wwPDB EM Validation Summary Report

Oct 26, 2026 – 12:10 PM EDT

PDB ID	:	9NRL / pdb_00009nrl
EMDB ID	:	EMD-49736
Title	:	Cryo-EM structure of UL52 catalytic core in complex with UL8 subunit from Herpes Simplex Virus 1
Authors	:	Bermek, O.; Krahn, J.M.; Viverette, E.G.; Peele, W.; Dandey, V.P.; Borgnia, M.J.; Williams, R.S.
Deposited on	:	2025-03-14
Resolution	:	3.40 Å(reported)
Based on initial model	:	.

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:

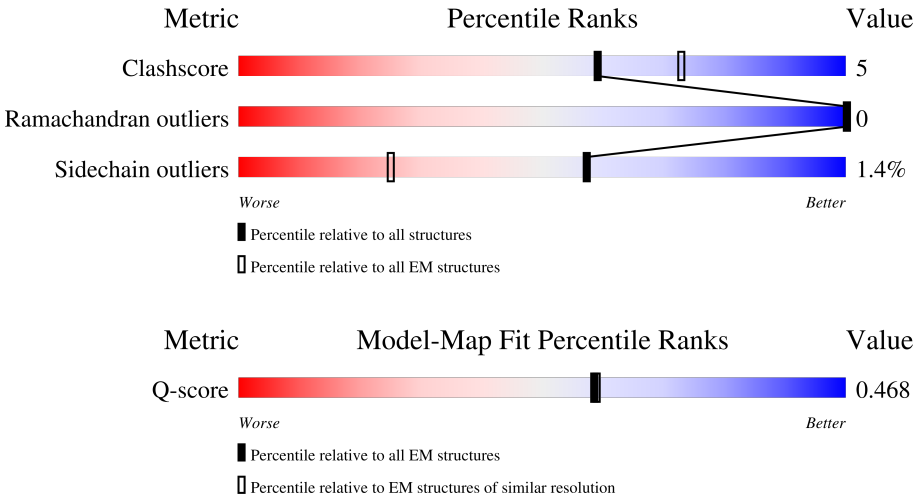
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.40 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	14717 (2.90 - 3.90)

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 <=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	768	16% 84% 12% .
2	B	1058	5% 29% . 66%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8332 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 UL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5580	3586	990	986	18		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A0A5J6DVE7
A	-16	ARG	-	expression tag	UNP A0A5J6DVE7
A	-15	GLY	-	expression tag	UNP A0A5J6DVE7
A	-14	SER	-	expression tag	UNP A0A5J6DVE7
A	-13	HIS	-	expression tag	UNP A0A5J6DVE7
A	-12	HIS	-	expression tag	UNP A0A5J6DVE7
A	-11	HIS	-	expression tag	UNP A0A5J6DVE7
A	-10	HIS	-	expression tag	UNP A0A5J6DVE7
A	-9	HIS	-	expression tag	UNP A0A5J6DVE7
A	-8	HIS	-	expression tag	UNP A0A5J6DVE7
A	-7	GLY	-	expression tag	UNP A0A5J6DVE7
A	-6	MET	-	expression tag	UNP A0A5J6DVE7
A	-5	GLU	-	expression tag	UNP A0A5J6DVE7
A	-4	ASN	-	expression tag	UNP A0A5J6DVE7
A	-3	LEU	-	expression tag	UNP A0A5J6DVE7
A	-2	TYR	-	expression tag	UNP A0A5J6DVE7
A	-1	PHE	-	expression tag	UNP A0A5J6DVE7
A	0	GLN	-	expression tag	UNP A0A5J6DVE7
A	467	ASP	ASN	conflict	UNP A0A5J6DVE7
A	565	ASN	SER	conflict	UNP A0A5J6DVE7
A	612	GLY	CYS	conflict	UNP A0A5J6DVE7
A	634	VAL	LEU	conflict	UNP A0A5J6DVE7

- Molecule 2 is a protein called UL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	359	Total	C	N	O	S	0	0
			2752	1769	500	471	12		

There are 7 discrepancies between the modelled and reference sequences:

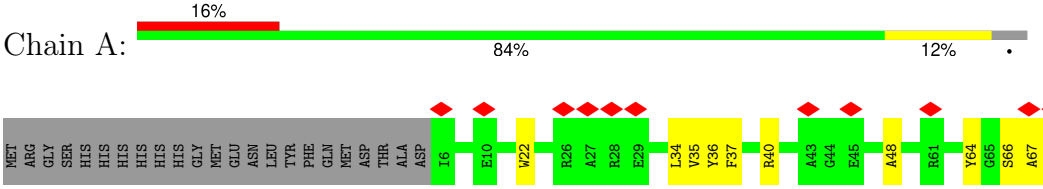
Chain	Residue	Modelled	Actual	Comment	Reference
B	129	GLU	ASP	conflict	UNP A0A2U9A692
B	166	VAL	ILE	conflict	UNP A0A2U9A692
B	385	SER	ASN	conflict	UNP A0A2U9A692
B	514	ASP	GLY	conflict	UNP A0A2U9A692
B	530	GLN	ARG	conflict	UNP A0A2U9A692
B	703	PRO	SER	conflict	UNP A0A2U9A692
B	719	ALA	THR	conflict	UNP A0A2U9A692

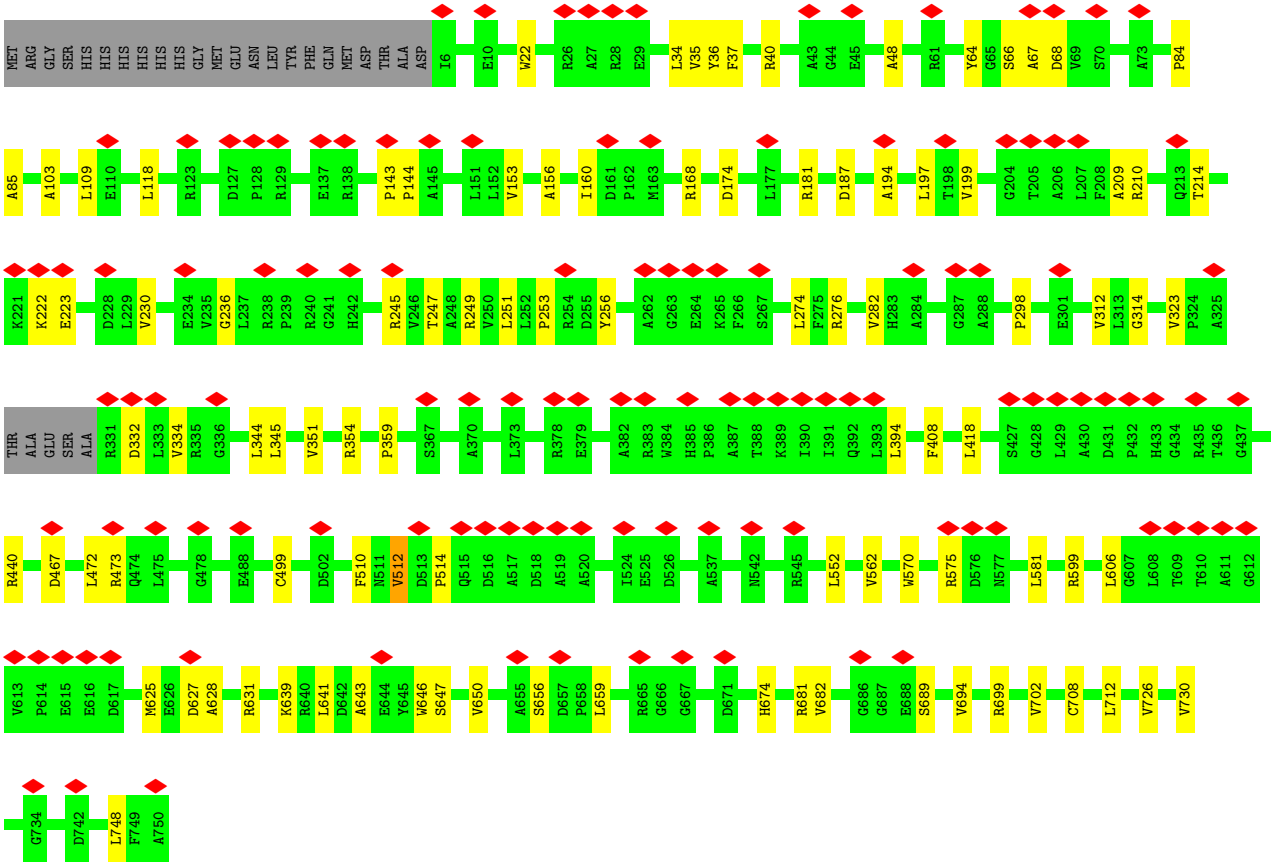
3 Residue-property plots (i)

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: UL8

Chain A:

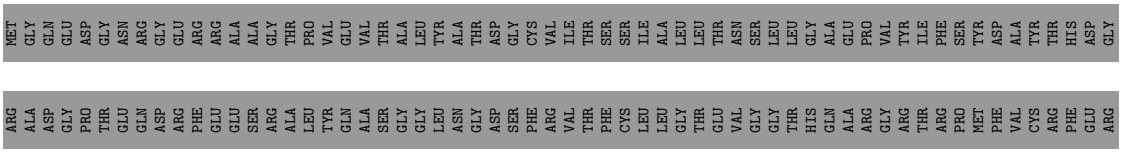


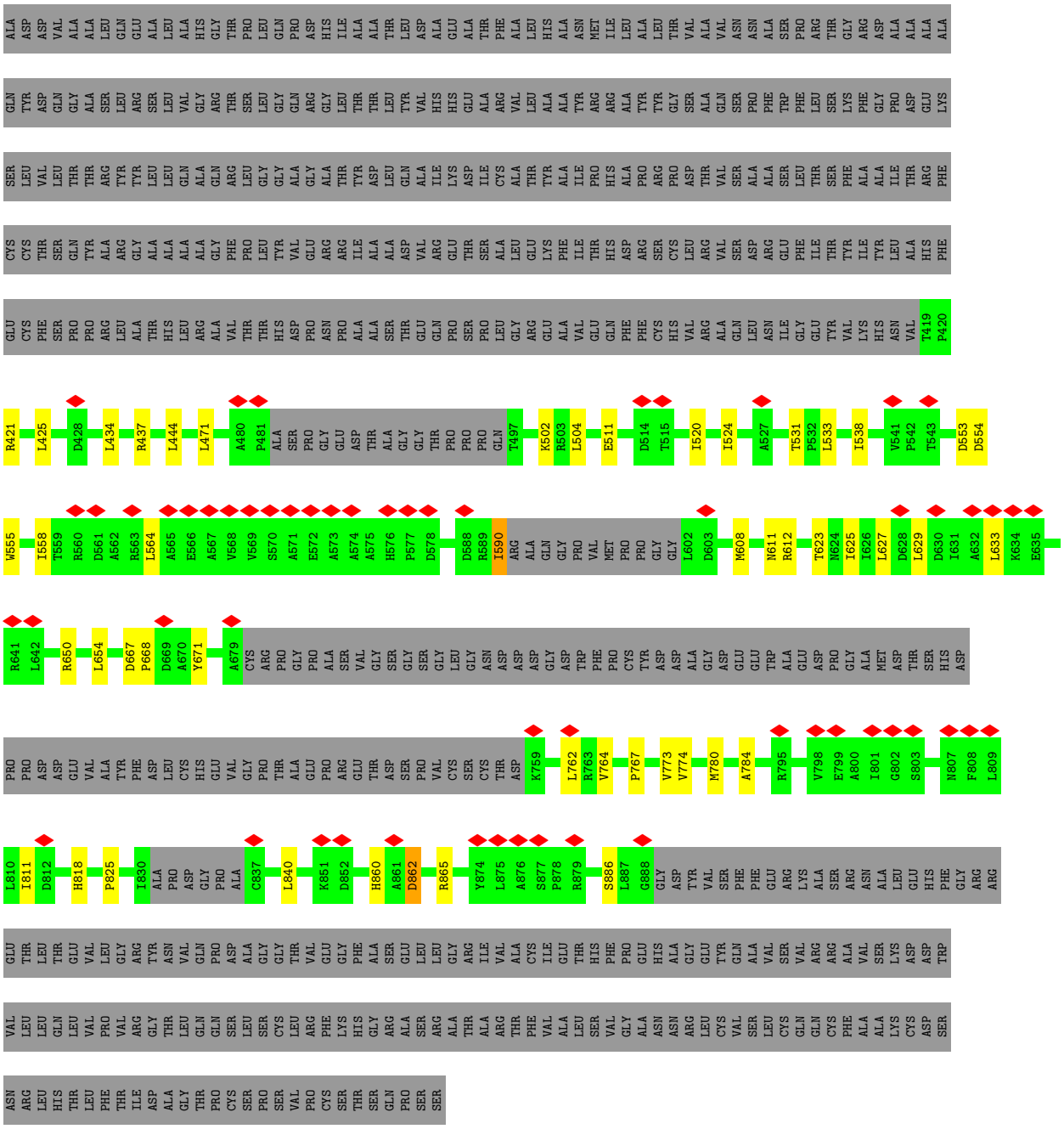


• Molecule 2: UL52

Chain B:






R421 L425 D428 L434 R437 L444 L471 A480 P481 T497 K502 R503 L504 E511 D514 T515 I520 I524 A527 T531 P532 L533 I538 V541 P542 T543 D553 D554
W555 I558 T559 R560 D561 A562 R563 L564 A565 E566 A567 V568 V569 S570 A571 E572 A573 A574 A575 H576 P577 D578 D588 R589 I590 L602 D603 M608 N611 R612 T623 N624 I625 I626 L627 D628 L629 D630 I631 A632 L633 K634 E635
R641 L642 R650 L654 D667 P668 D669 A670 Y671 A679 L762 R763 V764 P767 V773 V774 M780 A784 R795 V798 E799 A800 I801 G802 S803 N807 F808 L809
L810 I811 D812 H818 P825 I830 C837 L840 K851 D852 H860 A861 D862 R865 Y874 L875 A876 S877 P878 R879 S886 L887 G888

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108894	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	140	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	67.310	Depositor
Minimum map value	-41.635	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	9	Depositor
Map size (Å)	310.344, 310.344, 310.344	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2931, 1.2931, 1.2931	Depositor

5 Model quality

5.1 Standard geometry

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	0.13	0/5737	0.30	0/7864
2	B	0.14	0/2821	0.32	0/3846
All	All	0.13	0/8558	0.31	0/11710

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

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	5580	0	5555	55	0
2	B	2752	0	2791	26	0
All	All	8332	0	8346	77	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 5.

The worst 5 of 77 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:B:553:ASP:OD2	2:B:612:ARG:NH2	2.31	0.64
2:B:654:LEU:HD23	2:B:668:PRO:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:ARG:HB2	2:B:886:SER:HB3	1.83	0.61
2:B:538:ILE:HG23	2:B:611:ASN:HB3	1.84	0.59
2:B:538:ILE:HG12	2:B:608:MET:HA	1.83	0.59

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	736/768 (96%)	708 (96%)	28 (4%)	0	100	100
2	B	349/1058 (33%)	336 (96%)	13 (4%)	0	100	100
All	All	1085/1826 (59%)	1044 (96%)	41 (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	552/575 (96%)	549 (100%)	3 (0%)	81	81
2	B	277/832 (33%)	268 (97%)	9 (3%)	34	58
All	All	829/1407 (59%)	817 (99%)	12 (1%)	57	70

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	623	THR
2	B	633	LEU
2	B	862	ASP
2	B	774	VAL
2	B	504	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	613	ASN
2	B	643	HIS
2	B	807	ASN
2	B	885	HIS

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 oligosaccharides 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.

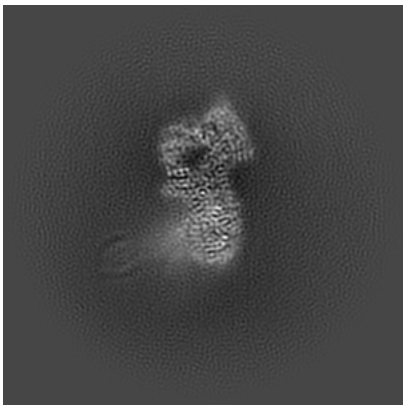
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49736. These allow visual inspection of the internal detail of the map and identification of artifacts.

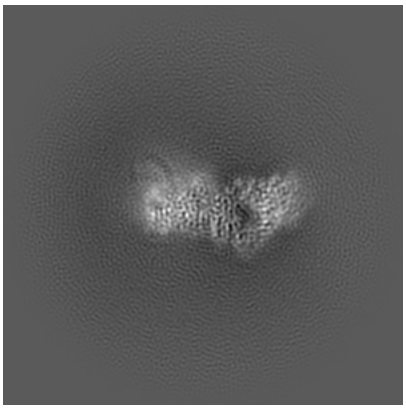
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

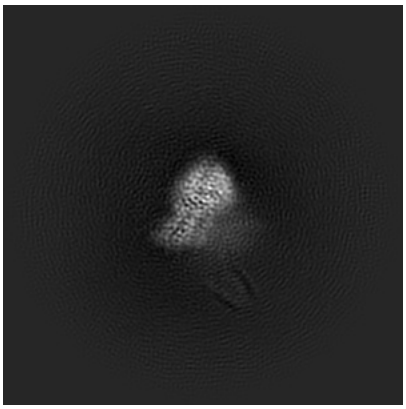
6.1.1 Primary map



X

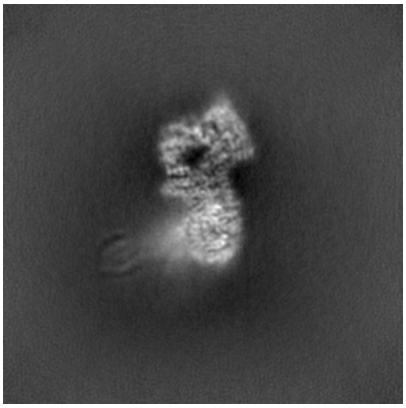


Y

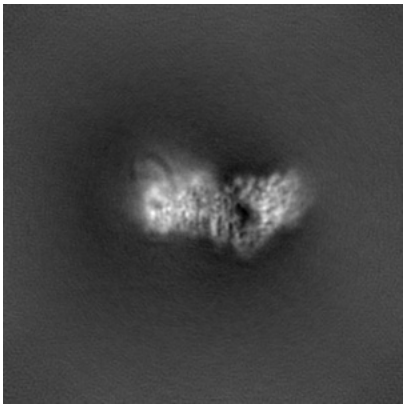


Z

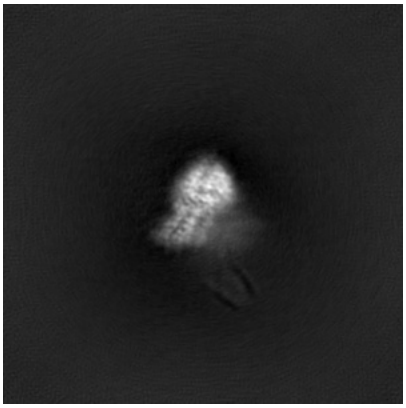
6.1.2 Raw map



X



Y

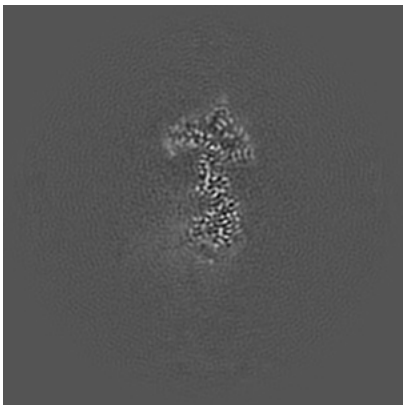


Z

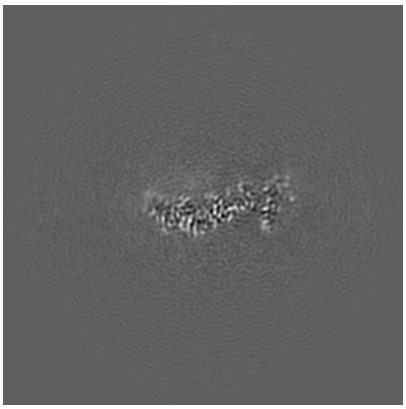
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

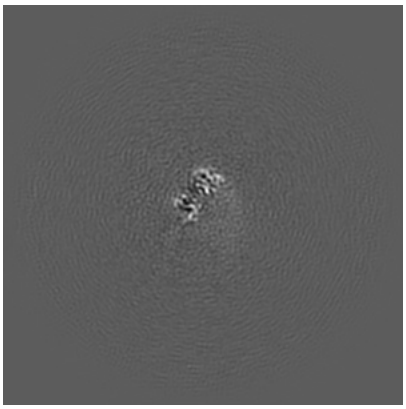
6.2.1 Primary map



X Index: 120

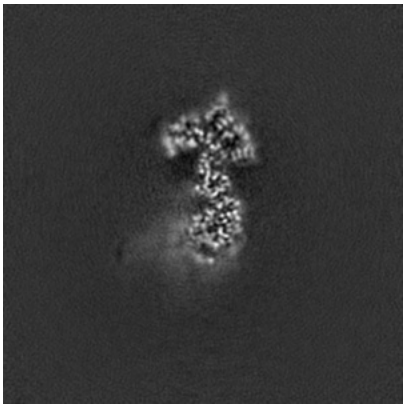


Y Index: 120

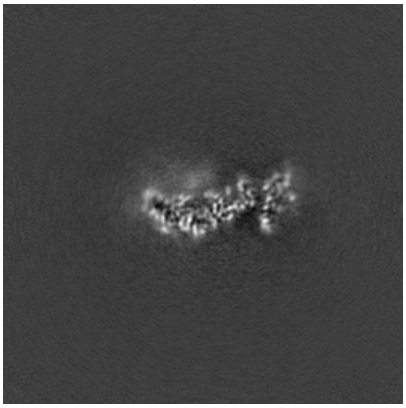


Z Index: 120

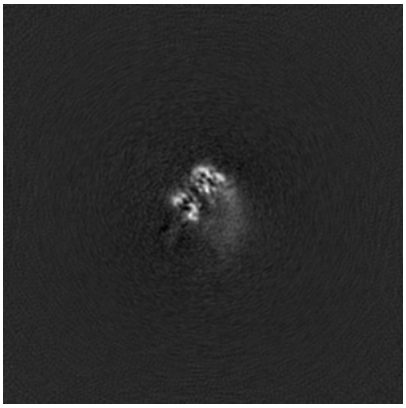
6.2.2 Raw map



X Index: 120



Y Index: 120

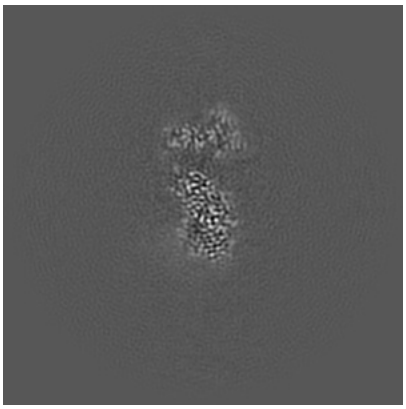


Z Index: 120

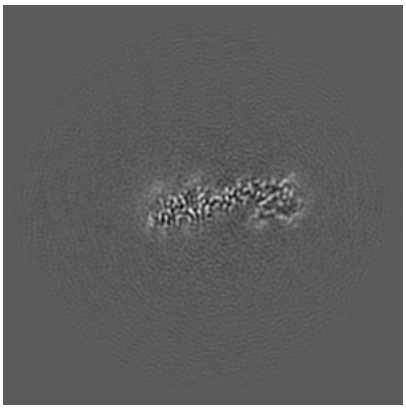
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

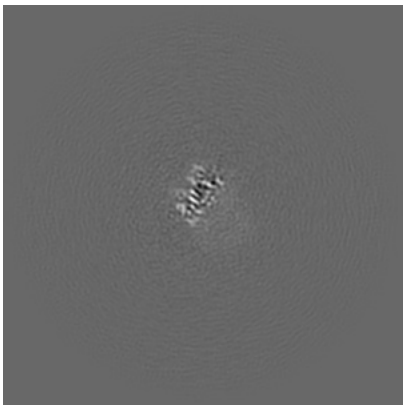
6.3.1 Primary map



X Index: 113

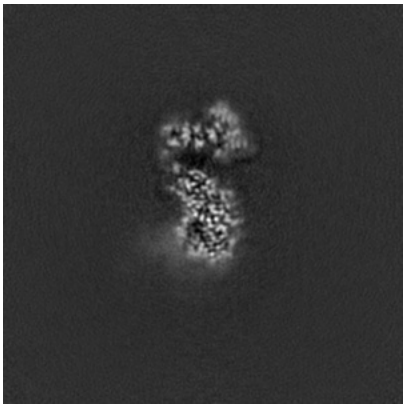


Y Index: 129

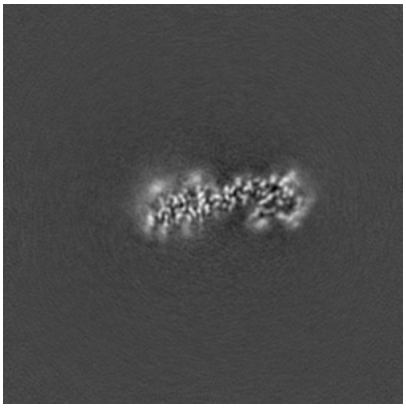


Z Index: 110

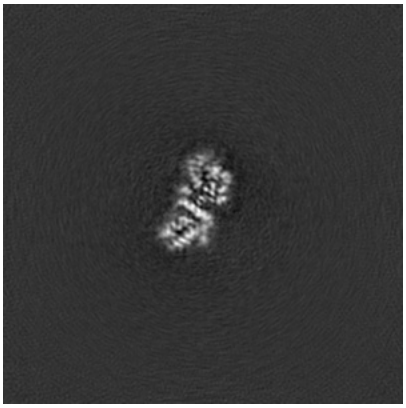
6.3.2 Raw map



X Index: 113



Y Index: 129

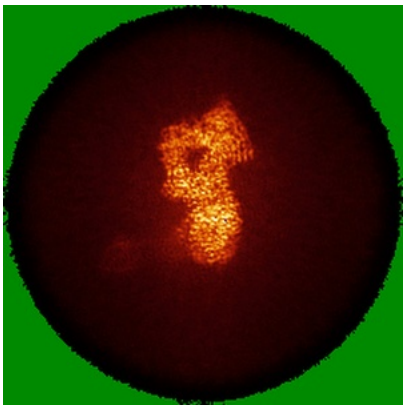


Z Index: 156

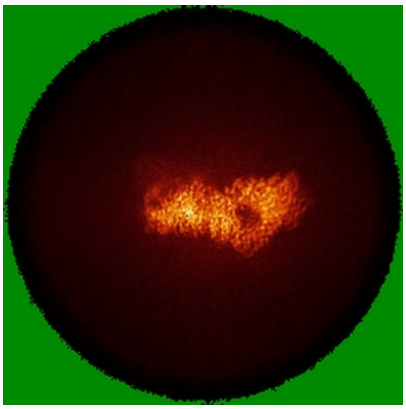
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

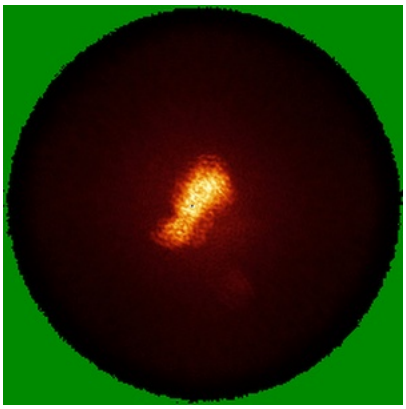
6.4.1 Primary map



X

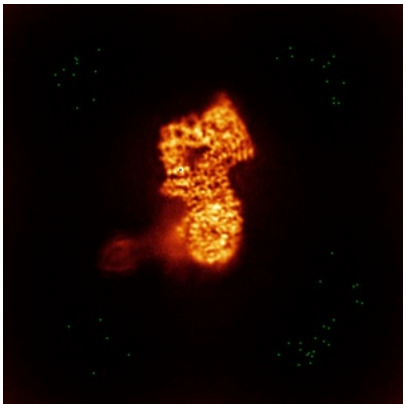


Y

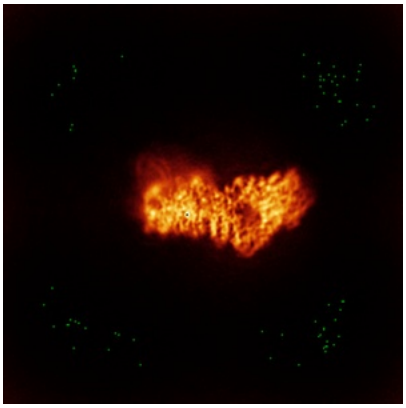


Z

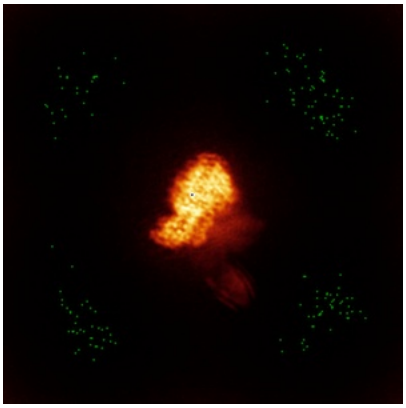
6.4.2 Raw map



X



Y

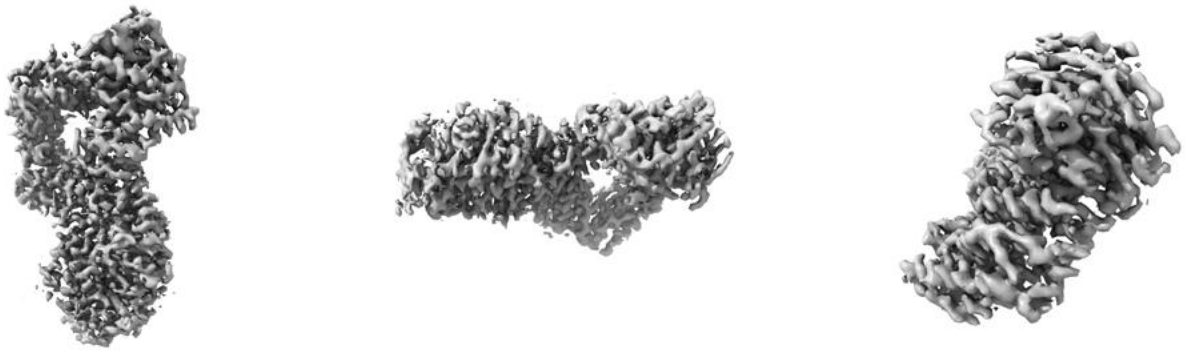


Z

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)

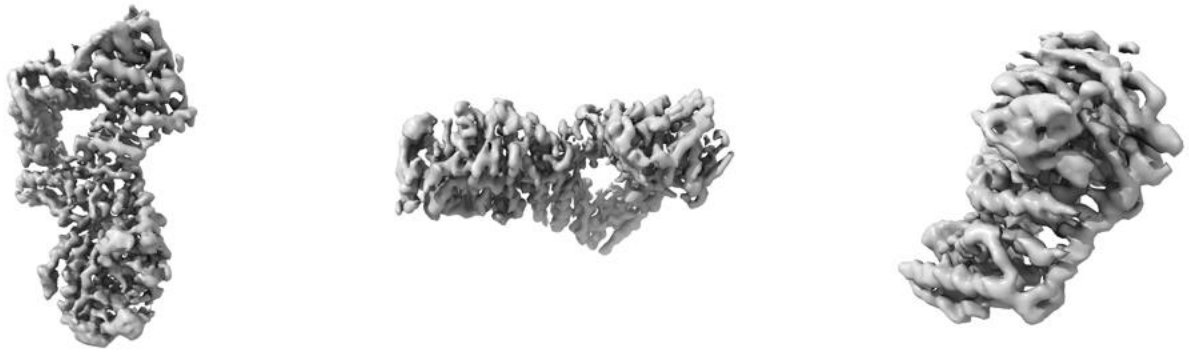
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 9.0. 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



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.

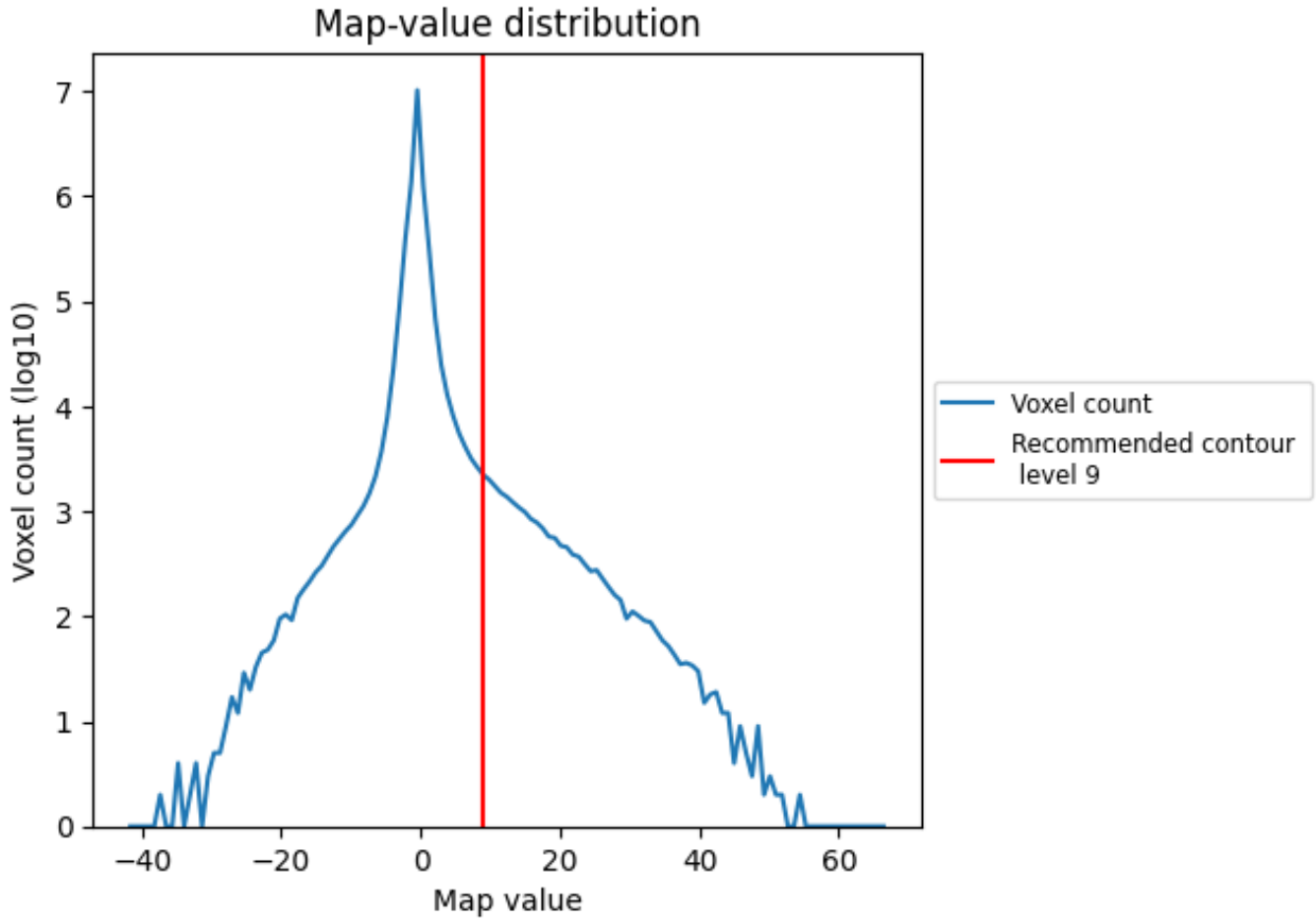
6.6 Mask visualisation (i)

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

7 Map analysis

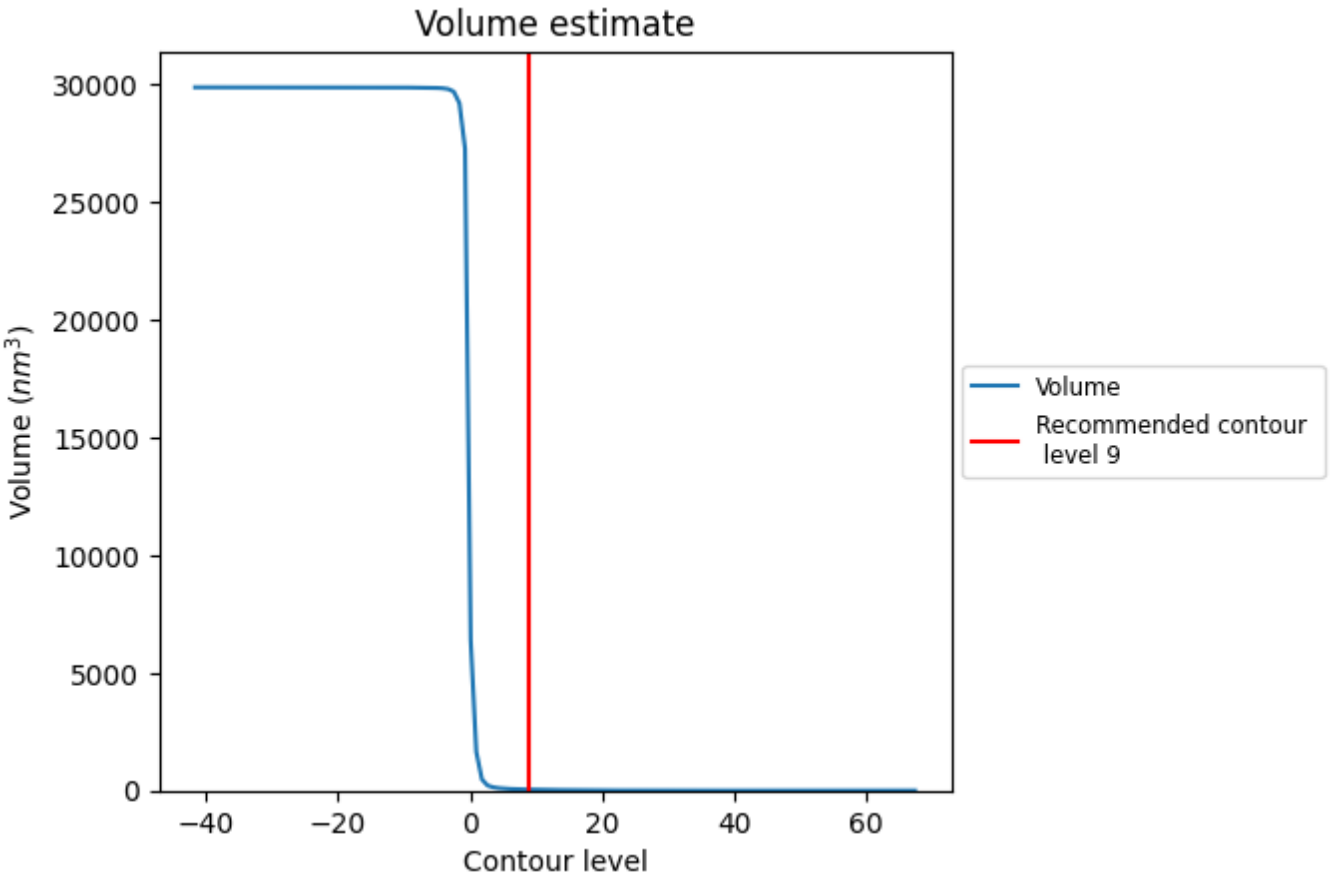
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

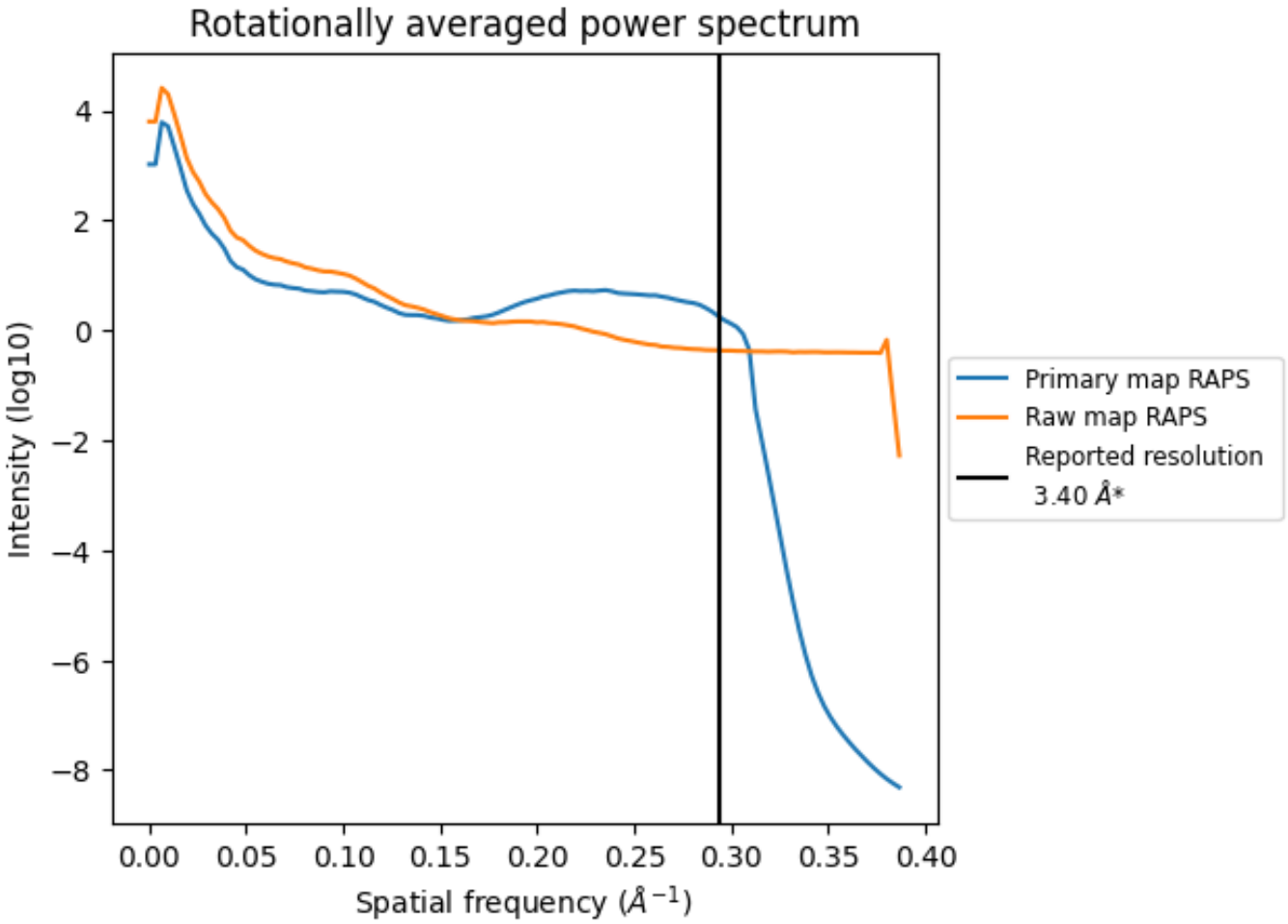
7.2 Volume estimate (i)



The volume at the recommended contour level is 43 nm^3; this corresponds to an approximate mass of 39 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)

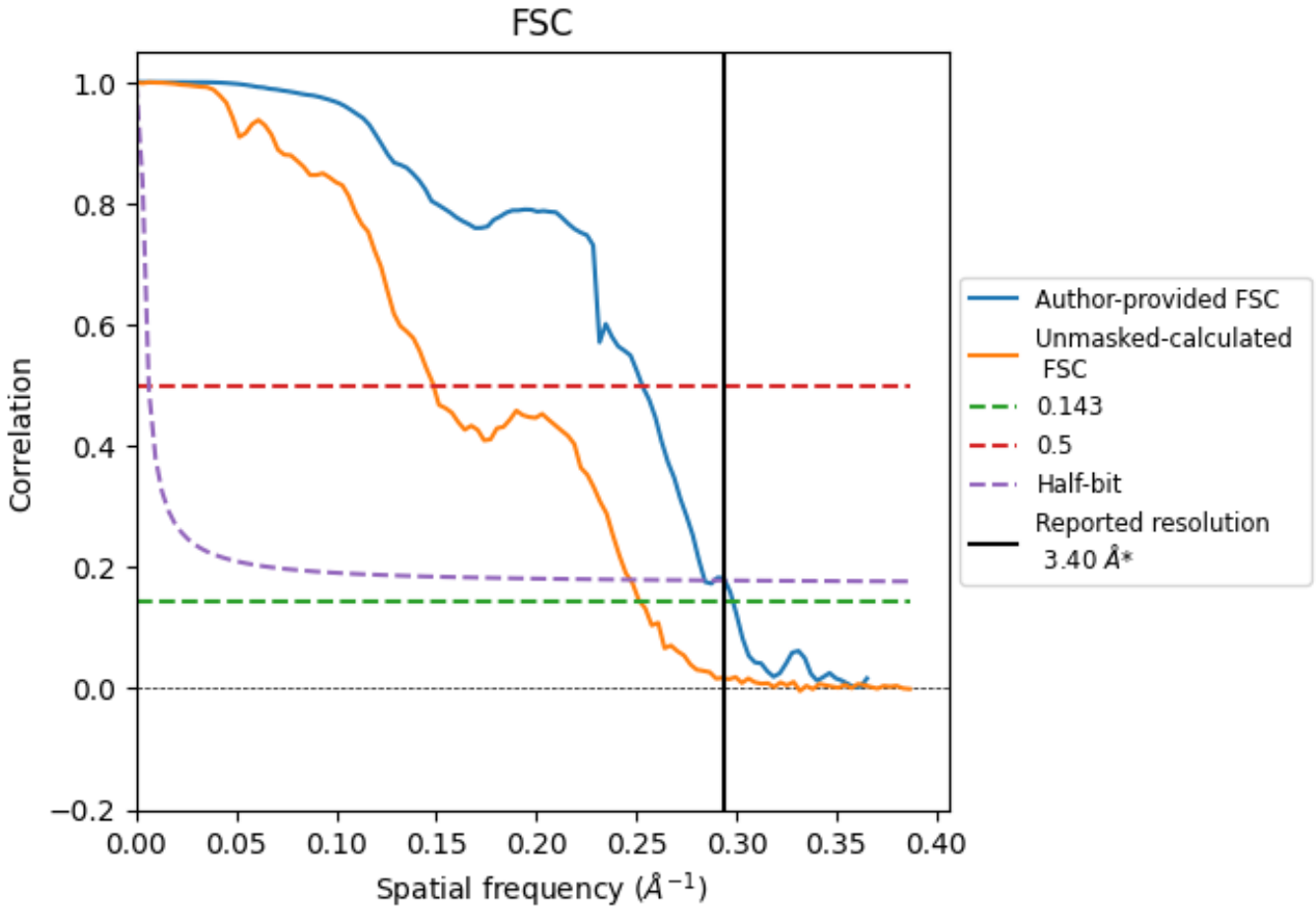


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.40	-
Author-provided FSC curve	3.35	3.95	3.52
Unmasked-calculated*	3.97	6.73	4.05

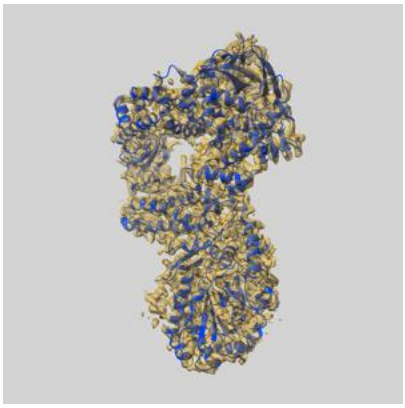
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 3.95 differs from the reported value 3.4 by more than 10 %

The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 6.73 differs from the reported value 3.4 by more than 10 %

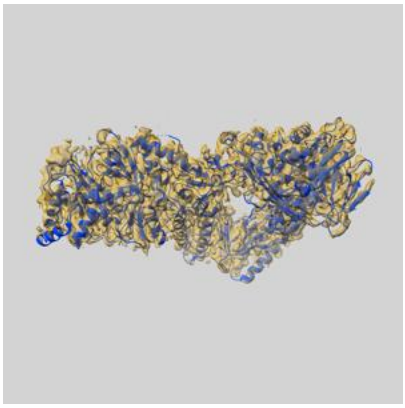
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49736 and PDB model 9NRL. Per-residue inclusion information can be found in section 3 on page 5.

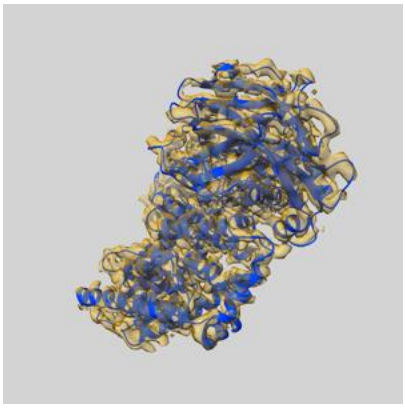
9.1 Map-model overlay



X



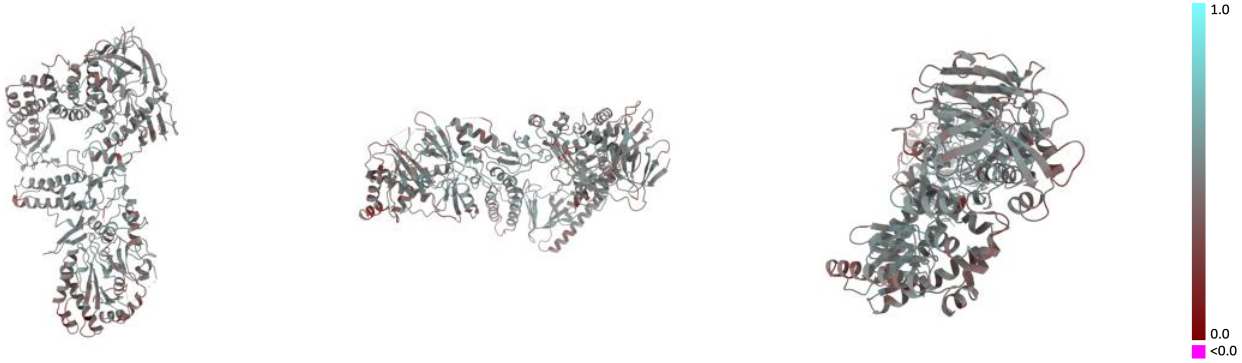
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 9.0 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.

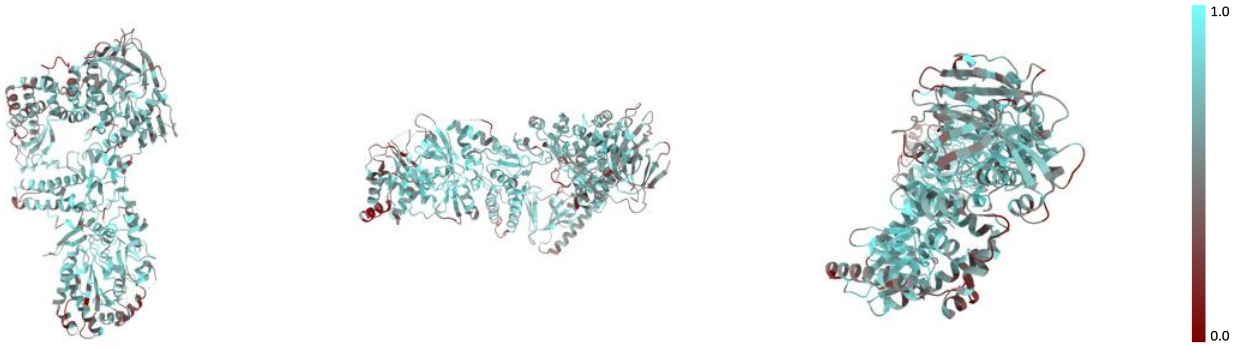
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

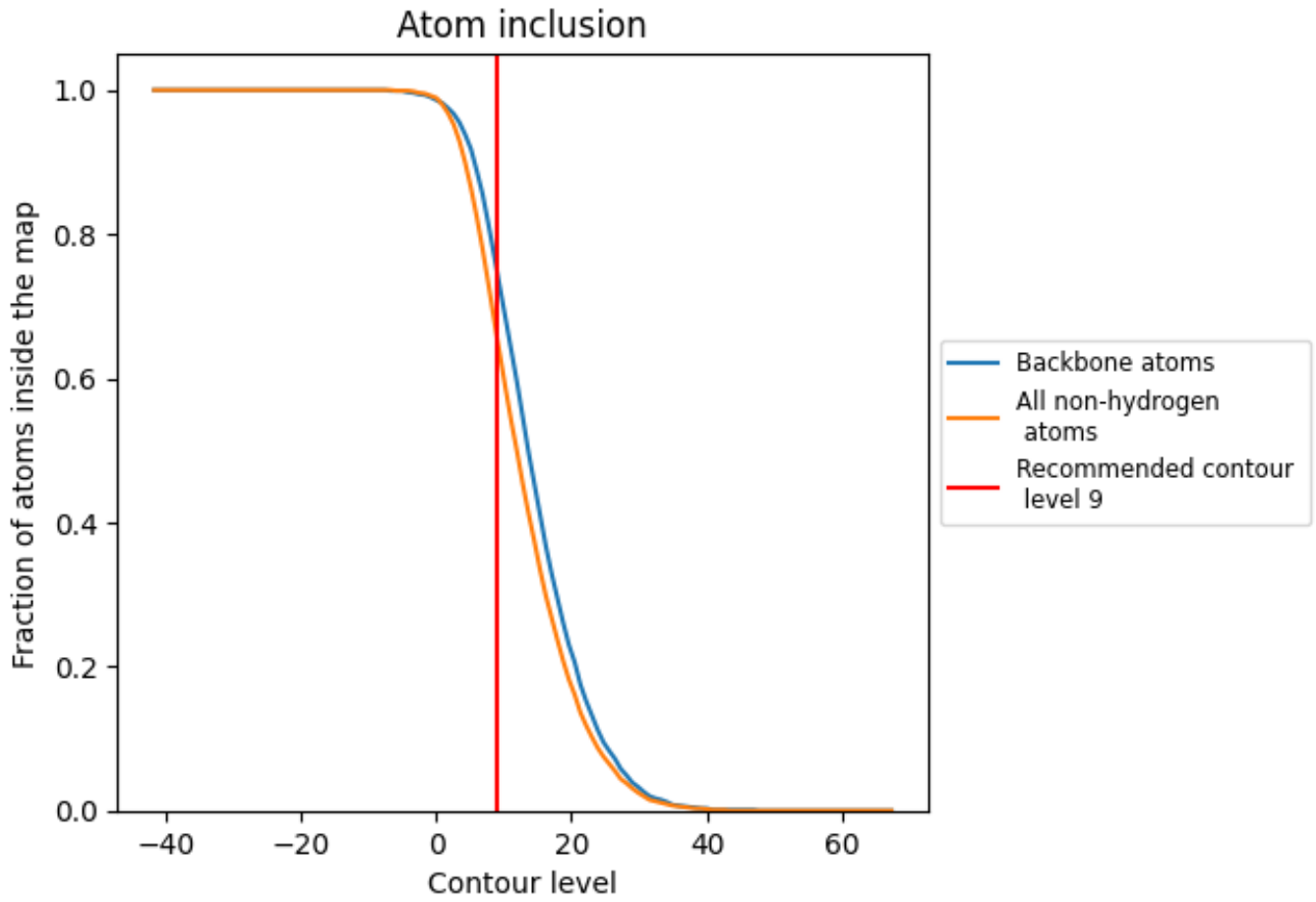
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (9).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 66% 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 (9) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6570	0.4680
A	0.6460	0.4740
B	0.6800	0.4560