



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 07:27 AM EST

PDB ID : 6PPF
EMDB ID : EMD-20435
Title : Bacterial 45SRbgA ribosomal particle class B
Authors : Ortega, J.; Seffouh, A.; Jain, N.; Jahagirdar, D.; Basu, K.; Razi, A.; Ni, X.;
Guarne, A.; Britton, R.A.
Deposited on : 2019-07-06
Resolution : 3.40 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:

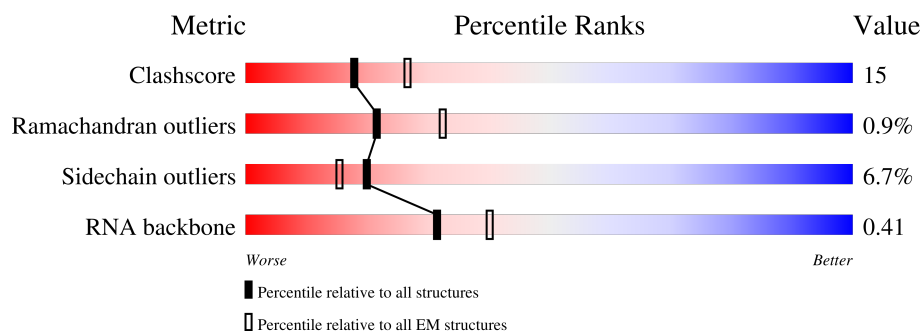
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.40 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
RNA backbone	4643	859

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	2927	<div> <div>9%</div> <div>45%</div> <div>31%</div> <div>8%</div> <div>16%</div> </div>
2	B	119	<div> <div>34%</div> <div>36%</div> <div>43%</div> <div>15%</div> <div>6%</div> </div>
3	C	277	<div> <div>6%</div> <div>51%</div> <div>26%</div> <div>20%</div> </div>
4	D	209	<div> <div>6%</div> <div>47%</div> <div>25%</div> <div>7%</div> <div>20%</div> </div>
5	E	207	<div> <div>10%</div> <div>56%</div> <div>35%</div> <div>6%</div> </div>
6	J	145	<div> <div>5%</div> <div>66%</div> <div>27%</div> </div>
7	K	122	<div> <div>22%</div> <div>66%</div> <div>34%</div> </div>

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Mol	Chain	Length	Quality of chain
8	L	145	
9	N	120	
10	O	120	
11	P	115	
12	Q	118	
13	R	102	
14	S	113	
15	T	95	
16	U	103	
17	V	94	
18	Z	59	
19	b	59	
20	Y	66	
21	d	44	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 71835 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2471	Total	C	N	O	P	0	0
			53094	23688	9835	17100	2471		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2395	1068	435	780	112		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	221	Total	C	N	O	S	0	0
			1684	1047	326	307	4		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	167	Total	C	N	O	S	0	0
			1265	802	220	240	3		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	194	Total	C	N	O	S	0	0
			1484	937	270	275	2		

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	141	Total	C	N	O	S	0	0
			1119	708	205	201	5		

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	128	Total	C	N	O	S	0	0
			952	594	179	177	2		

- Molecule 9 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 10 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	O	104	Total	C	N	O	0	0
			791	492	157	142		

- Molecule 11 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	P	103	Total	C	N	O	0	0
			846	540	162	144		

- Molecule 12 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 13 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	R	96	Total	C	N	O	0	0
			758	485	134	139		

- Molecule 14 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 15 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	88	Total	C	N	O	S	0	0
			707	441	131	132	3		

- Molecule 16 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	98	Total	C	N	O	S	0	0
			739	464	138	134	3		

- Molecule 17 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	73	Total	C	N	O		0	0
			555	344	106	105			

- Molecule 18 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 19 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	b	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 20 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 21 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

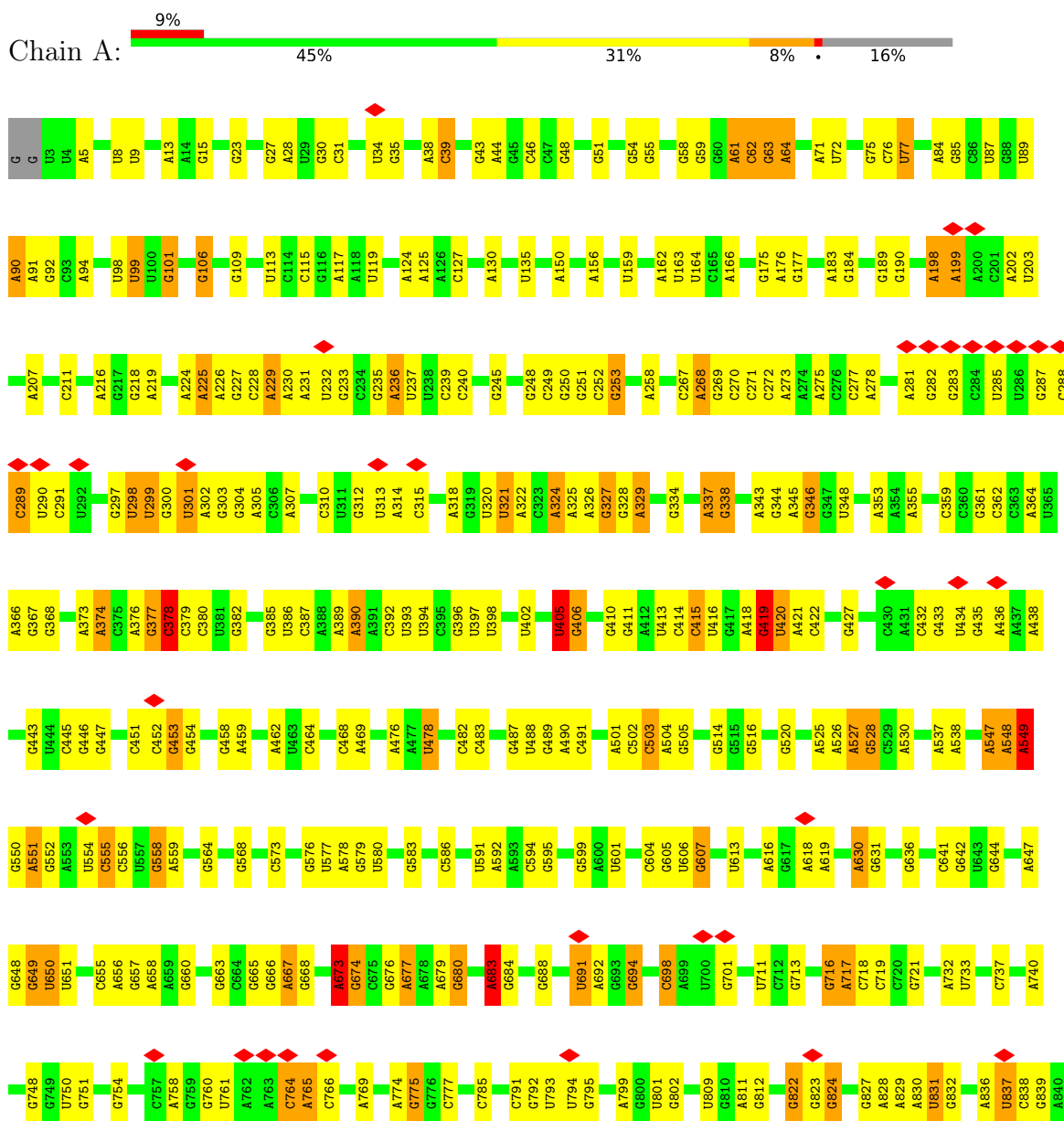
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	A	13	Total	O	0
			13	13	

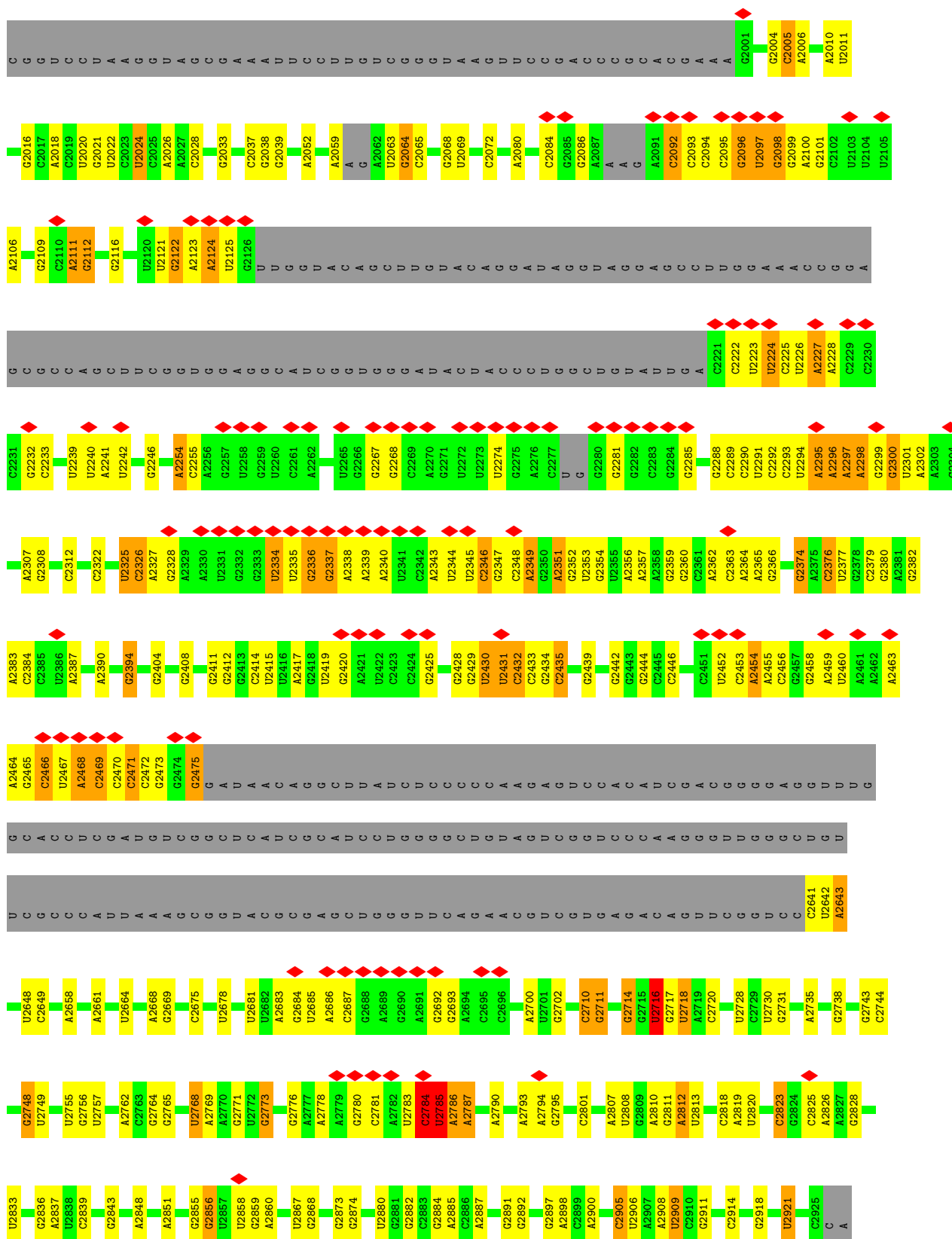
3 Residue-property plots

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: 23S rRNA



G	U1807	G1719	U1626	G1545	G1462	G1377	G1281	U1193	U1129	G1068	A991	A925	A841
C	U	C1720	U1629	G1546	C1463	G1378	A1286	A1194	A1130	U1069	G992	G	C842
C	A	A1724	G1630	U1554	A1464	U1379	A1287	A1197	A1131	A1072	A993	C	C843
C	C	U1725	A1631	A1555	A1473	U1380	U1288	C1198	A1132	A1073	G	C	A847
U	C	G1726	G1632	A1556	C1474	G1381	U1289	C1199	G1133	A1074	U995	C	G848
U	A	A1727	G1633	A1557	C1475	U1382	U1290	A1201	G1134	A1075	G996	C	G849
A	A	A1735	U1634	G1558	G1479	C1384	A1291	A1202	C987	G1076	C	C	
C	A1814	A1736	A1638	C1559	A1480	U1388	A1292	G1203	G998	G1077	C	C	G852
C	A1815	G1744	G1639	U1560	G1481	A1403	A1293	C1204	A999	U1078	C	C	C853
G	C1817	G1739	U1661	G1561	G1482	A1404	A1294	U1205	U1001	A1079	U	U	U854
U	A1818	G1740	A1662	A1562	A1483	A1405	A1295	G1206	G1002	G1080	C	C	G855
A	G1819	A1743	A1648	G1563	U1484	U1391	G1296		G1003	U1081	C	C	U856
A	A1820	G1745	C1649	C1564	A1485	A1392	C1297		A1004	G1082	C	C	U857
G		A1746	G1650	U1565	G1488	A1406			A1005	U1083	C	C	U858
C	C1829	G1747	C1652	U1566	A1491				A1006	G1084	C	C	C859
A	G1830		A1653	U1567					G1007	U1085	U	U	U860
A	A1831	G1752	A1654	G1568	G1494	C1409			A1008	U1086	A	A	C861
C	U1835	C1755	A1655	U1569	C1495				U1009	U1087	C	C	A866
G		U1756	G1660	G1570	G1496				C1010	G1088	C	C	U874
C	C1842	G1757	C1661	G1571	G1497	U1414			C1011	C1089			U875
C	G1843	U1758	A1662	G1572	U1498	A1221			U1012	C1090			A876
A	A1844	U1759	C1662	G1573	A1499	A1222			U1013	U1091			G877
A	A1845		A1667	A1574	U1500	C1223			A1014	A1092			G878
U				G1575	U1501				G1015				
U				C1577	G1502	G1227							
U	A1848	G1762	G1673	G1578	A1423				A1019	G1093			
G			G1674	G1579	A1424	G1231			A1020	C1095			A882
A	G1857	G1765	A1675	A1580	C1425	G1232				U1095			C885
A	A1858		G1676	A1581	U1506				A1027	G1096			
C		U1768		U1582	G1427	U1240			C1028	U1097			U892
C	C1861	G1769	A1679	A1583	G1428	C1241			A1029	C1098			A893
C	U1862	C1770	A1680	A	C1508	U1242			G1030	C1099			A894
C	U1863	G1771	U1681	U1584	C1509	A1244				A1100			U900
C			A1585	U1585		G1245			A1034	A1034			U901
C		A1774	G1682	G1586	A1434	G1246			C959	G1101			G902
C		G1775	C1683	U1587	U1435	C1247			U960	G1102			G903
U		A1776	U1684	U1588	U1436	G1248			C961	A1036			A904
A	G	G1777	A1685		C1437	C1249			C962	C1037			G905
A	A	U1778			U1438	U1249			G963				G906
A	A	G1779	G1688	A1592	U1440	G1250			A964	C1040			U907
C		C1780	U1689	U1595	G1441	U1251			A965	A1042			A908
C		G1781	G1690	U1596	A1442	G1252			G967	G1043			G909
G		U1782	A1691		C1443	C1257			C968	C1044			A910
C		C1783	G1692	G1600	G1444	U1258			C969	C1051			G911
C		A1784	C1693	A1601	A1445	A1259			A970	C1052			C912
G		G1785		U1602		A1260			A971	C1053			A913
C			G1696	U1603	A1524				U972	A1054			C914
C		A1791	A1697	U1607	G1525	G1263			G973	A1055			U915
C		G1792	G1698	C1607	U1448	G1264			A974	U1058			G916
U		G1793	A1699	A1608	C1449	U1265			C975	C1059			A917
U		C1794		C1609	C1450	G1264			U976	A1059			U918
A			G1711		U1455	U1274			C				U919
A		G1801	G1712	C1613	A1456	G1275			U1063				U920
U		A1802	A1713	U1457	U1457	G1276			U1064				G921
A		C1803	A1714	U1458	U1277	A1277			U1065				A922
U		U1804	A1615	U1459	G1278	G1279			C980				C923
A		G1805	G1616	G1460	C1279	G1280			A1067				U924
A		U1806	A1617	G1461	A1375				A987				
A			A1618		G1376								

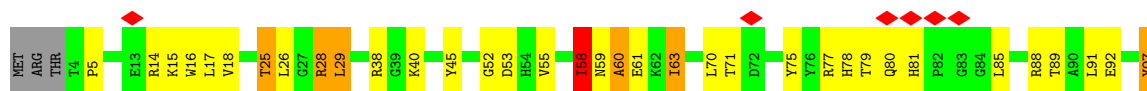


• Molecule 2: 5S rRNA

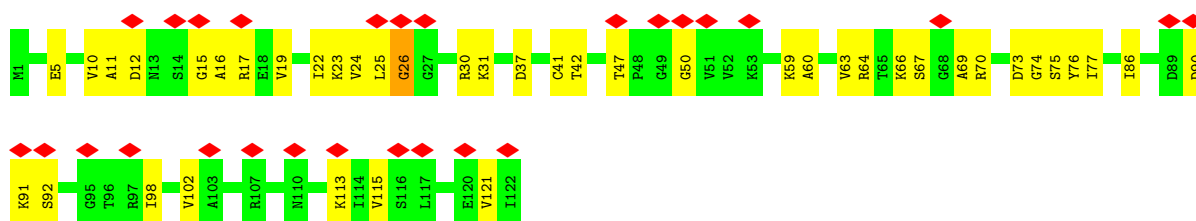




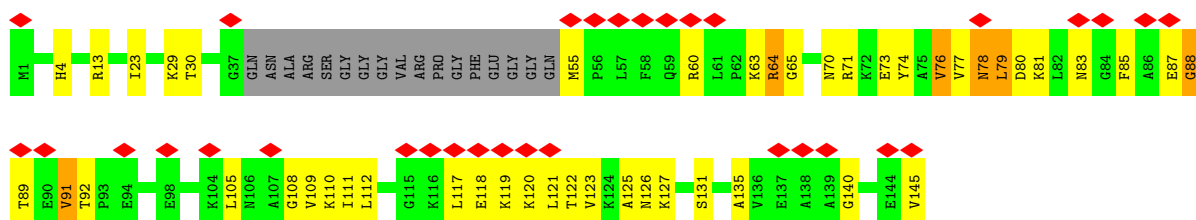
- Molecule 6: 50S ribosomal protein L13



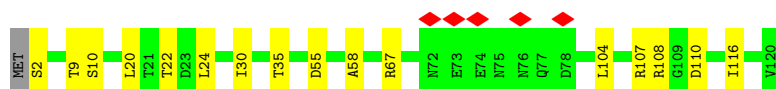
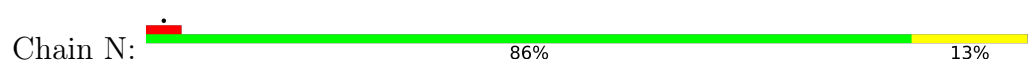
- Molecule 7: 50S ribosomal protein L14



- Molecule 8: 50S ribosomal protein L15

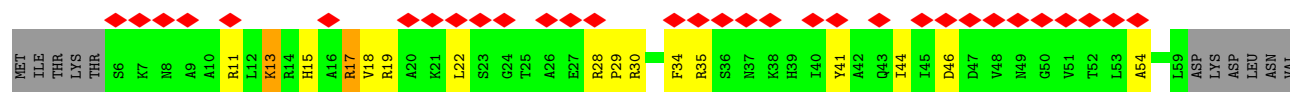


- Molecule 9: 50S ribosomal protein L17

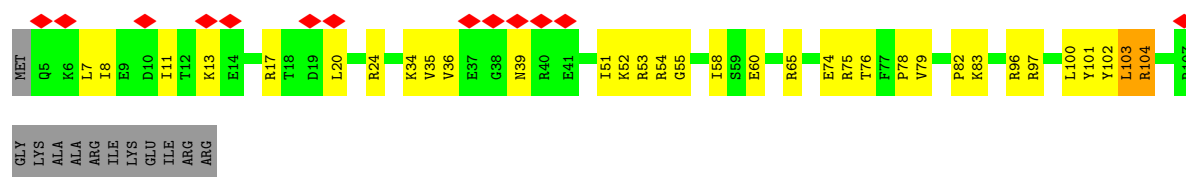


- Molecule 10: 50S ribosomal protein L18

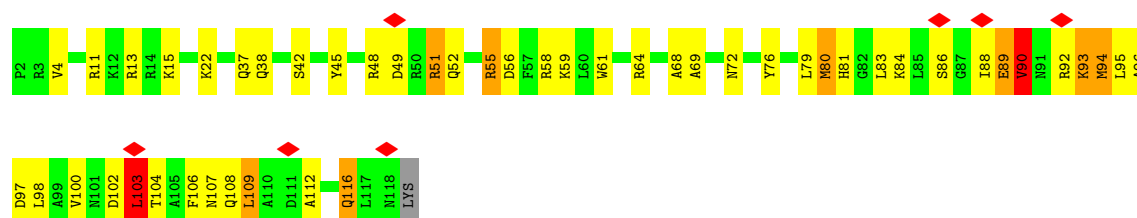




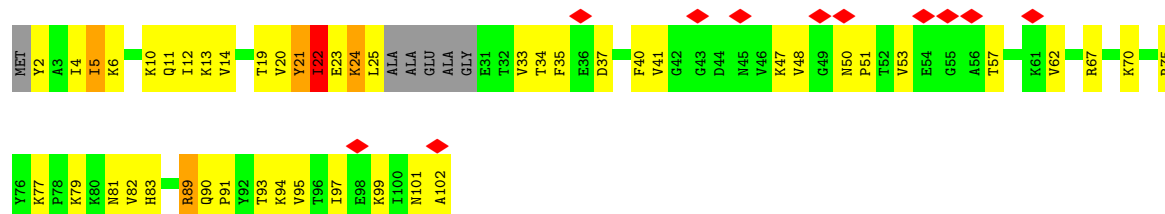
• Molecule 11: 50S ribosomal protein L19



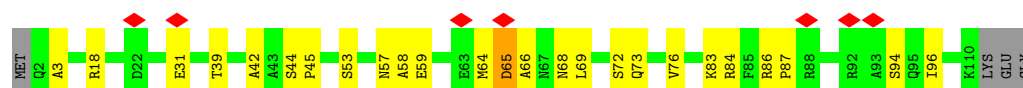
• Molecule 12: 50S ribosomal protein L20



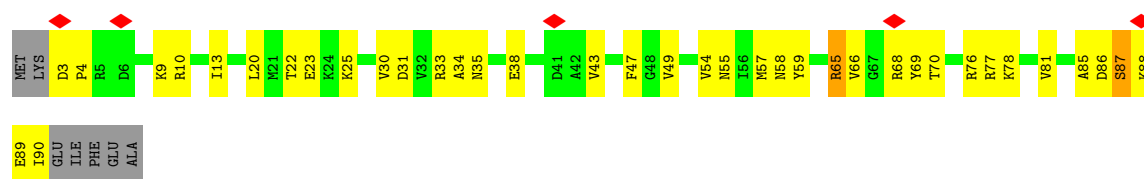
• Molecule 13: 50S ribosomal protein L21



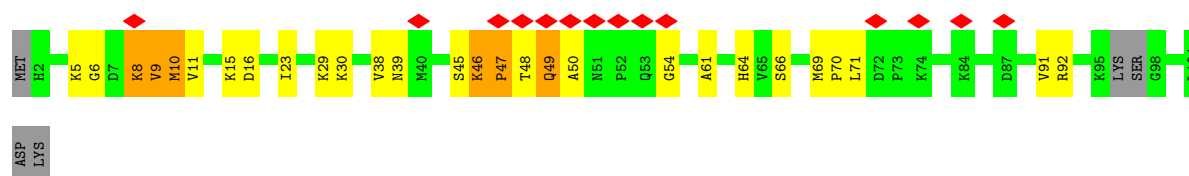
• Molecule 14: 50S ribosomal protein L22



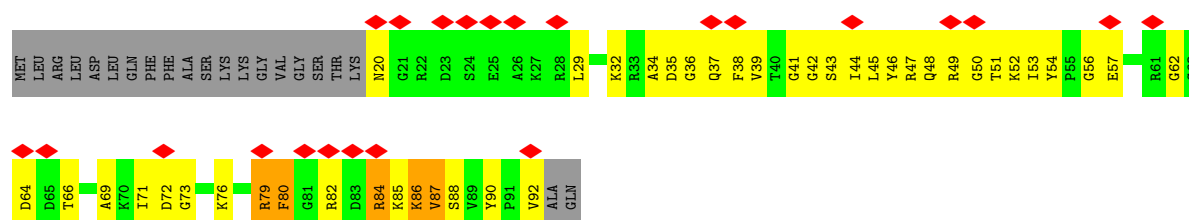
• Molecule 15: 50S ribosomal protein L23



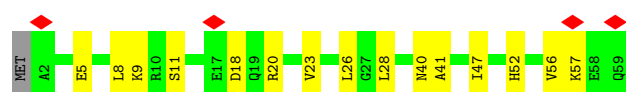
- Molecule 16: 50S ribosomal protein L24



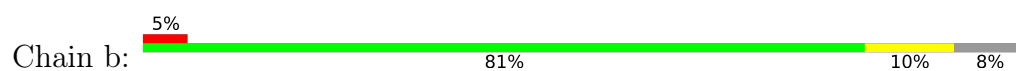
- Molecule 17: 50S ribosomal protein L27



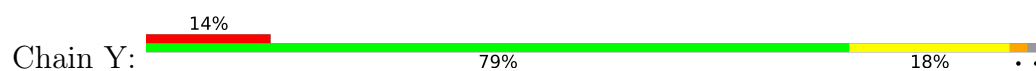
- Molecule 18: 50S ribosomal protein L30



- Molecule 19: 50S ribosomal protein L32



- Molecule 20: 50S ribosomal protein L29





• Molecule 21: 50S ribosomal protein L34



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	546297	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.640	Depositor
Minimum map value	-0.343	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0732	Depositor
Map size (Å)	360.52798, 360.52798, 360.52798	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.073, 1.073, 1.073	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.77	0/59472	1.00	137/92759 (0.1%)
2	B	0.33	0/2678	0.94	3/4174 (0.1%)
3	C	0.33	0/1709	0.53	2/2296 (0.1%)
4	D	0.35	0/1276	0.64	3/1709 (0.2%)
5	E	0.32	0/1501	0.60	4/2025 (0.2%)
6	J	0.36	0/1142	0.60	2/1537 (0.1%)
7	K	0.33	0/927	0.54	0/1245
8	L	0.29	0/961	0.78	7/1281 (0.5%)
9	N	0.40	0/960	0.54	0/1284
10	O	0.24	0/799	0.67	3/1070 (0.3%)
11	P	0.35	0/859	0.52	0/1152
12	Q	0.39	0/952	0.63	2/1266 (0.2%)
13	R	0.39	0/768	0.67	2/1029 (0.2%)
14	S	0.34	0/851	0.50	0/1146
15	T	0.36	0/713	0.46	0/951
16	U	0.34	0/748	0.51	0/1000
17	V	0.20	0/563	0.33	0/753
18	Z	0.33	0/457	0.54	0/613
19	b	0.34	0/433	0.45	0/574
20	Y	0.31	0/531	0.47	0/707
21	d	0.39	0/370	0.49	0/483
All	All	0.69	0/78670	0.94	165/119054 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
12	Q	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Q	103	LEU	CB-CA-C	15.54	139.72	110.20
1	A	1433	U	C2-N1-C1'	12.62	132.85	117.70
10	O	90	ILE	CB-CA-C	-12.23	87.14	111.60
8	L	85	PHE	CB-CA-C	-12.23	85.95	110.40
1	A	961	C	N1-C2-O2	11.32	125.69	118.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	56	LYS	Peptide
12	Q	103	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	53094	0	26707	695	0
2	B	2395	0	1212	52	0
3	C	1684	0	1754	81	0
4	D	1265	0	1332	102	0
5	E	1484	0	1565	80	0
6	J	1119	0	1159	47	0
7	K	920	0	977	54	0
8	L	952	0	1002	104	0
9	N	953	0	983	12	0
10	O	791	0	824	39	0
11	P	846	0	902	54	0
12	Q	940	0	1005	123	0
13	R	758	0	801	97	0
14	S	842	0	899	27	0
15	T	707	0	751	35	0
16	U	739	0	790	41	0
17	V	555	0	540	81	0
18	Z	455	0	491	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	b	426	0	445	0	0
20	Y	530	0	568	20	0
21	d	367	0	410	0	0
22	A	13	0	0	0	0
All	All	71835	0	45117	1512	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 1512 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)
12:Q:61:TRP:CZ2	12:Q:94:MET:HB2	1.27	1.60
12:Q:95:LEU:HD22	13:R:11:GLN:CB	1.28	1.57
1:A:901:U:H2'	1:A:902:G:C8	1.36	1.56
1:A:2465:G:H2'	1:A:2466:C:C5'	1.38	1.52
12:Q:95:LEU:CD2	13:R:11:GLN:HB3	1.30	1.52

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	
3	C	219/277 (79%)	199 (91%)	20 (9%)	0	100	100
4	D	161/209 (77%)	138 (86%)	20 (12%)	3 (2%)	8	31
5	E	188/207 (91%)	159 (85%)	28 (15%)	1 (0%)	29	61
6	J	139/145 (96%)	122 (88%)	14 (10%)	3 (2%)	6	29
7	K	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	19	51
8	L	124/145 (86%)	115 (93%)	6 (5%)	3 (2%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	N	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
10	O	100/120 (83%)	92 (92%)	7 (7%)	1 (1%)	15	46
11	P	101/115 (88%)	92 (91%)	9 (9%)	0	100	100
12	Q	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	17	49
13	R	92/102 (90%)	77 (84%)	15 (16%)	0	100	100
14	S	107/113 (95%)	100 (94%)	7 (6%)	0	100	100
15	T	86/95 (90%)	79 (92%)	7 (8%)	0	100	100
16	U	94/103 (91%)	82 (87%)	9 (10%)	3 (3%)	4	22
17	V	71/94 (76%)	62 (87%)	8 (11%)	1 (1%)	11	37
18	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
19	b	52/59 (88%)	47 (90%)	4 (8%)	1 (2%)	8	31
20	Y	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
21	d	42/44 (96%)	42 (100%)	0	0	100	100
All	All	2047/2313 (88%)	1844 (90%)	185 (9%)	18 (1%)	21	49

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	O	102	TYR
4	D	93	VAL
6	J	59	ASN
7	K	26	GLY
12	Q	90	VAL

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	
3	C	177/225 (79%)	168 (95%)	9 (5%)	24	54
4	D	135/170 (79%)	115 (85%)	20 (15%)	3	12
5	E	162/170 (95%)	148 (91%)	14 (9%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J	120/123 (98%)	113 (94%)	7 (6%)	20	50
7	K	101/101 (100%)	100 (99%)	1 (1%)	76	88
8	L	98/109 (90%)	92 (94%)	6 (6%)	18	48
9	N	99/100 (99%)	99 (100%)	0	100	100
10	O	78/93 (84%)	71 (91%)	7 (9%)	9	32
11	P	91/100 (91%)	87 (96%)	4 (4%)	28	58
12	Q	96/97 (99%)	83 (86%)	13 (14%)	4	14
13	R	82/84 (98%)	75 (92%)	7 (8%)	10	35
14	S	90/93 (97%)	87 (97%)	3 (3%)	38	66
15	T	79/85 (93%)	74 (94%)	5 (6%)	18	47
16	U	82/87 (94%)	78 (95%)	4 (5%)	25	55
17	V	54/74 (73%)	44 (82%)	10 (18%)	1	5
18	Z	52/53 (98%)	52 (100%)	0	100	100
19	b	48/53 (91%)	43 (90%)	5 (10%)	7	25
20	Y	56/57 (98%)	55 (98%)	1 (2%)	59	79
21	d	39/39 (100%)	39 (100%)	0	100	100
All	All	1739/1913 (91%)	1623 (93%)	116 (7%)	20	46

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	O	13	LYS
19	b	35	GLU
12	Q	80	MET
17	V	87	VAL
16	U	49	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
10	O	103	HIS
13	R	81	ASN
17	V	37	GLN
12	Q	37	GLN
14	S	60	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2458/2927 (83%)	792 (32%)	50 (2%)
2	B	111/119 (93%)	45 (40%)	3 (2%)
All	All	2569/3046 (84%)	837 (32%)	53 (2%)

5 of 837 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	13	A
1	A	15	G
1	A	23	G

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1245	G
1	A	1527	C
1	A	2812	A
1	A	1250	G
1	A	1362	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

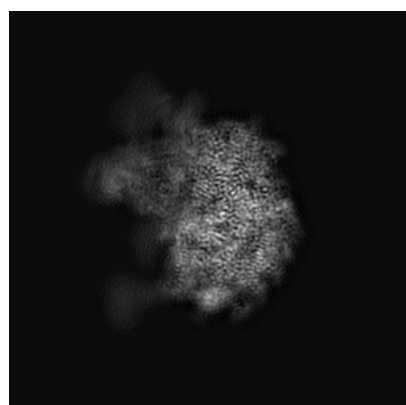
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20435. These allow visual inspection of the internal detail of the map and identification of artifacts.

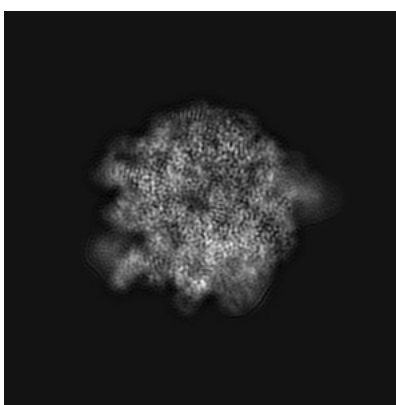
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

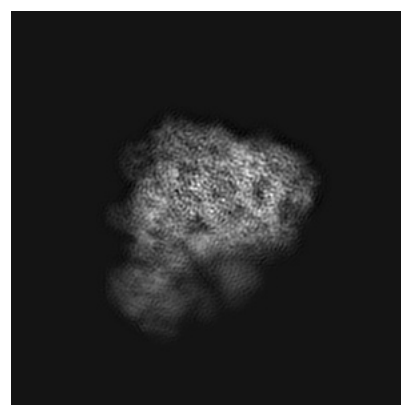
6.1.1 Primary map



X



Y

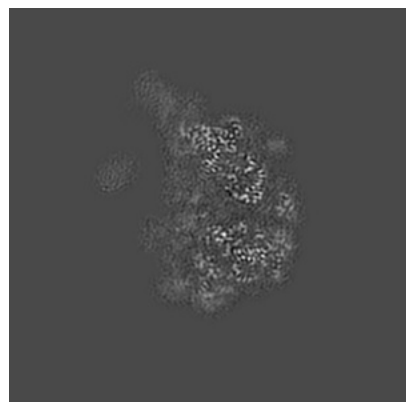


Z

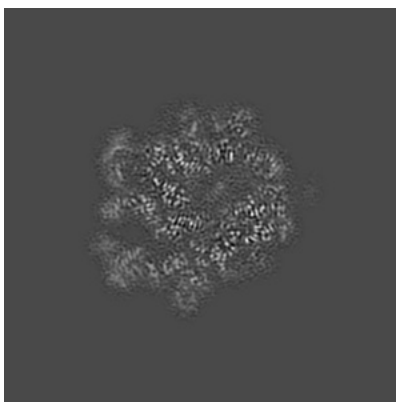
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

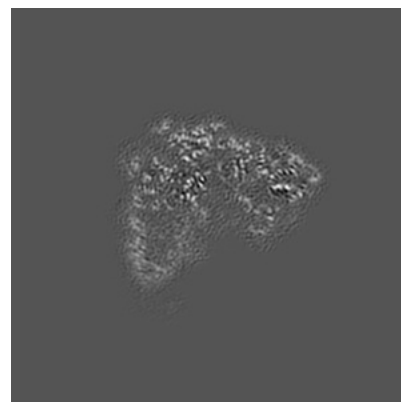
6.2.1 Primary map



X Index: 168



Y Index: 168

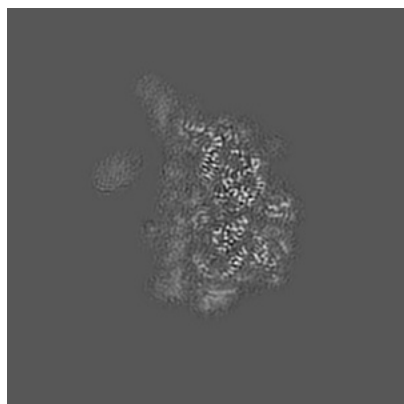


Z Index: 168

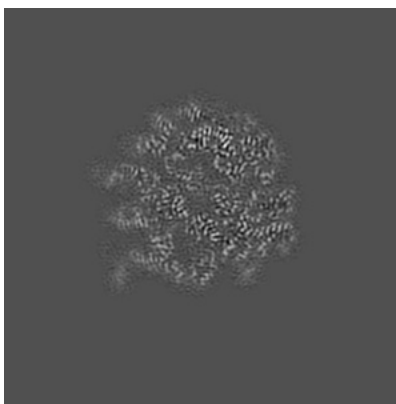
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

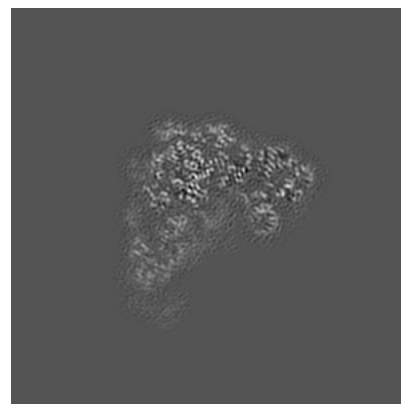
6.3.1 Primary map



X Index: 164



Y Index: 185

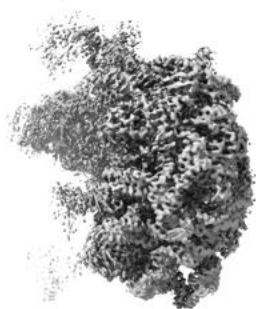


Z Index: 173

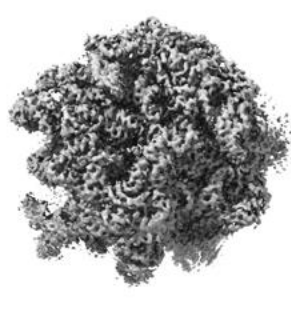
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0732. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

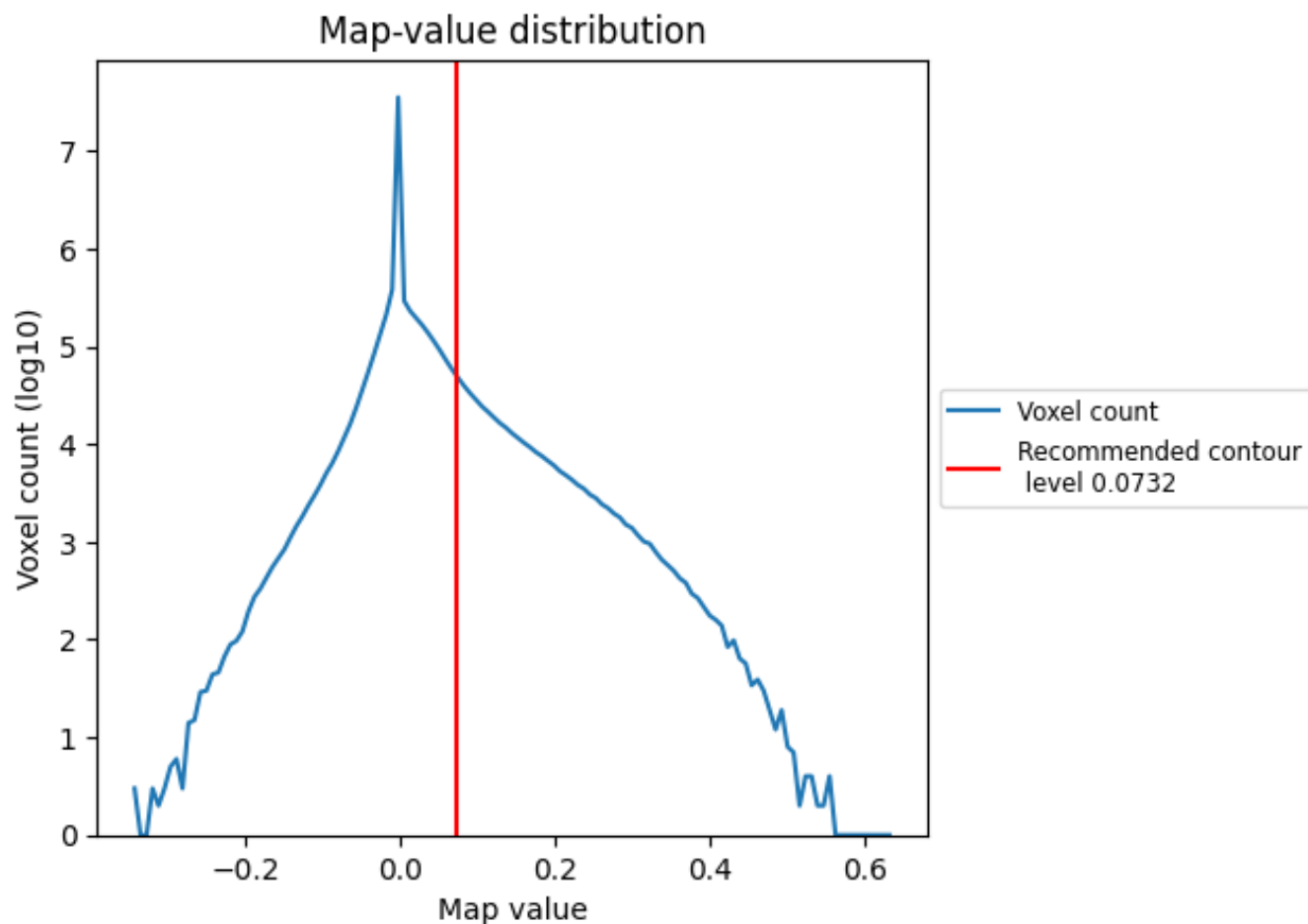
6.5 Mask visualisation

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

7 Map analysis [i](#)

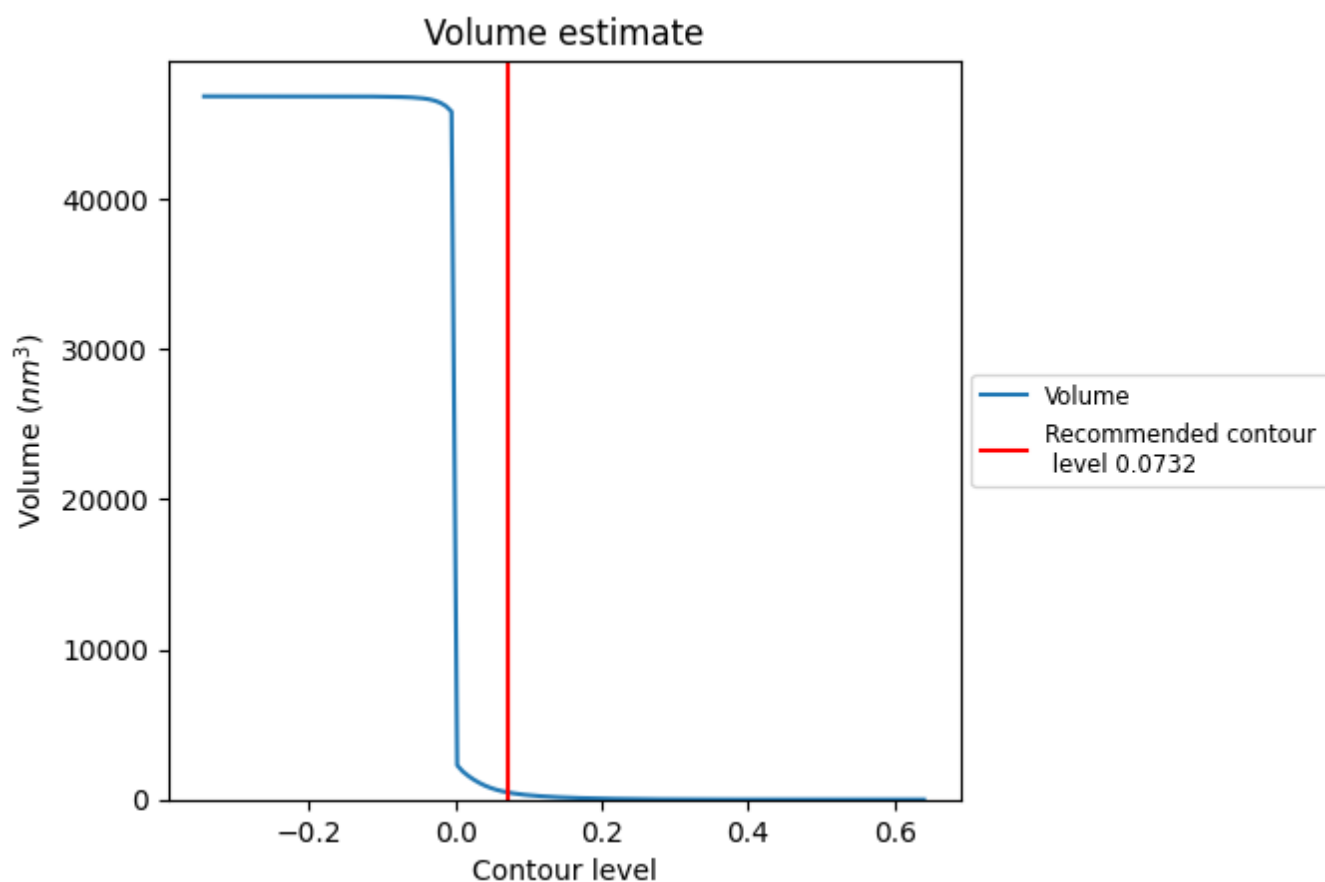
This section contains the results of statistical analysis of the map.

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.

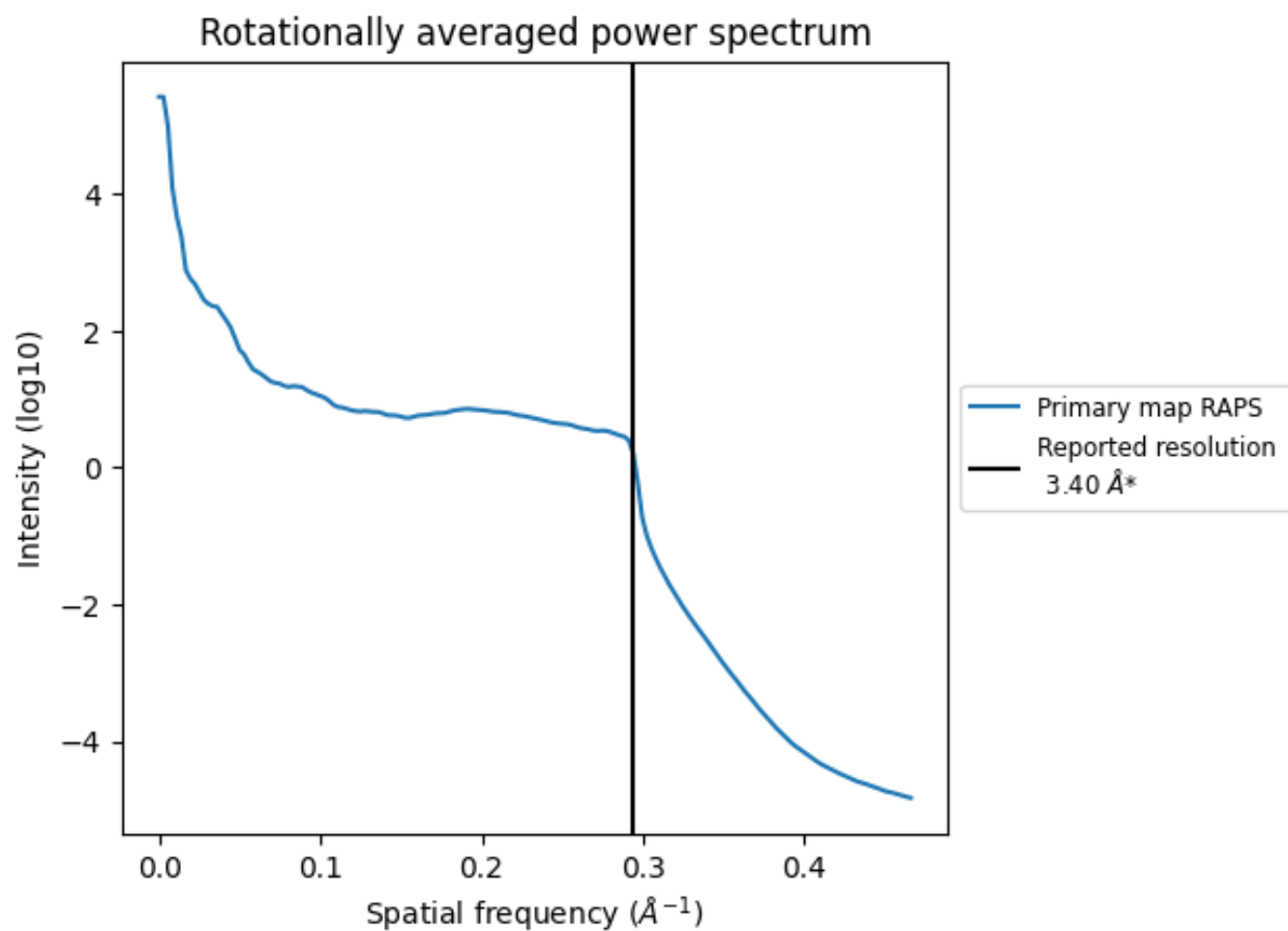
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 466 nm³; this corresponds to an approximate mass of 421 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 ⓘ

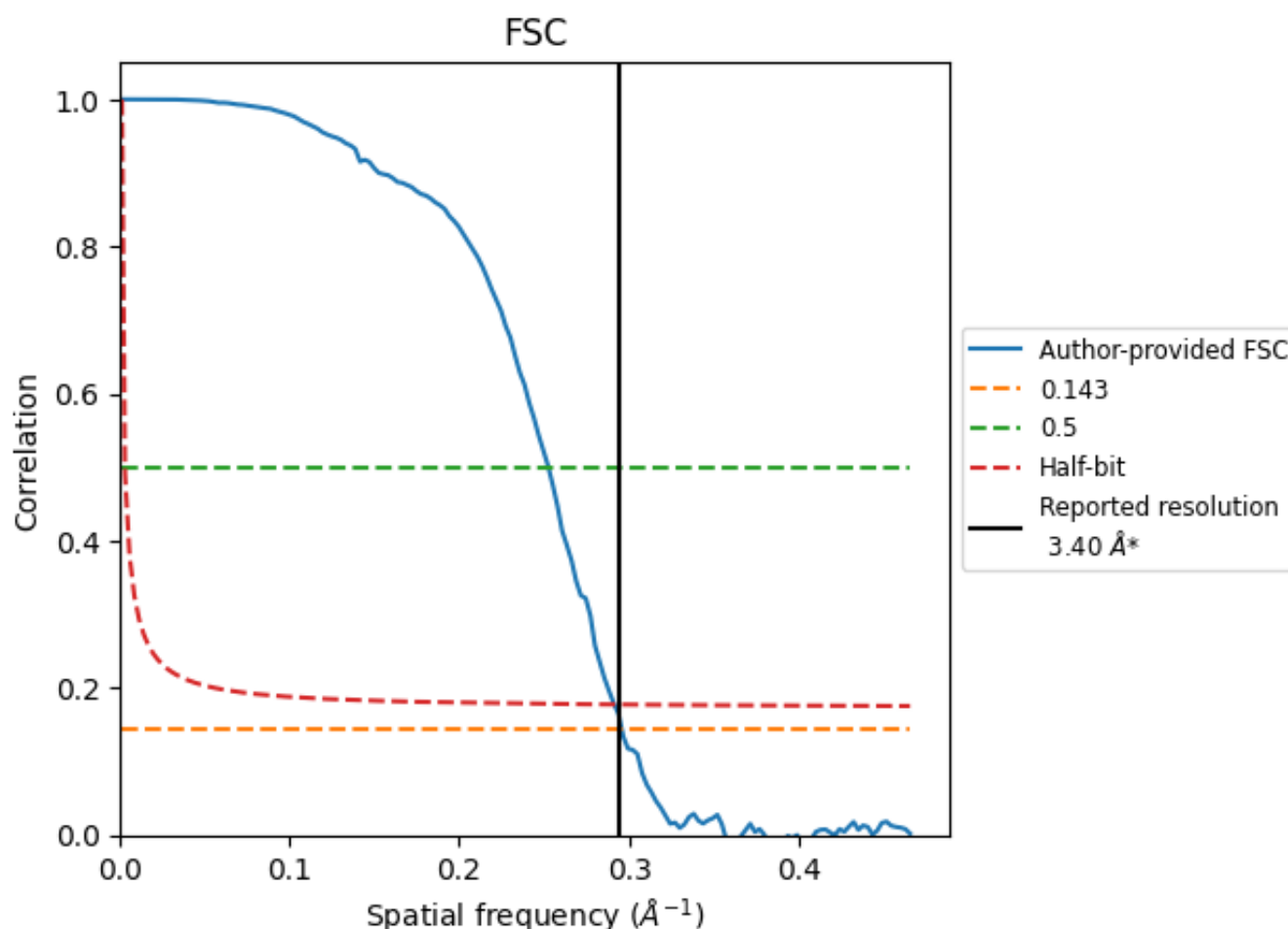


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

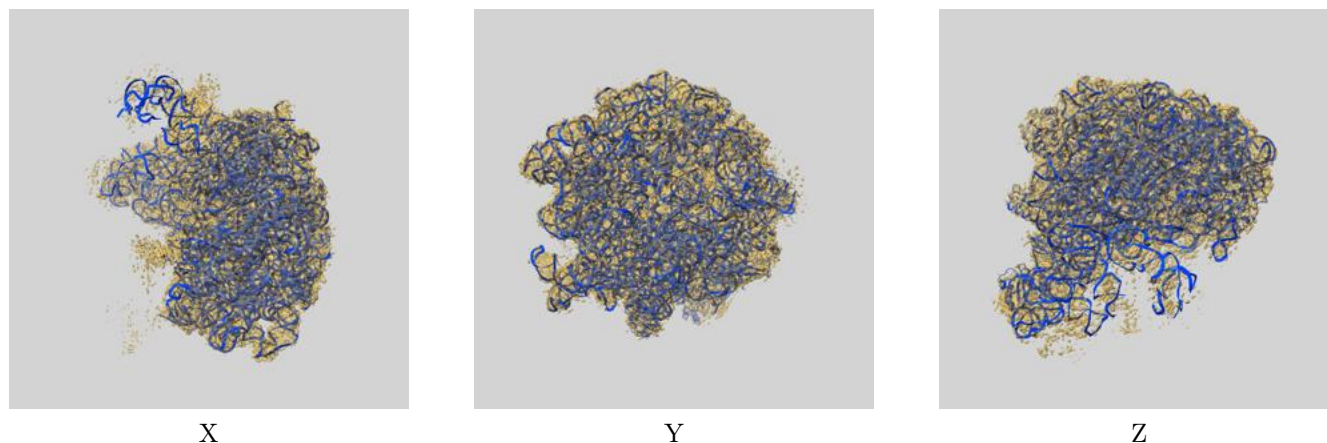
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	3.96	3.43
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

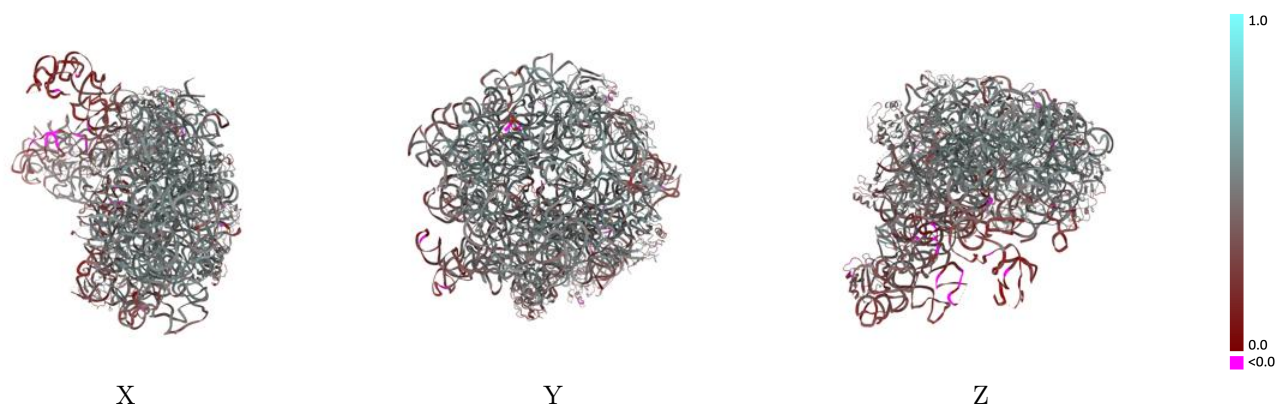
This section contains information regarding the fit between EMDB map EMD-20435 and PDB model 6PPF. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



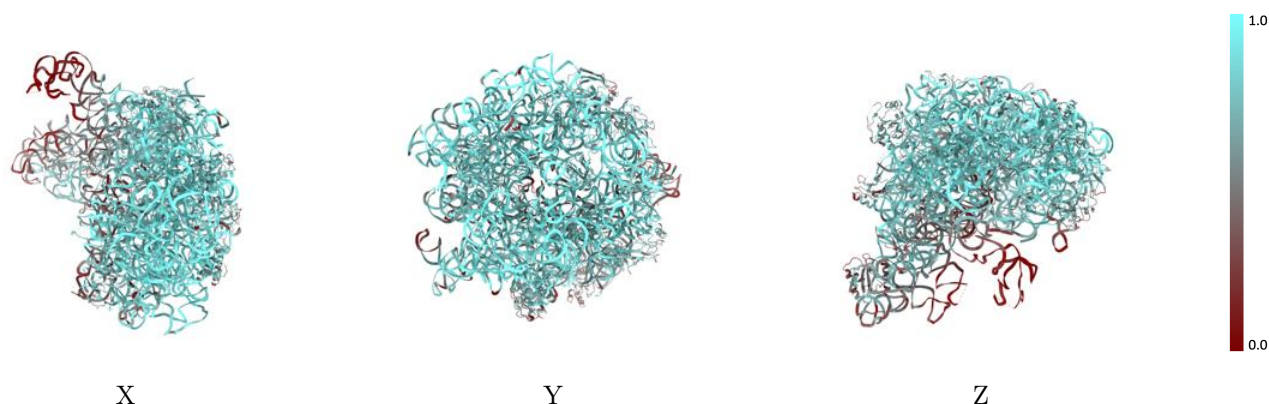
The images above show the 3D surface view of the map at the recommended contour level 0.0732 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



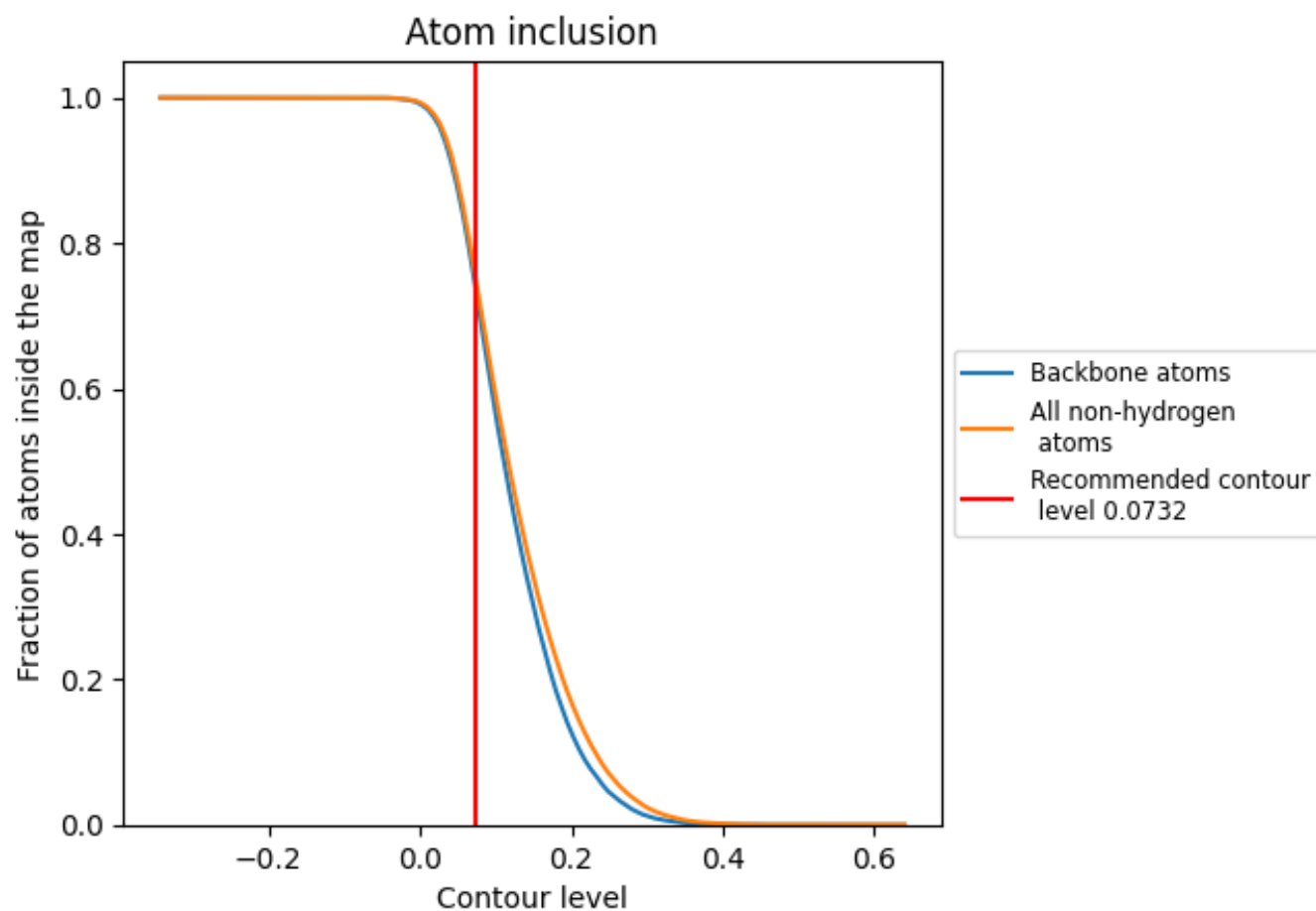
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0732).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.0732) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7551	 0.4360
A	 0.7926	 0.4390
B	 0.4919	 0.2950
C	 0.6977	 0.4540
D	 0.7242	 0.4550
E	 0.6845	 0.4380
J	 0.7541	 0.4760
K	 0.5842	 0.4320
L	 0.5827	 0.4040
N	 0.7950	 0.5070
O	 0.3551	 0.2810
P	 0.6732	 0.4300
Q	 0.7767	 0.4730
R	 0.6925	 0.4500
S	 0.7582	 0.4970
T	 0.7230	 0.4630
U	 0.6434	 0.4180
V	 0.4907	 0.3820
Y	 0.6537	 0.4400
Z	 0.6966	 0.4780
b	 0.7433	 0.4760
d	 0.7913	 0.5210

