wwPDB EM Validation Summary Report

Oct 19, 2026 – 02:31 PM JST

PDB ID	:	9X4Z / pdb_00009x4z
EMDB ID	:	EMD-66568
Title	:	Cryo-EM structure of ClassIII Lanthipeptide modification enzyme FaecKC in the presence of ATPrS.
Authors	:	Zhang, H.J.; Wang, B.C.
Deposited on	:	2025-10-12
Resolution	:	3.83 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:

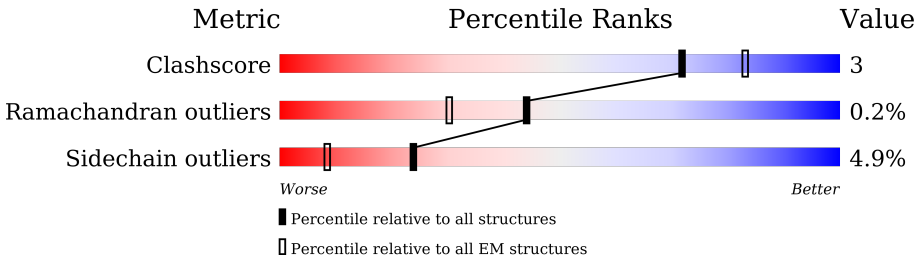
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

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

The reported resolution of this entry is 3.83 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	878	77% 84% 12%
1	B	878	75% 86% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13798 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 Lanthionine synthetase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	852	Total	C	N	O	S	0	0
			6925	4488	1137	1276	24		
1	B	842	Total	C	N	O	S	0	0
			6842	4439	1121	1258	24		

There are 40 discrepancies between the modelled and reference sequences:

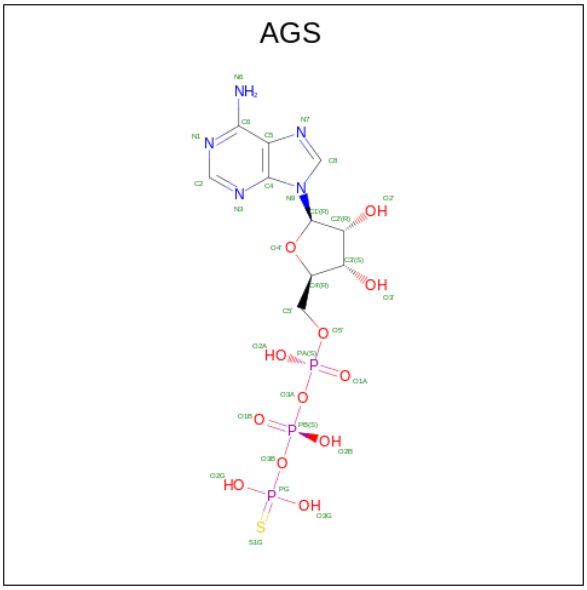
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	CYS	ASN	conflict	UNP A0A7V7GQX9
A	85	VAL	LEU	conflict	UNP A0A7V7GQX9
A	181	THR	ALA	conflict	UNP A0A7V7GQX9
A	186	THR	SER	conflict	UNP A0A7V7GQX9
A	198	GLU	ALA	conflict	UNP A0A7V7GQX9
A	210	ALA	PRO	conflict	UNP A0A7V7GQX9
A	212	LEU	SER	conflict	UNP A0A7V7GQX9
A	237	PRO	LEU	conflict	UNP A0A7V7GQX9
A	252	TYR	HIS	conflict	UNP A0A7V7GQX9
A	257	ASP	ASN	conflict	UNP A0A7V7GQX9
A	259	ARG	LYS	conflict	UNP A0A7V7GQX9
A	260	LEU	GLN	conflict	UNP A0A7V7GQX9
A	321	GLY	ASP	conflict	UNP A0A7V7GQX9
A	349	GLU	LYS	conflict	UNP A0A7V7GQX9
A	368	ASP	ASN	conflict	UNP A0A7V7GQX9
A	615	LYS	THR	conflict	UNP A0A7V7GQX9
A	621	ASN	SER	conflict	UNP A0A7V7GQX9
A	624	ASP	ASN	conflict	UNP A0A7V7GQX9
A	664	ILE	VAL	conflict	UNP A0A7V7GQX9
A	732	ASP	GLY	conflict	UNP A0A7V7GQX9
B	67	CYS	ASN	conflict	UNP A0A7V7GQX9
B	85	VAL	LEU	conflict	UNP A0A7V7GQX9
B	181	THR	ALA	conflict	UNP A0A7V7GQX9
B	186	THR	SER	conflict	UNP A0A7V7GQX9
B	198	GLU	ALA	conflict	UNP A0A7V7GQX9
B	210	ALA	PRO	conflict	UNP A0A7V7GQX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	212	LEU	SER	conflict	UNP A0A7V7GQX9
B	237	PRO	LEU	conflict	UNP A0A7V7GQX9
B	252	TYR	HIS	conflict	UNP A0A7V7GQX9
B	257	ASP	ASN	conflict	UNP A0A7V7GQX9
B	259	ARG	LYS	conflict	UNP A0A7V7GQX9
B	260	LEU	GLN	conflict	UNP A0A7V7GQX9
B	321	GLY	ASP	conflict	UNP A0A7V7GQX9
B	349	GLU	LYS	conflict	UNP A0A7V7GQX9
B	368	ASP	ASN	conflict	UNP A0A7V7GQX9
B	615	LYS	THR	conflict	UNP A0A7V7GQX9
B	621	ASN	SER	conflict	UNP A0A7V7GQX9
B	624	ASP	ASN	conflict	UNP A0A7V7GQX9
B	664	ILE	VAL	conflict	UNP A0A7V7GQX9
B	732	ASP	GLY	conflict	UNP A0A7V7GQX9

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
2	A	1	31	10	5	12	3	1	0

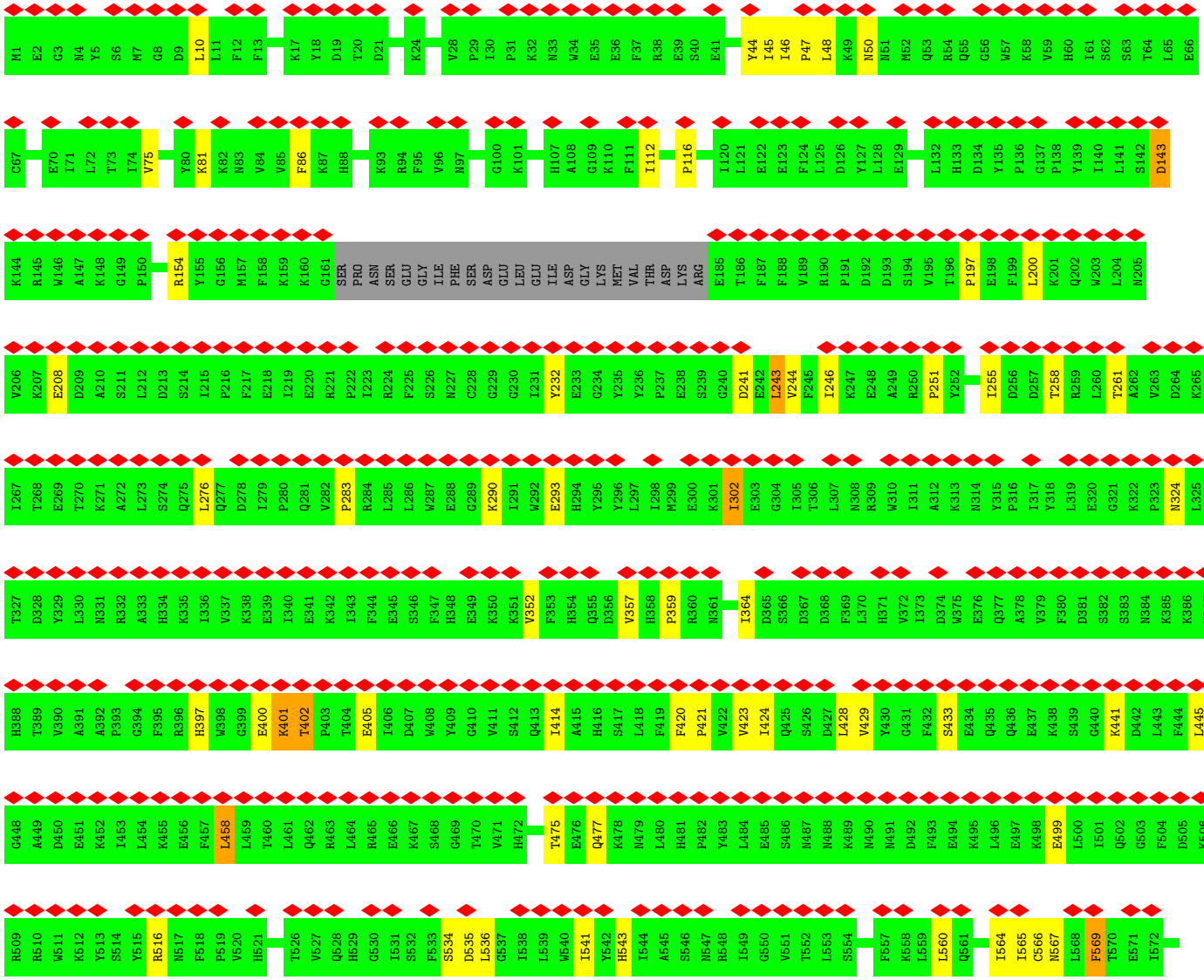
3 Residue-property plots (i)

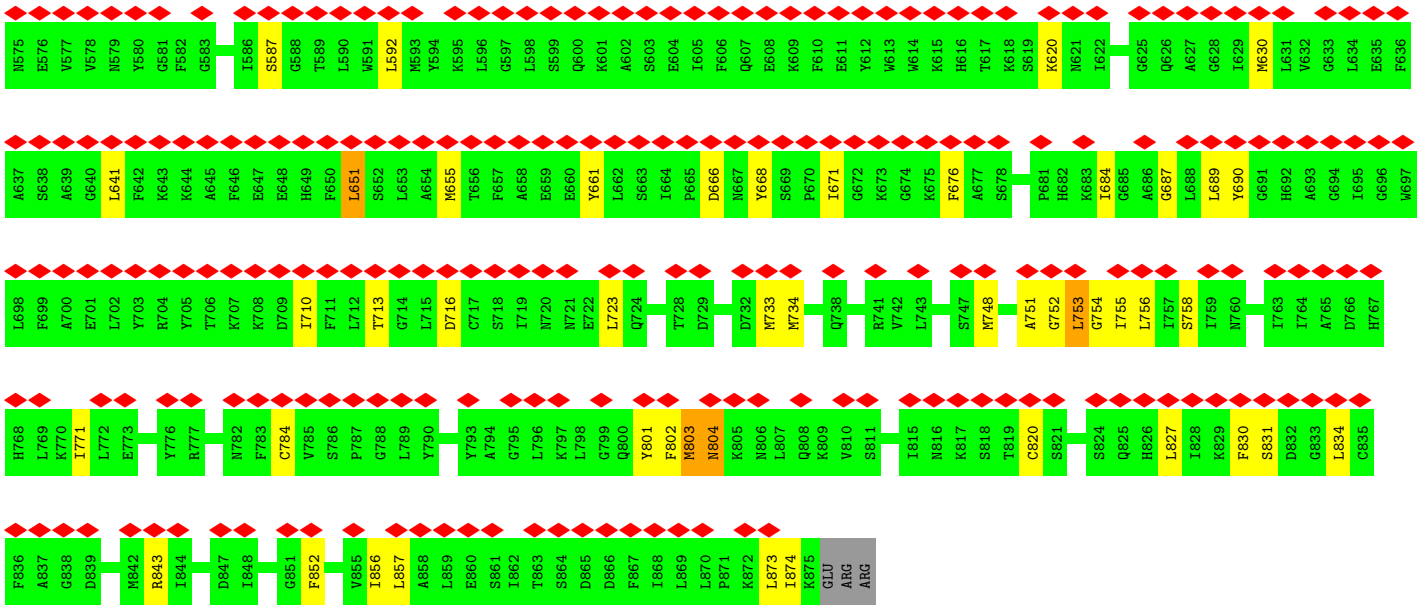
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Lanthionine synthetase

Chain A:



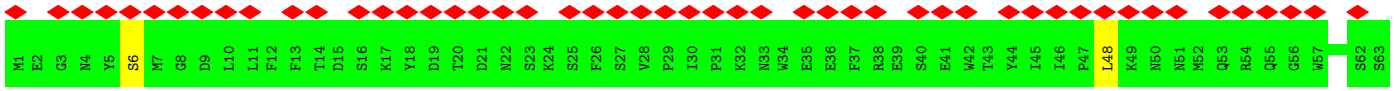


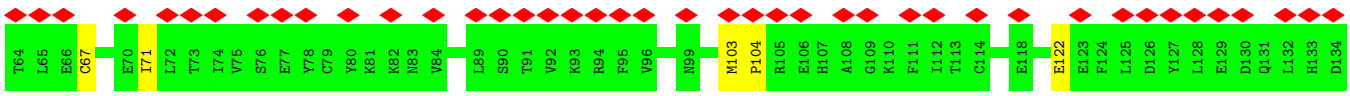


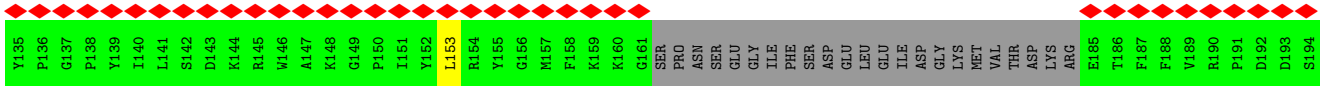
- Molecule 1: Lanthionine synthetase

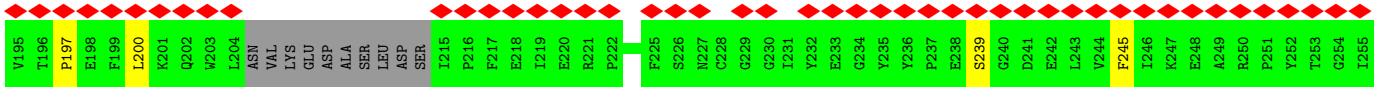
Chain B:

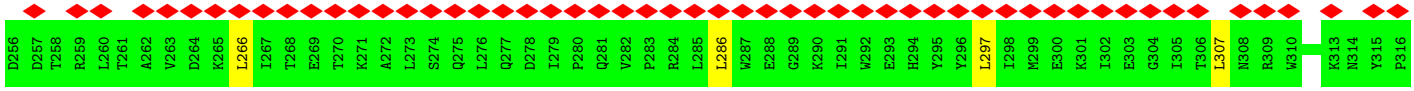


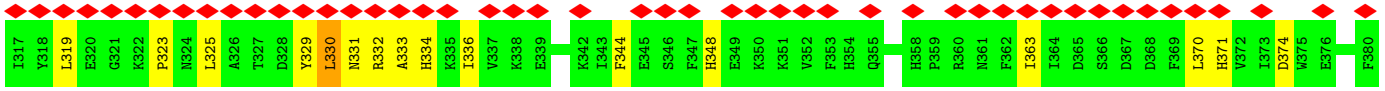


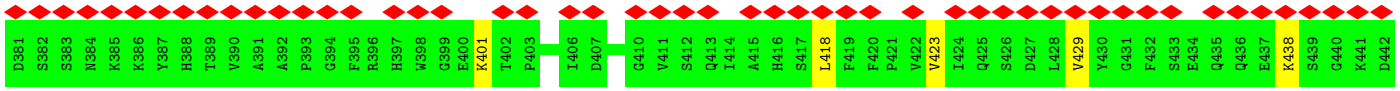


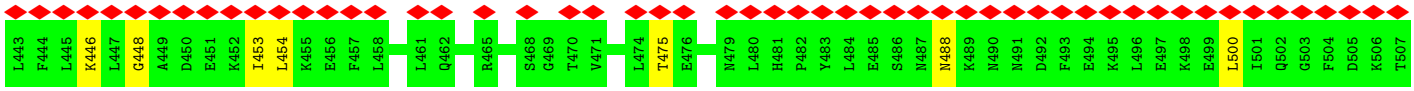


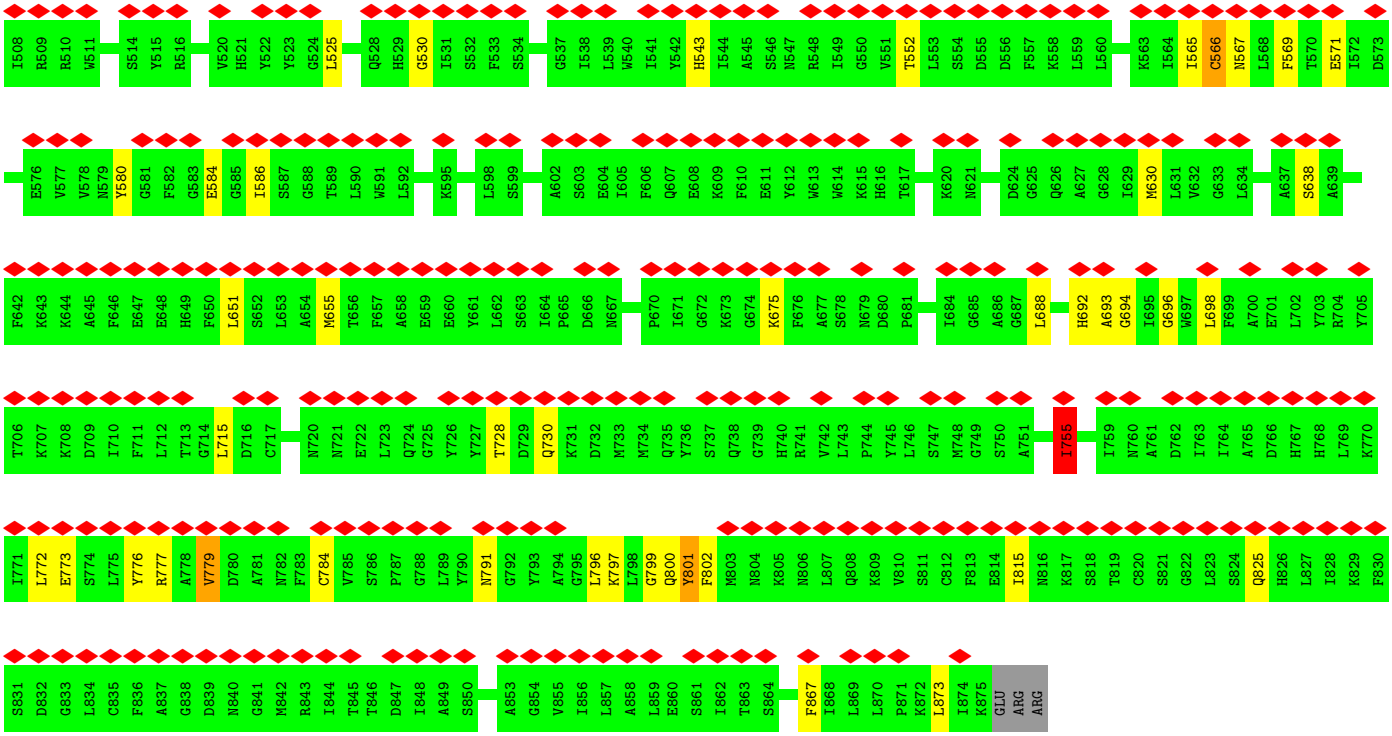











I508 R509 R510 W511 S514 Y515 R516 V520 H521 Y522 Y523 G524 L525 Q528 H529 G530 I531 S532 F533 S534 G537 I538 L539 W540 I541 Y542 H543 I544 A545 S546 N547 R548 I549 G550 V551 T552 L553 S554 D555 D556 F557 K558 L559 L560 K563 I564 I565 C566 N567 L568 F569 T570 E571 I572 D573
E576 V577 V578 N579 Y580 G581 F582 G583 E584 G585 I586 S587 G588 T589 L590 W591 L592 K595 L598 S599 A602 S603 E604 I605 F606 Q607 E608 K609 F610 E611 Y612 W613 W614 K615 H616 T617 K620 N621 D624 G625 Q626 A627 G628 I629 M630 L631 V632 G633 L634 A637 S638 A639
F642 K643 K644 A645 F646 E647 E648 H649 F650 L651 S652 L653 A654 M655 T656 F657 A658 E659 E660 Y661 L662 S663 I664 P665 D666 N667 P670 I671 G672 K673 G674 K675 F676 A677 S678 N679 D680 P681 I684 G685 A686 G687 L688 H692 A693 G694 I695 G696 W697 L698 F699 A700 E701 L702 Y703 R704 Y705
T706 K707 K708 D709 I710 F711 L712 T713 G714 L715 D716 C717 N720 N721 E722 L723 Q724 G725 Y726 Y727 T728 D729 Q730 K731 D732 M733 M734 Q735 Y736 S737 Q738 G739 H740 R741 V742 L743 P744 Y745 L746 S747 M748 G749 S750 A751 I755 I759 N760 A761 D762 I763 I764 A765 D766 H767 H768 L769 K770
I771 L772 E773 S774 L775 Y776 R777 A778 V779 D780 A781 N782 F783 C784 V785 S786 P787 G788 L789 Y790 N791 G792 Y793 A794 G795 L796 K797 L798 G799 Q800 Y801 F802 M803 N804 K805 N806 L807 Q808 K809 V810 S811 C812 F813 E814 I815 N816 K817 S818 T819 C820 S821 G822 L823 S824 Q825 H826 L827 I828 K829 F830
S831 D832 G833 L834 C835 F836 A837 G838 D839 N840 G841 M842 R843 I844 T845 T846 D847 I848 A849 S850 A853 G854 V855 I856 L857 A858 L859 E860 S861 I862 T863 S864 F867 I868 L869 L870 P871 K872 L873 I874 K875 GLU ARG ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	195132	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.416	Depositor
Minimum map value	-1.007	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.128	Depositor
Map size (Å)	250.112, 250.112, 250.112	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.977, 0.977, 0.977	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS

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	0.25	0/7110	0.55	4/9615 (0.0%)
1	B	0.24	0/7026	0.51	3/9501 (0.0%)
All	All	0.24	0/14136	0.53	7/19116 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	751	ALA	N-CA-C	-10.43	96.29	113.50
1	B	755	ILE	N-CA-C	-6.33	106.16	112.17
1	A	81	LYS	CA-C-N	-5.92	113.17	122.65
1	A	81	LYS	C-N-CA	-5.92	113.17	122.65
1	A	803	MET	N-CA-C	-5.79	104.77	112.94

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	6925	0	6769	52	0
1	B	6842	0	6678	41	0
2	A	31	0	12	0	0
All	All	13798	0	13459	93	0

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

The worst 5 of 93 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:B:776:TYR:HE1	1:B:800:GLN:HG3	1.54	0.73
1:B:755:ILE:HD11	1:B:799:GLY:HA2	1.73	0.71
1:B:333:ALA:O	1:B:336:ILE:N	2.28	0.65
1:B:776:TYR:CE1	1:B:800:GLN:HG3	2.31	0.65
1:B:319:LEU:HD11	1:B:325:LEU:HD23	1.80	0.63

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	848/878 (97%)	778 (92%)	66 (8%)	4 (0%)	24 59
1	B	836/878 (95%)	772 (92%)	64 (8%)	0	100 100
All	All	1684/1756 (96%)	1550 (92%)	130 (8%)	4 (0%)	44 74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	753	LEU
1	A	424	ILE
1	A	802	PHE
1	A	116	PRO

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	747/779 (96%)	704 (94%)	43 (6%)	18 45
1	B	736/779 (94%)	706 (96%)	30 (4%)	27 52
All	All	1483/1558 (95%)	1410 (95%)	73 (5%)	24 48

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	525	LEU
1	B	825	GLN
1	B	552	THR
1	B	728	THR
1	A	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	384	ASN
1	B	567	ASN
1	B	800	GLN
1	B	720	ASN
1	B	760	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	AGS	A	901	-	29,33,33	0.49	1 (3%)	39,52,52	0.66	1 (2%)

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	AGS	A	901	-	-	6/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	AGS	PG-S1G	2.18	1.95	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	AGS	PA-O3A-PB	-2.99	122.56	132.83

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	AGS	C5'-O5'-PA-O1A

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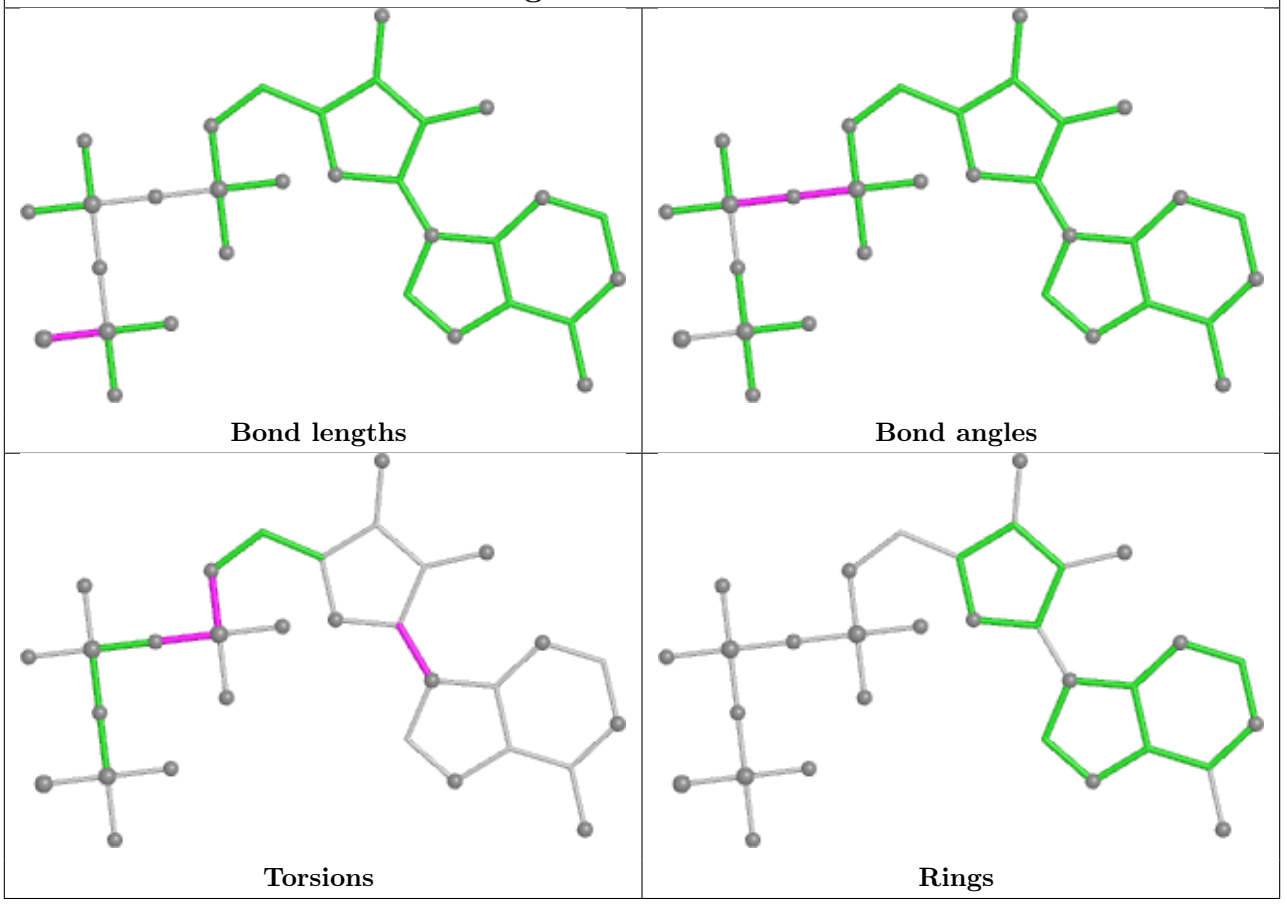
Mol	Chain	Res	Type	Atoms
2	A	901	AGS	C5'-O5'-PA-O3A
2	A	901	AGS	O4'-C1'-N9-C4
2	A	901	AGS	C5'-O5'-PA-O2A
2	A	901	AGS	PB-O3A-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AGS A 901



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.

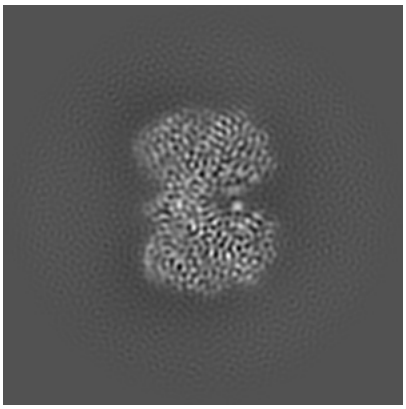
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66568. These allow visual inspection of the internal detail of the map and identification of artifacts.

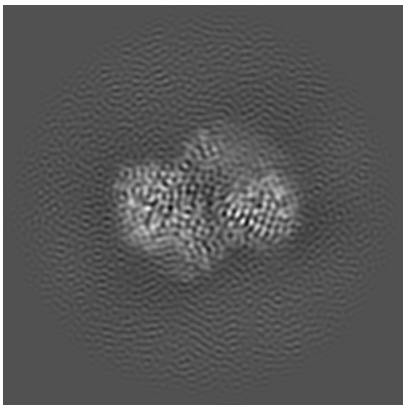
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

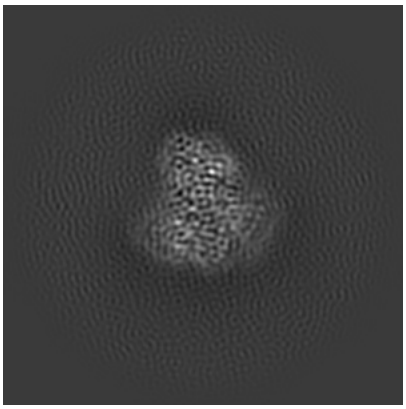
6.1.1 Primary map



X

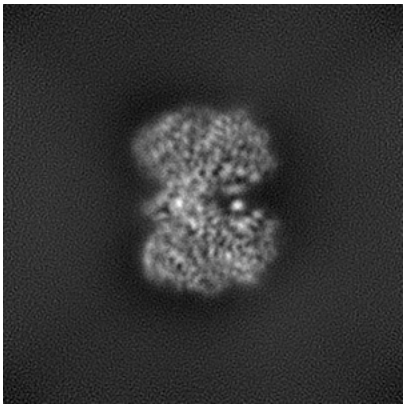


Y

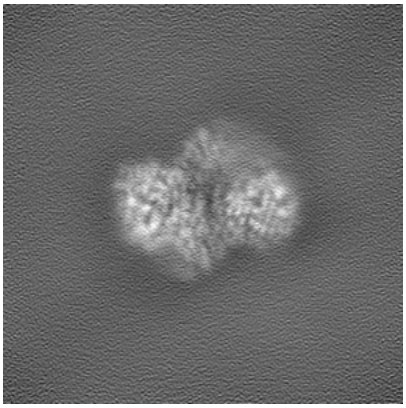


Z

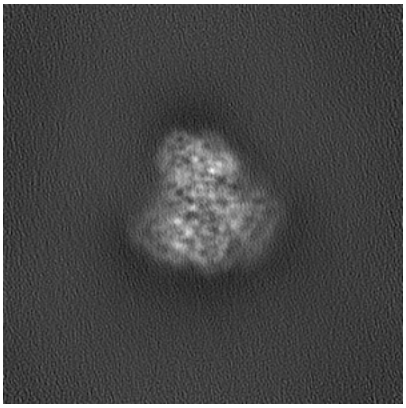
6.1.2 Raw map



X



Y

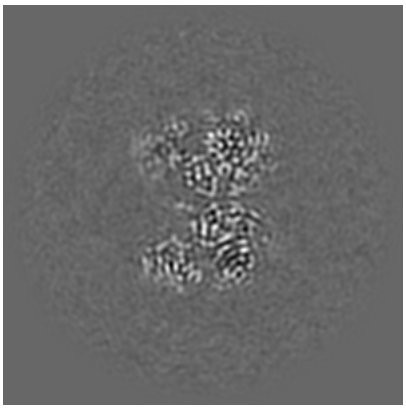


Z

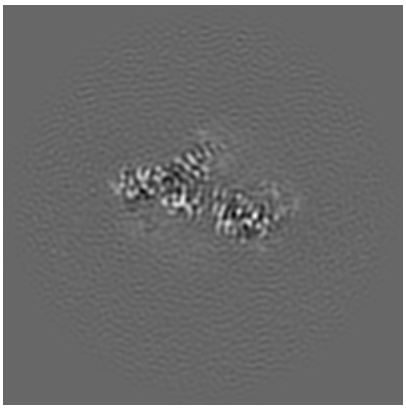
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

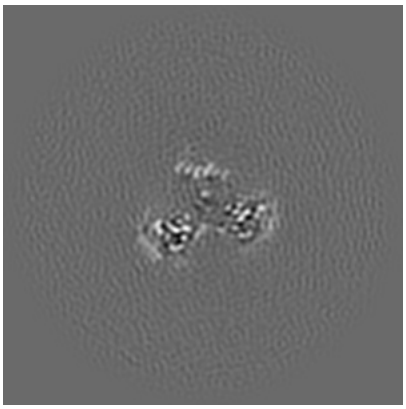
6.2.1 Primary map



X Index: 128

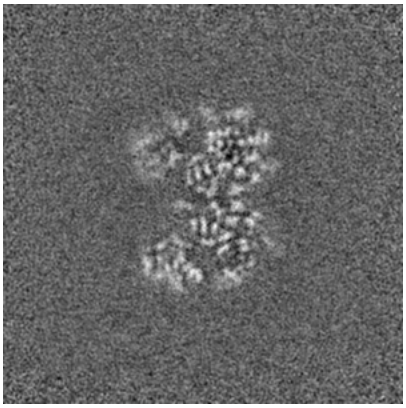


Y Index: 128

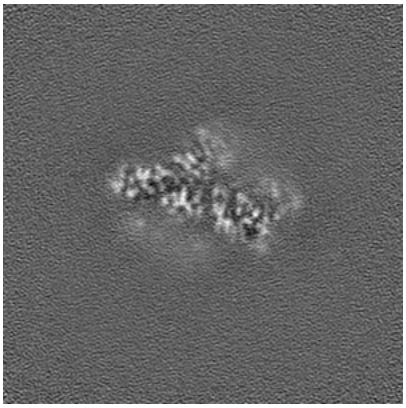


Z Index: 128

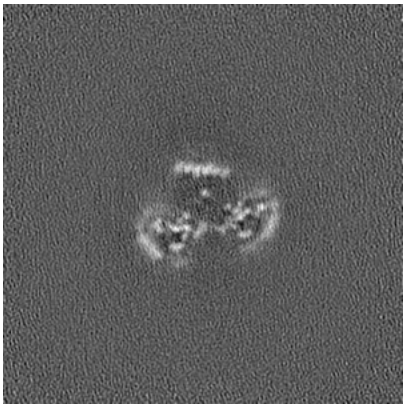
6.2.2 Raw map



X Index: 128



Y Index: 128

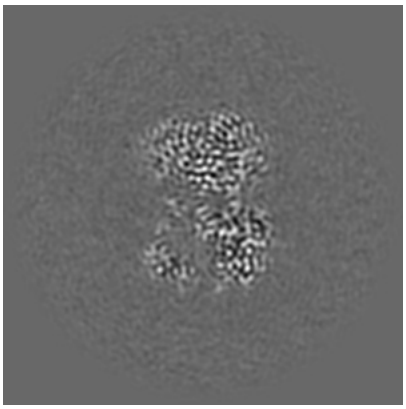


Z Index: 128

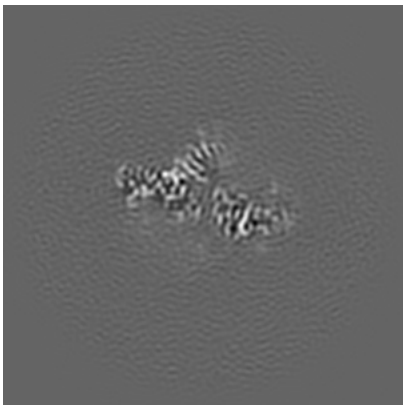
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

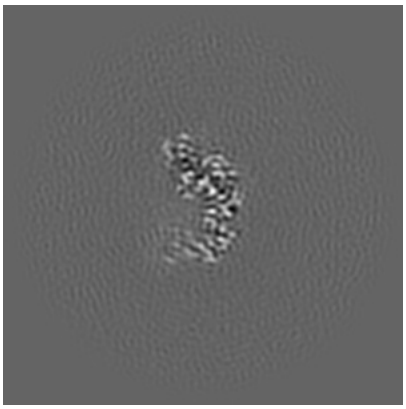
6.3.1 Primary map



X Index: 123

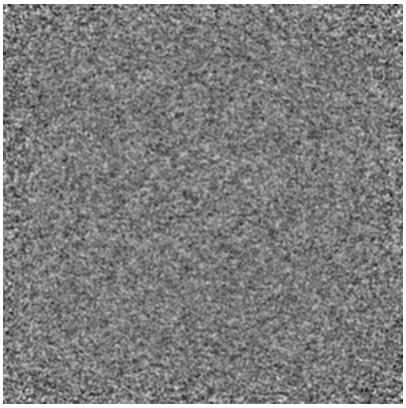


Y Index: 126

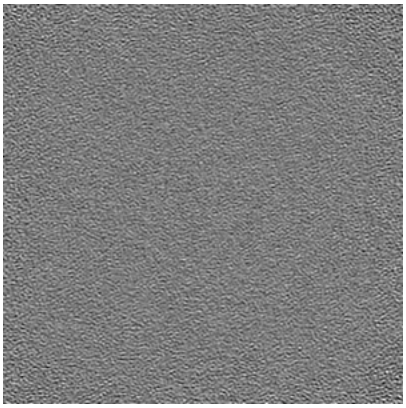


Z Index: 100

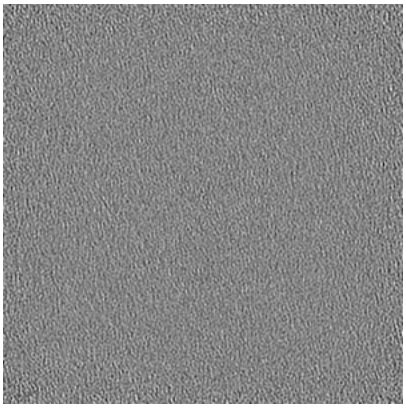
6.3.2 Raw map



X Index: 0



Y Index: 0

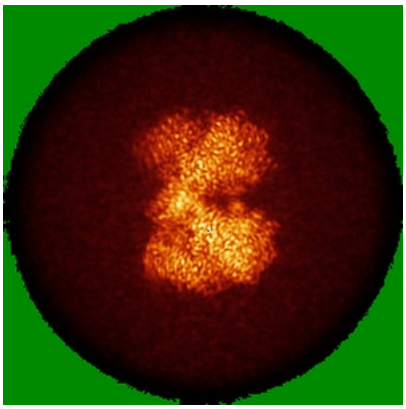


Z Index: 0

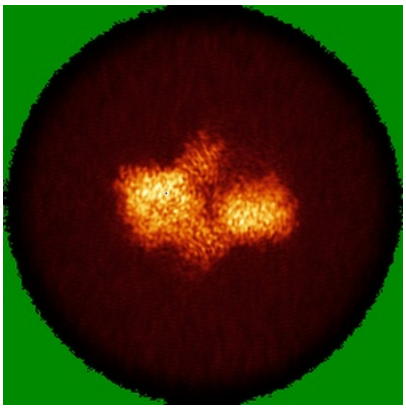
The images above show the largest variance slices of the map in three orthogonal directions.

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

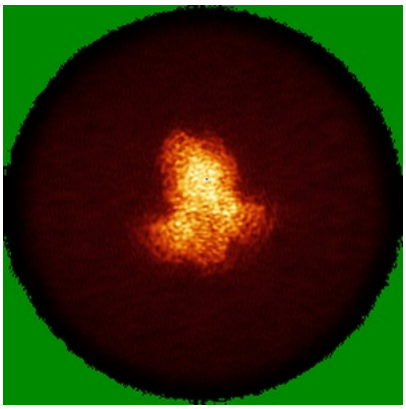
6.4.1 Primary map



X

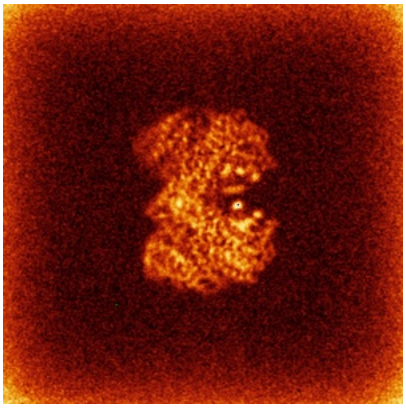


Y

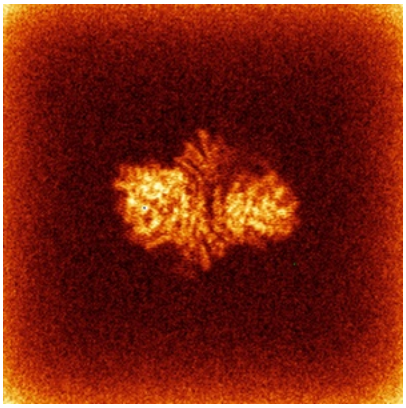


Z

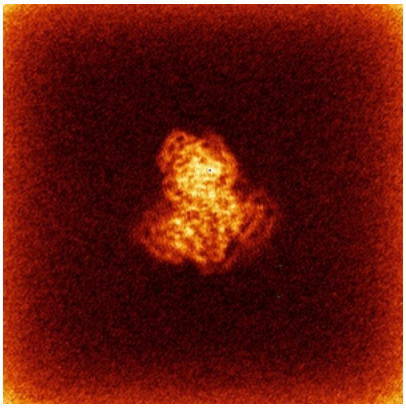
6.4.2 Raw map



X



Y

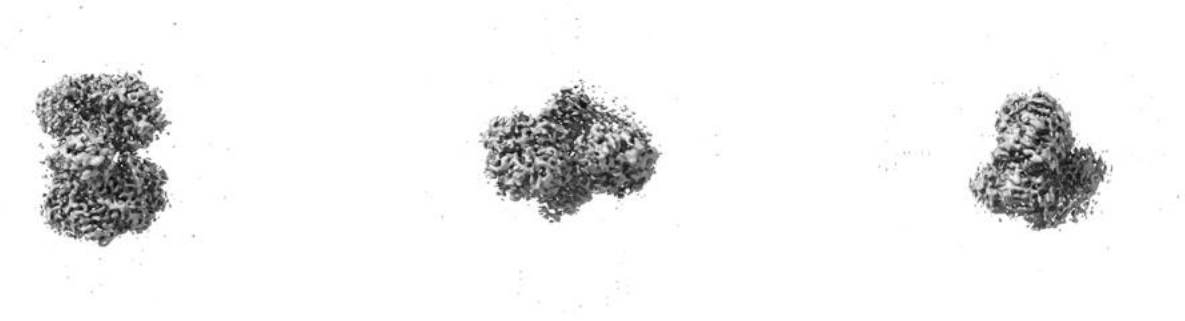


Z

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)

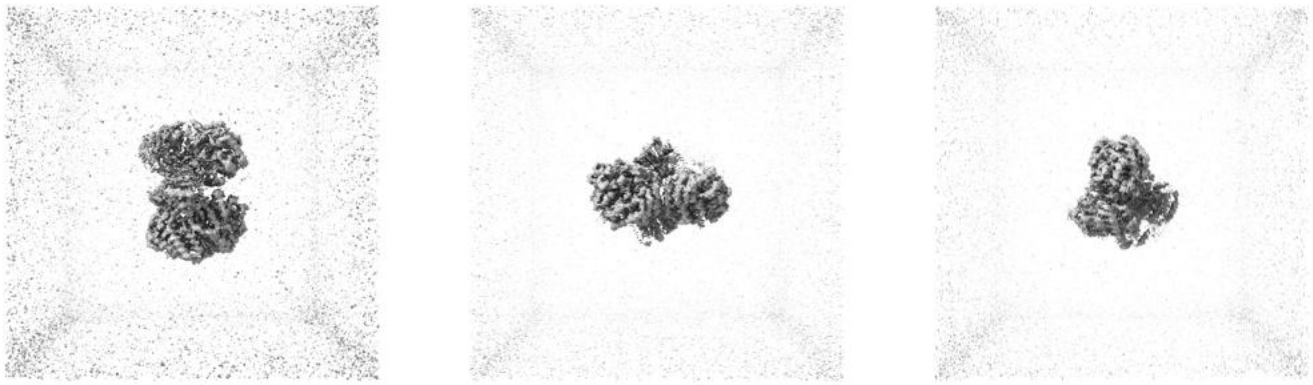
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.128. 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.

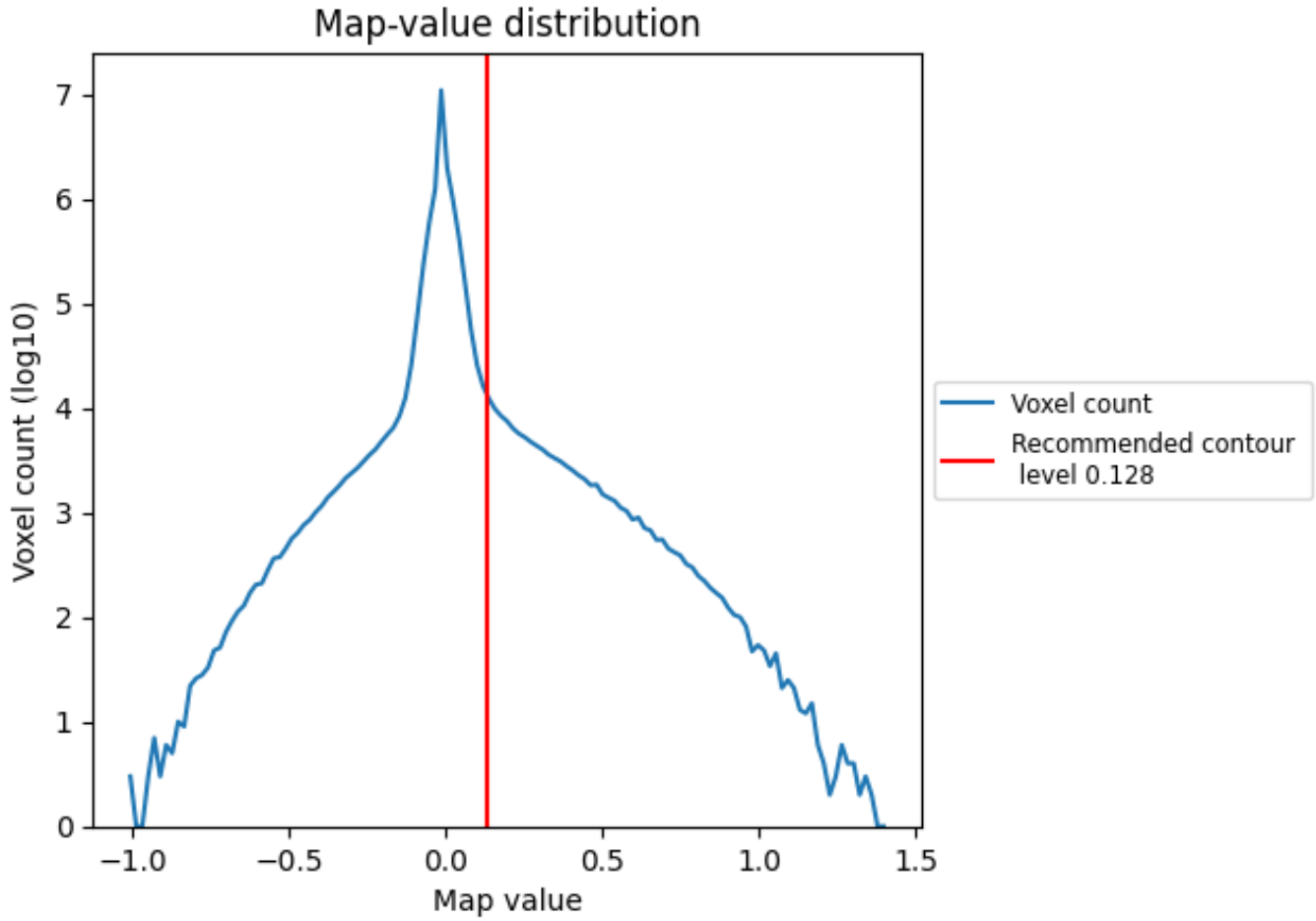
6.6 Mask visualisation (i)

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

7 Map analysis

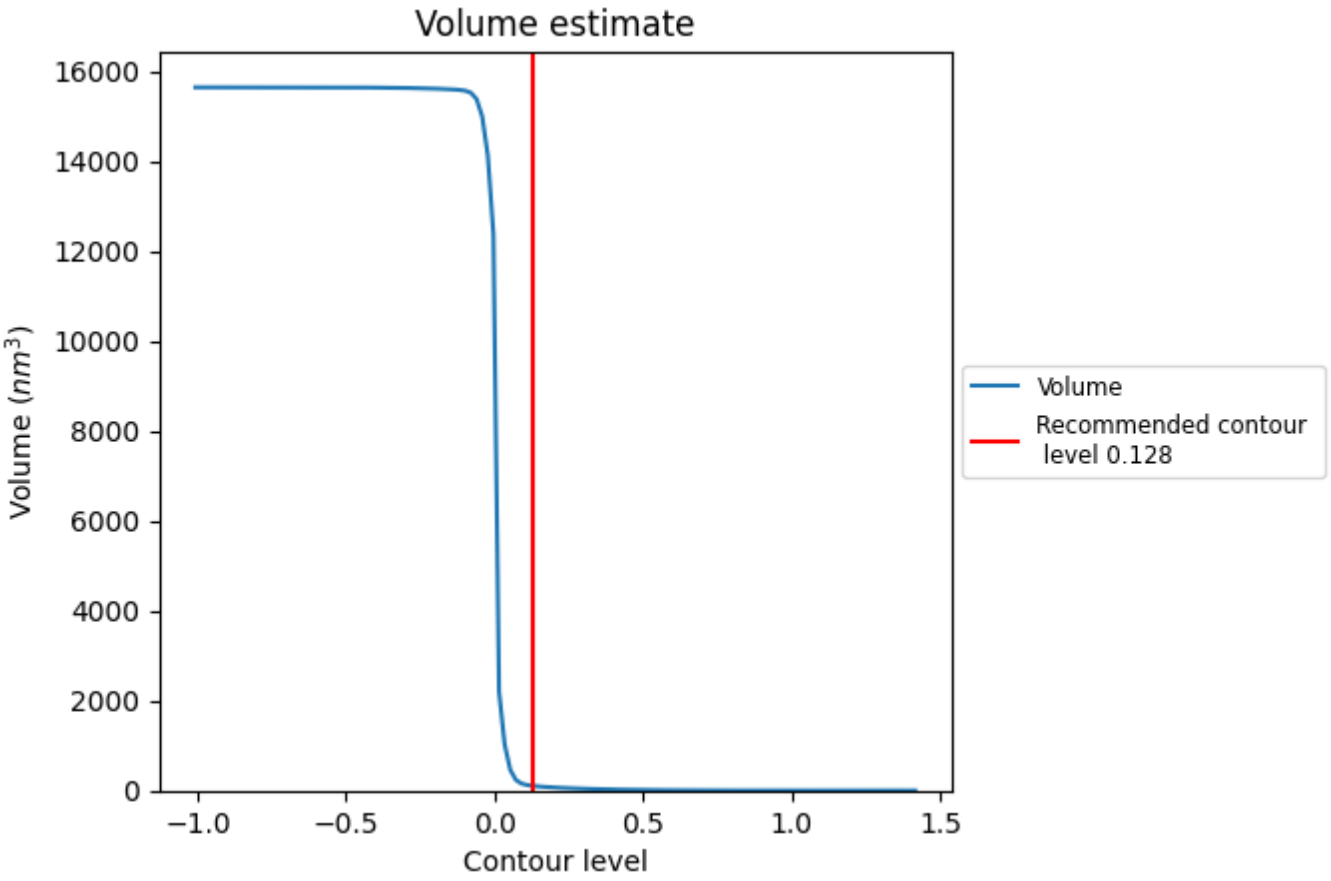
This section contains the results of statistical analysis of the map.

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.

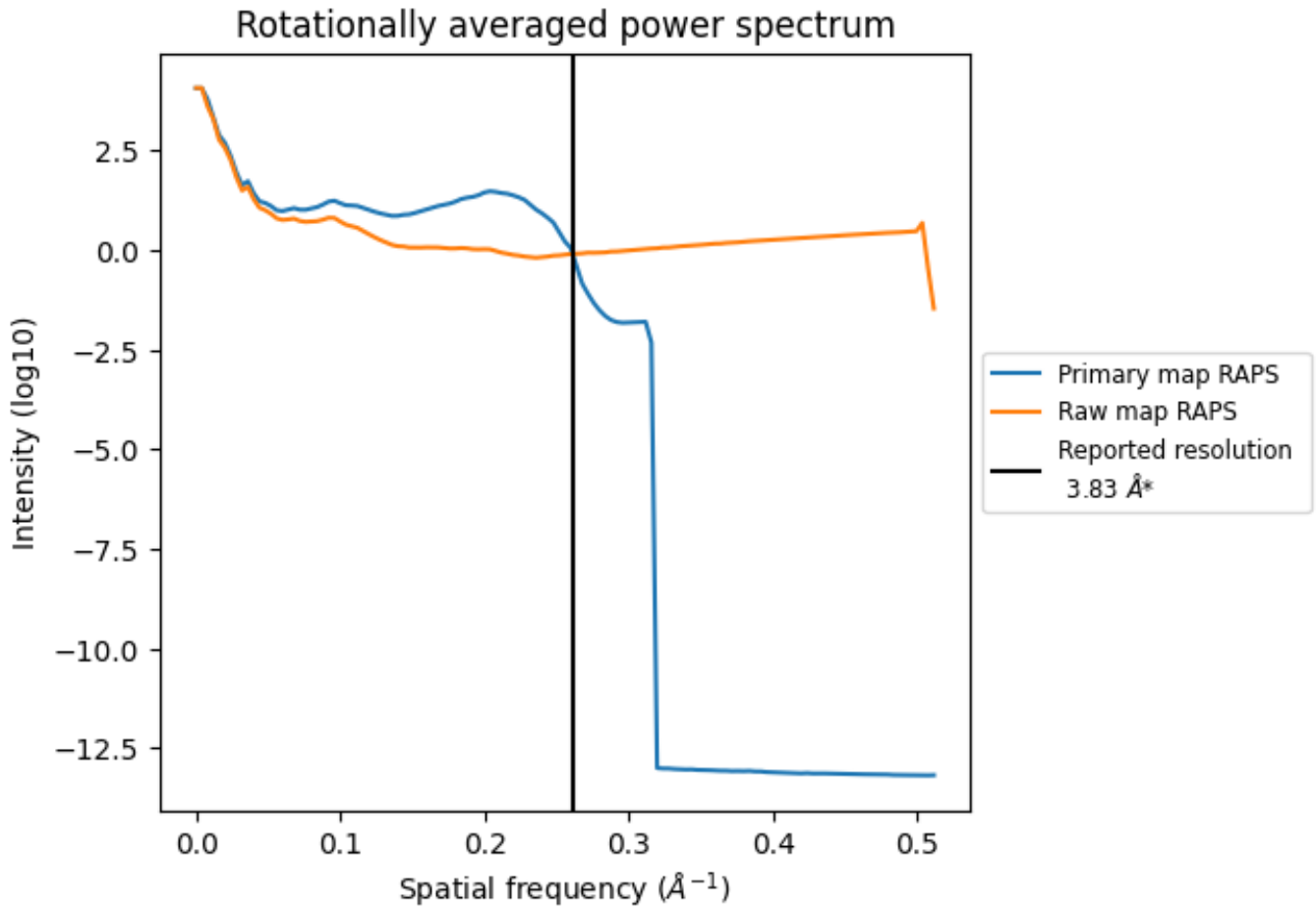
7.2 Volume estimate (i)



The volume at the recommended contour level is 105 nm^3; this corresponds to an approximate mass of 95 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)

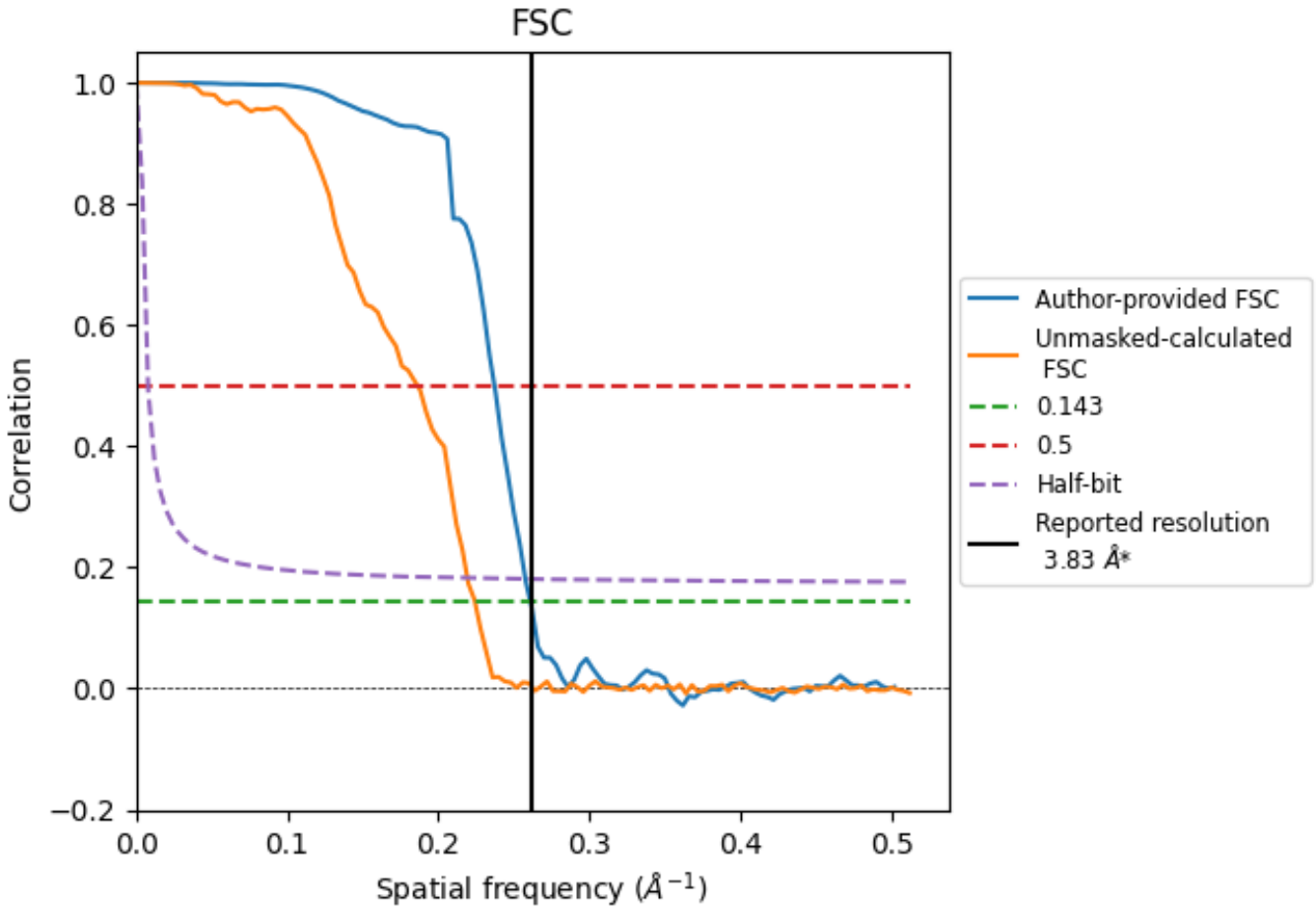


*Reported resolution corresponds to spatial frequency of 0.261 $Å^{-1}$

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 0.261 Å^{-1}

8.2 Resolution estimates (i)

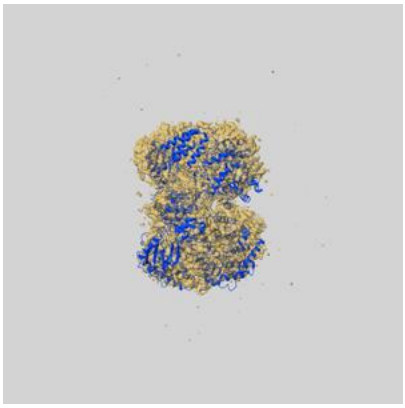
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	3.83	4.22	3.88
Unmasked-calculated*	4.46	5.37	4.56

*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 4.46 differs from the reported value 3.83 by more than 10 %

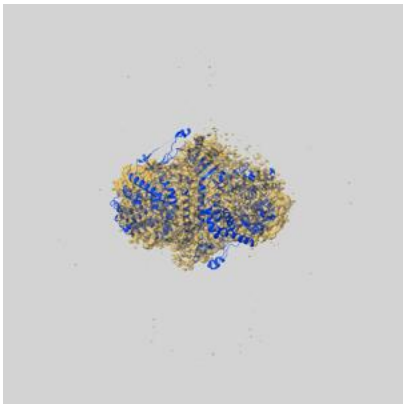
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66568 and PDB model 9X4Z. Per-residue inclusion information can be found in section 3 on page 5.

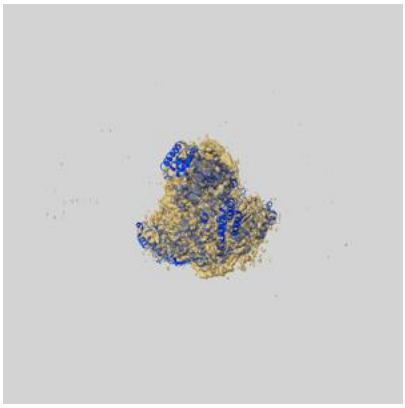
9.1 Map-model overlay



X



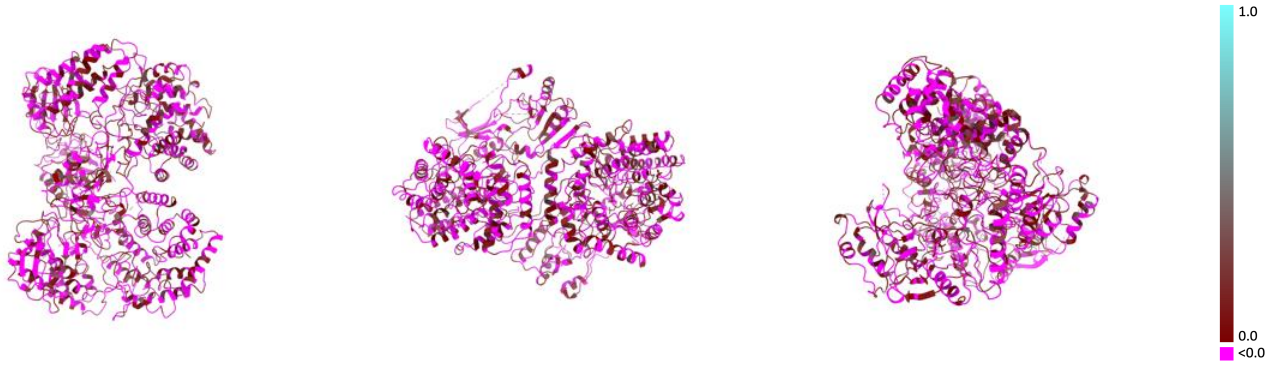
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.128 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.

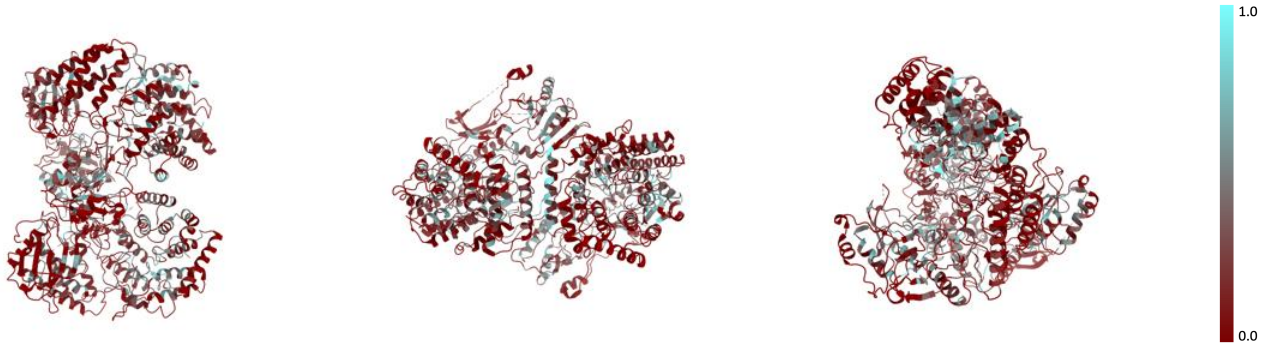
9.2 Q-score mapped to coordinate model (i)



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.

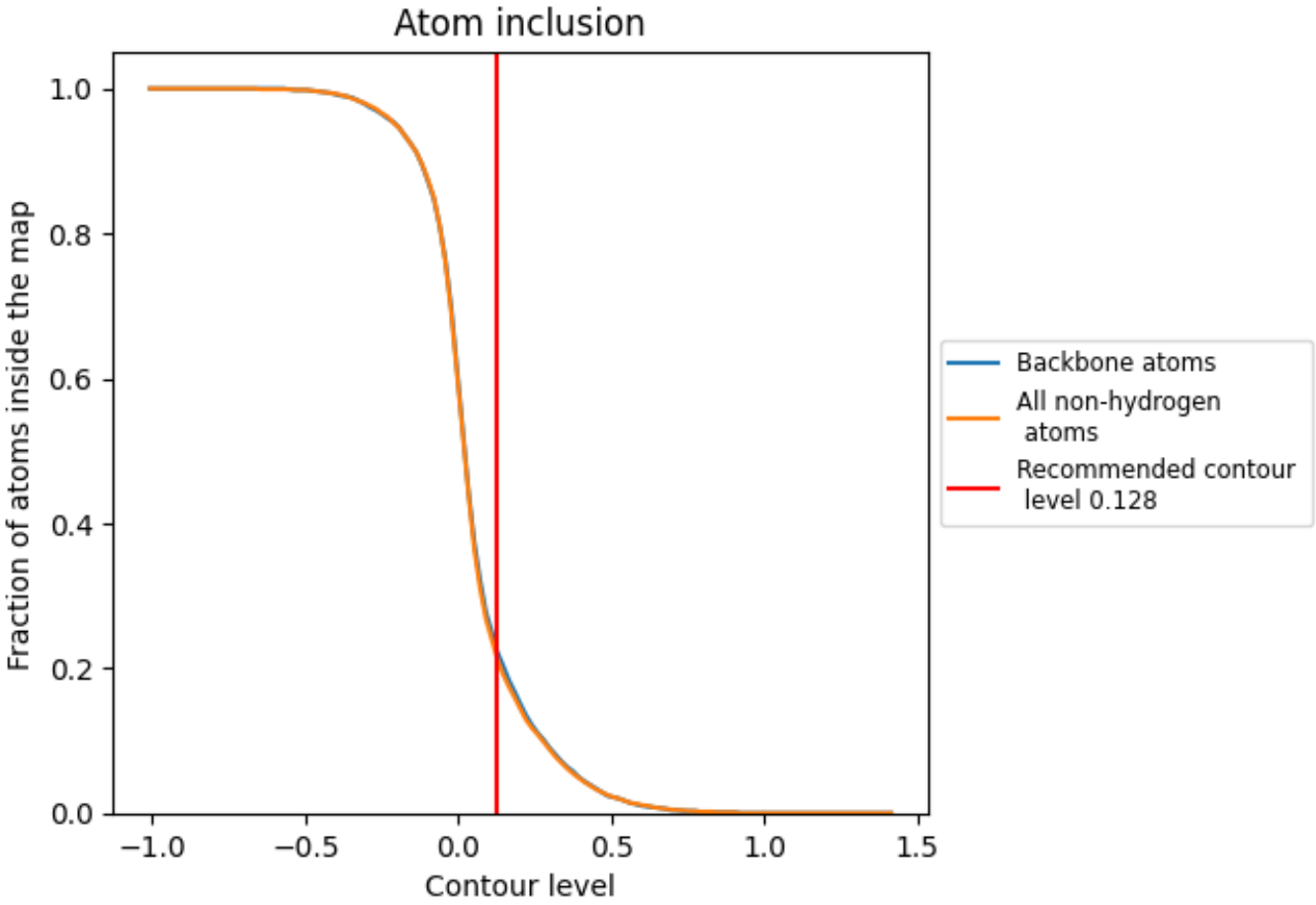
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.128).

9.4 Atom inclusion (i)



At the recommended contour level, 22% of all backbone atoms, 21% 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 (0.128) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.2120	-0.0010
A	0.2130	0.0090
B	0.2110	-0.0120