



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 11:41 PM UTC

PDB ID : 6N4C / pdb_00006n4c
EMDB ID : EMD-0340
Title : EM structure of the DNA wrapping in bacterial open transcription initiation complex
Authors : Florez-Ariza, A.; Cassago, A.; de Oliveira, P.S.L.; Guerra, D.G.; Portugal, R.V.
Deposited on : 2018-11-19
Resolution : 17.00 Å(reported)
Based on initial model : 4YLN

This is a Full wwPDB EM Validation 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 : **FAILED**
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

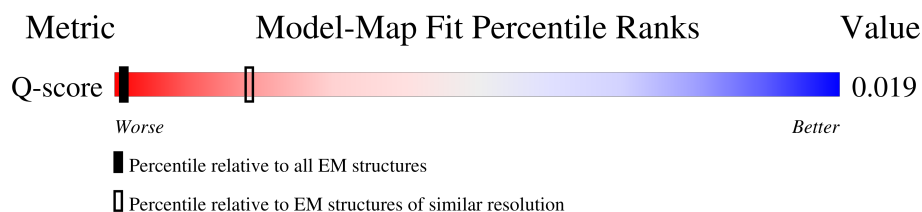
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.00 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	38 (16.50 - 17.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 68774 atoms, of which 33722 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 RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	F	558	Total	C	H	N	O	S	0	0
			9018	2799	4523	794	875	27		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	ALA	deletion	UNP P00579
F	?	-	PRO	deletion	UNP P00579
F	?	-	THR	deletion	UNP P00579
F	?	-	ALA	deletion	UNP P00579
F	?	-	THR	deletion	UNP P00579
F	?	-	HIS	deletion	UNP P00579
F	?	-	VAL	deletion	UNP P00579
F	?	-	GLY	deletion	UNP P00579
F	?	-	SER	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	SER	deletion	UNP P00579
F	?	-	GLN	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ASP	deletion	UNP P00579
F	?	-	GLY	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	SER	deletion	UNP P00579
F	?	-	ALA	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579
F	?	-	ILE	deletion	UNP P00579
F	?	-	ALA	deletion	UNP P00579
F	?	-	LYS	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	PRO	deletion	UNP P00579
F	521	ILE	-	insertion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	GLU	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	PRO	deletion	UNP P00579
F	?	-	LEU	deletion	UNP P00579
F	?	-	ASP	deletion	UNP P00579

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	1341	Total	C	H	N	O	S	0	0
			21172	6636	10595	1842	2056	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	1358	Total	C	H	N	O	S	0	0
			21296	6615	10758	1882	1991	50		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP A0A369F490
D	?	-	GLY	deletion	UNP A0A369F490
D	?	-	LYS	deletion	UNP A0A369F490
D	?	-	GLU	deletion	UNP A0A369F490

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	316	Total	C	H	N	O	S	0	0
			5001	1545	2528	436	484	8		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	310	Total	C	H	N	O	S	0	0
			4883	1508	2471	422	475	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	255	LEU	ARG	conflict	UNP P0A7Z4

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	90	Total	C	H	N	O	S	0	0
			1431	430	722	136	142	1		

- Molecule 7 is a DNA chain called DNA (94-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	a	94	Total	C	H	N	O	P	0	0
			2995	923	1064	349	566	93		

- Molecule 8 is a DNA chain called DNA (94-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	b	94	Total	C	H	N	O	P	0	0
			2978	917	1061	349	558	93		

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16015	Depositor
Resolution determination method	FSC 1/2 BIT CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL 2100	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	14.200	Depositor
Minimum map value	-6.374	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.42	Depositor
Map size ($\text{\AA}$)	320.4, 320.4, 320.4	wwPDB
Map dimensions	90, 90, 90	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	3.56, 3.56, 3.56	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0340. These allow visual inspection of the internal detail of the map and identification of artifacts.

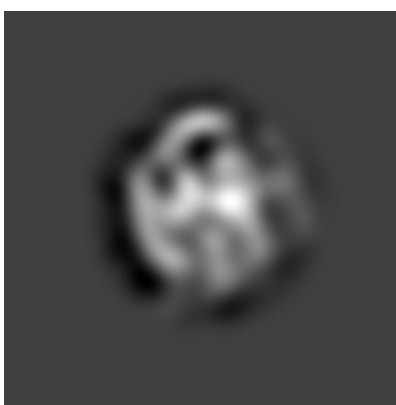
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

5.1.1 Primary map



X



Y

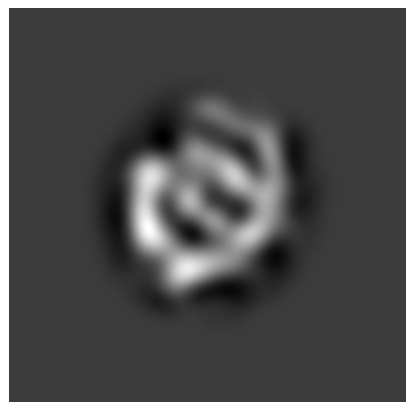


Z

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

5.2 Central slices [i](#)

5.2.1 Primary map



X Index: 45



Y Index: 45

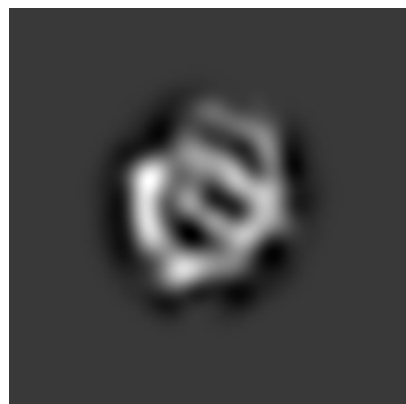


Z Index: 45

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

5.3 Largest variance slices [i](#)

5.3.1 Primary map



X Index: 47



Y Index: 40



Z Index: 48

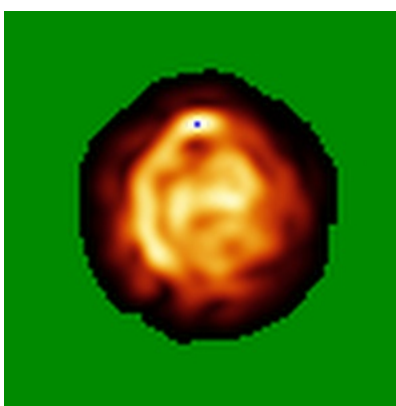
The images above show the largest variance slices of the map in three orthogonal directions.

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

5.4.1 Primary map



X



Y

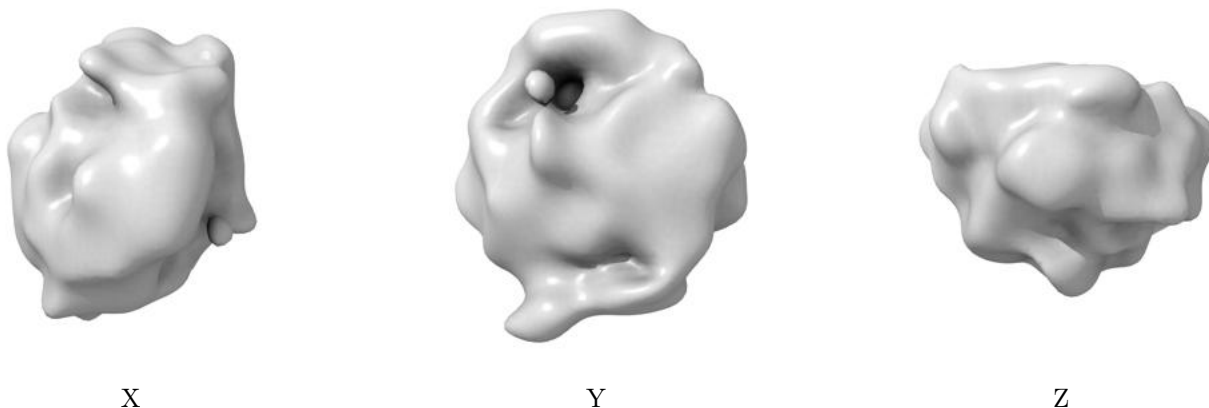


Z

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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

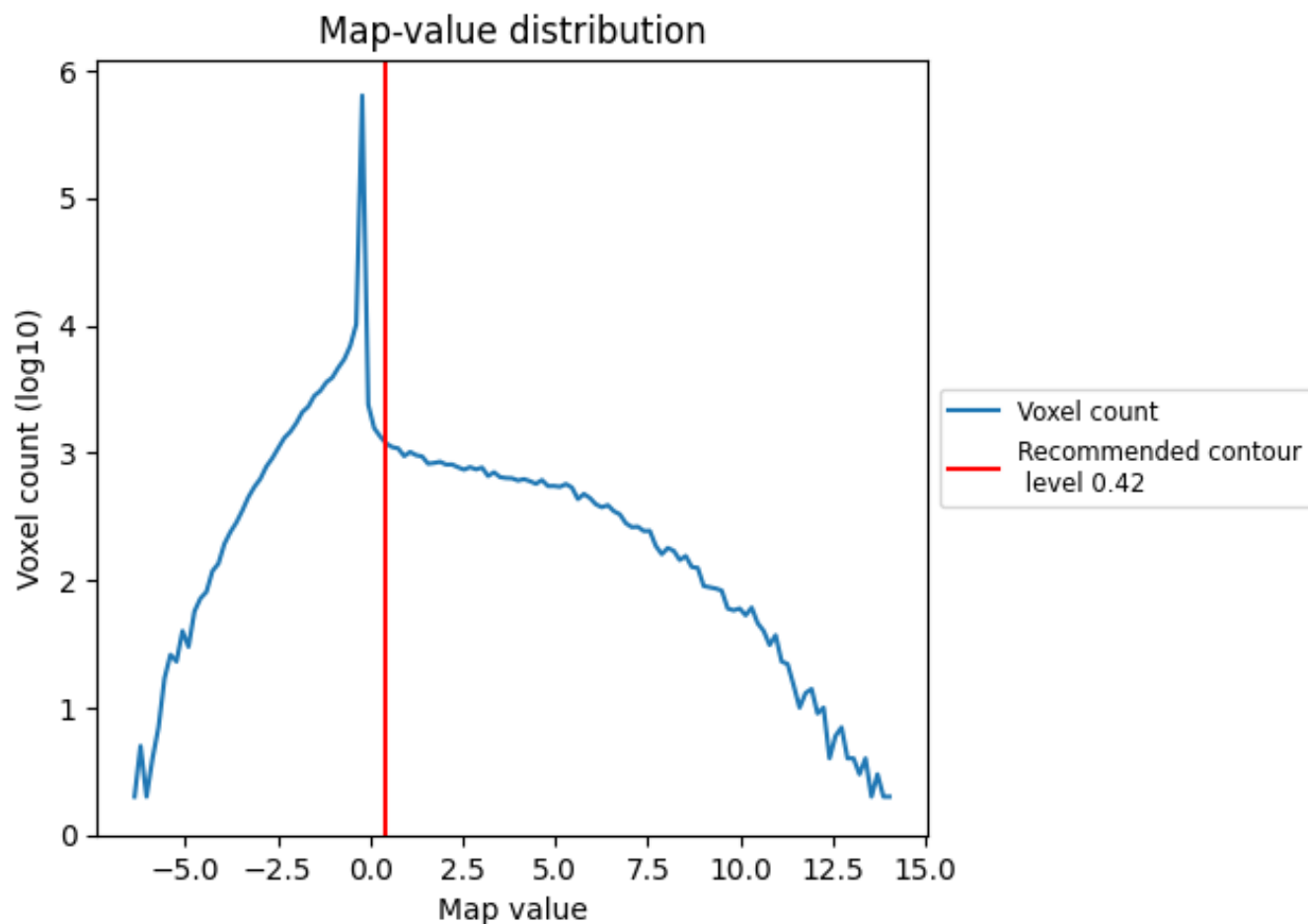
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

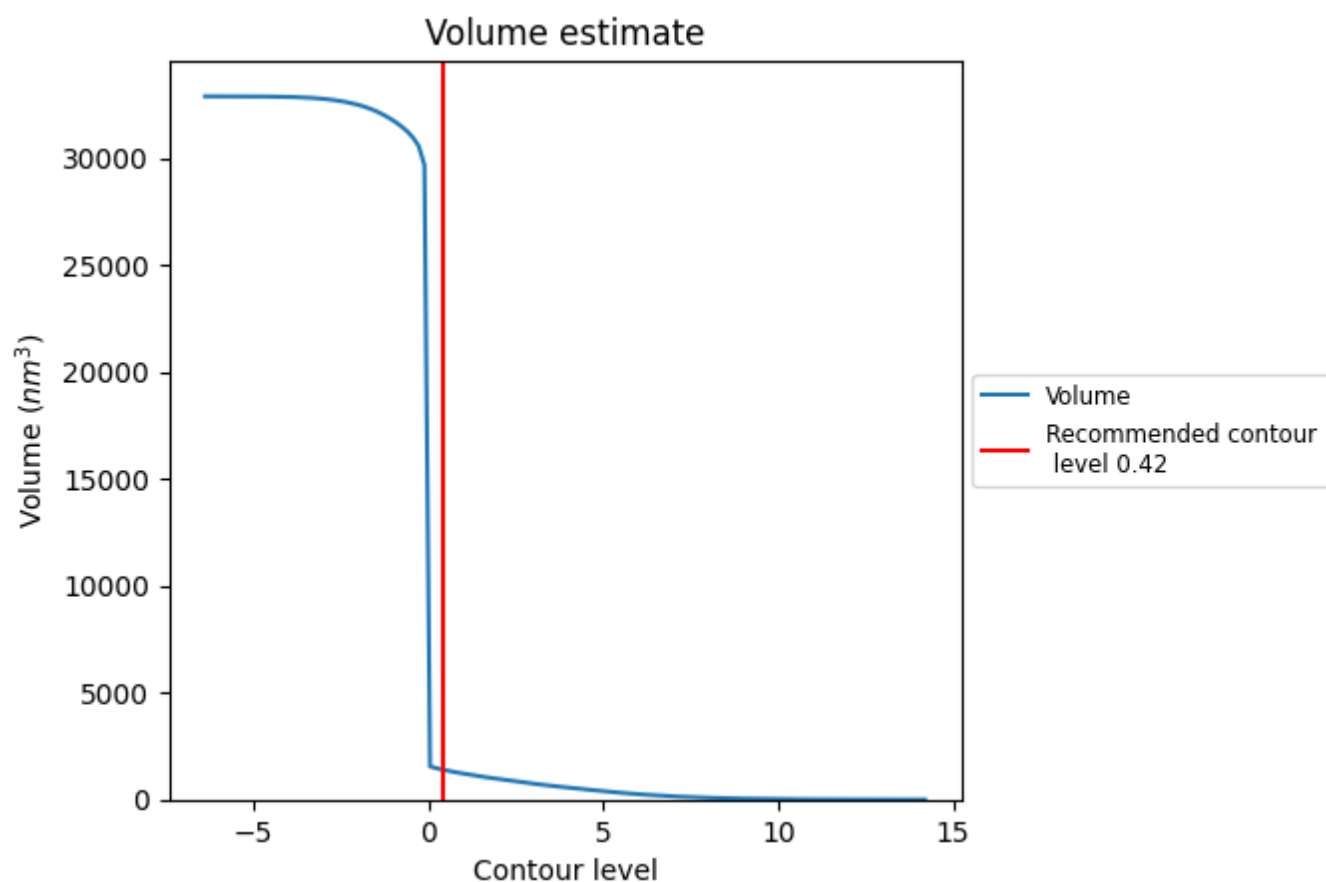
This section contains the results of statistical analysis of the map.

6.1 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.

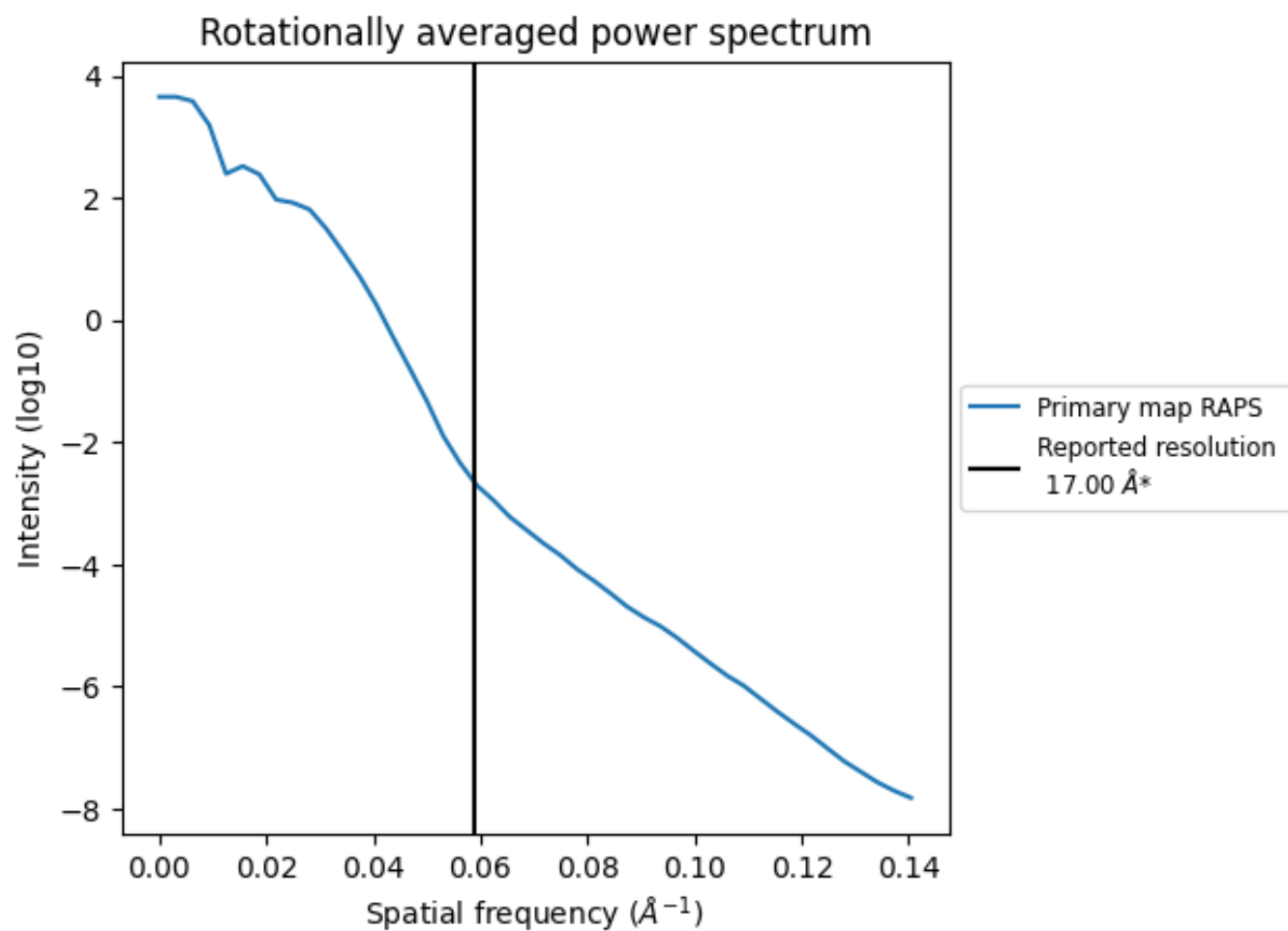
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 1394 nm³; this corresponds to an approximate mass of 1259 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.

6.3 Rotationally averaged power spectrum ⓘ

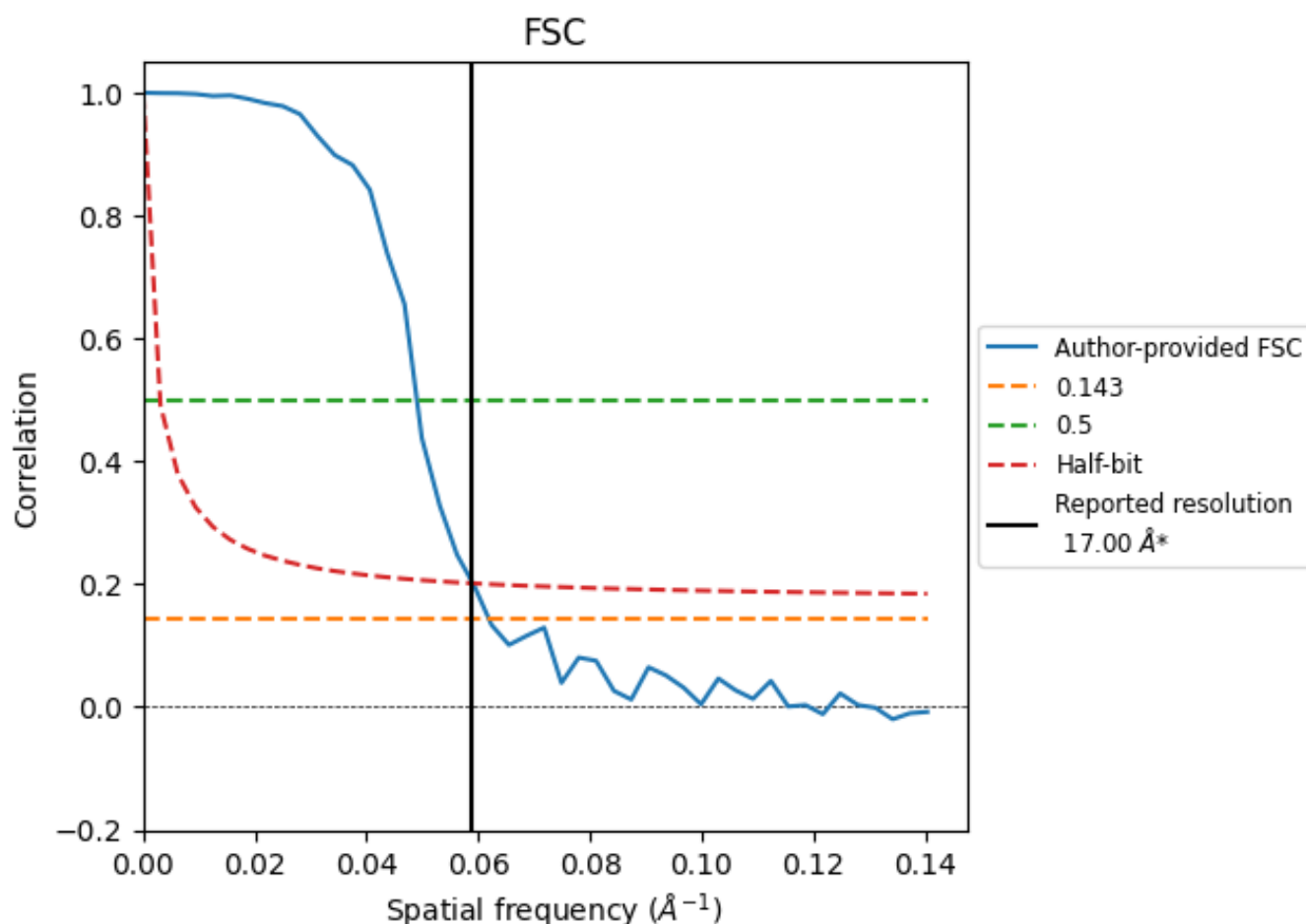


*Reported resolution corresponds to spatial frequency of 0.059 Å⁻¹

7 Fourier-Shell correlation [i](#)

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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.059 Å⁻¹

7.2 Resolution estimates [i](#)

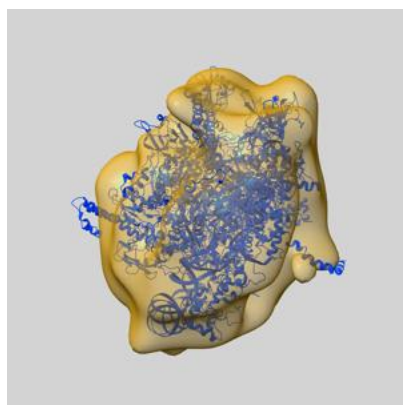
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	17.00
Author-provided FSC curve	16.16	20.41	16.95
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

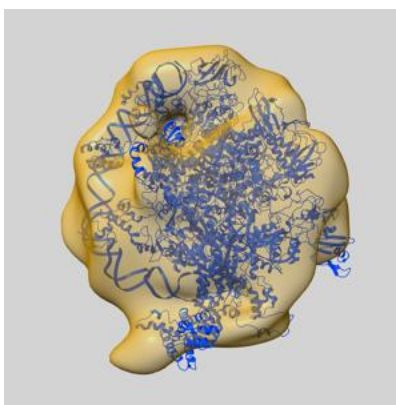
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0340 and PDB model 6N4C. Per-residue inclusion information can be found in section ?? on page ??.

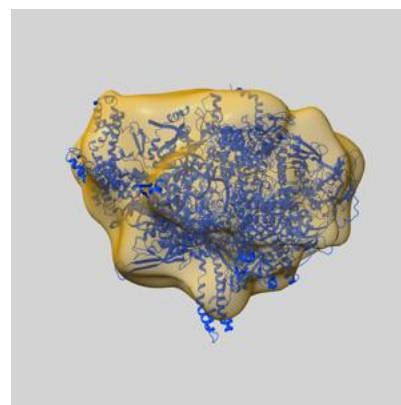
8.1 Map-model overlay [i](#)



X



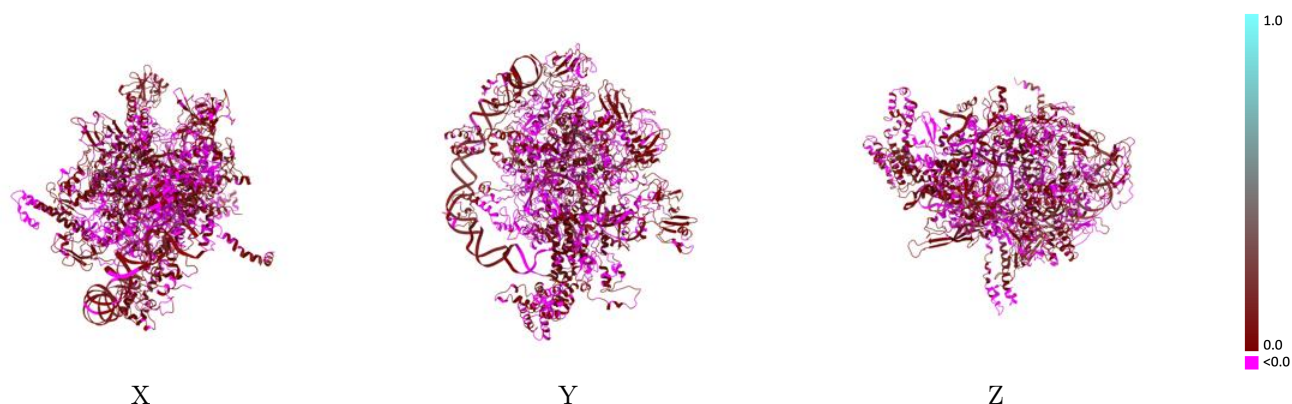
Y



Z

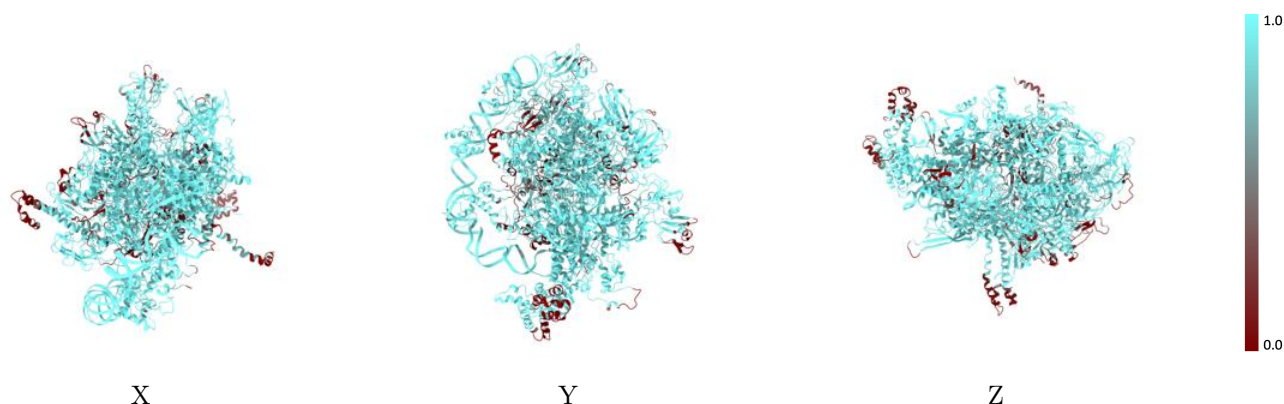
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



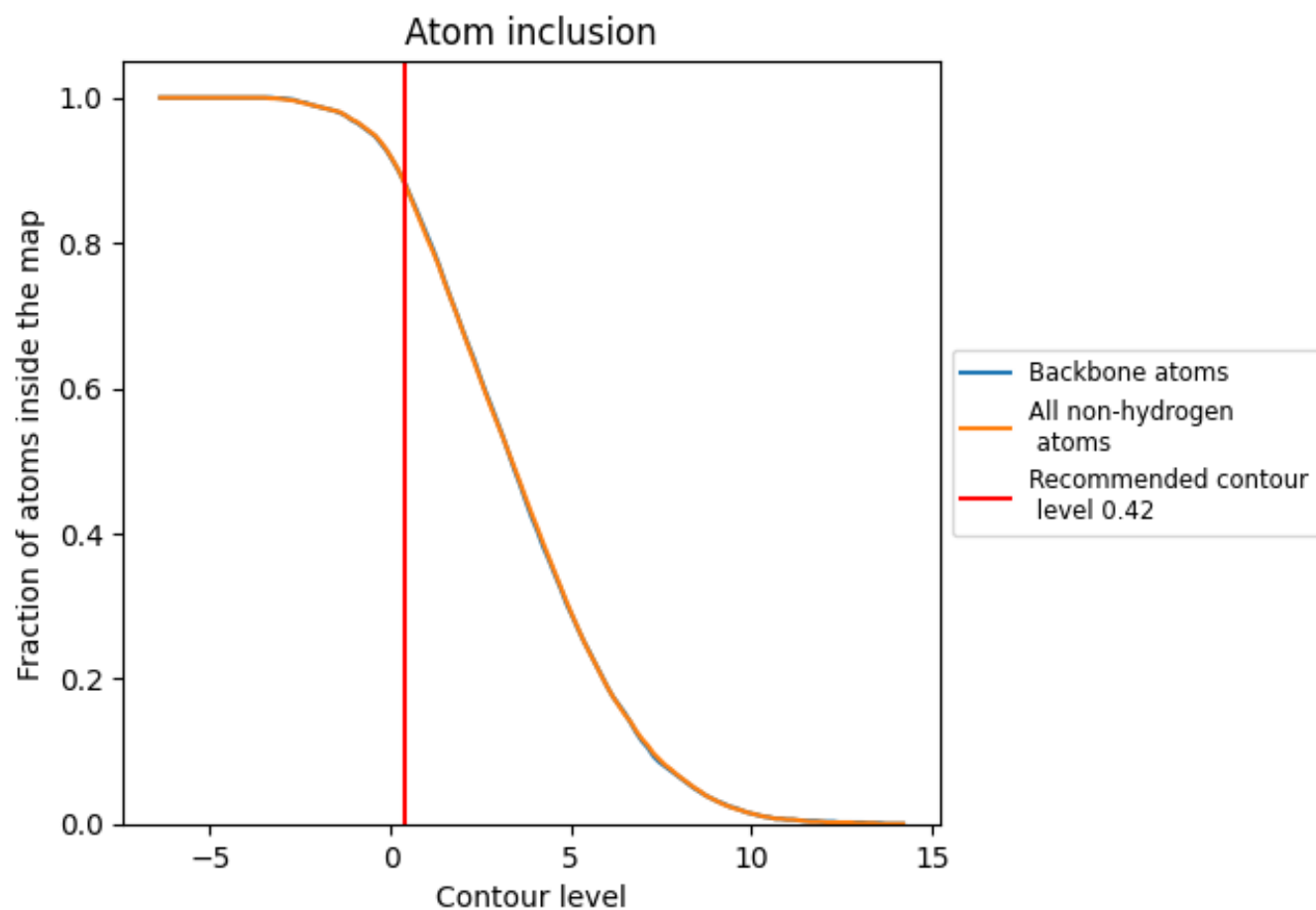
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 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 (0.42).

8.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.0190
A	0.8800	0.0210
B	0.8460	0.0110
C	0.8480	0.0190
D	0.9260	0.0140
E	0.6310	0.0120
F	0.8030	0.0170
a	0.9870	0.0410
b	0.9530	0.0440

1.0

0.0

<0.0