



## wwPDB EM Validation Summary Report ⓘ

Jan 16, 2025 – 01:14 am GMT

PDB ID : 9H3L  
EMDB ID : EMD-51829  
Title : 50S subunit precursor C\_(L29)-/(L22)-  
Authors : Lauer, S.; Nikolay, R.; Spahn, C.M.T.  
Deposited on : 2024-10-17  
Resolution : 5.84 Å(reported)  
Based on initial model : 8RPY

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.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) : 2.40

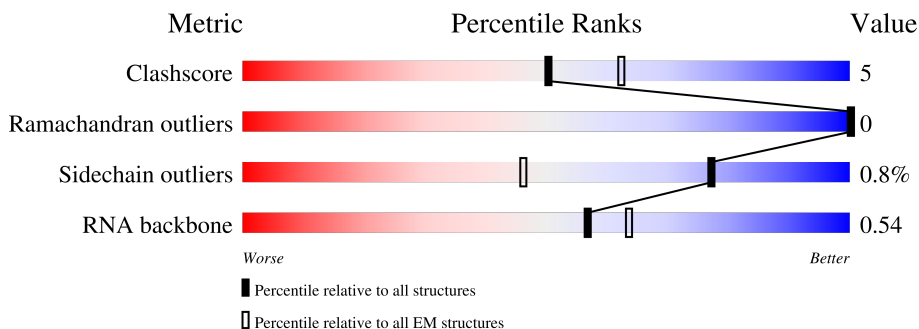
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.84 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
RNA backbone	6643	2191

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	2904	
2	D	209	
3	E	201	
4	J	142	
5	K	122	
6	L	143	
7	N	120	

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Mol	Chain	Length	Quality of chain
8	P	114	 89%11%
9	Q	117	 77%23%
10	R	103	 82%18%
11	U	102	 90%10%
12	Z	58	 60%88%10%
13	G	176	 72%83%15%

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 53578 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1946	Total	C	N	O	P	0	0
			41805	18648	7727	13484	1946		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	175	Total	C	N	O	S	0	0
			1306	820	235	247	4		

- Molecule 3 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	187	Total	C	N	O	S	0	0
			1438	904	255	274	5		

- Molecule 4 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 5 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 6 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	109	Total	C	N	O	0	0
			778	483	149	146		

- Molecule 7 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 8 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 9 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 10 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 11 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	102	Total	C	N	O	S	0	0
			780	492	146	142			

- Molecule 12 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

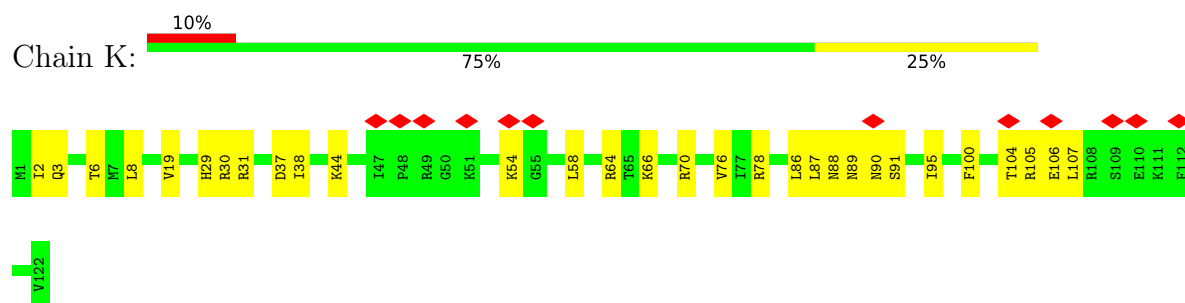


C	G	U	A	G1384	C1727	U1629	G1521	U1391	A1287	G1187	C974
C	C	U	A	C	C1728	A1630	G1521	U1391	G1288	G	A
U	U	A	C	A	U1729	A1631	U1523	A1392	U1198	A	G
U	G	C	A	G	G1730	A1632	U1524	A1393	U1199	G	A981
U	A	C	A	C	C1731	A1634	G1527	U1394	C1291	C	C
U	G	C	A	A	G1732	A1635	A1528	A1395	G1292	G	A982
U	G	C	A	A	G1733	U1636	A1529	U1396	U1203	G	A983
U	G	C	A	A	G1734	A1637	A1530	U1403	A1204	C	A984
U	U	A	A	G	G1735	C1638	A1532	A1415	U1205	C	A
U	A	A	A	U	G1736	C1639	C1533	U1416	G1206	U	A990
U	G	C	G	G	G1737	A1645	U1534	A1417	U1209	C	G
U	G	C	G	G	A1738	C1646	U1535	G1309	G1210	G	G993
U	A	A	C	C	A1739	U1647	A1536	G1310	C1211	C	G994
A	A	G	A	G	G1753	U1648	C1536	A1418	G1212	C	G995
A	G	C	A	G	A1754	G1649	A1537	A1419	U1213	U	A996
A	U	C	A	A	G1755	A1650	A1540	A1420	A1214	U	G997
A	U	C	A	A	A1756	C1658	G1543	A1421	U1313	A	A
A	U	C	A	A	A1757	G1659	A1544	G1422	G1314	G131	A
A	C	C	C	C	C	A1545	A1545	C1423	U1312	U132	A
A	C	C	C	C	C	G1546	A1546	G1424	A1133	G	A1000
A	U	U	G	G	C1760	U1662	G1555	A1427	G1225	A	C1006
A	U	U	G	G	G1763	G1663	C1556	C1320	U1232	G	C1007
A	U	U	G	G	C1764	A1664	A1557	C1321	G1336	A	A1008
A	U	U	C	C	G1768	G1665	C1558	C1322	G1337	G	A1009
A	U	U	C	C	C	G1666	C1559	C1323	G1338	C	A1010
A	U	U	C	C	C	A1667	G1560	U1325	G1339	C	G1011
A	U	U	C	C	C	A1668	C1561	U1326	C1140	U	U1012
A	U	U	C	C	C	G1674	C1562	A1327	C1141	A	C1013
A	U	U	C	C	C	C1675	C1563	U1328	U1141	C	A1014
A	U	U	C	C	C	G1681	G1564	A1329	A1142	A	A
A	U	U	C	C	C	G1682	A1570	U1329	A1143	C	A
A	U	U	C	C	C	G1686	A1571	U1240	A1144	C	A
A	U	U	C	C	C	G	C1576	G1333	C1243	U	A1020
A	U	U	C	C	C	U	C1577	G1334	A1244	U	A1021
A	U	U	C	C	C	A	U1578	U1344	G1149	U	G1022
A	U	U	C	C	C	U	U1579	U1345	C1150	U	U1023
A	U	U	C	C	C	A	A1580	C1346	A1151	A	G1024
A	U	U	C	C	C	U	G1581	C1351	G1153	A	G1025
A	U	U	C	C	C	U	C1582	A1352	G1154	G	G1026
A	U	U	C	C	C	C	A1583	A1353	A1156	A	A1027
A	U	U	C	C	C	G	U1584	G1157	A1157	A	A1028
A	U	U	C	C	C	G	C1585	G1255	G1162	C	G1031
A	U	U	C	C	C	G	A1586	A1359	U1256	G	A
A	U	U	C	C	C	G	G1587	A1365	C1261	C	U
A	U	U	C	C	C	A	A1588	A1366	A1262	G	U
A	U	U	C	C	C	A	G1589	G1371	G1171	U	U
A	U	U	C	C	C	A	U1173	U1173	A1172	A	G
A	U	U	C	C	C	A	G1174	U1174	U1173	A	G
A	U	U	C	C	C	A	A1175	U1175	A1175	C	A
A	U	U	C	C	C	A	U1176	U1176	G1177	C	A
A	U	U	C	C	C	A	G1177	U1177	U1177	U	C
A	U	U	C	C	C	A	U1181	U1181	U1181	C	C
A	U	U	C	C	C	A	G1182	U1182	G1182	U	C
A	U	U	C	C	C	A	U1183	U1183	U1183	C	A
A	U	U	C	C	C	A	G1185	U1185	G1185	G	G
A	U	U	C	C	C	A	U1186	G1186	G1186	U	A
A	U	U	C	C	C	A	A1286	C1386	A1286	C	A

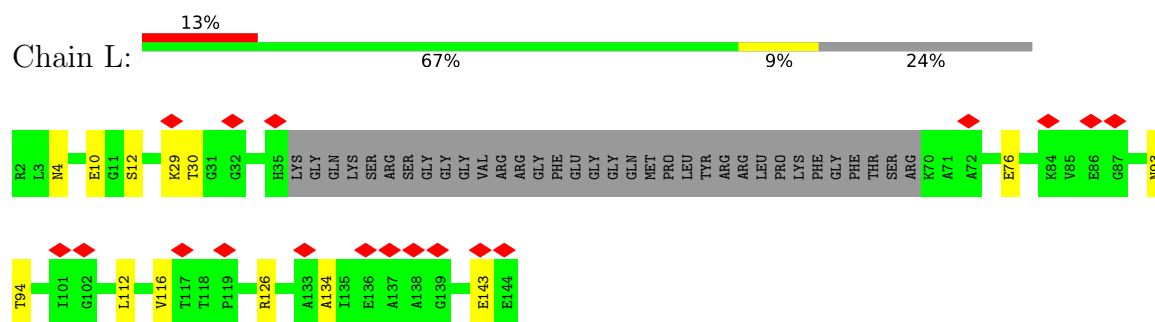




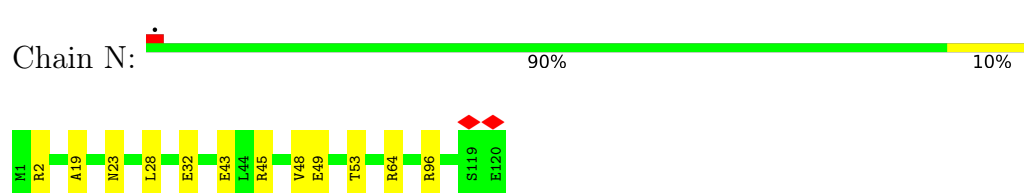
- Molecule 5: Large ribosomal subunit protein uL14



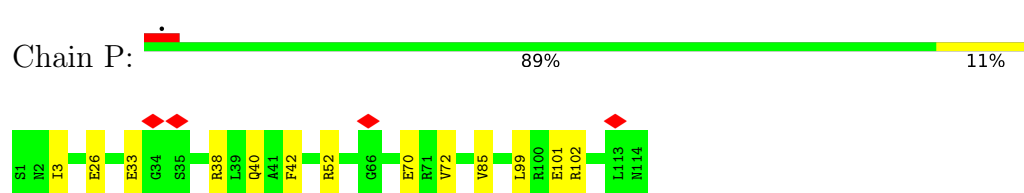
- Molecule 6: Large ribosomal subunit protein uL15



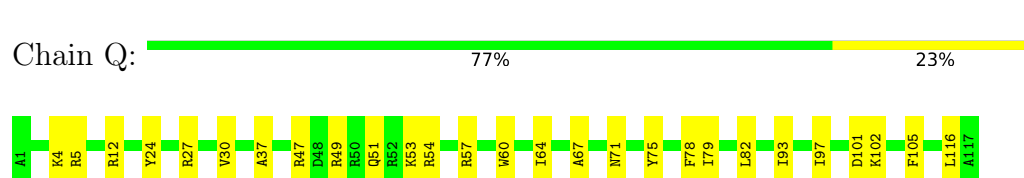
- Molecule 7: Large ribosomal subunit protein bL17



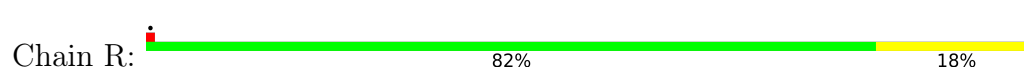
- Molecule 8: Large ribosomal subunit protein bL19



- Molecule 9: Large ribosomal subunit protein bL20

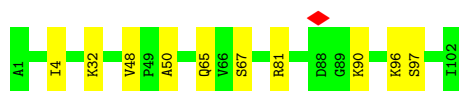
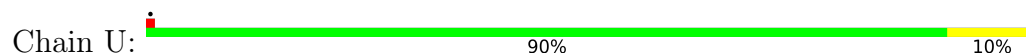


- Molecule 10: Large ribosomal subunit protein bL21

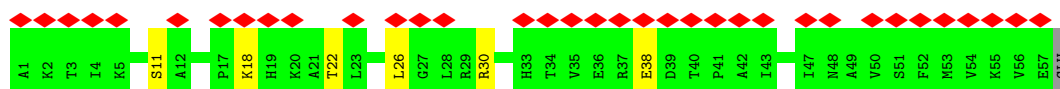
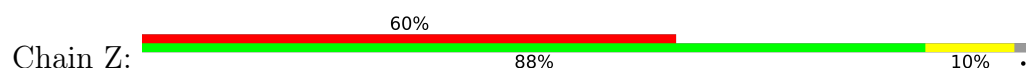




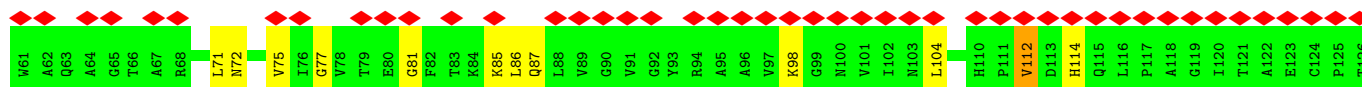
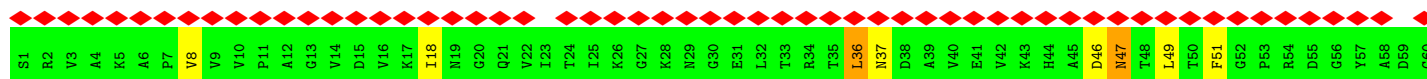
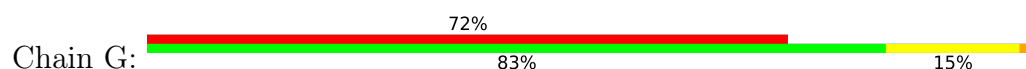
- Molecule 11: Large ribosomal subunit protein uL24



- Molecule 12: Large ribosomal subunit protein uL30



- Molecule 13: Large ribosomal subunit protein uL6



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5679	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)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.042	Depositor
Minimum map value	-0.217	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.255	Depositor
Map size (Å)	424.0, 424.0, 424.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4133333, 1.4133333, 1.4133333	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	0.26	4/46823 (0.0%)	1.25	22/73036 (0.0%)
2	D	0.24	0/1320	0.51	0/1776
3	E	0.24	0/1453	0.46	0/1956
4	J	0.24	0/1152	0.49	0/1551
5	K	0.24	0/948	0.54	0/1268
6	L	0.24	0/780	0.54	0/1041
7	N	0.24	0/974	0.58	0/1301
8	P	0.24	0/929	0.55	0/1242
9	Q	0.25	0/960	0.52	0/1278
10	R	0.25	0/829	0.53	0/1107
11	U	0.25	0/788	0.49	0/1051
12	Z	0.24	0/443	0.55	0/593
13	G	0.24	0/1343	0.49	0/1816
All	All	0.26	4/58742 (0.0%)	1.15	22/89016 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1310	G	C5-C4	-26.75	1.19	1.38
1	A	1310	G	N7-C5	23.64	1.53	1.39
1	A	1310	G	N9-C8	-23.23	1.21	1.37
1	A	1310	G	N9-C4	20.18	1.54	1.38

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1310	G	C4-C5-N7	-216.38	24.25	110.80
1	A	1310	G	N7-C8-N9	-120.30	52.95	113.10
1	A	1310	G	N9-C4-C5	-91.40	68.84	105.40
1	A	1310	G	C5-N7-C8	50.06	129.33	104.30
1	A	1310	G	C8-N9-C4	-46.38	87.85	106.40

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	41805	0	21035	312	0
2	D	1306	0	1355	21	0
3	E	1438	0	1494	16	0
4	J	1129	0	1162	14	0
5	K	939	0	1012	21	0
6	L	778	0	841	10	0
7	N	961	0	1000	10	0
8	P	917	0	965	11	0
9	Q	947	0	1022	23	0
10	R	816	0	839	15	0
11	U	780	0	834	8	0
12	Z	439	0	485	5	0
13	G	1323	0	1374	20	0
All	All	53578	0	33418	439	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 5.

The worst 5 of 439 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:571:U:O4	1:A:575:A:N7	2.02	0.93
1:A:175:G:O2'	1:A:176:A:O5'	1.87	0.92
1:A:1007:C:OP2	1:A:1008:A:O2'	1.90	0.89
1:A:2523:G:O2'	1:A:2765:A:N6	2.08	0.87
1:A:1521:G:OP2	1:A:1522:A:O2'	1.94	0.85

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	
2	D	171/209 (82%)	160 (94%)	11 (6%)	0	100	100
3	E	183/201 (91%)	178 (97%)	5 (3%)	0	100	100
4	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
5	K	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
6	L	105/143 (73%)	93 (89%)	12 (11%)	0	100	100
7	N	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
8	P	112/114 (98%)	106 (95%)	6 (5%)	0	100	100
9	Q	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
10	R	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
11	U	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
12	Z	55/58 (95%)	55 (100%)	0	0	100	100
13	G	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
All	All	1494/1607 (93%)	1420 (95%)	74 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
2	D	136/164 (83%)	132 (97%)	4 (3%)	37	56
3	E	155/165 (94%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	116/116 (100%)	115 (99%)	1 (1%)	75	83
5	K	103/103 (100%)	103 (100%)	0	100	100
6	L	76/102 (74%)	76 (100%)	0	100	100
7	N	100/100 (100%)	100 (100%)	0	100	100
8	P	99/99 (100%)	99 (100%)	0	100	100
9	Q	89/89 (100%)	89 (100%)	0	100	100
10	R	84/84 (100%)	84 (100%)	0	100	100
11	U	83/83 (100%)	83 (100%)	0	100	100
12	Z	47/48 (98%)	47 (100%)	0	100	100
13	G	137/137 (100%)	132 (96%)	5 (4%)	30	50
All	All	1225/1290 (95%)	1215 (99%)	10 (1%)	77	85

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	G	98	LYS
13	G	112	VAL
13	G	133	LYS
2	D	161	MET
4	J	96	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	42	ASN
13	G	103	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1938/2904 (66%)	322 (16%)	8 (0%)

5 of 322 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A

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Mol	Chain	Res	Type
1	A	12	U
1	A	25	U
1	A	27	G
1	A	46	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2763	G
1	A	1738	G
1	A	1394	U
1	A	1198	U
1	A	1420	A

#### 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.



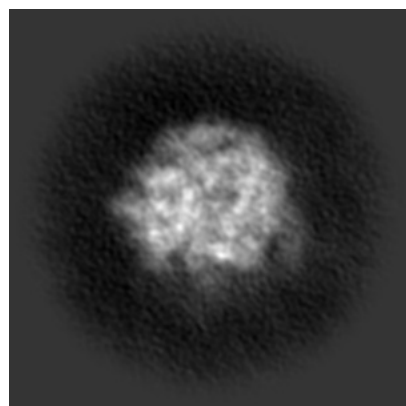
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51829. These allow visual inspection of the internal detail of the map and identification of artifacts.

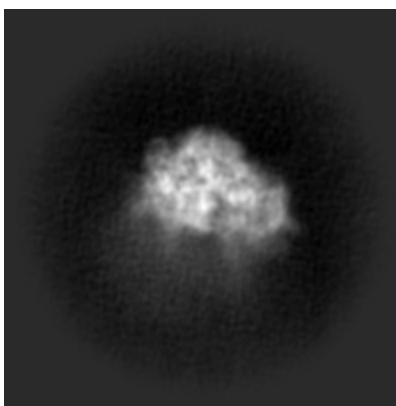
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

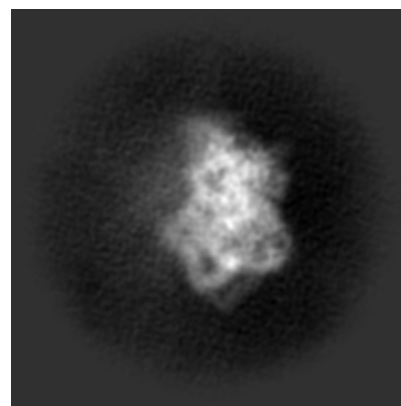
#### 6.1.1 Primary map



X

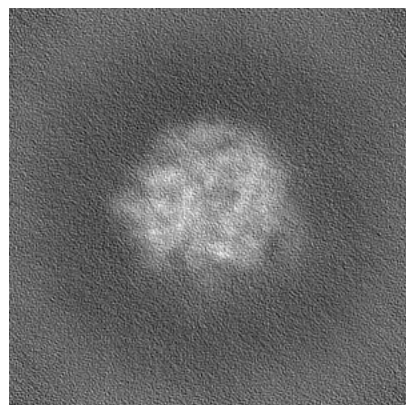


Y

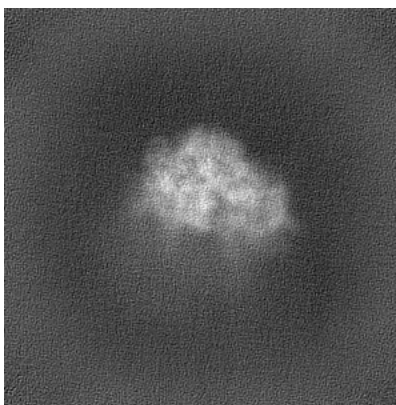


Z

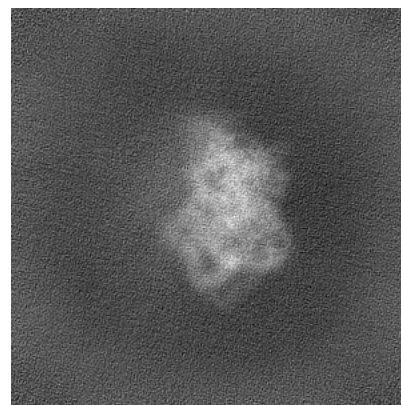
#### 6.1.2 Raw map



X



Y

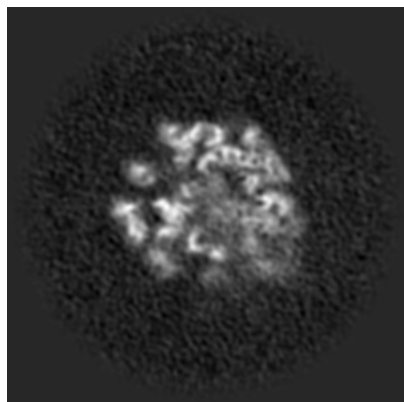


Z

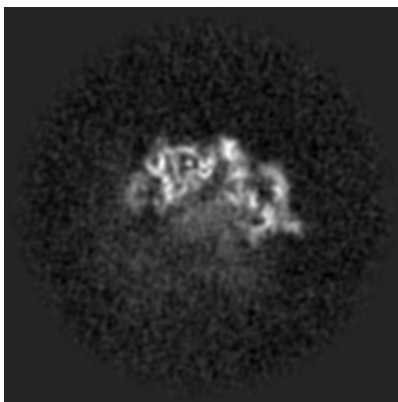
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

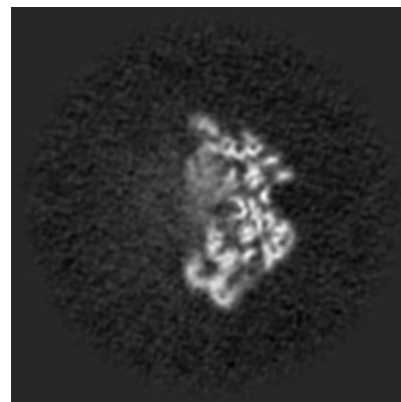
### 6.2.1 Primary map



X Index: 150

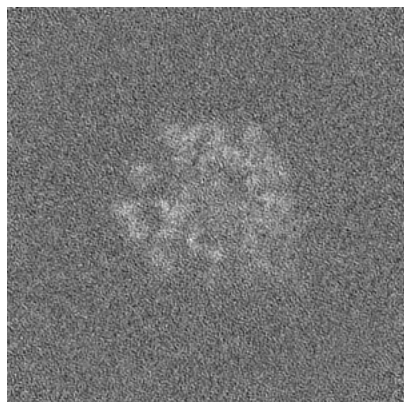


Y Index: 150

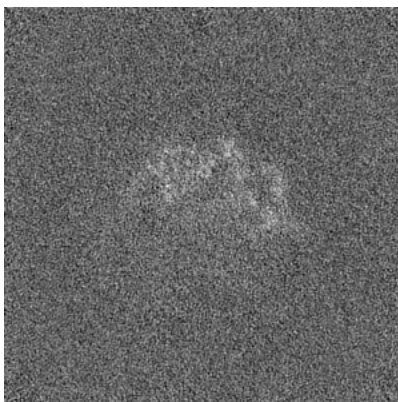


Z Index: 150

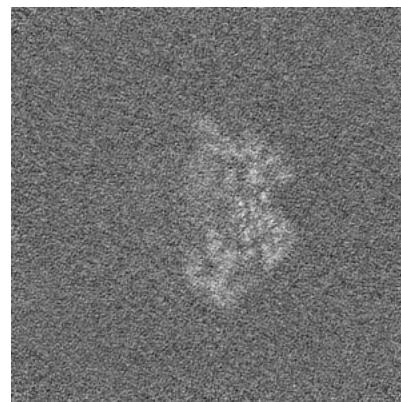
### 6.2.2 Raw map



X Index: 150



Y Index: 150

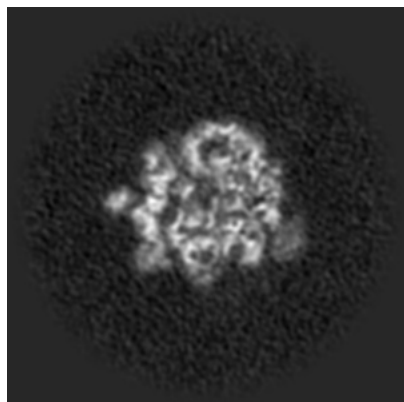


Z Index: 150

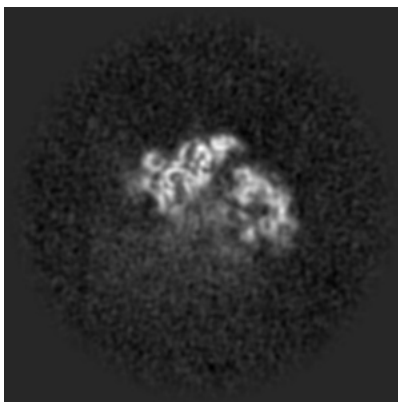
The images above show central slices of the map in three orthogonal directions.

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

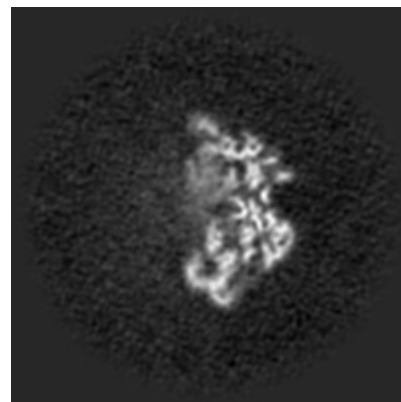
### 6.3.1 Primary map



X Index: 164

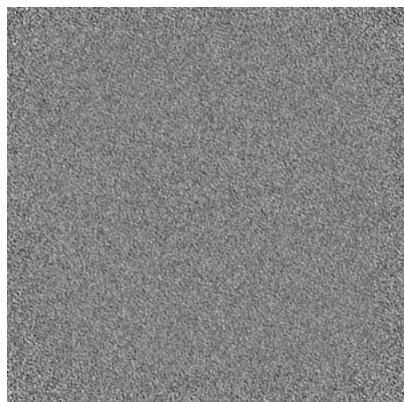


Y Index: 142

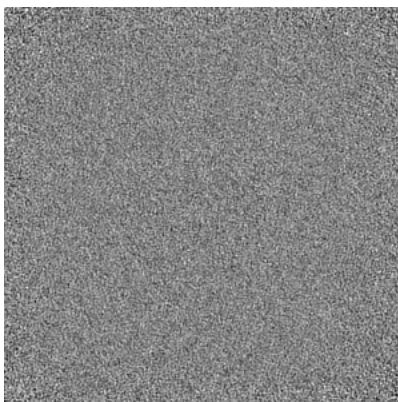


Z Index: 149

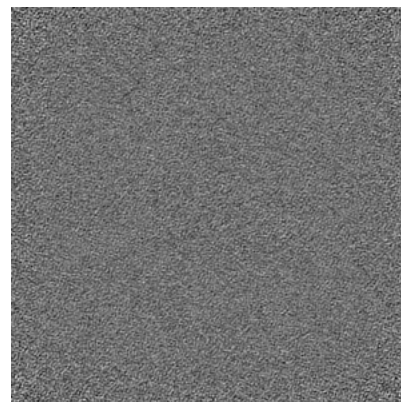
### 6.3.2 Raw map



X Index: 0



Y Index: 0



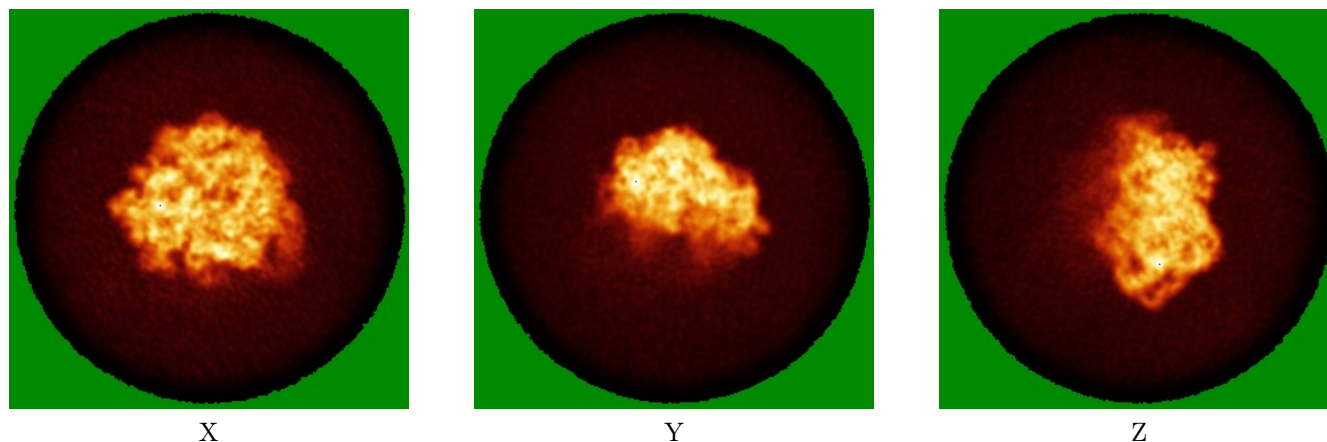
Z Index: 0

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

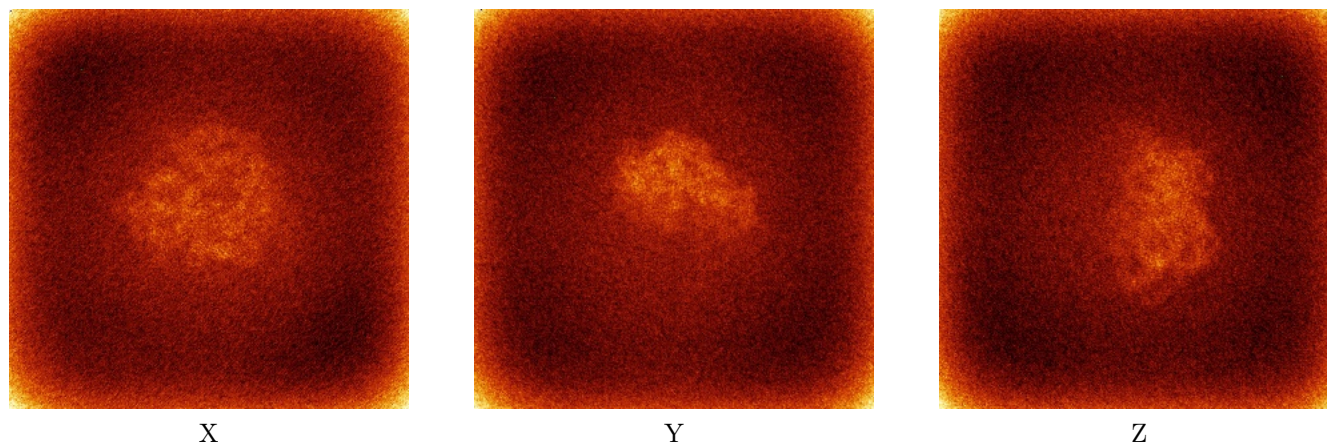


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



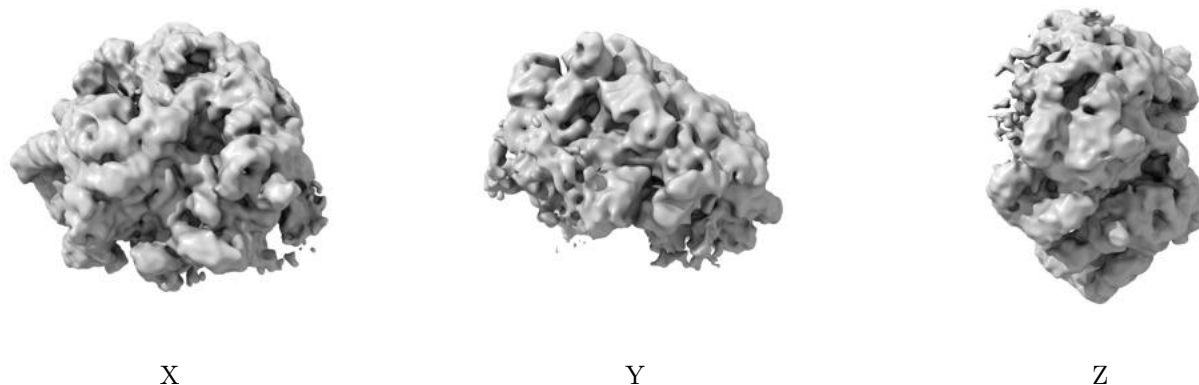
### 6.4.2 Raw map



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.

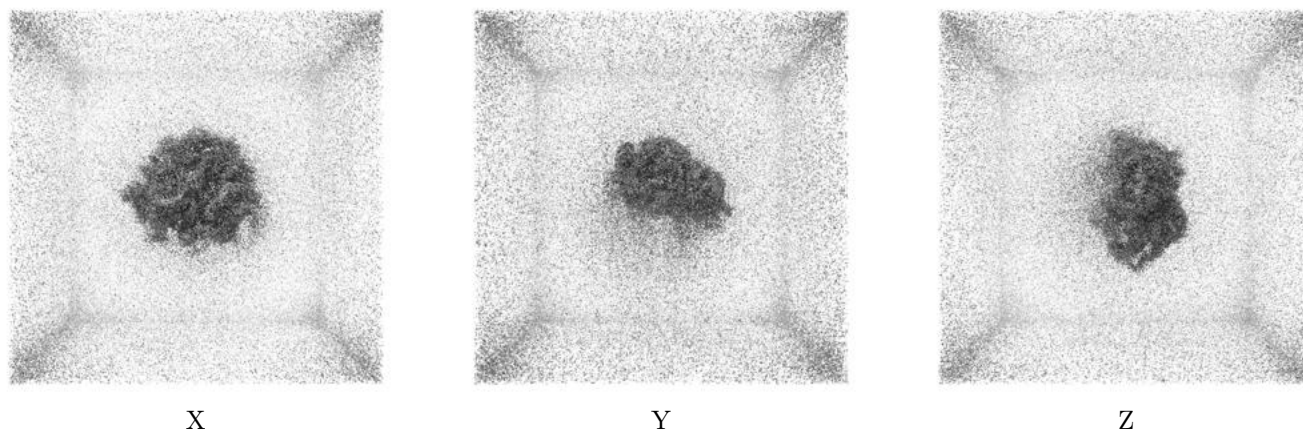
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.255. 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.

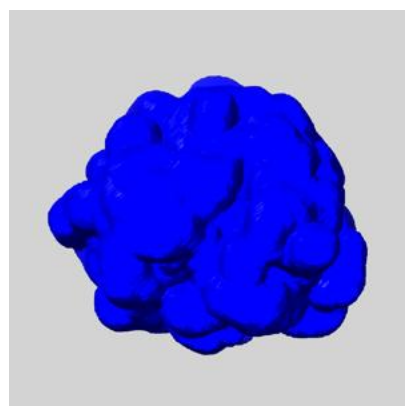
## 6.6 Mask visualisation [i](#)

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

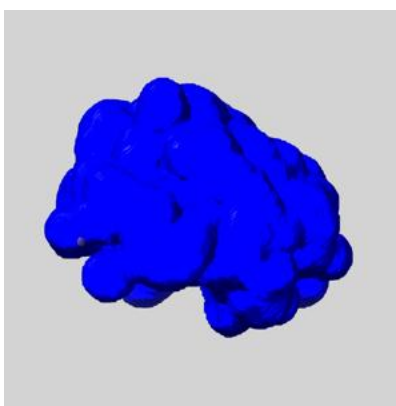
A mask typically either:

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

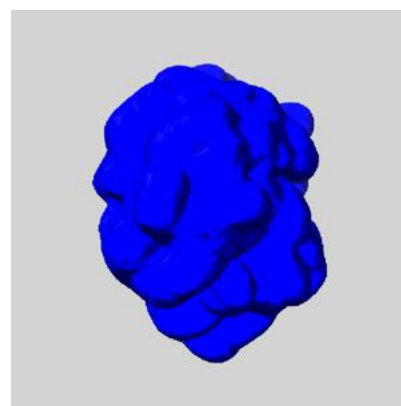
### 6.6.1 emd\_51829\_msk\_1.map [i](#)



X



Y

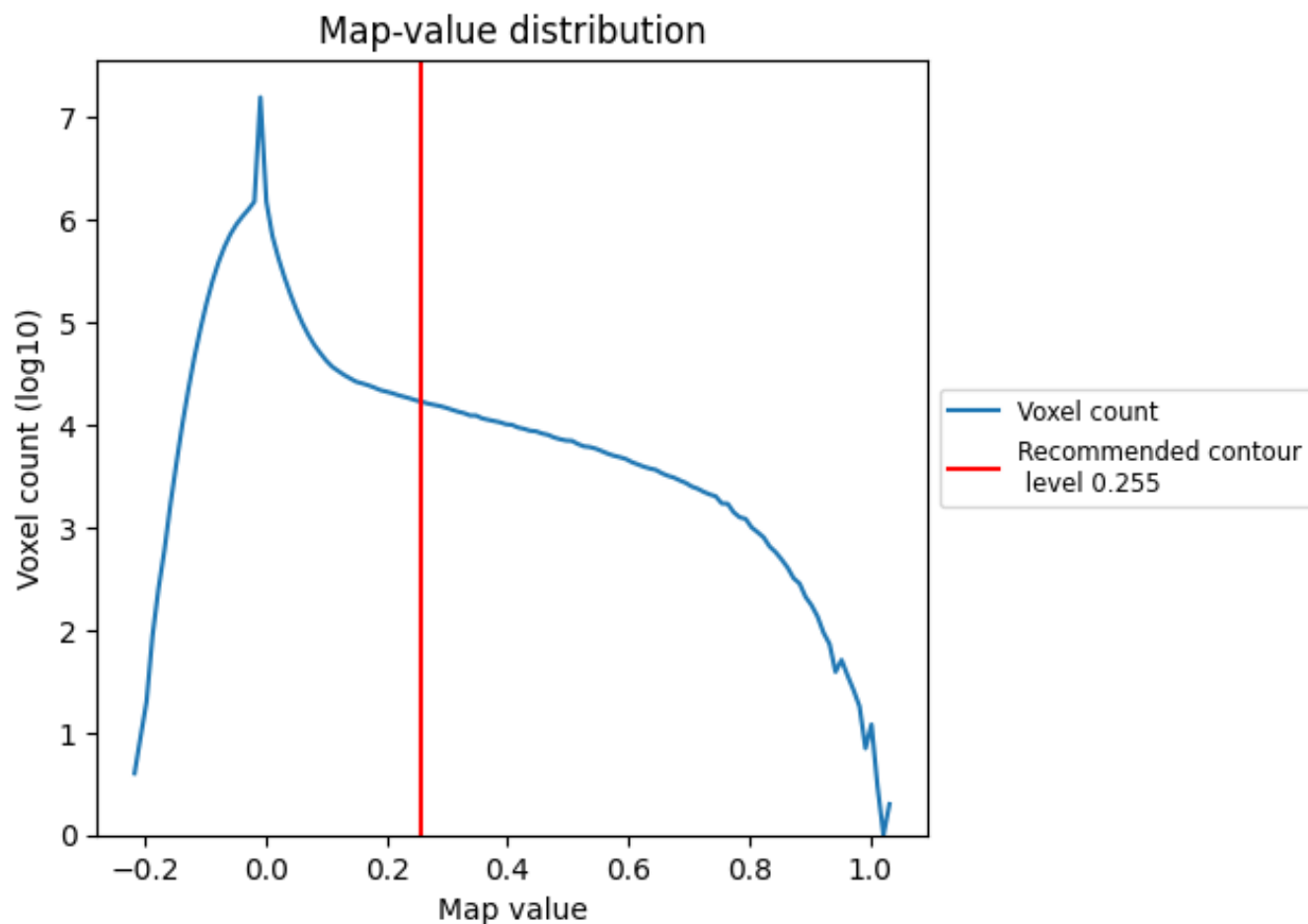


Z

## 7 Map analysis [i](#)

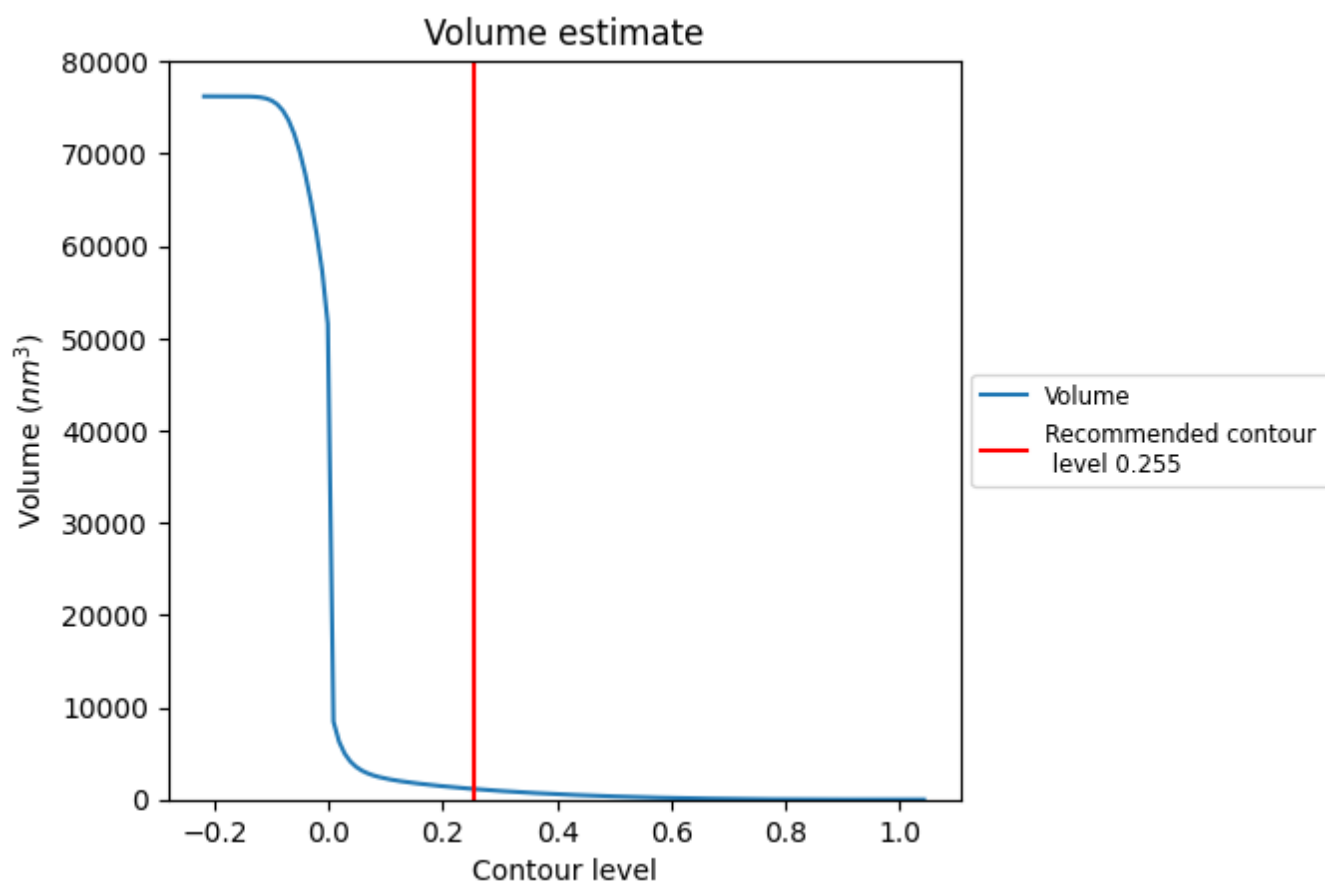
This section contains the results of statistical analysis of the map.

### 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](#)

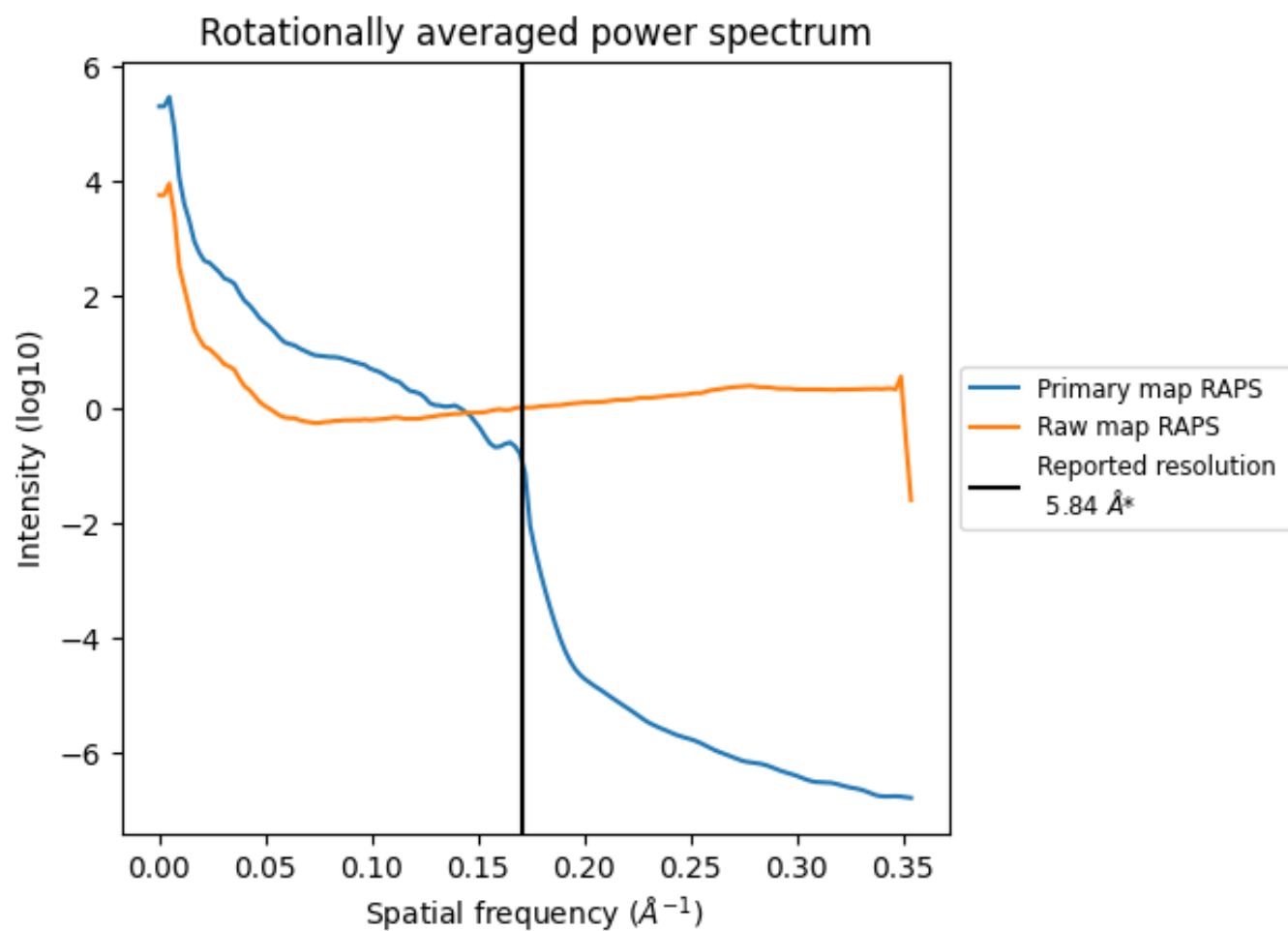


The volume at the recommended contour level is 1145 nm<sup>3</sup>; this corresponds to an approximate mass of 1034 kDa.

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 ⓘ

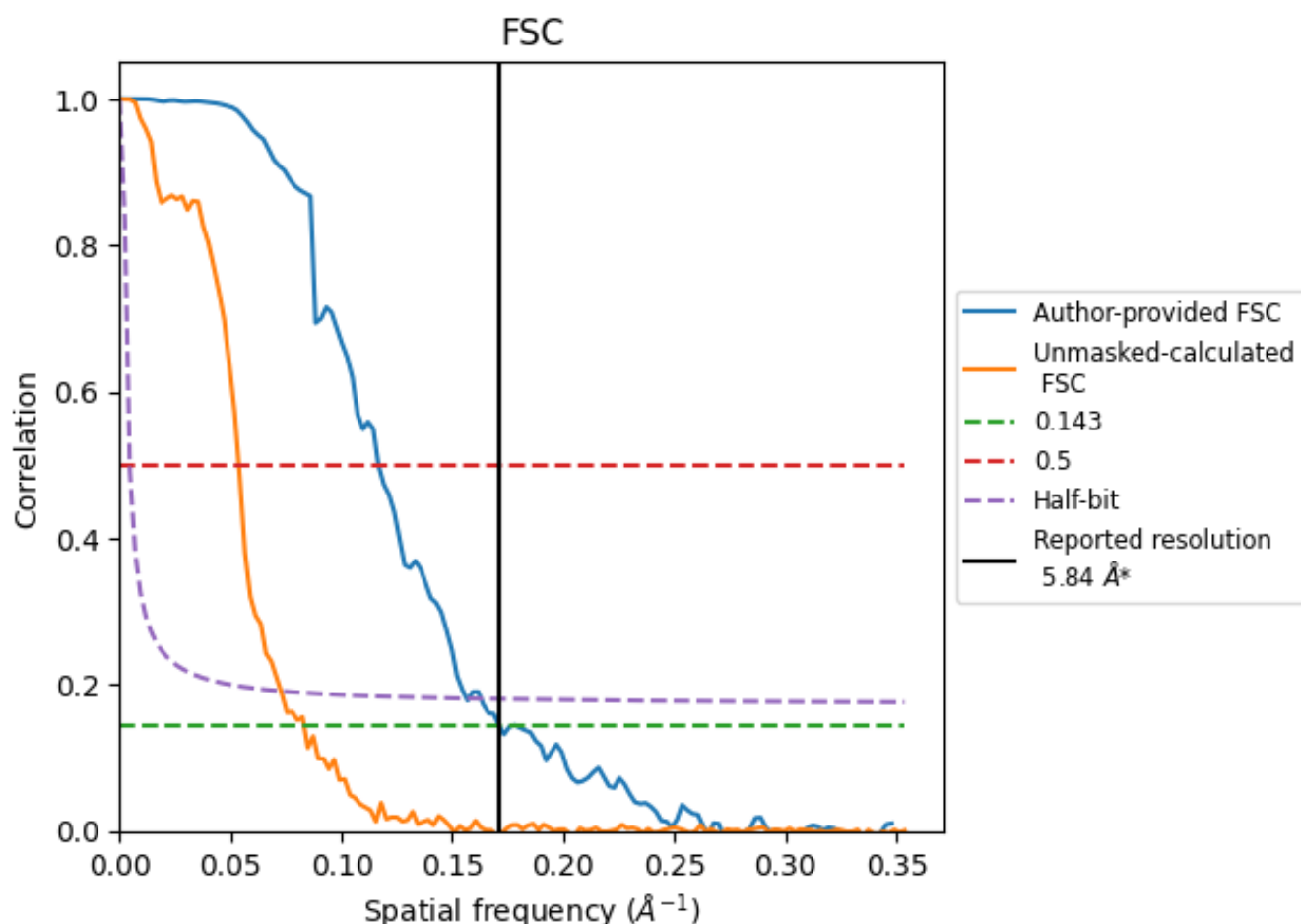


\*Reported resolution corresponds to spatial frequency of 0.171  $\text{\AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

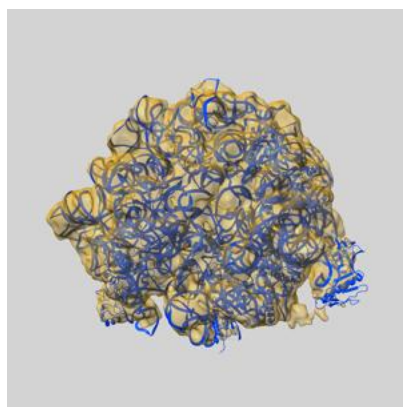
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.84	-	-
Author-provided FSC curve	5.84	8.57	6.39
Unmasked-calculated*	12.02	18.59	13.74

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 12.02 differs from the reported value 5.84 by more than 10 %

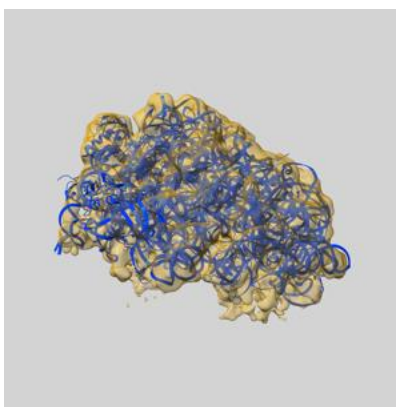
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51829 and PDB model 9H3L. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

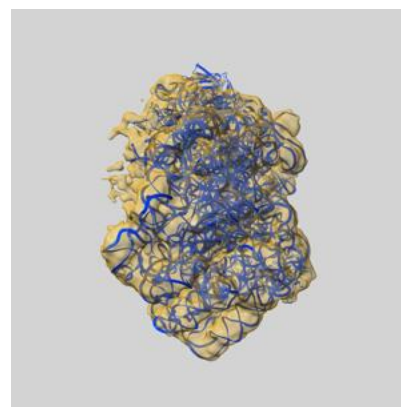
### 9.1 Map-model overlay [i](#)



X



Y



Z

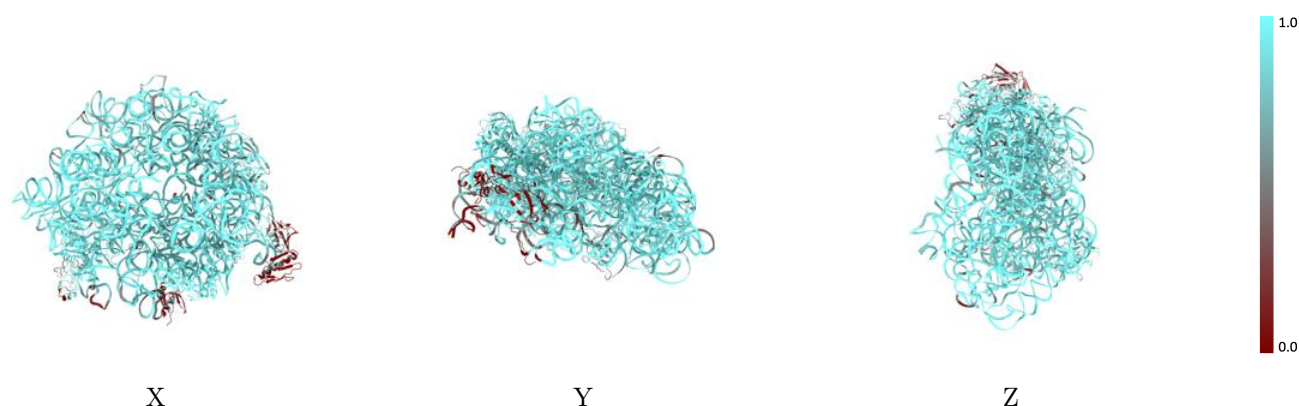
The images above show the 3D surface view of the map at the recommended contour level 0.255 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



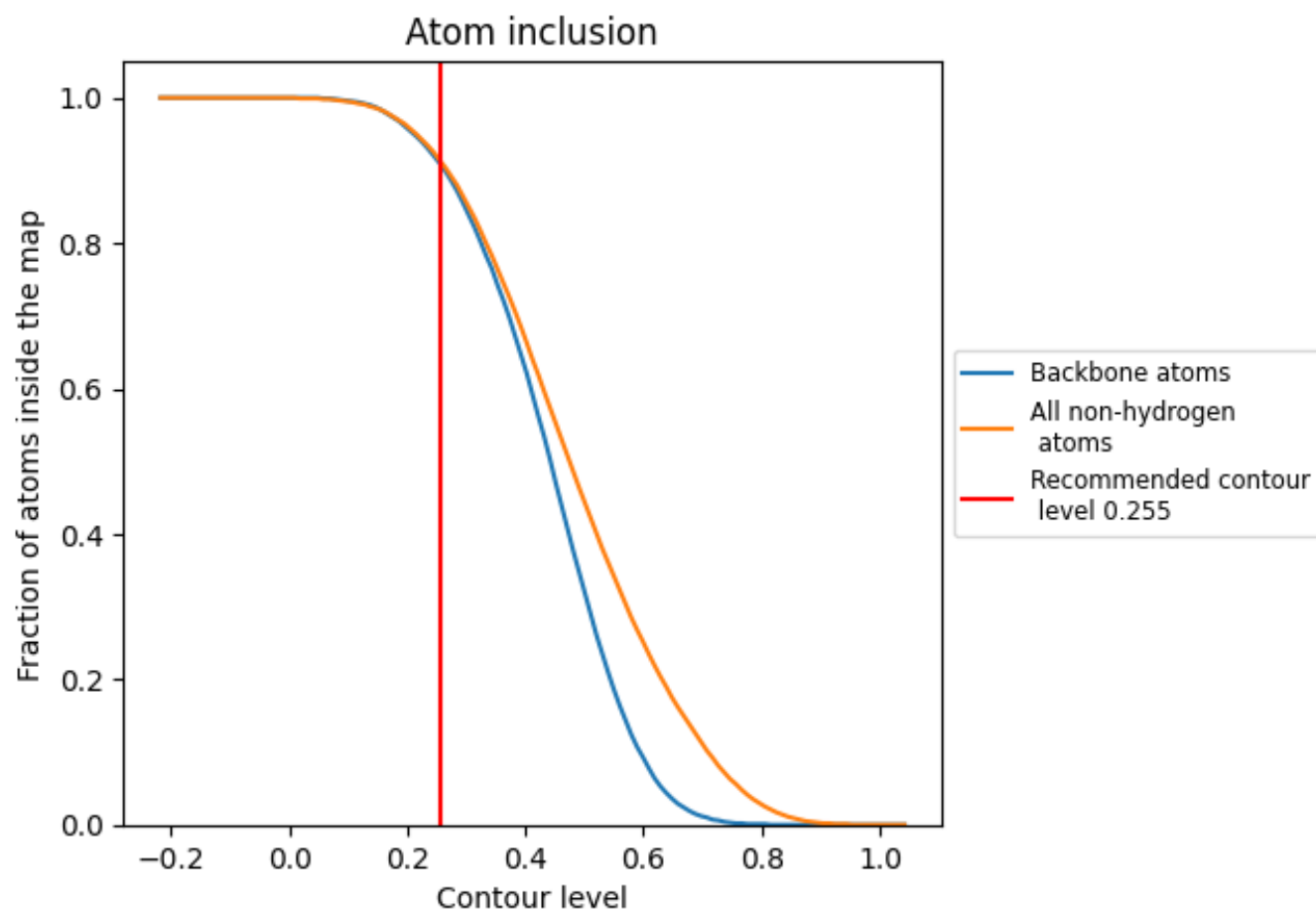
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.255).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.255) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.1540
A	 0.9450	 0.1630
D	 0.9170	 0.1320
E	 0.8920	 0.1300
G	 0.2570	 0.0780
J	 0.9360	 0.1490
K	 0.8280	 0.1080
L	 0.7440	 0.0730
N	 0.9130	 0.1170
P	 0.8960	 0.1420
Q	 0.9670	 0.1440
R	 0.9470	 0.1480
U	 0.9130	 0.1380
Z	 0.3330	 0.0840

