



wwPDB EM Validation Summary Report ⓘ

May 14, 2025 – 01:24 AM EDT

PDB ID : 7MPE / pdb_00007mpe
EMDB ID : EMD-23932
Title : Cryo-EM structure of the yeast cadmium factor 1 protein (Ycf1p)
Authors : Bickers, S.C.; Benlekbir, S.; Rubinstein, J.L.; Kanelis, V.
Deposited on : 2021-05-04
Resolution : 3.20 Å(reported)

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

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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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

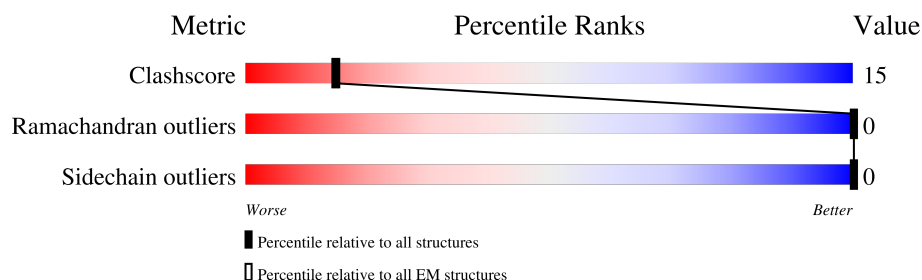
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 3.20 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	A	1537	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11214 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 Metal resistance protein YCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1428	Total	C	N	O	S	0	0
			11214	7251	1873	2039	51		

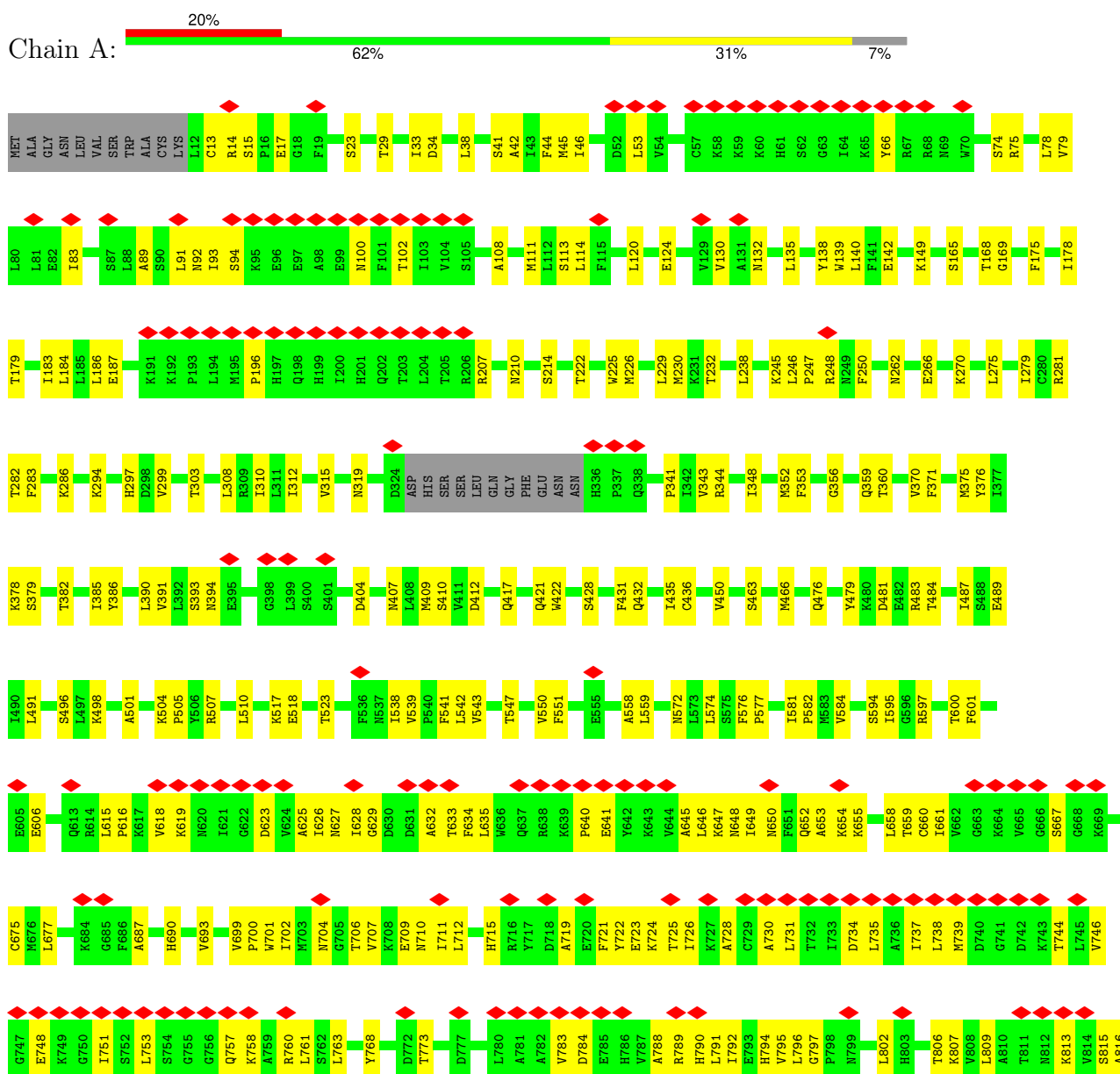
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1516	ASP	-	expression tag	UNP P39109
A	1517	TYR	-	expression tag	UNP P39109
A	1518	LYS	-	expression tag	UNP P39109
A	1519	ASP	-	expression tag	UNP P39109
A	1520	HIS	-	expression tag	UNP P39109
A	1521	ASP	-	expression tag	UNP P39109
A	1522	GLY	-	expression tag	UNP P39109
A	1523	ASP	-	expression tag	UNP P39109
A	1524	TYR	-	expression tag	UNP P39109
A	1525	LYS	-	expression tag	UNP P39109
A	1526	ASP	-	expression tag	UNP P39109
A	1527	HIS	-	expression tag	UNP P39109
A	1528	ASP	-	expression tag	UNP P39109
A	1529	ILE	-	expression tag	UNP P39109
A	1530	ASP	-	expression tag	UNP P39109
A	1531	TYR	-	expression tag	UNP P39109
A	1532	LYS	-	expression tag	UNP P39109
A	1533	ASP	-	expression tag	UNP P39109
A	1534	ASP	-	expression tag	UNP P39109
A	1535	ASP	-	expression tag	UNP P39109
A	1536	ASP	-	expression tag	UNP P39109
A	1537	LYS	-	expression tag	UNP P39109

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: Metal resistance protein YCF1



E1487	C1419	I1351	T1279	G1184	F1068	L940	E1487
F1488	L1420	I1352	R1280	L1189	V1084	E941	S918
D1489	A1421	Q1354	E1284	R1198	T1088	Y942	I819
S1490	R1422	D1355	L1285	L1199	T1089	K944	
P1491	L1425	S1356	D1286	L1204	T1097	A945	S822
G1492	V1426	Q1357	V1287	M1208	P1097	C946	I823
Q1493	P1427	V1358	L1288	V1209	P1098	N947	A824
L1494	S1428	F1359	K1289	L1213	P1099	P948	L825
L1495	K1429	E1360	H1291	Y1215	S1100	K949	L826
	I1430	G1361	I1292	S1214	Y1103	S951	D827
S1496	L1431	T1362	N1293	I1218	I1104	N828	N828
D1497	V1432	V1363	I1294	Q1218	Y1107	F954	G829
N1498	L1433	R1364	H1295	I1226	Y1110	I958	E830
K1499	D1434	I1367	I1296	V1227	Y1110	W975	I831
S1500	T1437	I1370	K1297	I1226	E1116	N979	T832
L1501	A1438	N1371	P1298	R1228	L1117	G983	Q833
F1502	A1439	Q1372	N1299	M1229	R1118	T836	Q834
Y1503	A1439	E1300	K1301	T1230	R1119	Y837	G835
S1504	V1440	Y1373			L1120	D838	
L1505	D1441	T1374			T1006	I840	
G1506	V1442	D1375	I1304	V1233	Q1009	T841	
M1507	E1442	E1376	V1305	E1234	I1019	K942	
E1508	E1443	A1377	G1306	T1235	H1020	D843	
A1509	T1444	A1377	R1307	T1236	Y1026	A844	
G1510	D1445	I1378	T1308	I1237			
G1511	K1446	W1379	G1309	R1242			
V1512	V1447	R1380	A1310	Y1246			
	V1448		G1311	E1252			
ASN	T1451	E1383	K1312				
GLU	I1452	L1384					
ASN	I1452	S1385	A1318	L1255			
ASP	R1453	H1386	L1319	I1256			
TYR	T1454		F1320	V1257			
LYS	A1455	E1389	R1321	E1258			
ASP	F1456	H1390	S1326	G1259			
HIS	K1457	V1391	E1327	H1260			
ASP	D1458	L1392	G1328	R1261			
GLY	R1459	S1393	N1329	P1262			
ASP	T1460	M1394	I1330	P1263			
TYR	T1461	S1395	V1331	K1264			
LYS		N1396		E1265			
ASP	A1465	D1397	N1334	V1266			
HIS	H1466	G1398	I1335	P1267			
ASP	R1467	L1399	A1336	S1268			
ILE	L1468	D1400	I1337	Q1269			
TYR	N1469	A1401	N1338	G1270			
ASP	T1470	Q1402	E1339	D1271			
ASP	M1472	L1403	I1340	I1272			
ASP	D1473	T1404	G1341	K1273			
LYS	S1474	E1405	L1342	F1274			
	D1475	G1406	Y1343	N1275			
		G1407	D1344	T1276			
		V1479	L1345	Y1277			
		L1480	R1346	S1278			
	D1481	N1482	K1347				
			K1348				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124864	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.508	Depositor
Minimum map value	-2.776	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.879	Depositor
Map size (Å)	263.68, 263.68, 263.68	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.20	0/11443	0.39	0/15530

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	11214	0	11296	336	0
All	All	11214	0	11296	336	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 15.

The worst 5 of 336 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:629:GLY:O	1:A:650:ASN:HA	1.47	1.11
1:A:391:VAL:HG12	1:A:606:GLU:HB2	1.60	0.84
1:A:78:LEU:HB2	1:A:183:ILE:HD12	1.65	0.79
1:A:1084:VAL:HG11	1:A:1215:TYR:HD2	1.51	0.75
1:A:1367:ILE:HG22	1:A:1425:LEU:HD22	1.68	0.75

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	1420/1537 (92%)	1322 (93%)	98 (7%)	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	1215/1353 (90%)	1215 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	834	GLN
1	A	1074	ASN
1	A	1299	ASN
1	A	1148	GLN
1	A	319	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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.

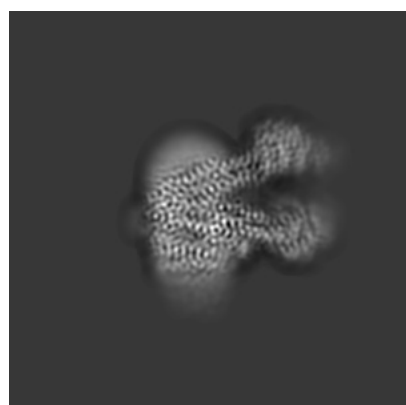
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23932. These allow visual inspection of the internal detail of the map and identification of artifacts.

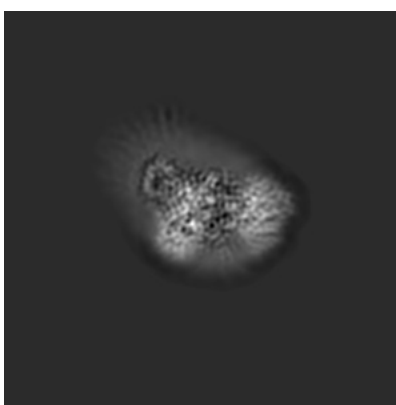
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

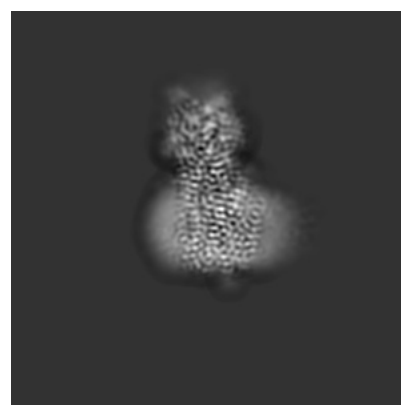
6.1.1 Primary map



X



Y

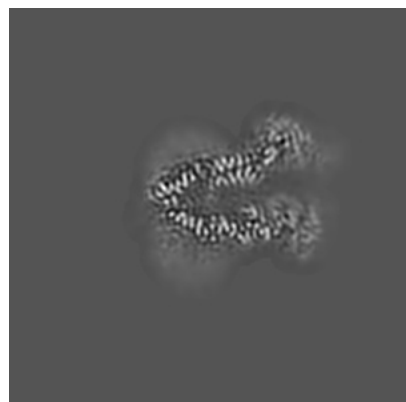


Z

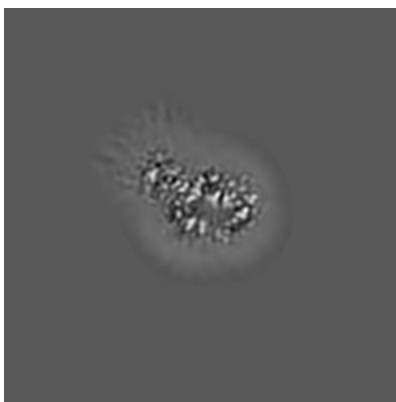
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128

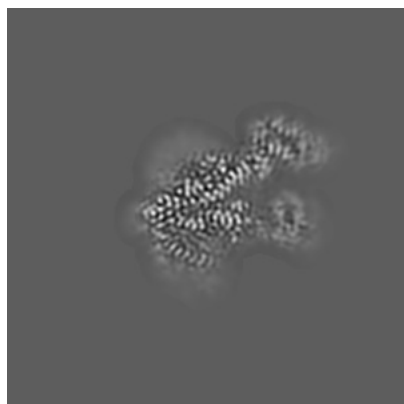


Z Index: 128

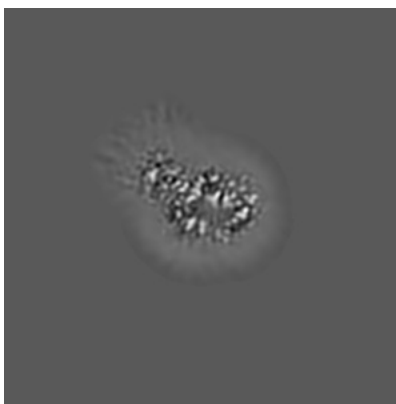
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

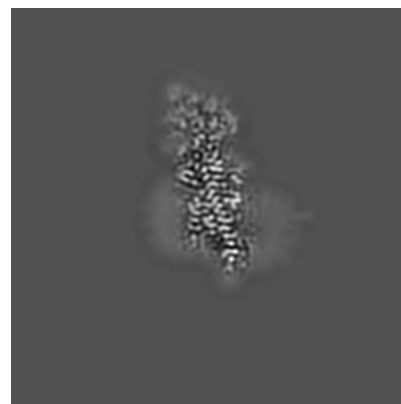
6.3.1 Primary map



X Index: 136



Y Index: 128

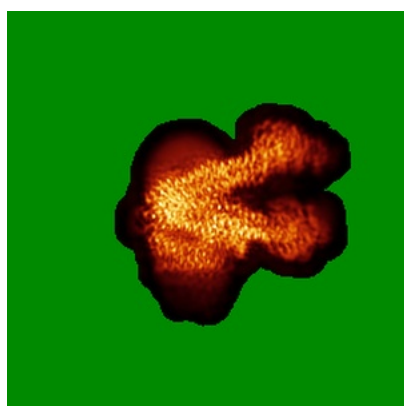


Z Index: 117

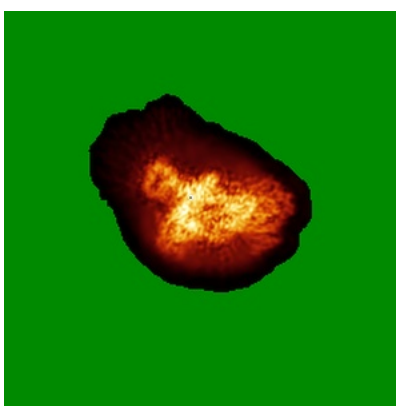
The images above show the largest variance slices of the map in three orthogonal directions.

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

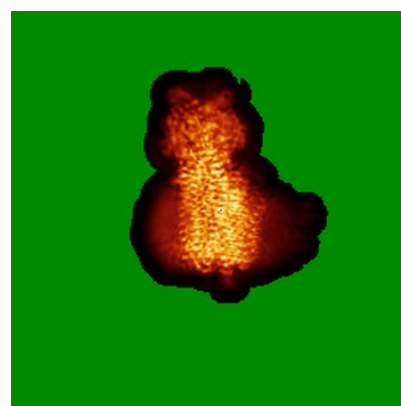
6.4.1 Primary map



X



Y

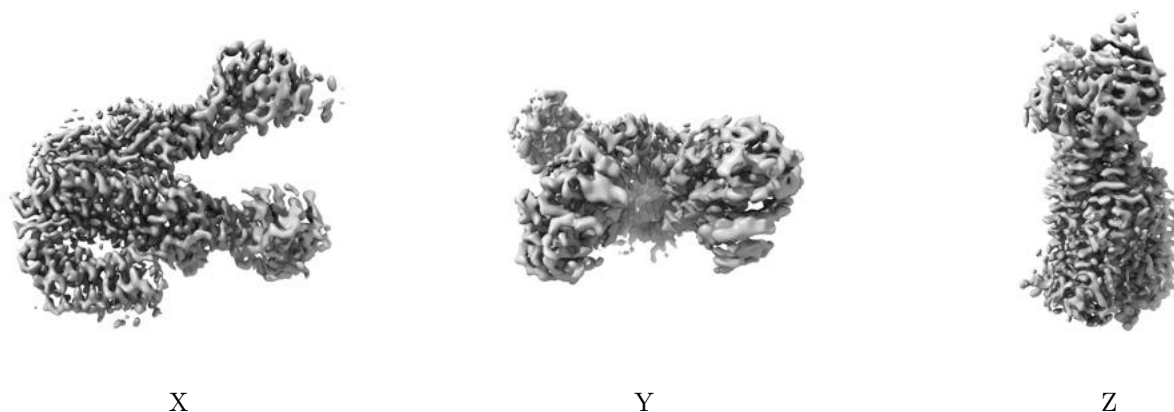


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.879. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

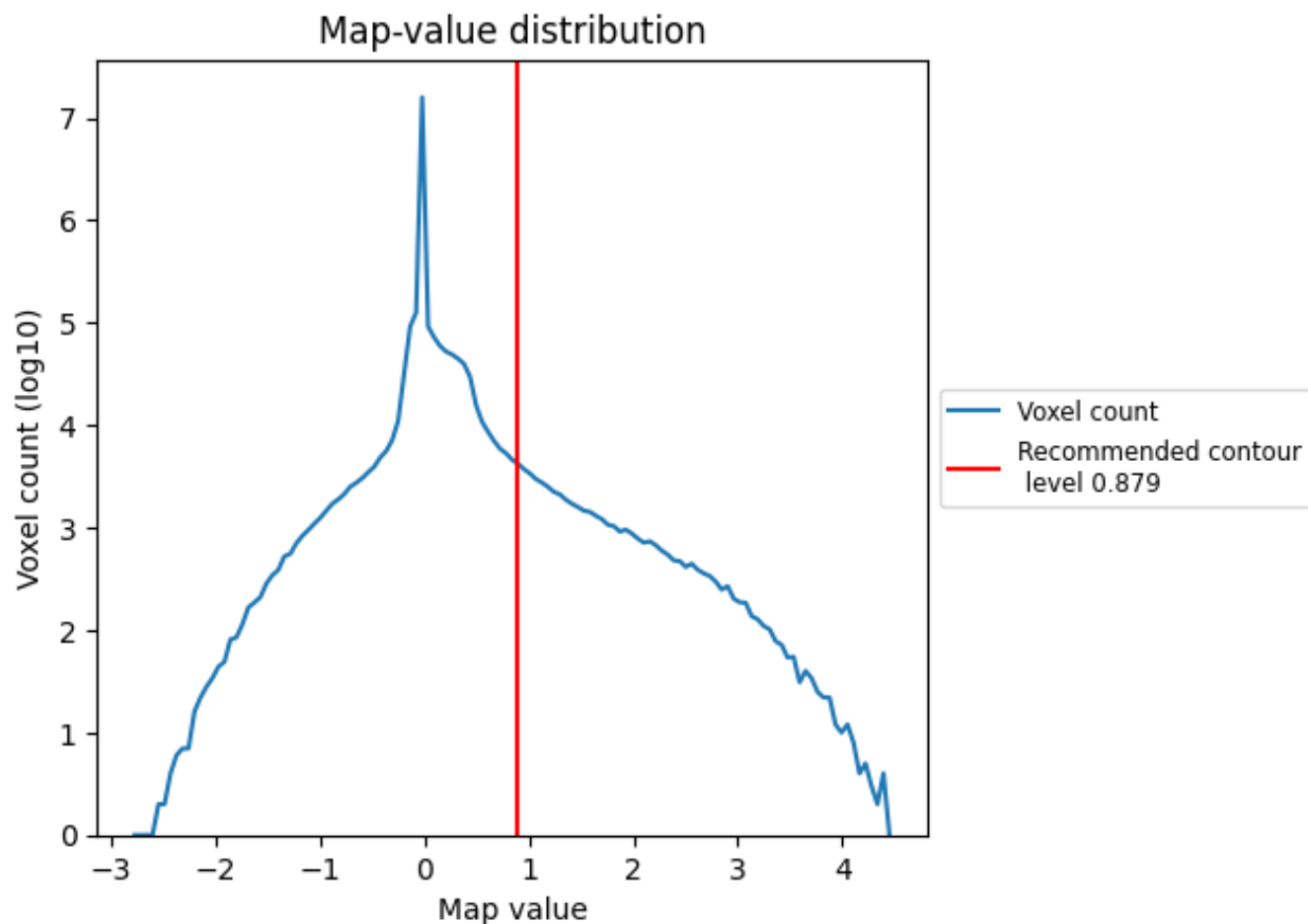
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

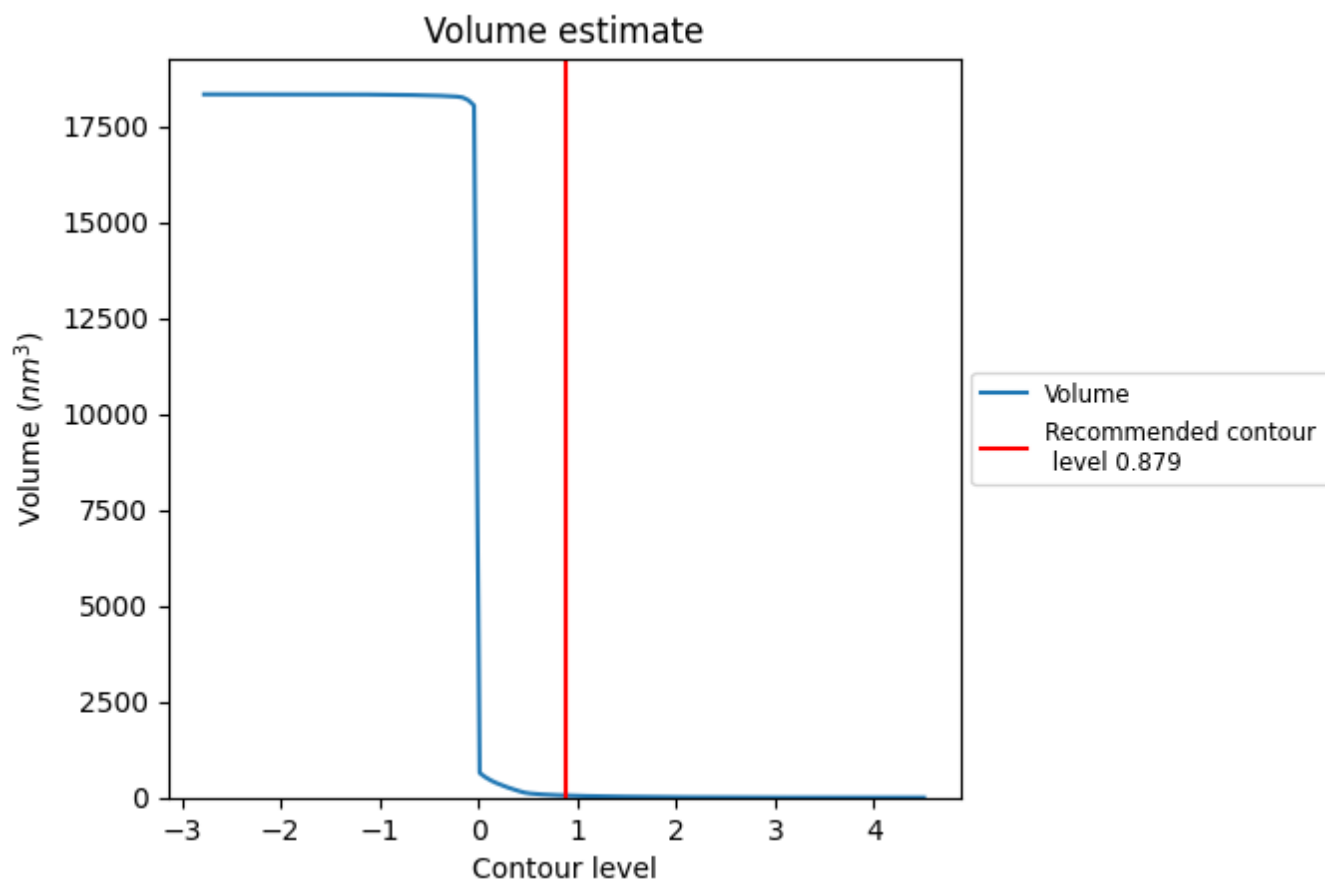
This section contains the results of statistical analysis of the map.

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.

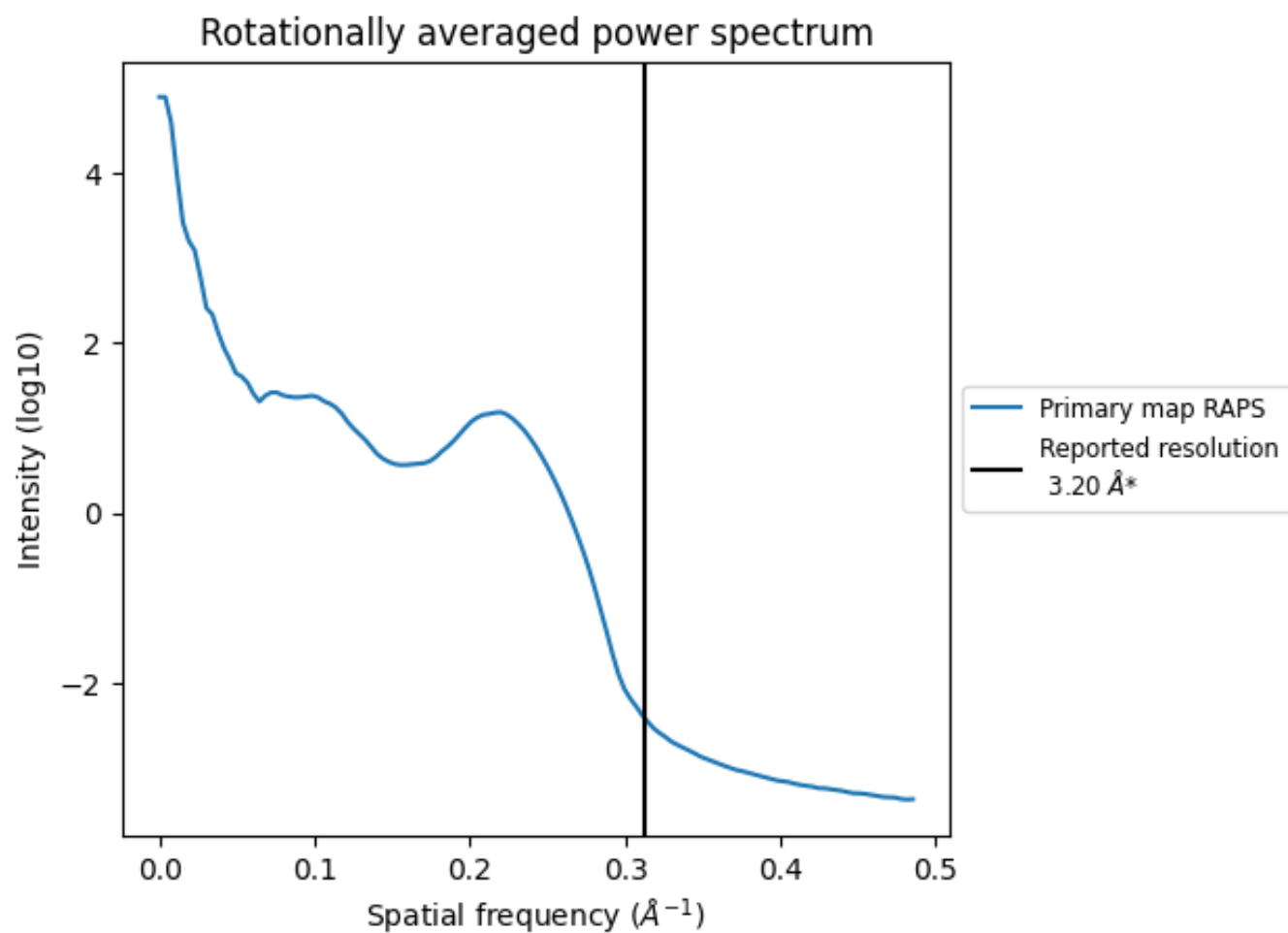
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 55 nm³; this corresponds to an approximate mass of 49 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 0.312 Å⁻¹

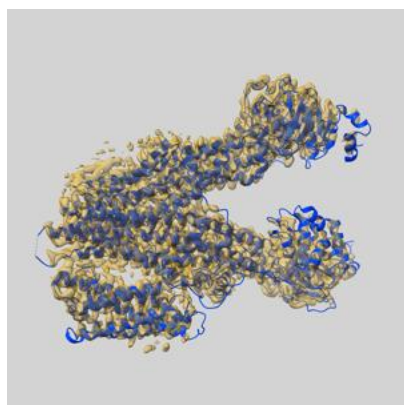
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

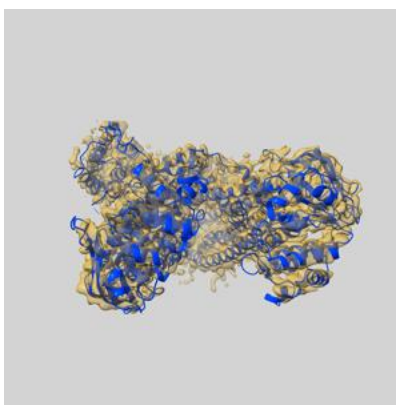
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23932 and PDB model 7MPE. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

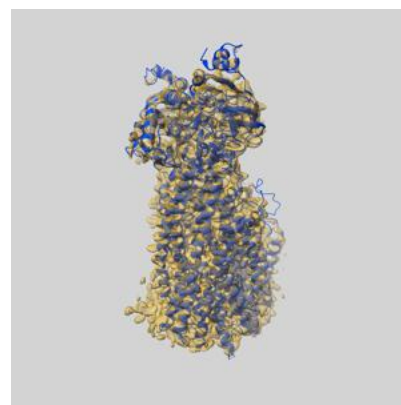
9.1 Map-model overlay [i](#)



X



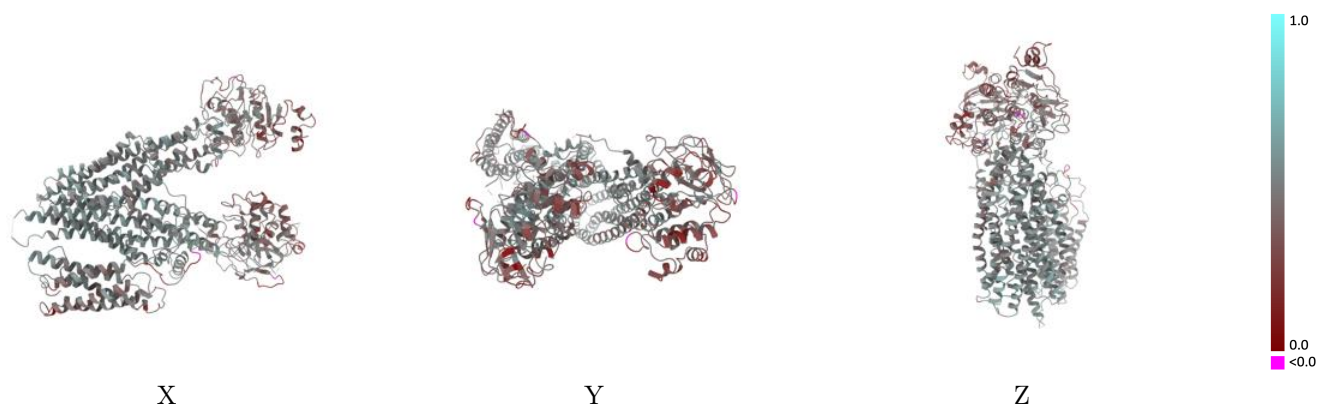
Y



Z

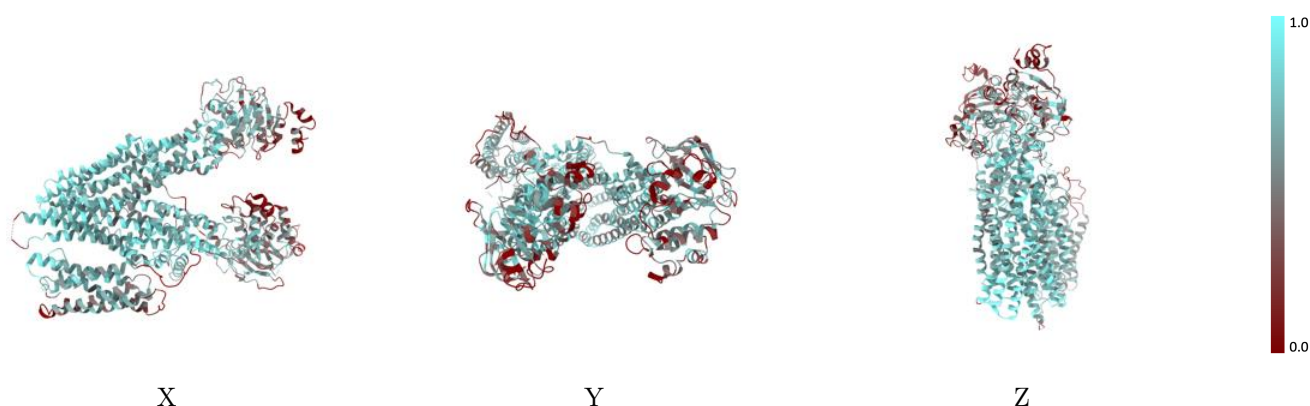
The images above show the 3D surface view of the map at the recommended contour level 0.879 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



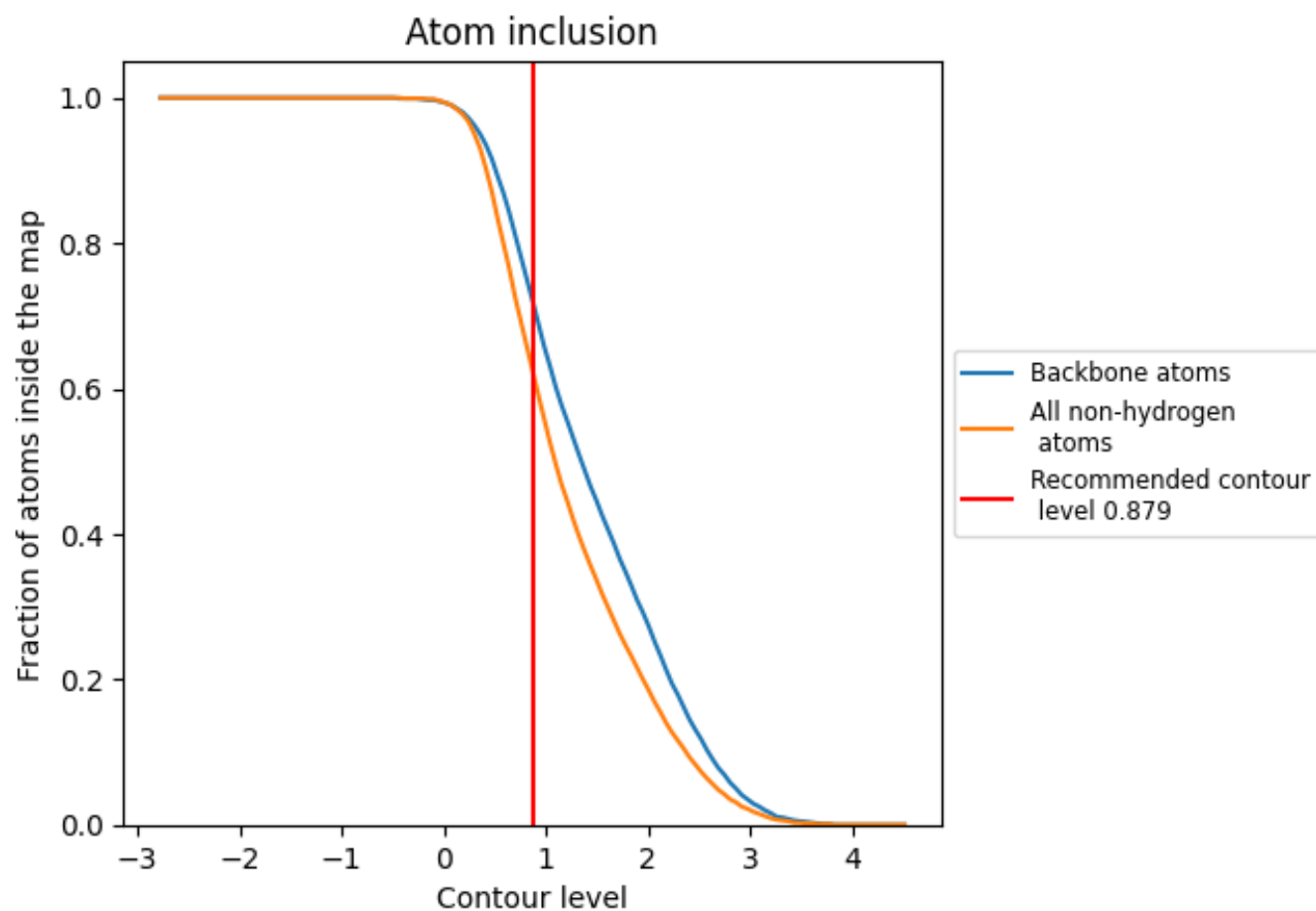
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.879).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 62% 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 (0.879) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6170	<div></div> 0.4560
A	<div></div> 0.6170	<div></div> 0.4560

