Full wwPDB EM Validation Report ⓘ

Oct 11, 2022 – 10:11 AM EDT

PDB ID	:	7M69
EMDB ID	:	EMD-23691
Title	:	E1435Q Ycf1 mutant in inward-facing wide conformation
Authors	:	Khandelwal, N.K.; Millan, C.R.; Thaker, T.M.; Tomasiak, T.M.
Deposited on	:	2021-03-25
Resolution	:	3.42 Å(reported)
Based on initial model	:	6JB1

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 ⓘ 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:

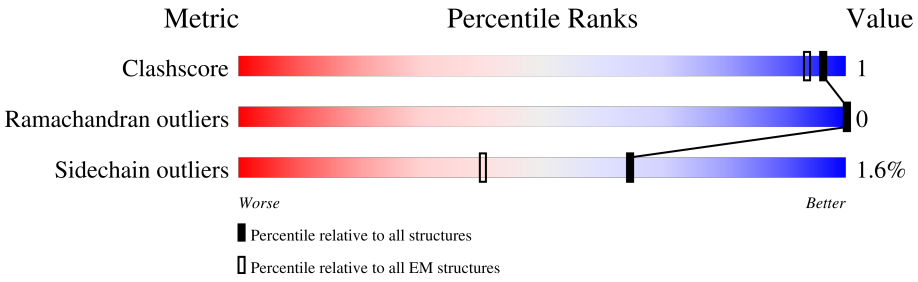
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.42 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	1559	36% 86% · 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21795 atoms, of which 10912 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 Metal resistance protein YCF1.

Mol	Chain	Residues	Atoms							AltConf	Trace
			Total	C	H	N	O	P	S		
1	A	1390	21795	7028	10912	1824	1981	3	47	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	ALA	-	expression tag	UNP P39109
A	-21	SER	-	expression tag	UNP P39109
A	-20	ASP	-	expression tag	UNP P39109
A	-19	TYR	-	expression tag	UNP P39109
A	-18	LYS	-	expression tag	UNP P39109
A	-17	ASP	-	expression tag	UNP P39109
A	-16	ASP	-	expression tag	UNP P39109
A	-15	ASP	-	expression tag	UNP P39109
A	-14	ASP	-	expression tag	UNP P39109
A	-13	LYS	-	expression tag	UNP P39109
A	-12	GLY	-	expression tag	UNP P39109
A	-11	ALA	-	expression tag	UNP P39109
A	-10	LEU	-	expression tag	UNP P39109
A	-9	GLU	-	expression tag	UNP P39109
A	-8	VAL	-	expression tag	UNP P39109
A	-7	LEU	-	expression tag	UNP P39109
A	-6	PHE	-	expression tag	UNP P39109
A	-5	GLN	-	expression tag	UNP P39109
A	-4	GLY	-	expression tag	UNP P39109
A	-3	PRO	-	expression tag	UNP P39109
A	-2	SER	-	expression tag	UNP P39109
A	-1	SER	-	expression tag	UNP P39109
A	0	PRO	-	expression tag	UNP P39109
A	1435	GLN	GLU	engineered mutation	UNP P39109
A	1516	GLY	-	expression tag	UNP P39109
A	1517	LEU	-	expression tag	UNP P39109
A	1518	VAL	-	expression tag	UNP P39109
A	1519	PRO	-	expression tag	UNP P39109

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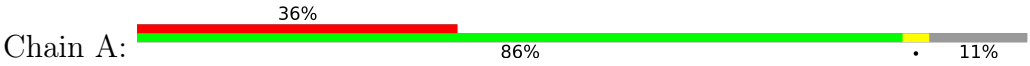
Chain	Residue	Modelled	Actual	Comment	Reference
A	1520	ARG	-	expression tag	UNP P39109
A	1521	GLY	-	expression tag	UNP P39109
A	1522	SER	-	expression tag	UNP P39109
A	1523	SER	-	expression tag	UNP P39109
A	1524	ALA	-	expression tag	UNP P39109
A	1525	HIS	-	expression tag	UNP P39109
A	1526	HIS	-	expression tag	UNP P39109
A	1527	HIS	-	expression tag	UNP P39109
A	1528	HIS	-	expression tag	UNP P39109
A	1529	HIS	-	expression tag	UNP P39109
A	1530	HIS	-	expression tag	UNP P39109
A	1531	HIS	-	expression tag	UNP P39109
A	1532	HIS	-	expression tag	UNP P39109
A	1533	HIS	-	expression tag	UNP P39109
A	1534	HIS	-	expression tag	UNP P39109
A	1535	GLY	-	expression tag	UNP P39109
A	1536	ALA	-	expression tag	UNP P39109

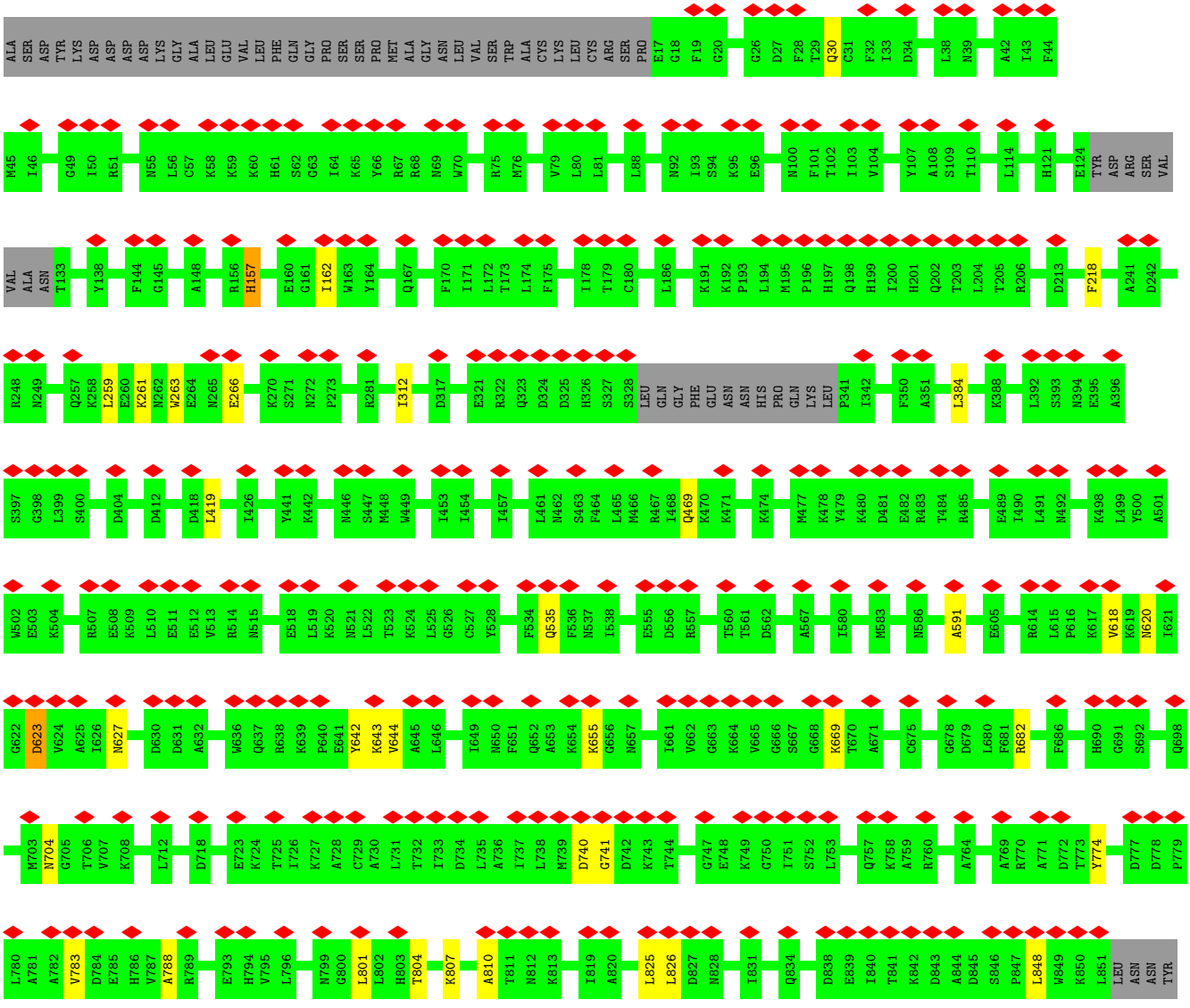
3 Residue-property plots (i)

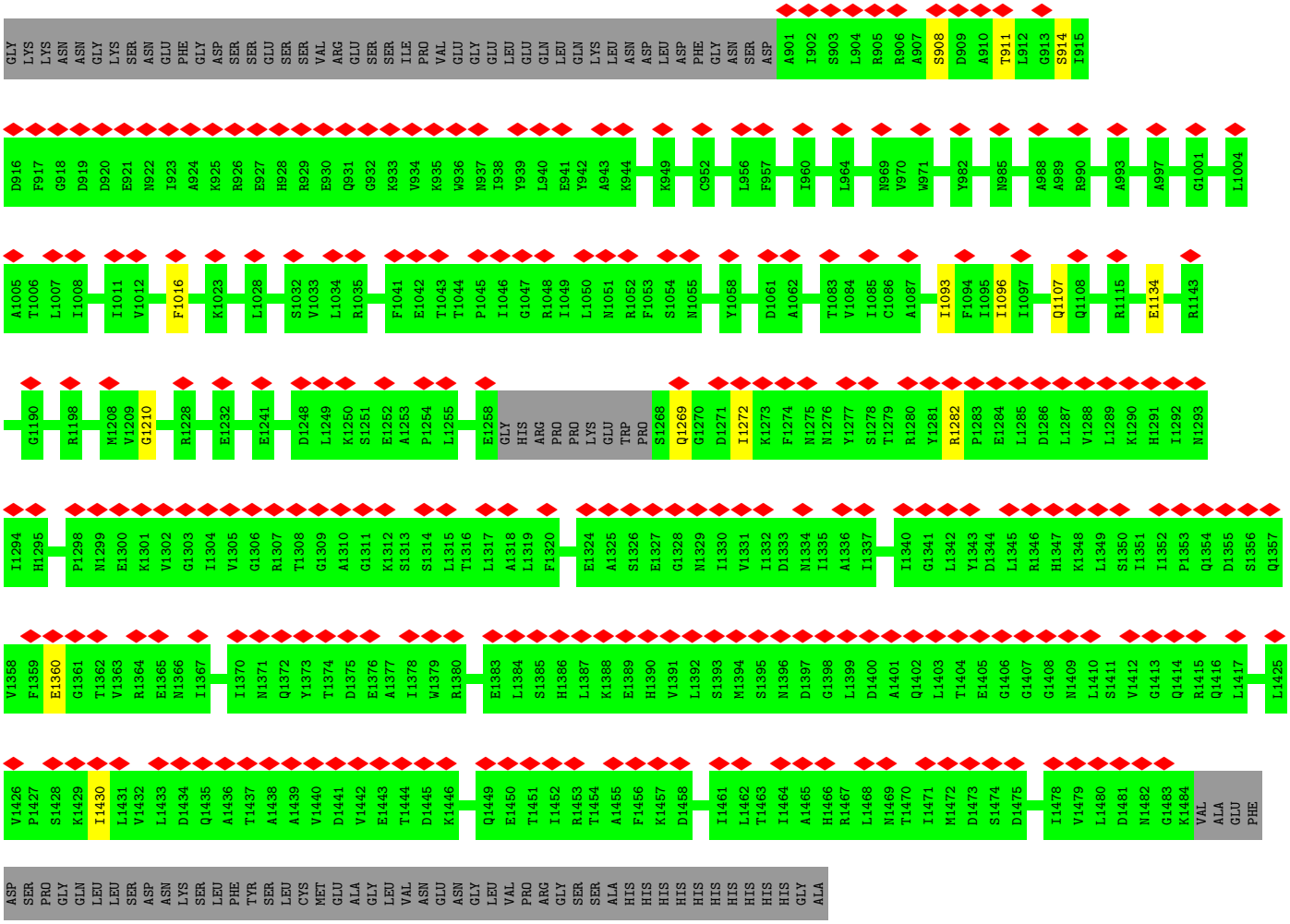
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Metal resistance protein YCF1

Chain A:






GLY LYS LYS ASN ASN GLY LYS SER ASN GLU PHE GLY ASP SER SER GLU SER SER VAL ARG GLU SER SER ILE PRO VAL GLU GLY GLU LEU GLU GLN LEU GLN LYS LEU ASN ASP LEU ASP PHE GLY ASN SER ASP
A901 I902 S903 L904 R905 R906 A907 S908 D909 A910 T911 L912 G913 S914 I915
D916 F917 G918 D919 D920 E921 N922 I923 A924 K925 R926 E927 H928 R929 E930 Q931 G932 K933 V934 K935 W936 N937 I938 Y939 L940 E941 Y942 A943 K944 K949 C952 L956 F957 I960 L964 N969 V970 W971 Y982 N985 A988 A989 R990 A993 A997 G1001 L1004
A1005 T1006 L1007 I1008 I1011 V1012 F1016 K1023 L1028 S1032 V1033 L1034 R1035 F1041 E1042 T1043 T1044 P1045 I1046 G1047 R1048 I1049 L1050 N1051 R1052 F1053 S1054 N1055 Y1058 D1061 A1062 T1083 V1084 I1085 C1086 A1087 I1093 F1094 I1095 I1096 I1097 Q1107 Q1108 R1115 E1134 R1143
G1190 R1198 M1208 V1209 G1210 R1228 E1232 E1241 D1248 L1249 K1250 S1251 E1252 A1253 P1254 L1255 E1258 GLY HIS ARG PRO PRO LYS GLU TRP PRO S1268 Q1269 G1270 D1271 I1272 K1273 F1274 N1275 N1276 Y1277 S1278 T1279 R1280 Y1281 R1282 P1283 E1284 L1285 D1286 L1287 V1288 L1289 K1290 H1291 I1292 N1293
I1294 H1295 P1298 N1299 E1300 K1301 V1302 G1303 I1304 V1305 G1306 R1307 T1308 G1309 A1310 G1311 K1312 S1313 S1314 L1315 T1316 L1317 A1318 L1319 F1320 E1324 A1325 S1326 E1327 G1328 N1329 I1330 V1331 I1332 D1333 N1334 I1335 A1336 I1337 I1340 G1341 L1342 Y1343 D1344 L1345 R1346 H1347 K1348 L1349 S1350 I1351 I1352 P1353 Q1354 D1355 S1356 Q1357
V1358 F1359 E1360 G1361 T1362 V1363 R1364 E1365 N1366 I1367 T1370 N1371 Q1372 Y1373 T1374 D1375 E1376 A1377 I1378 W1379 R1380 E1383 L1384 S1385 H1386 L1387 K1388 E1389 H1390 V1391 L1392 S1393 M1394 S1395 N1396 D1397 G1398 L1399 D1400 A1401 Q1402 L1403 T1404 E1405 G1406 G1407 G1408 N1409 L1410 S1411 V1412 G1413 Q1414 R1415 Q1416 L1417 L1425
V1426 P1427 S1428 K1429 I1430 L1431 V1432 L1433 D1434 Q1435 A1436 T1437 A1438 A1439 V1440 D1441 V1442 E1443 T1444 D1445 K1446 Q1449 E1450 T1451 I1452 R1453 T1454 A1455 F1456 K1457 D1458 I1461 L1462 T1463 I1464 A1465 H1466 R1467 L1468 N1469 T1470 I1471 M1472 D1473 S1474 D1475 I1478 V1479 L1480 D1481 N1482 G1483 K1484 VAL ALA GLU PHE
ASP SER PRO GLY GLN LEU LEU SER ASP ASN LYS SER LEU PHE TYR SER LEU CYS MET GLU ALA GLY LEU VAL ASN GLU ASN GLY GLY LEU VAL PRO ARG GLY SER SER ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS GLY GLY ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	114963	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 ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	16.055	Depositor
Minimum map value	-11.312	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.758	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	309.30002, 309.30002, 309.30002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.031, 1.031, 1.031	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP

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	0.31	0/11066	0.59	0/15008

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10883	10912	10947	17	0
All	All	10883	10912	10947	17	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 1.

All (17) 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:623:ASP:O	1:A:655:LYS:N	2.38	0.56
1:A:1272:ILE:HD11	1:A:1430:ILE:HD11	1.89	0.55
1:A:259:LEU:HD23	1:A:384:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ASN:N	1:A:1134:GLU:OE2	2.43	0.52
1:A:1269:GLN:HA	1:A:1272:ILE:HD13	1.91	0.52
1:A:642:TYR:HB3	1:A:644:VAL:HG23	1.92	0.51
1:A:669:LYS:HD3	1:A:810:ALA:HB1	1.94	0.49
1:A:620:ASN:HB2	1:A:623:ASP:OD1	2.13	0.47
1:A:1093:ILE:HA	1:A:1096:ILE:HG22	1.96	0.47
1:A:783:VAL:HG23	1:A:788:ALA:HB2	1.98	0.45
1:A:157:HIS:ND1	1:A:162:ILE:O	2.50	0.44
1:A:263:TRP:O	1:A:266:GLU:HB3	2.18	0.44
1:A:312:ILE:HD11	1:A:1210:GLY:CA	2.49	0.43
1:A:1360:GLU:OE1	1:A:1360:GLU:N	2.50	0.42
1:A:740:ASP:OD1	1:A:741:GLY:N	2.53	0.41
1:A:825:LEU:HD22	1:A:848:LEU:HB3	2.02	0.41
1:A:419:LEU:HD22	1:A:591:ALA:HB1	2.02	0.41

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	1377/1559 (88%)	1307 (95%)	70 (5%)	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	1167/1364 (86%)	1148 (98%)	19 (2%)	62 82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	157	HIS
1	A	218	PHE
1	A	261	LYS
1	A	469	GLN
1	A	535	GLN
1	A	618	VAL
1	A	623	ASP
1	A	627	ASN
1	A	643	LYS
1	A	682	ARG
1	A	774	TYR
1	A	801	LEU
1	A	804	THR
1	A	807	LYS
1	A	826	LEU
1	A	1016	PHE
1	A	1107	GLN
1	A	1282	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SEP	A	908	1	8,9,10	1.55	1 (12%)	8,12,14	1.64	2 (25%)
1	TPO	A	911	1	8,10,11	1.60	1 (12%)	10,14,16	1.73	1 (10%)
1	SEP	A	914	1	8,9,10	1.56	1 (12%)	8,12,14	1.66	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	908	1	-	1/5/8/10	-
1	TPO	A	911	1	-	3/9/11/13	-
1	SEP	A	914	1	-	2/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	911	TPO	P-O1P	3.40	1.61	1.50
1	A	914	SEP	P-O1P	3.39	1.61	1.50
1	A	908	SEP	P-O1P	3.38	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	911	TPO	P-OG1-CB	-4.63	109.23	123.21
1	A	914	SEP	OG-CB-CA	3.02	111.08	108.14
1	A	908	SEP	OG-CB-CA	3.00	111.06	108.14
1	A	914	SEP	P-OG-CB	-2.99	110.05	118.30
1	A	908	SEP	P-OG-CB	-2.96	110.15	118.30

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	908	SEP	N-CA-CB-OG
1	A	911	TPO	N-CA-CB-OG1
1	A	911	TPO	C-CA-CB-CG2
1	A	911	TPO	N-CA-CB-CG2
1	A	914	SEP	CA-CB-OG-P
1	A	914	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

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.

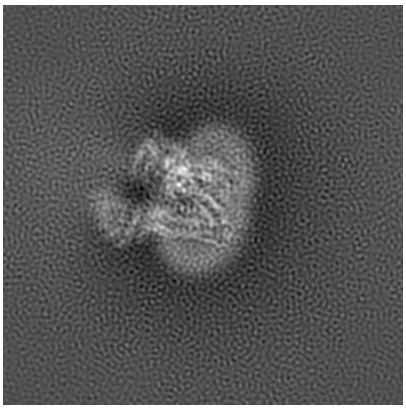
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23691. These allow visual inspection of the internal detail of the map and identification of artifacts.

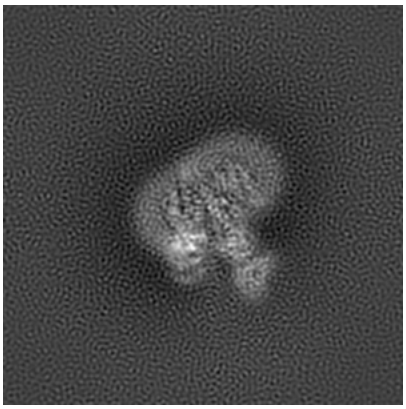
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

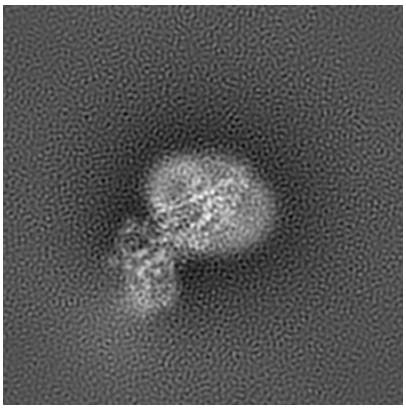
6.1.1 Primary map



X

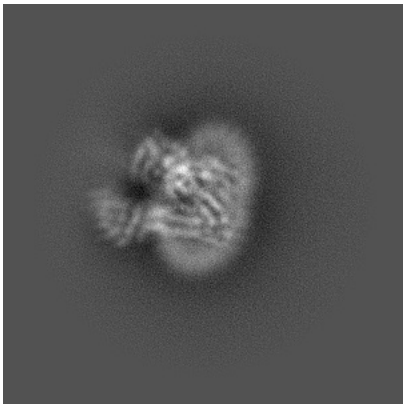


Y

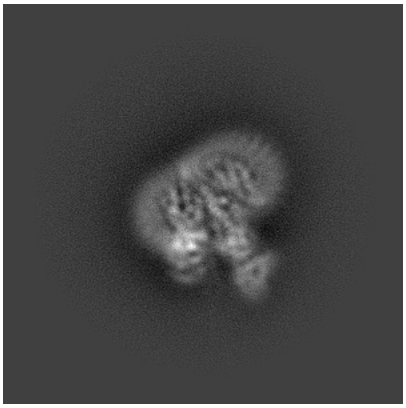


Z

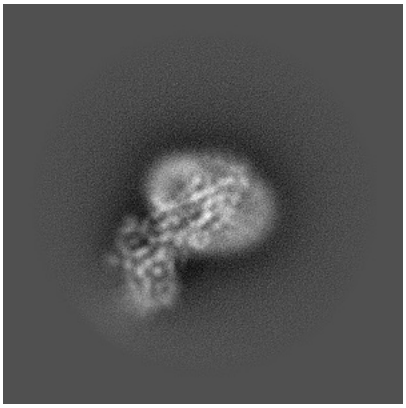
6.1.2 Raw map



X



Y

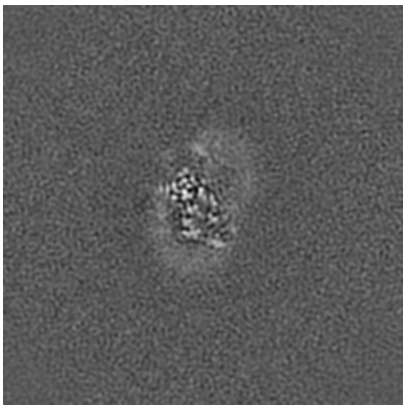


Z

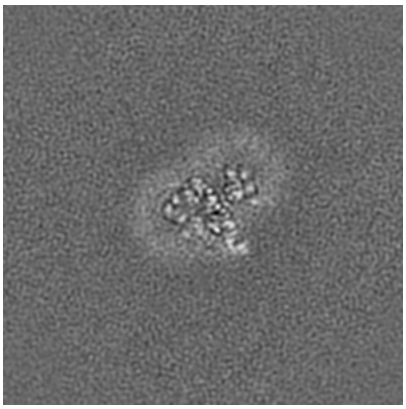
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

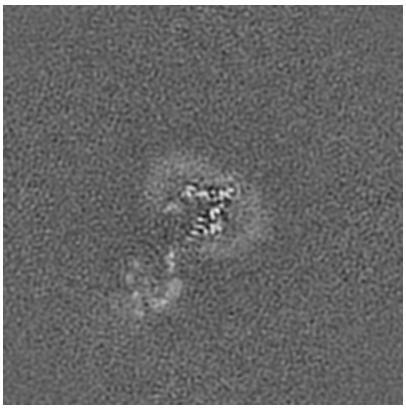
6.2.1 Primary map



X Index: 150

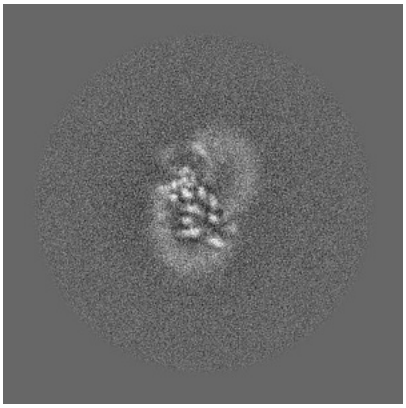


Y Index: 150

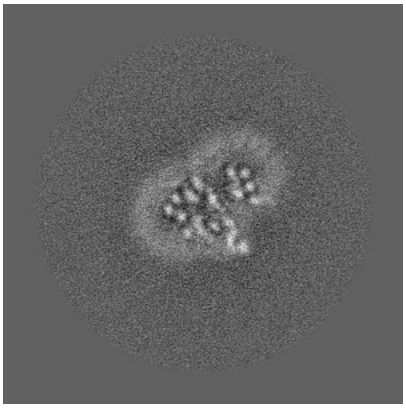


Z Index: 150

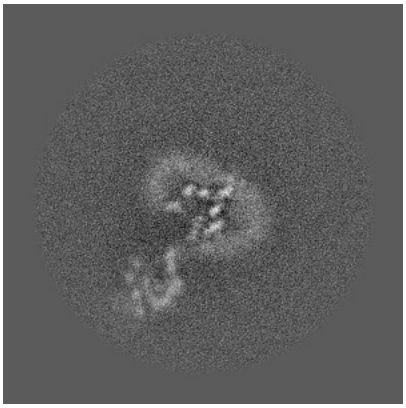
6.2.2 Raw map



X Index: 150



Y Index: 150

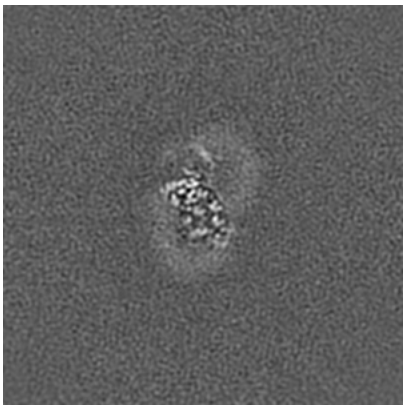


Z Index: 150

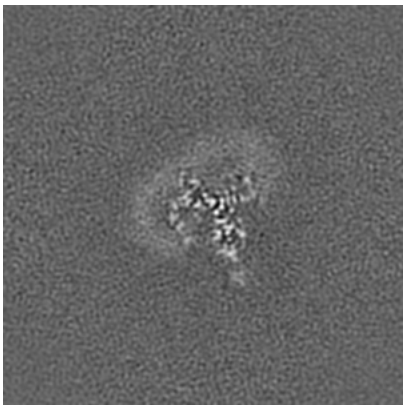
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

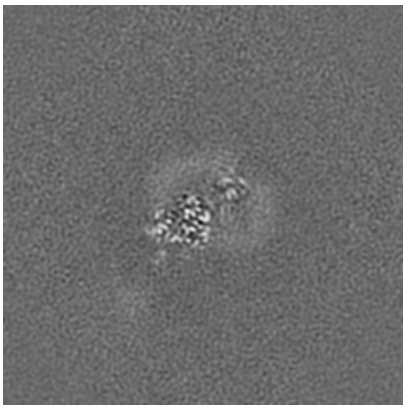
6.3.1 Primary map



X Index: 152

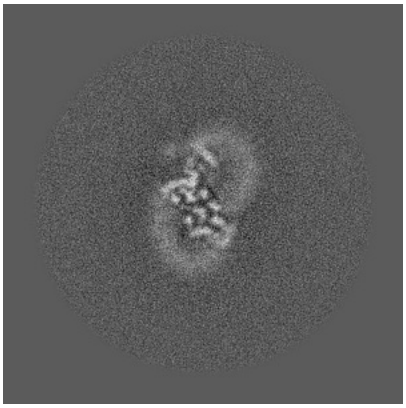


Y Index: 140

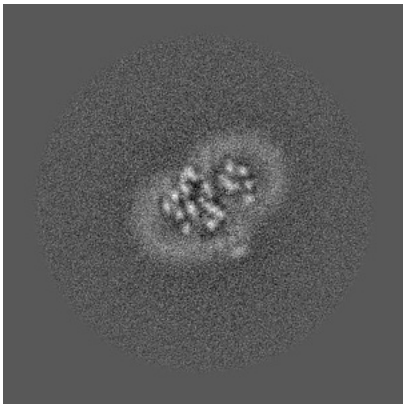


Z Index: 164

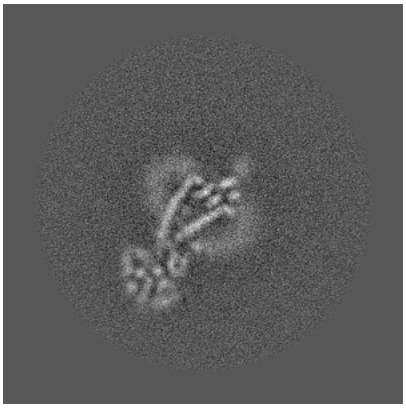
6.3.2 Raw map



X Index: 153



Y Index: 155



Z Index: 138

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

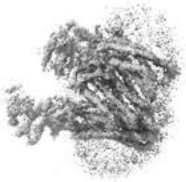
X

Y

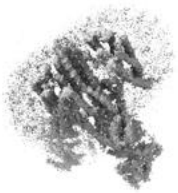
Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. 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.

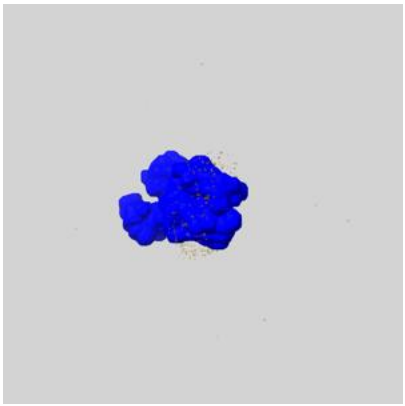
6.5 Mask visualisation (i)

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

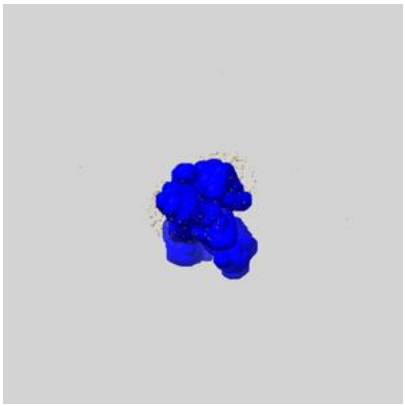
A mask typically either:

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

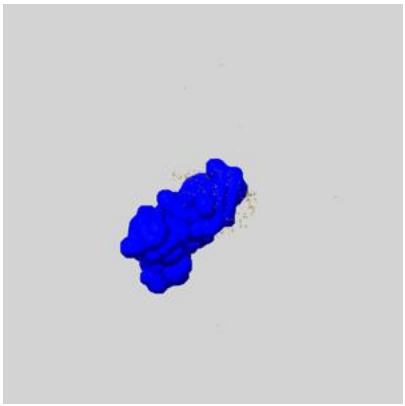
6.5.1 emd_23691_msk_1.map (i)



X



Y

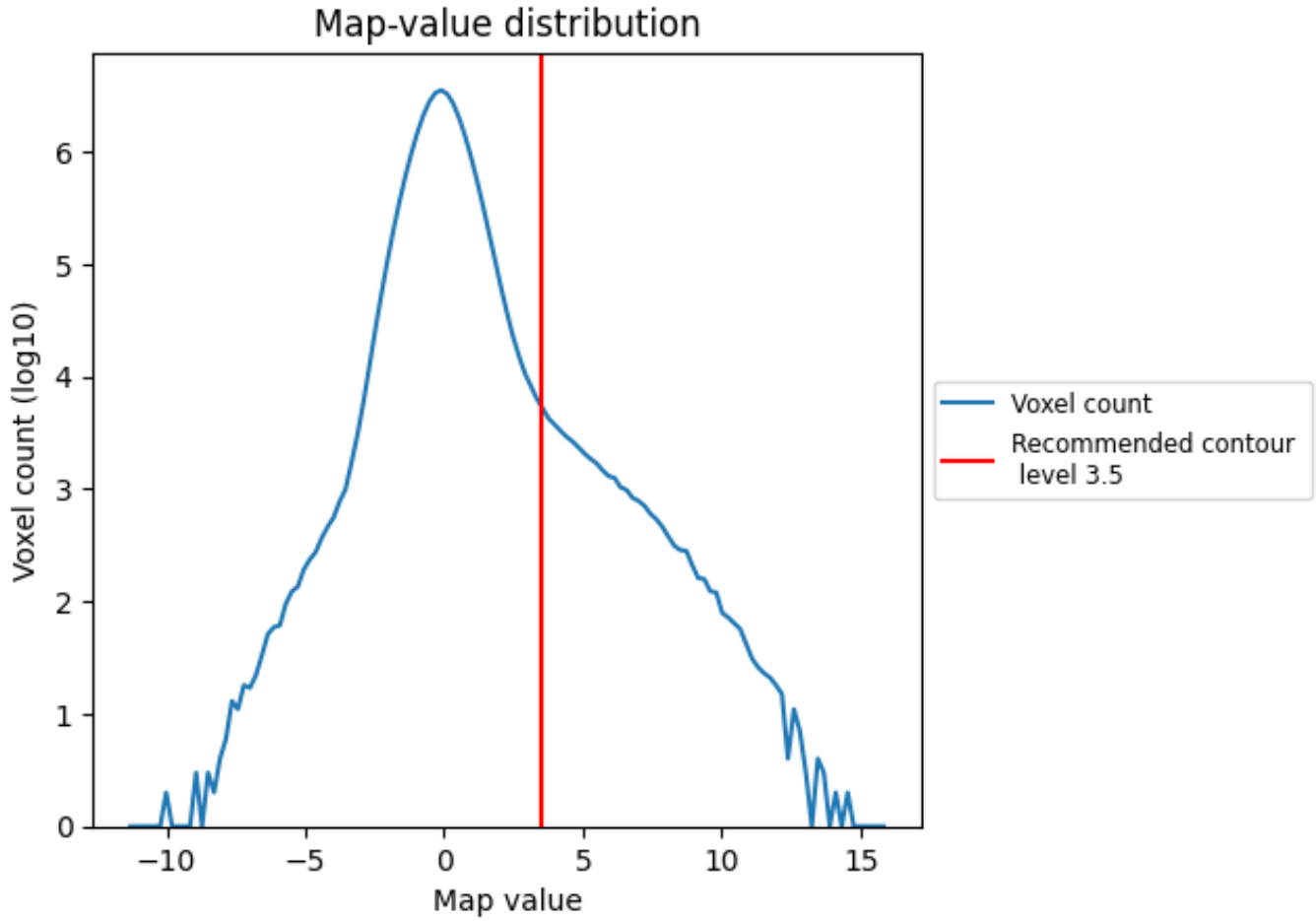


Z

7 Map analysis

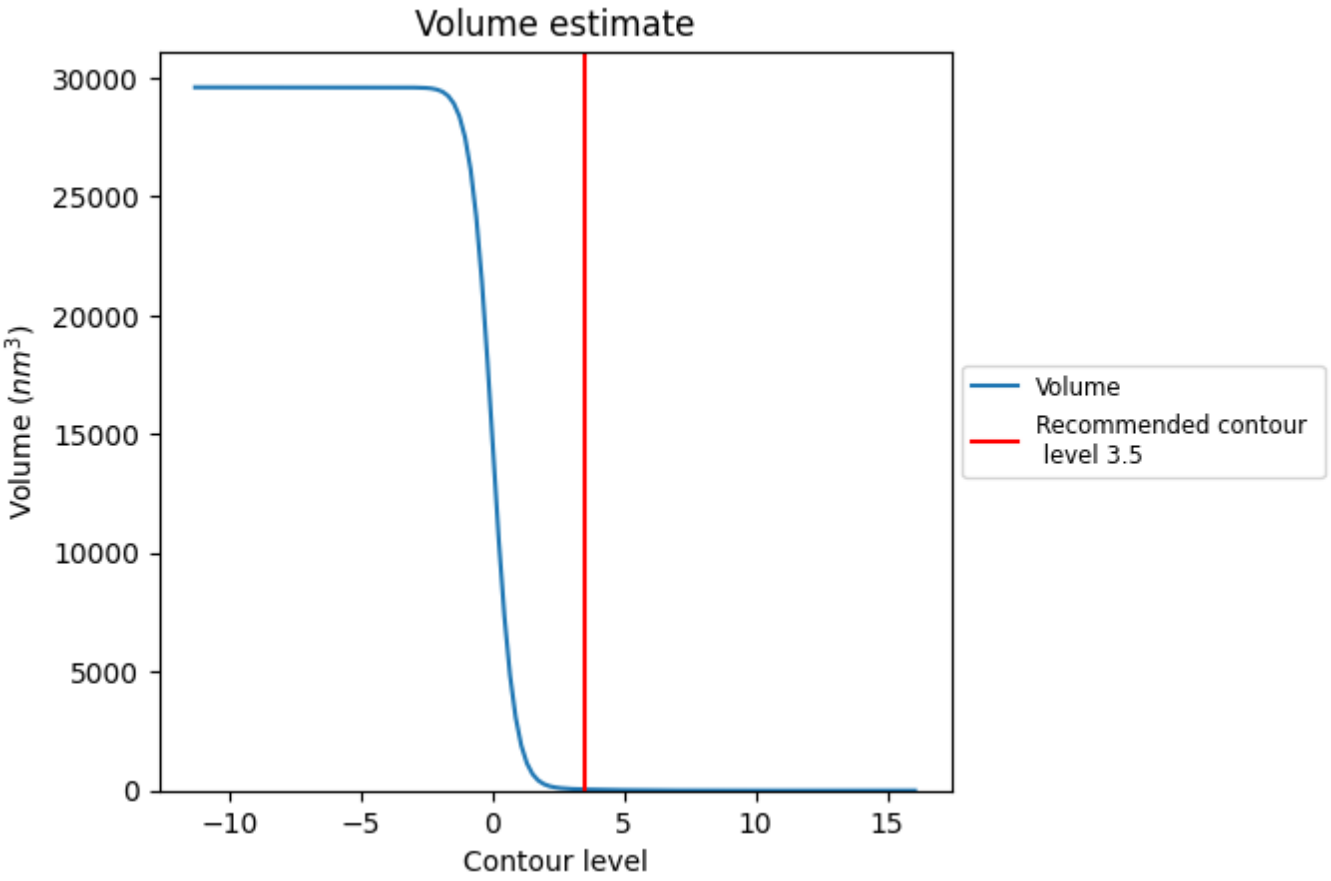
This section contains the results of statistical analysis of the map.

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.

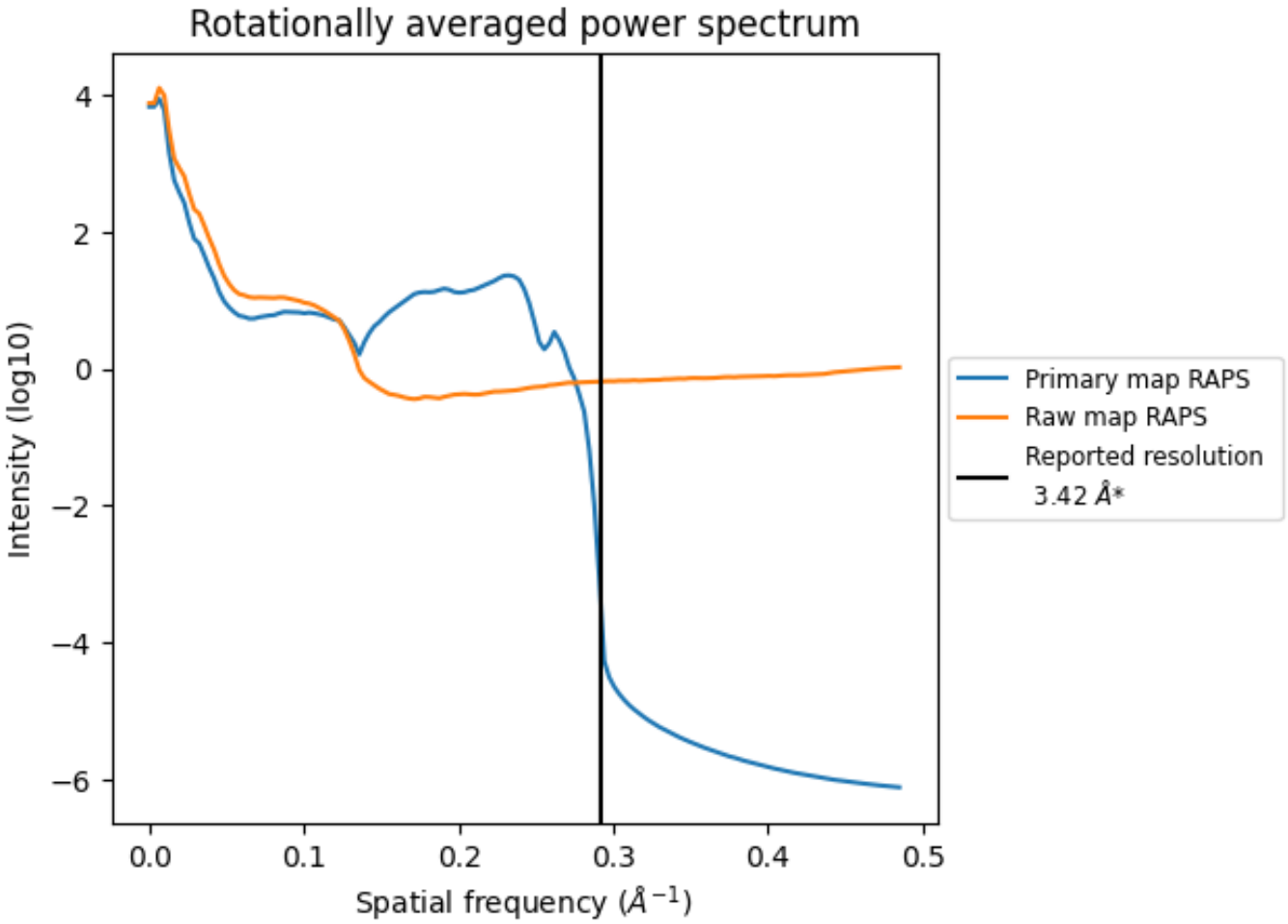
7.2 Volume estimate



The volume at the recommended contour level is 48 nm^3; this corresponds to an approximate mass of 43 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)

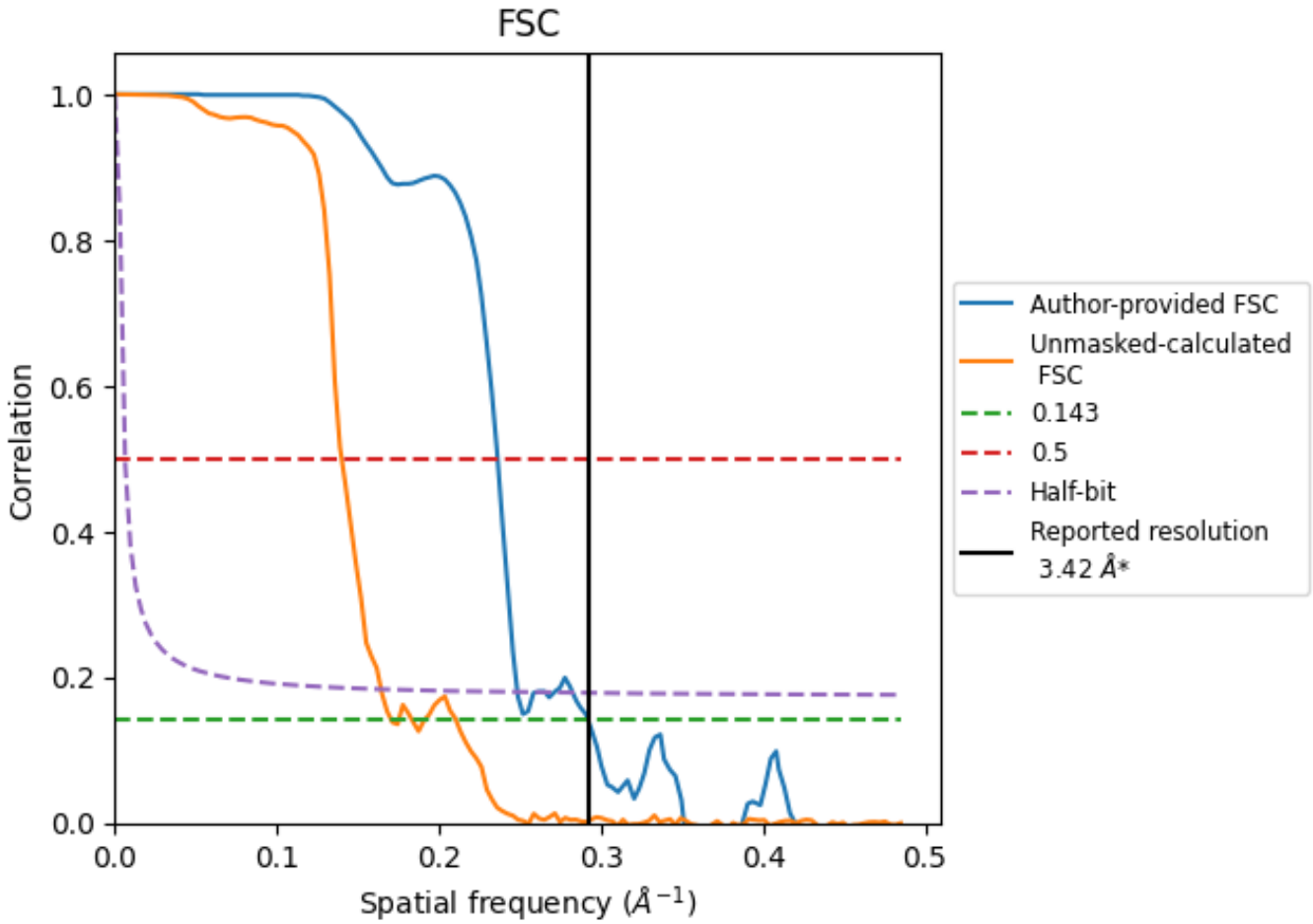


*Reported resolution corresponds to spatial frequency of 0.292 Å^{-1}

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 0.292 $Å^{-1}$

8.2 Resolution estimates (i)

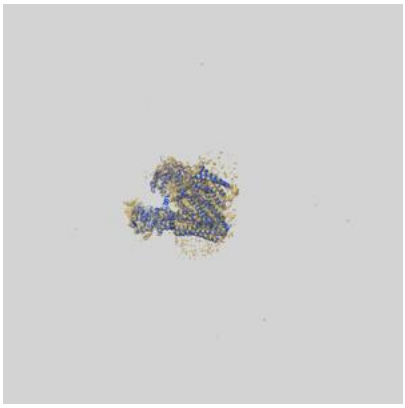
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.43	4.23	4.02
Unmasked-calculated*	5.88	7.14	6.09

*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 5.88 differs from the reported value 3.42 by more than 10 %

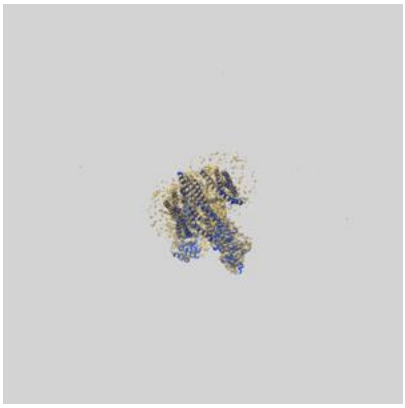
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23691 and PDB model 7M69. Per-residue inclusion information can be found in section 3 on page 5.

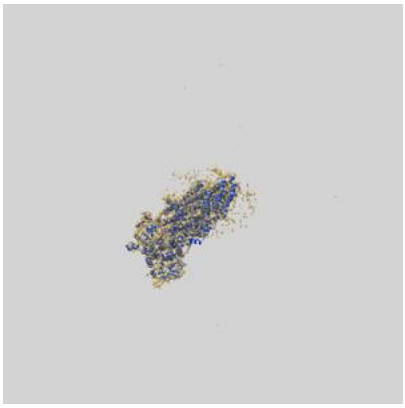
9.1 Map-model overlay



X



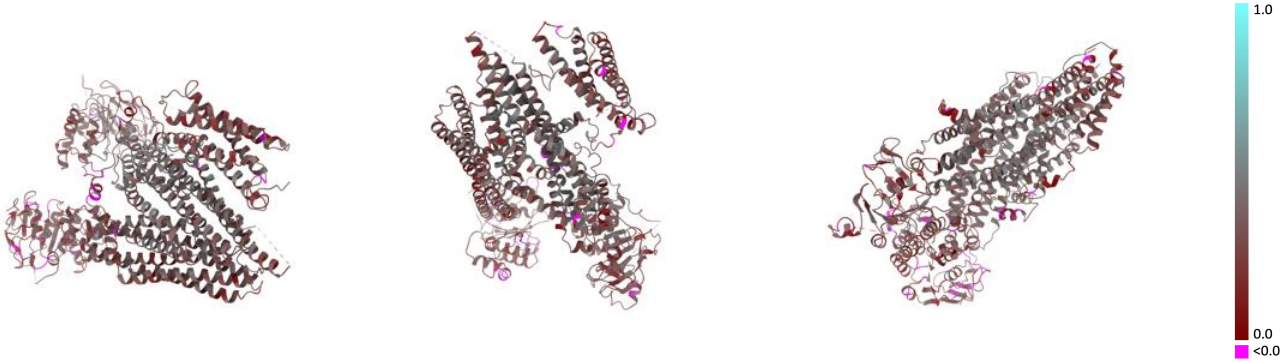
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5 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.

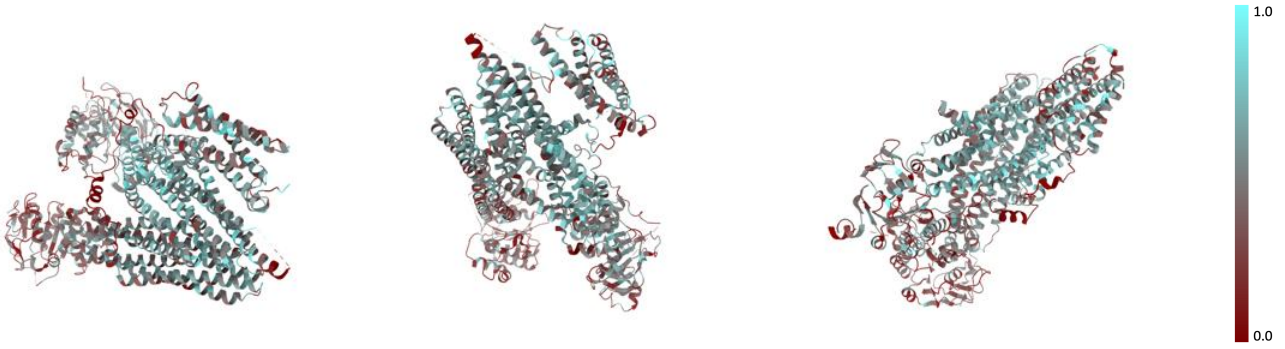
9.2 Q-score mapped to coordinate model (i)



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.

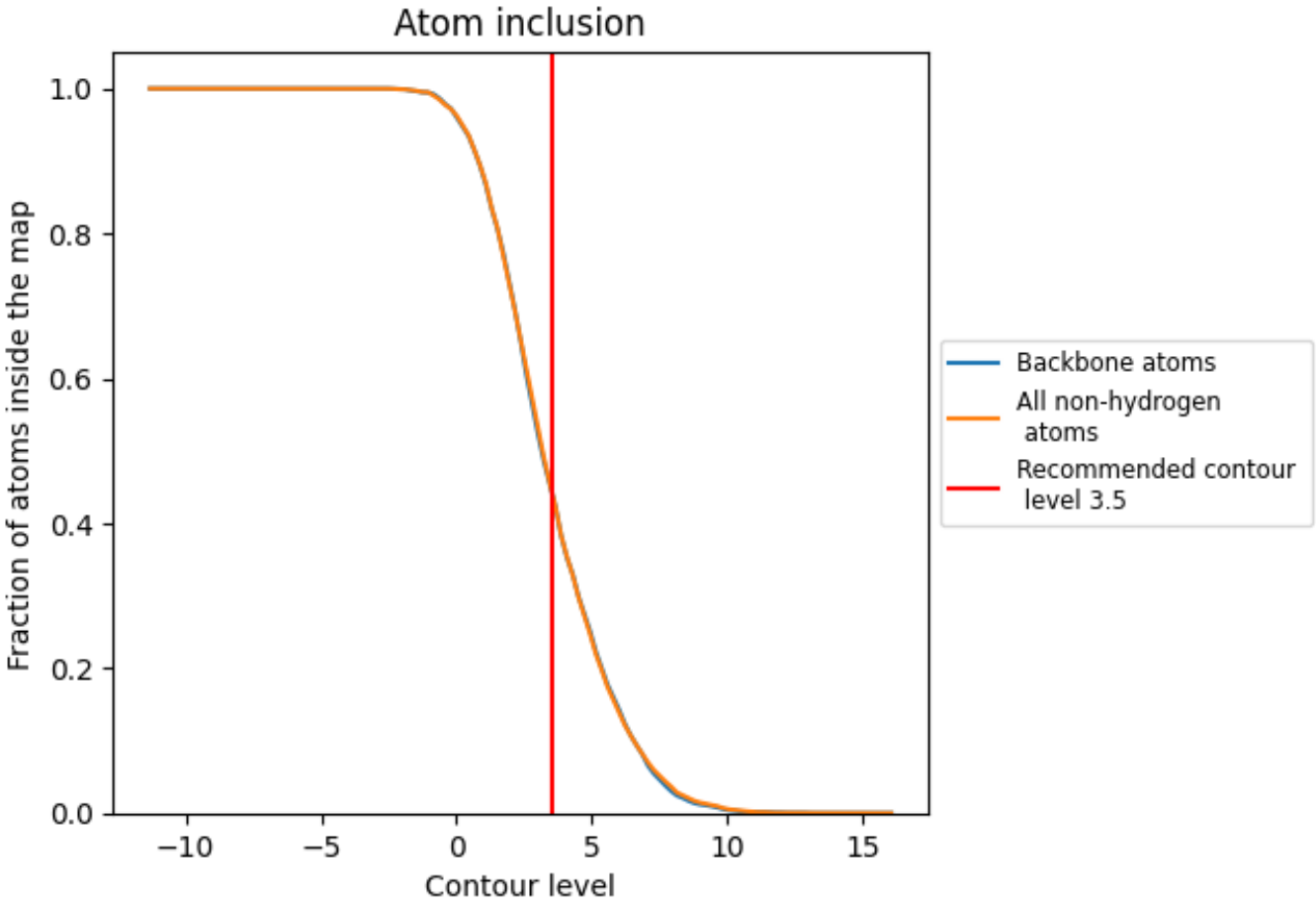
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 45% of all backbone atoms, 45% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4465	0.3180
A	0.4565	0.3180