wwPDB EM Validation Summary Report

Nov 11, 2026 – 02:25 PM EST

PDB ID	:	38BZ / pdb_000038bz
EMDB ID	:	EMD-78711
Title	:	Pseudomonas phage DEV gp71 vRNAP: Isolated RNAP Domain
Authors	:	Bellis, N.F.; Lokareddy, R.K.; Cingolani, G.
Deposited on	:	2026-08-19
Resolution	:	2.60 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:

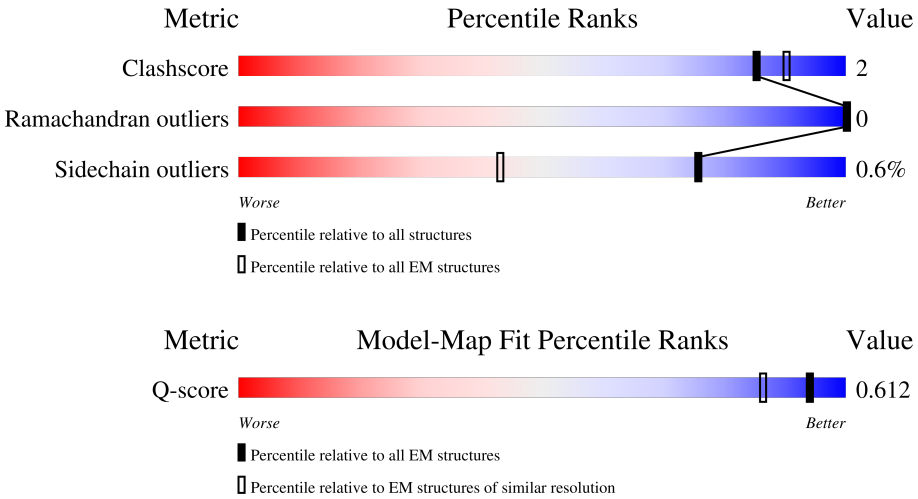
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.60 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	8728 (2.10 - 3.10)

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	3419	30% · 68%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8236 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 N4 gp50-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1080	8236	5137	1435	1634	30	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP X5KNB4
A	-19	GLY	-	expression tag	UNP X5KNB4
A	-18	HIS	-	expression tag	UNP X5KNB4
A	-17	HIS	-	expression tag	UNP X5KNB4
A	-16	HIS	-	expression tag	UNP X5KNB4
A	-15	HIS	-	expression tag	UNP X5KNB4
A	-14	HIS	-	expression tag	UNP X5KNB4
A	-13	HIS	-	expression tag	UNP X5KNB4
A	-12	HIS	-	expression tag	UNP X5KNB4
A	-11	HIS	-	expression tag	UNP X5KNB4
A	-10	HIS	-	expression tag	UNP X5KNB4
A	-9	HIS	-	expression tag	UNP X5KNB4
A	-8	SER	-	expression tag	UNP X5KNB4
A	-7	SER	-	expression tag	UNP X5KNB4
A	-6	GLY	-	expression tag	UNP X5KNB4
A	-5	HIS	-	expression tag	UNP X5KNB4
A	-4	ILE	-	expression tag	UNP X5KNB4
A	-3	GLU	-	expression tag	UNP X5KNB4
A	-2	GLY	-	expression tag	UNP X5KNB4
A	-1	ARG	-	expression tag	UNP X5KNB4
A	0	HIS	-	expression tag	UNP X5KNB4
A	2410	HIS	ARG	conflict	UNP X5KNB4

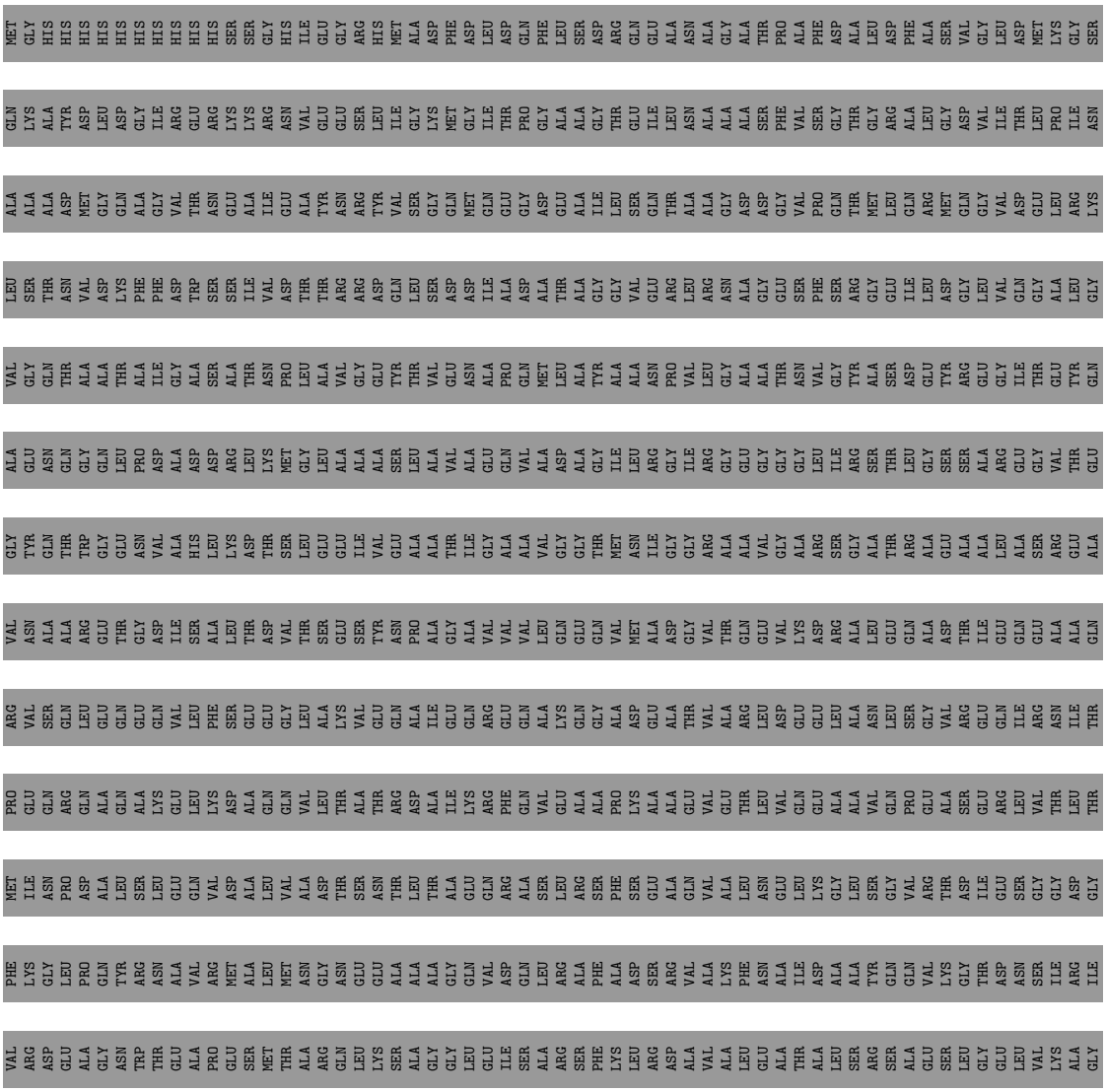
3 Residue-property plots (i)

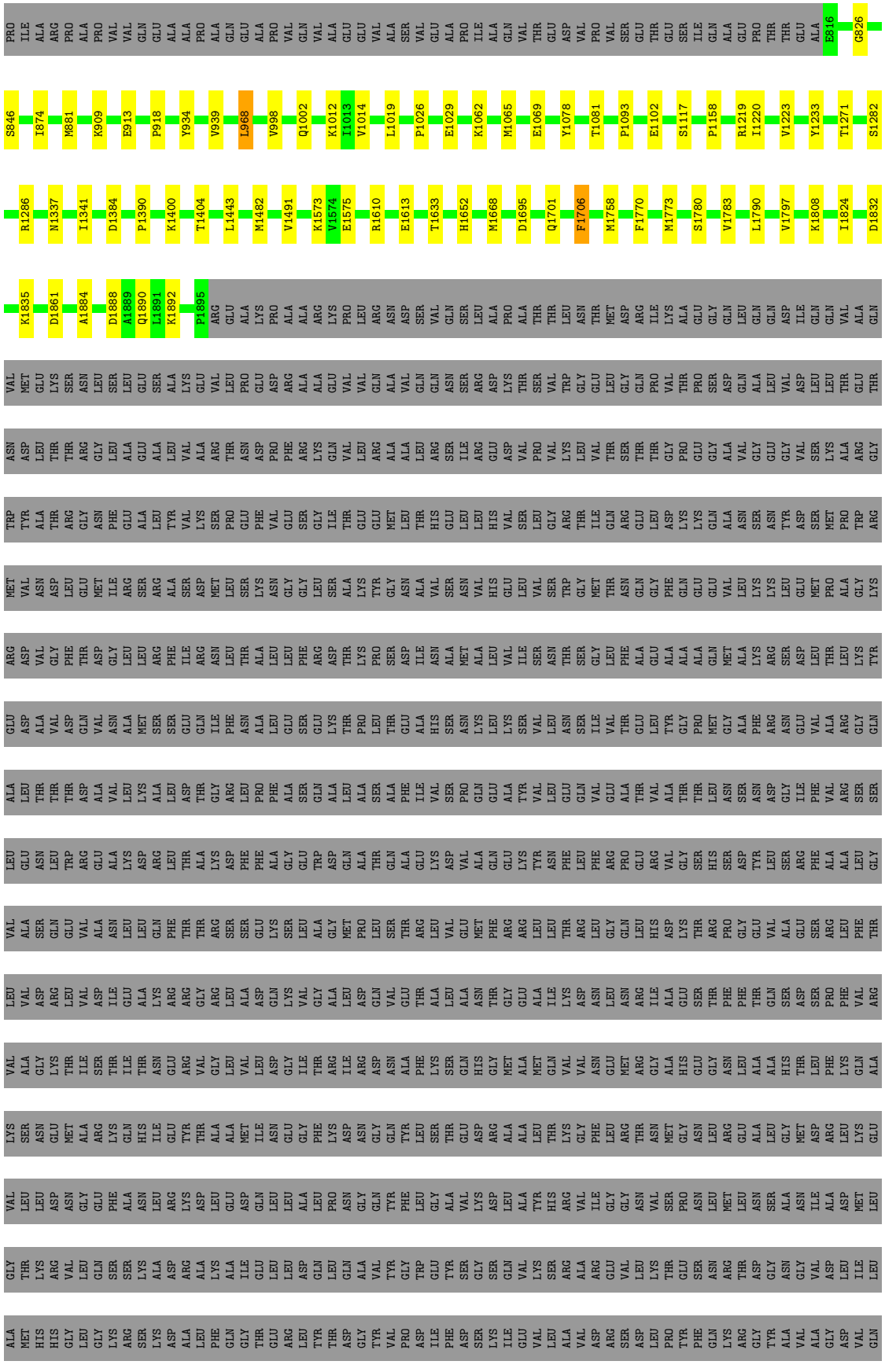
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

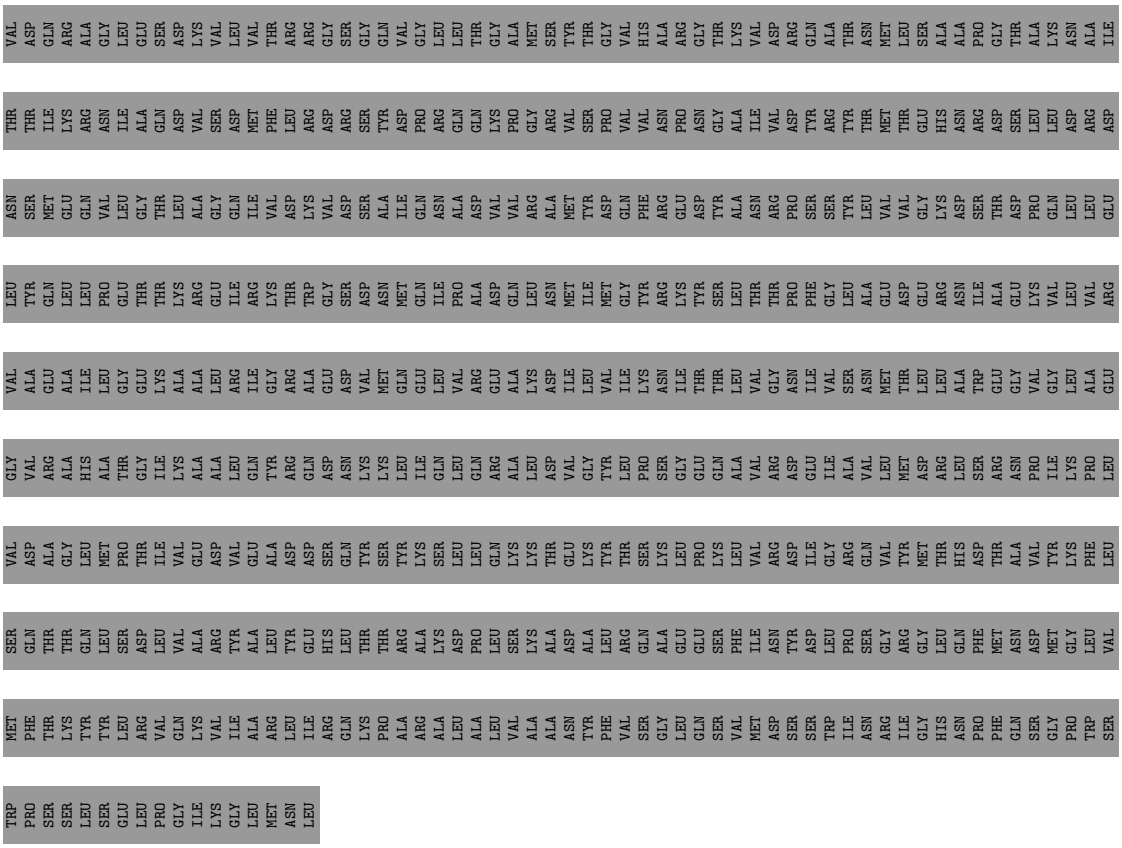
- Molecule 1: N4 gp50-like protein

Chain A:






S846 I874 M881 K909 E913 P918 Y934 V939 L968 V998 Q1002 K1012 I1013 V1014 L1019 P1026 E1029 K1062 M1065 E1069 Y1078 T1081 P1093 E1102 S1117 P1158 R1219 I1220 V1223 Y1233 T1271 S1282
R1286 N1337 I1341 D1384 P1390 K1400 T1404 L1443 M1482 V1491 K1573 V1574 E1575 R1610 E1613 T1633 H1652 M1668 D1695 Q1701 F1706 M1758 F1770 M1773 S1780 V1783 L1790 V1797 K1808 I1824 D1832
K1835 D1861 A1884 D1888 A1889 Q1890 L1891 K1892 P1895
E816 G826


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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	244430	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52.64	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.757	Depositor
Minimum map value	-0.376	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0365	Depositor
Map size (Å)	370.496, 370.496, 370.496	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	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	0.10	0/8366	0.25	0/11318

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	8236	0	8139	36	0
All	All	8236	0	8139	36	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 2.

The worst 5 of 36 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:1102:GLU:O	1:A:1219:ARG:NH1	2.33	0.59
1:A:1668:MET:HA	1:A:1668:MET:HE2	1.87	0.56
1:A:1002:GLN:HG2	1:A:1078:TYR:HB2	1.90	0.54
1:A:1491:VAL:HG21	1:A:1575:GLU:HB2	1.89	0.54
1:A:1773:MET:HB3	1:A:1835:LYS:HD2	1.90	0.53

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	1078/3419 (32%)	1068 (99%)	10 (1%)	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	868/2756 (32%)	863 (99%)	5 (1%)	78 91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	968	LEU
1	A	1065	MET
1	A	1271	THR
1	A	1652	HIS
1	A	1706	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1652	HIS
1	A	1728	HIS
1	A	1221	GLN
1	A	1312	ASN
1	A	1332	GLN

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.

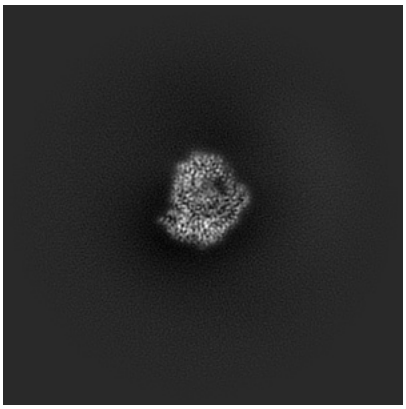
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-78711. These allow visual inspection of the internal detail of the map and identification of artifacts.

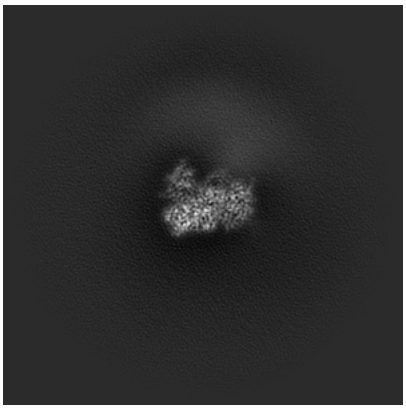
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

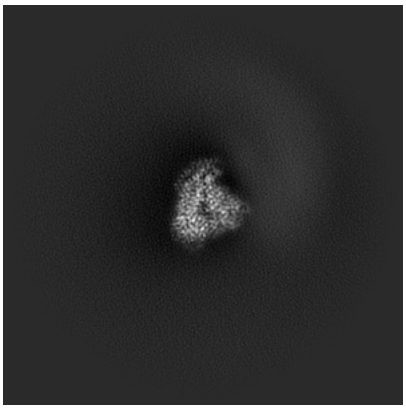
6.1.1 Primary map



X

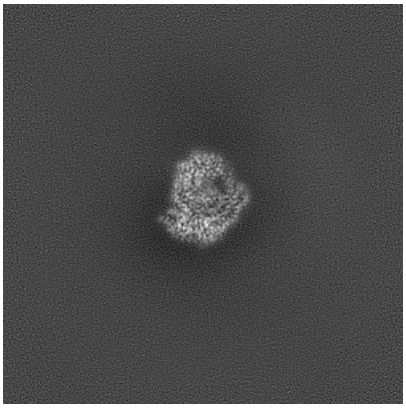


Y

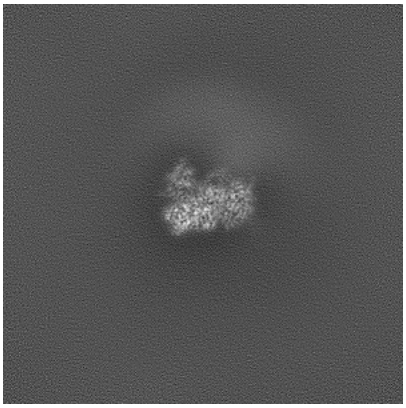


Z

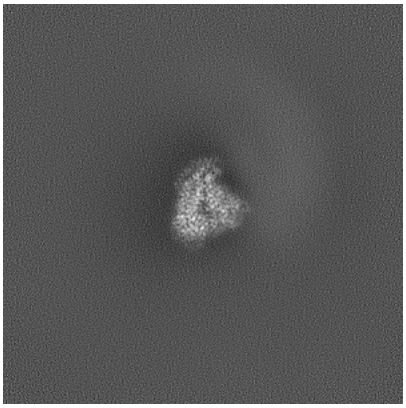
6.1.2 Raw map



X



Y

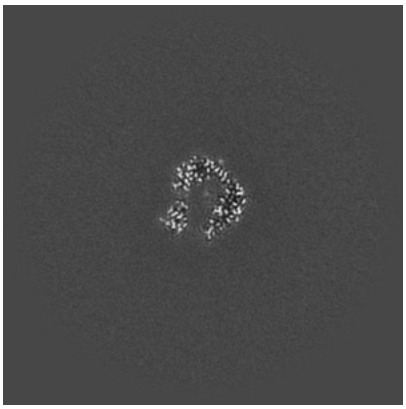


Z

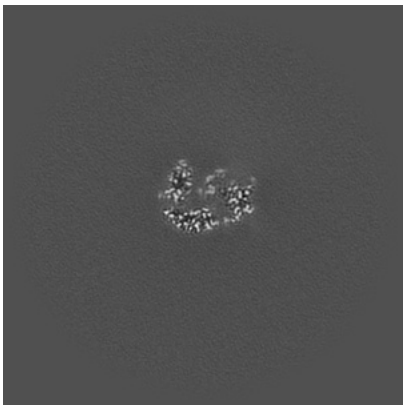
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

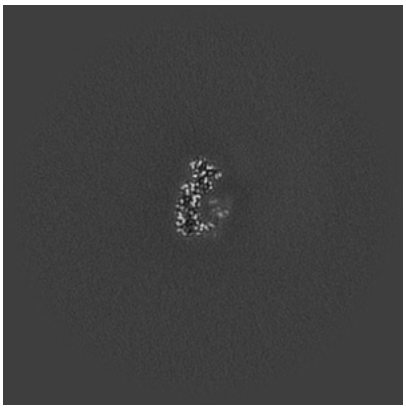
6.2.1 Primary map



X Index: 224

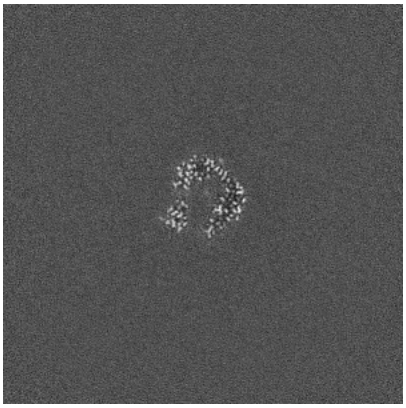


Y Index: 224

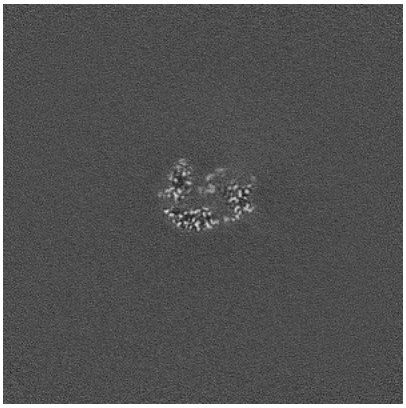


Z Index: 224

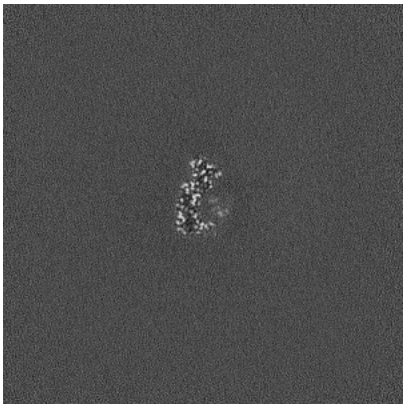
6.2.2 Raw map



X Index: 224



Y Index: 224

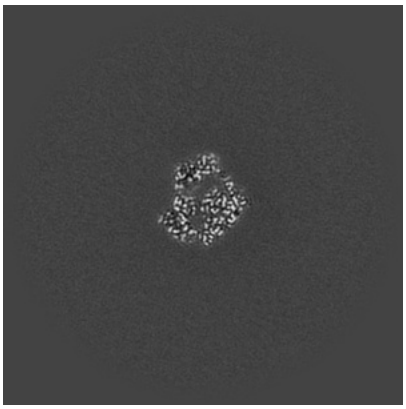


Z Index: 224

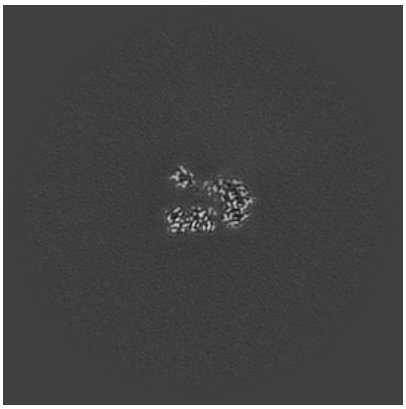
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

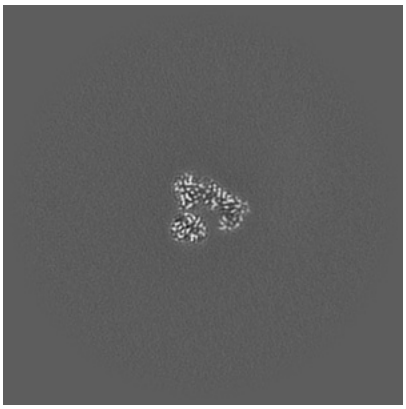
6.3.1 Primary map



X Index: 217

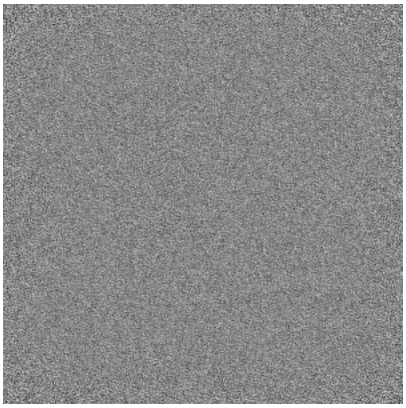


Y Index: 210

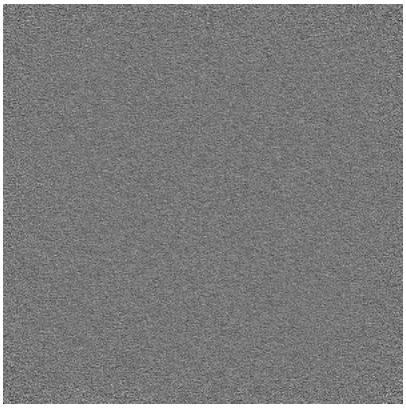


Z Index: 198

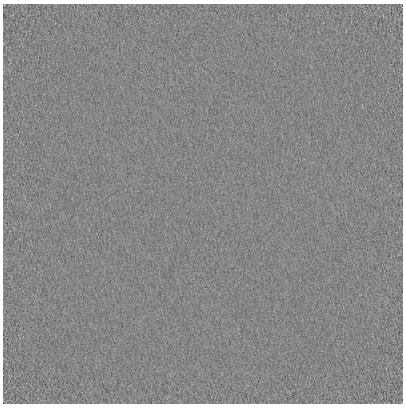
6.3.2 Raw map



X Index: 0



Y Index: 0

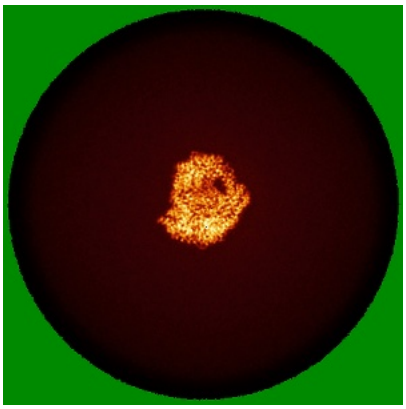


Z Index: 0

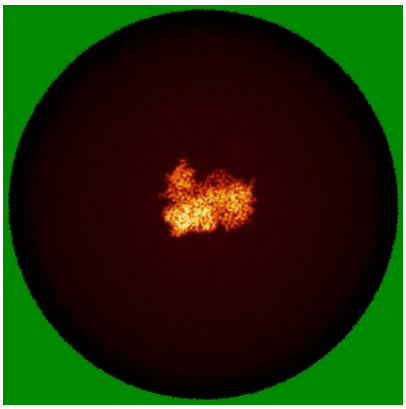
The images above show the largest variance slices of the map in three orthogonal directions.

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

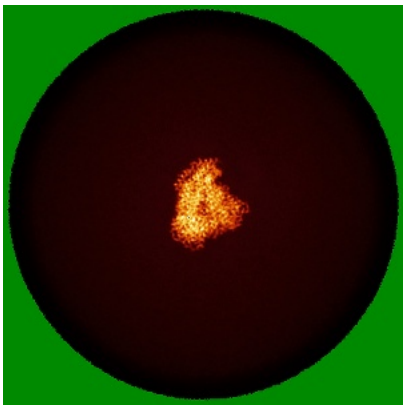
6.4.1 Primary map



X

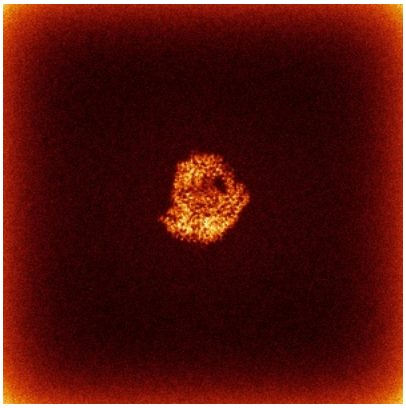


Y

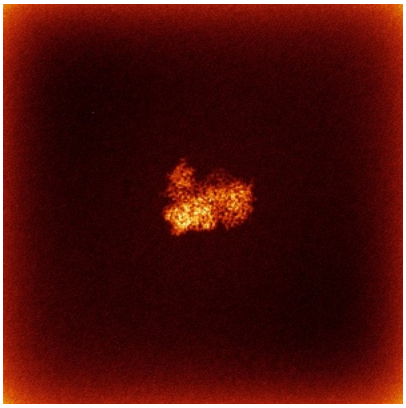


Z

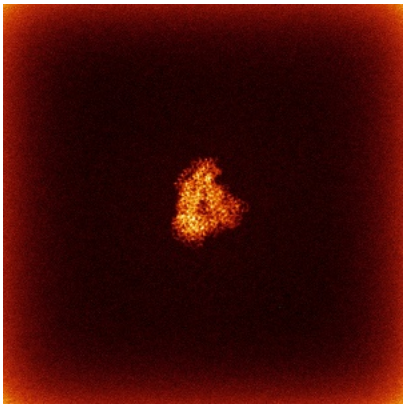
6.4.2 Raw map



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 0.0365. 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.

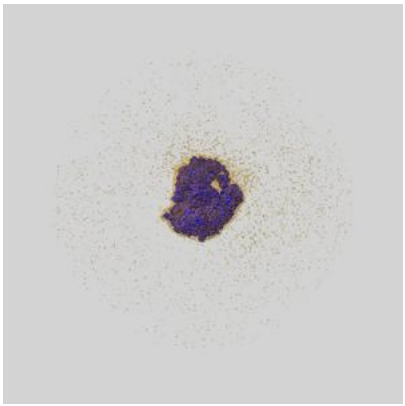
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

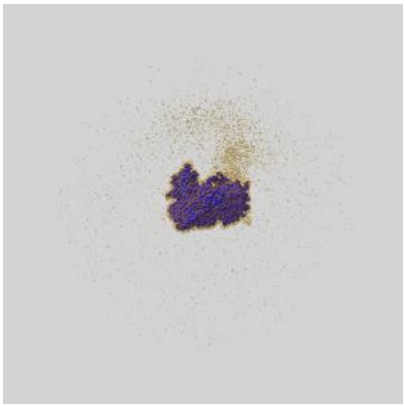
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

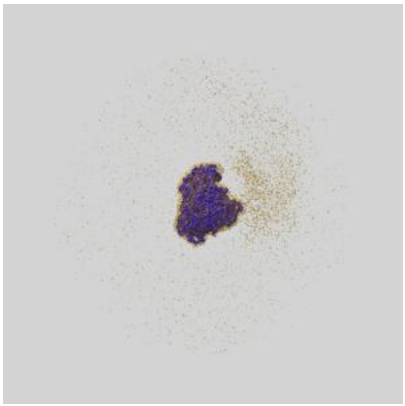
6.6.1 emd_78711_msk_1.map (i)



X



Y

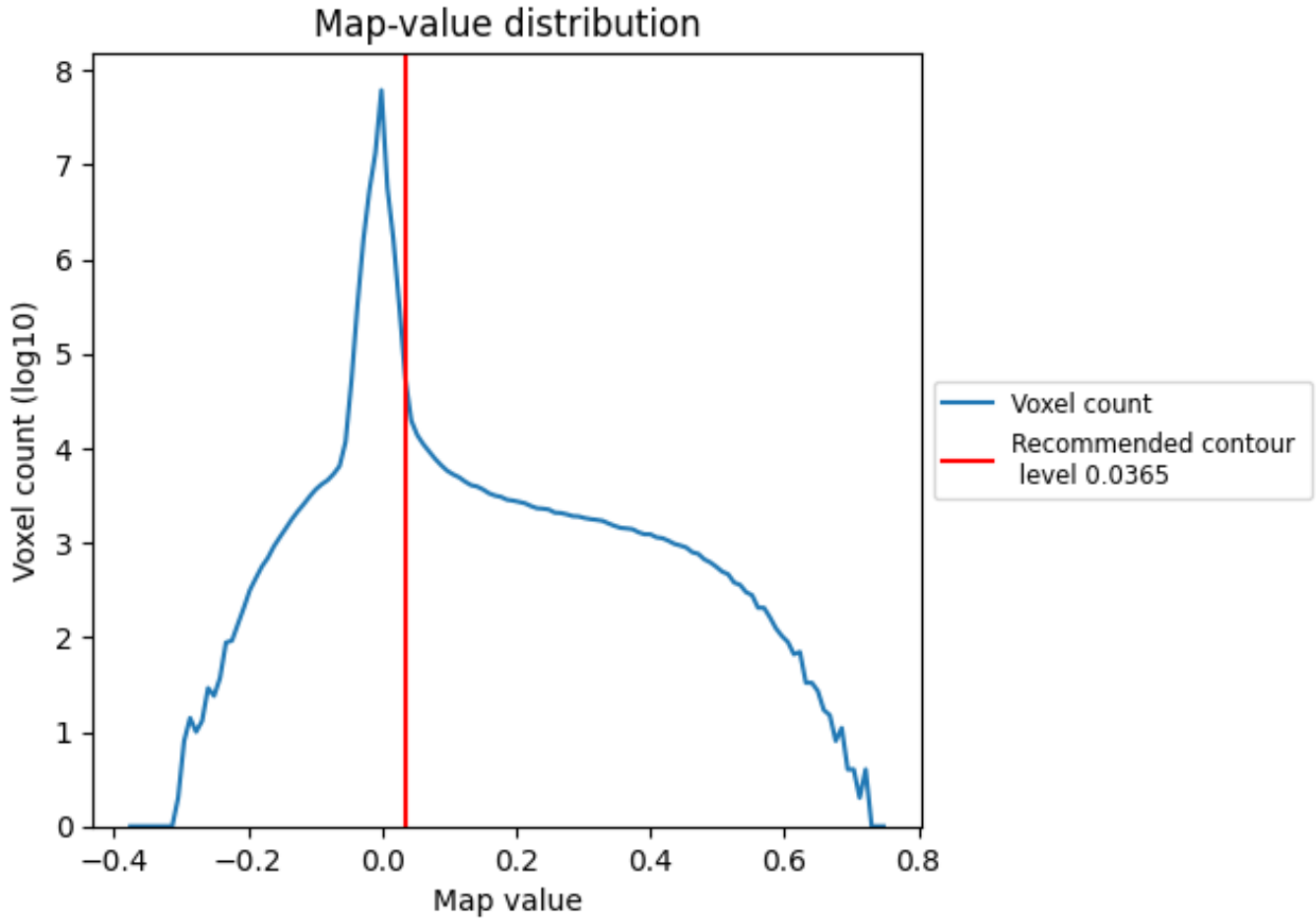


Z

7 Map analysis

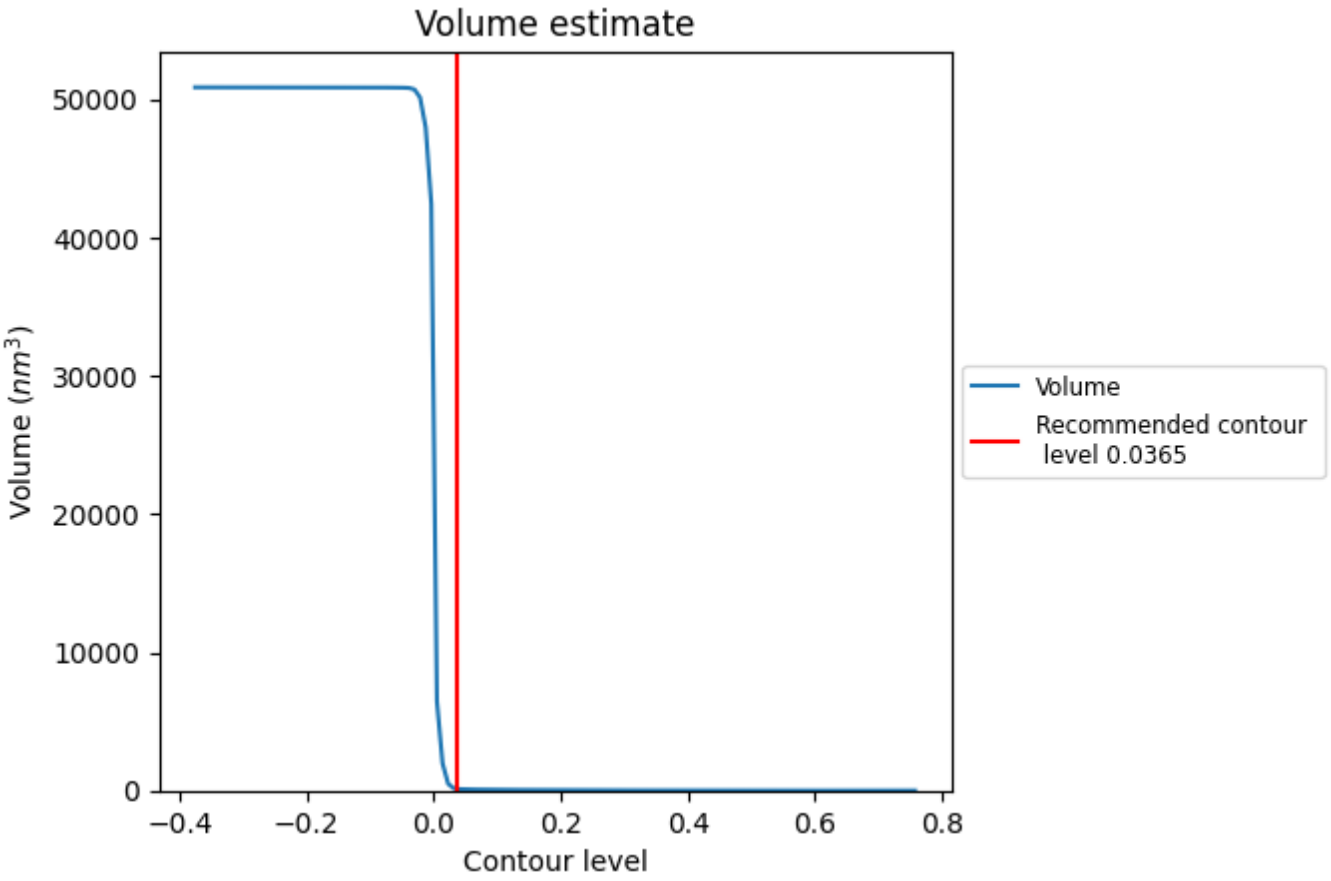
This section contains the results of statistical analysis of the map.

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.

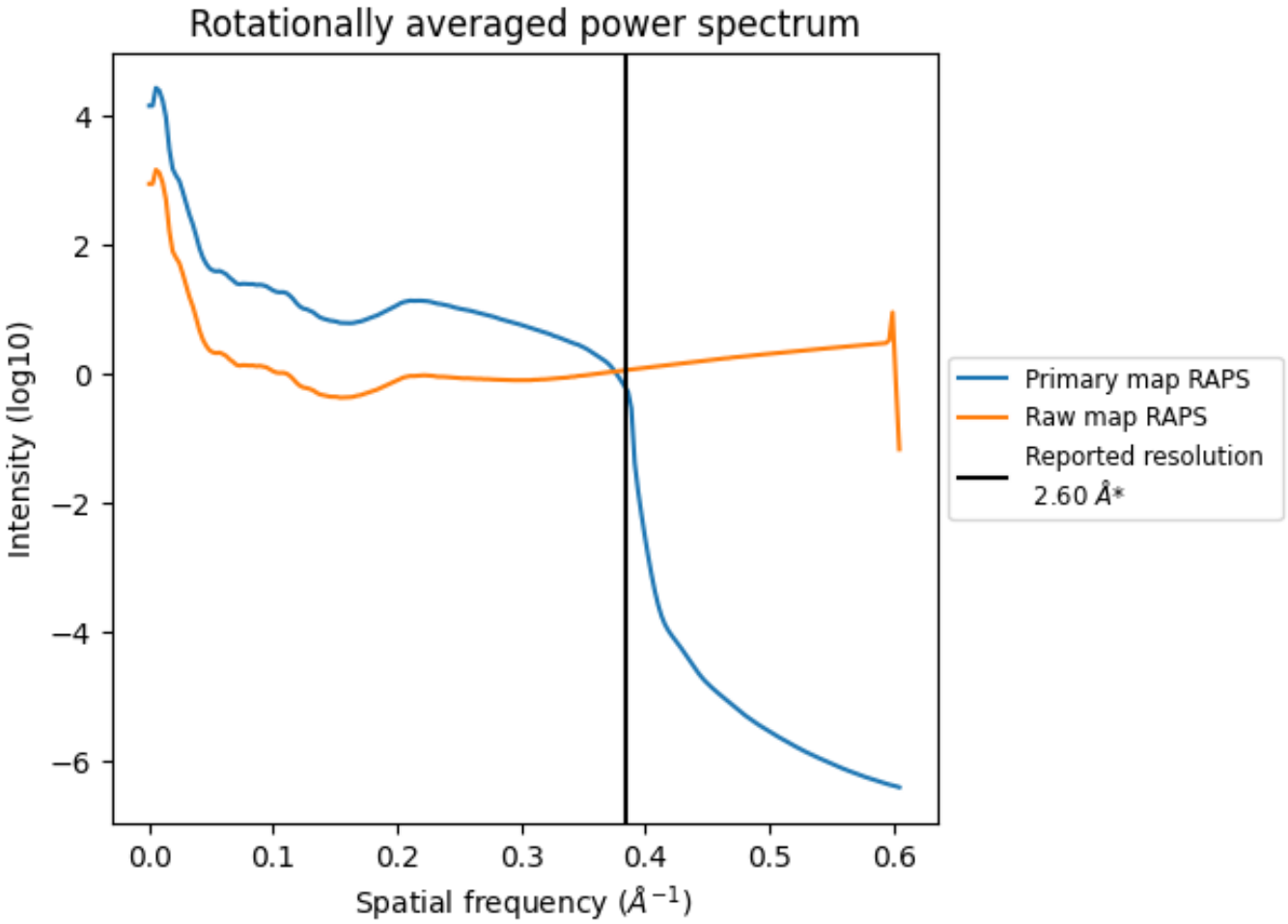
7.2 Volume estimate (i)



The volume at the recommended contour level is 128 nm^3; this corresponds to an approximate mass of 115 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)

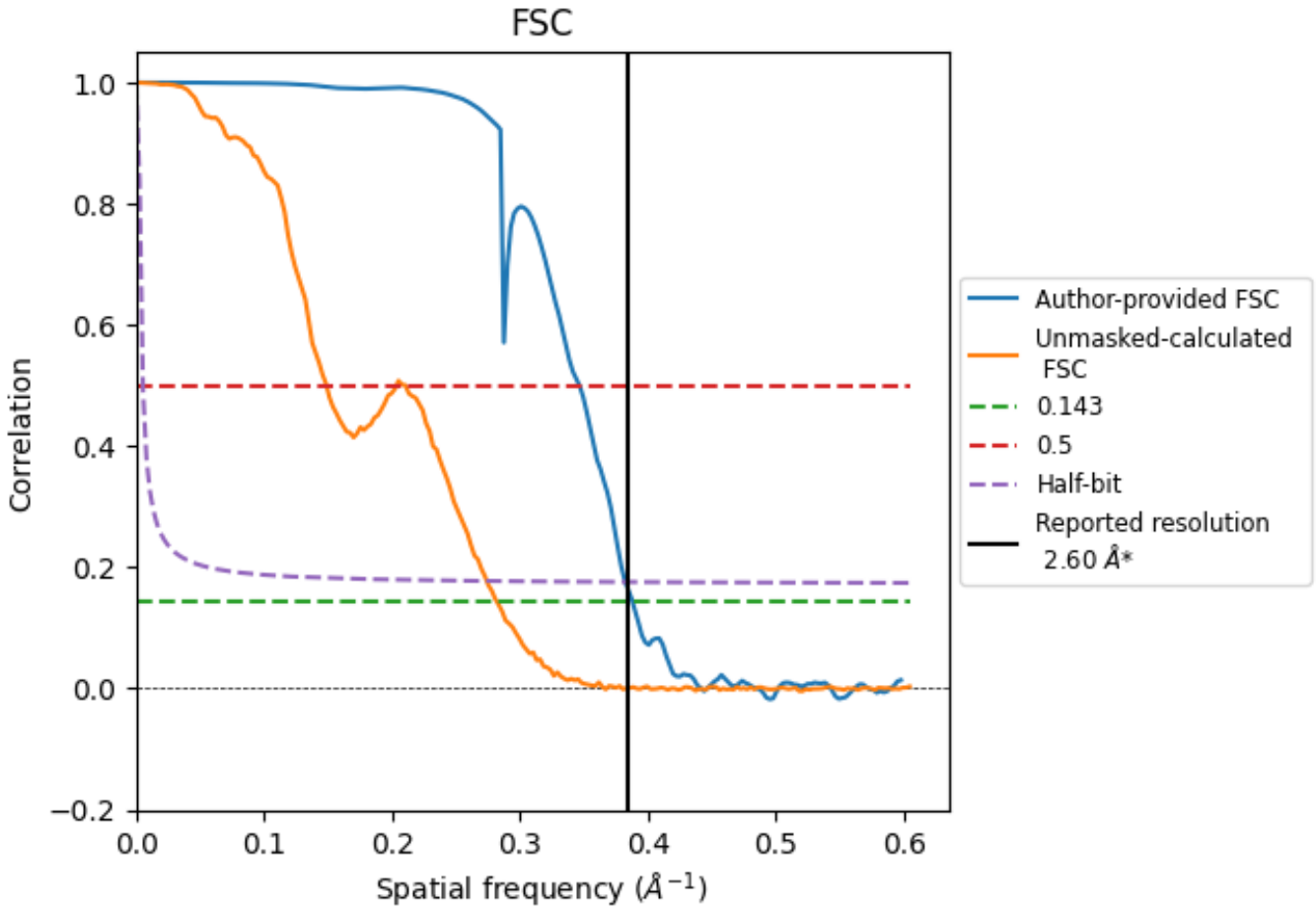


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

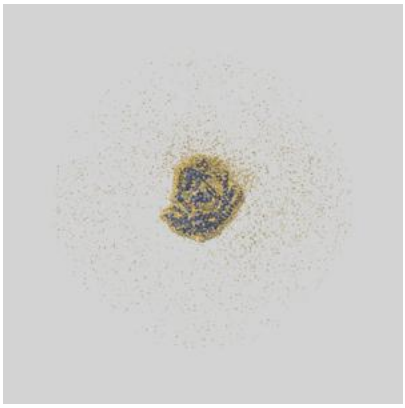
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.58	2.89	2.61
Unmasked-calculated*	3.54	6.72	3.65

*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 3.54 differs from the reported value 2.6 by more than 10 %

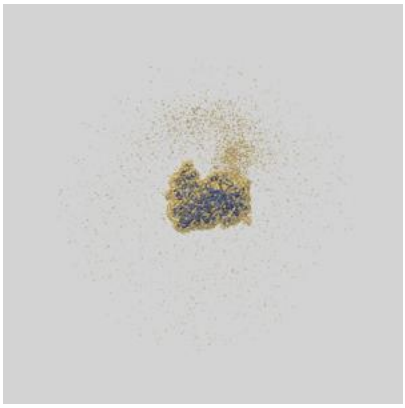
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-78711 and PDB model 38BZ. Per-residue inclusion information can be found in section 3 on page 4.

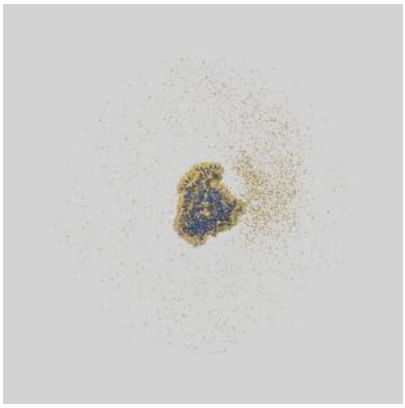
9.1 Map-model overlay



X



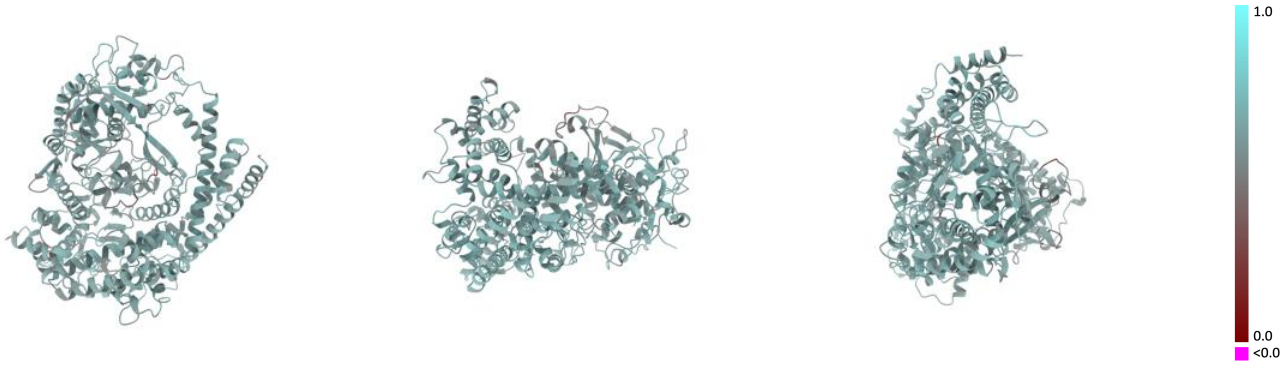
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0365 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.

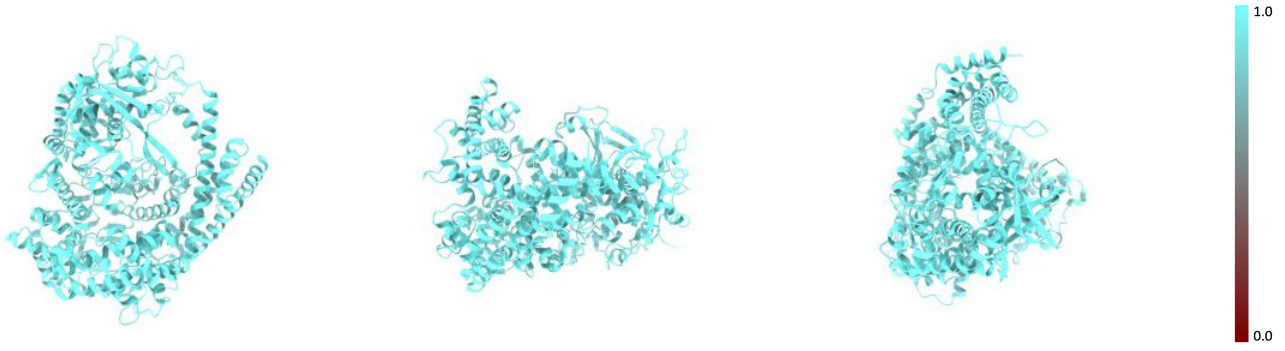
9.2 Q-score mapped to coordinate model (i)



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.

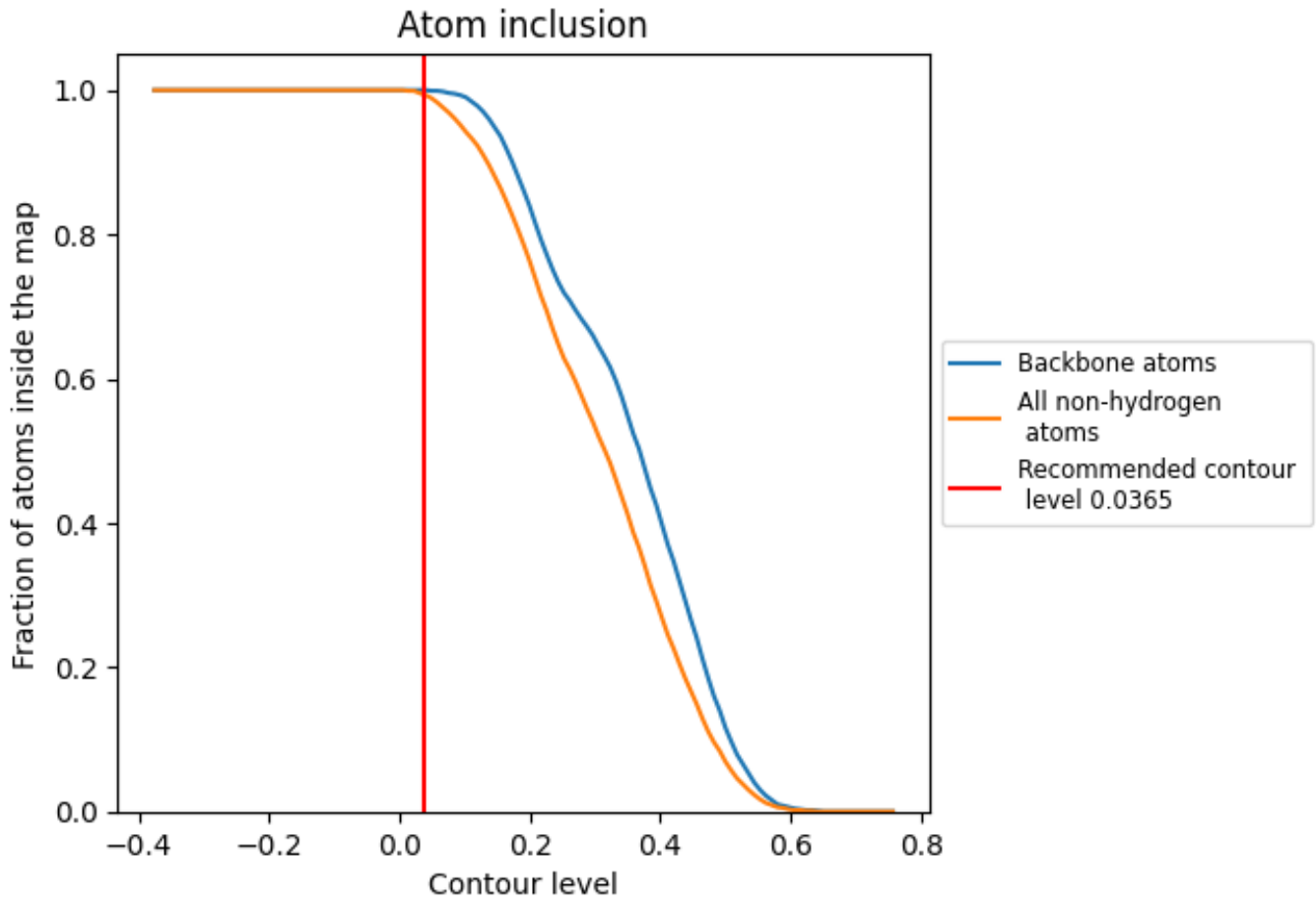
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0365).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0365) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9940	0.6120
A	0.9940	0.6120