Full wwPDB EM Validation Report (i)

Mar 9, 2024 – 08:08 AM EST

PDB ID	:	6O90
EMDB ID	:	EMD-0660
Title	:	Cryo-EM image reconstruction of the 70S Ribosome Enterococcus faecalis Class05
Authors	:	Jogl, G.; Khayat, R.
Deposited on	:	2019-03-12
Resolution	:	3.49 Å(reported)
Based on initial models	:	5LI0, 4YBB

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:

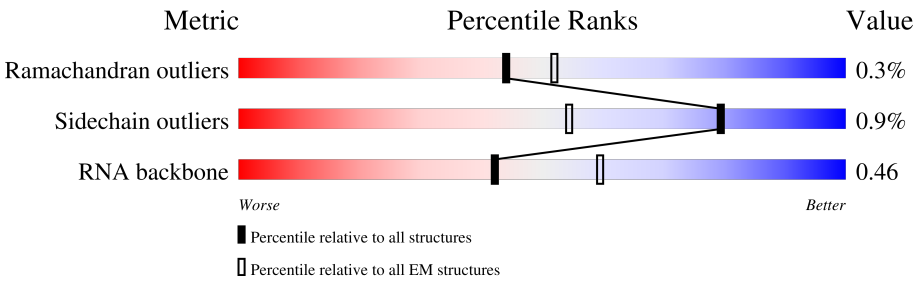
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.49 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	1528	67% 29% .
2	c	204	100%
3	d	201	13% 98% .
4	e	163	100%
5	f	97	100%
6	g	154	. 100%
7	h	131	100%
8	i	128	98% .

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Mol	Chain	Length	Quality of chain
9	j	99	98%
10	k	117	99%
11	l	136	5% 96%
12	m	112	99%
13	n	60	98%
14	o	88	98%
15	p	89	98%
16	q	83	96%
17	r	66	95% 5%
18	s	78	99%
19	t	81	7% 96%
20	A	2903	72% 25%
21	B	116	72% 25%
22	C	275	99%
23	D	207	97%
24	E	206	98%
25	F	177	99%
26	G	176	98%
27	K	145	99%
28	L	122	100%
29	M	146	96%
30	N	141	6% 97%
31	O	123	97%
32	P	117	97%
33	Q	114	98%

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Mol	Chain	Length	Quality of chain
34	R	118	98%
35	S	102	98%
36	T	112	100%
37	U	89	94%
38	V	101	95%
39	W	94	65% 98%
40	X	76	97%
41	Y	54	94% 6%
42	Z	61	98%
43	0	58	100%
44	1	83	99%
45	2	56	100%
46	3	49	100%
47	4	44	98%
48	5	64	100%
49	6	38	100%

2 Entry composition (i)

There are 50 unique types of molecules in this entry. The entry contains 138532 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1528	32746	14609	5979	10630	1528	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	c	204	1610	1012	303	292	3	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	201	1620	1016	303	297	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	e	163	1204	759	222	221	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f	97	795	501	137	154	3	0	0

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	g	154	1229	765	236	222	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	h	131	1041	662	184	193	2	0	0

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	i	128	990	615	197	177	1	0	0

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	j	99	800	504	147	147	2	0	0

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	k	117	863	533	165	161	4	0	0

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	l	136	1065	661	214	188	2	0	0

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	m	112	884	540	180	163	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	n	60	492	310	100	77	5	0	0

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	o	88	741	455	152	133	1	0	0

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	p	89	708	448	131	127	2	0	0

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	q	83	681	427	127	124	3	0	0

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	r	66	537	343	99	94	1	0	0

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	s	78	634	410	113	109	2	0	0

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	t	81	610	372	119	117	2	0	0

- Molecule 20 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	A	2903	62302	27811	11457	20131	2903	0	0

- Molecule 21 is a RNA chain called 4S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	B	116	2478	1106	444	812	116	0	0

- Molecule 22 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	C	275	2114	1310	416	381	7	0	0

- Molecule 23 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	D	207	1577	992	292	289	4	0	0

- Molecule 24 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	E	206	1573	984	290	297	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	F	177	1391	887	239	259	6	0	0

- Molecule 26 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	G	176	1344	842	243	255	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	K	145	1129	713	205	207	4	0	0

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	L	122	922	574	176	170	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	M	146	1094	676	212	205	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	N	141	1117	710	215	185	7	0	0

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	O	123	978	602	190	183	3	0	0

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	P	117	898	556	175	166	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Q	112	897	566	177	154	0	0

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	R	117	940	597	181	158	4	0	0

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	S	102	783	499	139	143	2	0	0

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	T	112	849	532	156	159	2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	U	89	719	457	127	132	3	0	0

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	V	101	763	486	135	140	2	0	0

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	W	94	757	479	135	139	4	0	0

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	X	76	571	351	108	112	0	0

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Y	54	425	265	86	72	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	51	ALA	THR	conflict	UNP A0A1B4XRZ8

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Z	61	504	314	94	95	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	0	58	434	270	81	82	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	1	83	673	424	114	133	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	2	56	429	262	88	73	6	0	0

- Molecule 46 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	3	49	418	253	85	76	4	0	0

- Molecule 47 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	4	44	374	227	91	54	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	5	64	522	320	122	78	2	0	0

- Molecule 49 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	6	38	303	188	66	43	6	0	0

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

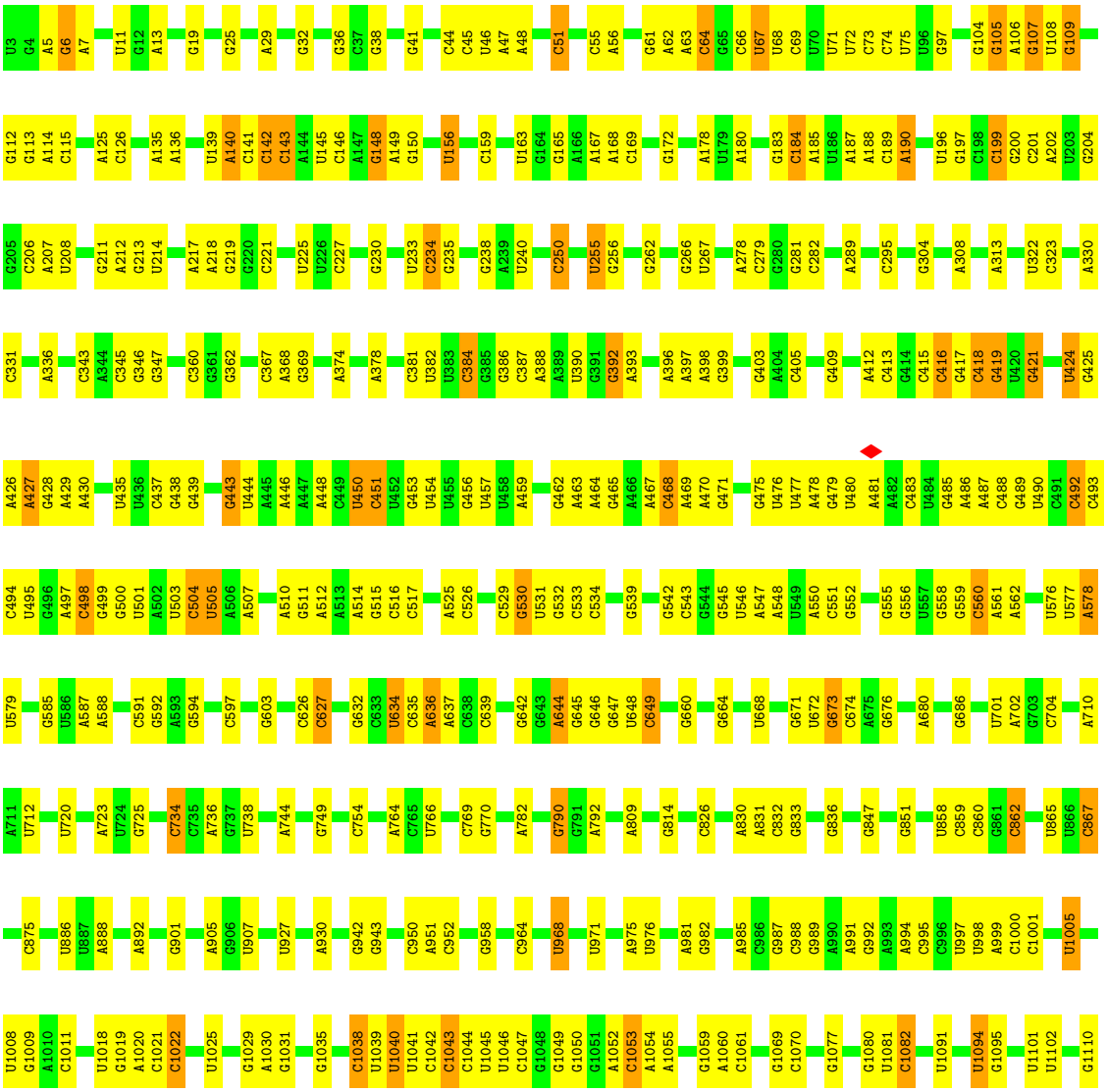
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
50	n	1	1	1	0
50	2	1	1	1	0
50	3	1	1	1	0
50	6	1	1	1	0

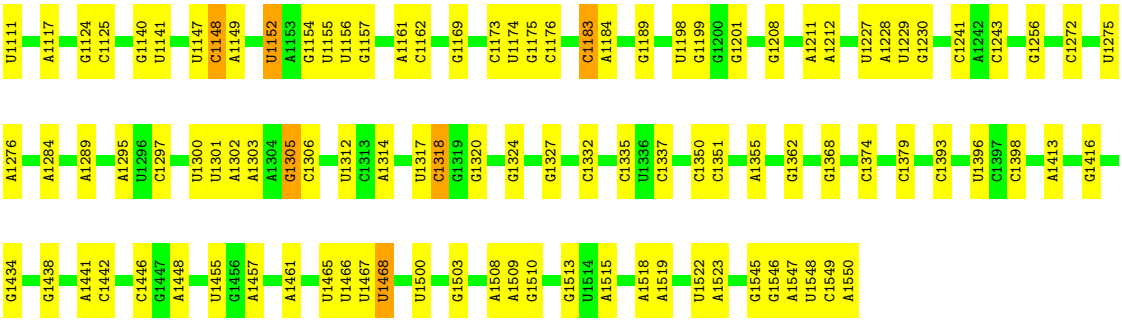
3 Residue-property plots (i)

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: 16S rRNA

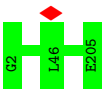
Chain a: 67% 29% •





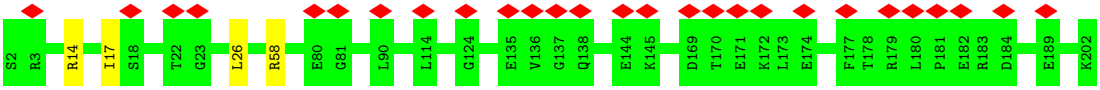
• Molecule 2: 30S ribosomal protein S3

Chain c: 100%



• Molecule 3: 30S ribosomal protein S4

Chain d: 13% 98%



• Molecule 4: 30S ribosomal protein S5

Chain e: 100%

There are no outlier residues recorded for this chain.

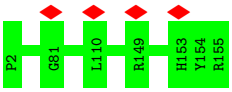
• Molecule 5: 30S ribosomal protein S6

Chain f: 100%

There are no outlier residues recorded for this chain.

• Molecule 6: 30S ribosomal protein S7

Chain g: 100%



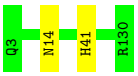
• Molecule 7: 30S ribosomal protein S8

Chain h: 100%

There are no outlier residues recorded for this chain.

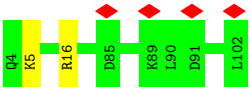
• Molecule 8: 30S ribosomal protein S9

Chain i: 98%



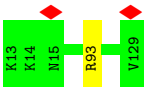
• Molecule 9: 30S ribosomal protein S10

Chain j: 98%



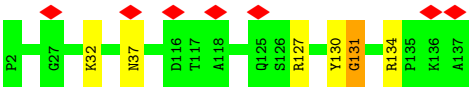
• Molecule 10: 30S ribosomal protein S11

Chain k: 99%



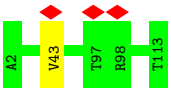
• Molecule 11: 30S ribosomal protein S12

Chain l: 5% 96%



• Molecule 12: 30S ribosomal protein S13

Chain m: 99%



• Molecule 13: 30S ribosomal protein S14 type Z

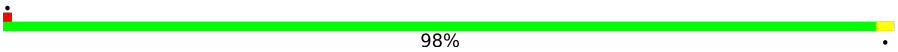
Chain n: 98%

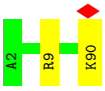
• Molecule 14: 30S ribosomal protein S15

Chain o: 98%

- Molecule 15: 30S ribosomal protein S16

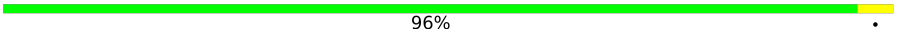
Chain p:

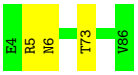




- Molecule 16: 30S ribosomal protein S17

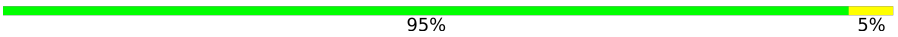
Chain q:





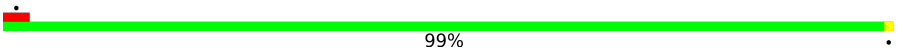
- Molecule 17: 30S ribosomal protein S18

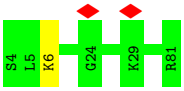
Chain r:



- Molecule 18: 30S ribosomal protein S19

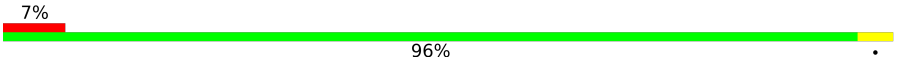
Chain s:

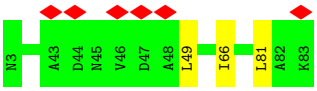




- Molecule 19: 30S ribosomal protein S20

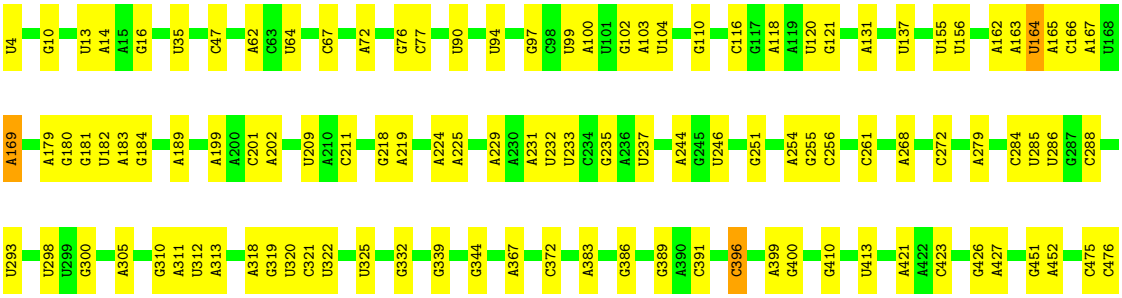
Chain t:





- Molecule 20: 23S rRNA

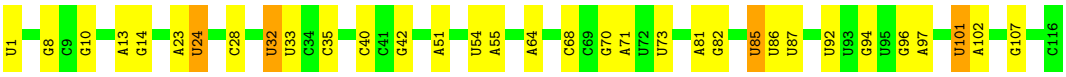
Chain A:



U488 C495 C496 U499 G507 G508 G509 A517 A518 A519 A520 G521 C527 A544 U547 C548 C549 U550 G559 U560 G561 C566 A567 A568 C569 A570 A571 G572 U573 A585 A586 U587 G588 G600 C601 C602 G607 G610 A611 A612 C621 G622 A623 G629
C638 G639 A640 U644 C649 G653 A654 G655 A656 C657 G669 A670 G673 A676 G677 U678 C679 U684 U693 G694 A695 G696 A708 G709 A710 C711 C712 A716 G722 U726 C730 U742 A755 A756 A757 A758 C759 G766 G769 A770 A775
C778 A779 C780 U787 G788 A792 G805 G808 G815 C816 G817 A822 A823 U824 G832 A833 A834 C835 A840 G845 C846 U847 G848 G849 C852 U867 U885 U886 G887 A888 G889 A890 A891 G897 G900 U901 G905 C906 A907 A919 G920 G921 G922
G923 C924 G925 C926 A927 U928 C931 G932 G933 G934 U935 C939 G940 A941 A942 U943 U944 C945 A946 A950 A951 A952 C953 U954 C955 C956 U960 G961 C962 C963 A964 U965 U966 U973 A974 U975 G978 A981 G982 U983 C984 A985 G986 G992 A993 A997 U998 A999 A1000 G1001 G1006
A1014 A1015 G1016 A1023 G1024 G1029 C1034 C1035 A1036 C1045 C1046 C1047 A1048 A1049 A1050 A1051 U1052 A1053 G1057 A1061 G1062 U1063 G1064 G1065 A1066 U1073 G1074 U1075 U1081 C1085 A1086 G1087 C1092 U1093 G1096 A1097 U1098 G1099 U1100 U1101 G1102 G1103 C1104 U1105 U1106 A1107 G1108 A1109
A1110 G1111 C1112 A1113 G1114 C1115 C1116 A1117 C1118 C1119 A1120 U1121 U1122 U1123 A1124 A1125 A1126 G1127 A1128 G1129 U1130 G1131 C1132 G1133 U1134 A1135 A1136 U1137 A1138 G1139 C1140 U1141 C1142 A1143 C1144 U1145 A1146 G1147 U1148 C1149 G1150 A1151 G1152 C1156 C1157 A1167 A1168 A1169 U1170 G1171 U1172 A1173 C1174 C1175 G1179 C1180 U1181
A1182 A1188 U1189 U1190 G1197 A1209 A1212 A1215 G1216 G1217 U1218 C1234 C1238 G1249 A1257 G1275 C1276 G1277 C1278 G1287 A1288 G1289 A1290 A1291 U1292 G1293 C1294 C1295 U1304 G1308 A1309 A1310 A1311 G1317 U1336 A1337 U1338 U1349 C1350 A1357 U1362
U1365 C1366 C1369 G1375 U1376 U1377 A1378 G1379 U1388 G1394 A1395 G1396 C1399 G1400 A1401 G1404 G1407 U1408 G1411 A1414 U1415 A1420 A1421 C1422 G1428 A1431 U1432 U1433 C1434 C1435 U1436 A1439 G1443 G1446 U1447 U1448 U1449 U1450 U1451 G1452 U1453 U1454 U1455 G1456 A1457
A1461 U1462 G1463 G1464 A1465 A1469 C1470 G1471 U1475 C1479 G1488 C1489 G1492 C1493 G1494 A1495 U1496 U1497 A1500 A1501 G1502 U1503 G1504 C1505 G1508 U1509 C1510 C1511 G1519 A1520 G1521 U1525 U1535 A1536 U1539 C1548 U1549 U1550 U1551 A1552 A1559 G1560 U1561 A1566 C1567
G1568 G1569 G1573 C1574 G1575 A1576 A1577 A1578 U1579 A1583 G1584 U1585 A1586 G1589 G1601 U1602 C1603 A1604 C1605 A1606 C1607 U1608 A1612 A1613 G1614 A1615 C1623 U1627 G1628 A1629 G1630 A1631 A1632 A1633 A1634 C1638 C1641 C1642 A1646 C1647 U1650 A1651 A1652 A1653 C1654 C1655 A1673 G1674
U1677 A1689 G1690 C1691 C1699 C1703 G1717 C1718 A1719 U1723 C1737 A1741 G1746 C1751 U1756 U1757 C1758 C1768 A1769 G1770 A1776 G1777 G1778 A1782 A1783 G1784 A1787 G1790 U1795 A1798 C1802 C1814 A1815 A1823 A1829 A1830 G1831 C1840
U1841 G1842 A1843 G1853 G1872 U1878 C1882 C1885 G1886 A1896 G1902 C1906 C1907 A1913 G1917 G1920 A1927 C1928 G1936 G1943 G1944 C1948 A1952 C1955 U1969 U1970 G1978 C1979 A1980 C1981 A1984 A1985 G1986 G1989 U1990 U1996 U2005
G2006 U2007 C2010 C2020 U2021 U2030 G2035 U2036 A2037 C2038 C2039 A2044 A2045 G2046 A2047 U2048 G2049 C2050 C2057 G2062 G2066 C2069 G2070 A2074 G2075 A2076 C2077 U2082 G2083 U2090 U2114 G2115 C2121 U2125 A2126 C2127 A2128 G2129 G2130 A2131 U2132 A2133 G2134 G2138
G2139 A2140 G2141 C2142 C2143 G2144 A2145 U2146 G2147 A2148 G2154 G2158 C2159 U2160 A2161 G2162 U2163 G2173 G2174 C2175 G2176 G2179 G2180 U2181 G2182 G2183 A2187 C2188 U2189 G2196 A2201 C2206 C2207 C2208 A2212 A2213 G2217 C2218 U2224 A2225 A2226 U2227 A2239 C2240 G2252 G2253
C2262 C2278 U2279 A2280 A2281 A2282 G2293 G2296 C2297 A2301 A2302 C2307 C2311 G2317 G2318 U2319 A2323 C2327 A2333 A2334 G2335 A2336 G2337 U2338 G2339 U2340 A2341 G2348 A2349 A2350 C2361 C2364 G2367 A2372 G2379 A2390 G2393 G2397 G2398 C2399

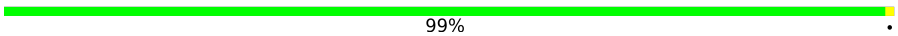
- Molecule 21: 4S rRNA

Chain B:



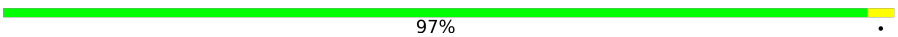
- Molecule 22: 50S ribosomal protein L2

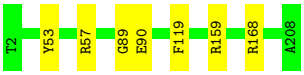
Chain C:



- Molecule 23: 50S ribosomal protein L3

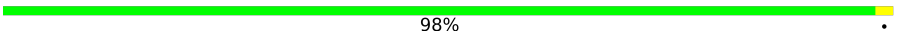
Chain D:

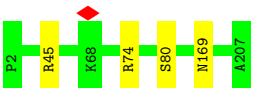




- Molecule 24: 50S ribosomal protein L4

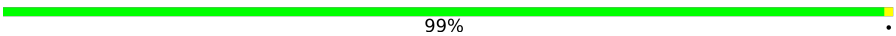
Chain E:





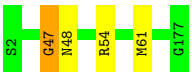
- Molecule 25: 50S ribosomal protein L5

Chain F:



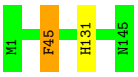
- Molecule 26: 50S ribosomal protein L6

Chain G: 98%



• Molecule 27: 50S ribosomal protein L13

Chain K: 99%



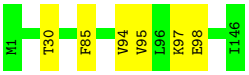
• Molecule 28: 50S ribosomal protein L14

Chain L: 100%

There are no outlier residues recorded for this chain.

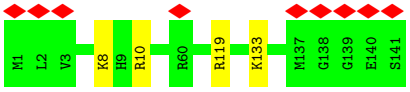
• Molecule 29: 50S ribosomal protein L15

Chain M: 96%



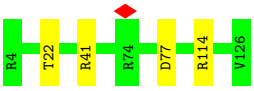
• Molecule 30: 50S ribosomal protein L16

Chain N: 6% 97%



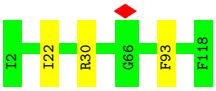
• Molecule 31: 50S ribosomal protein L17

Chain O: 97%



• Molecule 32: 50S ribosomal protein L18

Chain P: 97%



• Molecule 33: 50S ribosomal protein L19

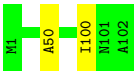
Chain Q: 98%

• Molecule 34: 50S ribosomal protein L20

Chain R: 98%

• Molecule 35: 50S ribosomal protein L21

Chain S: 98%



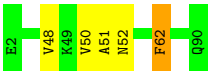
• Molecule 36: 50S ribosomal protein L22

Chain T: 100%

There are no outlier residues recorded for this chain.

• Molecule 37: 50S ribosomal protein L23

Chain U: 94%

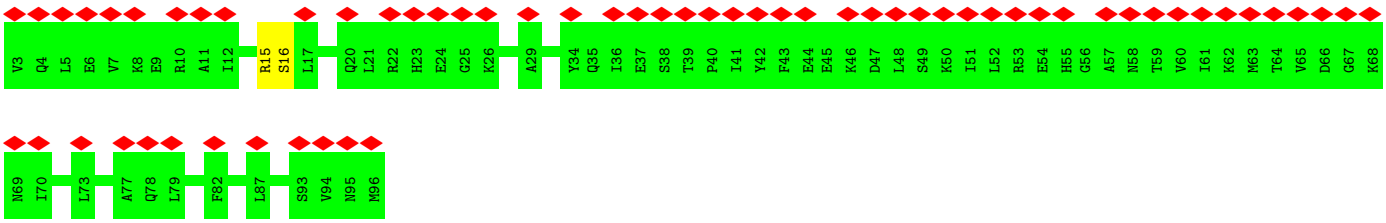


• Molecule 38: 50S ribosomal protein L24

Chain V: 95%

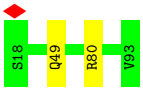
• Molecule 39: 50S ribosomal protein L25

Chain W: 65% 98%



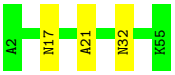
• Molecule 40: 50S ribosomal protein L27

Chain X: 97%



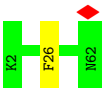
• Molecule 41: 50S ribosomal protein L28

Chain Y: 94% 6%



• Molecule 42: 50S ribosomal protein L29

Chain Z: 98%



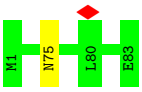
• Molecule 43: 50S ribosomal protein L30

Chain 0: 100%

There are no outlier residues recorded for this chain.

• Molecule 44: 50S ribosomal protein L31 type B

Chain 1: 99%



• Molecule 45: 50S ribosomal protein L32

Chain 2: 100%

There are no outlier residues recorded for this chain.

• Molecule 46: 50S ribosomal protein L33

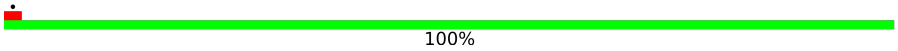
Chain 3: 100%

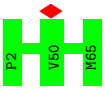
There are no outlier residues recorded for this chain.

• Molecule 47: 50S ribosomal protein L34

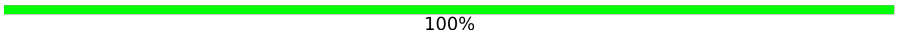
Chain 4: 98%

• Molecule 48: 50S ribosomal protein L35

Chain 5: 



• Molecule 49: 50S ribosomal protein L36

Chain 6: 

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46244	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.323	Depositor
Minimum map value	-0.893	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.238	Depositor
Map size (Å)	482.68, 482.68, 482.68	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.097, 1.097, 1.097	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: ZN

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	0.65	2/36657 (0.0%)	1.19	299/57173 (0.5%)
2	c	0.31	0/1635	0.54	0/2197
3	d	0.33	0/1650	0.64	2/2217 (0.1%)
4	e	0.34	0/1217	0.62	0/1641
5	f	0.30	0/807	0.53	0/1087
6	g	0.29	0/1249	0.52	0/1682
7	h	0.36	0/1054	0.60	0/1417
8	i	0.32	0/1003	0.59	0/1343
9	j	0.30	0/812	0.65	0/1093
10	k	0.30	0/878	0.58	0/1185
11	l	0.38	0/1082	0.72	1/1453 (0.1%)
12	m	0.28	0/890	0.58	0/1195
13	n	0.33	0/504	0.53	0/669
14	o	0.33	0/751	0.57	0/1001
15	p	0.38	0/720	0.59	0/966
16	q	0.40	0/689	0.66	0/920
17	r	0.31	0/544	0.61	0/728
18	s	0.33	0/650	0.58	0/872
19	t	0.36	0/612	0.64	2/818 (0.2%)
20	A	0.89	3/69785 (0.0%)	1.20	461/108842 (0.4%)
21	B	0.72	1/2770 (0.0%)	1.17	17/4311 (0.4%)
22	C	0.50	0/2148	0.72	1/2888 (0.0%)
23	D	0.51	0/1597	0.72	0/2143
24	E	0.47	0/1595	0.63	0/2157
25	F	0.33	0/1410	0.59	0/1895
26	G	0.40	0/1362	0.67	1/1831 (0.1%)
27	K	0.50	0/1148	0.71	0/1546
28	L	0.51	0/929	0.66	0/1247
29	M	0.43	0/1102	0.78	0/1467
30	N	0.47	0/1139	0.73	0/1515
31	O	0.50	0/984	0.80	2/1317 (0.2%)
32	P	0.41	0/907	0.63	0/1214

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Q	0.51	0/911	0.67	0/1227
34	R	0.52	0/951	0.70	1/1260 (0.1%)
35	S	0.47	0/794	0.65	0/1064
36	T	0.46	0/858	0.66	0/1157
37	U	0.48	0/725	0.73	0/969
38	V	0.41	0/772	0.75	1/1035 (0.1%)
39	W	0.29	0/768	0.65	0/1032
40	X	0.54	0/576	0.70	0/768
41	Y	0.35	0/431	0.58	0/574
42	Z	0.39	0/505	0.59	0/672
43	0	0.42	0/434	0.67	0/583
44	1	0.33	0/690	0.62	0/930
45	2	0.56	0/436	0.70	0/578
46	3	0.38	0/422	0.57	0/561
47	4	0.48	0/377	0.65	0/491
48	5	0.43	0/528	0.66	0/689
49	6	0.51	0/308	0.62	0/407
All	All	0.73	6/150766 (0.0%)	1.09	788/226027 (0.3%)

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
11	l	0	2
12	m	0	1
16	q	0	1
19	t	0	1
22	C	0	2
23	D	0	2
24	E	0	2
25	F	0	1
26	G	0	2
27	K	0	2
29	M	0	3
30	N	0	2
31	O	0	2
32	P	0	3
35	S	0	2
37	U	0	2
38	V	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	W	0	1
40	X	0	1
41	Y	0	1
47	4	0	1
All	All	0	36

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1	U	OP3-P	-10.56	1.48	1.61
20	A	1689	A	N9-C4	6.30	1.41	1.37
1	a	56	A	N9-C4	5.95	1.41	1.37
1	a	140	A	N9-C4	5.89	1.41	1.37
20	A	1288	A	N9-C4	-5.71	1.34	1.37
20	A	1414	A	N9-C4	-5.05	1.34	1.37

All (788) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	346	G	N7-C8-N9	11.73	118.96	113.10
20	A	1349	U	N3-C2-O2	-11.63	114.06	122.20
1	a	1548	U	N1-C2-O2	11.43	130.80	122.80
1	a	1082	C	N1-C2-O2	11.38	125.73	118.90
20	A	1551	U	C2-N1-C1'	11.38	131.36	117.70
20	A	1551	U	N1-C2-O2	11.22	130.65	122.80
20	A	644	U	N3-C2-O2	-10.82	114.63	122.20
1	a	1548	U	C2-N1-C1'	10.68	130.51	117.70
20	A	1130	U	N1-C2-O2	10.63	130.24	122.80
20	A	1130	U	C2-N1-C1'	10.49	130.29	117.70
1	a	109	G	O4'-C1'-N9	10.01	116.21	108.20
20	A	1551	U	N3-C2-O2	-9.99	115.21	122.20
20	A	1349	U	N1-C2-O2	9.90	129.73	122.80
1	a	1548	U	N3-C2-O2	-9.89	115.28	122.20
1	a	346	G	C8-N9-C4	-9.87	102.45	106.40
20	A	1130	U	N3-C2-O2	-9.71	115.40	122.20
1	a	1082	C	N3-C2-O2	-9.63	115.16	121.90
20	A	963	C	C6-N1-C2	-9.58	116.47	120.30
20	A	1106	U	N1-C2-O2	9.50	129.45	122.80
1	a	560	C	N1-C2-O2	9.49	124.59	118.90
1	a	826	C	C2-N1-C1'	9.43	129.17	118.80
1	a	579	U	N3-C2-O2	-9.38	115.63	122.20
1	a	1082	C	C2-N1-C1'	9.37	129.11	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	141	C	N1-C2-O2	9.37	124.52	118.90
1	a	142	C	N1-C2-O2	9.24	124.45	118.90
1	a	109	G	C8-N9-C1'	9.16	138.91	127.00
21	B	68	C	N1-C2-O2	9.16	124.40	118.90
1	a	346	G	C5-N7-C8	-9.15	99.72	104.30
21	B	68	C	C2-N1-C1'	9.15	128.87	118.80
20	A	644	U	N1-C2-O2	9.13	129.19	122.80
1	a	826	C	N1-C2-O2	9.06	124.34	118.90
20	A	901	U	C2-N1-C1'	9.05	128.56	117.70
20	A	1885	C	N1-C2-O2	9.03	124.32	118.90
20	A	2825	C	N1-C2-O2	9.01	124.31	118.90
1	a	108	U	N3-C2-O2	-8.99	115.91	122.20
20	A	1130	U	C5-C6-N1	8.96	127.18	122.70
1	a	1082	C	C6-N1-C2	-8.79	116.79	120.30
1	a	109	G	C4-N9-C1'	-8.73	115.15	126.50
1	a	56	A	C2-N3-C4	8.66	114.93	110.60
20	A	1489	C	C2-N3-C4	8.65	124.23	119.90
20	A	1349	U	C2-N1-C1'	8.62	128.05	117.70
1	a	492	C	N1-C2-O2	8.59	124.06	118.90
20	A	897	G	N3-C4-N9	-8.57	120.86	126.00
1	a	997	U	C2-N1-C1'	8.44	127.83	117.70
20	A	906	C	N1-C2-O2	8.43	123.96	118.90
20	A	849	G	N1-C6-O6	-8.40	114.86	119.90
1	a	579	U	N1-C2-O2	8.39	128.67	122.80
20	A	1148	U	N1-C2-O2	8.36	128.65	122.80
20	A	2825	C	N3-C2-O2	-8.36	116.05	121.90
20	A	1489	C	C5-C6-N1	8.33	125.17	121.00
20	A	1148	U	N3-C2-O2	-8.24	116.43	122.20
20	A	901	U	N1-C2-O2	8.22	128.55	122.80
1	a	1465	U	N1-C2-O2	8.19	128.53	122.80
20	A	1350	C	C2-N1-C1'	8.17	127.79	118.80
20	A	897	G	N9-C4-C5	8.17	108.67	105.40
1	a	468	C	C6-N1-C2	-8.15	117.04	120.30
20	A	261	C	N1-C2-O2	8.11	123.77	118.90
20	A	2697	C	N1-C2-O2	8.08	123.75	118.90
1	a	875	C	N1-C2-O2	8.06	123.73	118.90
1	a	505	U	C5-C6-N1	8.01	126.70	122.70
1	a	142	C	N3-C2-O2	-7.87	116.39	121.90
1	a	140	A	C2-N3-C4	7.87	114.53	110.60
20	A	1948	C	C2-N1-C1'	7.86	127.45	118.80
1	a	1173	C	C2-N1-C1'	7.84	127.43	118.80
1	a	826	C	C6-N1-C2	-7.79	117.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	730	C	C6-N1-C2	-7.79	117.19	120.30
20	A	1885	C	N3-C2-O2	-7.73	116.49	121.90
1	a	108	U	N1-C2-O2	7.71	128.19	122.80
1	a	141	C	N3-C2-O2	-7.70	116.51	121.90
1	a	1053	C	N1-C2-O2	7.69	123.51	118.90
1	a	826	C	N3-C2-O2	-7.68	116.53	121.90
1	a	109	G	N9-C4-C5	7.66	108.46	105.40
20	A	925	C	C2-N1-C1'	7.66	127.22	118.80
20	A	901	U	N3-C2-O2	-7.65	116.84	122.20
20	A	1758	C	C2-N1-C1'	7.60	127.16	118.80
20	A	1551	U	C6-N1-C1'	-7.59	110.58	121.20
1	a	1306	C	C2-N1-C1'	7.55	127.11	118.80
1	a	156	U	N1-C2-O2	7.53	128.07	122.80
1	a	184	C	N1-C2-O2	7.52	123.41	118.90
1	a	995	C	N1-C2-O2	7.52	123.41	118.90
20	A	2488	C	N1-C2-O2	7.51	123.41	118.90
20	A	2858	U	N3-C2-O2	-7.50	116.95	122.20
20	A	2753	U	N1-C2-O2	7.45	128.01	122.80
1	a	108	U	C5-C6-N1	7.44	126.42	122.70
20	A	2734	U	N3-C2-O2	-7.43	117.00	122.20
1	a	190	A	N7-C8-N9	7.42	117.51	113.80
1	a	579	U	C2-N1-C1'	7.42	126.61	117.70
20	A	549	C	N1-C2-O2	7.41	123.35	118.90
1	a	148	G	C2-N3-C4	7.41	115.60	111.90
1	a	1548	U	C6-N1-C1'	-7.38	110.87	121.20
20	A	1928	C	N1-C2-O2	7.38	123.33	118.90
20	A	1304	U	C2-N1-C1'	7.37	126.54	117.70
1	a	1059	G	N1-C6-O6	-7.36	115.48	119.90
1	a	1173	C	N1-C2-O2	7.36	123.32	118.90
1	a	632	G	N3-C4-N9	-7.36	121.58	126.00
20	A	1489	C	N1-C2-O2	7.36	123.32	118.90
20	A	2143	C	C5-C6-N1	7.36	124.68	121.00
20	A	1047	C	C6-N1-C2	-7.35	117.36	120.30
1	a	907	U	N1-C2-O2	7.34	127.94	122.80
20	A	2734	U	N1-C2-O2	7.34	127.94	122.80
20	A	246	U	N3-C2-O2	-7.33	117.07	122.20
1	a	790	G	N3-C4-N9	-7.33	121.61	126.00
1	a	109	G	C6-C5-N7	7.32	134.79	130.40
20	A	1497	U	N3-C2-O2	-7.31	117.08	122.20
1	a	1183	C	C2-N1-C1'	7.30	126.83	118.80
20	A	849	G	C5-C6-O6	7.30	132.98	128.60
1	a	1465	U	N3-C2-O2	-7.29	117.09	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	560	C	C2-N1-C1'	7.29	126.82	118.80
1	a	997	U	N3-C2-O2	-7.26	117.12	122.20
20	A	1885	C	C2-N1-C1'	7.26	126.78	118.80
1	a	234	C	N3-C2-O2	-7.25	116.83	121.90
20	A	2766	C	N1-C2-O2	7.25	123.25	118.90
1	a	860	C	N1-C2-O2	7.23	123.24	118.90
1	a	492	C	N3-C2-O2	-7.23	116.84	121.90
20	A	2143	C	C6-N1-C2	-7.22	117.41	120.30
20	A	654	A	C8-N9-C4	7.21	108.69	105.80
1	a	1152	U	N1-C2-O2	7.21	127.85	122.80
20	A	1350	C	C6-N1-C2	-7.21	117.42	120.30
1	a	529	C	C6-N1-C2	-7.20	117.42	120.30
20	A	2794	G	C4-N9-C1'	7.20	135.86	126.50
20	A	2753	U	N3-C2-O2	-7.19	117.17	122.20
1	a	64	C	C6-N1-C2	-7.17	117.43	120.30
1	a	279	C	C6-N1-C2	-7.17	117.43	120.30
1	a	907	U	N3-C2-O2	-7.16	117.19	122.20
20	A	272	C	C2-N1-C1'	7.16	126.68	118.80
20	A	1907	C	N3-C2-O2	-7.15	116.89	121.90
20	A	261	C	N3-C2-O2	-7.13	116.91	121.90
1	a	1053	C	N3-C2-O2	-7.13	116.91	121.90
1	a	66	C	C6-N1-C2	-7.12	117.45	120.30
20	A	272	C	C6-N1-C2	-7.12	117.45	120.30
21	B	68	C	N3-C2-O2	-7.11	116.92	121.90
20	A	935	U	N1-C2-O2	7.11	127.77	122.80
20	A	1907	C	N1-C2-O2	7.10	123.16	118.90
20	A	906	C	C2-N1-C1'	7.08	126.59	118.80
20	A	2858	U	N1-C2-O2	7.08	127.76	122.80
1	a	1152	U	C2-N1-C1'	7.07	126.19	117.70
1	a	67	U	C2-N1-C1'	7.04	126.14	117.70
1	a	115	C	N1-C2-O2	7.03	123.12	118.90
20	A	655	G	C8-N9-C4	7.03	109.21	106.40
1	a	451	C	N1-C2-O2	7.02	123.11	118.90
1	a	148	G	N3-C4-C5	-7.01	125.09	128.60
20	A	2697	C	N3-C2-O2	-7.01	117.00	121.90
1	a	468	C	N3-C2-O2	-7.00	117.00	121.90
20	A	246	U	N1-C2-O2	7.00	127.70	122.80
20	A	527	C	N1-C2-O2	7.00	123.10	118.90
1	a	196	U	N3-C2-O2	-7.00	117.30	122.20
20	A	935	U	C2-N1-C1'	6.99	126.09	117.70
1	a	1152	U	N3-C2-O2	-6.97	117.32	122.20
20	A	1604	A	P-O3'-C3'	6.96	128.06	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	504	C	N3-C2-O2	-6.96	117.03	121.90
20	A	1106	U	N3-C2-O2	-6.95	117.34	122.20
20	A	935	U	N3-C2-O2	-6.93	117.35	122.20
20	A	1689	A	C2-N3-C4	6.91	114.06	110.60
1	a	1059	G	C5-C6-O6	6.91	132.75	128.60
20	A	1157	C	C2-N1-C1'	6.90	126.39	118.80
1	a	1305	G	C4-N9-C1'	6.90	135.47	126.50
21	B	68	C	C6-N1-C1'	-6.89	112.53	120.80
1	a	995	C	C2-N1-C1'	6.87	126.35	118.80
20	A	1130	U	C6-N1-C2	-6.85	116.89	121.00
20	A	1574	C	N1-C2-O2	6.84	123.01	118.90
20	A	649	C	C5-C6-N1	6.81	124.41	121.00
1	a	418	C	N1-C2-O2	6.81	122.98	118.90
1	a	109	G	C4-C5-N7	-6.80	108.08	110.80
1	a	141	C	C6-N1-C2	-6.80	117.58	120.30
38	V	71	ILE	C-N-CA	6.79	138.68	121.70
1	a	450	U	C5-C6-N1	6.78	126.09	122.70
1	a	1022	C	N1-C2-O2	6.78	122.97	118.90
20	A	1641	C	C6-N1-C2	-6.78	117.59	120.30
1	a	649	C	C6-N1-C2	-6.78	117.59	120.30
20	A	1024	G	N3-C4-C5	-6.78	125.21	128.60
1	a	109	G	N3-C4-N9	-6.77	121.94	126.00
1	a	1038	C	N1-C2-O2	6.76	122.96	118.90
1	a	1082	C	C5-C6-N1	6.76	124.38	121.00
20	A	396	C	C2-N1-C1'	6.75	126.22	118.80
20	A	1948	C	N1-C2-O2	6.73	122.94	118.90
20	A	925	C	N1-C2-O2	6.73	122.94	118.90
1	a	1001	C	C2-N1-C1'	6.72	126.20	118.80
20	A	1148	U	C2-N1-C1'	6.72	125.77	117.70
20	A	1758	C	C6-N1-C2	-6.68	117.63	120.30
1	a	108	U	C6-N1-C2	-6.66	117.00	121.00
20	A	956	C	N1-C2-O2	6.66	122.89	118.90
20	A	2007	U	N3-C2-O2	-6.65	117.54	122.20
1	a	115	C	N3-C2-O2	-6.64	117.25	121.90
1	a	1173	C	N3-C2-O2	-6.63	117.26	121.90
20	A	963	C	N3-C2-O2	-6.63	117.26	121.90
20	A	1454	U	N3-C2-O2	-6.63	117.56	122.20
20	A	1197	G	N3-C4-N9	6.63	129.98	126.00
20	A	1217	G	O5'-P-OP1	-6.63	99.73	105.70
20	A	2729	C	C5-C6-N1	6.62	124.31	121.00
1	a	416	C	N1-C2-O2	6.62	122.87	118.90
21	B	35	C	C6-N1-C2	-6.61	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	527	C	N3-C2-O2	-6.61	117.28	121.90
20	A	1304	U	N1-C2-O2	6.60	127.42	122.80
1	a	511	G	C4-N9-C1'	6.60	135.08	126.50
1	a	140	A	N3-C4-N9	6.58	132.66	127.40
20	A	1024	G	N3-C4-N9	6.57	129.94	126.00
1	a	511	G	N3-C4-N9	6.57	129.94	126.00
20	A	2570	C	N1-C2-O2	6.57	122.84	118.90
1	a	418	C	C2-N1-C1'	6.56	126.02	118.80
1	a	1305	G	N3-C4-N9	6.56	129.94	126.00
20	A	1647	C	C6-N1-C2	-6.56	117.68	120.30
1	a	860	C	C2-N1-C1'	6.55	126.00	118.80
21	B	96	G	C4-N9-C1'	6.54	135.01	126.50
1	a	734	C	C2-N1-C1'	6.50	125.95	118.80
1	a	952	C	N1-C2-O2	6.50	122.80	118.90
1	a	734	C	N3-C2-O2	-6.49	117.36	121.90
20	A	2090	U	N1-C2-O2	6.49	127.34	122.80
1	a	578	A	C4-N9-C1'	6.48	137.97	126.30
1	a	1306	C	C6-N1-C2	-6.48	117.71	120.30
20	A	1561	U	C2-N1-C1'	6.48	125.47	117.70
20	A	931	C	C2-N1-C1'	6.48	125.93	118.80
20	A	906	C	N3-C2-O2	-6.46	117.38	121.90
20	A	1641	C	N1-C2-O2	6.46	122.77	118.90
20	A	1605	C	P-O3'-C3'	6.44	127.43	119.70
1	a	1094	U	N3-C2-O2	-6.43	117.70	122.20
20	A	310	G	C4-N9-C1'	6.43	134.85	126.50
1	a	55	C	C6-N1-C2	-6.41	117.74	120.30
1	a	1091	U	N3-C2-O2	-6.41	117.72	122.20
1	a	67	U	N1-C2-O2	6.40	127.28	122.80
20	A	1434	C	C2-N1-C1'	6.39	125.83	118.80
1	a	1306	C	C5-C6-N1	6.39	124.20	121.00
1	a	443	G	OP1-P-O3'	6.39	119.25	105.20
20	A	1882	C	C2-N1-C1'	6.39	125.83	118.80
1	a	649	C	N1-C2-O2	6.39	122.73	118.90
20	A	1970	U	N3-C2-O2	-6.39	117.73	122.20
1	a	1468	U	N1-C2-O2	6.37	127.26	122.80
1	a	184	C	N3-C2-O2	-6.37	117.44	121.90
1	a	511	G	C8-N9-C1'	-6.36	118.73	127.00
20	A	2819	U	N1-C2-O2	6.36	127.25	122.80
26	G	54	ARG	NE-CZ-NH1	-6.36	117.12	120.30
20	A	1212	A	C2-N3-C4	6.36	113.78	110.60
1	a	1039	U	C2-N1-C1'	6.36	125.33	117.70
20	A	549	C	C2-N1-C1'	6.35	125.78	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	504	C	C6-N1-C2	-6.35	117.76	120.30
20	A	2240	C	N1-C2-O2	6.34	122.71	118.90
20	A	104	U	N1-C2-O2	6.34	127.24	122.80
20	A	509	G	O4'-C1'-N9	6.34	113.27	108.20
1	a	1043	C	C6-N1-C2	-6.34	117.77	120.30
1	a	503	U	C5-C6-N1	6.33	125.87	122.70
1	a	997	U	N1-C2-O2	6.33	127.23	122.80
20	A	1885	C	C6-N1-C2	-6.33	117.77	120.30
20	A	2127	C	C2-N1-C1'	6.33	125.76	118.80
1	a	156	U	N3-C2-O2	-6.33	117.77	122.20
20	A	1584	G	P-O3'-C3'	6.33	127.29	119.70
20	A	1092	C	N1-C2-O2	6.32	122.69	118.90
20	A	2819	U	N3-C2-O2	-6.32	117.77	122.20
1	a	267	U	C2-N1-C1'	6.32	125.28	117.70
1	a	875	C	N3-C2-O2	-6.32	117.48	121.90
20	A	256	C	C6-N1-C2	-6.32	117.77	120.30
20	A	1369	C	N3-C2-O2	-6.32	117.48	121.90
20	A	1304	U	N3-C2-O2	-6.31	117.78	122.20
20	A	2881	C	C6-N1-C2	-6.31	117.78	120.30
20	A	1703	C	C6-N1-C2	-6.30	117.78	120.30
20	A	2307	C	C5-C6-N1	6.28	124.14	121.00
1	a	56	A	N3-C4-C5	-6.28	122.41	126.80
20	A	1156	C	C2-N1-C1'	6.27	125.70	118.80
1	a	1173	C	C6-N1-C2	-6.25	117.80	120.30
20	A	1024	G	C4-N9-C1'	6.24	134.62	126.50
20	A	423	C	N1-C2-O2	6.24	122.64	118.90
1	a	450	U	C2-N1-C1'	6.23	125.18	117.70
1	a	968	U	N3-C2-O2	-6.22	117.85	122.20
1	a	529	C	C5-C6-N1	6.20	124.10	121.00
20	A	2786	C	C6-N1-C2	-6.20	117.82	120.30
1	a	597	C	N1-C2-O2	6.19	122.62	118.90
20	A	1448	U	C2-N1-C1'	6.19	125.13	117.70
20	A	1130	U	C6-N1-C1'	-6.19	112.54	121.20
20	A	1435	C	N1-C2-O2	6.18	122.61	118.90
1	a	1125	C	N1-C2-O2	6.18	122.61	118.90
20	A	2488	C	C2-N1-C1'	6.18	125.60	118.80
20	A	602	C	C6-N1-C2	-6.18	117.83	120.30
20	A	1454	U	N1-C2-O2	6.17	127.12	122.80
20	A	901	U	C5-C6-N1	6.17	125.79	122.70
20	A	1238	C	C6-N1-C2	-6.17	117.83	120.30
20	A	2729	C	C6-N1-C2	-6.17	117.83	120.30
1	a	1091	U	C2-N1-C1'	6.16	125.10	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	826	C	C6-N1-C1'	-6.15	113.42	120.80
20	A	1641	C	C2-N1-C1'	6.15	125.56	118.80
20	A	2794	G	C8-N9-C1'	-6.15	119.01	127.00
20	A	1197	G	C4-N9-C1'	6.14	134.48	126.50
1	a	451	C	C5-C6-N1	6.14	124.07	121.00
20	A	1551	U	C5-C6-N1	6.14	125.77	122.70
1	a	255	U	O4'-C1'-N1	6.13	113.11	108.20
1	a	530	G	C4-N9-C1'	6.13	134.47	126.50
20	A	956	C	C2-N1-C1'	6.13	125.54	118.80
20	A	413	U	N3-C2-O2	-6.13	117.91	122.20
1	a	1318	C	C2-N1-C1'	6.12	125.53	118.80
20	A	1641	C	N3-C2-O2	-6.12	117.61	121.90
1	a	734	C	C6-N1-C2	-6.12	117.85	120.30
1	a	649	C	C2-N1-C1'	6.12	125.53	118.80
20	A	607	G	N3-C4-C5	-6.11	125.54	128.60
20	A	897	G	N1-C6-O6	-6.11	116.23	119.90
20	A	164	U	N1-C2-N3	6.10	118.56	114.90
20	A	310	G	N3-C4-N9	6.10	129.66	126.00
1	a	634	U	C2-N1-C1'	6.10	125.02	117.70
1	a	1305	G	C8-N9-C1'	-6.09	119.08	127.00
20	A	1399	C	C2-N1-C1'	6.09	125.50	118.80
1	a	140	A	N3-C4-C5	-6.08	122.54	126.80
20	A	709	G	C4-N9-C1'	6.07	134.40	126.50
20	A	47	C	C6-N1-C2	-6.07	117.87	120.30
20	A	2670	U	C2-N1-C1'	6.07	124.98	117.70
1	a	704	C	C6-N1-C2	-6.07	117.87	120.30
20	A	201	C	C2-N1-C1'	6.06	125.47	118.80
20	A	960	U	N3-C2-O2	-6.06	117.96	122.20
21	B	85	U	C5-C6-N1	6.05	125.73	122.70
1	a	468	C	N1-C2-O2	6.05	122.53	118.90
20	A	849	G	N9-C4-C5	6.05	107.82	105.40
1	a	142	C	C2-N1-C1'	6.05	125.45	118.80
1	a	322	U	N3-C2-O2	-6.04	117.97	122.20
1	a	1053	C	C6-N1-C2	-6.04	117.88	120.30
20	A	104	U	N3-C2-O2	-6.04	117.97	122.20
20	A	1497	U	N1-C2-O2	6.03	127.02	122.80
20	A	897	G	C5-C6-O6	6.02	132.22	128.60
1	a	995	C	N3-C2-O2	-6.02	117.68	121.90
20	A	209	U	N3-C2-O2	-6.02	117.99	122.20
20	A	1379	G	N3-C4-N9	6.02	129.61	126.00
20	A	1928	C	N3-C2-O2	-6.02	117.69	121.90
20	A	1970	U	N1-C2-O2	6.02	127.01	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	423	C	C2-N1-C1'	6.01	125.41	118.80
1	a	196	U	N1-C2-O2	6.00	127.00	122.80
20	A	2766	C	N3-C2-O2	-6.00	117.70	121.90
20	A	1830	A	N7-C8-N9	6.00	116.80	113.80
31	O	41	ARG	CA-CB-CG	5.99	126.59	113.40
20	A	924	C	C6-N1-C2	-5.99	117.90	120.30
20	A	1830	A	C8-N9-C4	-5.99	103.40	105.80
20	A	621	C	C5-C6-N1	5.98	123.99	121.00
1	a	865	U	N3-C2-O2	-5.98	118.02	122.20
1	a	1305	G	N3-C4-C5	-5.97	125.61	128.60
20	A	2766	C	C2-N1-C1'	5.97	125.36	118.80
1	a	649	C	N3-C2-O2	-5.97	117.72	121.90
1	a	143	C	N3-C2-O2	-5.96	117.73	121.90
20	A	325	U	N1-C2-O2	5.96	126.97	122.80
20	A	1574	C	N3-C2-O2	-5.96	117.73	121.90
20	A	1379	G	C4-N9-C1'	5.95	134.24	126.50
20	A	1489	C	C6-N1-C2	-5.95	117.92	120.30
20	A	256	C	C5-C6-N1	5.95	123.98	121.00
20	A	973	U	N3-C2-O2	-5.95	118.04	122.20
20	A	246	U	C2-N1-C1'	5.95	124.84	117.70
20	A	1453	U	C2-N1-C1'	5.95	124.83	117.70
20	A	272	C	N3-C2-O2	-5.94	117.74	121.90
1	a	1468	U	N3-C2-O2	-5.94	118.04	122.20
20	A	1758	C	N3-C2-O2	-5.94	117.74	121.90
20	A	602	C	N1-C2-O2	5.93	122.46	118.90
20	A	1830	A	C2-N3-C4	5.93	113.56	110.60
20	A	2826	C	C2-N1-C1'	5.93	125.32	118.80
1	a	279	C	C2-N1-C1'	5.92	125.32	118.80
20	A	1655	C	C6-N1-C2	-5.91	117.93	120.30
20	A	1197	G	C8-N9-C1'	-5.91	119.32	127.00
20	A	2127	C	N1-C2-O2	5.90	122.44	118.90
20	A	1081	U	N3-C2-O2	-5.90	118.07	122.20
1	a	632	G	N9-C4-C5	5.89	107.76	105.40
1	a	560	C	C6-N1-C1'	-5.89	113.73	120.80
20	A	712	C	C6-N1-C2	-5.89	117.94	120.30
20	A	925	C	C6-N1-C2	-5.89	117.95	120.30
20	A	2307	C	C6-N1-C2	-5.89	117.95	120.30
20	A	1878	U	N1-C2-O2	5.88	126.92	122.80
1	a	1183	C	N1-C2-O2	5.88	122.43	118.90
20	A	561	G	N3-C4-N9	5.88	129.53	126.00
1	a	769	C	C2-N1-C1'	5.88	125.26	118.80
20	A	1751	C	C6-N1-C2	-5.87	117.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	639	C	C6-N1-C1'	5.86	127.83	120.80
20	A	1996	U	N3-C2-O2	-5.86	118.10	122.20
1	a	346	G	C4-C5-N7	5.86	113.14	110.80
20	A	1479	C	C6-N1-C2	-5.85	117.96	120.30
20	A	1130	U	O4'-C1'-N1	5.85	112.88	108.20
20	A	2787	U	N3-C2-O2	-5.84	118.11	122.20
20	A	945	C	C2-N1-C1'	5.84	125.23	118.80
20	A	1349	U	C6-N1-C1'	-5.84	113.03	121.20
1	a	108	U	C2-N1-C1'	5.83	124.70	117.70
1	a	148	G	O4'-C1'-N9	5.83	112.87	108.20
20	A	495	C	N1-C2-O2	5.83	122.40	118.90
20	A	2007	U	N1-C2-O2	5.83	126.88	122.80
20	A	962	C	C6-N1-C2	-5.83	117.97	120.30
20	A	638	C	C2-N1-C1'	5.82	125.20	118.80
20	A	2240	C	N3-C2-O2	-5.82	117.83	121.90
20	A	848	G	C5-C6-O6	5.82	132.09	128.60
1	a	55	C	C2-N1-C1'	5.81	125.19	118.80
1	a	427	A	P-O3'-C3'	5.81	126.67	119.70
20	A	602	C	N3-C2-O2	-5.80	117.84	121.90
20	A	1758	C	N1-C2-O2	5.80	122.38	118.90
1	a	597	C	N3-C2-O2	-5.80	117.84	121.90
1	a	424	U	N3-C2-O2	-5.79	118.15	122.20
20	A	1045	C	N1-C2-O2	5.79	122.37	118.90
1	a	639	C	C6-N1-C2	-5.78	117.99	120.30
1	a	644	A	C4-N9-C1'	5.78	136.70	126.30
20	A	47	C	C2-N1-C1'	5.78	125.15	118.80
20	A	1955	C	N1-C2-O2	5.78	122.36	118.90
1	a	862	C	N1-C2-O2	5.77	122.36	118.90
21	B	101	U	N1-C2-O2	5.77	126.84	122.80
19	t	49	LEU	CA-CB-CG	5.77	128.57	115.30
20	A	956	C	N3-C2-O2	-5.77	117.86	121.90
20	A	1081	U	N1-C2-O2	5.76	126.84	122.80
20	A	1948	C	C6-N1-C2	-5.76	117.99	120.30
20	A	901	U	C6-N1-C1'	-5.75	113.14	121.20
20	A	162	A	C8-N9-C4	-5.75	103.50	105.80
1	a	860	C	N3-C2-O2	-5.75	117.87	121.90
20	A	2812	A	P-O3'-C3'	5.75	126.60	119.70
1	a	386	G	P-O3'-C3'	5.75	126.60	119.70
20	A	2142	C	N1-C2-O2	5.75	122.35	118.90
20	A	638	C	C6-N1-C2	-5.74	118.00	120.30
20	A	848	G	N1-C6-O6	-5.74	116.45	119.90
20	A	2518	U	C5-C6-N1	5.74	125.57	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	943	U	C2-N1-C1'	5.74	124.58	117.70
1	a	199	C	N3-C2-O2	-5.73	117.89	121.90
20	A	897	G	C8-N9-C1'	5.73	134.45	127.00
22	C	91	ILE	CG1-CB-CG2	-5.73	98.79	111.40
1	a	1548	U	C5-C6-N1	5.73	125.56	122.70
1	a	419	G	C4-N9-C1'	5.72	133.94	126.50
20	A	2142	C	C6-N1-C2	-5.72	118.01	120.30
20	A	679	C	C5-C6-N1	5.72	123.86	121.00
1	a	107	G	C5-C6-O6	5.72	132.03	128.60
20	A	1197	G	C6-C5-N7	-5.71	126.97	130.40
20	A	1969	U	C5-C6-N1	-5.71	119.85	122.70
1	a	720	U	N3-C2-O2	-5.71	118.21	122.20
1	a	578	A	C8-N9-C1'	-5.70	117.44	127.70
20	A	272	C	N1-C2-O2	5.70	122.32	118.90
1	a	927	U	N3-C2-O2	-5.69	118.22	122.20
20	A	1723	U	N3-C2-O2	-5.69	118.22	122.20
20	A	2208	C	C2-N1-C1'	5.69	125.06	118.80
20	A	1802	C	C6-N1-C2	-5.69	118.02	120.30
20	A	571	A	C2-N3-C4	5.69	113.44	110.60
20	A	1379	G	N3-C4-C5	-5.68	125.76	128.60
20	A	310	G	C8-N9-C1'	-5.68	119.61	127.00
20	A	849	G	C8-N9-C4	-5.68	104.13	106.40
20	A	1489	C	C2-N1-C1'	5.68	125.05	118.80
20	A	495	C	C2-N1-C1'	5.68	125.05	118.80
1	a	766	U	N3-C2-O2	-5.68	118.23	122.20
20	A	561	G	C6-C5-N7	-5.67	127.00	130.40
20	A	1128	A	C5-C6-N6	-5.67	119.16	123.70
20	A	549	C	C5-C6-N1	5.67	123.84	121.00
20	A	931	C	N1-C2-O2	5.66	122.30	118.90
20	A	1075	U	N1-C2-O2	5.66	126.76	122.80
1	a	384	C	C2-N1-C1'	5.65	125.02	118.80
1	a	952	C	C2-N1-C1'	5.65	125.02	118.80
1	a	1082	C	C6-N1-C1'	-5.65	114.02	120.80
1	a	660	G	C4-N9-C1'	5.65	133.84	126.50
20	A	780	C	C6-N1-C2	-5.64	118.04	120.30
20	A	1140	C	N1-C2-O2	5.64	122.29	118.90
1	a	267	U	N3-C2-O2	-5.64	118.25	122.20
1	a	204	G	N1-C6-O6	-5.64	116.52	119.90
1	a	968	U	N1-C2-O2	5.63	126.75	122.80
20	A	1699	C	C6-N1-C2	-5.63	118.05	120.30
20	A	1100	U	N3-C4-O4	5.63	123.34	119.40
20	A	413	U	N1-C2-O2	5.62	126.73	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	973	U	N1-C2-O2	5.62	126.73	122.80
20	A	1350	C	C5-C6-N1	5.62	123.81	121.00
20	A	1502	G	P-O3'-C3'	5.62	126.45	119.70
20	A	1723	U	C2-N1-C1'	5.62	124.44	117.70
1	a	862	C	C2-N1-C1'	5.61	124.97	118.80
20	A	2030	U	N3-C2-O2	-5.61	118.27	122.20
20	A	1902	G	O4'-C1'-N9	5.61	112.69	108.20
20	A	2724	C	N3-C2-O2	-5.61	117.97	121.90
21	B	96	G	C8-N9-C1'	-5.61	119.71	127.00
20	A	1936	G	N3-C4-N9	-5.60	122.64	126.00
20	A	823	A	C2-N3-C4	5.60	113.40	110.60
20	A	730	C	C2-N1-C1'	5.59	124.95	118.80
20	A	1505	C	N3-C2-O2	-5.59	117.98	121.90
20	A	1362	U	N3-C2-O2	-5.59	118.28	122.20
20	A	933	G	N3-C4-C5	-5.59	125.81	128.60
20	A	1399	C	C6-N1-C2	-5.59	118.06	120.30
3	d	26	LEU	CA-CB-CG	5.59	128.15	115.30
20	A	654	A	N7-C8-N9	-5.59	111.01	113.80
20	A	1502	G	OP1-P-O3'	5.59	117.49	105.20
20	A	310	G	N3-C4-C5	-5.58	125.81	128.60
1	a	156	U	C2-N1-C1'	5.58	124.40	117.70
1	a	279	C	N3-C2-O2	-5.58	117.99	121.90
1	a	424	U	N1-C2-O2	5.58	126.71	122.80
21	B	101	U	N3-C2-O2	-5.58	118.29	122.20
1	a	67	U	N3-C2-O2	-5.58	118.30	122.20
20	A	573	U	C5-C6-N1	5.57	125.49	122.70
20	A	1350	C	N1-C2-O2	5.56	122.24	118.90
20	A	1479	C	C2-N1-C1'	5.56	124.92	118.80
1	a	529	C	C2-N1-C1'	5.56	124.92	118.80
1	a	1091	U	N1-C2-O2	5.56	126.69	122.80
20	A	475	C	N1-C2-O2	5.56	122.23	118.90
20	A	1434	C	C5-C6-N1	5.56	123.78	121.00
1	a	109	G	N1-C6-O6	-5.55	116.57	119.90
20	A	2836	G	C6-C5-N7	-5.55	127.07	130.40
1	a	720	U	N1-C2-O2	5.55	126.68	122.80
1	a	585	G	C4-N9-C1'	5.54	133.71	126.50
1	a	1094	U	N1-C2-O2	5.54	126.68	122.80
20	A	2317	G	P-O3'-C3'	5.54	126.35	119.70
1	a	660	G	N3-C4-C5	-5.54	125.83	128.60
20	A	571	A	C4-N9-C1'	5.54	136.27	126.30
1	a	952	C	C6-N1-C2	-5.54	118.09	120.30
1	a	6	G	O4'-C1'-N9	5.53	112.63	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	709	G	N3-C4-N9	5.53	129.32	126.00
20	A	2700	G	N3-C4-C5	-5.53	125.83	128.60
20	A	657	C	C6-N1-C2	-5.53	118.09	120.30
20	A	2050	C	N1-C2-O2	5.53	122.22	118.90
1	a	56	A	N3-C4-N9	5.53	131.82	127.40
20	A	2825	C	C2-N1-C1'	5.53	124.88	118.80
1	a	279	C	N1-C2-O2	5.52	122.21	118.90
1	a	968	U	C2-N1-C1'	5.52	124.32	117.70
20	A	2670	U	N3-C2-O2	-5.52	118.34	122.20
1	a	560	C	C5-C6-N1	5.52	123.76	121.00
20	A	1948	C	N3-C2-O2	-5.52	118.04	121.90
1	a	148	G	C4-N9-C1'	5.51	133.67	126.50
1	a	1043	C	C5-C6-N1	5.51	123.76	121.00
20	A	1175	C	N1-C2-O2	5.51	122.21	118.90
20	A	137	U	N3-C2-O2	-5.51	118.34	122.20
20	A	2596	G	N3-C4-C5	-5.51	125.84	128.60
1	a	543	C	C6-N1-C2	-5.51	118.10	120.30
1	a	1040	U	C2-N1-C1'	5.51	124.31	117.70
1	a	627	C	C2-N1-C1'	5.51	124.86	118.80
1	a	660	G	N3-C4-N9	5.50	129.30	126.00
20	A	423	C	N3-C2-O2	-5.50	118.05	121.90
20	A	925	C	C5-C6-N1	5.50	123.75	121.00
20	A	1045	C	C2-N1-C1'	5.50	124.85	118.80
20	A	1831	G	C4-N9-C1'	5.50	133.65	126.50
1	a	875	C	C2-N1-C1'	5.50	124.85	118.80
20	A	209	U	N1-C2-O2	5.49	126.65	122.80
1	a	143	C	N1-C2-O2	5.49	122.19	118.90
20	A	1561	U	N1-C2-O2	5.49	126.64	122.80
1	a	392	G	N3-C4-C5	-5.49	125.86	128.60
1	a	1053	C	C2-N1-C1'	5.49	124.84	118.80
20	A	1561	U	N3-C2-O2	-5.48	118.36	122.20
20	A	1092	C	N3-C2-O2	-5.48	118.06	121.90
20	A	121	G	C6-C5-N7	-5.48	127.11	130.40
1	a	754	C	C5-C6-N1	5.47	123.74	121.00
20	A	2090	U	N3-C2-O2	-5.47	118.37	122.20
1	a	421	G	N3-C4-N9	5.47	129.28	126.00
20	A	1408	U	N3-C2-O2	-5.47	118.37	122.20
20	A	2408	C	N1-C2-O2	5.47	122.18	118.90
20	A	586	A	N1-C6-N6	-5.46	115.32	118.60
20	A	2206	C	N1-C2-O2	5.46	122.18	118.90
1	a	826	C	C5-C6-N1	5.46	123.73	121.00
11	l	131	GLY	N-CA-C	5.46	126.75	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	145	U	N3-C2-O2	-5.45	118.38	122.20
20	A	823	A	C4-N9-C1'	5.45	136.10	126.30
20	A	1157	C	N1-C2-O2	5.45	122.17	118.90
20	A	164	U	C2-N3-C4	-5.44	123.73	127.00
20	A	1047	C	C2-N1-C1'	5.44	124.79	118.80
1	a	734	C	N1-C2-O2	5.44	122.16	118.90
20	A	1492	G	N3-C4-N9	-5.44	122.74	126.00
20	A	1603	C	OP2-P-O3'	5.44	117.16	105.20
20	A	657	C	C2-N1-C1'	5.43	124.78	118.80
20	A	1689	A	N3-C4-N9	5.43	131.75	127.40
20	A	1216	G	N3-C4-N9	5.42	129.25	126.00
1	a	199	C	N1-C2-O2	5.42	122.15	118.90
20	A	943	U	N1-C2-O2	5.41	126.59	122.80
20	A	1435	C	C2-N1-C1'	5.41	124.76	118.80
1	a	995	C	C6-N1-C2	-5.41	118.14	120.30
1	a	952	C	C5-C6-N1	5.41	123.70	121.00
1	a	997	U	C6-N1-C1'	-5.41	113.62	121.20
20	A	2786	C	C5-C6-N1	5.41	123.70	121.00
1	a	250	C	N3-C2-O2	-5.41	118.12	121.90
1	a	140	A	C4-N9-C1'	5.40	136.03	126.30
1	a	107	G	N1-C6-O6	-5.40	116.66	119.90
20	A	137	U	N1-C2-O2	5.40	126.58	122.80
1	a	55	C	C5-C6-N1	5.40	123.70	121.00
1	a	632	G	C5-C6-O6	5.40	131.84	128.60
20	A	1928	C	C2-N1-C1'	5.39	124.73	118.80
20	A	2121	C	N3-C2-O2	-5.39	118.12	121.90
20	A	2697	C	C6-N1-C2	-5.39	118.14	120.30
20	A	2753	U	C2-N1-C1'	5.39	124.16	117.70
1	a	1040	U	N3-C2-O2	-5.38	118.43	122.20
20	A	1092	C	C6-N1-C2	-5.38	118.15	120.30
1	a	322	U	C6-N1-C2	-5.38	117.77	121.00
20	A	716	A	O4'-C1'-N9	5.38	112.51	108.20
1	a	419	G	N3-C4-C5	-5.38	125.91	128.60
20	A	2552	C	C6-N1-C2	-5.38	118.15	120.30
1	a	1005	U	N3-C2-O2	-5.38	118.43	122.20
20	A	2488	C	N3-C2-O2	-5.38	118.14	121.90
19	t	81	LEU	CA-CB-CG	5.37	127.66	115.30
20	A	169	A	O4'-C1'-N9	5.37	112.50	108.20
20	A	730	C	C5-C6-N1	5.37	123.69	121.00
1	a	1183	C	C6-N1-C1'	-5.37	114.36	120.80
21	B	24	U	N3-C2-O2	-5.37	118.44	122.20
20	A	2020	C	C2-N1-C1'	5.37	124.70	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	1024	G	C8-N9-C1'	-5.36	120.03	127.00
20	A	209	U	C2-N1-C1'	5.36	124.13	117.70
1	a	190	A	C8-N9-C4	-5.35	103.66	105.80
1	a	199	C	C6-N1-C2	-5.35	118.16	120.30
20	A	2020	C	C6-N1-C2	-5.35	118.16	120.30
1	a	927	U	N1-C2-O2	5.35	126.54	122.80
20	A	476	C	C6-N1-C2	-5.35	118.16	120.30
20	A	509	G	N7-C8-N9	5.35	115.77	113.10
1	a	146	C	C5-C6-N1	5.34	123.67	121.00
1	a	516	C	N3-C4-N4	-5.34	114.26	118.00
20	A	1362	U	N1-C2-O2	5.34	126.54	122.80
31	O	41	ARG	CB-CG-CD	-5.33	97.73	111.60
1	a	1446	C	N1-C2-O2	5.33	122.10	118.90
20	A	1689	A	C4-N9-C1'	5.33	135.90	126.30
20	A	906	C	C6-N1-C1'	-5.33	114.40	120.80
20	A	2262	C	C2-N1-C1'	5.33	124.66	118.80
20	A	2592	G	N1-C6-O6	-5.33	116.70	119.90
1	a	644	A	N7-C8-N9	5.32	116.46	113.80
20	A	121	G	N3-C4-N9	5.32	129.19	126.00
20	A	956	C	C6-N1-C2	-5.32	118.17	120.30
20	A	955	C	C6-N1-C2	-5.31	118.17	120.30
20	A	2206	C	N3-C2-O2	-5.31	118.18	121.90
1	a	1148	C	N1-C2-O2	5.31	122.08	118.90
20	A	1408	U	N1-C2-O2	5.31	126.52	122.80
20	A	1948	C	C6-N1-C1'	-5.31	114.43	120.80
20	A	1128	A	N1-C6-N6	5.31	121.78	118.60
20	A	1638	C	C2-N1-C1'	5.31	124.64	118.80
20	A	569	C	N1-C2-O2	5.30	122.08	118.90
20	A	1379	G	C8-N9-C1'	-5.30	120.11	127.00
20	A	939	C	N3-C2-O2	-5.30	118.19	121.90
20	A	2595	G	C4-N9-C1'	5.30	133.39	126.50
1	a	66	C	C5-C6-N1	5.30	123.65	121.00
1	a	234	C	N1-C2-O2	5.30	122.08	118.90
1	a	860	C	C6-N1-C2	-5.29	118.18	120.30
21	B	32	U	P-O3'-C3'	5.29	126.05	119.70
20	A	897	G	C6-C5-N7	5.29	133.57	130.40
20	A	1317	G	N3-C4-N9	5.29	129.17	126.00
20	A	1719	A	C8-N9-C4	-5.29	103.69	105.80
1	a	66	C	C2-N1-C1'	5.29	124.62	118.80
20	A	67	C	N1-C2-O2	5.29	122.07	118.90
20	A	1295	C	N3-C2-O2	-5.29	118.20	121.90
20	A	1304	U	C5-C6-N1	5.29	125.34	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	423	C	C6-N1-C2	-5.28	118.19	120.30
20	A	1569	G	N3-C4-N9	-5.28	122.83	126.00
20	A	1369	C	C6-N1-C2	-5.28	118.19	120.30
1	a	51	C	N1-C2-O2	5.28	122.06	118.90
20	A	1574	C	C2-N1-C1'	5.28	124.60	118.80
20	A	2794	G	N3-C4-N9	5.28	129.17	126.00
20	A	1906	C	C6-N1-C2	-5.27	118.19	120.30
20	A	2858	U	C2-N1-C1'	5.27	124.02	117.70
20	A	237	U	N3-C2-O2	-5.26	118.52	122.20
20	A	2188	C	N3-C2-O2	-5.26	118.22	121.90
20	A	835	C	C5-C6-N1	5.26	123.63	121.00
1	a	331	C	C2-N1-C1'	5.25	124.58	118.80
20	A	1853	G	C4-N9-C1'	5.25	133.33	126.50
20	A	2836	G	C4-C5-N7	5.25	112.90	110.80
21	B	35	C	N1-C2-O2	5.25	122.05	118.90
1	a	634	U	N3-C2-O2	-5.25	118.52	122.20
20	A	2854	G	N3-C4-N9	5.25	129.15	126.00
20	A	2090	U	C2-N1-C1'	5.25	124.00	117.70
20	A	1768	C	C6-N1-C2	-5.25	118.20	120.30
20	A	549	C	C6-N1-C2	-5.24	118.20	120.30
20	A	602	C	C2-N1-C1'	5.24	124.57	118.80
20	A	992	G	N3-C4-N9	5.24	129.15	126.00
20	A	121	G	C4-C5-N7	5.24	112.90	110.80
20	A	960	U	N1-C2-O2	5.24	126.47	122.80
20	A	1981	C	C2-N1-C1'	5.24	124.56	118.80
20	A	77	C	C6-N1-C2	-5.24	118.20	120.30
20	A	823	A	C8-N9-C4	-5.24	103.70	105.80
20	A	325	U	N3-C2-O2	-5.24	118.53	122.20
20	A	2606	G	N3-C4-N9	5.24	129.14	126.00
20	A	2021	U	N3-C2-O2	-5.23	118.54	122.20
20	A	561	G	C4-N9-C1'	5.23	133.29	126.50
1	a	498	C	C2-N1-C1'	5.22	124.55	118.80
20	A	709	G	C8-N9-C1'	-5.22	120.21	127.00
1	a	148	G	C8-N9-C4	-5.22	104.31	106.40
20	A	1492	G	N3-C4-C5	5.22	131.21	128.60
20	A	943	U	N3-C2-O2	-5.22	118.55	122.20
20	A	2474	U	N1-C2-O2	5.22	126.45	122.80
1	a	141	C	C2-N1-C1'	5.21	124.54	118.80
1	a	148	G	N3-C4-N9	5.21	129.13	126.00
1	a	418	C	C6-N1-C1'	-5.21	114.55	120.80
1	a	71	U	N1-C2-O2	5.20	126.44	122.80
20	A	4	U	C2-N1-C1'	5.20	123.94	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	2808	C	C6-N1-C2	-5.20	118.22	120.30
1	a	644	A	C8-N9-C1'	-5.20	118.34	127.70
20	A	607	G	N3-C4-N9	5.20	129.12	126.00
20	A	1108	G	N3-C4-C5	-5.20	126.00	128.60
20	A	499	U	N3-C2-O2	-5.20	118.56	122.20
20	A	2570	C	C2-N1-C1'	5.20	124.52	118.80
20	A	1723	U	N1-C2-O2	5.19	126.44	122.80
20	A	2552	C	C5-C6-N1	5.19	123.60	121.00
20	A	2766	C	C6-N1-C2	-5.19	118.22	120.30
20	A	549	C	N3-C2-O2	-5.18	118.27	121.90
1	a	639	C	N3-C2-O2	-5.18	118.27	121.90
20	A	1689	A	N3-C4-C5	-5.18	123.17	126.80
20	A	1197	G	C4-C5-N7	5.18	112.87	110.80
1	a	1022	C	N3-C2-O2	-5.18	118.28	121.90
20	A	2278	C	N3-C2-O2	-5.18	118.28	121.90
1	a	392	G	N3-C4-N9	5.18	129.11	126.00
1	a	634	U	N1-C2-O2	5.18	126.42	122.80
20	A	1603	C	P-O3'-C3'	5.17	125.91	119.70
1	a	71	U	N3-C2-O2	-5.17	118.58	122.20
1	a	559	G	P-O3'-C3'	5.17	125.90	119.70
20	A	77	C	C5-C6-N1	5.17	123.58	121.00
20	A	167	A	N1-C2-N3	-5.16	126.72	129.30
20	A	211	C	N1-C2-O2	5.16	122.00	118.90
20	A	550	U	C2-N1-C1'	5.16	123.90	117.70
20	A	1034	C	C6-N1-C2	-5.16	118.23	120.30
20	A	1501	A	C2-N3-C4	5.16	113.18	110.60
1	a	754	C	C6-N1-C2	-5.16	118.24	120.30
1	a	1022	C	C2-N1-C1'	5.16	124.47	118.80
20	A	1317	G	C4-N9-C1'	5.16	133.21	126.50
20	A	2670	U	N1-C2-O2	5.16	126.41	122.80
20	A	621	C	C6-N1-C2	-5.16	118.24	120.30
21	B	28	C	N1-C2-O2	5.16	121.99	118.90
1	a	392	G	C4-N9-C1'	5.15	133.20	126.50
1	a	346	G	C6-C5-N7	-5.15	127.31	130.40
1	a	559	G	N7-C8-N9	5.15	115.67	113.10
20	A	2188	C	N1-C2-O2	5.15	121.99	118.90
21	B	35	C	N3-C2-O2	-5.15	118.30	121.90
20	A	588	G	N3-C4-C5	-5.15	126.03	128.60
21	B	73	U	N3-C2-O2	-5.14	118.60	122.20
20	A	709	G	N3-C4-C5	-5.14	126.03	128.60
20	A	1642	C	C2-N1-C1'	5.14	124.46	118.80
20	A	2057	C	C2-N1-C1'	5.14	124.46	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	790	G	N3-C2-N2	-5.14	116.30	119.90
20	A	509	G	C5-N7-C8	-5.14	101.73	104.30
20	A	1399	C	C5-C6-N1	5.13	123.57	121.00
20	A	638	C	C5-C6-N1	5.13	123.57	121.00
20	A	742	U	N3-C2-O2	-5.13	118.61	122.20
20	A	1106	U	C2-N1-C1'	5.13	123.86	117.70
20	A	1278	C	C2-N1-C1'	5.13	124.44	118.80
20	A	1703	C	C5-C6-N1	5.13	123.57	121.00
20	A	2819	U	C2-N1-C1'	5.13	123.86	117.70
20	A	939	C	N1-C2-O2	5.13	121.98	118.90
1	a	585	G	N3-C4-N9	5.13	129.08	126.00
20	A	2812	A	OP1-P-O3'	5.13	116.48	105.20
20	A	1149	C	N1-C2-O2	5.13	121.98	118.90
20	A	286	U	C5-C6-N1	5.12	125.26	122.70
20	A	769	G	N3-C4-N9	-5.12	122.93	126.00
34	R	13	ARG	CB-CG-CD	-5.12	98.28	111.60
1	a	673	G	C8-N9-C4	-5.12	104.35	106.40
1	a	790	G	C2-N3-C4	-5.12	109.34	111.90
20	A	2896	C	C6-N1-C2	-5.12	118.25	120.30
1	a	1162	C	N1-C2-O2	5.11	121.97	118.90
20	A	1550	U	N1-C2-O2	5.11	126.38	122.80
20	A	655	G	N9-C4-C5	-5.11	103.36	105.40
20	A	1029	G	C4-N9-C1'	5.11	133.14	126.50
1	a	790	G	N3-C4-C5	5.11	131.15	128.60
20	A	2734	U	C2-N1-C1'	5.11	123.83	117.70
20	A	201	C	N1-C2-O2	5.11	121.96	118.90
20	A	1149	C	C2-N1-C1'	5.11	124.42	118.80
1	a	704	C	C5-C6-N1	5.10	123.55	121.00
1	a	108	U	C5-C4-O4	-5.10	122.84	125.90
20	A	975	U	N1-C2-O2	5.10	126.37	122.80
1	a	1442	C	C6-N1-C2	-5.10	118.26	120.30
20	A	1350	C	C6-N1-C1'	-5.10	114.68	120.80
20	A	1216	G	N3-C4-C5	-5.09	126.05	128.60
1	a	267	U	N1-C2-O2	5.09	126.36	122.80
1	a	1318	C	N1-C2-O2	5.09	121.95	118.90
20	A	963	C	C6-N1-C1'	5.09	126.90	120.80
20	A	1350	C	N3-C2-O2	-5.09	118.34	121.90
20	A	2062	G	C4-N9-C1'	5.08	133.11	126.50
1	a	867	C	N3-C2-O2	-5.08	118.35	121.90
20	A	2474	U	N3-C2-O2	-5.08	118.65	122.20
1	a	105	G	P-O3'-C3'	5.08	125.79	119.70
3	d	17	ILE	CG1-CB-CG2	-5.08	100.23	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	325	U	C2-N1-C1'	5.08	123.79	117.70
20	A	1928	C	C6-N1-C2	-5.07	118.27	120.30
20	A	2077	C	N1-C2-O2	5.07	121.94	118.90
20	A	848	G	N3-C4-N9	-5.07	122.96	126.00
20	A	769	G	C2-N3-C4	-5.07	109.37	111.90
20	A	1434	C	C6-N1-C2	-5.06	118.28	120.30
1	a	409	G	C4-N9-C1'	5.06	133.08	126.50
20	A	2138	G	C4-N9-C1'	5.06	133.08	126.50
1	a	415	C	N3-C2-O2	-5.06	118.36	121.90
1	a	1183	C	O4'-C1'-N1	5.06	112.25	108.20
20	A	261	C	C2-N1-C1'	5.06	124.36	118.80
20	A	992	G	C4-N9-C1'	5.06	133.07	126.50
20	A	1234	C	C6-N1-C2	-5.06	118.28	120.30
1	a	178	A	C8-N9-C4	-5.05	103.78	105.80
1	a	1005	U	N1-C2-O2	5.05	126.34	122.80
1	a	1465	U	C2-N1-C1'	5.05	123.77	117.70
1	a	790	G	C8-N9-C1'	5.05	133.56	127.00
20	A	1047	C	C5-C6-N1	5.04	123.52	121.00
20	A	2576	U	N3-C2-O2	-5.04	118.67	122.20
1	a	649	C	C5-C6-N1	5.04	123.52	121.00
20	A	2897	G	C4-N9-C1'	5.04	133.05	126.50
1	a	1306	C	N1-C2-O2	5.04	121.92	118.90
20	A	1128	A	N3-C4-N9	5.04	131.43	127.40
20	A	2785	C	C2-N1-C1'	5.04	124.34	118.80
20	A	1511	C	N3-C2-O2	-5.03	118.38	121.90
1	a	109	G	N3-C2-N2	-5.03	116.38	119.90
1	a	1173	C	C6-N1-C1'	-5.03	114.77	120.80
1	a	639	C	N1-C2-N3	5.02	122.72	119.20
20	A	2311	C	N3-C2-O2	-5.02	118.39	121.90
21	B	24	U	N1-C2-O2	5.02	126.31	122.80
20	A	1584	G	OP2-P-O3'	5.02	116.24	105.20
1	a	504	C	N1-C2-O2	5.02	121.91	118.90
20	A	1634	A	N3-C4-N9	5.02	131.41	127.40
20	A	2836	G	C5-N7-C8	-5.02	101.79	104.30
1	a	1077	G	C4-N9-C1'	5.02	133.02	126.50
1	a	464	A	C8-N9-C4	-5.01	103.80	105.80
20	A	638	C	N1-C2-O2	5.01	121.91	118.90
20	A	121	G	C4-N9-C1'	5.01	133.02	126.50
20	A	1132	C	C6-N1-C2	-5.01	118.30	120.30
1	a	1125	C	N3-C2-O2	-5.01	118.39	121.90
1	a	712	U	N3-C2-O2	-5.01	118.69	122.20
20	A	1115	C	N1-C2-O2	5.01	121.90	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	636	A	C2-N3-C4	5.00	113.10	110.60
20	A	2826	C	C6-N1-C2	-5.00	118.30	120.30
1	a	190	A	C5-N7-C8	-5.00	101.40	103.90
1	a	632	G	C8-N9-C1'	5.00	133.50	127.00
1	a	1038	C	N3-C2-O2	-5.00	118.40	121.90
20	A	778	C	C2-N1-C1'	5.00	124.30	118.80
1	a	530	G	C8-N9-C1'	-5.00	120.50	127.00
20	A	890	A	P-O3'-C3'	5.00	125.70	119.70
20	A	1234	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	4	3	ARG	Peptide
22	C	154	LEU	Peptide
22	C	195	VAL	Peptide
23	D	53	TYR	Peptide
23	D	89	GLY	Peptide
24	E	45	ARG	Peptide
24	E	80	SER	Peptide
25	F	121	ALA	Peptide
26	G	47	GLY	Peptide
26	G	61	MET	Peptide
27	K	131	HIS	Peptide
27	K	45	PHE	Peptide
29	M	30	THR	Peptide
29	M	85	PHE	Peptide
29	M	97	LYS	Peptide
30	N	133	LYS	Peptide
30	N	8	LYS	Peptide
31	O	22	THR	Peptide
31	O	77	ASP	Peptide
32	P	22	ILE	Peptide
32	P	30	ARG	Peptide
32	P	93	PHE	Peptide
35	S	100	ILE	Peptide
35	S	50	ALA	Peptide
37	U	50	VAL	Peptide
37	U	62	PHE	Peptide
38	V	72	ASP	Peptide
38	V	87	ASP	Peptide

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Mol	Chain	Res	Type	Group
39	W	15	ARG	Peptide
40	X	49	GLN	Peptide
41	Y	21	ALA	Peptide
11	l	130	TYR	Peptide
11	l	37	ASN	Peptide
12	m	43	VAL	Peptide
16	q	73	THR	Peptide
19	t	66	ILE	Peptide

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	
2	c	202/204 (99%)	178 (88%)	24 (12%)	0	100	100
3	d	199/201 (99%)	169 (85%)	30 (15%)	0	100	100
4	e	161/163 (99%)	142 (88%)	19 (12%)	0	100	100
5	f	95/97 (98%)	88 (93%)	7 (7%)	0	100	100
6	g	152/154 (99%)	138 (91%)	14 (9%)	0	100	100
7	h	129/131 (98%)	116 (90%)	13 (10%)	0	100	100
8	i	126/128 (98%)	110 (87%)	15 (12%)	1 (1%)	19	58
9	j	97/99 (98%)	87 (90%)	10 (10%)	0	100	100
10	k	115/117 (98%)	98 (85%)	17 (15%)	0	100	100
11	l	134/136 (98%)	106 (79%)	27 (20%)	1 (1%)	22	61
12	m	110/112 (98%)	86 (78%)	24 (22%)	0	100	100
13	n	58/60 (97%)	53 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	o	86/88 (98%)	79 (92%)	7 (8%)	0	100	100
15	p	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
16	q	81/83 (98%)	67 (83%)	14 (17%)	0	100	100
17	r	64/66 (97%)	53 (83%)	11 (17%)	0	100	100
18	s	76/78 (97%)	60 (79%)	16 (21%)	0	100	100
19	t	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
22	C	273/275 (99%)	236 (86%)	37 (14%)	0	100	100
23	D	205/207 (99%)	182 (89%)	22 (11%)	1 (0%)	29	68
24	E	204/206 (99%)	175 (86%)	29 (14%)	0	100	100
25	F	175/177 (99%)	149 (85%)	26 (15%)	0	100	100
26	G	172/176 (98%)	145 (84%)	25 (14%)	2 (1%)	13	50
27	K	142/145 (98%)	124 (87%)	18 (13%)	0	100	100
28	L	120/122 (98%)	98 (82%)	22 (18%)	0	100	100
29	M	143/146 (98%)	105 (73%)	35 (24%)	3 (2%)	7	38
30	N	137/141 (97%)	111 (81%)	26 (19%)	0	100	100
31	O	119/123 (97%)	95 (80%)	24 (20%)	0	100	100
32	P	115/117 (98%)	100 (87%)	15 (13%)	0	100	100
33	Q	110/114 (96%)	98 (89%)	12 (11%)	0	100	100
34	R	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
35	S	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
36	T	110/112 (98%)	95 (86%)	15 (14%)	0	100	100
37	U	87/89 (98%)	72 (83%)	13 (15%)	2 (2%)	6	36
38	V	99/101 (98%)	75 (76%)	21 (21%)	3 (3%)	4	30
39	W	92/94 (98%)	74 (80%)	17 (18%)	1 (1%)	14	52
40	X	73/76 (96%)	64 (88%)	9 (12%)	0	100	100
41	Y	52/54 (96%)	44 (85%)	8 (15%)	0	100	100
42	Z	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
43	0	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
44	1	81/83 (98%)	60 (74%)	21 (26%)	0	100	100
45	2	54/56 (96%)	47 (87%)	7 (13%)	0	100	100
46	3	47/49 (96%)	45 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	4	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
48	5	62/64 (97%)	55 (89%)	7 (11%)	0	100	100
49	6	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
All	All	5128/5235 (98%)	4406 (86%)	708 (14%)	14 (0%)	44	75

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	G	48	ASN
29	M	95	VAL
29	M	98	GLU
39	W	16	SER
11	l	131	GLY
26	G	47	GLY
38	V	73	PRO
38	V	88	GLY
37	U	51	ALA
23	D	90	GLU
38	V	72	ASP
8	i	41	HIS
37	U	52	ASN
29	M	94	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	162/162 (100%)	162 (100%)	0	100	100
3	d	175/175 (100%)	173 (99%)	2 (1%)	73	88
4	e	126/126 (100%)	126 (100%)	0	100	100
5	f	86/86 (100%)	86 (100%)	0	100	100
6	g	131/131 (100%)	131 (100%)	0	100	100
7	h	112/112 (100%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	101/101 (100%)	100 (99%)	1 (1%)	76	88
9	j	90/90 (100%)	88 (98%)	2 (2%)	52	78
10	k	91/91 (100%)	90 (99%)	1 (1%)	73	88
11	l	118/118 (100%)	115 (98%)	3 (2%)	47	75
12	m	95/95 (100%)	95 (100%)	0	100	100
13	n	51/51 (100%)	50 (98%)	1 (2%)	55	79
14	o	78/78 (100%)	76 (97%)	2 (3%)	46	74
15	p	79/79 (100%)	77 (98%)	2 (2%)	47	75
16	q	76/76 (100%)	74 (97%)	2 (3%)	46	74
17	r	57/57 (100%)	54 (95%)	3 (5%)	22	55
18	s	68/68 (100%)	67 (98%)	1 (2%)	65	84
19	t	62/62 (100%)	62 (100%)	0	100	100
22	C	224/225 (100%)	223 (100%)	1 (0%)	91	96
23	D	168/170 (99%)	164 (98%)	4 (2%)	49	76
24	E	172/172 (100%)	170 (99%)	2 (1%)	71	87
25	F	154/154 (100%)	154 (100%)	0	100	100
26	G	145/146 (99%)	145 (100%)	0	100	100
27	K	121/122 (99%)	120 (99%)	1 (1%)	81	91
28	L	98/98 (100%)	98 (100%)	0	100	100
29	M	111/112 (99%)	111 (100%)	0	100	100
30	N	112/112 (100%)	110 (98%)	2 (2%)	59	81
31	O	105/105 (100%)	104 (99%)	1 (1%)	76	88
32	P	91/91 (100%)	91 (100%)	0	100	100
33	Q	94/97 (97%)	94 (100%)	0	100	100
34	R	92/94 (98%)	92 (100%)	0	100	100
35	S	82/83 (99%)	82 (100%)	0	100	100
36	T	95/95 (100%)	95 (100%)	0	100	100
37	U	80/80 (100%)	78 (98%)	2 (2%)	47	75
38	V	85/85 (100%)	85 (100%)	0	100	100
39	W	85/85 (100%)	85 (100%)	0	100	100
40	X	60/61 (98%)	59 (98%)	1 (2%)	60	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Y	47/47 (100%)	45 (96%)	2 (4%)	29	62
42	Z	55/55 (100%)	54 (98%)	1 (2%)	59	81
43	0	48/49 (98%)	48 (100%)	0	100	100
44	1	75/75 (100%)	74 (99%)	1 (1%)	69	86
45	2	46/46 (100%)	46 (100%)	0	100	100
46	3	49/49 (100%)	49 (100%)	0	100	100
47	4	39/39 (100%)	39 (100%)	0	100	100
48	5	51/51 (100%)	51 (100%)	0	100	100
49	6	35/35 (100%)	35 (100%)	0	100	100
All	All	4377/4391 (100%)	4339 (99%)	38 (1%)	79	90

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	d	14	ARG
3	d	58	ARG
8	i	14	ASN
9	j	5	LYS
9	j	16	ARG
10	k	93	ARG
11	l	32	LYS
11	l	127	ARG
11	l	134	ARG
13	n	26	ARG
14	o	54	ARG
14	o	89	ARG
15	p	9	ARG
15	p	90	LYS
16	q	5	ARG
16	q	6	ASN
17	r	13	LYS
17	r	57	ARG
17	r	65	ARG
18	s	6	LYS
22	C	257	TYR
23	D	57	ARG
23	D	119	PHE
23	D	159	ARG
23	D	168	ARG

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Mol	Chain	Res	Type
24	E	74	ARG
24	E	169	ASN
27	K	45	PHE
30	N	10	ARG
30	N	119	ARG
31	O	114	ARG
37	U	48	VAL
37	U	62	PHE
40	X	80	ARG
41	Y	17	ASN
41	Y	32	ASN
42	Z	26	PHE
44	1	75	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
3	d	86	ASN
6	g	68	ASN
6	g	106	ASN
6	g	114	HIS
8	i	14	ASN
8	i	75	GLN
9	j	56	HIS
9	j	97	ASN
12	m	76	ASN
13	n	10	ASN
16	q	6	ASN
16	q	50	HIS
18	s	22	GLN
22	C	53	HIS
22	C	95	HIS
22	C	128	ASN
22	C	153	GLN
22	C	232	HIS
23	D	14	GLN
23	D	37	GLN
24	E	29	ASN
24	E	49	HIS
24	E	75	GLN
24	E	169	ASN
25	F	27	GLN

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Mol	Chain	Res	Type
25	F	37	ASN
26	G	106	ASN
28	L	13	ASN
32	P	20	ASN
32	P	32	ASN
34	R	81	HIS
35	S	88	HIS
36	T	102	ASN
38	V	44	HIS
40	X	87	GLN
41	Y	17	ASN
41	Y	23	ASN
41	Y	32	ASN
44	1	75	ASN
45	2	32	ASN
45	2	40	HIS
47	4	8	ASN
48	5	4	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1528 (99%)	441 (28%)	0
20	A	2895/2903 (99%)	650 (22%)	20 (0%)
21	B	113/116 (97%)	26 (23%)	2 (1%)
All	All	4534/4547 (99%)	1117 (24%)	22 (0%)

All (1117) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	5	A
1	a	6	G
1	a	7	A
1	a	11	U
1	a	13	A
1	a	19	G
1	a	25	G
1	a	29	A
1	a	32	G
1	a	36	G
1	a	38	G

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Mol	Chain	Res	Type
1	a	41	G
1	a	44	C
1	a	45	C
1	a	46	U
1	a	47	A
1	a	48	A
1	a	51	C
1	a	61	G
1	a	62	A
1	a	63	A
1	a	64	C
1	a	67	U
1	a	68	U
1	a	69	C
1	a	72	U
1	a	73	C
1	a	74	C
1	a	75	U
1	a	97	G
1	a	104	G
1	a	105	G
1	a	106	A
1	a	107	G
1	a	109	G
1	a	112	G
1	a	113	G
1	a	114	A
1	a	125	A
1	a	126	C
1	a	135	A
1	a	136	A
1	a	139	U
1	a	140	A
1	a	142	C
1	a	143	C
1	a	148	G
1	a	149	A
1	a	150	G
1	a	156	U
1	a	159	C
1	a	163	U
1	a	165	G

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Mol	Chain	Res	Type
1	a	167	A
1	a	168	A
1	a	169	C
1	a	172	G
1	a	180	A
1	a	183	G
1	a	184	C
1	a	185	A
1	a	187	A
1	a	188	A
1	a	189	C
1	a	190	A
1	a	197	G
1	a	199	C
1	a	200	G
1	a	201	C
1	a	202	A
1	a	206	C
1	a	207	A
1	a	208	U
1	a	211	G
1	a	212	A
1	a	213	G
1	a	214	U
1	a	217	A
1	a	218	A
1	a	219	G
1	a	221	C
1	a	225	U
1	a	227	C
1	a	230	G
1	a	233	U
1	a	234	C
1	a	235	G
1	a	238	G
1	a	240	U
1	a	250	C
1	a	255	U
1	a	256	G
1	a	262	G
1	a	266	G
1	a	278	A

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Mol	Chain	Res	Type
1	a	281	G
1	a	282	C
1	a	289	A
1	a	295	C
1	a	304	G
1	a	308	A
1	a	313	A
1	a	323	C
1	a	330	A
1	a	336	A
1	a	343	C
1	a	345	C
1	a	347	G
1	a	360	C
1	a	362	G
1	a	367	C
1	a	368	A
1	a	369	G
1	a	374	A
1	a	378	A
1	a	381	C
1	a	382	U
1	a	384	C
1	a	387	C
1	a	388	A
1	a	390	U
1	a	392	G
1	a	393	A
1	a	396	A
1	a	397	A
1	a	398	A
1	a	399	G
1	a	403	G
1	a	405	C
1	a	412	A
1	a	413	C
1	a	416	C
1	a	417	G
1	a	418	C
1	a	419	G
1	a	421	G
1	a	424	U

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Mol	Chain	Res	Type
1	a	425	G
1	a	426	A
1	a	427	A
1	a	428	G
1	a	429	A
1	a	430	A
1	a	435	U
1	a	437	C
1	a	438	G
1	a	439	G
1	a	443	G
1	a	444	U
1	a	446	A
1	a	448	A
1	a	450	U
1	a	451	C
1	a	453	G
1	a	454	U
1	a	456	G
1	a	457	U
1	a	459	A
1	a	462	G
1	a	463	A
1	a	465	G
1	a	467	A
1	a	468	C
1	a	469	A
1	a	470	A
1	a	471	G
1	a	475	G
1	a	476	U
1	a	477	U
1	a	478	A
1	a	479	G
1	a	480	U
1	a	481	A
1	a	483	C
1	a	485	G
1	a	486	A
1	a	487	A
1	a	488	C
1	a	489	G

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Mol	Chain	Res	Type
1	a	490	U
1	a	492	C
1	a	493	C
1	a	494	C
1	a	495	U
1	a	497	A
1	a	498	C
1	a	499	G
1	a	500	G
1	a	501	U
1	a	504	C
1	a	505	U
1	a	507	A
1	a	510	A
1	a	512	A
1	a	514	A
1	a	515	G
1	a	517	C
1	a	525	A
1	a	526	C
1	a	530	G
1	a	531	U
1	a	532	G
1	a	533	C
1	a	534	C
1	a	539	G
1	a	542	G
1	a	545	G
1	a	546	U
1	a	547	A
1	a	548	A
1	a	550	A
1	a	551	C
1	a	552	G
1	a	555	G
1	a	556	G
1	a	558	G
1	a	560	C
1	a	561	A
1	a	562	A
1	a	576	U
1	a	577	U

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Mol	Chain	Res	Type
1	a	578	A
1	a	587	A
1	a	588	A
1	a	591	C
1	a	592	G
1	a	594	G
1	a	603	G
1	a	626	C
1	a	627	C
1	a	634	U
1	a	635	C
1	a	636	A
1	a	637	A
1	a	642	G
1	a	644	A
1	a	645	G
1	a	646	G
1	a	647	G
1	a	648	U
1	a	649	C
1	a	664	G
1	a	668	U
1	a	671	G
1	a	672	U
1	a	673	G
1	a	674	C
1	a	676	G
1	a	680	A
1	a	686	G
1	a	701	U
1	a	702	A
1	a	710	A
1	a	723	A
1	a	725	G
1	a	734	C
1	a	736	A
1	a	738	U
1	a	744	A
1	a	749	G
1	a	764	A
1	a	770	G
1	a	782	A

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Mol	Chain	Res	Type
1	a	790	G
1	a	792	A
1	a	809	A
1	a	814	G
1	a	830	A
1	a	831	A
1	a	832	C
1	a	833	G
1	a	836	G
1	a	847	G
1	a	851	G
1	a	858	U
1	a	859	C
1	a	862	C
1	a	867	C
1	a	886	U
1	a	888	A
1	a	892	A
1	a	901	G
1	a	905	A
1	a	930	A
1	a	942	G
1	a	943	G
1	a	950	C
1	a	951	A
1	a	958	G
1	a	964	C
1	a	968	U
1	a	971	U
1	a	975	A
1	a	976	U
1	a	981	A
1	a	982	G
1	a	985	A
1	a	987	G
1	a	988	C
1	a	989	G
1	a	991	A
1	a	992	G
1	a	994	A
1	a	998	U
1	a	999	A

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Mol	Chain	Res	Type
1	a	1000	C
1	a	1005	U
1	a	1008	U
1	a	1009	G
1	a	1011	C
1	a	1018	U
1	a	1019	G
1	a	1020	A
1	a	1021	C
1	a	1022	C
1	a	1025	U
1	a	1029	G
1	a	1030	A
1	a	1031	G
1	a	1035	G
1	a	1038	C
1	a	1040	U
1	a	1041	U
1	a	1042	C
1	a	1043	C
1	a	1044	C
1	a	1045	U
1	a	1046	U
1	a	1047	C
1	a	1049	G
1	a	1050	G
1	a	1052	A
1	a	1053	C
1	a	1054	A
1	a	1055	A
1	a	1060	A
1	a	1061	C
1	a	1069	G
1	a	1070	C
1	a	1080	G
1	a	1081	U
1	a	1082	C
1	a	1094	U
1	a	1095	G
1	a	1101	U
1	a	1102	U
1	a	1110	G

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Mol	Chain	Res	Type
1	a	1111	U
1	a	1117	A
1	a	1124	G
1	a	1140	G
1	a	1141	U
1	a	1147	U
1	a	1148	C
1	a	1149	A
1	a	1152	U
1	a	1154	G
1	a	1155	U
1	a	1156	U
1	a	1157	G
1	a	1161	A
1	a	1169	G
1	a	1174	U
1	a	1175	G
1	a	1176	C
1	a	1183	C
1	a	1184	A
1	a	1189	G
1	a	1198	U
1	a	1199	G
1	a	1201	G
1	a	1208	G
1	a	1211	A
1	a	1212	A
1	a	1227	U
1	a	1228	A
1	a	1229	U
1	a	1230	G
1	a	1241	C
1	a	1243	C
1	a	1256	G
1	a	1272	C
1	a	1275	U
1	a	1276	A
1	a	1284	A
1	a	1289	A
1	a	1295	A
1	a	1297	C
1	a	1300	U

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Mol	Chain	Res	Type
1	a	1301	U
1	a	1302	A
1	a	1303	A
1	a	1305	G
1	a	1312	U
1	a	1314	A
1	a	1317	U
1	a	1318	C
1	a	1320	G
1	a	1324	G
1	a	1327	G
1	a	1332	C
1	a	1335	C
1	a	1337	C
1	a	1350	C
1	a	1351	C
1	a	1355	A
1	a	1362	G
1	a	1368	G
1	a	1374	C
1	a	1379	C
1	a	1393	C
1	a	1396	U
1	a	1398	C
1	a	1413	A
1	a	1416	G
1	a	1434	G
1	a	1438	G
1	a	1441	A
1	a	1448	A
1	a	1455	U
1	a	1457	A
1	a	1461	A
1	a	1466	U
1	a	1467	U
1	a	1468	U
1	a	1500	U
1	a	1503	G
1	a	1508	A
1	a	1509	A
1	a	1510	G
1	a	1513	G

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Mol	Chain	Res	Type
1	a	1515	A
1	a	1518	A
1	a	1519	A
1	a	1522	U
1	a	1523	A
1	a	1545	G
1	a	1546	G
1	a	1547	A
1	a	1549	C
1	a	1550	A
20	A	10	G
20	A	13	U
20	A	14	A
20	A	16	G
20	A	35	U
20	A	62	A
20	A	64	U
20	A	72	A
20	A	76	G
20	A	90	U
20	A	94	U
20	A	97	G
20	A	99	U
20	A	100	A
20	A	102	G
20	A	103	A
20	A	110	G
20	A	116	C
20	A	118	A
20	A	120	U
20	A	131	A
20	A	155	U
20	A	156	U
20	A	163	A
20	A	164	U
20	A	165	A
20	A	166	C
20	A	169	A
20	A	180	G
20	A	181	G
20	A	182	U
20	A	183	A

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Mol	Chain	Res	Type
20	A	184	G
20	A	189	A
20	A	199	A
20	A	202	A
20	A	218	G
20	A	219	A
20	A	224	A
20	A	225	A
20	A	229	A
20	A	231	A
20	A	232	U
20	A	233	U
20	A	235	G
20	A	244	A
20	A	251	G
20	A	254	A
20	A	255	G
20	A	268	A
20	A	279	A
20	A	284	C
20	A	285	U
20	A	288	C
20	A	293	U
20	A	298	U
20	A	300	G
20	A	305	A
20	A	311	A
20	A	312	U
20	A	313	A
20	A	318	A
20	A	319	G
20	A	321	C
20	A	322	U
20	A	332	G
20	A	339	G
20	A	344	G
20	A	367	A
20	A	372	C
20	A	383	A
20	A	389	G
20	A	391	C
20	A	396	C

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Mol	Chain	Res	Type
20	A	399	A
20	A	400	G
20	A	410	G
20	A	421	A
20	A	426	G
20	A	451	G
20	A	452	A
20	A	488	U
20	A	496	C
20	A	507	G
20	A	517	A
20	A	519	A
20	A	521	G
20	A	544	A
20	A	547	U
20	A	548	C
20	A	549	C
20	A	560	U
20	A	561	G
20	A	566	C
20	A	568	A
20	A	569	C
20	A	570	A
20	A	571	A
20	A	572	G
20	A	585	A
20	A	586	A
20	A	588	G
20	A	600	G
20	A	610	G
20	A	612	A
20	A	623	A
20	A	629	G
20	A	640	A
20	A	653	G
20	A	654	A
20	A	655	G
20	A	669	G
20	A	670	A
20	A	673	G
20	A	676	A
20	A	677	G

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Mol	Chain	Res	Type
20	A	684	U
20	A	693	U
20	A	694	G
20	A	696	G
20	A	708	A
20	A	710	A
20	A	711	C
20	A	712	C
20	A	722	G
20	A	726	U
20	A	756	A
20	A	757	A
20	A	759	C
20	A	766	G
20	A	769	G
20	A	770	A
20	A	775	A
20	A	778	C
20	A	787	U
20	A	788	G
20	A	792	A
20	A	805	G
20	A	808	G
20	A	815	G
20	A	816	C
20	A	817	G
20	A	822	A
20	A	823	A
20	A	824	U
20	A	832	G
20	A	833	A
20	A	840	A
20	A	845	G
20	A	846	C
20	A	849	G
20	A	852	C
20	A	867	U
20	A	885	U
20	A	886	U
20	A	887	G
20	A	888	A
20	A	891	A

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Mol	Chain	Res	Type
20	A	900	G
20	A	901	U
20	A	905	G
20	A	906	C
20	A	907	A
20	A	919	A
20	A	920	G
20	A	922	G
20	A	923	G
20	A	925	C
20	A	926	C
20	A	927	A
20	A	928	U
20	A	933	G
20	A	934	G
20	A	939	C
20	A	940	G
20	A	942	A
20	A	943	U
20	A	946	A
20	A	950	A
20	A	951	A
20	A	953	C
20	A	954	U
20	A	960	U
20	A	961	G
20	A	964	A
20	A	966	U
20	A	978	G
20	A	981	A
20	A	982	G
20	A	983	U
20	A	985	A
20	A	986	G
20	A	993	A
20	A	997	A
20	A	999	A
20	A	1001	G
20	A	1006	G
20	A	1014	A
20	A	1016	G
20	A	1023	A

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Mol	Chain	Res	Type
20	A	1036	A
20	A	1048	A
20	A	1049	A
20	A	1051	A
20	A	1052	U
20	A	1053	A
20	A	1057	G
20	A	1061	A
20	A	1062	G
20	A	1063	U
20	A	1064	G
20	A	1065	G
20	A	1066	A
20	A	1073	U
20	A	1085	C
20	A	1086	A
20	A	1087	G
20	A	1093	U
20	A	1096	G
20	A	1097	A
20	A	1098	U
20	A	1100	U
20	A	1101	U
20	A	1103	G
20	A	1104	C
20	A	1105	U
20	A	1106	U
20	A	1107	A
20	A	1108	G
20	A	1109	A
20	A	1110	A
20	A	1111	G
20	A	1113	A
20	A	1114	G
20	A	1116	C
20	A	1117	A
20	A	1118	C
20	A	1120	A
20	A	1122	U
20	A	1123	U
20	A	1124	A
20	A	1125	A

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Mol	Chain	Res	Type
20	A	1127	G
20	A	1128	A
20	A	1129	G
20	A	1131	G
20	A	1132	C
20	A	1134	U
20	A	1135	A
20	A	1136	A
20	A	1137	U
20	A	1138	A
20	A	1139	G
20	A	1140	C
20	A	1141	U
20	A	1142	C
20	A	1143	A
20	A	1144	C
20	A	1146	A
20	A	1147	G
20	A	1148	U
20	A	1149	C
20	A	1151	A
20	A	1152	G
20	A	1157	C
20	A	1167	A
20	A	1168	A
20	A	1170	U
20	A	1171	G
20	A	1172	U
20	A	1174	C
20	A	1175	C
20	A	1179	G
20	A	1181	U
20	A	1182	A
20	A	1188	A
20	A	1190	U
20	A	1209	A
20	A	1212	A
20	A	1215	A
20	A	1216	G
20	A	1217	G
20	A	1218	U
20	A	1249	G

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Mol	Chain	Res	Type
20	A	1257	A
20	A	1275	G
20	A	1277	G
20	A	1287	G
20	A	1290	A
20	A	1292	U
20	A	1293	G
20	A	1294	C
20	A	1308	G
20	A	1309	A
20	A	1310	A
20	A	1311	A
20	A	1336	U
20	A	1337	A
20	A	1338	U
20	A	1349	U
20	A	1357	A
20	A	1365	U
20	A	1366	C
20	A	1375	G
20	A	1377	U
20	A	1388	U
20	A	1394	G
20	A	1396	G
20	A	1401	A
20	A	1404	G
20	A	1407	G
20	A	1411	G
20	A	1415	U
20	A	1420	A
20	A	1422	C
20	A	1428	G
20	A	1431	A
20	A	1432	U
20	A	1436	U
20	A	1439	A
20	A	1443	G
20	A	1446	G
20	A	1447	U
20	A	1448	U
20	A	1449	U
20	A	1450	U

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Mol	Chain	Res	Type
20	A	1451	U
20	A	1452	G
20	A	1453	U
20	A	1455	U
20	A	1456	G
20	A	1457	A
20	A	1461	A
20	A	1462	U
20	A	1463	G
20	A	1465	A
20	A	1469	A
20	A	1470	C
20	A	1471	G
20	A	1475	U
20	A	1488	G
20	A	1489	C
20	A	1492	G
20	A	1493	C
20	A	1494	G
20	A	1495	A
20	A	1497	U
20	A	1500	A
20	A	1501	A
20	A	1502	G
20	A	1503	U
20	A	1504	G
20	A	1505	C
20	A	1508	G
20	A	1509	U
20	A	1510	C
20	A	1519	G
20	A	1521	G
20	A	1525	U
20	A	1535	U
20	A	1536	A
20	A	1539	U
20	A	1548	C
20	A	1551	U
20	A	1552	A
20	A	1559	A
20	A	1560	G
20	A	1566	A

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Mol	Chain	Res	Type
20	A	1567	C
20	A	1568	G
20	A	1573	G
20	A	1576	A
20	A	1577	A
20	A	1579	U
20	A	1584	G
20	A	1585	U
20	A	1586	A
20	A	1589	G
20	A	1601	G
20	A	1604	A
20	A	1605	C
20	A	1606	A
20	A	1608	U
20	A	1612	A
20	A	1613	A
20	A	1615	A
20	A	1623	C
20	A	1627	U
20	A	1629	A
20	A	1630	G
20	A	1631	A
20	A	1632	A
20	A	1633	A
20	A	1634	A
20	A	1646	A
20	A	1650	U
20	A	1651	A
20	A	1653	A
20	A	1673	A
20	A	1674	G
20	A	1677	U
20	A	1689	A
20	A	1690	G
20	A	1691	C
20	A	1717	G
20	A	1718	C
20	A	1737	C
20	A	1741	A
20	A	1746	G
20	A	1756	U

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Mol	Chain	Res	Type
20	A	1757	U
20	A	1770	G
20	A	1776	A
20	A	1777	G
20	A	1778	G
20	A	1782	A
20	A	1784	G
20	A	1787	A
20	A	1790	G
20	A	1795	U
20	A	1798	A
20	A	1814	C
20	A	1815	A
20	A	1823	A
20	A	1829	A
20	A	1830	A
20	A	1840	C
20	A	1841	U
20	A	1842	G
20	A	1843	A
20	A	1872	G
20	A	1882	C
20	A	1886	G
20	A	1896	A
20	A	1913	A
20	A	1917	G
20	A	1920	G
20	A	1927	A
20	A	1928	C
20	A	1943	G
20	A	1944	G
20	A	1948	C
20	A	1952	A
20	A	1969	U
20	A	1970	U
20	A	1978	G
20	A	1979	C
20	A	1980	A
20	A	1981	C
20	A	1984	A
20	A	1985	A
20	A	1986	G

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Mol	Chain	Res	Type
20	A	1989	G
20	A	1990	U
20	A	1996	U
20	A	2005	U
20	A	2006	G
20	A	2007	U
20	A	2010	C
20	A	2030	U
20	A	2035	G
20	A	2036	U
20	A	2037	A
20	A	2039	C
20	A	2044	A
20	A	2045	A
20	A	2046	G
20	A	2047	A
20	A	2048	U
20	A	2057	C
20	A	2066	G
20	A	2069	C
20	A	2070	G
20	A	2074	A
20	A	2075	G
20	A	2076	A
20	A	2082	U
20	A	2083	G
20	A	2114	U
20	A	2115	G
20	A	2125	U
20	A	2126	A
20	A	2127	C
20	A	2129	G
20	A	2131	A
20	A	2132	U
20	A	2133	A
20	A	2134	G
20	A	2139	G
20	A	2140	A
20	A	2141	G
20	A	2144	G
20	A	2145	A
20	A	2146	U

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Mol	Chain	Res	Type
20	A	2147	G
20	A	2148	A
20	A	2154	G
20	A	2158	G
20	A	2159	C
20	A	2160	U
20	A	2162	G
20	A	2163	U
20	A	2173	G
20	A	2174	G
20	A	2175	C
20	A	2176	G
20	A	2179	G
20	A	2180	G
20	A	2182	G
20	A	2183	G
20	A	2187	A
20	A	2189	U
20	A	2196	G
20	A	2201	A
20	A	2206	C
20	A	2207	C
20	A	2212	A
20	A	2213	A
20	A	2217	G
20	A	2218	C
20	A	2224	U
20	A	2225	A
20	A	2227	U
20	A	2239	A
20	A	2252	G
20	A	2253	G
20	A	2280	A
20	A	2281	A
20	A	2282	A
20	A	2293	G
20	A	2296	G
20	A	2297	C
20	A	2301	A
20	A	2302	A
20	A	2318	G
20	A	2319	U

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Mol	Chain	Res	Type
20	A	2323	A
20	A	2327	C
20	A	2333	A
20	A	2334	A
20	A	2336	A
20	A	2337	G
20	A	2339	G
20	A	2341	A
20	A	2348	G
20	A	2349	A
20	A	2350	A
20	A	2361	C
20	A	2364	C
20	A	2367	G
20	A	2372	A
20	A	2379	G
20	A	2390	A
20	A	2393	G
20	A	2397	G
20	A	2398	G
20	A	2399	C
20	A	2404	U
20	A	2405	G
20	A	2406	A
20	A	2417	C
20	A	2420	C
20	A	2433	U
20	A	2436	C
20	A	2437	U
20	A	2439	A
20	A	2441	C
20	A	2442	G
20	A	2443	G
20	A	2445	U
20	A	2455	C
20	A	2462	A
20	A	2473	A
20	A	2488	C
20	A	2489	C
20	A	2508	G
20	A	2517	A
20	A	2518	U

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Mol	Chain	Res	Type
20	A	2519	G
20	A	2521	C
20	A	2534	C
20	A	2548	C
20	A	2549	G
20	A	2557	G
20	A	2561	U
20	A	2563	G
20	A	2570	C
20	A	2571	G
20	A	2580	A
20	A	2581	G
20	A	2586	A
20	A	2587	C
20	A	2596	G
20	A	2599	U
20	A	2600	C
20	A	2616	A
20	A	2622	G
20	A	2623	U
20	A	2624	C
20	A	2627	U
20	A	2628	A
20	A	2629	U
20	A	2631	C
20	A	2650	U
20	A	2660	C
20	A	2675	G
20	A	2677	G
20	A	2696	G
20	A	2703	U
20	A	2722	G
20	A	2727	U
20	A	2728	G
20	A	2735	A
20	A	2740	U
20	A	2746	G
20	A	2747	A
20	A	2749	G
20	A	2753	U
20	A	2762	A
20	A	2766	C

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Mol	Chain	Res	Type
20	A	2771	A
20	A	2778	A
20	A	2779	A
20	A	2780	G
20	A	2792	A
20	A	2793	U
20	A	2804	A
20	A	2805	U
20	A	2812	A
20	A	2813	A
20	A	2814	G
20	A	2831	G
20	A	2835	U
20	A	2836	G
20	A	2841	G
20	A	2844	A
20	A	2845	G
20	A	2846	A
20	A	2850	G
20	A	2854	G
20	A	2858	U
20	A	2868	G
20	A	2870	G
20	A	2878	G
20	A	2883	G
20	A	2891	C
20	A	2895	U
20	A	2897	G
20	A	2902	A
20	A	2904	G
21	B	8	G
21	B	10	G
21	B	13	A
21	B	14	G
21	B	23	A
21	B	24	U
21	B	33	U
21	B	40	C
21	B	42	G
21	B	51	A
21	B	54	U
21	B	55	A

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Mol	Chain	Res	Type
21	B	64	A
21	B	70	G
21	B	71	A
21	B	81	A
21	B	82	G
21	B	85	U
21	B	86	U
21	B	87	U
21	B	92	U
21	B	94	G
21	B	97	A
21	B	101	U
21	B	102	A
21	B	107	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	179	A
20	A	311	A
20	A	320	U
20	A	386	G
20	A	427	A
20	A	559	G
20	A	654	A
20	A	755	A
20	A	890	A
20	A	960	U
20	A	963	C
20	A	1502	G
20	A	1584	G
20	A	1585	U
20	A	1604	A
20	A	1605	C
20	A	1628	G
20	A	2281	A
20	A	2317	G
20	A	2773	G
21	B	32	U
21	B	101	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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
20	A	2
1	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	928:U	O3'	931:C	P	16.19
1	a	75:U	O3'	96:U	P	13.98
1	A	1579:U	O3'	1583:A	P	9.00

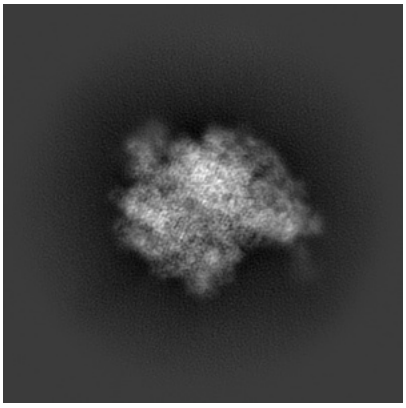
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0660. These allow visual inspection of the internal detail of the map and identification of artifacts.

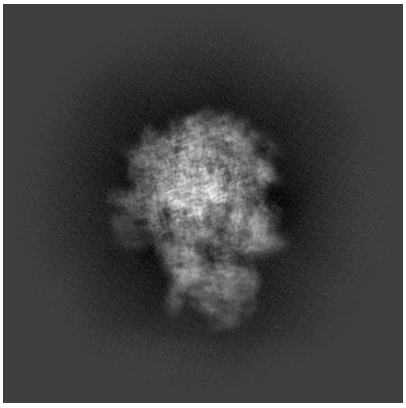
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

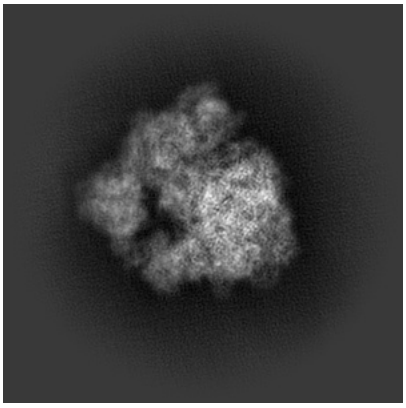
6.1.1 Primary map



X



Y

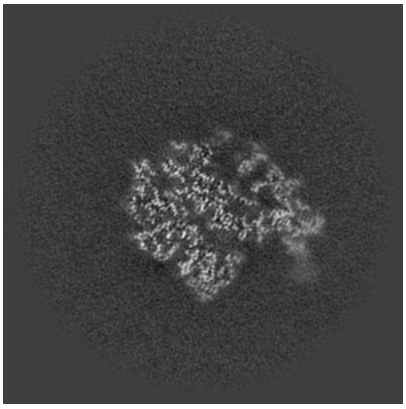


Z

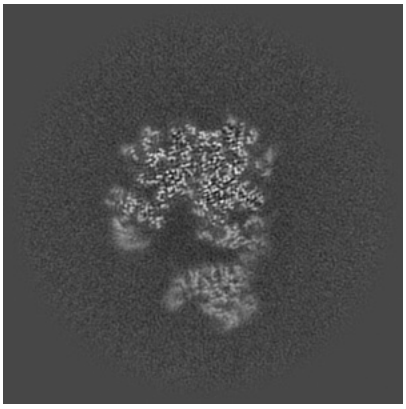
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

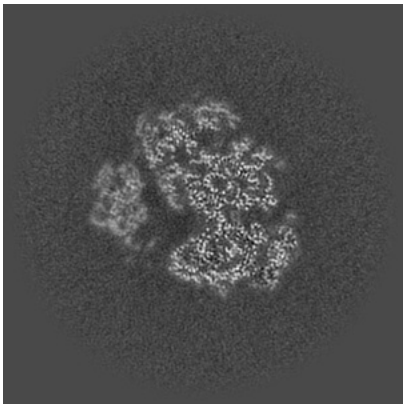
6.2.1 Primary map



X Index: 220



Y Index: 220

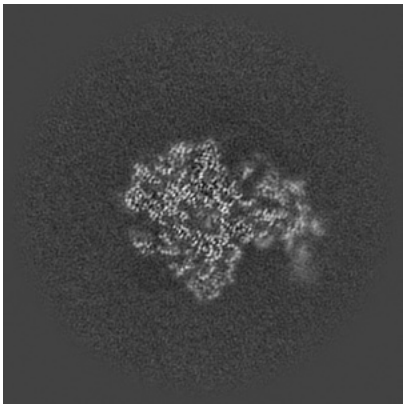


Z Index: 220

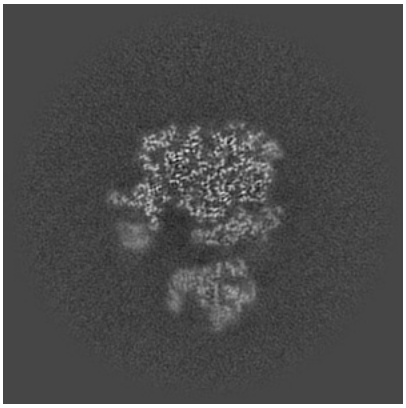
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

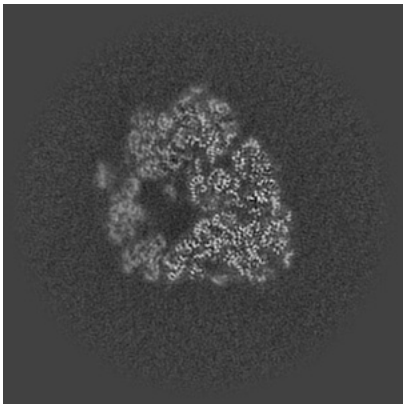
6.3.1 Primary map



X Index: 226



Y Index: 231

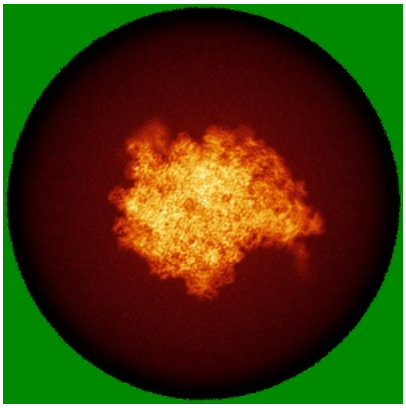


Z Index: 209

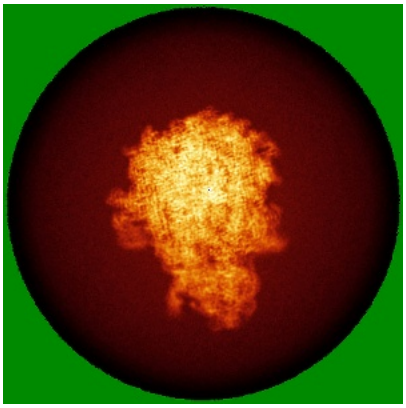
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

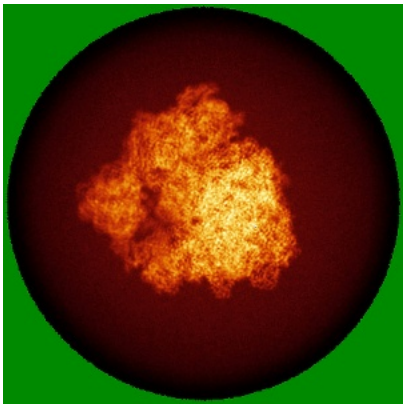
6.4.1 Primary map



X



Y

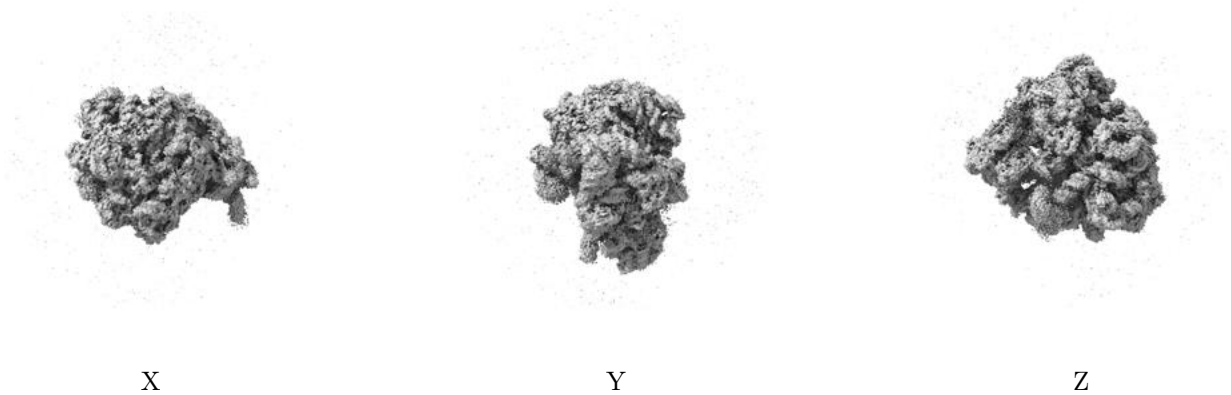


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.238. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

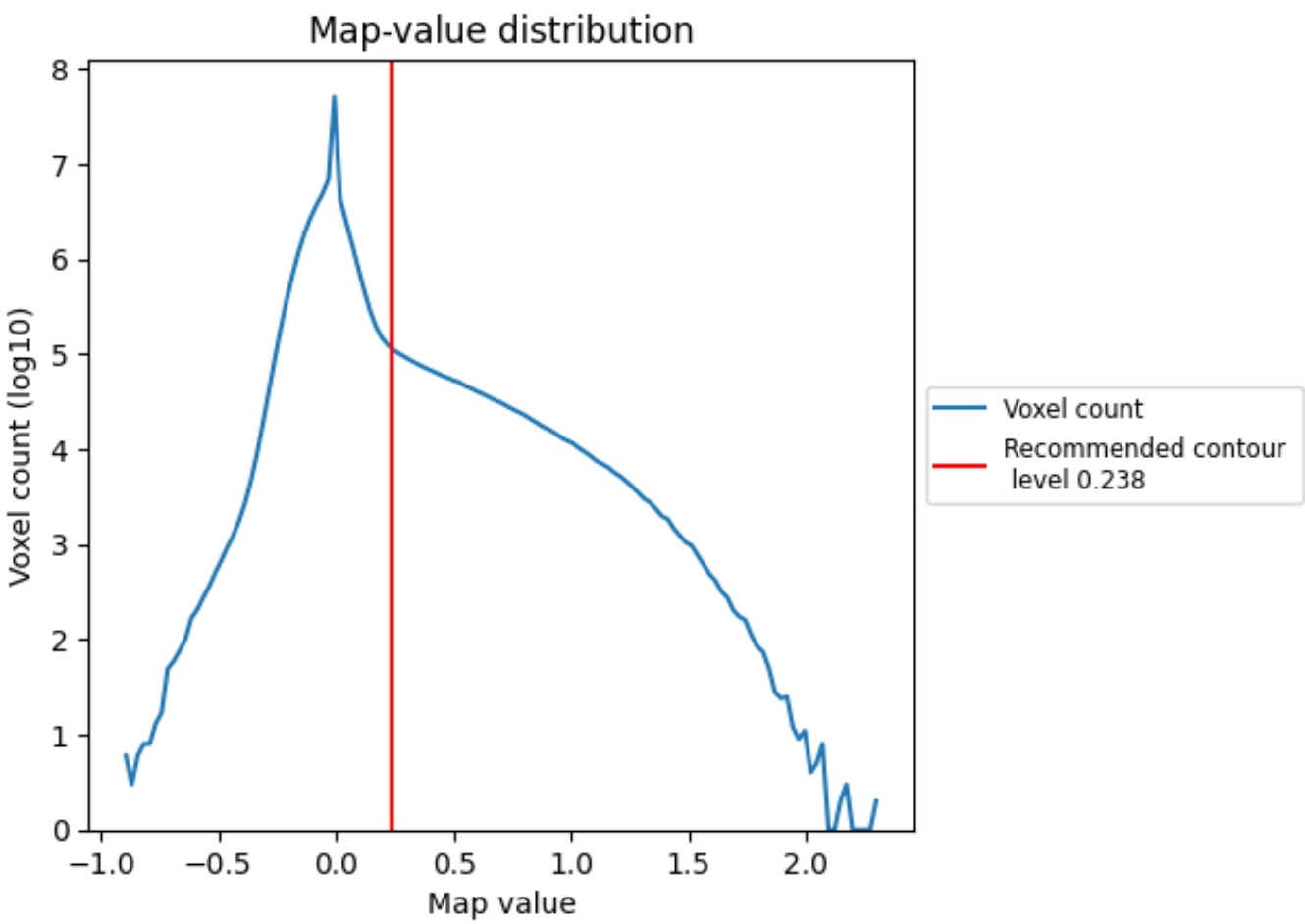
6.6 Mask visualisation (i)

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

7 Map analysis (i)

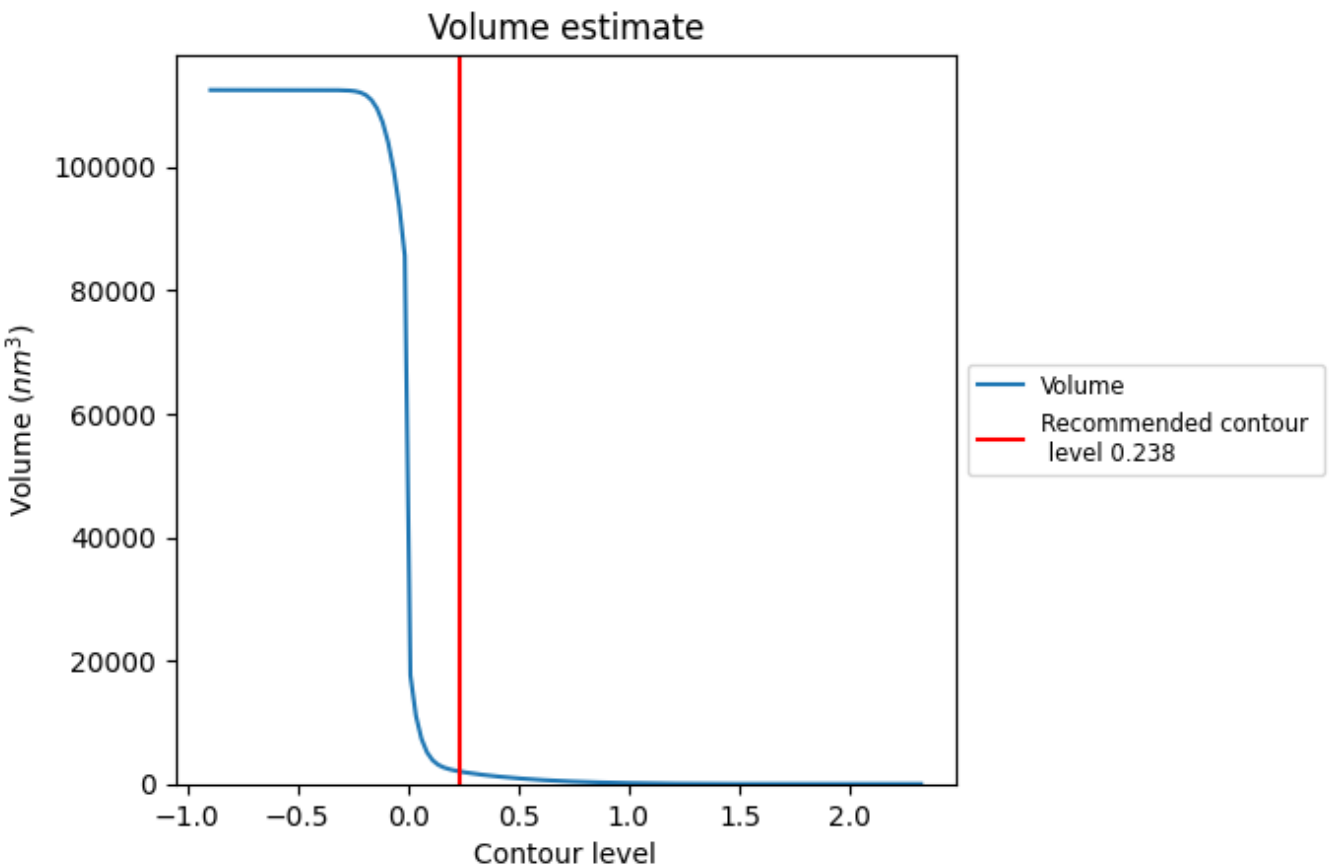
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

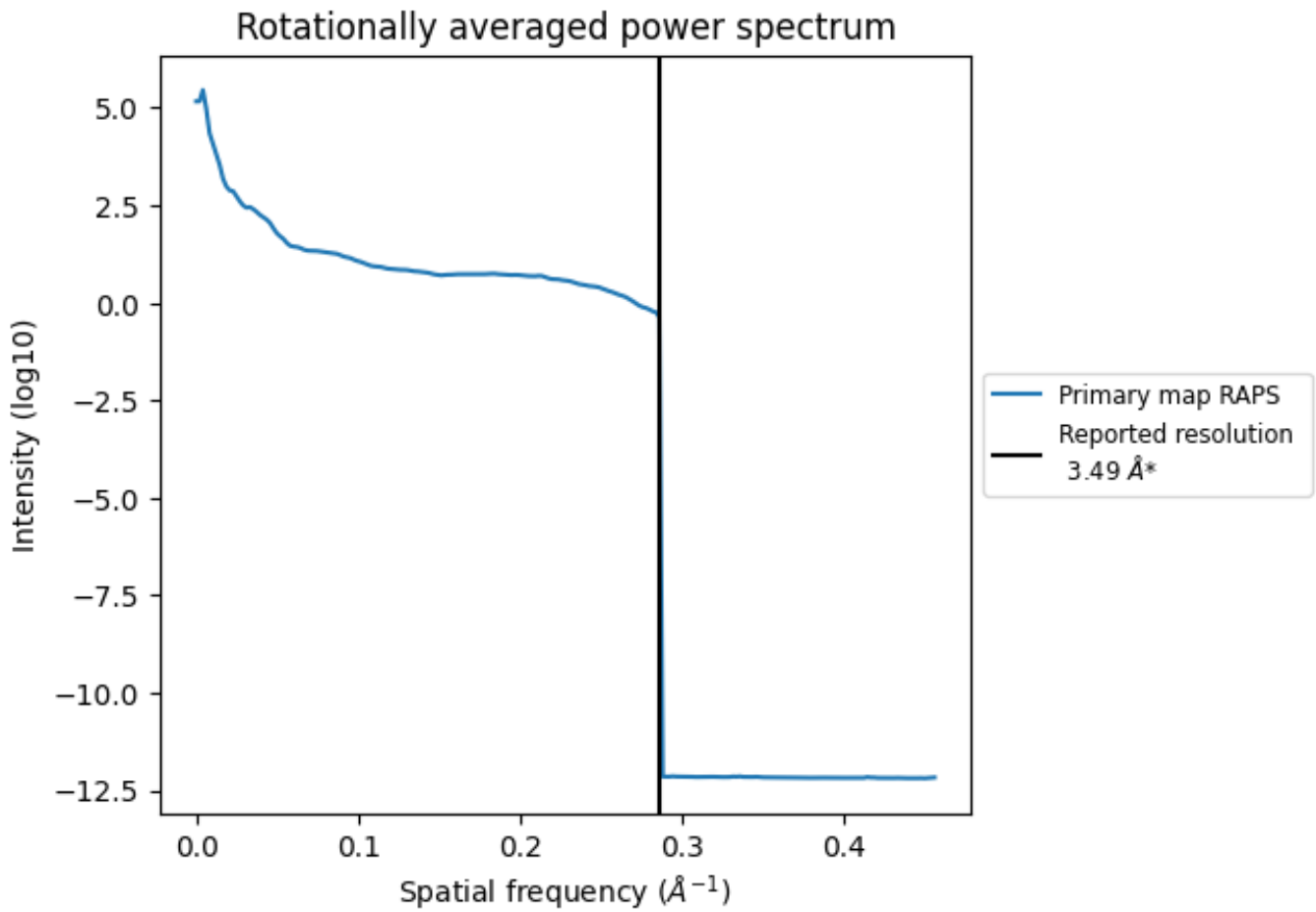
7.2 Volume estimate (i)



The volume at the recommended contour level is 2006 nm^3; this corresponds to an approximate mass of 1813 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 0.287 Å^{-1}

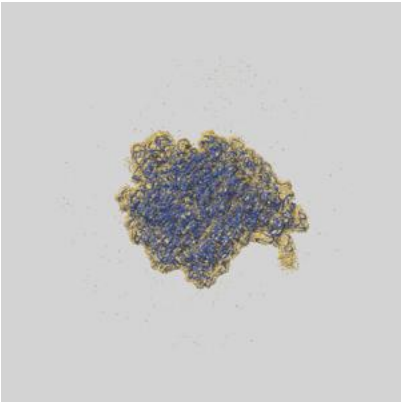
8 Fourier-Shell correlation (i)

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

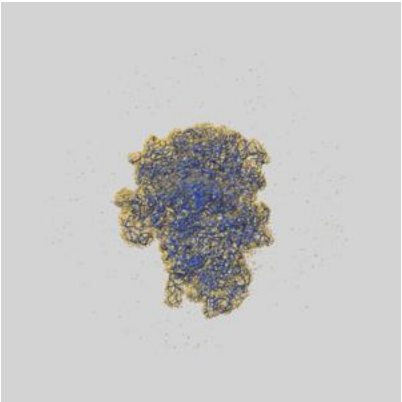
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0660 and PDB model 6O90. Per-residue inclusion information can be found in section 3 on page 13.

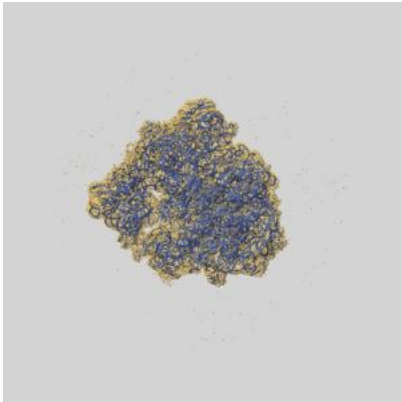
9.1 Map-model overlay (i)



X



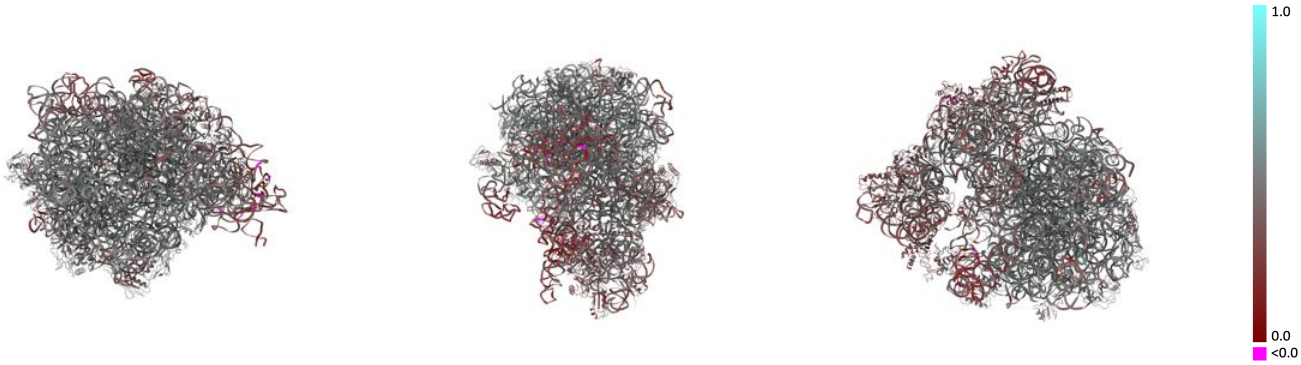
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.238 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.

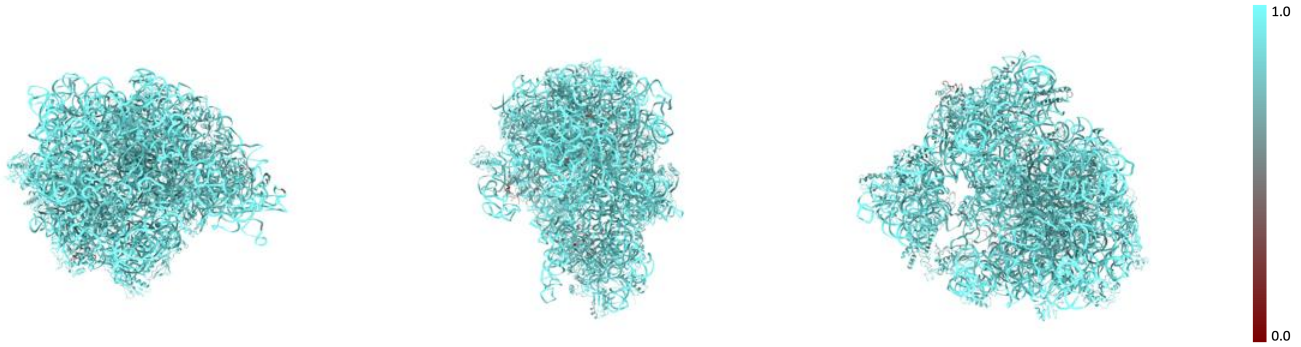
9.2 Q-score mapped to coordinate model (i)



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.

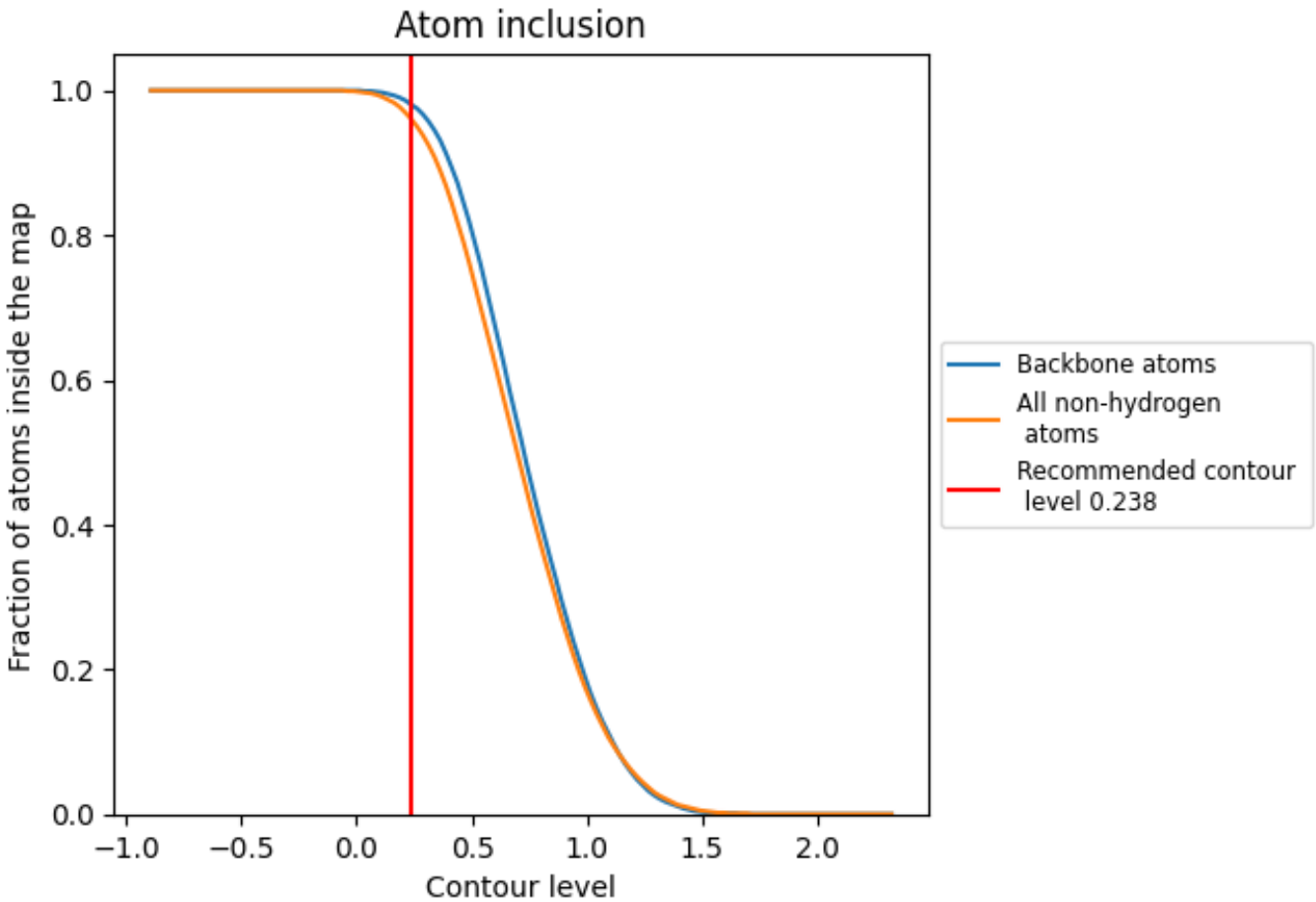
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.238).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.238) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9600	0.4280
0	0.9180	0.4660
1	0.8830	0.3050
2	0.9620	0.4940
3	0.9060	0.4700
4	0.9140	0.4700
5	0.9030	0.4930
6	0.9520	0.4820
A	0.9890	0.4580
B	0.9950	0.4200
C	0.9300	0.4780
D	0.9400	0.4980
E	0.9420	0.4690
F	0.8760	0.3670
G	0.9000	0.4090
K	0.9510	0.4820
L	0.9170	0.4930
M	0.9460	0.4790
N	0.8380	0.4370
O	0.9360	0.4670
P	0.8960	0.3990
Q	0.9260	0.4810
R	0.9260	0.4490
S	0.9160	0.4630
T	0.9340	0.4850
U	0.9190	0.4580
V	0.9000	0.4450
W	0.3410	0.2950
X	0.9280	0.4920
Y	0.9250	0.4820
Z	0.9290	0.4210
a	0.9910	0.3940
c	0.8900	0.3580
d	0.7230	0.2670
e	0.9010	0.4220

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Chain	Atom inclusion	Q-score
f	0.8800	0.3790
g	0.8730	0.3020
h	0.9220	0.4100
i	0.9380	0.3550
j	0.8740	0.3470
k	0.8780	0.3970
l	0.8400	0.3770
m	0.8740	0.2700
n	0.9430	0.3970
o	0.8810	0.3720
p	0.9020	0.3740
q	0.9030	0.4190
r	0.9100	0.3700
s	0.8850	0.3060
t	0.8160	0.3340