



wwPDB EM Validation Summary Report ⓘ

May 17, 2026 – 04:52 PM JST

PDB ID : 9UV7 / pdb_00009uv7
EMDB ID : EMD-64527
Title : Single-subunit apo Escherichia coli nicotinamide nucleotide transhydrogenase
Authors : Zhu, J.; Gennis, R.B.; Zhang, K.; Li, J.
Deposited on : 2025-05-09
Resolution : 3.43 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

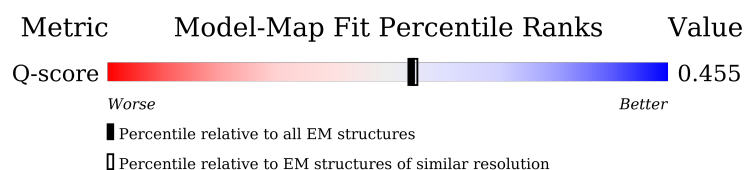
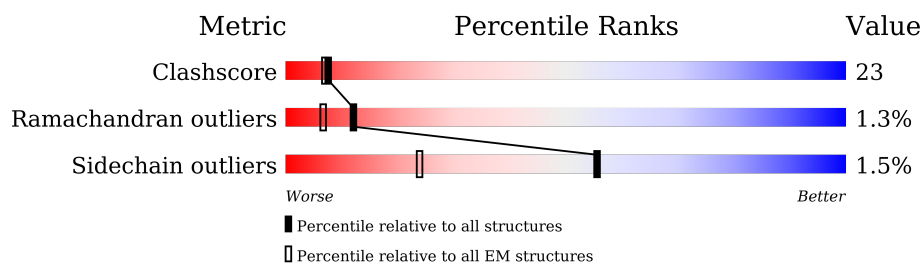
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 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	13927 (2.93 - 3.93)

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	
1	B	462	
2	C	99	
2	D	99	

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Mol	Chain	Length	Quality of chain
3	E	377	<div><div></div><div>54%</div><div></div><div>45%</div><div></div><div>48%</div><div></div><div>5%</div><div></div><div></div></div>
3	F	377	<div><div></div><div>47%</div><div></div><div>51%</div><div></div><div>44%</div><div></div><div></div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13484 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	438	Total	C	N	O	S	0	0
			3263	2116	542	583	22		
1	A	438	Total	C	N	O	S	0	0
			3263	2116	542	583	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	99	Total	C	N	O	S	0	0
			758	510	121	122	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		

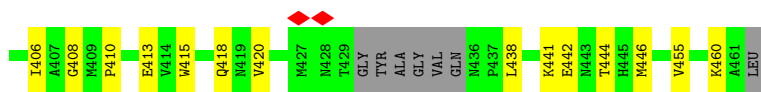
There are 6 discrepancies between the modelled and reference sequences:

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

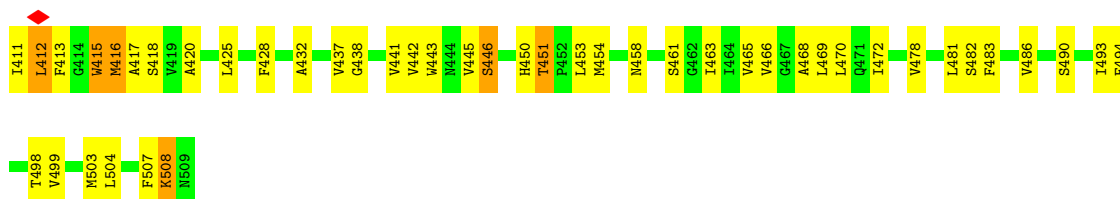
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Chain	Residue	Modelled	Actual	Comment	Reference
E	1000	HIS	-	expression tag	UNP P07001
E	1001	GLY	-	expression tag	UNP P07001
F	999	HIS	-	expression tag	UNP P07001
F	1000	HIS	-	expression tag	UNP P07001
F	1001	GLY	-	expression tag	UNP P07001



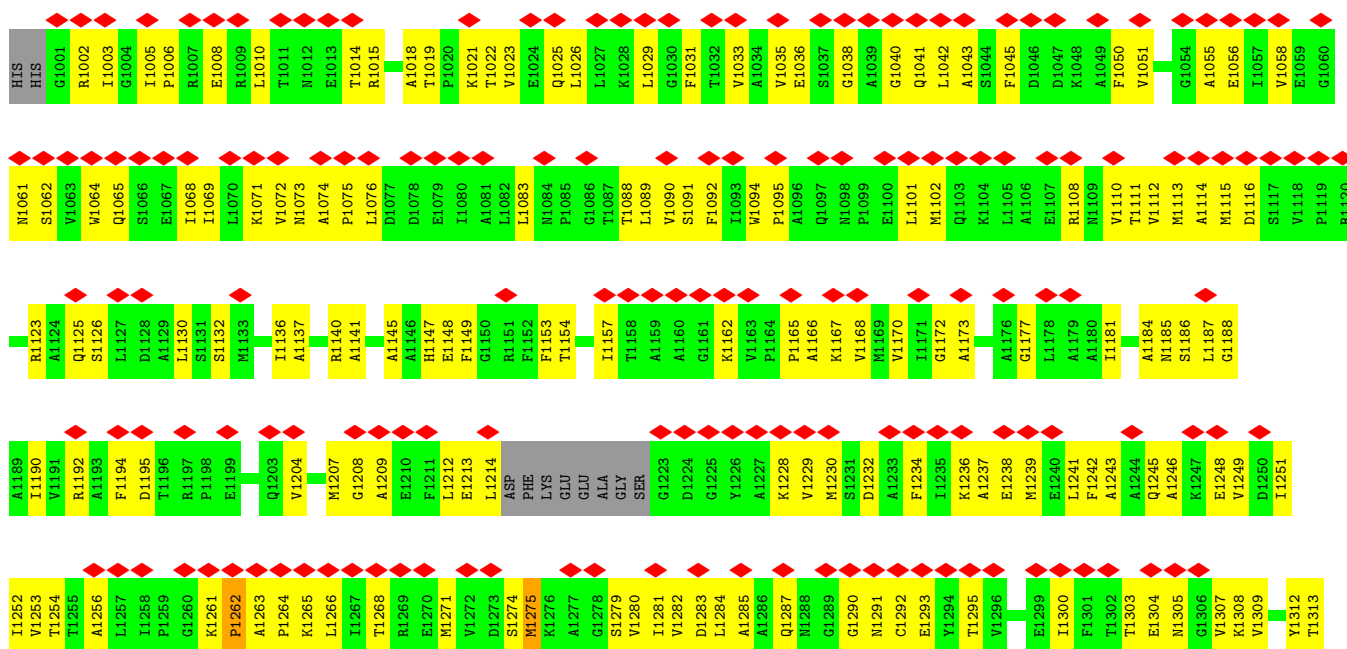
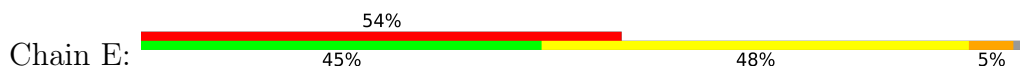
- Molecule 2: NAD(P) transhydrogenase subunit alpha

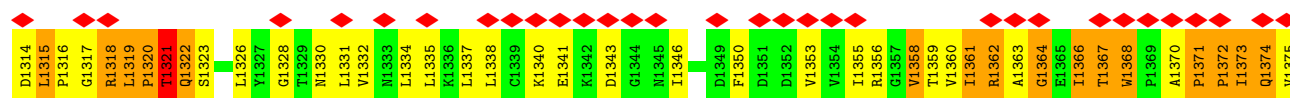


- Molecule 2: NAD(P) transhydrogenase subunit alpha

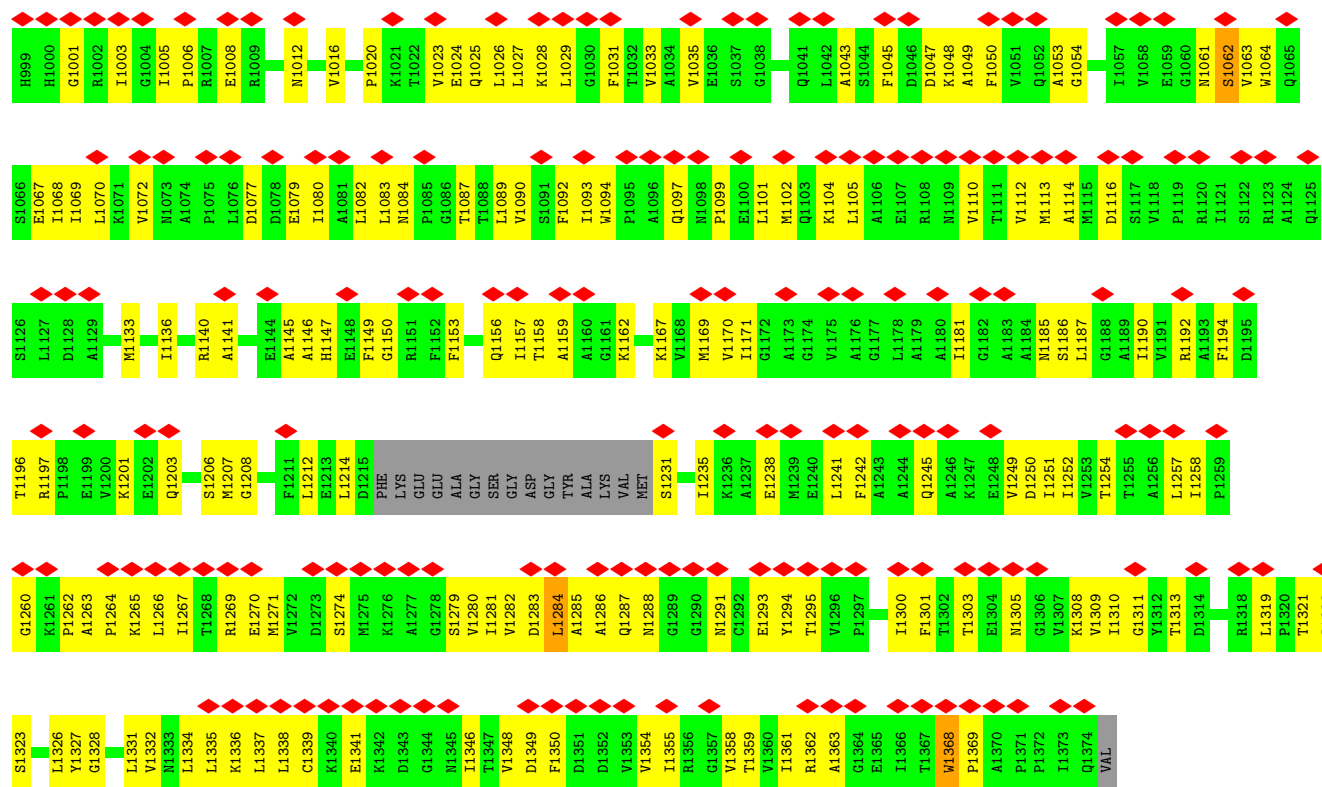


- Molecule 3: NAD(P) transhydrogenase subunit alpha





● Molecule 3: NAD(P) transhydrogenase subunit alpha



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42826	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 ($e^-/\text{\AA}^2$)	1.25	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	1.443	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.156	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	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	0.22	0/3324	0.39	0/4515
1	B	0.24	0/3324	0.45	2/4515 (0.0%)
2	C	0.33	0/779	0.62	2/1060 (0.2%)
2	D	0.29	0/779	0.50	0/1060
3	E	0.52	4/2781 (0.1%)	0.66	6/3777 (0.2%)
3	F	0.26	0/2746	0.47	1/3731 (0.0%)
All	All	0.32	4/13733 (0.0%)	0.51	11/18658 (0.1%)

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	1
3	F	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1262	PRO	CG-CD	-14.78	1.00	1.50
3	E	1262	PRO	N-CD	13.24	1.66	1.47
3	E	1261	LYS	C-N	9.57	1.56	1.33
3	E	1262	PRO	N-CA	-6.29	1.39	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1262	PRO	CA-N-CD	-19.80	84.28	112.00
3	F	1264	PRO	CA-N-CD	-11.13	96.42	112.00
3	E	1262	PRO	N-CD-CG	-9.04	89.65	103.20
3	E	1262	PRO	CA-CB-CG	-7.72	89.83	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1261	LYS	C-N-CD	7.29	154.87	125.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	THR	Peptide
3	F	1368	TRP	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	3263	0	3377	126	0
1	B	3263	0	3377	112	0
2	C	758	0	781	54	0
2	D	758	0	781	39	0
3	E	2739	0	2799	181	0
3	F	2703	0	2753	169	0
All	All	13484	0	13868	627	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 23.

The worst 5 of 627 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:E:1115:MET:HE2	3:E:1331:LEU:HD23	1.30	1.11
3:F:1099:PRO:HA	3:F:1102:MET:HE3	1.35	1.09
1:B:427:MET:HE1	1:B:439:PHE:HB3	1.26	1.08
3:F:1047:ASP:OD1	3:F:1048:LYS:HD3	1.54	1.08
3:F:1156:GLN:HE22	3:F:1158:THR:HA	1.23	1.04

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	432/462 (94%)	406 (94%)	26 (6%)	0	100	100
1	B	432/462 (94%)	404 (94%)	23 (5%)	5 (1%)	10	38
2	C	97/99 (98%)	88 (91%)	4 (4%)	5 (5%)	1	13
2	D	97/99 (98%)	85 (88%)	10 (10%)	2 (2%)	5	28
3	E	363/377 (96%)	317 (87%)	40 (11%)	6 (2%)	7	32
3	F	357/377 (95%)	316 (88%)	36 (10%)	5 (1%)	9	35
All	All	1778/1876 (95%)	1616 (91%)	139 (8%)	23 (1%)	12	37

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	SER
1	B	407	ALA
2	C	451	THR
3	E	1320	PRO
3	F	1062	SER

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	345/360 (96%)	343 (99%)	2 (1%)	78	80
1	B	345/360 (96%)	344 (100%)	1 (0%)	86	84
2	C	80/80 (100%)	79 (99%)	1 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	80/80 (100%)	79 (99%)	1 (1%)	61	72
3	E	290/298 (97%)	275 (95%)	15 (5%)	21	48
3	F	287/298 (96%)	286 (100%)	1 (0%)	86	84
All	All	1427/1476 (97%)	1406 (98%)	21 (2%)	55	71

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	1362	ARG
3	E	1368	TRP
3	F	1207	MET
3	E	1373	ILE
3	E	1367	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	1065	GLN
3	F	1156	GLN
3	F	1333	ASN
3	F	1185	ASN
3	F	1135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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.

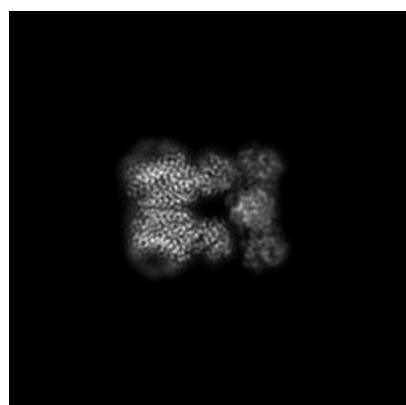
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64527. These allow visual inspection of the internal detail of the map and identification of artifacts.

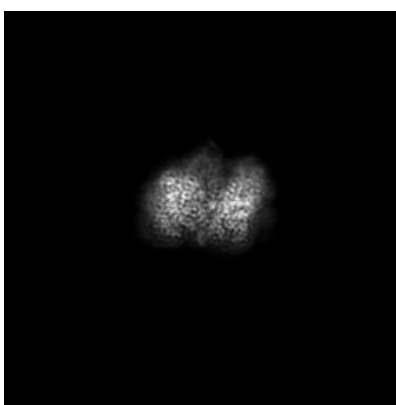
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

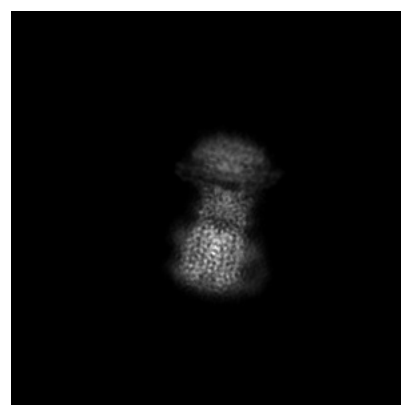
6.1.1 Primary map



X



Y

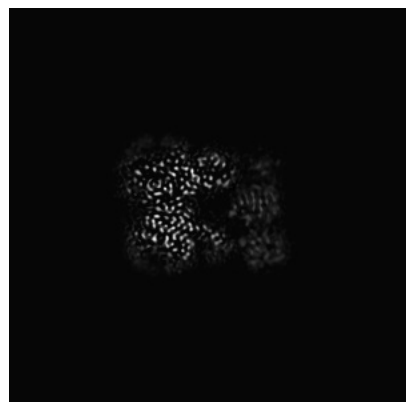


Z

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

6.2 Central slices [i](#)

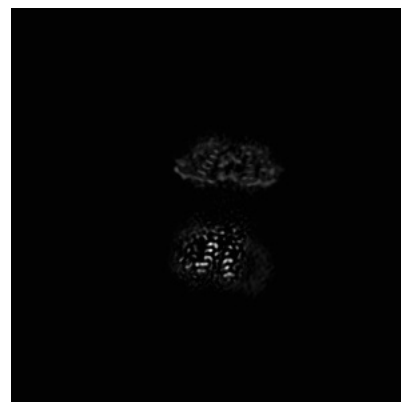
6.2.1 Primary map



X Index: 180



Y Index: 180

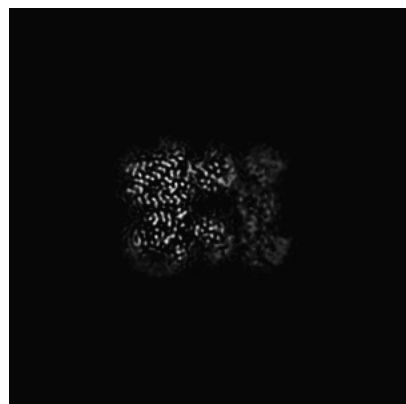


Z Index: 180

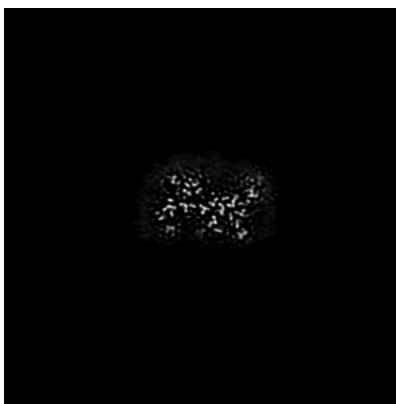
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 186



Y Index: 141

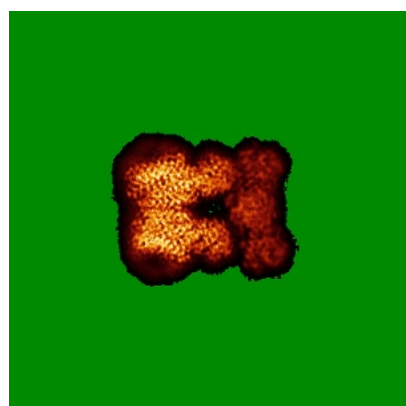


Z Index: 212

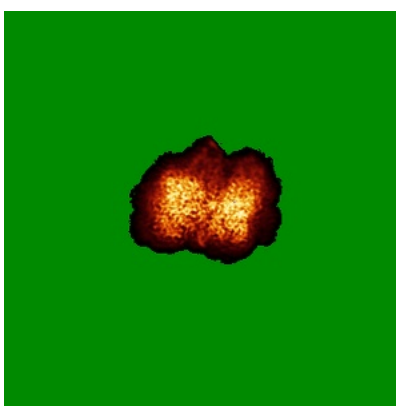
The images above show the largest variance slices of the map in three orthogonal directions.

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

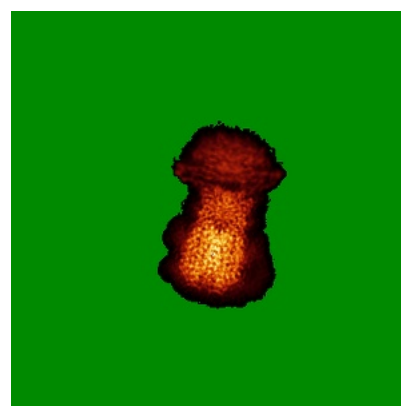
6.4.1 Primary map



X



Y

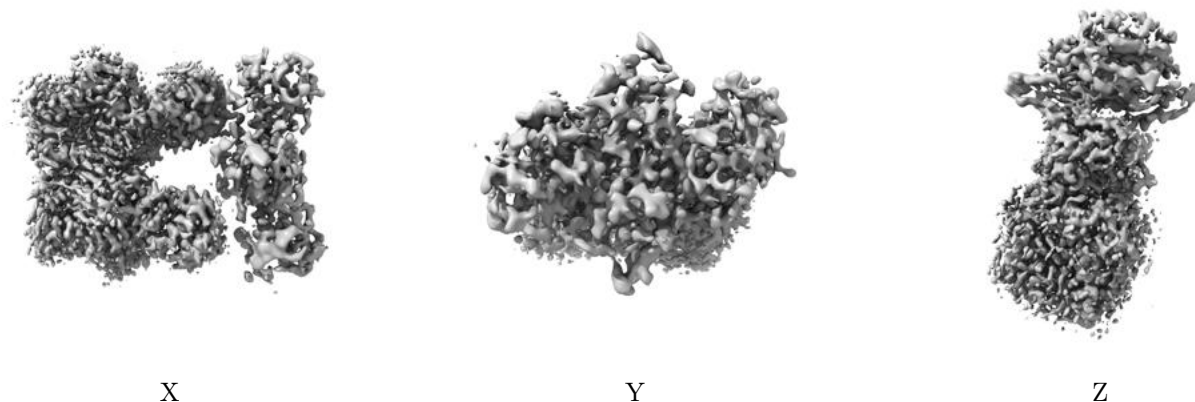


Z

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

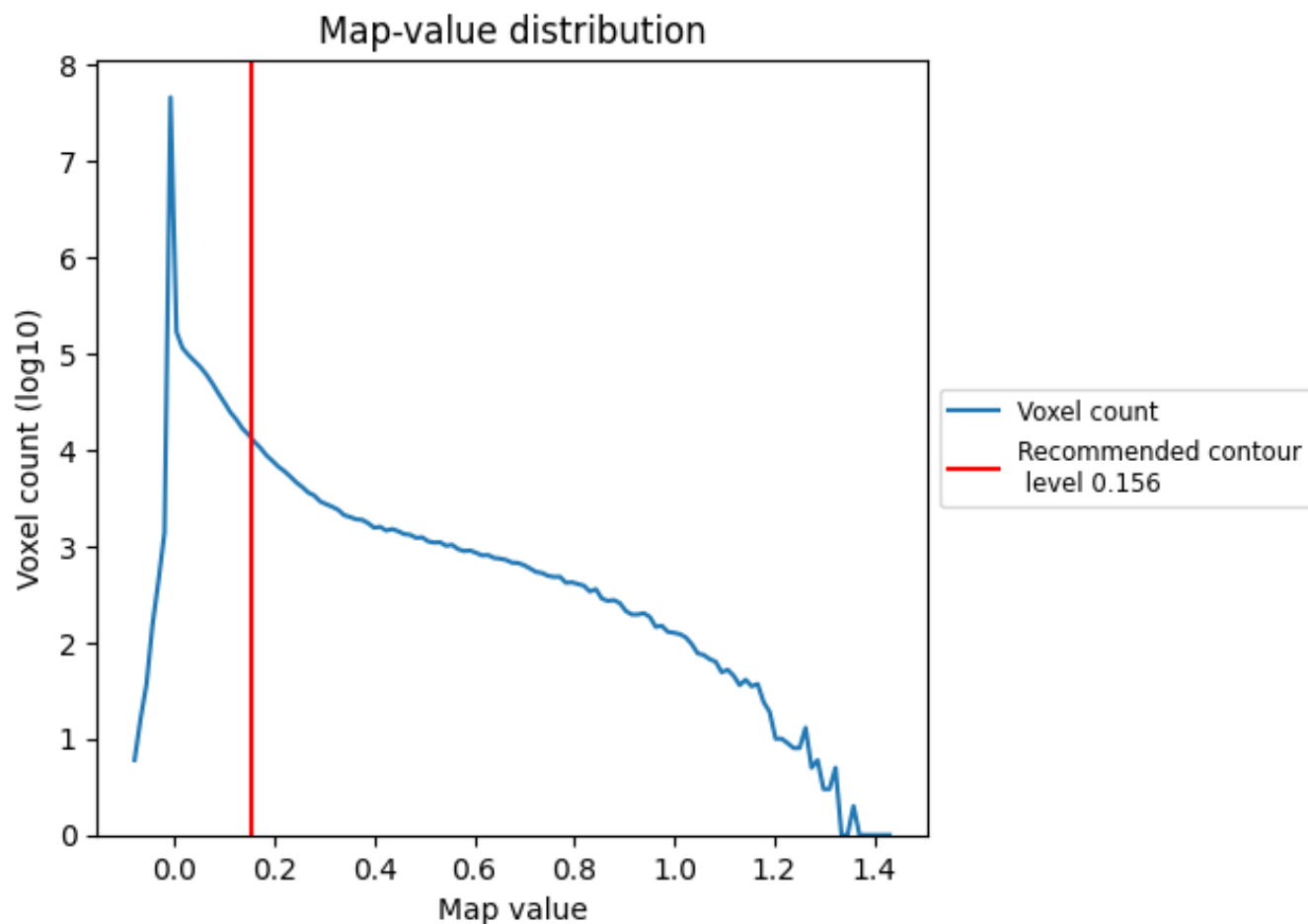
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

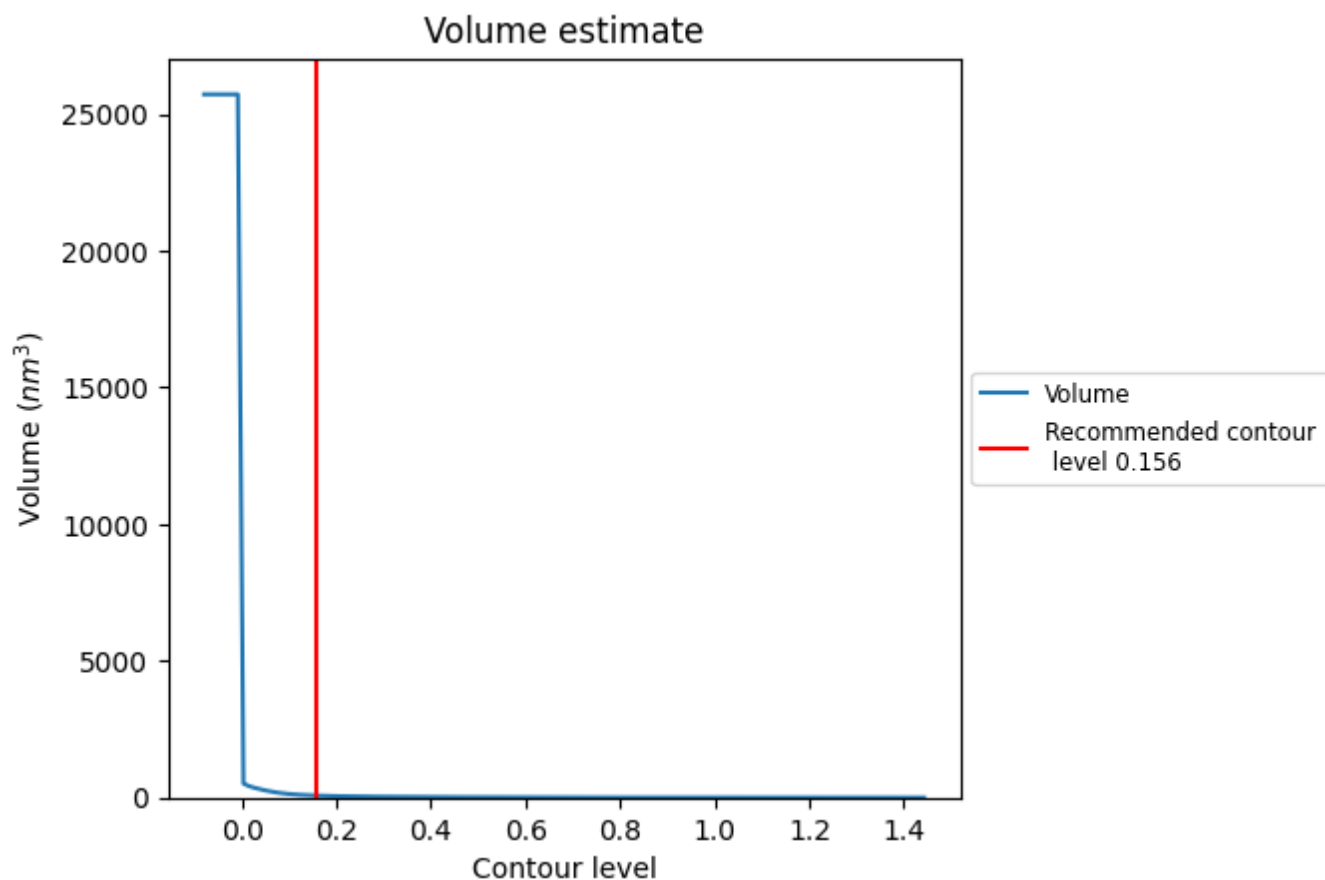
This section contains the results of statistical analysis of the map.

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.

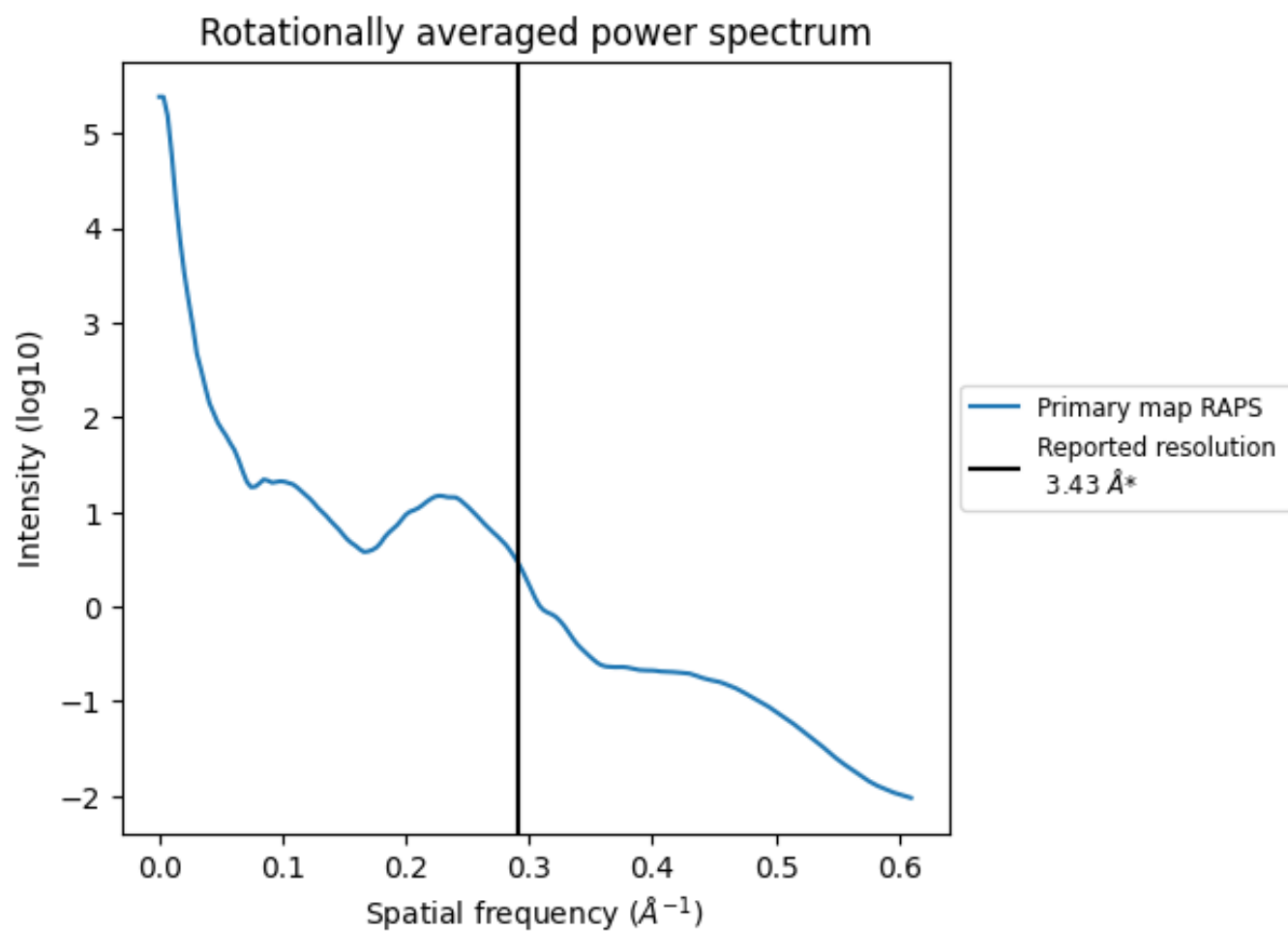
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm^3 ; this corresponds to an approximate mass of 67 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 0.292 Å⁻¹

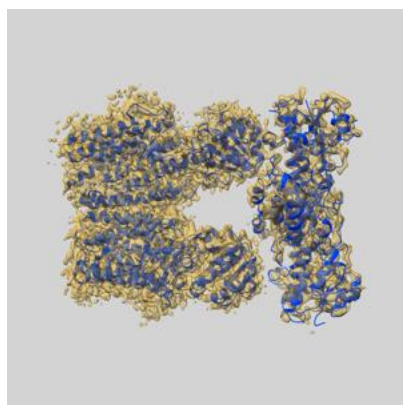
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

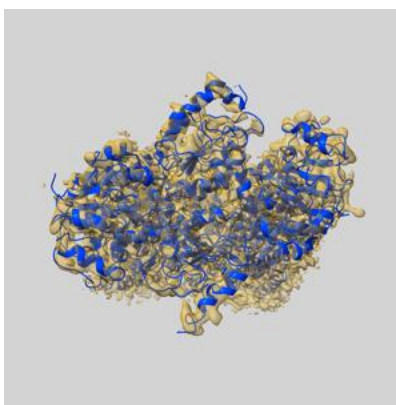
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64527 and PDB model 9UV7. Per-residue inclusion information can be found in section [3](#) on page [6](#).

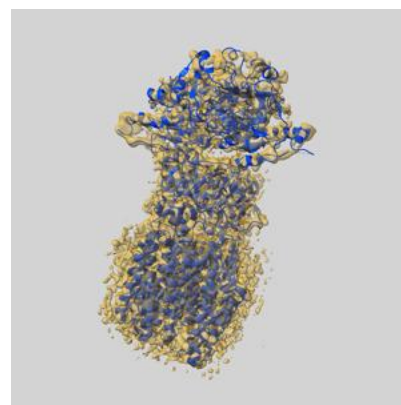
9.1 Map-model overlay [i](#)



X



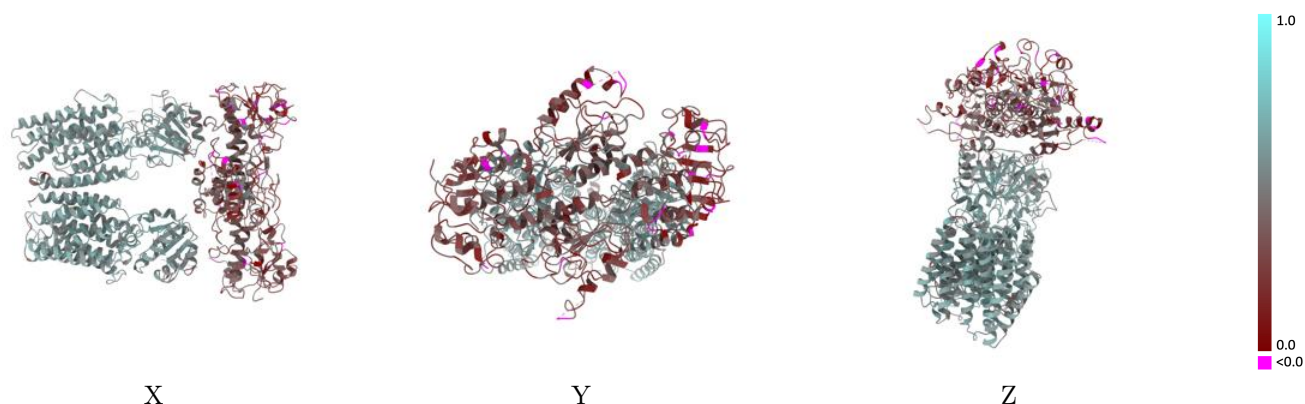
Y



Z

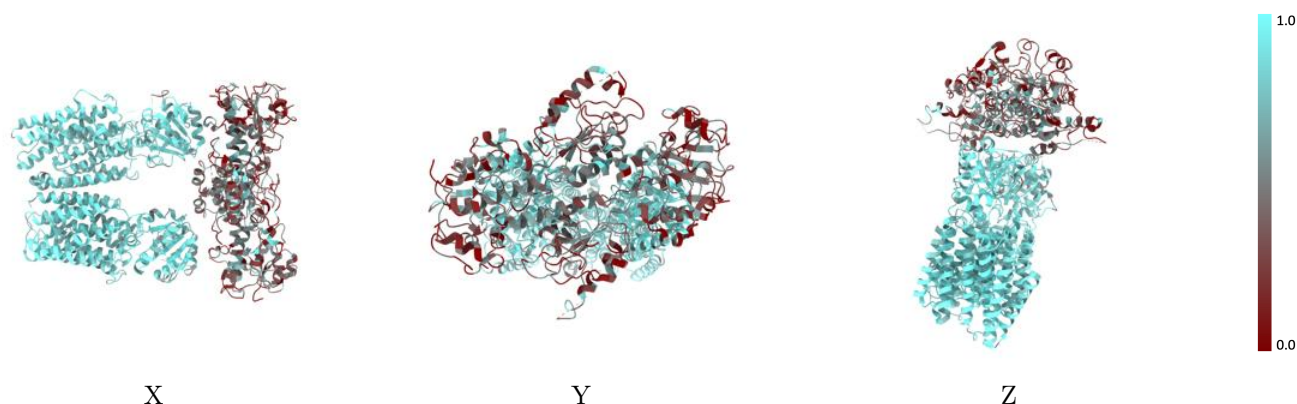
The images above show the 3D surface view of the map at the recommended contour level 0.156 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



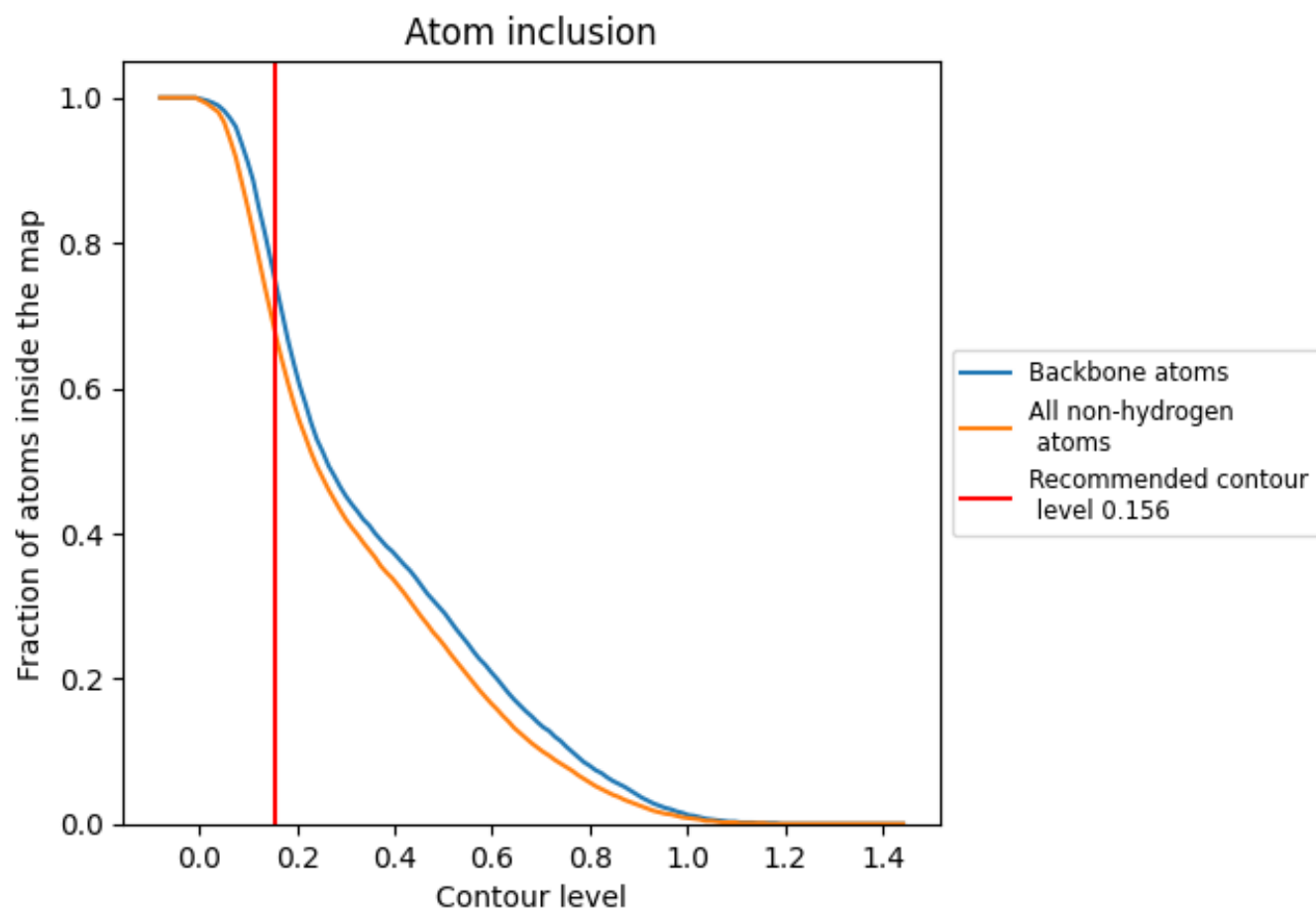
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.156).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 68% 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 (0.156) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6760	<div></div> 0.4550
A	<div></div> 0.8750	<div></div> 0.5630
B	<div></div> 0.8680	<div></div> 0.5620
C	<div></div> 0.8910	<div></div> 0.5660
D	<div></div> 0.8890	<div></div> 0.5620
E	<div></div> 0.3700	<div></div> 0.2890
F	<div></div> 0.3900	<div></div> 0.3030

1.0

0.0

<0.0