



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 05:08 AM UTC

PDB ID : 6YG8 / pdb_00006yg8
EMDB ID : EMD-10799
Title : Cryo-EM structure of a BcsB pentamer in the context of an assembled Bcs macrocomplex
Authors : Zouhir, S.; Krasteva, P.V.
Deposited on : 2020-03-27
Resolution : 3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

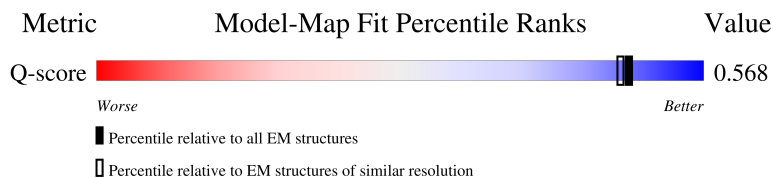
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	779	 66% 16% 17%
1	B	779	 67% 15% 18%
1	C	779	 69% 13% 18%
1	D	779	 68% 14% 18%

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Mol	Chain	Length	Quality of chain
1	E	779	59%15%26%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24330 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.

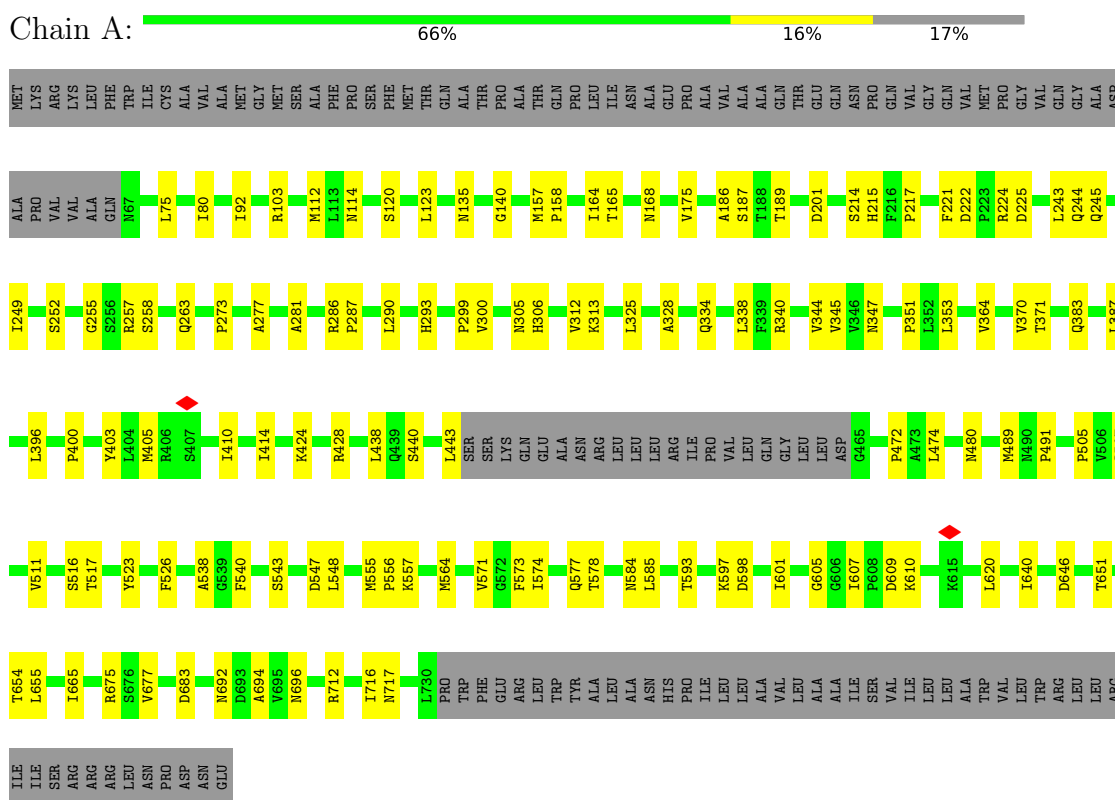
- Molecule 1 is a protein called Bacterial cellulose secretion regulator BcsB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	643	Total	C	N	O	S	0	0
			4996	3169	853	950	24		
1	B	637	Total	C	N	O	S	0	0
			4944	3136	842	943	23		
1	C	637	Total	C	N	O	S	0	0
			4944	3136	842	943	23		
1	D	639	Total	C	N	O	S	0	0
			4960	3146	844	947	23		
1	E	576	Total	C	N	O	S	0	0
			4486	2855	763	846	22		

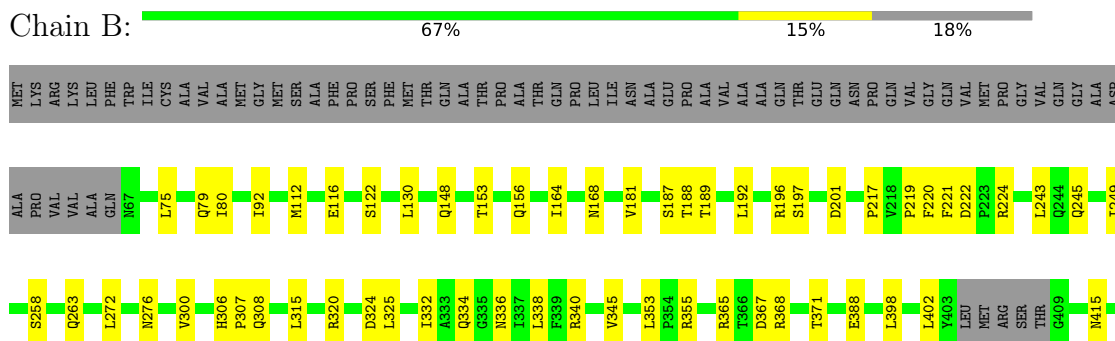
3 Residue-property plots

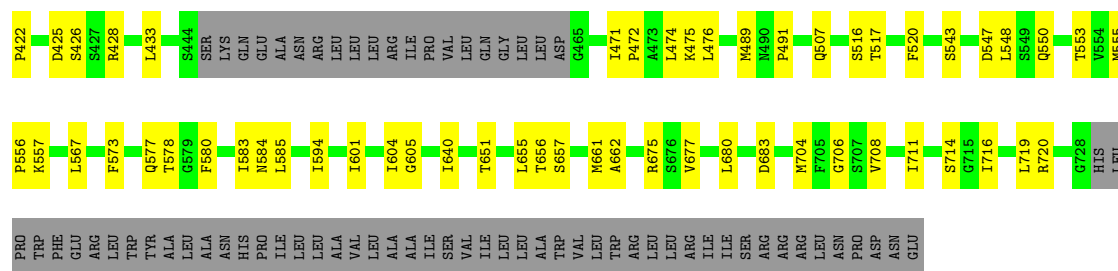
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Bacterial cellulose secretion regulator BcsB



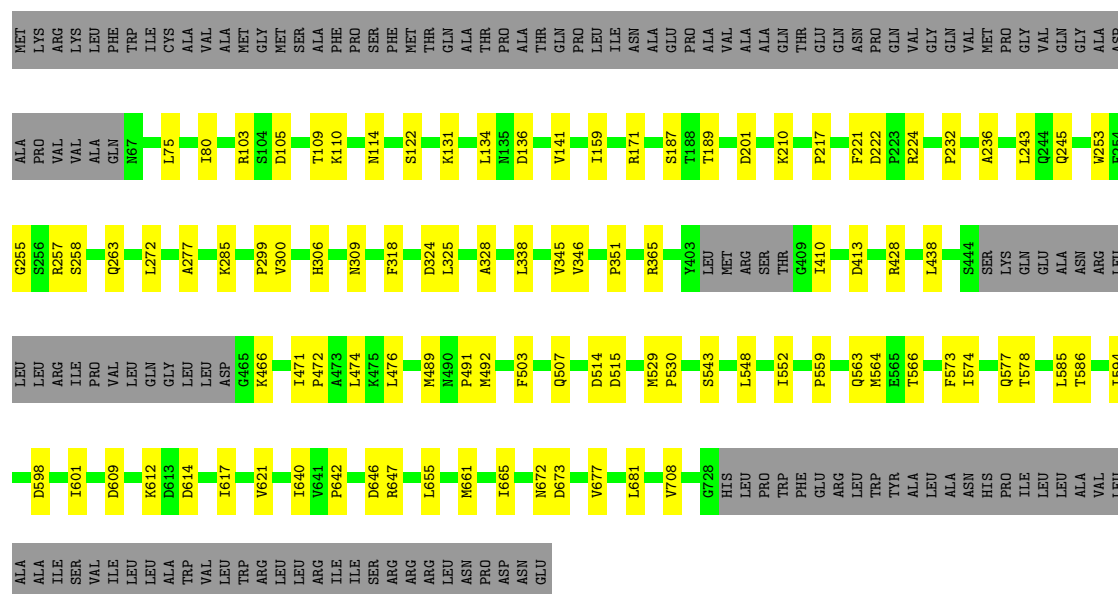
- Molecule 1: Bacterial cellulose secretion regulator BcsB





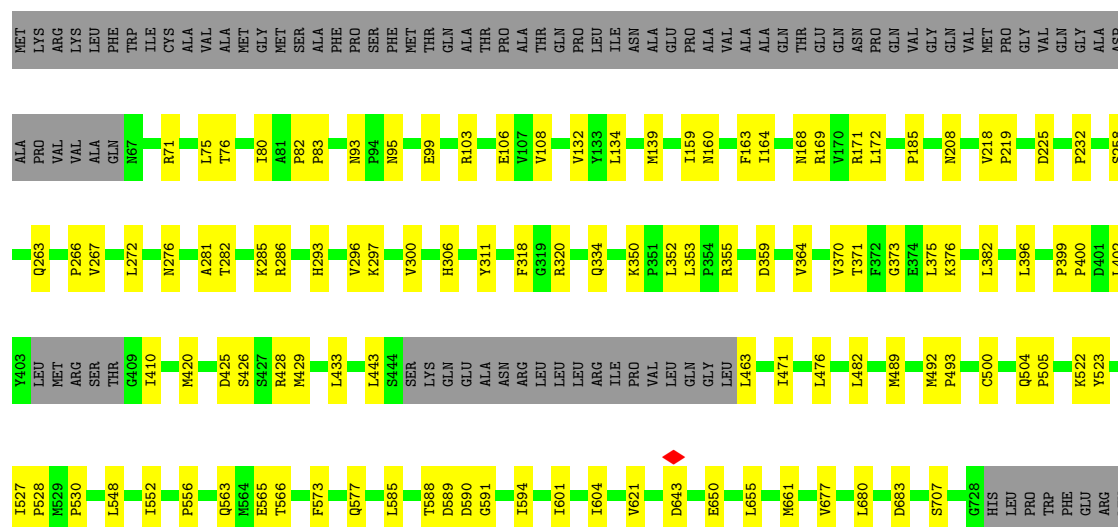
- Molecule 1: Bacterial cellulose secretion regulator BcsB

Chain C: 69% 13% 18%



- Molecule 1: Bacterial cellulose secretion regulator BcsB

Chain D: 68% 14% 18%



TRP
TYR
ALA
LEU
ALA
ASN
HIS
PRO
ILE
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LEU
ALA
VAL
VAL
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ALA
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SER
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TRP
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LEU
ARG
ILE
ILE
SER
ARG
ARG
LEU
ASN
PRO
ASP
ASN
GLU

- Molecule 1: Bacterial cellulose secretion regulator BcsB

Chain E: 59%15%26%

MET
LYS
ARG
LYS
LEU
ALA
PHE
TRP
ILE
CYS
ALA
VAL
VAL
ALA
MET
GLY
MET
SER
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MET
PRO
GLY
VAL
GLN
GLY
ALA
ASP

ALA
PRO
VAL
VAL
GLN
367
F77
A78
Q79
T80
A81
P82
P83
P84
S85
S86
S87
T98
S104
L115
T118
P119
S120
P121
S122
L123
L130
F167
N168
R169
L172
Y178
E183
N184
S187
T188
T189
L190
V191
L192
D193
R196
K210
N211
D212
L213

F220
R224
M233
P239
D240
L243
Q244
Q245
I249
S252
S258
Q263
N264
L272
P273
D274
R286
S120
H293
S122
K303
H306
L315
L325
I332
N336
R340
V344
R365
T371
Y403
LEU
ARG
SER
THR
I410
Y523

D413
I414
Y418
K424
D430
L438
L443
SER
LYS
GLN
GLU
ALA
ASN
ARG
LEU
LEU
LEU
ARG
ILE
PRO
VAL
GLN
GLY
N480
D485
N492
S496
V497
D498
N499
F503
Q507
S516
T517
I410
Y523

F526
F535
A536
A538
G539
M545
L548
S549
Q550
M555
P556
P559
M564
L568
N569
T570
V571
F572
F573
I574
Q577
T578
L585
I601
L604
G605
ILE
PRO
ASP
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Q668
R675
S676
V677
L678
A679
D683
S684
F705
V708
A709
V710
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	576455	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Gctf through the cryoSPARC v2 interface.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	55.833	Depositor
Minimum map value	-31.929	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.989	Depositor
Recommended contour level	4.5	Depositor
Map size ($\text{\AA}$)	431.51678, 431.51678, 431.51678	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05248, 1.05248, 1.05248	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	0.23	0/5111	0.35	0/6958
1	B	0.22	0/5057	0.34	0/6884
1	C	0.21	0/5057	0.34	0/6884
1	D	0.18	0/5073	0.36	0/6906
1	E	0.18	0/4590	0.35	0/6247
All	All	0.20	0/24888	0.35	0/33879

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	4996	0	4951	86	0
1	B	4944	0	4892	81	0
1	C	4944	0	4892	60	0
1	D	4960	0	4907	69	0
1	E	4486	0	4431	70	0
All	All	24330	0	24073	338	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 338 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:D:426:SER:HB3	1:D:489:MET:HB3	1.66	0.77
1:D:420:MET:HB2	1:D:463:LEU:HD13	1.67	0.75
1:C:428:ARG:NH2	1:E:507:GLN:O	2.20	0.74
1:A:300:VAL:HG12	1:A:345:VAL:HG22	1.72	0.72
1:E:258:SER:O	1:E:263:GLN:NE2	2.23	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	639/779 (82%)	612 (96%)	27 (4%)	0	100	100
1	B	631/779 (81%)	606 (96%)	25 (4%)	0	100	100
1	C	631/779 (81%)	610 (97%)	21 (3%)	0	100	100
1	D	633/779 (81%)	599 (95%)	34 (5%)	0	100	100
1	E	566/779 (73%)	527 (93%)	39 (7%)	0	100	100
All	All	3100/3895 (80%)	2954 (95%)	146 (5%)	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	557/669 (83%)	557 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	551/669 (82%)	551 (100%)	0	100	100
1	C	551/669 (82%)	551 (100%)	0	100	100
1	D	553/669 (83%)	553 (100%)	0	100	100
1	E	499/669 (75%)	499 (100%)	0	100	100
All	All	2711/3345 (81%)	2711 (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 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	509	HIS
1	E	508	ASN
1	D	622	GLN
1	E	334	GLN
1	B	442	ASN

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 ⓘ

There are no chain breaks in this entry.

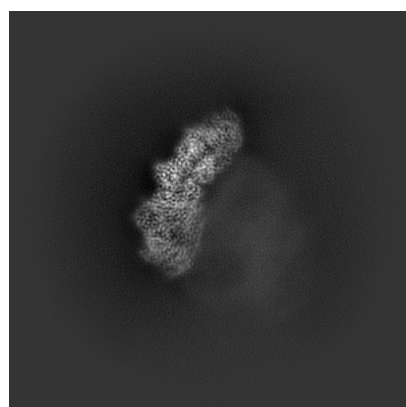
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10799. These allow visual inspection of the internal detail of the map and identification of artifacts.

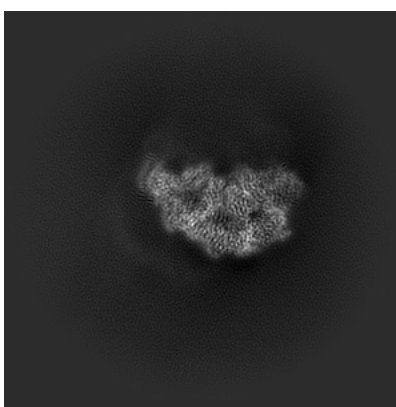
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

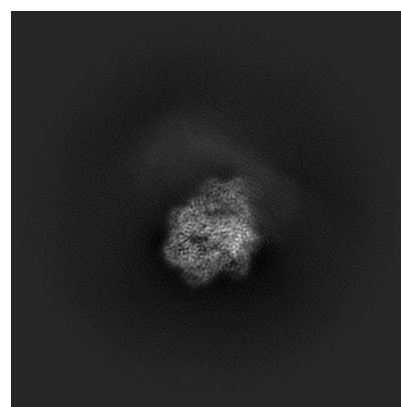
6.1.1 Primary map



X



Y

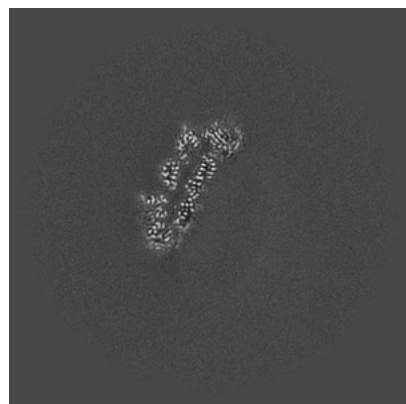


Z

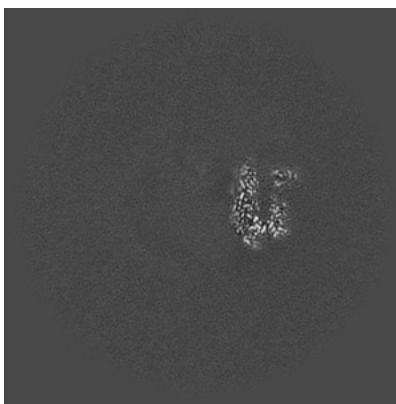
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

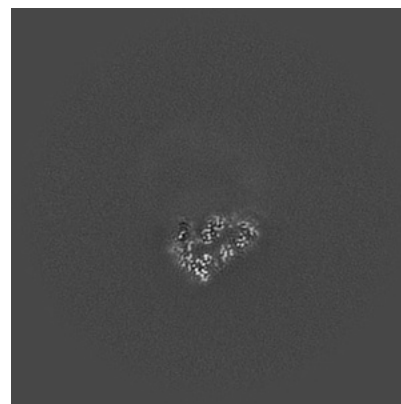
6.2.1 Primary map



X Index: 205



Y Index: 205

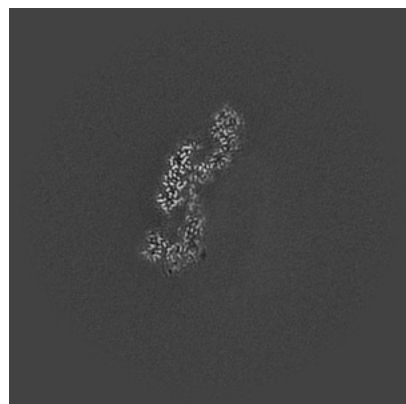


Z Index: 205

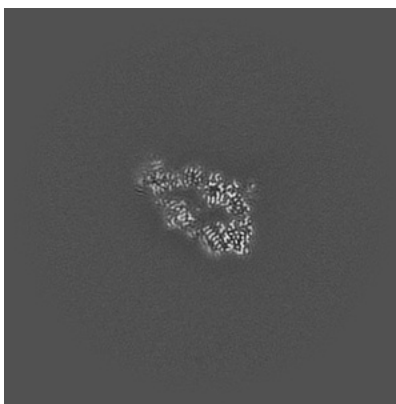
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

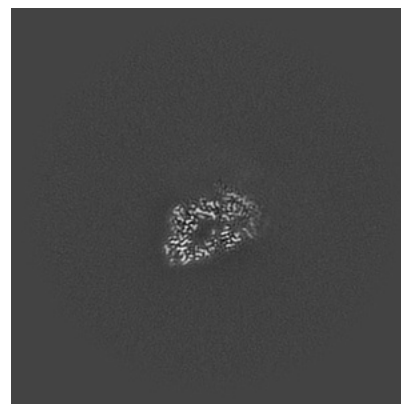
6.3.1 Primary map



X Index: 224



Y Index: 162

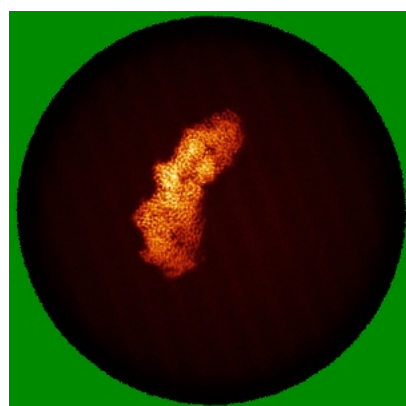


Z Index: 249

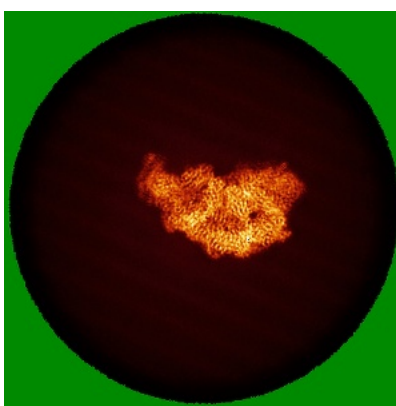
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

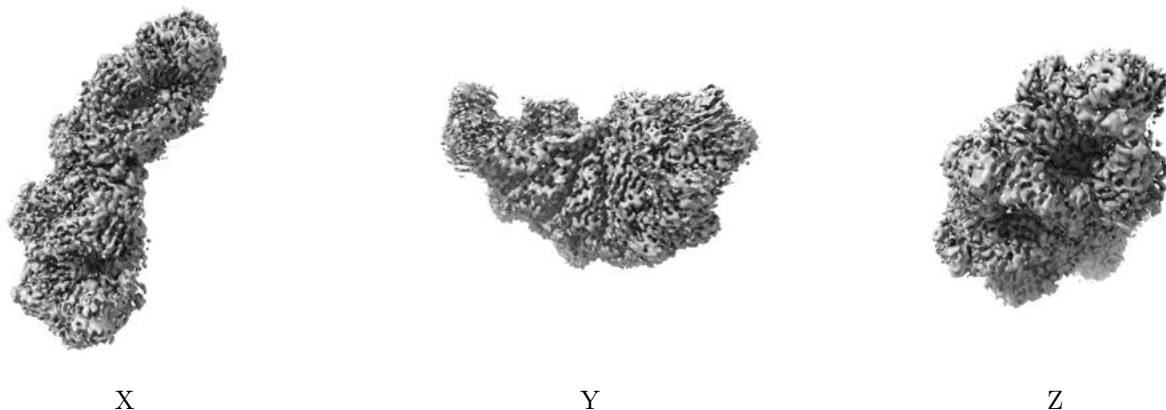


Z

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

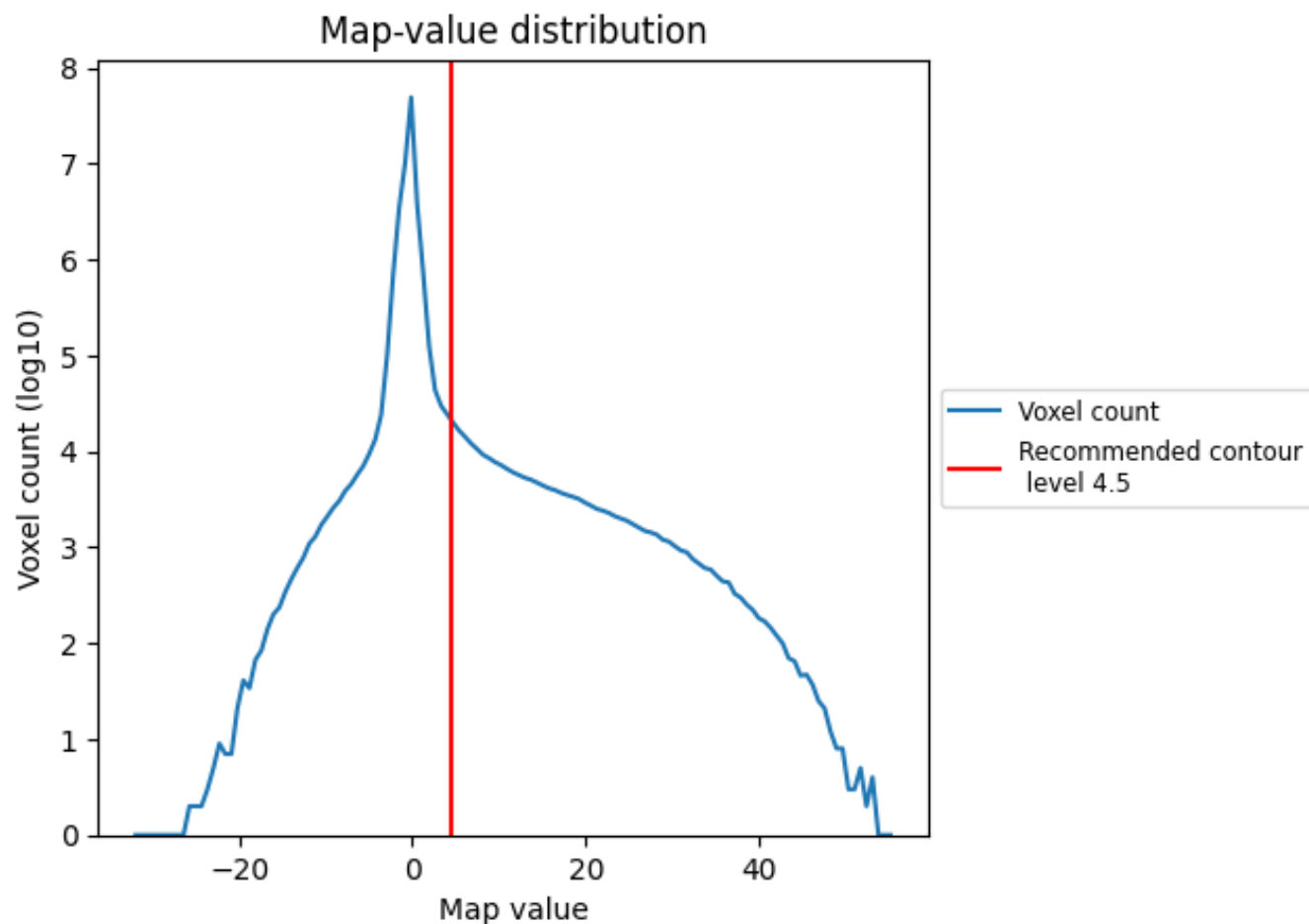
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

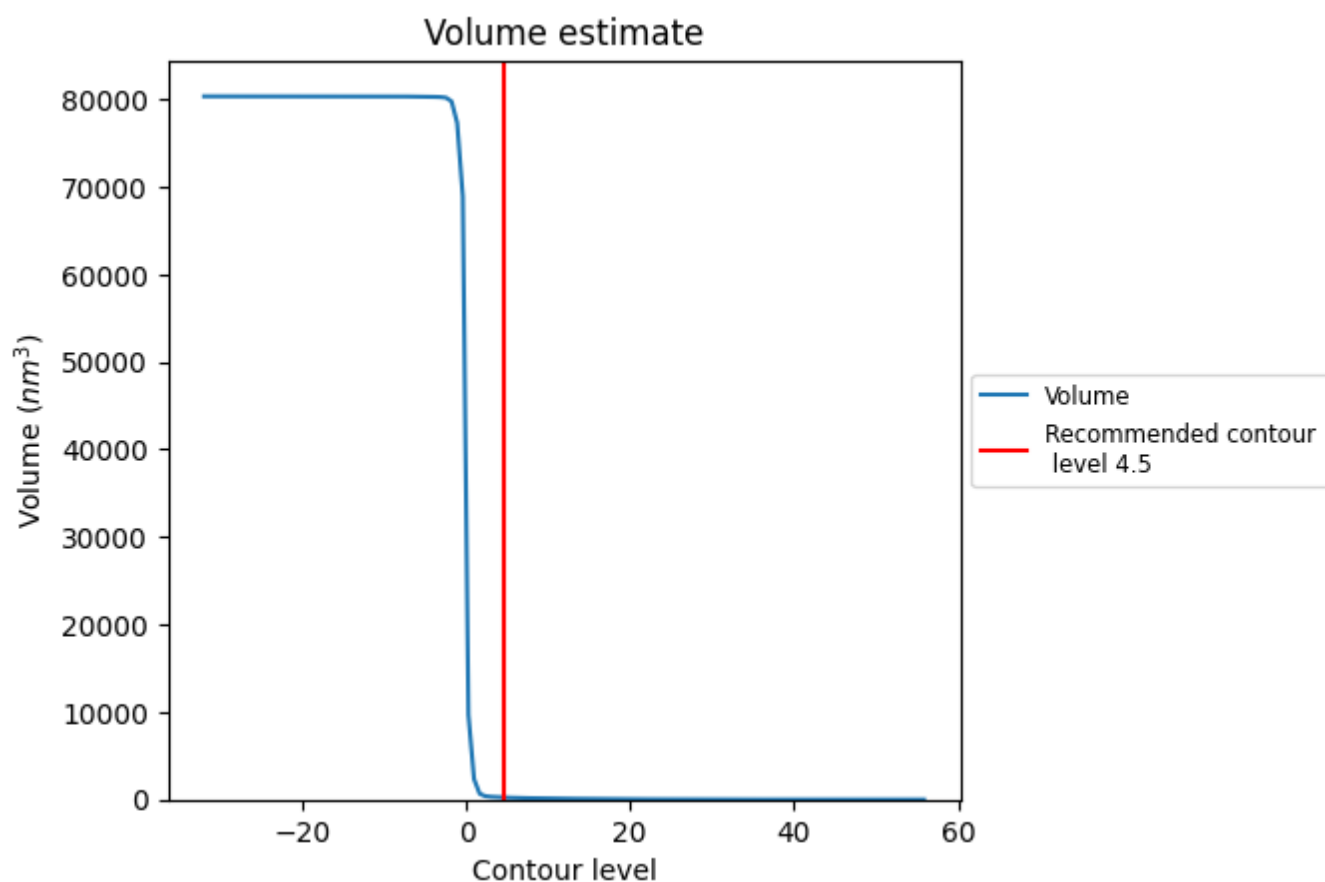
This section contains the results of statistical analysis of the map.

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.

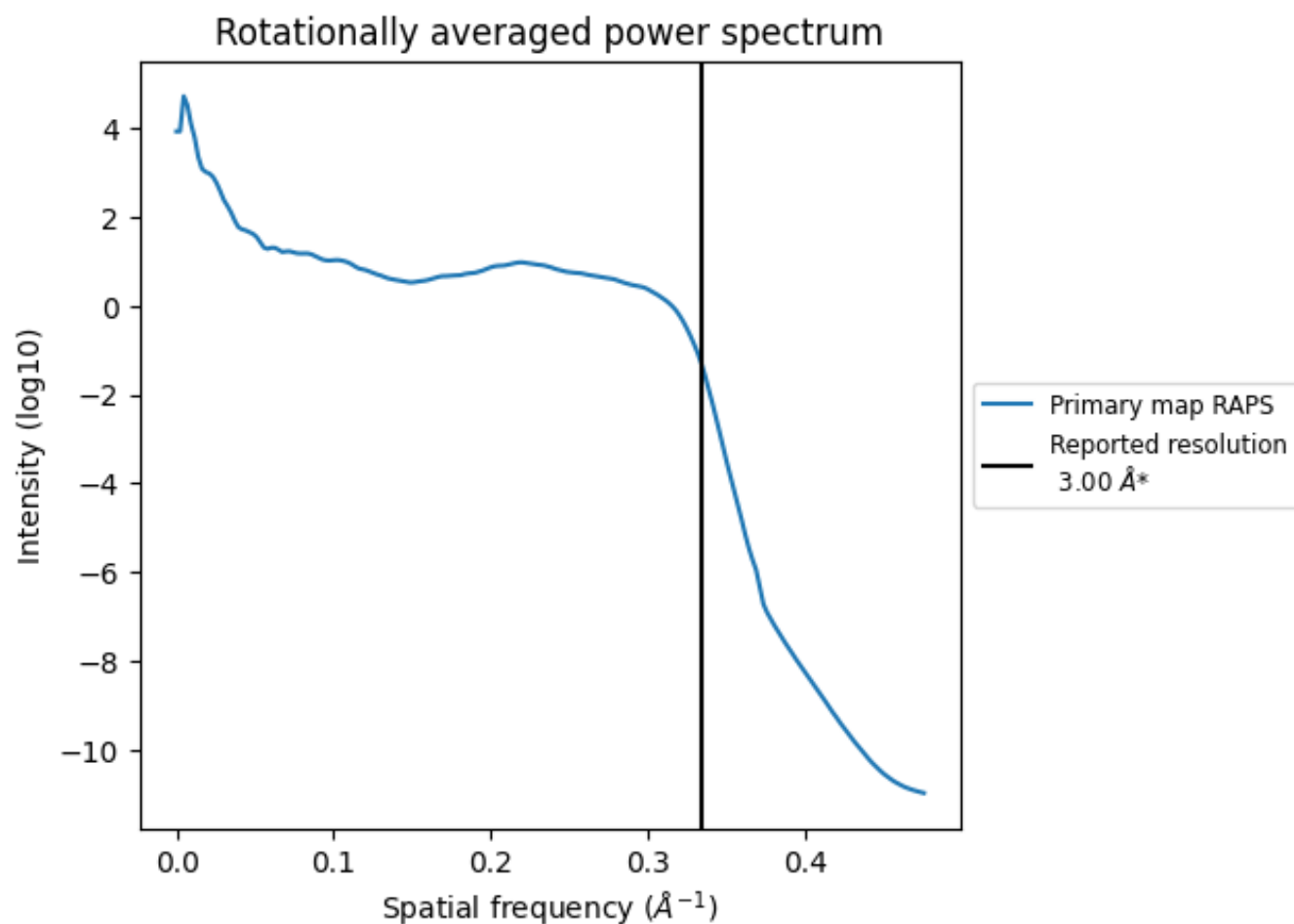
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 245 nm³; this corresponds to an approximate mass of 222 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 0.333 Å⁻¹

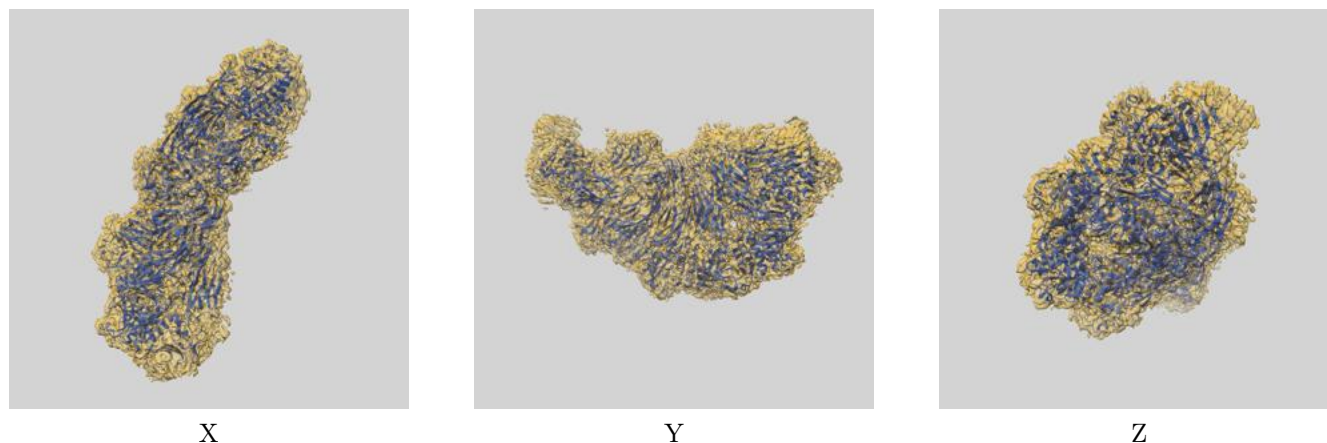
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

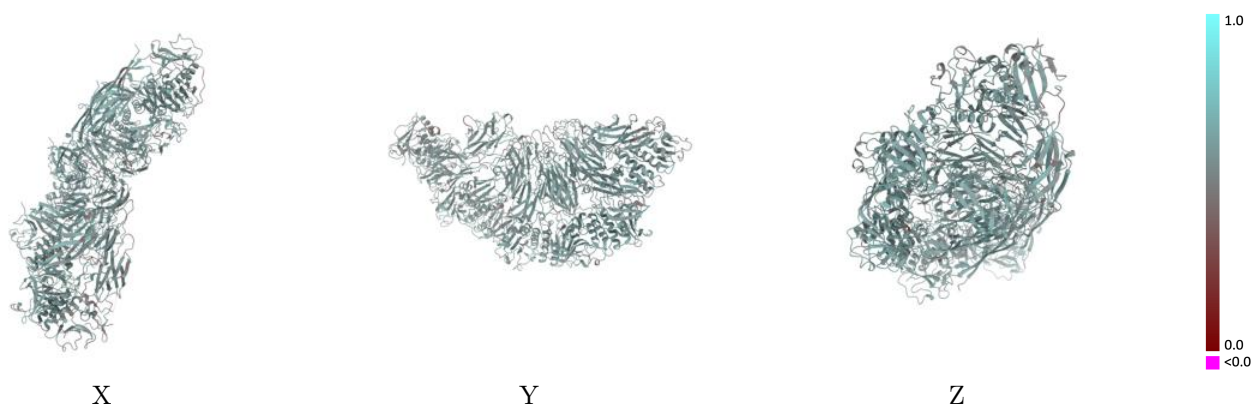
This section contains information regarding the fit between EMDB map EMD-10799 and PDB model 6YG8. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 4.5 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](#)



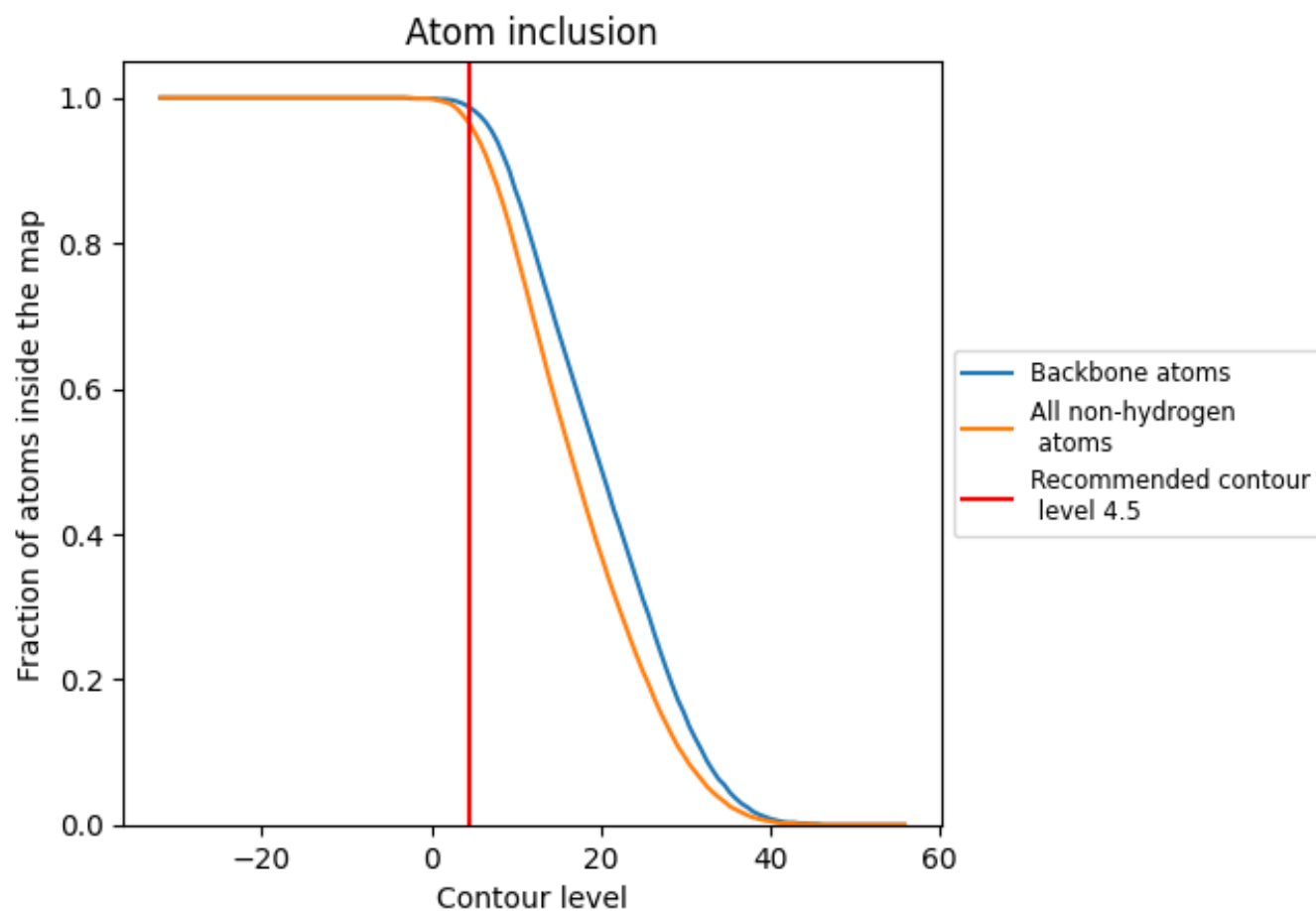
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9650	0.5680
A	0.9690	0.5800
B	0.9740	0.5800
C	0.9720	0.5730
D	0.9490	0.5580
E	0.9590	0.5450

