



# wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 03:07 PM EST

PDB ID : 3BBX  
EMDB ID : EMD-1455  
Title : The Hsp15 protein fitted into the low resolution Cryo-EM map of the 50S.nc-tRNA.Hsp15 complex  
Authors : Jiang, L.; Abrahams, J.P.  
Deposited on : 2007-11-11  
Resolution : 10.00 Å(reported)  
Based on initial model : 2AW4

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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) : 2.31.3

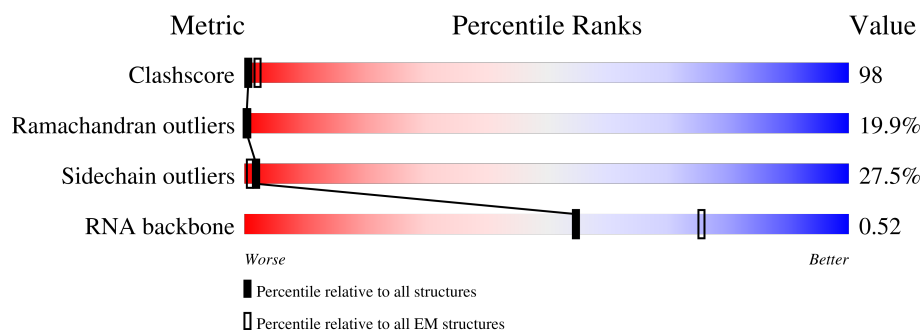
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.00 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  $\geq 3$ , 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	A	120	
2	B	2904	
3	V	94	
4	C	273	
5	D	209	
6	E	201	
7	F	178	

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Mol	Chain	Length	Quality of chain
8	G	176	
9	H	149	
10	J	142	
11	K	123	
12	L	144	
13	M	136	
14	N	127	
15	O	117	
16	P	114	
17	Q	117	
18	R	103	
19	S	110	
20	T	100	
21	U	103	
22	W	84	
23	X	63	
24	Y	58	
25	Z	70	
26	0	56	
27	1	54	
28	2	46	
29	3	64	
30	4	38	

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 89335 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	117	Total	C	N	O	P	0	0
			2507	1116	459	815	117		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2902	Total	C	N	O	P	0	61
			61056	27210	11229	19715	2902		

- Molecule 3 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	267	Total	C	N	O	S	0	0
			2053	1271	416	359	7		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	140	Total	C	N	O	S	0	0
			1112	704	210	194	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	121	Total	C	N	O	S	0	0
			930	582	179	164	5		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			777	491	145	139	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	102	Total	C	N	O		
			779	492	146	141	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	84	Total	C	N	O	S	
			634	391	129	113	1	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

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

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	70	Total	C	N	O	S	
			549	339	104	100	6	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	0	56	Total	C	N	O	S	
			444	269	94	80	1	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	1	54	Total	C	N	O		
			441	284	81	76	0	0

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	B	92	Total	Mg	0
			92	92	
31	C	1	Total	Mg	0
			1	1	
31	E	3	Total	Mg	0
			3	3	
31	L	4	Total	Mg	0
			4	4	
31	Q	2	Total	Mg	0
			2	2	
31	S	2	Total	Mg	0
			2	2	
31	T	2	Total	Mg	0
			2	2	
31	U	1	Total	Mg	0
			1	1	
31	2	3	Total	Mg	0
			3	3	

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	B	443	Total	O	0
			443	443	

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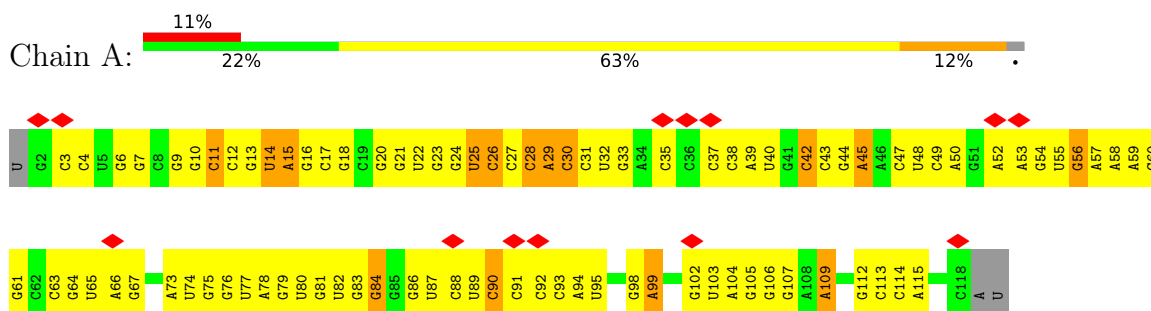
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Mol	Chain	Residues	Atoms		AltConf
32	C	1	Total 1	O 1	0
32	D	1	Total 1	O 1	0
32	E	18	Total 18	O 18	0
32	L	8	Total 8	O 8	0
32	Q	7	Total 7	O 7	0
32	S	7	Total 7	O 7	0
32	T	5	Total 5	O 5	0
32	U	5	Total 5	O 5	0
32	2	11	Total 11	O 11	0

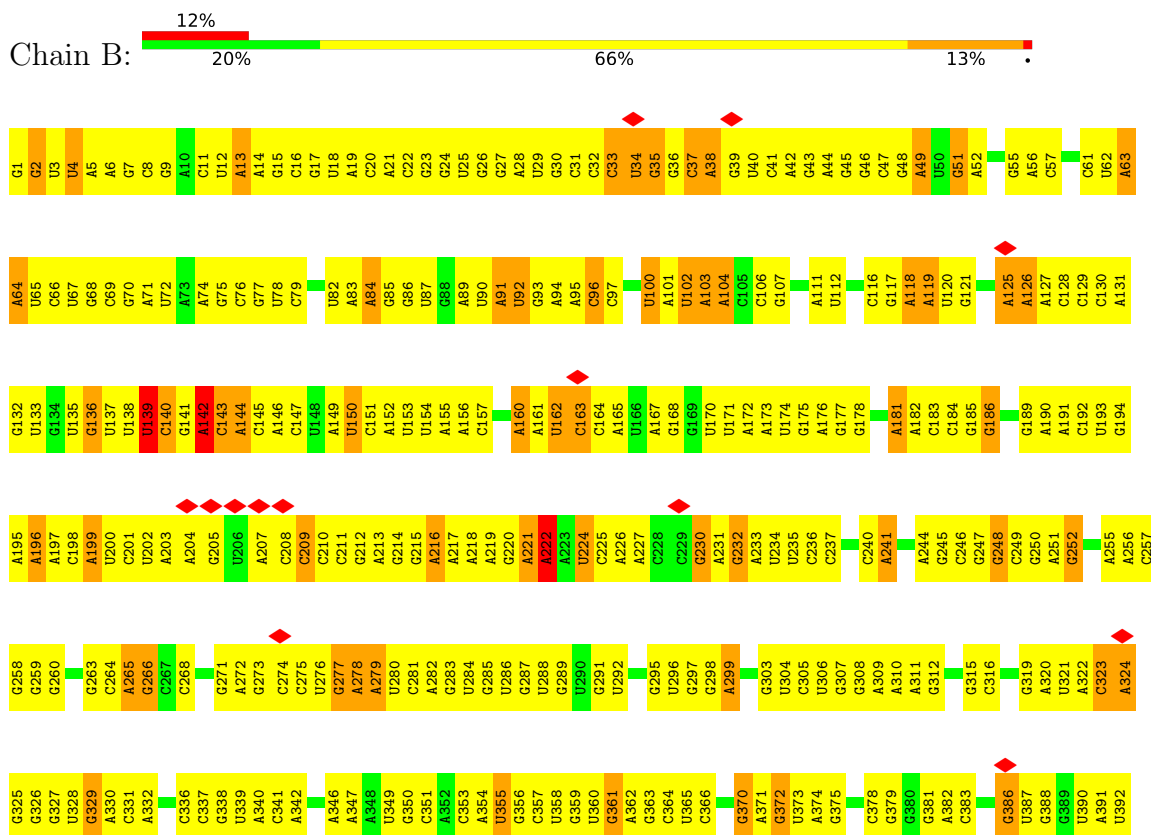
### 3 Residue-property plots

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: 5S ribosomal RNA



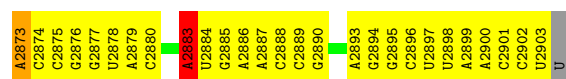
#### • Molecule 2: 23S ribosomal RNA



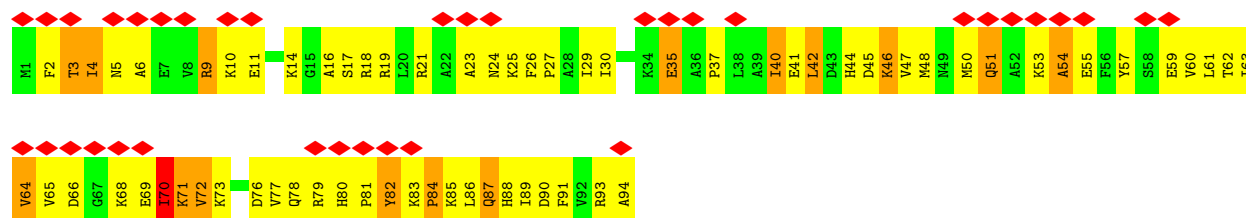


A1981	A1918	A1852	U1725	U1862	C1595	G1465	U1402	G1338	A1274	C1211
U1962	A1919	A1853	C1726	G1663	C1596	G1469	A1403	G1339	A1275	G1212
G1983	C1920	A1854	C1727	A1664	U1599	A1470	C1404	U1340	A1276	
G1984	G1921	U1855	C1728	A1665	A1535	A1471	C1406	G1341	G1277	G1215
C1985	G1922	U1856	U1729	G1666	G1601	G1472	G1407	U1278	G1278	G1216
U1923	U1923	G1857	C1730	A1668	A1603	G1473	G1408	G1279	G1280	U1217
A1987	C1924	A1858	G1731	A1669	C1604	U1474	U1409	G1281	G1281	G1218
G1988	A1927	U1859	G1732	A1670	C1605	U1475	G1410	U1219	G1282	U1219
G1989	A1928	C1796	G1733	C1670	G1540	U1476	U1411	G1220	G1283	G1220
C1990	U1929	U1796	G1734	A1671	C1541	U1477	U1412	C1221	G1284	U1221
U1991	G1932	U1798	G1735	G1672	C1542	U1478	A1413	G1222	A1285	U1222
G1992	A1933	G1799	U1736	G1673	U1543	G1479	C1414	G1223	A1286	G1223
C1993	G1933	C1800	U1737	C1675	A1544	C1480	U1415	G1224	A1287	U1224
G1994	C1934	A1801	G1738	A1676	A1545	U1481	G1416	G1225	G1288	G1225
C1995	G1935	A1802	A1739	A1677	G1546	G1482	A1418	A1226	A1353	A1226
A1997	A1936	A1803	G1740	A1678	G1547	U1483	U1419	G1227	A1354	G1227
C1998	A1937	C1804	C1741	G1681	A1548	U1484	A1420	G1228	A1355	G1228
A1998	A1938	A1805	U1742	U1682	A1549	U1485	G1421	U1229	G1360	U1229
C1999	A1939	C1806	G1743	U1683	A1550	U1486	G1422	U1230	G1361	A1230
C2000	U1940	G1807	A1744	C1684	A1551	U1487	A1423	U1231	C1362	U1231
C2001	A1871	U1808	A1745	C1685	A1552	U1488	G1424	G1232	C1363	G1232
G2002	A1872	A1809	A1746	U1686	U1553	U1489	G1425		G1296	G1236
A2003	G1873	A1810	A1747	U1687	G1554	C1489	G1426	G1237	A1237	A1237
G2004	C1874	U1811	U1748	U1688	G1555	C1490	G1427	G1298	G1238	G1238
A2005	U1875	U1812	C1748	A1689	C1556	A1491	G1428	G1299	G1239	G1239
C2006	A1876	G1813	A1749	C1690	C1557	G1492	G1429	G1300	U1240	U1240
U2007	U1877	G1814	G1750	C1691	U1558	G1493	G1430	A1301	A1241	A1241
C2008	A1878	A1815	U1751	U1692	U1559	G1494	G1431	C1302	C1243	C1243
A2009	G1879	C1816	G1752	U1693	G1560	C1495	A1434	G1303	A1244	A1244
G2010	U1880	G1817	G1753	C1694	C1561	A1496	G1437	G1304	G1245	G1245
U2011	C1881	U1818	A1754	G1695	U1562	U1495	U1438	G1305	A1246	A1246
A1952	U1882	U1819	U1755	G1696	C1563	A1496	A1439		G1247	G1247
A1953	U1883	U1820	G1756		U1564		U1440	G1311	A1248	A1248
G1954	A1884	A1821	U1757		C1565	G1500	G1441	U1312	U1249	U1249
U1955	U1885	U1822	U1758	A1700	C1566	G1501	U1442	U1313	G1250	G1250
U1956	A1886	G1823	A1759	G1702	G1567	G1502	U1443	C1314	C1251	C1251
C1957	U1887	U1824	C1760	G1703	G1568	A1502	U1444	U1315	G1252	G1252
G1958	G1887	U1825	U1765	C1704	A1569	A1503	G1445	U1316	A1253	A1253
A1960	U1888	G1826	U1766	C1705	A1570	A1504	G1446	G1317	U1254	U1254
C1961	A1889	U1827	G1767	G1706	A1571	A1505	C1447	U1318	U1255	U1255
U1962	G1890	C1828	C1768	G1707	A1572	U1506	G1448	C1319	G1256	G1256
U1963	A1891	U1829	C1769	U1708	G1573	U1507	A1321	C1320	C1257	C1257
G1964	C1892	G1830	U1770	U1709		A1385	A1322	U1258	U1258	U1258
C1965	U1893	C1831	U1771	U1710	U1578	A1508	C1386	U1259	U1259	U1259
A1966	A1894	C1832	G1772	A1711	U1579	A1509	A1387	A1260	A1260	A1260
G1967	U1895	C1833	A1773	U1712	A1580	G1510	G1388	C1261	C1261	C1261
C1968	C1896	G1839	C1774	A1713	G1581	G1511		A1262	A1262	A1262
A1969	A1900	U1839	U1775	U1714	C1582	C1512	A1454	U1326	U1263	U1263
U1970	G1904	C1842	G1776	G1715	U1583	U1513	G1455	A1327	A1264	A1264
G1971	C1905	C1843	U1777	U1716	U1584	U1514	G1456	U1328	A1265	A1265
C1972	G1906	G1844	U1778	A1717	C1585	U1515	U1457	U1329	A1266	A1266
G1973	U1909	U1845	U1779	G1718	U1586	A1516	U1458	C1330	G1267	G1267
C1974	G1910	C1846	U1780	G1719	A1587	G1517	G1459	G1331	A1268	A1268
U1975	U1911	A1847	A1781	U1720	U1588	U1518	U1460	G1332	A1269	A1269
G1976	A1912	U1848	U1782	A1721	G1589	C1518	C1398	G1333	C1270	C1270
U1977	A1913	A1849	U1783	A1722	U1590	G1524	C1461	G1334	G1271	G1271
A1978	C1914	U1851	A1784	G1723	A1591	A1525	C1462	C1335	A1272	A1272
U1979	U1915		A1785	G1724	A1592	C1526	G1463	A1336	U1273	U1273
G1980	A1916		A1786	G1725	U1593	G1527	G1464	G1337		
U2041	U1917				U1594	A1528				
						G1529				
						G1530				
						C1531				
						A1532				

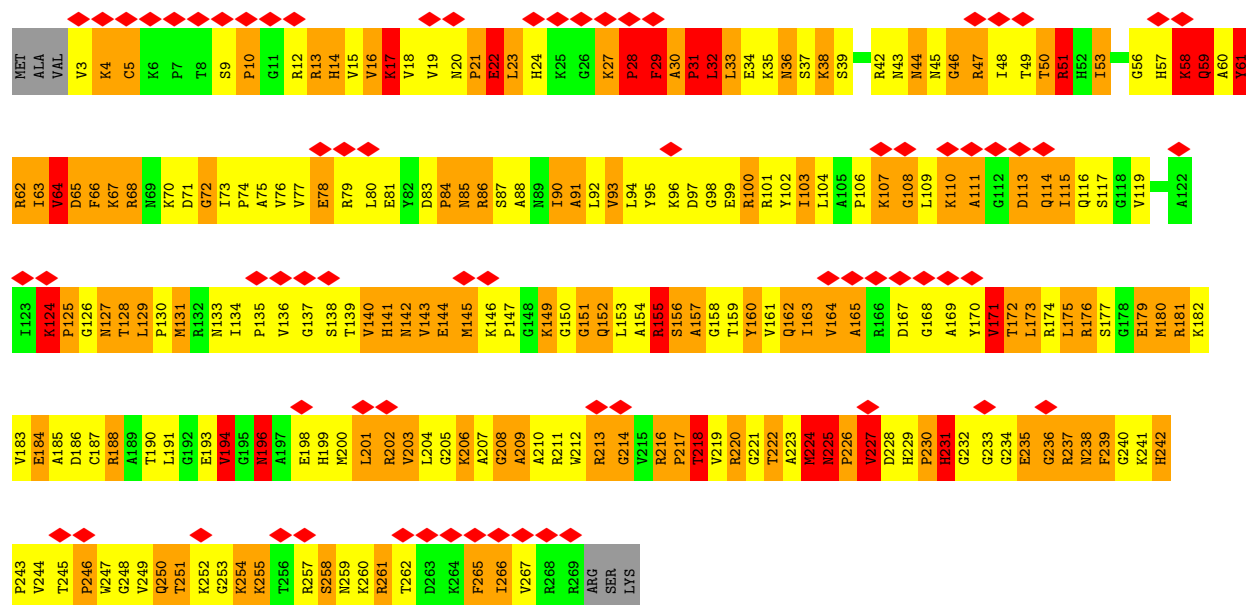




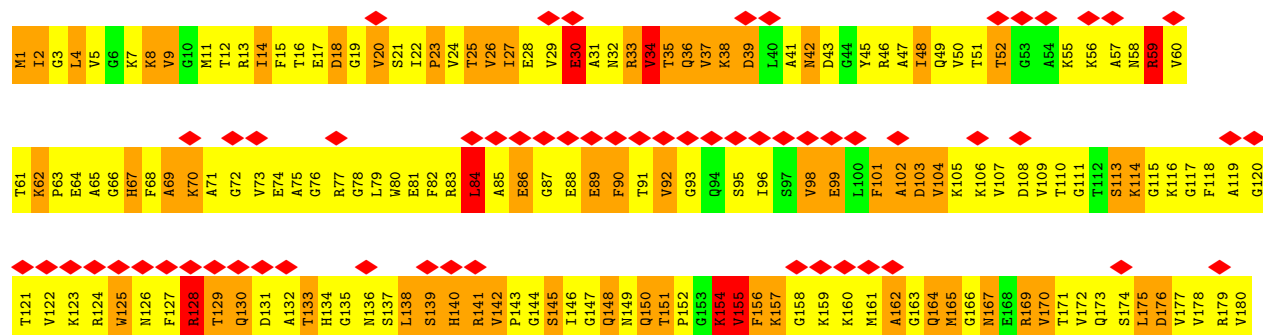
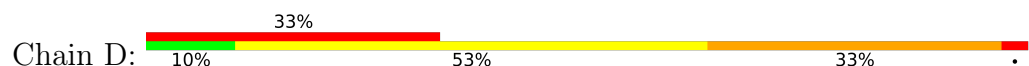
• Molecule 3: 50S ribosomal protein L25

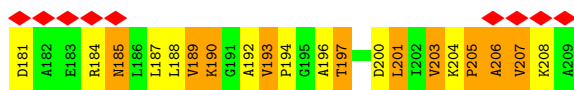


• Molecule 4: 50S ribosomal protein L2

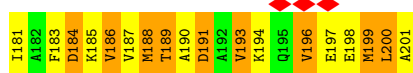
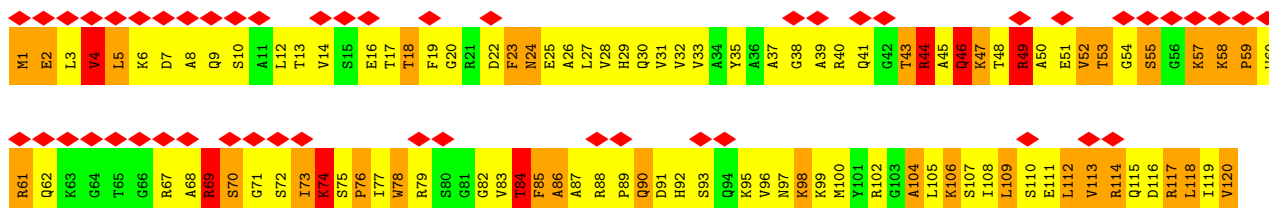
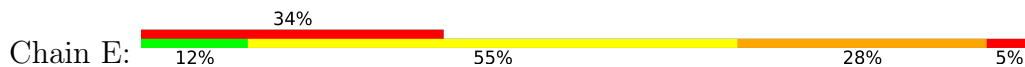


• Molecule 5: 50S ribosomal protein L3

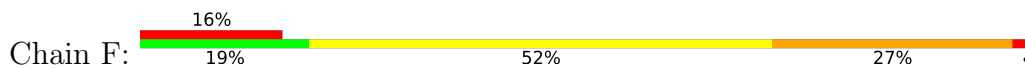




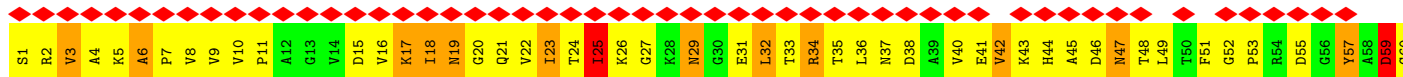
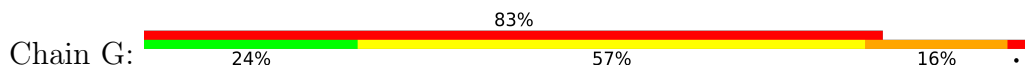
• Molecule 6: 50S ribosomal protein L4



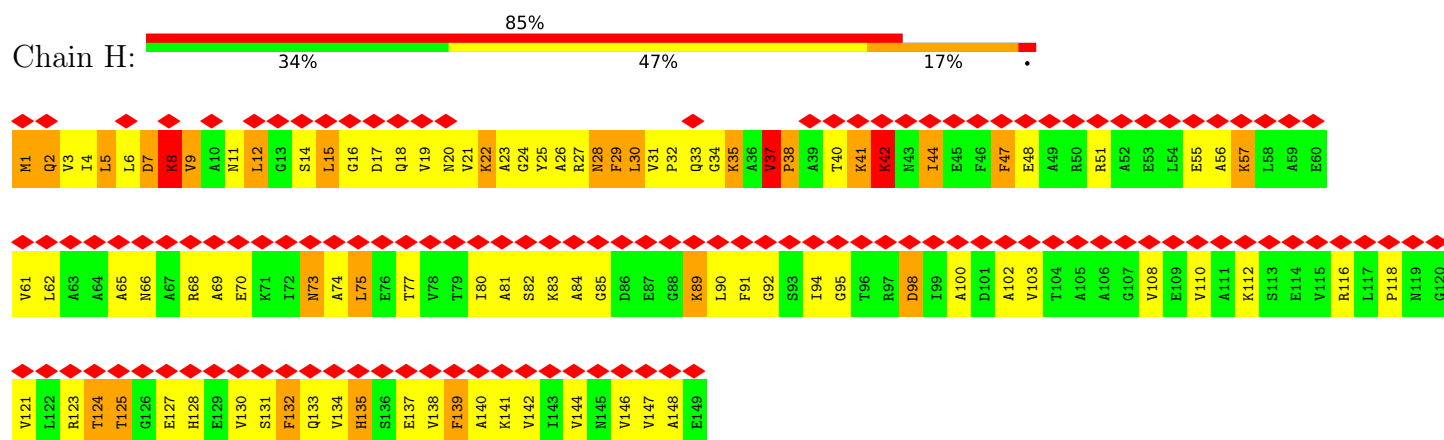
• Molecule 7: 50S ribosomal protein L5



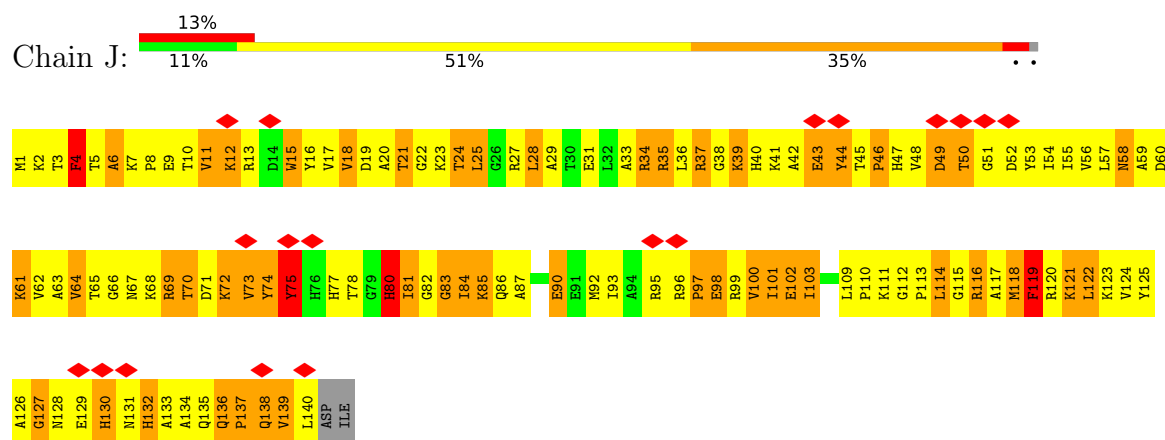
• Molecule 8: 50S ribosomal protein L6



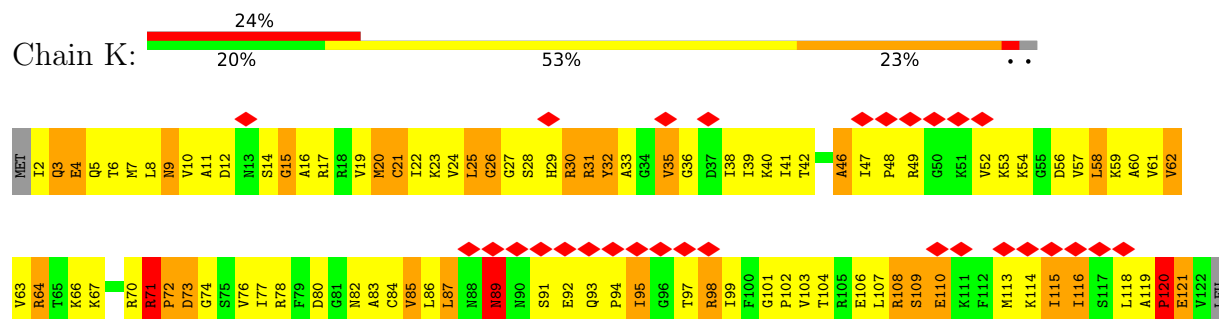
- Molecule 9: 50S ribosomal protein L9



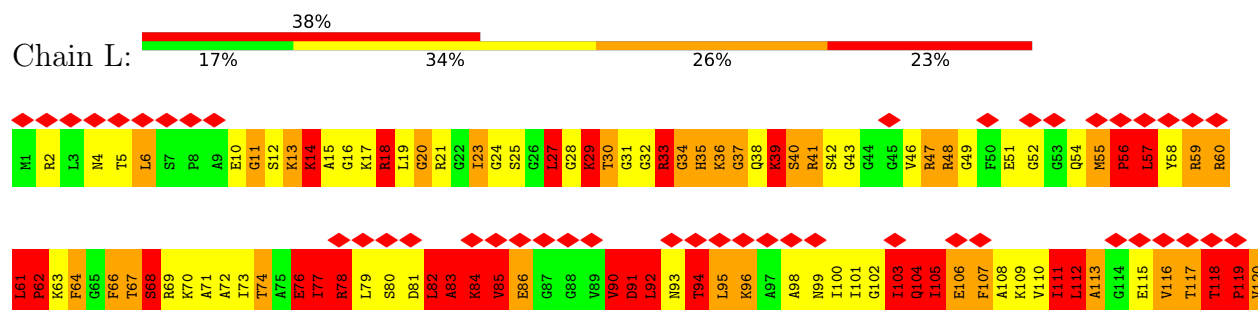
- Molecule 10: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L14

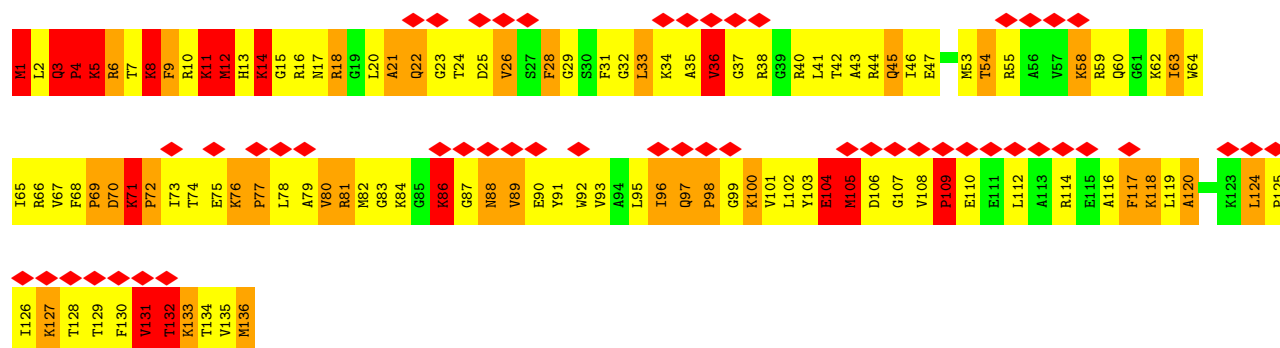
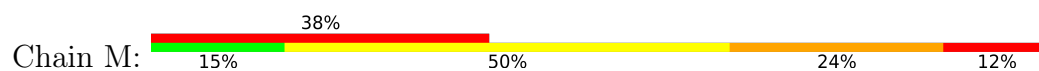


- Molecule 12: 50S ribosomal protein L15

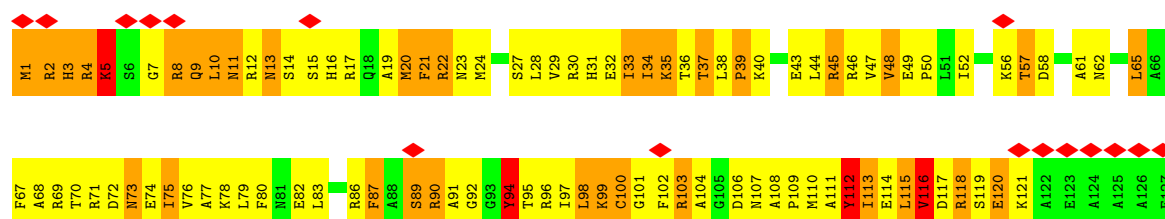
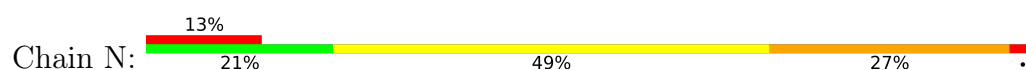




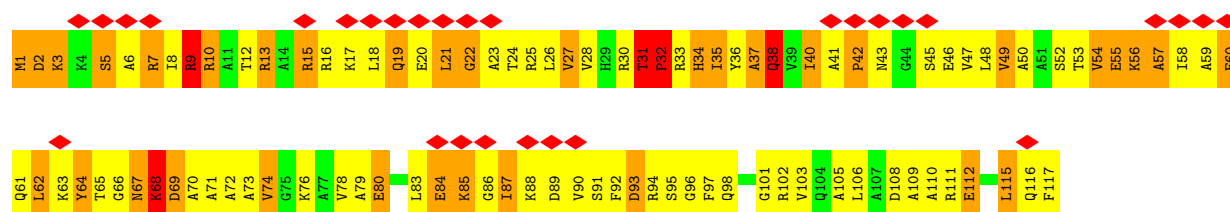
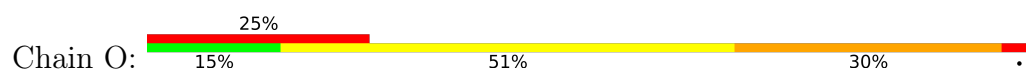
• Molecule 13: 50S ribosomal protein L16



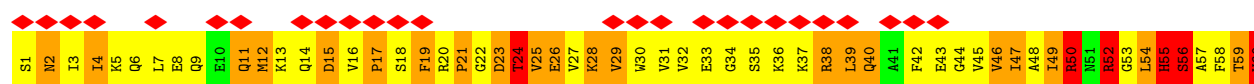
• Molecule 14: 50S ribosomal protein L17

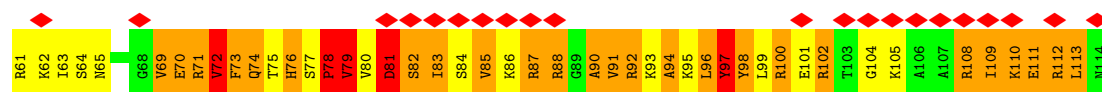


• Molecule 15: 50S ribosomal protein L18

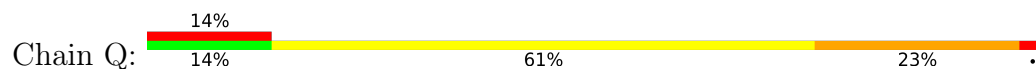


• Molecule 16: 50S ribosomal protein L19

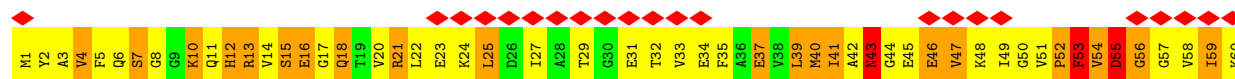
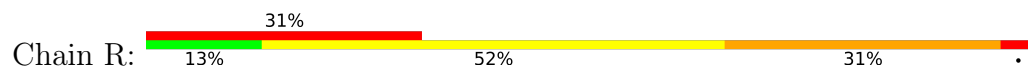




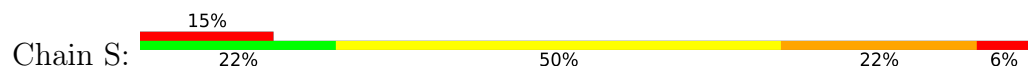
• Molecule 17: 50S ribosomal protein L20



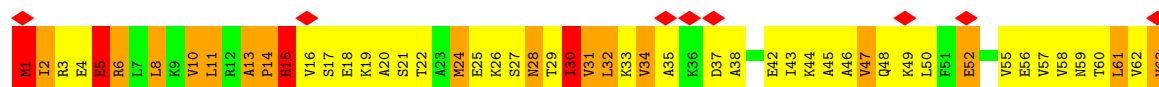
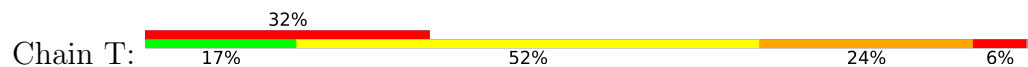
• Molecule 18: 50S ribosomal protein L21



• Molecule 19: 50S ribosomal protein L22

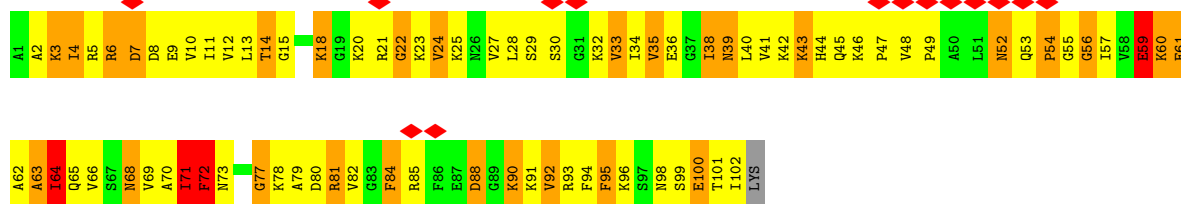
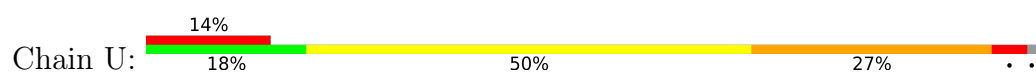


• Molecule 20: 50S ribosomal protein L23

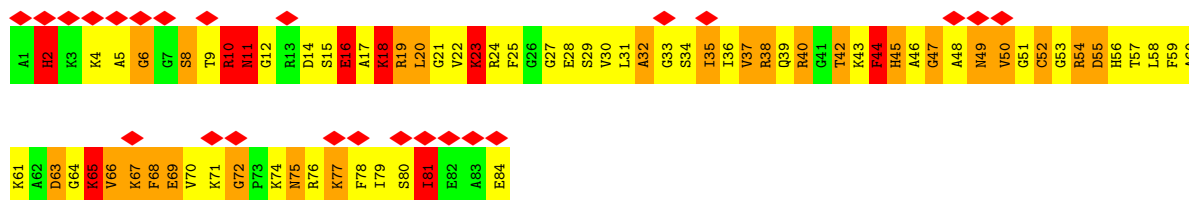
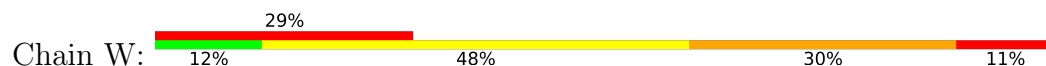


• Molecule 21: 50S ribosomal protein L24

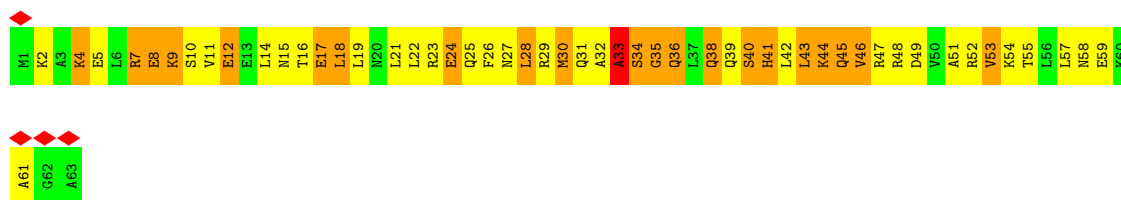
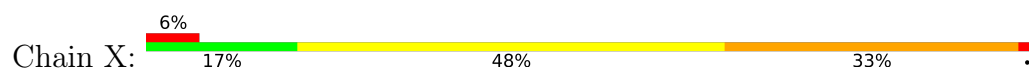




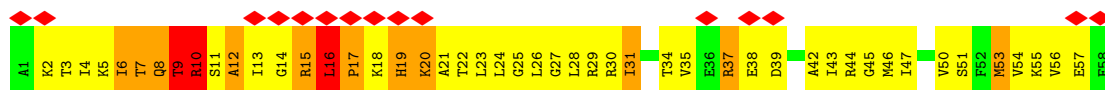
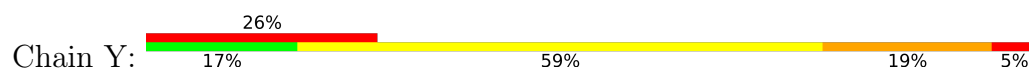
- Molecule 22: 50S ribosomal protein L27



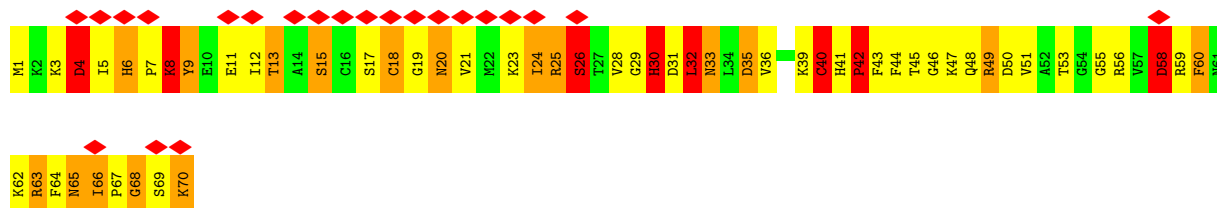
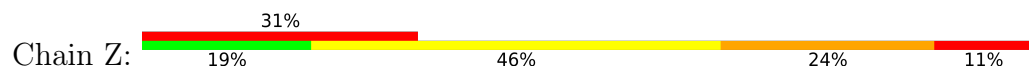
- Molecule 23: 50S ribosomal protein L29



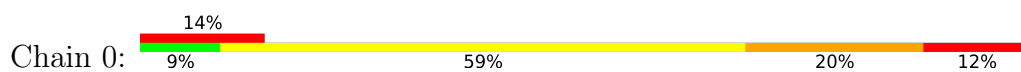
- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L31



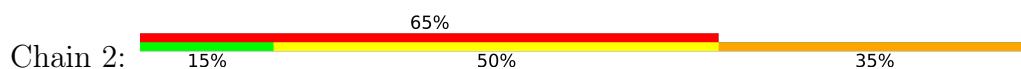
- Molecule 26: 50S ribosomal protein L32



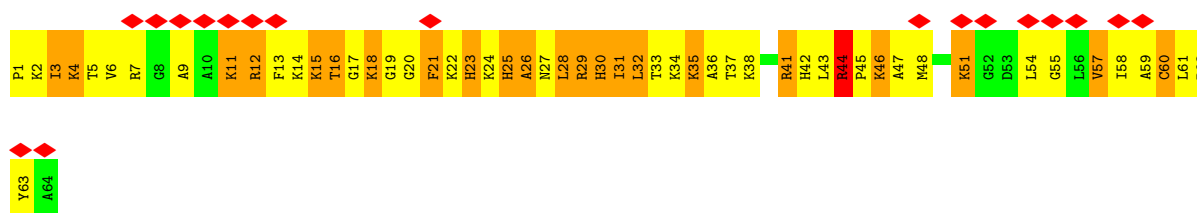
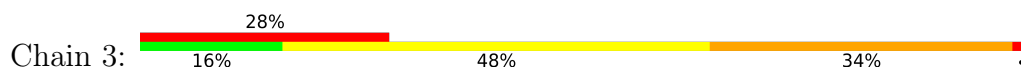
- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	CTF correction of each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	3.5	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	9.232	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.265	Depositor
Map value standard deviation	0.975	Depositor
Recommended contour level	2.48	Depositor
Map size ( $\text{\AA}$ )	325.12, 325.12, 325.12	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ( $^\circ$ )	90, 90, 90	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.54, 2.54, 2.54	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.29	0/2801	0.75	0/4363
2	B	0.45	23/68281 (0.0%)	0.93	94/106437 (0.1%)
3	V	0.31	0/766	0.53	0/1025
4	C	0.40	0/2092	0.88	7/2813 (0.2%)
5	D	0.40	0/1586	0.80	2/2134 (0.1%)
6	E	0.45	1/1571 (0.1%)	0.88	6/2113 (0.3%)
7	F	0.34	0/1444	0.87	5/1937 (0.3%)
8	G	0.31	0/1343	0.70	0/1816
9	H	1.99	0/1121	0.83	1/1512 (0.1%)
10	J	0.41	1/1135 (0.1%)	0.72	3/1529 (0.2%)
11	K	0.35	0/939	1.00	2/1258 (0.2%)
12	L	0.70	0/1062	1.60	30/1413 (2.1%)
13	M	0.48	0/1093	1.03	8/1460 (0.5%)
14	N	0.38	0/1021	0.92	7/1364 (0.5%)
15	O	0.30	0/910	0.67	0/1219
16	P	0.55	0/929	1.40	16/1242 (1.3%)
17	Q	0.41	0/960	0.86	2/1278 (0.2%)
18	R	1.06	6/829 (0.7%)	1.42	14/1107 (1.3%)
19	S	0.28	0/864	0.69	1/1156 (0.1%)
20	T	0.39	0/784	0.78	4/1048 (0.4%)
21	U	0.33	0/787	0.74	0/1051
22	W	0.37	0/642	0.96	5/848 (0.6%)
23	X	0.30	0/510	0.80	1/677 (0.1%)
24	Y	0.31	0/453	0.64	0/605
25	Z	0.48	0/559	1.04	5/745 (0.7%)
26	0	0.53	1/450 (0.2%)	1.15	7/599 (1.2%)
27	1	0.36	0/448	0.71	0/594
28	2	0.33	0/380	0.64	0/498
29	3	0.48	0/513	0.96	1/676 (0.1%)
30	4	0.40	0/303	0.73	0/397
All	All	0.49	32/96576 (0.0%)	0.92	221/144914 (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
2	B	0	61
4	C	0	3
10	J	0	2
12	L	0	1
16	P	0	1
17	Q	0	1
18	R	0	1
All	All	0	70

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2789	C	O3'-P	44.85	2.15	1.61
2	B	2390	U	O3'-P	-27.39	1.28	1.61
2	B	2626	C	O3'-P	23.56	1.89	1.61
2	B	2582	G	O3'-P	21.37	1.86	1.61
2	B	1417	C	O3'-P	-19.51	1.37	1.61

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1250	G	P-O3'-C3'	-66.83	39.50	119.70
2	B	2582	G	P-O3'-C3'	-54.08	54.80	119.70
2	B	1250	G	O3'-P-O5'	-47.15	14.41	104.00
2	B	1417	C	O3'-P-O5'	-41.83	24.52	104.00
2	B	1580	A	O3'-P-O5'	-38.06	31.68	104.00

There are no chirality outliers.

5 of 70 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	136	G	Sidechain
2	B	139	U	Sidechain
2	B	142	A	Sidechain
2	B	143	C	Sidechain
2	B	51	G	Sidechain

## 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	A	2507	0	1261	547	0
2	B	61056	0	30280	9648	0
3	V	753	0	777	235	0
4	C	2053	0	2111	760	0
5	D	1565	0	1597	807	0
6	E	1552	0	1611	578	0
7	F	1420	0	1451	471	0
8	G	1323	0	1367	217	0
9	H	1111	0	1146	140	0
10	J	1112	0	1141	313	0
11	K	930	0	997	291	0
12	L	1053	0	1114	673	0
13	M	1074	0	1136	507	0
14	N	1008	0	1040	285	0
15	O	900	0	927	259	0
16	P	917	0	958	316	0
17	Q	947	0	1016	425	0
18	R	816	0	830	336	0
19	S	857	0	915	293	0
20	T	777	0	832	278	0
21	U	779	0	832	210	0
22	W	634	0	654	294	0
23	X	509	0	528	238	0
24	Y	449	0	487	170	0
25	Z	549	0	546	175	0
26	0	444	0	444	324	0
27	1	441	0	485	153	0
28	2	377	0	408	327	0
29	3	504	0	563	259	0
30	4	302	0	336	147	0
31	2	3	0	0	0	0
31	B	92	0	0	0	0
31	C	1	0	0	0	0
31	E	3	0	0	0	0
31	L	4	0	0	0	0
31	Q	2	0	0	0	0
31	S	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	T	2	0	0	0	0
31	U	1	0	0	0	0
32	2	11	0	0	8	0
32	B	443	0	0	273	0
32	C	1	0	0	1	0
32	D	1	0	0	0	0
32	E	18	0	0	5	0
32	L	8	0	0	7	0
32	Q	7	0	0	2	0
32	S	7	0	0	0	0
32	T	5	0	0	16	0
32	U	5	0	0	6	0
All	All	89335	0	57790	14330	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 98.

The worst 5 of 14330 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)
2:B:1417:C:C5	2:B:1418:G:C5	1.77	1.72
2:B:827:U:P	2:B:2446:G:H5'	1.30	1.69
2:B:5:A:C2	2:B:2899:A:C5	1.79	1.68
1:A:57:A:C4	7:F:12:VAL:HG13	1.19	1.68
2:B:2848:G:C8	16:P:96:LEU:HD23	1.24	1.67

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	V	92/94 (98%)	62 (67%)	21 (23%)	9 (10%)	0	10
4	C	265/273 (97%)	103 (39%)	82 (31%)	80 (30%)	0	0
5	D	207/209 (99%)	90 (44%)	69 (33%)	48 (23%)	0	1
6	E	199/201 (99%)	99 (50%)	60 (30%)	40 (20%)	0	2
7	F	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	2
8	G	174/176 (99%)	118 (68%)	39 (22%)	17 (10%)	0	10
9	H	145/149 (97%)	86 (59%)	43 (30%)	16 (11%)	0	7
10	J	138/142 (97%)	69 (50%)	40 (29%)	29 (21%)	0	2
11	K	119/123 (97%)	71 (60%)	32 (27%)	16 (13%)	0	5
12	L	142/144 (99%)	60 (42%)	40 (28%)	42 (30%)	0	0
13	M	134/136 (98%)	69 (52%)	37 (28%)	28 (21%)	0	2
14	N	125/127 (98%)	73 (58%)	35 (28%)	17 (14%)	0	4
15	O	115/117 (98%)	64 (56%)	26 (23%)	25 (22%)	0	2
16	P	112/114 (98%)	39 (35%)	36 (32%)	37 (33%)	0	0
17	Q	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	0	8
18	R	101/103 (98%)	44 (44%)	31 (31%)	26 (26%)	0	1
19	S	108/110 (98%)	63 (58%)	27 (25%)	18 (17%)	0	3
20	T	97/100 (97%)	42 (43%)	40 (41%)	15 (16%)	0	3
21	U	100/103 (97%)	33 (33%)	46 (46%)	21 (21%)	0	2
22	W	82/84 (98%)	29 (35%)	26 (32%)	27 (33%)	0	0
23	X	61/63 (97%)	28 (46%)	21 (34%)	12 (20%)	0	2
24	Y	56/58 (97%)	29 (52%)	17 (30%)	10 (18%)	0	3
25	Z	68/70 (97%)	29 (43%)	26 (38%)	13 (19%)	0	2
26	0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	3
27	1	52/54 (96%)	19 (36%)	23 (44%)	10 (19%)	0	2
28	2	44/46 (96%)	23 (52%)	14 (32%)	7 (16%)	0	3
29	3	62/64 (97%)	30 (48%)	25 (40%)	7 (11%)	0	7
30	4	36/38 (95%)	18 (50%)	9 (25%)	9 (25%)	0	1
All	All	3179/3249 (98%)	1596 (50%)	950 (30%)	633 (20%)	0	2

5 of 633 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	21	PRO
4	C	22	GLU
4	C	28	PRO
4	C	29	PHE
4	C	31	PRO

### 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	
3	V	78/78 (100%)	66 (85%)	12 (15%)	2	14
4	C	213/218 (98%)	144 (68%)	69 (32%)	0	2
5	D	164/164 (100%)	112 (68%)	52 (32%)	0	2
6	E	165/165 (100%)	115 (70%)	50 (30%)	0	2
7	F	149/149 (100%)	118 (79%)	31 (21%)	1	6
8	G	137/137 (100%)	105 (77%)	32 (23%)	1	4
9	H	114/114 (100%)	83 (73%)	31 (27%)	0	3
10	J	114/116 (98%)	84 (74%)	30 (26%)	0	3
11	K	102/104 (98%)	78 (76%)	24 (24%)	1	4
12	L	103/103 (100%)	61 (59%)	42 (41%)	0	0
13	M	109/109 (100%)	77 (71%)	32 (29%)	0	2
14	N	103/103 (100%)	78 (76%)	25 (24%)	0	4
15	O	87/87 (100%)	58 (67%)	29 (33%)	0	2
16	P	99/99 (100%)	77 (78%)	22 (22%)	1	6
17	Q	89/89 (100%)	66 (74%)	23 (26%)	0	3
18	R	84/84 (100%)	68 (81%)	16 (19%)	1	8
19	S	93/93 (100%)	72 (77%)	21 (23%)	1	5
20	T	83/84 (99%)	60 (72%)	23 (28%)	0	3
21	U	83/84 (99%)	62 (75%)	21 (25%)	0	3
22	W	62/62 (100%)	46 (74%)	16 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	X	55/55 (100%)	40 (73%)	15 (27%)	0	3
24	Y	48/48 (100%)	36 (75%)	12 (25%)	0	3
25	Z	62/62 (100%)	44 (71%)	18 (29%)	0	2
26	0	47/47 (100%)	31 (66%)	16 (34%)	0	1
27	1	48/48 (100%)	33 (69%)	15 (31%)	0	2
28	2	38/38 (100%)	27 (71%)	11 (29%)	0	2
29	3	51/51 (100%)	33 (65%)	18 (35%)	0	1
30	4	34/34 (100%)	21 (62%)	13 (38%)	0	0
All	All	2614/2625 (100%)	1895 (72%)	719 (28%)	2	3

5 of 719 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	P	38	ARG
21	U	66	VAL
16	P	88	ARG
16	P	24	THR
19	S	3	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	81	ASN
20	T	72	GLN
15	O	67	ASN
17	Q	55	GLN
22	W	2	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	114/120 (95%)	22 (19%)	0
2	B	2805/2904 (96%)	445 (15%)	20 (0%)
All	All	2919/3024 (96%)	467 (15%)	20 (0%)

5 of 467 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	C
1	A	12	C
1	A	13	G
1	A	14	U
1	A	15	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	2258	C
2	B	2390	U
2	B	2756	U
2	B	2425	A
2	B	1205	A

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 110 ligands modelled in this entry, 110 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	44
1	A	2
9	H	1

The worst 5 of 47 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2450:A	O3'	2451:A	P	28.22
1	B	2059:A	O3'	2060:A	P	25.69
1	B	1679:A	O3'	1680:U	P	25.40
1	B	1760:C	O3'	1761:C	P	22.71
1	B	2433:A	O3'	2434:A	P	20.69

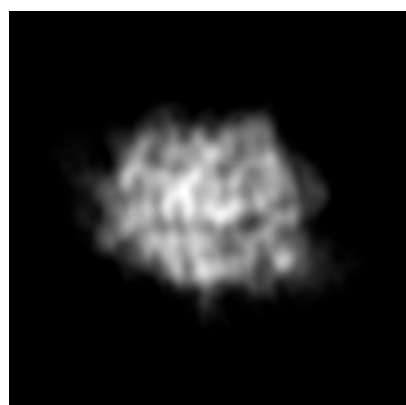
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1455. These allow visual inspection of the internal detail of the map and identification of artifacts.

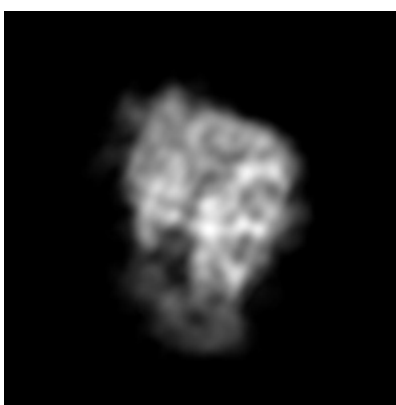
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

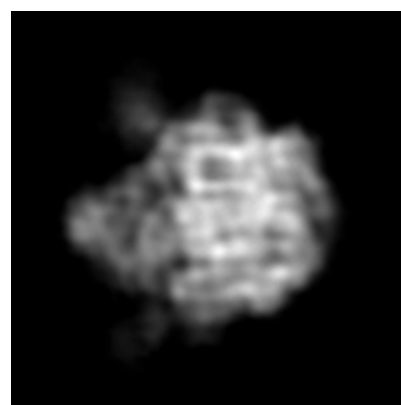
#### 6.1.1 Primary map



X



Y

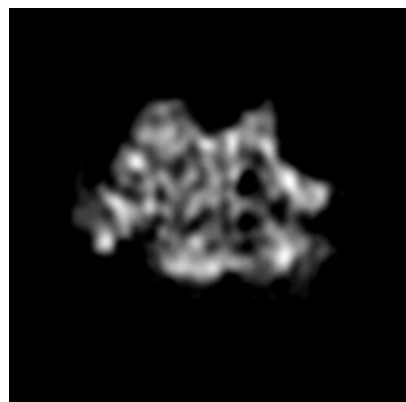


Z

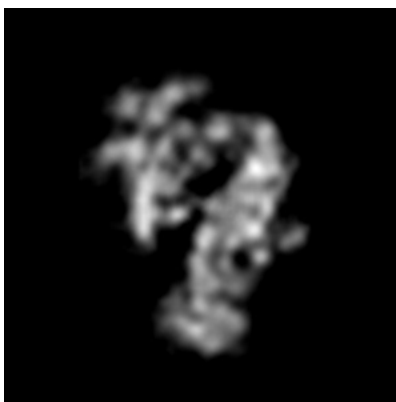
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64

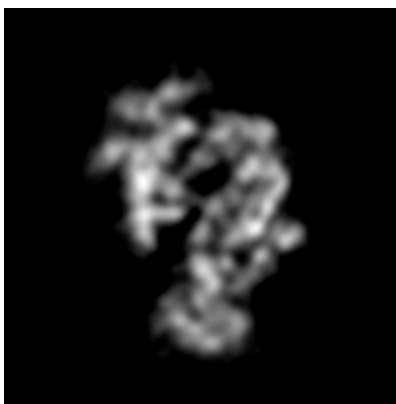
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 58



Y Index: 62

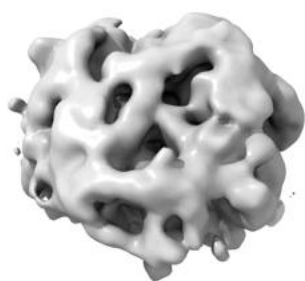


Z Index: 64

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

## 6.4 Orthogonal surface views [i](#)

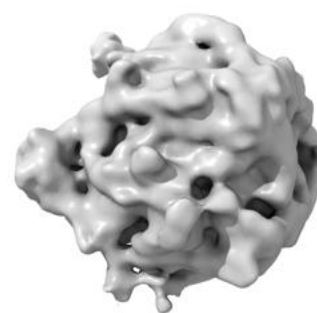
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.48. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

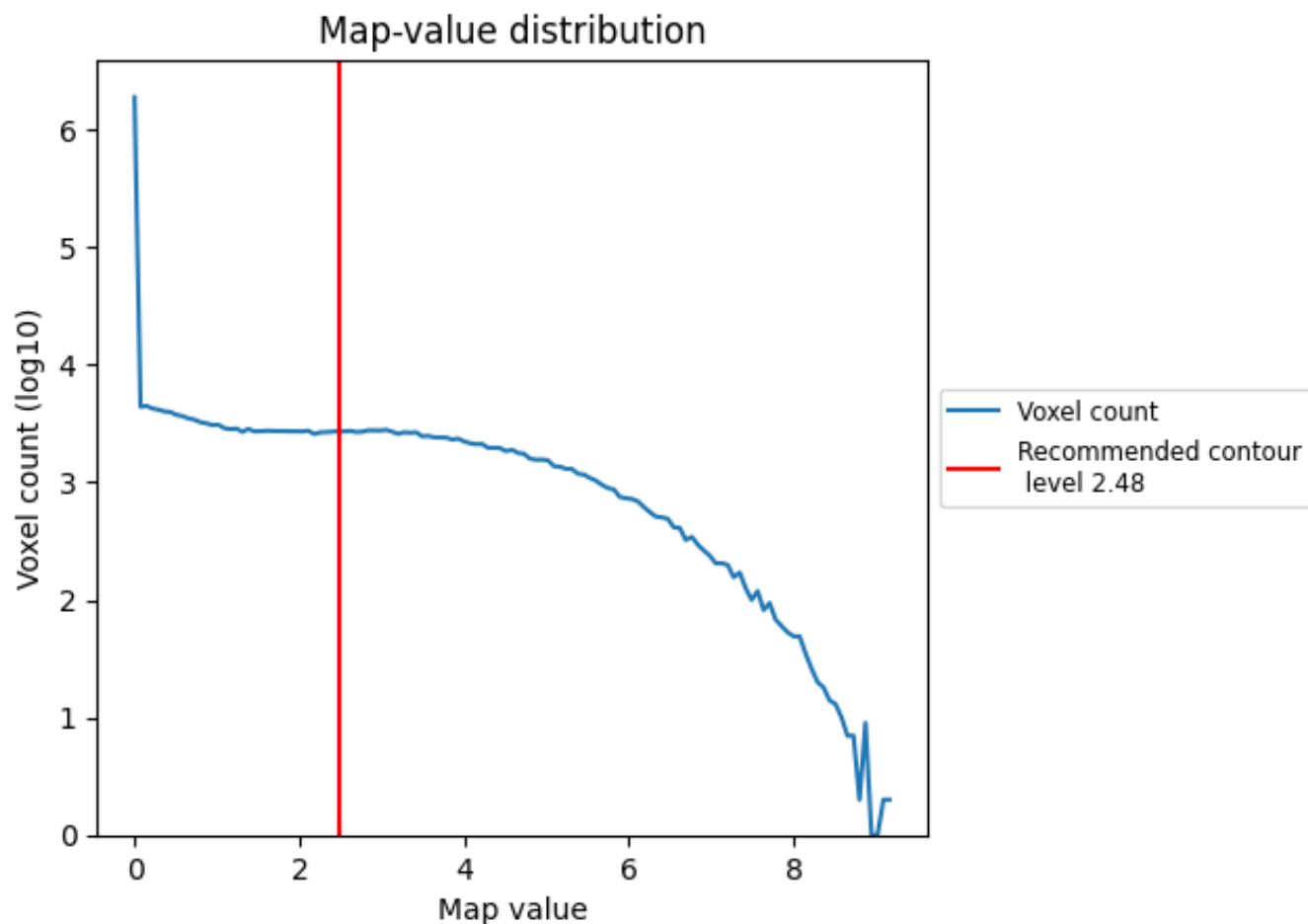
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

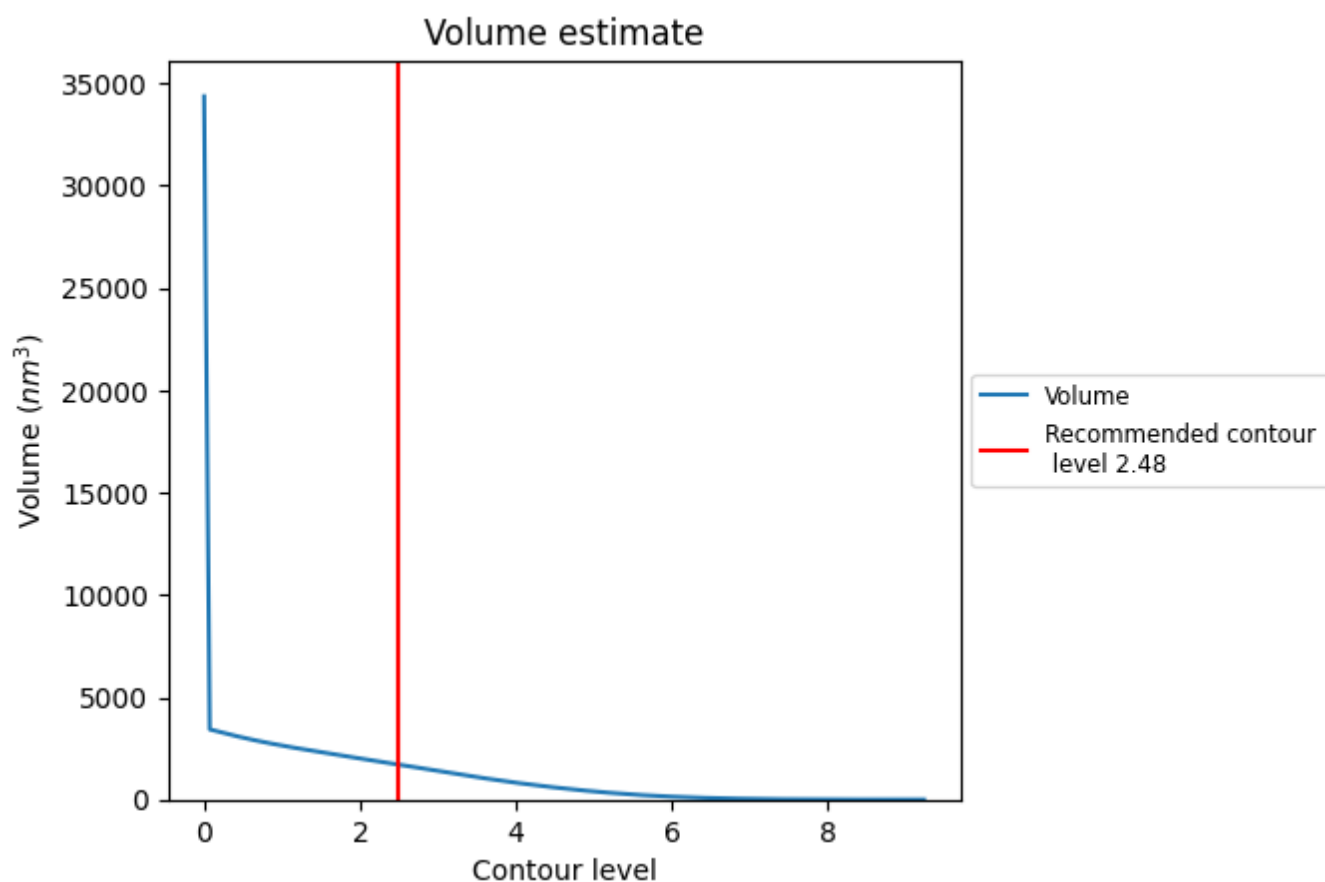
This section contains the results of statistical analysis of the map.

### 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.

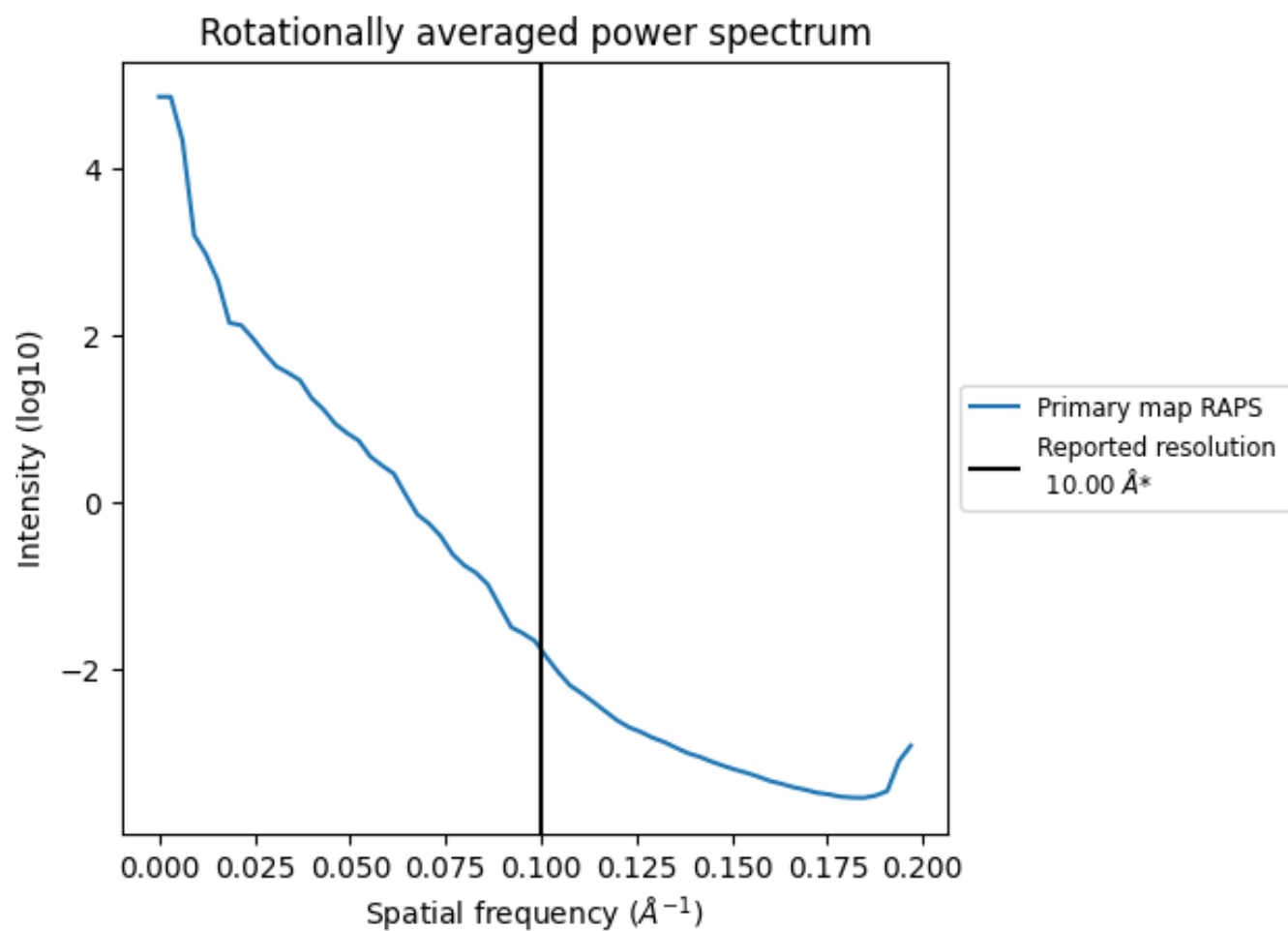
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1718  $\text{nm}^3$ ; this corresponds to an approximate mass of 1552 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 0.100 Å<sup>-1</sup>

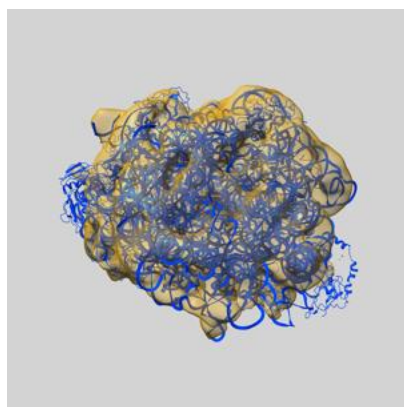
## 8 Fourier-Shell correlation

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

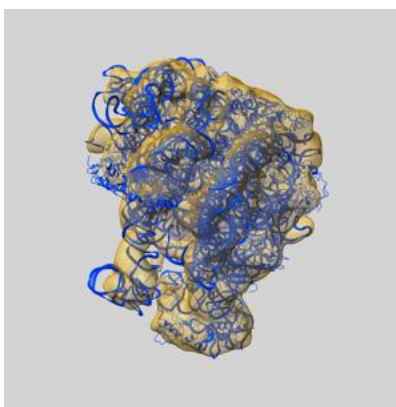
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1455 and PDB model 3BBX. Per-residue inclusion information can be found in section 3 on page 10.

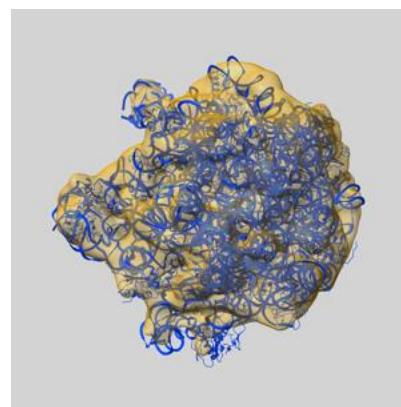
### 9.1 Map-model overlay [i](#)



X



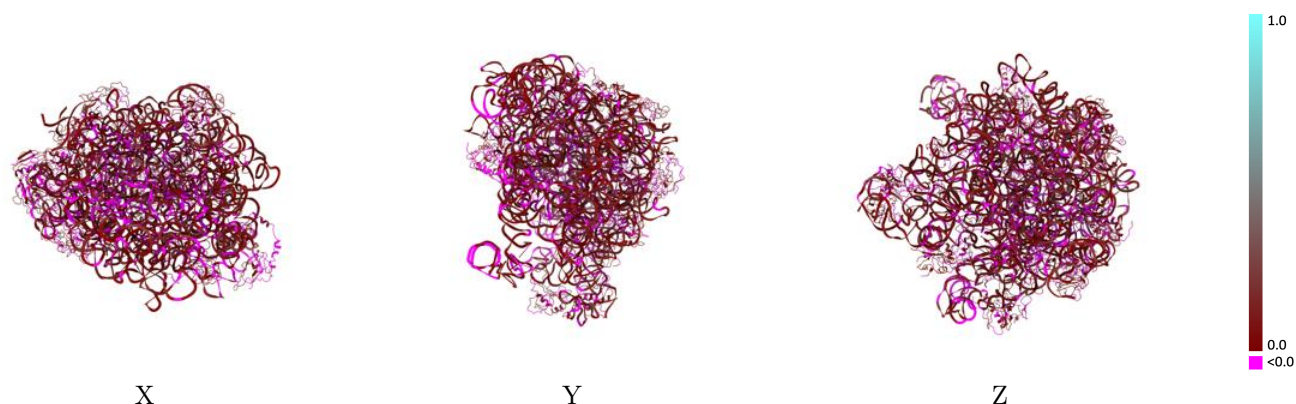
Y



Z

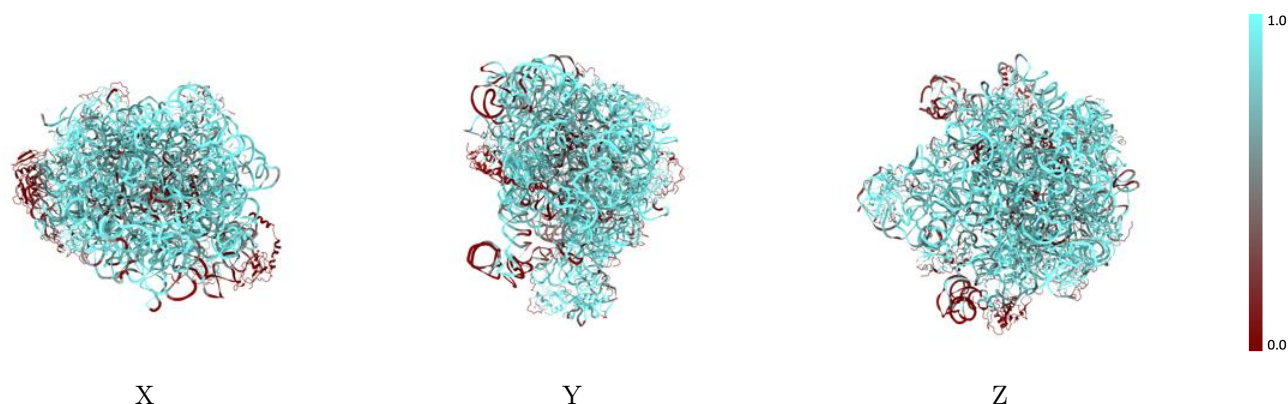
The images above show the 3D surface view of the map at the recommended contour level 2.48 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



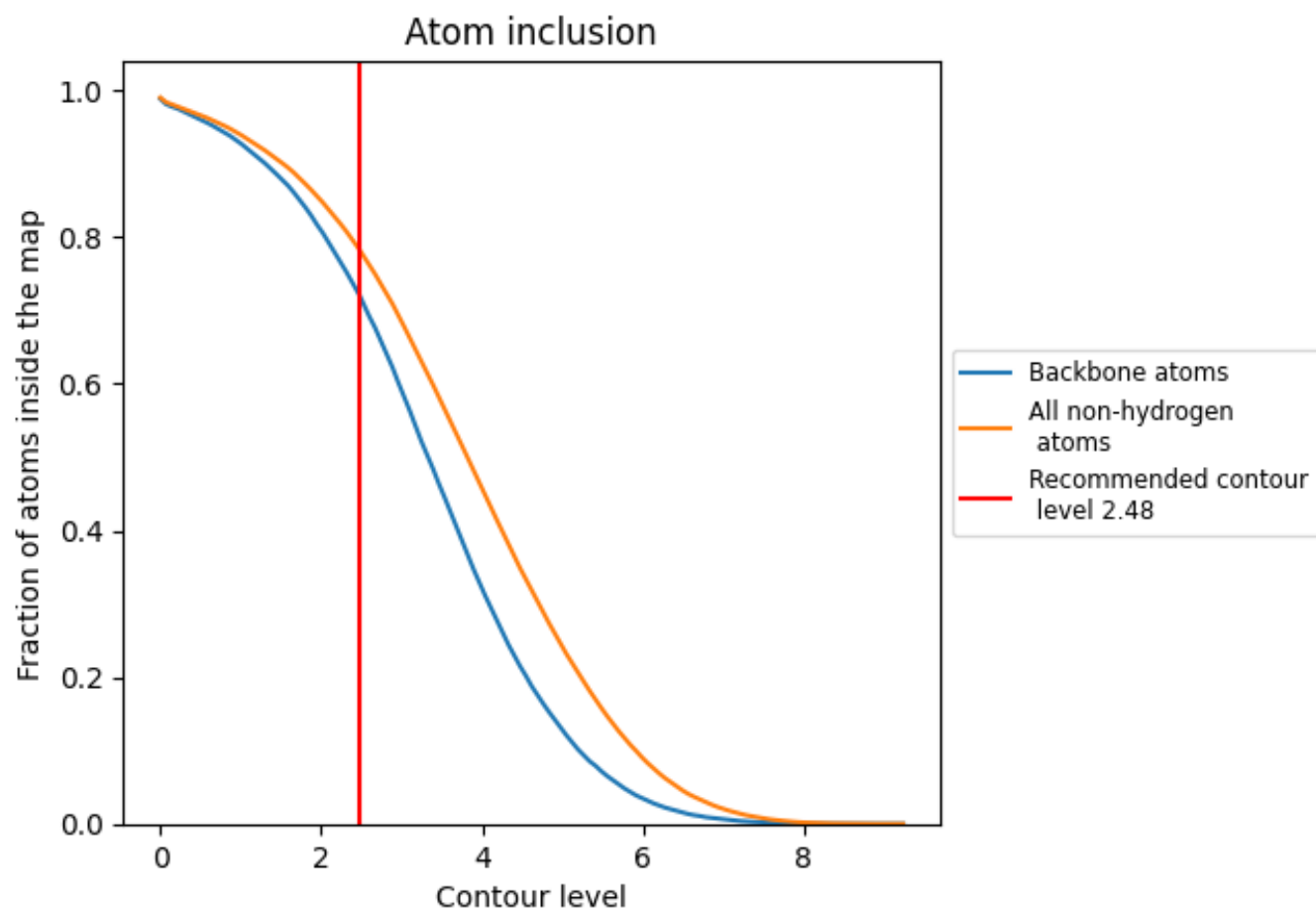
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.48).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 78% 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 (2.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7823	 0.0610
0	 0.8388	 0.0380
1	 0.3972	 -0.0230
2	 0.3575	 -0.0240
3	 0.6843	 -0.0280
4	 0.5445	 0.0040
A	 0.8285	 0.0870
B	 0.8389	 0.0740
C	 0.6920	 0.0250
D	 0.6229	 0.0220
E	 0.6376	 0.0220
F	 0.7802	 0.0580
G	 0.1511	 0.0540
H	 0.1542	 -0.0000
J	 0.8190	 0.0210
K	 0.7138	 0.0500
L	 0.5642	 0.0080
M	 0.6065	 0.0190
N	 0.8371	 0.0000
O	 0.7394	 0.0250
P	 0.5541	 0.0180
Q	 0.8341	 0.0240
R	 0.6550	 0.0470
S	 0.8103	 0.0580
T	 0.6579	 0.0050
U	 0.8008	 0.0630
V	 0.5894	 0.0760
W	 0.6926	 0.0300
X	 0.8873	 0.0530
Y	 0.7094	 0.0470
Z	 0.6468	 0.0080

