



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 02:59 PM JST

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

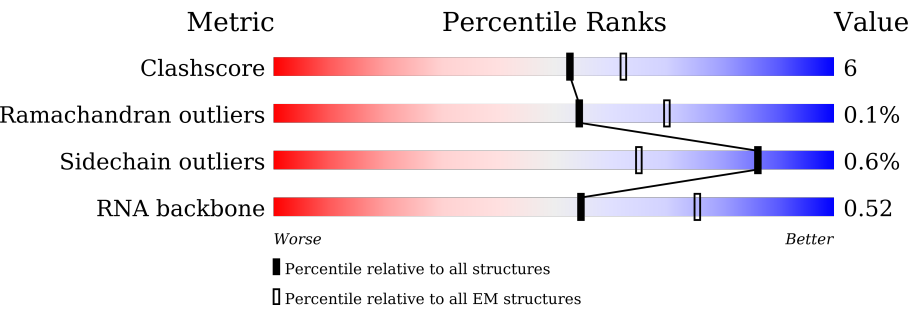
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	56	
2	2	65	
3	3	61	
4	4	73	
5	5	37	
6	6	142	
7	7	116	

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Mol	Chain	Length	Quality of chain
8	B	121	
9	C	271	
10	D	221	
11	E	243	
12	F	220	
13	G	182	
14	H	155	
15	K	197	
16	L	121	
17	M	192	
18	N	135	
19	O	116	
20	P	123	
21	Q	156	
22	R	127	
23	S	201	
24	T	199	
25	U	122	
26	V	145	
27	W	106	
28	X	137	
29	Y	77	
30	Z	109	
31	A	2810	
32	0	94	

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called protein cL37.

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

- Molecule 7 is a protein called protein cL38.

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

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

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

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

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

- Molecule 10 is a protein called protein L3.

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

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

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

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

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

- Molecule 13 is a protein called protein L6.

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

- Molecule 14 is a protein called protein L9.

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

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

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

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

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

- Molecule 17 is a protein called protein L15.

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

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

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

- Molecule 19 is a protein called protein L17.

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

- Molecule 20 is a protein called protein L18.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 28 is a protein called protein L27.

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

- Molecule 29 is a protein called protein L28.

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

- Molecule 30 is a protein called protein L29.

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

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

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

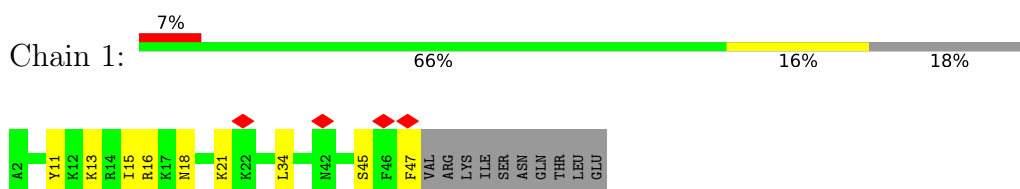
- Molecule 32 is a protein called 50S ribosomal protein L31.

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

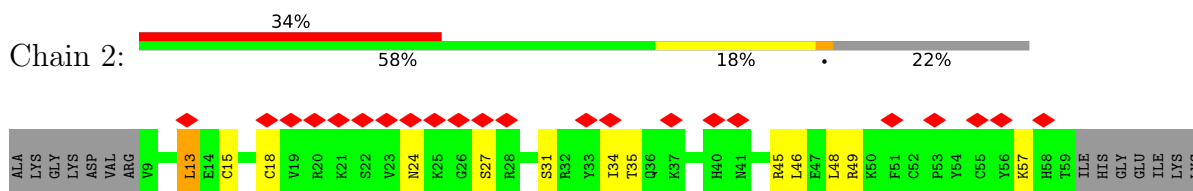
3 Residue-property plots [i](#)

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

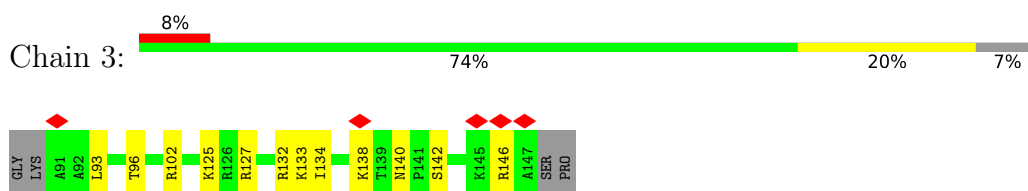
- Molecule 1: 50S ribosomal protein L32, chloroplastic



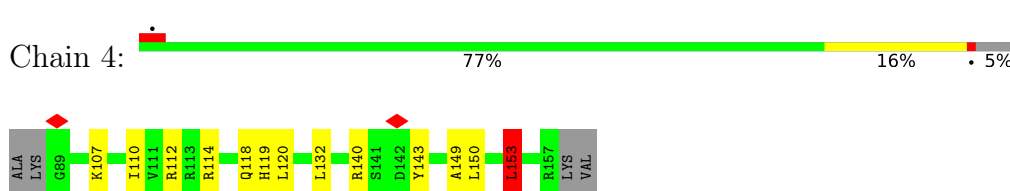
- Molecule 2: 50S ribosomal protein L33, chloroplastic



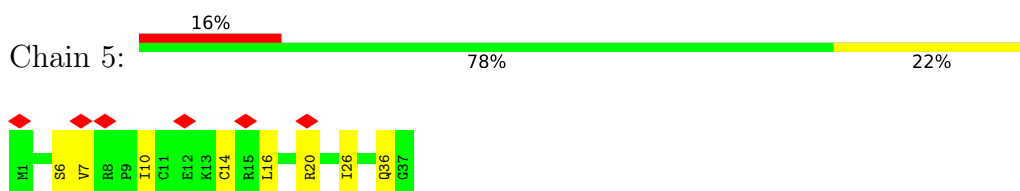
- Molecule 3: 50S ribosomal protein L34, chloroplastic



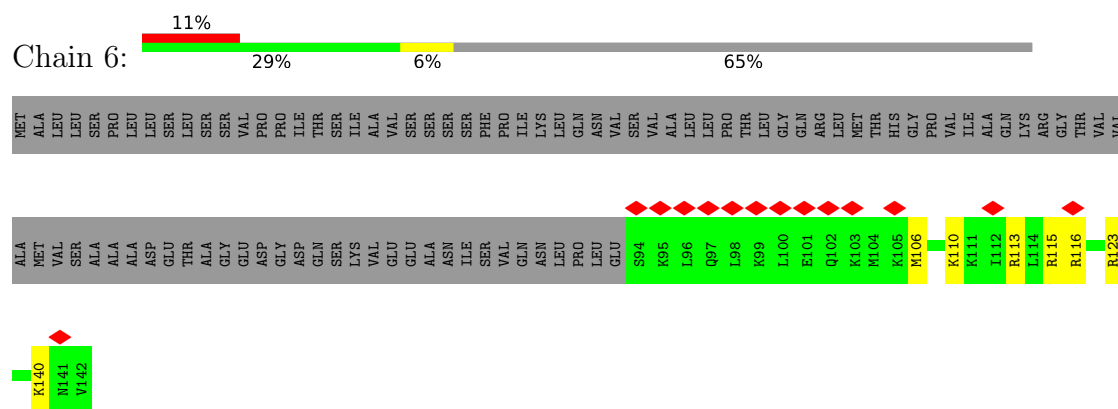
- Molecule 4: 50S ribosomal protein L35, chloroplastic



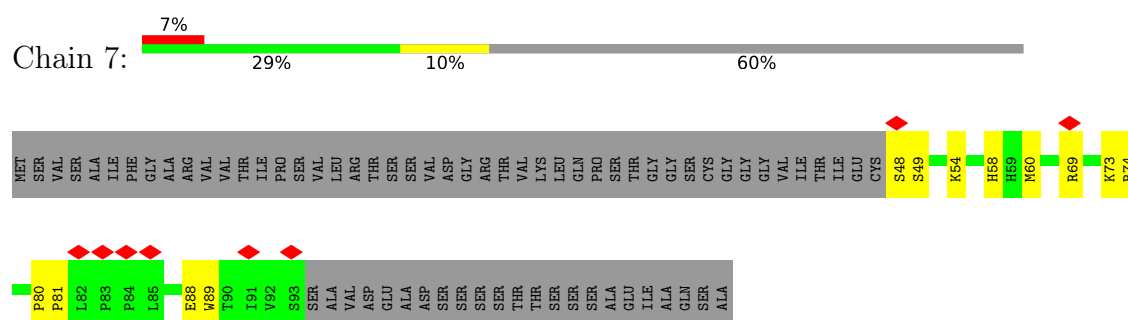
- Molecule 5: 50S ribosomal protein L36, chloroplastic



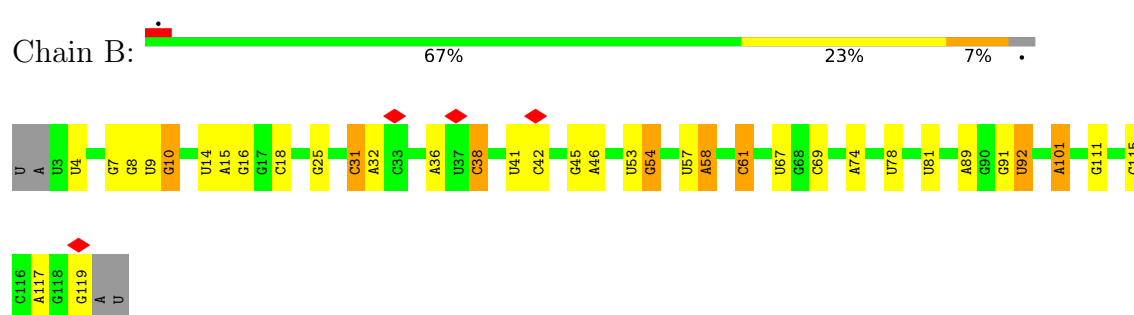
- Molecule 6: protein cL37



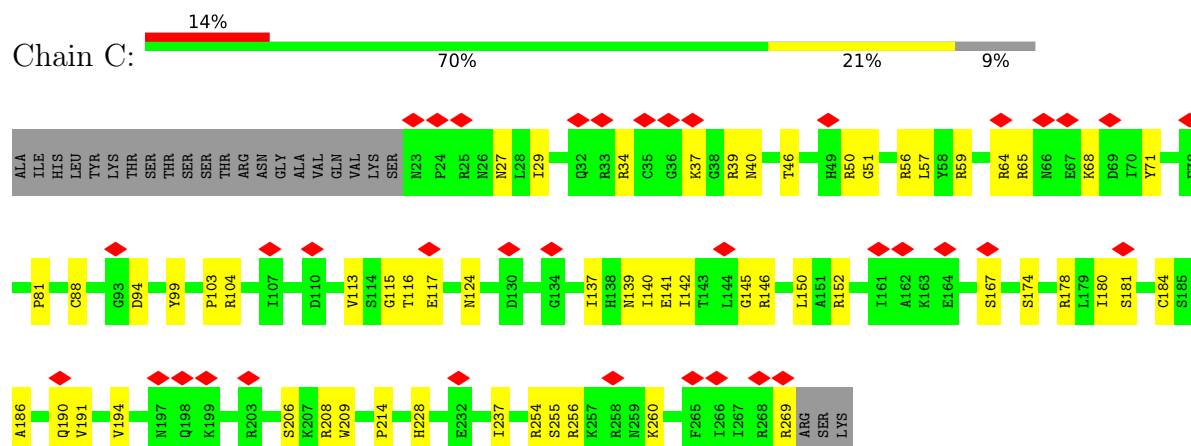
- Molecule 7: protein cL38



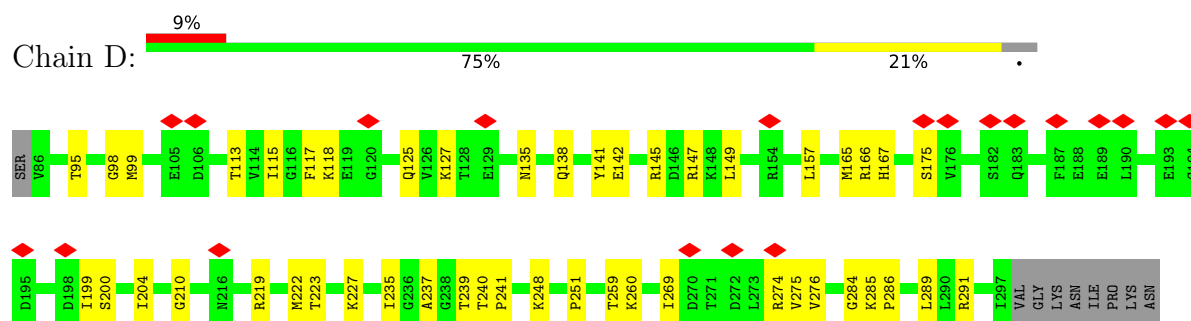
- Molecule 8: 5S rRNA



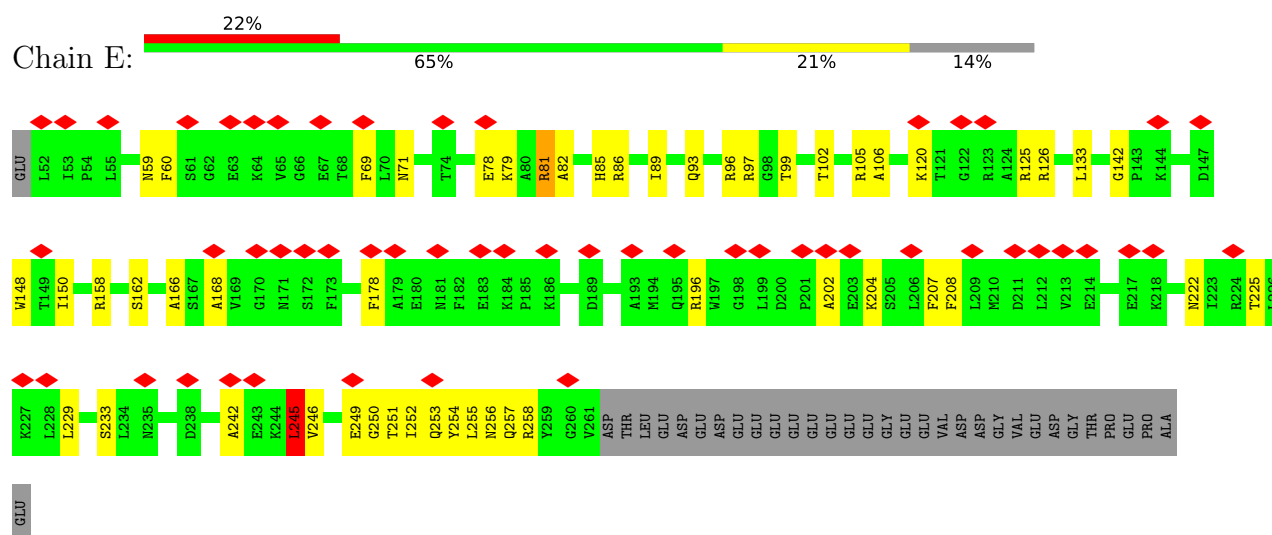
- Molecule 9: 50S ribosomal protein L2, chloroplastic



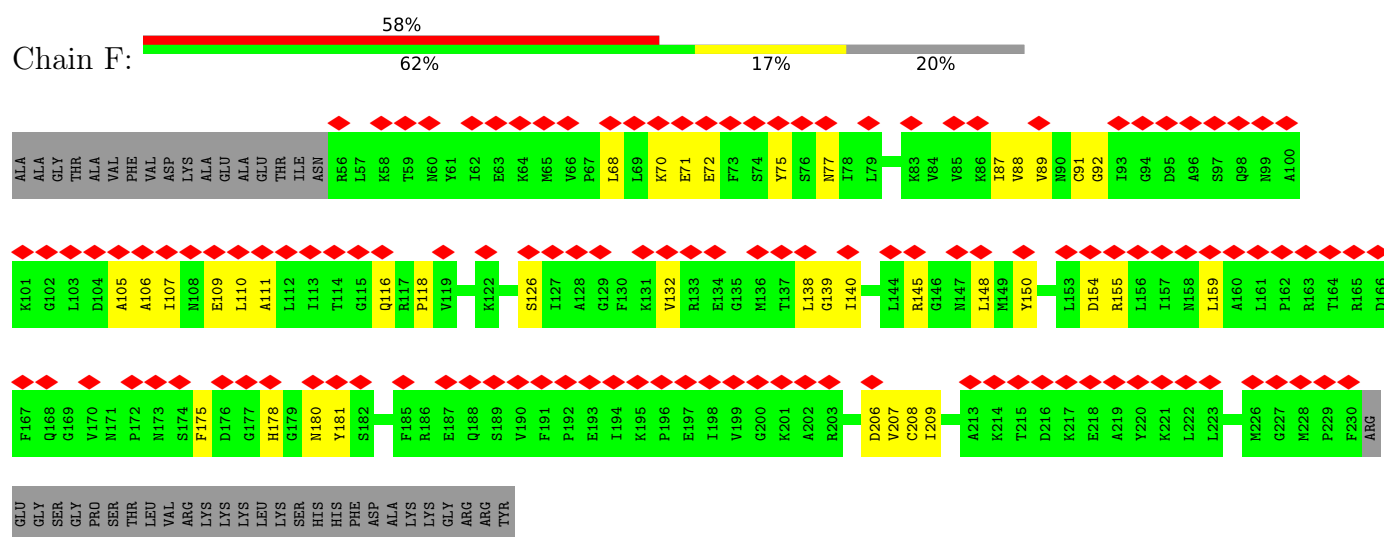
- Molecule 10: protein L3



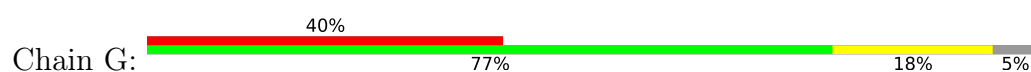
- Molecule 11: 50S ribosomal protein L4, chloroplastic

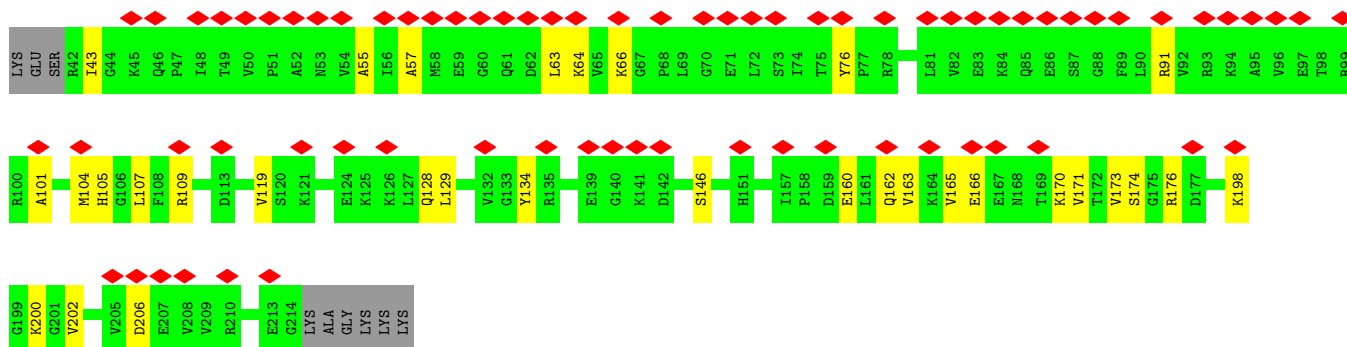


- Molecule 12: 50S ribosomal protein L5, chloroplastic

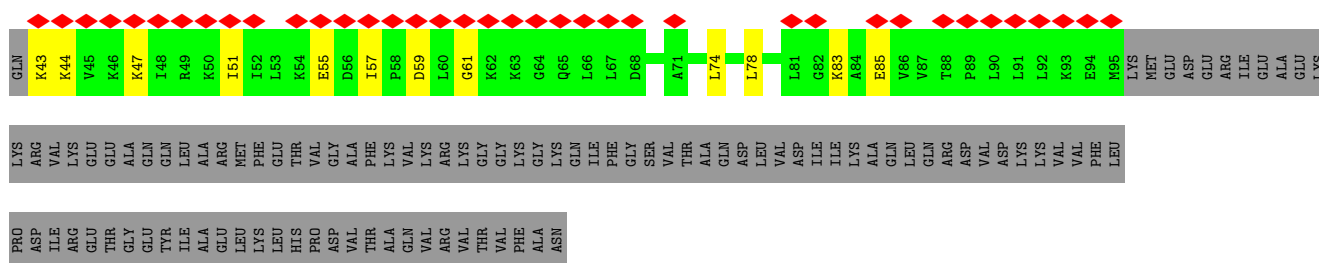


- Molecule 13: protein L6

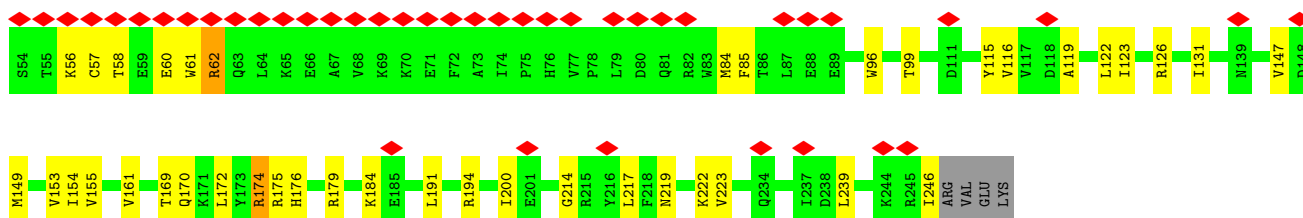




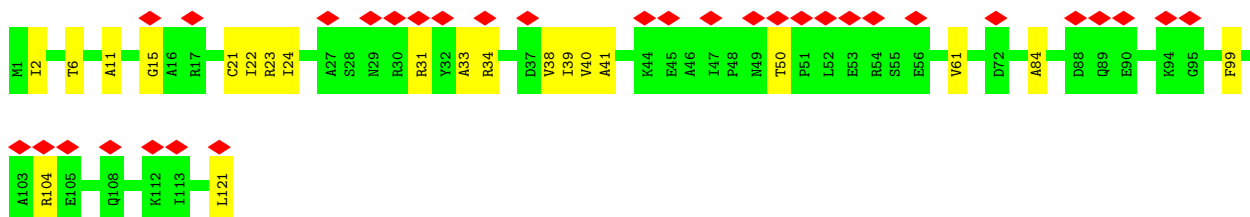
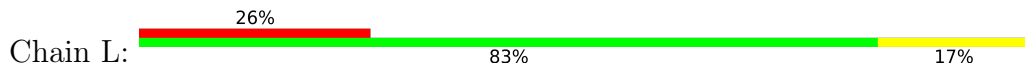
- Molecule 14: protein L9



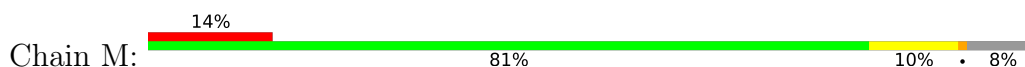
- Molecule 15: 50S ribosomal protein L13, chloroplastic

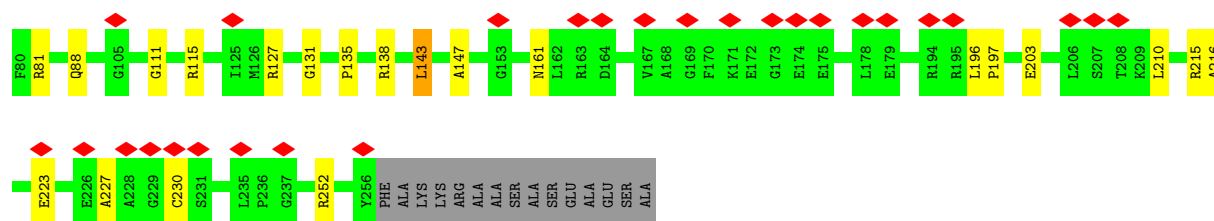


- Molecule 16: 50S ribosomal protein L14, chloroplastic



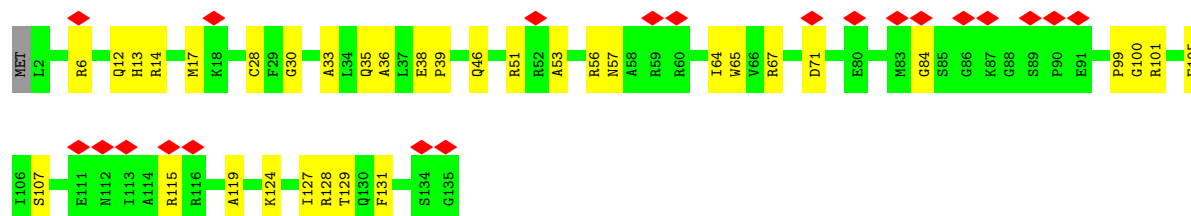
- Molecule 17: protein L15





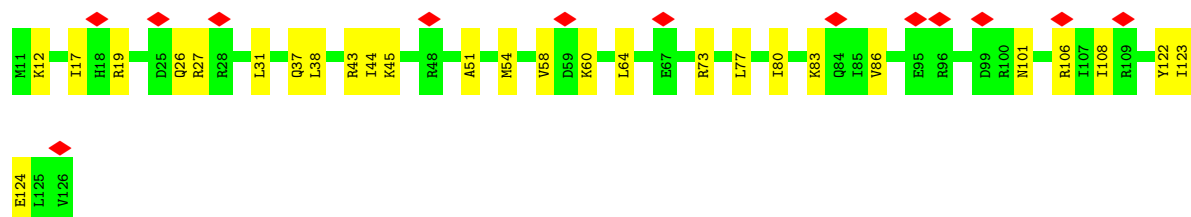
- Molecule 18: 50S ribosomal protein L16, chloroplastic

Chain N: 16% 74% 25%



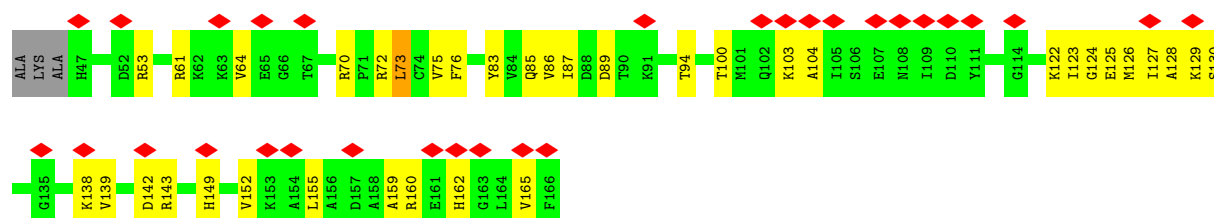
- Molecule 19: protein L17

Chain O: 11% 77% 23%



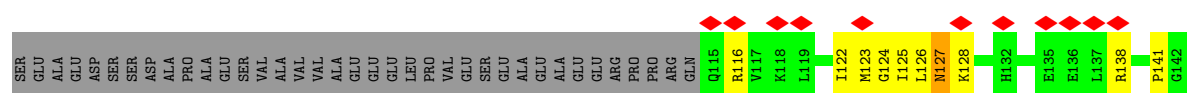
- Molecule 20: protein L18

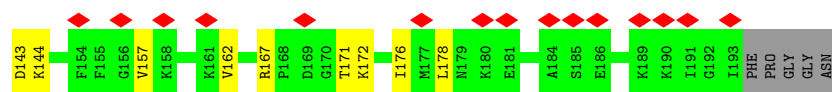
Chain P: 24% 67% 29%



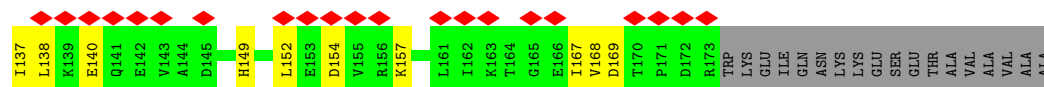
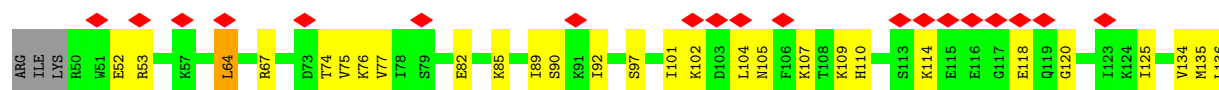
- Molecule 21: 50S ribosomal protein L19, chloroplastic

Chain Q: 15% 53% 22% 24%

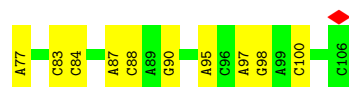
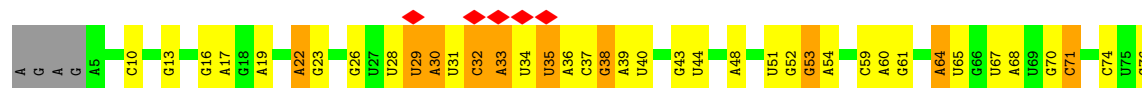




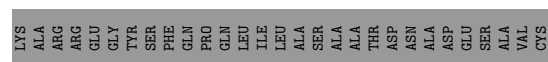
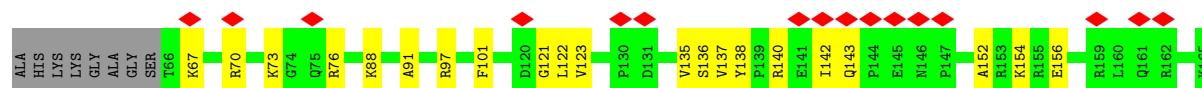
- Molecule 26: 50S ribosomal protein L24, chloroplastic



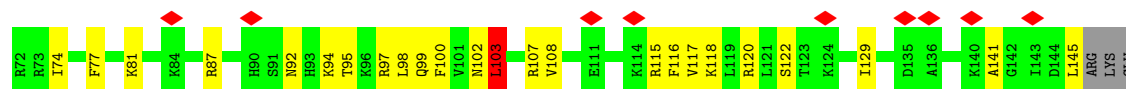
- Molecule 27: 4.8S rRNA



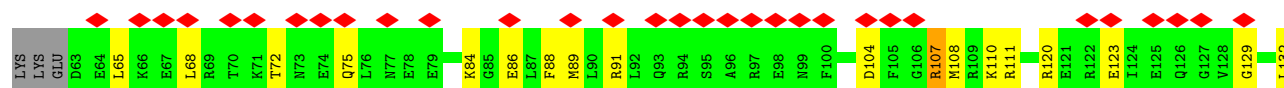
- Molecule 28: protein L27

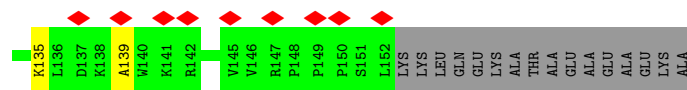


- Molecule 29: protein L28

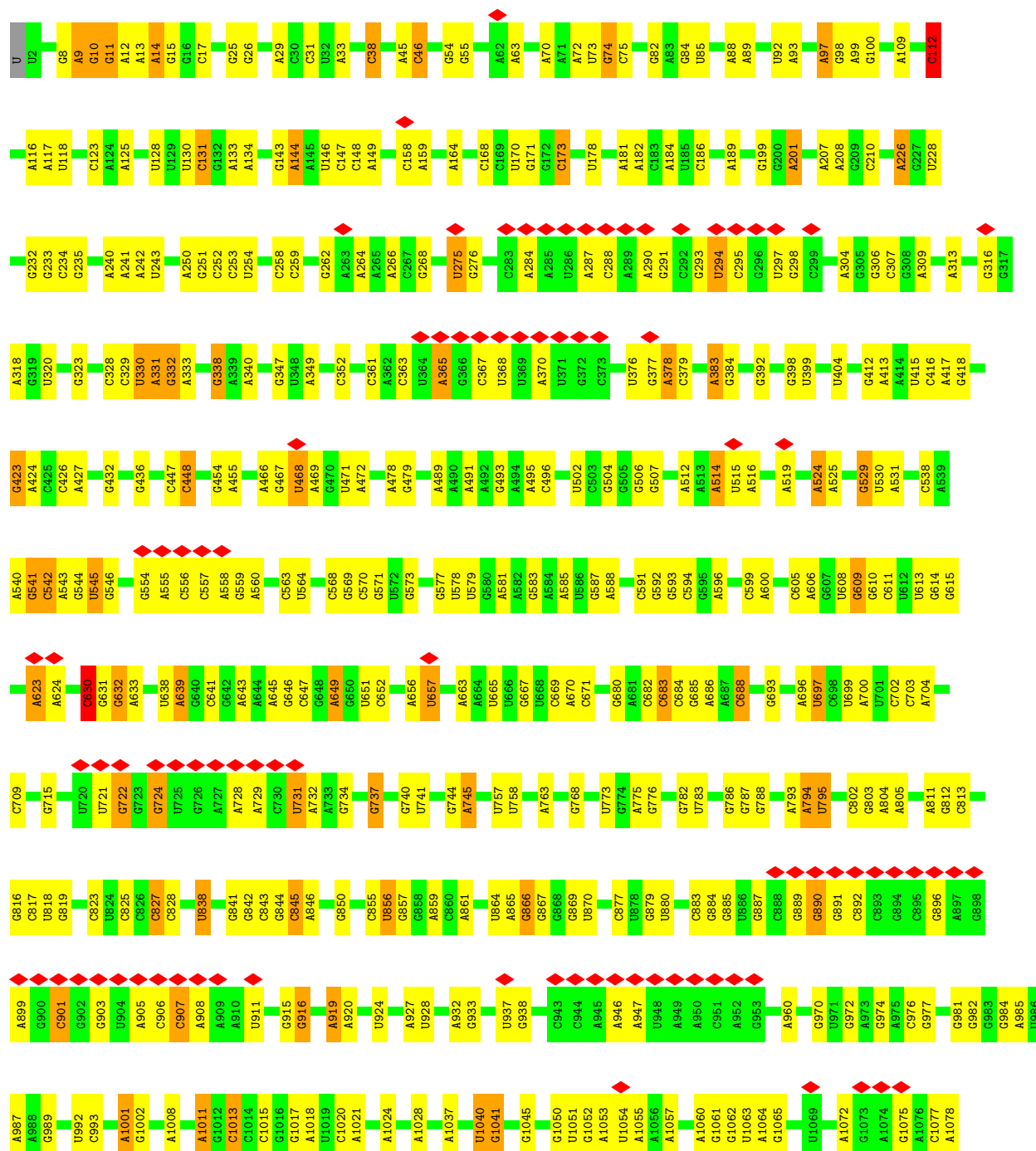


- Molecule 30: protein L29



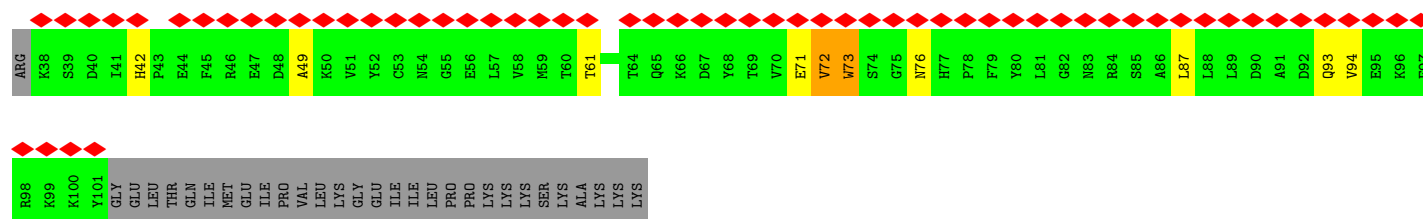


• Molecule 31: 23S rRNA



G1079	A1139	U1245	U1333	U1436	A1514	A1604	A1726	A1820	G1935	G2046	G2129	C2189
C1080	G1140	G1248	U1334	G1437	G1515	A1605	G1732	G1821	G1936	A2047	C2130	A2190
C1081	C1141	C1142	C1335	G1445	G1516	A1606	G1733	A1825	A1941	U2048	U2131	C2191
C1082	C1143	C1144	A1342	A1448	G1517	G1611	A1734	G1826	A1942	C2049	U2132	U2192
G1083	U1147	C1252	A1343	G1449	U1518	A1612	G1739	G1827	A1943	C2050	A2133	C2193
G1084	G1148	G1253	G1344	G1450	A1519	A1613	G1740	A1828	A1944	G2051	C2134	U2194
A1085	C1149	U1254	U1345	G1451	A1520	G1614	C1746	A1829	U1945	G2052	G2135	G2195
G1086	G1150	U1255	G1346	A1452	G1521	A1616	C1747	U1830	U1946	U2055	U2136	G2196
G1087	G1256	U1256	C1354	A1453	A1522	C1617	C1748	C1836	G1949	C2063	G2137	A2197
U1088	G1257	G1257	G1355	G1454	A1523	C1618	C1749	U1837	A1950	U2069	U2138	A2198
U1089	G1156	C1258	C1366	A1455	G1524	U1619	U1749	G1838	A1951	A2070	A2139	G2199
U1090	U1157	U1260	U1366	G1456	G1525	U1620	C1750	A1839	U1957	A2073	A2140	G2200
G1091	U1158	G1261	C1371	G1457	U1528	A1621	A1751	C1843	U1974	A2074	G2141	C2201
C1092	G1159	U1159	U1372	C1458	A1529	A1622	C1752	G1844	G1968	G2075	C2142	C2202
C1093	A1160	A1160	U1373	U1459	G1530	A1627	A1753	G1845	U1969	A2076	C2143	U2203
U1094	A1161	C1162	A1374	A1460	A1531	A1628	A1754	C1854	U1970	C2077	C2144	A2204
U1095	C1163	G1163	C1379	G1462	A1532	A1628	A1755	U1854	C1971	U2082	A2145	G2205
G1096	A1169	A1170	C1384	G1466	A1544	C1635	G1756	A1857	A1974	G2083	A2146	A2206
A1097	A1176	A1176	G1385	C1467	G1545	U1636	G1757	G1858	C1975	U2084	G2147	A2207
G1098	A1177	U1176	G1386	C1468	C1546	C1640	G1758	G1859	A1984	A2085	A2148	G2208
G1099	C1176	U1276	A1386	A1472	C1547	C1640	G1762	G1860	C1981	G2086	A2149	C2210
C1100	U1177	U1278	C1391	U1475	C1548	G1643	G1763	U1871	A1984	A2091	G2150	A2211
A1101	C1178	U1281	G1392	G1476	A1549	A1644	G1766	G1872	A1985	G2094	G2151	U2211
G1102	C1179	G1282	U1393	A1480	U1550	A1645	A1766	G1873	G1986	U2095	C2152	U2212
C1103	A1183	U1283	C1397	U1481	G1555	A1646	C1770	U1874	A1987	G2096	C2153	U2213
C1104	G1189	G1284	G1398	U1481	G1556	C1647	C1774	G1875	G1987	C2097	C2154	C2243
A1105	G1189	A1286	A1399	G1484	G1557	A1650	G1778	U1876	U1988	U2106	C2155	U2229
C1106	A1196	C1291	U1400	U1485	U1558	A1662	G1778	U1882	A1991	G2101	C2156	A2230
C1107	A1197	G1292	G1401	U1486	A1559	A1662	A1783	G1883	G1994	G2102	G2157	G2224
C1108	A1198	C1293	A1403	C1487	C1565	U1666	C1784	C1885	U1996	G2103	U2158	G2225
U1109	A1198	A1294	A1405	A1488	G1566	C1666	U1789	A1886	U2005	U2106	C2159	U2230
U1110	A1201	A1295	A1406	A1489	C1567	C1682	A1790	G1887	G2006	G2107	C2160	G2234
U1111	C1206	C1297	C1407	G1490	U1568	G1683	C1792	G1888	C2007	U2111	G2161	G2240
G1112	U1209	A1298	A1408	C1493	U1568	G1684	A1793	C1889	C2008	U2112	C2162	G2241
A1113	U1210	A1305	A1413	G1494	A1569	C1684	C1794	C1901	U2009	G2113	C2163	A2242
A1114	G1211	A1308	U1416	C1495	C1570	C1689	A1795	C1906	C2010	G2114	G2164	C2243
G1115	G1211	U1219	U1417	A1496	G1571	C1692	A1796	C1907	G2011	G2115	G2165	C2247
A1116	U1219	C1310	U1418	A1497	G1572	C1696	A1801	A1914	A2013	C2116	G2166	U2248
G1117	G1225	G1315	U1419	G1501	C1574	G1703	C1807	A1915	C2020	U2117	G2167	A2254
U1118	U1226	C1316	U1423	A1502	A1578	A1704	C1808	G1920	U2021	U2118	C2168	G2255
G1119	U1227	C1317	A1424	C1504	C1584	A1705	G1809	G1923	C2022	U2119	C2169	A2256
C1120	U1235	C1317	A1427	C1505	C1585	C1706	C1810	C1923	G2023	U2120	G2171	G2266
G1121	A1235	A1321	A1427	U1506	G1586	U1707	C1811	A1926	C2034	C2121	C2172	U2267
U1122	G1238	A1322	C1431	G1507	G1586	G1708	A1812	A1927	A2036	C2122	G2173	G2268
A1123	C1238	A1322	U1432	U1508	A1592	G1709	A1813	A1927	U2036	U2123	C2174	G2269
A1124	G1239	G1330	U1433	U1509	U1593	C1710	G1814	C1928	G2037	G2124	C2175	U2270
U1125	G1240	G1331	G1434	U1510	C1595	A1712	U1815	U1929	U2037	G2125	A2176	C2271
A1126	U1241	G1332	U1435	U1511	C1599	A1725	U1818	U1930	A2045	G2126	C2177	U2272
G1127	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	A2274
C1128	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279
U1129	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279
C1130	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279
G1132	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279
U1133	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279
G1134	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279
A1135	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279
U1136	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279
C1137	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279
G1138	U1241	G1332	U1435	U1512	A1600	A1725	U1819	U1931	U2045	C2127	C2178	U2279

- Molecule 32: 50S ribosomal protein L31



4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	M	0	1
21	Q	0	1
23	S	0	1
32	0	0	1
All	All	0	4

All (1) bond length outliers are listed below:

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

The worst 5 of 339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	2077	C	N1-C2-O2	11.06	125.54	118.90
31	A	2077	C	C2-N1-C1'	10.63	130.49	118.80
31	A	1747	C	N3-C2-O2	-9.95	114.94	121.90
31	A	2314	C	C2-N1-C1'	9.82	129.60	118.80
31	A	2314	C	N1-C2-O2	9.47	124.58	118.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	378	0	415	8	0
2	2	415	0	434	7	0
3	3	445	0	501	11	0
4	4	563	0	623	9	0
5	5	304	0	345	7	0
6	6	422	0	508	9	0
7	7	368	0	386	7	0
8	B	2500	0	1263	13	0
9	C	1904	0	1985	41	0
10	D	1620	0	1699	34	0
11	E	1655	0	1725	40	0
12	F	1351	0	1407	28	0
13	G	1353	0	1416	18	0
14	H	423	0	490	7	0
15	K	1568	0	1595	25	0
16	L	942	0	996	16	0
17	M	1342	0	1417	16	0
18	N	1067	0	1122	28	0
19	O	944	0	1004	25	0
20	P	947	0	966	30	0
21	Q	953	0	1045	25	0
22	R	996	0	1062	35	0
23	S	1171	0	1216	22	0
24	T	1149	0	1220	21	0
25	U	740	0	795	14	0
26	V	993	0	1055	25	0
27	W	2187	0	1102	17	0
28	X	810	0	847	14	0
29	Y	605	0	652	17	0
30	Z	754	0	808	13	0
31	A	60324	0	30377	432	0
32	0	521	0	499	4	0
All	All	91714	0	60975	829	0

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

The worst 5 of 829 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:293:G:H21	31:A:365:A:N6	1.61	0.98
31:A:293:G:N2	31:A:365:A:H62	1.61	0.98
31:A:1505:C:H42	31:A:1515:G:H1	1.09	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	44/56 (79%)	39 (89%)	5 (11%)	0	100	100
2	2	49/65 (75%)	39 (80%)	10 (20%)	0	100	100
3	3	55/61 (90%)	49 (89%)	6 (11%)	0	100	100
4	4	67/73 (92%)	59 (88%)	8 (12%)	0	100	100
5	5	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
6	6	47/142 (33%)	46 (98%)	1 (2%)	0	100	100
7	7	44/116 (38%)	41 (93%)	3 (7%)	0	100	100
9	C	245/271 (90%)	213 (87%)	32 (13%)	0	100	100
10	D	210/221 (95%)	188 (90%)	22 (10%)	0	100	100
11	E	208/243 (86%)	180 (86%)	28 (14%)	0	100	100
12	F	173/220 (79%)	161 (93%)	12 (7%)	0	100	100
13	G	171/182 (94%)	161 (94%)	10 (6%)	0	100	100
14	H	51/155 (33%)	47 (92%)	4 (8%)	0	100	100
15	K	191/197 (97%)	178 (93%)	13 (7%)	0	100	100
16	L	119/121 (98%)	103 (87%)	16 (13%)	0	100	100
17	M	175/192 (91%)	163 (93%)	11 (6%)	1 (1%)	25	57
18	N	132/135 (98%)	111 (84%)	21 (16%)	0	100	100

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

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	39/49 (80%)	39 (100%)	0	100	100
2	2	48/59 (81%)	46 (96%)	2 (4%)	30	60
3	3	47/50 (94%)	47 (100%)	0	100	100
4	4	59/62 (95%)	58 (98%)	1 (2%)	60	78
5	5	34/34 (100%)	34 (100%)	0	100	100

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

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	X	73	LYS
32	0	76	ASN
30	Z	107	ARG
15	K	174	ARG
26	V	64	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
22	R	99	GLN
32	O	76	ASN
23	S	145	GLN
24	T	52	GLN
12	F	77	ASN

5.3.3 RNA ⓘ

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

5 of 643 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	B	4	U
8	B	10	G
8	B	14	U
8	B	15	A
8	B	16	G

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	A	556	C
31	A	514	A
27	W	97	A
27	W	33	A
31	A	97	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

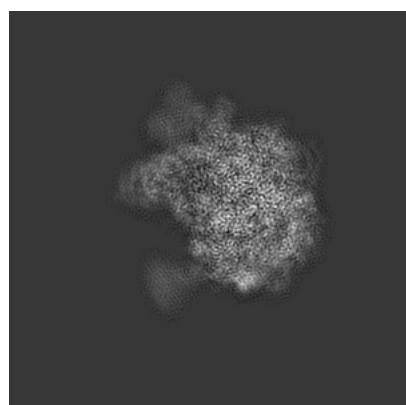
6 Map visualisation [i](#)

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

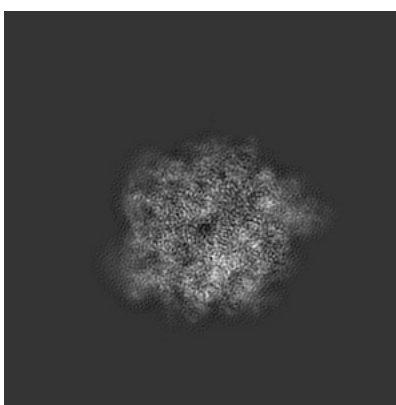
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

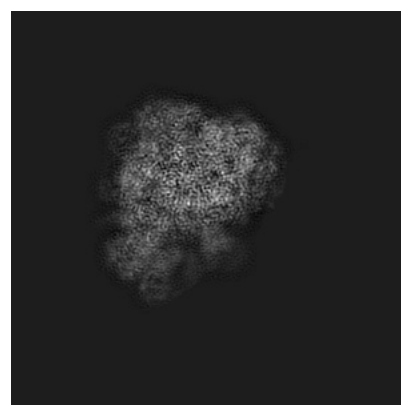
6.1.1 Primary map



X



Y

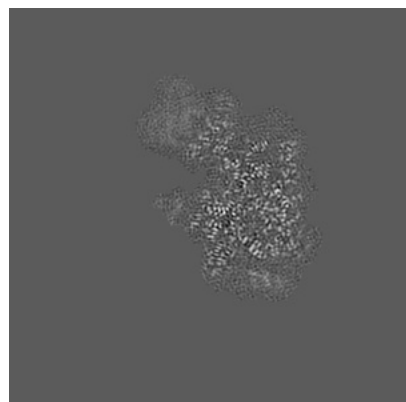


Z

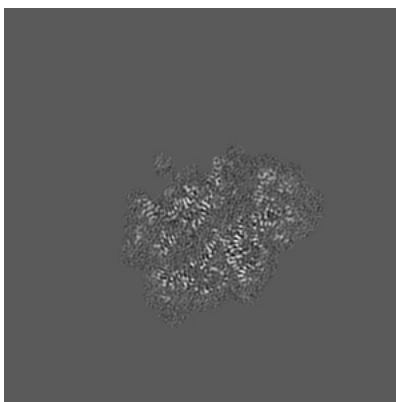
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

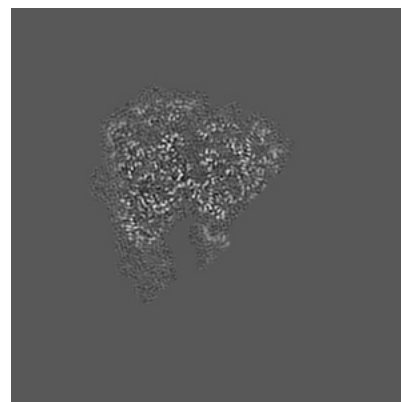
6.2.1 Primary map



X Index: 192



Y Index: 192

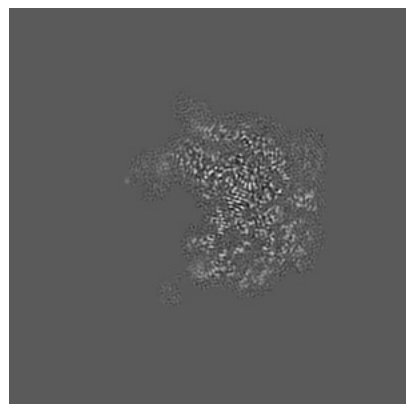


Z Index: 192

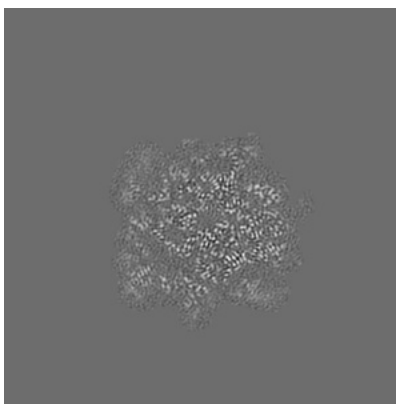
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

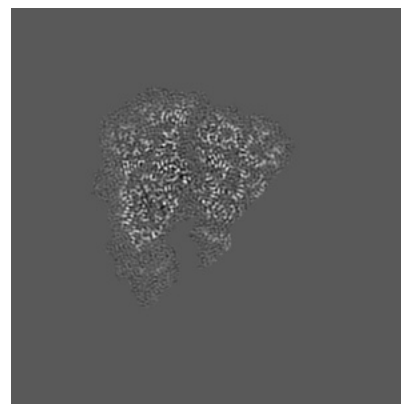
6.3.1 Primary map



X Index: 163



Y Index: 221



Z Index: 195

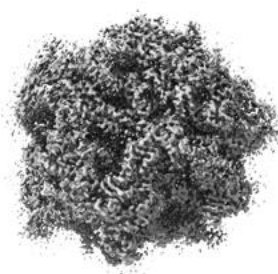
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

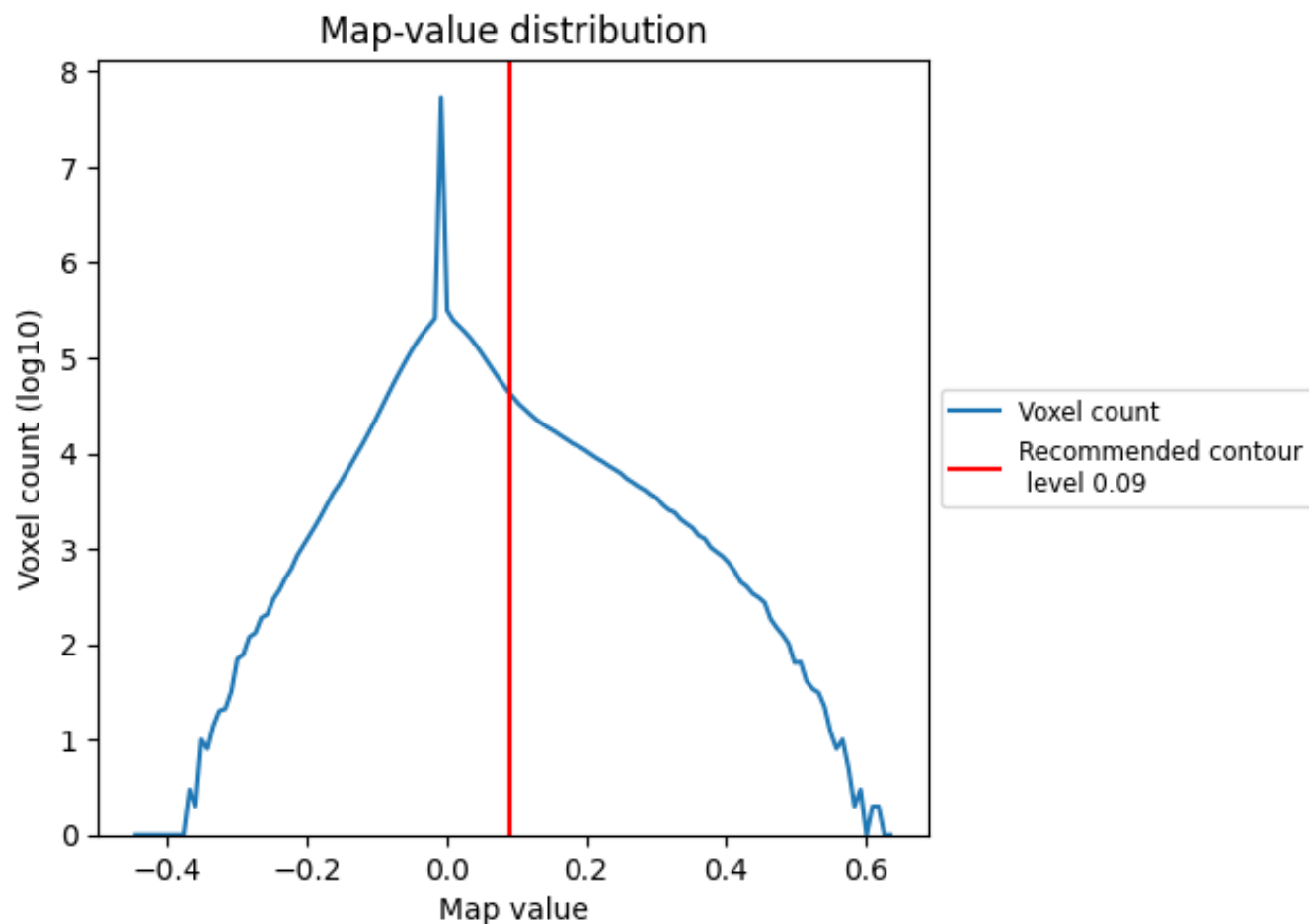
6.5 Mask visualisation

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

7 Map analysis [i](#)

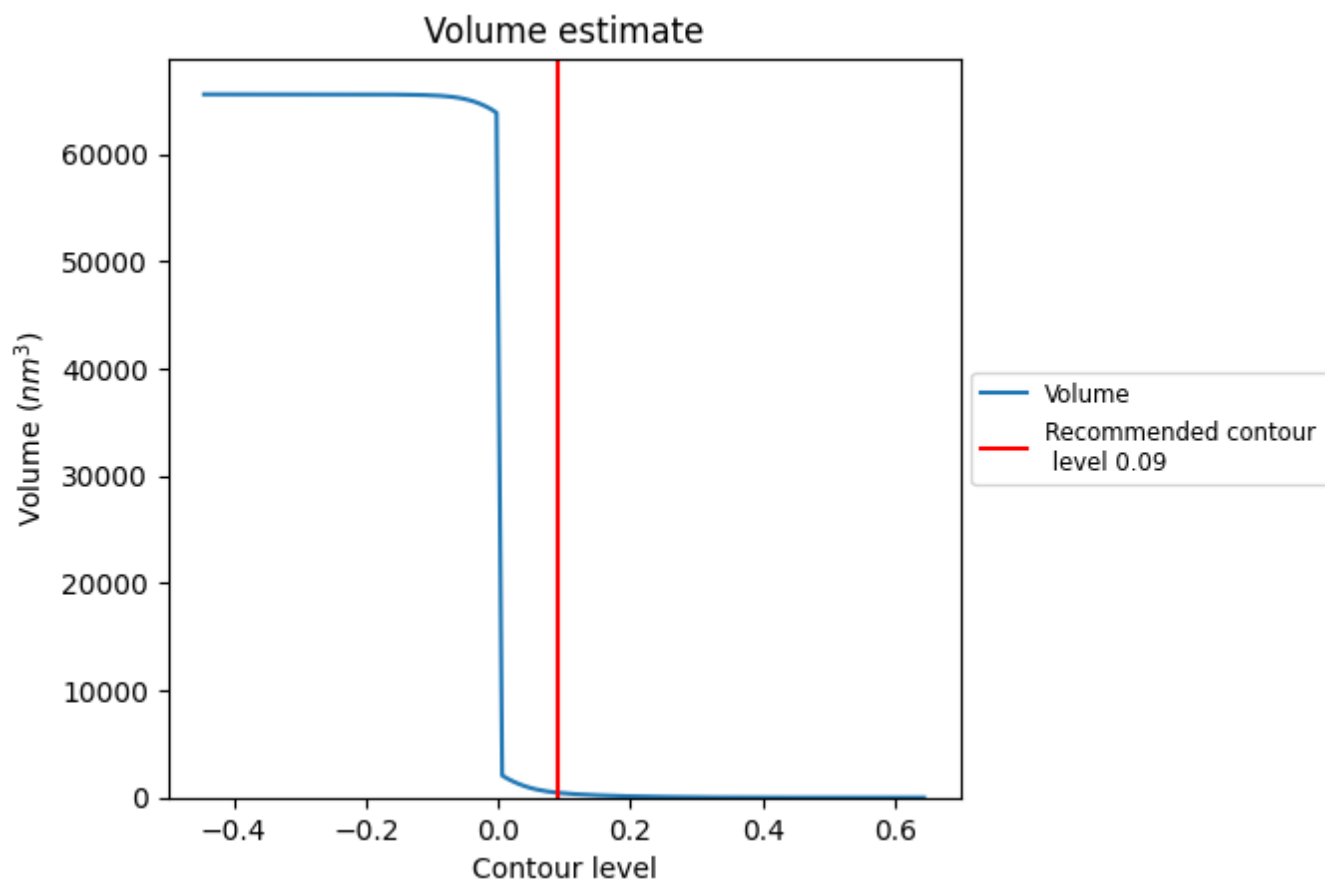
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

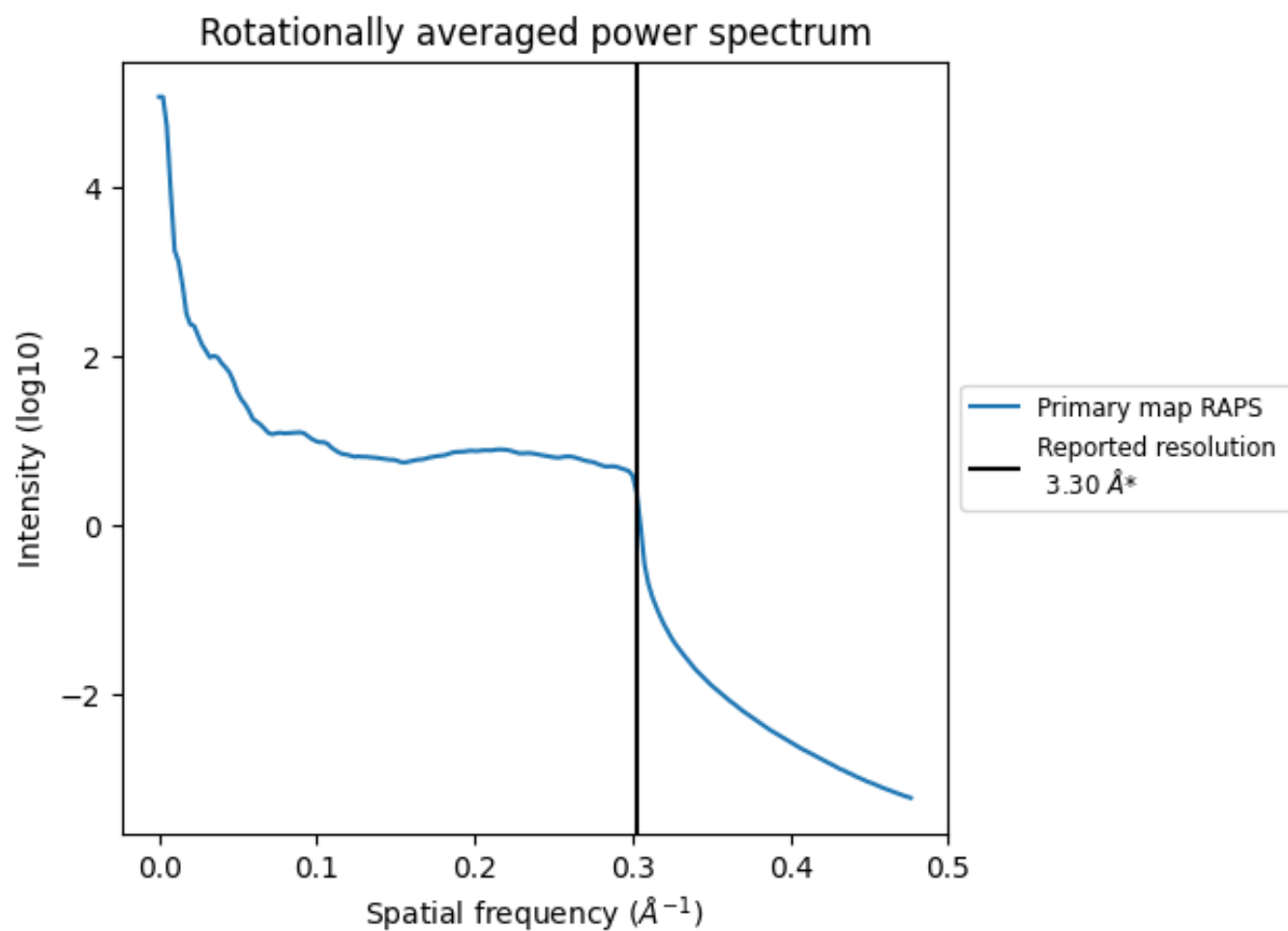
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 450 nm³; this corresponds to an approximate mass of 407 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

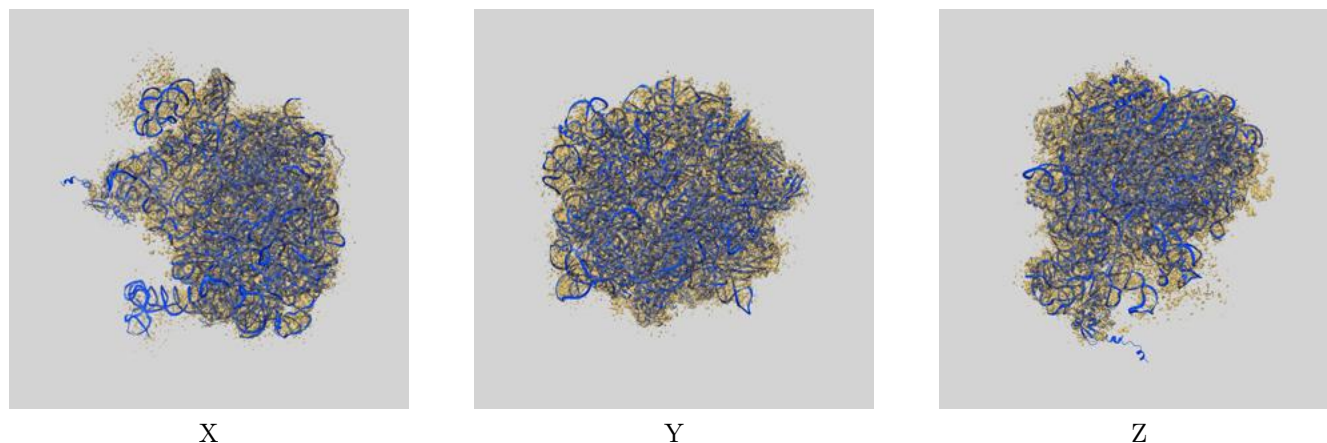
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

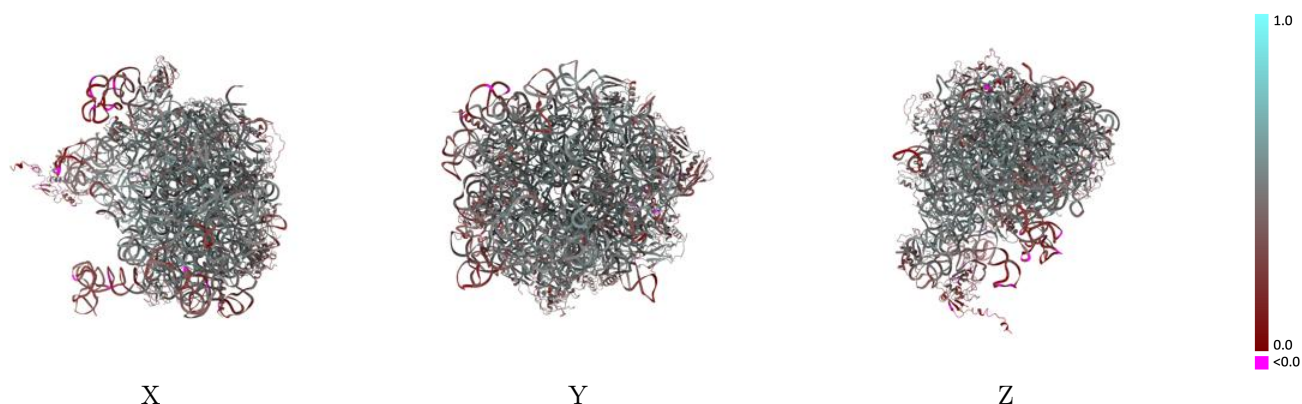
This section contains information regarding the fit between EMDB map EMD-6711 and PDB model 5X8T. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



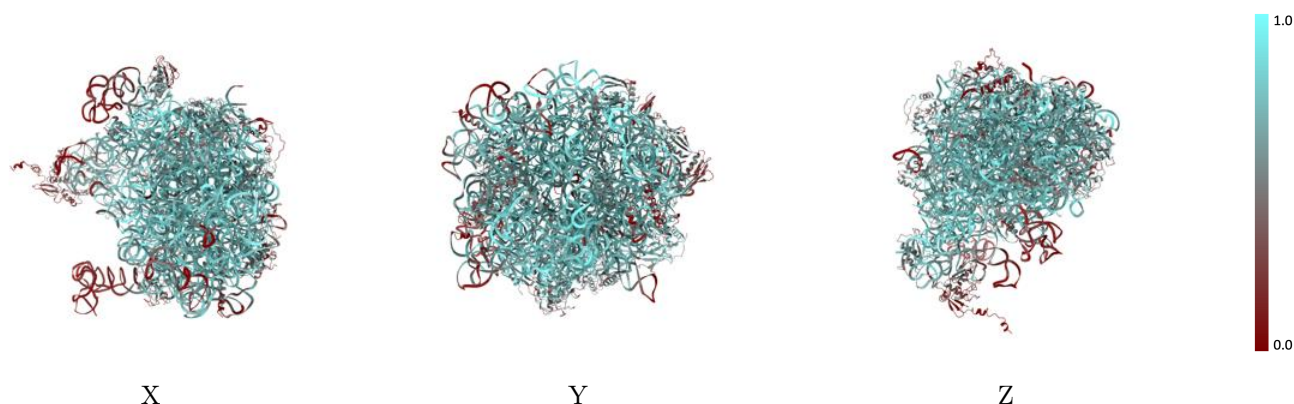
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



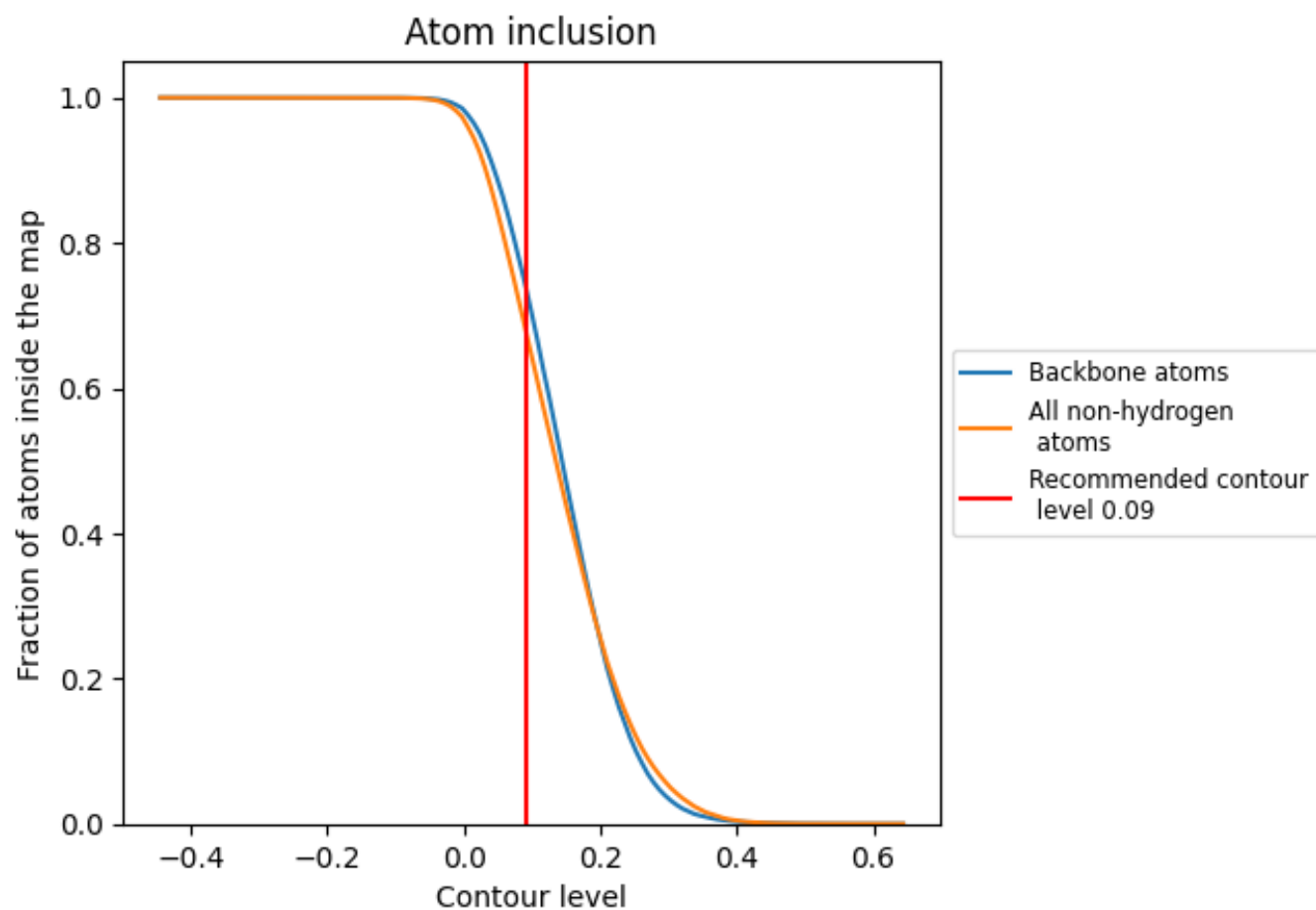
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6827	 0.4510
0	 0.0784	 0.1390
1	 0.6114	 0.4100
2	 0.5325	 0.3480
3	 0.6793	 0.4750
4	 0.7030	 0.4840
5	 0.6597	 0.4090
6	 0.4889	 0.3800
7	 0.6246	 0.4670
A	 0.7348	 0.4700
B	 0.7308	 0.4450
C	 0.6156	 0.4290
D	 0.6530	 0.4620
E	 0.5757	 0.4120
F	 0.2801	 0.2780
G	 0.4476	 0.3690
H	 0.2374	 0.3220
K	 0.5881	 0.4420
L	 0.5427	 0.4270
M	 0.6446	 0.4440
N	 0.6287	 0.4170
O	 0.6453	 0.4360
P	 0.5473	 0.3950
Q	 0.5604	 0.4240
R	 0.6568	 0.4170
S	 0.5419	 0.4110
T	 0.5260	 0.4070
U	 0.4890	 0.4060
V	 0.4985	 0.3810
W	 0.7641	 0.4760
X	 0.6031	 0.4270
Y	 0.6276	 0.4550
Z	 0.4717	 0.3770

