wwPDB EM Validation Summary Report

Oct 19, 2026 – 02:21 PM JST

PDB ID	:	24UO / pdb_000024uo
EMDB ID	:	EMD-69828
Title	:	Cryo-EM structure of AcrB in liposomes incubated with doxorubicin (class2-out)
Authors	:	Akisada, S.; Yokoyama, K.
Deposited on	:	2026-03-21
Resolution	:	3.75 Å(reported)
Based on initial model	:	4DX7

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:

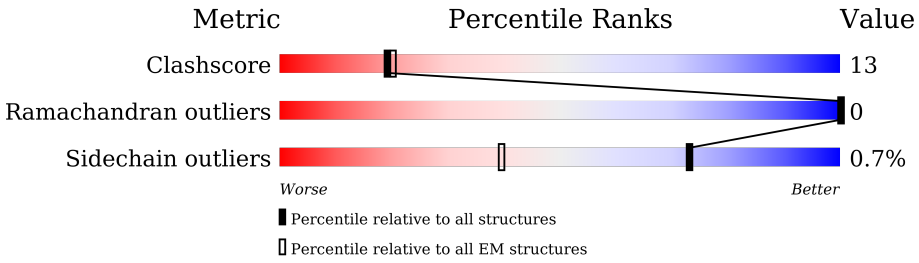
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

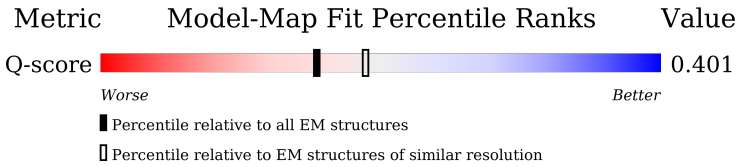
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.75 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	10301 (3.25 - 4.25)

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	1049	11% 74% 24%
1	B	1049	8% 74% 24%
1	C	1049	8% 72% 26%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23565 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 Multidrug efflux pump subunit AcrB.

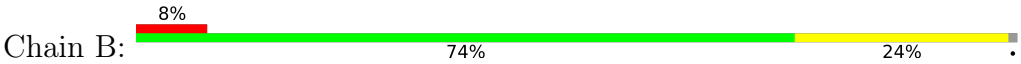
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1034	Total	C	N	O	S	0	0
			7855	5055	1296	1460	44		
1	C	1034	Total	C	N	O	S	0	0
			7855	5055	1296	1460	44		
1	A	1034	Total	C	N	O	S	0	0
			7855	5055	1296	1460	44		

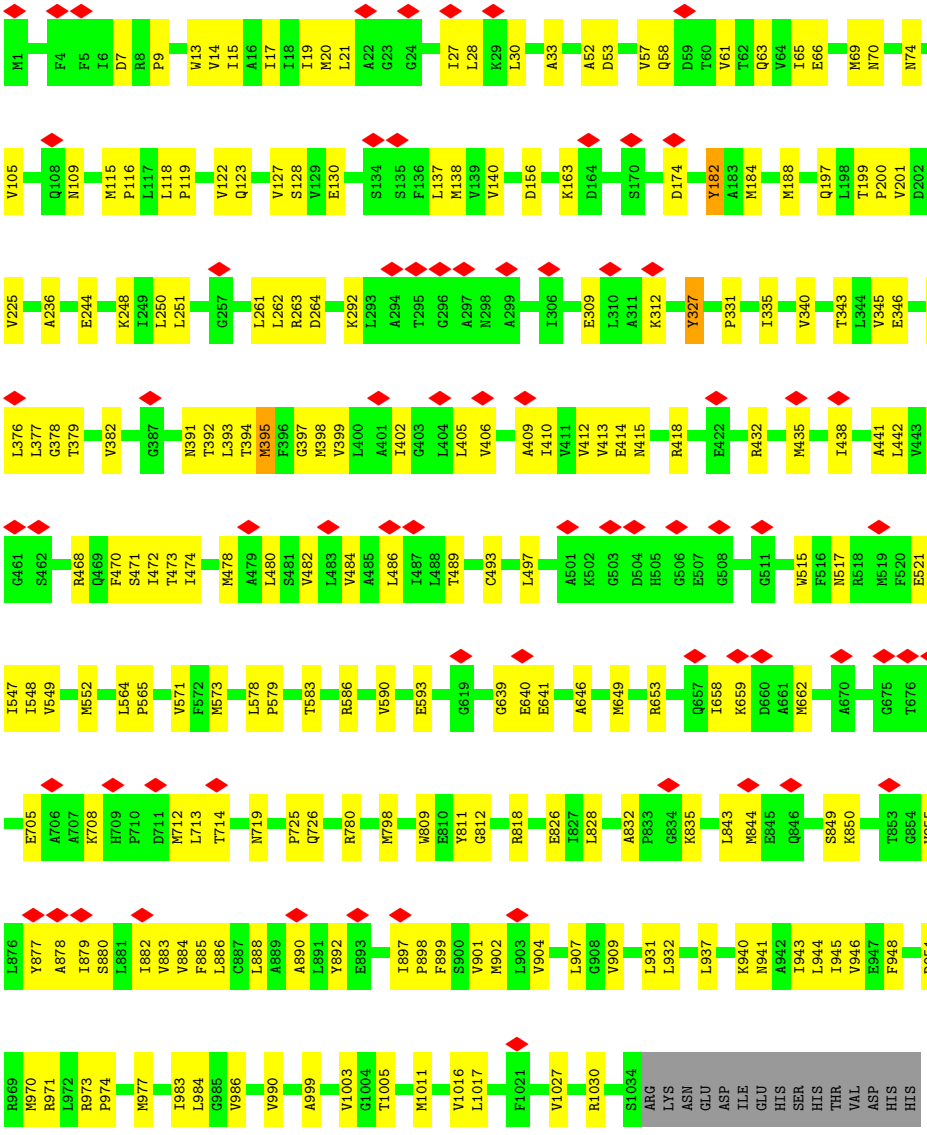
3 Residue-property plots (i)

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: Multidrug efflux pump subunit AcrB

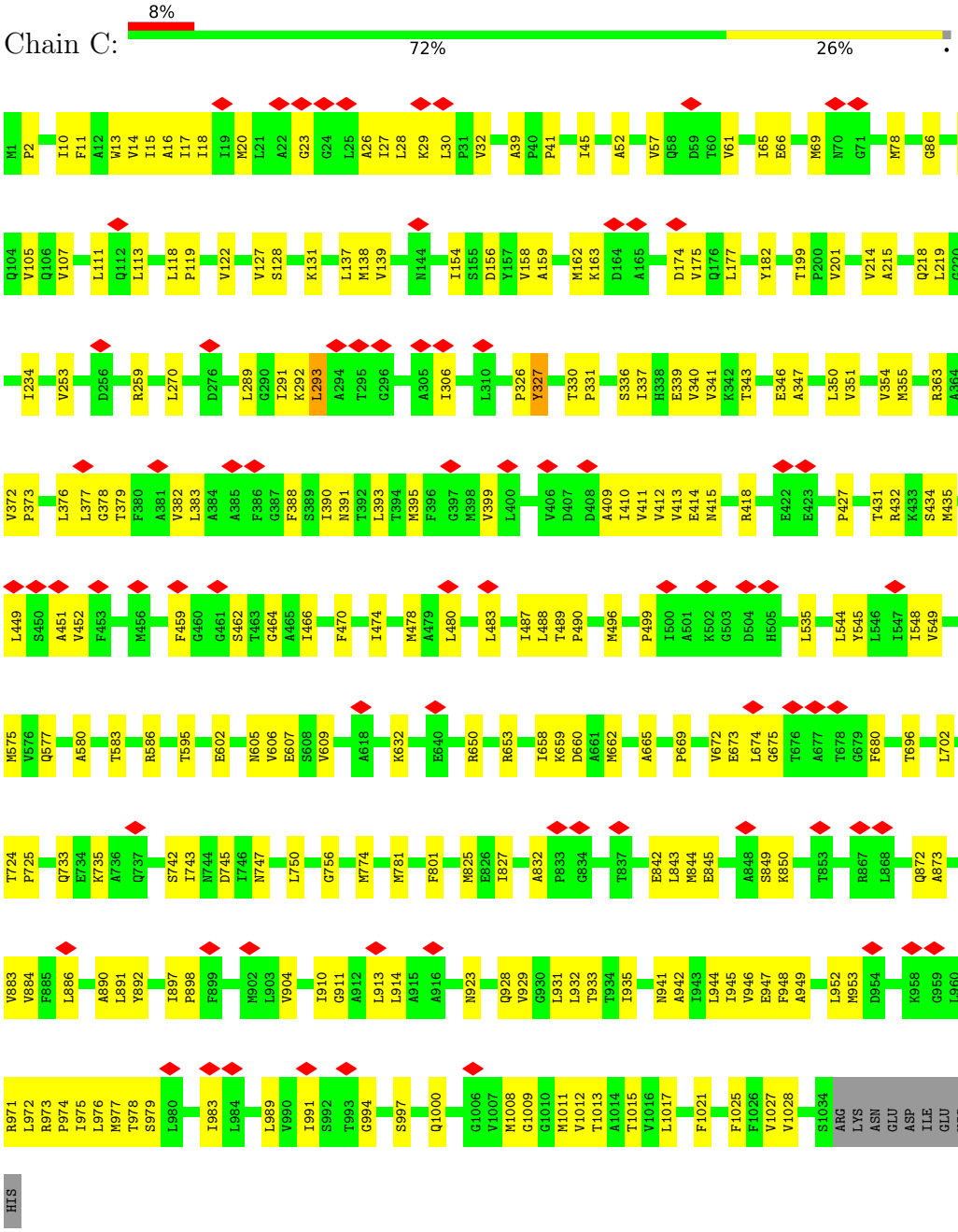
Chain B:





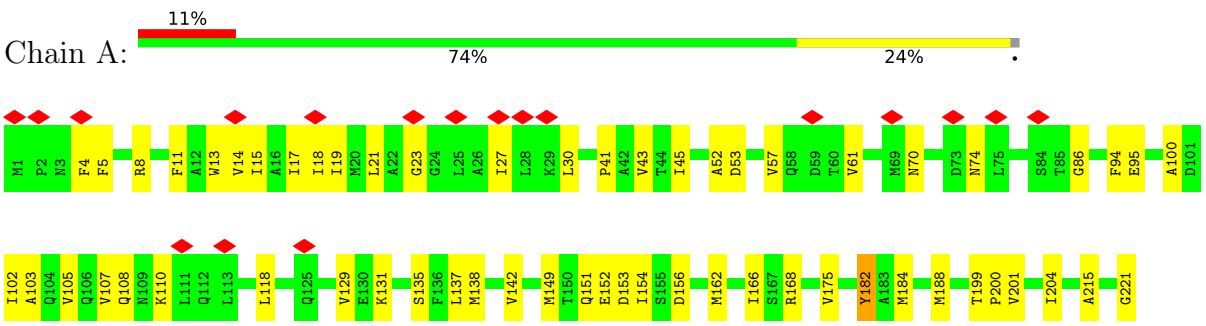
• Molecule 1: Multidrug efflux pump subunit AcrB

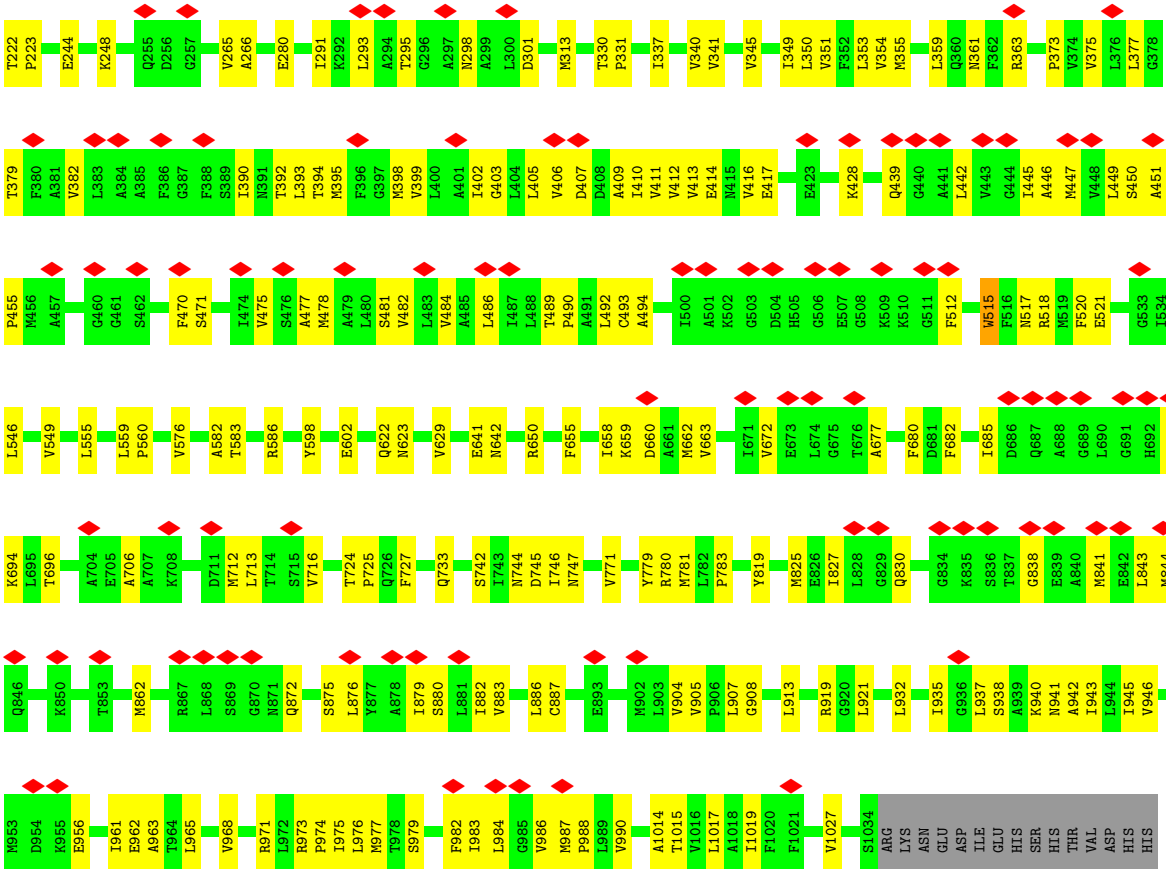
Chain C:



• Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:




T222 P223 E244 K248 Q255 D256 G257 V265 A266 E280 I291 K292 L293 A294 T295 G296 A297 N298 A299 L300 D301 M313 T330 P331 I337 V340 V341 V345 I349 L350 V351 F352 L353 V354 M355 L359 Q360 N361 F362 R363 P373 V374 V375 L376 L377 G378
T379 F380 A381 V382 L383 A384 A385 F386 G387 F388 S389 I390 N391 T392 L393 T394 M395 F396 G397 M398 V399 L400 A401 I402 G403 L404 L405 V406 D407 D408 A409 I410 V411 V412 V413 E414 N415 V416 E417 E423 K428 Q439 G440 A441 L442 V443 G444 I445 A446 M447 V448 L449 S450 A451 V452 F453 V454
P455 M456 A457 G460 G461 S462 F470 S471 I474 V475 S476 A477 M478 A479 L480 S481 V482 L483 V484 A485 L486 I487 L488 T489 P490 A491 L492 C493 A494 I500 A501 K502 G503 D504 H505 G506 E507 G508 K509 K510 G511 F512 W515 F516 N517 R518 M519 F520 E521 G533 I534 L535 R536
L546 V549 L555 L559 P560 V576 A582 T583 R586 Y598 E602 Q622 N623 V629 E641 N642 R650 F655 I658 K659 D660 A661 M662 V663 I671 V672 E673 L674 G675 T676 A677 F680 D681 F682 I685 D686 Q687 A688 G689 L690 G691 H692 E693
K694 L695 T696 A704 E705 A706 A707 K708 D711 M712 L713 T714 S715 V716 T724 P725 Q726 F727 Q733 S742 I743 N744 D745 I746 N747 V771 Y779 R780 M781 L782 P783 Y819 M825 E826 I827 L828 G829 Q830 G834 K835 S836 T837 G838 E839 A840 M841 E842 L843 M844 E845
Q846 K850 T853 M862 R867 L868 S869 G870 N871 Q872 S875 L876 Y877 A878 I879 S880 L881 I882 V883 L886 C887 E893 M902 L903 V904 V905 P906 L907 G908 L913 R919 G920 L921 L932 I935 G936 L937 S938 A939 K940 N941 A942 I943 L944 I945 V946 L952
M953 D954 K955 E956 I961 E962 A963 T964 L965 V968 R971 L972 R973 P974 I975 L976 M977 T978 S979 F982 I983 L984 G985 V986 M987 P988 L989 V990 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1027 S1034 ARG LYS ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32528	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)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.665	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	302.4, 302.4, 302.4	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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	0/8005	0.39	0/10871
1	B	0.14	0/8005	0.38	0/10871
1	C	0.14	0/8005	0.40	0/10871
All	All	0.14	0/24015	0.39	0/32613

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	7855	0	8005	202	0
1	B	7855	0	8006	208	0
1	C	7855	0	8006	217	0
All	All	23565	0	24017	605	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 13.

The worst 5 of 605 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:481:SER:O	1:A:484:VAL:HG12	1.36	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LEU:O	1:B:547:ILE:HG12	1.44	1.16
1:B:109:ASN:OD1	1:A:108:GLN:HG3	1.50	1.09
1:A:135:SER:OG	1:A:672:VAL:HG11	1.54	1.08
1:B:544:LEU:O	1:B:547:ILE:CG1	2.02	1.06

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	1032/1049 (98%)	999 (97%)	33 (3%)	0	100	100
1	B	1032/1049 (98%)	1000 (97%)	32 (3%)	0	100	100
1	C	1032/1049 (98%)	984 (95%)	48 (5%)	0	100	100
All	All	3096/3147 (98%)	2983 (96%)	113 (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	840/855 (98%)	836 (100%)	4 (0%)	81	81
1	B	840/855 (98%)	832 (99%)	8 (1%)	68	73
1	C	840/855 (98%)	834 (99%)	6 (1%)	76	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2520/2565 (98%)	2502 (99%)	18 (1%)	73 77

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	TYR
1	A	779	TYR
1	A	515	TRP
1	C	162	MET
1	C	965	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	733	GLN
1	A	1001	ASN
1	C	120	GLN
1	C	124	GLN
1	C	254	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)

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.

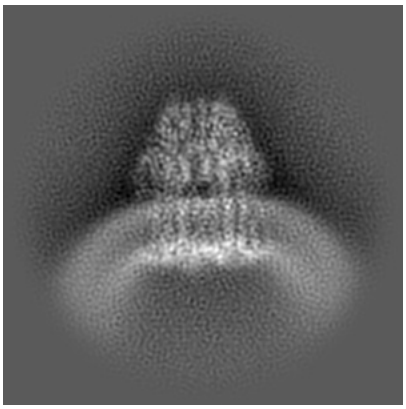
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-69828. These allow visual inspection of the internal detail of the map and identification of artifacts.

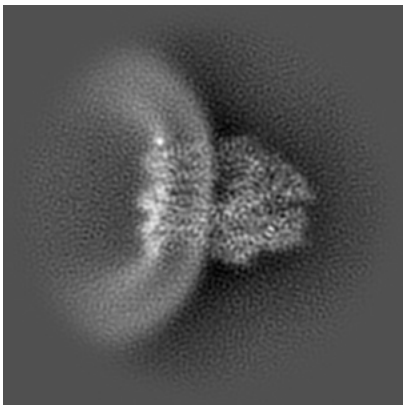
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

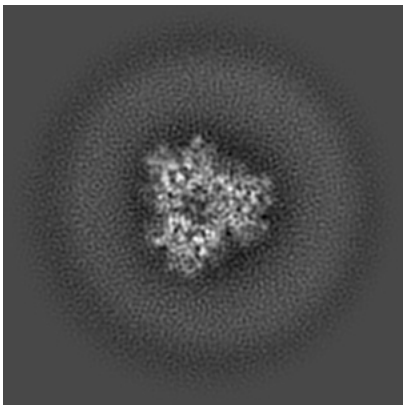
6.1.1 Primary map



X

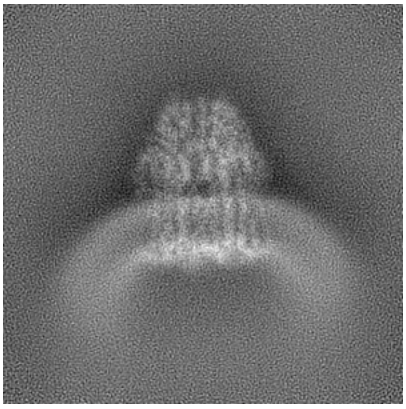


Y

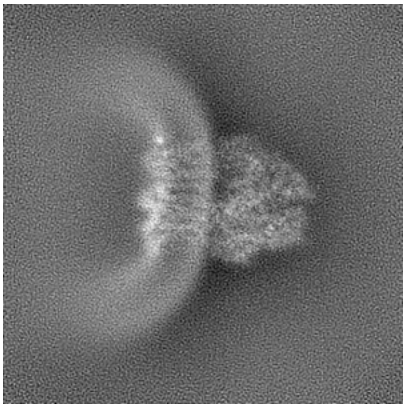


Z

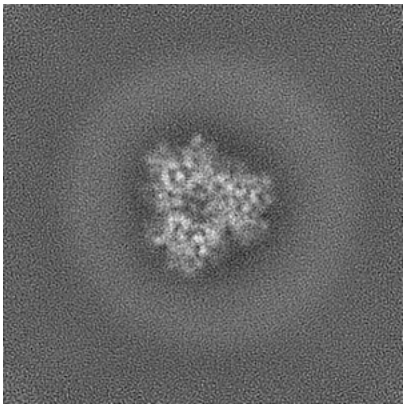
6.1.2 Raw map



X



Y

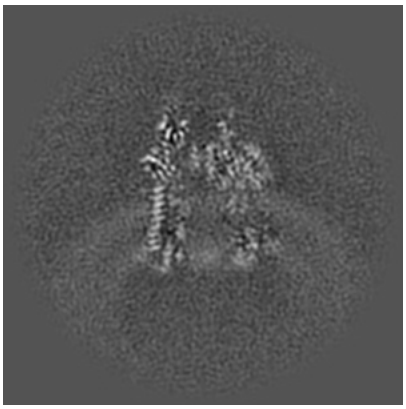


Z

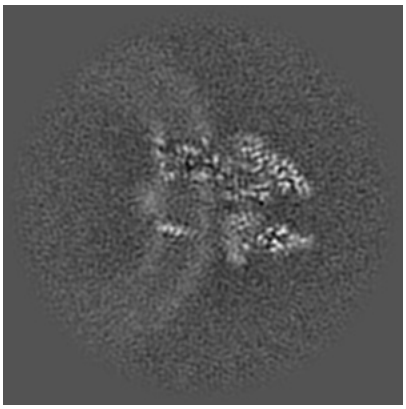
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

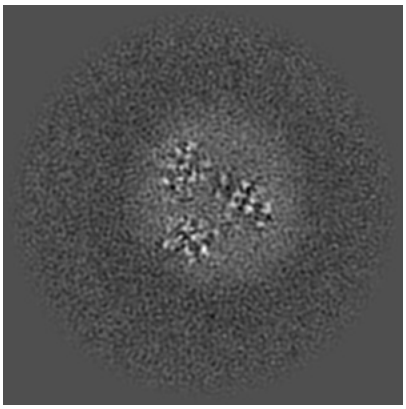
6.2.1 Primary map



X Index: 135

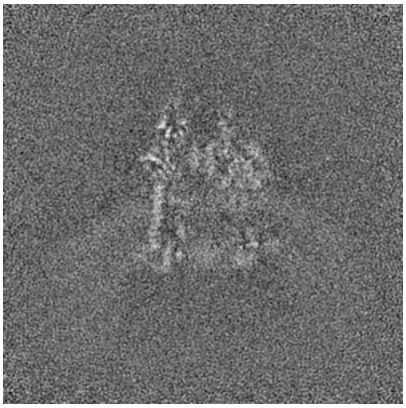


Y Index: 135

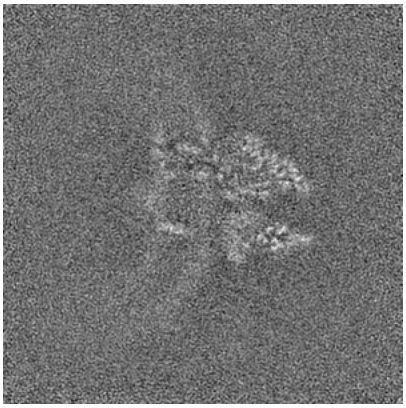


Z Index: 135

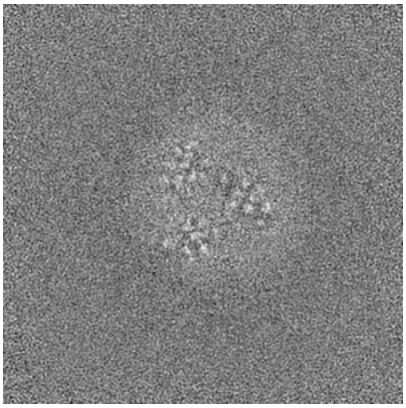
6.2.2 Raw map



X Index: 135



Y Index: 135

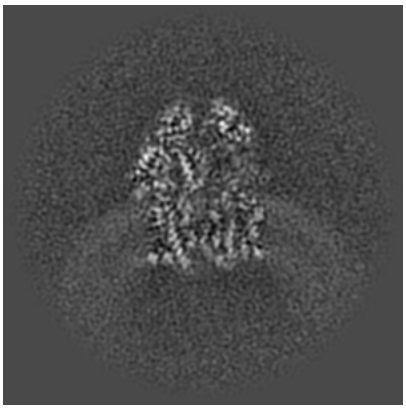


Z Index: 135

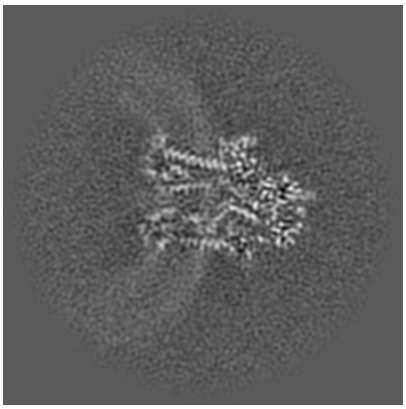
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

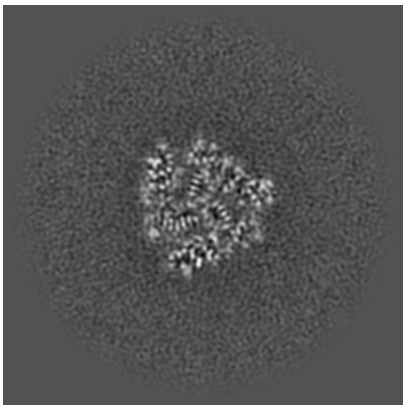
6.3.1 Primary map



X Index: 121

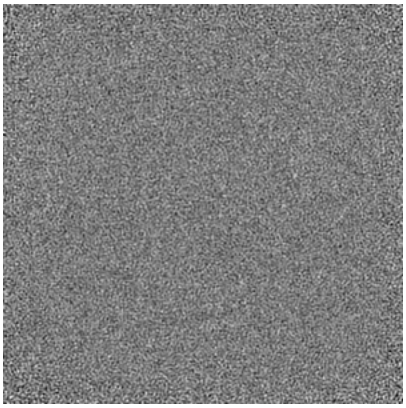


Y Index: 150

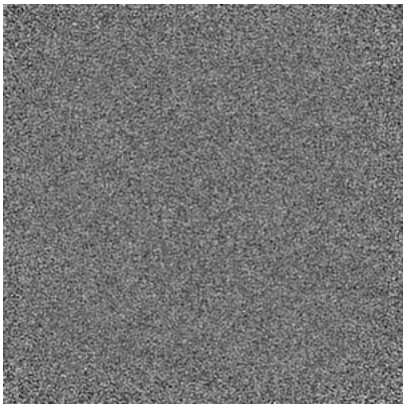


Z Index: 162

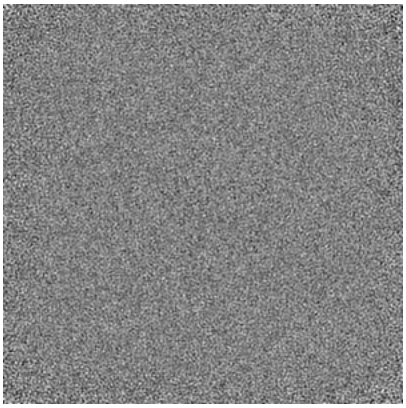
6.3.2 Raw map



X Index: 0



Y Index: 0

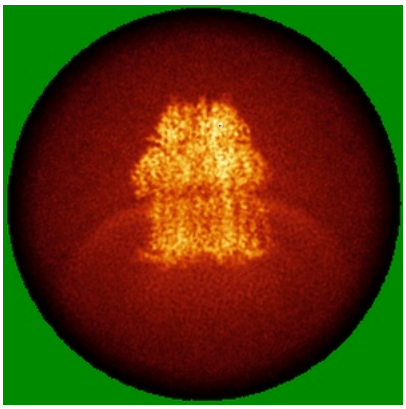


Z Index: 0

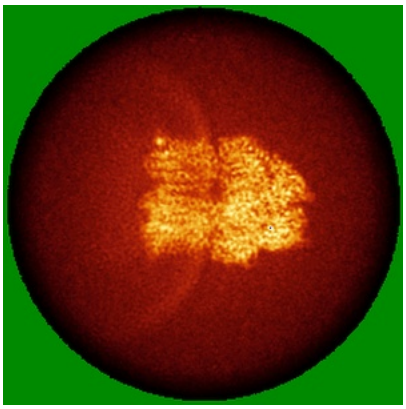
The images above show the largest variance slices of the map in three orthogonal directions.

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

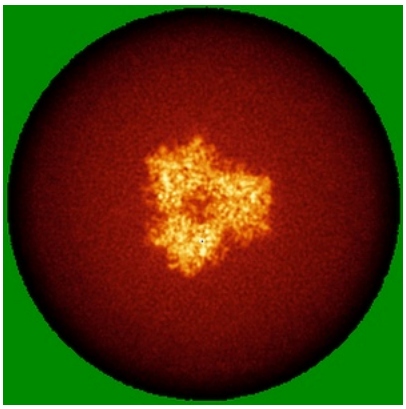
6.4.1 Primary map



X

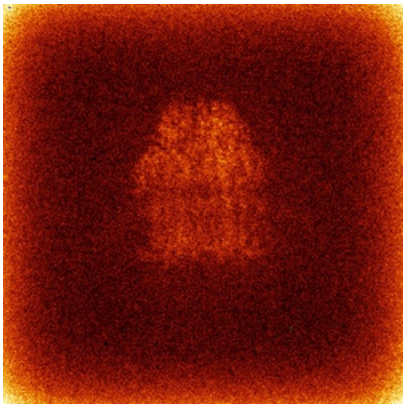


Y

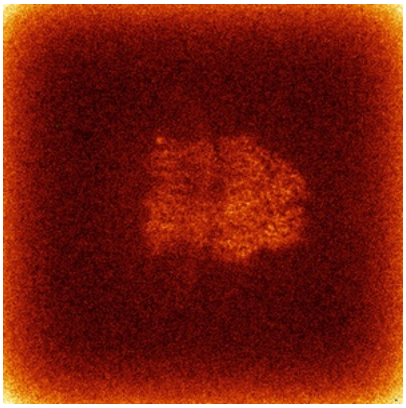


Z

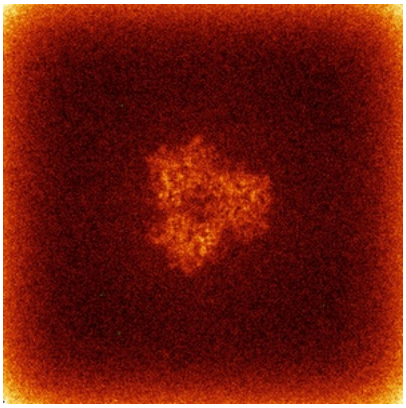
6.4.2 Raw map



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 0.12. 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.

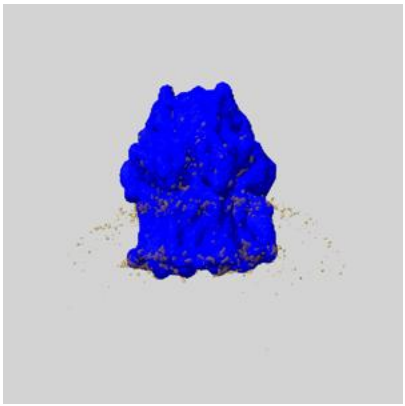
6.6 Mask visualisation

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

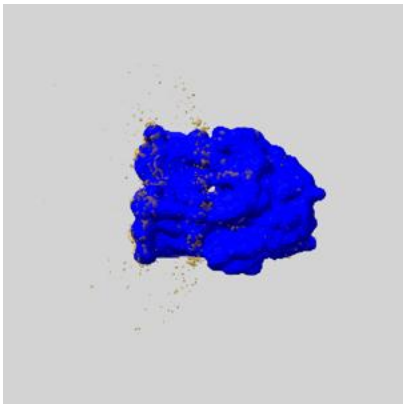
A mask typically either:

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

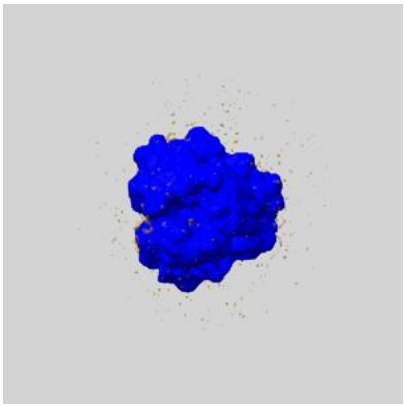
6.6.1 emd_69828_msk_1.map



X



Y

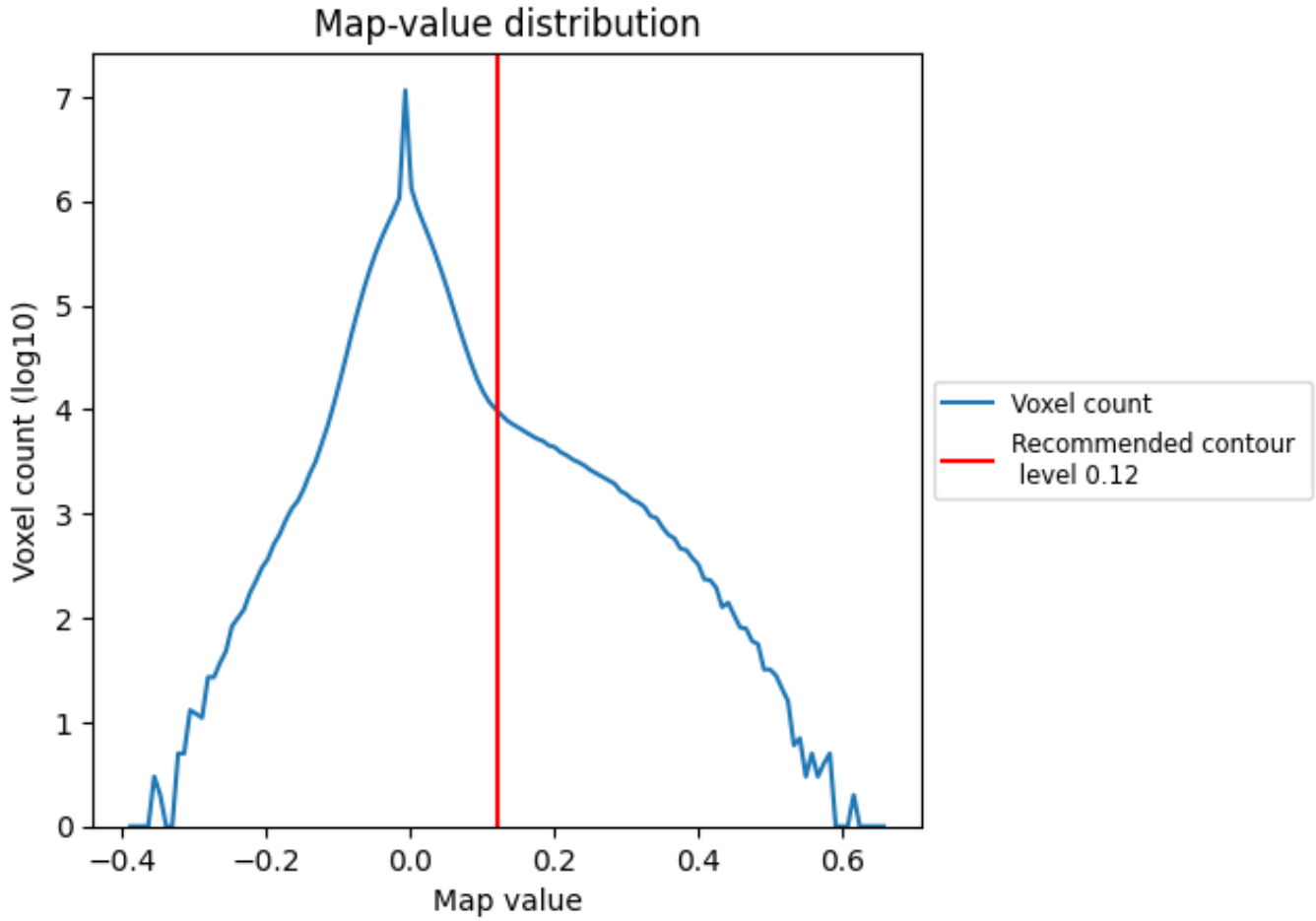


Z

7 Map analysis

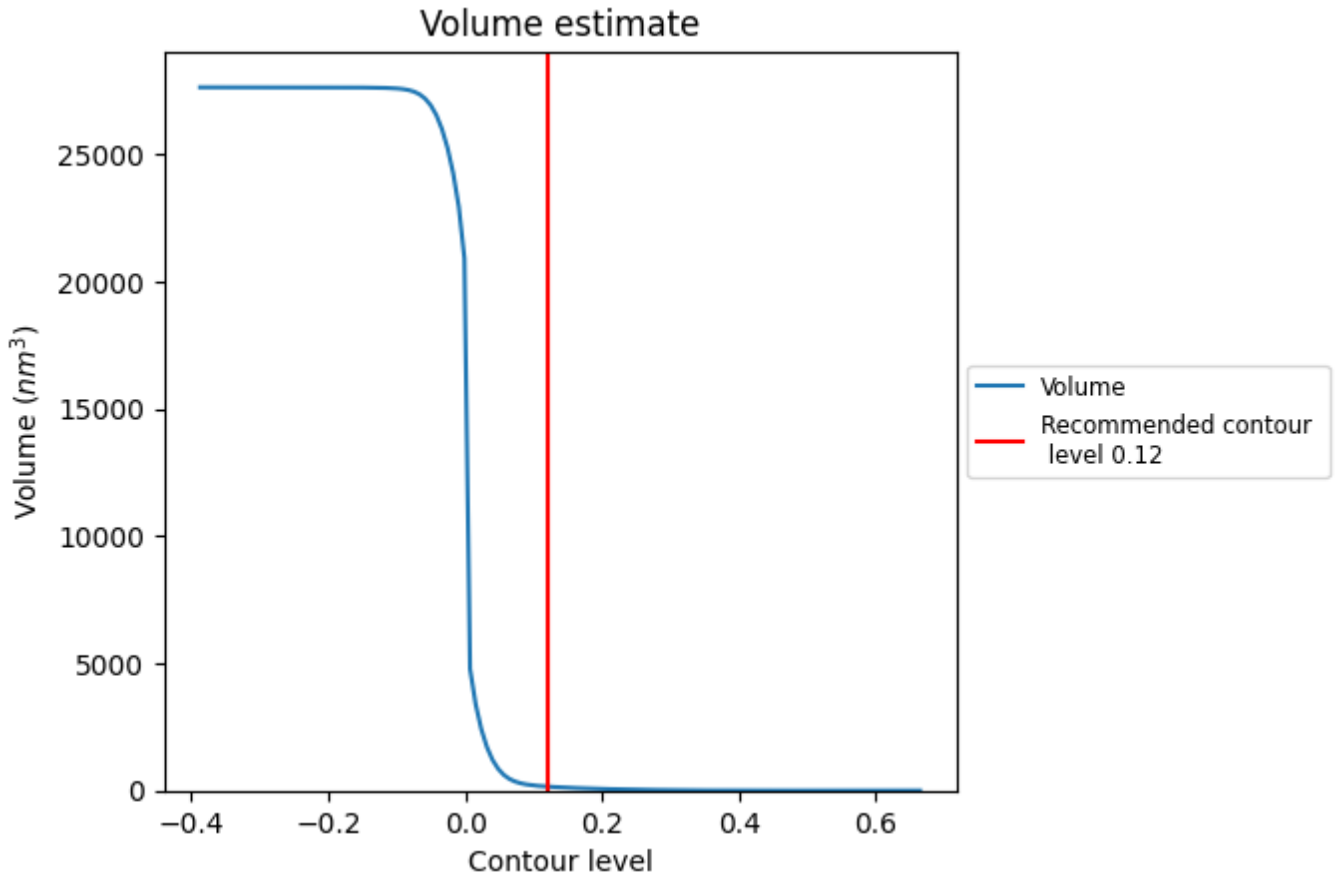
This section contains the results of statistical analysis of the map.

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.

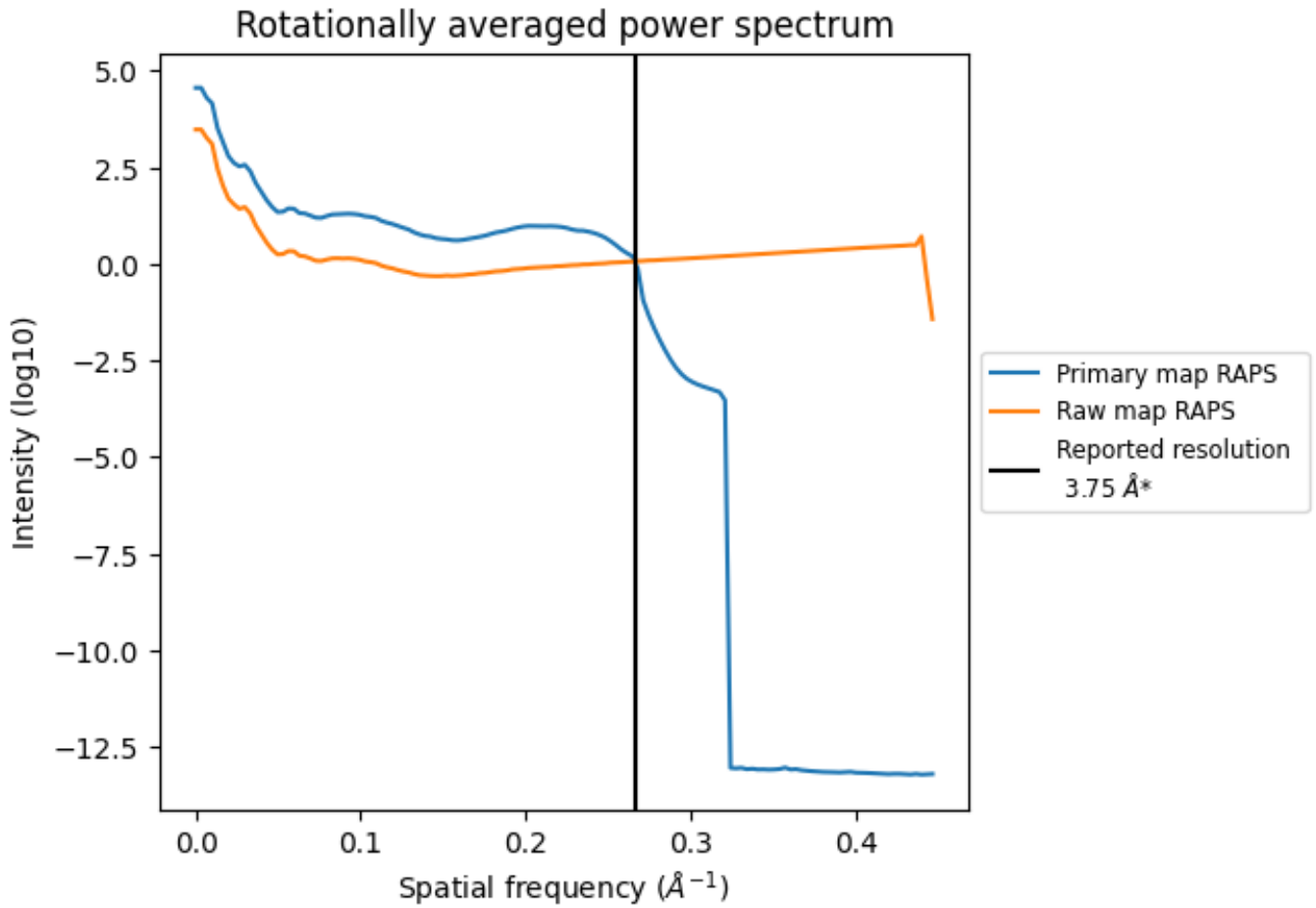
7.2 Volume estimate (i)



The volume at the recommended contour level is 156 nm^3; this corresponds to an approximate mass of 141 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)

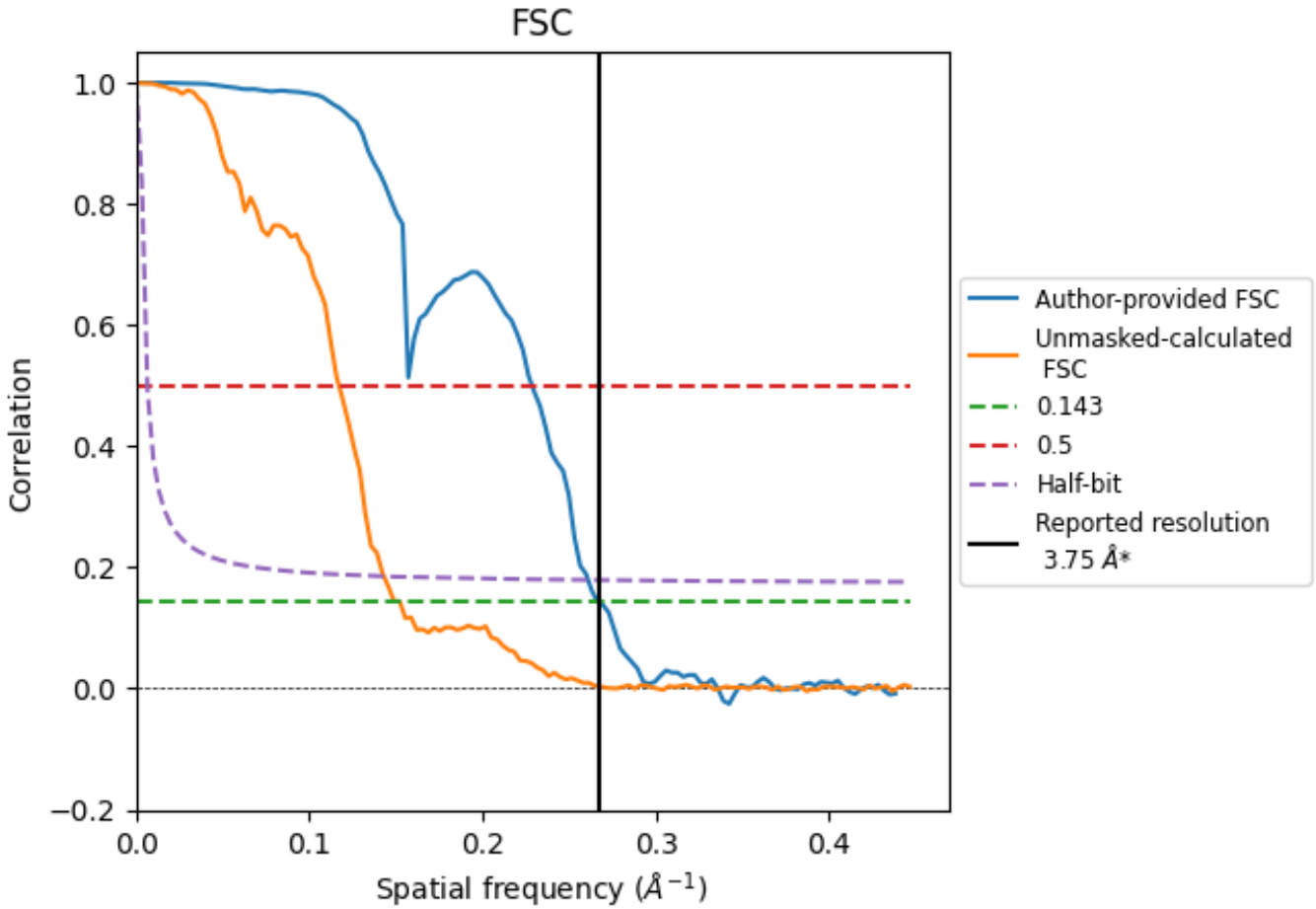


*Reported resolution corresponds to spatial frequency of 0.267 $Å^{-1}$

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 0.267 Å^{-1}

8.2 Resolution estimates (i)

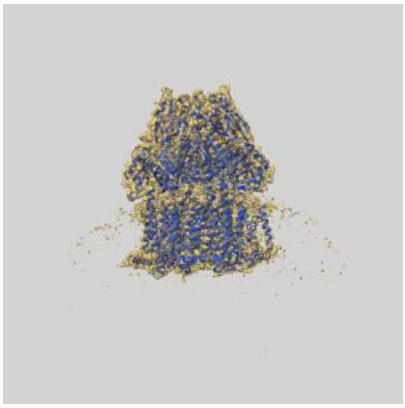
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.75	4.38	3.83
Unmasked-calculated*	6.57	8.54	6.99

*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 6.57 differs from the reported value 3.75 by more than 10 %

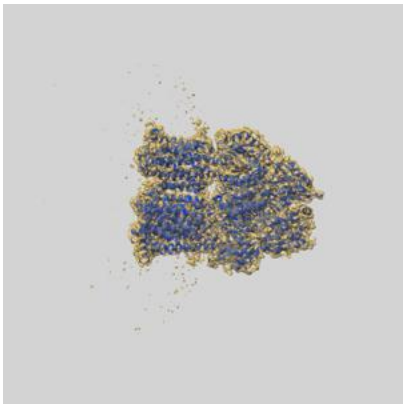
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-69828 and PDB model 24UO. Per-residue inclusion information can be found in section 3 on page 4.

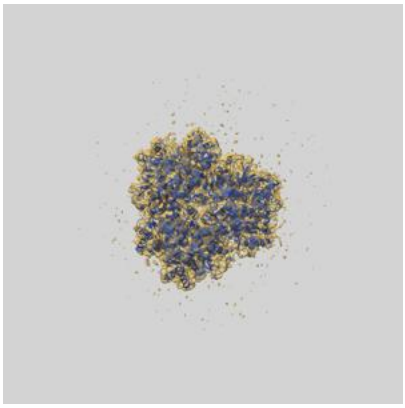
9.1 Map-model overlay



X



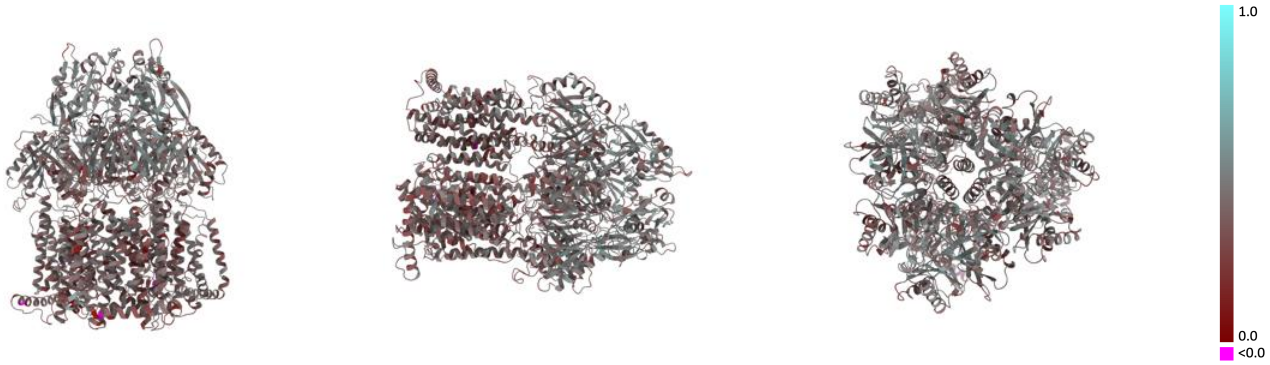
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

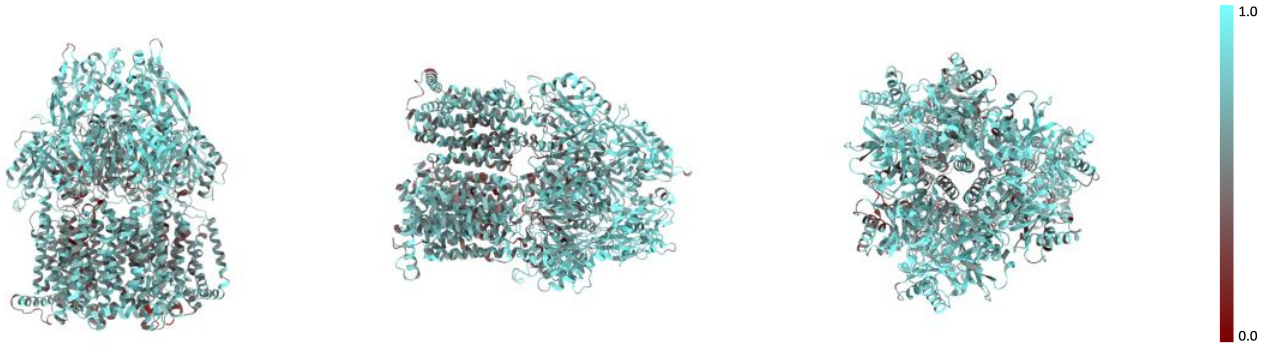
9.2 Q-score mapped to coordinate model



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.

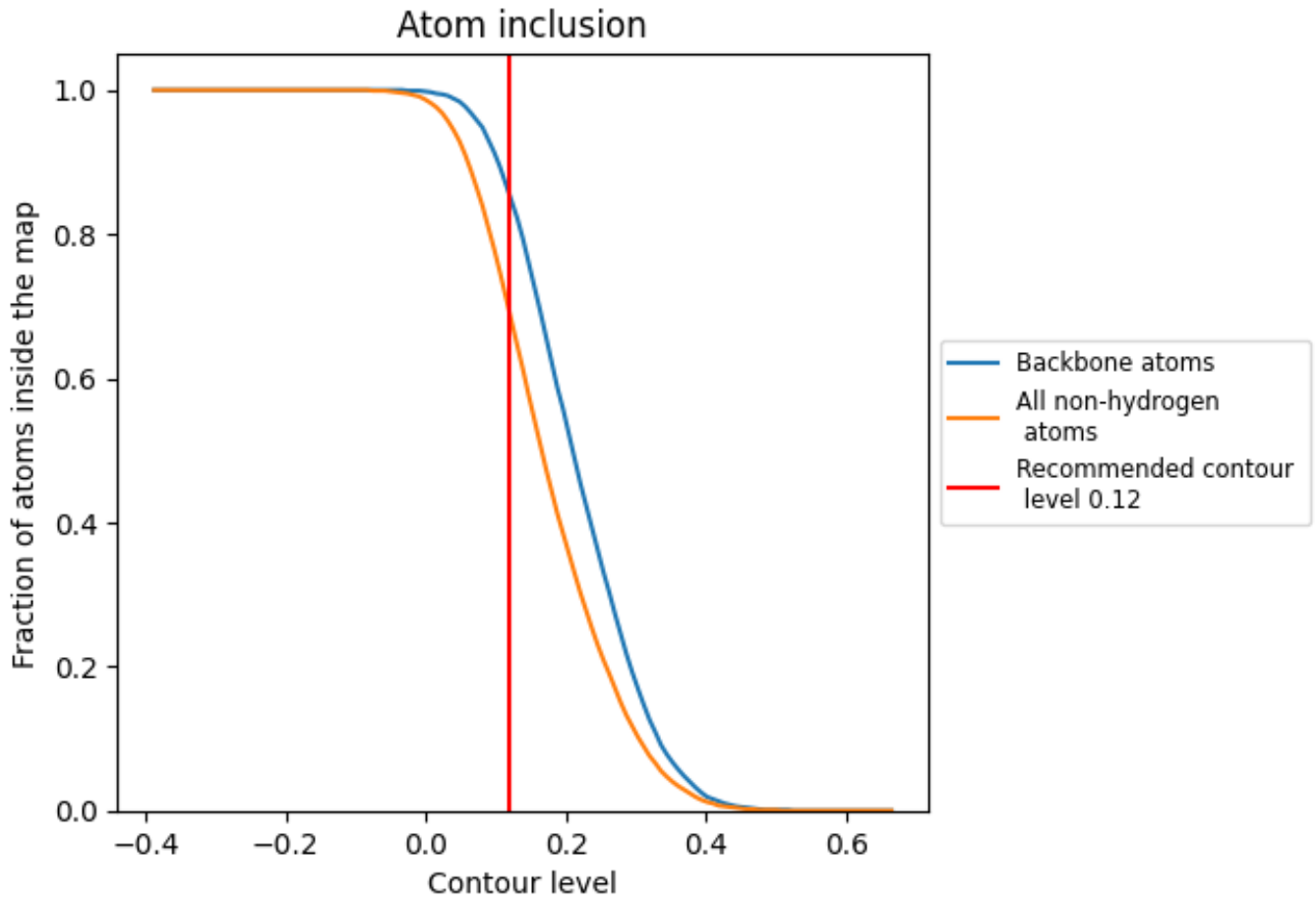
9.3 Atom inclusion mapped to coordinate model



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 69% 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 (0.12) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6900	0.4010
A	0.6800	0.3980
B	0.6940	0.4050
C	0.6950	0.4000