



wwPDB EM Validation Summary Report ⓘ

Sep 12, 2023 – 06:11 PM JST

PDB ID : 8IBX
EMDB ID : EMD-35348
Title : Structure of R2 with 3'UTR and DNA in unwinding state
Authors : Deng, P.; Tan, S.; Wang, J.; Liu, J.J.
Deposited on : 2023-02-10
Resolution : 3.74 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.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

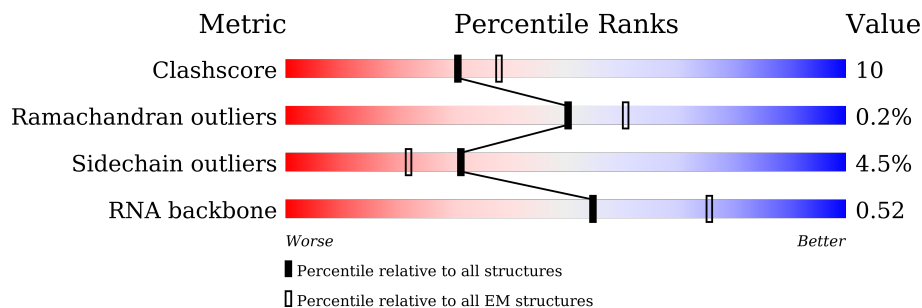
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.74 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	C	1114	 7% 61% 21% 17%
2	B	60	 7% 33% 27% 40%
3	A	60	 10% 42% 13% 45%
4	D	50	 44% 24% 10% 22%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9502 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 Reverse transcriptase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	922	7250	4541	1399	1272	38	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	628	TYR	ASP	conflict	UNP V9H052
C	996	ALA	ASP	conflict	UNP V9H052

- Molecule 2 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	36	730	348	126	220	36	0	0

- Molecule 3 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A	33	687	323	139	192	33	0	0

- Molecule 4 is a RNA chain called 3'UTR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	39	833	372	151	271	39	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	C	2	Total	Zn	0
			2	2	

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: Reverse transcriptase-like protein

Chain C: 

MET MET ALA ALA GLY THR ALA LEU SER LEU MET MET GLY ARG CYS ASN PRO ASP ASP GLY CYS THR ARG GLY HIS PRO VAL THR ALA ALA PRO MET ASP GLY PRO ASP PRO SER LEU ALA GLY THR PHE THR ASP GLY TRP GLY LEU ALA ILE PRO ALA ALA GLY LEU LEU LEU

ALA THR VAL GLY SER PHE PHE PRO VAL ALA LYS LYS SER ASN LYS ASN ASP ARG PRO PRO GLU ALA THR GLU SER GLN GLU ARG THR ASP GLY ASN VAL ARG GLY SER ALA GLY THR ASP PRO VAL ARG GLY SER ALA GLY THR PHE THR ASP PRO VAL

T141 M146 V148 H153 E156 L159 T163 R166 L167 L168 A169 E170 R171 G172 Q173 C174 S175 D178 L179 F180 L183 F186 G187 R188 E191 Q196 Y202 F213 G214 S215

ARG ALA SER GLY ALA GLU ALA GLY GLU GLU CYS ALA GLU ASP ALA ALA TTR ASP PRO SER VAL GLY GLN MET P261 D262 E272 G275 A279 C280 R281 W283

HIS LYS S306 R307 Q308 K309 R310 L320 Y321 R327 C337 G338 G339 V340 G341 H342 T365 A368 R374 ALA TRP HIS GLY ASN ARG ASP TYR T385 Q386 K389 P390 T396 S399 S406 Q416 V420 V432 G436 E437 P439 E440

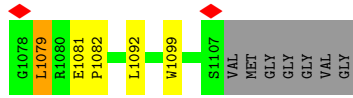
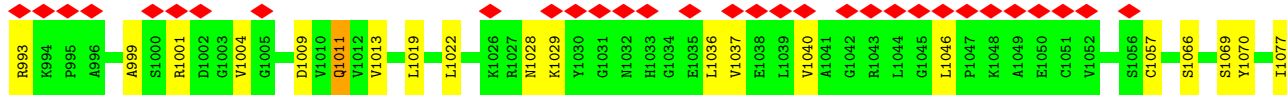
R443 Q444 C445 E454 R455 Q458 E461 V462 R463 P464 I465 I467 L472 R473 H474 F475 H476 S477 C486 D490 A491 R492 Q493 R494 C495 C498 A499 T502 L503 E504 V508 V512 R517 K518 R522 A526 D529 F530 G531 A532 A533 F534 T536

H539 V543 R549 S550 M551 Y558 H561 V564 W572 N573 N574 E575 M576 V586 R587 F597 D602 L603 L604 L605 A606 S607 R608 P609 E610 R611 V614 M618 A627 Y628 D629 M640 A646 C649 V650 V665 H673 R676 H677 I687

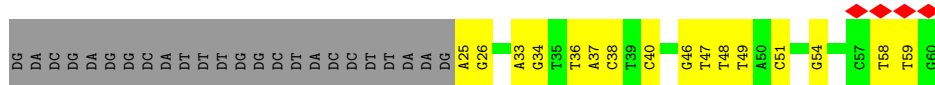
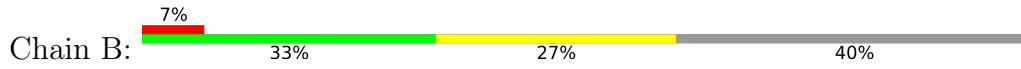
L692 R693 Q694 C697 V698 E699 R700 Y703 L704 L705 V706 S711 N712 C713 W714 L715 L716 E717 H718 S719 I720 Q736 R737 L738 L742 L745 F746 P747 R748 F749 Q750 W754 L755 G756 N757 D761 R762 L763 R764 D767 V768 W774 G775 Q776 R779 V784 P785

V793 Q794 L798 A799 V803 T807 I811 V812 D819 S820 D833 R836 K837 R838 R840 R841 W841 A842 R848 D853 Q854 S854 T855 T856 Q857 S860 P861 D874 E877 T886 S887 T888 R892 C895 A896 Q897 D902 F903 Q904 Q905 H908 T909 H910 I911 N912

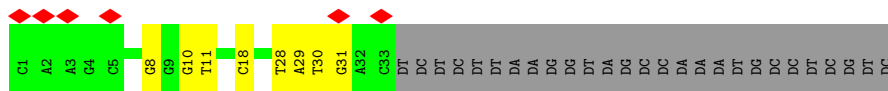
A913 L914 P915 S916 R919 G920 S921 R922 G923 R924 V925 G926 G927 G928 E929 S930 S931 K939 E942 I947 L948 Q949 G950 C951 H955 R958 P959 L960 R961 I965 V969 M973 E974 F975 N976 K977 R978 T979 V990 E991 L992 E993 P994 R995 L996 R997 T998 S999 G991 L992



• Molecule 2: DNA (60-MER)



• Molecule 3: DNA (60-MER)



• Molecule 4: 3'UTR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106634	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.572	Depositor
Minimum map value	-0.832	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	219.58, 219.58, 219.58	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	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	C	0.27	0/7397	0.56	0/9984
2	B	0.53	0/815	0.94	0/1254
3	A	0.50	0/774	0.81	0/1194
4	D	0.30	0/929	0.75	0/1441
All	All	0.32	0/9915	0.65	0/13873

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	C	7250	0	7356	161	0
2	B	730	0	407	15	0
3	A	687	0	368	8	0
4	D	833	0	424	10	0
5	C	2	0	0	0	0
All	All	9502	0	8555	177	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 10.

The worst 5 of 177 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:C:754:VAL:HG23	1:C:811:ILE:HG22	1.34	1.08
1:C:473:ARG:NH1	4:D:247:A:OP1	2.08	0.86
1:C:1028:ASN:OD1	1:C:1029:LYS:N	2.13	0.82
1:C:848:ARG:NH1	3:A:30:DT:OP1	2.14	0.81
1:C:175:SER:OG	3:A:8:DG:OP2	1.98	0.79

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	C	914/1114 (82%)	868 (95%)	44 (5%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	576	MET
1	C	586	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	760/906 (84%)	726 (96%)	34 (4%)	27 57

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	892	ARG
1	C	895	CYS
1	C	1070	TYR
1	C	573	ASN
1	C	572	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	694	GLN
1	C	857	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	36/50 (72%)	10 (27%)	0

5 of 10 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	31	U
4	D	32	A
4	D	37	A
4	D	125	C
4	D	126	C

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

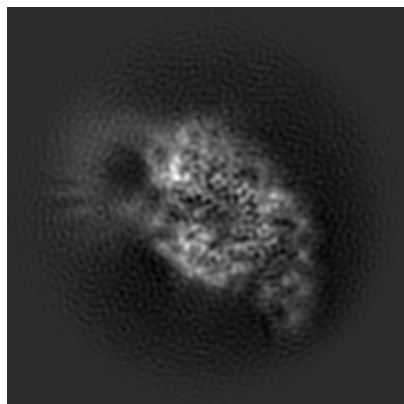
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35348. These allow visual inspection of the internal detail of the map and identification of artifacts.

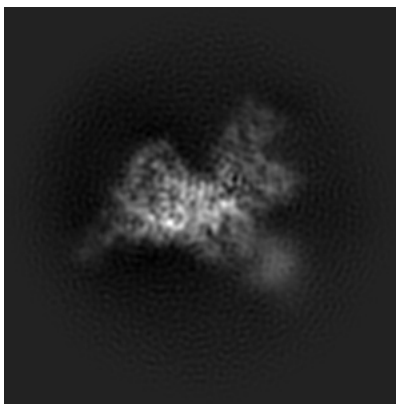
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

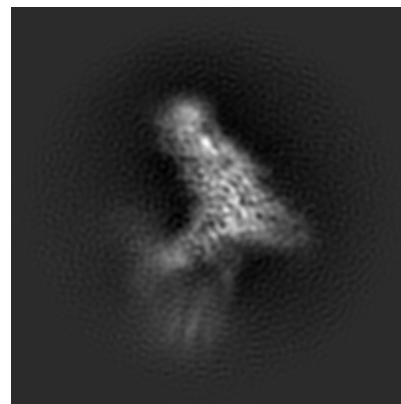
6.1.1 Primary map



X

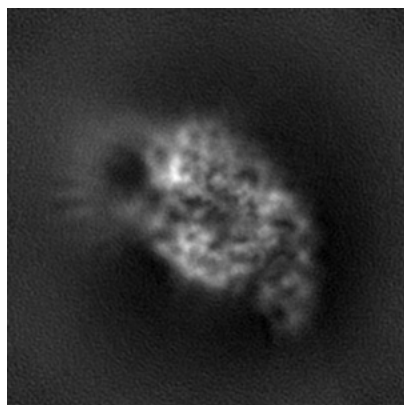


Y

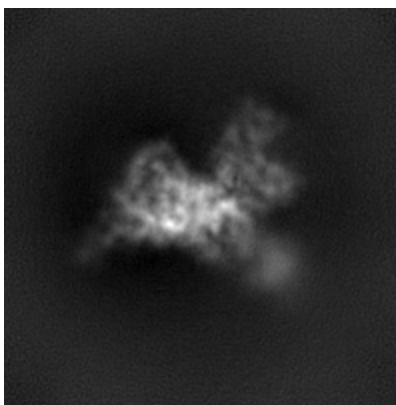


Z

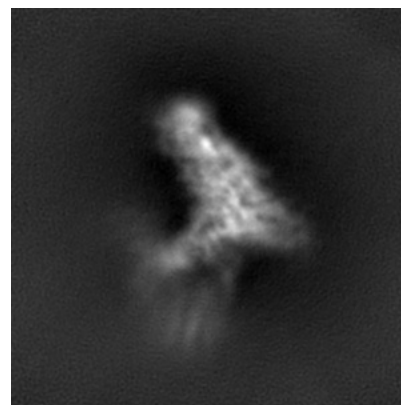
6.1.2 Raw map



X



Y

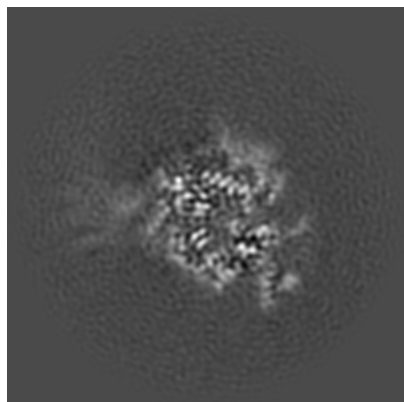


Z

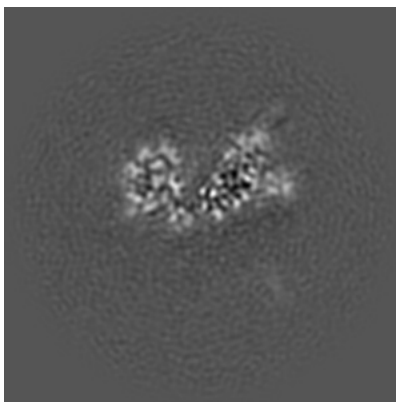
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

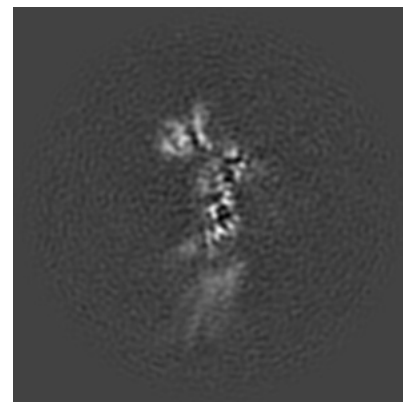
6.2.1 Primary map



X Index: 100

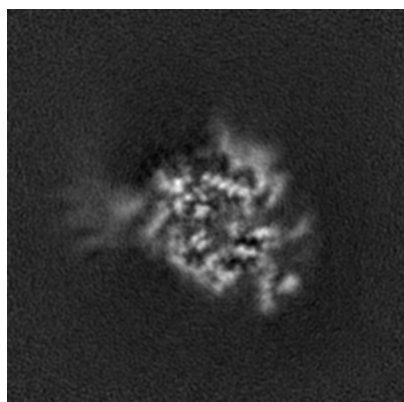


Y Index: 100

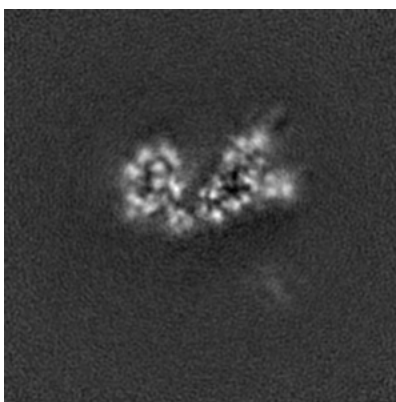


Z Index: 100

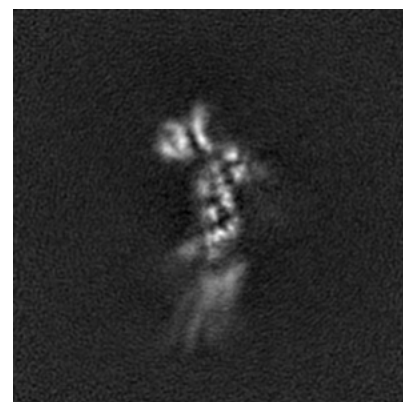
6.2.2 Raw map



X Index: 100



Y Index: 100

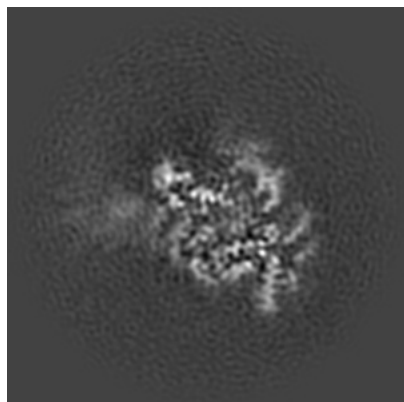


Z Index: 100

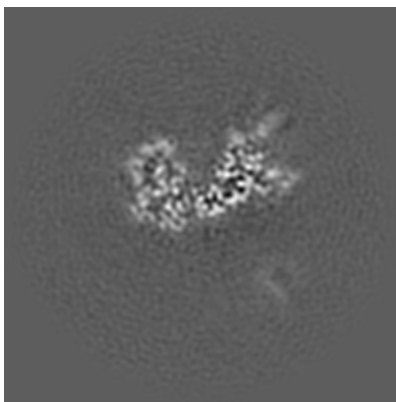
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

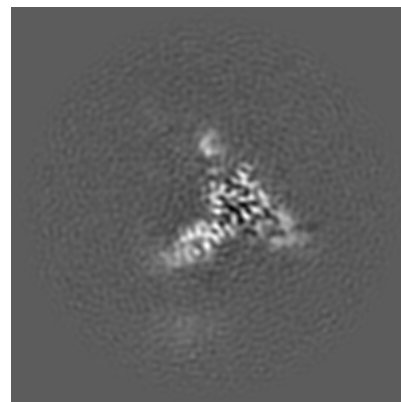
6.3.1 Primary map



X Index: 97

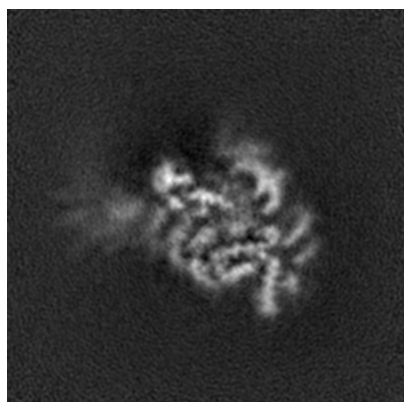


Y Index: 97

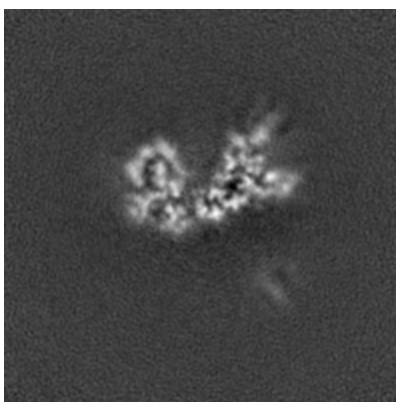


Z Index: 114

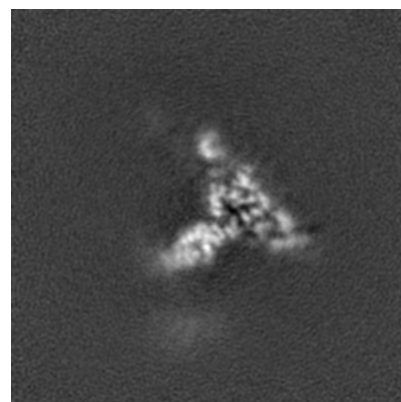
6.3.2 Raw map



X Index: 97



Y Index: 98

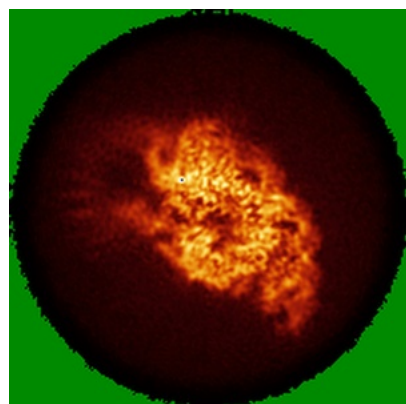


Z Index: 114

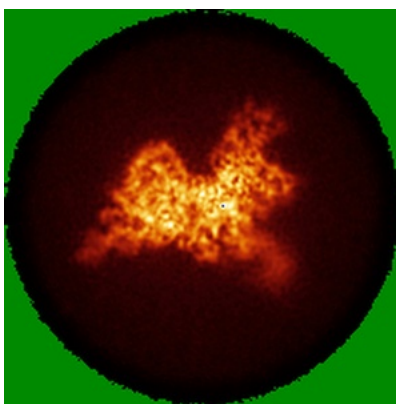
The images above show the largest variance slices of the map in three orthogonal directions.

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

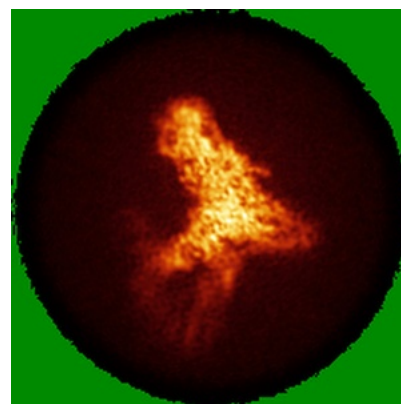
6.4.1 Primary map



X

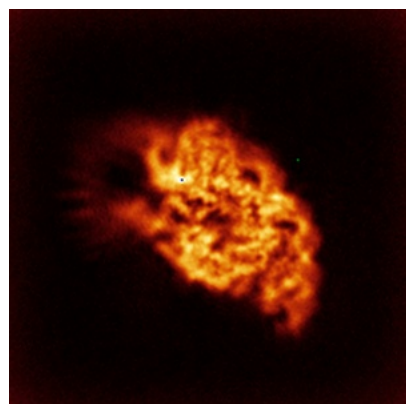


Y

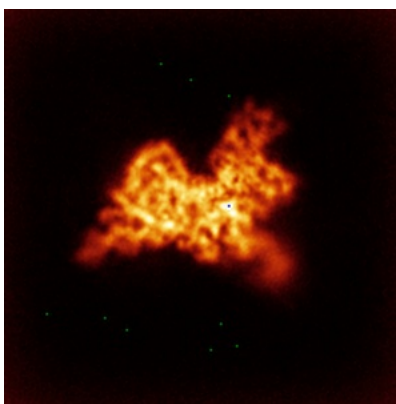


Z

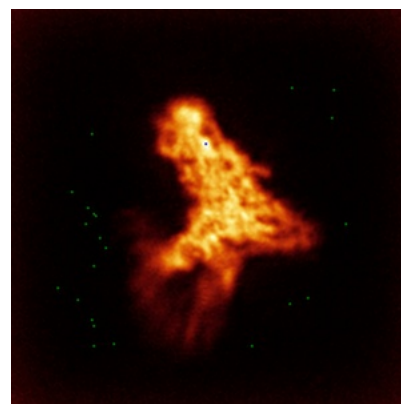
6.4.2 Raw map



X



Y

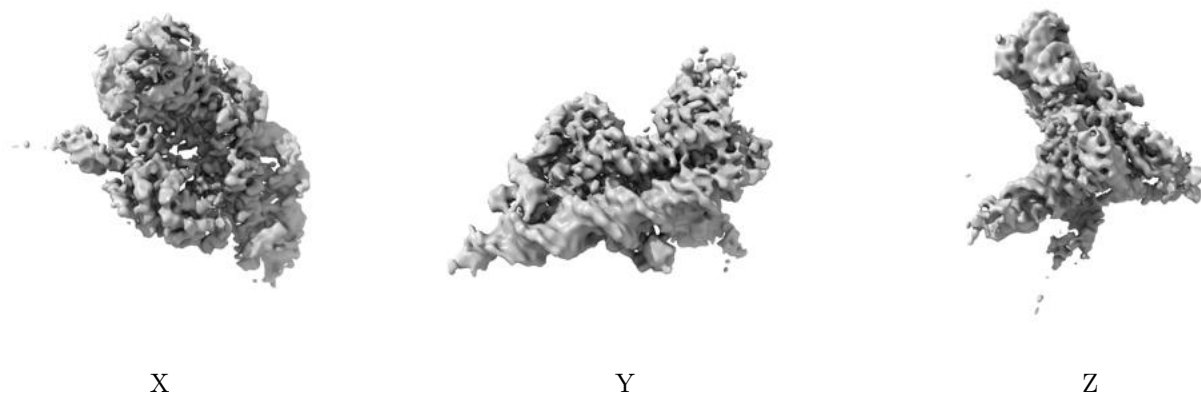


Z

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.

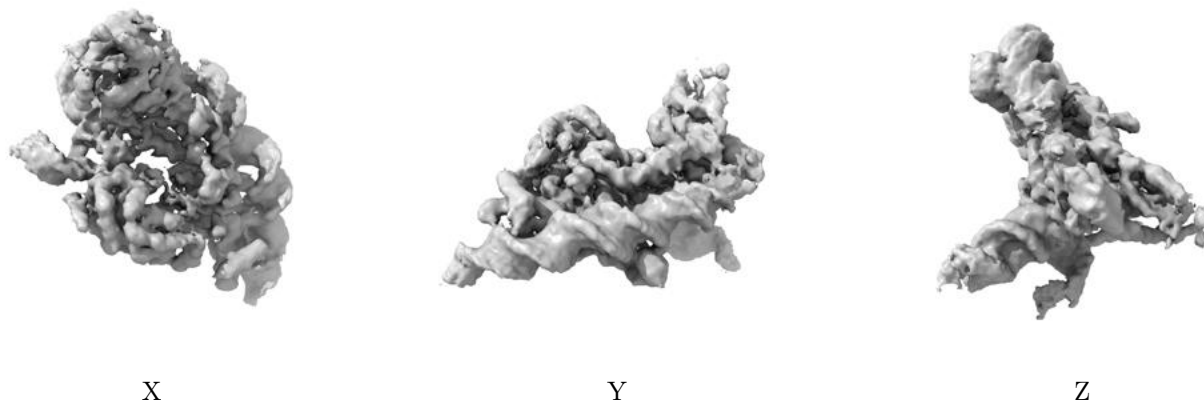
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

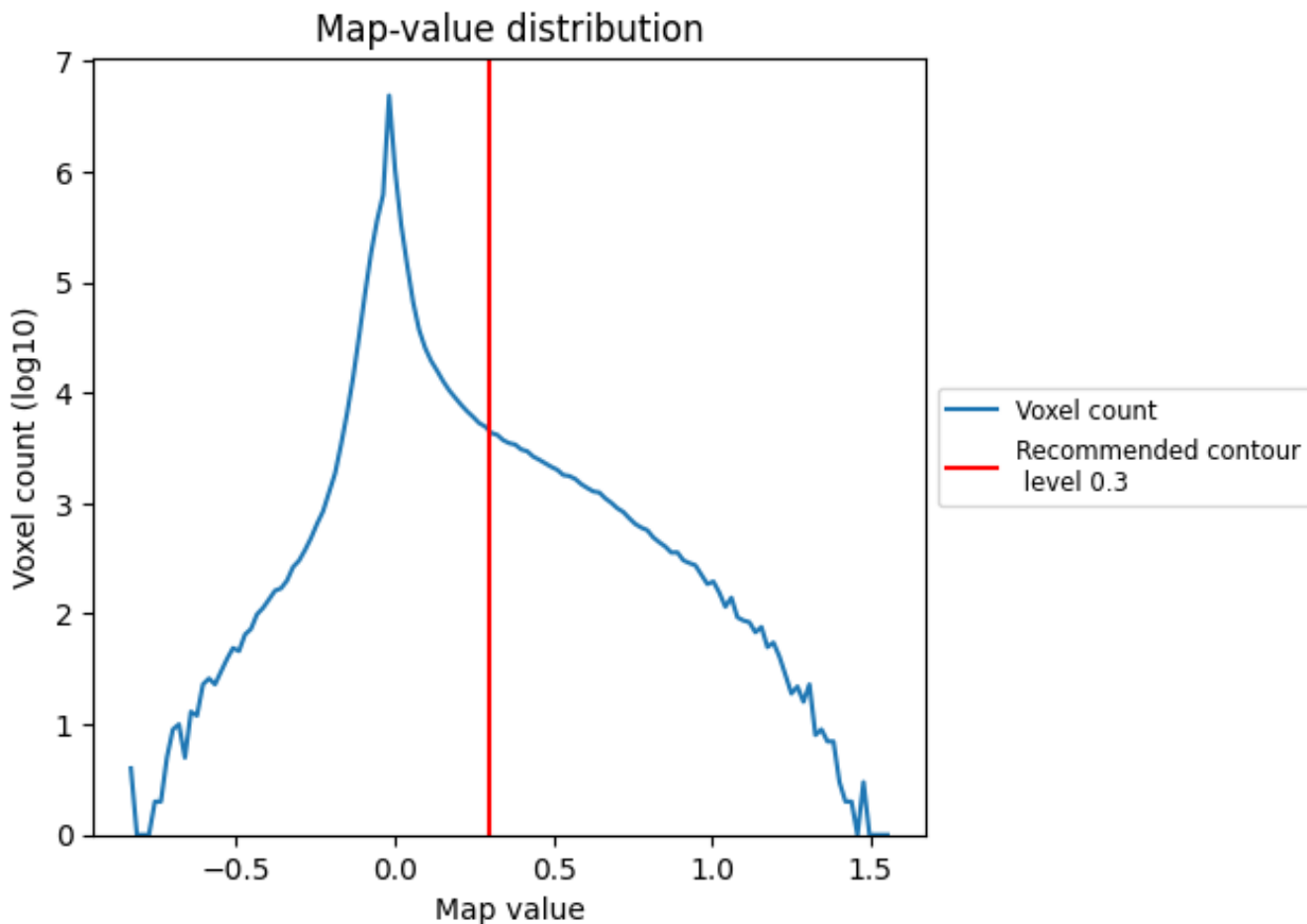
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

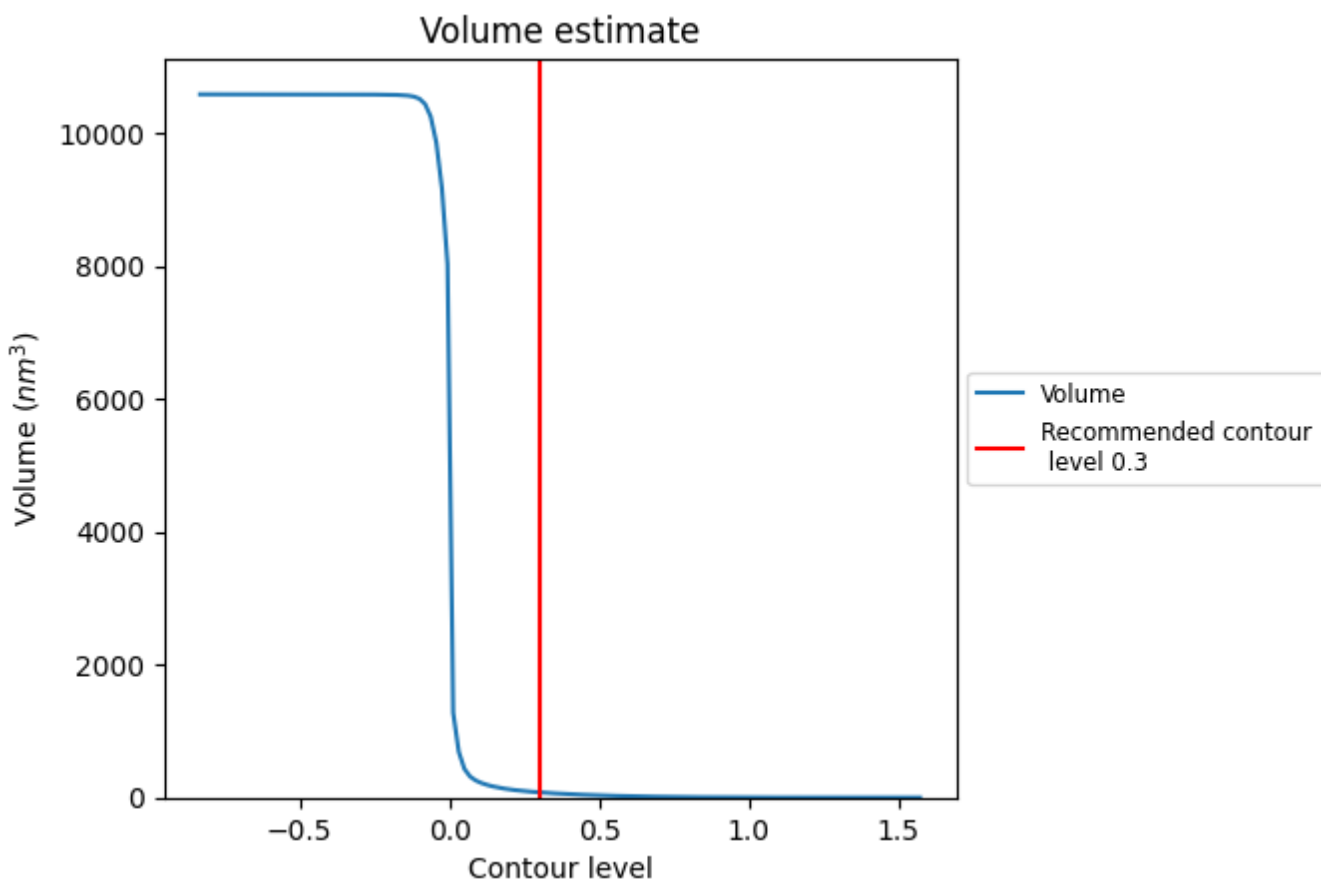
This section contains the results of statistical analysis of the map.

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.

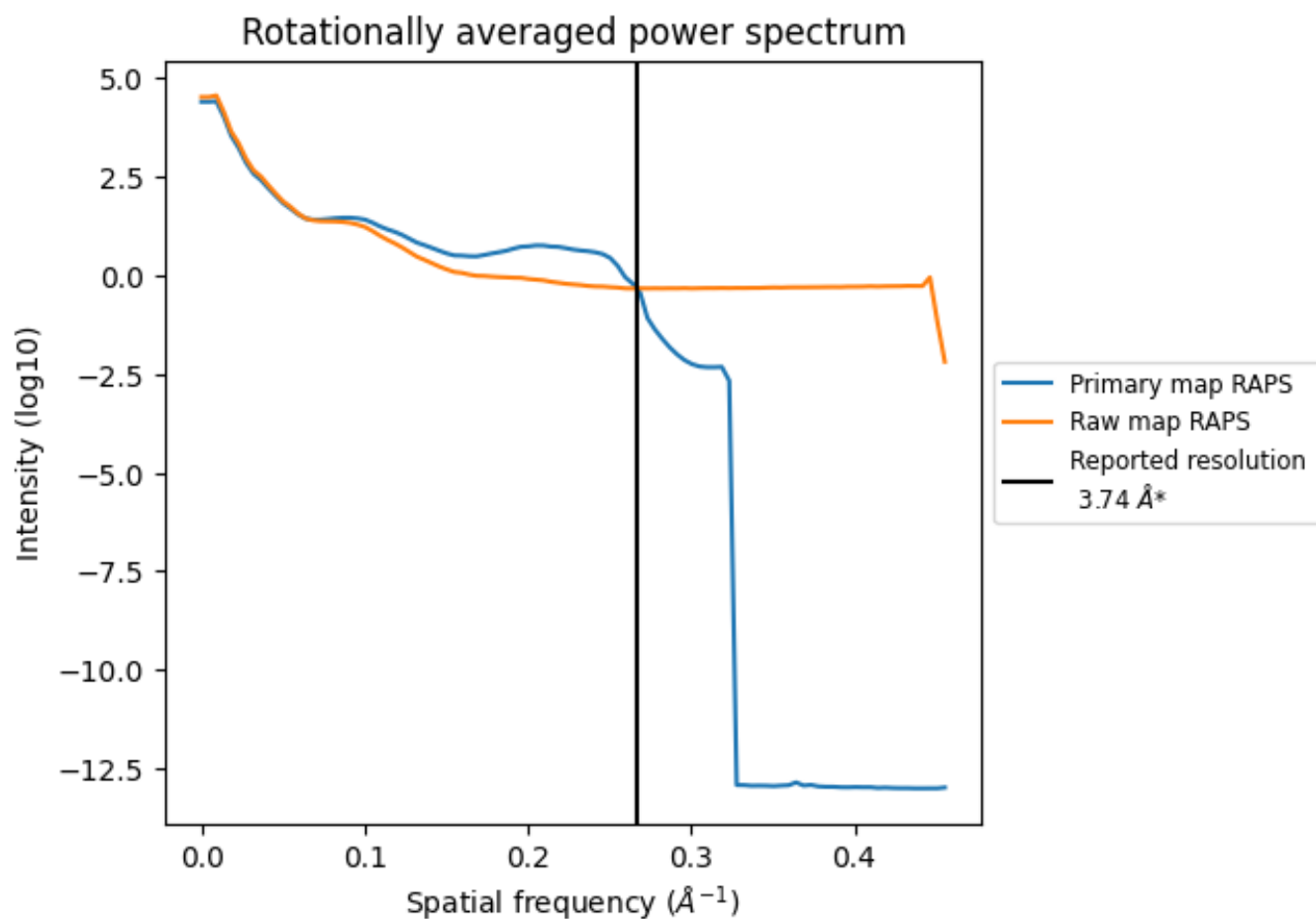
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm^3 ; this corresponds to an approximate mass of 71 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](#)

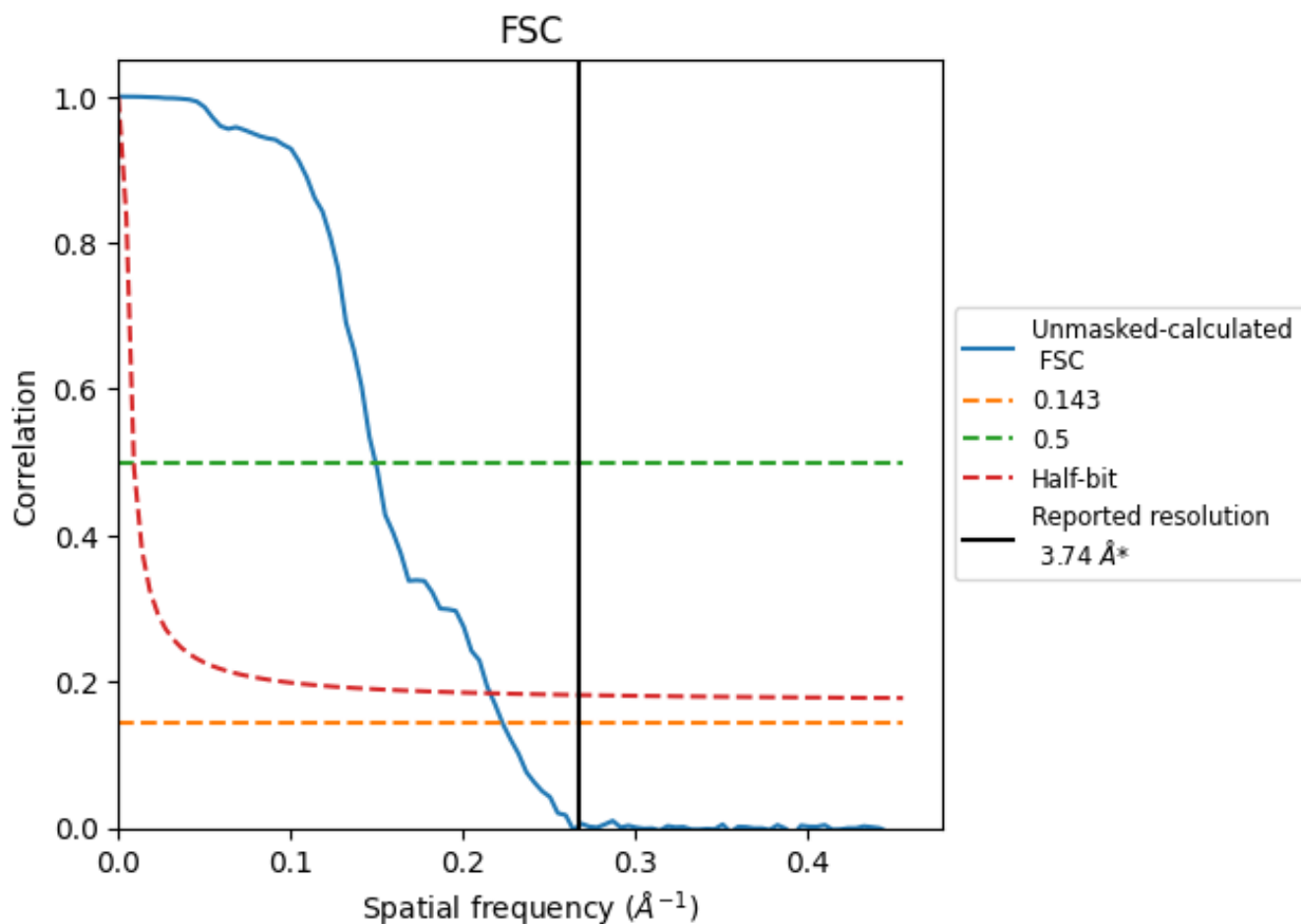


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

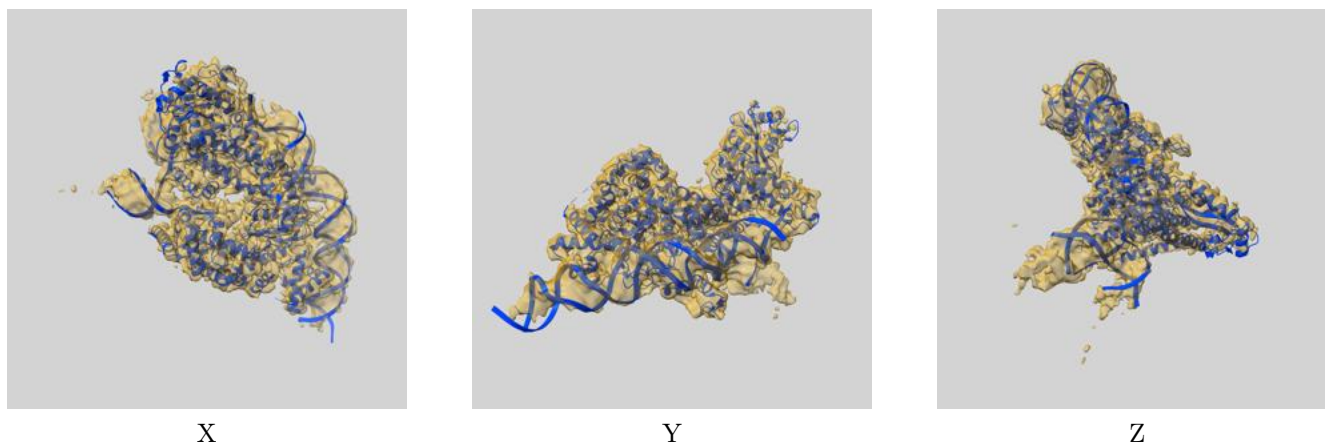
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.74	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	6.70	4.63

*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 4.49 differs from the reported value 3.74 by more than 10 %

9 Map-model fit [i](#)

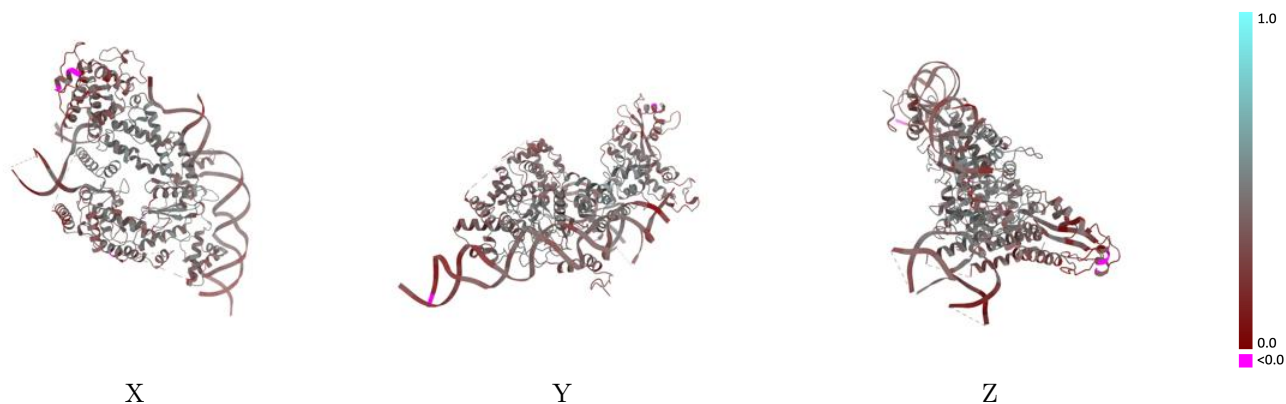
This section contains information regarding the fit between EMDB map EMD-35348 and PDB model 8IBX. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



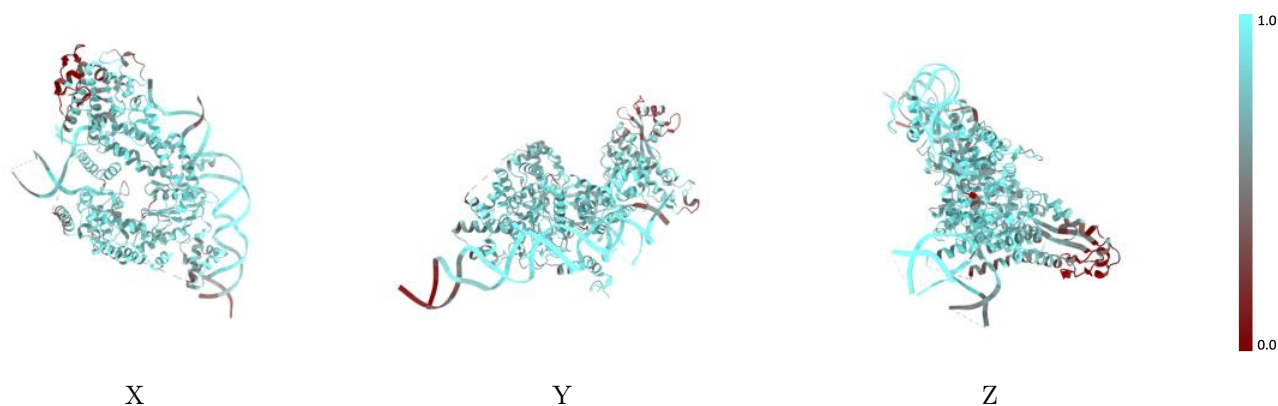
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



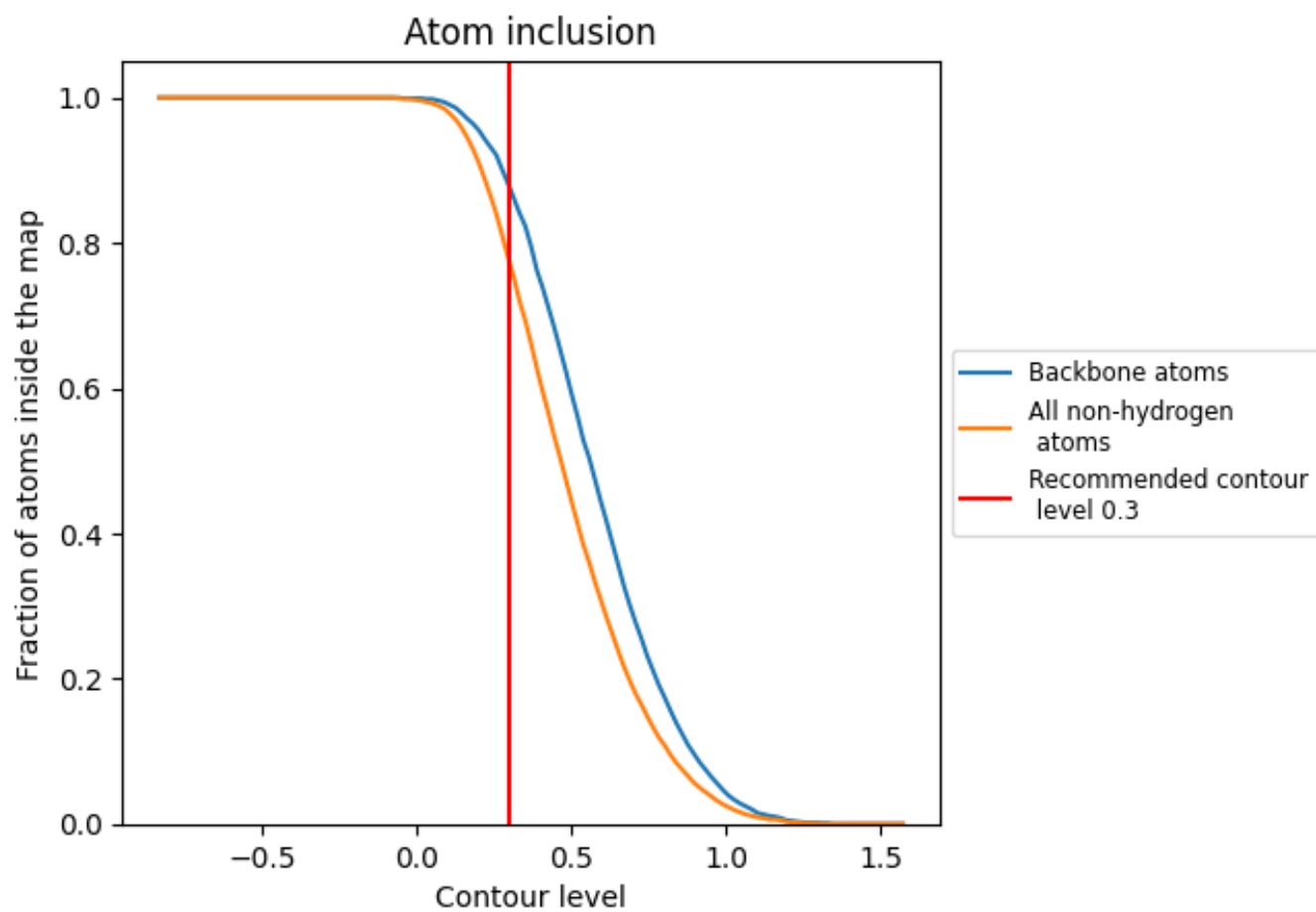
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).











9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.3850
A	 0.7320	 0.3130
B	 0.7730	 0.3140
C	 0.7670	 0.4040
D	 0.8600	 0.3450

