



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:18 AM GMT

PDB ID : 2WRO  
Title : THE CRYSTAL STRUCTURE OF THE 70S RIBOSOME BOUND TO EF-TU AND TRNA (PART 2 OF 4).  
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.  
Deposited on : 2009-09-01  
Resolution : 3.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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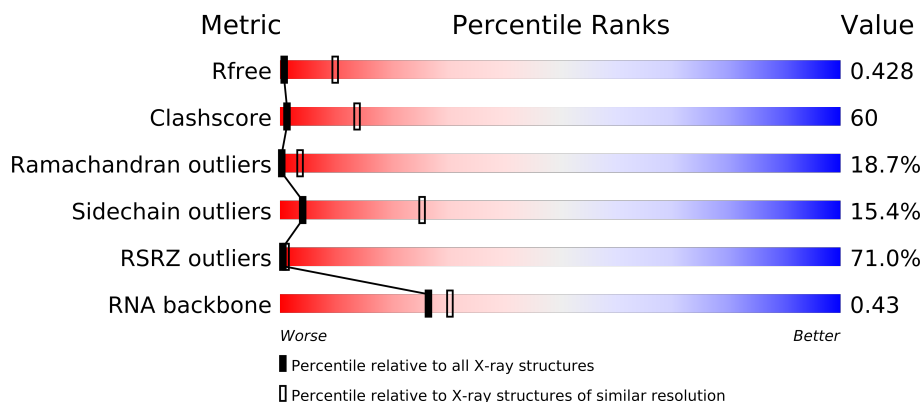
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.60 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.




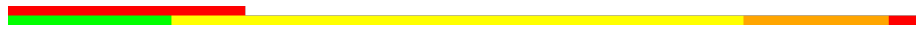









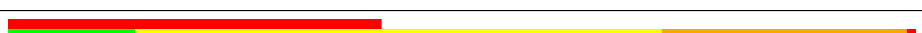




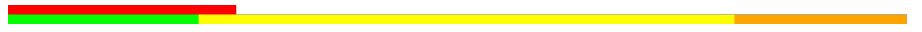




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)
RNA backbone	1838	1012 (4.40-2.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	85	
2	1	98	
3	2	72	
4	3	60	
5	4	71	
6	5	60	
7	6	54	
8	7	49	
9	8	65	
10	9	37	
11	A	2915	
12	B	122	

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Mol	Chain	Length	Quality of chain
13	C	229	
14	D	276	
15	E	206	
16	F	210	
17	G	182	
18	H	180	
19	J	173	
20	K	147	
21	N	140	
22	O	122	
23	P	150	
24	Q	141	
25	R	118	
26	S	112	
27	T	146	
28	U	118	
29	V	101	
30	W	113	
31	X	96	
32	Y	110	
33	Z	206	

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 93761 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 11 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	A	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- Molecule 12 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	D	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	E	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	F	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	H	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	J	131	Total	C	N	O		0	0	1
			651	390	131	130				

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	K	141	Total	C	N	O		0	0	1
			701	420	141	140				

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	N	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	P	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	S	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	T	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	U	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	W	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	X	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	Y	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L25.

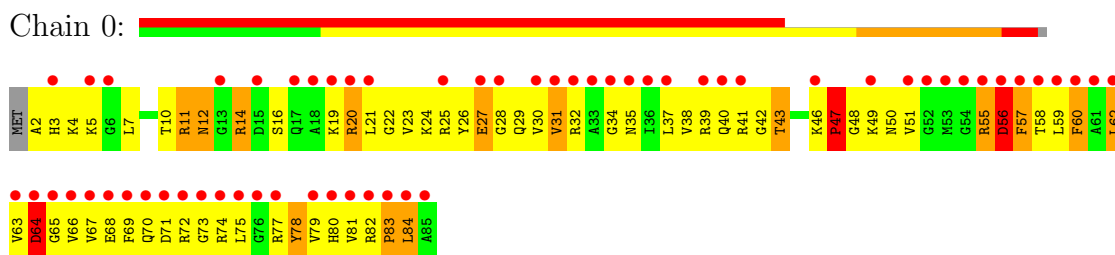
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	Z	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			



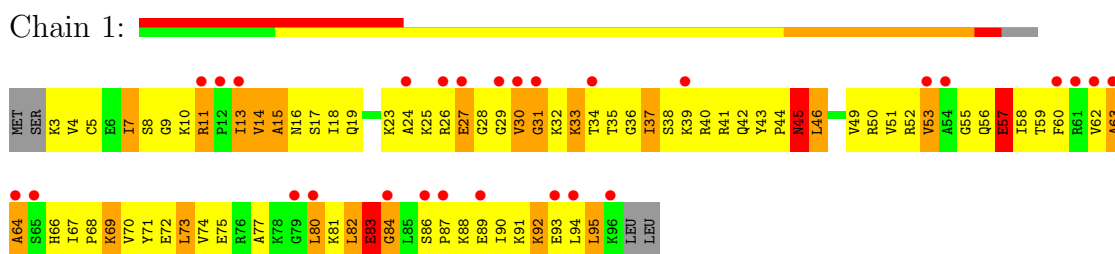
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

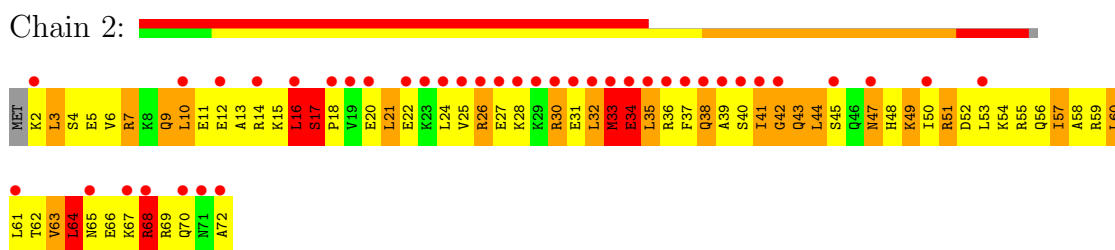
- Molecule 1: 50S RIBOSOMAL PROTEIN L27



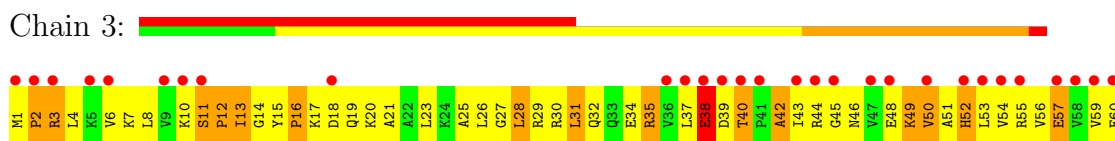
- Molecule 2: 50S RIBOSOMAL PROTEIN L28



- Molecule 3: 50S RIBOSOMAL PROTEIN L29

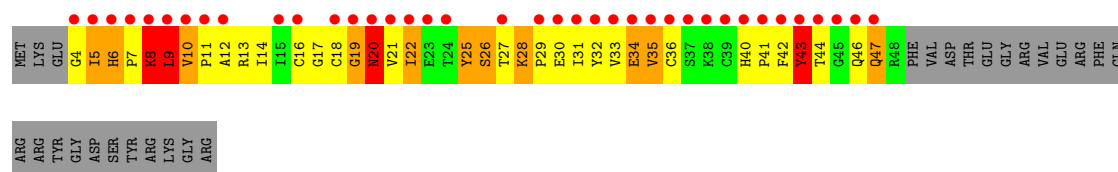


- Molecule 4: 50S RIBOSOMAL PROTEIN L30



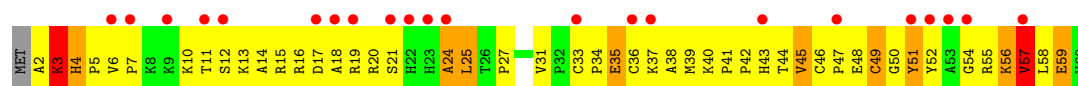
- Molecule 5: 50S RIBOSOMAL PROTEIN L31





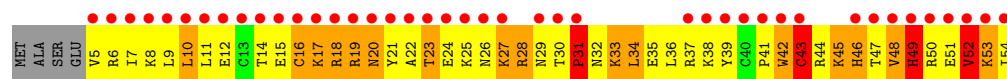
• Molecule 6: 50S RIBOSOMAL PROTEIN L32

Chain 5:



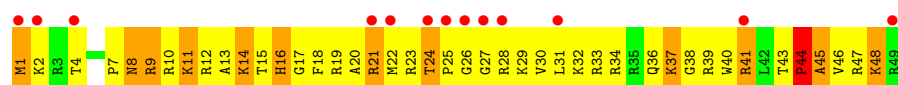
• Molecule 7: 50S RIBOSOMAL PROTEIN L33

Chain 6:



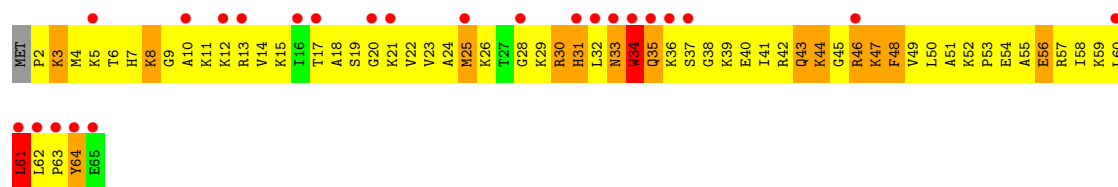
• Molecule 8: 50S RIBOSOMAL PROTEIN L34

Chain 7:



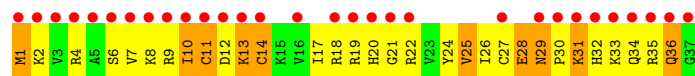
• Molecule 9: 50S RIBOSOMAL PROTEIN L35

Chain 8:



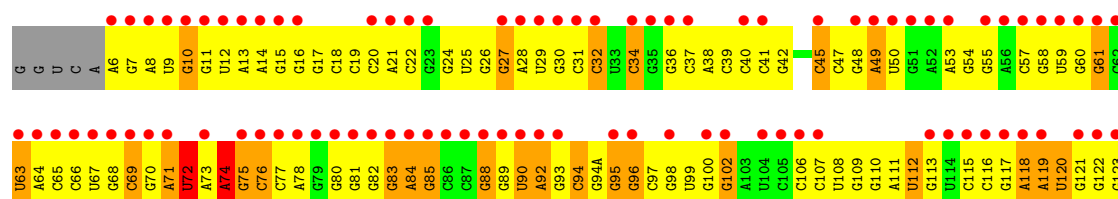
• Molecule 10: 50S RIBOSOMAL PROTEIN L36

Chain 9:



• Molecule 11: 23S RIBOSOMAL RNA

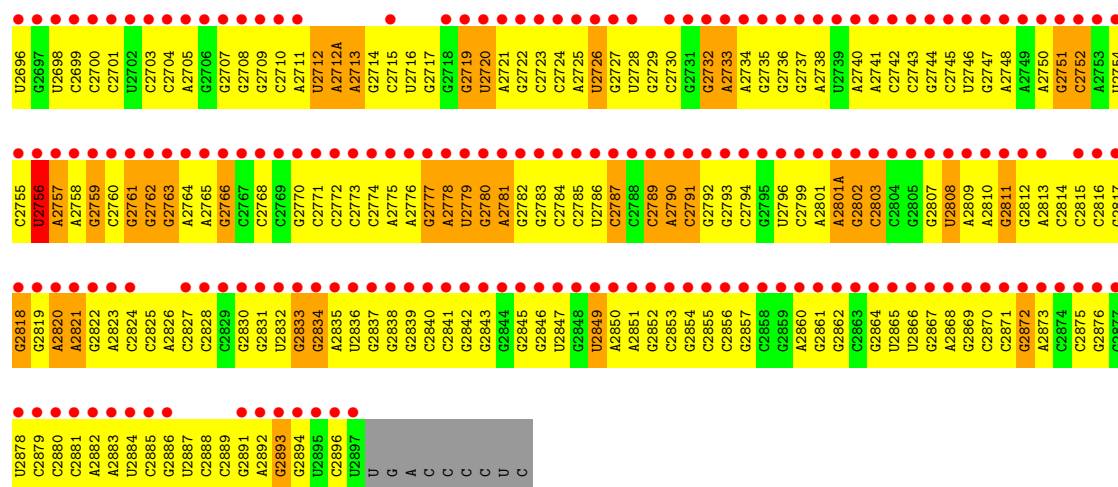
Chain A:





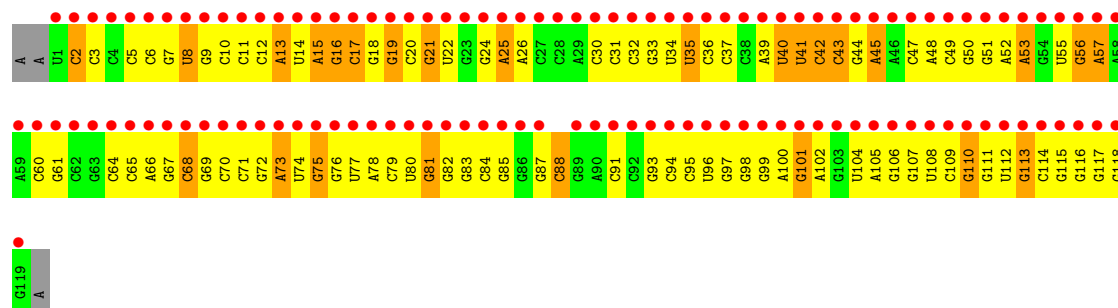
C1774	C1698	C1699	C1638	C1639	C1458	C1399	C1339	G1279	A1220	U1159	G1099	G1039	G979
U1775	G1699	A1700	U1639	A1578	G1459	G1400	U1340	G1280	C1221	G1160	C1100	C1040	A980
U1776	A1641	G1581	A1640	A1580	A1461	G1401	A1342	G1281	C1221A	C1161	C1101	C1041	A981
U1777	G1642	C1582	C1643	G1583	C1462	C1402	A1342	G1282	C1222	G1162	C1102	C1042	C982
G1703	G1643	C1583	G1644	A1584	C1463	C1403	G1344	G1283	C1223	G1163	A1103	C1043	A983
U1779	G1704	C1584	C1644	G1585	C1464	C1404	G1345	G1284	C1224	G1164	C1104	C1044	A984
A1780	G1705	A1586	G1645	G1586	C1465	U1405	C1346	G1285	G1225	U1165	U1105	A1045	C985
C1781	G1706	A1587	G1646	G1587	C1466	U1406	C1347	G1286	G1226	C1166	C1106	A1046	C986
U1782	G1707	C1588	G1647	A1588	C1467	C1407	G1348	G1287	G1227	U1167	G1107	A1047	C987
A1783	C1708	C1589	G1648	A1589	C1468	C1408	G1349	U1288	G1228	G1168	U1108	A1048	A988
A1784	G1709	C1590	G1649	A1590	C1469	C1409	A1350	U1289	G1229	G1169	C1109	C1049	C989
U1785	C1710	U1591	G1650	G1591	C1470	C1411	C1351	C1290	C1230	G1170	G1110	A1050	A990
A1786	C1711	C1592	G1651	A1592	A1471	A1412	U1352	U1292	G1232	G1171	A1111	A1051	C991
A1787	G1712	G1593	A1652	A1472	G1413	G1414	A1353	G1173	C1233	C1172	G1112	C1052	C992
C1788	U1713	G1594	G1653	G1473	G1414	G1415	A1354	U1175	C1234	U1174	U1113	A1053	C993
A1789	G1714	C1595	U1654	C1474	U1415	U1416	G1355	U1176	G1235	G1175	G1114	C1054	C994
C1790	G1715	A1596	A1655	G1475	G1416	G1417	G1356	G1177	G1236	U1177	C1115	G1055	C995
A1791	G1716	A1597	C1656	C1476	U1417	G1418	U1357	C1178	A1237	C1178	C1116	G1056	A996
G1792	G1717	C1598	C1657	A1477	G1419	G1420	G1358	C1179	G1238	C1179	C1117	A1057	C997
U1793	U1720	C1599	G1658	G1478	A1419	U1421	A1359	C1180	G1239	C1180	C1118	G1058	C998
C1795	G1721	G1600	C1659	G1479	U1420	A1421	A1360	U1181	U1240	G1181	G1120	U1060	U999
U1796	A1722	C1601	C1680	G1480	G1422	G1423	G1361	C1182	A1241	U1182	C1121	U1061	A1000
C1797	G1739	U1602	G1681	U1481	G1423	G1424	C1362	C1183	G1242	A1183	G1122	G1062	A1001
U1798	G1740	A1603	C1682	G1482	G1424	G1425	C1363	G1303	A1243	G1184	C1123	G1063	G1002
G1799	A1741	C1604	C1683	G1484	G1425	G1426	G1364	C1304	G1244	C1185	C1124	C1064	C1004
C1800	G1742	C1605	A1684	G1485	G1426	G1427	A1365	C1305	G1245	G1186	G1125	U1065	C1005
G1801	C1743	A1606	A1685	A1486	G1427	G1428	A1366	C1306	A1246	A1126	A1126	U1066	C1006
A1802	G1744	C1607	G1686	G1487	A1427	C1428	G1367	A1307	G1247	U1187	A1127	A1067	C1007
C1803	C1745	A1608	C1687	G1488	C1428	G1429	G1368	A1308	A1248	A1188	A1128	G1068	C1008
U1804	G1746	A1609	A1688	U1489	G1429	C1430	G1369	G1309	U1249	G1190	A1129	A1069	A1009
C1805	C1747	A1610	A1689	A1490	C1430	C1431	C1370	G1310	G1250	G1191	U1130	A1070	A1010
U1806	G1747	C1611	C1670	G1491	U1431	U1432	G1371	G1311	G1251	G1192	G1131	G1071	G1011
G1807	G1748	G1612	U1671	G1492	U1432	U1433	G1372	G1312	G1252	A1193	A1132	A1072	C1012
U1808	C1749	G1613	C1672	C1493	C1433	C1434	A1373	A1194	A1253	G1195	U1133	C1073	C1013
A1809	A1749	A1614	U1673	A1494	A1434	G1435	G1374	C1314	A1254	C1196	C1135	G1074	U1014
A1810	G1750	C1615	G1674	A1495	G1435	G1436	C1375	G1315	U1255	G1197	G1136	G1075	G1015
G1811	C1751	A1616	C1675	A1496	G1436	U1437	C1376	U1316	G1256	G1198	G1137	C1076	G1016
A1812	G1752	C1617	U1676	U1497	U1437	C1438	G1377	A1317	C1257	U1199	G1138	A1077	G1017
G1813	C1753	A1618	A1677	C1498	U1438	A1439	A1378	C1318	G1258	U1198	G1139	U1078	C1018
A1814	C1754	G1619	G1678	C1499	A1439	G1440	A1379	G1319	G1259	C1200	U1141	C1080	U1019
U1815	A1755	G1620	U1679	G1500	G1440	G1441	G1380	C1320	G1260	C1201	C1140	C1081	A1020
G1816	G1756	U1621	G1680	C1501	G1441	G1442	G1381	A1321	A1261	C1202	U1142	U1082	A1021
A1817	U1757	G1622	G1681	G1502	G1442	G1443	G1382	A1322	A1262	G1203	A1142A	U1083	G1022
U1818	G1758	G1623	G1682	U1503	G1443	G1444	C1383	U1323	U1263	A1204	A1143	U1084	U1023
A1819	A1759	G1624	C1683	C1504	G1444	A1445	A1384	G1324	G1264	U1205	G1144	A1085	G1024
U1820	C1760	C1625	C1684	C1505	A1445	C1446A	G1385	G1325	A1265	G1206	C1145	A1086	G1025
A1821	C1761	G1626	C1685	C1506	C1446A	C1447	C1386	U1326	G1266	C1207	C1146	A1087	U1026
G1822	A1762	G1627	C1686	A1507	C1446	C1447	G1387	G1327	U1267	G1208	C1147	G1087	A1027
G1823	G1763	A1628	G1687	A1508	C1447	G1448	G1388	U1328	A1268	G1209	A1148	A1088	A1028
A1824	G1764	U1629	U1688	C1509	G1448	G1449	G1389	U1329	A1269	A1210	G1149	G1089	A1029
U1825	C1765	G1630	A1689	A1509A	G1449	A1450	U1390	C1330	C1270	U1211	C1150	U1090	G1030
G1826	U1766	A1631	A1690	A1509B	A1450	C1450A	U1391	A1331	G1271	G1212	G1151	G1091	G1031
C1827	C1767	G1631A	C1691	G1510	C1450A	C1451	A1392	G1332	A1272	A1213	C1152	C1092	A1032
G1828	U1768	A1632	U1692	C1511	C1451	A1452	A1393	U1333	U1273	G1214	C1153	G1093	U1033
A1829	G1769	G1633	G1693	U1512	A1452	U1453	A1394	G1334	A1274	G1215	G1154	U1094	G1034
C1830	C1770	A1634	C1694	G1513	U1453	G1454	A1395	U1335	A1275	G1216	A1155	A1095	U1035
A1831	G1771	G1635	G1695	U1514	G1454	G1455	U1396	A1336	G1277	C1217	A1156	A1096	G1036
C1832	G1772	U1515	U1576	G1516	G1456	A1457	U1397	G1337	A1278	G1218	U1097	G1037	G1037
U1833	A1773	C1516	C1577	C1516	A1457		C1398	G1338		G1219	C1158	A1098	C1038

U2636	G2576	G2516	C2456	G2396	A2336	G2276	C2206	C2146	C2086	C2026	U1963	G1903	U1834
U2637	A2577	C2617	U2457	G2397	G2337	G2277	G2207	C2147	U2086	C2027	G1964	G1904	G1835
A2638	G2578	U2518	G2458	U2398	G2338	A2278	A2208	G2148	G2087	U2027	C1965	G1905	C1836
A2639	G2579	U2519	A2459	G2399	G2339	G2279	U2218	G2149	G2088	U2028	A1966	G1906	C1837
U2640	U2580	G2520	U2460	G2400	G2340	G2280	G2220	U2150	U2089	G2029	G1967	G1907	G1838
G2641	G2581	C2521	C2461	U2401	G2341	G2281	G2221	G2151	G2090	A2030	G1968	G1908	G1839
G2642	G2582	U2522	U2462	G2402	C2342	G2282	G2222	G2152	U2091	A2031	A1969	G1909	G1840
G2643	G2583	G2523	C2463	C2403	C2343	G2283	G2223	G2153	U2092	G2032	A1970	U1910	U1841
G2644	U2584	G2524	C2464	G2404	C2344	C2284	G2224	G2154	G2093	A2033	A1971	U1911	G1842
G2645	U2585	G2525	C2465	G2405	G2345	C2285	G2225	G2155	G2094	U2034	A1972	C1943	C1843
G2646	U2586	G2526	C2466	U2406	A2346	A2286	A2226	G2156	C2095	G2035	G1973	A1913	G1844
U2647	G2587	G2527	C2467	G2407	C2347	A2287	G2227	G2157	U2096	C2036	G1974	G1914	G1845
G2648	U2588	U2528	G2468	U2408	U2348	A2288	A2228	G2158	C2097	G2037	G1975	U1915	G1846
U2649	A2589	G2529	A2469	G2409	G2349	G2289	G2229	A2158	U2098	G2038	U1976	A1916	A1847
U2650	A2590	A2530	G2470	G2410	C2350	G2290	G2230	G2159	U2099	C2039	A1977	U1917	A1848
C2651	C2591	G2531	C2471	A2411	G2351	U2291	G2231	G2160	G2100	C2040	A1978	A1918	G1849
C2652	G2592	G2532	G2472	G2412	A2352	C2292	C2232	G2161	G2101	U2041	G1979	G1919	G1850
U2653	U2593	U2533	U2473	G2413	G2353	C2293	U2233	G2162	A2102	A2042	G1980	C1920	U1851
A2654	G2594	A2534	C2474	G2414	G2354	G2294	U2234	G2163	C2103	C2043	A1981	G1921	C1852
G2655	G2595	G2535	C2475	G2415	C2355	G2295	G2235	G2164	G2104	C2044	C1982	G1922	A1853
U2656	U2596	G2536	A2476	C2416	G2356	U2296	G2236	G2165	C2105	C2045	C1983	G1923	G1854
A2657	G2597	U2537	C2477	A2417	U2357	A2297	G2237	G2166	G2106	G2046	G1984	C1924	G1855
C2658	A2598	C2538	C2478	A2418	G2358	A2298	G2238	U2167	C2107	U2047	G1985	C1925	G1856
G2659	U2599	G2539	G2479	U2419	C2359	G2299	G2239	A2168	C2108	G2048	A1986	U1926	G1857
A2660	A2600	C2540	C2480	C2420	A2360	G2300	G2240	A2169	U2109	G2049	G1987	A1927	G1858
G2661	C2601	A2541	G2481	G2421	A2361	G2301	C2241	A2170	G2110	C2050	C1988	A1928	A1859
A2662	A2602	U2542	G2482	A2422	G2362	G2302	A2242	U2171	C2111	A2051	G1989	G1929	G1860
G2663	G2603	C2543	C2483	U2423	C2363	G2303	G2243	U2172	G2112	G2052	C1990	G1930	G1861
G2664	U2604	G2544	G2484	A2424	G2364	G2304	U2244	A2173	U2113	G2053	G1991	G1931	G1862
A2665	U2605	G2545	G2485	A2425	G2365	A2305	U2245	C2174	A2114	A2054	G1992	A1932	G1863
G2666	G2606	U2546	G2486	A2426	A2366	C2306	U2246	C2175	G2115	C2055	U1993	G1933	U1864
C2667	G2607	U2547	G2487	G2427	G2367	G2307	G2247	A2176	G2116	G2056	C1994	C1934	G1865
G2668	G2608	U2548	A2488	G2428	C2368	G2308	A2248	C2177	A2117	C2057	U1995	G1935	G1866
G2669	U2609	G2549	G2489	A2429	A2369	A2309	G2249	C2178	U2118	A2058	C1996	A1876	G1867
A2670	C2610	G2550	G2490	G2430	G2370	A2310	U2249	C2179	A2119	A2059	G1997	A1937	A1877
G2671	U2611	C2551	U2491	U2431	G2371	A2311	G2250	U2180	G2120	A2060	C1998	U1938	G1878
G2672	G2612	U2552	U2492	A2432	G2372	U2312	G2251	G2181	G2121	G2061	G1999	U1939	G1879
G2673	U2613	G2553	U2493	A2433	G2373	C2313	G2252	G2182	U2122	A2062	G2000	U1940	C1880
A2674	U2614	U2554	G2494	A2434	C2374	G2314	G2253	G2183	G2123	C2063	A2001	C1941	C1881
U2675	U2615	U2555	G2495	A2435	G2375	G2315	G2254	G2184	G2124	C2064	G2005	C1942	C1882
G2676	G2616	G2556	C2496	A2436	A2376	C2316	G2255	C2185	G2125	C2065	C2006	U1943	G1883
G2677	U2617	G2557	A2497	U2437	A2377	C2317	G2256	G2186	A2126	C2066	G2007	U1944	A1884
G2678	G2618	C2558	G2498	U2438	A2378	G2318	U2257	G2187	G2127	G2067	C2008	U1945	A1885
A2679	C2619	C2559	C2499	U2439	G2379	G2319	G2258	C2188	C2128	U2068	G2009	U1946	C1886
C2680	C2620	G2560	U2500	G2440	C2380	A2320	G2259	U2189	C2129	G2069	G2010	C1947	C1887
C2681	A2621	A2561	C2501	G2441	C2381	G2321	G2260	G2190	U2130	G2070	G2011	G1948	G1888
U2682	G2622	U2562	G2502	C2442	G2382	A2322	C2261	G2191	G2131	A2071	U2011	G1949	C1889
C2683	G2623	U2563	C2503	G2443	G2383	G2323	U2262	G2192	U2132	G2072	G2012	G1950	C1890
U2684	G2624	A2564	U2504	G2444	G2384	G2324	C2263	G2193	G2133	C2073	A2013	U1951	G1891
G2685	G2625	A2565	G2505	G2445	C2385	G2325	G2264	G2194	A2134	U2074	A2014	A1952	C1892
G2686	G2626	A2566	U2506	G2446	C2386	G2326	G2265	C2195	A2135	U2075	A2015	A1953	C1893
U2687	U2627	G2567	C2507	G2447	U2387	A2327	A2267	C2196	C2136	U2076	U2016	G1954	C1894
U2688	G2628	C2568	G2508	A2448	A2388	A2328	A2268	U2197	C2137	A2077	U2017	G1955	G1895
U2689	A2629	G2569	G2509	U2449	G2389	G2329	A2269	A2198	C2138	C2078	G2018	U1956	G1896
C2690	G2630	G2570	C2510	A2450	U2390	G2330	G2270	A2199	C2139	U2079	A2019	G1957	U1897
C2691	G2631	C2571	U2511	G2451	G2391	G2331	G2271	G2200	C2140	G2080	A2020	C1958	U1898
C2692	A2632	A2572	C2512	G2452	A2392	U2332	U2272	C2201	G2141	C2081	C2021	G1959	G1899
A2693	G2633	C2573	G2513	A2453	A2393	A2333	A2273	C2202	C2142	A2082	U2022	G1960	G1899
G2694	U2634	G2574	U2514	G2454	C2394	G2334	A2274	U2203	C2143	G2083	G2023	A1901	C1900
C2695	G2635	C2575	C2515	G2455	C2395	A2335	G2275	C2205	U2144	C2084	G2024	C1962	C1902



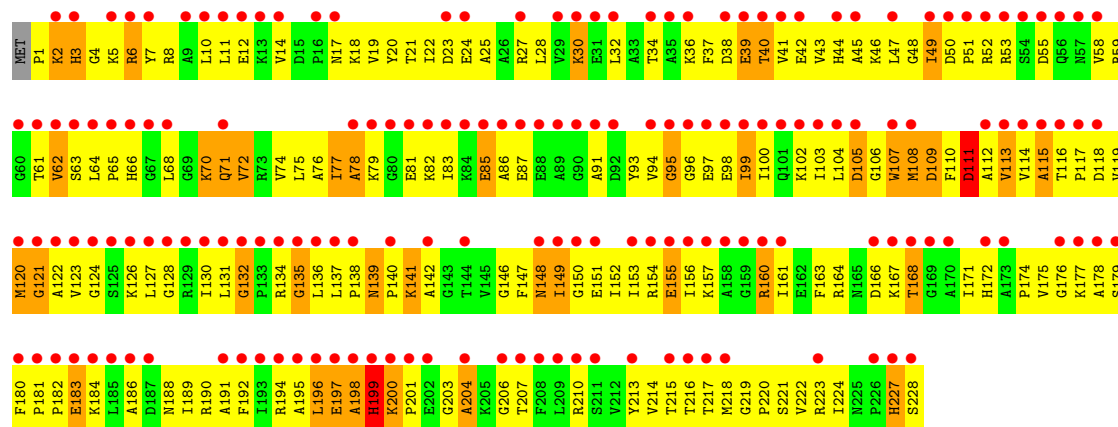
• Molecule 12: 5S RIBOSOMAL RNA

Chain B:



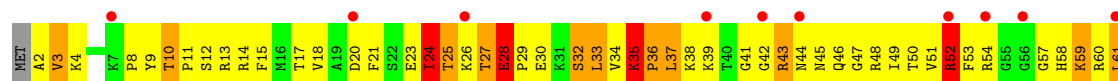
• Molecule 13: 50S RIBOSOMAL PROTEIN L1

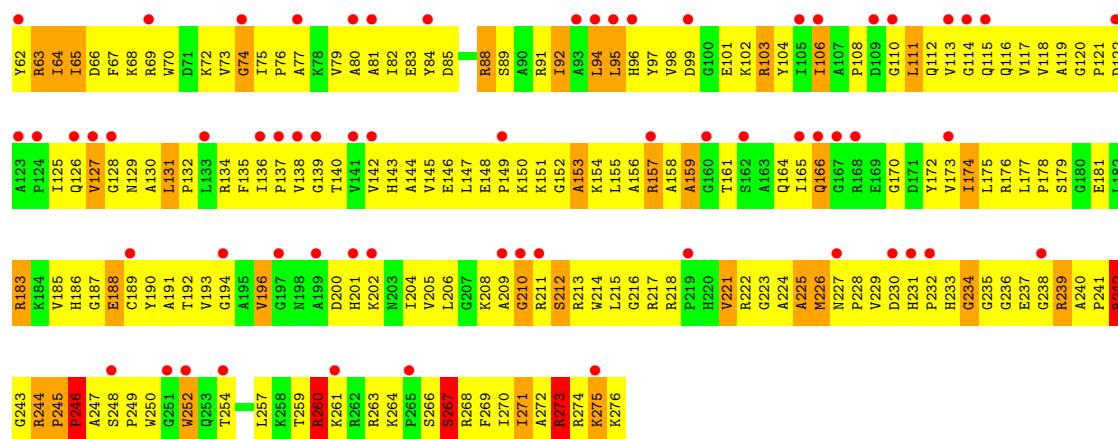
Chain C:



• Molecule 14: 50S RIBOSOMAL PROTEIN L2

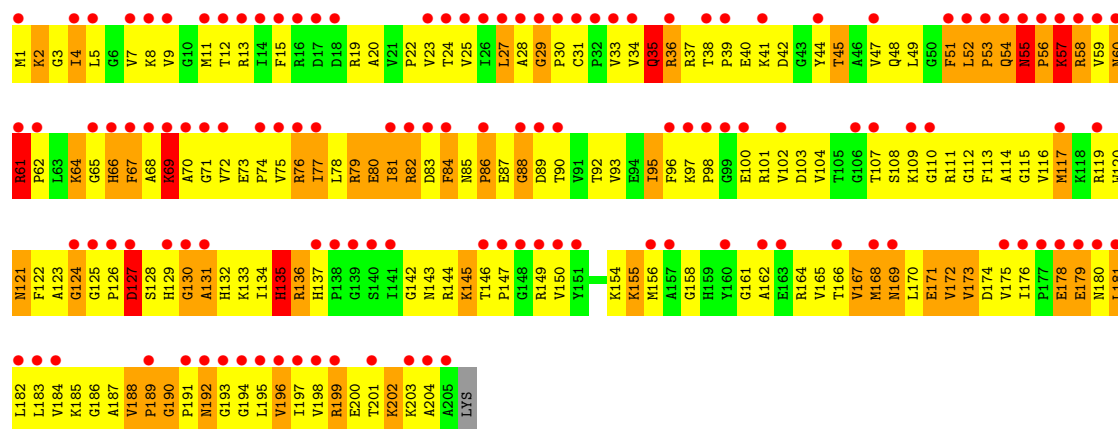
Chain D:





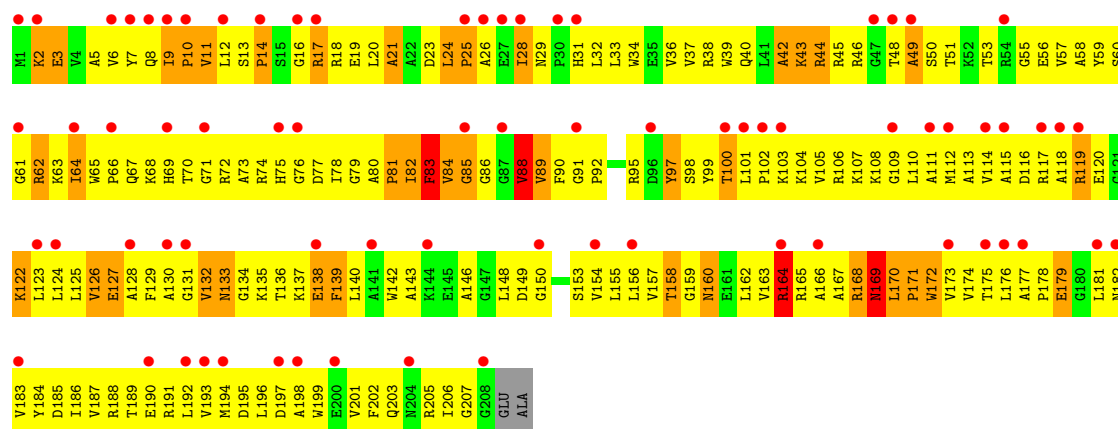
• Molecule 15: 50S RIBOSOMAL PROTEIN L3

Chain E:



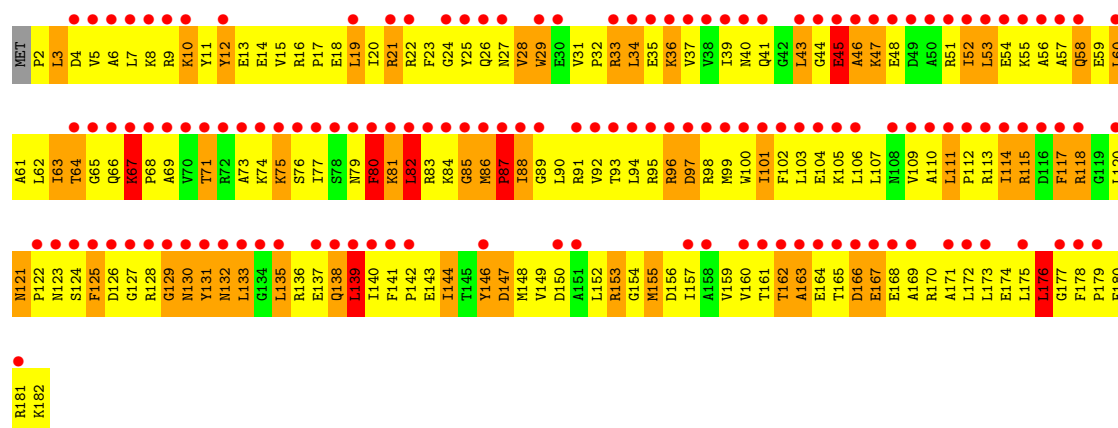
• Molecule 16: 50S RIBOSOMAL PROTEIN L4

Chain F:



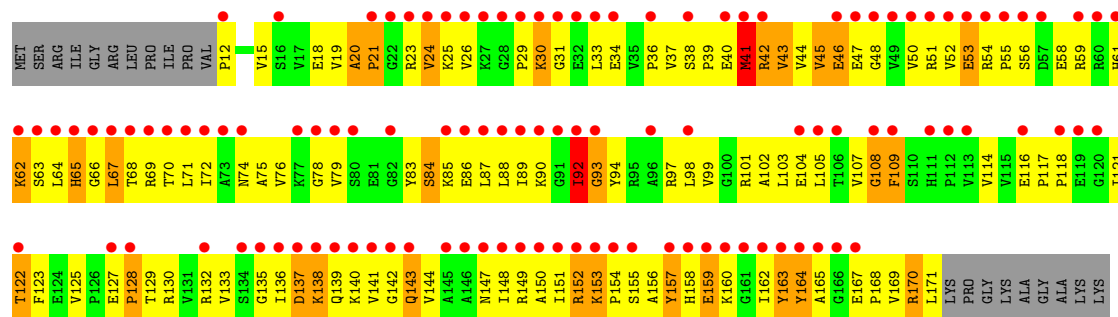
• Molecule 17: 50S RIBOSOMAL PROTEIN L5

Chain G:



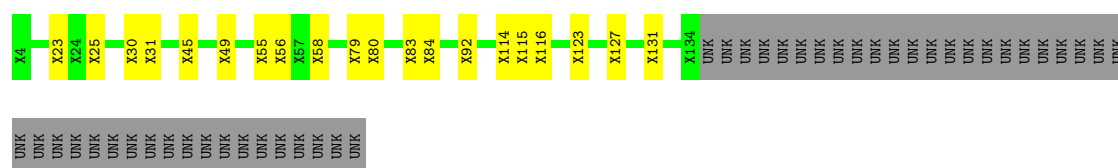
• Molecule 18: 50S RIBOSOMAL PROTEIN L6

Chain H:



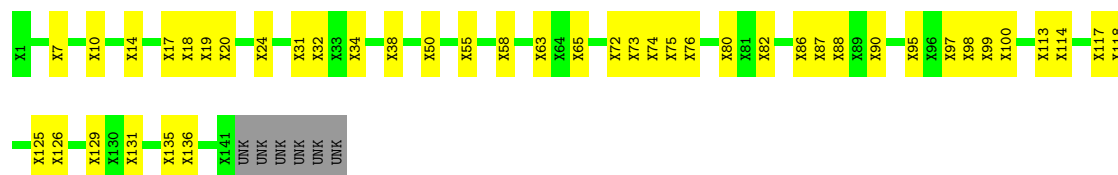
• Molecule 19: 50S RIBOSOMAL PROTEIN L10

Chain J:



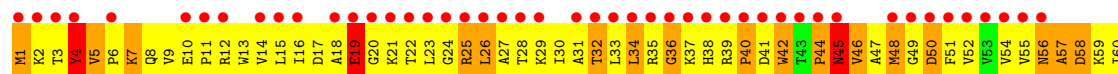
• Molecule 20: 50S RIBOSOMAL PROTEIN L11

Chain K:

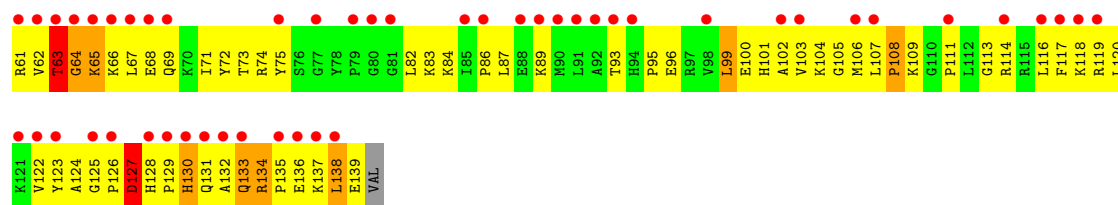


• Molecule 21: 50S RIBOSOMAL PROTEIN L13

Chain N:

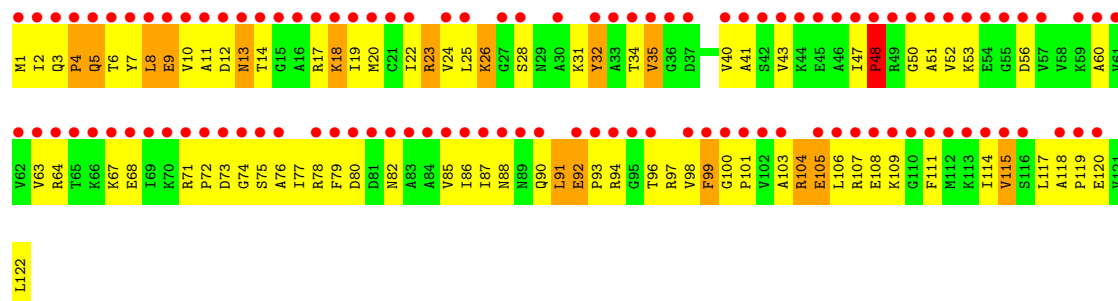






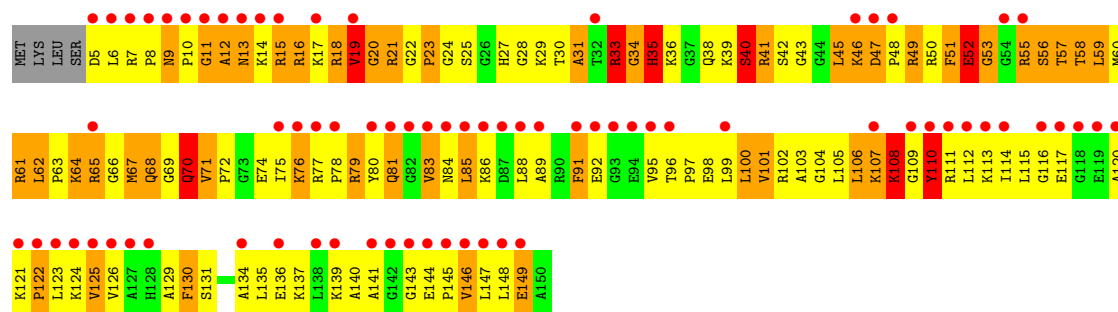
• Molecule 22: 50S RIBOSOMAL PROTEIN L14

Chain O:



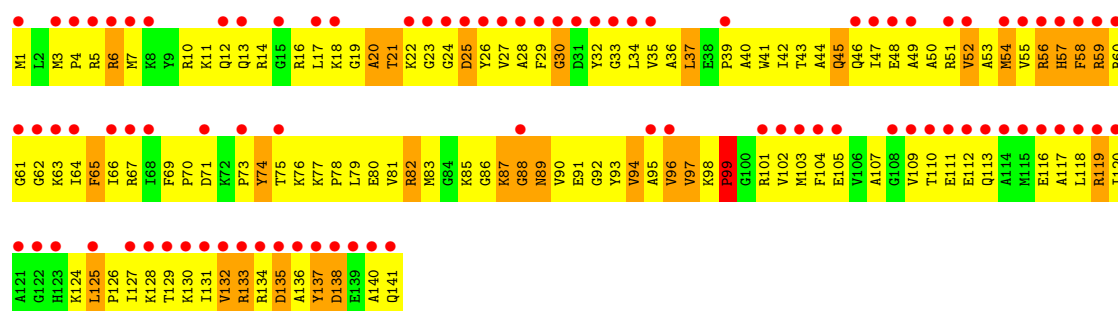
• Molecule 23: 50S RIBOSOMAL PROTEIN L15

Chain P:



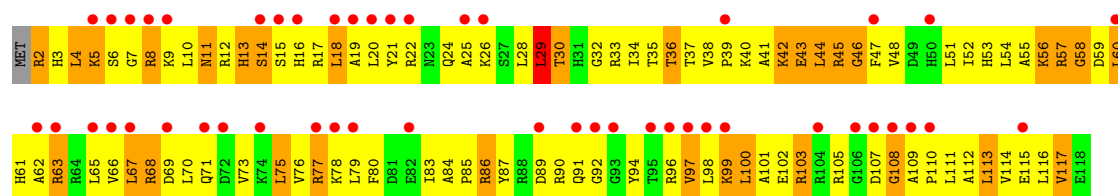
• Molecule 24: 50S RIBOSOMAL PROTEIN L16

Chain Q:



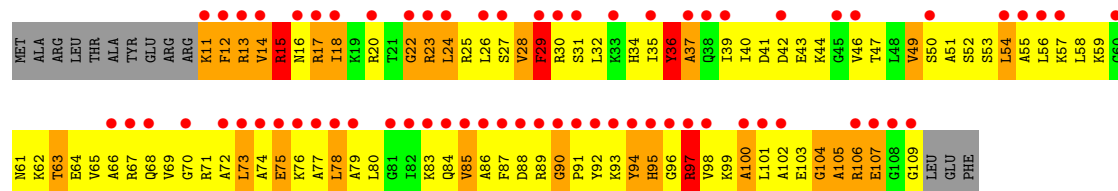
• Molecule 25: 50S RIBOSOMAL PROTEIN L17

Chain R:



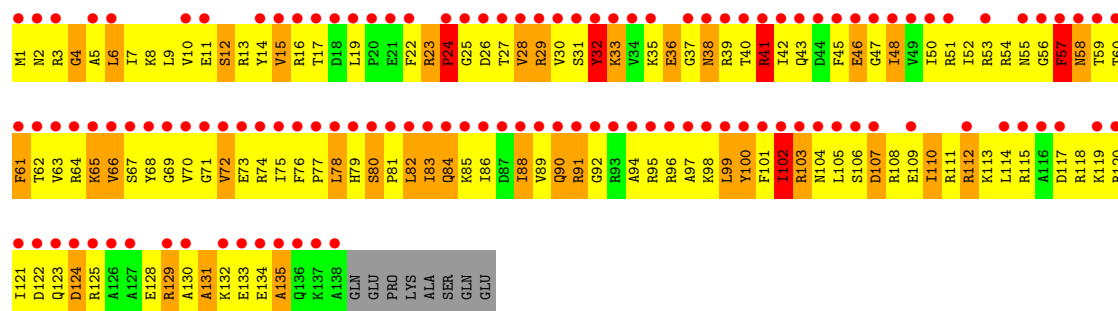
• Molecule 26: 50S RIBOSOMAL PROTEIN L18

Chain S:



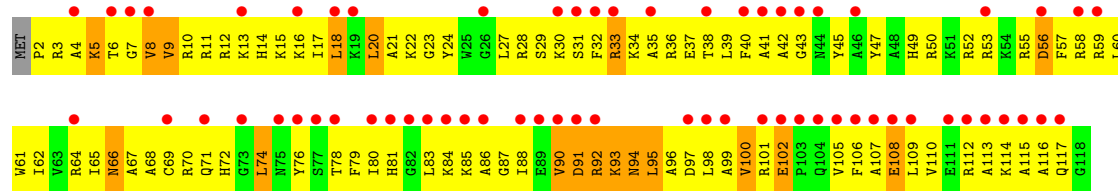
• Molecule 27: 50S RIBOSOMAL PROTEIN L19

Chain T:



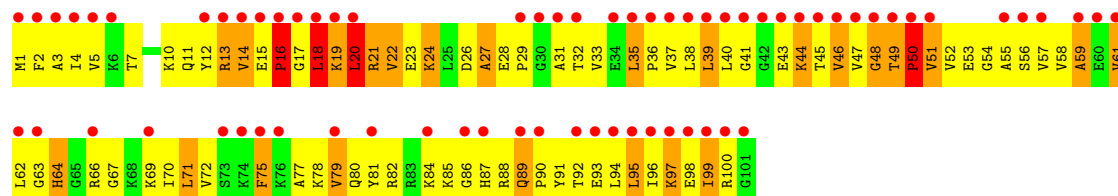
• Molecule 28: 50S RIBOSOMAL PROTEIN L20

Chain U:

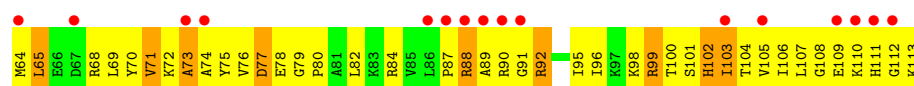


• Molecule 29: 50S RIBOSOMAL PROTEIN L21

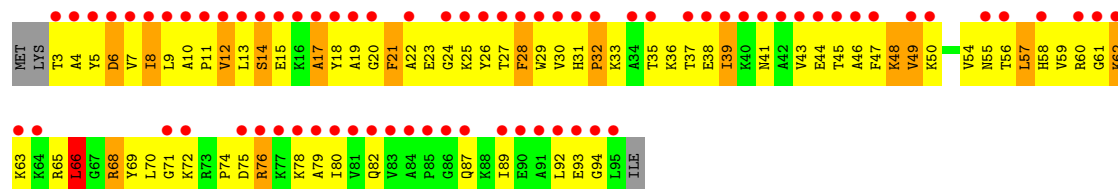
Chain V:



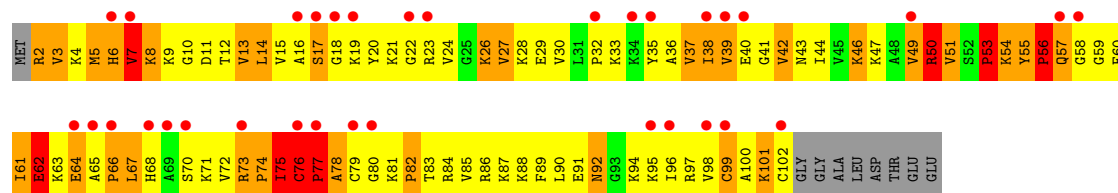
• Molecule 30: 50S RIBOSOMAL PROTEIN L22



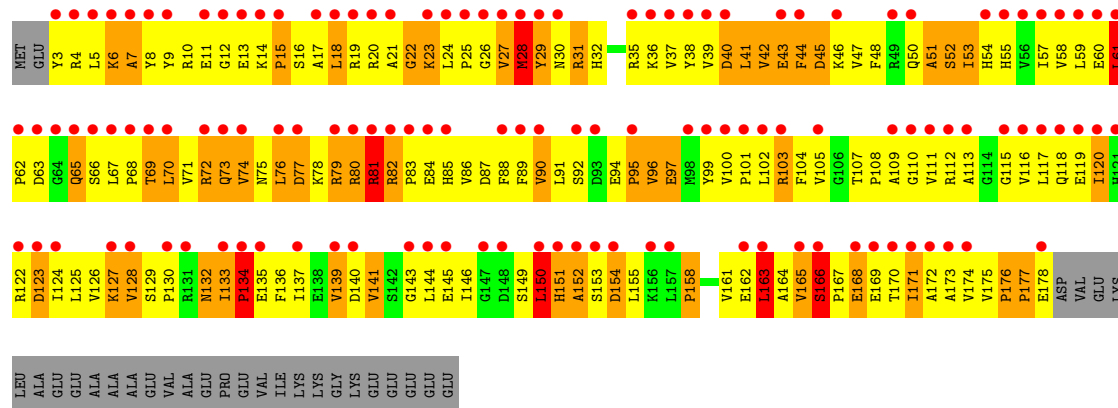
- Molecule 31: 50S RIBOSOMAL PROTEIN L23



- Molecule 32: 50S RIBOSOMAL PROTEIN L24



- Molecule 33: 50S RIBOSOMAL PROTEIN L25



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.57Å 268.36Å 403.88Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 49.91 – 3.48	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-3.60) 87.3 (49.91-3.48)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.281 , 0.315 0.422 , 0.428	Depositor DCC
$R_{free}$ test set	35772 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 91.5	EDS
Estimated twinning fraction	0.098 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 714740 reflections	Xtriage
$F_o, F_c$ correlation	0.52	EDS
Total number of atoms	93761	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0	0.40	0/671	0.67	0/892
2	1	0.57	0/739	0.91	0/983
3	2	0.44	0/600	0.87	2/793 (0.3%)
4	3	0.44	0/473	0.74	0/636
5	4	0.71	0/350	0.79	0/476
6	5	0.44	0/473	0.72	0/639
7	6	0.53	0/440	0.91	0/586
8	7	0.50	0/427	0.75	0/563
9	8	0.51	0/516	0.78	0/681
10	9	0.42	0/310	0.66	0/407
11	A	0.61	2/69972 (0.0%)	0.76	36/109237 (0.0%)
12	B	0.46	0/2853	0.72	0/4451
13	C	0.45	2/1774 (0.1%)	0.69	0/2391
14	D	0.59	0/2195	0.86	1/2955 (0.0%)
15	E	0.48	0/1597	0.75	0/2155
16	F	0.45	0/1659	0.73	0/2246
17	G	0.46	0/1499	0.81	3/2016 (0.1%)
18	H	0.37	0/1246	0.70	0/1684
21	N	0.42	0/1132	0.75	1/1527 (0.1%)
22	O	0.49	0/943	0.79	0/1269
23	P	0.49	0/1131	1.00	7/1504 (0.5%)
24	Q	0.44	0/1143	0.71	0/1527
25	R	0.41	0/974	0.74	0/1302
26	S	0.41	0/779	0.72	0/1038
27	T	0.47	0/1156	0.75	0/1544
28	U	0.43	0/975	0.74	0/1297
29	V	0.39	0/790	0.73	0/1057
30	W	0.44	0/907	0.71	0/1216
31	X	0.47	0/740	0.71	0/995
32	Y	0.44	0/789	0.81	1/1053 (0.1%)
33	Z	0.43	0/1435	0.77	0/1949
All	All	0.57	4/100688 (0.0%)	0.77	51/151069 (0.0%)

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
5	4	0	1
11	A	2	84
21	N	0	1
All	All	2	86

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	218	MET	CG-SD	6.21	1.97	1.81
13	C	120	MET	CG-SD	5.97	1.96	1.81
11	A	761	A	C5-C6	-5.87	1.35	1.41
11	A	733	G	C5-C6	-5.61	1.36	1.42

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1799	G	C2'-C3'-O3'	8.77	128.80	109.50
11	A	1819	A	C2'-C3'-O3'	8.63	128.48	109.50
11	A	2346	A	N9-C1'-C2'	8.34	124.85	114.00
23	P	41	ARG	N-CA-C	-8.16	88.97	111.00
11	A	1653	G	C2'-C3'-O3'	8.01	127.11	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	1799	G	C3'
11	A	1819	A	C3'

5 of 86 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	4	43	TYR	Sidechain
11	A	250	G	Sidechain
11	A	269	U	Sidechain
11	A	63	U	Sidechain
11	A	72	U	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	662	0	688	110	0
2	1	732	0	808	156	0
3	2	598	0	653	166	0
4	3	468	0	523	74	0
5	4	341	0	339	70	0
6	5	459	0	480	98	0
7	6	433	0	461	157	0
8	7	419	0	467	71	0
9	8	508	0	576	141	0
10	9	307	0	338	74	0
11	A	62474	0	31497	4282	0
12	B	2551	0	1295	152	0
13	C	1742	0	1800	263	0
14	D	2145	0	2234	441	0
15	E	1564	0	1629	331	0
16	F	1624	0	1677	362	0
17	G	1474	0	1535	385	0
18	H	1223	0	1282	214	0
19	J	651	0	136	11	0
20	K	701	0	157	35	0
21	N	1105	0	1180	233	0
22	O	933	0	996	121	0
23	P	1114	0	1187	309	0
24	Q	1122	0	1179	240	0
25	R	960	0	1021	198	0
26	S	771	0	832	195	0
27	T	1142	0	1202	260	0
28	U	958	0	1015	223	0
29	V	779	0	852	167	0
30	W	896	0	953	153	0
31	X	726	0	778	118	0
32	Y	776	0	870	208	0
33	Z	1403	0	1432	320	0
All	All	93761	0	62072	9334	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 60.

The worst 5 of 9334 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:1:41:ARG:NH2	11:A:1365:A:H5''	1.53	1.24
7:6:45:LYS:H	7:6:45:LYS:CD	1.48	1.19
32:Y:46:LYS:H	32:Y:62:GLU:HG2	1.10	1.16
11:A:1887:C:H2'	11:A:1888:G:H5''	1.22	1.15
2:1:13:ILE:HD11	11:A:396:G:H5'	1.14	1.14

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	0	82/85 (96%)	54 (66%)	20 (24%)	8 (10%)	1	18
2	1	92/98 (94%)	55 (60%)	22 (24%)	15 (16%)	0	6
3	2	69/72 (96%)	43 (62%)	10 (14%)	16 (23%)	0	2
4	3	58/60 (97%)	28 (48%)	15 (26%)	15 (26%)	0	1
5	4	43/71 (61%)	20 (46%)	15 (35%)	8 (19%)	0	4
6	5	57/60 (95%)	33 (58%)	13 (23%)	11 (19%)	0	3
7	6	48/54 (89%)	17 (35%)	14 (29%)	17 (35%)	0	0
8	7	47/49 (96%)	27 (57%)	12 (26%)	8 (17%)	0	5
9	8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	3
10	9	35/37 (95%)	18 (51%)	9 (26%)	8 (23%)	0	2
13	C	226/229 (99%)	143 (63%)	53 (24%)	30 (13%)	0	10
14	D	273/276 (99%)	176 (64%)	63 (23%)	34 (12%)	1	12
15	E	203/206 (98%)	109 (54%)	45 (22%)	49 (24%)	0	1
16	F	206/210 (98%)	120 (58%)	47 (23%)	39 (19%)	0	3
17	G	179/182 (98%)	86 (48%)	52 (29%)	41 (23%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	H	158/180 (88%)	98 (62%)	36 (23%)	24 (15%)	0	7
21	N	137/140 (98%)	75 (55%)	39 (28%)	23 (17%)	0	5
22	O	120/122 (98%)	91 (76%)	17 (14%)	12 (10%)	1	17
23	P	144/150 (96%)	72 (50%)	35 (24%)	37 (26%)	0	1
24	Q	139/141 (99%)	77 (55%)	46 (33%)	16 (12%)	1	13
25	R	115/118 (98%)	68 (59%)	25 (22%)	22 (19%)	0	3
26	S	97/112 (87%)	37 (38%)	35 (36%)	25 (26%)	0	1
27	T	136/146 (93%)	63 (46%)	40 (29%)	33 (24%)	0	1
28	U	115/118 (98%)	69 (60%)	34 (30%)	12 (10%)	1	16
29	V	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	3
30	W	111/113 (98%)	73 (66%)	24 (22%)	14 (13%)	0	11
31	X	91/96 (95%)	55 (60%)	20 (22%)	16 (18%)	0	4
32	Y	99/110 (90%)	37 (37%)	29 (29%)	33 (33%)	0	0
33	Z	174/206 (84%)	87 (50%)	47 (27%)	40 (23%)	0	2
All	All	3415/3607 (95%)	1926 (56%)	852 (25%)	637 (19%)	0	3

5 of 637 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	47	PRO
1	0	55	ARG
1	0	56	ASP
2	1	27	GLU
2	1	45	ASN

### 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 X-ray entries followed by that with respect to entries of similar resolution. 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	0	66/67 (98%)	52 (79%)	14 (21%)	1	10
2	1	78/83 (94%)	59 (76%)	19 (24%)	1	7
3	2	66/67 (98%)	49 (74%)	17 (26%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	51/52 (98%)	44 (86%)	7 (14%)	5	31
5	4	39/63 (62%)	26 (67%)	13 (33%)	0	3
6	5	51/52 (98%)	47 (92%)	4 (8%)	18	65
7	6	49/52 (94%)	41 (84%)	8 (16%)	3	22
8	7	41/42 (98%)	32 (78%)	9 (22%)	1	9
9	8	53/55 (96%)	45 (85%)	8 (15%)	4	27
10	9	34/34 (100%)	30 (88%)	4 (12%)	8	39
13	C	180/181 (99%)	157 (87%)	23 (13%)	6	35
14	D	217/218 (100%)	180 (83%)	37 (17%)	3	20
15	E	165/166 (99%)	142 (86%)	23 (14%)	5	31
16	F	165/166 (99%)	152 (92%)	13 (8%)	18	64
17	G	155/156 (99%)	130 (84%)	25 (16%)	3	23
18	H	132/148 (89%)	118 (89%)	14 (11%)	10	46
21	N	117/119 (98%)	103 (88%)	14 (12%)	7	38
22	O	100/100 (100%)	90 (90%)	10 (10%)	11	50
23	P	112/116 (97%)	88 (79%)	24 (21%)	1	10
24	Q	111/111 (100%)	91 (82%)	20 (18%)	2	16
25	R	100/101 (99%)	86 (86%)	14 (14%)	5	30
26	S	77/88 (88%)	66 (86%)	11 (14%)	5	29
27	T	120/127 (94%)	99 (82%)	21 (18%)	3	18
28	U	92/94 (98%)	84 (91%)	8 (9%)	15	59
29	V	82/82 (100%)	66 (80%)	16 (20%)	2	13
30	W	91/92 (99%)	79 (87%)	12 (13%)	6	33
31	X	74/78 (95%)	67 (90%)	7 (10%)	12	52
32	Y	84/91 (92%)	68 (81%)	16 (19%)	2	14
33	Z	155/179 (87%)	127 (82%)	28 (18%)	2	16
All	All	2857/2980 (96%)	2418 (85%)	439 (15%)	4	25

5 of 439 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	F	169	ASN
21	N	45	ASN

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Mol	Chain	Res	Type
32	Y	67	LEU
17	G	36	LYS
17	G	166	ASP

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

Mol	Chain	Res	Type
16	F	69	HIS
18	H	147	ASN
31	X	55	ASN
16	F	75	HIS
16	F	204	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	2900/2915 (99%)	647 (22%)	55 (1%)
12	B	118/122 (96%)	29 (24%)	1 (0%)
All	All	3018/3037 (99%)	676 (22%)	56 (1%)

5 of 676 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	10	G
11	A	15	G
11	A	27	G
11	A	32	C
11	A	34	C

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1069	A
11	A	1541	G
11	A	2610	C
11	A	1210	A
11	A	1301	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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(Å²)	Q<0.9	
1	0	84/85 (98%)	3.80	60 (71%)	0 1	104, 116, 128, 137	0
2	1	94/98 (95%)	1.48	28 (29%)	1 1	41, 71, 107, 111	0
3	2	71/72 (98%)	2.93	40 (56%)	0 1	84, 115, 128, 130	0
4	3	60/60 (100%)	2.50	29 (48%)	1 1	106, 122, 132, 148	0
5	4	45/71 (63%)	5.42	38 (84%)	0 1	107, 169, 196, 198	0
6	5	59/60 (98%)	1.83	22 (37%)	1 1	89, 116, 175, 187	0
7	6	50/54 (92%)	3.50	42 (84%)	0 1	78, 119, 146, 152	0
8	7	49/49 (100%)	1.25	13 (26%)	1 2	59, 77, 144, 152	0
9	8	64/65 (98%)	1.58	24 (37%)	1 1	80, 104, 124, 138	0
10	9	37/37 (100%)	5.15	30 (81%)	0 1	104, 117, 124, 128	0
11	A	2901/2915 (99%)	5.14	2477 (85%)	0 1	31, 100, 192, 200	0
12	B	119/122 (97%)	7.68	118 (99%)	0 0	103, 142, 169, 175	0
13	C	228/229 (99%)	3.81	169 (74%)	0 1	92, 122, 168, 178	0
14	D	275/276 (99%)	1.37	73 (26%)	1 2	30, 67, 96, 110	0
15	E	205/206 (99%)	2.90	126 (61%)	0 1	67, 106, 143, 154	0
16	F	208/210 (99%)	1.76	73 (35%)	1 1	61, 123, 160, 167	0
17	G	181/182 (99%)	4.00	140 (77%)	0 1	103, 128, 146, 163	0
18	H	160/180 (88%)	3.50	113 (70%)	0 1	131, 155, 174, 176	0
19	J	0/173	-	-	-	-	-
20	K	0/147	-	-	-	-	-
21	N	139/140 (99%)	3.58	96 (69%)	0 1	103, 123, 148, 155	0
22	O	122/122 (100%)	4.10	108 (88%)	0 1	60, 80, 96, 105	0
23	P	146/150 (97%)	2.33	74 (50%)	0 1	71, 113, 133, 140	0
24	Q	141/141 (100%)	3.26	90 (63%)	0 1	73, 106, 130, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9	
25	R	117/118 (99%)	2.01	48 (41%)	1 1	81, 105, 123, 143	0
26	S	99/112 (88%)	3.85	67 (67%)	0 1	96, 133, 155, 162	0
27	T	138/146 (94%)	3.86	121 (87%)	0 1	72, 112, 166, 181	0
28	U	117/118 (99%)	2.73	64 (54%)	0 1	87, 120, 141, 147	0
29	V	101/101 (100%)	3.71	68 (67%)	0 1	105, 144, 159, 164	0
30	W	113/113 (100%)	1.47	28 (24%)	1 2	81, 109, 132, 136	0
31	X	93/96 (96%)	3.57	73 (78%)	0 1	96, 108, 124, 128	0
32	Y	101/110 (91%)	1.79	33 (32%)	1 1	124, 145, 165, 170	0
33	Z	176/206 (85%)	4.06	127 (72%)	0 1	107, 133, 161, 164	0
All	All	6493/6964 (93%)	4.01	4612 (71%)	0 1	30, 111, 168, 200	0

The worst 5 of 4612 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	A	1051	G	25.2
11	A	2758	A	21.4
11	A	2114	A	20.7
11	A	2792	G	19.8
11	A	2466	C	18.9

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.