wwPDB EM Validation Summary Report

Nov 11, 2026 – 02:22 PM EST

PDB ID	:	38CA / pdb_000038ca
EMDB ID	:	EMD-78712
Title	:	Pseudomonas phage DEV gp71 vRNAP: Isolated RNAP Domain with PE1 promoter
Authors	:	Bellis, N.F.; Lokareddy, R.K.; Cingolani, G.
Deposited on	:	2026-08-19
Resolution	:	2.90 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:

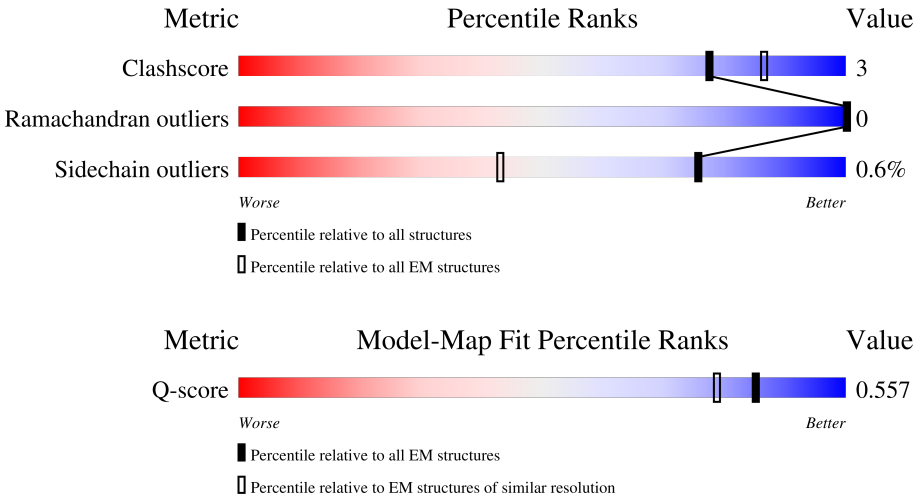
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & 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 2.90 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	13054 (2.40 - 3.40)

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	29% · 68%
2	B	19	89% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8625 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

- Molecule 2 is a DNA chain called PE1 Promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	19	389	183	78	109	19	0	0

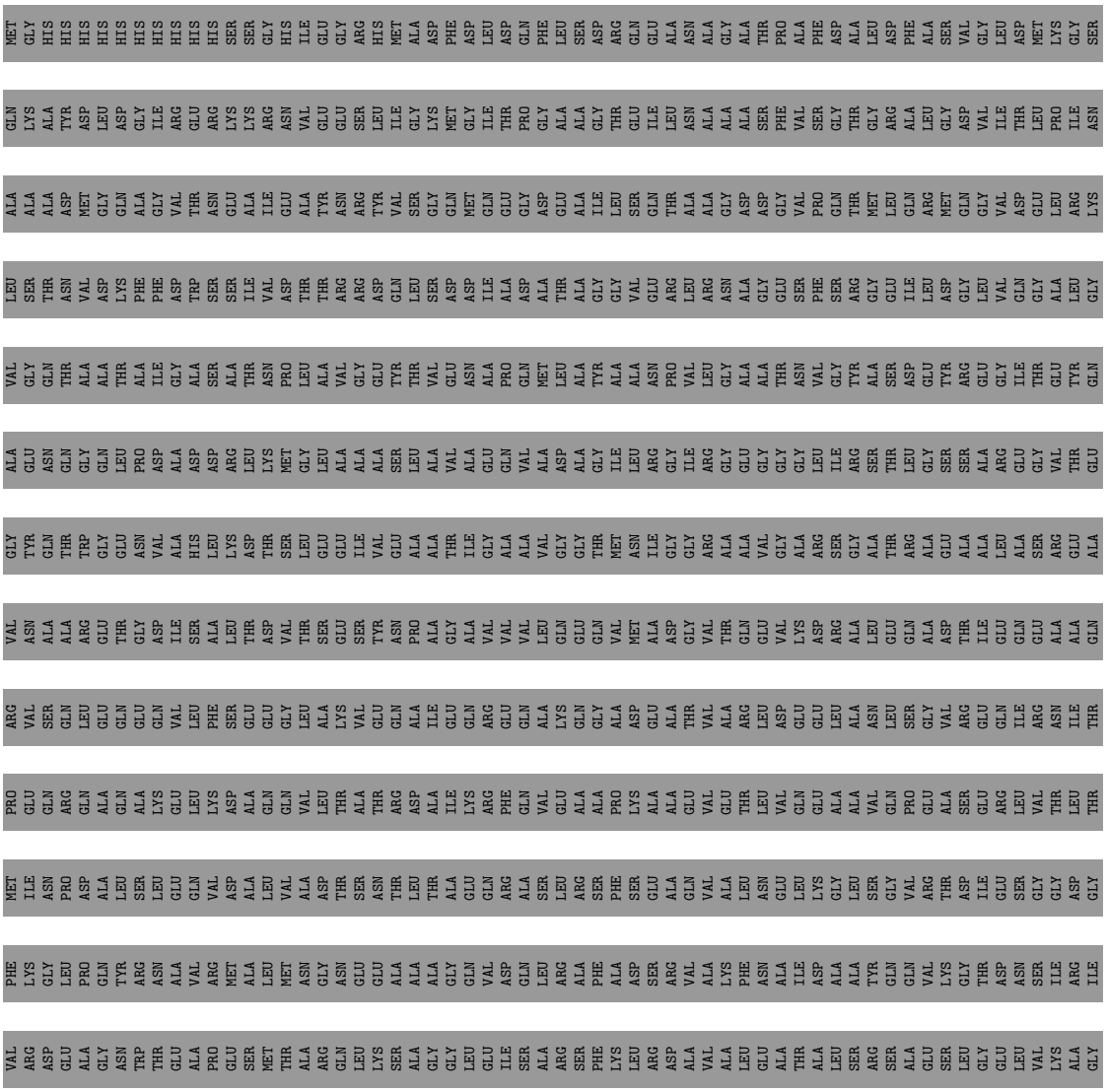
3 Residue-property plots (i)

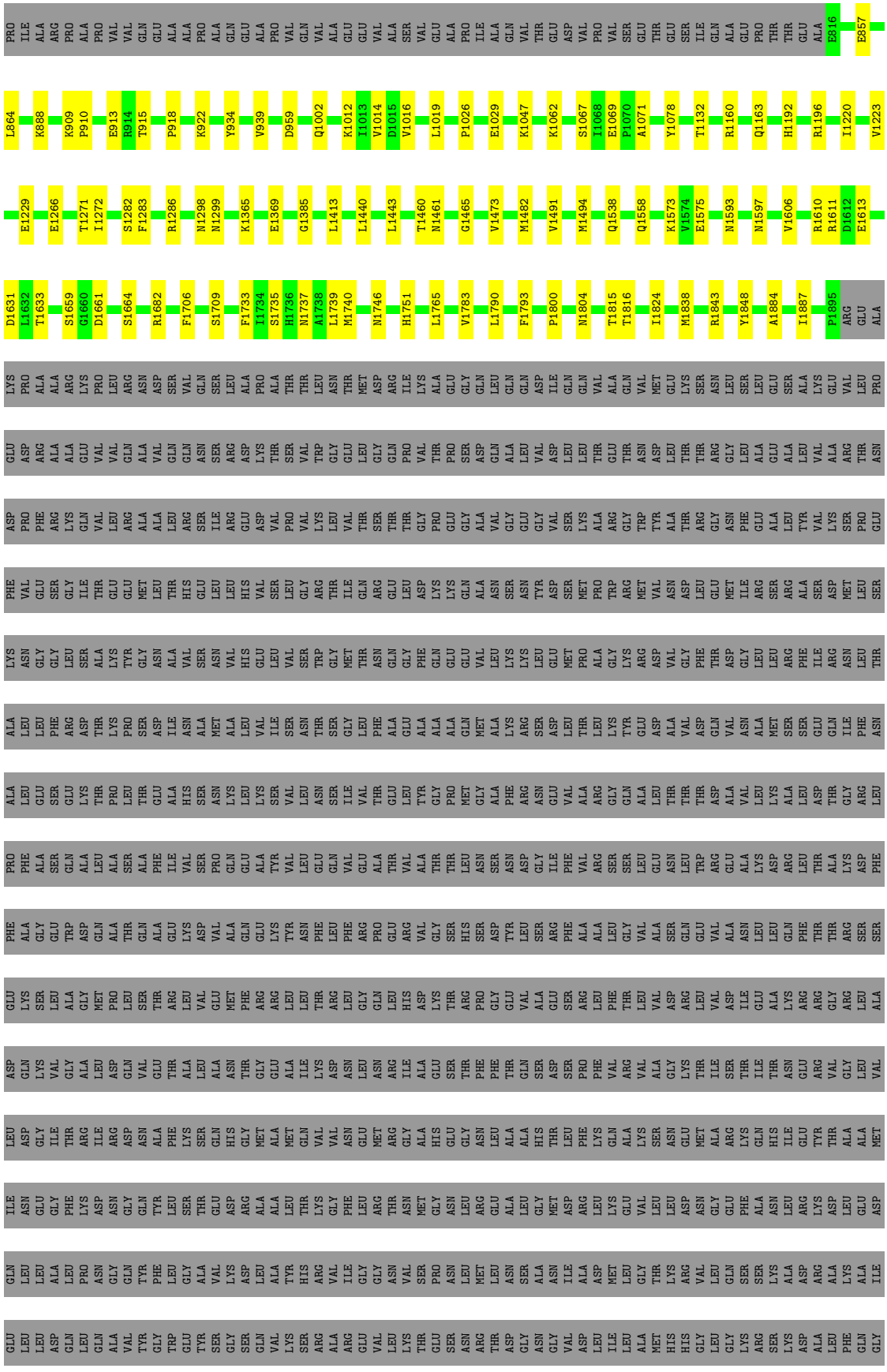
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

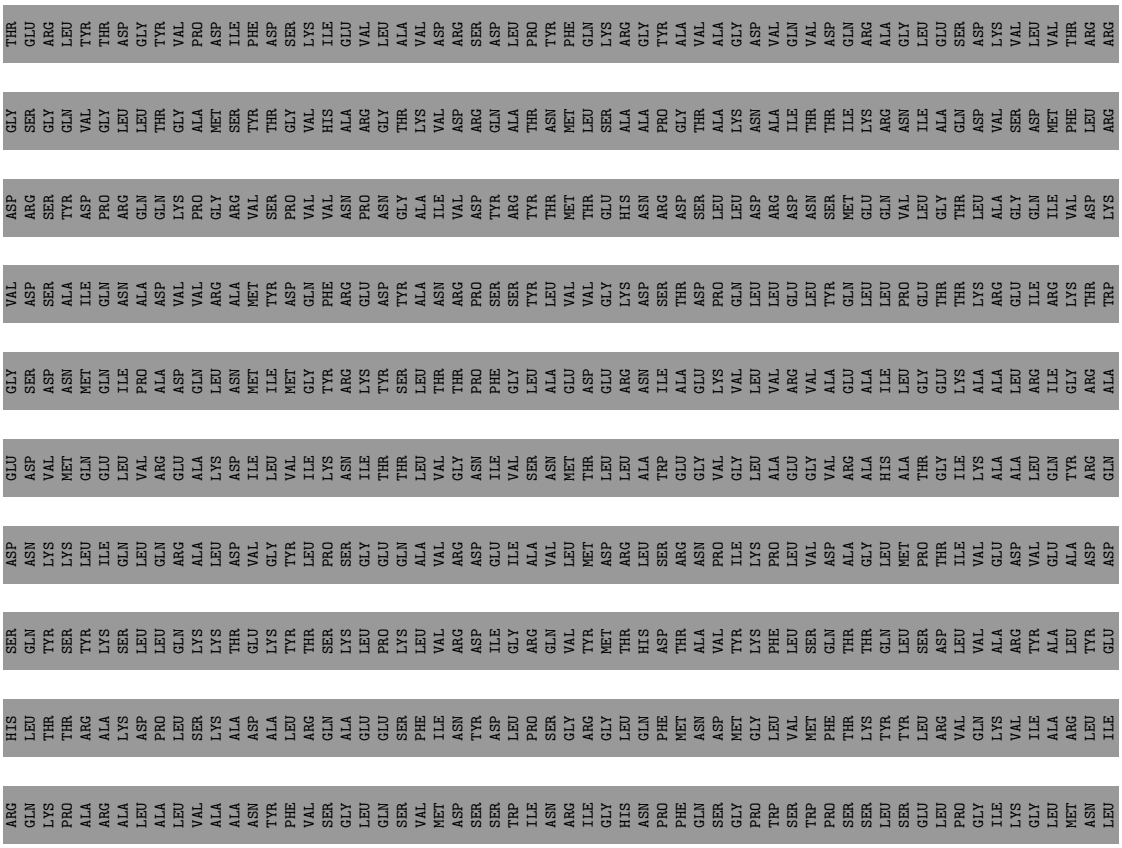
- Molecule 1: N4 gp50-like protein

Chain A:






PRO ILE ALA ARG PRO ALA PRO VAL VAL GLN GLU GLU ALA ALA PRO ALA GLN GLU ALA PRO VAL GLN VAL ALA GLU GLU VAL ALA SER VAL GLU ALA PRO ILE ALA GLN VAL THR GLU ASP VAL PRO VAL SER GLU THR GLU SER ILE GLN ALA GLU PRO THR THR GLU ALA E816 E857
L864 K888 K909 P910 E913 R914 T915 P918 K922 Y934 V939 D959 Q1002 K1012 I1013 V1014 D1015 V1016 L1019 P1026 E1029 K1047 K1062 S1067 I1068 E1069 P1070 A1071 Y1078 T1132 R1160 Q1163 H1192 R1196 I1220 V1223
E1229 E1266 T1271 I1272 S1282 F1283 R1286 N1298 N1299 K1365 E1369 G1385 L1413 L1440 L1443 T1460 N1461 G1465 V1473 M1482 V1491 M1494 Q1538 Q1558 K1573 V1574 E1575 N1593 N1597 V1606 R1610 R1611 D1612 E1613
D1631 L1632 T1633 S1659 G1660 D1661 S1664 R1682 F1706 S1709 F1733 I1734 S1735 H1736 N1737 A1738 L1739 M1740 N1746 H1751 L1765 V1783 L1790 F1793 P1800 N1804 T1815 T1816 I1824 M1838 R1843 Y1848 A1884 I1887 P1895 ARG GLU ALA
LYS PRO ALA ALA ARG LYS PRO LEU ARG ASN ASP SER VAL GLN SER LEU ALA PRO ALA THR THR LEU ASN THR MET ASP ARG ILE LYS ALA GLU GLY GLN GLN GLN ASP ILE GLN GLN VAL ALA GLN VAL MET GLU LYS SER ASN LEU SER LEU GLU GLU SER ALA LEU LEU ARG PRO
GLU ASP ARG ALA ALA GLU VAL VAL GLN ALA VAL GLN ASN SER ARG ASP LYS THR SER VAL TRP GLY GLU LEU GLY GLN PRO VAL THR PRO SER ASP GLN ALA LEU VAL ASP LEU LEU THR GLU THR ASN ASP LEU THR THR ARG GLY LEU ALA GLU GLU ALA LEU TYR VAL LYS GLU ASN
ASP PRO PHE ARG LYS GLN VAL LEU ARG ALA ALA LEU ARG SER ILE ARG GLU ASP PRO VAL LYS LEU VAL THR SER THR THR GLY VAL SER LYS ALA ARG GLY TRP TYR ALA THR ARG GLY ASN PHE GLU ALA LEU TYR VAL LYS PRO GLU
PHE VAL GLU SER GLY ILE GLU GLU MET LEU THR GLY HIS GLU ASP LYS GLN LYS GLN ALA ASN SER ASN TYR ASP SER MET PRO ALA GLY LYS ARG ASP VAL GLY PHE THR GLU MET ILE ARG SER ARG PHE ILE ARG ASN LEU THR
LYS ASN GLY GLY LEU SER VAL TYR GLY ASN ALA VAL SER SER ASN VAL HIS GLU LEU VAL SER TRP GLY MET THR ASN GLN GLY PHE GLN GLU GLU GLU VAL LYS LYS LEU GLU MET PRO ALA GLY LYS ARG ASP VAL GLY PHE THR ASN ASP LEU GLU MET ILE GLY LEU LEU LEU ARG PHE ILE ARG ASN LEU THR
ALA LEU LEU PHE ARG ASP THR LYS PRO LEU GLU ALA ALA LEU VAL ILE SER ASN THR SER GLY LEU PHE ALA GLU ALA ALA ALA GLN MET ALA ALA LYS ARG SER ASP LEU THR LEU LYS TYR GLU ASP ALA VAL GLY PHE THR ASP GLN VAL ASN ALA ALA MET SER SER GLU GLN GLN ILE PHE ASN
ALA LEU GLU SER GLU LYS THR PRO LEU THR GLU ALA HIS SER ASN LYS LEU LYS SER VAL LEU ASN SER ILE VAL THR GLY PRO MET GLY ALA PHE ARG ASN GLU VAL ASP LEU THR THR THR ASP ALA VAL ASN LEU ARG GLU ALA VAL ASN ALA ILE ASP ARG LEU
PRO PHE ALA SER GLN ALA LEU GLU GLN ALA SER ALA THR VAL ALA ALA THR HIS LEU ASN SER SER GLY LEU ASN TRP ASP ARG SER SER LEU GLU LEU ASN LEU TRP ARG GLU ALA ALA LEU ASP ASP ARG LEU THR ALA LYS ASP PHE
PHE ALA GLY GLU TRP ASP GLN ALA ALA GLU LYS TYR ASN PHE LEU PHE ARG PRO GLU ARG VAL GLY SER HIS SER ASP TYR LEU SER ARG PHE ALA ALA LEU GLY VAL ALA SER GLN GLU VAL ALA ASN LEU LEU GLN PHE THR THR ARG PHE
GLU LYS SER LEU ALA GLY MET PRO LEU SER THR ARG LEU GLY GLN LEU HIS ASP LYS THR ARG PRO GLY GLU VAL ALA ALA GLU SER ARG LEU PHE THR LEU VAL ASP ARG LEU VAL ASP ALA ARG GLY ARG GLY ARG LEU ALA
ASP GLN LYS VAL GLY ALA ASP GLN VAL GLU THR PHE LEU ASN ASN ARG ILE ALA GLU SER THR PHE PHE THR GLN SER ALA LEU GLU ASP SER PRO PHE VAL ALA ASP ARG SER ILE ALA THR ASP ILE THR ILE ASN THR LYS GLU ARG VAL GLY LEU
LEU ASP GLY ILE THR ARG ASP ASN ALA PHE LYS SER THR HIS GLU GLY ASN LEU ALA ALA HIS THR LEU PHE LYS GLN ALA LYS SER ASN GLU MET ALA ARG LYS GLN HIS ILE GLU TYR THR ALA ALA MET
ILE ASN GLU GLY PHE LYS ASP ASN GLY TYR LEU SER THR GLU ASP ARG ALA ALA LEU THR LYS GLY PHE LEU ARG GLY THR ASN MET GLY ASN LEU ARG GLU ALA LEU GLY MET ASP ARG LEU LYS GLU VAL LEU LEU LEU ASP ASP ASN GLU MET ALA ARG GLU PHE LEU ASN ALA ASP ASP LEU ILE ASP
GLN LEU LEU ALA PRO ASN GLY ALA GLN TYR PHE LEU GLY ALA TYR HIS ARG VAL ILE GLY GLY ASN VAL SER PRO ASN LEU MET LEU ASN SER ALA ASP MET ILE LEU GLY THR LYS ARG VAL LEU GLN GLY SER SER LYS ALA ASP ARG ALA LYS ALA ILE
GLU LEU LEU ASP GLN ALA VAL TYR GLY TRP GLU TYR SER GLY SER GLN VAL LYS SER ARG ALA ARG GLU VAL LEU LYS THR GLU SER ASN ARG GLY VAL ASP LEU ILE LEU ALA MET HIS HIS GLY LEU GLY LYS ARG SER LYS ASP ALA LEU PHE GLN GLY
WORLDWIDE PDB PROTEIN DATA BANK



• Molecule 2: PE1 Promoter

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210675	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.444	Depositor
Minimum map value	-0.224	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0259	Depositor
Map size (Å)	292.0, 292.0, 292.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	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	0.07	0/8366	0.19	0/11318
2	B	0.62	0/437	0.63	0/671
All	All	0.15	0/8803	0.24	0/11989

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	47	0
2	B	389	0	211	1	0
All	All	8625	0	8350	48	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 3.

The worst 5 of 48 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:1682:ARG:NH1	1:A:1709:SER:OG	2.32	0.62
1:A:1014:VAL:HG13	1:A:1019:LEU:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:ARG:NH1	1:A:1266:GLU:OE2	2.33	0.60
1:A:959:ASP:OD2	1:A:1012:LYS:NZ	2.33	0.59
1:A:1593:ASN:O	1:A:1597:ASN:ND2	2.34	0.59

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%)	1071 (99%)	7 (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	93

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

Mol	Chain	Res	Type
1	A	1271	THR
1	A	1482	MET
1	A	1706	PHE

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Mol	Chain	Res	Type
1	A	1740	MET
1	A	1838	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1826	HIS
1	A	1608	GLN
1	A	1167	GLN
1	A	1135	ASN
1	A	1270	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 (i)

There are no chain breaks in this entry.

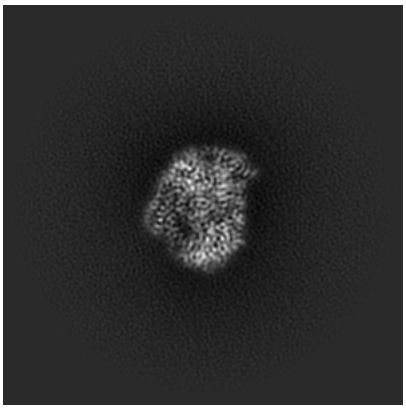
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-78712. These allow visual inspection of the internal detail of the map and identification of artifacts.

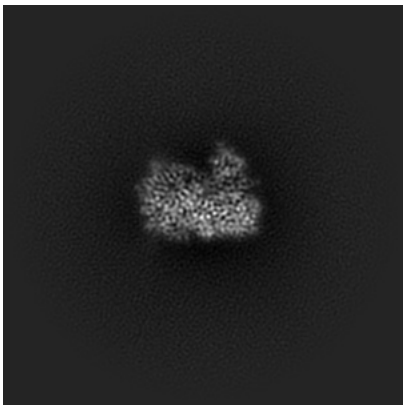
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

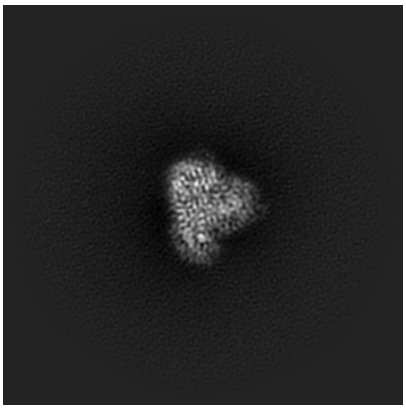
6.1.1 Primary map



X

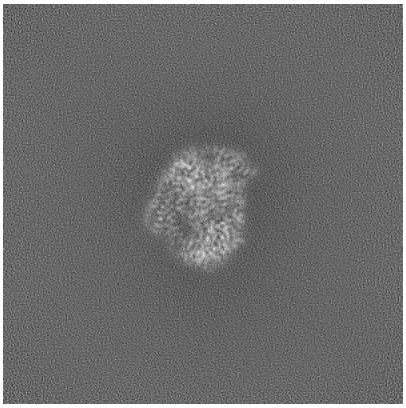


Y

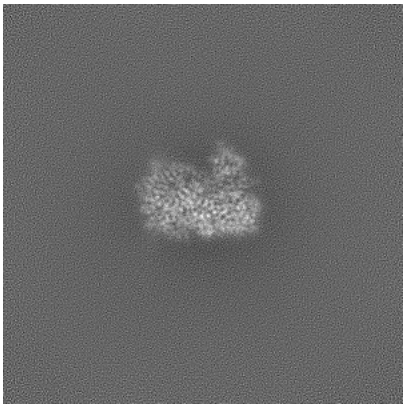


Z

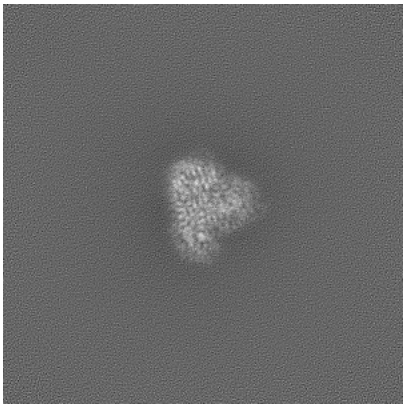
6.1.2 Raw map



X



Y

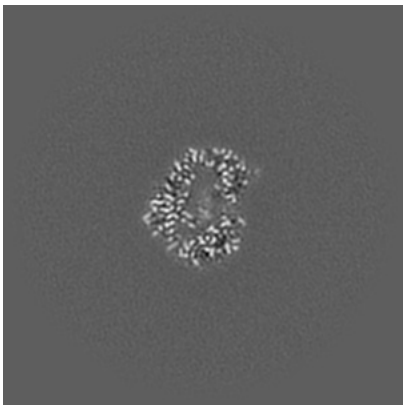


Z

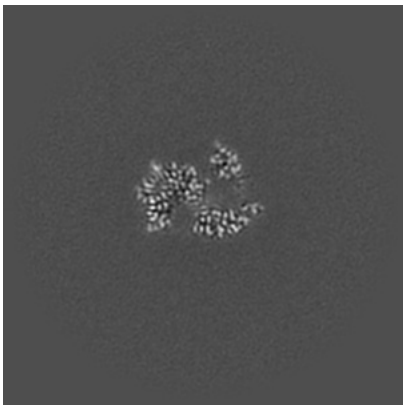
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

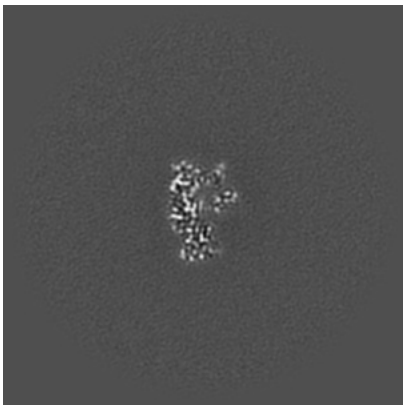
6.2.1 Primary map



X Index: 200

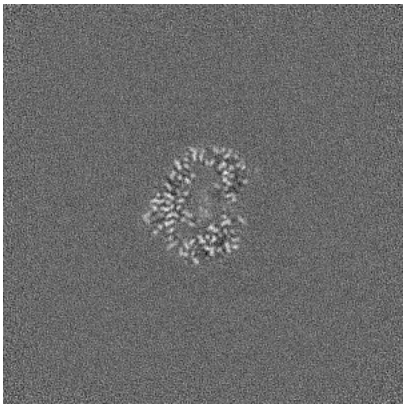


Y Index: 200

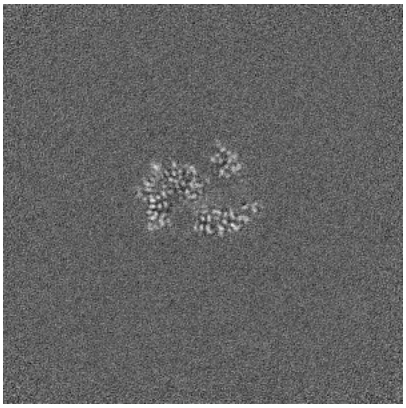


Z Index: 200

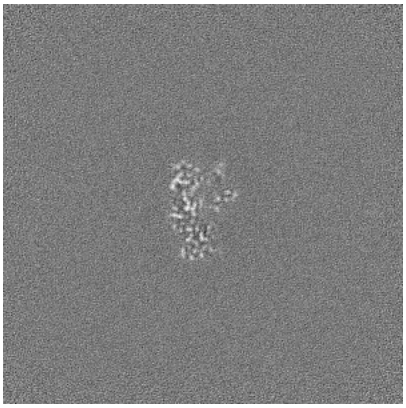
6.2.2 Raw map



X Index: 200



Y Index: 200

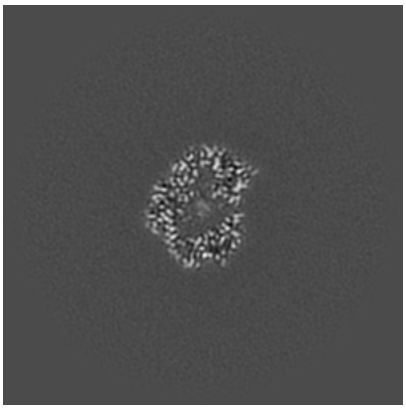


Z Index: 200

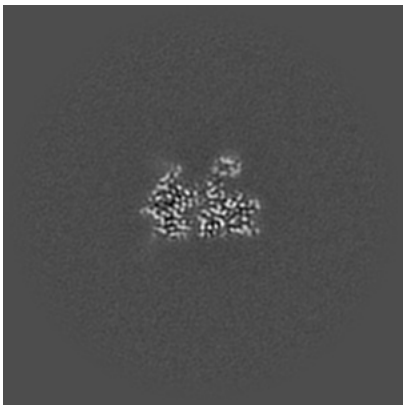
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

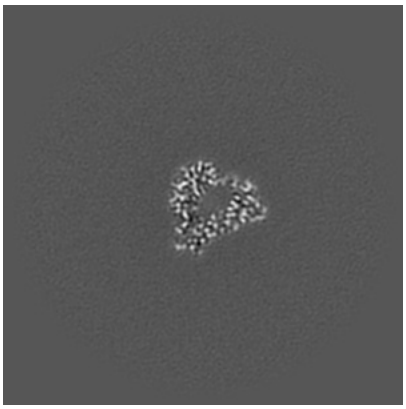
6.3.1 Primary map



X Index: 196

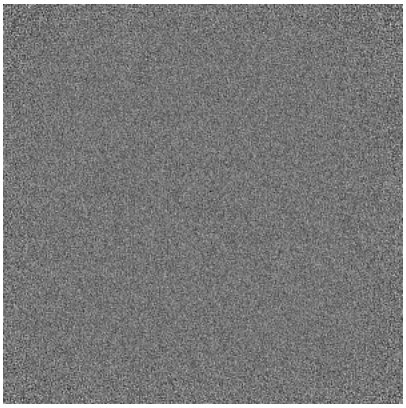


Y Index: 221

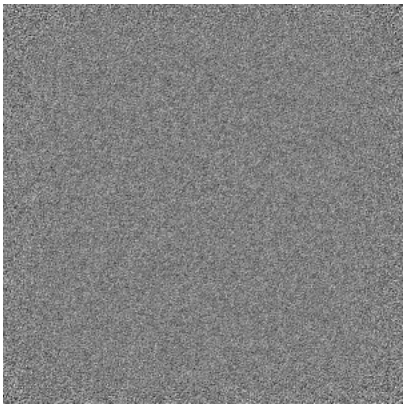


Z Index: 219

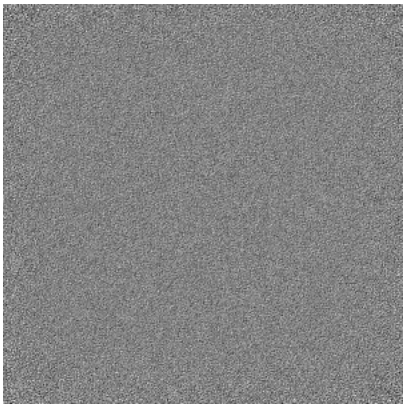
6.3.2 Raw map



X Index: 0



Y Index: 0

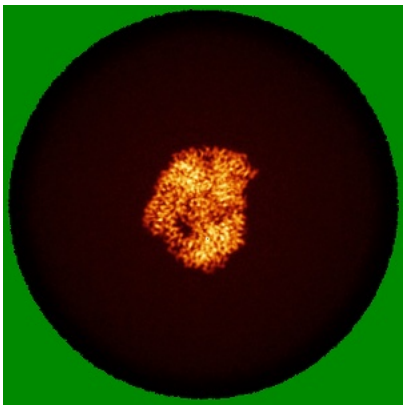


Z Index: 0

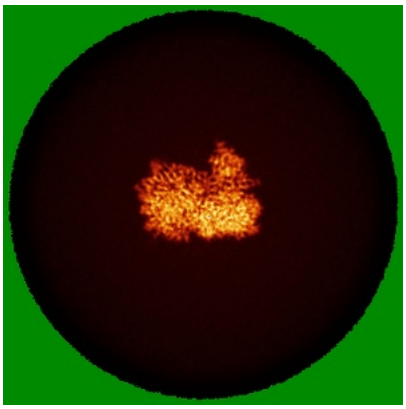
The images above show the largest variance slices of the map in three orthogonal directions.

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

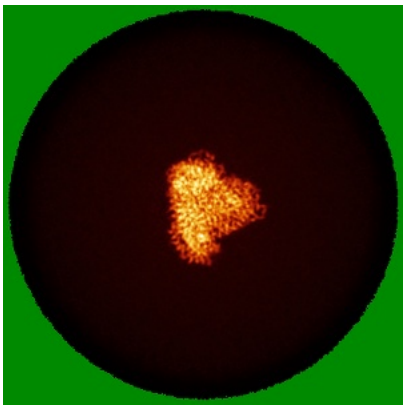
6.4.1 Primary map



X

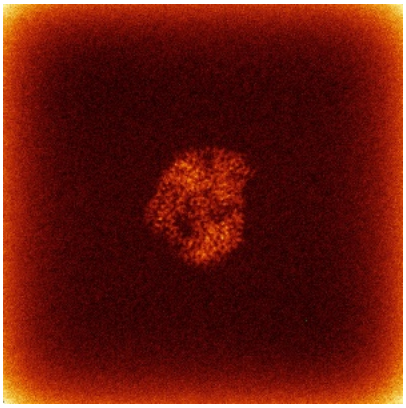


Y

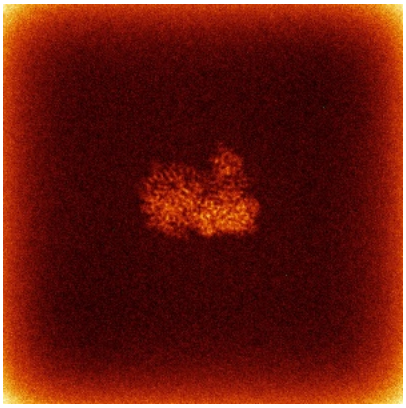


Z

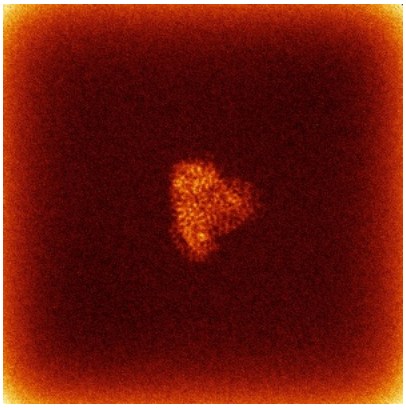
6.4.2 Raw map



X



Y

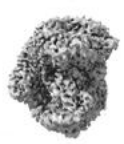


Z

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



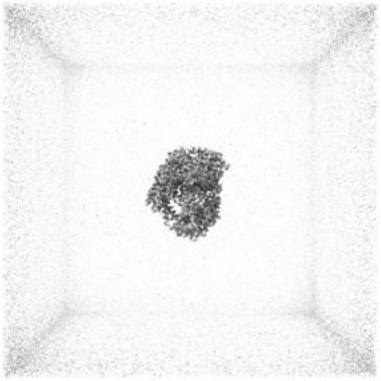
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0259. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

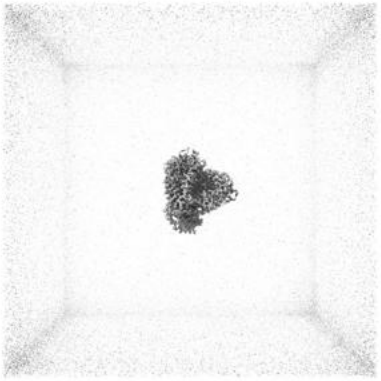
6.5.2 Raw map



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.

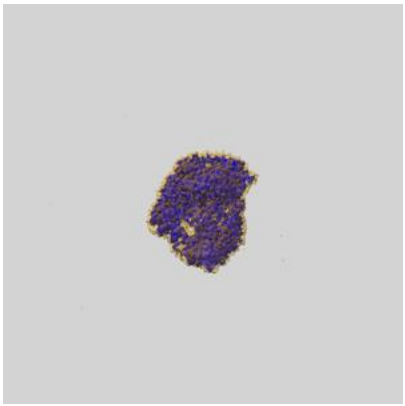
6.6 Mask visualisation (i)

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

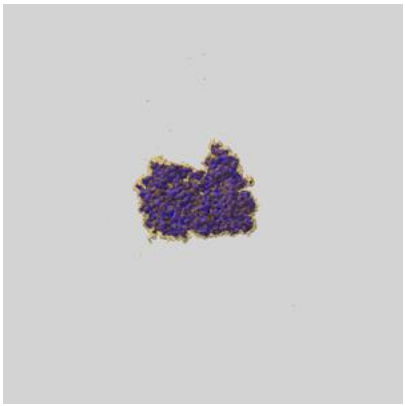
A mask typically either:

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

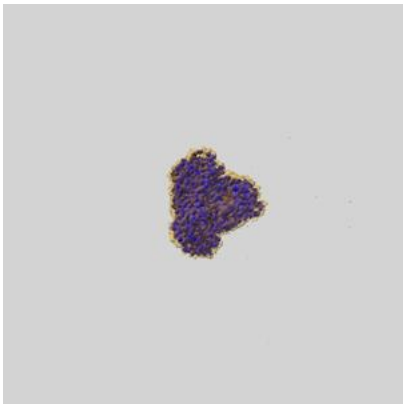
6.6.1 emd_78712_msk_1.map (i)



X



Y

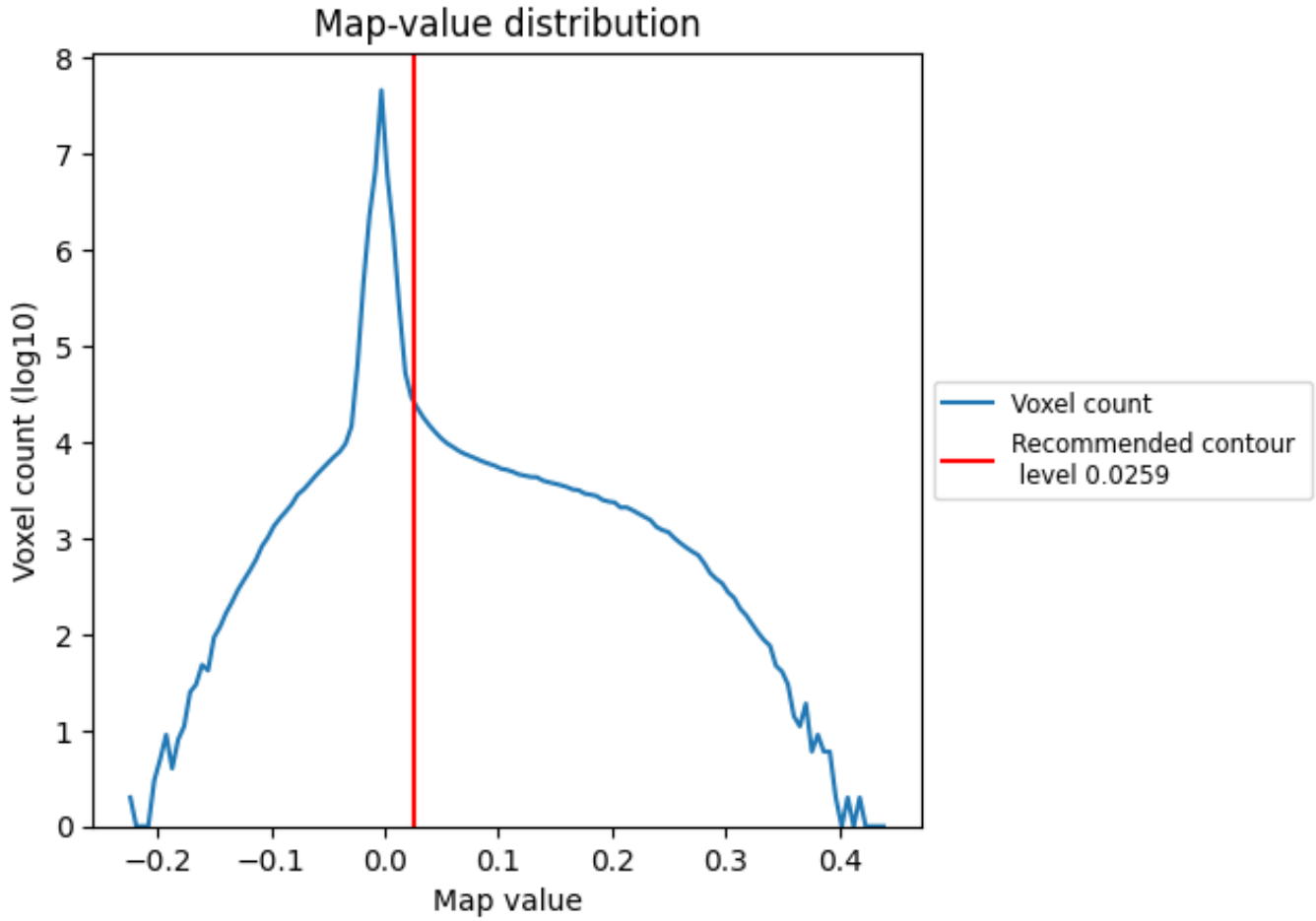


Z

7 Map analysis

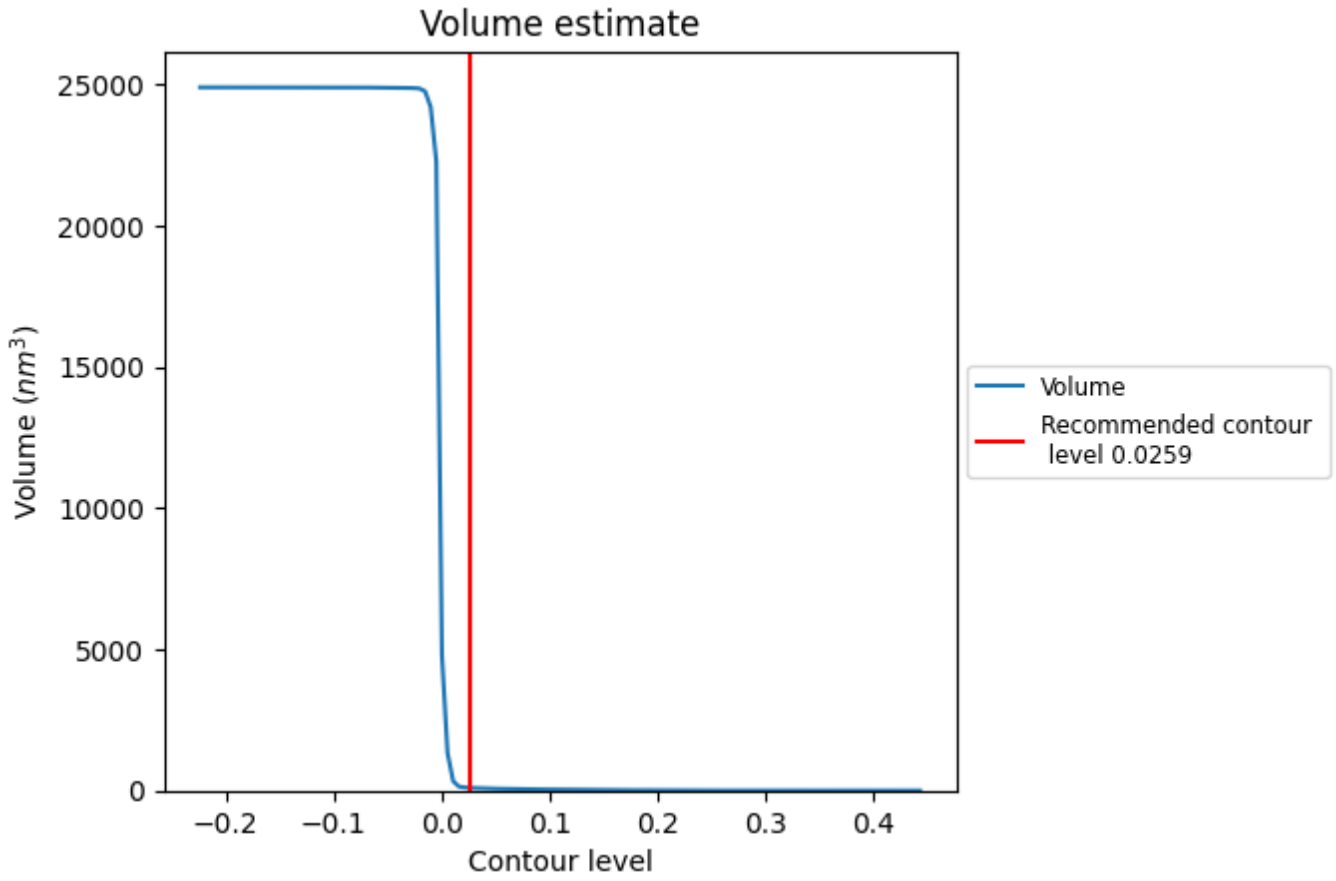
This section contains the results of statistical analysis of the map.

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.

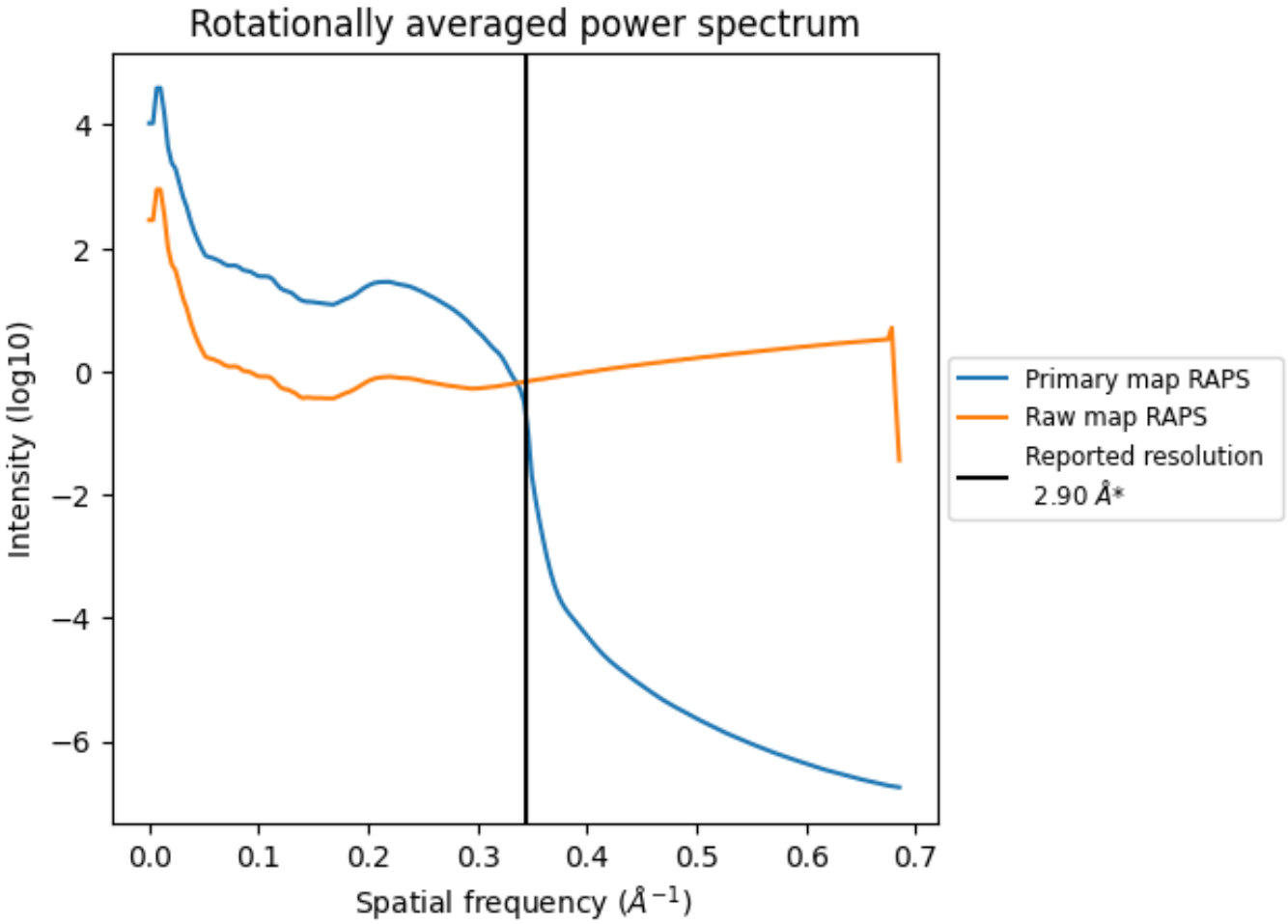
7.2 Volume estimate (i)



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 90 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)

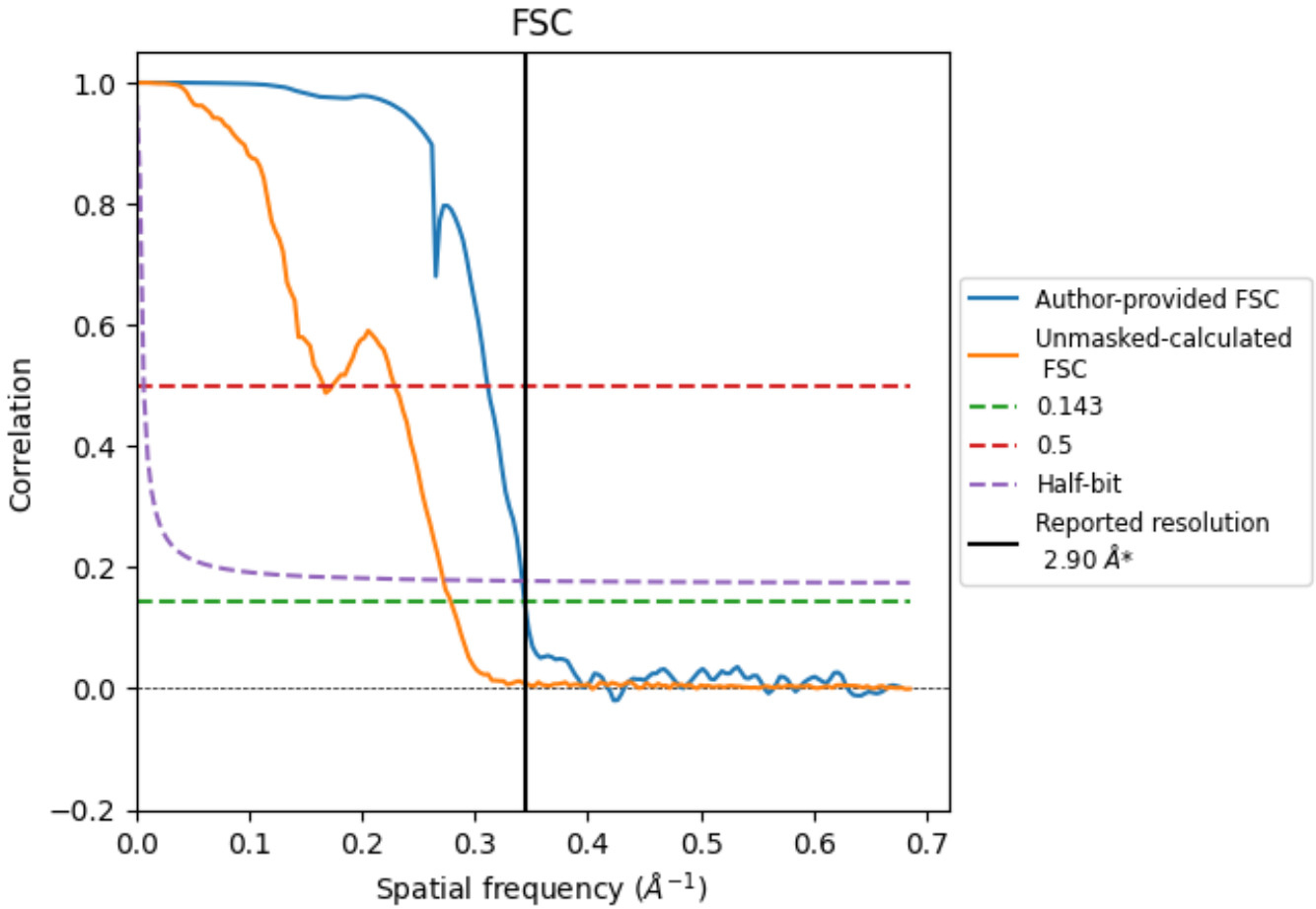


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

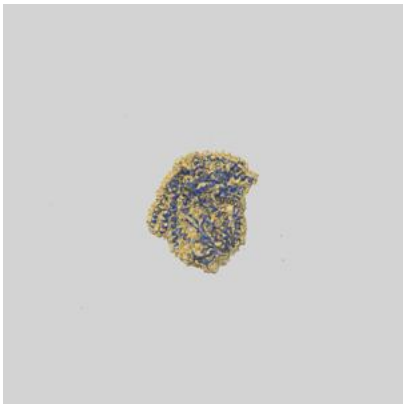
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.21	2.92
Unmasked-calculated*	3.59	6.04	3.68

*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 3.59 differs from the reported value 2.9 by more than 10 %

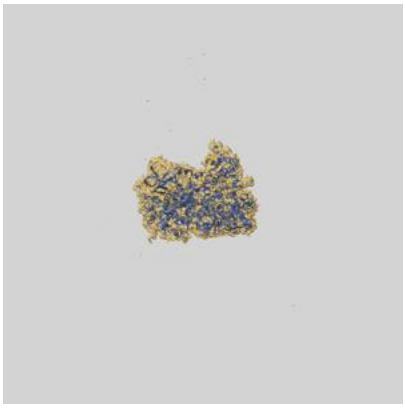
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-78712 and PDB model 38CA. Per-residue inclusion information can be found in section 3 on page 4.

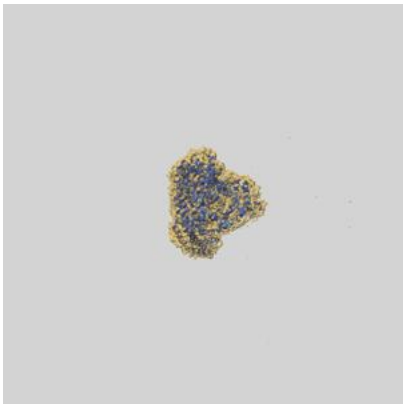
9.1 Map-model overlay



X



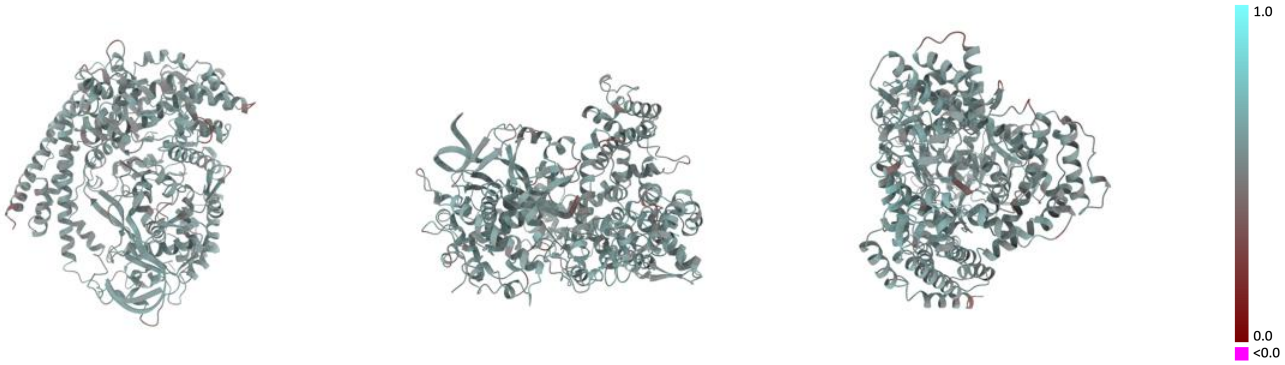
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0259 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.

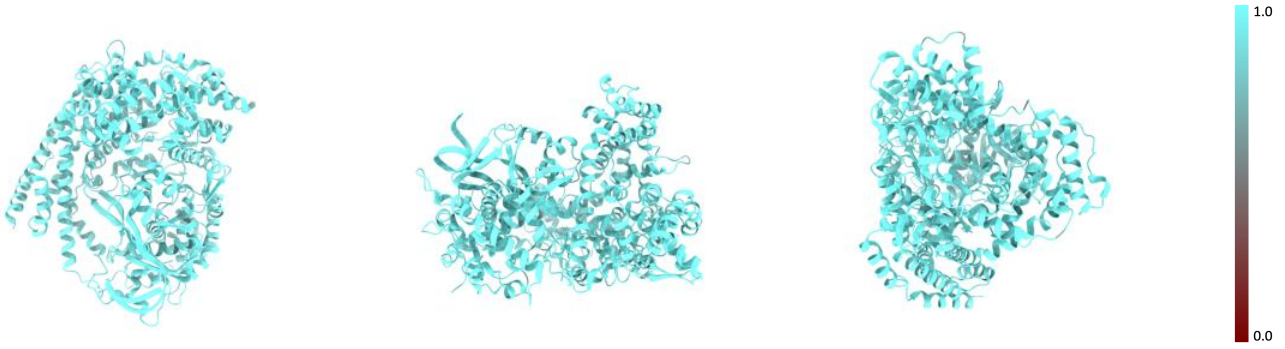
9.2 Q-score mapped to coordinate model (i)



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.

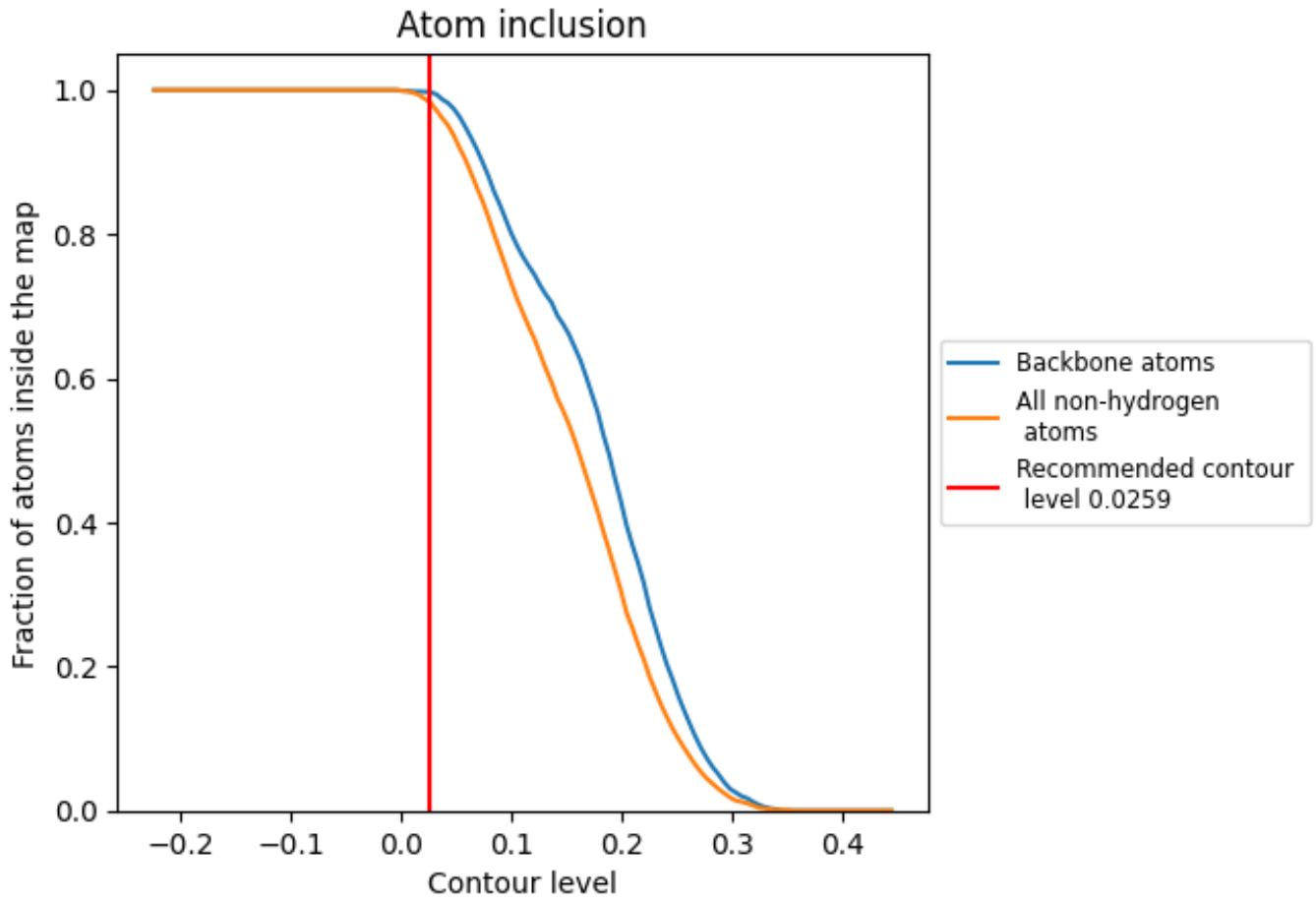
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0259).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.0259) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9830	0.5570
A	0.9820	0.5570
B	0.9950	0.5530