wwPDB EM Validation Summary Report

Nov 4, 2026 – 04:57 PM JST

PDB ID	:	24VA / pdb_000024va
EMDB ID	:	EMD-69834
Title	:	Cryo-EM structure of recombinant Botulinum neurotoxin A
Authors	:	Xu, L.
Deposited on	:	2026-03-22
Resolution	:	3.24 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:

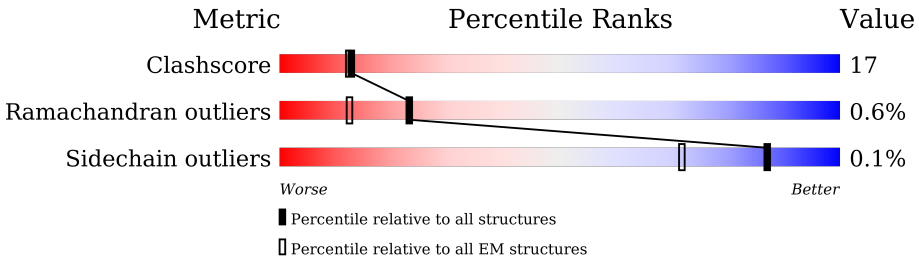
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

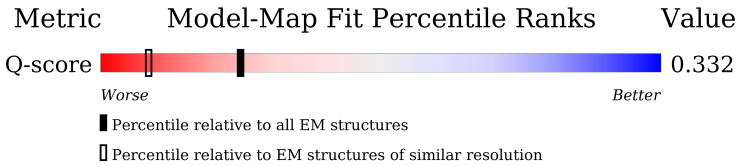
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.24 Å.

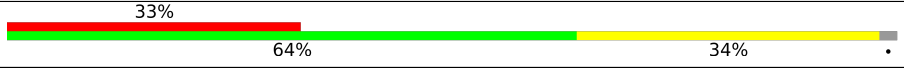
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





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	14594 (2.74 - 3.74)

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	448	
2	B	850	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10327 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3490	2256	568	657	9	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P0DPI1
A	2	PRO	-	expression tag	UNP P0DPI1
A	3	LEU	-	expression tag	UNP P0DPI1
A	4	GLY	-	expression tag	UNP P0DPI1
A	5	SER	-	expression tag	UNP P0DPI1
A	443	LEU	-	expression tag	UNP P0DPI1
A	444	GLU	-	expression tag	UNP P0DPI1
A	445	VAL	-	expression tag	UNP P0DPI1
A	446	LEU	-	expression tag	UNP P0DPI1
A	447	PHE	-	expression tag	UNP P0DPI1
A	448	GLN	-	expression tag	UNP P0DPI1

- Molecule 2 is a protein called Botulinum neurotoxin A heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	836	6837	4370	1136	1308	23	0	0

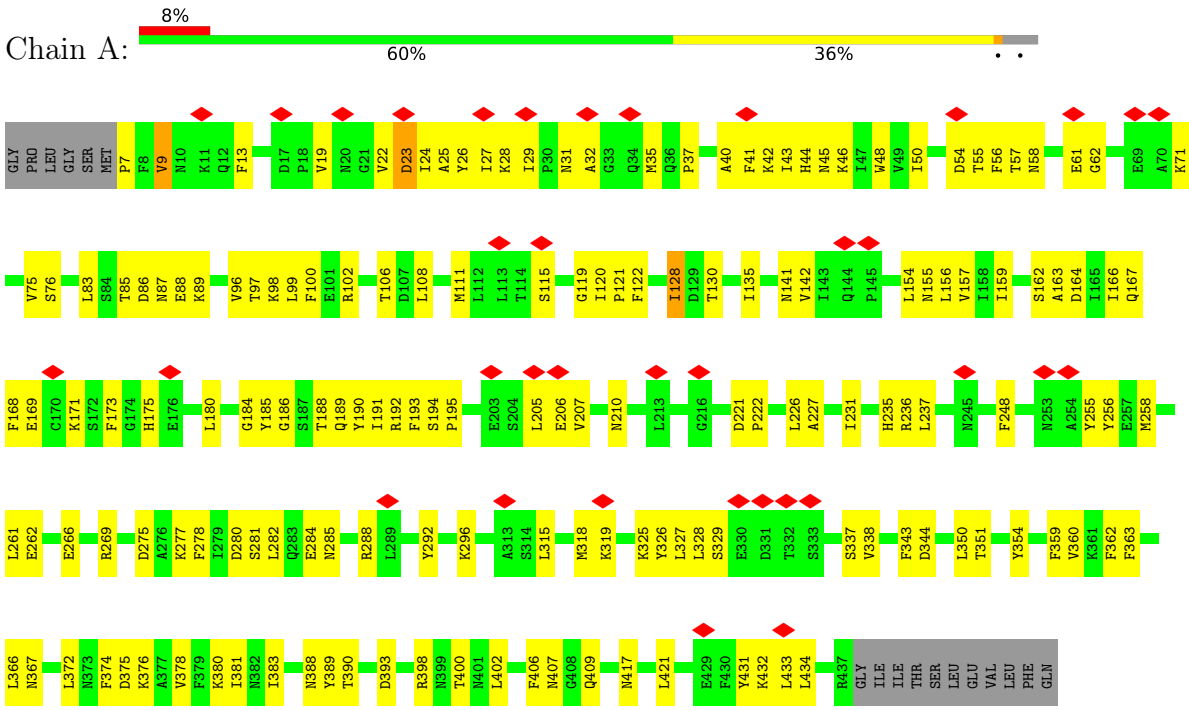
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP P0DPI1
B	2	PRO	-	expression tag	UNP P0DPI1

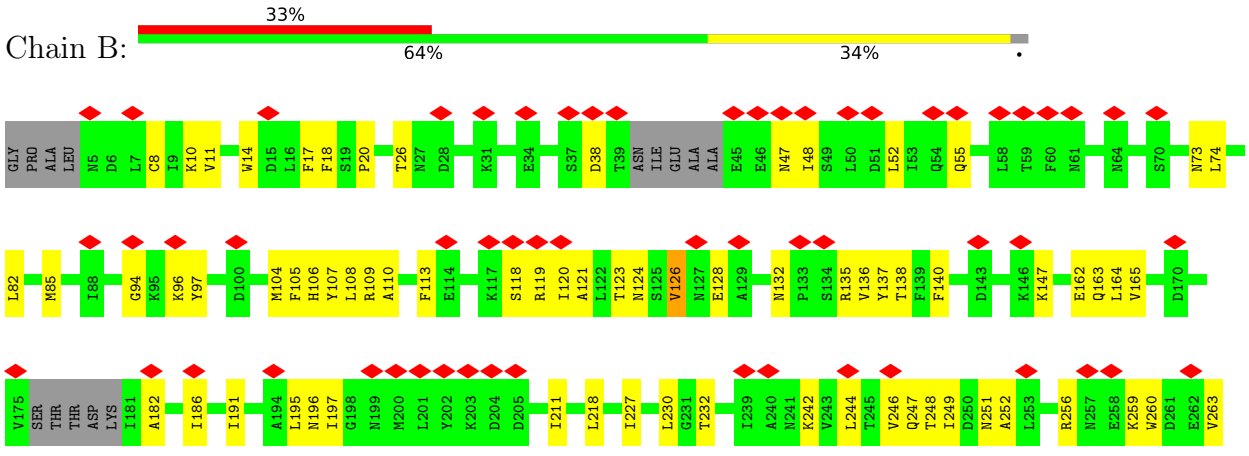
3 Residue-property plots (i)

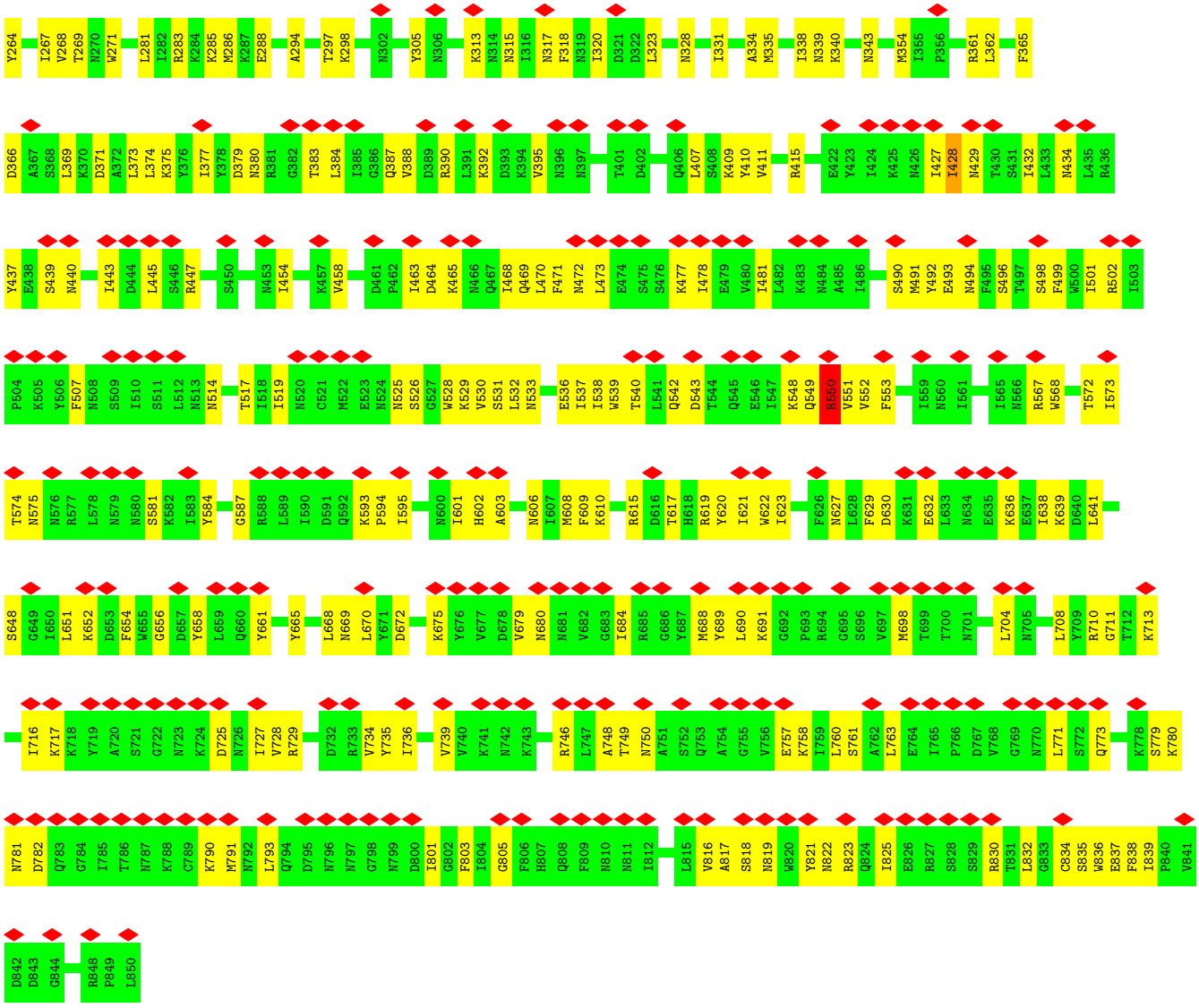
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Botulinum neurotoxin type A



• Molecule 2: Botulinum neurotoxin A heavy chain




Y264 I267 V268 T269 N270 W271 L281 I282 R283 K284 K285 M286 K287 E288 A294 T297 K298 N302 Y305 N306 K313 N314 N315 I316 N317 F318 N319 I320 D321 D322 L323 N328 I331 A334 M335 I338 N339 K340 N343 M354 I355 P356 R361 L362 F365
D366 A367 S368 L369 K370 D371 A372 L373 L374 K375 Y376 I377 Y378 D379 N380 R381 G382 T383 L384 I385 G386 Q387 V388 D389 R390 L391 K392 D393 K394 V395 N396 N397 T401 D402 Q406 L407 S408 K409 Y410 V411 R415 E422 Y423 I424 K425 N426 I427 T428 N429 T430 S431 I432 L433 N434 L435 R436
Y437 E438 S439 N440 I443 D444 L445 S446 R447 S450 N453 I454 K457 V458 D461 P462 I463 D464 K465 N466 Q467 I468 Q469 L470 F471 N472 L473 E474 S475 S476 K477 I478 E479 V480 I481 L482 K483 N484 A485 I486 S490 N491 Y492 E493 N494 F495 S496 T497 S498 F499 W500 I501 R502 I503
P504 K505 Y506 F507 N508 S509 I510 S511 L512 N513 N514 T517 I518 I519 N520 C521 M522 E523 N524 N525 S526 G527 W528 K529 V530 S531 L532 N533 E536 I537 I538 W539 T540 L541 Q542 D543 T544 Q545 E546 I547 K548 Q549 R550 V551 V552 F553 I559 N560 I561 I565 N566 R567 W568 T572 I573
T574 N575 N576 R577 L578 N579 N580 S581 K582 I583 Y584 G587 R588 L589 I590 D591 Q592 K593 P594 I595 N600 I601 H602 A603 N606 I607 M608 F609 K610 R615 D616 T617 H618 R619 Y620 I621 W622 I623 F626 N627 L628 F629 D630 K631 E632 L633 N634 E635 K636 E637 I638 K639 D640 L641
S648 G649 I650 L651 K652 D653 F654 W655 G656 D657 Y658 L659 Q660 Y661 Y665 L668 N669 L670 Y671 D672 K675 Y676 V677 D678 V679 N680 N681 V682 G683 I684 R685 G686 Y687 M688 Y689 L690 K691 G692 P693 R694 G695 S696 V697 M698 T699 T700 N701 L704 N705 L708 Y709 R710 G711 T712 K713
I716 K717 K718 Y719 A720 S721 G722 N723 K724 D725 N726 I727 V728 R729 D732 R733 V734 Y735 I736 V739 V740 K741 N742 K743 R746 L747 A748 T749 N750 A751 S752 Q753 A754 G755 V756 E757 K758 I759 L760 S761 A762 L763 E764 I765 P766 D767 V768 G769 N770 L771 S772 Q773 K778 S779 K780
N781 D782 Q783 G784 I785 T786 N787 K788 C789 K790 M791 N792 L793 Q794 D795 N796 N797 G798 N799 D800 I801 G802 F803 I804 G805 F806 H807 Q808 F809 N810 N811 I812 L815 V816 A817 S818 N819 W820 Y821 N822 R823 Q824 I825 E826 R827 S828 S829 R830 T831 L832 G833 C834 S835 W836 E837 F838 I839 P840 V841
D842 D843 G844 R848 P849 L850

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	237907	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	0.032	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0038	Depositor
Map size (Å)	197.76, 197.76, 197.76	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	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	0.17	0/3574	0.36	0/4838
2	B	0.16	0/6972	0.39	0/9437
All	All	0.16	0/10546	0.38	0/14275

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	550	ARG	Sidechain

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	3490	0	3436	131	0
2	B	6837	0	6756	230	0
All	All	10327	0	10192	340	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 17.

The worst 5 of 340 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:27:ILE:HD13	1:A:40:ALA:HB3	1.51	0.91
2:B:230:LEU:HG	2:B:259:LYS:HZ1	1.40	0.86
2:B:507:PHE:H	2:B:619:ARG:HH22	1.23	0.86
1:A:26:TYR:HB3	1:A:37:PRO:HB2	1.59	0.84
1:A:19:VAL:HG13	1:A:25:ALA:HA	1.62	0.81

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	429/448 (96%)	403 (94%)	23 (5%)	3 (1%)	18	50
2	B	830/850 (98%)	761 (92%)	64 (8%)	5 (1%)	21	53
All	All	1259/1298 (97%)	1164 (92%)	87 (7%)	8 (1%)	23	53

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	128	ILE
2	B	126	VAL
2	B	315	ASN
2	B	317	ASN

5.3.2 Protein sidechains

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	385/400 (96%)	385 (100%)	0	100 100
2	B	767/778 (99%)	766 (100%)	1 (0%)	88 90
All	All	1152/1178 (98%)	1151 (100%)	1 (0%)	87 90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	550	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	514	ASN
2	B	730	ASN
2	B	794	GLN
2	B	731	ASN
2	B	251	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

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.

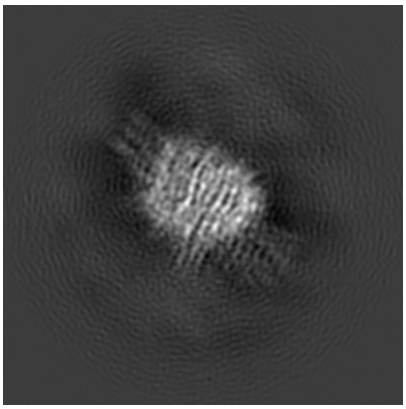
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-69834. These allow visual inspection of the internal detail of the map and identification of artifacts.

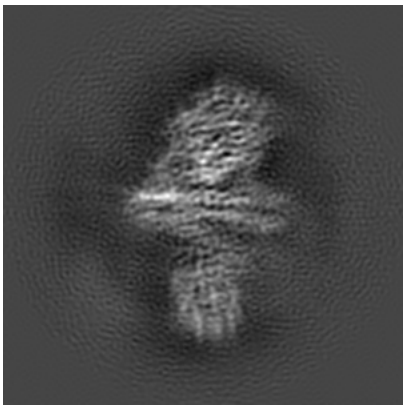
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

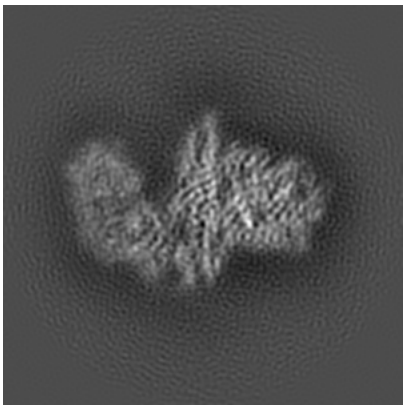
6.1.1 Primary map



X

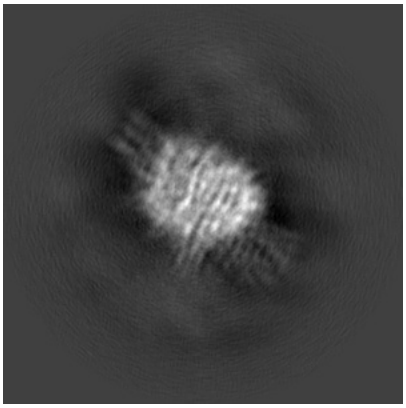


Y

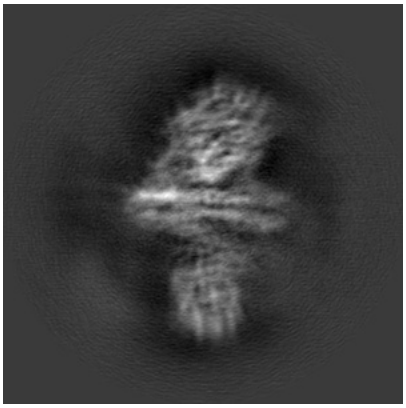


Z

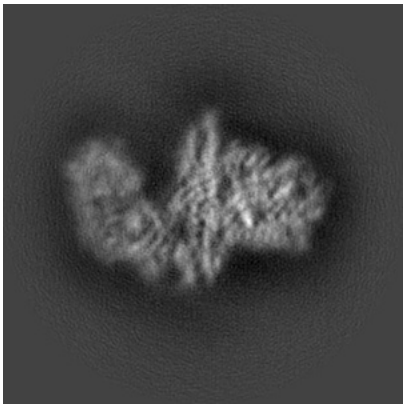
6.1.2 Raw map



X



Y

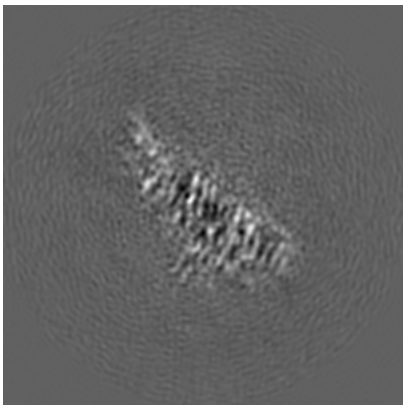


Z

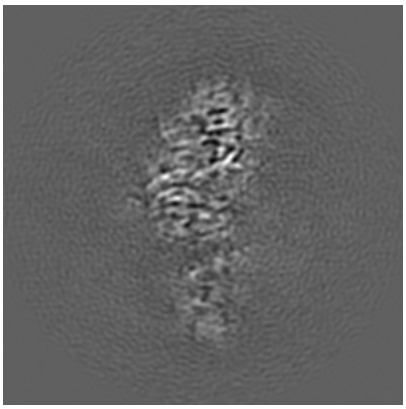
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

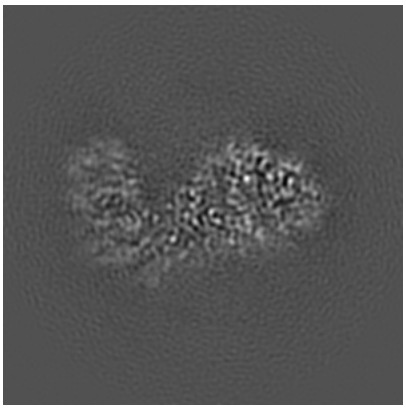
6.2.1 Primary map



X Index: 120

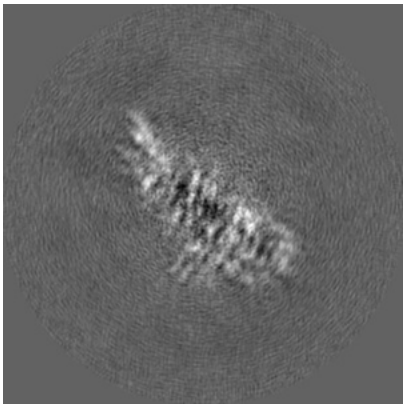


Y Index: 120

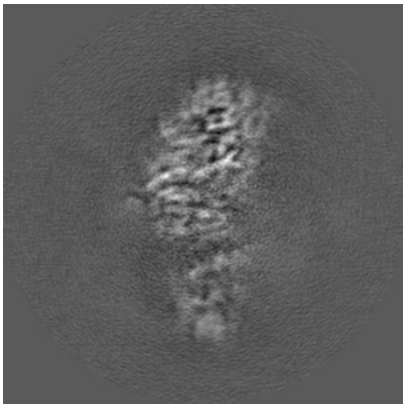


Z Index: 120

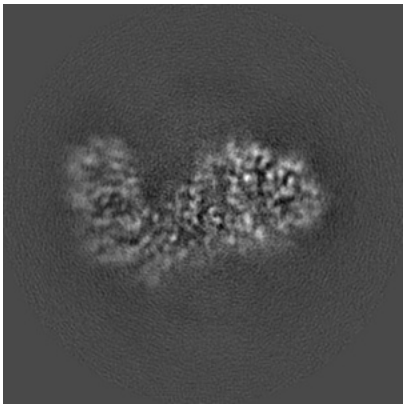
6.2.2 Raw map



X Index: 120



Y Index: 120

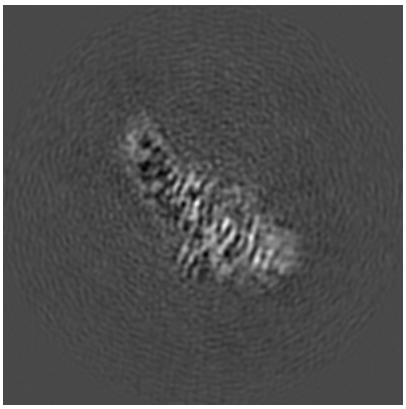


Z Index: 120

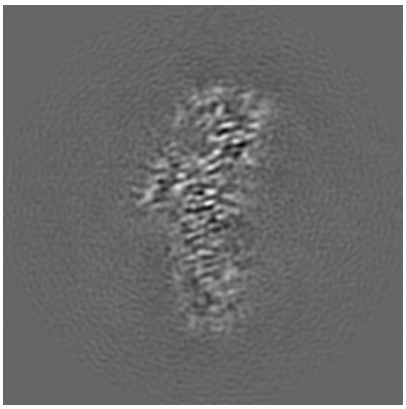
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

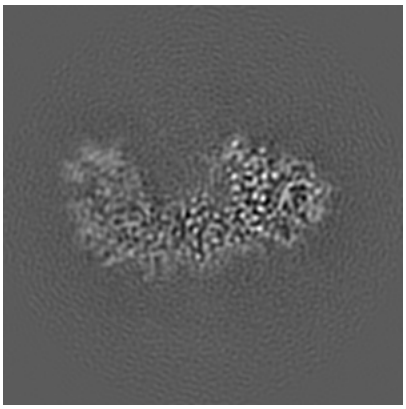
6.3.1 Primary map



X Index: 125

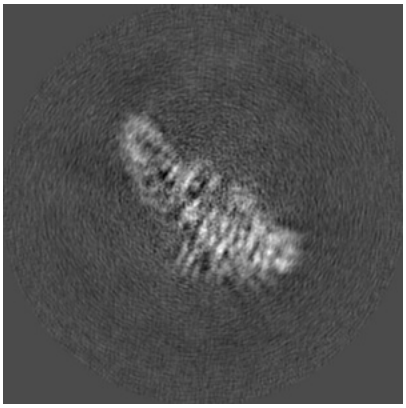


Y Index: 112

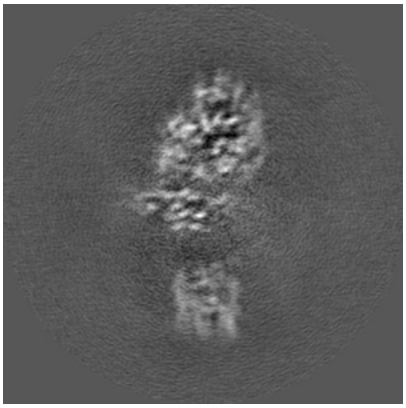


Z Index: 127

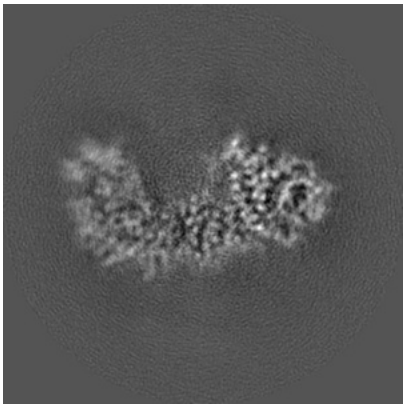
6.3.2 Raw map



X Index: 124



Y Index: 126

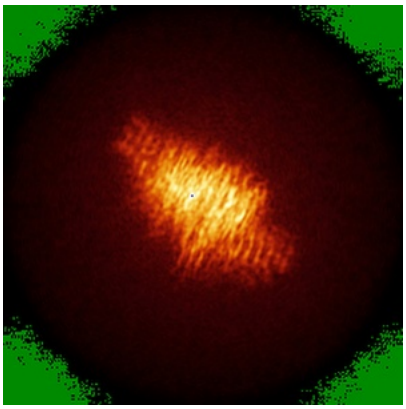


Z Index: 127

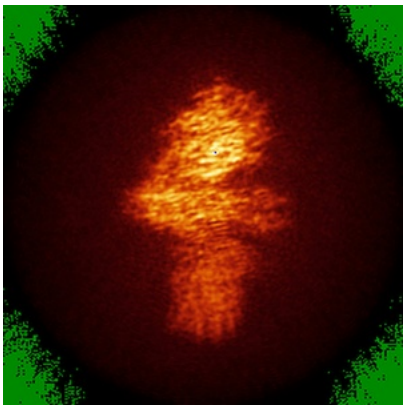
The images above show the largest variance slices of the map in three orthogonal directions.

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

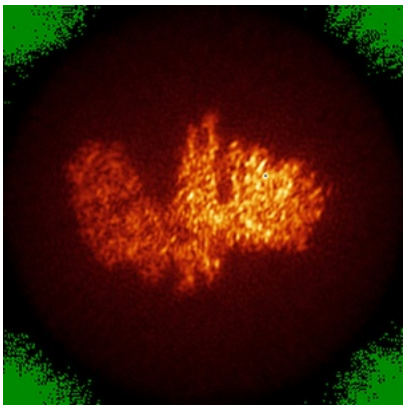
6.4.1 Primary map



X

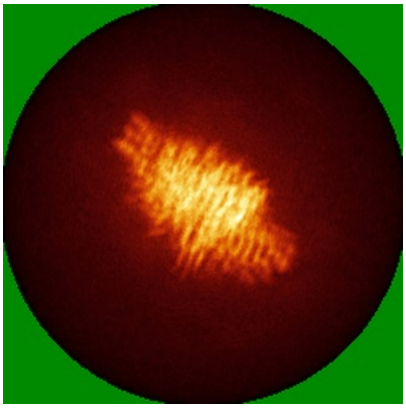


Y

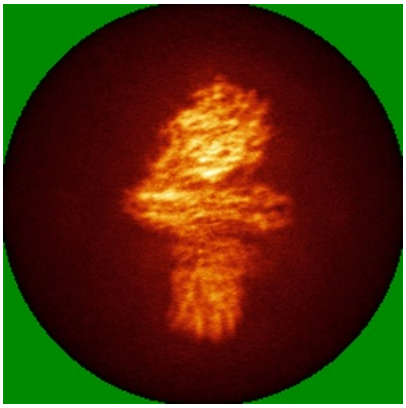


Z

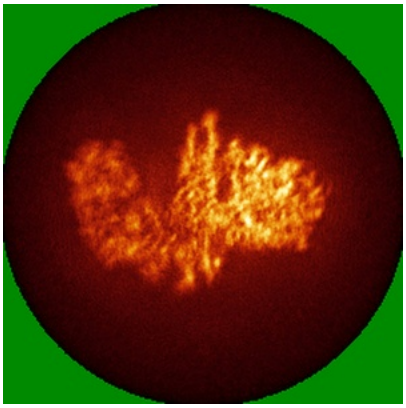
6.4.2 Raw map



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 0.0038. 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.

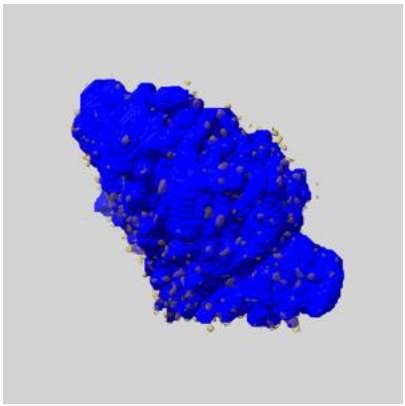
6.6 Mask visualisation

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

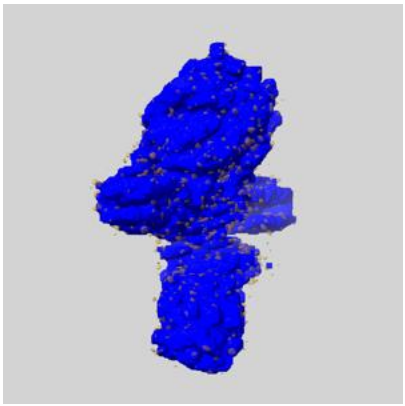
A mask typically either:

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

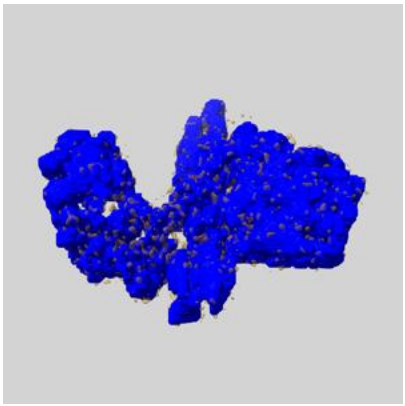
6.6.1 emd_69834_msk_1.map



X



Y

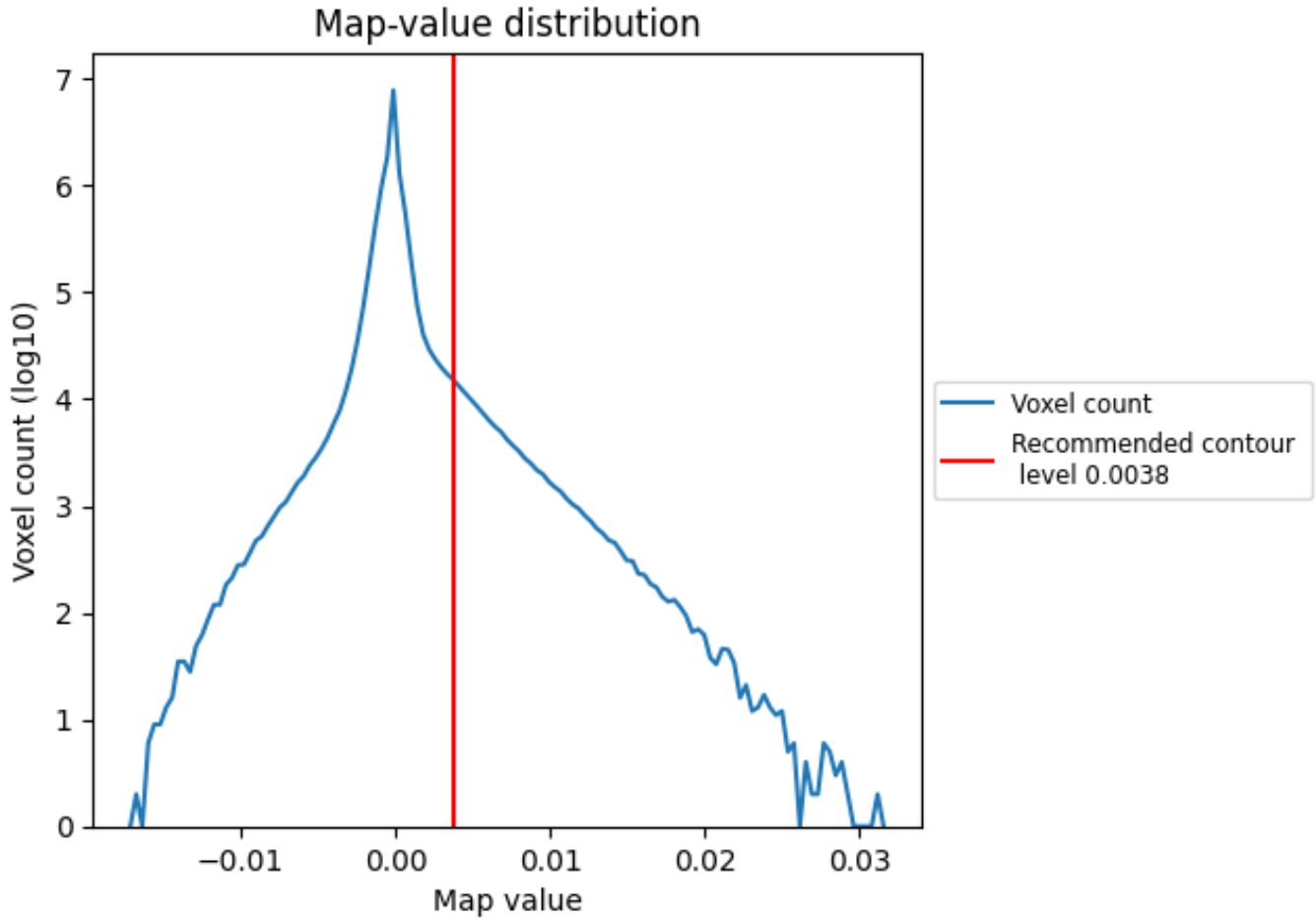


Z

7 Map analysis

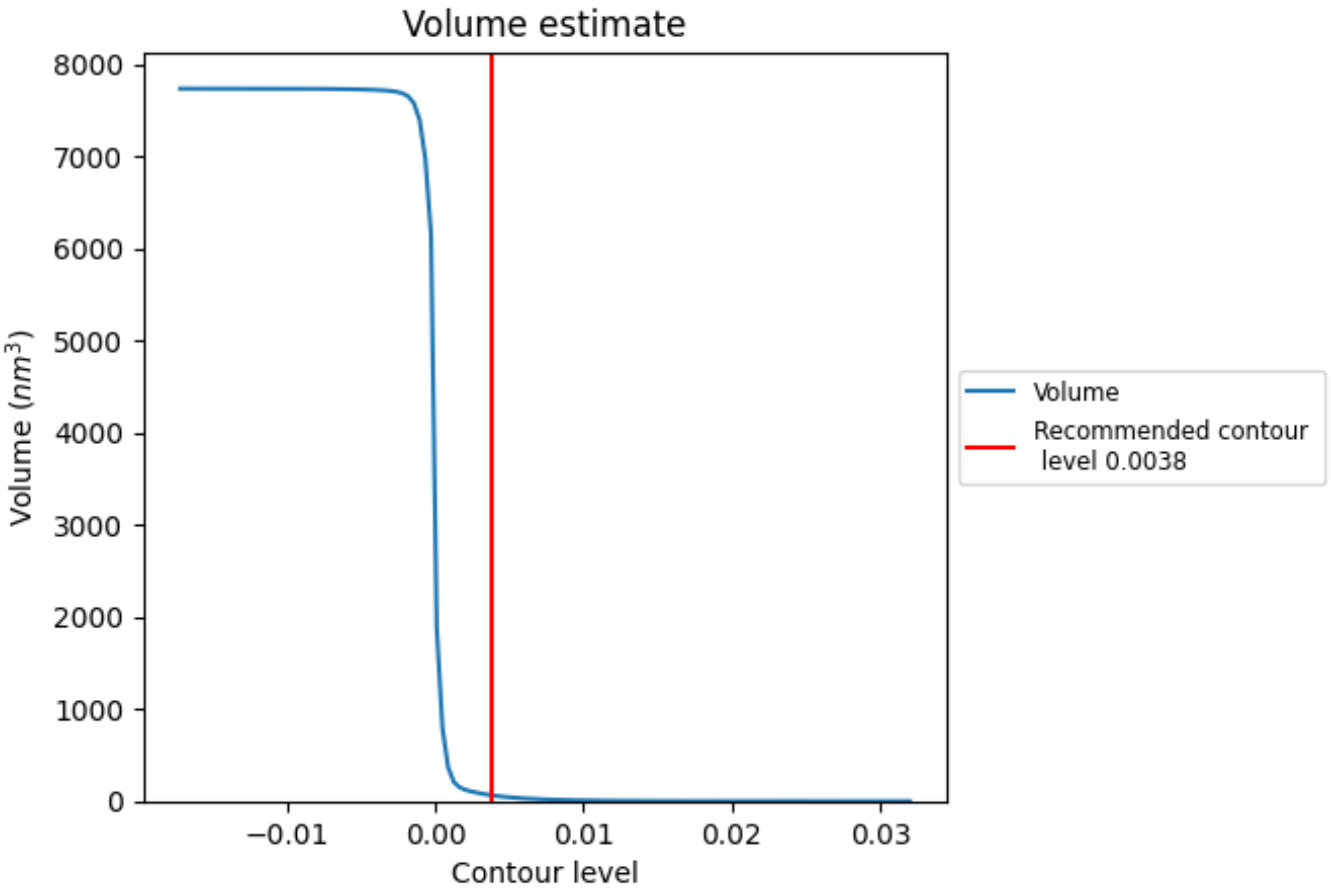
This section contains the results of statistical analysis of the map.

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.

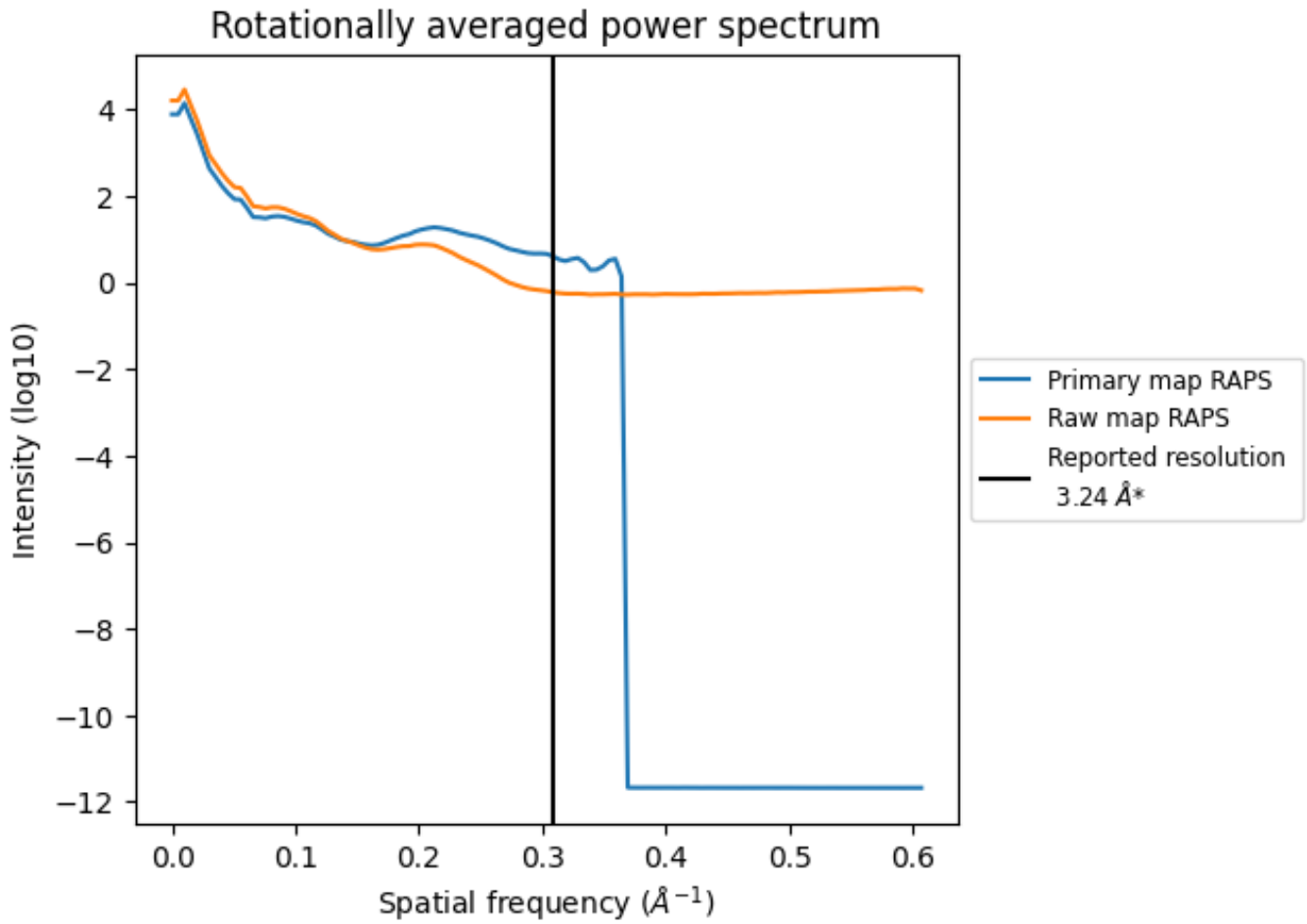
7.2 Volume estimate (i)



The volume at the recommended contour level is 64 nm^3; this corresponds to an approximate mass of 58 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)

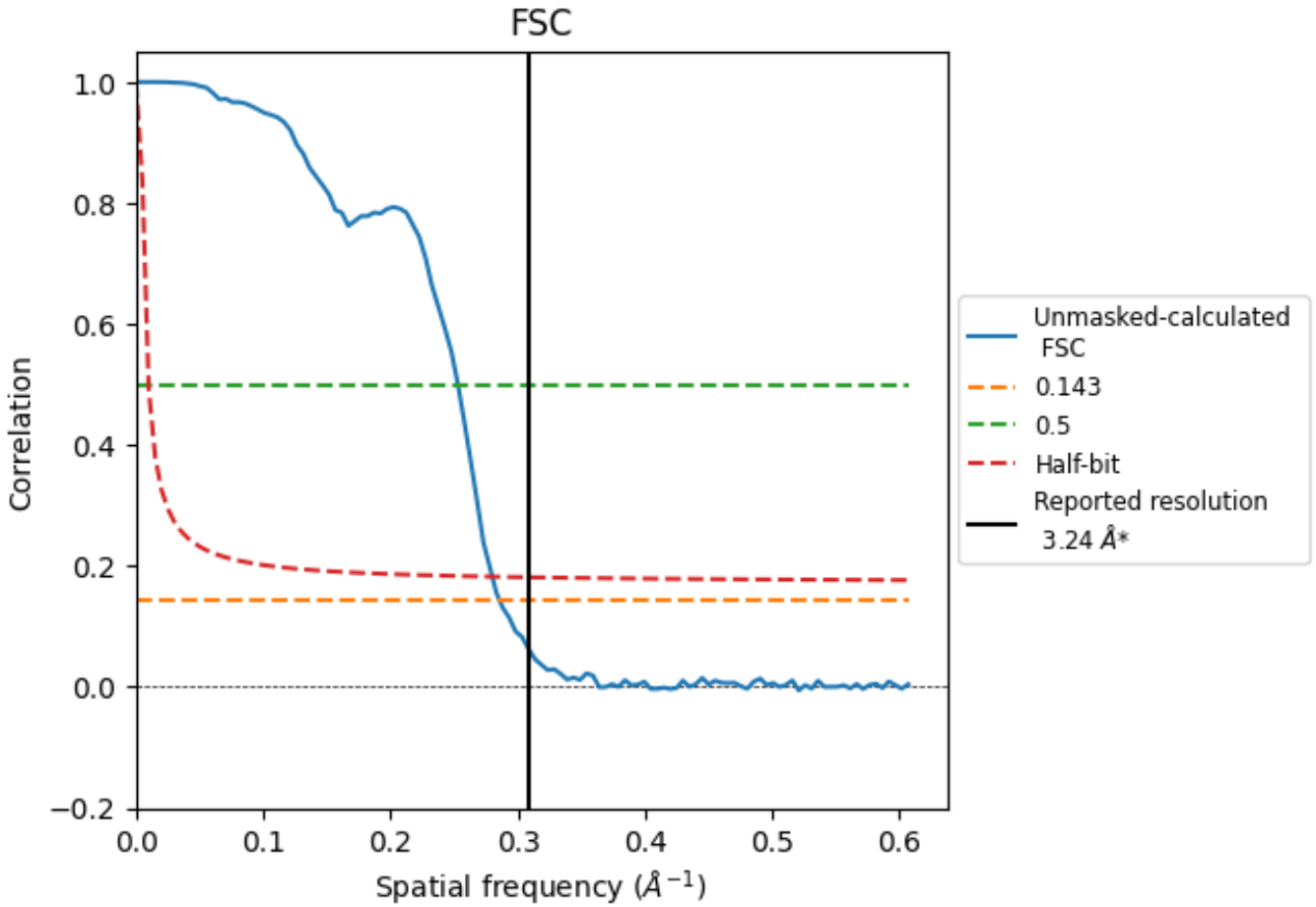


*Reported resolution corresponds to spatial frequency of 0.309 Å^{-1}

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 0.309 Å^{-1}

8.2 Resolution estimates (i)

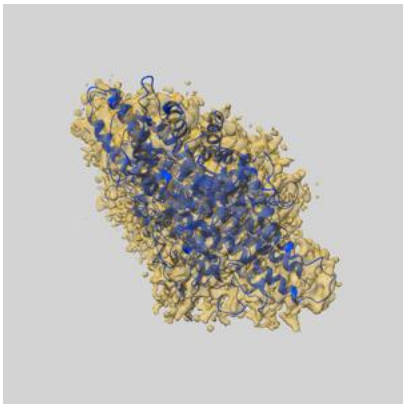
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	3.95	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

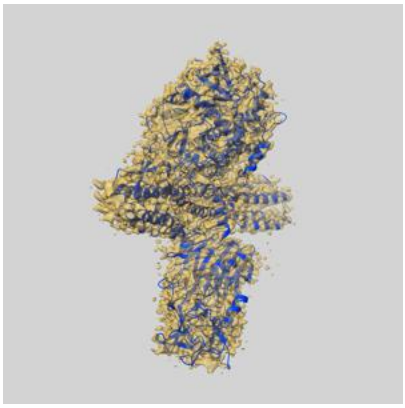
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-69834 and PDB model 24VA. Per-residue inclusion information can be found in section 3 on page 4.

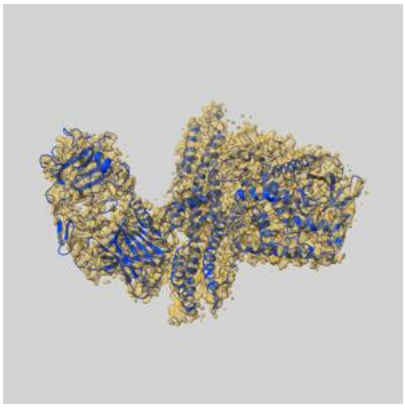
9.1 Map-model overlay



X



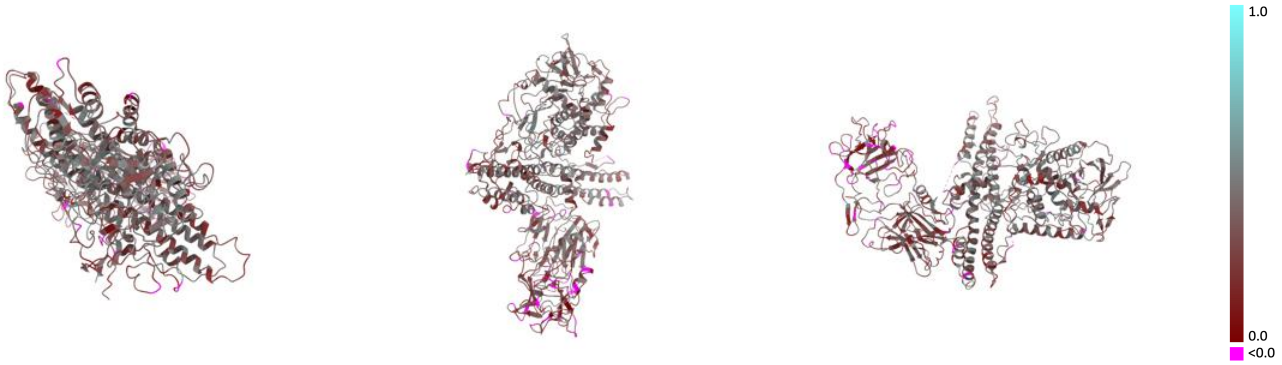
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0038 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.

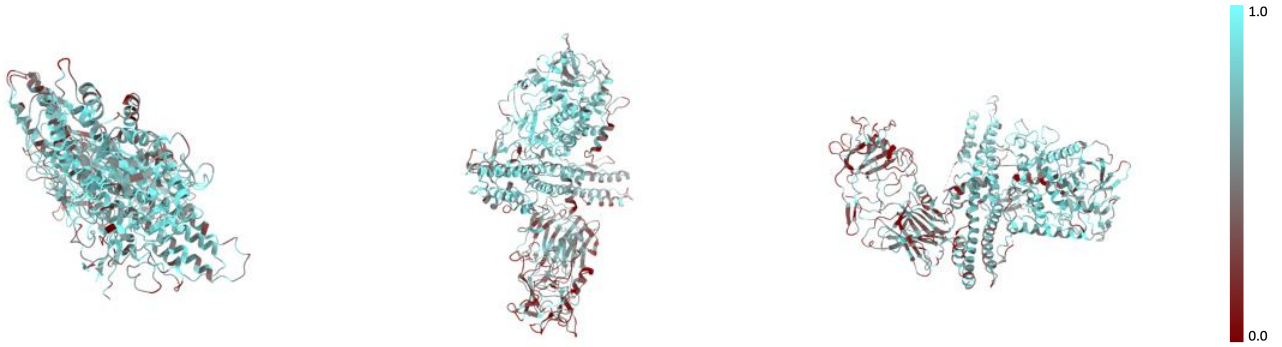
9.2 Q-score mapped to coordinate model (i)



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.

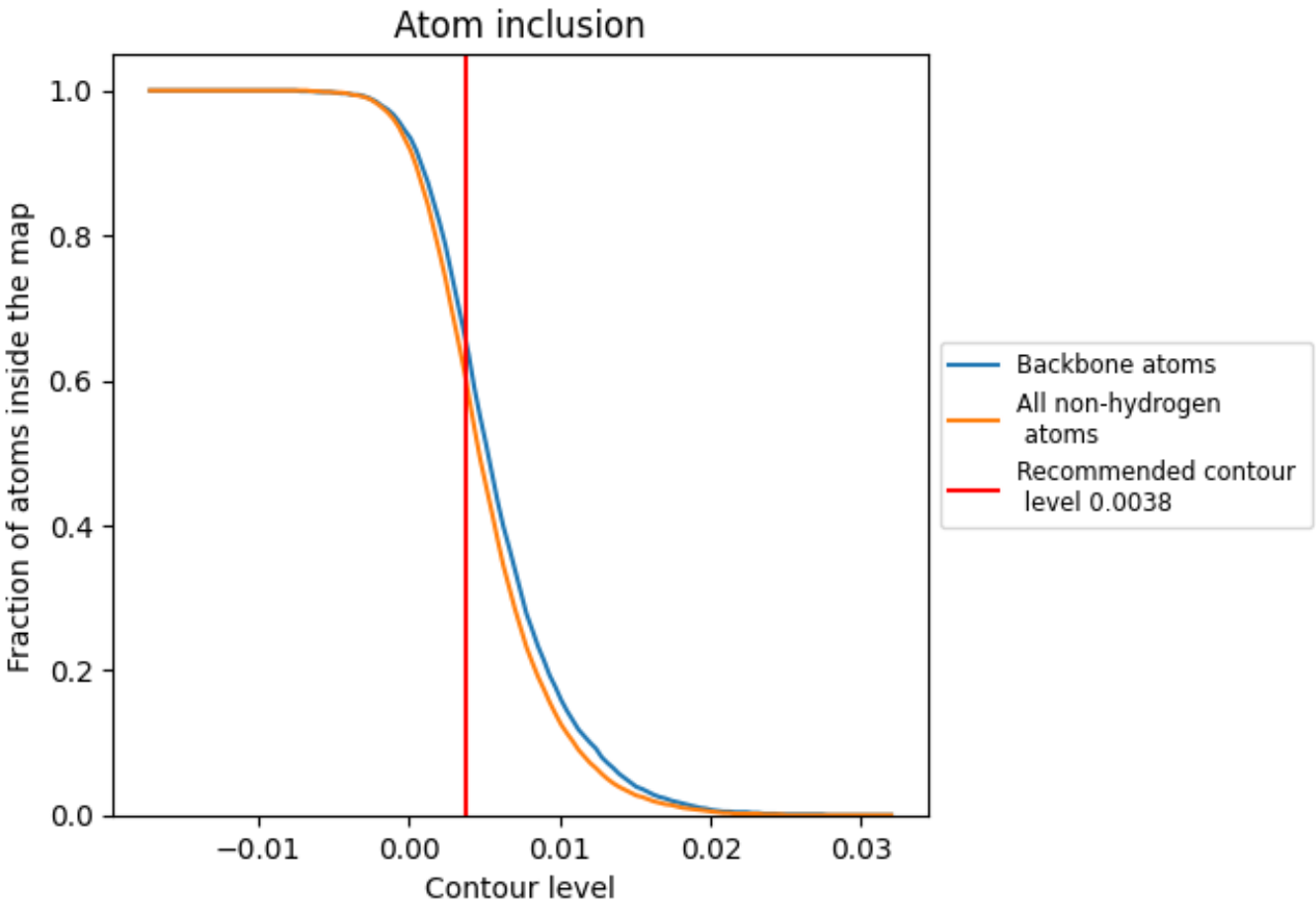
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0038).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 60% 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 (0.0038) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.6000	0.3320
A	0.7290	0.3880
B	0.5330	0.3040