wwPDB EM Validation Summary Report

Aug 15, 2026 – 12:45 PM EDT

PDB ID	:	9Q69 / pdb_00009q69
EMDB ID	:	EMD-72260
Title	:	Cryo-electron microscopy structure of PfRIPR bound to monoclonal antibodies RP.047, RP.057 and RP.035
Authors	:	Barrett, J.R.; Ward, A.B.
Deposited on	:	2025-08-21
Resolution	:	3.35 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:

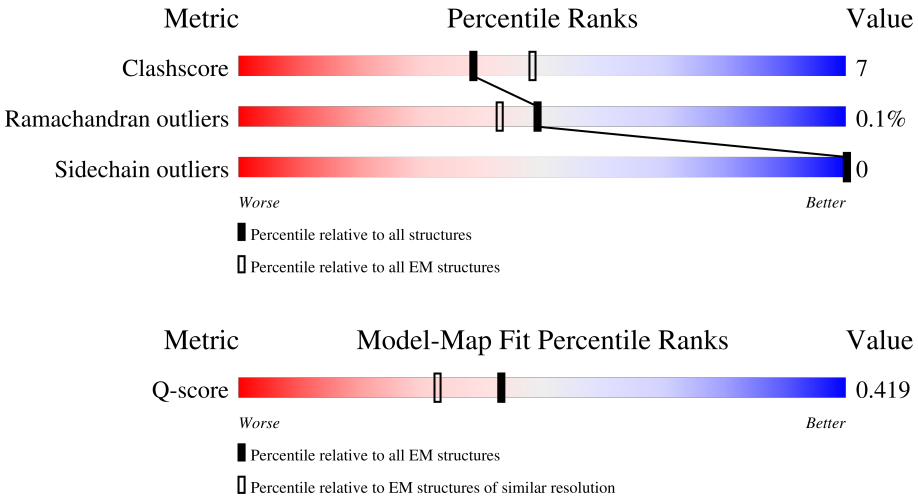
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.35 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	14390 (2.85 - 3.85)

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	117	79% 21%
2	B	108	84% 16%
3	C	120	23% 84% 16%
4	D	107	14% 84% 16%

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Mol	Chain	Length	Quality of chain
5	E	121	
6	F	110	
7	G	1070	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6429 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 RP.047 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	117	914	577	161	172	4	0	0

- Molecule 2 is a protein called RP.047 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	108	811	515	135	159	2	0	0

- Molecule 3 is a protein called RP.057 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	120	901	563	153	180	5	0	0

- Molecule 4 is a protein called RP.057 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	107	808	506	132	167	3	0	0

- Molecule 5 is a protein called RP.035 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	121	954	610	156	183	5	0	0

- Molecule 6 is a protein called RP.035 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	110	833	527	140	164	2	0	0

- Molecule 7 is a protein called Rh5-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	152	Total	C	N	O	S	0	0
			1208	733	210	242	23		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	103	GLN	ASN	conflict	UNP O97302
G	144	GLN	ASN	conflict	UNP O97302
G	228	GLN	ASN	conflict	UNP O97302
G	334	GLN	ASN	conflict	UNP O97302
G	480	GLN	ASN	conflict	UNP O97302
G	498	GLN	ASN	conflict	UNP O97302
G	506	GLN	ASN	conflict	UNP O97302
G	526	GLN	ASN	conflict	UNP O97302
G	646	GLN	ASN	conflict	UNP O97302
G	647	GLN	ASN	conflict	UNP O97302
G	964	GLN	ASN	conflict	UNP O97302
G	1021	GLN	ASN	conflict	UNP O97302
G	1087	GLU	-	expression tag	UNP O97302
G	1088	PRO	-	expression tag	UNP O97302
G	1089	GLU	-	expression tag	UNP O97302
G	1090	ALA	-	expression tag	UNP O97302

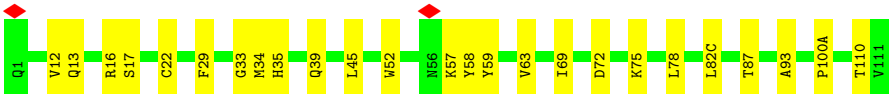
3 Residue-property plots (i)

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: RP.047 Heavy Chain

Chain A:





- Molecule 2: RP.047 Light Chain

Chain B:

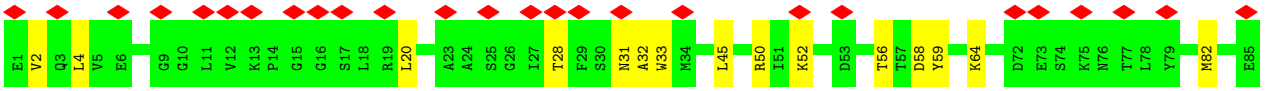


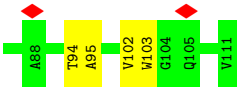


- Molecule 3: RP.057 Heavy Chain

Chain C:



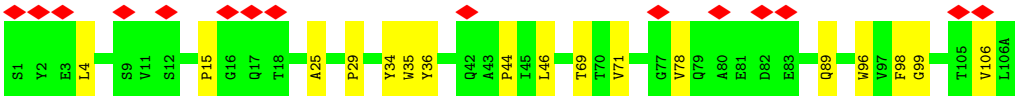




- Molecule 4: RP.057 Light Chain

Chain D:





- Molecule 5: RP.035 Heavy Chain

Chain E:



Q1 V12 T17 L18 T19 L20 P40 K43 W47 L48 T49 L50 I51 D54 D55 D56 K57 P61 L67 T68 I69 K75 L80 T82A D83 P84 V85 Y100B Q105 G106 T107 V111

- Molecule 6: RP.035 Light Chain

Chain F: 77% 23%

Q1 L4 P7 P8 P15 V19 N27B I28 V33 Y34 W35 Y36 Q37 A43 L46 L47 I48 Y49 R61 A71 S76 G77 L78 R79 S80 C88 A89 V90 L95 V97 F98 L104 L106A

- Molecule 7: Rh5-interacting protein

Chain G: 12% 86%

ASP LEU ILE GLU GLY ILE PHE TYR GLU LYS ASN GLU ILE ASP LYS LEU THR PHE SER LEU ASP HIS ARG VAL ARG ASP ASN LEU LYS THR ASP LEU ILE LEU ASN ASN GLY GLU ASN ASP TYR ALA TYR LEU ASN LYS TYR VAL TYR THR ILE LEU ASN ARG ASP SER THR GLU LYS

ILE LYS THR PHE PHE SER HIS ASN LYS ASP MET LYS SER CYS ASP TYR PHE ILE SER LYS GLU TYR GLN SER SER ASP LYS THR ASN GLN ILE CYS TYR LYS LYS THR PHE CYS GLY VAL VAL ILE PRO ASN SER GLU GLU ILE LYS THR ASN LYS ILE THR ASN ASP LYS LEU TYR CYS

ALA HIS PHE GLN SER THR HIS ILE ILE ILE TYR TYR ILE SER GLN PRO LEU LEU LEU GLU PRO HIS VAL VAL TYR GLU GLU THR PHE PHE GLU LYS GLY LYS ASN ASP GLN ILE ASN CYS GLN GLY MET TYR ILE SER LEU ARG SER VAL HIS VAL HIS THR HIS ASN ALA ILE LEU GLN

GLN GLU THR LEU THR TYR ILE LYS ASN LEU CYS ASP GLY LYS ASN ASN CYS LYS PHE ASP PHE ASP SER ILE LYS TYR GLU GLN LYS SER LEU THR HIS TYR LEU PHE PHE ILE ASN ILE GLN TYR GLN CYS ILE SER PRO LEU ASN LEU GLN GLU ASN GLU MET CYS ASP VAL TYR ASN

ASP ASP THR HIS LYS ALA THR CYS LYS TYR GLY PHE ASN LYS ILE GLU LEU LEU LYS ASN VAL CYS GLU GLU ASN TYR ARG CYS THR GLN ASP ILE CYS SER VAL ASN GLN PHE CYS ASP GLY GLU ASN GLU THR CYS THR CYS LYS THR SER LEU LEU PRO SER ALA LYS ASN ASN CYS

GLU TYR ASN ASP LEU CYS THR VAL LEU ASN CYS PRO GLU GLN SER THR CYS GLU GLN ILE GLY ASN GLY LYS LYS ALA GLU CYS LYS CYS GLU ASN GLY LYS TYR TYR HIS ASN ASN LYS CYS TYR THR LYS ASN ASP LEU GLU LEU ALA ILE LYS ILE GLU PRO HIS LYS LYS GLU LYS

PHE TYR LYS ASN ASN LEU TYR GLN GLY LYS ALA LEU LYS PRO GLU TYR ILE PHE MET GLN CYS GLU ASN GLY PHE SER ILE GLU VAL ILE ASN ALA TYR VAL SER CYS TYR ARG VAL SER PHE ASN LEU ASN LYS LEU LYS TYR VAL THR GLU SER LEU LYS LYS MET CYS ASP GLY LYS

THR LYS CYS ALA TYR GLY ASN THR ILE ASP PRO ILE ASP ASP LEU ASN HIS HIS ASN ILE CYS ASN ASN PHE ASN THR ILE PHE LYS TYR ASP TYR LEU CYS VAL PHE ASN ASN GLN ILE THR SER ASP LYS ASN SER HIS LEU HIS SER ASN ILE PRO SER LEU TYR GLN SER SER

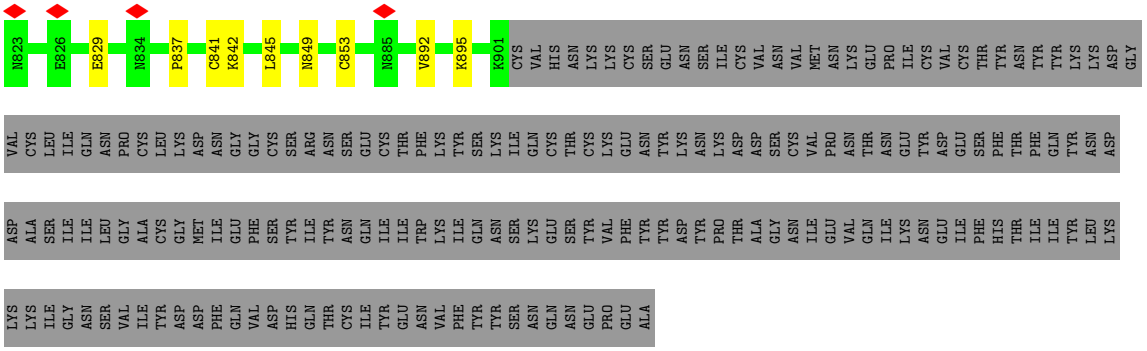
ILE LEU PRO ASP ILE GLN LYS SER LYS PHE HIS LEU ILE SER ARG ASN SER ARG THR ASN GLN TYR PRO HIS ASN GLN ILE SER MET LEU GLU ILE GLN ASN GLU ILE SER SER HIS ASN SER ASN GLN PHE SER THR ASP PRO HIS THR ASN SER ASN ASN ILE ASN ASN MET ASN ILE

LYS LYS VAL GLU ILE PHE ARG SER ARG PHE SER SER LYS LEU GLN CYS GLN GLY GLY LYS ILE ASN ILE ASP LYS ALA ILE LEU LYS GLY GLY GLU GLY CYS ASN ASP LEU LEU LEU THR ASN SER LEU LYS SER TYR CYS ASN ASP LEU SER GLU CYS ASP ILE GLY LEU ILE TYR HIS

PHE ASP THR TYR CYS ILE ASN ASP GLN TYR LEU PHE VAL SER TYR SER CYS SER ASN LEU CYS ASN LYS CYS HIS GLN GLN SER THR CYS TYR GLY ASN ARG PHE ASN TYR ASP CYS PHE CYS ASP ASN PRO TYR ILE SER LYS TYR GLY ASN LYS LEU CYS GLU ARG PRO ASN ASP CYS

GLU SER VAL LEU CYS SER GLN ASN GLN VAL CYS GLN ILE LEU PRO ASN ASP LYS LEU ILE CYS GLN CYS GLU GLU GLY TYR LYS ASN VAL LYS GLY LYS CYS VAL PRO ASP ASN LYS CYS ASP LEU SER CYS PRO SER ASN LYS VAL CYS VAL ILE GLU ASN GLY LYS GLN THR CYS LYS

CYS SER GLU ARG PHE VAL LEU GLU ASN G750 V751 C752 I753 C754 A755 N756 D757 Y758 K759 M760 E761 D762 G763 I764 N765 C766 I767 A768 K769 N770 K773 R774 K775 E776 Y777 E778 N779 M787 Y790 N791 E792 E793 T794 V797 C801 K802 Y805 D817 Y818 C819 K820 D821 I822


N823
E826
E829
N834
P837
C841
K842
L845
N849
C853
N885
V892
K895
K901
CYS VAL HIS ASN LYS LYS CYS SER GLU ASN SER ILE CYS VAL ASN VAL MET ASN LYS GLU PRO ILE CYS VAL CYS THR TYR ASN TYR TYR LYS LYS ASP GLY
VAL CYS LEU ILE GLN ASN PRO CYS LEU LYS ASP ASN GLY GLY CYS SER ARG ASN SER GLU CYS THR PHE LYS TYR SER LYS ILE GLN CYS THR CYS LYS GLU ASN TYR LYS ASN LYS ASP ASP SER CYS VAL PRO ASN THR ASN GLU TYR ASP GLU SER PHE THR PHE GLN TYR ASN ASP
ASP ALA SER ILE ILE LEU GLY ALA CYS GLY MET ILE GLU PHE SER TYR ILE TYR ASN GLN ILE ILE TRP LYS ILE GLN ASN SER LYS GLU SER TYR VAL PHE TYR TYR ASP TYR PRO THR ALA GLY ASN ILE GLU VAL GLN ILE LYS ASN GLU ILE PHE HIS THR ILE ILE TYR LEU LYS
LYS LYS ILE GLY ASN SER VAL ILE TYR ASP ASP PHE GLN VAL ASP HIS GLN THR CYS ILE TYR GLU ASN VAL PHE TYR TYR SER ASN GLN ASN GLU PRO GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.099	Depositor
Minimum map value	-0.649	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	367.616, 367.616, 367.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.718, 0.718, 0.718	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	0/937	0.40	0/1270
2	B	0.20	0/829	0.36	0/1123
3	C	0.22	0/918	0.61	0/1245
4	D	0.21	0/829	0.45	0/1132
5	E	0.23	0/981	0.45	0/1344
6	F	0.22	0/856	0.45	0/1167
7	G	0.18	0/1224	0.45	0/1638
All	All	0.21	0/6574	0.46	0/8919

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

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	914	0	874	18	0
2	B	811	0	802	13	0
3	C	901	0	884	11	0
4	D	808	0	764	12	0
5	E	954	0	931	17	0
6	F	833	0	799	16	0
7	G	1208	0	1140	19	0
All	All	6429	0	6194	92	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 7.

The worst 5 of 92 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:100(A):PRO:HD2	2:B:49:TYR:HB2	1.62	0.80
5:E:61:PRO:HG3	6:F:95:LEU:HB2	1.73	0.71
1:A:33:GLY:HA3	7:G:793:GLU:HB3	1.74	0.70
2:B:34:ALA:HB3	2:B:89:GLN:HB3	1.81	0.62
2:B:65:SER:HB2	2:B:72:THR:HB	1.83	0.61

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	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
2	B	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
3	C	118/120 (98%)	113 (96%)	4 (3%)	1 (1%)	16	44
4	D	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
5	E	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
6	F	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
7	G	150/1070 (14%)	146 (97%)	4 (3%)	0	100	100
All	All	821/1753 (47%)	794 (97%)	26 (3%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	2	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/95 (100%)	95 (100%)	0	100	100
2	B	89/89 (100%)	89 (100%)	0	100	100
3	C	96/96 (100%)	96 (100%)	0	100	100
4	D	90/90 (100%)	90 (100%)	0	100	100
5	E	108/108 (100%)	108 (100%)	0	100	100
6	F	91/91 (100%)	91 (100%)	0	100	100
7	G	141/1011 (14%)	141 (100%)	0	100	100
All	All	710/1580 (45%)	710 (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 8 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	865	ASN
6	F	53	GLN
5	E	100	HIS
3	C	105	GLN
5	E	105	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

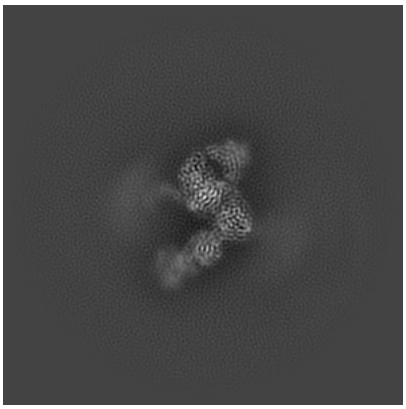
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-72260. These allow visual inspection of the internal detail of the map and identification of artifacts.

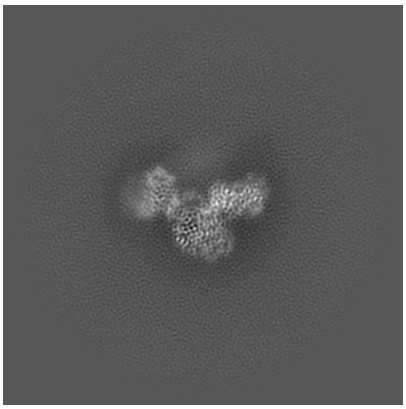
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

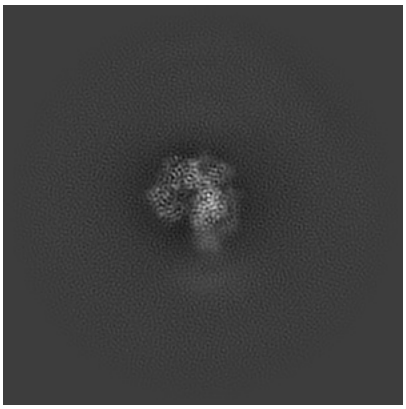
6.1.1 Primary map



X

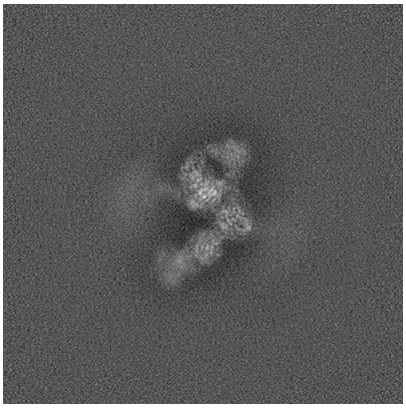


Y

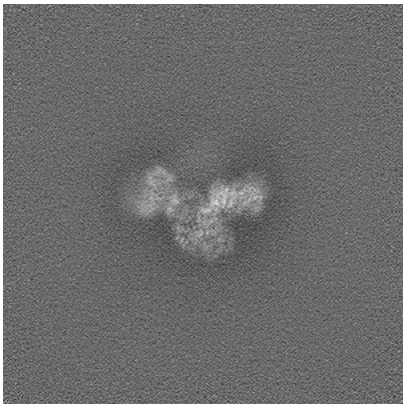


Z

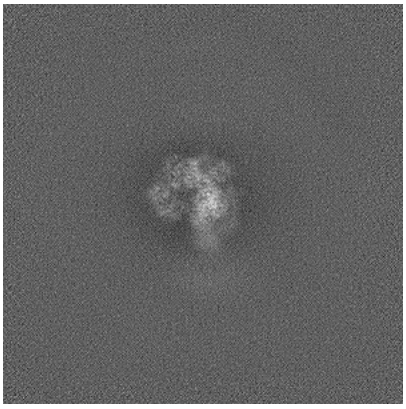
6.1.2 Raw map



X



Y

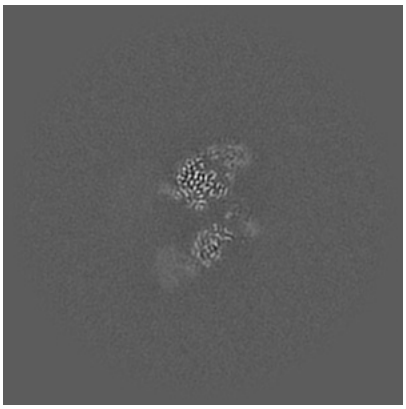


Z

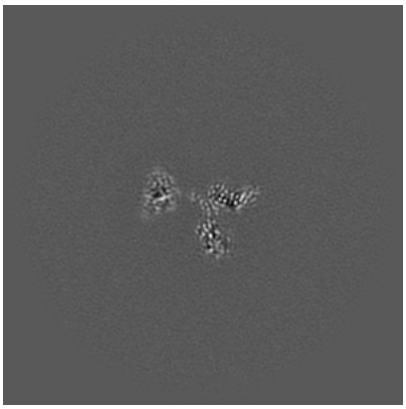
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

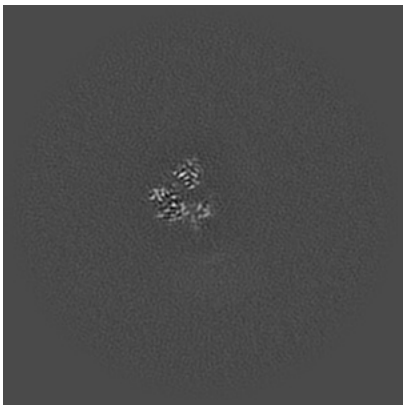
6.2.1 Primary map



X Index: 256

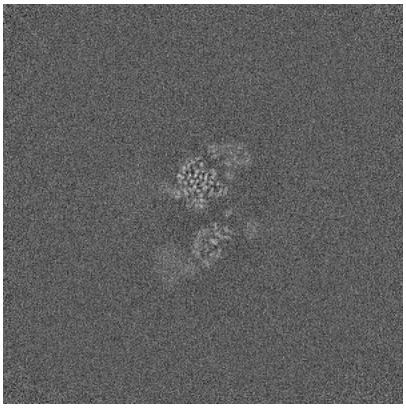


Y Index: 256

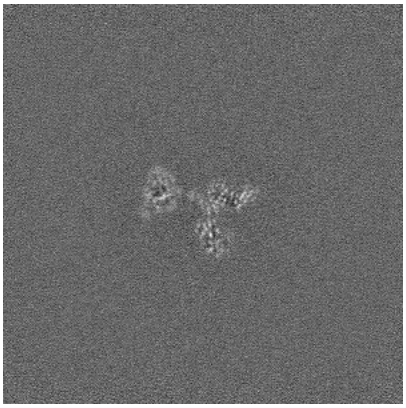


Z Index: 256

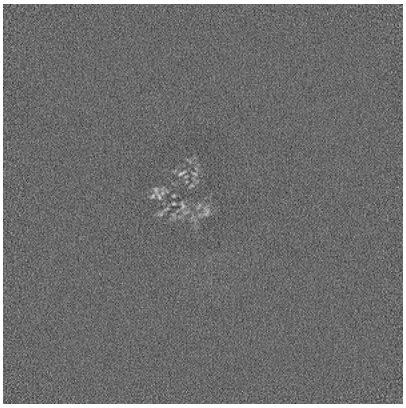
6.2.2 Raw map



X Index: 256



Y Index: 256

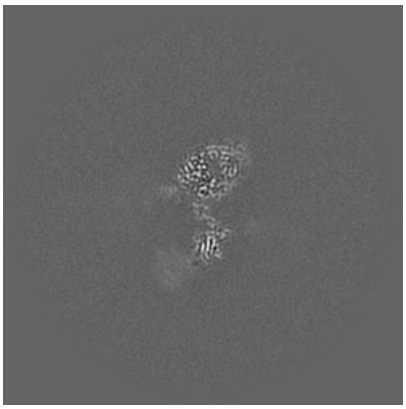


Z Index: 256

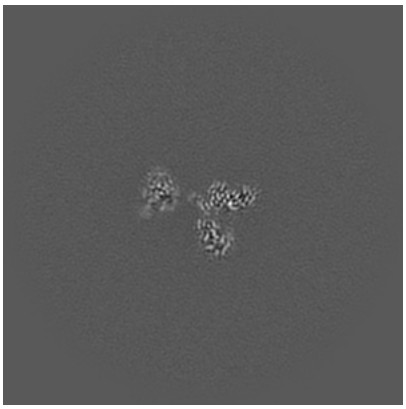
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

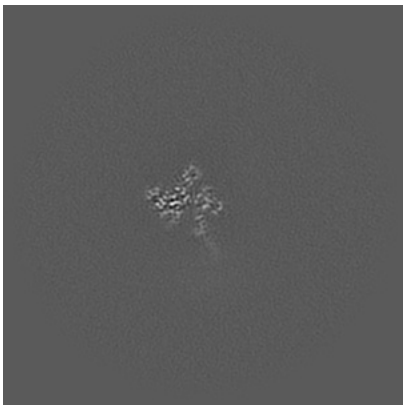
6.3.1 Primary map



X Index: 263

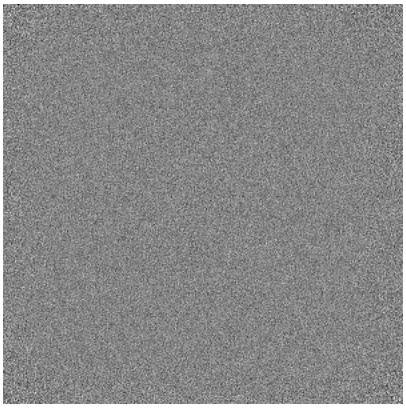


Y Index: 253

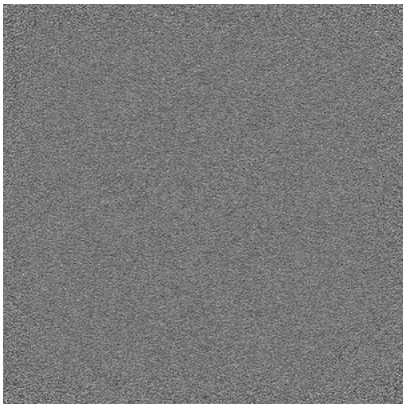


Z Index: 266

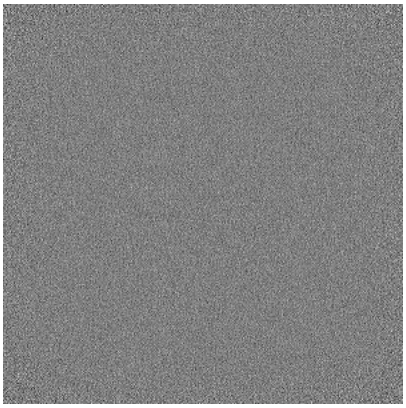
6.3.2 Raw map



X Index: 0



Y Index: 0

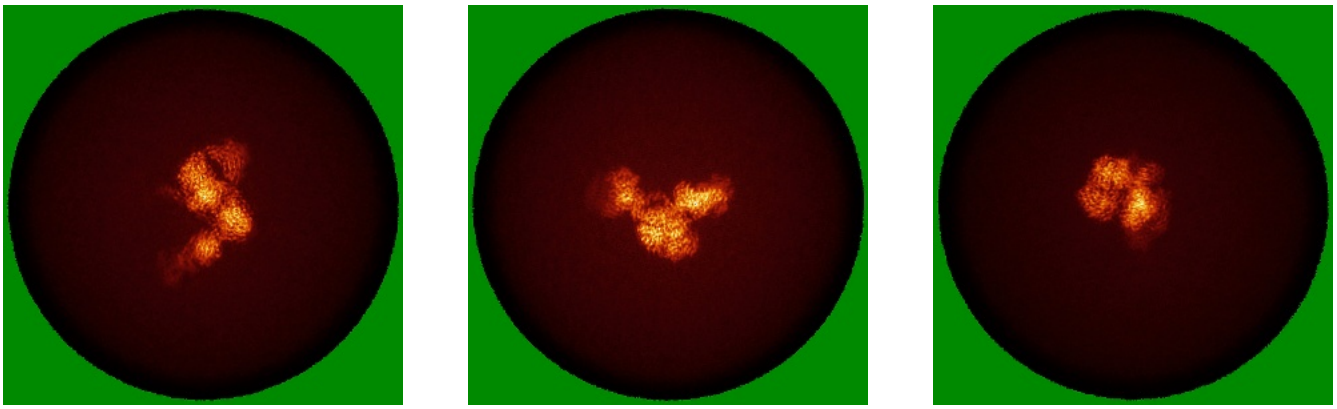


Z Index: 0

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

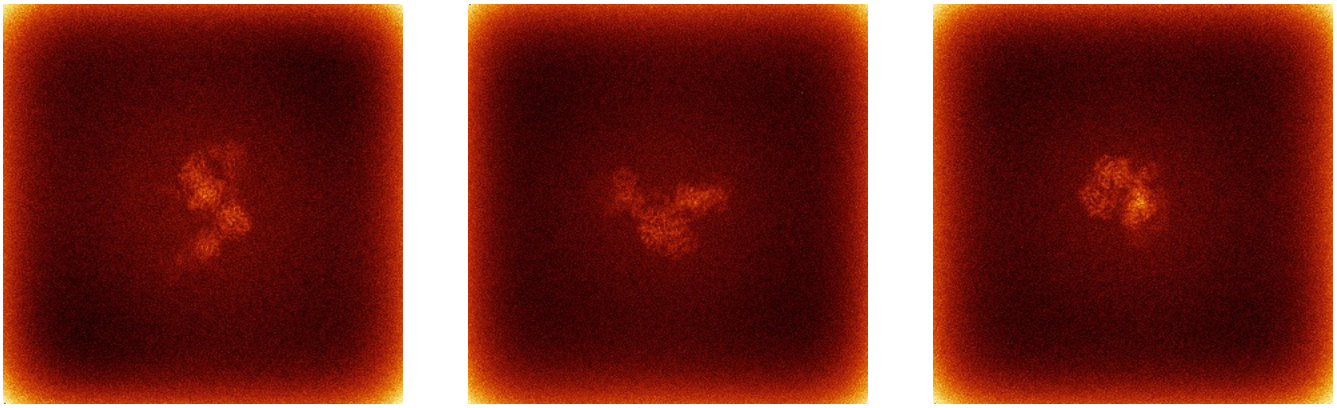
6.4 Orthogonal standard-deviation projections (False-color) (i)

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

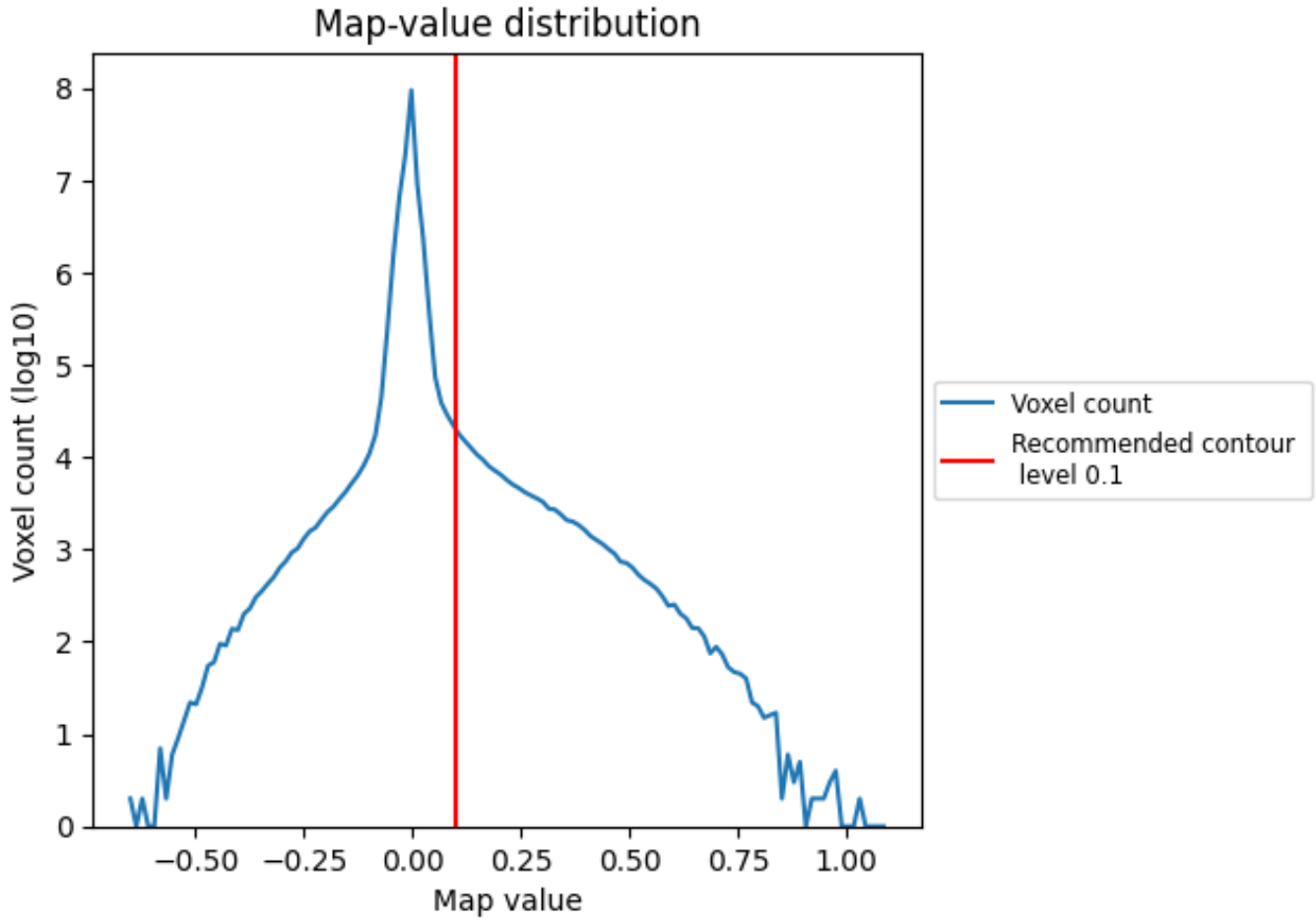
6.6 Mask visualisation (i)

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

7 Map analysis

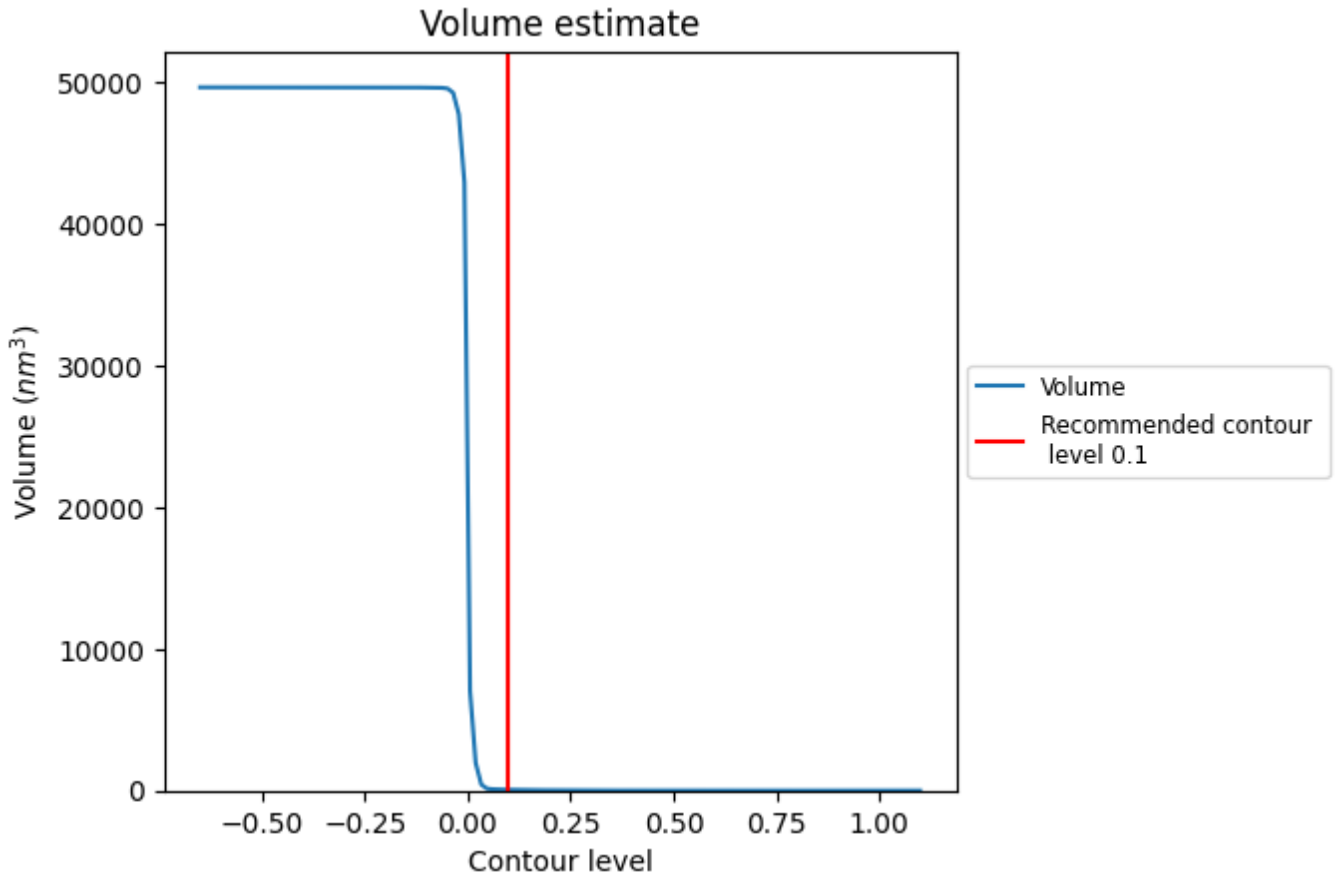
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

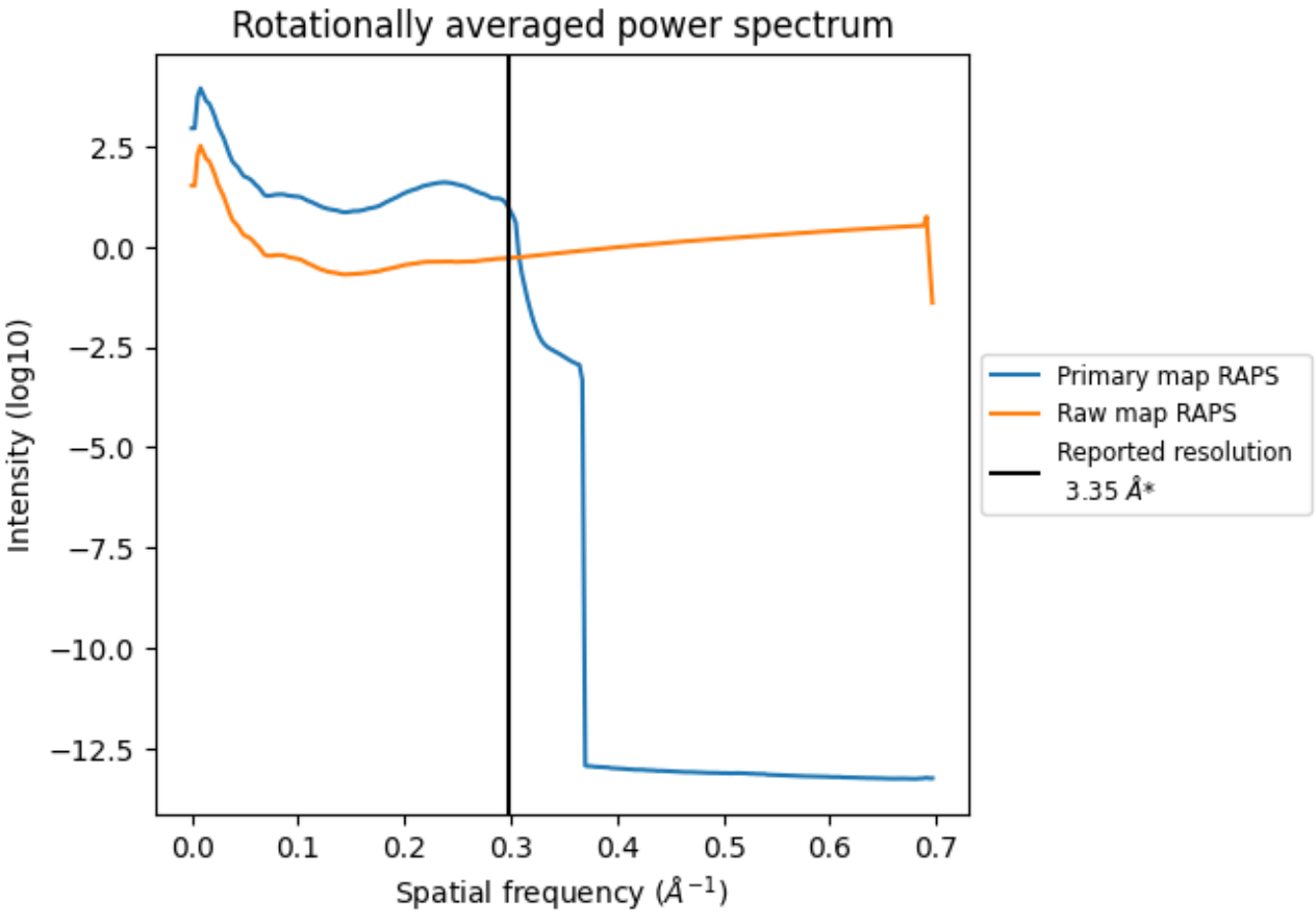
7.2 Volume estimate (i)



The volume at the recommended contour level is 58 nm^3; this corresponds to an approximate mass of 52 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)

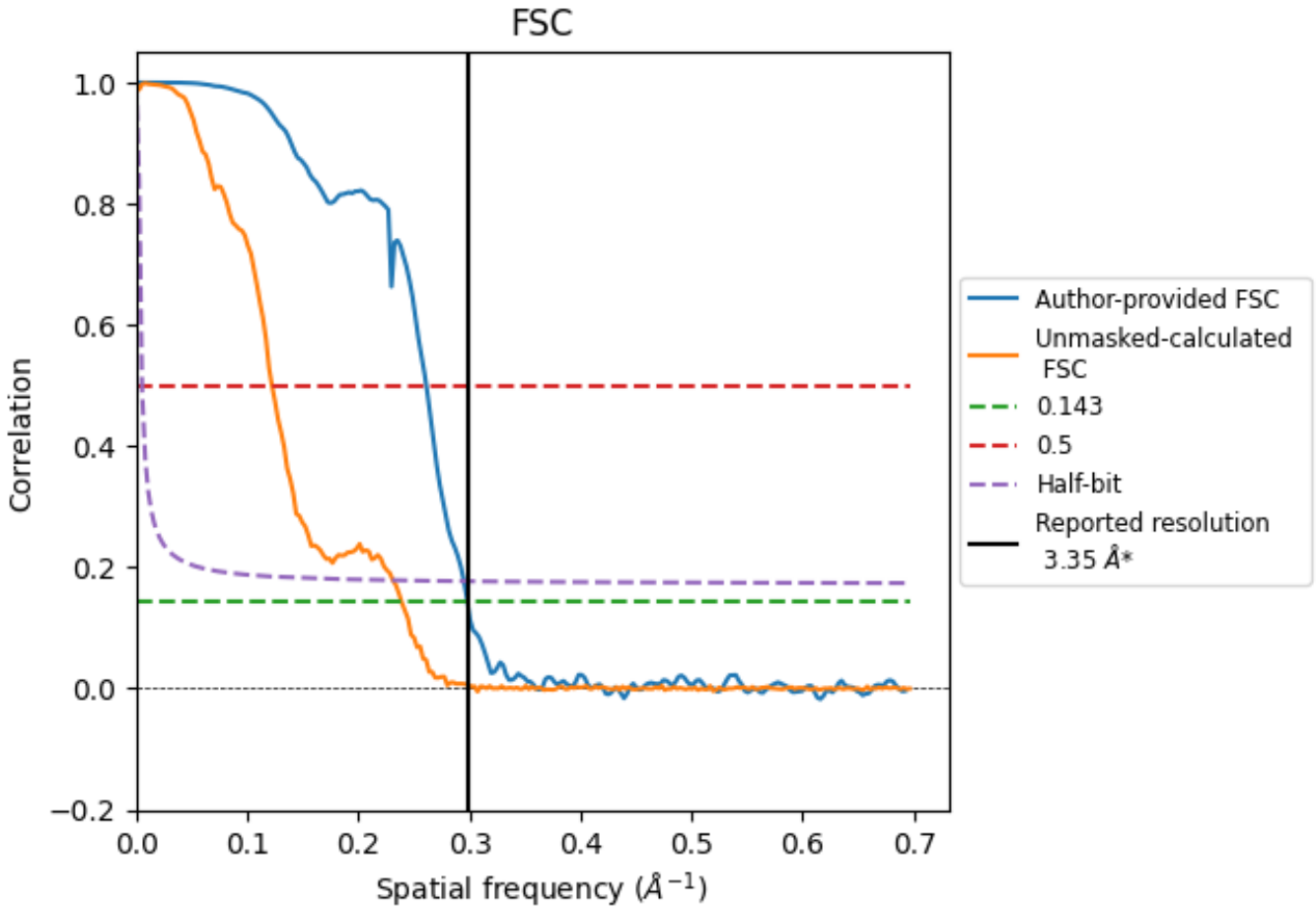


*Reported resolution corresponds to spatial frequency of 0.299 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

8.2 Resolution estimates (i)

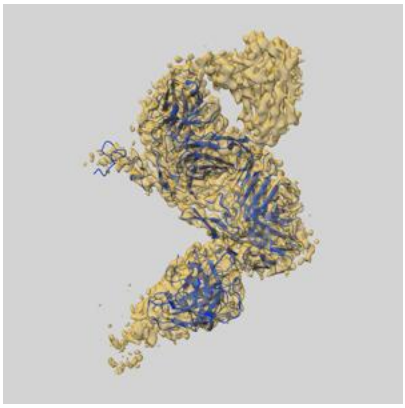
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.35	3.83	3.39
Unmasked-calculated*	4.18	8.18	4.33

*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 4.18 differs from the reported value 3.35 by more than 10 %

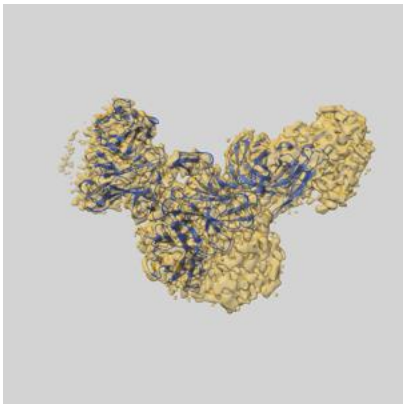
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-72260 and PDB model 9Q69. Per-residue inclusion information can be found in section 3 on page 6.

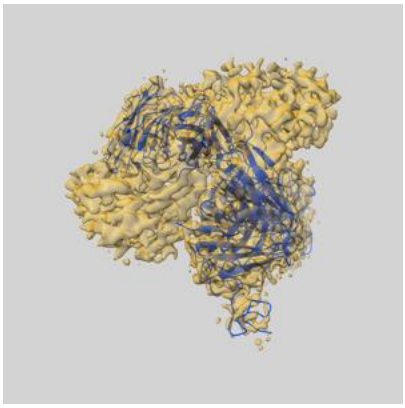
9.1 Map-model overlay



X



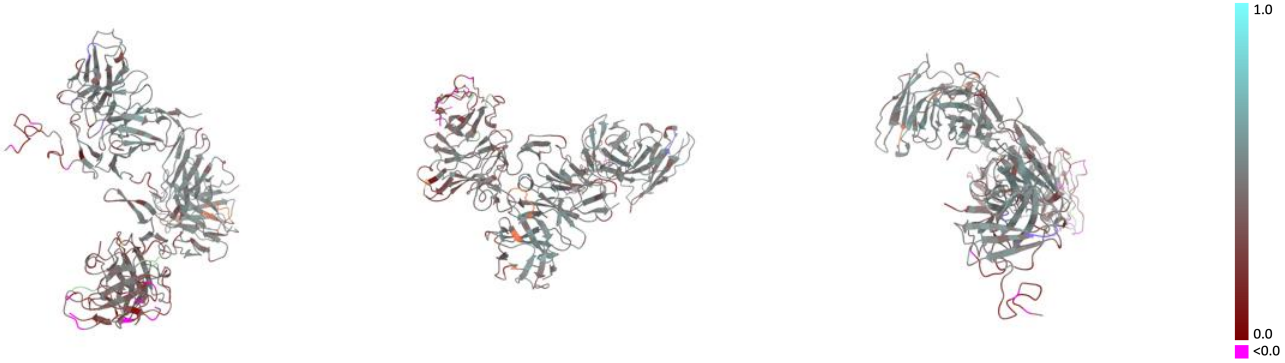
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

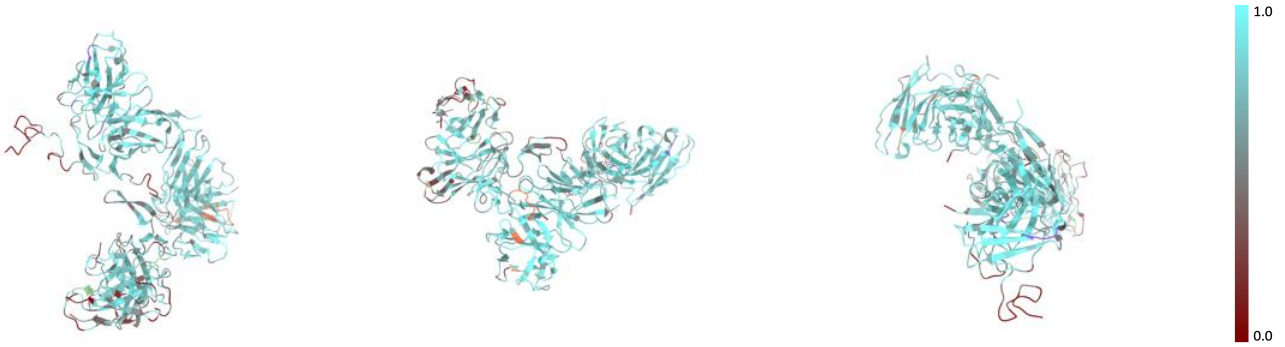
9.2 Q-score mapped to coordinate model (i)



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.

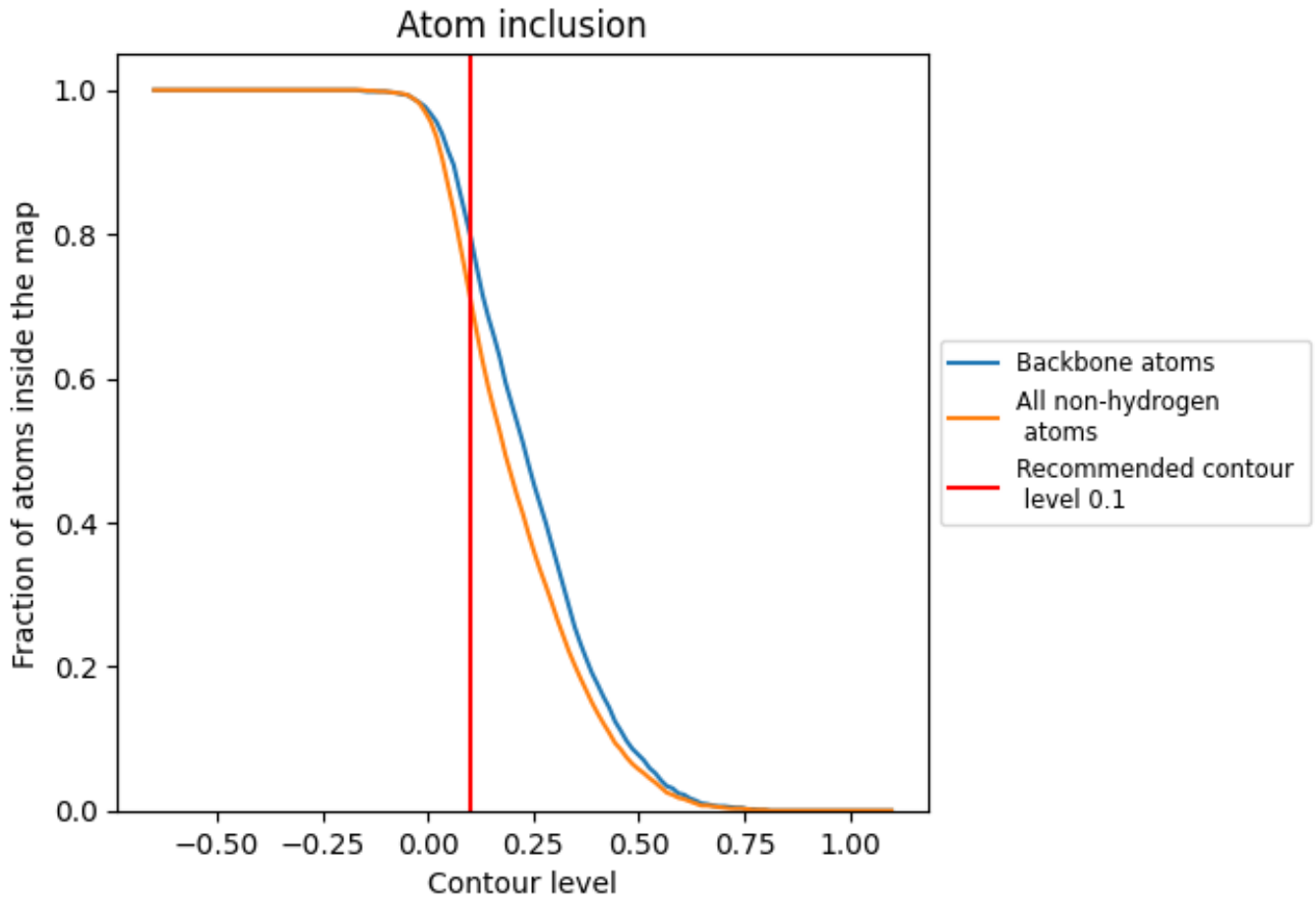
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7100	0.4190
A	0.8020	0.4620
B	0.7720	0.4840
C	0.5770	0.2960
D	0.6720	0.3810
E	0.8080	0.4810
F	0.7790	0.4760
G	0.6000	0.3730

