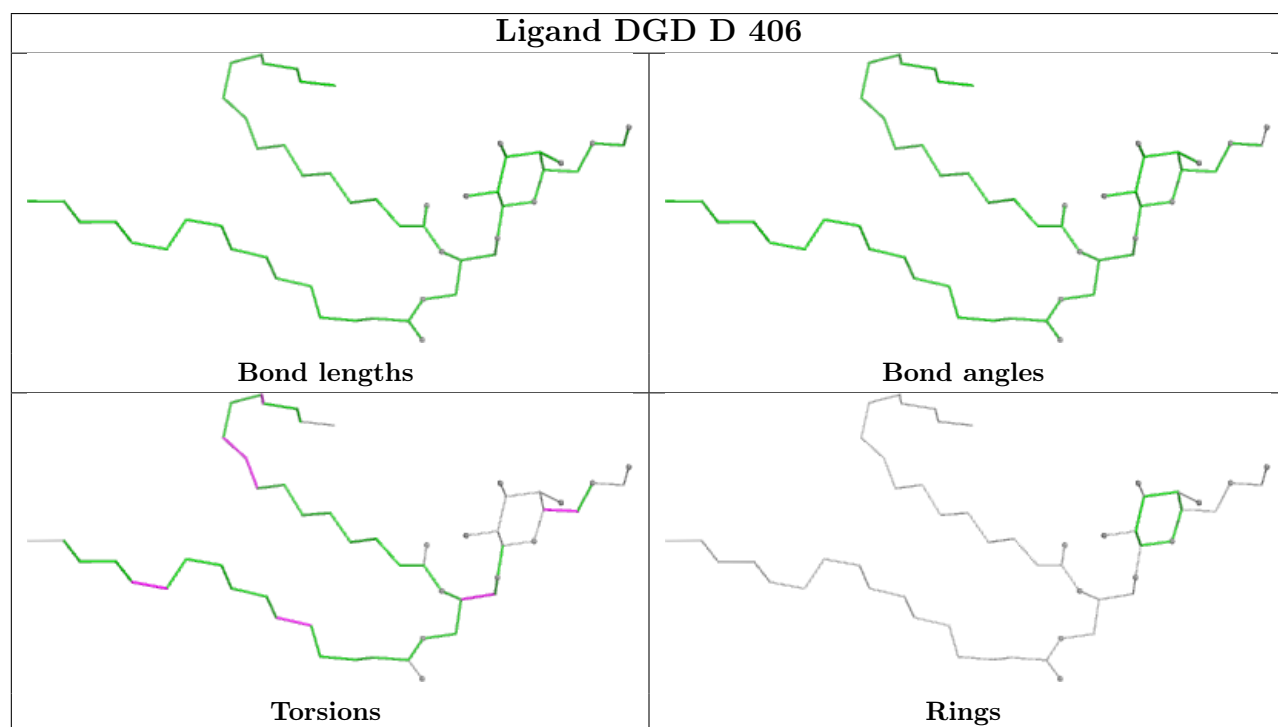
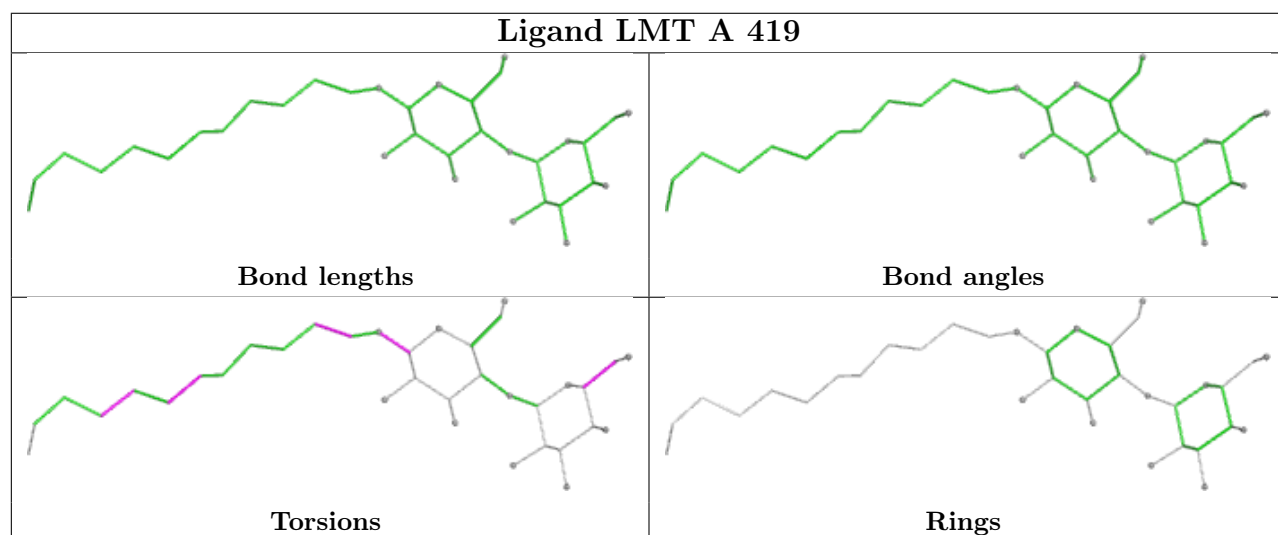
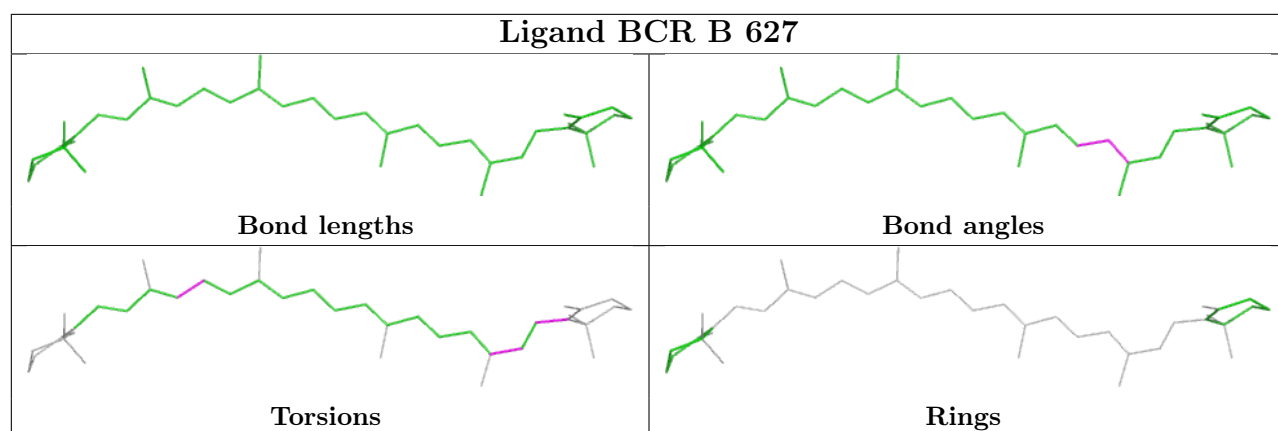


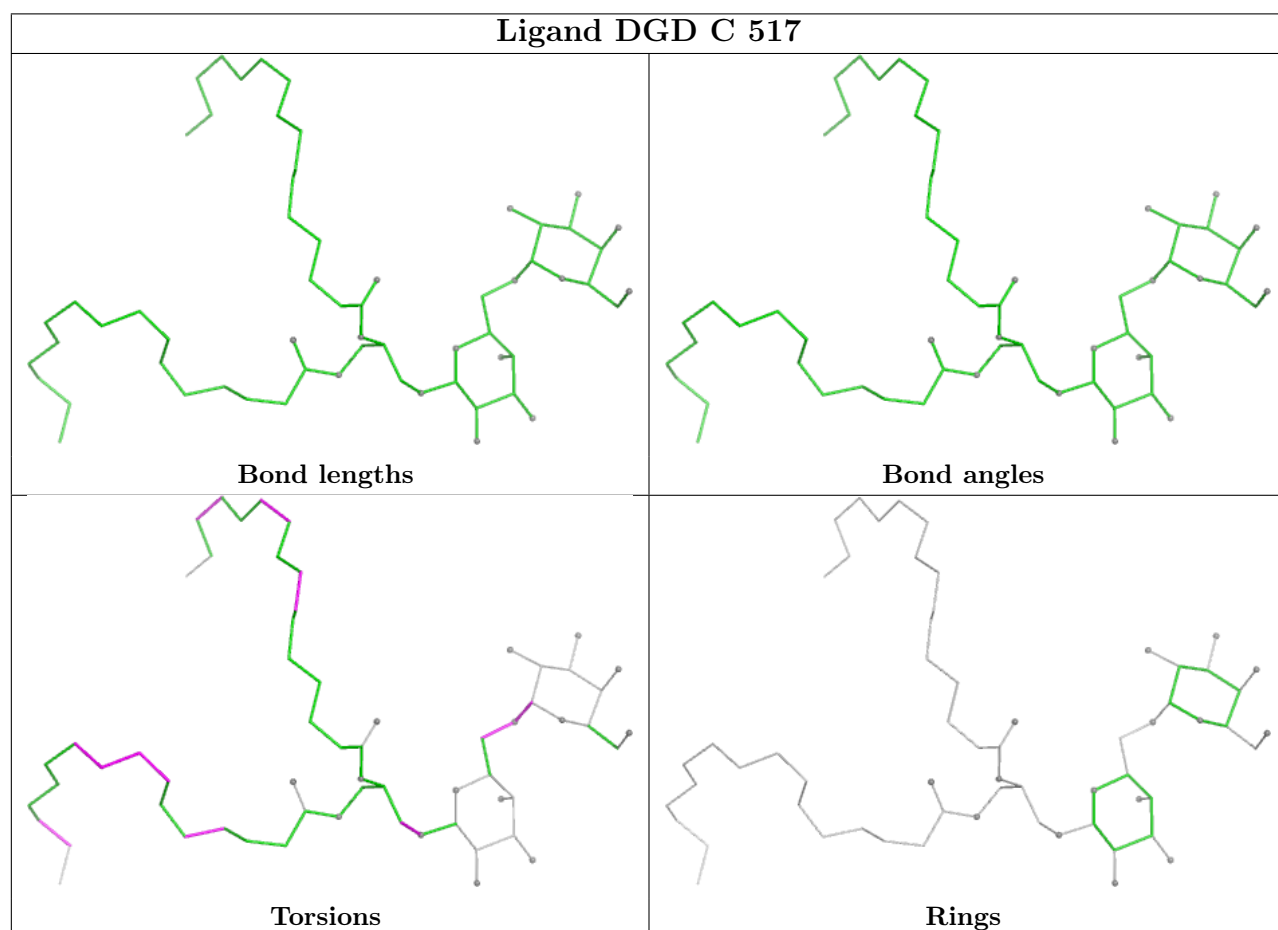
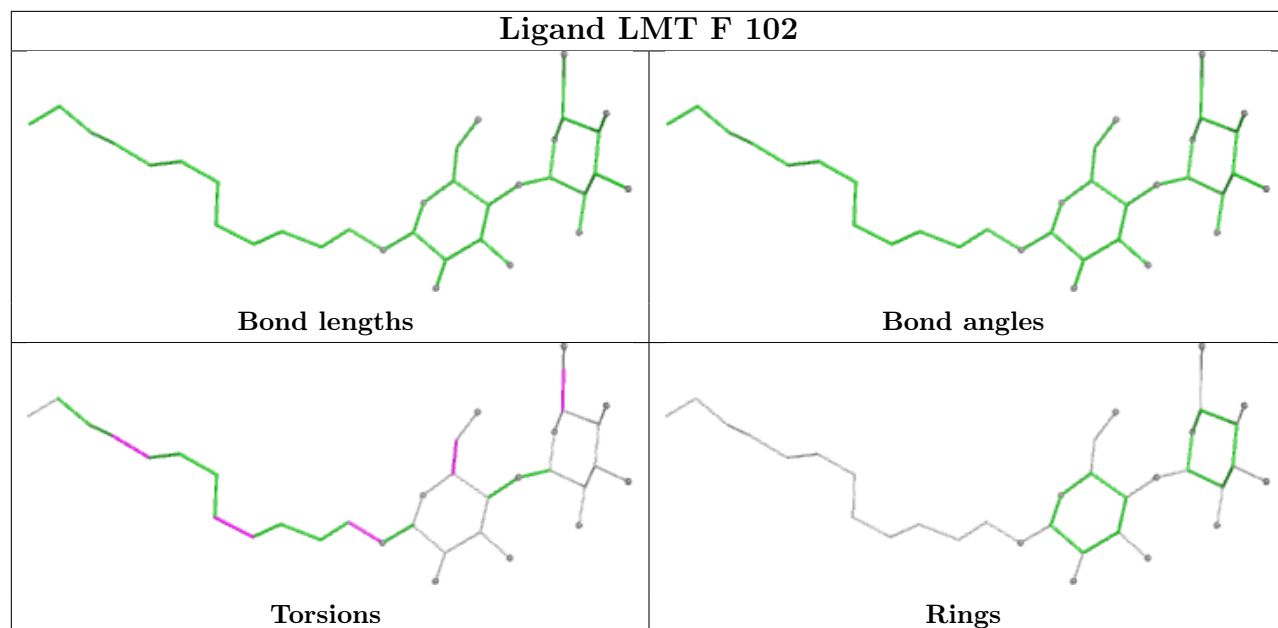
Ligand CLA C 513

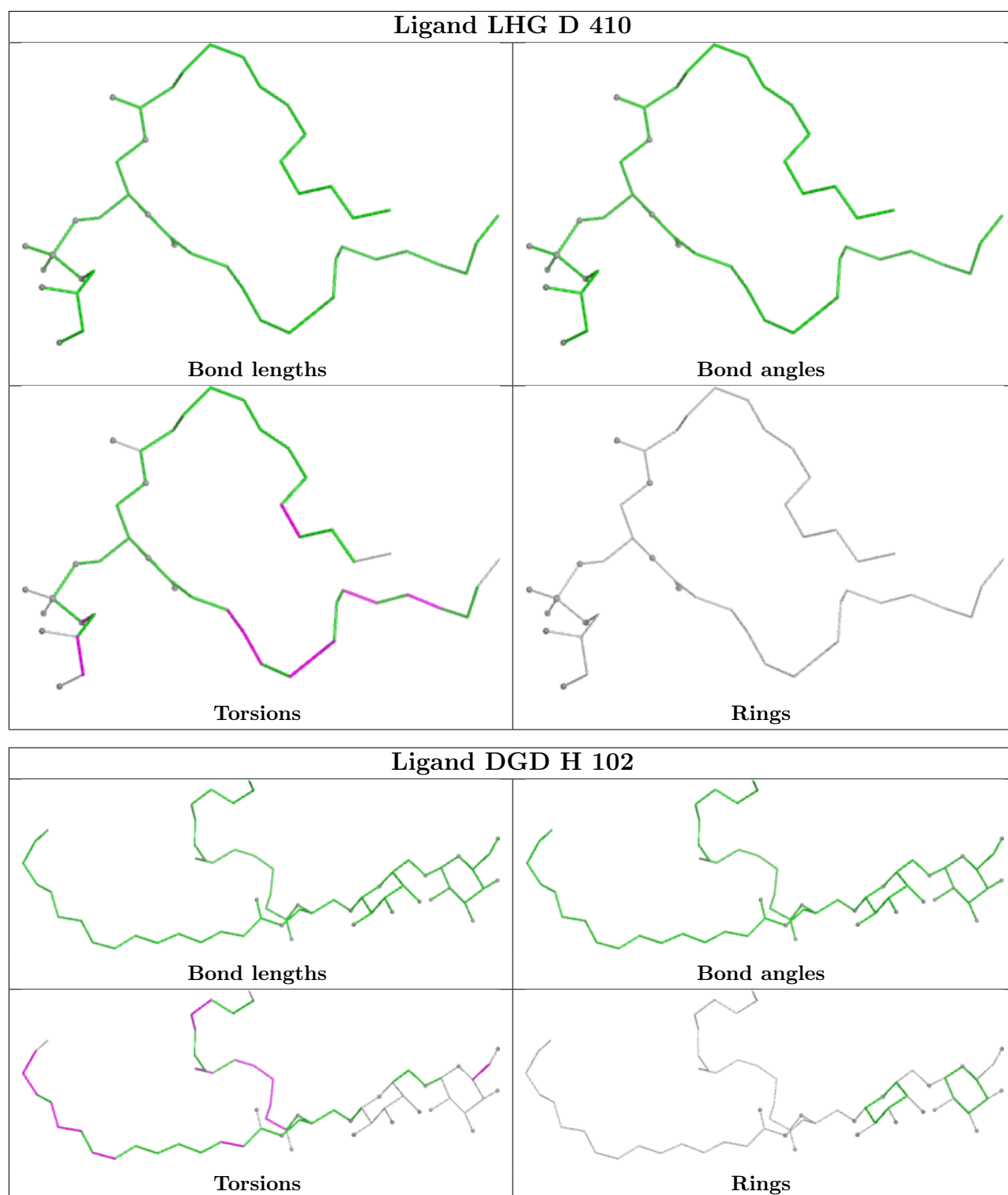


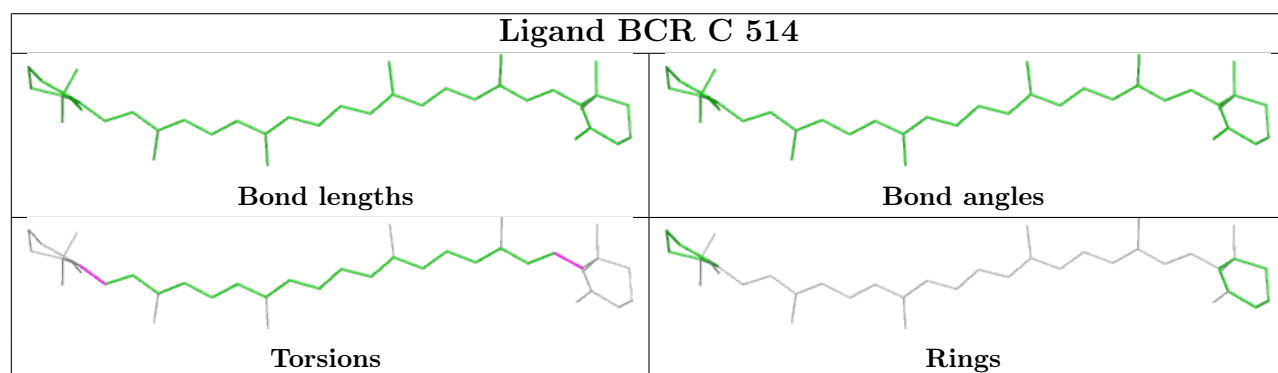
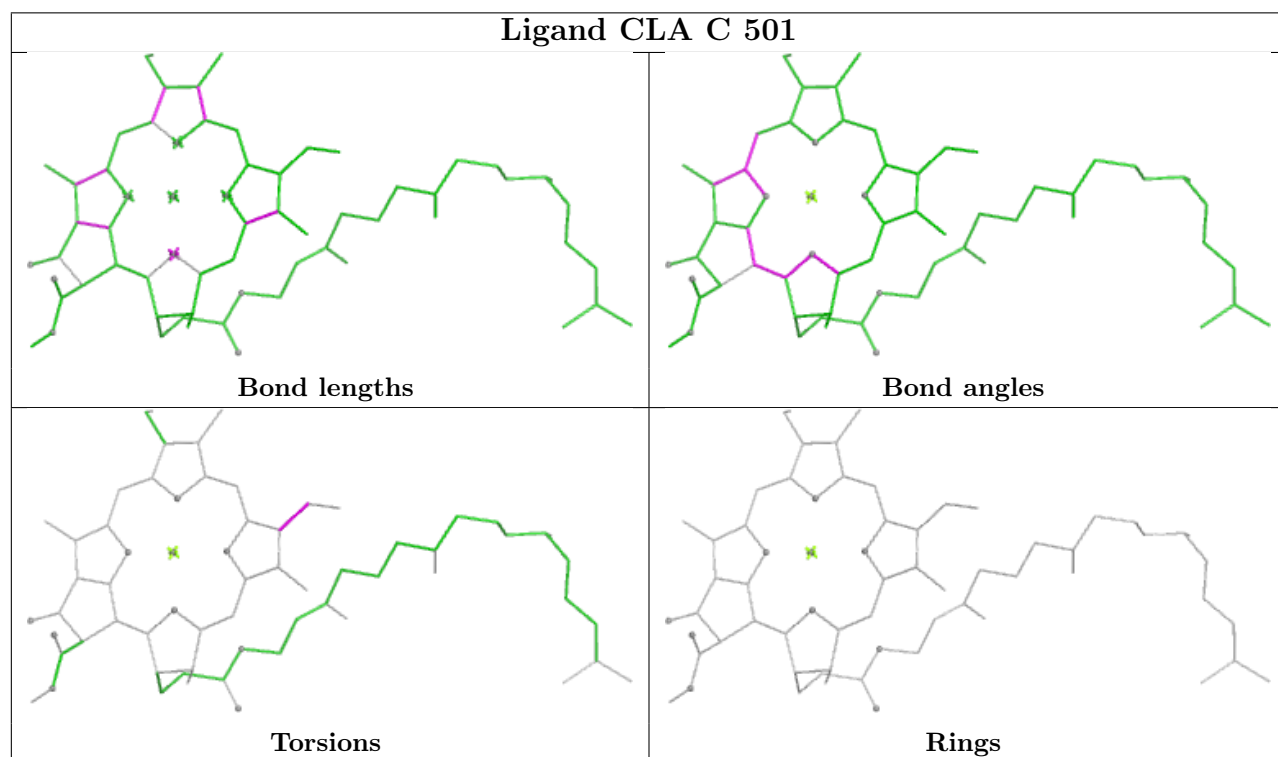
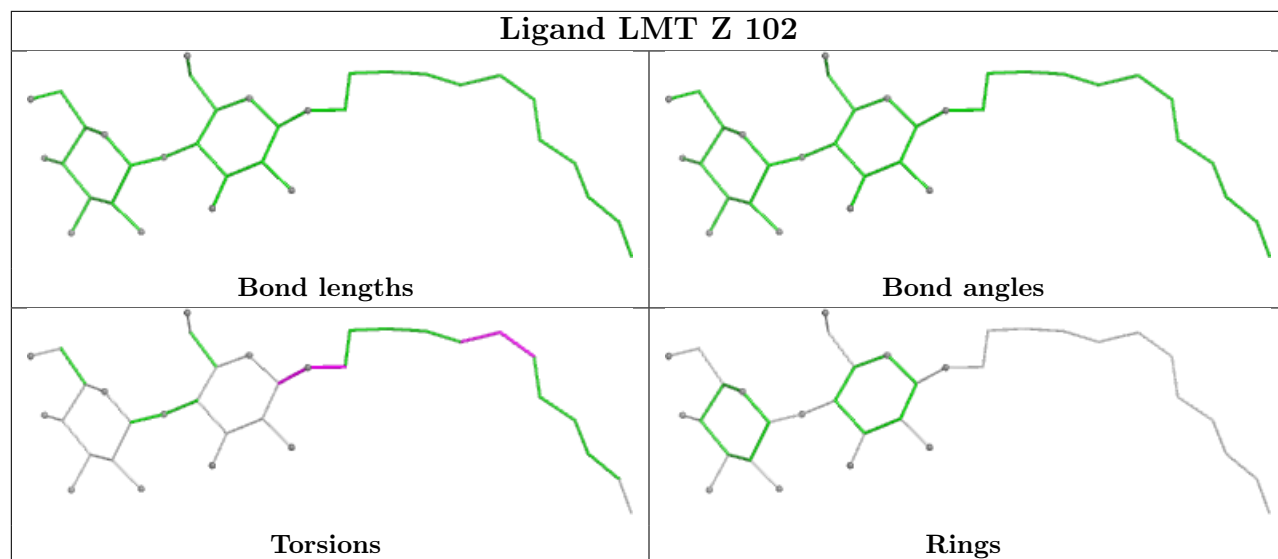
Ligand SQD L 103

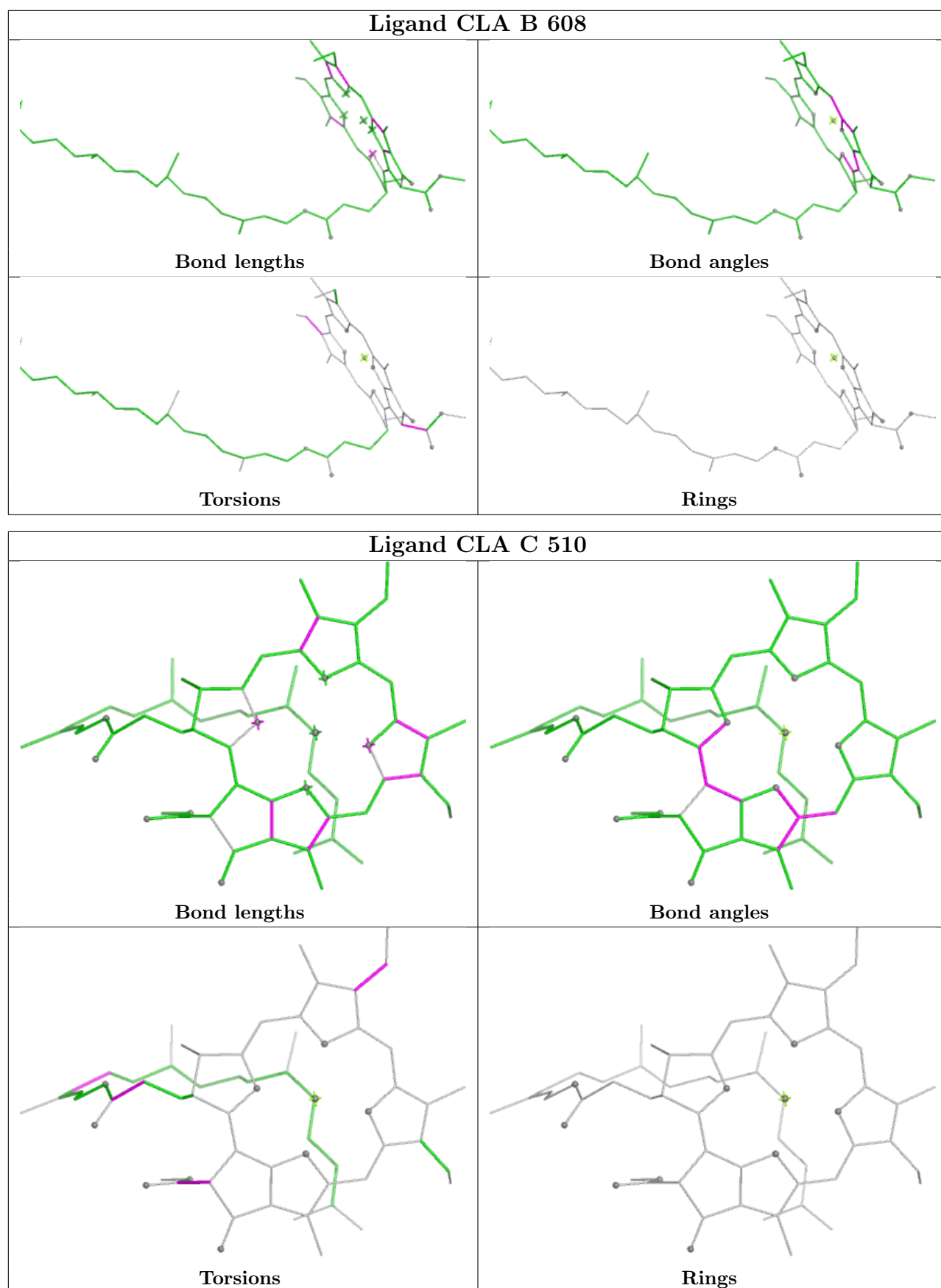


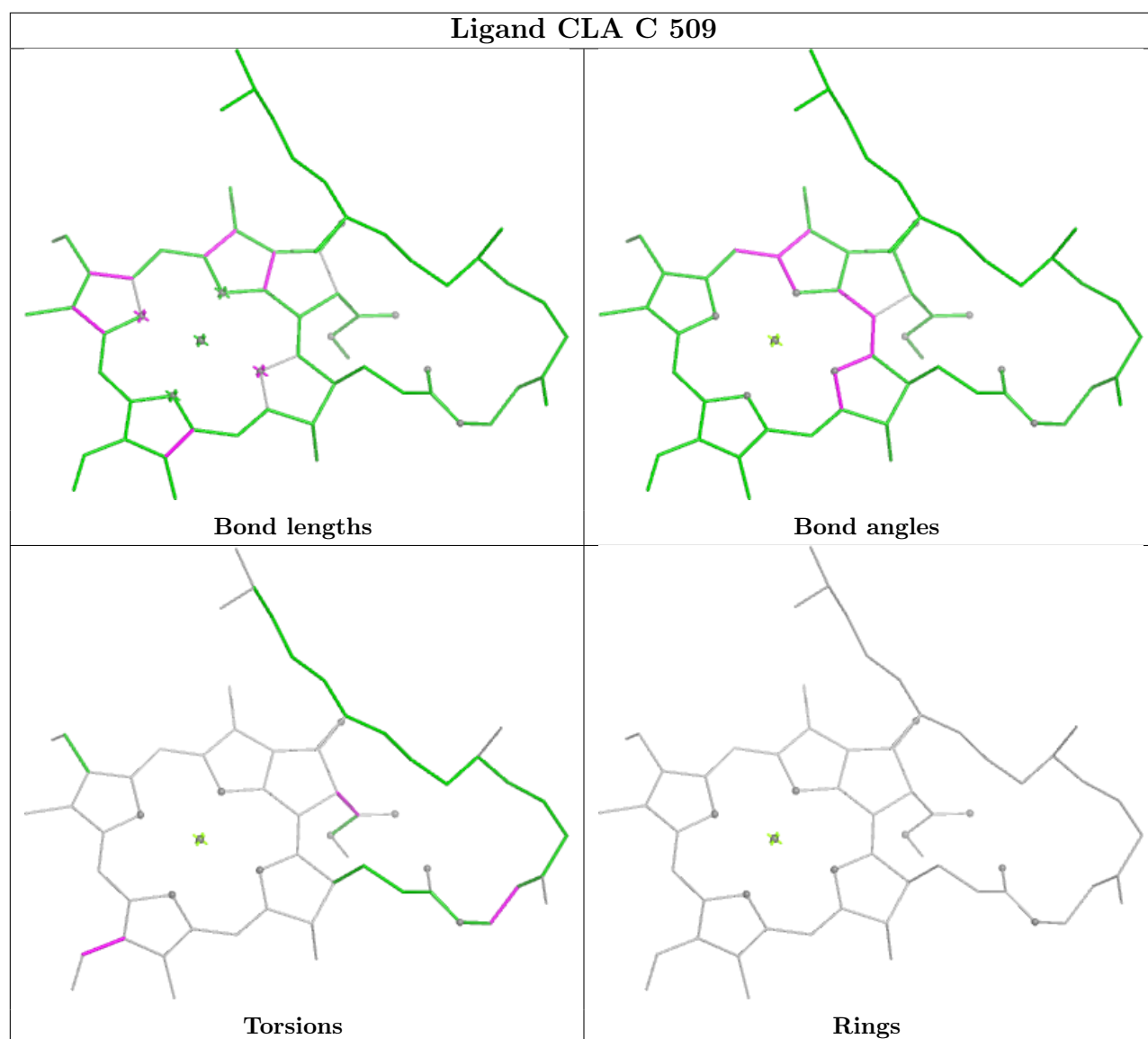












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

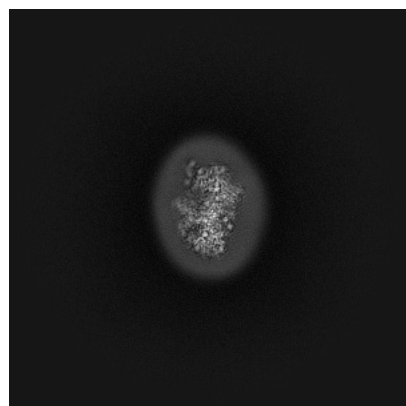
6 Map visualisation [i](#)

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.

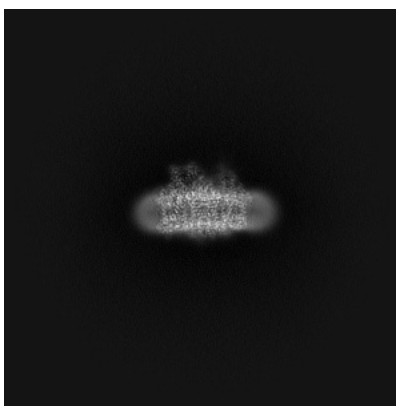
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

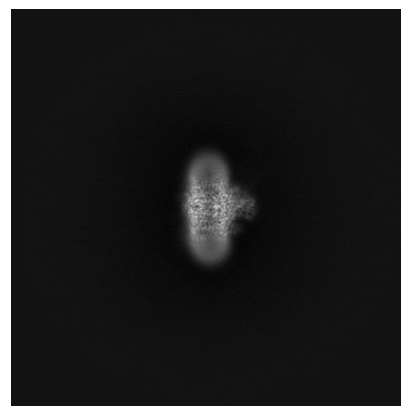
6.1.1 Primary map



X

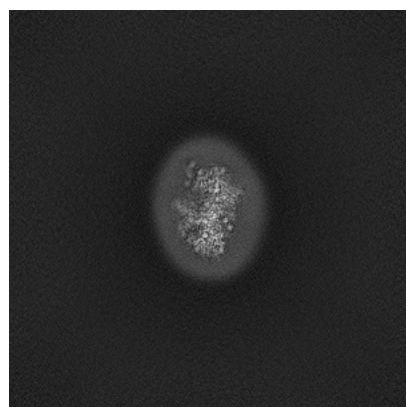


Y

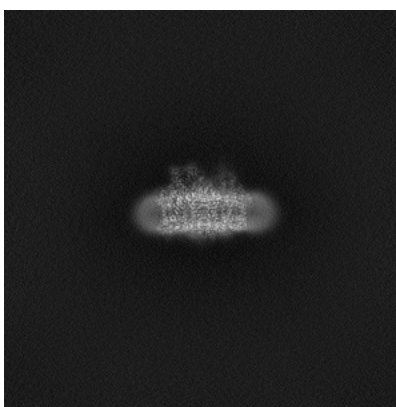


Z

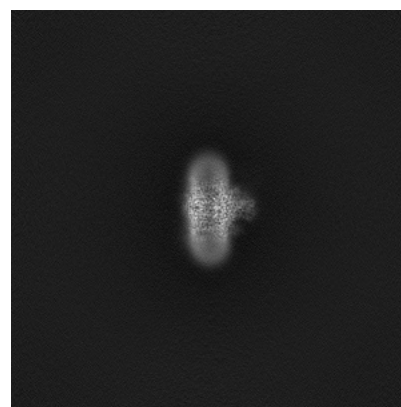
6.1.2 Raw map



X



Y

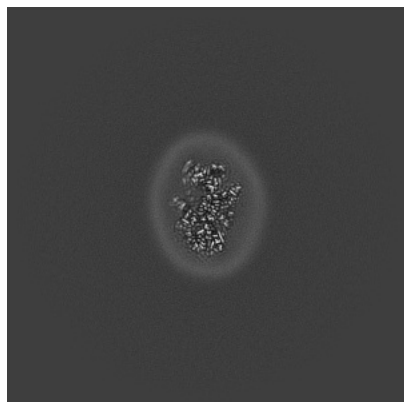


Z

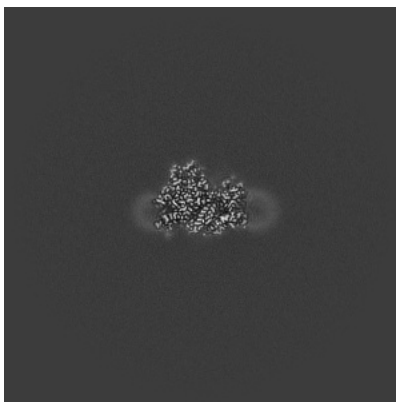
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

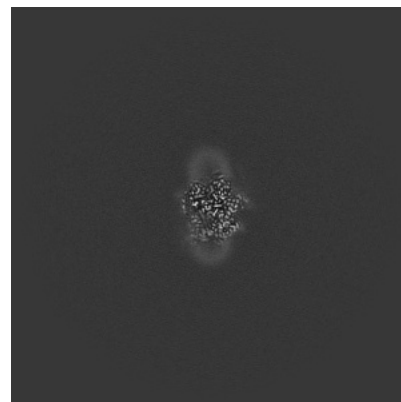
6.2.1 Primary map



X Index: 300

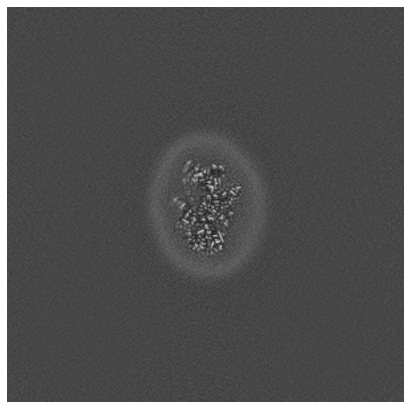


Y Index: 300

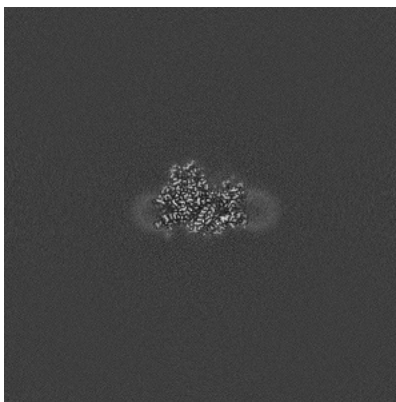


Z Index: 300

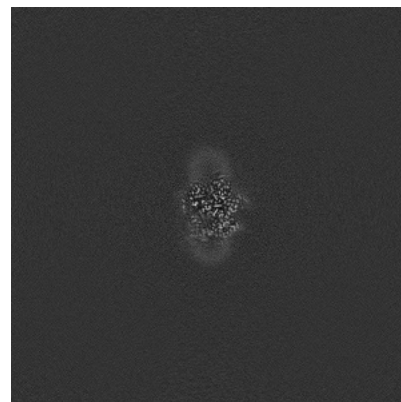
6.2.2 Raw map



X Index: 300



Y Index: 300

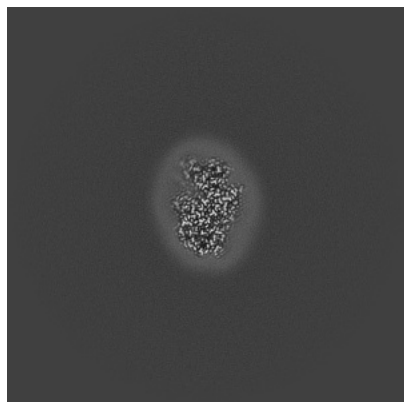


Z Index: 300

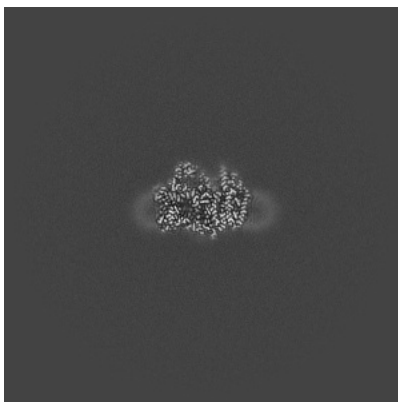
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

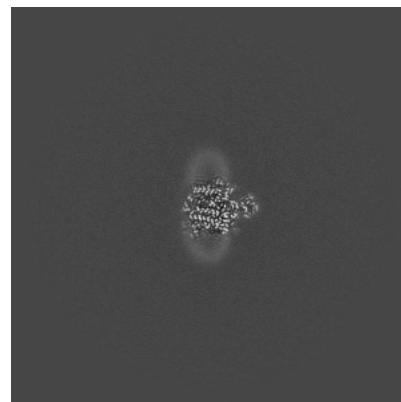
6.3.1 Primary map



X Index: 315

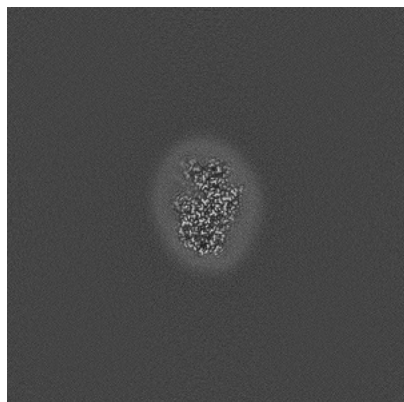


Y Index: 312

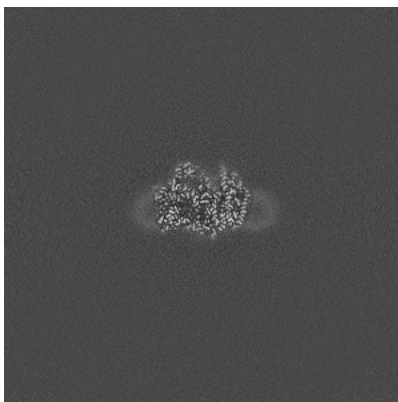


Z Index: 283

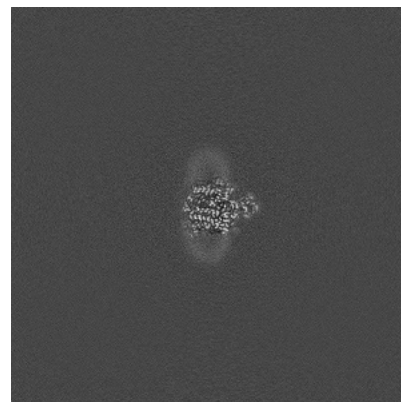
6.3.2 Raw map



X Index: 315



Y Index: 312

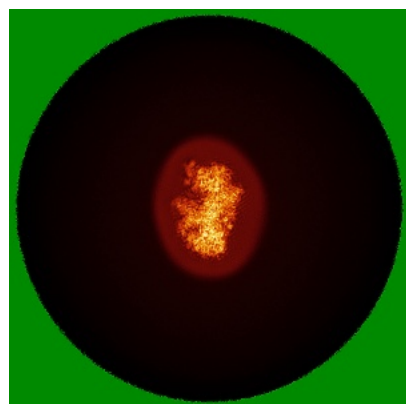


Z Index: 283

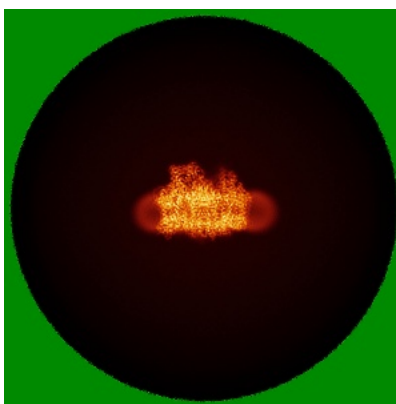
The images above show the largest variance slices of the map in three orthogonal directions.

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

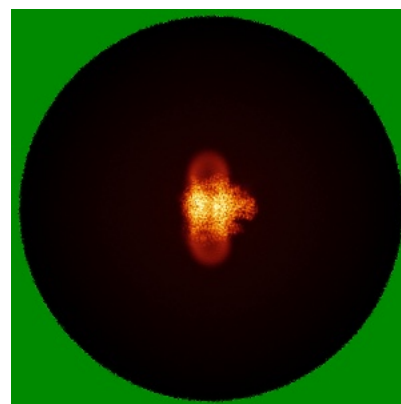
6.4.1 Primary map



X

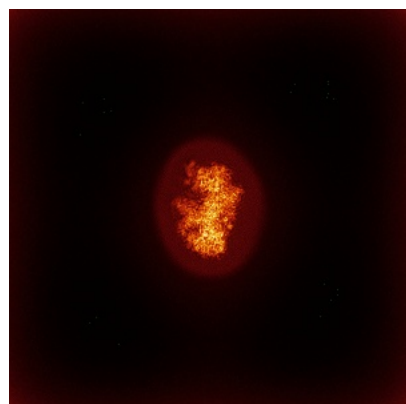


Y

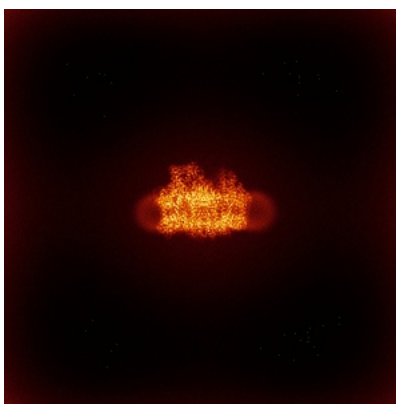


Z

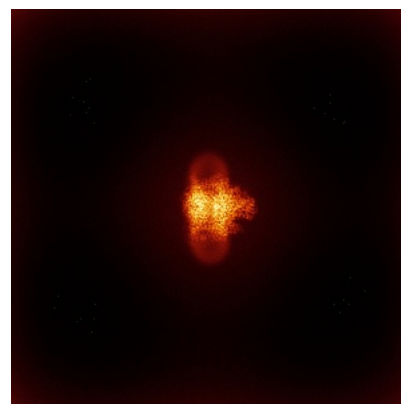
6.4.2 Raw map



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.

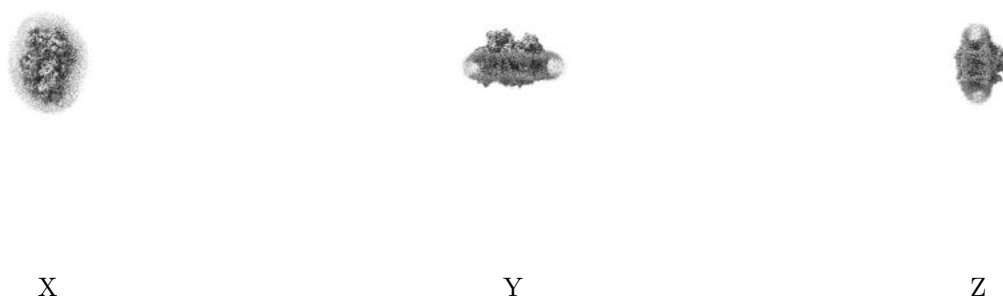
6.5 Orthogonal surface views [i](#)

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.

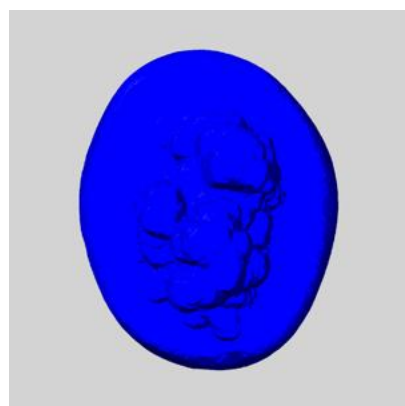
6.6 Mask visualisation [i](#)

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

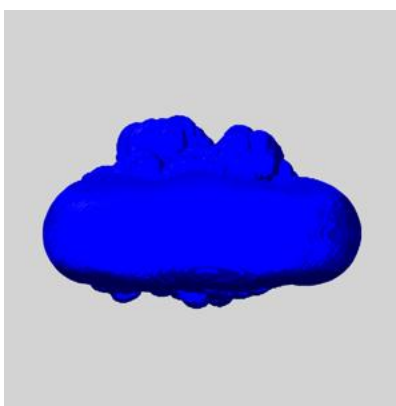
A mask typically either:

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

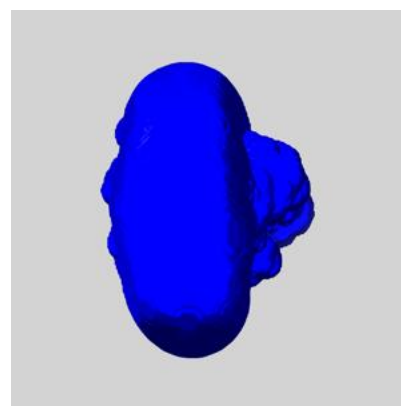
6.6.1 emd_55594_msk_1.map [i](#)



X



Y

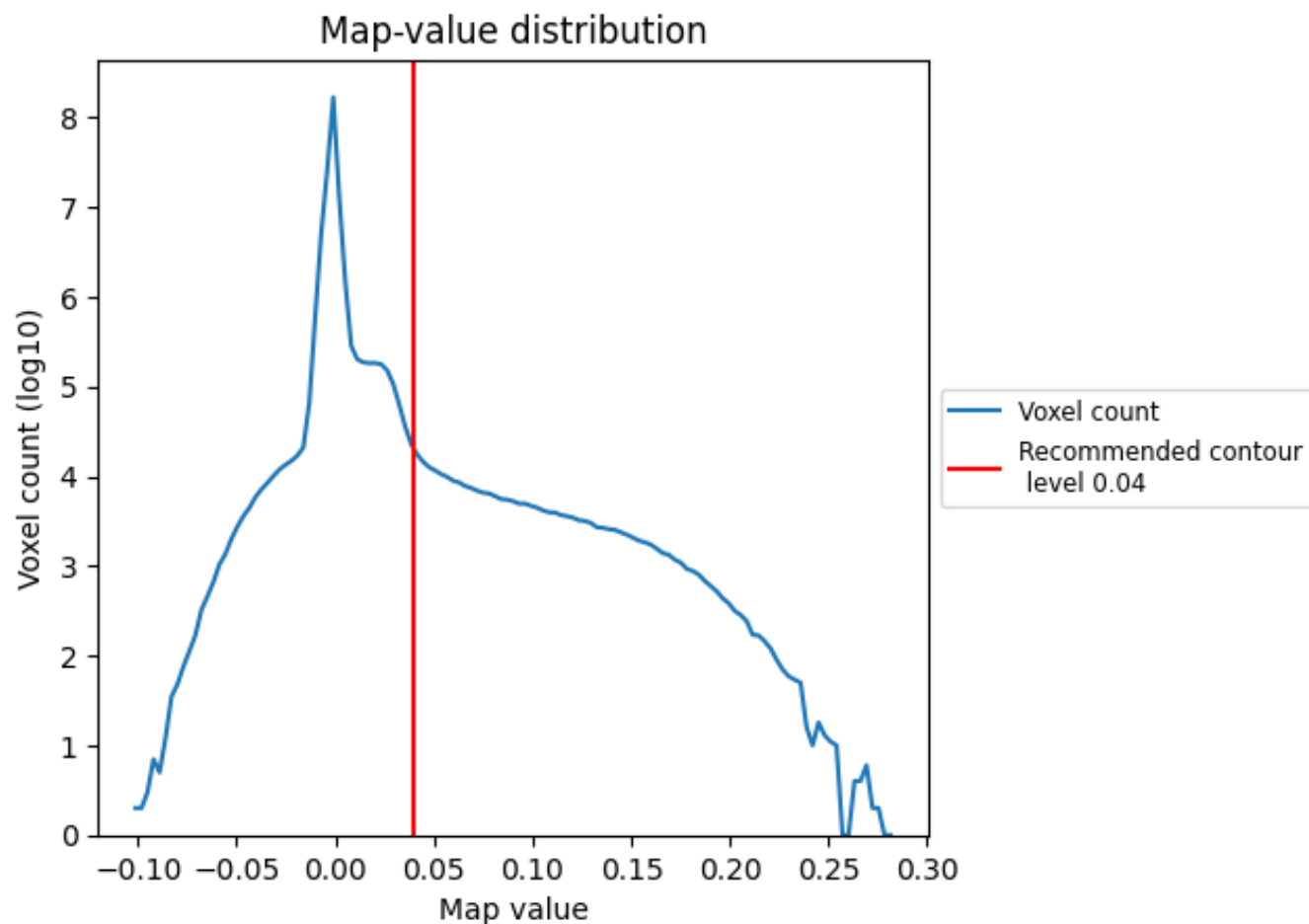


Z

7 Map analysis [i](#)

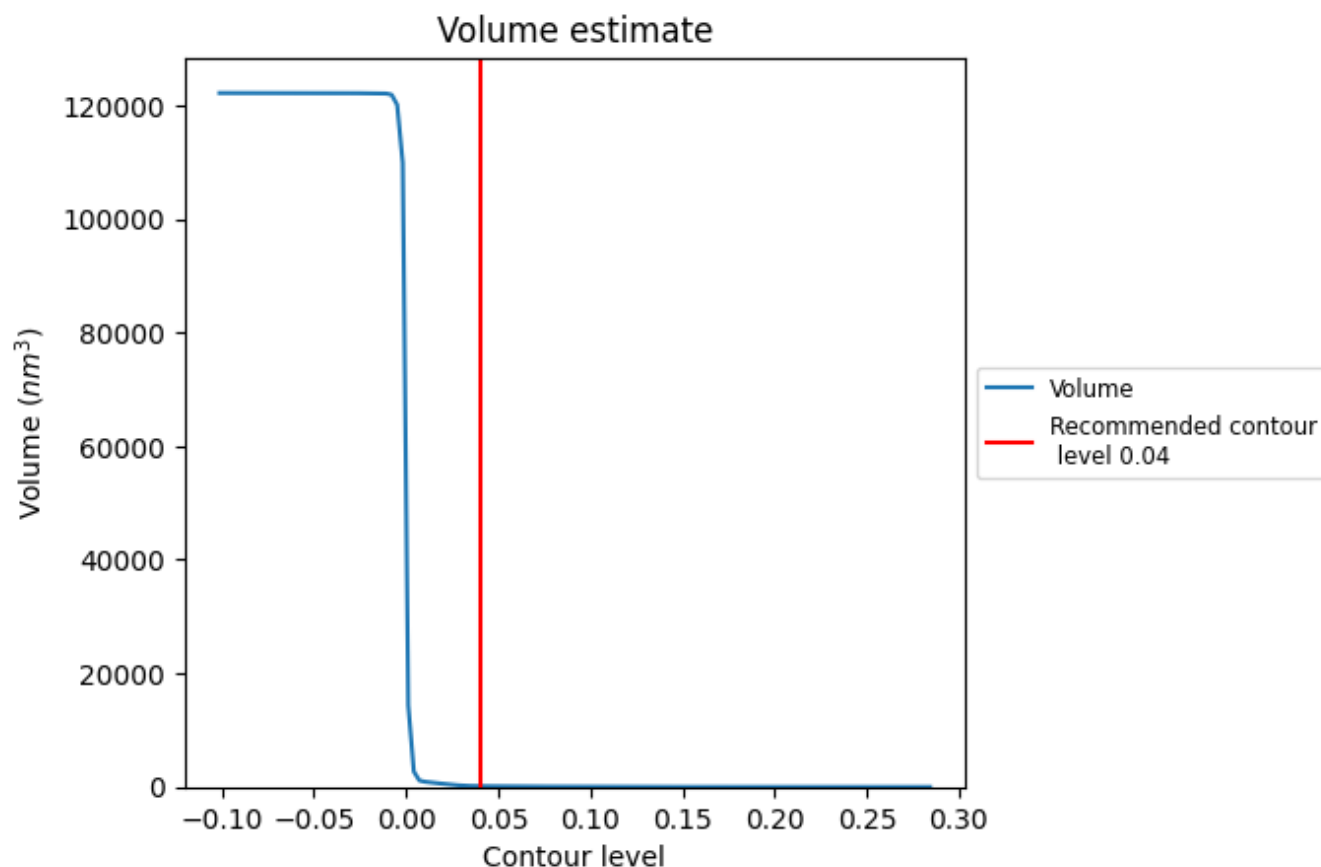
This section contains the results of statistical analysis of the map.

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.

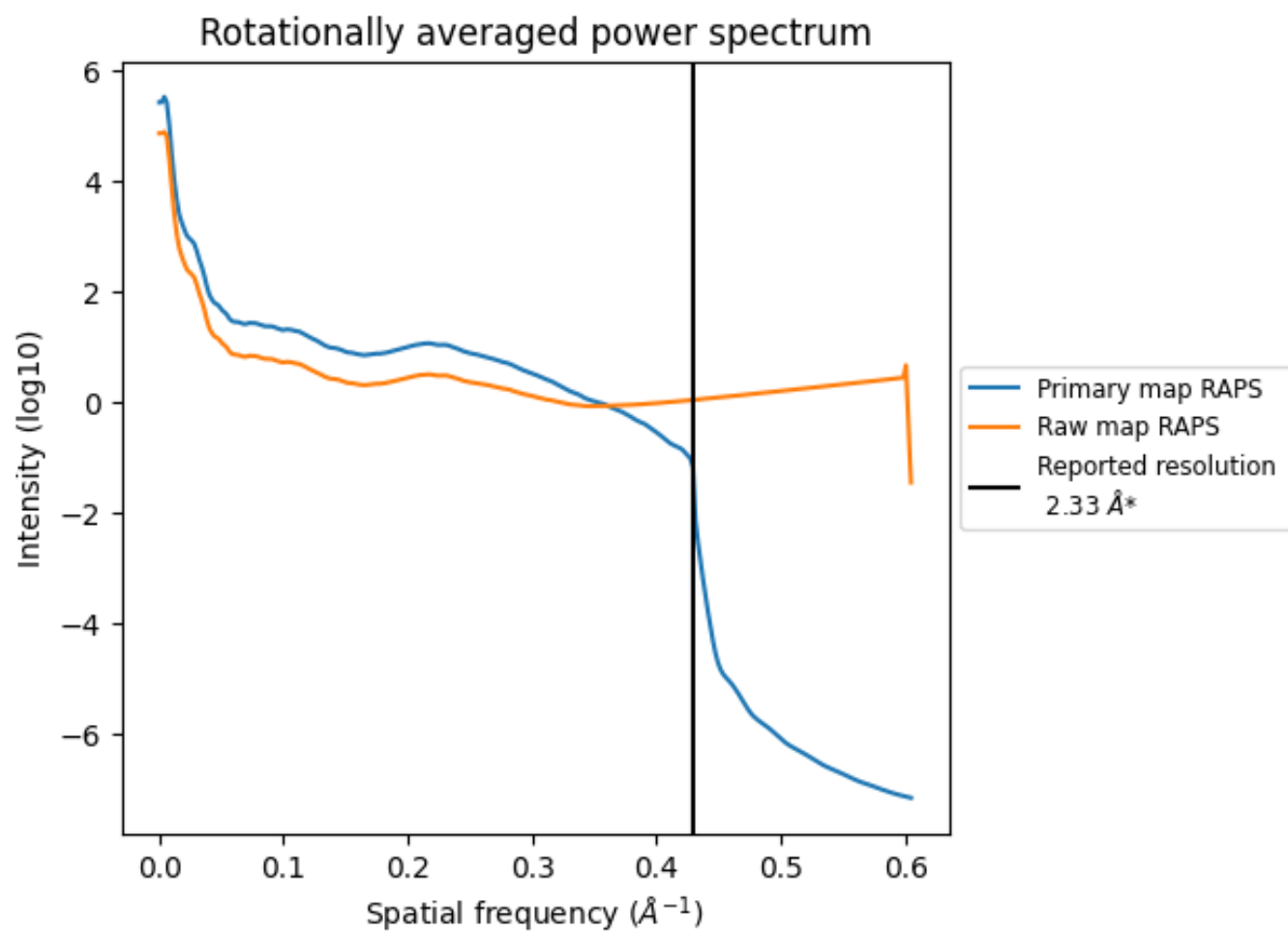
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm^3 ; 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 ⓘ

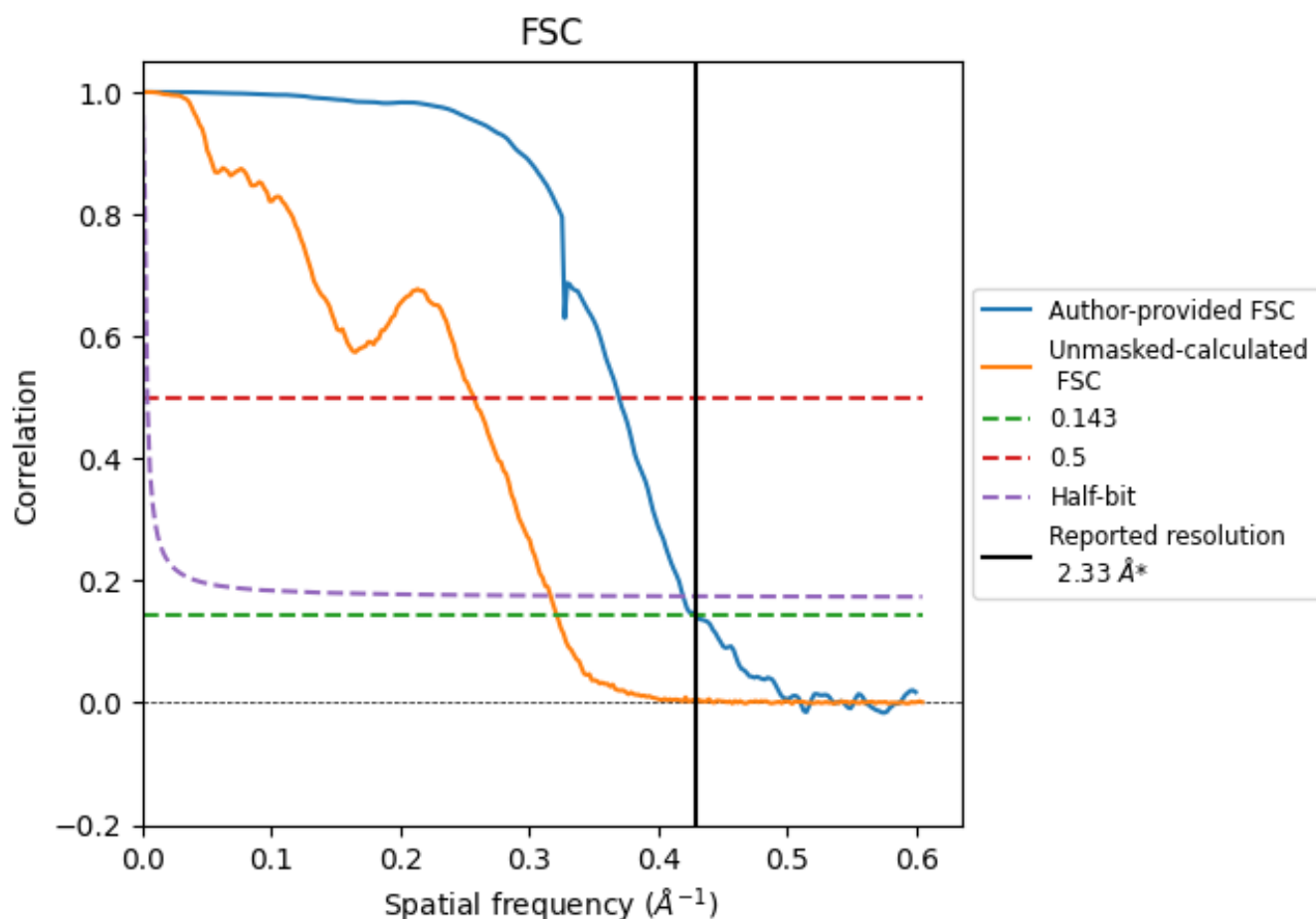


*Reported resolution corresponds to spatial frequency of 0.429 $\text{\AA}^{-1}$

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

8.2 Resolution estimates [i](#)

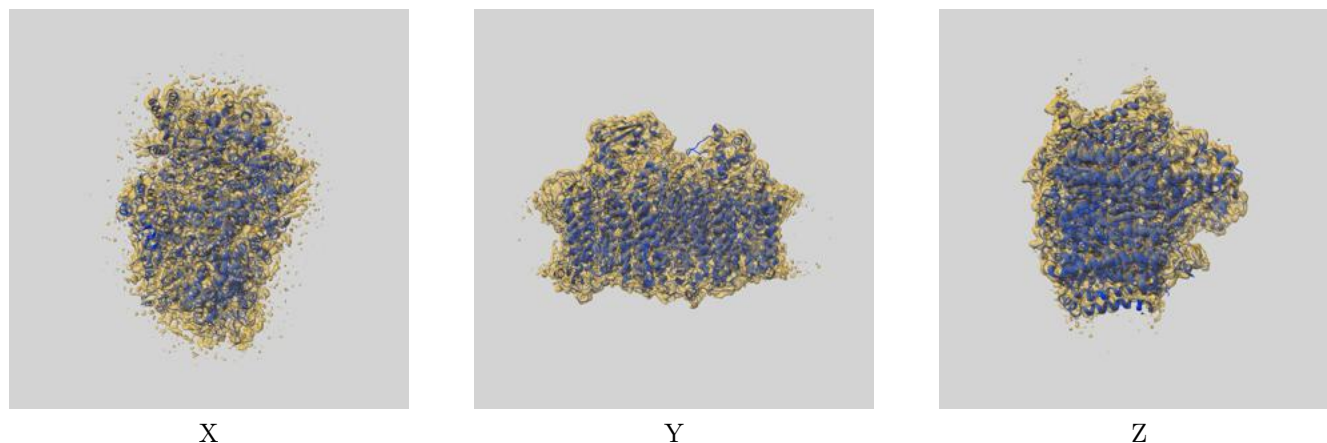
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.33	2.71	2.38
Unmasked-calculated*	3.11	3.89	3.16

*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](#)

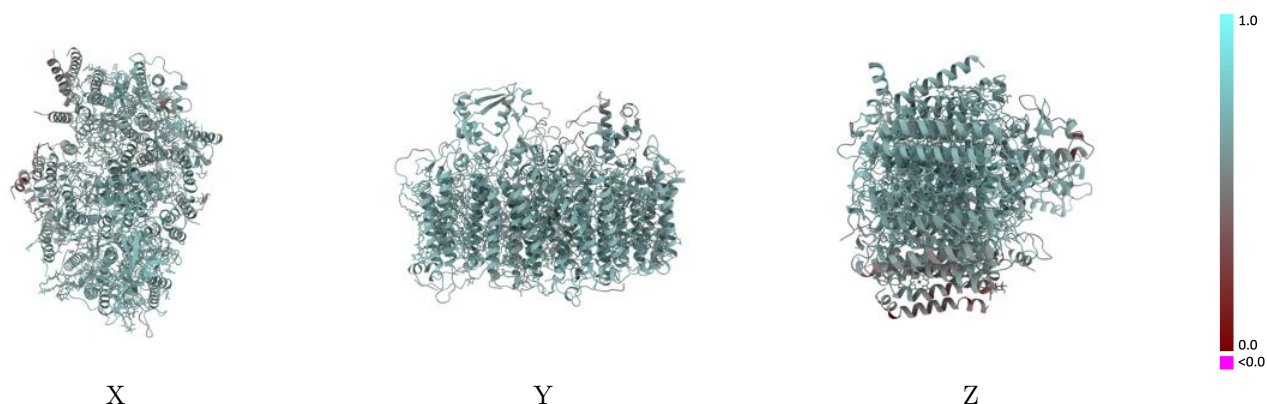
This section contains information regarding the fit between EMDB map EMD-55594 and PDB model 9T5U. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

9.1 Map-model overlay [i](#)



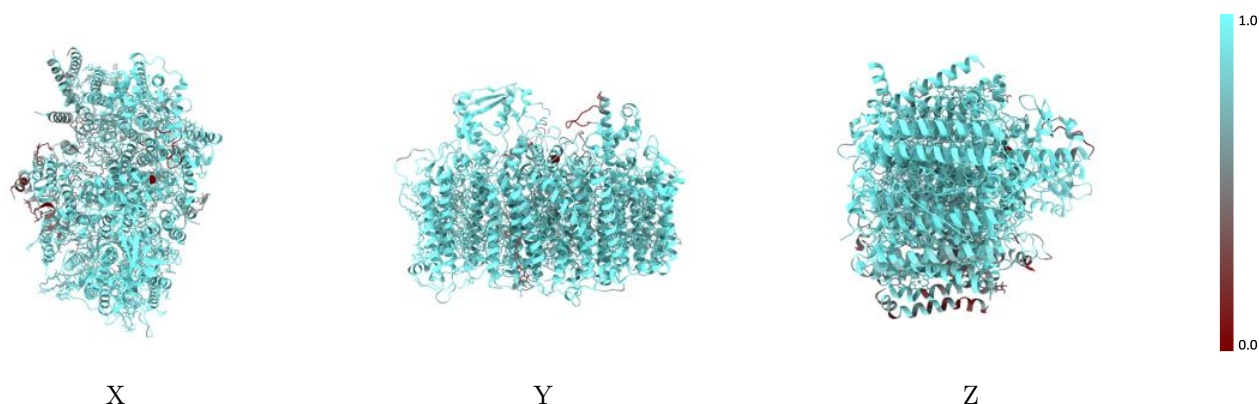
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



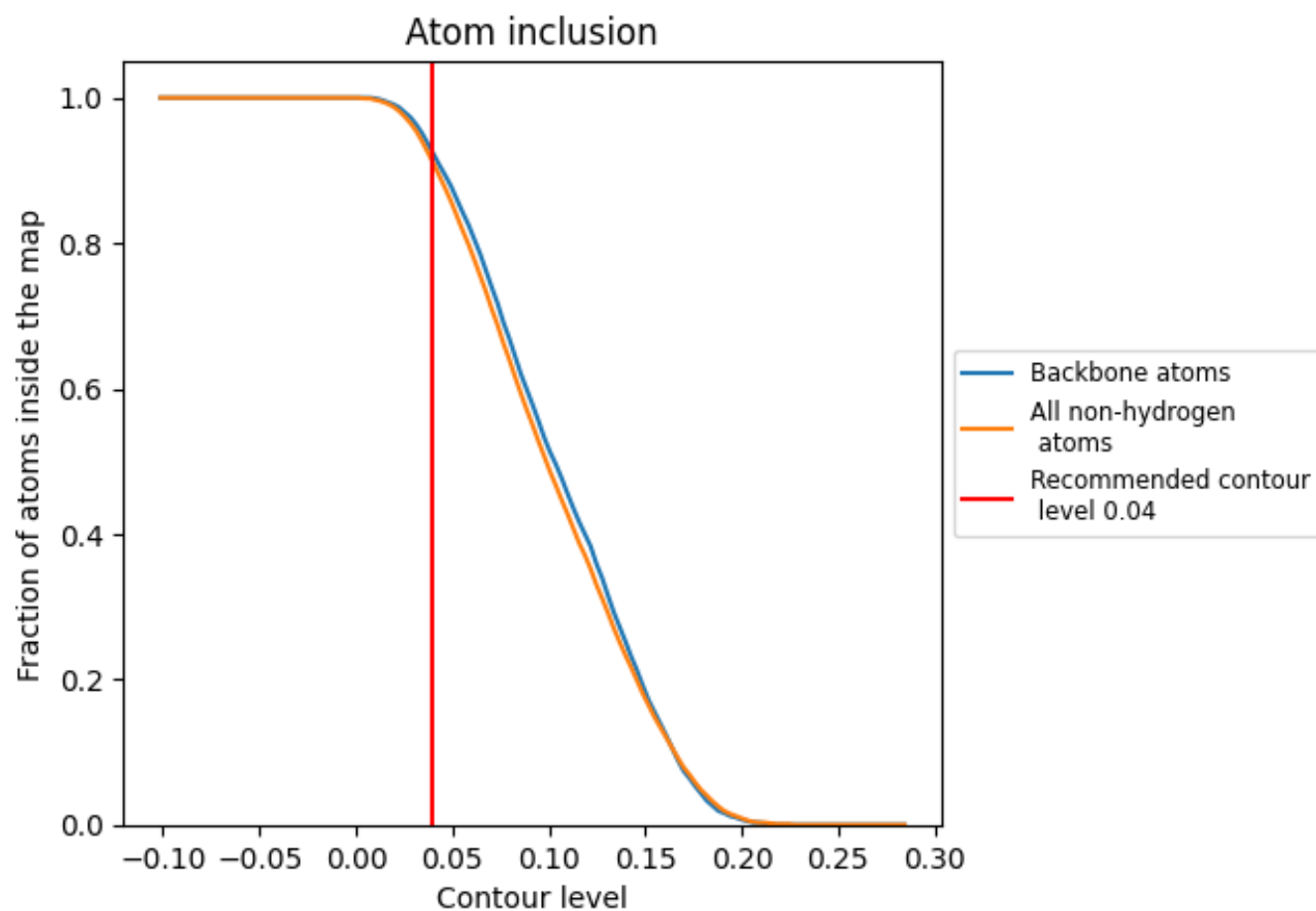
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.9110	0.6210
A	0.9400	0.6390
B	0.9500	0.6420
C	0.9130	0.6220
D	0.9410	0.6430
E	0.7550	0.5550
F	0.8160	0.5220
H	0.9680	0.6320
I	0.9560	0.6050
J	0.6570	0.5800
K	0.8920	0.5920
L	0.8690	0.6200
M	0.9260	0.6160
R	0.4890	0.4310
T	0.9260	0.6160
X	0.8830	0.5930
Y	0.7130	0.5080
Z	0.7760	0.5070

