



## wwPDB EM Validation Summary Report ⓘ

Mar 10, 2024 – 04:18 PM EDT

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](mailto: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>.

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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

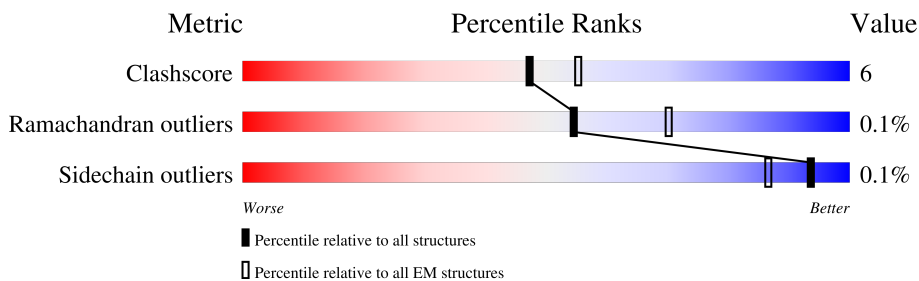
# 1 Overall quality at a glance

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  $\geq 3$ , 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	<p>62% (Upper red bar), 83% (Green), 16% (Yellow), 1% (Grey)</p>
2	B	42	<p>95% (Upper red bar), 86% (Green), 14% (Yellow)</p>

## 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	
			Total	C	H	N	O			S
1	A	2099	33865	10792	16965	2931	3097	80	0	0

- Molecule 2 is a protein called Phosphoprotein,Phosphoprotein.

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

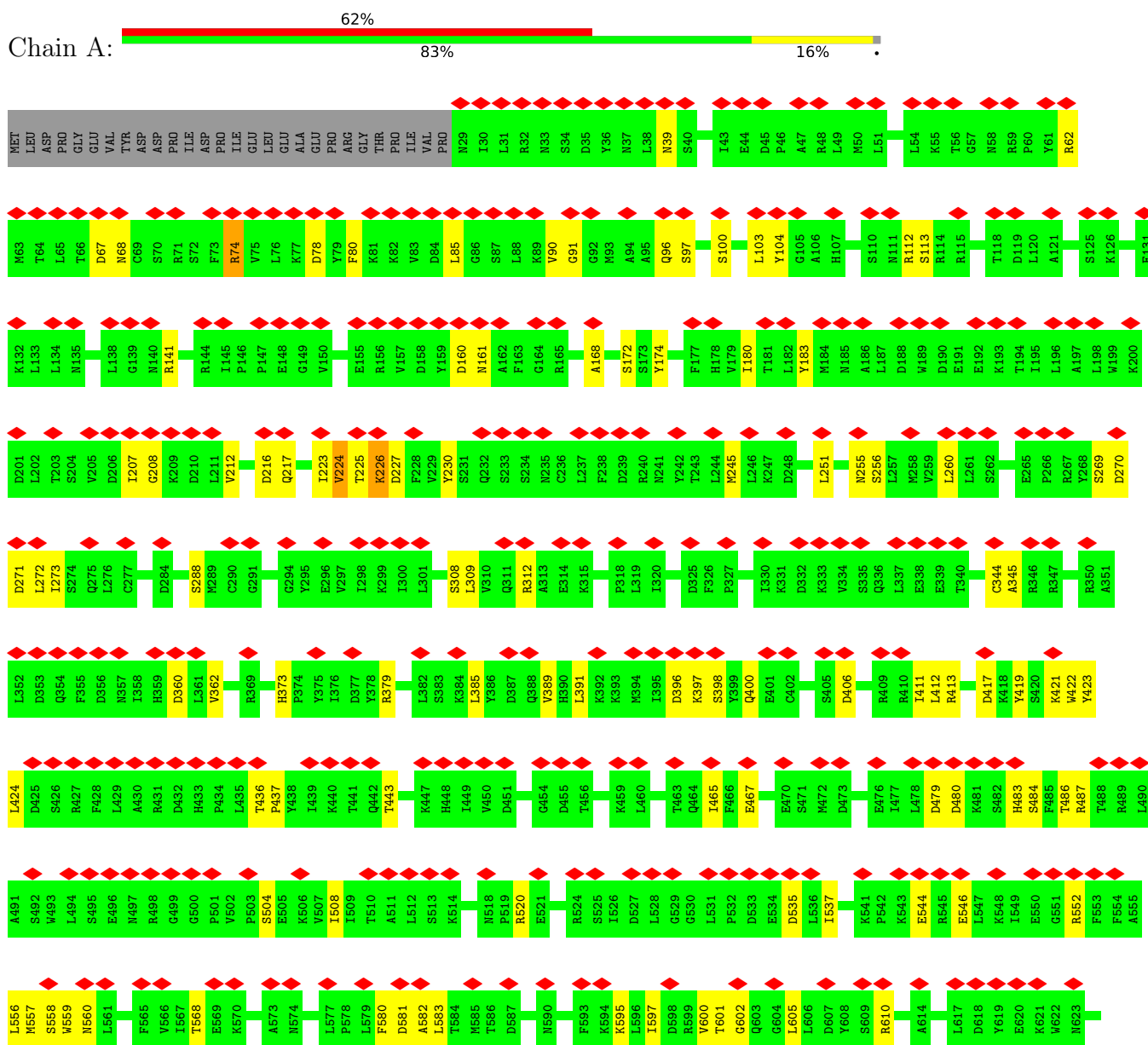
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

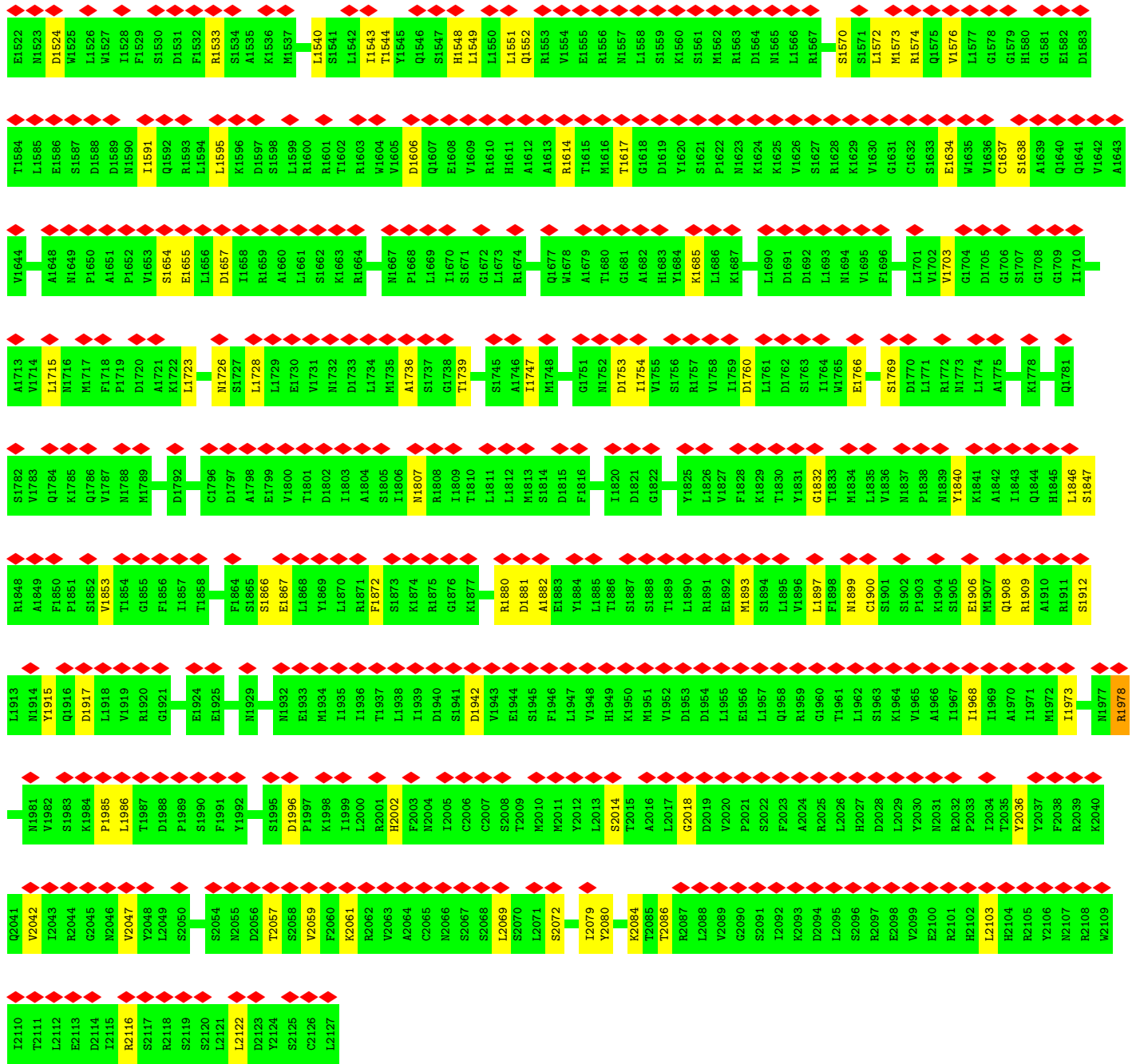
### 3 Residue-property plots

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.

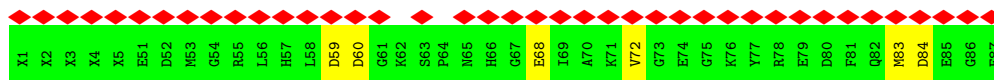
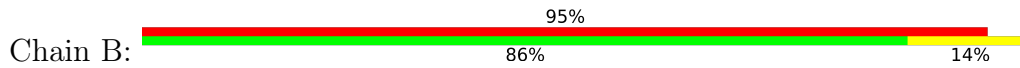
- Molecule 1: Large structural protein



R627	L628	E629	S630	E632	D633	V634	F635	D639	Q640	L644	K645	R646	F648	S649	R650	E653	F654	F655	W659	S663	D664	R665	S666	D667	L668	I669	G670	L671	R672	E673	D674	Q675	I676	Y677	C678	L679	D680	A681	S682	M683	G684	W688	M689	G690	Q691	D692	G693	G694	L695	E696	G697						
L698	R699	Q700	K701	T631	M703	S704	L705	L709	M710	I711	D712	R713	E714	S715	Q716	I717	R718	T720	R721	T722	K723	I724	L725	A726	Q727	G728	D729	N730	L733	C734	I669	T735	T736	Y737	M738	L739	S740	P741	G742	L743	S744	Q745	E746	G747	L748	L749	E751	L752	E753	R754	T755	S756	R757	N758	L760		
R764	E767	E768	G769	A770	G774	L775	I776	I777	K778	K779	E780	E781	T782	M783	S866	F787	F788	K793	L796	R798	L802	E805	S806	K807	R808	W809	A810	R811	V812	S813	C814	V815	S816	M817	D818	Q819	I820	V821	N822	L823	A824	M825	S828	T829	N833	T836	Q839										
H840	S841	Q842	S843	L844	I845	K846	P847	M848	R849	D850	M854	Q857	Y862	L863	L864	F865	P867	K870	G871	K875	I876	L877	S878	E880	G881	E882	S883	F884	A887	M888	I891	D895	L898	G899	Q900	I901	S902	G903	M904	S905	L906	G907	R908	F909	H910	I911	R912	Q913									
F914	S915	D916	P917	E920	G921	R926	E927	I928	W929	L930	S931	Q932	Q933	E934	S935	W936	I937	H938	Q942	E943	N946	P947	L949	G950	E951	R952	T953	L954	S955	S956	F957	T958	R959	L960	L961	E962	D963	P964	T965	T966	L967	N968	R970	G971	G972	A973	S974	P975	T976	I977	L978	L979	K980				
D981	A982	I983	R984	K985	A986	L987	Y988	D989	E990	V991	D992	K993	V994	E995	M996	S997	E998	F999	R1000	E1001	A1002	I1003	L1005	S1006	K1007	T1008	H1009	G950	E951	R952	T953	L954	S955	S956	F957	T958	R959	L960	L961	E962	D963	P964	T965	T966	L967	N968	R970	G971	G972	A973	S974	P975	T976	I977	L978	L979	K980
G1045	L1046	I1047	Q1048	M1049	S1050	R1051	T1052	R1053	R1054	R1055	Q1056	F1057	R1058	K1059	S1060	S1062	K1063	T1064	L1065	E1067	S1068	Y1070	M1071	G950	E951	R952	T953	L954	S955	S956	F957	T958	R959	L960	L961	E962	D963	P964	T965	T966	L967	N968	R970	G971	G972	A973	S974	P975	T976	I977	L978	L979	K980				
H1117	L1124	L1125	P1126	K1127	I1130	S1131	C1132	T1133	C1134	G1135	I1136	T1137	G1138	G1139	M1141	P1142	R1143	V1146	S1147	P1150	D1153	Q1154	S1155	F1156	F1157	S1158	R1159	L1162	K1163	G1164	Y1165	G1167	S1168	S1169	T1170	S1171	M1172	S1173	T1174	Q1175	L1176	F1177	H1178	A1179	W1180	E1181	K1182	V1183	T1184	N1185							
V1186	H1187	V1188	V1189	K1190	R1191	A1192	L1193	S1194	L1195	K1196	E1197	S1198	I1199	M1200	W1201	F1202	R1205	D1206	S1207	M208	L1209	A1210	Q1211	A1212	L1213	I1214	R1215	M1216	I1217	F1218	S1219	G1222	P1223	D1224	F1225	P1226	L1227	E1228	E1229	A1230	P1231	V1232	F1233	K1234	R1235	T1236	G1237	S1238	A1239	L1240	H1241	R1242	F1243	M1244	S1245	A1246	R1247
Y1248	S1249	E1250	G1251	Y1253	C1257	P1258	L1261	S1262	H1263	I1264	S1265	D1269	M1271	S1272	D1273	L1274	T1275	Q1276	D1277	K1278	G1279	N1280	Y1281	D1282	F1283	M1284	F1285	L1288	M1289	L1290	Y1291	A1292	T1296	S1297	E1298	Q1301	R1302	D1303	T1304	R1305	L1306	R1307	D1308	S1309	L1310	F1311	H1312	R1316	C1317	M1318							
R1319	C1320	V1321	R1322	P1323	I1324	L1325	D1326	V1327	E1330	T1331	S1332	Q1333	I1334	F1335	E1336	F1337	P1338	D1339	V1340	S1341	K1342	R1343	I1344	S1345	R1346	S1349	G1350	P1353	H1354	F1355	Q1356	R1357	L1358	P1359	D1360	I1361	R1362	L1363	R1364	P1365	G1366	D1367	F1368	E1369	S1370	L1371	S1372	G1373	L1374	E1375	K1376	G1381	S1382	L1386			
H1395	D1396	S1397	G1398	Y1399	M1400	D1401	G1402	T1403	L1404	F1405	P1406	V1407	M1408	I1409	Y1410	G1411	K1412	V1413	S1414	P1415	R1416	D1417	Y1418	L1419	R1424	V1426	I1428	G1429	S1430	M1431	I1432	F1433	F1434	L1435	T1436	R1437	M1438	T1439	M1440	I1441	M1442	I1443	R1444	M1445	F1446	L1447	E1448	L1449	V1450	S1451	G1452	V1453	I1457	L1458			
L1459	R1460	L1461	D1462	M1463	H1464	L1467	Y1468	I1469	M1470	L1471	R1472	E1473	P1474	S1475	L1476	R1477	G1478	E1479	I1480	F1481	S1482	I1483	P1484	Q1485	K1486	A1489	A1490	Y1491	P1492	T1493	T1494	M1495	S1496	I1497	F1498	L1499	R1500	S1501	I1502	L1503	C1504	Y1505	L1506	Q1507	H1508	R1511	Y1512	E1513	R1514	E1515	I1516	I1517	T1518	A1519	S1520	P1521	



● 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 ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	1.234, 1.234, 1.234	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

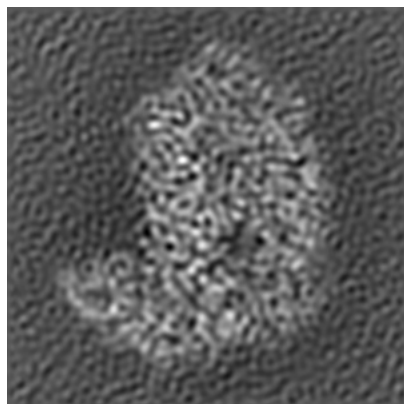
## 6 Map visualisation [i](#)

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.

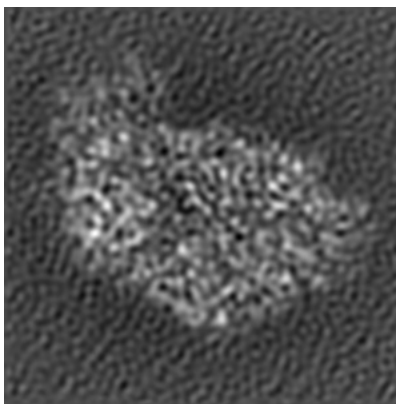
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

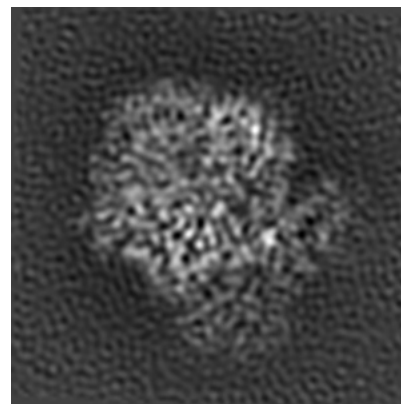
#### 6.1.1 Primary map



X



Y

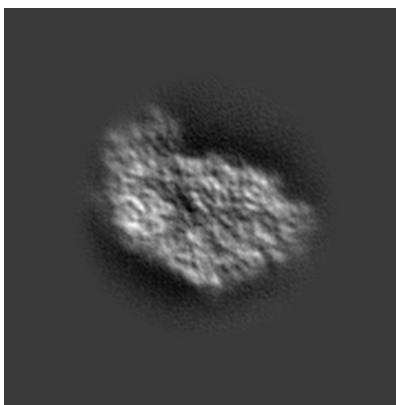


Z

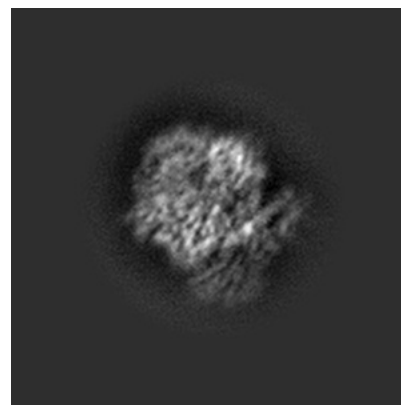
#### 6.1.2 Raw map



X



Y

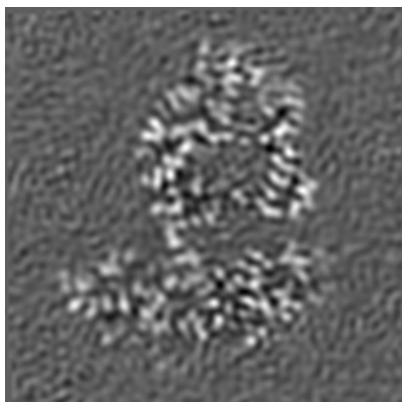


Z

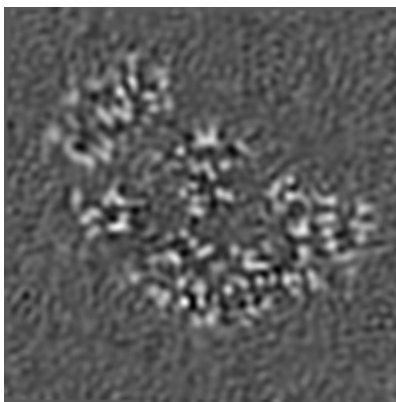
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

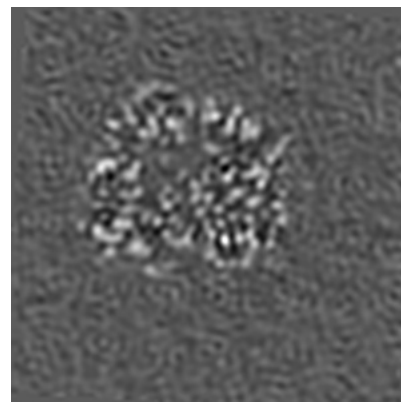
### 6.2.1 Primary map



X Index: 58

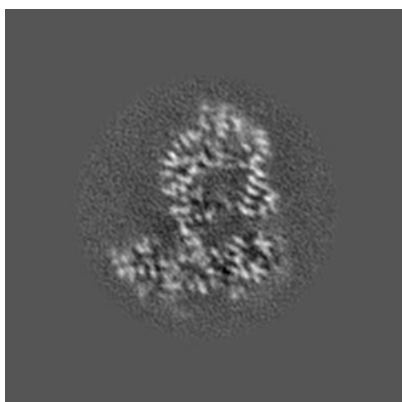


Y Index: 58

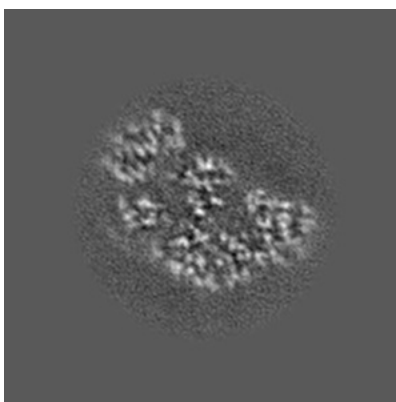


Z Index: 58

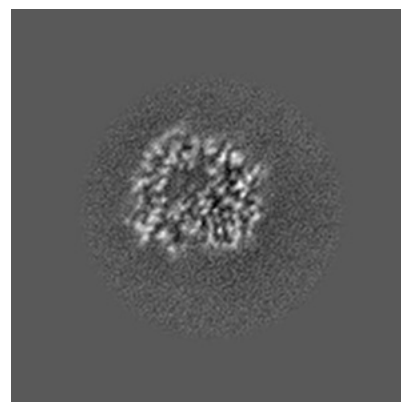
### 6.2.2 Raw map



X Index: 90



Y Index: 90

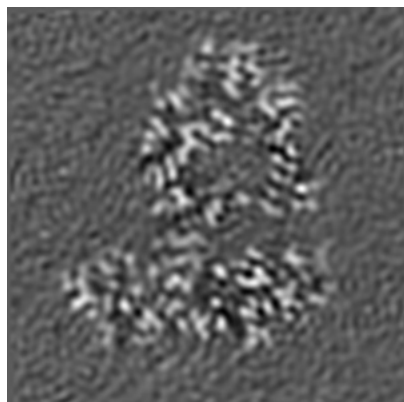


Z Index: 90

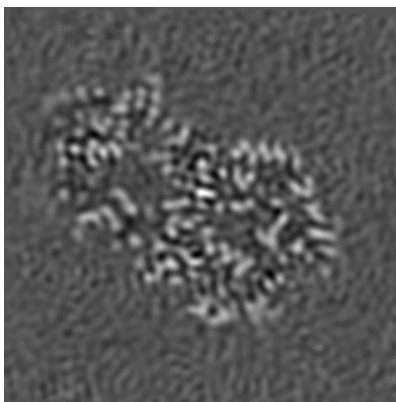
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

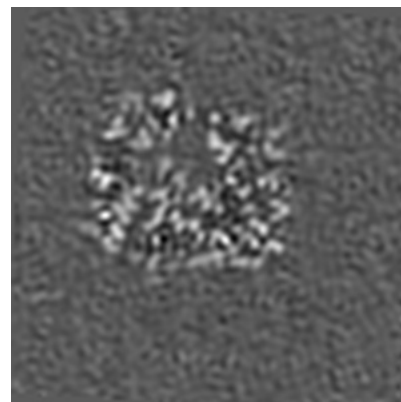
### 6.3.1 Primary map



X Index: 57

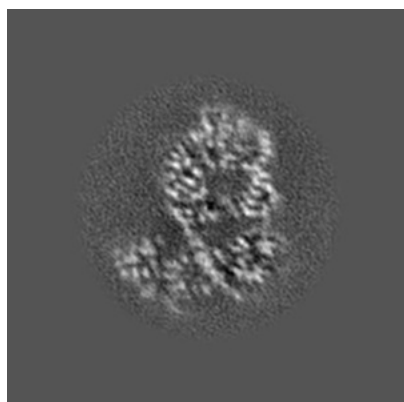


Y Index: 48

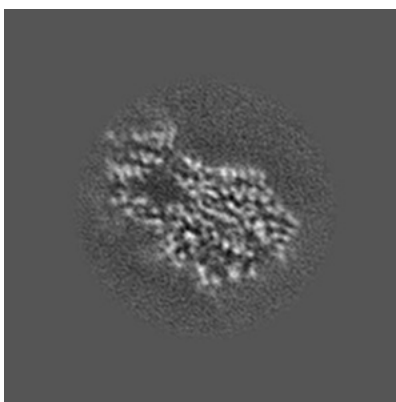


Z Index: 56

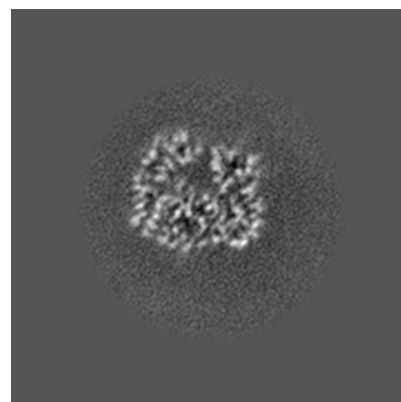
### 6.3.2 Raw map



X Index: 91



Y Index: 82

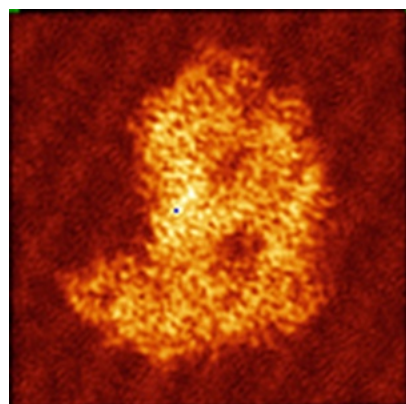


Z Index: 87

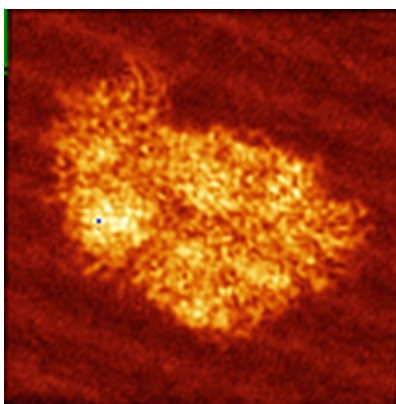
The images above show the largest variance slices of the map in three orthogonal directions.

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

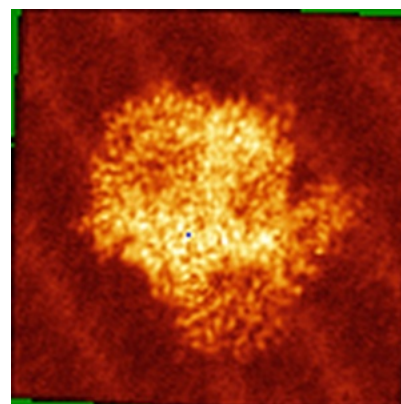
### 6.4.1 Primary map



X

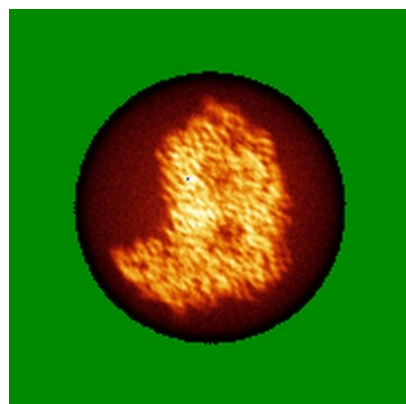


Y

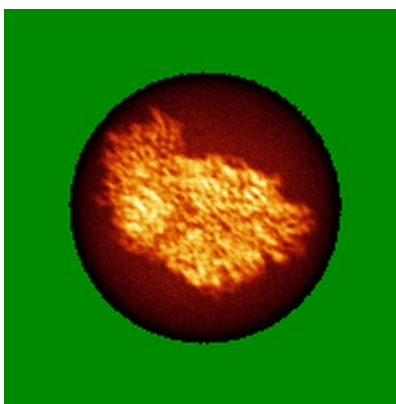


Z

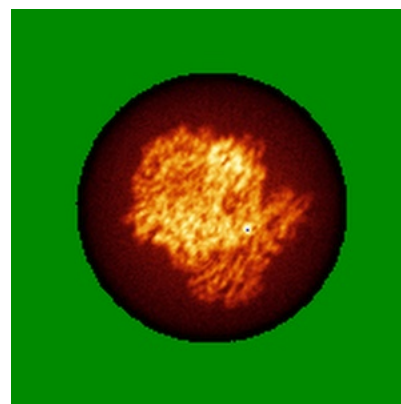
### 6.4.2 Raw map



X



Y



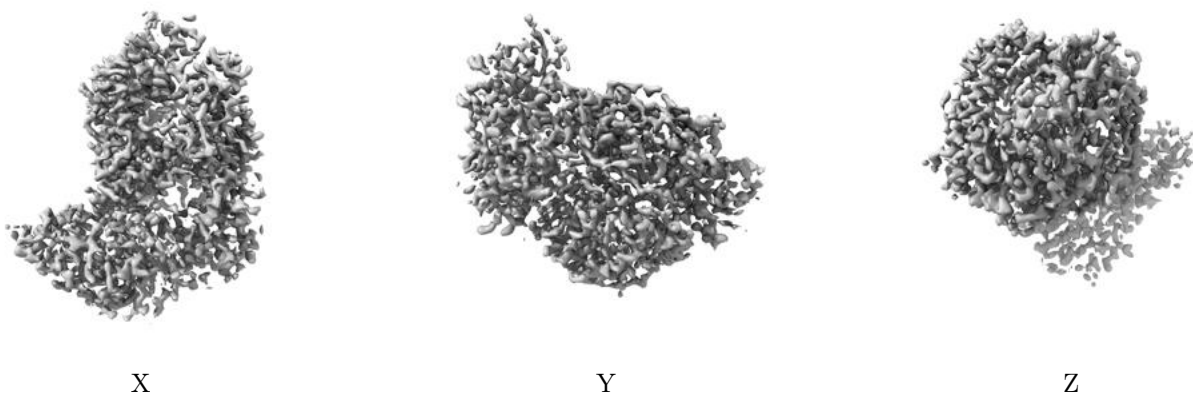
Z

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.



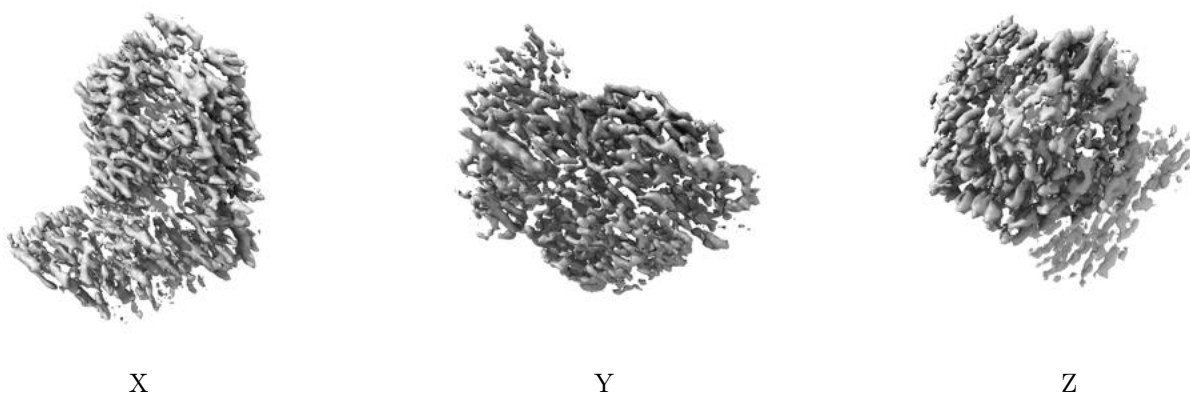
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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.

### 6.5.2 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.

## 6.6 Mask visualisation [i](#)

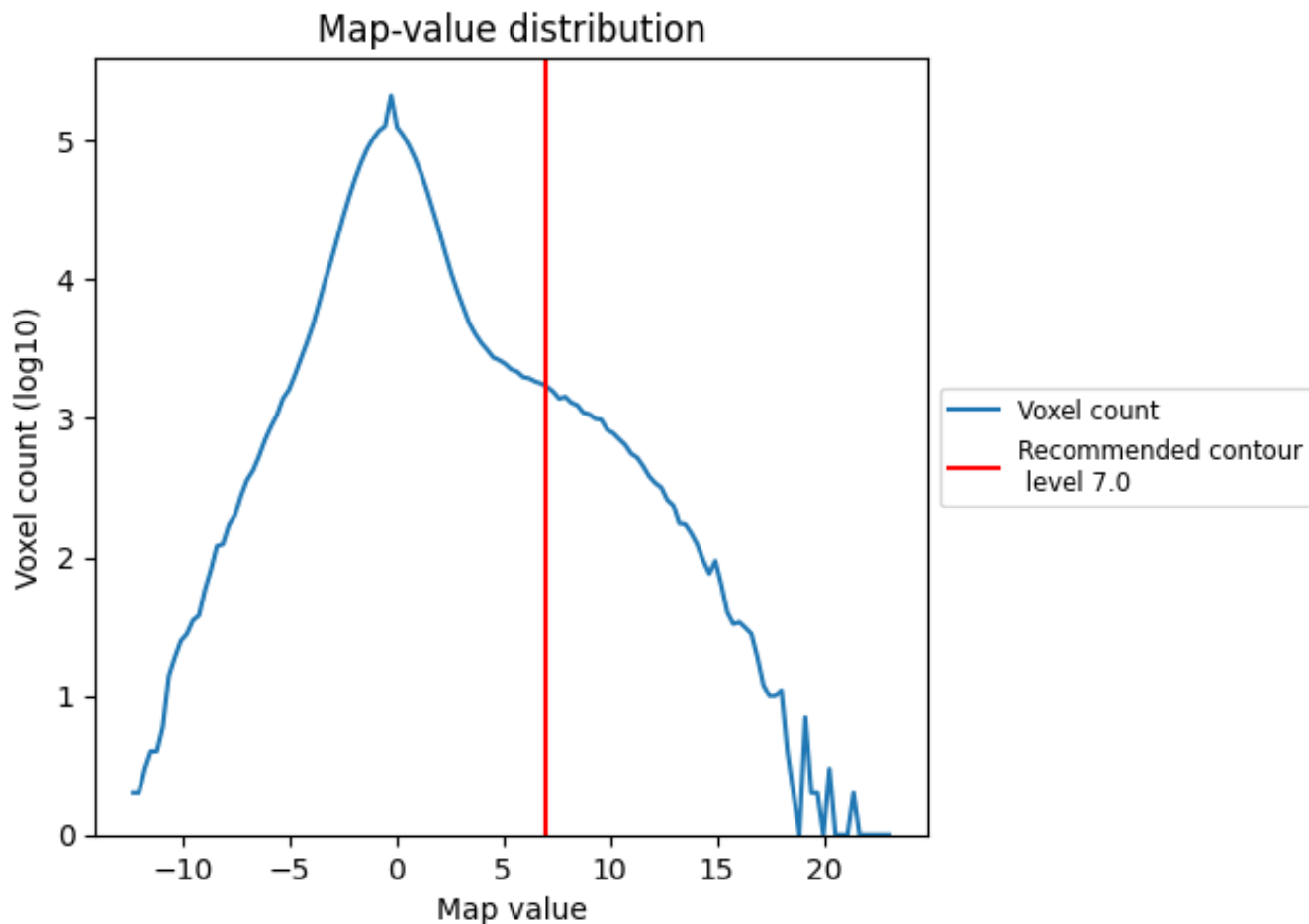
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

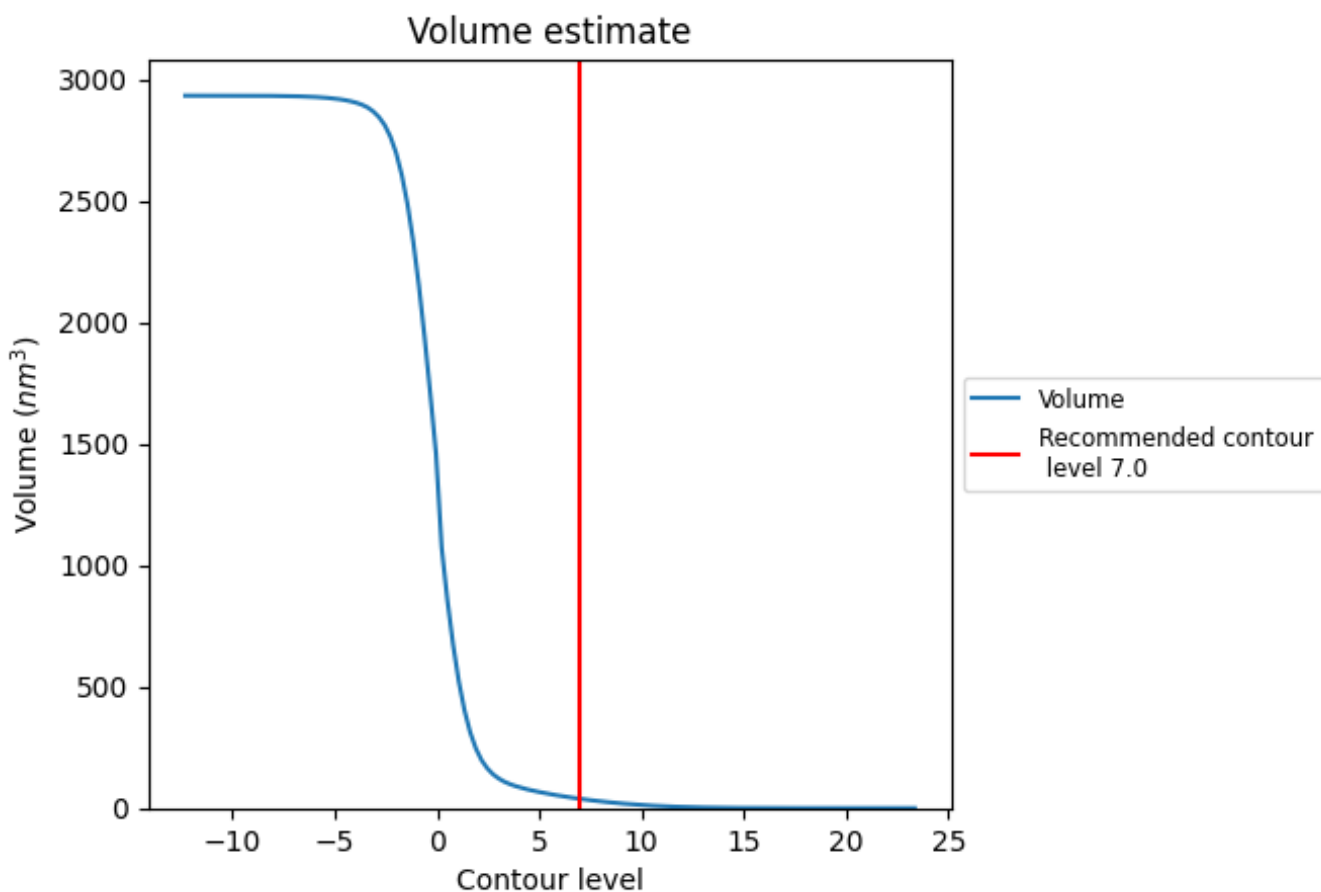
This section contains the results of statistical analysis of the map.

### 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.

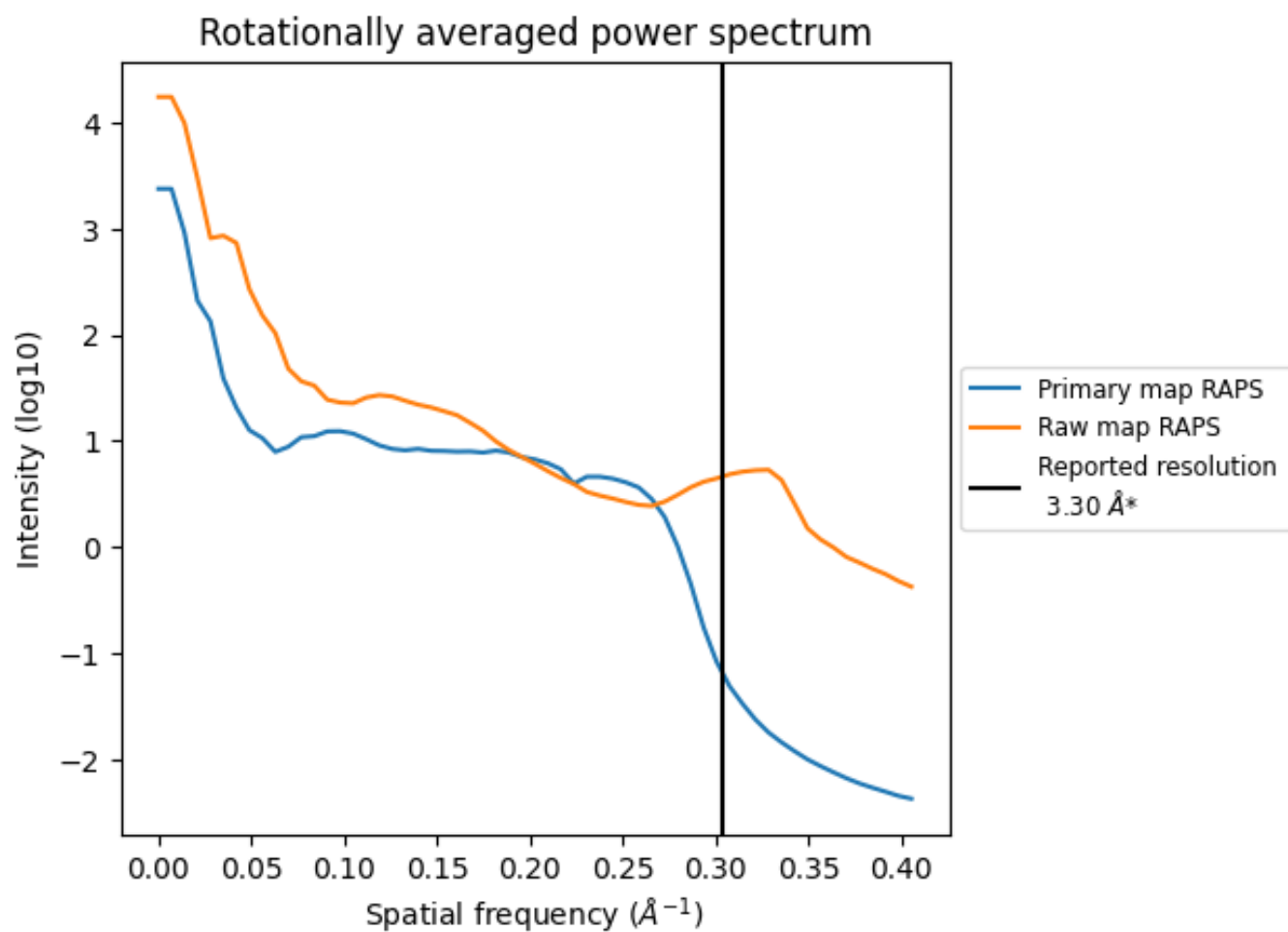
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 38 nm<sup>3</sup>; 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 i

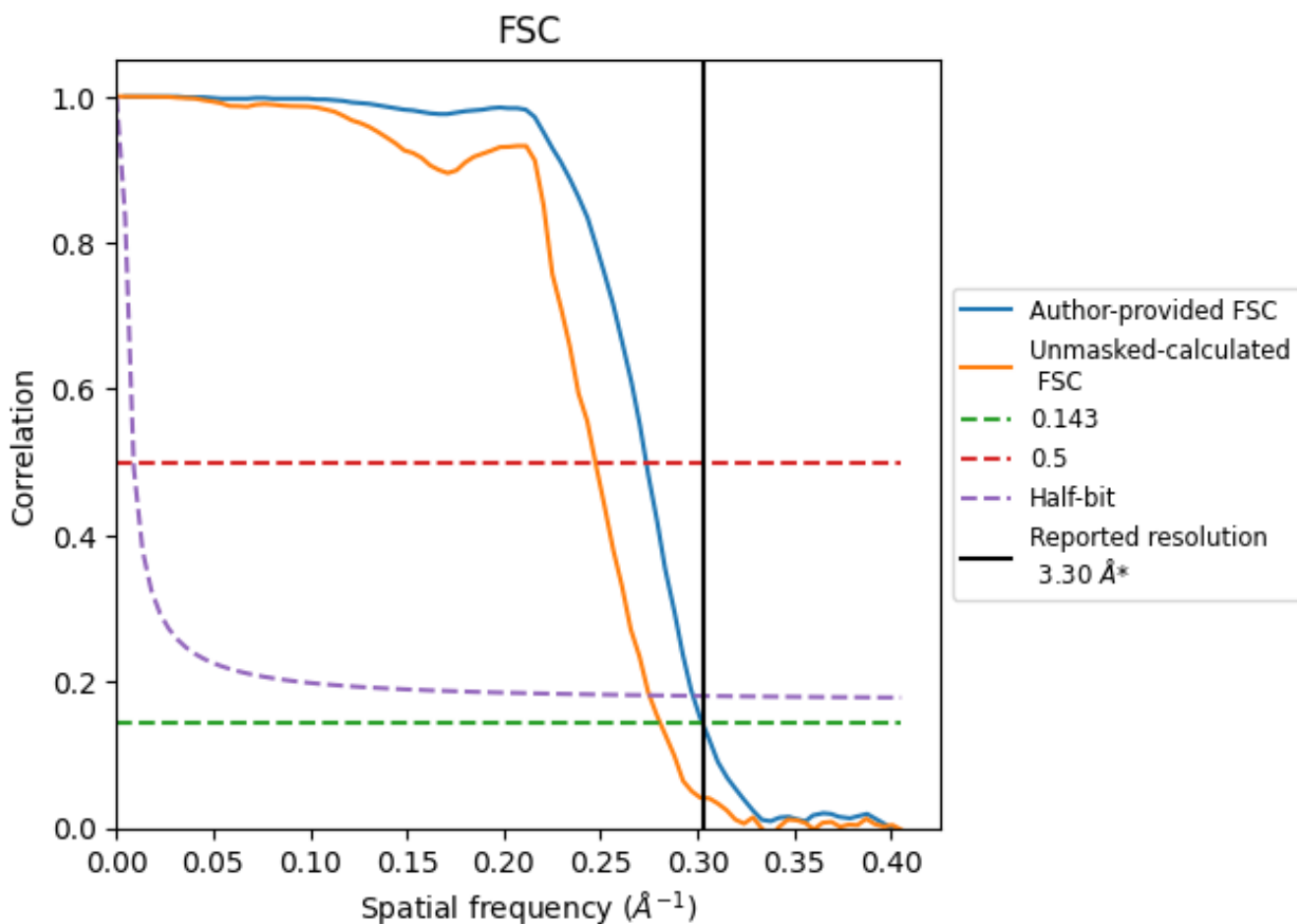


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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  $0.303 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

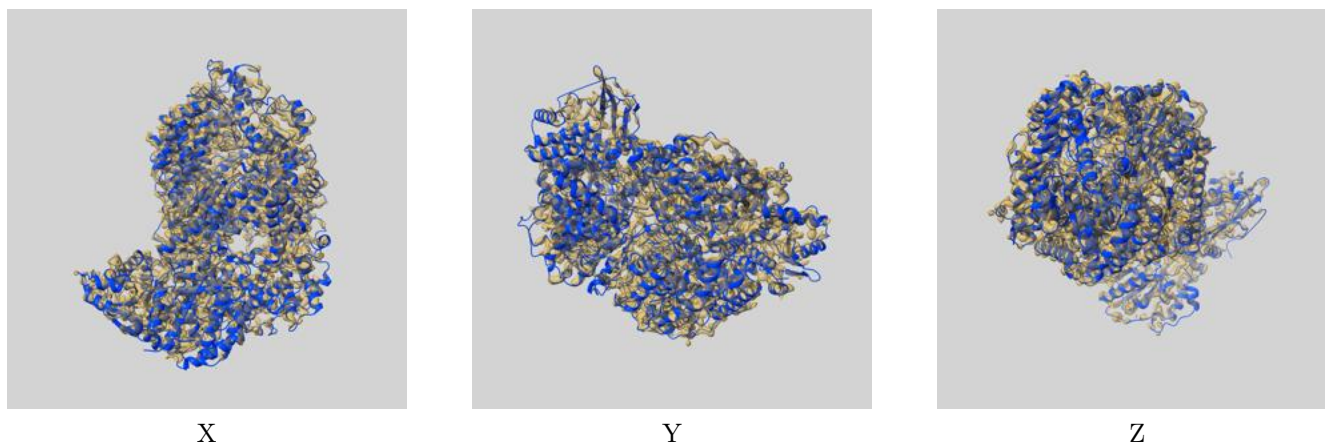
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.65	3.36
Unmasked-calculated*	3.56	4.04	3.63

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

## 9 Map-model fit [i](#)

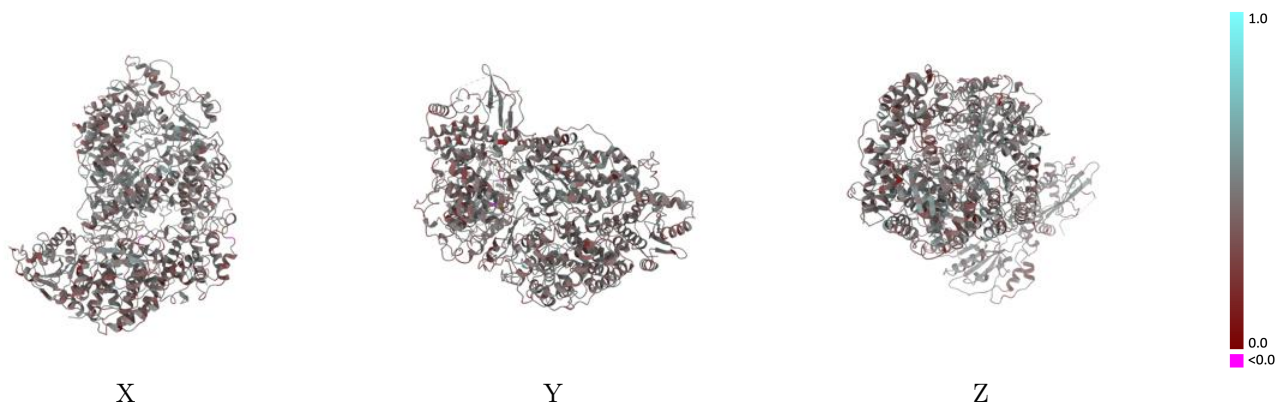
This section contains information regarding the fit between EMDB map EMD-20753 and PDB model 6UEB. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlay [i](#)



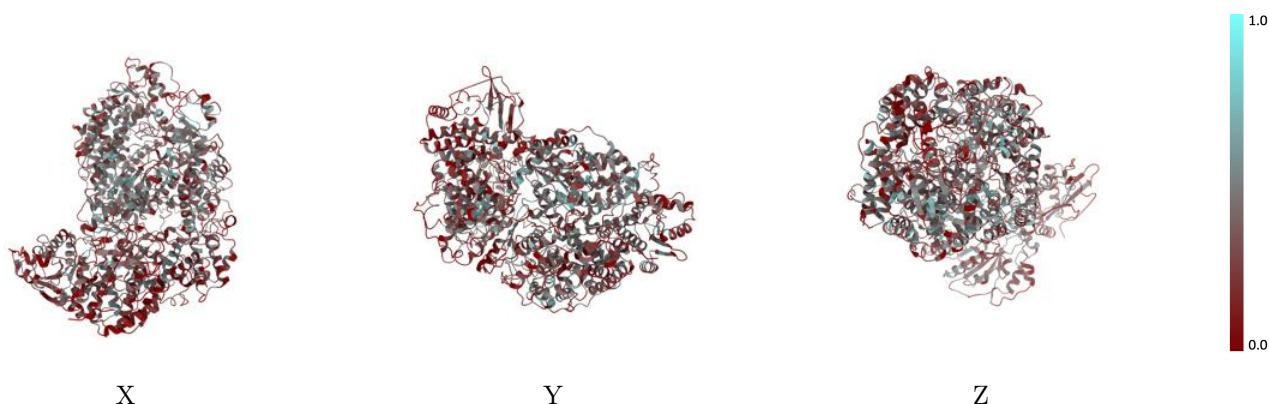
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



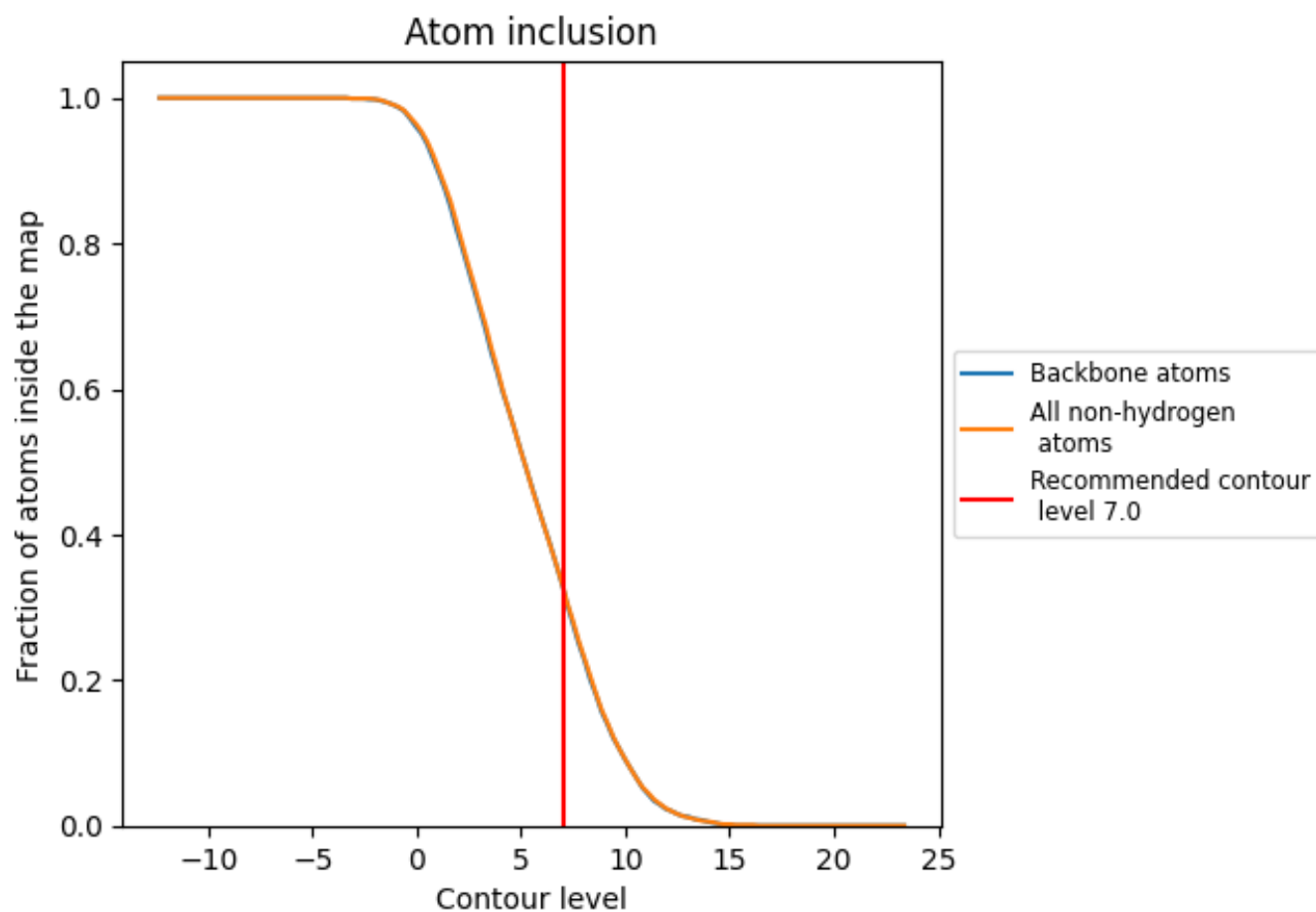
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	 0.3300	 0.4350
A	 0.3390	 0.4360
B	 0.0900	 0.3840

