



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:55 PM UTC

PDB ID : 8OJC / pdb_00008ojc
EMDB ID : EMD-16911
Title : HSV-1 DNA polymerase active site in alternative exonuclease state
Authors : Gustavsson, E.; Grunewald, K.; Elias, P.; Hallberg, B.M.
Deposited on : 2023-03-24
Resolution : 2.08 Å(reported)
Based on initial model : 7LUF

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

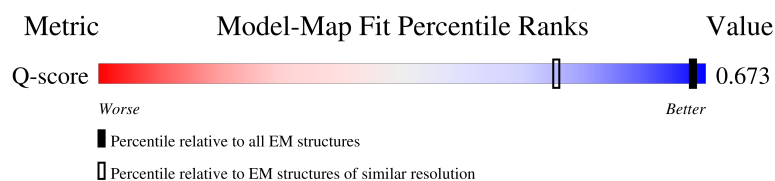
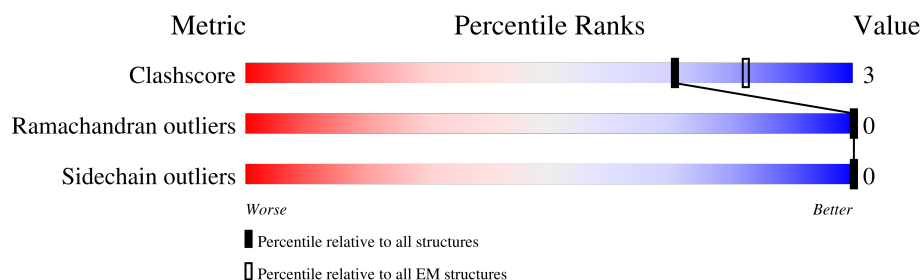
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1976 (1.58 - 2.58)

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	C	47	 94%
2	A	1235	 30% 68%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3501 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 DNA (47-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	3	Total	C	N	O	P	S	0	0
			63	30	15	14	3	1		

- Molecule 2 is a protein called DNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	395	Total	C	N	O	S	6	0
			3148	2024	532	577	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	ARG	ALA	variant	UNP P04293

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	

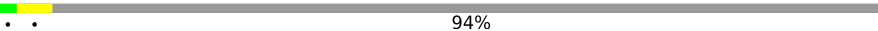
- Molecule 4 is water.

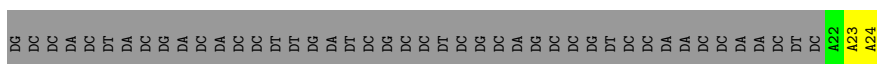
Mol	Chain	Residues	Atoms		AltConf
4	C	11	Total	O	0
			11	11	
4	A	277	Total	O	0
			277	277	

3 Residue-property plots

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.

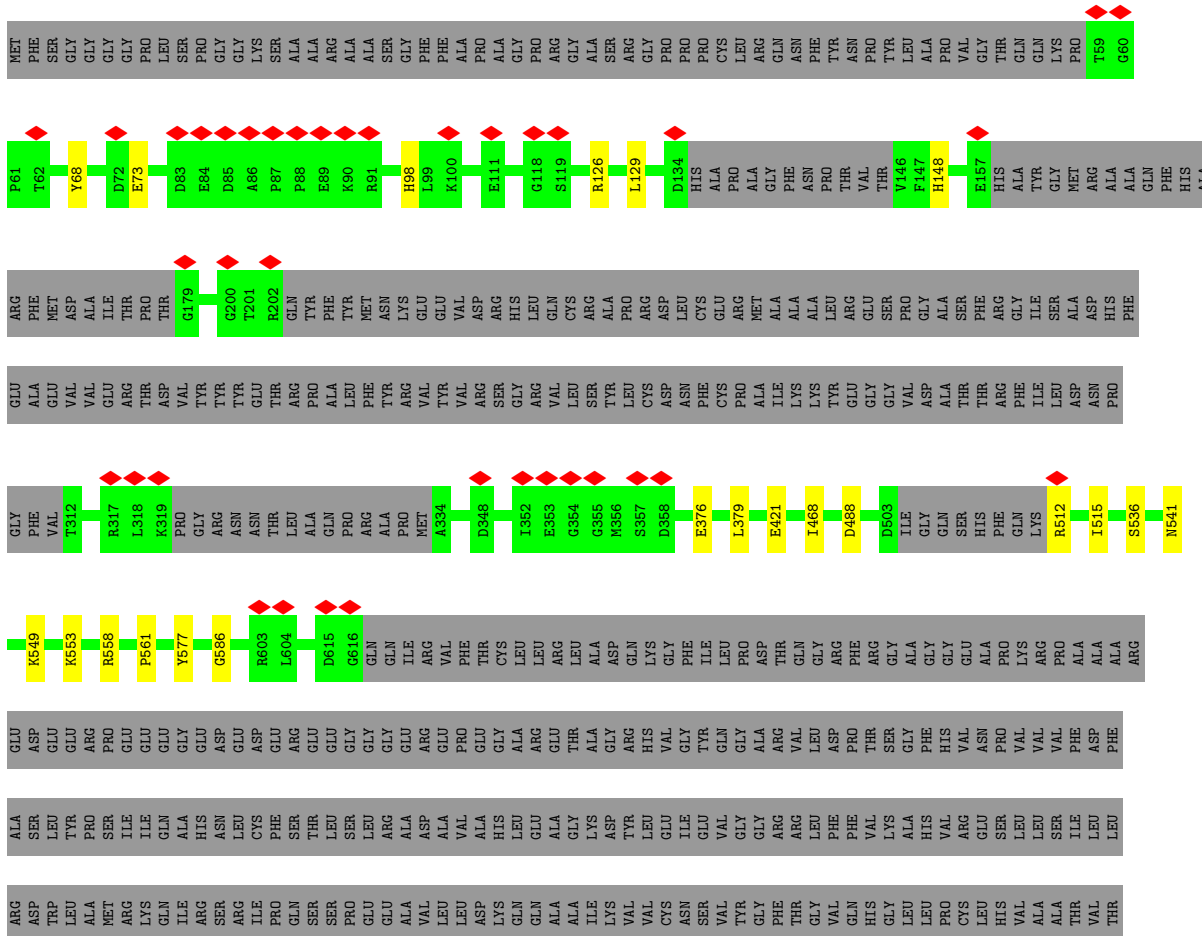
• Molecule 1: DNA (47-MER)

Chain C:  94%



• Molecule 2: DNA polymerase catalytic subunit

Chain A:  30% 68%



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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48633	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.412	Depositor
Minimum map value	-2.491	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.6	Depositor
Map size ($\text{\AA}$)	353.5, 353.5, 353.5	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.73645836, 0.73645836, 0.73645836	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: CA, AS

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	C	0.53	0/47	0.73	0/70
2	A	0.60	1/3240 (0.0%)	0.90	2/4388 (0.0%)
All	All	0.60	1/3287 (0.0%)	0.90	2/4458 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	148	HIS	CG-CD2	-5.21	1.30	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	421	GLU	CB-CA-C	-5.63	101.80	110.81
2	A	126	ARG	NE-CZ-NH1	-5.13	116.37	121.50

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	C	63	0	34	2	0
2	A	3148	0	3090	20	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	277	0	0	19	0
4	C	11	0	0	0	0
All	All	3501	0	3124	22	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.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:536:SER:HB2	4:A:1590:HOH:O	1.90	0.70
2:A:68:TYR:O	4:A:1401:HOH:O	2.12	0.67
2:A:488:ASP:OD2	4:A:1402:HOH:O	2.13	0.65
2:A:577[B]:TYR:OH	4:A:1403:HOH:O	2.15	0.63
2:A:512:ARG:HB2	4:A:1619:HOH:O	2.00	0.62
1:C:23:DA:H4'	4:A:1454:HOH:O	2.01	0.60
2:A:549:LYS:HB3	4:A:1512:HOH:O	2.02	0.59
2:A:541:ASN:HB3	4:A:1596:HOH:O	2.03	0.58
1:C:24:AS:OP1	1:C:24:AS:H8	2.07	0.55
2:A:376:GLU:HB2	4:A:1594:HOH:O	2.05	0.55
2:A:73:GLU:HB2	2:A:98[B]:HIS:CE1	2.43	0.53
2:A:549:LYS:CB	4:A:1512:HOH:O	2.57	0.51
2:A:586:GLY:HA2	4:A:1565:HOH:O	2.12	0.50
2:A:379:LEU:HD21	4:A:1634:HOH:O	2.11	0.49
2:A:376:GLU:HB3	4:A:1421:HOH:O	2.15	0.46
2:A:376:GLU:CB	4:A:1594:HOH:O	2.64	0.46
2:A:512:ARG:CB	4:A:1619:HOH:O	2.63	0.44
2:A:558:ARG:NH2	4:A:1423:HOH:O	2.52	0.43
2:A:129:LEU:HD12	4:A:1514:HOH:O	2.19	0.42
2:A:553:LYS:N	4:A:1425:HOH:O	2.52	0.42
2:A:561:PRO:HG2	4:A:1586:HOH:O	2.17	0.42
2:A:468:ILE:HD12	2:A:515:ILE:HG21	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	389/1235 (32%)	383 (98%)	6 (2%)	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	
2	A	337/996 (34%)	337 (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. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	63	GLN
2	A	155	ASN
2	A	344	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
1	AS	C	24	1	20,23,24	0.26	0	28,33,36	0.40	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
1	AS	C	24	1	-	4/7/21/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	24	AS	O4'-C4'-C5'-O5'
1	C	24	AS	C3'-C4'-C5'-O5'
1	C	24	AS	C2'-C1'-N9-C4
1	C	24	AS	O4'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	24	AS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

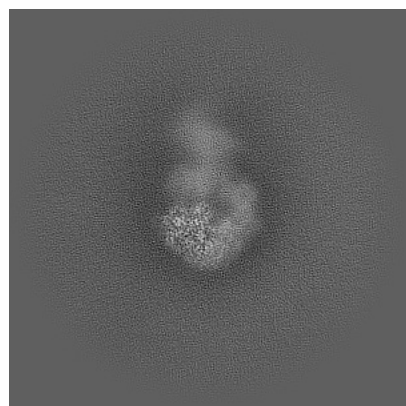
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16911. These allow visual inspection of the internal detail of the map and identification of artifacts.

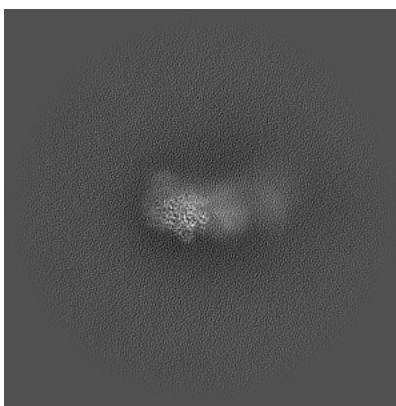
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

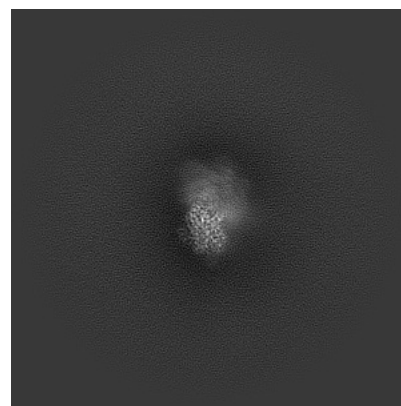
6.1.1 Primary map



X

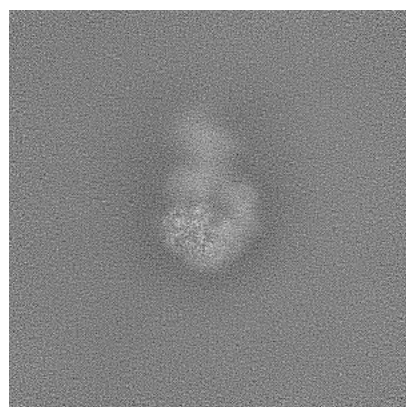


Y

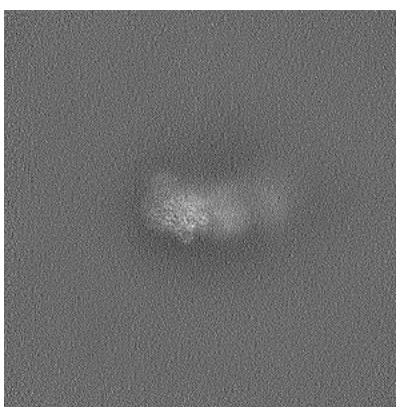


Z

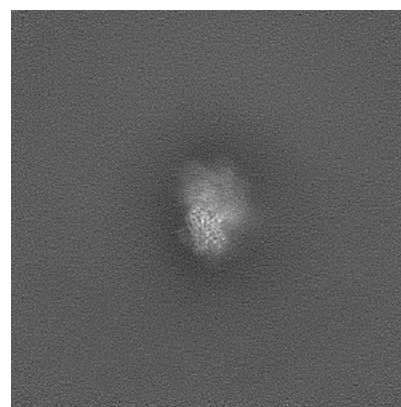
6.1.2 Raw map



X



Y

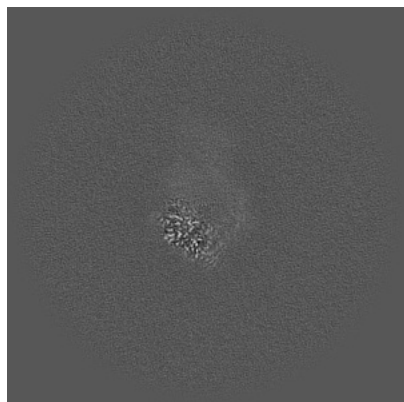


Z

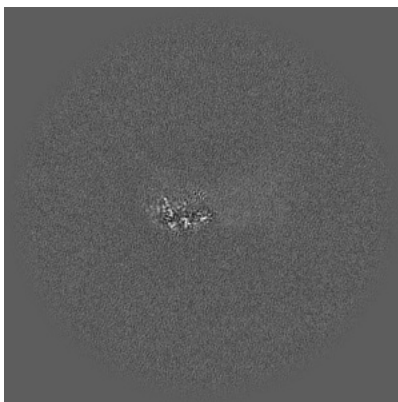
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

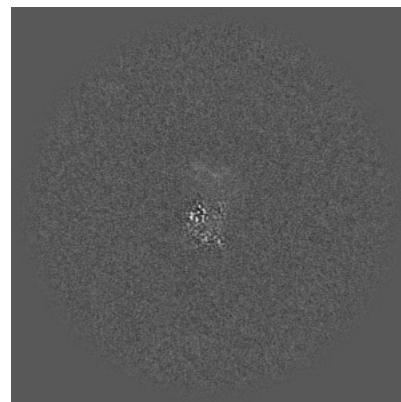
6.2.1 Primary map



X Index: 240

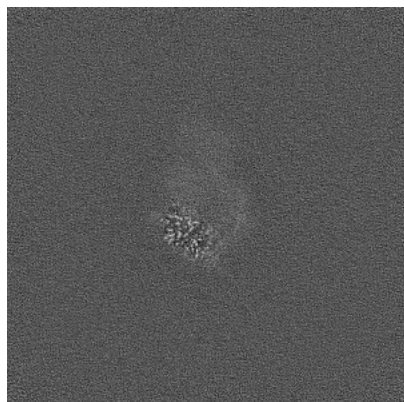


Y Index: 240



Z Index: 240

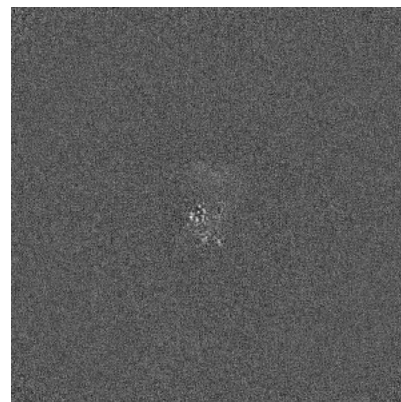
6.2.2 Raw map



X Index: 240



Y Index: 240

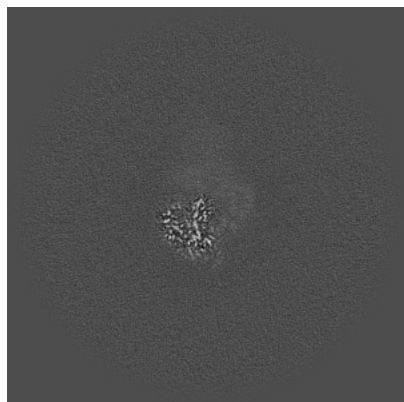


Z Index: 240

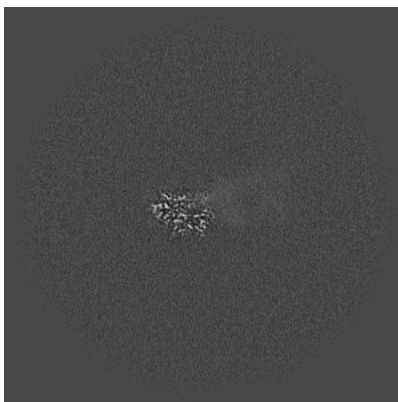
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

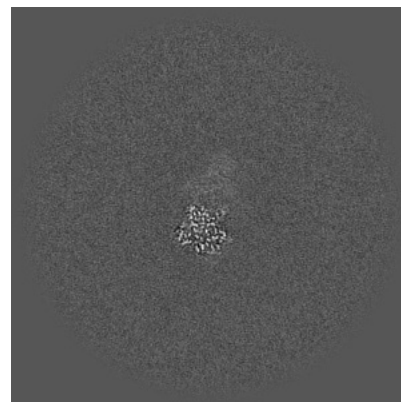
6.3.1 Primary map



X Index: 229

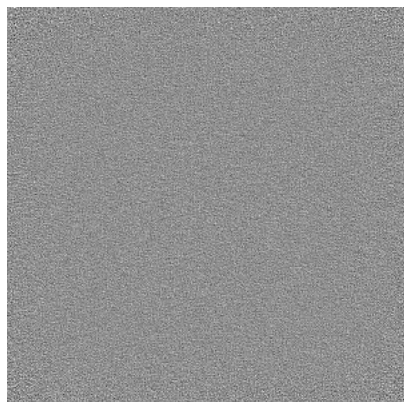


Y Index: 227

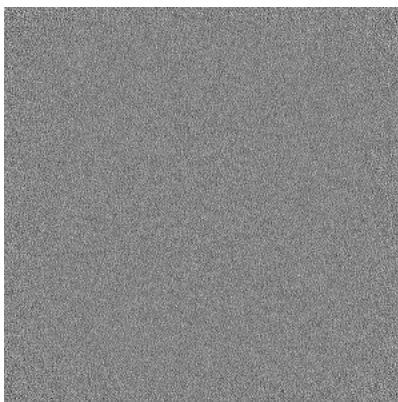


Z Index: 223

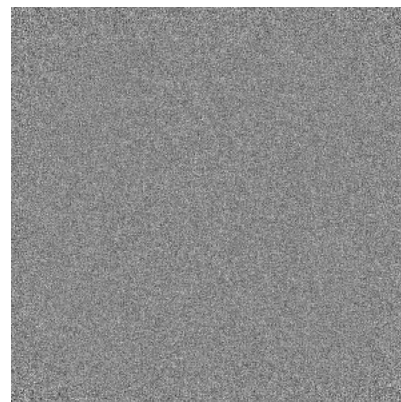
6.3.2 Raw map



X Index: 0



Y Index: 0

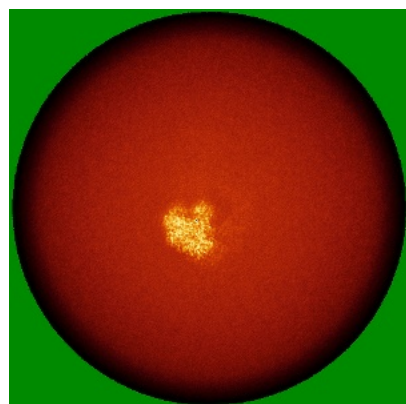


Z Index: 0

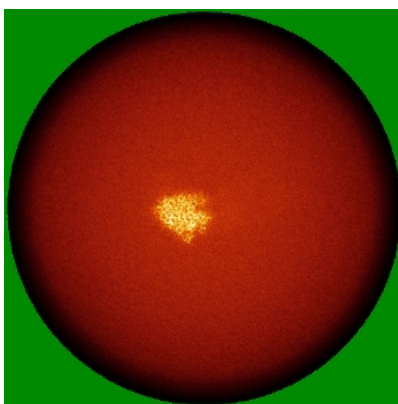
The images above show the largest variance slices of the map in three orthogonal directions.

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

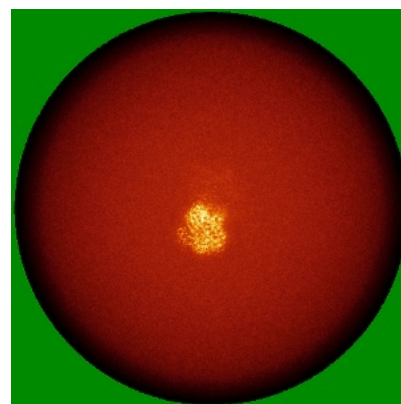
6.4.1 Primary map



X

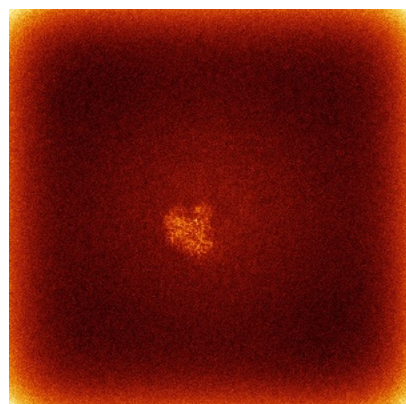


Y

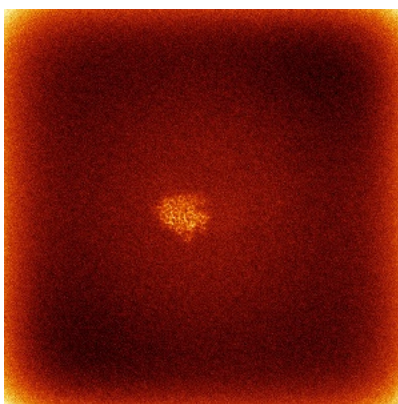


Z

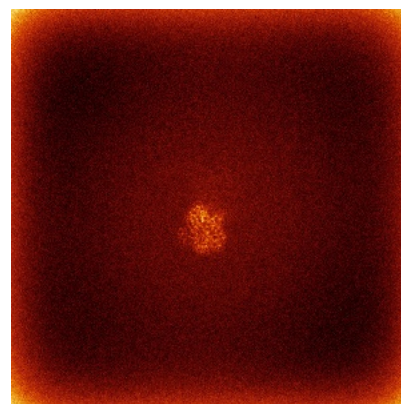
6.4.2 Raw map



X



Y

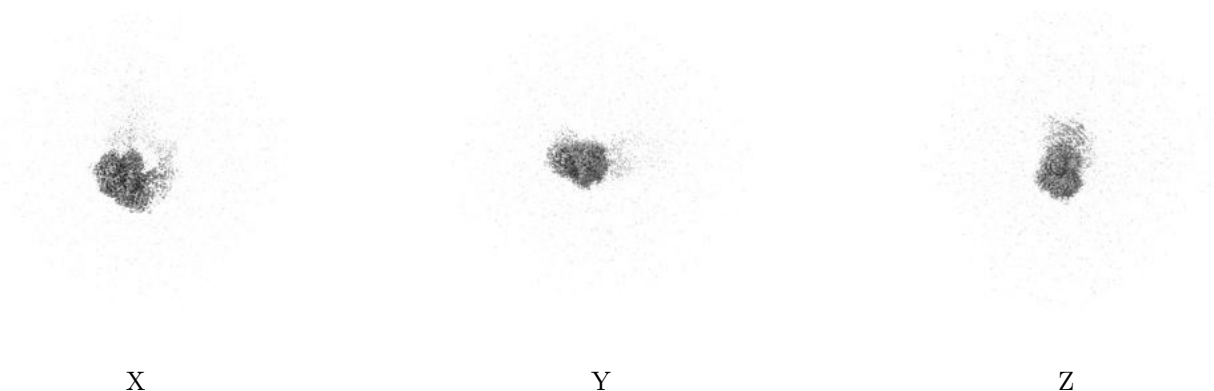


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

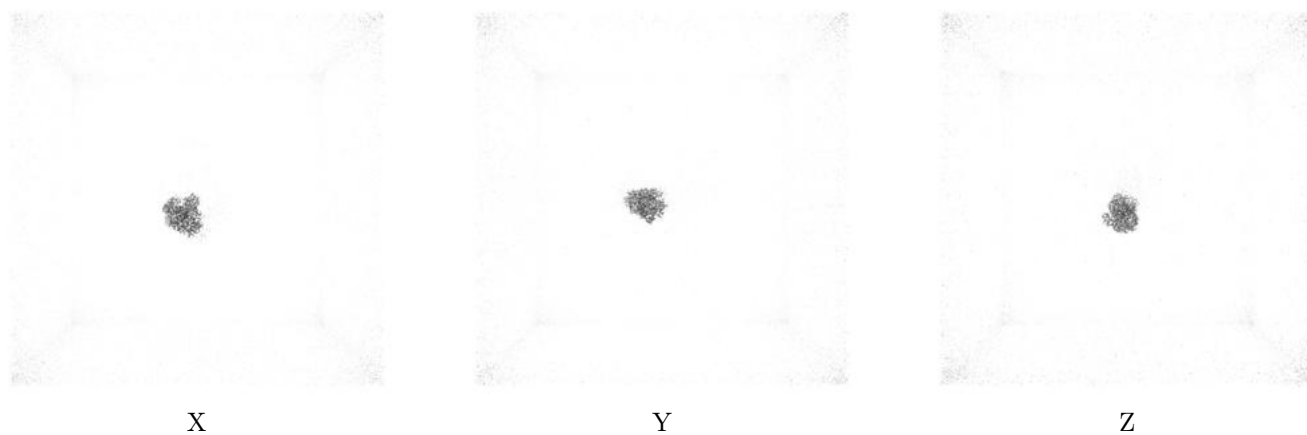
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

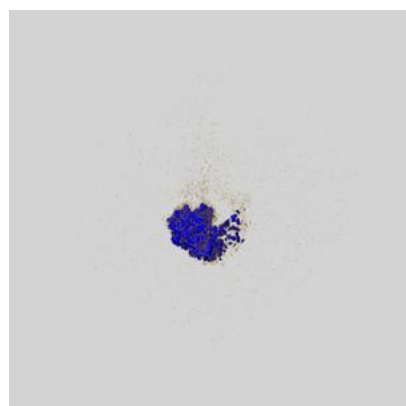
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

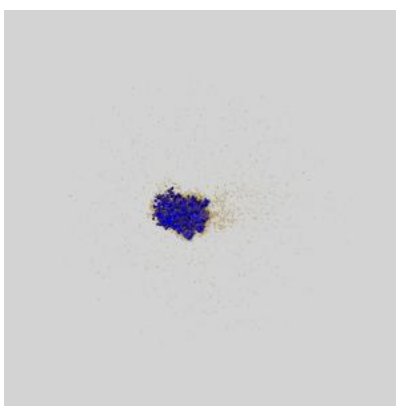
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

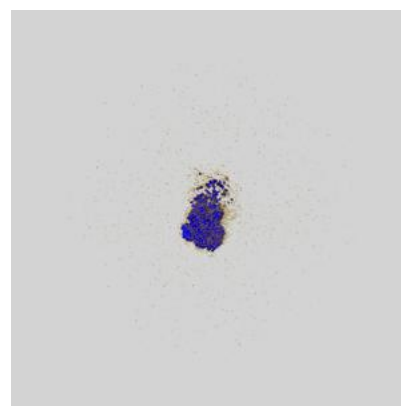
6.6.1 emd_16911_msk_1.map [i](#)



X



Y

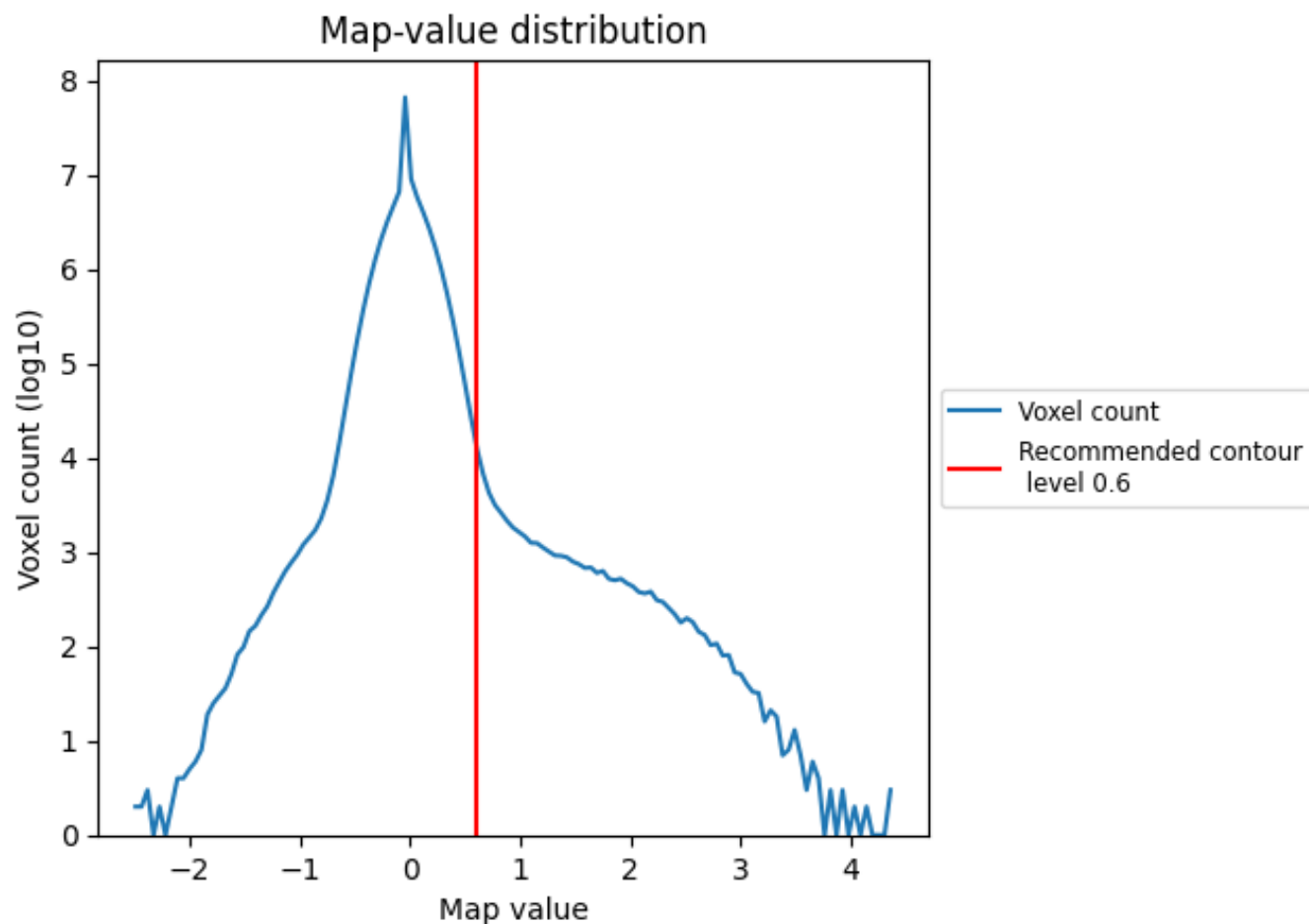


Z

7 Map analysis [i](#)

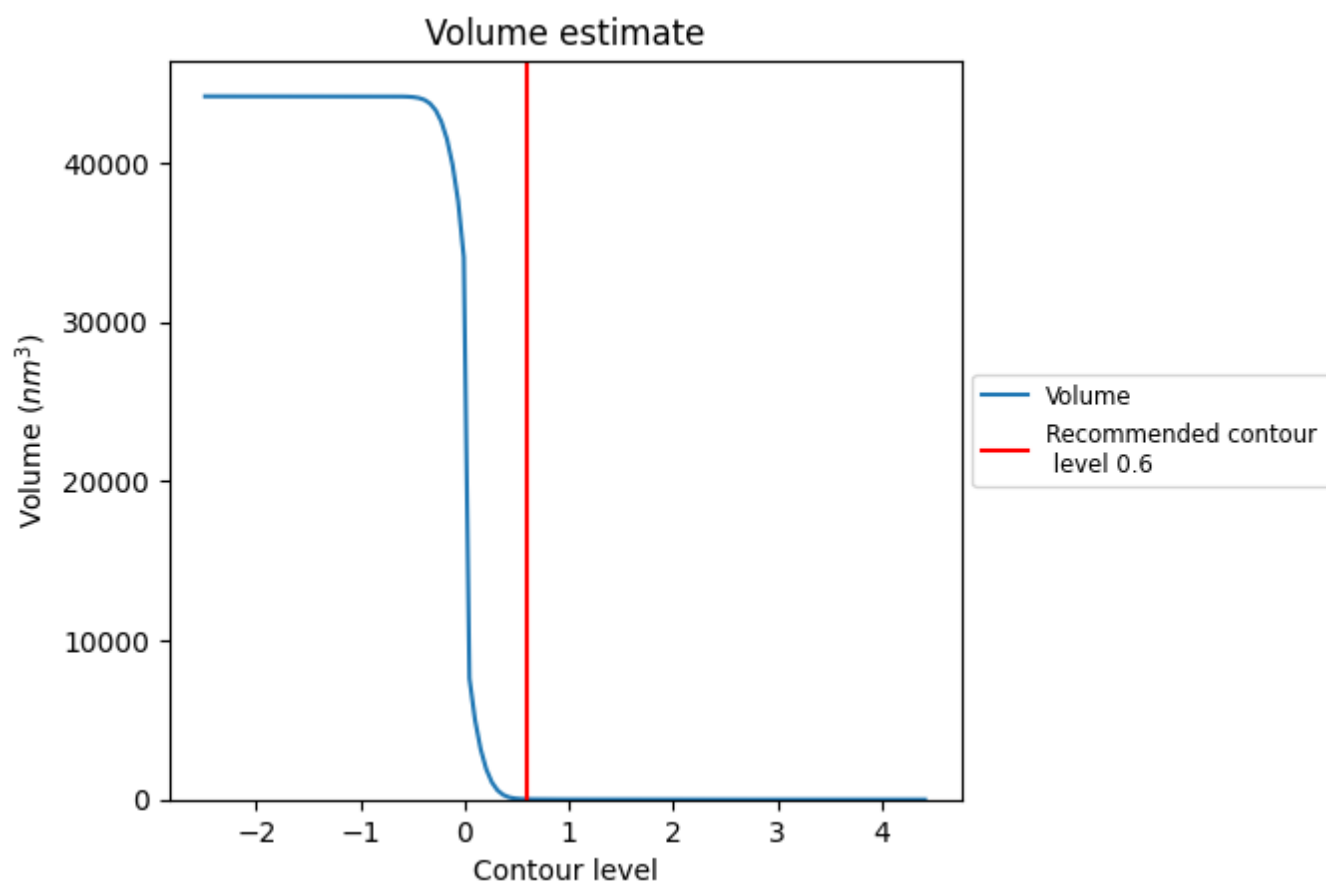
This section contains the results of statistical analysis of the map.

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.

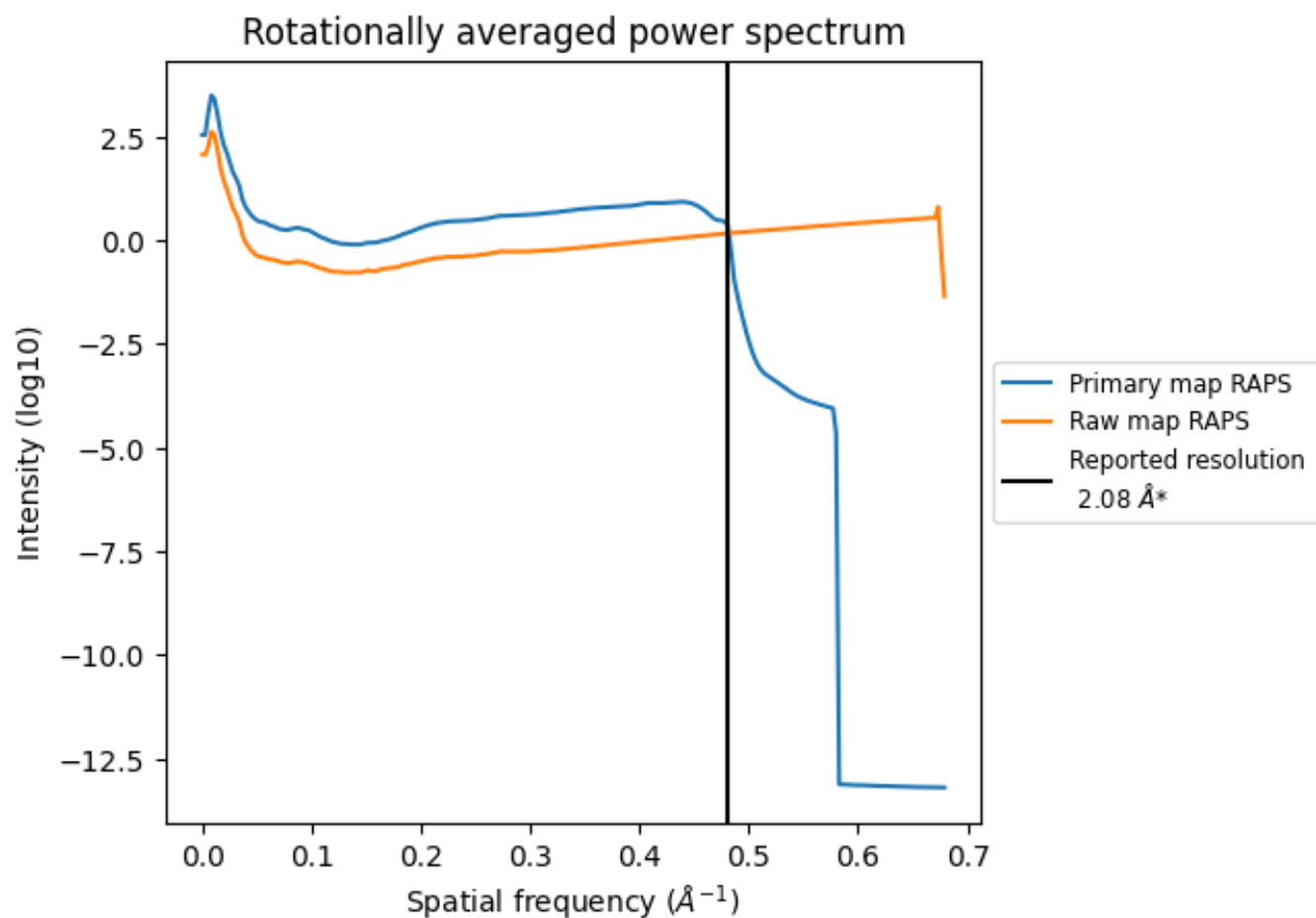
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 23 nm³; this corresponds to an approximate mass of 21 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 ⓘ

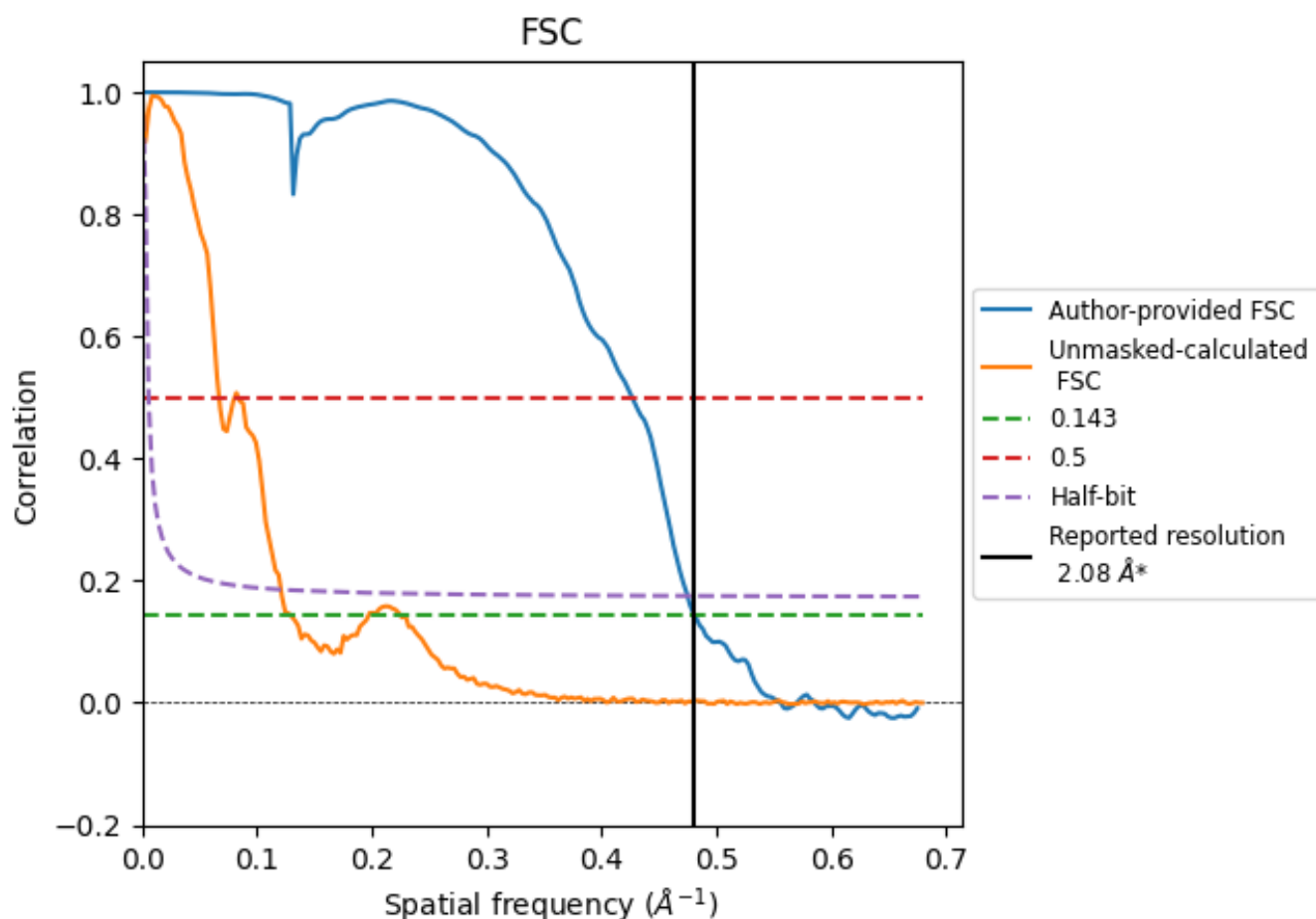


*Reported resolution corresponds to spatial frequency of 0.481 $\text{\AA}^{-1}$

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 0.481 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

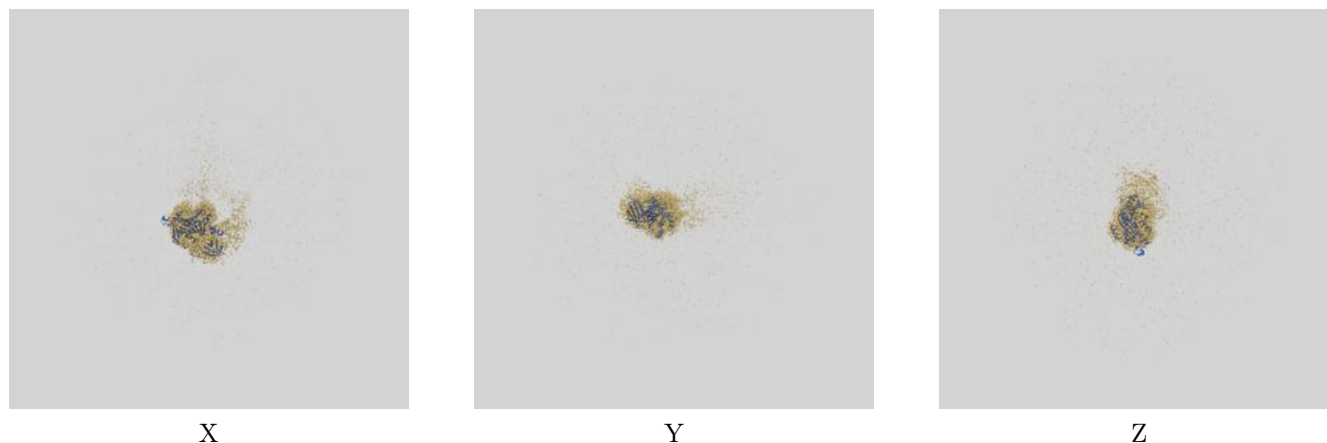
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.08	2.34	2.11
Unmasked-calculated*	7.74	14.95	8.28

*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 7.74 differs from the reported value 2.08 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16911 and PDB model 8OJC. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



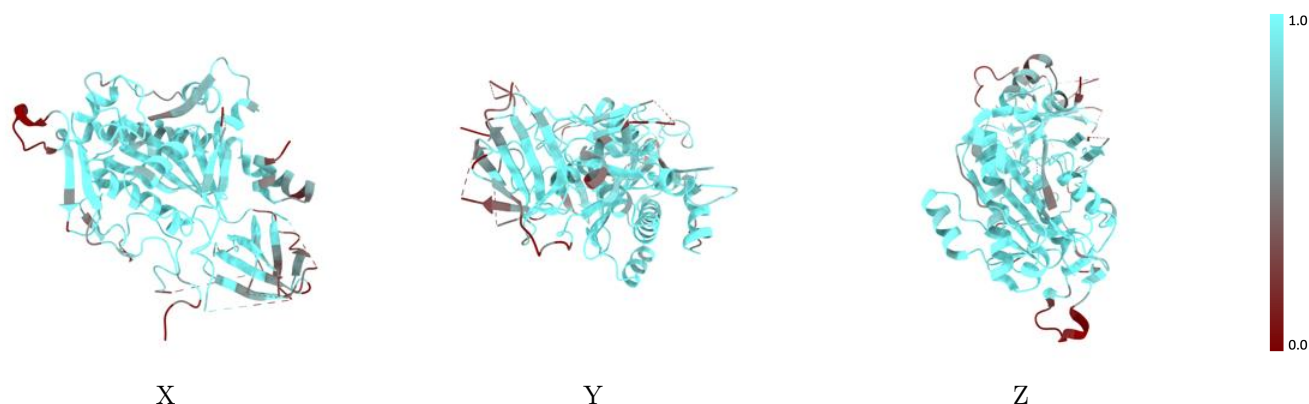
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



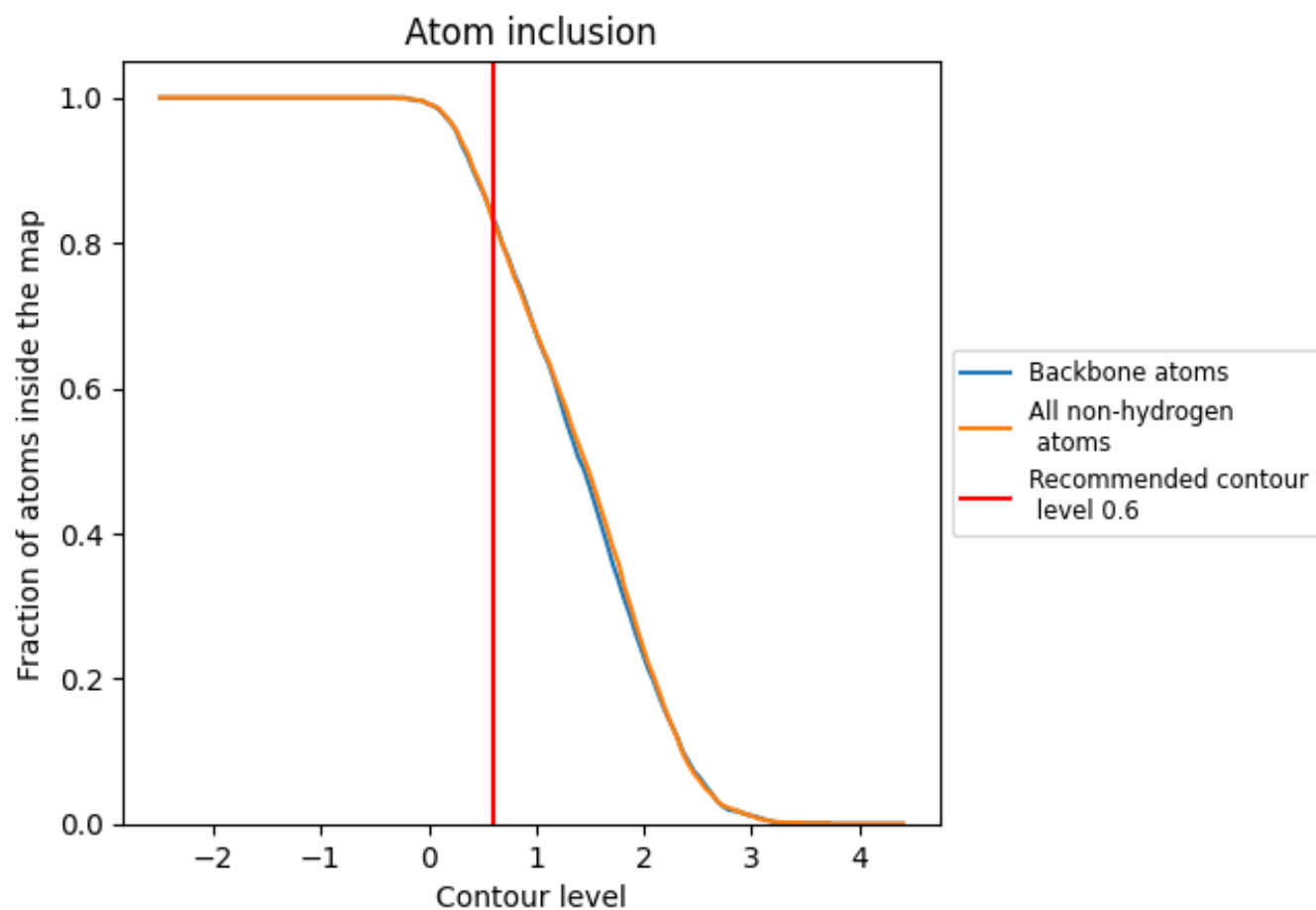
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.6730
A	0.8420	0.6770
C	0.5710	0.4800

