



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2023 – 03:47 pm GMT

PDB ID : 8PC5
EMDB ID : EMD-17594
Title : H3K36me3 nucleosome-LEDGF/p75 PWWP domain complex
Authors : Koutna, E.; Kouba, T.; Veverka, V.
Deposited on : 2023-06-09
Resolution : 3.02 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.dev70
Mogul : 1.8.4, 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

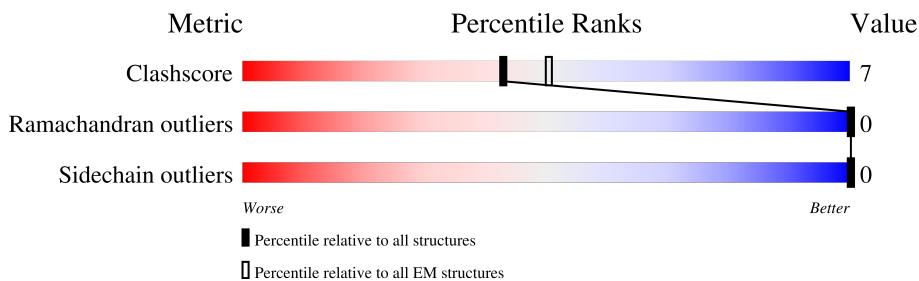
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 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 ≥ 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	I	147	
2	A	135	
2	E	135	
3	B	102	
3	F	102	
4	C	129	
4	G	129	
5	D	122	

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Mol	Chain	Length	Quality of chain
5	H	122	 <p>68% 9% 23%</p>
6	K	530	 <p>11% 6% 84%</p>
7	J	147	 <p>70% 30%</p>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12836 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 Widom 601 DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	I	147	2996	1423	545	881	147	0	0

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	100	829	525	160	141	3	0	0
2	E	97	801	506	155	138	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	CYS	conflict	UNP A0A310TTQ1
E	110	ALA	CYS	conflict	UNP A0A310TTQ1

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	82	657	416	128	112	1	0	0
3	F	86	694	436	140	117	1	0	0

- Molecule 4 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	C	107	823	519	161	143	0	0
4	G	107	823	519	161	143	0	0

- Molecule 5 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	94	Total	C	N	O	S	0	0
			736	463	132	139	2		
5	H	94	Total	C	N	O	S	0	0
			736	463	132	139	2		

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is a protein called PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	86	Total	C	N	O	S	0	0
			710	467	119	122	2		

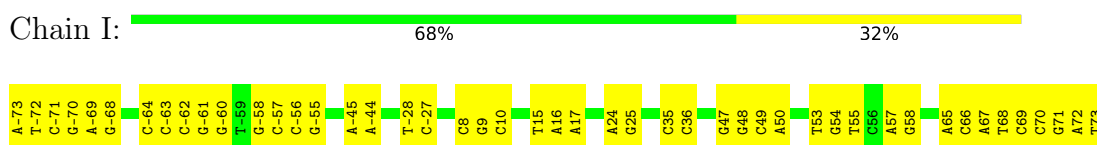
- Molecule 7 is a DNA chain called Widom 601 DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	147	Total	C	N	O	P	0	0
			3031	1435	566	883	147		

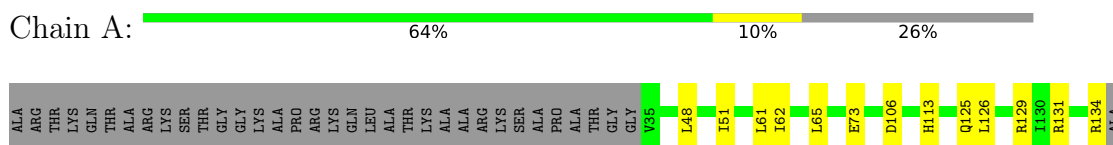
3 Residue-property plots [i](#)

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.

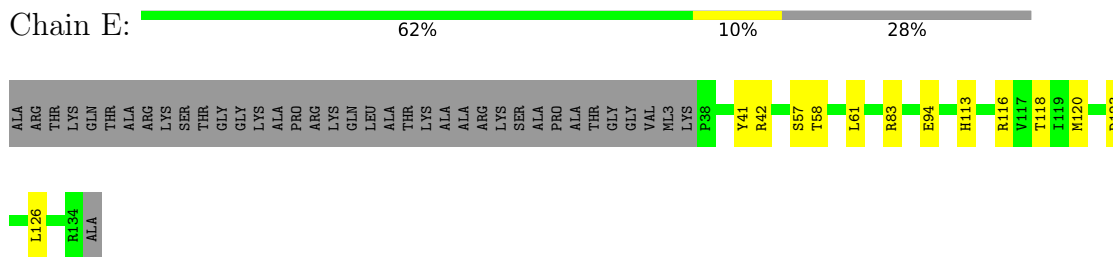
- Molecule 1: Widom 601 DNA (147-MER)



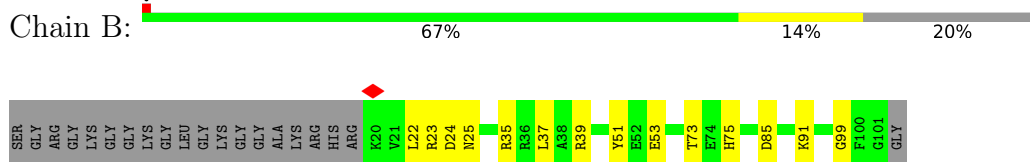
- Molecule 2: Histone H3



- Molecule 2: Histone H3

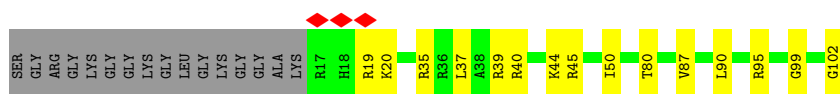


- Molecule 3: Histone H4

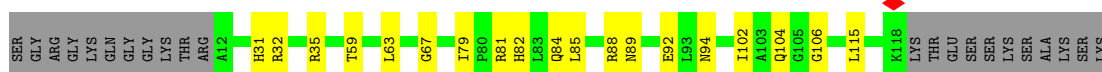


- Molecule 3: Histone H4

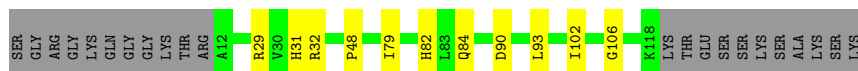




• Molecule 4: Histone H2A



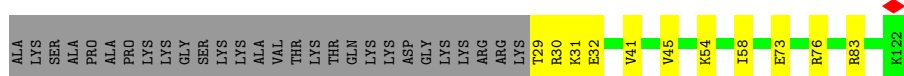
• Molecule 4: Histone H2A



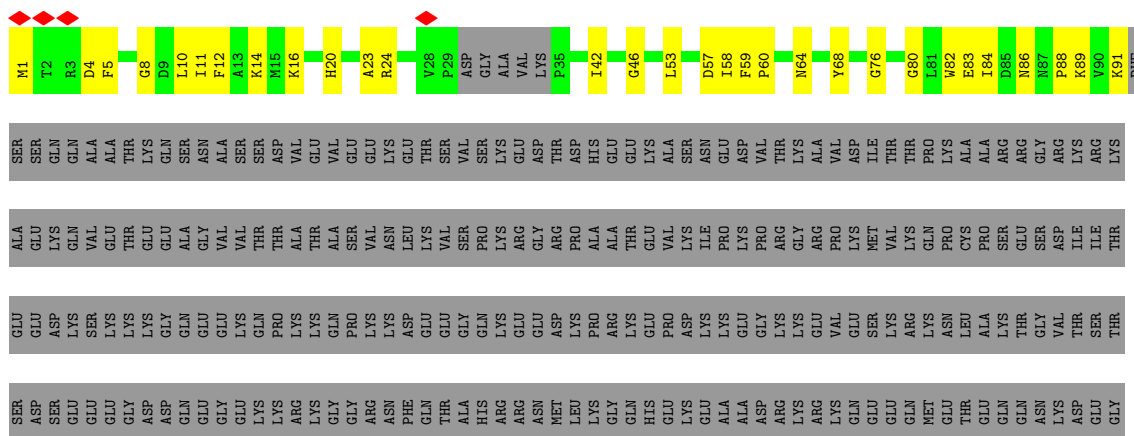
• Molecule 5: Histone H2B 1.1



• Molecule 5: Histone H2B 1.1



• Molecule 6: PC4 and SFRS1-interacting protein



LYS	HIS
LYS	THR
PRO	GLU
GLU	MET
VAL	ILE
LYS	THR
LYS	THR
VAL	LEU
GLU	LEU
LYS	LYS
LYS	ILE
LYS	ILE
ARG	PRO
ARG	ARG
GLU	ARG
THR	PHE
SER	LYS
MET	VAL
ASP	GLN
SER	VAL
ARG	ILE
LEU	MET
GLN	THR
ARG	GLY
ILE	SER
GLY	LYS
ILE	HIS
ALA	THR
GLU	THR
ILE	MET
LYS	LEU
LYS	TYR
ASN	GLY
ASN	GLY
SER	SER
SER	LYS
LEU	PHE
LYS	LYS
ILE	ASN
ILE	ASN
ASP	MET
GLY	PHE
ASN	GLY
LEU	ASN
ASP	VAL
VAL	VAL
ASN	GLY
ASN	GLU
ARG	GLY
ARG	ASP
LYS	SER
ALA	ILE
LEU	THR
GLN	VAL
ASP	GLN
ASN	VAL
ASN	LEU
LEU	LEU
ALA	ALA
SER	LYS
LEU	ASP
GLN	SER
HIS	ASN
ASN	LYS
GLY	ASP
LEU	ASN
VAL	SER
ASP	THR
ILE	ILE
THR	THR
GLN	GLN
ASP	VAL
GLU	LEU
ASP	LEU
LYS	LEU
ASP	ASN
ASN	LYS
HIS	HIS
GLU	VAL
ALA	ALA
ALA	THR
SER	GLN
THR	MET
THR	GLN
LYS	ARG
LYS	GLN
LYS	GLN
GLN	HIS
LYS	GLU
PRO	LYS
PRO	GLU

• Molecule 7: Widom 601 DNA (147-MER)

Chain J:  70% 30%

A-73	A-73
T-72	T-72
C-71	C-71
G-70	G-70
G-69	G-69
A-68	A-68
T-67	T-67
G-66	G-66
T-63	T-63
A-62	A-62
T-61	T-61
A-60	A-60
T-59	T-59
C-54	C-54
A-53	A-53
T-50	T-50
G-49	G-49
A-43	A-43
G-42	G-42
G-33	G-33
T-23	T-23
G-22	G-22
C11	C11
A17	A17
G20	G20
G21	G21
C24	C24
T25	T25
G32	G32
T33	T33
C34	C34
T35	T35
C49	C49
G50	G50
T54	T54
C55	C55
G62	G62
G63	G63
G64	G64
A65	A65
T66	T66
T67	T67
C68	C68
T69	T69
C70	C70
G71	G71

A72	A72
T73	T73

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36211	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 ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.740	Depositor
Minimum map value	-0.238	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	350.112, 350.112, 350.112	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8336, 0.8336, 0.8336	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: ML3

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	I	0.72	0/3357	1.01	0/5174
2	A	0.33	0/828	0.56	0/1110
2	E	0.30	0/813	0.54	0/1091
3	B	0.35	0/664	0.58	0/889
3	F	0.31	0/702	0.57	0/937
4	C	0.27	0/833	0.51	0/1124
4	G	0.33	0/833	0.55	0/1124
5	D	0.30	0/747	0.47	0/1004
5	H	0.33	0/747	0.50	0/1004
6	K	0.28	0/736	0.47	0/992
7	J	0.70	0/3403	1.00	0/5255
All	All	0.55	0/13663	0.82	0/19704

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	I	2996	0	1650	38	0
2	A	829	0	878	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	801	0	841	14	0
3	B	657	0	706	12	0
3	F	694	0	742	12	0
4	C	823	0	882	15	0
4	G	823	0	882	7	0
5	D	736	0	760	14	0
5	H	736	0	760	8	0
6	K	710	0	701	21	0
7	J	3031	0	1651	42	0
All	All	12836	0	10453	161	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 161 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)
1:I:-62:DC:H2'	1:I:-61:DG:C8	2.06	0.90
7:J:66:DT:H2''	7:J:67:DT:H5''	1.54	0.87
2:E:83:ARG:HB2	3:F:80:THR:HG22	1.63	0.78
7:J:65:DA:H2''	7:J:66:DT:H5''	1.67	0.77
3:B:75:HIS:O	5:D:89:ARG:NH2	2.20	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	
2	A	97/135 (72%)	96 (99%)	1 (1%)	0	100	100
2	E	95/135 (70%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	80/102 (78%)	78 (98%)	2 (2%)	0	100	100
3	F	84/102 (82%)	83 (99%)	1 (1%)	0	100	100
4	C	105/129 (81%)	103 (98%)	2 (2%)	0	100	100
4	G	105/129 (81%)	103 (98%)	2 (2%)	0	100	100
5	D	92/122 (75%)	91 (99%)	1 (1%)	0	100	100
5	H	92/122 (75%)	92 (100%)	0	0	100	100
6	K	82/530 (16%)	77 (94%)	5 (6%)	0	100	100
All	All	832/1506 (55%)	816 (98%)	16 (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	86/108 (80%)	86 (100%)	0	100	100
2	E	84/108 (78%)	84 (100%)	0	100	100
3	B	68/78 (87%)	68 (100%)	0	100	100
3	F	71/78 (91%)	71 (100%)	0	100	100
4	C	84/101 (83%)	84 (100%)	0	100	100
4	G	84/101 (83%)	84 (100%)	0	100	100
5	D	80/102 (78%)	80 (100%)	0	100	100
5	H	80/102 (78%)	80 (100%)	0	100	100
6	K	76/470 (16%)	76 (100%)	0	100	100
All	All	713/1248 (57%)	713 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	$\# Z > 2$
2	ML3	A	36	2	10,11,12	0.73	0	10,14,16	0.88	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
2	ML3	A	36	2	-	0/8/10/12	-

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.

5.5 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.

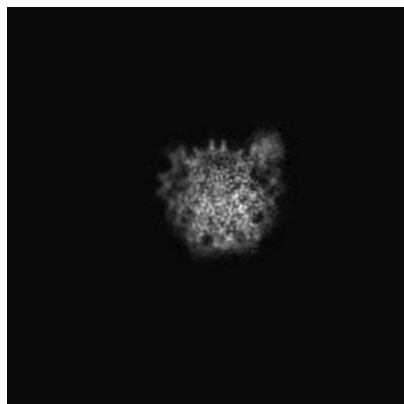
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17594. These allow visual inspection of the internal detail of the map and identification of artifacts.

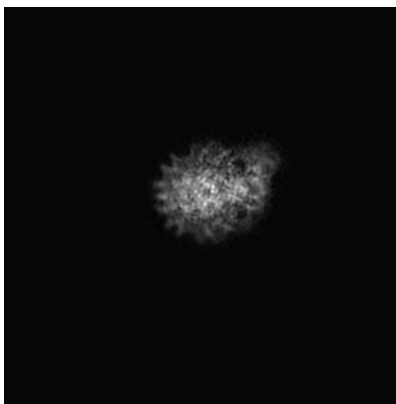
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

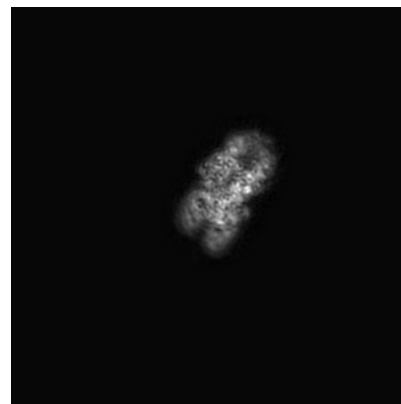
6.1.1 Primary map



X

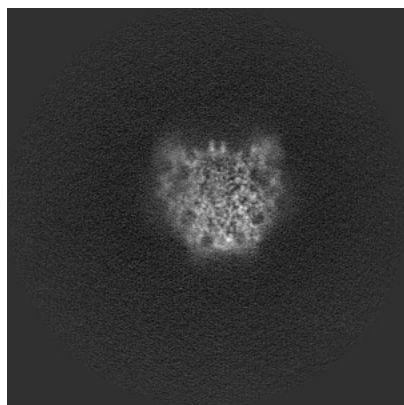


Y

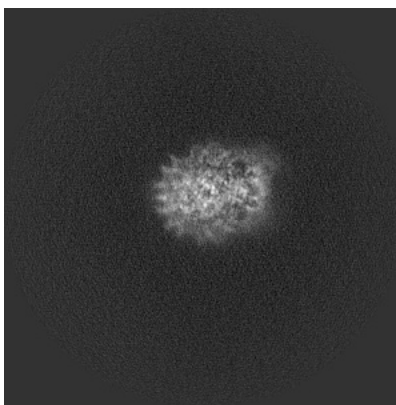


Z

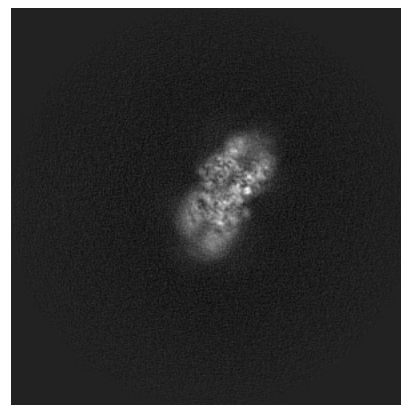
6.1.2 Raw map



X



Y

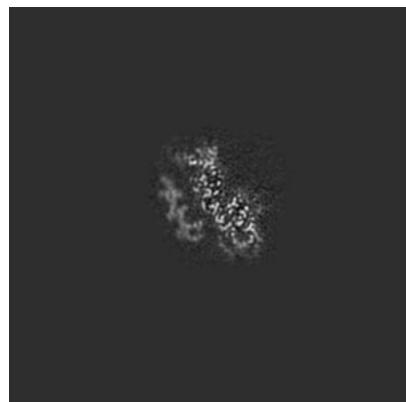


Z

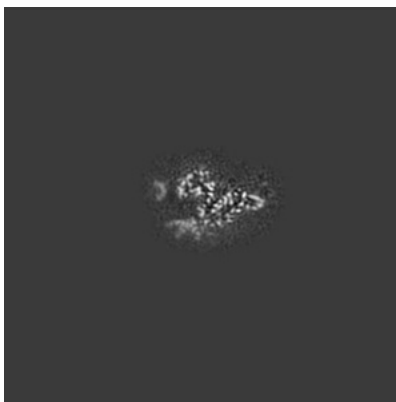
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

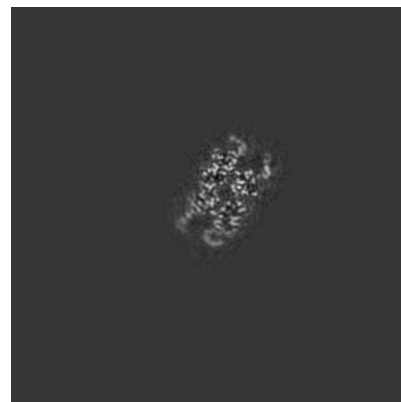
6.2.1 Primary map



X Index: 210

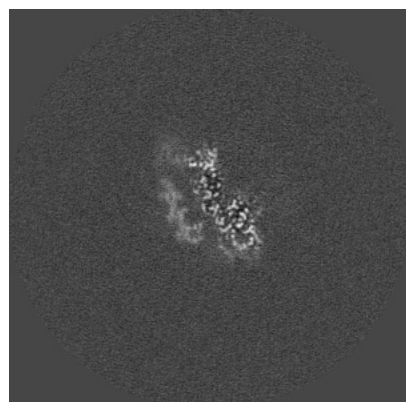


Y Index: 210

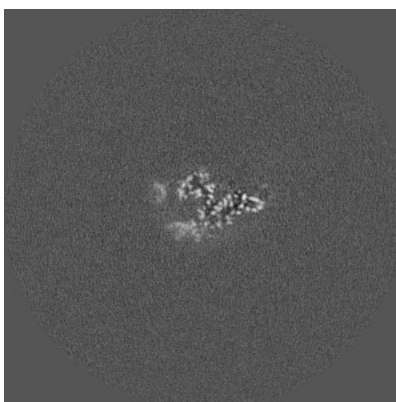


Z Index: 210

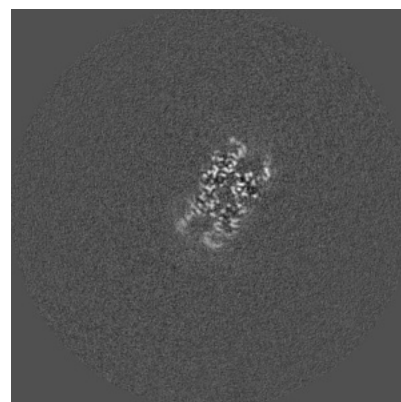
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

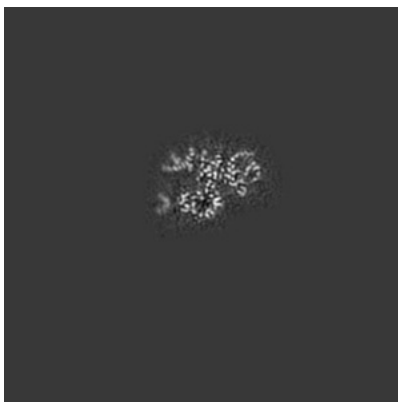
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

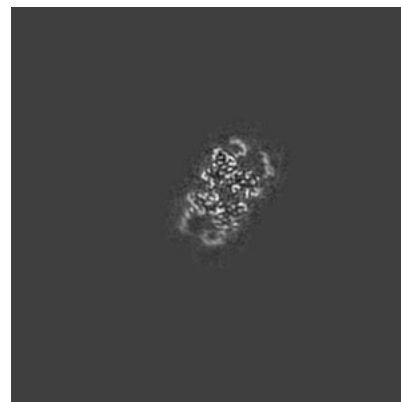
6.3.1 Primary map



X Index: 220

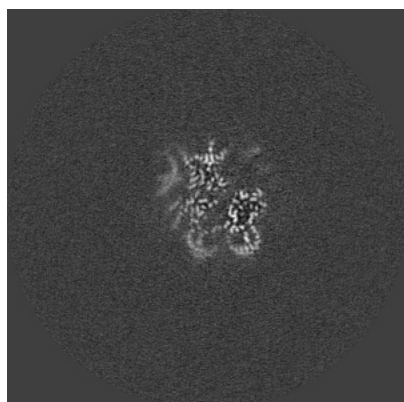


Y Index: 241

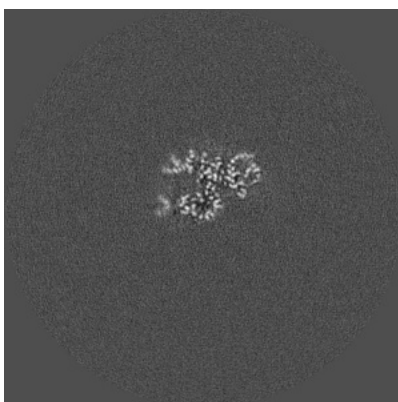


Z Index: 212

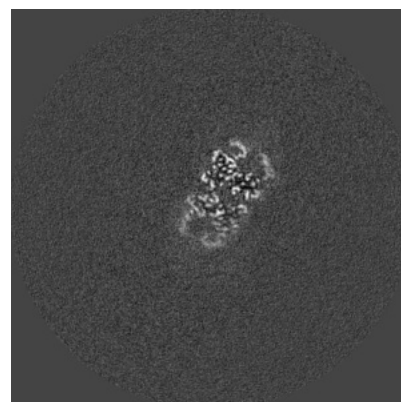
6.3.2 Raw map



X Index: 220



Y Index: 241

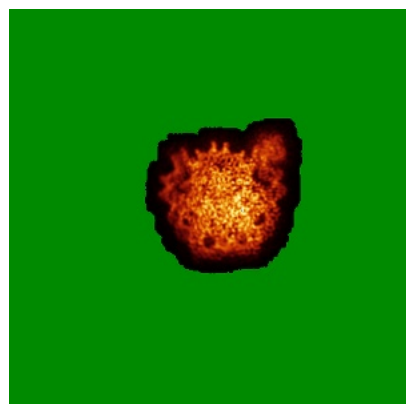


Z Index: 212

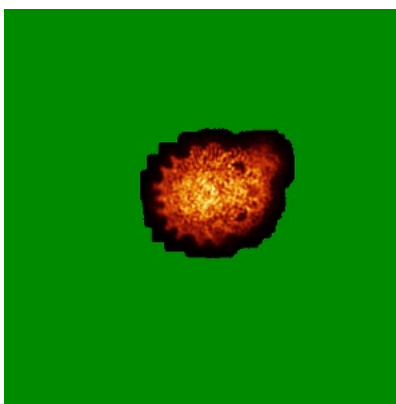
The images above show the largest variance slices of the map in three orthogonal directions.

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

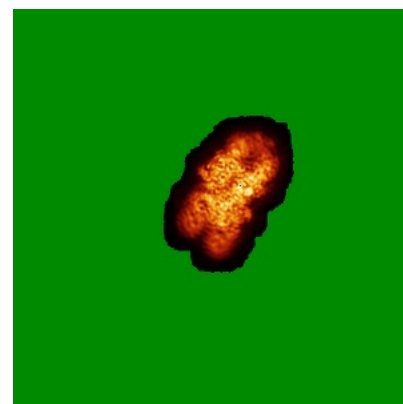
6.4.1 Primary map



X

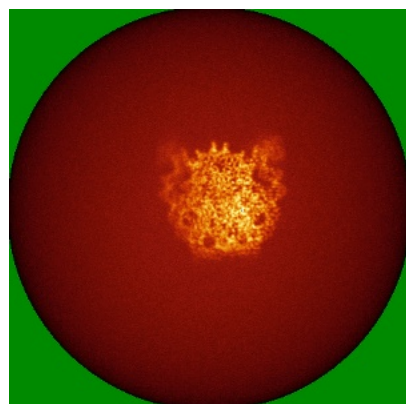


Y

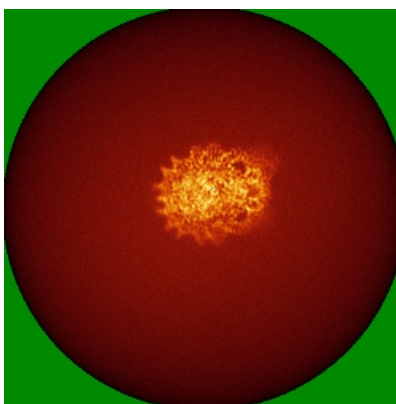


Z

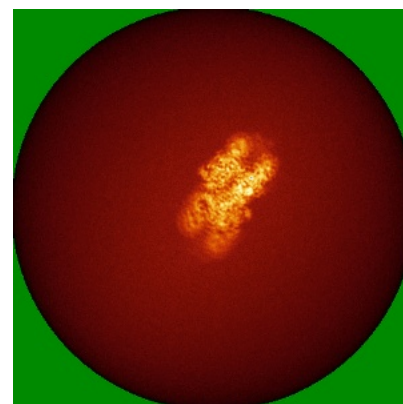
6.4.2 Raw map



X



Y

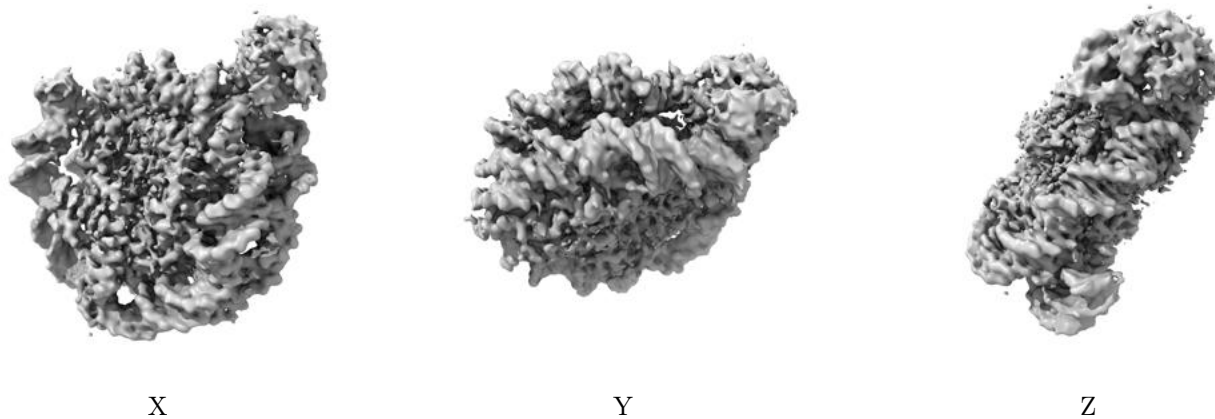


Z

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.

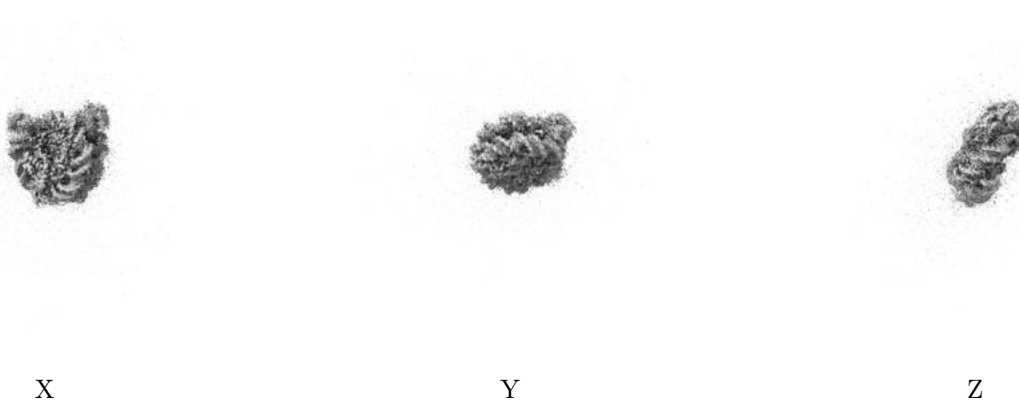
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

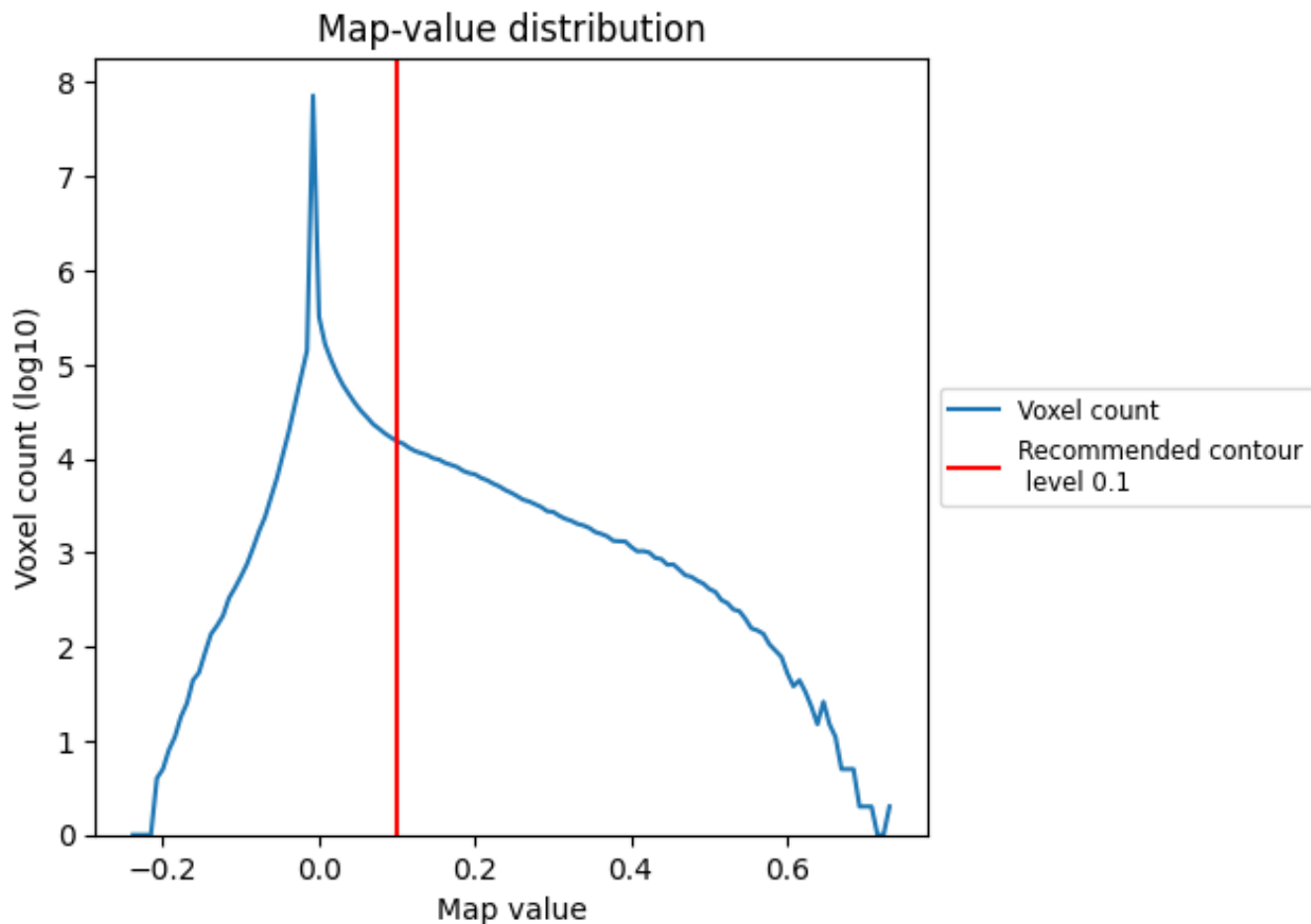
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

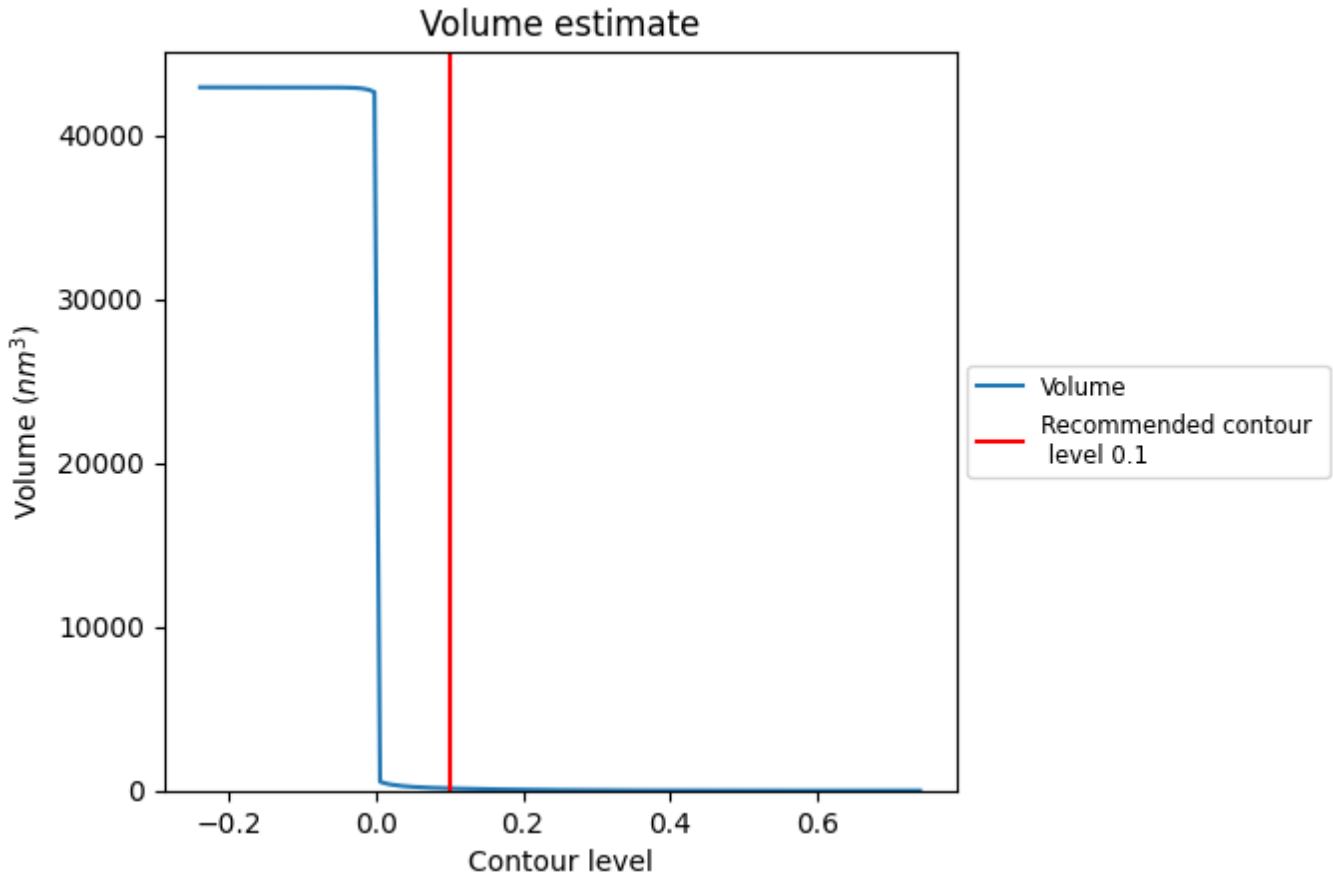
This section contains the results of statistical analysis of the map.

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.

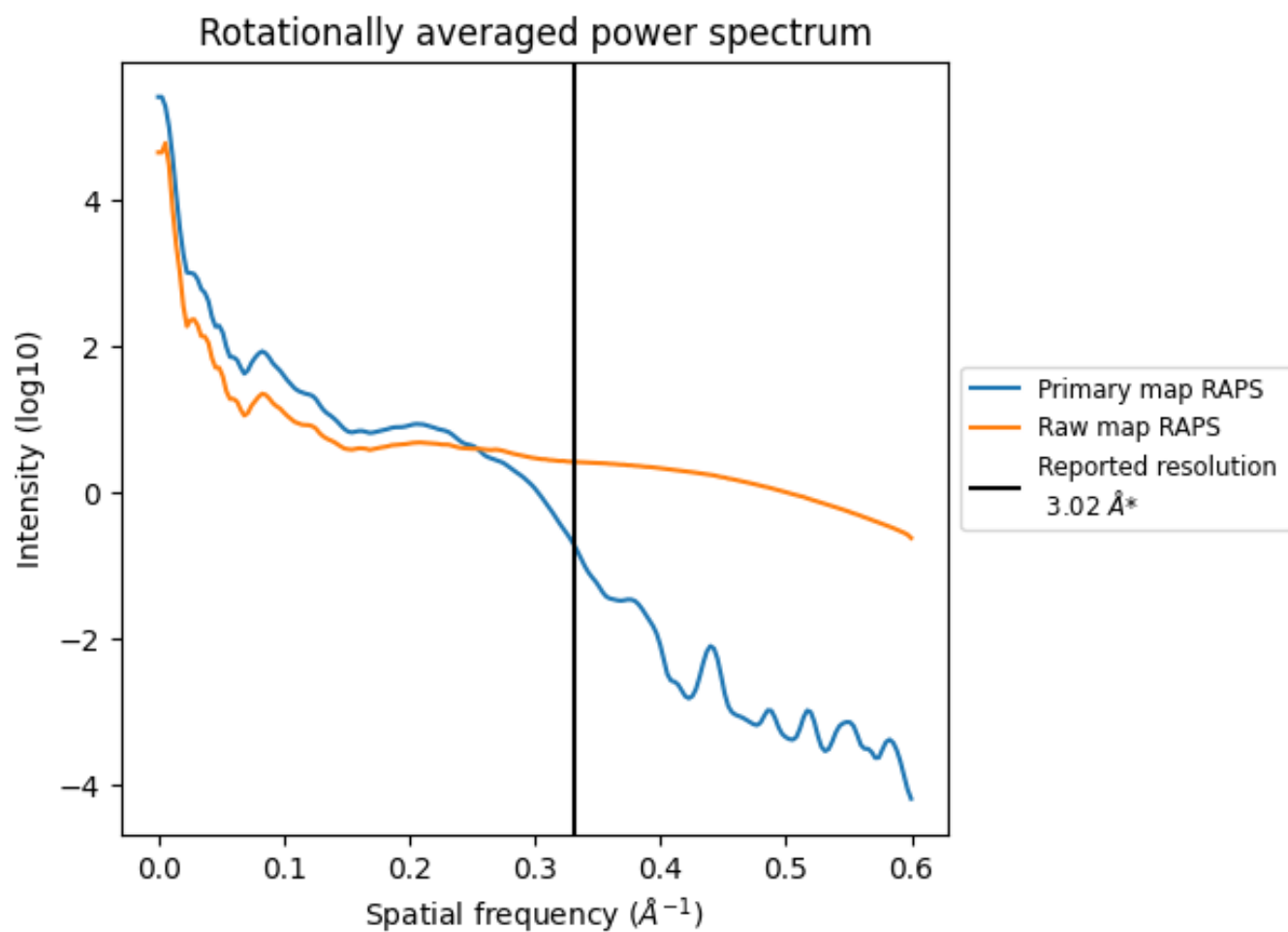
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 136 nm³; this corresponds to an approximate mass of 123 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

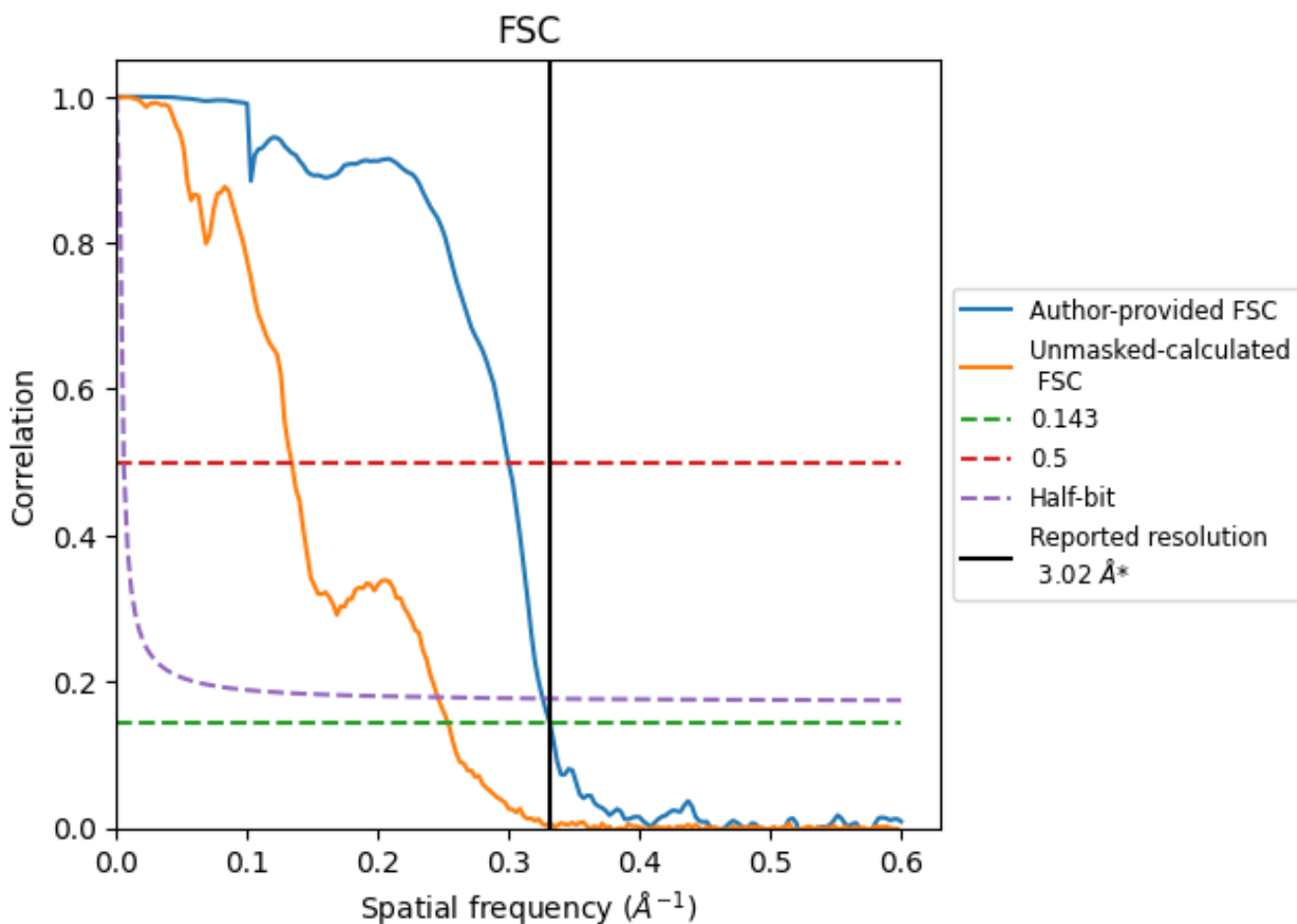


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

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 0.331 Å⁻¹

8.2 Resolution estimates [i](#)

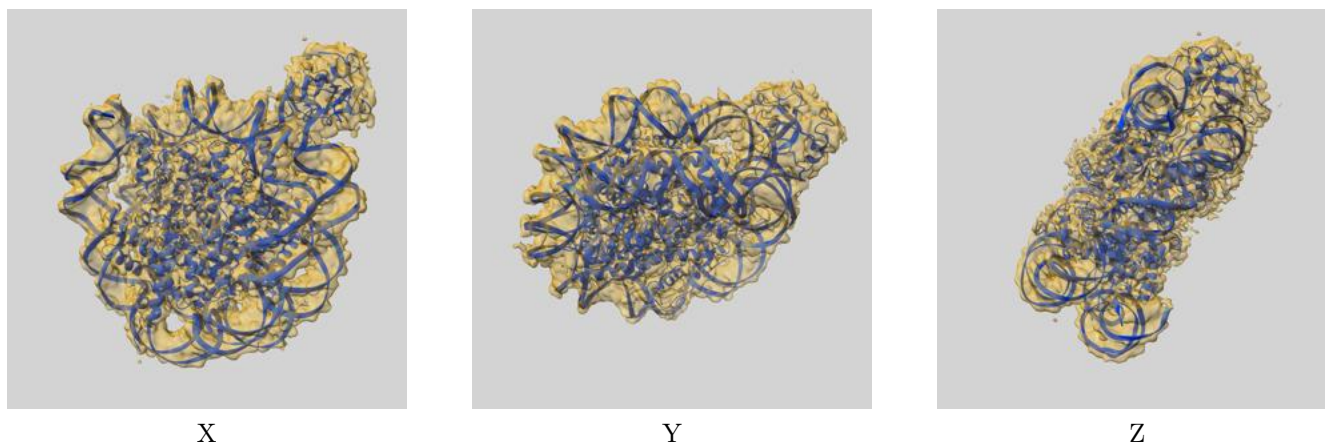
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.34	3.07
Unmasked-calculated*	3.94	7.46	4.07

*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 3.94 differs from the reported value 3.02 by more than 10 %

9 Map-model fit [i](#)

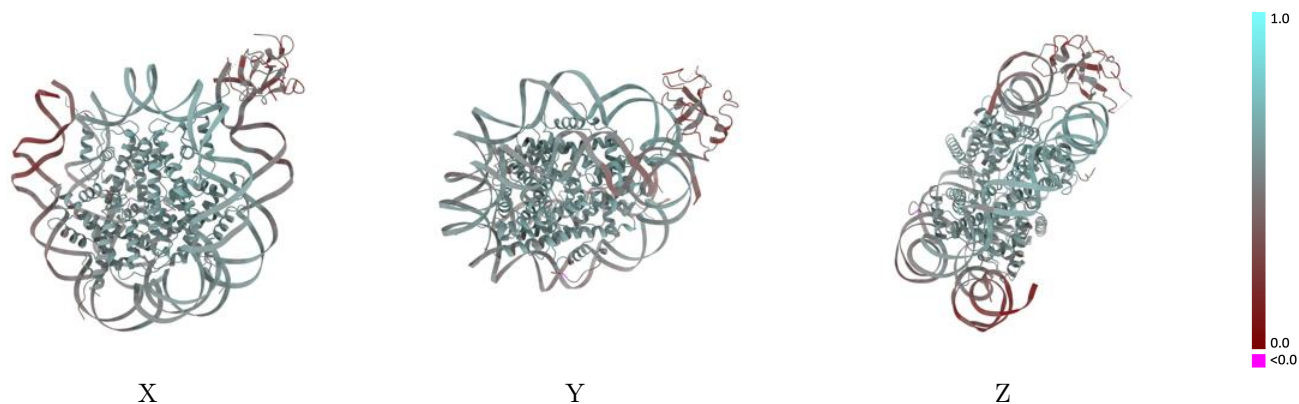
This section contains information regarding the fit between EMDB map EMD-17594 and PDB model 8PC5. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)



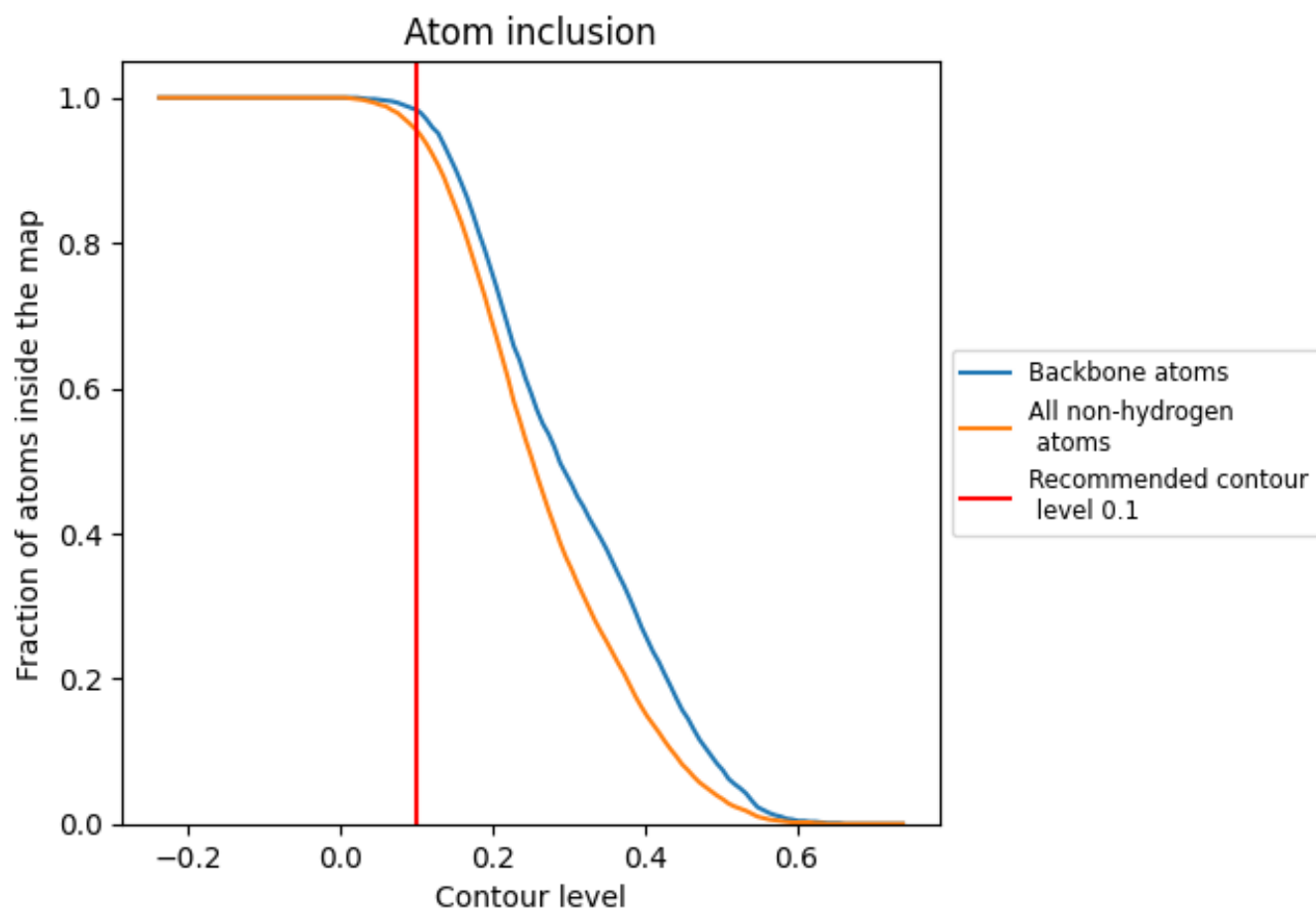
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.5210
A	 0.9760	 0.5980
B	 0.9600	 0.5990
C	 0.9490	 0.5510
D	 0.9460	 0.5480
E	 0.9730	 0.5690
F	 0.9290	 0.5500
G	 0.9670	 0.5900
H	 0.9680	 0.5740
I	 0.9640	 0.4860
J	 0.9660	 0.4890
K	 0.8380	 0.3700

