



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 09:33 AM EDT

PDB ID : 6WRU  
EMDB ID : EMD-21888  
Title : Structure of the 50S subunit of the ribosome from Methicillin Resistant Staphylococcus aureus in complex with an isomer of the tedizolid  
Authors : Belousoff, M.J.  
Deposited on : 2020-04-30  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
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)	:	2.39

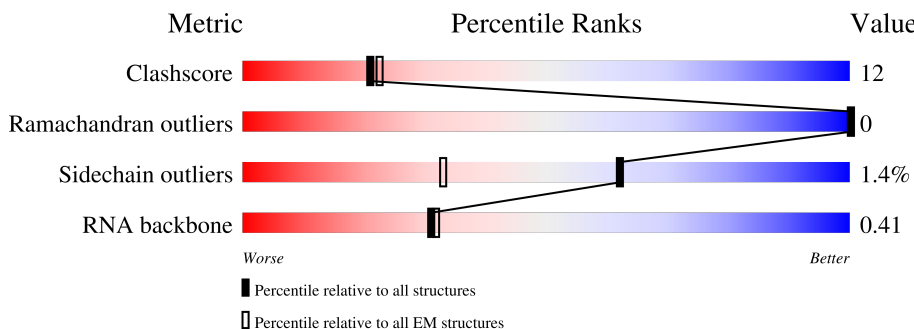
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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	116	
2	B	277	
3	C	118	
4	D	105	
5	E	117	
6	F	91	
7	G	105	

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Mol	Chain	Length	Quality of chain
8	H	107	
9	J	62	
10	K	72	
11	L	217	
12	M	58	
13	N	57	
14	O	49	
15	P	50	
16	Q	65	
17	R	37	
18	S	207	
19	U	175	
20	V	145	
21	W	122	
22	X	146	
23	Y	144	
24	Z	122	
25	a	119	
26	1	2923	
27	2	115	
28	I	85	

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 81707 atoms, of which 14 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 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	113	Total	C	N	O	0	0
			915	576	184	155		

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	275	Total	C	N	O	S	0	0
			2103	1309	417	372	5		

- Molecule 3 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 4 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	100	Total	C	N	O	S	0	0
			785	499	139	146	1		

- Molecule 5 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	110	ALA	GLY	variant	UNP A0A077UKF9

- Molecule 6 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			711	447	128	132	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	87	ASP	ILE	variant	UNP W8TUB4

- Molecule 7 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	89	Total	C	N	O	S	0	0
			689	437	126	125	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	54	SER	GLY	variant	UNP W8TRD5

- Molecule 8 is a protein called uL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			727	465	129	132	1		

- Molecule 9 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	59	Total	C	N	O	S	0	0
			463	287	99	76	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	62	ALA	-	insertion	UNP A0A077URJ8

- Molecule 10 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	58	Total	C	N	O	0	0
			481	296	92	93		

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	215	Total	C	N	O	S	0	0
			1628	1018	299	306	5		

- Molecule 12 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	56	Total	C	N	O	0	0
			432	269	82	81		

- Molecule 13 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	50	Total	C	N	O	S	0	0
			397	241	83	68	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	54	ALA	VAL	variant	UNP A0A077UWR7

- Molecule 14 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	47	Total	C	N	O	S	0	0
			390	233	79	73	5		

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	44	Total	C	N	O	S	0	0
			372	228	90	53	1		

- Molecule 16 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 17 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 18 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	192	Total	C	N	O	S	0	0
			1472	924	271	275	2		

- Molecule 19 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	174	Total	C	N	O	S	0	0
			1360	845	249	263	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	18	SER	THR	variant	UNP W8U3X2

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	143	Total	C	N	O	S	0	0
			1138	710	209	217	2		

- Molecule 21 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	121	Total	C	N	O	S	0	0
			911	566	173	168	4		

- Molecule 22 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	144	Total	C	N	O	0	0
			1082	669	213	200		

- Molecule 23 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	114	Total	C	N	O	S	0	0
			899	554	175	169	1		

- Molecule 25 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	116	Total	C	N	O		0	0
			899	560	171	168			

- Molecule 26 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	2665	Total	C	N	O	P	0	0
			57132	25513	10463	18496	2660		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1866	A	G	conflict	GB 1760383645

- Molecule 27 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	112	Total	C	N	O	P	0	0
			2381	1066	427	777	111		

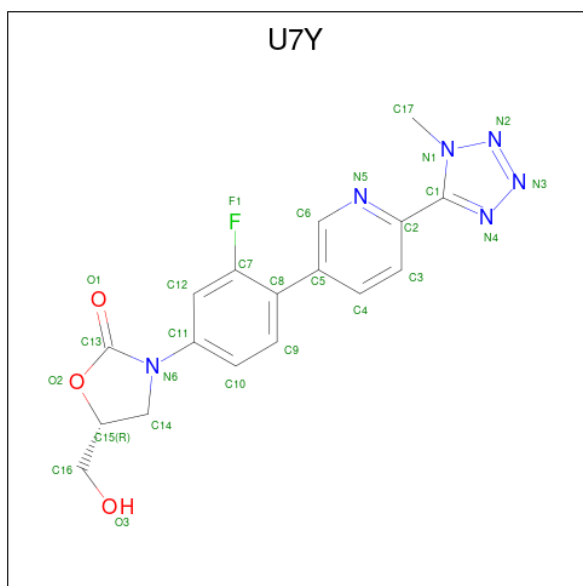
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	80	C	G	variant	GB 1750990749
2	109	C	G	variant	GB 1750990749
2	111	A	C	variant	GB 1750990749
2	112	G	A	variant	GB 1750990749

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	I	78	Total	C	N	O	0	0
			597	367	116	114		

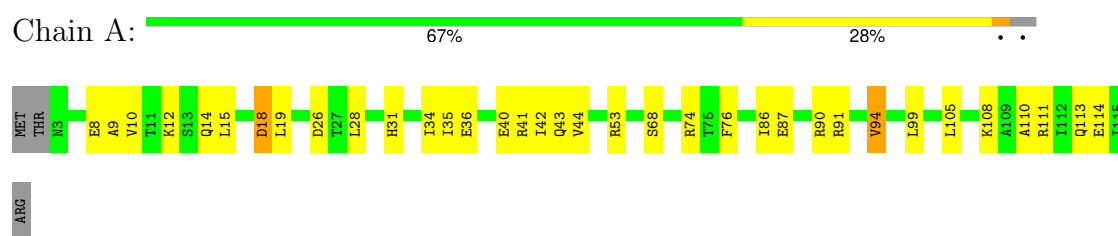
- Molecule 29 is Tedizolid isomer (three-letter code: U7Y) (formula:  $C_{17}H_{15}FN_6O_3$ ) (labeled as "Ligand of Interest" by depositor).



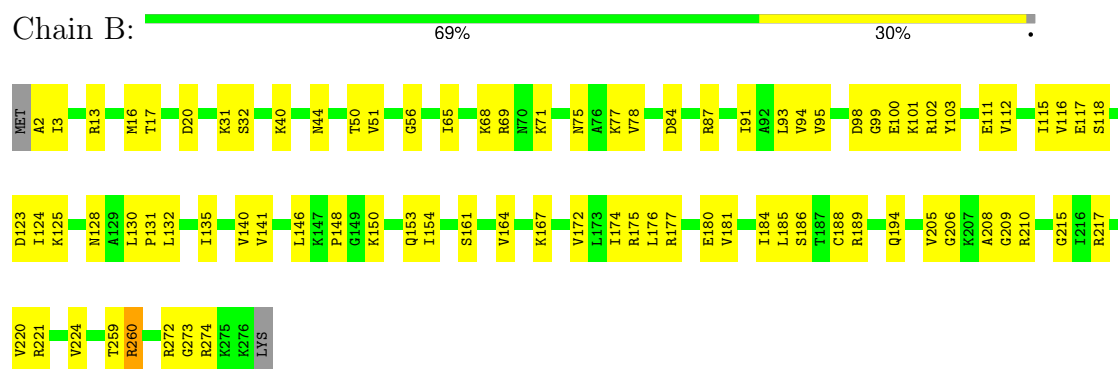
### 3 Residue-property plots

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.

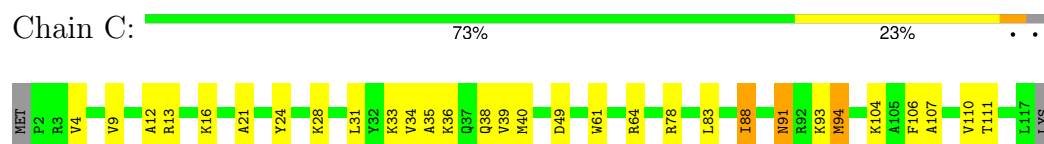
#### • Molecule 1: 50S ribosomal protein L19



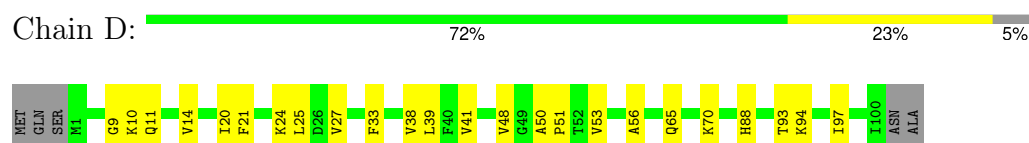
#### • Molecule 2: 50S ribosomal protein L2



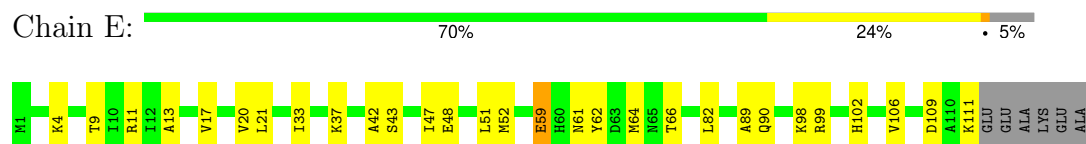
#### • Molecule 3: 50S ribosomal protein L20



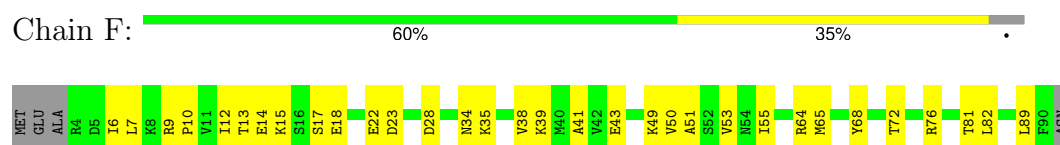
#### • Molecule 4: 50S ribosomal protein L21



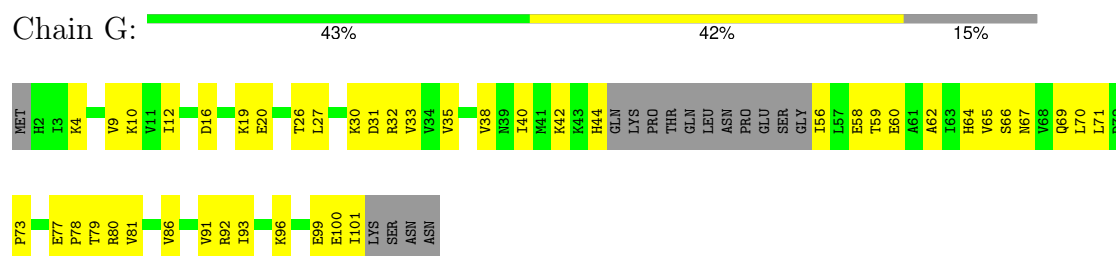
- Molecule 5: 50S ribosomal protein L22



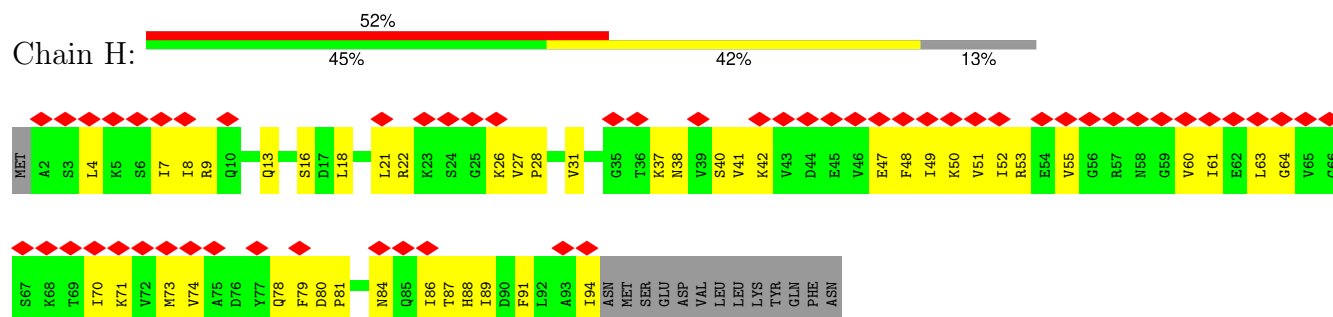
- Molecule 6: 50S ribosomal protein L23



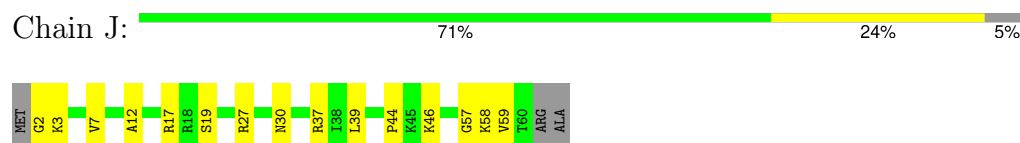
- Molecule 7: 50S ribosomal protein L24



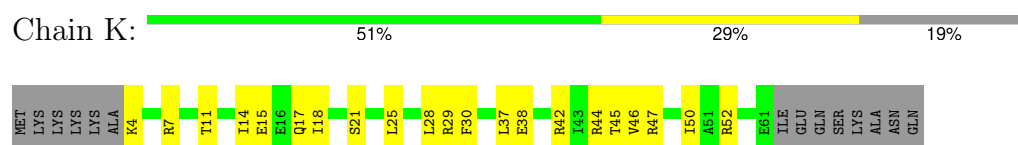
- Molecule 8: uL25




- Molecule 9: 50S ribosomal protein L28

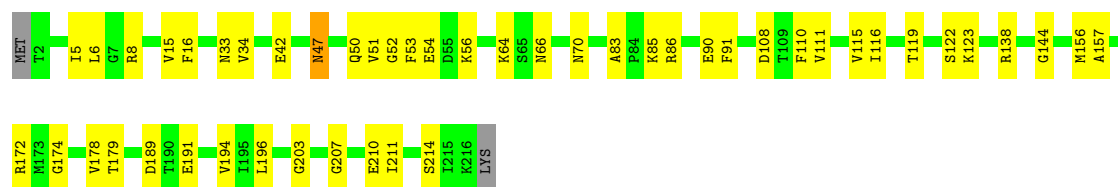


- Molecule 10: 50S ribosomal protein L29



- Molecule 11: 50S ribosomal protein L3

Chain L:  77% 22%



- Molecule 12: 50S ribosomal protein L30

Chain M:  72% 22%



- Molecule 13: 50S ribosomal protein L32

Chain N:  72% 16% 12%



- Molecule 14: 50S ribosomal protein L33

Chain O:  59% 37%



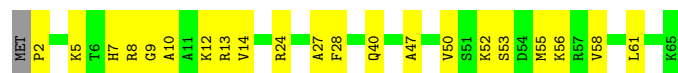
- Molecule 15: 50S ribosomal protein L34

Chain P:  72% 16% 12%



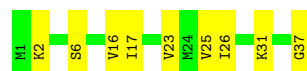
- Molecule 16: 50S ribosomal protein L35

Chain Q:  66% 32%



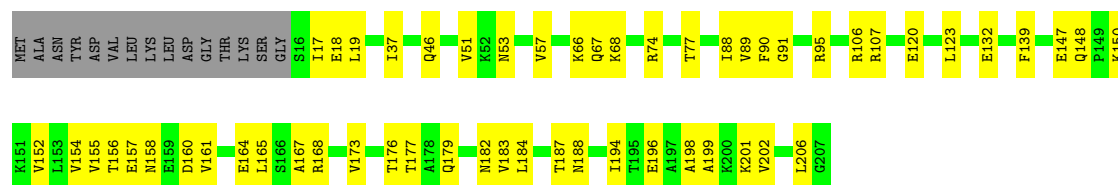
- Molecule 17: 50S ribosomal protein L36

Chain R:  76% 24%



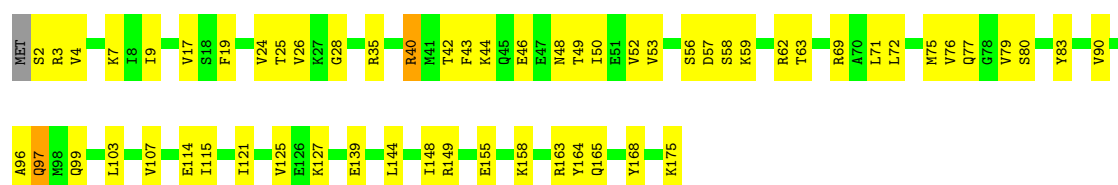
- Molecule 18: 50S ribosomal protein L4

Chain S: 



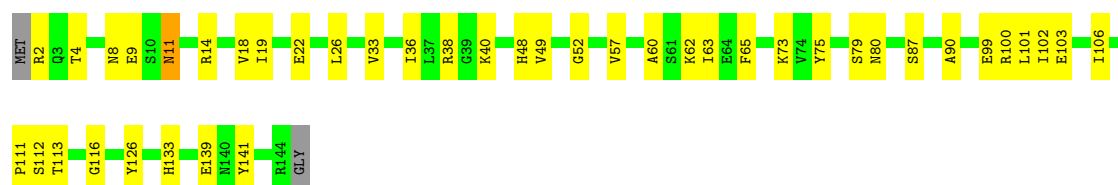
- Molecule 19: 50S ribosomal protein L6

Chain U: 



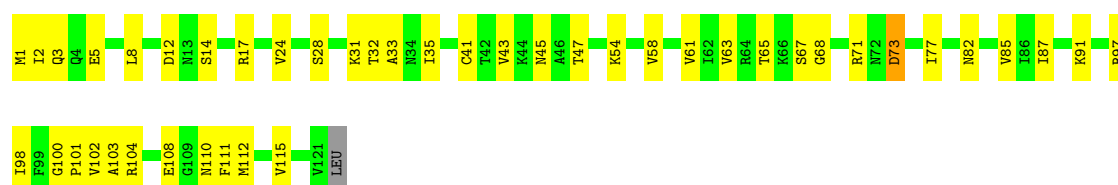
- Molecule 20: 50S ribosomal protein L13

Chain V: 



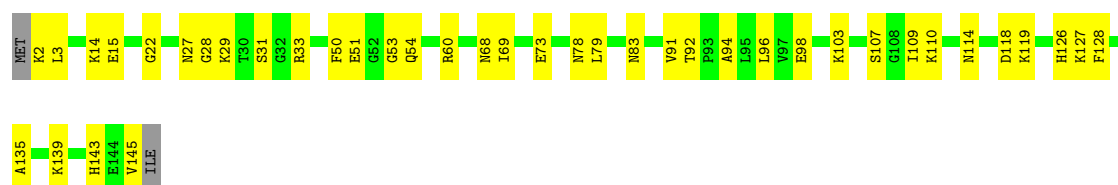
- Molecule 21: 50S ribosomal protein L14

Chain W: 



- Molecule 22: 50S ribosomal protein L15

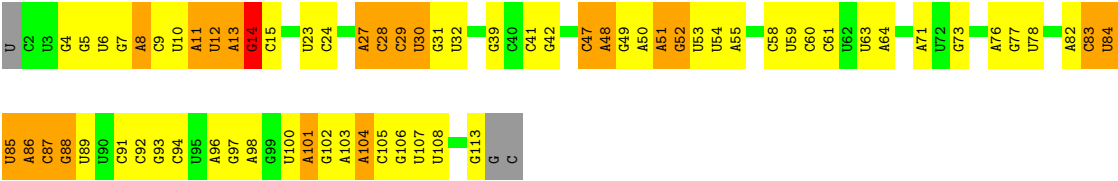
Chain X: 



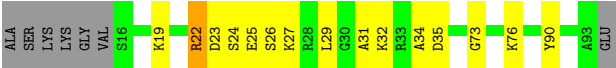


G1716	G1566	U1504	U1428	G1329	A1231	A	A	A1001	G	G	C831	G749	G665	G578
G1717	A1567	G1505	G1429	U1330	G1232	G1156	C	U1002	G	G	C832	A750	A666	U579
G1718	U1568	C1506	A1430	U1331	U1233	A1159	U	A1003	G	G	A833	A751	A667	A583
G1719	G1569	A1507	U1431	U1332	U1234	C1160	G	A1004	G	G	A834	G752	C668	
A1720	C1570	C1508	A1432	G1336	A1241	G1166	G	G1005	C	C	U835	U753	C587	C587
A1721	G1571	G1509	U1433	U1337	A1242	G1167	G	U1013	C	C	C836	U754	A672	C588
A1722	G1572	U1510	U1434	U1338	A1243	G1168	U	U1014	C	C	G837	C755	G673	G589
A1723	A1573	C1511	A1443	U1339	G1245	C1169	G	U1018	C	C	A838	A756	C674	U590
G1724	U1574	U1512	C1444	U1340	G1246	A1170	U	A1018	C	C	G839	G757	U591	A591
A1725	A1575	A1513	A1445	A1344	C1247	A1171	U	A1024	C	C	G846	A760	A678	A592
G1726	A1576	G1514	U1447	A1345	A1251	A1172	G	A1025	C	C	A847	A761	G679	U593
G1727	A1577	C1515	U1448	G1346	A1252	A1173	G	C1026	G	G	U848	C762	C680	G594
C1730	C1578	A1517	A	G1347	G1253	A1173	C	A1027	G	G	A849	A763	G681	
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G1738	U1581	U1519	U	U1349	G1257	A1177	U	G1028	U	U	G854	U765	G683	U598
G1739	U1582	A1520	C	C1350	A1258	C1178	G	C1029	A	A	U855	A768	A599	U600
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G1741	U1584	G1522	U	A1352	A1263		A	A1044	C	C	C857	A772	G687	G604
A1742	G1585	G1523	U	G1353		U1185	A	A1045	G	G	U858	G773	U605	U605
	U1586	C	U	G1354	U1272	A1186	A	A1051	C	C	U859	A774	G688	G606
	C1587	U	U	G1355	G1273	A1187	C	A1055	C	C	C859	A775	A689	
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G1746	U1589	A	A	G1357	A1275	C1189	G	A1057	C	C	U871		G692	U614
	C1590	G	A	A1358	G1276	A1190	C	A1058	C	C	C872		G693	A615
	U1591	U	G	A1359	G1277	U1191	C	A1059	C	C	U873		G694	A616
	G1592	A	U	G1360	G1278	A1195	C	A1063	C	C	U874		G695	A617
G1750	U1593	U	U	G1361	G1279	C1196	C	A1064	C	C	C875		G696	A618
C1752	U1594	U	U	G1362	G1280	C1197	C	A1065	C	C	U876		G697	G620
	C1595	A	G	G1363	U1281	G1201	U	A1066	C	C	C883		U698	A621
U1756	U1596	A	G	U1364	A1285	C1202	U	A1067	C	C	U877		A700	A622
A1758	U1597	G	U	U1365	G1286	U1203	U	A1068	C	C	U878		G701	C623
G1759	U1598	C	U	U1366	U1287	C1204	U	A1069	C	C	U879		U702	A629
G1760	U1599	U	U	G1375	A1291	U1205	A	U1067	C	C	U880		A703	G630
U1762	A1600	A	U	U1376	U1292	A1208	G	U1068	C	C	U881		U704	U631
	U1601	U	G	U1377	U1293	U1209	A	G1069	C	C	U882		U705	
	A1605	U	G	U1378	G1294	U1210	G	A1070	C	C	U883		U712	A632
	C1606	A	U	U1379	C1295	U1211	C	A1071	C	C	U884		A633	
		A	G	G1375	G1300	U1212	C	A1072	C	C	U885		A646	A646
		U	G	U1477	A1303	C1214	U	G1074	C	C	U886		A720	G647
		A	U	U1478	G1304	U1215	A	U1077	C	C	U887		A721	G648
		C	U	A1479	U1305	U1216	A	U1078	C	C	U888		A722	U649
		G	U	A1480	A1306	U1217	C	U1079	C	C	U889		C723	U650
		U	U	A1481	G1307	G1218	U	A1079	C	C	U890		C724	A651
		A	A	G1405	U1308	G1219	A	A1080	C	C	A901		A652	A652
		A	U	G1490	C1309	A1220	C	G1083	C	C	A902		A730	G653
		G	U	A1415	A1310	G1221	C	U1084	C	C	U893		U731	C654
		U	U	U1416	A1311	A1222	U	U1085	C	C	U894		C732	A655
		U	U	U1417	G1313	A1223	C	C1086	C	C	U895		U657	A656
		U	U	A1421	U1320	G1225	C	C1087	C	C	G821		U738	A658
		U	U	A1422	G1321	G1226	C	C1088	C	C	U896		U739	A659
		U	U	A1423	G1322	U1227	C	C	C	C	G822		A744	A660
		U	U	A1424	U1323	U1228	C	A	C	C	A911		G745	U661
		U	U	G1425	A1324	G1229	C	A	C	C	A920		G746	U662
		U	U	U1427	U1325	U1325	C	A	C	C	G		U747	U663
		U	U				C	A	C	C	A		U748	G664





• Molecule 28: 50S ribosomal protein L27



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	11.419	Depositor
Minimum map value	-7.604	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.292	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	419.04, 419.04, 419.04	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U7Y

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	0.47	0/927	0.59	0/1239
2	B	0.48	0/2138	0.55	0/2869
3	C	0.56	0/955	0.58	0/1265
4	D	0.45	0/795	0.55	0/1062
5	E	0.44	0/861	0.58	0/1159
6	F	0.45	0/719	0.57	0/959
7	G	0.36	0/695	0.48	0/926
8	H	0.28	0/735	0.45	0/986
9	J	0.42	0/469	0.52	0/625
10	K	0.47	0/482	0.58	0/642
11	L	0.53	0/1652	0.64	0/2216
12	M	0.58	0/434	0.64	0/585
13	N	0.50	0/404	0.53	0/537
14	O	0.39	0/393	0.54	0/523
15	P	0.53	0/376	0.56	0/491
16	Q	0.50	0/526	0.55	0/690
17	R	0.43	0/299	0.54	0/393
18	S	0.47	0/1494	0.58	0/2018
19	U	0.37	0/1378	0.53	0/1853
20	V	0.50	0/1160	0.54	0/1563
21	W	0.48	0/918	0.58	0/1232
22	X	0.45	0/1096	0.56	0/1461
23	Y	0.47	0/1113	0.52	0/1493
24	Z	0.46	0/902	0.55	0/1202
25	a	0.37	0/908	0.50	0/1215
26	1	0.84	0/63978	1.00	90/99764 (0.1%)
27	2	0.57	0/2662	0.95	1/4146 (0.0%)
28	I	0.53	0/603	0.60	0/801
All	All	0.75	0/89072	0.92	91/133915 (0.1%)

There are no bond length outliers.

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	2902	A	N9-C1'-C2'	-8.91	102.20	112.00
26	1	2539	C	N1-C1'-C2'	-8.10	103.09	112.00
26	1	1522	G	C4'-C3'-O3'	7.63	128.25	113.00
26	1	675	G	N9-C1'-C2'	-7.37	103.89	112.00
26	1	167	U	N1-C1'-C2'	-7.19	104.09	112.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	915	0	987	30	0
2	B	2103	0	2218	74	0
3	C	943	0	1014	24	0
4	D	785	0	825	21	0
5	E	853	0	912	21	0
6	F	711	0	743	23	0
7	G	689	0	748	36	0
8	H	727	0	777	46	0
9	J	463	0	501	11	0
10	K	481	0	508	15	0
11	L	1628	0	1667	38	0
12	M	432	0	472	11	0
13	N	397	0	407	7	0
14	O	390	0	396	19	0
15	P	372	0	420	6	0
16	Q	521	0	586	14	0
17	R	296	0	340	5	0
18	S	1472	0	1520	48	0
19	U	1360	0	1390	54	0
20	V	1138	0	1130	30	0
21	W	911	0	970	38	0
22	X	1082	0	1119	29	0
23	Y	1089	0	1155	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Z	899	0	954	22	0
25	a	899	0	940	0	0
26	1	57132	0	28744	938	0
27	2	2381	0	1209	41	0
28	I	597	0	607	12	0
29	1	27	14	0	1	0
All	All	81693	14	53259	1522	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 12.

The worst 5 of 1522 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)
26:1:275:A:H62	26:1:296:G:N2	1.53	1.05
10:K:17:GLN:O	10:K:21:SER:HB2	1.59	1.03
26:1:699:U:H4'	26:1:700:A:H5'	1.43	1.00
2:B:95:VAL:HG22	2:B:101:LYS:HG2	1.44	0.98
4:D:65:GLN:HG3	4:D:93:THR:HG22	1.46	0.95

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	111/116 (96%)	101 (91%)	10 (9%)	0	100	100
2	B	273/277 (99%)	247 (90%)	26 (10%)	0	100	100
3	C	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
4	D	98/105 (93%)	87 (89%)	11 (11%)	0	100	100
5	E	109/117 (93%)	103 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	85/91 (93%)	73 (86%)	12 (14%)	0	100	100
7	G	85/105 (81%)	79 (93%)	6 (7%)	0	100	100
8	H	91/107 (85%)	88 (97%)	3 (3%)	0	100	100
9	J	57/62 (92%)	52 (91%)	5 (9%)	0	100	100
10	K	56/72 (78%)	52 (93%)	4 (7%)	0	100	100
11	L	213/217 (98%)	199 (93%)	14 (7%)	0	100	100
12	M	54/58 (93%)	50 (93%)	4 (7%)	0	100	100
13	N	48/57 (84%)	41 (85%)	7 (15%)	0	100	100
14	O	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
15	P	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
16	Q	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
17	R	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
18	S	190/207 (92%)	177 (93%)	13 (7%)	0	100	100
19	U	172/175 (98%)	152 (88%)	20 (12%)	0	100	100
20	V	141/145 (97%)	134 (95%)	7 (5%)	0	100	100
21	W	119/122 (98%)	107 (90%)	12 (10%)	0	100	100
22	X	142/146 (97%)	124 (87%)	18 (13%)	0	100	100
23	Y	134/144 (93%)	130 (97%)	4 (3%)	0	100	100
24	Z	110/122 (90%)	104 (94%)	6 (6%)	0	100	100
25	a	114/119 (96%)	98 (86%)	16 (14%)	0	100	100
28	I	76/85 (89%)	69 (91%)	7 (9%)	0	100	100
All	All	2776/2968 (94%)	2551 (92%)	225 (8%)	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	
1	A	99/102 (97%)	96 (97%)	3 (3%)	36	64
2	B	222/224 (99%)	221 (100%)	1 (0%)	86	92
3	C	96/98 (98%)	92 (96%)	4 (4%)	25	56
4	D	85/89 (96%)	85 (100%)	0	100	100
5	E	90/94 (96%)	87 (97%)	3 (3%)	33	62
6	F	79/82 (96%)	77 (98%)	2 (2%)	42	69
7	G	76/91 (84%)	75 (99%)	1 (1%)	65	82
8	H	81/95 (85%)	81 (100%)	0	100	100
9	J	49/51 (96%)	49 (100%)	0	100	100
10	K	53/65 (82%)	52 (98%)	1 (2%)	52	75
11	L	173/175 (99%)	168 (97%)	5 (3%)	37	65
12	M	50/52 (96%)	49 (98%)	1 (2%)	50	74
13	N	45/49 (92%)	45 (100%)	0	100	100
14	O	45/47 (96%)	45 (100%)	0	100	100
15	P	39/45 (87%)	39 (100%)	0	100	100
16	Q	55/56 (98%)	55 (100%)	0	100	100
17	R	35/35 (100%)	35 (100%)	0	100	100
18	S	158/170 (93%)	155 (98%)	3 (2%)	52	75
19	U	152/153 (99%)	150 (99%)	2 (1%)	65	82
20	V	122/123 (99%)	120 (98%)	2 (2%)	58	79
21	W	99/100 (99%)	98 (99%)	1 (1%)	73	86
22	X	110/112 (98%)	108 (98%)	2 (2%)	54	76
23	Y	113/119 (95%)	113 (100%)	0	100	100
24	Z	94/102 (92%)	94 (100%)	0	100	100
25	a	92/95 (97%)	91 (99%)	1 (1%)	70	84
28	I	61/66 (92%)	60 (98%)	1 (2%)	58	79
All	All	2373/2490 (95%)	2340 (99%)	33 (1%)	62	81

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	W	73	ASP
22	X	29	LYS
28	I	22	ARG

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Mol	Chain	Res	Type
6	F	68	TYR
6	F	65	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
18	S	46	GLN
19	U	77	GLN
18	S	119	GLN
18	S	179	GLN
20	V	48	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	1	2654/2923 (90%)	749 (28%)	236 (8%)
27	2	111/115 (96%)	36 (32%)	17 (15%)
All	All	2765/3038 (91%)	785 (28%)	253 (9%)

5 of 785 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	1	11	U
26	1	18	C
26	1	20	C
26	1	27	G
26	1	28	A

5 of 253 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1	1491	C
26	1	2639	C
26	1	1712	A
26	1	2637	C
27	2	8	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
29	U7Y	1	3001	-	28,30,30	5.51	19 (67%)	39,43,43	2.35	14 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	U7Y	1	3001	-	-	7/14/26/26	0/4/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	3001	U7Y	N4-N3	13.36	1.55	1.35
29	1	3001	U7Y	C13-N6	11.11	1.48	1.36
29	1	3001	U7Y	C12-C7	8.77	1.52	1.37
29	1	3001	U7Y	C9-C8	8.22	1.52	1.40
29	1	3001	U7Y	C6-C5	7.40	1.52	1.39

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	3001	U7Y	C17-N1-C1	-6.95	121.60	129.43
29	1	3001	U7Y	C14-N6-C13	-5.25	107.28	111.17
29	1	3001	U7Y	O2-C13-N6	-4.35	106.26	109.92
29	1	3001	U7Y	O2-C13-O1	3.68	126.71	122.40
29	1	3001	U7Y	C14-N6-C11	3.56	127.53	121.36

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

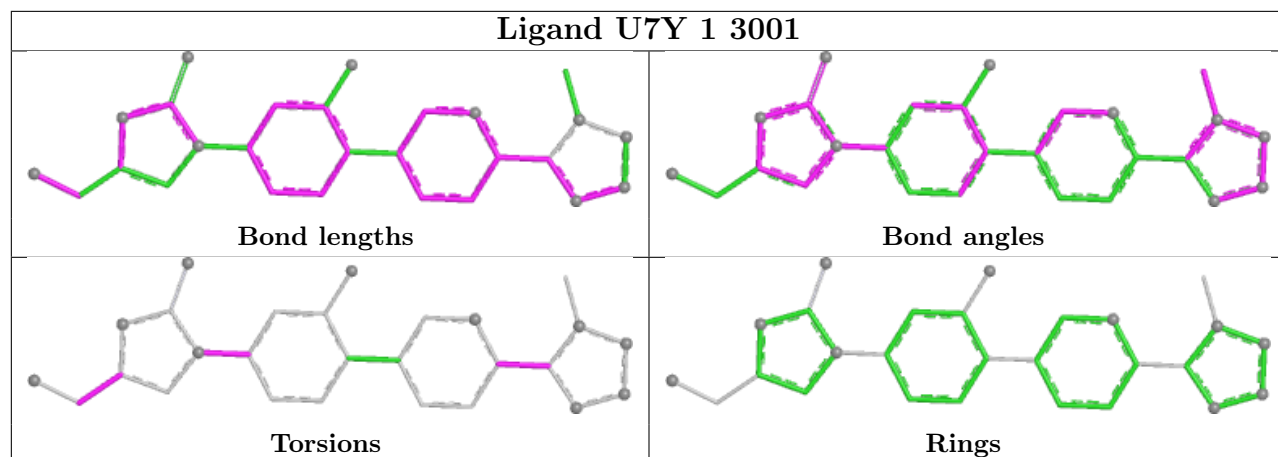
Mol	Chain	Res	Type	Atoms
29	1	3001	U7Y	N1-C1-C2-C3
29	1	3001	U7Y	N1-C1-C2-N5
29	1	3001	U7Y	N4-C1-C2-C3
29	1	3001	U7Y	N4-C1-C2-N5
29	1	3001	U7Y	C14-C15-C16-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1	3001	U7Y	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

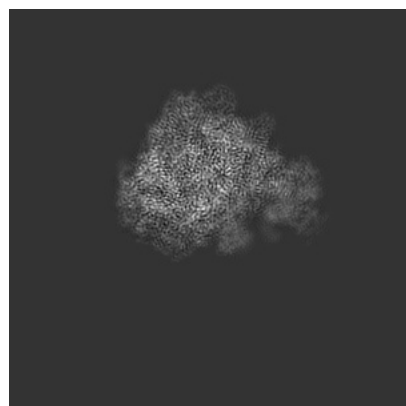
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21888. These allow visual inspection of the internal detail of the map and identification of artifacts.

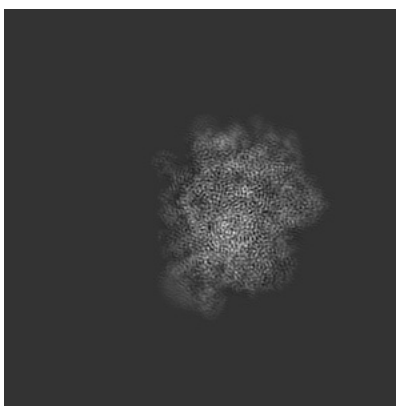
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

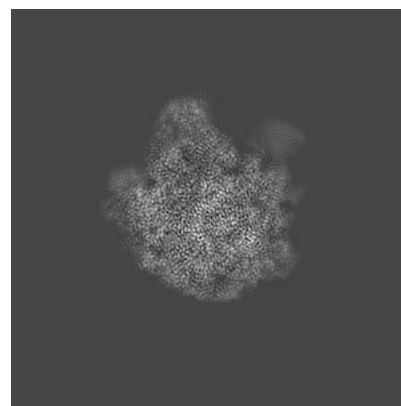
#### 6.1.1 Primary map



X

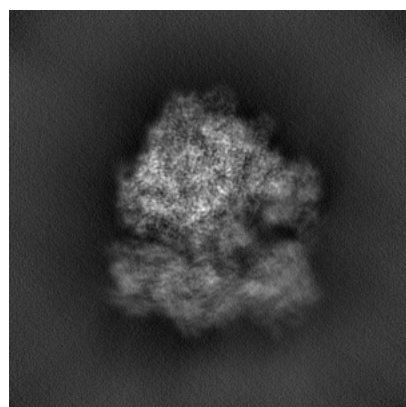


Y

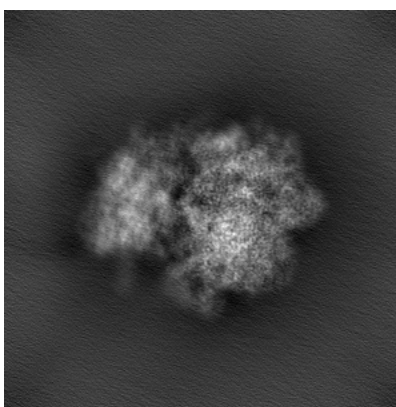


Z

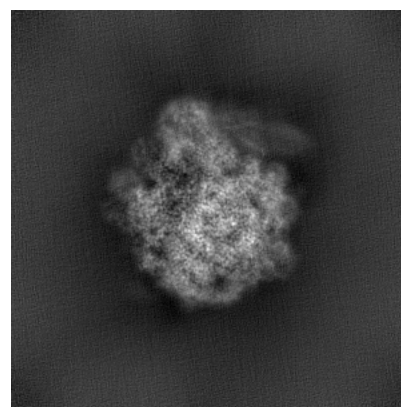
#### 6.1.2 Raw map



X



Y

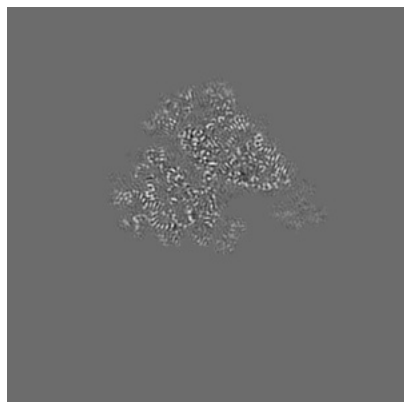


Z

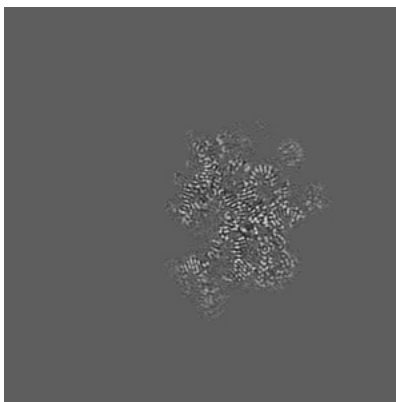
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

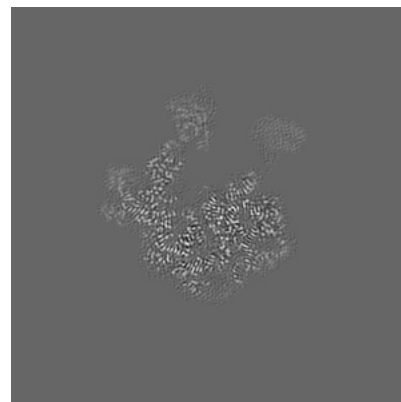
### 6.2.1 Primary map



X Index: 216

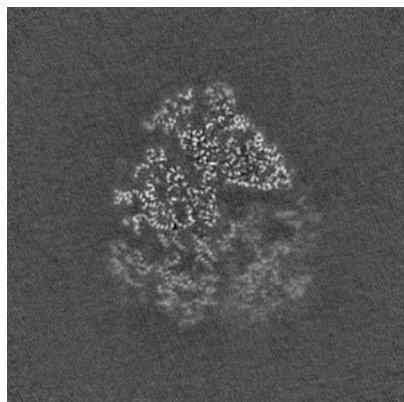


Y Index: 216

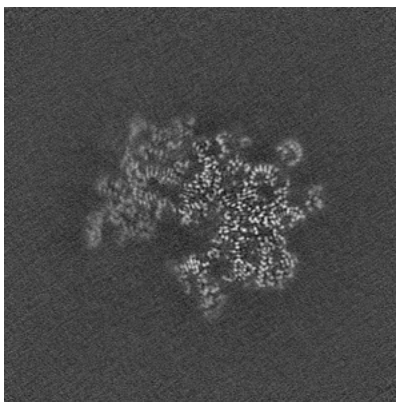


Z Index: 216

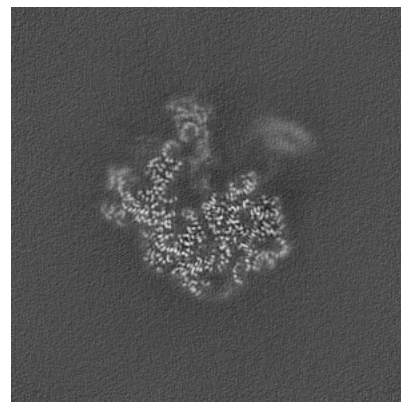
### 6.2.2 Raw map



X Index: 216



Y Index: 216

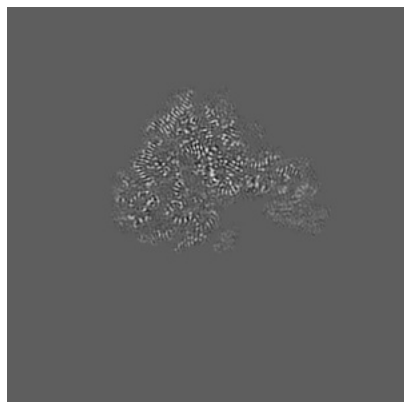


Z Index: 216

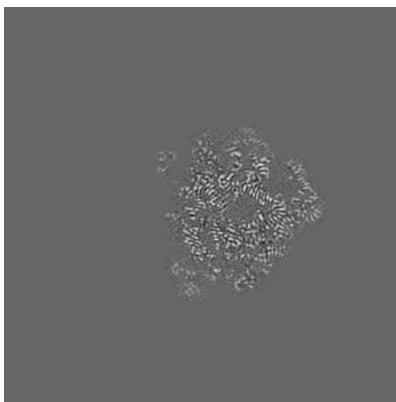
The images above show central slices of the map in three orthogonal directions.

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

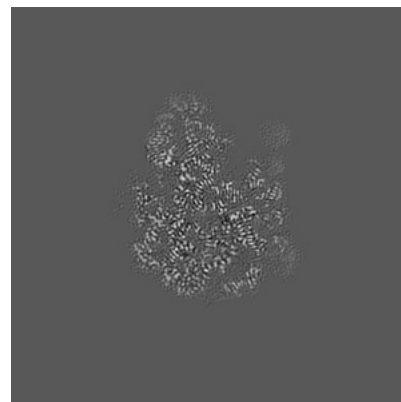
### 6.3.1 Primary map



X Index: 206

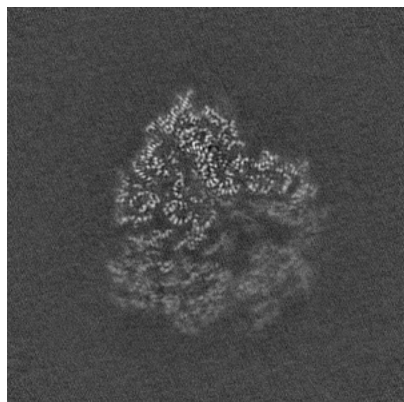


Y Index: 195

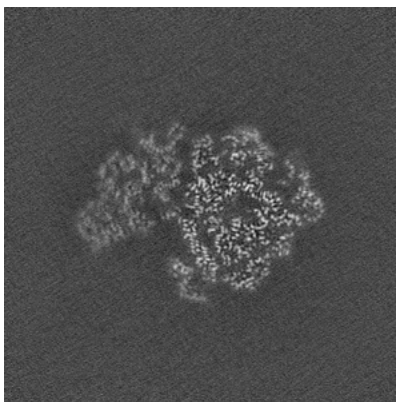


Z Index: 242

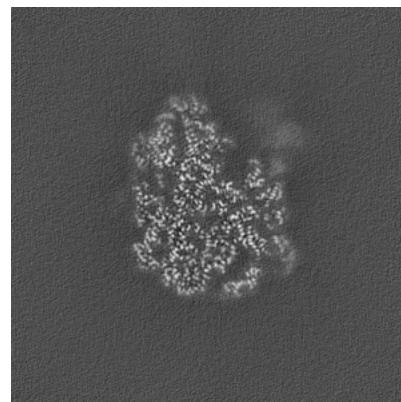
### 6.3.2 Raw map



X Index: 205



Y Index: 199

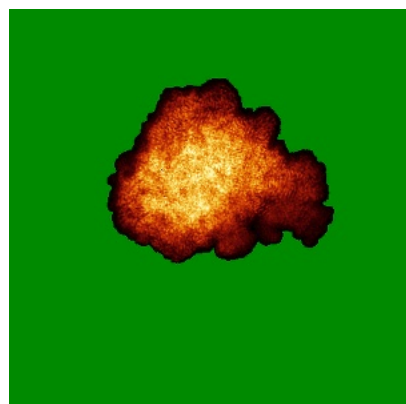


Z Index: 242

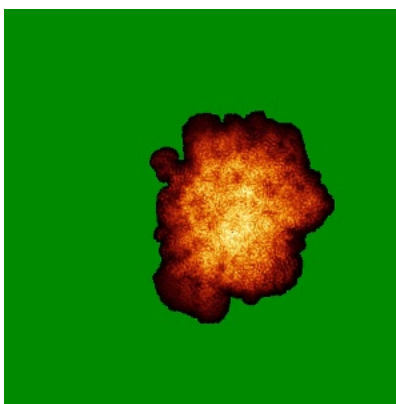
The images above show the largest variance slices of the map in three orthogonal directions.

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

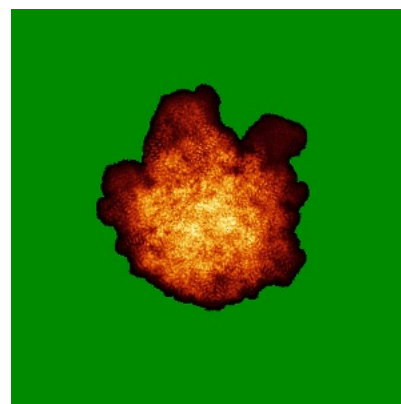
### 6.4.1 Primary map



X

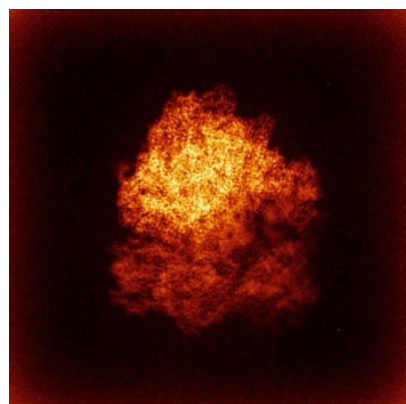


Y

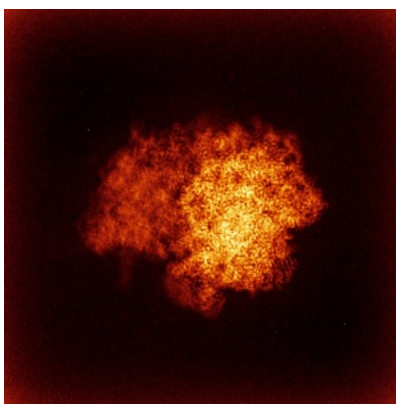


Z

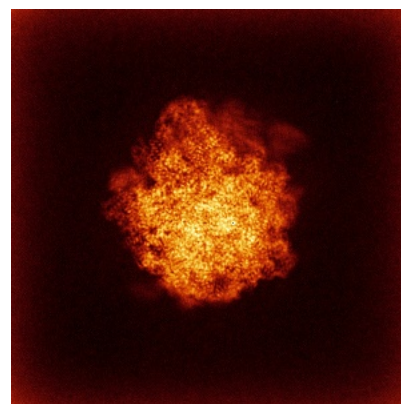
### 6.4.2 Raw map



X



Y

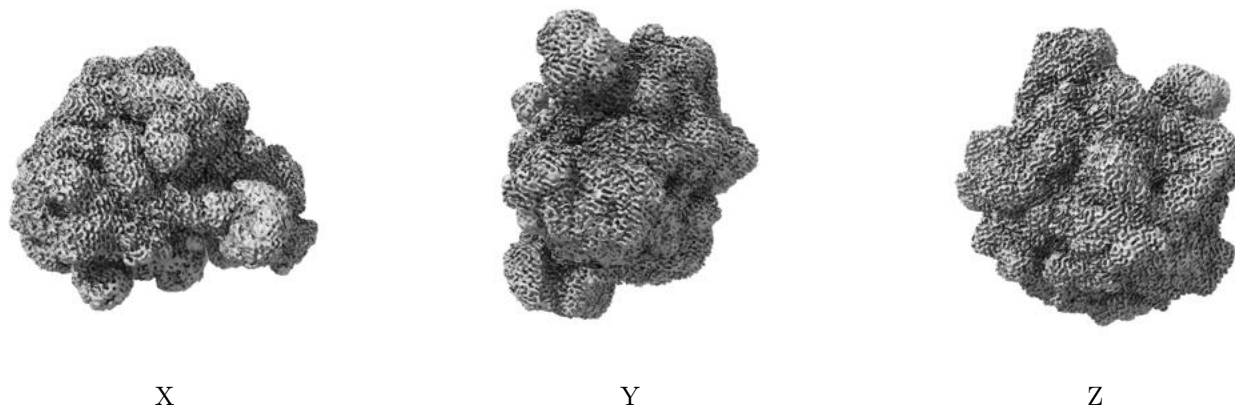


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

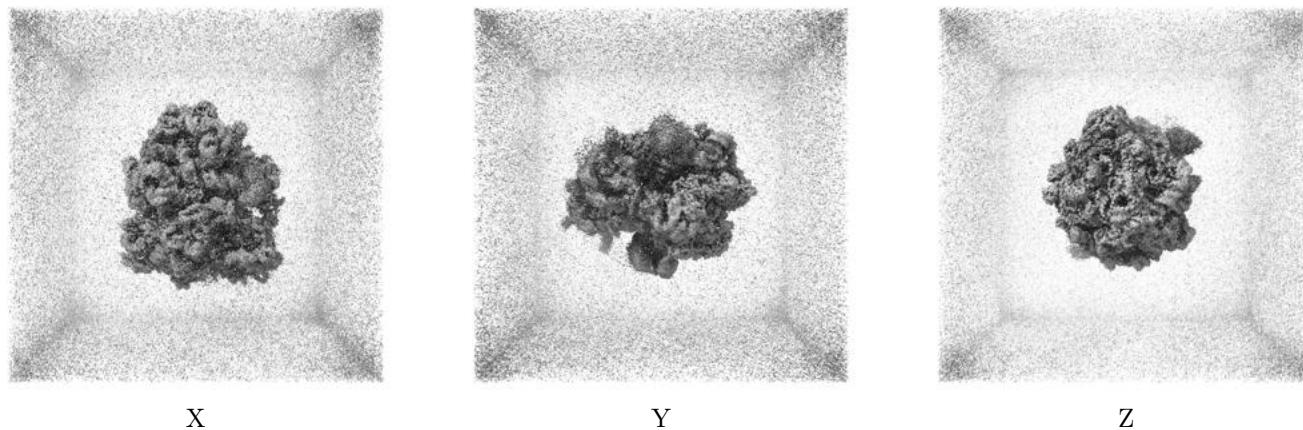
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

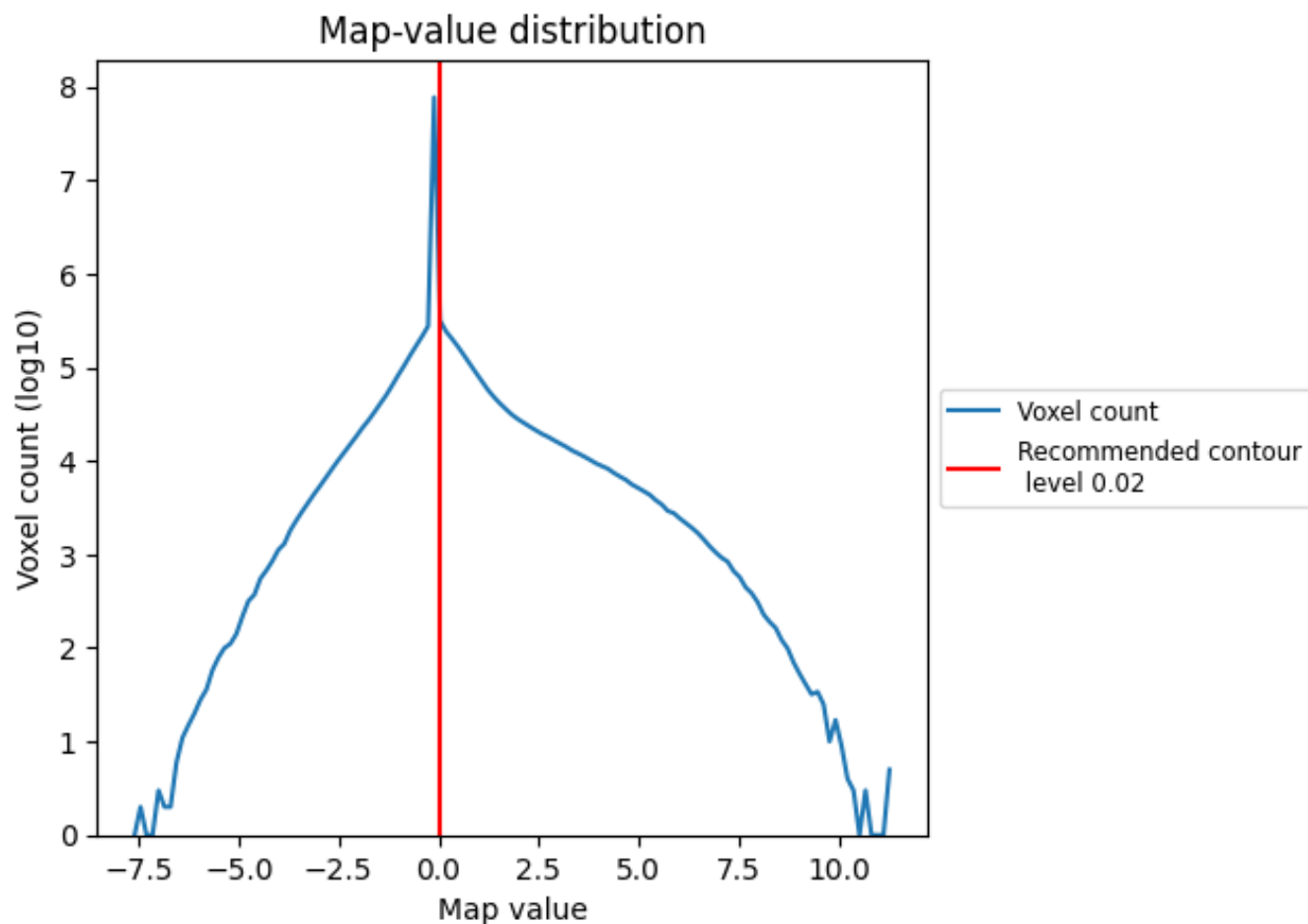
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

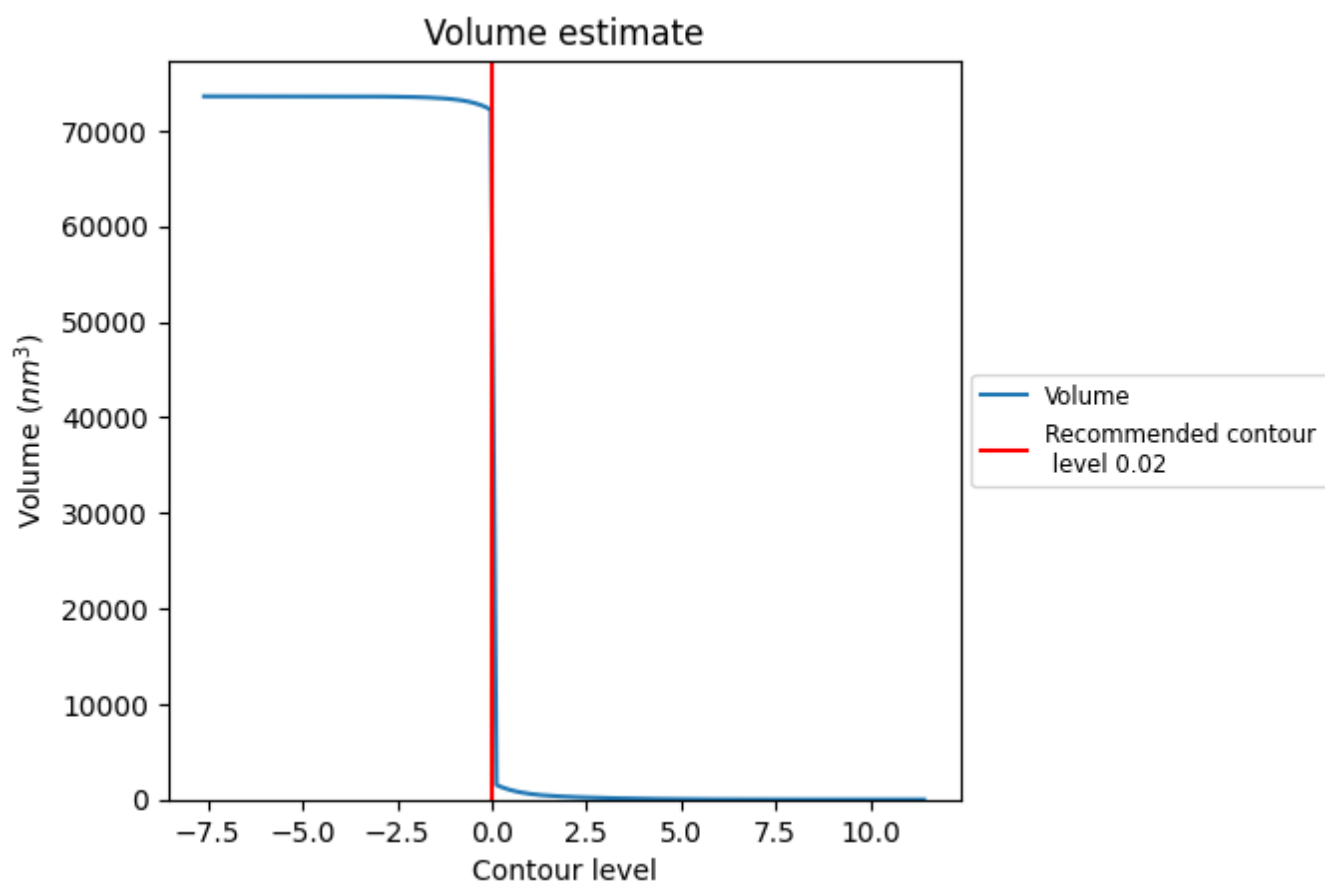
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

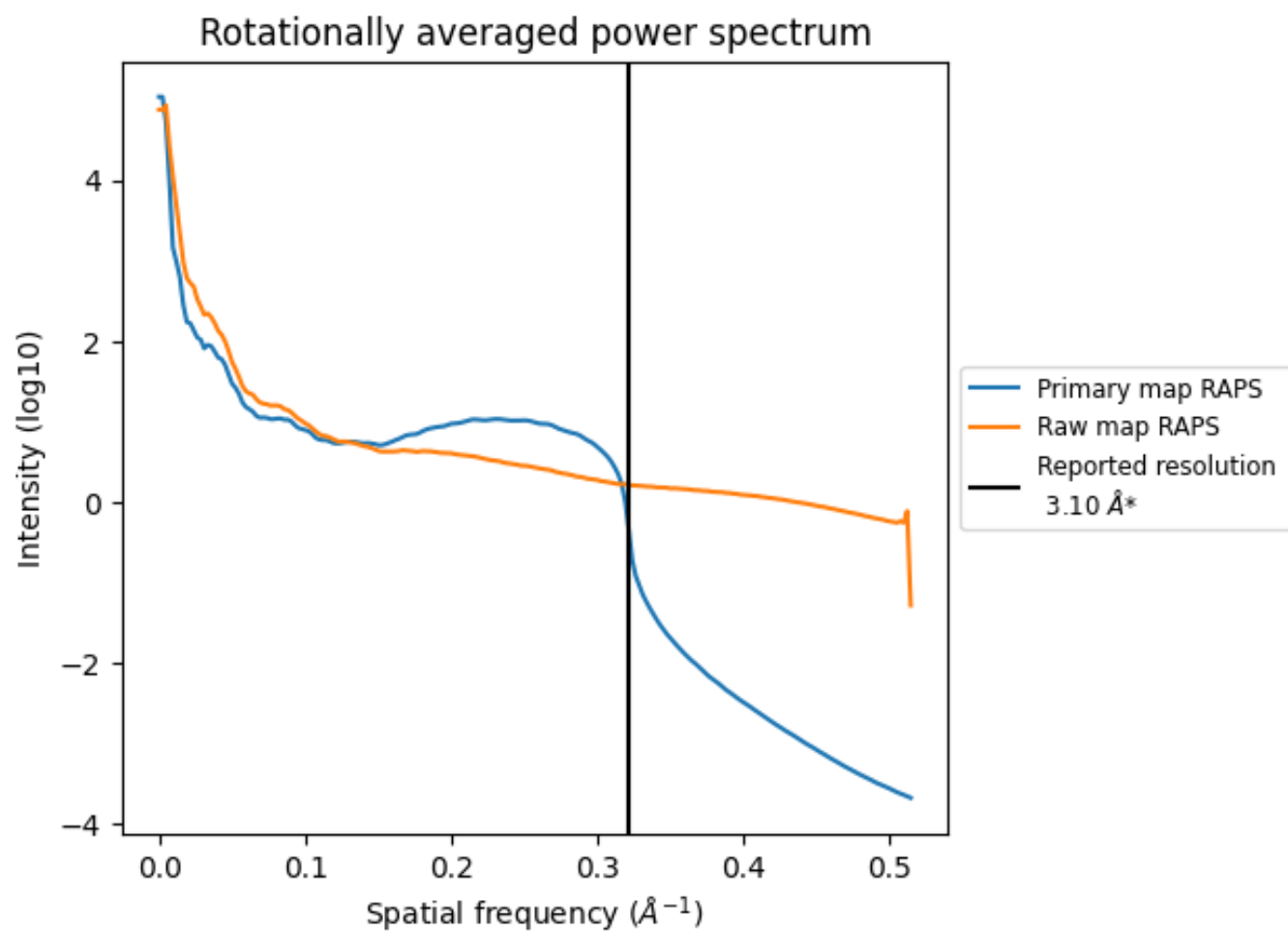
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51111  $\text{nm}^3$ ; this corresponds to an approximate mass of 46170 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 ⓘ

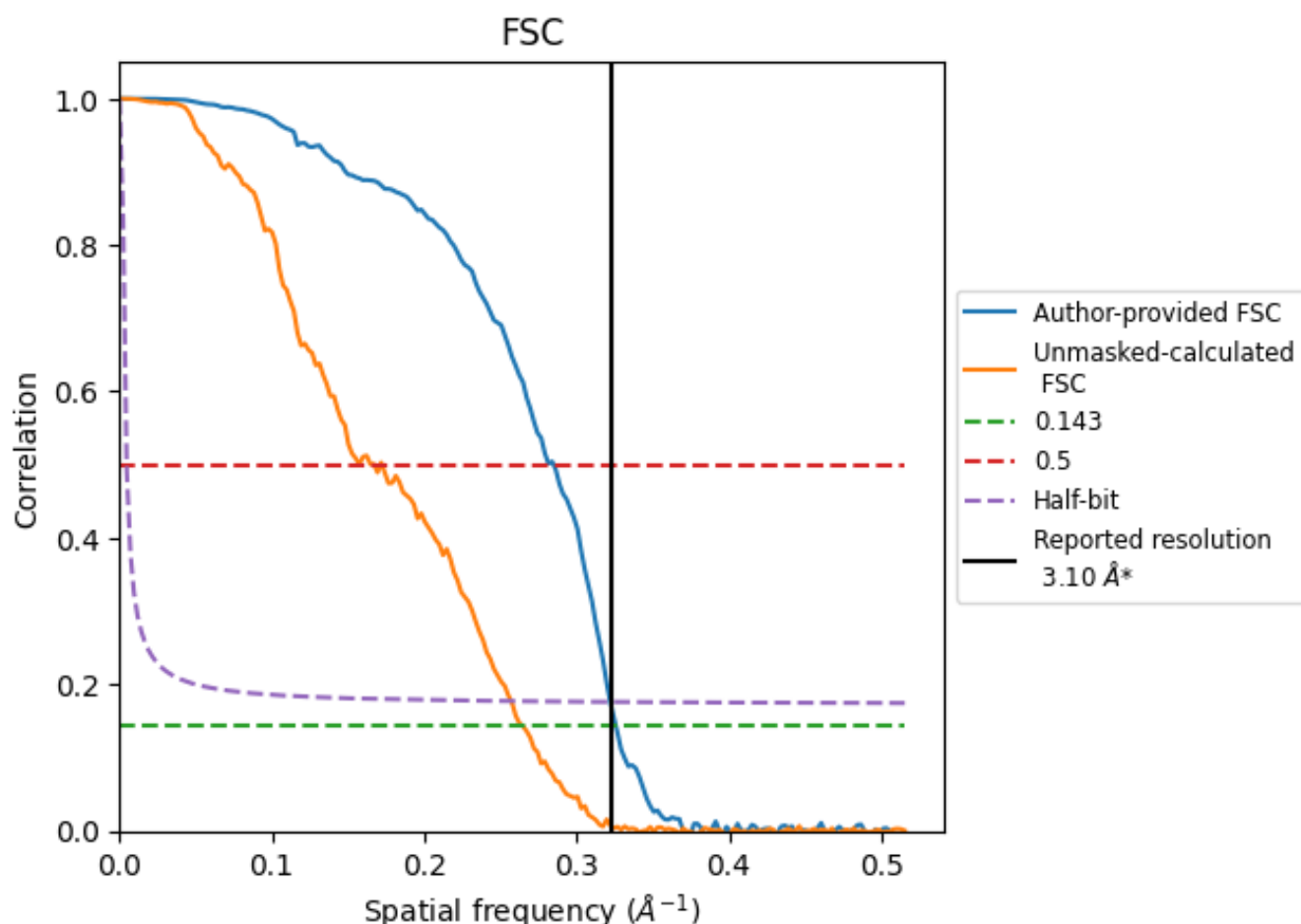


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

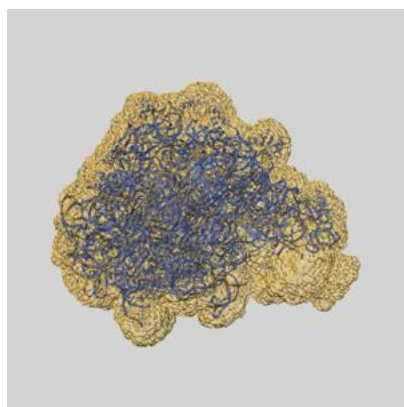
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.51	3.10
Unmasked-calculated*	3.78	5.98	3.89

\*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 3.78 differs from the reported value 3.1 by more than 10 %

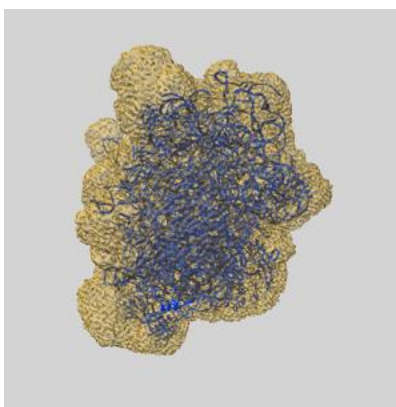
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21888 and PDB model 6WRU. Per-residue inclusion information can be found in section [3](#) on page [10](#).

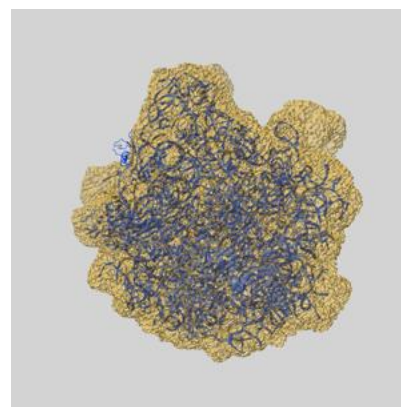
### 9.1 Map-model overlay [i](#)



X



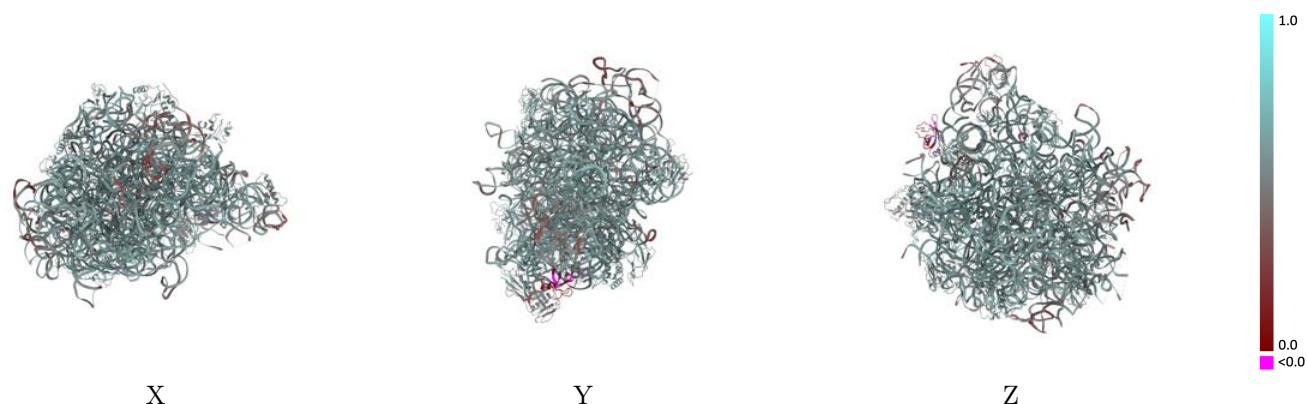
Y



Z

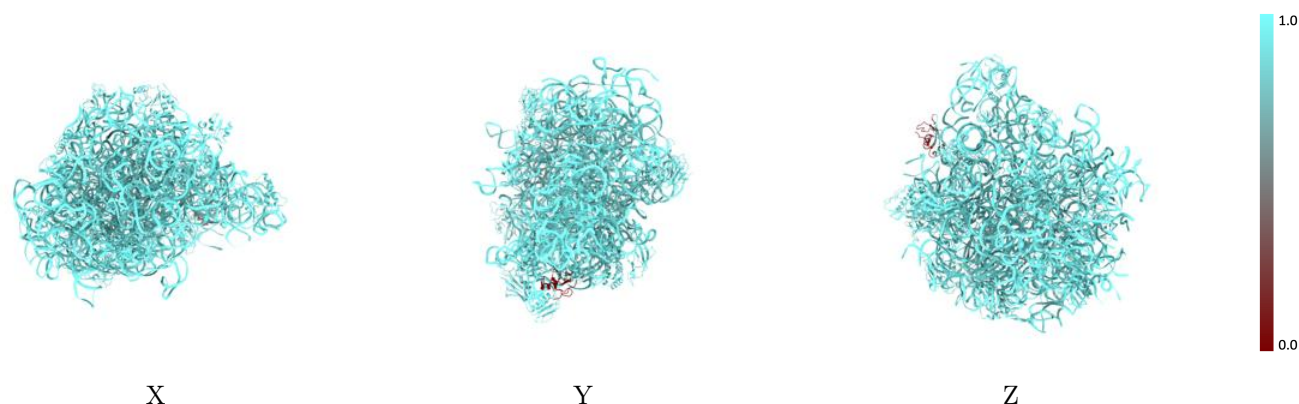
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



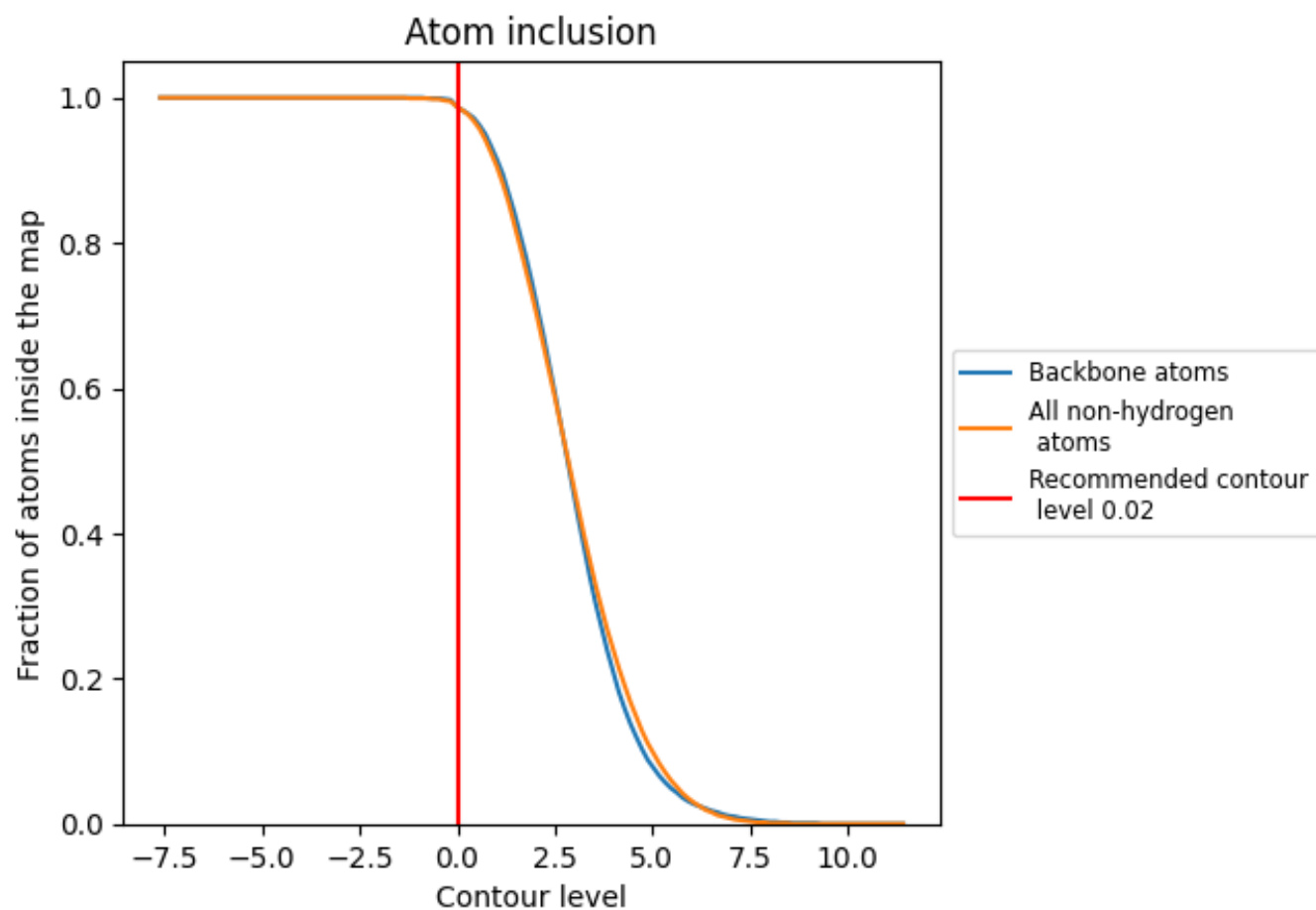
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9860	 0.5670
1	 0.9920	 0.5730
2	 0.9900	 0.4860
A	 0.9940	 0.5800
B	 0.9890	 0.5890
C	 0.9910	 0.5910
D	 0.9970	 0.5820
E	 0.9940	 0.5940
F	 0.9840	 0.5540
G	 0.9940	 0.5620
H	 0.3800	 0.1680
I	 0.9880	 0.5810
J	 0.9910	 0.5570
K	 0.9870	 0.5310
L	 0.9820	 0.5700
M	 0.9840	 0.5730
N	 0.9950	 0.5930
O	 0.9790	 0.5610
P	 0.9890	 0.6100
Q	 0.9980	 0.6180
R	 1.0000	 0.5920
S	 0.9870	 0.5690
U	 0.9850	 0.4980
V	 0.9930	 0.5920
W	 0.9880	 0.5730
X	 0.9900	 0.5760
Y	 0.9950	 0.5910
Z	 0.9920	 0.5870
a	 0.9890	 0.5220

