



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 03:25 AM UTC

PDB ID : 9PNW / pdb_00009pnw
EMDB ID : EMD-71774
Title : N4 vRNAP gp50 bound to P1 promoter - closed complex
Authors : Bellis, N.F.; Lokareddy, R.K.; Cingolani, G.
Deposited on : 2025-07-21
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.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

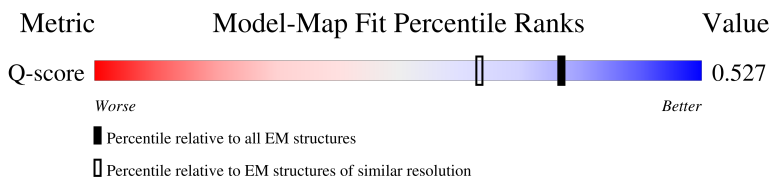
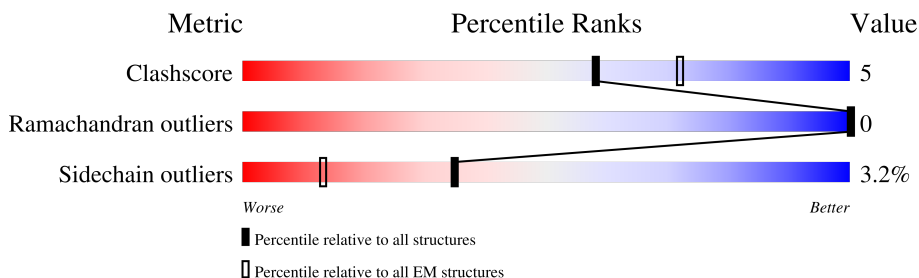
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 $\leq 5\%$. 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	B	34	18% 53% 44%
2	A	3500	61% 9% 30%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19392 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 DNA chain called N4 P1 DNA Promoter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	19	Total	C	N	O	P	0	0
			392	186	78	109	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2443	Total	C	N	O	S	0	0
			19000	11931	3297	3681	91		

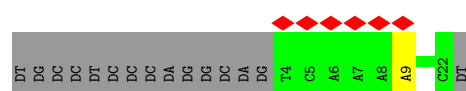
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3218	ALA	SER	conflict	UNP Q859P9

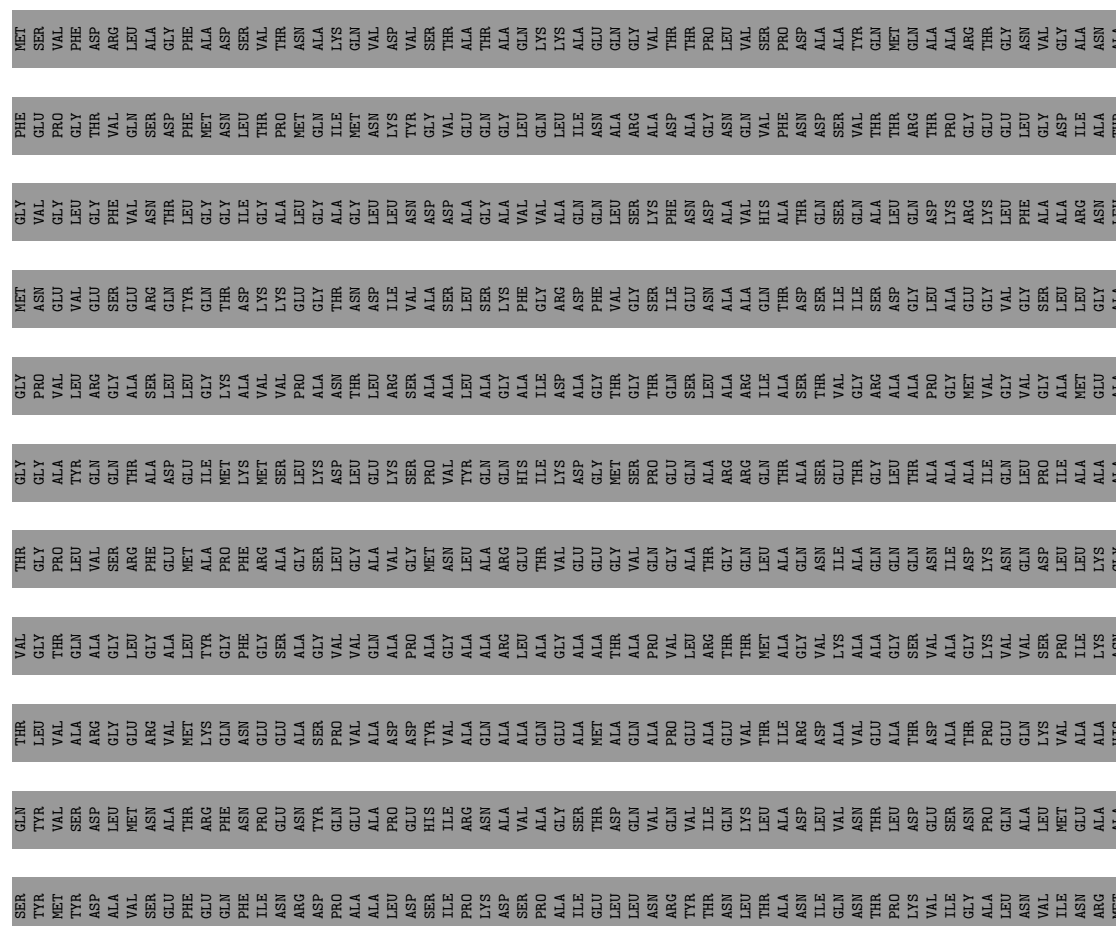
3 Residue-property plots [i](#)

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.

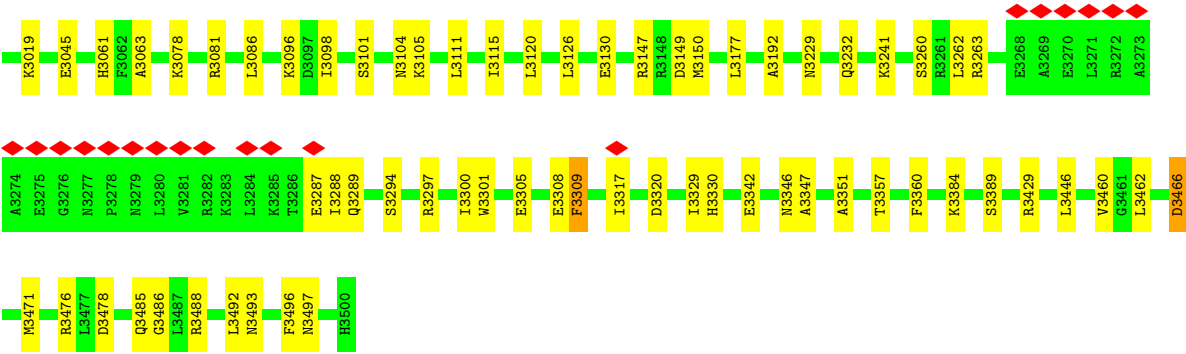
- Molecule 1: N4 P1 DNA Promoter



- Molecule 2: Virion DNA-directed RNA polymerase



V2723	K2559	F2360	Q2186	L2072	L1671	M1480	L1200	K1042	ALA
D2730	K2560	S2361	T2190	S2073	S1688	S1481	M1235	S1043	ILE
H2737	T2570	L2363	E2086	K2086	S1688	S1481	M1235	L1052	LYS
T2740	M2584	M2371	E2196	E2090	I1711	L1487	M1256	A1056	PRO
T2760	K2589	R2372	E2198	V2099	R1750	N1491	I1259	Q1057	GLN
Q2761	D2598	S2373	A2200	A2100	K1751	L1492	D1280	R1062	ASN
K2764	E2602	Q2374	Q2201	ALA	K1764	N1511	D1262	A1063	ILE
T2765	M2605	P2375	Q2201	ALA	G1765	A1512	M1263	R1064	GLY
R2771	Y2615	E2396	G2203	ARG	A1781	V1513	I1272	N1075	ASN
S2786	D2616	Q2400	G2204	ALA	A1781	M1517	I1272	ASP	THR
K2787	A2617	V2409	M2204	GLU	M1785	R1523	S1283	K1084	ALA
K2790	T2620	R2414	I2205	VAL	M1786	K1524	S1283	R1085	GLN
L2796	S2641	V2418	D2212	THR	Q1820	D1543	L1293	L1089	LYS
K2816	E2642	T2419	D2213	VAL	K1835	K1544	T1297	M1090	ASP
N2848	T2642	E2420	S2221	SER	T1841	S1545	F1301	E1094	ASN
L2868	THR	R2423	V2219	LYS	K1841	T1549	V1309	L1108	GLN
E2886	VAL	M2485	S2220	GLU	T1852	V1553	T1322	D1112	VAL
E2902	ILE	E2491	M2223	VAL	A1867	M1566	V1339	K1115	THR
D2909	GLY	M2494	E2257	ASN	E1871	M1567	V1339	N1124	GLU
T2912	ASP	Y2507	R2267	PHE	M1900	T1570	L1358	N1133	ALA
T2921	LYS	T2515	I2271	MET	T1575	T1575	D1371	T1134	LEU
P2922	VAL	N2519	S2272	V2124	P1576	D1577	K1375	V1135	LEU
Y2953	ALA	L2520	K2273	S2137	D1577	I1582	L1391	D1140	THR
R2960	GLY	V2521	R2328	A2138	I1582	N1587	Q1401	T1141	LYS
K2964	VAL	GLU	S2329	I2141	K1945	S1601	H1411	F1142	THR
L2981	A2684	ASP	Q2333	R2142	T1946	S1601	H1411	R1160	GLU
L2982	Q2678	ALA	D2337	N2143	D1948	D1607	T1417	A1163	VAL
Q2983	E2680	LYS	K2344	L2144	S1971	Q1636	V1418	T1167	THR
Q2990	K2684	ARG	E2347	A2145	E2010	Q1636	V1418	K1170	VAL
D2993	T2697	S2530	G2348	E2160	Y2011	L1648	G1420	D1171	GLY
T2996	P2698	L2531	R2349	Q2154	T2018	G1654	P1430	D1174	LYS
R3007	H2700	I2549	Q2350	E2174	L2052	E1655	Q1431	T1179	THR
I3008	E2713	K2554	Q2351	T2176	S2053	N1656	V1436	Q1183	VAL
T3009	V2716	P2556	A2352	T2176	M2057	A1658	R1437	L1196	GLN
		K2556	L2355	V2180	N2066	E1660	S1450	L1190	THR
		T2556	G2356	A2181	N2067	L1661	Q1461	F1194	VAL
			E2357	E2182	K2069	K1662	L1468	D1195	VAL
					I2070	R1663	M1475		
					D2071	K1667			
						N1668			



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128569	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.306	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0431	Depositor
Map size (Å)	389.44, 389.44, 389.44	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.217, 1.217, 1.217	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	B	0.14	0/441	0.26	0/678
2	A	0.08	0/19302	0.23	0/26087
All	All	0.08	0/19743	0.23	0/26765

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	B	392	0	213	1	0
2	A	19000	0	19100	182	0
All	All	19392	0	19313	182	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 5.

The worst 5 of 182 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)
2:A:2223:MET:HA	2:A:2223:MET:HE2	1.74	0.68
2:A:3007:ARG:NH2	2:A:3460:VAL:O	2.26	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2141:ILE:HG22	2:A:2142:ARG:HH21	1.62	0.65
2:A:3192:ALA:HB2	2:A:3330:HIS:HB2	1.81	0.62
2:A:2529:THR:HG23	2:A:2531:LEU:H	1.65	0.61

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	
2	A	2419/3500 (69%)	2379 (98%)	40 (2%)	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	
2	A	2047/2874 (71%)	1982 (97%)	65 (3%)	34	68

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3130	GLU
2	A	3260	SER
2	A	2073	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	2053	SER
2	A	3308	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	2737	HIS
2	A	3255	ASN
2	A	3232	GLN
2	A	3277	ASN
2	A	1979	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.

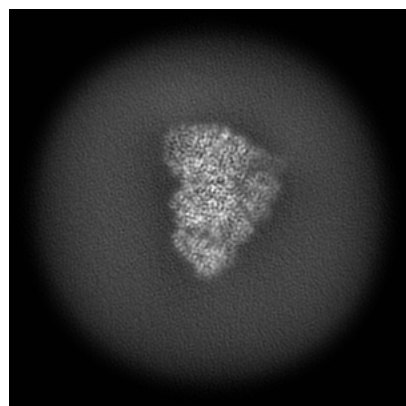
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71774. These allow visual inspection of the internal detail of the map and identification of artifacts.

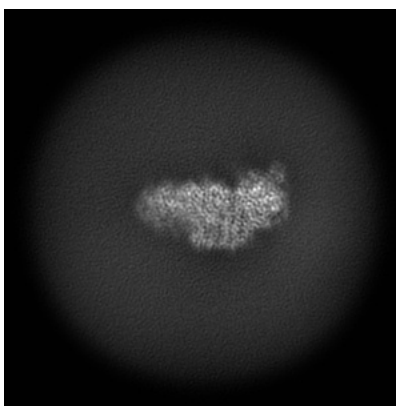
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

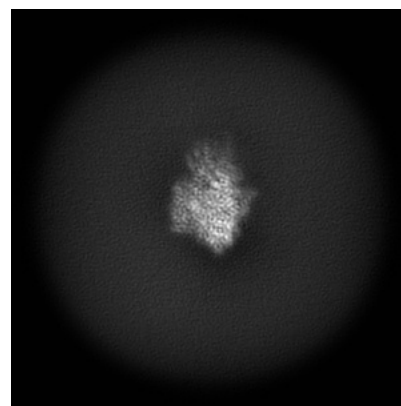
6.1.1 Primary map



X

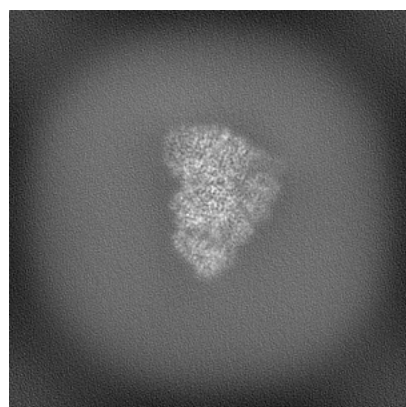


Y

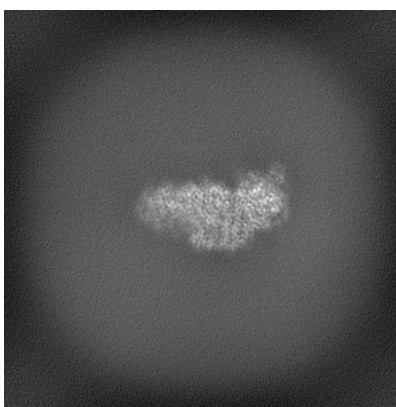


Z

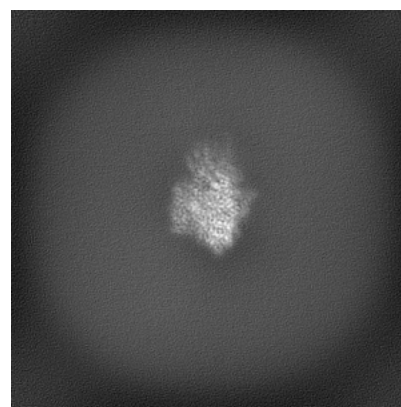
6.1.2 Raw map



X



Y

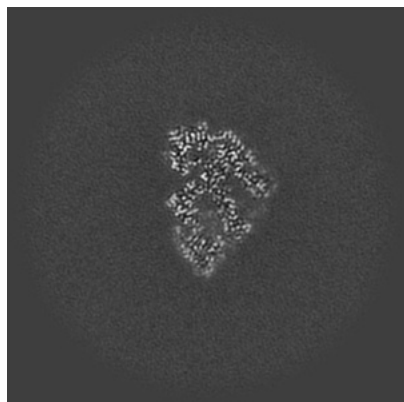


Z

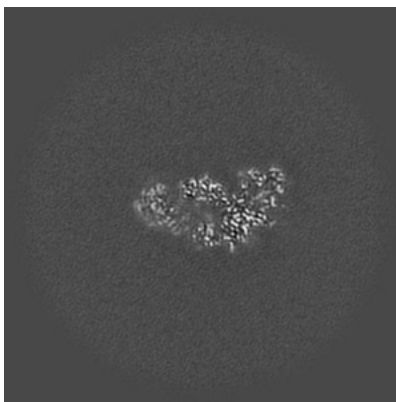
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

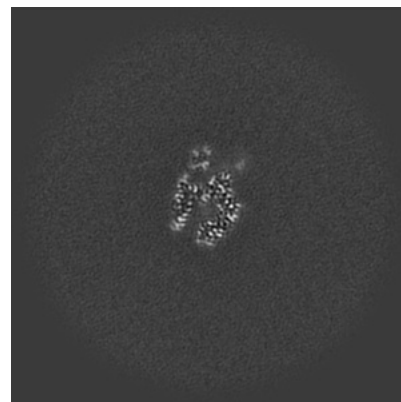
6.2.1 Primary map



X Index: 160

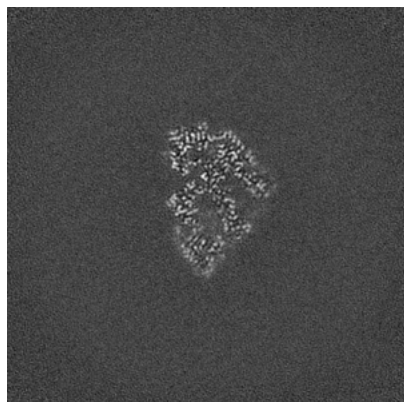


Y Index: 160

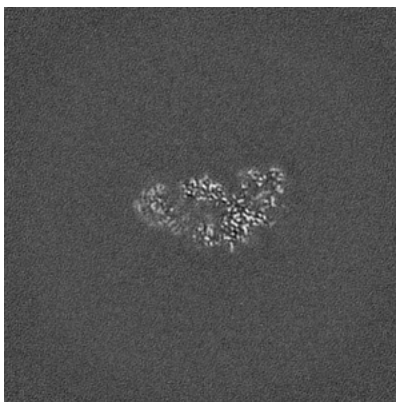


Z Index: 160

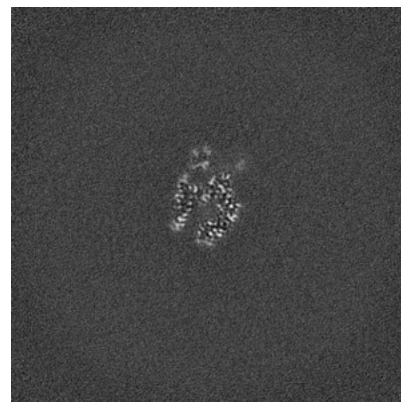
6.2.2 Raw map



X Index: 160



Y Index: 160

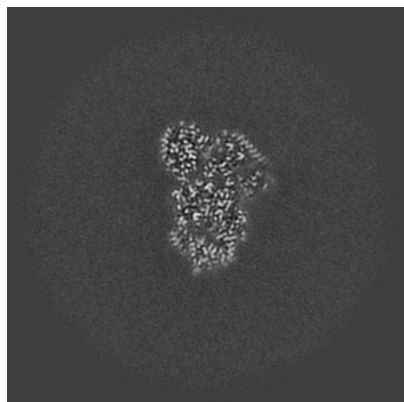


Z Index: 160

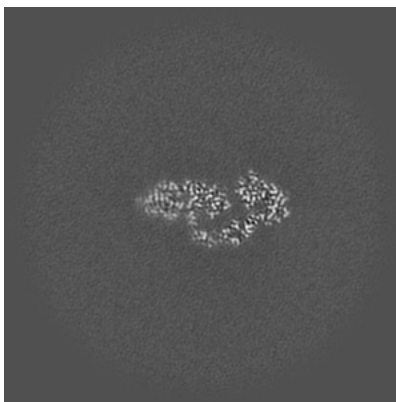
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

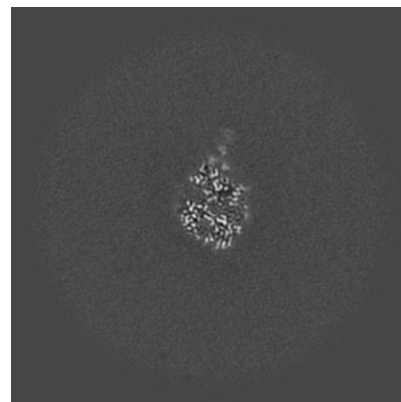
6.3.1 Primary map



X Index: 166

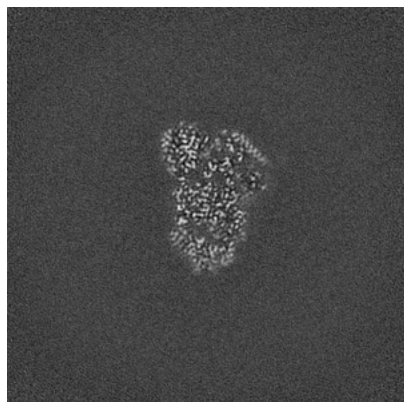


Y Index: 149

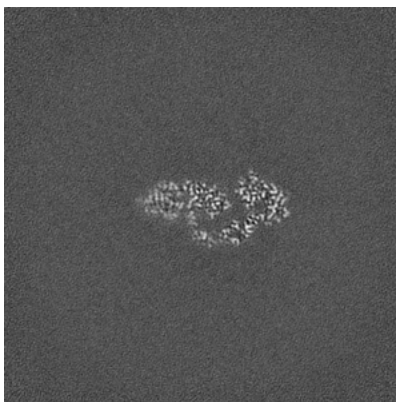


Z Index: 195

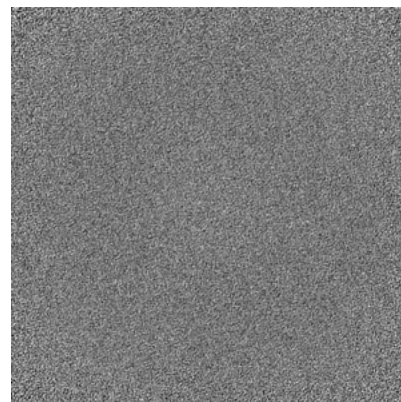
6.3.2 Raw map



X Index: 167



Y Index: 149

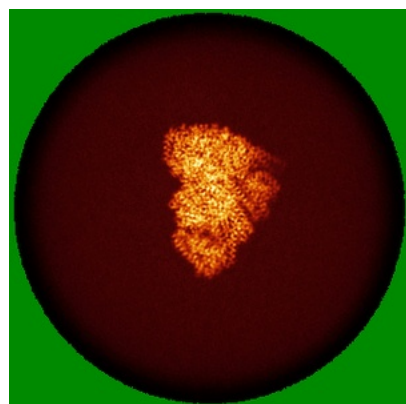


Z Index: 0

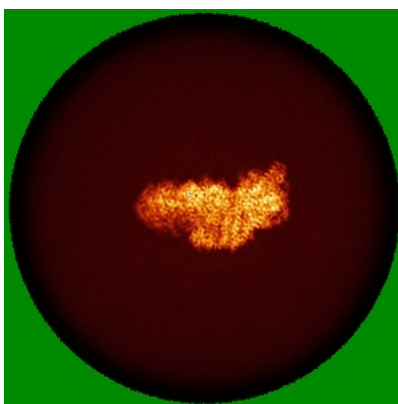
The images above show the largest variance slices of the map in three orthogonal directions.

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

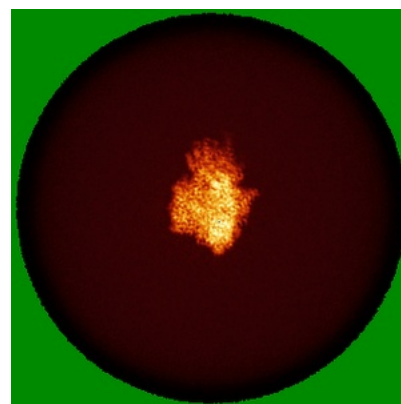
6.4.1 Primary map



X

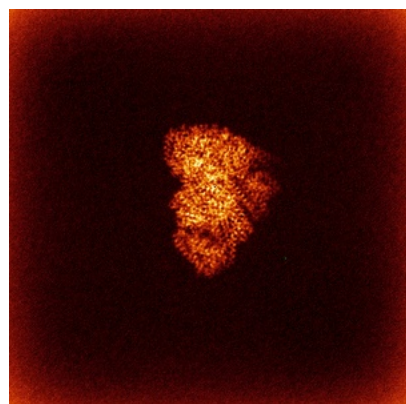


Y

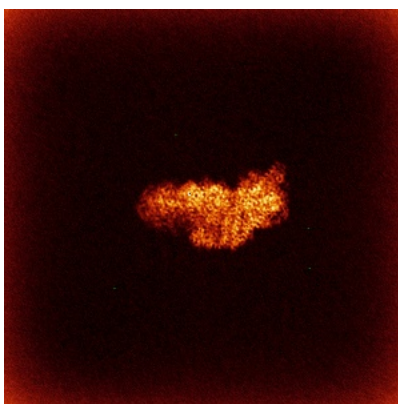


Z

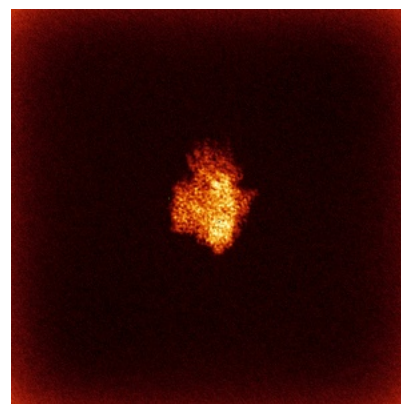
6.4.2 Raw map



X



Y

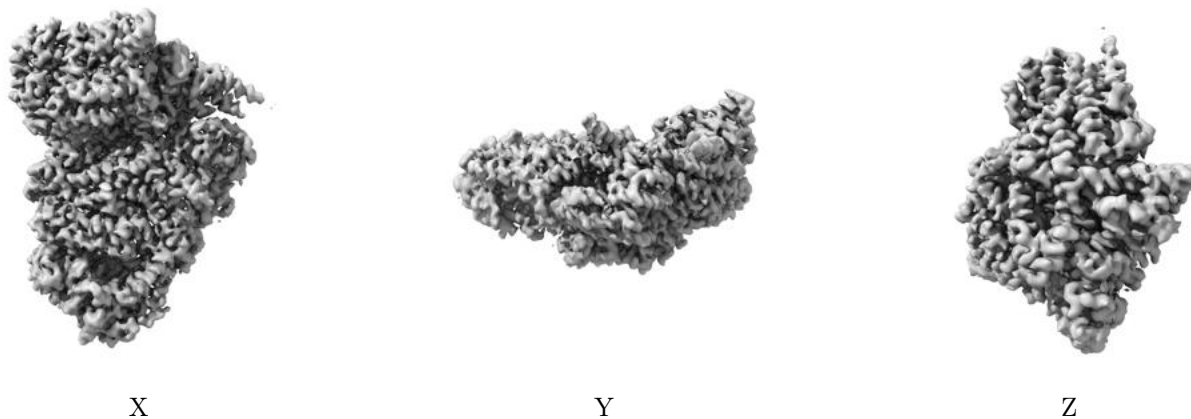


Z

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.

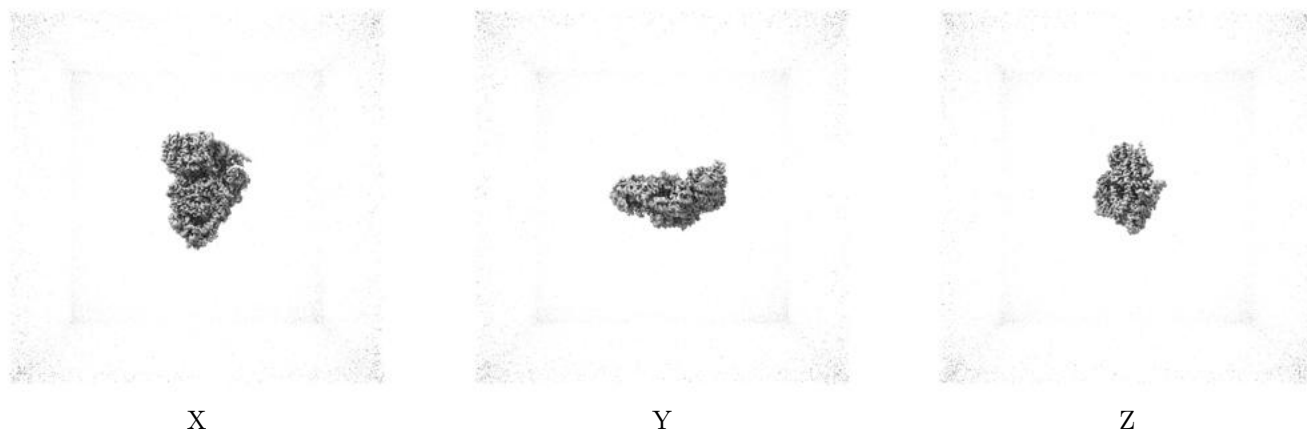
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0431. 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



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.

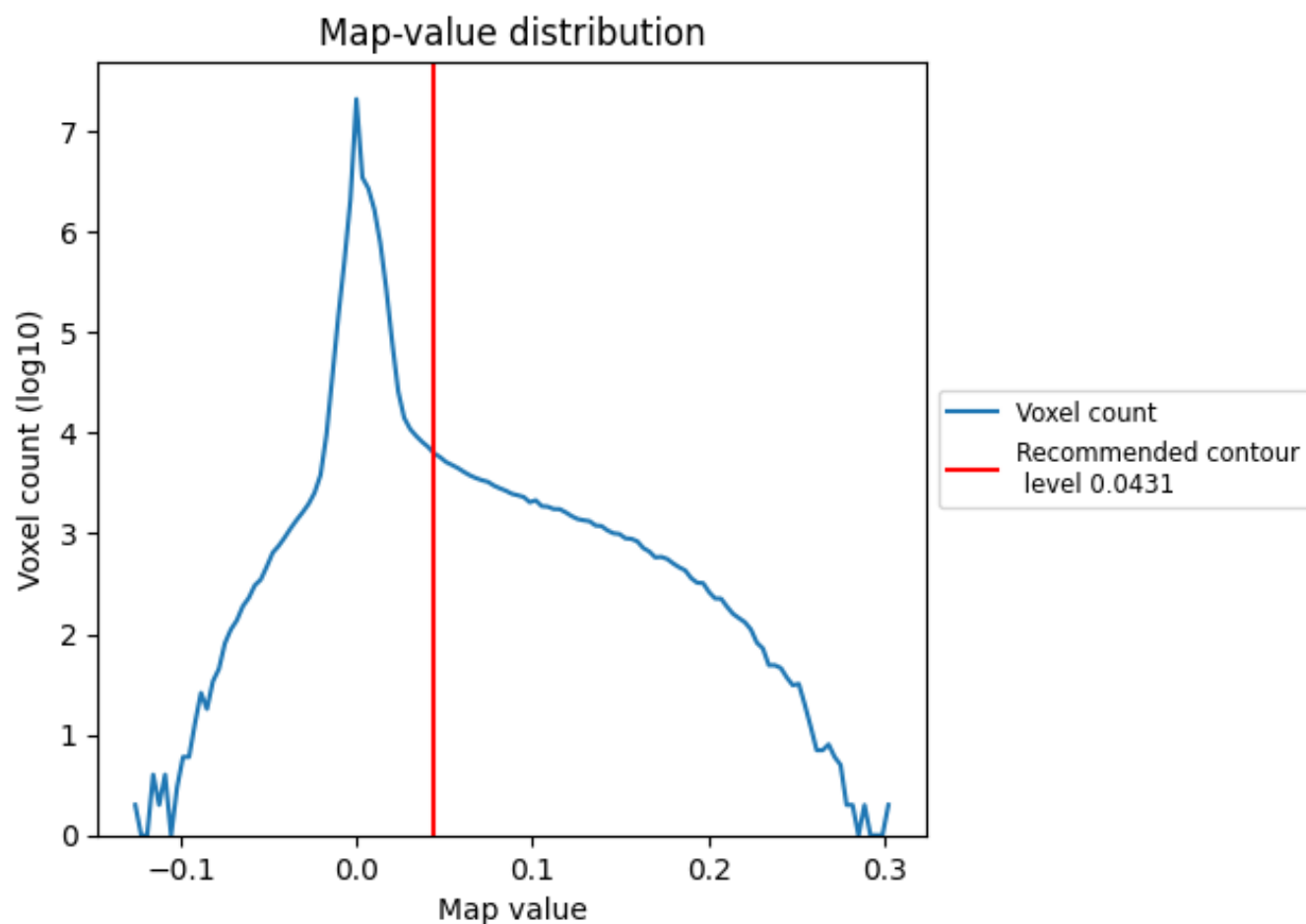
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

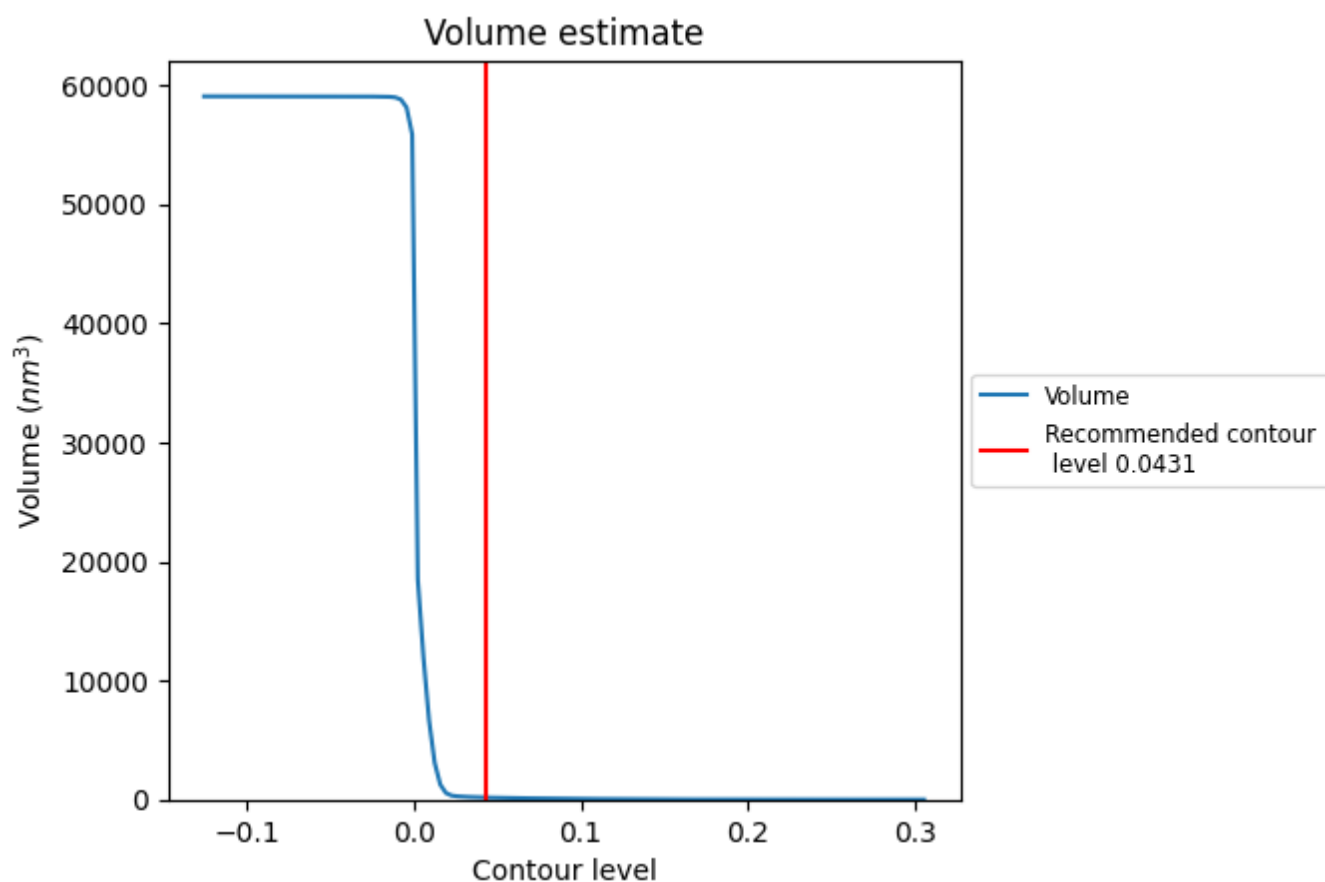
This section contains the results of statistical analysis of the map.

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.

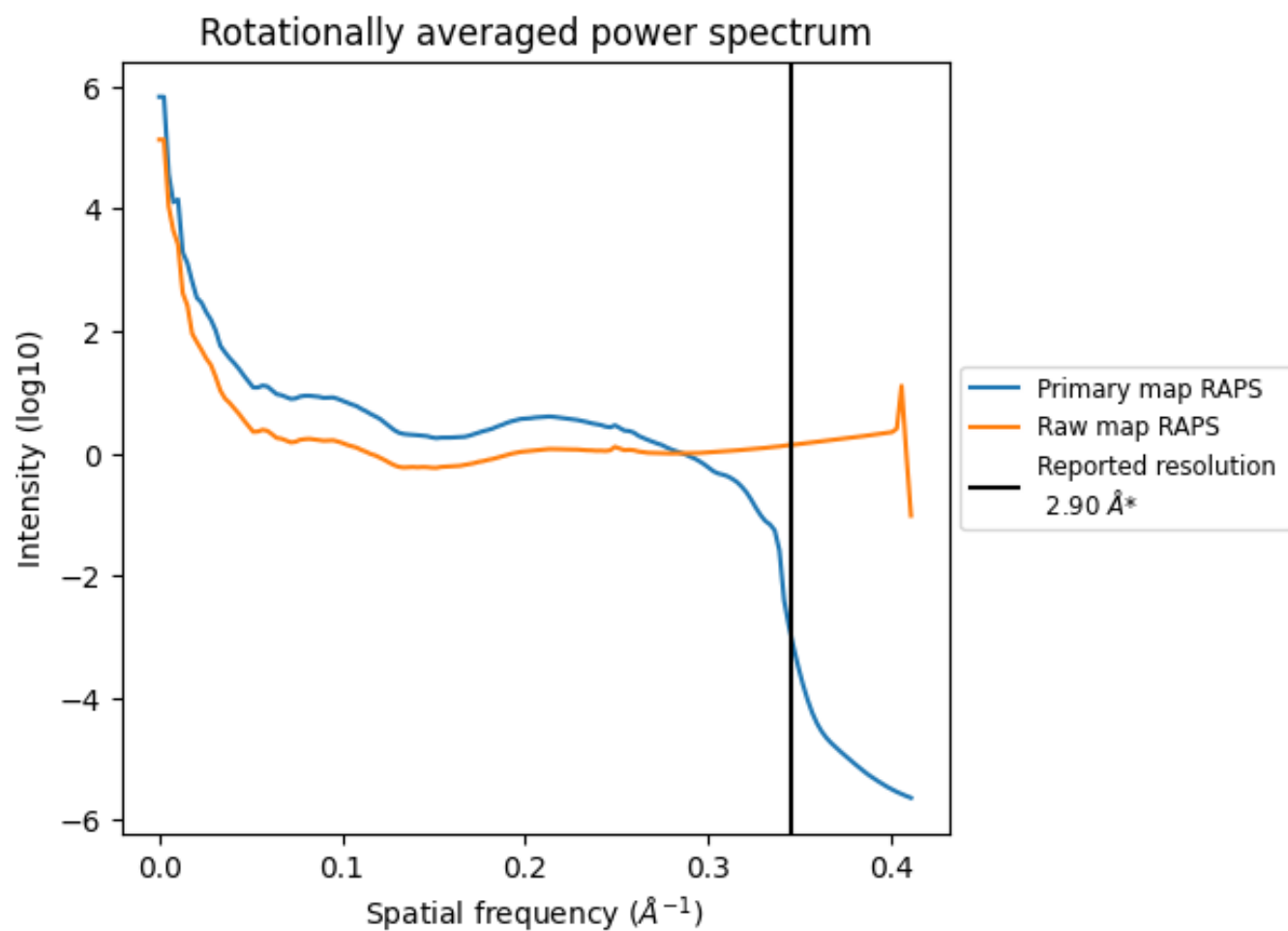
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm³; this corresponds to an approximate mass of 157 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 ⓘ

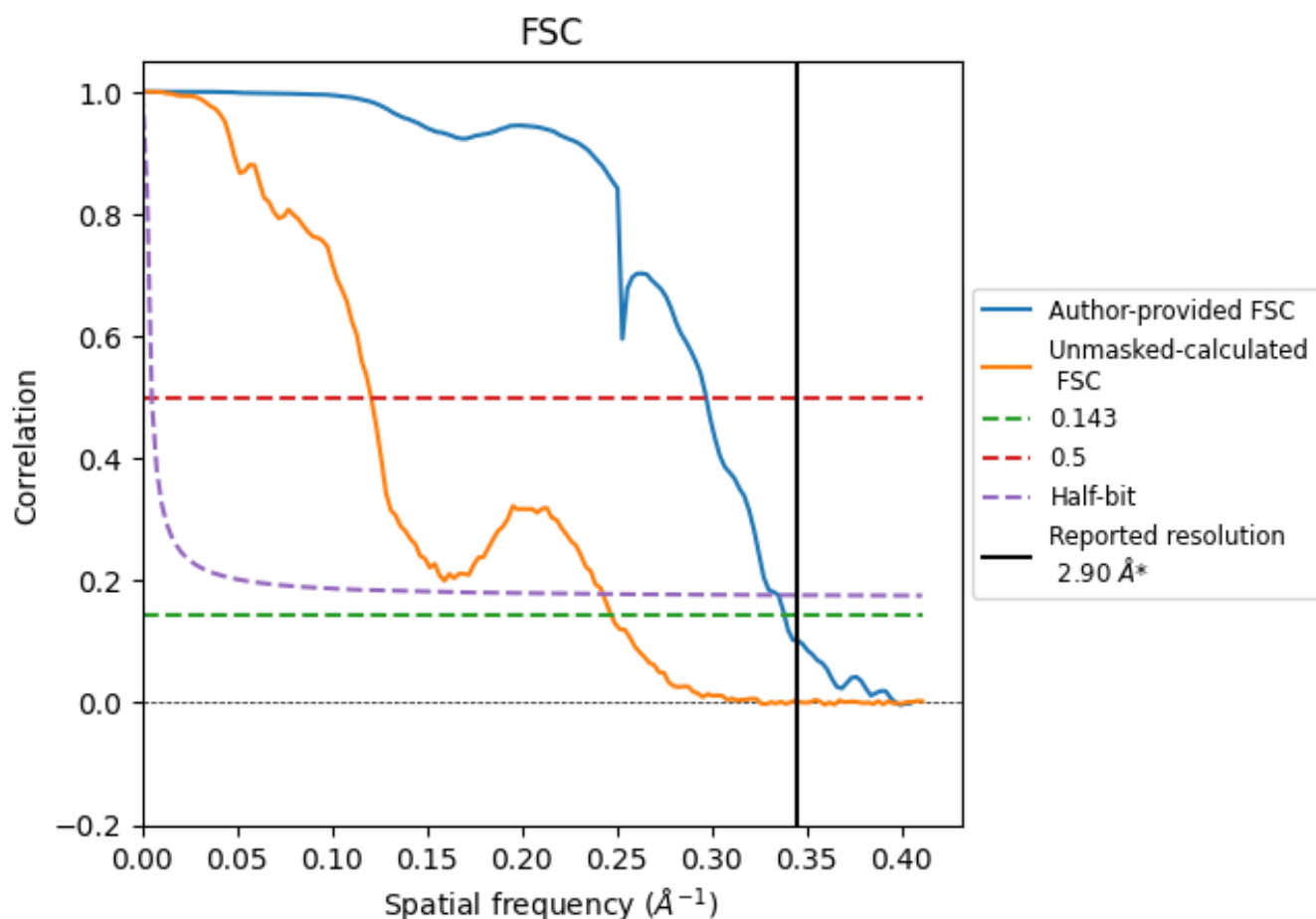


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 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.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

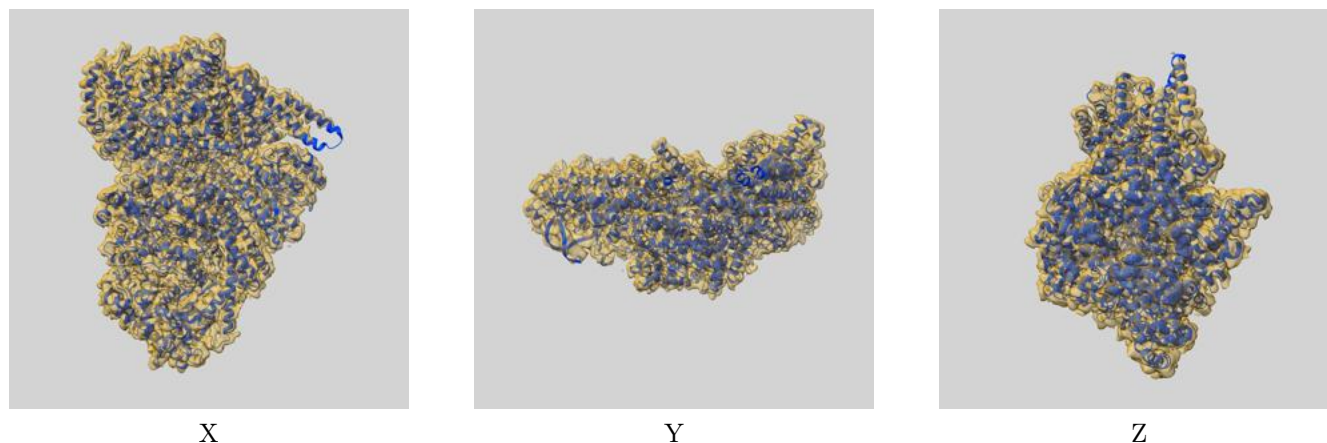
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.96	3.37	2.98
Unmasked-calculated*	4.05	8.30	4.12

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

9 Map-model fit [i](#)

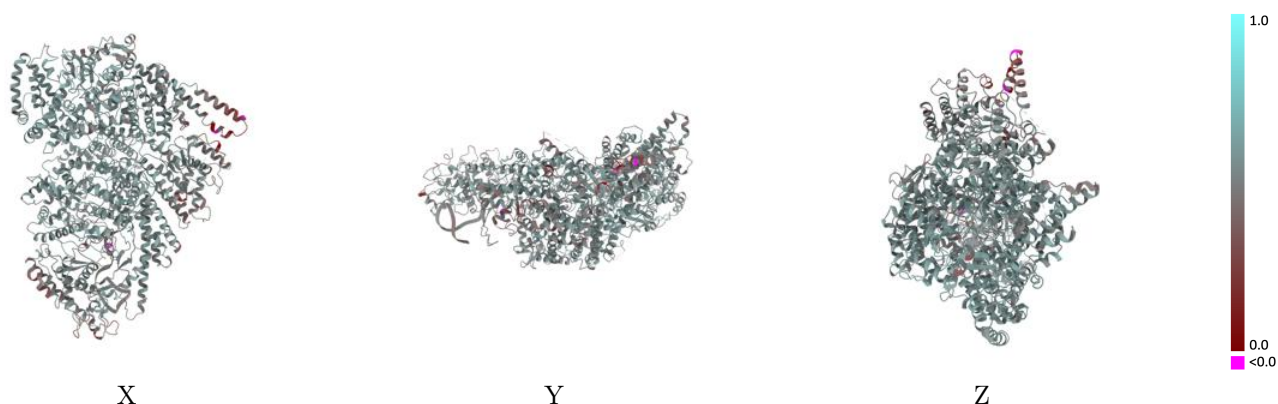
This section contains information regarding the fit between EMDB map EMD-71774 and PDB model 9PNW. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



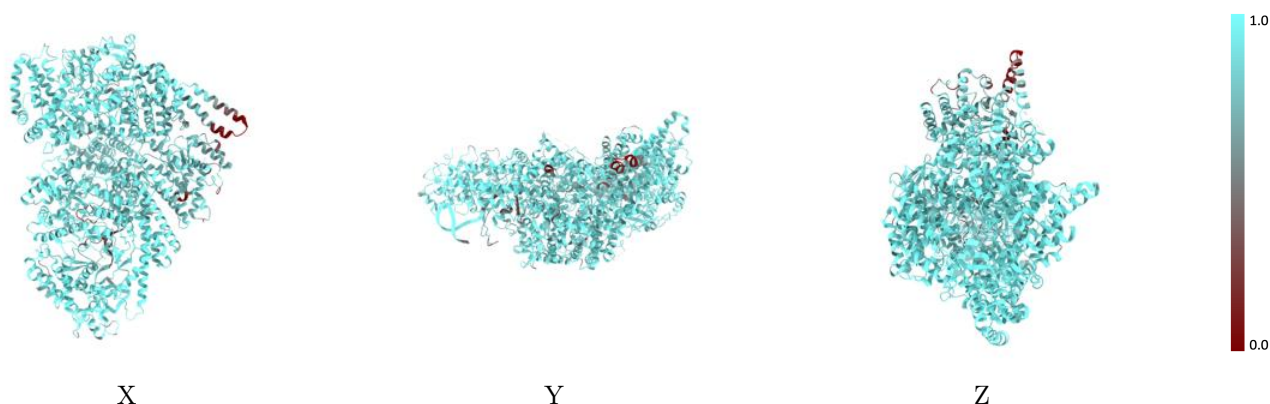
The images above show the 3D surface view of the map at the recommended contour level 0.0431 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



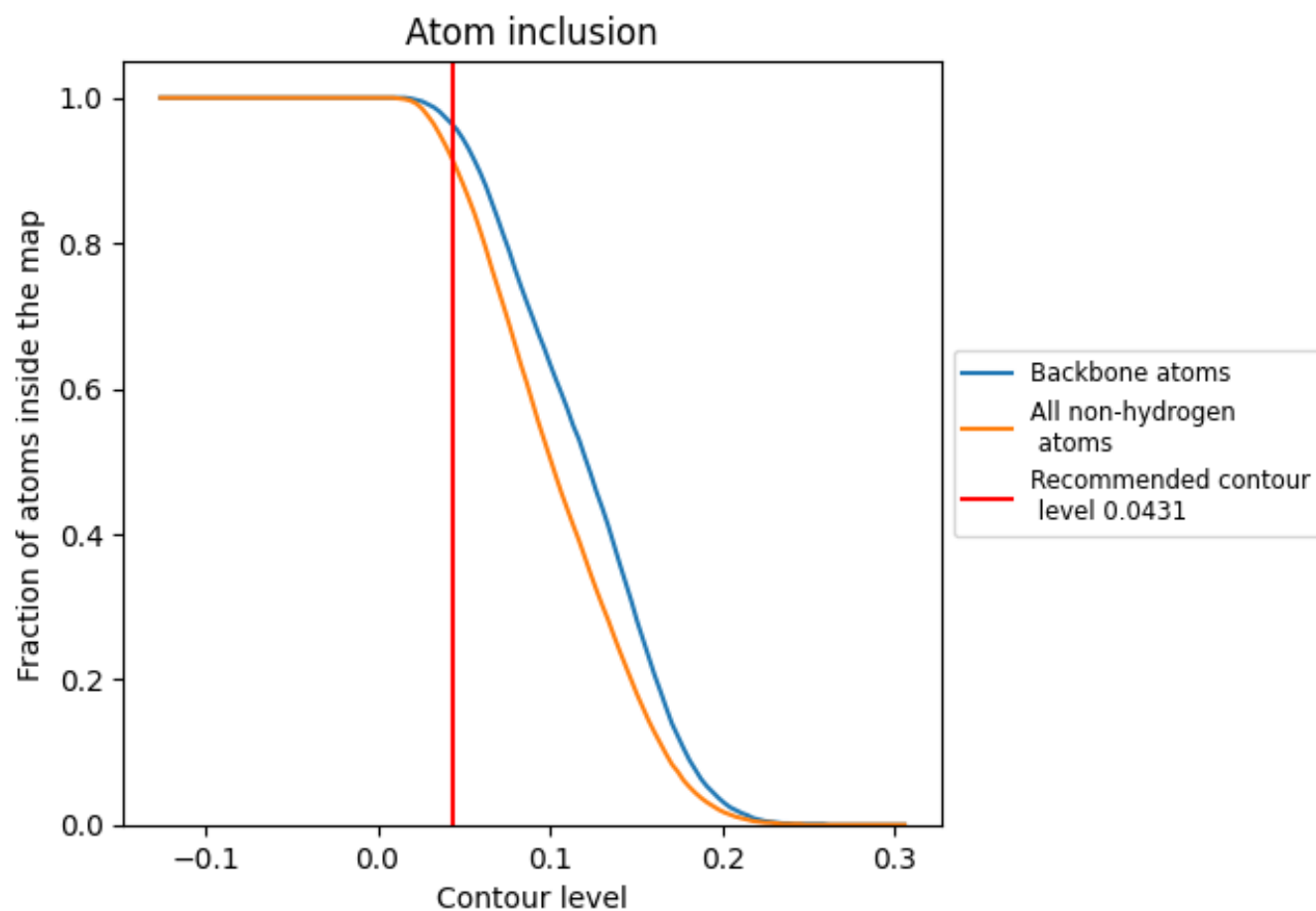
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0431).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.0431) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9170	0.5270
A	0.9210	0.5290
B	0.7170	0.4330

