Full wwPDB EM Validation Report (i)

Oct 12, 2026 – 05:36 PM EDT

PDB ID	:	9YPN / pdb_00009ypn
EMDB ID	:	EMD-73301
Title	:	Pseudomonas aeruginosa 50S ribosome (L1 stalk in 'out' conformation and missing uL1 and tRNA)
Authors	:	Findlay, J.L.; Kanik, M.; Gauvin, C.C.; Franklin, M.J.; Lawrence, C.M.
Deposited on	:	2025-10-14
Resolution	:	2.25 Å(reported)
Based on initial model	:	7UNW

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 (1)) were used in the production of this report:

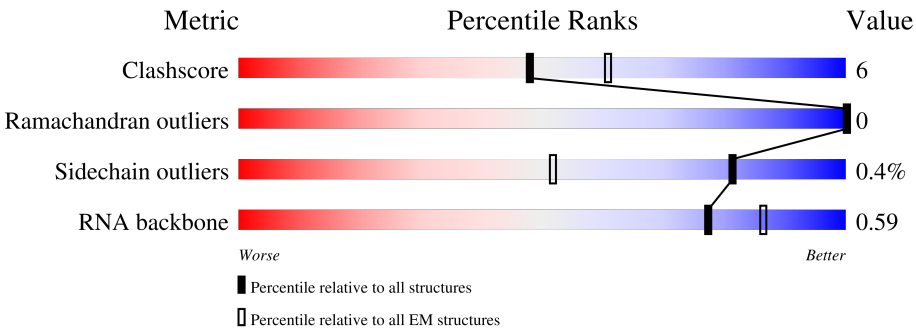
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

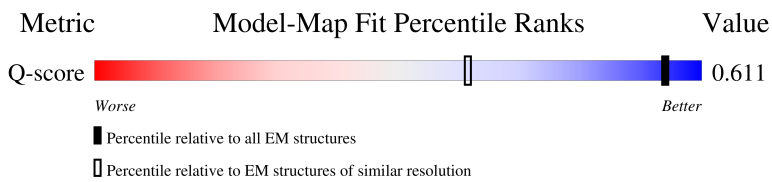
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3458 (1.75 - 2.75)

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

Mol	Chain	Length	Quality of chain
1	A	2892	63% 32%
2	B	121	61% 31% 6%
3	D	273	82% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	211	87% 11%
5	F	200	85% 14%
6	G	179	75% 25%
7	H	177	83% 15%
8	I	148	26% 73% 5% 22%
9	L	142	88% 12%
10	M	122	86% 14%
11	N	144	88% 12%
12	O	137	74% 26%
13	P	129	80% 12% 8%
14	Q	116	87% 12%
15	R	116	6% 84% 14%
16	S	118	86% 14%
17	T	103	89% 11%
18	U	110	87% 13%
19	V	99	68% 27% 5%
20	W	104	86% 6% 9%
21	X	204	80% 13% 7%
22	Y	85	82% 8% 9%
23	Z	78	85% 14%
24	1	63	86% 11%
25	2	58	93%
26	4	60	75% 15% 10%
27	5	51	78% 22%
28	6	44	84% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	7	64	81% 17%
30	8	38	89% 11%
31	J	166	17% 51% 16% 33%
32	K	143	29% 83% 17%

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 95807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2837	60895	27173	11178	19708	2836	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	119	2535	1132	452	832	119	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	272	2072	1276	426	364	6	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	208	1564	968	298	293	5	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	200	1521	955	283	280	3	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	179	1435	914	256	260	5	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	174	1314	828	242	242	2	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	115	858	539	152	166	1	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	142	1130	718	206	202	4	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	122	938	587	180	165	6	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	144	1066	654	215	194	3	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	O	137	1085	689	211	181	4	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	P	119	952	595	191	161	5	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Q	115	881	544	174	161	2	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	R	114	901	567	171	162	1	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	S	117	936	592	196	148	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	103	822	521	156	143	2	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	U	110	833	515	161	153	4	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	V	94	739	472	134	132	1	0	0

- Molecule 20 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	W	95	738	466	142	129	1	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	X	190	1445	915	262	265	3	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	Y	77	581	367	112	102	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Z	77	630	391	134	103	2	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	1	61	490	301	96	91	2	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	2	56	440	275	86	77	2	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	4	54	431	258	91	81	1	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	5	51	426	272	78	75	1	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	6	44	365	222	87	54	2	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	7	63	506	314	108	81	3	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	8	38	307	186	69	48	4	0	0

- Molecule 31 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	J	111	840	533	151	155	1	0	0

- Molecule 32 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	K	143	1046	655	186	201	4	0	0

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
33	A	196	196	196	0
33	B	3	3	3	0
33	D	1	1	1	0
33	E	1	1	1	0
33	4	1	1	1	0

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
34	8	1	1	1	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
35	A	4032	4032	4032	0
			Total	O	
35	B	76	76	76	0
			Total	O	
35	D	89	89	89	0
			Total	O	
35	E	78	78	78	0
			Total	O	
35	F	47	47	47	0
			Total	O	
35	G	12	12	12	0
			Total	O	
35	H	3	3	3	0
			Total	O	
35	I	1	1	1	0
			Total	O	
35	L	34	34	34	0
			Total	O	
35	M	18	18	18	0
			Total	O	
35	N	64	64	64	0
			Total	O	
35	O	37	37	37	0
			Total	O	
35	P	36	36	36	0
			Total	O	
35	Q	6	6	6	0
			Total	O	
35	R	25	25	25	0
			Total	O	
35	S	44	44	44	0
			Total	O	
35	T	32	32	32	0
			Total	O	
35	U	40	40	40	0
			Total	O	
35	V	26	26	26	0

Continued on next page...

Continued from previous page...

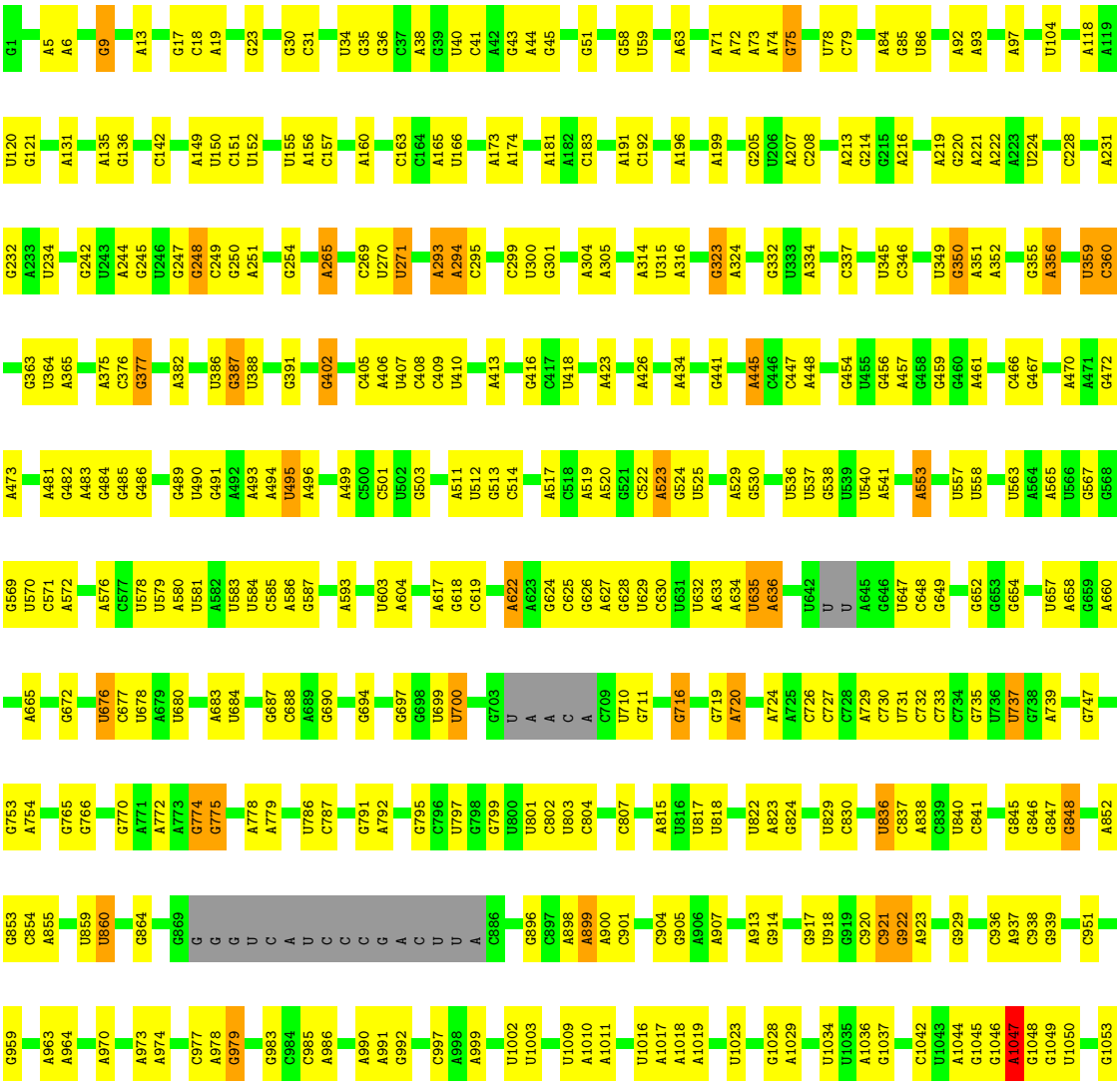
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
35	W	11	11	11	0
			Total	O	
35	X	22	22	22	0
			Total	O	
35	Y	24	24	24	0
			Total	O	
35	Z	20	20	20	0
			Total	O	
35	1	3	3	3	0
			Total	O	
35	2	16	16	16	0
			Total	O	
35	4	32	32	32	0
			Total	O	
35	5	1	1	1	0
			Total	O	
35	6	23	23	23	0
			Total	O	
35	7	22	22	22	0
			Total	O	
35	8	8	8	8	0

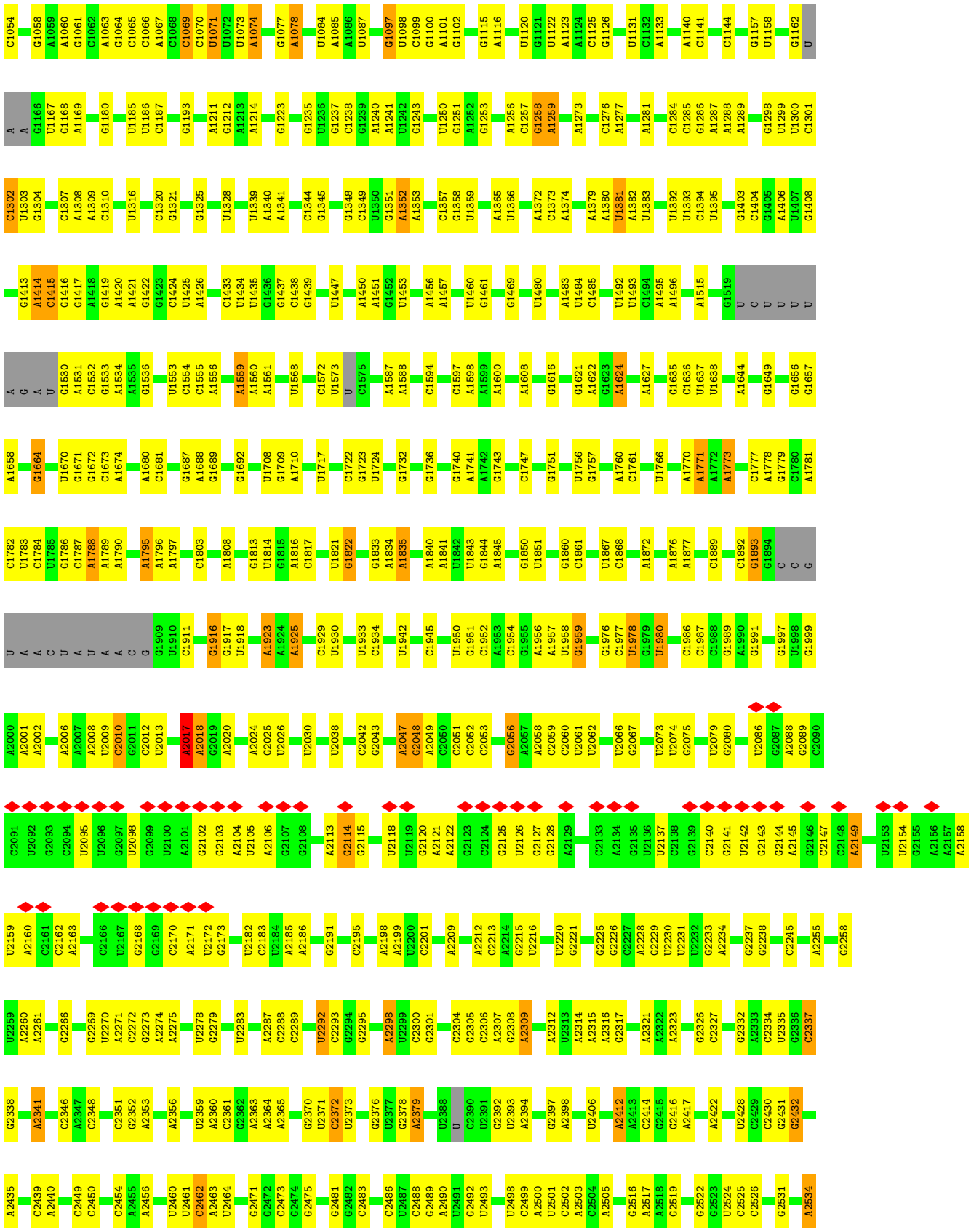
3 Residue-property plots (i)

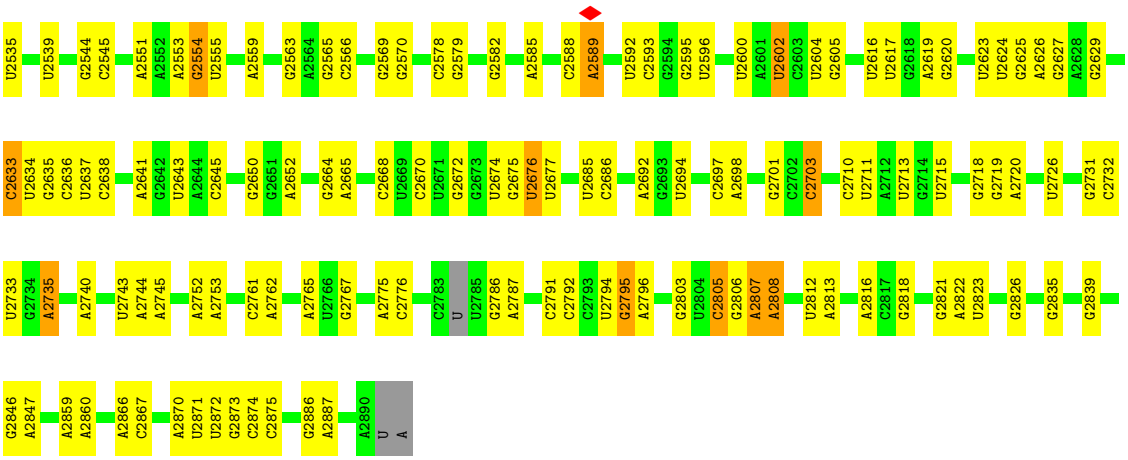
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S rRNA

Chain A:

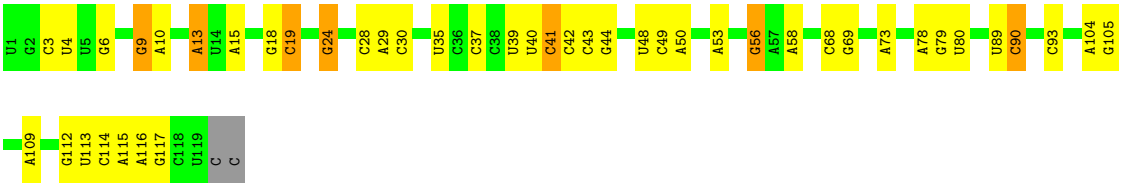



C1054 G1058 A1059 A1060 G1061 C1062 A1063 G1064 C1065 C1066 A1067 C1068 C1069 C1070 U1071 U1072 U1073 A1074 G1077 A1078 U1084 A1085 A1086 U1087 G1097 U1098 C1099 G1100 A1101 G1102 G1115 A1116 U1120 G1121 U1122 A1123 A1124 C1125 G1126 U1131 C1132 A1133 A1140 C1141 C1144 G1157 U1158 G1162 U
A A G1166 U1167 G1168 A1169 G1180 U1185 U1186 C1187 G1193 A1211 G1212 A1213 A1214 G1223 G1235 U1236 G1237 C1238 G1239 A1240 A1241 U1242 G1243 U1250 G1251 A1252 G1253 A1256 C1257 G1258 A1259 A1273 C1276 A1277 A1281 C1284 C1285 G1286 A1287 A1288 A1289 G1298 U1299 U1300 C1301
C1302 U1303 G1304 C1307 A1308 A1309 C1310 U1316 C1320 G1321 G1325 U1328 U1339 A1340 A1341 C1344 G1345 G1348 C1349 U1350 G1351 A1352 A1353 C1357 G1358 U1359 A1365 U1366 A1372 C1373 A1374 A1379 A1380 U1381 A1382 U1383 U1392 U1393 C1394 U1395 G1403 C1404 G1405 A1406 U1407 G1408
G1413 A1414 C1415 G1416 G1417 A1418 G1419 A1420 A1421 G1422 G1423 C1424 U1425 A1426 C1433 U1434 U1435 G1436 G1437 C1438 G1439 U1447 A1450 A1451 G1452 U1453 A1456 A1457 U1460 G1461 G1469 U1480 A1483 U1484 C1485 U1492 U1493 C1494 A1495 A1496 A1515 G1519 U C U U U U
A G A U G1530 A1531 C1532 G1533 A1534 A1535 G1536 U1553 C1554 C1555 A1556 A1559 A1560 A1561 U1568 C1572 U1573 U C1575 A1587 A1588 C1594 C1597 A1598 A1599 A1600 A1608 G1616 G1621 A1622 G1623 A1624 A1627 G1635 C1636 U1637 U1638 A1644 G1649 G1656 G1657
A1658 G1664 U1670 G1671 G1672 C1673 A1674 A1680 C1681 G1687 A1688 G1689 G1692 U1708 G1709 A1710 U1717 C1722 G1723 U1724 G1732 G1736 G1740 A1741 A1742 G1743 C1747 G1751 U1756 G1757 A1760 C1761 U1766 A1770 A1771 A1772 A1773 C1777 A1778 G1779 C1780 A1781
C1782 U1783 C1784 U1785 G1786 C1787 A1788 A1789 A1790 A1795 A1796 A1797 C1803 A1808 G1813 U1814 G1815 A1816 C1817 U1821 G1822 G1833 A1834 A1835 A1840 A1841 U1842 U1843 G1844 A1845 G1850 U1851 G1860 C1861 U1867 C1868 A1872 A1876 A1877 C1889 C1892 G1893 G1894 C C G
U A A C U A U A A C G G1909 U1910 C1911 G1916 G1917 U1918 A1923 A1924 A1925 C1929 U1930 U1933 C1934 U1942 C1945 U1950 G1951 C1952 A1953 C1954 G1955 A1956 A1957 U1958 G1959 G1976 C1977 U1978 G1979 U1980 C1986 C1987 C1988 G1989 A1990 G1991 G1997 U1998 G1999
A2000 A2001 A2002 A2006 A2007 A2008 U2009 C2010 G2011 C2012 U2013 A2017 A2018 G2019 A2020 A2024 G2025 U2026 U2030 U2038 C2042 G2043 A2047 G2048 A2049 C2050 C2051 C2052 C2053 G2056 A2057 A2058 C2059 C2060 U2061 U2062 U2066 G2067 U2073 U2074 G2075 U2079 G2080 U2086 G2087 A2088 G2089 C2090
C2091 U2092 G2093 C2094 U2095 U2096 G2097 U2098 G2099 U2100 A2101 G2102 G2103 A2104 U2105 A2106 G2107 G2108 A2113 G2114 G2115 U2118 U2119 G2120 A2121 A2122 G2123 C2124 G2125 U2126 G2127 G2128 A2129 C2133 A2134 G2135 U2136 U2137 C2138 G2139 C2140 G2141 U2142 G2143 G2144 A2145 G2146 C2147 C2148 A2149 U2153 U2154 G2155 A2156 A2157 A2158
U2159 A2160 C2161 C2162 A2163 C2166 U2167 G2168 G2169 C2170 A2171 U2172 G2173 U2182 C2183 U2184 A2185 A2186 G2191 C2195 A2198 A2199 U2200 C2201 A2209 A2212 C2213 A2214 G2215 U2216 U2220 G2221 G2225 G2226 C2227 A2228 G2229 U2230 U2231 U2232 G2233 A2234 G2237 G2238 C2245 A2255 G2258
U2259 A2260 A2261 G2266 G2269 U2270 A2271 C2272 G2273 A2274 A2275 U2278 G2279 U2283 A2287 C2288 C2289 U2292 C2293 G2294 G2295 A2298 U2299 C2300 G2301 C2304 G2305 C2306 A2307 G2308 A2309 A2312 U2313 A2314 A2315 A2316 G2317 A2321 A2322 A2323 G2326 C2327 G2332 A2333 C2334 U2335 G2336 C2337
G2338 A2341 C2346 A2347 C2348 C2351 G2352 A2353 A2356 U2359 A2360 C2361 G2362 A2363 A2364 A2365 G2370 U2371 C2372 U2373 G2376 U2377 G2378 A2379 U2388 U C2390 U2391 G2392 U2393 A2394 G2397 A2398 U2406 A2412 A2413 C2414 G2415 G2416 A2417 A2422 U2428 C2429 C2430 G2431 G2432
A2435 C2439 A2440 C2449 C2450 C2454 A2455 A2456 U2460 U2461 C2462 A2463 U2464 G2471 G2472 C2473 G2474 G2475 G2481 G2482 C2483 C2486 U2487 C2488 G2489 A2490 U2491 G2492 U2493 U2498 C2499 A2500 U2501 C2502 A2503 C2504 A2505 G2516 A2517 A2518 G2519 G2522 G2523 U2524 C2525 C2526 G2531 A2534



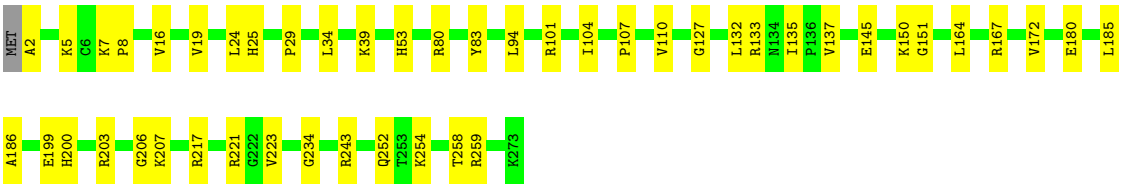
- Molecule 2: 5S rRNA

Chain B:



- Molecule 3: Large ribosomal subunit protein uL2

Chain D:



- Molecule 4: Large ribosomal subunit protein uL3

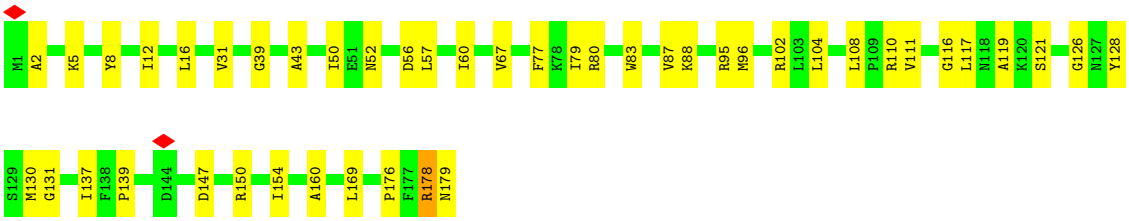
Chain E:

- Molecule 5: Large ribosomal subunit protein uL4

Chain F:

- Molecule 6: Large ribosomal subunit protein uL5

Chain G:

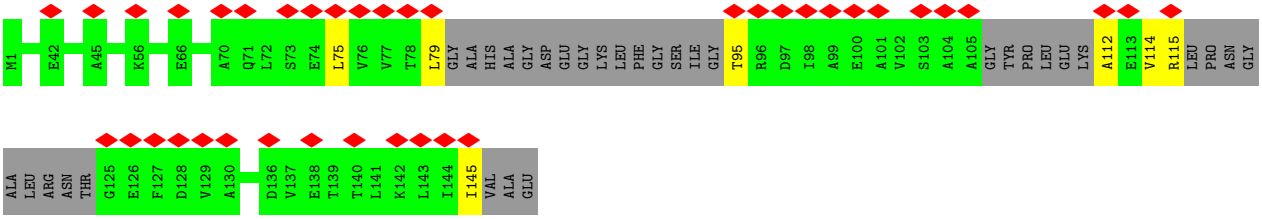


- Molecule 7: Large ribosomal subunit protein uL6

Chain H:

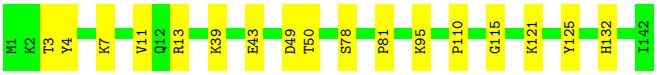
- Molecule 8: Large ribosomal subunit protein bL9

Chain I:



- Molecule 9: Large ribosomal subunit protein uL13

Chain L:

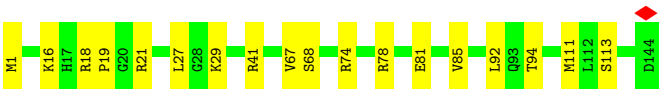


- Molecule 10: Large ribosomal subunit protein uL14

Chain M:

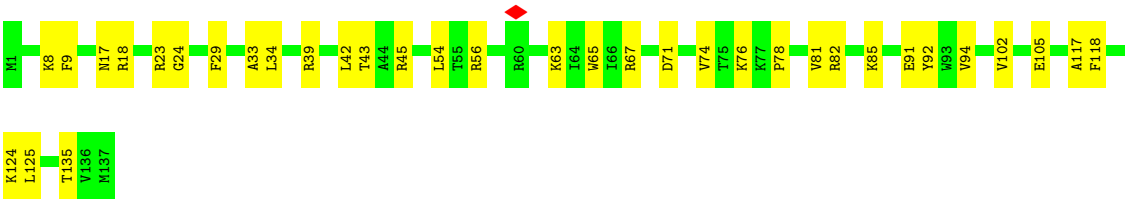
- Molecule 11: Large ribosomal subunit protein uL15

Chain N:



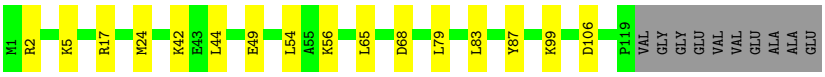
- Molecule 12: Large ribosomal subunit protein uL16

Chain O:



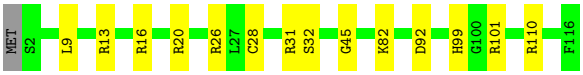
• Molecule 13: Large ribosomal subunit protein bL17

Chain P:



• Molecule 14: Large ribosomal subunit protein uL18

Chain Q:

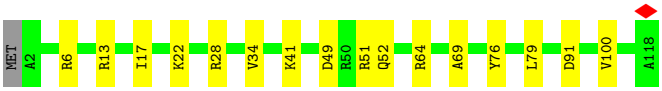


• Molecule 15: Large ribosomal subunit protein bL19

Chain R:

• Molecule 16: Large ribosomal subunit protein bL20

Chain S:

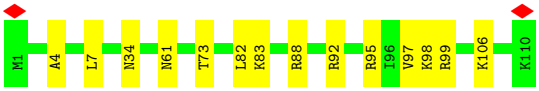


• Molecule 17: Large ribosomal subunit protein bL21

Chain T:

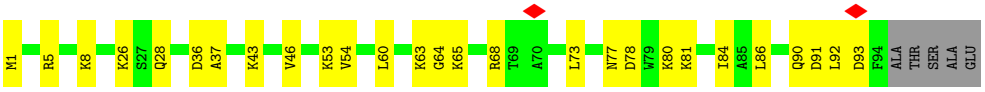
• Molecule 18: Large ribosomal subunit protein uL22

Chain U:



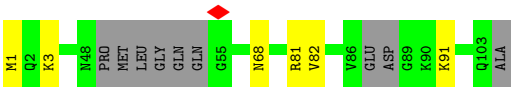
• Molecule 19: Large ribosomal subunit protein uL23

Chain V:



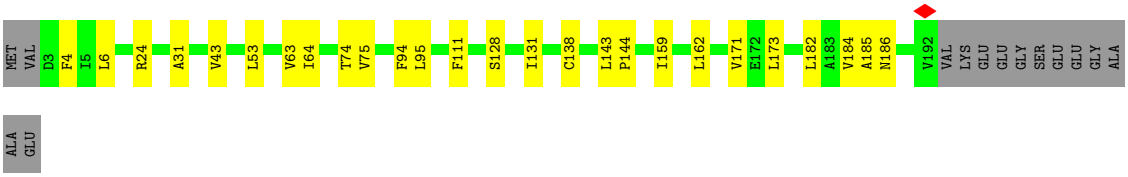
• Molecule 20: Large ribosomal subunit protein uL24

Chain W:



• Molecule 21: Large ribosomal subunit protein bL25

Chain X:

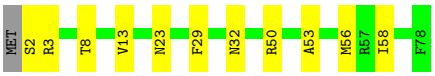


• Molecule 22: Large ribosomal subunit protein bL27

Chain Y:

• Molecule 23: Large ribosomal subunit protein bL28

Chain Z:

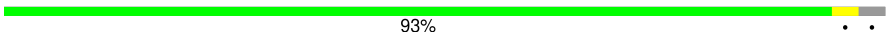


• Molecule 24: Large ribosomal subunit protein uL29

Chain 1:

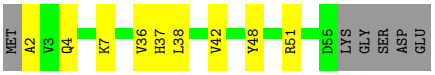
• Molecule 25: Large ribosomal subunit protein uL30

Chain 2:



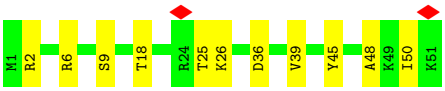
• Molecule 26: Large ribosomal subunit protein bL32

Chain 4:



• Molecule 27: Large ribosomal subunit protein bL33

Chain 5:

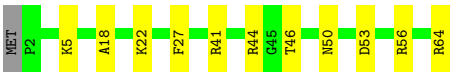


• Molecule 28: Large ribosomal subunit protein bL34

Chain 6:

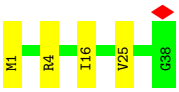
• Molecule 29: Large ribosomal subunit protein bL35

Chain 7:



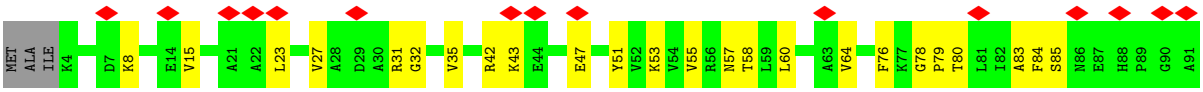
• Molecule 30: Large ribosomal subunit protein bL36A

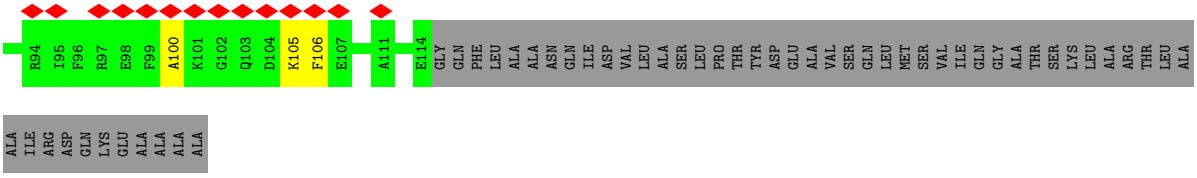
Chain 8:



• Molecule 31: Large ribosomal subunit protein uL10

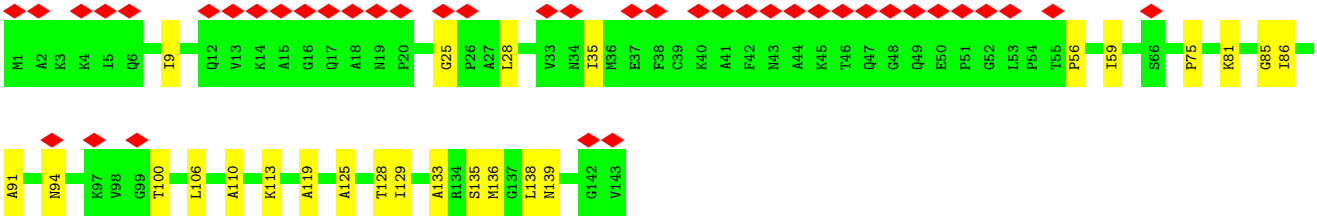
Chain J:





• Molecule 32: Large ribosomal subunit protein uL10

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	642285	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	54.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	81.284	Depositor
Minimum map value	-47.287	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.038	Depositor
Recommended contour level	3	Depositor
Map size (Å)	468.408, 468.408, 468.408	wwPDB
Map dimensions	696, 696, 696	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.673, 0.673, 0.673	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 7MG, 1MG, 2MA, 5MC, ZN, 2MG, OMG, 5MU, MG, OMC, 6MZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.28	0/67882	0.74	17/105870 (0.0%)
2	B	0.31	0/2833	0.67	1/4413 (0.0%)
3	D	0.15	0/2108	0.27	0/2831
4	E	0.20	0/1587	0.34	0/2138
5	F	0.17	0/1541	0.28	0/2075
6	G	0.25	0/1456	0.37	0/1953
7	H	0.09	0/1332	0.22	0/1794
8	I	0.11	0/861	0.24	0/1159
9	L	0.24	0/1156	0.38	0/1559
10	M	0.11	0/947	0.27	0/1268
11	N	0.11	0/1078	0.28	0/1436
12	O	0.12	0/1105	0.26	0/1476
13	P	0.19	0/968	0.31	0/1294
14	Q	0.18	0/888	0.29	0/1183
15	R	0.16	0/910	0.34	0/1218
16	S	0.14	0/946	0.30	0/1257
17	T	0.09	0/835	0.23	0/1117
18	U	0.09	0/837	0.23	0/1114
19	V	0.08	0/749	0.22	0/1002
20	W	0.09	0/743	0.24	0/988
21	X	0.09	0/1468	0.21	0/1987
22	Y	0.09	0/589	0.24	0/782
23	Z	0.16	0/641	0.23	0/854
24	1	0.17	0/491	0.31	0/654
25	2	0.08	0/444	0.23	0/597
26	4	0.31	0/437	0.55	0/583
27	5	0.09	0/433	0.24	0/576
28	6	0.16	0/368	0.36	0/482
29	7	0.16	0/511	0.27	0/668
30	8	0.08	0/308	0.22	0/404
31	J	0.48	0/850	0.63	0/1142
32	K	0.33	0/1061	0.42	0/1435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.26	0/98363	0.65	18/147309 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1911	C	C2-N1-C1'	-7.12	110.97	118.80
1	A	1097	G	N3-C4-N9	-6.80	121.92	126.00
1	A	9	G	O4'-C1'-N9	6.40	113.32	108.20
1	A	503	G	O4'-C1'-N9	6.11	113.09	108.20
1	A	1071	U	N3-C2-O2	-6.06	117.96	122.20
1	A	1097	G	C6-C5-N7	6.04	134.02	130.40
1	A	1923	A	N9-C4-C5	-5.88	103.45	105.80
1	A	1047	A	N9-C4-C5	-5.87	103.45	105.80
1	A	1300	U	N1-C2-O2	5.81	126.87	122.80
1	A	1042	C	C2-N1-C1'	5.71	125.08	118.80
1	A	1300	U	C2-N1-C1'	5.54	124.35	117.70
1	A	2807	A	P-O3'-C3'	5.51	126.31	119.70
1	A	1761	C	N3-C2-O2	-5.32	118.17	121.90
1	A	2835	G	O4'-C1'-N9	5.27	112.42	108.20
1	A	1911	C	C6-N1-C1'	5.27	127.12	120.80
1	A	1893	G	N3-C4-N9	5.08	129.05	126.00
1	A	1071	U	C2-N3-C4	-5.07	123.96	127.00
2	B	42	C	C2-N1-C1'	5.04	124.34	118.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60895	0	30644	586	0
2	B	2535	0	1283	30	0
3	D	2072	0	2152	38	0
4	E	1564	0	1575	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1521	0	1581	26	0
6	G	1435	0	1504	30	0
7	H	1314	0	1373	17	0
8	I	858	0	890	4	0
9	L	1130	0	1160	15	0
10	M	938	0	1012	12	0
11	N	1066	0	1112	14	0
12	O	1085	0	1157	25	0
13	P	952	0	996	12	0
14	Q	881	0	920	15	0
15	R	901	0	958	10	0
16	S	936	0	1025	16	0
17	T	822	0	858	7	0
18	U	833	0	897	10	0
19	V	739	0	788	18	0
20	W	738	0	806	5	0
21	X	1445	0	1486	18	0
22	Y	581	0	603	6	0
23	Z	630	0	653	8	0
24	1	490	0	520	5	0
25	2	440	0	469	2	0
26	4	431	0	424	7	0
27	5	426	0	457	8	0
28	6	365	0	409	6	0
29	7	506	0	569	10	0
30	8	307	0	342	3	0
31	J	840	0	867	21	0
32	K	1046	0	1089	23	0
33	4	1	0	0	0	0
33	A	196	0	0	0	0
33	B	3	0	0	0	0
33	D	1	0	0	0	0
33	E	1	0	0	0	0
34	8	1	0	0	0	0
35	1	3	0	0	0	0
35	2	16	0	0	0	0
35	4	32	0	0	1	0
35	5	1	0	0	0	0
35	6	23	0	0	1	0
35	7	22	0	0	0	0
35	8	8	0	0	0	0
35	A	4032	0	0	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	76	0	0	2	0
35	D	89	0	0	1	0
35	E	78	0	0	0	0
35	F	47	0	0	3	0
35	G	12	0	0	0	0
35	H	3	0	0	0	0
35	I	1	0	0	0	0
35	L	34	0	0	0	0
35	M	18	0	0	0	0
35	N	64	0	0	0	0
35	O	37	0	0	2	0
35	P	36	0	0	0	0
35	Q	6	0	0	1	0
35	R	25	0	0	0	0
35	S	44	0	0	1	0
35	T	32	0	0	0	0
35	U	40	0	0	1	0
35	V	26	0	0	0	0
35	W	11	0	0	0	0
35	X	22	0	0	2	0
35	Y	24	0	0	0	0
35	Z	20	0	0	0	0
All	All	95807	0	60579	864	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 (864) 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:J:43:LYS:HG2	31:J:47:GLU:OE1	1.80	0.82
6:G:119:ALA:HB3	6:G:179:ASN:HB2	1.64	0.80
1:A:558:U:H1'	1:A:2017:6MZ:H9C1	1.68	0.76
1:A:1045:G:H5'	31:J:32:GLY:HA2	1.70	0.73
1:A:1097:G:O2'	31:J:78:GLY:HA2	1.89	0.73
1:A:1070:C:O2'	32:K:128:THR:HA	1.88	0.72
1:A:1587:A:H5"	1:A:1588:A:H5'	1.73	0.70
1:A:2154:U:N3	1:A:2158:A:N6	2.38	0.70
1:A:459:G:N7	28:6:39:ARG:NH2	2.39	0.69
1:A:2292:U:H5"	6:G:131:GLY:HA3	1.74	0.69
1:A:1766:U:OP2	1:A:1771:A:N6	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:63:VAL:HG23	35:X:307:HOH:O	1.93	0.69
32:K:100:THR:HG22	32:K:139:ASN:HB2	1.74	0.69
1:A:694:G:O2'	1:A:716:G:N2	2.21	0.68
1:A:649:G:H4'	5:F:94:LYS:HG2	1.76	0.68
1:A:2095:U:H3	1:A:2168:G:H1	1.39	0.68
7:H:164:TYR:HB2	7:H:167:GLU:HB2	1.76	0.67
28:6:1:MET:SD	28:6:3:ARG:NH2	2.67	0.67
1:A:2645:C:OP1	7:H:160:LYS:NZ	2.28	0.66
3:D:221:ARG:NH2	35:D:403:HOH:O	2.27	0.66
5:F:2:GLN:NE2	5:F:12:GLU:OE1	2.28	0.66
1:A:2360:A:N7	35:A:3191:HOH:O	2.29	0.65
1:A:2154:U:C2	1:A:2158:A:N6	2.65	0.65
31:J:27:VAL:HG13	31:J:80:THR:HG23	1.77	0.65
32:K:9:ILE:HB	32:K:59:ILE:HB	1.78	0.64
1:A:2321:A:OP2	14:Q:13:ARG:NH2	2.30	0.64
1:A:2278:U:H2'	1:A:2279:G:C8	2.33	0.64
1:A:2454:C:O2	12:O:124:LYS:NZ	2.28	0.64
1:A:2753:A:N7	35:A:3206:HOH:O	2.30	0.64
1:A:1692:G:N7	35:A:3223:HOH:O	2.30	0.63
10:M:25:LEU:HD12	10:M:38:ILE:HG22	1.81	0.63
1:A:2103:G:N2	1:A:2149:A:OP2	2.32	0.63
7:H:40:SER:HB2	7:H:61:THR:HG23	1.81	0.63
1:A:1298:G:OP2	1:A:1298:G:N2	2.25	0.62
1:A:2162:C:H2'	1:A:2163:A:H8	1.63	0.62
6:G:56:ASP:OD2	6:G:150:ARG:NH1	2.32	0.62
1:A:2283:U:O2'	1:A:2307:A:N6	2.32	0.62
1:A:896:G:H5'	12:O:23:ARG:HB3	1.82	0.62
1:A:1273:A:N3	35:A:3237:HOH:O	2.31	0.62
1:A:1515:A:N6	1:A:1533:G:O2'	2.33	0.62
1:A:2010:C:H5'	1:A:2604:U:H4'	1.81	0.62
5:F:3:LEU:HD12	5:F:13:VAL:HG11	1.80	0.62
17:T:14:VAL:HG13	17:T:98:ILE:HG13	1.82	0.62
1:A:160:A:N3	1:A:2195:C:O2'	2.31	0.61
1:A:1406:A:O2'	1:A:1408:G:N7	2.32	0.61
1:A:2315:A:H2'	1:A:2316:A:C8	2.35	0.61
1:A:2432:2MG:OP1	5:F:68:ARG:NH1	2.32	0.61
15:R:101:LEU:HD11	15:R:111:ILE:HD11	1.82	0.61
17:T:6:VAL:HG22	17:T:11:GLN:HG2	1.83	0.61
26:4:2:ALA:N	35:4:203:HOH:O	2.34	0.61
1:A:359:U:H5"	1:A:360:C:H5'	1.81	0.61
1:A:2775:A:H2'	1:A:2776:C:C6	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:C:N4	6:G:67:VAL:O	2.34	0.61
5:F:147:ILE:HG23	5:F:186:LEU:HD23	1.81	0.61
1:A:1180:G:N7	35:A:3228:HOH:O	2.31	0.60
12:O:76:LYS:HB2	12:O:91:GLU:HG3	1.82	0.60
1:A:896:G:OP1	12:O:24:GLY:N	2.34	0.60
1:A:992:G:N7	35:A:3241:HOH:O	2.31	0.60
35:B:342:HOH:O	14:Q:28:CYS:SG	2.57	0.60
1:A:688:C:O2'	1:A:724:A:N6	2.35	0.60
1:A:2170:C:H2'	1:A:2171:A:C8	2.36	0.60
1:A:2498:U:H5"	4:E:128:ARG:HG3	1.84	0.60
32:K:28:LEU:HD12	32:K:35:ILE:HG23	1.84	0.60
1:A:2454:C:OP2	30:8:4:ARG:NH2	2.35	0.60
1:A:1419:G:H2'	1:A:1420:A:C8	2.37	0.59
1:A:2170:C:H2'	1:A:2171:A:H8	1.67	0.59
3:D:132:LEU:HD23	3:D:135:ILE:HD12	1.82	0.59
11:N:78:ARG:HB2	11:N:81:GLU:HG3	1.83	0.59
1:A:1259:A:H1'	35:A:4491:HOH:O	2.03	0.59
21:X:162:LEU:HD12	21:X:182:LEU:H	1.67	0.59
1:A:797:U:OP2	11:N:41:ARG:NH2	2.34	0.59
1:A:1036:A:H4'	31:J:58:THR:HB	1.85	0.59
6:G:119:ALA:CB	6:G:179:ASN:HB2	2.31	0.59
5:F:1:MET:HG3	5:F:13:VAL:HG23	1.84	0.59
27:5:6:ARG:NH2	27:5:50:ILE:O	2.36	0.59
1:A:1067:A:H4'	32:K:94:ASN:HB2	1.85	0.59
1:A:1373:C:H2'	1:A:1374:A:C8	2.38	0.58
5:F:169:ARG:NH1	5:F:175:ASP:OD1	2.32	0.58
29:7:53:ASP:OD1	29:7:56:ARG:NH2	2.37	0.58
1:A:1989:G:OP1	13:P:17:ARG:NH2	2.36	0.58
1:A:929:G:OP1	29:7:64:ARG:NH2	2.36	0.58
1:A:244:A:H5"	11:N:67:VAL:HG11	1.86	0.58
1:A:2260:A:H2'	1:A:2261:A:C8	2.39	0.58
1:A:1049:G:O2'	32:K:113:LYS:HE2	2.04	0.58
1:A:1821:U:H5"	1:A:1822:2MG:H5'	1.84	0.58
21:X:128:SER:OG	21:X:186:ASN:OD1	2.20	0.58
1:A:786:U:H2'	1:A:787:C:C6	2.39	0.57
14:Q:28:CYS:HA	14:Q:92:ASP:HB3	1.85	0.57
7:H:121:ILE:HD11	7:H:140:LEU:HG	1.84	0.57
1:A:2114:G:H2'	1:A:2115:G:H8	1.69	0.57
21:X:24:ARG:NH2	35:X:303:HOH:O	2.36	0.57
3:D:53:HIS:HA	3:D:217:ARG:HB2	1.85	0.57
1:A:2605:G:H21	4:E:155:VAL:HG21	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:31:VAL:HG12	6:G:96:MET:SD	2.45	0.57
1:A:219:A:N3	1:A:234:U:O2'	2.35	0.56
1:A:963:A:H5"	17:T:81:LYS:HD2	1.87	0.56
1:A:2406:U:H4'	27:5:18:THR:HG21	1.87	0.56
1:A:747:G:N7	35:A:3285:HOH:O	2.33	0.56
1:A:921:C:H4'	1:A:922:G:H5'	1.86	0.56
1:A:1766:U:H5	1:A:1771:A:N7	2.04	0.56
1:A:2301:G:OP1	6:G:88:LYS:NZ	2.27	0.56
5:F:97:LYS:NZ	35:F:309:HOH:O	2.37	0.56
32:K:56:PRO:HD3	32:K:75:PRO:HD3	1.87	0.56
1:A:1788:A:OP2	3:D:150:LYS:NZ	2.34	0.56
1:A:2114:G:N2	1:A:2149:A:O2'	2.38	0.56
1:A:2300:C:H5"	6:G:88:LYS:HD2	1.88	0.56
1:A:2121:A:H2'	1:A:2122:A:H8	1.70	0.56
1:A:2172:U:H2'	1:A:2173:G:H8	1.70	0.56
1:A:2623:U:H4'	4:E:82:GLU:OE1	2.06	0.56
12:O:78:PRO:HG2	12:O:81:VAL:HG21	1.88	0.56
14:Q:13:ARG:HH22	22:Y:75:PHE:HZ	1.53	0.56
1:A:441:G:N1	1:A:445:A:OP2	2.33	0.56
1:A:570:U:H2'	1:A:571:C:C6	2.41	0.55
1:A:1097:G:H4'	31:J:78:GLY:C	2.31	0.55
1:A:1710:A:N7	1:A:1724:U:O2'	2.38	0.55
3:D:19:VAL:HG23	3:D:203:ARG:HB3	1.88	0.55
19:V:37:ALA:O	19:V:80:LYS:NZ	2.37	0.55
1:A:59:U:OP2	19:V:77:ASN:ND2	2.39	0.55
10:M:120:GLU:OE1	15:R:66:SER:OG	2.24	0.55
1:A:815:A:N7	35:A:3291:HOH:O	2.33	0.55
1:A:1018:A:N3	1:A:2473:C:O2'	2.35	0.55
1:A:1420:A:H2'	1:A:1421:A:C8	2.40	0.55
3:D:94:LEU:HD11	3:D:104:ILE:HD13	1.88	0.55
1:A:486:G:H21	18:U:61:ASN:HD21	1.54	0.55
35:A:4741:HOH:O	3:D:39:LYS:HD2	2.05	0.55
2:B:13:A:N1	2:B:69:G:O2'	2.38	0.55
1:A:2102:G:H2'	1:A:2104:A:N7	2.22	0.55
1:A:2643:U:O2	1:A:2652:A:N7	2.39	0.55
6:G:108:LEU:HD21	6:G:130:MET:HE1	1.89	0.55
19:V:5:ARG:NH2	19:V:36:ASP:OD1	2.39	0.55
1:A:2534:A:H2'	1:A:2535:U:C6	2.42	0.55
21:X:63:VAL:HG13	21:X:74:THR:HG23	1.89	0.55
1:A:2272:C:OP2	27:5:2:ARG:HD3	2.07	0.54
1:A:1237:G:O6	11:N:18:ARG:NH2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2554:G:H2'	1:A:2555:U:C6	2.42	0.54
1:A:823:A:H2'	1:A:824:G:C8	2.42	0.54
2:B:114:C:H2'	2:B:115:A:H8	1.71	0.54
1:A:853:G:H2'	1:A:854:C:C6	2.41	0.54
1:A:1781:A:H2'	1:A:1782:C:C6	2.43	0.54
1:A:2676:U:H5	35:A:5383:HOH:O	1.90	0.54
12:O:67:ARG:NH1	12:O:105:GLU:OE2	2.40	0.54
1:A:569:G:O2'	1:A:2006:A:OP1	2.25	0.54
1:A:859:U:H2'	1:A:860:U:H5"	1.88	0.54
1:A:1097:G:O2'	31:J:79:PRO:HD3	2.08	0.54
1:A:1740:G:H5"	15:R:94:ARG:HD2	1.89	0.54
1:A:1073:U:O3'	31:J:42:ARG:NH2	2.40	0.54
1:A:192:C:O2'	1:A:792:A:N3	2.41	0.54
1:A:983:G:OP2	16:S:51:ARG:NH2	2.40	0.54
1:A:2461:U:OP2	1:A:2462:C:N4	2.28	0.54
13:P:54:LEU:HD21	13:P:65:LEU:HB3	1.89	0.54
1:A:405:C:H2'	1:A:406:A:C8	2.42	0.54
1:A:622:A:H5'	11:N:68:SER:HB2	1.90	0.54
1:A:2230:U:H2'	1:A:2231:U:C6	2.42	0.54
7:H:124:GLU:HB2	7:H:132:LEU:HB3	1.89	0.54
12:O:65:TRP:HB2	12:O:105:GLU:HB2	1.90	0.54
1:A:899:A:H2'	1:A:900:A:C8	2.43	0.54
2:B:9:G:OP1	14:Q:20:ARG:NH2	2.41	0.54
3:D:132:LEU:HA	3:D:135:ILE:HD12	1.88	0.54
9:L:43:GLU:HG3	16:S:100:VAL:HG13	1.90	0.54
14:Q:32:SER:O	14:Q:101:ARG:NH2	2.31	0.54
1:A:733:C:O2'	1:A:1649:G:OP1	2.24	0.53
1:A:665:A:N3	1:A:2430:C:O2'	2.41	0.53
1:A:293:A:H2'	1:A:294:A:C8	2.43	0.53
1:A:985:C:O2	9:L:3:THR:OG1	2.22	0.53
1:A:1851:U:OP1	1:A:2397:G:O2'	2.26	0.53
1:A:2735:A:H5'	7:H:4:VAL:HG21	1.91	0.53
27:5:25:THR:HG22	27:5:26:LYS:HE3	1.91	0.53
1:A:191:A:H2'	1:A:192:C:C6	2.44	0.53
5:F:142:LEU:HD13	5:F:145:VAL:HG21	1.90	0.53
1:A:571:C:H2'	1:A:572:A:C8	2.43	0.53
1:A:1779:G:O2'	1:A:1817:C:OP1	2.25	0.53
13:P:79:LEU:HA	13:P:83:LEU:HB2	1.90	0.53
23:Z:13:VAL:HG23	23:Z:29:PHE:HB2	1.90	0.53
1:A:1453:U:O3'	1:A:1536:G:O2'	2.27	0.53
6:G:52:ASN:ND2	6:G:147:ASP:OD2	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:C:OP2	20:W:81:ARG:NH2	2.42	0.53
1:A:1253:G:O2'	1:A:1999:G:O6	2.24	0.53
1:A:2803:G:H5"	13:P:99:LYS:HE3	1.91	0.53
9:L:4:TYR:O	16:S:64:ARG:NH1	2.35	0.53
1:A:2051:C:H2'	1:A:2052:C:C6	2.44	0.53
4:E:156:PHE:HB3	9:L:81:PRO:HG3	1.90	0.53
1:A:1044:A:H2'	1:A:1045:G:C8	2.43	0.52
1:A:38:A:N3	5:F:42:SER:HB3	2.24	0.52
1:A:265:A:N1	1:A:418:U:O2'	2.41	0.52
1:A:739:A:H4'	1:A:1258:G:N3	2.24	0.52
2:B:15:A:OP2	2:B:69:G:N2	2.34	0.52
1:A:567:G:O2'	1:A:1241:A:OP1	2.26	0.52
1:A:2341:A:H4'	22:Y:35:ASN:ND2	2.24	0.52
2:B:43:C:N3	35:B:305:HOH:O	2.33	0.52
10:M:98:ILE:HD13	10:M:114:ILE:HG23	1.92	0.52
1:A:19:A:H5"	16:S:22:LYS:HG2	1.92	0.52
19:V:93:ASP:OD1	19:V:93:ASP:N	2.43	0.52
1:A:2578:C:H2'	1:A:2579:G:C8	2.45	0.52
3:D:133:ARG:HA	3:D:167:ARG:HH12	1.75	0.52
6:G:111:VAL:HG22	6:G:137:ILE:HG21	1.92	0.52
1:A:1616:G:OP2	1:A:1616:G:N2	2.29	0.52
1:A:1786:G:OP1	3:D:259:ARG:NH1	2.36	0.52
1:A:1074:A:OP2	31:J:53:LYS:HG3	2.09	0.52
1:A:2061:U:H2'	1:A:2062:U:C6	2.45	0.52
1:A:2220:U:H2'	1:A:2221:G:C8	2.45	0.52
1:A:2602:U:H1'	26:4:4:GLN:HB3	1.92	0.52
15:R:89:ARG:NH2	15:R:111:ILE:O	2.34	0.52
1:A:1834:A:O2'	1:A:1835:A:N7	2.43	0.51
1:A:2052:C:H2'	1:A:2053:C:H6	1.75	0.51
1:A:2602:U:C2	26:4:4:GLN:HA	2.45	0.51
1:A:907:A:N3	2:B:80:U:O2'	2.40	0.51
1:A:1185:U:H2'	1:A:1186:U:C6	2.45	0.51
10:M:24:VAL:HG13	10:M:33:ALA:HB2	1.92	0.51
1:A:937:A:H2'	1:A:938:C:C6	2.45	0.51
1:A:2544:G:H2'	1:A:2545:C:C6	2.45	0.51
1:A:2585:A:H5"	3:D:234:GLY:HA3	1.93	0.51
1:A:334:A:O2'	5:F:161:ARG:NH2	2.43	0.51
1:A:466:C:H4'	1:A:501:C:H5'	1.91	0.51
4:E:41:GLU:HG3	4:E:47:ARG:HG3	1.93	0.51
8:I:79:LEU:HD21	8:I:145:ILE:HG12	1.92	0.51
1:A:323:G:OP2	20:W:68:ASN:ND2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1756:U:O2'	1:A:1945:C:OP1	2.28	0.51
17:T:59:VAL:HG22	17:T:101:ILE:HG23	1.93	0.51
1:A:697:G:N7	35:A:3345:HOH:O	2.35	0.51
6:G:110:ARG:HH12	6:G:139:PRO:HA	1.76	0.51
12:O:43:THR:HG22	12:O:94:VAL:HG12	1.91	0.51
21:X:75:VAL:HB	21:X:94:PHE:HB3	1.93	0.51
31:J:32:GLY:HA3	31:J:105:LYS:HD2	1.93	0.51
1:A:388:U:H5"	23:Z:32:ASN:HB2	1.93	0.51
1:A:1783:U:H2'	1:A:1784:C:C6	2.46	0.51
1:A:72:A:H61	24:1:58:ASN:HD22	1.59	0.51
1:A:1078:A:N6	32:K:135:SER:HB3	2.27	0.51
1:A:1424:C:H2'	1:A:1425:U:C6	2.46	0.51
1:A:845:G:H2'	1:A:846:G:C8	2.46	0.50
1:A:1434:U:H2'	1:A:1435:U:C6	2.46	0.50
1:A:1672:G:H2'	1:A:1673:C:C6	2.47	0.50
28:6:12:ARG:HE	28:6:44:VAL:HG12	1.76	0.50
1:A:2711:U:OP1	4:E:123:LYS:NZ	2.43	0.50
1:A:349:U:O2'	1:A:350:G:H8	1.94	0.50
1:A:729:A:H1'	1:A:730:C:H5	1.76	0.50
1:A:1658:A:O2'	1:A:1664:G:N7	2.41	0.50
2:B:48:U:H2'	2:B:49:C:C6	2.47	0.50
9:L:110:PRO:O	9:L:115:GLY:HA3	2.10	0.50
1:A:652:G:H5'	11:N:16:LYS:HB3	1.94	0.50
1:A:2582:G:N2	1:A:2585:A:OP2	2.35	0.50
1:A:2592:U:H2'	1:A:2593:C:C6	2.47	0.50
3:D:135:ILE:O	3:D:167:ARG:NH2	2.45	0.50
12:O:34:LEU:HD13	12:O:118:PHE:HB3	1.93	0.50
1:A:576:A:N1	1:A:799:G:O2'	2.39	0.50
1:A:979:G:OP2	25:2:11:SER:OG	2.28	0.50
1:A:2307:A:H8	1:A:2309:A:C5	2.30	0.50
1:A:2821:G:H2'	1:A:2866:A:H61	1.76	0.50
1:A:629:U:H2'	1:A:630:C:C6	2.46	0.50
1:A:2079:U:OP1	1:A:2186:A:O2'	2.23	0.50
12:O:135:THR:HG23	35:O:201:HOH:O	2.11	0.50
1:A:1140:A:H2'	1:A:1141:C:C6	2.46	0.50
1:A:1843:U:H2'	1:A:1844:G:O4'	2.12	0.50
1:A:364:U:H2'	1:A:365:A:H8	1.77	0.50
1:A:797:U:O2'	1:A:2047:A:N1	2.40	0.50
1:A:848:G:O2'	1:A:905:G:O6	2.22	0.50
1:A:1235:G:OP1	5:F:43:LYS:NZ	2.45	0.50
1:A:1393:U:H2'	1:A:1394:C:H6	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2337:C:OP2	29:7:44:ARG:NH1	2.45	0.50
14:Q:9:LEU:O	14:Q:13:ARG:HG3	2.11	0.50
1:A:1018:A:H2'	1:A:1019:A:C8	2.47	0.49
1:A:1850:G:H4'	1:A:2398:A:H4'	1.93	0.49
1:A:2570:G:N7	35:A:3346:HOH:O	2.35	0.49
1:A:2685:U:H2'	1:A:2686:C:C6	2.47	0.49
2:B:39:U:H2'	2:B:40:U:C6	2.47	0.49
21:X:131:ILE:HD11	21:X:184:VAL:HG22	1.94	0.49
1:A:300:U:H2'	1:A:301:G:O4'	2.11	0.49
1:A:2228:A:H2'	1:A:2229:G:C8	2.47	0.49
19:V:64:GLY:N	19:V:78:ASP:OD1	2.30	0.49
1:A:23:G:OP1	1:A:495:U:N3	2.38	0.49
1:A:1348:G:H2'	1:A:1349:C:C6	2.47	0.49
1:A:1416:G:H2'	1:A:1417:G:H8	1.76	0.49
7:H:87:LEU:HB2	7:H:131:ILE:HB	1.95	0.49
16:S:28:ARG:NH1	35:S:204:HOH:O	2.41	0.49
1:A:294:A:OP2	20:W:81:ARG:NH1	2.43	0.49
1:A:803:U:H2'	1:A:804:C:C6	2.47	0.49
1:A:2273:G:N7	35:A:3363:HOH:O	2.35	0.49
7:H:16:GLU:HB2	7:H:27:LYS:HB3	1.95	0.49
1:A:719:G:H5'	1:A:720:A:H5"	1.94	0.49
1:A:2627:G:OP1	9:L:95:LYS:NZ	2.40	0.49
1:A:1781:A:H2'	1:A:1782:C:H6	1.78	0.49
1:A:2154:U:H3	1:A:2158:A:N6	2.09	0.49
18:U:4:ALA:HB2	18:U:106:LYS:HG2	1.94	0.49
31:J:64:VAL:HG11	31:J:76:PHE:HZ	1.77	0.49
1:A:1034:U:OP1	31:J:8:LYS:NZ	2.45	0.49
1:A:1186:U:H2'	1:A:1187:C:C6	2.47	0.49
6:G:126:GLY:HA3	6:G:160:ALA:HB3	1.94	0.49
1:A:837:C:H2'	1:A:838:A:C8	2.48	0.49
1:A:1084:U:H1'	1:A:1087:U:H5	1.77	0.49
1:A:1393:U:H2'	1:A:1394:C:C6	2.47	0.49
1:A:647:U:H2'	1:A:648:C:C6	2.47	0.49
1:A:2121:A:H2'	1:A:2122:A:C8	2.47	0.49
1:A:557:U:OP2	11:N:29:LYS:NZ	2.39	0.48
1:A:977:C:O2'	1:A:990:A:N3	2.39	0.48
1:A:2073:U:H2'	1:A:2074:U:C6	2.47	0.48
1:A:2118:U:O4'	1:A:2145:A:N6	2.46	0.48
1:A:2293:C:H42	6:G:39:GLY:HA3	1.77	0.48
13:P:2:ARG:HA	13:P:5:LYS:HE3	1.94	0.48
19:V:8:LYS:NZ	24:1:25:GLN:OE1	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:8:16:ILE:HD13	30:8:25:VAL:HG22	1.94	0.48
1:A:1741:A:N1	1:A:2703:C:O2'	2.37	0.48
1:A:2417:A:H1'	35:A:6991:HOH:O	2.13	0.48
1:A:2846:G:H2'	1:A:2847:A:C8	2.48	0.48
3:D:200:HIS:CD2	3:D:203:ARG:HE	2.31	0.48
1:A:247:G:H4'	1:A:377:G:C5	2.48	0.48
1:A:1053:G:N2	32:K:91:ALA:O	2.38	0.48
1:A:1796:A:H2'	1:A:1797:A:C8	2.49	0.48
1:A:2563:G:O2'	1:A:2566:C:OP2	2.26	0.48
5:F:116:ARG:NH1	11:N:1:MET:O	2.41	0.48
18:U:88:ARG:HB2	18:U:92:ARG:HB3	1.95	0.48
1:A:1381:U:H2'	1:A:1382:A:O4'	2.13	0.48
1:A:2052:C:H2'	1:A:2053:C:C6	2.48	0.48
1:A:2316:A:H2'	1:A:2317:G:C8	2.48	0.48
18:U:82:LEU:HB2	18:U:98:LYS:HB2	1.95	0.48
21:X:162:LEU:HD22	21:X:173:LEU:HD13	1.95	0.48
1:A:75:G:H4'	24:1:48:ARG:NH2	2.28	0.48
1:A:580:A:H2'	1:A:581:U:C6	2.49	0.48
1:A:733:C:OP1	4:E:135:GLY:HA2	2.14	0.48
1:A:1115:G:OP2	1:A:1116:A:O2'	2.26	0.48
1:A:2001:A:H2'	1:A:2002:A:C8	2.48	0.48
5:F:17:THR:OG1	5:F:200:GLY:O	2.32	0.48
16:S:49:ASP:HA	16:S:52:GLN:HB2	1.95	0.48
1:A:1784:C:HO2'	3:D:258:THR:HG1	1.59	0.48
1:A:2126:U:H2'	1:A:2127:G:H8	1.79	0.48
18:U:97:VAL:HG12	18:U:99:ARG:HG2	1.96	0.48
19:V:46:VAL:HG21	19:V:84:ILE:HD13	1.96	0.48
1:A:13:A:O4'	1:A:517:A:N6	2.46	0.48
1:A:254:G:N7	29:7:5:LYS:NZ	2.61	0.48
1:A:293:A:H8	1:A:293:A:OP2	1.96	0.48
1:A:1434:U:O2'	1:A:1534:A:N3	2.37	0.48
1:A:1786:G:O2'	3:D:180:GLU:OE2	2.28	0.48
1:A:2233:G:H2'	1:A:2234:A:C8	2.48	0.48
1:A:2775:A:O2'	1:A:2796:A:N3	2.37	0.48
10:M:77:ILE:HG12	15:R:73:ARG:HD2	1.95	0.48
5:F:147:ILE:HD12	5:F:168:VAL:HG22	1.96	0.48
9:L:11:VAL:HG11	9:L:50:THR:HA	1.95	0.48
1:A:618:G:H5"	29:7:18:ALA:HB2	1.95	0.48
1:A:938:C:H2'	1:A:939:G:H8	1.79	0.48
1:A:1635:G:H5"	1:A:1636:C:H5'	1.95	0.48
2:B:28:C:OP1	14:Q:32:SER:OG	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:26:LYS:HB3	19:V:28:GLN:HG3	1.96	0.48
1:A:1284:C:O2'	1:A:1289:A:N1	2.40	0.48
1:A:2245:C:O2'	1:A:2414:C:OP2	2.30	0.48
1:A:2629:G:OP1	9:L:78:SER:OG	2.22	0.48
11:N:19:PRO:HA	11:N:27:LEU:HB3	1.96	0.48
21:X:111:PHE:HE2	21:X:185:ALA:HB2	1.78	0.48
1:A:245:G:O2'	1:A:375:A:N1	2.37	0.47
1:A:1353:A:OP1	23:Z:2:SER:OG	2.21	0.47
1:A:1708:U:H2'	1:A:1709:G:O4'	2.14	0.47
1:A:1840:A:H2'	1:A:1841:A:C8	2.49	0.47
1:A:1795:A:H3'	1:A:1796:A:C8	2.49	0.47
1:A:2449:C:H2'	1:A:2450:C:C6	2.49	0.47
3:D:252:GLN:HE22	3:D:254:LYS:HB2	1.77	0.47
1:A:634:A:H2'	1:A:636:A:N7	2.29	0.47
19:V:1:MET:HB3	19:V:5:ARG:HB3	1.97	0.47
23:Z:53:ALA:HA	23:Z:56:MET:HE3	1.96	0.47
1:A:840:U:H2'	1:A:841:C:C6	2.48	0.47
1:A:1421:A:H2'	1:A:1422:G:O4'	2.14	0.47
1:A:2379:A:H5'	29:7:27:PHE:CD2	2.50	0.47
1:A:2501:U:H2'	1:A:2502:C:C6	2.50	0.47
6:G:8:TYR:HA	6:G:12:ILE:HB	1.94	0.47
1:A:155:U:H2'	1:A:156:A:H8	1.79	0.47
1:A:228:C:N4	1:A:2394:A:N3	2.63	0.47
1:A:1456:A:H2'	1:A:1457:A:C8	2.49	0.47
3:D:29:PRO:HG2	3:D:34:LEU:HD11	1.96	0.47
1:A:454:G:N2	1:A:457:A:OP2	2.40	0.47
1:A:774:G:H5'	1:A:775:G:OP1	2.15	0.47
1:A:1789:A:H2'	1:A:1790:A:C8	2.50	0.47
1:A:2298:A:N3	6:G:79:ILE:HD11	2.30	0.47
1:A:2531:G:H1'	1:A:2633:C:H5'	1.96	0.47
2:B:29:A:H2'	2:B:30:C:C6	2.49	0.47
9:L:49:ASP:OD1	9:L:121:LYS:NZ	2.48	0.47
12:O:74:VAL:HG12	35:O:236:HOH:O	2.15	0.47
27:5:6:ARG:O	27:5:48:ALA:N	2.46	0.47
27:5:36:ASP:HB3	27:5:39:VAL:HG22	1.96	0.47
31:J:100:ALA:HB2	31:J:106:PHE:HD2	1.79	0.47
1:A:58:G:O2'	1:A:73:A:N1	2.41	0.47
1:A:467:G:N1	1:A:470:A:OP2	2.38	0.47
1:A:619:C:O2	1:A:629:U:O2'	2.30	0.47
1:A:1078:A:C6	32:K:135:SER:HB3	2.50	0.47
1:A:847:G:N3	1:A:2255:A:H2'	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2715:U:H4'	35:A:6089:HOH:O	2.14	0.47
12:O:8:LYS:HG2	12:O:9:PHE:CE2	2.50	0.47
1:A:690:G:O2'	1:A:1622:A:N3	2.43	0.47
1:A:1687:G:OP2	1:A:1688:A:O2'	2.27	0.47
1:A:1757:G:N7	35:A:3357:HOH:O	2.35	0.47
1:A:2066:U:O2'	23:Z:23:ASN:ND2	2.43	0.47
3:D:164:LEU:HD11	3:D:172:VAL:CG1	2.45	0.47
19:V:91:ASP:OD1	19:V:92:LEU:N	2.48	0.47
2:B:37:C:O2	14:Q:99:HIS:NE2	2.33	0.46
32:K:110:ALA:HB1	32:K:125:ALA:HB1	1.97	0.46
1:A:822:U:H2'	1:A:823:A:C8	2.50	0.46
1:A:1017:A:C2	1:A:2475:G:H5'	2.50	0.46
1:A:1167:U:H2'	1:A:1168:G:C8	2.50	0.46
1:A:1284:C:OP1	1:A:2697:C:H4'	2.16	0.46
19:V:60:LEU:HD21	19:V:81:LYS:HD2	1.97	0.46
1:A:1351:G:OP2	23:Z:50:ARG:NH1	2.46	0.46
1:A:1892:C:H4'	1:A:1916:G:H8	1.80	0.46
2:B:90:C:H5'	12:O:18:ARG:HG2	1.96	0.46
5:F:61:GLN:NE2	5:F:68:ARG:HD2	2.30	0.46
19:V:86:LEU:HD11	19:V:92:LEU:HG	1.96	0.46
1:A:155:U:H2'	1:A:156:A:C8	2.50	0.46
1:A:938:C:H2'	1:A:939:G:C8	2.51	0.46
1:A:1018:A:N6	1:A:1115:G:H2'	2.29	0.46
1:A:1058:G:N2	1:A:1085:A:O2'	2.49	0.46
1:A:1450:A:H2'	1:A:1451:A:C8	2.50	0.46
6:G:43:ALA:HB1	6:G:50:ILE:HD11	1.97	0.46
12:O:54:LEU:HD12	12:O:117:ALA:HB1	1.97	0.46
26:4:42:VAL:HG22	26:4:48:TYR:HB2	1.98	0.46
1:A:624:G:H2'	1:A:625:C:C6	2.51	0.46
1:A:837:C:H2'	1:A:838:A:H8	1.80	0.46
1:A:2103:G:H2'	1:A:2104:A:N7	2.31	0.46
1:A:2209:A:H4'	3:D:185:LEU:HD11	1.97	0.46
1:A:2619:A:H2'	1:A:2620:G:C8	2.51	0.46
2:B:40:U:N3	2:B:44:G:OP2	2.33	0.46
20:W:1:MET:HE3	20:W:91:LYS:HE3	1.97	0.46
1:A:491:G:N1	1:A:494:A:OP2	2.45	0.46
1:A:632:U:O2'	1:A:634:A:N7	2.39	0.46
1:A:1168:G:H2'	1:A:1169:A:C8	2.50	0.46
1:A:1657:G:O2'	1:A:1978:U:O4	2.28	0.46
1:A:2626:A:H2'	1:A:2627:G:O4'	2.16	0.46
3:D:16:VAL:HG22	3:D:206:GLY:HA3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:U:O2	1:A:2001:A:H1'	2.16	0.46
1:A:836:U:H5	1:A:923:A:N7	2.13	0.46
1:A:1069:C:H2'	1:A:1070:C:O4'	2.16	0.46
1:A:2278:U:H2'	1:A:2279:G:H8	1.78	0.46
6:G:16:LEU:HD11	6:G:169:LEU:HA	1.96	0.46
1:A:363:G:O2'	1:A:391:G:O6	2.31	0.46
1:A:829:U:H2'	1:A:830:C:C6	2.51	0.46
1:A:1394:C:H2'	1:A:1395:U:H6	1.80	0.46
1:A:1784:C:O2'	3:D:258:THR:OG1	2.30	0.46
1:A:2038:U:H5'	1:A:2565:G:O4'	2.14	0.46
7:H:18:LYS:HB3	7:H:25:SER:HB2	1.98	0.46
31:J:27:VAL:HG21	31:J:76:PHE:HE1	1.81	0.46
1:A:250:G:H2'	1:A:251:A:C8	2.51	0.46
1:A:625:C:O2'	1:A:629:U:OP1	2.31	0.46
1:A:1010:A:N1	1:A:1131:U:O2'	2.45	0.46
1:A:1980:U:H4'	4:E:133:THR:OG1	2.16	0.46
2:B:49:C:H2'	2:B:50:A:C8	2.51	0.46
8:I:95:THR:HB	8:I:114:VAL:HB	1.97	0.46
12:O:42:LEU:HD22	12:O:125:LEU:HD22	1.97	0.46
23:Z:8:THR:HG22	23:Z:58:ILE:HD12	1.97	0.46
1:A:121:G:H4'	1:A:149:A:H5'	1.98	0.46
1:A:1594:C:O2'	1:A:1600:A:N1	2.43	0.46
1:A:1621:G:N1	1:A:1624:A:OP2	2.43	0.46
5:F:61:GLN:HE22	5:F:68:ARG:HD2	1.81	0.46
1:A:5:A:H2'	1:A:6:A:C8	2.51	0.45
1:A:710:U:H2'	1:A:711:G:H8	1.81	0.45
1:A:2517:A:N6	7:H:156:PRO:HG3	2.31	0.45
1:A:2624:U:H2'	1:A:2625:G:O4'	2.16	0.45
1:A:2692:A:O2'	1:A:2839:G:OP1	2.31	0.45
2:B:9:G:C2	2:B:10:A:C8	3.03	0.45
3:D:145:GLU:HG2	3:D:151:GLY:C	2.41	0.45
7:H:105:LEU:HB2	7:H:113:VAL:HB	1.97	0.45
18:U:92:ARG:NH1	35:U:208:HOH:O	2.48	0.45
30:8:1:MET:HE3	30:8:1:MET:HB2	1.87	0.45
1:A:293:A:N1	1:A:316:A:O2'	2.47	0.45
1:A:1303:U:H2'	1:A:1304:G:C8	2.52	0.45
1:A:2271:A:H5"	35:A:4820:HOH:O	2.15	0.45
3:D:133:ARG:HB2	3:D:186:ALA:HB1	1.97	0.45
1:A:490:U:H2'	1:A:491:G:O4'	2.15	0.45
1:A:557:U:H2'	1:A:558:U:O4'	2.16	0.45
1:A:672:G:H5'	28:6:26:ASN:CG	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:U:H3	1:A:711:G:H1	1.64	0.45
1:A:1956:A:H2'	1:A:1959:G:H21	1.81	0.45
7:H:72:VAL:HA	7:H:75:MET:HE2	1.98	0.45
1:A:78:U:H2'	1:A:79:C:C6	2.52	0.45
1:A:351:A:H2'	1:A:352:A:C8	2.52	0.45
1:A:467:G:H4'	1:A:493:A:N1	2.31	0.45
1:A:658:A:H2'	1:A:660:A:H62	1.81	0.45
1:A:1299:U:O4	19:V:63:LYS:HD2	2.17	0.45
1:A:2058:A:H2'	1:A:2059:C:C6	2.51	0.45
6:G:77:PHE:HB2	6:G:79:ILE:HG13	1.98	0.45
1:A:1063:A:H2'	1:A:1064:G:H8	1.81	0.45
3:D:2:ALA:N	3:D:199:GLU:OE2	2.49	0.45
19:V:43:LYS:HG3	19:V:54:VAL:HB	1.98	0.45
1:A:525:U:O2'	16:S:49:ASP:OD2	2.27	0.45
1:A:1783:U:H2'	1:A:1784:C:H6	1.81	0.45
1:A:1808:A:OP1	3:D:200:HIS:HE1	1.99	0.45
1:A:2142:U:H2'	1:A:2143:G:O4'	2.17	0.45
6:G:80:ARG:HD2	6:G:83:TRP:CZ2	2.51	0.45
9:L:121:LYS:HB2	9:L:121:LYS:HE2	1.83	0.45
1:A:173:A:H2'	1:A:174:A:C8	2.52	0.45
1:A:1009:U:O2'	1:A:1011:A:N7	2.42	0.45
1:A:1424:C:H2'	1:A:1425:U:H6	1.80	0.45
1:A:2186:A:N1	1:A:2213:C:N4	2.65	0.45
1:A:2360:A:H2'	1:A:2361:C:C6	2.51	0.45
6:G:104:LEU:HD23	6:G:108:LEU:HD12	1.99	0.45
14:Q:16:ARG:HG2	14:Q:26:ARG:HH11	1.82	0.45
1:A:86:U:H4'	1:A:104:U:H1'	1.98	0.45
1:A:584:U:H2'	1:A:585:C:C6	2.51	0.45
1:A:2334:C:H2'	1:A:2335:U:C6	2.52	0.45
1:A:2392:G:O2'	1:A:2398:A:N6	2.48	0.45
1:A:2636:C:H2'	1:A:2637:U:H6	1.82	0.45
1:A:2818:G:H1'	1:A:2870:A:H2'	1.99	0.45
2:B:68:C:H2'	2:B:69:G:O4'	2.17	0.45
31:J:15:VAL:HG21	31:J:55:VAL:HG21	1.99	0.45
1:A:151:C:H2'	1:A:152:U:C6	2.51	0.45
1:A:1392:U:H2'	1:A:1393:U:C6	2.52	0.45
1:A:2018:A:N7	35:A:3386:HOH:O	2.36	0.45
1:A:2220:U:H2'	1:A:2221:G:H8	1.82	0.45
1:A:332:G:N7	35:A:3399:HOH:O	2.36	0.45
1:A:852:A:H2'	1:A:853:G:C8	2.52	0.45
1:A:1627:A:H5'	1:A:1747:C:O2'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2258:G:OP1	22:Y:18:SER:HB2	2.17	0.45
22:Y:26:PHE:H	22:Y:29:GLN:HE21	1.65	0.45
1:A:513:G:H2'	1:A:514:C:C6	2.52	0.44
1:A:719:G:C5	3:D:207:LYS:HB2	2.52	0.44
1:A:1415:C:C5	1:A:1559:A:H5"	2.52	0.44
2:B:114:C:H2'	2:B:115:A:C8	2.50	0.44
17:T:2:TYR:CD1	17:T:13:LYS:HE2	2.52	0.44
1:A:224:U:O4	1:A:410:U:O2'	2.35	0.44
1:A:579:U:H2'	1:A:580:A:C8	2.52	0.44
1:A:2024:A:H2'	1:A:2025:G:C8	2.52	0.44
1:A:2025:G:H2'	1:A:2026:U:O4'	2.17	0.44
1:A:2519:G:N2	1:A:2650:G:O2'	2.50	0.44
10:M:8:LEU:HD11	10:M:84:ALA:HB2	1.99	0.44
12:O:17:ASN:O	12:O:39:ARG:HD3	2.17	0.44
1:A:913:A:H2'	1:A:914:G:C8	2.52	0.44
1:A:1028:G:H2'	1:A:1029:A:C8	2.52	0.44
1:A:1211:A:H2'	1:A:1212:G:C8	2.53	0.44
1:A:1553:U:H2'	1:A:1554:C:C6	2.52	0.44
6:G:147:ASP:OD1	6:G:150:ARG:NH2	2.49	0.44
7:H:137:ASP:OD1	7:H:137:ASP:N	2.50	0.44
13:P:56:LYS:HE2	13:P:87:TYR:O	2.18	0.44
20:W:3:LYS:HD3	20:W:82:VAL:HB	1.99	0.44
24:1:3:ALA:HA	24:1:6:LEU:HD12	1.99	0.44
1:A:1212:G:N7	35:A:3383:HOH:O	2.36	0.44
1:A:2378:G:C6	1:A:2414:C:H1'	2.52	0.44
1:A:687:G:H2'	1:A:688:C:C6	2.52	0.44
1:A:719:G:O2'	1:A:753:G:H4'	2.17	0.44
1:A:1460:U:H2'	1:A:1461:G:O4'	2.17	0.44
1:A:1777:C:H2'	1:A:1778:A:C5	2.52	0.44
1:A:1991:G:N7	35:A:3410:HOH:O	2.36	0.44
1:A:2114:G:N1	1:A:2149:A:H1'	2.33	0.44
1:A:2326:G:H2'	1:A:2327:C:C6	2.53	0.44
3:D:25:HIS:CG	3:D:80:ARG:HD2	2.52	0.44
6:G:67:VAL:HA	6:G:87:VAL:HG12	1.98	0.44
32:K:133:ALA:HB1	32:K:138:LEU:HB2	1.99	0.44
1:A:355:G:OP2	1:A:356:A:O2'	2.27	0.44
1:A:1433:C:H2'	1:A:1434:U:C6	2.52	0.44
3:D:107:PRO:HG3	3:D:127:GLY:HA2	2.00	0.44
4:E:121:THR:HB	4:E:127:PHE:CD2	2.53	0.44
21:X:131:ILE:HG12	21:X:184:VAL:HA	2.00	0.44
1:A:583:U:H2'	1:A:584:U:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1276:C:H2'	1:A:1277:A:C8	2.53	0.44
1:A:1416:G:H2'	1:A:1417:G:C8	2.53	0.44
1:A:1833:G:H2'	1:A:1834:A:O4'	2.17	0.44
1:A:2551:A:OP1	1:A:2635:G:O2'	2.27	0.44
1:A:2740:A:N7	35:A:3394:HOH:O	2.36	0.44
6:G:116:GLY:HA3	6:G:178:ARG:HB3	2.00	0.44
9:L:7:LYS:O	9:L:11:VAL:HG23	2.17	0.44
12:O:63:LYS:HD3	12:O:65:TRP:CZ2	2.52	0.44
13:P:24:MET:HB3	13:P:44:LEU:HD13	2.00	0.44
1:A:314:A:H4'	1:A:316:A:N7	2.32	0.44
1:A:356:A:OP1	1:A:416:G:O2'	2.29	0.44
1:A:1018:A:H61	1:A:1115:G:H2'	1.83	0.44
1:A:1372:A:O2'	1:A:1383:U:O2	2.36	0.44
1:A:2012:C:H2'	1:A:2013:U:C6	2.53	0.44
1:A:2269:G:H4'	1:A:2376:G:O2'	2.18	0.44
1:A:2636:C:H2'	1:A:2637:U:C6	2.53	0.44
3:D:137:VAL:HA	3:D:164:LEU:HD23	1.99	0.44
4:E:39:LYS:NZ	4:E:82:GLU:OE2	2.47	0.44
1:A:586:A:H2'	1:A:587:G:C8	2.53	0.44
1:A:1933:U:H2'	1:A:1934:C:C6	2.53	0.44
1:A:2122:A:H4'	1:A:2147:C:H4'	1.99	0.44
1:A:2337:C:H5"	29:7:41:ARG:HD2	2.00	0.44
1:A:2670:C:O2	10:M:70:ARG:NH1	2.39	0.44
24:1:2:LYS:HE3	24:1:2:LYS:HB3	1.74	0.44
1:A:2182:U:H2'	1:A:2183:C:H6	1.83	0.43
1:A:2812:U:H3'	1:A:2813:A:H8	1.83	0.43
15:R:8:GLN:O	15:R:12:GLU:HG3	2.18	0.43
28:6:19:ARG:NH2	35:6:103:HOH:O	2.51	0.43
1:A:719:G:C6	3:D:207:LYS:HB2	2.53	0.43
1:A:731:U:H2'	1:A:732:C:C6	2.53	0.43
1:A:990:A:H2'	1:A:991:A:C8	2.53	0.43
1:A:2588:C:H4'	1:A:2589:A:N1	2.33	0.43
2:B:24:G:N7	2:B:56:G:H2'	2.33	0.43
2:B:48:U:H4'	14:Q:99:HIS:HD2	1.83	0.43
4:E:26:THR:HG21	4:E:193:VAL:HB	1.99	0.43
1:A:405:C:H2'	1:A:406:A:H8	1.82	0.43
1:A:408:C:H2'	1:A:409:C:C6	2.54	0.43
1:A:807:C:O2'	1:A:829:U:H5"	2.18	0.43
1:A:1929:C:OP2	1:A:1930:U:O2'	2.23	0.43
4:E:9:LYS:NZ	4:E:195:GLY:O	2.42	0.43
4:E:36:THR:HG22	4:E:74:VAL:HG21	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:112:ALA:O	8:I:115:ARG:NH1	2.51	0.43
13:P:106:ASP:OD1	13:P:106:ASP:N	2.51	0.43
1:A:1167:U:H2'	1:A:1168:G:H8	1.84	0.43
1:A:2238:OMG:HM23	1:A:2238:OMG:H1'	1.70	0.43
1:A:2502:C:H2'	1:A:2503:A:H8	1.84	0.43
1:A:2886:G:H2'	1:A:2887:A:C8	2.53	0.43
2:B:93:C:H5"	21:X:24:ARG:CZ	2.48	0.43
31:J:23:LEU:N	31:J:85:SER:O	2.46	0.43
31:J:51:TYR:HD2	31:J:84:PHE:HD2	1.65	0.43
1:A:864:G:H5"	21:X:159:ILE:HD12	2.01	0.43
1:A:1394:C:H2'	1:A:1395:U:C6	2.54	0.43
1:A:1554:C:H2'	1:A:1555:C:C6	2.52	0.43
1:A:1656:G:O2'	10:M:6:SER:OG	2.30	0.43
1:A:2048:G:H2'	1:A:2488:C:O2'	2.19	0.43
1:A:2463:A:H2'	1:A:2464:U:C6	2.53	0.43
1:A:2826:G:O2'	13:P:49:GLU:OE1	2.26	0.43
18:U:34:ASN:HD21	26:4:36:VAL:HG21	1.84	0.43
1:A:540:U:H2'	1:A:541:A:C8	2.54	0.43
1:A:803:U:H2'	1:A:804:C:H6	1.84	0.43
1:A:1325:G:N7	19:V:65:LYS:NZ	2.48	0.43
4:E:84:ARG:HD2	4:E:84:ARG:HA	1.87	0.43
1:A:683:A:H2'	1:A:684:U:C6	2.54	0.43
1:A:1050:U:OP2	32:K:75:PRO:HA	2.19	0.43
1:A:1157:G:H2'	1:A:1158:U:C6	2.53	0.43
1:A:1492:U:H2'	1:A:1493:U:C6	2.54	0.43
1:A:1976:G:H2'	1:A:1977:C:O4'	2.17	0.43
1:A:2215:G:H2'	1:A:2216:U:C6	2.53	0.43
9:L:13:ARG:NH2	9:L:49:ASP:O	2.51	0.43
19:V:1:MET:HE3	19:V:1:MET:HB2	1.95	0.43
21:X:6:LEU:HG	21:X:53:LEU:HD22	2.01	0.43
1:A:2059:C:H2'	1:A:2060:C:H6	1.84	0.43
2:B:48:U:H2'	2:B:49:C:H6	1.83	0.43
12:O:71:ASP:OD1	12:O:71:ASP:N	2.52	0.43
16:S:69:ALA:HB2	16:S:79:LEU:HD22	2.01	0.43
16:S:91:ASP:HB2	17:T:11:GLN:CD	2.44	0.43
17:T:24:LYS:HD3	17:T:92:TRP:HB3	2.01	0.43
18:U:83:LYS:HB3	18:U:95:ARG:HD2	2.00	0.43
1:A:36:G:N3	1:A:441:G:O2'	2.50	0.43
1:A:150:U:H2'	1:A:151:C:C6	2.54	0.43
1:A:207:A:H2'	1:A:208:C:O4'	2.19	0.43
1:A:1997:G:N7	35:A:3402:HOH:O	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2006:A:H4'	16:S:34:VAL:HG21	2.01	0.43
1:A:2272:C:OP2	27:5:2:ARG:NH1	2.50	0.43
1:A:2364:A:H2'	1:A:2365:A:C8	2.54	0.43
1:A:2816:A:N7	35:A:3415:HOH:O	2.37	0.43
3:D:94:LEU:O	3:D:101:ARG:HA	2.19	0.43
21:X:138:CYS:HB3	21:X:171:VAL:HA	2.00	0.43
32:K:25:GLY:HA2	32:K:35:ILE:HD13	2.01	0.43
1:A:269:C:H5"	1:A:271:U:H5'	2.00	0.43
1:A:301:G:N1	1:A:304:A:OP2	2.45	0.43
1:A:386:U:O2'	1:A:387:G:N7	2.46	0.43
1:A:1773:A:H1'	1:A:1925:A:N6	2.33	0.43
1:A:2353:A:H4'	22:Y:62:LYS:HE2	2.00	0.43
1:A:2874:C:H2'	1:A:2875:C:C6	2.54	0.43
19:V:53:LYS:HB2	19:V:90:GLN:HE22	1.84	0.43
32:K:86:ILE:HD13	32:K:138:LEU:HD21	2.00	0.43
1:A:626:G:N2	11:N:111:MET:SD	2.92	0.42
1:A:1325:G:O2'	1:A:1380:A:N1	2.39	0.42
1:A:1673:C:H2'	1:A:1674:A:C8	2.54	0.42
1:A:2304:C:H2'	1:A:2305:G:O4'	2.18	0.42
4:E:23:ILE:HG23	4:E:190:LYS:HG3	2.01	0.42
12:O:29:PHE:HB3	12:O:65:TRP:CE2	2.54	0.42
1:A:1644:A:O2'	4:E:118:PHE:O	2.31	0.42
1:A:2806:G:H2'	1:A:2808:A:N7	2.34	0.42
14:Q:82:LYS:HE3	14:Q:82:LYS:HB3	1.88	0.42
1:A:732:C:H2'	1:A:733:C:C6	2.54	0.42
1:A:917:G:H2'	1:A:918:U:C6	2.54	0.42
1:A:2128:G:H1	1:A:2137:U:H3	1.68	0.42
1:A:2697:C:H2'	1:A:2698:A:C8	2.54	0.42
2:B:104:A:H4'	21:X:95:LEU:HD13	2.00	0.42
6:G:2:ALA:HB3	6:G:5:LYS:HB2	2.00	0.42
1:A:413:A:H5"	35:A:6813:HOH:O	2.19	0.42
1:A:1054:C:O2'	32:K:91:ALA:HB2	2.18	0.42
1:A:2674:U:H2'	1:A:2675:G:O4'	2.19	0.42
26:4:7:LYS:HE3	26:4:7:LYS:HB2	1.90	0.42
1:A:156:A:H2'	1:A:157:C:C6	2.55	0.42
1:A:456:G:H2'	1:A:457:A:C8	2.54	0.42
1:A:1044:A:H1'	31:J:31:ARG:HG2	2.01	0.42
1:A:1047:A:H1'	31:J:35:VAL:HG11	2.01	0.42
1:A:1560:A:H2'	1:A:1561:A:C8	2.55	0.42
1:A:1986:C:H5"	1:A:2710:C:O2'	2.19	0.42
1:A:1987:C:OP1	13:P:5:LYS:NZ	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2346:C:H5”	29:7:50:ASN:ND2	2.34	0.42
1:A:2821:G:H1’	1:A:2870:A:N6	2.35	0.42
1:A:617:A:N7	11:N:113:SER:HB2	2.34	0.42
1:A:997:C:OP1	9:L:39:LYS:NZ	2.52	0.42
1:A:1097:G:H2’	1:A:1098:U:C6	2.53	0.42
1:A:1238:C:OP1	16:S:13:ARG:NH2	2.48	0.42
10:M:122:LEU:HD13	15:R:71:VAL:HG11	2.00	0.42
27:5:9:SER:HB3	27:5:45:TYR:CZ	2.54	0.42
1:A:448:A:N1	1:A:461:A:H5”	2.34	0.42
1:A:791:G:C8	5:F:49:SER:HB3	2.54	0.42
1:A:1186:U:H2’	1:A:1187:C:H6	1.84	0.42
1:A:1814:U:OP2	3:D:221:ARG:NE	2.51	0.42
21:X:4:PHE:HB3	21:X:64:ILE:HG12	2.02	0.42
1:A:523:A:H4’	1:A:524:G:C8	2.55	0.42
1:A:578:U:H2’	1:A:579:U:C6	2.55	0.42
1:A:635:U:O2’	1:A:636:A:OP1	2.33	0.42
1:A:1065:C:H2’	1:A:1066:C:C6	2.55	0.42
1:A:1309:A:C5	1:A:1310:C:C5	3.08	0.42
1:A:1672:G:OP2	1:A:1689:G:N2	2.52	0.42
1:A:2009:U:O2’	1:A:2604:U:H5’	2.20	0.42
1:A:2641:A:N1	1:A:2652:A:H5”	2.34	0.42
2:B:112:G:H2’	2:B:113:U:C6	2.55	0.42
5:F:1:MET:HE3	5:F:19:GLY:HA3	2.01	0.42
18:U:73:THR:HB	18:U:106:LYS:HD2	2.01	0.42
1:A:553:A:OP1	16:S:41:LYS:NZ	2.53	0.42
1:A:898:A:H2’	1:A:901:C:C5	2.55	0.42
1:A:1437:G:H2’	1:A:1438:C:C6	2.55	0.42
1:A:2363:A:N3	14:Q:110:ARG:NH2	2.65	0.42
1:A:2439:C:H2’	1:A:2440:A:C8	2.55	0.42
6:G:57:LEU:HD23	6:G:57:LEU:HA	1.89	0.42
6:G:130:MET:HG3	6:G:154:ILE:HB	2.01	0.42
32:K:81:LYS:O	32:K:85:GLY:N	2.51	0.42
1:A:1214:A:N3	35:A:3392:HOH:O	2.36	0.42
1:A:1352:A:OP1	23:Z:3:ARG:NH1	2.42	0.42
1:A:1722:C:H2’	1:A:1723:G:O4’	2.19	0.42
1:A:1844:G:H1’	1:A:1872:A:H61	1.85	0.42
1:A:2314:A:H2’	1:A:2315:A:C8	2.55	0.42
1:A:2733:U:H5”	7:H:138:LYS:HB3	2.02	0.42
2:B:49:C:H2’	2:B:50:A:H8	1.85	0.42
6:G:117:LEU:HD12	6:G:176:PRO:HD2	2.02	0.42
1:A:519:A:N6	35:A:3629:HOH:O	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:A:H2'	1:A:530:G:O4'	2.19	0.41
1:A:1144:C:H5'	16:S:76:TYR:HE2	1.85	0.41
1:A:1285:C:H2'	1:A:1286:G:O4'	2.20	0.41
1:A:1876:A:H2'	1:A:1877:A:C8	2.55	0.41
1:A:2010:C:H4'	1:A:2604:U:O3'	2.19	0.41
1:A:2088:A:H2'	1:A:2089:G:H8	1.84	0.41
1:A:2668:C:OP2	4:E:114:LYS:NZ	2.51	0.41
2:B:18:G:H2'	2:B:19:C:C6	2.55	0.41
1:A:483:A:H2'	1:A:484:G:O4'	2.20	0.41
1:A:624:G:N7	11:N:74:ARG:NH1	2.68	0.41
1:A:633:A:N1	1:A:2356:A:O2'	2.46	0.41
1:A:1328:U:OP2	1:A:1381:U:O2'	2.33	0.41
1:A:1357:C:H2'	1:A:1358:G:O4'	2.20	0.41
1:A:1530:G:H2'	1:A:1531:A:C8	2.54	0.41
1:A:1670:U:H2'	1:A:1671:G:O4'	2.20	0.41
1:A:1867:U:H2'	1:A:1868:C:C6	2.55	0.41
1:A:2017:6MZ:C2	1:A:2486:C:H5"	2.49	0.41
1:A:2307:A:H8	1:A:2309:A:C6	2.37	0.41
1:A:2378:G:O6	1:A:2412:A:H8	2.03	0.41
11:N:85:VAL:HB	11:N:94:THR:HG22	2.03	0.41
15:R:34:LYS:HB2	15:R:39:GLN:HE21	1.85	0.41
1:A:1813:G:OP1	3:D:223:VAL:HG13	2.20	0.41
1:A:2761:C:H2'	1:A:2762:A:O4'	2.20	0.41
3:D:24:LEU:HD13	3:D:83:TYR:HB2	2.02	0.41
5:F:172:GLN:HE21	5:F:198:LEU:HD21	1.85	0.41
12:O:33:ALA:HB1	12:O:102:VAL:HG13	2.02	0.41
1:A:213:A:H2'	1:A:214:G:C8	2.55	0.41
1:A:511:A:H2'	1:A:512:U:C6	2.55	0.41
1:A:628:G:H2'	1:A:629:U:C6	2.55	0.41
1:A:977:C:H2'	1:A:978:A:O4'	2.21	0.41
1:A:1372:A:H1'	1:A:1373:C:C6	2.56	0.41
1:A:1770:A:H5'	1:A:2595:G:H4'	2.02	0.41
1:A:2456:A:H4'	12:O:56:ARG:HD2	2.01	0.41
1:A:2637:U:H2'	1:A:2638:C:H6	1.85	0.41
2:B:112:G:H2'	2:B:113:U:H6	1.86	0.41
5:F:129:LYS:HA	5:F:129:LYS:HD2	1.94	0.41
6:G:121:SER:HB2	6:G:128:TYR:CE1	2.55	0.41
7:H:28:GLY:HA3	7:H:79:VAL:HB	2.03	0.41
8:I:79:LEU:H	8:I:79:LEU:HD23	1.84	0.41
21:X:31:ALA:HB3	21:X:43:VAL:HG23	2.02	0.41
1:A:1844:G:H1'	1:A:1872:A:N6	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2172:U:H2'	1:A:2173:G:C8	2.53	0.41
1:A:2471:G:OP1	12:O:45:ARG:NH1	2.39	0.41
1:A:2578:C:H2'	1:A:2579:G:H8	1.84	0.41
10:M:98:ILE:HD12	10:M:117:LEU:HB2	2.01	0.41
19:V:68:ARG:HH21	19:V:73:LEU:HD22	1.86	0.41
32:K:106:LEU:HD22	32:K:129:ILE:HG22	2.02	0.41
1:A:974:A:N3	1:A:974:A:H2'	2.35	0.41
1:A:1054:C:H1'	32:K:91:ALA:HA	2.03	0.41
1:A:2059:C:H2'	1:A:2060:C:C6	2.56	0.41
1:A:43:G:H2'	1:A:44:A:C8	2.56	0.41
1:A:571:C:H2'	1:A:572:A:H8	1.84	0.41
1:A:959:G:O3'	25:2:14:GLY:HA2	2.21	0.41
1:A:2140:C:H2'	1:A:2141:G:C8	2.55	0.41
5:F:68:ARG:HG3	35:F:321:HOH:O	2.20	0.41
10:M:63:VAL:HG12	10:M:106:LEU:HD11	2.02	0.41
12:O:76:LYS:HE2	12:O:92:TYR:HE1	1.86	0.41
29:7:22:LYS:HB2	29:7:46:THR:HG22	2.02	0.41
1:A:299:C:H2'	1:A:300:U:C6	2.56	0.41
1:A:677:C:H2'	1:A:678:U:O4'	2.21	0.41
1:A:1320:C:H2'	1:A:1321:G:H8	1.86	0.41
1:A:2288:C:H2'	1:A:2289:C:C6	2.55	0.41
1:A:2372:C:H2'	1:A:2373:U:C6	2.56	0.41
1:A:2525:C:H2'	1:A:2526:C:H6	1.85	0.41
1:A:2643:U:C2	1:A:2652:A:N7	2.88	0.41
35:A:6775:HOH:O	16:S:13:ARG:HD3	2.19	0.41
2:B:3:C:H2'	2:B:4:U:C6	2.55	0.41
9:L:4:TYR:CD2	16:S:100:VAL:HG11	2.56	0.41
15:R:16:LYS:HE3	15:R:18:ILE:HD11	2.03	0.41
15:R:21:PHE:O	15:R:51:LYS:NZ	2.40	0.41
1:A:17:G:H2'	1:A:18:C:C6	2.56	0.41
1:A:35:G:H1'	1:A:445:A:C4	2.56	0.41
1:A:135:A:H2'	1:A:136:G:C8	2.56	0.41
1:A:151:C:H2'	1:A:152:U:H6	1.86	0.41
1:A:183:C:O2'	1:A:423:A:N3	2.44	0.41
1:A:248:G:O5'	1:A:249:C:H5"	2.21	0.41
1:A:801:U:H2'	11:N:21:ARG:HA	2.03	0.41
1:A:1302:C:O2'	1:A:1379:A:N3	2.52	0.41
1:A:1340:A:H2'	1:A:1341:A:C8	2.56	0.41
1:A:1359:U:O2'	1:A:2199:A:N3	2.53	0.41
1:A:2371:U:OP2	22:Y:55:LYS:HE3	2.20	0.41
1:A:2499:C:H2'	1:A:2500:A:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2499:C:P	4:E:128:ARG:HG2	2.60	0.41
1:A:2805:C:OP2	13:P:42:LYS:HE2	2.20	0.41
2:B:3:C:H2'	2:B:4:U:H6	1.85	0.41
3:D:5:LYS:HB2	3:D:5:LYS:HE2	1.87	0.41
3:D:107:PRO:HG2	3:D:110:VAL:HG21	2.02	0.41
9:L:125:TYR:OH	9:L:132:HIS:NE2	2.34	0.41
10:M:38:ILE:HD11	10:M:111:PHE:HZ	1.86	0.41
31:J:51:TYR:O	31:J:83:ALA:HA	2.21	0.41
1:A:92:A:H2'	1:A:93:A:C8	2.57	0.41
1:A:456:G:OP1	28:6:12:ARG:NH2	2.54	0.41
1:A:570:U:H2'	1:A:571:C:H6	1.85	0.41
1:A:680:U:O2'	1:A:770:G:OP1	2.30	0.41
1:A:2074:U:H2'	1:A:2075:G:H8	1.86	0.41
1:A:2337:C:H2'	1:A:2338:G:O4'	2.21	0.41
1:A:2794:U:H2'	1:A:2795:G:H5'	2.02	0.41
2:B:78:A:H2'	2:B:79:G:O4'	2.21	0.41
14:Q:20:ARG:HH21	14:Q:45:GLY:HA3	1.86	0.41
1:A:18:C:H2'	1:A:19:A:C8	2.56	0.40
1:A:30:G:H2'	1:A:31:C:C6	2.57	0.40
1:A:231:A:H2'	1:A:232:G:O4'	2.21	0.40
1:A:466:C:O2	1:A:470:A:N6	2.39	0.40
1:A:1256:A:H2'	1:A:1257:C:C6	2.55	0.40
1:A:1344:C:H2'	1:A:1345:G:O4'	2.21	0.40
1:A:1413:G:H3'	1:A:1414:A:H2'	2.03	0.40
1:A:1860:G:H2'	1:A:1861:C:C6	2.56	0.40
1:A:2633:C:H2'	1:A:2634:U:O4'	2.21	0.40
1:A:2694:U:O2'	13:P:68:ASP:OD1	2.24	0.40
6:G:60:ILE:O	6:G:102:ARG:NH1	2.52	0.40
21:X:143:LEU:HD12	21:X:144:PRO:HD2	2.03	0.40
26:4:37:HIS:ND1	26:4:38:LEU:O	2.53	0.40
32:K:136:MET:HE2	32:K:136:MET:HB3	1.96	0.40
1:A:40:U:H2'	1:A:41:C:C6	2.56	0.40
1:A:345:U:H2'	1:A:346:C:C6	2.55	0.40
1:A:382:A:H1'	1:A:402:G:O4'	2.20	0.40
1:A:654:G:N2	29:7:64:ARG:O	2.54	0.40
1:A:1049:G:N2	32:K:128:THR:HG23	2.35	0.40
1:A:1071:U:O2'	32:K:119:ALA:HA	2.21	0.40
1:A:1097:G:OP1	31:J:57:ASN:N	2.54	0.40
1:A:1483:A:H2'	1:A:1485:C:C5	2.55	0.40
1:A:1532:C:H2'	1:A:1533:G:O4'	2.21	0.40
1:A:1680:A:H2'	1:A:1681:C:O4'	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2237:G:OP1	12:O:85:LYS:NZ	2.44	0.40
1:A:2430:C:H2'	1:A:2431:G:C8	2.56	0.40
1:A:2718:G:H2'	1:A:2719:G:C8	2.56	0.40
1:A:2732:C:O2	7:H:139:GLN:NE2	2.51	0.40
1:A:2745:A:H1'	7:H:64:MET:SD	2.62	0.40
5:F:17:THR:HA	5:F:105:ARG:HG2	2.03	0.40
5:F:105:ARG:NH2	35:F:315:HOH:O	2.46	0.40
16:S:17:ILE:HD13	16:S:17:ILE:HA	1.96	0.40
1:A:484:G:O2'	18:U:7:LEU:HA	2.21	0.40
1:A:1250:U:C4	1:A:1251:G:C6	3.10	0.40
1:A:2791:C:H2'	1:A:2792:C:H6	1.86	0.40
4:E:121:THR:HG21	4:E:143:PRO:HB3	2.01	0.40
5:F:31:VAL:HG13	5:F:177:VAL:HG22	2.03	0.40
14:Q:31:ARG:NH1	35:Q:203:HOH:O	2.44	0.40
1:A:473:A:H1'	1:A:489:G:N2	2.36	0.40
1:A:676:U:H6	1:A:778:A:N1	2.19	0.40
1:A:699:U:H2'	1:A:700:U:O4'	2.21	0.40
1:A:1303:U:H2'	1:A:1304:G:H8	1.87	0.40
1:A:2066:U:H2'	1:A:2067:G:O4'	2.21	0.40
1:A:2524:U:H2'	1:A:2525:C:C6	2.56	0.40
3:D:7:LYS:HA	3:D:8:PRO:HD3	1.92	0.40
1:A:657:U:H2'	1:A:658:A:O4'	2.21	0.40
1:A:726:C:H2'	1:A:727:C:C6	2.57	0.40
1:A:1053:G:H4'	32:K:136:MET:HG2	2.04	0.40
1:A:1425:U:H2'	1:A:1426:A:C8	2.56	0.40
1:A:1889:C:H4'	3:D:243:ARG:O	2.22	0.40
1:A:2125:G:H2'	1:A:2126:U:C6	2.57	0.40
1:A:2287:A:H2'	1:A:2288:C:C6	2.56	0.40
1:A:2351:C:H2'	1:A:2352:G:O4'	2.21	0.40
1:A:2483:C:OP2	12:O:82:ARG:HD3	2.21	0.40
1:A:2664:G:H2'	1:A:2665:A:C8	2.57	0.40
1:A:2791:C:H2'	1:A:2792:C:C6	2.56	0.40
5:F:3:LEU:HD23	5:F:3:LEU:HA	1.91	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	
3	D	270/273 (99%)	266 (98%)	4 (2%)	0	100	100
4	E	206/211 (98%)	201 (98%)	5 (2%)	0	100	100
5	F	198/200 (99%)	198 (100%)	0	0	100	100
6	G	177/179 (99%)	174 (98%)	3 (2%)	0	100	100
7	H	172/177 (97%)	172 (100%)	0	0	100	100
8	I	107/148 (72%)	103 (96%)	4 (4%)	0	100	100
9	L	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
10	M	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
11	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
12	O	135/137 (98%)	134 (99%)	1 (1%)	0	100	100
13	P	117/129 (91%)	115 (98%)	2 (2%)	0	100	100
14	Q	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
15	R	112/116 (97%)	108 (96%)	4 (4%)	0	100	100
16	S	115/118 (98%)	115 (100%)	0	0	100	100
17	T	101/103 (98%)	101 (100%)	0	0	100	100
18	U	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
19	V	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
20	W	89/104 (86%)	87 (98%)	2 (2%)	0	100	100
21	X	188/204 (92%)	185 (98%)	3 (2%)	0	100	100
22	Y	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
23	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
24	1	59/63 (94%)	59 (100%)	0	0	100	100
25	2	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
26	4	52/60 (87%)	51 (98%)	1 (2%)	0	100	100
27	5	49/51 (96%)	49 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	6	42/44 (96%)	42 (100%)	0	0	100	100
29	7	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
30	8	36/38 (95%)	36 (100%)	0	0	100	100
31	J	109/166 (66%)	105 (96%)	4 (4%)	0	100	100
32	K	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
All	All	3455/3682 (94%)	3400 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	212/213 (100%)	212 (100%)	0	100	100
4	E	160/162 (99%)	160 (100%)	0	100	100
5	F	157/158 (99%)	156 (99%)	1 (1%)	78	84
6	G	153/153 (100%)	151 (99%)	2 (1%)	61	72
7	H	137/141 (97%)	137 (100%)	0	100	100
8	I	85/107 (79%)	84 (99%)	1 (1%)	63	74
9	L	119/119 (100%)	119 (100%)	0	100	100
10	M	102/102 (100%)	102 (100%)	0	100	100
11	N	106/106 (100%)	105 (99%)	1 (1%)	70	79
12	O	110/110 (100%)	110 (100%)	0	100	100
13	P	98/104 (94%)	98 (100%)	0	100	100
14	Q	86/87 (99%)	86 (100%)	0	100	100
15	R	96/98 (98%)	95 (99%)	1 (1%)	68	77
16	S	87/88 (99%)	86 (99%)	1 (1%)	65	75
17	T	86/86 (100%)	86 (100%)	0	100	100
18	U	87/87 (100%)	87 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	V	79/82 (96%)	79 (100%)	0	100	100
20	W	81/88 (92%)	81 (100%)	0	100	100
21	X	154/164 (94%)	154 (100%)	0	100	100
22	Y	57/61 (93%)	57 (100%)	0	100	100
23	Z	66/67 (98%)	66 (100%)	0	100	100
24	1	54/55 (98%)	53 (98%)	1 (2%)	50	61
25	2	48/49 (98%)	48 (100%)	0	100	100
26	4	47/52 (90%)	46 (98%)	1 (2%)	47	58
27	5	47/47 (100%)	47 (100%)	0	100	100
28	6	37/37 (100%)	37 (100%)	0	100	100
29	7	54/55 (98%)	54 (100%)	0	100	100
30	8	34/34 (100%)	34 (100%)	0	100	100
31	J	82/122 (67%)	81 (99%)	1 (1%)	63	74
32	K	110/110 (100%)	110 (100%)	0	100	100
All	All	2831/2944 (96%)	2821 (100%)	10 (0%)	81	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	94	LYS
6	G	95	ARG
6	G	178	ARG
8	I	75	LEU
11	N	92	LEU
15	R	40	ARG
16	S	6	ARG
24	1	7	ARG
26	4	51	ARG
31	J	60	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	22	GLN
3	D	90	HIS
3	D	226	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	65	GLN
4	E	126	ASN
4	E	148	GLN
4	E	150	GLN
4	E	185	ASN
5	F	2	GLN
5	F	28	HIS
7	H	22	GLN
7	H	73	ASN
7	H	97	GLN
7	H	111	HIS
10	M	91	GLN
11	N	17	HIS
11	N	99	ASN
11	N	102	ASN
11	N	104	HIS
11	N	106	GLN
13	P	9	HIS
15	R	53	ASN
16	S	44	GLN
16	S	72	ASN
17	T	43	ASN
17	T	69	HIS
18	U	23	GLN
18	U	61	ASN
19	V	61	ASN
19	V	87	GLN
19	V	90	GLN
21	X	161	HIS
21	X	175	GLN
22	Y	29	GLN
23	Z	23	ASN
23	Z	34	GLN
26	4	5	GLN
28	6	26	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2827/2892 (97%)	311 (11%)	6 (0%)
2	B	118/121 (97%)	17 (14%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2945/3013 (97%)	328 (11%)	6 (0%)

All (328) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	34	U
1	A	45	G
1	A	51	G
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	85	G
1	A	97	A
1	A	118	A
1	A	120	U
1	A	131	A
1	A	142	C
1	A	163	C
1	A	165	A
1	A	166	U
1	A	181	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	216	A
1	A	220	G
1	A	221	A
1	A	222	A
1	A	242	G
1	A	248	G
1	A	265	A
1	A	270	U
1	A	271	U
1	A	293	A
1	A	294	A
1	A	305	A
1	A	315	U
1	A	323	G
1	A	324	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	337	C
1	A	350	G
1	A	356	A
1	A	359	U
1	A	360	C
1	A	376	C
1	A	377	G
1	A	387	G
1	A	402	G
1	A	407	U
1	A	426	A
1	A	434	A
1	A	445	A
1	A	447	C
1	A	472	G
1	A	481	A
1	A	482	G
1	A	485	G
1	A	495	U
1	A	496	A
1	A	499	A
1	A	520	A
1	A	522	C
1	A	523	A
1	A	536	U
1	A	537	U
1	A	538	G
1	A	553	A
1	A	563	U
1	A	565	A
1	A	593	A
1	A	603	U
1	A	604	A
1	A	622	A
1	A	627	A
1	A	635	U
1	A	636	A
1	A	676	U
1	A	700	U
1	A	716	G
1	A	720	A
1	A	737	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	754	A
1	A	765	G
1	A	766	G
1	A	772	A
1	A	774	G
1	A	775	G
1	A	779	A
1	A	795	G
1	A	802	C
1	A	817	U
1	A	818	U
1	A	836	U
1	A	848	G
1	A	855	A
1	A	860	U
1	A	899	A
1	A	904	C
1	A	920	C
1	A	921	C
1	A	922	G
1	A	936	C
1	A	951	C
1	A	964	A
1	A	970	A
1	A	973	A
1	A	979	G
1	A	986	A
1	A	999	A
1	A	1002	U
1	A	1003	U
1	A	1016	U
1	A	1023	U
1	A	1037	G
1	A	1046	G
1	A	1047	A
1	A	1048	G
1	A	1060	A
1	A	1061	G
1	A	1069	C
1	A	1074	A
1	A	1077	G
1	A	1078	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1099	C
1	A	1100	G
1	A	1101	A
1	A	1102	G
1	A	1120	U
1	A	1122	U
1	A	1123	A
1	A	1125	C
1	A	1126	G
1	A	1133	A
1	A	1162	G
1	A	1193	G
1	A	1223	G
1	A	1240	A
1	A	1243	G
1	A	1258	G
1	A	1259	A
1	A	1281	A
1	A	1287	A
1	A	1288	A
1	A	1301	C
1	A	1302	C
1	A	1308	A
1	A	1316	U
1	A	1339	U
1	A	1352	A
1	A	1365	A
1	A	1366	U
1	A	1381	U
1	A	1403	G
1	A	1404	C
1	A	1414	A
1	A	1415	C
1	A	1439	G
1	A	1447	U
1	A	1469	G
1	A	1480	U
1	A	1484	U
1	A	1495	A
1	A	1496	A
1	A	1556	A
1	A	1559	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1568	U
1	A	1572	C
1	A	1573	U
1	A	1597	C
1	A	1598	A
1	A	1624	A
1	A	1637	U
1	A	1638	U
1	A	1664	G
1	A	1717	U
1	A	1732	G
1	A	1736	G
1	A	1743	G
1	A	1751	G
1	A	1760	A
1	A	1771	A
1	A	1773	A
1	A	1787	C
1	A	1788	A
1	A	1795	A
1	A	1803	C
1	A	1816	A
1	A	1822	2MG
1	A	1835	A
1	A	1845	A
1	A	1893	G
1	A	1916	G
1	A	1917	G
1	A	1918	U
1	A	1923	A
1	A	1925	A
1	A	1942	U
1	A	1950	U
1	A	1951	G
1	A	1952	C
1	A	1954	C
1	A	1957	A
1	A	1958	U
1	A	1959	G
1	A	1978	U
1	A	1980	U
1	A	2008	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2010	C
1	A	2017	6MZ
1	A	2018	A
1	A	2020	A
1	A	2030	U
1	A	2042	C
1	A	2043	G
1	A	2047	A
1	A	2048	G
1	A	2049	A
1	A	2056	7MG
1	A	2080	G
1	A	2086	U
1	A	2098	U
1	A	2105	U
1	A	2106	A
1	A	2113	A
1	A	2114	G
1	A	2120	G
1	A	2144	G
1	A	2149	A
1	A	2159	U
1	A	2160	A
1	A	2185	A
1	A	2191	G
1	A	2198	A
1	A	2201	C
1	A	2212	A
1	A	2225	G
1	A	2226	G
1	A	2266	G
1	A	2270	U
1	A	2274	A
1	A	2275	A
1	A	2292	U
1	A	2295	G
1	A	2298	A
1	A	2306	C
1	A	2308	G
1	A	2309	A
1	A	2312	A
1	A	2323	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2332	G
1	A	2337	C
1	A	2341	A
1	A	2348	C
1	A	2359	U
1	A	2370	G
1	A	2372	C
1	A	2379	A
1	A	2393	U
1	A	2412	A
1	A	2416	G
1	A	2422	A
1	A	2428	U
1	A	2432	2MG
1	A	2435	A
1	A	2460	U
1	A	2462	C
1	A	2481	G
1	A	2489	G
1	A	2492	G
1	A	2493	U
1	A	2505	A
1	A	2516	G
1	A	2522	G
1	A	2534	A
1	A	2553	A
1	A	2554	G
1	A	2559	A
1	A	2569	G
1	A	2589	A
1	A	2596	U
1	A	2600	U
1	A	2602	U
1	A	2616	U
1	A	2617	U
1	A	2633	C
1	A	2672	G
1	A	2676	U
1	A	2677	U
1	A	2701	G
1	A	2703	C
1	A	2713	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2720	A
1	A	2726	U
1	A	2731	G
1	A	2735	A
1	A	2744	A
1	A	2752	A
1	A	2765	A
1	A	2767	G
1	A	2786	G
1	A	2787	A
1	A	2795	G
1	A	2805	C
1	A	2807	A
1	A	2808	A
1	A	2822	A
1	A	2823	U
1	A	2859	A
1	A	2860	A
1	A	2867	C
1	A	2871	U
1	A	2872	U
1	A	2873	G
2	B	6	G
2	B	9	G
2	B	13	A
2	B	19	C
2	B	24	G
2	B	35	U
2	B	41	C
2	B	53	A
2	B	56	G
2	B	58	A
2	B	73	A
2	B	89	U
2	B	90	C
2	B	105	G
2	B	109	A
2	B	116	A
2	B	117	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	221	A
1	A	635	U
1	A	774	G
1	A	1046	G
1	A	1307	C
1	A	2743	U

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	6MZ	A	1608	1	22,25,26	2.39	4 (18%)	29,36,39	2.33	9 (31%)
1	2MG	A	1822	1	23,26,27	0.43	0	33,38,41	0.47	0
1	6MZ	A	2017	1	22,25,26	2.34	5 (22%)	29,36,39	2.50	11 (37%)
1	OMG	A	2238	1	23,26,27	0.44	0	32,38,41	0.45	0
1	OMU	A	2539	1	19,22,23	3.10	8 (42%)	25,31,34	1.82	4 (16%)
1	2MA	A	2490	1,33	22,25,26	1.70	5 (22%)	32,37,40	3.65	12 (37%)
1	5MU	A	1926	1	19,22,23	0.42	0	27,32,35	0.58	0
1	OMC	A	2485	1,33	19,22,23	0.48	0	25,31,34	0.64	0
1	1MG	A	735	1	23,26,27	3.16	8 (34%)	33,39,42	1.84	9 (27%)
1	5MC	A	1949	1	19,22,23	0.54	0	26,32,35	0.63	0
1	2MG	A	2432	1	23,26,27	0.49	0	33,38,41	0.49	0
1	7MG	A	2056	1	23,26,27	1.13	1 (4%)	27,39,42	0.86	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	A	1608	1	-	0/9/27/28	0/3/3/3
1	2MG	A	1822	1	-	2/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	A	2017	1	-	2/9/27/28	0/3/3/3
1	OMG	A	2238	1	-	1/9/27/28	0/3/3/3
1	OMU	A	2539	1	-	0/9/27/28	0/2/2/2
1	2MA	A	2490	1,33	-	1/7/25/26	0/3/3/3
1	5MU	A	1926	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2485	1,33	-	0/9/27/28	0/2/2/2
1	1MG	A	735	1	-	0/7/25/26	0/3/3/3
1	5MC	A	1949	1	-	0/7/25/26	0/2/2/2
1	2MG	A	2432	1	-	2/9/27/28	0/3/3/3
1	7MG	A	2056	1	-	1/7/37/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1608	6MZ	C6-N6	9.73	1.45	1.34
1	A	735	1MG	C2-N3	9.65	1.48	1.33
1	A	2017	6MZ	C6-N6	9.35	1.44	1.34
1	A	2539	OMU	C2-N1	8.09	1.51	1.38
1	A	735	1MG	C4-N3	6.95	1.50	1.34
1	A	2539	OMU	C2-N3	6.68	1.49	1.38
1	A	735	1MG	C2-N2	6.24	1.45	1.34
1	A	2539	OMU	C6-C5	5.54	1.47	1.35
1	A	2490	2MA	C6-N6	5.20	1.47	1.34
1	A	2056	7MG	C5-N7	4.77	1.41	1.35
1	A	2539	OMU	C4-N3	3.48	1.44	1.38
1	A	2490	2MA	C6-N1	-3.27	1.30	1.35
1	A	735	1MG	C5-C6	3.21	1.53	1.45
1	A	735	1MG	C2-N1	3.17	1.43	1.37
1	A	2539	OMU	C5-C4	3.15	1.50	1.43
1	A	2017	6MZ	C5-C4	-3.02	1.33	1.39
1	A	1608	6MZ	C5-C4	-2.88	1.33	1.39
1	A	735	1MG	C6-N1	2.84	1.46	1.40
1	A	2539	OMU	O4-C4	-2.82	1.19	1.24
1	A	2490	2MA	C5-N7	-2.65	1.34	1.39
1	A	735	1MG	O6-C6	-2.60	1.17	1.23
1	A	1608	6MZ	C5-N7	-2.57	1.34	1.39
1	A	2539	OMU	O2-C2	-2.47	1.18	1.23
1	A	2017	6MZ	C5-N7	-2.45	1.34	1.39
1	A	2539	OMU	C6-N1	2.17	1.43	1.38
1	A	735	1MG	C5-N7	-2.16	1.34	1.39
1	A	1608	6MZ	C8-N9	-2.13	1.33	1.37
1	A	2490	2MA	C5-C4	-2.09	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2017	6MZ	C4-N9	-2.08	1.33	1.37
1	A	2490	2MA	C8-N9	-2.08	1.34	1.37
1	A	2017	6MZ	C8-N9	-2.04	1.34	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2490	2MA	N6-C6-N1	-9.23	104.58	117.03
1	A	2490	2MA	CM2-C2-N3	9.13	130.79	117.13
1	A	2490	2MA	C5-C4-N3	-8.59	118.13	127.18
1	A	2017	6MZ	C9-N6-C6	-6.95	116.40	122.85
1	A	2490	2MA	N3-C4-N9	6.36	135.06	126.99
1	A	2490	2MA	CM2-C2-N1	-6.16	107.91	117.13
1	A	2539	OMU	C4-N3-C2	-5.78	119.44	126.61
1	A	2017	6MZ	N1-C2-N3	-5.71	119.93	128.58
1	A	1608	6MZ	N1-C2-N3	-5.51	120.23	128.58
1	A	1608	6MZ	C5-C4-N3	-5.00	119.83	126.72
1	A	735	1MG	C5-C4-N3	-4.70	120.91	128.39
1	A	2490	2MA	C5-C6-N6	4.68	134.88	123.29
1	A	2490	2MA	C4-N9-C1'	-4.68	115.69	126.63
1	A	2490	2MA	C1'-N9-C8	4.56	137.21	127.09
1	A	2017	6MZ	N9-C8-N7	-4.40	107.69	113.94
1	A	1608	6MZ	C9-N6-C6	-4.24	118.92	122.85
1	A	2017	6MZ	C5-C4-N3	-4.21	120.92	126.72
1	A	1608	6MZ	N9-C8-N7	-4.08	108.14	113.94
1	A	735	1MG	C1'-N9-C4	-3.96	114.77	126.49
1	A	2539	OMU	C5-C4-N3	3.94	120.33	114.80
1	A	1608	6MZ	C4-C5-C6	3.74	119.89	116.78
1	A	2539	OMU	N3-C2-N1	3.63	119.61	114.89
1	A	735	1MG	C1'-N9-C8	3.41	136.43	126.73
1	A	735	1MG	C2-N3-C4	3.37	119.55	111.98
1	A	1608	6MZ	C2-N3-C4	3.37	120.05	111.83
1	A	1608	6MZ	N3-C4-N9	3.35	132.87	127.17
1	A	2017	6MZ	C2-N3-C4	3.20	119.64	111.83
1	A	735	1MG	N9-C8-N7	-3.15	107.56	113.40
1	A	2539	OMU	O4-C4-C5	-3.04	119.91	125.16
1	A	2490	2MA	N9-C8-N7	-3.01	109.67	113.94
1	A	2017	6MZ	C4-N9-C8	2.95	108.83	105.74
1	A	735	1MG	N9-C4-N3	2.86	131.66	125.95
1	A	2490	2MA	C6-C5-C4	2.77	120.96	117.18
1	A	1608	6MZ	C5-N7-C8	2.68	107.66	103.45
1	A	2017	6MZ	N3-C4-N9	2.64	131.66	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2017	6MZ	C4-N9-C1'	-2.62	120.50	126.63
1	A	735	1MG	C5-C6-N1	2.61	119.83	115.02
1	A	2017	6MZ	C4-C5-C6	2.60	118.94	116.78
1	A	2017	6MZ	C5-N7-C8	2.55	107.45	103.45
1	A	2490	2MA	N3-C2-N1	-2.53	121.30	125.77
1	A	2056	7MG	C4-C5-N7	2.52	108.35	105.38
1	A	1608	6MZ	C4-N9-C8	2.47	108.33	105.74
1	A	2490	2MA	C5-N7-C8	2.46	107.32	103.45
1	A	2017	6MZ	C5-C6-N1	2.20	120.51	118.15
1	A	735	1MG	O6-C6-C5	-2.09	119.21	124.59
1	A	735	1MG	C8-N7-C5	2.01	107.84	104.26

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2238	OMG	C1'-C2'-O2'-CM2
1	A	1822	2MG	C3'-C4'-C5'-O5'
1	A	2432	2MG	C3'-C4'-C5'-O5'
1	A	1822	2MG	O4'-C4'-C5'-O5'
1	A	2017	6MZ	O4'-C4'-C5'-O5'
1	A	2432	2MG	O4'-C4'-C5'-O5'
1	A	2017	6MZ	C3'-C4'-C5'-O5'
1	A	2490	2MA	C4'-C5'-O5'-P
1	A	2056	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1822	2MG	1	0
1	A	2017	6MZ	2	0
1	A	2238	OMG	1	0
1	A	2432	2MG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 203 ligands modelled in this entry, 203 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

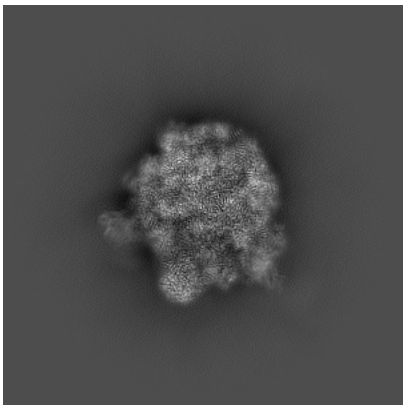
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-73301. These allow visual inspection of the internal detail of the map and identification of artifacts.

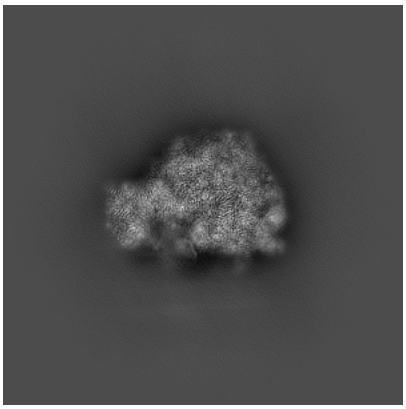
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

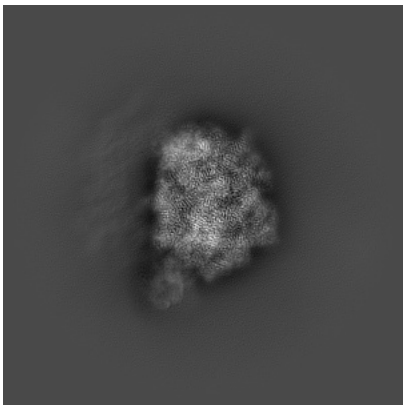
6.1.1 Primary map



X

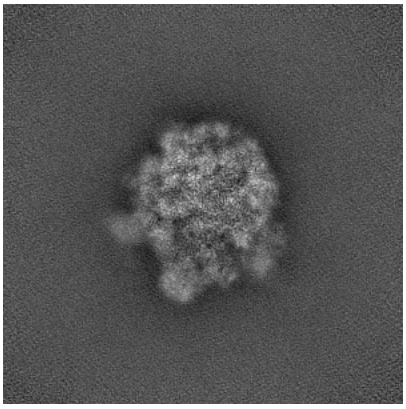


Y

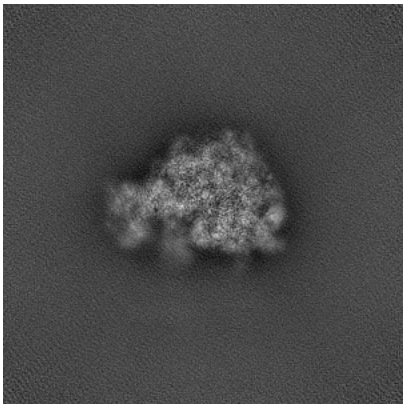


Z

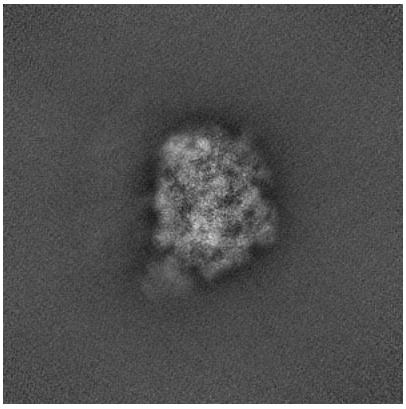
6.1.2 Raw map



X



Y

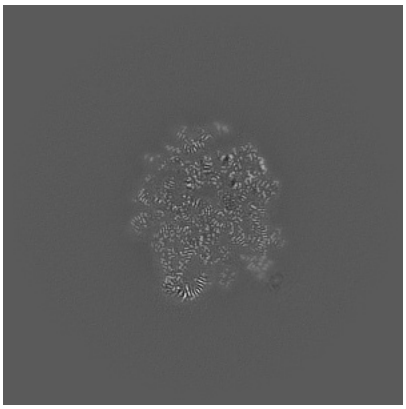


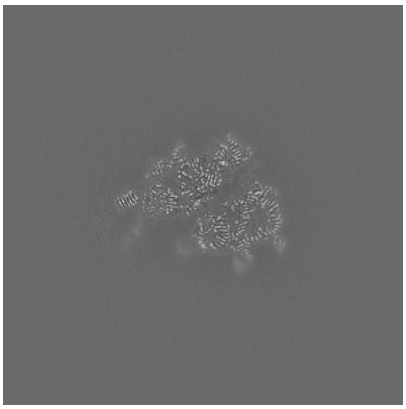
Z

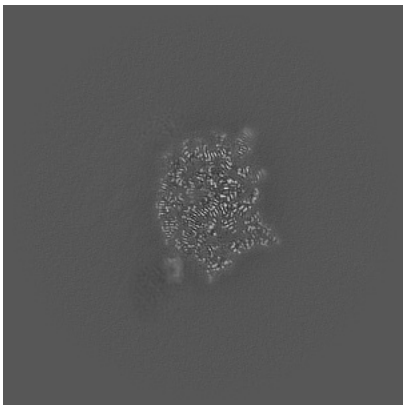
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

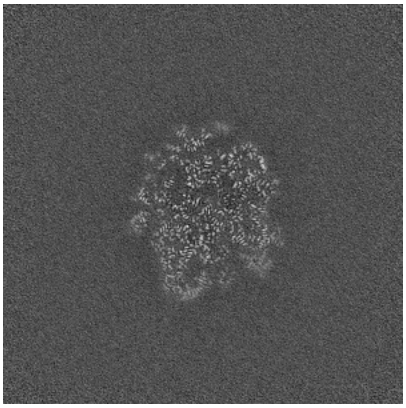
6.2.1 Primary map

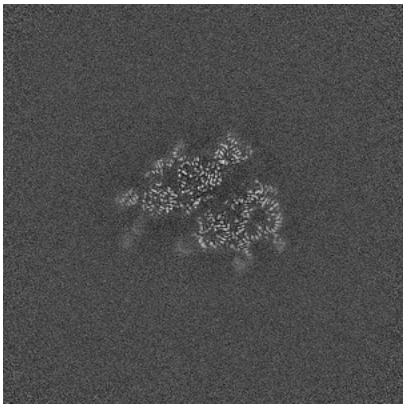

X Index: 348

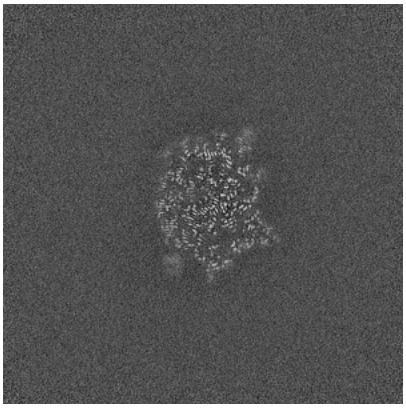

Y Index: 348


Z Index: 348

6.2.2 Raw map


X Index: 348

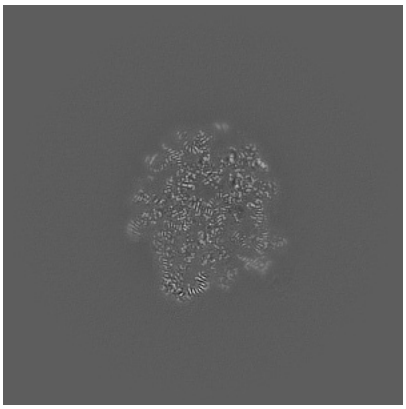

Y Index: 348


Z Index: 348

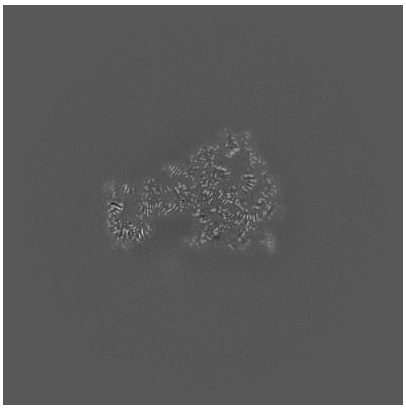
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

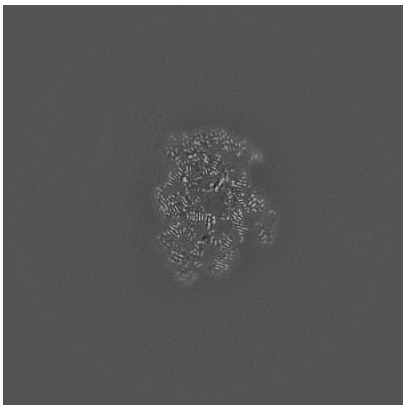
6.3.1 Primary map



X Index: 353

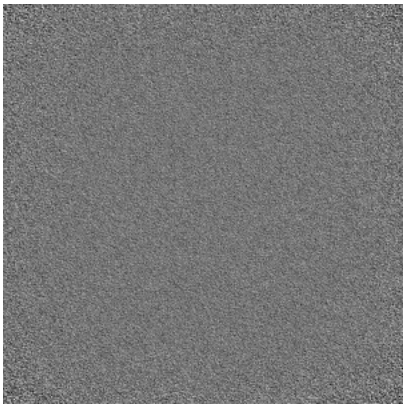


Y Index: 319

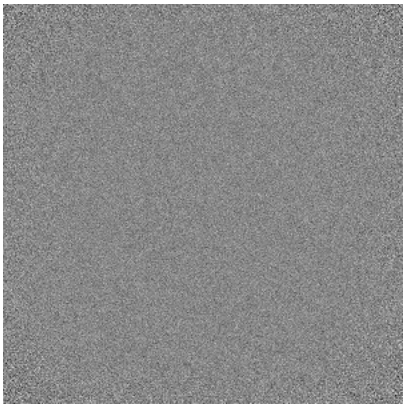


Z Index: 380

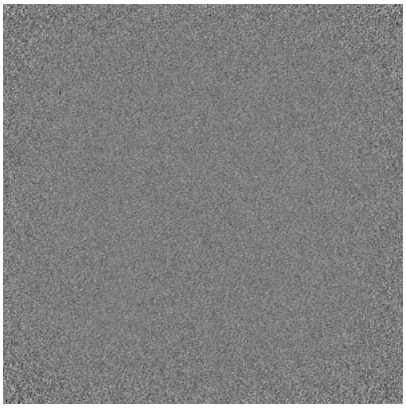
6.3.2 Raw map



X Index: 0



Y Index: 0

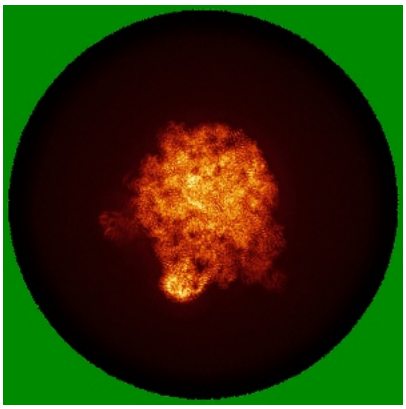


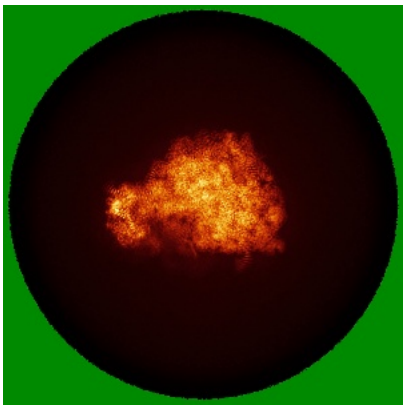
Z Index: 0

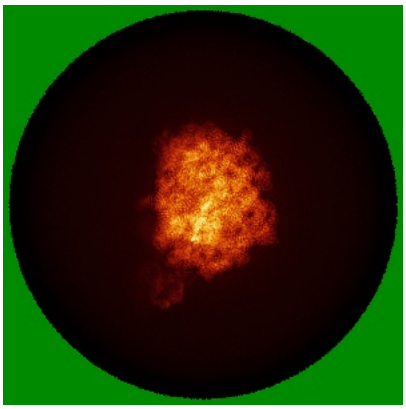
The images above show the largest variance slices of the map in three orthogonal directions.

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

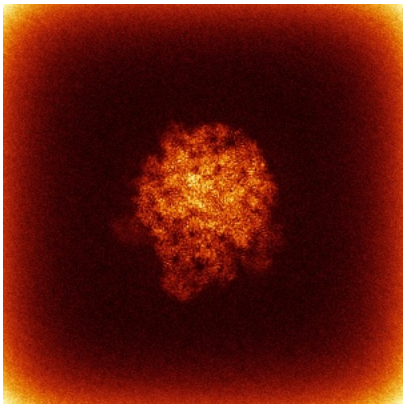
6.4.1 Primary map

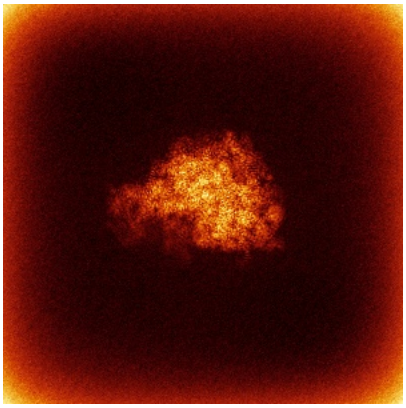

X

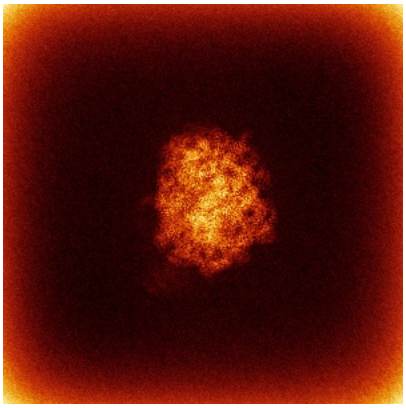

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

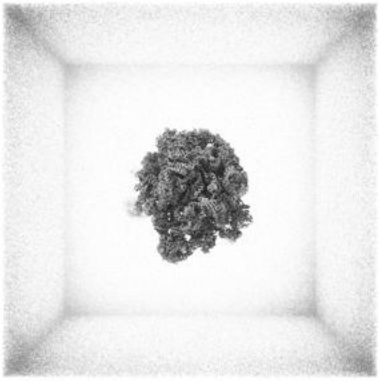
X

Y

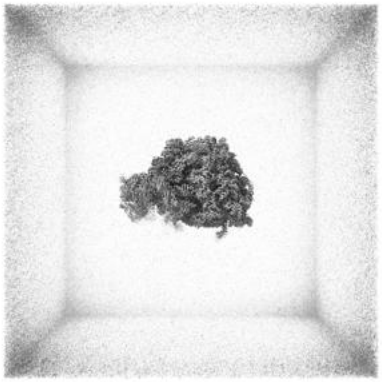
Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

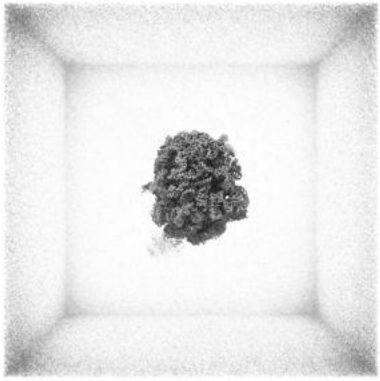
6.5.2 Raw map



X



Y



Z

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

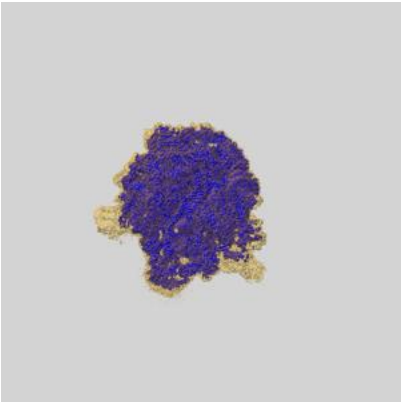
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

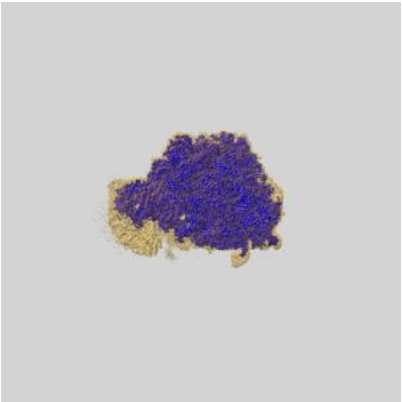
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

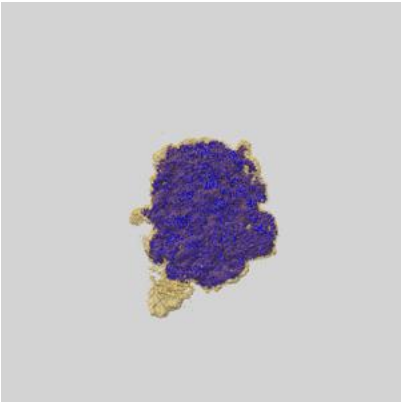
6.6.1 emd_73301_msk_1.map (i)



X



Y

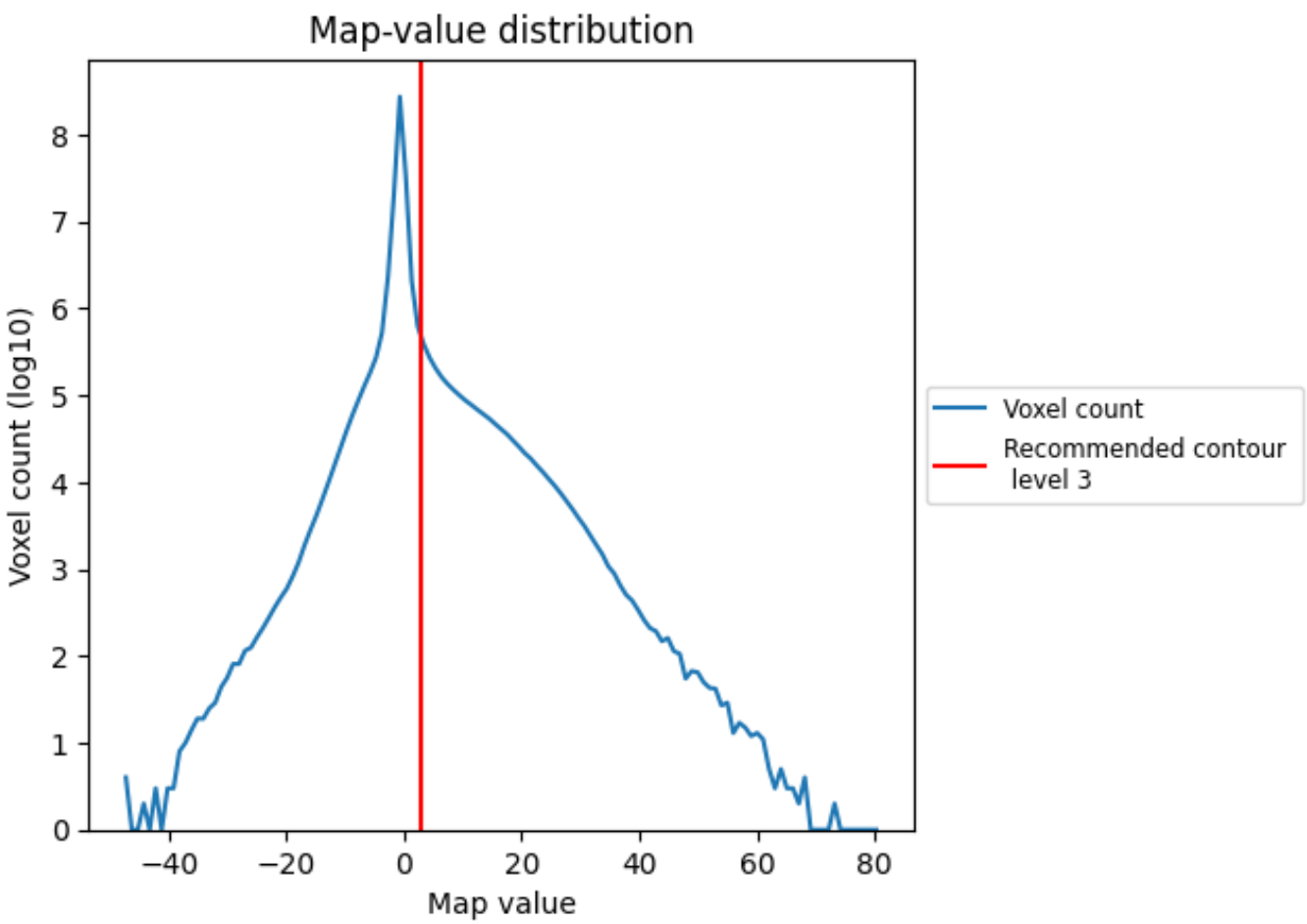


Z

7 Map analysis (i)

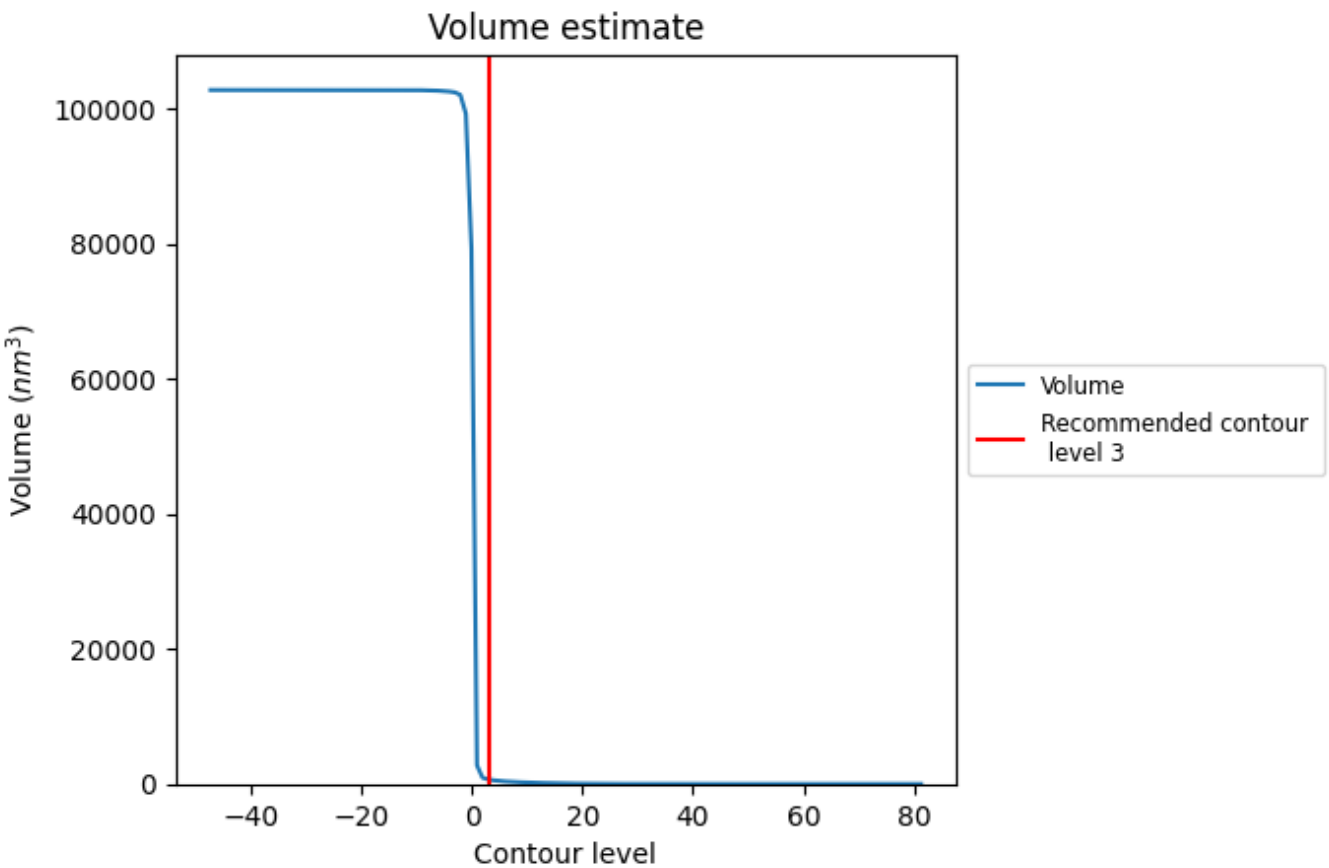
This section contains the results of statistical analysis of the map.

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.

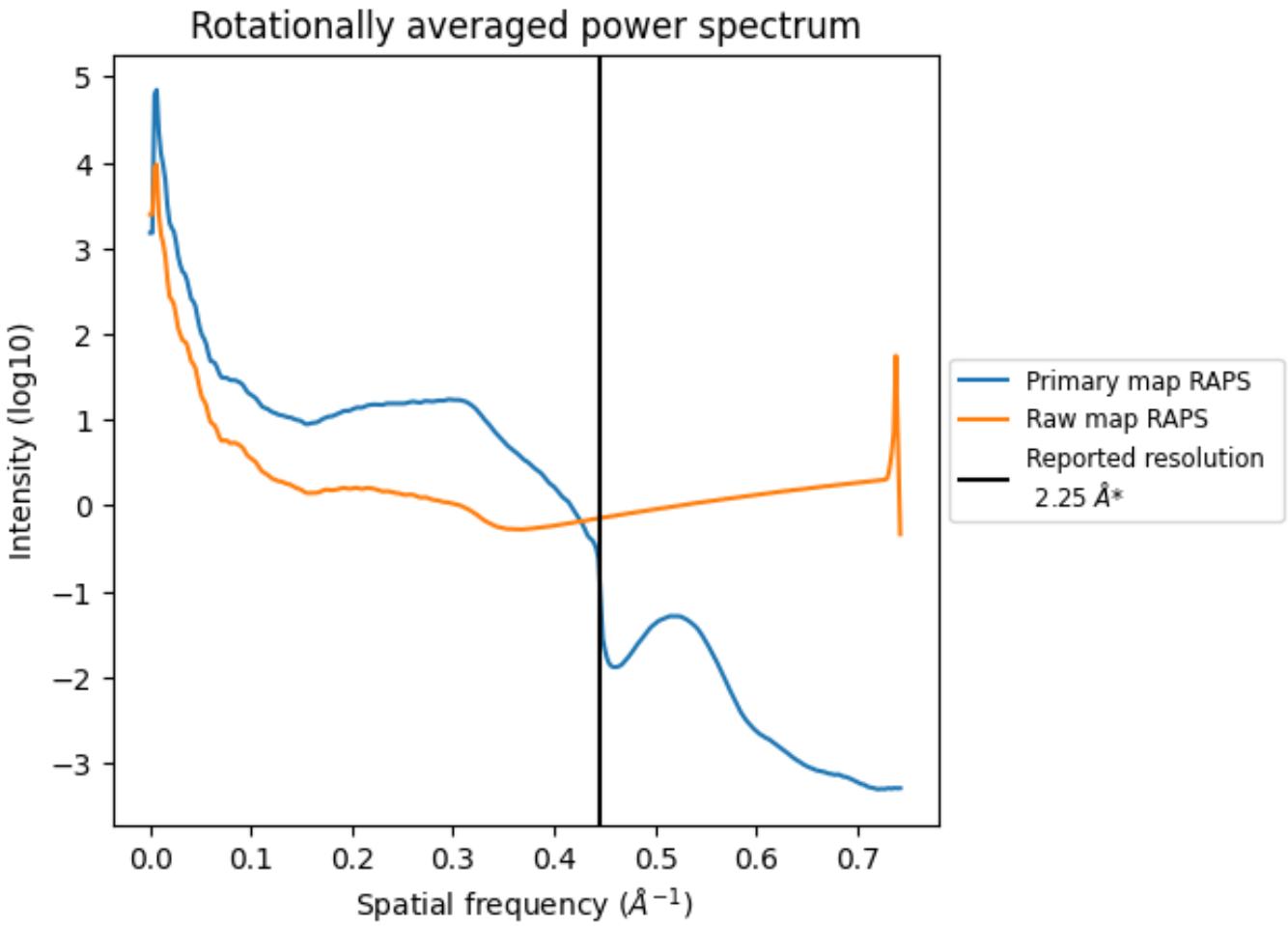
7.2 Volume estimate (i)



The volume at the recommended contour level is 675 nm^3; this corresponds to an approximate mass of 610 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)

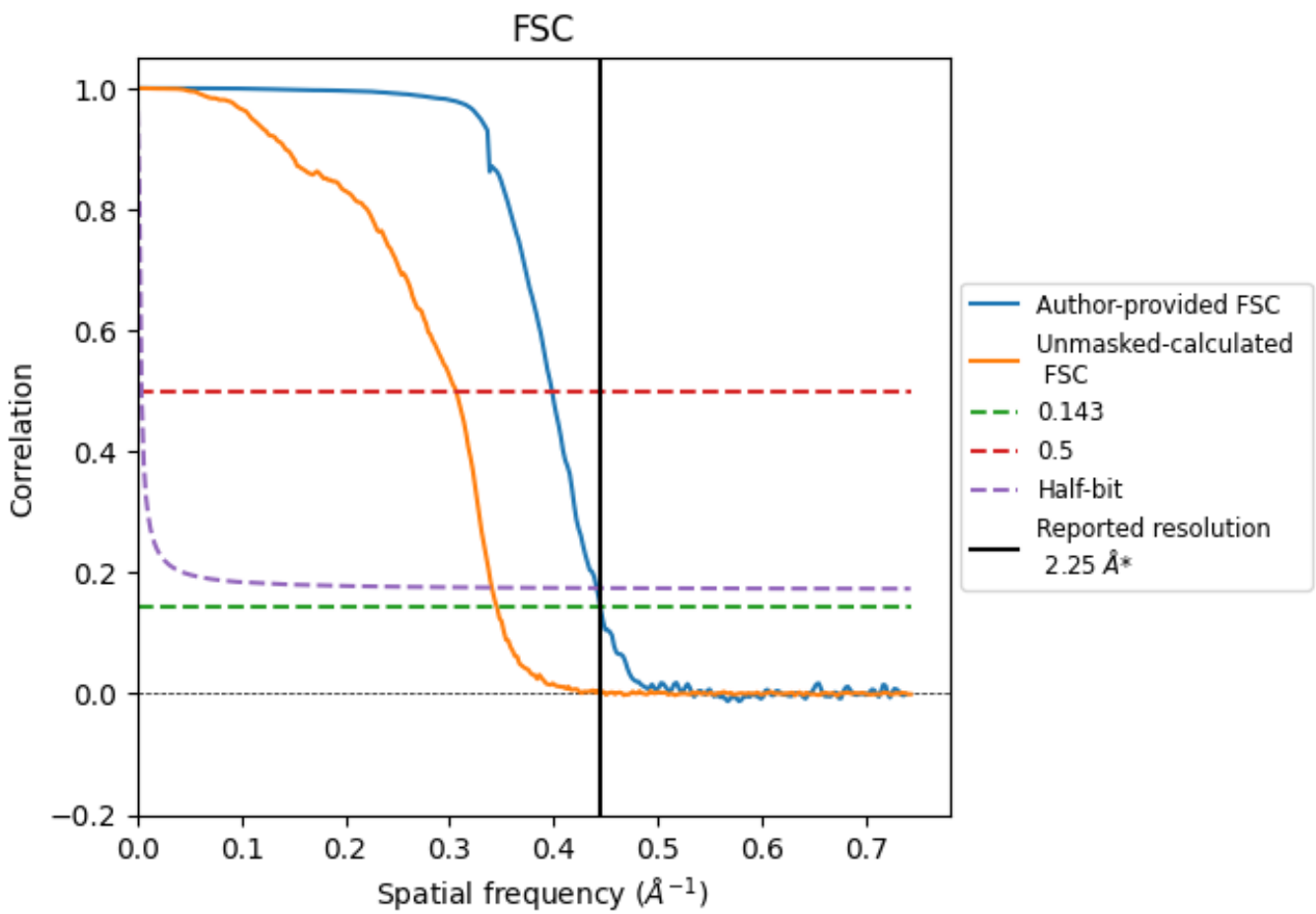


*Reported resolution corresponds to spatial frequency of 0.444 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.444 Å^{-1}

8.2 Resolution estimates (i)

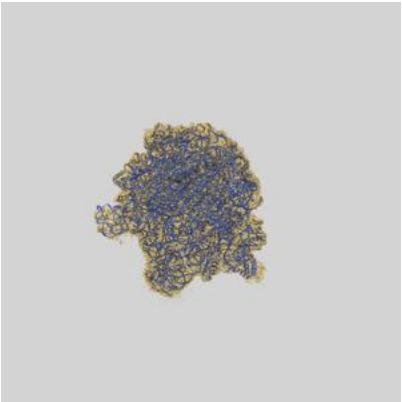
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.51	2.27
Unmasked-calculated*	2.89	3.27	2.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.89 differs from the reported value 2.25 by more than 10 %

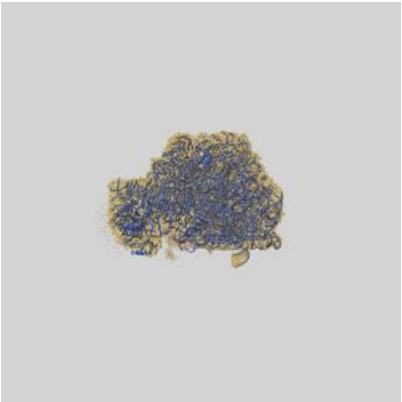
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-73301 and PDB model 9YPN. Per-residue inclusion information can be found in section 3 on page 12.

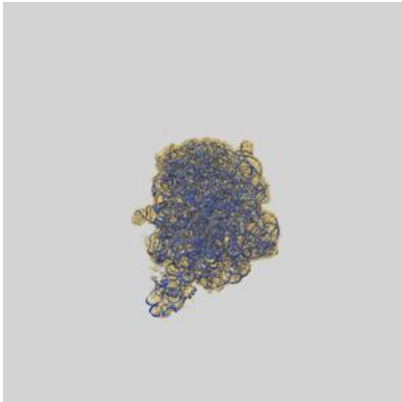
9.1 Map-model overlay (i)



X



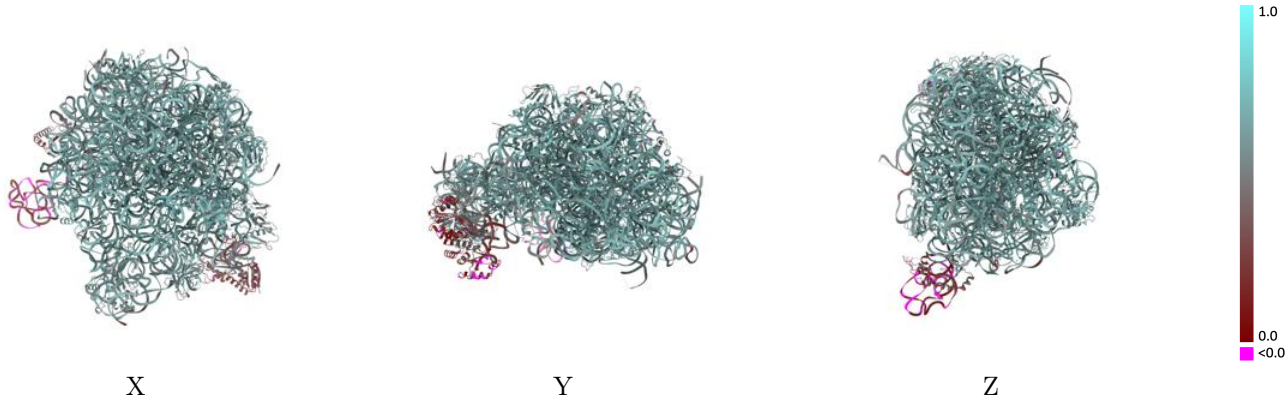
Y



Z

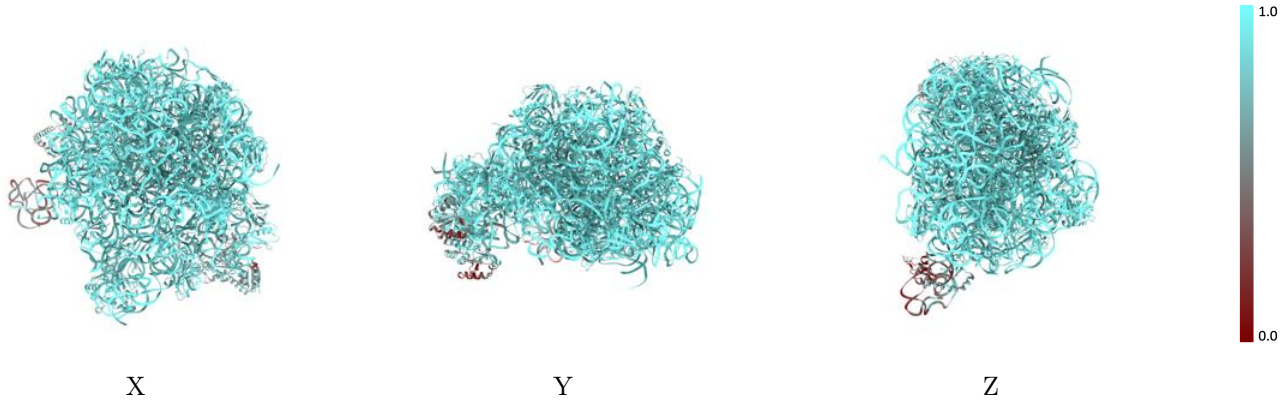
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



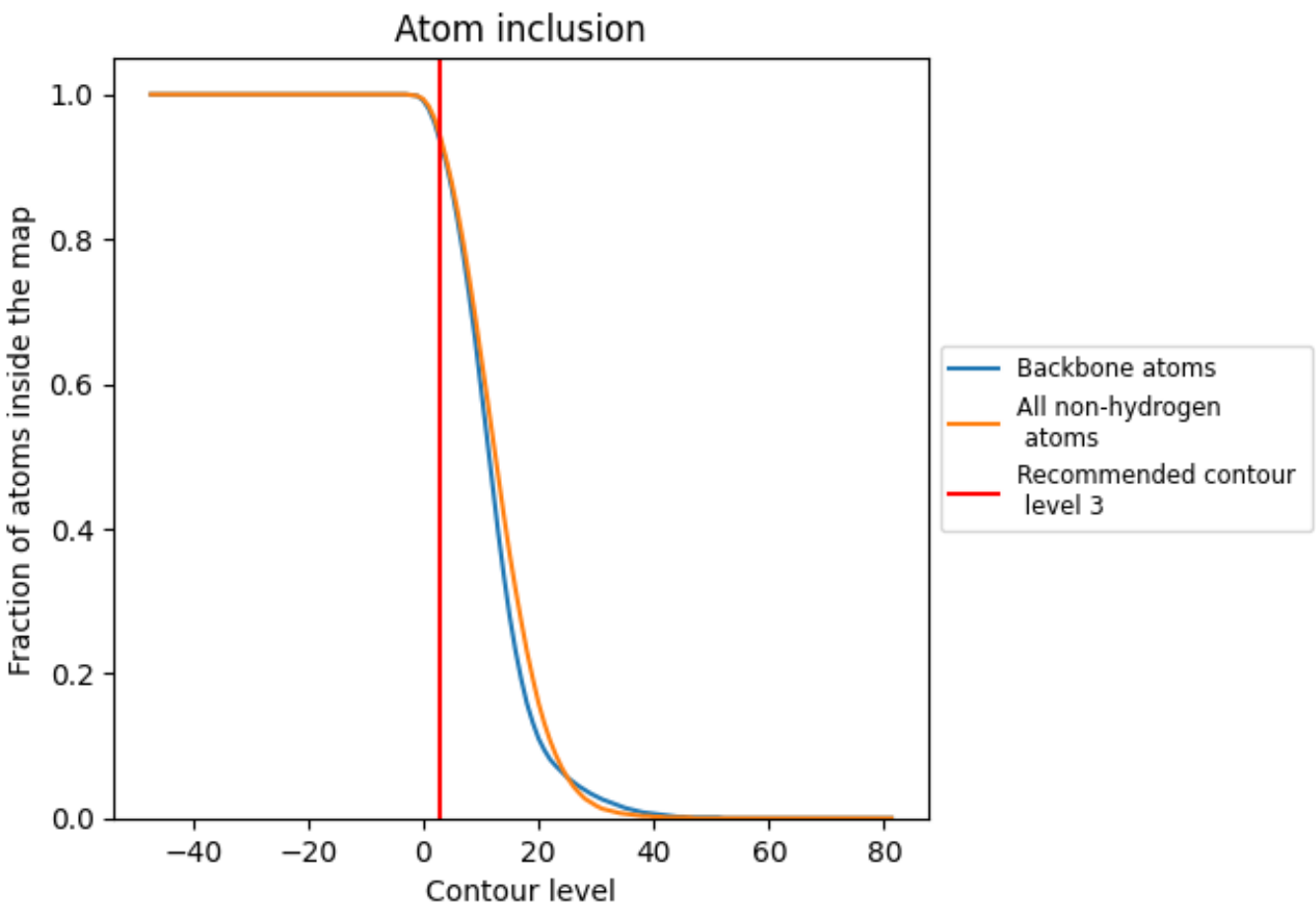
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9400	0.6110
1	0.9170	0.6020
2	0.9530	0.6460
4	0.9330	0.6200
5	0.8460	0.5770
6	0.9450	0.6690
7	0.9610	0.6660
8	0.9490	0.6450
A	0.9610	0.6230
B	0.9780	0.6050
D	0.9570	0.6600
E	0.9500	0.6510
F	0.9480	0.6400
G	0.8930	0.5280
H	0.8940	0.5500
I	0.5420	0.3930
J	0.5490	0.2230
K	0.5550	0.1940
L	0.9450	0.6470
M	0.9080	0.6150
N	0.9470	0.6500
O	0.9250	0.6430
P	0.9670	0.6580
Q	0.9400	0.6040
R	0.8900	0.6030
S	0.9660	0.6630
T	0.9320	0.6240
U	0.9150	0.6390
V	0.9090	0.6040
W	0.9090	0.5780
X	0.8860	0.5720
Y	0.9290	0.6490
Z	0.9350	0.6430