



wwPDB EM Validation Summary Report ⓘ

May 17, 2026 – 05:02 PM JST

PDB ID : 9UVA / pdb_00009uva
EMDB ID : EMD-64529
Title : Structures of multiple states of the nicotinamide nucleotide transhydrogenase from Escherichia coli
Authors : Zhu, J.; Gennis, R.B.; Zhang, K.; Li, J.
Deposited on : 2025-05-09
Resolution : 3.73 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

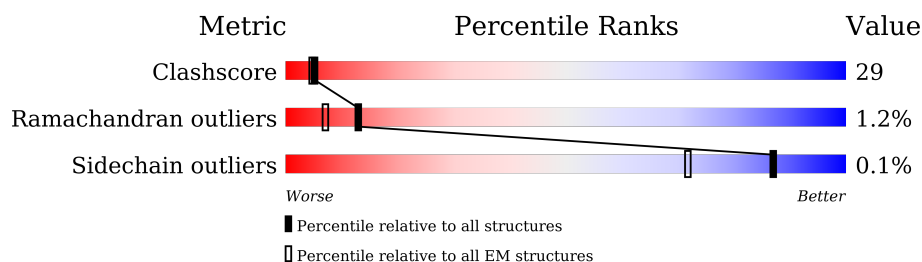
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.73 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	462	<div> <div>44%</div> <div>49%</div> <div>46%</div> <div>• •</div> </div>
1	B	462	<div> <div>26%</div> <div>42%</div> <div>43%</div> <div>• 14%</div> </div>
2	C	99	<div> <div>28%</div> <div>38%</div> <div>57%</div> <div>• •</div> </div>
2	D	99	<div> <div>22%</div> <div>37%</div> <div>61%</div> <div>•</div> </div>
3	E	377	<div> <div>88%</div> <div>56%</div> <div>41%</div> <div>•</div> </div>
3	F	377	<div> <div>84%</div> <div>59%</div> <div>36%</div> <div>• •</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13177 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 NAD(P) transhydrogenase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	396	Total	C	N	O	S	0	0
			2943	1913	489	522	19		
1	A	444	Total	C	N	O	S	0	0
			3304	2143	549	590	22		

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	96	Total	C	N	O	S	0	0
			730	491	116	118	5		
2	D	99	Total	C	N	O	S	0	0
			758	510	121	122	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	508	LYS	-	expression tag	UNP P07001
C	509	ASN	-	expression tag	UNP P07001
D	508	LYS	-	expression tag	UNP P07001
D	509	ASN	-	expression tag	UNP P07001

- Molecule 3 is a protein called NAD(P) transhydrogenase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	367	Total	C	N	O	S	0	0
			2739	1738	464	525	12		
3	F	361	Total	C	N	O	S	0	0
			2703	1713	461	518	11		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	999	HIS	-	expression tag	UNP P07001

Continued on next page...

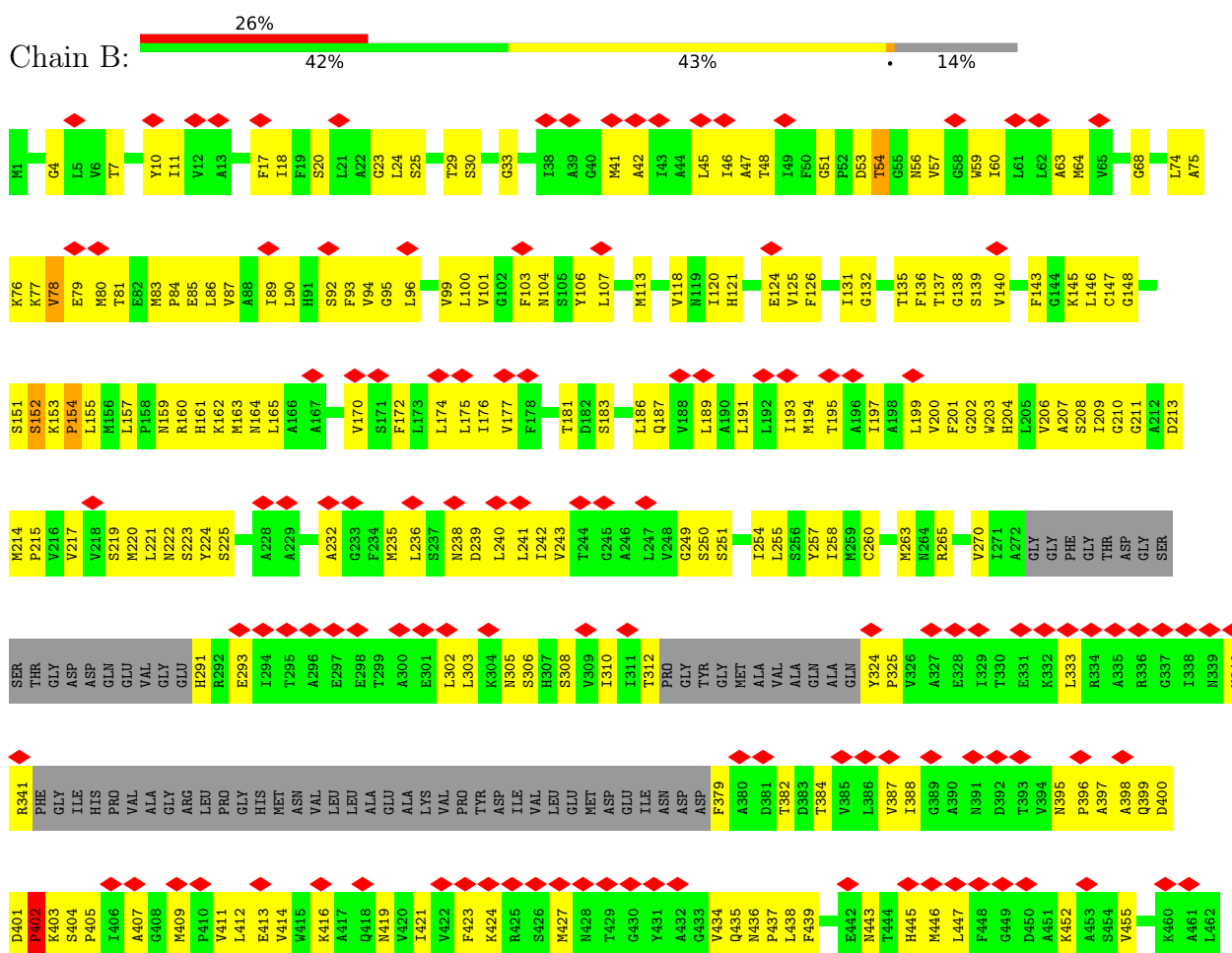
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1000	HIS	-	expression tag	UNP P07001
E	1001	GLY	-	expression tag	UNP P07001
F	999	HIS	-	expression tag	UNP P07001
F	1000	HIS	-	expression tag	UNP P07001
F	1001	GLY	-	expression tag	UNP P07001

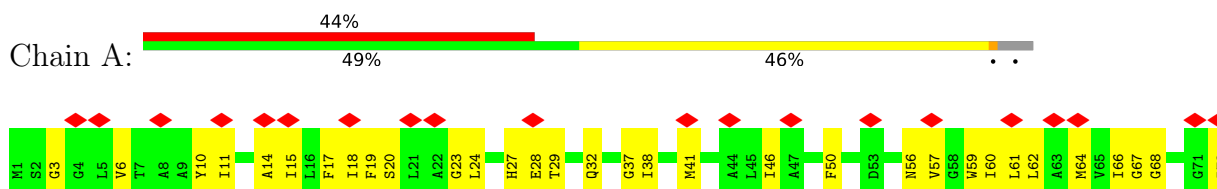
3 Residue-property plots

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: NAD(P) transhydrogenase subunit beta



• Molecule 1: NAD(P) transhydrogenase subunit beta



G1364	I1300
E1365	F1301
I1366	T1302
T1367	T1303
W1368	E1304
P1369	W1305
A1370	G1306
P1371	W1307
P1372	K1308
I1373	W1309
Q1374	I1310
VAL	G1311
	Y1312
	R1318
	L1319
	T1320
	T1321
	Q1322
	S1323
	S1324
	Q1325
	L1326
	Y1327
	G1328
	T1329
	N1330
	L1331
	V1332
	N1333
	L1334
	L1335
	K1336
	L1337
	L1338
	C1339
	K1340
	E1341
	L1342
	D1343
	G1344
	N1345
	L1346
	T1347
	V1348
	D1349
	F1350
	D1351
	D1352
	V1353
	V1354
	I1355
	R1356
	G1357
	V1358
	T1359
	V1360
	I1361
	R1362
	V1363

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55221	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 ($e^-/\text{\AA}^2$)	1.378	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.454	Depositor
Minimum map value	-0.286	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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	0.23	0/3367	0.67	2/4574 (0.0%)
1	B	0.25	0/2995	0.73	2/4063 (0.0%)
2	C	0.30	0/750	0.87	0/1022
2	D	0.27	0/779	0.72	1/1060 (0.1%)
3	E	0.15	0/2781	0.42	0/3777
3	F	0.14	0/2746	0.36	0/3731
All	All	0.21	0/13418	0.61	5/18227 (0.0%)

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
1	B	0	1
3	E	0	1
3	F	0	2
All	All	0	8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	SER	CA-C-N	8.47	132.17	120.65
1	B	152	SER	C-N-CA	8.47	132.17	120.65
1	A	402	PRO	N-CA-C	6.38	125.60	112.47
1	A	202	GLY	N-CA-C	-5.40	106.25	112.73
2	D	495	GLY	O-C-N	5.10	124.71	121.85

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	SER	Peptide
1	A	402	PRO	Peptide
1	A	404	SER	Peptide
1	A	410	PRO	Peptide
1	B	402	PRO	Peptide

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	3304	0	3420	245	0
1	B	2943	0	3067	232	0
2	C	730	0	753	84	0
2	D	758	0	781	73	0
3	E	2739	0	2799	124	0
3	F	2703	0	2753	100	0
All	All	13177	0	13573	774	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 774 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:90:LEU:HD12	2:D:492:ASN:HA	1.53	0.91
1:B:101:VAL:HG23	2:D:471:GLN:HE22	1.38	0.86
3:F:1047:ASP:OD1	3:F:1048:LYS:NZ	2.08	0.86
1:B:210:GLY:H	1:B:402:PRO:HA	1.41	0.85
1:B:153:LYS:O	1:B:401:ASP:N	2.08	0.85

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	440/462 (95%)	383 (87%)	56 (13%)	1 (0%)	43	71
1	B	388/462 (84%)	331 (85%)	52 (13%)	5 (1%)	9	38
2	C	94/99 (95%)	75 (80%)	16 (17%)	3 (3%)	3	25
2	D	97/99 (98%)	78 (80%)	17 (18%)	2 (2%)	5	31
3	E	363/377 (96%)	325 (90%)	35 (10%)	3 (1%)	16	47
3	F	357/377 (95%)	315 (88%)	36 (10%)	6 (2%)	7	34
All	All	1739/1876 (93%)	1507 (87%)	212 (12%)	20 (1%)	13	39

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	SER
1	B	78	VAL
2	C	416	MET
2	C	451	THR
2	D	507	PHE

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	348/360 (97%)	347 (100%)	1 (0%)	86	83
1	B	311/360 (86%)	311 (100%)	0	100	100
2	C	77/80 (96%)	77 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	80/80 (100%)	80 (100%)	0	100	100
3	E	290/298 (97%)	290 (100%)	0	100	100
3	F	287/298 (96%)	287 (100%)	0	100	100
All	All	1393/1476 (94%)	1392 (100%)	1 (0%)	87	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	1203	GLN
3	F	1103	GLN
3	F	1041	GLN
1	A	395	ASN
2	D	471	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

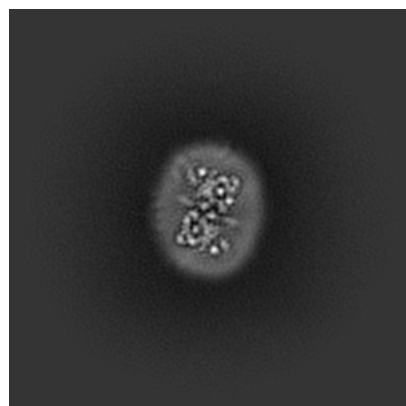
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64529. These allow visual inspection of the internal detail of the map and identification of artifacts.

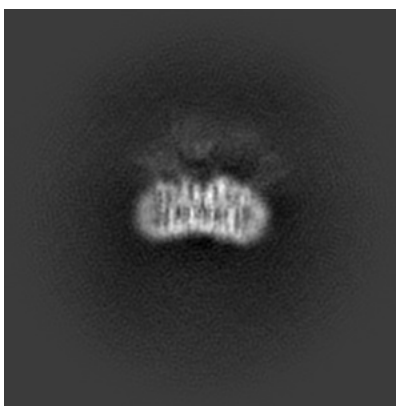
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

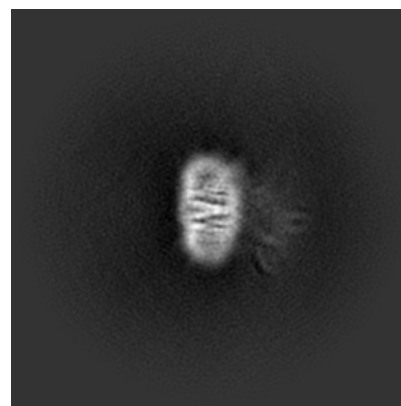
6.1.1 Primary map



X

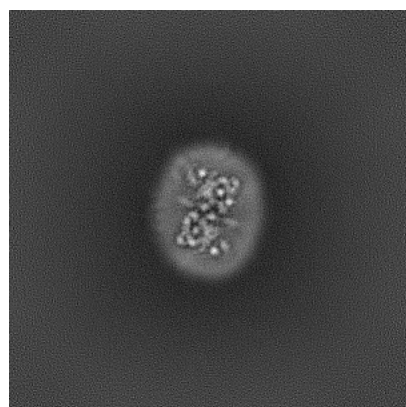


Y

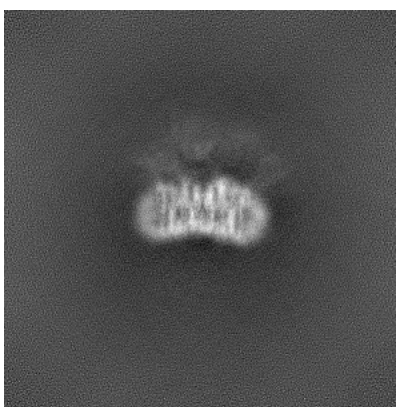


Z

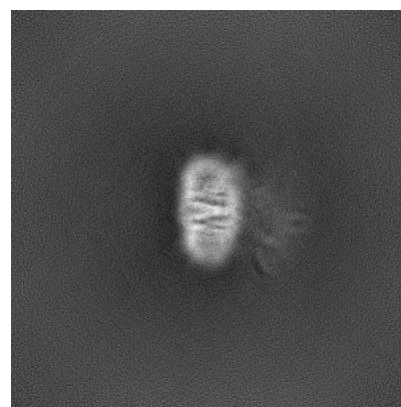
6.1.2 Raw map



X



Y

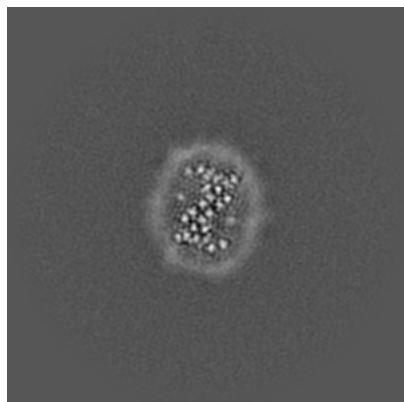


Z

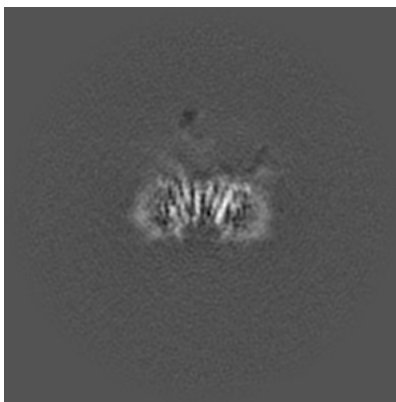
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

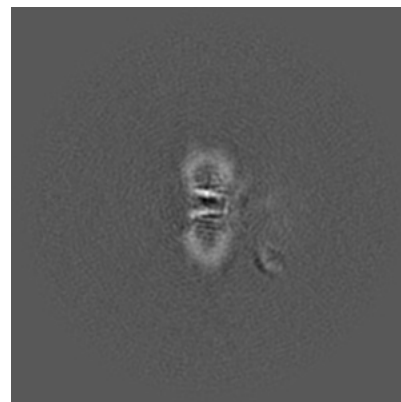
6.2.1 Primary map



X Index: 200

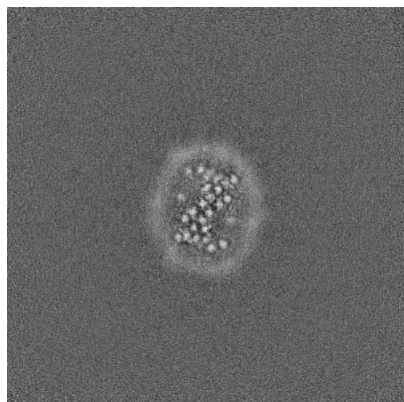


Y Index: 200

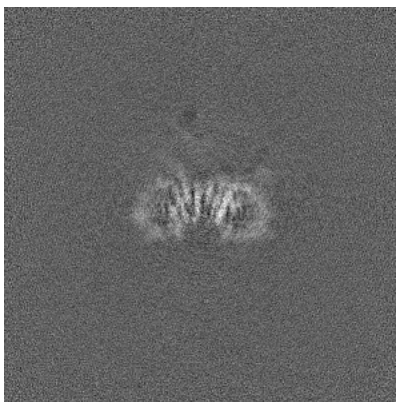


Z Index: 200

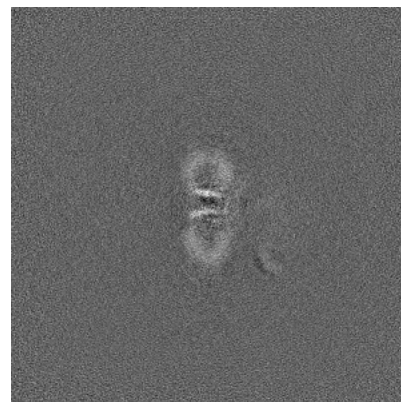
6.2.2 Raw map



X Index: 200



Y Index: 200

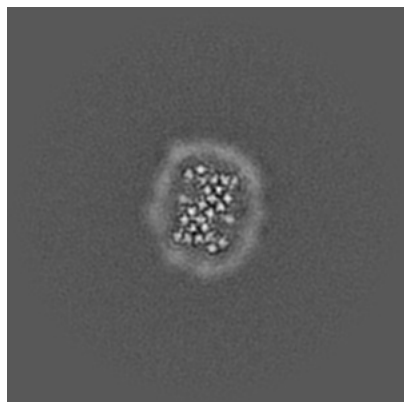


Z Index: 200

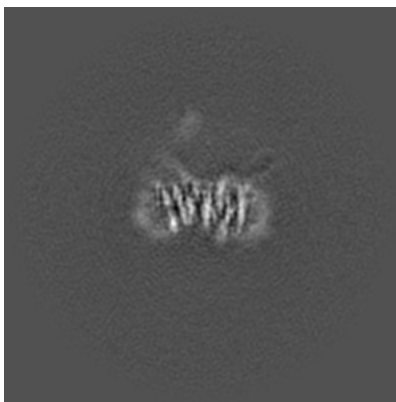
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

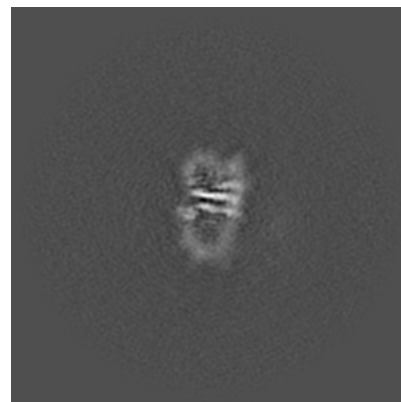
6.3.1 Primary map



X Index: 194

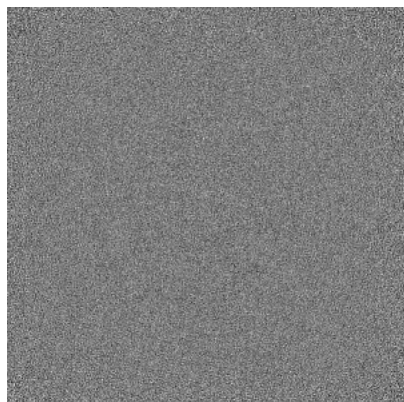


Y Index: 195

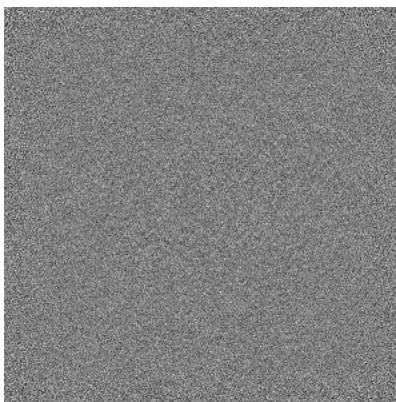


Z Index: 217

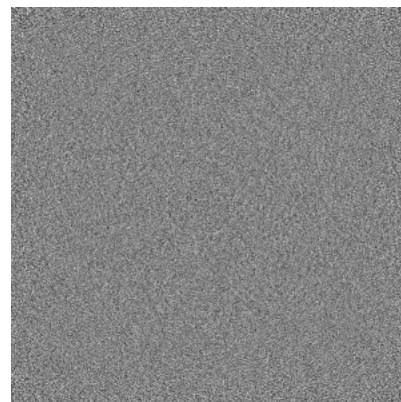
6.3.2 Raw map



X Index: 0



Y Index: 0

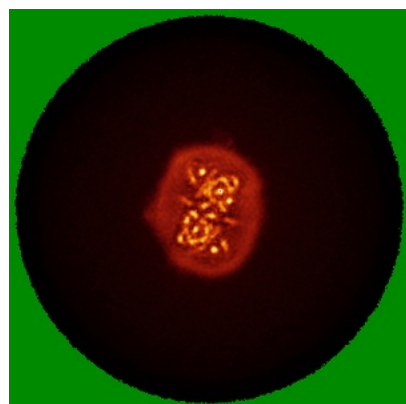


Z Index: 399

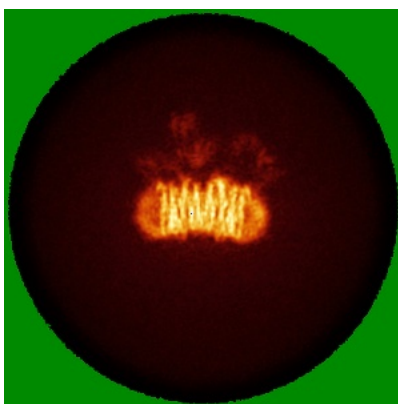
The images above show the largest variance slices of the map in three orthogonal directions.

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

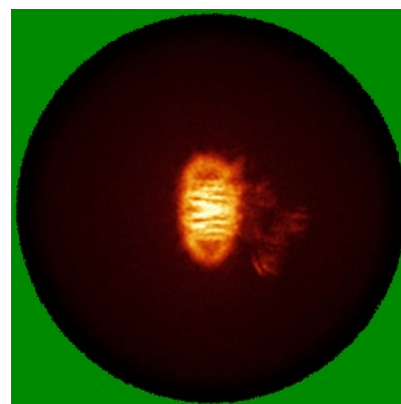
6.4.1 Primary map



X

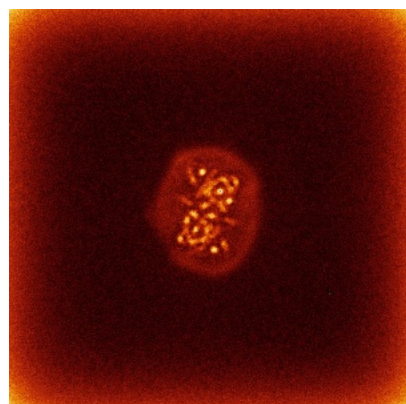


Y

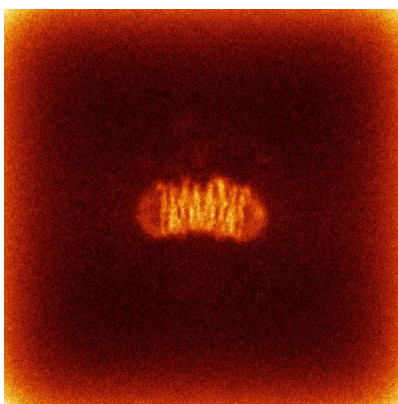


Z

6.4.2 Raw map



X



Y

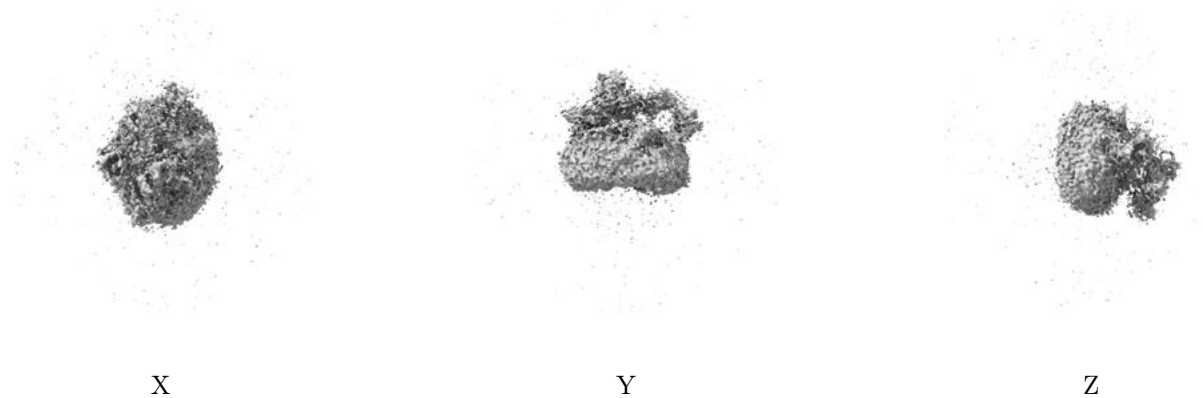


Z

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.

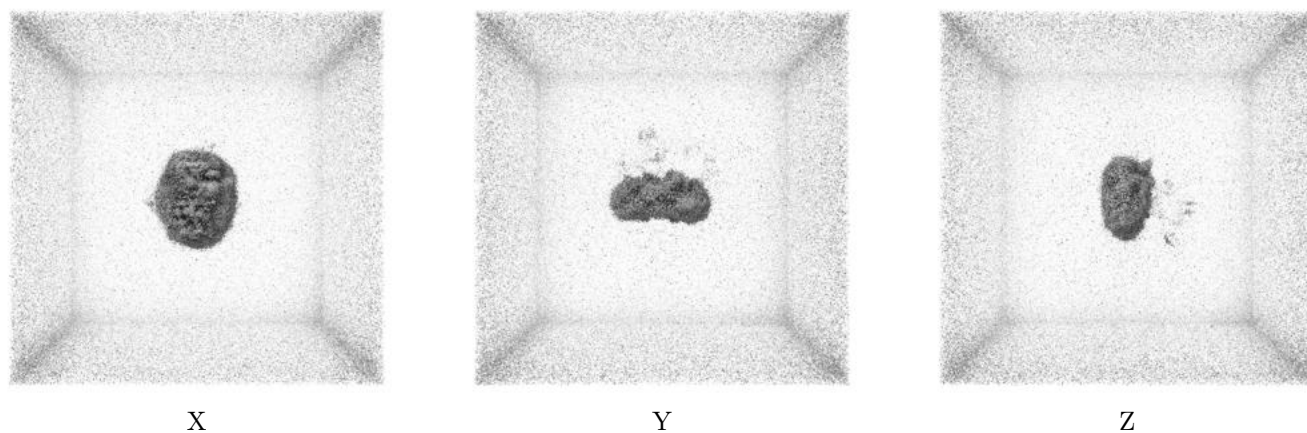
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

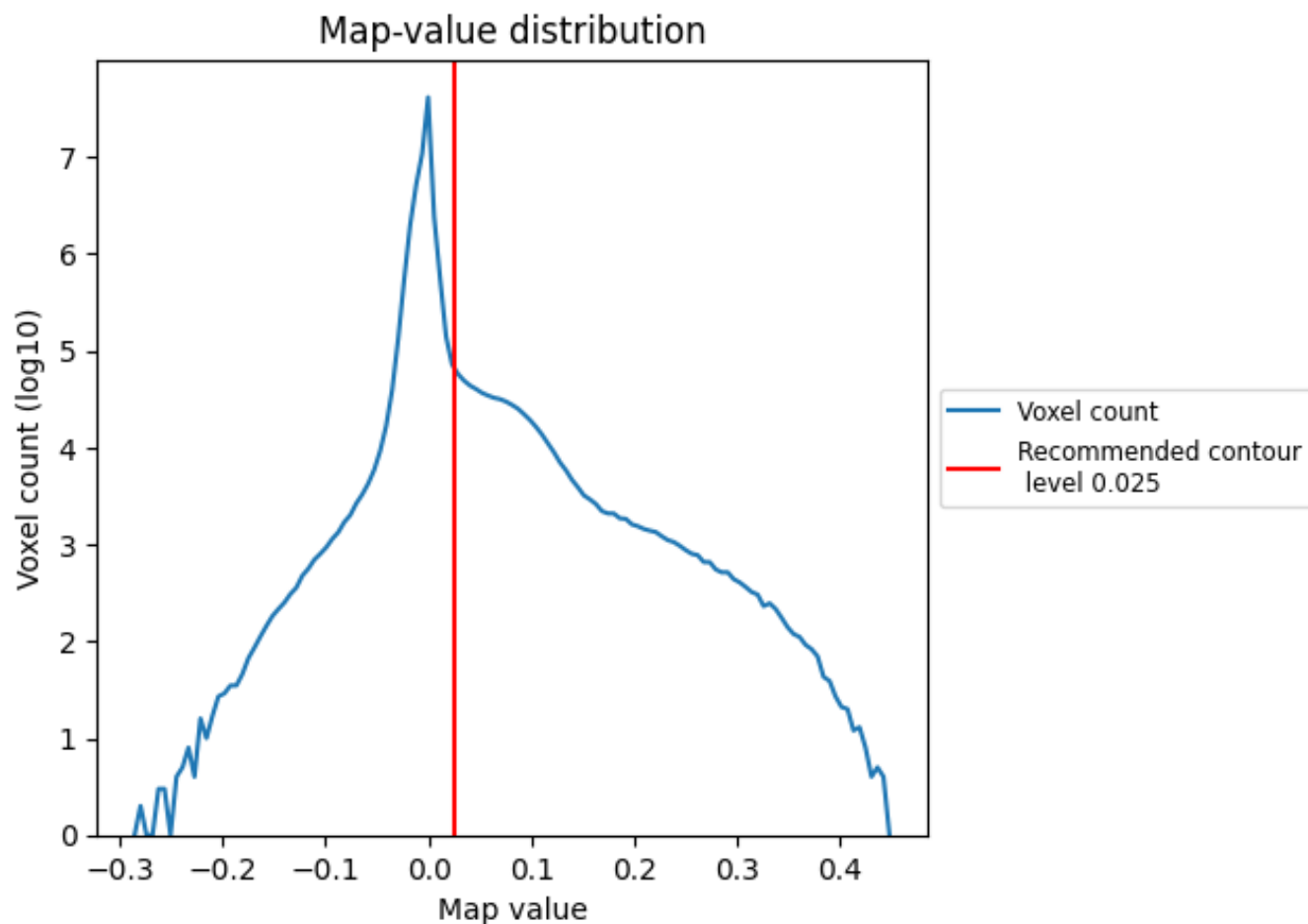
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

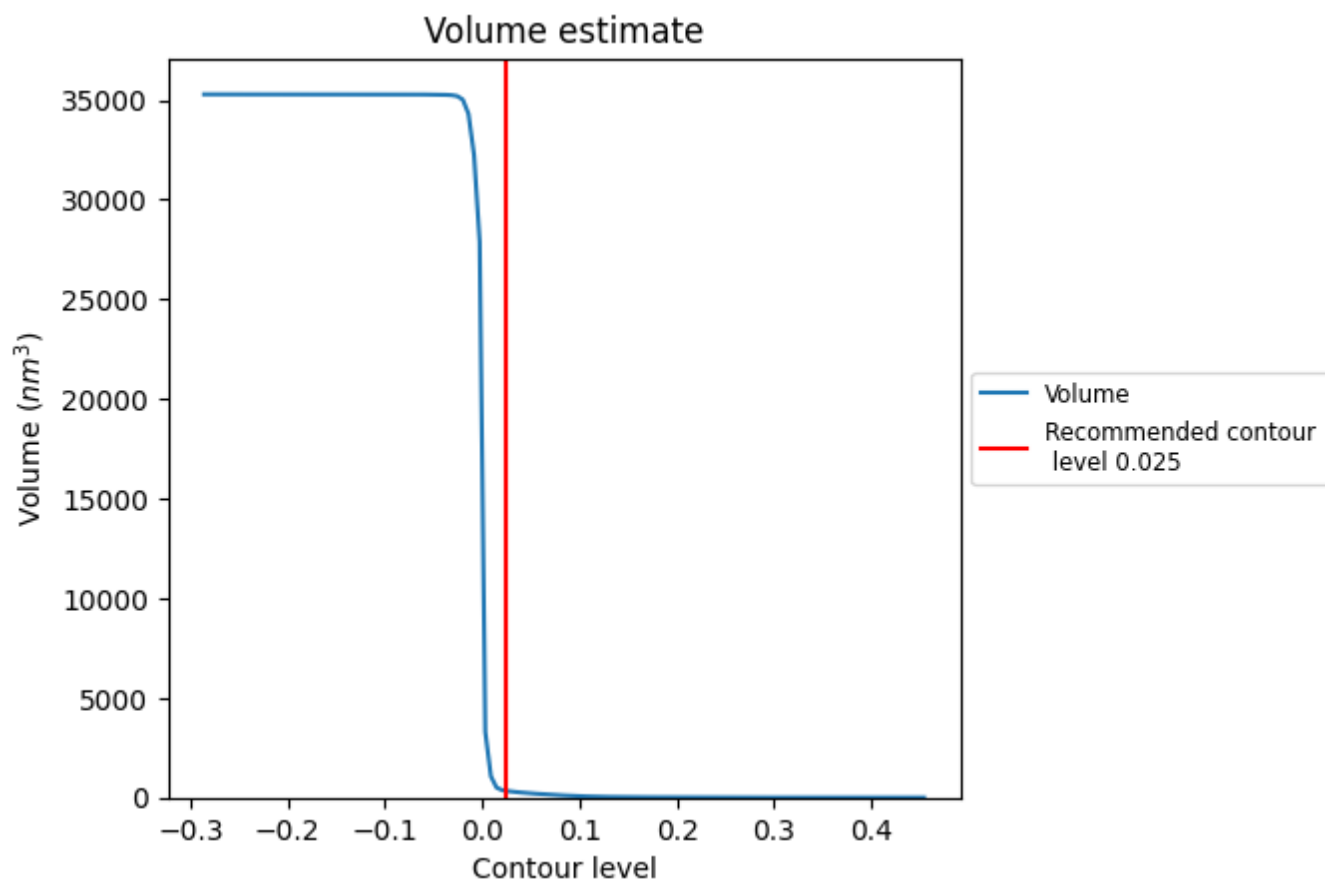
This section contains the results of statistical analysis of the map.

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.

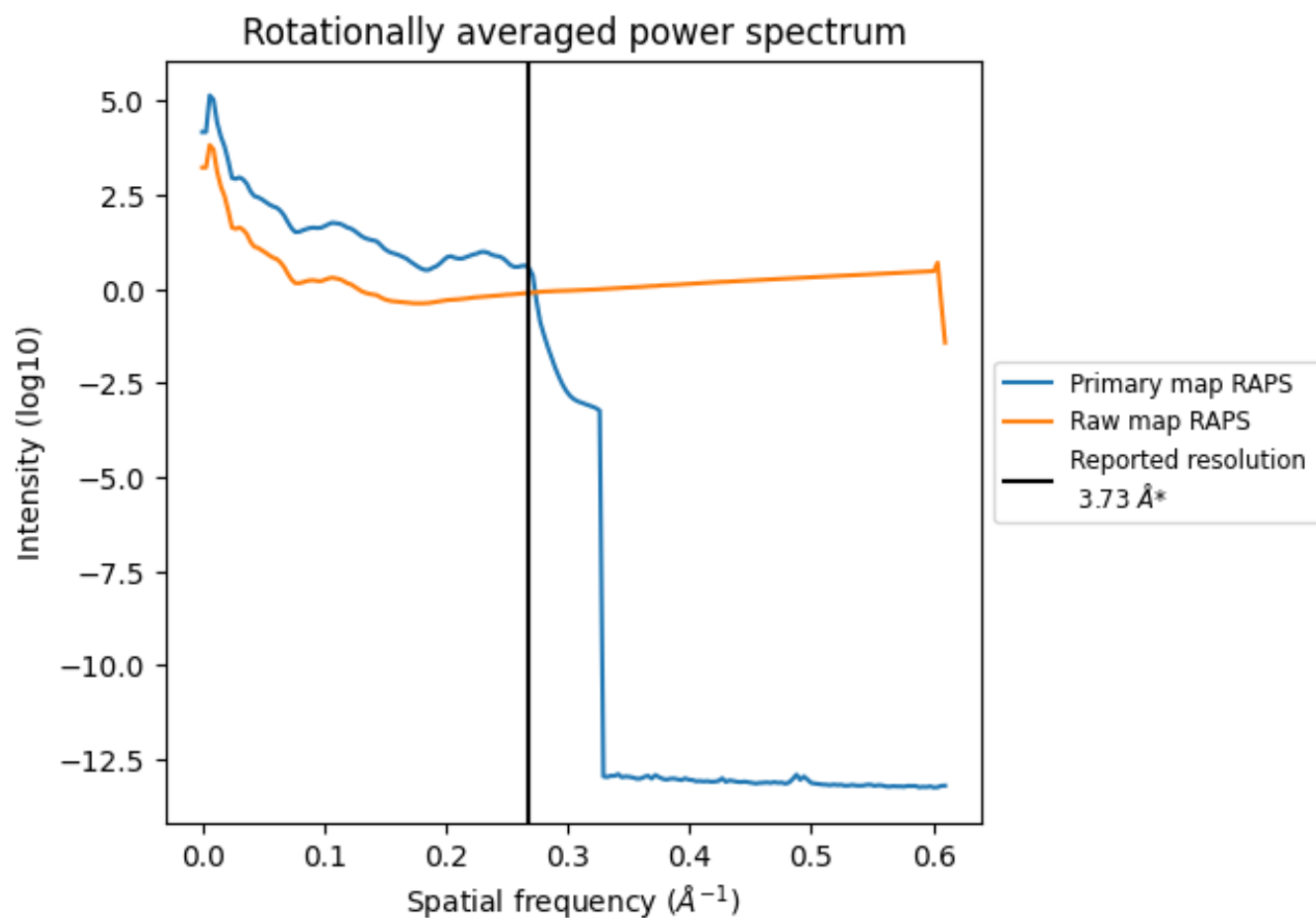
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm³; this corresponds to an approximate mass of 304 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 ⓘ

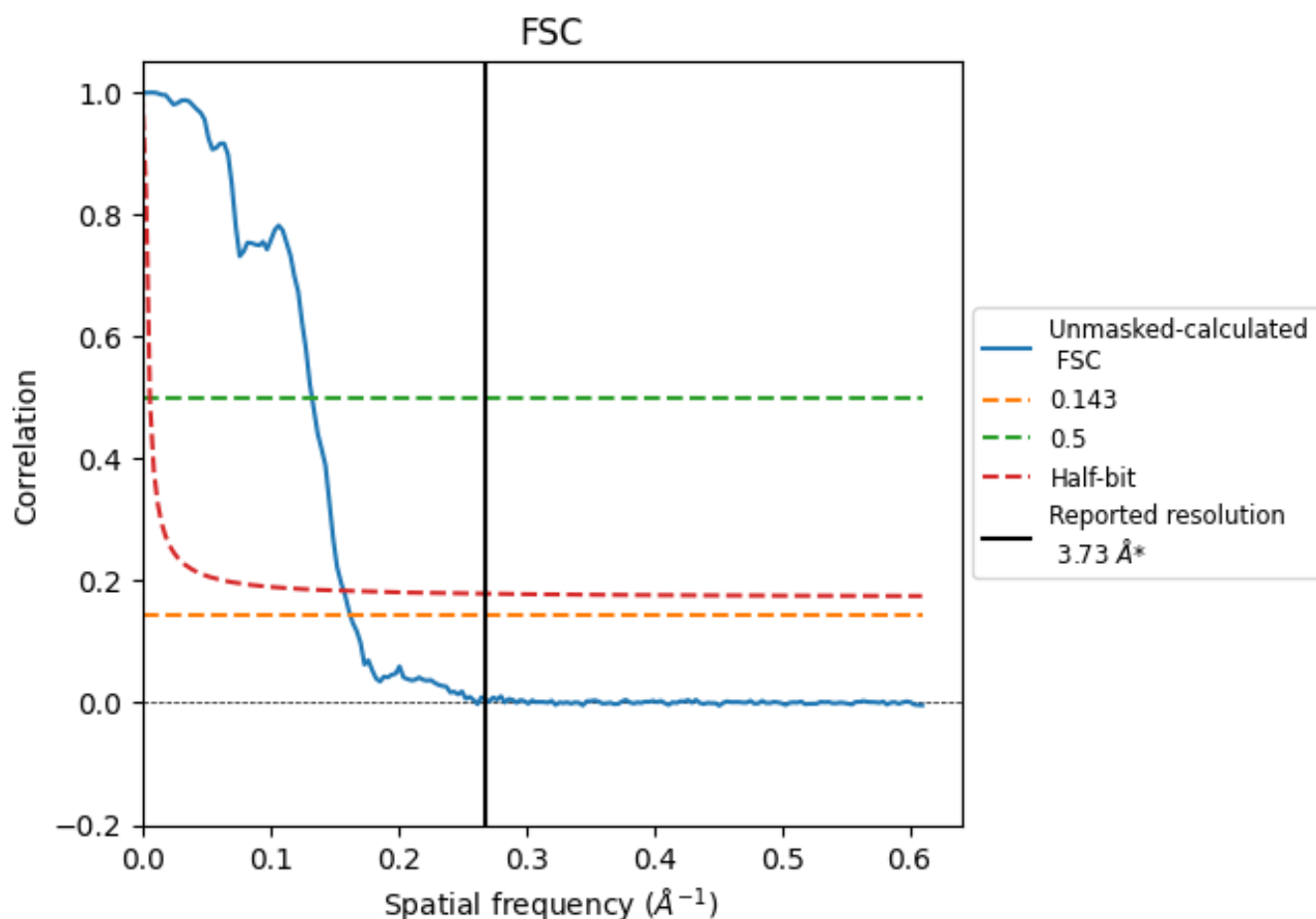


*Reported resolution corresponds to spatial frequency of 0.268 \AA^{-1}

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 0.268 Å⁻¹

8.2 Resolution estimates [i](#)

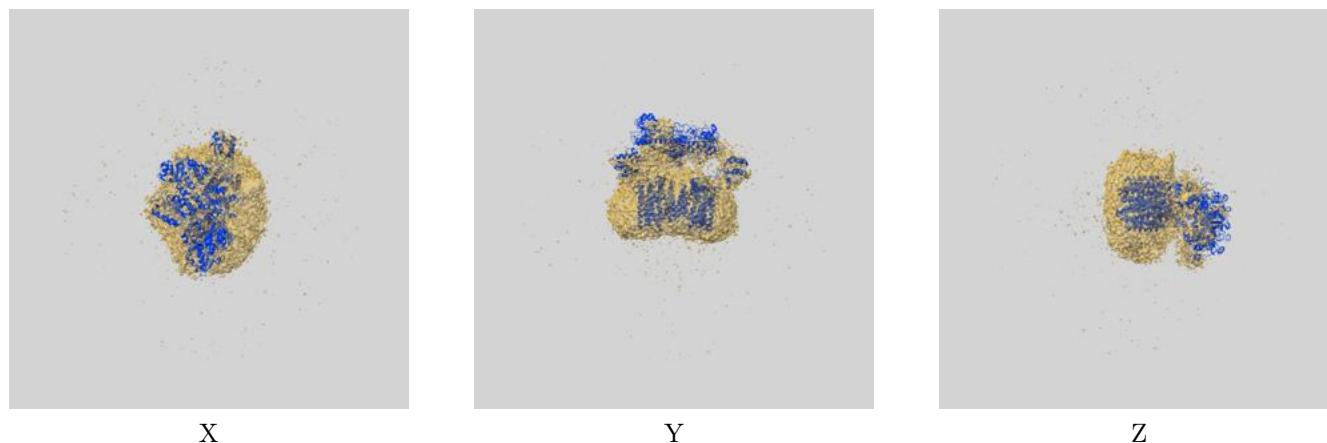
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.15	7.54	6.35

*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 6.15 differs from the reported value 3.73 by more than 10 %

9 Map-model fit [i](#)

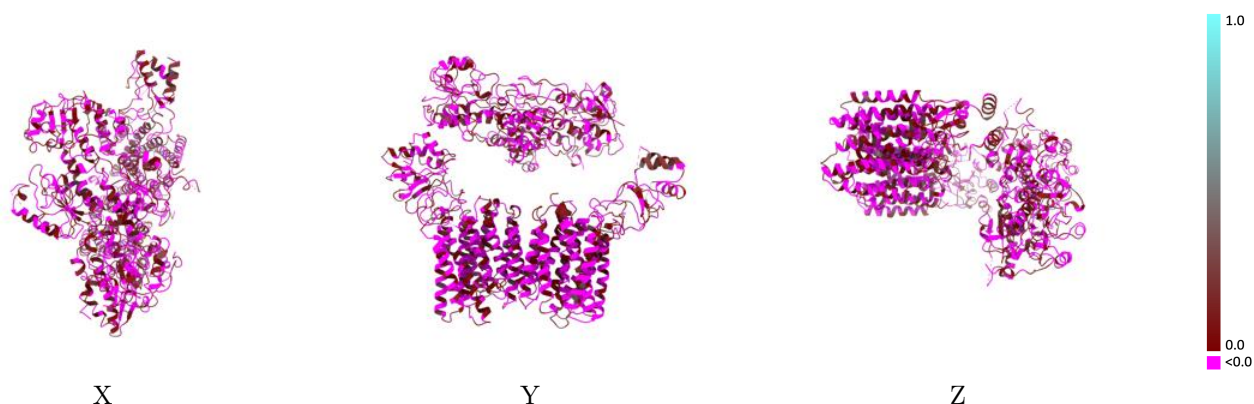
This section contains information regarding the fit between EMDB map EMD-64529 and PDB model 9UVA. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



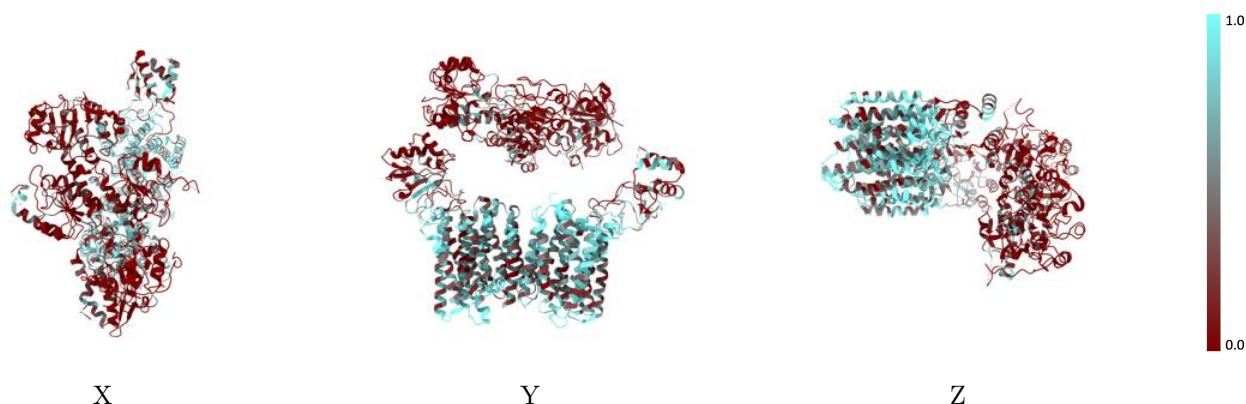
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



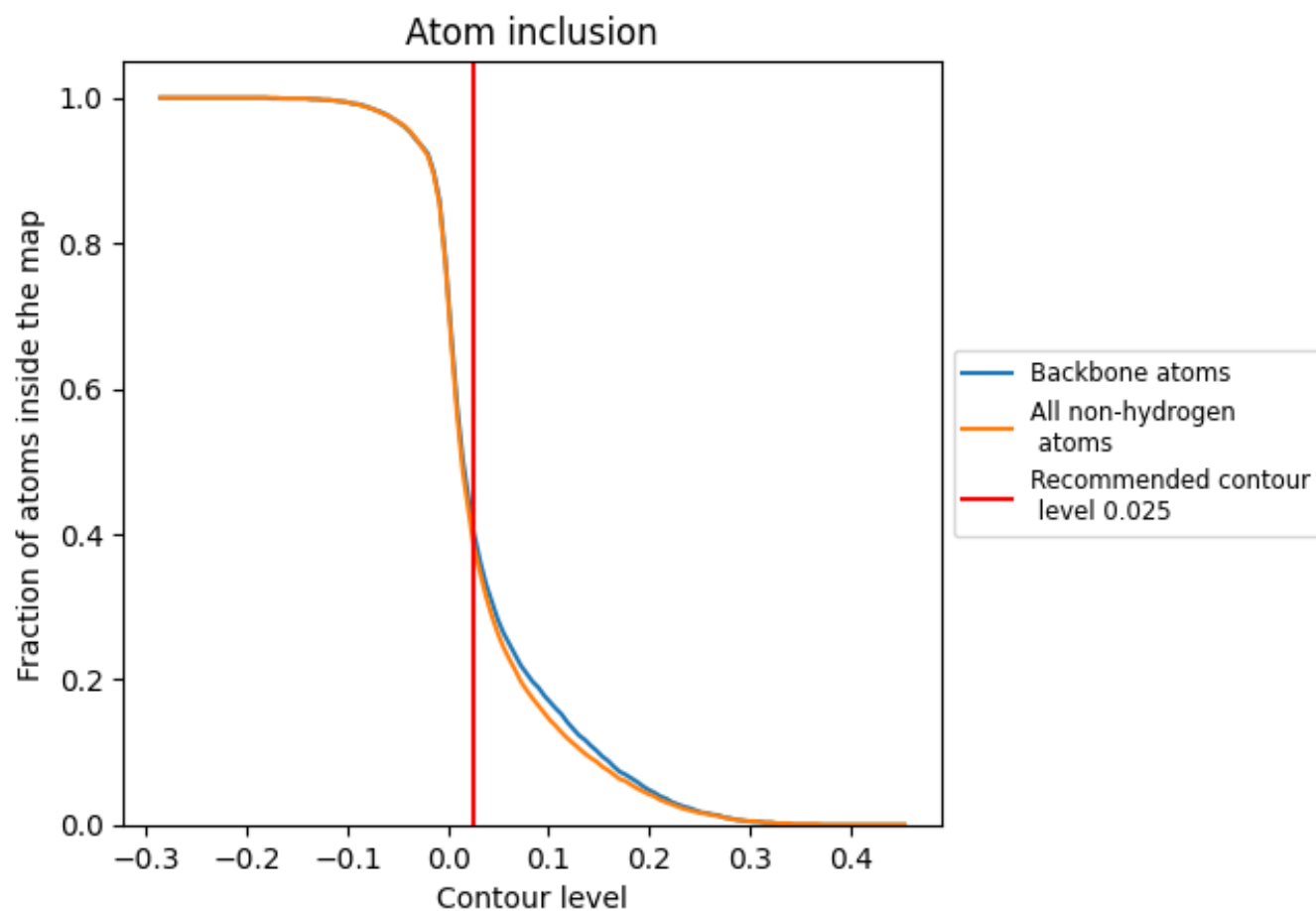
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 39% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3900	<div></div> -0.0030
A	<div></div> 0.5200	<div></div> -0.0100
B	<div></div> 0.6270	<div></div> 0.0110
C	<div></div> 0.6380	<div></div> -0.0110
D	<div></div> 0.6710	<div></div> -0.0450
E	<div></div> 0.1030	<div></div> 0.0000
F	<div></div> 0.1180	<div></div> 0.0020

1.0
0.0
-0.0