wwPDB EM Validation Summary Report

Apr 1, 2024 – 06:13 PM JST

PDB ID	:	8IZR
EMDB ID	:	EMD-35869
Title	:	Multidrug resistance-associated protein 3
Authors	:	Yun, C.H.; Gao, H.M.
Deposited on	:	2023-04-07
Resolution	:	3.62 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:

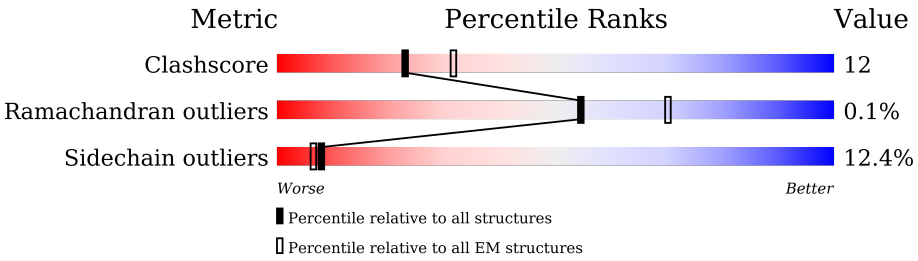
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.62 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	1589	15% 60% 25% • 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11116 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 ATP-binding cassette sub-family C member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1400	11116	7213	1842	2004	57	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PHE	TYR	variant	UNP Q92887
A	1546	LEU	-	expression tag	UNP Q92887
A	1547	GLU	-	expression tag	UNP Q92887
A	1548	GLU	-	expression tag	UNP Q92887
A	1549	ASN	-	expression tag	UNP Q92887
A	1550	LEU	-	expression tag	UNP Q92887
A	1551	TYR	-	expression tag	UNP Q92887
A	1552	PHE	-	expression tag	UNP Q92887
A	1553	GLN	-	expression tag	UNP Q92887
A	1554	GLY	-	expression tag	UNP Q92887
A	1555	SER	-	expression tag	UNP Q92887
A	1556	GLY	-	expression tag	UNP Q92887
A	1557	GLY	-	expression tag	UNP Q92887
A	1558	GLY	-	expression tag	UNP Q92887
A	1559	GLY	-	expression tag	UNP Q92887
A	1560	GLY	-	expression tag	UNP Q92887
A	1561	GLY	-	expression tag	UNP Q92887
A	1562	ASP	-	expression tag	UNP Q92887
A	1563	TYR	-	expression tag	UNP Q92887
A	1564	LYS	-	expression tag	UNP Q92887
A	1565	ASP	-	expression tag	UNP Q92887
A	1566	HIS	-	expression tag	UNP Q92887
A	1567	ASP	-	expression tag	UNP Q92887
A	1568	GLY	-	expression tag	UNP Q92887
A	1569	ASP	-	expression tag	UNP Q92887
A	1570	TYR	-	expression tag	UNP Q92887
A	1571	LYS	-	expression tag	UNP Q92887
A	1572	ASP	-	expression tag	UNP Q92887

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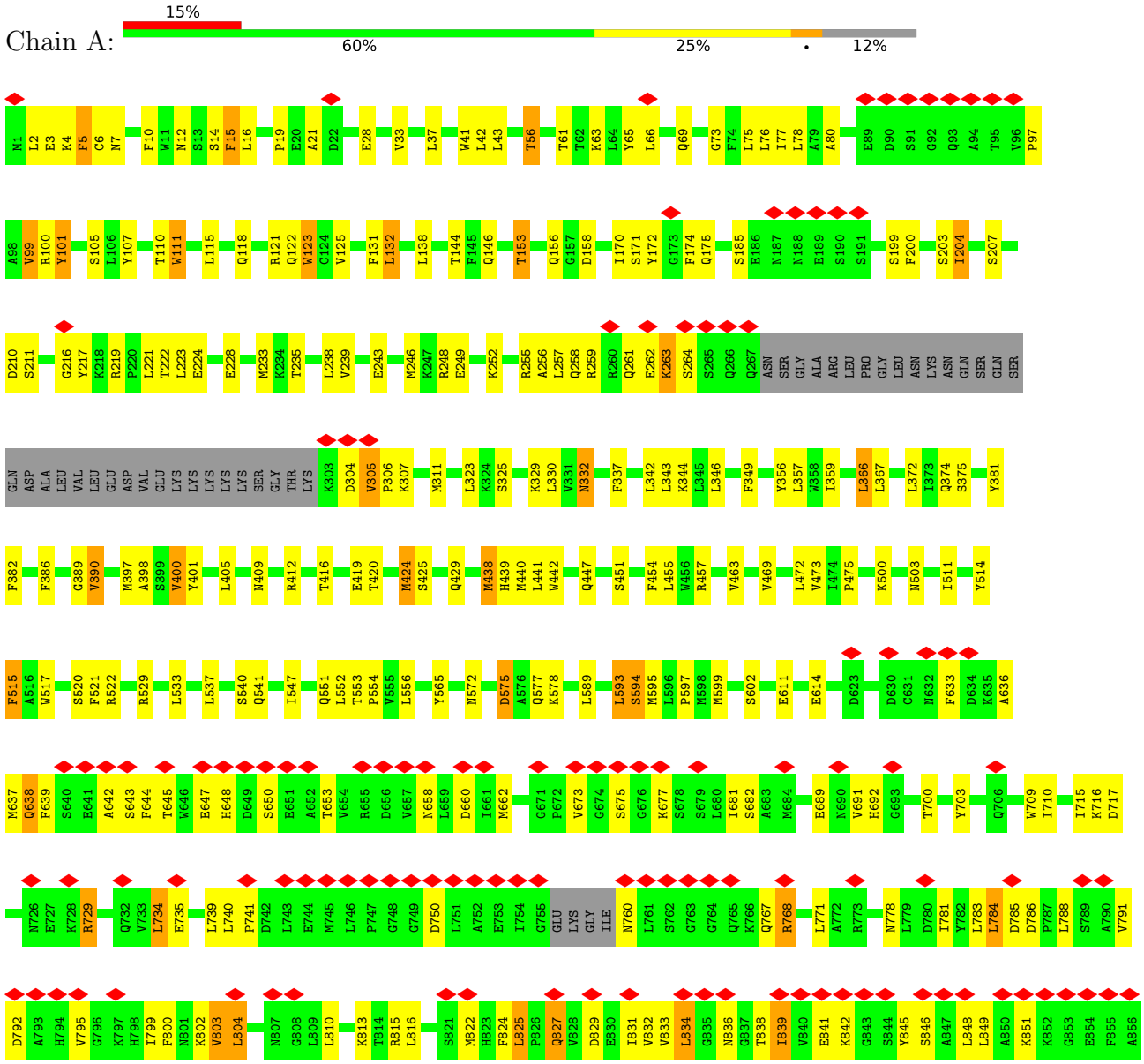
Chain	Residue	Modelled	Actual	Comment	Reference
A	1573	HIS	-	expression tag	UNP Q92887
A	1574	ASP	-	expression tag	UNP Q92887
A	1575	ILE	-	expression tag	UNP Q92887
A	1576	ASP	-	expression tag	UNP Q92887
A	1577	TYR	-	expression tag	UNP Q92887
A	1578	LYS	-	expression tag	UNP Q92887
A	1579	ASP	-	expression tag	UNP Q92887
A	1580	ASP	-	expression tag	UNP Q92887
A	1581	ASP	-	expression tag	UNP Q92887
A	1582	ASP	-	expression tag	UNP Q92887
A	1583	LYS	-	expression tag	UNP Q92887
A	1584	HIS	-	expression tag	UNP Q92887
A	1585	HIS	-	expression tag	UNP Q92887
A	1586	HIS	-	expression tag	UNP Q92887
A	1587	HIS	-	expression tag	UNP Q92887
A	1588	HIS	-	expression tag	UNP Q92887
A	1589	HIS	-	expression tag	UNP Q92887

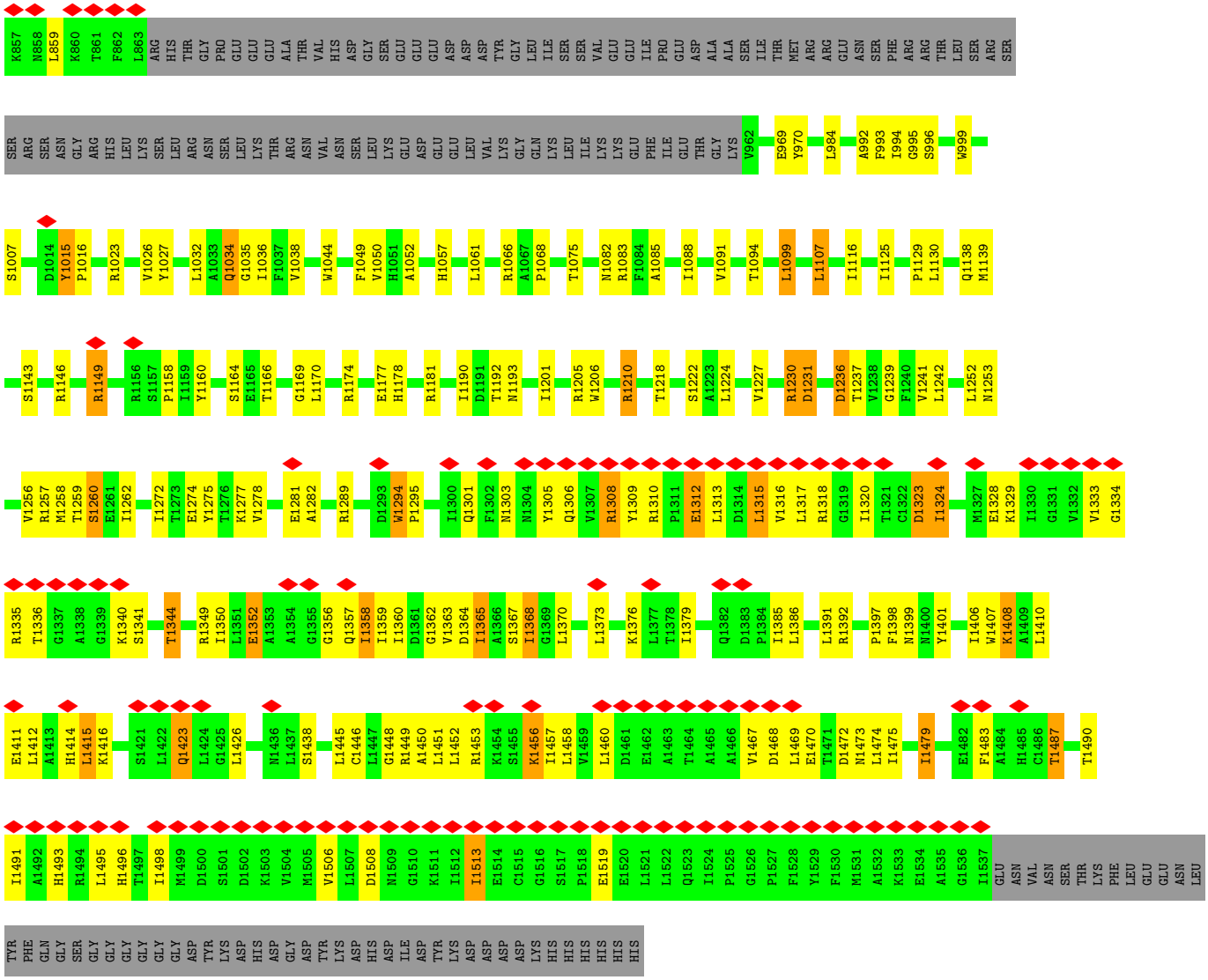
3 Residue-property plots (i)

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: ATP-binding cassette sub-family C member 2

Chain A:




K857 N858 L859 K860 T861 F862 L863 ARG HIS THR GLY PRO GLU GLU GLU ALA THR VAL HIS ASP GLY SER GLU GLU GLU ASP ASP TYR GLY LEU ILE SER SER VAL GLU GLU ILE PRO GLU ASP ALA ALA SER ILE THR MET ARG ARG GLU ASN SER PHE ARG ARG THR LEU SER ARG SER
SER ARG SER ASN GLY ARG HIS LEU LYS SER LEU LEU ARG ASN SER LEU LYS THR ARG ASN VAL ASN SER LEU LYS GLU GLU LEU LYS LEU ILE LYS LYS GLU PHE ILE GLU THR GLY LYS V962 E969 Y970 L984 A992 F993 I994 G995 S996 W999
S1007 D1014 Y1015 P1016 R1023 V1026 Y1027 L1032 A1033 Q1034 G1035 I1036 F1037 V1038 W1044 F1049 V1050 H1051 A1052 H1057 L1061 R1066 A1067 P1068 T1075 N1082 R1083 F1084 A1085 I1088 V1091 T1094 L1099 L1107 I1116 I1125 P1129 L1130 Q1138 M1139
S1143 R1146 R1149 R1156 S1157 P1158 I1159 Y1160 S1164 E1165 T1166 G1169 L1170 R1174 E1177 H1178 R1181 I1190 D1191 T1192 N1193 I1201 R1205 W1206 R1210 T1218 S1222 A1223 L1224 V1227 R1230 D1231 D1236 T1237 V1238 G1239 F1240 V1241 L1242 L1252 N1253
V1256 R1257 M1258 T1259 S1260 E1261 I1262 I1272 T1273 E1274 Y1275 T1276 K1277 V1278 E1281 A1282 R1289 D1293 W1294 P1295 I1300 Q1301 F1302 N1303 N1304 Y1305 Q1306 V1307 R1308 Y1309 R1310 P1311 E1312 L1313 D1314 L1315 V1316 L1317 R1318 G1319 I1320 T1321 C1322 D1323 I1324 M1327 E1328 K1329 I1330 G1331 V1332 V1333 G1334
R1335 T1336 G1337 A1338 G1339 K1340 S1341 T1344 R1349 I1350 L1351 E1352 A1353 A1354 G1355 G1356 Q1357 T1358 I1359 I1360 D1361 G1362 V1363 D1364 I1365 A1366 S1367 I1368 G1369 L1370 L1373 K1376 L1377 T1378 I1379 Q1382 D1383 P1384 I1385 L1386 L1391 R1392 P1397 F1398 N1399 N1400 Y1401 I1406 W1407 K1408 A1409 L1410
E1411 L1412 A1413 H1414 L1415 K1416 S1421 L1422 Q1423 L1424 G1425 L1426 N1436 L1437 S1438 L1445 C1446 L1447 G1448 R1449 A1450 L1451 L1452 R1453 K1454 S1455 K1456 I1457 L1458 V1459 L1460 D1461 E1462 A1463 T1464 A1465 A1466 V1467 D1468 L1469 E1470 T1471 D1472 N1473 L1474 I1475 I1479 E1482 F1483 A1484 H1485 C1486 T1487 T1490
I1491 A1492 H1493 R1494 L1495 H1496 T1497 I1498 M1499 D1500 S1501 D1502 K1503 V1504 M1505 V1506 L1507 D1508 N1509 G1510 K1511 I1512 I1513 E1514 C1515 G1516 S1517 P1518 E1519 E1520 L1521 L1522 Q1523 I1524 P1525 G1526 P1527 F1528 Y1529 F1530 M1531 A1532 K1533 E1534 A1535 G1536 I1537 GLU ASN VAL ASN SER THR LYS PHE LEU GLU GLU ASN LEU
TYR PHE GLN GLY SER GLY GLY GLY GLY GLY ASP TYR LYS ASP HIS ASP GLY ASP TYR LYS ASP HIS ASP ILE ASP TYR LYS ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.612	Depositor
Minimum map value	-0.379	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.103	Depositor
Map size (Å)	273.92, 273.92, 273.92	wwPDB
Map dimensions	256, 256, 256	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	0.65	0/11350	0.89	0/15389

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	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
1	A	1230	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	11116	0	11376	279	0
All	All	11116	0	11376	279	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 12.

The worst 5 of 279 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:1365:ILE:HG13	1:A:1373:LEU:HD22	1.52	0.90
1:A:1358:ILE:HG23	1:A:1363:VAL:H	1.40	0.86
1:A:78:LEU:CD1	1:A:170:ILE:HG22	2.09	0.82
1:A:1303:ASN:O	1:A:1356:GLY:HA2	1.80	0.82
1:A:97:PRO:HD2	1:A:100:ARG:HD2	1.63	0.80

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	1392/1589 (88%)	1347 (97%)	43 (3%)	2 (0%)	51 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1015	TYR
1	A	1231	ASP

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1241/1408 (88%)	1087 (88%)	154 (12%)	4 25

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1210	ARG
1	A	1423	GLN
1	A	1242	LEU
1	A	1324	ILE
1	A	1487	THR

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	997	ASN
1	A	1247	ASN
1	A	694	HIS
1	A	711	GLN
1	A	760	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 monosaccharides 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.

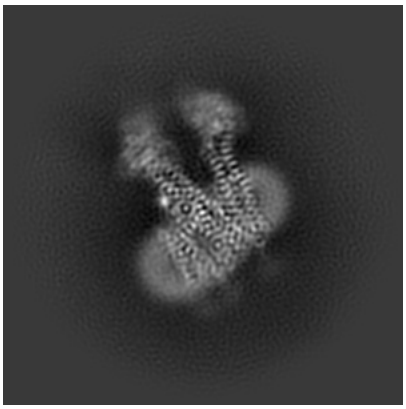
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35869. These allow visual inspection of the internal detail of the map and identification of artifacts.

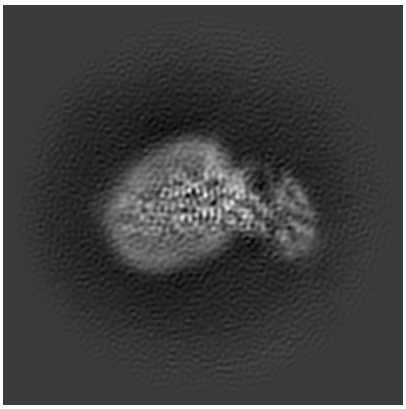
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

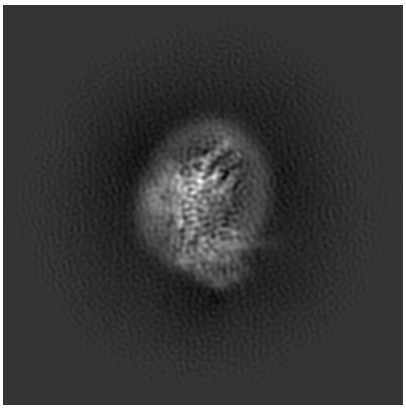
6.1.1 Primary map



X

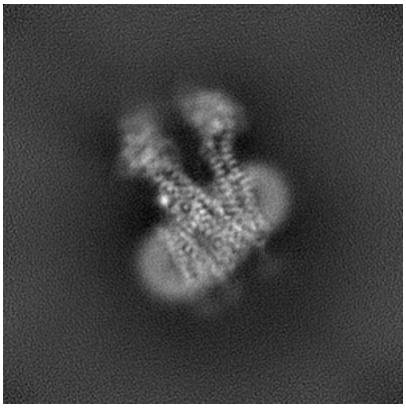


Y

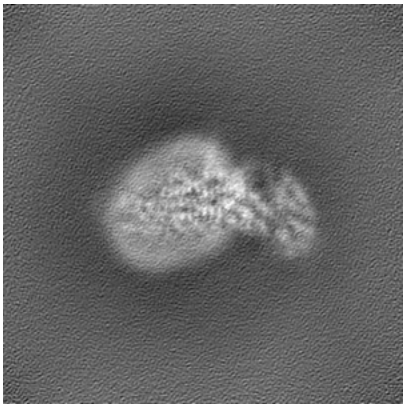


Z

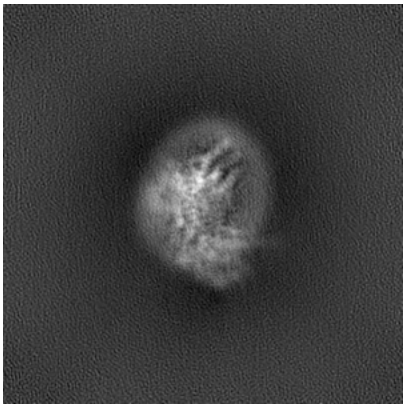
6.1.2 Raw map



X



Y

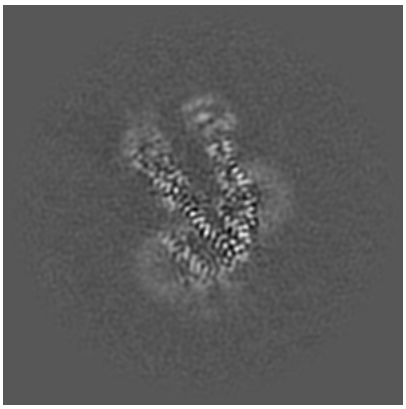


Z

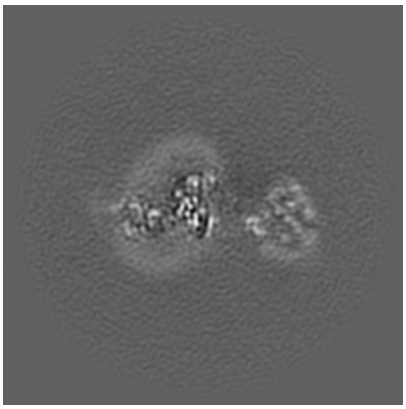
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

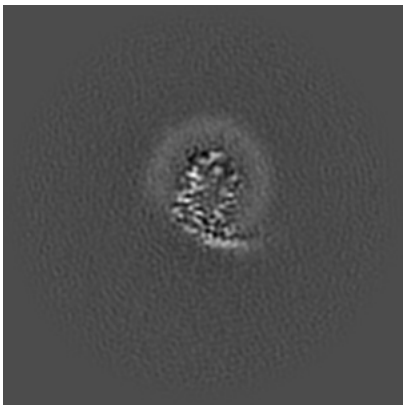
6.2.1 Primary map



X Index: 128

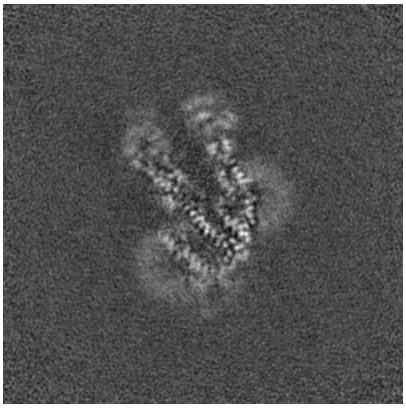


Y Index: 128

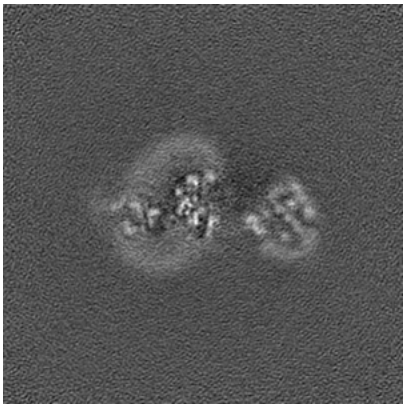


Z Index: 128

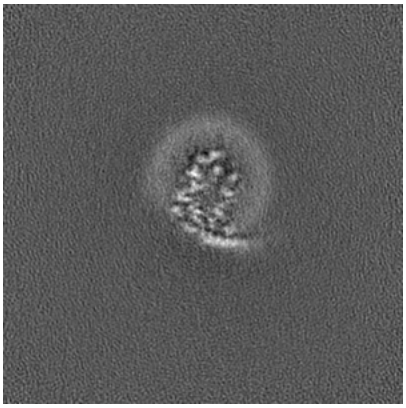
6.2.2 Raw map



X Index: 128



Y Index: 128

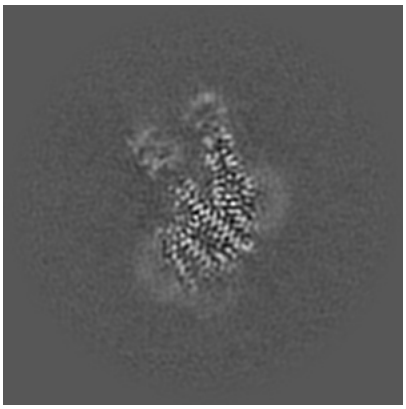


Z Index: 128

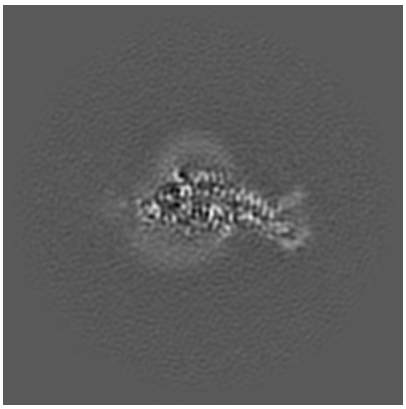
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

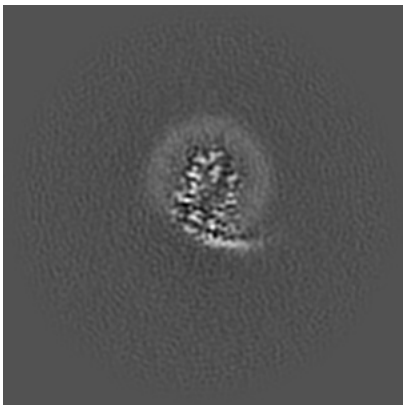
6.3.1 Primary map



X Index: 121

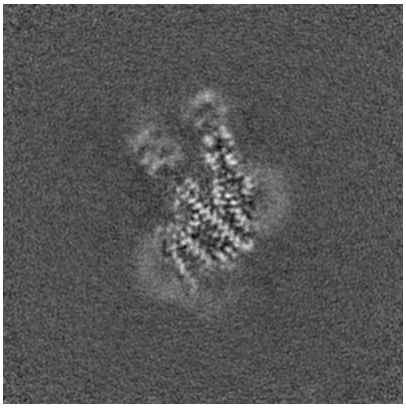


Y Index: 144

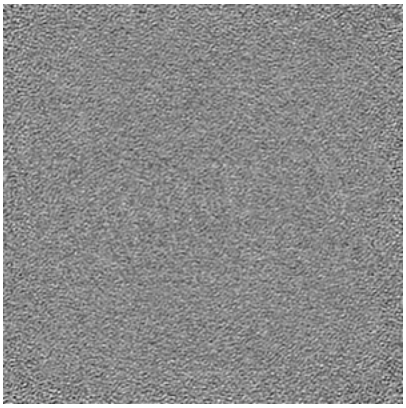


Z Index: 129

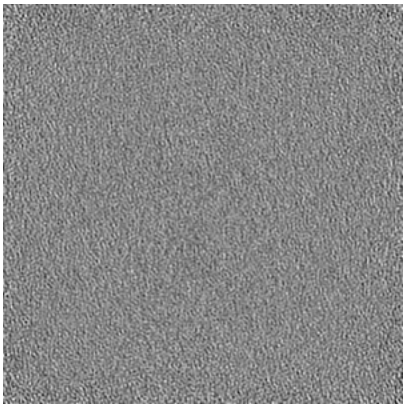
6.3.2 Raw map



X Index: 121



Y Index: 0

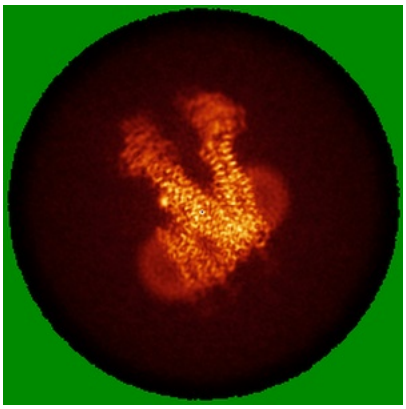


Z Index: 0

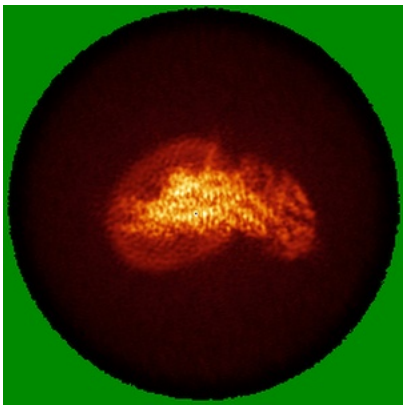
The images above show the largest variance slices of the map in three orthogonal directions.

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

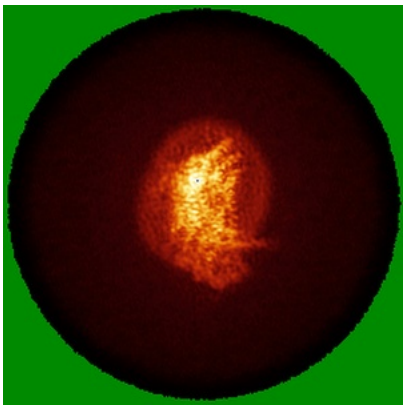
6.4.1 Primary map



X

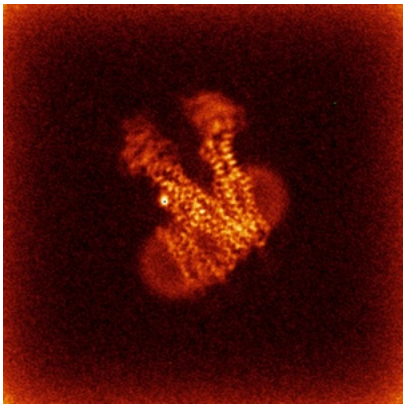


Y

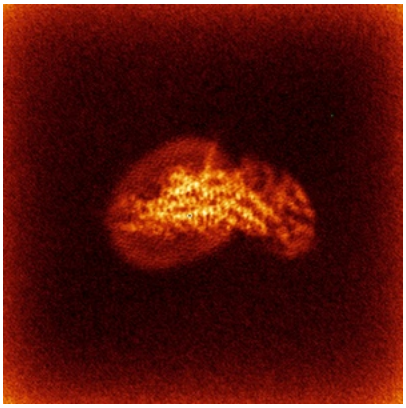


Z

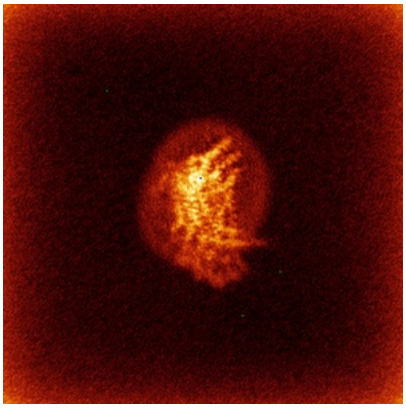
6.4.2 Raw map



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 0.103. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

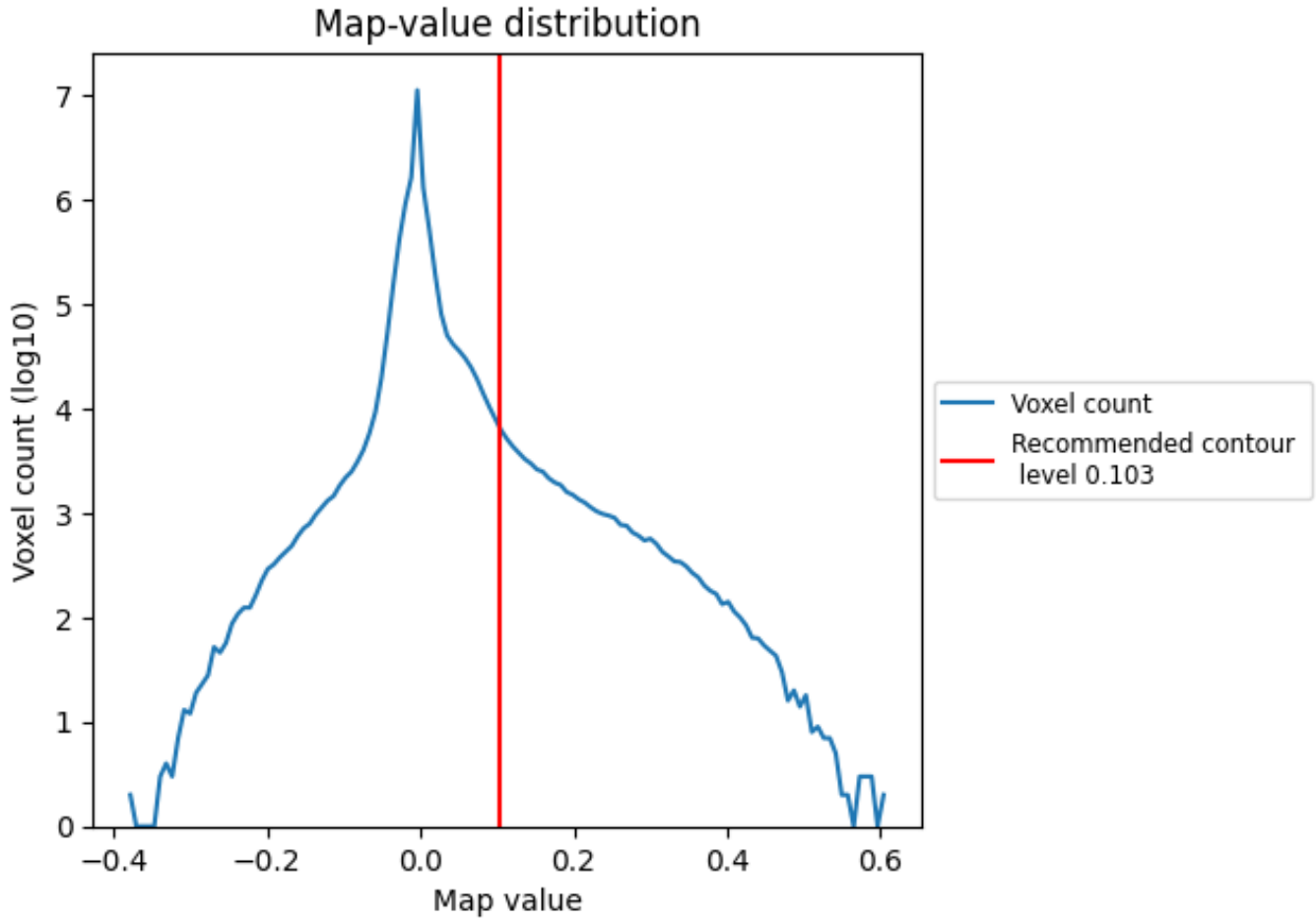
6.6 Mask visualisation (i)

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

7 Map analysis

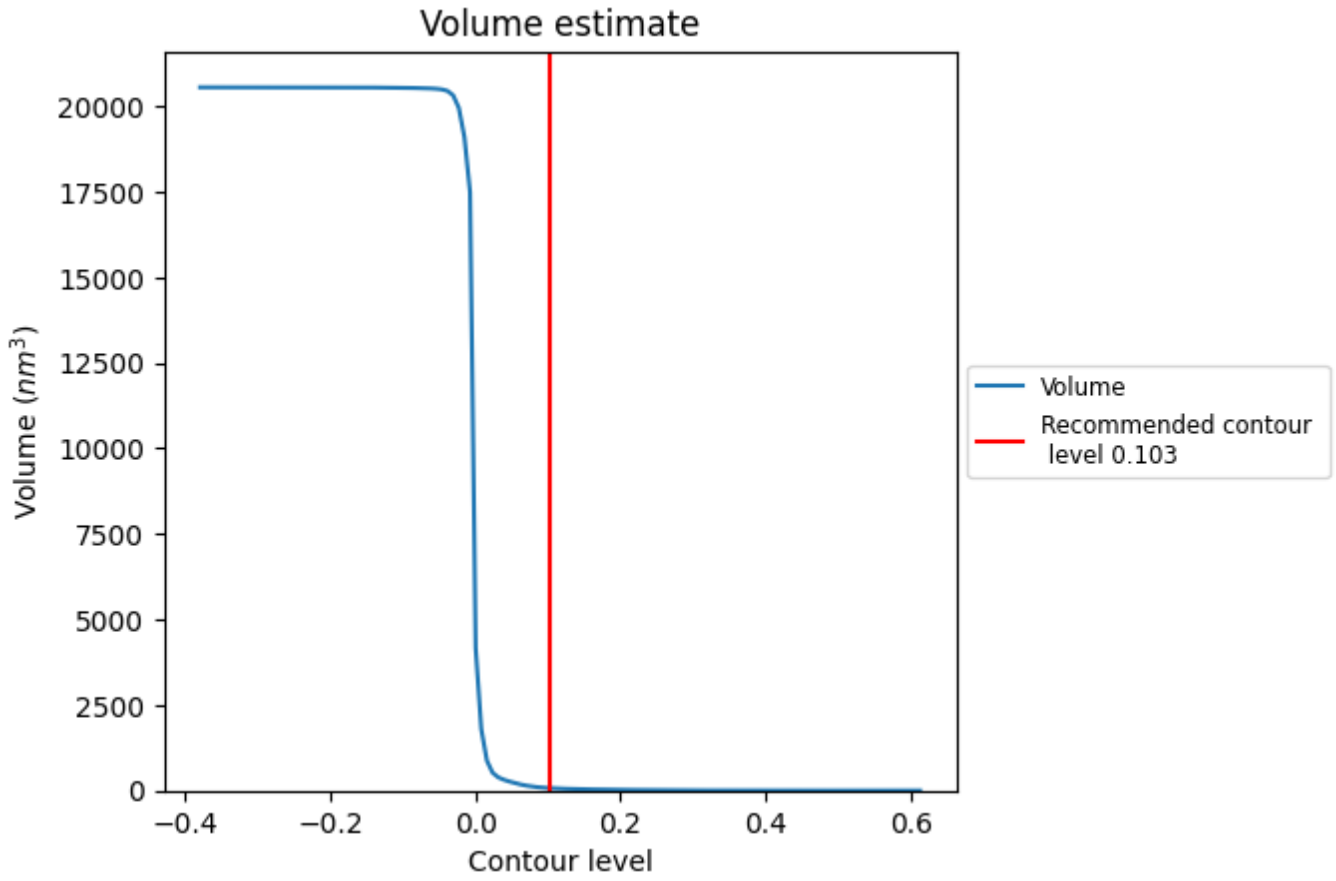
This section contains the results of statistical analysis of the map.

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.

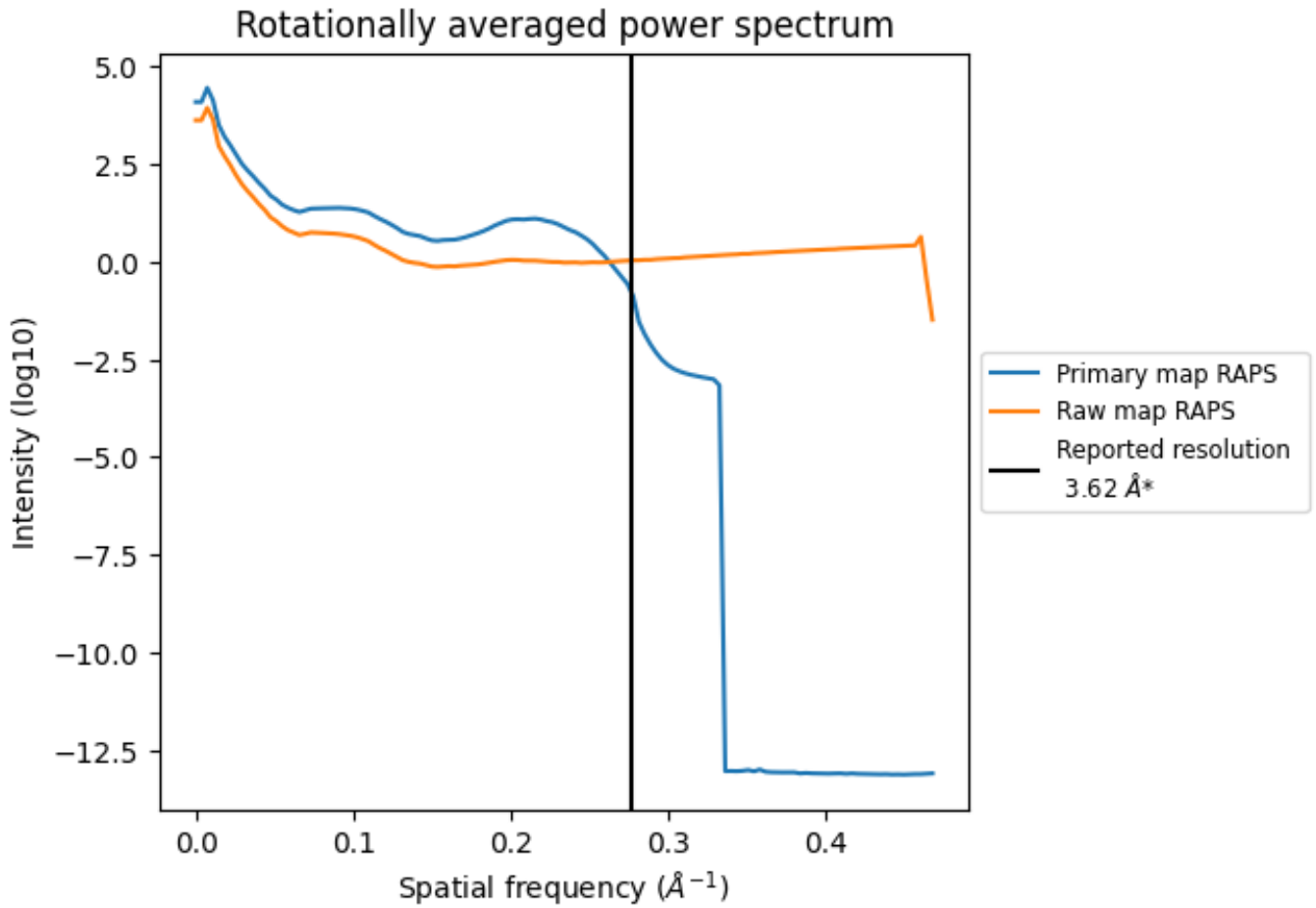
7.2 Volume estimate (i)



The volume at the recommended contour level is 71 nm^3; this corresponds to an approximate mass of 64 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)

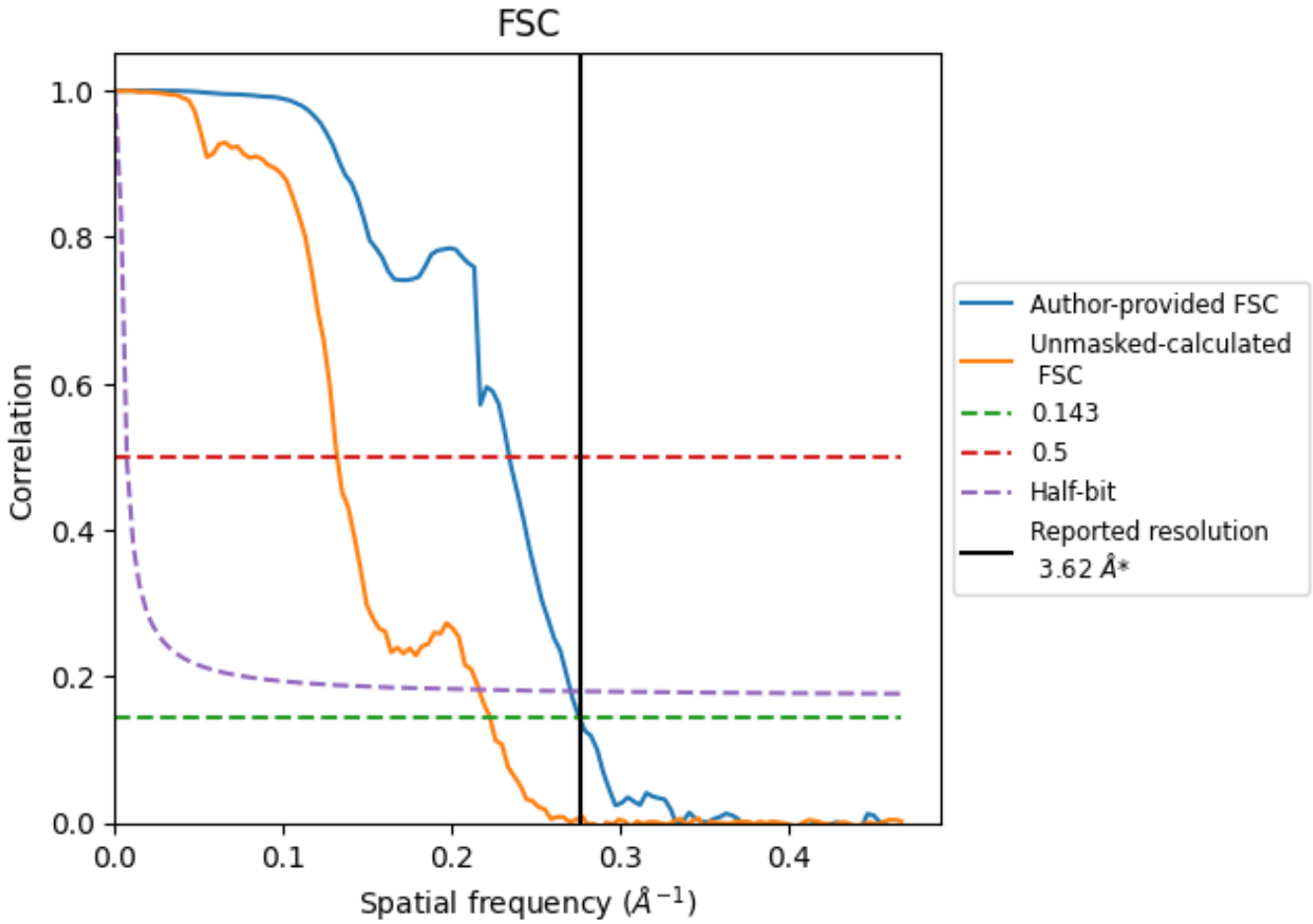


*Reported resolution corresponds to spatial frequency of 0.276 $Å^{-1}$

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 0.276 Å^{-1}

8.2 Resolution estimates (i)

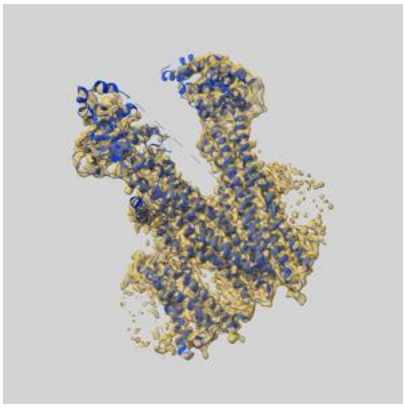
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.62	4.27	3.69
Unmasked-calculated*	4.48	7.57	4.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.48 differs from the reported value 3.62 by more than 10 %

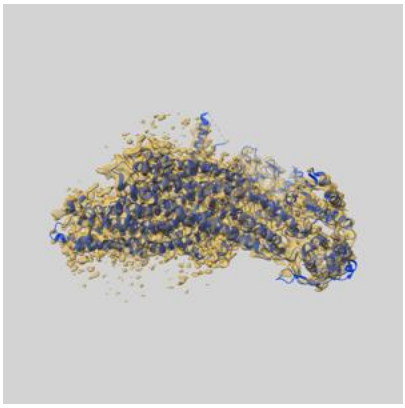
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35869 and PDB model 8IZR. Per-residue inclusion information can be found in section 3 on page 5.

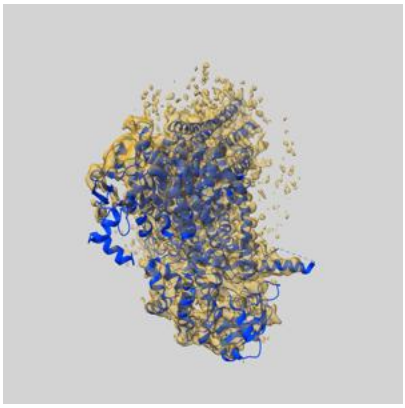
9.1 Map-model overlay



X



Y



Z

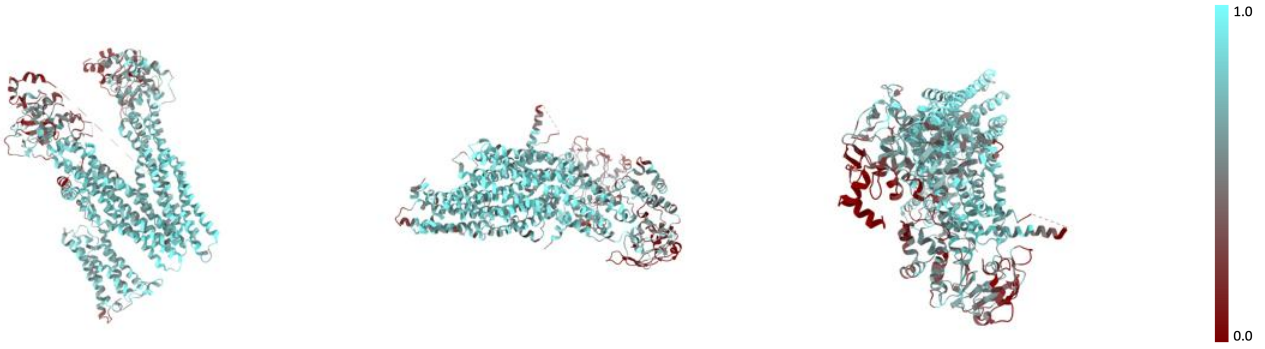
The images above show the 3D surface view of the map at the recommended contour level 0.103 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

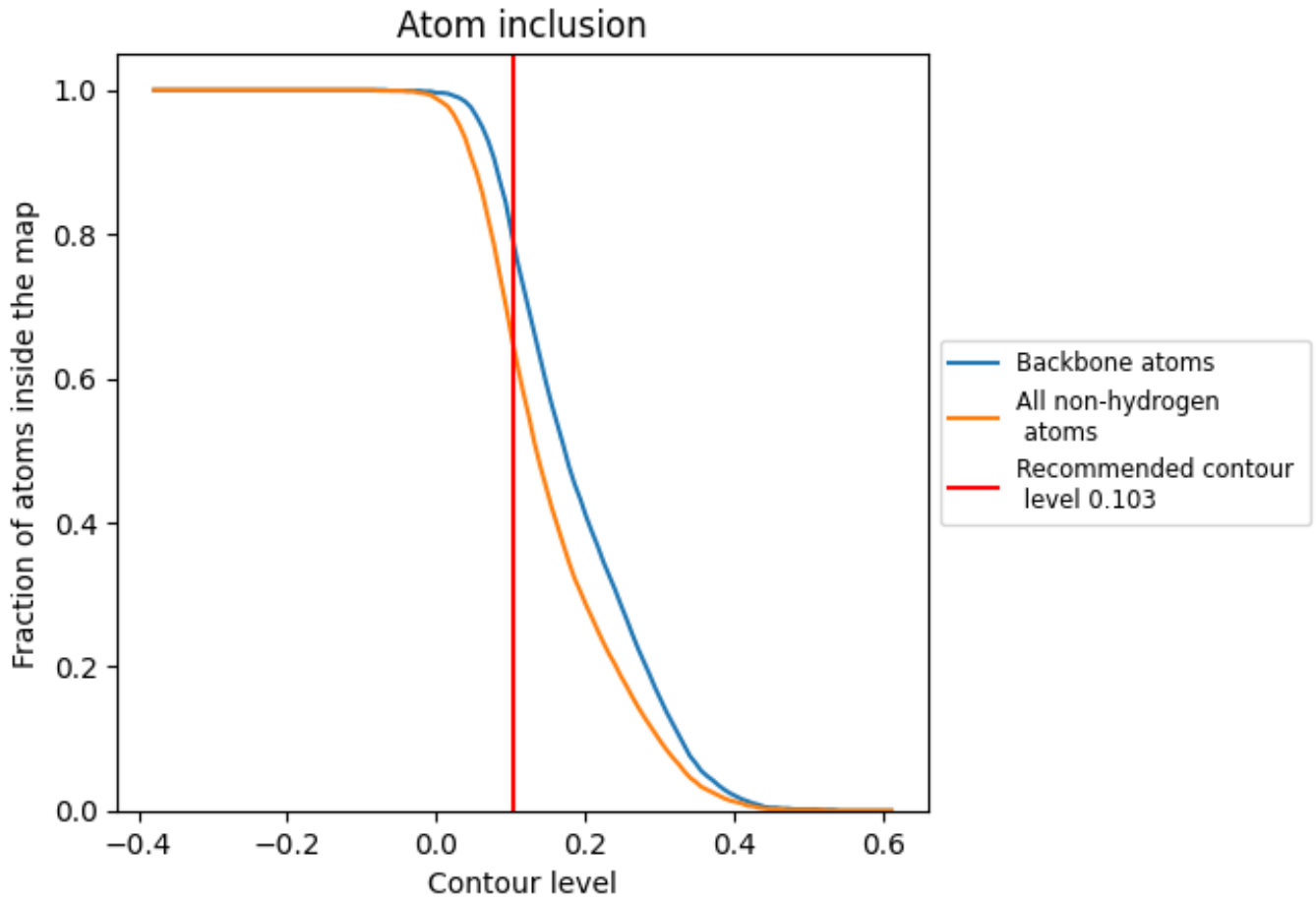
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.103).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 65% 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 (0.103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.4240
A	0.6500	0.4240