



# Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 05:21 pm BST

PDB ID : 8P7B  
EMDB ID : EMD-17528  
Title : CryoEM structure of METTL6 tRNA SerRS complex in a 1:2:2 stoichiometry  
Authors : Throll, P.; Dolce, L.G.; Kowalinski, E.  
Deposited on : 2023-05-30  
Resolution : 2.42 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

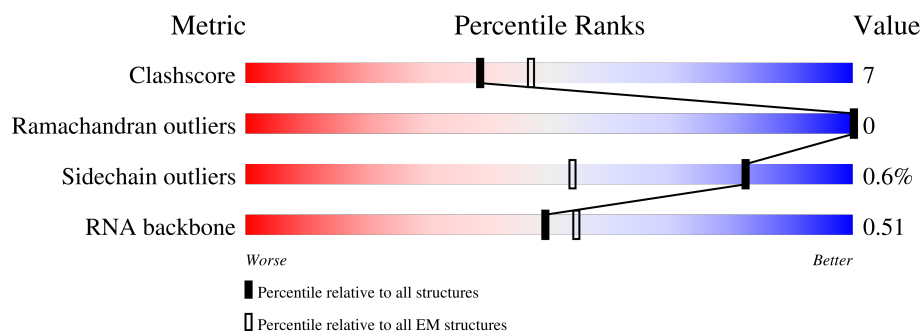
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.42 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	B	514	
1	D	514	
2	A	284	
3	T	85	
4	R	85	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12363 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 Serine-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	455	Total	C	N	O	S	0	0
			3540	2262	625	633	20		
1	D	448	Total	C	N	O	S	0	0
			3486	2226	616	626	18		

- Molecule 2 is a protein called tRNA N(3)-methylcytidine methyltransferase METTL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	239	Total	C	N	O	S	0	0
			1870	1217	315	329	9		

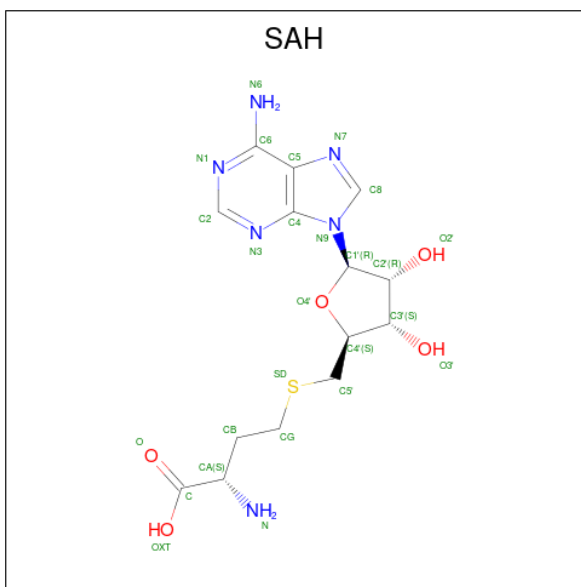
- Molecule 3 is a RNA chain called Serine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	78	Total	C	N	O	P	0	0
			1660	742	292	548	78		

- Molecule 4 is a RNA chain called Serine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	83	Total	C	N	O	P	0	0
			1773	796	311	583	83		

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	T	3	Total	Mg	0
			3	3	
6	R	3	Total	Mg	0
			3	3	

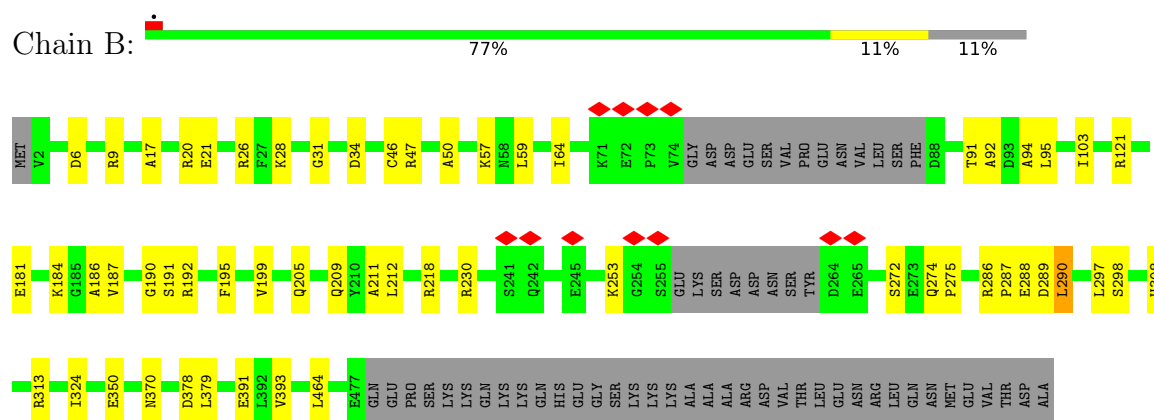
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	T	1	Total	O	0
			1	1	
7	R	1	Total	O	0
			1	1	

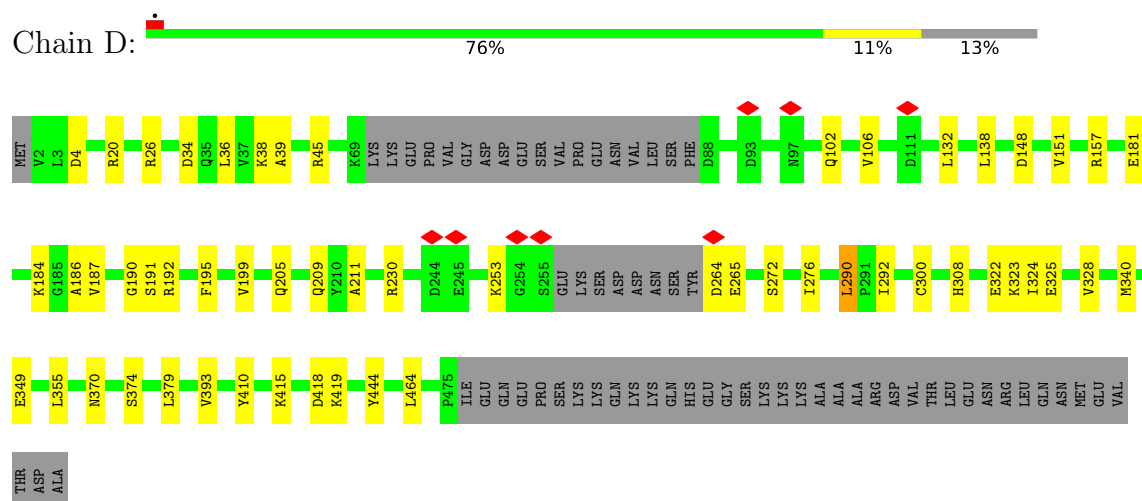
### 3 Residue-property plots

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: Serine–tRNA ligase, cytoplasmic

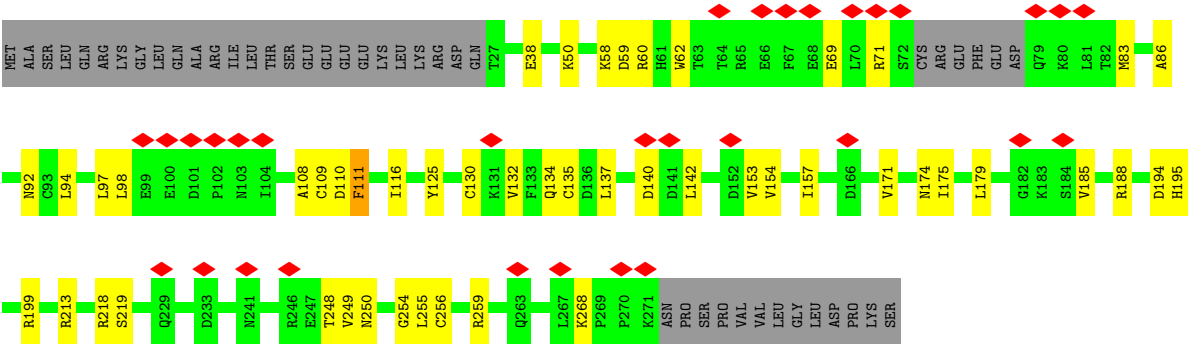


- Molecule 1: Serine–tRNA ligase, cytoplasmic

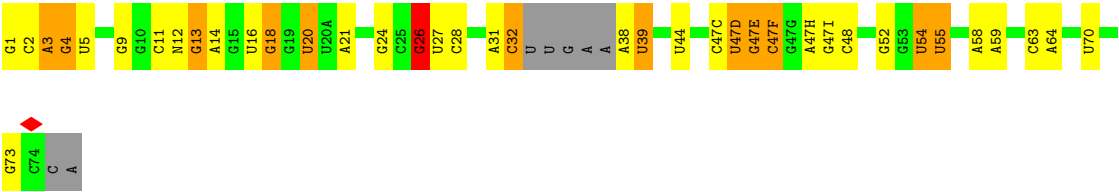


- Molecule 2: tRNA N(3)-methylcytidine methyltransferase METTL6

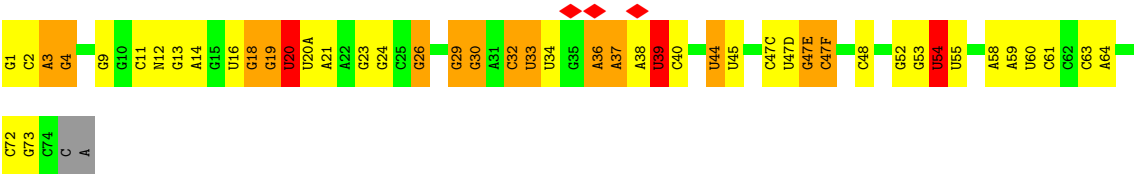




• Molecule 3: Serine tRNA



• Molecule 4: Serine tRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	460853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	63.27	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.531	Depositor
Minimum map value	-0.550	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	354.75, 354.75, 354.75	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.645, 0.645, 0.645	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: M2G, MG, H2U, 5MC, SAH, OMG, 5MU, PSU, JMH, 4AC, 6IA, 1MA, OMU

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	B	0.51	0/3610	0.49	0/4877
1	D	0.52	0/3555	0.53	0/4805
2	A	0.45	0/1919	0.56	0/2608
3	T	0.84	1/1609 (0.1%)	0.88	0/2502
4	R	0.82	0/1681	0.93	0/2612
All	All	0.61	1/12374 (0.0%)	0.66	0/17404

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	59	A	O3'-P	-5.19	1.54	1.61

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	B	3540	0	3490	36	0
1	D	3486	0	3414	34	0
2	A	1870	0	1752	35	0
3	T	1660	0	853	28	0
4	R	1773	0	905	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	26	0	19	3	0
6	R	3	0	0	0	0
6	T	3	0	0	0	0
7	R	1	0	0	0	0
7	T	1	0	0	0	0
All	All	12363	0	10433	155	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 7.

All (155) 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)
4:R:9:G:C8	4:R:12:4AC:HM72	2.09	0.87
4:R:26:M2G:HM23	4:R:44:OMU:O2	1.74	0.87
4:R:37:6IA:H3'	4:R:37:6IA:OP2	1.80	0.82
4:R:11:C:H2'	4:R:12:4AC:H6	1.61	0.81
2:A:249:VAL:HA	2:A:255:LEU:O	1.84	0.77
4:R:37:6IA:O4'	4:R:39:PSU:H1'	1.86	0.75
2:A:60:ARG:NH2	4:R:32:JMH:O2	2.21	0.73
1:D:157:ARG:NH1	1:D:349:GLU:OE2	2.23	0.72
1:D:290:LEU:O	1:D:292:ILE:N	2.22	0.71
4:R:9:G:N7	4:R:12:4AC:HM72	2.07	0.69
1:B:26:ARG:NH2	1:B:370:ASN:O	2.25	0.69
1:B:218:ARG:NH2	1:B:350:GLU:OE1	2.27	0.68
1:B:20:ARG:NH1	1:B:34:ASP:OD1	2.27	0.68
4:R:60:U:H5''	4:R:61:C:H5	1.58	0.66
4:R:12:4AC:H6	4:R:12:4AC:O5'	1.95	0.66
1:B:287:PRO:HA	1:B:290:LEU:HD23	1.79	0.64
1:D:26:ARG:NH2	1:D:370:ASN:O	2.31	0.64
1:B:287:PRO:O	1:B:290:LEU:HB2	1.98	0.64
4:R:36:A:N3	4:R:36:A:H5''	2.14	0.63
1:D:308:HIS:NE2	4:R:73:G:O6	2.30	0.63
4:R:26:M2G:CM2	4:R:44:OMU:O2	2.46	0.63
1:D:20:ARG:NH1	1:D:34:ASP:OD1	2.32	0.62
3:T:12:4AC:H2'	3:T:13:G:C8	2.34	0.62
1:B:199:VAL:HG12	1:B:464:LEU:HD21	1.81	0.61
1:B:64:ILE:HD11	1:B:103:ILE:HB	1.83	0.61
3:T:32:C:C5'	3:T:32:C:C6	2.84	0.60
1:D:379:LEU:HB3	1:D:393:VAL:HB	1.82	0.60
4:R:12:4AC:H2'	4:R:13:G:O4'	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:2:C:O2'	4:R:3:A:O5'	2.18	0.59
4:R:19:G:H4'	4:R:20:H2U:OP2	2.03	0.59
1:B:181:GLU:HB3	1:B:195:PHE:HB2	1.85	0.58
1:D:181:GLU:HB3	1:D:195:PHE:HB2	1.85	0.58
3:T:2:C:O2'	3:T:3:A:H8	1.87	0.58
1:B:230:ARG:NH1	1:D:187:VAL:O	2.36	0.57
3:T:12:4AC:H6	3:T:12:4AC:OP2	2.05	0.57
3:T:11:C:O2'	3:T:12:4AC:H5'	2.04	0.56
3:T:32:C:H6	3:T:32:C:O5'	1.89	0.56
2:A:59:ASP:OD1	2:A:92:ASN:ND2	2.39	0.55
1:B:253:LYS:HD2	4:R:1:G:H5'	1.87	0.55
3:T:38:A:P	3:T:38:A:C8	3.00	0.54
5:A:301:SAH:SD	4:R:32:JMH:C31	2.96	0.54
1:B:272:SER:HB3	1:B:298:SER:OG	2.07	0.53
2:A:60:ARG:HG2	4:R:33:U:H5''	1.90	0.53
2:A:199:ARG:CZ	4:R:37:6IA:H151	2.39	0.53
2:A:140:ASP:O	2:A:174:ASN:ND2	2.41	0.53
2:A:199:ARG:CZ	4:R:37:6IA:C15	2.87	0.53
4:R:48:5MC:C2	4:R:59:A:H1'	2.44	0.53
3:T:47(E):G:H2'	3:T:47(F):C:C6	2.43	0.52
1:B:17:ALA:O	1:B:21:GLU:HG3	2.10	0.52
2:A:50:LYS:HE2	4:R:47(E):G:P	2.50	0.52
2:A:259:ARG:NH2	4:R:32:JMH:OP1	2.43	0.52
1:B:205:GLN:O	1:B:209:GLN:HG2	2.10	0.52
2:A:199:ARG:NE	4:R:37:6IA:H151	2.24	0.52
1:D:211:ALA:HB3	1:D:324:ILE:HD12	1.90	0.52
1:D:323:LYS:NZ	1:D:325:GLU:OE1	2.43	0.52
2:A:179:LEU:HD23	2:A:268:LYS:HB2	1.92	0.52
2:A:83:MET:HG3	2:A:153:VAL:HG13	1.92	0.51
3:T:26:M2G:H8	3:T:26:M2G:H5''	1.74	0.50
2:A:110:ASP:O	2:A:134:GLN:HA	2.12	0.50
4:R:29:G:HO2'	4:R:30:G:H8	1.60	0.50
4:R:11:C:H2'	4:R:12:4AC:C6	2.37	0.50
1:D:36:LEU:HD11	1:D:132:LEU:HD13	1.94	0.49
1:B:91:THR:H	1:B:94:ALA:HB3	1.76	0.49
3:T:32:C:C6	3:T:32:C:H5''	2.47	0.49
3:T:31:A:H3'	3:T:32:C:H6	1.78	0.49
1:D:186:ALA:HA	1:D:190:GLY:O	2.13	0.49
1:B:211:ALA:HB3	1:B:324:ILE:HD12	1.95	0.49
2:A:195:HIS:ND1	4:R:37:6IA:H161	2.27	0.49
1:B:379:LEU:HB3	1:B:393:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:9:G:C5	4:R:12:4AC:HM72	2.47	0.48
2:A:157:ILE:O	5:A:301:SAH:N	2.46	0.48
1:B:187:VAL:O	1:D:230:ARG:NH1	2.44	0.48
1:B:191:SER:O	1:B:192:ARG:HB2	2.14	0.48
1:B:59:LEU:HD21	1:B:92:ALA:HA	1.96	0.48
1:B:313:ARG:NH1	3:T:70:U:OP2	2.47	0.47
1:D:181:GLU:HG3	1:D:184:LYS:HB2	1.96	0.47
1:D:308:HIS:HE1	4:R:73:G:N7	2.13	0.47
2:A:108:ALA:HB3	2:A:132:VAL:HA	1.96	0.47
4:R:39:PSU:H2'	4:R:40:C:C6	2.49	0.47
3:T:2:C:O2'	3:T:3:A:O5'	2.30	0.47
3:T:47(E):G:O2'	3:T:47(F):C:O5'	2.32	0.47
2:A:86:ALA:HB1	2:A:137:LEU:HD11	1.97	0.46
1:B:308:HIS:NE2	3:T:73:G:N7	2.60	0.46
2:A:97:LEU:C	2:A:97:LEU:HD12	2.35	0.46
4:R:53:G:C5	4:R:54:5MU:H72	2.50	0.46
3:T:12:4AC:H2'	3:T:13:G:H8	1.79	0.46
3:T:26:M2G:H5''	3:T:26:M2G:C8	2.50	0.46
1:D:102:GLN:O	1:D:106:VAL:HG23	2.16	0.46
1:B:46:CYS:SG	1:B:121:ARG:HB2	2.56	0.46
3:T:27:U:H2'	3:T:28:C:C6	2.50	0.46
3:T:32:C:H2'	3:T:32:C:O2	2.15	0.45
4:R:29:G:O2'	4:R:30:G:H8	1.98	0.45
1:B:47:ARG:NH1	1:B:50:ALA:HB3	2.31	0.45
2:A:110:ASP:HB3	2:A:116:ILE:HD11	1.98	0.45
2:A:94:LEU:O	2:A:98:LEU:HB2	2.16	0.45
3:T:63:C:H2'	3:T:64:A:C8	2.52	0.45
1:D:272:SER:O	1:D:276:ILE:HG12	2.17	0.45
1:D:415:LYS:HB2	1:D:418:ASP:HB3	1.98	0.45
4:R:47(E):G:H2'	4:R:47(F):C:C6	2.51	0.45
1:D:199:VAL:HG12	1:D:464:LEU:HD11	1.99	0.45
1:D:355:LEU:O	1:D:444:TYR:OH	2.21	0.45
2:A:60:ARG:NH1	5:A:301:SAH:OXT	2.50	0.45
3:T:38:A:C8	3:T:38:A:OP2	2.70	0.44
4:R:37:6IA:C4'	4:R:39:PSU:H1'	2.47	0.44
1:D:290:LEU:O	1:D:290:LEU:HD12	2.17	0.44
4:R:63:C:H2'	4:R:64:A:C8	2.52	0.44
1:B:212:LEU:HD11	1:B:297:LEU:HD22	2.00	0.44
2:A:109:CYS:SG	2:A:135:CYS:HB3	2.58	0.43
4:R:47(E):G:H2'	4:R:47(F):C:H6	1.82	0.43
2:A:142:LEU:HD11	2:A:175:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:32:C:C6	3:T:32:C:O5'	2.70	0.43
4:R:60:U:H5''	4:R:61:C:C5	2.46	0.43
1:B:378:ASP:OD2	1:B:391:GLU:HG3	2.19	0.43
1:D:191:SER:O	1:D:192:ARG:HB2	2.19	0.43
1:D:264:ASP:OD1	1:D:265:GLU:N	2.48	0.43
1:B:288:GLU:O	1:B:289:ASP:HB2	2.19	0.43
1:B:31:GLY:HA2	1:B:34:ASP:OD2	2.19	0.43
1:B:57:LYS:HB3	1:B:57:LYS:HE2	1.79	0.43
1:B:274:GLN:HB2	1:B:275:PRO:HD3	2.01	0.43
1:D:205:GLN:O	1:D:209:GLN:HG2	2.19	0.43
1:D:264:ASP:CG	1:D:265:GLU:H	2.22	0.43
2:A:154:VAL:HG13	2:A:185:VAL:HG23	2.00	0.43
3:T:63:C:H2'	3:T:64:A:H8	1.83	0.43
1:D:148:ASP:OD2	1:D:151:VAL:HG12	2.19	0.42
2:A:137:LEU:HB3	2:A:171:VAL:HG13	2.01	0.42
2:A:58:LYS:HB2	4:R:33:U:O4'	2.19	0.42
2:A:194:ASP:OD1	2:A:195:HIS:N	2.53	0.42
3:T:47(D):U:H5''	3:T:47(E):G:C8	2.54	0.42
2:A:62:TRP:CH2	2:A:188:ARG:HD2	2.55	0.42
1:B:181:GLU:HG3	1:B:184:LYS:HB2	2.02	0.41
2:A:213:ARG:NH2	2:A:219:SER:OG	2.53	0.41
2:A:38:GLU:HA	2:A:218:ARG:HH12	1.85	0.41
1:B:272:SER:O	1:B:275:PRO:HD2	2.20	0.41
1:D:290:LEU:HD13	1:D:290:LEU:HA	1.72	0.41
1:B:28:LYS:HA	1:B:28:LYS:HD3	1.88	0.41
3:T:3:A:O2'	3:T:4:G:O5'	2.28	0.41
1:D:4:ASP:OD2	1:D:419:LYS:NZ	2.53	0.41
1:B:59:LEU:HD22	1:B:95:LEU:HD12	2.02	0.41
1:B:186:ALA:HA	1:B:190:GLY:O	2.21	0.41
1:D:38:LYS:HG3	1:D:39:ALA:N	2.36	0.41
2:A:69:GLU:C	2:A:71:ARG:H	2.23	0.41
1:D:138:LEU:O	1:D:374:SER:HB2	2.20	0.41
1:D:253:LYS:HD2	3:T:1:G:H5'	2.03	0.41
1:D:300:CYS:SG	1:D:323:LYS:HE3	2.61	0.41
1:D:328:VAL:HG11	1:D:340:MET:HG2	2.02	0.41
2:A:248:THR:O	2:A:256:CYS:HA	2.20	0.41
3:T:38:A:P	3:T:38:A:O4'	2.79	0.41
1:B:286:ARG:HA	1:B:287:PRO:HD3	1.90	0.41
2:A:125:TYR:CE1	2:A:130:CYS:HB2	2.56	0.40
1:B:6:ASP:OD1	1:B:9:ARG:NH1	2.55	0.40
2:A:111:PHE:HA	2:A:134:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:250:ASN:O	2:A:254:GLY:N	2.55	0.40
1:D:290:LEU:HD23	1:D:410:TYR:CE1	2.56	0.40
4:R:3:A:O2'	4:R:4:G:O5'	2.34	0.40
3:T:4:G:H2'	3:T:5:U:C6	2.56	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	B	449/514 (87%)	437 (97%)	12 (3%)	0	100	100
1	D	442/514 (86%)	430 (97%)	12 (3%)	0	100	100
2	A	235/284 (83%)	224 (95%)	11 (5%)	0	100	100
All	All	1126/1312 (86%)	1091 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	B	363/453 (80%)	362 (100%)	1 (0%)	91	96
1	D	355/453 (78%)	352 (99%)	3 (1%)	79	89
2	A	189/262 (72%)	188 (100%)	1 (0%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	907/1168 (78%)	902 (99%)	5 (1%)	82	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	290	LEU
1	D	45	ARG
1	D	290	LEU
1	D	322	GLU
2	A	111	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	235	GLN
1	B	303	GLN
1	B	353	GLN
1	B	424	HIS
1	D	131	ASN
2	A	42	GLN
2	A	92	ASN
2	A	209	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	T	75/85 (88%)	21 (28%)	5 (6%)
4	R	79/85 (92%)	25 (31%)	4 (5%)
All	All	154/170 (90%)	46 (29%)	9 (5%)

All (46) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	3	A
3	T	4	G
3	T	9	G
3	T	13	G
3	T	14	A
3	T	16	U

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Mol	Chain	Res	Type
3	T	18	OMG
3	T	20	H2U
3	T	21	A
3	T	24	G
3	T	26	M2G
3	T	32	C
3	T	39	PSU
3	T	47(C)	C
3	T	47(D)	U
3	T	47(E)	G
3	T	47(F)	C
3	T	47(I)	G
3	T	52	G
3	T	54	5MU
3	T	55	PSU
4	R	3	A
4	R	4	G
4	R	14	A
4	R	16	U
4	R	18	OMG
4	R	19	G
4	R	20	H2U
4	R	20(A)	U
4	R	21	A
4	R	23	G
4	R	24	G
4	R	29	G
4	R	30	G
4	R	33	U
4	R	34	U
4	R	36	A
4	R	38	A
4	R	39	PSU
4	R	45	U
4	R	47(C)	C
4	R	47(D)	U
4	R	47(F)	C
4	R	52	G
4	R	54	5MU
4	R	72	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	T	3	A
3	T	26	M2G
3	T	47(D)	U
3	T	47(E)	G
3	T	47(H)	A
4	R	3	A
4	R	18	OMG
4	R	39	PSU
4	R	47(E)	G

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

22 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
4	4AC	R	12	6,4	21,24,25	0.43	0	29,34,37	0.24	0
3	PSU	T	55	3	18,21,22	1.15	2 (11%)	22,30,33	1.11	2 (9%)
3	4AC	T	12	3,6	21,24,25	0.41	0	29,34,37	0.62	0
4	H2U	R	20	4	18,21,22	0.69	1 (5%)	21,30,33	1.30	1 (4%)
4	5MC	R	48	6,4	18,22,23	0.34	0	26,32,35	0.50	0
4	PSU	R	39	4	18,21,22	1.79	5 (27%)	22,30,33	2.67	11 (50%)
4	JMH	R	32	4	18,22,23	4.03	10 (55%)	21,32,35	1.50	5 (23%)
3	M2G	T	26	3	20,27,28	1.08	3 (15%)	22,40,43	0.68	0
3	1MA	T	58	3	16,25,26	1.69	4 (25%)	18,37,40	1.53	5 (27%)
4	6IA	R	37	4	22,29,30	0.80	0	22,41,44	1.78	5 (22%)
4	OMU	R	44	4	19,22,23	1.20	2 (10%)	26,31,34	1.81	6 (23%)
4	1MA	R	58	4	16,25,26	1.57	2 (12%)	18,37,40	1.43	3 (16%)
4	5MU	R	54	4	19,22,23	2.68	8 (42%)	28,32,35	4.08	11 (39%)
3	OMG	T	18	3	18,26,27	1.63	3 (16%)	19,38,41	1.53	5 (26%)
3	5MC	T	48	3,6	18,22,23	0.60	1 (5%)	26,32,35	0.60	0
4	PSU	R	55	4	18,21,22	0.87	1 (5%)	22,30,33	0.64	0
4	OMG	R	18	4	18,26,27	1.00	2 (11%)	19,38,41	1.08	3 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMU	T	44	3	19,22,23	4.26	11 (57%)	26,31,34	1.96	6 (23%)
3	H2U	T	20	3	18,21,22	1.68	3 (16%)	21,30,33	2.09	5 (23%)
3	PSU	T	39	3	18,21,22	1.57	5 (27%)	22,30,33	2.60	5 (22%)
4	M2G	R	26	4	20,27,28	1.08	3 (15%)	22,40,43	0.64	0
3	5MU	T	54	3	19,22,23	2.68	8 (42%)	28,32,35	3.95	11 (39%)

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
4	4AC	R	12	6,4	-	4/11/29/30	0/2/2/2
3	PSU	T	55	3	-	2/7/25/26	0/2/2/2
3	4AC	T	12	3,6	-	5/11/29/30	0/2/2/2
4	H2U	R	20	4	-	5/7/38/39	0/2/2/2
4	5MC	R	48	6,4	-	0/7/25/26	0/2/2/2
4	PSU	R	39	4	-	3/7/25/26	0/2/2/2
4	JMH	R	32	4	-	2/7/25/26	0/2/2/2
3	M2G	T	26	3	-	2/7/29/30	0/3/3/3
3	1MA	T	58	3	-	0/3/25/26	0/3/3/3
4	6IA	R	37	4	-	3/9/31/32	0/3/3/3
4	OMU	R	44	4	-	0/9/27/28	0/2/2/2
4	1MA	R	58	4	-	0/3/25/26	0/3/3/3
4	5MU	R	54	4	-	2/7/25/26	0/2/2/2
3	OMG	T	18	3	-	2/5/27/28	0/3/3/3
3	5MC	T	48	3,6	-	0/7/25/26	0/2/2/2
4	PSU	R	55	4	-	0/7/25/26	0/2/2/2
4	OMG	R	18	4	-	1/5/27/28	0/3/3/3
3	OMU	T	44	3	-	0/9/27/28	0/2/2/2
3	H2U	T	20	3	-	6/7/38/39	0/2/2/2
3	PSU	T	39	3	-	0/7/25/26	0/2/2/2
4	M2G	R	26	4	-	0/7/29/30	0/3/3/3
3	5MU	T	54	3	-	2/7/25/26	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	44	OMU	C3'-C4'	-9.93	1.27	1.53
4	R	32	JMH	O4'-C4'	-9.08	1.24	1.45
4	R	32	JMH	C2'-C1'	-8.00	1.27	1.53
3	T	44	OMU	C2'-C1'	-7.86	1.32	1.53
4	R	32	JMH	O4'-C1'	7.12	1.58	1.42
3	T	44	OMU	O4-C4	6.90	1.37	1.24
3	T	54	5MU	C2-N1	-6.44	1.28	1.38
4	R	54	5MU	C2-N1	-6.16	1.28	1.38
3	T	44	OMU	O4'-C4'	5.64	1.57	1.45
4	R	32	JMH	C2-N1	-5.12	1.31	1.38
4	R	54	5MU	C6-N1	-5.11	1.29	1.38
3	T	54	5MU	C6-N1	-5.05	1.29	1.38
3	T	18	OMG	C6-N1	-4.94	1.30	1.37
3	T	44	OMU	C4-N3	-4.77	1.30	1.38
4	R	58	1MA	C2-N3	4.55	1.34	1.29
4	R	54	5MU	C2-N3	-4.54	1.29	1.38
3	T	44	OMU	C3'-C2'	4.36	1.62	1.52
3	T	54	5MU	C2-N3	-4.34	1.30	1.38
4	R	32	JMH	C2-N3	-4.31	1.30	1.39
4	R	54	5MU	C4-N3	-4.24	1.31	1.38
3	T	54	5MU	C4-N3	-4.03	1.31	1.38
3	T	44	OMU	O4'-C1'	3.99	1.51	1.42
4	R	39	PSU	C4-N3	-3.97	1.31	1.38
3	T	44	OMU	C2-N1	-3.79	1.32	1.38
3	T	20	H2U	C4-N3	-3.78	1.31	1.37
4	R	54	5MU	O4-C4	-3.62	1.16	1.23
4	R	32	JMH	C4-N4	3.61	1.43	1.28
3	T	54	5MU	O4-C4	-3.52	1.16	1.23
3	T	20	H2U	C2-N3	-3.52	1.31	1.38
3	T	20	H2U	C2-N1	-3.47	1.30	1.35
3	T	55	PSU	C6-C5	3.44	1.39	1.35
4	R	55	PSU	C6-C5	3.40	1.39	1.35
3	T	39	PSU	C4-N3	-3.38	1.32	1.38
4	R	58	1MA	C6-N6	3.30	1.35	1.27
4	R	32	JMH	C6-N1	-3.28	1.30	1.38
4	R	39	PSU	C2-N3	-3.25	1.31	1.37
3	T	58	1MA	C2-N3	3.16	1.32	1.29
3	T	54	5MU	C6-C5	3.11	1.39	1.34
3	T	58	1MA	C2'-C1'	-3.05	1.49	1.53
3	T	55	PSU	O5'-C5'	-3.04	1.37	1.44
4	R	54	5MU	C6-C5	2.98	1.39	1.34
3	T	44	OMU	C2-N3	-2.81	1.33	1.38
3	T	39	PSU	C2'-C1'	-2.78	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	32	JMH	O2-C2	-2.78	1.17	1.22
4	R	32	JMH	O2'-C2'	2.75	1.49	1.43
3	T	58	1MA	C6-N6	2.72	1.34	1.27
4	R	39	PSU	C2-N1	-2.67	1.33	1.36
3	T	18	OMG	C2-N1	-2.66	1.31	1.37
3	T	26	M2G	C5-C6	-2.65	1.42	1.47
4	R	18	OMG	C5-C6	-2.62	1.42	1.47
4	R	26	M2G	C5-C6	-2.61	1.42	1.47
3	T	44	OMU	C6-N1	-2.52	1.31	1.38
3	T	44	OMU	O3'-C3'	2.49	1.48	1.43
4	R	44	OMU	C4-N3	-2.43	1.34	1.38
4	R	54	5MU	O2-C2	-2.42	1.18	1.23
4	R	39	PSU	C2'-C1'	-2.39	1.50	1.53
3	T	39	PSU	C2-N3	-2.37	1.33	1.37
3	T	54	5MU	O2-C2	-2.35	1.18	1.23
4	R	32	JMH	C5-C4	-2.25	1.37	1.42
3	T	39	PSU	C2-N1	-2.23	1.33	1.36
4	R	20	H2U	C2-N3	-2.19	1.34	1.38
4	R	54	5MU	C5M-C5	2.10	1.55	1.50
4	R	44	OMU	C2-N3	-2.08	1.34	1.38
3	T	26	M2G	C8-N7	-2.08	1.31	1.35
3	T	54	5MU	C5M-C5	2.08	1.55	1.50
3	T	58	1MA	C2-N1	-2.07	1.31	1.35
3	T	48	5MC	O5'-C5'	-2.07	1.39	1.44
4	R	18	OMG	C8-N7	-2.06	1.31	1.35
3	T	26	M2G	C5-C4	-2.04	1.37	1.43
4	R	26	M2G	C8-N7	-2.04	1.31	1.35
3	T	39	PSU	C6-N1	-2.03	1.32	1.36
3	T	18	OMG	O4'-C4'	-2.02	1.40	1.45
4	R	39	PSU	C6-N1	-2.02	1.32	1.36
4	R	26	M2G	C5-C4	-2.02	1.37	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	54	5MU	C5M-C5-C4	9.65	129.39	118.77
3	T	54	5MU	C5M-C5-C4	9.49	129.21	118.77
4	R	54	5MU	C4-N3-C2	-8.95	115.77	127.35
3	T	54	5MU	C4-N3-C2	-8.68	116.11	127.35
4	R	54	5MU	N3-C2-N1	8.24	125.83	114.89
3	T	54	5MU	N3-C2-N1	8.15	125.71	114.89
4	R	54	5MU	C5-C6-N1	-7.72	115.39	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	54	5MU	C5M-C5-C6	-7.57	112.74	122.85
3	T	39	PSU	N1-C2-N3	7.52	123.65	115.13
3	T	54	5MU	C5M-C5-C6	-7.34	113.04	122.85
3	T	54	5MU	C5-C6-N1	-7.33	115.80	123.34
3	T	20	H2U	C4-N3-C2	-7.26	119.77	125.79
4	R	39	PSU	N1-C2-N3	7.02	123.08	115.13
4	R	54	5MU	C5-C4-N3	6.80	121.12	115.31
3	T	54	5MU	C5-C4-N3	6.42	120.79	115.31
3	T	44	OMU	N3-C2-N1	5.51	122.21	114.89
3	T	39	PSU	C4-N3-C2	-5.48	118.44	126.34
3	T	39	PSU	O2-C2-N1	-5.31	116.95	122.79
4	R	39	PSU	C2'-C3'-C4'	-5.23	92.47	102.64
4	R	20	H2U	C4-N3-C2	-5.17	121.50	125.79
3	T	44	OMU	C4-N3-C2	-4.88	120.14	126.58
4	R	39	PSU	C4-N3-C2	-4.83	119.38	126.34
4	R	44	OMU	C4-N3-C2	-4.46	120.70	126.58
4	R	37	6IA	C2-N1-C6	4.43	120.39	116.59
4	R	54	5MU	O4-C4-N3	-4.35	111.78	120.12
3	T	58	1MA	O4'-C1'-C2'	-4.09	100.95	106.93
3	T	54	5MU	O4-C4-N3	-4.07	112.32	120.12
4	R	44	OMU	N3-C2-N1	4.03	120.24	114.89
4	R	37	6IA	O4'-C1'-C2'	-3.89	101.25	106.93
3	T	54	5MU	O2-C2-N1	-3.77	117.77	122.79
4	R	58	1MA	C5-C6-N1	3.71	119.43	113.90
3	T	55	PSU	O3'-C3'-C4'	-3.68	100.40	111.05
4	R	44	OMU	C5-C4-N3	3.57	120.19	114.84
4	R	54	5MU	O2-C2-N1	-3.34	118.34	122.79
4	R	58	1MA	N1-C2-N3	-3.26	122.22	126.02
3	T	20	H2U	C3'-C2'-C1'	3.23	107.57	101.43
4	R	39	PSU	O2-C2-N1	-3.16	119.31	122.79
3	T	44	OMU	C5-C4-N3	3.11	119.50	114.84
4	R	54	5MU	O2-C2-N3	-3.05	115.83	121.50
3	T	39	PSU	C5-C6-N1	-3.03	117.57	122.11
3	T	18	OMG	C5-C6-N1	3.01	119.27	113.95
4	R	37	6IA	C4-C5-N7	-3.00	106.27	109.40
4	R	39	PSU	O4'-C4'-C5'	2.98	119.18	109.37
4	R	44	OMU	O4-C4-C5	-2.96	119.96	125.16
4	R	44	OMU	C2'-C1'-N1	-2.89	108.62	114.22
4	R	39	PSU	C5-C6-N1	-2.82	117.88	122.11
4	R	37	6IA	N3-C2-N1	-2.75	124.38	128.68
3	T	18	OMG	O3'-C3'-C4'	-2.73	103.15	111.05
4	R	54	5MU	C6-N1-C2	2.71	124.04	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	32	JMH	C31-N3-C2	2.69	122.03	117.31
3	T	54	5MU	O2-C2-N3	-2.68	116.52	121.50
3	T	44	OMU	O4-C4-C5	-2.60	120.59	125.16
4	R	54	5MU	C1'-N1-C6	-2.60	116.80	121.12
3	T	20	H2U	O3'-C3'-C2'	2.56	120.12	111.82
3	T	18	OMG	C8-N7-C5	2.56	107.86	102.99
4	R	32	JMH	O4'-C1'-C2'	-2.53	101.12	106.64
3	T	54	5MU	C6-N1-C2	2.52	123.85	121.30
4	R	18	OMG	C3'-C2'-C1'	-2.51	98.17	102.89
4	R	32	JMH	C1'-N1-C2	2.48	121.18	116.99
3	T	44	OMU	O2-C2-N1	-2.48	119.49	122.79
3	T	39	PSU	O4'-C1'-C2'	2.46	108.62	105.14
3	T	18	OMG	O4'-C1'-C2'	-2.42	102.39	106.59
4	R	39	PSU	C4'-O4'-C1'	-2.42	102.48	108.55
3	T	20	H2U	C5-C6-N1	-2.35	103.87	111.61
3	T	58	1MA	N1-C2-N3	-2.31	123.33	126.02
3	T	44	OMU	C5-C6-N1	-2.29	117.97	121.81
3	T	54	5MU	C1'-N1-C6	-2.29	117.31	121.12
4	R	39	PSU	O4'-C4'-C3'	-2.26	100.64	105.11
4	R	18	OMG	O3'-C3'-C2'	-2.25	104.78	111.17
3	T	55	PSU	C2'-C3'-C4'	-2.24	98.29	102.64
4	R	39	PSU	O2-C2-N3	-2.24	117.60	121.82
4	R	37	6IA	C3'-C2'-C1'	2.21	104.31	100.98
4	R	44	OMU	O2-C2-N1	-2.20	119.86	122.79
4	R	39	PSU	O2'-C2'-C1'	-2.19	106.00	111.23
3	T	58	1MA	C8-N7-C5	2.16	107.10	102.99
3	T	58	1MA	C5-C6-N1	2.14	117.09	113.90
4	R	32	JMH	O2-C2-N3	-2.13	118.34	121.34
4	R	32	JMH	O4'-C1'-N1	-2.11	103.55	108.36
3	T	20	H2U	O2-C2-N1	-2.09	120.48	123.11
4	R	39	PSU	C3'-C2'-C1'	2.07	104.05	101.64
3	T	58	1MA	C5'-C4'-C3'	-2.05	107.51	115.18
4	R	58	1MA	C8-N7-C5	2.04	106.87	102.99
3	T	18	OMG	C2-N1-C6	-2.02	121.38	125.10
4	R	18	OMG	O6-C6-C5	2.00	128.29	124.37

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	T	12	4AC	N3-C4-N4-C7
3	T	12	4AC	C5-C4-N4-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	T	12	4AC	O7-C7-N4-C4
3	T	12	4AC	CM7-C7-N4-C4
3	T	20	H2U	O4'-C1'-N1-C6
3	T	26	M2G	C3'-C4'-C5'-O5'
3	T	55	PSU	C3'-C4'-C5'-O5'
3	T	55	PSU	O4'-C4'-C5'-O5'
4	R	12	4AC	N3-C4-N4-C7
4	R	12	4AC	C5-C4-N4-C7
4	R	12	4AC	O7-C7-N4-C4
4	R	12	4AC	CM7-C7-N4-C4
4	R	20	H2U	O4'-C4'-C5'-O5'
4	R	20	H2U	O4'-C1'-N1-C6
3	T	18	OMG	O4'-C4'-C5'-O5'
4	R	18	OMG	O4'-C4'-C5'-O5'
4	R	20	H2U	C3'-C4'-C5'-O5'
3	T	18	OMG	C3'-C4'-C5'-O5'
3	T	20	H2U	O4'-C4'-C5'-O5'
3	T	26	M2G	O4'-C4'-C5'-O5'
4	R	32	JMH	C3'-C4'-C5'-O5'
4	R	32	JMH	O4'-C4'-C5'-O5'
4	R	39	PSU	O4'-C4'-C5'-O5'
3	T	20	H2U	C3'-C4'-C5'-O5'
4	R	39	PSU	C3'-C4'-C5'-O5'
3	T	54	5MU	O4'-C4'-C5'-O5'
4	R	54	5MU	O4'-C4'-C5'-O5'
4	R	37	6IA	C12-C13-C14-C15
4	R	54	5MU	C3'-C4'-C5'-O5'
3	T	54	5MU	C3'-C4'-C5'-O5'
4	R	37	6IA	C12-C13-C14-C16
4	R	39	PSU	C4'-C5'-O5'-P
3	T	12	4AC	C4'-C5'-O5'-P
4	R	37	6IA	C4'-C5'-O5'-P
3	T	20	H2U	C2'-C1'-N1-C6
3	T	20	H2U	C2'-C1'-N1-C2
3	T	20	H2U	O4'-C1'-N1-C2
4	R	20	H2U	O4'-C1'-N1-C2
4	R	20	H2U	C2'-C1'-N1-C2

There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	12	4AC	7	0
3	T	12	4AC	4	0
4	R	20	H2U	1	0
4	R	48	5MC	1	0
4	R	39	PSU	3	0
4	R	32	JMH	3	0
3	T	26	M2G	2	0
4	R	37	6IA	7	0
4	R	44	OMU	2	0
4	R	54	5MU	1	0
4	R	26	M2G	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z  > 2$
5	SAH	A	301	-	24,28,28	1.23	3 (12%)	25,40,40	1.73	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SAH	A	301	-	-	4/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	SAH	C2-N3	3.46	1.37	1.32
5	A	301	SAH	OXT-C	-2.23	1.23	1.30
5	A	301	SAH	C2-N1	2.14	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	SAH	N3-C2-N1	-5.46	120.15	128.68
5	A	301	SAH	C5'-SD-CG	-4.22	89.62	102.27
5	A	301	SAH	OXT-C-O	-2.36	118.73	124.09
5	A	301	SAH	OXT-C-CA	2.04	120.33	113.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	SAH	C-CA-CB-CG
5	A	301	SAH	N-CA-CB-CG
5	A	301	SAH	O-C-CA-CB
5	A	301	SAH	OXT-C-CA-CB

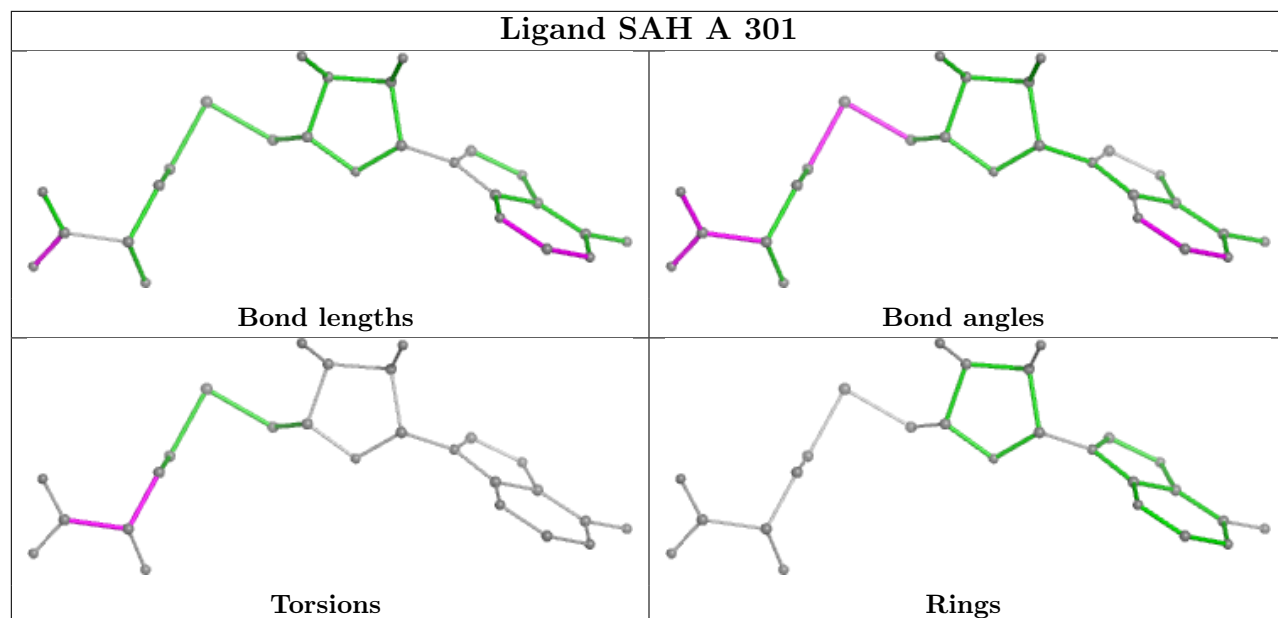
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	301	SAH	3	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.

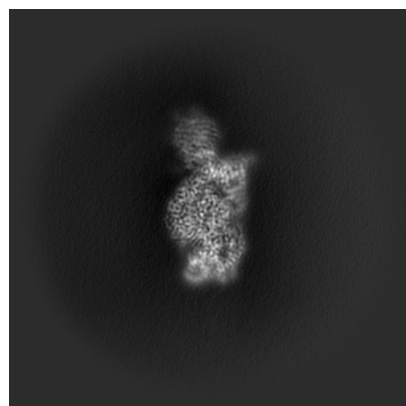
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17528. These allow visual inspection of the internal detail of the map and identification of artifacts.

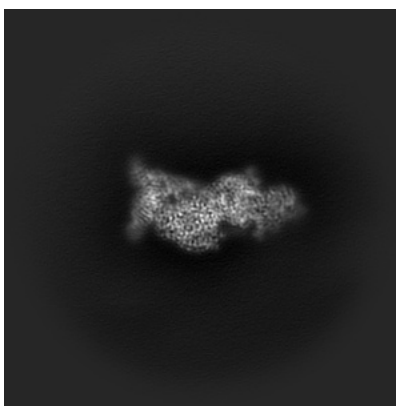
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

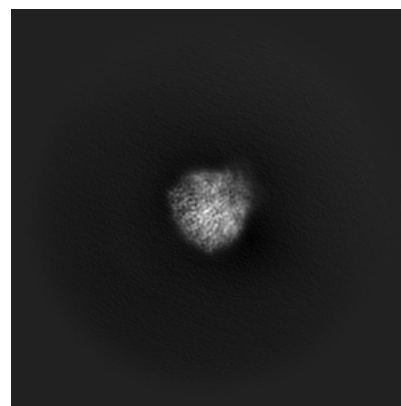
#### 6.1.1 Primary map



X

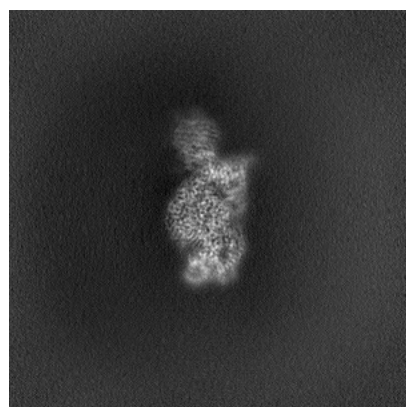


Y

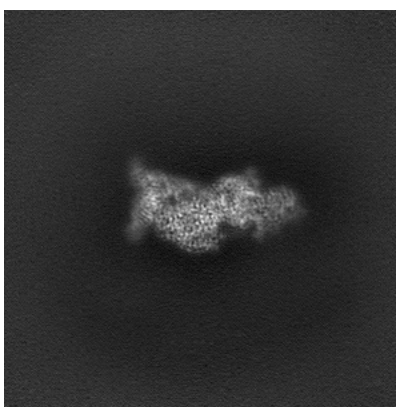


Z

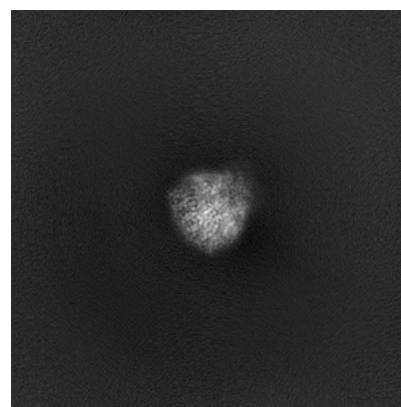
#### 6.1.2 Raw map



X



Y

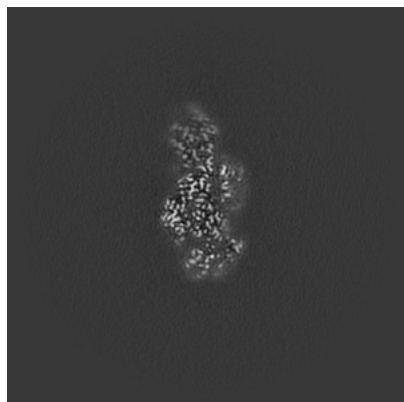


Z

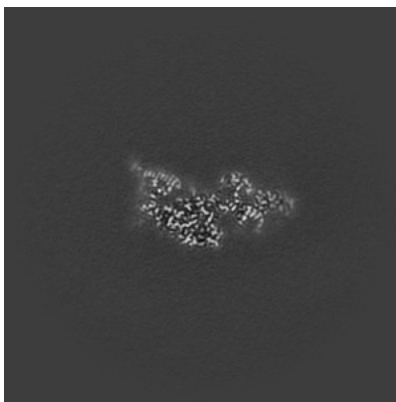
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

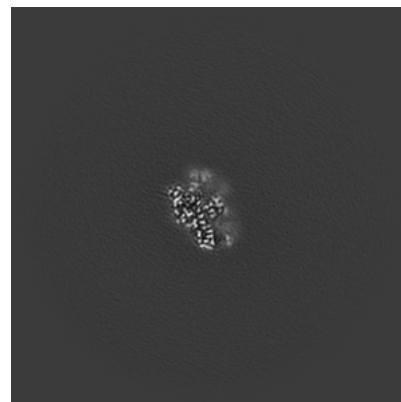
### 6.2.1 Primary map



X Index: 275

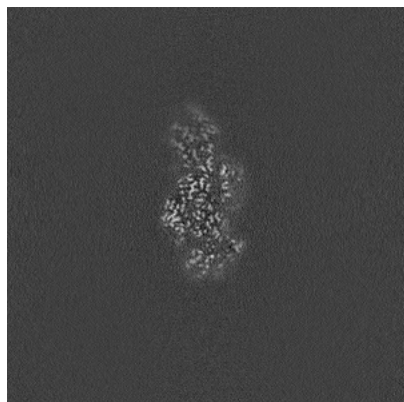


Y Index: 275

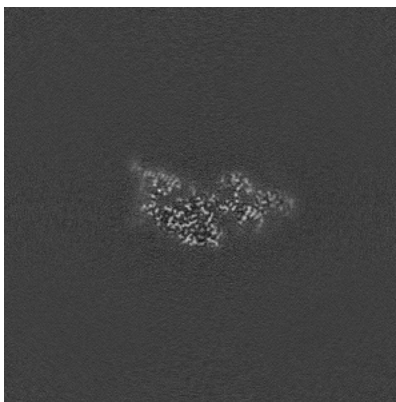


Z Index: 275

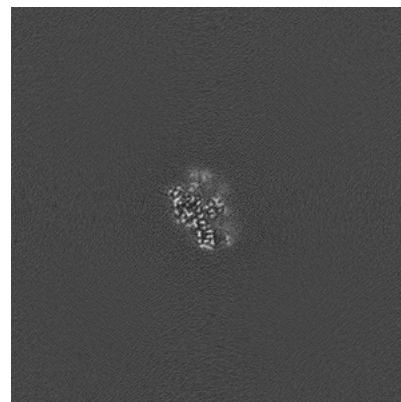
### 6.2.2 Raw map



X Index: 275



Y Index: 275

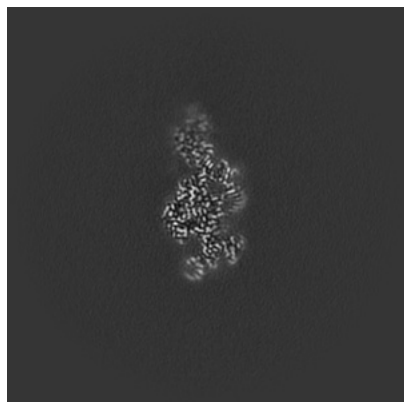


Z Index: 275

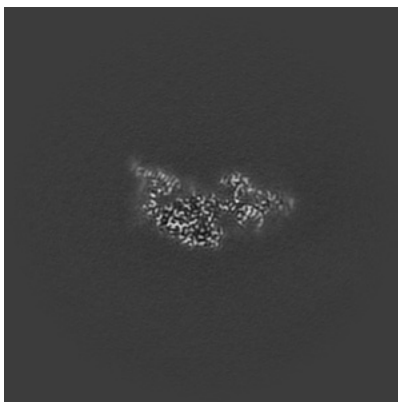
The images above show central slices of the map in three orthogonal directions.

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

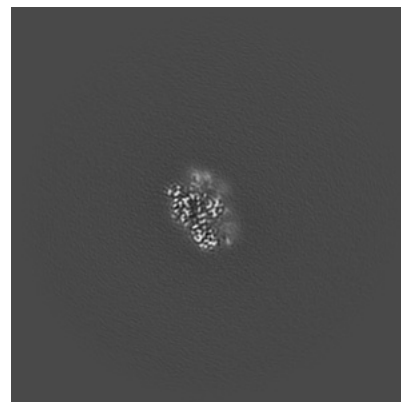
### 6.3.1 Primary map



X Index: 267

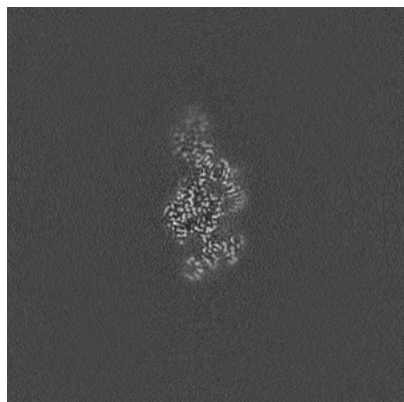


Y Index: 276

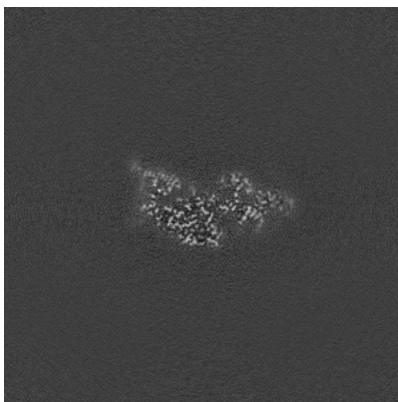


Z Index: 273

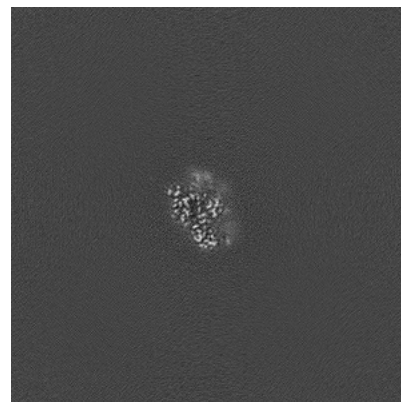
### 6.3.2 Raw map



X Index: 266



Y Index: 275

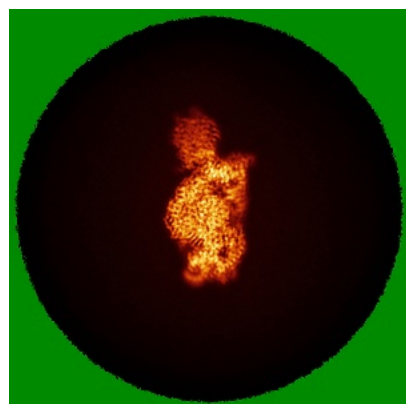


Z Index: 273

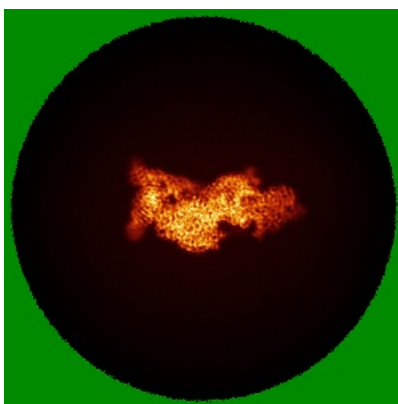
The images above show the largest variance slices of the map in three orthogonal directions.

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

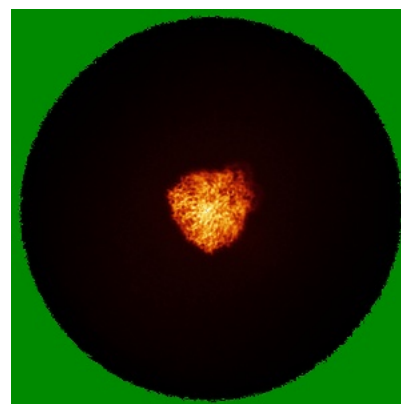
### 6.4.1 Primary map



X

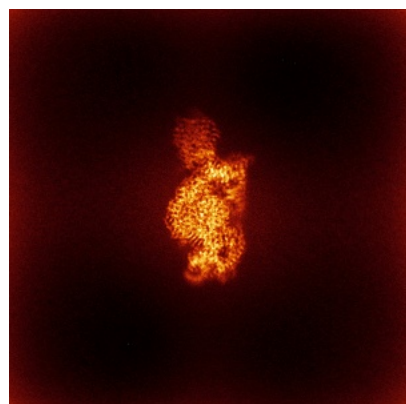


Y

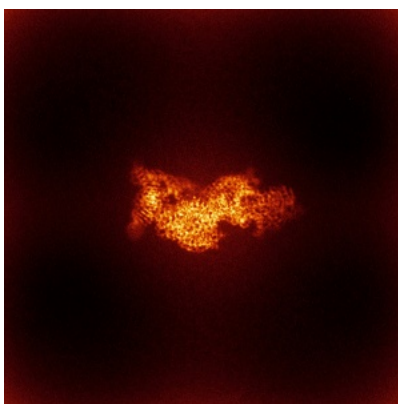


Z

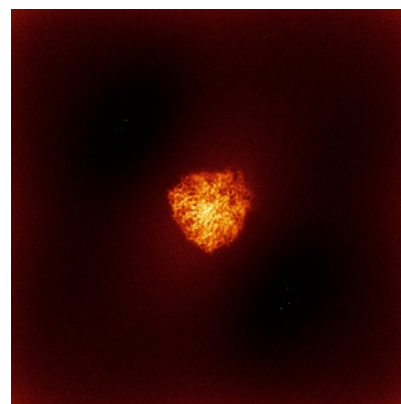
### 6.4.2 Raw map



X



Y

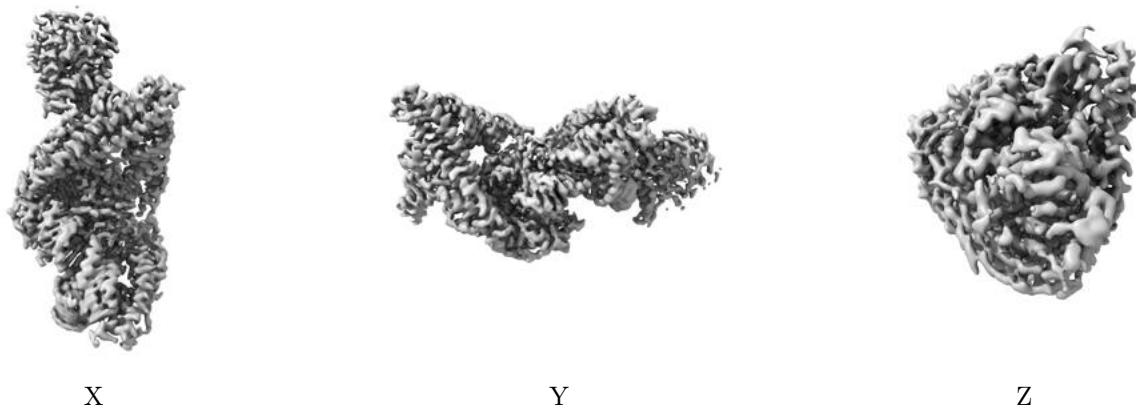


Z

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.

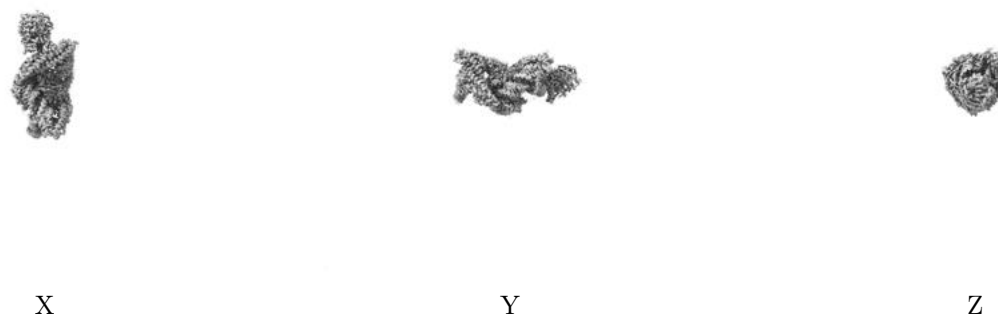
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.



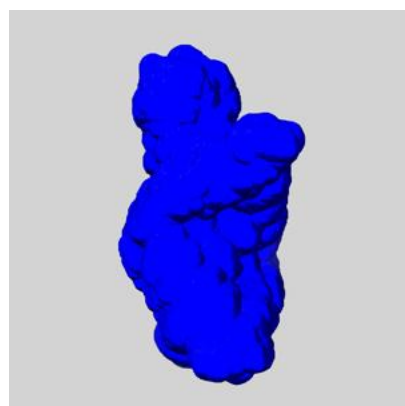
## 6.6 Mask visualisation [i](#)

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

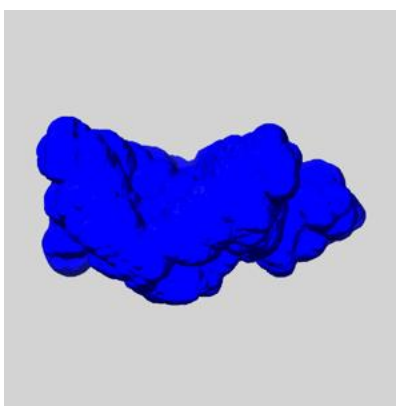
A mask typically either:

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

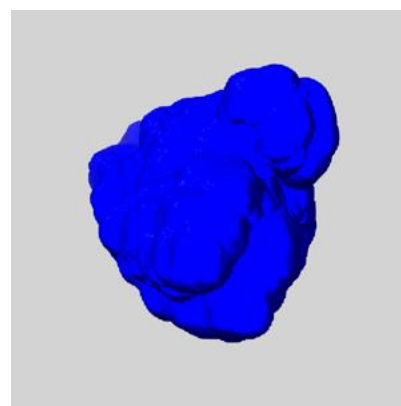
### 6.6.1 emd\_17528\_msk\_1.map [i](#)



X



Y

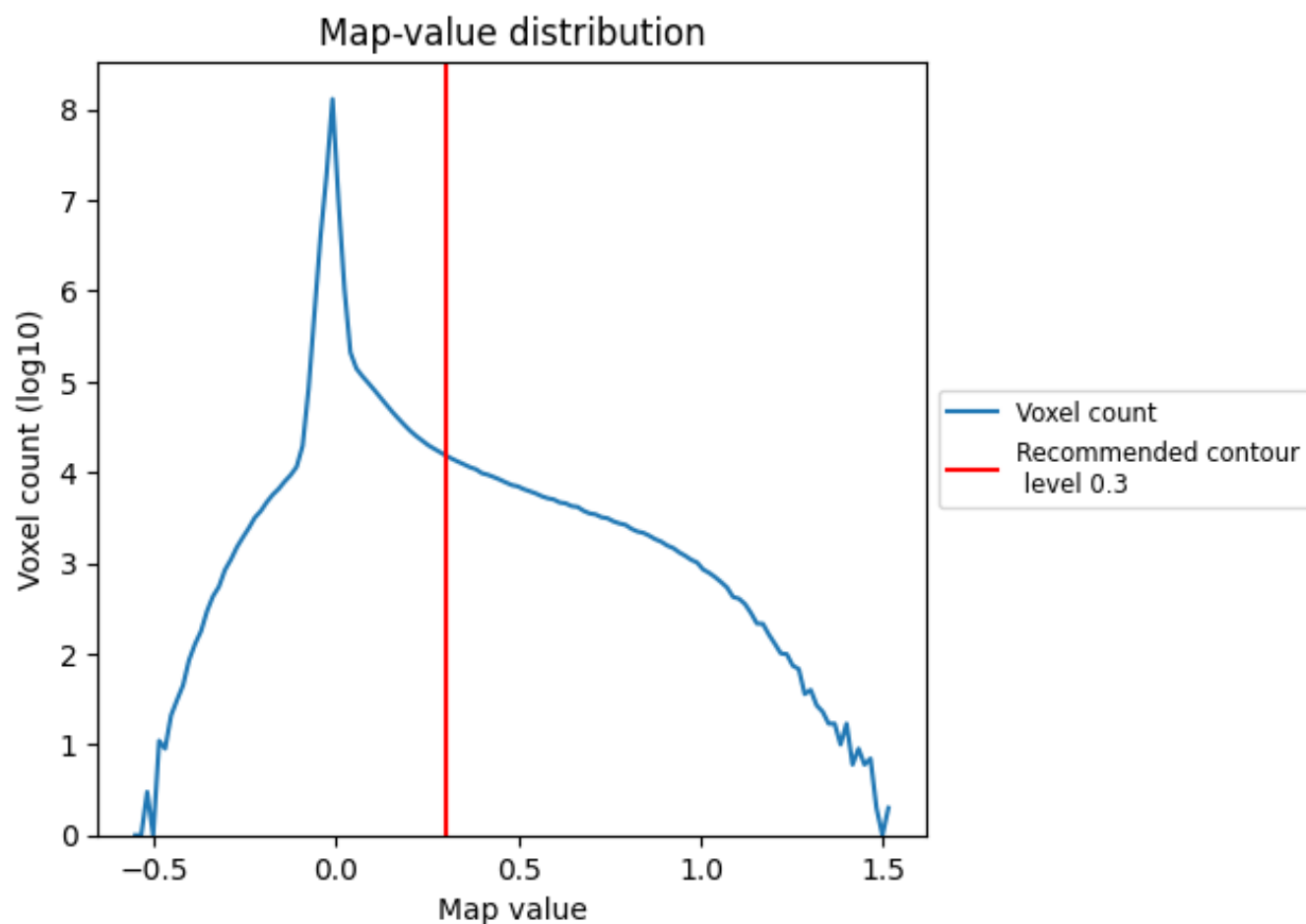


Z

## 7 Map analysis [i](#)

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

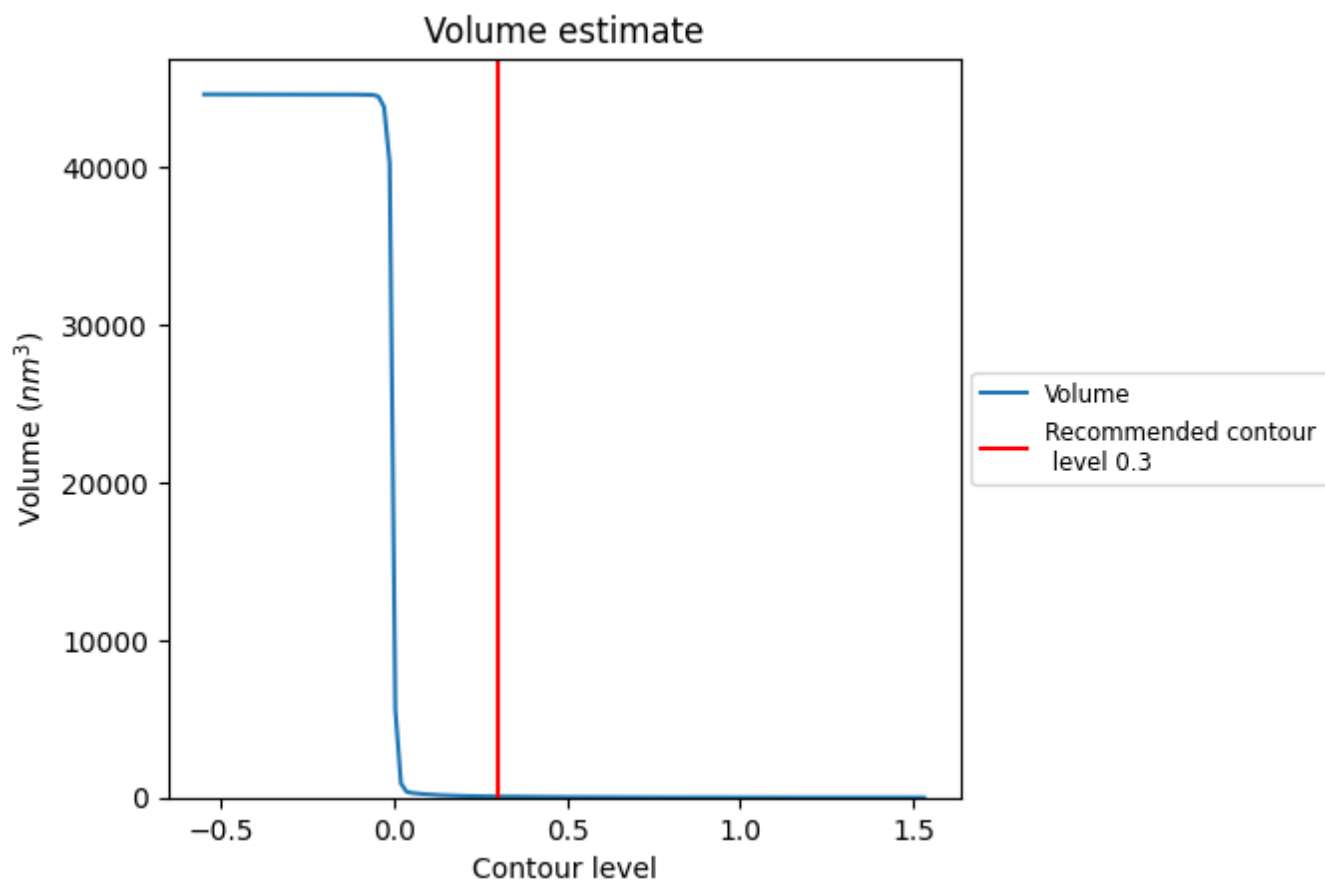
### 7.1 Map-value distribution [i](#)



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.



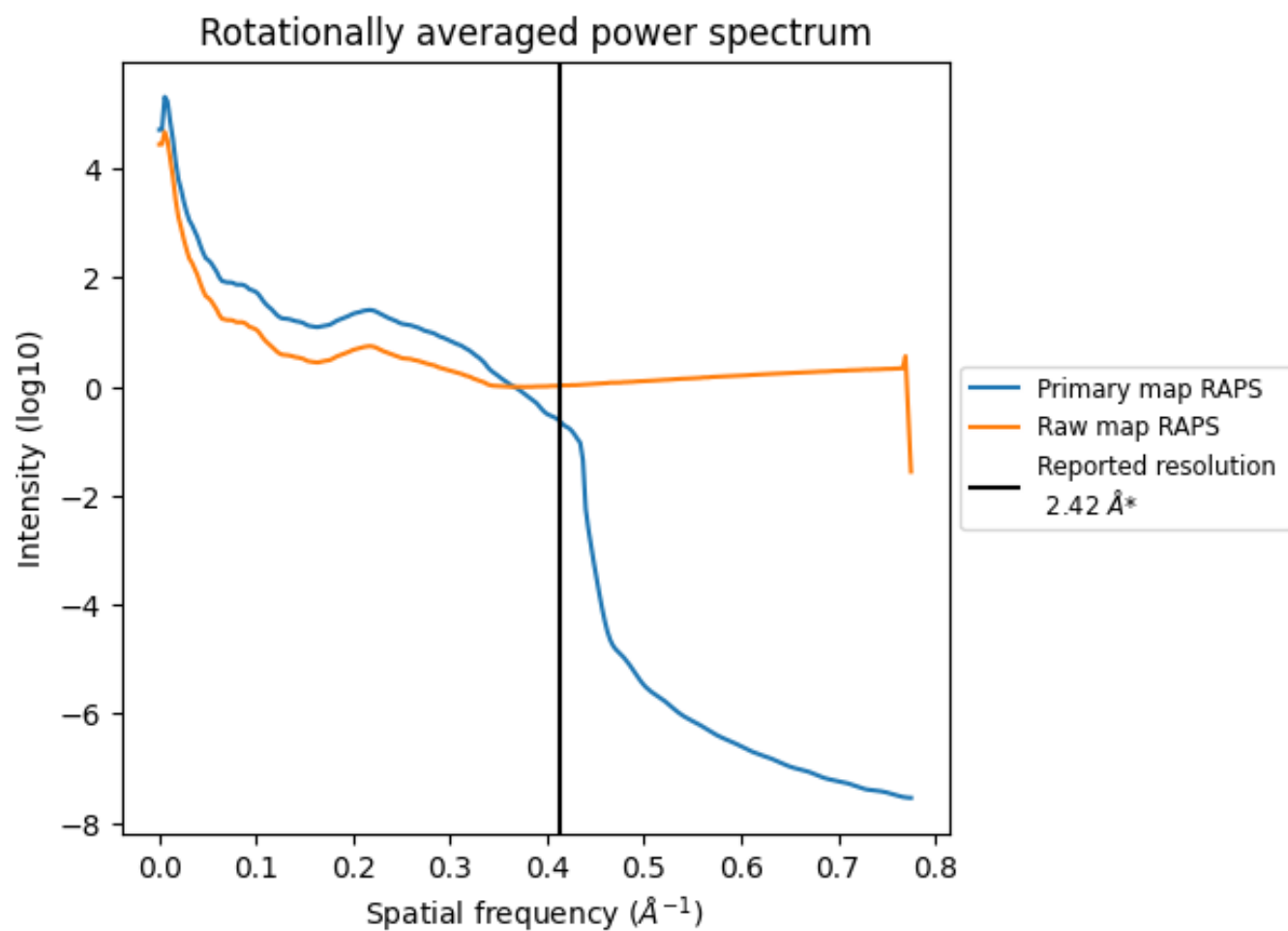
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65  $\text{nm}^3$ ; this corresponds to an approximate mass of 58 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 ⓘ

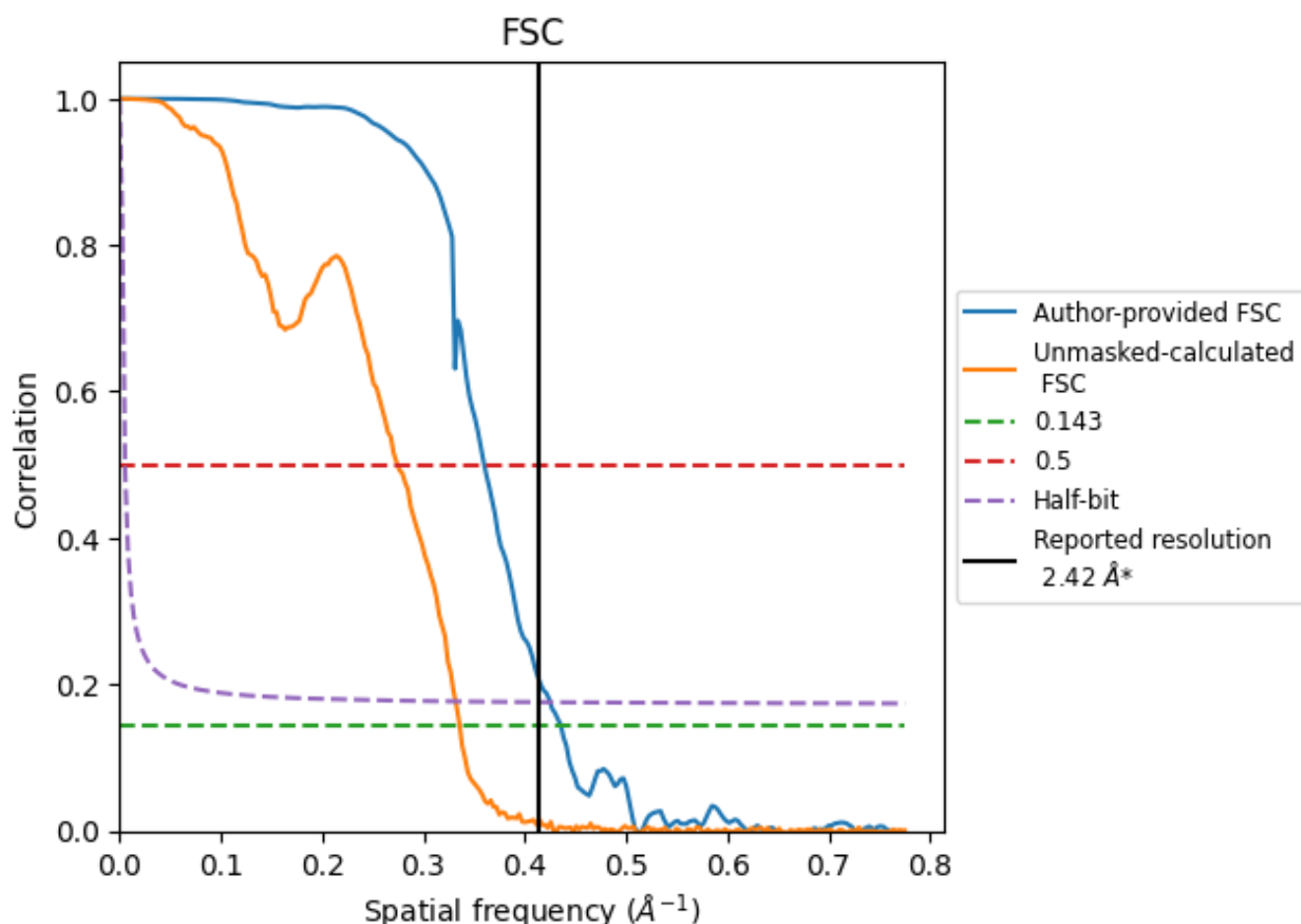


\*Reported resolution corresponds to spatial frequency of 0.413 Å<sup>-1</sup>

## 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 0.413 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

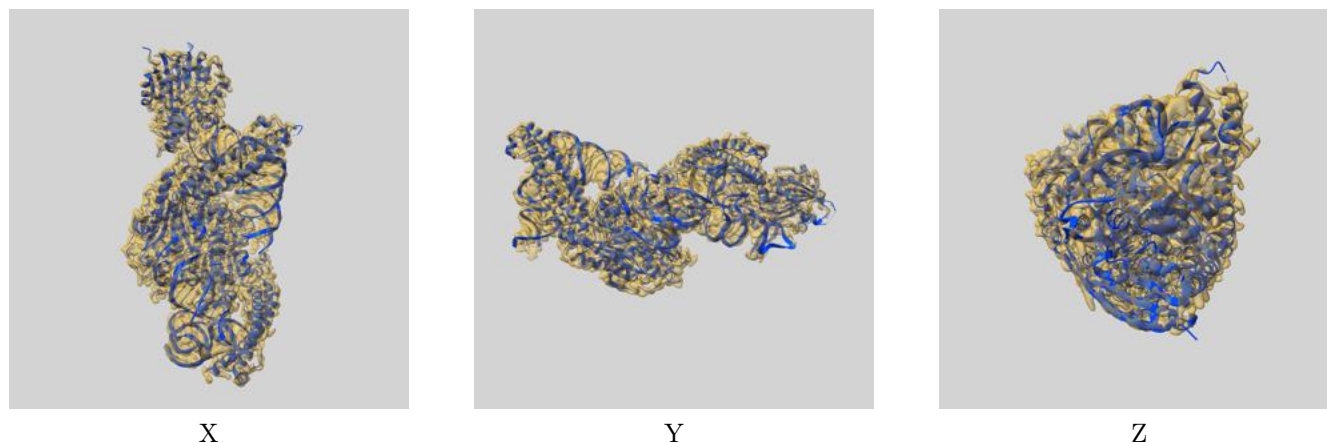
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.29	2.78	2.35
Unmasked-calculated*	2.98	3.64	3.01

\*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 2.98 differs from the reported value 2.42 by more than 10 %

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

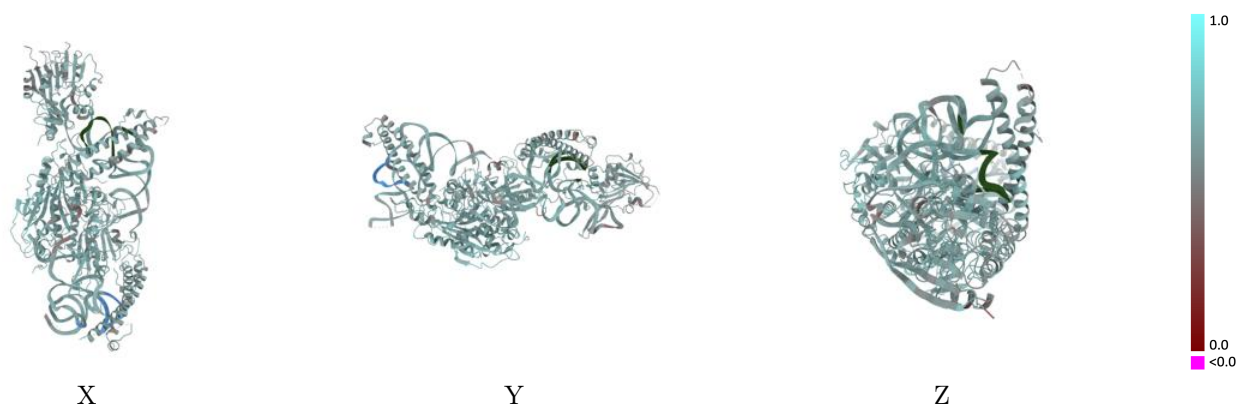
This section contains information regarding the fit between EMDB map EMD-17528 and PDB model 8P7B. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



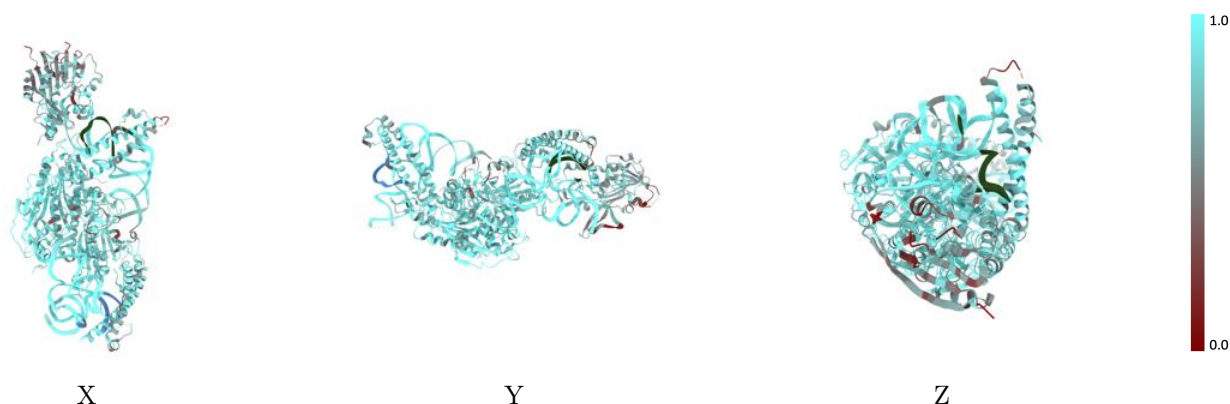
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



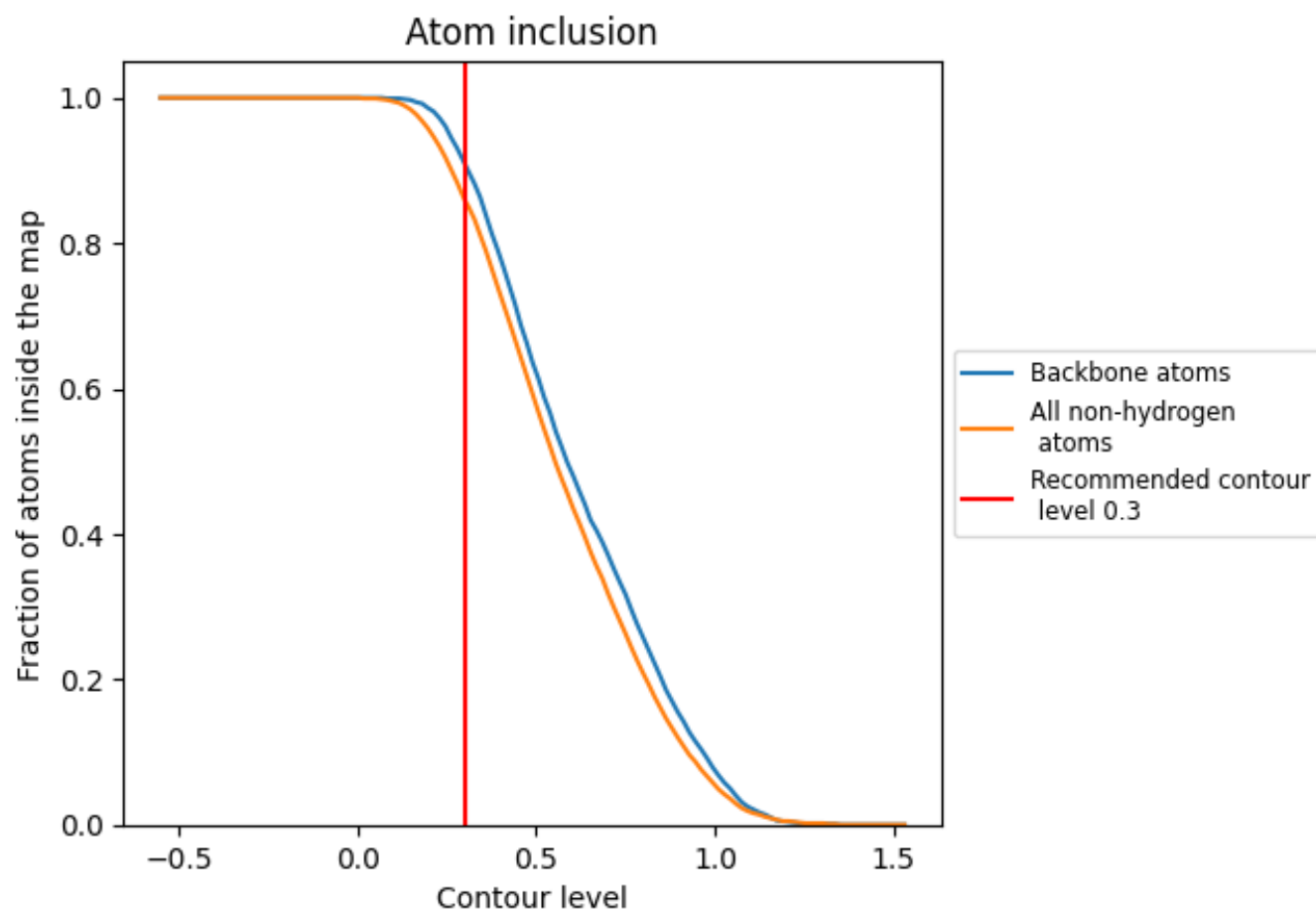
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8600	<div></div> 0.6150
A	<div></div> 0.6610	<div></div> 0.5800
B	<div></div> 0.8860	<div></div> 0.6290
D	<div></div> 0.8880	<div></div> 0.6300
R	<div></div> 0.9040	<div></div> 0.6070
T	<div></div> 0.9280	<div></div> 0.6020

