Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 01:55 am GMT

PDB ID	:	6GC6
EMDB ID	:	EMD-4381
Title	:	50S ribosomal subunit assembly intermediate state 2
Authors	:	Nikolay, R.; Hilal, T.; Qin, B.; Loerke, J.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on	:	2018-04-17
Resolution	:	4.30 Å(reported)

This is a Full wwPDB EM Validation 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 (i)) were used in the production of this report:

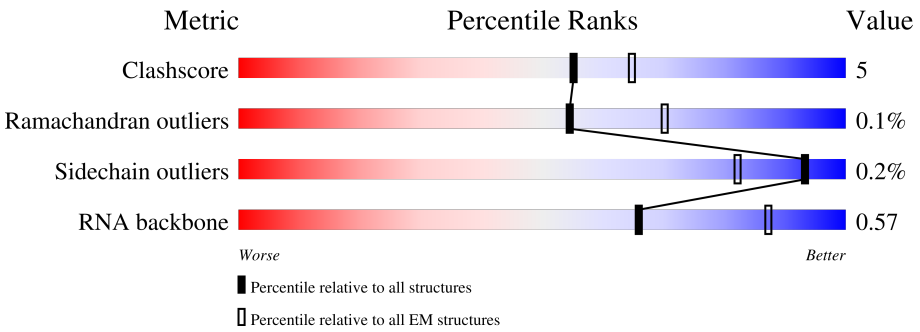
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2904	6%, 47%, 23%, •, 28%
2	C	223	43%, 70%, 22%, 9%
3	D	209	9%, 71%, 16%, 13%
4	E	201	13%, 84%, 16%
5	G	176	99%, 88%, 12%
6	J	142	11%, 89%, 11%
7	K	122	29%, 87%, 13%

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Mol	Chain	Length	Quality of chain
8	L	143	50% 65% 10% • 24%
9	N	120	• 83% 16% •
10	P	114	25% 71% 29%
11	Q	117	• 82% 18%
12	R	103	11% 84% 16%
13	S	110	15% 80% 20%
14	T	93	• 80% 20%
15	U	102	8% 80% 20%
16	Y	63	11% 79% 19% •
17	0	56	20% 91% 9%
18	2	46	7% 91% 9%
19	Z	58	22% 83% 17%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 61404 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2092	44960	20059	8333	14476	2092	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	204	1561	975	305	275	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	182	1366	863	245	254	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	201	1552	974	283	290	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called 50S ribosomal protein L19.

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

- Molecule 11 is a protein called 50S ribosomal protein L20.

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

- Molecule 12 is a protein called 50S ribosomal protein L21.

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

- Molecule 13 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	S	110	857	532	166	156	3	0	0

- Molecule 14 is a protein called 50S ribosomal protein L23.

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

- Molecule 15 is a protein called 50S ribosomal protein L24.

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

- Molecule 16 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Y	63	509	313	99	95	2	0	0

- Molecule 17 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	0	56	444	269	94	80	1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	2	46	377	228	90	57	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L30.

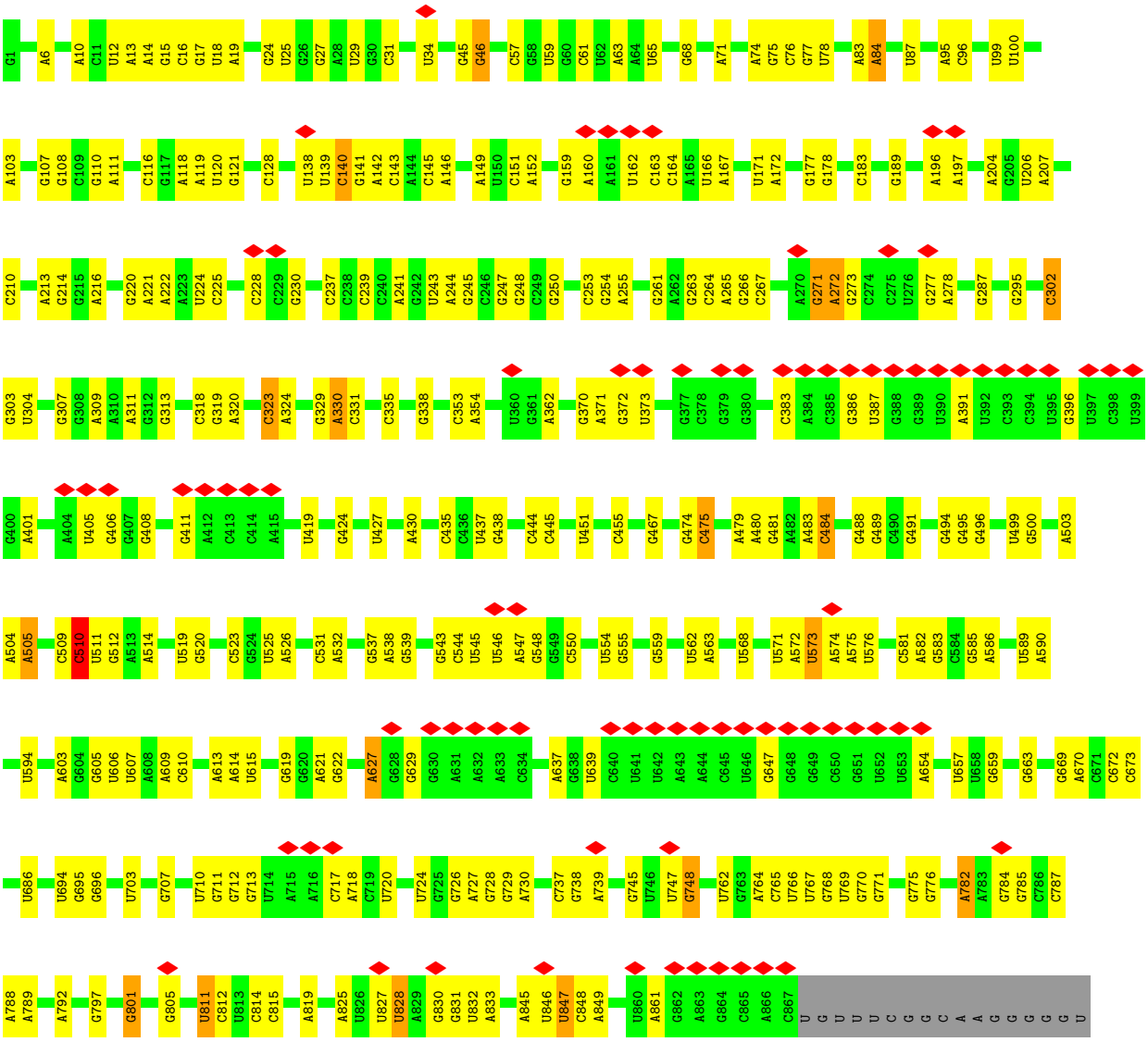
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	58	449	281	87	79	2	0	0

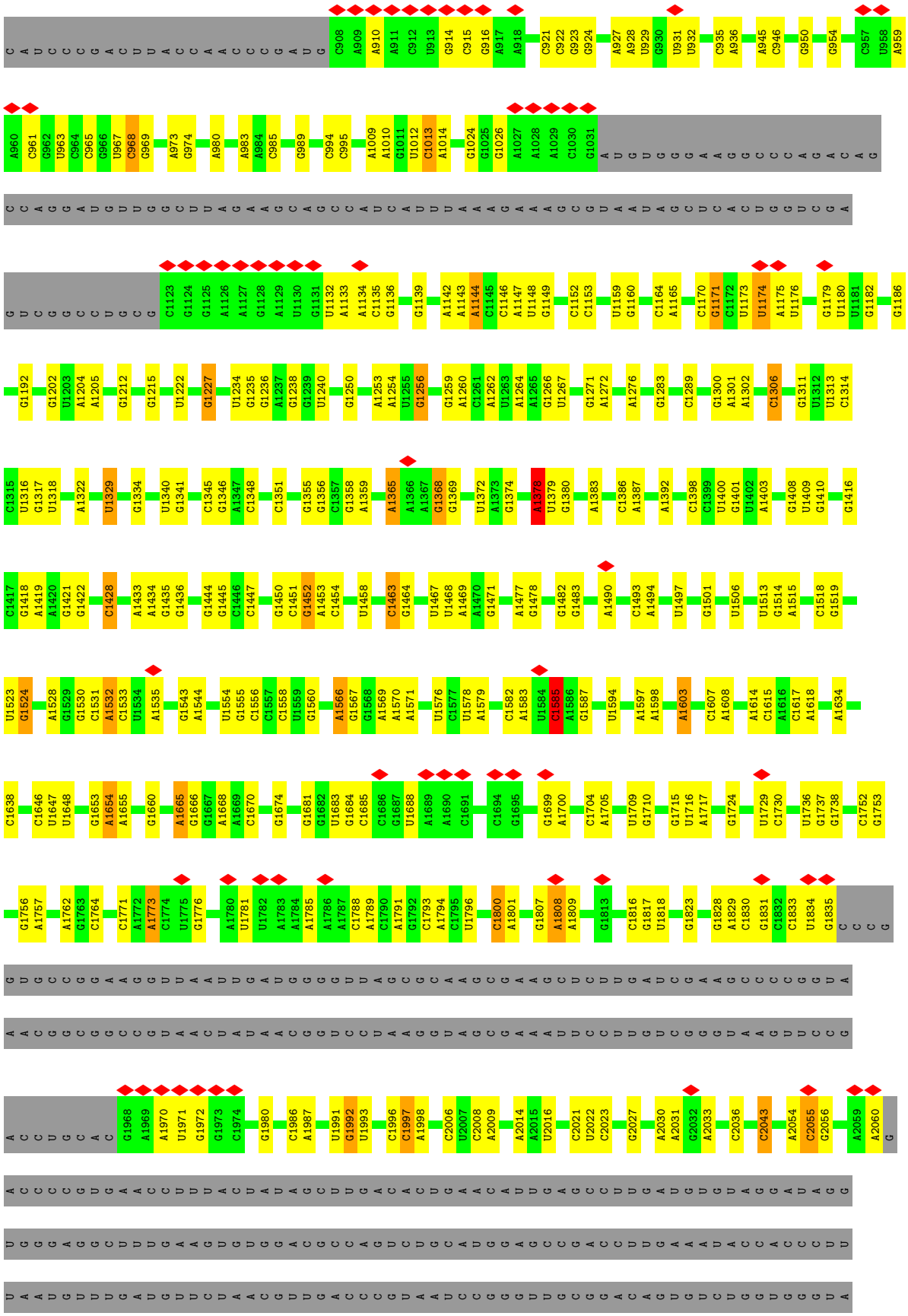
3 Residue-property plots (i)

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: 23S ribosomal RNA

Chain A: 6% 47% 23% • 28%

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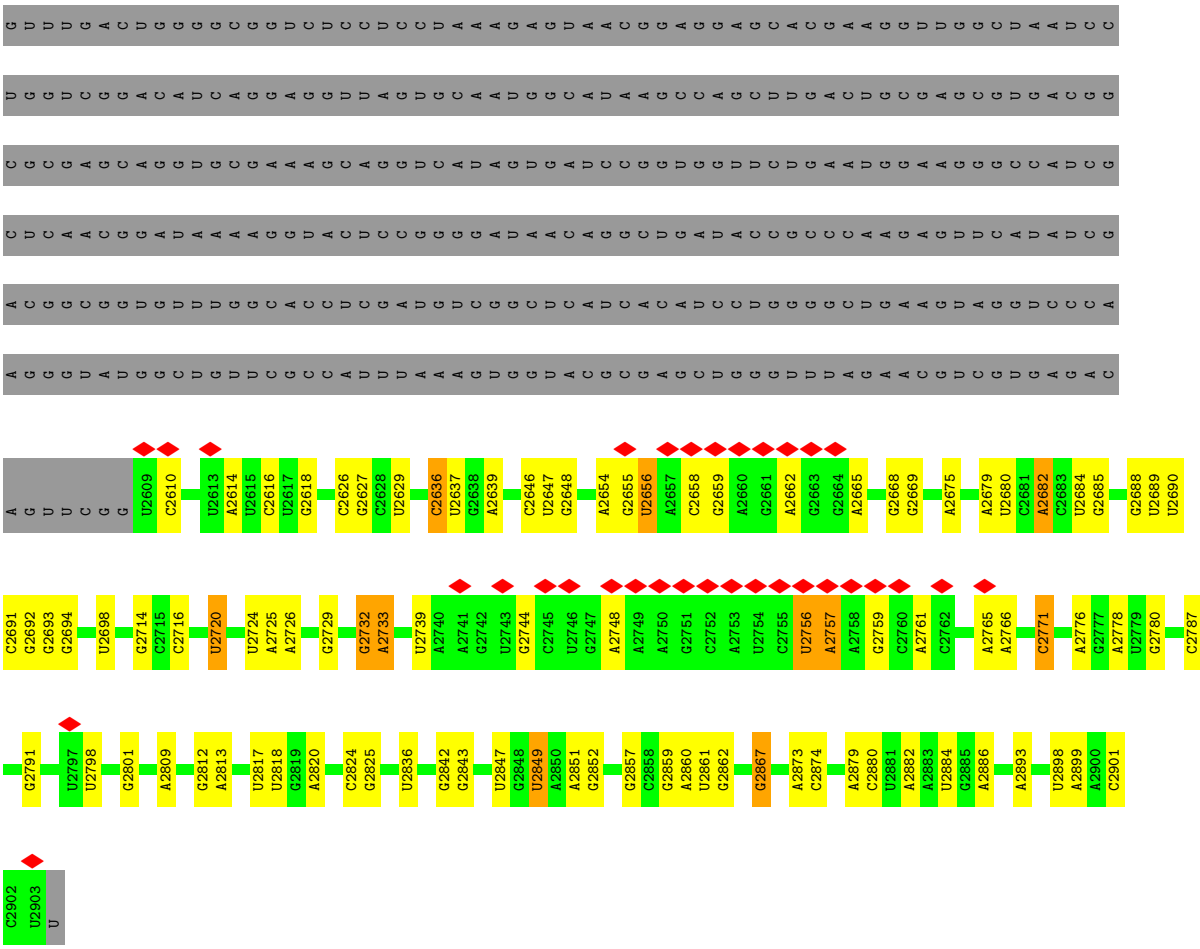
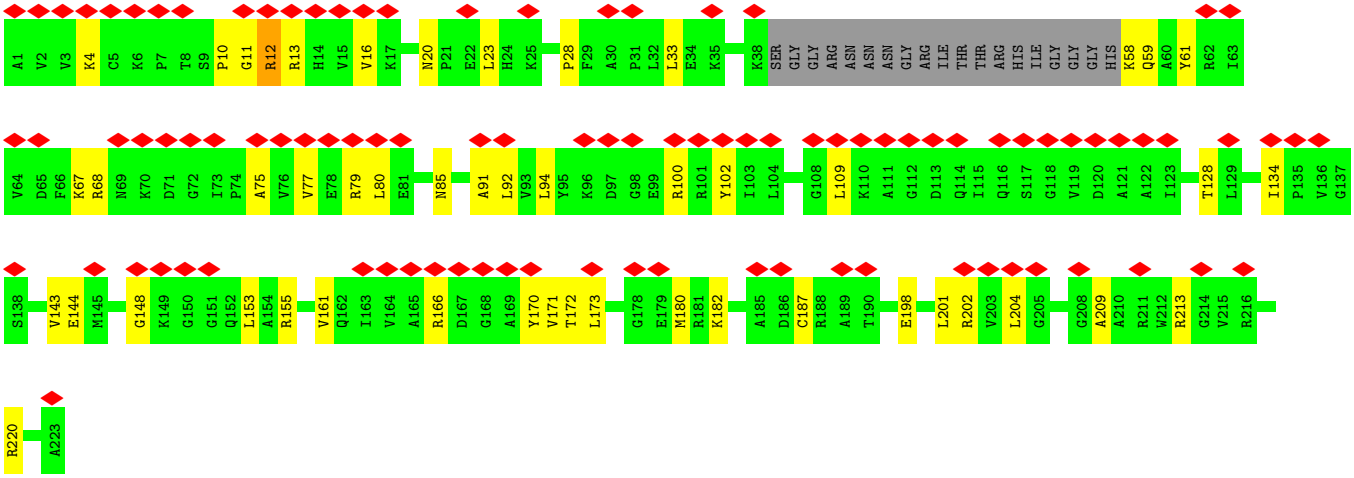
A960 C961 G962 U963 C964 C965 G966 U967 C968 G969 A973 G974 A980 A983 A984 C985 G989 C994 C995 A1009 A1010 G1011 U1012 C1013 A1014 G1024 G1025 G1026 A1027 A1028 A1029 C1030 G1031
C1123 G1124 G1125 A1126 A1127 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1139 A1142 A1143 A1144 C1145 C1146 A1147 U1148 G1149 C1152 C1153 U1159 G1160 C1164 A1165 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1179 U1180 U1181 G1182 G1186
G1192 G1202 U1203 A1204 A1205 G1212 G1215 U1222 G1227 U1234 G1235 G1236 A1237 G1238 G1239 U1240 G1250 A1253 A1254 U1255 C1256 G1259 A1260 C1261 A1262 U1263 A1264 A1265 G1266 U1267 G1271 A1272 A1276 G1283 C1289 G1300 A1301 A1302 C1306 G1311 U1312 U1313 C1314
C1315 U1316 G1317 U1318 A1322 U1329 G1334 U1340 G1341 C1345 G1346 A1347 C1348 C1351 G1355 G1356 C1357 G1358 A1359 A1365 A1366 A1367 G1368 G1369 U1372 A1373 G1374 A1378 U1379 G1380 A1383 C1386 A1387 A1392 C1398 C1399 U1400 G1401 U1402 A1403 G1408 U1409 G1410 G1416
C1417 G1418 A1419 A1420 G1421 G1422 C1428 A1433 A1434 G1435 G1436 G1444 G1445 C1446 C1447 G1450 C1451 G1452 A1453 C1454 U1458 C1463 G1464 U1467 U1468 A1469 A1470 G1471 A1477 G1478 G1482 G1483 A1490 C1493 A1494 U1497 G1501 U1506 U1513 G1514 A1515 C1518 G1519
U1523 G1524 A1528 G1529 G1530 C1531 A1532 C1533 U1534 A1535 G1543 A1544 U1554 G1555 C1556 C1557 C1558 U1559 G1560 A1566 G1567 G1568 A1569 A1570 A1571 U1576 C1577 U1578 A1579 C1582 A1583 U1584 C1585 A1586 G1587 U1594 A1597 A1598 A1603 C1607 A1608 A1614 C1615 A1616 C1617 A1618 A1634
C1638 C1646 U1647 U1648 G1653 A1654 A1655 G1660 A1665 G1666 G1667 A1668 A1669 C1670 G1674 G1681 G1682 U1683 G1684 C1685 C1686 G1687 U1688 A1689 A1690 C1691 C1694 G1695 G1699 A1700 C1704 A1705 U1709 G1710 G1715 U1716 A1717 G1724 U1729 C1730 U1736 G1737 G1738 C1752 G1753
G1756 A1757 A1762 G1763 C1764 C1771 A1772 A1773 C1774 U1775 G1776 A1780 U1781 U1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 A1794 C1795 U1796 C1800 A1801 G1807 A1808 A1809 G1813 C1816 G1817 U1818 G1823 G1828 A1829 C1830 G1831 C1832 C1833 U1834 G1835 C C C G
G U G C C G G A A C G G U U A A C U U G A U G G G C U U G G C U A G A A G C A G C C A U U U A A A G A A A G C G U A U A G C U U G G U C G A
A A C G C G C G C A C G U G G U U U G A A G G C A C A U U C A A U U G C C C A U U G C A A A G G C U C C C A G A C A G
A C C U G C A C G1968 A1969 A1970 U1971 G1972 G1973 C1974 G1980 C1986 A1987 U1991 G1992 U1993 C1996 C1997 A1998 C2006 U2007 C2008 A2009 A2014 A2015 U2016 C2021 U2022 C2023 G2027 A2030 A2031 G2032 A2033 C2036 C2043 A2054 C2055 G2056 A2059 A2060 G
A C C C G G C U U G A A C C A G U U G A A C C U U G A U U A A G G C C U G A A U G U U G C C G A C A G U G U U G A A U G U U G A C C U U G A A C C U G G G A A U G G C U A
U G G G A G G C U U G A U U C G A U G C U U G C C U U G A C A U G G G A A C A U G C C A U G C C U G U A A C G U U G A C C C U G G G G U A



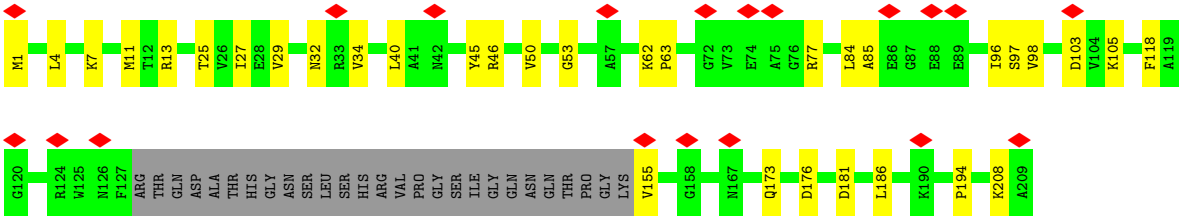
• Molecule 2: 50S ribosomal protein L2

Chain C:



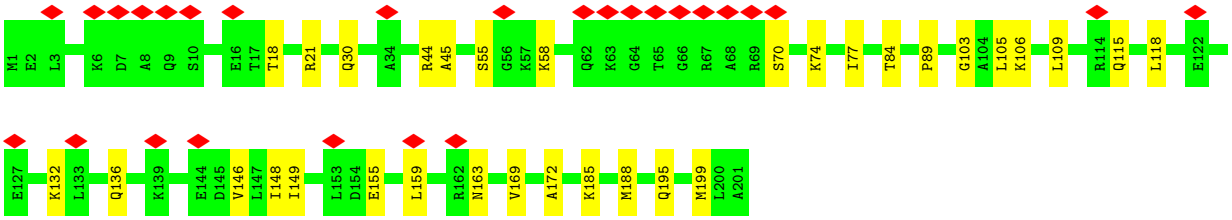
• Molecule 3: 50S ribosomal protein L3

Chain D:



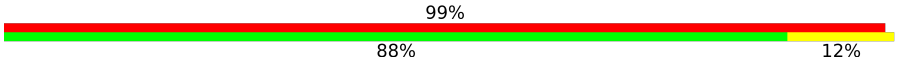
• Molecule 4: 50S ribosomal protein L4

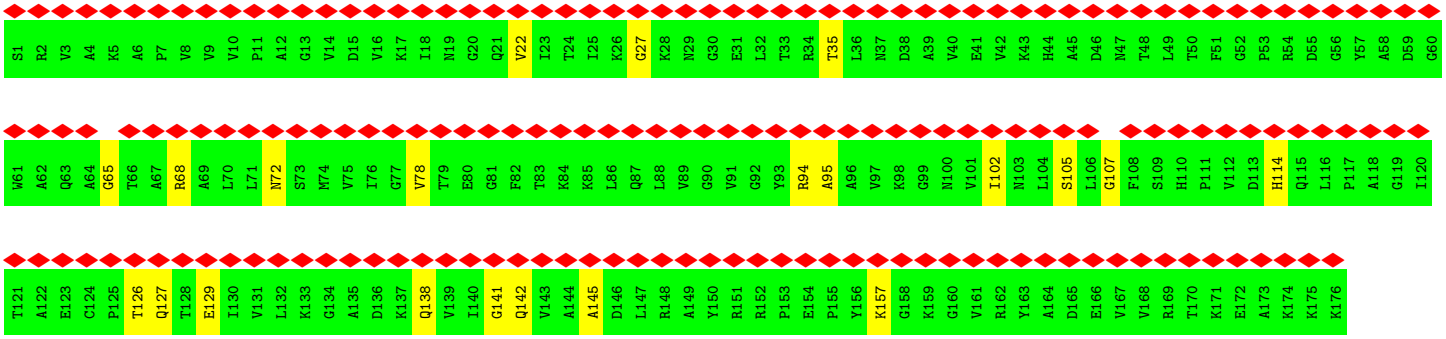
Chain E:



• Molecule 5: 50S ribosomal protein L6

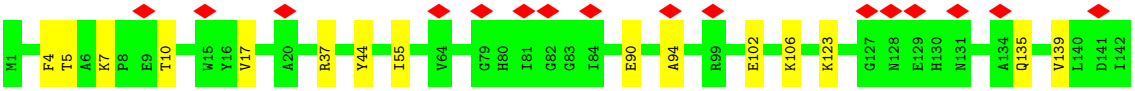
Chain G:





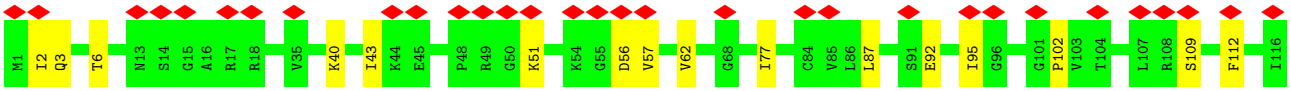
• Molecule 6: 50S ribosomal protein L13

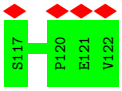
Chain J:



• Molecule 7: 50S ribosomal protein L14

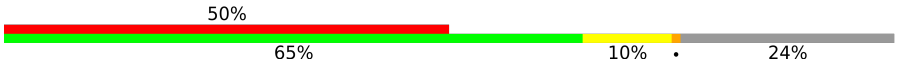
Chain K:

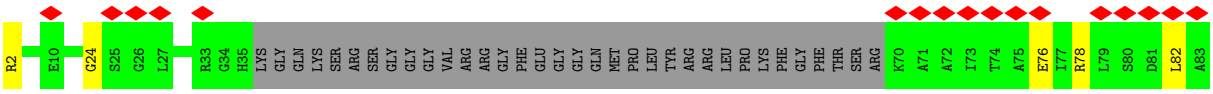


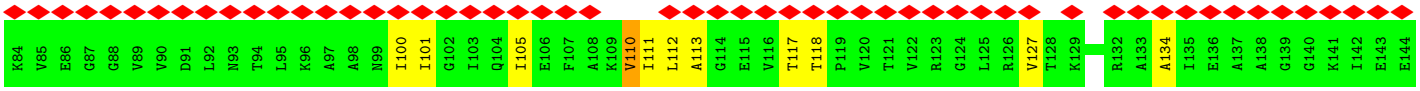


- Molecule 8: 50S ribosomal protein L15

Chain L:





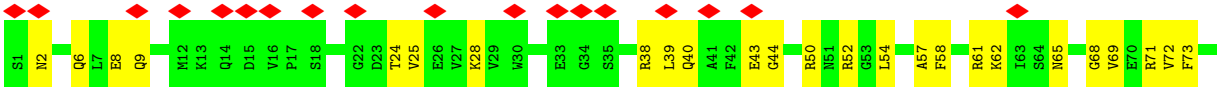


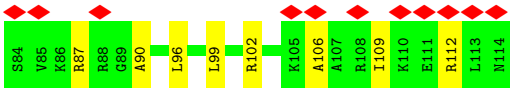
- Molecule 9: 50S ribosomal protein L17

Chain N:

- Molecule 10: 50S ribosomal protein L19

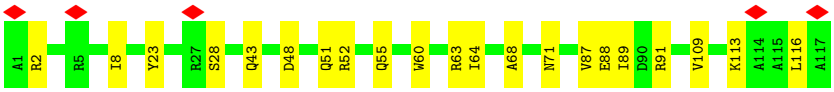
Chain P:





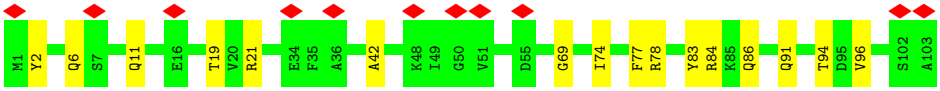
- Molecule 11: 50S ribosomal protein L20

Chain Q:



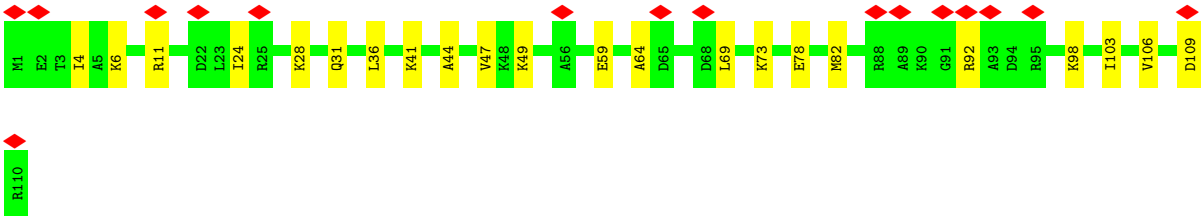
- Molecule 12: 50S ribosomal protein L21

Chain R:



- Molecule 13: 50S ribosomal protein L22

Chain S:



- Molecule 14: 50S ribosomal protein L23

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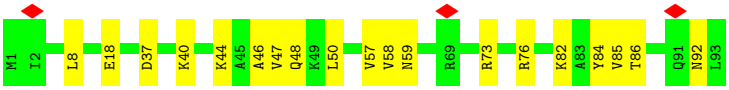
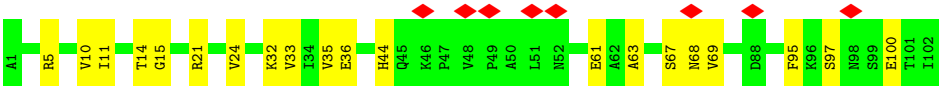


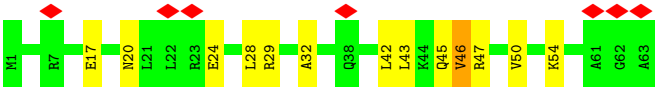
- Molecule 15: 50S ribosomal protein L24

Chain U:



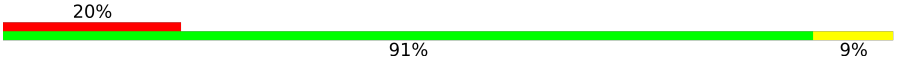
- Molecule 16: 50S ribosomal protein L29

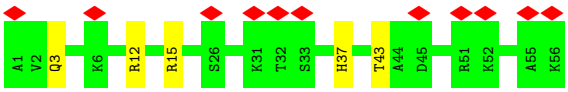
Chain Y:



- Molecule 17: 50S ribosomal protein L32

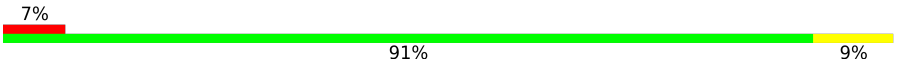
Chain 0:

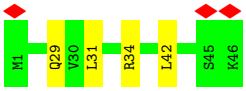




- Molecule 18: 50S ribosomal protein L34

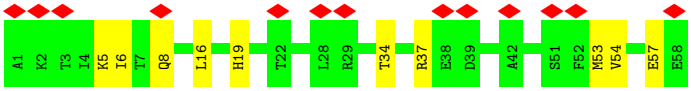
Chain 2:





- Molecule 19: 50S ribosomal protein L30

Chain Z:


A1
K2
T3
I4
K5
I6
T7
Q8
L16
H19
T22
L28
R29
T34
R37
E38
D39
A42
S51
F52
M53
V54
E57
E58

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	9.969	Depositor
Minimum map value	-3.764	Depositor
Average map value	0.070	Depositor
Map value standard deviation	0.487	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	334.8, 334.8, 334.8	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/50368	0.94	71/78571 (0.1%)
2	C	0.25	0/1586	0.52	0/2135
3	D	0.26	0/1382	0.49	0/1856
4	E	0.25	0/1571	0.49	0/2113
5	G	0.25	0/1343	0.47	0/1816
6	J	0.24	0/1152	0.44	0/1551
7	K	0.26	0/948	0.52	0/1268
8	L	0.27	0/780	0.63	1/1041 (0.1%)
9	N	0.27	0/974	0.56	0/1301
10	P	0.25	0/929	0.47	0/1242
11	Q	0.25	0/960	0.41	0/1278
12	R	0.25	0/829	0.49	0/1107
13	S	0.24	0/864	0.48	0/1156
14	T	0.25	0/745	0.51	0/994
15	U	0.28	0/788	0.56	1/1051 (0.1%)
16	Y	0.26	0/510	0.57	0/677
17	0	0.24	0/450	0.52	0/599
18	2	0.24	0/380	0.46	0/498
19	Z	0.24	0/453	0.46	0/605
All	All	0.26	0/67012	0.87	73/100859 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
8	L	0	1
9	N	0	1
All	All	0	3

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1306	C	N3-C2-O2	-9.63	115.16	121.90
1	A	1313	U	N3-C2-O2	-9.12	115.82	122.20
1	A	1306	C	N1-C2-O2	9.02	124.31	118.90
1	A	965	C	N1-C2-O2	8.93	124.26	118.90
1	A	1313	U	N1-C2-O2	8.50	128.75	122.80
1	A	1313	U	C2-N1-C1'	8.38	127.76	117.70
1	A	1289	C	N1-C2-O2	7.74	123.55	118.90
1	A	1170	C	N1-C2-O2	7.60	123.46	118.90
1	A	143	C	N1-C2-O2	7.39	123.33	118.90
1	A	965	C	N3-C2-O2	-7.32	116.78	121.90
1	A	1348	C	N1-C2-O2	7.23	123.24	118.90
1	A	965	C	C2-N1-C1'	7.02	126.53	118.80
1	A	965	C	C6-N1-C2	-6.78	117.59	120.30
1	A	2720	U	N3-C2-O2	-6.73	117.49	122.20
1	A	1170	C	C2-N1-C1'	6.71	126.19	118.80
1	A	1378	A	P-O3'-C3'	6.70	127.73	119.70
1	A	1267	U	N3-C2-O2	-6.60	117.58	122.20
1	A	183	C	N1-C2-O2	6.59	122.86	118.90
1	A	1267	U	N1-C2-O2	6.53	127.37	122.80
1	A	271	G	P-O3'-C3'	6.53	127.53	119.70
1	A	1289	C	N3-C2-O2	-6.51	117.34	121.90
1	A	1585	C	N1-C2-O2	6.40	122.74	118.90
1	A	143	C	N3-C2-O2	-6.39	117.43	121.90
1	A	166	U	N1-C2-O2	6.35	127.24	122.80
1	A	545	U	C2-N1-C1'	6.27	125.22	117.70
1	A	607	U	N3-C2-O2	-6.26	117.82	122.20
1	A	2720	U	N1-C2-O2	6.18	127.13	122.80
1	A	717	C	N1-C2-O2	6.18	122.61	118.90
1	A	166	U	N3-C2-O2	-6.12	117.92	122.20
1	A	96	C	C2-N1-C1'	6.09	125.50	118.80
1	A	1378	A	OP1-P-O3'	6.09	118.60	105.20
1	A	2636	C	C2-N1-C1'	6.08	125.49	118.80
1	A	2616	C	C2-N1-C1'	6.07	125.47	118.80
1	A	510	C	N1-C2-O2	5.97	122.48	118.90
1	A	2616	C	C6-N1-C2	-5.91	117.94	120.30
1	A	1267	U	C2-N1-C1'	5.88	124.76	117.70
1	A	143	C	C6-N1-C2	-5.88	117.95	120.30
1	A	1170	C	N3-C2-O2	-5.84	117.81	121.90
1	A	1348	C	N3-C2-O2	-5.75	117.87	121.90
1	A	607	U	N1-C2-O2	5.74	126.82	122.80
1	A	915	C	N1-C2-O2	5.73	122.34	118.90
1	A	96	C	N1-C2-O2	5.72	122.33	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	C	C2-N1-C1'	5.71	125.08	118.80
1	A	1685	C	N1-C2-O2	5.66	122.30	118.90
1	A	545	U	N3-C2-O2	-5.60	118.28	122.20
1	A	1306	C	C6-N1-C2	-5.57	118.07	120.30
1	A	323	C	N1-C2-O2	5.51	122.21	118.90
1	A	1776	G	C4-N9-C1'	5.48	133.62	126.50
1	A	968	C	N1-C2-O2	5.47	122.18	118.90
8	L	82	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	1398	C	C2-N1-C1'	5.43	124.77	118.80
1	A	545	U	N1-C2-O2	5.41	126.59	122.80
1	A	1463	C	N1-C2-O2	5.36	122.12	118.90
1	A	183	C	C6-N1-C2	-5.33	118.17	120.30
1	A	225	C	C2-N1-C1'	5.32	124.66	118.80
1	A	183	C	N3-C2-O2	-5.31	118.18	121.90
1	A	1314	C	C2-N1-C1'	5.31	124.64	118.80
1	A	921	C	N1-C2-O2	5.31	122.08	118.90
1	A	968	C	N3-C2-O2	-5.28	118.21	121.90
1	A	25	U	C2-N1-C1'	5.26	124.01	117.70
1	A	1289	C	C2-N1-C1'	5.25	124.58	118.80
15	U	97	SER	C-N-CA	5.24	134.79	121.70
1	A	1348	C	C6-N1-C2	-5.22	118.21	120.30
1	A	140	C	N1-C2-O2	5.17	122.00	118.90
1	A	1348	C	C2-N1-C1'	5.16	124.48	118.80
1	A	965	C	C5-C6-N1	5.13	123.56	121.00
1	A	847	U	N1-C2-O2	5.11	126.38	122.80
1	A	484	C	N1-C2-O2	5.11	121.96	118.90
1	A	1776	G	N3-C4-C5	-5.10	126.05	128.60
1	A	847	U	N3-C2-O2	-5.06	118.66	122.20
1	A	717	C	N3-C2-O2	-5.05	118.36	121.90
1	A	1174	U	C2-N1-C1'	5.04	123.75	117.70
1	A	96	C	C6-N1-C2	-5.01	118.30	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	11	GLY	Peptide
8	L	110	VAL	Peptide
9	N	10	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	44960	0	22614	313	0
2	C	1561	0	1638	31	0
3	D	1366	0	1424	23	0
4	E	1552	0	1619	21	0
5	G	1323	0	1374	16	0
6	J	1129	0	1162	13	0
7	K	939	0	1012	10	0
8	L	778	0	841	10	0
9	N	961	0	1000	14	0
10	P	917	0	965	18	0
11	Q	947	0	1022	16	0
12	R	816	0	839	10	0
13	S	857	0	922	15	0
14	T	739	0	807	15	0
15	U	780	0	834	12	0
16	Y	509	0	543	10	0
17	0	444	0	461	4	0
18	2	377	0	418	3	0
19	Z	449	0	491	6	0
All	All	61404	0	39986	483	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (483) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:G:N2	1:A:718:A:H62	1.60	0.99
1:A:713:G:H21	1:A:718:A:N6	1.61	0.98
1:A:954:G:H1	1:A:963:U:H3	1.13	0.94
1:A:1800:C:H42	1:A:1817:G:N2	1.69	0.90
1:A:950:G:H1	1:A:967:U:H3	0.94	0.90
1:A:1800:C:N4	1:A:1817:G:H22	1.71	0.88
1:A:408:G:H1	1:A:419:U:H3	1.21	0.88
1:A:1800:C:H42	1:A:1817:G:H22	1.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:U:H3	1:A:108:G:H1	0.88	0.87
1:A:713:G:H21	1:A:718:A:H62	0.88	0.87
1:A:695:G:H1	1:A:767:U:H3	1.20	0.84
1:A:304:U:H3	1:A:313:G:H1	1.19	0.84
1:A:585:G:H21	1:A:1254:A:N6	1.75	0.83
1:A:703:U:H3	1:A:728:G:H1	1.26	0.81
1:A:585:G:H21	1:A:1254:A:H62	1.26	0.81
1:A:244:A:H62	1:A:254:G:H21	1.25	0.81
1:A:2685:G:H1	1:A:2724:U:H3	1.25	0.81
1:A:1359:A:H62	1:A:1372:U:H3	1.29	0.80
1:A:585:G:N2	1:A:1254:A:H62	1.80	0.79
14:T:46:ALA:O	14:T:50:LEU:HB2	1.84	0.77
1:A:1483:G:H1	1:A:1506:U:H3	1.34	0.75
12:R:74:ILE:O	12:R:86:GLN:HA	1.89	0.72
19:Z:6:ILE:O	19:Z:34:THR:HA	1.90	0.71
1:A:861:A:H62	1:A:916:G:H21	1.40	0.69
4:E:155:GLU:O	4:E:159:LEU:HB2	1.92	0.69
10:P:24:THR:HA	10:P:44:GLY:O	1.93	0.68
2:C:173:LEU:O	2:C:180:MET:HA	1.94	0.68
1:A:1800:C:N3	1:A:1817:G:N1	2.41	0.67
1:A:1222:U:H3	1:A:1227:G:H1	1.43	0.66
10:P:25:VAL:O	10:P:43:GLU:HA	1.95	0.65
1:A:609:A:H62	1:A:619:G:N2	1.95	0.65
1:A:1433:A:H61	1:A:1560:G:H1	1.41	0.65
4:E:195:GLN:O	4:E:199:MET:HB2	1.96	0.64
10:P:61:ARG:HA	10:P:69:VAL:O	1.98	0.64
15:U:33:VAL:O	15:U:63:ALA:HA	1.98	0.64
1:A:1215:G:H1	1:A:1234:U:H3	1.46	0.64
1:A:320:A:N3	4:E:163:ASN:ND2	2.46	0.64
1:A:1992:G:N2	1:A:1996:C:O2'	2.32	0.63
10:P:28:LYS:HA	10:P:40:GLN:O	1.99	0.62
1:A:711:G:H1	1:A:720:U:H3	1.48	0.61
3:D:46:ARG:HB3	3:D:84:LEU:HD12	1.82	0.61
1:A:99:U:H5"	1:A:100:U:H5'	1.82	0.61
2:C:10:PRO:HA	2:C:13:ARG:HB2	1.83	0.61
1:A:1796:U:H3	1:A:1823:G:H1	1.49	0.60
5:G:141:GLY:O	5:G:145:ALA:HB2	2.00	0.60
1:A:309:A:H4'	15:U:15:GLY:HA2	1.82	0.60
1:A:627:A:H62	8:L:113:ALA:HB2	1.68	0.59
1:A:814:C:N4	8:L:24:GLY:O	2.35	0.59
1:A:1478:G:H1	1:A:1513:U:H3	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:A:OP1	15:U:5:ARG:NH1	2.35	0.59
1:A:1834:U:H5"	1:A:1835:G:H5'	1.84	0.59
1:A:659:G:H21	4:E:30:GLN:HE22	1.51	0.59
1:A:1986:C:H2'	1:A:1987:A:H8	1.68	0.58
1:A:2720:U:OP1	10:P:52:ARG:NH2	2.35	0.58
2:C:28:PRO:HG2	2:C:33:LEU:HD11	1.85	0.58
1:A:373:U:O2	1:A:401:A:N7	2.37	0.58
3:D:11:MET:HG2	3:D:25:THR:HG22	1.86	0.58
13:S:73:LYS:HB2	13:S:106:VAL:HB	1.86	0.58
1:A:729:G:N2	2:C:10:PRO:O	2.37	0.58
1:A:707:G:H1	1:A:724:U:H3	1.52	0.58
1:A:1403:A:HO2'	1:A:1471:G:HO2'	1.51	0.58
2:C:171:VAL:O	2:C:182:LYS:HA	2.04	0.57
3:D:53:GLY:HA3	3:D:77:ARG:HE	1.69	0.57
1:A:484:C:H42	1:A:496:G:H1	1.49	0.57
1:A:1153:C:OP1	11:Q:91:ARG:NH2	2.37	0.57
5:G:94:ARG:H	5:G:105:SER:HB2	1.68	0.57
1:A:629:G:N3	1:A:639:U:O2'	2.37	0.57
2:C:75:ALA:HA	2:C:94:LEU:O	2.05	0.57
3:D:7:LYS:O	3:D:27:ILE:HA	2.05	0.57
4:E:132:LYS:O	4:E:136:GLN:HB2	2.04	0.57
7:K:40:LYS:HE2	7:K:57:VAL:HG12	1.86	0.57
3:D:32:ASN:HB2	3:D:96:ILE:HB	1.87	0.57
1:A:696:G:H1	1:A:766:U:H3	1.52	0.57
1:A:787:C:H5"	1:A:788:A:H5'	1.87	0.56
1:A:832:U:H2'	1:A:833:A:H8	1.70	0.56
1:A:627:A:OP1	8:L:78:ARG:NH1	2.37	0.56
1:A:1408:G:H1	1:A:1594:U:H3	1.53	0.56
11:Q:43:GLN:HE21	12:R:77:PHE:HB3	1.69	0.56
2:C:209:ALA:O	2:C:213:ARG:NH1	2.38	0.56
13:S:28:LYS:H	13:S:31:GLN:HE21	1.54	0.56
1:A:2009:A:OP1	13:S:41:LYS:NZ	2.39	0.56
6:J:4:PHE:O	11:Q:63:ARG:NH2	2.37	0.56
1:A:61:C:H5"	16:Y:43:LEU:HD12	1.87	0.56
1:A:210:C:OP1	18:2:29:GLN:NE2	2.39	0.56
1:A:2680:U:O2	1:A:2682:A:N6	2.38	0.56
1:A:488:G:H4'	13:S:49:LYS:HD2	1.88	0.56
2:C:77:VAL:HG11	2:C:109:LEU:HD21	1.88	0.56
10:P:62:LYS:O	10:P:68:GLY:HA2	2.05	0.55
1:A:1791:A:N6	1:A:1828:G:O2'	2.39	0.55
10:P:90:ALA:HB2	10:P:112:ARG:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:24:ILE:HD13	13:S:36:LEU:HD11	1.86	0.55
12:R:78:ARG:HB3	12:R:83:TYR:HB3	1.88	0.55
1:A:2851:A:O2'	9:N:64:ARG:NH2	2.39	0.55
4:E:115:GLN:HG3	8:L:2:ARG:HE	1.71	0.55
1:A:1724:G:O6	1:A:1737:G:N2	2.38	0.55
4:E:21:ARG:NH1	4:E:103:GLY:O	2.40	0.55
1:A:767:U:H2'	1:A:768:G:H8	1.72	0.55
1:A:6:A:N3	6:J:135:GLN:NE2	2.54	0.55
12:R:6:GLN:HB2	12:R:11:GLN:HG2	1.89	0.55
1:A:994:C:OP1	11:Q:52:ARG:NH1	2.40	0.55
1:A:1681:G:H21	1:A:1762:A:H3'	1.71	0.54
5:G:95:ALA:O	5:G:127:GLN:NE2	2.40	0.54
1:A:483:A:H5'	15:U:44:HIS:HB3	1.89	0.54
1:A:1351:C:O2'	1:A:1571:A:O2'	2.23	0.54
19:Z:16:LEU:HB2	19:Z:19:HIS:HD2	1.73	0.54
3:D:40:LEU:HG	3:D:46:ARG:HG3	1.89	0.54
1:A:1566:A:OP1	2:C:213:ARG:NH2	2.41	0.54
1:A:2691:C:H2'	1:A:2692:G:H8	1.72	0.54
1:A:162:U:H1'	1:A:164:C:H41	1.73	0.54
1:A:1322:A:OP2	13:S:11:ARG:NH2	2.40	0.54
5:G:102:ILE:HB	5:G:114:HIS:HB2	1.89	0.54
11:Q:23:TYR:H	11:Q:28:SER:HB3	1.73	0.53
14:T:40:LYS:NZ	14:T:58:VAL:O	2.41	0.53
1:A:1428:C:N4	1:A:1570:A:OP2	2.40	0.53
19:Z:5:LYS:HB2	19:Z:57:GLU:HB2	1.90	0.53
1:A:1830:C:H2'	1:A:1831:G:H8	1.73	0.53
3:D:181:ASP:HB3	3:D:186:LEU:HB3	1.91	0.53
14:T:44:LYS:O	14:T:48:GLN:HB2	2.08	0.53
13:S:82:MET:HB2	13:S:98:LYS:HB2	1.89	0.53
1:A:2027:G:H1	1:A:2036:C:H42	1.57	0.53
1:A:444:C:OP1	4:E:44:ARG:NH2	2.42	0.53
1:A:24:G:N2	13:S:78:GLU:OE2	2.42	0.53
1:A:2759:G:N2	5:G:138:GLN:OE1	2.42	0.53
1:A:2655:G:N2	1:A:2665:A:OP2	2.41	0.53
11:Q:88:GLU:O	12:R:11:GLN:NE2	2.41	0.53
8:L:76:GLU:HG3	8:L:111:ILE:HD13	1.90	0.53
16:Y:28:LEU:O	16:Y:32:ALA:HB2	2.08	0.53
1:A:87:U:H3	1:A:95:A:H61	1.57	0.52
1:A:815:C:H42	1:A:1192:G:H1	1.54	0.52
1:A:1494:A:H2	1:A:1579:A:H1'	1.74	0.52
1:A:1528:A:N6	1:A:1543:G:O2'	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2008:C:H2'	1:A:2009:A:H8	1.74	0.52
3:D:103:ASP:OD1	3:D:105:LYS:NZ	2.42	0.52
1:A:1450:G:N2	1:A:1452:G:O6	2.40	0.52
1:A:1688:U:O2'	1:A:1700:A:N7	2.39	0.52
4:E:105:LEU:O	4:E:109:LEU:HB2	2.09	0.52
1:A:162:U:O2	1:A:164:C:N4	2.42	0.52
1:A:2658:C:OP1	5:G:157:LYS:NZ	2.43	0.52
1:A:171:U:H2'	1:A:172:A:H8	1.74	0.52
4:E:146:VAL:HG12	4:E:185:LYS:HB2	1.90	0.52
1:A:2787:C:H4'	3:D:62:LYS:HG2	1.91	0.52
1:A:159:G:O2'	1:A:167:A:N6	2.43	0.52
1:A:609:A:H62	1:A:619:G:H21	1.57	0.52
1:A:797:G:OP1	4:E:55:SER:OG	2.28	0.52
1:A:1311:G:H21	1:A:1603:A:H62	1.58	0.52
1:A:244:A:H62	1:A:254:G:N2	2.01	0.51
13:S:59:GLU:HA	13:S:64:ALA:HB2	1.92	0.51
1:A:318:C:H2'	1:A:319:G:H8	1.75	0.51
1:A:511:U:H4'	1:A:1235:G:H4'	1.92	0.51
13:S:6:LYS:HA	13:S:103:ILE:O	2.10	0.51
1:A:2874:C:OP1	9:N:4:ARG:NH2	2.43	0.51
1:A:673:C:OP1	1:A:801:G:N2	2.42	0.51
1:A:2857:G:N2	1:A:2860:A:OP2	2.39	0.51
14:T:59:ASN:HB2	14:T:84:TYR:HB2	1.92	0.51
1:A:1668:A:N3	1:A:1670:C:N4	2.58	0.51
1:A:1997:C:H2'	1:A:1998:A:H8	1.76	0.51
1:A:1773:A:H62	1:A:1791:A:H2	1.58	0.51
10:P:102:ARG:HD3	10:P:106:ALA:HB1	1.92	0.51
1:A:954:G:N2	1:A:963:U:O2	2.34	0.51
1:A:974:G:O2'	1:A:989:G:N2	2.43	0.51
9:N:49:GLU:HG2	9:N:94:TYR:HB2	1.92	0.51
16:Y:43:LEU:HB3	16:Y:47:ARG:HH12	1.76	0.51
1:A:324:A:N6	1:A:338:G:O2'	2.44	0.51
1:A:1614:A:N6	13:S:92:ARG:O	2.41	0.51
2:C:143:VAL:HB	2:C:153:LEU:HD12	1.93	0.51
1:A:1422:G:H1	1:A:1576:U:H3	1.57	0.50
6:J:90:GLU:O	6:J:94:ALA:HB2	2.10	0.50
10:P:87:ARG:NH2	10:P:109:ILE:O	2.40	0.50
16:Y:20:ASN:O	16:Y:24:GLU:HB2	2.10	0.50
1:A:2771:C:O2'	3:D:173:GLN:NE2	2.43	0.50
3:D:34:VAL:HA	3:D:50:VAL:HG12	1.92	0.50
9:N:43:GLU:OE2	9:N:46:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:38:ARG:NH2	10:P:39:LEU:O	2.44	0.50
1:A:514:A:N3	1:A:581:C:O2'	2.40	0.50
1:A:1264:A:N6	1:A:2014:A:OP2	2.45	0.50
3:D:4:LEU:HD23	3:D:29:VAL:HG11	1.94	0.50
1:A:408:G:O6	1:A:419:U:O4	2.30	0.50
1:A:576:U:OP2	1:A:2055:C:N4	2.45	0.50
7:K:77:ILE:HD11	10:P:71:ARG:HH11	1.76	0.50
1:A:78:U:O4	1:A:108:G:O6	2.30	0.49
7:K:43:ILE:HD12	7:K:56:ASP:HB2	1.92	0.49
8:L:117:THR:HG23	8:L:118:THR:HG23	1.95	0.49
1:A:189:G:H21	1:A:207:A:H62	1.59	0.49
1:A:605:G:N3	1:A:657:U:O2'	2.44	0.49
1:A:237:C:N4	1:A:261:G:O6	2.45	0.49
1:A:539:G:OP1	6:J:7:LYS:NZ	2.45	0.49
1:A:559:G:N2	11:Q:51:GLN:OE1	2.44	0.49
1:A:505:A:HO2'	1:A:509:C:HO2'	1.58	0.49
1:A:571:U:O2'	1:A:573:U:OP2	2.30	0.49
7:K:51:LYS:HD3	7:K:95:ILE:HG22	1.93	0.49
7:K:102:PRO:HD3	10:P:65:ASN:HD22	1.75	0.49
1:A:239:C:O2'	1:A:622:G:O2'	2.26	0.49
1:A:1654:A:N6	1:A:2006:C:O4'	2.45	0.49
1:A:1392:A:N6	14:T:18:GLU:OE2	2.44	0.49
15:U:11:ILE:HB	15:U:21:ARG:HG2	1.94	0.49
1:A:206:U:H2'	1:A:207:A:H8	1.77	0.49
1:A:737:C:H2'	1:A:738:G:C8	2.48	0.49
9:N:114:GLU:OE1	9:N:118:ARG:NH2	2.45	0.49
1:A:2898:U:H2'	1:A:2899:A:H8	1.78	0.49
1:A:78:U:O2	1:A:108:G:N2	2.39	0.48
1:A:1653:G:H1	9:N:11:ASN:HD21	1.60	0.48
5:G:68:ARG:HH12	5:G:72:ASN:HD22	1.60	0.48
14:T:47:VAL:HG11	14:T:85:VAL:HG11	1.94	0.48
1:A:1164:C:H2'	1:A:1165:A:H8	1.78	0.48
1:A:609:A:N6	1:A:619:G:H21	2.10	0.48
1:A:1683:U:H2'	1:A:1684:G:H8	1.79	0.48
1:A:335:C:O2	15:U:67:SER:OG	2.31	0.48
1:A:1318:U:H3	1:A:1334:G:H1	1.61	0.48
1:A:1665:A:H2'	1:A:1666:G:H8	1.77	0.48
1:A:24:G:O2'	13:S:78:GLU:O	2.31	0.48
1:A:1256:G:N2	4:E:77:ILE:O	2.37	0.48
1:A:494:G:H2'	1:A:495:G:H8	1.77	0.48
1:A:1340:U:OP2	14:T:82:LYS:NZ	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1567:G:OP1	2:C:59:GLN:NE2	2.46	0.48
12:R:19:THR:HA	12:R:96:VAL:O	2.14	0.48
1:A:1386:C:H2'	1:A:1387:A:H8	1.79	0.48
4:E:55:SER:O	4:E:74:LYS:NZ	2.47	0.48
9:N:45:ARG:O	9:N:49:GLU:HB2	2.13	0.48
1:A:968:C:H2'	1:A:969:G:H8	1.78	0.47
1:A:2618:G:O2'	3:D:155:VAL:O	2.32	0.47
1:A:2656:U:O2	1:A:2665:A:N7	2.47	0.47
1:A:2665:A:N6	5:G:107:GLY:O	2.41	0.47
1:A:1477:A:H62	1:A:1514:G:H21	1.62	0.47
1:A:2693:G:H2'	1:A:2694:G:H8	1.79	0.47
2:C:134:ILE:O	2:C:166:ARG:NH2	2.47	0.47
5:G:22:VAL:HG12	5:G:35:THR:HA	1.96	0.47
7:K:2:ILE:HG13	7:K:62:VAL:HG21	1.95	0.47
10:P:8:GLU:HA	10:P:54:LEU:HD22	1.95	0.47
1:A:1159:U:H2'	1:A:1160:G:H8	1.79	0.47
8:L:100:ILE:HG23	8:L:101:ILE:HG12	1.95	0.47
1:A:539:G:O6	1:A:555:G:N2	2.48	0.47
1:A:589:U:H2'	1:A:590:A:H8	1.77	0.47
1:A:1666:G:H4'	7:K:6:THR:HG23	1.97	0.47
2:C:68:ARG:NH1	2:C:128:THR:OG1	2.48	0.47
1:A:121:G:H4'	1:A:149:A:H5'	1.96	0.47
1:A:263:G:H21	1:A:430:A:H2	1.62	0.47
1:A:304:U:O4	1:A:313:G:O6	2.32	0.47
6:J:102:GLU:O	6:J:106:LYS:HB3	2.14	0.47
1:A:13:A:O2'	1:A:15:G:N7	2.46	0.47
1:A:319:G:H1	1:A:323:C:H42	1.63	0.47
5:G:138:GLN:O	5:G:142:GLN:HB2	2.15	0.47
1:A:523:C:O2	1:A:554:U:O2'	2.31	0.47
1:A:950:G:O6	1:A:967:U:O4	2.33	0.47
1:A:1386:C:O2'	1:A:1469:A:N3	2.44	0.47
1:A:1582:C:O2'	1:A:1585:C:N3	2.38	0.47
6:J:17:VAL:HB	6:J:139:VAL:HA	1.96	0.47
12:R:21:ARG:HA	12:R:94:THR:O	2.15	0.47
15:U:14:THR:OG1	15:U:68:ASN:ND2	2.48	0.47
1:A:59:U:H3	1:A:68:G:H1	1.62	0.47
1:A:1358:G:N2	1:A:1372:U:OP2	2.47	0.47
6:J:102:GLU:O	6:J:106:LYS:CB	2.62	0.47
1:A:247:G:O2'	1:A:250:G:O6	2.31	0.47
1:A:1654:A:O2'	3:D:118:PHE:O	2.33	0.47
1:A:2682:A:O2'	3:D:13:ARG:NH1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2788:C:O2'	1:A:2809:A:N3	2.41	0.47
2:C:172:THR:HG22	2:C:182:LYS:HG2	1.97	0.47
4:E:45:ALA:HB2	4:E:89:PRO:HD3	1.96	0.47
1:A:261:G:HO2'	1:A:610:C:HO2'	1.63	0.46
1:A:727:A:N3	2:C:12:ARG:NH1	2.63	0.46
1:A:1666:G:N3	7:K:3:GLN:NE2	2.63	0.46
1:A:2861:U:H2'	1:A:2862:G:H8	1.80	0.46
1:A:1800:C:O2	1:A:1817:G:O6	2.32	0.46
1:A:2659:G:N2	1:A:2662:A:OP2	2.41	0.46
5:G:95:ALA:H	5:G:127:GLN:HE21	1.62	0.46
10:P:58:PHE:O	10:P:72:VAL:HA	2.15	0.46
1:A:83:A:O2'	1:A:103:A:N6	2.48	0.46
1:A:243:U:H2'	1:A:244:A:H8	1.81	0.46
6:J:7:LYS:HD2	6:J:10:THR:HG23	1.97	0.46
9:N:18:GLN:O	9:N:22:ARG:HB2	2.15	0.46
13:S:44:ALA:HA	13:S:47:VAL:HG12	1.97	0.46
5:G:27:GLY:HA3	5:G:78:VAL:HB	1.96	0.46
1:A:782:A:H3'	1:A:1788:C:H4'	1.97	0.46
1:A:559:G:N2	11:Q:48:ASP:OD1	2.46	0.46
1:A:1654:A:H2'	1:A:1655:A:H8	1.80	0.46
2:C:67:LYS:NZ	2:C:148:GLY:O	2.48	0.46
4:E:118:LEU:HD11	4:E:188:MET:HG2	1.97	0.46
5:G:65:GLY:O	5:G:68:ARG:HB3	2.16	0.46
1:A:31:C:H42	1:A:474:G:H1	1.64	0.46
1:A:65:U:H4'	14:T:73:ARG:HE	1.79	0.46
1:A:1400:U:H2'	1:A:1401:G:C8	2.51	0.46
5:G:141:GLY:O	5:G:145:ALA:CB	2.64	0.46
1:A:177:G:H3'	1:A:178:G:H8	1.81	0.46
1:A:302:C:H2'	1:A:303:G:H8	1.80	0.46
1:A:1468:U:O2	1:A:1524:G:O6	2.33	0.46
1:A:2780:G:N1	6:J:102:GLU:OE2	2.46	0.46
4:E:58:LYS:NZ	4:E:70:SER:O	2.41	0.46
1:A:500:G:N1	1:A:503:A:OP2	2.40	0.46
1:A:1013:C:H2'	1:A:1014:A:H8	1.80	0.46
1:A:1753:G:N2	1:A:1756:G:O5'	2.48	0.46
1:A:220:G:H1	1:A:427:U:H3'	1.81	0.46
1:A:861:A:H62	1:A:916:G:N2	2.09	0.46
1:A:1598:A:H5"	14:T:40:LYS:HD3	1.98	0.46
9:N:33:ILE:HD12	9:N:118:ARG:HH22	1.81	0.45
14:T:44:LYS:O	14:T:48:GLN:CB	2.64	0.45
1:A:16:C:H2'	1:A:17:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:G:H2'	1:A:1369:G:H8	1.80	0.45
10:P:6:GLN:HA	10:P:9:GLN:HG2	1.97	0.45
1:A:559:G:N3	11:Q:55:GLN:NE2	2.63	0.45
1:A:594:U:H3	1:A:663:G:H1	1.63	0.45
1:A:1597:A:H5"	1:A:1598:A:H5'	1.97	0.45
2:C:92:LEU:HD11	2:C:100:ARG:HB3	1.98	0.45
16:Y:46:VAL:O	16:Y:50:VAL:N	2.45	0.45
1:A:922:C:H2'	1:A:923:G:H8	1.81	0.45
1:A:1752:C:H2'	1:A:1753:G:C8	2.51	0.45
1:A:2679:A:H4'	3:D:194:PRO:HG3	1.98	0.45
1:A:2824:C:H3'	1:A:2825:G:H21	1.80	0.45
1:A:571:U:N3	1:A:575:A:N7	2.64	0.45
1:A:770:G:H2'	1:A:771:G:H8	1.81	0.45
1:A:935:C:H2'	1:A:936:A:C8	2.51	0.45
2:C:170:TYR:HB2	2:C:182:LYS:HE3	1.99	0.45
16:Y:28:LEU:O	16:Y:32:ALA:CB	2.65	0.45
1:A:2733:A:C6	3:D:208:LYS:HG2	2.51	0.45
4:E:155:GLU:O	4:E:159:LEU:CB	2.63	0.45
11:Q:113:LYS:HA	11:Q:116:LEU:HB2	1.98	0.45
1:A:538:A:H62	1:A:555:G:H21	1.65	0.45
1:A:2842:G:H2'	1:A:2843:G:H8	1.82	0.45
11:Q:60:TRP:HB3	11:Q:91:ARG:HB3	1.99	0.45
5:G:126:THR:HB	5:G:129:GLU:HB3	1.99	0.44
1:A:499:U:H3	1:A:503:A:H62	1.65	0.44
1:A:1365:A:H5"	1:A:1808:A:H62	1.83	0.44
1:A:244:A:N6	1:A:254:G:H21	2.05	0.44
1:A:694:U:OP1	2:C:58:LYS:NZ	2.40	0.44
1:A:1171:G:N2	1:A:1179:G:N7	2.66	0.44
1:A:1378:A:O2'	1:A:1380:G:OP2	2.34	0.44
1:A:1434:A:H2'	1:A:1435:G:C8	2.53	0.44
1:A:1789:A:OP2	2:C:220:ARG:NH1	2.49	0.44
1:A:2852:G:H5'	9:N:64:ARG:HH22	1.82	0.44
8:L:110:VAL:HG21	8:L:127:VAL:HG22	1.99	0.44
1:A:213:A:H2'	1:A:214:G:C8	2.52	0.44
12:R:2:TYR:H	12:R:42:ALA:HB3	1.82	0.44
1:A:848:C:H2'	1:A:849:A:C8	2.53	0.44
1:A:2817:U:OP1	9:N:42:LYS:NZ	2.50	0.44
3:D:1:MET:HA	3:D:85:ALA:HB2	1.98	0.44
7:K:109:SER:HB3	7:K:112:PHE:HD2	1.83	0.44
1:A:383:C:H42	1:A:391:A:H62	1.65	0.44
1:A:1818:U:H2'	2:C:155:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:69:LEU:HA	13:S:109:ASP:HA	1.99	0.44
1:A:1024:G:HO2'	1:A:1144:A:HO2'	1.65	0.43
1:A:2849:U:H5'	1:A:2867:G:H21	1.83	0.43
8:L:101:ILE:HD12	8:L:105:ILE:HG21	1.98	0.43
1:A:116:C:H5"	1:A:128:C:H41	1.82	0.43
2:C:202:ARG:HG2	2:C:204:LEU:HD12	2.00	0.43
9:N:63:ARG:HH12	9:N:77:ALA:HA	1.82	0.43
1:A:145:C:H2'	1:A:146:A:H8	1.82	0.43
1:A:1264:A:OP1	17:0:15:ARG:NH1	2.43	0.43
1:A:1316:U:H2'	1:A:1317:G:H8	1.82	0.43
1:A:2692:G:N3	1:A:2847:U:O2'	2.46	0.43
15:U:36:GLU:HA	15:U:61:GLU:HG2	2.01	0.43
1:A:272:A:H2'	1:A:273:G:H8	1.81	0.43
1:A:1483:G:O6	1:A:1506:U:O4	2.35	0.43
1:A:537:G:H4'	6:J:5:THR:HG21	2.00	0.43
4:E:149:ILE:HD11	4:E:172:ALA:HA	2.01	0.43
19:Z:8:GLN:HA	19:Z:54:VAL:HG12	2.01	0.43
1:A:245:G:H1	1:A:253:C:H42	1.67	0.43
1:A:582:A:H2'	1:A:583:G:H8	1.83	0.43
1:A:1386:C:H2'	1:A:1387:A:C8	2.54	0.43
1:A:1771:C:H42	1:A:1980:G:H1	1.67	0.43
1:A:2668:G:H2'	1:A:2669:G:H8	1.83	0.43
1:A:2684:U:OP2	10:P:50:ARG:NH1	2.51	0.43
2:C:4:LYS:HA	2:C:16:VAL:HG22	1.99	0.43
2:C:20:ASN:HB3	2:C:23:LEU:HD13	2.00	0.43
4:E:18:THR:HG23	4:E:106:LYS:HG2	2.01	0.43
7:K:87:LEU:HD22	7:K:92:GLU:HB3	2.01	0.43
1:A:18:U:H2'	1:A:19:A:C8	2.53	0.43
1:A:1421:G:H2'	1:A:1422:G:H8	1.84	0.43
1:A:1435:G:H2'	1:A:1436:G:C8	2.54	0.43
1:A:2812:G:H2'	1:A:2813:A:H8	1.83	0.43
10:P:57:ALA:HA	10:P:73:PHE:O	2.18	0.43
1:A:57:C:OP2	14:T:76:ARG:NH2	2.52	0.43
1:A:475:C:H4'	1:A:510:C:H5'	1.99	0.43
1:A:1518:C:H2'	1:A:1519:G:H8	1.82	0.43
16:Y:42:LEU:O	16:Y:45:GLN:NE2	2.40	0.43
1:A:107:G:H2'	1:A:108:G:H8	1.84	0.43
1:A:1501:G:H4'	2:C:94:LEU:HD11	2.01	0.43
1:A:287:G:O6	1:A:354:A:N6	2.52	0.42
1:A:1709:U:O2'	1:A:2859:G:N3	2.47	0.42
1:A:2680:U:O2'	3:D:11:MET:SD	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:37:ASP:OD1	14:T:37:ASP:N	2.52	0.42
1:A:606:U:H3	1:A:622:G:H1	1.67	0.42
9:N:28:LEU:HD23	9:N:48:VAL:HG21	2.00	0.42
11:Q:71:ASN:HD22	11:Q:109:VAL:HG21	1.84	0.42
1:A:710:U:H2'	1:A:711:G:H8	1.84	0.42
1:A:1447:C:O2'	1:A:1544:A:N3	2.39	0.42
1:A:1704:C:H2'	1:A:1705:A:H8	1.84	0.42
1:A:2016:U:O2'	17:0:3:GLN:O	2.37	0.42
2:C:80:LEU:HD21	2:C:109:LEU:HD22	2.01	0.42
14:T:8:LEU:O	16:Y:29:ARG:NH1	2.52	0.42
1:A:324:A:OP2	1:A:1205:A:N6	2.53	0.42
1:A:1146:C:H2'	1:A:1147:A:H8	1.84	0.42
1:A:2637:U:H3	1:A:2776:A:H62	1.67	0.42
4:E:148:ILE:HB	4:E:169:VAL:HG22	2.01	0.42
1:A:526:A:O2'	1:A:2043:C:O2	2.30	0.42
1:A:1716:U:H2'	1:A:1717:A:H8	1.85	0.42
6:J:55:ILE:HA	6:J:123:LYS:O	2.19	0.42
11:Q:8:ILE:H	11:Q:8:ILE:HG13	1.77	0.42
15:U:95:PHE:HB2	15:U:100:GLU:HB3	2.00	0.42
1:A:711:G:H2'	1:A:712:G:H8	1.84	0.42
1:A:968:C:H2'	1:A:969:G:C8	2.53	0.42
1:A:1793:C:H2'	1:A:1794:A:H8	1.84	0.42
2:C:144:GLU:HB3	2:C:187:CYS:HB3	2.02	0.42
14:T:57:VAL:HG12	14:T:86:THR:HB	2.01	0.42
1:A:15:G:H1	1:A:525:U:H3	1.67	0.42
6:J:37:ARG:NE	6:J:44:TYR:OH	2.50	0.42
19:Z:53:MET:HG3	19:Z:54:VAL:HG13	2.02	0.42
1:A:171:U:H2'	1:A:172:A:C8	2.54	0.42
1:A:437:U:H2'	1:A:438:G:H8	1.85	0.42
2:C:91:ALA:O	2:C:102:TYR:HA	2.20	0.42
14:T:8:LEU:HD23	14:T:50:LEU:HD21	2.02	0.42
1:A:1418:G:N1	1:A:1579:A:OP2	2.49	0.42
15:U:24:VAL:HG22	15:U:35:VAL:HG22	2.01	0.42
1:A:980:A:N6	1:A:2027:G:O2'	2.52	0.42
1:A:1152:C:H2'	1:A:1153:C:H6	1.85	0.42
1:A:1409:U:H2'	1:A:1410:G:H8	1.85	0.42
2:C:61:TYR:HA	2:C:85:ASN:HD21	1.85	0.42
8:L:112:LEU:HD21	8:L:134:ALA:HB3	2.00	0.42
15:U:10:VAL:HB	15:U:69:VAL:HB	2.02	0.42
16:Y:17:GLU:OE2	16:Y:54:LYS:NZ	2.40	0.42
18:2:34:ARG:NH1	18:2:42:LEU:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:G:H2'	1:A:748:G:H21	1.84	0.41
1:A:1638:C:O2	1:A:2698:U:O2'	2.37	0.41
1:A:695:G:O6	1:A:767:U:O4	2.38	0.41
1:A:1665:A:H2'	1:A:1666:G:C8	2.56	0.41
1:A:1013:C:H2'	1:A:1014:A:C8	2.55	0.41
1:A:1139:G:O2'	1:A:1143:A:N1	2.48	0.41
1:A:1316:U:H2'	1:A:1317:G:C8	2.56	0.41
1:A:2761:A:O2'	5:G:142:GLN:NE2	2.53	0.41
11:Q:87:VAL:HG12	11:Q:89:ILE:H	1.85	0.41
18:2:31:LEU:HD22	18:2:42:LEU:HD23	2.02	0.41
1:A:307:G:H21	1:A:330:A:H61	1.67	0.41
1:A:445:C:H5"	11:Q:2:ARG:HB3	2.02	0.41
1:A:110:G:H2'	1:A:111:A:H8	1.86	0.41
1:A:151:C:H2'	1:A:152:A:H8	1.86	0.41
1:A:2882:A:OP1	9:N:96:ARG:NH2	2.52	0.41
3:D:97:SER:OG	3:D:98:VAL:N	2.52	0.41
6:J:90:GLU:O	6:J:94:ALA:CB	2.68	0.41
17:0:12:ARG:HG3	17:0:15:ARG:HH11	1.86	0.41
1:A:519:U:H2'	1:A:520:G:C8	2.55	0.41
1:A:1830:C:H2'	1:A:1831:G:C8	2.53	0.41
1:A:703:U:O4	1:A:728:G:O6	2.38	0.41
1:A:2861:U:H2'	1:A:2862:G:C8	2.55	0.41
13:S:4:ILE:HG12	13:S:106:VAL:HG22	2.02	0.41
1:A:672:C:H5"	4:E:84:THR:HG21	2.02	0.41
1:A:1531:C:H2'	1:A:1532:A:C8	2.56	0.41
1:A:2626:C:H2'	1:A:2627:G:C8	2.56	0.41
1:A:2898:U:H2'	1:A:2899:A:C8	2.55	0.41
15:U:32:LYS:HB3	15:U:63:ALA:HB1	2.03	0.41
1:A:76:C:H2'	1:A:77:G:H8	1.86	0.41
1:A:769:U:H2'	1:A:770:G:H8	1.85	0.41
1:A:811:U:N3	1:A:1250:G:OP1	2.48	0.41
1:A:848:C:H2'	1:A:849:A:H8	1.86	0.41
1:A:927:A:H2'	1:A:928:A:C8	2.56	0.41
1:A:1359:A:N7	1:A:1372:U:O4	2.54	0.41
1:A:2675:A:H61	1:A:2732:G:H1	1.69	0.41
2:C:198:GLU:HA	2:C:201:LEU:HD13	2.02	0.41
3:D:40:LEU:HD23	3:D:45:TYR:HA	2.03	0.41
1:A:923:G:H2'	1:A:924:G:H8	1.86	0.41
1:A:1283:G:H21	1:A:1329:U:H3	1.69	0.41
1:A:1463:C:H2'	1:A:1464:G:H8	1.86	0.41
1:A:2787:C:H1'	3:D:63:PRO:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:96:LEU:HB3	10:P:99:LEU:HD12	2.04	0.41
1:A:45:G:H5'	1:A:46:G:H5'	2.02	0.40
1:A:929:U:H4'	19:Z:37:ARG:HH22	1.86	0.40
12:R:69:GLY:N	12:R:91:GLN:O	2.47	0.40
17:0:37:HIS:HB3	17:0:43:THR:HG22	2.03	0.40
1:A:1148:U:H2'	1:A:1149:G:C8	2.56	0.40
1:A:1615:C:OP2	1:A:1617:C:N4	2.55	0.40
1:A:2647:U:H2'	1:A:2648:G:H8	1.85	0.40
3:D:176:ASP:OD1	3:D:176:ASP:N	2.54	0.40
1:A:29:U:O4	1:A:512:G:N2	2.55	0.40
1:A:437:U:H2'	1:A:438:G:C8	2.57	0.40
1:A:1259:G:H2'	1:A:1260:A:C8	2.56	0.40
1:A:1355:G:H2'	1:A:1356:G:C8	2.56	0.40
1:A:1444:G:H2'	1:A:1445:G:H8	1.87	0.40
16:Y:43:LEU:HD22	16:Y:47:ARG:HH22	1.86	0.40
1:A:302:C:H2'	1:A:303:G:C8	2.55	0.40
11:Q:64:ILE:O	11:Q:68:ALA:CB	2.70	0.40
12:R:77:PHE:HD1	12:R:84:ARG:HB3	1.87	0.40
1:A:581:C:H2'	1:A:582:A:H8	1.86	0.40
1:A:828:U:O2'	1:A:831:G:O6	2.39	0.40
1:A:2688:G:N1	1:A:2720:U:OP2	2.36	0.40
1:A:2756:U:H1'	1:A:2757:A:H5"	2.04	0.40
1:A:2842:G:H2'	1:A:2843:G:C8	2.56	0.40
2:C:161:VAL:HG11	2:C:173:LEU:HD23	2.03	0.40

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
2	C	200/223 (90%)	190 (95%)	9 (4%)	1 (0%)	29 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	178/209 (85%)	171 (96%)	7 (4%)	0	100	100
4	E	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
5	G	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
6	J	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
7	K	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
8	L	105/143 (73%)	93 (89%)	12 (11%)	0	100	100
9	N	118/120 (98%)	104 (88%)	14 (12%)	0	100	100
10	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
11	Q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
12	R	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
13	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
14	T	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
15	U	100/102 (98%)	86 (86%)	14 (14%)	0	100	100
16	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	45
17	0	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
18	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
19	Z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
All	All	2076/2198 (94%)	1950 (94%)	124 (6%)	2 (0%)	54	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	12	ARG
16	Y	46	VAL

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	
2	C	162/175 (93%)	161 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	142/164 (87%)	142 (100%)	0	100	100
4	E	165/165 (100%)	165 (100%)	0	100	100
5	G	137/137 (100%)	137 (100%)	0	100	100
6	J	116/116 (100%)	116 (100%)	0	100	100
7	K	103/103 (100%)	103 (100%)	0	100	100
8	L	76/102 (74%)	76 (100%)	0	100	100
9	N	100/100 (100%)	99 (99%)	1 (1%)	76	86
10	P	99/99 (100%)	98 (99%)	1 (1%)	76	86
11	Q	89/89 (100%)	89 (100%)	0	100	100
12	R	84/84 (100%)	84 (100%)	0	100	100
13	S	93/93 (100%)	93 (100%)	0	100	100
14	T	80/80 (100%)	79 (99%)	1 (1%)	69	82
15	U	83/83 (100%)	83 (100%)	0	100	100
16	Y	55/55 (100%)	55 (100%)	0	100	100
17	0	47/47 (100%)	47 (100%)	0	100	100
18	2	38/38 (100%)	38 (100%)	0	100	100
19	Z	48/48 (100%)	48 (100%)	0	100	100
All	All	1717/1778 (97%)	1713 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	79	ARG
9	N	118	ARG
10	P	2	ASN
14	T	92	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	85	ASN
3	D	164	GLN
3	D	173	GLN
4	E	30	GLN
5	G	37	ASN

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Mol	Chain	Res	Type
5	G	72	ASN
5	G	127	GLN
5	G	142	GLN
9	N	11	ASN
10	P	2	ASN
10	P	65	ASN
11	Q	19	GLN
11	Q	43	GLN
11	Q	71	ASN
12	R	91	GLN
13	S	31	GLN
13	S	57	ASN
14	T	48	GLN
14	T	92	ASN
15	U	68	ASN
19	Z	19	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2085/2904 (71%)	307 (14%)	4 (0%)

All (307) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	14	A
1	A	27	G
1	A	34	U
1	A	46	G
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	138	U
1	A	139	U

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Mol	Chain	Res	Type
1	A	140	C
1	A	141	G
1	A	142	A
1	A	160	A
1	A	163	C
1	A	196	A
1	A	197	A
1	A	204	A
1	A	216	A
1	A	221	A
1	A	222	A
1	A	224	U
1	A	228	C
1	A	230	G
1	A	241	A
1	A	248	G
1	A	255	A
1	A	264	C
1	A	265	A
1	A	266	G
1	A	267	C
1	A	271	G
1	A	272	A
1	A	277	G
1	A	278	A
1	A	295	G
1	A	302	C
1	A	311	A
1	A	329	G
1	A	330	A
1	A	331	C
1	A	353	C
1	A	362	A
1	A	370	G
1	A	371	A
1	A	372	G
1	A	386	G
1	A	387	U
1	A	396	G
1	A	405	U
1	A	406	G
1	A	411	G

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Mol	Chain	Res	Type
1	A	424	G
1	A	435	C
1	A	451	U
1	A	455	C
1	A	467	G
1	A	475	C
1	A	479	A
1	A	480	A
1	A	481	G
1	A	489	G
1	A	491	G
1	A	504	A
1	A	505	A
1	A	510	C
1	A	531	C
1	A	532	A
1	A	543	G
1	A	544	C
1	A	546	U
1	A	547	A
1	A	548	G
1	A	550	C
1	A	562	U
1	A	563	A
1	A	568	U
1	A	572	A
1	A	573	U
1	A	574	A
1	A	586	A
1	A	603	A
1	A	613	A
1	A	614	A
1	A	615	U
1	A	621	A
1	A	627	A
1	A	637	A
1	A	647	G
1	A	654	A
1	A	669	G
1	A	670	A
1	A	686	U
1	A	726	G

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Mol	Chain	Res	Type
1	A	730	A
1	A	739	A
1	A	747	U
1	A	748	G
1	A	762	U
1	A	764	A
1	A	765	C
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	789	A
1	A	792	A
1	A	801	G
1	A	805	G
1	A	811	U
1	A	812	C
1	A	819	A
1	A	825	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	910	A
1	A	914	G
1	A	931	U
1	A	932	U
1	A	945	A
1	A	946	C
1	A	959	A
1	A	961	C
1	A	973	A
1	A	983	A
1	A	985	C
1	A	995	C
1	A	1009	A
1	A	1010	A
1	A	1012	U
1	A	1013	C

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Mol	Chain	Res	Type
1	A	1026	G
1	A	1132	U
1	A	1133	A
1	A	1134	A
1	A	1135	C
1	A	1136	G
1	A	1142	A
1	A	1144	A
1	A	1171	G
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1180	U
1	A	1182	G
1	A	1186	G
1	A	1202	G
1	A	1204	A
1	A	1212	G
1	A	1227	G
1	A	1236	G
1	A	1238	G
1	A	1240	U
1	A	1253	A
1	A	1256	G
1	A	1262	A
1	A	1266	G
1	A	1271	G
1	A	1272	A
1	A	1276	A
1	A	1300	G
1	A	1301	A
1	A	1302	A
1	A	1306	C
1	A	1329	U
1	A	1341	G
1	A	1345	C
1	A	1346	G
1	A	1365	A
1	A	1368	G
1	A	1374	G
1	A	1378	A

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Mol	Chain	Res	Type
1	A	1379	U
1	A	1383	A
1	A	1416	G
1	A	1419	A
1	A	1428	C
1	A	1451	C
1	A	1452	G
1	A	1453	A
1	A	1454	C
1	A	1458	U
1	A	1467	U
1	A	1482	G
1	A	1490	A
1	A	1493	C
1	A	1497	U
1	A	1515	A
1	A	1523	U
1	A	1524	G
1	A	1530	G
1	A	1532	A
1	A	1533	C
1	A	1535	A
1	A	1554	U
1	A	1555	G
1	A	1556	C
1	A	1558	C
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1583	A
1	A	1585	C
1	A	1587	G
1	A	1603	A
1	A	1607	C
1	A	1608	A
1	A	1618	A
1	A	1634	A
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1654	A
1	A	1660	G

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Mol	Chain	Res	Type
1	A	1665	A
1	A	1674	G
1	A	1699	G
1	A	1710	G
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1736	U
1	A	1738	G
1	A	1757	A
1	A	1764	C
1	A	1773	A
1	A	1781	U
1	A	1785	A
1	A	1800	C
1	A	1801	A
1	A	1807	G
1	A	1808	A
1	A	1809	A
1	A	1816	C
1	A	1829	A
1	A	1833	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1997	C
1	A	2021	C
1	A	2022	U
1	A	2023	C
1	A	2030	A
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2054	A
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2610	C
1	A	2614	A

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Mol	Chain	Res	Type
1	A	2629	U
1	A	2636	C
1	A	2639	A
1	A	2646	C
1	A	2654	A
1	A	2656	U
1	A	2682	A
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2716	C
1	A	2725	A
1	A	2726	A
1	A	2729	G
1	A	2732	G
1	A	2733	A
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2757	A
1	A	2765	A
1	A	2766	A
1	A	2771	C
1	A	2778	A
1	A	2791	G
1	A	2798	U
1	A	2801	G
1	A	2818	U
1	A	2820	A
1	A	2836	U
1	A	2849	U
1	A	2867	G
1	A	2873	A
1	A	2879	A
1	A	2880	C
1	A	2884	U
1	A	2886	A
1	A	2893	A
1	A	2901	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	271	G
1	A	479	A
1	A	1378	A
1	A	2756	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2045:C	O3'	2046:G	P	3.57
1	A	973:A	O3'	974:G	P	3.36

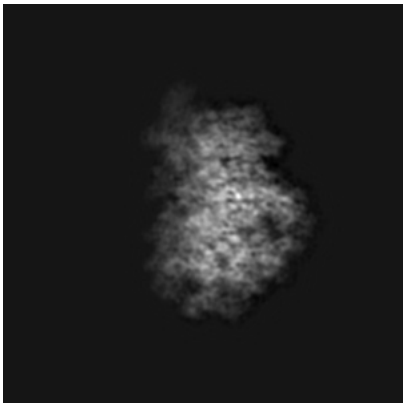
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4381. These allow visual inspection of the internal detail of the map and identification of artifacts.

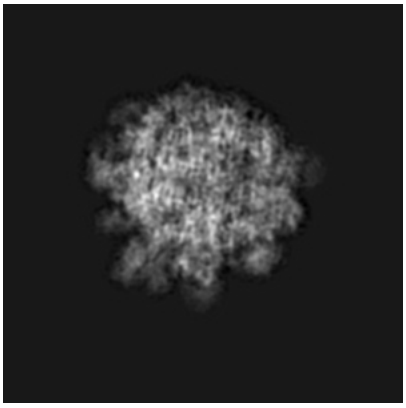
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

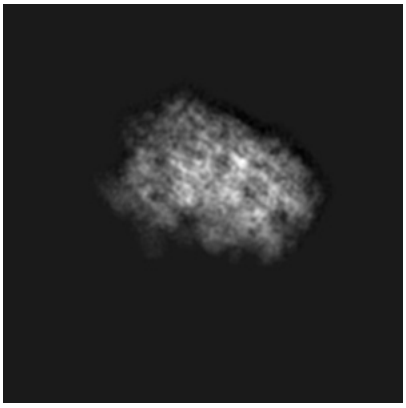
6.1.1 Primary map



X



Y

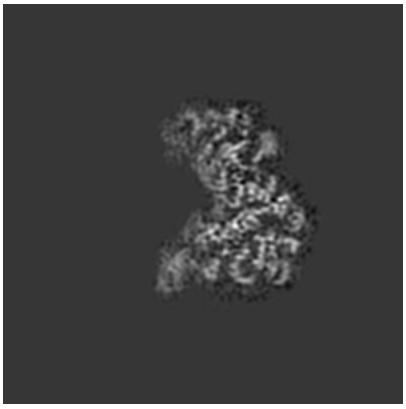


Z

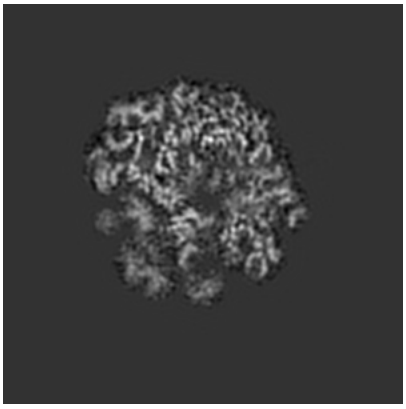
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

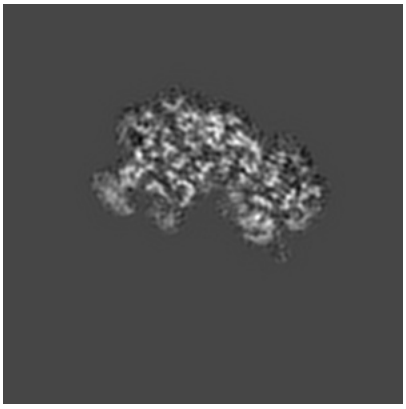
6.2.1 Primary map



X Index: 135



Y Index: 135

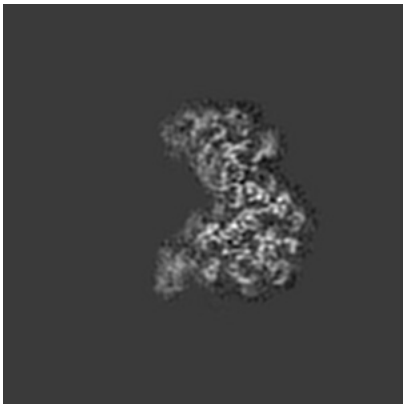


Z Index: 135

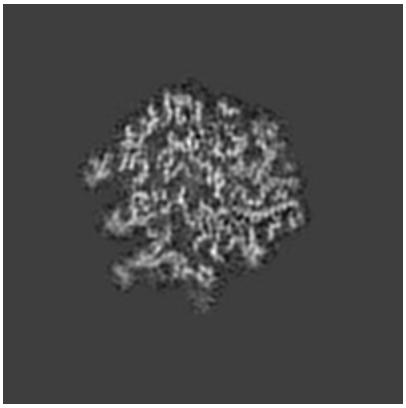
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

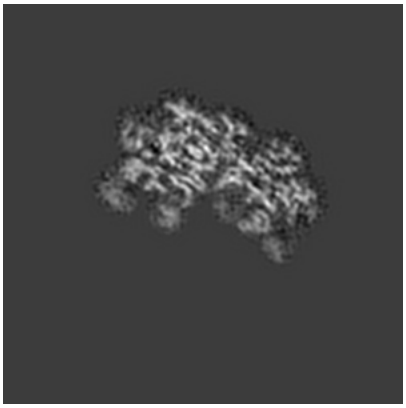
6.3.1 Primary map



X Index: 136



Y Index: 154



Z Index: 140

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 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

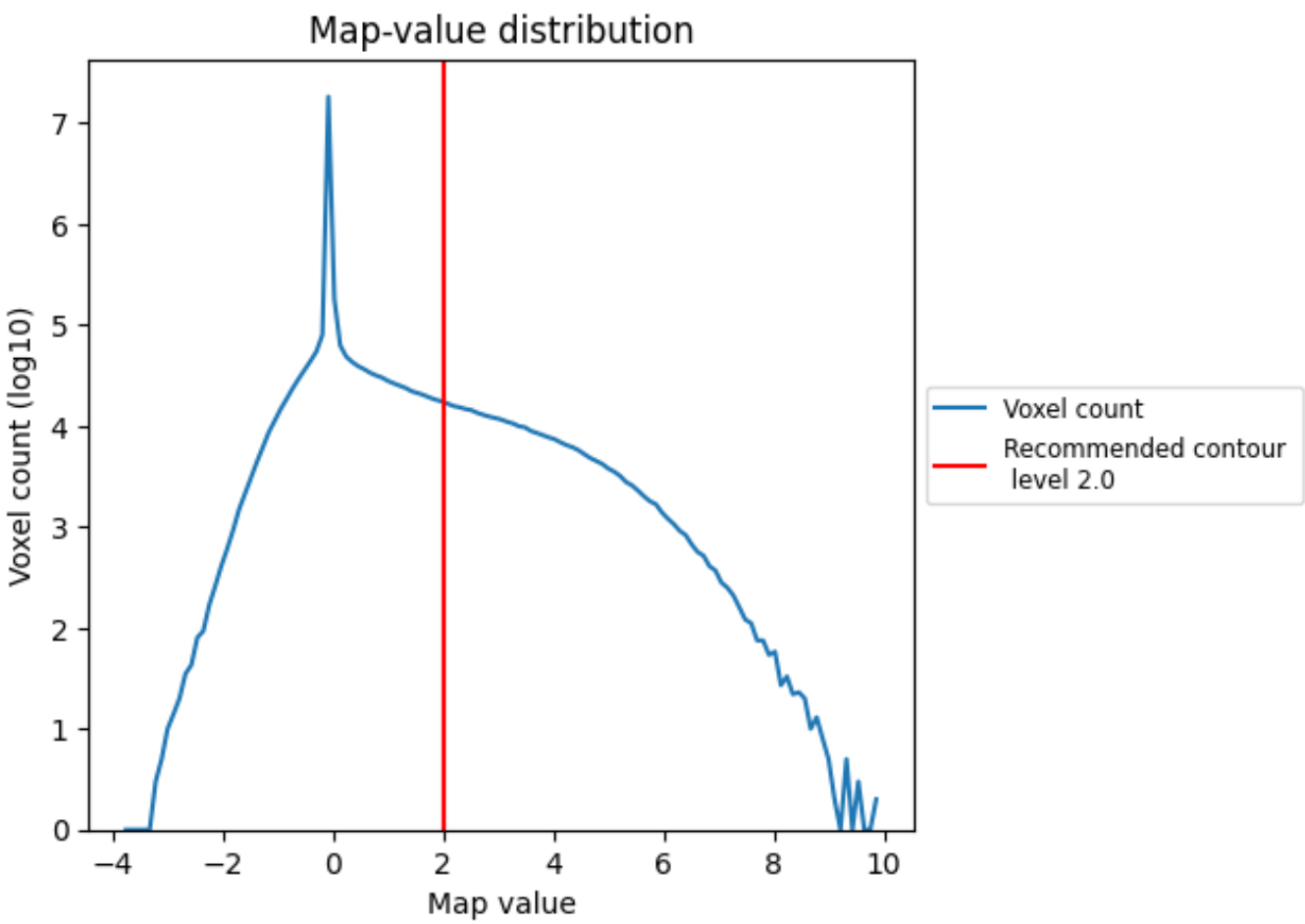
6.5 Mask visualisation (i)

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

7 Map analysis (i)

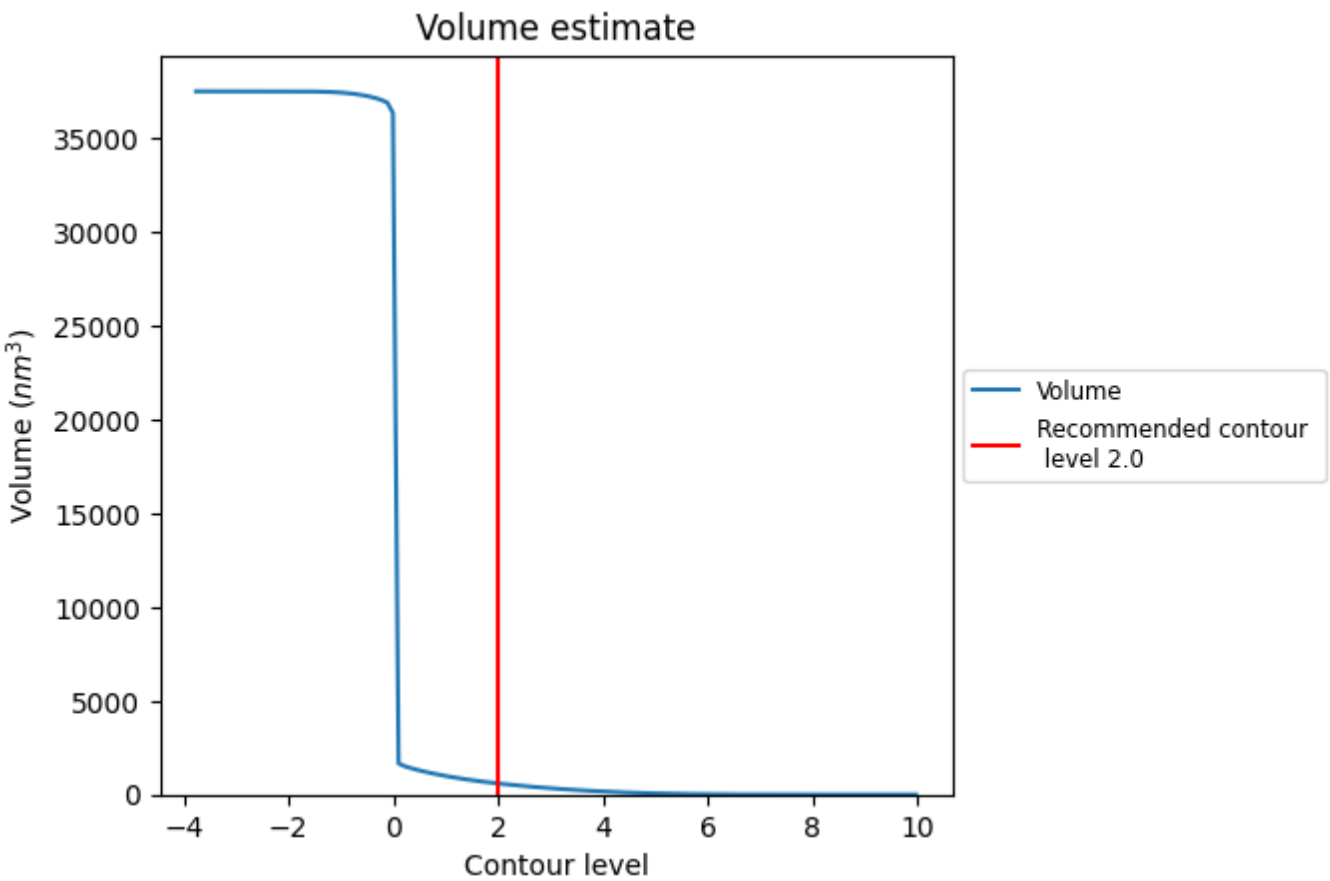
This section contains the results of statistical analysis of the map.

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.

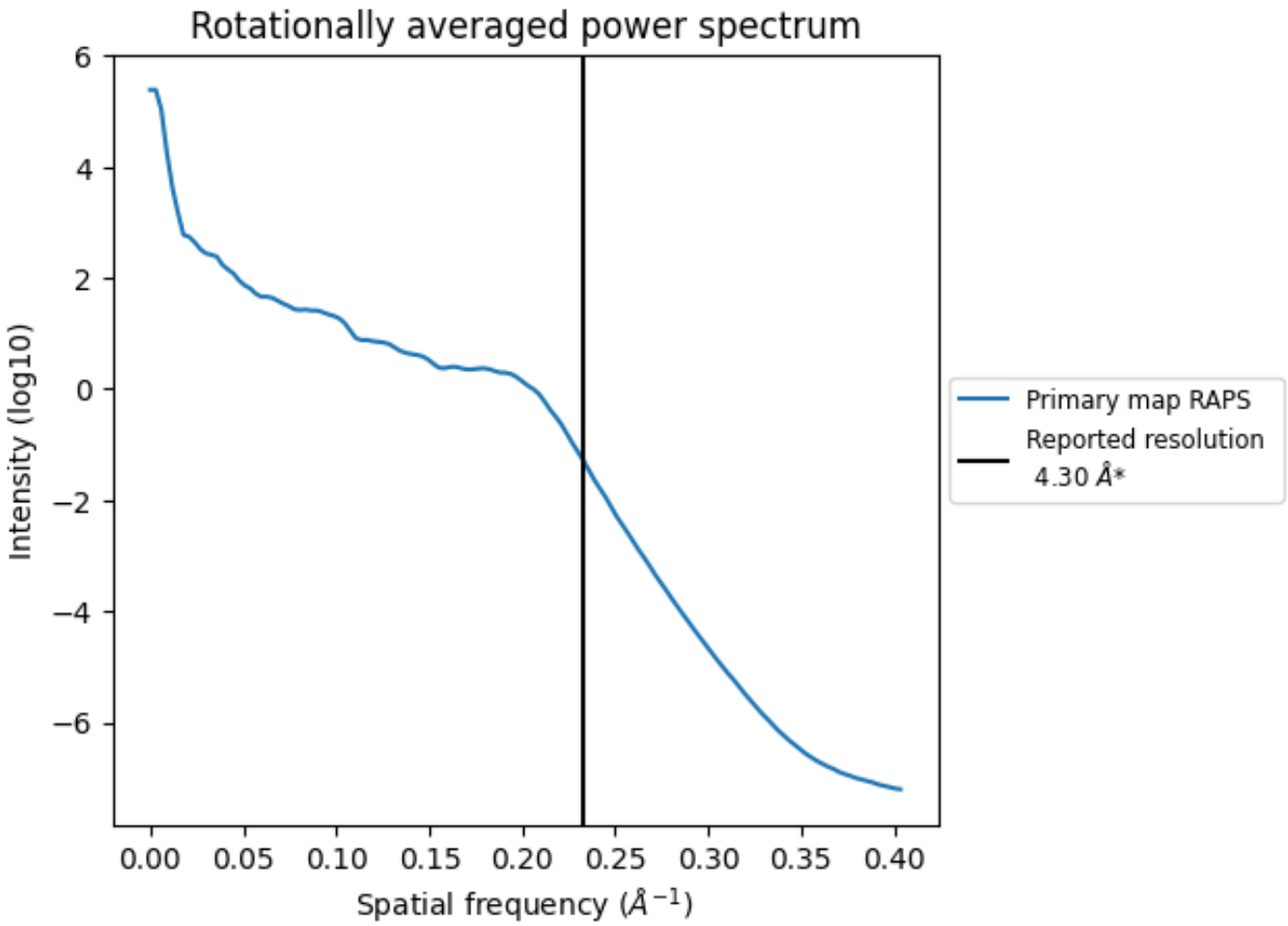
7.2 Volume estimate (i)



The volume at the recommended contour level is 592 nm^3; this corresponds to an approximate mass of 535 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 0.233 Å^{-1}

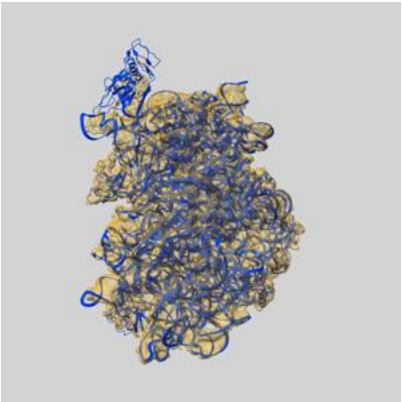
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

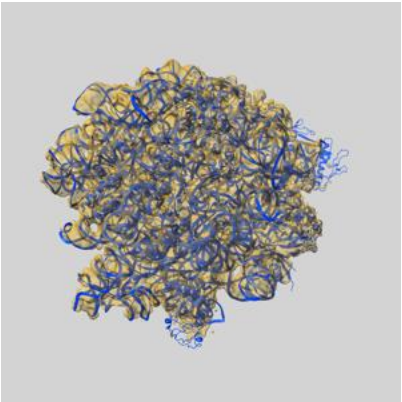
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4381 and PDB model 6GC6. Per-residue inclusion information can be found in section 3 on page 7.

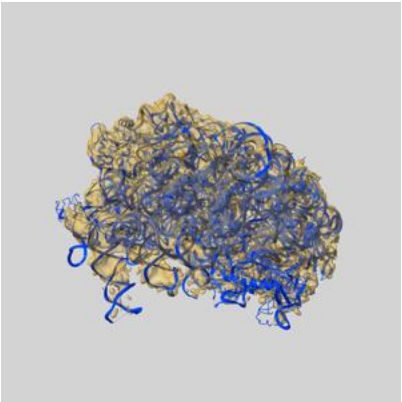
9.1 Map-model overlay (i)



X



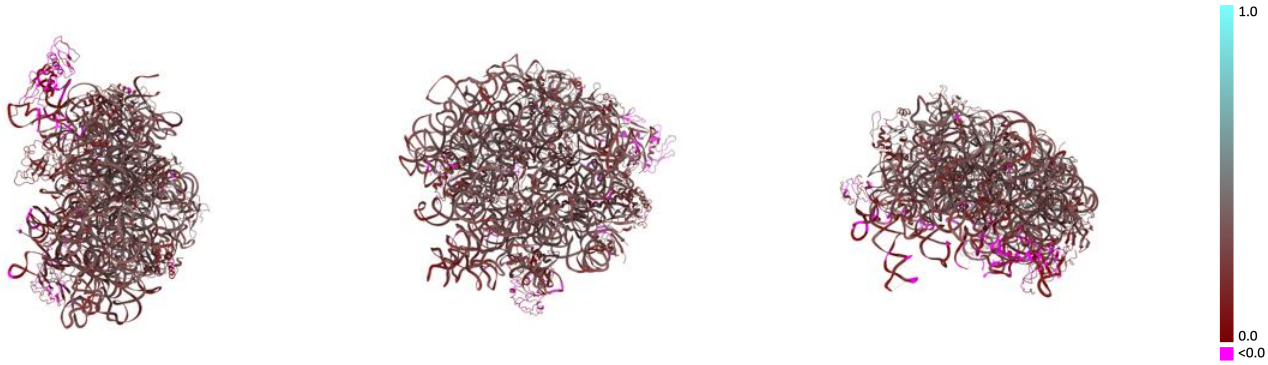
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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.

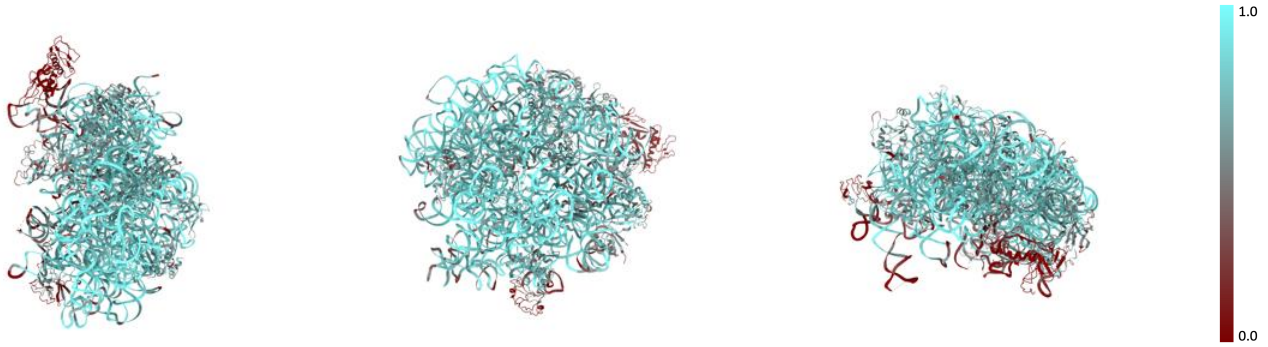
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

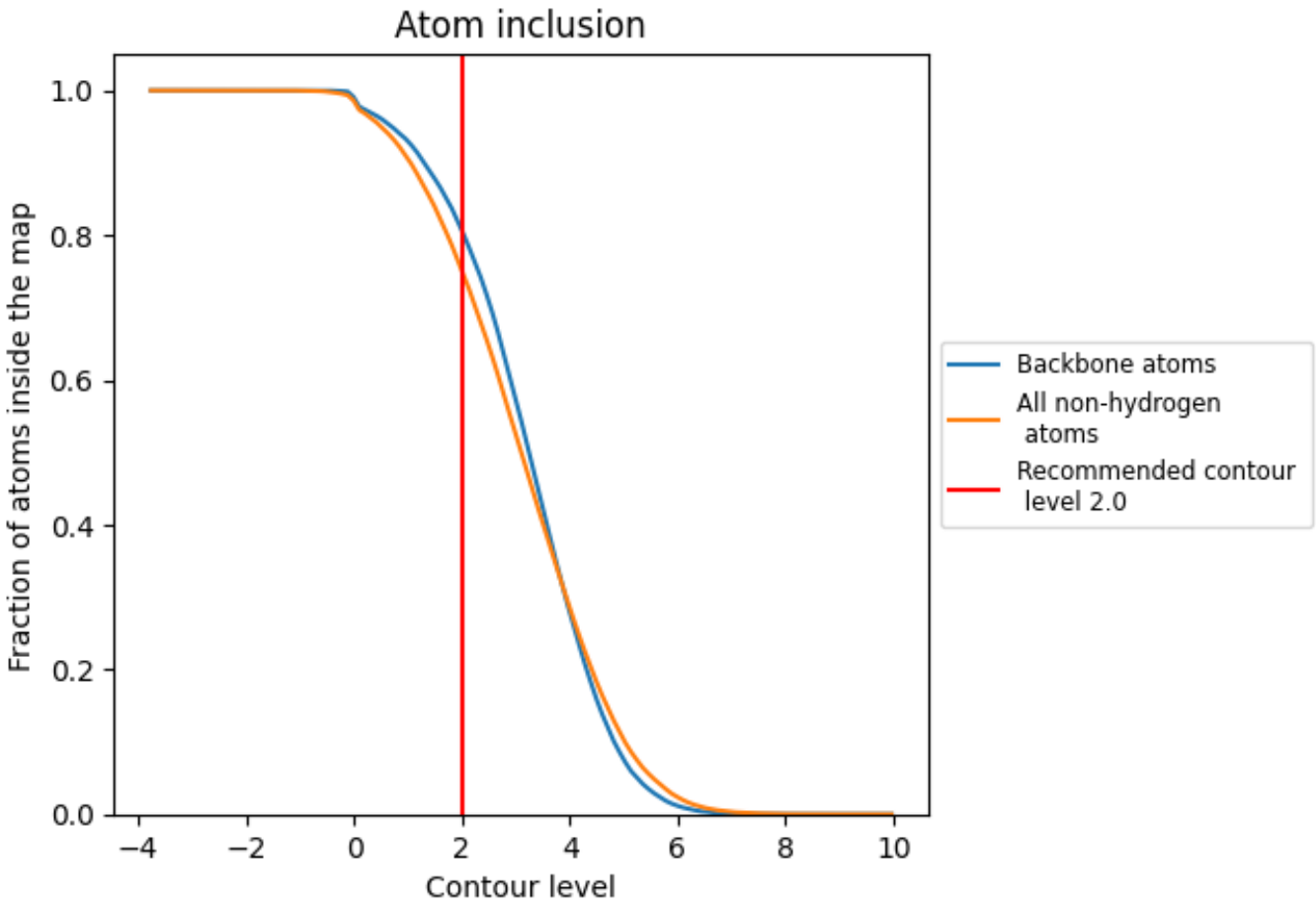
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 75% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7515	0.2610
0	0.6379	0.2610
2	0.7746	0.2690
A	0.8213	0.2750
C	0.4247	0.1480
D	0.6463	0.2780
E	0.6454	0.2400
G	0.0116	0.0260
J	0.6209	0.2480
K	0.5317	0.2250
L	0.2598	0.1250
N	0.7194	0.2830
P	0.5495	0.2470
Q	0.6982	0.2540
R	0.6775	0.2920
S	0.6483	0.2660
T	0.7234	0.2890
U	0.6680	0.2670
Y	0.6378	0.1950
Z	0.5675	0.2250