Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 01:33 PM JST

PDB ID	:	5X8T
EMDB ID	:	EMD-6711
Title	:	Structure of the 50S large subunit of chloroplast ribosome from spinach
Authors	:	Ahmed, T.; Shi, J.; Bhushan, S.
Deposited on	:	2017-03-03
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

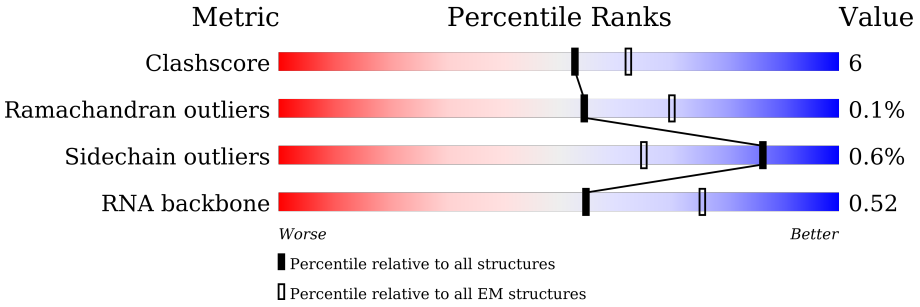
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	56	7%, 66%, 16%, 18%
2	2	65	34%, 58%, 18%, •, 22%
3	3	61	8%, 74%, 20%, 7%
4	4	73	•, 77%, 16%, • 5%
5	5	37	16%, 78%, 22%
6	6	142	11%, 29%, 6%, 65%
7	7	116	7%, 29%, 10%, 60%

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Mol	Chain	Length	Quality of chain
8	B	121	67% 23% 7%
9	C	271	14% 70% 21% 9%
10	D	221	9% 75% 21%
11	E	243	22% 65% 21% 14%
12	F	220	58% 62% 17% 20%
13	G	182	40% 77% 18% 5%
14	H	155	25% 26% 8% 66%
15	K	197	21% 77% 20%
16	L	121	26% 83% 17%
17	M	192	14% 81% 10% 8%
18	N	135	16% 74% 25%
19	O	116	11% 77% 23%
20	P	123	24% 67% 29%
21	Q	156	15% 53% 22% 24%
22	R	127	12% 62% 28% 9%
23	S	201	17% 58% 15% 27%
24	T	199	19% 59% 13% 28%
25	U	122	28% 60% 15% 25%
26	V	145	28% 59% 26% 14%
27	W	106	6% 50% 37% 9%
28	X	137	12% 58% 15% 27%
29	Y	77	12% 65% 30%
30	Z	109	37% 64% 17% 17%
31	A	2810	12% 61% 32% 6%
32	0	94	65% 57% 9% 32%

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 91714 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	1	46	378	250	70	58	0	0

- Molecule 2 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	51	415	258	83	70	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	57	445	268	103	71	3	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	69	563	353	119	90	1	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	37	304	186	70	44	4	0	0

- Molecule 6 is a protein called protein cL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	49	422	268	92	57	5	0	0

- Molecule 7 is a protein called protein cL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	46	368	237	71	59	1	0	0

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	B	117	2500	1116	452	815	117	0	0

- Molecule 9 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	247	1904	1181	390	327	6	0	0

- Molecule 10 is a protein called protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	212	1620	1025	295	289	11	0	0

- Molecule 11 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E	210	1655	1052	308	292	3	0	0

- Molecule 12 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	175	1351	862	233	248	8	0	0

- Molecule 13 is a protein called protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	173	1353	855	249	245	4	0	0

- Molecule 14 is a protein called protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	H	53	423	280	74	68	1	0	0

- Molecule 15 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	193	1568	1000	289	274	5	0	0

- Molecule 16 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L	121	942	588	179	170	5	0	0

- Molecule 17 is a protein called protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M	177	1342	836	264	236	6	0	0

- Molecule 18 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	134	1067	672	217	173	5	0	0

- Molecule 19 is a protein called protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	O	116	944	592	193	155	4	0	0

- Molecule 20 is a protein called protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P	120	947	589	183	170	5	0	0

- Molecule 21 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	118	953	610	186	156	1	0	0

- Molecule 22 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	115	996	633	208	153	2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	S	147	1171	759	202	210	0	0

- Molecule 24 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	T	144	1149	731	210	200	8	0	0

- Molecule 25 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	U	92	740	477	129	132	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	V	124	993	624	187	180	2	0	0

- Molecule 27 is a RNA chain called 4.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
27	W	102	2187	977	403	705	102	0	0

- Molecule 28 is a protein called protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	X	100	810	511	159	140	0	0

- Molecule 29 is a protein called protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	74	605	385	121	98	1	0	0

- Molecule 30 is a protein called protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	90	754	470	150	131	3	0	0

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	A	2809	60324	26912	11166	19437	2809	0	0

- Molecule 32 is a protein called 50S ribosomal protein L31.

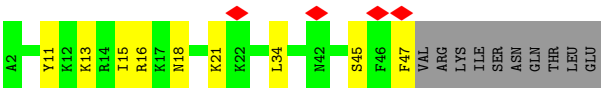
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	0	64	521	330	89	100	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

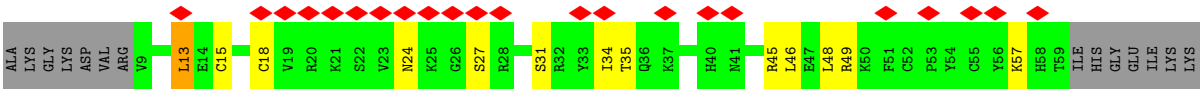
- Molecule 1: 50S ribosomal protein L32, chloroplastic

Chain 1:



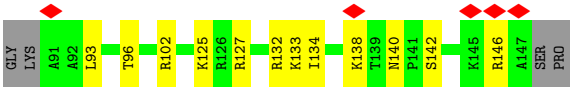
- Molecule 2: 50S ribosomal protein L33, chloroplastic

Chain 2:



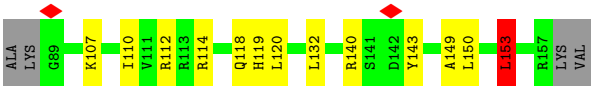
- Molecule 3: 50S ribosomal protein L34, chloroplastic

Chain 3:



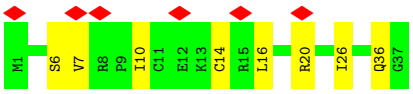
- Molecule 4: 50S ribosomal protein L35, chloroplastic

Chain 4:



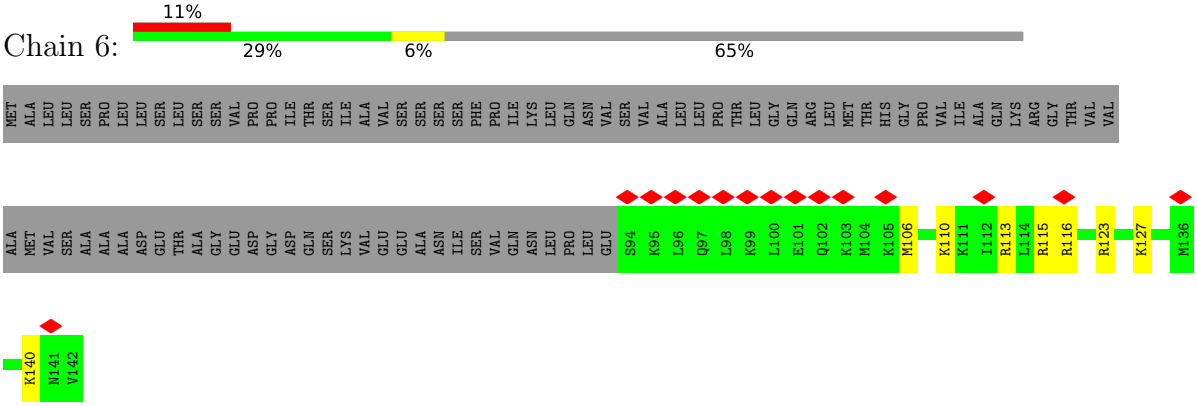
- Molecule 5: 50S ribosomal protein L36, chloroplastic

Chain 5:



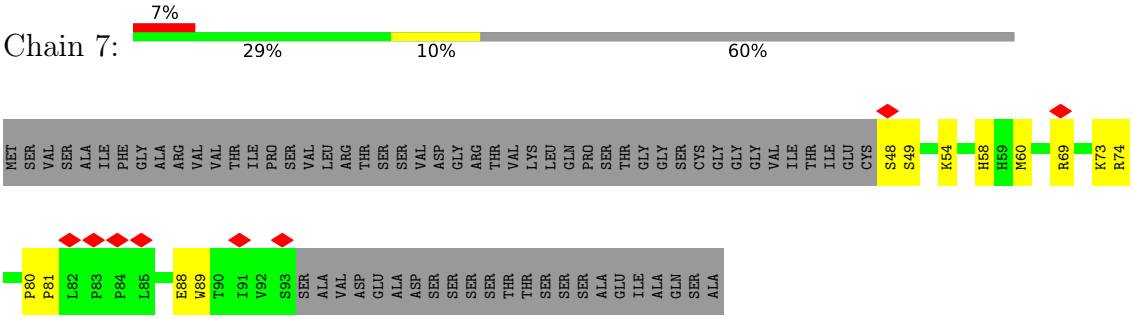
- Molecule 6: protein cL37

Chain 6:



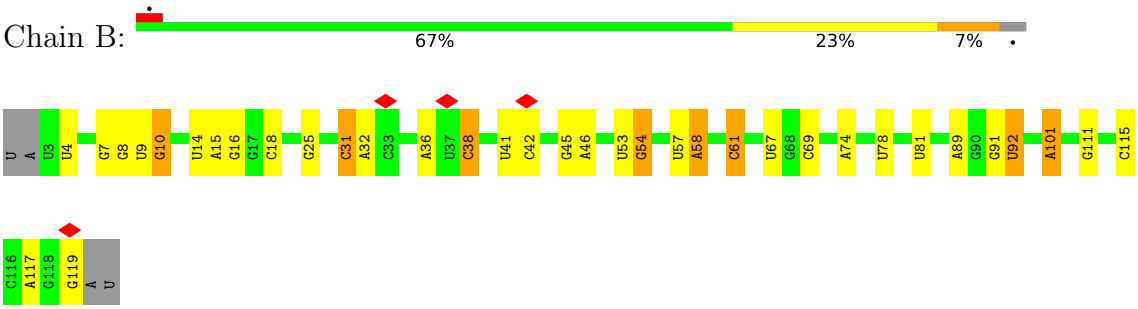
- Molecule 7: protein cL38

Chain 7:



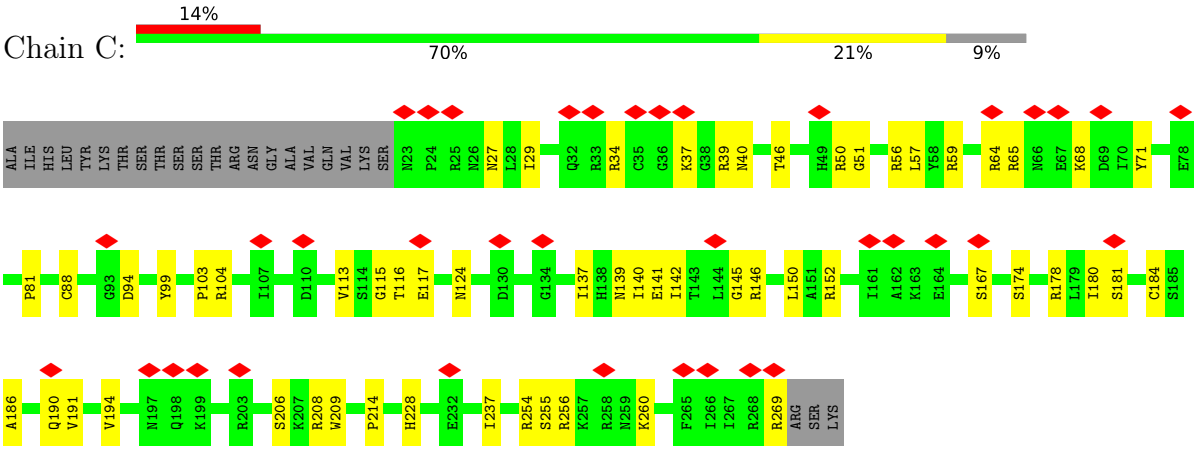
- Molecule 8: 5S rRNA

Chain B:



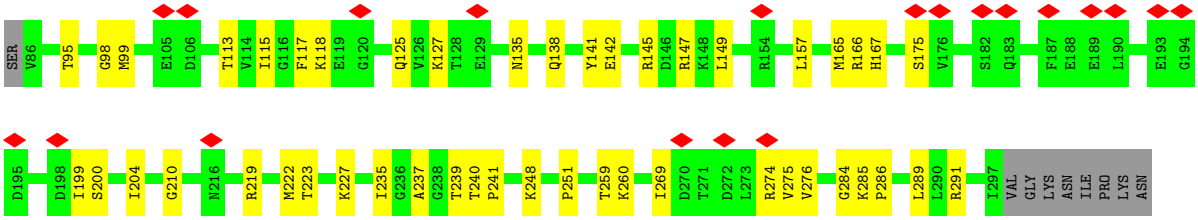
- Molecule 9: 50S ribosomal protein L2, chloroplastic

Chain C:



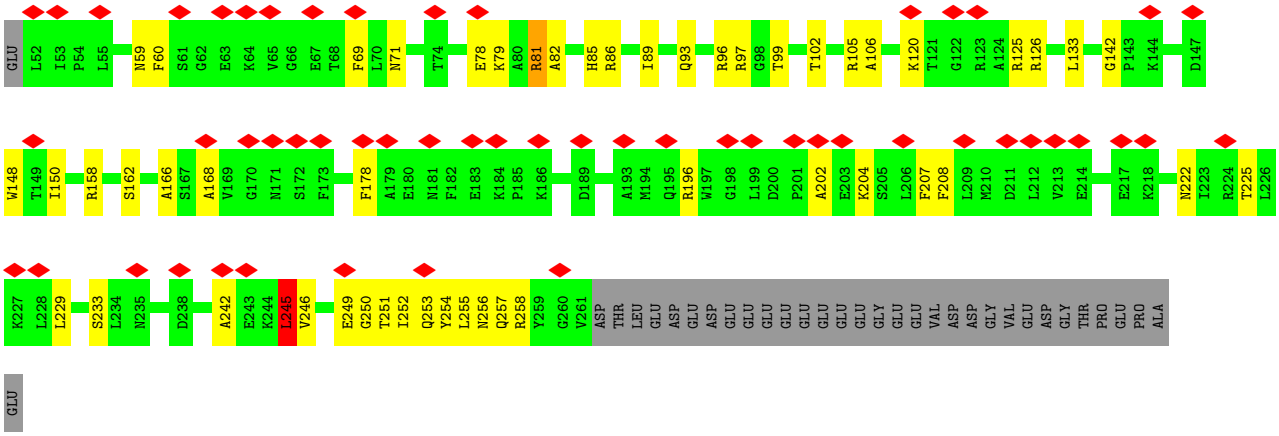
• Molecule 10: protein L3

Chain D:



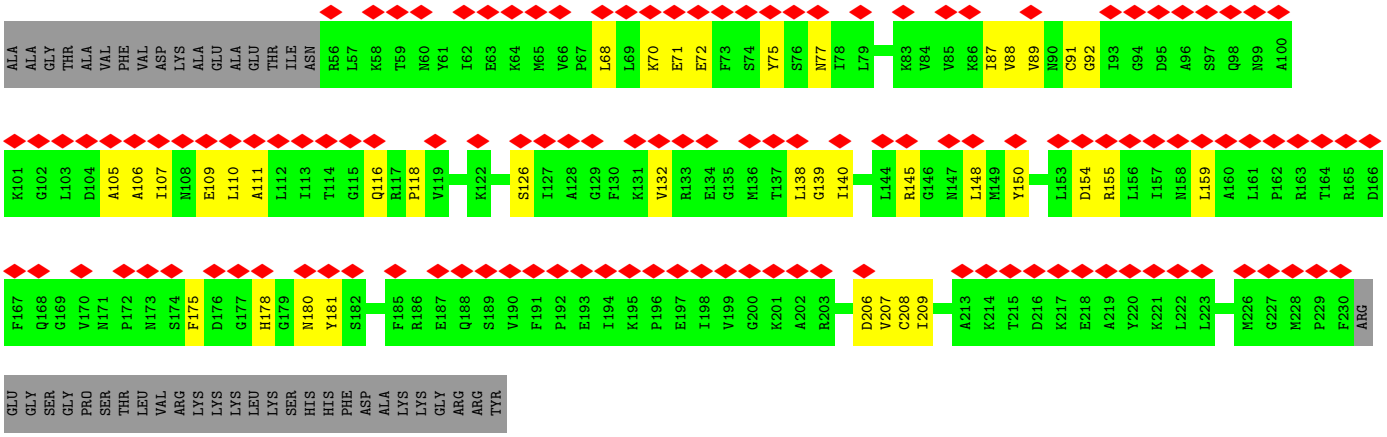
• Molecule 11: 50S ribosomal protein L4, chloroplastic

Chain E:



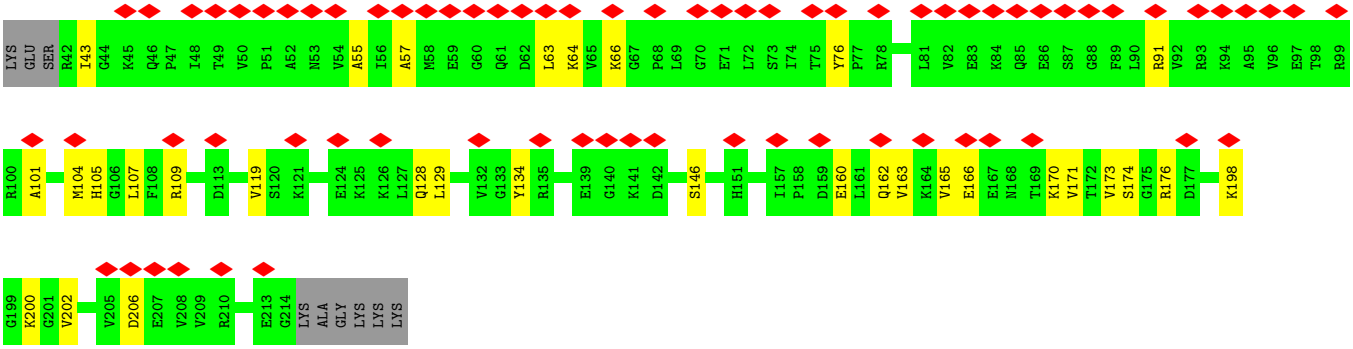
• Molecule 12: 50S ribosomal protein L5, chloroplastic

Chain F:



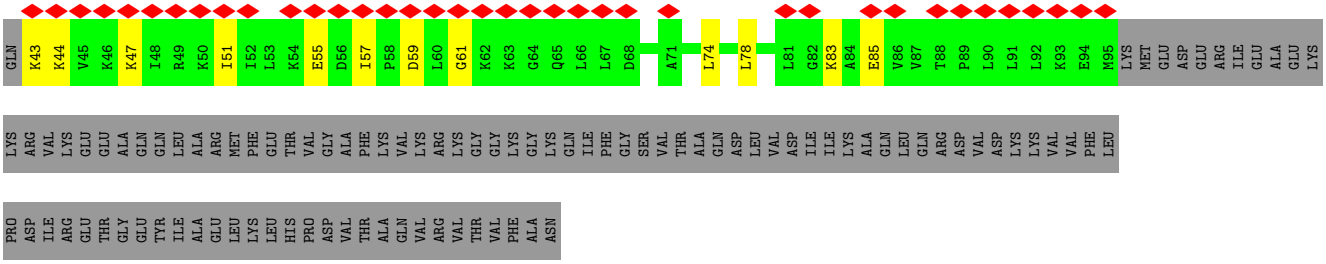
• Molecule 13: protein L6

Chain G:



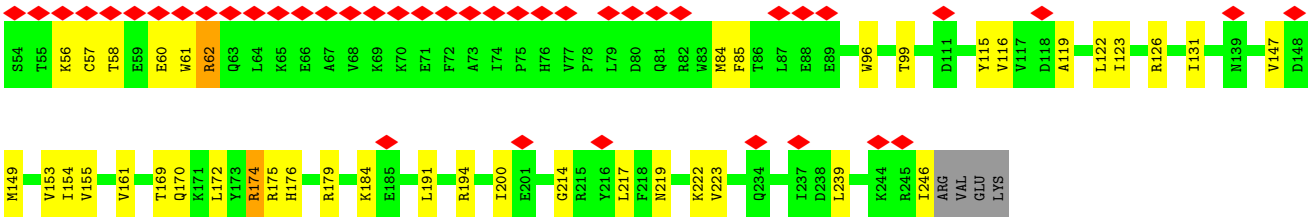
- Molecule 14: protein L9

Chain H:



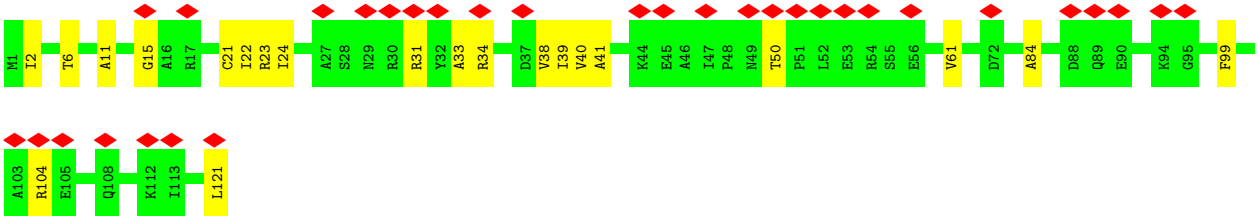
- Molecule 15: 50S ribosomal protein L13, chloroplastic

Chain K:



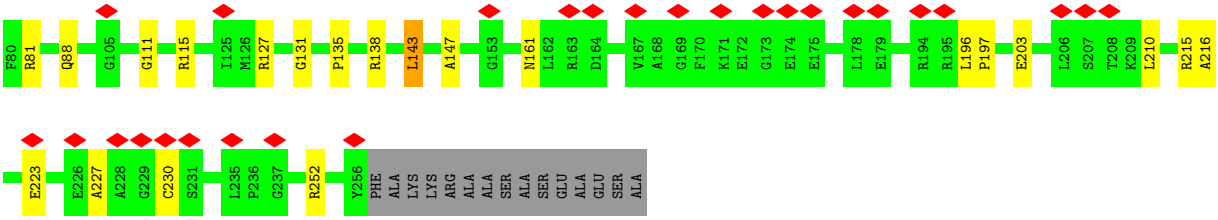
- Molecule 16: 50S ribosomal protein L14, chloroplastic

Chain L:



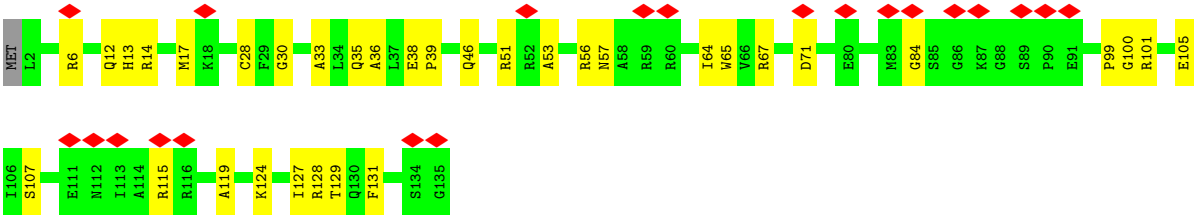
- Molecule 17: protein L15

Chain M:



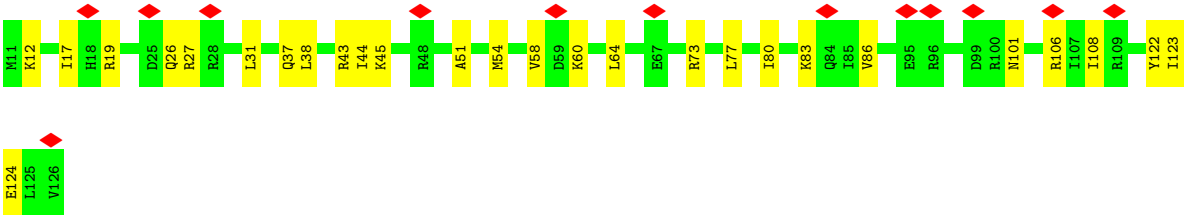
- Molecule 18: 50S ribosomal protein L16, chloroplastic

Chain N:



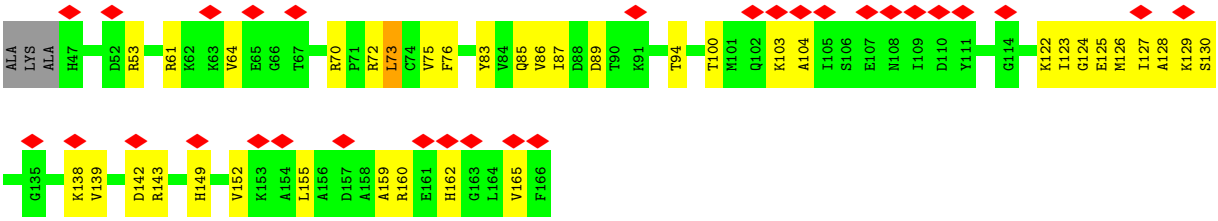
- Molecule 19: protein L17

Chain O:



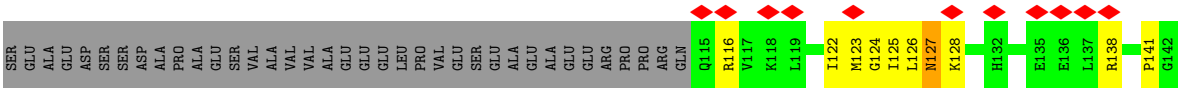
- Molecule 20: protein L18

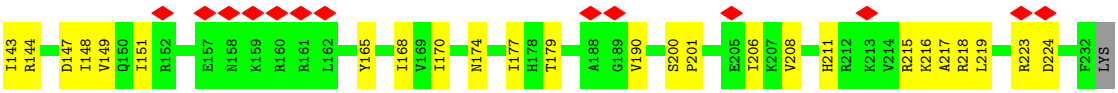
Chain P:



- Molecule 21: 50S ribosomal protein L19, chloroplastic

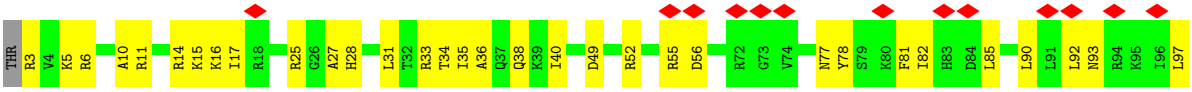
Chain Q:

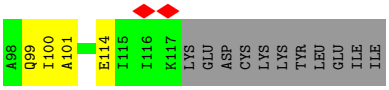




- Molecule 22: 50S ribosomal protein L20, chloroplastic

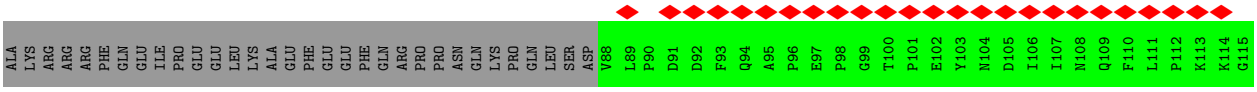
Chain R:

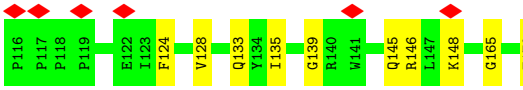


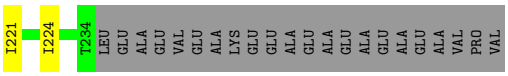


- Molecule 23: 50S ribosomal protein L21, chloroplastic

Chain S:

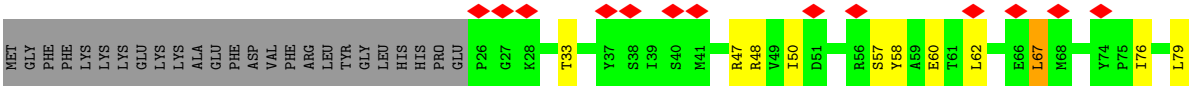


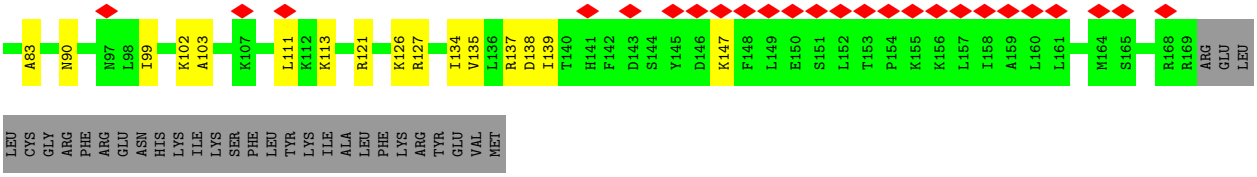




- Molecule 24: 50S ribosomal protein L22, chloroplastic

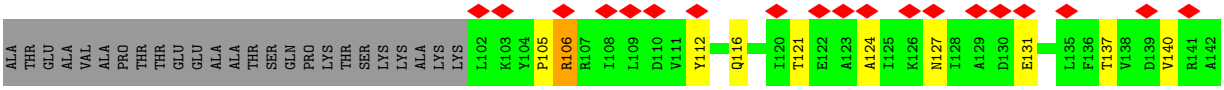
Chain T:

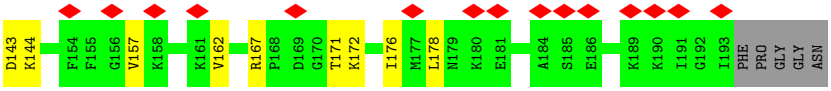




- Molecule 25: 50S ribosomal protein L23, chloroplastic

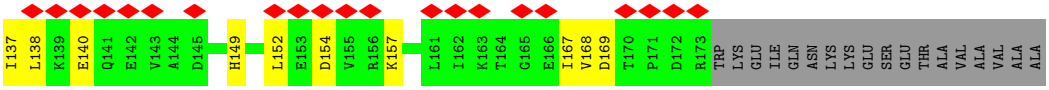
Chain U:





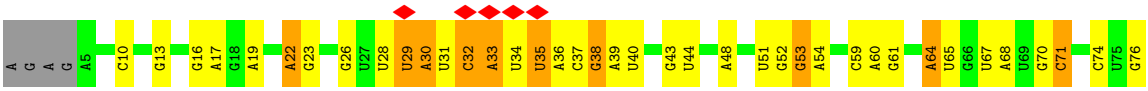
- Molecule 26: 50S ribosomal protein L24, chloroplastic

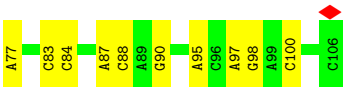
Chain V:



- Molecule 27: 4.8S rRNA

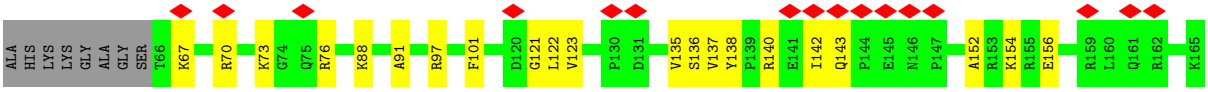
Chain W:





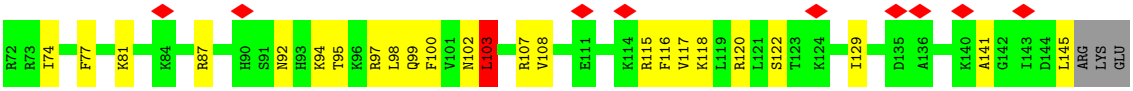
- Molecule 28: protein L27

Chain X:



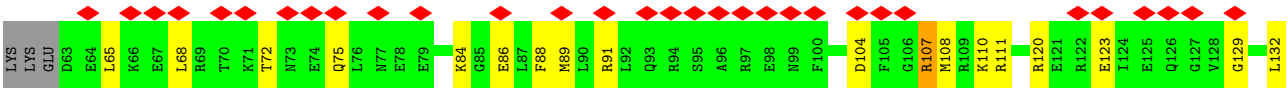
- Molecule 29: protein L28

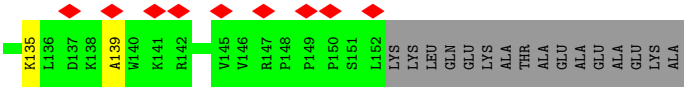
Chain Y:



- Molecule 30: protein L29

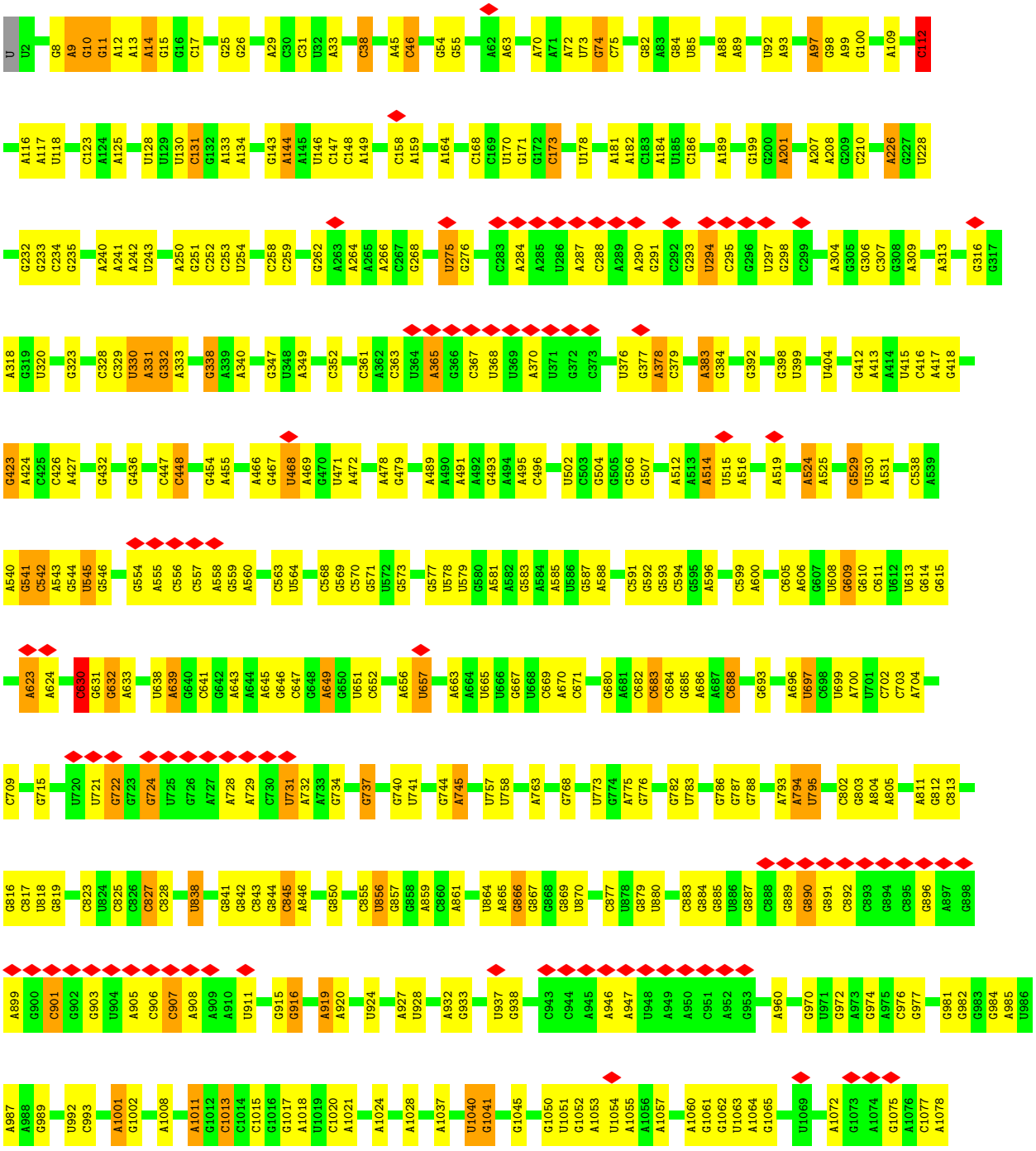
Chain Z:

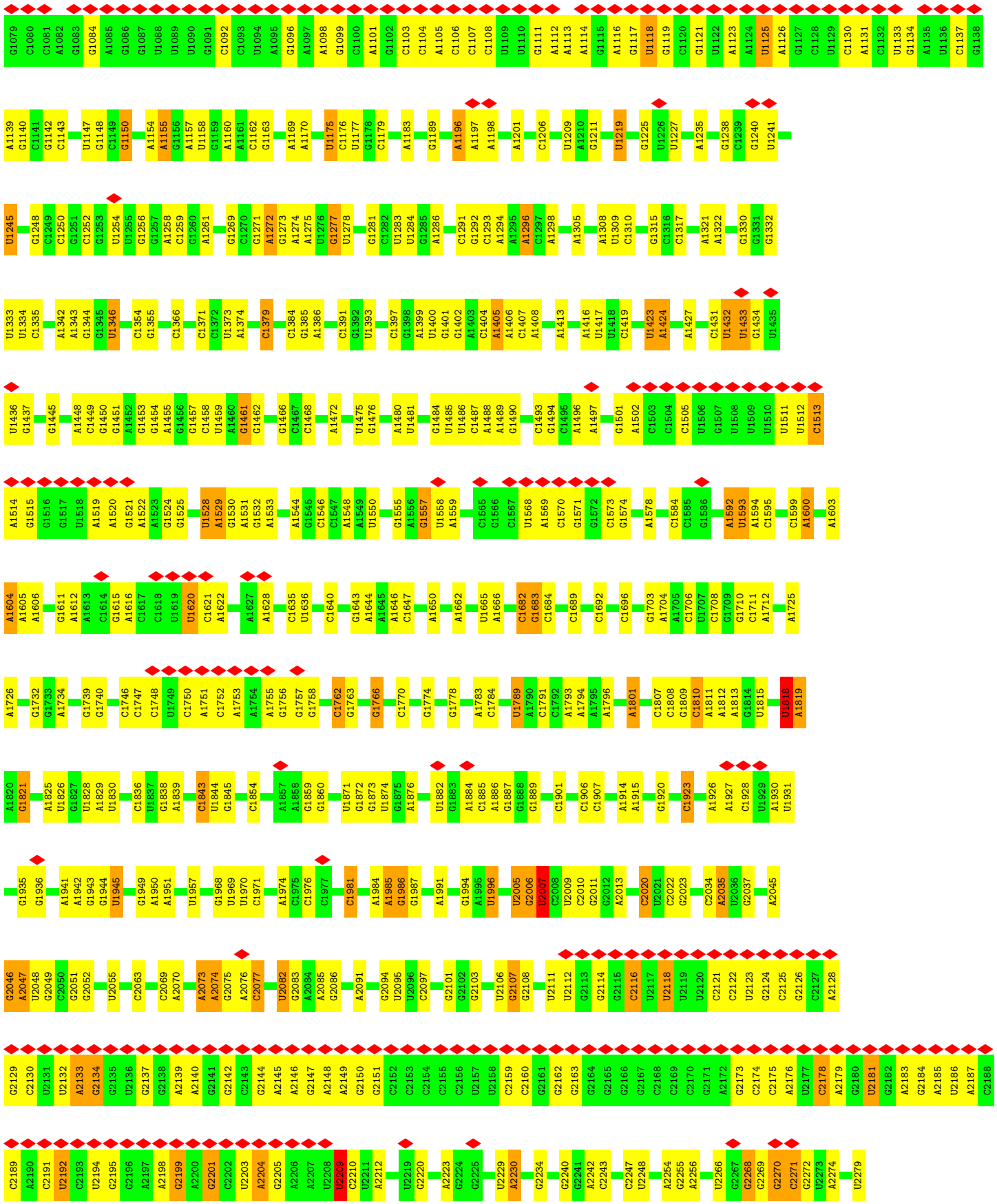


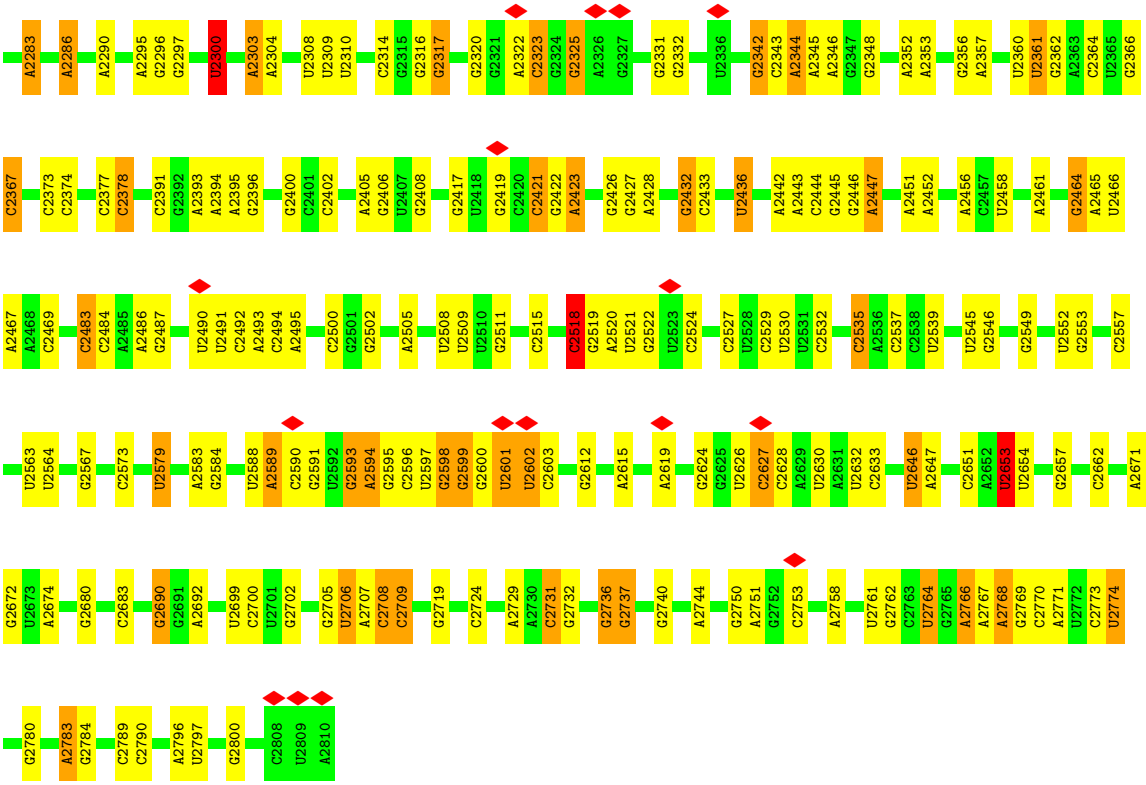


• Molecule 31: 23S rRNA

Chain A:

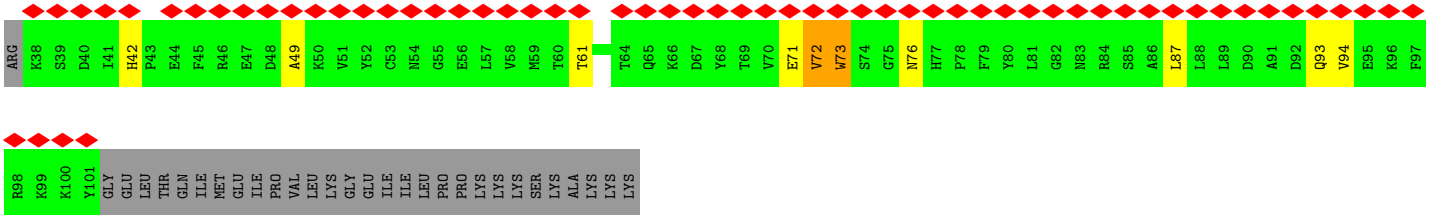



G1079 C1080 C1081 A1082 G1083 G1084 A1085 G1086 G1087 U1088 U1089 U1090 G1091 C1092 C1093 U1094 A1095 G1096 A1097 A1098 G1099 C1100 A1101 G1102 C1103 C1104 A1105 C1106 C1107 C1108 U1109 U1110 G1111 A1112 A1113 A1114 G1115 A1116 G1117 U1118 G1119 C1120 G1121 U1122 A1123 A1124 U1125 A1126 G1127 C1128 U1129 C1130 A1131 C1132 U1133 G1134 A1135 U1136 C1137 G1138
A1139 G1140 C1141 G1142 C1143 U1147 G1148 C1149 G1150 A1154 A1155 G1156 A1157 U1158 G1159 A1160 A1161 C1162 G1163 A1169 A1170 U1175 C1176 U1177 G1178 C1179 A1183 G1189 A1196 A1197 A1198 A1201 C1206 U1209 A1210 G1211 U1219 G1225 U1226 U1227 A1235 G1238 C1239 G1240 U1241
U1245 G1248 C1249 C1250 G1251 C1252 G1253 U1254 U1255 G1256 G1257 A1258 C1259 G1260 A1261 G1269 C1270 G1271 A1272 G1273 A1274 A1275 U1276 G1277 U1278 G1281 C1282 U1283 U1284 G1285 A1286 C1291 G1292 C1293 A1294 A1295 A1296 C1297 A1298 A1305 A1308 U1309 C1310 G1315 C1316 C1317 A1321 A1322 G1330 G1331 G1332
U1333 U1334 C1335 A1342 A1343 G1344 G1345 U1346 C1354 G1355 C1366 C1371 C1372 U1373 A1374 C1379 C1384 G1385 A1386 C1391 G1392 U1393 C1397 G1398 A1399 U1400 G1401 G1402 A1403 C1404 A1405 A1406 C1407 A1408 A1413 A1416 U1417 U1418 C1419 U1423 A1424 A1427 C1431 U1432 U1433 G1434 U1435
U1436 G1437 G1445 A1448 C1449 G1450 G1451 A1452 G1453 G1454 A1455 G1456 G1457 C1458 U1459 A1460 G1461 G1462 G1466 C1467 C1468 A1472 U1475 G1476 A1480 U1481 G1484 U1485 U1486 C1487 A1488 A1489 G1490 C1493 G1494 C1495 A1496 A1497 G1501 A1502 C1503 C1504 C1505 U1506 G1507 U1508 U1509 U1510 U1511 U1512 C1513
A1514 G1515 G1516 G1517 U1518 A1519 A1520 G1521 A1522 A1523 G1524 G1525 U1528 A1529 G1530 A1531 G1532 A1533 A1544 G1545 C1546 C1547 A1548 A1549 U1550 G1555 A1556 G1557 U1558 A1559 C1565 G1566 C1567 U1568 A1569 C1570 G1571 G1572 C1573 G1574 A1578 C1584 C1585 G1586 A1592 U1593 A1594 C1595 C1599 A1600 A1603
A1604 A1605 A1606 G1611 A1612 A1613 C1614 G1615 A1616 C1617 C1618 U1619 U1620 C1621 A1622 A1627 A1628 C1635 U1636 C1640 G1643 A1644 A1645 A1646 C1647 A1650 A1662 U1665 A1666 C1682 G1683 C1684 C1689 C1692 C1696 G1703 A1704 A1705 C1706 U1707 C1708 G1709 G1710 C1711 A1712 A1725
A1726 G1732 G1733 A1734 G1739 G1740 C1746 C1747 C1748 U1749 C1750 A1751 C1752 A1753 A1754 A1755 G1756 G1757 G1758 C1762 G1763 G1766 C1770 G1774 G1778 A1783 C1784 U1789 A1790 C1791 C1792 A1793 A1794 A1795 A1796 A1801 C1807 C1808 G1809 C1810 A1811 A1812 A1813 G1814 U1815 U1818 A1819
A1820 G1821 A1825 U1826 G1827 U1828 A1829 U1830 C1836 U1837 G1838 A1839 C1843 U1844 G1845 C1854 A1857 A1858 G1859 G1860 U1871 G1872 G1873 U1874 G1875 A1876 U1882 G1883 A1884 C1885 A1886 G1887 G1888 G1889 C1901 C1906 C1907 A1914 A1915 G1920 C1923 A1926 A1927 C1928 U1929 A1930 U1931
G1935 G1936 A1941 A1942 G1943 G1944 U1945 G1949 A1950 A1951 U1957 G1968 U1969 U1970 C1971 A1974 G1975 C1976 C1977 C1981 A1984 A1985 G1986 G1987 A1991 G1994 A1995 U1996 U2005 G2006 U2007 C2008 U2009 C2010 G2011 G2012 A2013 C2020 U2021 C2022 G2023 C2034 A2035 U2036 G2037 A2045
G2046 A2047 U2048 G2049 C2050 G2051 G2052 U2055 C2063 C2069 A2070 A2073 A2074 G2075 A2076 C2077 U2082 G2083 A2084 A2085 G2086 A2091 G2094 U2095 U2096 C2097 G2101 G2102 G2103 U2106 G2107 G2108 U2111 U2112 G2113 G2114 G2115 C2116 U2117 U2118 U2119 U2120 C2121 C2122 U2123 G2124 C2125 G2126 C2127 A2128
G2129 C2130 U2131 U2132 A2133 G2134 G2135 U2136 G2137 G2138 A2139 A2140 G2141 G2142 C2143 G2144 A2145 A2146 A2147 A2148 A2149 G2150 G2151 C2152 C2153 C2154 C2155 C2156 U2157 U2158 C2159 C2160 G2161 G2162 G2163 G2164 G2165 G2166 G2167 C2168 C2169 C2170 G2171 A2172 G2173 C2174 C2175 A2176 U2177 C2178 A2179 G2180 U2181 G2182 A2183 G2184 A2185 U2186 A2187 C2188
C2189 A2190 C2191 U2192 C2193 U2194 G2195 G2196 A2197 A2198 G2199 A2200 G2201 C2202 U2203 A2204 G2205 A2206 A2207 U2208 U2209 C2210 U2211 A2212 U2219 G2220 A2223 G2224 G2225 U2229 A2230 G2234 G2240 G2241 A2242 C2243 C2247 U2248 A2254 G2255 A2256 U2266 G2267 G2268 G2269 G2270 C2271 G2272 U2273 A2274 U2279



- Molecule 32: 50S ribosomal protein L31

Chain 0:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81305	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	133333	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.644	Depositor
Minimum map value	-0.445	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.27	0/387	0.51	0/513
2	2	0.32	0/422	0.75	1/564 (0.2%)
3	3	0.27	0/447	0.66	1/588 (0.2%)
4	4	0.30	0/569	0.66	1/752 (0.1%)
5	5	0.30	0/306	0.67	0/403
6	6	0.25	0/425	0.46	0/551
7	7	0.28	0/382	0.54	0/520
8	B	0.31	0/2796	1.05	12/4357 (0.3%)
9	C	0.29	0/1938	0.64	0/2603
10	D	0.31	0/1646	0.65	0/2201
11	E	0.31	0/1687	0.65	1/2271 (0.0%)
12	F	0.28	0/1372	0.61	0/1848
13	G	0.26	0/1374	0.55	1/1849 (0.1%)
14	H	0.26	0/427	0.59	0/568
15	K	0.28	0/1608	0.57	2/2174 (0.1%)
16	L	0.31	0/951	0.59	0/1282
17	M	0.28	0/1361	0.53	0/1806
18	N	0.31	0/1089	0.61	0/1461
19	O	0.28	0/959	0.61	0/1280
20	P	0.26	0/963	0.55	1/1293 (0.1%)
21	Q	0.31	0/967	0.71	2/1300 (0.2%)
22	R	0.33	0/1013	0.61	0/1351
23	S	0.31	0/1199	0.61	0/1633
24	T	0.29	0/1168	0.60	1/1566 (0.1%)
25	U	0.27	0/749	0.58	0/1006
26	V	0.27	0/1006	0.64	1/1343 (0.1%)
27	W	0.35	0/2449	1.07	9/3817 (0.2%)
28	X	0.30	0/825	0.57	0/1099
29	Y	0.28	0/615	0.65	2/819 (0.2%)
30	Z	0.27	0/762	0.57	0/1012
31	A	0.35	1/67572 (0.0%)	1.05	303/105421 (0.3%)
32	0	0.29	0/533	0.66	1/718 (0.1%)
All	All	0.33	1/99967 (0.0%)	0.96	339/149969 (0.2%)

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
17	M	0	1
21	Q	0	1
23	S	0	1
32	0	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	2447	A	N9-C4	5.09	1.41	1.37

All (339) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	2077	C	N1-C2-O2	11.06	125.54	118.90
31	A	2077	C	C2-N1-C1'	10.63	130.49	118.80
31	A	1747	C	N3-C2-O2	-9.95	114.94	121.90
31	A	2314	C	C2-N1-C1'	9.82	129.60	118.80
31	A	2314	C	N1-C2-O2	9.47	124.58	118.90
31	A	2662	C	N1-C2-O2	9.29	124.47	118.90
31	A	2077	C	C6-N1-C2	-9.23	116.61	120.30
31	A	2077	C	N3-C2-O2	-9.10	115.53	121.90
31	A	2268	G	C4-N9-C1'	8.91	138.08	126.50
31	A	294	U	N1-C2-O2	8.85	128.99	122.80
31	A	1334	U	C2-N1-C1'	8.85	128.32	117.70
31	A	1334	U	N1-C2-O2	8.71	128.90	122.80
31	A	2314	C	C6-N1-C2	-8.71	116.82	120.30
8	B	61	C	N1-C2-O2	8.57	124.05	118.90
31	A	46	C	N1-C2-O2	8.53	124.02	118.90
31	A	2662	C	C2-N1-C1'	8.49	128.15	118.80
31	A	2709	C	N3-C2-O2	-8.32	116.08	121.90
31	A	1784	C	N3-C2-O2	-8.32	116.08	121.90
31	A	1923	C	N3-C2-O2	-8.29	116.09	121.90
31	A	294	U	N3-C2-O2	-8.26	116.42	122.20
31	A	1334	U	N3-C2-O2	-8.18	116.47	122.20
31	A	1843	C	N3-C2-O2	-8.17	116.18	121.90
29	Y	103	LEU	CA-CB-CG	8.14	134.02	115.30
31	A	1970	U	N1-C2-O2	8.11	128.48	122.80

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	1283	U	N3-C2-O2	-8.05	116.57	122.20
21	Q	224	ASP	CB-CG-OD1	8.03	125.53	118.30
31	A	294	U	C2-N1-C1'	8.01	127.31	117.70
31	A	1970	U	N3-C2-O2	-7.99	116.61	122.20
31	A	2268	G	C8-N9-C1'	-7.84	116.81	127.00
31	A	112	C	N1-C2-O2	7.82	123.59	118.90
31	A	2314	C	N3-C2-O2	-7.68	116.52	121.90
8	B	69	C	N1-C2-O2	7.60	123.46	118.90
31	A	1818	U	C2-N1-C1'	7.58	126.80	117.70
31	A	1784	C	N1-C2-O2	7.56	123.44	118.90
31	A	448	C	N1-C2-O2	7.54	123.43	118.90
31	A	1013	C	N1-C2-O2	7.54	123.42	118.90
31	A	2683	C	N1-C2-O2	7.44	123.37	118.90
31	A	168	C	N1-C2-O2	7.43	123.36	118.90
31	A	38	C	N1-C2-O2	7.36	123.31	118.90
4	4	153	LEU	CA-CB-CG	7.33	132.16	115.30
31	A	46	C	C6-N1-C2	-7.33	117.37	120.30
31	A	1107	C	N1-C2-O2	7.33	123.30	118.90
26	V	64	LEU	CA-CB-CG	7.32	132.13	115.30
31	A	2662	C	N3-C2-O2	-7.29	116.80	121.90
31	A	2077	C	C5-C6-N1	7.28	124.64	121.00
31	A	2121	C	N1-C2-O2	7.28	123.27	118.90
31	A	1283	U	N1-C2-O2	7.23	127.86	122.80
31	A	1595	C	N1-C2-O2	7.19	123.22	118.90
31	A	1432	U	N3-C2-O2	-7.14	117.20	122.20
31	A	1432	U	C2-N1-C1'	7.12	126.24	117.70
31	A	1459	U	N1-C2-O2	7.12	127.78	122.80
31	A	2314	C	C5-C6-N1	7.11	124.55	121.00
31	A	112	C	C2-N1-C1'	7.10	126.61	118.80
31	A	1335	C	C2-N1-C1'	7.06	126.57	118.80
31	A	2268	G	N3-C4-N9	7.05	130.23	126.00
31	A	2518	C	C6-N1-C2	-7.04	117.48	120.30
31	A	1432	U	N1-C2-O2	6.98	127.69	122.80
31	A	46	C	N3-C2-O2	-6.95	117.03	121.90
31	A	1818	U	N1-C2-O2	6.95	127.67	122.80
11	E	245	LEU	CA-CB-CG	6.95	131.28	115.30
31	A	2268	G	N3-C4-C5	-6.94	125.13	128.60
31	A	2209	U	N3-C2-O2	-6.94	117.34	122.20
31	A	688	C	C2-N1-C1'	6.93	126.42	118.80
31	A	1419	C	N1-C2-O2	6.92	123.05	118.90
31	A	2709	C	C6-N1-C2	-6.87	117.55	120.30
31	A	2706	U	N1-C2-O2	6.85	127.59	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	630	C	N1-C2-O2	6.83	123.00	118.90
31	A	2209	U	N1-C2-O2	6.82	127.58	122.80
31	A	2116	C	N1-C2-O2	6.82	122.99	118.90
31	A	2209	U	C2-N1-C1'	6.81	125.87	117.70
31	A	1620	U	N1-C2-O2	6.74	127.52	122.80
31	A	1528	U	N1-C2-O2	6.71	127.50	122.80
31	A	31	C	N1-C2-O2	6.70	122.92	118.90
31	A	2378	C	N1-C2-O2	6.70	122.92	118.90
31	A	38	C	N3-C2-O2	-6.69	117.22	121.90
31	A	2706	U	N3-C2-O2	-6.67	117.53	122.20
8	B	61	C	N3-C2-O2	-6.66	117.23	121.90
31	A	877	C	N1-C2-O2	6.66	122.89	118.90
31	A	1818	U	C5-C6-N1	6.62	126.01	122.70
31	A	1397	C	N1-C2-O2	6.61	122.87	118.90
31	A	2077	C	C6-N1-C1'	-6.60	112.88	120.80
31	A	2483	C	N1-C2-O2	6.57	122.84	118.90
2	2	13	LEU	CA-CB-CG	6.56	130.38	115.30
27	W	33	A	P-O3'-C3'	6.53	127.54	119.70
31	A	1528	U	N3-C2-O2	-6.52	117.64	122.20
31	A	928	U	N1-C2-O2	6.51	127.36	122.80
31	A	1459	U	N3-C2-O2	-6.50	117.65	122.20
8	B	61	C	C2-N1-C1'	6.50	125.95	118.80
31	A	2121	C	C2-N1-C1'	6.49	125.94	118.80
31	A	1620	U	N3-C2-O2	-6.49	117.66	122.20
31	A	46	C	C2-N1-C1'	6.45	125.90	118.80
31	A	2447	A	C2-N3-C4	6.44	113.82	110.60
31	A	363	C	N1-C2-O2	6.44	122.77	118.90
31	A	1335	C	C6-N1-C2	-6.43	117.73	120.30
8	B	69	C	N3-C2-O2	-6.41	117.41	121.90
31	A	168	C	N3-C2-O2	-6.39	117.42	121.90
31	A	1528	U	C2-N1-C1'	6.35	125.32	117.70
27	W	32	C	P-O3'-C3'	6.35	127.32	119.70
31	A	1013	C	N3-C2-O2	-6.35	117.46	121.90
31	A	253	C	C2-N1-C1'	6.33	125.76	118.80
31	A	31	C	C2-N1-C1'	6.32	125.76	118.80
31	A	1250	C	C5-C6-N1	6.29	124.14	121.00
31	A	783	U	N1-C2-O2	6.29	127.20	122.80
31	A	112	C	N3-C2-O2	-6.27	117.51	121.90
31	A	448	C	N3-C2-O2	-6.23	117.54	121.90
31	A	2097	C	N1-C2-O2	6.20	122.62	118.90
31	A	2598	G	C4-C5-N7	6.20	113.28	110.80
31	A	1335	C	C5-C6-N1	6.19	124.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	1907	C	N1-C2-O2	6.18	122.61	118.90
31	A	1108	C	N3-C2-O2	-6.18	117.58	121.90
31	A	2469	C	N1-C2-O2	6.16	122.59	118.90
31	A	38	C	C6-N1-C2	-6.15	117.84	120.30
31	A	2683	C	N3-C2-O2	-6.13	117.61	121.90
8	B	69	C	C6-N1-C2	-6.11	117.86	120.30
31	A	856	U	N3-C2-O2	-6.09	117.94	122.20
15	K	239	LEU	CA-CB-CG	6.06	129.24	115.30
31	A	448	C	C2-N1-C1'	6.06	125.47	118.80
31	A	2700	C	N1-C2-O2	6.06	122.53	118.90
31	A	2314	C	C6-N1-C1'	-6.06	113.53	120.80
31	A	253	C	C6-N1-C2	-6.03	117.89	120.30
31	A	2724	C	N1-C2-O2	6.03	122.52	118.90
31	A	1620	U	C2-N1-C1'	6.00	124.90	117.70
31	A	38	C	C2-N1-C1'	5.98	125.38	118.80
31	A	46	C	C5-C6-N1	5.98	123.99	121.00
31	A	1013	C	C2-N1-C1'	5.98	125.38	118.80
31	A	186	C	N1-C2-O2	5.97	122.48	118.90
31	A	1209	U	N1-C2-O2	5.96	126.97	122.80
31	A	1142	G	N3-C4-C5	-5.96	125.62	128.60
31	A	1309	U	N3-C2-O2	-5.95	118.03	122.20
31	A	2789	C	N1-C2-O2	5.94	122.46	118.90
31	A	112	C	C6-N1-C2	-5.93	117.93	120.30
31	A	1142	G	C4-N9-C1'	5.92	134.20	126.50
27	W	100	C	N1-C2-O2	5.92	122.45	118.90
20	P	73	LEU	CA-CB-CG	5.90	128.87	115.30
31	A	1770	C	N1-C2-O2	5.90	122.44	118.90
31	A	1748	C	N3-C2-O2	-5.89	117.78	121.90
31	A	856	U	N1-C2-O2	5.89	126.92	122.80
31	A	901	C	C2-N1-C1'	5.89	125.28	118.80
31	A	243	U	N3-C2-O2	-5.89	118.08	122.20
31	A	2662	C	C6-N1-C1'	-5.88	113.74	120.80
31	A	173	C	N1-C2-O2	5.88	122.43	118.90
13	G	206	ASP	CB-CG-OD1	5.87	123.58	118.30
31	A	2706	U	C2-N1-C1'	5.87	124.75	117.70
27	W	29	U	P-O3'-C3'	5.87	126.74	119.70
31	A	243	U	N1-C2-O2	5.87	126.91	122.80
3	3	93	LEU	CA-CB-CG	5.86	128.78	115.30
31	A	2654	U	C2-N1-C1'	5.86	124.73	117.70
31	A	901	C	N1-C2-O2	5.85	122.41	118.90
31	A	1784	C	C6-N1-C2	-5.84	117.96	120.30
31	A	1219	U	N3-C2-O2	-5.83	118.12	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	647	C	C6-N1-C2	-5.83	117.97	120.30
31	A	1107	C	C2-N1-C1'	5.83	125.21	118.80
31	A	1419	C	N3-C2-O2	-5.81	117.83	121.90
31	A	9	A	C2-N3-C4	5.80	113.50	110.60
31	A	186	C	N3-C2-O2	-5.80	117.84	121.90
31	A	2654	U	N1-C2-O2	5.80	126.86	122.80
31	A	514	A	P-O3'-C3'	5.80	126.66	119.70
27	W	74	C	C6-N1-C2	-5.79	117.98	120.30
31	A	2121	C	N3-C2-O2	-5.79	117.85	121.90
31	A	2598	G	C5-N7-C8	-5.79	101.41	104.30
31	A	1746	C	N1-C2-O2	5.78	122.37	118.90
31	A	178	U	N3-C2-O2	-5.78	118.15	122.20
31	A	2007	U	N3-C2-O2	-5.78	118.15	122.20
8	B	31	C	N1-C2-O2	5.78	122.37	118.90
31	A	210	C	N1-C2-O2	5.78	122.37	118.90
31	A	2491	U	C2-N1-C1'	5.78	124.63	117.70
31	A	1747	C	C6-N1-C2	-5.77	117.99	120.30
8	B	7	G	O4'-C1'-N9	5.76	112.81	108.20
31	A	254	U	N3-C2-O2	-5.76	118.17	122.20
31	A	1923	C	N1-C2-O2	5.75	122.35	118.90
31	A	1595	C	C2-N1-C1'	5.75	125.12	118.80
31	A	1945	U	N1-C2-O2	5.74	126.82	122.80
31	A	928	U	N3-C2-O2	-5.72	118.20	122.20
31	A	2178	C	N1-C2-O2	5.71	122.33	118.90
31	A	2653	U	N1-C2-O2	5.71	126.79	122.80
31	A	2111	U	C2-N1-C1'	5.70	124.54	117.70
31	A	1334	U	C6-N1-C1'	-5.70	113.22	121.20
31	A	1595	C	N3-C2-O2	-5.70	117.91	121.90
31	A	2588	U	N1-C2-O2	5.67	126.77	122.80
31	A	367	C	P-O3'-C3'	5.67	126.50	119.70
31	A	1459	U	C2-N1-C1'	5.67	124.50	117.70
31	A	1923	C	C6-N1-C2	-5.66	118.03	120.30
31	A	2708	C	N1-C2-O2	5.66	122.30	118.90
31	A	541	G	C4-N9-C1'	5.65	133.85	126.50
31	A	794	A	C2-N3-C4	5.65	113.42	110.60
31	A	367	C	OP1-P-O3'	5.64	117.61	105.20
31	A	1843	C	C2-N3-C4	-5.63	117.08	119.90
31	A	594	C	C5-C6-N1	5.63	123.81	121.00
31	A	2421	C	N1-C2-O2	5.62	122.27	118.90
27	W	10	C	N1-C2-O2	5.61	122.26	118.90
31	A	1945	U	C2-N1-C1'	5.61	124.43	117.70
8	B	38	C	N1-C2-O2	5.60	122.26	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	1981	C	N1-C2-O2	5.60	122.26	118.90
8	B	69	C	C2-N1-C1'	5.59	124.95	118.80
31	A	2683	C	C2-N1-C1'	5.58	124.94	118.80
31	A	1906	C	N1-C2-O2	5.58	122.25	118.90
31	A	1142	G	N3-C4-N9	5.57	129.34	126.00
31	A	688	C	N1-C2-O2	5.56	122.24	118.90
31	A	594	C	C6-N1-C2	-5.56	118.08	120.30
32	0	87	LEU	CA-CB-CG	5.56	128.09	115.30
31	A	2573	C	N1-C2-O2	5.56	122.24	118.90
31	A	1945	U	N3-C2-O2	-5.55	118.32	122.20
31	A	683	C	N1-C2-O2	5.54	122.23	118.90
31	A	2325	G	N3-C4-N9	5.53	129.32	126.00
31	A	448	C	C6-N1-C2	-5.52	118.09	120.30
31	A	496	C	N1-C2-O2	5.52	122.21	118.90
27	W	22	A	OP1-P-O3'	5.51	117.32	105.20
31	A	1692	C	C6-N1-C2	-5.51	118.10	120.30
31	A	210	C	C6-N1-C2	-5.50	118.10	120.30
31	A	1137	C	N1-C2-O2	5.50	122.20	118.90
31	A	2789	C	N3-C2-O2	-5.50	118.05	121.90
31	A	1317	C	C6-N1-C2	-5.49	118.11	120.30
31	A	688	C	C6-N1-C2	-5.48	118.11	120.30
31	A	2662	C	C6-N1-C2	-5.47	118.11	120.30
31	A	813	C	N1-C2-O2	5.46	122.18	118.90
31	A	1397	C	N3-C2-O2	-5.46	118.07	121.90
31	A	1818	U	N3-C2-O2	-5.46	118.38	122.20
31	A	2007	U	N1-C2-O2	5.46	126.62	122.80
31	A	1309	U	N1-C2-O2	5.45	126.61	122.80
31	A	630	C	C2-N1-C1'	5.44	124.78	118.80
31	A	2300	U	C2-N1-C1'	5.44	124.23	117.70
31	A	688	C	N3-C2-O2	-5.44	118.09	121.90
31	A	2325	G	N3-C4-C5	-5.43	125.89	128.60
31	A	2378	C	N3-C2-O2	-5.42	118.10	121.90
31	A	1604	A	N1-C6-N6	5.42	121.85	118.60
31	A	2303	A	O4'-C1'-N9	-5.42	103.87	108.20
31	A	2097	C	N3-C2-O2	-5.42	118.11	121.90
31	A	2325	G	C4-N9-C1'	5.42	133.54	126.50
31	A	2774	U	C5-C4-O4	5.41	129.15	125.90
24	T	67	LEU	CA-CB-CG	5.41	127.73	115.30
31	A	1283	U	C2-N1-C1'	5.40	124.18	117.70
31	A	856	U	C2-N1-C1'	5.40	124.18	117.70
31	A	1309	U	C2-N1-C1'	5.39	124.17	117.70
31	A	2535	C	N1-C2-O2	5.39	122.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	2699	U	N3-C2-O2	-5.39	118.42	122.20
31	A	2300	U	C5-C6-N1	5.39	125.40	122.70
31	A	877	C	N3-C2-O2	-5.39	118.13	121.90
31	A	2020	C	N1-C2-O2	5.39	122.13	118.90
31	A	870	U	N1-C2-O2	5.38	126.56	122.80
31	A	703	C	N1-C2-O2	5.37	122.12	118.90
31	A	178	U	N1-C2-O2	5.36	126.55	122.80
31	A	186	C	C6-N1-C2	-5.35	118.16	120.30
31	A	2491	U	N1-C2-O2	5.35	126.54	122.80
31	A	2545	U	N1-C2-O2	5.35	126.54	122.80
8	B	31	C	C2-N1-C1'	5.33	124.67	118.80
31	A	2360	U	N1-C2-O2	5.33	126.53	122.80
31	A	363	C	C2-N1-C1'	5.32	124.66	118.80
31	A	2378	C	C6-N1-C2	-5.32	118.17	120.30
31	A	2653	U	N3-C2-O2	-5.32	118.47	122.20
31	A	1397	C	C2-N1-C1'	5.32	124.65	118.80
31	A	2530	U	N3-C2-O2	-5.32	118.48	122.20
31	A	1175	U	N1-C2-O2	5.31	126.52	122.80
31	A	496	C	C5-C6-N1	5.31	123.65	121.00
31	A	2737	G	N1-C6-O6	-5.30	116.72	119.90
31	A	907	C	N1-C2-O2	5.30	122.08	118.90
31	A	684	C	C2-N3-C4	-5.29	117.25	119.90
31	A	1335	C	N1-C2-O2	5.29	122.08	118.90
31	A	2300	U	N3-C2-O2	-5.29	118.50	122.20
8	B	18	C	N1-C2-O2	5.29	122.07	118.90
21	Q	223	ARG	C-N-CA	5.29	134.91	121.70
31	A	294	U	C5-C6-N1	5.28	125.34	122.70
31	A	1419	C	C2-N1-C1'	5.28	124.61	118.80
31	A	2116	C	N3-C2-O2	-5.27	118.21	121.90
31	A	2529	C	C6-N1-C2	-5.27	118.19	120.30
27	W	74	C	C5-C6-N1	5.27	123.63	121.00
31	A	1843	C	N1-C2-N3	5.26	122.88	119.20
31	A	2530	U	C2-N1-C1'	5.26	124.01	117.70
31	A	563	C	N1-C2-O2	5.25	122.05	118.90
31	A	2651	C	N1-C2-O2	5.25	122.05	118.90
31	A	1209	U	C5-C6-N1	5.25	125.33	122.70
31	A	2699	U	N1-C2-O2	5.25	126.48	122.80
31	A	2737	G	C5-C6-O6	5.25	131.75	128.60
31	A	630	C	N3-C2-O2	-5.25	118.23	121.90
31	A	1595	C	C6-N1-C2	-5.25	118.20	120.30
31	A	1550	U	N1-C2-O2	5.24	126.47	122.80
31	A	1907	C	N3-C2-O2	-5.24	118.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	2483	C	N3-C2-O2	-5.24	118.23	121.90
31	A	2708	C	C6-N1-C2	-5.24	118.20	120.30
31	A	972	G	C4-N9-C1'	5.24	133.31	126.50
31	A	2270	G	N3-C4-N9	5.23	129.14	126.00
31	A	541	G	N3-C4-N9	5.23	129.14	126.00
31	A	228	U	N1-C2-O2	5.22	126.46	122.80
31	A	1696	C	N1-C2-O2	5.22	122.03	118.90
27	W	29	U	OP2-P-O3'	5.22	116.68	105.20
31	A	1901	C	N1-C2-O2	5.22	122.03	118.90
31	A	1107	C	N3-C2-O2	-5.21	118.25	121.90
31	A	541	G	N3-C4-C5	-5.19	126.00	128.60
31	A	2447	A	N3-C4-N9	5.18	131.54	127.40
31	A	173	C	N3-C2-O2	-5.17	118.28	121.90
31	A	1175	U	N3-C2-O2	-5.16	118.59	122.20
31	A	1219	U	C6-N1-C2	-5.16	117.90	121.00
31	A	2360	U	C2-N1-C1'	5.15	123.88	117.70
31	A	2593	G	N3-C2-N2	5.14	123.50	119.90
31	A	2654	U	N3-C2-O2	-5.14	118.60	122.20
31	A	2683	C	C6-N1-C2	-5.14	118.24	120.30
31	A	404	U	N1-C2-O2	5.14	126.39	122.80
31	A	1092	C	N1-C2-O2	5.14	121.98	118.90
31	A	1419	C	C6-N1-C2	-5.13	118.25	120.30
15	K	191	LEU	CA-CB-CG	5.12	127.08	115.30
31	A	210	C	N3-C2-O2	-5.12	118.31	121.90
31	A	275	U	C2-N1-C1'	5.12	123.85	117.70
31	A	2527	C	N1-C2-O2	5.12	121.97	118.90
31	A	2432	G	C4-N9-C1'	5.11	133.15	126.50
31	A	112	C	C5-C6-N1	5.11	123.55	121.00
31	A	1604	A	N7-C8-N9	5.10	116.35	113.80
31	A	2121	C	C6-N1-C2	-5.10	118.26	120.30
31	A	258	C	N1-C2-O2	5.10	121.96	118.90
31	A	2300	U	N1-C2-O2	5.10	126.37	122.80
31	A	827	C	N1-C2-O2	5.10	121.96	118.90
31	A	845	C	C6-N1-C2	-5.10	118.26	120.30
31	A	258	C	N3-C2-O2	-5.09	118.33	121.90
31	A	1317	C	N3-C2-O2	-5.08	118.34	121.90
31	A	683	C	C6-N1-C2	-5.08	118.27	120.30
31	A	703	C	N3-C2-O2	-5.08	118.34	121.90
31	A	1546	C	N1-C2-O2	5.07	121.94	118.90
31	A	2367	C	N1-C2-O2	5.07	121.94	118.90
31	A	2518	C	C5-C4-N4	5.07	123.75	120.20
31	A	1550	U	N3-C2-O2	-5.06	118.66	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	97	A	P-O3'-C3'	5.06	125.77	119.70
31	A	1013	C	C6-N1-C2	-5.06	118.28	120.30
31	A	288	C	N1-C2-O2	5.05	121.93	118.90
31	A	2469	C	N3-C2-O2	-5.05	118.36	121.90
29	Y	98	LEU	CA-CB-CG	5.05	126.92	115.30
31	A	502	U	N1-C2-O2	5.05	126.33	122.80
31	A	2243	C	N1-C2-O2	5.04	121.93	118.90
31	A	1789	U	C2-N1-C1'	5.04	123.75	117.70
31	A	2724	C	C2-N1-C1'	5.04	124.34	118.80
31	A	1747	C	N1-C2-O2	5.04	121.92	118.90
31	A	2063	C	C2-N1-C1'	5.04	124.34	118.80
31	A	253	C	C5-C6-N1	5.04	123.52	121.00
31	A	1770	C	N3-C2-O2	-5.04	118.38	121.90
31	A	2270	G	N3-C4-C5	-5.03	126.09	128.60
31	A	363	C	N3-C2-O2	-5.02	118.39	121.90
31	A	1971	C	N1-C2-O2	5.02	121.91	118.90
31	A	2360	U	N3-C2-O2	-5.01	118.69	122.20
31	A	2447	A	N3-C4-C5	-5.01	123.29	126.80
31	A	855	C	N1-C2-O2	5.01	121.90	118.90
31	A	563	C	N3-C2-O2	-5.00	118.40	121.90
31	A	783	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	0	73	TRP	Peptide
17	M	143	LEU	Peptide
21	Q	190	VAL	Peptide
23	S	174	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	378	0	415	8	0
2	2	415	0	434	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	445	0	501	11	0
4	4	563	0	623	9	0
5	5	304	0	345	7	0
6	6	422	0	508	9	0
7	7	368	0	386	7	0
8	B	2500	0	1263	13	0
9	C	1904	0	1985	41	0
10	D	1620	0	1699	34	0
11	E	1655	0	1725	40	0
12	F	1351	0	1407	28	0
13	G	1353	0	1416	18	0
14	H	423	0	490	7	0
15	K	1568	0	1595	25	0
16	L	942	0	996	16	0
17	M	1342	0	1417	16	0
18	N	1067	0	1122	28	0
19	O	944	0	1004	25	0
20	P	947	0	966	30	0
21	Q	953	0	1045	25	0
22	R	996	0	1062	35	0
23	S	1171	0	1216	22	0
24	T	1149	0	1220	21	0
25	U	740	0	795	14	0
26	V	993	0	1055	25	0
27	W	2187	0	1102	17	0
28	X	810	0	847	14	0
29	Y	605	0	652	17	0
30	Z	754	0	808	13	0
31	A	60324	0	30377	432	0
32	0	521	0	499	4	0
All	All	91714	0	60975	829	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (829) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:63:A:H61	31:A:89:A:N6	1.59	1.01
31:A:2118:U:H3	31:A:2199:G:H1	1.08	0.99
31:A:293:G:H21	31:A:365:A:N6	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:293:G:N2	31:A:365:A:H62	1.61	0.98
31:A:1505:C:H42	31:A:1515:G:H1	1.09	0.98
31:A:63:A:H61	31:A:89:A:H61	0.98	0.96
31:A:1121:G:H21	31:A:1126:A:H62	1.09	0.95
31:A:1084:G:H21	31:A:1131:A:N6	1.65	0.94
31:A:313:A:H2	31:A:323:G:H1	1.02	0.93
31:A:1084:G:N2	31:A:1131:A:H62	1.67	0.92
31:A:63:A:N6	31:A:89:A:H61	1.66	0.91
12:F:106:ALA:O	12:F:110:LEU:HB3	1.72	0.90
20:P:73:LEU:HA	20:P:85:GLN:O	1.73	0.86
31:A:1235:A:H62	31:A:1256:G:H21	1.24	0.86
31:A:1196:A:H61	31:A:1201:A:H61	1.25	0.85
31:A:1084:G:H21	31:A:1131:A:H62	0.88	0.84
31:A:313:A:C2	31:A:323:G:N1	2.45	0.84
13:G:57:ALA:HB3	13:G:64:LYS:O	1.77	0.83
31:A:313:A:H2	31:A:323:G:N1	1.77	0.83
32:0:49:ALA:HB3	32:0:61:THR:O	1.79	0.81
12:F:105:ALA:O	12:F:109:GLU:HB2	1.80	0.81
31:A:1505:C:N4	31:A:1515:G:H1	1.78	0.80
13:G:101:ALA:O	13:G:105:HIS:HB2	1.82	0.79
13:G:162:GLN:O	13:G:174:SER:HB2	1.85	0.77
31:A:293:G:H21	31:A:365:A:H62	0.83	0.77
31:A:2764:U:O4	31:A:2774:U:C4	2.38	0.76
11:E:251:THR:O	11:E:255:LEU:HB2	1.88	0.74
22:R:81:PHE:O	22:R:85:LEU:HB2	1.86	0.74
31:A:2107:G:H1	31:A:2210:C:H42	1.34	0.74
31:A:1121:G:N2	31:A:1126:A:H62	1.85	0.73
31:A:721:U:H3	31:A:732:A:H61	1.33	0.73
31:A:722:G:H1	31:A:731:U:H3	1.37	0.72
10:D:260:LYS:HD2	31:A:2790:C:H5"	1.72	0.71
31:A:1462:G:H1	31:A:1584:C:H42	1.38	0.71
31:A:2112:U:H3	31:A:2205:G:H1	1.39	0.70
10:D:127:LYS:O	10:D:135:ASN:HA	1.92	0.70
31:A:2764:U:O4	31:A:2774:U:C5	2.45	0.69
14:H:57:ILE:HG22	14:H:59:ASP:H	1.58	0.69
14:H:51:ILE:HA	14:H:85:GLU:O	1.94	0.68
16:L:22:ILE:HB	16:L:40:VAL:O	1.94	0.68
31:A:55:G:H1	31:A:112:C:H42	1.42	0.68
31:A:2707:A:H62	31:A:2737:G:N2	1.92	0.68
28:X:121:GLY:HA3	28:X:138:TYR:O	1.94	0.67
31:A:2464:G:H1	31:A:2467:A:H62	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:167:SER:HA	9:C:180:ILE:O	1.93	0.67
31:A:2492:C:H42	31:A:2546:G:H22	1.41	0.67
26:V:75:VAL:HA	26:V:135:MET:O	1.95	0.67
31:A:2134:G:H22	31:A:2192:U:H3	1.42	0.67
18:N:35:GLN:HE21	18:N:100:GLY:HA2	1.60	0.66
18:N:30:GLY:HA2	18:N:107:SER:HB3	1.77	0.66
21:Q:148:ILE:HG12	21:Q:168:ILE:HG12	1.77	0.66
10:D:98:GLY:H	10:D:286:PRO:HB3	1.59	0.66
10:D:275:VAL:HG21	21:Q:122:ILE:HG21	1.78	0.66
31:A:2764:U:C4	31:A:2774:U:O4	2.49	0.66
27:W:53:G:H8	27:W:70:G:H21	1.44	0.66
18:N:65:TRP:HB2	18:N:105:GLU:HB2	1.77	0.65
12:F:91:CYS:O	12:F:139:GLY:HA2	1.96	0.65
16:L:2:ILE:HB	16:L:33:ALA:HB3	1.78	0.65
31:A:1385:G:H4'	31:A:1818:U:H3	1.60	0.65
5:5:14:CYS:HA	5:5:26:ILE:O	1.97	0.65
23:S:198:PHE:HA	23:S:208:ARG:O	1.97	0.65
31:A:1235:A:H62	31:A:1256:G:N2	1.93	0.65
13:G:91:ARG:HA	13:G:109:ARG:HH22	1.62	0.65
12:F:89:VAL:HA	12:F:206:ASP:O	1.97	0.65
31:A:1196:A:N6	31:A:1201:A:H61	1.93	0.65
10:D:125:GLN:O	10:D:138:GLN:HB3	1.97	0.65
11:E:86:ARG:NH2	31:A:670:A:N3	2.45	0.65
21:Q:216:LYS:HG3	21:Q:218:ARG:H	1.61	0.65
31:A:2764:U:O4	31:A:2774:U:O4	2.14	0.65
9:C:37:LYS:HE3	9:C:50:ARG:HE	1.61	0.64
15:K:56:LYS:O	15:K:60:GLU:HB2	1.97	0.64
19:O:108:ILE:O	19:O:122:TYR:HB3	1.98	0.64
3:3:146:ARG:HH22	25:U:140:VAL:HG21	1.64	0.63
31:A:1505:C:N3	31:A:1515:G:N2	2.43	0.63
22:R:97:LEU:O	22:R:101:ALA:HB2	1.99	0.63
31:A:1060:A:H2	31:A:1150:G:H1	1.43	0.62
23:S:211:GLY:H	31:A:1245:U:H4'	1.64	0.62
9:C:146:ARG:NH2	31:A:1811:A:OP2	2.33	0.62
17:M:203:GLU:HB3	31:A:649:A:H5"	1.82	0.62
21:Q:123:MET:O	21:Q:127:ASN:HB2	1.99	0.62
9:C:29:ILE:HG22	9:C:57:LEU:HD22	1.81	0.62
14:H:57:ILE:HB	14:H:61:GLY:H	1.65	0.62
26:V:76:LYS:O	26:V:134:VAL:HA	1.99	0.62
31:A:540:A:H62	31:A:2055:U:H3	1.48	0.62
4:4:110:ILE:H	4:4:143:TYR:HE1	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:14:ARG:NH1	31:A:984:G:N7	2.48	0.61
22:R:6:ARG:NH2	31:A:29:A:OP2	2.33	0.61
13:G:104:MET:HA	13:G:107:LEU:HB3	1.81	0.61
23:S:214:GLN:HE22	31:A:1189:G:H21	1.47	0.61
9:C:139:ASN:O	9:C:186:ALA:HA	2.00	0.61
11:E:97:ARG:NH1	31:A:38:C:O2	2.33	0.61
22:R:16:LYS:NZ	31:A:1248:G:N7	2.48	0.61
8:B:58:A:H5'	12:F:77:ASN:HD22	1.65	0.61
28:X:123:VAL:HG12	28:X:137:VAL:HG22	1.83	0.60
31:A:2492:C:H42	31:A:2546:G:N2	1.99	0.60
9:C:137:ILE:HG21	9:C:186:ALA:HB1	1.84	0.60
31:A:892:C:H42	31:A:903:G:H1	1.47	0.60
12:F:155:ARG:O	12:F:159:LEU:HB2	2.01	0.60
15:K:123:ILE:HG12	15:K:246:ILE:HG23	1.84	0.60
31:A:1133:U:H2'	31:A:1134:G:H8	1.67	0.60
31:A:721:U:H3	31:A:732:A:N6	1.99	0.60
28:X:142:ILE:HG22	28:X:143:GLN:HG3	1.84	0.60
13:G:198:LYS:HG3	13:G:200:LYS:HB3	1.82	0.60
15:K:84:MET:HG2	15:K:96:TRP:HE1	1.66	0.60
19:O:17:ILE:HD12	31:A:2707:A:H4'	1.84	0.60
26:V:152:LEU:HD12	26:V:154:ASP:H	1.67	0.60
31:A:1196:A:H61	31:A:1201:A:N6	1.97	0.60
10:D:200:SER:HA	10:D:259:THR:O	2.02	0.59
31:A:1121:G:H21	31:A:1126:A:N6	1.92	0.59
12:F:92:GLY:HA3	31:A:2323:C:H42	1.67	0.59
31:A:1238:G:H1	31:A:1252:C:H42	1.47	0.59
31:A:525:A:N3	31:A:591:C:O2'	2.35	0.59
22:R:92:LEU:O	23:S:133:GLN:NE2	2.36	0.59
3:3:140:ASN:ND2	31:A:125:A:OP2	2.36	0.59
10:D:227:LYS:HB3	31:A:2596:C:H4'	1.84	0.59
19:O:60:LYS:O	19:O:64:LEU:HB2	2.03	0.59
21:Q:151:ILE:HB	21:Q:165:TYR:HB2	1.85	0.59
3:3:127:ARG:NH2	31:A:478:A:OP1	2.35	0.58
31:A:984:G:H2'	31:A:985:A:H2'	1.85	0.58
31:A:313:A:N1	31:A:323:G:O6	2.36	0.58
31:A:1789:U:OP2	31:A:1794:A:N6	2.36	0.58
12:F:68:LEU:O	12:F:72:GLU:HB2	2.03	0.58
22:R:33:ARG:O	31:A:1273:G:N2	2.36	0.58
31:A:2456:A:N6	31:A:2602:U:OP1	2.37	0.58
24:T:47:ARG:HA	24:T:50:ILE:HG22	1.86	0.58
29:Y:102:ASN:HB3	31:A:2247:C:H1'	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:39:PRO:HB3	18:N:99:PRO:HD3	1.85	0.58
31:A:2707:A:H62	31:A:2737:G:H21	1.51	0.58
3:3:125:LYS:HE2	31:A:164:A:H5"	1.86	0.58
4:4:114:ARG:HE	4:4:132:LEU:HD23	1.69	0.58
16:L:23:ARG:NH1	31:A:2579:U:O2'	2.37	0.58
23:S:197:VAL:HG23	23:S:210:ILE:HG13	1.85	0.58
11:E:126:ARG:HH21	31:A:1278:U:H5"	1.68	0.58
20:P:152:VAL:HA	20:P:155:LEU:HB3	1.85	0.58
6:6:106:MET:O	6:6:110:LYS:HB2	2.04	0.58
29:Y:87:ARG:NH1	31:A:2095:U:OP1	2.36	0.58
12:F:116:GLN:HE21	12:F:148:LEU:HD21	1.68	0.57
31:A:17:C:O2'	31:A:564:U:OP1	2.21	0.57
14:H:43:LYS:HG2	14:H:44:LYS:HG2	1.85	0.57
2:2:34:ILE:HG12	31:A:2303:A:H61	1.68	0.57
4:4:150:LEU:HD22	4:4:153:LEU:HG	1.86	0.57
17:M:138:ARG:NH2	31:A:235:G:O2'	2.37	0.57
27:W:52:G:N2	27:W:71:C:O2'	2.37	0.57
31:A:1291:C:H5"	31:A:1292:G:H5'	1.86	0.57
9:C:142:ILE:HA	9:C:180:ILE:HD11	1.85	0.57
30:Z:110:LYS:NZ	31:A:75:C:OP1	2.38	0.57
31:A:1130:C:H2'	31:A:1131:A:H8	1.68	0.57
22:R:11:ARG:O	22:R:15:LYS:HB2	2.05	0.57
25:U:162:VAL:HG12	25:U:176:ILE:HG22	1.86	0.57
31:A:1296:A:OP2	31:A:1682:C:N4	2.37	0.57
10:D:240:THR:HG23	31:A:2046:G:H21	1.69	0.57
11:E:99:THR:OG1	31:A:454:G:N3	2.38	0.57
12:F:107:ILE:O	12:F:111:ALA:CB	2.53	0.57
31:A:1020:C:H2'	31:A:1021:A:H8	1.70	0.57
31:A:1103:C:C4	31:A:1104:C:N4	2.73	0.57
3:3:127:ARG:NH1	3:3:134:ILE:O	2.37	0.56
11:E:69:PHE:O	11:E:256:ASN:ND2	2.39	0.56
26:V:85:LYS:HD3	26:V:104:LEU:HD13	1.87	0.56
26:V:107:LYS:HB2	26:V:125:ILE:O	2.05	0.56
31:A:2599:G:OP2	31:A:2600:G:N2	2.38	0.56
9:C:206:SER:HA	9:C:209:TRP:HD1	1.69	0.56
11:E:204:LYS:HA	11:E:225:THR:HB	1.88	0.56
21:Q:143:ILE:HD11	21:Q:206:ILE:HD13	1.87	0.56
31:A:2705:G:OP1	31:A:2731:C:N4	2.38	0.56
31:A:2707:A:N6	31:A:2737:G:H21	2.03	0.56
14:H:55:GLU:OE1	14:H:83:LYS:NZ	2.37	0.56
31:A:1111:G:N2	31:A:1114:A:OP2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:235:ILE:O	10:D:248:LYS:NZ	2.37	0.56
20:P:64:VAL:HG11	20:P:142:ASP:HB3	1.87	0.56
6:6:123:ARG:NH2	31:A:1405:A:OP2	2.37	0.56
19:O:27:ARG:NH1	31:A:2707:A:OP2	2.38	0.56
10:D:275:VAL:HG11	21:Q:126:LEU:HD11	1.87	0.56
11:E:253:GLN:O	11:E:257:GLN:HB2	2.05	0.56
12:F:89:VAL:HG22	12:F:207:VAL:HG22	1.88	0.56
21:Q:124:GLY:O	21:Q:128:LYS:HB2	2.05	0.56
31:A:1573:C:H2'	31:A:1574:G:H8	1.71	0.56
23:S:146:ARG:NH1	31:A:1189:G:OP1	2.39	0.56
1:1:34:LEU:HD23	24:T:67:LEU:HD21	1.88	0.56
10:D:210:GLY:HA2	10:D:251:PRO:HB3	1.88	0.56
28:X:123:VAL:HA	28:X:136:SER:O	2.06	0.56
31:A:2464:G:N2	31:A:2467:A:N7	2.53	0.56
22:R:25:ARG:HH22	31:A:2035:A:H5'	1.71	0.56
26:V:105:ASN:OD1	26:V:107:LYS:NZ	2.39	0.55
23:S:204:LYS:HG2	31:A:1001:A:H5'	1.89	0.55
16:L:31:ARG:HH11	31:A:2009:U:H1'	1.70	0.55
12:F:208:CYS:SG	31:A:2320:G:N2	2.80	0.55
31:A:1343:A:N1	31:A:1354:C:O2'	2.38	0.55
19:O:37:GLN:HE22	31:A:1298:A:H2	1.55	0.55
19:O:51:ALA:HA	19:O:123:ILE:HD11	1.89	0.55
22:R:3:ARG:N	31:A:1269:G:N7	2.55	0.55
29:Y:107:ARG:HG2	29:Y:116:PHE:HB3	1.89	0.55
31:A:1041:G:H1	31:A:1176:C:H42	1.55	0.55
6:6:123:ARG:HH22	31:A:1404:C:H3'	1.72	0.55
22:R:49:ASP:OD1	22:R:52:ARG:NH1	2.38	0.55
31:A:318:A:N3	31:A:338:G:O2'	2.36	0.55
11:E:168:ALA:HB1	11:E:245:LEU:HD11	1.89	0.55
23:S:128:VAL:HG22	23:S:133:GLN:HG2	1.89	0.55
31:A:641:C:O2	31:A:651:U:O2'	2.25	0.55
3:3:127:ARG:HE	3:3:132:ARG:HG3	1.72	0.55
23:S:214:GLN:HE21	31:A:1021:A:H1'	1.72	0.55
26:V:76:LYS:HB2	26:V:137:ILE:HD11	1.89	0.55
31:A:423:G:OP2	31:A:2423:A:O2'	2.24	0.55
16:L:34:ARG:NH1	31:A:2690:G:OP1	2.41	0.54
31:A:2300:U:O2	31:A:2342:G:O6	2.24	0.54
31:A:1793:A:H1'	31:A:2624:G:H21	1.72	0.54
31:A:1801:A:N6	31:A:1838:G:O2'	2.36	0.54
20:P:100:THR:O	20:P:104:ALA:HB2	2.06	0.54
31:A:542:C:OP1	31:A:571:G:N1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1096:G:N2	31:A:1123:A:O2'	2.39	0.54
31:A:992:U:O2'	31:A:2290:A:N3	2.37	0.54
31:A:2761:U:OP2	31:A:2773:C:N4	2.38	0.54
11:E:79:LYS:NZ	31:A:609:G:OP1	2.39	0.54
16:L:61:VAL:O	16:L:84:ALA:HA	2.06	0.54
28:X:70:ARG:NH1	31:A:2274:A:O2'	2.41	0.54
9:C:256:ARG:HE	9:C:260:LYS:HD3	1.72	0.54
11:E:222:ASN:ND2	31:A:329:C:O2'	2.36	0.54
16:L:24:ILE:HG21	16:L:33:ALA:HB2	1.89	0.54
31:A:2612:G:N2	31:A:2615:A:OP2	2.36	0.54
23:S:139:GLY:H	23:S:221:ILE:HB	1.72	0.54
31:A:2107:G:H1	31:A:2210:C:N4	2.05	0.54
15:K:219:ASN:O	15:K:222:LYS:NZ	2.41	0.54
28:X:97:ARG:HH22	31:A:2279:U:H5"	1.72	0.54
31:A:1155:A:N7	31:A:2505:A:O2'	2.39	0.54
31:A:1379:C:N4	31:A:1393:U:OP2	2.41	0.54
5:5:6:SER:HB3	31:A:2483:C:H5"	1.89	0.54
15:K:58:THR:O	15:K:62:ARG:HB2	2.07	0.54
18:N:128:ARG:NH1	31:A:1057:A:OP1	2.40	0.54
19:O:19:ARG:NH1	31:A:1689:C:O2'	2.41	0.54
7:7:74:ARG:NH1	31:A:1177:U:O4	2.40	0.54
11:E:105:ARG:NH2	31:A:685:G:OP1	2.38	0.54
20:P:61:ARG:NH2	20:P:89:ASP:OD1	2.41	0.54
31:A:259:C:H42	31:A:268:G:H1	1.56	0.54
8:B:10:G:O5'	20:P:61:ARG:NH1	2.41	0.53
11:E:207:PHE:HB2	11:E:246:VAL:HG22	1.91	0.53
22:R:77:ASN:ND2	31:A:1040:U:OP1	2.41	0.53
31:A:656:A:H61	31:A:2366:G:H21	1.55	0.53
31:A:724:G:H21	31:A:729:A:H62	1.56	0.53
13:G:63:LEU:HB2	13:G:76:TYR:HE1	1.73	0.53
20:P:75:VAL:HA	20:P:83:TYR:O	2.08	0.53
23:S:148:LYS:HB2	31:A:1189:G:H5'	1.90	0.53
18:N:46:GLN:NE2	31:A:2502:G:OP1	2.41	0.53
21:Q:174:ASN:HA	21:Q:179:THR:HA	1.89	0.53
29:Y:115:ARG:HH12	29:Y:145:LEU:HD21	1.74	0.53
3:3:133:LYS:HE3	31:A:471:U:H5"	1.91	0.53
12:F:87:ILE:HG22	12:F:209:ILE:HA	1.90	0.53
15:K:99:THR:HA	22:R:99:GLN:HE22	1.73	0.53
21:Q:122:ILE:HA	21:Q:125:ILE:HG22	1.91	0.53
31:A:1615:G:H2'	31:A:1616:A:H8	1.73	0.53
1:1:16:ARG:NH2	31:A:2633:C:OP1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:114:LYS:HD3	26:V:118:GLU:HB2	1.90	0.53
31:A:709:C:O2'	31:A:745:A:N6	2.38	0.53
31:A:1117:G:N2	31:A:1118:U:O4	2.42	0.53
31:A:2300:U:O2	31:A:2342:G:C6	2.61	0.53
2:2:24:ASN:HB2	2:2:27:SER:HB3	1.91	0.53
31:A:763:A:OP2	31:A:1791:C:N4	2.42	0.53
31:A:1393:U:O2'	31:A:2230:A:N3	2.37	0.53
6:6:140:LYS:HE2	31:A:1461:G:H5'	1.90	0.53
16:L:24:ILE:HG22	16:L:39:ILE:HG22	1.90	0.53
19:O:44:ILE:HG22	19:O:123:ILE:HB	1.91	0.53
26:V:89:ILE:HG22	26:V:101:ILE:HG22	1.91	0.53
31:A:1533:A:N3	31:A:1611:G:O2'	2.42	0.53
9:C:181:SER:OG	9:C:184:CYS:SG	2.67	0.53
12:F:87:ILE:HA	12:F:208:CYS:O	2.08	0.53
16:L:104:ARG:NH1	16:L:121:LEU:O	2.42	0.53
9:C:152:ARG:HG2	31:A:1828:U:H2'	1.91	0.52
22:R:10:ALA:O	22:R:14:ARG:HB2	2.09	0.52
24:T:57:SER:HA	24:T:99:ILE:HA	1.90	0.52
31:A:88:A:H3'	31:A:89:A:H2'	1.92	0.52
9:C:103:PRO:HA	9:C:191:VAL:HA	1.90	0.52
24:T:90:ASN:ND2	31:A:506:G:O2'	2.42	0.52
31:A:208:A:O2'	31:A:432:G:N3	2.42	0.52
31:A:1876:A:H62	31:A:1889:G:H21	1.57	0.52
2:2:35:THR:O	31:A:2303:A:N6	2.41	0.52
10:D:204:ILE:HG23	10:D:284:GLY:HA2	1.91	0.52
31:A:2495:A:O2'	31:A:2553:G:N2	2.42	0.52
8:B:81:U:O2'	31:A:927:A:N3	2.42	0.52
16:L:22:ILE:O	16:L:40:VAL:HB	2.09	0.52
31:A:1462:G:H1	31:A:1584:C:N4	2.05	0.52
10:D:99:MET:HG2	10:D:113:THR:HG22	1.92	0.52
15:K:172:LEU:HB2	15:K:174:ARG:HH11	1.75	0.52
31:A:182:A:N6	31:A:2447:A:O2'	2.43	0.52
31:A:1836:C:O2'	31:A:1985:A:OP2	2.27	0.52
16:L:6:THR:HG1	16:L:21:CYS:HG	1.58	0.52
19:O:77:LEU:HD11	19:O:83:LYS:HD2	1.91	0.52
30:Z:135:LYS:O	30:Z:139:ALA:HB2	2.10	0.52
31:A:376:U:O2'	31:A:378:A:N1	2.38	0.52
31:A:845:C:H2'	31:A:846:A:H8	1.74	0.52
31:A:1886:A:H2'	31:A:1887:G:H8	1.75	0.52
6:6:115:ARG:HH12	31:A:1490:G:H5"	1.74	0.52
11:E:120:LYS:HA	31:A:2073:A:H4'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:73:ARG:HH21	31:A:1475:U:H4'	1.73	0.52
20:P:72:ARG:NH1	20:P:142:ASP:OD2	2.41	0.52
21:Q:170:ILE:HG23	21:Q:219:LEU:HB2	1.92	0.52
24:T:79:LEU:HD22	24:T:134:ILE:HD12	1.92	0.52
25:U:144:LYS:NZ	25:U:162:VAL:O	2.43	0.52
25:U:167:ARG:NH1	25:U:171:THR:OG1	2.42	0.52
26:V:109:LYS:HD3	26:V:125:ILE:HD12	1.91	0.52
9:C:141:GLU:HB2	9:C:184:CYS:HB3	1.92	0.52
15:K:58:THR:O	15:K:62:ARG:CB	2.58	0.52
18:N:71:ASP:OD2	31:A:916:G:N2	2.42	0.52
21:Q:138:ARG:HH12	21:Q:201:PRO:HA	1.75	0.52
22:R:40:ILE:HG23	23:S:198:PHE:HE2	1.74	0.52
24:T:57:SER:OG	24:T:60:GLU:OE1	2.25	0.52
31:A:2133:A:N6	31:A:2181:U:O2'	2.40	0.52
11:E:78:GLU:O	17:M:88:GLN:NE2	2.43	0.52
31:A:579:U:O2'	31:A:1011:A:N1	2.40	0.52
31:A:1949:G:N2	31:A:1976:C:O2'	2.43	0.52
9:C:64:ARG:NH2	9:C:145:GLY:O	2.43	0.52
31:A:1457:G:O2'	31:A:1496:A:N1	2.43	0.52
2:2:15:CYS:O	2:2:31:SER:HA	2.10	0.51
8:B:9:U:OP1	20:P:53:ARG:NH2	2.39	0.51
8:B:38:C:O2	20:P:149:HIS:NE2	2.42	0.51
9:C:178:ARG:NH1	31:A:1810:C:OP2	2.43	0.51
20:P:87:ILE:HG22	20:P:94:THR:HG22	1.91	0.51
26:V:76:LYS:HE2	26:V:137:ILE:HD11	1.92	0.51
1:1:47:PHE:HZ	19:O:45:LYS:HE2	1.75	0.51
7:7:48:SER:OG	7:7:49:SER:N	2.43	0.51
15:K:194:ARG:NH1	31:A:2657:G:OP2	2.42	0.51
20:P:128:ALA:HB2	20:P:159:ALA:HA	1.93	0.51
24:T:121:ARG:O	31:A:1650:A:N6	2.44	0.51
10:D:142:GLU:OE1	10:D:166:ARG:NH2	2.38	0.51
10:D:239:THR:OG1	31:A:2589:A:N7	2.35	0.51
12:F:116:GLN:OE1	32:0:42:HIS:ND1	2.43	0.51
19:O:43:ARG:HA	19:O:123:ILE:O	2.10	0.51
21:Q:144:ARG:HH12	27:W:53:G:H22	1.57	0.51
31:A:817:C:O2	31:A:2461:A:O2'	2.28	0.51
32:0:71:GLU:HG3	32:0:72:VAL:HG13	1.92	0.51
12:F:70:LYS:HD2	12:F:75:TYR:HB2	1.91	0.51
26:V:167:ILE:HG22	26:V:169:ASP:H	1.75	0.51
14:H:47:LYS:NZ	31:A:412:G:OP2	2.37	0.51
16:L:6:THR:OG1	16:L:21:CYS:SG	2.65	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:112:TYR:HB2	30:Z:84:LYS:HE2	1.91	0.51
27:W:61:G:N2	27:W:64:A:OP2	2.44	0.51
10:D:199:ILE:O	10:D:260:LYS:HA	2.11	0.51
30:Z:129:GLY:H	30:Z:132:LEU:HD12	1.76	0.51
31:A:290:A:H2'	31:A:291:G:H8	1.76	0.51
31:A:1424:A:HO2'	31:A:1490:G:HO2'	1.55	0.51
15:K:169:THR:HG23	15:K:170:GLN:HG2	1.93	0.51
18:N:124:LYS:NZ	31:A:2500:C:N3	2.48	0.51
26:V:52:GLU:HG3	26:V:53:ARG:HG3	1.92	0.51
26:V:138:LEU:HG	26:V:140:GLU:H	1.76	0.51
31:A:232:G:OP2	31:A:234:C:N4	2.43	0.51
31:A:1332:G:OP2	31:A:1332:G:N2	2.44	0.51
9:C:140:ILE:HD11	9:C:150:LEU:HD12	1.93	0.51
19:O:101:ASN:O	27:W:43:G:N2	2.43	0.51
24:T:99:ILE:HD11	24:T:137:ARG:HD3	1.92	0.51
27:W:30:A:O2'	27:W:38:G:O2'	2.28	0.51
2:2:45:ARG:NH2	31:A:2361:U:OP1	2.44	0.51
12:F:180:ASN:HB3	31:A:2332:G:H4'	1.92	0.51
1:1:45:SER:HA	19:O:108:ILE:HG23	1.93	0.50
31:A:545:U:H2'	31:A:546:G:H8	1.76	0.50
11:E:250:GLY:O	11:E:254:TYR:CB	2.60	0.50
20:P:103:LYS:HE3	20:P:122:LYS:HB3	1.92	0.50
31:A:804:A:OP2	31:A:2085:A:O2'	2.29	0.50
31:A:2492:C:N4	31:A:2546:G:H22	2.06	0.50
3:3:102:ARG:NH2	3:3:138:LYS:O	2.44	0.50
25:U:127:ASN:ND2	25:U:131:GLU:OE1	2.43	0.50
31:A:2108:G:H1	31:A:2209:U:H3	1.59	0.50
15:K:56:LYS:O	24:T:147:LYS:NZ	2.45	0.50
19:O:106:ARG:HE	19:O:124:GLU:HG3	1.76	0.50
20:P:125:GLU:OE2	20:P:162:HIS:NE2	2.42	0.50
4:4:118:GLN:NE2	31:A:2436:U:O4	2.45	0.50
9:C:56:ARG:HG3	9:C:81:PRO:HB2	1.92	0.50
13:G:119:VAL:HG12	13:G:176:ARG:HD2	1.93	0.50
18:N:115:ARG:O	18:N:119:ALA:HB3	2.12	0.50
6:6:113:ARG:NH1	31:A:1548:A:OP1	2.45	0.50
6:6:127:LYS:NZ	31:A:1402:G:OP2	2.45	0.50
9:C:194:VAL:HG13	31:A:1830:U:H3	1.77	0.50
21:Q:147:ASP:OD1	21:Q:211:HIS:ND1	2.40	0.50
26:V:67:ARG:HH12	26:V:92:ILE:HD11	1.77	0.50
9:C:27:ASN:ND2	31:A:1445:G:OP2	2.45	0.50
27:W:19:A:N3	31:A:2020:C:O2'	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:239:THR:N	31:A:2589:A:OP2	2.45	0.50
13:G:55:ALA:HB3	13:G:66:LYS:HB2	1.94	0.50
17:M:143:LEU:O	17:M:147:ALA:N	2.44	0.50
31:A:1391:C:O2'	31:A:1821:G:O2'	2.28	0.50
31:A:2308:U:O2'	31:A:2391:C:O2	2.30	0.50
15:K:155:VAL:HB	15:K:223:VAL:HG22	1.94	0.50
25:U:106:ARG:NH2	25:U:143:ASP:OD1	2.43	0.50
11:E:60:PHE:O	11:E:196:ARG:NH1	2.45	0.49
11:E:249:GLU:HA	11:E:252:ILE:HG22	1.94	0.49
22:R:52:ARG:O	22:R:56:ASP:HB2	2.11	0.49
30:Z:65:LEU:HB3	30:Z:68:LEU:HD13	1.93	0.49
31:A:2118:U:O2	31:A:2199:G:N2	2.37	0.49
22:R:11:ARG:NH2	31:A:524:A:O2'	2.45	0.49
22:R:17:ILE:HG22	22:R:35:ILE:HG22	1.94	0.49
27:W:54:A:OP2	27:W:70:G:N2	2.35	0.49
29:Y:92:ASN:OD1	29:Y:94:LYS:NZ	2.39	0.49
30:Z:86:GLU:HA	30:Z:89:MET:HE2	1.93	0.49
4:4:149:ALA:HB2	17:M:127:ARG:HG3	1.94	0.49
12:F:150:TYR:O	12:F:154:ASP:HB2	2.13	0.49
15:K:85:PHE:HB3	15:K:96:TRP:HZ2	1.78	0.49
26:V:75:VAL:HB	26:V:134:VAL:HB	1.93	0.49
31:A:883:C:H2'	31:A:884:G:H8	1.77	0.49
10:D:200:SER:HB2	10:D:291:ARG:HB2	1.94	0.49
31:A:1454:G:H2'	31:A:1455:A:H8	1.76	0.49
15:K:176:HIS:NE2	15:K:179:ARG:O	2.45	0.49
31:A:704:A:O2'	31:A:1374:A:N3	2.41	0.49
10:D:237:ALA:HB3	10:D:241:PRO:HG3	1.94	0.49
20:P:70:ARG:HH12	31:A:2395:A:H5"	1.78	0.49
24:T:111:LEU:HB2	24:T:127:ARG:HB3	1.93	0.49
31:A:864:U:H2'	31:A:865:A:H8	1.77	0.49
31:A:1874:U:OP1	31:A:2427:G:O2'	2.28	0.49
5:5:20:ARG:NH1	31:A:2758:A:OP1	2.46	0.49
9:C:46:THR:OG1	31:A:1815:U:O2	2.31	0.49
26:V:74:THR:OG1	26:V:137:ILE:O	2.31	0.49
31:A:596:A:H62	31:A:1272:A:H2	1.61	0.49
9:C:51:GLY:HA3	31:A:702:C:H5"	1.94	0.49
10:D:219:ARG:HH12	31:A:2006:G:H21	1.61	0.49
12:F:118:PRO:HB2	12:F:140:ILE:HG22	1.94	0.49
29:Y:87:ARG:HD2	29:Y:97:ARG:HD3	1.93	0.49
31:A:2114:G:H1	31:A:2203:U:H3	1.61	0.49
31:A:2422:G:O2'	31:A:2428:A:N6	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:101:ASN:OD1	27:W:44:U:O2'	2.30	0.48
24:T:79:LEU:O	24:T:83:ALA:HB2	2.13	0.48
31:A:699:U:H2'	31:A:700:A:H8	1.78	0.48
31:A:1935:G:H2'	31:A:1936:G:C8	2.48	0.48
11:E:250:GLY:O	11:E:254:TYR:HB2	2.13	0.48
17:M:135:PRO:HD2	17:M:138:ARG:HD2	1.94	0.48
21:Q:215:ARG:HD3	31:A:1763:G:H5"	1.95	0.48
22:R:78:TYR:CZ	22:R:82:ILE:HD11	2.49	0.48
31:A:1103:C:N4	31:A:1104:C:N4	2.61	0.48
31:A:2692:A:H61	31:A:2750:G:H1	1.61	0.48
10:D:117:PHE:O	10:D:274:ARG:NH2	2.47	0.48
29:Y:118:LYS:NZ	31:A:2234:G:OP1	2.38	0.48
31:A:693:G:O6	31:A:805:A:N6	2.46	0.48
31:A:2557:C:O2'	31:A:2758:A:N3	2.41	0.48
23:S:124:PHE:HE1	23:S:135:ILE:HG23	1.77	0.48
31:A:1401:G:H21	31:A:1604:A:H2	1.61	0.48
19:O:26:GLN:NE2	31:A:1296:A:O4'	2.46	0.48
31:A:827:C:OP1	31:A:1206:C:O2'	2.29	0.48
31:A:1052:G:H5"	31:A:1053:A:H5"	1.93	0.48
1:1:21:LYS:HG2	24:T:48:ARG:HB3	1.96	0.48
2:2:18:CYS:O	2:2:49:ARG:NH2	2.47	0.48
9:C:71:TYR:HA	9:C:113:VAL:HB	1.95	0.48
11:E:150:ILE:HG23	31:A:671:C:H5"	1.95	0.48
21:Q:138:ARG:NH1	21:Q:200:SER:O	2.47	0.48
31:A:2118:U:N3	31:A:2199:G:N1	2.51	0.48
3:3:96:THR:O	31:A:697:U:O2'	2.30	0.48
18:N:115:ARG:O	18:N:119:ALA:CB	2.62	0.48
22:R:114:GLU:HG3	23:S:172:ILE:HD13	1.94	0.48
31:A:932:A:H2'	31:A:933:G:H8	1.79	0.48
11:E:81:ARG:O	11:E:85:HIS:CB	2.61	0.48
23:S:145:GLN:HE21	31:A:1189:G:H1'	1.78	0.48
31:A:2490:U:OP1	31:A:2546:G:N2	2.44	0.48
9:C:116:THR:OG1	9:C:117:GLU:OE1	2.31	0.48
11:E:125:ARG:HE	31:A:685:G:H1'	1.78	0.48
11:E:222:ASN:O	31:A:332:G:O2'	2.28	0.48
18:N:51:ARG:HG3	18:N:64:ILE:HD11	1.94	0.48
19:O:31:LEU:HD23	19:O:54:MET:HE1	1.96	0.48
23:S:165:GLY:HA2	23:S:170:THR:HA	1.96	0.48
24:T:50:ILE:HD13	24:T:76:ILE:HD12	1.94	0.48
26:V:77:VAL:HG11	26:V:82:GLU:HG2	1.96	0.48
31:A:1757:G:H2'	31:A:1758:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:89:ILE:O	11:E:93:GLN:HB2	2.14	0.47
22:R:52:ARG:HG2	22:R:55:ARG:HE	1.78	0.47
31:A:615:G:H21	31:A:669:C:H5'	1.79	0.47
31:A:976:C:H2'	31:A:977:G:H8	1.78	0.47
31:A:2296:G:HO2'	31:A:2344:A:HO2'	1.62	0.47
31:A:2563:U:H5"	31:A:2564:U:H5'	1.97	0.47
9:C:254:ARG:NH2	31:A:1854:C:O3'	2.47	0.47
11:E:208:PHE:HB3	11:E:229:LEU:HB2	1.96	0.47
21:Q:124:GLY:O	21:Q:128:LYS:CB	2.63	0.47
31:A:133:A:O2'	31:A:134:A:N7	2.45	0.47
15:K:57:CYS:O	15:K:61:TRP:HB2	2.15	0.47
29:Y:120:ARG:NH1	31:A:1385:G:OP2	2.48	0.47
5:5:16:LEU:HD21	31:A:1060:A:H4'	1.96	0.47
10:D:204:ILE:HG21	10:D:285:LYS:HG2	1.96	0.47
15:K:123:ILE:HD11	15:K:126:ARG:HD2	1.97	0.47
15:K:131:ILE:HG23	15:K:153:VAL:HG21	1.96	0.47
21:Q:116:ARG:HH22	27:W:35:U:H5"	1.79	0.47
29:Y:87:ARG:HB3	29:Y:97:ARG:HE	1.79	0.47
31:A:744:G:N2	31:A:745:A:N7	2.63	0.47
31:A:2013:A:O3'	31:A:2740:G:N2	2.47	0.47
8:B:45:G:H3'	12:F:145:ARG:HH12	1.79	0.47
19:O:43:ARG:NE	19:O:124:GLU:OE1	2.44	0.47
31:A:182:A:H2	31:A:2451:A:H62	1.61	0.47
15:K:175:ARG:HH21	15:K:184:LYS:HD3	1.80	0.47
22:R:97:LEU:HA	22:R:100:ILE:HG12	1.96	0.47
31:A:2594:A:H5"	31:A:2595:G:H5'	1.97	0.47
1:1:13:LYS:HD3	31:A:1284:U:H5"	1.95	0.47
15:K:161:VAL:HG21	15:K:200:ILE:HD11	1.95	0.47
18:N:101:ARG:NH1	31:A:916:G:O2'	2.39	0.47
25:U:106:ARG:NH1	31:A:128:U:OP2	2.48	0.47
26:V:120:GLY:O	31:A:495:A:O2'	2.24	0.47
29:Y:108:VAL:HG21	29:Y:129:ILE:HD13	1.97	0.47
31:A:737:G:O5'	31:A:1453:G:O2'	2.31	0.47
31:A:1235:A:N6	31:A:1256:G:H21	2.01	0.47
31:A:1703:G:O2'	31:A:2005:U:O4	2.30	0.47
9:C:255:SER:OG	31:A:1813:A:O2'	2.32	0.47
10:D:223:THR:HG21	31:A:1712:A:H1'	1.97	0.47
31:A:599:C:H2'	31:A:600:A:H8	1.79	0.47
31:A:1513:C:H2'	31:A:1514:A:H8	1.79	0.47
31:A:2345:A:H2'	31:A:2346:A:C8	2.50	0.47
9:C:208:ARG:HD3	9:C:214:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:242:ALA:HB3	17:M:81:ARG:HD3	1.97	0.47
12:F:107:ILE:O	12:F:111:ALA:HB3	2.15	0.47
21:Q:217:ALA:HB2	27:W:52:G:C8	2.50	0.47
23:S:194:LYS:HG2	23:S:213:ARG:HD3	1.97	0.47
30:Z:107:ARG:HA	30:Z:110:LYS:HB3	1.97	0.47
31:A:1859:G:H2'	31:A:1860:G:H8	1.80	0.47
9:C:104:ARG:HB3	9:C:190:GLN:HG3	1.95	0.47
22:R:90:LEU:HD23	22:R:93:ASN:HD21	1.79	0.47
30:Z:135:LYS:O	30:Z:139:ALA:CB	2.63	0.47
31:A:890:G:H2'	31:A:891:G:H8	1.80	0.47
31:A:1407:C:H2'	31:A:1408:A:H8	1.80	0.47
31:A:1725:A:H2'	31:A:1726:A:H8	1.80	0.47
17:M:111:GLY:HA2	31:A:1211:G:H5"	1.96	0.46
17:M:131:GLY:O	31:A:842:G:N2	2.47	0.46
22:R:5:LYS:NZ	31:A:1219:U:O2	2.37	0.46
29:Y:74:ILE:HG22	29:Y:81:LYS:HG2	1.97	0.46
31:A:1466:G:O6	31:A:1485:U:O2	2.33	0.46
31:A:1844:U:O4	31:A:1914:A:N6	2.48	0.46
31:A:2270:G:H5"	31:A:2271:C:H5	1.80	0.46
3:3:146:ARG:HH12	25:U:140:VAL:HG11	1.80	0.46
6:6:123:ARG:NH1	31:A:1404:C:OP2	2.49	0.46
18:N:38:GLU:HB3	18:N:127:ILE:HB	1.97	0.46
31:A:8:G:O2'	31:A:2646:U:O4	2.28	0.46
31:A:1487:C:H42	31:A:1557:G:N2	2.13	0.46
9:C:34:ARG:NH2	9:C:40:ASN:O	2.49	0.46
24:T:138:ASP:OD1	24:T:139:ILE:N	2.49	0.46
28:X:152:ALA:O	28:X:156:GLU:HB2	2.16	0.46
10:D:115:ILE:O	10:D:275:VAL:HA	2.15	0.46
16:L:38:VAL:HG12	16:L:61:VAL:HG22	1.97	0.46
17:M:215:ARG:HG3	17:M:216:ALA:H	1.81	0.46
20:P:160:ARG:NH1	31:A:2393:A:O2'	2.31	0.46
31:A:55:G:H1	31:A:112:C:N4	2.11	0.46
31:A:715:G:O2'	31:A:737:G:N2	2.43	0.46
15:K:84:MET:HE2	15:K:84:MET:HB2	1.56	0.46
22:R:81:PHE:O	22:R:85:LEU:CB	2.60	0.46
28:X:88:LYS:HB2	28:X:91:ALA:HB2	1.98	0.46
9:C:57:LEU:O	9:C:59:ARG:NH2	2.47	0.46
22:R:10:ALA:O	22:R:14:ARG:CB	2.63	0.46
7:7:60:MET:SD	31:A:977:G:O2'	2.66	0.46
8:B:41:U:H1'	8:B:46:A:H61	1.80	0.46
31:A:309:A:N3	31:A:328:C:O2'	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G:128:GLN:HA	13:G:170:LYS:HA	1.97	0.46
17:M:115:ARG:NH1	31:A:578:U:OP1	2.49	0.46
20:P:138:LYS:HA	20:P:165:VAL:HB	1.98	0.46
9:C:174:SER:OG	31:A:1809:G:O6	2.30	0.46
9:C:269:ARG:HH22	31:A:1808:C:H5	1.63	0.46
18:N:39:PRO:HD3	18:N:99:PRO:HG3	1.98	0.46
28:X:76:ARG:HD2	31:A:2373:C:H4'	1.98	0.46
31:A:652:C:N4	31:A:657:U:O4	2.49	0.46
31:A:1384:C:O2'	31:A:1819:A:N3	2.46	0.46
11:E:148:TRP:CD1	11:E:150:ILE:HG12	2.51	0.45
19:O:38:LEU:HD22	19:O:58:VAL:HG21	1.97	0.45
31:A:1406:A:O2'	31:A:1417:U:O2	2.30	0.45
31:A:1423:U:O2'	31:A:1555:G:O2'	2.33	0.45
31:A:1640:C:O2'	31:A:1646:A:N1	2.38	0.45
10:D:222:MET:HB3	31:A:2007:U:H5'	1.98	0.45
11:E:82:ALA:HB2	17:M:88:GLN:HG3	1.99	0.45
21:Q:218:ARG:HG2	31:A:2736:G:H4'	1.99	0.45
26:V:136:LEU:HD13	26:V:168:VAL:HG11	1.99	0.45
31:A:2085:A:H2'	31:A:2086:G:H8	1.80	0.45
9:C:256:ARG:NH1	31:A:1809:G:OP1	2.50	0.45
18:N:56:ARG:NE	31:A:2486:A:O2'	2.49	0.45
24:T:113:LYS:HE2	31:A:1344:G:H5"	1.97	0.45
31:A:1871:U:H2'	31:A:1872:G:H8	1.81	0.45
31:A:2051:G:H2'	31:A:2052:G:C8	2.52	0.45
31:A:2116:C:N3	31:A:2201:G:O6	2.49	0.45
31:A:2417:G:H1	31:A:2433:C:H42	1.63	0.45
11:E:59:ASN:HB3	11:E:178:PHE:HE1	1.82	0.45
12:F:178:HIS:HB2	12:F:181:TYR:HA	1.98	0.45
13:G:165:VAL:HG22	13:G:171:VAL:HG22	1.99	0.45
20:P:100:THR:O	20:P:104:ALA:CB	2.64	0.45
22:R:52:ARG:HD2	22:R:55:ARG:HH11	1.81	0.45
22:R:82:ILE:HA	22:R:85:LEU:HB3	1.98	0.45
29:Y:100:PHE:CE2	31:A:2247:C:H5"	2.51	0.45
31:A:1844:U:H5"	31:A:1845:G:H5'	1.99	0.45
9:C:37:LYS:NZ	31:A:1825:A:OP2	2.47	0.45
19:O:106:ARG:HB3	19:O:124:GLU:HB2	1.97	0.45
22:R:33:ARG:NH2	31:A:588:A:O2'	2.49	0.45
31:A:1433:U:H2'	31:A:1434:G:C8	2.52	0.45
31:A:2009:U:H3'	31:A:2010:C:H2'	1.99	0.45
13:G:163:VAL:HG12	13:G:173:VAL:HA	1.98	0.45
18:N:28:CYS:HB2	18:N:67:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:116:GLN:HB2	25:U:137:THR:O	2.16	0.45
26:V:67:ARG:HD3	26:V:97:SER:HA	1.98	0.45
31:A:170:U:H2'	31:A:171:G:H8	1.82	0.45
31:A:241:A:H2'	31:A:242:A:H8	1.81	0.45
31:A:471:U:H2'	31:A:472:A:H8	1.81	0.45
11:E:81:ARG:O	11:E:85:HIS:HB2	2.17	0.45
24:T:111:LEU:O	24:T:126:LYS:HA	2.17	0.45
9:C:37:LYS:HD3	9:C:56:ARG:HH22	1.81	0.45
31:A:313:A:N1	31:A:323:G:C6	2.85	0.45
31:A:1732:G:N2	31:A:1991:A:O2'	2.50	0.45
4:4:119:HIS:CE1	4:4:120:LEU:HD13	2.52	0.45
25:U:121:THR:HG23	25:U:124:ALA:H	1.82	0.45
26:V:110:HIS:HB3	31:A:495:A:H5'	1.99	0.45
4:4:107:LYS:HB2	31:A:663:A:H5'	1.99	0.45
5:5:7:VAL:HG12	5:5:36:GLN:HE22	1.82	0.45
21:Q:149:VAL:HG12	21:Q:208:VAL:HA	1.98	0.45
30:Z:120:ARG:NE	30:Z:123:GLU:OE1	2.50	0.45
31:A:309:A:N1	31:A:331:A:O2'	2.37	0.45
31:A:1454:G:H2'	31:A:1455:A:C8	2.52	0.45
31:A:1529:A:H2'	31:A:1530:G:C8	2.52	0.45
31:A:1599:C:O2	31:A:1600:A:O2'	2.31	0.45
26:V:157:LYS:NZ	31:A:306:G:O3'	2.50	0.44
31:A:1408:A:H5'	31:A:1488:A:H1'	1.99	0.44
31:A:1604:A:H2'	31:A:1605:A:C8	2.52	0.44
5:5:6:SER:O	5:5:6:SER:OG	2.26	0.44
8:B:8:G:O6	8:B:115:C:N4	2.50	0.44
9:C:65:ARG:HH12	9:C:124:ASN:HA	1.81	0.44
11:E:162:SER:O	11:E:166:ALA:HB2	2.17	0.44
15:K:115:TYR:HB2	15:K:153:VAL:HG12	2.00	0.44
16:L:11:ALA:O	16:L:99:PHE:N	2.46	0.44
24:T:58:TYR:O	24:T:62:LEU:HB2	2.17	0.44
26:V:90:SER:HB2	26:V:102:LYS:HD3	2.00	0.44
31:A:1077:C:H2'	31:A:1078:A:H8	1.82	0.44
1:1:18:ASN:ND2	31:A:14:A:O3'	2.48	0.44
8:B:92:U:OP1	18:N:17:MET:N	2.50	0.44
10:D:145:ARG:HE	10:D:147:ARG:HD2	1.82	0.44
11:E:202:ALA:HA	11:E:225:THR:HG21	1.98	0.44
17:M:161:ASN:HD21	31:A:639:A:H62	1.65	0.44
20:P:126:MET:HA	20:P:129:LYS:HG2	2.00	0.44
26:V:149:HIS:HB2	31:A:307:C:H5"	2.00	0.44
31:A:199:G:N2	31:A:201:A:N3	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:1739:G:H2'	31:A:1740:G:H8	1.82	0.44
17:M:203:GLU:HG2	31:A:649:A:H8	1.83	0.44
18:N:124:LYS:NZ	31:A:2484:C:O2	2.46	0.44
19:O:77:LEU:HA	19:O:86:VAL:HG21	1.98	0.44
31:A:885:G:H1	31:A:911:U:H3	1.63	0.44
31:A:1994:G:O2'	31:A:1996:U:OP2	2.32	0.44
3:3:142:SER:O	31:A:1636:U:O2'	2.28	0.44
31:A:605:C:H2'	31:A:606:A:H8	1.82	0.44
31:A:1238:G:H1	31:A:1252:C:N4	2.15	0.44
31:A:1605:A:H2'	31:A:1606:A:C8	2.52	0.44
15:K:116:VAL:HG22	15:K:154:ILE:HB	2.00	0.44
16:L:15:GLY:HA3	16:L:50:THR:HG21	1.99	0.44
20:P:128:ALA:HB1	20:P:162:HIS:HB2	1.99	0.44
28:X:122:LEU:O	28:X:137:VAL:HA	2.17	0.44
31:A:1468:C:O2'	31:A:1578:A:N3	2.39	0.44
31:A:1665:U:O4	31:A:1666:A:N6	2.51	0.44
31:A:1873:G:H4'	31:A:2428:A:H4'	1.99	0.44
29:Y:77:PHE:HA	29:Y:141:ALA:HB2	1.99	0.44
31:A:631:G:OP2	31:A:632:G:N2	2.51	0.44
31:A:1354:C:H2'	31:A:1355:G:H8	1.83	0.44
31:A:1968:G:H5'	31:A:2567:G:H21	1.82	0.44
9:C:152:ARG:NE	31:A:1828:U:OP2	2.50	0.44
18:N:33:ALA:O	18:N:131:PHE:HA	2.17	0.44
25:U:157:VAL:HG21	25:U:178:LEU:HD13	1.99	0.44
31:A:144:A:N3	31:A:2223:A:O2'	2.48	0.44
31:A:545:U:H2'	31:A:546:G:C8	2.53	0.44
31:A:1157:A:O2'	31:A:2532:C:O2	2.31	0.44
19:O:80:ILE:HD12	19:O:86:VAL:HG22	2.01	0.43
23:S:145:GLN:NE2	23:S:214:GLN:OE1	2.51	0.43
8:B:91:G:N2	18:N:38:GLU:OE2	2.46	0.43
11:E:158:ARG:NH1	31:A:630:C:OP2	2.51	0.43
11:E:251:THR:O	11:E:255:LEU:CB	2.62	0.43
31:A:818:U:O2'	31:A:2074:A:N1	2.51	0.43
31:A:2022:C:H2'	31:A:2023:G:H8	1.82	0.43
31:A:2601:U:H5'	31:A:2602:U:H5'	2.00	0.43
10:D:125:GLN:O	10:D:138:GLN:CB	2.63	0.43
21:Q:217:ALA:HB2	27:W:52:G:H8	1.83	0.43
23:S:188:GLU:OE2	23:S:218:ARG:NH1	2.52	0.43
31:A:570:C:H2'	31:A:571:G:C8	2.53	0.43
31:A:794:A:H2'	31:A:795:U:H4'	2.01	0.43
31:A:1487:C:H42	31:A:1557:G:H22	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:106:ALA:HB2	31:A:812:G:H8	1.83	0.43
12:F:68:LEU:HA	12:F:71:GLU:HG2	2.00	0.43
31:A:1015:C:O2'	31:A:1028:A:N3	2.43	0.43
31:A:1704:A:N3	31:A:1706:C:N4	2.66	0.43
31:A:2464:G:C8	31:A:2518:C:H5"	2.53	0.43
31:A:2627:C:H4'	31:A:2628:C:H5'	2.00	0.43
18:N:36:ALA:HA	18:N:129:THR:HG22	2.00	0.43
22:R:31:LEU:HD12	22:R:31:LEU:HA	1.84	0.43
31:A:1407:C:H2'	31:A:1408:A:C8	2.53	0.43
20:P:73:LEU:HD23	20:P:139:VAL:HG21	2.00	0.43
31:A:330:U:O2'	31:A:349:A:N3	2.52	0.43
31:A:426:C:H2'	31:A:427:A:C8	2.54	0.43
31:A:591:C:H2'	31:A:592:G:C8	2.54	0.43
31:A:645:A:O2'	31:A:2421:C:OP1	2.32	0.43
19:O:38:LEU:HD11	19:O:123:ILE:HG21	1.99	0.43
31:A:1118:U:H2'	31:A:1119:G:C8	2.54	0.43
31:A:1154:A:H4'	31:A:1155:A:H5"	2.00	0.43
31:A:2204:A:H3'	31:A:2205:G:H8	1.84	0.43
31:A:2599:G:C2	31:A:2600:G:H1'	2.53	0.43
2:2:46:LEU:HB2	2:2:57:LYS:HD2	2.00	0.43
4:4:112:ARG:NH1	31:A:2377:C:OP1	2.51	0.43
13:G:43:ILE:HG12	31:A:2769:G:H4'	2.01	0.43
27:W:13:G:N2	27:W:40:U:O2'	2.43	0.43
13:G:129:LEU:HG	13:G:202:VAL:HG22	2.00	0.43
29:Y:107:ARG:HA	29:Y:117:VAL:O	2.19	0.43
30:Z:107:ARG:O	30:Z:111:ARG:HB2	2.19	0.43
31:A:92:U:H2'	31:A:93:A:C8	2.54	0.43
31:A:226:A:H61	31:A:240:A:H5"	1.84	0.43
31:A:1986:G:H2'	31:A:1987:G:C8	2.54	0.43
30:Z:72:THR:OG1	30:Z:75:GLN:OE1	2.37	0.42
31:A:919:A:H2'	31:A:920:A:C8	2.54	0.42
31:A:2316:G:H2'	31:A:2317:G:C8	2.54	0.42
31:A:2539:U:C2	31:A:2783:A:N7	2.87	0.42
4:4:140:ARG:HA	4:4:143:TYR:HB3	2.01	0.42
6:6:116:ARG:NH2	31:A:1405:A:OP1	2.49	0.42
15:K:214:GLY:HA2	15:K:217:LEU:HG	2.01	0.42
20:P:73:LEU:HB3	20:P:86:VAL:HG22	2.01	0.42
31:A:74:G:H22	31:A:109:A:H2	1.67	0.42
31:A:592:G:H2'	31:A:593:G:H8	1.84	0.42
31:A:825:C:O2'	31:A:1245:U:O2	2.29	0.42
10:D:135:ASN:HD22	10:D:175:SER:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:88:VAL:HG11	31:A:2331:G:H5'	2.01	0.42
16:L:21:CYS:HA	16:L:41:ALA:HA	2.01	0.42
31:A:383:A:H61	31:A:413:A:H3'	1.84	0.42
20:P:124:GLY:HA2	20:P:127:ILE:HG22	2.02	0.42
31:A:468:U:O2	31:A:471:U:O2'	2.35	0.42
31:A:1450:G:H2'	31:A:1451:G:C8	2.55	0.42
7:7:88:GLU:HG3	7:7:89:TRP:CD1	2.54	0.42
8:B:92:U:H5'	18:N:17:MET:HB2	2.00	0.42
9:C:68:LYS:HB3	9:C:115:GLY:HA2	2.01	0.42
13:G:166:GLU:OE2	13:G:170:LYS:NZ	2.52	0.42
30:Z:88:PHE:HA	30:Z:91:ARG:HE	1.85	0.42
31:A:867:G:N2	31:A:2286:A:O4'	2.51	0.42
31:A:2283:A:N6	31:A:2290:A:OP2	2.52	0.42
10:D:269:ILE:HG22	10:D:276:VAL:HG13	2.01	0.42
13:G:43:ILE:HG13	31:A:2766:A:H5'	2.02	0.42
18:N:53:ALA:O	18:N:57:ASN:HB2	2.19	0.42
31:A:25:G:H4'	31:A:1281:G:H4'	2.02	0.42
8:B:78:U:O2	8:B:101:A:N7	2.53	0.42
31:A:2308:U:H2'	31:A:2309:U:C6	2.55	0.42
11:E:133:LEU:O	31:A:1277:G:N2	2.53	0.42
15:K:147:VAL:HG23	15:K:149:MET:HG2	2.00	0.42
18:N:6:ARG:HB3	31:A:880:U:H5"	2.01	0.42
31:A:146:U:O2	31:A:148:C:N4	2.45	0.42
31:A:587:G:O2'	31:A:1275:A:OP1	2.38	0.42
31:A:818:U:H2'	31:A:819:G:C8	2.55	0.42
31:A:843:C:H2'	31:A:844:G:C8	2.54	0.42
31:A:1125:U:H3'	31:A:1126:A:H8	1.84	0.42
31:A:1874:U:O3'	31:A:2426:G:N2	2.50	0.42
18:N:12:GLN:HA	31:A:919:A:H62	1.84	0.42
20:P:70:ARG:NH2	20:P:139:VAL:O	2.40	0.42
21:Q:127:ASN:HD21	21:Q:177:ILE:N	2.18	0.42
31:A:10:G:H2'	31:A:11:G:C8	2.55	0.42
31:A:2047:A:O2'	31:A:2049:G:OP2	2.31	0.42
12:F:126:SER:HA	12:F:132:VAL:HG12	2.02	0.42
21:Q:141:PRO:HD2	21:Q:206:ILE:HD11	2.02	0.42
28:X:122:LEU:HG	28:X:140:ARG:HG3	2.01	0.42
29:Y:99:GLN:HG3	31:A:2248:U:H5"	2.02	0.42
31:A:932:A:H2'	31:A:933:G:C8	2.55	0.42
9:C:228:HIS:CE1	9:C:237:ILE:HG13	2.55	0.41
10:D:95:THR:HG21	10:D:118:LYS:HE3	2.02	0.41
18:N:13:HIS:CD2	31:A:982:G:H5"	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:27:ALA:O	22:R:34:THR:OG1	2.36	0.41
7:7:69:ARG:HG3	7:7:73:LYS:NZ	2.35	0.41
23:S:182:VAL:HG22	23:S:224:ILE:HG12	2.02	0.41
28:X:101:PHE:HB3	28:X:135:VAL:HG23	2.02	0.41
31:A:1060:A:N1	31:A:1150:G:O6	2.53	0.41
31:A:1843:C:H42	31:A:1986:G:H1	1.68	0.41
11:E:102:THR:HG21	11:E:142:GLY:HA3	2.02	0.41
17:M:223:GLU:O	17:M:227:ALA:HB2	2.20	0.41
24:T:103:ALA:HA	24:T:134:ILE:HA	2.02	0.41
10:D:141:TYR:CD2	10:D:142:GLU:HG3	2.55	0.41
11:E:96:ARG:HD2	31:A:455:A:C6	2.55	0.41
20:P:125:GLU:HG3	20:P:129:LYS:HE3	2.01	0.41
31:A:1063:U:H2'	31:A:1064:A:C8	2.55	0.41
7:7:54:LYS:O	7:7:58:HIS:N	2.50	0.41
17:M:210:LEU:H	17:M:230:CYS:HB2	1.85	0.41
24:T:47:ARG:HH22	31:A:529:G:P	2.43	0.41
25:U:105:PRO:O	31:A:131:C:N4	2.54	0.41
31:A:656:A:H61	31:A:2366:G:N2	2.19	0.41
31:A:2316:G:H2'	31:A:2317:G:H8	1.85	0.41
8:B:32:A:H61	8:B:54:G:H21	1.69	0.41
20:P:143:ARG:HH11	31:A:2310:U:H5"	1.85	0.41
22:R:33:ARG:HG2	31:A:1273:G:H21	1.86	0.41
23:S:202:LYS:HG3	23:S:203:LYS:H	1.86	0.41
29:Y:95:THR:HG21	31:A:2095:U:H4'	2.01	0.41
31:A:1330:G:H21	31:A:1647:C:H5'	1.85	0.41
31:A:2767:A:H3'	31:A:2768:A:H5"	2.01	0.41
10:D:149:LEU:HD21	10:D:157:LEU:HD12	2.02	0.41
13:G:134:TYR:HA	13:G:146:SER:O	2.21	0.41
22:R:49:ASP:OD1	31:A:569:G:N2	2.53	0.41
24:T:102:LYS:HG2	24:T:135:VAL:HB	2.02	0.41
27:W:26:G:H8	27:W:87:A:H2	1.67	0.41
27:W:51:U:O2	31:A:2709:C:O2'	2.39	0.41
31:A:838:U:O2'	31:A:2082:U:N3	2.53	0.41
12:F:107:ILE:O	12:F:111:ALA:HB2	2.18	0.41
12:F:175:PHE:HA	31:A:2320:G:H4'	2.02	0.41
22:R:28:HIS:HB3	22:R:38:GLN:HG3	2.01	0.41
31:A:530:U:H2'	31:A:531:A:H8	1.86	0.41
31:A:865:A:H2'	31:A:866:G:H8	1.85	0.41
5:5:10:ILE:HG21	31:A:2494:C:H42	1.85	0.41
9:C:88:CYS:O	9:C:99:TYR:HA	2.21	0.41
19:O:12:LYS:HB2	31:A:1689:C:H3'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:W:67:U:H2'	27:W:68:A:C8	2.56	0.41
31:A:538:C:N4	31:A:2797:U:OP2	2.40	0.41
31:A:682:C:H2'	31:A:683:C:H6	1.85	0.41
31:A:1762:C:H42	31:A:1766:G:H1	1.69	0.41
10:D:167:HIS:CD2	10:D:289:LEU:HD22	2.56	0.41
14:H:74:LEU:HA	14:H:78:LEU:HB2	2.01	0.41
24:T:33:THR:HG22	24:T:135:VAL:HG22	2.02	0.41
27:W:59:C:H2'	27:W:60:A:H8	1.86	0.41
28:X:154:LYS:NZ	31:A:960:A:N1	2.69	0.41
15:K:119:ALA:HA	15:K:122:LEU:HD12	2.03	0.40
20:P:126:MET:O	20:P:130:SER:HB3	2.21	0.40
29:Y:103:LEU:HA	29:Y:122:SER:HA	2.03	0.40
31:A:1487:C:N4	31:A:1557:G:H22	2.18	0.40
7:7:80:PRO:HA	7:7:81:PRO:HD3	1.93	0.40
9:C:94:ASP:HA	31:A:1530:G:H21	1.86	0.40
10:D:157:LEU:HD13	10:D:165:MET:H	1.87	0.40
11:E:254:TYR:OH	11:E:258:ARG:NH1	2.39	0.40
12:F:132:VAL:HG22	12:F:138:LEU:HD21	2.03	0.40
13:G:160:GLU:OE1	13:G:176:ARG:NH2	2.49	0.40
20:P:76:PHE:HB3	20:P:83:TYR:HB2	2.03	0.40
20:P:127:ILE:HD12	20:P:127:ILE:HA	1.98	0.40
22:R:36:ALA:O	22:R:40:ILE:HG12	2.22	0.40
31:A:577:G:H21	31:A:581:A:H8	1.68	0.40
31:A:1488:A:H2'	31:A:1489:A:C8	2.56	0.40
31:A:2356:G:H2'	31:A:2357:A:H8	1.86	0.40
31:A:2653:U:H3	31:A:2800:G:H1	1.69	0.40
20:P:123:ILE:HD12	20:P:123:ILE:HA	1.87	0.40
31:A:1941:A:H2'	31:A:1942:A:C8	2.56	0.40
9:C:255:SER:HG	31:A:1807:C:HO2'	1.68	0.40
21:Q:174:ASN:HB3	21:Q:179:THR:HG23	2.02	0.40
25:U:140:VAL:HA	25:U:172:LYS:HE3	2.04	0.40
30:Z:104:ASP:O	30:Z:108:MET:HB2	2.21	0.40
31:A:568:C:H2'	31:A:569:G:C8	2.57	0.40
31:A:864:U:H2'	31:A:865:A:C8	2.57	0.40
31:A:1592:A:H4'	31:A:1593:U:H3'	2.02	0.40
31:A:2118:U:O4	31:A:2199:G:O6	2.40	0.40
31:A:2149:A:H3'	31:A:2150:G:H8	1.87	0.40
31:A:2464:G:N7	31:A:2518:C:H2'	2.36	0.40
32:0:93:GLN:HG2	32:0:94:VAL:HG23	2.04	0.40
1:1:11:TYR:O	1:1:15:ILE:HG12	2.22	0.40
11:E:233:SER:OG	31:A:623:A:N6	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:84:GLY:HA3	28:X:67:LYS:NZ	2.37	0.40
22:R:82:ILE:HD12	31:A:1179:C:H4'	2.04	0.40
23:S:192:ASP:HB3	23:S:216:ILE:HD13	2.04	0.40
31:A:426:C:H2'	31:A:427:A:H8	1.85	0.40
31:A:828:C:O2'	31:A:850:G:OP1	2.33	0.40
31:A:1346:U:OP1	31:A:1683:G:O2'	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	44/56 (79%)	39 (89%)	5 (11%)	0	100	100
2	2	49/65 (75%)	39 (80%)	10 (20%)	0	100	100
3	3	55/61 (90%)	49 (89%)	6 (11%)	0	100	100
4	4	67/73 (92%)	59 (88%)	8 (12%)	0	100	100
5	5	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
6	6	47/142 (33%)	46 (98%)	1 (2%)	0	100	100
7	7	44/116 (38%)	41 (93%)	3 (7%)	0	100	100
9	C	245/271 (90%)	213 (87%)	32 (13%)	0	100	100
10	D	210/221 (95%)	188 (90%)	22 (10%)	0	100	100
11	E	208/243 (86%)	180 (86%)	28 (14%)	0	100	100
12	F	173/220 (79%)	161 (93%)	12 (7%)	0	100	100
13	G	171/182 (94%)	161 (94%)	10 (6%)	0	100	100
14	H	51/155 (33%)	47 (92%)	4 (8%)	0	100	100
15	K	191/197 (97%)	178 (93%)	13 (7%)	0	100	100
16	L	119/121 (98%)	103 (87%)	16 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	M	175/192 (91%)	163 (93%)	11 (6%)	1 (1%)	25	57
18	N	132/135 (98%)	111 (84%)	21 (16%)	0	100	100
19	O	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
20	P	118/123 (96%)	116 (98%)	2 (2%)	0	100	100
21	Q	116/156 (74%)	100 (86%)	16 (14%)	0	100	100
22	R	113/127 (89%)	105 (93%)	8 (7%)	0	100	100
23	S	145/201 (72%)	118 (81%)	27 (19%)	0	100	100
24	T	142/199 (71%)	126 (89%)	16 (11%)	0	100	100
25	U	90/122 (74%)	86 (96%)	4 (4%)	0	100	100
26	V	122/145 (84%)	109 (89%)	13 (11%)	0	100	100
28	X	98/137 (72%)	87 (89%)	11 (11%)	0	100	100
29	Y	72/77 (94%)	66 (92%)	6 (8%)	0	100	100
30	Z	88/109 (81%)	87 (99%)	1 (1%)	0	100	100
32	0	62/94 (66%)	54 (87%)	6 (10%)	2 (3%)	4	22
All	All	3296/4093 (80%)	2967 (90%)	326 (10%)	3 (0%)	54	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	0	72	VAL
17	M	197	PRO
32	0	73	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	39/49 (80%)	39 (100%)	0	100	100
2	2	48/59 (81%)	46 (96%)	2 (4%)	30	60
3	3	47/50 (94%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	59/62 (95%)	58 (98%)	1 (2%)	60	78
5	5	34/34 (100%)	34 (100%)	0	100	100
6	6	46/124 (37%)	46 (100%)	0	100	100
7	7	40/96 (42%)	40 (100%)	0	100	100
9	C	195/216 (90%)	194 (100%)	1 (0%)	88	93
10	D	174/182 (96%)	174 (100%)	0	100	100
11	E	176/205 (86%)	173 (98%)	3 (2%)	60	78
12	F	148/183 (81%)	148 (100%)	0	100	100
13	G	147/154 (96%)	147 (100%)	0	100	100
14	H	47/134 (35%)	47 (100%)	0	100	100
15	K	167/171 (98%)	165 (99%)	2 (1%)	71	83
16	L	101/101 (100%)	101 (100%)	0	100	100
17	M	135/144 (94%)	133 (98%)	2 (2%)	65	81
18	N	107/108 (99%)	107 (100%)	0	100	100
19	O	96/96 (100%)	96 (100%)	0	100	100
20	P	99/100 (99%)	99 (100%)	0	100	100
21	Q	104/135 (77%)	103 (99%)	1 (1%)	76	86
22	R	102/114 (90%)	102 (100%)	0	100	100
23	S	129/174 (74%)	129 (100%)	0	100	100
24	T	126/176 (72%)	126 (100%)	0	100	100
25	U	81/103 (79%)	80 (99%)	1 (1%)	71	83
26	V	112/129 (87%)	111 (99%)	1 (1%)	78	87
28	X	85/111 (77%)	84 (99%)	1 (1%)	71	83
29	Y	64/67 (96%)	63 (98%)	1 (2%)	62	79
30	Z	83/97 (86%)	82 (99%)	1 (1%)	71	83
32	0	56/83 (68%)	55 (98%)	1 (2%)	59	78
All	All	2847/3457 (82%)	2829 (99%)	18 (1%)	86	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	13	LEU
2	2	48	LEU

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Mol	Chain	Res	Type
4	4	153	LEU
9	C	39	ARG
11	E	71	ASN
11	E	81	ARG
11	E	245	LEU
15	K	62	ARG
15	K	174	ARG
17	M	196	LEU
17	M	252	ARG
21	Q	127	ASN
25	U	106	ARG
26	V	64	LEU
28	X	73	LYS
29	Y	103	LEU
30	Z	107	ARG
32	0	76	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	58	HIS
4	4	95	HIS
4	4	118	GLN
4	4	145	ASN
9	C	54	HIS
9	C	84	ASN
10	D	167	HIS
10	D	209	GLN
11	E	71	ASN
11	E	118	GLN
11	E	153	ASN
12	F	60	ASN
12	F	77	ASN
12	F	116	GLN
13	G	103	GLN
15	K	97	ASN
15	K	139	ASN
16	L	3	GLN
16	L	73	ASN
16	L	82	ASN
17	M	161	ASN
18	N	13	HIS

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Mol	Chain	Res	Type
19	O	37	GLN
20	P	81	HIS
21	Q	127	ASN
22	R	28	HIS
22	R	77	ASN
22	R	93	ASN
22	R	99	GLN
23	S	145	GLN
23	S	212	HIS
23	S	214	GLN
24	T	52	GLN
24	T	106	ASN
26	V	130	HIS
32	0	76	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	W	101/106 (95%)	30 (29%)	4 (3%)
31	A	2808/2810 (99%)	592 (21%)	3 (0%)
8	B	116/121 (95%)	21 (18%)	1 (0%)
All	All	3025/3037 (99%)	643 (21%)	8 (0%)

All (643) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	B	4	U
8	B	10	G
8	B	14	U
8	B	15	A
8	B	16	G
8	B	25	G
8	B	31	C
8	B	36	A
8	B	42	C
8	B	53	U
8	B	54	G
8	B	58	A
8	B	61	C
8	B	67	U
8	B	74	A

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Mol	Chain	Res	Type
8	B	89	A
8	B	92	U
8	B	101	A
8	B	111	G
8	B	117	A
8	B	119	G
27	W	16	G
27	W	17	A
27	W	22	A
27	W	23	G
27	W	28	U
27	W	29	U
27	W	30	A
27	W	31	U
27	W	32	C
27	W	33	A
27	W	34	U
27	W	35	U
27	W	36	A
27	W	37	C
27	W	38	G
27	W	39	A
27	W	48	A
27	W	53	G
27	W	64	A
27	W	65	U
27	W	71	C
27	W	76	G
27	W	77	A
27	W	83	C
27	W	84	C
27	W	88	C
27	W	90	G
27	W	95	A
27	W	97	A
27	W	98	G
31	A	9	A
31	A	10	G
31	A	11	G
31	A	12	A
31	A	13	A
31	A	14	A

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Mol	Chain	Res	Type
31	A	15	G
31	A	26	G
31	A	33	A
31	A	45	A
31	A	46	C
31	A	54	G
31	A	70	A
31	A	72	A
31	A	73	U
31	A	74	G
31	A	82	G
31	A	84	G
31	A	85	U
31	A	98	G
31	A	99	A
31	A	100	G
31	A	112	C
31	A	116	A
31	A	117	A
31	A	118	U
31	A	123	C
31	A	130	U
31	A	131	C
31	A	143	G
31	A	144	A
31	A	147	C
31	A	149	A
31	A	158	C
31	A	159	A
31	A	173	C
31	A	181	A
31	A	184	A
31	A	189	A
31	A	201	A
31	A	207	A
31	A	226	A
31	A	233	G
31	A	250	A
31	A	251	G
31	A	252	C
31	A	262	G
31	A	264	A

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Mol	Chain	Res	Type
31	A	266	A
31	A	275	U
31	A	276	G
31	A	284	A
31	A	287	A
31	A	294	U
31	A	295	C
31	A	297	U
31	A	298	G
31	A	304	A
31	A	316	G
31	A	320	U
31	A	330	U
31	A	331	A
31	A	332	G
31	A	333	A
31	A	338	G
31	A	340	A
31	A	347	G
31	A	352	C
31	A	361	C
31	A	365	A
31	A	368	U
31	A	370	A
31	A	377	G
31	A	378	A
31	A	379	C
31	A	383	A
31	A	384	G
31	A	392	G
31	A	398	G
31	A	399	U
31	A	415	U
31	A	416	C
31	A	417	A
31	A	418	G
31	A	423	G
31	A	424	A
31	A	436	G
31	A	447	C
31	A	448	C
31	A	466	A

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Mol	Chain	Res	Type
31	A	467	G
31	A	468	U
31	A	469	A
31	A	479	G
31	A	489	A
31	A	491	A
31	A	493	G
31	A	504	G
31	A	507	G
31	A	512	A
31	A	515	U
31	A	516	A
31	A	519	A
31	A	524	A
31	A	529	G
31	A	541	G
31	A	542	C
31	A	543	A
31	A	544	G
31	A	545	U
31	A	554	G
31	A	555	A
31	A	557	C
31	A	558	A
31	A	559	G
31	A	560	A
31	A	573	G
31	A	583	G
31	A	585	A
31	A	608	U
31	A	609	G
31	A	610	G
31	A	611	C
31	A	613	U
31	A	614	G
31	A	623	A
31	A	624	A
31	A	630	C
31	A	632	G
31	A	633	A
31	A	638	U
31	A	639	A

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Mol	Chain	Res	Type
31	A	643	A
31	A	646	G
31	A	649	A
31	A	657	U
31	A	665	U
31	A	667	G
31	A	680	G
31	A	686	A
31	A	688	C
31	A	696	A
31	A	697	U
31	A	722	G
31	A	724	G
31	A	728	A
31	A	731	U
31	A	734	G
31	A	737	G
31	A	740	G
31	A	741	U
31	A	745	A
31	A	757	U
31	A	758	U
31	A	768	G
31	A	773	U
31	A	775	A
31	A	776	G
31	A	782	G
31	A	786	G
31	A	787	G
31	A	788	G
31	A	793	A
31	A	795	U
31	A	802	C
31	A	803	G
31	A	811	A
31	A	816	G
31	A	823	C
31	A	838	U
31	A	841	G
31	A	856	U
31	A	857	G
31	A	859	A

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Mol	Chain	Res	Type
31	A	861	A
31	A	866	G
31	A	869	G
31	A	879	G
31	A	887	G
31	A	889	G
31	A	890	G
31	A	896	G
31	A	899	A
31	A	901	C
31	A	905	A
31	A	906	C
31	A	907	C
31	A	908	A
31	A	915	G
31	A	916	G
31	A	919	A
31	A	924	U
31	A	937	U
31	A	938	G
31	A	946	A
31	A	947	A
31	A	970	G
31	A	974	G
31	A	981	G
31	A	987	A
31	A	989	G
31	A	993	C
31	A	1001	A
31	A	1002	G
31	A	1008	A
31	A	1011	A
31	A	1013	C
31	A	1017	G
31	A	1018	A
31	A	1024	A
31	A	1037	A
31	A	1040	U
31	A	1041	G
31	A	1045	G
31	A	1050	G
31	A	1051	U

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Mol	Chain	Res	Type
31	A	1054	U
31	A	1055	A
31	A	1061	G
31	A	1062	G
31	A	1065	G
31	A	1072	A
31	A	1075	G
31	A	1098	A
31	A	1099	G
31	A	1101	A
31	A	1105	A
31	A	1106	C
31	A	1112	A
31	A	1113	A
31	A	1116	A
31	A	1118	U
31	A	1125	U
31	A	1139	A
31	A	1140	G
31	A	1143	C
31	A	1147	U
31	A	1148	G
31	A	1150	G
31	A	1155	A
31	A	1158	U
31	A	1160	A
31	A	1162	C
31	A	1163	G
31	A	1169	A
31	A	1170	A
31	A	1175	U
31	A	1183	A
31	A	1196	A
31	A	1197	A
31	A	1198	A
31	A	1225	G
31	A	1227	U
31	A	1240	G
31	A	1241	U
31	A	1245	U
31	A	1254	U
31	A	1258	A

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Mol	Chain	Res	Type
31	A	1259	C
31	A	1261	A
31	A	1271	G
31	A	1272	A
31	A	1274	A
31	A	1277	G
31	A	1286	A
31	A	1293	C
31	A	1294	A
31	A	1296	A
31	A	1305	A
31	A	1308	A
31	A	1310	C
31	A	1315	G
31	A	1321	A
31	A	1322	A
31	A	1333	U
31	A	1342	A
31	A	1346	U
31	A	1366	C
31	A	1371	C
31	A	1373	U
31	A	1379	C
31	A	1386	A
31	A	1399	A
31	A	1400	U
31	A	1405	A
31	A	1413	A
31	A	1416	A
31	A	1423	U
31	A	1424	A
31	A	1427	A
31	A	1431	C
31	A	1432	U
31	A	1433	U
31	A	1436	U
31	A	1437	G
31	A	1448	A
31	A	1449	C
31	A	1458	C
31	A	1461	G
31	A	1472	A

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Mol	Chain	Res	Type
31	A	1476	G
31	A	1480	A
31	A	1481	U
31	A	1484	G
31	A	1486	U
31	A	1493	C
31	A	1494	G
31	A	1497	A
31	A	1501	G
31	A	1502	A
31	A	1511	U
31	A	1512	U
31	A	1513	C
31	A	1519	A
31	A	1520	A
31	A	1521	G
31	A	1522	A
31	A	1524	G
31	A	1525	G
31	A	1528	U
31	A	1529	A
31	A	1531	A
31	A	1532	G
31	A	1544	A
31	A	1557	G
31	A	1558	U
31	A	1559	A
31	A	1568	U
31	A	1569	A
31	A	1570	C
31	A	1571	G
31	A	1592	A
31	A	1593	U
31	A	1594	A
31	A	1600	A
31	A	1603	A
31	A	1612	A
31	A	1620	U
31	A	1621	C
31	A	1622	A
31	A	1628	A
31	A	1635	C

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Mol	Chain	Res	Type
31	A	1643	G
31	A	1644	A
31	A	1662	A
31	A	1682	C
31	A	1683	G
31	A	1684	C
31	A	1708	C
31	A	1710	G
31	A	1711	C
31	A	1734	A
31	A	1750	C
31	A	1751	A
31	A	1752	C
31	A	1753	A
31	A	1755	A
31	A	1756	G
31	A	1762	C
31	A	1766	G
31	A	1774	G
31	A	1778	G
31	A	1783	A
31	A	1796	A
31	A	1801	A
31	A	1810	C
31	A	1812	A
31	A	1818	U
31	A	1819	A
31	A	1821	G
31	A	1826	U
31	A	1829	A
31	A	1839	A
31	A	1882	U
31	A	1884	A
31	A	1885	C
31	A	1915	A
31	A	1920	G
31	A	1923	C
31	A	1926	A
31	A	1927	A
31	A	1928	C
31	A	1930	A
31	A	1931	U

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Mol	Chain	Res	Type
31	A	1943	G
31	A	1944	G
31	A	1945	U
31	A	1950	A
31	A	1951	A
31	A	1957	U
31	A	1969	U
31	A	1974	A
31	A	1981	C
31	A	1984	A
31	A	1985	A
31	A	1986	G
31	A	1996	U
31	A	2005	U
31	A	2006	G
31	A	2007	U
31	A	2011	G
31	A	2034	C
31	A	2035	A
31	A	2037	G
31	A	2045	A
31	A	2046	G
31	A	2047	A
31	A	2048	U
31	A	2069	C
31	A	2070	A
31	A	2073	A
31	A	2074	A
31	A	2075	G
31	A	2076	A
31	A	2077	C
31	A	2082	U
31	A	2083	G
31	A	2091	A
31	A	2094	G
31	A	2101	G
31	A	2103	G
31	A	2106	U
31	A	2107	G
31	A	2118	U
31	A	2122	C
31	A	2123	U

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Mol	Chain	Res	Type
31	A	2124	G
31	A	2125	C
31	A	2126	G
31	A	2128	A
31	A	2129	G
31	A	2130	C
31	A	2132	U
31	A	2133	A
31	A	2134	G
31	A	2137	G
31	A	2139	A
31	A	2140	A
31	A	2142	G
31	A	2144	G
31	A	2145	A
31	A	2146	A
31	A	2147	G
31	A	2148	A
31	A	2151	G
31	A	2159	C
31	A	2160	C
31	A	2162	G
31	A	2163	G
31	A	2173	G
31	A	2174	C
31	A	2175	C
31	A	2176	A
31	A	2178	C
31	A	2179	A
31	A	2181	U
31	A	2183	A
31	A	2184	G
31	A	2185	A
31	A	2186	U
31	A	2187	A
31	A	2189	C
31	A	2191	C
31	A	2192	U
31	A	2194	U
31	A	2195	G
31	A	2198	A
31	A	2199	G

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Mol	Chain	Res	Type
31	A	2201	G
31	A	2204	A
31	A	2209	U
31	A	2212	A
31	A	2220	G
31	A	2229	U
31	A	2230	A
31	A	2240	G
31	A	2242	A
31	A	2254	A
31	A	2255	G
31	A	2256	A
31	A	2266	U
31	A	2268	G
31	A	2269	G
31	A	2271	C
31	A	2272	G
31	A	2283	A
31	A	2286	A
31	A	2295	A
31	A	2297	G
31	A	2300	U
31	A	2304	A
31	A	2317	G
31	A	2322	A
31	A	2323	C
31	A	2325	G
31	A	2342	G
31	A	2343	C
31	A	2344	A
31	A	2348	G
31	A	2352	A
31	A	2353	A
31	A	2361	U
31	A	2362	G
31	A	2364	C
31	A	2367	C
31	A	2374	C
31	A	2378	C
31	A	2394	A
31	A	2396	G
31	A	2400	G

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Mol	Chain	Res	Type
31	A	2402	C
31	A	2405	A
31	A	2406	G
31	A	2408	G
31	A	2419	G
31	A	2423	A
31	A	2432	G
31	A	2436	U
31	A	2442	A
31	A	2443	A
31	A	2444	C
31	A	2445	G
31	A	2446	G
31	A	2452	A
31	A	2458	U
31	A	2464	G
31	A	2465	A
31	A	2466	U
31	A	2487	G
31	A	2493	A
31	A	2508	U
31	A	2509	U
31	A	2511	G
31	A	2515	C
31	A	2518	C
31	A	2519	G
31	A	2520	A
31	A	2521	U
31	A	2522	G
31	A	2524	C
31	A	2535	C
31	A	2537	C
31	A	2549	G
31	A	2552	U
31	A	2579	U
31	A	2583	A
31	A	2584	G
31	A	2589	A
31	A	2590	C
31	A	2591	G
31	A	2593	G
31	A	2594	A

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Mol	Chain	Res	Type
31	A	2597	U
31	A	2598	G
31	A	2599	G
31	A	2601	U
31	A	2602	U
31	A	2603	C
31	A	2619	A
31	A	2626	U
31	A	2627	C
31	A	2630	U
31	A	2632	U
31	A	2646	U
31	A	2647	A
31	A	2653	U
31	A	2671	A
31	A	2672	G
31	A	2674	A
31	A	2680	G
31	A	2690	G
31	A	2702	G
31	A	2706	U
31	A	2708	C
31	A	2719	G
31	A	2729	A
31	A	2731	C
31	A	2732	G
31	A	2736	G
31	A	2744	A
31	A	2751	A
31	A	2753	C
31	A	2762	G
31	A	2764	U
31	A	2766	A
31	A	2768	A
31	A	2770	C
31	A	2771	A
31	A	2780	G
31	A	2783	A
31	A	2784	G
31	A	2796	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	B	57	U
27	W	29	U
27	W	32	C
27	W	33	A
27	W	97	A
31	A	97	A
31	A	514	A
31	A	556	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

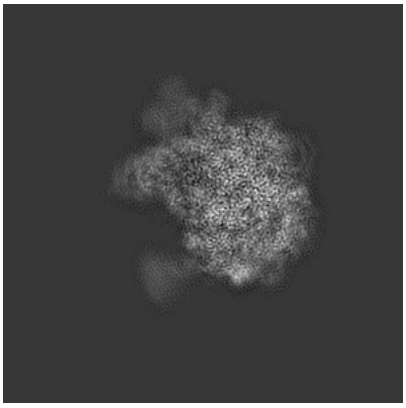
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6711. These allow visual inspection of the internal detail of the map and identification of artifacts.

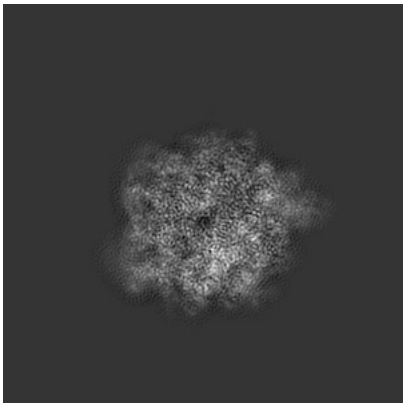
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

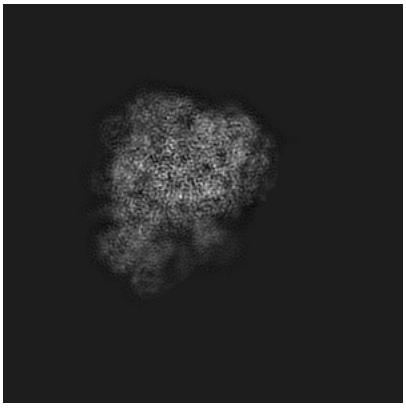
6.1.1 Primary map



X



Y

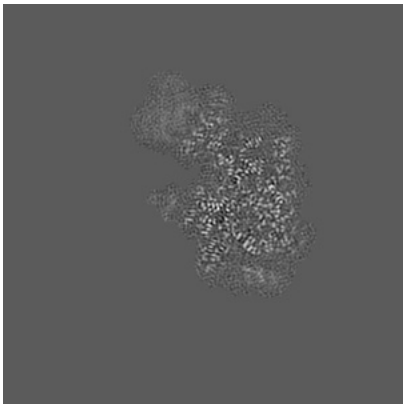


Z

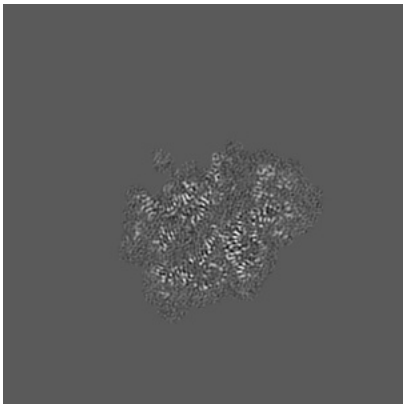
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 192



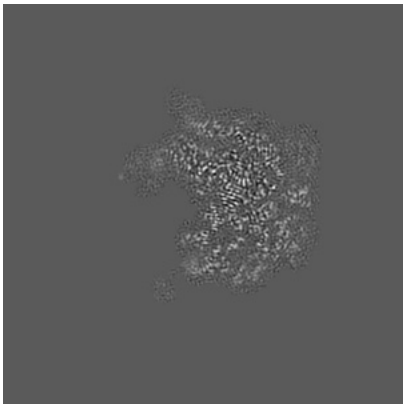
Y Index: 192

Z Index: 192

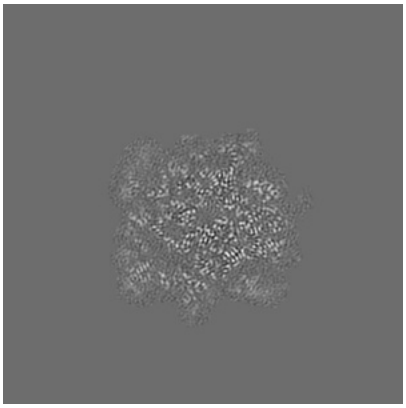
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 163



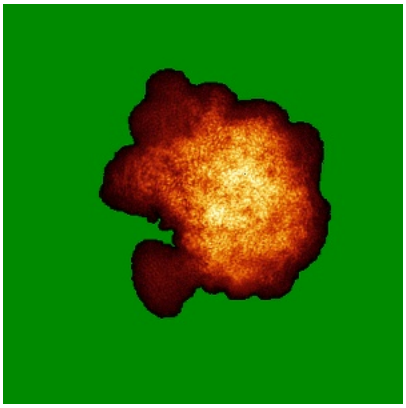
Y Index: 221

Z Index: 195

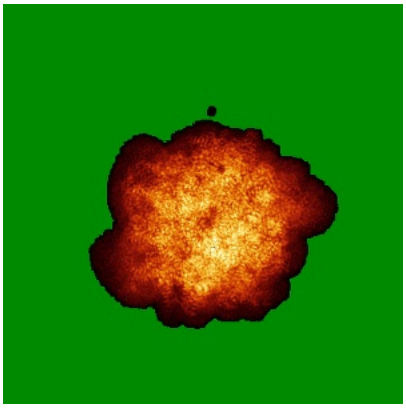
The images above show the largest variance slices of the map in three orthogonal directions.

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

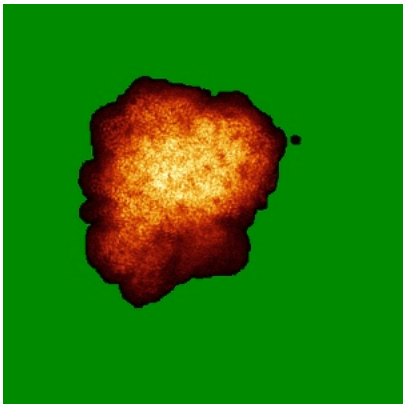
6.4.1 Primary map



X



Y

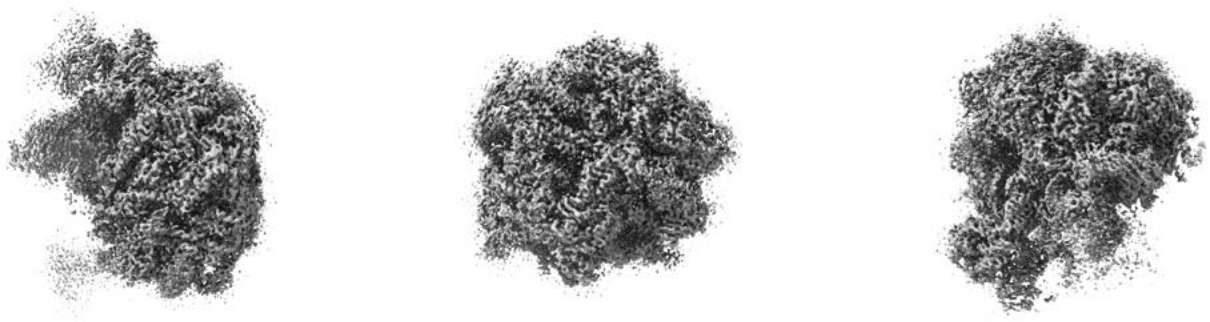


Z

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

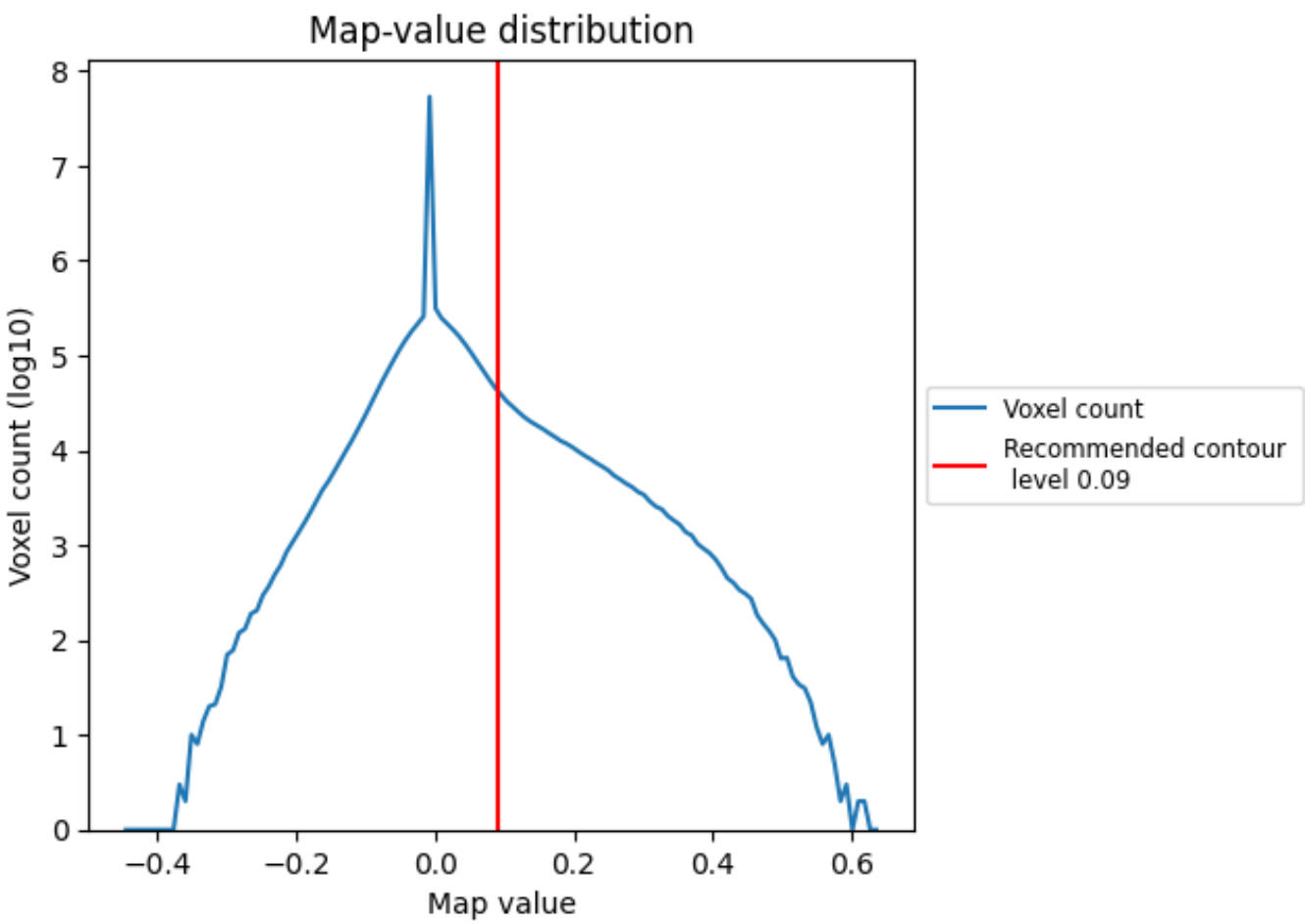
6.6 Mask visualisation (i)

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

7 Map analysis (i)

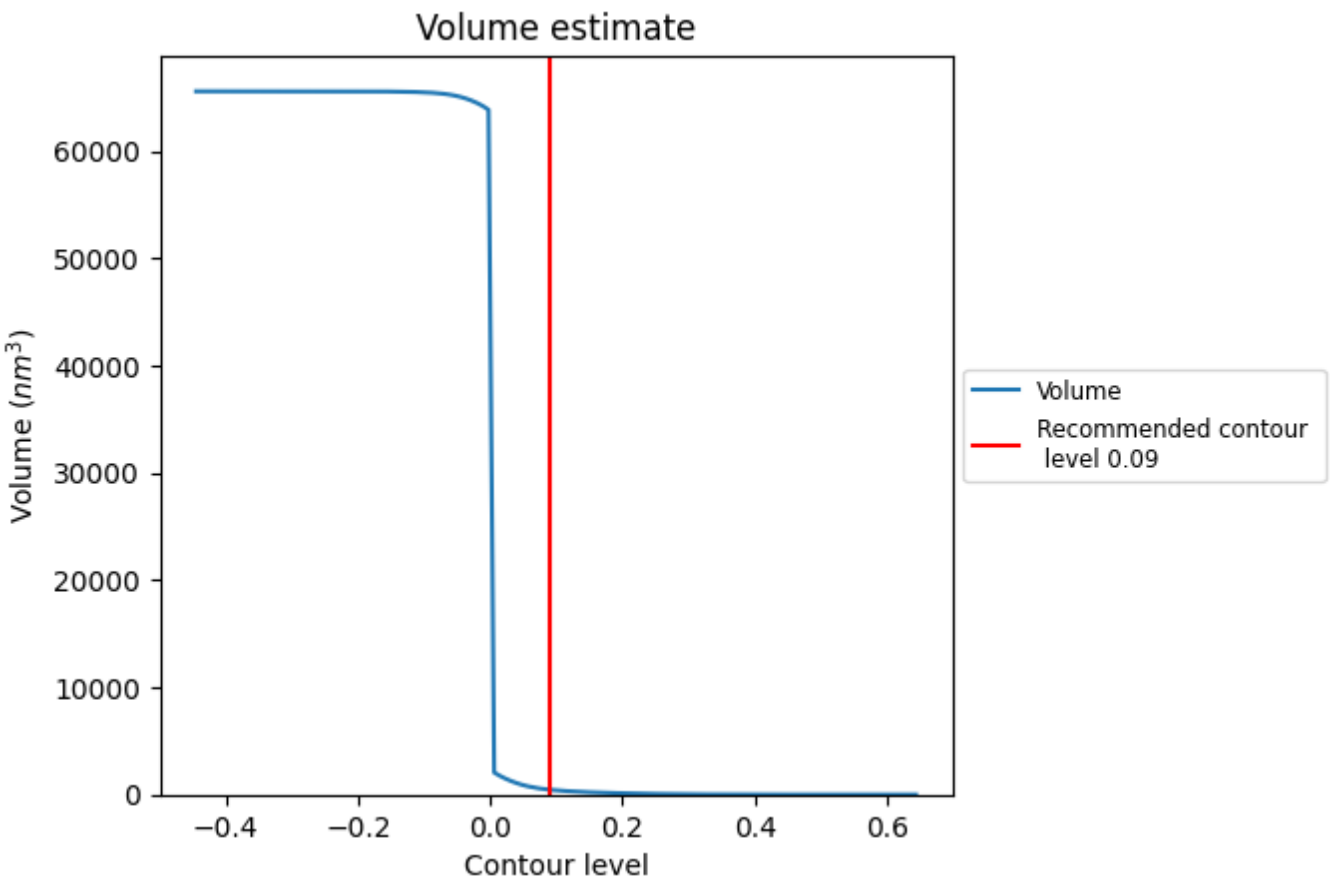
This section contains the results of statistical analysis of the map.

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.

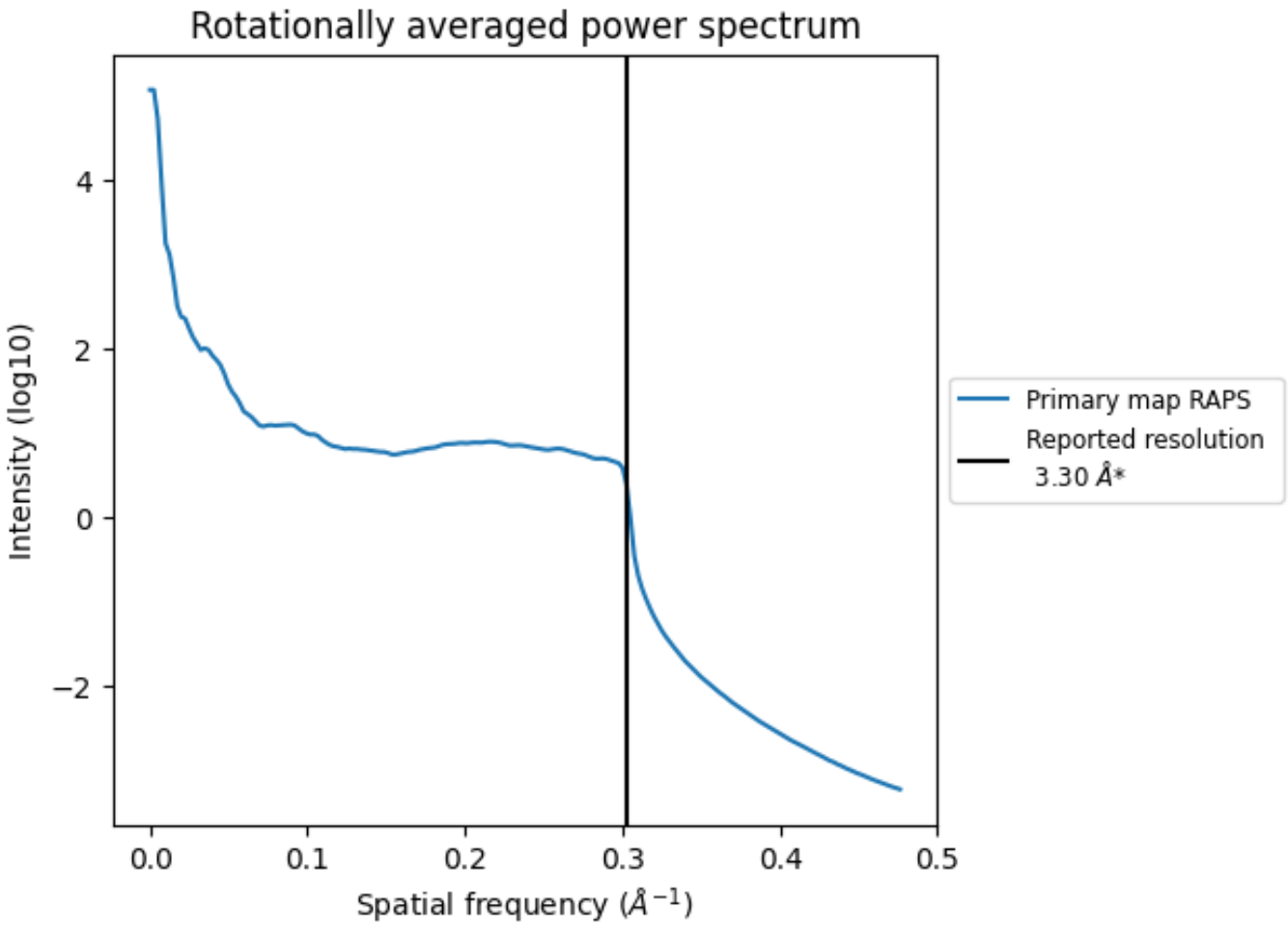
7.2 Volume estimate (i)



The volume at the recommended contour level is 450 nm^3; this corresponds to an approximate mass of 407 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 0.303 Å^{-1}

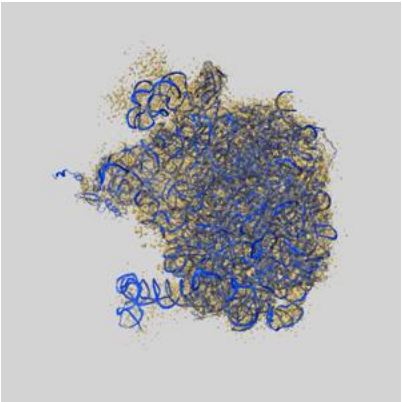
8 Fourier-Shell correlation (i)

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

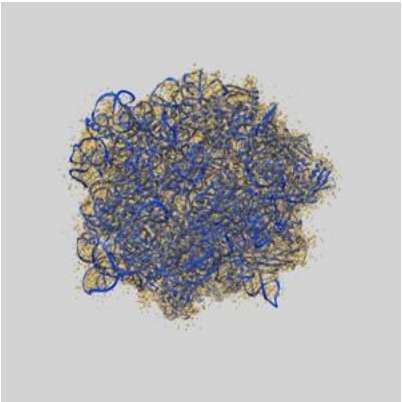
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6711 and PDB model 5X8T. Per-residue inclusion information can be found in section 3 on page 9.

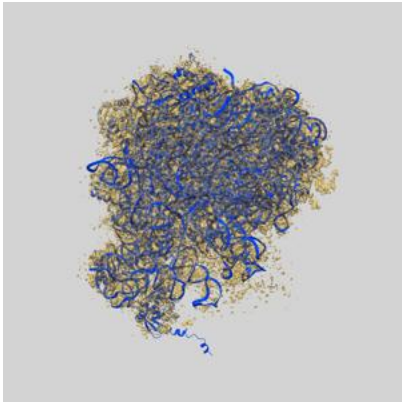
9.1 Map-model overlay (i)



X



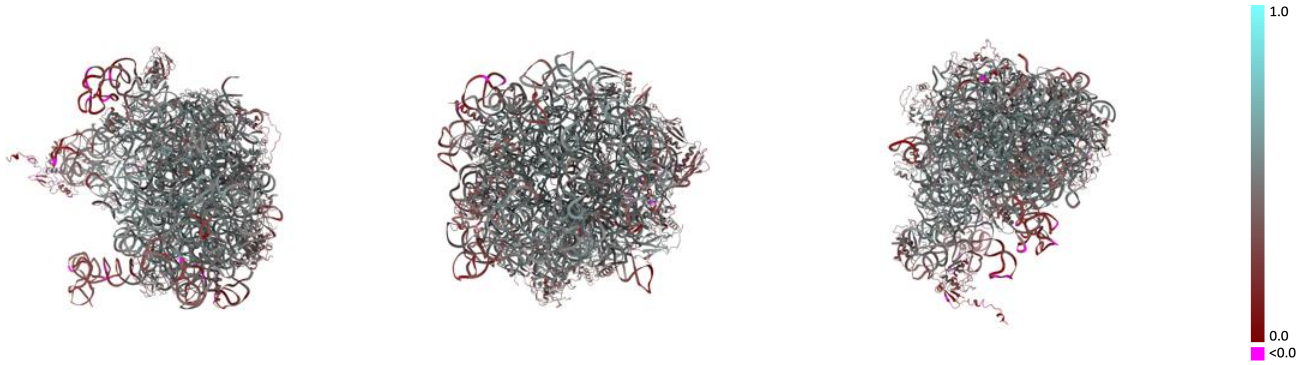
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

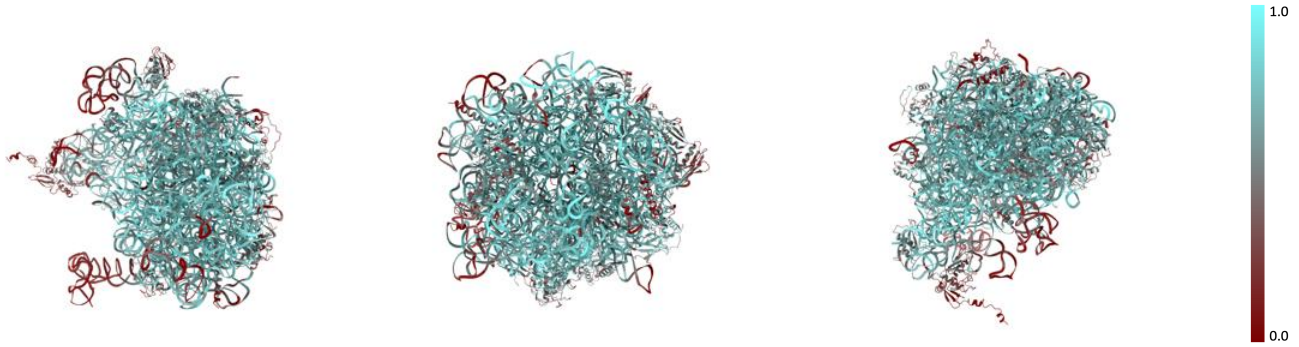
9.2 Q-score mapped to coordinate model (i)



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.

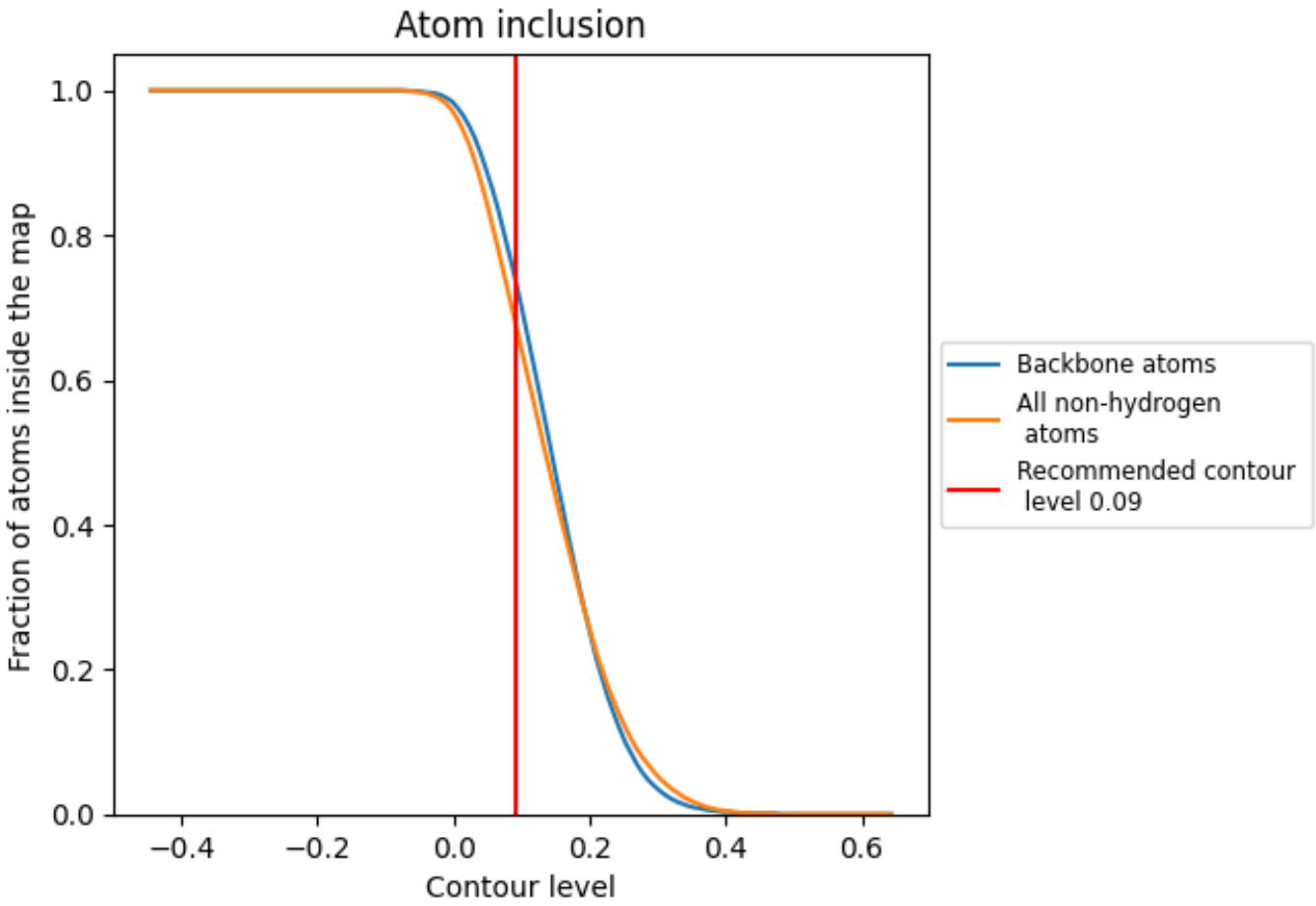
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.4510
0	0.0780	0.1390
1	0.6110	0.4100
2	0.5320	0.3480
3	0.6790	0.4750
4	0.7030	0.4840
5	0.6600	0.4090
6	0.4890	0.3800
7	0.6250	0.4670
A	0.7350	0.4700
B	0.7310	0.4450
C	0.6160	0.4290
D	0.6530	0.4620
E	0.5760	0.4120
F	0.2800	0.2780
G	0.4480	0.3690
H	0.2370	0.3220
K	0.5880	0.4420
L	0.5430	0.4270
M	0.6450	0.4440
N	0.6290	0.4170
O	0.6450	0.4360
P	0.5470	0.3950
Q	0.5600	0.4240
R	0.6570	0.4170
S	0.5420	0.4110
T	0.5260	0.4070
U	0.4890	0.4060
V	0.4980	0.3810
W	0.7640	0.4760
X	0.6030	0.4270
Y	0.6280	0.4550
Z	0.4720	0.3770