



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 05:06 PM UTC

PDB ID : 9HA4 / pdb_00009ha4
EMDB ID : EMD-51976
Title : Pooled 50S subunit C-CP_(L22)- precursor states supplemented with Api137
Authors : Lauer, S.; Nikolay, R.; Spahn, C.M.T.
Deposited on : 2024-11-01
Resolution : 4.26 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:

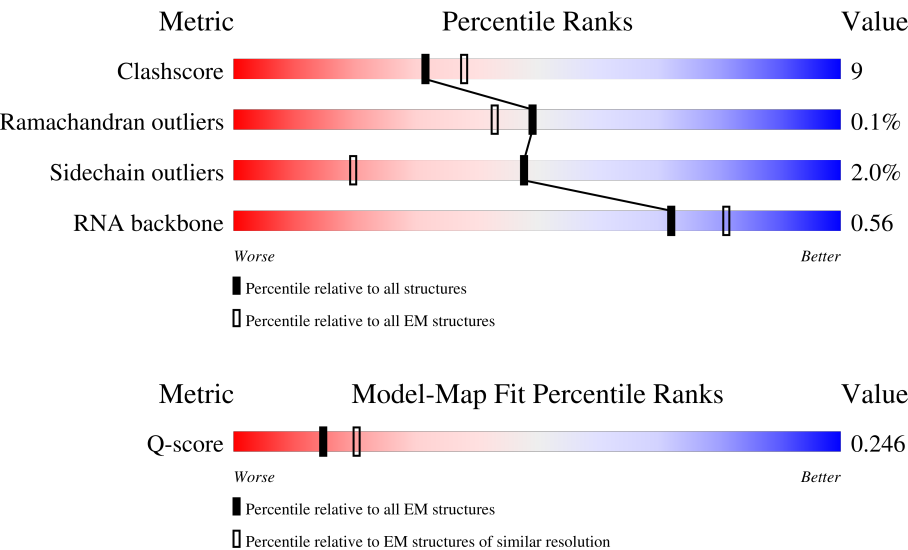
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.26 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4601 (3.76 - 4.76)

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	2	46	9% 65% 22% 13%
2	B	120	52% 43% • •
3	D	209	52% 5% 44%

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Mol	Chain	Length	Quality of chain
4	F	177	
5	J	142	
6	K	122	
7	N	120	
8	O	116	
9	P	114	
10	Q	117	
11	R	103	
12	T	93	
13	U	102	
14	V	94	
15	W	75	
16	Y	63	
17	Z	58	
18	y	17	
19	A	2903	
20	E	201	
21	L	143	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 60234 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 Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	40	Total	C	N	O	S	0	0
			322	193	79	49	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	118	Total	C	N	O	S	0	0
			887	560	156	169	2		

- Molecule 4 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 5 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL14.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	111	Total	C	N	O	S	0	0
			882	548	174	156	4		

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 9 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 10 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 11 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 13 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 14 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 15 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	69	Total	C	N	O	S	0	0
			522	328	103	90	1		

- Molecule 16 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	61	Total	C	N	O	S	0	0
			499	308	97	92	2		

- Molecule 17 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 18 is a protein called Apidaecins type 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	y	17	Total	C	N	O	0	0
			148	94	33	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	10	ARG	GLN	conflict	UNP P35581

- Molecule 19 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	1977	Total	C	N	O	P	0	0
			42496	18957	7879	13683	1977		

- Molecule 20 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	168	Total	C	N	O	S	0	0
			1307	824	231	247	5		

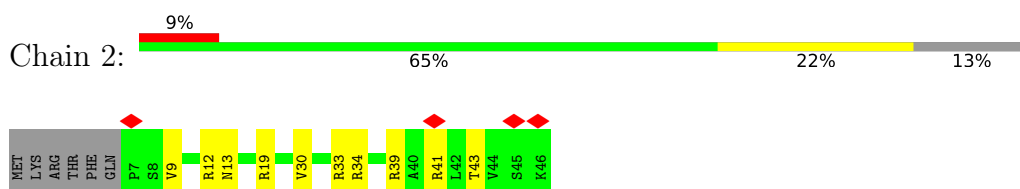
- Molecule 21 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	L	118	Total	C	N	O	0	0
			850	530	163	157		

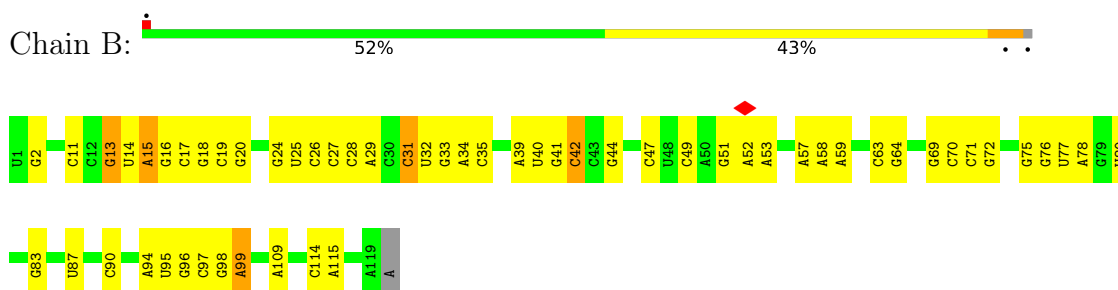
3 Residue-property plots

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.

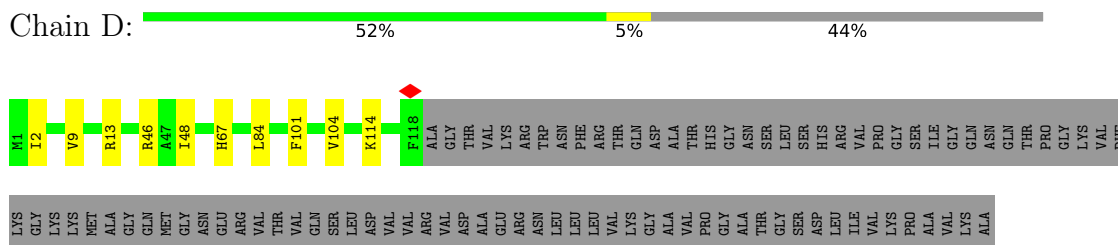
- Molecule 1: Large ribosomal subunit protein bL34



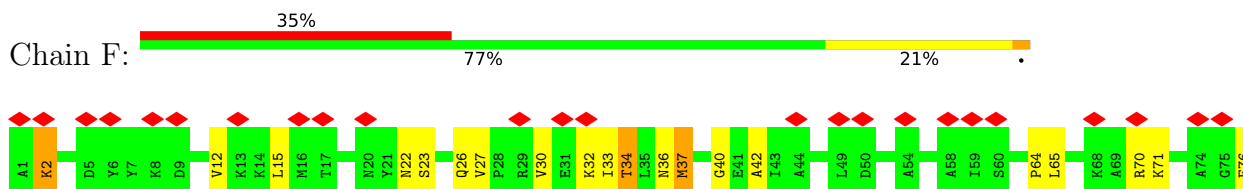
- Molecule 2: 5S ribosomal RNA

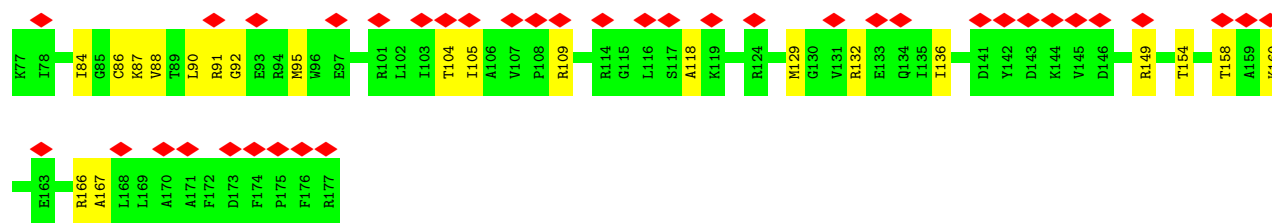


- Molecule 3: 50S ribosomal protein L3

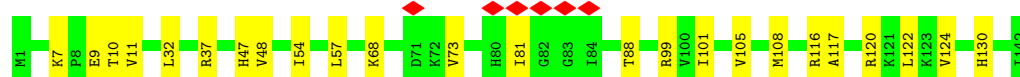
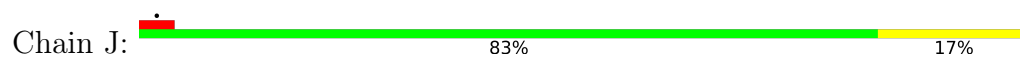


- Molecule 4: Large ribosomal subunit protein uL5

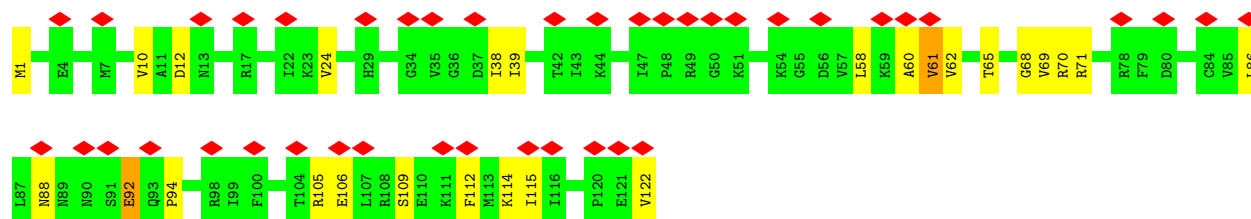
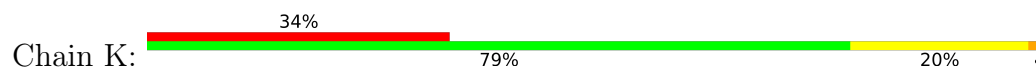




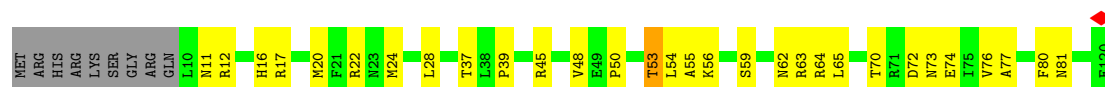
- Molecule 5: Large ribosomal subunit protein uL13



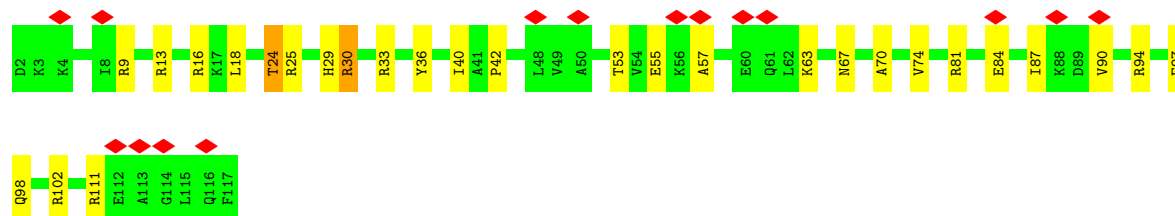
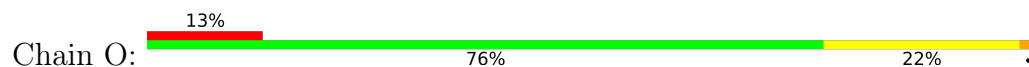
- Molecule 6: Large ribosomal subunit protein uL14



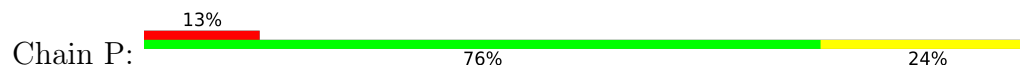
- Molecule 7: Large ribosomal subunit protein bL17

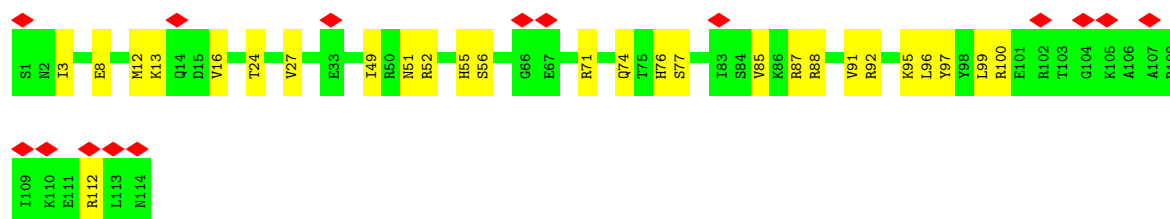


- Molecule 8: Large ribosomal subunit protein uL18

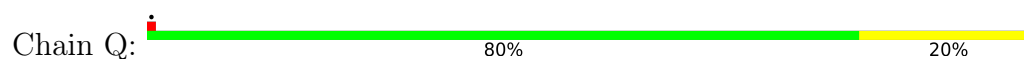


- Molecule 9: Large ribosomal subunit protein bL19

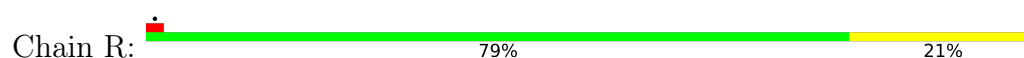




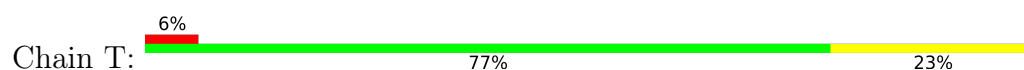
- Molecule 10: Large ribosomal subunit protein bL20



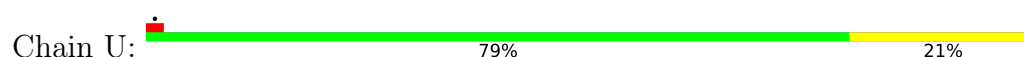
- Molecule 11: Large ribosomal subunit protein bL21



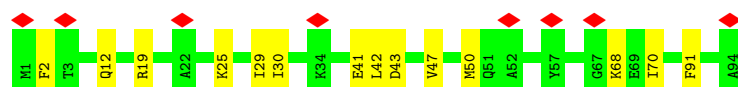
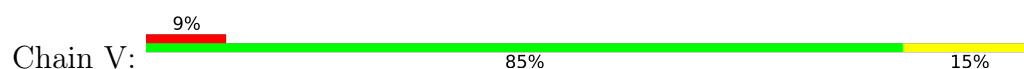
- Molecule 12: Large ribosomal subunit protein uL23



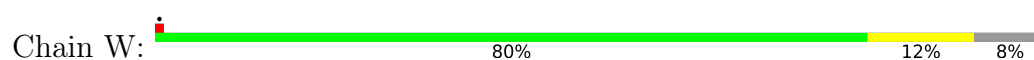
- Molecule 13: Large ribosomal subunit protein uL24



- Molecule 14: Large ribosomal subunit protein bL25



- Molecule 15: Large ribosomal subunit protein bL27





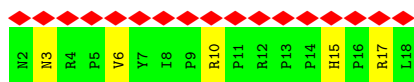
- Molecule 16: Large ribosomal subunit protein uL29



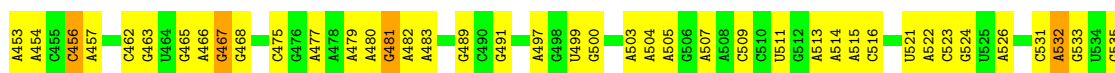
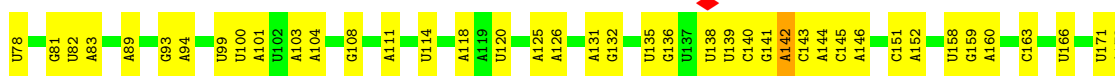
- Molecule 17: Large ribosomal subunit protein uL30



- Molecule 18: Apidaecins type 22

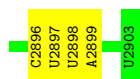


- Molecule 19: 23S ribosomal RNA

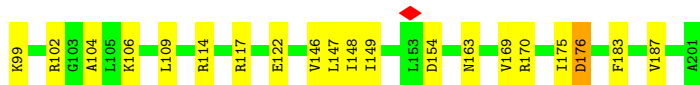
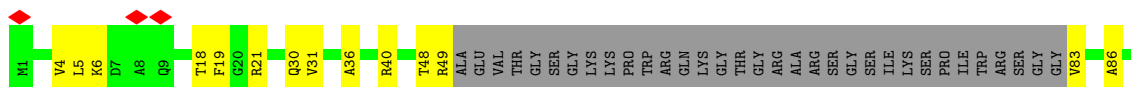


G1601	U1506	U1415	C1330	A1244	C1167	U	G	C965	U	G818	A	C	G	A614	G536
U1602	G1510	G1416	G1331	G1245	G1168	C	G	G966	C	A819	A	U	C	U615	A537
A1603	G1510	G1417	G1332	A1246	G1171	A	C	U967	C	C923	U	C	G	A616	A538
C1604	G1514	G1418	G1333	A1247	C1172	C	C	C968	C	A825	G	G	G	G622	C540
C1605	G1514	A1419	G1334	G1248	U1173	U	C	G969	A	U828	C	C	C	A627	A541
C1606	A1515	G1421	A1336	A1253	U1174	G	G	G971	C	U829	C	C	C	G643	C542
C1607	C1518	G1422	G1337	A1254	A1175	U	C	G974	U	A828	G	G	A	U546	G549
A1608	G1519	G1423	G1338	U1255	U1176	C	C	A975	C	A830	G	G	G	G628	C550
A1609	U1520	G1424	G1339	G1256	G1177	G	A	G976	A	G831	U	U	A	G629	G551
A1610	G1521	G1425	U1340	A1262	C1178	A	G	G977	C	U832	U	C	G	G630	U552
A1616	G1522	G1426	G1341	U1263	G1179	C	C	A981	C	A833	G	C	C	A631	U554
G1619	U1523	C1427	G1342	U1264	U1180	U	A	G982	A	G834	C	A	A	G632	G548
G1620	G1524	G1428	U1343	A1265	U1181	C	C	A983	C	U839	U	U	C	A633	C549
U1629	A1528	G1432	G1344	G1266	G1186	G	G	A984	C	U840	C	C	G	C634	C550
A1630	C1533	A1433	G1345	U1267	G1187	G	G	C987	C	G841	U	U	G	A637	U551
G1631	U1534	G1434	U1346	A1268	U1188	C	U	A988	C	U842	G	G	U	G638	G553
A1632	A1535	G1435	C1350	G1271	A1189	U	A	G989	U	G843	G	A	U	U639	U554
A1634	C1536	U1438	G1355	A1272	G1190	C	U	C995	G	A844	C	C	G	A643	G555
A1634	C1537	A1439	G1356	G1277	G1187	G	G	G996	C	U845	U	U	C	A644	A556
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A1634	A1539	G1453	G1358	G1279	A1189	U	A	C998	C	U847	U	A	A	C646	G561
A1634	A1359	A1453	A1359	G1279	G1190	G	U	C999	U	G848	G	C	C	U646	U562
A1637	G1538	U1458	A1365	U1282	C1200	C	G	C995	G	U849	G	C	C	G647	A563
C1638	U1539	C1458	U1372	U1287	U1201	A	A	G996	C	U850	U	U	A	G648	C564
C1646	G1540	C1461	U1373	G1288	G1202	C	C	G997	C	U851	G	C	C	G649	G565
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G	A1551	A1469	U1378	G1292	A1213	U	C	C1007	C	G857	A	C	C	A655	U573
G	G1555	G1471	G1380	G1295	A1214	C	C	A1008	C	G858	G	U	U	A656	G579
G	G1560	C1472	G1381	G1296	C1217	C	C	A1009	C	G859	G	C	C	A657	U580
A	A	G1473	G1382	G1297	U1217	U	U	A1010	C	U931	U	C	C	U658	C581
C	U1566	U1474	G1383	C1298	G1218	C	C	U1011	C	U932	C	C	C	G664	A582
U	G1567	G1475	A1386	G1299	U1222	U	U	A1012	C	A933	A	A	A	U665	G583
C	G1568	U1481	C1387	G1300	G1223	U	U	A1020	C	G939	A	C	C	A666	A586
G	A1569	G1482	A1387	A1301	U1224	U	U	G1022	C	U940	C	C	C	G669	U588
G	A1570	U1483	G1388	G1311	G1225	A	A	U1023	C	A941	C	C	C	C672	U596
U	A1571	U1484	A1392	U1312	A1226	A	A	G1024	C	A945	C	C	C	C673	G597
U	G1572	U1485	A1393	U1313	G1227	A	A	G1025	C	C946	C	C	C	G674	U598
A	C1574	U1486	U1394	C1314	G1228	G	G	A1026	C	G947	C	C	C	A675	A599
A	C1575	C1488	A1395	C1315	C1229	A	A	A1027	C	C	C	C	C	C680	G600
G	U1576	C1489	A1396	U1316	U1230	A	A	A1028	C	U	C	C	C	C681	C601
A	C1577	A1490	C1398	G1317	U1231	C	C	G1031	C	A	A	A	A	G684	A603
A	G1581	G1491	G1401	C1320	G1232	G	G	A	C	G808	C	C	C	A	G605
C	C1582	G1492	U1402	A1321	G1233	C	C	U	C	G809	C	C	C	U	C
A	A1583	C1493	U1406	A1322	U1234	U	U	U	C	U810	C	C	C	U	C
G	U1584	A1496	U1407	C1323	G1235	U	U	U	C	G	C	C	C	U	C
C	C1585	C1497	G1407	A1324	U1236	A	A	U	C	G	C	C	C	U	C
A	A1586	U1498	U1412	G1325	A1237	U	U	G	C	G	C	C	C	U	C
A	G1587	C1499	A1413	U1325	G1238	U	A	G	C	U957	C	C	C	U	C
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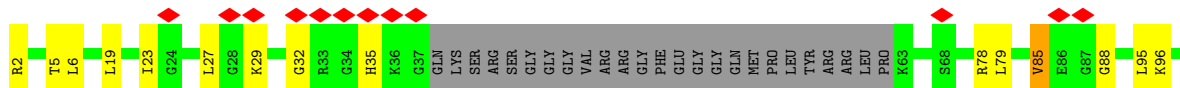




- Molecule 20: Large ribosomal subunit protein uL4



- Molecule 21: Large ribosomal subunit protein uL15



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31417	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 ($e^-/\text{\AA}^2$)	46.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.406	Depositor
Minimum map value	-0.124	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.068	Depositor
Map size (Å)	399.6, 399.6, 399.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332, 1.332, 1.332	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	2	0.09	0/324	0.23	0/424
2	B	0.07	0/2850	0.17	0/4444
3	D	0.08	0/898	0.20	0/1207
4	F	0.09	0/1435	0.25	0/1926
5	J	0.07	0/1152	0.18	0/1551
6	K	0.09	0/948	0.25	0/1268
7	N	0.10	0/894	0.29	0/1198
8	O	0.08	0/902	0.23	0/1209
9	P	0.07	0/929	0.21	0/1242
10	Q	0.08	0/960	0.19	0/1278
11	R	0.08	0/829	0.22	0/1107
12	T	0.10	0/745	0.30	0/994
13	U	0.09	0/788	0.26	0/1051
14	V	0.07	0/766	0.20	0/1025
15	W	0.07	0/529	0.19	0/699
16	Y	0.10	0/500	0.30	0/665
17	Z	0.07	0/453	0.19	0/605
18	y	0.15	0/155	0.38	0/212
19	A	0.07	0/47606	0.17	0/74262
20	E	0.08	0/1319	0.21	0/1775
21	L	0.09	0/854	0.35	0/1137
All	All	0.07	0/65836	0.19	0/99279

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	322	0	357	7	0
2	B	2549	0	1291	44	0
3	D	887	0	912	7	0
4	F	1411	0	1447	29	0
5	J	1129	0	1162	14	0
6	K	939	0	1012	16	0
7	N	882	0	913	19	0
8	O	892	0	923	24	0
9	P	917	0	965	18	0
10	Q	947	0	1022	21	0
11	R	816	0	839	12	0
12	T	739	0	807	16	0
13	U	780	0	834	16	0
14	V	753	0	780	9	0
15	W	522	0	543	6	0
16	Y	499	0	535	13	0
17	Z	449	0	491	9	0
18	y	148	0	152	4	0
19	A	42496	0	21375	595	0
20	E	1307	0	1365	24	0
21	L	850	0	916	19	0
All	All	60234	0	38641	833	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 9.

The worst 5 of 833 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)
19:A:377:G:H1	19:A:397:U:H3	1.14	0.96
19:A:2747:G:H21	19:A:2758:A:H62	1.15	0.90
19:A:1323:C:O2	19:A:1331:G:N2	2.12	0.81
19:A:1282:U:H3	19:A:1286:A:H62	1.25	0.81
19:A:1350:C:N3	19:A:1381:G:N1	2.29	0.80

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	
1	2	38/46 (83%)	35 (92%)	3 (8%)	0	100	100
3	D	116/209 (56%)	112 (97%)	4 (3%)	0	100	100
4	F	175/177 (99%)	164 (94%)	11 (6%)	0	100	100
5	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
6	K	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
7	N	109/120 (91%)	104 (95%)	5 (5%)	0	100	100
8	O	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
9	P	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
10	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
11	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
12	T	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
13	U	100/102 (98%)	88 (88%)	12 (12%)	0	100	100
14	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
15	W	67/75 (89%)	67 (100%)	0	0	100	100
16	Y	59/63 (94%)	53 (90%)	5 (8%)	1 (2%)	7	35
17	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
18	y	15/17 (88%)	12 (80%)	3 (20%)	0	100	100
20	E	164/201 (82%)	159 (97%)	5 (3%)	0	100	100
21	L	114/143 (80%)	104 (91%)	10 (9%)	0	100	100
All	All	1898/2112 (90%)	1800 (95%)	97 (5%)	1 (0%)	49	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Y	46	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	
1	2	32/38 (84%)	32 (100%)	0	100	100
3	D	92/164 (56%)	92 (100%)	0	100	100
4	F	148/148 (100%)	144 (97%)	4 (3%)	39	60
5	J	116/116 (100%)	115 (99%)	1 (1%)	70	76
6	K	103/103 (100%)	99 (96%)	4 (4%)	28	50
7	N	92/100 (92%)	91 (99%)	1 (1%)	65	73
8	O	86/86 (100%)	83 (96%)	3 (4%)	32	53
9	P	99/99 (100%)	96 (97%)	3 (3%)	36	57
10	Q	89/89 (100%)	89 (100%)	0	100	100
11	R	84/84 (100%)	82 (98%)	2 (2%)	43	63
12	T	80/80 (100%)	79 (99%)	1 (1%)	61	71
13	U	83/83 (100%)	82 (99%)	1 (1%)	63	73
14	V	78/78 (100%)	78 (100%)	0	100	100
15	W	51/57 (90%)	50 (98%)	1 (2%)	48	66
16	Y	55/55 (100%)	54 (98%)	1 (2%)	51	66
17	Z	48/48 (100%)	45 (94%)	3 (6%)	16	38
18	y	17/17 (100%)	16 (94%)	1 (6%)	18	41
20	E	141/165 (86%)	140 (99%)	1 (1%)	76	78
21	L	83/102 (81%)	79 (95%)	4 (5%)	23	45
All	All	1577/1712 (92%)	1546 (98%)	31 (2%)	48	66

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	P	27	VAL
21	L	85	VAL
11	R	47	VAL
21	L	116	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Z	56	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
14	V	75	GLN
20	E	115	GLN
18	y	3	ASN
10	Q	71	ASN
13	U	98	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	A	1969/2903 (67%)	285 (14%)	7 (0%)
2	B	118/120 (98%)	14 (11%)	0
All	All	2087/3023 (69%)	299 (14%)	7 (0%)

5 of 299 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	13	G
2	B	15	A
2	B	16	G
2	B	25	U

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
19	A	848	C
19	A	929	U
19	A	2425	A
19	A	1328	A
19	A	828	U

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.

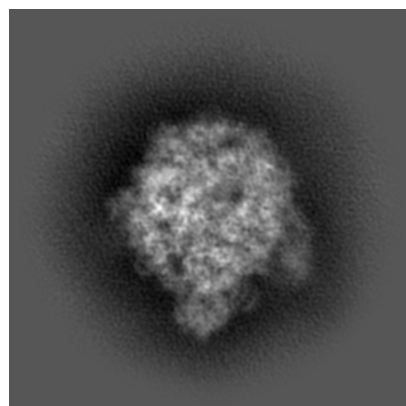
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51976. These allow visual inspection of the internal detail of the map and identification of artifacts.

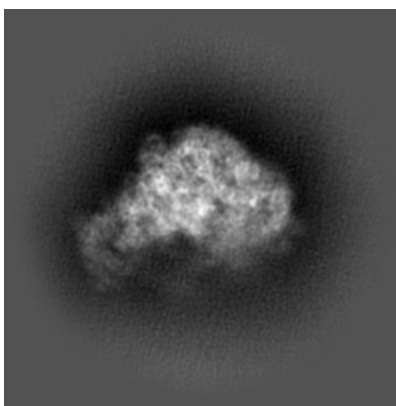
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

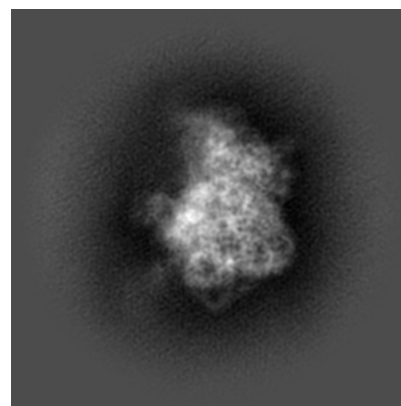
6.1.1 Primary map



X

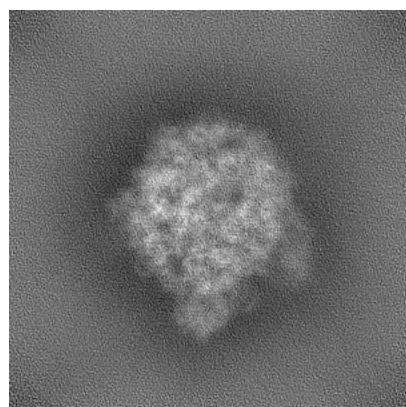


Y

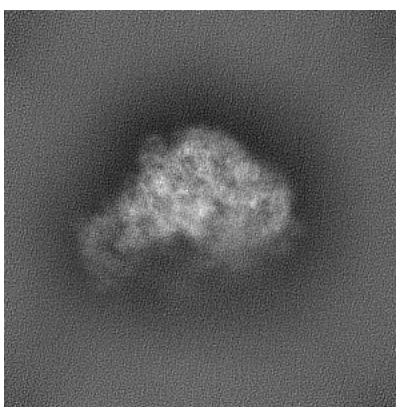


Z

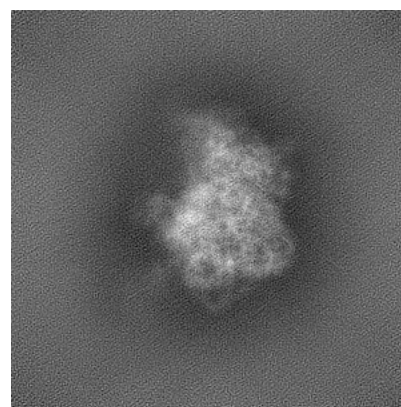
6.1.2 Raw map



X



Y

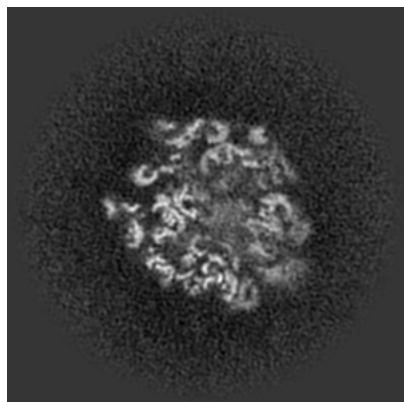


Z

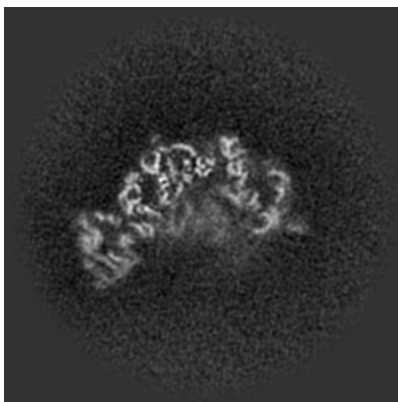
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

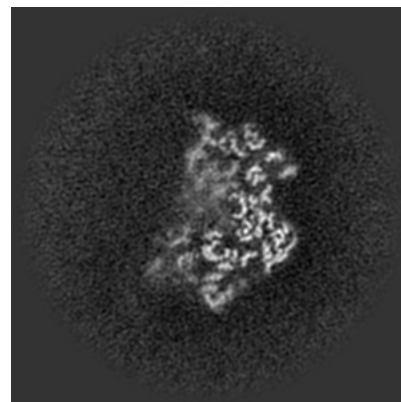
6.2.1 Primary map



X Index: 150

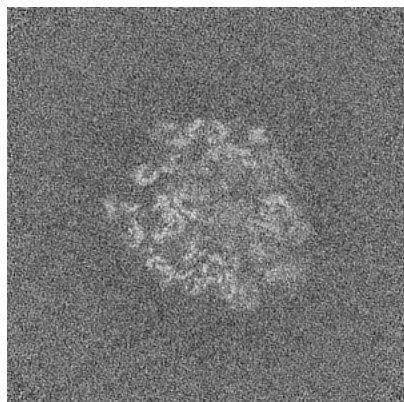


Y Index: 150

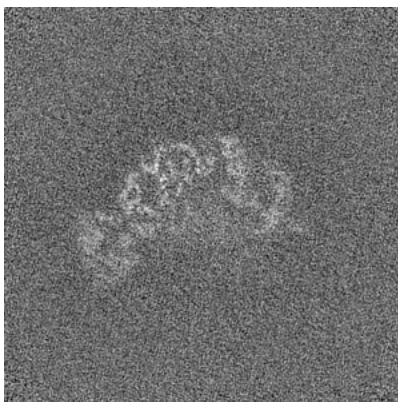


Z Index: 150

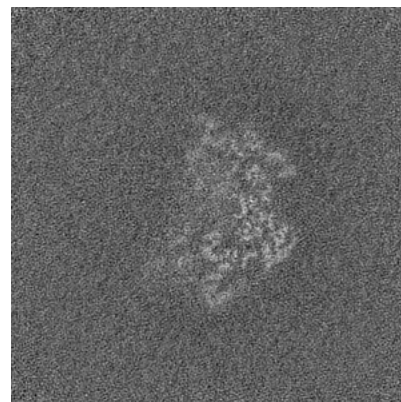
6.2.2 Raw map



X Index: 150



Y Index: 150

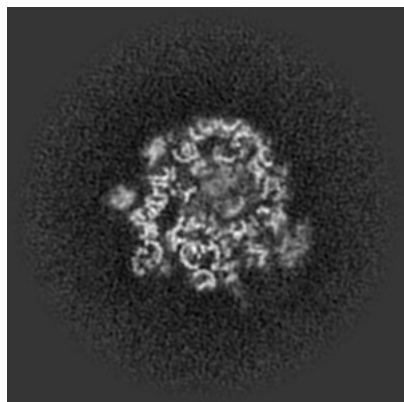


Z Index: 150

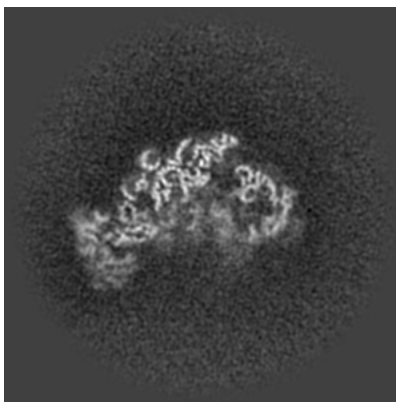
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

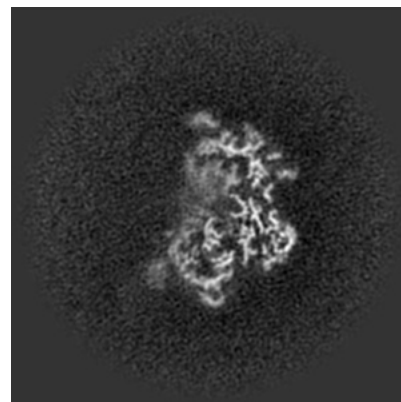
6.3.1 Primary map



X Index: 163

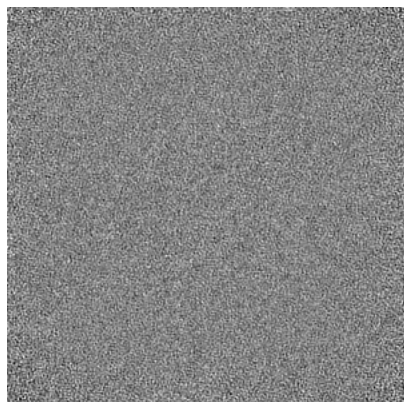


Y Index: 143

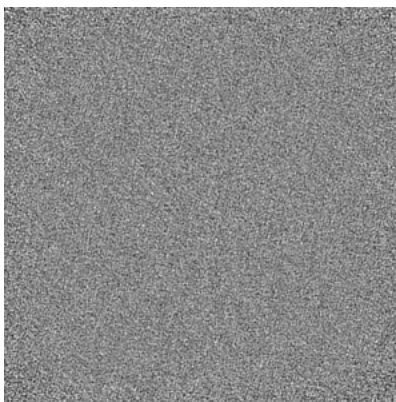


Z Index: 147

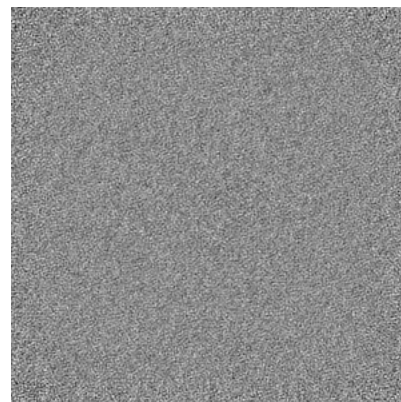
6.3.2 Raw map



X Index: 0



Y Index: 0

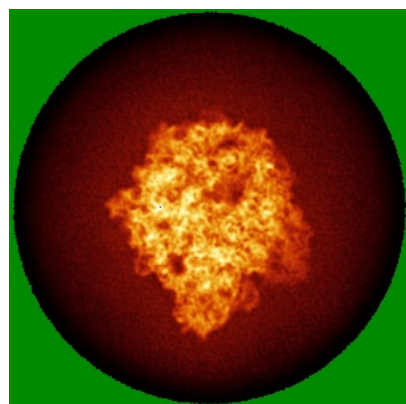


Z Index: 0

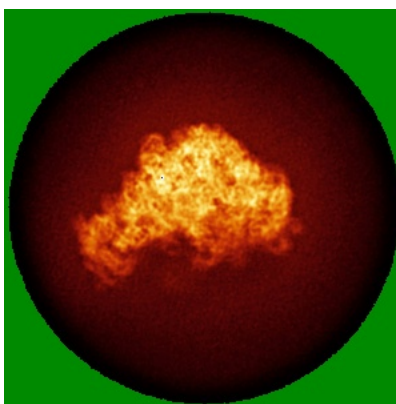
The images above show the largest variance slices of the map in three orthogonal directions.

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

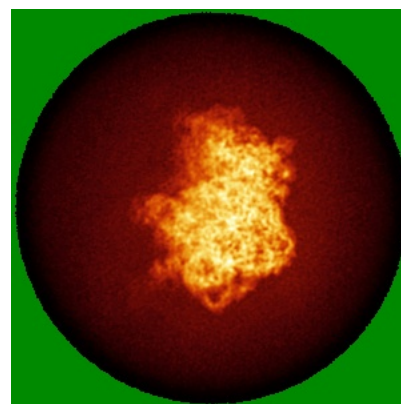
6.4.1 Primary map



X

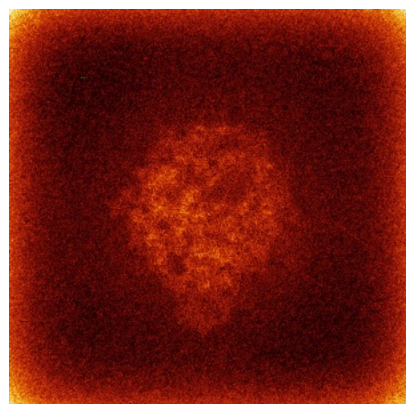


Y

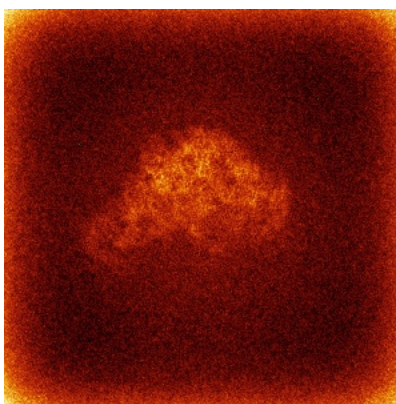


Z

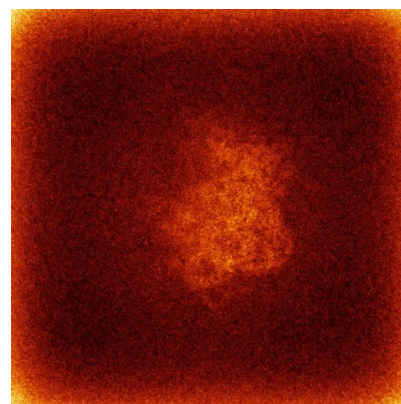
6.4.2 Raw map



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](#)

This section was not generated.

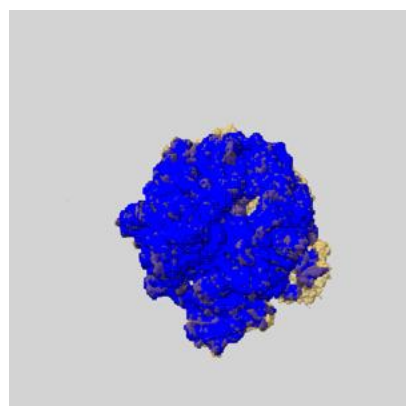
6.6 Mask visualisation [i](#)

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

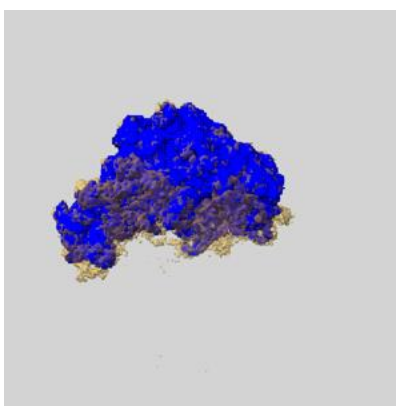
A mask typically either:

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

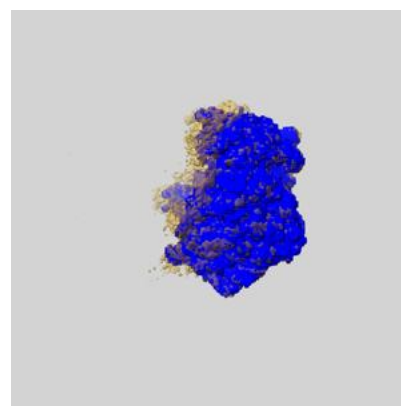
6.6.1 emd_51976_msk_1.map [i](#)



X



Y

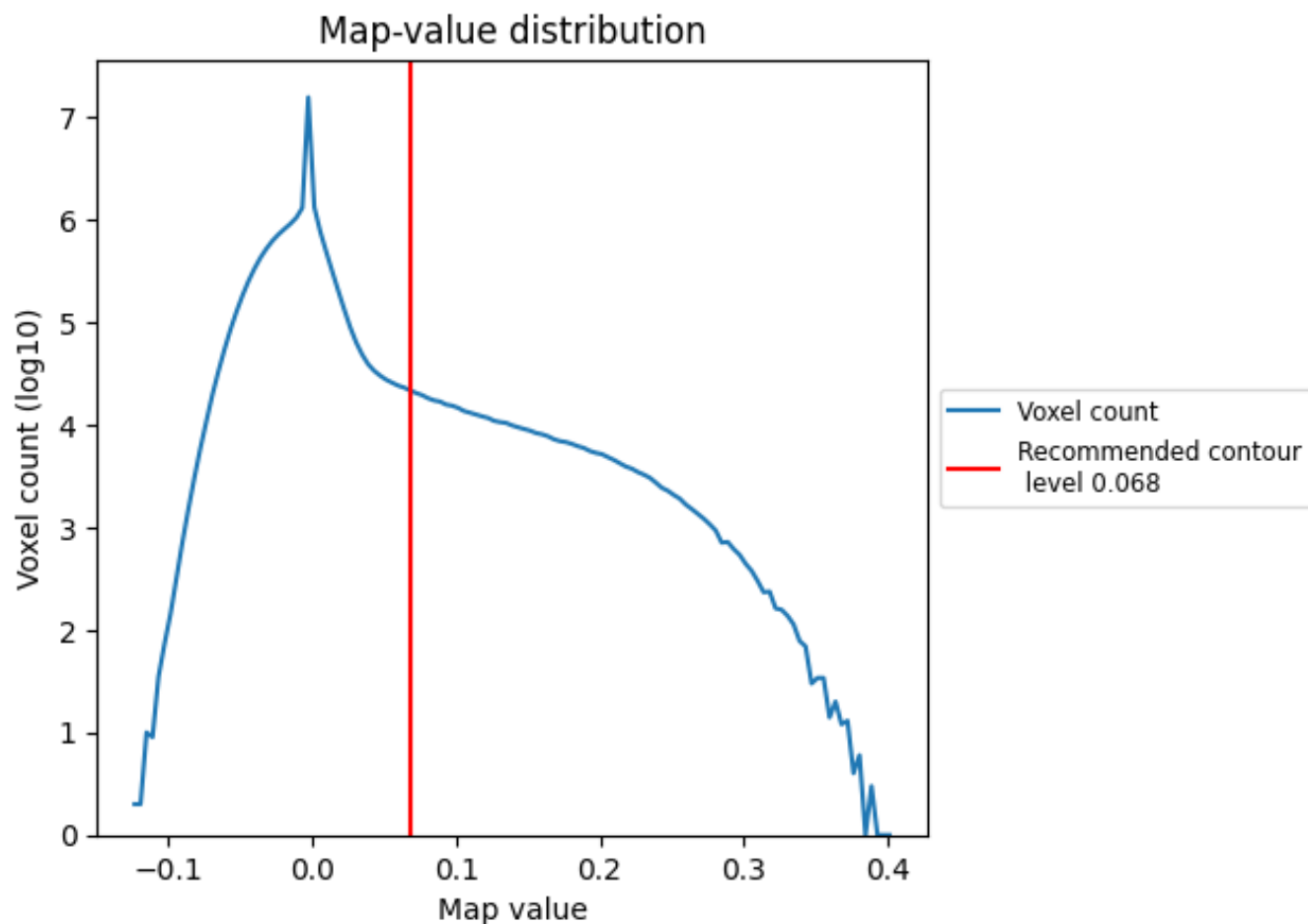


Z

7 Map analysis [i](#)

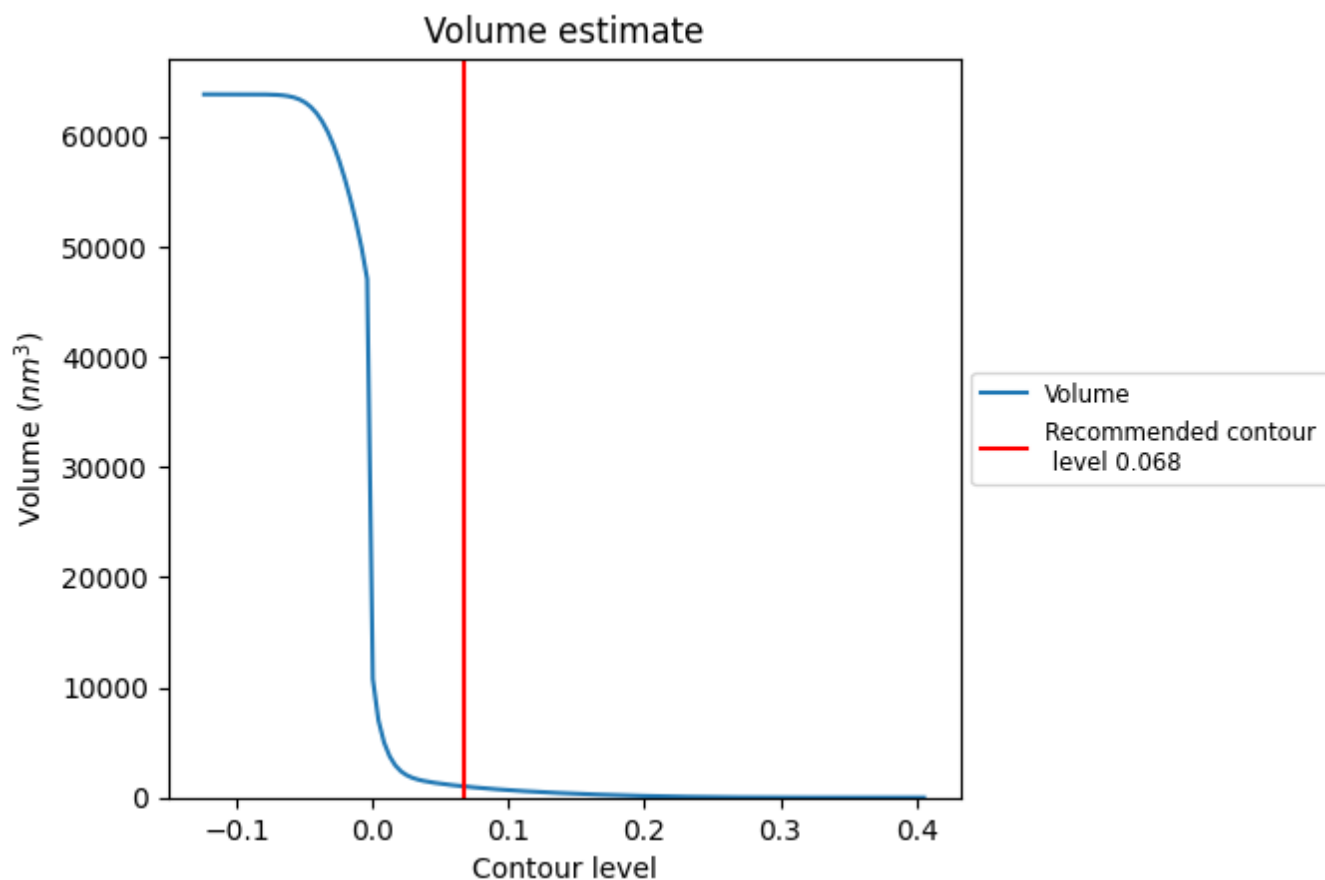
This section contains the results of statistical analysis of the map.

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.

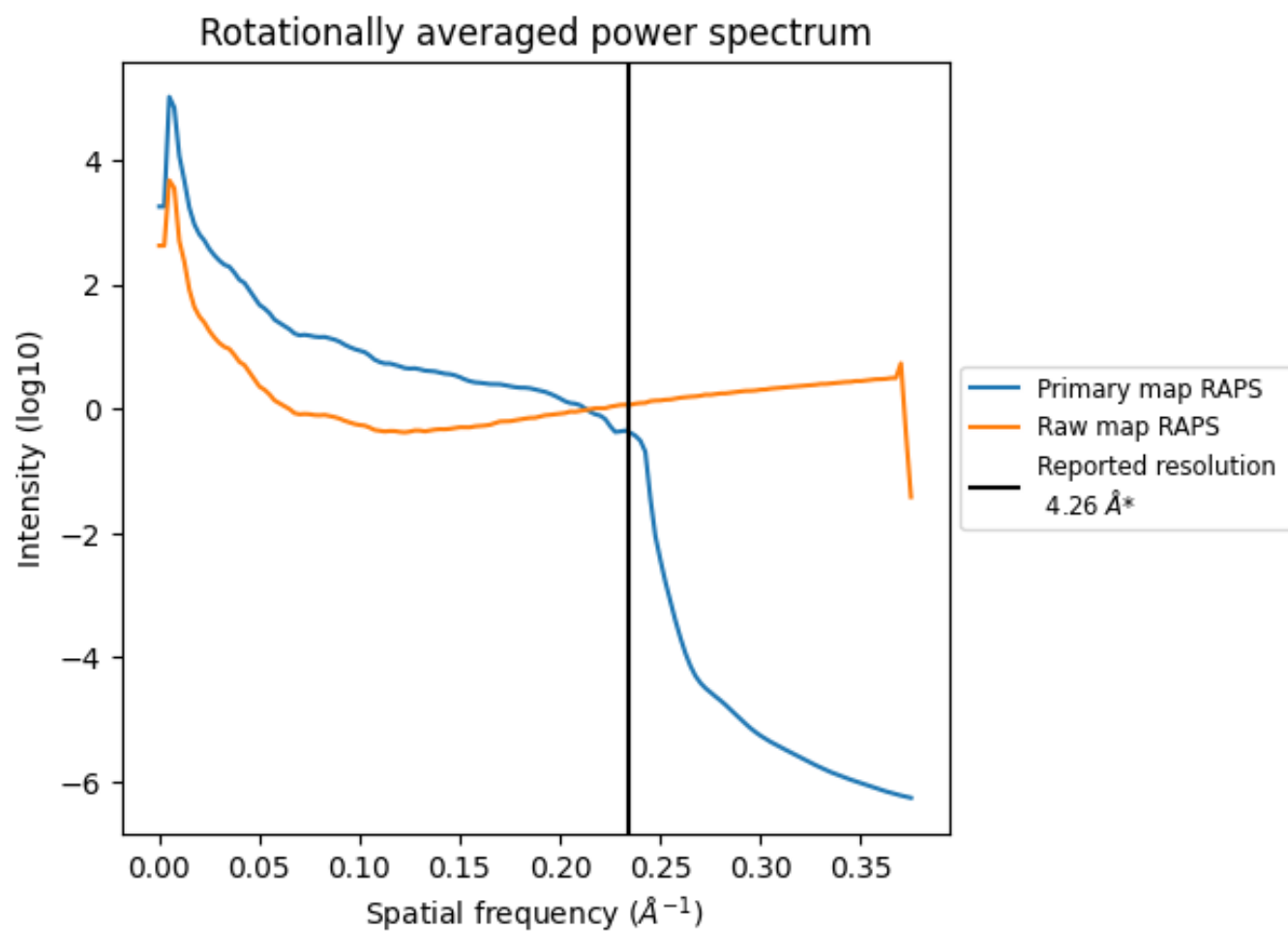
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1007 nm³; this corresponds to an approximate mass of 909 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 ⓘ

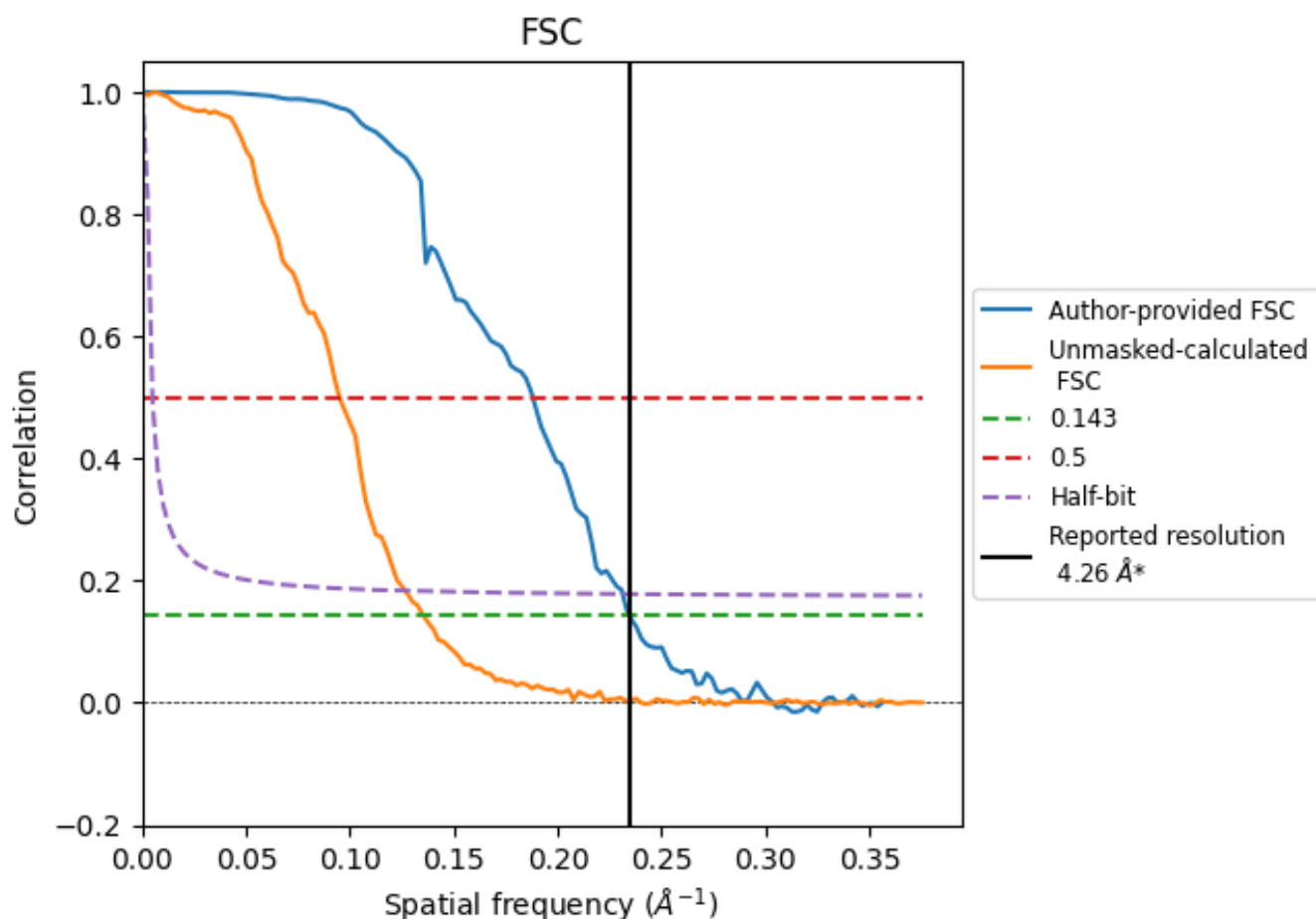


*Reported resolution corresponds to spatial frequency of 0.235 Å⁻¹

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 0.235 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.26	-	-
Author-provided FSC curve	4.26	5.32	4.33
Unmasked-calculated*	7.39	10.54	7.89

*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 7.39 differs from the reported value 4.26 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51976 and PDB model 9HA4. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

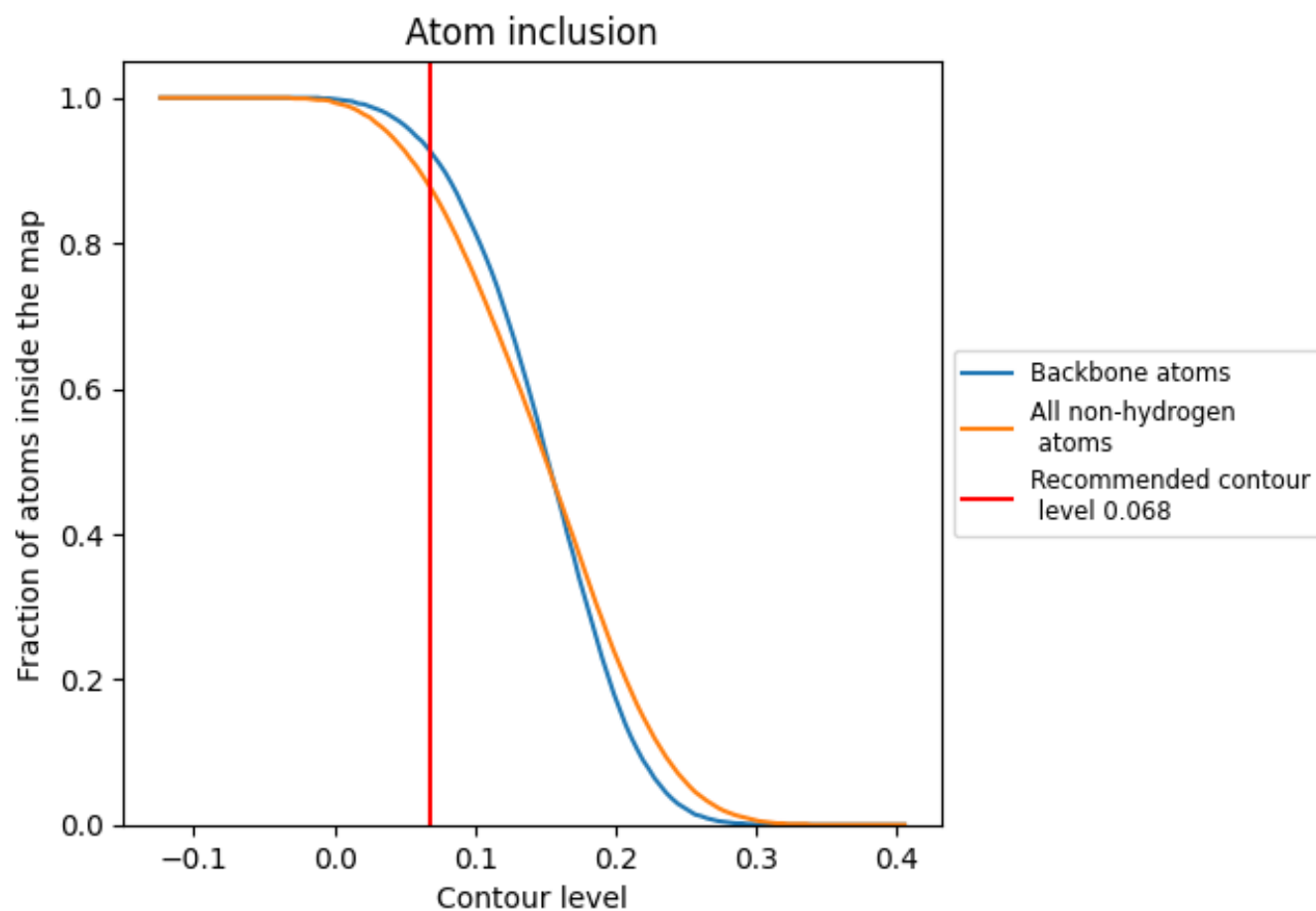


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.2460
2	 0.7220	 0.2150
A	 0.9270	 0.2560
B	 0.9340	 0.2180
D	 0.8350	 0.2810
E	 0.7720	 0.2660
F	 0.5400	 0.0790
J	 0.7870	 0.2590
K	 0.5420	 0.1750
L	 0.7090	 0.2160
N	 0.8170	 0.2360
O	 0.7030	 0.1250
P	 0.6590	 0.2030
Q	 0.8280	 0.2630
R	 0.7750	 0.2850
T	 0.7400	 0.2720
U	 0.8160	 0.2890
V	 0.7290	 0.1860
W	 0.8040	 0.2740
Y	 0.7700	 0.2040
Z	 0.8350	 0.2950
y	 0.0220	 0.0420

