wwPDB EM Validation Summary Report (i)

Nov 13, 2022 – 08:11 AM EST

PDB ID	:	6WRS
EMDB ID	:	EMD-21887
Title	:	Structure of the 50S subunit of the ribosome from Methicillin Resistant Staphylococcus aureus in complex with the antibiotic, tedizolid
Authors	:	Belousoff, M.J.
Deposited on	:	2020-04-30
Resolution	:	3.20 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 (i) 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 (1)) were used in the production of this report:

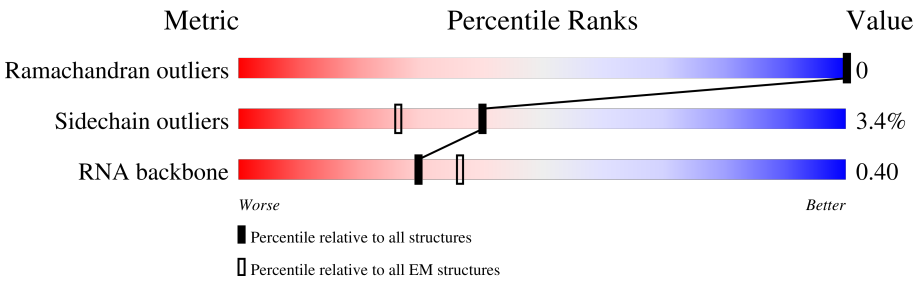
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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 <=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	97%
2	B	277	95%
3	C	118	94%
4	D	105	91% 5%
5	E	117	91% 5%
6	F	91	85% 11%
7	G	105	95% 5%
8	H	107	78% 9% 13%

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Mol	Chain	Length	Quality of chain
9	J	62	90% 5% 5%
10	K	72	79% 19%
11	L	217	96%
12	M	58	97%
13	N	57	86% 12%
14	O	49	92%
15	P	50	88% 12%
16	Q	65	98%
17	R	37	100%
18	S	207	92% 7%
19	V	145	97%
20	W	122	98%
21	X	146	95%
22	Y	144	93% 6%
23	Z	122	98%
24	a	119	90% 8%
25	1	2923	66% 26% 8%
26	2	115	57% 38%
27	I	85	92% 8%

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 81130 atoms, of which 15 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
			Total	C	N	O		
1	A	113	915	576	184	155	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	274	2094	1303	415	371	5	0	0

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

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

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

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

- Molecule 5 is a protein called uL22.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	110	ALA	GLY	variant	UNP A7X5F6

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

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

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
			Total	C	N	O	S		
7	G	100	770	486	141	142	1	0	0

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
			Total	C	N	O	S		
8	H	93	727	465	129	132	1	0	0

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

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

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
			Total	C	N	O		
10	K	58	481	296	92	93	0	0

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

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

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

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

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

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

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
			Total	C	N	O	S		
14	O	47	390	233	79	73	5	0	0

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

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

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

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

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

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

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

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

- Molecule 19 is a protein called 50S ribosomal protein L13.

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

- Molecule 20 is a protein called 50S ribosomal protein L14.

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

- Molecule 21 is a protein called 50S ribosomal protein L15.

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

- Molecule 22 is a protein called 50S ribosomal protein L16.

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

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Z	121	955	586	183	185	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	a	110	857	536	165	156	0	0

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	1	2698	57851	25835	10608	18715	2693	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	2	111	2358	1056	422	770	110	0	0

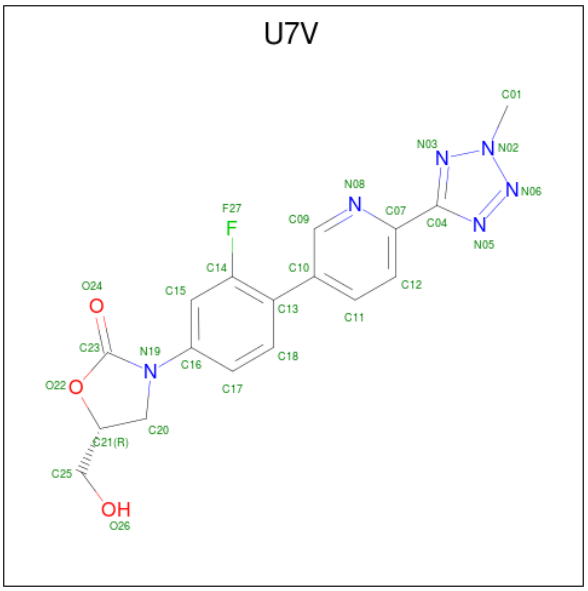
There are 4 discrepancies between the modelled and reference sequences:

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 27 is a protein called 50S ribosomal protein L27.

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

- Molecule 28 is Tedizolid (three-letter code: U7V) (formula: $C_{17}H_{15}FN_6O_3$) (labeled as "Ligand of Interest" by depositor).



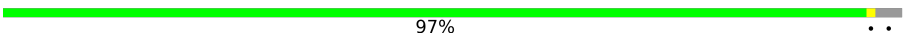
Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	H	N	O	
28	1	1	42	17	1	15	6	3	0

3 Residue-property plots (i)

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.

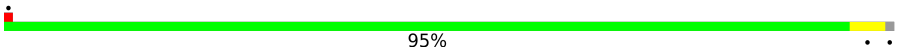
- Molecule 1: 50S ribosomal protein L19

Chain A:



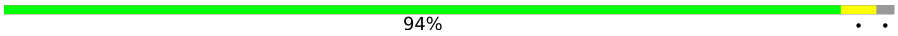
- Molecule 2: 50S ribosomal protein L2

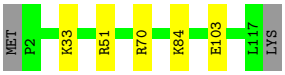
Chain B:



- Molecule 3: 50S ribosomal protein L20

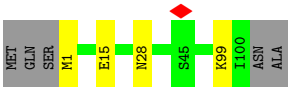
Chain C:





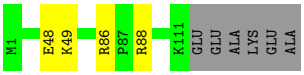
- Molecule 4: 50S ribosomal protein L21

Chain D:



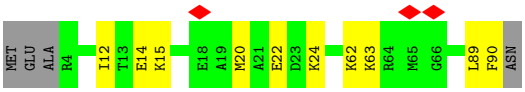
- Molecule 5: uL22

Chain E:



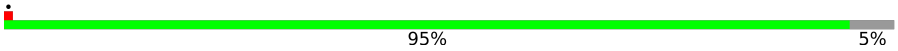
- Molecule 6: 50S ribosomal protein L23

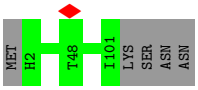
Chain F:



- Molecule 7: 50S ribosomal protein L24

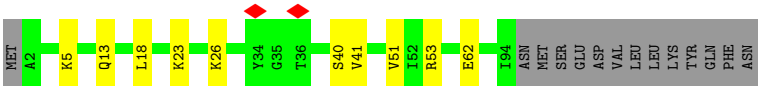
Chain G:





- Molecule 8: uL25

Chain H:

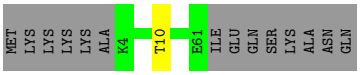


- Molecule 9: 50S ribosomal protein L28

Chain J:

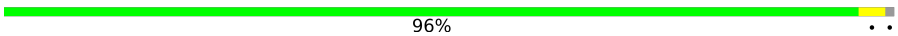
- Molecule 10: 50S ribosomal protein L29

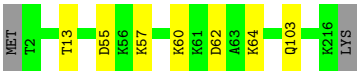
Chain K:



- Molecule 11: 50S ribosomal protein L3

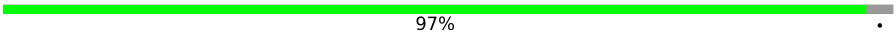
Chain L:





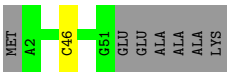
- Molecule 12: 50S ribosomal protein L30

Chain M:



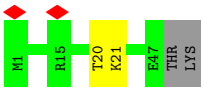
- Molecule 13: 50S ribosomal protein L32

Chain N: 86% 12%



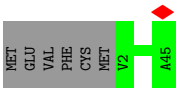
• Molecule 14: 50S ribosomal protein L33

Chain O: 92%



• Molecule 15: 50S ribosomal protein L34

Chain P: 88% 12%



• Molecule 16: 50S ribosomal protein L35

Chain Q: 98%

• Molecule 17: 50S ribosomal protein L36

Chain R: 100%

There are no outlier residues recorded for this chain.

• Molecule 18: 50S ribosomal protein L4

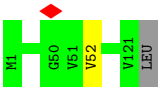
Chain S: 92% 7%

• Molecule 19: 50S ribosomal protein L13

Chain V: 97%

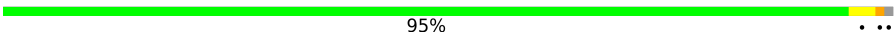
• Molecule 20: 50S ribosomal protein L14

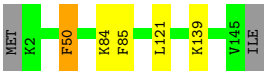
Chain W: 98%



- Molecule 21: 50S ribosomal protein L15

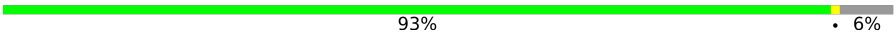
Chain X:





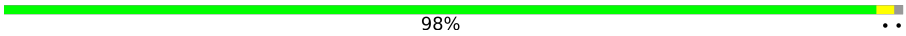
- Molecule 22: 50S ribosomal protein L16

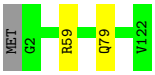
Chain Y:



- Molecule 23: 50S ribosomal protein L17

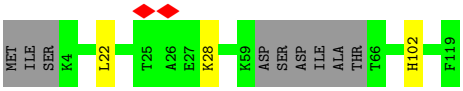
Chain Z:





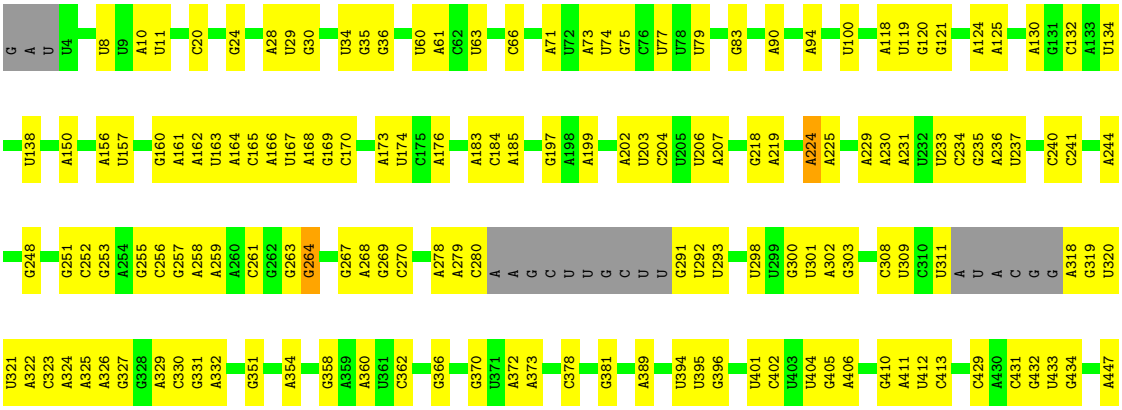
- Molecule 24: 50S ribosomal protein L18

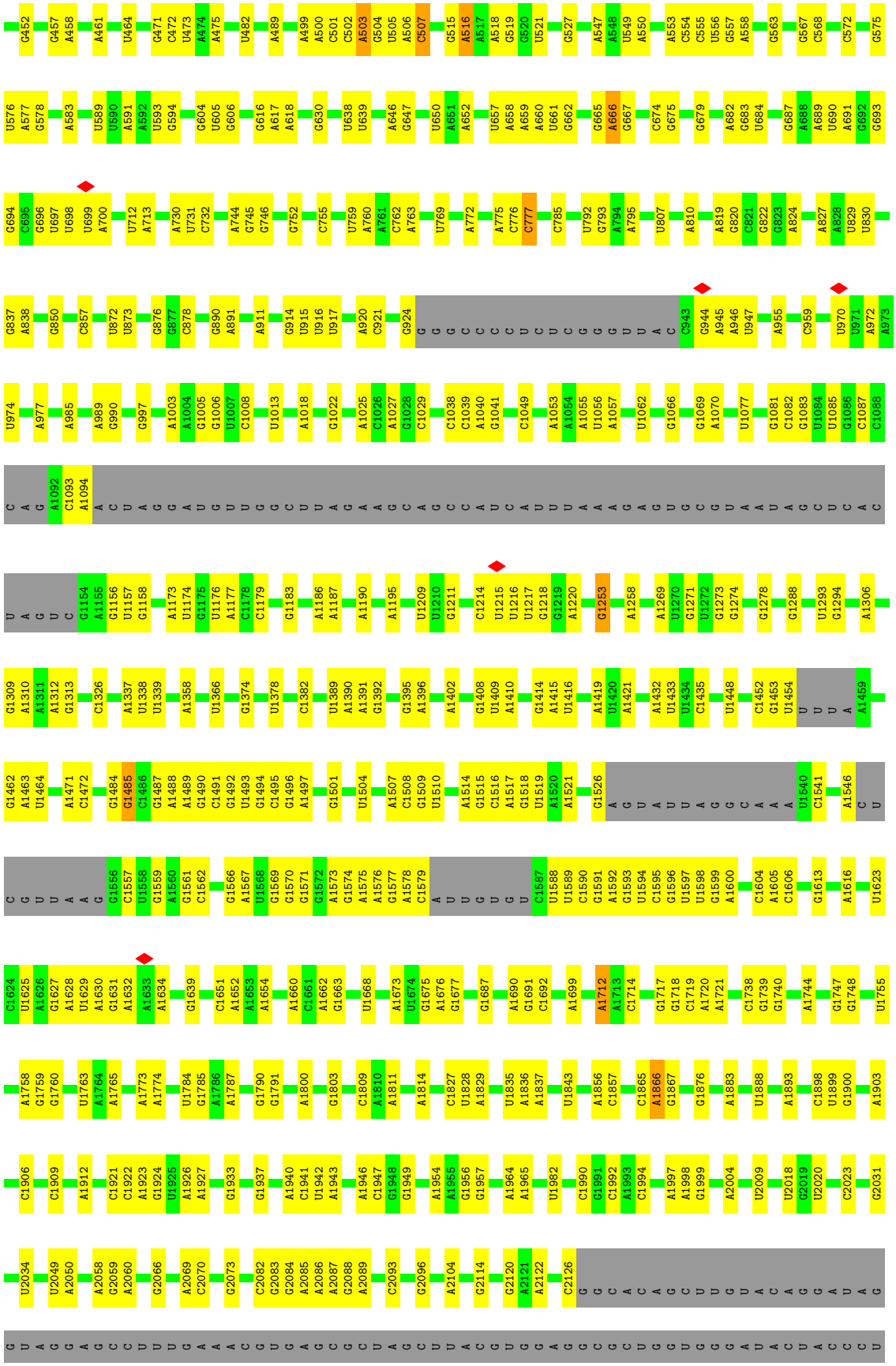
Chain a:

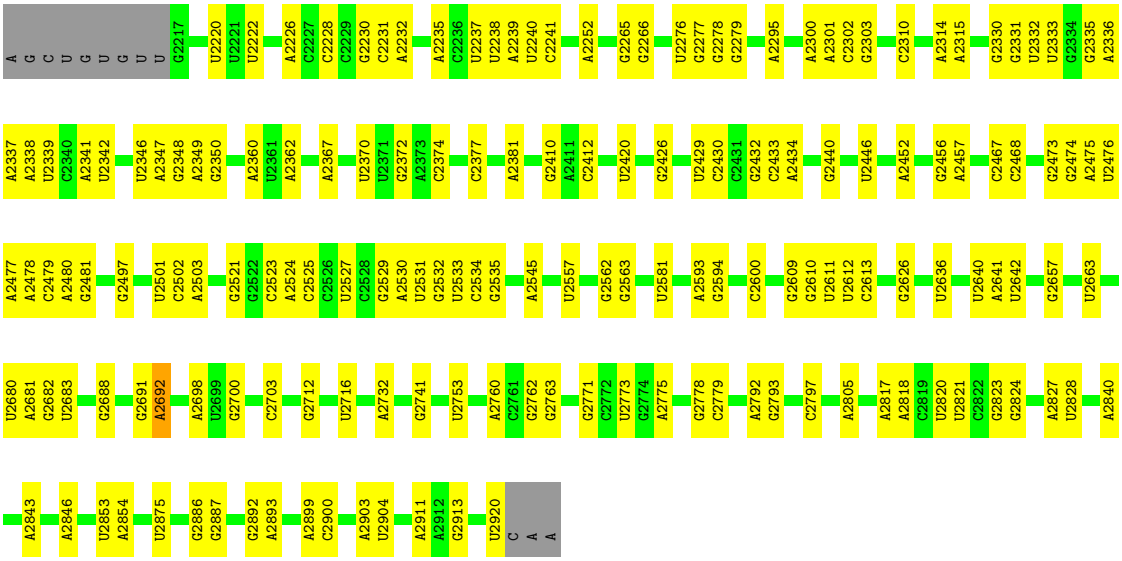


- Molecule 25: 23S rRNA

Chain 1:

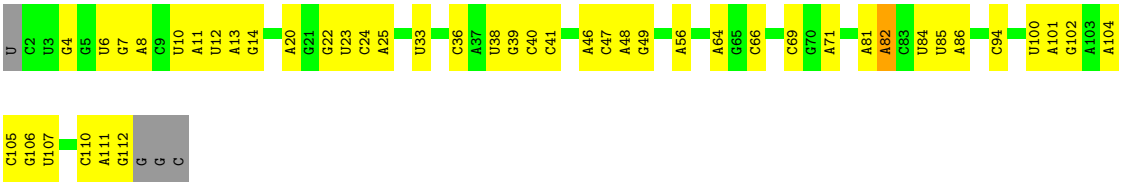



G452
G457 A458
A461
U464
G471 C472 U473 A474 A475
U482
A489
A499 A500 C501 C502 A503 G504 U505 A506 C507
G515 A516 A517 A518 G519 G520 U521
G527
A547 A548 U549 A550
A553 C554 C555 U556 G557 A558
G563
G567 C568
C572
G575
U576 A577 G578
A583
U589 U590 A591 A592 U593 G594
G604 U605 G606
G616 A617 A618
G630
U638 U639
A646 G647
U650 A651 A652
U657 A658 A659 A660 U661 G662
G665 A666 G667
C674 G675
G679
A682 G683 U684
G687 A688 A689 U690 A691 G692 G693
G694 C695 G696 U697 U698 U699 A700
U712 A713
A730 U731 C732
A744 G745 G746
G752
C755
U759 A760 A761 C762 A763
U769
A772
A775 C776 C777
C785
U792 G793 A794 A795
U807
A810
A819 G820 C821 G822 G823 A824
A827 A828 U829 U830
G837 A838
G850
C857
U872 U873
G876 G877 C878
G890 A891
A911
G914 U915 U916 U917
A920 C921
G924
G G G C C C U C U U A C C943 G944 A945 A946 U947
A955
C959
U970 U971 A972 A973
U974
A977
A985
A989 G990
G997
A1003 A1004 G1005 G1006 U1007 C1008
U1013
A1018
G1022
A1025 C1026 A1027 G1028 C1029
C1038 C1039 A1040 G1041
C1049
A1053 A1054 A1055 U1056 A1057
U1062
G1066
G1069 A1070
U1077
G1081 C1082 G1083 U1084 U1085 G1086 C1087 C1088
C A G A1092 C1093 A1094 A C U A G G A U G U U G G C C U A A G A A G C A G C U U U C A A A G A G U G U A C C U C A C
U A G U C G1154 A1155 G1156 U1157 G1158
A1173 U1174 G1175 U1176 A1177 C1178 C1179
G1183
A1186 A1187
A1190
A1195
U1209 U1210 G1211
C1214
U1215 U1216 U1217 G1218 G1219 A1220
G1253
A1258
A1269 U1270 G1271 U1272 G1273 G1274
G1278
G1288
U1293 G1294
A1306
G1309 A1310 A1311 A1312 G1313
C1326
A1337 U1338 U1339
A1358
U1366
G1374
U1378
C1382
U1389 A1390 A1391 G1392
G1395 A1396
A1402
G1408 U1409 A1410
G1414 A1415 U1416
A1419 U1420 A1421
A1432 U1433 U1434 C1435
U1448
C1452 G1453 U1454 U U U A A1459
G1462 A1463 U1464
A1471 C1472
G1484 G1485 C1486 G1487 A1488 A1489 G1490 C1491 G1492 U1493 G1494 C1495 G1496 A1497
G1501
U1504
A1507 C1508 G1509 U1510
A1514 G1515 C1516 A1517 G1518 U1519 A1520 A1521
G1526
A G U A U U A G G C A A A U1540 C1541
A1546
C U
C G U U A A G G1556 C1557 U1558 G1559 A1560 G1561 C1562
G1566 A1567 U1568 G1569 G1570 G1571 G1572 A1573 G1574 A1575 A1576 G1577 A1578 C1579
A U U G U G U C1587 U1588 U1589 C1590 G1591 A1592 G1593 U1594 C1595 G1596 U1597 U1598 G1599 A1600
C1604 A1605 C1606
G1613
A1616
U1623
C1624 U1625 A1626 G1627 A1628 U1629 A1630 G1631 A1632 A1633 A1634
G1639
C1651 A1652 A1653 A1654
A1660 C1661 A1662 G1663
U1668
A1673 U1674 G1675 A1676 G1677
G1687
A1690 G1691 C1692
A1699
A1712 A1713 C1714
G1717 G1718 C1719 A1720 A1721
C1738 G1739 G1740
A1744
G1747 G1748
U1755
A1758 G1759 G1760
U1763 A1764 A1765
A1773 A1774
U1784 G1785 A1786 A1787
G1790 G1791
A1800
G1803
C1809 A1810 A1811
A1814
C1827 U1828 A1829
U1835 A1836 A1837
U1843
A1856 C1857
C1865 A1866 G1867
G1876
A1883
U1888
A1893
C1898 U1899 G1900
A1903
C1906
C1909
A1912
C1921 C1922 A1923 G1924
U1925 A1926 A1927
G1933
G1937
A1940 C1941 U1942 A1943
A1946 C1947 G1948 G1949
A1954
A1955 G1956 G1957
A1964 A1965
U1982
C1990 G1991 C1992 A1993 C1994
A1997 A1998 G1999
A2004
U2009
U2018 G2019 U2020
C2023
G2031
U2034
U2049 A2050
A2058 G2059 A2060
G2066
A2069 C2070
G2073
C2082 G2083 G2084 A2085 A2086 A2087 G2088 A2089
C2093
G2096
A2104
G2114
G2120 A2121 A2122
C2126
G G C A C A G G U U G U A A C A G A A U A C U G A C U



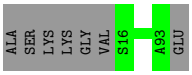
- Molecule 26: 5S rRNA

Chain 2:



- Molecule 27: 50S ribosomal protein L27

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	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	0.432	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	410.4, 410.4, 410.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: U7V

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	0.38	0/927	0.50	0/1239
2	B	0.48	0/2129	0.54	0/2858
3	C	0.44	0/955	0.47	0/1265
4	D	0.40	0/795	0.52	0/1062
5	E	0.36	0/861	0.49	0/1159
6	F	0.40	0/719	0.51	0/959
7	G	0.34	0/779	0.51	0/1042
8	H	0.33	0/735	0.52	0/986
9	J	0.36	0/469	0.56	0/625
10	K	0.40	0/482	0.53	0/642
11	L	0.41	0/1652	0.59	0/2216
12	M	0.42	0/434	0.56	0/585
13	N	0.41	0/404	0.52	0/537
14	O	0.36	0/393	0.56	0/523
15	P	0.47	0/376	0.51	0/491
16	Q	0.44	0/526	0.52	0/690
17	R	0.36	0/299	0.48	0/393
18	S	0.42	0/1494	0.55	0/2018
19	V	0.47	0/1160	0.56	0/1563
20	W	0.38	0/918	0.53	0/1232
21	X	0.42	0/1096	0.58	1/1461 (0.1%)
22	Y	0.42	0/1113	0.51	0/1493
23	Z	0.42	0/959	0.56	0/1282
24	a	0.35	0/865	0.50	0/1154
25	1	0.86	0/64789	0.89	30/101033 (0.0%)
26	2	0.54	0/2636	0.94	3/4105 (0.1%)
27	I	0.45	0/603	0.51	0/801
All	All	0.77	0/88568	0.83	34/133414 (0.0%)

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	1	2235	A	C4'-C3'-O3'	5.96	124.93	113.00
25	1	777	C	C4'-C3'-O3'	5.95	124.89	113.00
25	1	257	G	N9-C1'-C2'	-5.91	105.50	112.00
25	1	516	A	N9-C1'-C2'	-5.88	105.54	112.00
26	2	82	A	C4'-C3'-O3'	5.72	124.44	113.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	103 (93%)	8 (7%)	0	100	100
2	B	272/277 (98%)	248 (91%)	24 (9%)	0	100	100
3	C	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
4	D	98/105 (93%)	90 (92%)	8 (8%)	0	100	100
5	E	109/117 (93%)	103 (94%)	6 (6%)	0	100	100
6	F	85/91 (93%)	73 (86%)	12 (14%)	0	100	100
7	G	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
8	H	91/107 (85%)	86 (94%)	5 (6%)	0	100	100
9	J	57/62 (92%)	52 (91%)	5 (9%)	0	100	100
10	K	56/72 (78%)	55 (98%)	1 (2%)	0	100	100
11	L	213/217 (98%)	194 (91%)	19 (9%)	0	100	100
12	M	54/58 (93%)	50 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	48/57 (84%)	44 (92%)	4 (8%)	0	100	100
14	O	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
15	P	42/50 (84%)	42 (100%)	0	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%)	174 (92%)	16 (8%)	0	100	100
19	V	141/145 (97%)	133 (94%)	8 (6%)	0	100	100
20	W	119/122 (98%)	109 (92%)	10 (8%)	0	100	100
21	X	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
22	Y	134/144 (93%)	122 (91%)	12 (9%)	0	100	100
23	Z	119/122 (98%)	108 (91%)	11 (9%)	0	100	100
24	a	106/119 (89%)	97 (92%)	9 (8%)	0	100	100
27	I	76/85 (89%)	70 (92%)	6 (8%)	0	100	100
All	All	2617/2793 (94%)	2424 (93%)	193 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	99/102 (97%)	98 (99%)	1 (1%)	76	90
2	B	221/224 (99%)	210 (95%)	11 (5%)	24	60
3	C	96/98 (98%)	91 (95%)	5 (5%)	23	59
4	D	85/89 (96%)	81 (95%)	4 (5%)	26	62
5	E	90/94 (96%)	86 (96%)	4 (4%)	28	64
6	F	79/82 (96%)	69 (87%)	10 (13%)	4	20
7	G	85/91 (93%)	85 (100%)	0	100	100
8	H	81/95 (85%)	71 (88%)	10 (12%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	49/51 (96%)	46 (94%)	3 (6%)	18	54
10	K	53/65 (82%)	52 (98%)	1 (2%)	57	81
11	L	173/175 (99%)	166 (96%)	7 (4%)	31	66
12	M	50/52 (96%)	50 (100%)	0	100	100
13	N	45/49 (92%)	44 (98%)	1 (2%)	52	79
14	O	45/47 (96%)	43 (96%)	2 (4%)	28	64
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%)	156 (99%)	2 (1%)	69	87
19	V	122/123 (99%)	120 (98%)	2 (2%)	62	84
20	W	99/100 (99%)	98 (99%)	1 (1%)	76	90
21	X	110/112 (98%)	105 (96%)	5 (4%)	27	63
22	Y	113/119 (95%)	111 (98%)	2 (2%)	59	82
23	Z	101/102 (99%)	99 (98%)	2 (2%)	55	80
24	a	87/95 (92%)	84 (97%)	3 (3%)	37	70
27	I	61/66 (92%)	61 (100%)	0	100	100
All	All	2231/2337 (96%)	2155 (97%)	76 (3%)	40	70

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	O	20	THR
23	Z	59	ARG
18	S	23	VAL
21	X	84	LYS
24	a	102	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
17	R	36	GLN
18	S	158	ASN
23	Z	79	GLN
18	S	121	ASN

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Mol	Chain	Res	Type
19	V	48	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	1	2689/2923 (91%)	742 (27%)	137 (5%)
26	2	110/115 (95%)	41 (37%)	10 (9%)
All	All	2799/3038 (92%)	783 (27%)	147 (5%)

5 of 783 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	1	8	U
25	1	11	U
25	1	20	C
25	1	24	G
25	1	28	A

5 of 147 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	1	2277	G
26	2	47	C
25	1	2302	C
25	1	2610	G
25	1	502	C

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 monosaccharides 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	$\#\|Z\| > 2$
28	U7V	1	3001	-	28,30,30	2.52	4 (14%)	35,43,43	3.56	21 (60%)

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
28	U7V	1	3001	-	-	6/14/26/26	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	3001	U7V	C23-N19	9.68	1.46	1.36
28	1	3001	U7V	O22-C23	6.37	1.43	1.35
28	1	3001	U7V	C20-N19	-3.70	1.40	1.47
28	1	3001	U7V	O22-C21	-3.51	1.41	1.46

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	1	3001	U7V	C20-N19-C23	-8.50	106.36	111.28
28	1	3001	U7V	C21-O22-C23	-8.25	103.64	110.15
28	1	3001	U7V	O22-C23-N19	-6.72	105.20	109.83
28	1	3001	U7V	C20-N19-C16	5.99	131.59	121.45
28	1	3001	U7V	C04-C07-N08	5.67	123.23	116.75

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	1	3001	U7V	N05-C04-C07-N08
28	1	3001	U7V	C15-C16-N19-C23

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Mol	Chain	Res	Type	Atoms
28	1	3001	U7V	C17-C16-N19-C23
28	1	3001	U7V	N03-C04-C07-N08
28	1	3001	U7V	N05-C04-C07-C12

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand U7V 1 3001

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.

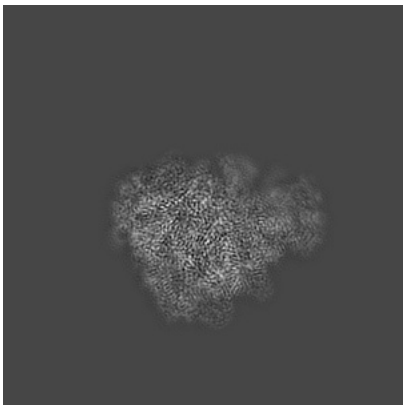
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21887. These allow visual inspection of the internal detail of the map and identification of artifacts.

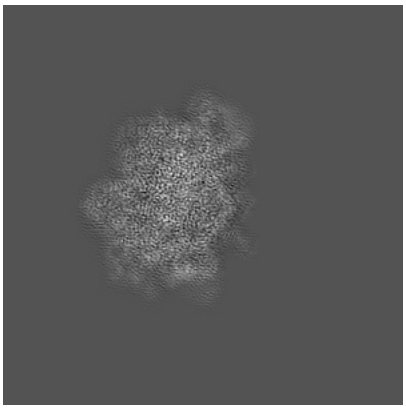
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

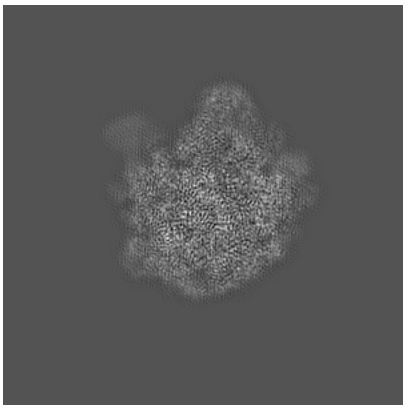
6.1.1 Primary map



X

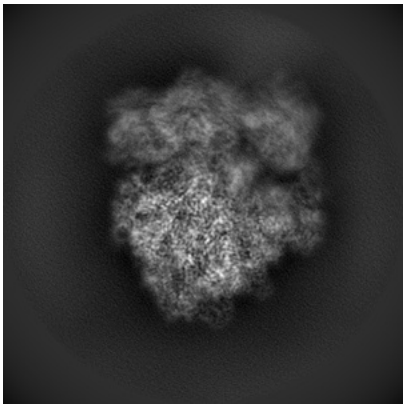


Y

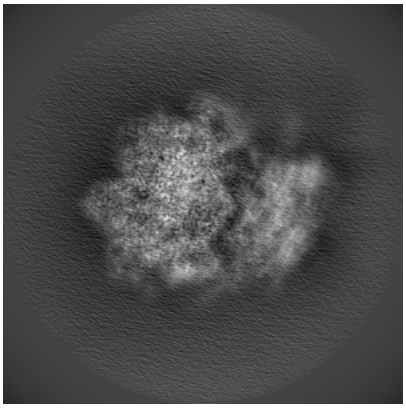


Z

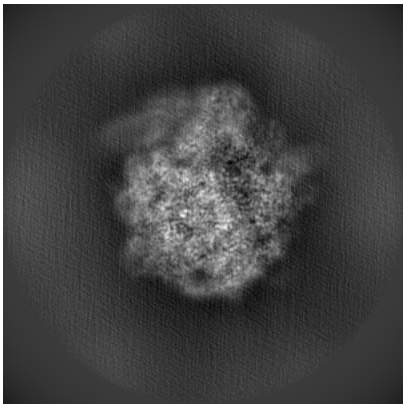
6.1.2 Raw map



X



Y

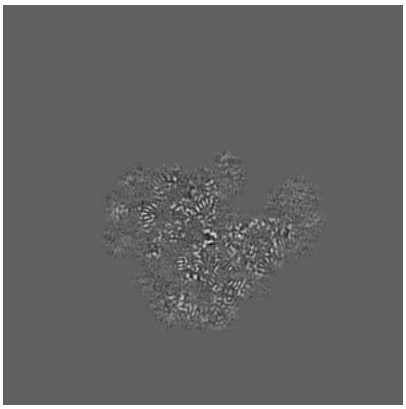


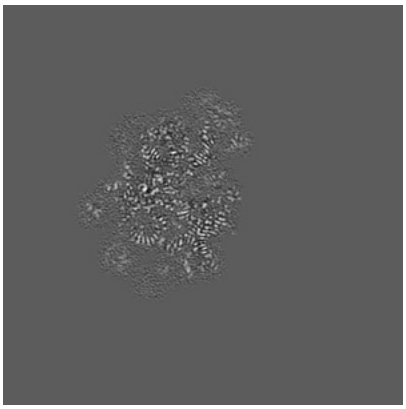
Z

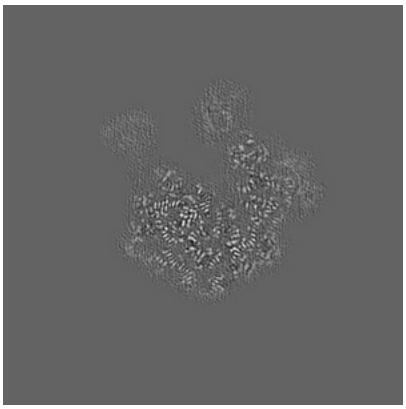
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

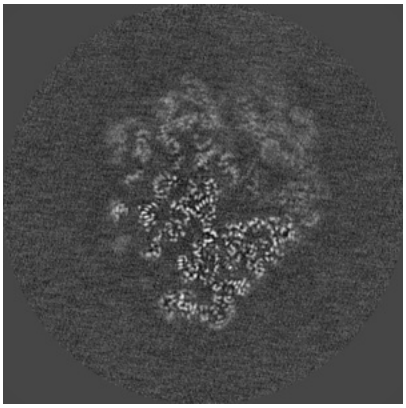
6.2.1 Primary map

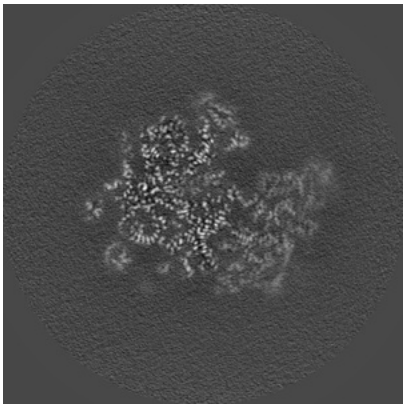

X Index: 180

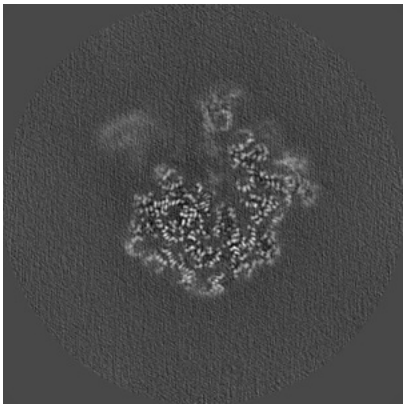

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

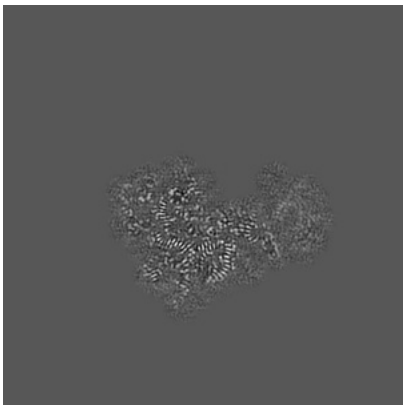

Y Index: 180


Z Index: 180

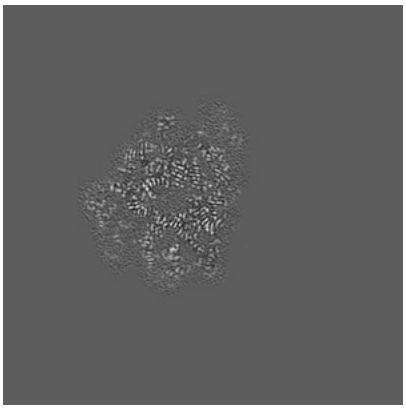
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

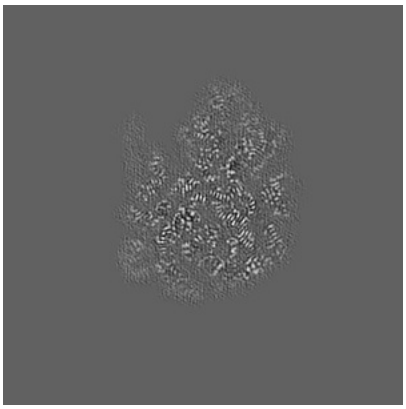
6.3.1 Primary map



X Index: 202

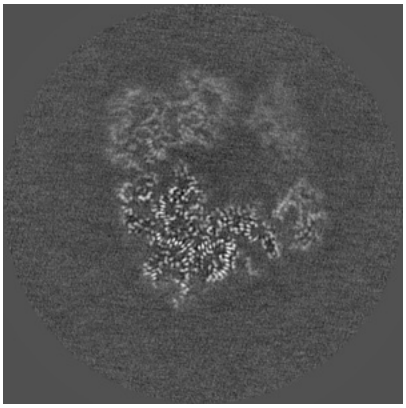


Y Index: 168

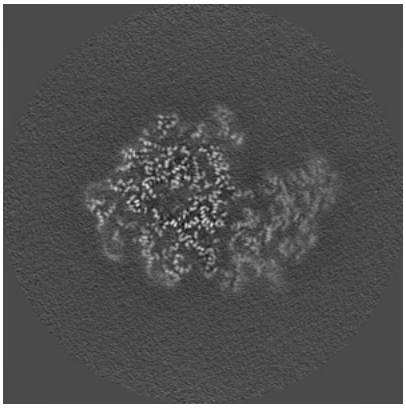


Z Index: 157

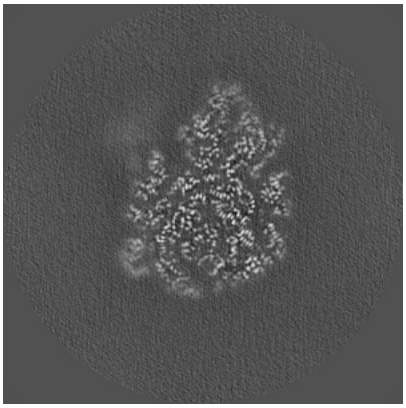
6.3.2 Raw map



X Index: 202



Y Index: 169

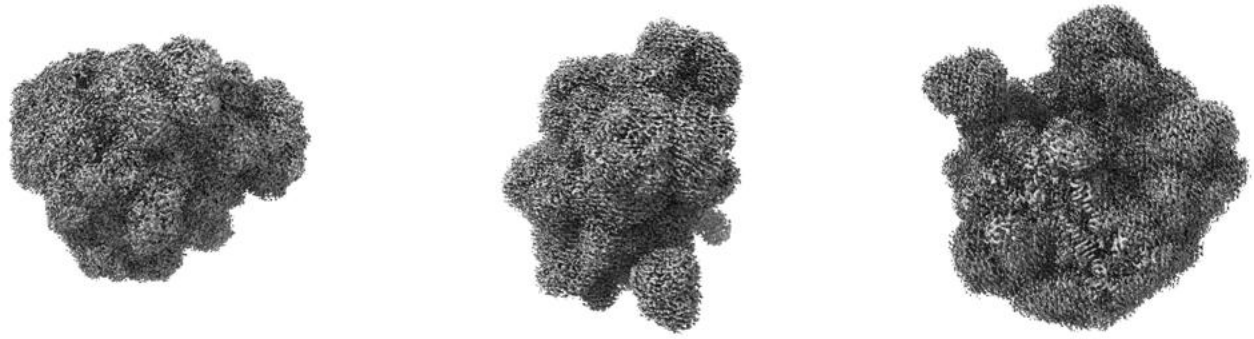


Z Index: 157

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

6.4 Orthogonal surface views (i)

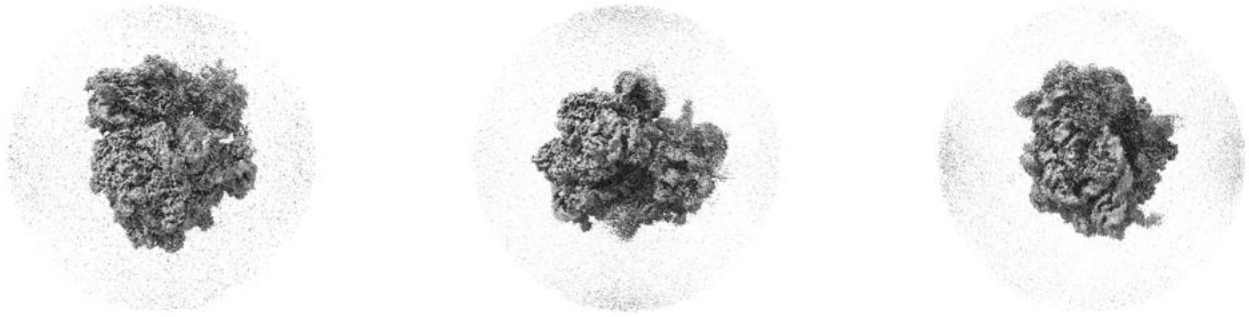
6.4.1 Primary map



X Y Z

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

6.4.2 Raw map



X Y Z

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.

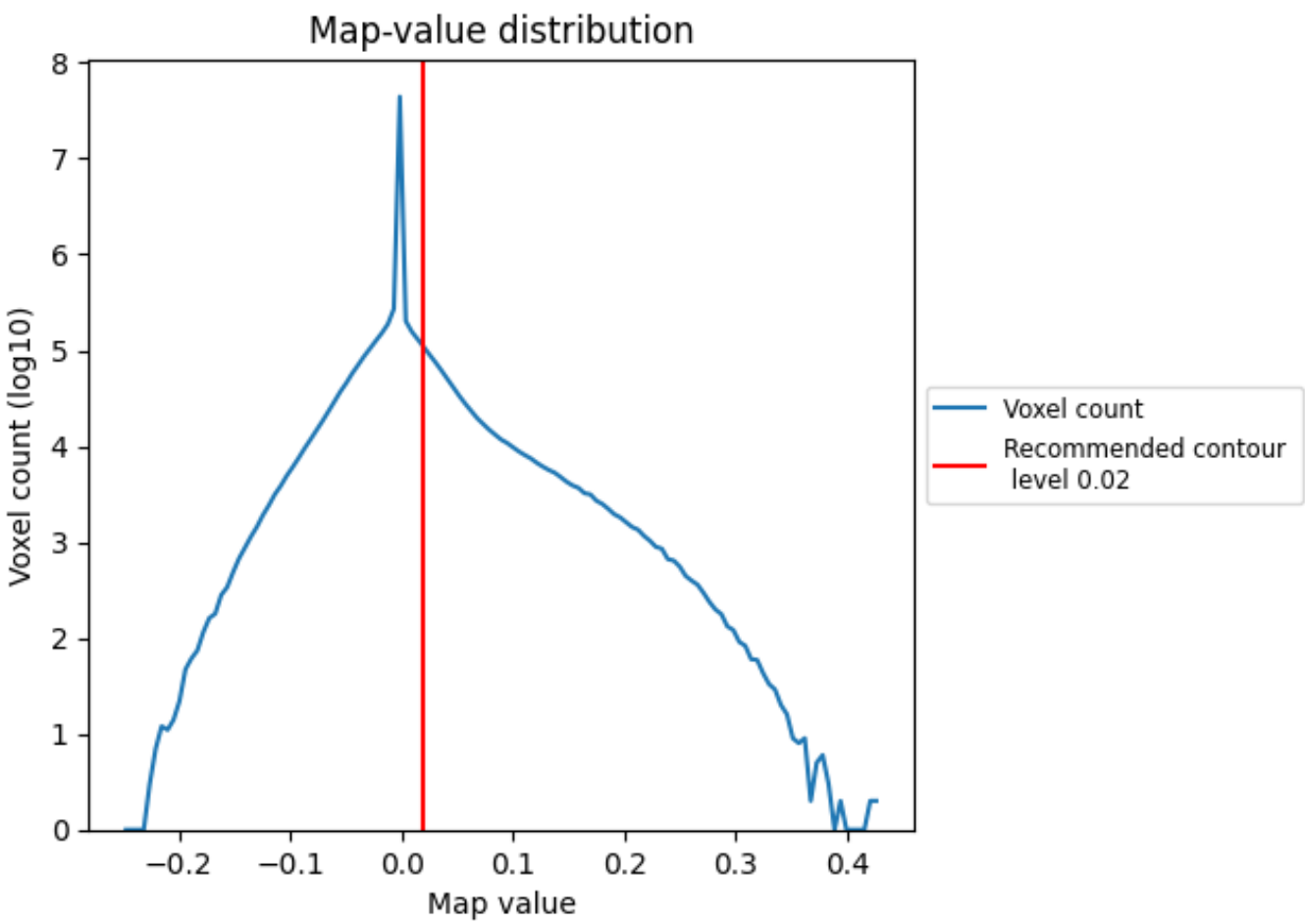
6.5 Mask visualisation (i)

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

7 Map analysis (i)

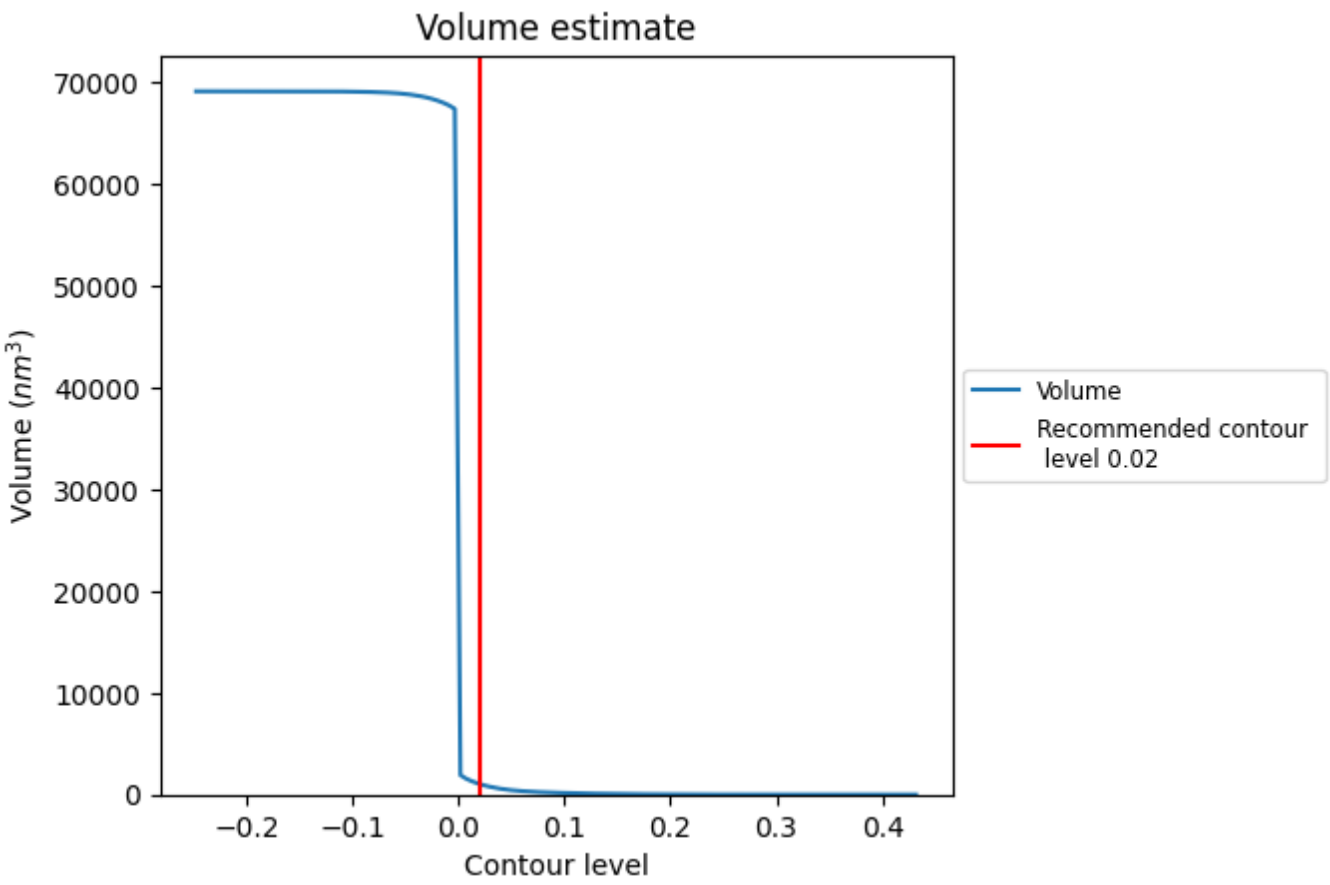
This section contains the results of statistical analysis of the map.

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.

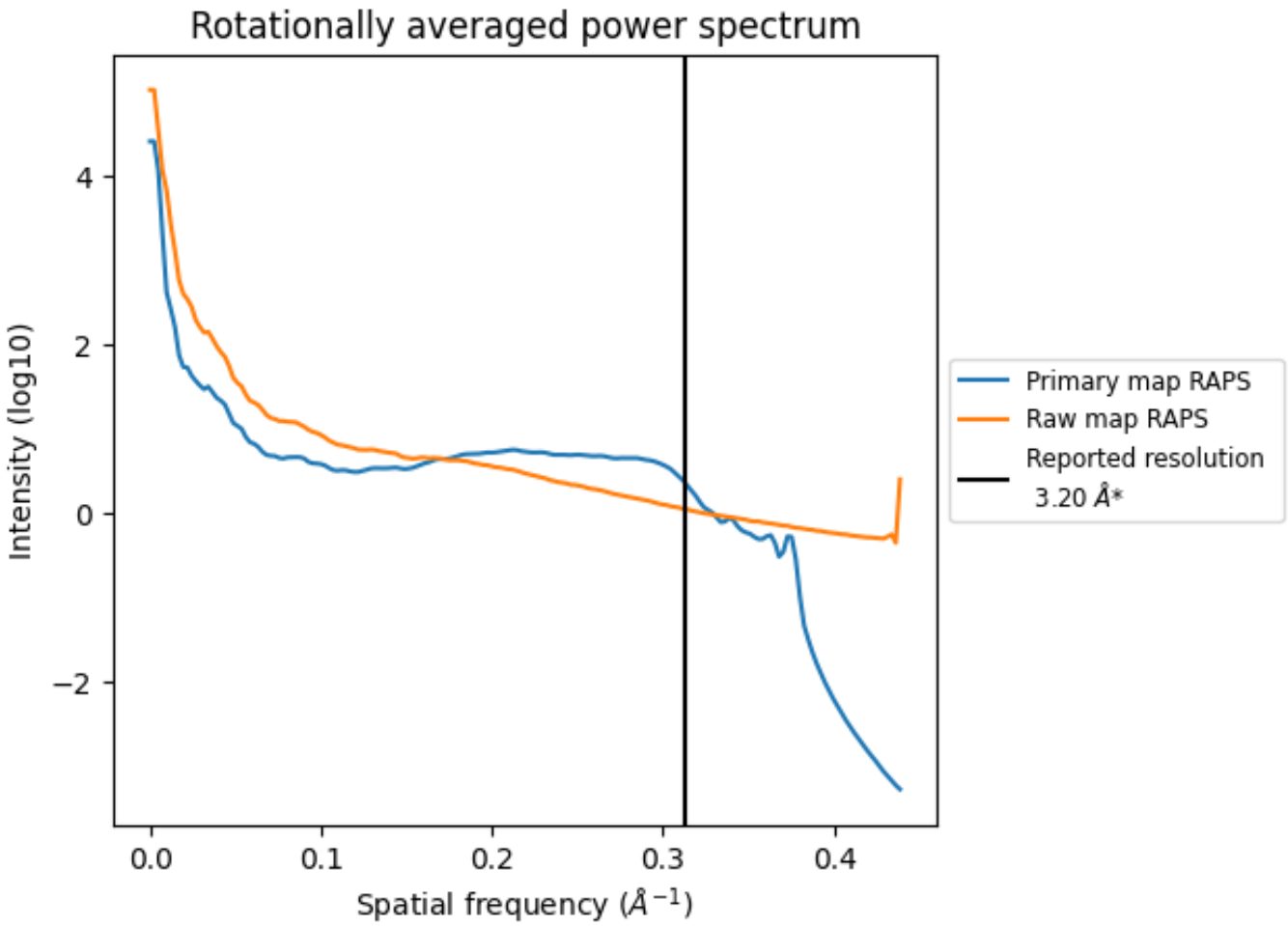
7.2 Volume estimate (i)



The volume at the recommended contour level is 1046 nm^3; this corresponds to an approximate mass of 945 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 (i)

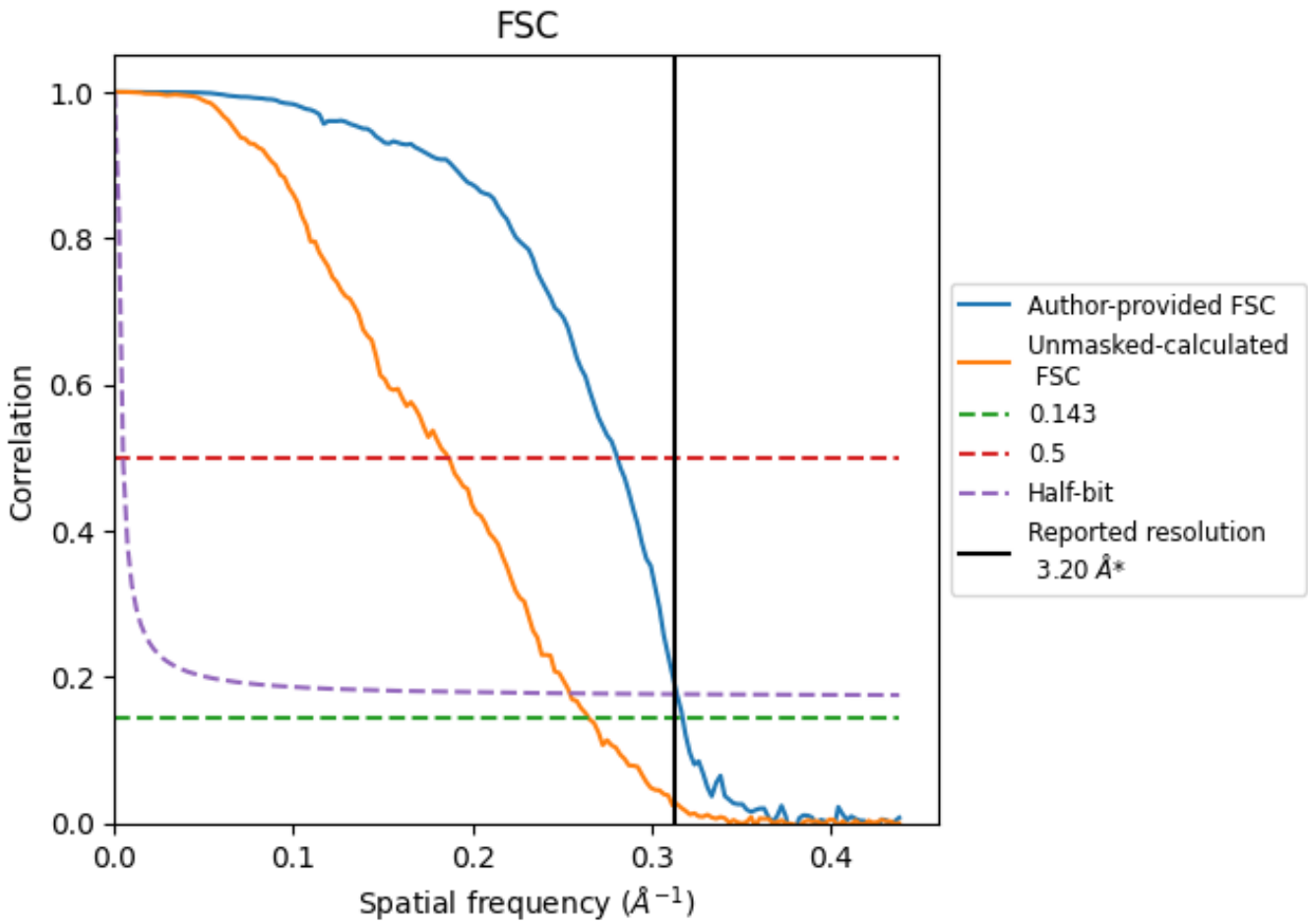


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

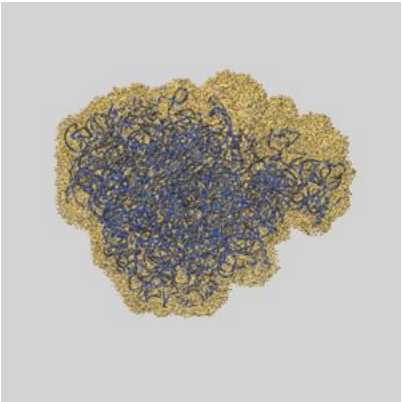
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.56	3.18
Unmasked-calculated*	3.77	5.36	3.93

*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 3.77 differs from the reported value 3.2 by more than 10 %

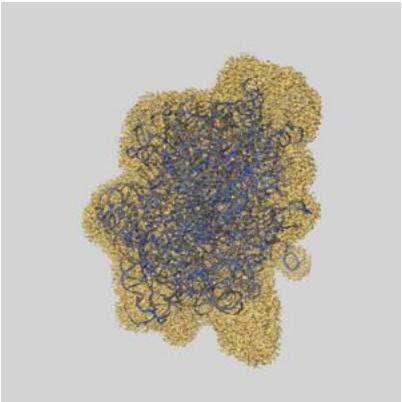
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21887 and PDB model 6WRS. Per-residue inclusion information can be found in section 3 on page 10.

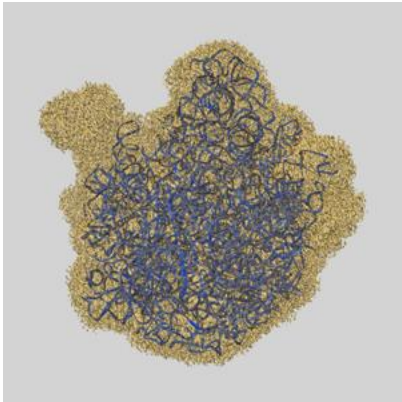
9.1 Map-model overlay (i)



X



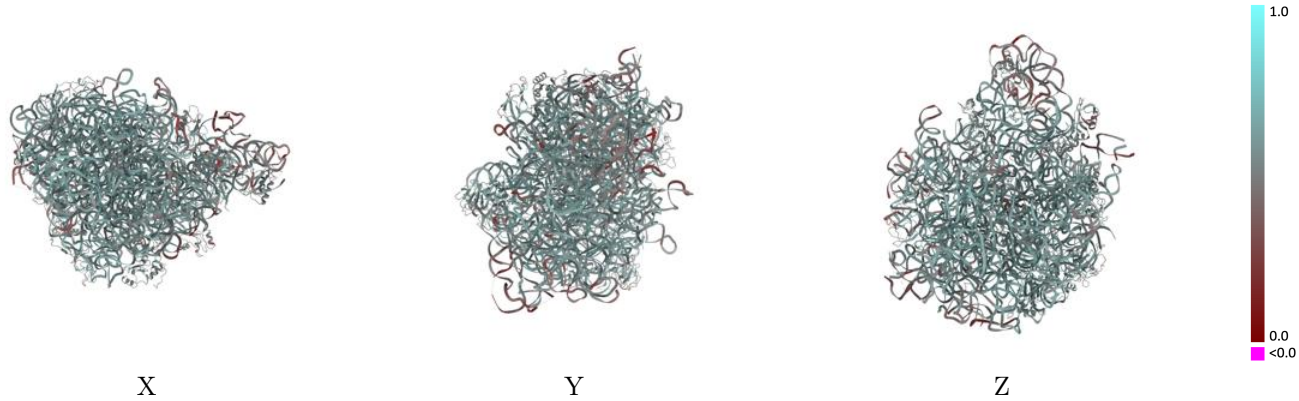
Y



Z

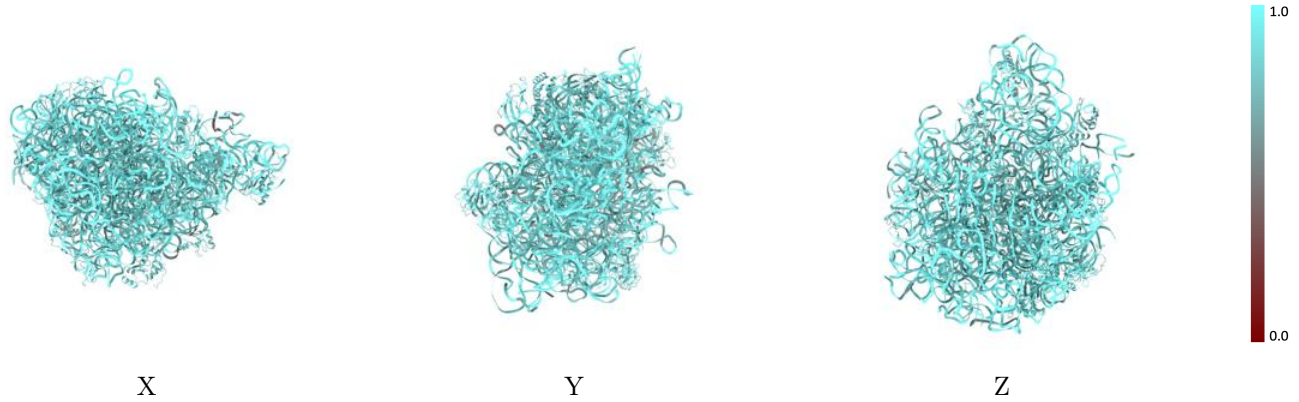
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



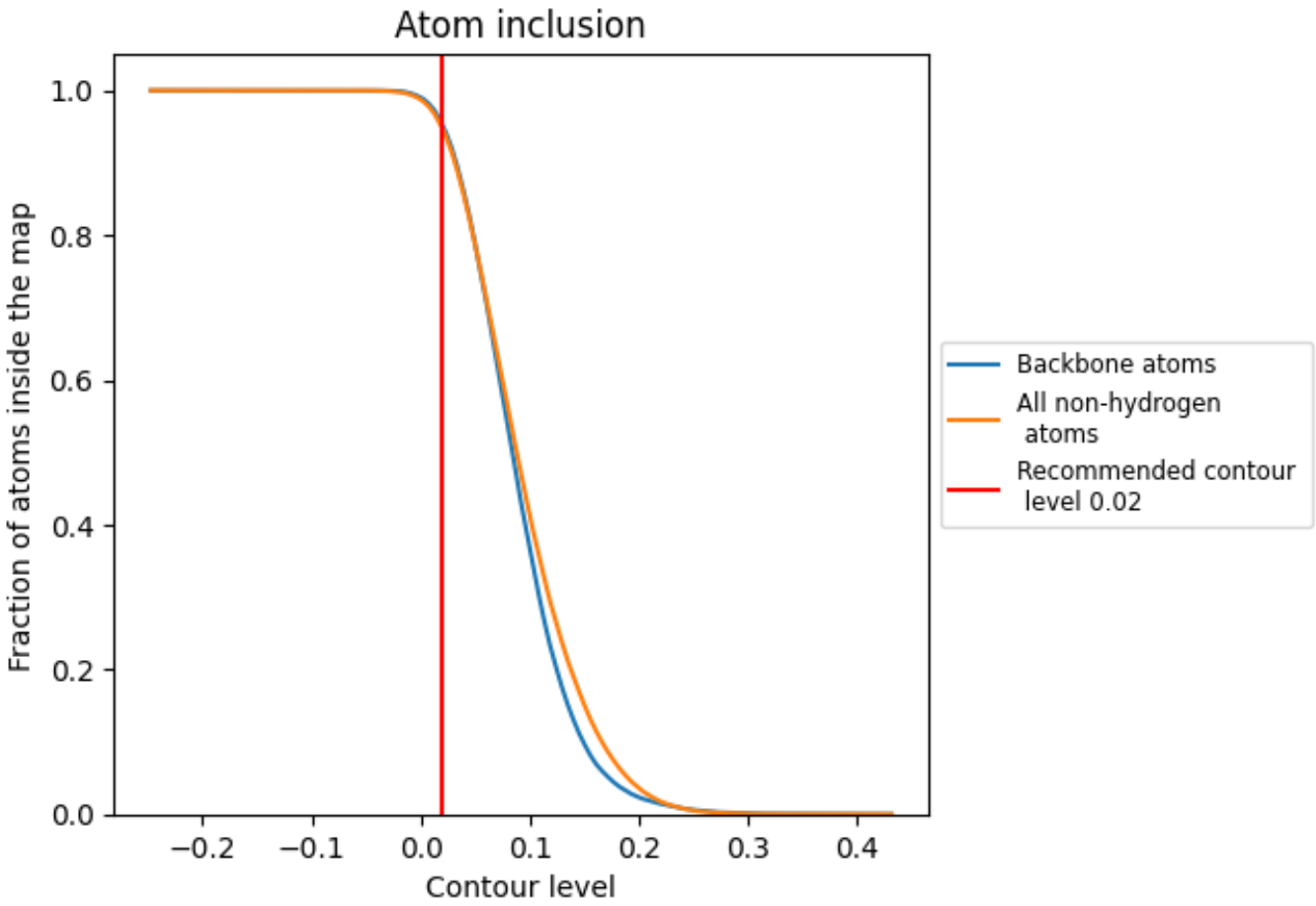
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.9474	0.5610
1	0.9585	0.5690
2	0.9122	0.4700
A	0.9317	0.5620
B	0.9308	0.5720
C	0.9253	0.5680
D	0.9224	0.5480
E	0.9543	0.5810
F	0.8918	0.5220
G	0.8938	0.5010
H	0.8109	0.4400
I	0.9550	0.5820
J	0.8949	0.5260
K	0.8710	0.4890
L	0.9171	0.5520
M	0.9363	0.5660
N	0.9426	0.5680
O	0.8727	0.5130
P	0.9715	0.6180
Q	0.9741	0.6060
R	0.9379	0.5630
S	0.9223	0.5600
V	0.9459	0.5610
W	0.9088	0.5440
X	0.9169	0.5430
Y	0.9298	0.5540
Z	0.9241	0.5620
a	0.8970	0.4970