



## wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 12:32 AM UTC

PDB ID : 9QLI / pdb\_00009qli  
EMDB ID : EMD-53228  
Title : YerA41 family-A DNA polymerase  
Authors : Missouri, S.; Delarue, M.  
Deposited on : 2025-03-21  
Resolution : 5.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

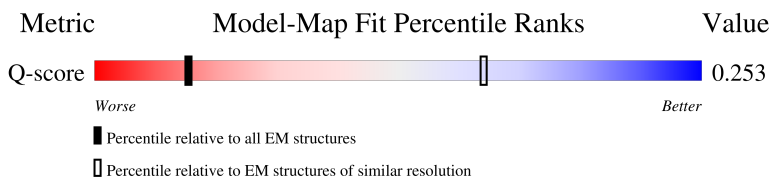
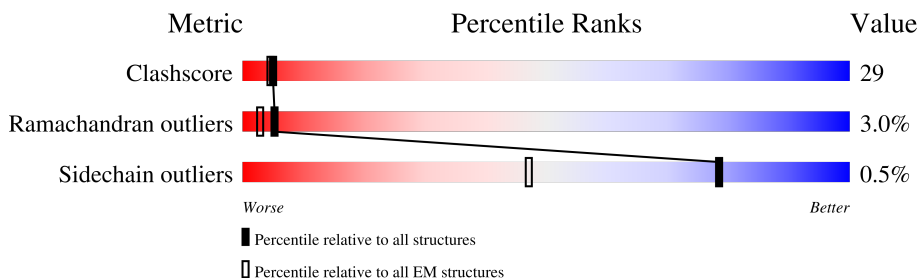
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.00 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	1057 ( 4.50 - 5.50 )

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

Mol	Chain	Length	Quality of chain
1	A	1306	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10352 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 DNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1257	Total	C	N	O	S	0	0
			10352	6690	1701	1922	39		

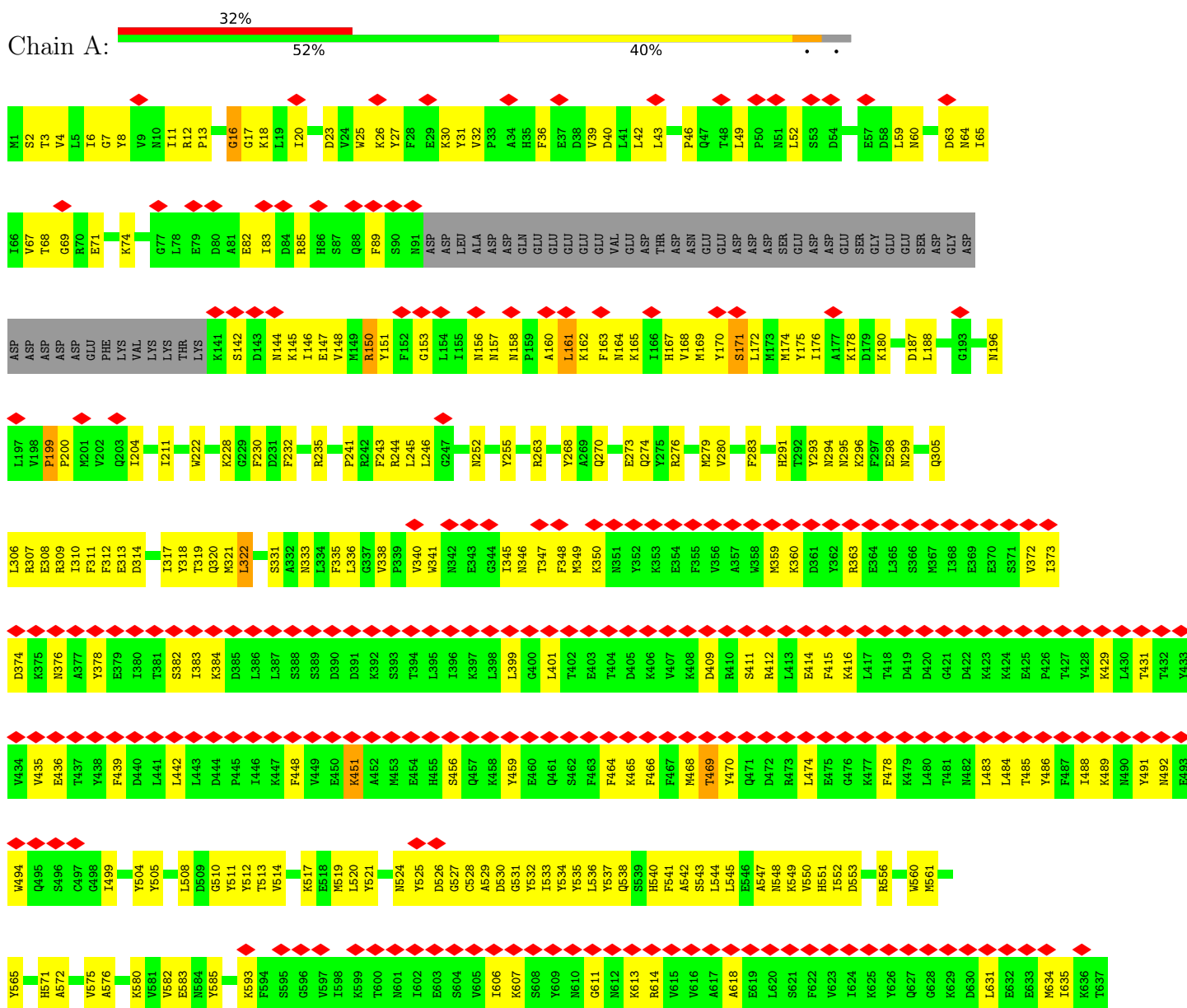
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	VAL	ASN	conflict	UNP A0AA86MGY1
A	402	THR	ILE	conflict	UNP A0AA86MGY1
A	420	ASP	-	insertion	UNP A0AA86MGY1
A	533	ILE	VAL	conflict	UNP A0AA86MGY1
A	595	SER	ASN	conflict	UNP A0AA86MGY1
A	647	LYS	ARG	conflict	UNP A0AA86MGY1
A	673	GLU	GLY	conflict	UNP A0AA86MGY1
A	717	LEU	VAL	conflict	UNP A0AA86MGY1
A	761	GLU	ASP	conflict	UNP A0AA86MGY1
A	915	VAL	ALA	conflict	UNP A0AA86MGY1

### 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: DNA polymerase



Y1283	P1205	Y1126	M1052	C974	V903	A822	A762	G698	Y638
K1284	S1206	S1127	L1053	F975	E905	G823	R763	T699	Y639
P1285	F1210	I1128	T1054	T976	E905	Q824	L764	T699	E640
C1287	E1211	K1129	F1055	P977	E905	G825	R765	N700	E641
R1288	L1212	Q1130	A1056	R978	L908	K826	T766	P701	H641
F1289	R1216	K1131	I1057	K979	G909	R827	N767	P702	L642
R1290	Y1217	G1132	L1058	E980	G910	N768	A769	I703	A643
E1291	S1218	I1136	Y1059	Q981	G911	L828	N770	A704	V644
V1293	G1219	Q1137	G1060	F984	S912	A830	V770	D705	G645
T1294	M1227	Q1138	V1063	H985	F913	A831	I771	R706	R646
Y1297	D1228	N1139	G1064	H986	I914	D832	A773	I707	K647
V1298	D1229	L1140	S1065	M987	V915	K833	G774	A708	A648
S1300	K1230	S1142	I1066	E988	S916	I834	H775	V709	L649
A1301	K1231	L1144	A1067	M989	H917	I835	E776	I710	V650
I1302	S1232	T1145	Q1069	Q991	K918	L836	M777	S711	D651
I1303	A1233	A1146	K1072	R995	D919	A842	I778	Q712	H652
G1304	A1234	Y1147	P1073	I996	S920	T845	I779	F713	I653
L1305	I1235	T1148	F1074	A999	H921	L846	L780	I714	N654
K1306	I1236	A1149	D1075	E1003	P923	T846	F782	N715	E655
	K1236	Y1150	E1076	E1003	I924	G852	L783	H716	T656
	L1237	A1151	A1077	E1003	G925	E853	L784	L717	G657
	E1238	L1152	K1078	L1006	P926	K854	L785	Y718	N658
	I1239	R1157	K1079	I1007	K927	L855	N786	N719	A659
	K1240	Y1160	I1080	I1010	T928	G856	R787	R720	K660
	D1241	E1163	Y1081	L1011	S929	K857	K789	A721	L661
	Y1242	I1164	D1082	I1016	D932	H858	T791	E722	T662
	I1243	Q1165	G1083	F1019	I933	L860	S792	G723	K663
	H1244	L1166	Y1084	F1020	E934	R861	T793	M724	T664
	D1245	L1167	F1085	F1021	N935	T862	H795	V725	Q665
	K1246	G1168	M1086	A1023	E936	I863	E796	N726	K666
	E1247	F1169	A1087	A1024	P937	V867	F797	I727	G667
	D1248	V1170	N1088	F1025	E938	D868	T798	T728	K668
	L1250	H1171	P1089	D1026	D939	F869	D799	Y729	I669
	K1251	D1172	N1090	L1027	Q941	R873	M801	E730	I670
	L1252	E1175	F1091	Q1028	T942	K874	S803	D731	G671
	M1253	F1176	K1092	F1029	T944	N875	D804	V732	K672
	S1256	E1177	E1096	A1030	K945	S876	E805	K733	E673
	F1257	K1181	N1105	E1031	Y948	L877	F806	Y736	F674
	E1261	D1182	F1106	D1032	V949	D878	G807	L737	I680
	K1265	L1183	N1109	E1033	Q950	E879	E808	D738	I681
	K1266	F1184	Y1110	L1034	N951	Y880	Y809	R739	H682
	H1269	I1185	Y1111	Y1035	T955	F883	L810	V740	K683
		L1187	L1111	K1036	L956	I884	V811	D745	D677
			R1117	I1037	R957	L886	D812	I746	K679
			F1118	K1038	V958	L889	L813	Y747	I680
			Y1119	Q1039	P966		V814	D748	I681
			I1120	D1040	S967		K815	I749	H682
			G1121	P1041	T968		R816	D750	K683
			N1122	E1042	L969		N817	R751	F684
			Y1123	L1043	D970		N818	Y752	I685
			H1125	D1044			A820	E754	E686
				Q1045			E821	F755	I687
				L1046				S756	I688
				R1047				S757	D689
								T758	K690
								R759	K691
								H760	Y692
								E761	K693
									L694
									F696
									F697

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.707	Depositor
Minimum map value	-1.145	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.172	Depositor
Map size (Å)	328.32, 328.32, 328.32	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.49	0/10601	0.93	23/14285 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	918	LYS	N-CA-C	-8.92	101.45	114.39
1	A	199	PRO	N-CA-CB	8.20	111.03	103.08
1	A	200	PRO	N-CA-CB	7.16	110.77	103.25
1	A	925	GLY	C-N-CD	-6.68	97.59	125.00
1	A	914	ILE	N-CA-C	-6.59	103.82	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1290	ARG	Sidechain
1	A	150	ARG	Sidechain
1	A	765	ARG	Sidechain
1	A	787	ARG	Sidechain

## 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	10352	0	10185	601	0
All	All	10352	0	10185	601	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 29.

The worst 5 of 601 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:A:764:LEU:HA	1:A:768:ASN:HD22	1.10	1.05
1:A:912:SER:HB2	1:A:940:THR:HA	1.42	1.01
1:A:803:SER:HA	1:A:806:PHE:HD1	1.26	1.00
1:A:995:ARG:HH12	1:A:1016:ILE:HG21	1.30	0.95
1:A:800:LYS:HD3	1:A:804:ASP:HB2	1.51	0.93

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	1253/1306 (96%)	1104 (88%)	112 (9%)	37 (3%)	<b>3</b> <b>22</b>

5 of 37 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	199	PRO
1	A	805	GLU
1	A	806	PHE
1	A	808	GLU
1	A	869	PHE

### 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	1120/1179 (95%)	1114 (100%)	6 (0%)	<a href="#">81</a> <a href="#">82</a>

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1023	ASN
1	A	1187	LEU
1	A	1261	GLU
1	A	469	THR
1	A	168	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	734	GLN
1	A	818	ASN
1	A	1274	HIS
1	A	950	GLN
1	A	320	GLN

### 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 [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	239:PHE	C	240:GLU	N	1.16
1	A	236:ASN	C	237:PHE	N	1.13

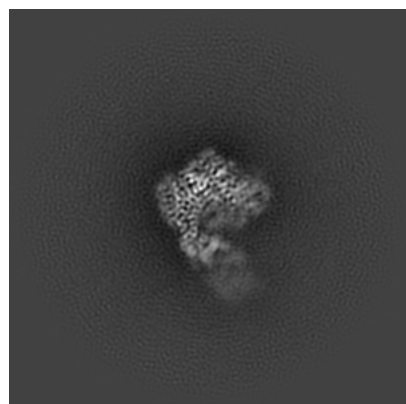
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53228. These allow visual inspection of the internal detail of the map and identification of artifacts.

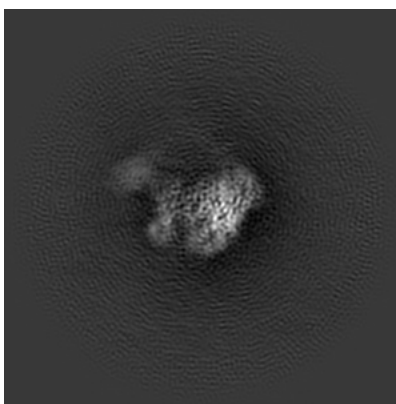
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

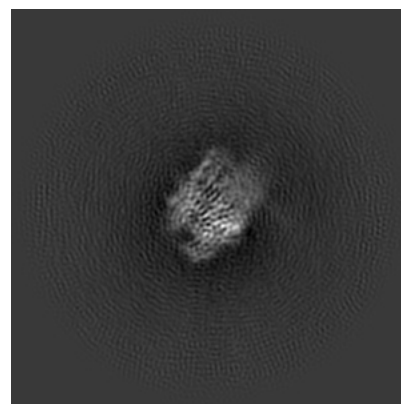
#### 6.1.1 Primary map



X

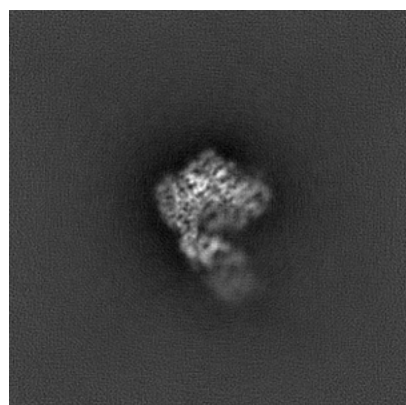


Y

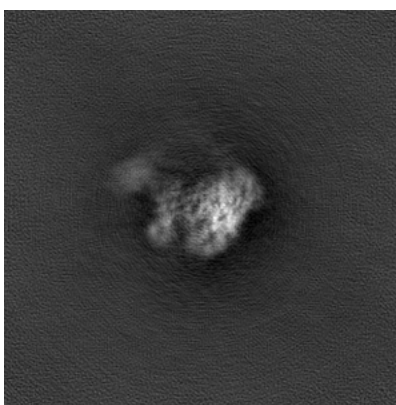


Z

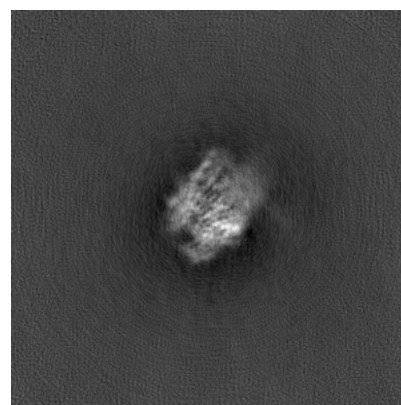
#### 6.1.2 Raw map



X



Y

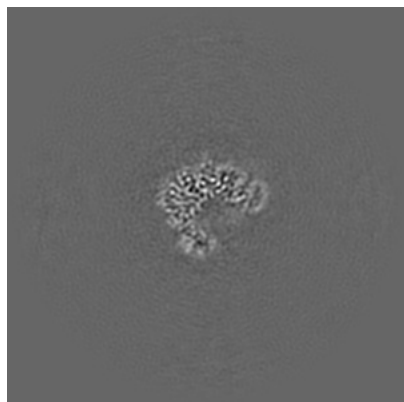


Z

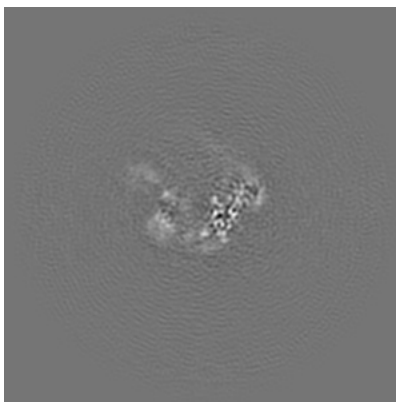
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

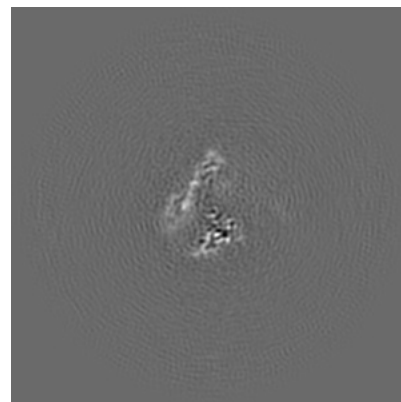
### 6.2.1 Primary map



X Index: 144

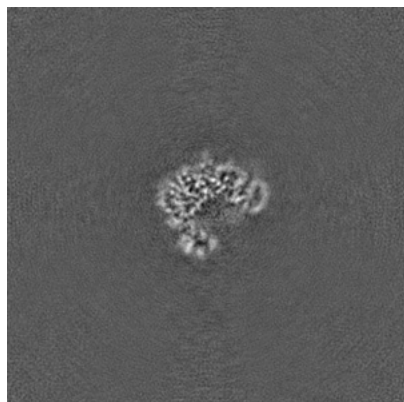


Y Index: 144

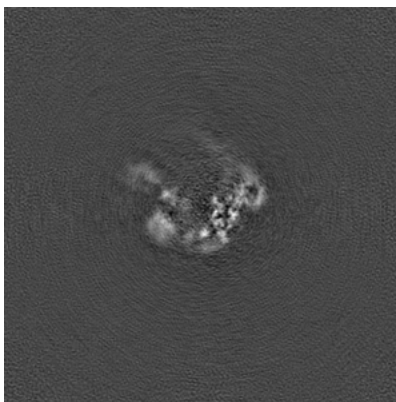


Z Index: 144

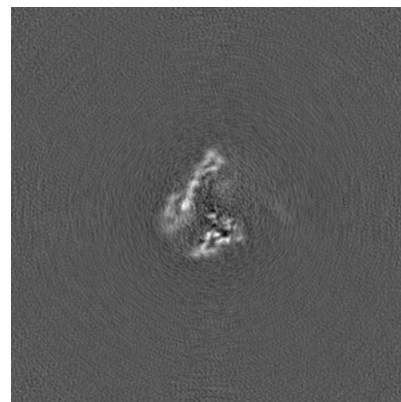
### 6.2.2 Raw map



X Index: 144



Y Index: 144

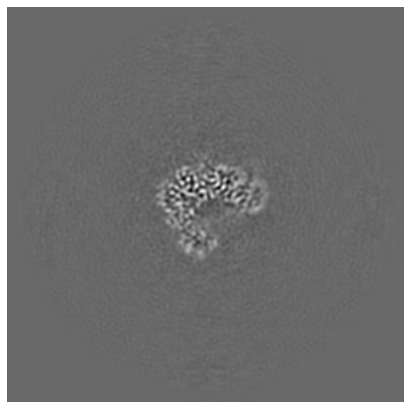


Z Index: 144

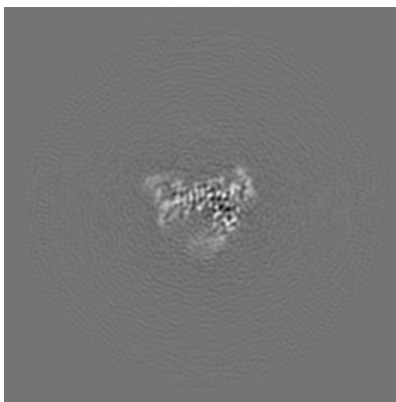
The images above show central slices of the map in three orthogonal directions.

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

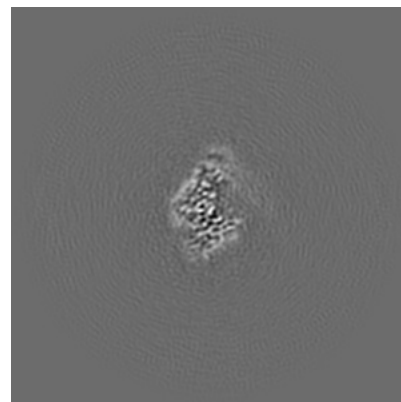
### 6.3.1 Primary map



X Index: 143

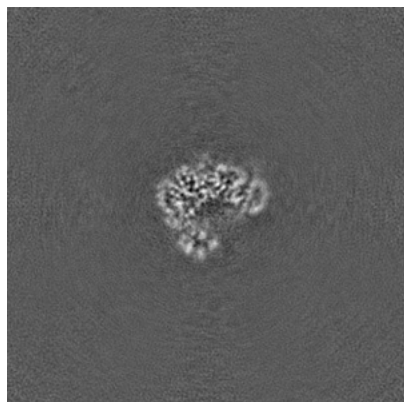


Y Index: 132

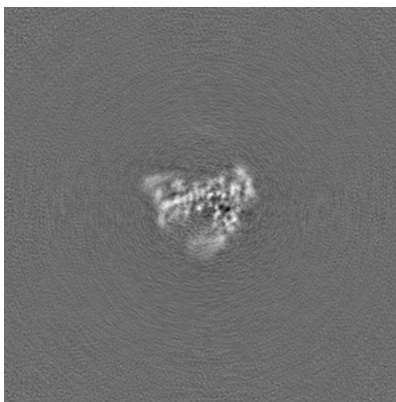


Z Index: 155

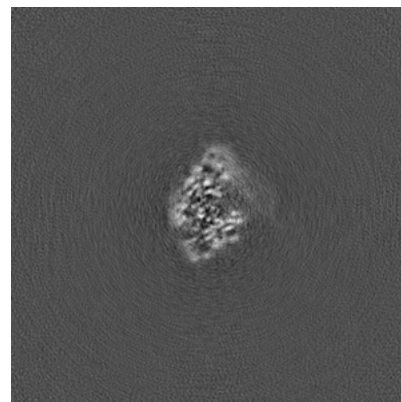
### 6.3.2 Raw map



X Index: 143



Y Index: 132

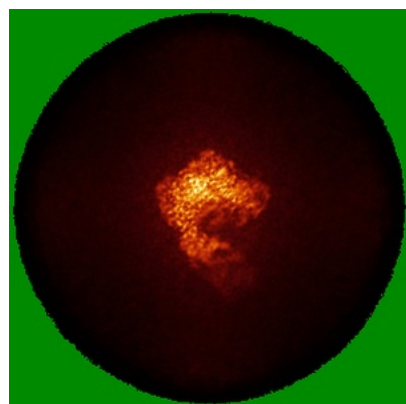


Z Index: 157

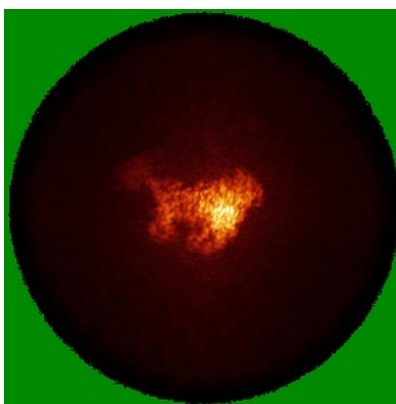
The images above show the largest variance slices of the map in three orthogonal directions.

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

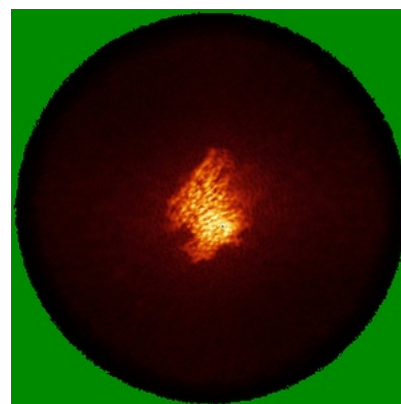
### 6.4.1 Primary map



X

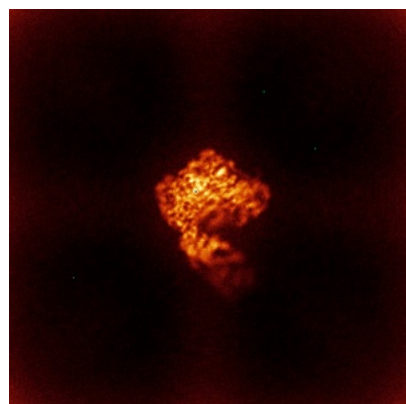


Y

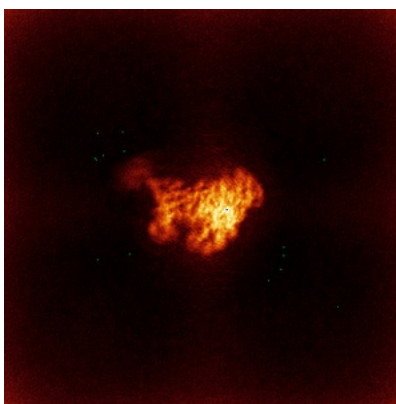


Z

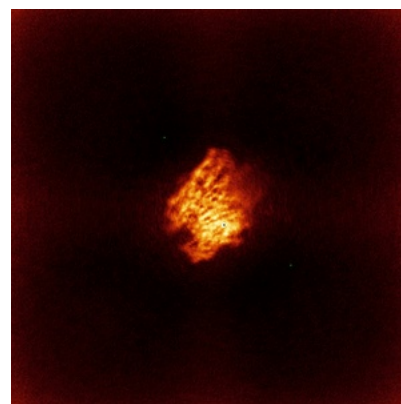
### 6.4.2 Raw map



X



Y



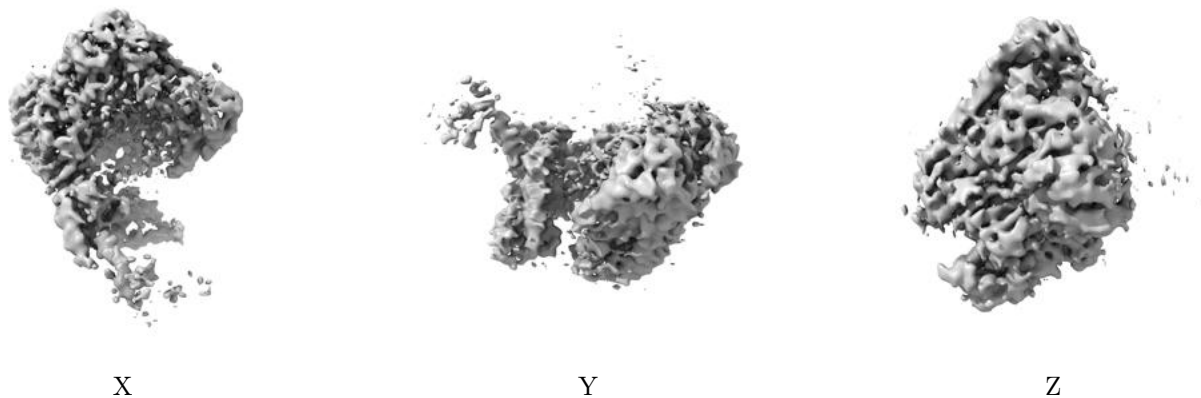
Z

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.



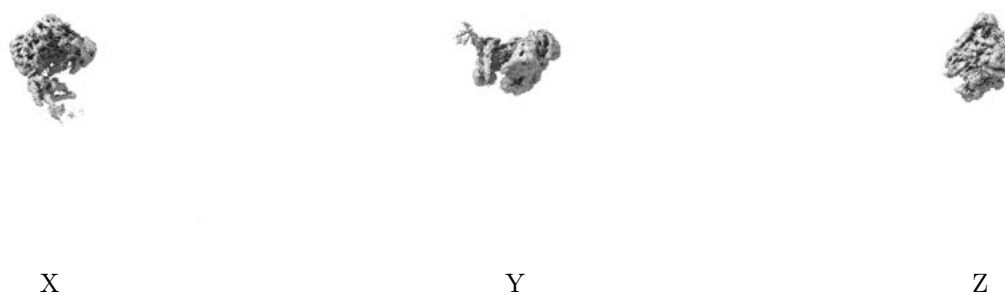
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.172. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

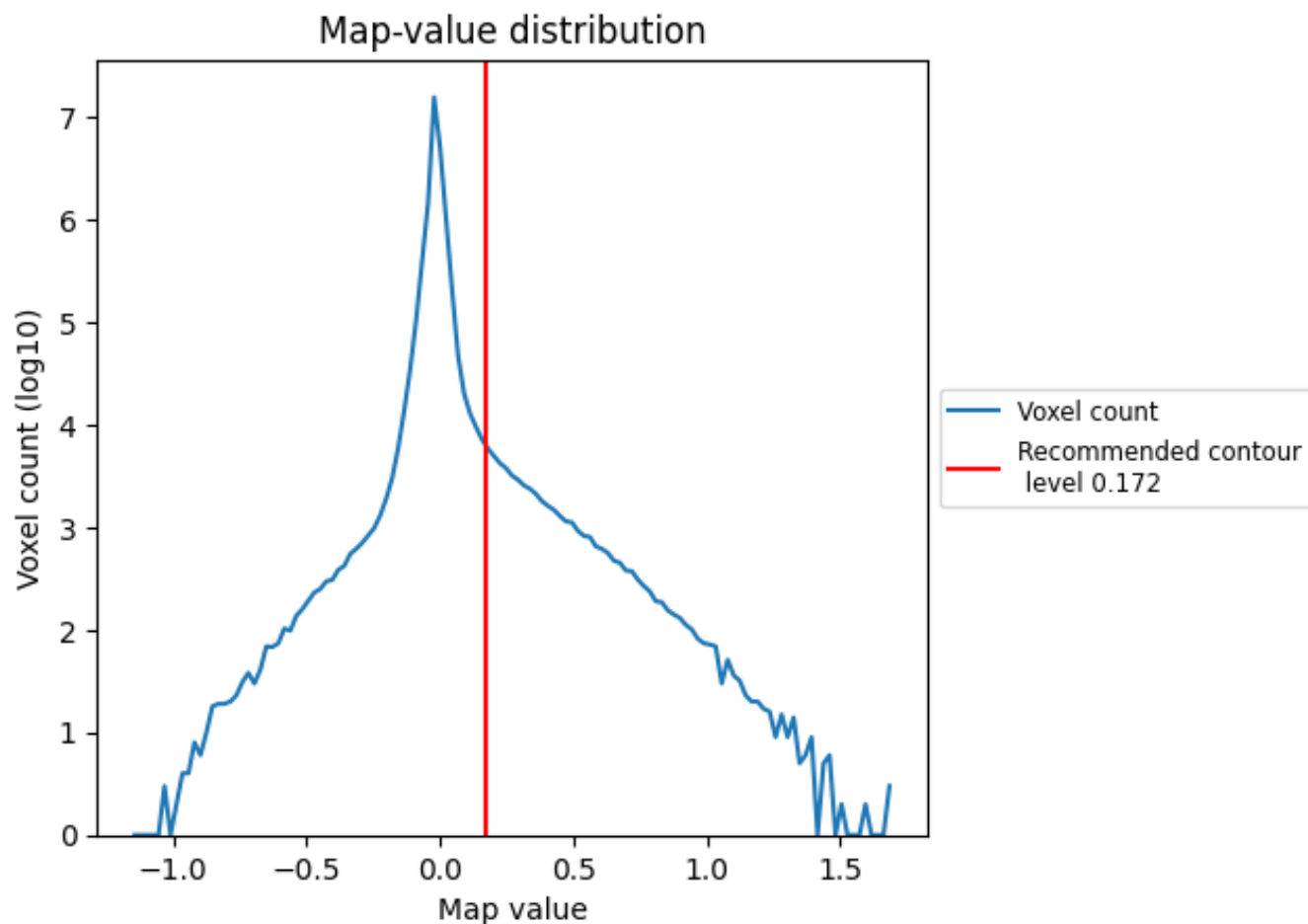
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

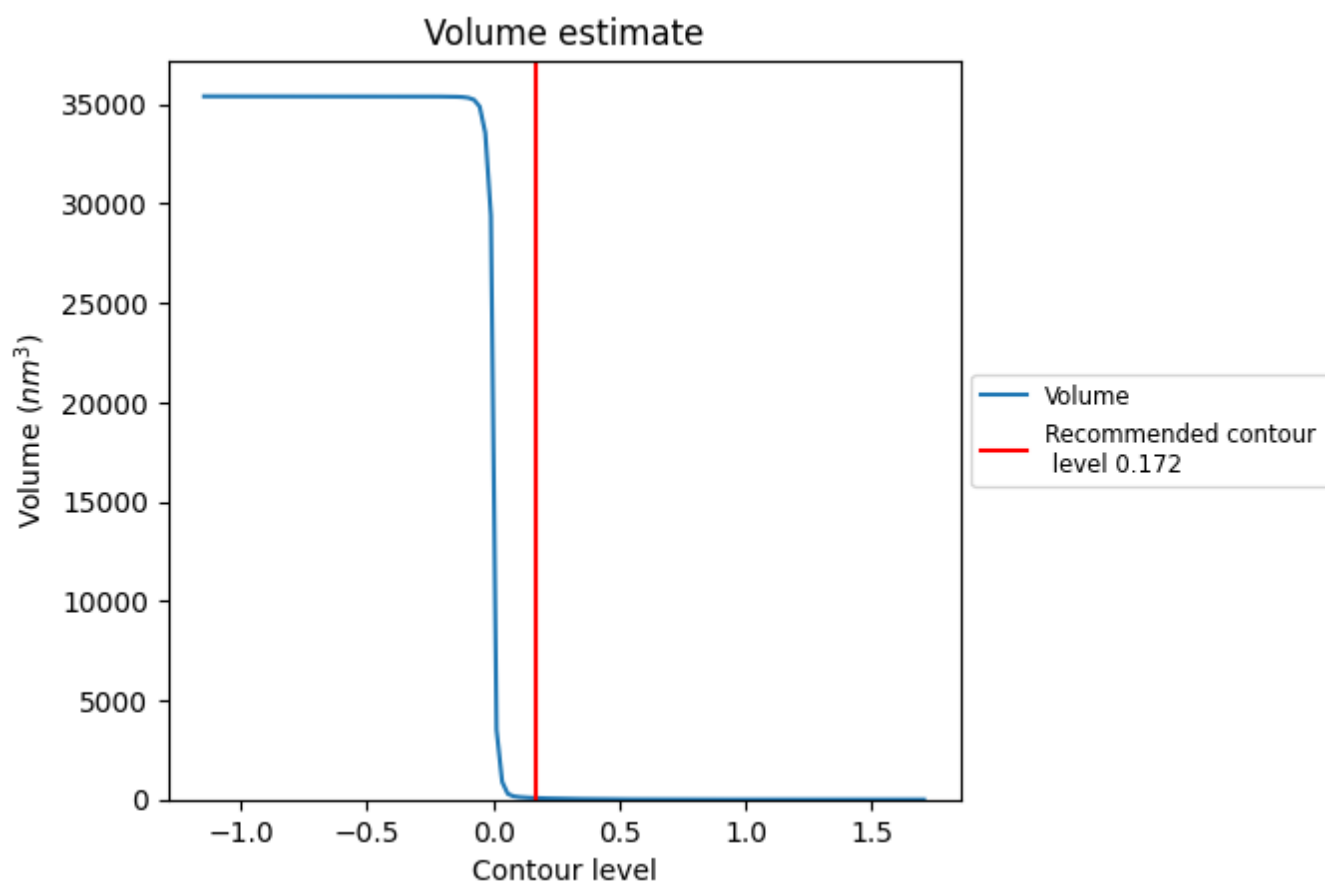
### 7.1 Map-value distribution [i](#)



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



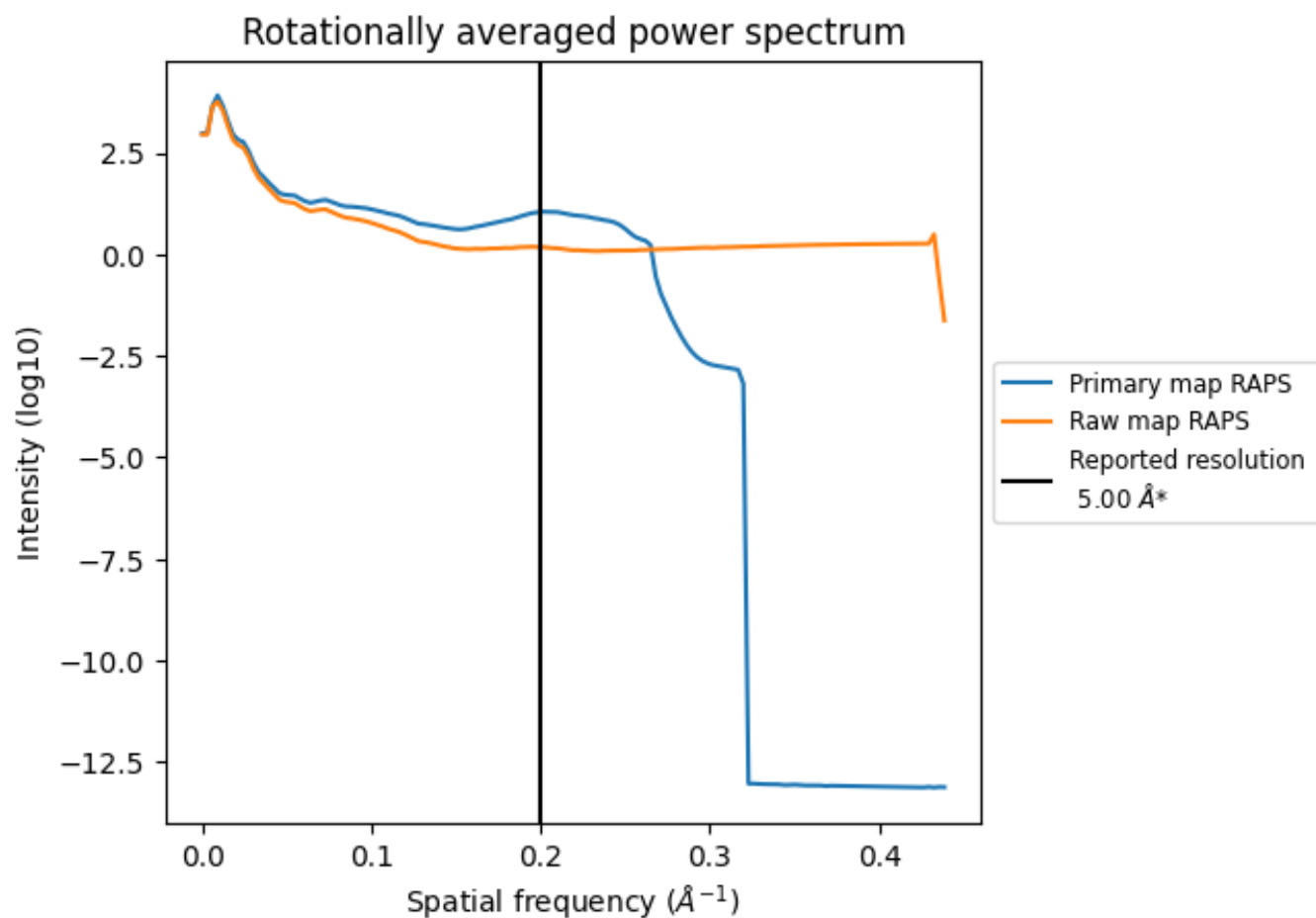
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 76 nm<sup>3</sup>; this corresponds to an approximate mass of 69 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 ⓘ

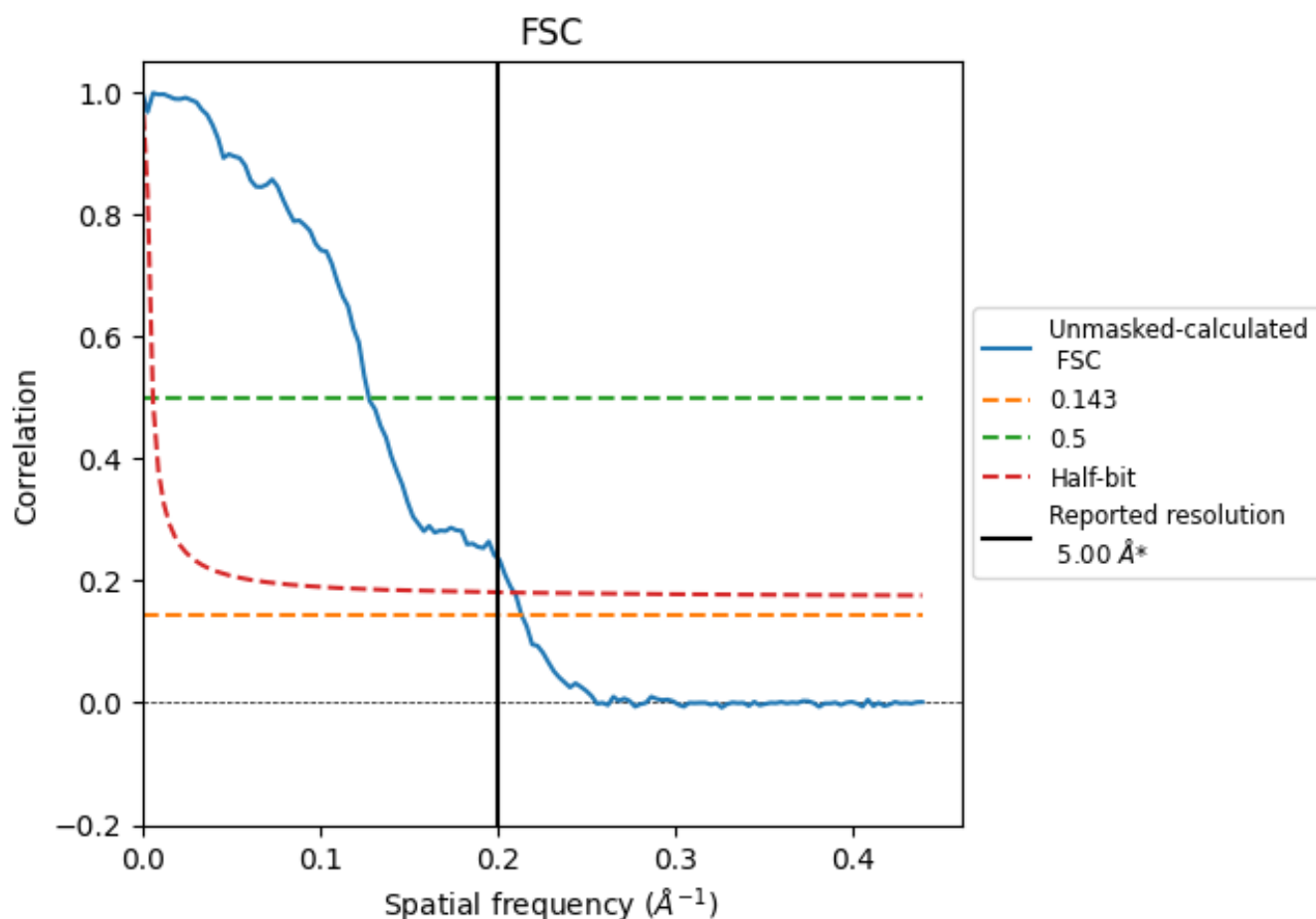


\*Reported resolution corresponds to spatial frequency of 0.200 Å<sup>-1</sup>

## 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 0.200 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

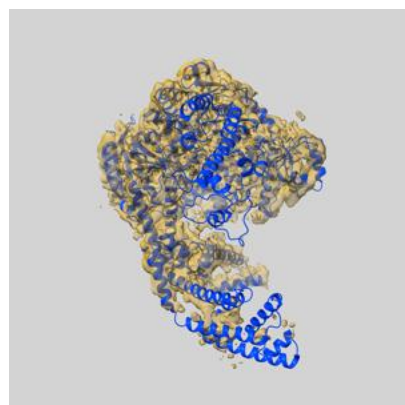
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.69	7.84	4.78

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

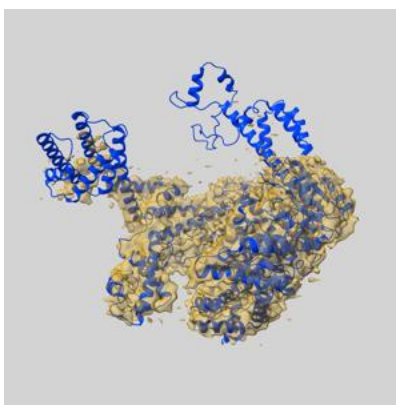
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53228 and PDB model 9QLI. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

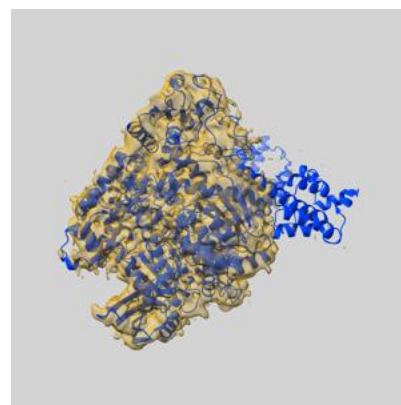
### 9.1 Map-model overlay [i](#)



X



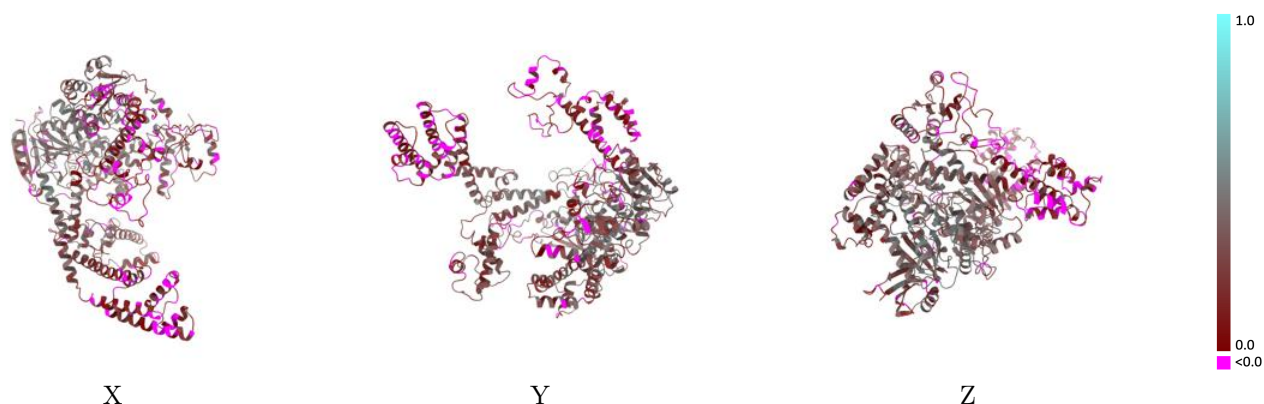
Y



Z

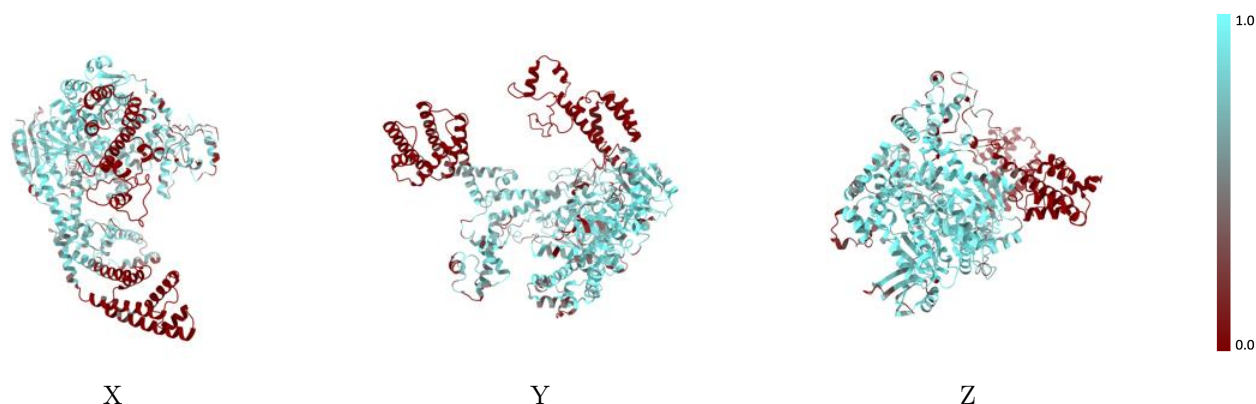
The images above show the 3D surface view of the map at the recommended contour level 0.172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



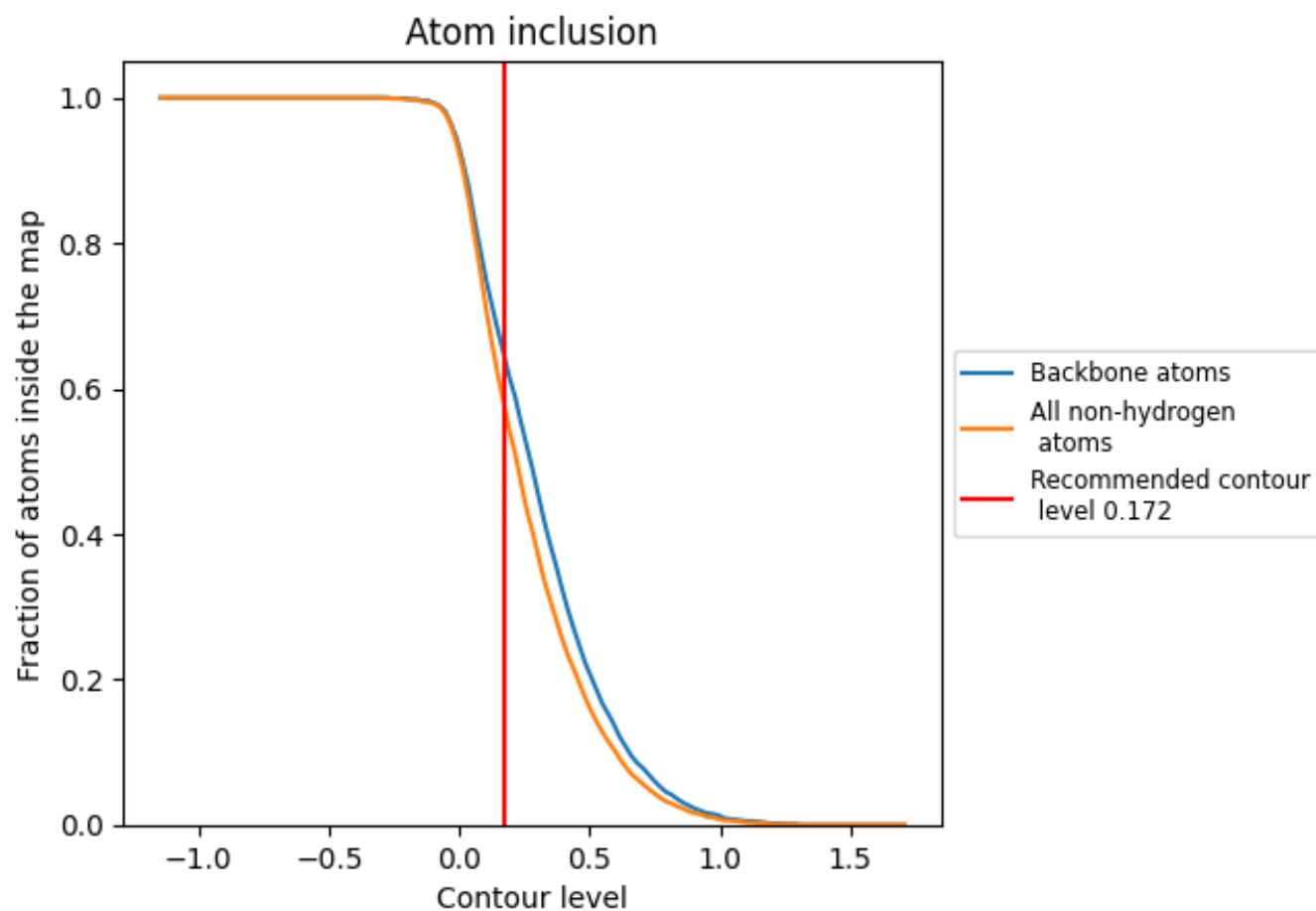
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.172).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 58% 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 (0.172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5780	<div></div> 0.2530
A	<div></div> 0.5790	<div></div> 0.2530

