



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 03:47 PM JST

PDB ID : 6M71
EMDB ID : EMD-30127
Title : SARS-Cov-2 RNA-dependent RNA polymerase in complex with cofactors
Authors : Gao, Y.; Yan, L.; Huang, Y.; Liu, F.; Cao, L.; Wang, T.; Wang, Q.; Lou, Z.;
Rao, Z.
Deposited on : 2020-03-16
Resolution : 2.90 Å(reported)
Based on initial model : 6NUR

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.dev43
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) : 2.31.2

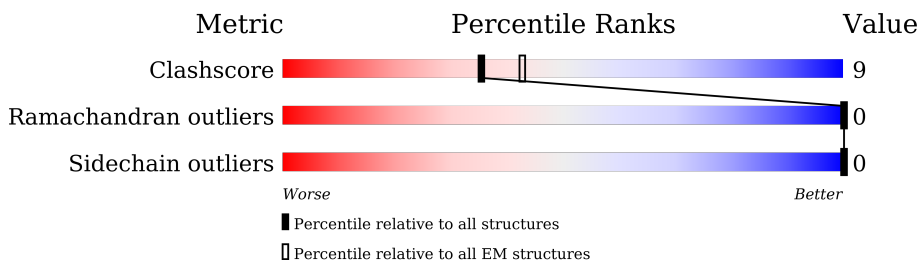
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	A	942	
2	C	83	
3	B	198	
3	D	198	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8614 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	859	6903	4424	1154	1279	46	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	933	HIS	-	expression tag	UNP P0DTD1
A	934	HIS	-	expression tag	UNP P0DTD1
A	935	HIS	-	expression tag	UNP P0DTD1
A	936	HIS	-	expression tag	UNP P0DTD1
A	937	HIS	-	expression tag	UNP P0DTD1
A	938	HIS	-	expression tag	UNP P0DTD1
A	939	HIS	-	expression tag	UNP P0DTD1
A	940	HIS	-	expression tag	UNP P0DTD1
A	941	HIS	-	expression tag	UNP P0DTD1
A	942	HIS	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	70	538	341	89	103	5	0	0

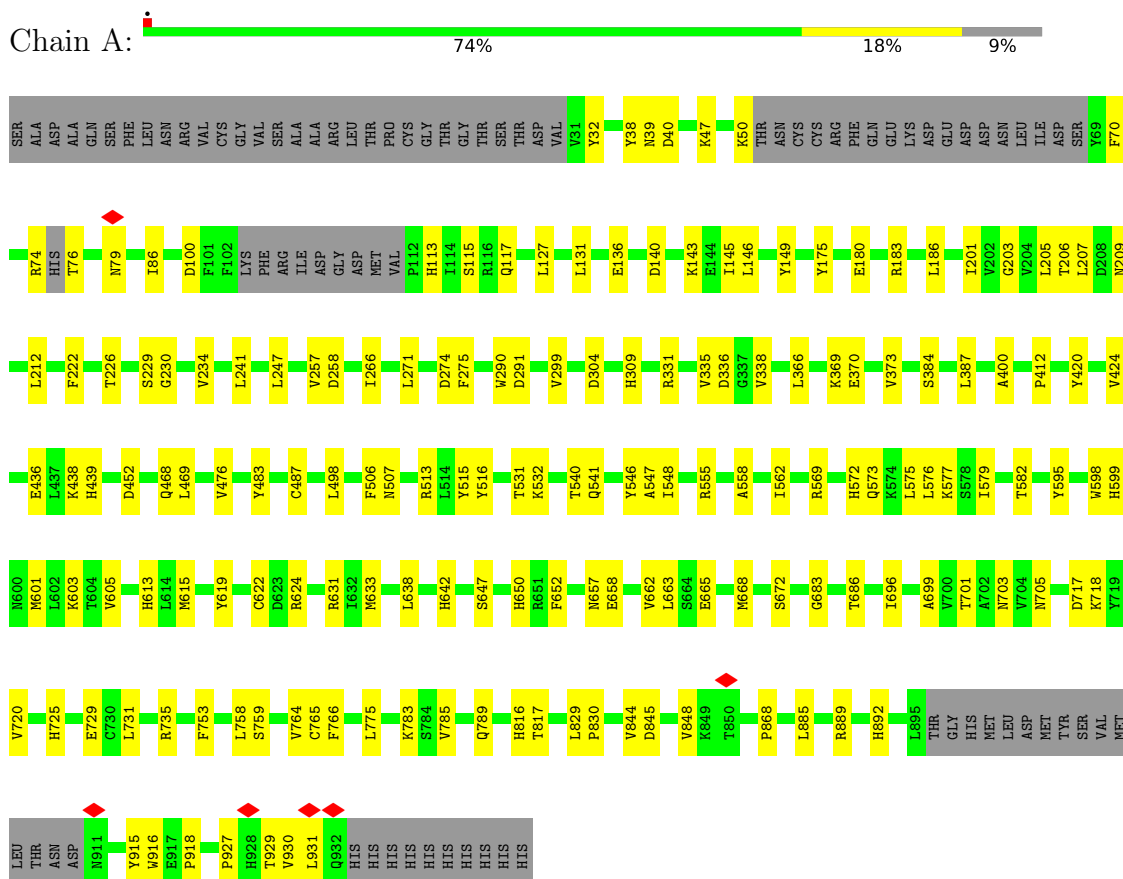
- Molecule 3 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	43	315	199	51	60	5	0	0
3	B	113	858	543	142	166	7	0	0

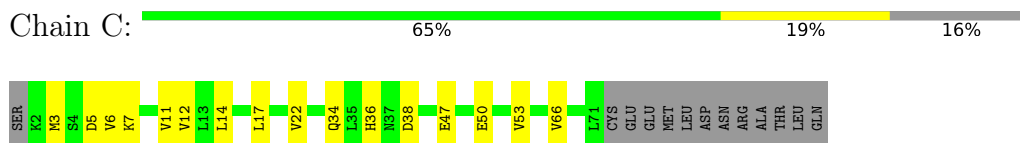
3 Residue-property plots

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: RNA-directed RNA polymerase



- Molecule 2: Non-structural protein 7



- Molecule 3: Non-structural protein 8



ALA	ALA	ALA	ALA	GLU	PHE	SER	SER	SER	LEU	PRO	TYR	ALA	ALA	PHE	THR	THR	ALA	ALA	GLN	GLU	VAL	VAL	VAL	ALA	ALA	ALA	GLY	GLY	ASP	SER	GLU	VAL	VAL	VAL	VAL	LEU	LEU	LYS	LYS	LEU	LYS	LYS	LEU	LEU	ASN	VAL	VAL	ALA	ALA	LYS	LYS	GLU	PHE	ASP	ARG	ARG	ARG	ARG	ALA	ALA	ALA	TYR	ASN	ALA	ALA	GLN	ARG	GLN	ARG	LYS	LYS	LEU	THR	CYS	GLU
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LYS	MET	ALA	ASP	GLN	ALA	MET	THR	MET	THR	ALA	TYR	LYS	GLN	ALA	ALA	ARG	SER	GLN	VAL	GLU	ASP	LYS	ARG	ALA	ASP	LYS	VAL	T84	T88	T89	M90	L91	F92	L95	L96	D101	A102	L106	M106	M108	L122	THR	THR	THR	ALA	ALA	ALA	LYS	LYS	M129	M132	M132	PRO	ASP	ASP	VAL	TYR	ASN	ALA	LYS	THR	TYR	LYS	TYR	LYS	ASN	LEU	THR	CYS
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ASP	GLY	THR	THR	PHE	THR	TYR	ALA	SER	LEU	ALA	PRO	SER	TYR	TRP	LYS	GLU	ILE	GLN	VAL	VAL	ASP	ALA	ALA	ASP	SER	LYS	VAL	ILE	VAL	GLN	LEU	SER	ASP	GLY	ILE	SER	MET	GLU	ASP	ASN	ASN	VAL	VAL	LEU	SER	PRO	LYS	ASN	LEU	ALA	ALA	TRP	PRO	LEU	ILE	ILE	VAL	THR	THR	ALA	ALA	LYS	LEU	LEU	ARG	ALA	ALA	ASN	ASP	SER	ALA	VAL	VAL	LYS	LEU	LEU	GLN
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● Molecule 3: Non-structural protein 8

Chain B: 46% 11% 43%

ALA	ILE	ALA	SER	GLU	PHE	SER	SER	LEU	GLN	PRO	SER	TYR	LYS	ALA	ALA	PHE	ARG	SER	THR	VAL	GLU	ASP	GLN	ALA	ALA	GLU	TYR	GLU	GLN	ALA	VAL	VAL	ALA	ASN	ASN	GLY	ASP	SER	GLU	VAL	VAL	VAL	VAL	LEU	LEU	LYS	LYS	LEU	LEU	ASN	VAL	VAL	ALA	LYS	SER	SER	GLU	PHE	ASP	ASP	ARG	ASP	ALA	ALA	ALA	MET	LEU	GLN	ARG	LYS	LEU	GLU
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LYS	MET	ASP	ASN	ALA	ALA	THR	GLN	MET	TYR	LYS	GLN	ALA	ALA	ARG	SER	GLU	D78	V83	L95	M105	I106	M109	G113	I120	T124	A125	L128	I132	P133	D134	Y138	G144	THR	T146	V159	V160	S164	S177	P178	N179	L180	L184	I185	V186
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R190	A191	ASN	SER	ALA	VAL	LYS	LEU	GLN
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The CTF correction was done by patch CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.709	Depositor
Minimum map value	-1.093	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	246.0, 246.0, 246.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.28	0/7078	0.42	0/9609
2	C	0.24	0/541	0.41	0/729
3	B	0.24	0/870	0.44	0/1189
3	D	0.24	0/316	0.39	0/429
All	All	0.27	0/8805	0.42	0/11956

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	6903	0	6648	120	0
2	C	538	0	574	13	0
3	B	858	0	857	14	0
3	D	315	0	318	7	0
All	All	8614	0	8397	145	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 9.

The worst 5 of 145 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:A:487:CYS:SG	1:A:642:HIS:ND1	2.44	0.90
1:A:335:VAL:O	1:A:336:ASP:OD1	1.97	0.83
1:A:927:PRO:O	1:A:930:VAL:CG2	2.35	0.74
1:A:844:VAL:HG12	1:A:845:ASP:N	2.04	0.73
1:A:844:VAL:HG11	1:A:848:VAL:HG22	1.71	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	849/942 (90%)	814 (96%)	35 (4%)	0	100	100
2	C	68/83 (82%)	66 (97%)	2 (3%)	0	100	100
3	B	109/198 (55%)	103 (94%)	6 (6%)	0	100	100
3	D	39/198 (20%)	37 (95%)	2 (5%)	0	100	100
All	All	1065/1421 (75%)	1020 (96%)	45 (4%)	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	749/833 (90%)	749 (100%)	0	100	100
2	C	65/77 (84%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	95/167 (57%)	95 (100%)	0	100	100
3	D	36/167 (22%)	36 (100%)	0	100	100
All	All	945/1244 (76%)	945 (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. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	892	HIS
2	C	36	HIS
3	B	140	ASN
3	D	100	ASN
1	A	360	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

There are no chain breaks in this entry.

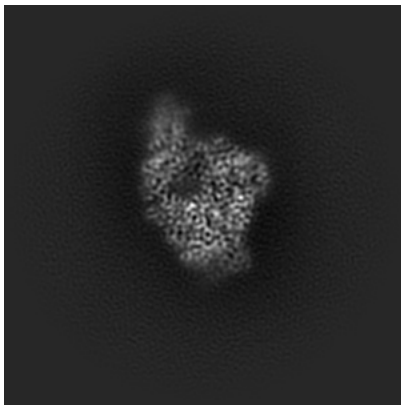
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30127. These allow visual inspection of the internal detail of the map and identification of artifacts.

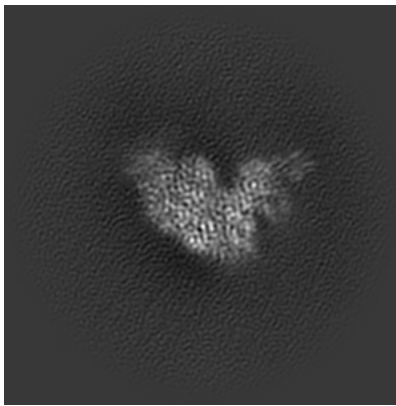
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

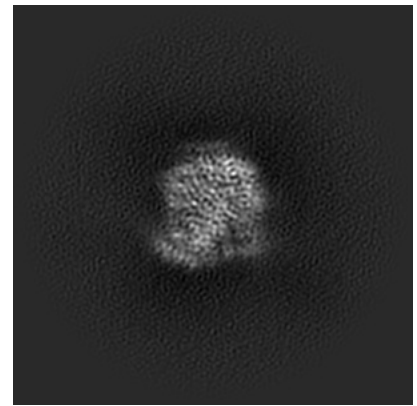
6.1.1 Primary map



X

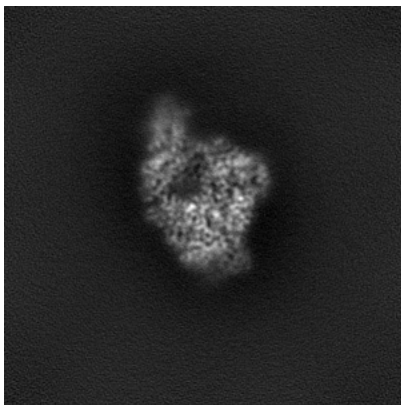


Y

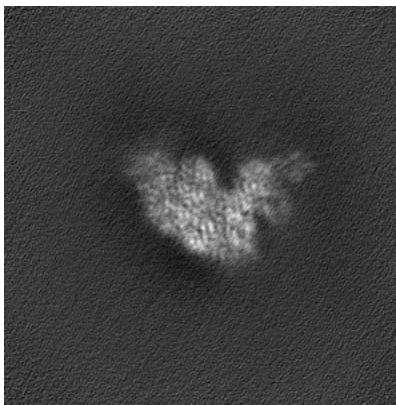


Z

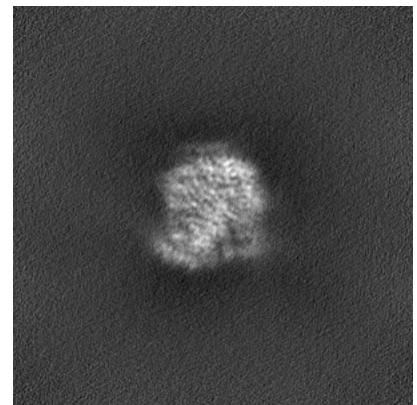
6.1.2 Raw map



X



Y

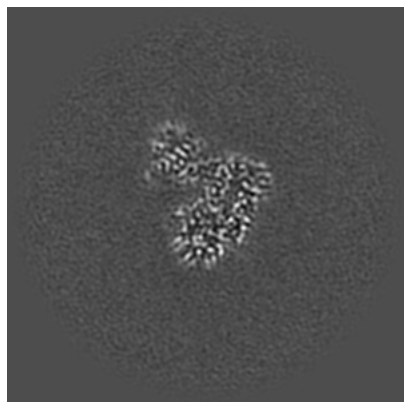


Z

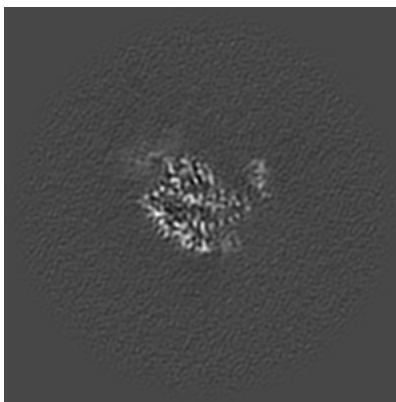
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

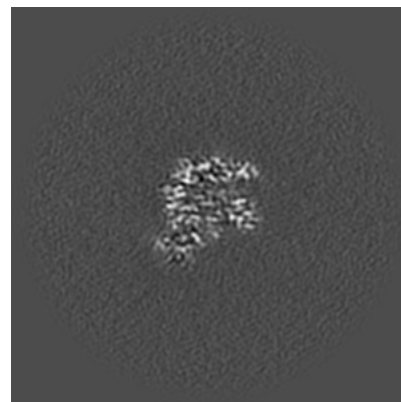
6.2.1 Primary map



X Index: 150

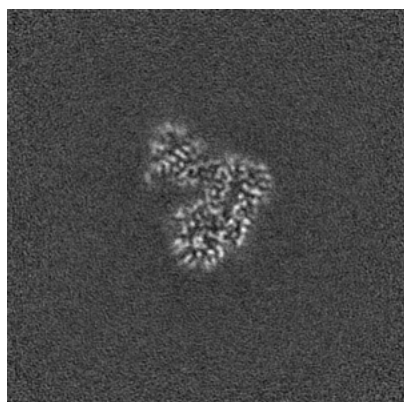


Y Index: 150

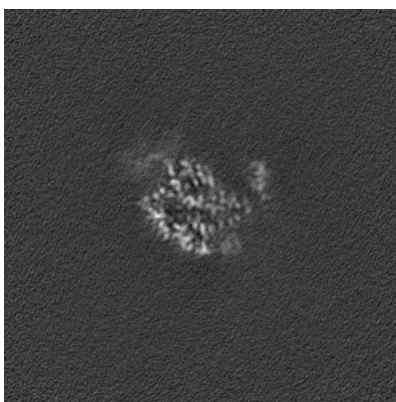


Z Index: 150

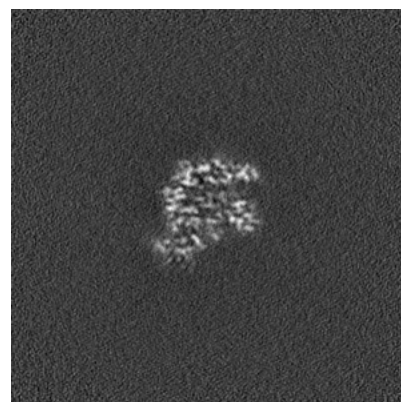
6.2.2 Raw map



X Index: 150



Y Index: 150

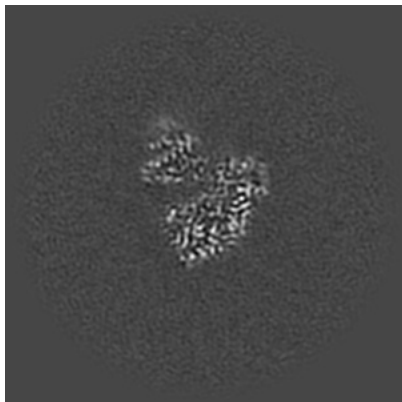


Z Index: 150

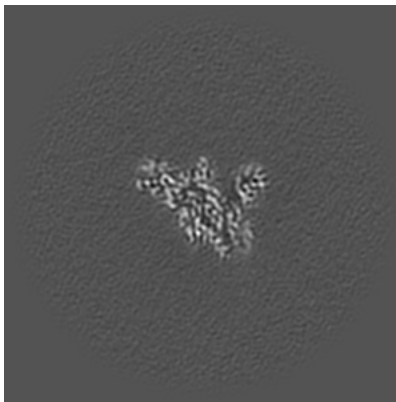
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

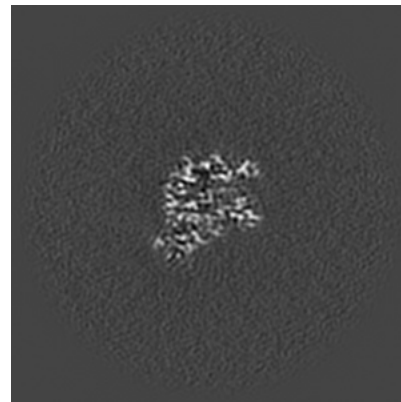
6.3.1 Primary map



X Index: 147

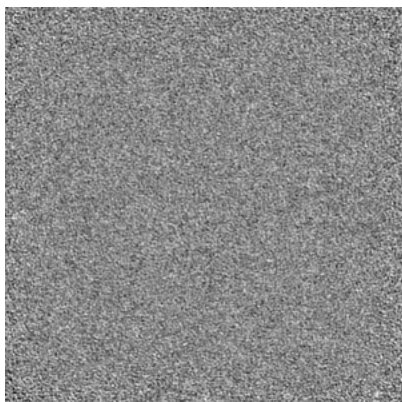


Y Index: 174

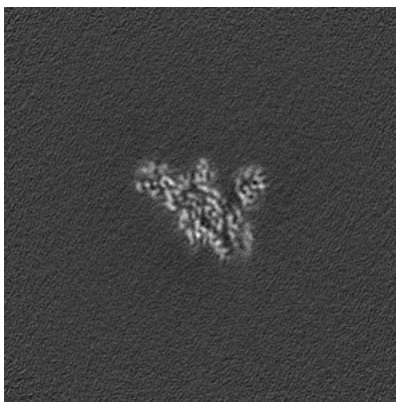


Z Index: 149

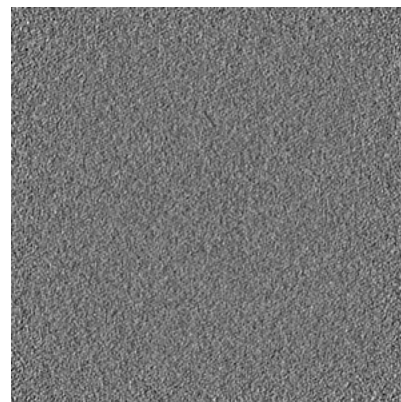
6.3.2 Raw map



X Index: 0



Y Index: 174



Z Index: 0

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

6.4 Orthogonal surface views [i](#)

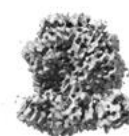
6.4.1 Primary map



X



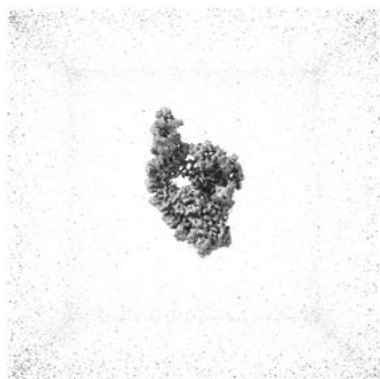
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X



Y



Z

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.

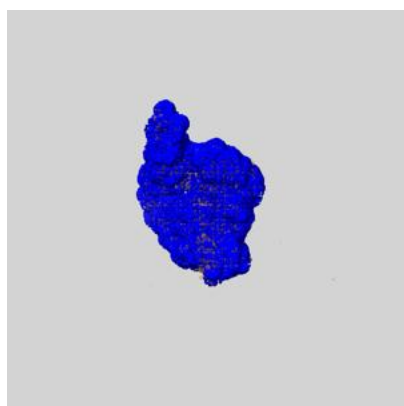
6.5 Mask visualisation [i](#)

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

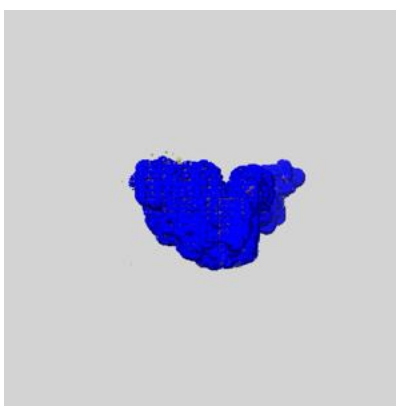
A mask typically either:

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

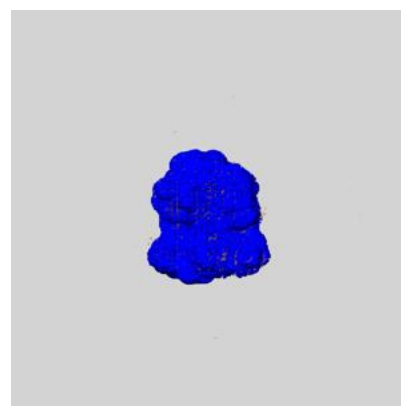
6.5.1 emd_30127_msk_1.map [i](#)



X



Y

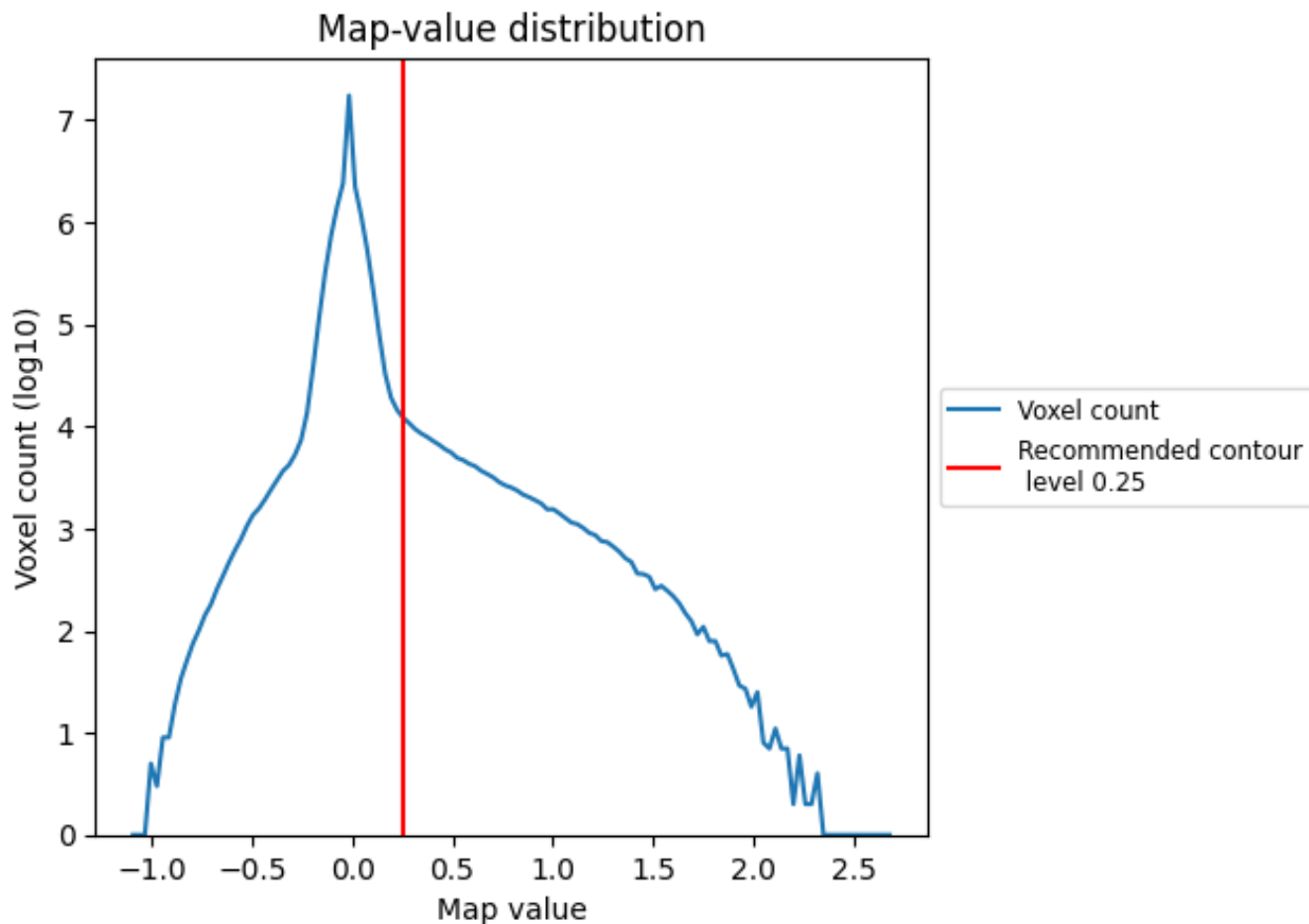


Z

7 Map analysis [i](#)

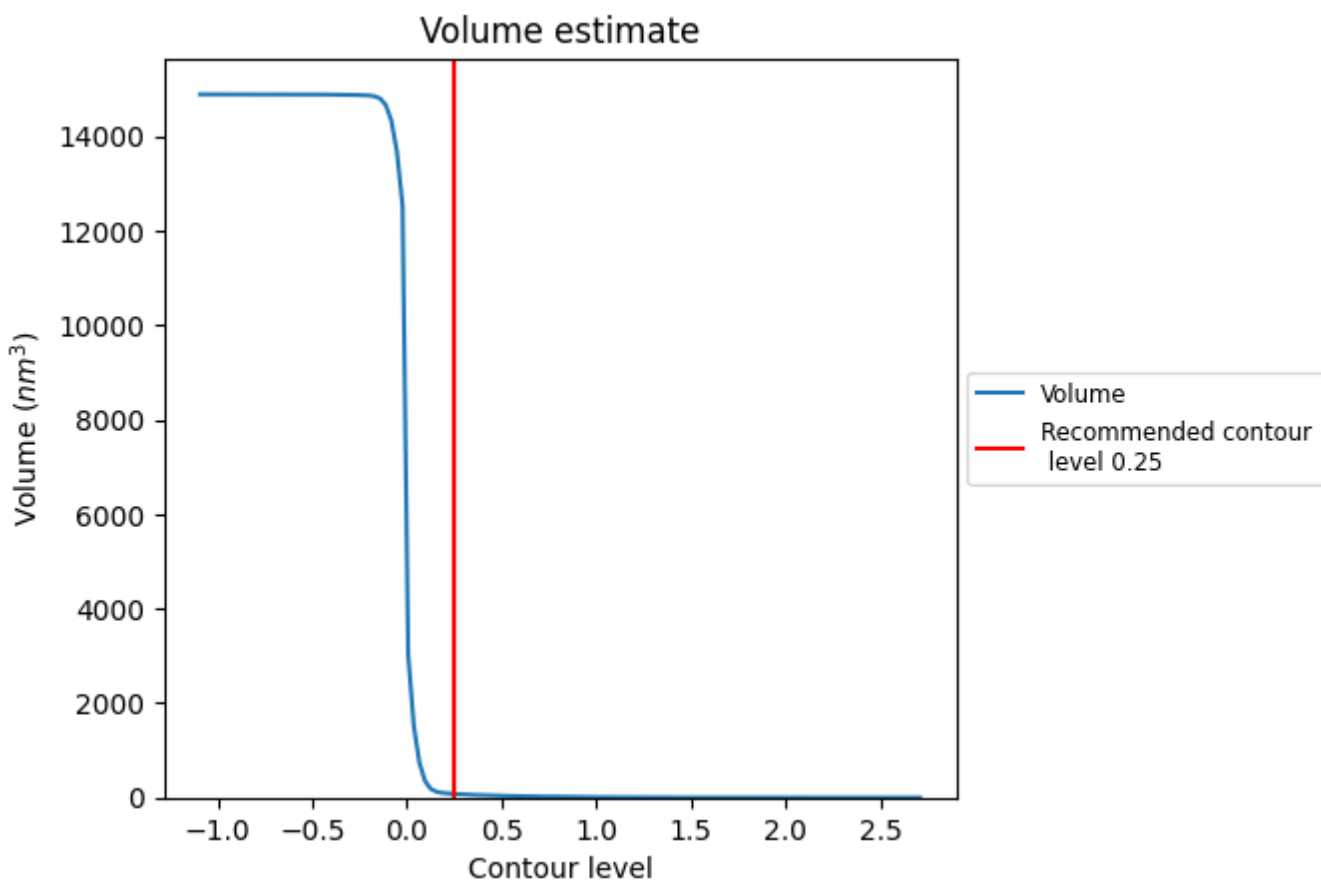
This section contains the results of statistical analysis of the map.

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.

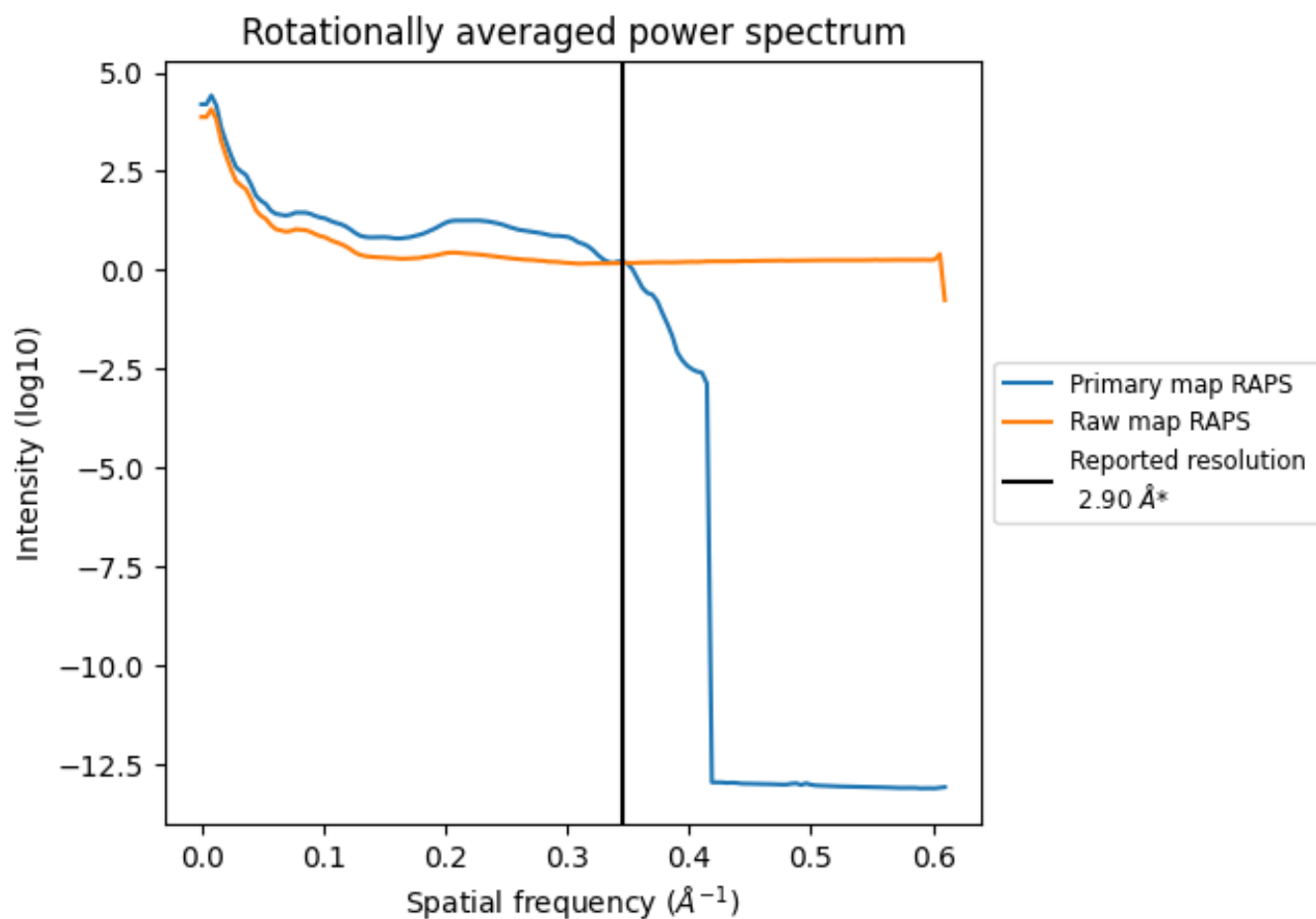
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm^3 ; this corresponds to an approximate mass of 70 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](#)

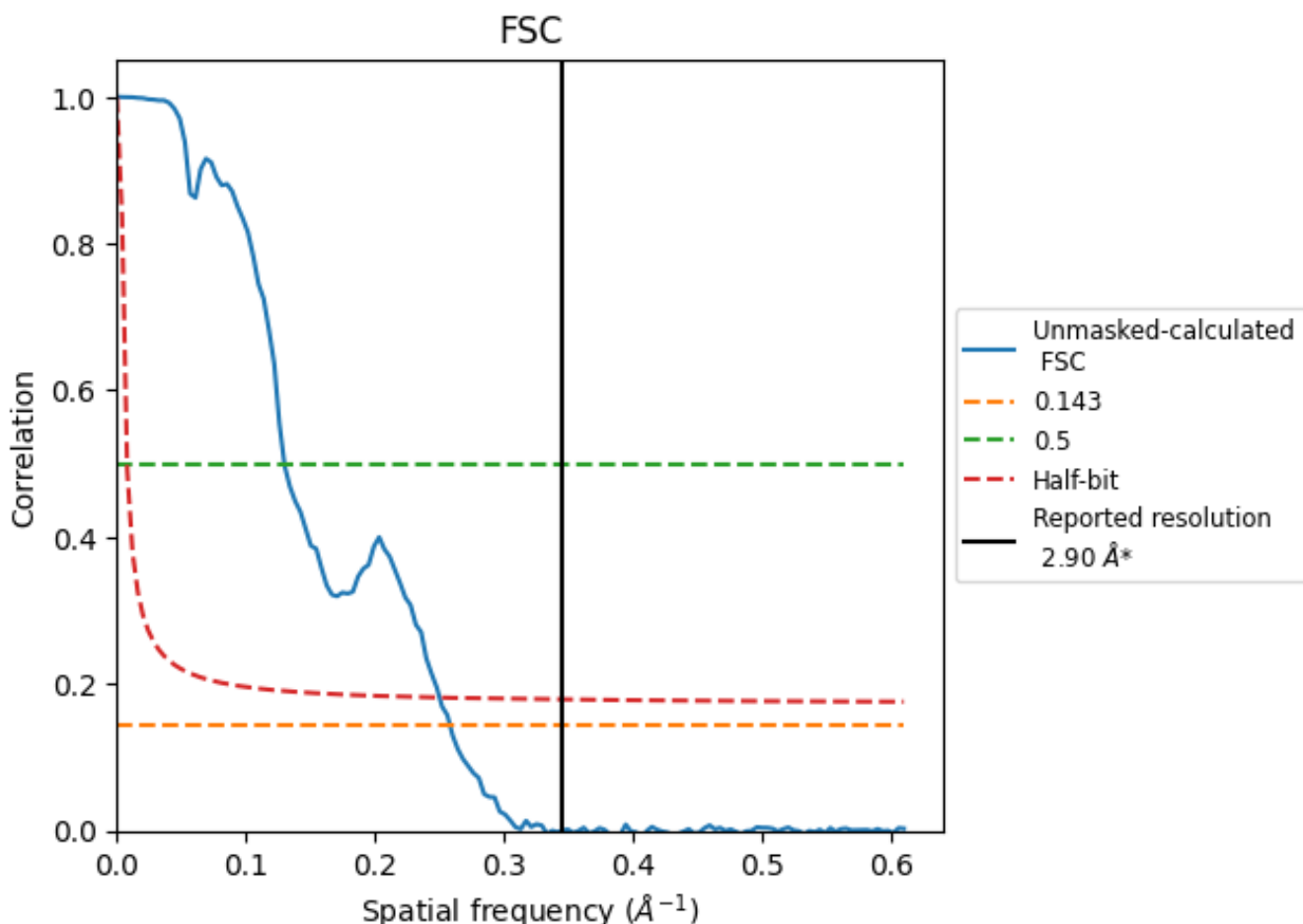


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

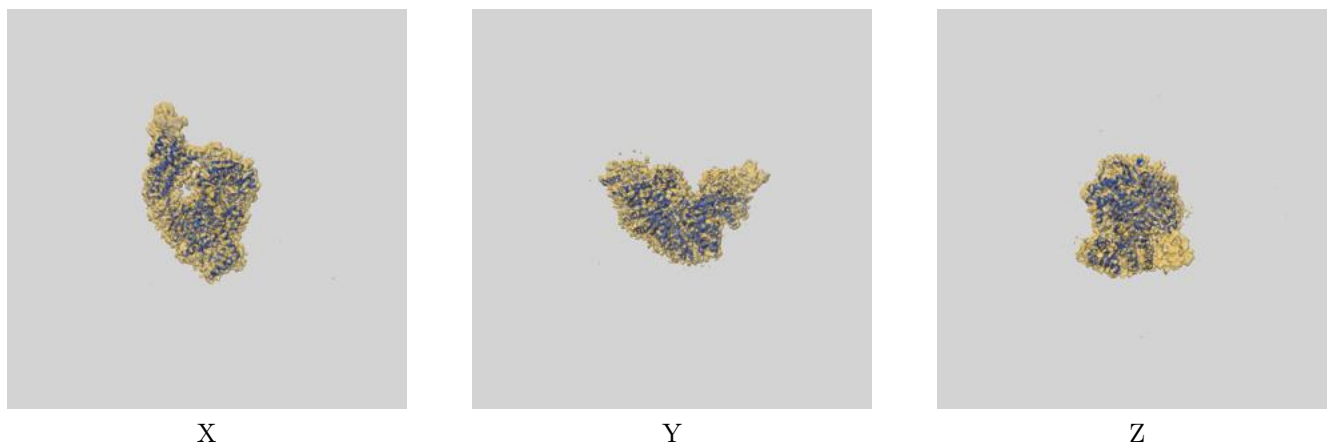
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	7.70	4.00

*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 3.87 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

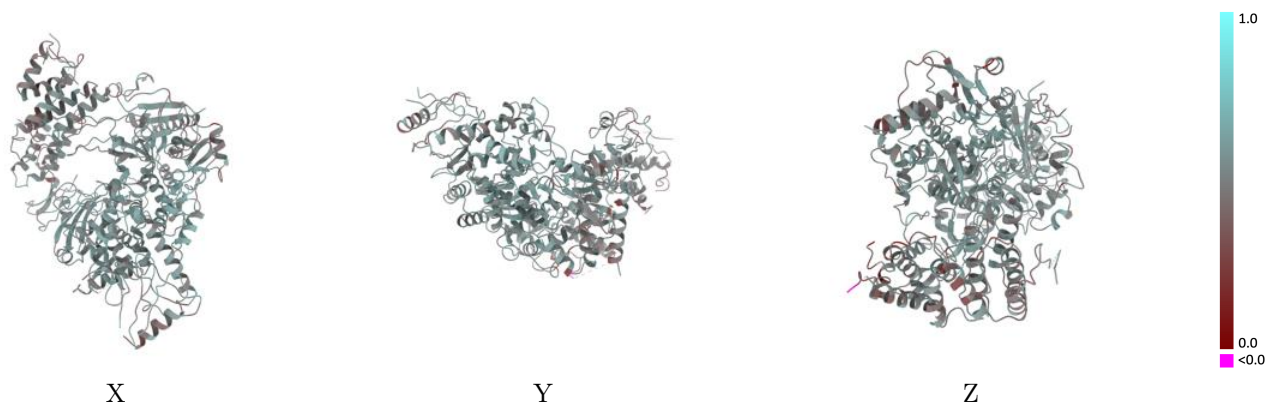
This section contains information regarding the fit between EMDB map EMD-30127 and PDB model 6M71. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



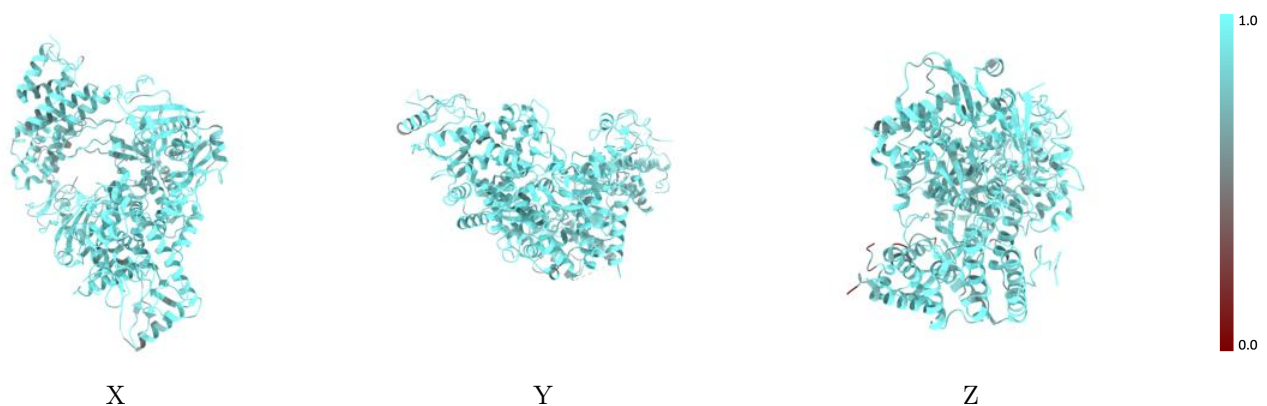
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



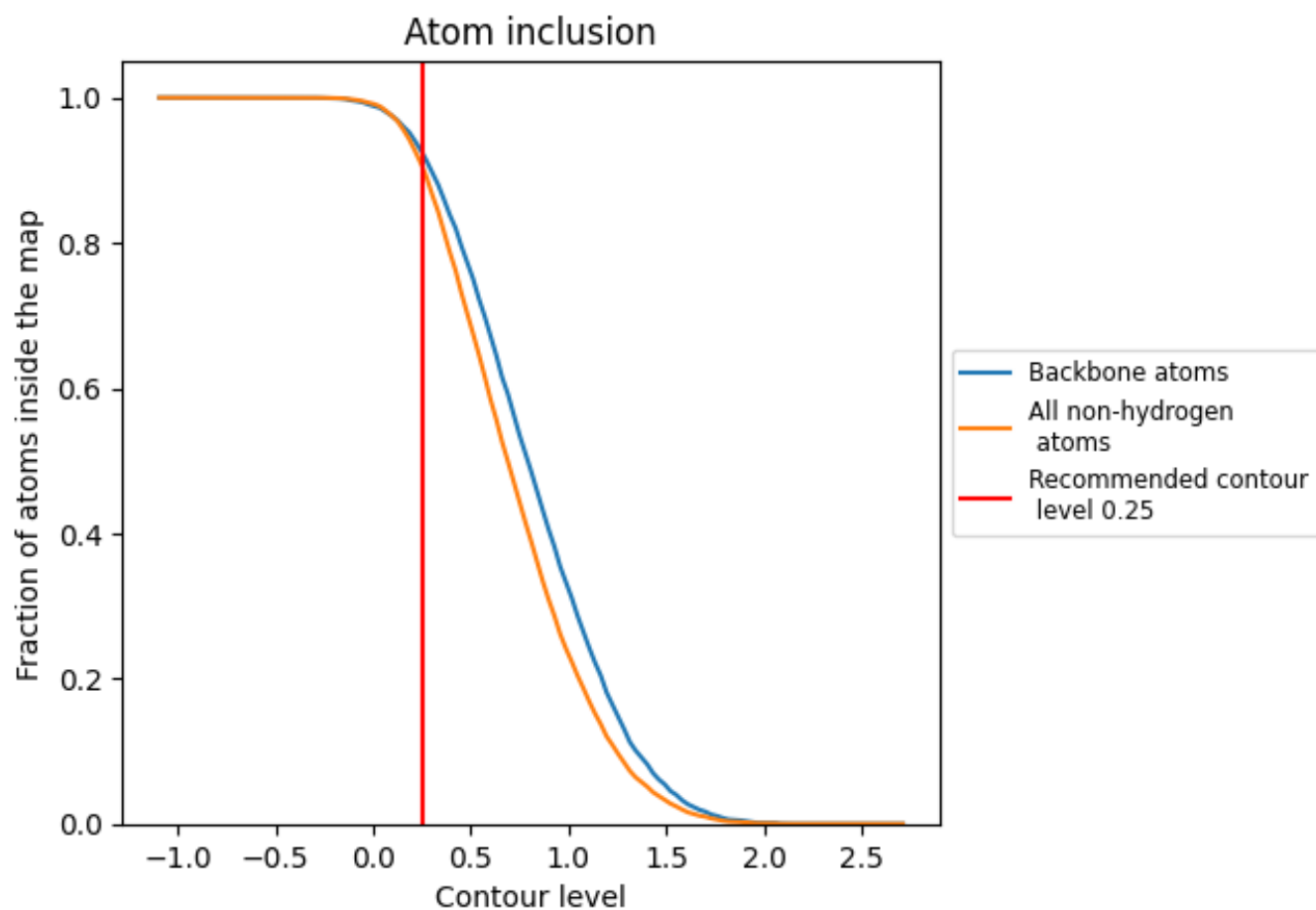
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).











9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9059	 0.5190
A	 0.9150	 0.5290
B	 0.8914	 0.4890
C	 0.8486	 0.4800
D	 0.8476	 0.4660

