Full wwPDB EM Validation Report

Mar 30, 2021 – 11:05 am BST

PDB ID	:	7ADK
EMDB ID	:	EMD-11729
Title	:	Structure of the mycoplasma MIB and MIP proteins
Authors	:	Nottelet, P.; Bataille, L.; Gourgues, G.; Anger, R.; Lartigue, C.; Sirand-Pugnet, P.; Marza, E.; Fronzes, R.; Arfi, Y.
Deposited on	:	2020-09-15
Resolution	:	2.80 Å(reported)

This is a Full wwPDB EM Validation 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 following versions of software and data (see references (1)) were used in the production of this report:

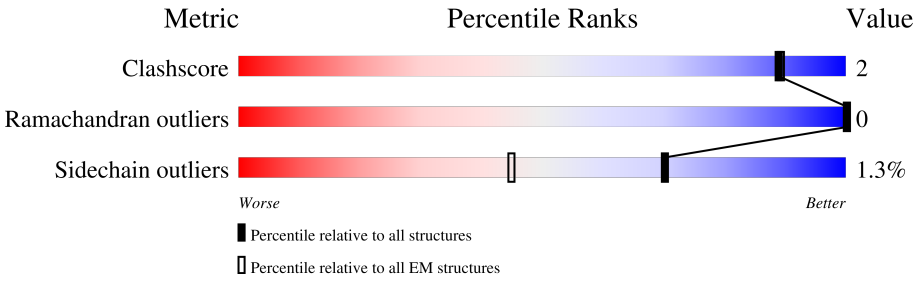
EMDB validation analysis	:	0.0.0.dev75
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	750	9% 76% 5% 18%
2	B	861	19% 75% 6% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20869 atoms, of which 10260 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 Putative immunoglobulin-blocking virulence protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	613	Total	C	H	N	O	S	0	0
			9710	3078	4790	850	989	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP A0A446C0S7
A	418	VAL	UNK	conflict	UNP A0A446C0S7
A	513	LYS	UNK	conflict	UNP A0A446C0S7

- Molecule 2 is a protein called Lipoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	704	Total	C	H	N	O	S	0	0
			11159	3612	5470	932	1139	6		

There is a discrepancy between the modelled and reference sequences:

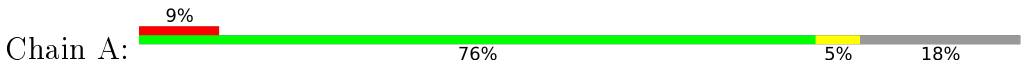
Chain	Residue	Modelled	Actual	Comment	Reference
B	810	LEU	UNK	conflict	UNP A0A446C0V0

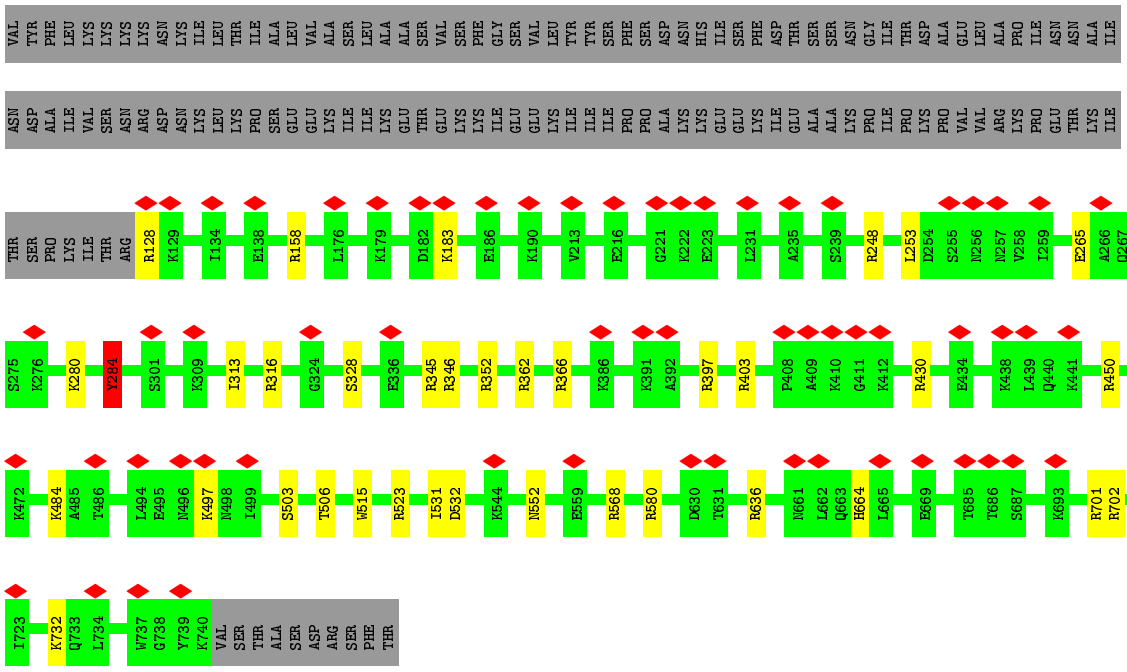
3 Residue-property plots (i)

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: Putative immunoglobulin-blocking virulence protein

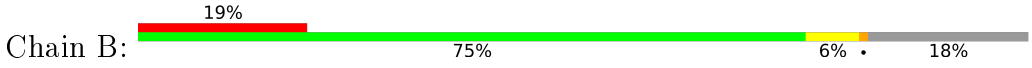
Chain A:

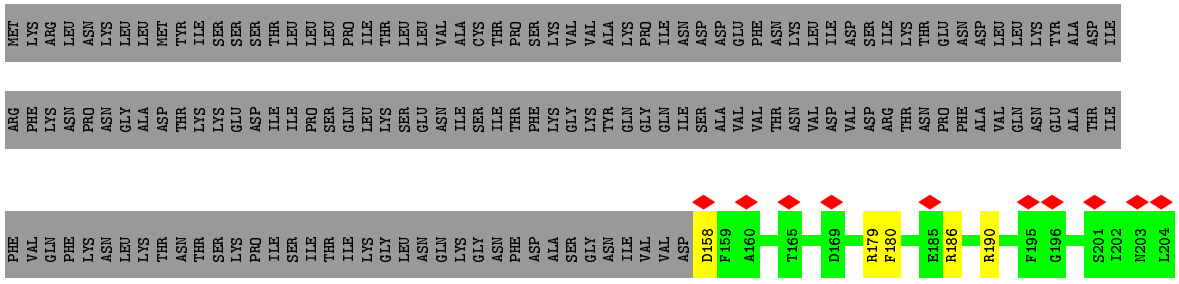


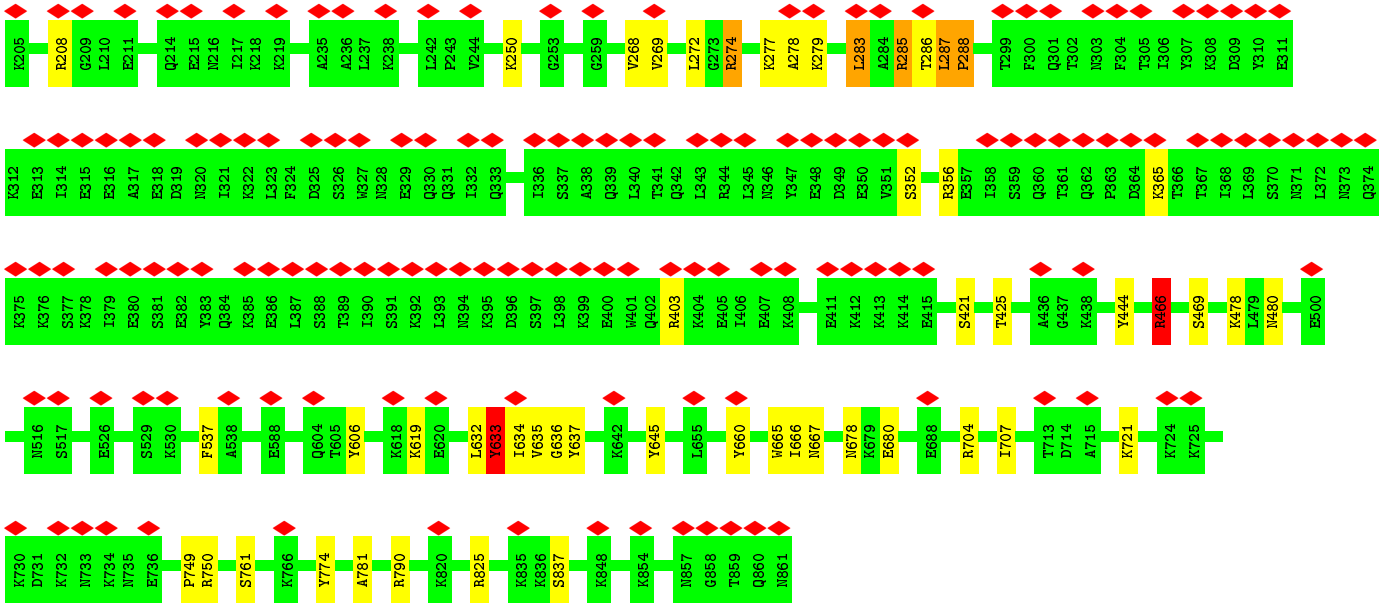


- Molecule 2: Lipoprotein

Chain B:






K205 R208 G209 L210 E211 Q214 E215 N216 I217 K218 K219 A235 A236 L237 K238 L242 P243 V244 K250 G253 G259 V268 V269 L272 G273 R274 K277 A278 K279 L283 A284 R285 T286 L287 P288 T299 F300 Q301 T302 N303 F304 T305 I306 Y307 K308 D309 Y310 E311
K312 E313 I314 E315 E316 A317 E318 D319 N320 I321 K322 L323 F324 D325 S326 W327 N328 E329 Q330 Q331 I332 Q333 I336 S337 A338 Q339 L340 T341 Q342 L343 R344 L345 N346 Y347 E348 D349 E350 V351 S352 R356 E357 I358 S359 Q360 T361 Q362 P363 D364 K365 T366 T367 I368 L369 S370 N371 L372 N373 Q374
K375 K376 S377 K378 I379 E380 S381 E382 Y383 Q384 K385 E386 L387 S388 T389 I390 S391 K392 L393 N394 K395 D396 S397 L398 K399 E400 W401 Q402 R403 K404 E405 I406 E407 K408 E411 K412 K413 K414 E415 S421 T425 A436 G437 K438 Y444 R466 S469 K478 L479 N480 E500
N516 S517 E526 S529 K530 F537 A538 E588 Q604 T605 V606 K618 K619 E620 L632 V633 I634 V635 G636 Y637 K642 Y645 L655 Y660 W665 I666 N667 N678 K679 E680 E688 R704 I707 T713 D714 A715 K721 K724 K725
K730 D731 K732 N733 K734 N735 E736 P749 R750 S761 K766 Y774 A781 R790 K820 R825 K835 K836 S837 K848 K854 N857 G858 T859 Q860 N861

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	255911	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 ($e^-/Å^2$)	1.45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.810	Depositor
Minimum map value	-24.764	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	212.48, 212.48, 212.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	0.71	0/5014	1.10	26/6760 (0.4%)
2	B	0.71	0/5807	1.08	16/7809 (0.2%)
All	All	0.71	0/10821	1.09	42/14569 (0.3%)

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
2	B	0	9
All	All	0	11

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	450	ARG	NE-CZ-NH2	9.81	125.20	120.30
1	A	450	ARG	NE-CZ-NH1	-9.61	115.49	120.30
1	A	284	TYR	CB-CG-CD2	-8.87	115.68	121.00
1	A	568	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	346	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	397	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	A	284	TYR	CB-CA-C	7.39	125.18	110.40
1	A	362	ARG	NE-CZ-NH2	7.31	123.96	120.30
1	A	316	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	430	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	A	715	ARG	NE-CZ-NH2	7.03	123.82	120.30
1	A	580	ARG	NE-CZ-NH2	6.91	123.76	120.30
2	B	356	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	B	208	ARG	NE-CZ-NH1	6.74	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	274	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	A	523	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	345	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	636	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	284	TYR	CA-CB-CG	6.26	125.29	113.40
2	B	790	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	352	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	B	403	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	702	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	B	825	ARG	NE-CZ-NH1	6.07	123.33	120.30
2	B	179	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	B	704	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	128	ARG	NE-CZ-NH2	5.89	123.25	120.30
2	B	285	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	158	ARG	NE-CZ-NH1	5.83	123.22	120.30
2	B	750	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	B	208	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	701	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	403	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	450	ARG	CD-NE-CZ	5.54	131.35	123.60
1	A	248	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	366	ARG	NE-CZ-NH2	5.40	123.00	120.30
2	B	660	TYR	CB-CG-CD2	-5.26	117.84	121.00
2	B	186	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	397	ARG	NE-CZ-NH1	-5.21	117.69	120.30
2	B	287	LEU	CB-CA-C	5.15	119.99	110.20
2	B	466	ARG	NE-CZ-NH2	5.03	122.82	120.30
2	B	190	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	TYR	Sidechain
1	A	497	LYS	Peptide
2	B	285	ARG	Sidechain
2	B	288	PRO	Peptide
2	B	421	SER	Peptide
2	B	444	TYR	Sidechain
2	B	466	ARG	Sidechain
2	B	606	TYR	Sidechain
2	B	633	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	637	TYR	Sidechain
2	B	774	TYR	Sidechain

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	4920	4790	4789	13	0
2	B	5689	5470	5463	32	0
All	All	10609	10260	10252	37	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 2.

All (37) 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:484:LYS:HE3	2:B:478:LYS:CD	2.03	0.86
2:B:286:THR:HG21	2:B:635:VAL:HG12	1.64	0.79
1:A:484:LYS:HE3	2:B:478:LYS:HD2	1.72	0.71
2:B:286:THR:CG2	2:B:635:VAL:HG12	2.30	0.60
2:B:269:VAL:HG23	2:B:665:TRP:CE3	2.38	0.59
1:A:462:ALA:HA	2:B:680:GLU:OE2	2.04	0.58
2:B:283:LEU:HD21	2:B:469:SER:HA	1.86	0.57
2:B:635:VAL:HG23	2:B:761:SER:HB3	1.87	0.56
1:A:506:THR:HG21	1:A:515:TRP:CZ2	2.40	0.56
2:B:274:ARG:HH11	2:B:632:LEU:HD11	1.71	0.56
1:A:719:LYS:NZ	2:B:158:ASP:OD2	2.39	0.56
2:B:279:LYS:HA	2:B:283:LEU:HD22	1.92	0.51
2:B:666:ILE:CG1	2:B:667:ASN:H	2.25	0.50
2:B:283:LEU:C	2:B:283:LEU:HD23	2.31	0.50
2:B:666:ILE:HG12	2:B:667:ASN:H	1.77	0.49
2:B:286:THR:HG21	2:B:635:VAL:CG1	2.39	0.49
1:A:484:LYS:HE3	2:B:478:LYS:HD3	1.93	0.48
1:A:280:LYS:HA	1:A:280:LYS:HE2	1.96	0.48
1:A:274:LYS:HE2	2:B:352:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:PHE:CG	2:B:707:ILE:HG23	2.50	0.47
2:B:287:LEU:HG	2:B:288:PRO:HD3	1.97	0.46
2:B:272:LEU:HD22	2:B:278:ALA:CB	2.46	0.46
2:B:425:THR:HG21	2:B:636:GLY:H	1.81	0.45
2:B:633:TYR:CZ	2:B:749:PRO:HB3	2.51	0.45
2:B:286:THR:OG1	2:B:635:VAL:HG12	2.17	0.45
2:B:268:VAL:HA	2:B:645:TYR:CZ	2.52	0.44
2:B:250:LYS:HB2	2:B:781:ALA:HB2	1.98	0.44
1:A:253:LEU:HD23	1:A:284:TYR:CD2	2.53	0.43
1:A:484:LYS:CE	2:B:478:LYS:CD	2.81	0.43
2:B:277:LYS:HE2	2:B:666:ILE:HD11	2.00	0.43
2:B:286:THR:CB	2:B:635:VAL:HG12	2.49	0.42
1:A:531:ILE:HG22	1:A:532:ASP:H	1.84	0.42
1:A:460:ASP:OD2	2:B:678:ASN:ND2	2.51	0.42
2:B:635:VAL:CG2	2:B:761:SER:HB3	2.49	0.41
2:B:180:PHE:CE1	2:B:707:ILE:HD12	2.54	0.41
2:B:634:ILE:HD11	2:B:666:ILE:HD12	2.03	0.40
1:A:313:ILE:HG23	1:A:328:SER:HB3	2.03	0.40

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	611/750 (82%)	569 (93%)	42 (7%)	0	100	100
2	B	702/861 (82%)	620 (88%)	82 (12%)	0	100	100
All	All	1313/1611 (82%)	1189 (91%)	124 (9%)	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	544/668 (81%)	538 (99%)	6 (1%)	73 92
2	B	613/768 (80%)	604 (98%)	9 (2%)	65 89
All	All	1157/1436 (81%)	1142 (99%)	15 (1%)	70 91

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LYS
1	A	265	GLU
1	A	503	SER
1	A	552	ASN
1	A	664	HIS
1	A	732	LYS
2	B	283	LEU
2	B	365	LYS
2	B	466	ARG
2	B	480	ASN
2	B	537	PHE
2	B	619	LYS
2	B	633	TYR
2	B	721	LYS
2	B	837	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	461	GLN
1	A	590	HIS
1	A	711	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.

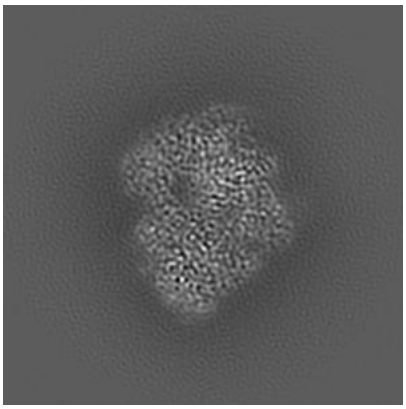
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11729. These allow visual inspection of the internal detail of the map and identification of artifacts.

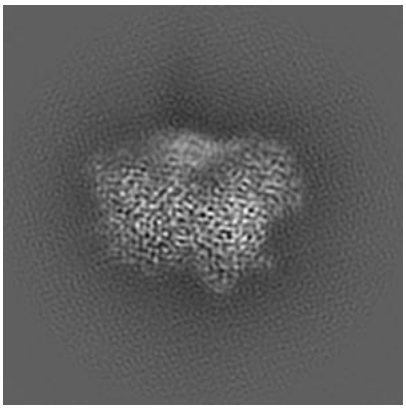
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

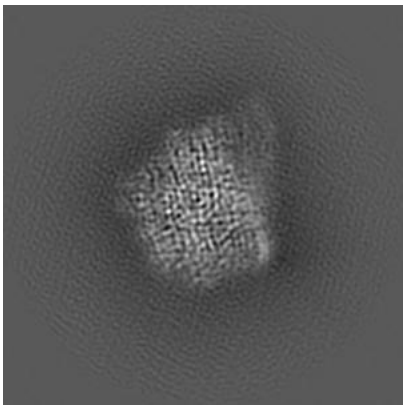
6.1.1 Primary map



X

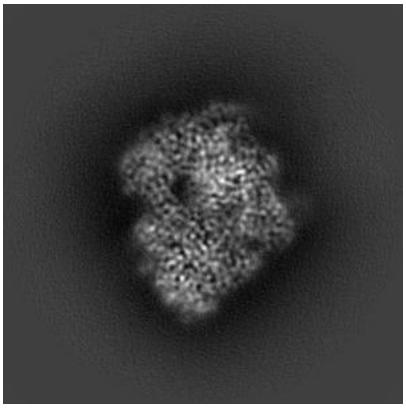


Y

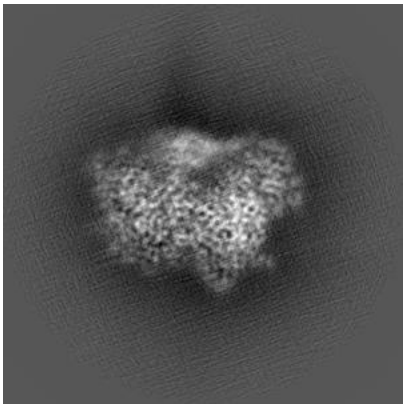


Z

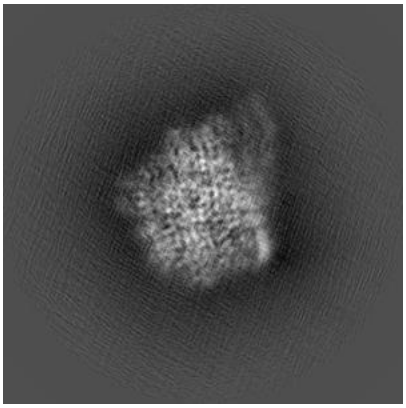
6.1.2 Raw map



X



Y

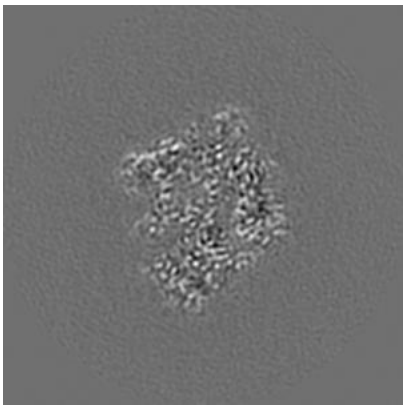


Z

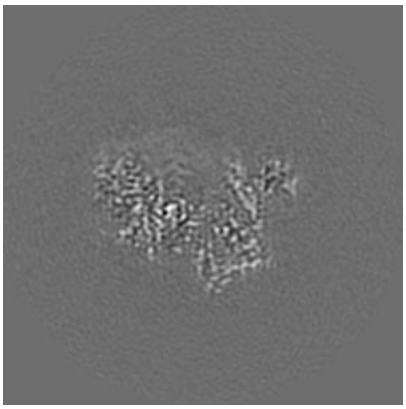
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

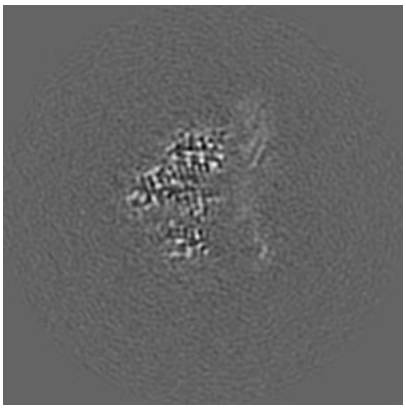
6.2.1 Primary map



X Index: 128

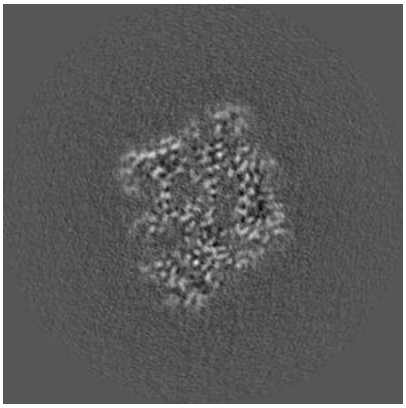


Y Index: 128

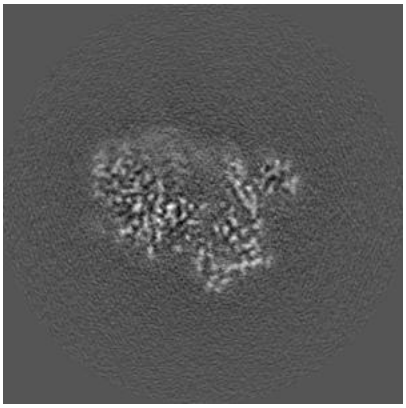


Z Index: 128

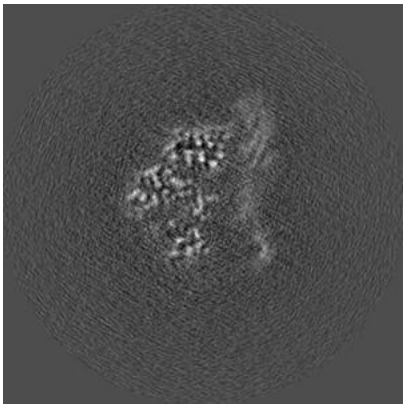
6.2.2 Raw map



X Index: 128



Y Index: 128

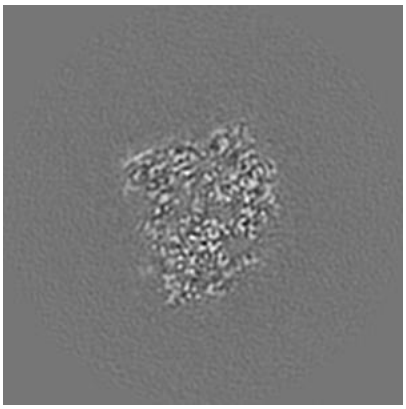


Z Index: 128

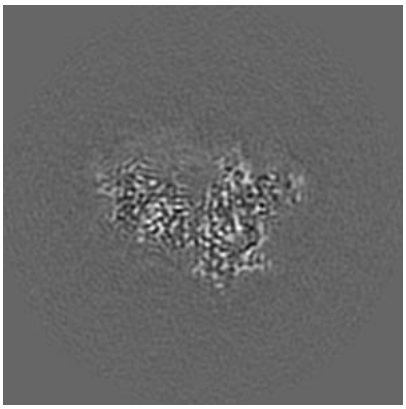
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

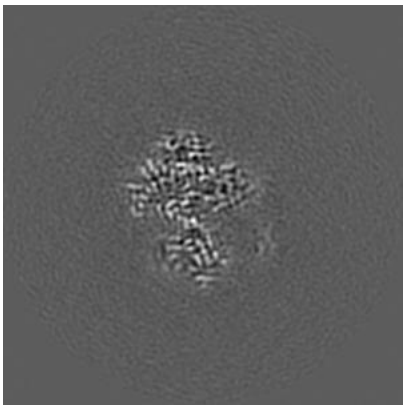
6.3.1 Primary map



X Index: 122

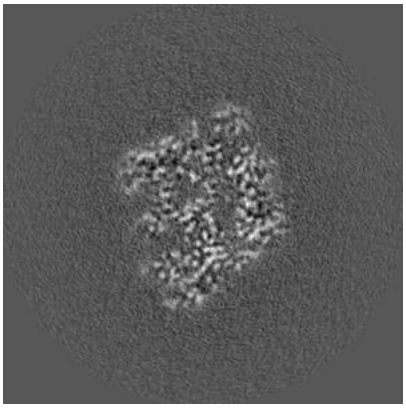


Y Index: 134

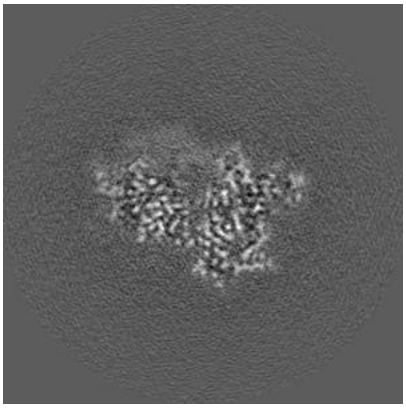


Z Index: 148

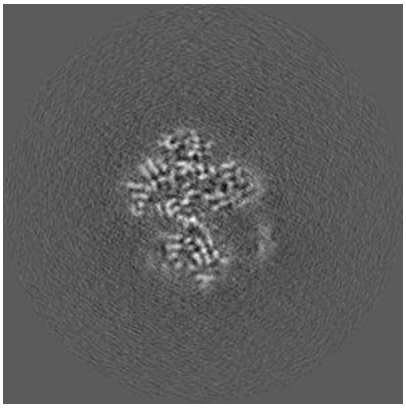
6.3.2 Raw map



X Index: 127



Y Index: 134



Z Index: 148

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

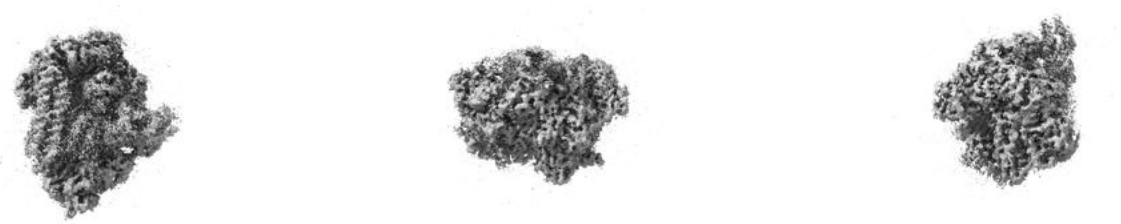
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

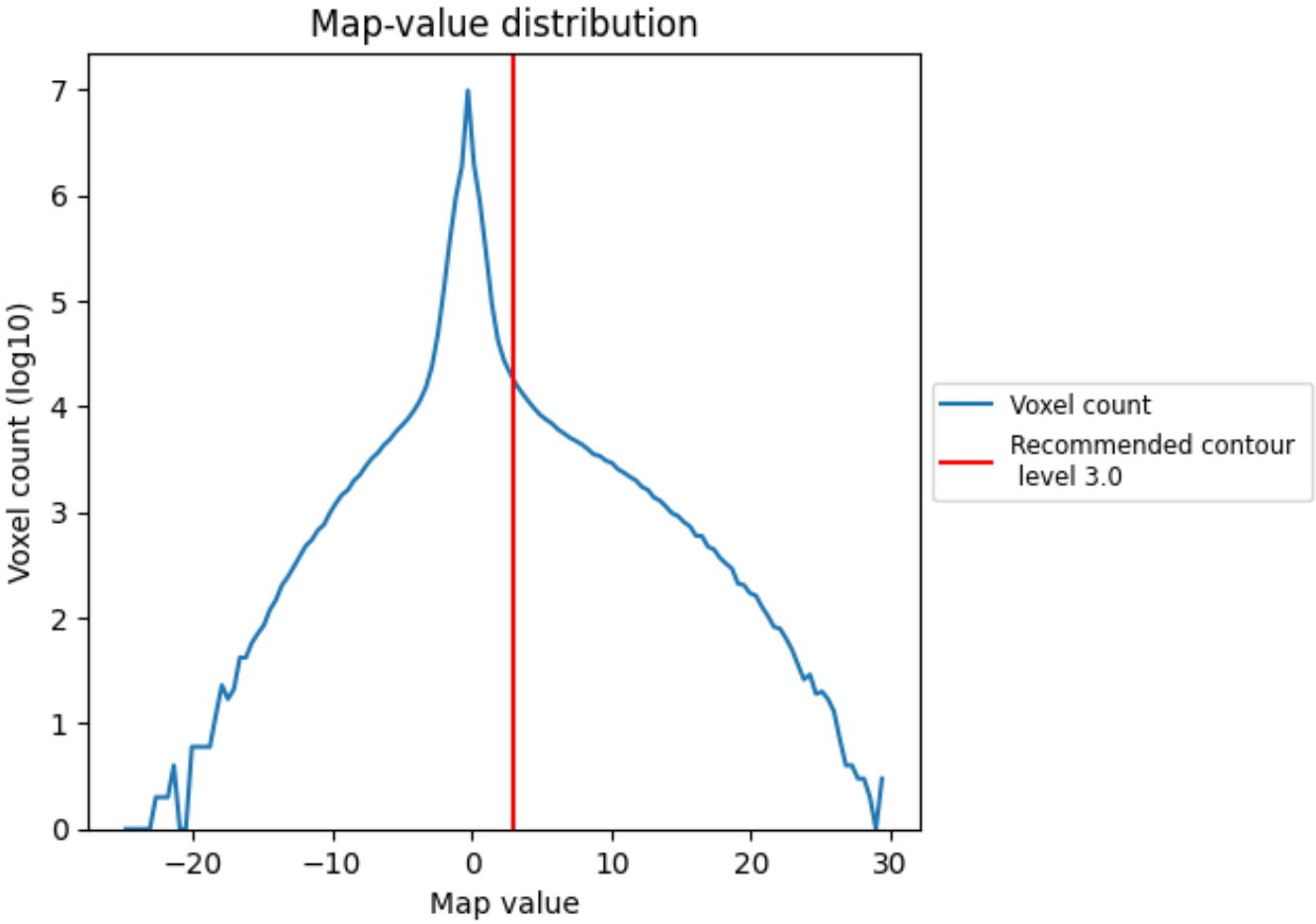
6.5 Mask visualisation (i)

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

7 Map analysis

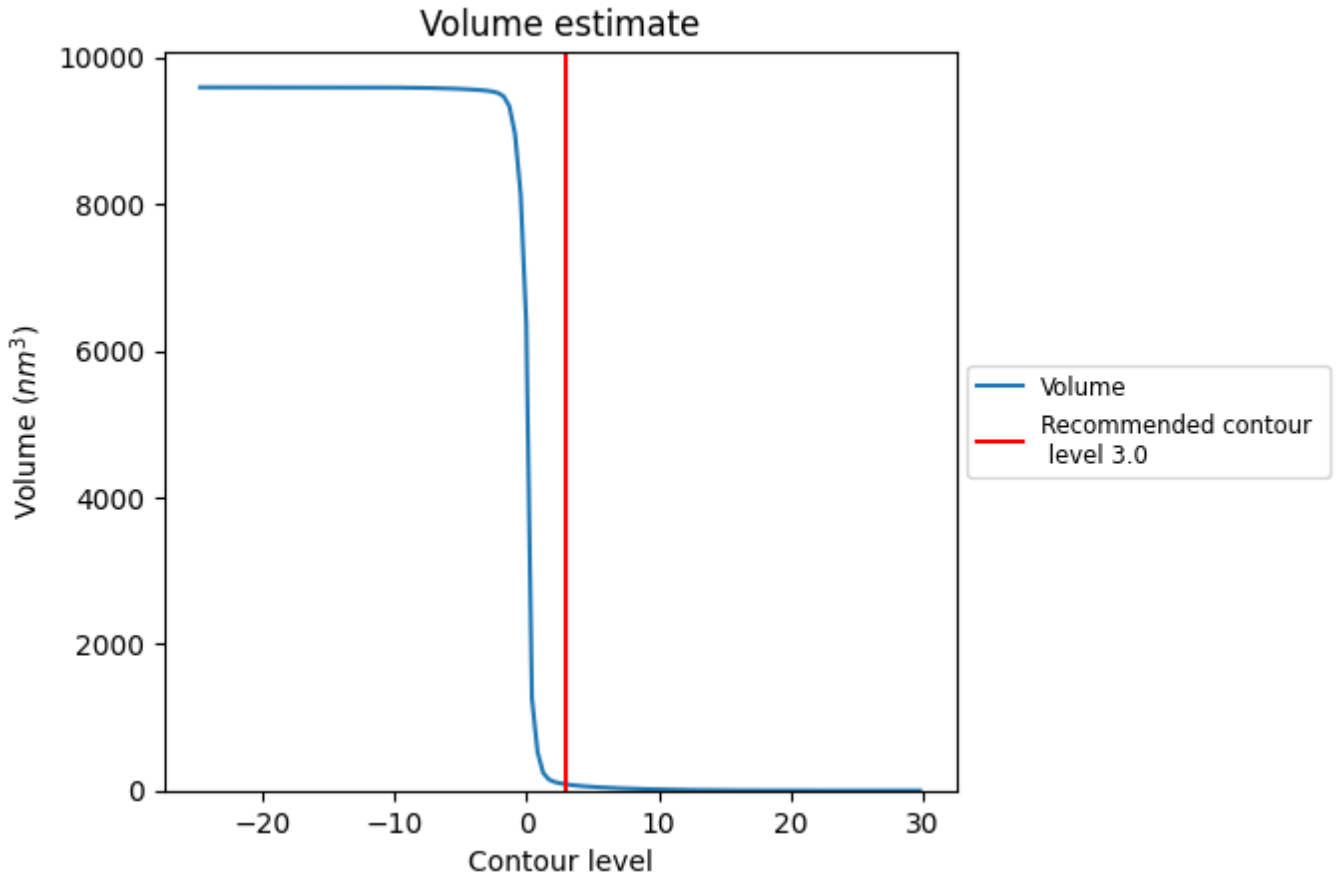
This section contains the results of statistical analysis of the map.

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.

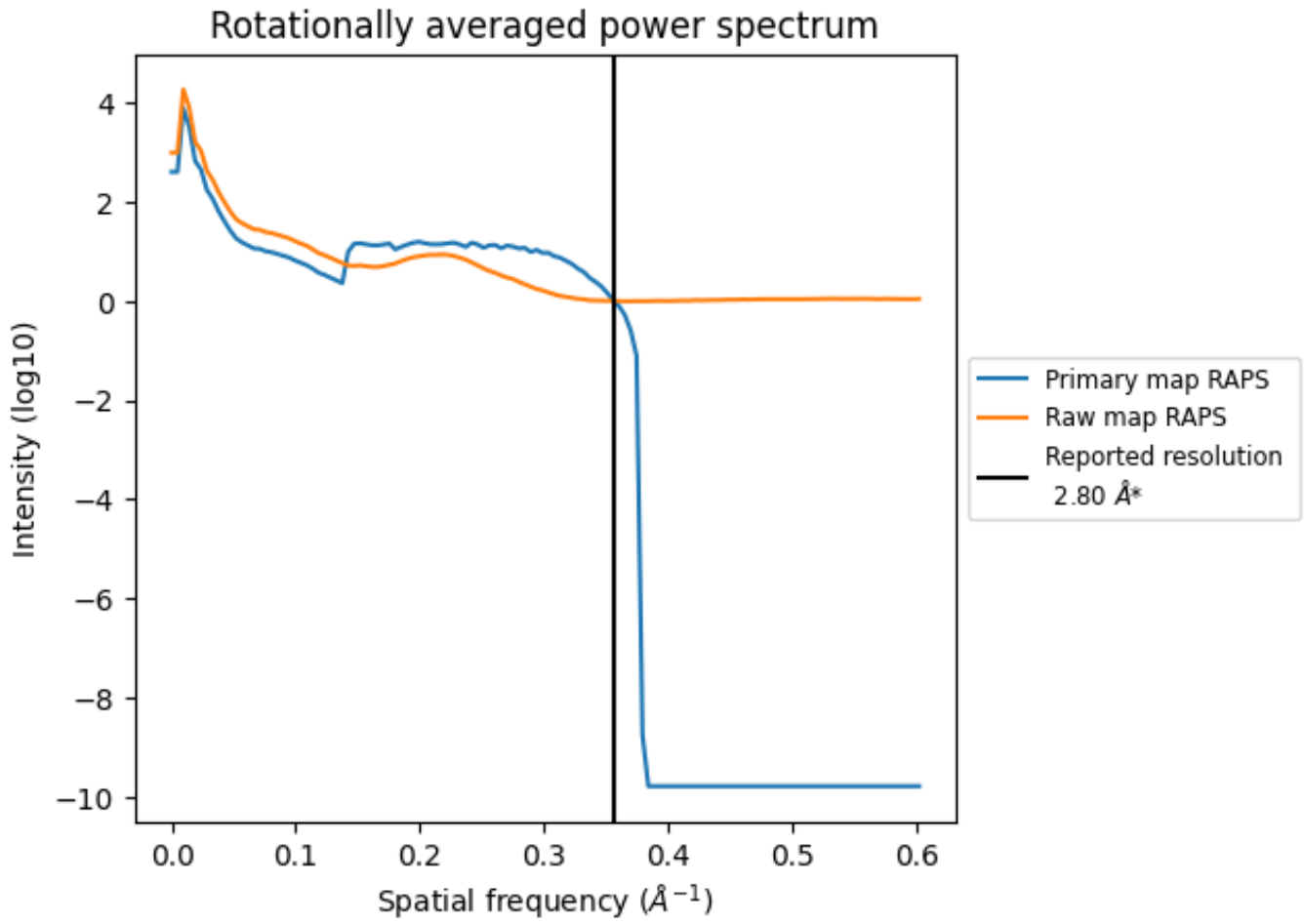
7.2 Volume estimate



The volume at the recommended contour level is 85 nm^3; this corresponds to an approximate mass of 77 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)

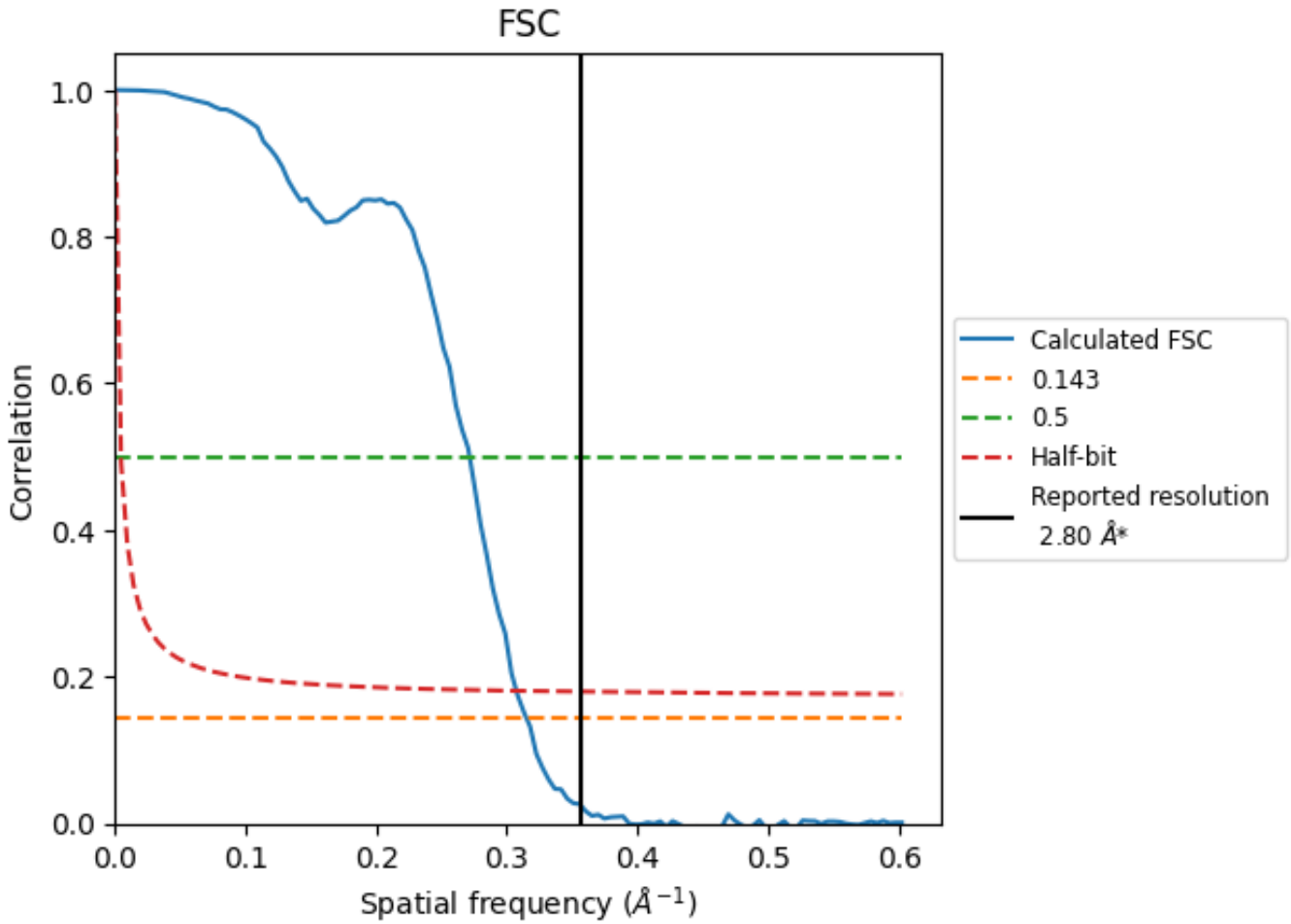


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

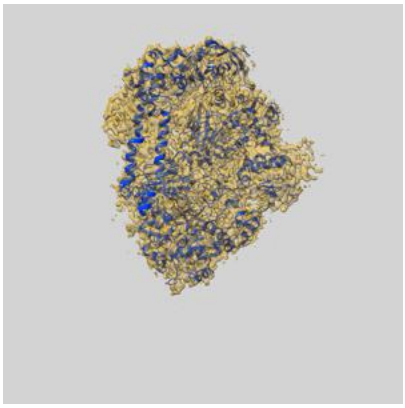
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Calculated*	3.17	3.68	3.25

*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 3.17 differs from the reported value 2.8 by more than 10 %

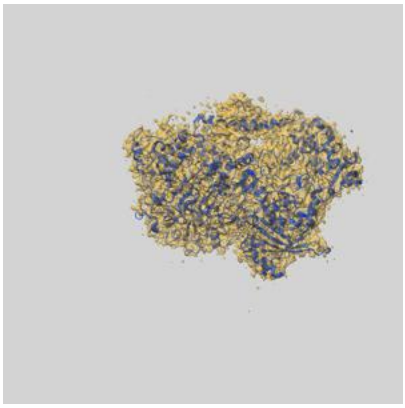
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11729 and PDB model 7ADK. Per-residue inclusion information can be found in section 3 on page 4.

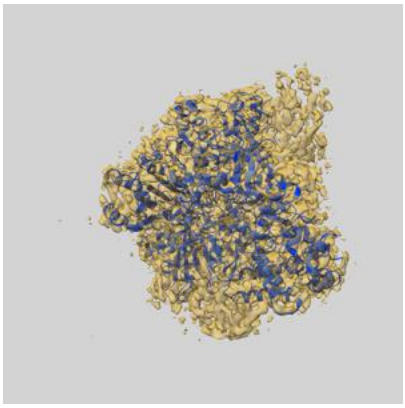
9.1 Map-model overlay



X



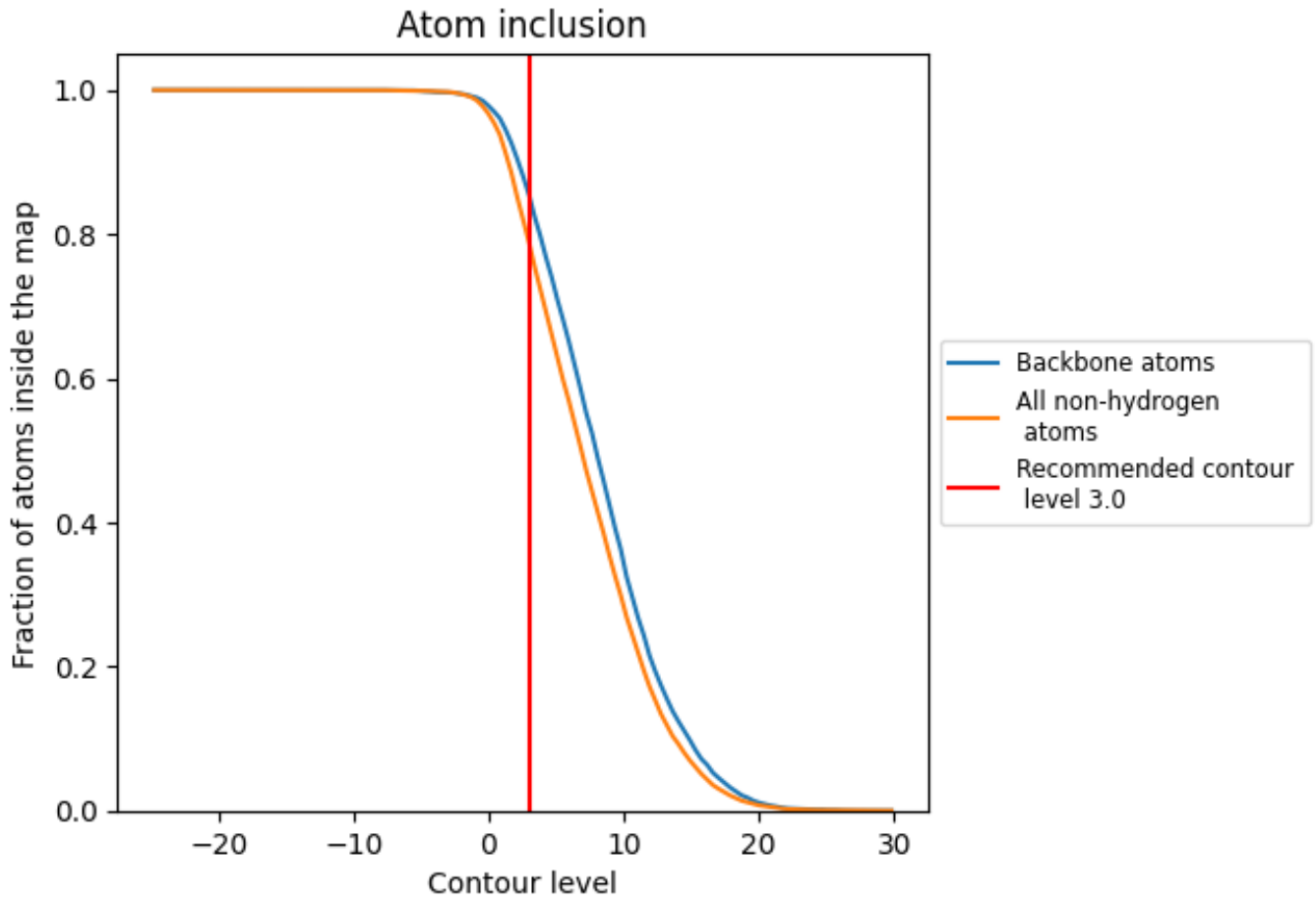
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.