



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 09:23 AM EST

PDB ID : 6UEB
EMDB ID : EMD-20753
Title : Structure of Rabies SAD-B19 L-P complex from cryo-EM
Authors : Horwitz, J.A.; Harrison, S.C.
Deposited on : 2019-09-20
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

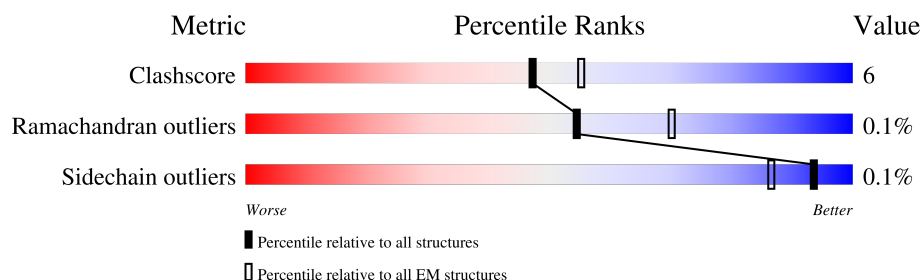
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 $\leq 5\%$. 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	A	2127	<div> <div>62%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	B	42	<div> <div>95%</div> <div>86%</div> <div>14%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34451 atoms, of which 17232 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 Large structural protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2099	Total	C	H	N	O	S	0	0
			33865	10792	16965	2931	3097	80		

- Molecule 2 is a protein called Phosphoprotein,Phosphoprotein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	42	Total	C	H	N	O	S	0	0
			584	190	267	57	68	2		

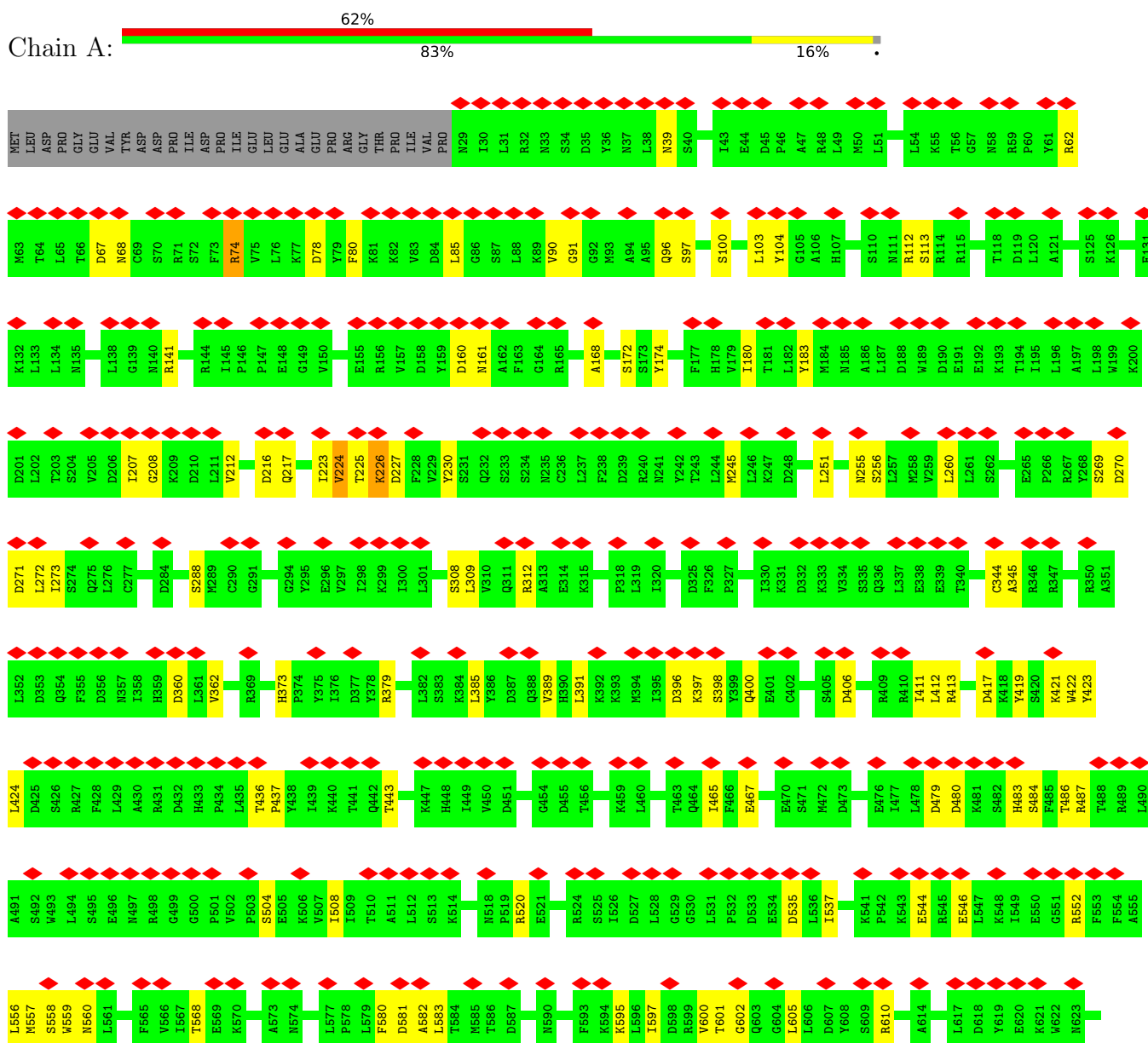
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

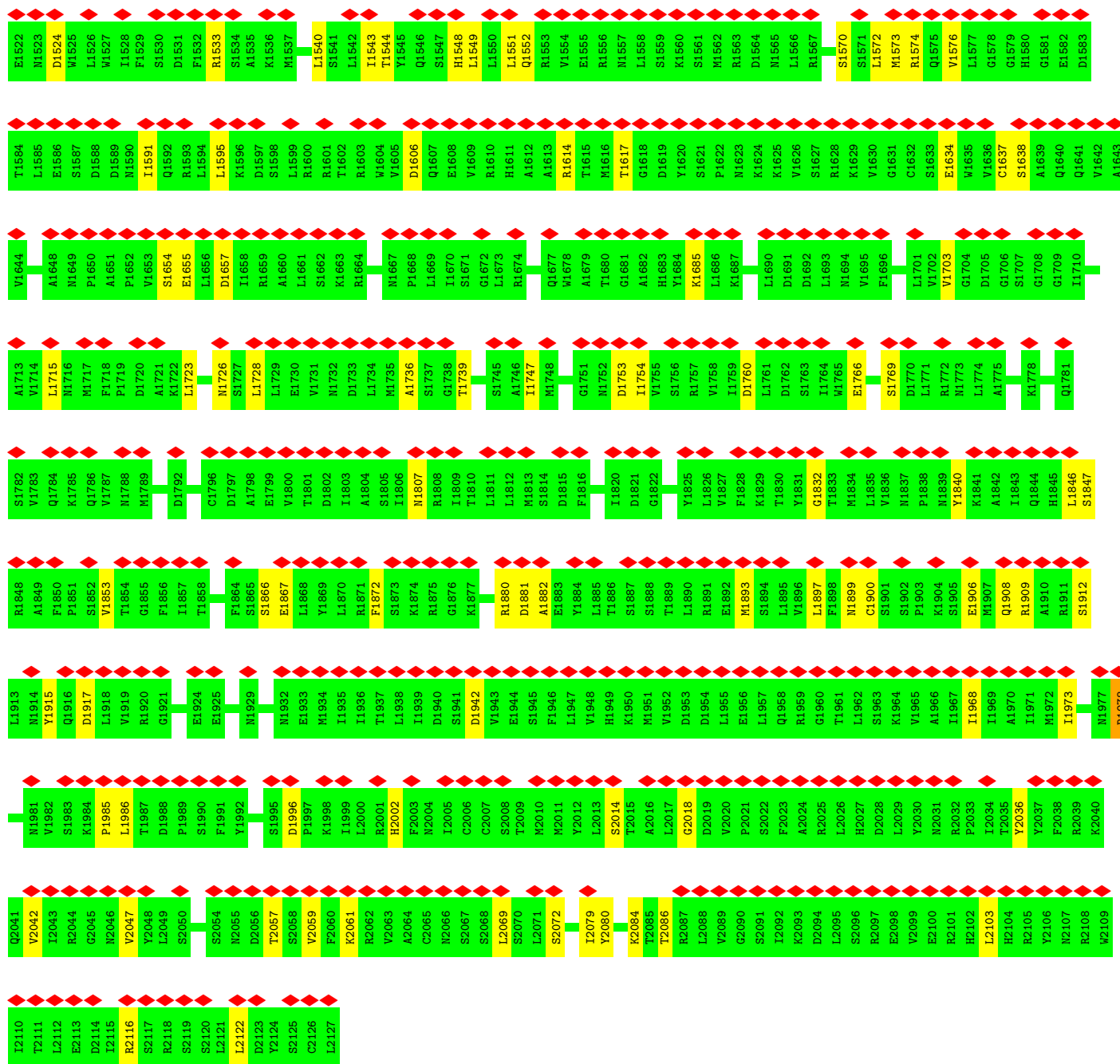
3 Residue-property plots

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.

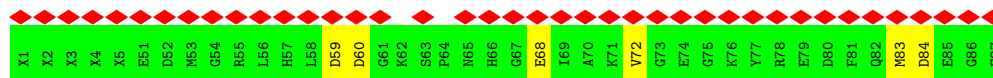
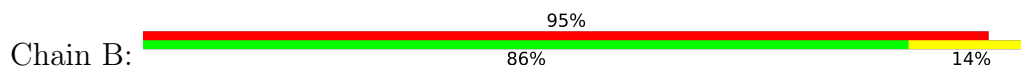
- Molecule 1: Large structural protein



L1459	H1395	R1319	V1248	V1186	H1117	G1045	D981	F914	H840	R764	L698
R1460	D1396	C1320	S1249	H1187	L1124	L1046	A982	S915	Q842	E767	R699
L1461	S1397	V1321	E1250	V1188	P1126	L1048	I983	D916	S843	E768	K701
L1462	D1398	R1322	G1251	K1190	P1125	Q1048	R984	P917	L844	G769	T702
H1463	Y1399	I1324	G1252	R1191	K1127	S1050	K985	E920	L845	A770	S704
H1464	N1400	D1325	Y1253	A1192	L1127	S1050	L987	G921	K846	R774	L705
L1467	D1401	D1326	C1257	L1193	I1130	T1052	Y988	R926	M848	L775	L709
Y1468	G1402	V1394	P1258	S1194	S1131	I1053	D989	E927	R849	I776	M710
L1469	T1403	L1195	L1261	L1196	C1132	R1054	E990	I928	D850	I777	I711
M1470	L1404	K1196	S1262	K1197	T1133	R1054	V991	W929	M854	K778	D712
R1471	F1405	E1197	H1263	E1198	C1134	Q1056	D992	L930	Q857	K779	R713
P1472	P1406	S1198	H1264	I1199	G1135	F1057	K993	S931	Q857	E780	E714
Y1473	V1407	N1200	S1265	Y1201	A1136	R1058	V994	S932	Y862	T782	S715
M1408	N1408	I1334	S1265	W1201	I1137	R1059	E995	Q933	L863	I717	V647
S1475	I1409	F1335	D1269	F1202	G1138	S1060	N996	E934	L864	M783	F648
L1476	Y1410	E1336	T1270	F1202	G1139	S1062	S997	E936	F865	R718	S649
R1477	G1411	F1337	M1271	R1205	H1139	L1061	E998	W936	P867	W719	R650
G1478	P1412	P1338	S1272	D1206	G1140	S1062	S997	I937	F788	T720	T721
E1479	L1413	D1339	S1273	S1207	M1141	K1063	R1000	H938	K793	T722	T723
Y1480	V1340	V1340	D1273	N1208	P1142	T1064	E1001	Q942	G871	K724	K724
F1481	S1341	K1342	L1274	L1209	R1143	L1065	A1002	E943	K875	L725	L725
L1482	P1415	K1342	T1275	A1210	V1146	E1067	I1003	E943	L876	R797	A726
I1483	R1416	R1343	Q1276	Q1211	S1147	S1068	L1004	W946	R798	L802	Q727
Q1485	L1417	I1344	D1277	A1212	P1150	F1069	L1005	P947	E805	E806	W730
K1486	Y1418	S1345	G1278	L1213	P1150	Y1070	L1006	D948	S806	K807	L733
	L1419	R1346	K1279	I1214		M1071	T1008	L949	E880	R808	C734
			M1280	R1215	D1153	S1072	H1009	E950	E881	W809	P735
A1489	G1425	G1350	Y1281	R1216	Q1154	E1073	R1010	E951	E882	R811	G770
A1490	V1426		D1282	I1217	S1155	I1074	D1011	R952	S883	V812	L671
Y1491	L1427		F1283	M1218	F1156	H1075	M1012	T953	F884	S813	R672
T1492	I1428	P1353	M1284	S1219	F1157	G1076	F1013	E955	A887	C814	E873
L1493	G1429	H1354	F1285		S1158			S956	M888	V815	D674
T1494	S1430	F1355			R1159			I891	S816	E746	A681
M1495	S1431	Q1356			L1162	R1079	L1017	D895	N817	G747	S682
I1496	I1432	R1357	L1288	G1222	K1163	M1080	V1020	L960	D818	L748	M683
E1497	G1433	L1358	M1289	D1224	G1164	T1081	E1021	L961	Q819	Y750	G684
F1498	F1434	P1359	L1290	F1225	Y1165	Q1062	L1022	E962	I820	E751	W688
N1499	L1435	D1360	Y1291	P1226	L1166	Q1085	L1023	D963	V821	L752	M689
R1500	T1436	I1361	A1292	L1227	G1167	V1087	F1024	P964	N822	E753	Q691
S1501	R1437	R1362	T1296	E1228	S1297	G1089	R1026	T965	L833	R754	D692
I1502	M1438	L1363	S1297	E1229	E1298	V1090	F1027	T966	E903	S756	G693
L1503	T1439	R1364	L1298	A1230	T1174	R1097	L1028	L967	M904	T757	G694
Y1505	C1504	P1365	E1298	P1231	Q1176	A1098	E1030	N968	S905	R912	L696
L1441	I1441	P1366	Q1301	V1232	L1175	L1098	F1032	I969	L906	Q839	G697
Q1507	M1442	G1366	R1302	V1233	Q1176	D1099	S1033	G971	G907	W833	E596
H1508	I1443	D1367	D1303	F1233	F1177	L1100	F1036	A973	R908	T757	G697
	L1444	F1368	T1304	K1234	H1178	L1101	L1037	S974	H910	R912	L696
	R1445	E1369	R1305	R1235	A1179	E1102	G1038	P975	I911	R912	E596
	P1446	S1370	L1306	T1236	W1180	L1104	I1039	T976	Q913		G697
Y1512	L1447	L1371	R1307	G1237	L1175	L1009	F1032	G971			
E1513	E1448	S1372	D1308	S1238	F1177	L1101	S1033	T829			
R1514	L1449	G1373	S1309	A1239	H1178	R1102	A973	R908			
E1515	V1450	L1374	T1310	L1240	H1178	E1103	S974	H910			
I1517	S1451	E1375	F1311	H1241	A1179	L1104	L1037	I911			
T1518	G1452	K1376	H1312	R1242	W1180	I1104	G1038	T976			
A1519	Y1453		R1316	F1243	E1181	G1107	P1040	R912			
S1520	I1457	G1381	C1317	K1244	K1182	R1108	E1041	L978			
P1521	L1458	S1382	M1318	S1245	V1183	K1109	S1042	L979			
				A1246	T1184	G1112	I1043	K980			
				R1247	M1185		I1043				



• Molecule 2: Phosphoprotein, Phosphoprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72	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	23.362	Depositor
Minimum map value	-12.309	Depositor
Average map value	0.015	Depositor
Map value standard deviation	1.889	Depositor
Recommended contour level	7.0	Depositor
Map size (\AA)	143.144, 143.144, 143.144	wwPDB
Map dimensions	116, 116, 116	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.234, 1.234, 1.234	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.34	0/17290	0.52	0/23418
2	B	0.28	0/296	0.59	0/392
All	All	0.34	0/17586	0.52	0/23810

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	16900	16965	16964	218	0
2	B	317	267	268	5	0
3	A	2	0	0	0	0
All	All	17219	17232	17232	220	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 6.

The worst 5 of 220 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:180:ILE:HD12	1:A:224:VAL:HG21	1.53	0.89
1:A:2042:VAL:HG12	1:A:2047:VAL:HG12	1.58	0.82
1:A:1469:ILE:HD11	1:A:1739:THR:HG21	1.61	0.82
1:A:255:ASN:ND2	1:A:809:TRP:O	2.13	0.81
1:A:68:ASN:HB3	1:A:227:ASP:OD2	1.83	0.78

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	2097/2127 (99%)	2085 (99%)	10 (0%)	2 (0%)	51	81
2	B	35/42 (83%)	34 (97%)	1 (3%)	0	100	100
All	All	2132/2169 (98%)	2119 (99%)	11 (0%)	2 (0%)	54	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	VAL
1	A	226	LYS

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	1901/1927 (99%)	1899 (100%)	2 (0%)	93	97
2	B	30/30 (100%)	30 (100%)	0	100	100
All	All	1931/1957 (99%)	1929 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	1978	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](#)

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	5:UNK	C	51:GLU	N	20.90

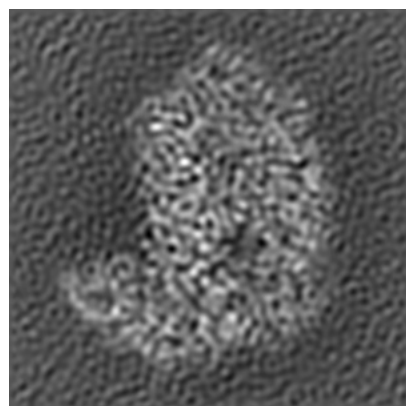
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20753. These allow visual inspection of the internal detail of the map and identification of artifacts.

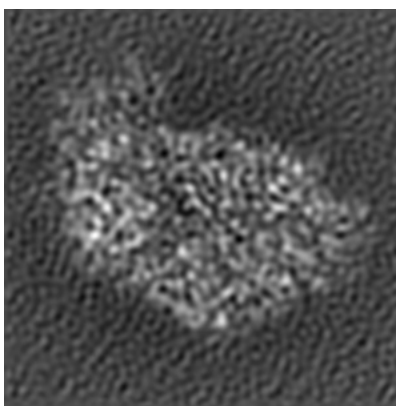
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

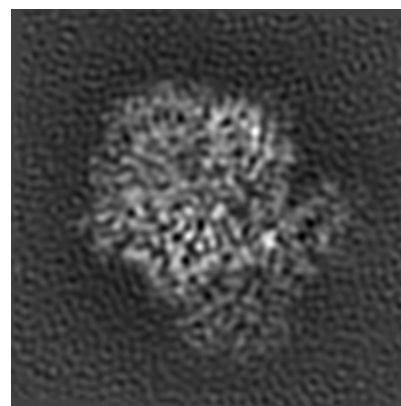
6.1.1 Primary map



X

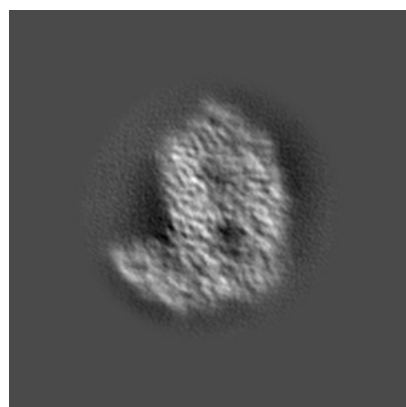


Y

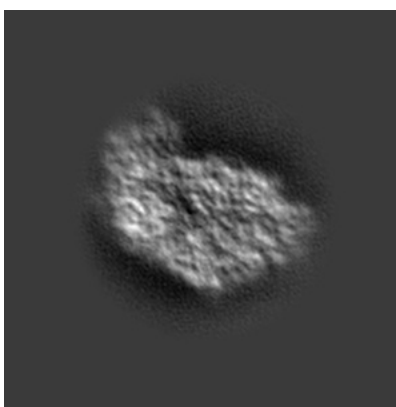


Z

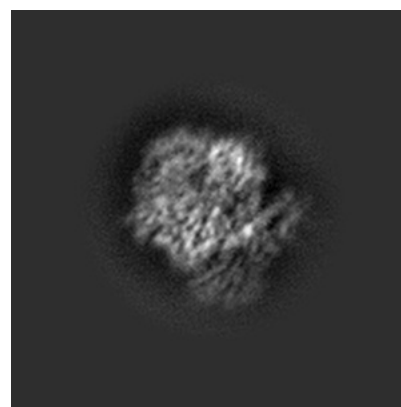
6.1.2 Raw map



X



Y

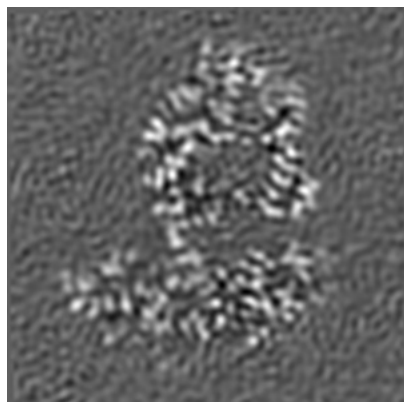


Z

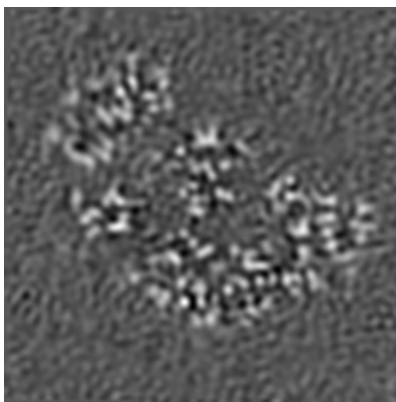
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

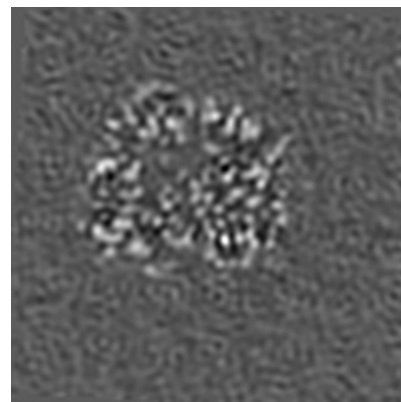
6.2.1 Primary map



X Index: 58

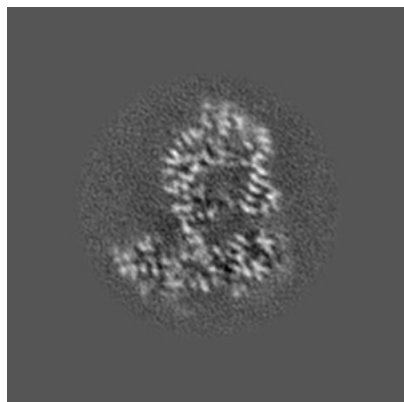


Y Index: 58

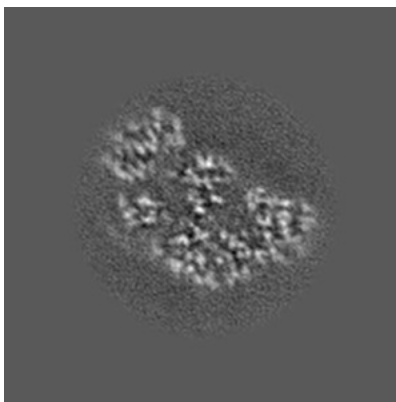


Z Index: 58

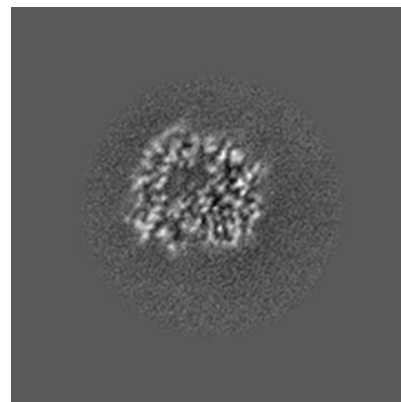
6.2.2 Raw map



X Index: 90



Y Index: 90

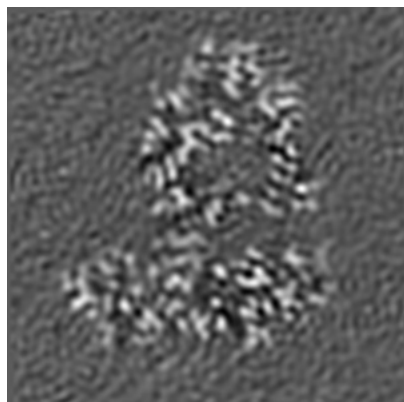


Z Index: 90

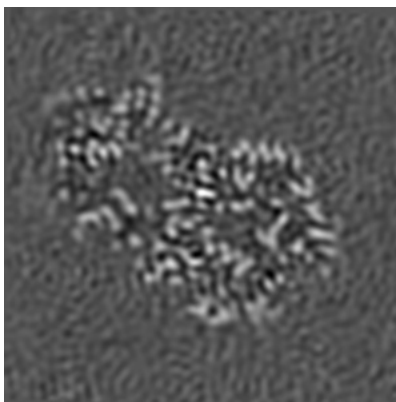
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

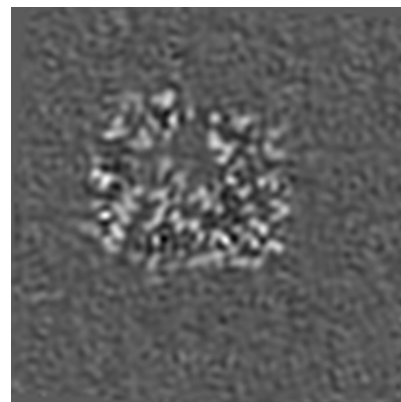
6.3.1 Primary map



X Index: 57

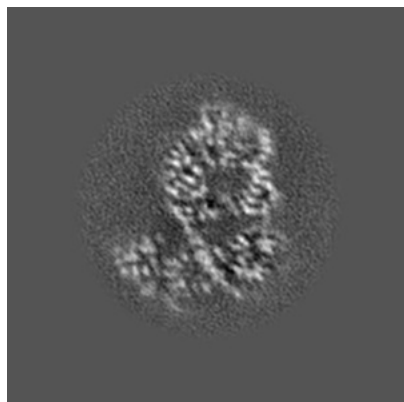


Y Index: 48

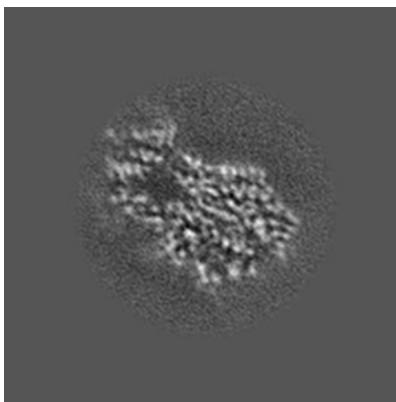


Z Index: 56

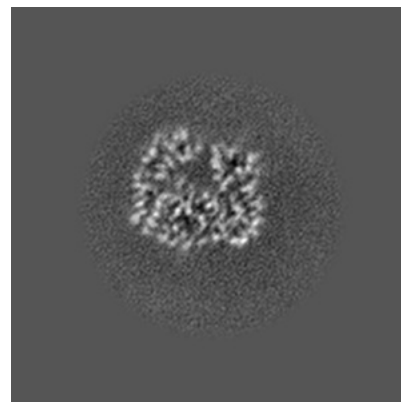
6.3.2 Raw map



X Index: 91



Y Index: 82

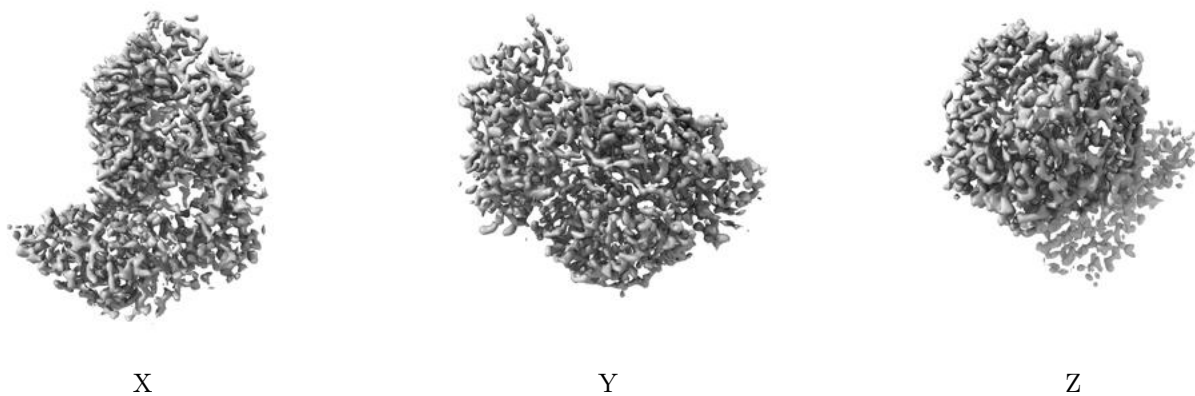


Z Index: 87

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

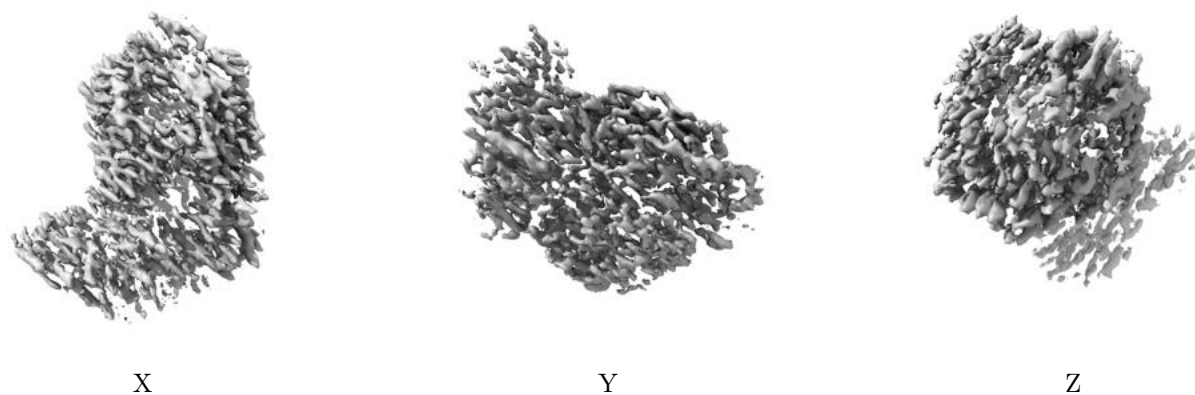
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.0. 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



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.

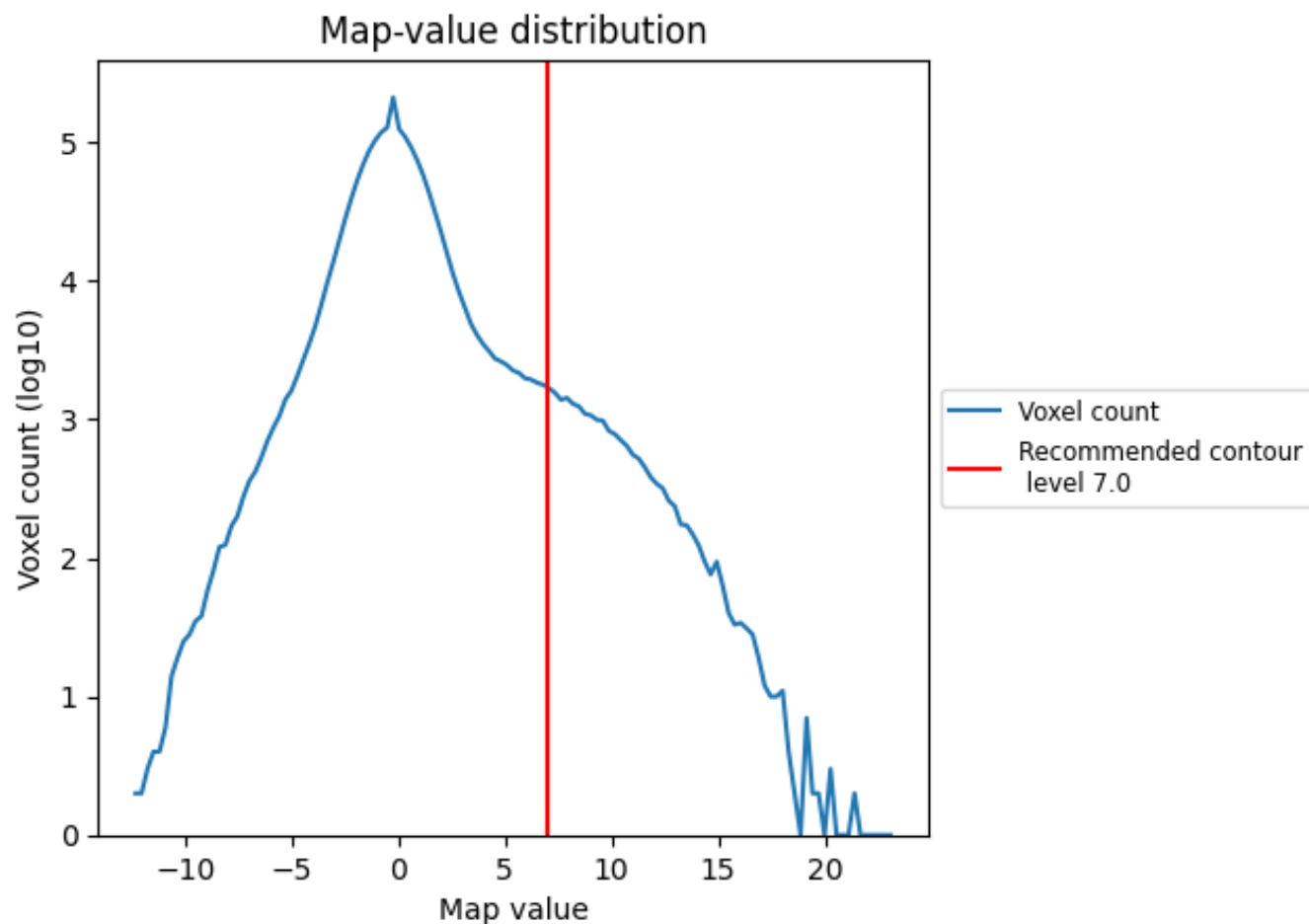
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

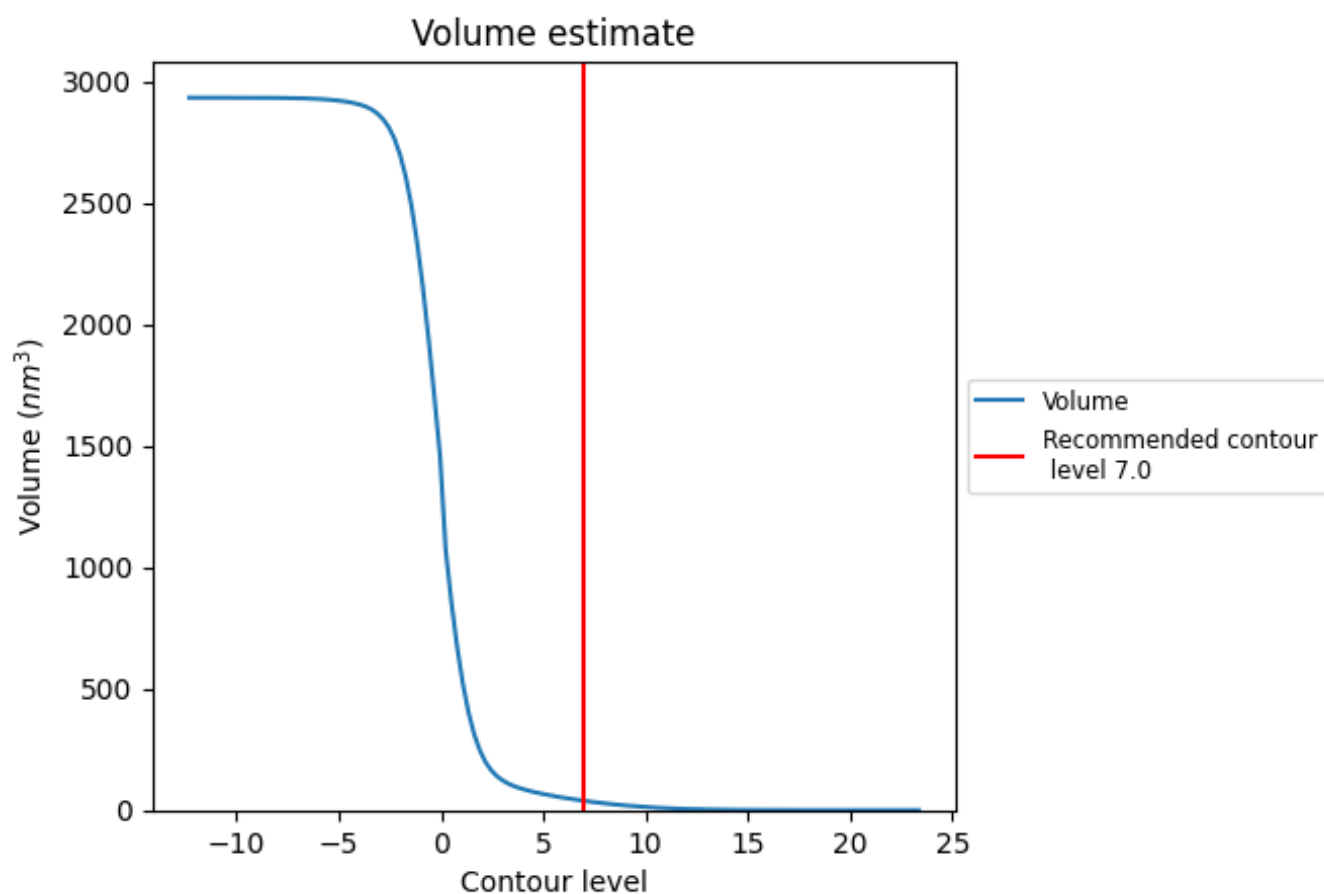
This section contains the results of statistical analysis of the map.

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.

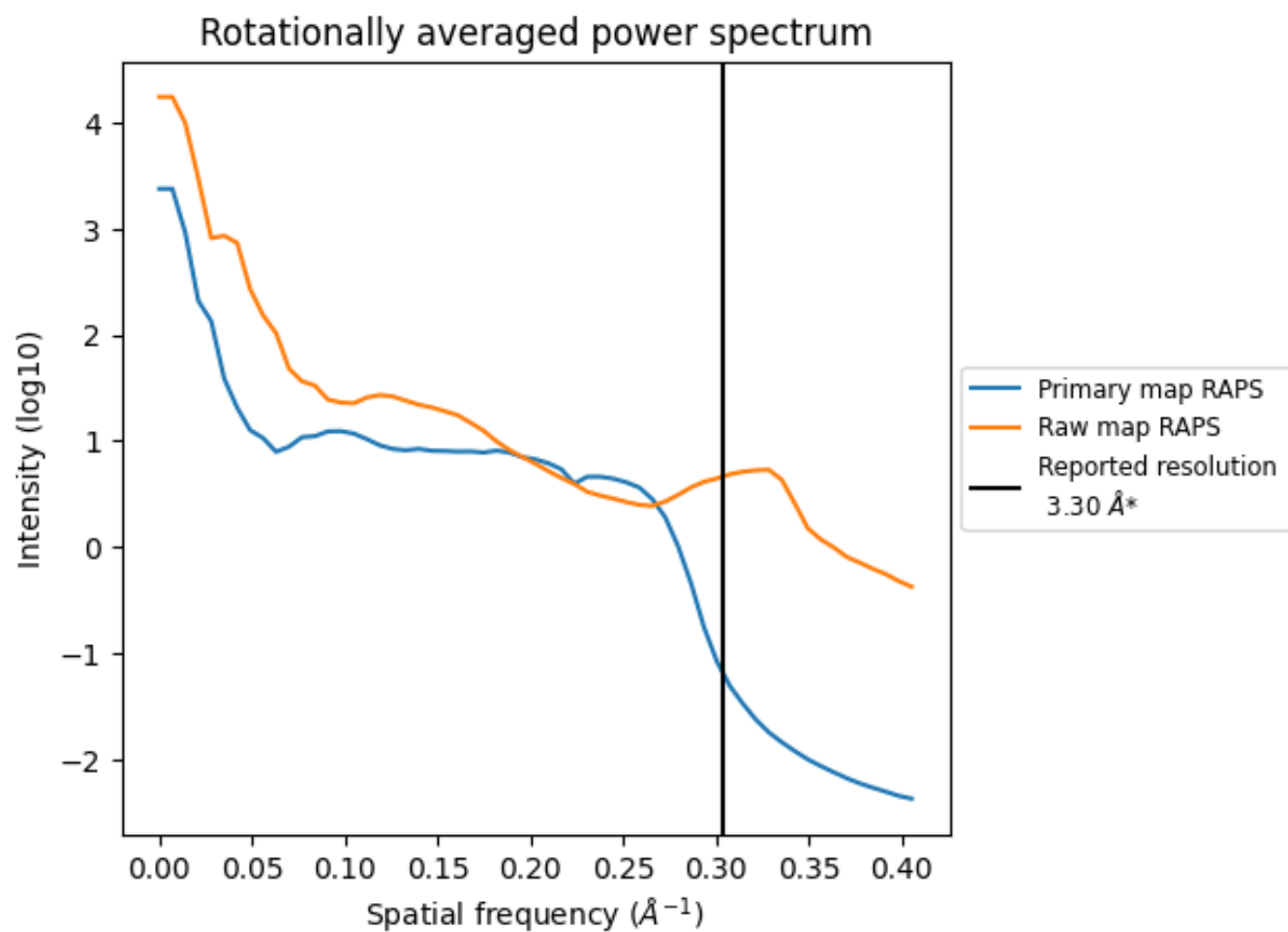
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 38 nm³; this corresponds to an approximate mass of 35 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 ⓘ

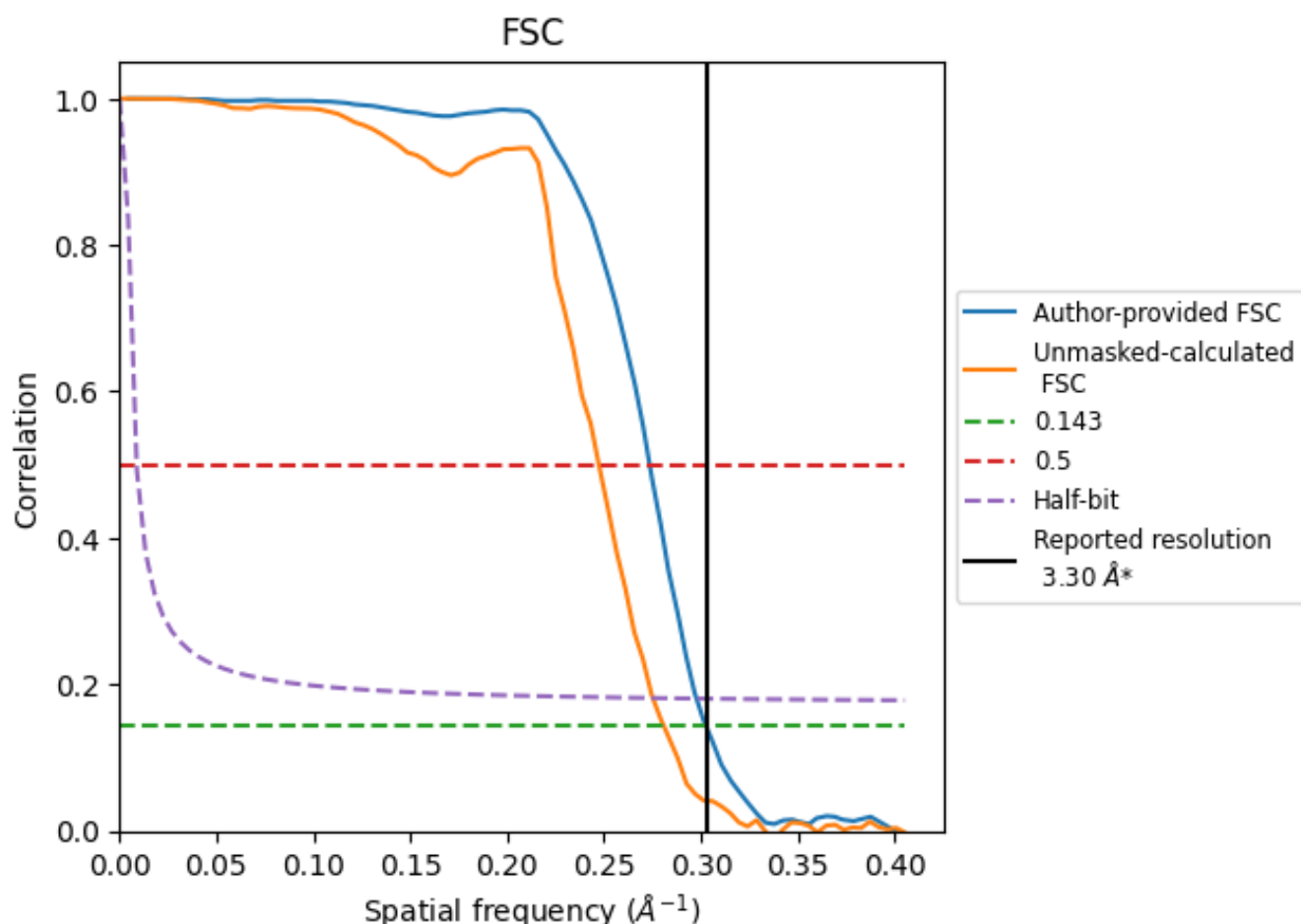


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

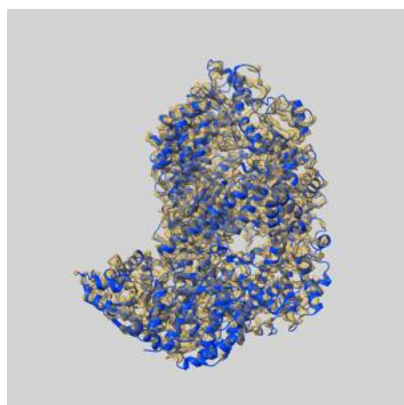
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.65	3.36
Unmasked-calculated*	3.56	4.04	3.63

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

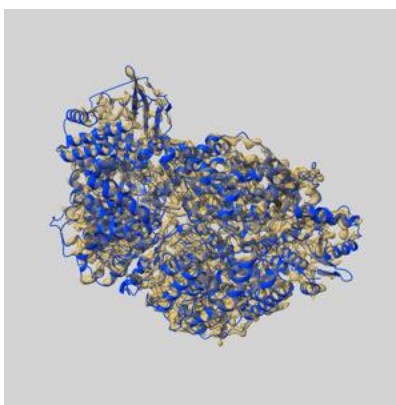
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20753 and PDB model 6UEB. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

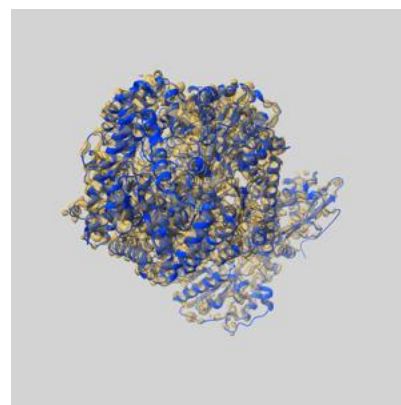
9.1 Map-model overlay [i](#)



X



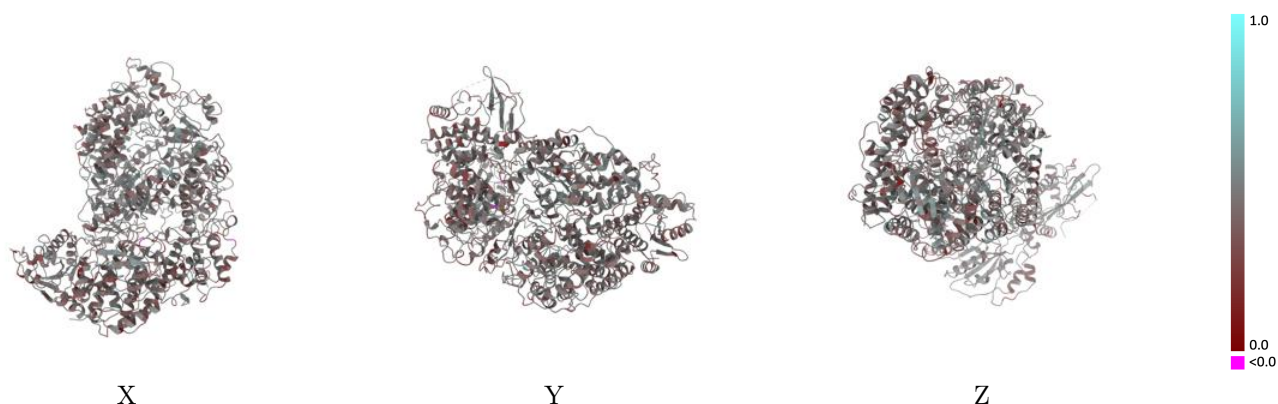
Y



Z

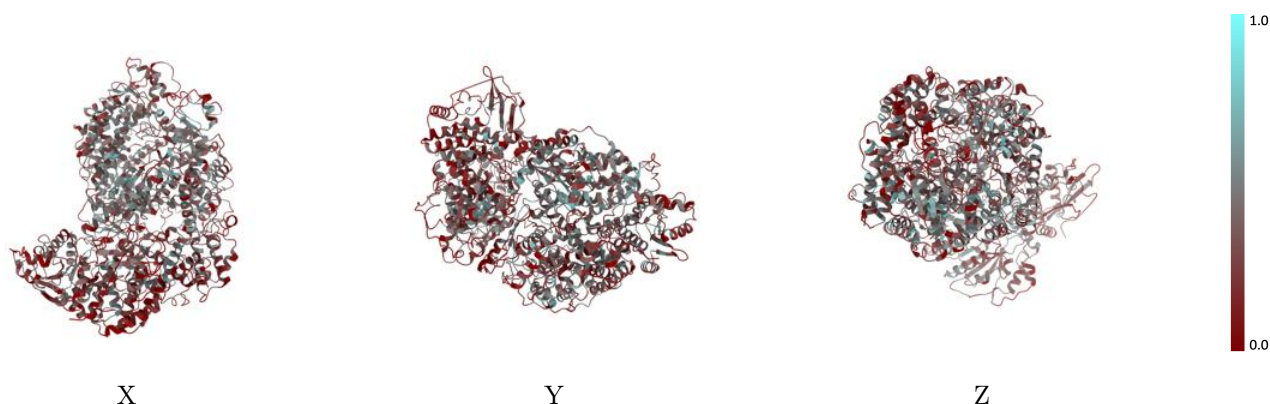
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



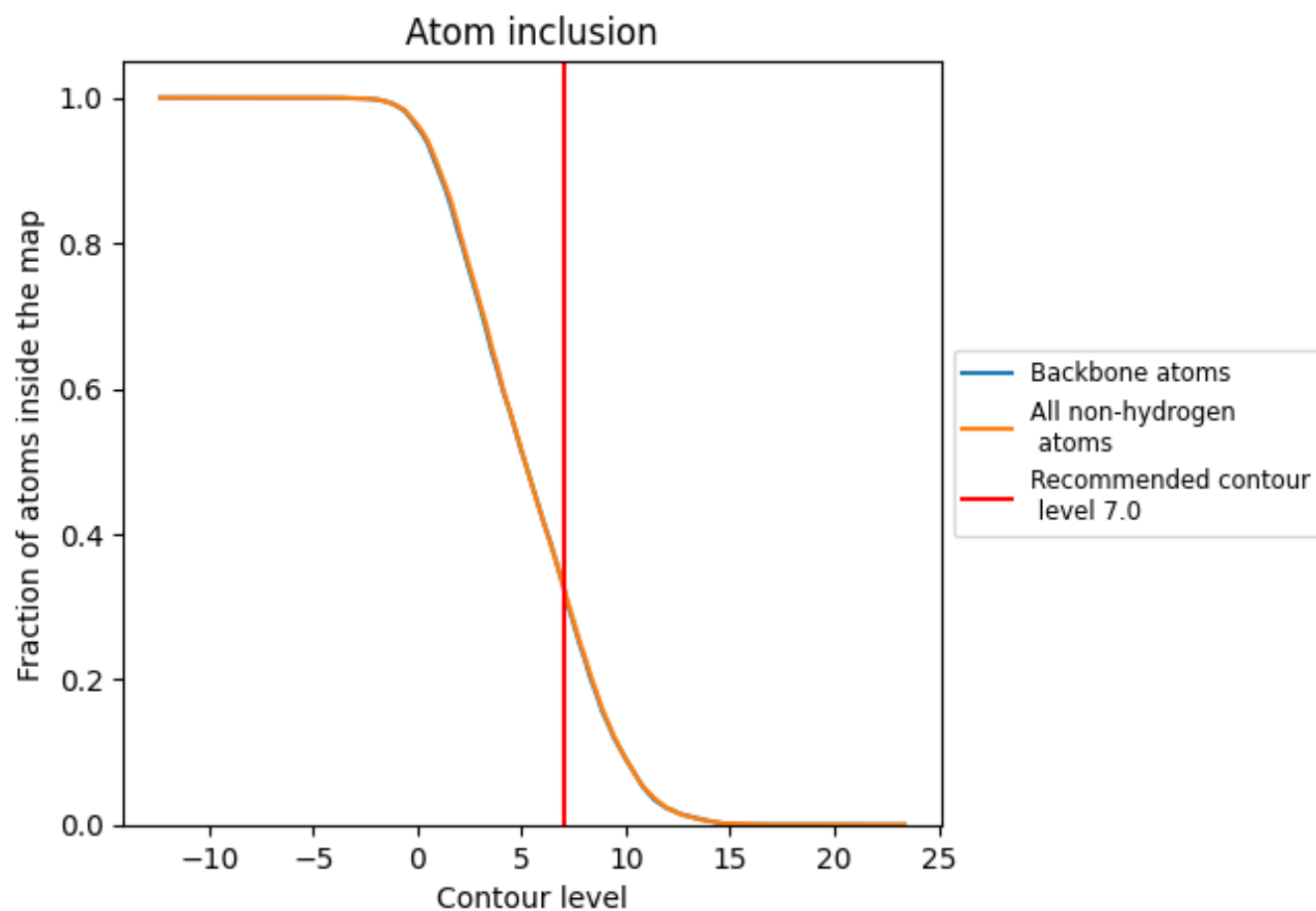
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (7.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 33% of all backbone atoms, 33% 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 (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3300	<div></div> 0.4350
A	<div></div> 0.3390	<div></div> 0.4360
B	<div></div> 0.0897	<div></div> 0.3840

