wwPDB EM Validation Summary Report (i)

Nov 11, 2026 – 12:53 PM EST

PDB ID	:	7U5U / pdb_00007u5u
EMDB ID	:	EMD-26359
Title	:	Structure of the SK/DHQase/DHSD dimer from Candida albicans Aro1
Authors	:	Quade, B.; Borek, D.; Otwinowski, Z.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2022-03-02
Resolution	:	3.16 Å(reported)
Based on initial model	:	7TBV

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 (i) 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 (i)) were used in the production of this report:

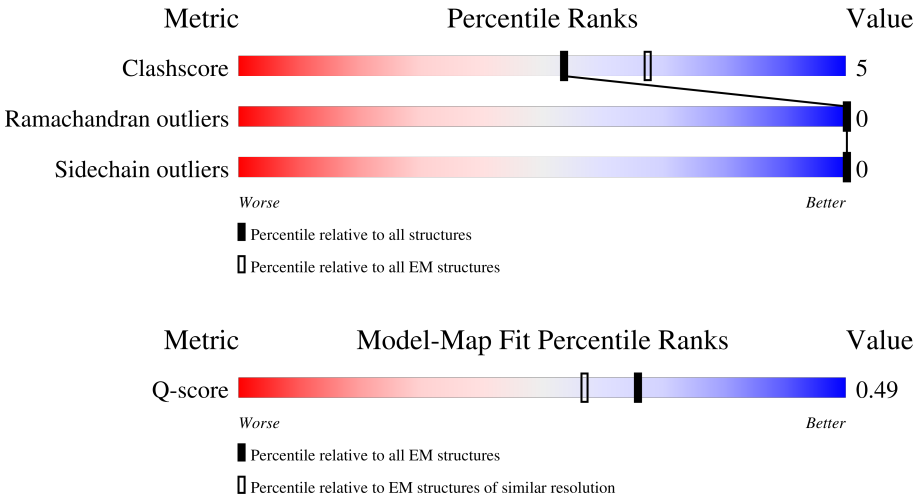
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 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	14474 (2.66 - 3.66)

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 <=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	1551	6% 36% 5% 59%
1	B	1551	36% 5% 58%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 10035 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 Pentafunctional AROM polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	638	Total	C	N	O	S	0	0
			4983	3181	844	944	14		
1	B	645	Total	C	N	O	S	0	0
			5052	3230	853	956	13		

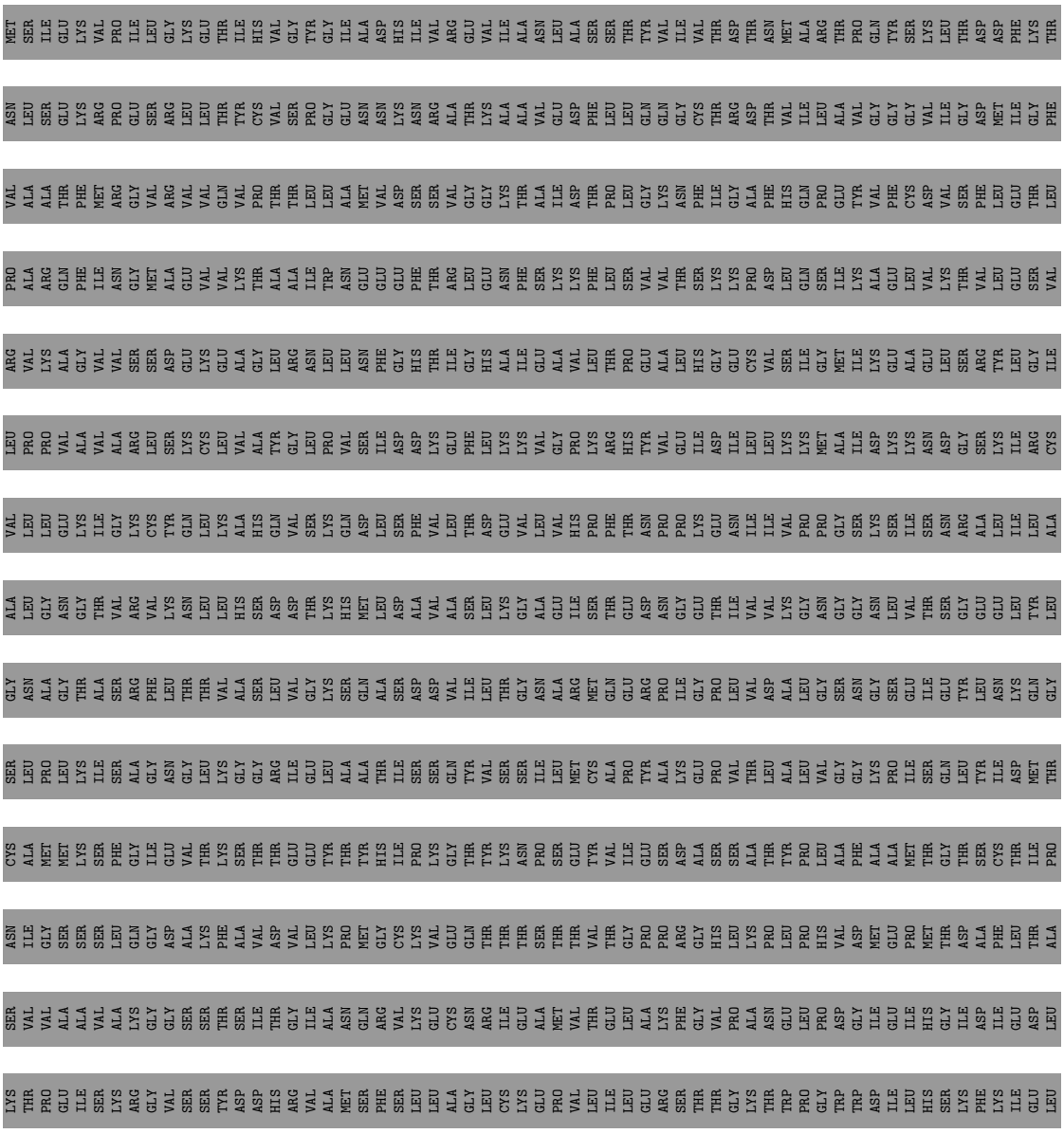
3 Residue-property plots (i)

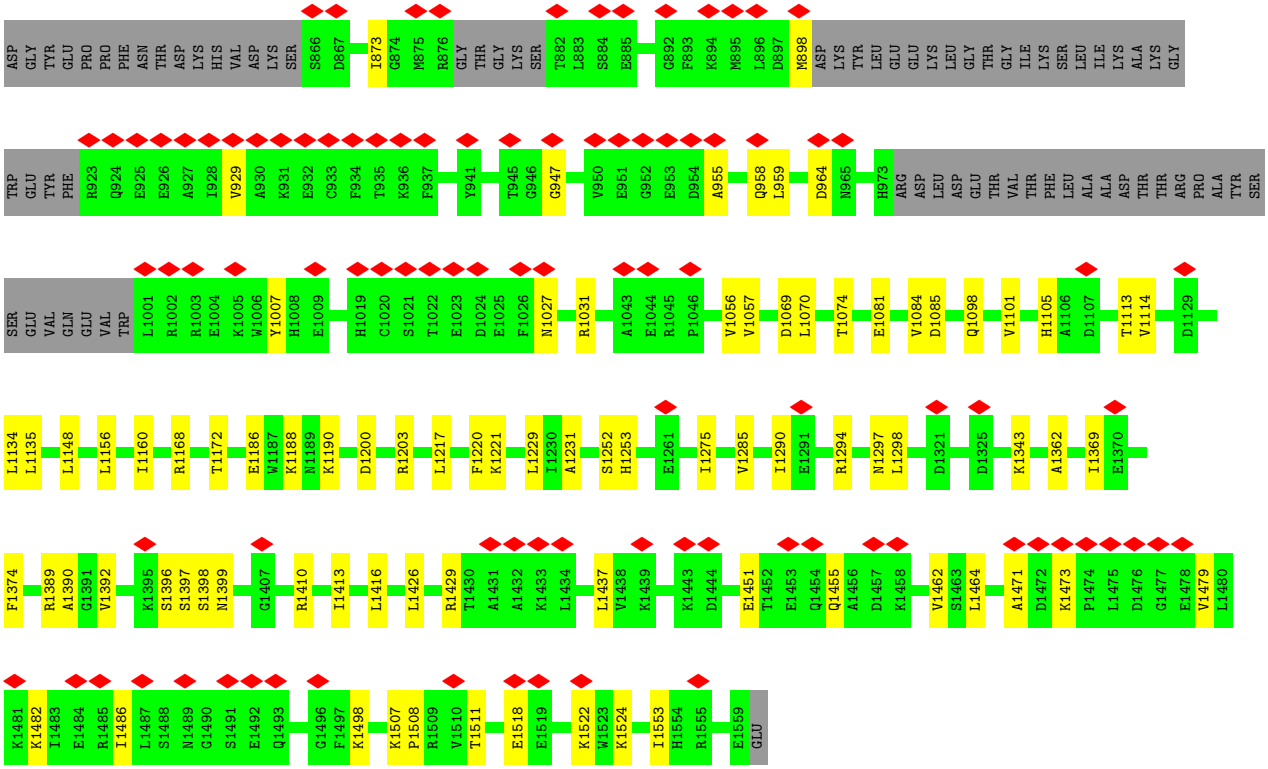
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:



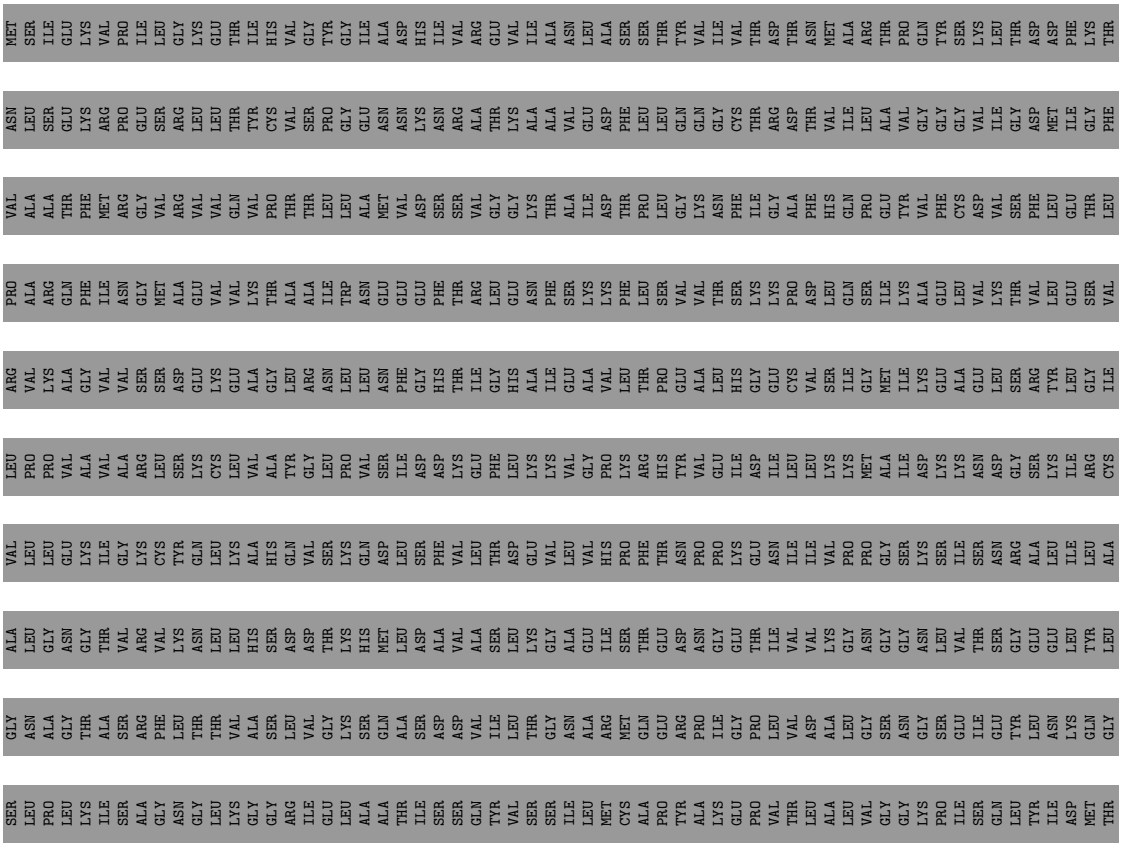


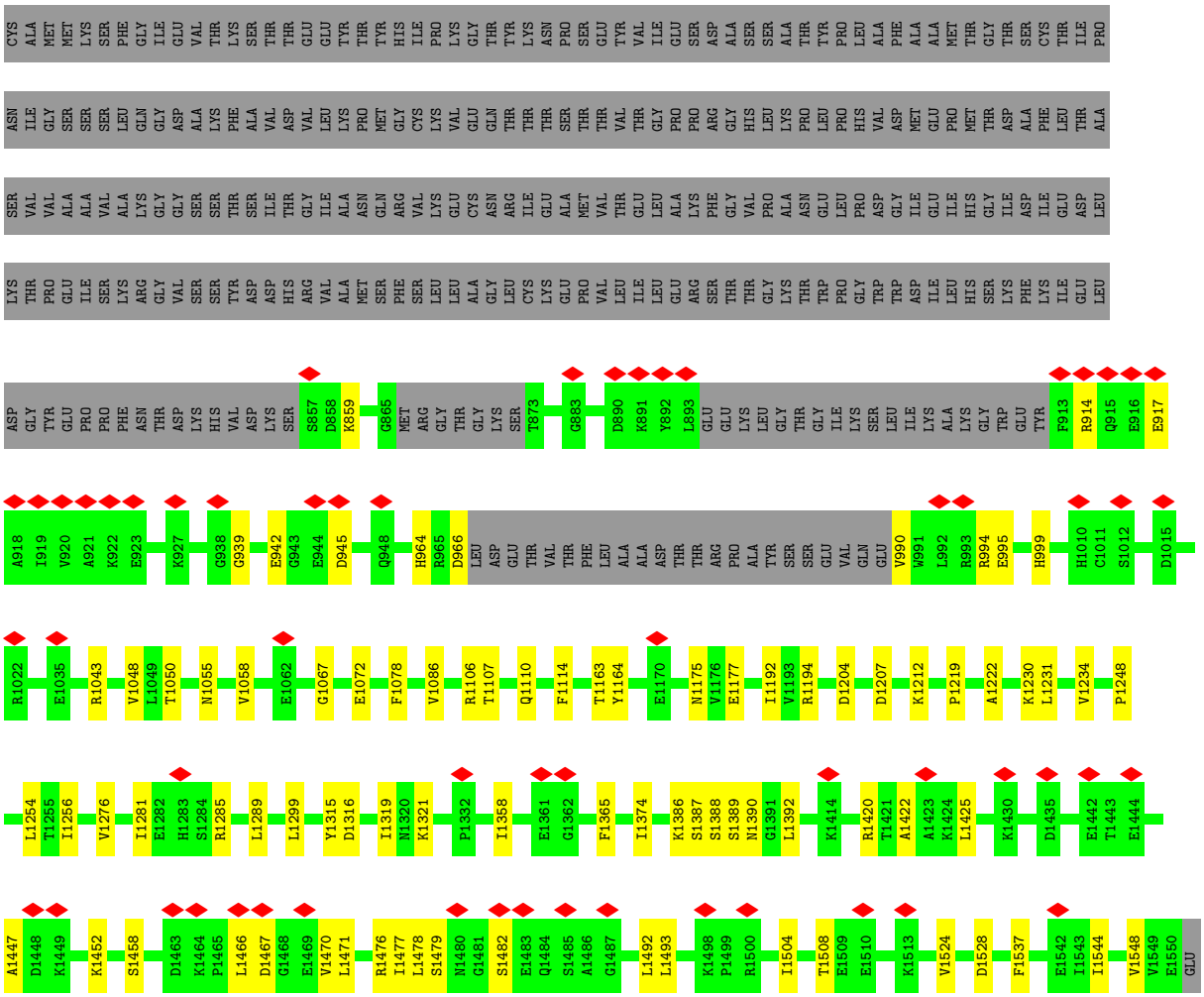


• Molecule 1: Pentafunctional AROM polypeptide

Chain B:






CYS ALA MET MET LYS SER PHE GLY ILE GLU VAL THR LYS SER THR THR GLU GLU TYR THR TYR HIS ILE PRO LYS GLY THR TYR LYS ASN PRO SER GLU TYR VAL ILE GLU SER ASP ALA SER SER ALA THR TYR PRO LEU ALA PHE ALA ALA MET THR GLY THR SER CYS THR ILE PRO
ASN ILE GLY SER SER SER LEU GLN GLY ASP ALA LYS PHE ALA VAL ASP VAL LEU LYS PRO MET GLY CYS LYS VAL GLU GLN THR THR THR SER THR THR VAL THR GLY PRO PRO ARG GLY HIS LEU LYS PRO LEU PRO HIS VAL ASP MET GLU PRO MET THR ASP ALA PHE LEU THR ALA
SER VAL VAL ALA ALA VAL ALA LYS GLY GLY SER SER SER THR SER ILE THR GLY ILE ALA ASN GLN ARG VAL LYS GLU CYS ASN ARG ILE GLU ALA MET VAL THR GLU LEU ALA LYS PHE GLY VAL PRO ALA ASN GLU LEU PRO PRO ASP GLY ILE GLU GLU ILE HIS GLY ILE ASP ILE GLU ASP LEU
LYS THR PRO GLU ILE SER LYS ARG GLY VAL SER SER TYR ASP ASP HIS ARG VAL ALA MET SER PHE SER LEU LEU ALA GLY LEU CYS LYS GLU PRO VAL LEU ILE LEU GLU ARG SER THR THR GLY LYS THR TRP PRO GLY TRP TRP ASP ILE LEU LYS PHE LYS ILE GLU GLU LEU
ASP GLY TYR GLU PRO PRO PHE ASN THR ASP LYS HIS VAL ASP LYS SER S857 D858 K859 G865 MET ARG GLY THR GLY LYS SER T873 G883 D890 K891 Y892 L893 GLU GLU LYS LEU GLY THR GLY ILE LYS SER LEU ILE LYS ALA LYS GLY TRP GLU TYR F913 R914 Q915 E916 E917
A918 I919 V920 A921 K922 E923 K927 G938 G939 E942 G943 E944 D945 Q948 H964 R965 D966 LEU ASP GLU THR VAL THR PHE LEU ALA ALA ASP THR THR ARG PRO ALA TYR SER SER GLU VAL GLN GLU V990 W991 L992 R993 R994 E995 H999 H1010 C1011 S1012 D1015
R1022 E1035 R1043 V1048 L1049 T1050 N1055 V1058 E1062 G1067 E1072 F1078 V1086 R1106 T1107 Q1110 F1114 T1163 Y1164 E1170 N1175 V1176 E1177 I1192 V1193 R1194 D1204 D1207 K1212 P1219 A1222 K1230 L1231 V1234 P1248
L1254 T1255 I1256 V1276 I1281 E1282 H1283 S1284 R1285 L1289 L1299 Y1315 D1316 I1319 N1320 K1321 P1332 I1358 E1361 G1362 F1365 I1374 K1386 S1387 S1388 S1389 N1390 G1391 L1392 K1414 R1420 T1421 A1422 A1423 K1424 L1425 K1430 D1435 E1442 T1443 E1444
A1447 D1448 K1449 K1452 S1458 D1463 K1464 P1465 L1466 D1467 G1468 E1469 V1470 L1471 R1476 I1477 L1478 S1479 N1480 G1481 S1482 E1483 Q1484 S1485 A1486 G1487 L1492 L1493 K1498 P1499 R1500 I1504 T1508 E1509 E1510 K1513 V1524 D1528 F1537 E1542 I1543 I1544 V1548 V1549 E1550 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	87484	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 ($e^-/Å^2$)	83.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.128	Depositor
Minimum map value	-1.292	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.32	Depositor
Map size (Å)	499.80002, 499.80002, 499.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2495, 1.2495, 1.2495	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	0.33	0/5080	0.53	0/6873
1	B	0.32	0/5153	0.46	0/6974
All	All	0.32	0/10233	0.50	0/13847

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4983	0	5003	55	0
1	B	5052	0	5063	50	0
All	All	10035	0	10066	104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 104 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1212:LYS:HE3	1:B:1222:ALA:HB3	1.79	0.64
1:B:1420:ARG:HH21	1:B:1467:ASP:HB2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:ILE:HD11	1:A:959:LEU:CD2	2.31	0.61
1:A:1056:VAL:HG11	1:A:1074:THR:HG22	1.83	0.59
1:B:1163:THR:HG22	1:B:1194:ARG:HB3	1.85	0.58

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	630/1551 (41%)	592 (94%)	38 (6%)	0	100	100
1	B	637/1551 (41%)	605 (95%)	32 (5%)	0	100	100
All	All	1267/3102 (41%)	1197 (94%)	70 (6%)	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	A	542/1311 (41%)	542 (100%)	0	100	100
1	B	549/1311 (42%)	549 (100%)	0	100	100
All	All	1091/2622 (42%)	1091 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1175	ASN
1	B	1244	HIS
1	B	1368	ASN
1	B	962	HIS
1	B	1110	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)

There are no chain breaks in this entry.

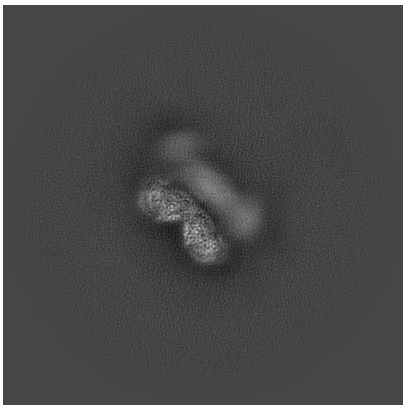
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26359. These allow visual inspection of the internal detail of the map and identification of artifacts.

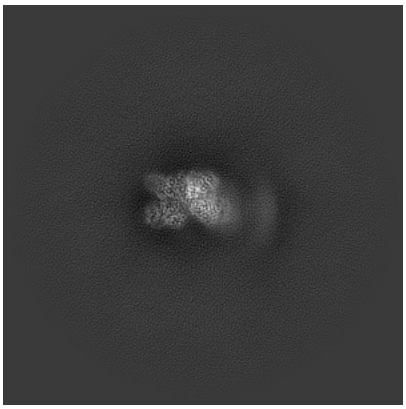
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

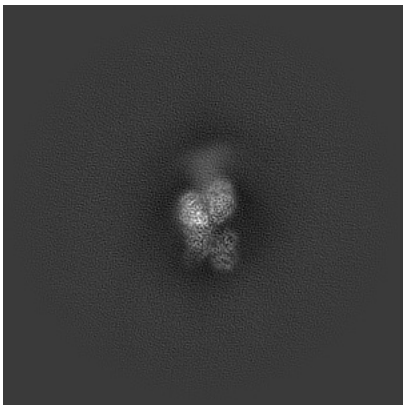
6.1.1 Primary map



X

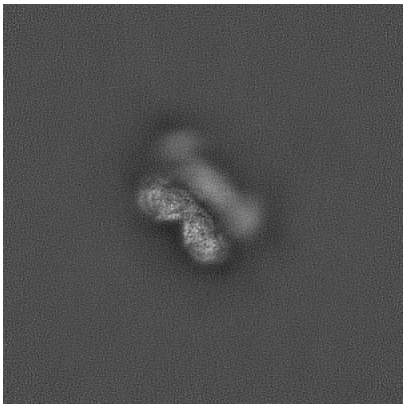


Y



Z

6.1.2 Raw map



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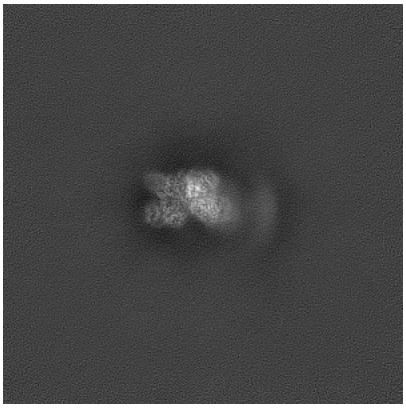

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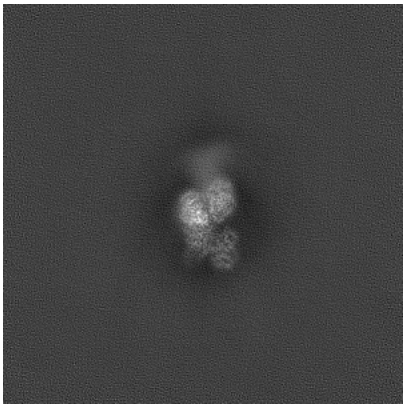
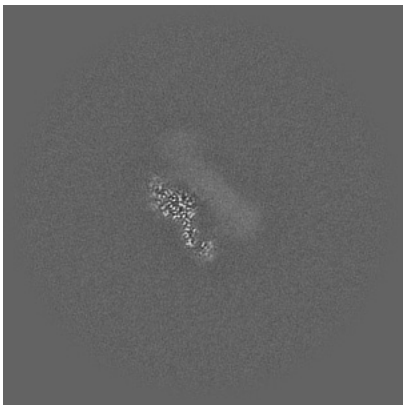


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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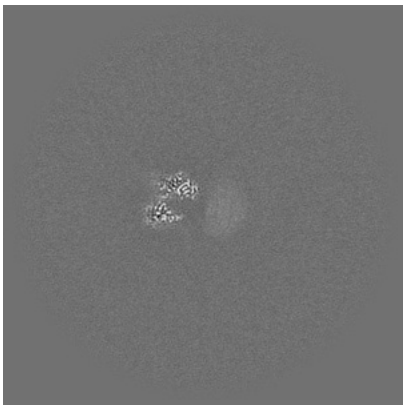

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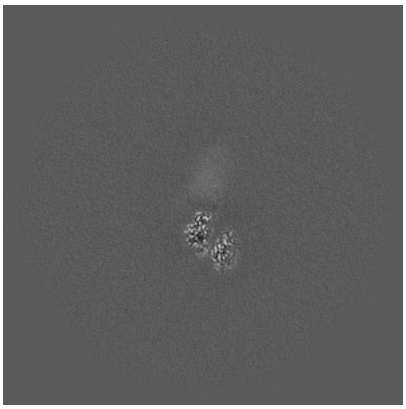
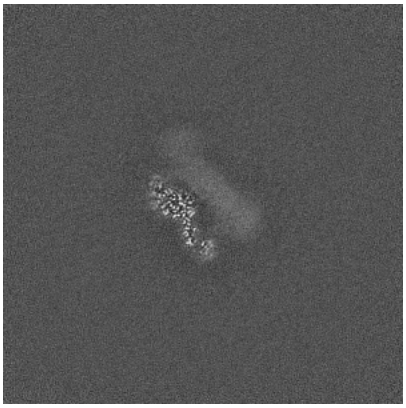
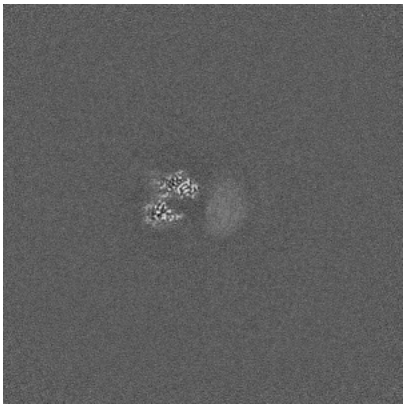


Z Index: 200

6.2.2 Raw map



X Index: 200



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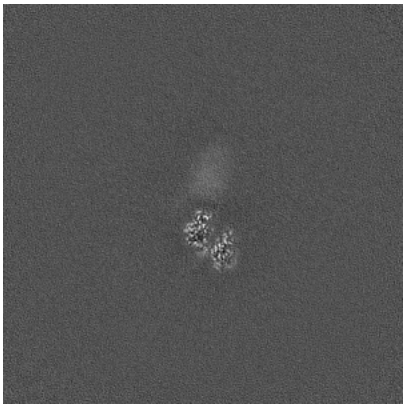
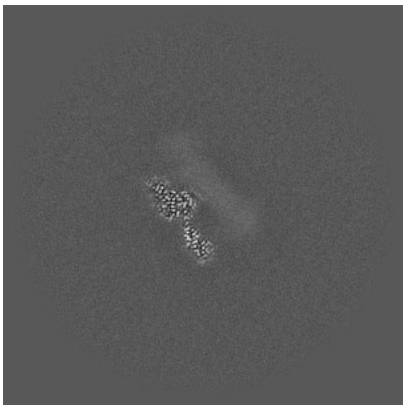


Z Index: 200

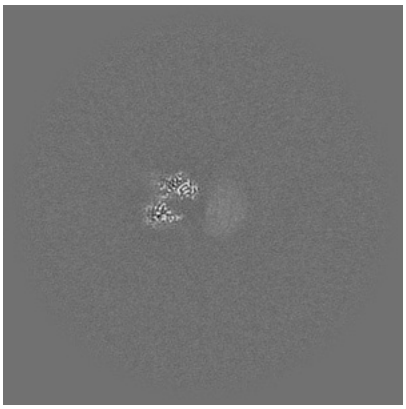
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 196



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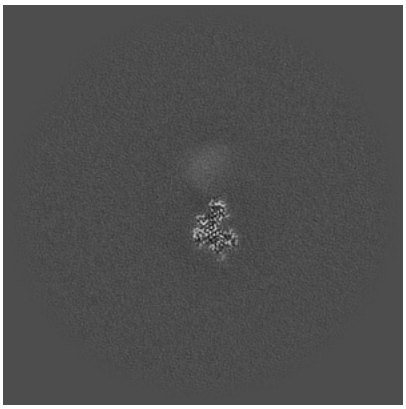
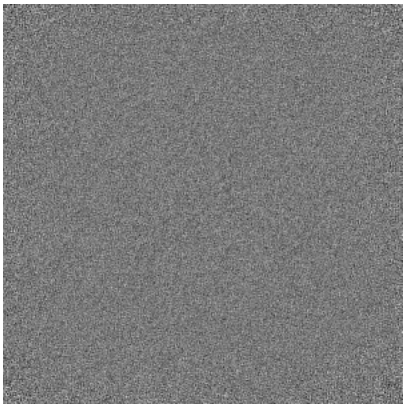
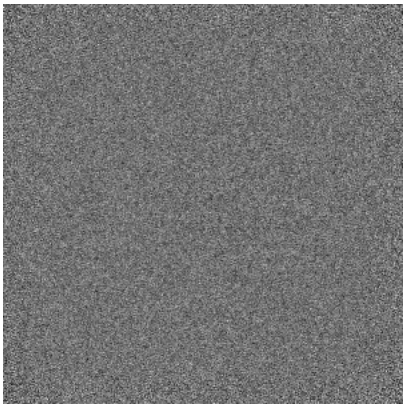


Z Index: 189

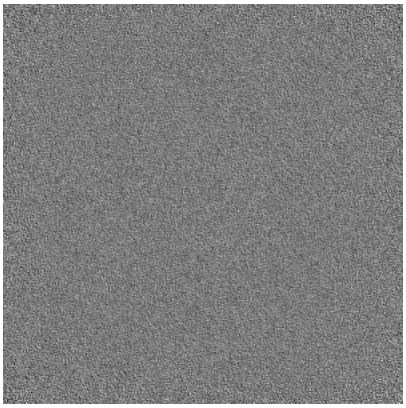
6.3.2 Raw map



X Index: 0



Y Index: 0

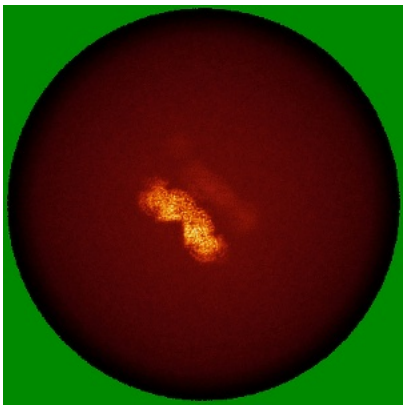


Z Index: 0

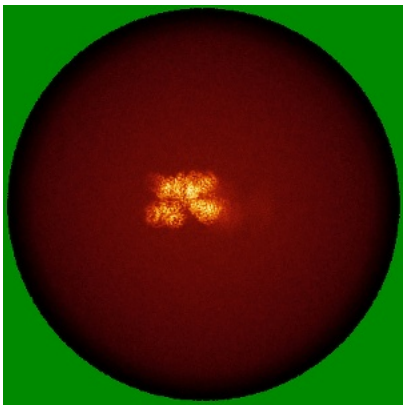
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

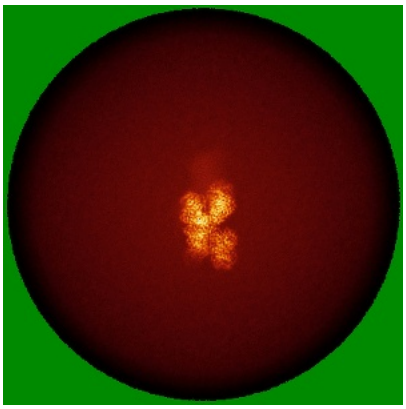
6.4.1 Primary map



X

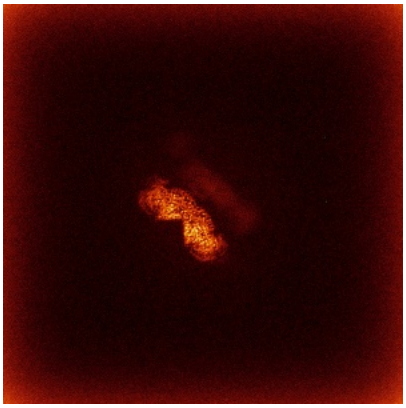


Y



Z

6.4.2 Raw map



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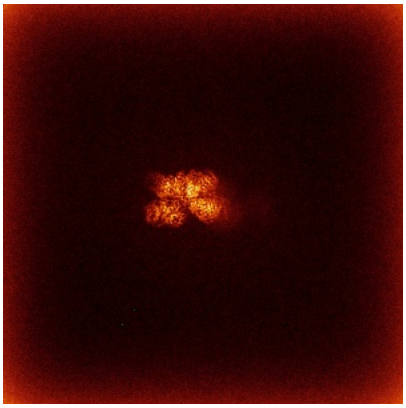
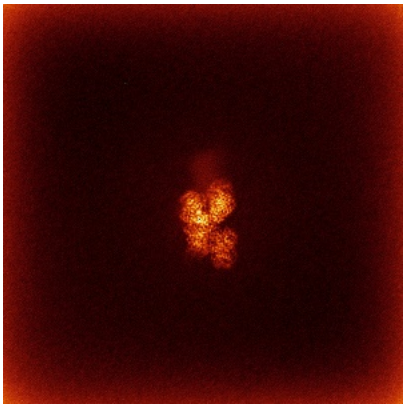


Y



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.32. 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



X Y Z

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.

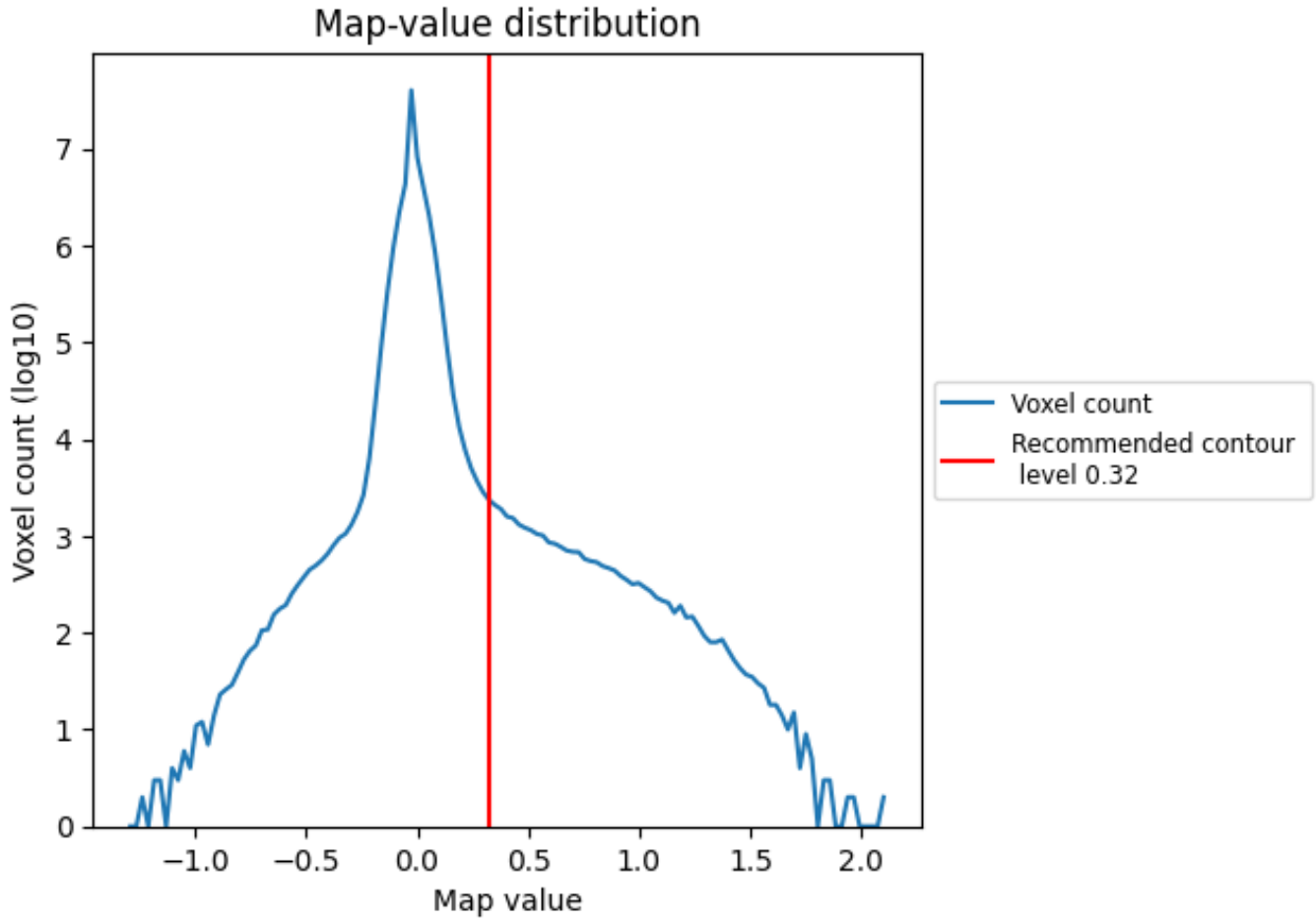
6.6 Mask visualisation (i)

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

7 Map analysis

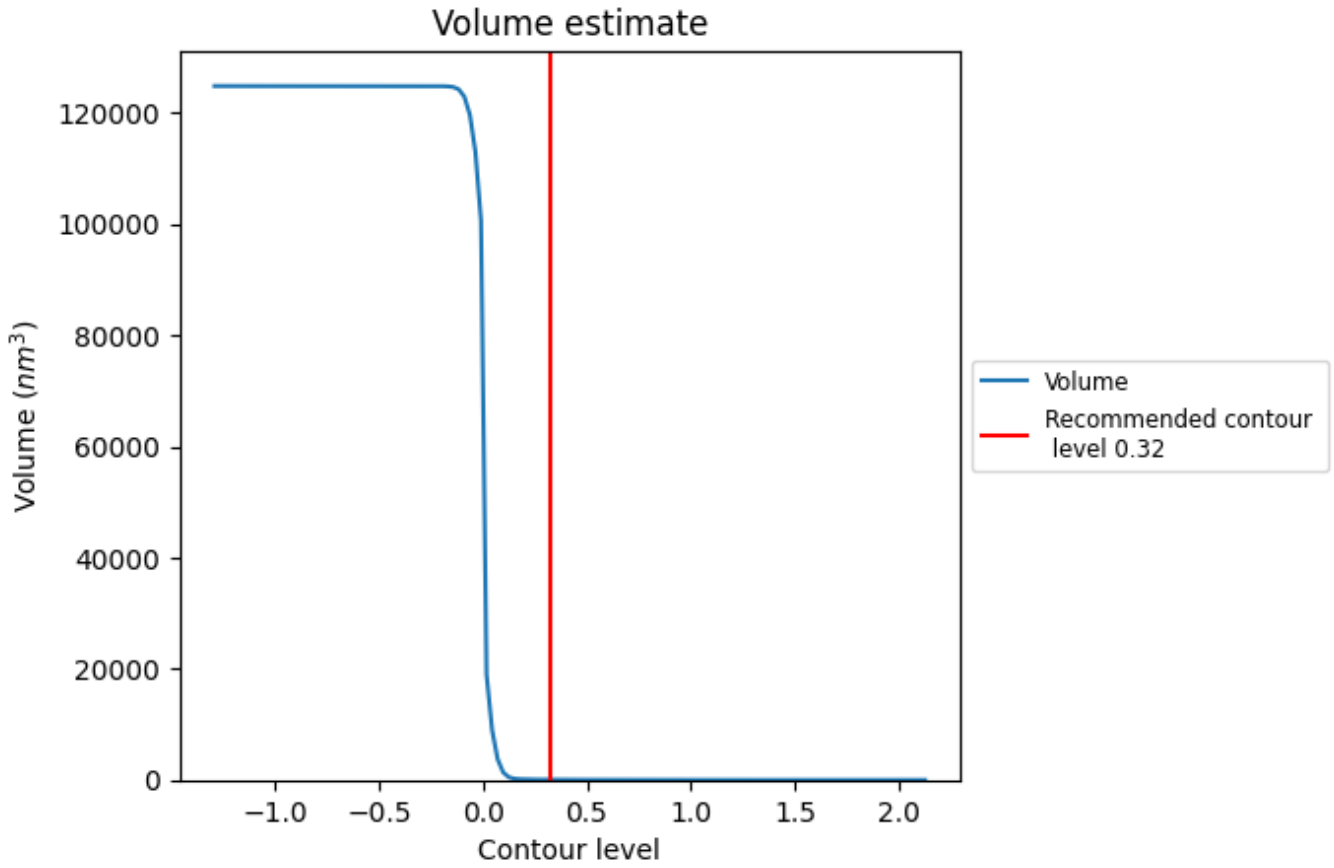
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

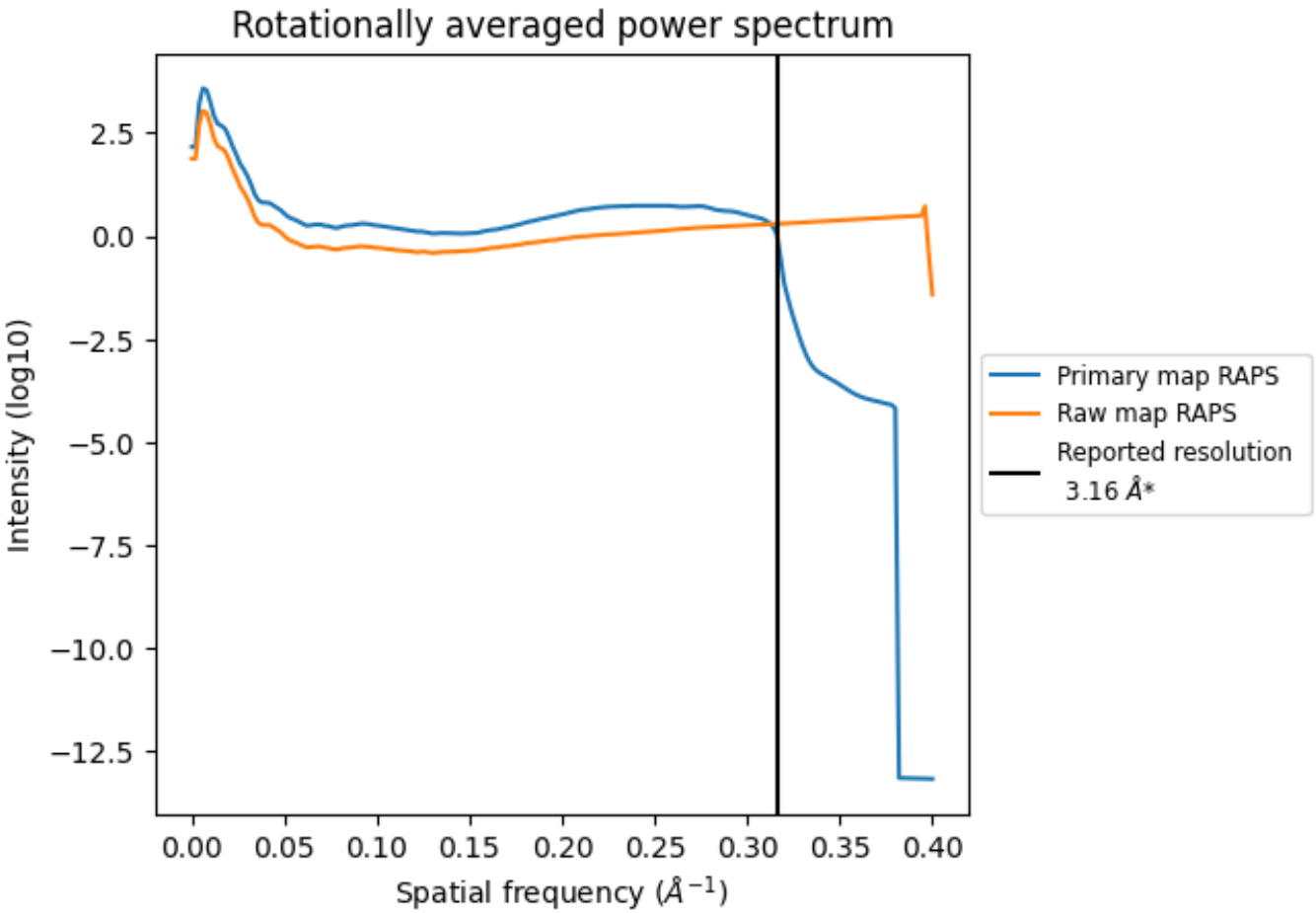
7.2 Volume estimate (i)



The volume at the recommended contour level is 53 nm^3; this corresponds to an approximate mass of 48 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

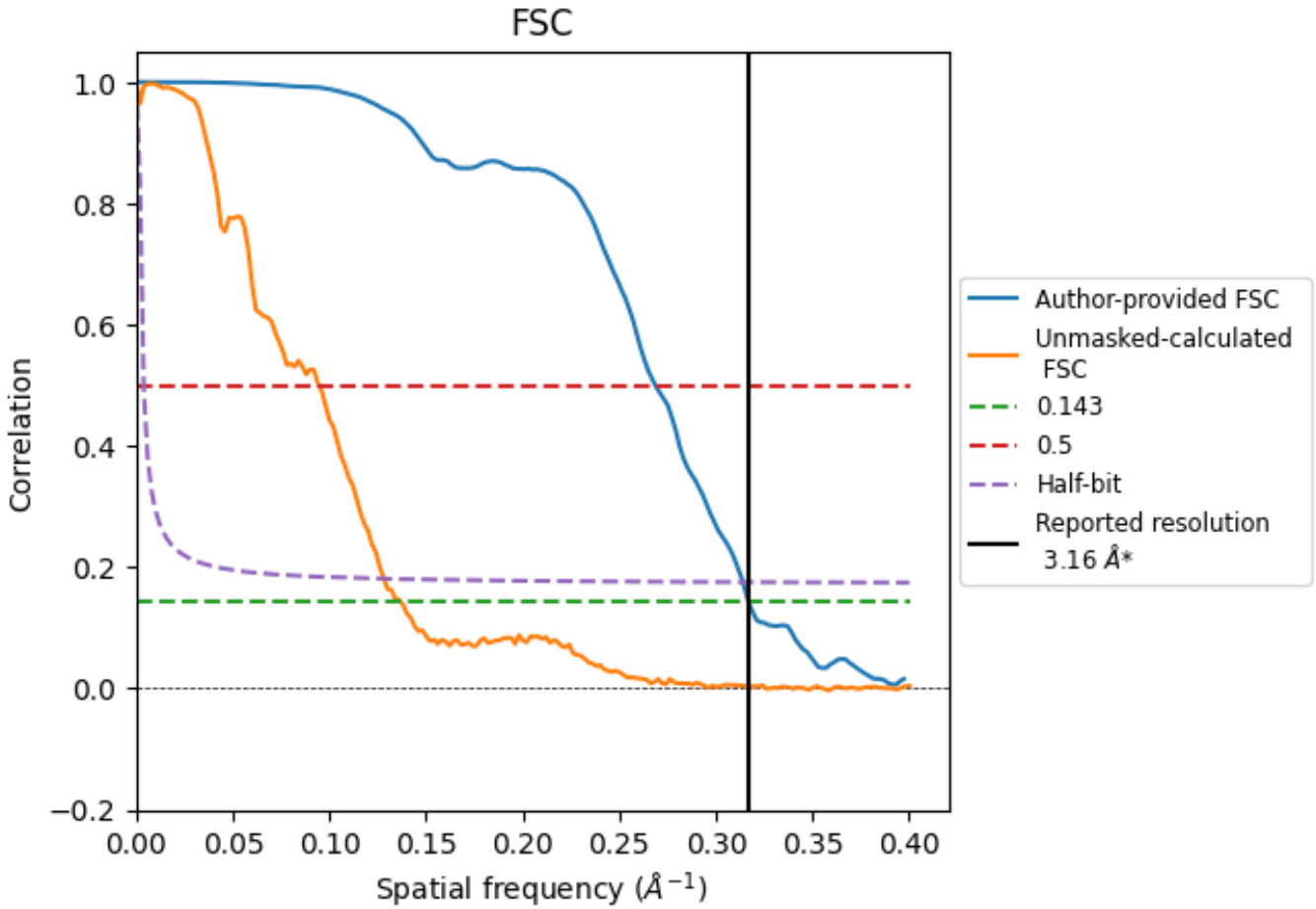


*Reported resolution corresponds to spatial frequency of 0.316 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8.2 Resolution estimates (i)

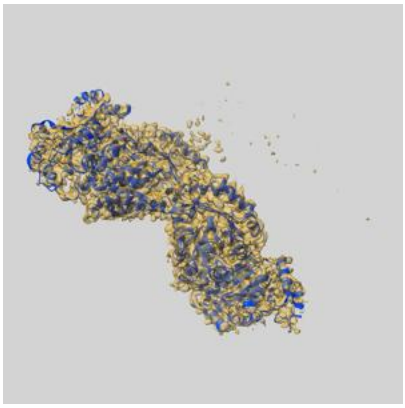
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.16	3.72	3.19
Unmasked-calculated*	7.31	10.57	7.80

*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 7.31 differs from the reported value 3.16 by more than 10 %

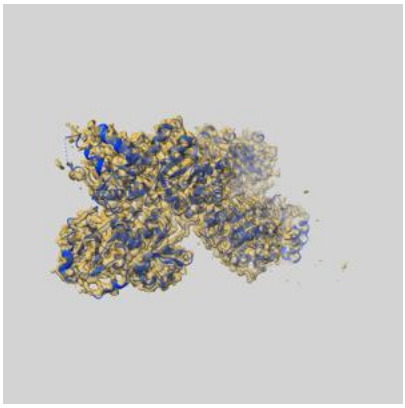
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26359 and PDB model 7U5U. Per-residue inclusion information can be found in section 3 on page 4.

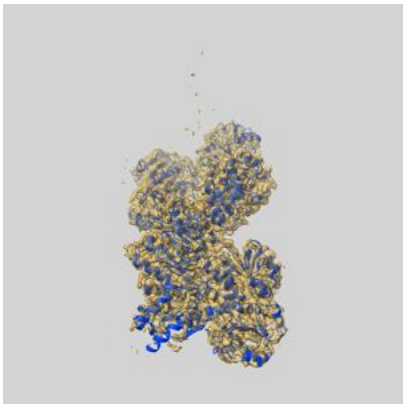
9.1 Map-model overlay



X



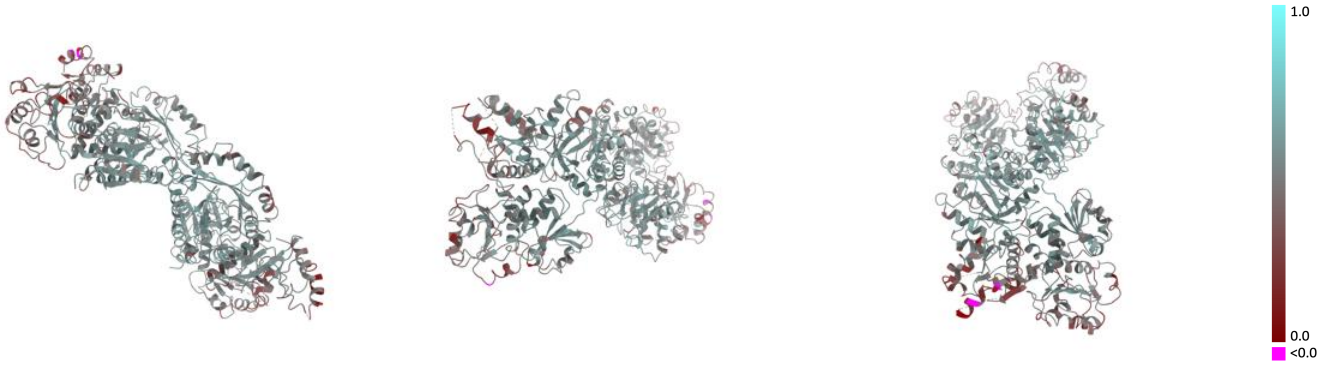
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.32 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.

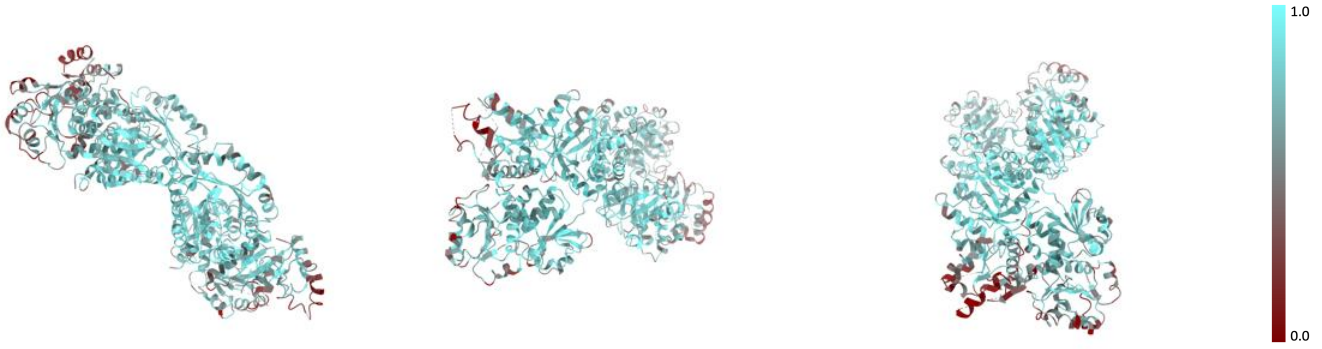
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

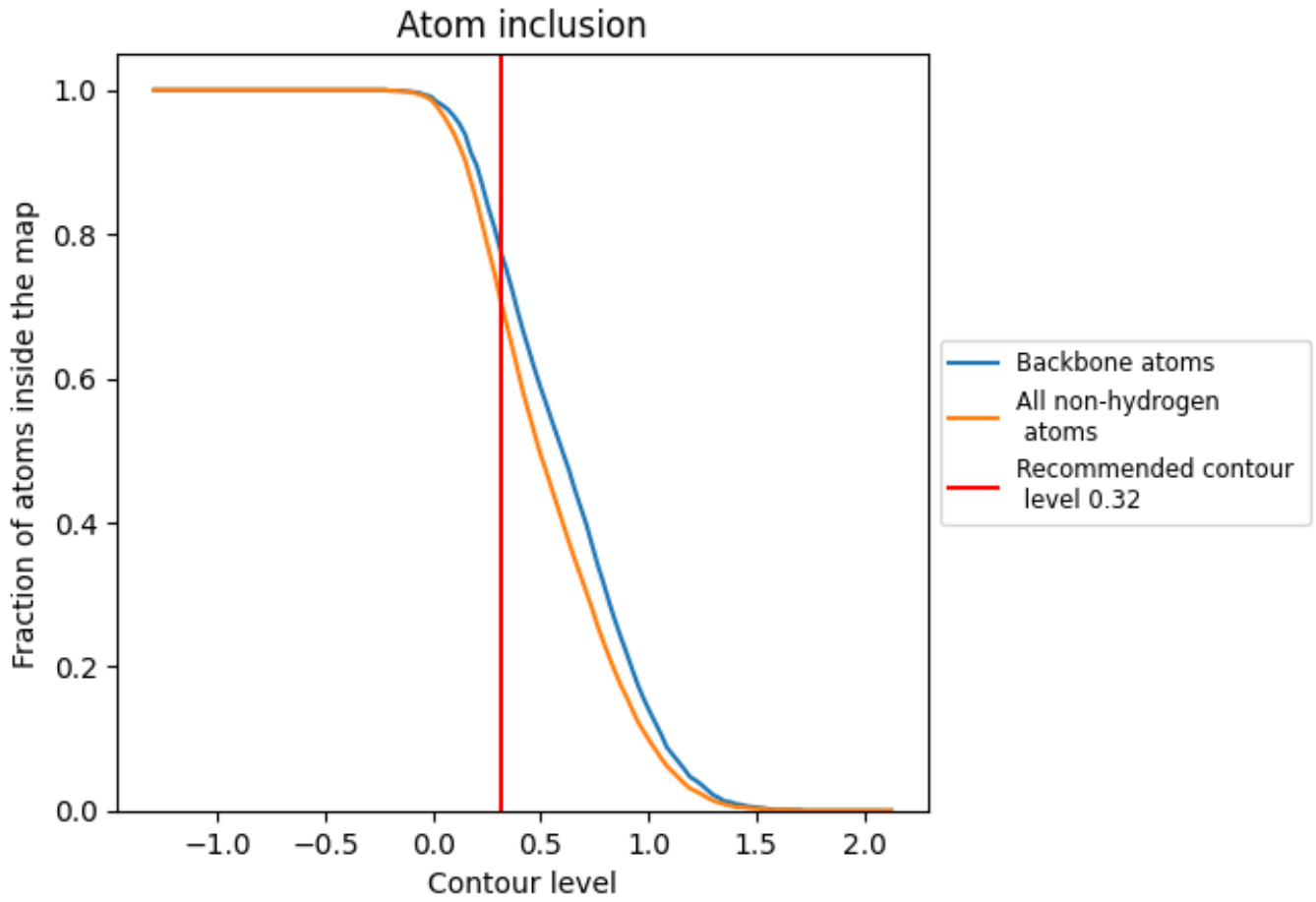
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.32).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 70% 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 (0.32) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7020	0.4900
A	0.6750	0.4820
B	0.7290	0.4980