



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:29 PM GMT

PDB ID : 1FFK  
Title : CRYSTAL STRUCTURE OF THE LARGE RIBOSOMAL SUBUNIT FROM HALOARCUA MARISMORTUI AT 2.4 ANGSTROM RESOLUTION  
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Deposited on : 2000-07-25  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

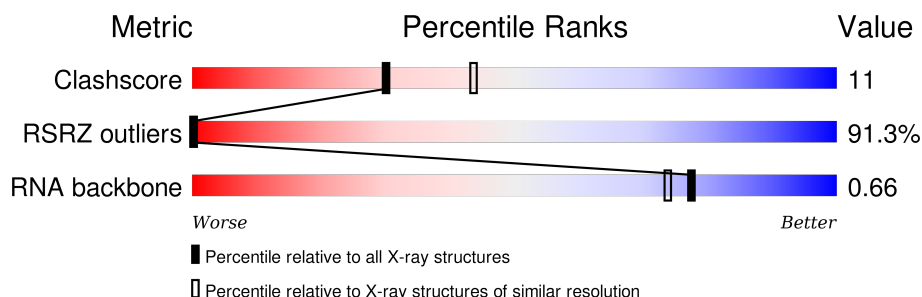
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)
RNA backbone	2183	1073 (2.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>74%</div> <div> <div>49%</div> <div>34%</div> <div>8%</div> <div>7%</div> </div> </div>
2	9	122	<div> <div>93%</div> <div> <div>43%</div> <div>43%</div> <div>11%</div> </div> </div>
3	A	239	<div> <div>99%</div> <div>98%</div> </div>
4	B	337	<div> <div>99%</div> <div>99%</div> </div>
5	C	246	<div> <div>100%</div> <div>100%</div> </div>
6	D	176	<div> <div>79%</div> <div>80%</div> <div>20%</div> </div>
7	E	119	<div> <div>97%</div> <div>97%</div> </div>
8	F	157	<div> <div>100%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
9	G	145	98% 
10	H	132	100% 
11	I	194	100% 
12	J	164	87% 
13	K	186	100% 
14	L	115	100% 
15	M	148	97% 
16	N	95	100% 
17	O	154	97% 
18	P	84	93% 
19	Q	119	100% 
20	R	66	80% 
21	S	70	93% 
22	T	154	100% 
23	U	91	93% 
24	V	143	99% 
25	W	73	100% 
26	X	56	100% 
27	Y	49	63% 
28	Z	92	100% 
29	1	177	97% 

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 64281 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	0	2706	Total	C	N	O	P	0	0	0
			58012	25885	10685	18737	2705			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	A	237	Total	C	0	0	237
			237	237			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	B	337	Total	C	0	0	337
			337	337			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	DELETION	UNP P20279
B	311	PHE	-	INSERTION	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	C	246	Total C 246 246	0	0	246

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	D	140	Total C 140 140	0	0	140

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	E	118	Total C 118 118	0	0	118

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	108	LEU	-	INSERTION	UNP P12743
E	109	GLU	-	INSERTION	UNP P12743
E	110	GLU	-	INSERTION	UNP P12743

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	F	157	Total C 157 157	0	0	157

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	G	142	Total C 142 142	0	0	142

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	H	132	Total C 132 132	0	0	132

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	I	194	Total C 194 194	0	0	194

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	J	143	Total C 143 143	0	0	143

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	K	186	Total C 186 186	0	0	186

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	186	LEU	-	INSERTION	UNP P14123

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	L	115	Total C 115 115	0	0	115

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	M	143	Total C 143 143	0	0	143

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	N	95	Total C 95 95	0	0	95

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	O	150	Total C 150 150	0	0	150

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	P	78	Total C 78 78	0	0	78

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	Q	119	Total C 119 119	0	0	119

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	R	53	Total C 53 53	0	0	53

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	65	Total C 65 65	0	0	65

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	T	154	Total C 154 154	0	0	154

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	85	Total C 85 85	0	0	85

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	V	143	Total C 143 143	0	0	143

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	109	ASN	ALA	CONFLICT	UNP P12736

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	W	73	Total C 73 73	0	0	73

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	X	56	Total C 56 56	0	0	56

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Y	31	Total C 31 31	0	0	31

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	11	LYS	LEU	CONFLICT	UNP P22452
Y	24	TYR	TRP	CONFLICT	UNP P22452
Y	42	TRP	TYR	CONFLICT	UNP P22452

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L44E.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	Z	92	Total C 92 92	0	0	92

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	1	172	Total C 172 172	0	0	172

- Molecule 30 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	1	Total Cd 1 1	0	0
30	W	1	Total Cd 1 1	0	0
30	R	1	Total Cd 1 1	0	0
30	Z	1	Total Cd 1 1	0	0

- Molecule 31 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	0	1	Total K 1 1	0	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	2	Total Mg 2 2	0	0

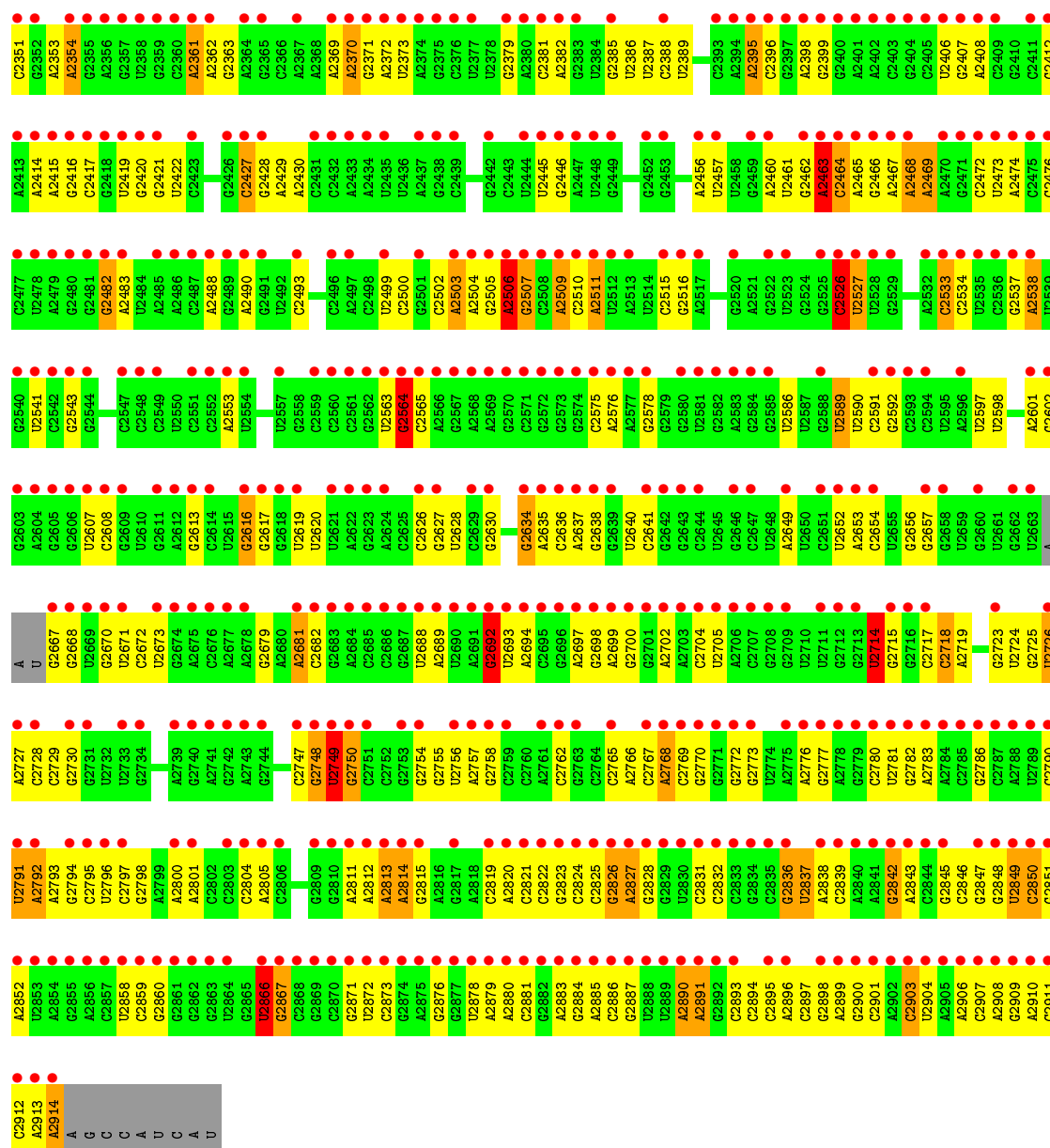
- Molecule 33 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	6	Total O 6 6	0	0

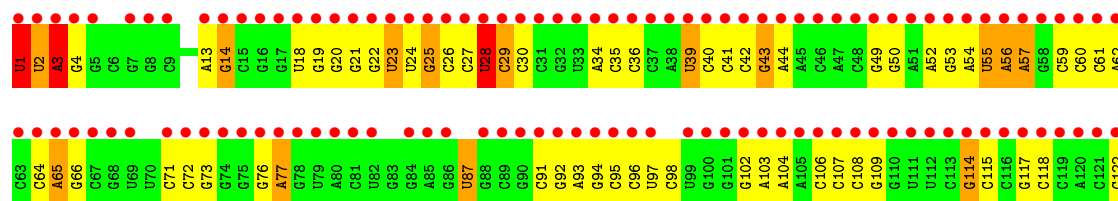


G1421	A1355	A1294	A1232	G1112	G1049	G	A926	A746	A686	U626
U1422	A1356	G1295	A1236	G1113	G1050	A	A929	G747	G687	G627
C1423	A1357	A1296	U1237	U1114	G1051	G	A930	C748	A688	A628
A1424	U1297	U1297	U1237	U1115	G1052	U	G931	G749	G689	G629
G1425	U1298	C1238	G1239	U1116	G1053	C	C932	A750	G690	A630
A1426	G1299	A1239	G1239	U1117	G1054	C	C933	A751	G691	A631
A1427	G1300	G1240	G1240	U1118	G1055	G	C934	G752	A692	A632
G1430	U1301	G1241	G1241	U1119	U1056	C	G935	U753	C633	C633
G1433	U1304	A1242	A1242	U1120	U1057	A	C936	G754	A693	C634
A1434	U1305	C1243	C1243	G1121	A1058	C	G937	G755	A694	A635
A1437	U1306	U1244	U1244	U1122	G1059	A	G938	G756	C695	A636
G1439	U1307	C1245	C1245	A1123	C1060	C	A939	G757	G697	C637
G1440	A1307	A1246	A1246	C1124	C1061	C	G940	A758	A698	C638
G1442	U1308	A1247	A1247	U1125	U1062	U	G941	C759	C699	A639
G1443	U1309	A1248	A1248	C1126	U1063	C	U942	G760	A700	G640
G1444	U1310	U1249	U1249	U1127	U1064	U	A943	A761	U701	G641
G1445	G1311	C1250	C1250	U1128	G1065	A	G944	C762	G702	G642
G1446	G1312	C1251	C1251	U1129	U1066	A	U945	G763	G703	A643
G1447	A1313	A1252	A1252	G1130	A1067	A	C946	C764	C704	G644
G1448	U1314	C1253	C1253	G1131	C1068	G	U947	G765	G705	U645
G1449	U1315	A1254	A1254	A1132	G1069	A	A948	A766	G706	G646
G1450	G1316	A1255	A1255	A1133	A1070	A	U949	A767	C707	U647
G1451	A1317	C1256	C1256	G1134	G1071	A	G950	U768	A708	G648
G1452	A1318	G1257	G1257	A1072	A1072	G	A951	C769	G709	U649
G1453	G1319	C1258	C1258	U1135	A1073	C	G952	G770	G710	C650
G1454	U1320	A1259	A1259	G1137	G1074	G	G953	G771	G711	U651
G1455	A1321	G1260	G1260	U1138	G1075	A	U954	G772	G712	G652
G1456	G1322	A1261	A1261	U1139	A1076	U	A955	A773	C713	C653
G1457	G1323	C1262	C1262	A1140	U1016	A	G956	G774	U714	A654
G1458	G1324	C1263	C1263	U1141	U1017	C	U957	G775	U	U655
G1459	A1325	U1264	U1264	C1142	A1081	G	G958	A776	G716	G656
G1460	U1326	G1265	G1265	G1143	A1082	A	C959	U777	C717	G657
G1461	G1327	U1266	U1266	A1144	A1083	C	G960	G778	C718	C658
G1462	A1328	C1267	C1267	G1145	C1084	U	A961	U779	C719	A659
G1463	G1329	A1268	A1268	C1146	C1084	U	G962	A780	G720	A660
G1464	U1330	U1269	U1269	G1147	G1087	A	C963	C781	A721	G661
G1465	A1331	A1270	A1270	U1148	A1088	C	G964	G782	G722	U662
G1466	G1332	U1271	U1271	U1149	G1089	A	A965	C783	G723	C663
G1467	U1333	C1272	C1272	A1150	A1090	C	U966	A784	G724	U664
G1468	G1334	G1273	G1273	G1151	U1091	A	G967	U785	C725	A665
G1469	U1335	A1274	A1274	C1152	A1092	C	G968	G786	G726	A666
G1470	C1336	C1275	C1275	U1153	G1093	U	U969	G787	G727	C667
G1471	A1337	U1276	U1276	A1154	G1094	A	U970	A788	G728	C668
G1472	U1338	C1277	C1277	G1155	U1095	C	U	C729	G729	G669
G1473	G1339	A1278	A1278	C1156	U1096	C	U	A790	G730	G670
G1474	U1340	U1279	U1279	G1157	A1097	C	U	A791	U731	A671
G1475	A1341	A1280	A1280	U1158	A1098	C	U	G792	C732	U672
G1476	C1342	C1281	C1281	G1159	G1099	C	U	A793	U733	U673
G1477	G1343	U1282	U1282	U1160	G1100	C	C	G794	U734	A674
G1478	A1344	G1283	G1283	A	U101	C	C	G795	C735	U675
G1479	U1345	A1284	A1284	G1160	C1102	C	U	A796	A736	C676
G1480	G1346	U1285	U1285	G	C1103	C	U	A797	A737	C677
G1481	U1347	A1286	A1286	U	A1040	C	U	G798	U738	G678
G1482	A1348	U1287	U1287	G	C1104	C	U	G799	G739	G679
G1483	G1349	A1288	A1288	C1105	U1042	C	C	G800	G740	G680
G1484	U1350	C1289	C1289	A	C1043	C	C	A801	C741	G681
G1485	G1351	U1290	U1290	A1107	A1044	C	G	G802	G742	A682
G1486	A1352	A1291	A1291	G1108	G1045	A	A	C803	G743	G683
G1487	U1353	G1292	G1292	U1109	U1046	C	G	G804	G744	G684
G1488	C1354	A1293	A1293	U	G1048	C	G	G805	G745	C685

G2287	C	U	G	C2104	U2042	G1979	H1918	A1857	G1795	A1733	U1671	G1610	G1546	G1484
G2288	C	C	A	C2105	U2043	U1960	A1919	A1858	A1796	C1734	G1672	G1611	A1947	A1485
G2289	G	G	G	C2106	G2044	A1981	A1920	A1859	A1797	C1735	U1673	A1612	A1947	
U2290	G	A	A	U2107	G2045	U1982	A1921	U1860	C1798	A1736		G1613	U1488	
A2291	U	C	C	A2108	G2046	C1983	G1923	C1862	G1799	A1737	U1676	G1614	C1551	G1489
C2292	G	A	A	U2109	C2047		G1924	G1863	G1800	C1738	U1677	A1615	C1552	G1490
G2293	C	C	C	G2110			A1925	C1864	A1801	G1739	U1678	A1616	C1553	C1491
G2294	C	U	U	G2111	G2050		G1926	C1865	G1802	C1679	U1679	C1617	U1564	A1492
U2297	C	U	A	A2112	G2051		A1927	A1866	A1804	C1740	C1680	G1618	C1555	A1493
A2300	C	C	A	C2113	U2052		G1928	G1867	A1806	C1742	A1681	C1620	C1556	A1494
A2301	C	C	C	C2114	G2053		G1929	G1868	G1806	G1743	A1682	G1621	C1557	C1495
A2302	C	C	C	U2115	A2054		A1930	A1869	U1807	G1744	A1683	G1622	C1558	G1496
A2303	C	C	C	U2116	A2055		A1931	A1870	C1806	A1746	A1685	G1623	U	G1497
A2304	C	C	C	U2117	C2056		G1932							G1498
A2305	C	C	C	C2118	U2057		G1933	G1873	C1809	C1750	C1686	U1624	U1561	
G2309	C	C	C	C2119	G2058		A1934	U1874	C1810	C1687	U1562	U1625	A1501	
G2310	C	C	C	U2120	U2059		A1935	A1875	A1811	G1751	C1563	A1626	A1502	
G2311	C	C	C	G2121	A1997		G1936	C1876	G1812	C1752	C1564	G1627	U1503	
G2312	C	C	C	G2122	A1998		C1937	G1877	A1815	C1753	C1565	G1628	U1504	
G2313	C	C	C	U2123	G2060		U1938	G1878	A1816	A1754	C1566	G1629	U1505	
G2314	C	C	C	C2124	U2061		G1939	U1879	C1817	A1756	A1567	A1631	U1506	
G2315	C	C	C	G2125	G2062		C1940	U1880	A1818	C1757	C1568	A1632	C1507	
G2316	C	C	C	U2126	U2063		G1941	A1886	C1824	U1758	U1569	G1633	U1508	
G2317	C	C	C	C2127	C2064		U1939	U1887	U1825	C1763	C1570	G1634	C1509	
G2318	C	C	C	U2128	C2065		A1942	A1888	G1820	A1759	C1571	G1635	G1510	
G2319	C	C	C	U2129	A2066		G1943	A1889	A1821	G1760	A1572	U1636	U1511	
G2320	C	C	C	C2130	U2067		G1944	U1890	A1822	C1761	A1573	G1637	G1512	
G2321	C	C	C	U2131	G2068		G1945	A1891	G1823	C1762	C1574	C1575	C1513	
G2322	C	C	C	U2132	U2069		A1946	A1892	A1824	C1763	C1575	C1576	C1514	
G2323	C	C	C	U2133	C2070		G1947	A1893	U1826	C1764	U1577	G1576	C1515	
G2324	C	C	C	U2134	U2071		G1948	U1894	U1827	C1765	U1578	C1577	C1516	
G2325	C	C	C	A2135	G2072		U1949	U1895	G1828	A1766	U1579	C1578	C1517	
G2326	C	C	C	G2136	A2073		G1950	U1896	A1829	C1767	U1580	A1581	C1518	
G2327	C	C	C	A	A2074		G1951	U1897	A1830	C1768	U1581	A1582	U1519	
G2328	C	C	C	C	G2075		U	U1898	U1831	C1769	G1706	A1583	G1520	
G2329	C	C	C	C	G2076		A	U1899	U1832	C1770	G1707	G1584	C1521	
G2330	C	C	C	C	C2077		A	U1900	U1833	C1771	U1585	C1585	U1522	
G2331	C	C	C	C	U2078		C	U1901	U1834	C1772	G1708	C1586	G1523	
G2332	C	C	C	C	A2016		C	U1902	U1835	C1773	A1710	C1587	U1524	
G2333	C	C	C	C	U2017		U	U1903	U1836	C1774	C1650	C1588	G1525	
G2334	C	C	C	C	U2018		A	U1904	U1837	C1775	C1651	U1589	A1526	
G2335	C	C	C	C	A2019		A	U1905	U1838	C1776	C1652	C1590	A1527	
G2336	C	C	C	C	G2080		C	U1906	U1839	C1777	U1654	C1594	A1528	
G2337	C	C	C	C	A2081		C	U1907	A1840	A1778	U1655	A1591	G1529	
G2338	C	C	C	C	U2082		C	U1908	A1841	A1779	G1656	A1592	U1530	
A	C	C	C	C	G2083		U1964	A1842	A1843	C1780	G1717	C1592	U1531	
C	C	C	C	C	A2084		C1965	A1844	A1845	C1781	G1718	C1593	G1532	
A	C	C	C	C	G2085		C1966	A1846	A1847	C1782	G1719	C1594	A1533	
A	C	C	C	C	U2086		U1967	U1848	U1849	A1783	A1659	G1595	C1534	
A	C	C	C	C	G2087		A1968	U1849	A1847	U1784	U1722	G1660	G1535	
A	C	C	C	C	A2088		A1969	A1848	A1847	G1785	G1723	A1661	C1536	
A	C	C	C	C	U2089		G1970	A1849	A1847	C1786	U1724	G1662	C1537	
A	C	C	C	C	G2090		G1971	U1850	U1850	C1787	C1725	G1663	C1538	
A	C	C	C	C	A2091		U1972	U1851	U1851	G1788	A1604	U1539	U1539	
A	C	C	C	C	G2092		A1973	A1852	A1852	G1789	G1605	G1540	G1540	
A	C	C	C	C	U2093		G1974	A1853	A1853	C1790	G1606	G1541	G1541	
A	C	C	C	C	A2100		C1975	C1853	C1853	U1791	A1607	G1542	G1542	
A	C	C	C	C	U2101		G1976	A1854	A1854	C1792	U1608	G1543	G1543	
A	C	C	C	C	G2102		U1977	A1855	A1855	C1793	A1609	U1544	U1544	
A	C	C	C	C	A2103		A1978	A1856	A1856	A1794	A1732	G1670	G1545	

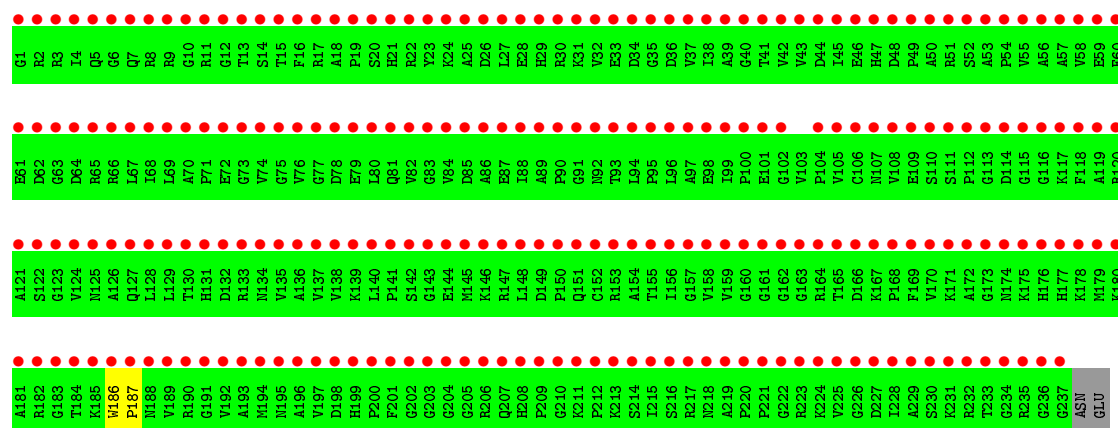


- Molecule 2: 5S RRNA

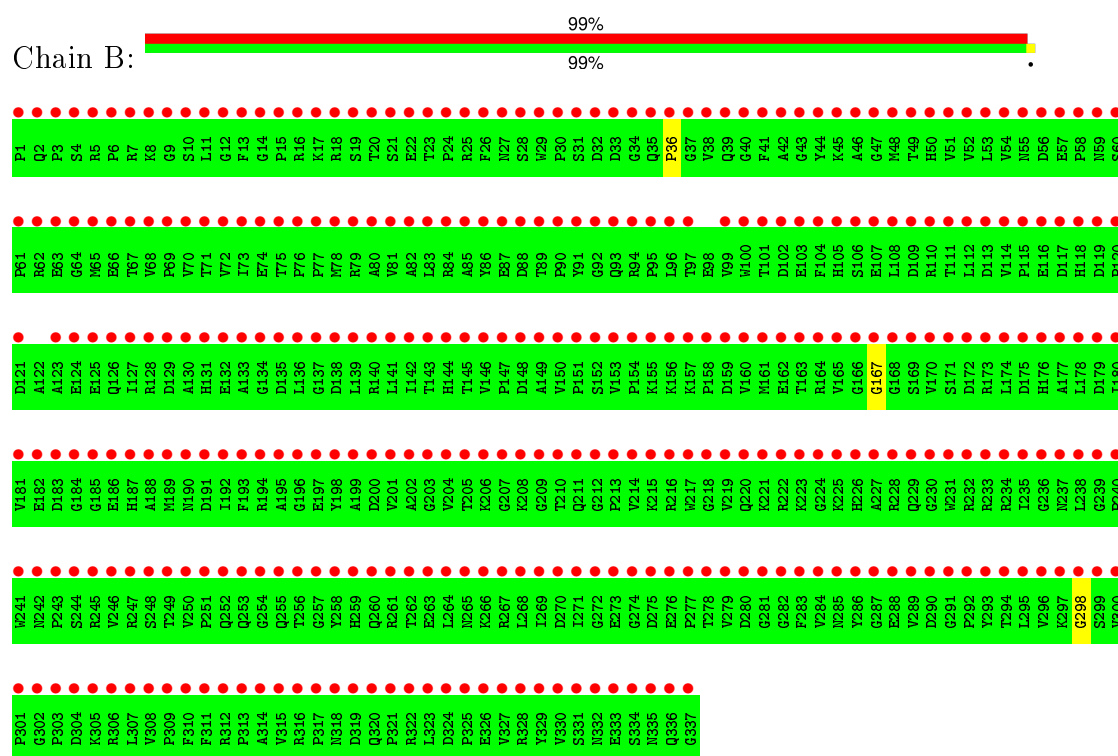


- Molecule 3: RIBOSOMAL PROTEIN L2

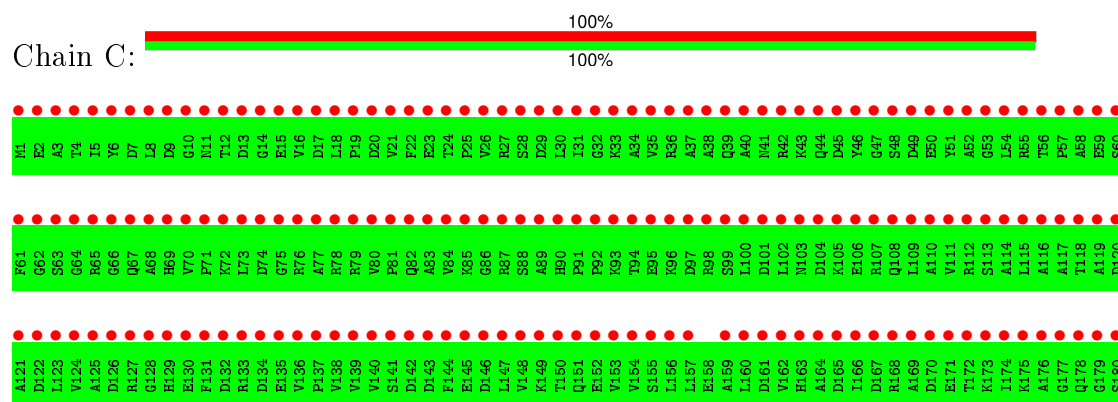


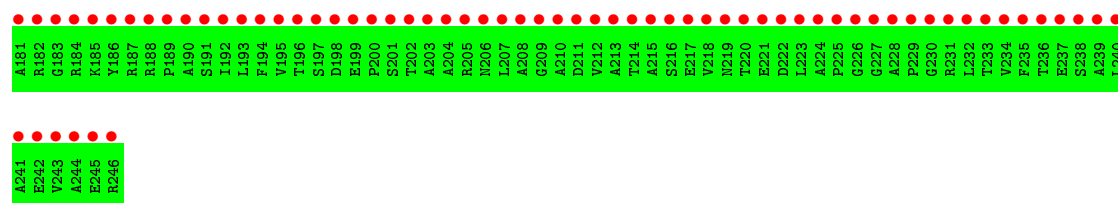


### ● Molecule 4: RIBOSOMAL PROTEIN L3

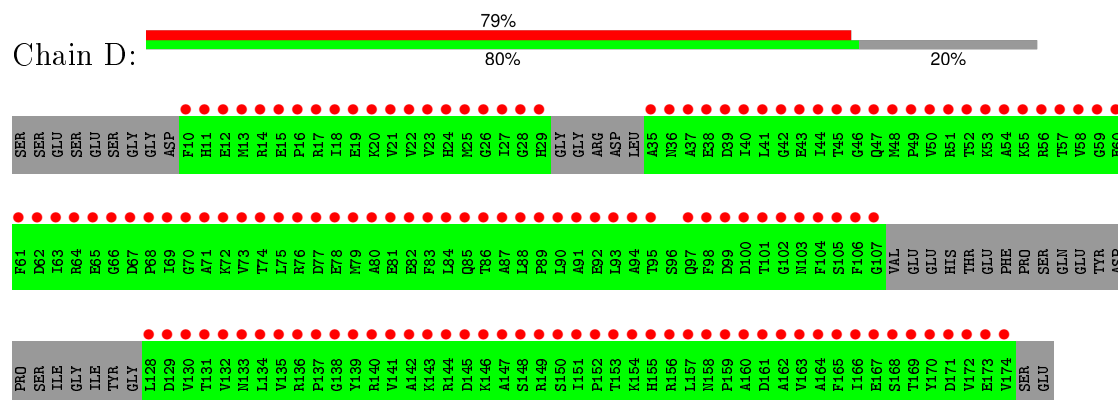


### ● Molecule 5: RIBOSOMAL PROTEIN L4

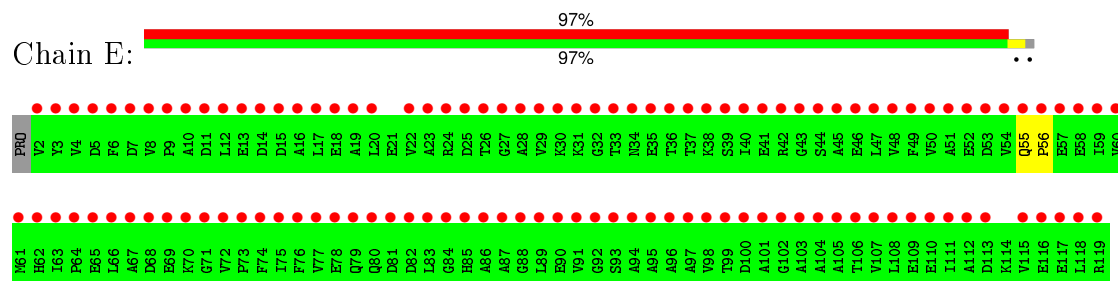




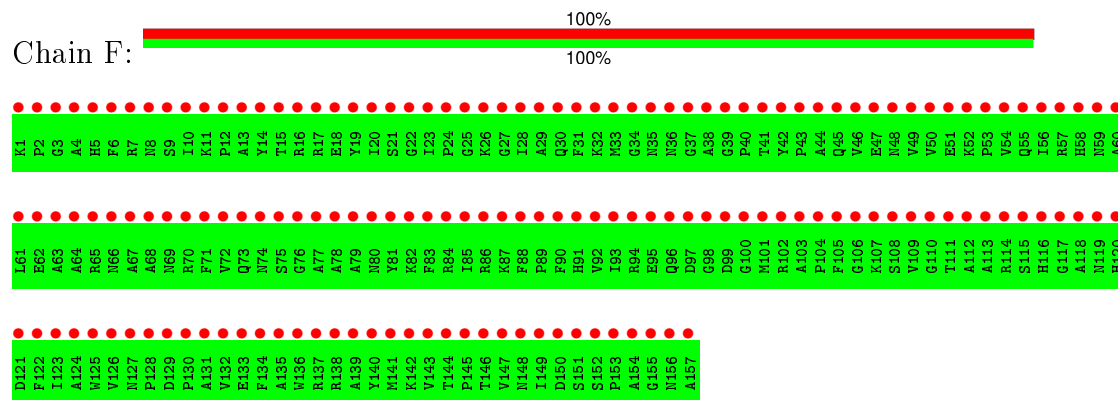
• Molecule 6: RIBOSOMAL PROTEIN L5



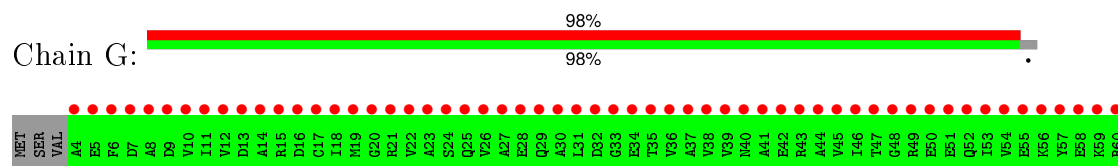
• Molecule 7: RIBOSOMAL PROTEIN L7AE

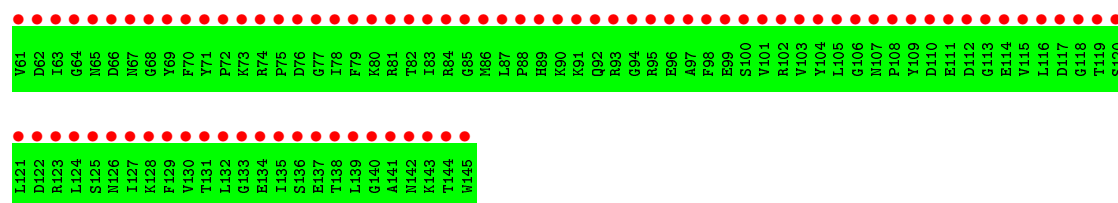


• Molecule 8: RIBOSOMAL PROTEIN L10E

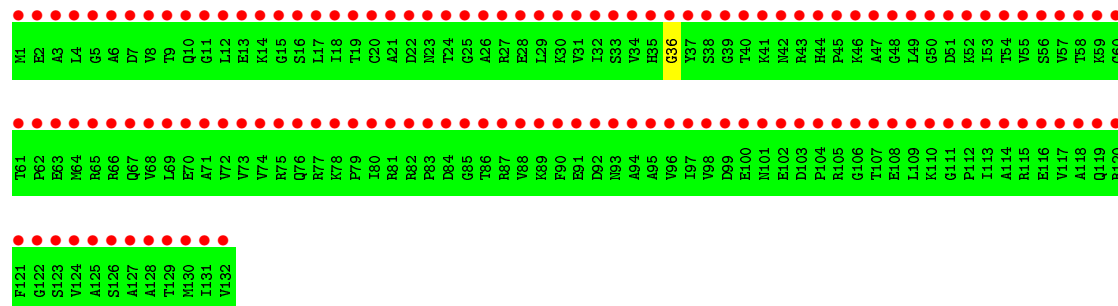


• Molecule 9: RIBOSOMAL PROTEIN L13

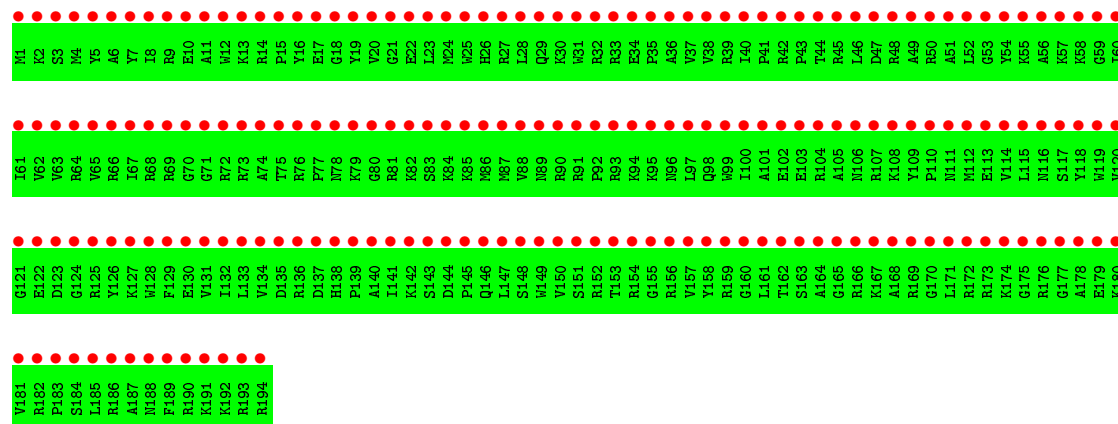




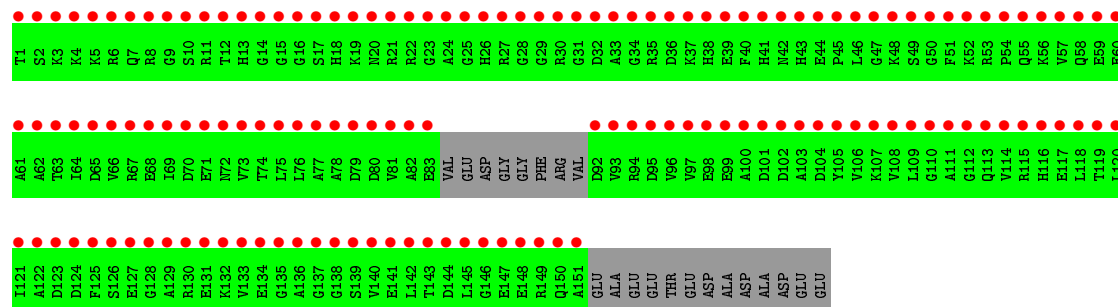
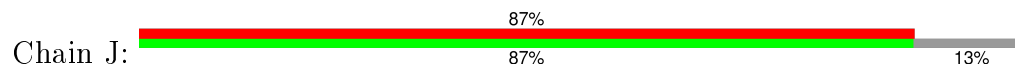
• Molecule 10: RIBOSOMAL PROTEIN L14



• Molecule 11: RIBOSOMAL PROTEIN L15E

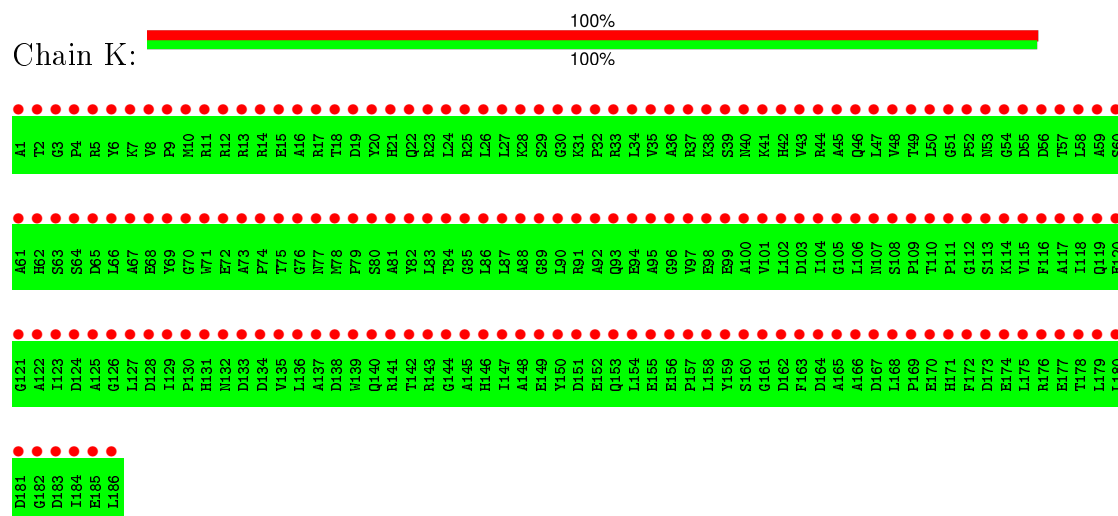


• Molecule 12: RIBOSOMAL PROTEIN L15

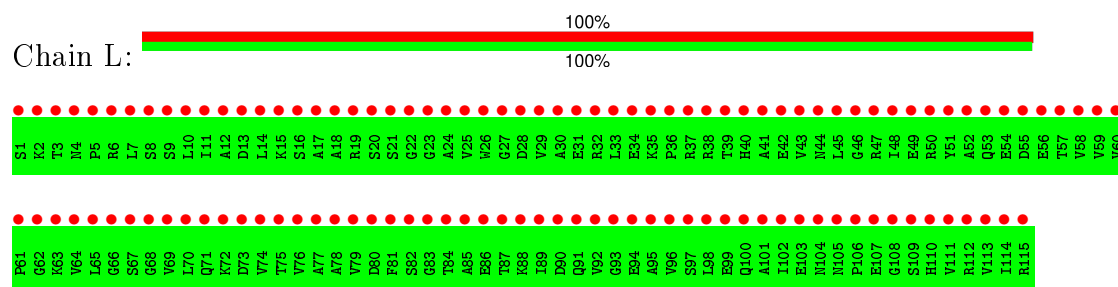




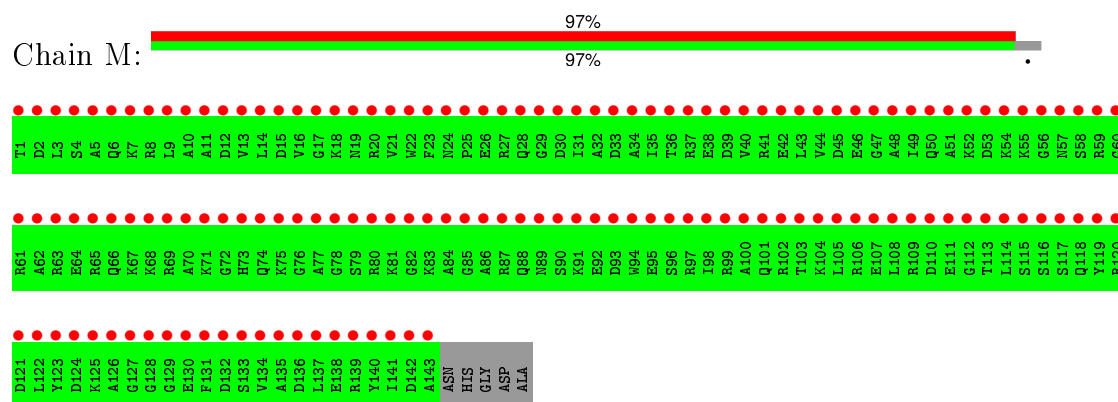
- Molecule 13: RIBOSOMAL PROTEIN L18



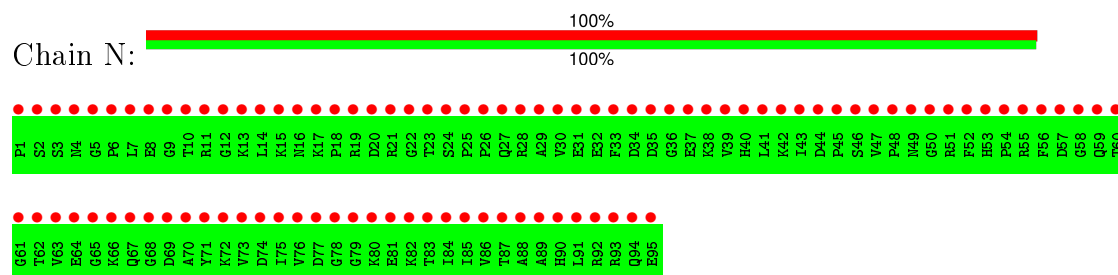
- Molecule 14: RIBOSOMAL PROTEIN L18E



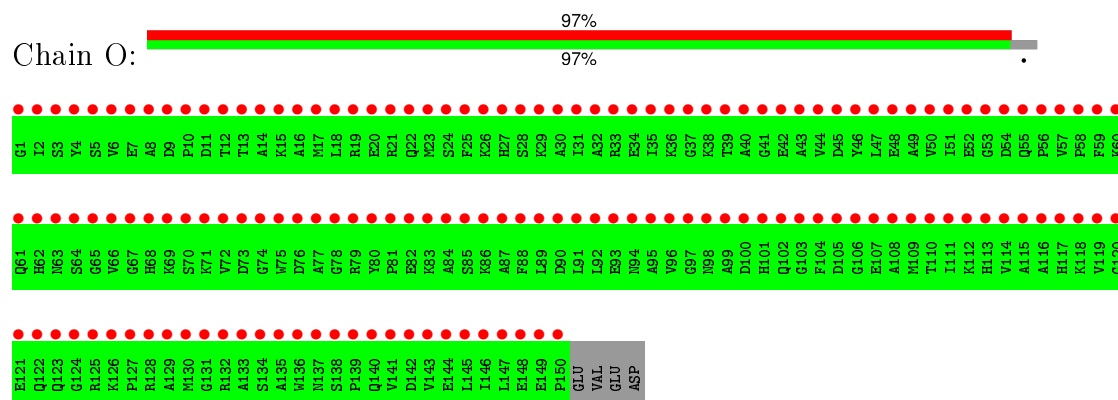
- Molecule 15: RIBOSOMAL PROTEIN L19



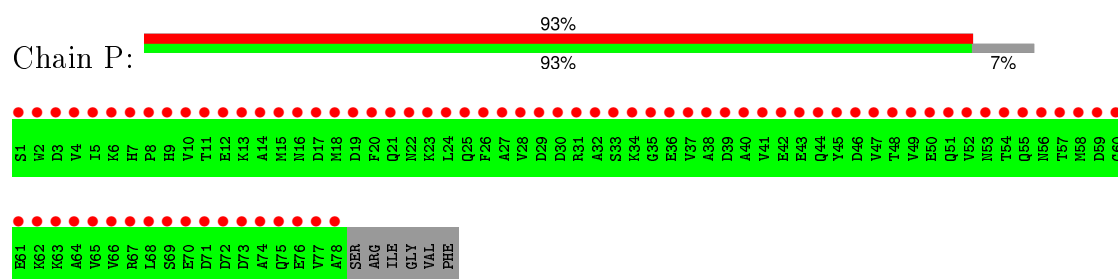
- Molecule 16: RIBOSOMAL PROTEIN L21E



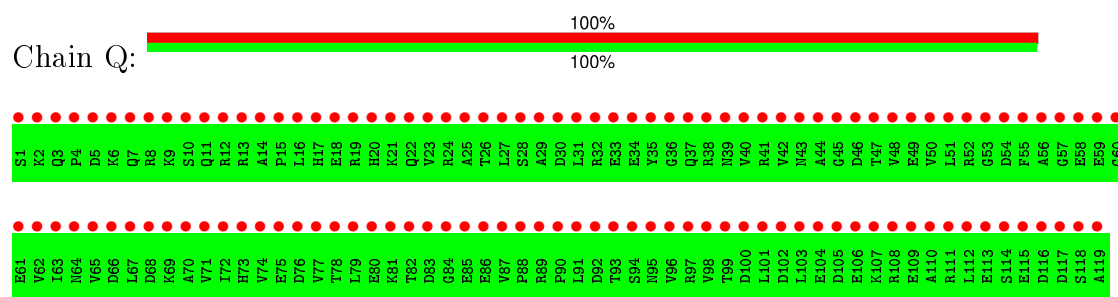
- Molecule 17: RIBOSOMAL PROTEIN L22



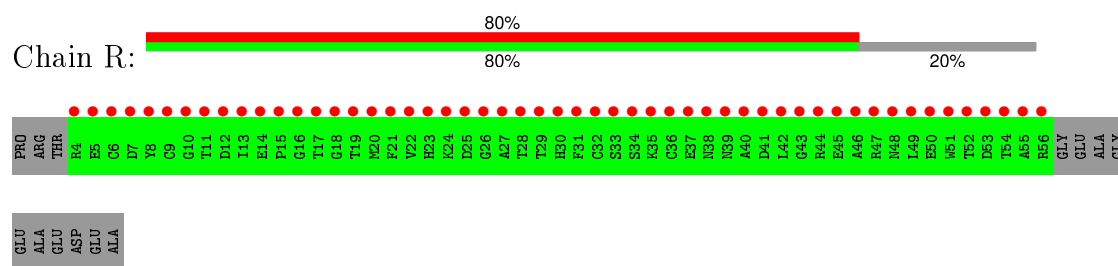
- Molecule 18: RIBOSOMAL PROTEIN L23

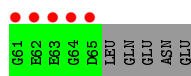


- Molecule 19: RIBOSOMAL PROTEIN L24

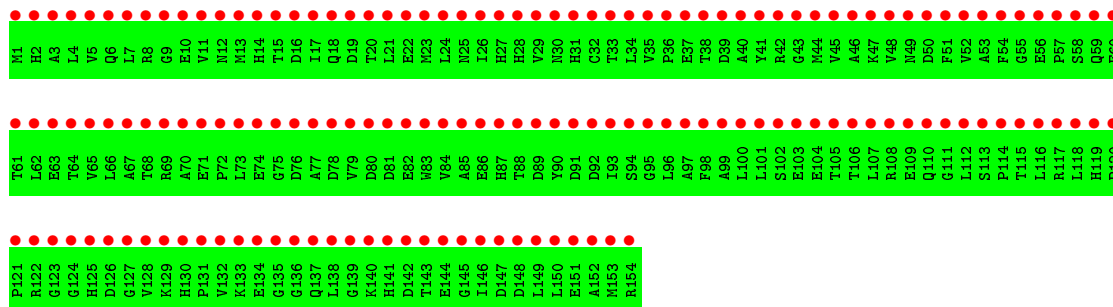


- Molecule 20: RIBOSOMAL PROTEIN L24E

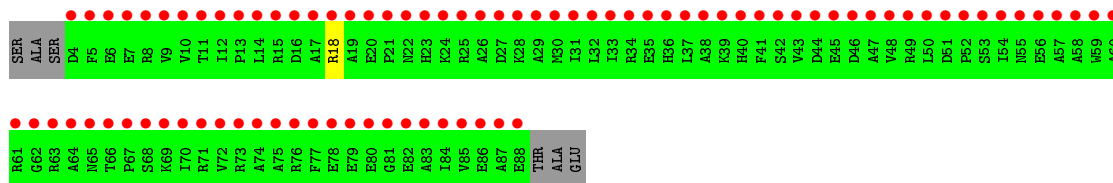
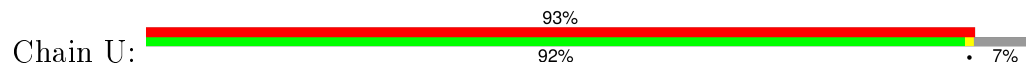




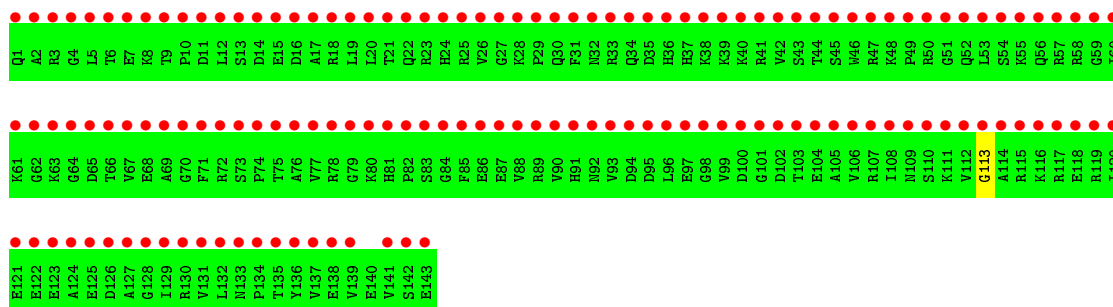
• Molecule 22: RIBOSOMAL PROTEIN L30



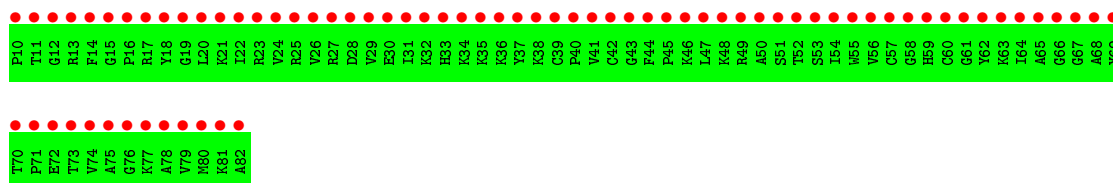
• Molecule 23: RIBOSOMAL PROTEIN L31E



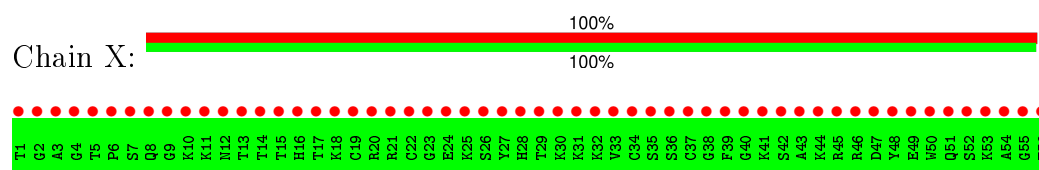
• Molecule 24: RIBOSOMAL PROTEIN L32E



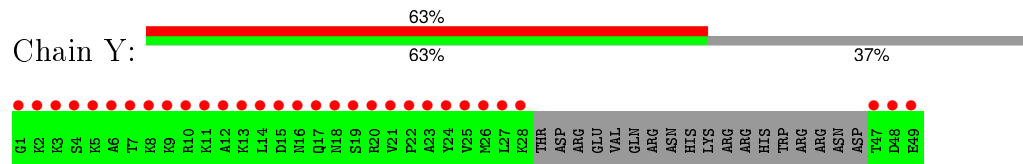
• Molecule 25: RIBOSOMAL PROTEIN L37AE



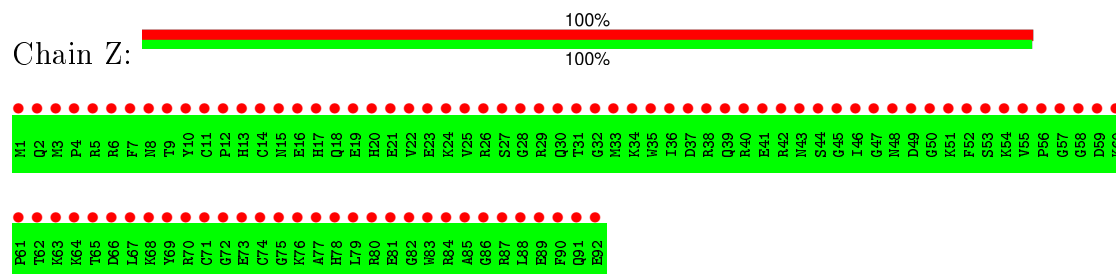
• Molecule 26: RIBOSOMAL PROTEIN L37E



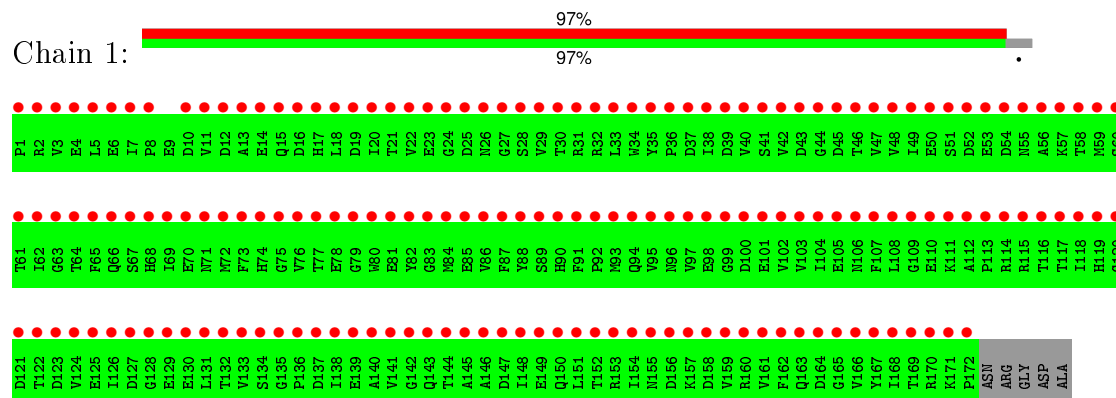
• Molecule 27: RIBOSOMAL PROTEIN L39E



• Molecule 28: RIBOSOMAL PROTEIN L44E



• Molecule 29: RIBOSOMAL PROTEIN L6



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.00 – 2.40 89.24 – 2.40	Depositor EDS
% Data completeness (in resolution range)	82.3 (90.00-2.40) 95.5 (89.24-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.40Å)	Xtriage
Refinement program	TNT, CNS	Depositor
R, $R_{free}$	0.252 , 0.261 0.337 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.04 , -7.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 701272 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	64281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: K, MG, CD

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	0	0.47	0/64945	0.72	73/101281 (0.1%)
2	9	0.35	0/2905	0.75	4/4528 (0.1%)
All	All	0.46	0/67850	0.72	77/105809 (0.1%)

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
1	0	18	45
2	9	2	0
All	All	20	45

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	0	2749	U	C2'-C3'-O3'	11.07	133.85	109.50
1	0	904	U	C2'-C3'-O3'	10.39	132.35	109.50
1	0	1981	A	C2'-C3'-O3'	10.23	132.00	109.50
1	0	2692	G	N9-C1'-C2'	10.09	127.12	114.00
2	9	3	A	C2'-C3'-O3'	9.58	130.57	109.50

5 of 20 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	191	A	C3'
1	0	282	C	C3'
1	0	600	G	C3'

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Mol	Chain	Res	Type	Atom
1	0	894	A	C3'
1	0	904	U	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	138	U	Sidechain
1	0	189	A	Sidechain
1	0	262	A	Sidechain
1	0	270	U	Sidechain
1	0	333	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	0	58012	0	29282	976	0
2	9	2600	0	1326	62	0
3	A	237	0	0	1	0
4	B	337	0	0	2	0
5	C	246	0	0	0	0
6	D	140	0	0	0	0
7	E	118	0	0	1	0
8	F	157	0	0	0	0
9	G	142	0	0	0	0
10	H	132	0	0	1	0
11	I	194	0	0	0	0
12	J	143	0	0	0	0
13	K	186	0	0	0	0
14	L	115	0	0	0	0
15	M	143	0	0	0	0
16	N	95	0	0	0	0
17	O	150	0	0	0	0
18	P	78	0	0	0	0
19	Q	119	0	0	0	0
20	R	53	0	0	0	0
21	S	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	154	0	0	0	0
23	U	85	0	0	1	0
24	V	143	0	0	2	0
25	W	73	0	0	0	0
26	X	56	0	0	0	0
27	Y	31	0	0	0	0
28	Z	92	0	0	0	0
29	1	172	0	0	0	0
30	R	1	0	0	0	0
30	W	1	0	0	0	0
30	X	1	0	0	0	0
30	Z	1	0	0	0	0
31	0	1	0	0	0	0
32	0	2	0	0	0	0
33	0	6	0	0	0	0
All	All	64281	0	30608	1040	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 11.

The worst 5 of 1040 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)
2:9:76:G:H3'	2:9:77:A:H5''	1.29	1.10
1:0:1682:A:H2	1:0:1696:U:H3	1.05	1.01
1:0:795:G:H2'	1:0:817:G:H22	1.25	1.00
1:0:326:G:H1	1:0:330:C:H5	1.03	1.00
1:0:1355:A:O2'	1:0:1356:A:H3'	1.60	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.



### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2697/2922 (92%)	334 (12%)	107 (3%)
2	9	122/122 (100%)	17 (13%)	5 (4%)
All	All	2819/3044 (92%)	351 (12%)	112 (3%)

5 of 351 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	70	A

5 of 112 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1379	A
1	0	1690	C
1	0	2836	G
1	0	1408	U
1	0	1534	C

## 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2706/2922 (92%)	2.87	2156 (79%) 0 0	12, 29, 60, 87	0
2	9	122/122 (100%)	3.77	114 (93%) 0 0	22, 42, 67, 106	0
3	A	237/239 (99%)	8.12	236 (99%) 0 0	16, 35, 64, 78	0
4	B	337/337 (100%)	8.74	335 (99%) 0 0	18, 42, 65, 72	0
5	C	246/246 (100%)	8.36	245 (99%) 0 0	14, 31, 54, 76	0
6	D	140/176 (79%)	7.87	139 (99%) 0 0	49, 80, 90, 94	0
7	E	118/119 (99%)	5.77	116 (98%) 0 0	32, 51, 69, 72	0
8	F	157/157 (100%)	9.68	157 (100%) 0 0	33, 56, 81, 93	0
9	G	142/145 (97%)	8.81	142 (100%) 0 0	22, 38, 58, 68	0
10	H	132/132 (100%)	7.59	132 (100%) 0 0	20, 37, 55, 63	0
11	I	194/194 (100%)	10.95	194 (100%) 0 0	22, 36, 54, 66	0
12	J	143/164 (87%)	9.10	143 (100%) 0 0	21, 46, 73, 85	0
13	K	186/186 (100%)	8.86	186 (100%) 0 0	40, 65, 83, 87	0
14	L	115/115 (100%)	6.64	115 (100%) 0 0	28, 38, 55, 65	0
15	M	143/148 (96%)	9.10	143 (100%) 0 0	24, 38, 49, 58	0
16	N	95/95 (100%)	9.85	95 (100%) 0 0	20, 32, 53, 65	0
17	O	150/154 (97%)	9.44	150 (100%) 0 0	19, 31, 49, 58	0
18	P	78/84 (92%)	6.86	78 (100%) 0 0	27, 38, 63, 65	0
19	Q	119/119 (100%)	6.31	119 (100%) 0 0	28, 39, 56, 67	0
20	R	53/66 (80%)	6.98	53 (100%) 0 0	29, 43, 55, 58	0
21	S	65/70 (92%)	6.91	65 (100%) 0 0	35, 51, 77, 83	0
22	T	154/154 (100%)	8.60	154 (100%) 0 0	24, 35, 51, 56	0
23	U	85/91 (93%)	10.03	85 (100%) 0 0	29, 47, 73, 80	0
24	V	143/143 (100%)	7.67	142 (99%) 0 0	18, 33, 62, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	73/73 (100%)	8.47	73 (100%) 0 0	36, 43, 57, 62	0
26	X	56/56 (100%)	13.37	56 (100%) 0 0	17, 27, 35, 41	0
27	Y	31/49 (63%)	9.74	31 (100%) 0 0	25, 33, 55, 61	0
28	Z	92/92 (100%)	8.48	92 (100%) 0 0	23, 40, 51, 63	0
29	1	172/177 (97%)	6.37	171 (99%) 0 0	31, 48, 64, 71	0
All	All	6484/6825 (95%)	6.04	5917 (91%) 0 0	12, 36, 70, 106	0

The worst 5 of 5917 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	86	THR	34.8
6	D	63	ILE	30.5
12	J	81	VAL	29.8
13	K	166	ALA	26.3
6	D	106	PHE	25.9

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	0	2926	1/1	0.60	0.27	-2.02	30,30,30,30	0
32	MG	0	2925	1/1	0.75	0.14	-5.90	30,30,30,30	0
31	K	0	2924	1/1	0.87	0.09	-12.79	30,30,30,30	0
30	CD	Z	104	1/1	0.96	0.23	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	CD	R	101	1/1	0.96	0.12	-	39,39,39,39	0
30	CD	X	102	1/1	0.81	0.21	-	48,48,48,48	0
30	CD	W	103	1/1	0.95	0.13	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.