



## wwPDB EM Validation Summary Report ⓘ

Oct 30, 2023 – 04:51 PM JST

PDB ID : 7XFM  
EMDB ID : EMD-33176  
Title : Structure of nucleosome-AAG complex (A-53I, post-catalytic state)  
Authors : Zheng, L.; Tsai, B.; Gao, N.  
Deposited on : 2022-04-01  
Resolution : 3.10 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

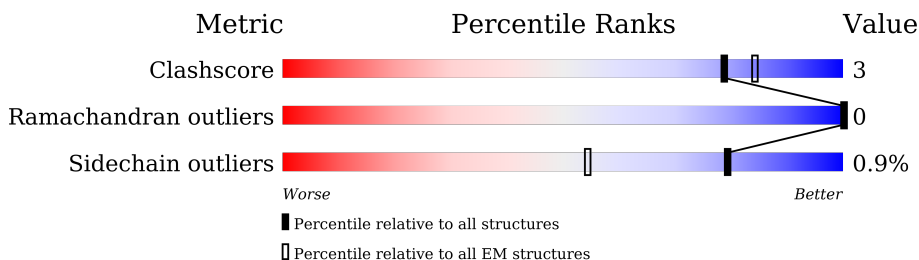
EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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.



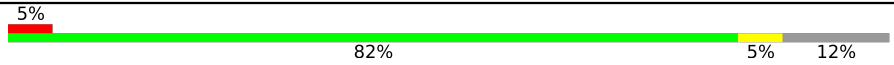


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	 68% 29%
1	E	136	 60% 10% 31%
2	B	103	 72% 7% 21%
2	F	103	 68% 10% 22%
3	C	130	 69% 11% 20%
3	G	130	 78% 5% 18%
4	D	126	 61% 11% 28%
4	H	126	 65% 8% 27%

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Mol	Chain	Length	Quality of chain
5	I	152	 <p>5% 82% 5% 12%</p>
6	J	152	 <p>6% 81% 6% 12%</p>
7	K	298	 <p>66% 58% 8% 33%</p>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12914 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
			Total	C	N	O	S		
1	A	97	801	505	155	138	3	0	0
1	E	94	773	488	147	135	3	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	81	646	407	126	112	1	0	0
2	F	80	638	401	125	111	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	104	800	504	156	140	0	0
3	G	107	823	519	161	143	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	91	708	447	125	134	2	0	0

*Continued on next page...*

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	92	719	453	129	135	2	0	0

- Molecule 5 is a DNA chain called DNA (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	133	2730	1290	509	798	133	0	0

- Molecule 6 is a DNA chain called DNA (152-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	133	2710	1286	496	796	132	0	0

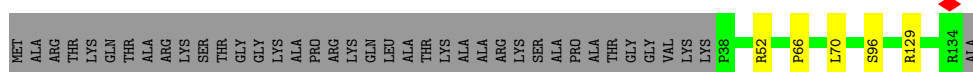
- Molecule 7 is a protein called DNA-3-methyladenine glycosylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	200	1566	986	290	281	9	0	0

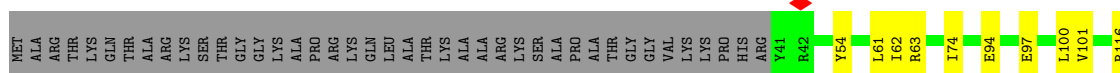
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

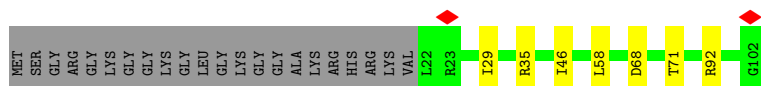
- Molecule 1: Histone H3.2



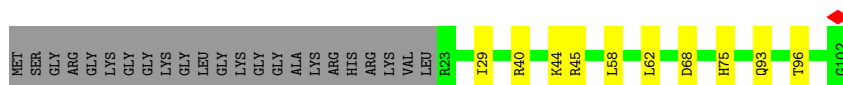
- Molecule 1: Histone H3.2



- Molecule 2: Histone H4



- Molecule 2: Histone H4

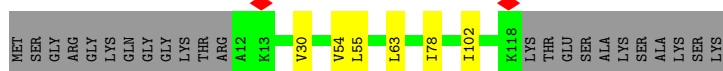
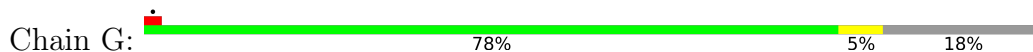


- Molecule 3: Histone H2A type 1

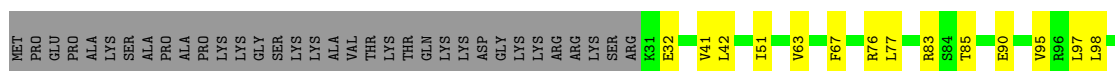




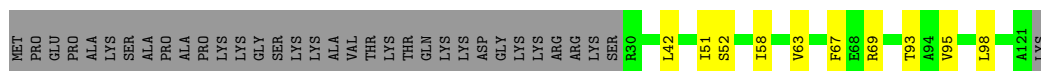
• Molecule 3: Histone H2A type 1



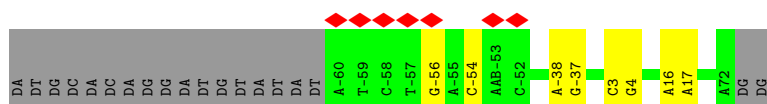
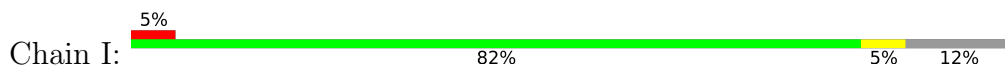
• Molecule 4: Histone H2B 1.1



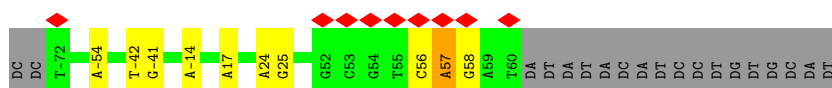
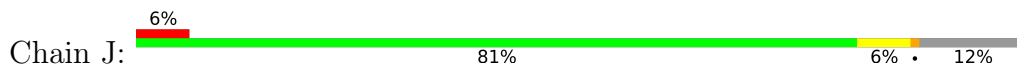
• Molecule 4: Histone H2B 1.1



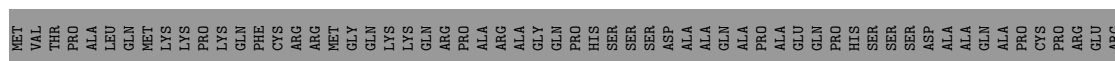
• Molecule 5: DNA (152-MER)



• Molecule 6: DNA (152-MER)



• Molecule 7: DNA-3-methyladenine glycosylase



CYS	LEU	GLY	PRO	THR	THR	PRO	GLY	PRO	TYR	ARG	SER	ILE	TYR	PHE	SER	SER	PRO	LYS	GLY	H82	L83	T84	R85	L86	G87	L88	E89	F90	F91	D92	Q93	P94	A95	V96	P97	L98	A99	R100	A101	F102	L103	G104	Q105	V106	L107	V108	R109	R110	L111	P112	N113	G114	T115	E116	L117	R118	G119	R120	
I121	V122	E123	T124	E125	A126	Y127	L128	G129	P130	E131	D132	E133	A134	A135	H136	S137	R138	G139	G140	R141	Q142	T143	P144	R145	M146	R147	G148	M149	F150	M151	K152	P153	G154	T155	L156	Y157	V158	Y159	I160	I161	Y162	G163	M164	Y165	F166	C167	M168	N169	I170	S171	S172	Q173	G174	D175	G176	A177	C178	V179	L180
L181	R182	A183	L184	E185	P186	L187	E188	G189	L190	E191	T192	M193	R194	Q195	L196	R197	S198	T199	LEU	ARG	LYS	GLY	THR	ALA	SER	ARG	V208	L209	K210	D211	R212	E213	L214	C215	S216	G217	P218	S219	K220	L221	C222	Q223	A224	L225	A226	I227	N228	K229	S230	F231	D232	Q233	R234	D235	L236	A237	Q238	D239	E240
A241	V242	W243	L244	E245	R246	G247	P248	LEU	GLU	PRO	SER	GLU	PRO	A255	V256	V257	A258	A259	A260	R261	V262	G263	V264	G265	H266	A267	G268	E269	W270	A271	R272	K273	P274	L275	R276	F277	Y278	V279	R280	G281	S282	F283	W284	V285	S286	V287	V288	D289	R290	V291	A292	E293	Q294	D295	THR	GLN	ALA		



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98691	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	64	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.281	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0315	Depositor
Map size ( $\text{\AA}$ )	210.40001, 210.40001, 210.40001	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.052, 1.052, 1.052	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: AAB

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	0.34	0/813	0.67	1/1090 (0.1%)
1	E	0.34	0/783	0.59	0/1050
2	B	0.36	0/653	0.62	0/873
2	F	0.39	0/645	0.69	0/862
3	C	0.32	0/810	0.58	0/1095
3	G	0.32	0/833	0.61	0/1124
4	D	0.32	0/719	0.55	0/969
4	H	0.32	0/730	0.58	0/983
5	I	0.70	0/3050	0.95	0/4706
6	J	0.72	0/3037	0.97	3/4682 (0.1%)
7	K	0.29	0/1596	0.65	0/2155
All	All	0.53	0/13669	0.80	4/19589 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	J	57	DA	OP1-P-O3'	-11.57	79.75	105.20
6	J	57	DA	OP2-P-O3'	-6.72	90.42	105.20
6	J	58	DG	OP1-P-OP2	6.50	129.35	119.60
1	A	52	ARG	CA-CB-CG	5.21	124.86	113.40

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	801	0	839	3	0
1	E	773	0	811	10	0
2	B	646	0	687	6	0
2	F	638	0	676	10	0
3	C	800	0	851	12	0
3	G	823	0	882	6	0
4	D	708	0	727	11	0
4	H	719	0	740	9	0
5	I	2730	0	1488	9	0
6	J	2710	0	1492	8	0
7	K	1566	0	1568	19	0
All	All	12914	0	10761	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 67 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)
5:I:-54:DC:H2''	7:K:162:TYR:CE2	1.75	1.21
5:I:-54:DC:H2''	7:K:162:TYR:CD2	2.07	0.88
5:I:-54:DC:H2''	7:K:162:TYR:HE2	1.43	0.81
7:K:127:TYR:O	7:K:177:ALA:HA	1.88	0.74
5:I:-54:DC:C2'	7:K:162:TYR:CE2	2.67	0.73

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	95/136 (70%)	95 (100%)	0	0	100	100
1	E	92/136 (68%)	91 (99%)	1 (1%)	0	100	100
2	B	79/103 (77%)	78 (99%)	1 (1%)	0	100	100
2	F	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
3	C	102/130 (78%)	100 (98%)	2 (2%)	0	100	100
3	G	105/130 (81%)	101 (96%)	4 (4%)	0	100	100
4	D	89/126 (71%)	85 (96%)	4 (4%)	0	100	100
4	H	90/126 (71%)	87 (97%)	3 (3%)	0	100	100
7	K	194/298 (65%)	186 (96%)	8 (4%)	0	100	100
All	All	924/1288 (72%)	898 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/111 (77%)	84 (99%)	1 (1%)	71	88
1	E	82/111 (74%)	81 (99%)	1 (1%)	71	88
2	B	66/79 (84%)	66 (100%)	0	100	100
2	F	65/79 (82%)	65 (100%)	0	100	100
3	C	82/101 (81%)	82 (100%)	0	100	100
3	G	84/101 (83%)	84 (100%)	0	100	100
4	D	77/106 (73%)	76 (99%)	1 (1%)	69	87
4	H	78/106 (74%)	78 (100%)	0	100	100
7	K	162/242 (67%)	158 (98%)	4 (2%)	47	75
All	All	781/1036 (75%)	774 (99%)	7 (1%)	79	91

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	K	147	ARG
7	K	152	LYS
7	K	290	ARG
7	K	162	TYR
1	E	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	AAB	I	-53	5	10,12,13	0.76	0	7,16,19	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AAB	I	-53	5	-	1/3/17/18	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	-53	AAB	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

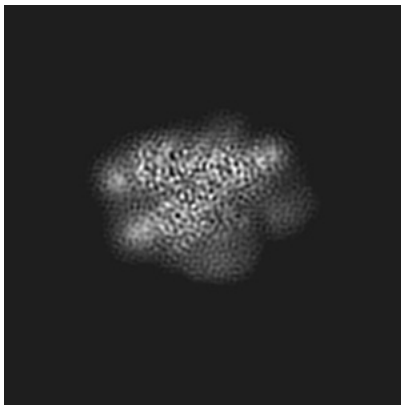
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33176. These allow visual inspection of the internal detail of the map and identification of artifacts.

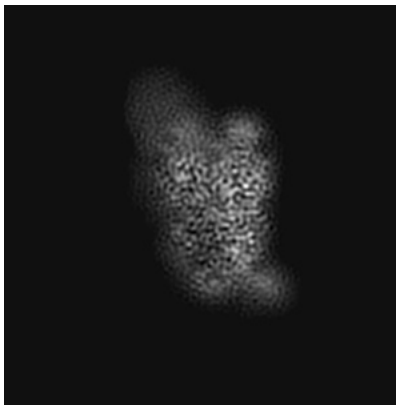
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

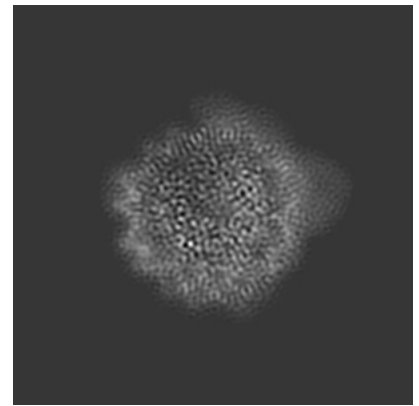
#### 6.1.1 Primary map



X

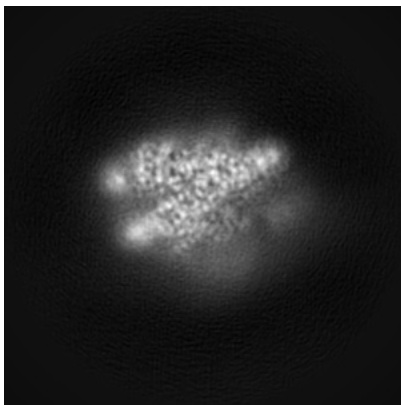


Y

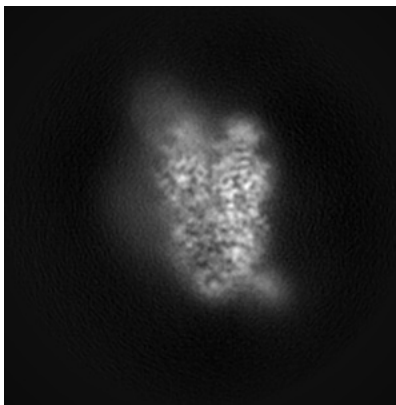


Z

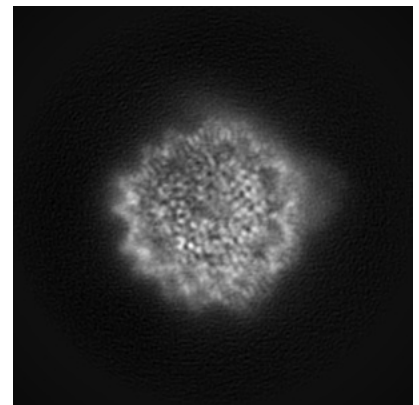
#### 6.1.2 Raw map



X



Y

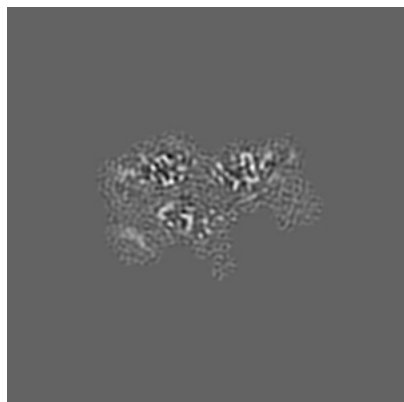


Z

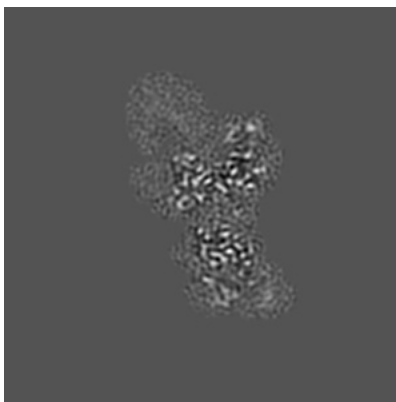
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

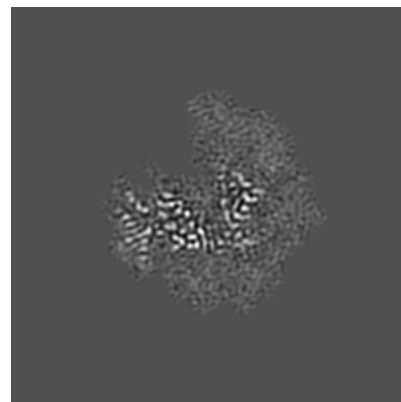
### 6.2.1 Primary map



X Index: 100

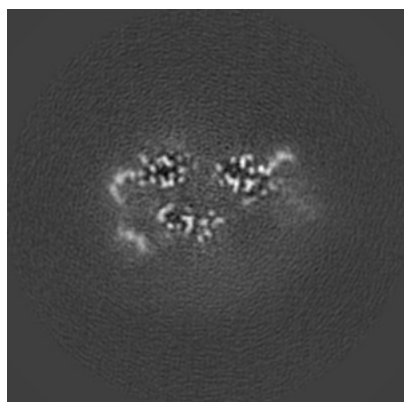


Y Index: 100

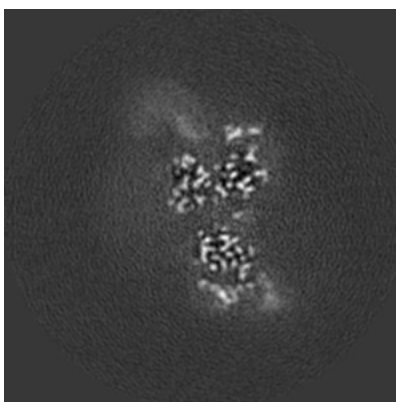


Z Index: 100

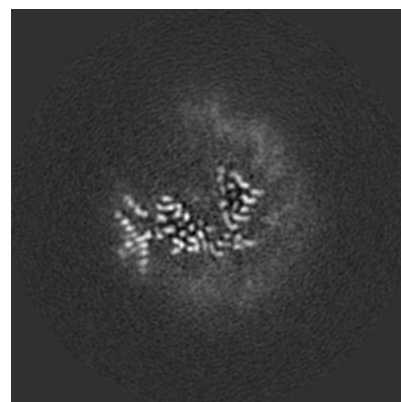
### 6.2.2 Raw map



X Index: 100



Y Index: 100



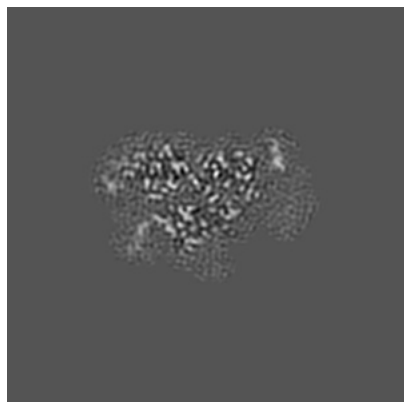
Z Index: 100

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

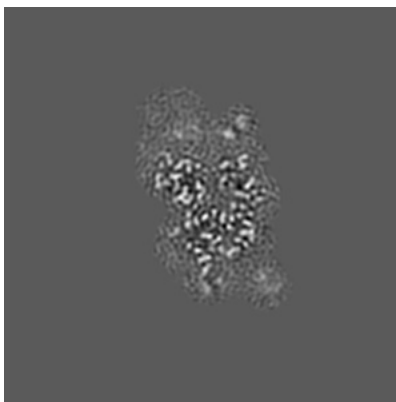


## 6.3 Largest variance slices [i](#)

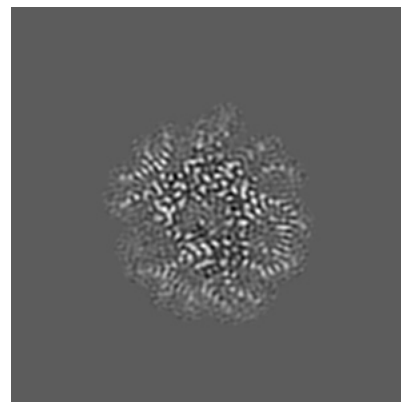
### 6.3.1 Primary map



X Index: 109

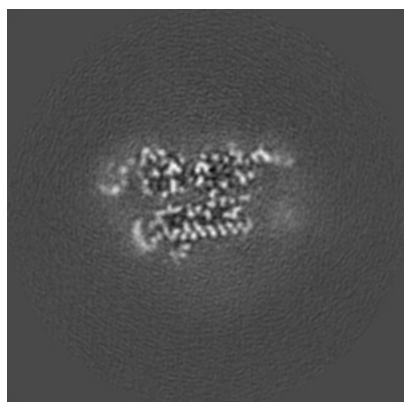


Y Index: 87

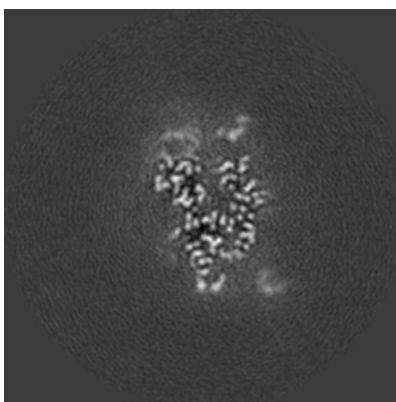


Z Index: 115

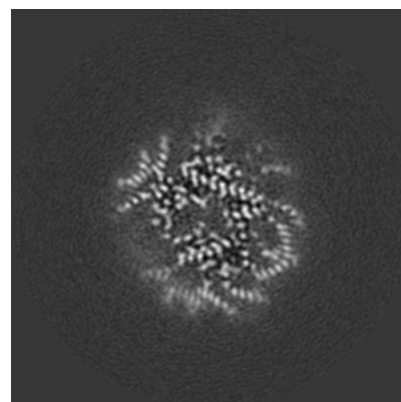
### 6.3.2 Raw map



X Index: 113



Y Index: 87

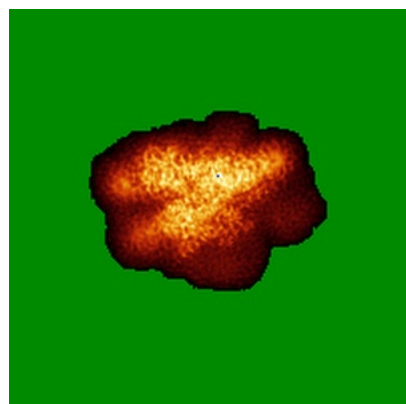


Z Index: 114

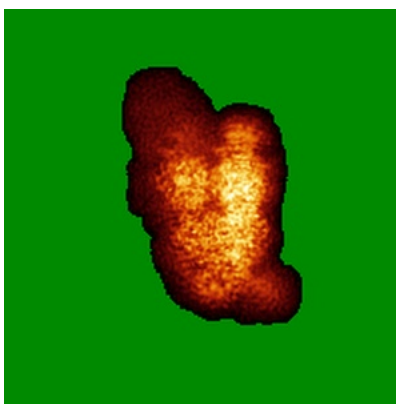
The images above show the largest variance slices of the map in three orthogonal directions.

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

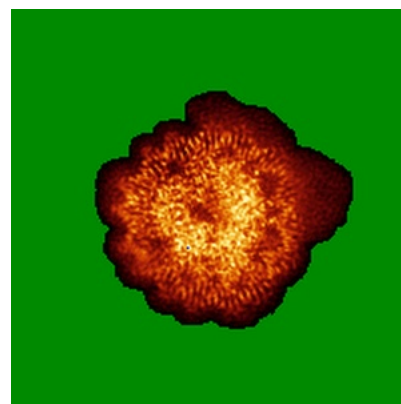
### 6.4.1 Primary map



X

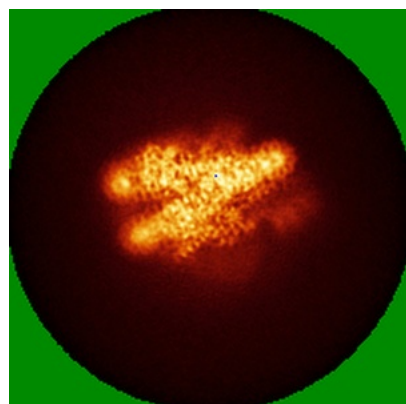


Y

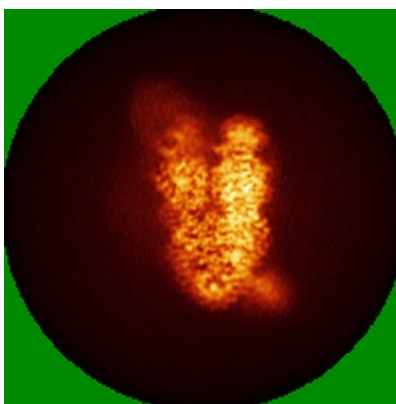


Z

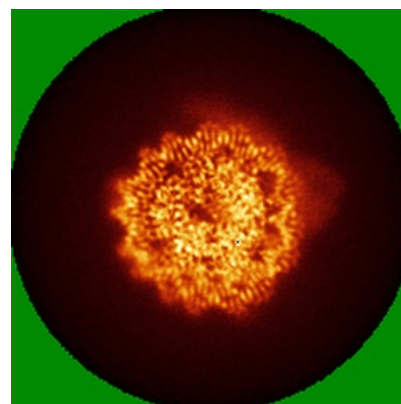
### 6.4.2 Raw map



X



Y

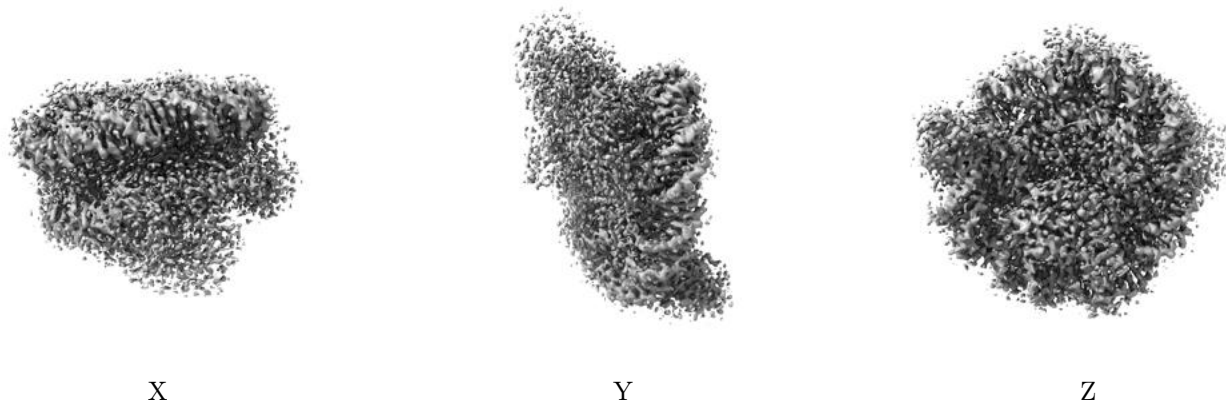


Z

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.

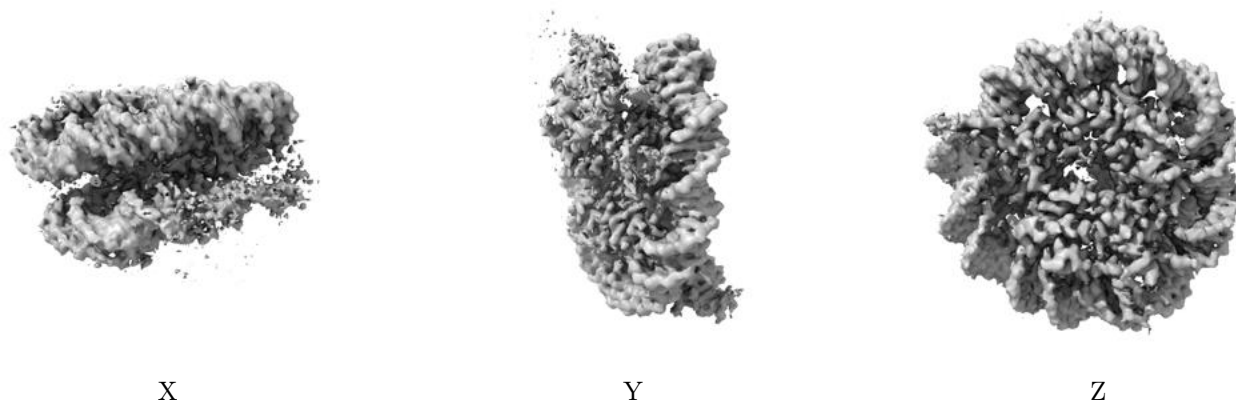
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0315. 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.

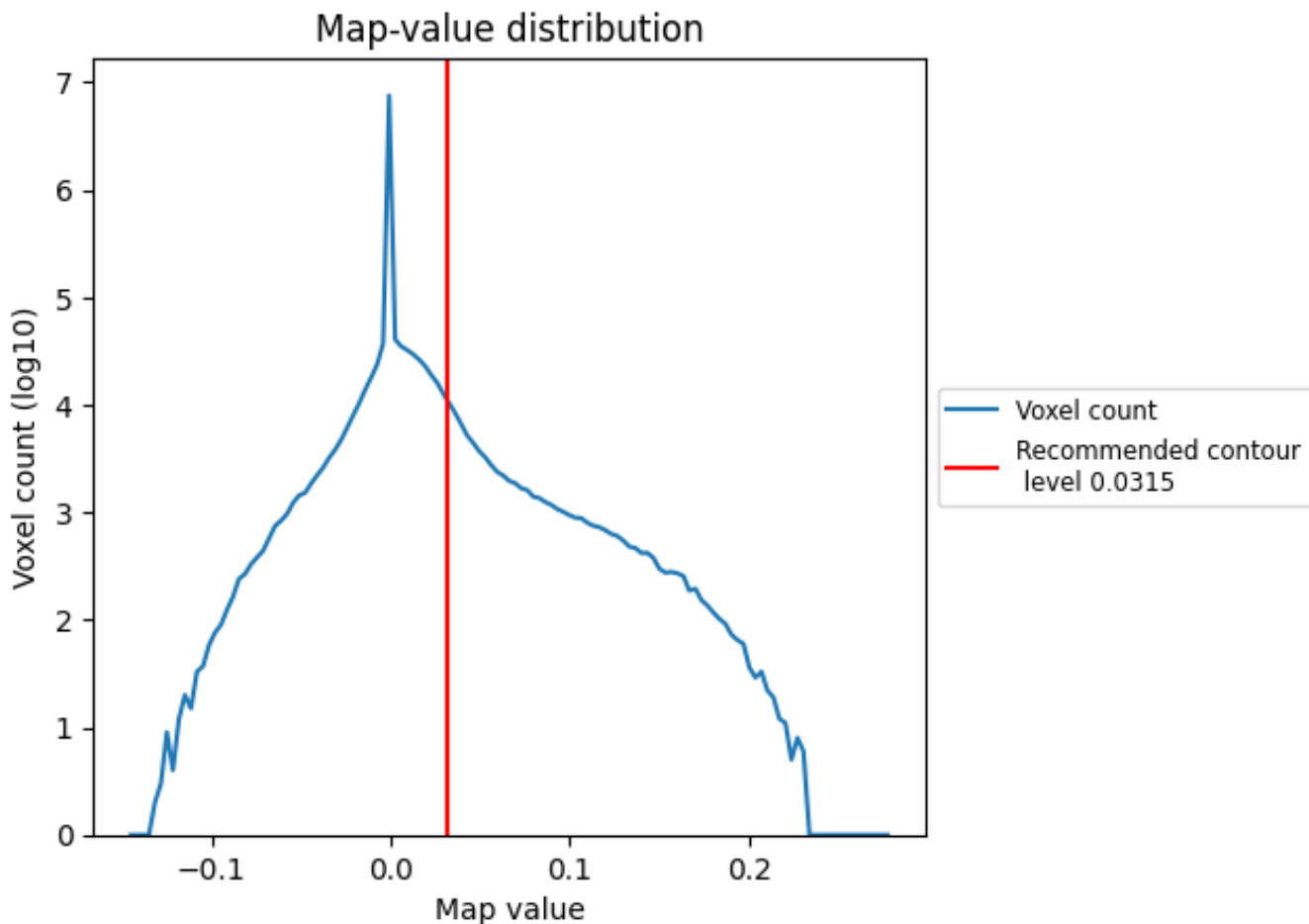
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

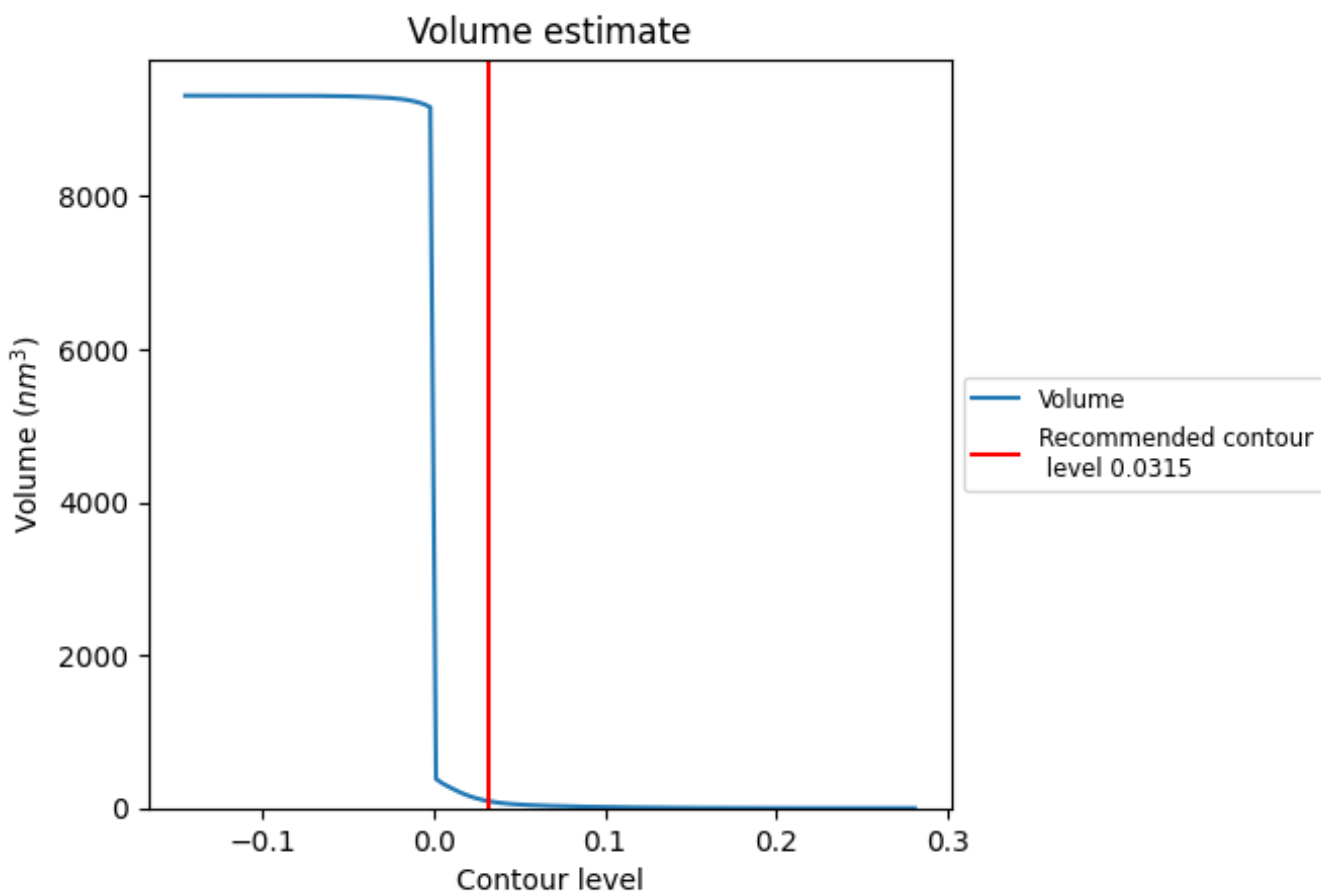
This section contains the results of statistical analysis of the map.

### 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.

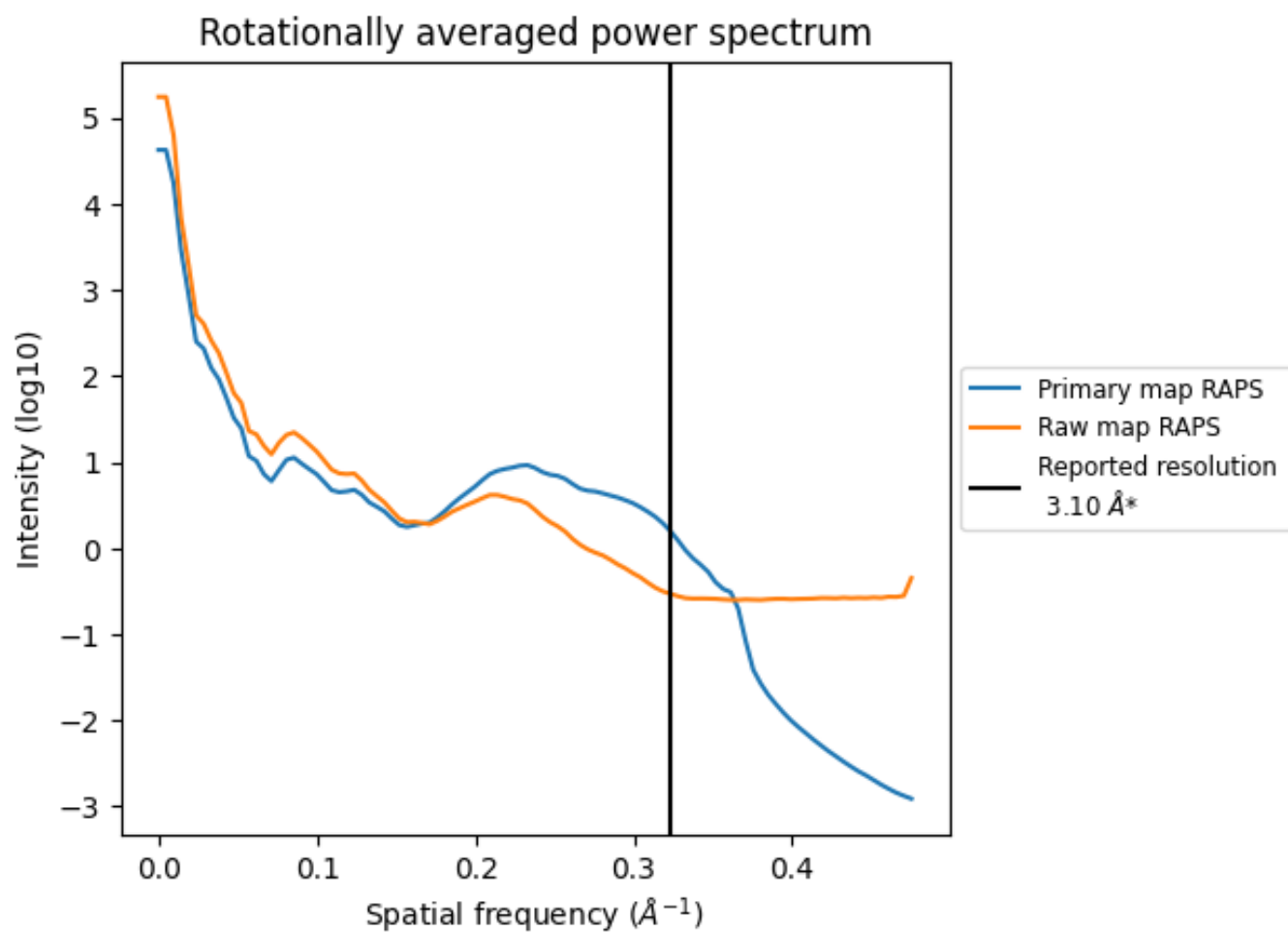
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 94  $\text{nm}^3$ ; this corresponds to an approximate mass of 85 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

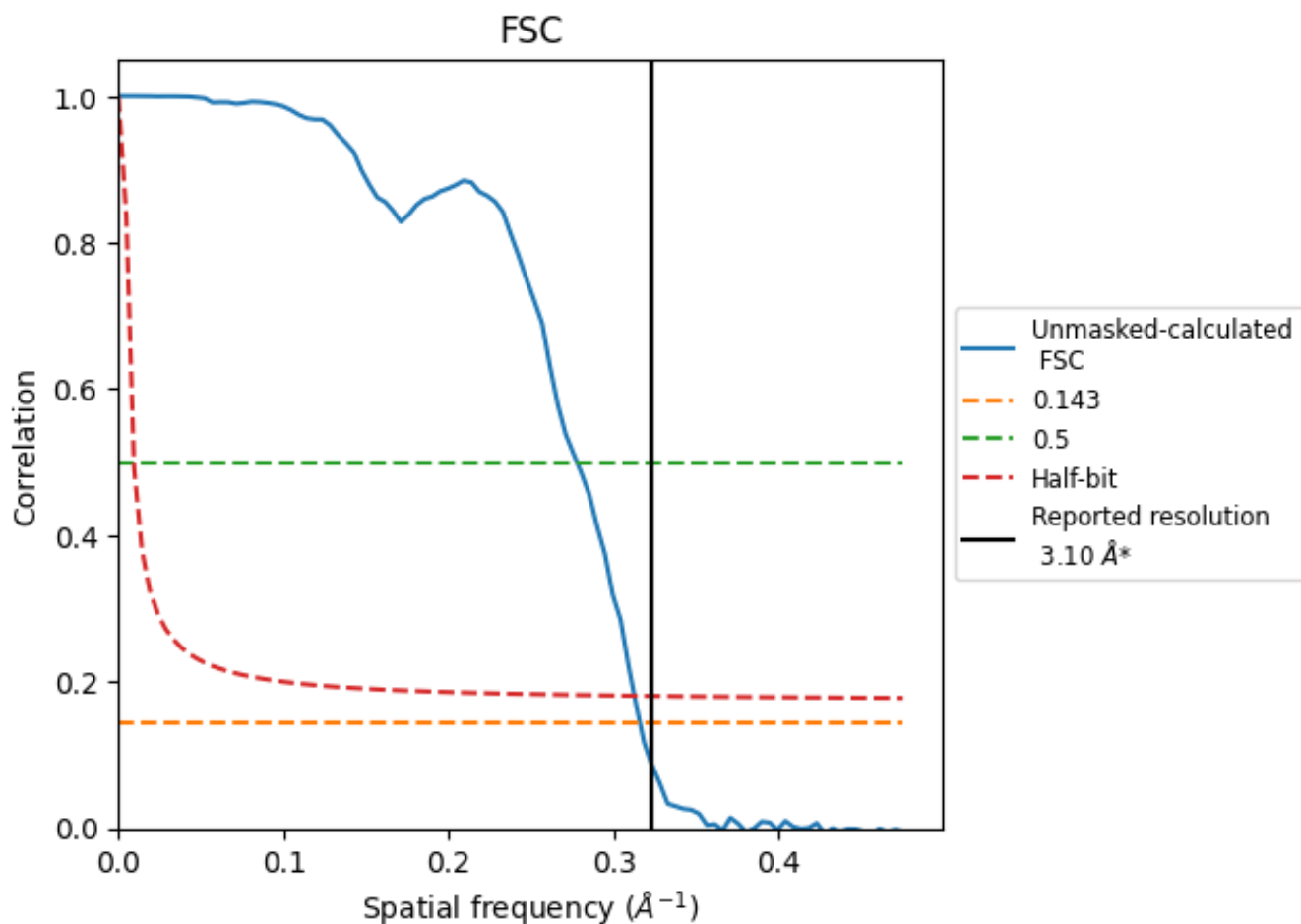


\*Reported resolution corresponds to spatial frequency of  $0.323 \text{ \AA}^{-1}$

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	3.60	3.20

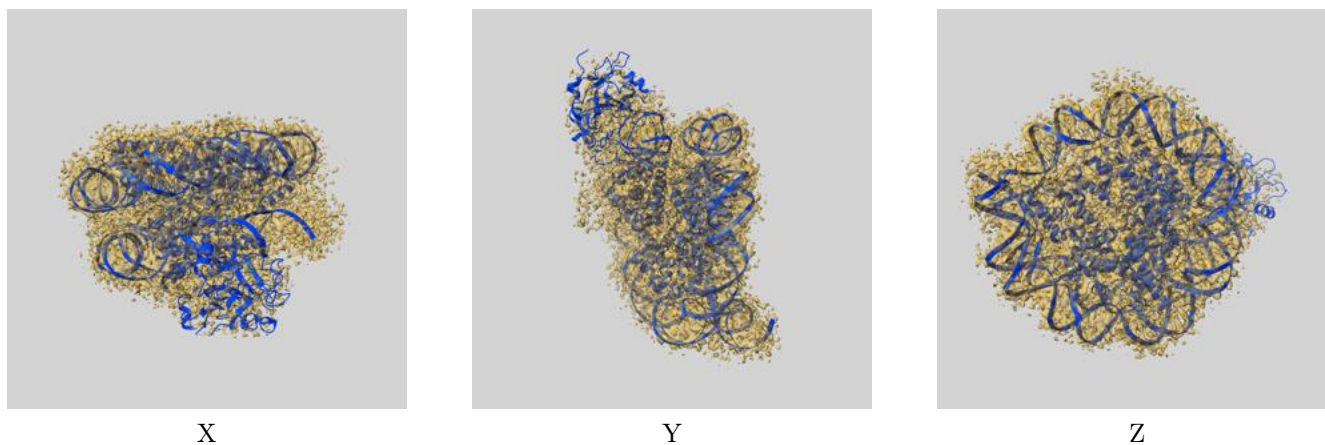
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

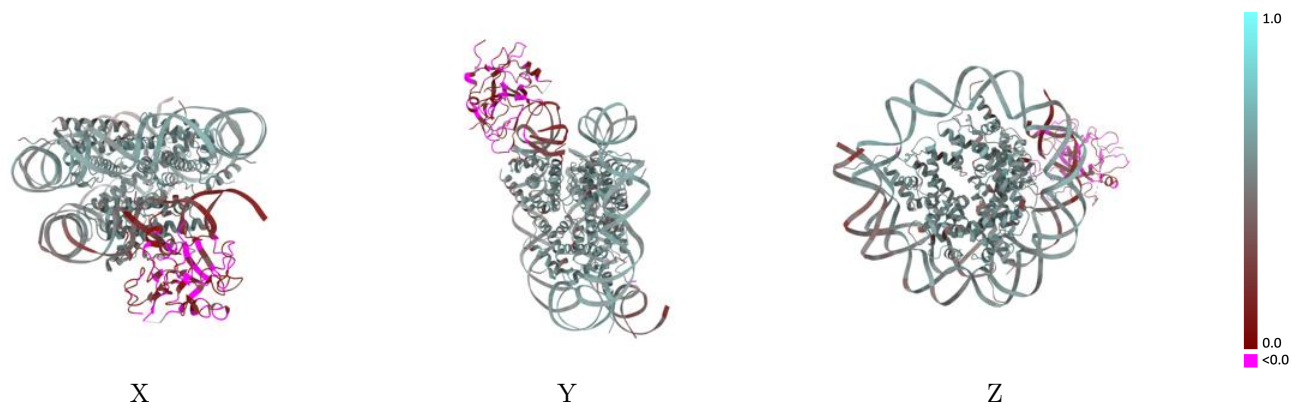
This section contains information regarding the fit between EMDB map EMD-33176 and PDB model 7XFM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



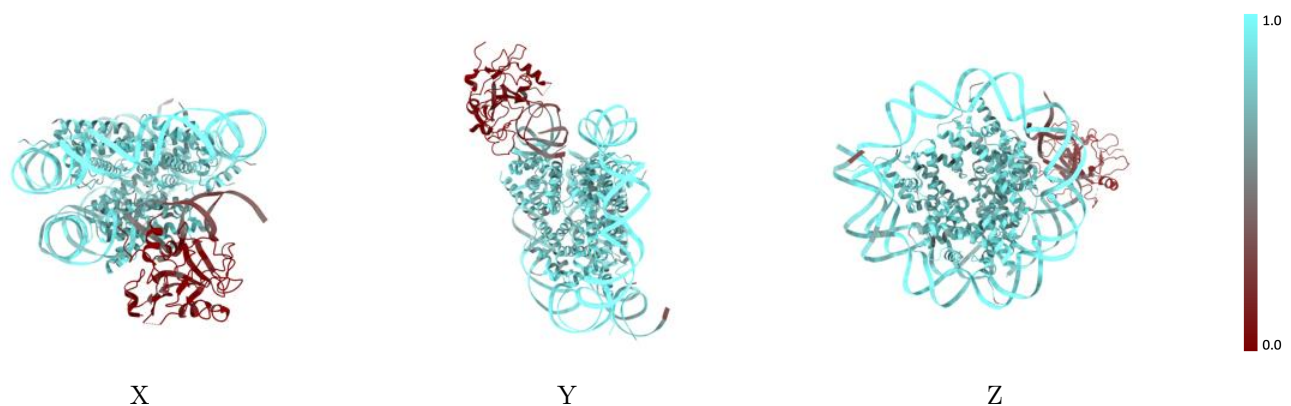
The images above show the 3D surface view of the map at the recommended contour level 0.0315 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



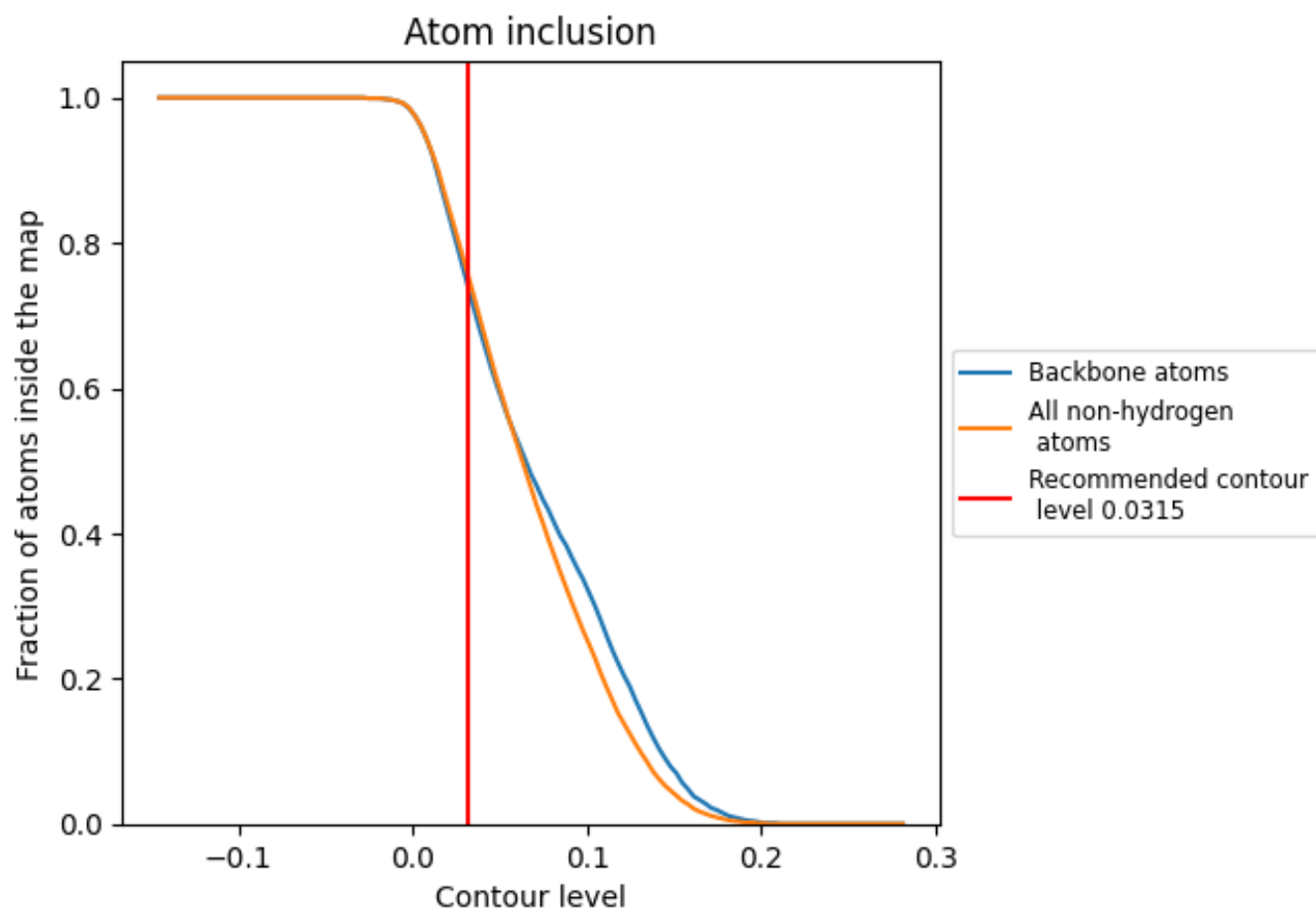
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0315).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.0315) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.4660
A	 0.8830	 0.5540
B	 0.8710	 0.5570
C	 0.8530	 0.5480
D	 0.8370	 0.5260
E	 0.8580	 0.5540
F	 0.8770	 0.5600
G	 0.8420	 0.5350
H	 0.8500	 0.5330
I	 0.8550	 0.4920
J	 0.8400	 0.4910
K	 0.0560	 0.0730

