



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 03:18 pm GMT

PDB ID : 7Z12
EMDB ID : EMD-14438
Title : VAR2 complex with PAM1.4
Authors : Raghavan, S.S.R.; Wang, K.T.
Deposited on : 2022-02-24
Resolution : 3.00 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

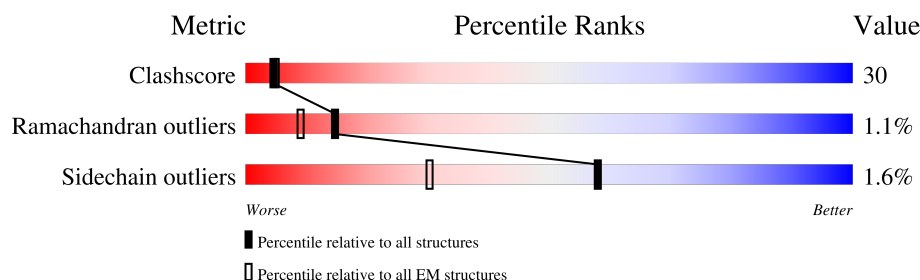
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	B	472	
2	C	233	
3	A	2040	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18352 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 PAM1.4, Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	221	Total	C	N	O	S	0	0
			1650	1042	283	319	6		

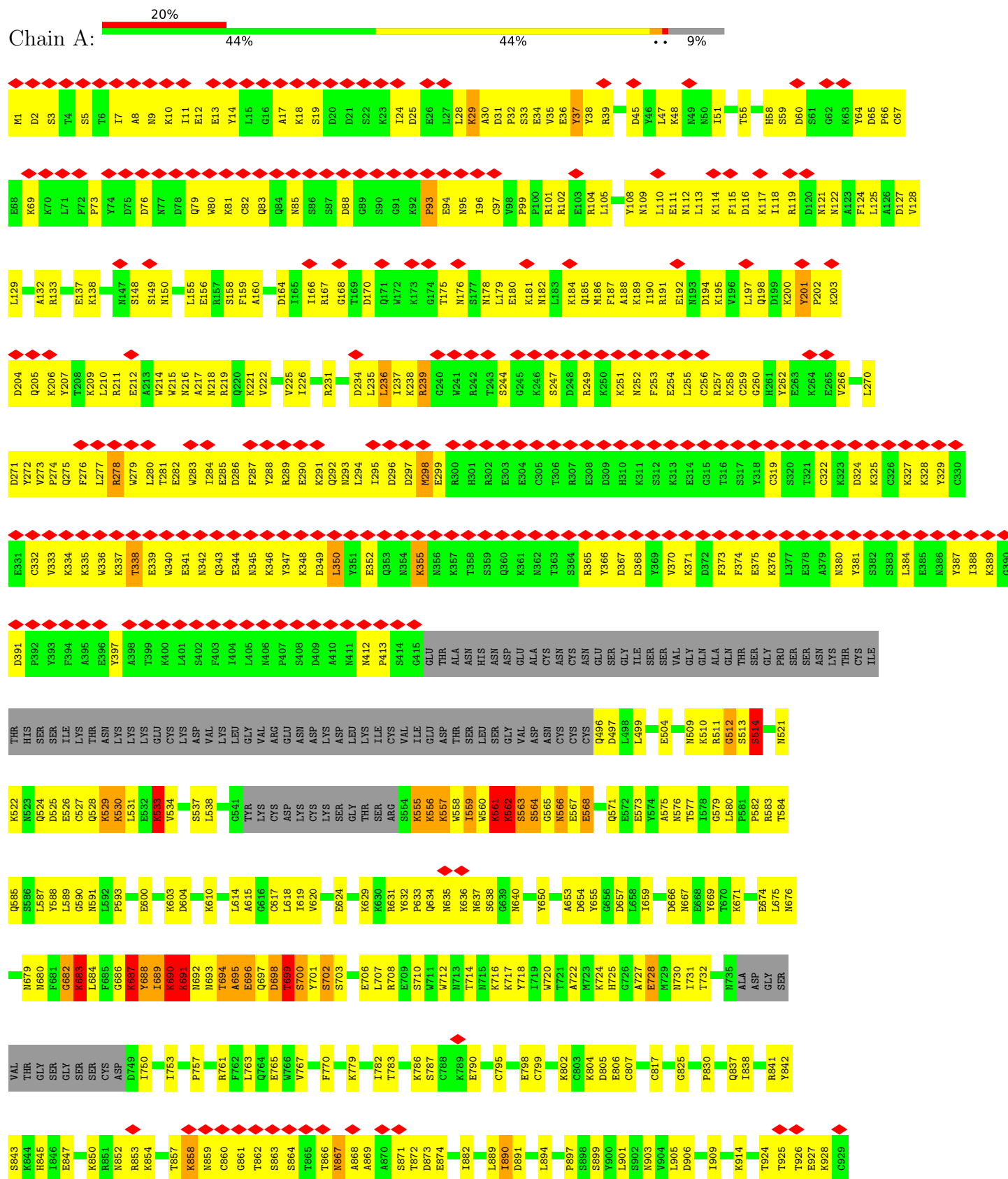
- Molecule 2 is a protein called PAM1.4, light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	212	Total	C	N	O	S	0	0
			1631	1021	279	326	5		

- Molecule 3 is a protein called VAR2CSA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1853	Total	C	N	O	S	0	0
			15071	9402	2597	2973	99		

● Molecule 3: VAR2CSA



N930	R995	SER	A1129	E1206	N1271	G1332	V1394	R1465	N1556	R1664	Q1765	E1875
K931	G996	ASP	M1130	S1207	L1272	K1333	G1395	L1466	N1561	E1665	R1769	D1879
E932	Y997	GLU	K1131	T1208	C1273	M1334	S1396	R1467	Y1561	A1666	Y1770	Y1880
R933	Y997	THR	G1132	D1209	G1274	D1335	S1397	Y1468	Y1561	Y1667	P1780	L1883
D934	N999	PRQ	S1133	E1210	E1275	P1336	T1398	E1470	Y1564	Y1669	L1781	M1884
K935	D1000	LVS	Q1134	N1211	G1276	L1339	E1399	R1471	Y1564	K1470	M1780	L1888
S936	M1001	VAL	K1136	T1212	E1277	P1340	N1400	I1472	D1569	I1473	L1781	M1888
K937	E1002	ARG	K1137	I1212	L1278	K1341	A1401	Y1473	S1572	A1474	C1762	M1888
S938	L1004	GLY	Y1138	N1213	D1279	G1342	A1402	A1475	I1573	C1476	G1769	L1888
Q939	C1005	TJR	W1139	K1214	K1280	F1343	W1404	T1477	Q1578	T1478	I1788	M1888
S940	K1006	GLU	S1140	S1215	Y1282	H1345	W1405	I1478	Y1581	I1479	H1790	M1888
V946	K1007	GLY	L1141	E1216	G1283	V1347	K1406	K1479	Y1582	K1480	A1791	M1888
V947	Y1007	ASP	S1142	N1217	G1284	Q1348	G1407	R1481	Y1584	R1482	Q1794	M1888
V948	M1008	ARG	M1143	S1218	R1285	S1350	E1409	E1483	Y1584	R1482	R1797	M1888
V949	G1009	ASN	F1145	C1219	N1287	S1351	E1410	E1484	E1588	R1482	L1798	M1888
P950	V1010	ASN	F1147	D1220	I1288	T1352	E1411	E1485	K1589	K1484	L1799	M1888
S951	D1011	THR	S1148	L1221	I1288	D1353	A1412	K1485	K1590	D1697	E1800	M1888
P952	Y1012	THR	W1150	N1222	N1290	Y1354	D1414	K1485	K1590	L1698	E1801	M1888
P952	T1015	GLN	I1154	A1223	D1291	K1355	A1415	S1489	S1594	I1701	F1814	M1888
P952	T1016	THR	Q1155	N1225	E1294	M1357	V1416	K1490	L1595	D1706	K1818	M1888
P952	R1018	C1093	K1156	Y1226	L1295	I1358	R1417	Q1493	C1596	E1711	C1821	M1888
P952	S1019	E1094	M1159	I1227	L1296	L1359	A1418	E1493	K1599	Y1712	D1822	M1888
P952	M1020	E1095	G1160	R1228	K1297	G1360	E1419	K1496	K1612	E1712	P1823	M1888
P952	S1021	C1096	D1161	G1229	E1298	T1361	T1421	I1497	K1612	Y1715	P1824	M1888
P952	G1026	K1098	W1162	C1230	K1300	S1362	K1422	Q1498	N1615	K1719	R1825	M1888
P952	Y1029	C1099	S1163	Q1231	K1301	N1364	I1423	G1499	G1616	L1720	K1826	M1888
P952	M1033	K1101	I1165	Y1235	N1302	E1365	K1425	C1501	R1617	N1721	A1827	M1888
P952	E1041	L1102	I1167	G1237	I1304	I1369	K1426	K1502	P1626	W1720	D1828	M1888
P952	I1042	W1103	M1167	E1236	I1304	I1369	N1427	R1503	R1627	I1722	T1829	M1888
P952	Q1045	K1106	I1168	G1241	K1306	E1370	N1429	K1504	K1629	I1723	C1830	M1888
P952	I1046	D1107	E1174	P1242	E1307	G1370	E1432	K1507	Q1630	S1726	D1832	M1888
P952	I1047	N1108	F1175	G1243	T1308	K1371	F1432	Y1508	L1633	T1729	N1833	M1888
P952	E1048	Q1110	L1176	K1243	L1310	E1374	N1433	Y1511	Y1634	R1738	C1838	M1888
P952	M1049	W1111	I1177	E1246	L1311	D1375	E1436	E1519	E1635	W1741	K1839	M1888
P952	M1050	K1113	S1184	K1247	Y1312	I1376	E1437	D1520	L1636	T1746	A1843	M1888
P952	N1052	Q1114	G1187	Q1248	E1313	K1377	C1437	K1521	F1637	P1752	M1847	M1888
P952	A1053	N1115	G1187	T1249	H1315	K1378	P1442	Q1522	I1639	R1753	R1853	M1888
P952	N1054	D1116	I1190	C1251	D1316	I1379	T1443	K1525	I1641	K1754	L1854	M1888
P952	I1055	N1117	E1193	K1252	T1317	E1381	G1444	Y1526	K1642	T1755	E1855	M1888
P952	S1056	Y1118	K1194	D1253	G1318	K1382	N1445	Y1530	L1655	R1757	M1859	M1888
P952	C1057	N1119	M1197	T1254	T1319	G1383	D1446	Y1538	E1656	Q1758	M1863	M1888
P952	I1058	F1121	A1198	I1255	A1320	T1384	Q1449	L1538	T1657	W1761	Y1863	M1888
P952	T1059	R1122	E1199	I1256	I1321	T1384	F1454	N1542	T1660	D1762	K1953	M1888
P952	GLY	S1123	E1199	H1257	I1322	T1385	E1456	K1388	V1661	A1763	Y1954	M1888
P952	LVS	K1124	K1200	G1258	K1323	Q1386	W1457	D1389	E1663	M1764	Y1867	M1888
P952	GLU	Q1125	K1201	D1259	K1324	Q1387	Q1460	K1390	T1660		N1871	M1888
P952	GLU	I1126	C1202	T1260	M1325	K1388	E1464	K1391	V1661			M1888
P952	VAL	Y1127	K1203	T1261	K1326	K1389		I1391	E1663			M1888
P952	LEU	D1128	E1204	G1262	K1327	D1389		G1392				M1888
P952	ASP		M1205		Q1330	G1393		G1393				M1888
P952	SER				K1331							M1888
P952	VAL											M1888

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.352	Depositor
Minimum map value	-0.906	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	366.08002, 366.08002, 366.08002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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	B	0.39	0/1688	0.53	0/2297
2	C	0.36	0/1665	0.51	0/2263
3	A	0.38	0/15370	0.57	2/20668 (0.0%)
All	All	0.38	0/18723	0.56	2/25228 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	A	0	31
All	All	0	32

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	562	LYS	CB-CA-C	-7.20	95.99	110.40
3	A	1203	LYS	N-CA-C	6.14	127.59	111.00

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	201	TYR	Peptide
3	A	236	LEU	Peptide
3	A	239	ARG	Peptide
3	A	37	TYR	Peptide
2	C	48	ILE	Peptide

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	B	1650	0	1628	59	0
2	C	1631	0	1599	60	0
3	A	15071	0	14624	984	0
All	All	18352	0	17851	1093	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 30.

The worst 5 of 1093 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)
3:A:924:THR:HA	3:A:946:VAL:O	1.27	1.31
3:A:251:LYS:HB3	3:A:566:ASN:HB2	1.21	1.12
3:A:325:LYS:O	3:A:329:TYR:HB2	1.60	0.99
3:A:83:GLN:HB3	3:A:95:ASN:HD21	1.28	0.97
3:A:559:ILE:HG22	3:A:561:LYS:HG2	1.48	0.95

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	B	219/472 (46%)	205 (94%)	14 (6%)	0	100	100
2	C	210/233 (90%)	189 (90%)	21 (10%)	0	100	100
3	A	1843/2040 (90%)	1512 (82%)	305 (16%)	26 (1%)	9	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2272/2745 (83%)	1906 (84%)	340 (15%)	26 (1%)	15	44

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	563	SER
3	A	566	ASN
3	A	683	LYS
3	A	690	LYS
3	A	699	THR

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	B	181/411 (44%)	180 (99%)	1 (1%)	84	93
2	C	184/201 (92%)	182 (99%)	2 (1%)	70	87
3	A	1674/1839 (91%)	1644 (98%)	30 (2%)	54	80
All	All	2039/2451 (83%)	2006 (98%)	33 (2%)	58	82

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1156	LYS
3	A	1490	LYS
3	A	1980	ILE
3	A	561	LYS
3	A	559	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	1400	ASN
3	A	1427	ASN

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Mol	Chain	Res	Type
3	A	1972	GLN
3	A	1957	HIS
3	A	1305	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

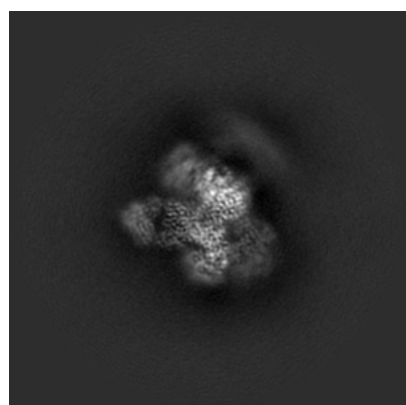
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14438. These allow visual inspection of the internal detail of the map and identification of artifacts.

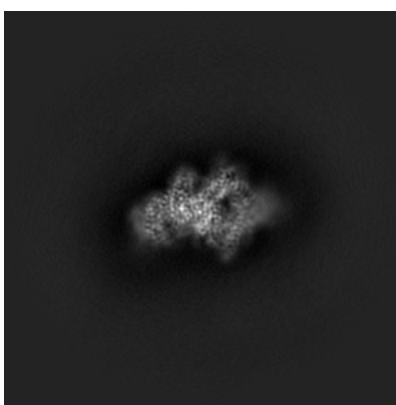
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

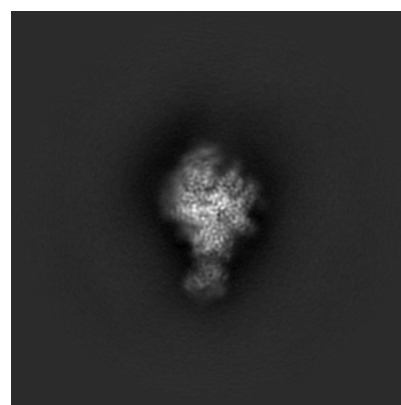
6.1.1 Primary map



X



Y

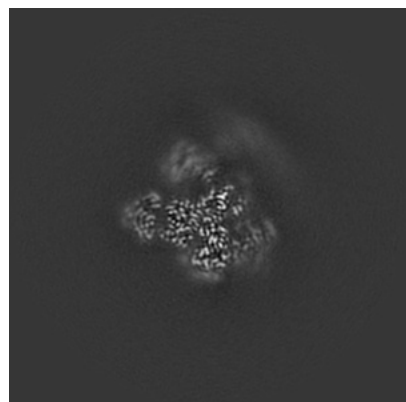


Z

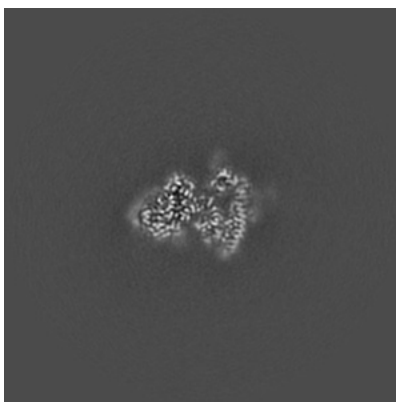
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

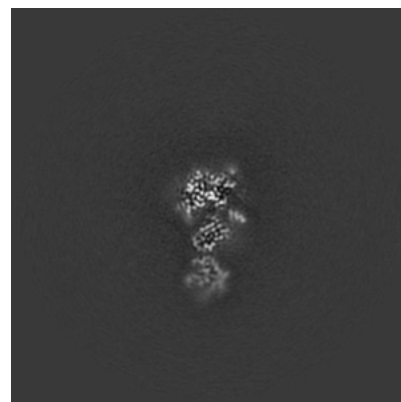
6.2.1 Primary map



X Index: 220



Y Index: 220

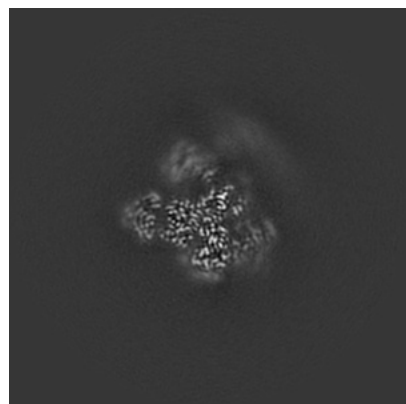


Z Index: 220

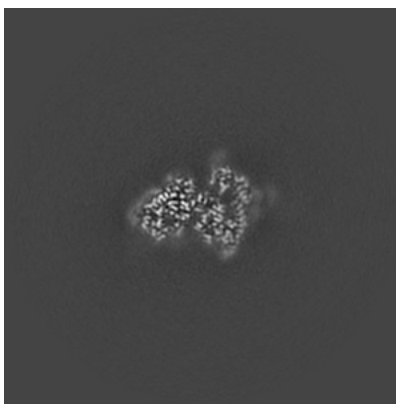
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

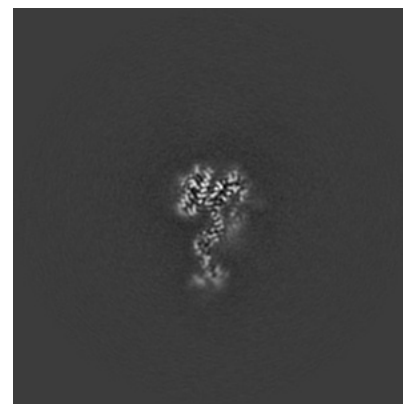
6.3.1 Primary map



X Index: 220



Y Index: 223

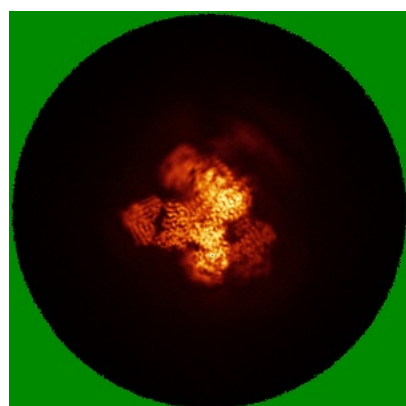


Z Index: 225

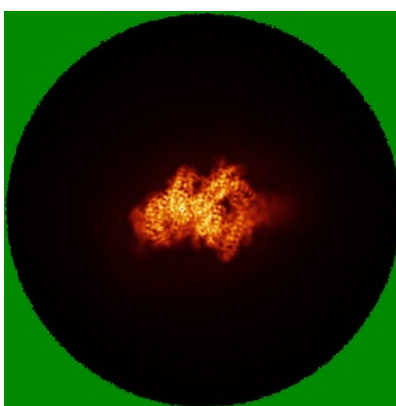
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

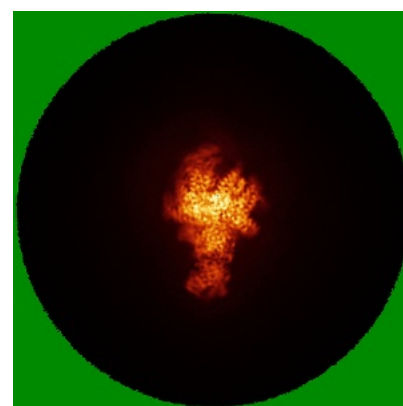
6.4.1 Primary map



X



Y

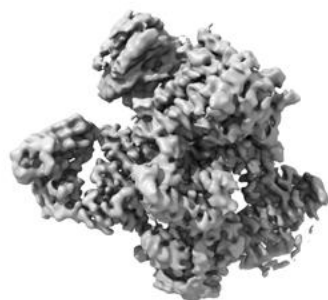


Z

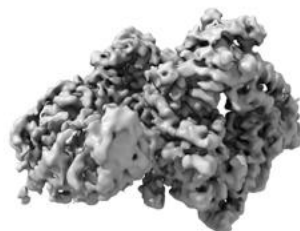
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

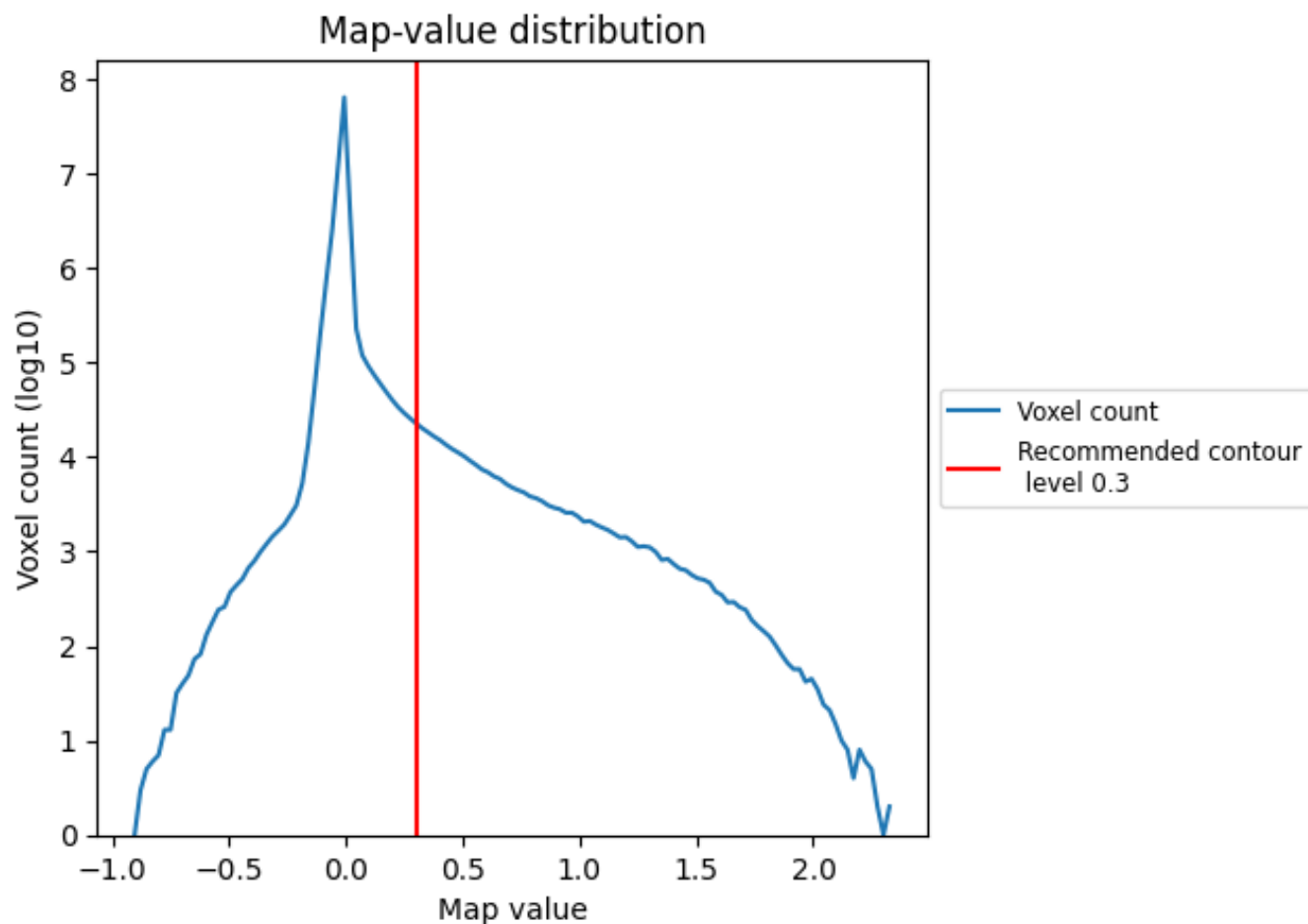
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

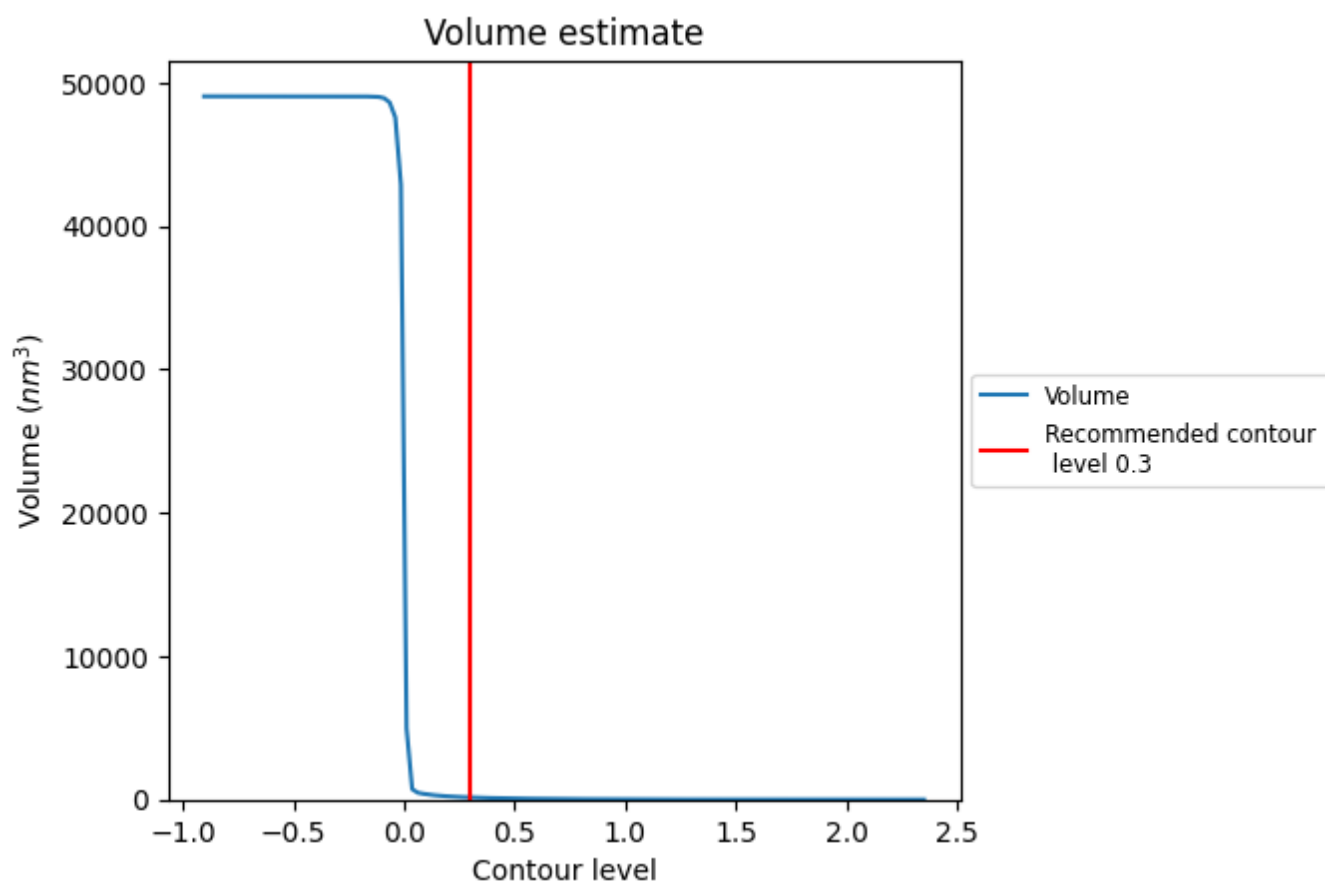
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

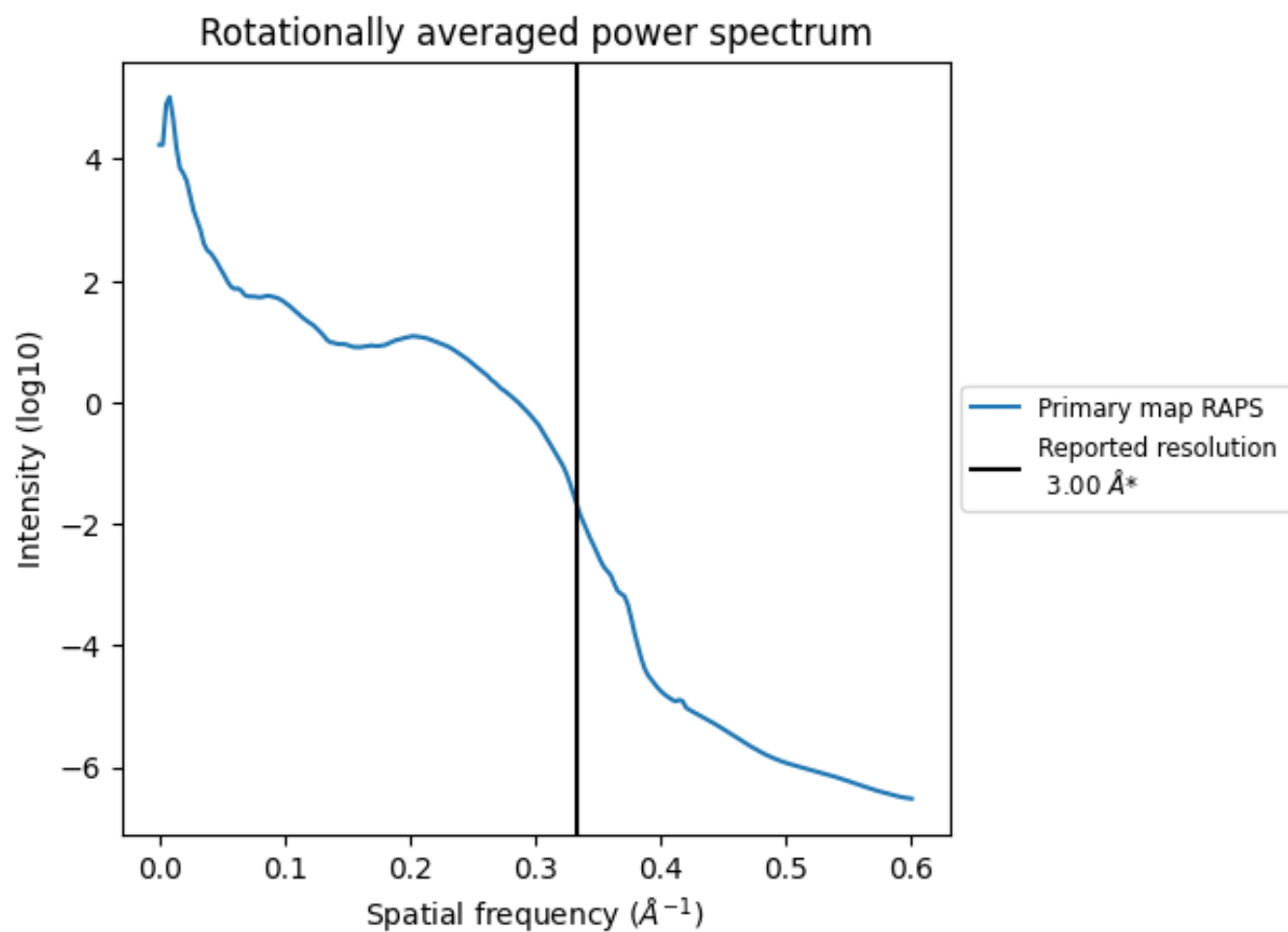
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm³; this corresponds to an approximate mass of 134 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 ⓘ

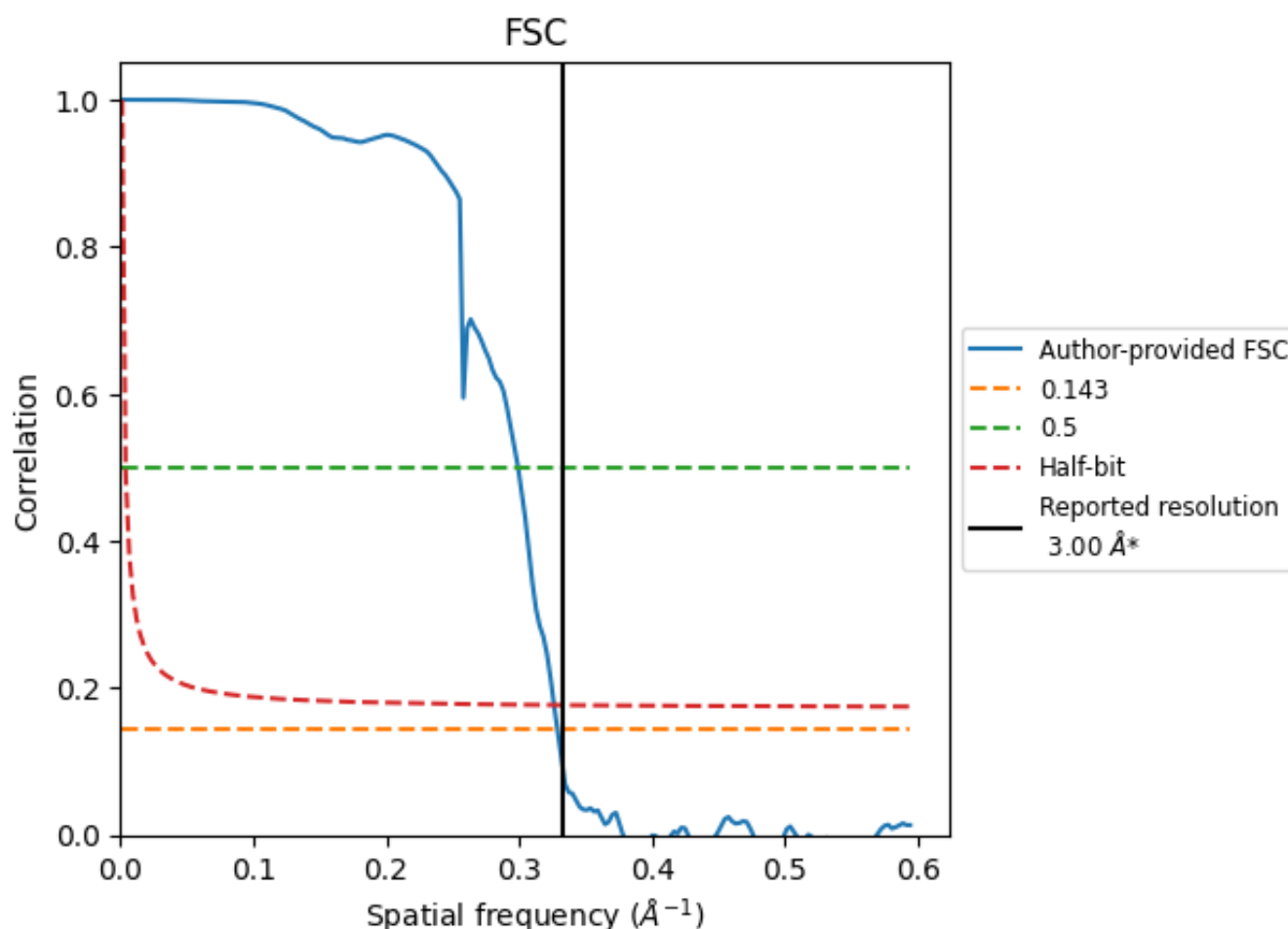


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

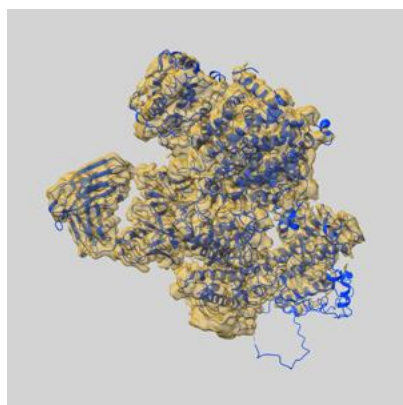
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.34	3.06
Unmasked-calculated*	-	-	-

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

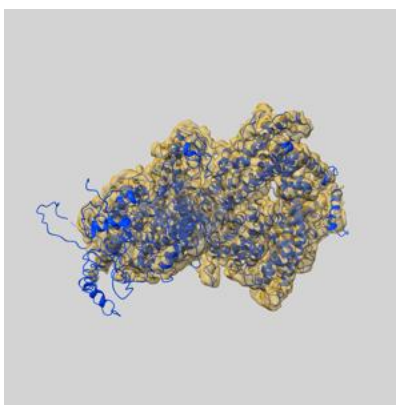
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14438 and PDB model 7Z12. Per-residue inclusion information can be found in section [3](#) on page [4](#).

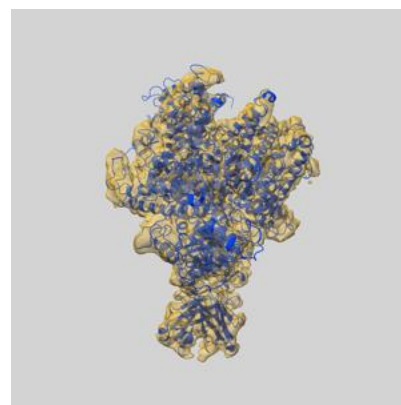
9.1 Map-model overlay [i](#)



X



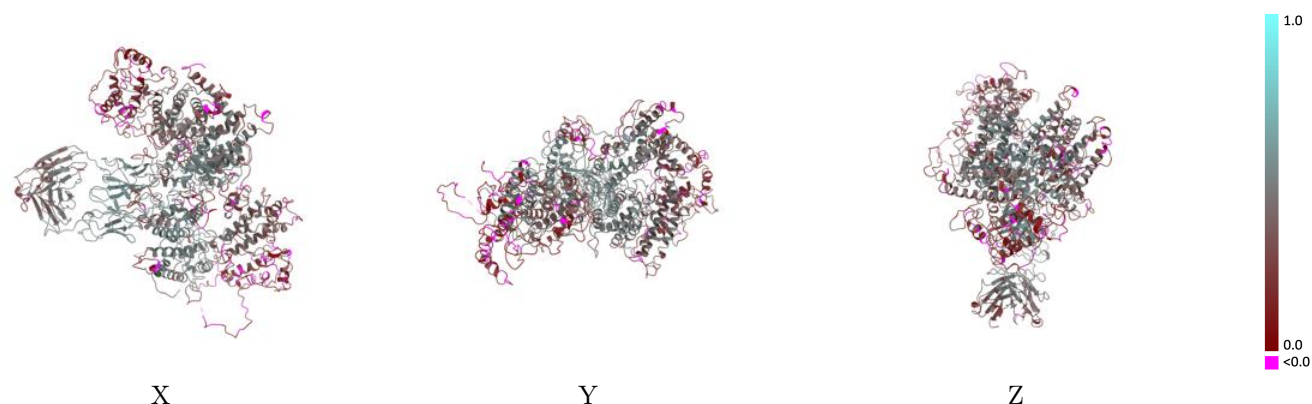
Y



Z

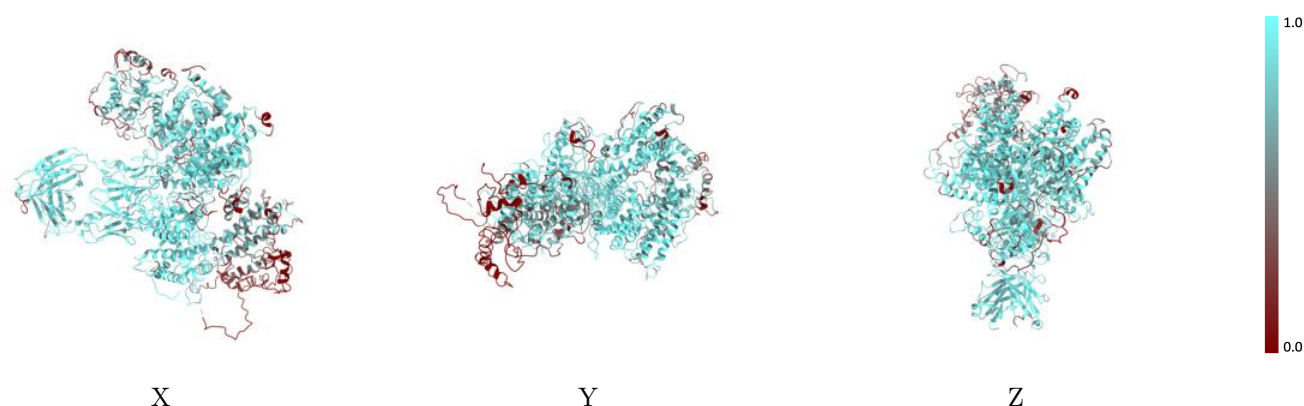
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



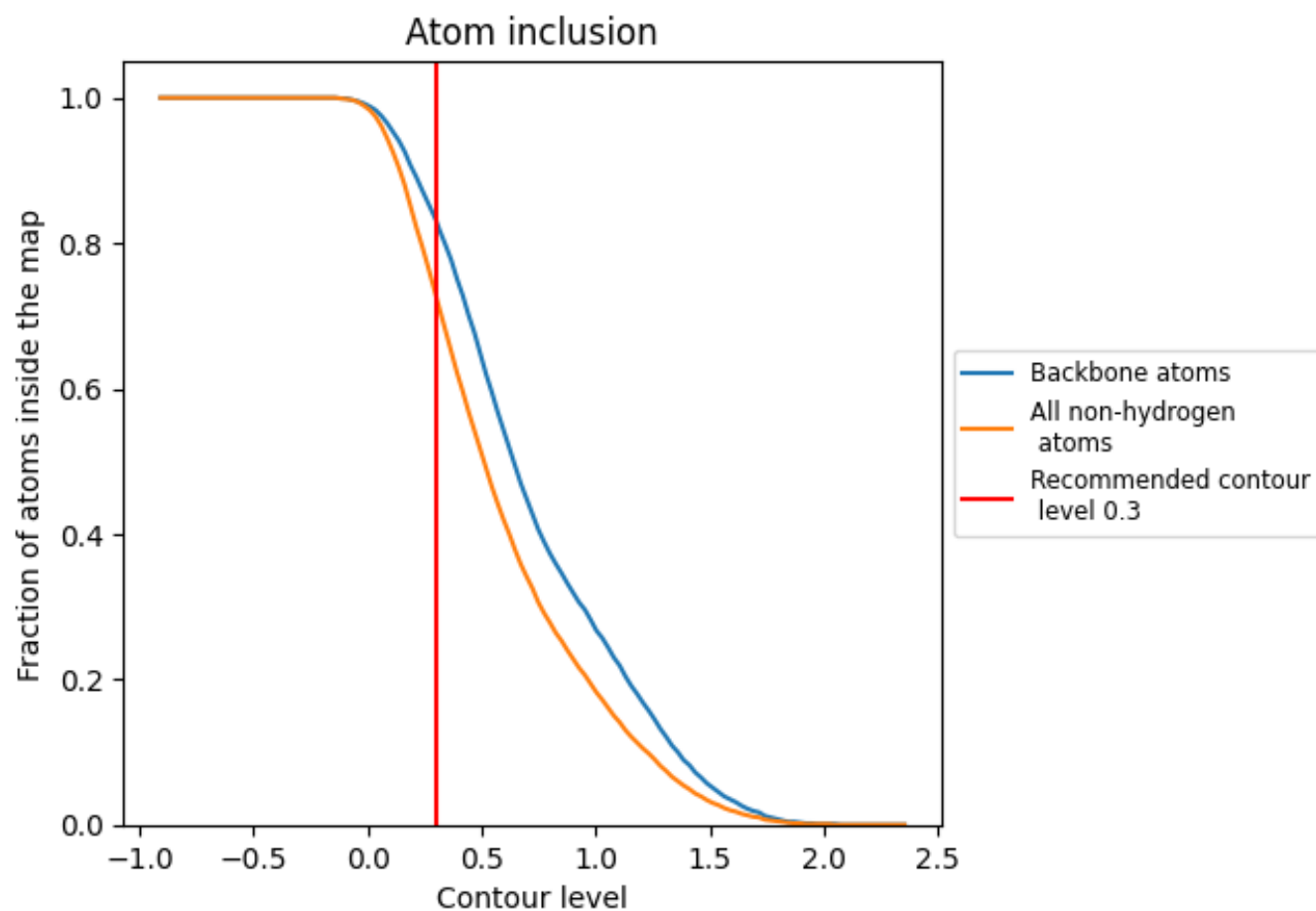
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 73% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7280	<div></div> 0.3620
A	<div></div> 0.6940	<div></div> 0.3360
B	<div></div> 0.8900	<div></div> 0.4880
C	<div></div> 0.8770	<div></div> 0.4750

