



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:35 AM UTC

PDB ID : 7KPX / pdb_00007kpx
EMDB ID : EMD-22991
Title : Structure of the yeast CKM
Authors : Li, Y.C.; Chao, T.C.; Kim, H.J.; Cholko, T.; Chen, S.F.; Nakanishi, K.; Chang, C.E.; Murakami, K.; Garcia, B.A.; Boyer, T.G.; Tsai, K.L.
Deposited on : 2020-11-12
Resolution : 4.40 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

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:

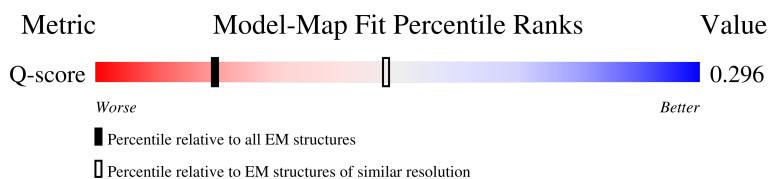
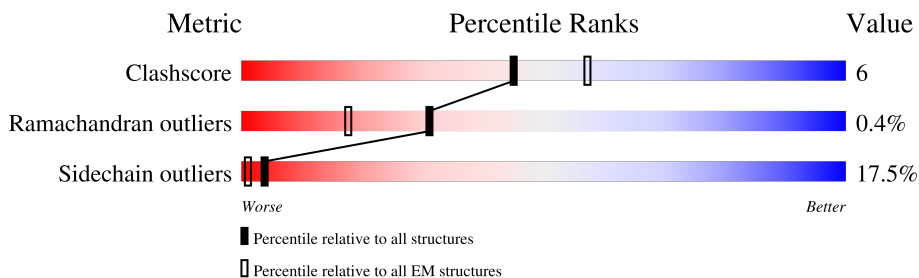
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.40 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	3132 (3.91 - 4.90)

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	555	
2	B	352	
3	C	1427	
4	D	1420	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20762 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 Meiotic mRNA stability protein kinase SSN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	357	Total	C	N	O	S	0	0
			2952	1919	512	507	14		

- Molecule 2 is a protein called RNA polymerase II holoenzyme cyclin-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	290	Total	C	N	O	S	0	0
			2436	1591	404	429	12		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	324	SER	-	expression tag	UNP P47821
B	325	MET	-	expression tag	UNP P47821
B	326	GLU	-	expression tag	UNP P47821
B	327	LYS	-	expression tag	UNP P47821
B	328	ARG	-	expression tag	UNP P47821
B	329	ARG	-	expression tag	UNP P47821
B	330	TRP	-	expression tag	UNP P47821
B	331	LYS	-	expression tag	UNP P47821
B	332	LYS	-	expression tag	UNP P47821
B	333	ASN	-	expression tag	UNP P47821
B	334	PHE	-	expression tag	UNP P47821
B	335	ILE	-	expression tag	UNP P47821
B	336	ALA	-	expression tag	UNP P47821
B	337	VAL	-	expression tag	UNP P47821
B	338	SER	-	expression tag	UNP P47821
B	339	ALA	-	expression tag	UNP P47821
B	340	ALA	-	expression tag	UNP P47821
B	341	ASN	-	expression tag	UNP P47821
B	342	ARG	-	expression tag	UNP P47821
B	343	PHE	-	expression tag	UNP P47821
B	344	LYS	-	expression tag	UNP P47821

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Chain	Residue	Modelled	Actual	Comment	Reference
B	345	LYS	-	expression tag	UNP P47821
B	346	ILE	-	expression tag	UNP P47821
B	347	SER	-	expression tag	UNP P47821
B	348	SER	-	expression tag	UNP P47821
B	349	SER	-	expression tag	UNP P47821
B	350	GLY	-	expression tag	UNP P47821
B	351	ALA	-	expression tag	UNP P47821
B	352	LEU	-	expression tag	UNP P47821

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1352	Total	C	N	O	S	0	0
			8362	5201	1544	1600	17		

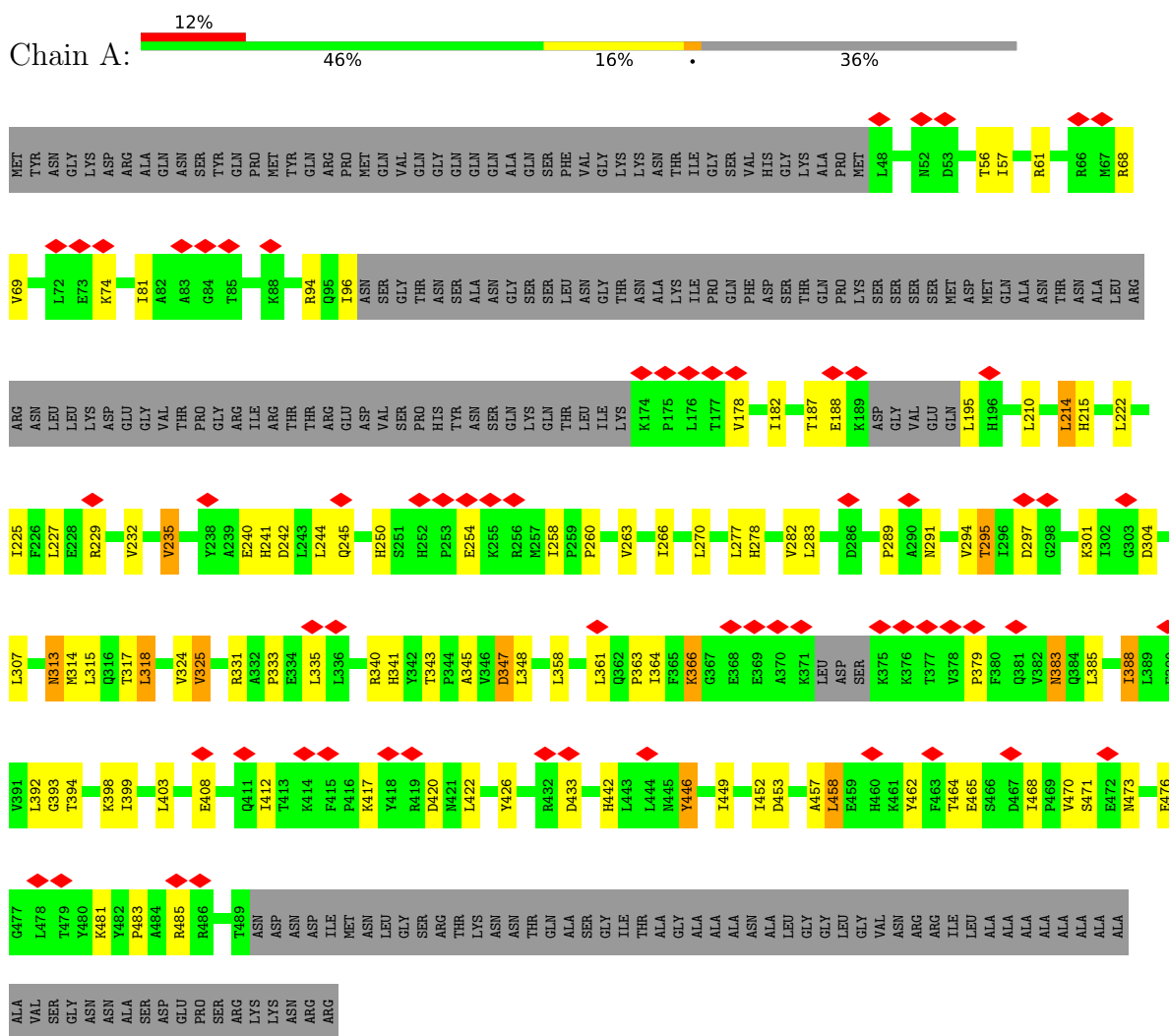
- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	876	Total	C	N	O	S	0	0
			7012	4530	1176	1272	34		

3 Residue-property plots

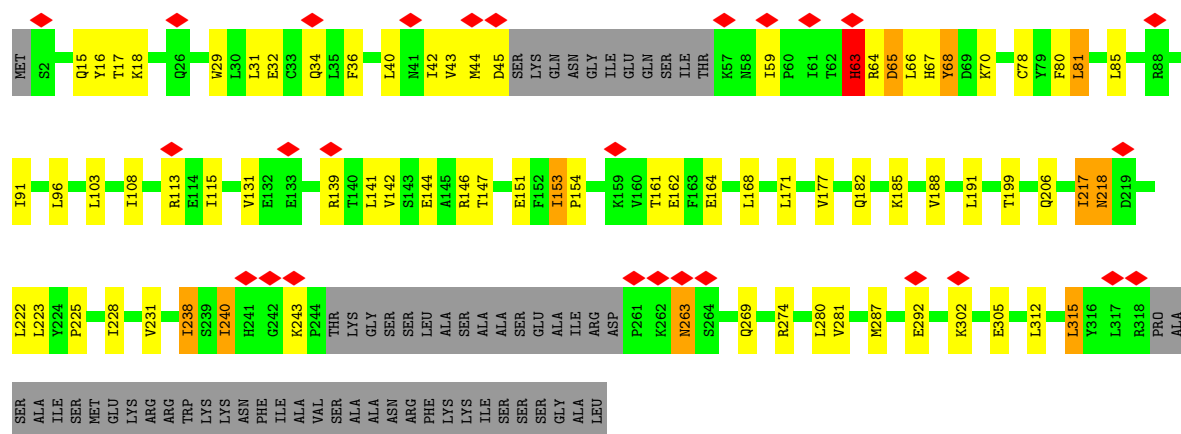
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Meiotic mRNA stability protein kinase SSN3

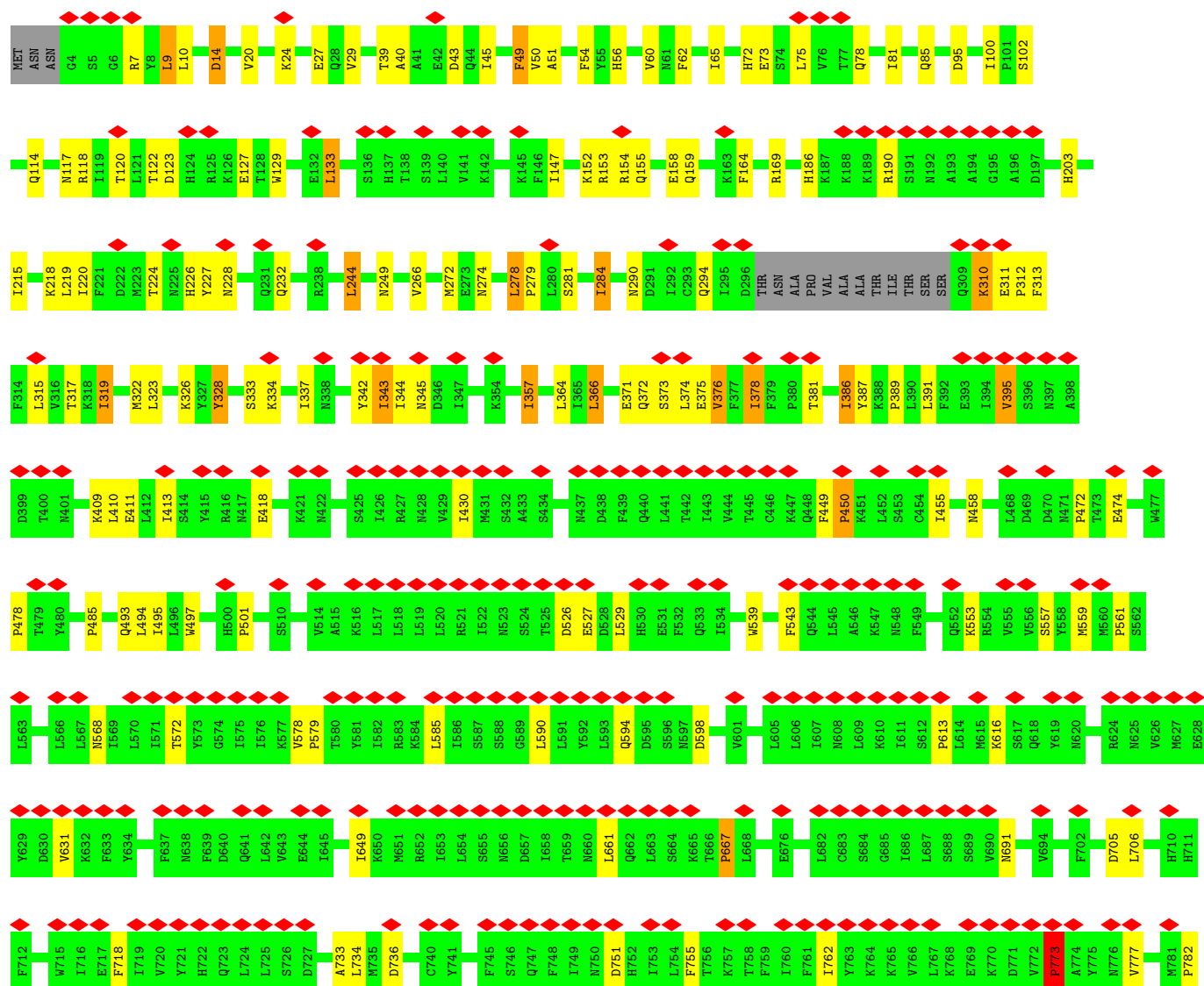
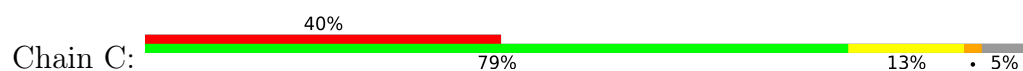


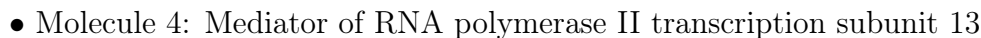
- Molecule 2: RNA polymerase II holoenzyme cyclin-like subunit





• Molecule 3: Mediator of RNA polymerase II transcription subunit 12





C1342	V1244	GLN	THR	ILE	PRO	THR	VAL	ASN	GLY
F1343	V1245	GLN	PRO	PRO	ASP	THR	ASP	ASN	LEU
H1344	G1246	GLN	ALA	GLN	ASP	THR	ASN	ASN	LEU
S1345	D1247	GLN	ASP	GLU	ILE	GLY	LYS	LYS	SER
D1346	D1248	GLN	PRO	SER	PRO	SER	LYS	PRO	SER
S1347	D1249	GLN	ASN	LEU	ASN	ASN	ILE	ASN	ILE
L1364	K1252	ASN	SER	PHE	THR	GLY	GLY	ALA	ALA
L1370	S1253	ASN	GLU	GLY	THR	ARG	LYS	THR	GLY
E1374	F1254	THR	SER	VAL	ILE	ARG	LYS	ALA	ASN
D1375	I1255	GLY	ASP	VAL	HIS	THR	LYS	PRO	PRO
G1376	I1256	S1142	S814	SER	GLU	LEU	ALA	ALA	LEU
H1377	D1257	S1143	S815	SER	GLU	THR	PHE	ASP	SER
I1378	E1258	S1144	S816	SER	GLU	THR	PHE	ASP	SER
I1382	F1259	I1145	L821	GLN	TYR	PRO	GLN	LEU	ASN
V1385	K1260	I1041	L826	ILE	ASN	ILE	LYS	PRO	THR
M1389	L1261	E1042	L832	GLU	TYR	GLU	GLU	MET	ASN
V1393	K1266	K1046	L835	SER	SER	GLU	GLU	ASP	THR
R1396	D1271	R1158	L836	ASN	SER	GLU	GLU	GLN	GLU
V1397	T1272	S1159	P836	ILE	ILE	LEU	LEU	ARG	GLN
A1400	F1273	D1160	T837	LYS	PRO	GLY	ASN	ASN	ASN
ASN	D1274	K1162	V840	MET	SER	THR	GLN	ASN	ASN
THR	G1275	L1169	P842	LEU	GLN	PRO	GLU	GLU	GLU
SER	G1276	Q1175	P943	GLU	ASN	LEU	ASN	ASN	LEU
ALA	G1277	G1176	N948	ASP	SER	MET	LYS	PHE	THR
VAL	G1278	S1177	L852	ASN	ILE	ALA	ASP	ASP	THR
HIS	D1279	T1181	K855	VAL	LYS	LEU	LEU	ARG	ILE
THR	L1282	S1187	Q856	THR	GLN	SER	LYS	LYS	SER
ALA	F1191	K1190	V857	ASN	ASN	PRO	GLN	ASN	GLN
THR	D1192	D1192	T859	THR	ASN	GLU	ASN	ASP	THR
ALA	W1199	W1199	L863	PHE	VAL	GLU	GLU	ASP	THR
SER	L1205	L1205	L867	THR	ASP	ASP	GLU	ASP	THR
SER	I1213	I1213	Q869	ASN	ALA	GLU	GLU	LEU	LEU
ILE	L1215	L1215	L869	VAL	ILE	GLU	ASP	GLY	ASN
ILE	L1216	L1216	P870	ASN	THR	GLY	ASN	GLY	ASN
LEU	L1217	L1217	K871	SER	SER	ARG	GLY	ASP	THR
SER	Q1310	Q1310	V877	GLU	ASN	LYS	ASP	ILE	ASN
ASP	H1311	H1311	K878	SER	GLY	VAL	PRO	LEU	LEU
LYS	A1312	A1312	D879	ASN	PHE	LEU	ASP	SER	LEU
	I1315	I1315	C880	PRO	ASN	LYS	LYS	PHE	ALA
	I1321	I1321	Q881	LYS	SER	ASN	ASN	GLY	ASP
	C1326	C1326	E882	LYS	ILE	LEU	LYS	GLY	PHE
	D1327	D1327	Q883	LYS	TRP	ASN	ASN	ARG	SER
	G1328	G1328	L884	SER	LYS	VAL	ASN	ASN	ASN
	D1329	D1329	T886	GLY	ILE	ARG	LYS	LYS	PHE
	W1332	W1332	V889	ILE	PRO	ASP	ILE	ARG	THR
			L898	THR	GLN	ASP	ILE	THR	GLY
			K1002	ILE	ASN	MET	ASN	ASN	ILE
			L1005	PRO	GLN	ASN	LYS	VAL	ASN
			L1006	PHE	PHE	THR	ASN	THR	ASN
			K1020	ASN	ASP	LYS	THR	ASN	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138178	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 ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	410.88, 410.88, 410.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.21	0/3030	0.57	2/4098 (0.0%)
2	B	0.22	0/2505	0.53	1/3407 (0.0%)
3	C	0.51	1/8467 (0.0%)	0.99	56/11647 (0.5%)
4	D	0.23	0/7183	0.57	3/9753 (0.0%)
All	All	0.37	1/21185 (0.0%)	0.76	62/28905 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	661	LEU	C-O	5.06	1.30	1.24

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	494	LEU	N-CA-C	15.24	127.60	111.14
3	C	495	ILE	N-CA-C	12.20	124.91	113.20
4	D	1027	PRO	N-CA-C	10.88	123.97	110.70
3	C	1073	ASP	N-CA-C	10.81	123.07	111.28
4	D	1027	PRO	CA-C-N	-9.54	109.94	119.76

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	2952	0	2987	39	0
2	B	2436	0	2430	27	0
3	C	8362	0	5809	102	0
4	D	7012	0	7104	91	0
All	All	20762	0	18330	247	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 6.

The worst 5 of 247 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)
3:C:373:SER:HB2	3:C:1318:GLN:CB	1.77	1.15
3:C:102:SER:CB	3:C:1413:ASN:HD21	1.60	1.13
3:C:373:SER:CB	3:C:1318:GLN:CB	2.29	1.10
3:C:102:SER:HB2	3:C:1413:ASN:HD21	1.05	1.09
3:C:311:GLU:CG	3:C:312:PRO:HD3	1.88	1.03

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	349/555 (63%)	308 (88%)	41 (12%)	0	100	100
2	B	284/352 (81%)	259 (91%)	25 (9%)	0	100	100
3	C	1344/1427 (94%)	1267 (94%)	67 (5%)	10 (1%)	18	55
4	D	870/1420 (61%)	782 (90%)	88 (10%)	0	100	100
All	All	2847/3754 (76%)	2616 (92%)	221 (8%)	10 (0%)	31	66

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1105	GLU
3	C	1106	PRO
3	C	1255	PRO
3	C	1316	PRO
3	C	667	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/474 (67%)	260 (82%)	57 (18%)	2	10
2	B	274/323 (85%)	226 (82%)	48 (18%)	2	11
3	C	460/1357 (34%)	385 (84%)	75 (16%)	2	12
4	D	793/1300 (61%)	651 (82%)	142 (18%)	2	10
All	All	1844/3454 (53%)	1522 (82%)	322 (18%)	4	11

5 of 322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	826	LEU
4	D	1181	THR
4	D	858	VAL
4	D	989	GLU
4	D	1249	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	29	HIS
4	D	198	HIS
4	D	120	ASN
4	D	205	GLN
2	B	63	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 [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](#)

There are no chain breaks in this entry.

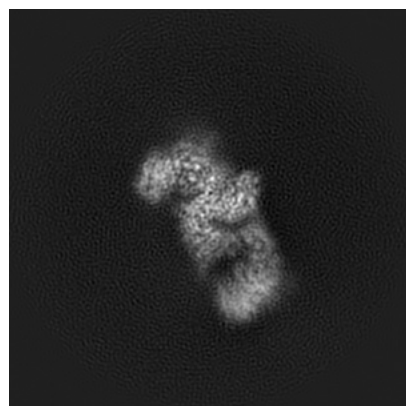
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22991. These allow visual inspection of the internal detail of the map and identification of artifacts.

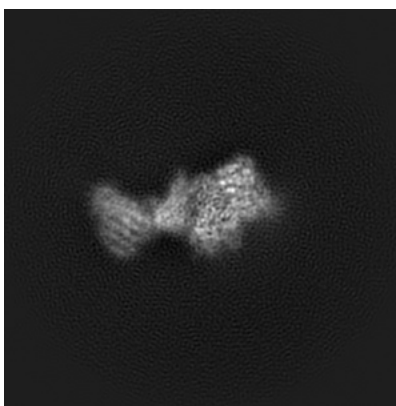
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

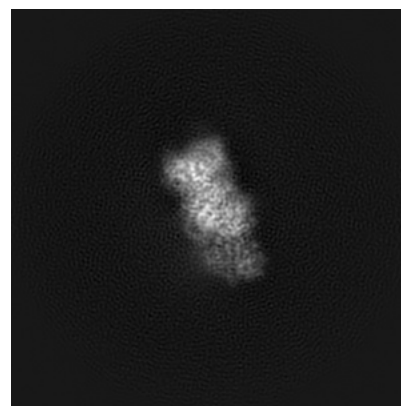
6.1.1 Primary map



X

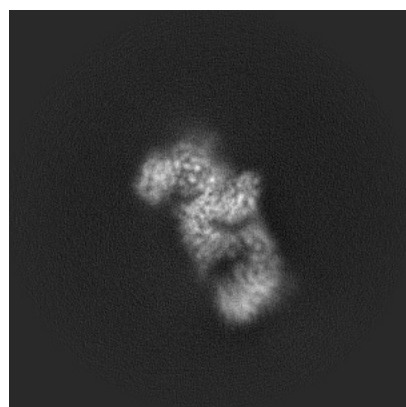


Y

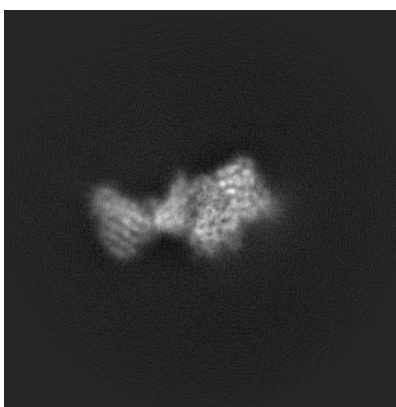


Z

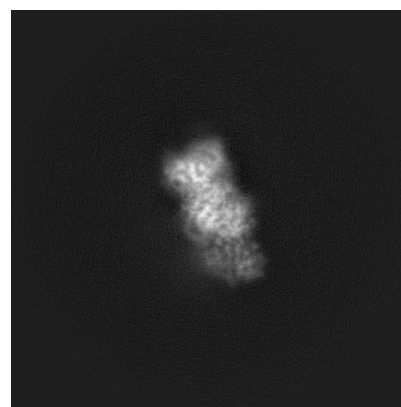
6.1.2 Raw map



X



Y

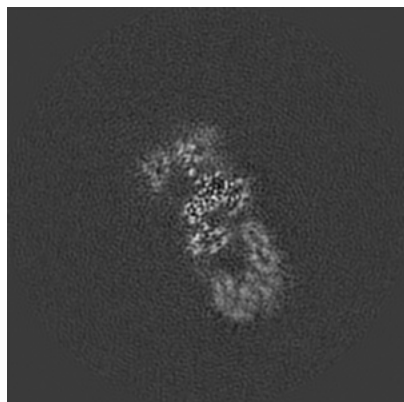


Z

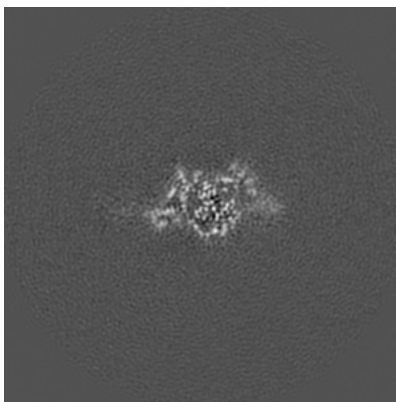
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

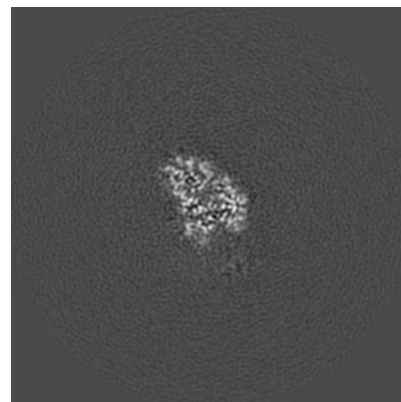
6.2.1 Primary map



X Index: 192

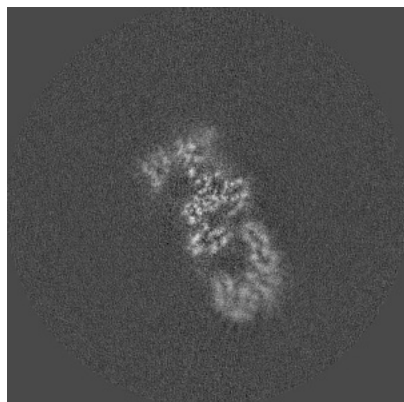


Y Index: 192

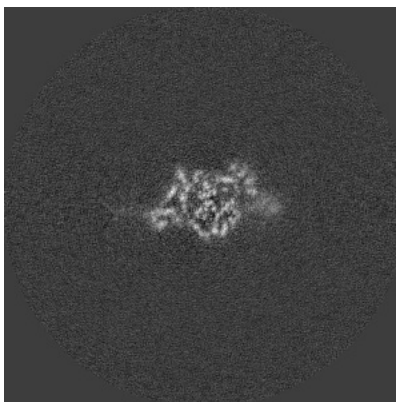


Z Index: 192

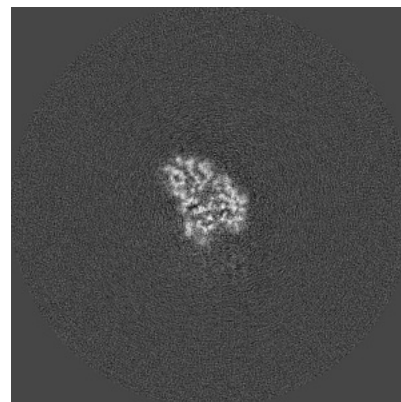
6.2.2 Raw map



X Index: 192



Y Index: 192

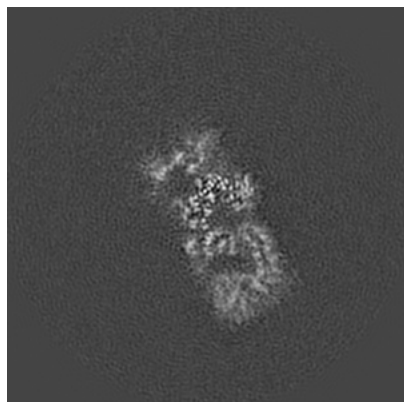


Z Index: 192

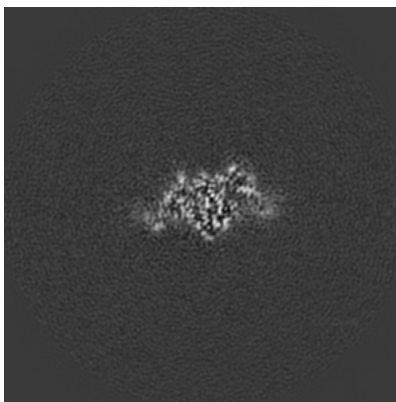
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

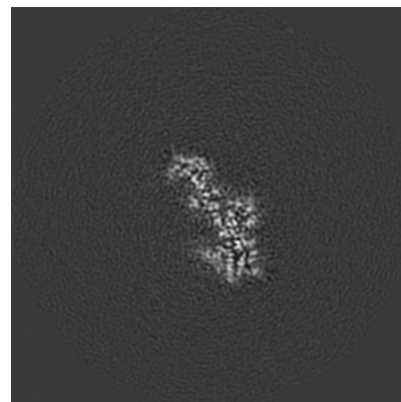
6.3.1 Primary map



X Index: 188

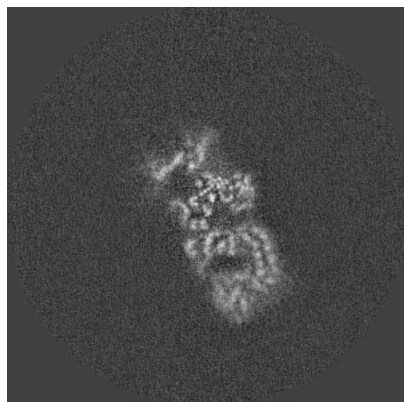


Y Index: 189

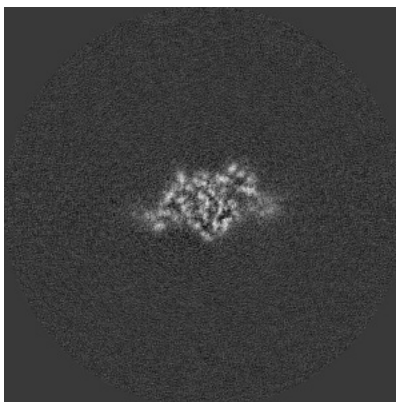


Z Index: 219

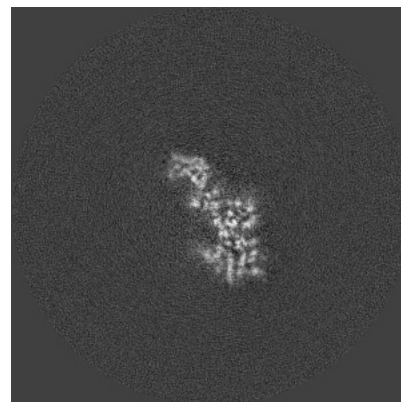
6.3.2 Raw map



X Index: 187



Y Index: 190

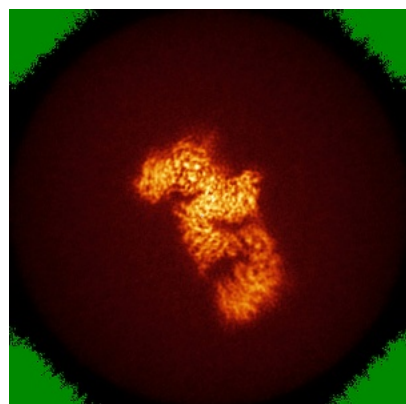


Z Index: 220

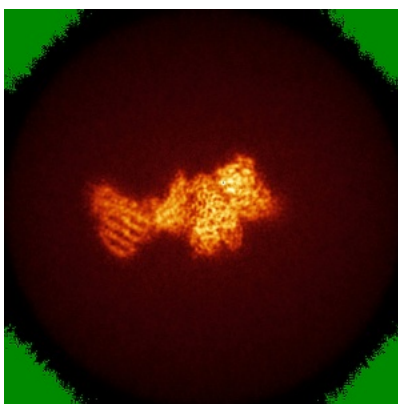
The images above show the largest variance slices of the map in three orthogonal directions.

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

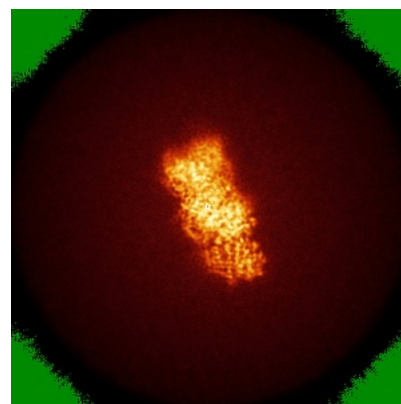
6.4.1 Primary map



X

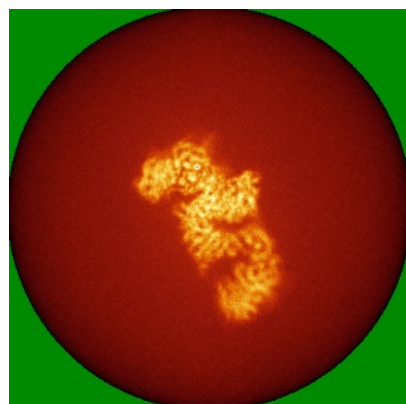


Y

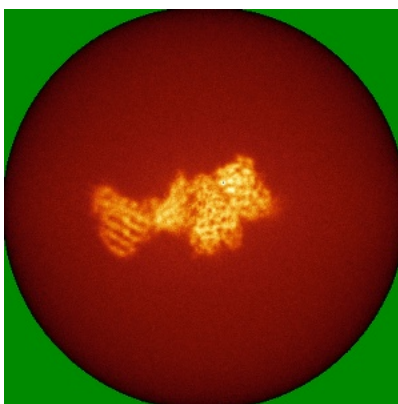


Z

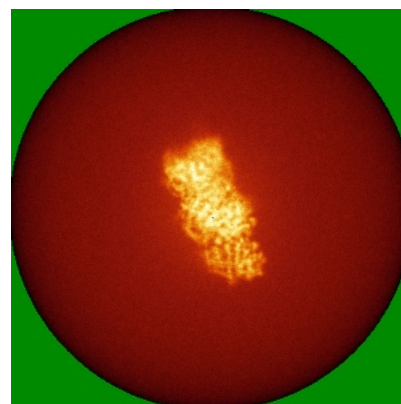
6.4.2 Raw map



X



Y

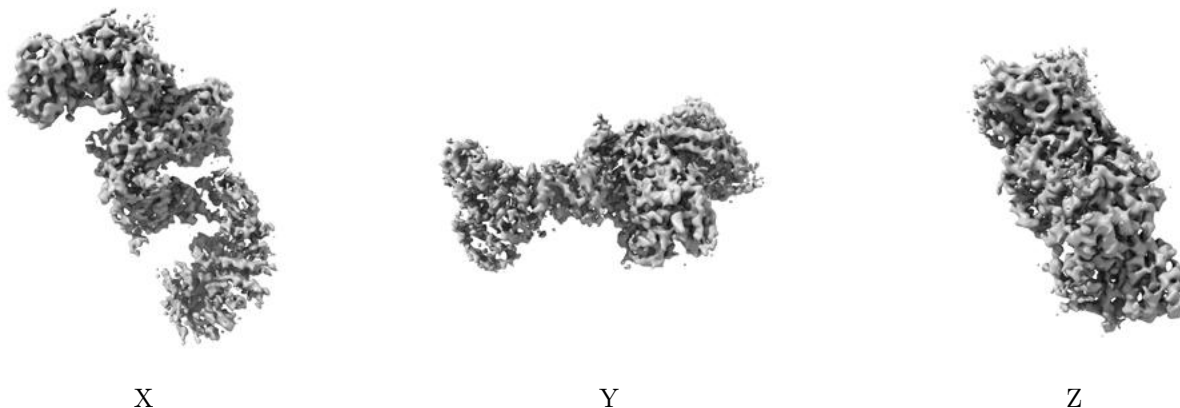


Z

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

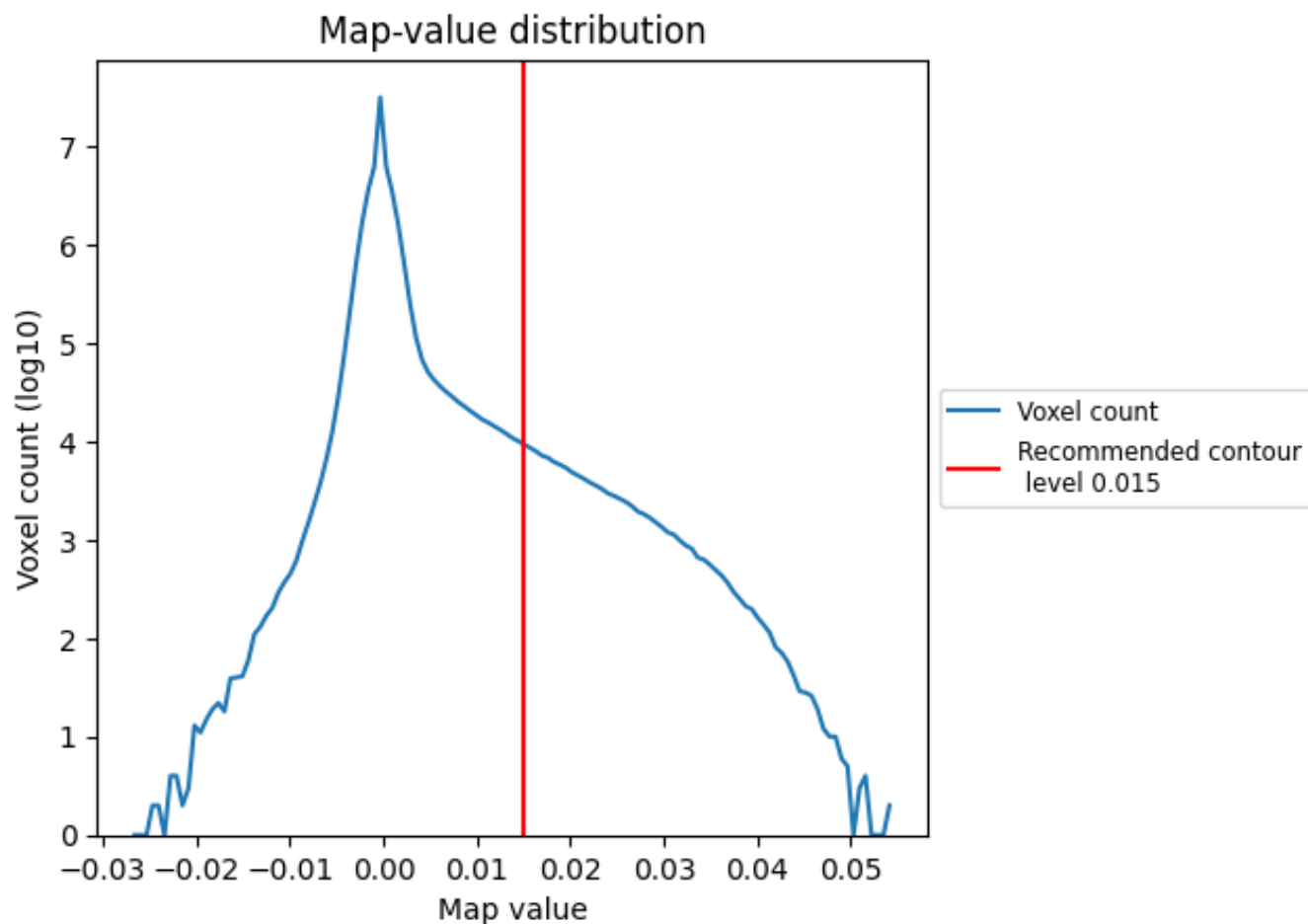
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

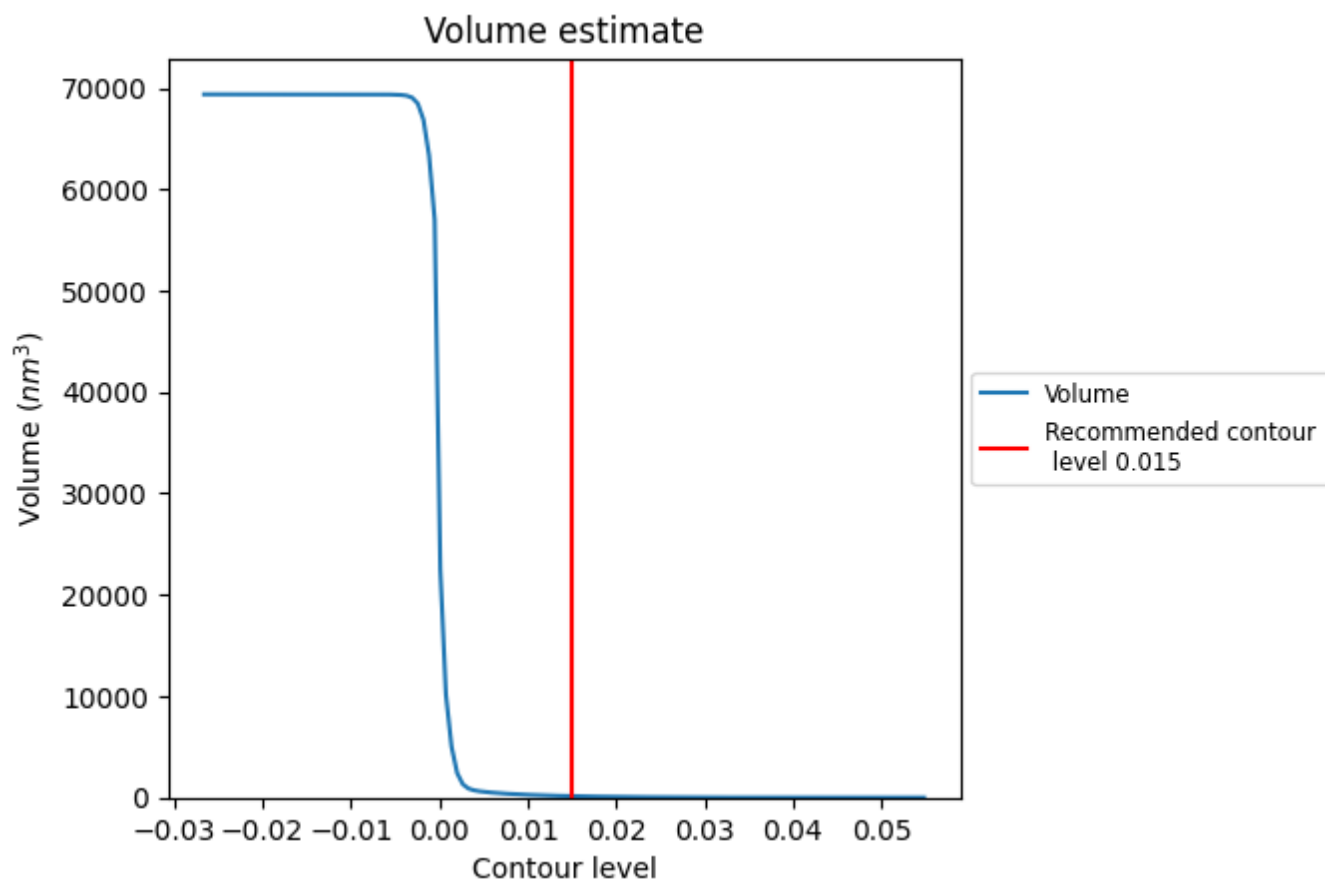
This section contains the results of statistical analysis of the map.

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.

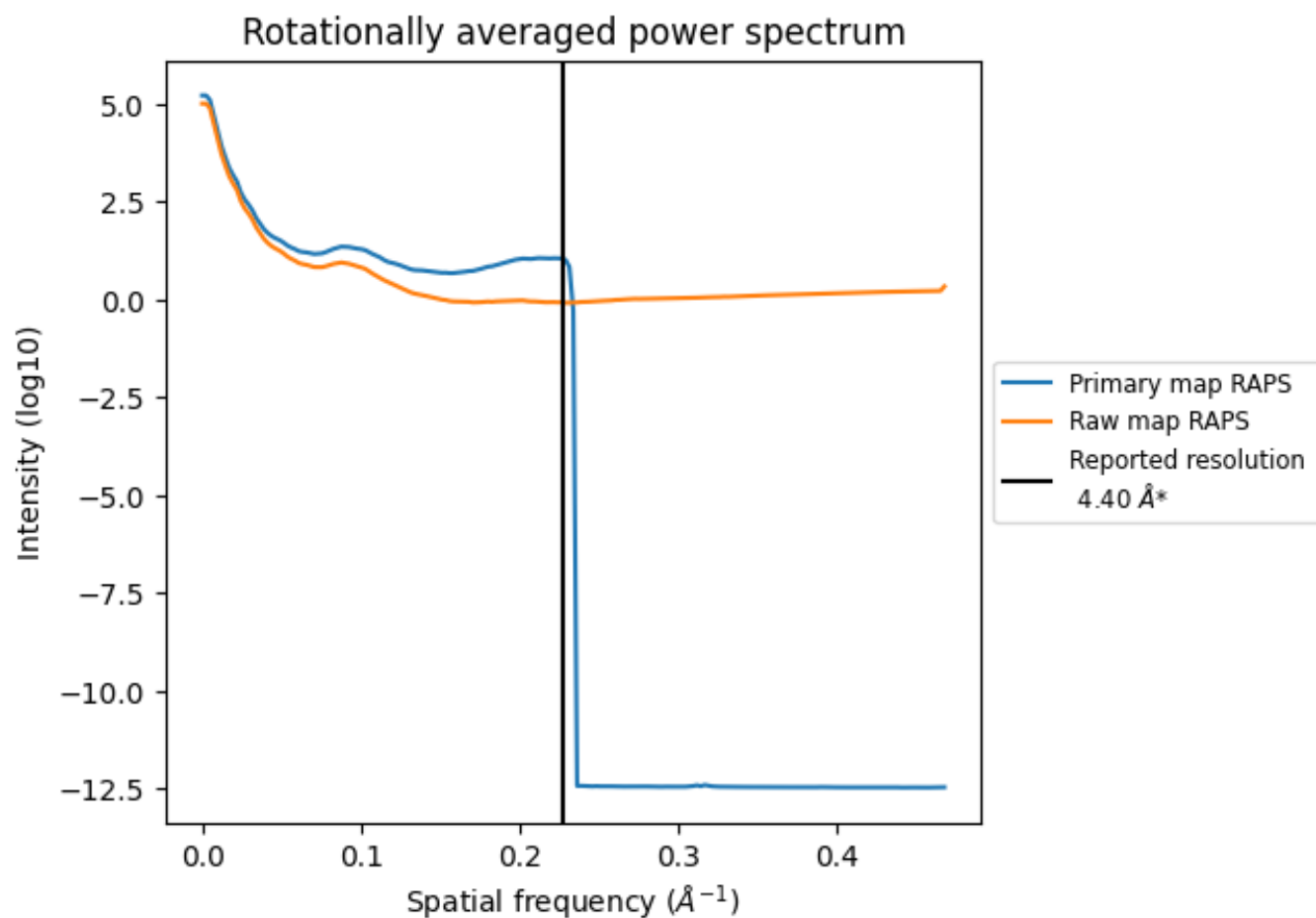
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm³; this corresponds to an approximate mass of 126 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 ⓘ

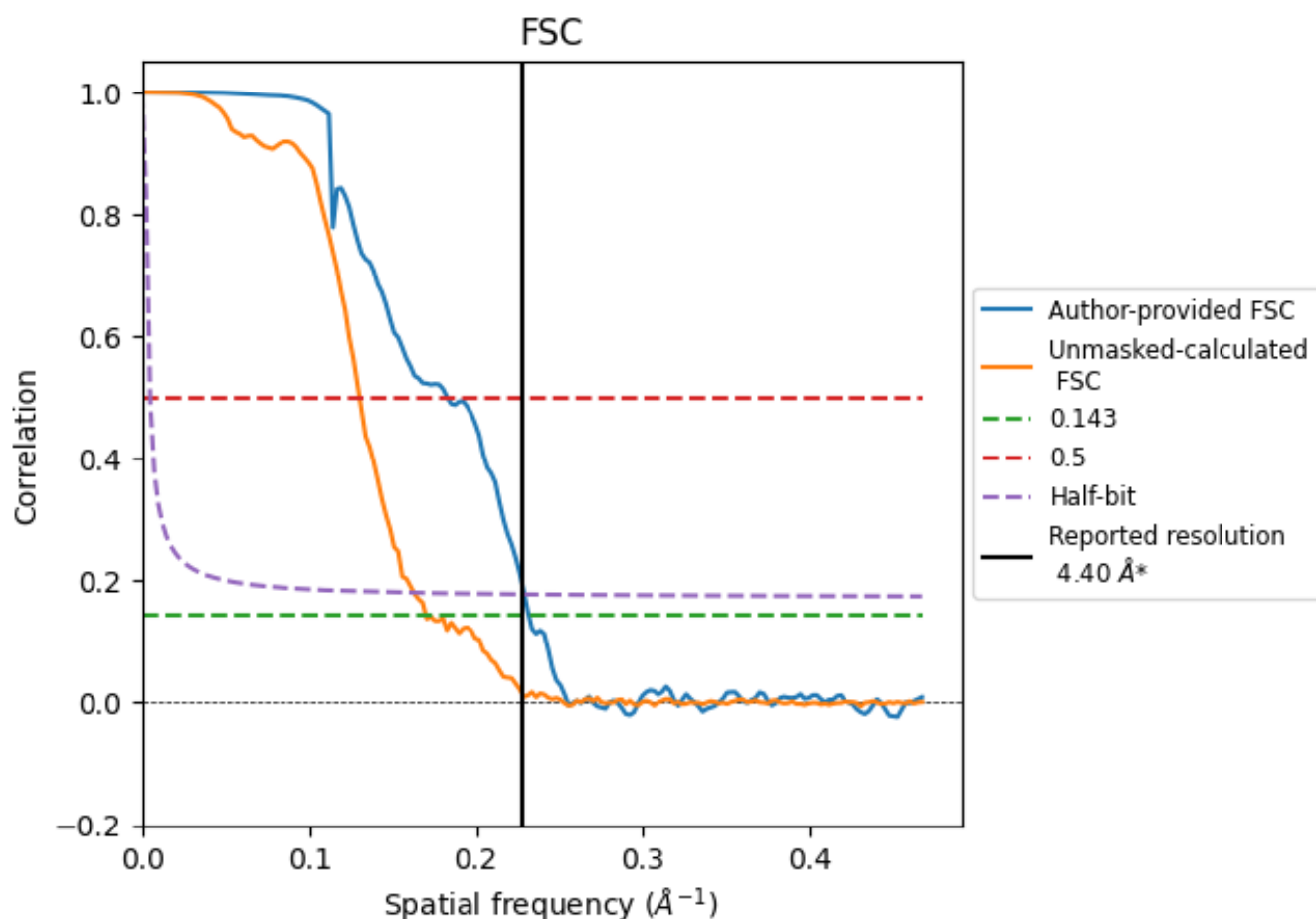


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 $0.227 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

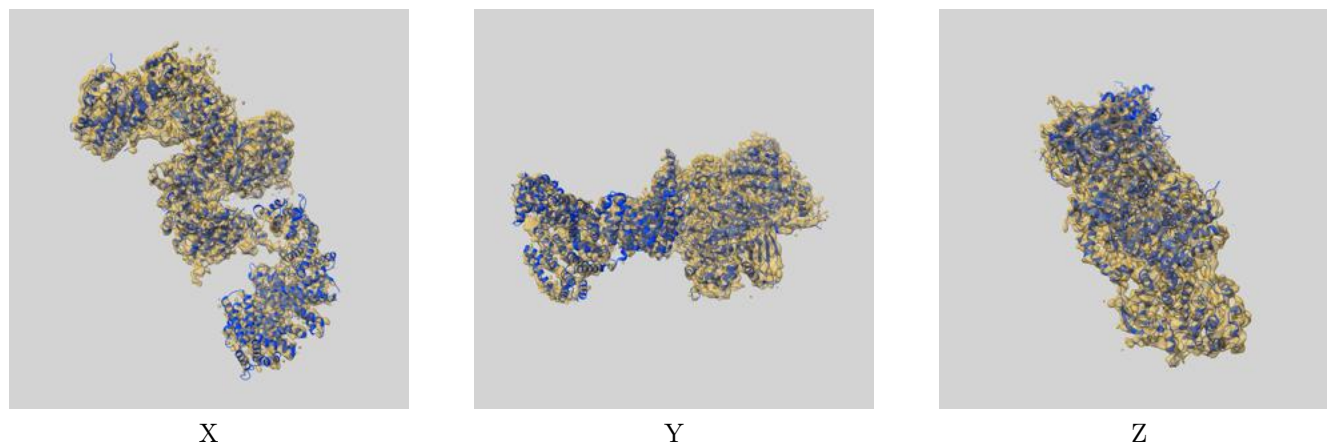
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.32	5.47	4.37
Unmasked-calculated*	5.89	7.68	6.15

*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 5.89 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

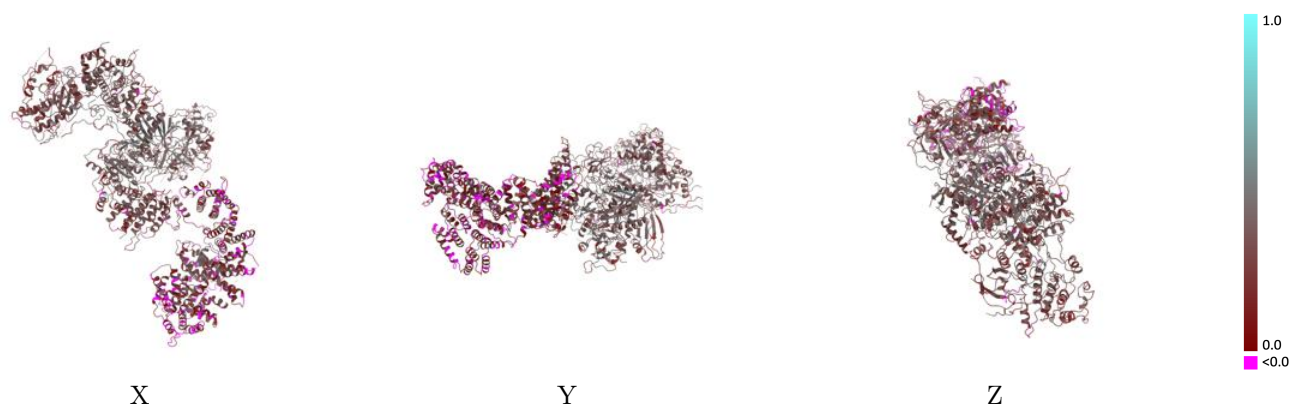
This section contains information regarding the fit between EMDB map EMD-22991 and PDB model 7KPX. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



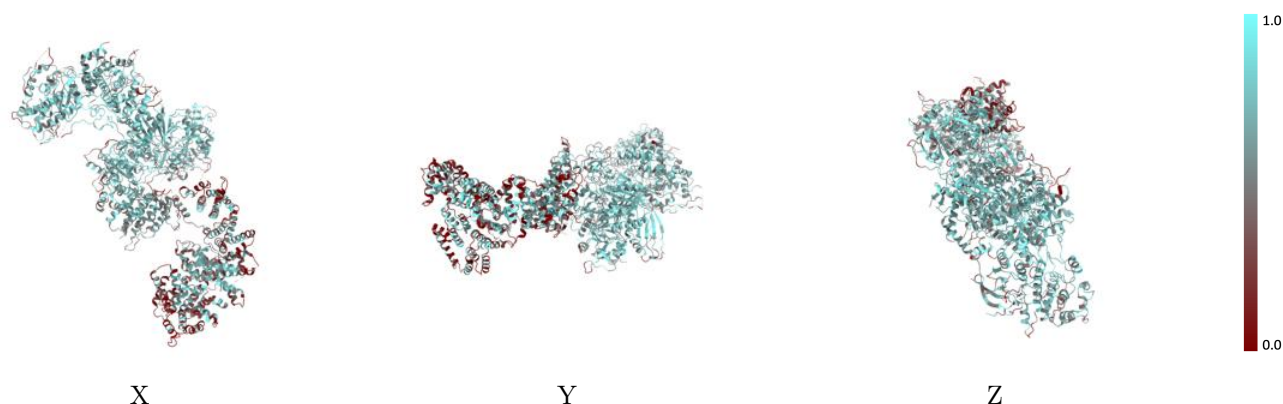
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



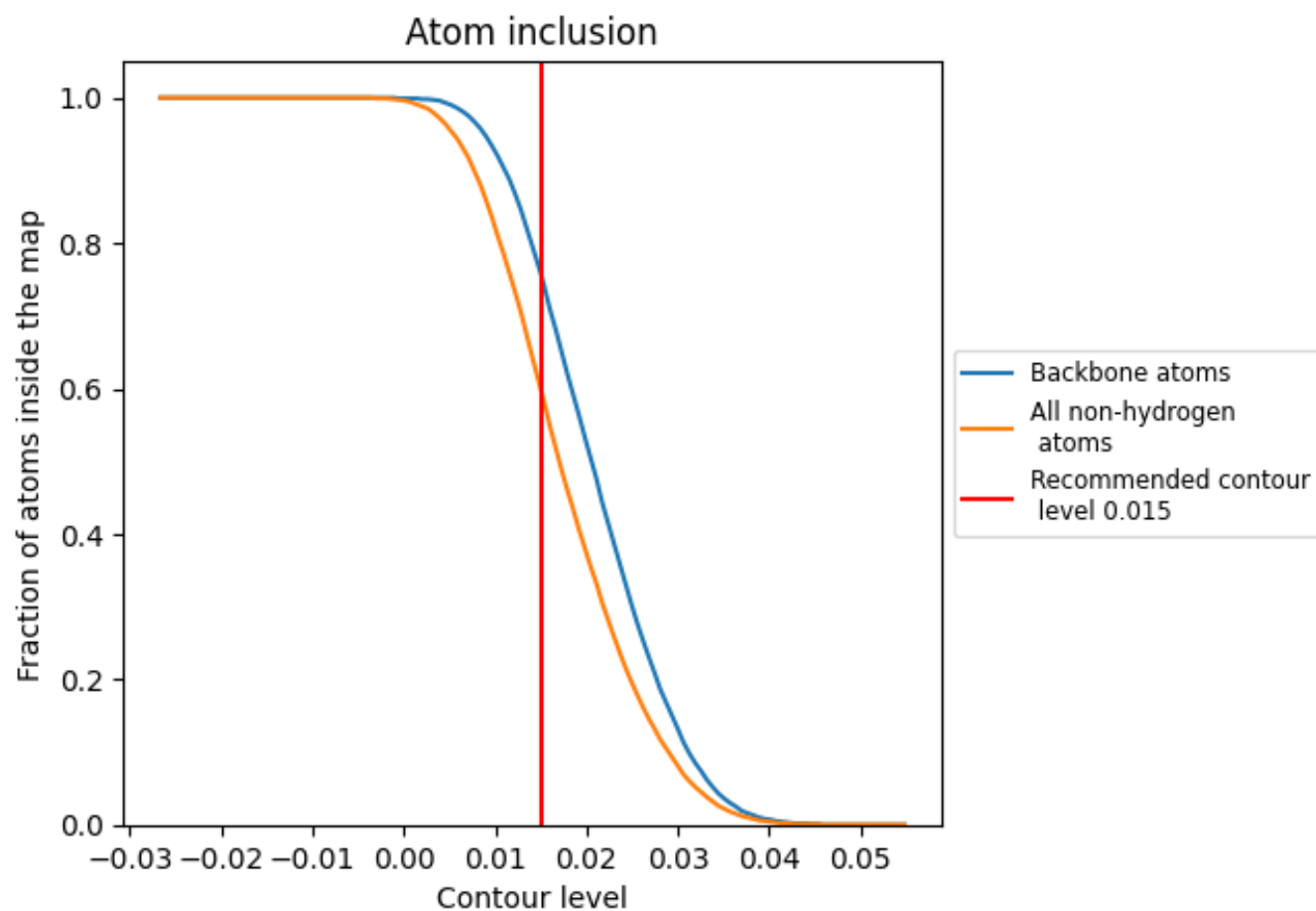
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 60% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5990	0.2960
A	0.6120	0.2970
B	0.6640	0.3280
C	0.5120	0.2290
D	0.6770	0.3630

