wwPDB EM Validation Summary Report

Dec 17, 2022 – 08:19 am GMT

PDB ID	:	6Z12
EMDB ID	:	EMD-4460
Title	:	Salmonella AcrB solubilised in the SMA copolymer
Authors	:	Muench, s.p.; Johnson, R.M.
Deposited on	:	2020-05-11
Resolution	:	4.60 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:

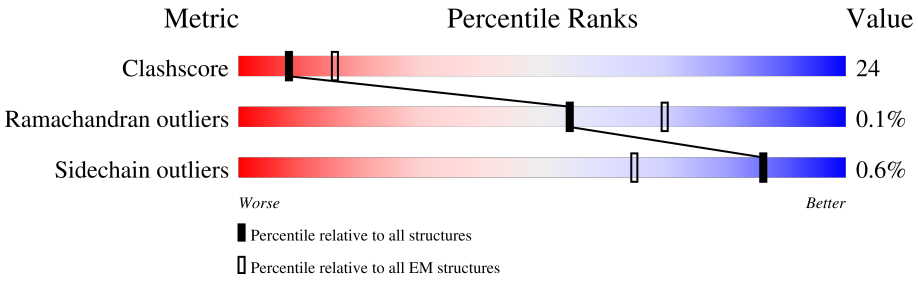
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.60 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	1049	56% 41% .
1	B	1049	55% 41% . .
1	C	1049	53% 43% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 44768 atoms, of which 21585 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1015	Total	C	H	N	O	S	0	0
			15044	4994	7303	1269	1437	41		
1	B	1019	Total	C	H	N	O	S	0	0
			15064	5006	7300	1273	1444	41		
1	C	1010	Total	C	H	N	O	S	0	0
			14660	4954	6982	1257	1426	41		

There are 3 discrepancies between the modelled and reference sequences:

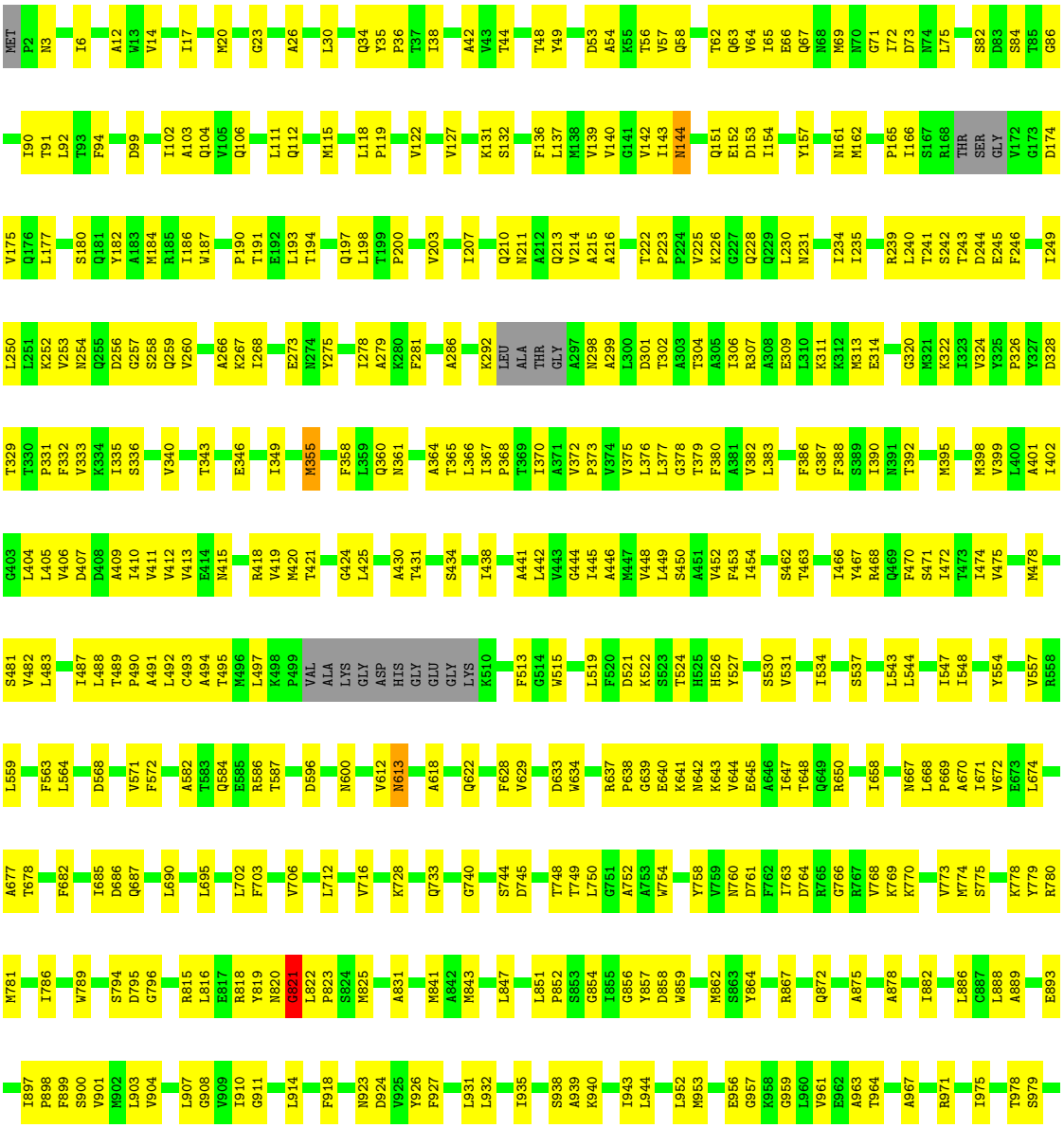
Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ASP	GLY	conflict	UNP A0A3U3J7F4
B	288	ASP	GLY	conflict	UNP A0A3U3J7F4
C	288	ASP	GLY	conflict	UNP A0A3U3J7F4

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.

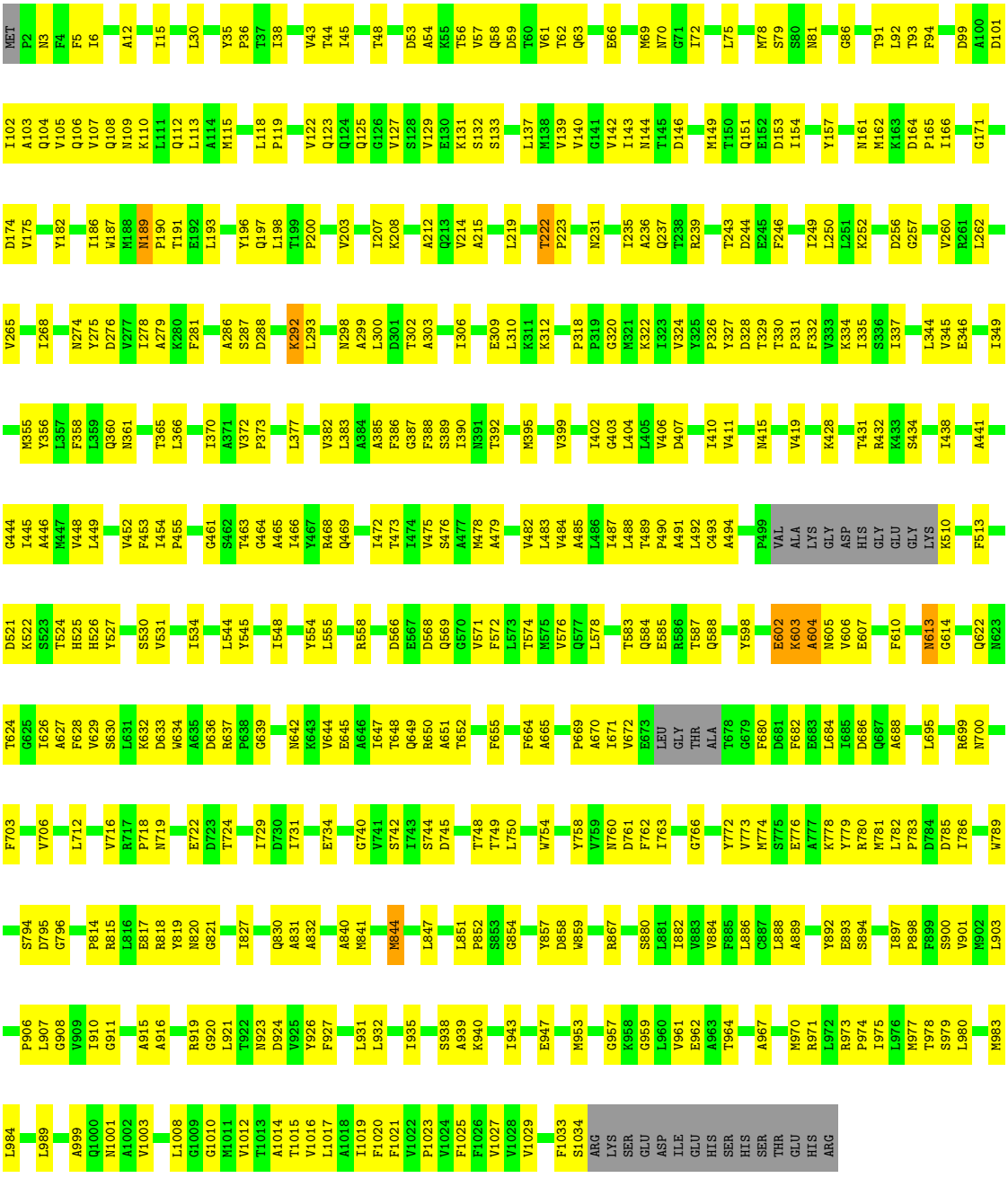
- Molecule 1: Efflux pump membrane transporter

Chain A:



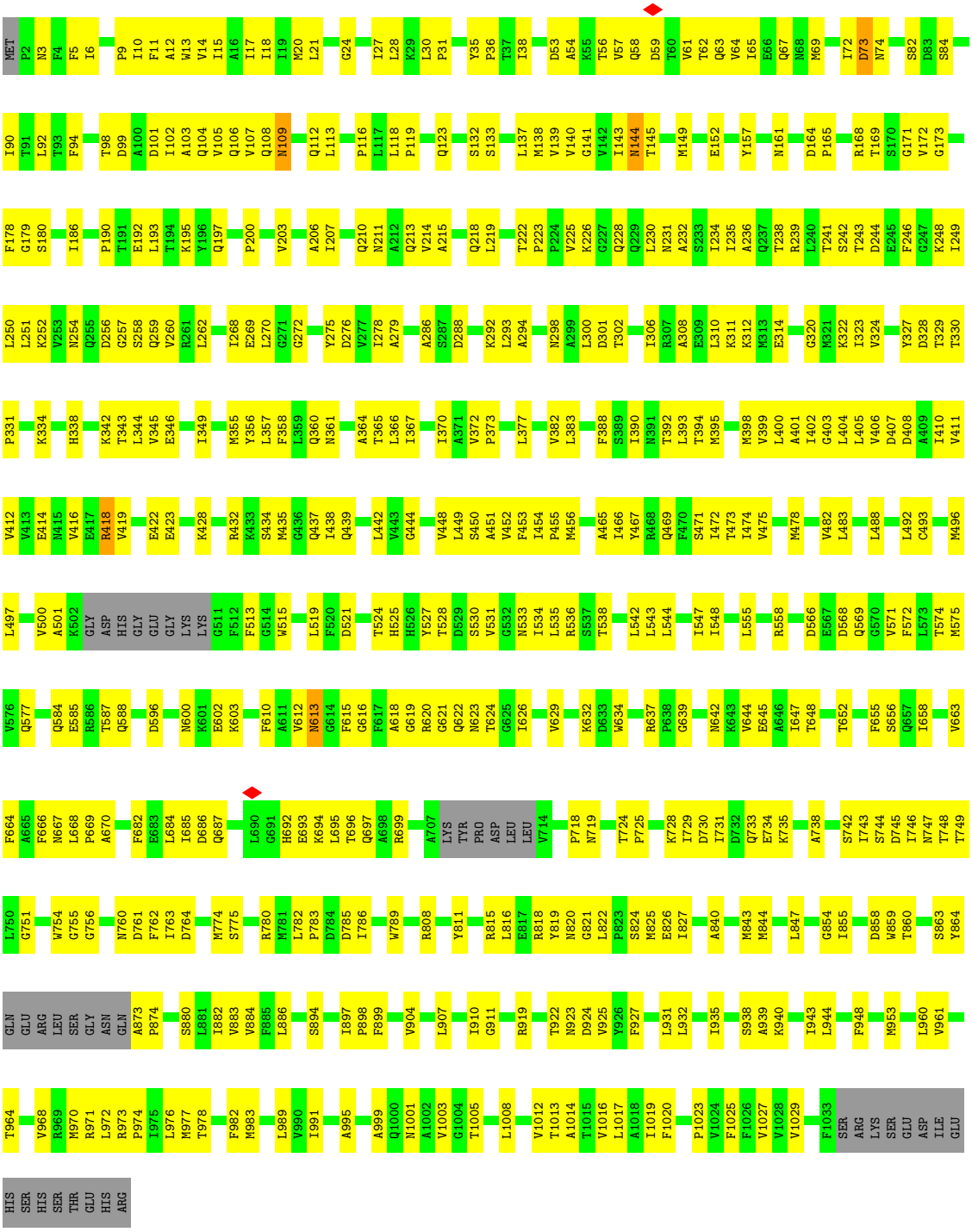
• Molecule 1: Efflux pump membrane transporter

Chain B:



• Molecule 1: Efflux pump membrane transporter

Chain C:


MET P2 N3 F4 F5 I6 P9 I10 F11 A12 W13 V14 I15 A16 I17 I18 I19 M20 L21 G24 I27 L28 K29 L30 P31 Y35 P36 T37 I38 D53 A54 K55 T56 V57 Q58 D59 T60 V61 T62 Q63 V64 I65 E66 Q67 N68 M69 I72 D73 N74 S82 D83 S84
I90 T91 L92 T93 F94 T98 D99 A100 D101 I102 A103 Q104 V105 Q106 V107 Q108 N109 Q112 L113 P116 L117 L118 P119 Q123 S132 S133 L137 M138 V139 V140 G141 V142 I143 N144 T145 M149 E152 Y157 N161 D164 P165 R168 T169 S170 G171 V172 G173
F178 G179 S180 I186 P190 T191 E192 L193 T194 K195 Y196 Q197 P200 V203 A206 I207 Q210 N211 A212 Q213 V214 A215 Q218 L219 T222 P223 P224 V225 K226 G227 Q228 Q229 L230 N231 A232 S233 I234 I235 A236 Q237 T238 R239 L240 T241 S242 T243 D244 E245 F246 G247 K248 I249
L250 L251 K252 V253 N254 Q255 D256 G257 S258 Q259 V260 R261 L262 I268 E269 L270 G271 G272 Y275 D276 V277 I278 A279 A286 S287 D288 K292 L293 A294 N298 A299 L300 D301 T302 I306 R307 A308 E309 L310 K311 K312 M313 E314 G320 M321 K322 I323 V324 Y327 D328 T329 T330
P331 K334 H338 K342 T343 L344 V345 E346 I349 M355 Y356 L357 F358 L359 Q360 N361 A364 T365 L366 I367 I370 A371 V372 P373 L377 V382 L383 F388 S389 I390 N391 T392 L393 T394 M395 M398 V399 L400 A401 I402 G403 L404 L405 V406 D407 D408 A409 I410 V411
V412 V413 E414 N415 V416 E417 R418 V419 E422 E423 K428 R432 K433 S434 M435 G436 Q437 I438 Q439 A364 T365 L442 V443 G444 I370 A371 V448 L449 S450 A451 V452 F453 I454 P455 M456 V382 L383 A465 I466 Y467 R468 Q469 F470 S471 I472 T473 I474 V475 M478 V482 L483 L488 L492 C493 M496
L497 V500 A501 K502 GLY ASP HIS GLY GLU GLY LYS LYS G511 F512 F513 G514 W515 L519 F520 D521 T524 H525 H526 Y527 T528 D529 S530 V531 G532 N533 I534 L535 R536 S537 T538 L542 L543 L544 I547 I548 L555 R558 D566 E567 D568 Q569 G570 V571 F572 L573 T574 M575
V576 Q577 Q584 E585 R586 T587 Q588 D596 N600 K601 E602 K603 F610 A611 V612 N613 G614 F615 G616 F617 A618 G619 R620 G621 Q622 N623 T624 G625 I626 V629 K632 D633 W634 R637 P638 G639 N642 K643 V644 E645 A646 I647 T648 T652 F655 S656 Q657 I658 V663
F664 A665 F666 N667 L668 P669 A670 F682 E683 L684 I685 D686 Q687 L690 G691 H692 E693 K694 L695 T696 Q697 A698 R699 A707 LYS TYR PRO ASP LEU LEU V714 P718 N719 T724 P725 K728 I729 D730 I731 D732 Q733 E734 K735 A738 S742 I743 S744 D745 I746 N747 T748 T749
L750 G751 W754 G755 G756 N760 D761 F762 I763 D764 M774 S775 R780 M781 L782 P783 D784 D785 I786 W789 R808 Y811 R815 L816 E817 R818 Y819 N820 G821 L822 P823 S824 M825 E826 I827 A840 M843 M844 L847 G854 I855 D858 W859 T860 S863 Y864
GLN GLU ARG LEU SER GLY ASN GLN A873 P874 S880 L881 I882 V883 V884 F885 L886 S894 I897 P898 F899 V904 L907 I910 G911 R919 T922 N923 D924 V925 Y926 F927 L931 L932 I935 S938 A939 K940 I943 L944 G954 I955 D958 W959 T960 S963 Y964
T964 V968 R969 M970 R971 L972 R973 P974 I975 L976 M977 T978 F982 M983 L989 V990 I991 A995 A999 Q1000 N1001 A1002 V1003 G1004 T1005 L1008 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 P1023 V1024 F1025 F1026 V1027 V1028 V1029 F1033 SER ARG LYS SER GLU ASP ILE GLU
HIS SER HIS SER THR GLU HIS ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	316000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0196	Depositor
Map size (Å)	214.00002, 214.00002, 214.00002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.44	0/7889	0.52	0/10714
1	B	0.45	0/7913	0.52	0/10748
1	C	0.45	0/7824	0.51	0/10628
All	All	0.45	0/23626	0.52	0/32090

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
1	A	0	2
1	B	0	3
1	C	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	559	LEU	Peptide
1	A	821	GLY	Peptide
1	B	287	SER	Peptide
1	B	292	LYS	Peptide
1	B	602	GLU	Peptide

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	7741	7303	7893	366	0
1	B	7764	7300	7914	390	0
1	C	7678	6982	7833	415	0
All	All	23183	21585	23640	1144	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 24.

The worst 5 of 1144 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:576:VAL:O	1:B:624:THR:OG1	1.80	1.00
1:B:406:VAL:HG12	1:B:410:ILE:HD11	1.45	0.97
1:A:766:GLY:O	1:B:63:GLN:NE2	1.98	0.96
1:A:240:LEU:HB2	1:A:246:PHE:HE1	1.29	0.96
1:B:584:GLN:N	1:B:622:GLN:OE1	1.98	0.96

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1007/1049 (96%)	881 (88%)	125 (12%)	1 (0%)	51 85
1	B	1013/1049 (97%)	871 (86%)	140 (14%)	2 (0%)	47 81
1	C	1002/1049 (96%)	879 (88%)	123 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3022/3147 (96%)	2631 (87%)	388 (13%)	3 (0%)	54 85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	604	ALA
1	B	603	LYS
1	A	821	GLY

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	832/859 (97%)	829 (100%)	3 (0%)	91 94
1	B	835/859 (97%)	829 (99%)	6 (1%)	84 90
1	C	824/859 (96%)	819 (99%)	5 (1%)	86 92
All	All	2491/2577 (97%)	2477 (99%)	14 (1%)	86 92

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	719	ASN
1	B	844	MET
1	C	613	ASN
1	C	144	ASN
1	C	418	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	ASN
1	C	584	GLN
1	C	104	GLN

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Mol	Chain	Res	Type
1	C	161	ASN
1	C	613	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

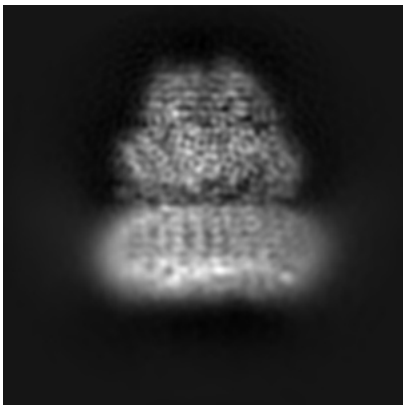
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4460. These allow visual inspection of the internal detail of the map and identification of artifacts.

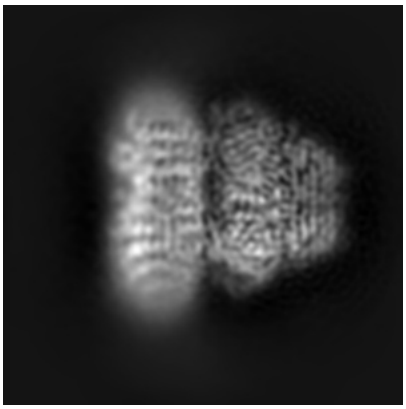
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

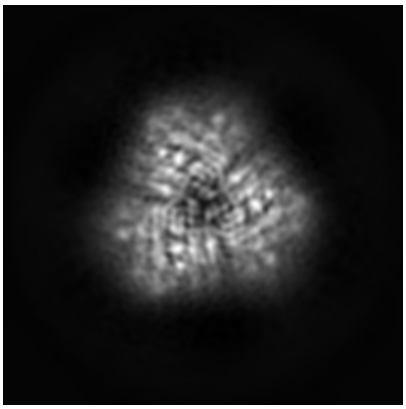
6.1.1 Primary map



X

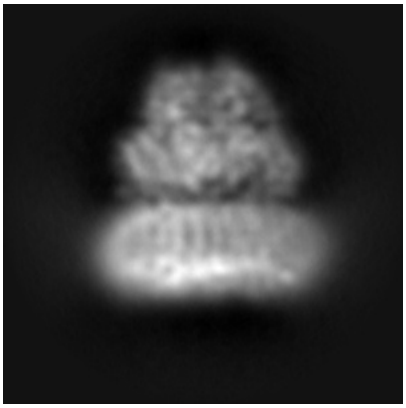


Y

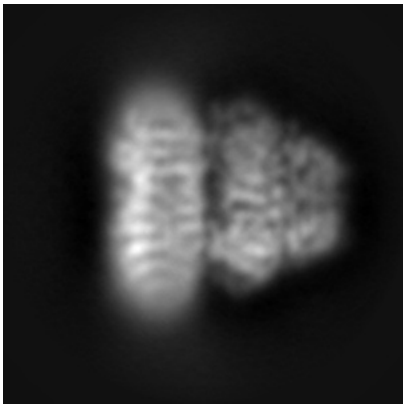


Z

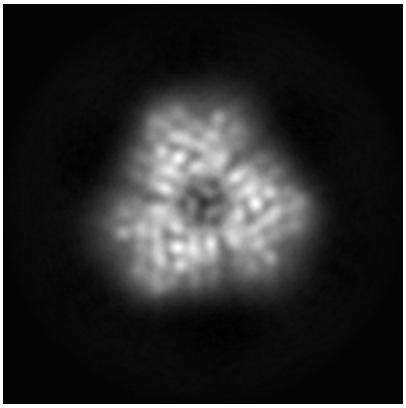
6.1.2 Raw map



X



Y

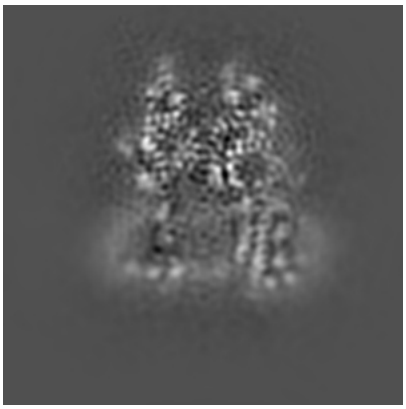


Z

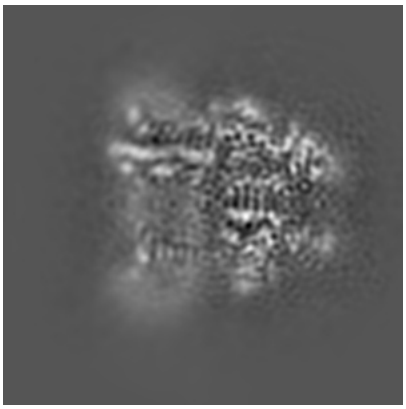
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

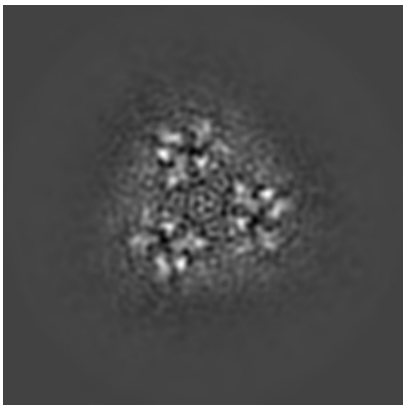
6.2.1 Primary map



X Index: 100

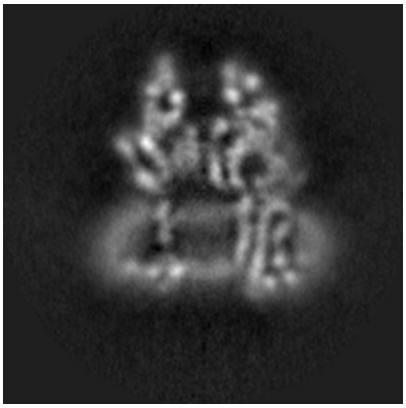


Y Index: 100

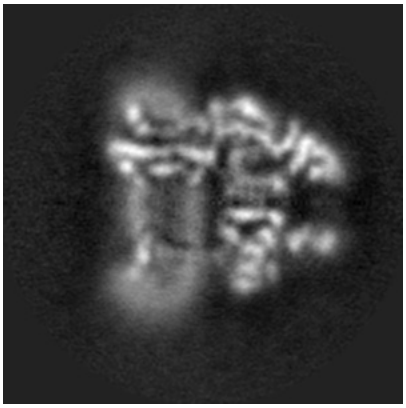


Z Index: 100

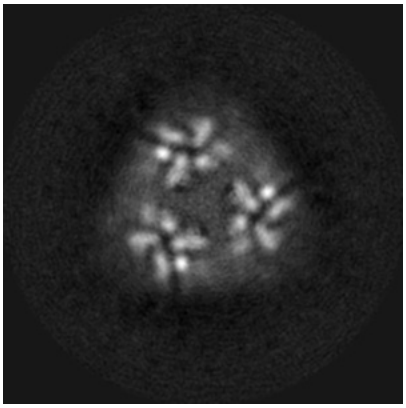
6.2.2 Raw map



X Index: 100



Y Index: 100

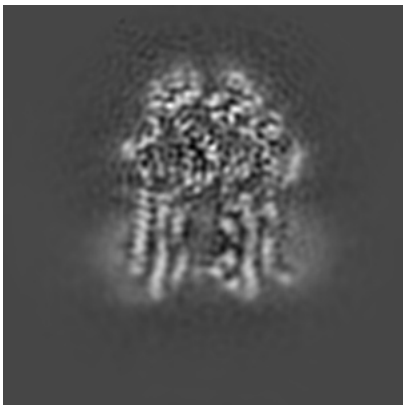


Z Index: 100

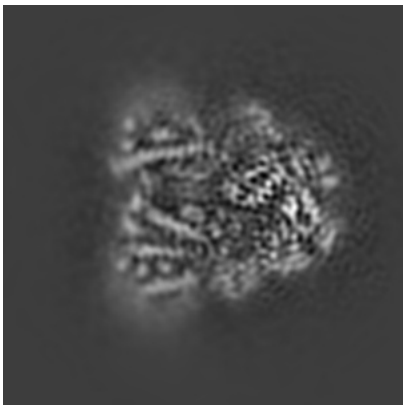
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

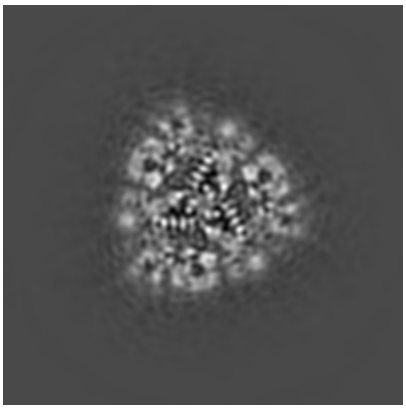
6.3.1 Primary map



X Index: 87

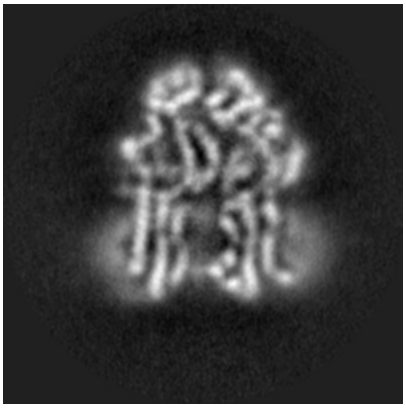


Y Index: 86

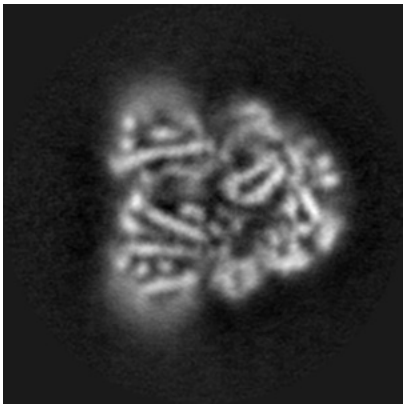


Z Index: 128

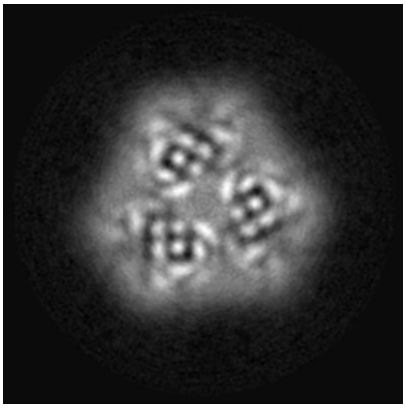
6.3.2 Raw map



X Index: 87



Y Index: 86

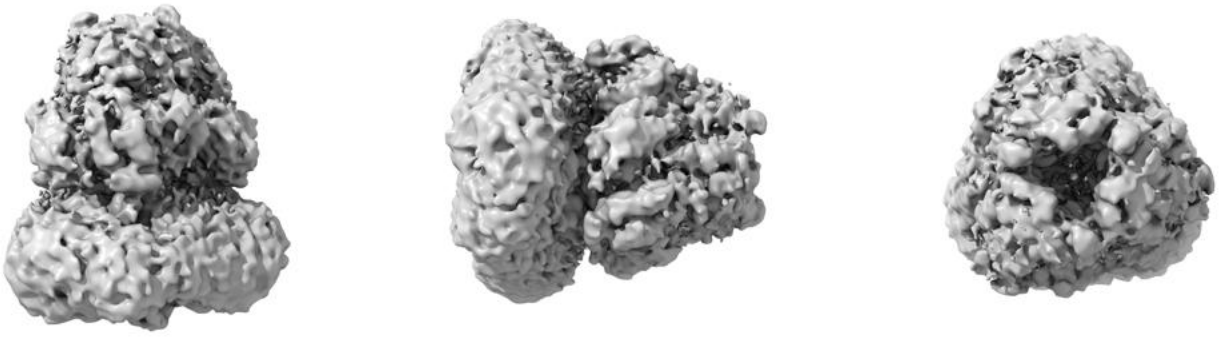


Z Index: 67

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0196. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

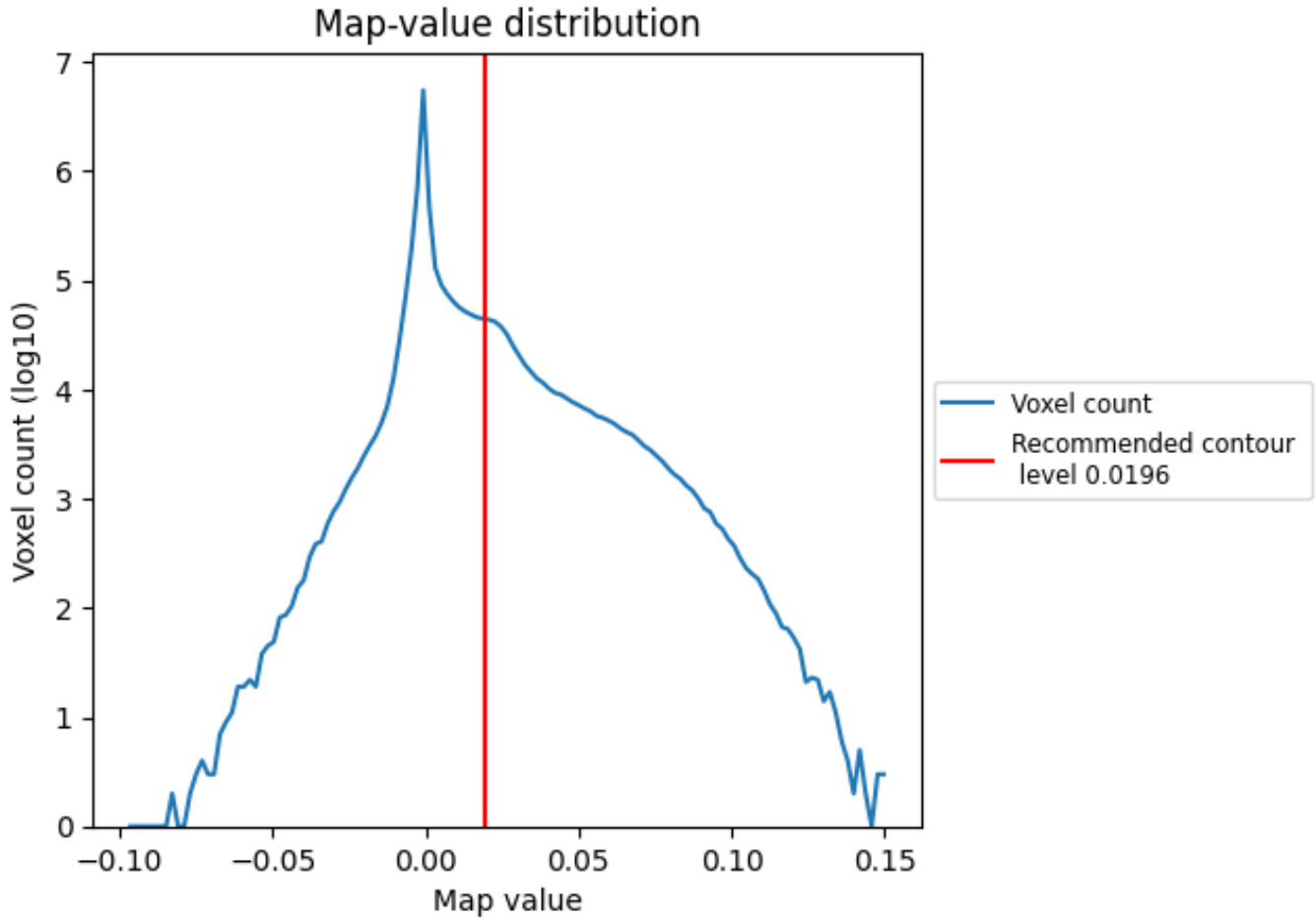
6.5 Mask visualisation (i)

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

7 Map analysis

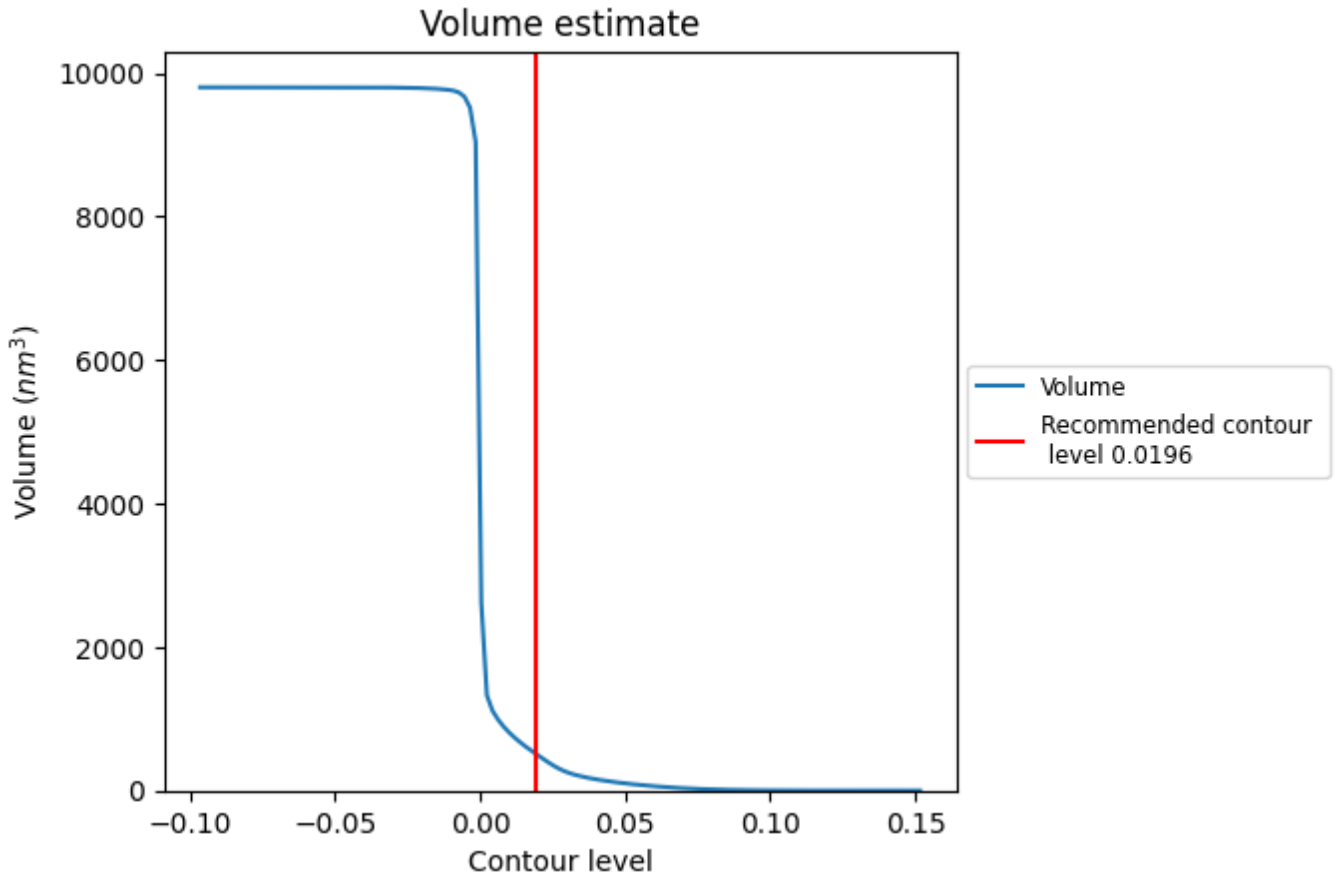
This section contains the results of statistical analysis of the map.

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.

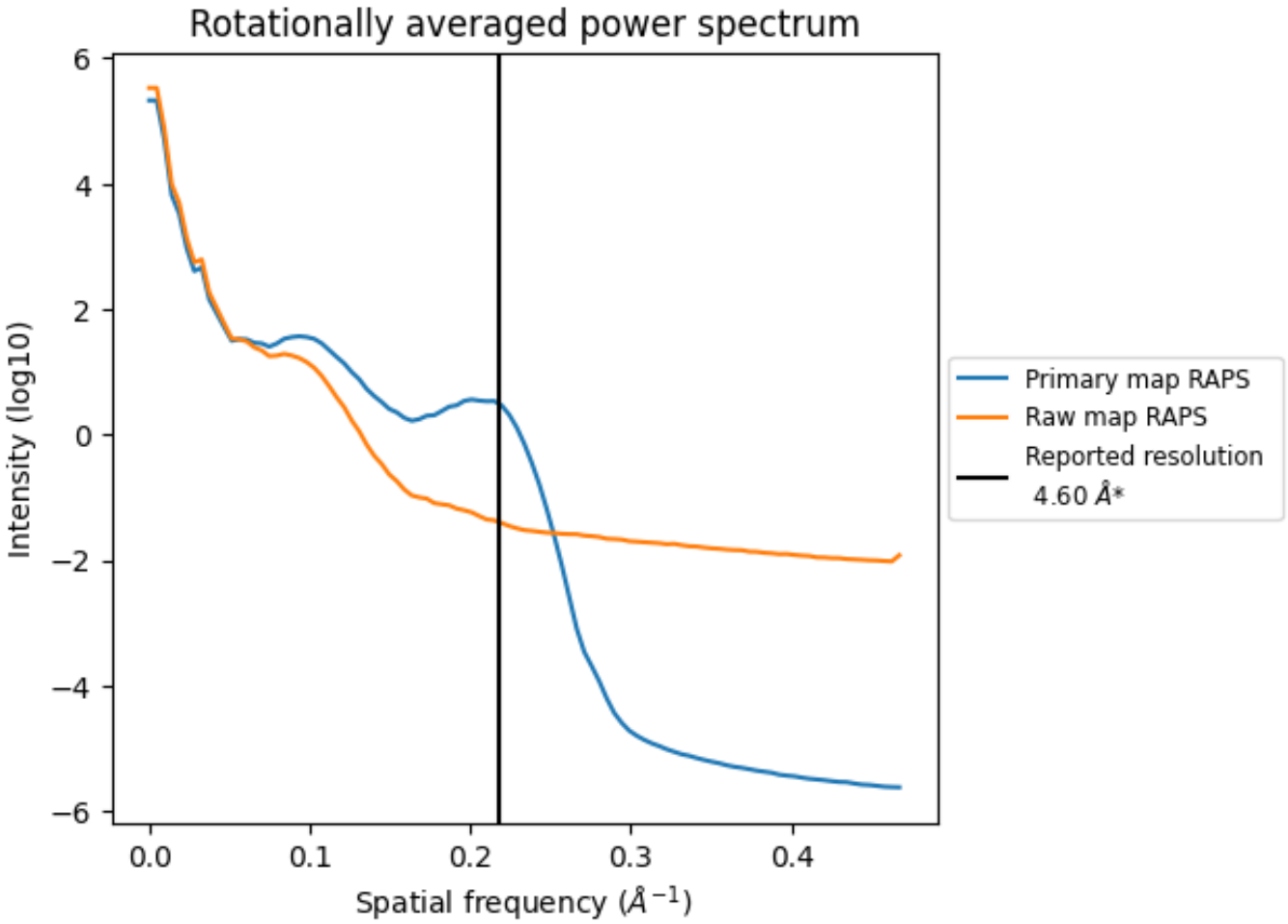
7.2 Volume estimate (i)



The volume at the recommended contour level is 503 nm^3; this corresponds to an approximate mass of 454 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)

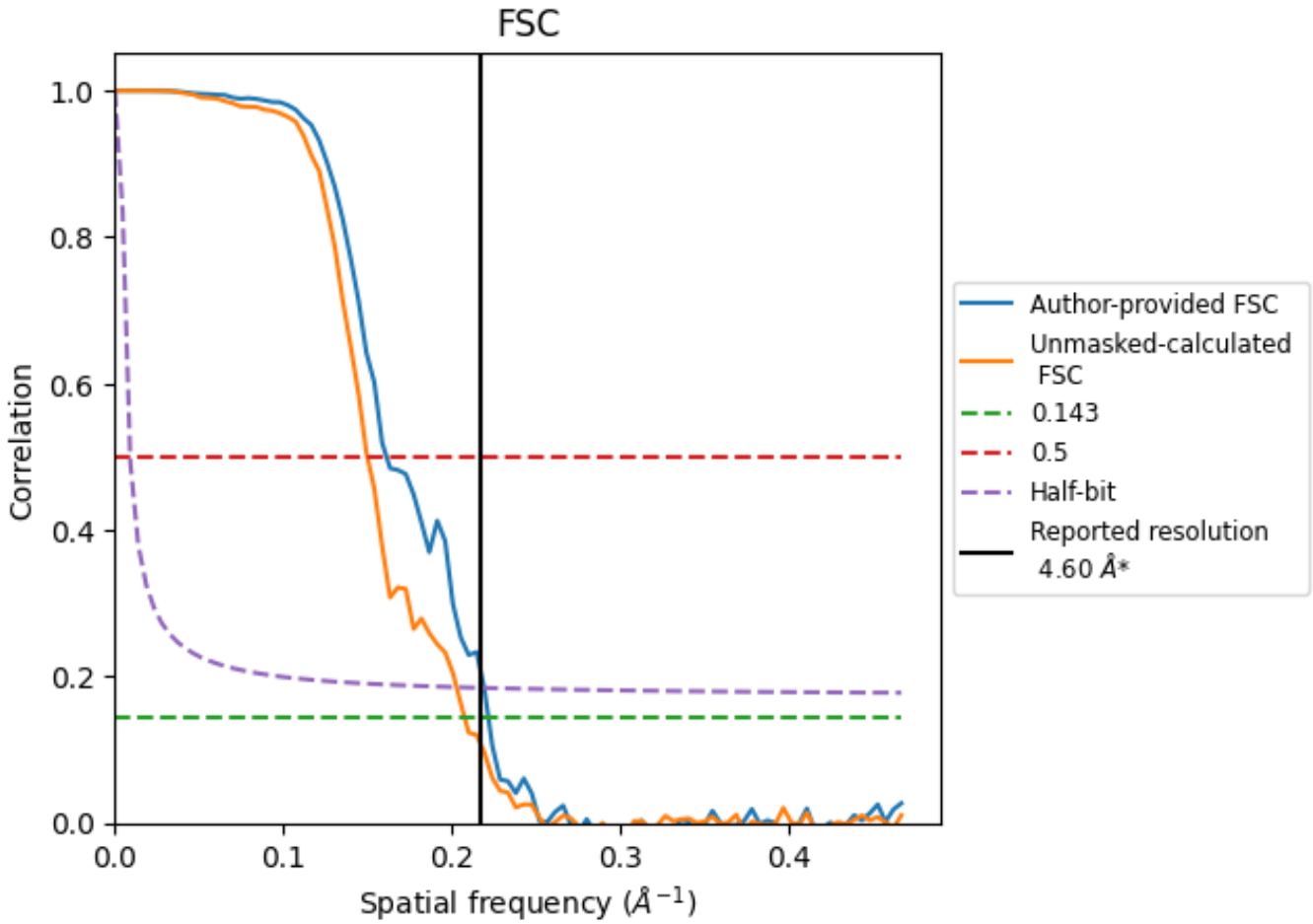


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

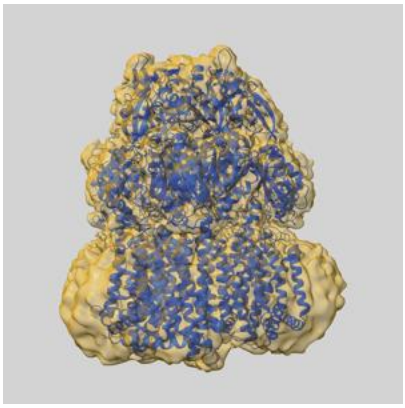
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.50	6.20	4.56
Unmasked-calculated*	4.81	6.66	4.92

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

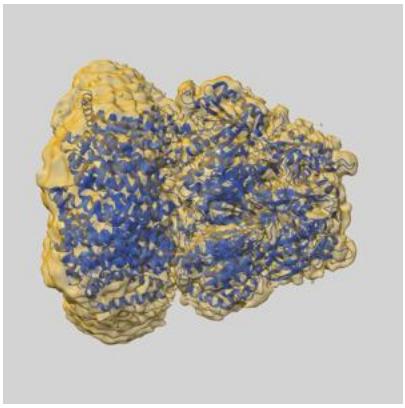
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4460 and PDB model 6Z12. Per-residue inclusion information can be found in section 3 on page 4.

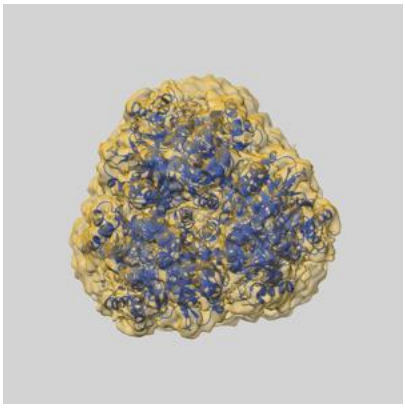
9.1 Map-model overlay



X



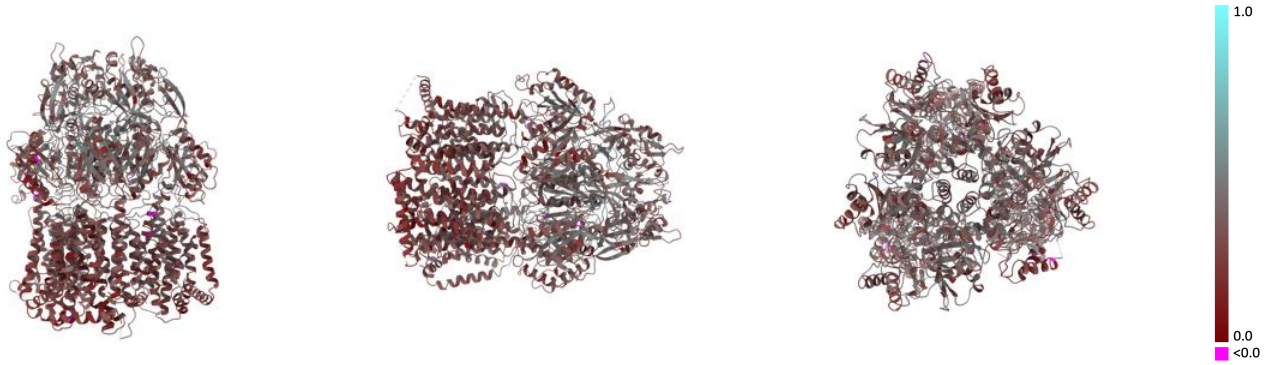
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0196 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.

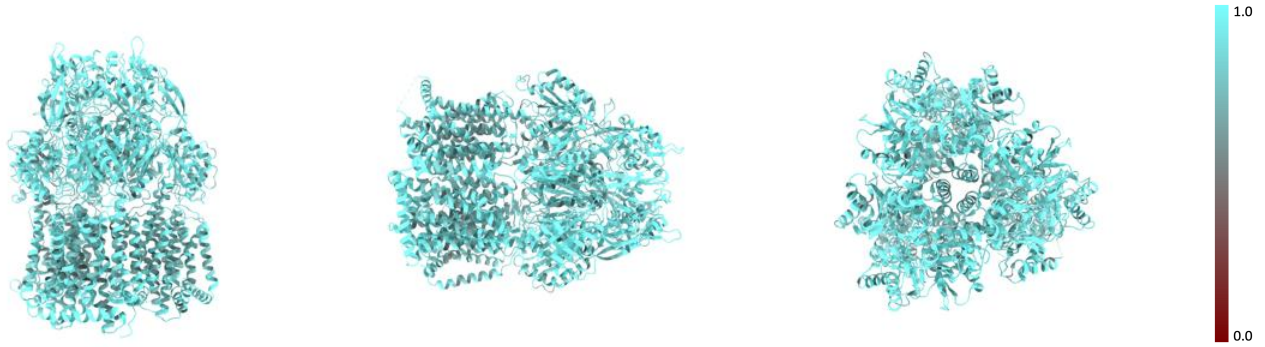
9.2 Q-score mapped to coordinate model (i)



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.

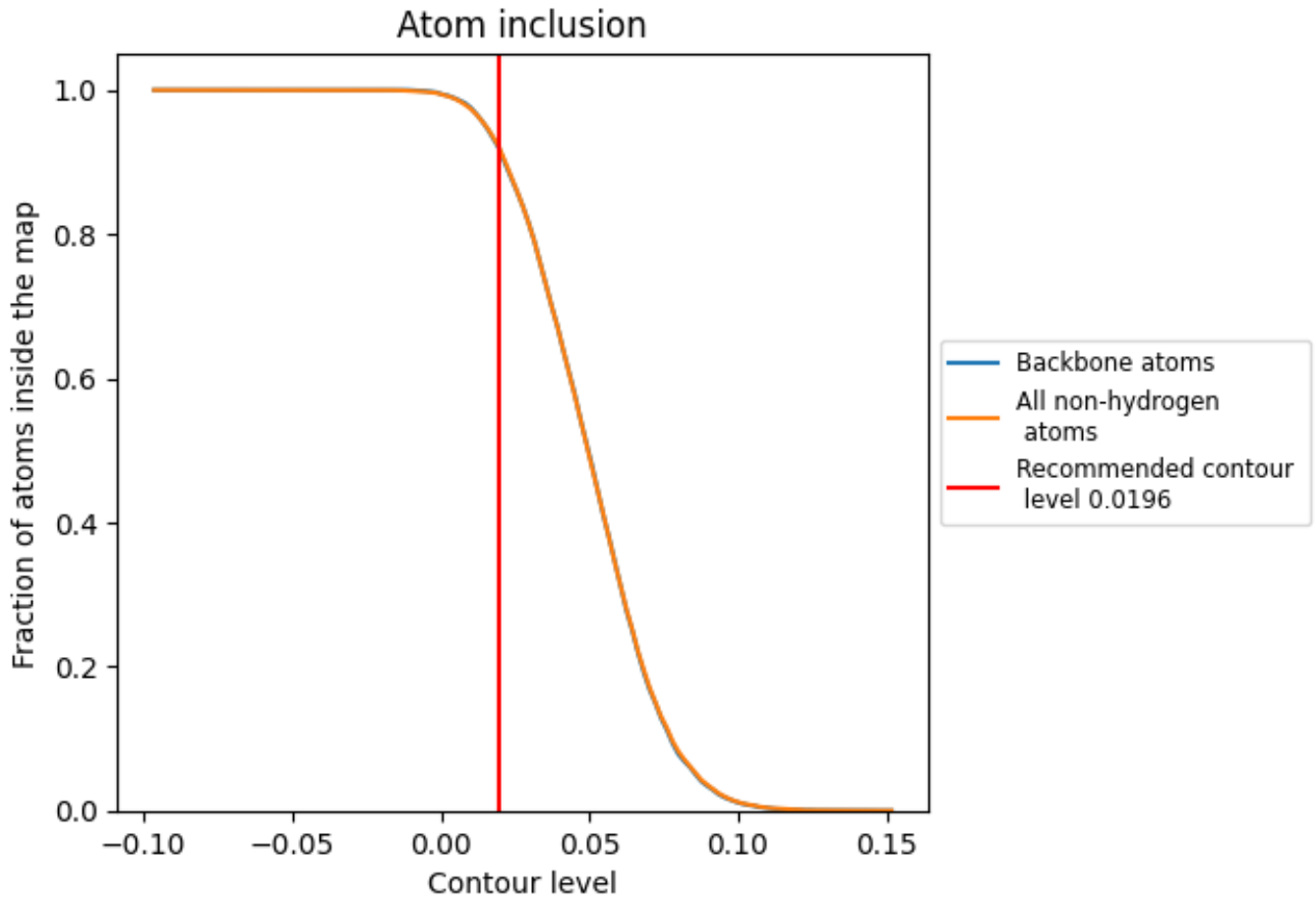
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0196).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.0196) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9213	0.3310
A	0.9207	0.3310
B	0.9200	0.3320
C	0.9174	0.3290