



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:32 PM UTC

PDB ID : 9IR4 / pdb_00009ir4
EMDB ID : EMD-60800
Title : Cryo-EM structure of Nipah virus L-P (H1165Y) polymerase complex
Authors : Shi, Y.; Peng, Q.
Deposited on : 2024-07-14
Resolution : 3.01 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:

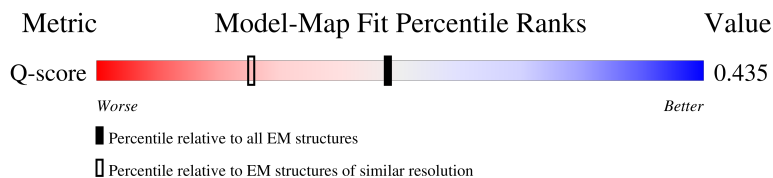
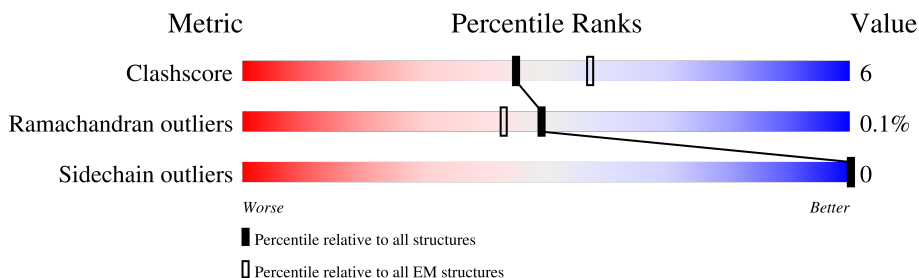
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.01 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	13882 (2.51 - 3.51)

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	2244	
2	C	709	
2	D	709	
2	E	709	

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Mol	Chain	Length	Quality of chain
2	F	709	 8% 91%
2	G	709	 5% 5% 91%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12604 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1260	Total	C	N	O	S	0	0
			10150	6473	1734	1877	66		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1165	TYR	HIS	engineered mutation	UNP Q997F0

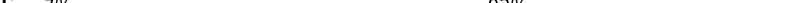
- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	69	Total	C	N	O	S	0	0
			557	344	94	118	1		
2	D	58	Total	C	N	O	S	0	0
			436	271	77	85	3		
2	E	65	Total	C	N	O	S	0	0
			484	309	81	90	4		
2	F	67	Total	C	N	O	S	0	0
			494	311	86	93	4		
2	G	65	Total	C	N	O	S	0	0
			481	302	82	93	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

- Molecule 2: Phosphoprotein

Chain D:  7% 92%

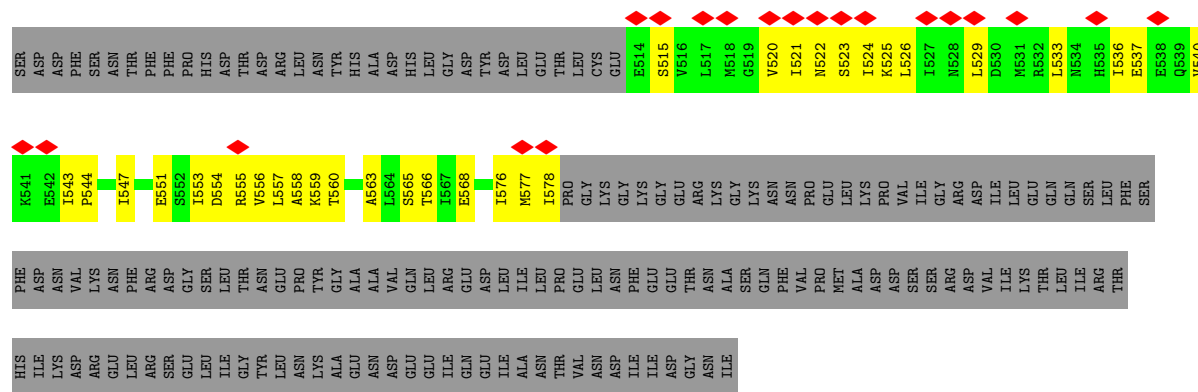




Position	Residue	Score
1547	SER	1547
1548	LEU	1548
1549	THR	1549
1550	ASN	1550
1551	GLU	1551
1552	PRO	1552
1553	TYR	1553
1554	GLY	1554
1555	ALA	1555
1556	ALA	1556
1557	ASN	1557
1558	ASP	1558
1559	VAL	1559
1560	GLN	1560
1561	LEU	1561
1562	ARG	1562
1563	GLU	1563
1564	GLN	1564
1565	GLU	1565
1566	LEU	1566
1567	ILE	1567
1568	ALA	1568
1569	ASN	1569
1570	THR	1570
1571	VAL	1571
1572	ASP	1572
1573	ASN	1573
1574	GLU	1574
1575	LEU	1575
1576	GLY	1576
1577	ASN	1577
1578	GLU	1578
1579	ASN	1579
1580	GLY	1580
1581	GLU	1581
1582	ASP	1582
1583	LYS	1583
1584	GLY	1584
1585	GLU	1585
1586	ARG	1586
1587	LYS	1587
1588	GLY	1588
1589	LYS	1589
1590	ASN	1590
1591	ASN	1591
1592	PRO	1592
1593	VAL	1593
1594	PRO	1594
1595	MET	1595
1596	ALA	1596
1597	ASP	1597
1598	ASP	1598
1599	SER	1599
1600	SER	1600
1601	ARG	1601
1602	ASP	1602
1603	VAL	1603
1604	ILE	1604
1605	LYS	1605
1606	THR	1606
1607	LEU	1607
1608	ILE	1608
1609	ARG	1609
1610	THR	1610
1611	HIS	1611
1612	ILE	1612
1613	LYS	1613
1614	ASP	1614
1615	ARG	1615
1616	GLU	1616
1617	LEU	1617
1618	ARG	1618
1619	SER	1619
1620	GLU	1620

Chain G:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56199	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.787	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.11	0/10358	0.28	0/14002
2	C	0.10	0/562	0.28	0/760
2	D	0.17	0/438	0.36	0/591
2	E	0.18	0/486	0.41	0/656
2	F	0.16	0/497	0.42	0/670
2	G	0.16	0/483	0.42	0/652
All	All	0.12	0/12824	0.30	0/17331

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 [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	10150	0	10189	119	0
2	C	557	0	544	7	0
2	D	436	0	438	6	0
2	E	484	0	513	14	0
2	F	494	0	504	8	0
2	G	481	0	487	23	0
3	A	2	0	0	0	0
All	All	12604	0	12675	160	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 160 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:TRP:HB3	1:A:1373:SER:HB3	1.74	0.69
1:A:468:SER:O	1:A:472:LYS:NZ	2.27	0.68
1:A:919:LEU:HD21	1:A:1072:ILE:HD12	1.76	0.68
2:C:668:ILE:HG23	2:C:672:ILE:HD12	1.76	0.68
1:A:1249:PHE:HB2	1:A:1420:TYR:HB3	1.78	0.65

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	1250/2244 (56%)	1218 (97%)	31 (2%)	1 (0%)	48	79
2	C	67/709 (9%)	64 (96%)	3 (4%)	0	100	100
2	D	56/709 (8%)	55 (98%)	1 (2%)	0	100	100
2	E	63/709 (9%)	63 (100%)	0	0	100	100
2	F	65/709 (9%)	60 (92%)	5 (8%)	0	100	100
2	G	63/709 (9%)	60 (95%)	3 (5%)	0	100	100
All	All	1564/5789 (27%)	1520 (97%)	43 (3%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	832	ASP

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	1129/2046 (55%)	1129 (100%)	0	100	100
2	C	64/625 (10%)	64 (100%)	0	100	100
2	D	48/625 (8%)	48 (100%)	0	100	100
2	E	54/625 (9%)	54 (100%)	0	100	100
2	F	53/625 (8%)	53 (100%)	0	100	100
2	G	53/625 (8%)	53 (100%)	0	100	100
All	All	1401/5171 (27%)	1401 (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 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	528	ASN
2	F	528	ASN
2	F	535	HIS
2	F	534	ASN
1	A	1029	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

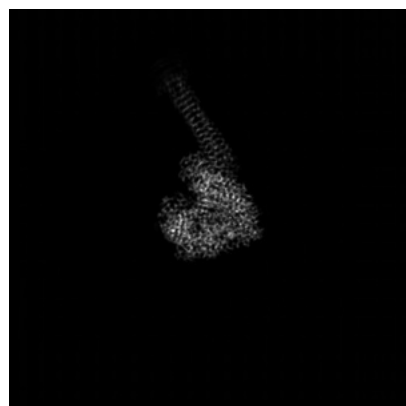
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60800. These allow visual inspection of the internal detail of the map and identification of artifacts.

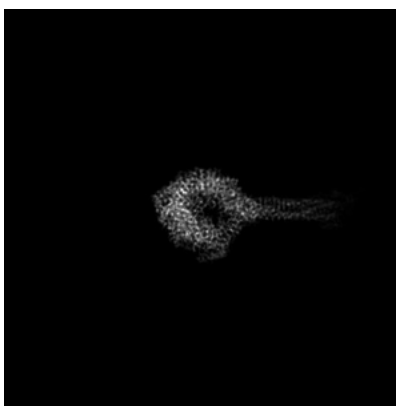
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

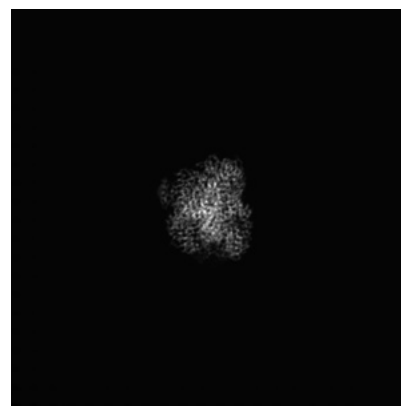
6.1.1 Primary map



X

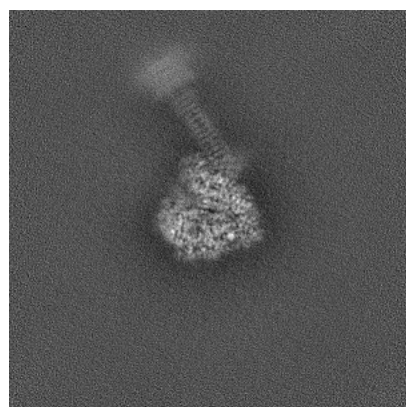


Y

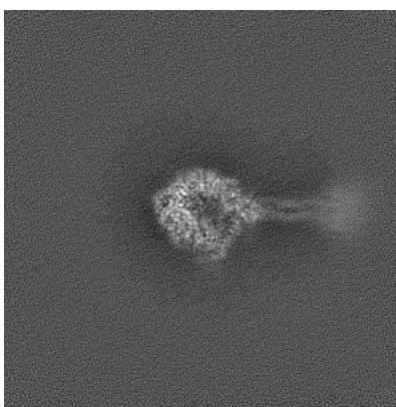


Z

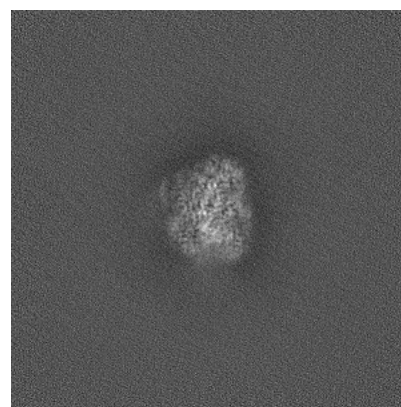
6.1.2 Raw map



X



Y



Z

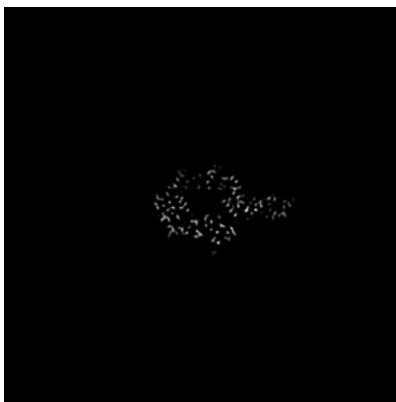
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210

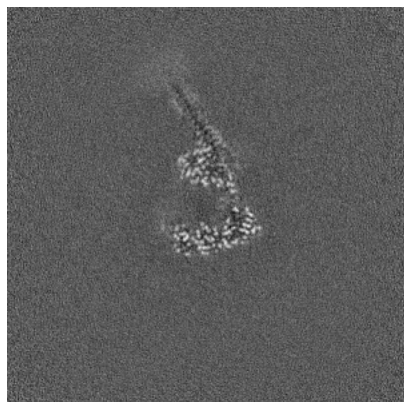


Y Index: 210

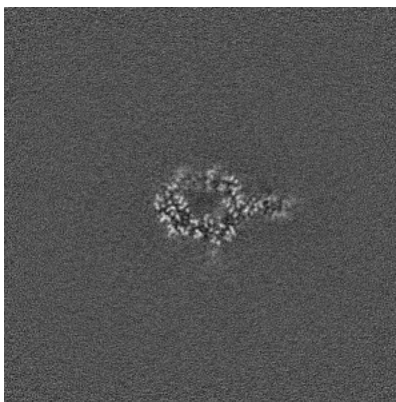


Z Index: 210

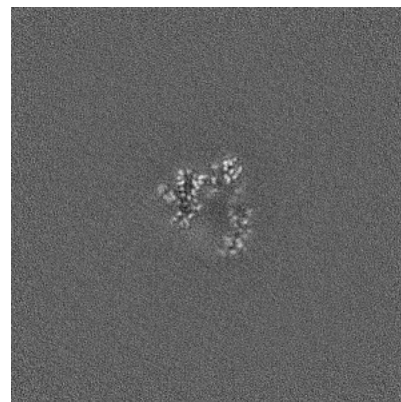
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

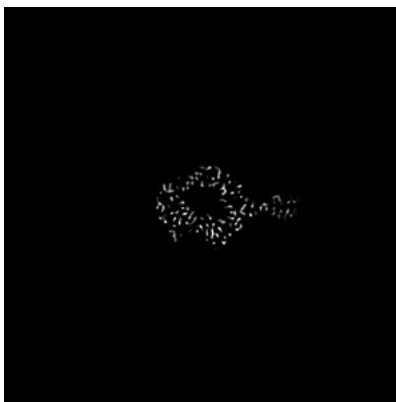
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 208

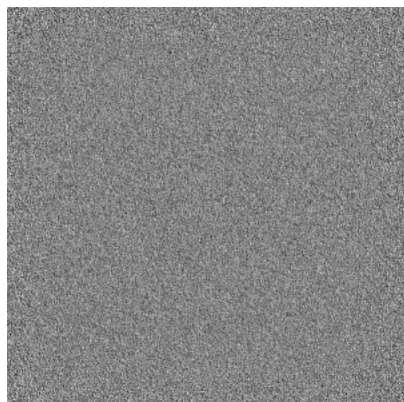


Y Index: 206

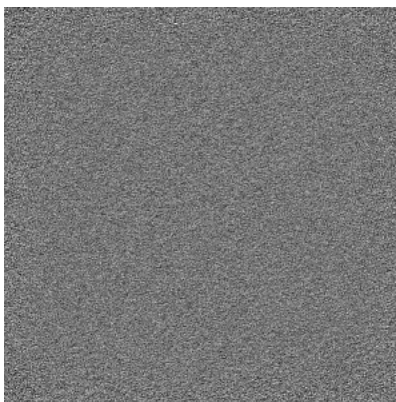


Z Index: 187

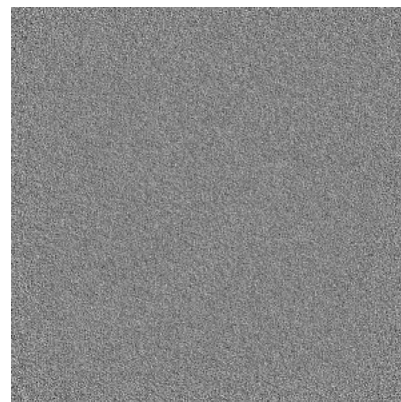
6.3.2 Raw map



X Index: 0



Y Index: 0

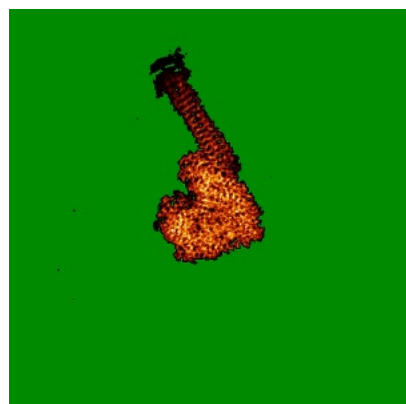


Z Index: 0

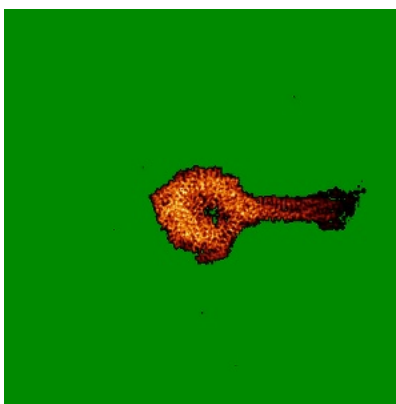
The images above show the largest variance slices of the map in three orthogonal directions.

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

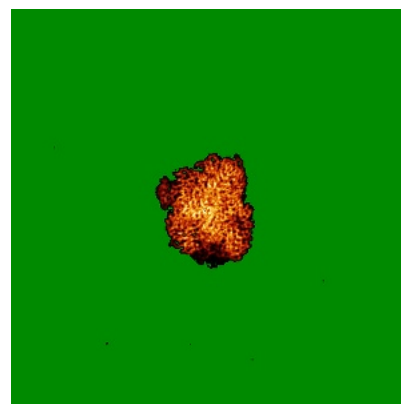
6.4.1 Primary map



X

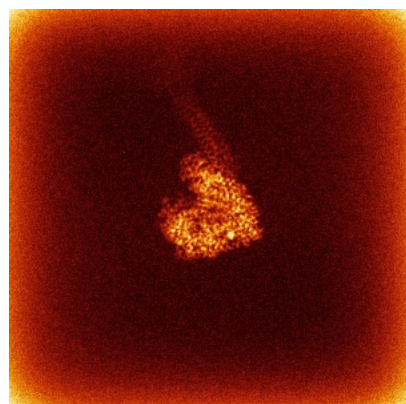


Y

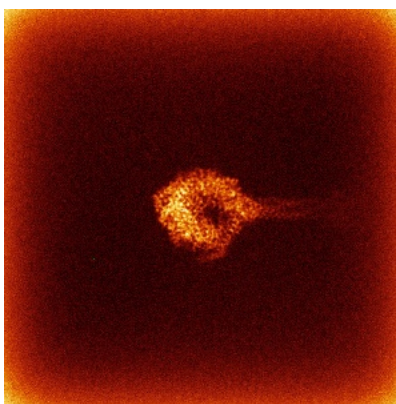


Z

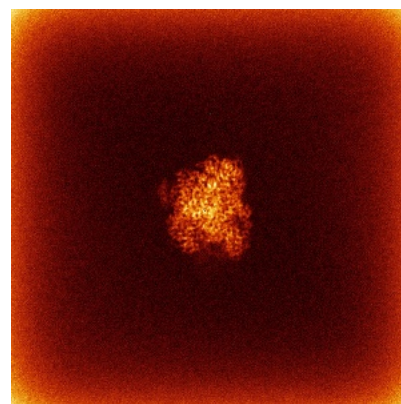
6.4.2 Raw map



X



Y

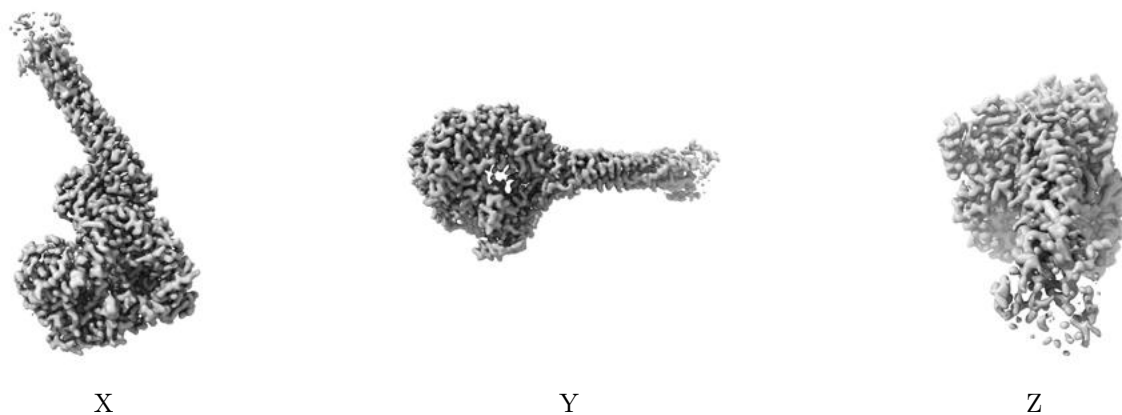


Z

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.

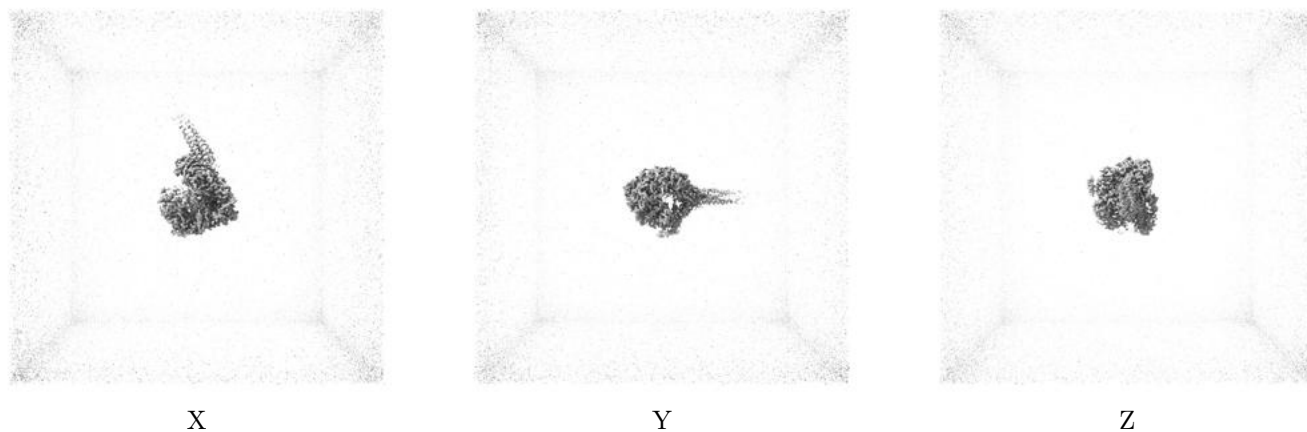
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

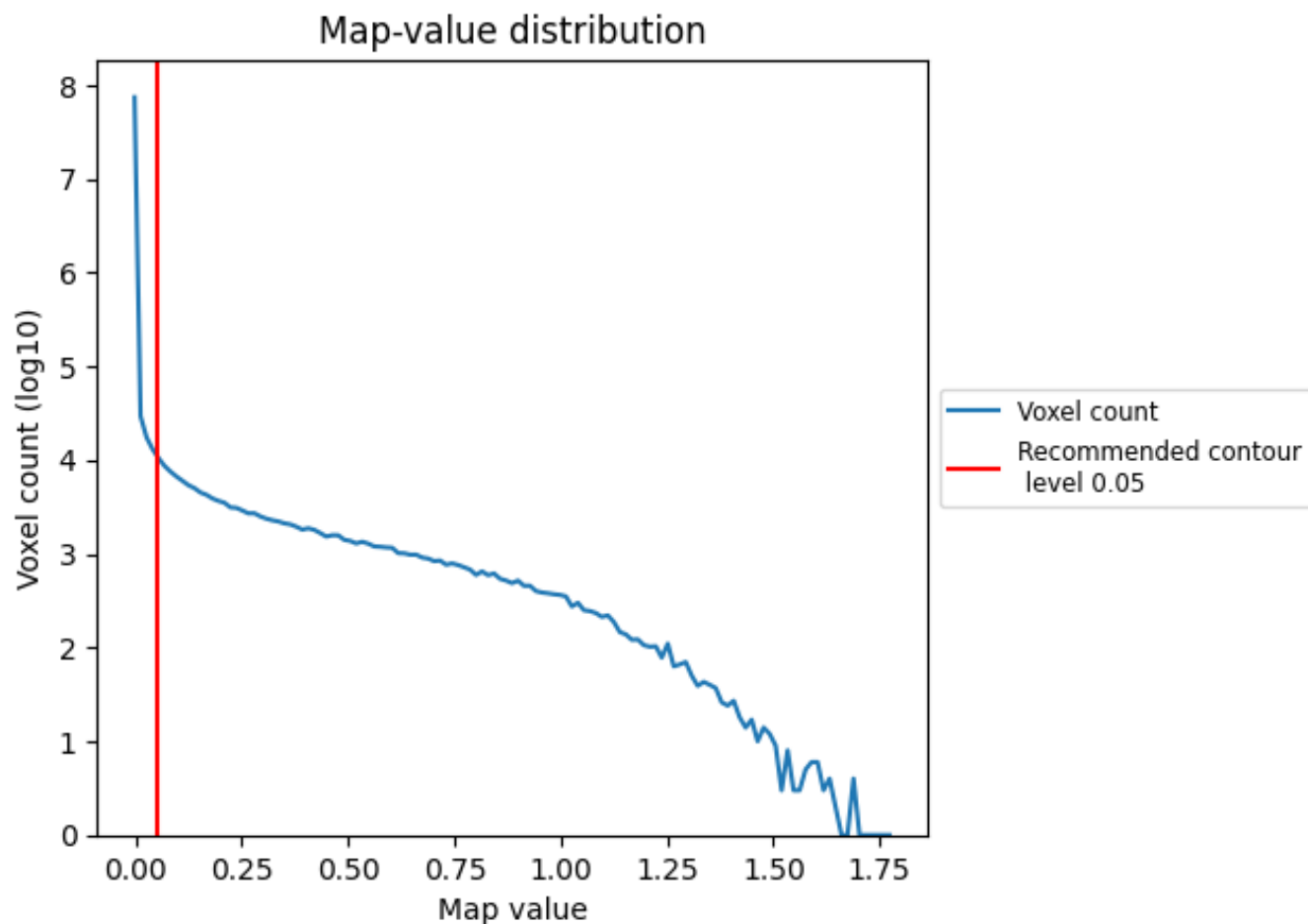
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

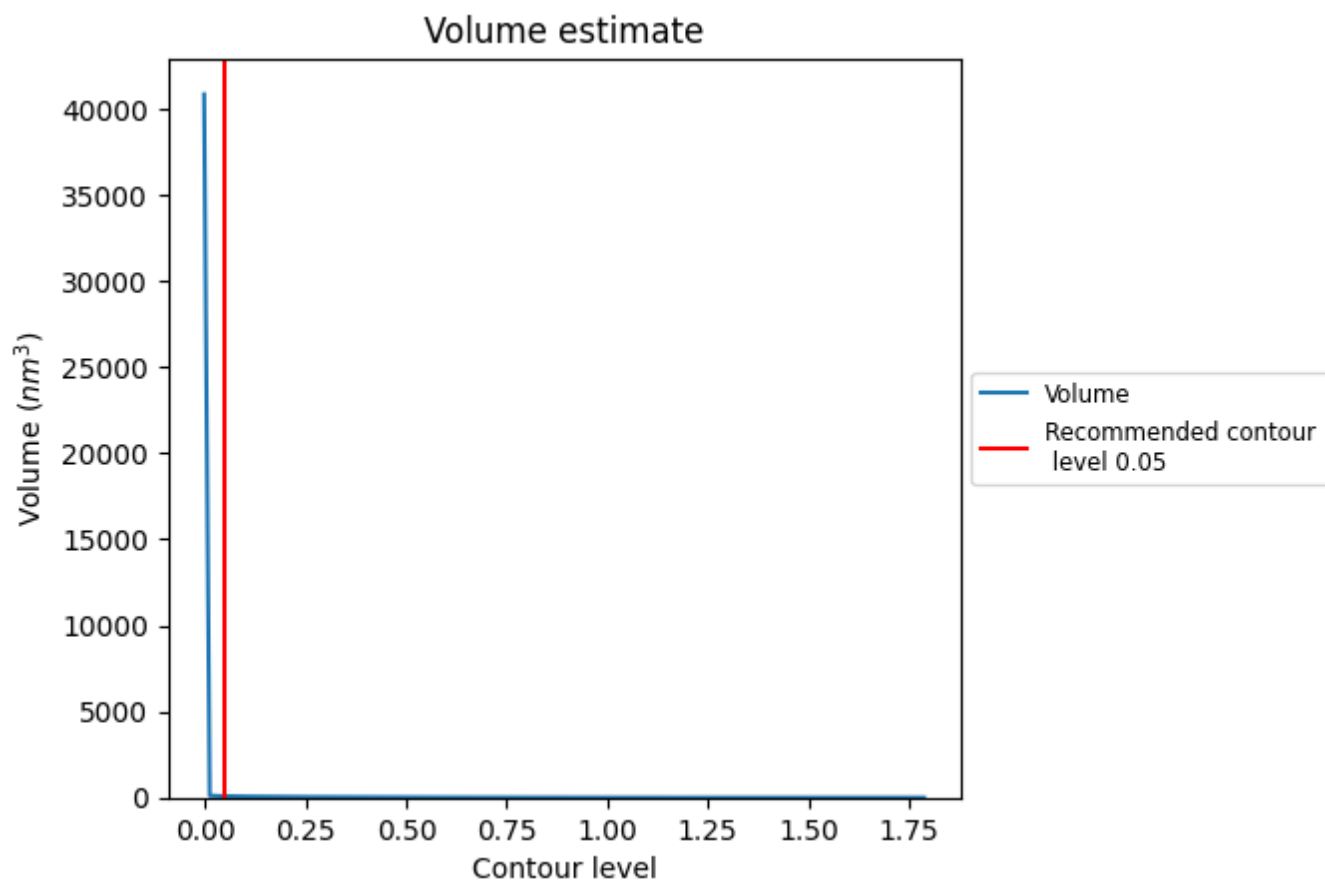
This section contains the results of statistical analysis of the map.

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.

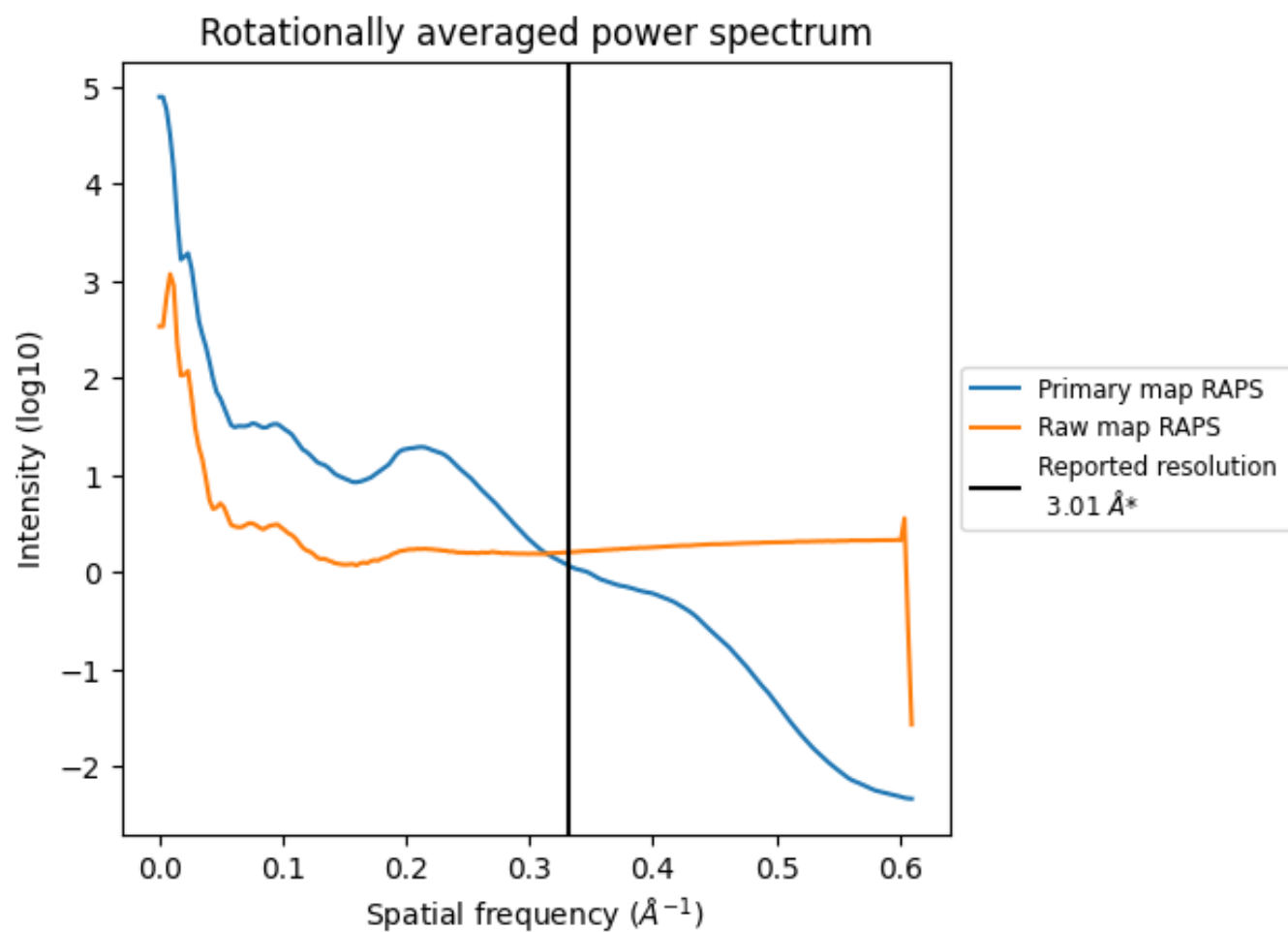
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm^3 ; this corresponds to an approximate mass of 74 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 ⓘ

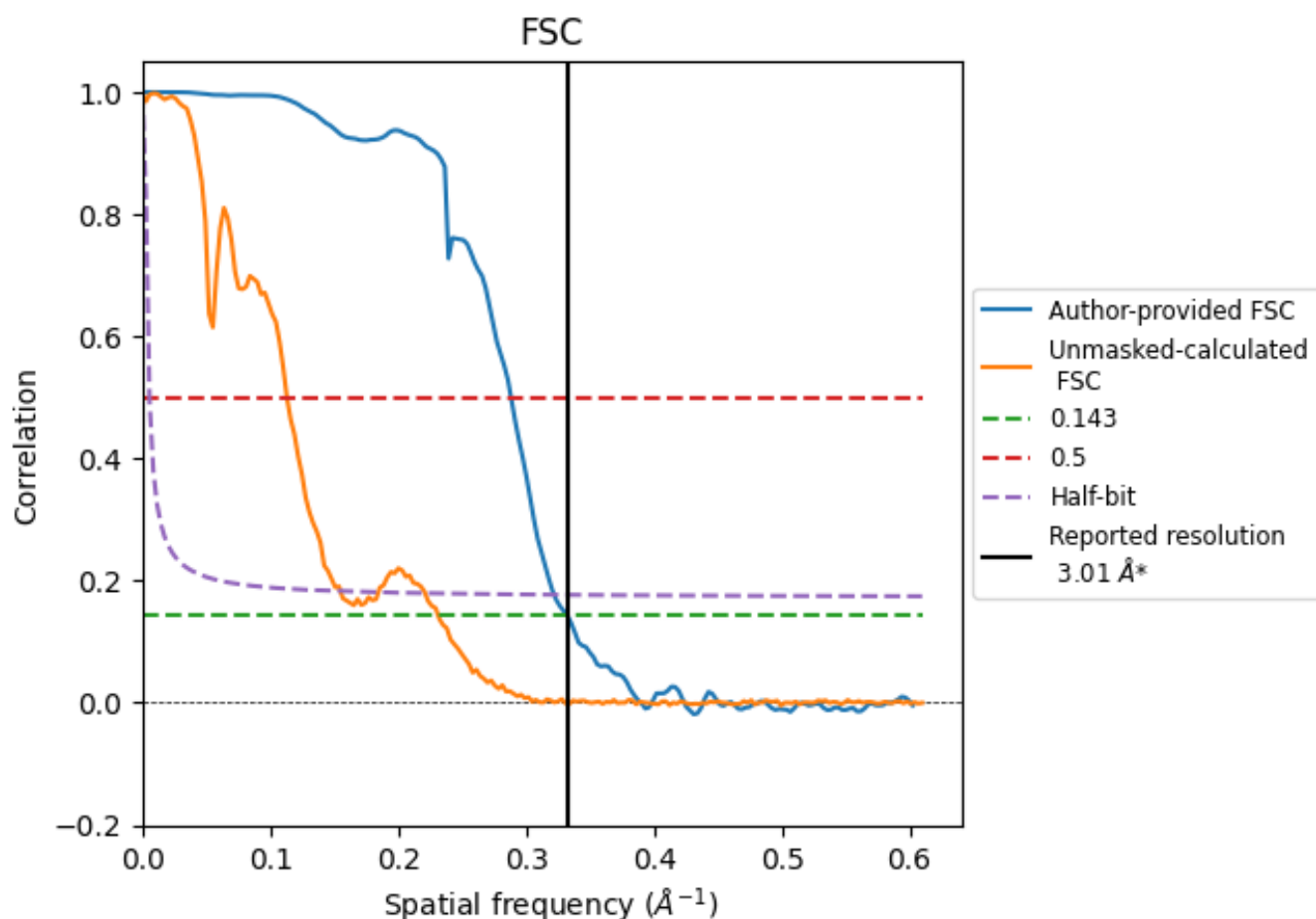


*Reported resolution corresponds to spatial frequency of 0.332 $\text{\AA}^{-1}$

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 0.332 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

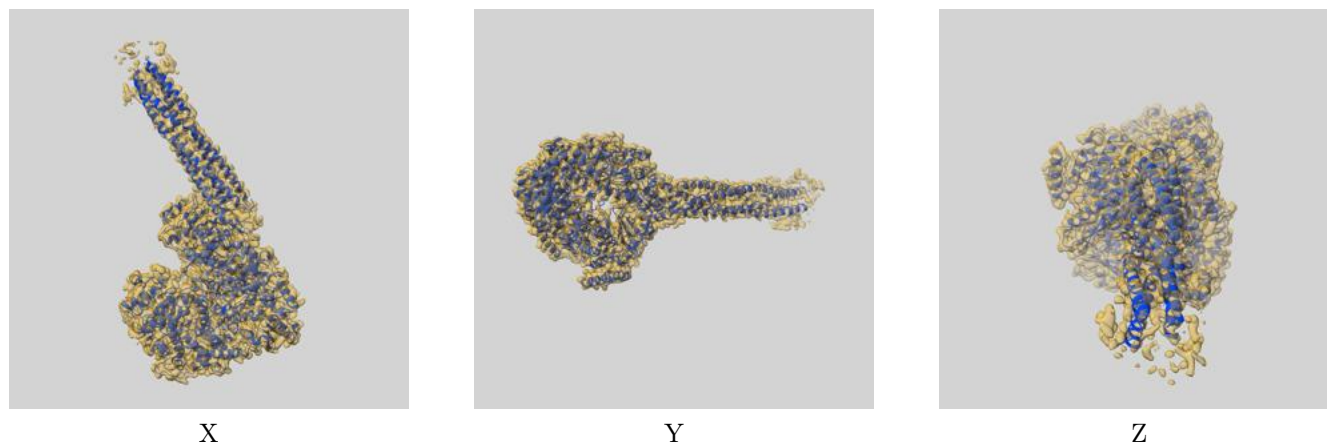
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.01	3.47	3.10
Unmasked-calculated*	4.32	8.83	6.45

*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 4.32 differs from the reported value 3.01 by more than 10 %

9 Map-model fit [i](#)

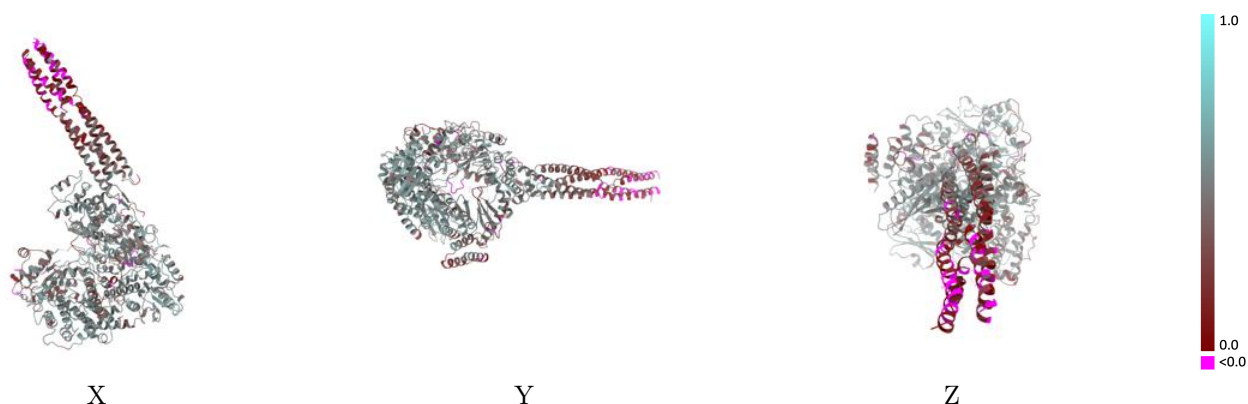
This section contains information regarding the fit between EMDB map EMD-60800 and PDB model 9IR4. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



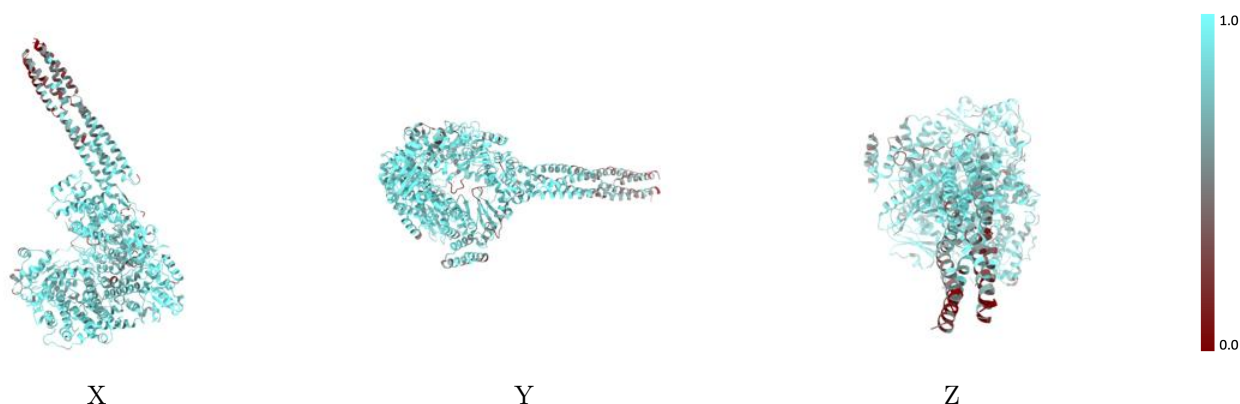
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



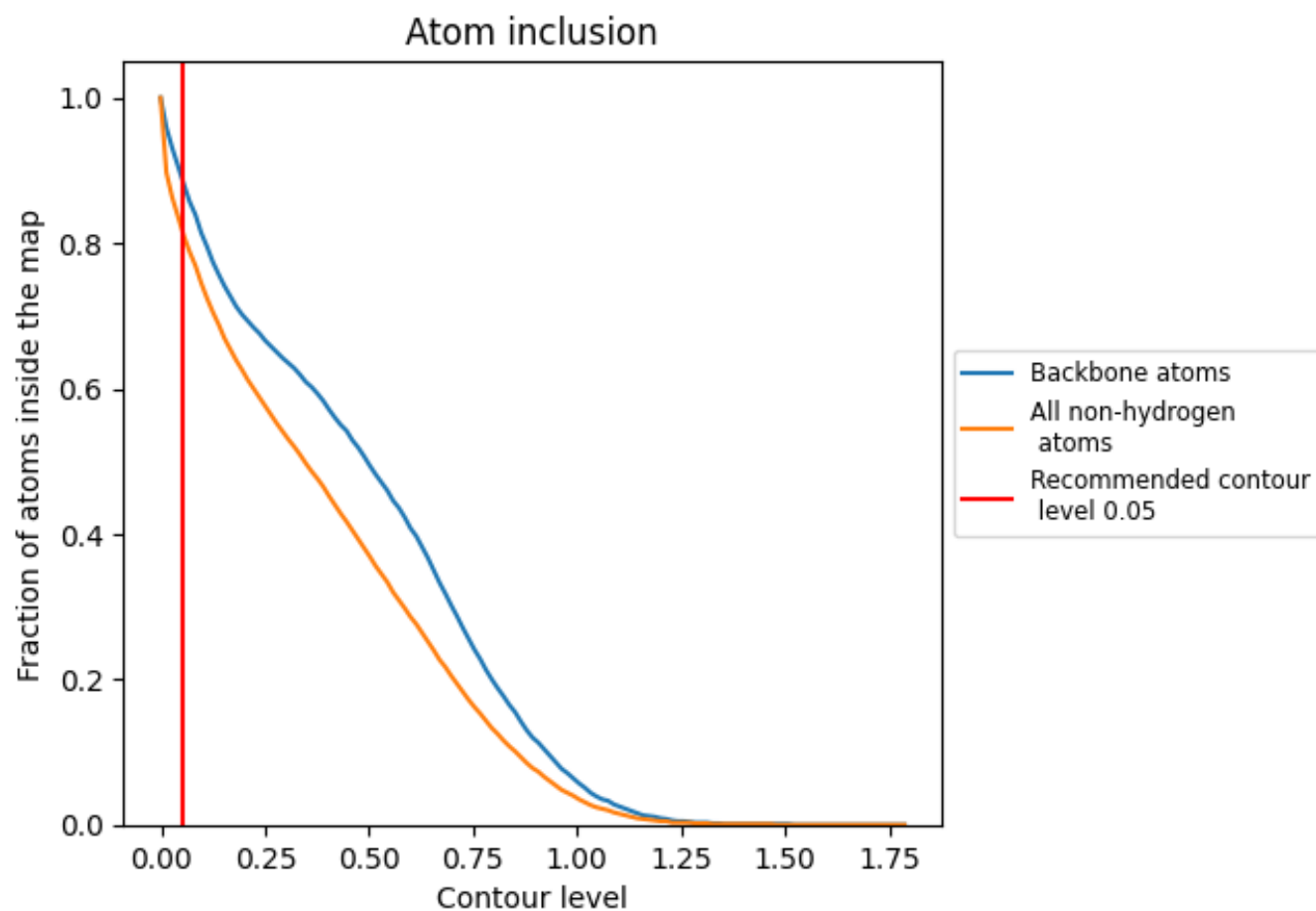
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.4350
A	0.8660	0.4840
C	0.6220	0.3140
D	0.6300	0.2180
E	0.6520	0.2300
F	0.6370	0.2190
G	0.5530	0.1810

