



wwPDB EM Validation Summary Report ⓘ

Nov 12, 2024 – 06:28 PM EST

PDB ID : 9DBY
EMDB ID : EMD-46728
Title : ncPRC1RYBP bound to singly modified H2AK119Ub nucleosome
Authors : Godinez-Lopez, V.; Valencia-Sanchez, M.I.; Armache, J.P.; Armache, K.-J.
Deposited on : 2024-08-24
Resolution : 2.80 Å (reported)
Based on initial models : 8H1T, 1UBQ, ., 8SVF, 2D9G, 3tu4, 4R8P

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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

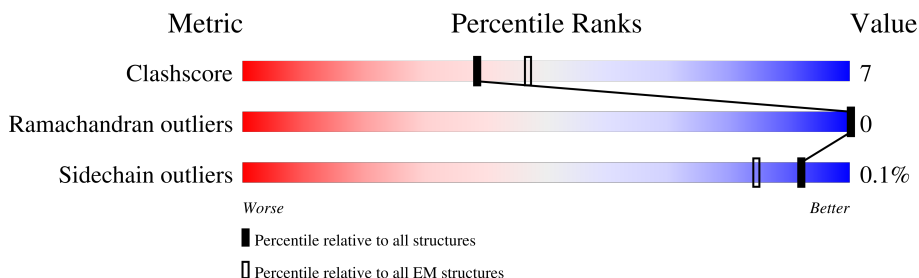
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.




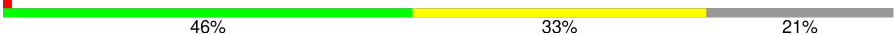




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	136	
1	E	136	
2	B	103	
2	F	103	
3	C	130	
4	D	126	
4	H	126	
5	G	130	

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Mol	Chain	Length	Quality of chain
6	I	187	
7	J	187	
8	K	326	
9	L	336	
10	M	228	
11	N	76	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 14368 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 Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			801	506	153	139	3		
1	E	95	Total	C	N	O	S	0	0
			779	492	148	136	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	engineered mutation	UNP P84233
E	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	83	Total	C	N	O	S	0	0
			658	416	128	113	1		
2	F	85	Total	C	N	O	S	0	0
			668	421	130	116	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	107	Total	C	N	O	0	0
			811	510	158	143		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	engineered mutation	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			718	451	128	137	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	engineered mutation	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281

- Molecule 5 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	108	Total	C	N	O	S	0	0
			821	516	160	144	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	99	ARG	GLY	engineered mutation	UNP P06897
G	118	CYS	LYS	engineered mutation	UNP P06897

- Molecule 6 is a DNA chain called DNA (187-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	148	Total	C	N	O	P	0	0
			3054	1445	574	887	148		

- Molecule 7 is a DNA chain called DNA (187-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	148	Total	C	N	O	P	0	0
			3014	1432	545	889	148		

- Molecule 8 is a protein called Polycomb complex protein BMI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	102	Total	C	N	O	S	0	0
			774	498	132	136	8		

- Molecule 9 is a protein called E3 ubiquitin-protein ligase RING2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	101	Total	C	N	O	S	0	0
			766	480	135	141	10		

- Molecule 10 is a protein called RING1 and YY1-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	42	Total	C	N	O	S	0	0
			312	194	59	55	4		

- Molecule 11 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	N	74	Total	C	N	O	0	0
			461	285	86	90		

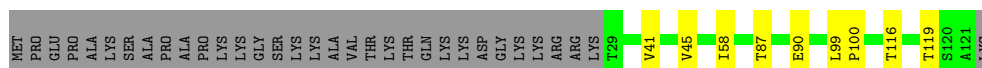
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	76	CYS	GLY	engineered mutation	UNP P0CG47

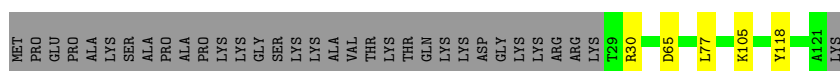
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	K	2	Total	Zn	0
			2	2	
12	L	2	Total	Zn	0
			2	2	
12	M	1	Total	Zn	0
			1	1	

- Molecule 4: Histone H2B 1.1



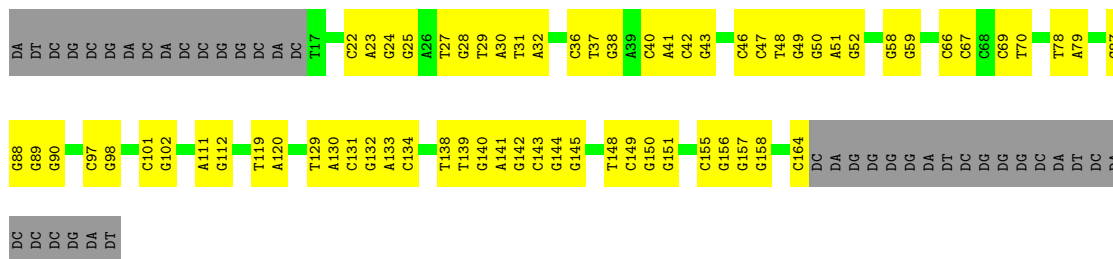
- Molecule 4: Histone H2B 1.1



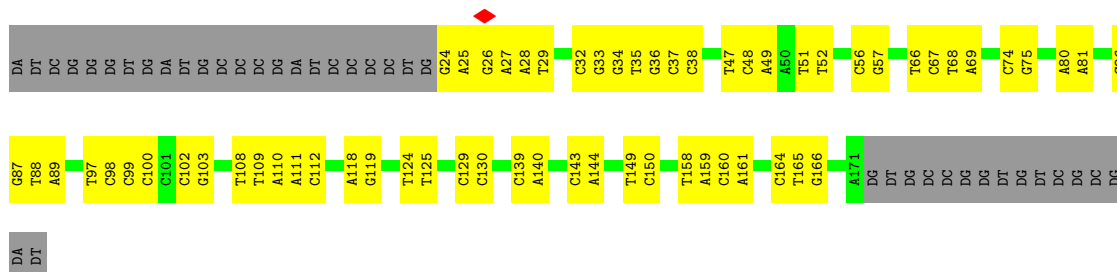
- Molecule 5: Histone H2A type 1



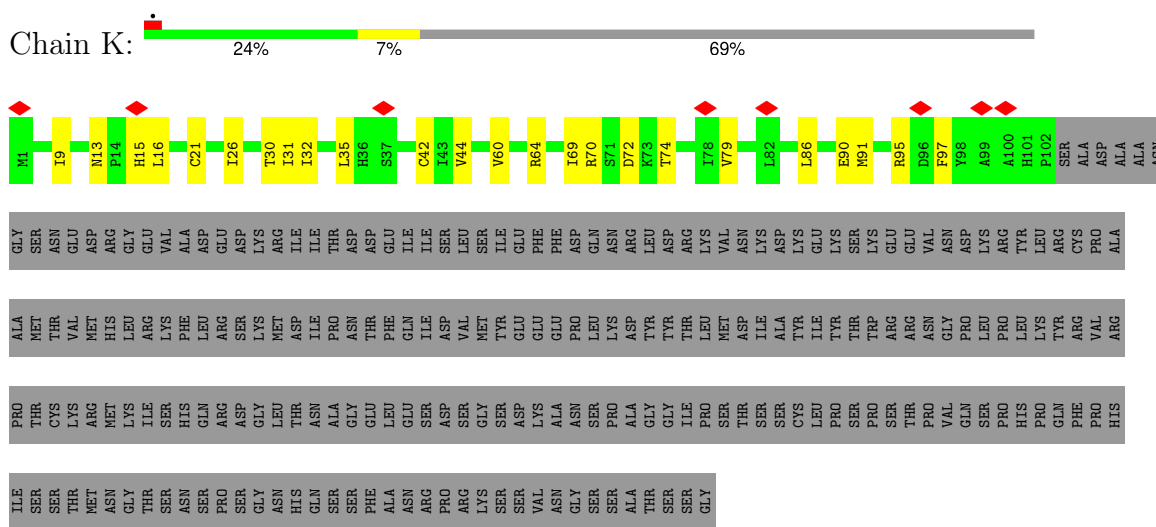
- Molecule 6: DNA (187-MER)



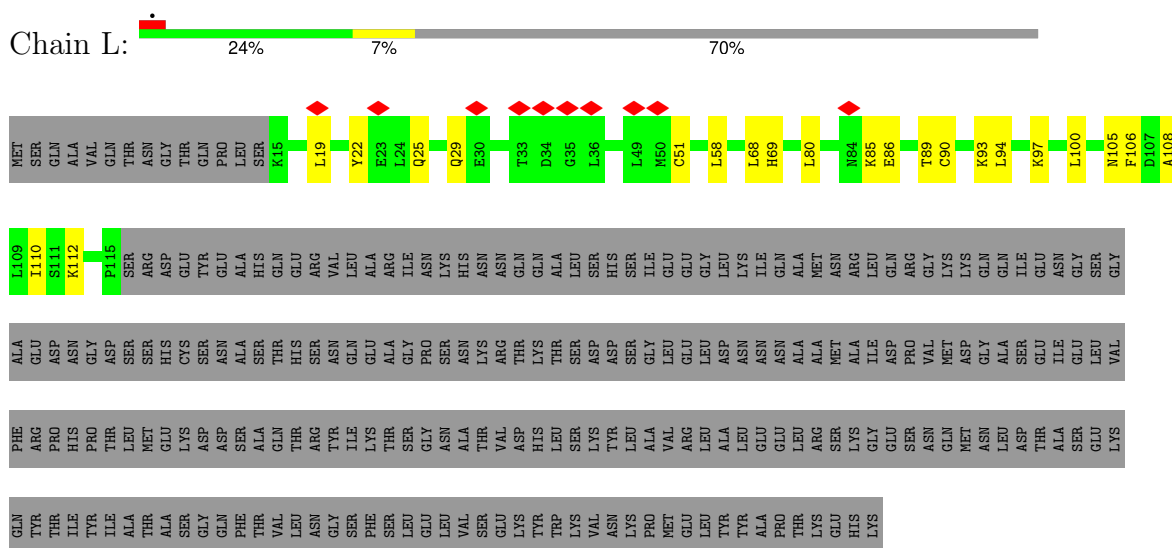
- Molecule 7: DNA (187-MER)



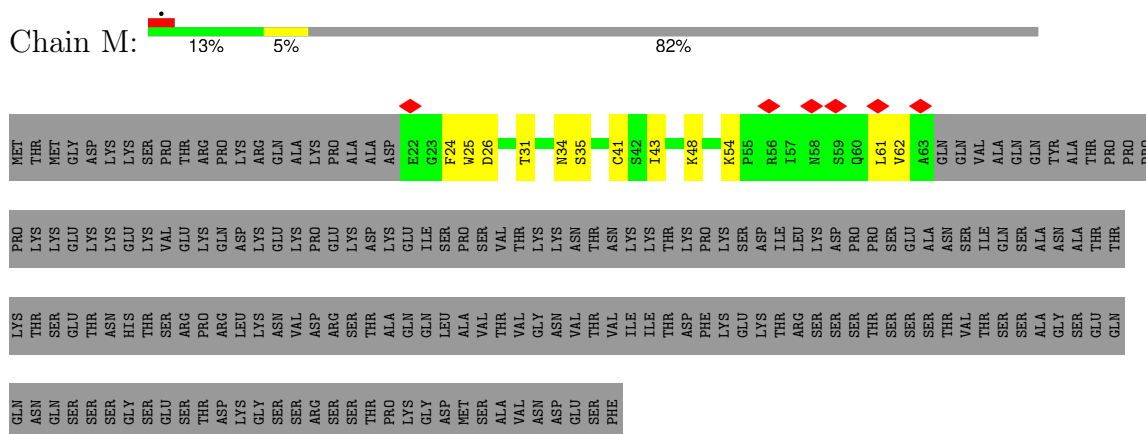
- Molecule 8: Polycomb complex protein BMI-1



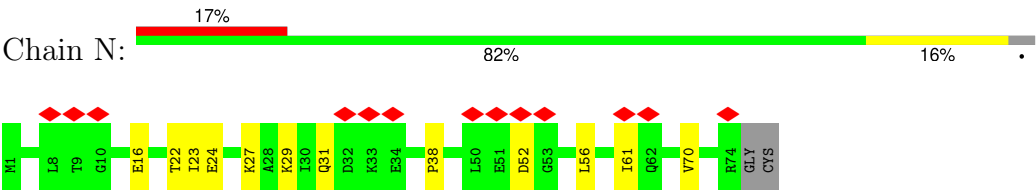
- Molecule 9: E3 ubiquitin-protein ligase RING2



- Molecule 10: RING1 and YY1-binding protein



● Molecule 11: Ubiquitin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	206339	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 ($e^-/\text{\AA}^2$)	50.70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.533	Depositor
Minimum map value	0.000	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.182	Depositor
Map size (Å)	277.1456, 277.1456, 277.1456	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0826, 1.0826, 1.0826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.27	0/813	0.53	0/1093
1	E	0.27	0/789	0.53	0/1059
2	B	0.31	0/665	0.58	0/892
2	F	0.34	0/675	0.56	0/904
3	C	0.37	0/821	0.54	0/1112
4	D	0.27	0/729	0.45	0/985
4	H	0.27	0/737	0.47	0/993
5	G	0.26	0/831	0.55	0/1124
6	I	0.52	0/3430	0.88	0/5297
7	J	0.54	0/3376	0.94	0/5203
8	K	0.30	0/792	0.57	0/1083
9	L	0.25	0/780	0.59	0/1058
10	M	0.27	0/317	0.54	0/426
11	N	0.23	0/463	0.50	0/638
All	All	0.41	0/15218	0.74	0/21867

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	801	0	831	11	0
1	E	779	0	815	5	0
2	B	658	0	697	7	0
2	F	668	0	702	9	0
3	C	811	0	849	5	0
4	D	718	0	725	6	0
4	H	726	0	747	6	0
5	G	821	0	865	7	0
6	I	3054	0	1661	44	0
7	J	3014	0	1662	46	0
8	K	774	0	736	27	0
9	L	766	0	748	22	0
10	M	312	0	299	11	0
11	N	461	0	381	7	0
12	K	2	0	0	0	0
12	L	2	0	0	0	0
12	M	1	0	0	0	0
All	All	14368	0	11718	183	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 183 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)
8:K:30:THR:CG2	9:L:68:LEU:HD21	2.04	0.86
8:K:16:LEU:HD11	8:K:79:VAL:HG12	1.65	0.79
8:K:30:THR:HG21	9:L:68:LEU:HD21	1.67	0.75
10:M:61:LEU:HG	10:M:62:VAL:H	1.51	0.73
10:M:61:LEU:HG	10:M:62:VAL:N	2.05	0.71

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	96/136 (71%)	95 (99%)	1 (1%)	0	100	100
1	E	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
2	B	81/103 (79%)	76 (94%)	5 (6%)	0	100	100
2	F	83/103 (81%)	79 (95%)	4 (5%)	0	100	100
3	C	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
4	D	91/126 (72%)	90 (99%)	1 (1%)	0	100	100
4	H	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
5	G	106/130 (82%)	103 (97%)	3 (3%)	0	100	100
8	K	100/326 (31%)	98 (98%)	2 (2%)	0	100	100
9	L	99/336 (30%)	94 (95%)	5 (5%)	0	100	100
10	M	40/228 (18%)	40 (100%)	0	0	100	100
11	N	72/76 (95%)	71 (99%)	1 (1%)	0	100	100
All	All	1057/1956 (54%)	1030 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	84/111 (76%)	84 (100%)	0	100	100
1	E	82/111 (74%)	82 (100%)	0	100	100
2	B	67/79 (85%)	67 (100%)	0	100	100
2	F	67/79 (85%)	67 (100%)	0	100	100
3	C	81/101 (80%)	81 (100%)	0	100	100
4	D	77/106 (73%)	77 (100%)	0	100	100
4	H	79/106 (74%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	G	83/101 (82%)	83 (100%)	0	100	100
8	K	82/296 (28%)	82 (100%)	0	100	100
9	L	85/297 (29%)	84 (99%)	1 (1%)	67	89
10	M	33/205 (16%)	33 (100%)	0	100	100
11	N	33/69 (48%)	33 (100%)	0	100	100
All	All	853/1661 (51%)	852 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	L	51	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	93	GLN
9	L	105	ASN
11	N	31	GLN

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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

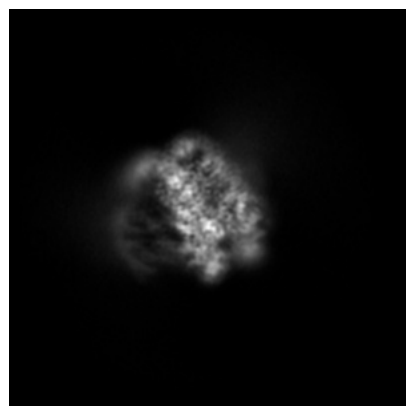
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46728. These allow visual inspection of the internal detail of the map and identification of artifacts.

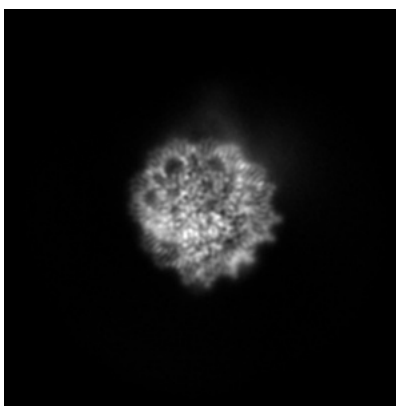
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

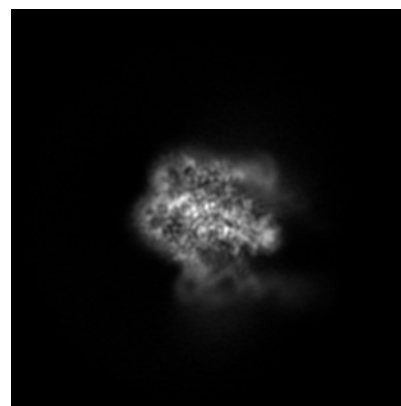
6.1.1 Primary map



X

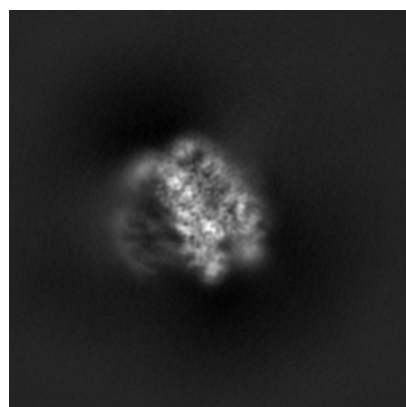


Y

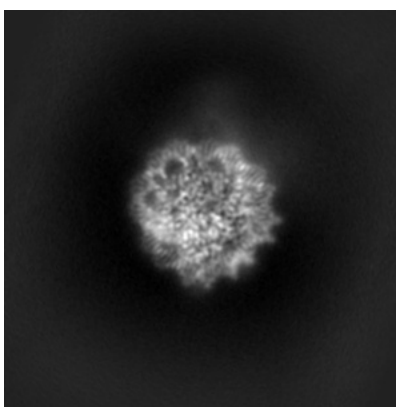


Z

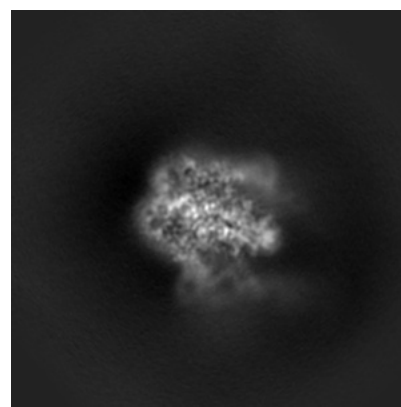
6.1.2 Raw map



X



Y

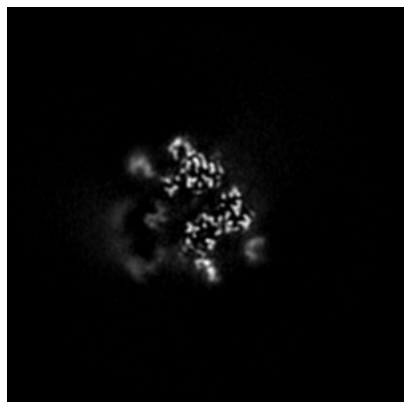


Z

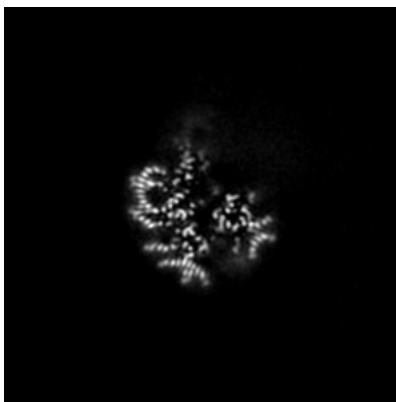
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

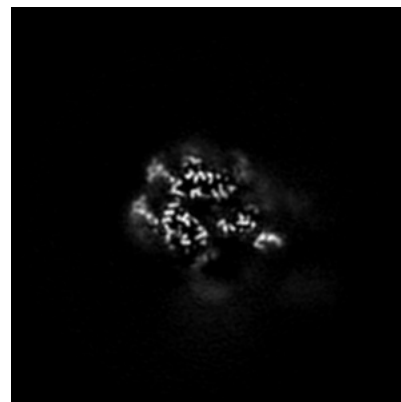
6.2.1 Primary map



X Index: 128

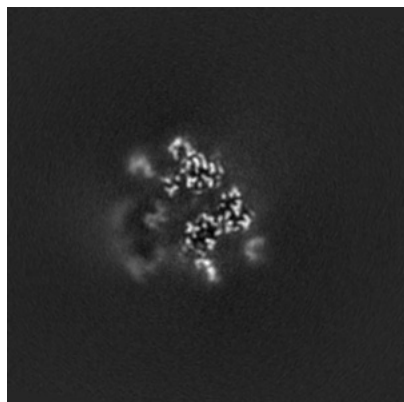


Y Index: 128

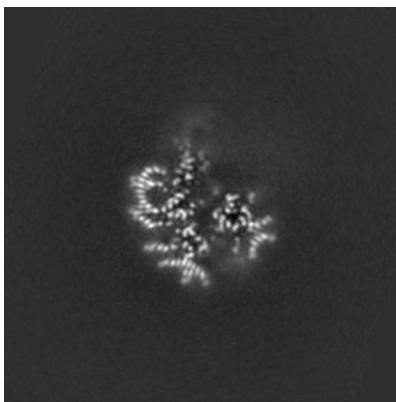


Z Index: 128

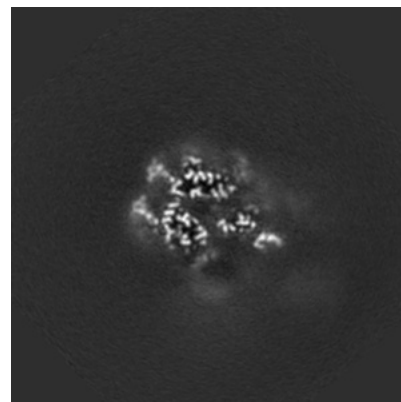
6.2.2 Raw map



X Index: 128



Y Index: 128

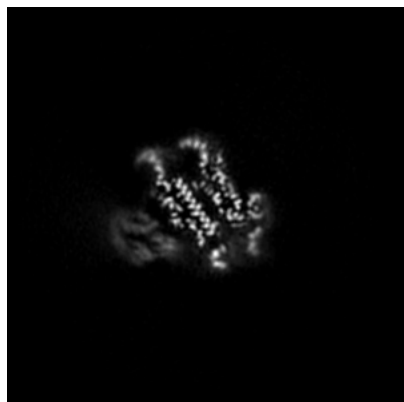


Z Index: 128

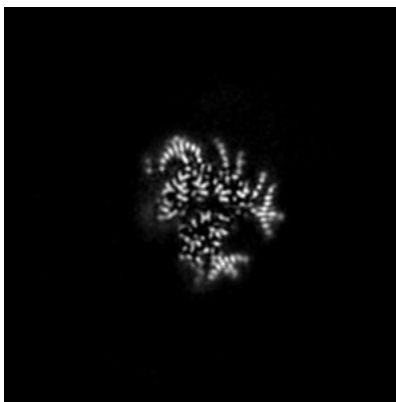
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

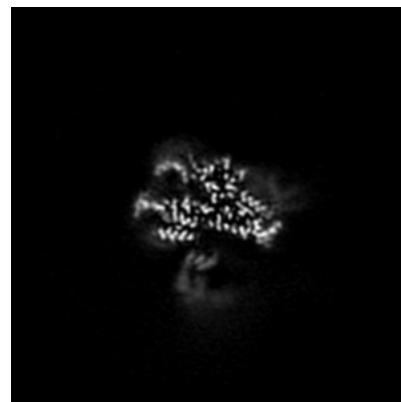
6.3.1 Primary map



X Index: 112

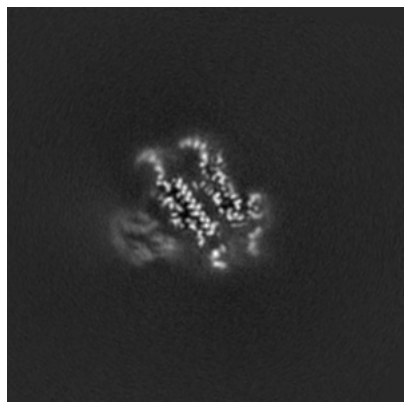


Y Index: 114

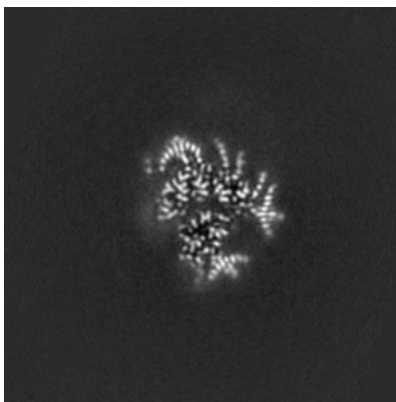


Z Index: 116

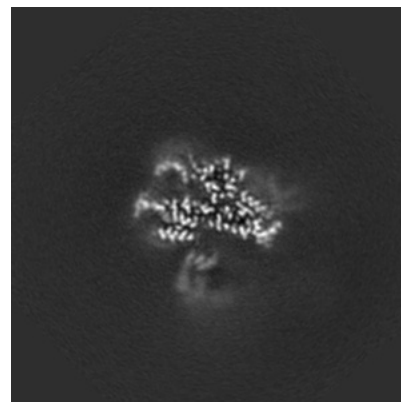
6.3.2 Raw map



X Index: 112



Y Index: 114

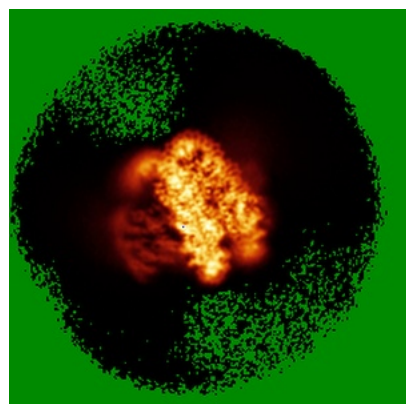


Z Index: 116

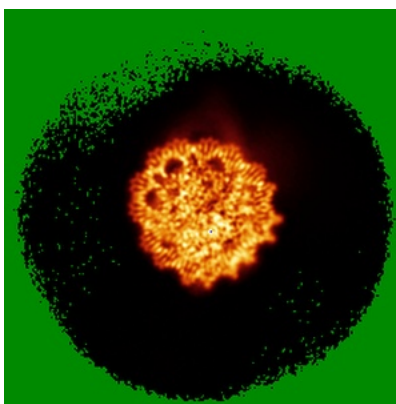
The images above show the largest variance slices of the map in three orthogonal directions.

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

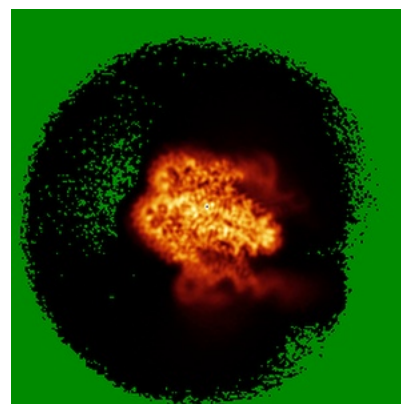
6.4.1 Primary map



X

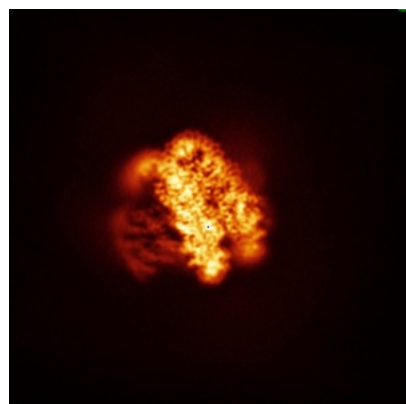


Y

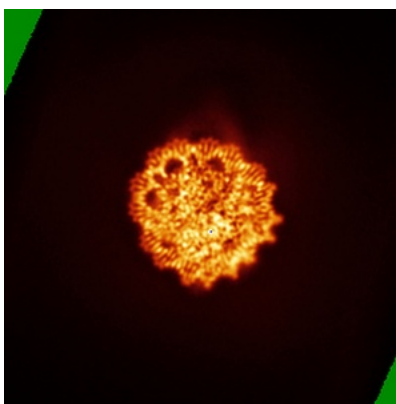


Z

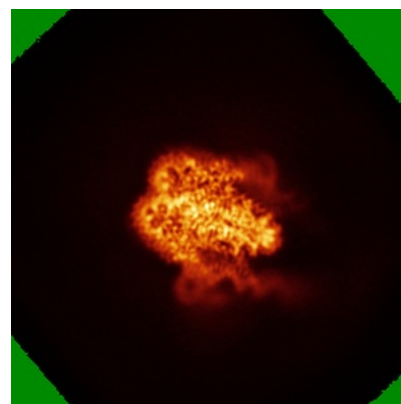
6.4.2 Raw map



X



Y

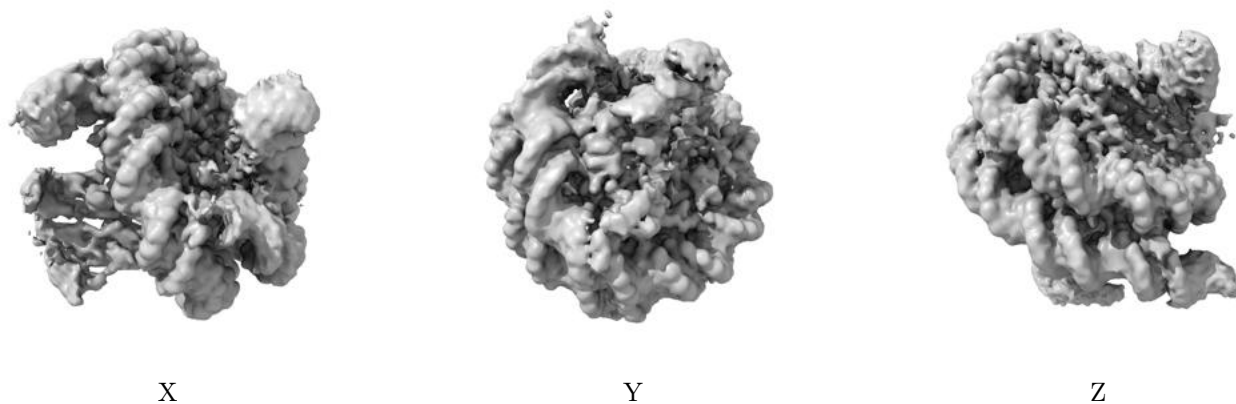


Z

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 0.182. 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.

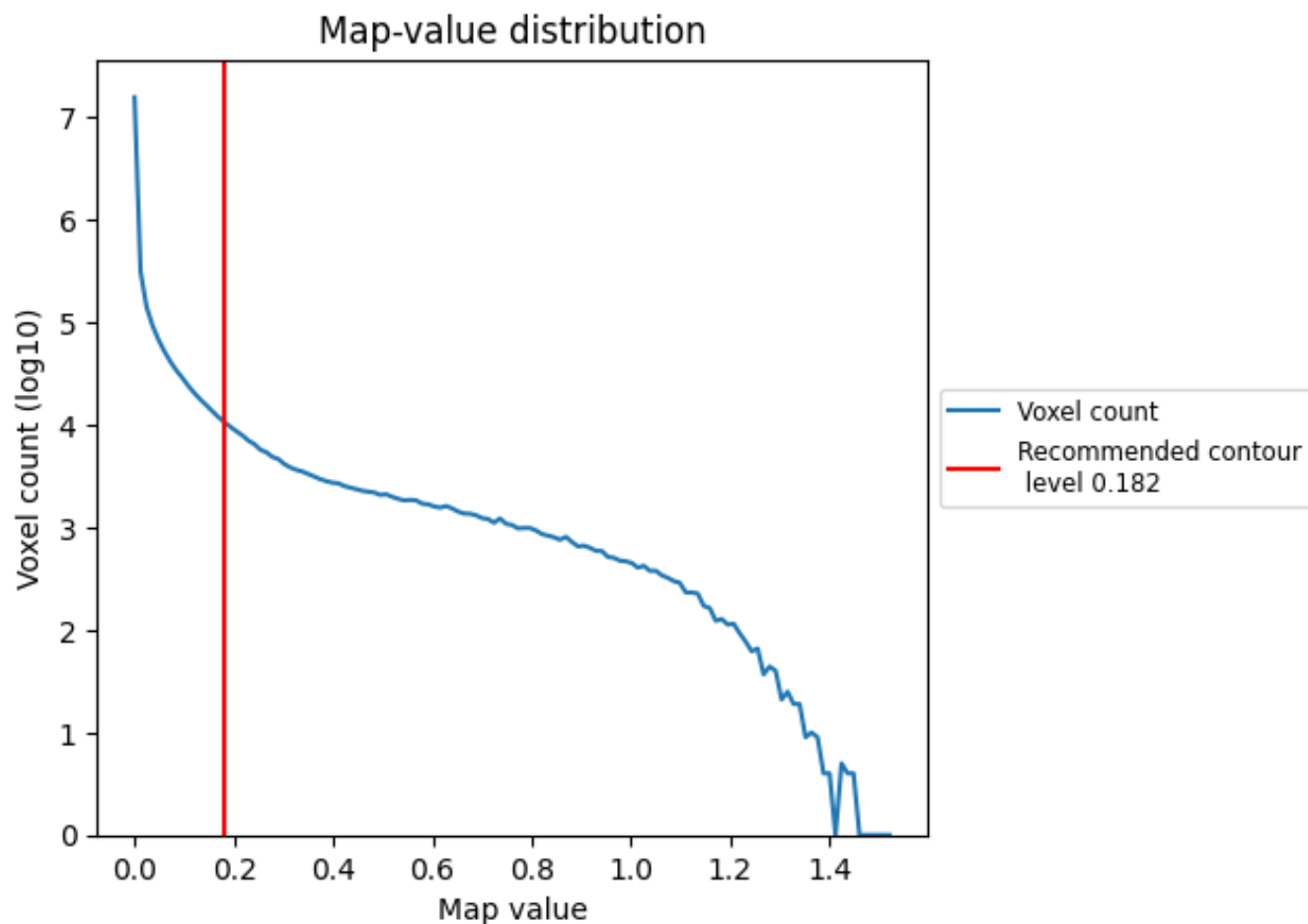
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

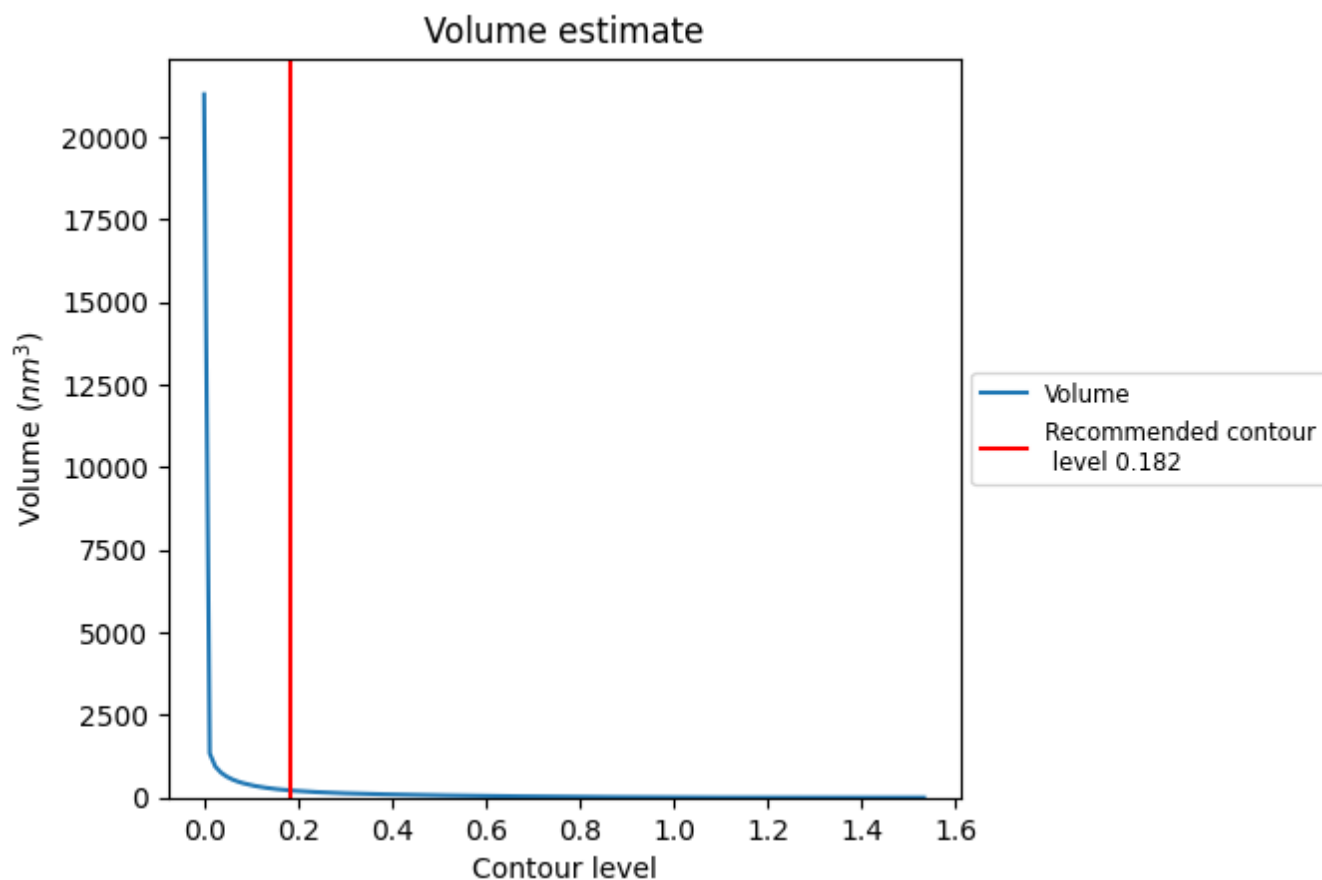
This section contains the results of statistical analysis of the map.

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.

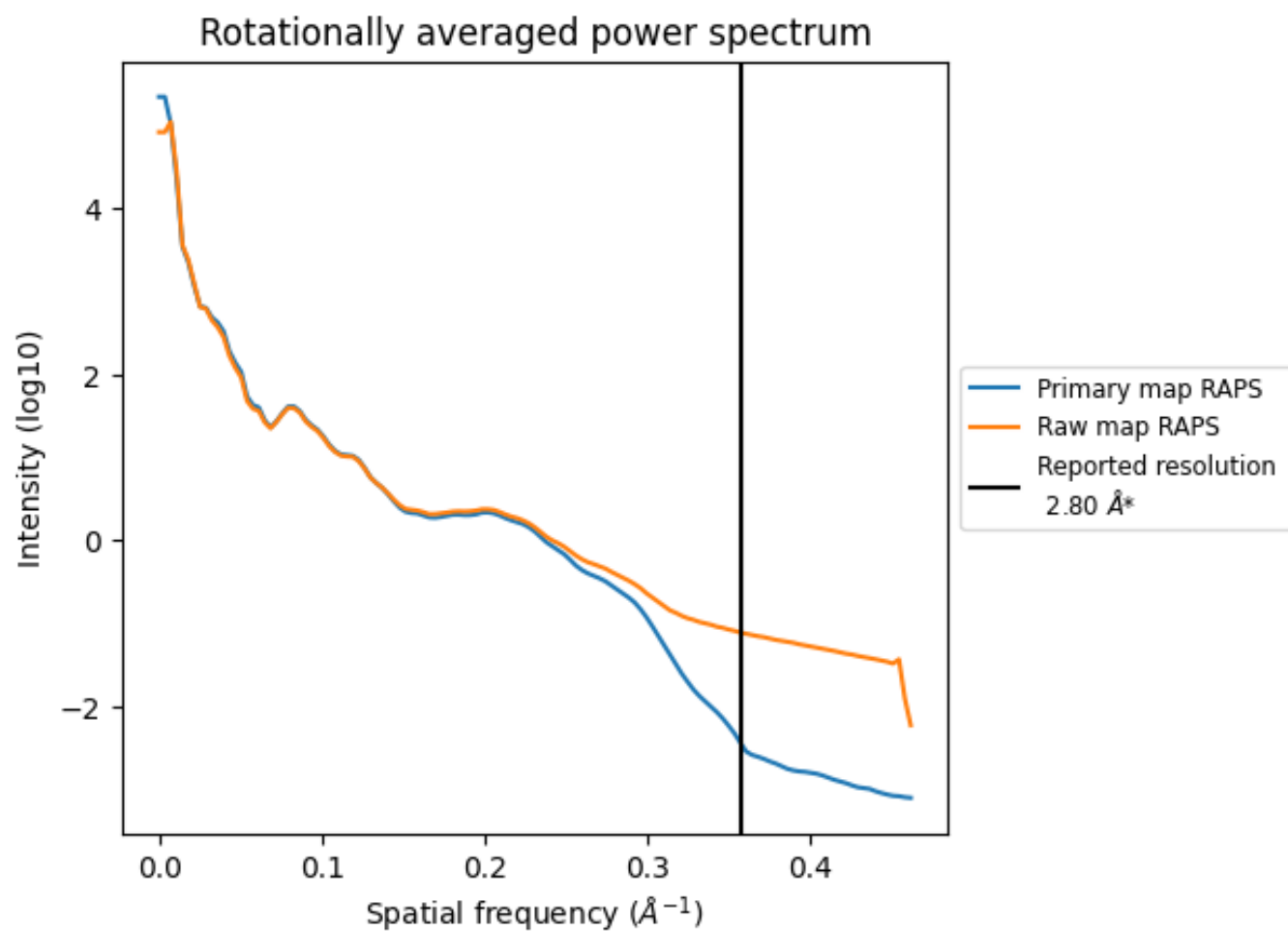
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 218 nm^3 ; this corresponds to an approximate mass of 197 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 ⓘ

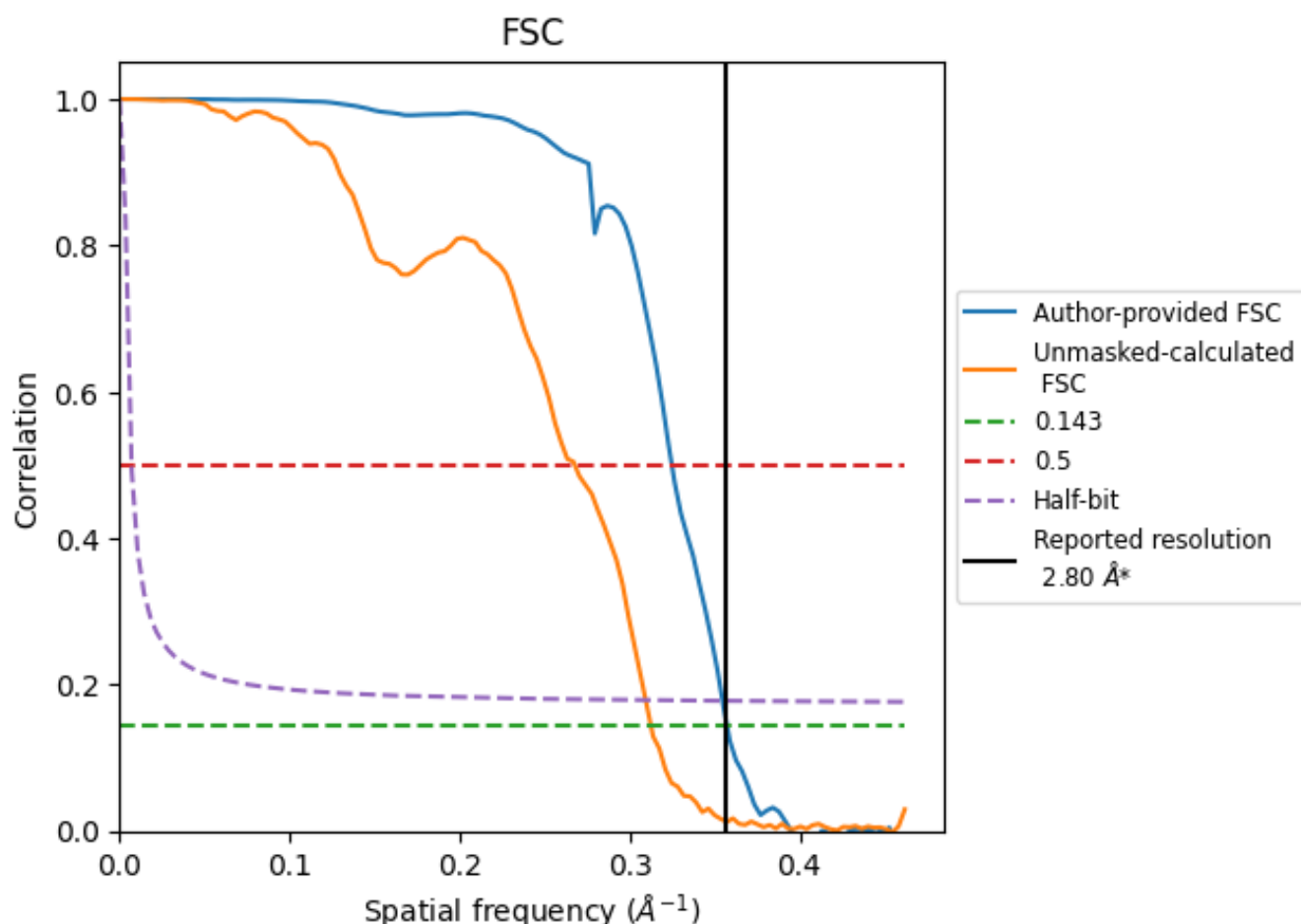


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

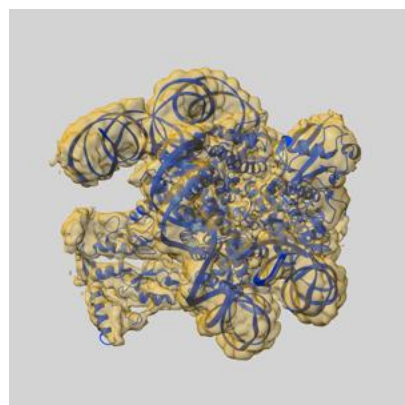
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.08	2.82
Unmasked-calculated*	3.20	3.73	3.23

*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 3.20 differs from the reported value 2.8 by more than 10 %

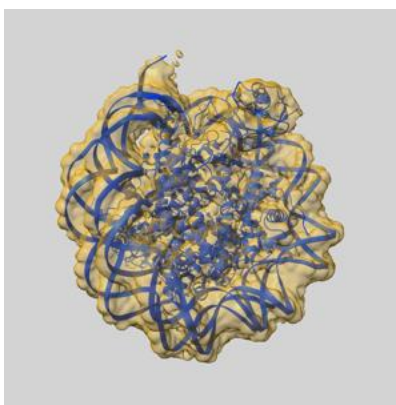
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46728 and PDB model 9DBY. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

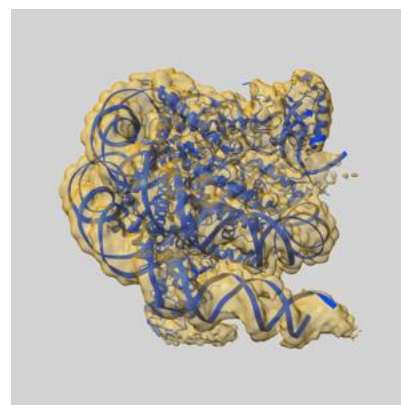
9.1 Map-model overlay [i](#)



X



Y



Z

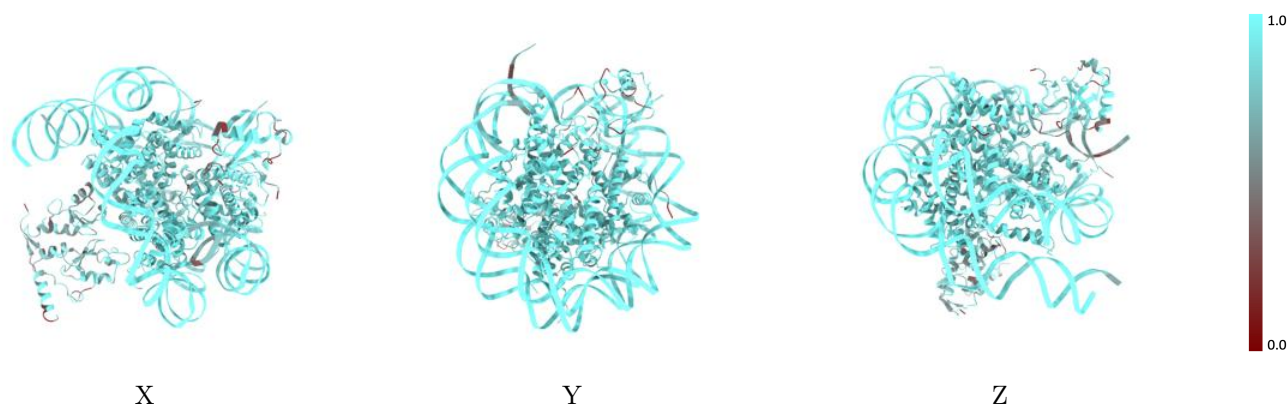
The images above show the 3D surface view of the map at the recommended contour level 0.182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



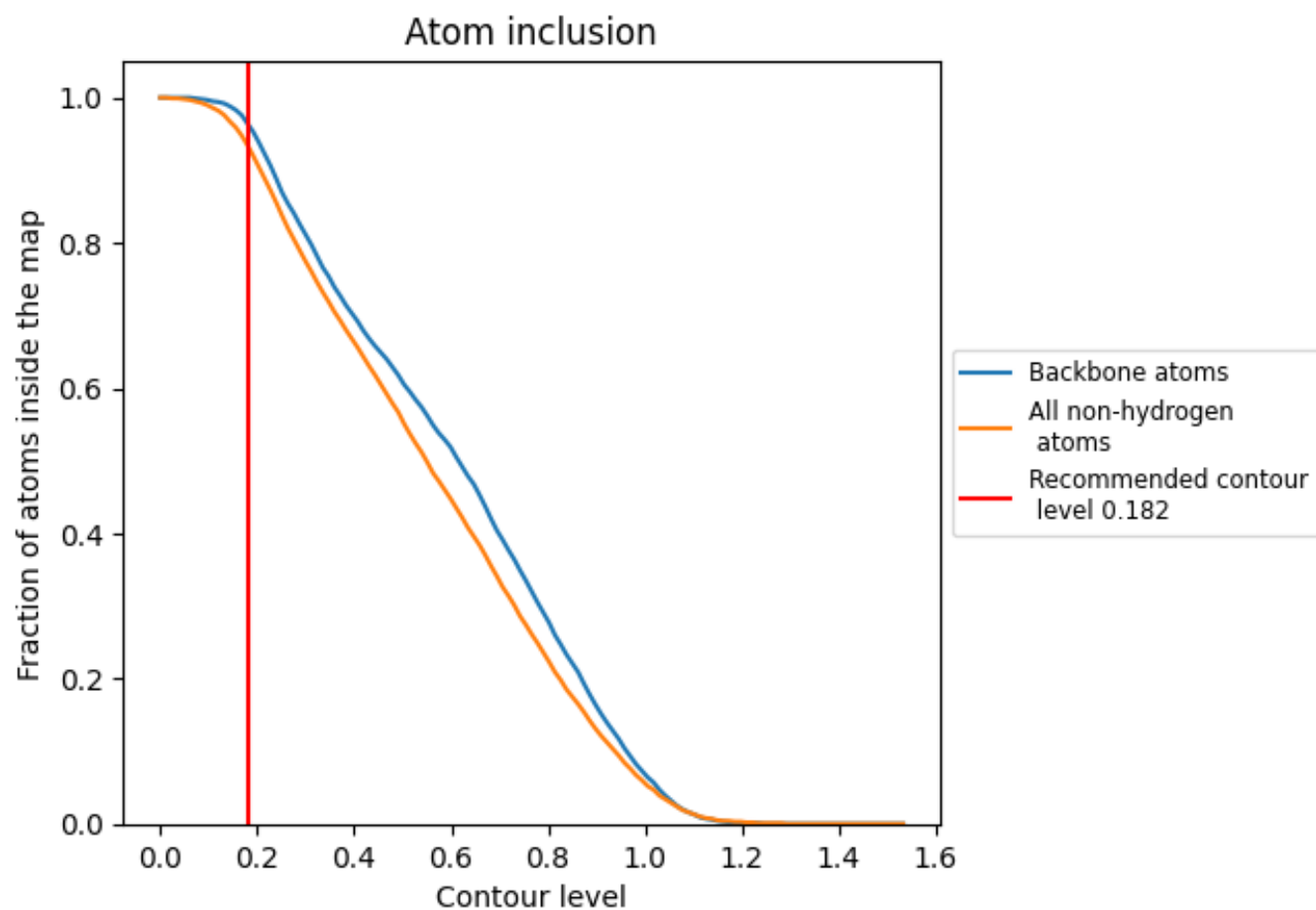
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.182).































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.3900
A	 0.9590	 0.4520
B	 0.9620	 0.4610
C	 0.9490	 0.4480
D	 0.9670	 0.4420
E	 0.9600	 0.4560
F	 0.9190	 0.4430
G	 0.9410	 0.4430
H	 0.9610	 0.4500
I	 0.9790	 0.3740
J	 0.9720	 0.3880
K	 0.7890	 0.2490
L	 0.7320	 0.2850
M	 0.7890	 0.3220
N	 0.7640	 0.2010

