



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 05:16 PM JST

PDB ID : 7E9F
EMDB ID : EMD-31030
Title : Cryo-EM structure of the 2:1 Orc1 BAH domain in complex with nucleosome
Authors : Jiang, H.; Yu, C.; Liu, C.P.; Han, X.; Yu, Z.; Xu, R.M.
Deposited on : 2021-03-04
Resolution : 4.00 Å(reported)
Based on initial models : 1ID3, 1M4Z, 3LZ0, 6OM3

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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

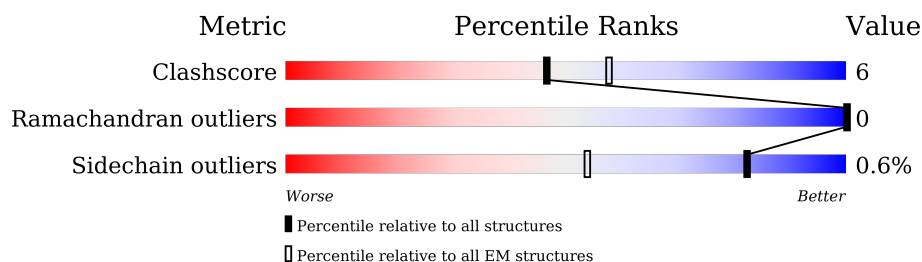
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.





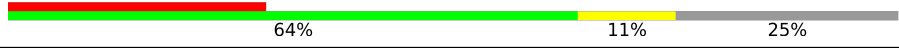

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	134	 5% 55% 13% 32%
1	E	134	 49% 16% 35%
2	B	103	 60% 20% 19%
2	F	103	 63% 16% 21%
3	C	132	 61% 15% 23%
3	G	132	 5% 60% 17% 23%
4	D	131	 58% 13% 29%
4	H	131	 63% 8% 29%

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Mol	Chain	Length	Quality of chain
5	I	147	 69% 15% 16%
6	J	147	 70% 16% 14%
7	K	219	 29% 64% 11% 25%
7	L	219	 29% 63% 12% 25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13279 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.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	91	Total	C	N	O	0	0
			734	467	140	127		
1	E	87	Total	C	N	O	0	0
			710	452	136	122		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	83	Total	C	N	O	0	0
			659	417	127	115		
2	F	81	Total	C	N	O	0	0
			643	408	122	113		

- Molecule 3 is a protein called Histone H2A.2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	101	Total	C	N	O	0	0
			776	486	153	137		
3	G	102	Total	C	N	O	0	0
			781	490	153	138		

- Molecule 4 is a protein called Histone H2B.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	93	Total	C	N	O	S	0	0
			714	450	125	138	1		
4	H	93	Total	C	N	O	S	0	0
			714	450	125	138	1		

- Molecule 5 is a DNA chain called DNA (147-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	123	Total	C	N	O	P	0	0
			2506	1188	456	739	123		

- Molecule 6 is a DNA chain called DNA (147-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	126	Total	C	N	O	P	0	0
			2600	1228	491	755	126		

- Molecule 7 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	164	Total	C	N	O	S	0	0
			1221	776	220	224	1		
7	L	164	Total	C	N	O	S	0	0
			1221	776	220	224	1		

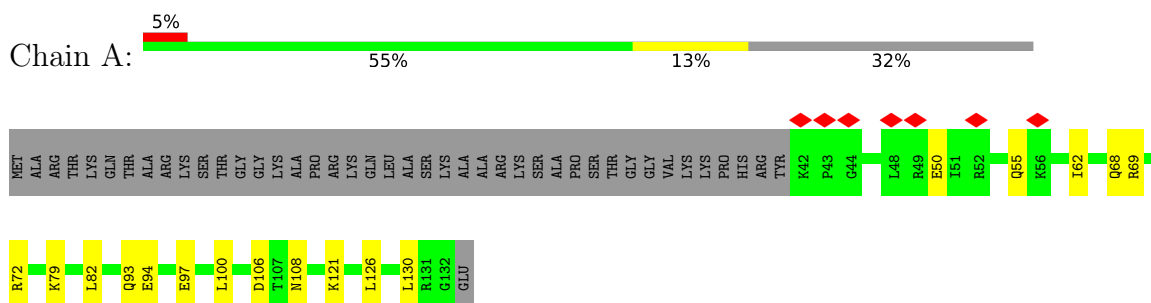
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	ACE	-	acetylation	UNP P54784
L	1	ACE	-	acetylation	UNP P54784

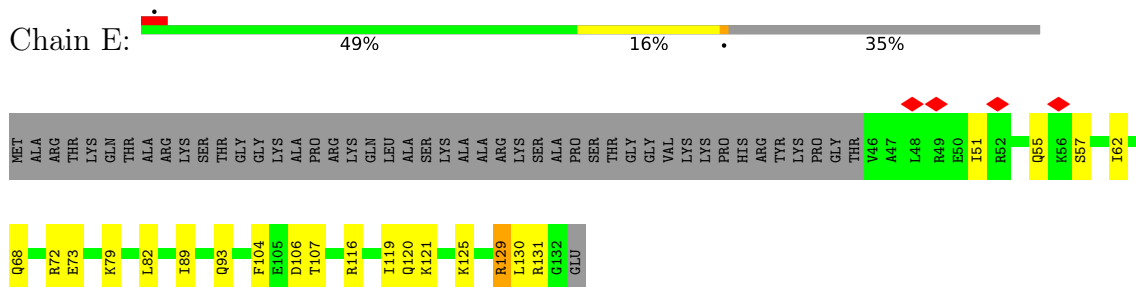
3 Residue-property plots [i](#)

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.

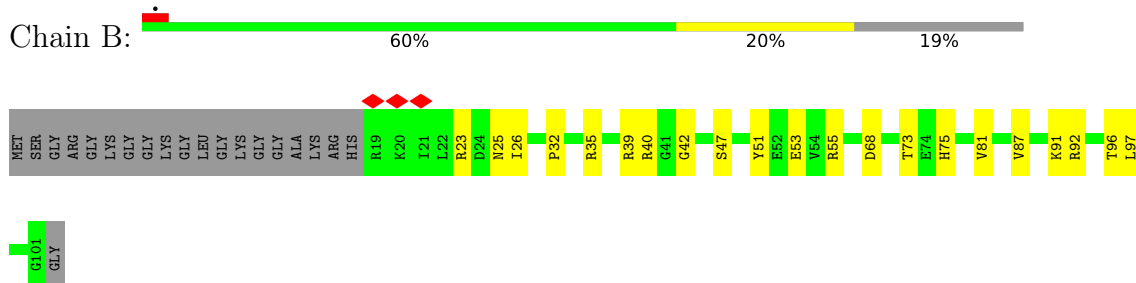
• Molecule 1: Histone H3



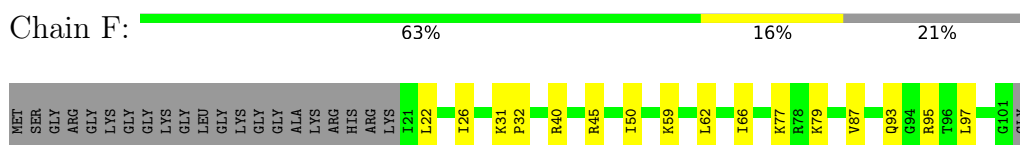
• Molecule 1: Histone H3



• Molecule 2: Histone H4

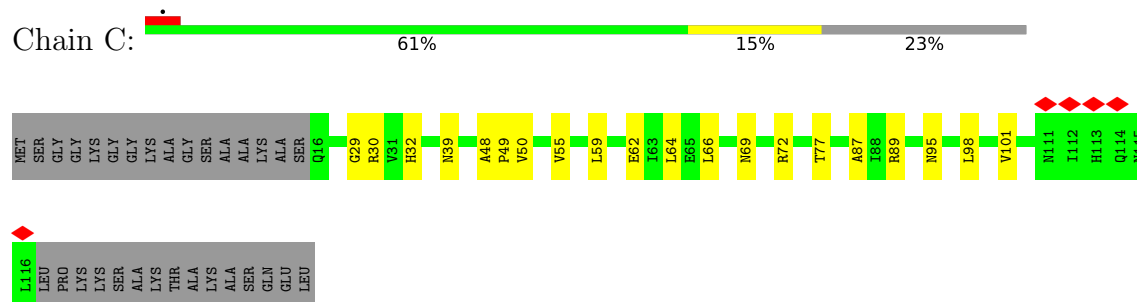


• Molecule 2: Histone H4



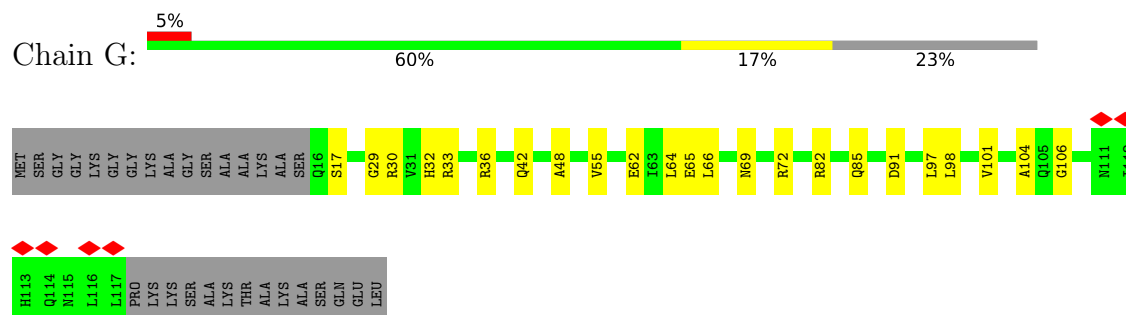
• Molecule 3: Histone H2A.2

Chain C:



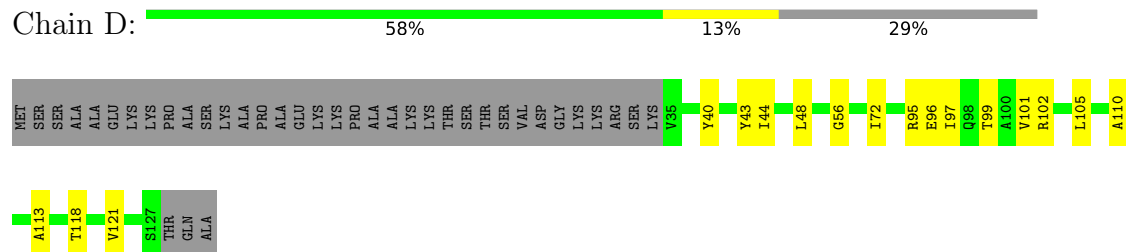
• Molecule 3: Histone H2A.2

Chain G:



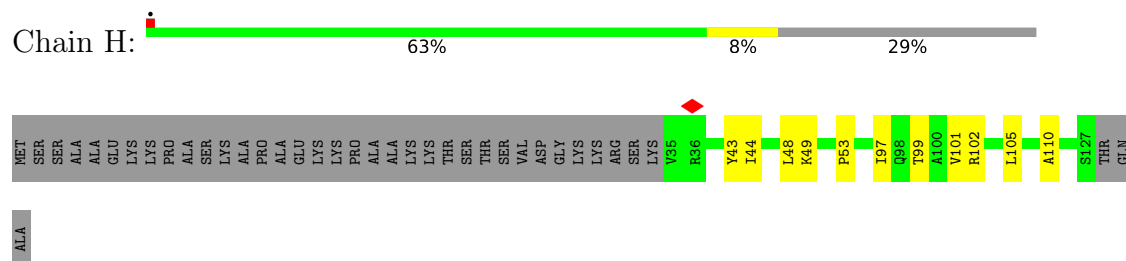
• Molecule 4: Histone H2B.2

Chain D:



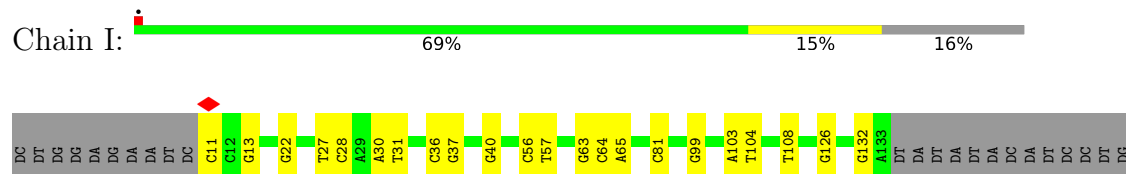
• Molecule 4: Histone H2B.2

Chain H:



• Molecule 5: DNA (147-mer)

Chain I:



DT

- Molecule 6: DNA (147-mer)

Chain J: 

DA DC DA DA DG DG DA DT DG DT DA DA DT DA DT DA DT DA DT C15 C16 C22 C27 T28 G29 G30 G41 T42 A43 A44 T45 C46 C47 C48 C49 T50 C54 G55 G82 G101 T109 C123 G124 C127 C134 C135 G136 G137 G138 A139 T140 DT DC DT DC

DC DA DG

- Molecule 7: Origin recognition complex subunit 1

Chain K: 

ACE1 T4 L5 K6 Q9 E18 Q19 G20 N21 D24 G25 R31 R32 R33 G34 A35 H39 S44 S45 D46 G47 I48 V56 H59 N60 E61 A62 A63 G64 T65 Y66 S67 Y68 Y69 L74 L79 N80 N81 Y90 L91 L92 W93 F94 GLU VAL ASN PRO LEU

ALA HIS TYR ARG GLN PHE ASN ASP ASP ALA ASN ILE LEU G181 ASN ARG PRO PRO LEU ASN TVR TYR LEU LEU PHE SER GLU THR ALA ASN LYS N130 Y133 L134 T135 A136 E137 L138 A139 E140 L141 F144 N145 F146 I147 M153 D154 G155 SER LYS TRP VAL LEU LYS GLY ASN VAL

ASP PRO ARG D170 I176 C177 E178 T180 T181 E182 K183 F184 V185 D186 I187 N188 E200 P201 R202 E203 A204 Y207 L208 D210 L213 PRO SER LYS LYS LYS

- Molecule 7: Origin recognition complex subunit 1

Chain L: 

ACE1 T4 L5 K6 Q9 T15 E18 Q19 G20 N21 D24 G25 G26 Q27 L30 R31 R32 R33 G34 A35 S44 S45 D46 G47 I48 H59 N60 E61 A62 A63 G64 T65 Y66 S67 Y68 Y69 R75 L79 N80 N81 Y90 L91 R92 W93 F94 GLU VAL ASN PRO

LEU ALA HIS TYR ARG GLN PHE ASN ASP ASP ALA ASN ILE LEU G181 ASN ARG PRO PRO LEU ASN TVR TYR LEU LYS PHE SER GLU THR ALA ASN LYS N130 Y133 L134 T135 A136 E137 L138 A139 E140 L141 F144 N145 F146 I147 M153 D154 G155 SER LYS TRP VAL LEU LYS GLY ASN

VAL ASP PRO GLU ARG D170 V173 R174 Y175 I176 C177 E178 F179 T180 G181 E182 K183 F184 V185 D186 I187 N188 E200 P201 R202 E203 A204 Y207 L208 D209 L213 PRO SER LYS LYS LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	119206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	192.0, 192.0, 192.0	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/742	0.43	0/994
1	E	0.25	0/717	0.46	0/959
2	B	0.25	0/666	0.51	0/893
2	F	0.24	0/650	0.49	0/872
3	C	0.25	0/786	0.45	0/1063
3	G	0.25	0/791	0.49	0/1071
4	D	0.23	0/724	0.43	0/977
4	H	0.25	0/724	0.45	0/977
5	I	0.57	0/2807	1.01	0/4326
6	J	0.54	0/2920	0.93	0/4509
7	K	0.24	0/1237	0.51	0/1681
7	L	0.24	0/1237	0.51	0/1681
All	All	0.40	0/14001	0.74	0/20003

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 [i](#)

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	734	0	782	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	710	0	761	14	0
2	B	659	0	700	15	0
2	F	643	0	685	12	0
3	C	776	0	810	20	0
3	G	781	0	812	20	0
4	D	714	0	729	17	0
4	H	714	0	729	10	0
5	I	2506	0	1379	19	0
6	J	2600	0	1412	21	0
7	K	1221	0	1141	15	0
7	L	1221	0	1141	16	0
All	All	13279	0	11081	136	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 6.

The worst 5 of 136 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)
3:G:85:GLN:HE21	3:G:106:GLY:HA3	1.65	0.60
5:I:103:DA:N1	6:J:45:DT:C4	2.71	0.59
6:J:16:DC:H6	6:J:16:DC:H5''	1.68	0.58
2:B:73:THR:HG21	2:B:81:VAL:HG22	1.86	0.57
4:D:105:LEU:HB2	4:D:110:ALA:HB2	1.86	0.57

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	89/134 (66%)	89 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	85/134 (63%)	83 (98%)	2 (2%)	0	100	100
2	B	81/103 (79%)	76 (94%)	5 (6%)	0	100	100
2	F	79/103 (77%)	77 (98%)	2 (2%)	0	100	100
3	C	99/132 (75%)	96 (97%)	3 (3%)	0	100	100
3	G	100/132 (76%)	97 (97%)	3 (3%)	0	100	100
4	D	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
4	H	91/131 (70%)	89 (98%)	2 (2%)	0	100	100
7	K	158/219 (72%)	152 (96%)	6 (4%)	0	100	100
7	L	158/219 (72%)	151 (96%)	7 (4%)	0	100	100
All	All	1031/1438 (72%)	1000 (97%)	31 (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	77/111 (69%)	77 (100%)	0	100	100
1	E	75/111 (68%)	74 (99%)	1 (1%)	65	77
2	B	69/81 (85%)	69 (100%)	0	100	100
2	F	68/81 (84%)	68 (100%)	0	100	100
3	C	79/99 (80%)	79 (100%)	0	100	100
3	G	79/99 (80%)	79 (100%)	0	100	100
4	D	78/110 (71%)	78 (100%)	0	100	100
4	H	78/110 (71%)	78 (100%)	0	100	100
7	K	112/193 (58%)	110 (98%)	2 (2%)	54	71
7	L	112/193 (58%)	110 (98%)	2 (2%)	54	71
All	All	827/1188 (70%)	822 (99%)	5 (1%)	82	88

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

Mol	Chain	Res	Type
1	E	129	ARG
7	K	33	ARG
7	K	208	LEU
7	L	33	ARG
7	L	208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	90	ASN
7	K	27	GLN
7	L	81	ASN
7	K	81	ASN
2	B	93	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

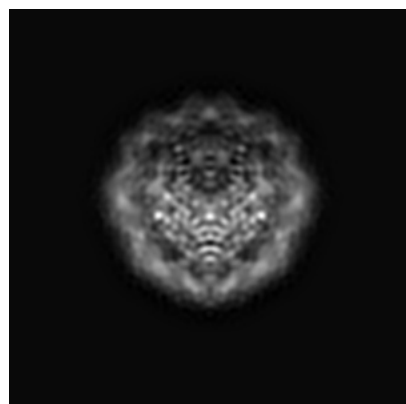
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31030. These allow visual inspection of the internal detail of the map and identification of artifacts.

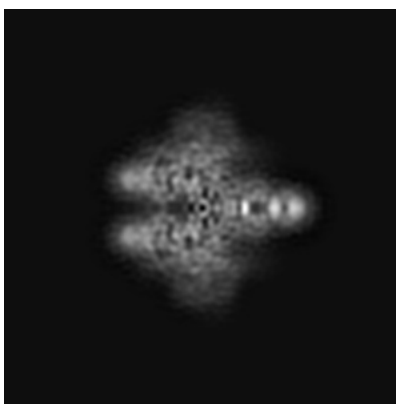
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

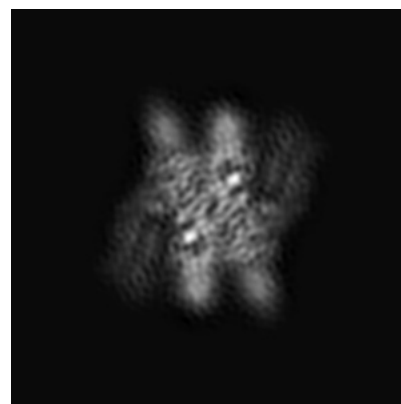
6.1.1 Primary map



X

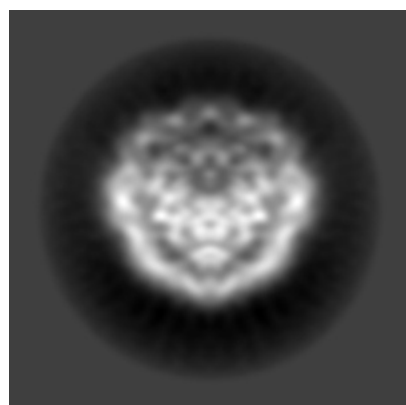


Y

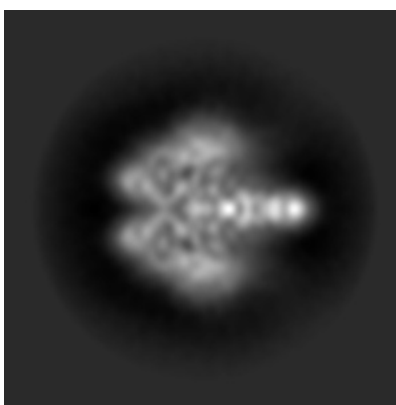


Z

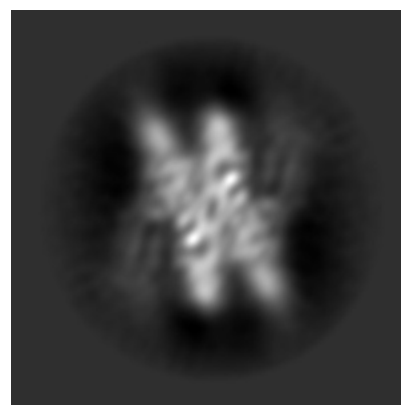
6.1.2 Raw map



X



Y

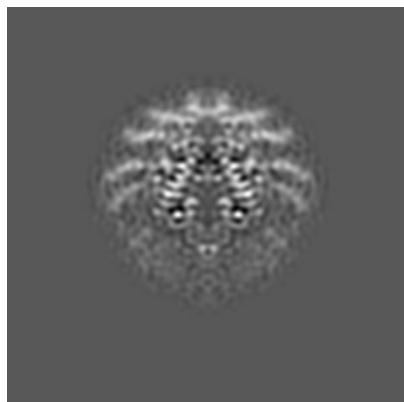


Z

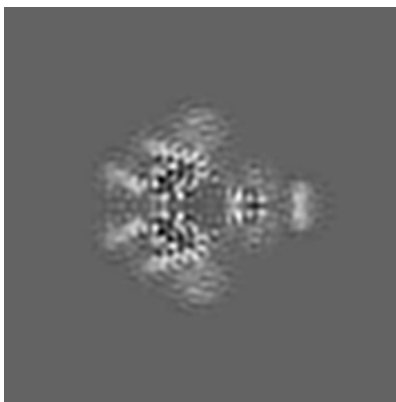
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

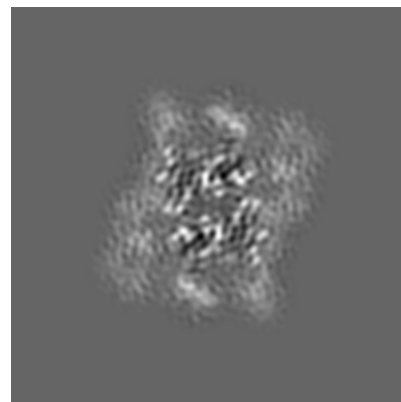
6.2.1 Primary map



X Index: 96



Y Index: 96

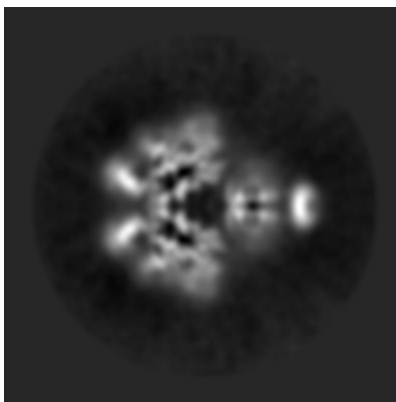


Z Index: 96

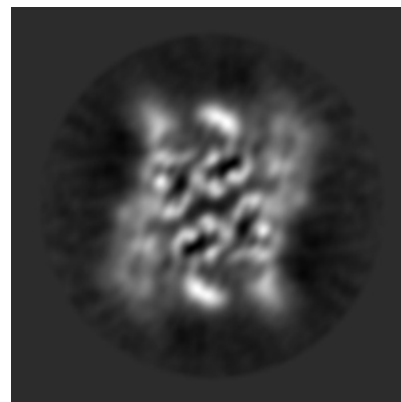
6.2.2 Raw map



X Index: 96



Y Index: 96



Z Index: 96

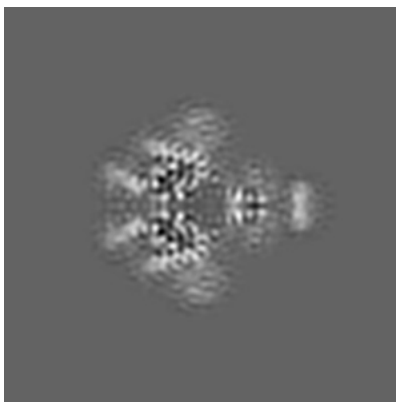
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

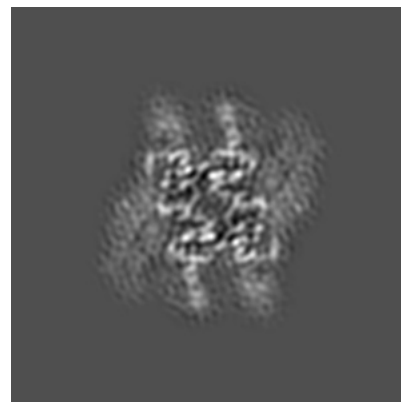
6.3.1 Primary map



X Index: 99



Y Index: 96

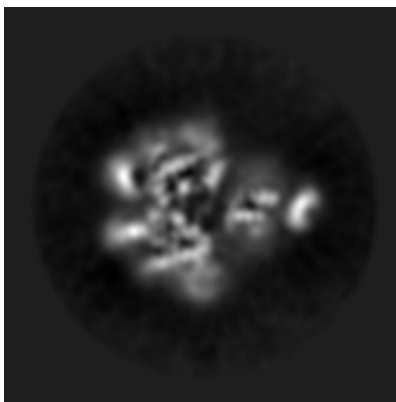


Z Index: 92

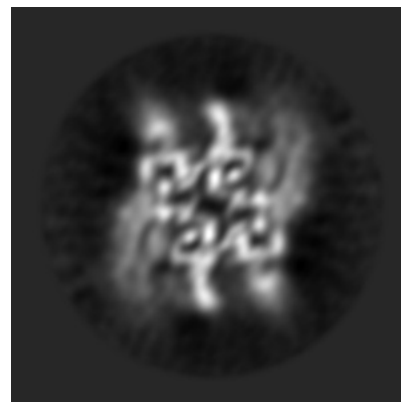
6.3.2 Raw map



X Index: 96



Y Index: 93

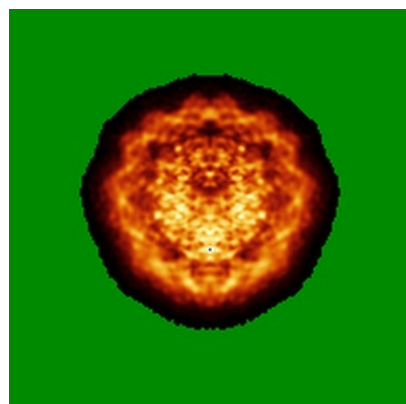


Z Index: 92

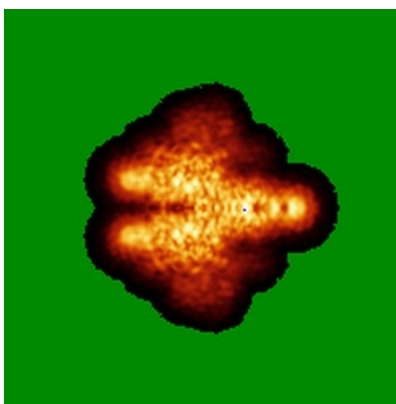
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

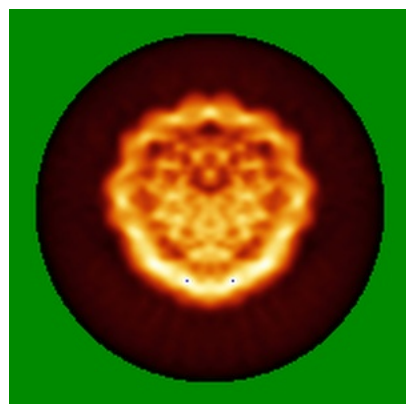


Y

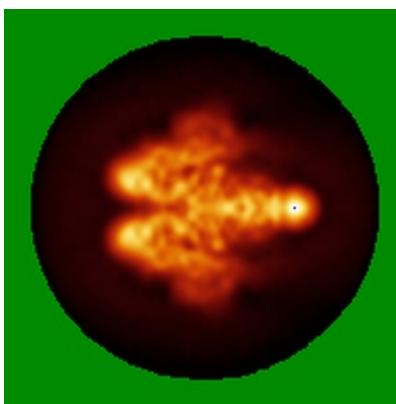


Z

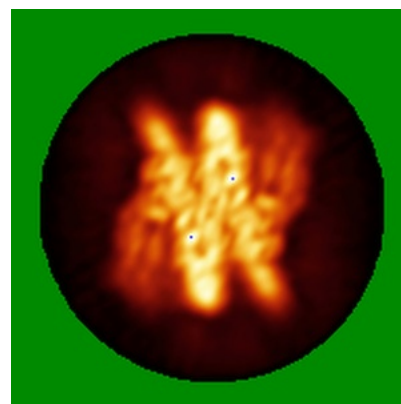
6.4.2 Raw map



X



Y

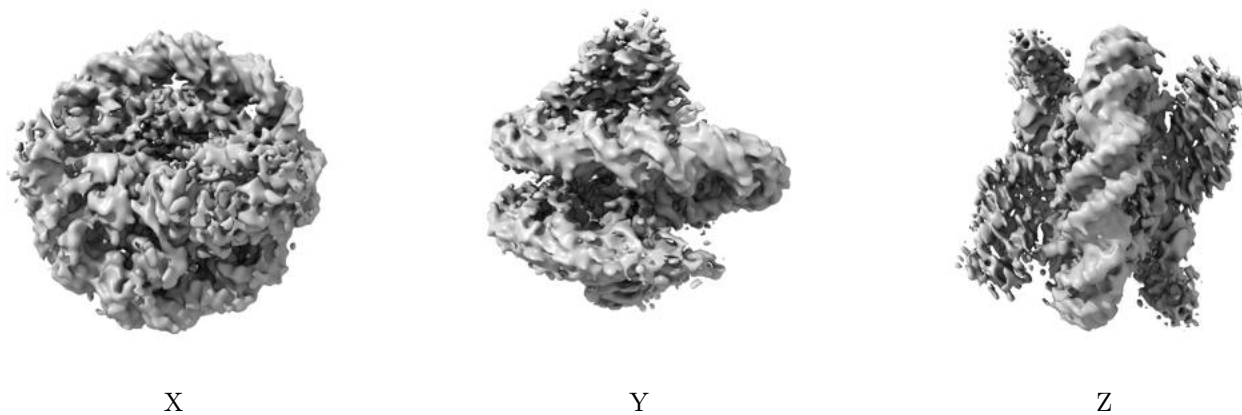


Z

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.

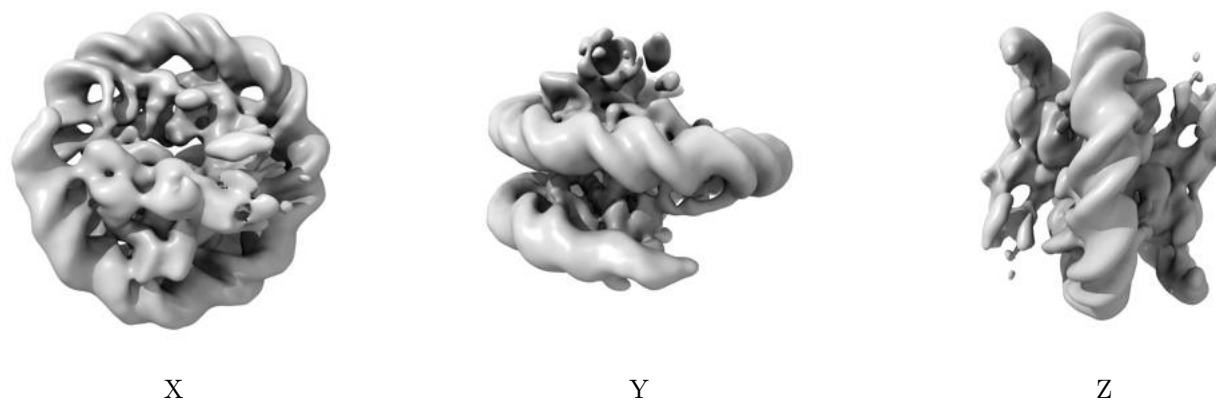
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

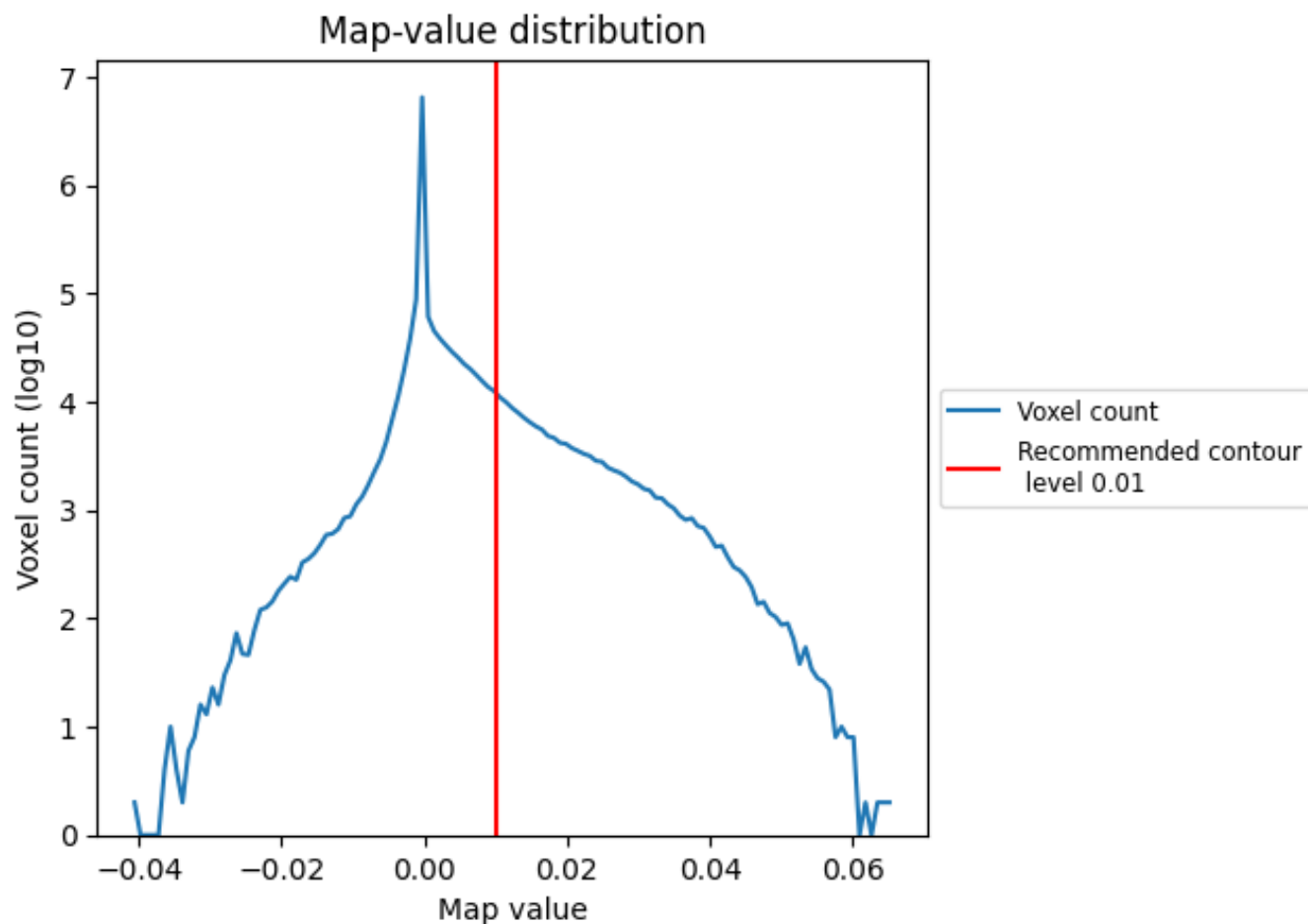
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

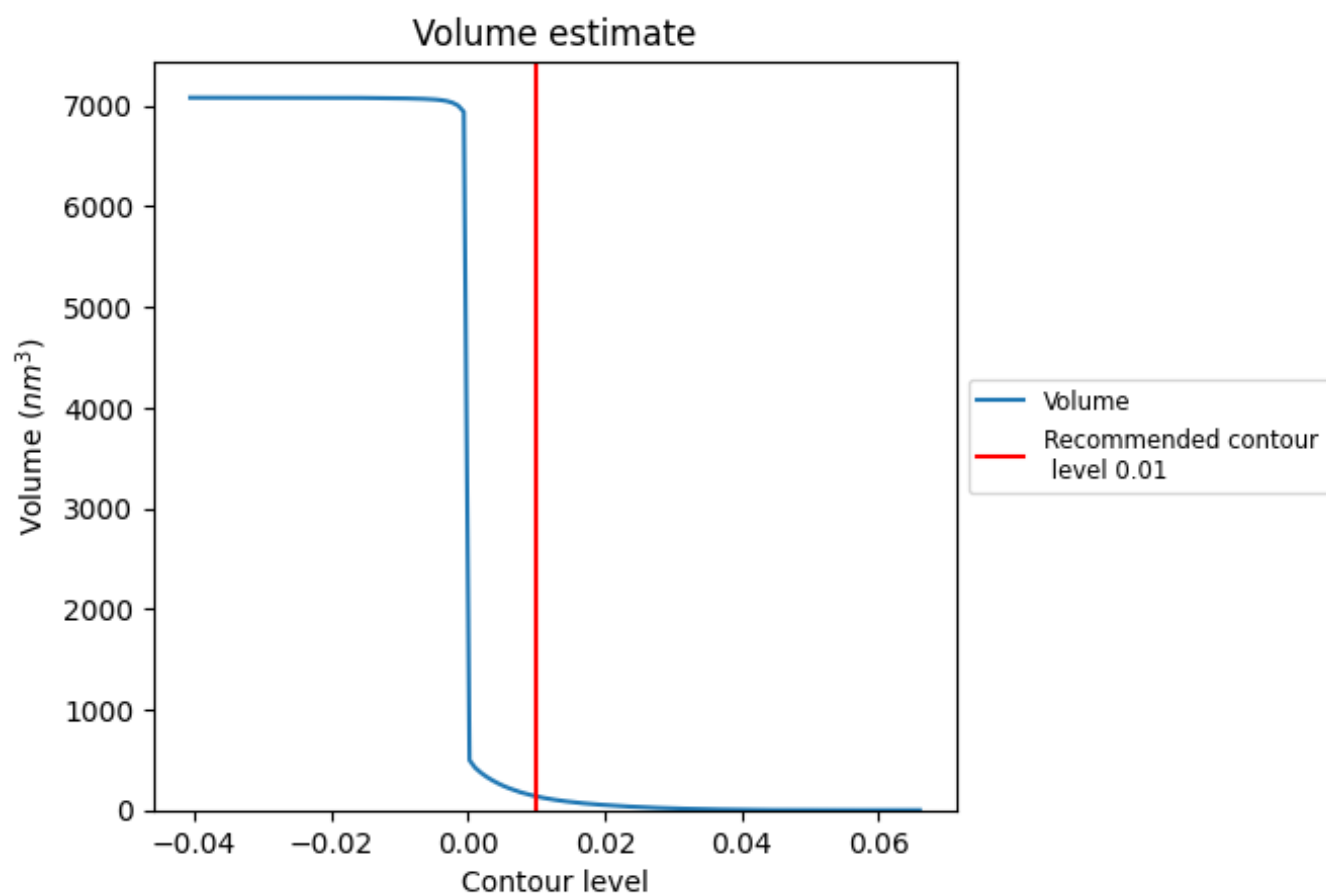
This section contains the results of statistical analysis of the map.

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.

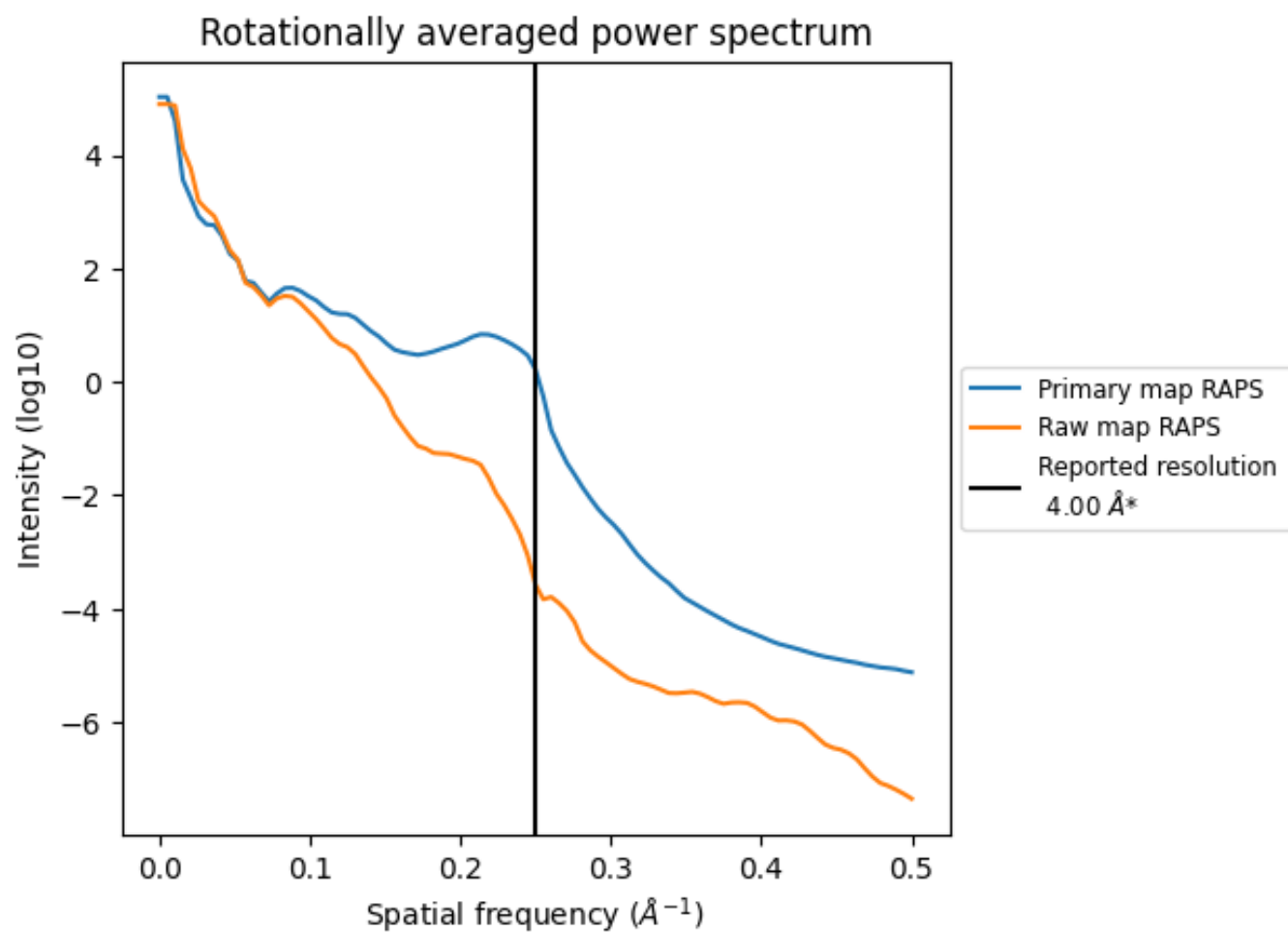
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm³; this corresponds to an approximate mass of 124 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 ⓘ

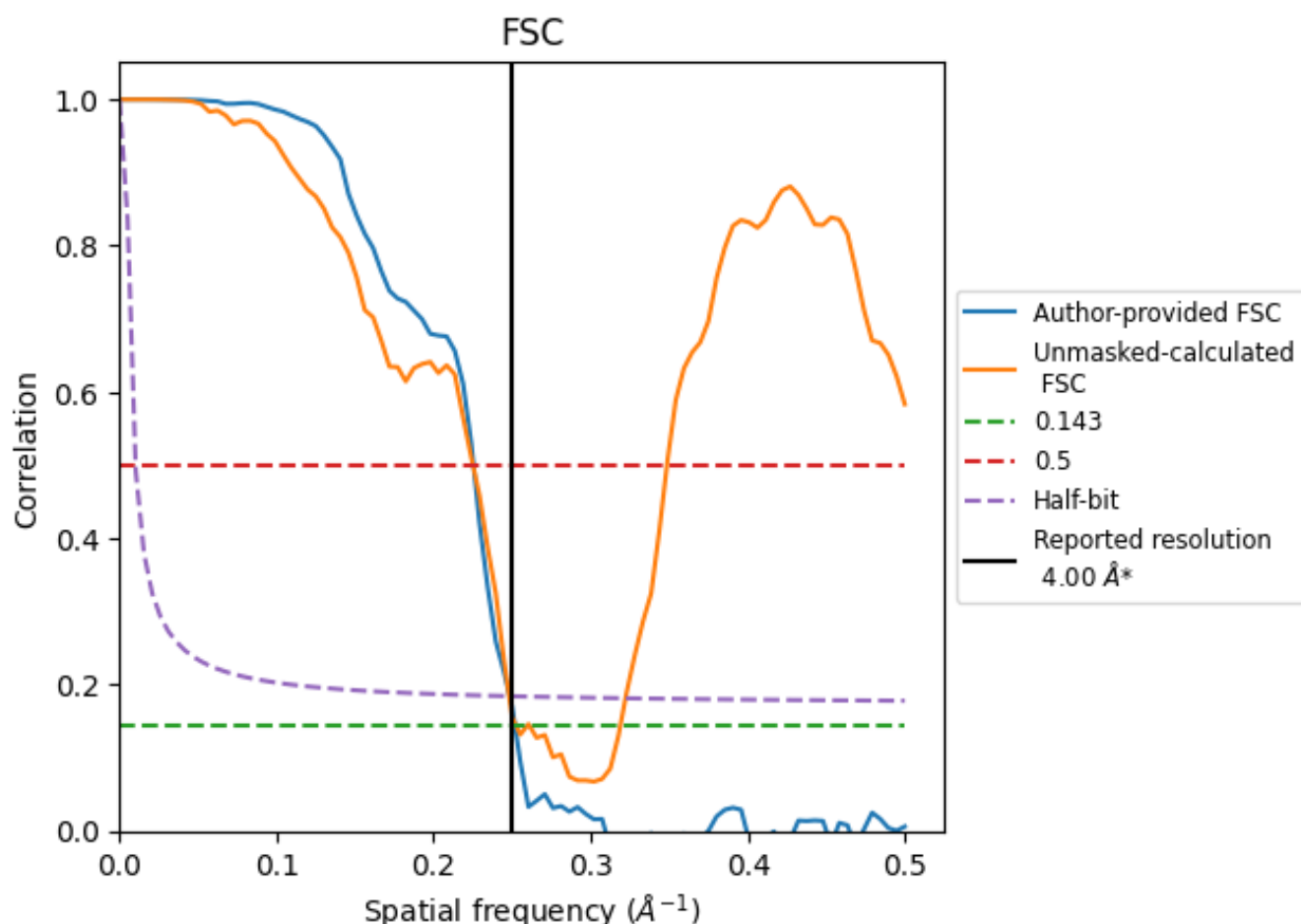


*Reported resolution corresponds to spatial frequency of 0.250 \AA^{-1}

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

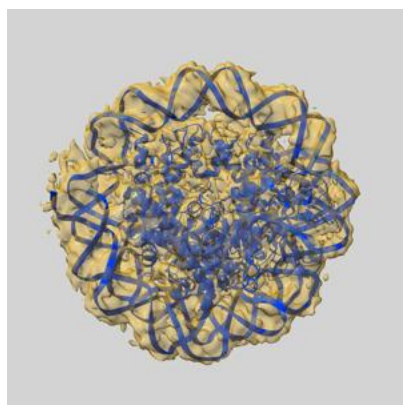
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.97	4.44	4.02
Unmasked-calculated*	3.96	4.44	4.03

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

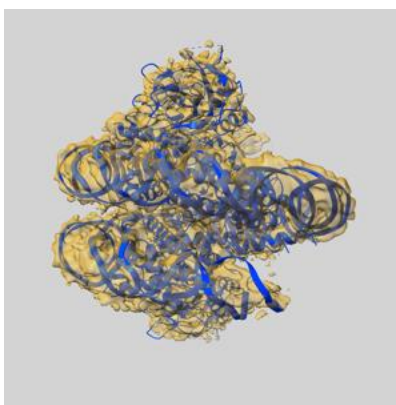
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31030 and PDB model 7E9F. Per-residue inclusion information can be found in section [3](#) on page [6](#).

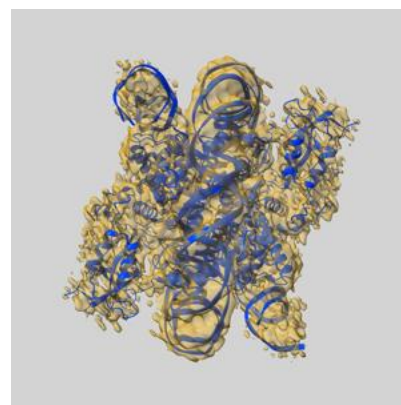
9.1 Map-model overlay [i](#)



X



Y



Z

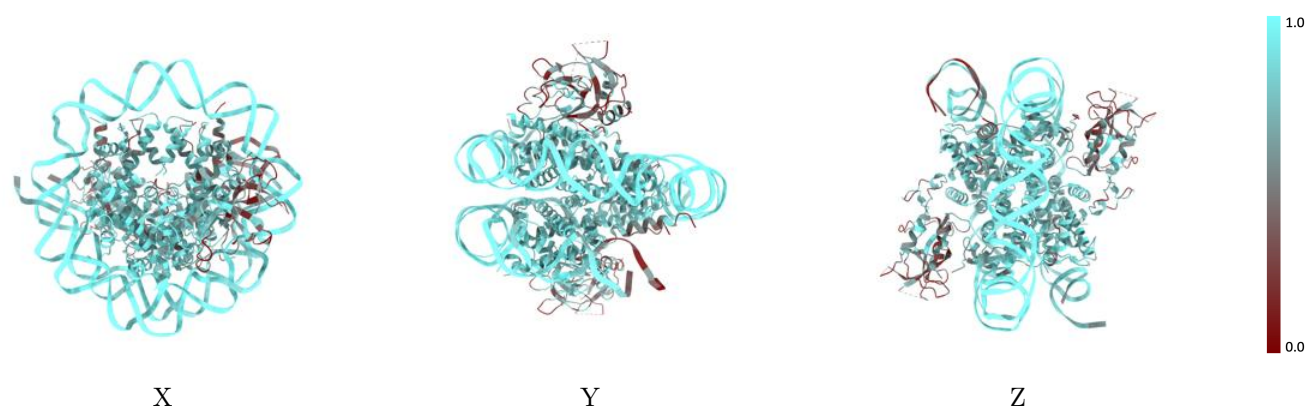
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



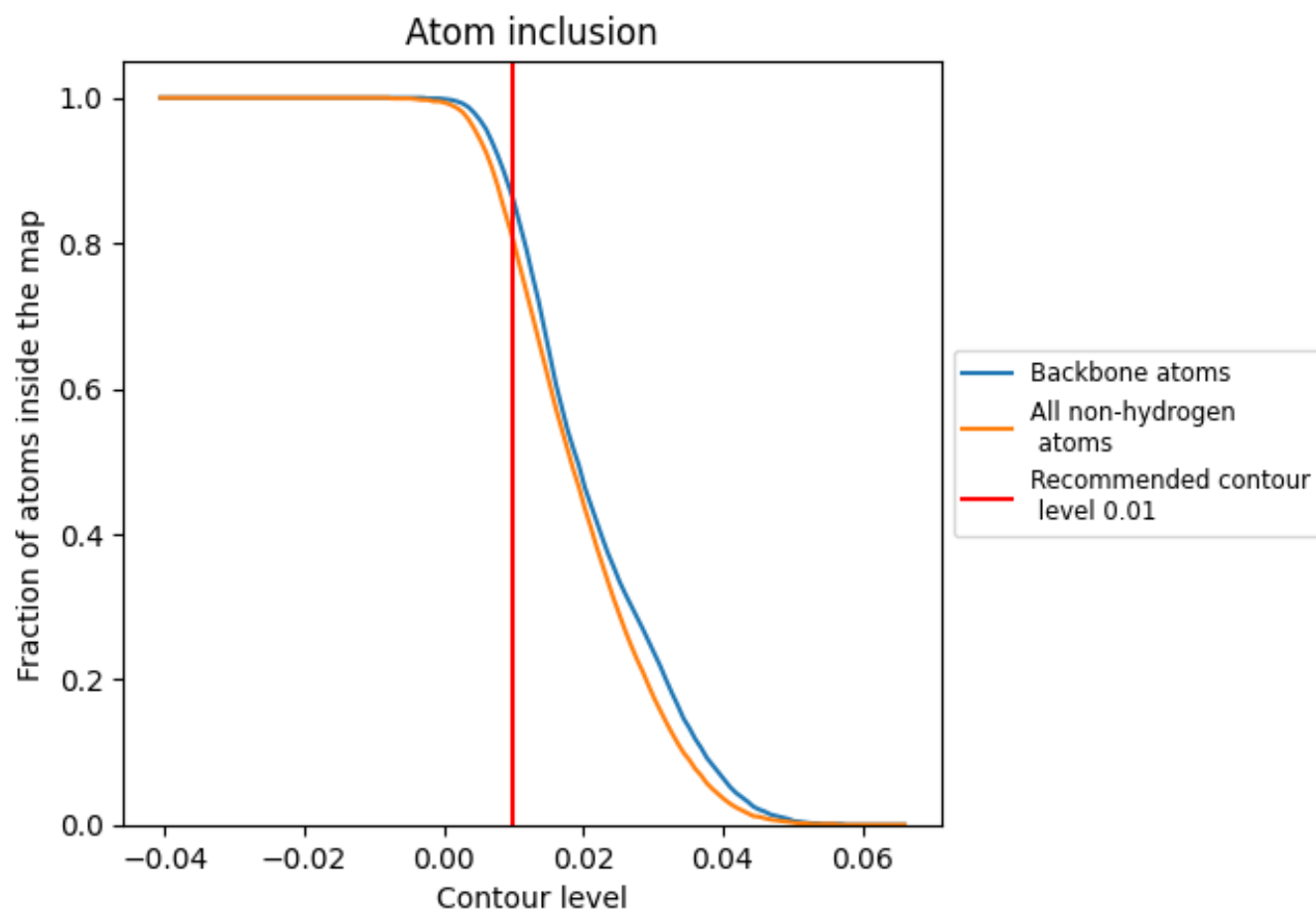
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8030</div>	<div><div></div>0.3190</div>
A	<div><div></div>0.7690</div>	<div><div></div>0.3740</div>
B	<div><div></div>0.8250</div>	<div><div></div>0.3860</div>
C	<div><div></div>0.8190</div>	<div><div></div>0.3930</div>
D	<div><div></div>0.8570</div>	<div><div></div>0.3920</div>
E	<div><div></div>0.7960</div>	<div><div></div>0.3830</div>
F	<div><div></div>0.8480</div>	<div><div></div>0.3930</div>
G	<div><div></div>0.8180</div>	<div><div></div>0.3830</div>
H	<div><div></div>0.8640</div>	<div><div></div>0.3910</div>
I	<div><div></div>0.9330</div>	<div><div></div>0.2910</div>
J	<div><div></div>0.8950</div>	<div><div></div>0.2800</div>
K	<div><div></div>0.5170</div>	<div><div></div>0.2340</div>
L	<div><div></div>0.5160</div>	<div><div></div>0.2300</div>

1.0

0.0

<0.0