



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 02:16 AM UTC

PDB ID : 6JPU / pdb_00006jpu
EMDB ID : EMD-9871
Title : CryoEM structure of Abo1 hexamer - apo complex
Authors : Cho, C.; Jang, J.; Song, J.J.
Deposited on : 2019-03-28
Resolution : 4.27 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

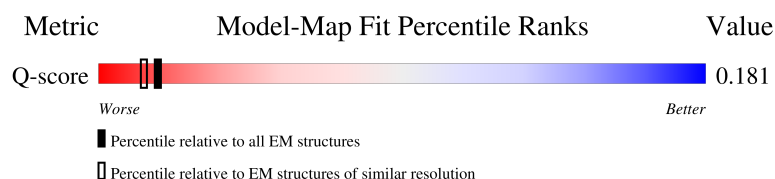
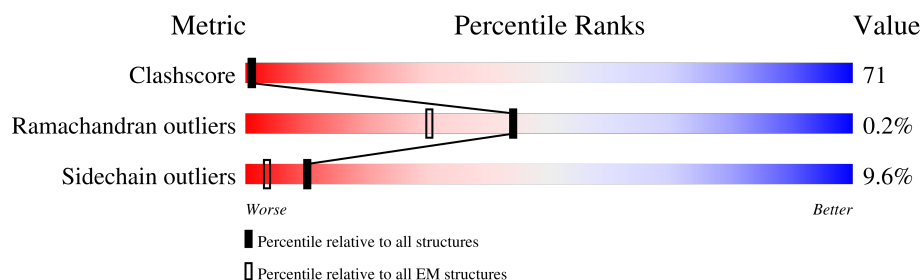
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.27 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	4567 (3.77 - 4.76)

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	1198	15% 10% 35% 52%
1	B	1198	17% 10% 35% 52%
1	C	1198	15% 11% 35% 52%
1	D	1198	14% 11% 35% 52%

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Mol	Chain	Length	Quality of chain
1	E	1198	17% 11% 35% 52%
1	F	1198	14% 10% 35% 52%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30378 atoms, of which 2610 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 Uncharacterized AAA domain-containing protein C31G5.19.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	B	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	C	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	D	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	E	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		
1	F	577	Total	C	H	N	O	S	0	0
			5063	2963	435	789	854	22		

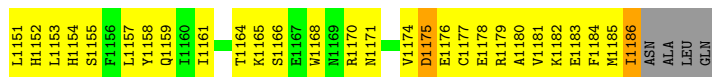
There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP O14114
A	-6	ALA	-	expression tag	UNP O14114
A	-5	MET	-	expression tag	UNP O14114
A	-4	GLY	-	expression tag	UNP O14114
A	-3	SER	-	expression tag	UNP O14114
A	-2	GLY	-	expression tag	UNP O14114
A	-1	ILE	-	expression tag	UNP O14114
A	0	GLN	-	expression tag	UNP O14114
B	-7	GLY	-	expression tag	UNP O14114
B	-6	ALA	-	expression tag	UNP O14114
B	-5	MET	-	expression tag	UNP O14114
B	-4	GLY	-	expression tag	UNP O14114
B	-3	SER	-	expression tag	UNP O14114
B	-2	GLY	-	expression tag	UNP O14114
B	-1	ILE	-	expression tag	UNP O14114
B	0	GLN	-	expression tag	UNP O14114
C	-7	GLY	-	expression tag	UNP O14114
C	-6	ALA	-	expression tag	UNP O14114

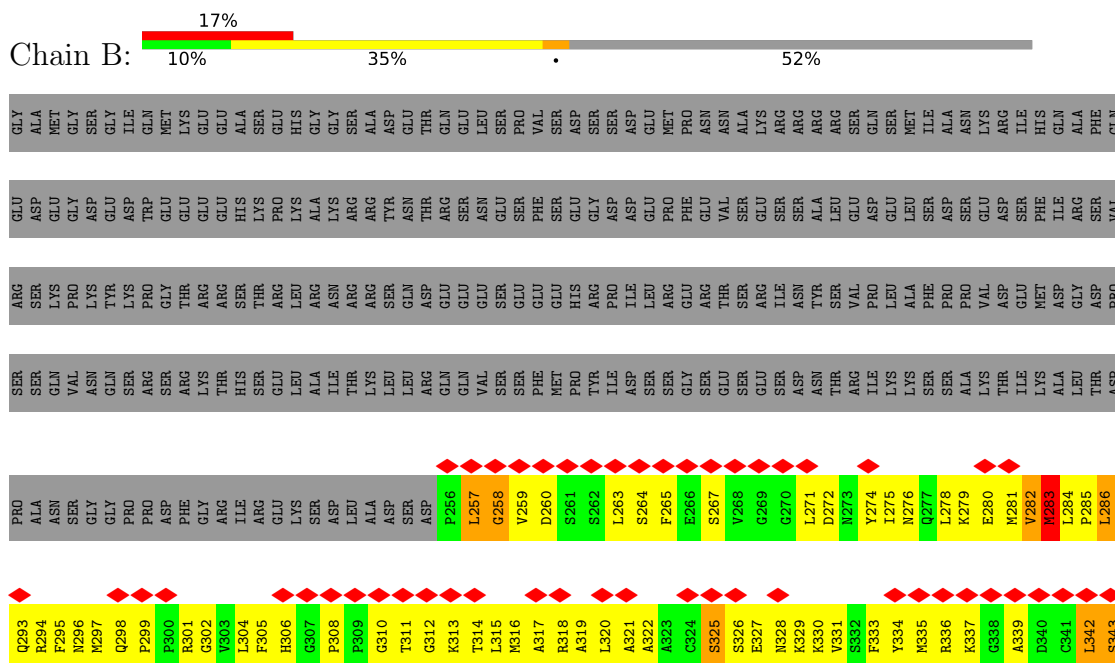
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MET	-	expression tag	UNP O14114
C	-4	GLY	-	expression tag	UNP O14114
C	-3	SER	-	expression tag	UNP O14114
C	-2	GLY	-	expression tag	UNP O14114
C	-1	ILE	-	expression tag	UNP O14114
C	0	GLN	-	expression tag	UNP O14114
D	-7	GLY	-	expression tag	UNP O14114
D	-6	ALA	-	expression tag	UNP O14114
D	-5	MET	-	expression tag	UNP O14114
D	-4	GLY	-	expression tag	UNP O14114
D	-3	SER	-	expression tag	UNP O14114
D	-2	GLY	-	expression tag	UNP O14114
D	-1	ILE	-	expression tag	UNP O14114
D	0	GLN	-	expression tag	UNP O14114
E	-7	GLY	-	expression tag	UNP O14114
E	-6	ALA	-	expression tag	UNP O14114
E	-5	MET	-	expression tag	UNP O14114
E	-4	GLY	-	expression tag	UNP O14114
E	-3	SER	-	expression tag	UNP O14114
E	-2	GLY	-	expression tag	UNP O14114
E	-1	ILE	-	expression tag	UNP O14114
E	0	GLN	-	expression tag	UNP O14114
F	-7	GLY	-	expression tag	UNP O14114
F	-6	ALA	-	expression tag	UNP O14114
F	-5	MET	-	expression tag	UNP O14114
F	-4	GLY	-	expression tag	UNP O14114
F	-3	SER	-	expression tag	UNP O14114
F	-2	GLY	-	expression tag	UNP O14114
F	-1	ILE	-	expression tag	UNP O14114
F	0	GLN	-	expression tag	UNP O14114

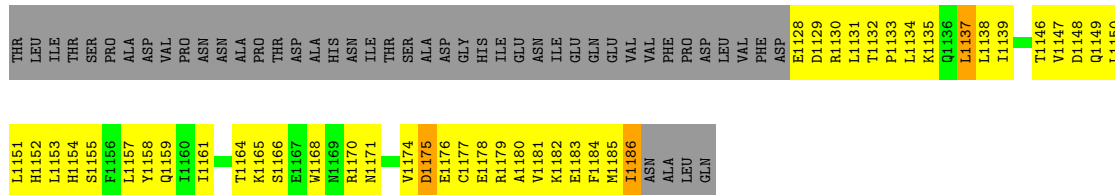


- Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19



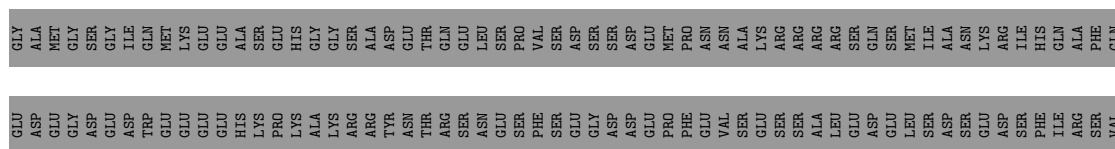






Chain D:







LEU	LEU
ILE	ILE
THR	THR
SER	SER
PRO	PRO
ALA	ALA
ASP	ASP
VAL	VAL
PRO	PRO
ASN	ASN
ASN	ASN
ALA	ALA
PRO	PRO
THR	THR
ASP	ASP
ALA	ALA
HIS	HIS
ASN	ASN
ILE	ILE
THR	THR
SER	SER
ALA	ALA
ASP	ASP
GLY	GLY
HIS	HIS
ILE	ILE
GLU	GLU
ASN	ASN
ILE	ILE
GLU	GLU
GLN	GLN
GLU	GLU
VAL	VAL
VAL	VAL
PHE	PHE
PRO	PRO
ASP	ASP
LEU	LEU
VAL	VAL
PHE	PHE
ASP	ASP
E1128	E1128
D1129	D1129
R1130	R1130
L1131	L1131
T1132	T1132
P1133	P1133
L1134	L1134
K1135	K1135
Q1136	Q1136
L1137	L1137
L1138	L1138
L1139	L1139
T1146	T1146
V1147	V1147
D1148	D1148
Q1149	Q1149
L1150	L1150
L1151	L1151

H1152
L1153
H1154
S1155
F1156
L1157
Y1158
Q1159
I1160
I1161
T1164
K1165
S1166
E1167
W1168
N1169
R1170
N1171
V1174
D1175
E1176
C1177
E1178
R1179
A1180
V1181
K1182
E1183
F1184
M1185
I1186
ASN
ALA
LEU
GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	125874	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 ($e^-/\text{\AA}^2$)	1.5	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	8.458	Depositor
Minimum map value	-3.915	Depositor
Average map value	-0.011	Depositor
Map value standard deviation	0.371	Depositor
Recommended contour level	2	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.30	0/4734	0.60	0/6411
1	B	0.30	0/4734	0.60	1/6411 (0.0%)
1	C	0.30	0/4734	0.60	1/6411 (0.0%)
1	D	0.30	0/4734	0.60	1/6411 (0.0%)
1	E	0.30	0/4734	0.60	1/6411 (0.0%)
1	F	0.30	0/4734	0.60	1/6411 (0.0%)
All	All	0.30	0/28404	0.60	5/38466 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	MET	CA-CB-CG	5.02	124.13	114.10
1	E	283	MET	CA-CB-CG	5.02	124.14	114.10
1	D	283	MET	CA-CB-CG	5.01	124.12	114.10
1	C	283	MET	CA-CB-CG	5.00	124.11	114.10
1	F	283	MET	CA-CB-CG	5.00	124.11	114.10

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	LEU	Peptide
1	A	511	THR	Peptide
1	B	257	LEU	Peptide
1	B	511	THR	Peptide
1	C	257	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4628	435	4700	682	0
1	B	4628	435	4700	718	0
1	C	4628	435	4700	707	0
1	D	4628	435	4700	664	0
1	E	4628	435	4700	674	0
1	F	4628	435	4700	666	0
All	All	27768	2610	28200	3947	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 71.

The worst 5 of 3947 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:B:482:LEU:HD23	1:B:526:MET:HE3	1.37	1.05
1:E:482:LEU:HD23	1:E:526:MET:HE3	1.37	1.05
1:A:482:LEU:HD23	1:A:526:MET:HE3	1.37	1.04
1:E:440:ASP:HA	1:E:472:LYS:HE2	1.40	1.04
1:F:440:ASP:HA	1:F:472:LYS:HE2	1.40	1.04

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	43	77
1	B	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	43	77
1	C	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	43	77
1	D	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	43	77
1	E	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	43	77
1	F	573/1198 (48%)	516 (90%)	56 (10%)	1 (0%)	43	77
All	All	3438/7188 (48%)	3096 (90%)	336 (10%)	6 (0%)	44	77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLY
1	B	258	GLY
1	C	258	GLY
1	D	258	GLY
1	E	258	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	522/1086 (48%)	472 (90%)	50 (10%)	8	26
1	B	522/1086 (48%)	472 (90%)	50 (10%)	8	26
1	C	522/1086 (48%)	472 (90%)	50 (10%)	8	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	522/1086 (48%)	472 (90%)	50 (10%)	8	26
1	E	522/1086 (48%)	472 (90%)	50 (10%)	8	26
1	F	522/1086 (48%)	472 (90%)	50 (10%)	8	26
All	All	3132/6516 (48%)	2832 (90%)	300 (10%)	10	26

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	533	SER
1	F	633	SER
1	E	656	LEU
1	F	343	SER
1	B	1166	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	489	ASN
1	F	1149	GLN
1	D	1149	GLN
1	F	1136	GLN
1	F	489	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

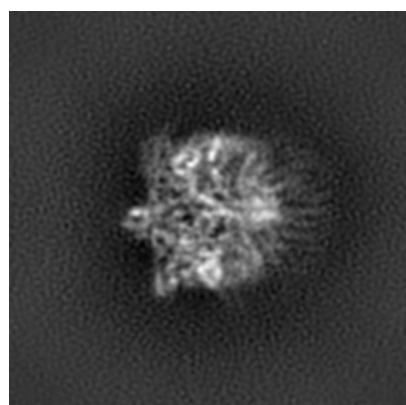
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9871. These allow visual inspection of the internal detail of the map and identification of artifacts.

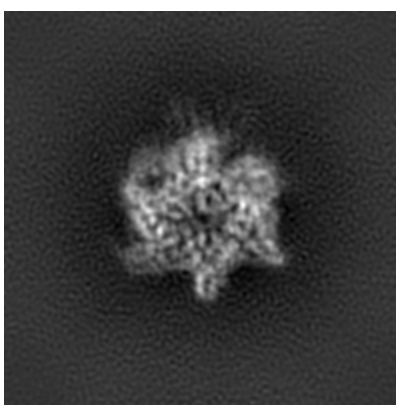
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

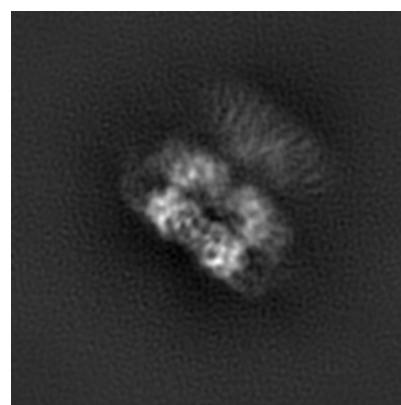
6.1.1 Primary map



X



Y

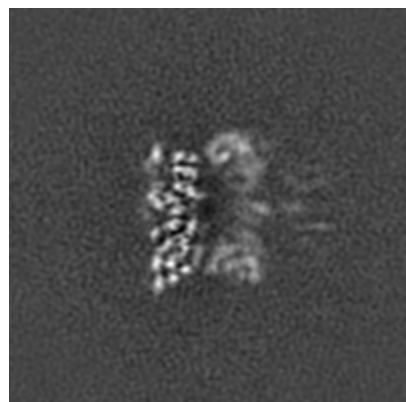


Z

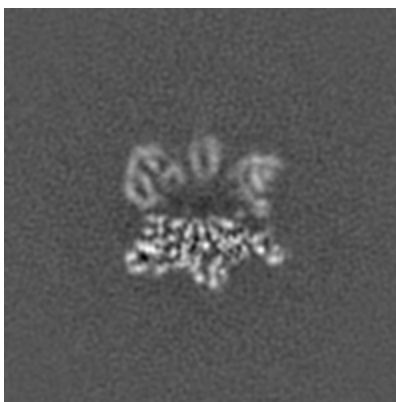
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

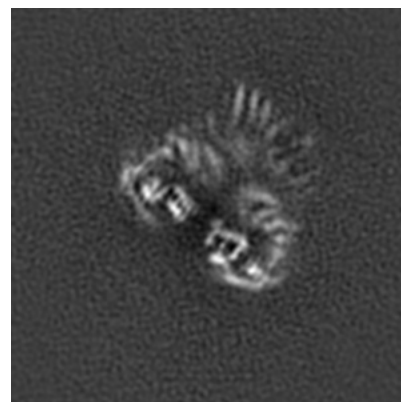
6.2.1 Primary map



X Index: 150



Y Index: 150

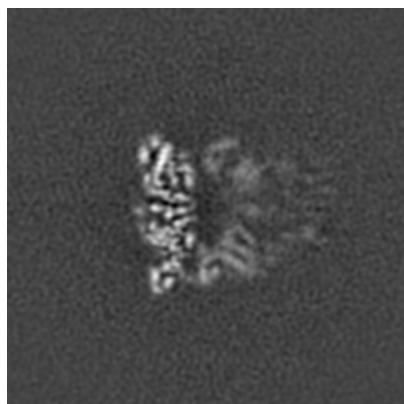


Z Index: 150

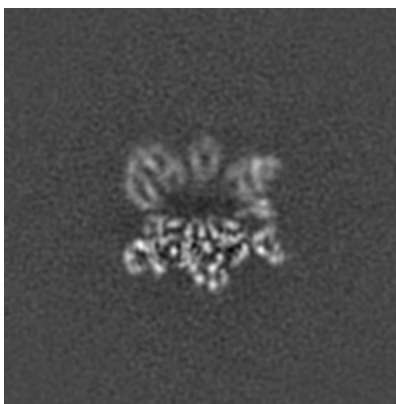
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

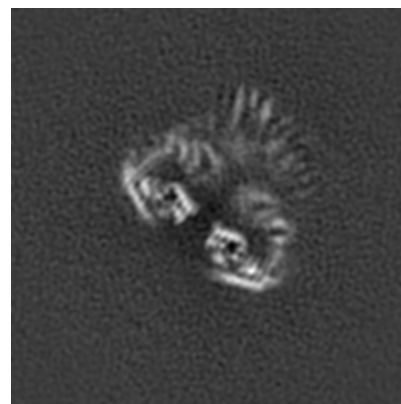
6.3.1 Primary map



X Index: 157



Y Index: 152

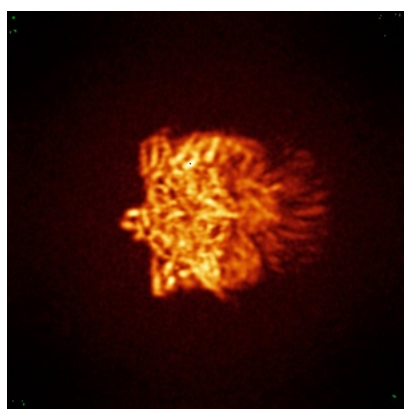


Z Index: 148

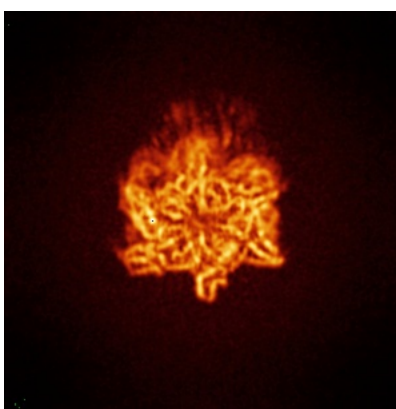
The images above show the largest variance slices of the map in three orthogonal directions.

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

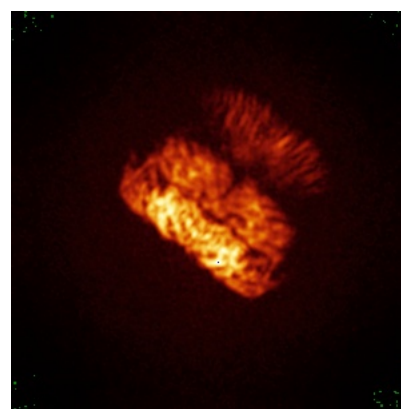
6.4.1 Primary map



X



Y

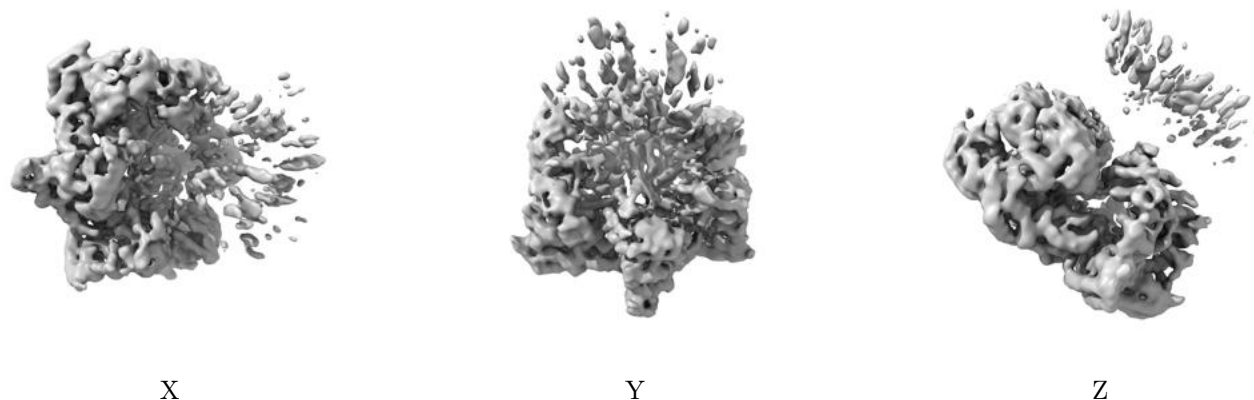


Z

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

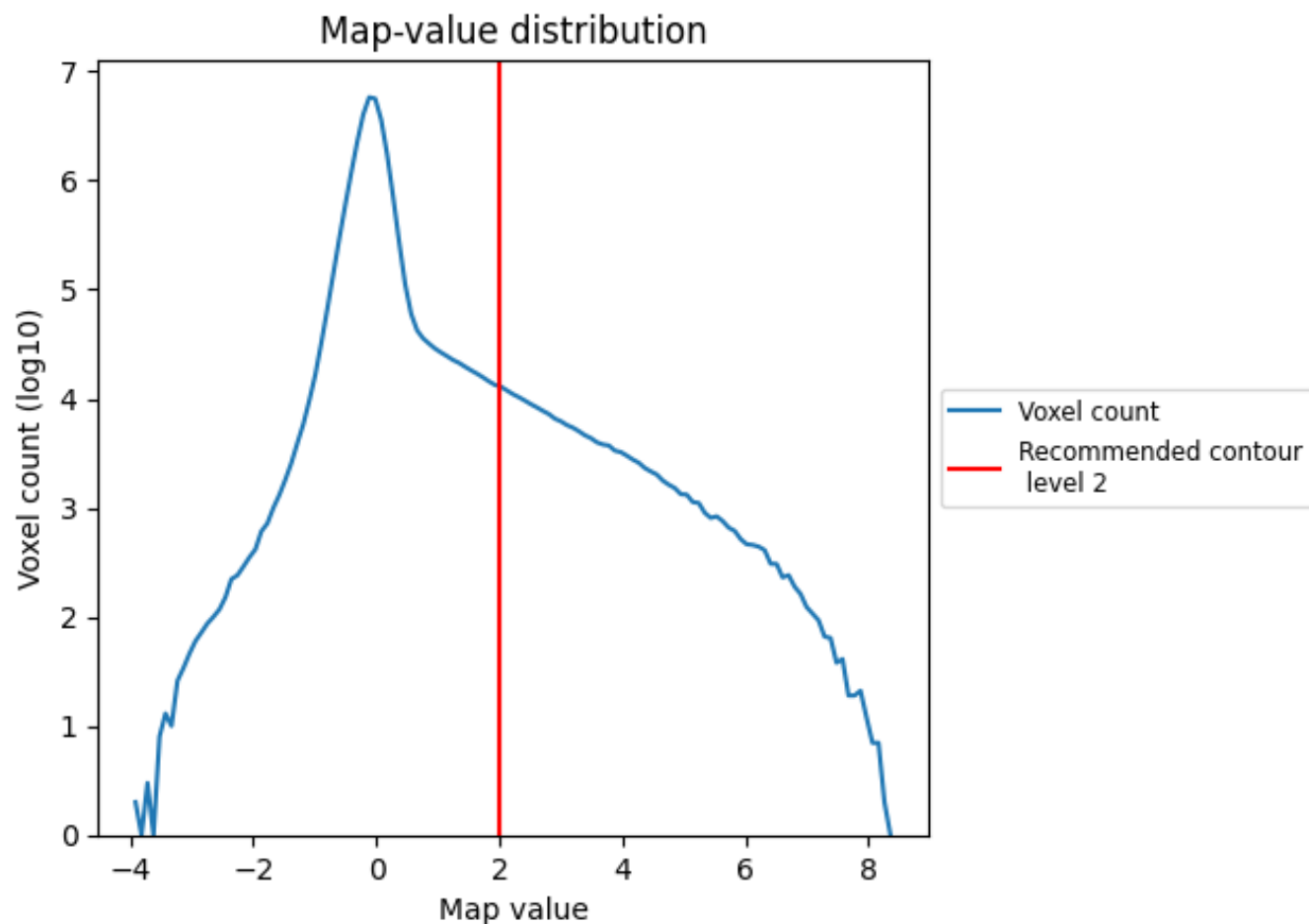
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

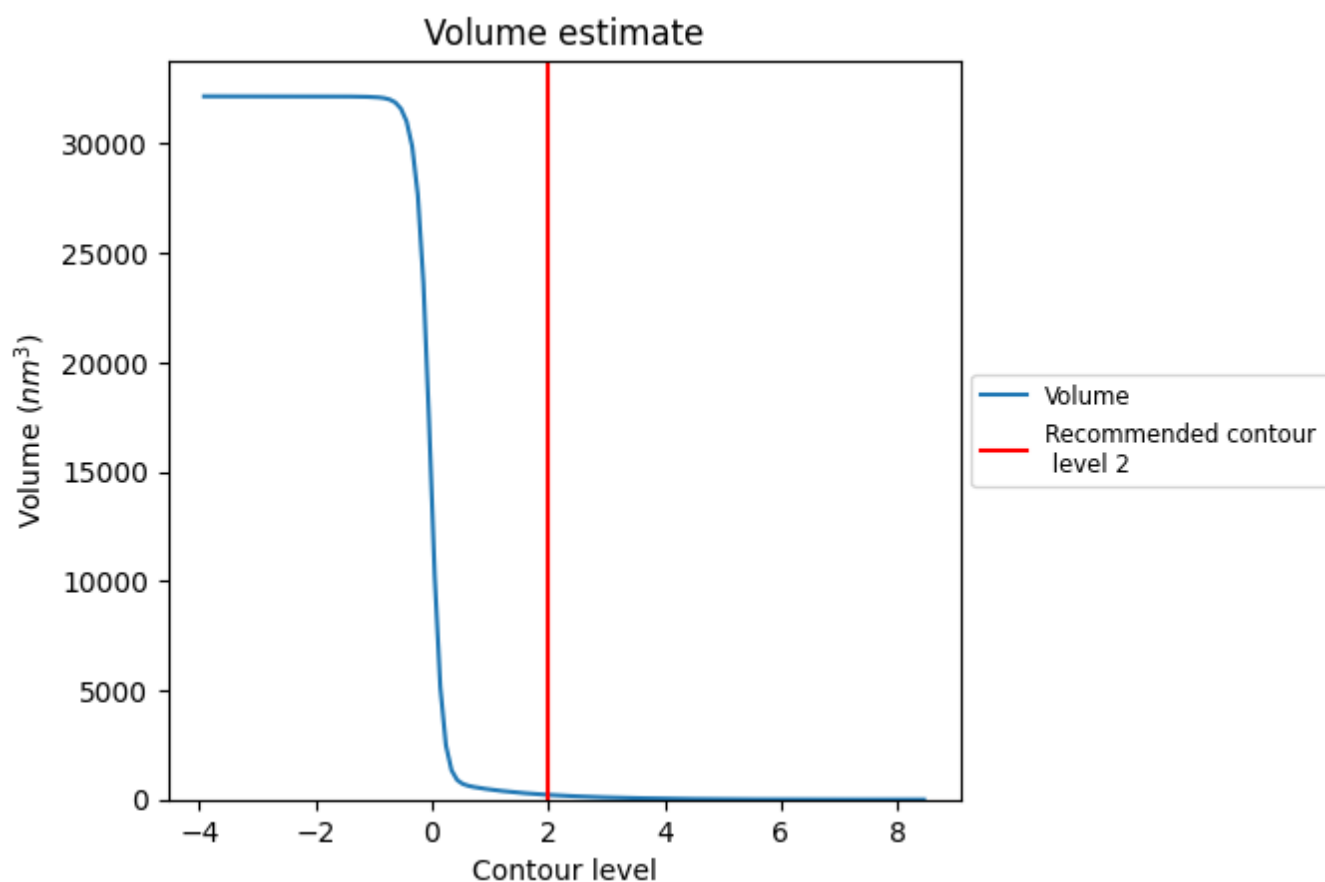
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

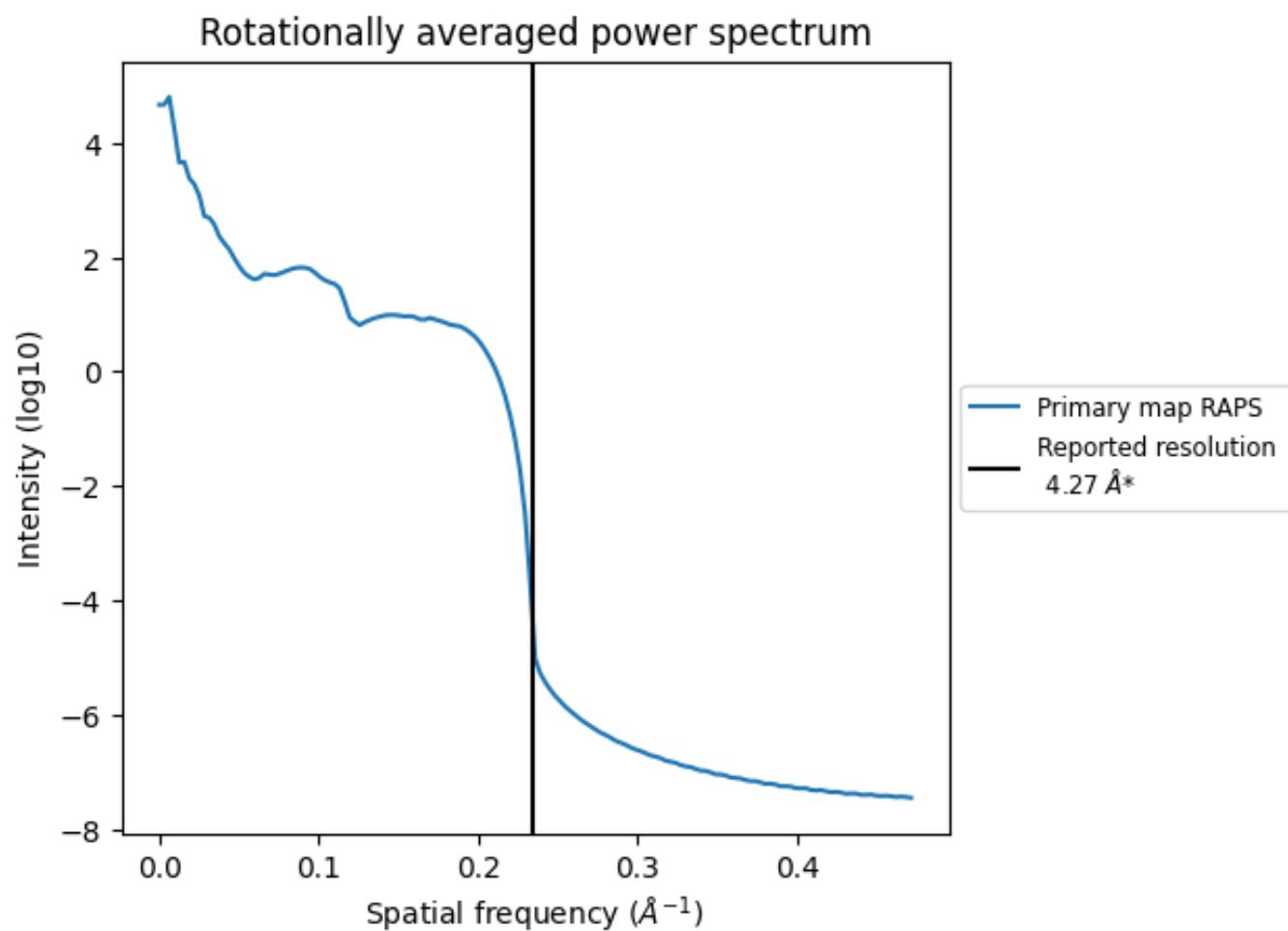
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm^3 ; this corresponds to an approximate mass of 195 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 0.234 Å⁻¹

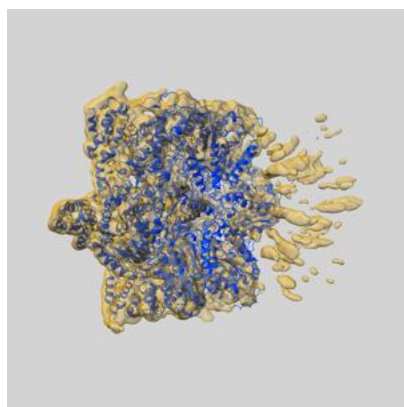
8 Fourier-Shell correlation

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

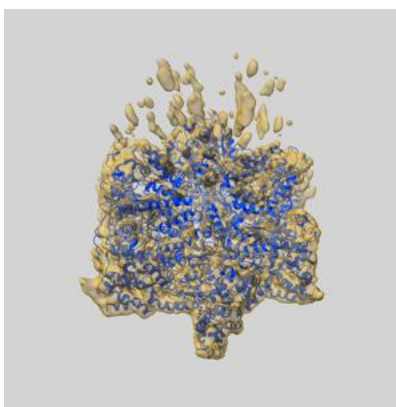
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9871 and PDB model 6JPU. Per-residue inclusion information can be found in section [3](#) on page [6](#).

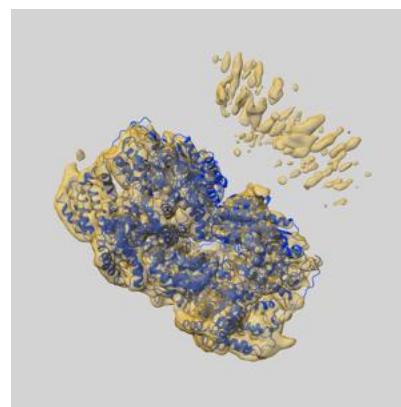
9.1 Map-model overlay [i](#)



X



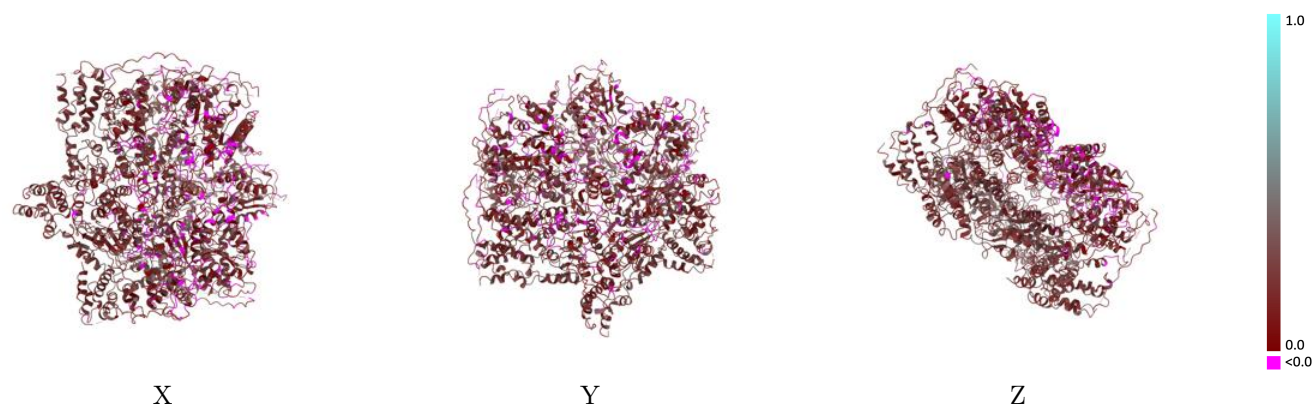
Y



Z

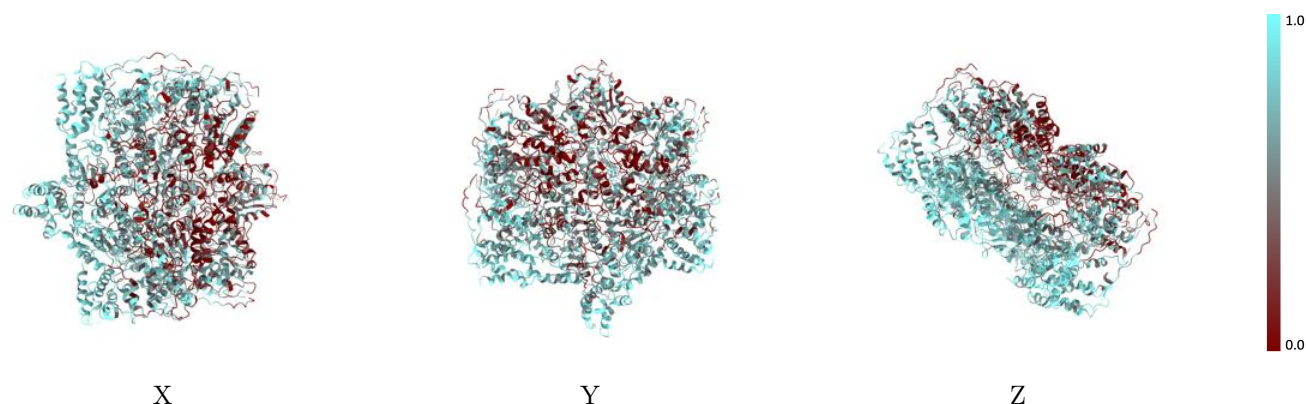
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



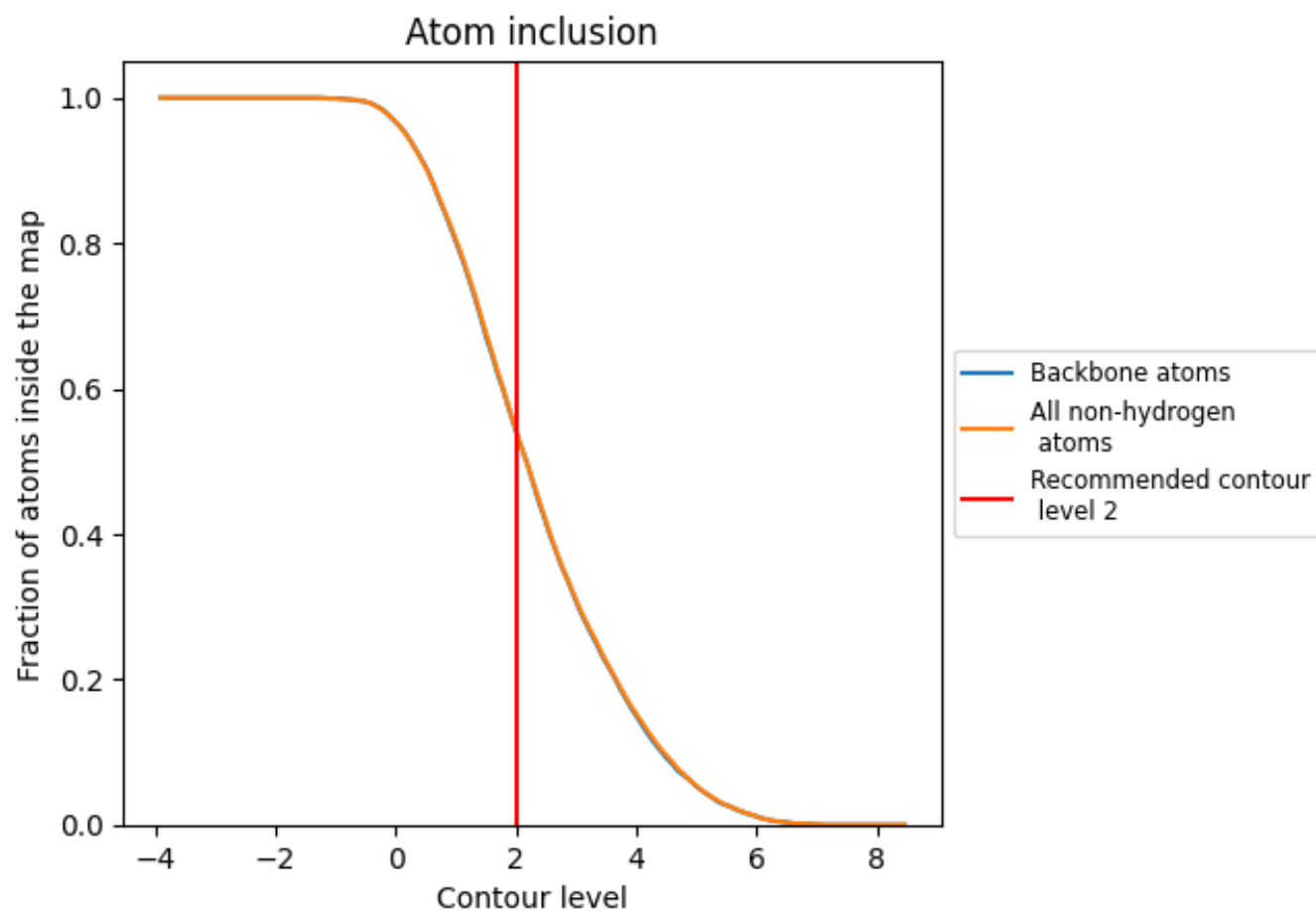
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5410	0.1810
A	0.5670	0.1860
B	0.5160	0.1740
C	0.5450	0.1850
D	0.5650	0.1800
E	0.5280	0.1800
F	0.5740	0.1830

1.0

0.0

<0.0