



Full wwPDB EM Validation Report ⓘ

Jun 29, 2026 – 02:28 pm BST

PDB ID : 31EW / pdb_000031ew
EMDB ID : EMD-58351
Title : UapA (WT) in DDM, Apo state
Authors : Broutzakis, G.; Gatsogiannis, C.
Deposited on : 2026-06-01
Resolution : 2.06 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:

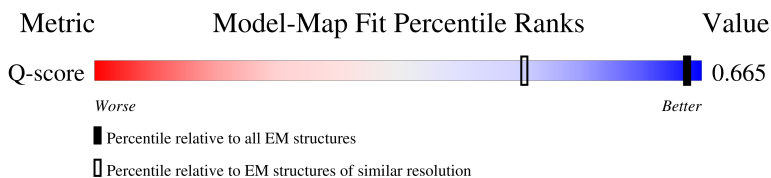
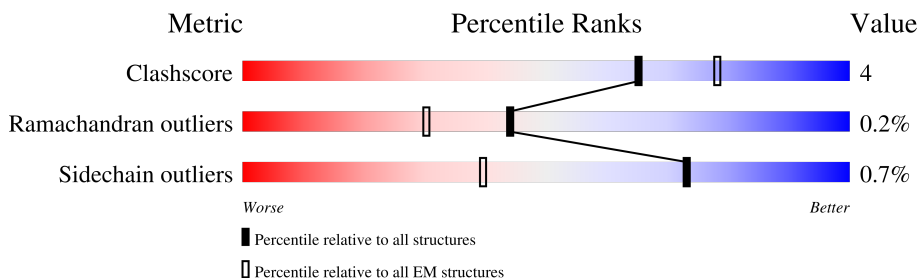
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.06 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	1895 (1.56 - 2.56)

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	566	
1	B	566	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9690 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.

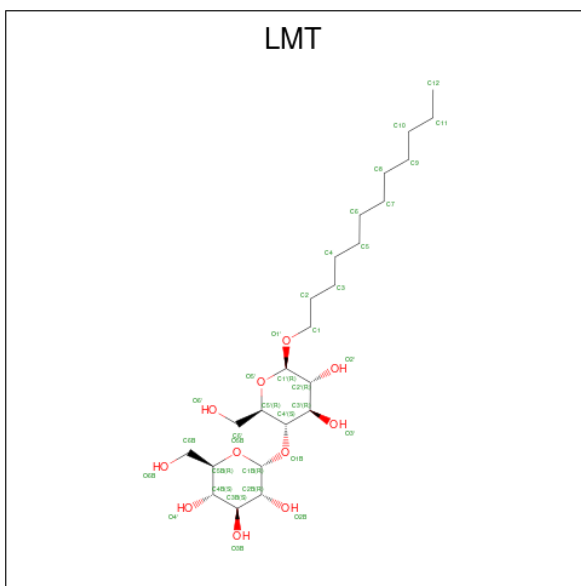
- Molecule 1 is a protein called Uric acid-xanthine permease.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	519	Total 3866	C 2528	N 623	O 679	S 36	0	0
1	B	519	Total 3866	C 2528	N 623	O 679	S 36	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP Q07307
B	9	MET	-	initiating methionine	UNP Q07307

- Molecule 2 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



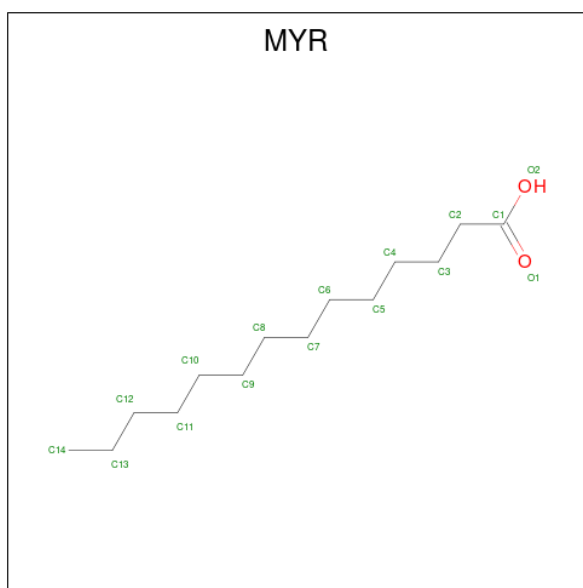
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	Total 35	C 24	O 11	0
2	A	1	Total 35	C 24	O 11	0

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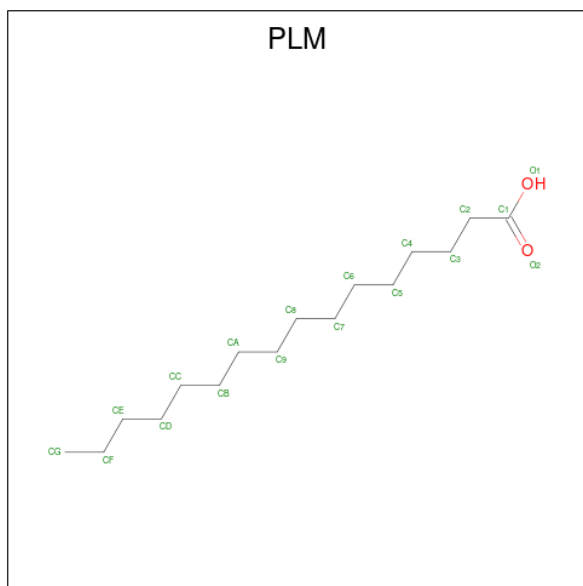
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	24	11	
2	A	1	Total	C	O	0
			35	24	11	
2	A	1	Total	C	O	0
			35	24	11	
2	A	1	Total	C	O	0
			35	24	11	
2	A	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	
2	B	1	Total	C	O	0
			35	24	11	

- Molecule 3 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



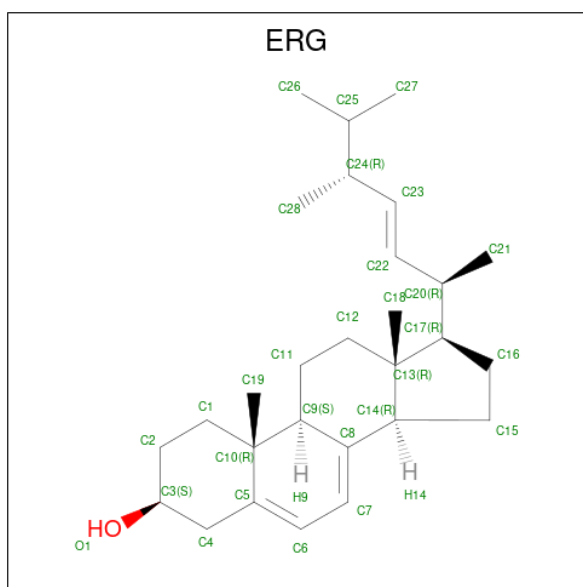
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			16	14	2	
3	A	1	Total	C	O	0
			16	14	2	
3	A	1	Total	C	O	0
			16	14	2	
3	A	1	Total	C	O	0
			16	14	2	
3	A	1	Total	C	O	0
			16	14	2	
3	A	1	Total	C	O	0
			16	14	2	
3	A	1	Total	C	O	0
			16	14	2	
3	A	1	Total	C	O	0
			16	14	2	
3	A	1	Total	C	O	0
			16	14	2	
3	A	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	
3	B	1	Total	C	O	0
			16	14	2	

- Molecule 4 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



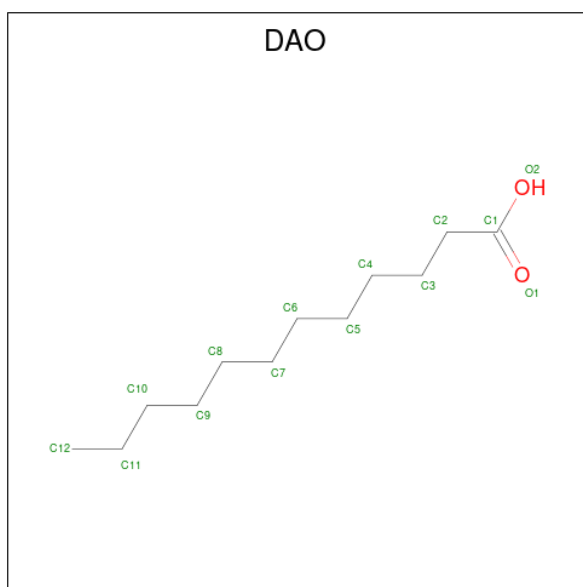
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	A	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	
4	B	1	Total	C	O	0
			18	16	2	

- Molecule 5 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



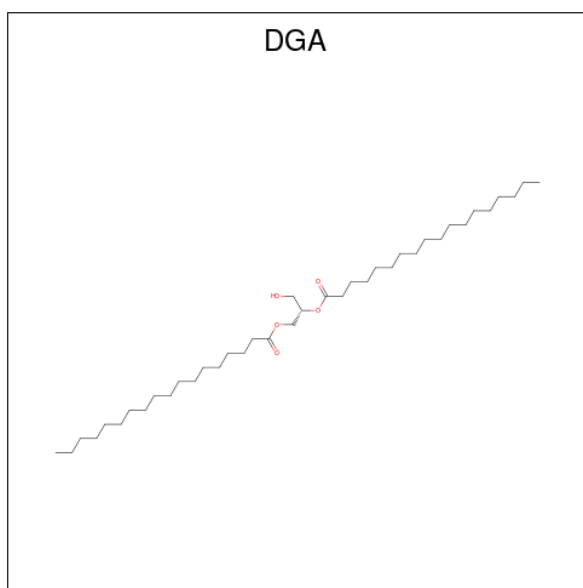
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	A	1	Total	C	O	0
			29	28	1	
5	B	1	Total	C	O	0
			29	28	1	
5	B	1	Total	C	O	0
			29	28	1	
5	B	1	Total	C	O	0
			29	28	1	

- Molecule 6 is LAURIC ACID (CCD ID: DAO) (formula: C₁₂H₂₄O₂).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			14	12	2	
6	A	1	Total	C	O	0
			14	12	2	
6	A	1	Total	C	O	0
			14	12	2	
6	A	1	Total	C	O	0
			14	12	2	
6	A	1	Total	C	O	0
			14	12	2	
6	A	1	Total	C	O	0
			14	12	2	
6	B	1	Total	C	O	0
			14	12	2	
6	B	1	Total	C	O	0
			14	12	2	
6	B	1	Total	C	O	0
			14	12	2	
6	B	1	Total	C	O	0
			14	12	2	
6	B	1	Total	C	O	0
			14	12	2	
6	B	1	Total	C	O	0
			14	12	2	

- Molecule 7 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			44	39	5	
7	A	1	Total	C	O	0
			44	39	5	
7	B	1	Total	C	O	0
			44	39	5	
7	B	1	Total	C	O	0
			44	39	5	

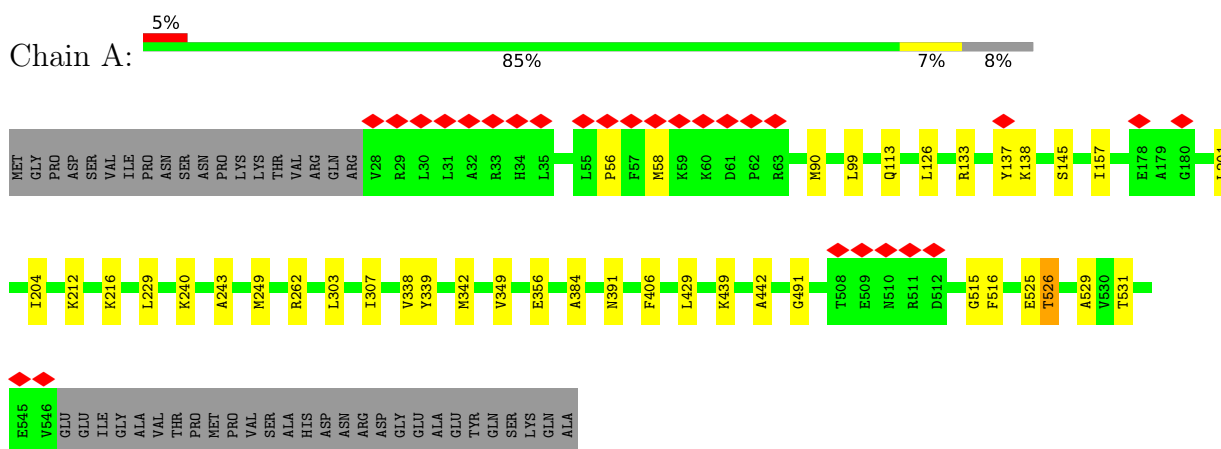
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	202	Total	O	0
			202	202	
8	B	202	Total	O	0
			202	202	

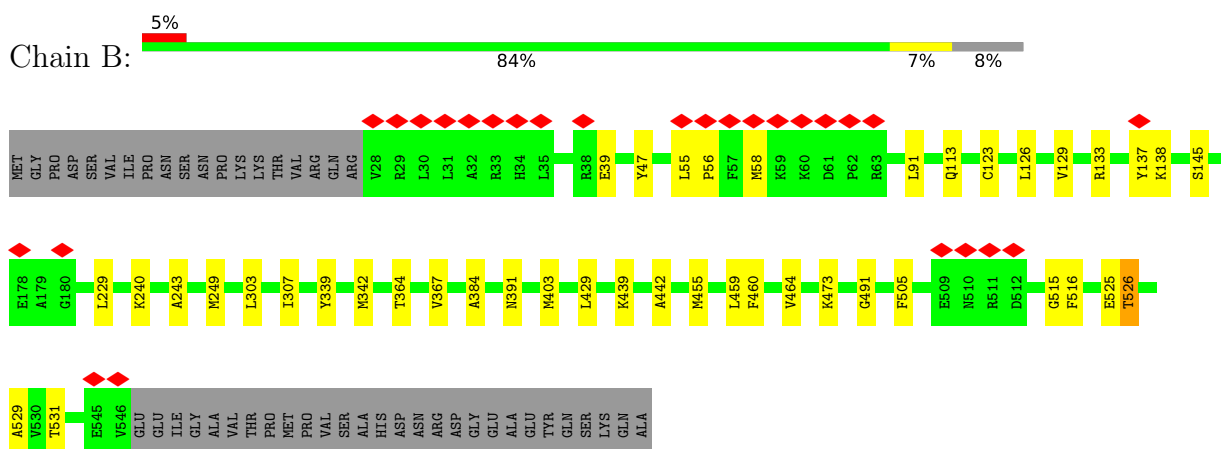
3 Residue-property plots [i](#)

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: Uric acid-xanthine permease



- Molecule 1: Uric acid-xanthine permease



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	499617	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.320	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.069	Depositor
Map size (Å)	257.6, 257.6, 257.6	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.736, 0.736, 0.736	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: DAO, PLM, LMT, ERG, DGA, MYR

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	0.17	0/3958	0.32	0/5397
1	B	0.17	0/3958	0.33	0/5397
All	All	0.17	0/7916	0.33	0/10794

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	3866	0	3969	32	0
1	B	3866	0	3969	34	0
2	A	245	0	322	7	0
2	B	245	0	322	6	0
3	A	176	0	297	5	0
3	B	176	0	297	5	0
4	A	54	0	93	1	0
4	B	54	0	93	3	0
5	A	116	0	176	3	0
5	B	116	0	176	4	0
6	A	98	0	161	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	98	0	161	4	0
7	A	88	0	152	1	0
7	B	88	0	152	2	0
8	A	202	0	0	0	0
8	B	202	0	0	0	0
All	All	9690	0	10340	79	0

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

All (79) 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)
1:B:55:LEU:HB2	1:B:58:MET:HG2	1.61	0.83
1:A:138:LYS:HZ2	7:A:622:DGA:HA32	1.45	0.82
1:A:240:LYS:HD3	1:A:249:MET:HE1	1.64	0.77
1:B:303:LEU:O	1:B:307:ILE:HD12	1.91	0.71
1:A:303:LEU:O	1:A:307:ILE:HD12	1.91	0.69
1:B:138:LYS:HZ2	7:B:624:DGA:HA32	1.59	0.67
1:B:123:CYS:HB2	1:B:403:MET:HE1	1.77	0.67
1:A:262:ARG:HG3	1:A:262:ARG:HH11	1.63	0.64
1:A:145:SER:HB3	1:A:384:ALA:HB2	1.81	0.62
1:B:145:SER:HB3	1:B:384:ALA:HB2	1.82	0.61
1:B:243:ALA:HB2	2:B:601:LMT:H52	1.83	0.59
1:A:243:ALA:HB2	2:A:633:LMT:H52	1.87	0.56
3:A:607:MYR:H41	6:A:628:DAO:H31	1.87	0.56
1:A:58:MET:N	1:A:58:MET:HE2	2.20	0.56
1:B:439:LYS:HB2	4:B:617:PLM:H62	1.88	0.55
1:A:307:ILE:HG13	6:A:632:DAO:H101	1.89	0.55
1:A:439:LYS:HB2	4:A:615:PLM:H62	1.88	0.55
1:A:526:THR:HG22	1:A:529:ALA:H	1.71	0.55
2:B:612:LMT:H72	6:B:619:DAO:H61	1.88	0.54
3:B:623:MYR:H82	5:B:633:ERG:H271	1.89	0.54
1:A:126:LEU:HD13	1:A:391:ASN:HB3	1.90	0.54
1:A:212:LYS:H	1:A:212:LYS:HE2	1.73	0.54
1:B:126:LEU:HD13	1:B:391:ASN:HB3	1.90	0.54
3:B:609:MYR:H41	6:B:630:DAO:H31	1.90	0.54
1:B:307:ILE:HG13	6:B:634:DAO:H101	1.89	0.53
2:A:610:LMT:H72	6:A:617:DAO:H61	1.91	0.53
1:B:58:MET:N	1:B:58:MET:HE2	2.23	0.53
1:B:526:THR:HG22	1:B:529:ALA:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:621:MYR:H82	5:A:631:ERG:H271	1.90	0.53
1:A:339:TYR:HB3	1:A:342:MET:HE2	1.91	0.52
1:B:339:TYR:HB3	1:B:342:MET:HE2	1.91	0.51
1:A:429:LEU:HD21	2:A:601:LMT:H123	1.92	0.51
6:A:612:DAO:H111	2:A:625:LMT:H121	1.93	0.50
3:A:616:MYR:H92	5:A:624:ERG:H263	1.96	0.48
1:B:91:LEU:HD22	4:B:617:PLM:HG2	1.96	0.48
1:B:429:LEU:HD21	2:B:603:LMT:H123	1.96	0.48
1:A:240:LYS:HD3	1:A:249:MET:CE	2.40	0.48
1:B:113:GLN:HG2	1:B:442:ALA:HA	1.96	0.48
1:B:473:LYS:NZ	2:B:620:LMT:H6'1	2.29	0.47
1:A:58:MET:HE2	1:A:58:MET:H	1.80	0.47
1:B:240:LYS:HD3	1:B:249:MET:HE1	1.97	0.47
3:A:607:MYR:H61	6:A:628:DAO:H51	1.97	0.46
1:B:473:LYS:HE2	1:B:473:LYS:HB2	1.71	0.46
1:A:356:GLU:HG3	2:A:618:LMT:H2'	1.96	0.46
1:A:515:GLY:HA3	6:A:617:DAO:H31	1.99	0.45
1:A:338:VAL:HG23	3:A:629:MYR:H62	1.99	0.45
1:A:113:GLN:HG2	1:A:442:ALA:HA	1.99	0.44
1:B:339:TYR:HB3	1:B:342:MET:CE	2.48	0.44
1:A:56:PRO:HB3	2:A:634:LMT:H2'	1.98	0.44
1:A:339:TYR:HB3	1:A:342:MET:CE	2.48	0.44
1:B:137:TYR:CE2	1:B:138:LYS:HD3	2.53	0.44
1:A:137:TYR:CE2	1:A:138:LYS:HD3	2.53	0.44
1:B:505:PHE:HB3	3:B:613:MYR:H72	1.99	0.44
3:B:618:MYR:H92	5:B:626:ERG:H263	1.99	0.44
2:B:603:LMT:H71	5:B:633:ERG:H283	1.99	0.43
1:A:157:ILE:HD13	1:A:349:VAL:HG11	2.00	0.43
1:A:516:PHE:H	1:A:516:PHE:HD1	1.67	0.43
1:A:516:PHE:CD1	1:A:516:PHE:N	2.87	0.43
1:B:455:MET:HE3	1:B:459:LEU:HD12	2.01	0.43
1:A:216:LYS:HE3	1:A:216:LYS:HB2	1.76	0.42
1:B:129:VAL:HG22	3:B:622:MYR:H121	2.02	0.42
1:A:262:ARG:HG3	1:A:262:ARG:NH1	2.33	0.42
1:A:491:GLY:HA3	1:A:531:THR:OG1	2.20	0.42
1:B:516:PHE:CD2	1:B:516:PHE:N	2.88	0.42
1:B:39:GLU:H	1:B:39:GLU:CD	2.28	0.41
1:B:56:PRO:HB3	2:B:602:LMT:H2'	2.02	0.41
1:B:515:GLY:HA3	6:B:619:DAO:H31	2.02	0.41
1:A:201:LEU:HA	1:A:204:ILE:HD12	2.01	0.41
2:A:601:LMT:H6E	5:A:631:ERG:H12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:TYR:HB3	7:B:608:DGA:HB81	2.03	0.41
1:B:240:LYS:HD3	1:B:249:MET:CE	2.51	0.41
1:B:491:GLY:HA3	1:B:531:THR:OG1	2.20	0.41
1:B:516:PHE:HD2	1:B:516:PHE:H	1.68	0.41
1:B:364:THR:HA	1:B:367:VAL:HG12	2.02	0.41
1:B:429:LEU:HD23	1:B:429:LEU:HA	1.95	0.41
1:B:460:PHE:O	1:B:464:VAL:HG23	2.21	0.41
1:A:90:MET:HE1	1:A:406:PHE:CE2	2.56	0.40
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.90	0.40
4:B:605:PLM:H62	5:B:606:ERG:H152	2.03	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	517/566 (91%)	512 (99%)	4 (1%)	1 (0%)	43 38
1	B	517/566 (91%)	513 (99%)	3 (1%)	1 (0%)	43 38
All	All	1034/1132 (91%)	1025 (99%)	7 (1%)	2 (0%)	44 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	ARG
1	B	133	ARG

5.3.2 Protein sidechains [i](#)

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	415/455 (91%)	412 (99%)	3 (1%)	76	79
1	B	415/455 (91%)	412 (99%)	3 (1%)	76	79
All	All	830/910 (91%)	824 (99%)	6 (1%)	73	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	LEU
1	A	525	GLU
1	A	526	THR
1	B	229	LEU
1	B	525	GLU
1	B	526	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	181	ASN
1	B	34	HIS
1	B	215	GLN
1	B	317	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

68 ligands 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
3	MYR	B	622	-	15,15,15	0.71	0	15,15,15	0.66	0
3	MYR	A	620	-	15,15,15	0.71	0	15,15,15	0.66	0
3	MYR	B	623	-	15,15,15	0.69	0	15,15,15	0.65	0
7	DGA	B	608	-	43,43,43	0.36	0	45,45,45	0.33	0
5	ERG	B	626	-	31,32,32	0.47	0	47,50,50	0.76	0
3	MYR	B	629	-	15,15,15	0.69	0	15,15,15	0.66	0
4	PLM	A	603	-	17,17,17	0.65	0	17,17,17	0.60	0
3	MYR	A	629	-	15,15,15	0.70	0	15,15,15	0.66	0
2	LMT	A	633	-	36,36,36	0.54	0	47,47,47	0.71	0
3	MYR	A	616	-	15,15,15	0.70	0	15,15,15	0.66	0
6	DAO	A	617	-	13,13,13	0.69	0	13,13,13	0.63	0
3	MYR	B	604	-	15,15,15	0.71	0	15,15,15	0.66	0
2	LMT	A	610	-	36,36,36	0.54	0	47,47,47	0.67	0
3	MYR	B	631	-	15,15,15	0.70	0	15,15,15	0.66	0
3	MYR	A	607	-	15,15,15	0.69	0	15,15,15	0.68	0
6	DAO	B	630	-	13,13,13	0.70	0	13,13,13	0.63	0
6	DAO	A	612	-	13,13,13	0.70	0	13,13,13	0.63	0
5	ERG	A	604	-	31,32,32	0.49	0	47,50,50	0.93	2 (4%)
5	ERG	A	631	-	31,32,32	0.47	0	47,50,50	0.80	0
7	DGA	A	622	-	43,43,43	0.34	0	45,45,45	0.39	0
2	LMT	B	621	-	36,36,36	0.54	0	47,47,47	0.63	0
3	MYR	A	627	-	15,15,15	0.70	0	15,15,15	0.66	0
2	LMT	A	618	-	36,36,36	0.55	0	47,47,47	0.81	0
2	LMT	B	603	-	36,36,36	0.58	0	47,47,47	0.63	0
2	LMT	B	602	-	36,36,36	0.53	0	47,47,47	0.64	0
6	DAO	B	607	-	13,13,13	0.71	0	13,13,13	0.64	0
6	DAO	B	619	-	13,13,13	0.69	0	13,13,13	0.63	0
4	PLM	A	626	-	17,17,17	0.64	0	17,17,17	0.62	0
3	MYR	B	611	-	15,15,15	0.70	0	15,15,15	0.64	0
5	ERG	A	624	-	31,32,32	0.47	0	47,50,50	0.77	0
7	DGA	B	624	-	43,43,43	0.35	0	45,45,45	0.38	0
5	ERG	B	606	-	31,32,32	0.48	0	47,50,50	0.94	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMT	B	601	-	36,36,36	0.54	0	47,47,47	0.72	0
3	MYR	B	615	-	15,15,15	0.70	0	15,15,15	0.64	0
3	MYR	B	613	-	15,15,15	0.72	0	15,15,15	0.62	0
3	MYR	B	625	-	15,15,15	0.70	0	15,15,15	0.66	0
6	DAO	A	605	-	13,13,13	0.70	0	13,13,13	0.64	0
6	DAO	A	632	-	13,13,13	0.68	0	13,13,13	0.66	0
4	PLM	B	617	-	17,17,17	0.66	0	17,17,17	0.58	0
6	DAO	B	614	-	13,13,13	0.70	0	13,13,13	0.63	0
3	MYR	A	602	-	15,15,15	0.69	0	15,15,15	0.66	0
6	DAO	B	634	-	13,13,13	0.69	0	13,13,13	0.66	0
2	LMT	A	625	-	36,36,36	0.51	0	47,47,47	1.14	4 (8%)
3	MYR	A	611	-	15,15,15	0.72	0	15,15,15	0.62	0
5	ERG	B	610	-	31,32,32	0.48	0	47,50,50	0.74	0
3	MYR	A	623	-	15,15,15	0.70	0	15,15,15	0.65	0
3	MYR	B	609	-	15,15,15	0.69	0	15,15,15	0.67	0
2	LMT	A	601	-	36,36,36	0.58	0	47,47,47	0.63	0
2	LMT	B	612	-	36,36,36	0.54	0	47,47,47	0.67	0
2	LMT	A	634	-	36,36,36	0.53	0	47,47,47	0.65	0
4	PLM	B	628	-	17,17,17	0.64	0	17,17,17	0.62	0
2	LMT	B	627	-	36,36,36	0.51	0	47,47,47	1.15	4 (8%)
6	DAO	B	616	-	13,13,13	0.70	0	13,13,13	0.62	0
6	DAO	A	628	-	13,13,13	0.71	0	13,13,13	0.63	0
2	LMT	A	619	-	36,36,36	0.55	0	47,47,47	0.63	0
5	ERG	B	633	-	31,32,32	0.47	0	47,50,50	0.79	0
3	MYR	A	621	-	15,15,15	0.70	0	15,15,15	0.65	0
3	MYR	A	609	-	15,15,15	0.71	0	15,15,15	0.65	0
6	DAO	A	630	-	13,13,13	0.71	0	13,13,13	0.62	0
5	ERG	A	608	-	31,32,32	0.48	0	47,50,50	0.74	0
6	DAO	B	632	-	13,13,13	0.70	0	13,13,13	0.62	0
4	PLM	B	605	-	17,17,17	0.65	0	17,17,17	0.60	0
6	DAO	A	614	-	13,13,13	0.70	0	13,13,13	0.62	0
7	DGA	A	606	-	43,43,43	0.36	0	45,45,45	0.33	0
3	MYR	A	613	-	15,15,15	0.71	0	15,15,15	0.63	0
2	LMT	B	620	-	36,36,36	0.54	0	47,47,47	0.82	0
3	MYR	B	618	-	15,15,15	0.70	0	15,15,15	0.66	0
4	PLM	A	615	-	17,17,17	0.65	0	17,17,17	0.58	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
3	MYR	B	622	-	-	5/13/13/13	-
3	MYR	A	620	-	-	5/13/13/13	-
3	MYR	B	623	-	-	3/13/13/13	-
7	DGA	B	608	-	-	17/45/45/45	-
5	ERG	B	626	-	-	2/13/71/71	0/4/4/4
3	MYR	B	629	-	-	1/13/13/13	-
4	PLM	A	603	-	-	4/15/15/15	-
3	MYR	A	629	-	-	2/13/13/13	-
2	LMT	A	633	-	-	5/21/61/61	0/2/2/2
3	MYR	A	616	-	-	2/13/13/13	-
6	DAO	A	617	-	-	3/11/11/11	-
3	MYR	B	604	-	-	3/13/13/13	-
2	LMT	A	610	-	-	7/21/61/61	0/2/2/2
3	MYR	B	631	-	-	1/13/13/13	-
3	MYR	A	607	-	-	2/13/13/13	-
6	DAO	B	630	-	-	2/11/11/11	-
6	DAO	A	612	-	-	2/11/11/11	-
5	ERG	A	604	-	-	4/13/71/71	0/4/4/4
5	ERG	A	631	-	-	6/13/71/71	0/4/4/4
7	DGA	A	622	-	-	13/45/45/45	-
2	LMT	B	621	-	-	6/21/61/61	0/2/2/2
3	MYR	A	627	-	-	2/13/13/13	-
2	LMT	A	618	-	-	9/21/61/61	0/2/2/2
2	LMT	B	603	-	-	3/21/61/61	0/2/2/2
2	LMT	B	602	-	-	6/21/61/61	0/2/2/2
6	DAO	B	607	-	-	0/11/11/11	-
6	DAO	B	619	-	-	4/11/11/11	-
4	PLM	A	626	-	-	3/15/15/15	-
3	MYR	B	611	-	-	0/13/13/13	-
5	ERG	A	624	-	-	2/13/71/71	0/4/4/4
7	DGA	B	624	-	-	12/45/45/45	-
5	ERG	B	606	-	-	4/13/71/71	0/4/4/4
2	LMT	B	601	-	-	5/21/61/61	0/2/2/2
3	MYR	B	615	-	-	3/13/13/13	-
3	MYR	B	613	-	-	3/13/13/13	-
3	MYR	B	625	-	-	3/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DAO	A	605	-	-	0/11/11/11	-
6	DAO	A	632	-	-	1/11/11/11	-
4	PLM	B	617	-	-	5/15/15/15	-
6	DAO	B	614	-	-	2/11/11/11	-
3	MYR	A	602	-	-	3/13/13/13	-
6	DAO	B	634	-	-	1/11/11/11	-
2	LMT	A	625	-	-	10/21/61/61	0/2/2/2
3	MYR	A	611	-	-	3/13/13/13	-
5	ERG	B	610	-	-	5/13/71/71	0/4/4/4
3	MYR	A	623	-	-	3/13/13/13	-
3	MYR	B	609	-	-	2/13/13/13	-
2	LMT	A	601	-	-	3/21/61/61	0/2/2/2
2	LMT	B	612	-	-	7/21/61/61	0/2/2/2
2	LMT	A	634	-	-	6/21/61/61	0/2/2/2
4	PLM	B	628	-	-	3/15/15/15	-
2	LMT	B	627	-	-	8/21/61/61	0/2/2/2
6	DAO	B	616	-	-	3/11/11/11	-
6	DAO	A	628	-	-	3/11/11/11	-
2	LMT	A	619	-	-	6/21/61/61	0/2/2/2
5	ERG	B	633	-	-	6/13/71/71	0/4/4/4
3	MYR	A	621	-	-	2/13/13/13	-
3	MYR	A	609	-	-	0/13/13/13	-
6	DAO	A	630	-	-	0/11/11/11	-
5	ERG	A	608	-	-	5/13/71/71	0/4/4/4
6	DAO	B	632	-	-	0/11/11/11	-
4	PLM	B	605	-	-	4/15/15/15	-
6	DAO	A	614	-	-	3/11/11/11	-
7	DGA	A	606	-	-	14/45/45/45	-
3	MYR	A	613	-	-	3/13/13/13	-
2	LMT	B	620	-	-	11/21/61/61	0/2/2/2
3	MYR	B	618	-	-	2/13/13/13	-
4	PLM	A	615	-	-	5/15/15/15	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	627	LMT	C1B-O5B-C5B	4.14	121.82	113.69
2	A	625	LMT	C1B-O5B-C5B	4.02	121.58	113.69
2	A	625	LMT	C1B-O1B-C4'	2.73	124.71	117.96
2	B	627	LMT	C1B-O1B-C4'	2.69	124.62	117.96
5	B	606	ERG	C13-C17-C20	2.65	122.85	119.43
5	A	604	ERG	C13-C17-C20	2.62	122.81	119.43
2	A	625	LMT	O1B-C1B-O5B	2.17	116.74	110.67
5	B	606	ERG	C21-C20-C17	2.16	117.43	113.06
2	B	627	LMT	O1B-C1B-O5B	2.15	116.68	110.67
5	A	604	ERG	C21-C20-C17	2.10	117.29	113.06
2	B	627	LMT	O5B-C1B-C2B	2.06	114.72	110.35
2	A	625	LMT	O5B-C1B-C2B	2.03	114.65	110.35

There are no chirality outliers.

All (283) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	ERG	C13-C17-C20-C21
5	A	604	ERG	C17-C20-C22-C23
5	A	631	ERG	C23-C24-C25-C26
5	A	631	ERG	C23-C24-C25-C27
5	A	631	ERG	C28-C24-C25-C26
5	A	631	ERG	C28-C24-C25-C27
5	B	606	ERG	C13-C17-C20-C21
5	B	606	ERG	C17-C20-C22-C23
5	B	633	ERG	C23-C24-C25-C26
5	B	633	ERG	C23-C24-C25-C27
5	B	633	ERG	C28-C24-C25-C26
7	A	622	DGA	CB2-CB1-OG2-CG2
7	A	622	DGA	OB1-CB1-OG2-CG2
7	B	624	DGA	OB1-CB1-OG2-CG2
7	B	624	DGA	OA1-CA1-OG1-CG1
7	A	606	DGA	CA2-CA1-OG1-CG1
7	A	606	DGA	OA1-CA1-OG1-CG1
7	A	622	DGA	OA1-CA1-OG1-CG1
7	B	608	DGA	OA1-CA1-OG1-CG1
2	A	625	LMT	O5B-C1B-O1B-C4'
2	B	627	LMT	O5B-C1B-O1B-C4'
7	A	622	DGA	CA2-CA1-OG1-CG1
7	B	608	DGA	CA2-CA1-OG1-CG1
7	B	624	DGA	CA2-CA1-OG1-CG1
7	B	624	DGA	CB2-CB1-OG2-CG2
2	B	621	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
2	A	619	LMT	C3'-C4'-O1B-C1B
2	A	619	LMT	C2'-C1'-O1'-C1
2	B	621	LMT	C2'-C1'-O1'-C1
5	A	631	ERG	C17-C20-C22-C23
5	B	633	ERG	C17-C20-C22-C23
2	A	618	LMT	O5'-C5'-C6'-O6'
2	B	620	LMT	O5'-C5'-C6'-O6'
7	A	622	DGA	CB1-CB2-CB3-CB4
3	B	631	MYR	C5-C6-C7-C8
3	A	629	MYR	C5-C6-C7-C8
5	B	633	ERG	C28-C24-C25-C27
2	A	619	LMT	O1'-C1-C2-C3
2	B	621	LMT	O1'-C1-C2-C3
2	A	610	LMT	C2'-C1'-O1'-C1
2	B	612	LMT	C2'-C1'-O1'-C1
2	B	627	LMT	C2'-C1'-O1'-C1
2	A	625	LMT	C11-C10-C9-C8
3	B	629	MYR	C6-C7-C8-C9
7	A	622	DGA	CCA-CDA-CEA-CFA
2	A	610	LMT	O5'-C1'-O1'-C1
2	A	625	LMT	O5'-C1'-O1'-C1
2	B	612	LMT	O5'-C1'-O1'-C1
2	B	627	LMT	O5'-C1'-O1'-C1
5	A	604	ERG	C16-C17-C20-C22
5	B	606	ERG	C16-C17-C20-C22
2	A	618	LMT	C2-C1-O1'-C1'
2	B	620	LMT	C2-C1-O1'-C1'
6	A	628	DAO	C4-C5-C6-C7
2	A	625	LMT	O5'-C5'-C6'-O6'
2	A	625	LMT	C2B-C1B-O1B-C4'
2	A	625	LMT	C4'-C5'-C6'-O6'
7	B	624	DGA	CCA-CDA-CEA-CFA
2	A	633	LMT	C4-C5-C6-C7
2	B	612	LMT	C7-C8-C9-C10
7	B	624	DGA	CB1-CB2-CB3-CB4
2	A	610	LMT	C7-C8-C9-C10
2	B	627	LMT	C2B-C1B-O1B-C4'
4	B	605	PLM	C2-C3-C4-C5
7	B	608	DGA	CA6-CA7-CA8-CA9
4	A	603	PLM	C2-C3-C4-C5
7	A	606	DGA	CAA-CBA-CCA-CDA
2	B	620	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
2	B	601	LMT	C4-C5-C6-C7
4	A	615	PLM	CA-CB-CC-CD
4	B	617	PLM	CA-CB-CC-CD
2	B	603	LMT	O1'-C1-C2-C3
2	A	625	LMT	C2'-C1'-O1'-C1
2	B	601	LMT	C2-C3-C4-C5
2	A	619	LMT	C5'-C4'-O1B-C1B
2	B	621	LMT	C5'-C4'-O1B-C1B
6	B	619	DAO	C3-C4-C5-C6
7	A	622	DGA	CB7-CB8-CB9-CAB
2	B	603	LMT	C1-C2-C3-C4
7	B	608	DGA	CAA-CBA-CCA-CDA
2	A	601	LMT	C1-C2-C3-C4
2	A	601	LMT	O1'-C1-C2-C3
2	A	633	LMT	C2-C3-C4-C5
7	A	622	DGA	OG1-CG1-CG2-CG3
2	B	627	LMT	C2-C3-C4-C5
4	B	605	PLM	C3-C4-C5-C6
2	B	627	LMT	O5B-C5B-C6B-O6B
4	B	617	PLM	C8-C9-CA-CB
7	B	624	DGA	CB7-CB8-CB9-CAB
2	A	625	LMT	C2-C3-C4-C5
2	A	625	LMT	O5B-C5B-C6B-O6B
2	A	633	LMT	O5B-C5B-C6B-O6B
2	B	601	LMT	O5B-C5B-C6B-O6B
4	A	615	PLM	C8-C9-CA-CB
6	A	617	DAO	C3-C4-C5-C6
2	A	610	LMT	O5B-C5B-C6B-O6B
2	B	612	LMT	O5B-C5B-C6B-O6B
7	B	608	DGA	CA3-CA4-CA5-CA6
2	A	633	LMT	C6-C7-C8-C9
4	A	603	PLM	C3-C4-C5-C6
2	B	601	LMT	C6-C7-C8-C9
7	A	622	DGA	CA9-CAA-CBA-CCA
7	A	606	DGA	CA3-CA4-CA5-CA6
7	B	608	DGA	CB2-CB1-OG2-CG2
3	B	615	MYR	C2-C3-C4-C5
2	A	625	LMT	C2-C1-O1'-C1'
2	B	627	LMT	C2-C1-O1'-C1'
4	A	615	PLM	C3-C4-C5-C6
7	A	606	DGA	OG1-CG1-CG2-CG3
7	B	608	DGA	OG1-CG1-CG2-CG3

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Mol	Chain	Res	Type	Atoms
7	B	624	DGA	OG1-CG1-CG2-CG3
5	A	608	ERG	C23-C24-C25-C26
5	B	610	ERG	C23-C24-C25-C26
7	A	606	DGA	CA6-CA7-CA8-CA9
7	A	606	DGA	CB2-CB1-OG2-CG2
2	A	618	LMT	O5'-C1'-O1'-C1
3	A	613	MYR	C2-C3-C4-C5
7	A	606	DGA	CA4-CA5-CA6-CA7
2	B	602	LMT	O1'-C1-C2-C3
4	B	617	PLM	C3-C4-C5-C6
7	A	606	DGA	CEB-CFB-CGB-CHB
7	A	622	DGA	CA1-CA2-CA3-CA4
6	B	619	DAO	C2-C3-C4-C5
7	B	608	DGA	OB1-CB1-OG2-CG2
3	A	627	MYR	C6-C7-C8-C9
2	B	627	LMT	C11-C10-C9-C8
7	B	608	DGA	CEB-CFB-CGB-CHB
7	A	606	DGA	OB1-CB1-OG2-CG2
2	A	634	LMT	C1-C2-C3-C4
7	A	606	DGA	OG1-CG1-CG2-OG2
7	A	622	DGA	OG1-CG1-CG2-OG2
7	B	608	DGA	OG1-CG1-CG2-OG2
7	B	624	DGA	OG1-CG1-CG2-OG2
2	A	618	LMT	C4'-C5'-C6'-O6'
2	A	634	LMT	O1'-C1-C2-C3
7	B	624	DGA	CA1-CA2-CA3-CA4
2	B	620	LMT	C4'-C5'-C6'-O6'
2	B	602	LMT	C1-C2-C3-C4
5	A	604	ERG	C16-C17-C20-C21
5	B	606	ERG	C16-C17-C20-C21
4	A	615	PLM	C9-CA-CB-CC
6	A	617	DAO	C2-C3-C4-C5
6	B	616	DAO	C3-C4-C5-C6
2	A	618	LMT	C7-C8-C9-C10
3	A	623	MYR	C4-C5-C6-C7
4	B	617	PLM	C9-CA-CB-CC
3	B	625	MYR	C4-C5-C6-C7
6	A	614	DAO	C3-C4-C5-C6
2	B	620	LMT	C7-C8-C9-C10
7	B	608	DGA	CBB-CCB-CDB-CEB
7	A	606	DGA	CB4-CB5-CB6-CB7
2	B	612	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	613	MYR	C1-C2-C3-C4
6	A	617	DAO	C4-C5-C6-C7
2	A	634	LMT	O5'-C1'-O1'-C1
2	A	618	LMT	C2'-C1'-O1'-C1
2	B	620	LMT	C2'-C1'-O1'-C1
6	B	634	DAO	C9-C10-C11-C12
5	A	608	ERG	C28-C24-C25-C26
5	A	608	ERG	C28-C24-C25-C27
5	B	610	ERG	C28-C24-C25-C26
5	B	610	ERG	C28-C24-C25-C27
7	B	608	DGA	CB4-CB5-CB6-CB7
6	B	619	DAO	C4-C5-C6-C7
2	A	610	LMT	C1-C2-C3-C4
6	A	632	DAO	C9-C10-C11-C12
7	B	608	DGA	CA4-CA5-CA6-CA7
2	A	618	LMT	C3-C4-C5-C6
3	B	615	MYR	C1-C2-C3-C4
4	B	628	PLM	O1-C1-C2-C3
2	B	602	LMT	O5'-C1'-O1'-C1
3	B	604	MYR	C7-C8-C9-C10
3	A	602	MYR	C7-C8-C9-C10
3	B	622	MYR	O1-C1-C2-C3
2	B	602	LMT	C6-C7-C8-C9
2	B	602	LMT	C7-C8-C9-C10
3	A	620	MYR	C4-C5-C6-C7
3	B	609	MYR	O1-C1-C2-C3
4	A	626	PLM	O1-C1-C2-C3
2	A	634	LMT	C2'-C1'-O1'-C1
7	A	622	DGA	CBB-CAB-CB9-CB8
4	B	628	PLM	O2-C1-C2-C3
2	B	620	LMT	C3-C4-C5-C6
3	A	620	MYR	C5-C6-C7-C8
7	B	624	DGA	CBB-CAB-CB9-CB8
3	A	613	MYR	C5-C6-C7-C8
3	B	622	MYR	C4-C5-C6-C7
2	B	612	LMT	C6-C7-C8-C9
4	B	628	PLM	CD-CE-CF-CG
3	B	622	MYR	C5-C6-C7-C8
2	B	620	LMT	C4B-C5B-C6B-O6B
4	A	626	PLM	O2-C1-C2-C3
6	A	614	DAO	O2-C1-C2-C3
3	A	611	MYR	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	612	DAO	O1-C1-C2-C3
6	B	616	DAO	O2-C1-C2-C3
2	A	610	LMT	C6-C7-C8-C9
7	B	624	DGA	CB2-CB3-CB4-CB5
4	A	626	PLM	CD-CE-CF-CG
6	B	619	DAO	C6-C7-C8-C9
3	A	607	MYR	O1-C1-C2-C3
3	B	622	MYR	O2-C1-C2-C3
6	B	614	DAO	O2-C1-C2-C3
3	A	611	MYR	C6-C7-C8-C9
5	A	624	ERG	C22-C23-C24-C28
3	A	607	MYR	O2-C1-C2-C3
3	A	620	MYR	O1-C1-C2-C3
3	B	613	MYR	O1-C1-C2-C3
6	A	614	DAO	O1-C1-C2-C3
3	A	611	MYR	O1-C1-C2-C3
4	A	603	PLM	O1-C1-C2-C3
4	A	603	PLM	O2-C1-C2-C3
4	B	605	PLM	O1-C1-C2-C3
4	B	605	PLM	O2-C1-C2-C3
6	A	612	DAO	O2-C1-C2-C3
6	B	616	DAO	O1-C1-C2-C3
5	A	608	ERG	C23-C24-C25-C27
5	B	610	ERG	C23-C24-C25-C27
6	B	614	DAO	O1-C1-C2-C3
3	B	609	MYR	O2-C1-C2-C3
6	B	630	DAO	O2-C1-C2-C3
3	A	621	MYR	O2-C1-C2-C3
3	B	613	MYR	O2-C1-C2-C3
3	B	623	MYR	O2-C1-C2-C3
6	A	628	DAO	O2-C1-C2-C3
7	A	606	DGA	CBB-CCB-CDB-CEB
3	B	615	MYR	C5-C6-C7-C8
5	B	626	ERG	C22-C23-C24-C28
3	B	623	MYR	C1-C2-C3-C4
6	B	630	DAO	O1-C1-C2-C3
2	B	601	LMT	C11-C10-C9-C8
3	A	602	MYR	O2-C1-C2-C3
2	A	610	LMT	C4-C5-C6-C7
2	B	612	LMT	C4-C5-C6-C7
2	B	602	LMT	C9-C10-C11-C12
3	B	623	MYR	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	A	634	LMT	C7-C8-C9-C10
3	B	604	MYR	O2-C1-C2-C3
5	A	624	ERG	C21-C20-C22-C23
5	B	626	ERG	C21-C20-C22-C23
3	A	621	MYR	O1-C1-C2-C3
2	B	621	LMT	O5'-C1'-O1'-C1
6	A	628	DAO	O1-C1-C2-C3
2	A	634	LMT	C6-C7-C8-C9
3	B	604	MYR	O1-C1-C2-C3
3	A	602	MYR	O1-C1-C2-C3
2	A	633	LMT	C11-C10-C9-C8
3	B	625	MYR	O1-C1-C2-C3
3	A	623	MYR	O1-C1-C2-C3
3	A	620	MYR	O2-C1-C2-C3
7	B	608	DGA	CB9-CAB-CBB-CCB
2	B	621	LMT	C5-C6-C7-C8
3	B	625	MYR	O2-C1-C2-C3
7	A	606	DGA	CB9-CAB-CBB-CCB
2	B	620	LMT	O5B-C5B-C6B-O6B
3	A	623	MYR	O2-C1-C2-C3
7	B	608	DGA	CA1-CA2-CA3-CA4
2	A	619	LMT	C5-C6-C7-C8
5	A	608	ERG	C21-C20-C22-C23
5	B	610	ERG	C21-C20-C22-C23
2	A	601	LMT	C7-C8-C9-C10
7	A	622	DGA	CAA-CBA-CCA-CDA
2	B	603	LMT	C2-C3-C4-C5
2	A	619	LMT	O5'-C1'-O1'-C1
2	A	618	LMT	C9-C10-C11-C12
3	A	616	MYR	O2-C1-C2-C3
7	B	608	DGA	CA2-CA3-CA4-CA5
4	B	617	PLM	C1-C2-C3-C4
2	A	618	LMT	C5-C6-C7-C8
7	B	608	DGA	CCA-CDA-CEA-CFA
5	A	631	ERG	C21-C20-C22-C23
5	B	633	ERG	C21-C20-C22-C23
2	B	620	LMT	C9-C10-C11-C12
2	B	620	LMT	C2B-C1B-O1B-C4'
3	B	613	MYR	C6-C7-C8-C9
3	B	622	MYR	C9-C10-C11-C12
3	A	616	MYR	O1-C1-C2-C3
4	A	615	PLM	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	627	MYR	O1-C1-C2-C3
3	B	618	MYR	O2-C1-C2-C3
3	A	629	MYR	C3-C4-C5-C6
3	A	620	MYR	C9-C10-C11-C12
3	B	618	MYR	O1-C1-C2-C3

There are no ring outliers.

38 monomers are involved in 34 short contacts:

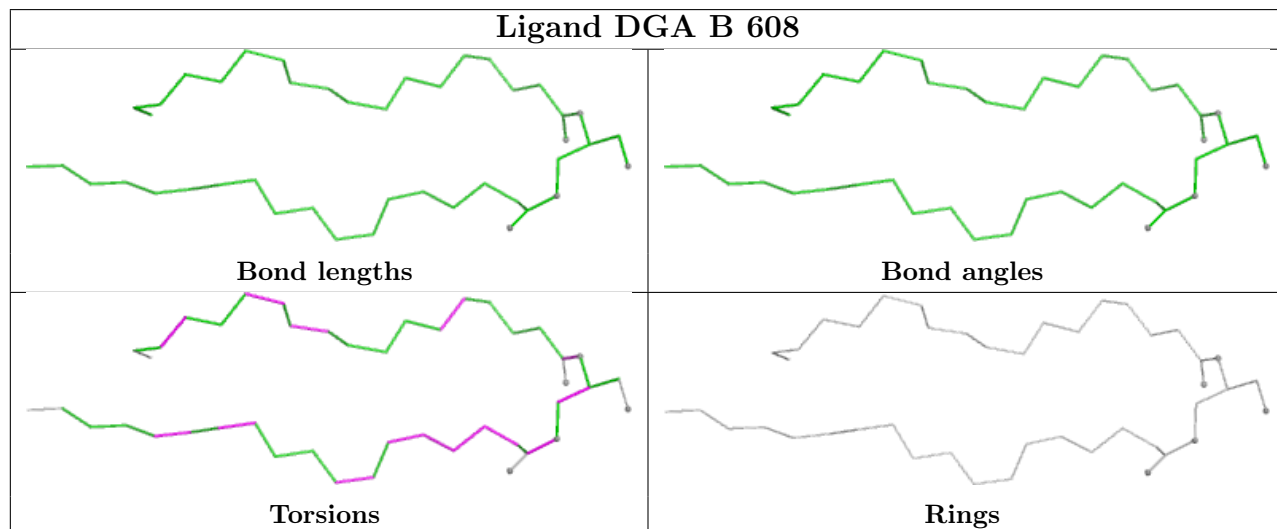
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	622	MYR	1	0
3	B	623	MYR	1	0
7	B	608	DGA	1	0
5	B	626	ERG	1	0
3	A	629	MYR	1	0
2	A	633	LMT	1	0
3	A	616	MYR	1	0
6	A	617	DAO	2	0
2	A	610	LMT	1	0
3	A	607	MYR	2	0
6	B	630	DAO	1	0
6	A	612	DAO	1	0
5	A	631	ERG	2	0
7	A	622	DGA	1	0
2	A	618	LMT	1	0
2	B	603	LMT	2	0
2	B	602	LMT	1	0
6	B	619	DAO	2	0
5	A	624	ERG	1	0
7	B	624	DGA	1	0
5	B	606	ERG	1	0
2	B	601	LMT	1	0
3	B	613	MYR	1	0
6	A	632	DAO	1	0
4	B	617	PLM	2	0
6	B	634	DAO	1	0
2	A	625	LMT	1	0
3	B	609	MYR	1	0
2	A	601	LMT	2	0
2	B	612	LMT	1	0
2	A	634	LMT	1	0
6	A	628	DAO	2	0

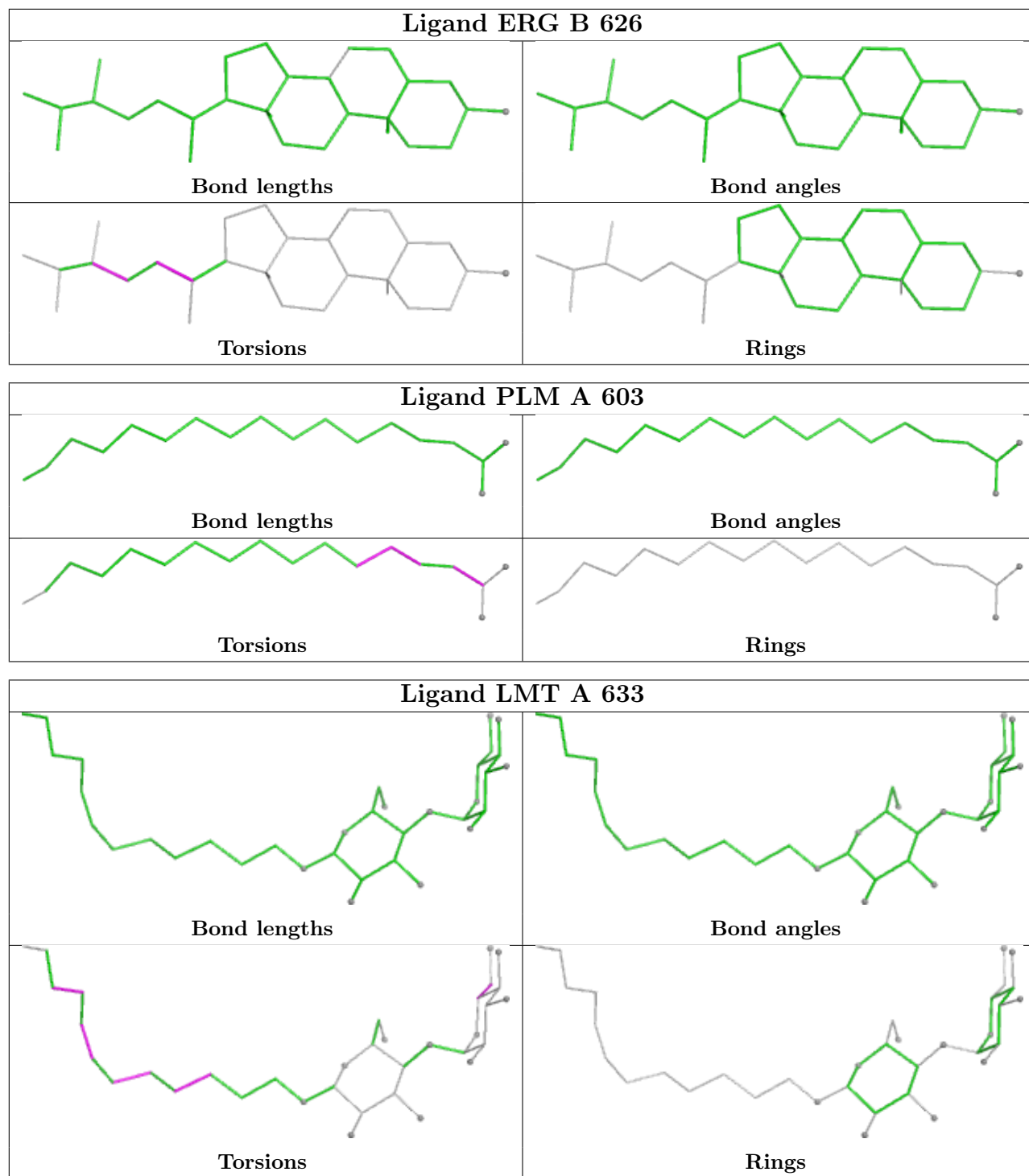
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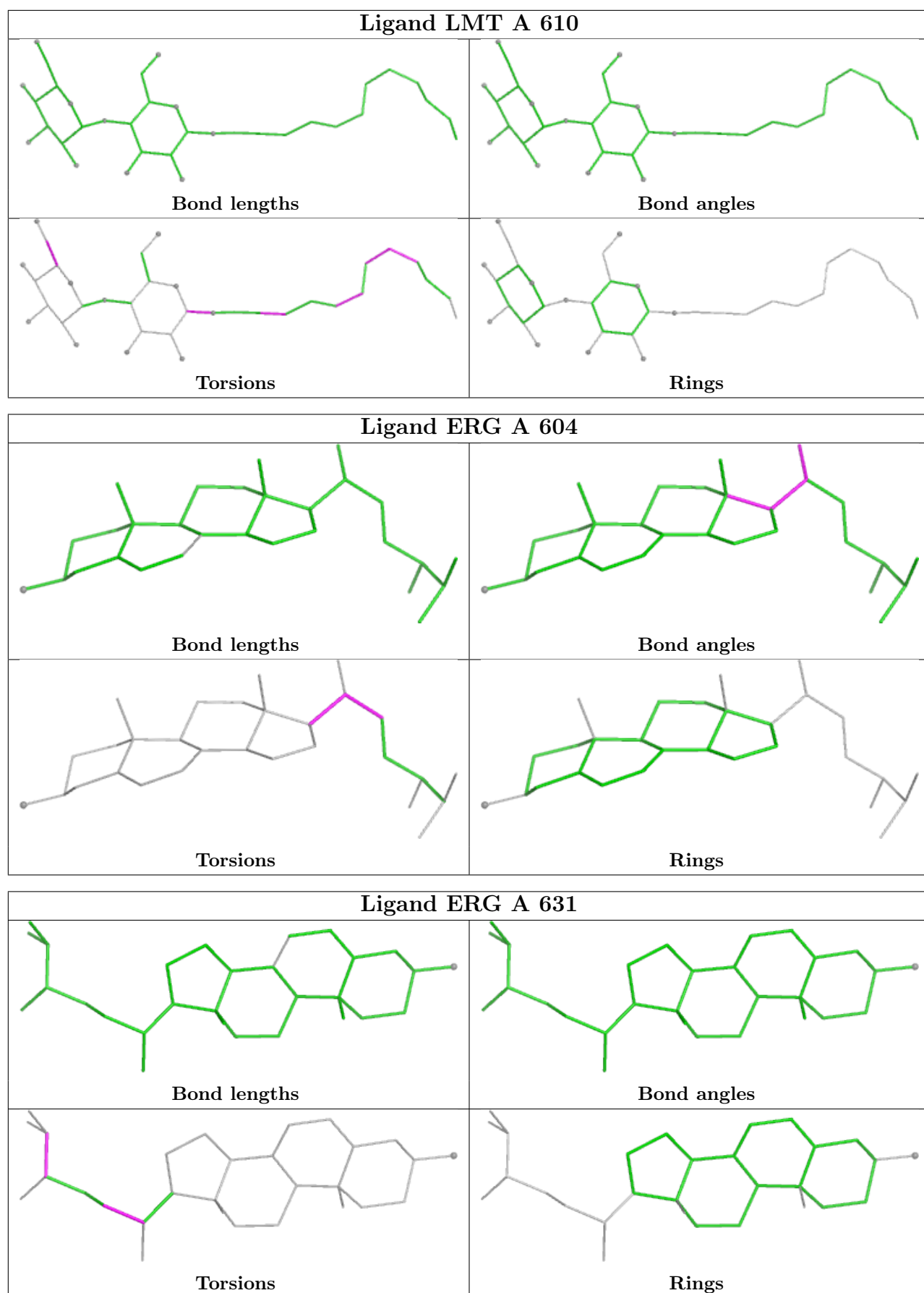
Continued from previous page...

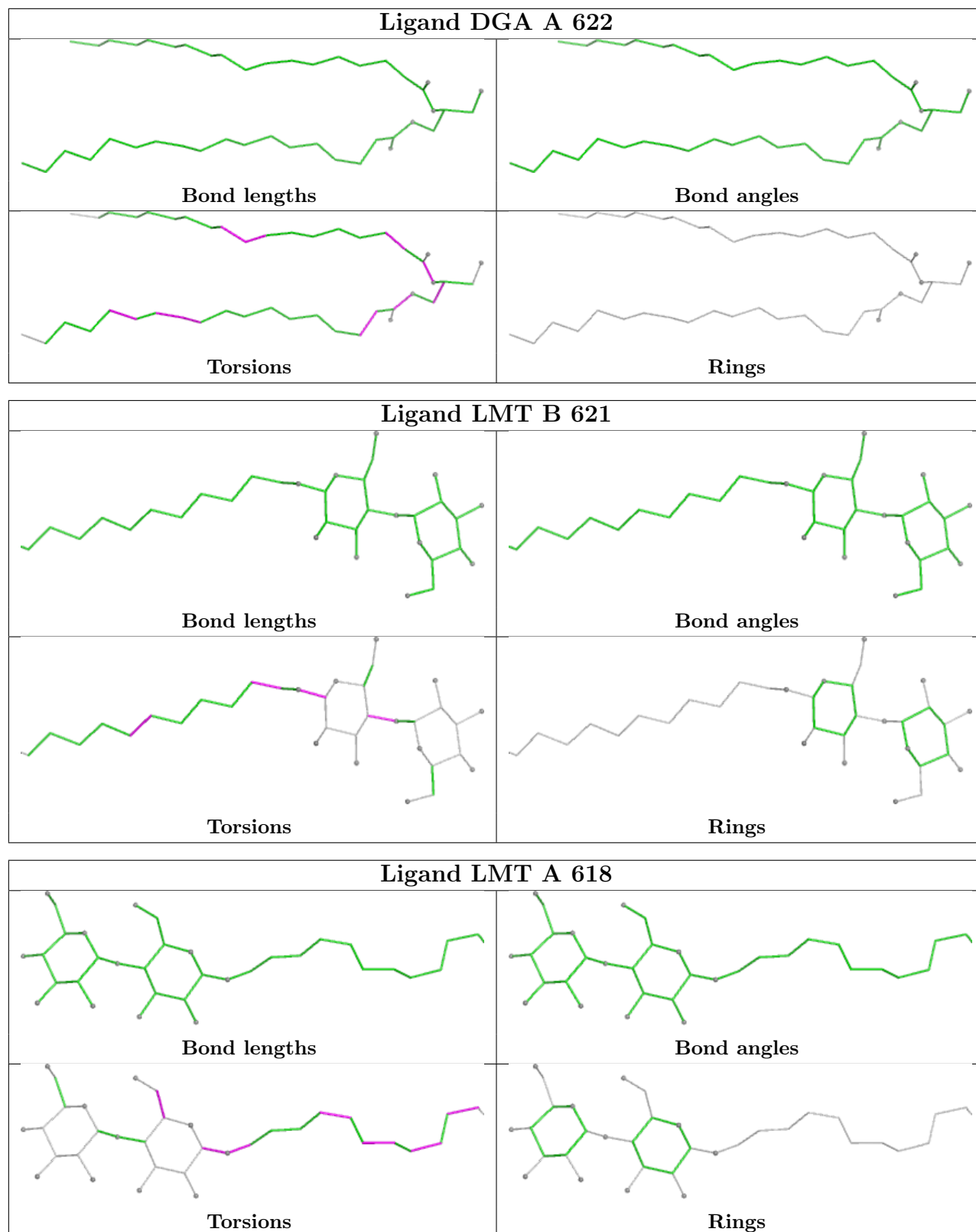
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	633	ERG	2	0
3	A	621	MYR	1	0
4	B	605	PLM	1	0
2	B	620	LMT	1	0
3	B	618	MYR	1	0
4	A	615	PLM	1	0

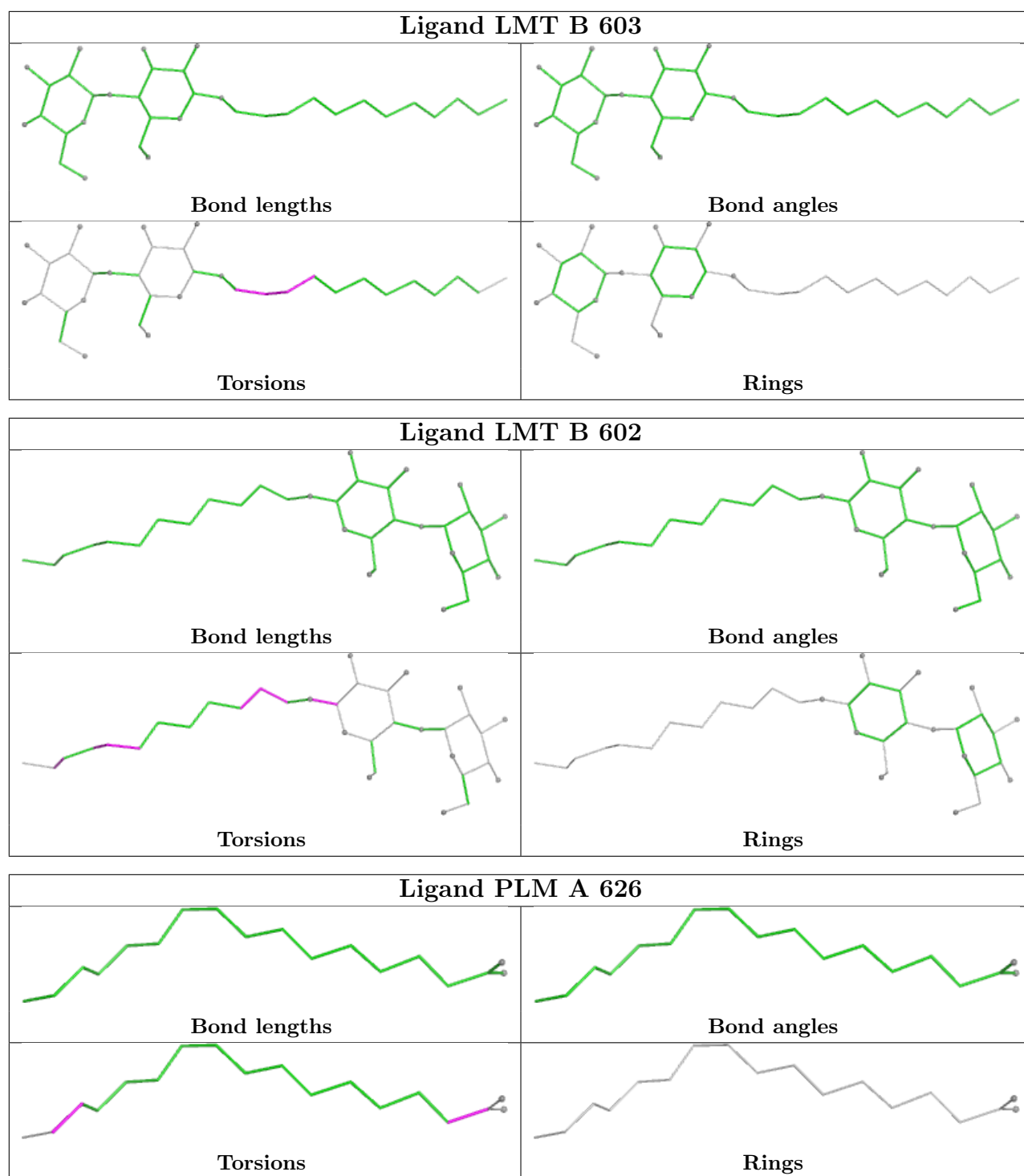
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

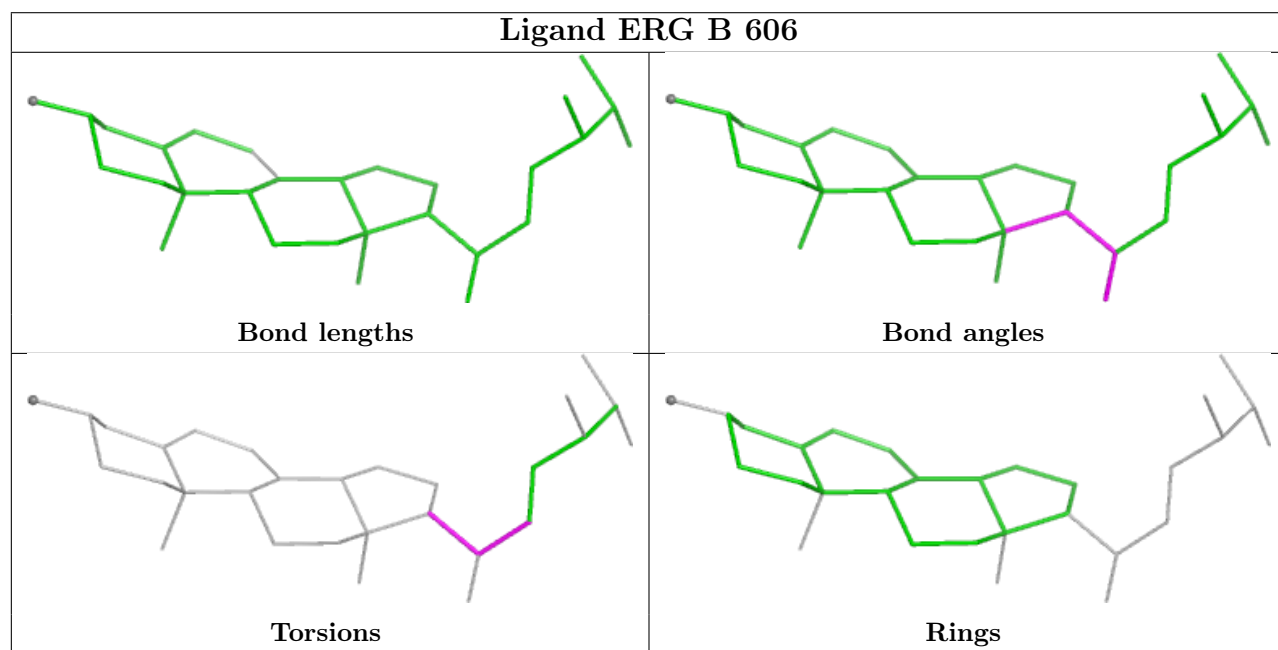
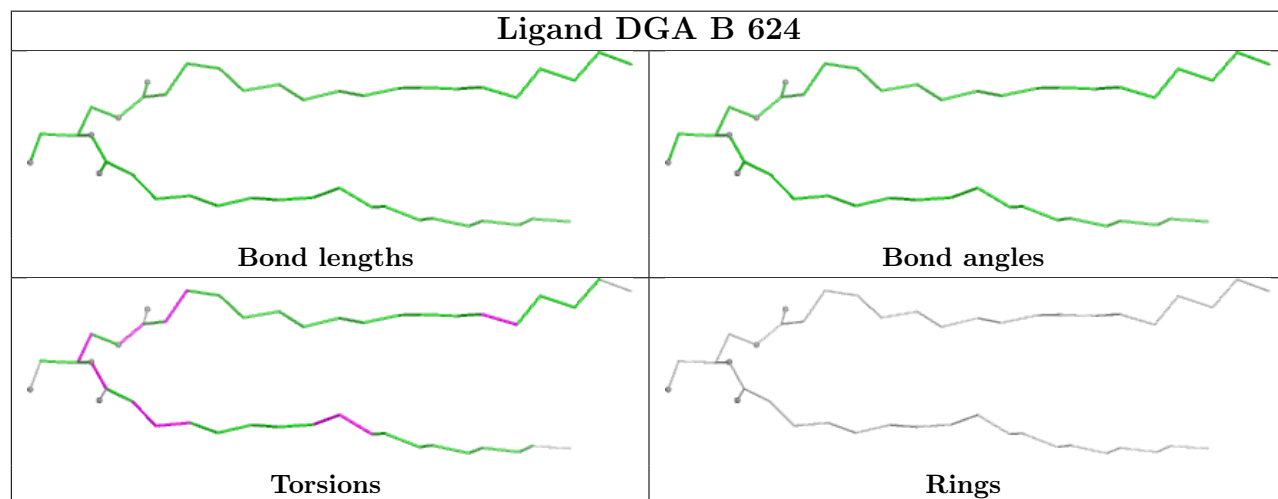
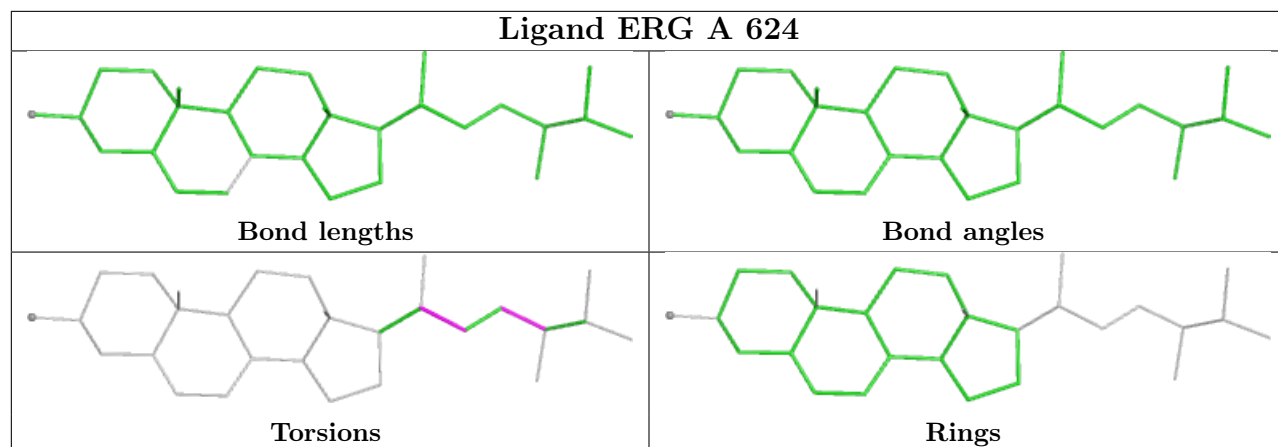


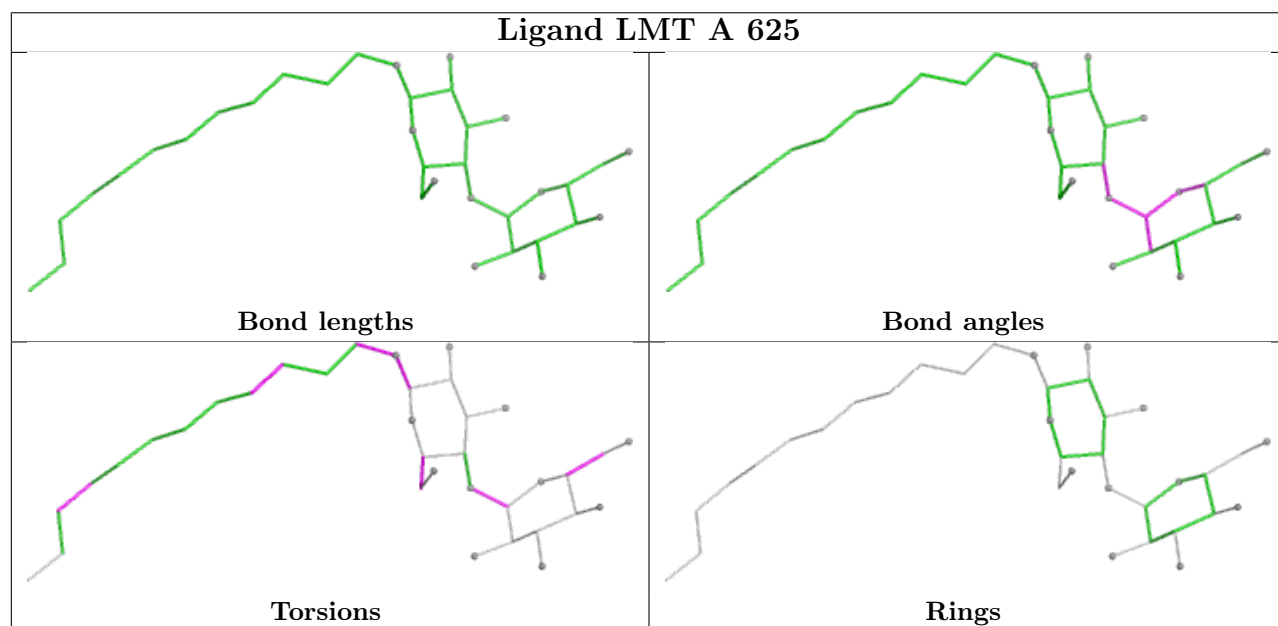
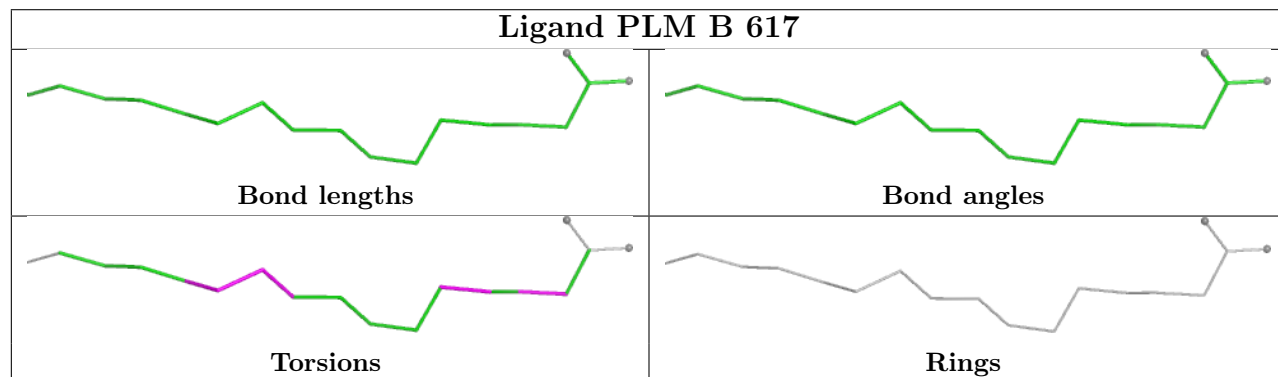
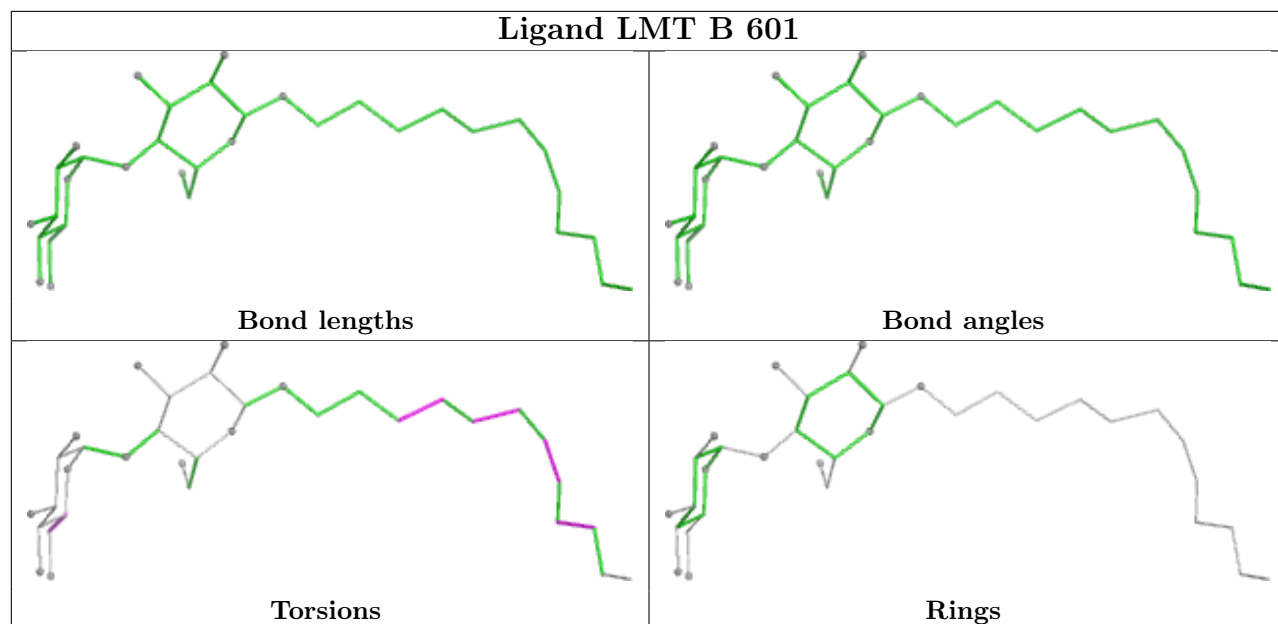


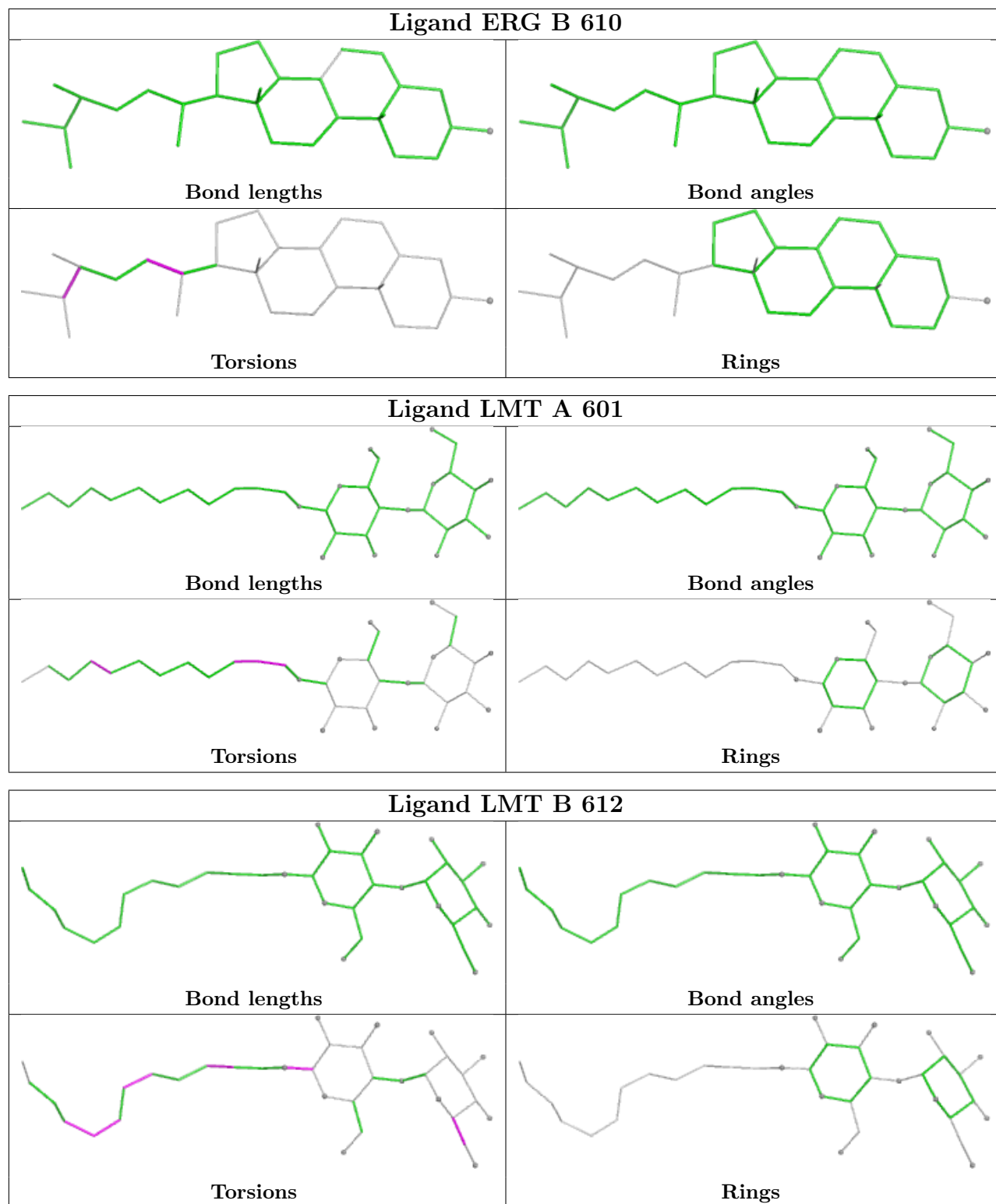


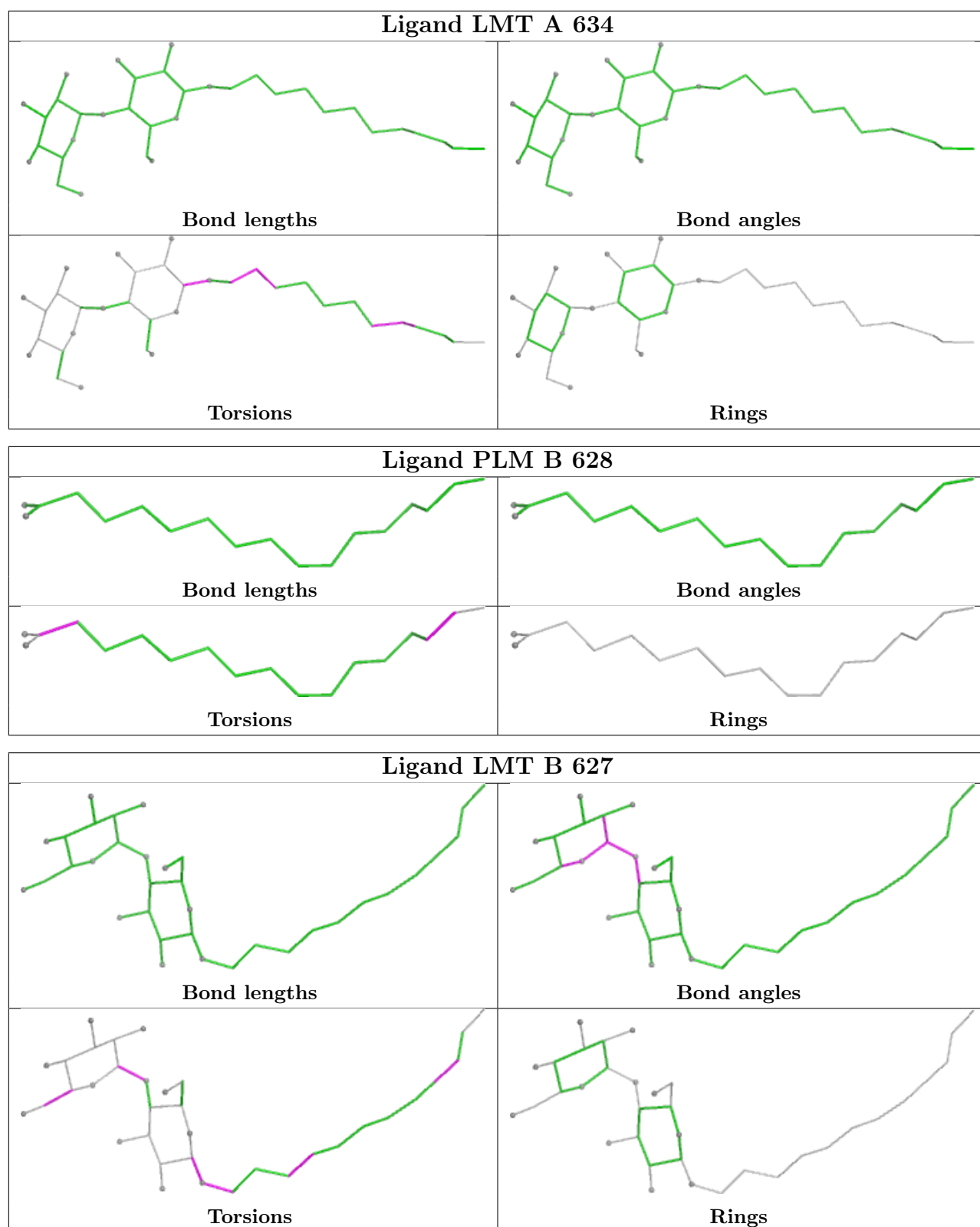


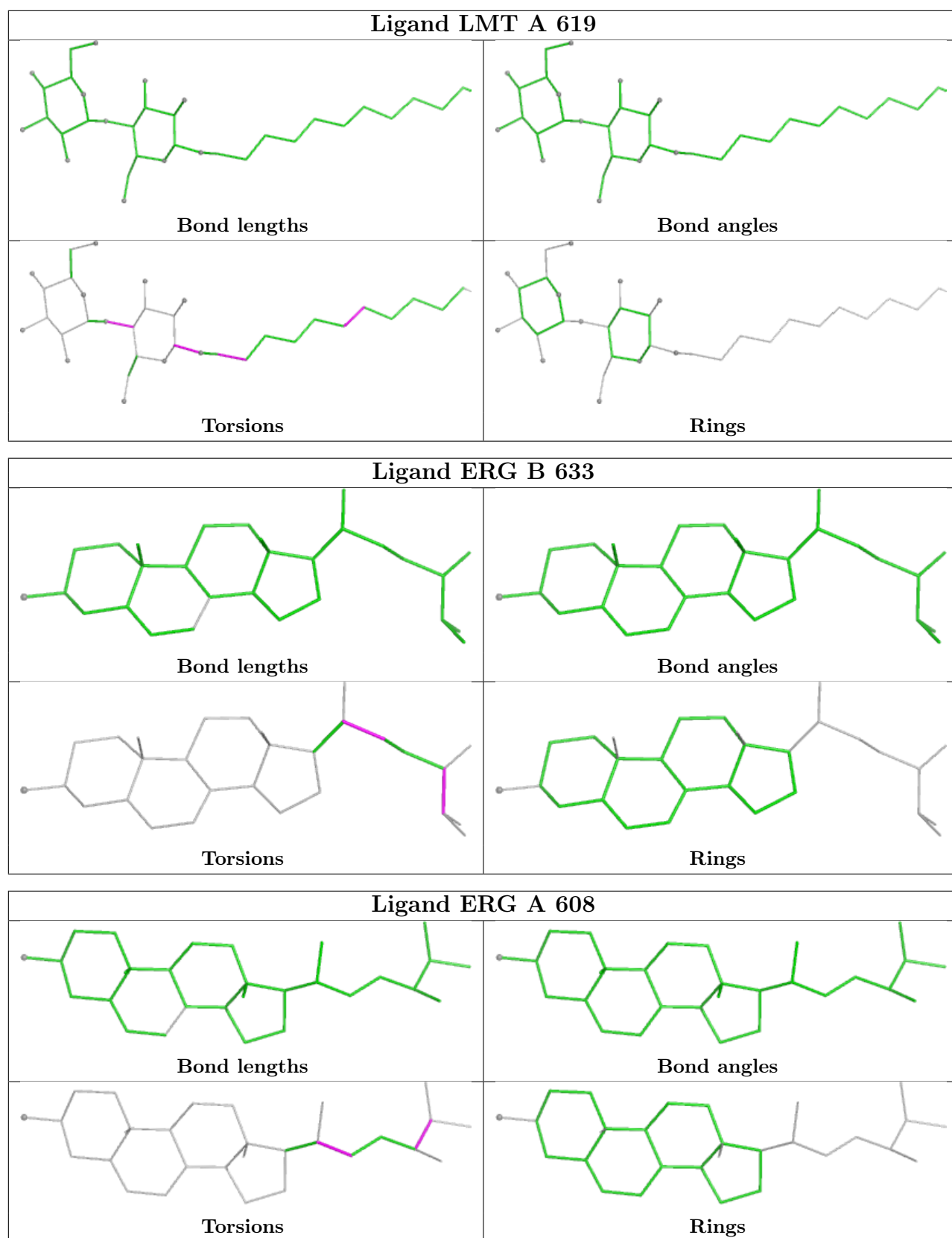


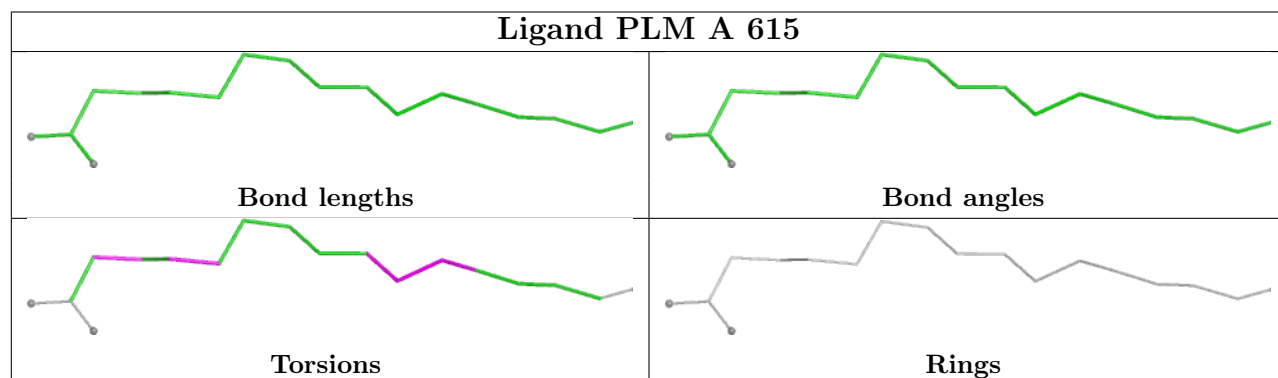
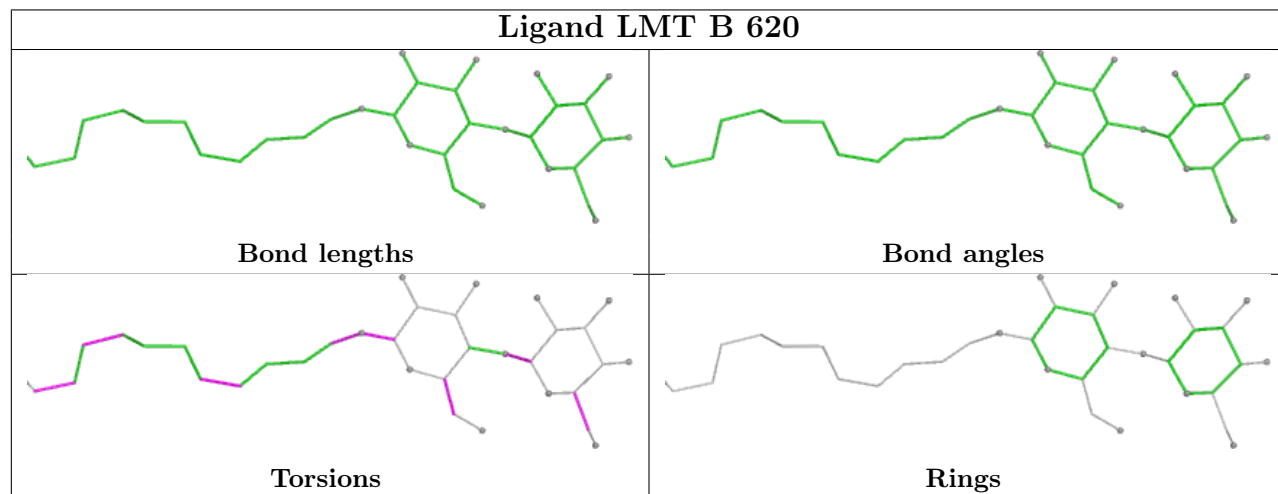
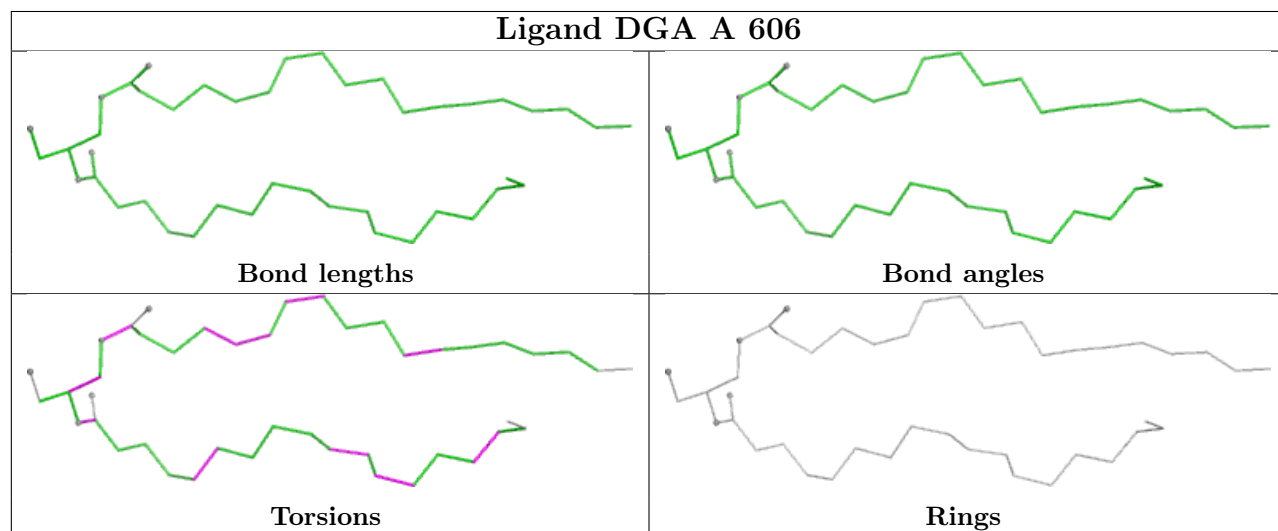
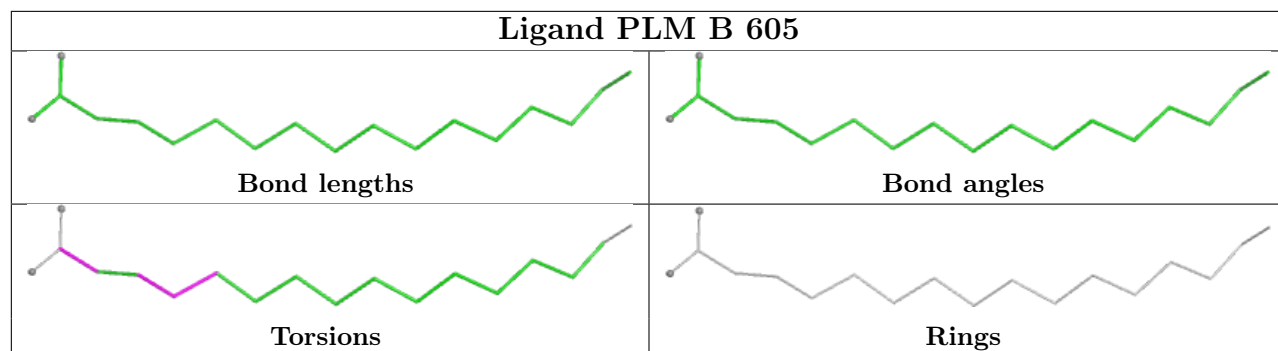












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

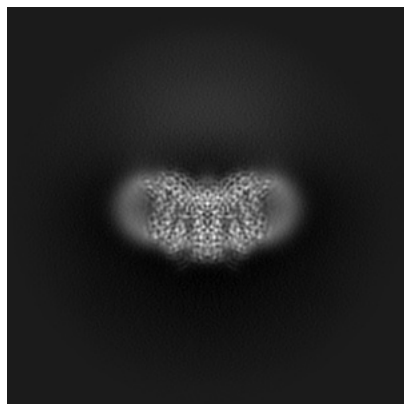
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-58351. These allow visual inspection of the internal detail of the map and identification of artifacts.

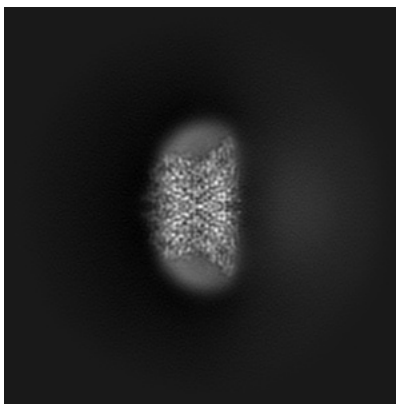
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

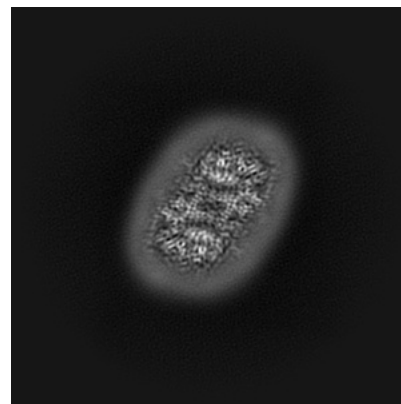
6.1.1 Primary map



X

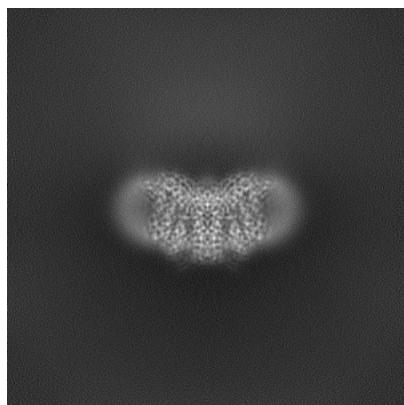


Y

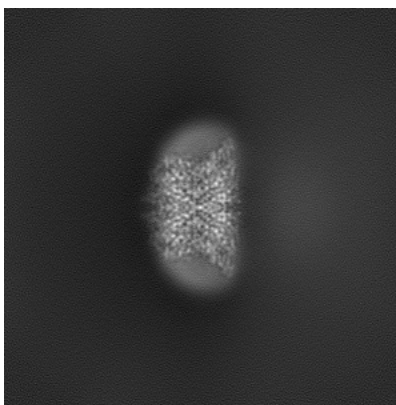


Z

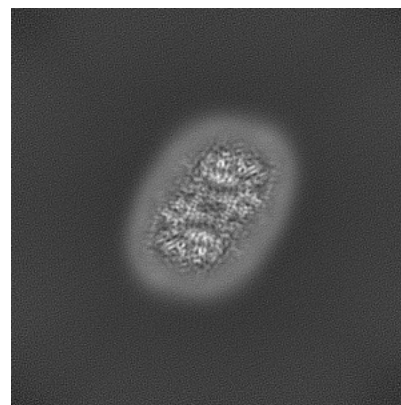
6.1.2 Raw map



X



Y

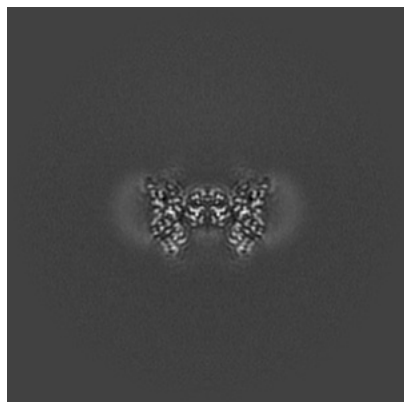


Z

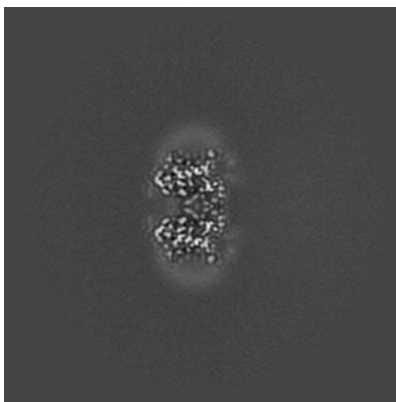
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

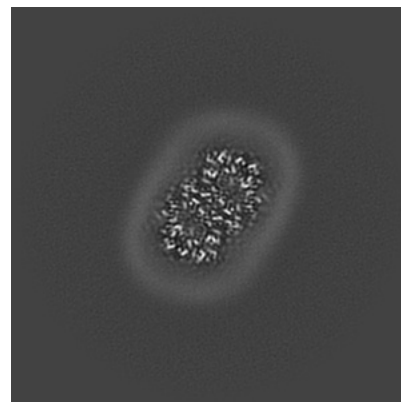
6.2.1 Primary map



X Index: 175

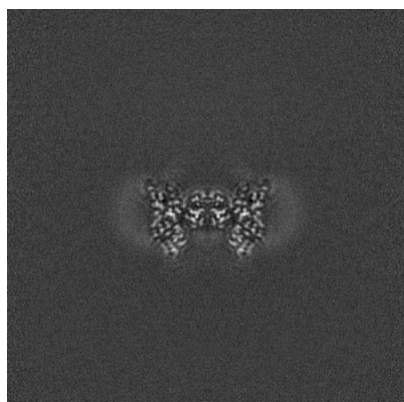


Y Index: 175

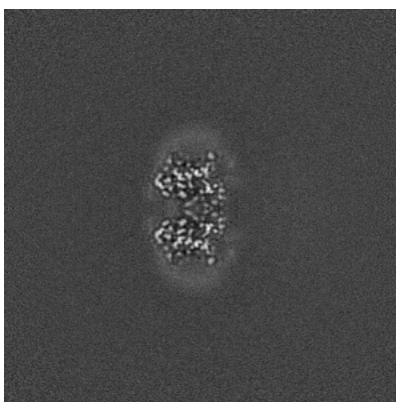


Z Index: 175

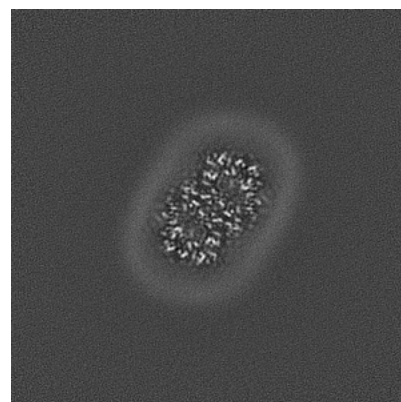
6.2.2 Raw map



X Index: 175



Y Index: 175

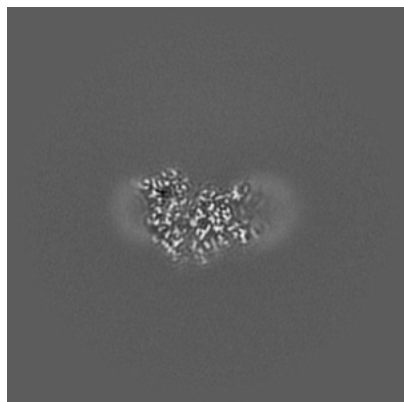


Z Index: 175

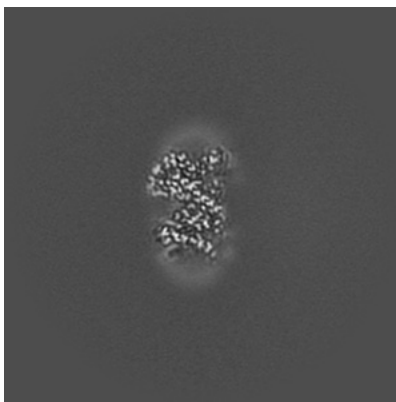
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

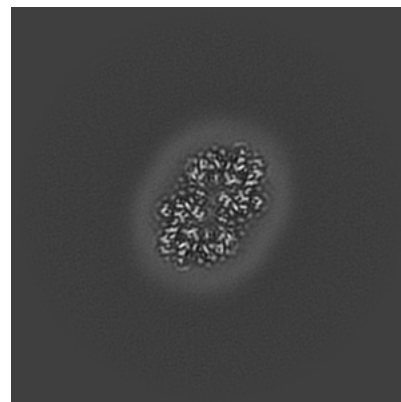
6.3.1 Primary map



X Index: 162

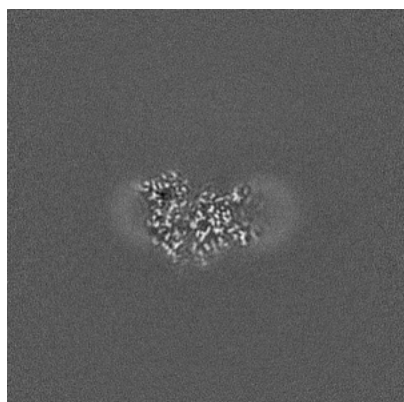


Y Index: 180

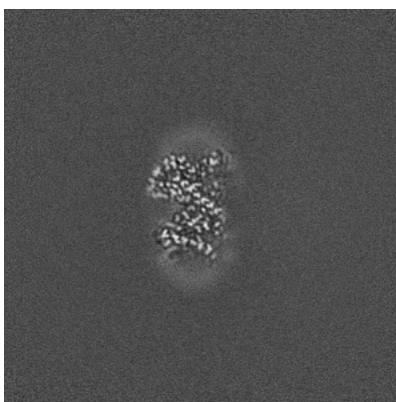


Z Index: 153

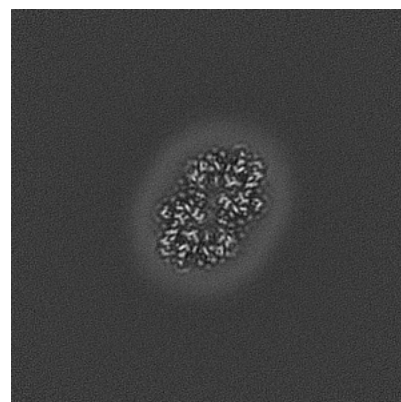
6.3.2 Raw map



X Index: 162



Y Index: 180

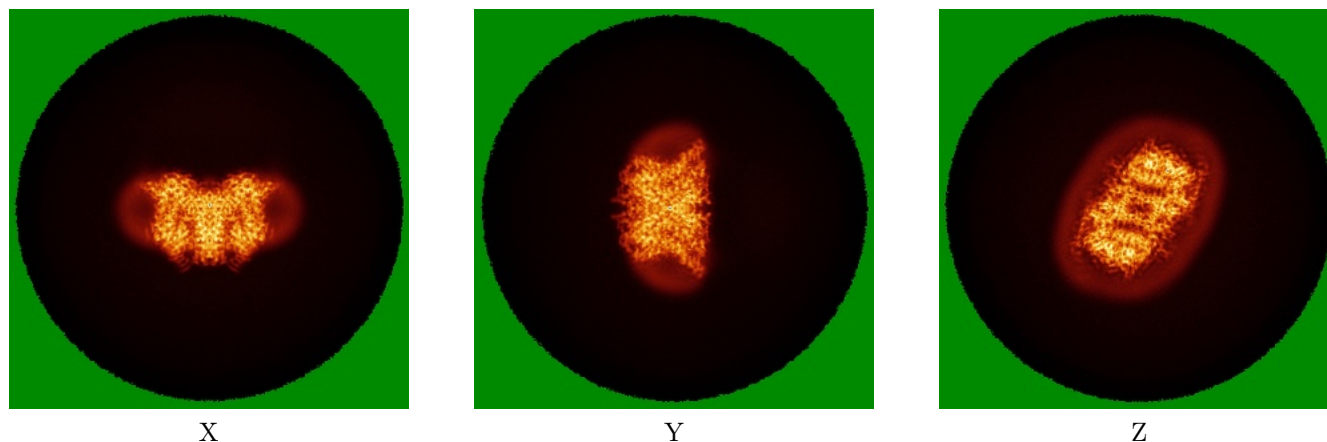


Z Index: 153

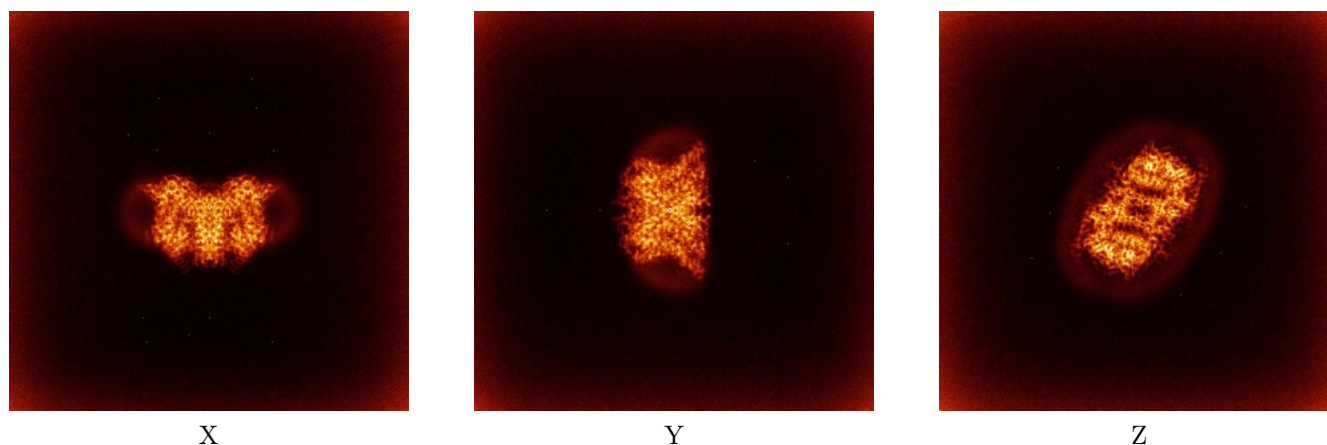
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



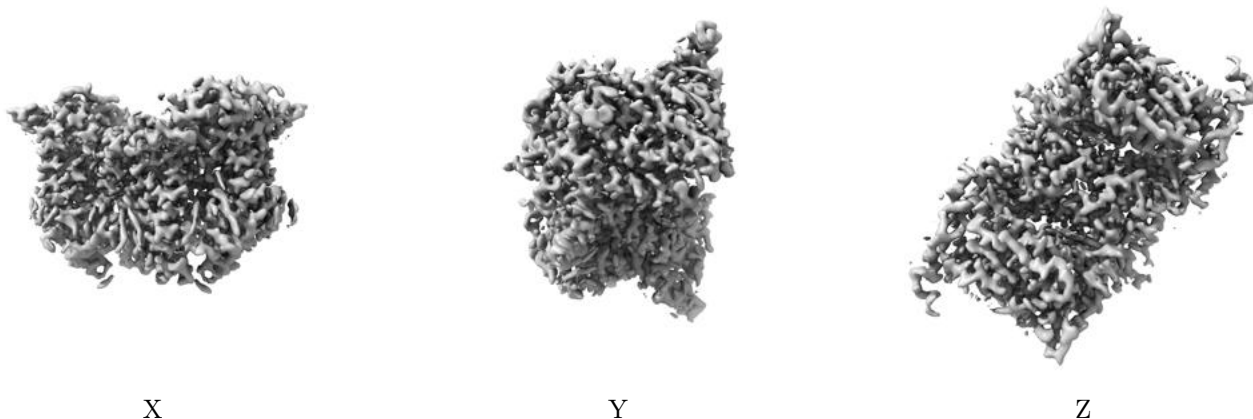
6.4.2 Raw map



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.

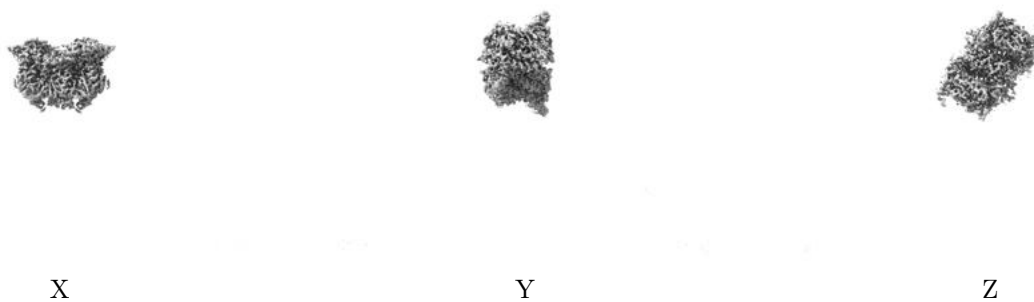
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.069. 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.

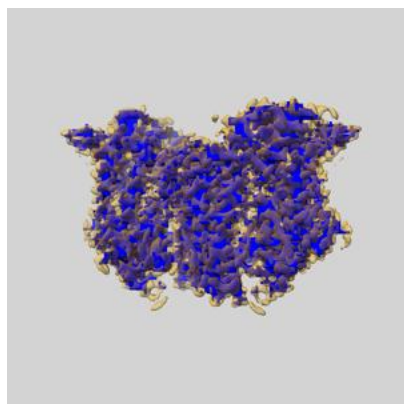
6.6 Mask visualisation [i](#)

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

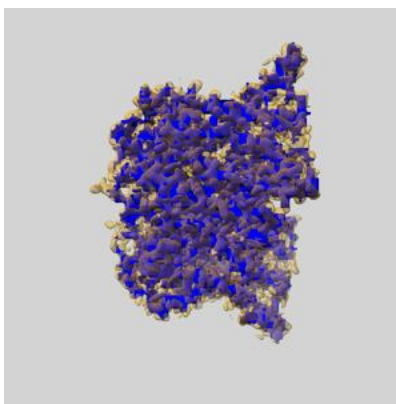
A mask typically either:

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

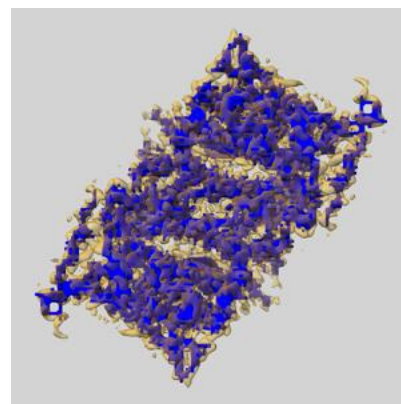
6.6.1 emd_58351_msk_1.map [i](#)



X



Y

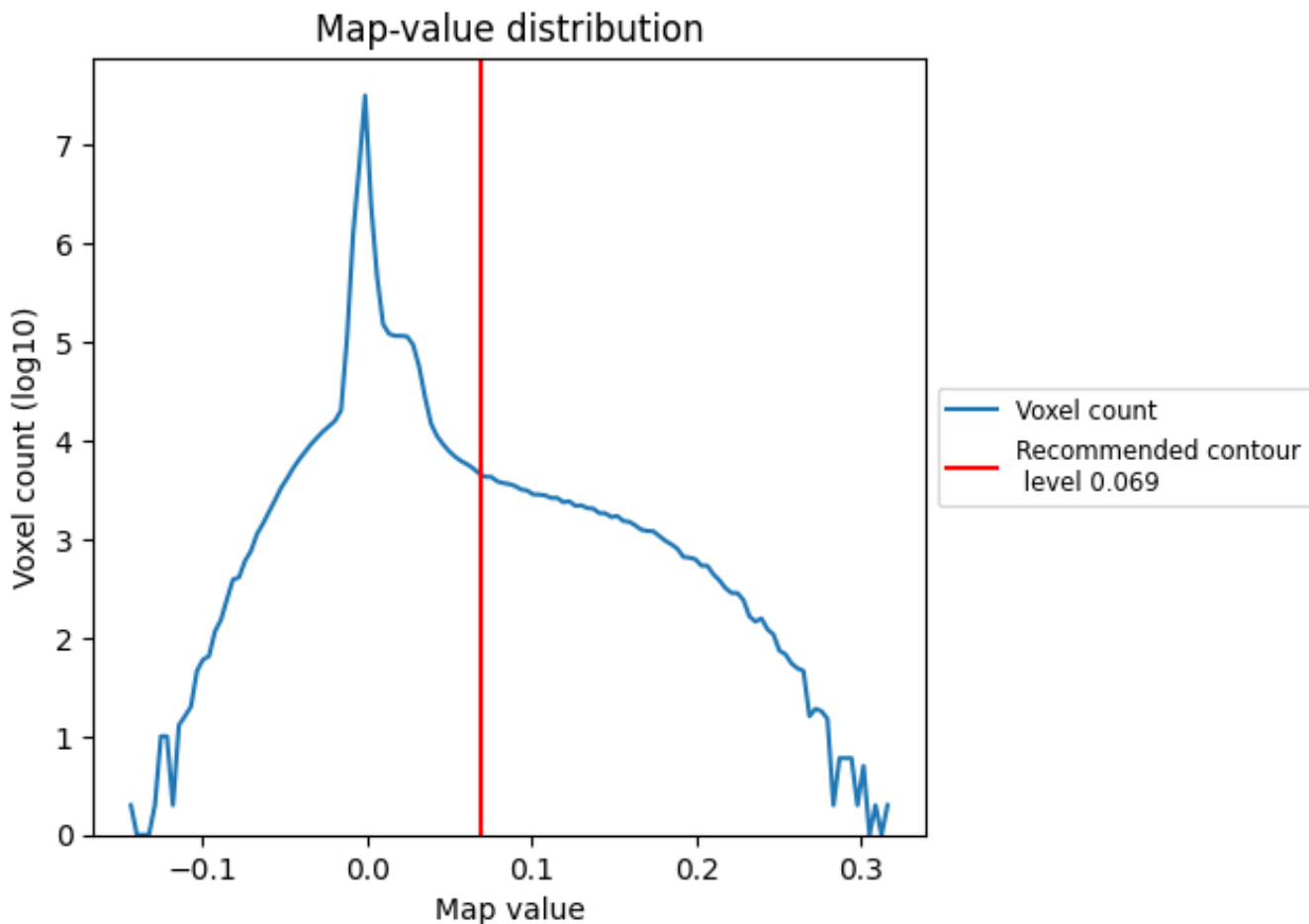


Z

7 Map analysis [i](#)

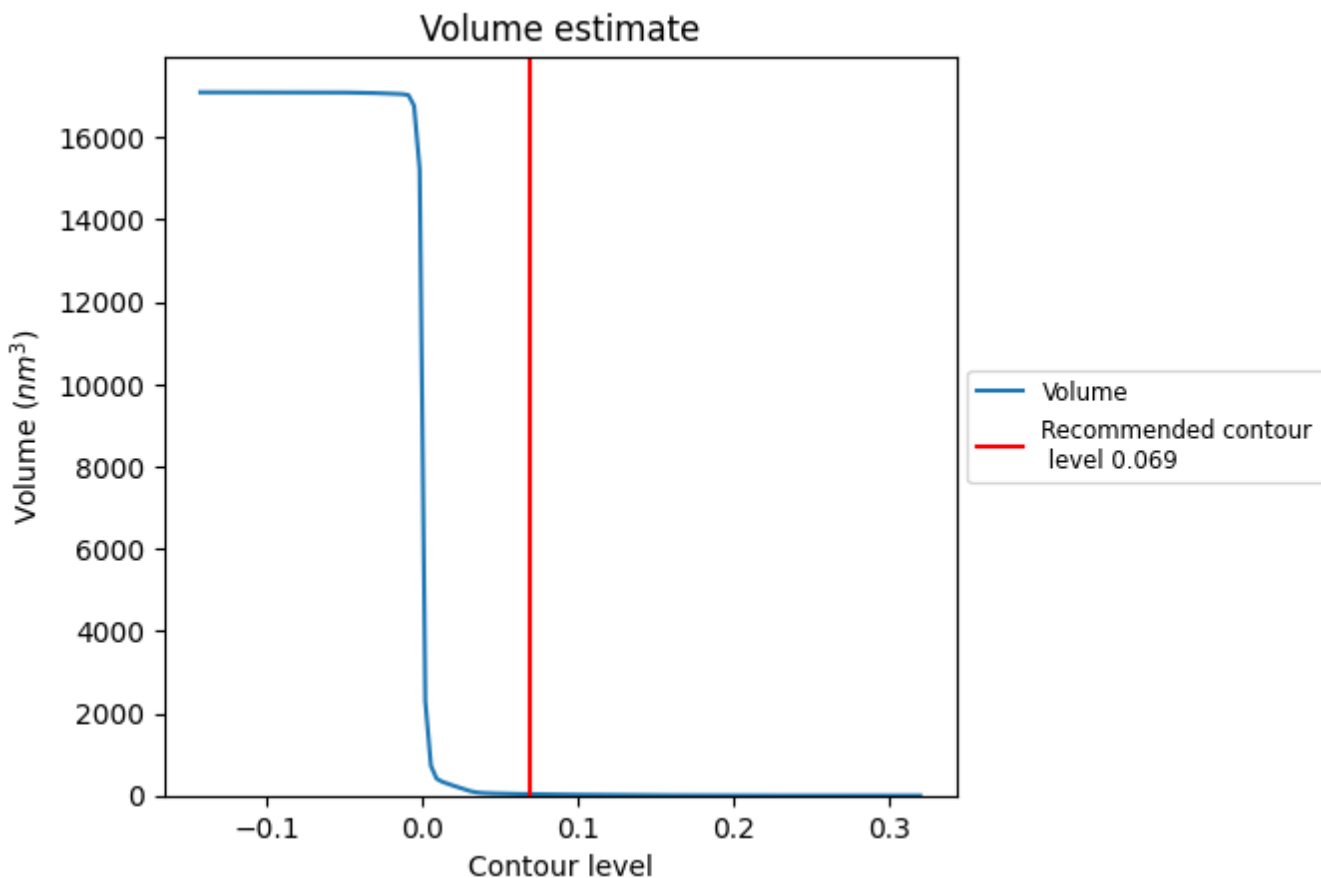
This section contains the results of statistical analysis of the map.

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.

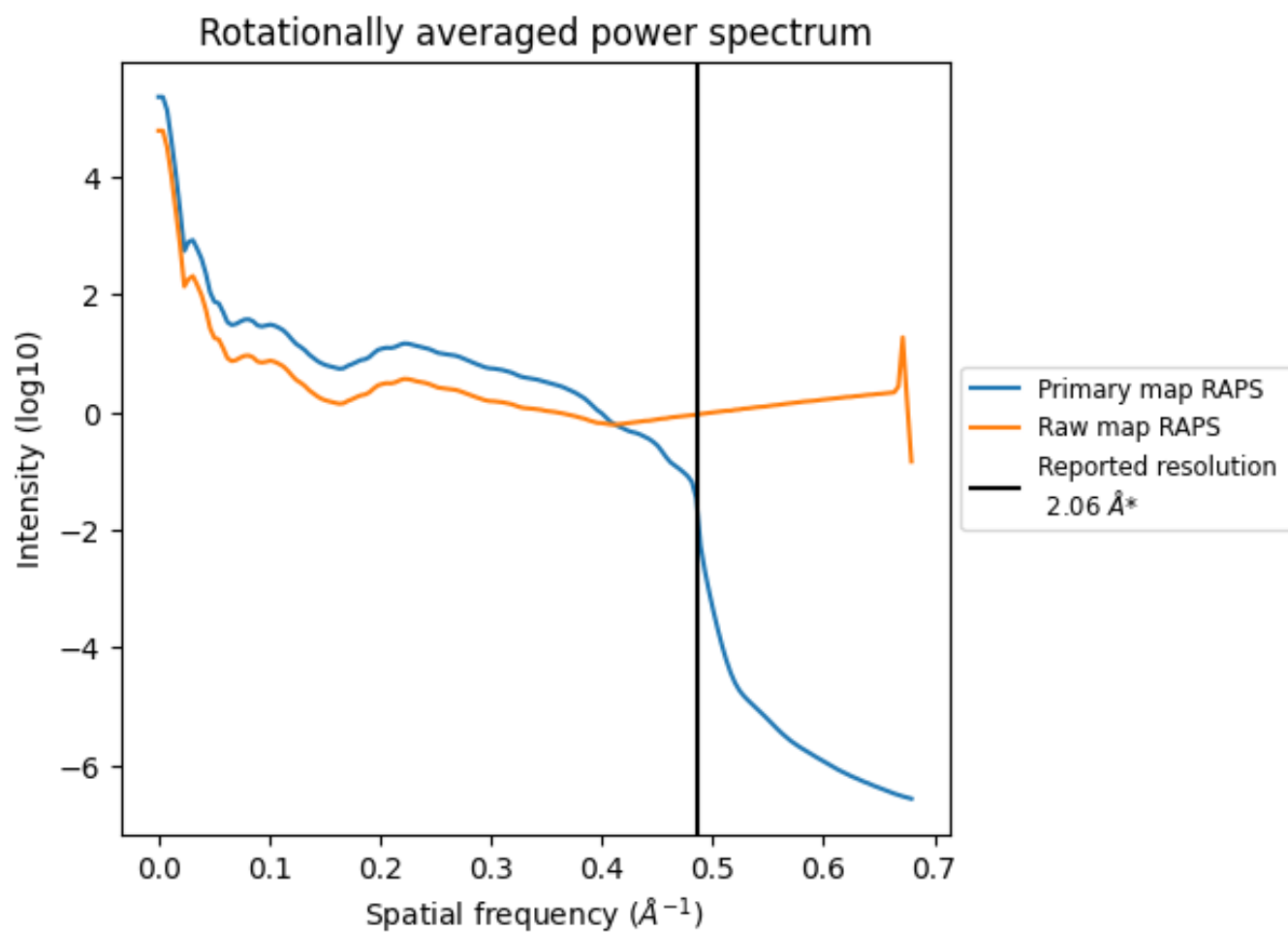
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm³; this corresponds to an approximate mass of 31 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 i

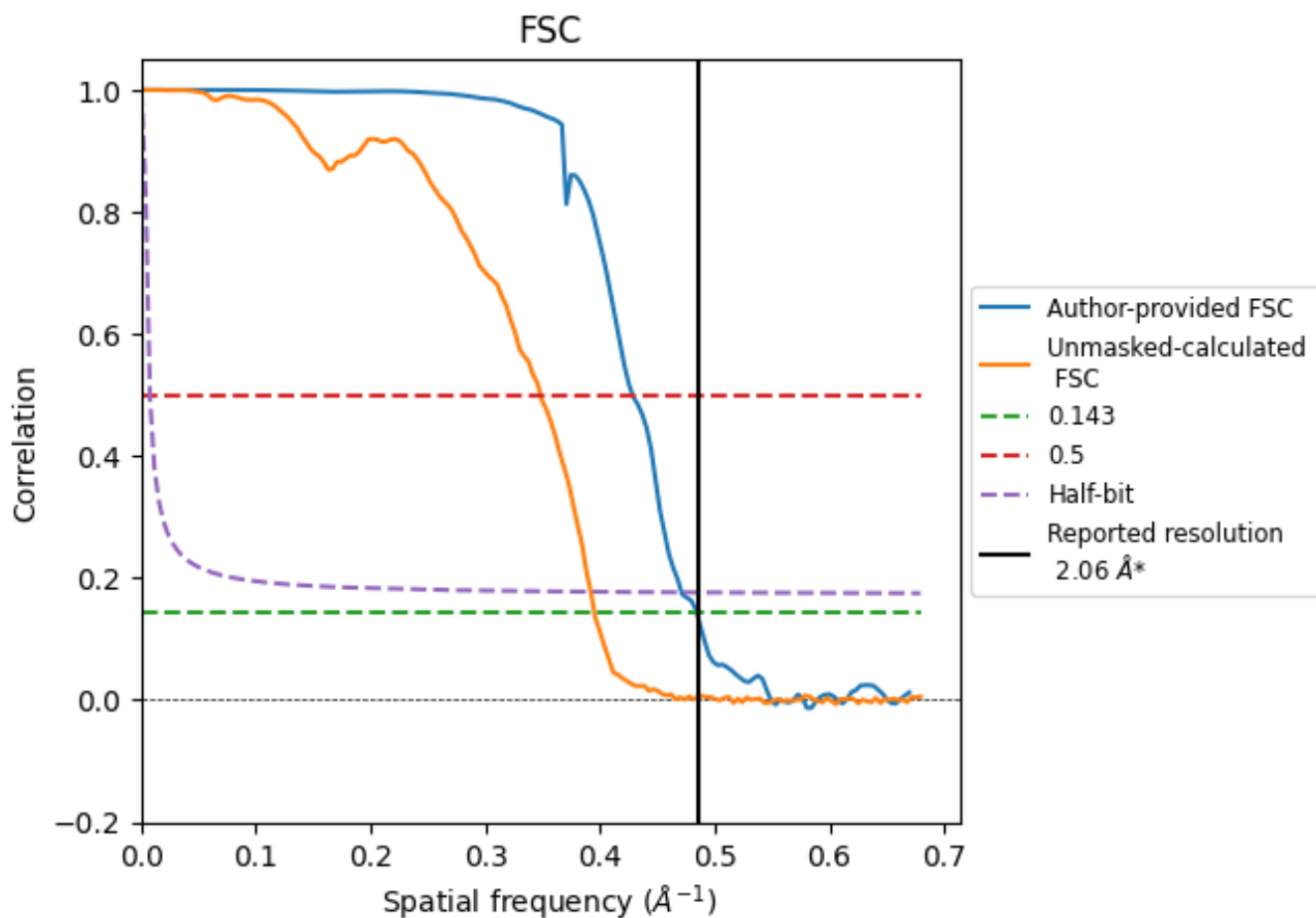


*Reported resolution corresponds to spatial frequency of 0.485 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.485 Å⁻¹

8.2 Resolution estimates [i](#)

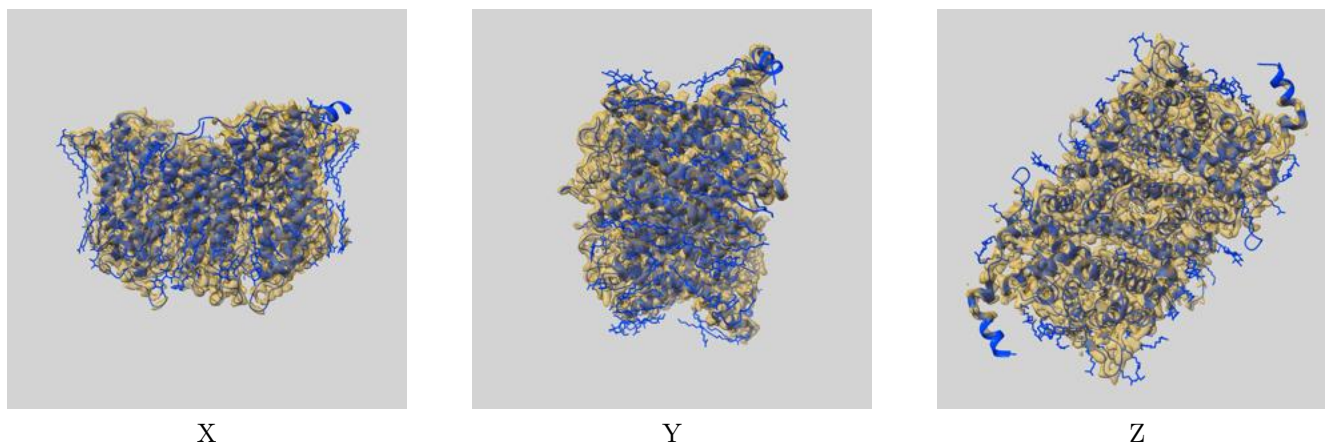
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.33	2.12
Unmasked-calculated*	2.53	2.87	2.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.53 differs from the reported value 2.06 by more than 10 %

9 Map-model fit [i](#)

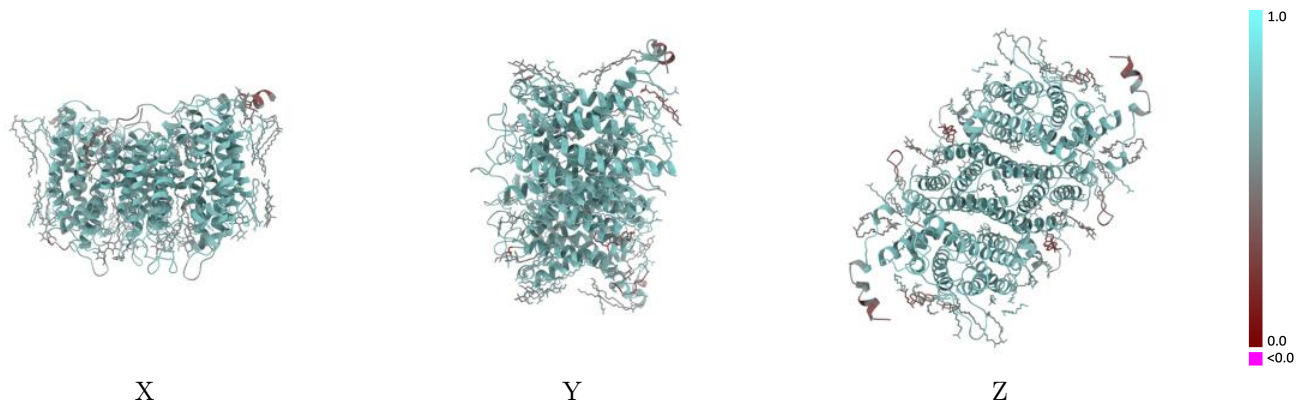
This section contains information regarding the fit between EMDB map EMD-58351 and PDB model 31EW. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



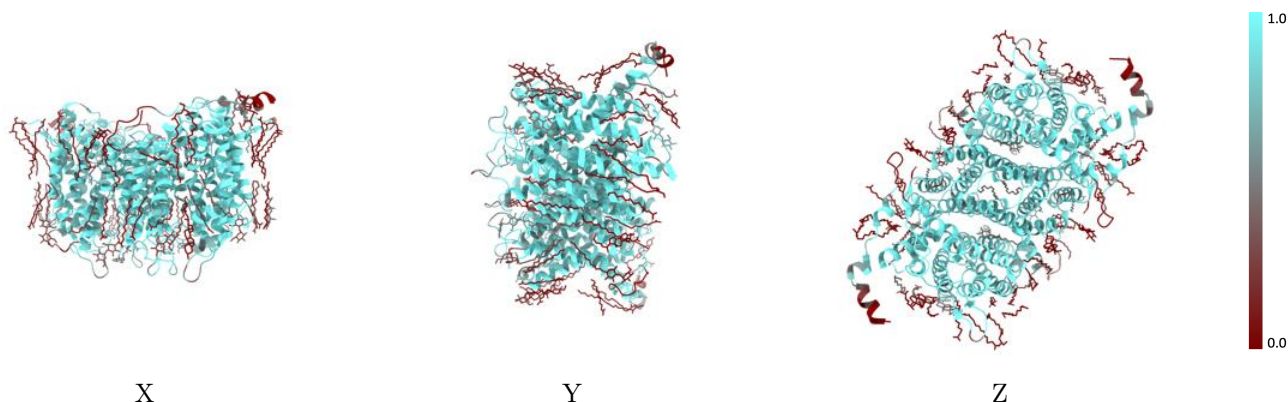
The images above show the 3D surface view of the map at the recommended contour level 0.069 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



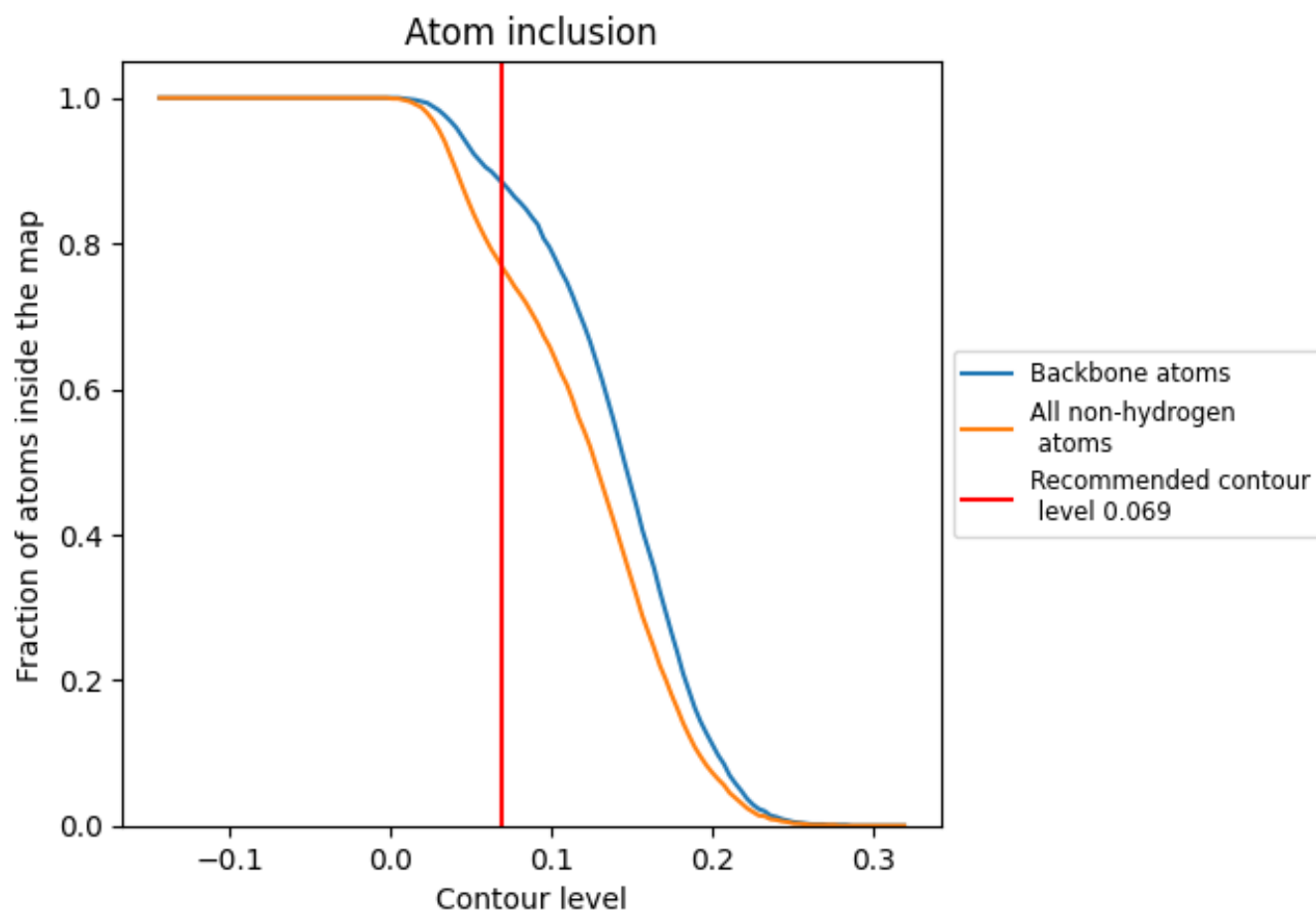
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.069).







9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.069) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.6650
A	 0.7730	 0.6640
B	 0.7710	 0.6650

