wwPDB EM Validation Summary Report (i)

Mar 3, 2024 – 08:42 AM EST

PDB ID	:	6BGI
EMDB ID	:	EMD-7095
Title	:	Cryo-EM structure of the TMEM16A calcium-activated chloride channel in nanodisc
Authors	:	Dang, S.; Feng, S.; Tien, J.; Peters, C.J.; Bulkley, D.; Lolicato, M.; Zhao, J.; Zuberbuhler, K.; Ye, W.; Qi, J.; Chen, T.; Craik, C.S.; Jan, Y.N.; Minor Jr., D.L.; Cheng, Y.; Jan, L.Y.
Deposited on	:	2017-10-28
Resolution	:	3.80 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 (i) 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 (i)) were used in the production of this report:

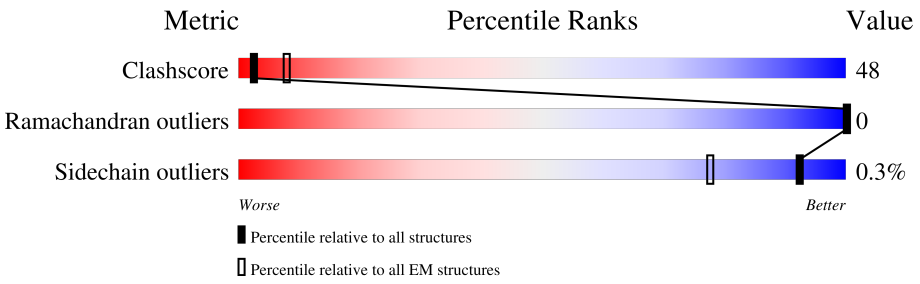
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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 <=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	912	20% 25% 31% 44%
1	B	912	20% 25% 30% 44%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7774 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 Anoctamin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	510	3885	2560	633	667	25	0	0
1	B	510	3885	2560	633	667	25	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	904	SER	-	expression tag	UNP Q8BHY3
A	905	ASN	-	expression tag	UNP Q8BHY3
A	906	SER	-	expression tag	UNP Q8BHY3
A	907	LEU	-	expression tag	UNP Q8BHY3
A	908	GLU	-	expression tag	UNP Q8BHY3
A	909	VAL	-	expression tag	UNP Q8BHY3
A	910	LEU	-	expression tag	UNP Q8BHY3
A	911	PHE	-	expression tag	UNP Q8BHY3
A	912	GLN	-	expression tag	UNP Q8BHY3
B	904	SER	-	expression tag	UNP Q8BHY3
B	905	ASN	-	expression tag	UNP Q8BHY3
B	906	SER	-	expression tag	UNP Q8BHY3
B	907	LEU	-	expression tag	UNP Q8BHY3
B	908	GLU	-	expression tag	UNP Q8BHY3
B	909	VAL	-	expression tag	UNP Q8BHY3
B	910	LEU	-	expression tag	UNP Q8BHY3
B	911	PHE	-	expression tag	UNP Q8BHY3
B	912	GLN	-	expression tag	UNP Q8BHY3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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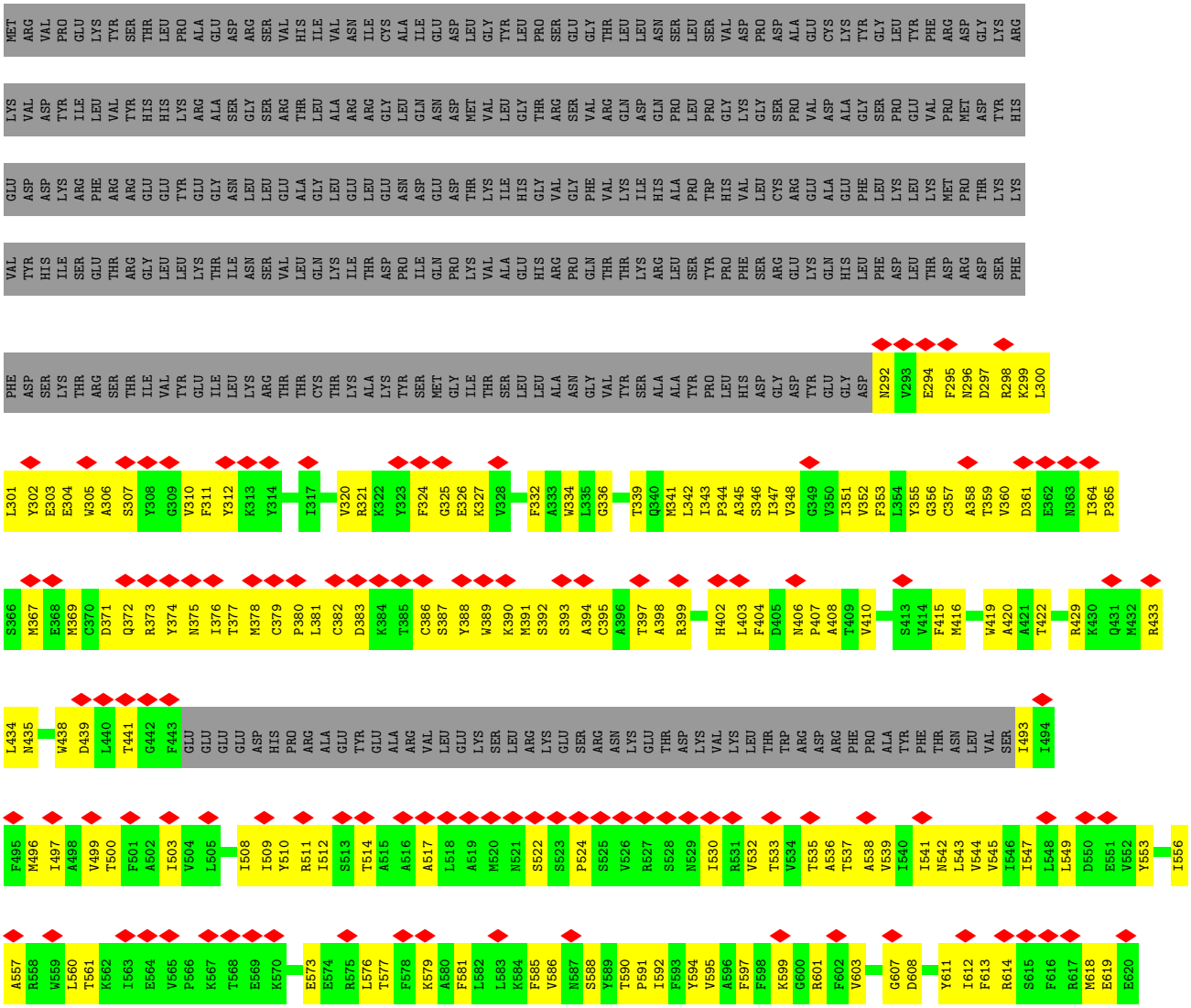
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
2	B	2	2	2	0

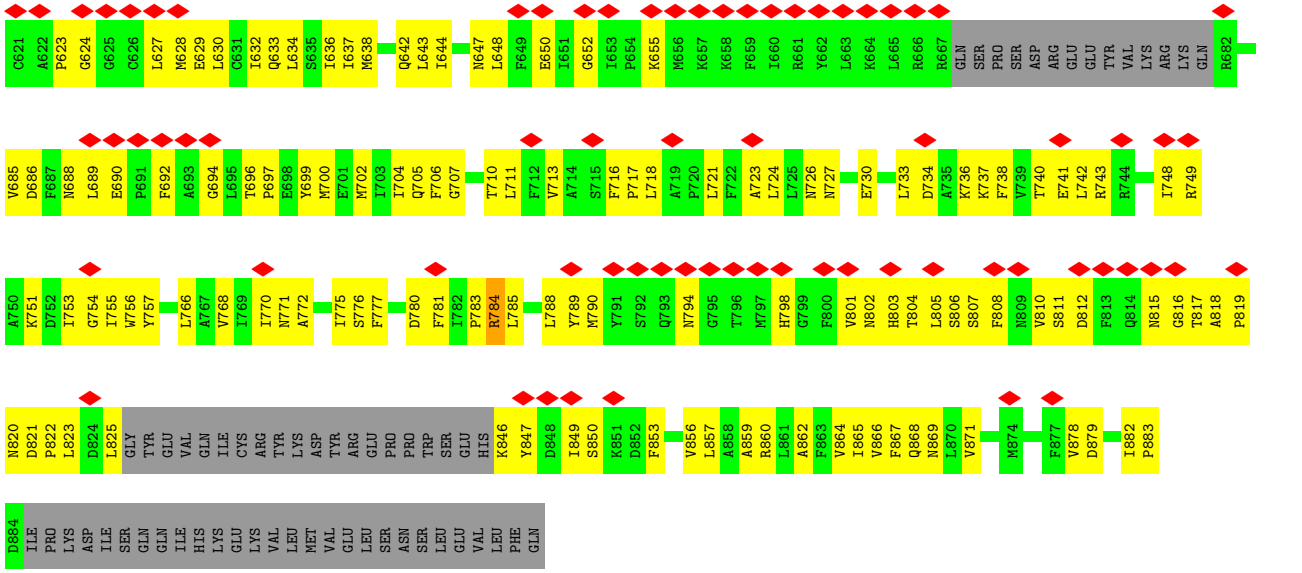
3 Residue-property plots (i)

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: Anoctamin-1

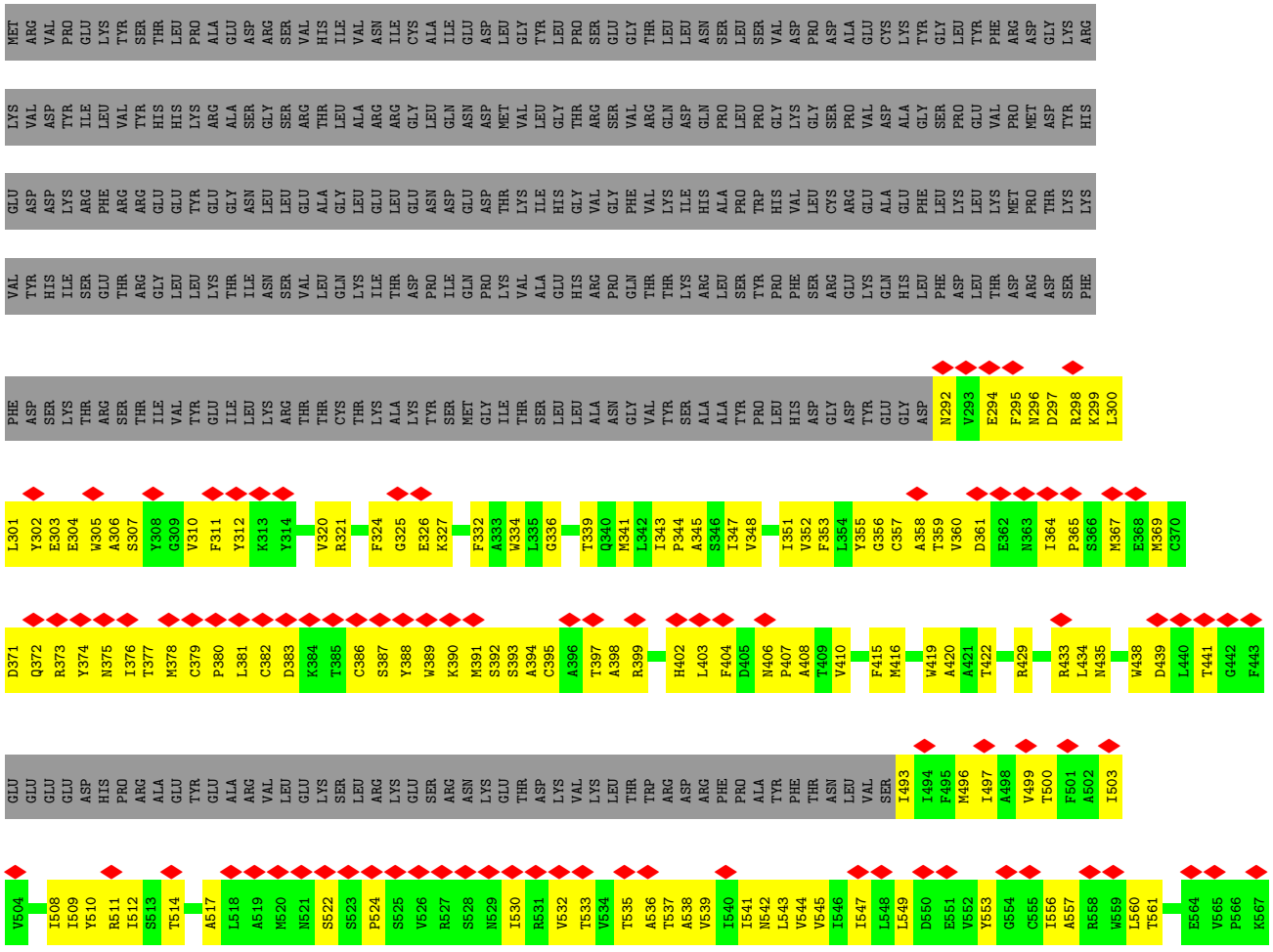
Chain A: 20% 25% 31% 44%

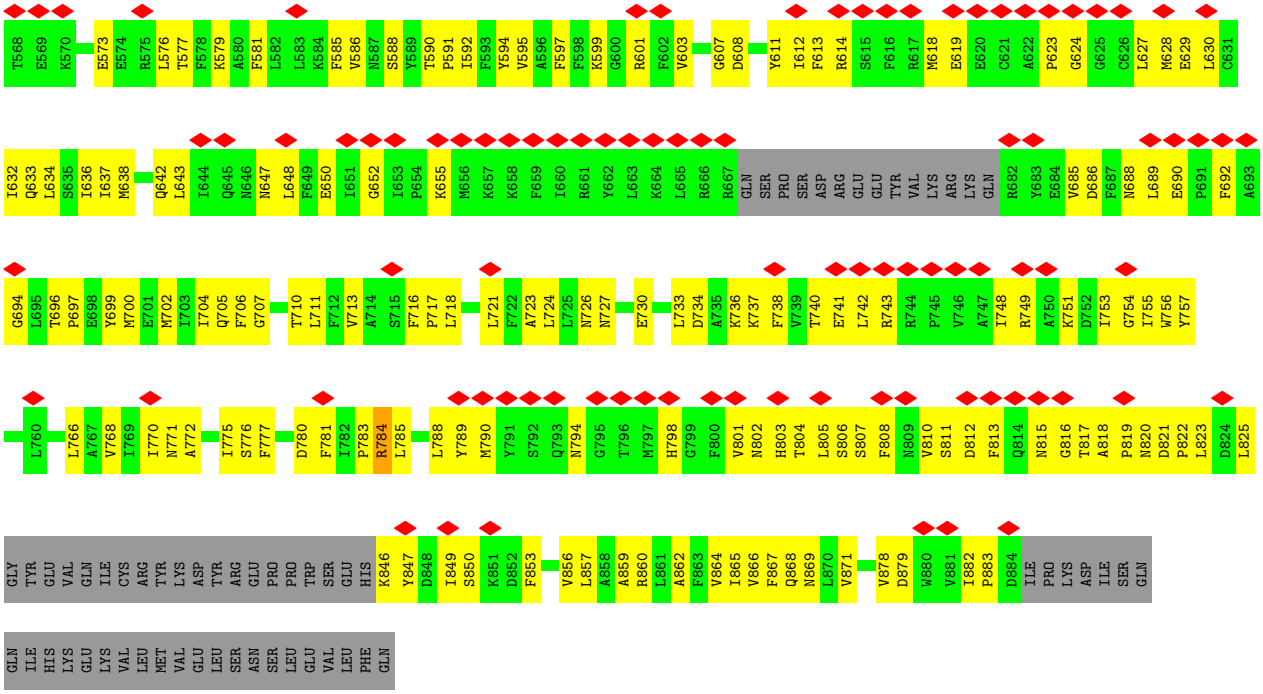




- Molecule 1: Anoctamin-1

Chain B:




T568 E569 K570 E573 E574 R575 L576 T577 F578 K579 A580 F581 L582 L583 K584 F585 V586 N587 S588 Y589 T590 P591 I592 F593 Y594 V595 A596 F597 F598 K599 G600 R601 F602 V603 G607 D608 Y611 I612 F613 R614 S615 F616 R617 M618 E619 E620 C621 A622 P623 G624 G625 C626 L627 M628 E629 L630 C631
I632 Q633 L634 S635 I636 I637 M638 Q642 L643 I644 Q645 N646 N647 L648 F649 E650 I651 G652 I653 F654 K655 M656 K657 K658 F659 I660 R661 Y662 L663 K664 L665 R666 R667 GLN SER PRO SER ASP ARG GLU GLU TYR VAL LYS ARG LYS GLN R682 Y683 E684 V685 D686 F687 N688 L689 E690 P691 F692 A693
G694 L695 T696 P697 E698 Y699 M700 E701 M702 I703 I704 Q705 F706 G707 T710 L711 F712 V713 A714 S715 F716 P717 L718 L721 F722 A723 L724 L725 N726 N727 E730 L733 D734 A735 K736 K737 F738 V739 T740 E741 L742 R743 R744 P745 V746 A747 I748 R749 A750 K751 D752 I753 G754 I755 W756 Y757
L760 L766 A767 V768 I769 I770 N771 A772 I775 S776 F777 D780 F781 I782 P783 R784 L785 L788 Y789 M790 Y791 S792 Q793 N794 G795 T796 M797 H798 G799 F800 V801 N802 H803 T804 L805 S806 S807 F808 N809 V810 S811 D812 F813 Q814 N815 G816 T817 A818 P819 N820 D821 P822 L823 D824 L825
GLY TYR GLU VAL GLN ILE CYS ARG TYR LYS ASP TYR ARG GLU PRO PRO TRP SER GLU HIS K846 Y847 D848 I849 S850 K851 D852 F853 V856 L857 A858 A859 R860 L861 A862 F863 V864 I865 V866 F867 Q868 N869 L870 V871 V878 D879 W880 V881 I882 P883 D884 ILE PRO LYS ASP ILE SER GLN
GLN ILE HIS LYS GLU LYS VAL LEU MET VAL GLU LEU SER ASN SER LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	251851	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	26.889	Depositor
Minimum map value	-20.315	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.0	Depositor
Map size (Å)	261.12, 261.12, 261.12	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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

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	0.41	0/3982	0.52	0/5418
1	B	0.41	0/3982	0.52	0/5418
All	All	0.41	0/7964	0.52	0/10836

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	3885	0	3740	363	0
1	B	3885	0	3740	369	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
All	All	7774	0	7480	727	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 48.

The worst 5 of 727 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:378:MET:HB2	1:B:391:MET:HG2	1.38	1.02
1:A:378:MET:HB2	1:A:391:MET:HG2	1.38	1.01
1:B:410:VAL:HA	1:B:775:ILE:HD11	1.45	0.99
1:B:298:ARG:HA	1:B:301:LEU:HB2	1.45	0.97
1:A:410:VAL:HA	1:A:775:ILE:HD11	1.45	0.97

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	502/912 (55%)	421 (84%)	81 (16%)	0	100	100
1	B	502/912 (55%)	421 (84%)	81 (16%)	0	100	100
All	All	1004/1824 (55%)	842 (84%)	162 (16%)	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	382/812 (47%)	381 (100%)	1 (0%)	92	96
1	B	382/812 (47%)	381 (100%)	1 (0%)	92	96
All	All	764/1624 (47%)	762 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	784	ARG
1	B	784	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	798	HIS
1	B	868	GLN
1	A	869	ASN
1	B	375	ASN
1	B	431	GLN

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)

Of 4 ligands modelled in this entry, 4 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.

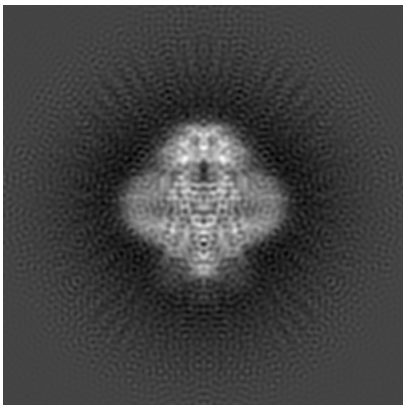
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7095. 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



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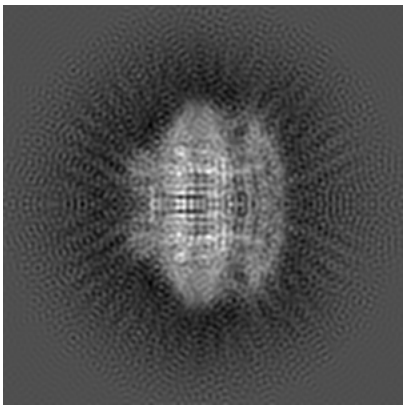
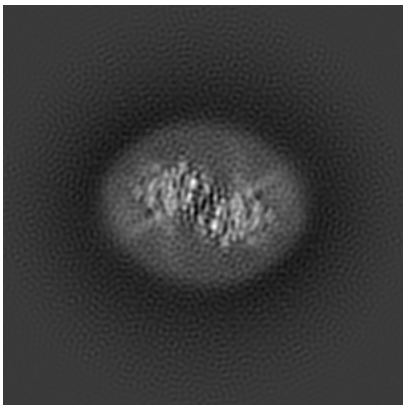
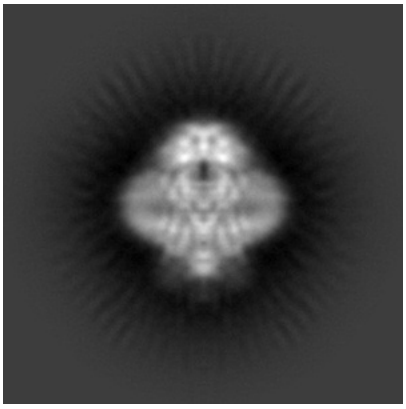


Y



Z

6.1.2 Raw map



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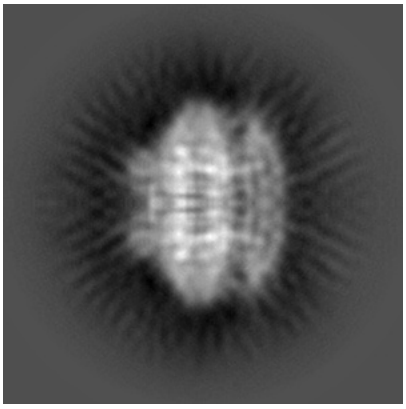
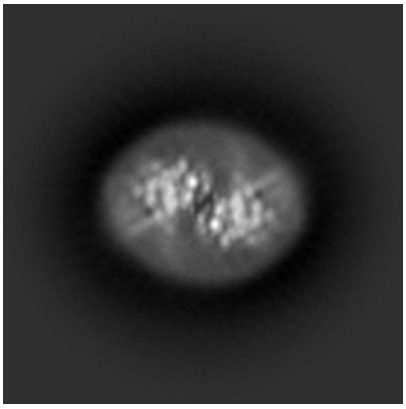


Y

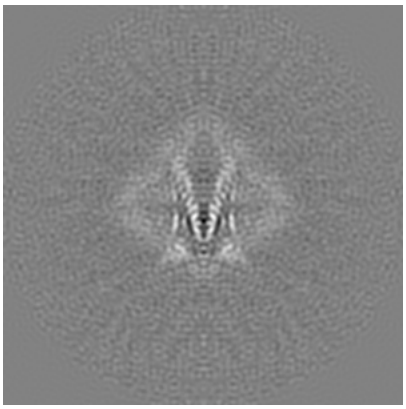


Z

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

6.2 Central slices (i)

6.2.1 Primary map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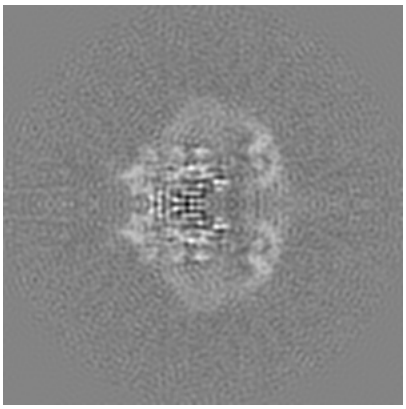
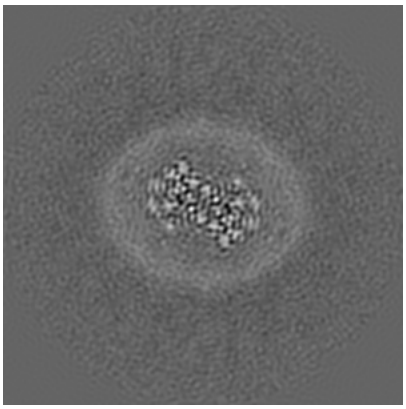
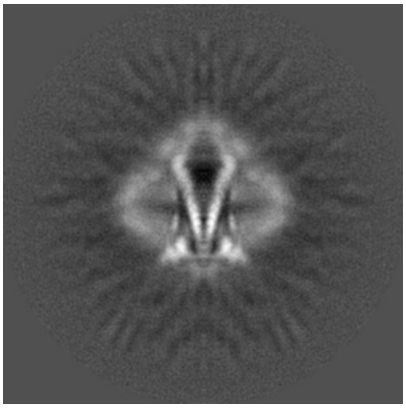

Y Index: 128


Z Index: 128

6.2.2 Raw map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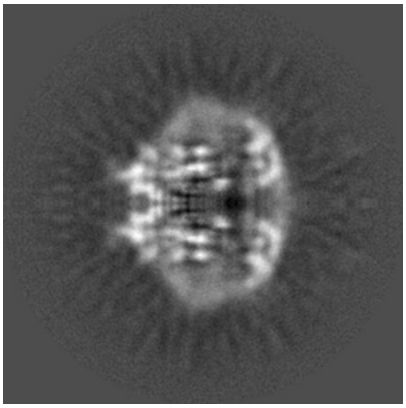
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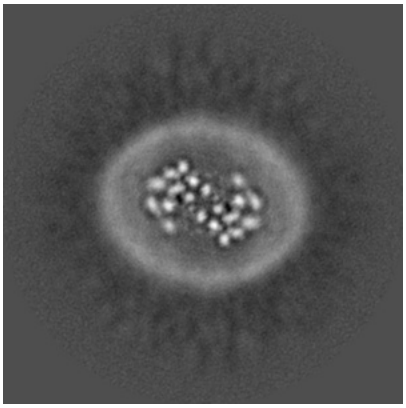
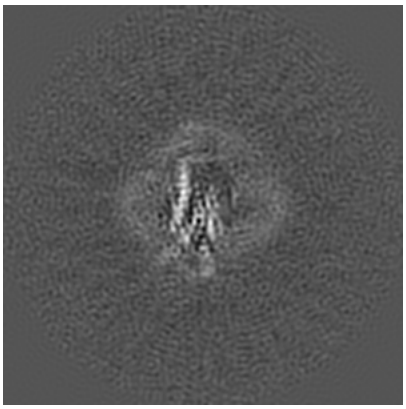

Z Index: 128

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

6.3 Largest variance slices (i)

6.3.1 Primary map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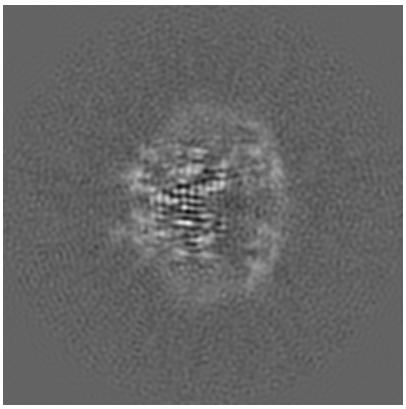
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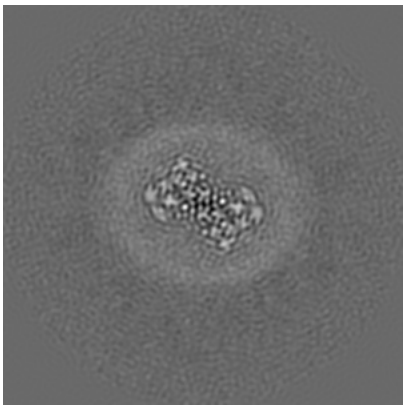
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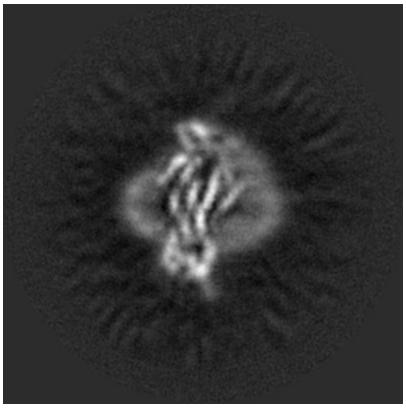
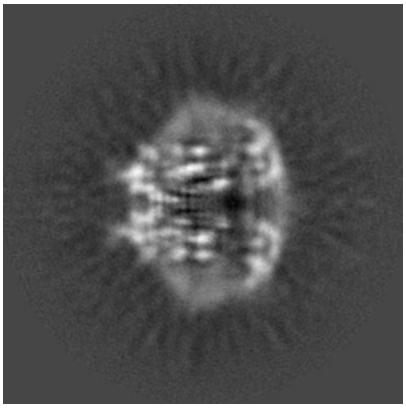
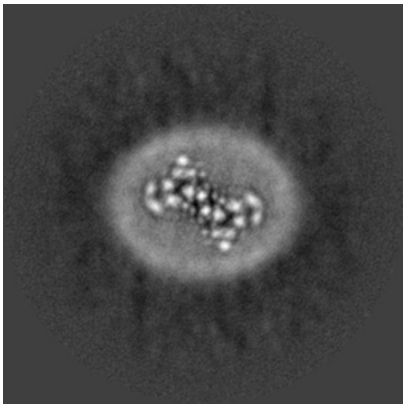
6.3.2 Raw map


X Index: 149

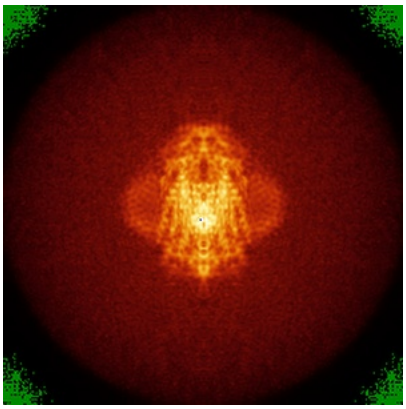

Y Index: 127


Z Index: 113

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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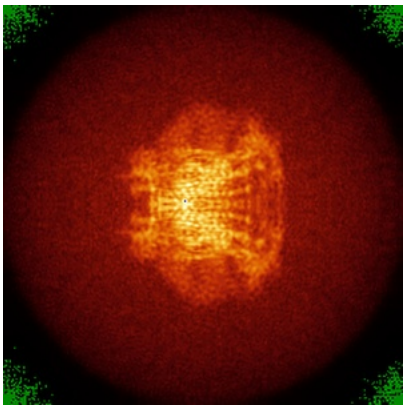
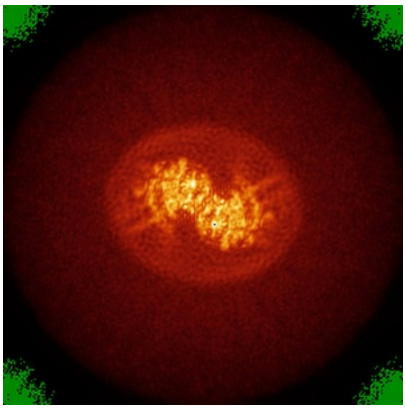
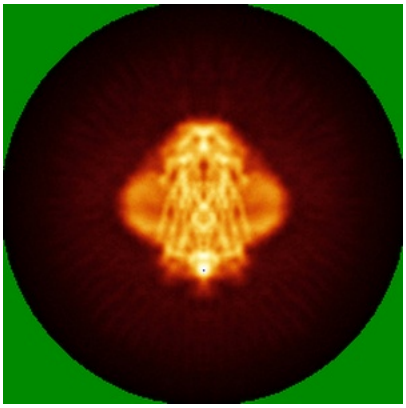
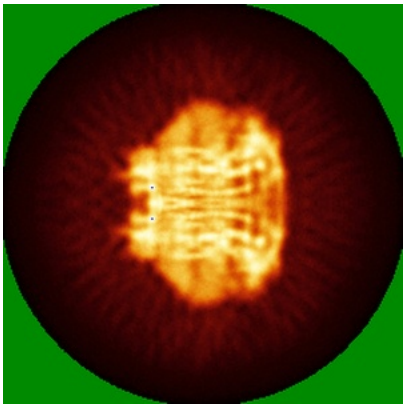
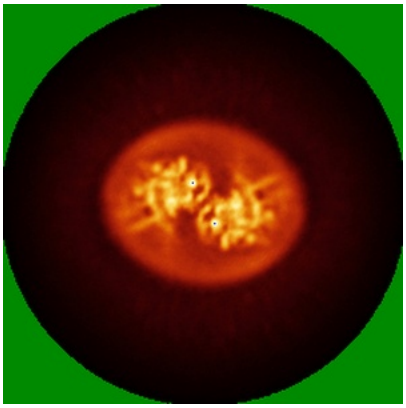

Y


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.

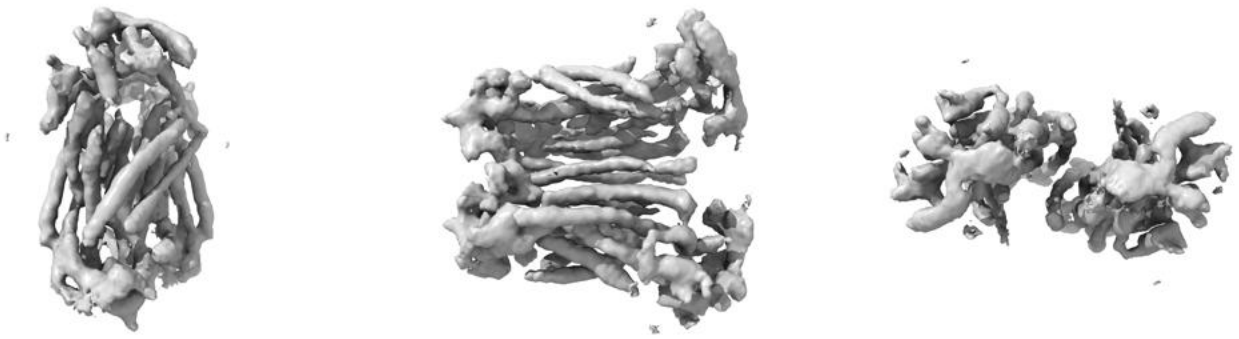
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. 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.

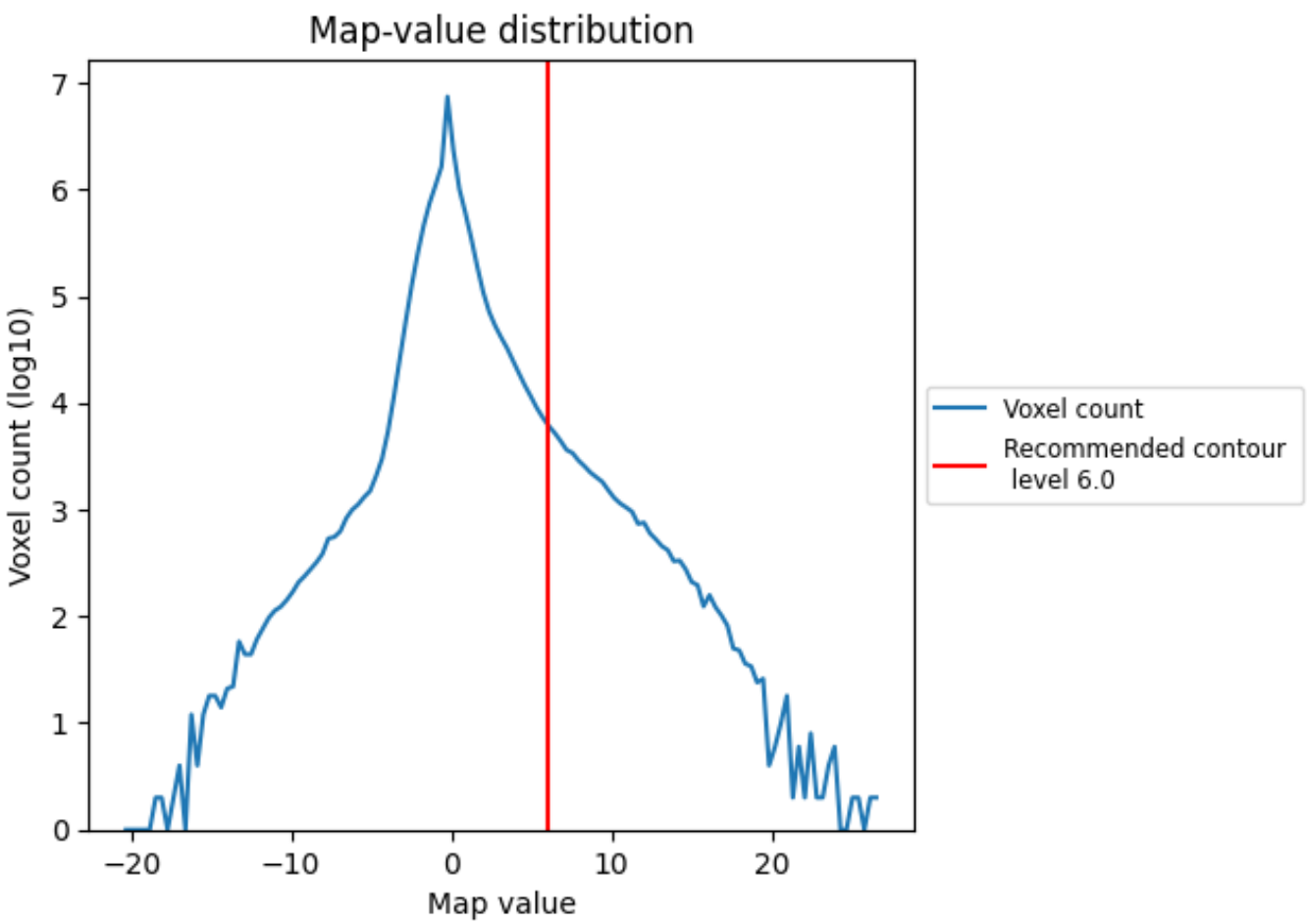
6.6 Mask visualisation (i)

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

7 Map analysis (i)

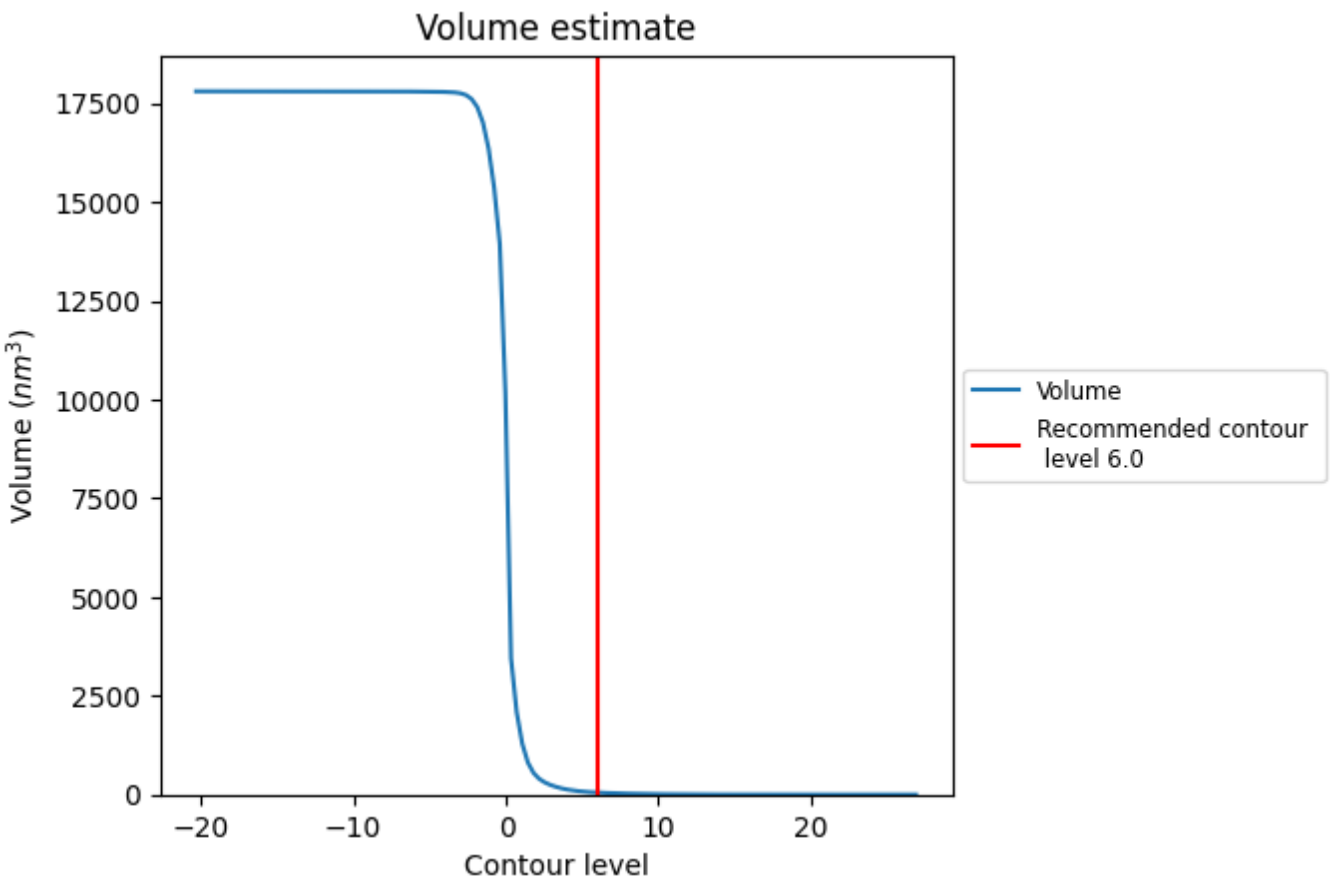
This section contains the results of statistical analysis of the map.

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.

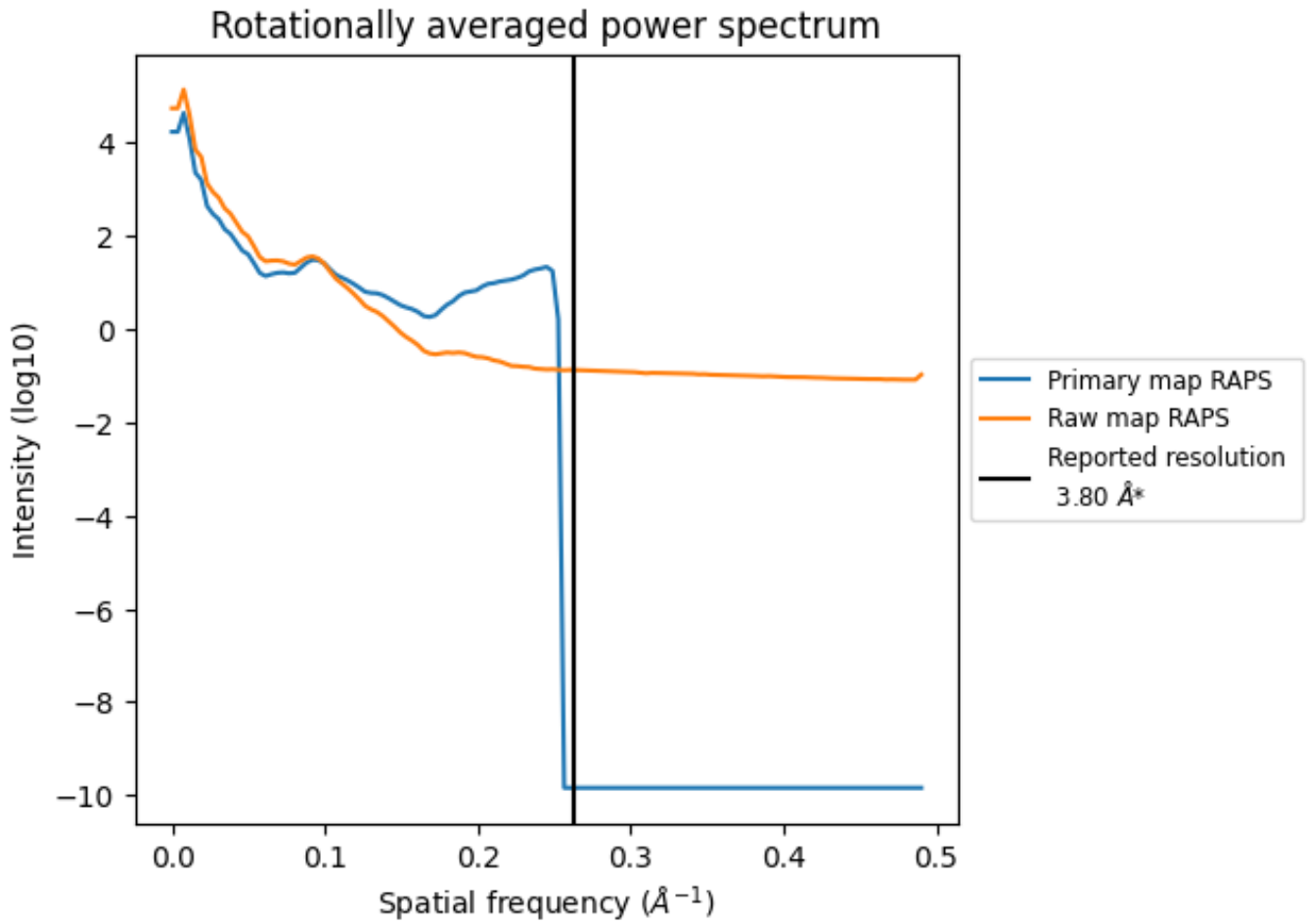
7.2 Volume estimate (i)



The volume at the recommended contour level is 50 nm^3; this corresponds to an approximate mass of 45 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)

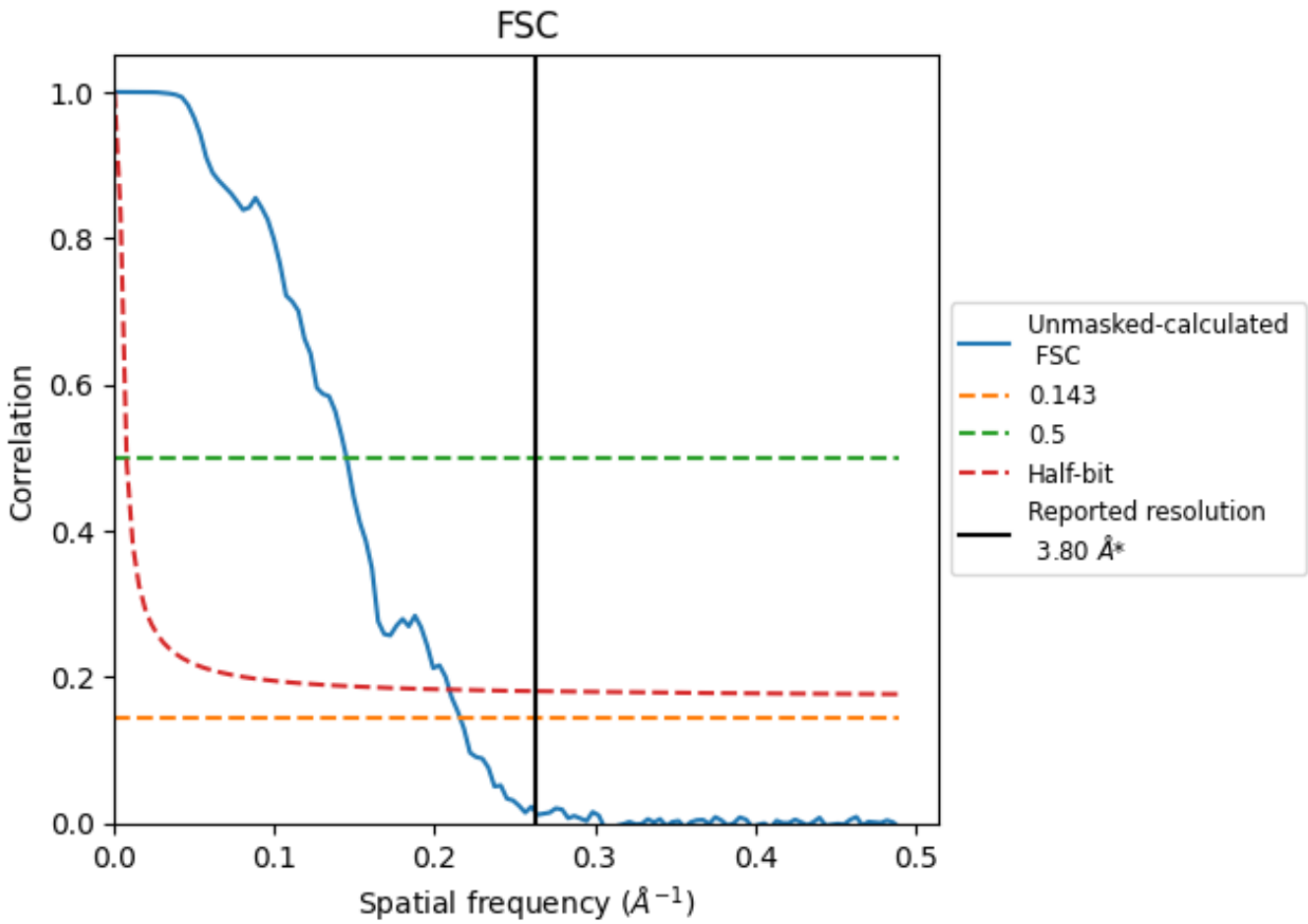


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

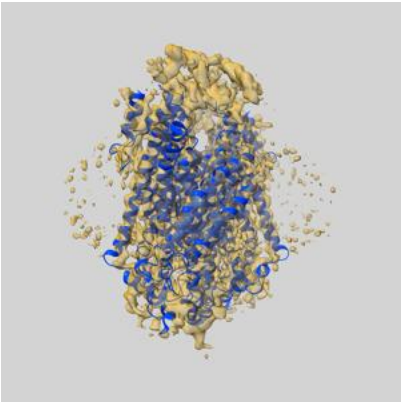
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.63	6.90	4.78

*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 4.63 differs from the reported value 3.8 by more than 10 %

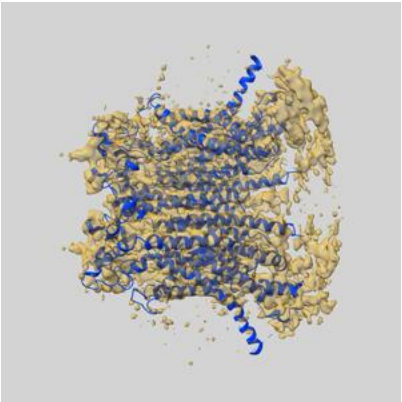
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7095 and PDB model 6BGI. Per-residue inclusion information can be found in section 3 on page 5.

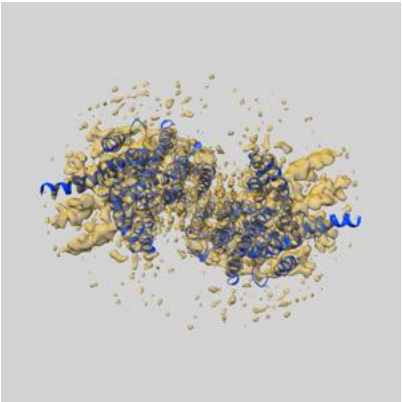
9.1 Map-model overlay (i)



X



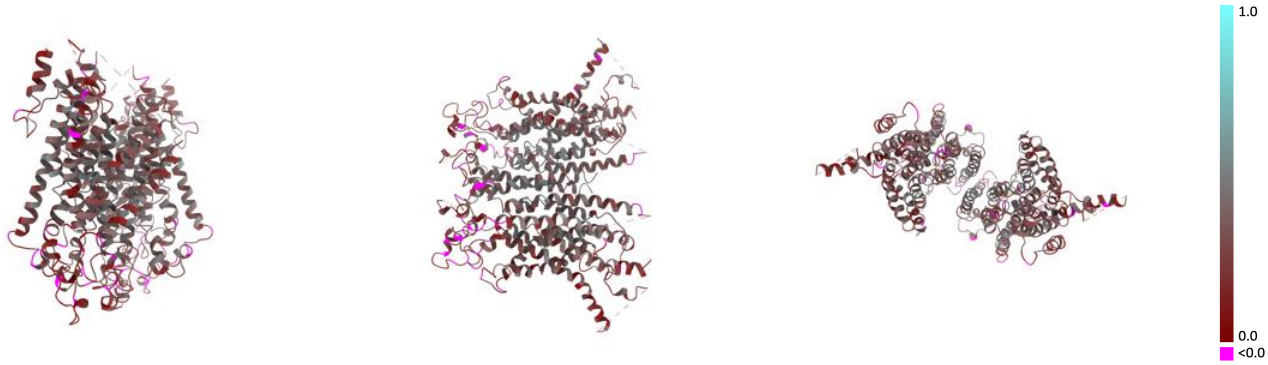
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0 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.

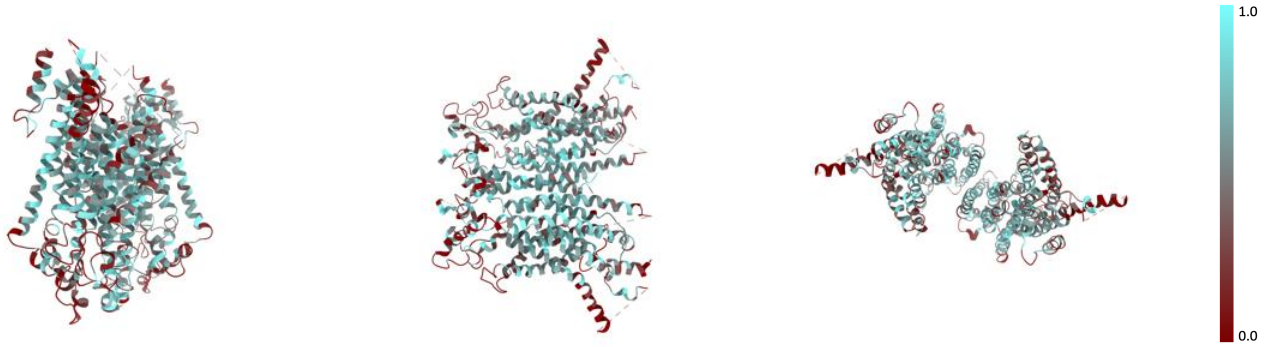
9.2 Q-score mapped to coordinate model (i)



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.

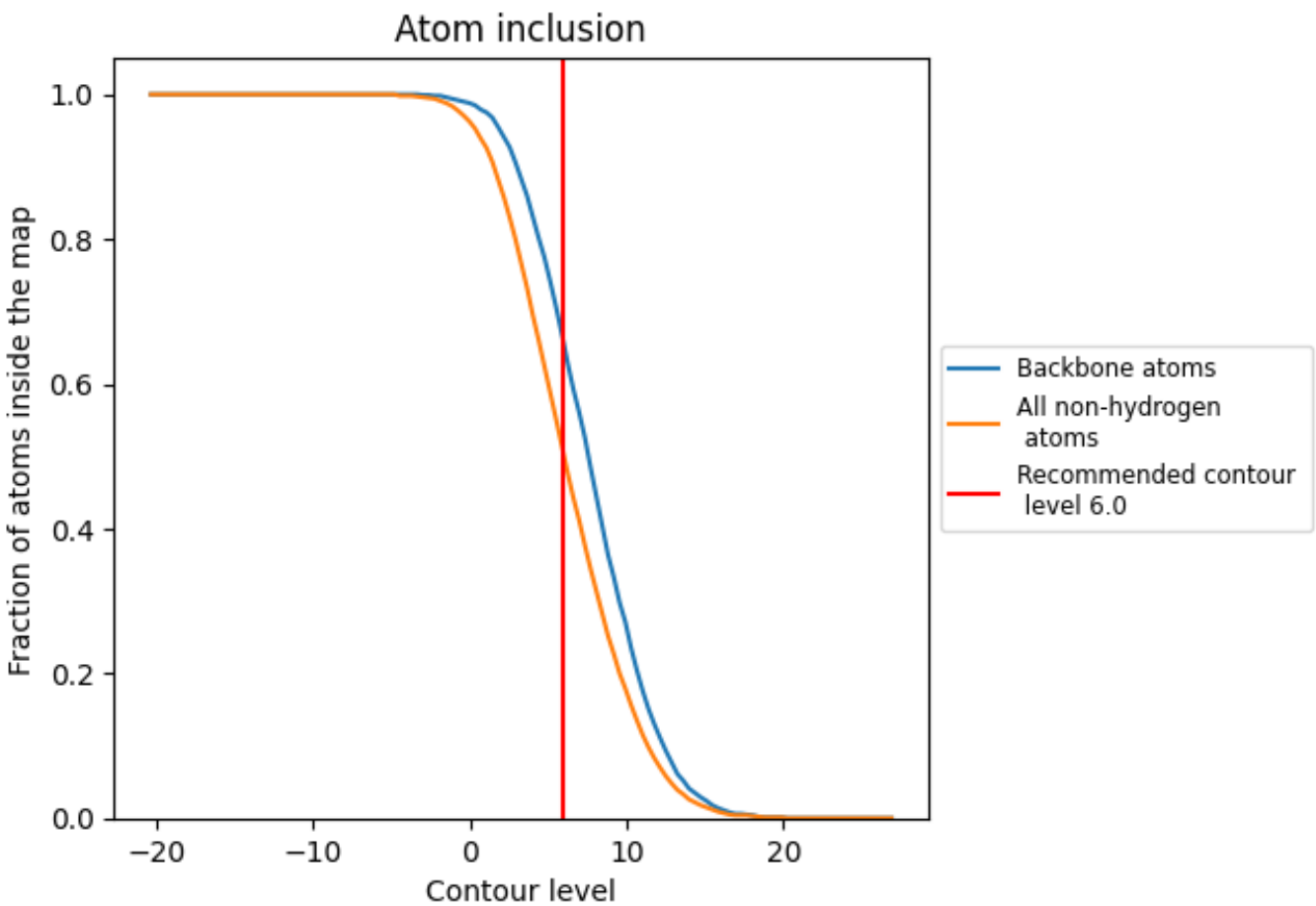
9.3 Atom inclusion mapped to coordinate model (i)



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 (6.0).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 50% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5020	0.2930
A	0.5000	0.2890
B	0.5040	0.2970