wwPDB EM Validation Summary Report (i)

Jul 3, 2024 – 09:52 am BST

PDB ID	:	7AA3
EMDB ID	:	EMD-11689
Title	:	T275P after heme uptake from M. tuberculosis
Authors	:	Blundell, T.L.; Chaplin, A.K.; Munir, A.
Deposited on	:	2020-09-03
Resolution	:	3.56 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

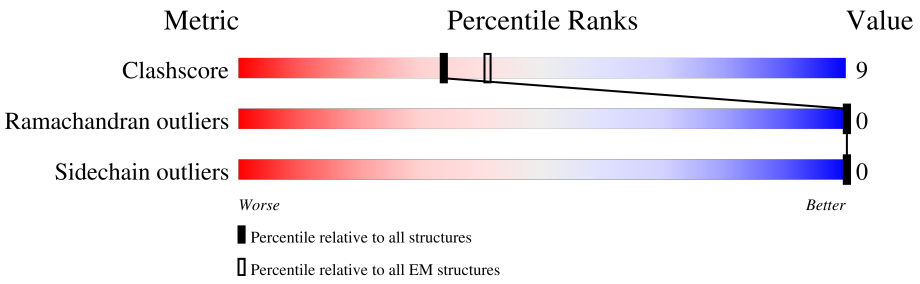
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.56 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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	740	6% 59% 16% 26%
1	B	740	6% 58% 16% 26%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8389 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 Catalase-peroxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	550	4211	2675	722	799	15	0	0
1	B	544	4178	2661	716	787	14	0	0

There are 2 discrepancies between the modelled and reference sequences:

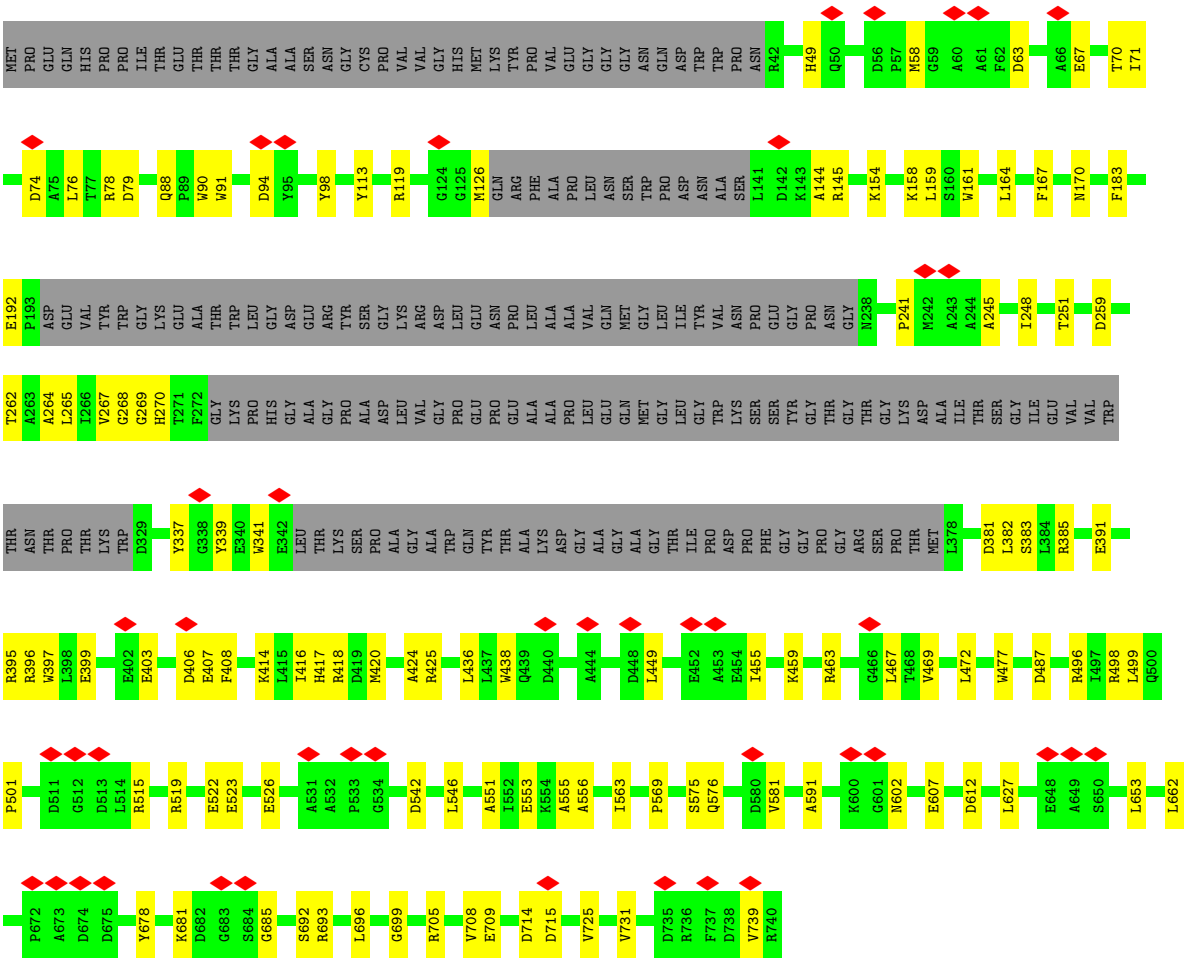
Chain	Residue	Modelled	Actual	Comment	Reference
A	275	PRO	THR	engineered mutation	UNP A0A0D5ZBI4
B	275	PRO	THR	engineered mutation	UNP A0A0D5ZBI4

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

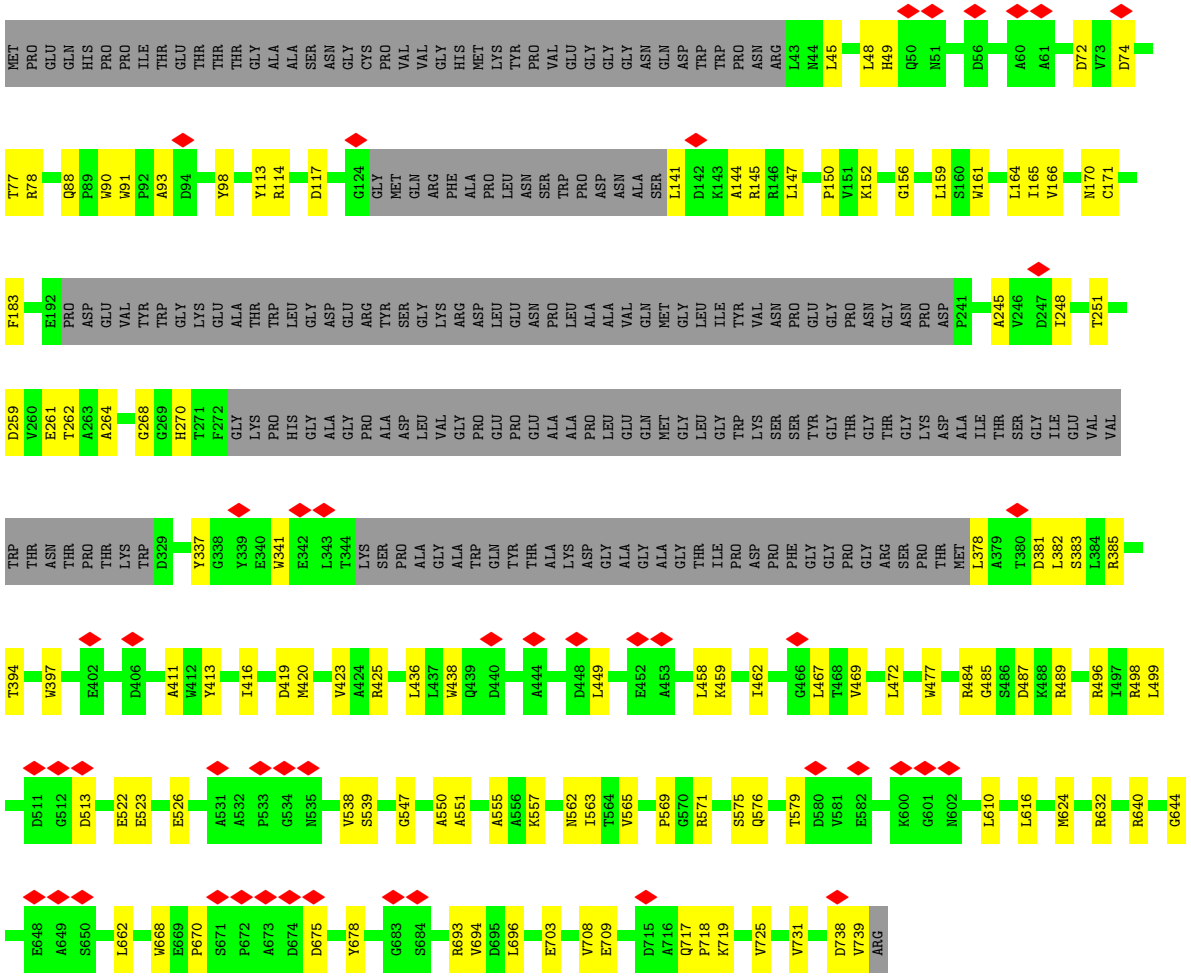
- Molecule 1: Catalase-peroxidase

Chain A:



- Molecule 1: Catalase-peroxidase

Chain B:


MET PRO GLU GLN HIS PRO PRO ILE THR GLU THR THR THR GLY ALA ALA SER ASN GLY CYS PRO VAL VAL GLY HIS MET LYS TYR PRO VAL GLU GLY GLY GLY ASN GLN ASP TRP TRP PRO ASN ARG L43 N44 L45 L48 H49 Q50 N51 D56 A60 A61 D72 V73 D74
T77 R78 Q88 P89 W90 W91 P92 A93 D94 Y98 Y113 R114 D117 G124 GLY MET GLN ARG PHE ALA PRO LEU ASN SER TRP PRO ASP ASN ALA SER L141 D142 K143 A144 R145 R146 L147 P150 V151 K152 G156 L159 S160 W161 L164 I165 V166 N170 C171
F183 E192 PRO ASP GLU VAL TYR TRP GLY LYS GLU ALA THR TRP LEU GLY ASP GLU ARG TYR SER GLY LYS ARG ASP LEU GLU ASN PRO LEU ALA ALA VAL GLN MET GLY LEU ILE TYR VAL ASN PRO GLU GLY PRO ASN GLY ASN PRO ASP P241 A245 V246 D247 I248 T251
D259 V260 E261 T262 A263 A264 G268 G269 H270 T271 F272 GLY LYS PRO HIS GLY ALA GLY PRO ALA ASP LEU VAL GLY PRO GLU PRO GLU ALA ALA PRO LEU GLU GLN MET GLY LEU GLY TRP LYS SER SER TYR GLY THR GLY THR GLY LYS ASP ALA ILE THR SER GLY ILE GLU VAL VAL
TRP THR ASN THR PRO THR LYS TRP D329 Y337 G338 Y339 E340 W341 E342 L343 T344 LYS SER PRO ALA GLY ALA TRP GLN TYR THR ALA LYS ASP GLY ALA GLY ALA GLY THR ILE PRO ASP PRO PHE GLY GLY PRO GLY ARG SER PRO THR MET L378 A379 T380 D381 L382 S383 L384 R385
T394 W397 E402 D406 A411 W412 Y413 I416 D419 M420 V423 A424 R425 L436 L437 W438 Q439 D440 A444 D448 L449 E452 A453 L458 K459 I462 G466 L467 T468 V469 L472 W477 R484 G485 S486 D487 K488 R489 R496 I497 R498 L499
D511 G512 D513 E522 E523 E526 A531 A532 P533 G534 N535 V538 S539 G547 A550 A551 A555 A556 K557 N562 I563 T564 V565 P569 G570 R571 S575 Q576 T579 D580 V581 E582 K600 G601 N602 L610 L616 M624 R632 R640 G644
E648 A649 S650 L662 W668 E669 P670 S671 P672 A673 D674 D675 V678 G683 S684 R693 V694 D695 L696 E703 V708 E709 D715 A716 Q717 P718 K719 V725 V731 D738 V739 ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	165609	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.576	Depositor
Minimum map value	-0.949	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.305	Depositor
Map size (Å)	304.5, 304.5, 304.5	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.29	0/4311	0.44	0/5866
1	B	0.29	0/4278	0.46	0/5821
All	All	0.29	0/8589	0.45	0/11687

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	4211	0	4039	77	0
1	B	4178	0	4020	76	0
All	All	8389	0	8059	148	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 9.

The worst 5 of 148 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:414:LYS:HD3	1:A:418:ARG:HH21	1.47	0.76
1:B:337:TYR:HB3	1:B:385:ARG:HE	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:TYR:OH	1:B:394:THR:O	2.05	0.74
1:A:170:ASN:HD22	1:A:183:PHE:HD2	1.36	0.73
1:A:58:MET:SD	1:B:719:LYS:NZ	2.63	0.72

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	540/740 (73%)	490 (91%)	50 (9%)	0	100	100
1	B	534/740 (72%)	475 (89%)	59 (11%)	0	100	100
All	All	1074/1480 (73%)	965 (90%)	109 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/584 (73%)	426 (100%)	0	100	100
1	B	423/584 (72%)	423 (100%)	0	100	100
All	All	849/1168 (73%)	849 (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. There are no such sidechains identified.

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 monosaccharides 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.

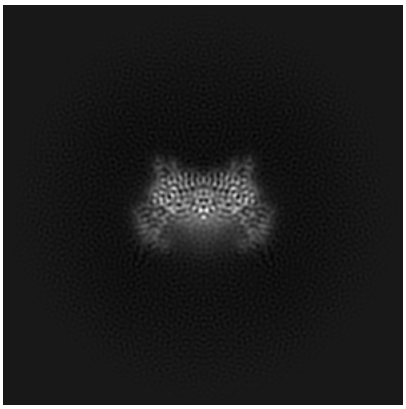
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11689. These allow visual inspection of the internal detail of the map and identification of artifacts.

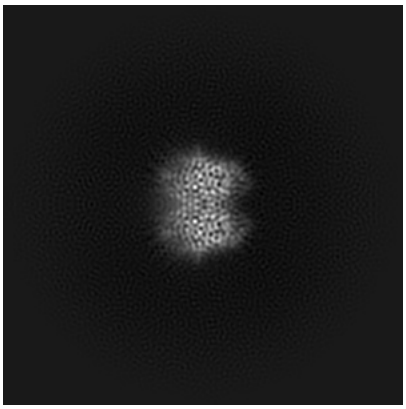
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

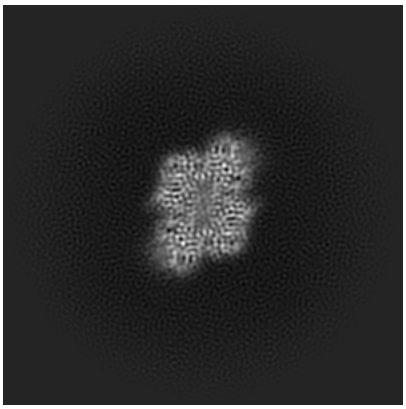
6.1.1 Primary map



X

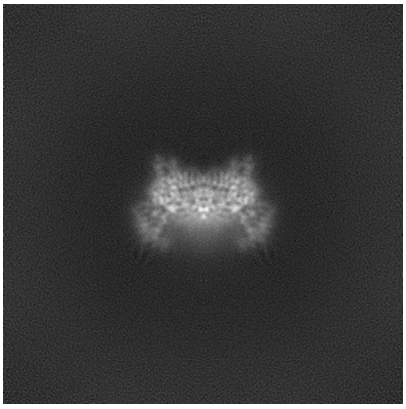


Y

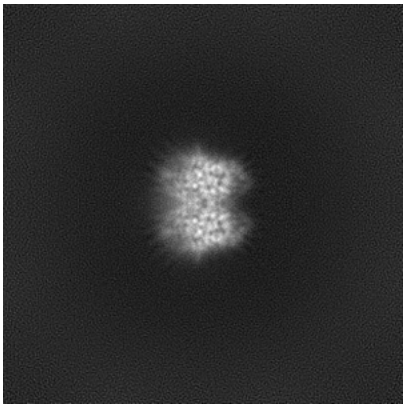


Z

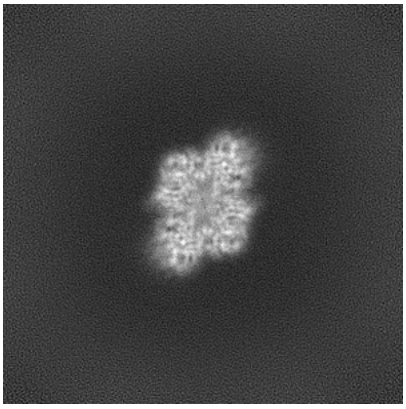
6.1.2 Raw map



X



Y

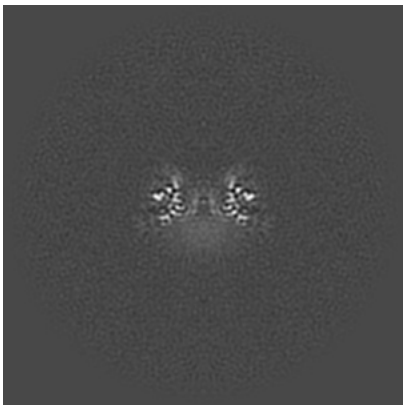


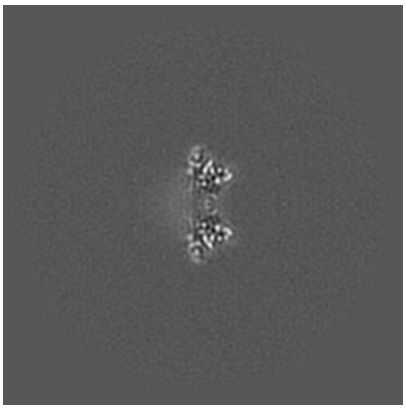
Z

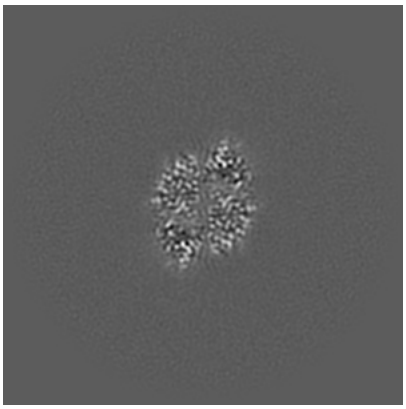
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

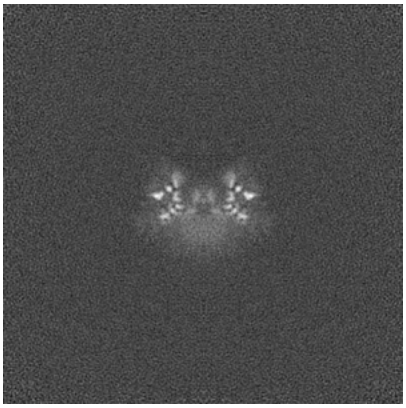
6.2.1 Primary map

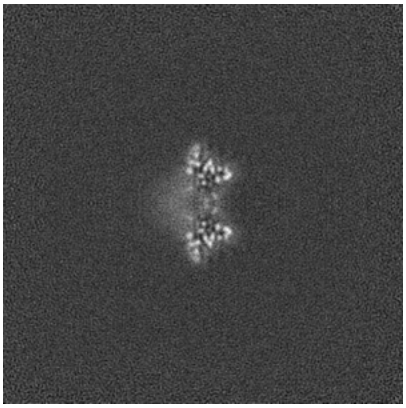

X Index: 145

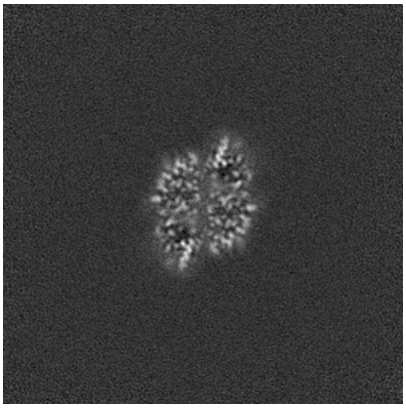

Y Index: 145


Z Index: 145

6.2.2 Raw map


X Index: 145

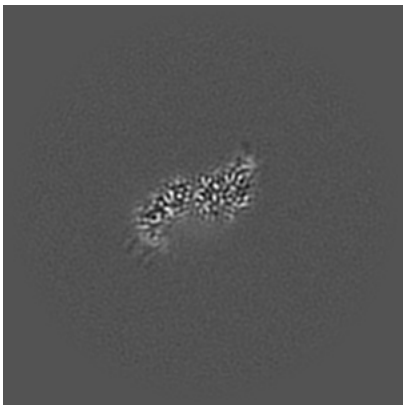

Y Index: 145

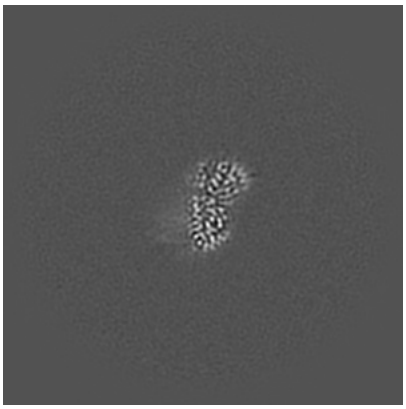

Z Index: 145

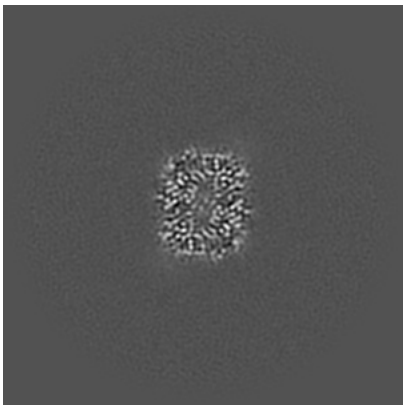
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

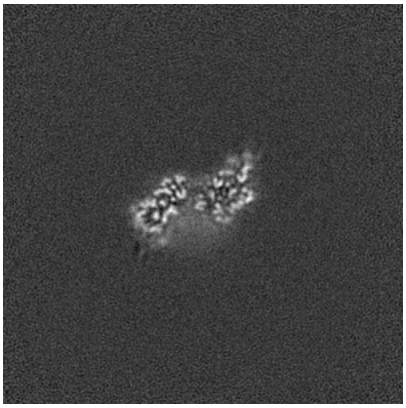
6.3.1 Primary map

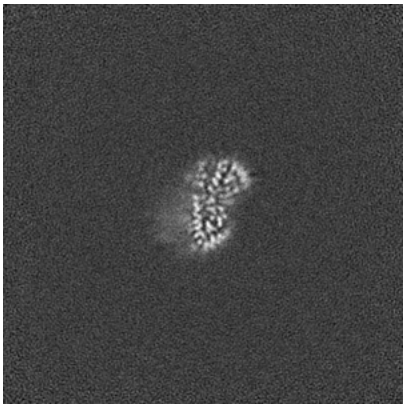

X Index: 126

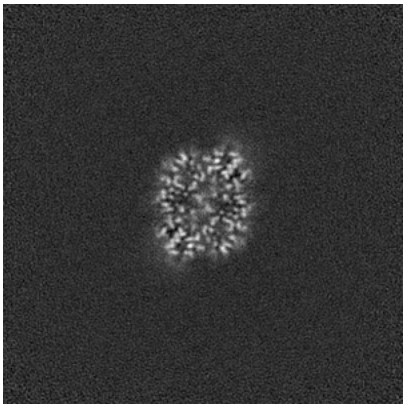

Y Index: 123


Z Index: 152

6.3.2 Raw map


X Index: 131

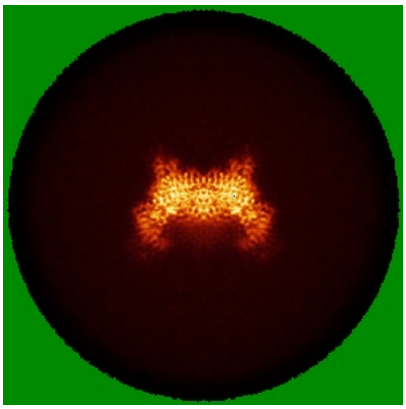

Y Index: 123

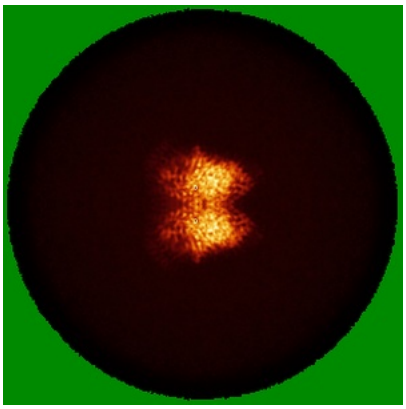

Z Index: 148

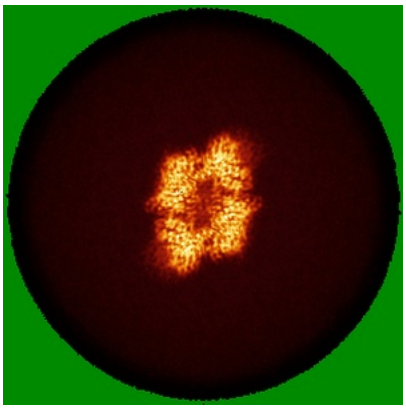
The images above show the largest variance slices of the map in three orthogonal directions.

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

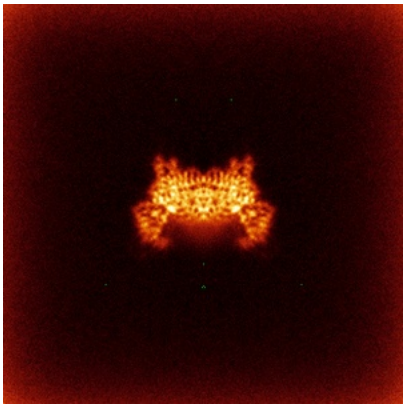
6.4.1 Primary map

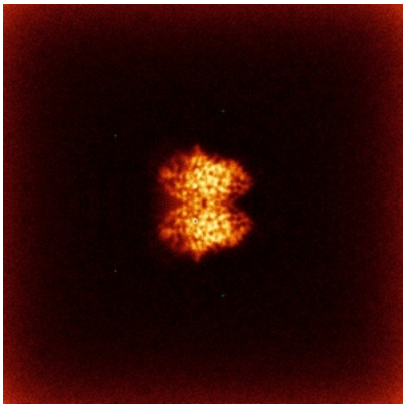

X

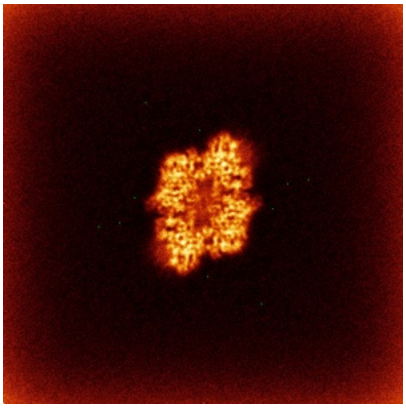

Y


Z

6.4.2 Raw map


X

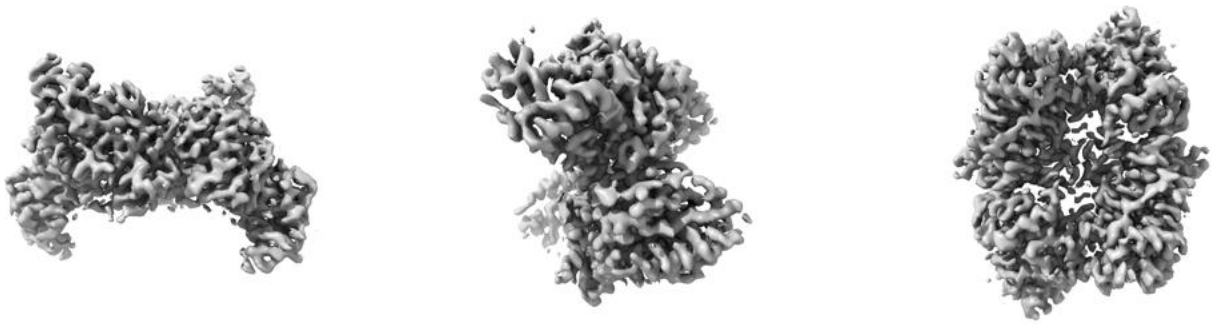

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.305. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

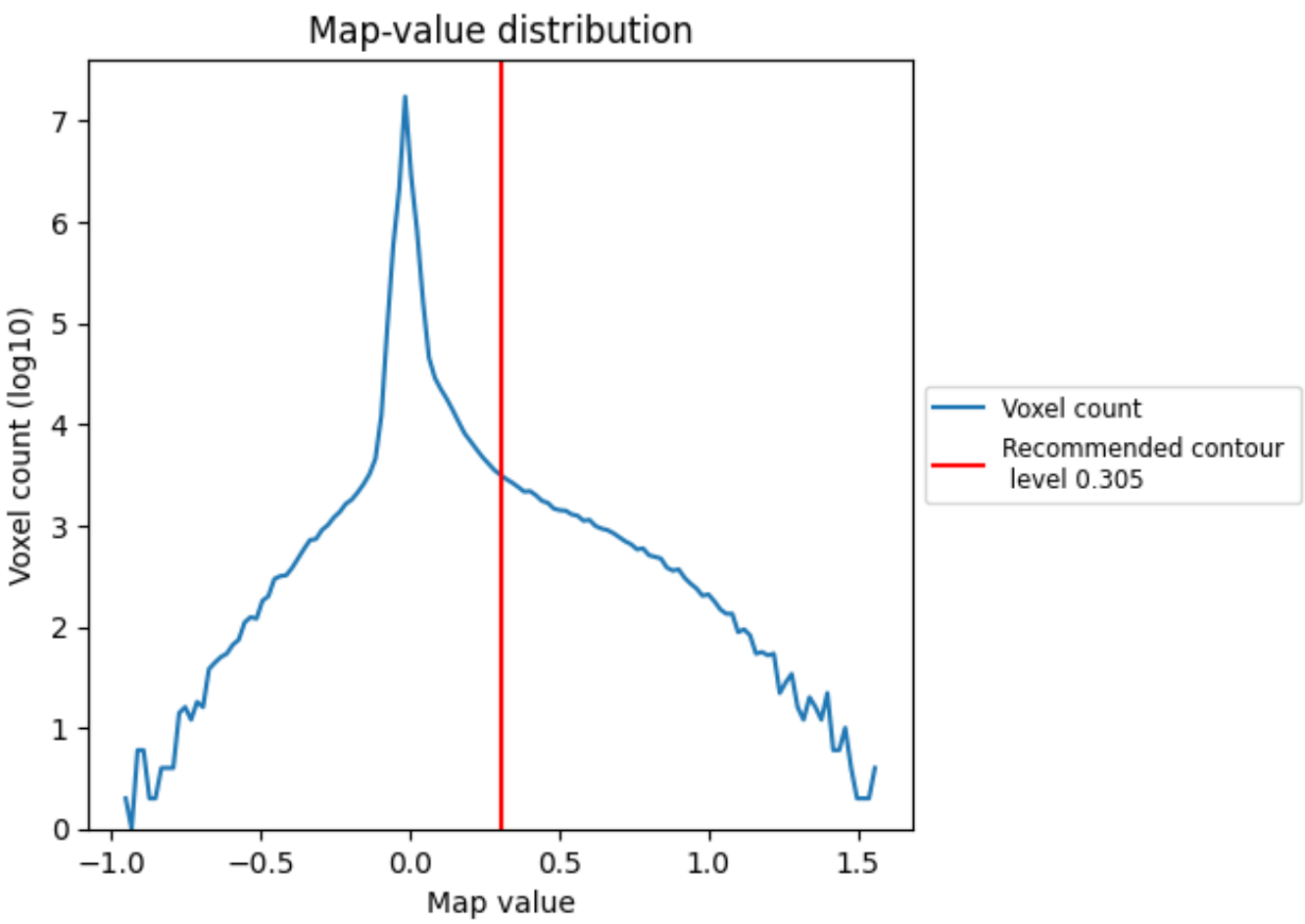
6.6 Mask visualisation (i)

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

7 Map analysis (i)

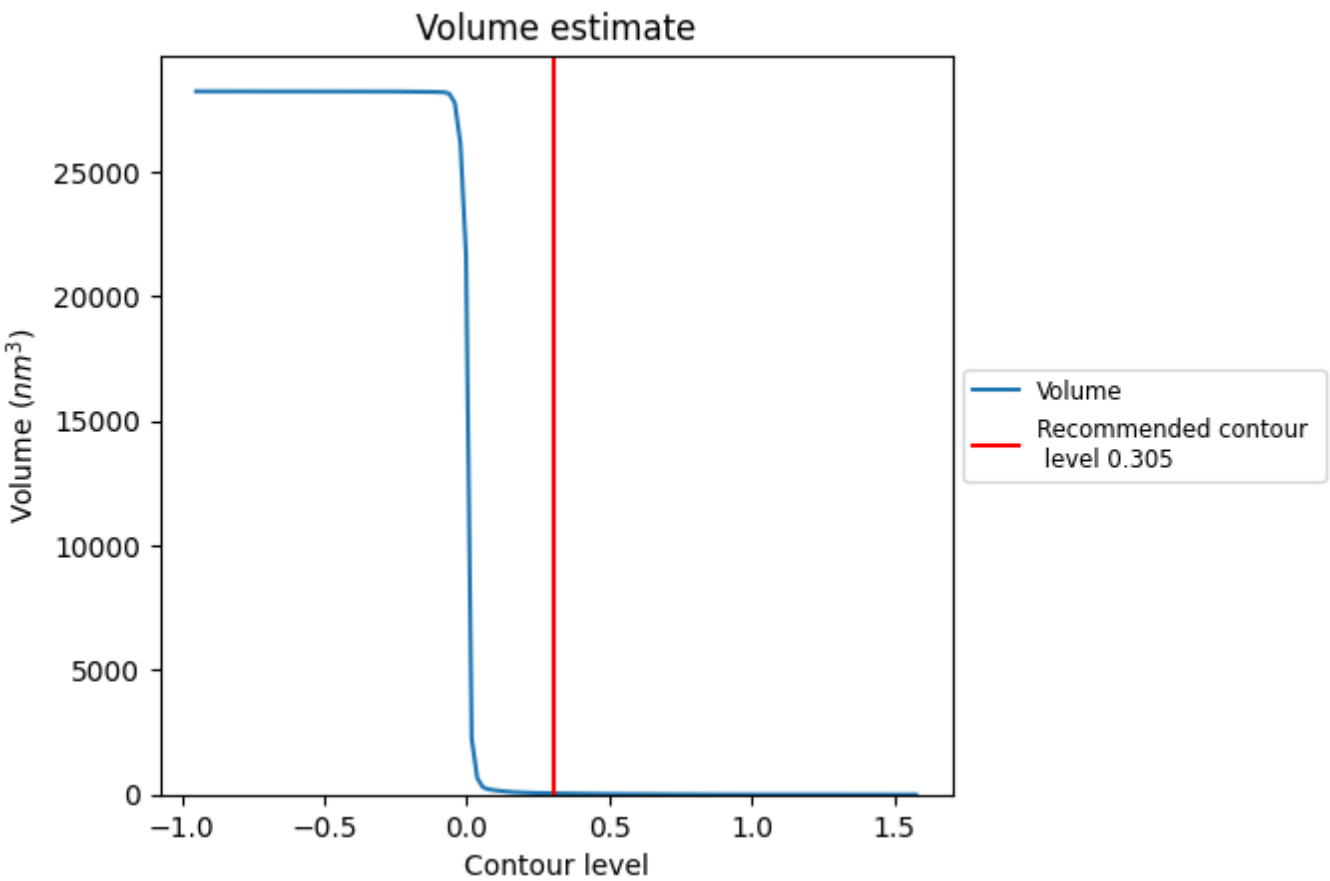
This section contains the results of statistical analysis of the map.

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.

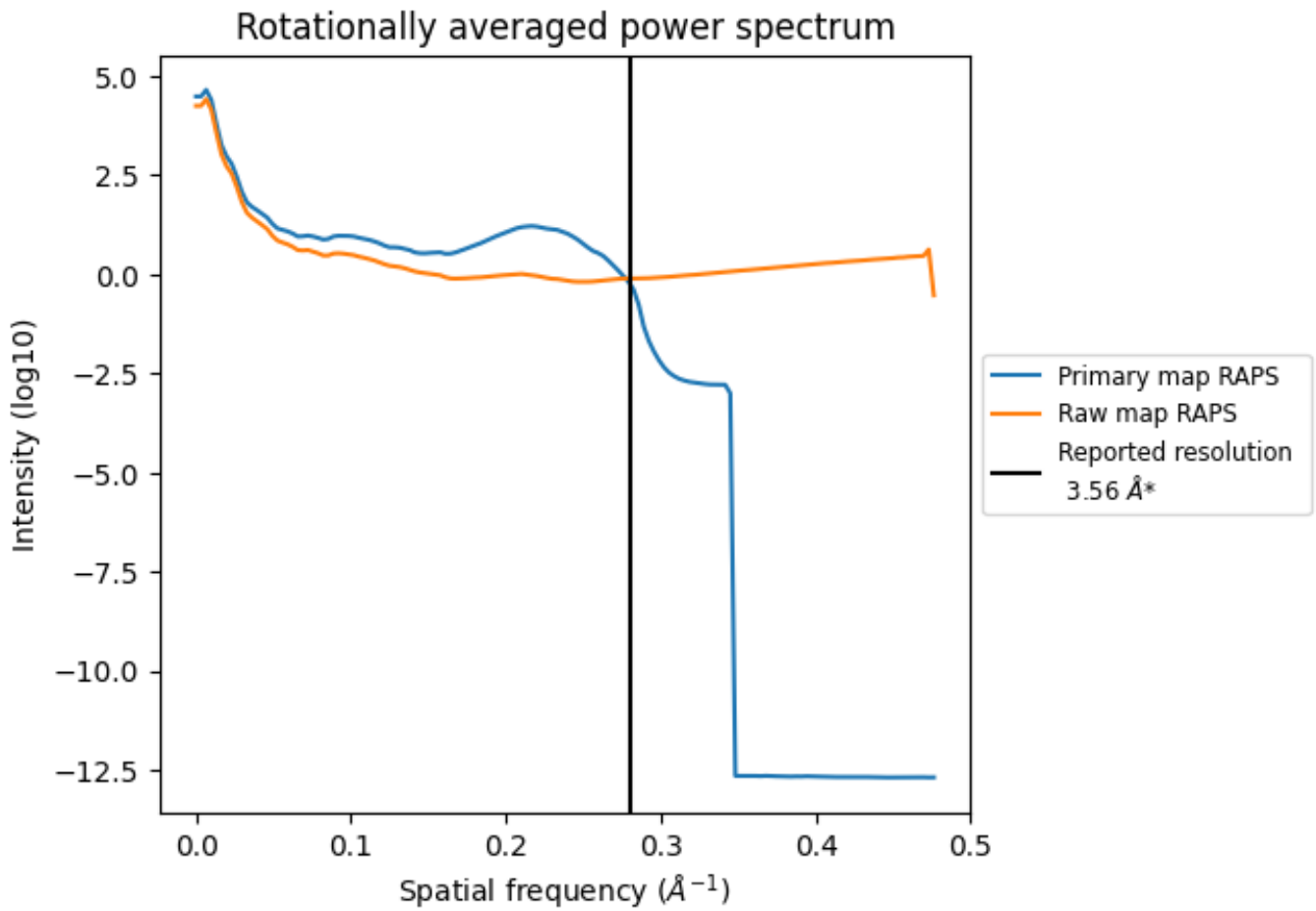
7.2 Volume estimate (i)



The volume at the recommended contour level is 48 nm^3; this corresponds to an approximate mass of 44 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)

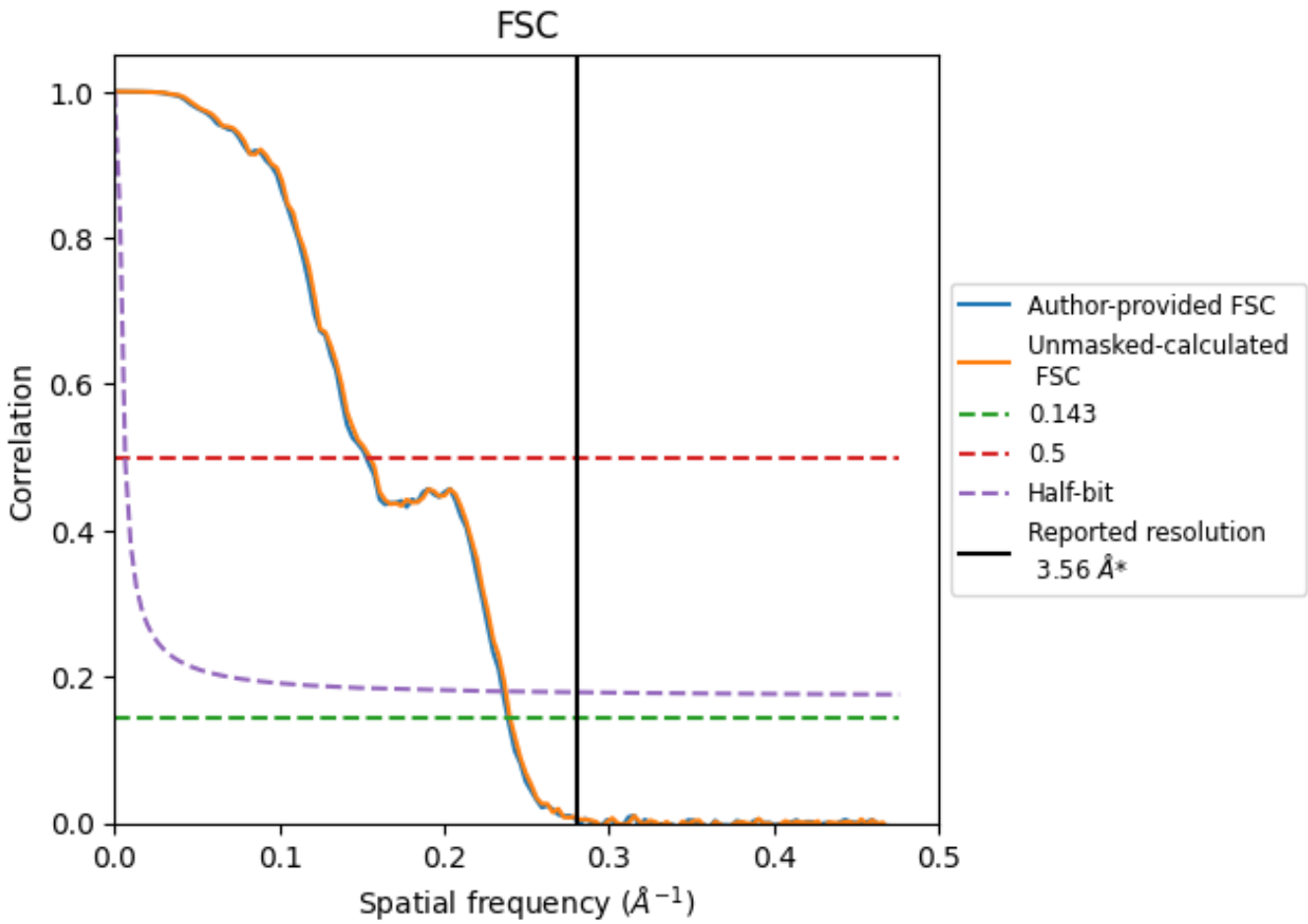


*Reported resolution corresponds to spatial frequency of 0.281 Å^{-1}

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 0.281 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.56	-	-
Author-provided FSC curve	4.19	6.55	4.24
Unmasked-calculated*	4.16	6.46	4.21

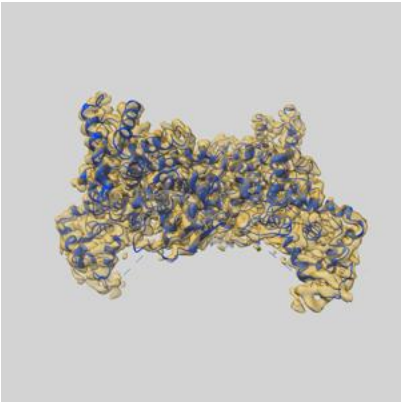
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.19 differs from the reported value 3.56 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 3.56 by more than 10 %

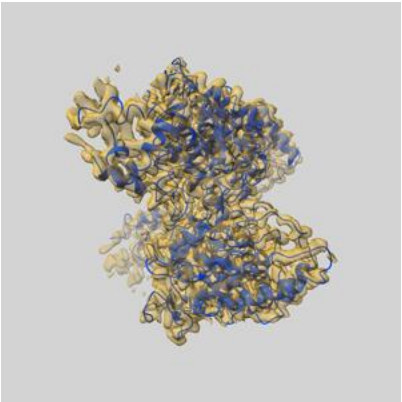
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11689 and PDB model 7AA3. Per-residue inclusion information can be found in section 3 on page 4.

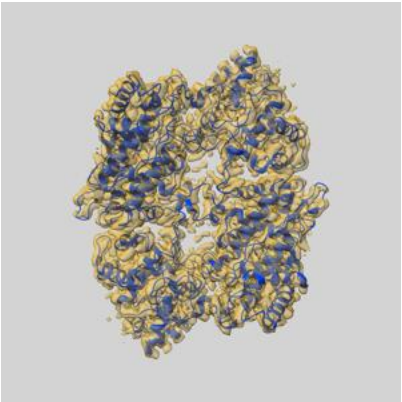
9.1 Map-model overlay (i)



X



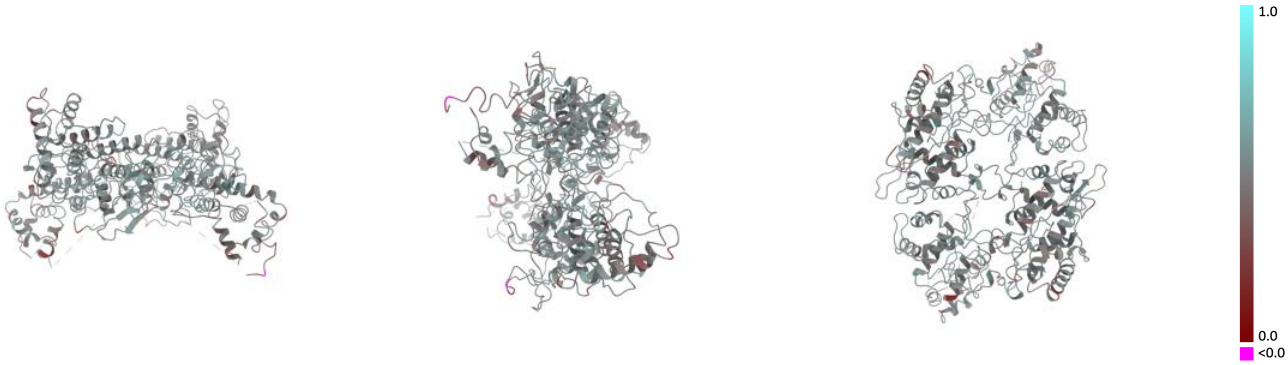
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.305 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

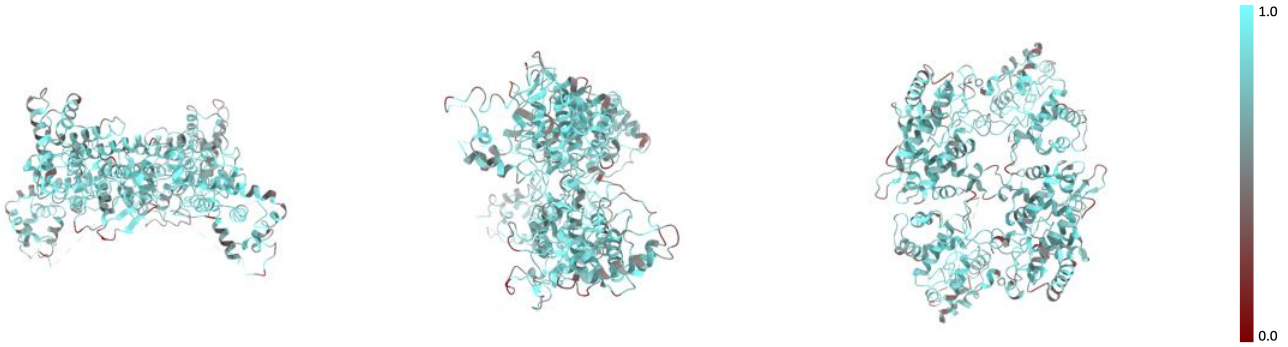
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

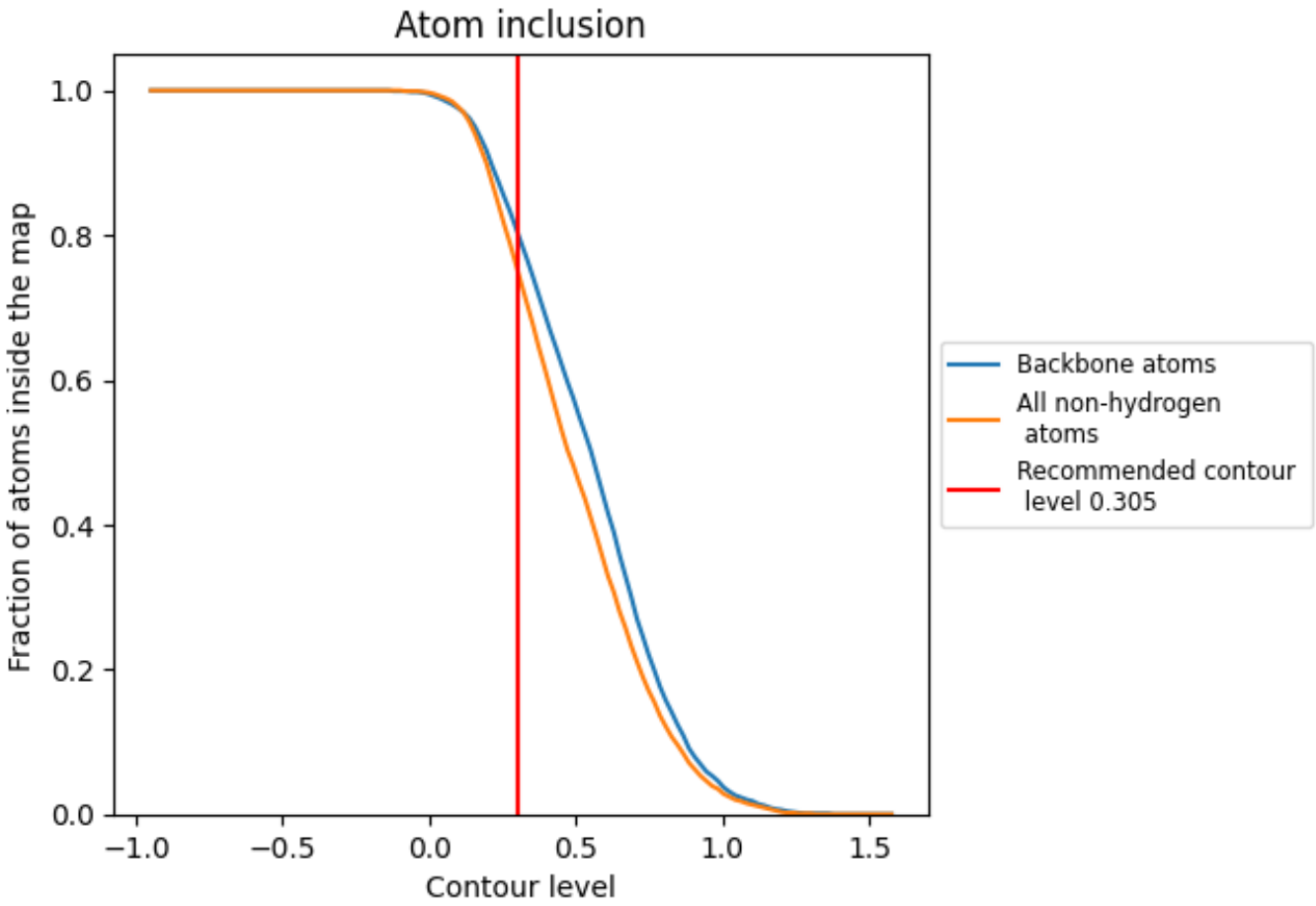
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.305).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.305) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.5000
A	0.7420	0.4990
B	0.7480	0.5010