



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:24 AM GMT

PDB ID : 2HGJ
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome showing how the 16S 3'-end mimicks mRNA E and P codons. This entry 2HGJ contains 50S ribosomal subunit. The 30S ribosomal subunit can be found in PDB entry 2HGI.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 5.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

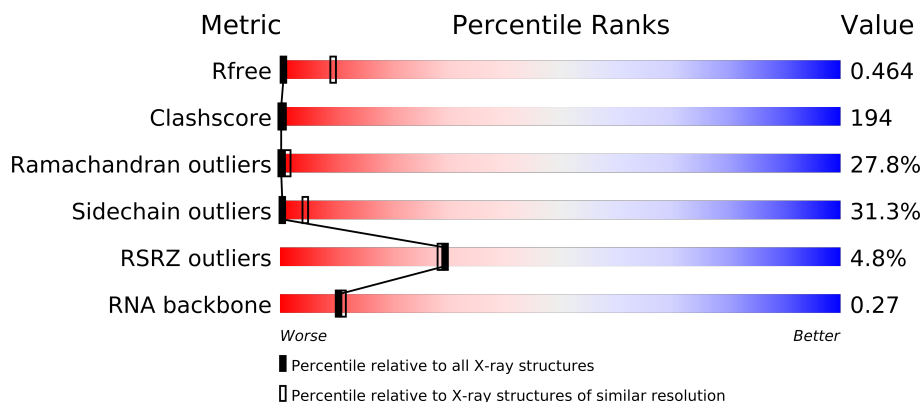
The following versions of software and data (see [references](#)) were used in the production of this report:

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 5.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1052 (6.50-3.50)
Clashscore	79885	1327 (6.50-3.50)
Ramachandran outliers	78287	1242 (6.50-3.50)
Sidechain outliers	78261	1221 (6.50-3.50)
RSRZ outliers	66119	1051 (6.50-3.50)
RNA backbone	1838	1037 (7.00-2.80)

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 ≥ 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	A	2916	
2	B	123	
3	C	229	
4	D	276	
5	E	206	
6	F	210	
7	G	182	
8	H	180	
9	K	148	
10	L	147	
11	M	140	
12	N	122	

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Mol	Chain	Length	Quality of chain
13	O	150	
14	P	141	
15	Q	118	
16	R	112	
17	S	146	
18	T	118	
19	U	101	
20	V	113	
21	W	96	
22	X	110	
23	Y	206	
24	Z	85	
25	1	67	
26	2	60	
27	3	71	
28	4	60	
29	5	54	
30	6	49	
31	7	65	
32	8	37	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 94012 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2889	Total	C	N	O	P	0	0	0
			62218	27691	11629	20009	2889			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	G	-	INSERTION	GB 48268

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total	C	N	O	P	0	0	0
			2641	1175	488	855	123			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	A	-	INSERTION	GB 48271
B	120	U	-	INSERTION	GB 48271

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	228	Total	C	N	O	S	0	0	0
			1742	1102	318	319	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	272	Total	C	N	O	S	0	0	0
			2124	1339	424	358	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	206	Total	C	N	O	S	0	0	0
			1578	997	302	273	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	208	Total	C	N	O	S	0	0	0
			1625	1034	303	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	182	Total	C	N	O	S	0	0	0
			1482	947	269	261	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	174	Total	C	N	O	S	0	0	0
			1328	844	248	235	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	148	Total	C	N	O	S	0	0	0
			1155	737	205	212	1			

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	138	Total	C	N	O	S	0	0	0
			1025	654	181	185	5			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	139	Total	C	N	O	S	0	0	0
			1113	717	207	186	3			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	N	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	145	Total	C	N	O	S	0	0	0
			1106	688	226	190	2			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	Q	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	R	110	Total	C	N	O	S	0	0	0
			877	553	175	149				

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	S	117	Total	C	N	O	S	0	0	0
			976	614	197	164	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	T	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	V	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	W	94	Total	C	N	O	S	0	0	0
			742	483	133	126				

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	110	Total	C	N	O	S	0	0	0
			844	539	158	141	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	180	Total	C	N	O	S	0	0	0
			1435	916	256	260	3			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Z	85	Total	C	N	O	S	0	0	0
			670	415	141	112	2			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1	67	Total	C	N	O	S	0	0	0
			567	350	116	99	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	2	59	Total	C	N	O			
			469	298	90	81	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	71	Total	C	N	O	S			
			581	364	108	104	5	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	57	Total	C	N	O	S			
			445	279	87	74	5	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	5	49	Total	C	N	O	S			
			426	265	87	70	4	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	6	49	Total	C	N	O	S			
			430	263	108	57	2	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	7	64	Total	C	N	O	S			
			515	331	102	79	3	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L36.

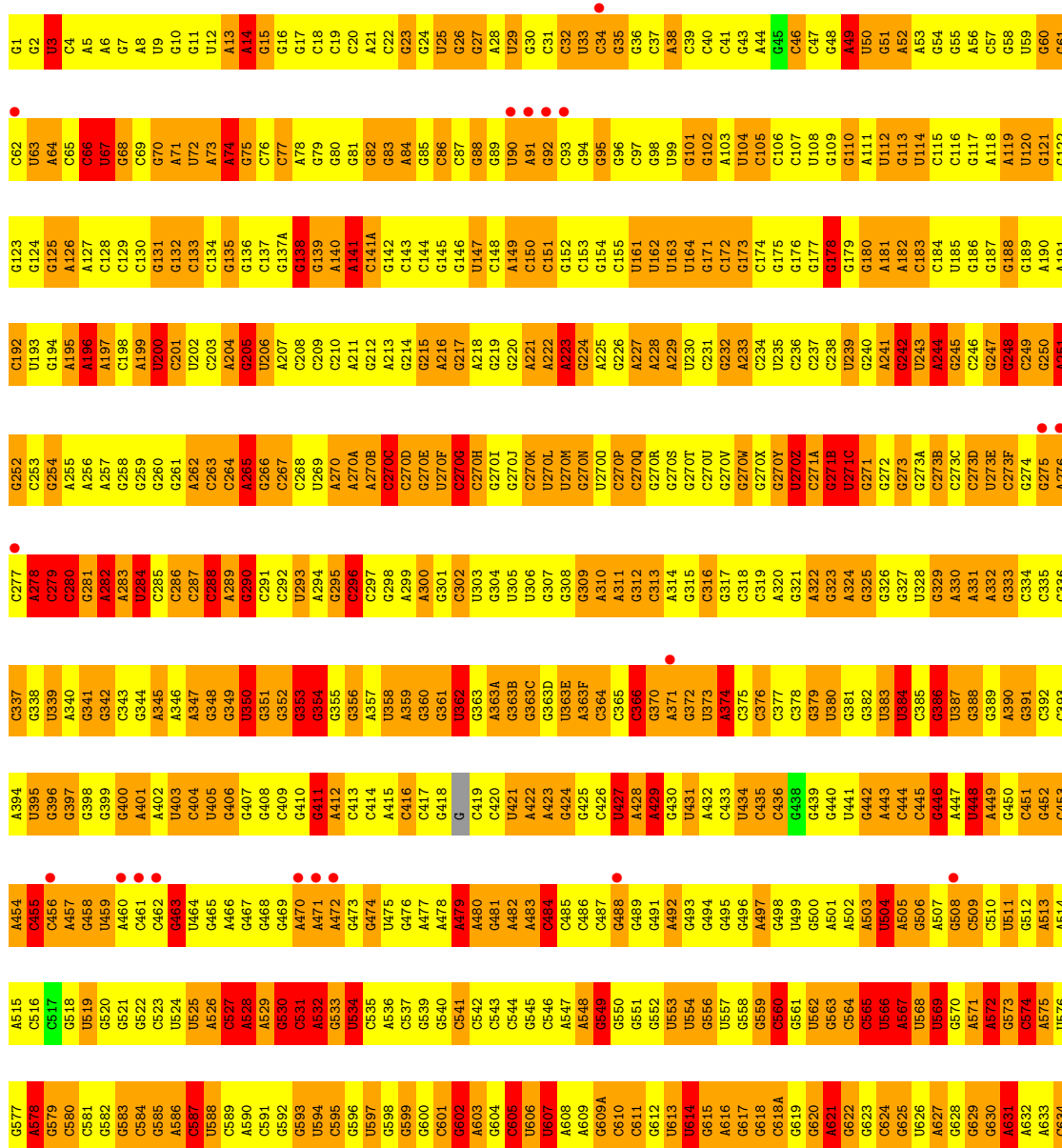
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	8	37	Total	C	N	O	S			
			307	188	68	47	4	0	0	0

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.

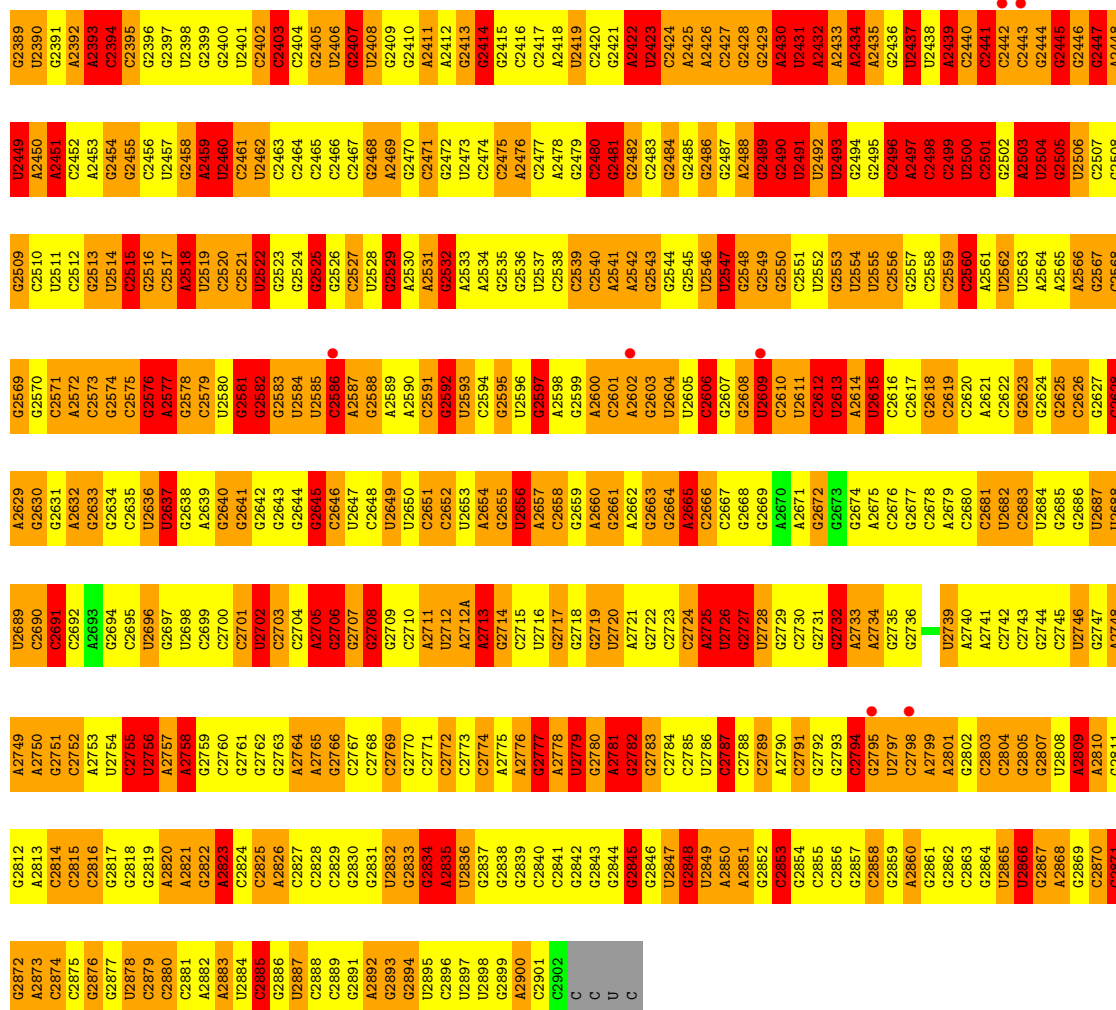
• Molecule 1: 23S ribosomal RNA

Chain A: 



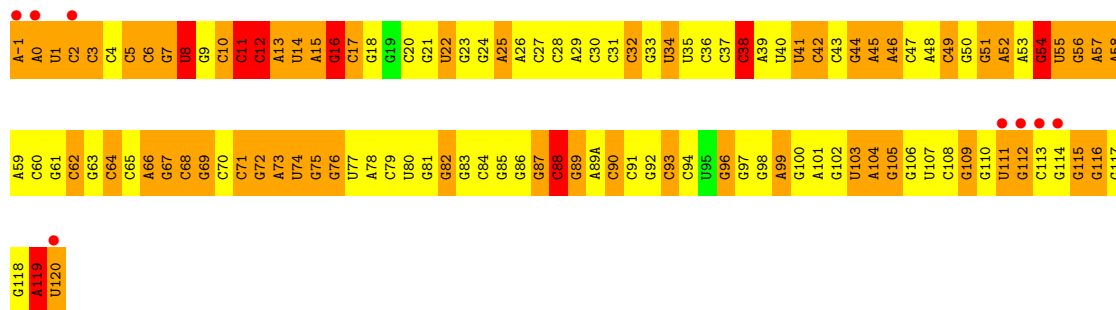
U1454	A1395	G1215	G1154	U1094	G1034	C974A	C914	G853	A793	G733	G673	G635
G1455	U1396	G1216	A1155	A1095	U1035	G975	C915	G854	G794	A734	G674	G636
A1456	U1397	C1217	A1156	A1096	G1036	C976	G916	G855	C795	A735	A675	A637
G1457	C1398	C1218	G1157	U1097	G1037	G977	A917	C856	C796	C736	A676	A638
C1458	C1399	G1219	A1158	A1098	U1038	G978	A918	C857	C797	C737	G677	U639
G1459	G1400	A1220	U1159	G1099	G1039	G979	G919	U858	G798	G738	G678	C640
A1460	G1401	C1221	G1160	C1100	C1040	A980	G920	C859	G799	G739	G679	G641
G1461	A1342	C1222	C1161	U1101	G1041	A981	G921	U860	A900	U740	G680	G642
C1462	G1343	C1223	G1162	C1102	A1042	C982	U922	A861	G801	G741	G681	A643
C1463	G1344	G1224	G1163	A1103	C1043	A983	C923	G862	A802	G742	G682	A644
C1464	C1345	C1225	G1164	A1104	A1044	A984	C924	A863	U803	G743	C683	C645
U1465	U1406	G1226	U1165	U1105	A1045	C985	C925	G864	A804	G744	G684	A646
G1466	G1346	A1227	C1166	G1106	A1046	C986	G926	C865	G805	G745	A685	A647
G1467	A1287	G1227	U1167	G1107	G1047	G987	G928	A866	C806	A746	G686	G648
A1468	U1288	G1228	U1168	U1108	A1048	A988	G929	C867	U807	U747	G687	G649
G1469	C1289	G1229	G1169	C1109	A1049	G989	U930	U868	G808	G748	G688	C
A1470	C1290	C1230	G1170	G1110	A1050	A990	G931	G869	G809	C749	A689	G
A1471	C1291	G1231	G1171	A1111	G1051	C991	G932	A870	U810	A750	G690	C
A1472	C1292	C1232	G1172	U1112	G1052	C992	A933	U871	U811	A751	C691	A
G1473	C1293	C1233	A1173	U1113	A1053	G993	G934	A872	C812	A752	C692	A
U1474	U1234	U1235	U1174	G1114	A1054	C994	C935	U873	U813	C753	C693	G
G1475	G1235	G1236	G1175	G1115	G1055	C995	C936	G874	C814	C754	G694	C
C1476	A1237	A1177	G1176	C1116	G1056	A996	U937	G875	C815	C755	G695	G
A1477	G1238	G1178	C1177	G1117	A1057	G997	G938	C876	C816	C756	G696	G
G1478	G1239	G1179	G1178	C1118	G1058	C998	G939	U877	C817	U757	G697	G
U1479	U1240	U1240	C1180	G1119	G1059	U999	G940	A878	G818	C758	C698	C
G1480	A1241	A1241	C1181	G1120	U1060	A1000	A941	G879	A819	G759	A699	C
U1481	C1242	A1242	A1182	C1121	U1061	A1001	G942	G880	U820	G760	G700	G
G1482	G1243	G1243	G1183	G1122	G1062	G1002	U943	G881	A821	A761	G701	C
A1483	C1304	G1244	G1184	C1123	G1063	G1003	G944	G882	U822	U762	G702	A
G1484	G1245	G1245	C1185	C1124	C1064	C1004	A945	G883	G823	G763	U703	C
G1485	C1305	C1246	G1186	G1125	U1065	G1005	G946	C884	A824	A764	G704	G
A1486	C1306	A1246	G1187	A1126	U1066	C1006	G947	C885	C825	G765	A705	C
G1487	U1247	A1247	U1187	A1127	A1067	C1007	G948	A886	U826	C766	A706	G
A1488	G1248	U1248	A1188	A1128	G1068	C1008	C949	A887	U827	U767	G707	G
U1489	U1249	G1250	A1189	A1129	A1069	A1009	G950	C888	U828	G768	C708	C
A1490	C1307	C1251	G1190	U1130	A1070	A1010	C951	C889	A829	G769	U709	C
G1491	G1311	C1251	G1191	G1131	G1071	G1011	G952	A890	G830	G770	G710	C
C1492	U1312	G1252	G1192	A1132	C1072	U1012	A953	G892	G831	C771	G711	C
G1493	U1313	A1253	G1193	U1133	A1073	C1013	G954	C893	G832	C772	G712	C
A1494	C1314	A1254	G1194	G1134	G1074	U1014	C955	C894	U833	U773	G713	C
A1495	G1315	U1255	C1195	C1135	C1075	G1015	G956	U895	C834	A774	U714	A653
A1496	C1376	C1256	C1196	G1136	C1076	G1016	A957	A896	A835	G775	G715	A655
U1497	A1317	C1257	G1197	G1137	A1077	G1017	U958	C897	G836	G776	A716	A656
C1498	C1318	C1258	U1198	G1138	U1078	C1018	A959	C898	C837	A777	G717	U657
U1499	G1319	G1259	U1199	G1139	U1079	U1019	A960	A899	C838	G778	A718	C658
G1500	C1320	G1260	C1200	C1140	C1080	A1020	C961	A900	U839	U779	C719	C659
C1501	A1261	C1261	C1201	U1141	U1081	G962	G962	A901	C940	G780	C720	G660
U1502	A1262	A1262	C1202	U1142	U1082	G1022	U963	C902	A841	A781	C721	C661
C1503	U1263	U1263	G1203	U1143	U1083	U1023	C964	C903	G842	A782	A722	G662
A1504	G1264	G1264	A1204	A1142A	A1084	G1024	C965	C904	G843	A783	G723	G663
C1505	A1265	A1265	U1205	A1143	A1085	G1025	G966	U905	C944	A784	U724	C664
C1506	G1266	G1266	G1206	G1144	A1086	U1026	C967	G906	G845	G785	G725	C665
A1507	U1267	C1207	C1207	C1145	A1087	G1027	G968	U907	C946	C786	G726	G666
A1508	A1268	C1208	C1208	C1146	G1087	A1027	U969	G908	U847	U787	G727	C667
C1509	U1269	A1269	G1209	A1148	A1088	A1028	C970	A909	G848	A788	G728	G668
A1510	C1330	C1270	A1210	G1149	G1089	A1029	C971	A849	A849	A789	G729	G669
U1511	G1271	G1271	U1211	C1150	U1090	G1030	G972	A910	C950	C790	C730	A670
G1449A	A1331	A1331	U1212	G1151	G1091	G1031	A973	A911	C912	C791	C671	C672
C1512	U1272	U1272	A1213	C1152	C1092	A1032	G974	U913	G852	G792	G732	C672
C1513	C1333	C1333	A1213	C1152	C1092	A1032	G974	U913	G852	G792	G732	C672
U1514	A1453	A1274	A1214	C1153	G1093	U1033	G974	U913	G852	G792	G732	C672

G2329	A2269	A2199	C2139	U2079	A2019	G1959	C1899	C1830	G1770	C1694	A1634	C1574	G1515
G2330	G2270	C2205	C2140	G2080	A2020	A1960	A1900	G1831	C1771	G1695	G1635	C1675	U1516
G2331	G2271	C2206	G2141	A2081	C2021	C1961	A1901	G1832	C1772	G1696	C1636	U1576	G1517
U2332	U2272	C2207	C2142	A2082	U2022	C1962	C1902	U1833	A1773	G1697	A1637	C1577	C1518
A2333	U2208	U2208	C2143	G2083	G2023	G1963	G1903	U1834	C1774	A1698	C1638	U1578	U1519
G2334	A2274	G2209	C2144	C2084	G2024	G1964	G1904	G1835	U1775	G1699	U1639	A1579	U1520
A2335	C2275	G2210	C2145	C2085	C2025	C1965	C1905	C1836	G1776	A1700	C1640	A1580	G1521
A2336	G2276	G2211	C2146	U2086	C2026	A1966	G1906	C1837	U1777	A1701	C1641	G1522	G1523
G2337	G2277	A2212	G2147	G2087	G2027	C1967	G1907	C1838	U1778	G1702	G1642	C1582	U1524
G2338	U2213	U2213	G2148	G2088	U2028	G1968	C1908	G1839	A1779	G1703	G1643	A1583	G1525
G2339	G2278	G2215	G2149	G2089	G2029	A1969	C1909	G1840	U1780	G1704	C1644	C1585	G1526
G2340	G2280	G2216	U2150	G2090	A2030	A1971	G1910	U1841	C1781	G1705	G1645	A1586	G1527
G2341	C2281	G2217	G2151	G2091	A2031	A1972	U1911	G1842	C1782	U1706	G1646	A1587	G1528
C2342	G2282	G2218	G2152	U2092	G2032	A1973	A1912	C1843	A1783	G1707	G1647	C1588	A1529
U2343	C2283	G2219	G2153	G2093	A2033	G1973	A1913	G1844	A1784	C1708	C1648	C1589	U1530
U2344	G2284	G2224	G2154	G2094	U2034	C1974	A1914	G1845	A1785	U1709	G1649	U1590	C1531
G2345	C2285	A2225	G2155	C2095	G2035	G1975	A1915	G1846	A1786	C1710	G1650	C1591	C1532
A2346	A2286	G2226	G2156	U2096	G2036	U1976	A1916	A1847	A1787	C1711	G1651	C1592	C1533
A2347	U2287	A2227	G2157	C2097	G2037	A1977	U1917	A1848	C1788	C1712	A1652	G1593	C1534
U2348	A2288	G2228	A2158	U2098	G2038	A1978	A1918	G1849	A1789	U1716	G1653	G1594	U1535
G2349	G2289	C2229	G2159	U2099	C2039	C1979	A1919	G1850	C1790	G1717	A1654	G1595	U1536
C2350	G2290	G2230	G2160	G2100	C2040	G1980	A1920	U1851	A1791	G1718	A1655	A1596	C1537
G2351	U2291	C2231	G2161	G2101	U2041	A1981	G1921	C1852	G1792	G1725	C1656	A1597	C1538
A2352	C2292	U2232	G2162	U2102	A2042	C1982	A1922	A1853	U1793	G1726	C1657	C1598	G1539
G2353	C2293	U2233	C2163	C2103	C2043	C1983	U1923	A1854	C1794	U1727	C1658	C1599	G1540
G2354	C2294	G2234	C2164	G2104	G2044	G1984	C1924	G1855	C1795	G1728	U1659	C1600	U1541
C2355	G2295	G2235	G2165	C2105	G2045	G1985	C1925	G1856	U1796	A1729	C1660	U1601	G1542
C2356	U2296	G2236	G2166	G2106	G2046	A1986	U1926	G1857	C1797	G1730	G1661	U1602	A1543
U2357	G2297	U2167	C2167	C2107	U2047	G1987	A1927	G1858	U1798	G1731	C1662	A1603	C1544
G2358	A2298	G2237	G2168	C2108	G2048	C1988	A1928	A1859	G1799	A1732	C1663	C1604	A1545
G2359	G2299	G2239	A2169	U2109	G2049	G1989	G1929	G1860	C1800	G1733	A1664	C1605	A1546
C2360	G2300	C2240	A2170	G2110	G2050	C1990	G1930	G1861	G1801	C1734	A1665	C1606	A1547
A2361	C2301	A2241	A2051	C2111	A2051	U1991	U1991	G1862	A1802	C1735	G1666	C1607	C1548
G2362	G2302	G2242	U2172	G2112	G2052	G1992	A1932	G1863	A1803	C1741	G1667	A1608	C1549
G2363	G2303	U2243	A2173	U2113	G2053	U1993	G1933	U1864	C1804	C1742	A1668	A1609	C1550
C2364	G2304	U2244	A2054	A2114	A2054	C1994	C1934	G1869	U1805	G1743	A1669	C1611	C1551
G2365	A2305	U2245	G2055	G2115	G2055	U1995	G1935	C1870	C1806	G1746	C1670	C1612	G1552
A2366	C2306	G2246	G2056	G2116	G2056	C1996	A1936	A1871	G1807	G1747	U1671	G1613	A1553
G2367	G2307	A2247	A2057	A2117	A2057	G1997	A1937	A1872	U1808	G1748	C1672	A1614	A1554
G2368	G2308	C2248	C2178	U2118	A2058	G1998	A1938	G1878	A1809	A1749	U1673	C1615	G1555
A2369	A2309	U2249	C2179	A2119	A2059	C1999	U1939	C1879	G1810	G1750	G1674	A1616	C1556
G2370	A2310	G2250	U2180	G2120	A2060	G2000	U1940	C1880	G1811	C1751	C1675	C1617	C1557
A2371	G2311	G2251	G2181	G2121	G2061	A2001	C1941	C1881	A1812	G1752	A1676	A1618	A1558
G2372	U2312	G2252	G2182	U2122	A2062	G2002	C1942	C1882	G1813	G1753	C1677	G1619	G1559
G2373	C2313	G2253	C2183	G2123	C2063	G2003	U1943	G1883	G1814	C1754	G1678	U1620	G1560
C2374	G2314	C2254	G2184	G2124	C2064	G2004	U1944	A1884	A1815	A1755	U1679	G1621	G1561
G2375	G2315	G2255	C2185	G2125	C2065	A2005	G1945	A1885	G1816	G1756	U1680	G1622	A1562
A2376	G2316	G2256	G2186	A2126	C2066	C2006	U1946	C1886	G1817	U1757	G1681	G1623	G1563
A2377	C2317	U2257	G2187	G2127	G2067	C2007	C1947	C1887	U1818	G1758	G1682	G1624	G1564
A2378	G2318	C2258	C2188	C2128	U2068	C2008	G1948	G1888	A1819	A1759	C1683	C1625	C1565
G2379	G2319	G2259	U2189	C2129	G2069	G1949	G1949	A1889	U1820	A1760	C1684	G1626	A1566
C2380	A2320	C2260	G2190	U2130	G2070	G2010	G1950	A1890	A1821	C1761	C1685	G1627	A1567
C2381	G2321	C2261	G2191	U2131	A2071	U2011	U1951	A1891	G1822	A1762	C1686	G1628	G1568
A2382	U2322	U2262	G2192	U2132	G2072	G2012	A1952	C1892	G1823	G1763	C1687	U1629	A1569
G2383	G2323	C2263	G2193	C2133	U2073	A2013	A1953	C1893	G1824	G1764	U1688	G1630	C1630A
G2384	C2324	C2264	G2194	A2134	C2074	A2014	G1954	C1894	A1825	C1765	A1689	A1570	A1571
C2385	U2265	U2265	C2195	A2135	U2075	A2015	U1955	C1895	G1826	U1766	C1691	A1631	A1572
C2386	A2266	A2266	C2196	C2136	U2076	U2016	U1956	G1896	G1827	C1767	U1692	A1632	A1573
U2387	U2327	A2077	C2137	U2137	A2077	G1828	C1957	G1897	G1828	U1768	C1692	G1633	
A2388	A2328	A2268	A2198	C2138	C2078	G2018	C1958	U1898	A1829	G1769	U1693		



• Molecule 2: 5S ribosomal RNA

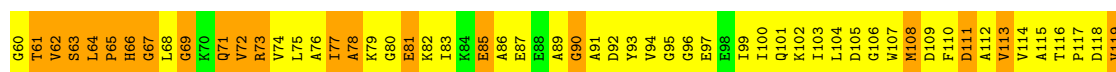
Chain B:



• Molecule 3: 50S ribosomal protein L1

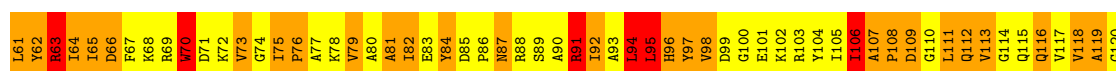
Chain C:





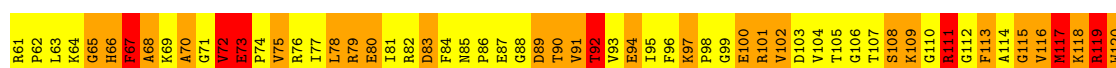
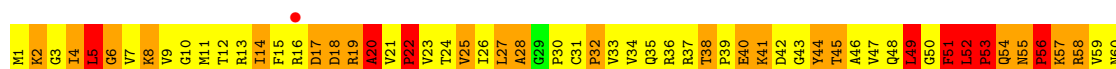
• Molecule 4: 50S ribosomal protein L2

Chain D:



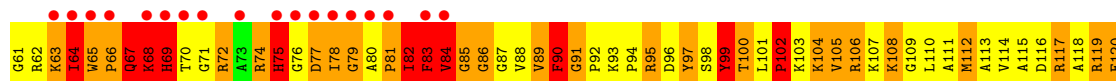
• Molecule 5: 50S ribosomal protein L3

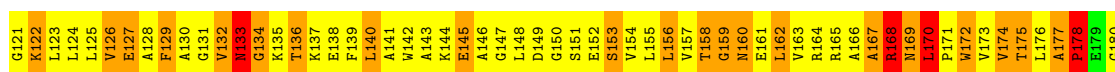
Chain E:



• Molecule 6: 50S ribosomal protein L4

Chain F:





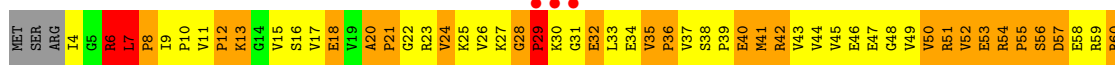
• Molecule 7: 50S ribosomal protein L5

Chain G:



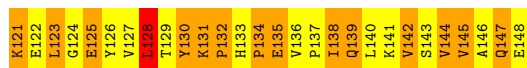
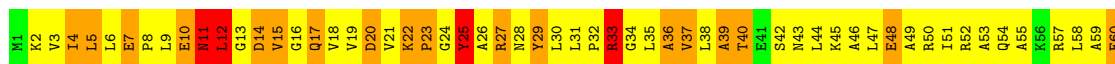
• Molecule 8: 50S ribosomal protein L6

Chain H:



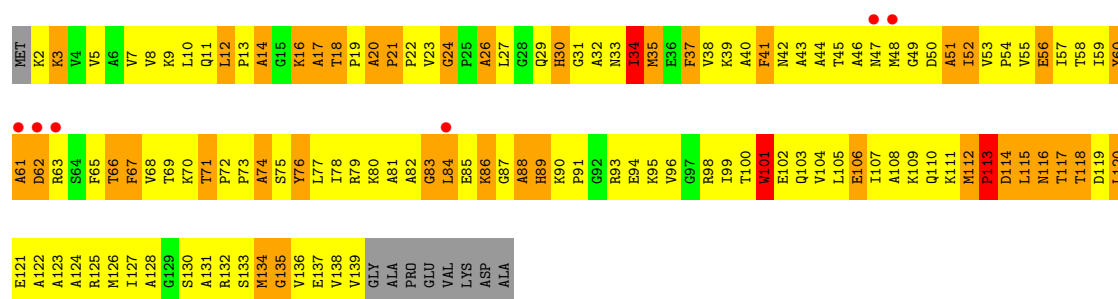
• Molecule 9: 50S ribosomal protein L9

Chain K:



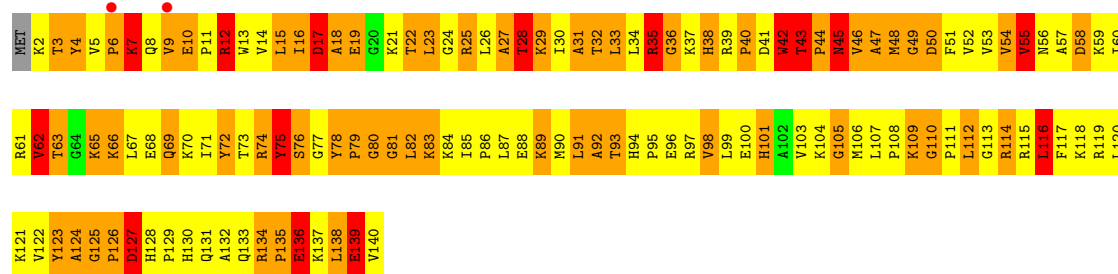
• Molecule 10: 50S ribosomal protein L11

Chain L:



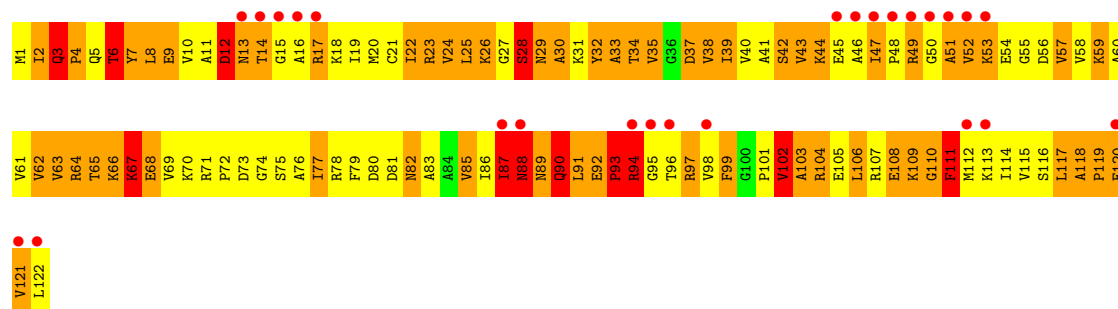
• Molecule 11: 50S ribosomal protein L13

Chain M:



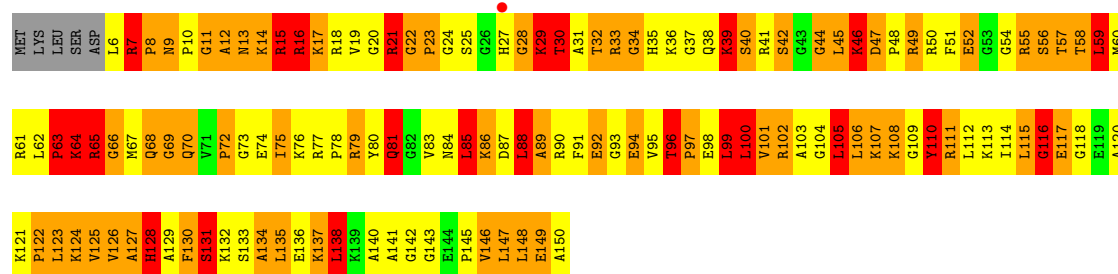
• Molecule 12: 50S ribosomal protein L14

Chain N:



• Molecule 13: 50S ribosomal protein L15

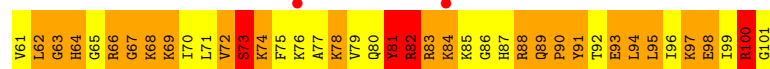
Chain O:



• Molecule 14: 50S ribosomal protein L16

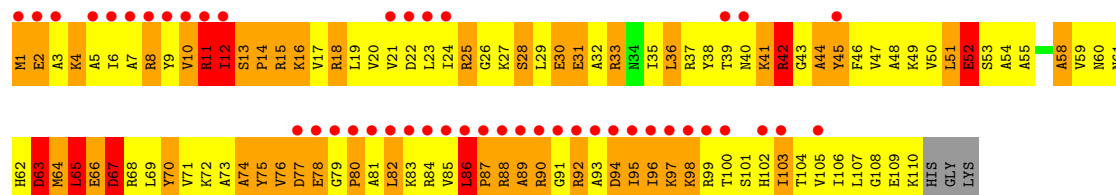
Chain P:

Responsibility	Percentage
Current government	85%
Opposition	15%



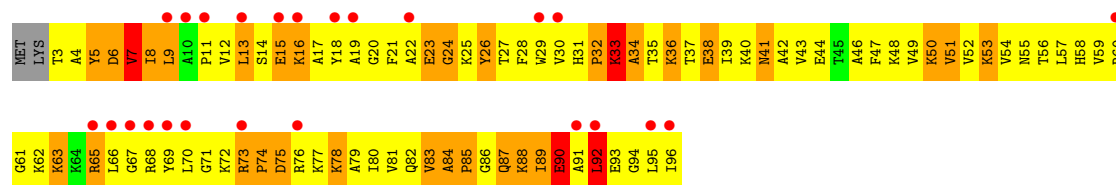
- Molecule 20: 50S ribosomal protein L22

Age Group	Percentage
18-24	~45%
25-34	~5%
35-44	~55%
45-54	~40%
55-64	~5%
65-74	~5%
75-84	~5%
85+	~5%



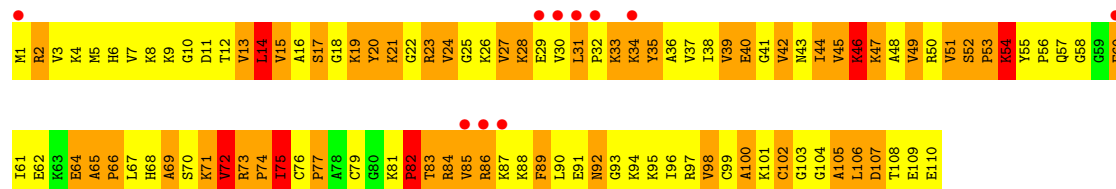
- Molecule 21: 50S ribosomal protein L23

Age Group	Percentage
18-24	~25%
25-34	~5%
35-44	~55%
45-54	~25%
55-64	~10%
65-74	~2%
75-84	~1%
85+	~1%

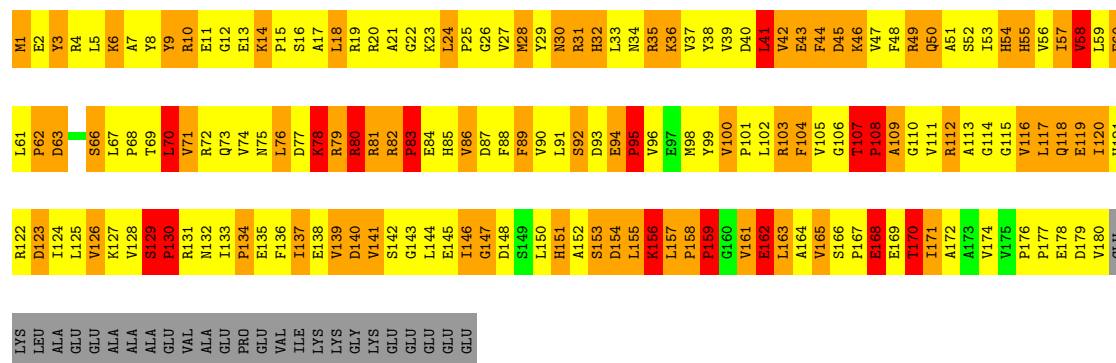


- Molecule 22: 50S ribosomal protein L24

Age Group	Percentage
18-24	10%
25-34	5%
35-44	45%
45-54	35%
55-64	10%
65-74	5%
75-84	2%
85+	0%

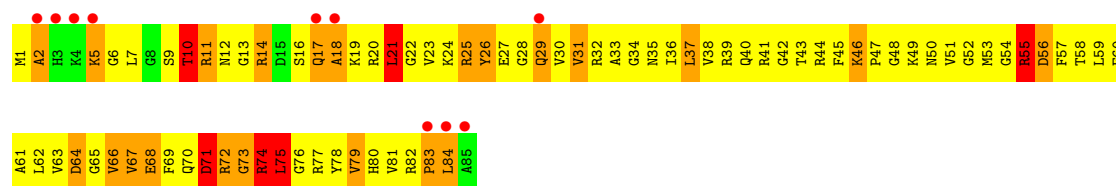


- Molecule 23: 50S ribosomal protein L25



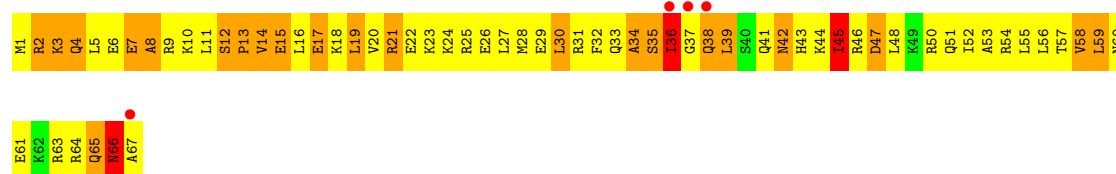
- Molecule 24: 50S ribosomal protein L27

Chain Z:



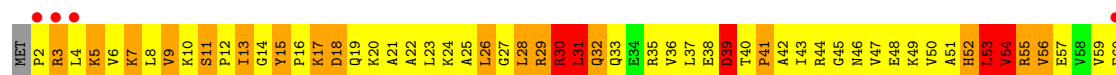
- Molecule 25: 50S ribosomal protein L29

Chain 1:



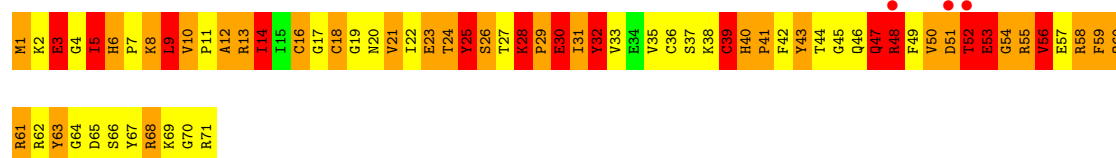
- Molecule 26: 50S ribosomal protein L30

Chain 2:



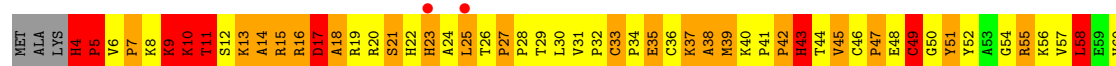
- Molecule 27: 50S ribosomal protein L31

Chain 3:



- Molecule 28: 50S ribosomal protein L32

Chain 4:



- Molecule 29: 50S ribosomal protein L33

Chain 5:



- Molecule 30: 50S ribosomal protein L34

Chain 6:



● Molecule 31: 50S ribosomal protein L35

Chain 7: A horizontal bar chart for Chain 7. The bar is mostly yellow, with a small red segment at the beginning and a small orange segment at the end.



● Molecule 32: 50S ribosomal protein L36

Chain 8: A horizontal bar chart for Chain 8. The bar is mostly yellow, with a small red segment at the beginning and a small orange segment at the end.



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	509.52Å 509.52Å 804.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.00 430.52 – 4.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (300.00-5.00) 96.7 (430.52-4.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.323 0.435 , 0.464	Depositor DCC
R_{free} test set	10525 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	99.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 18.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	1 of 252174 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	94012	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	A	1.06	154/69685 (0.2%)	1.16	463/108786 (0.4%)
2	B	0.86	4/2954 (0.1%)	1.01	8/4606 (0.2%)
3	C	0.50	0/1775	0.89	2/2393 (0.1%)
4	D	0.83	3/2174 (0.1%)	1.25	12/2927 (0.4%)
5	E	0.86	2/1611 (0.1%)	1.29	13/2171 (0.6%)
6	F	0.69	0/1660	1.11	8/2247 (0.4%)
7	G	0.63	0/1507	1.05	4/2027 (0.2%)
8	H	0.62	0/1354	1.06	5/1831 (0.3%)
9	K	0.69	0/1170	1.08	2/1581 (0.1%)
10	L	0.49	0/1044	0.90	1/1415 (0.1%)
11	M	0.83	1/1140 (0.1%)	1.19	8/1537 (0.5%)
12	N	1.00	0/942	1.39	8/1268 (0.6%)
13	O	0.79	0/1123	1.27	15/1493 (1.0%)
14	P	0.85	1/1100 (0.1%)	1.27	6/1470 (0.4%)
15	Q	0.69	0/974	1.08	2/1302 (0.2%)
16	R	0.78	0/887	1.11	2/1180 (0.2%)
17	S	0.95	0/990	1.44	13/1325 (1.0%)
18	T	0.79	0/982	1.18	6/1306 (0.5%)
19	U	0.90	1/790 (0.1%)	1.44	11/1057 (1.0%)
20	V	0.78	0/886	1.11	2/1189 (0.2%)
21	W	0.57	0/756	0.91	0/1015
22	X	0.53	0/857	1.09	4/1142 (0.4%)
23	Y	0.66	0/1467	1.13	6/1992 (0.3%)
24	Z	0.72	0/679	1.11	2/902 (0.2%)
25	1	0.64	0/569	0.91	0/751
26	2	0.63	0/474	1.08	1/635 (0.2%)
27	3	1.00	2/594 (0.3%)	1.37	8/795 (1.0%)
28	4	0.74	1/459 (0.2%)	1.12	2/621 (0.3%)
29	5	0.91	0/433	1.61	7/576 (1.2%)
30	6	0.81	0/438	1.03	1/575 (0.2%)
31	7	0.70	0/523	1.23	3/690 (0.4%)
32	8	0.69	0/310	1.19	2/407 (0.5%)
All	All	0.97	169/102307 (0.2%)	1.16	627/153212 (0.4%)

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	A	0	546
2	B	0	16
4	D	0	2
5	E	0	1
6	F	0	1
8	H	0	1
14	P	0	3
17	S	0	2
19	U	0	2
20	V	0	1
21	W	0	1
27	3	0	2
All	All	0	578

The worst 5 of 169 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1203	G	O3'-P	-34.70	1.19	1.61
1	A	607	U	N3-C4	-31.59	1.10	1.38
1	A	2501	C	O3'-P	24.61	1.90	1.61
1	A	607	U	C2-N3	-22.10	1.22	1.37
1	A	607	U	C4-C5	19.62	1.61	1.43

The worst 5 of 627 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	U	N3-C4-O4	-29.32	98.87	119.40
1	A	1203	G	P-O3'-C3'	27.75	153.00	119.70
1	A	607	U	C5-C4-O4	20.38	138.13	125.90
1	A	2756	U	P-O3'-C3'	18.31	141.67	119.70
1	A	2501	C	O3'-P-O5'	-17.22	71.28	104.00

There are no chirality outliers.

5 of 578 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	A	Sidechain
1	A	25	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	3	U	Sidechain
1	A	32	C	Sidechain
1	A	67	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	A	62218	0	31353	14943	0
2	B	2641	0	1337	589	1
3	C	1742	0	1796	843	0
4	D	2124	0	2207	1513	0
5	E	1578	0	1647	1071	0
6	F	1625	0	1666	891	0
7	G	1482	0	1546	922	0
8	H	1328	0	1408	737	0
9	K	1155	0	1244	550	0
10	L	1025	0	1074	489	0
11	M	1113	0	1183	765	0
12	N	932	0	994	687	0
13	O	1106	0	1183	834	0
14	P	1080	0	1127	704	0
15	Q	960	0	1021	511	0
16	R	877	0	938	586	0
17	S	976	0	1033	660	0
18	T	964	0	1022	665	0
19	U	779	0	852	580	0
20	V	876	0	941	448	0
21	W	742	0	800	376	0
22	X	844	0	930	504	0
23	Y	1435	0	1463	735	0
24	Z	670	0	700	368	0
25	1	567	0	621	314	0
26	2	469	0	518	304	0
27	3	581	0	577	358	0
28	4	445	0	459	296	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	5	426	0	452	291	0
30	6	430	0	480	261	0
31	7	515	0	587	388	0
32	8	307	0	335	148	0
All	All	94012	0	63494	30536	1

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 194.

The worst 5 of 30536 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:27:VAL:HG23	23:Y:85:HIS:CE1	1.45	1.50
23:Y:27:VAL:CG2	23:Y:85:HIS:CE1	1.95	1.45
12:N:64:ARG:HH11	12:N:68:GLU:N	1.15	1.44
1:A:775:G:H2'	1:A:794:G:C8	1.54	1.42
1:A:1201:C:N4	1:A:1241:A:H61	1.15	1.39

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:-1:A:O2'	2:B:-1:A:O2'[15_545]	2.14	0.06

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
3	C	226/229 (99%)	110 (49%)	62 (27%)	54 (24%)	0 3
4	D	270/276 (98%)	110 (41%)	66 (24%)	94 (35%)	0 0
5	E	204/206 (99%)	108 (53%)	40 (20%)	56 (28%)	0 1
6	F	206/210 (98%)	106 (52%)	45 (22%)	55 (27%)	0 2
7	G	180/182 (99%)	71 (39%)	52 (29%)	57 (32%)	0 0
8	H	172/180 (96%)	75 (44%)	50 (29%)	47 (27%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	146/148 (99%)	85 (58%)	36 (25%)	25 (17%)	0	7
10	L	136/147 (92%)	68 (50%)	38 (28%)	30 (22%)	0	3
11	M	137/140 (98%)	63 (46%)	28 (20%)	46 (34%)	0	0
12	N	120/122 (98%)	60 (50%)	24 (20%)	36 (30%)	0	1
13	O	143/150 (95%)	52 (36%)	40 (28%)	51 (36%)	0	0
14	P	134/141 (95%)	53 (40%)	36 (27%)	45 (34%)	0	0
15	Q	115/118 (98%)	60 (52%)	37 (32%)	18 (16%)	0	8
16	R	108/112 (96%)	43 (40%)	35 (32%)	30 (28%)	0	1
17	S	115/146 (79%)	55 (48%)	27 (24%)	33 (29%)	0	1
18	T	115/118 (98%)	46 (40%)	40 (35%)	29 (25%)	0	2
19	U	99/101 (98%)	53 (54%)	19 (19%)	27 (27%)	0	1
20	V	108/113 (96%)	64 (59%)	20 (18%)	24 (22%)	0	3
21	W	92/96 (96%)	53 (58%)	18 (20%)	21 (23%)	0	3
22	X	108/110 (98%)	39 (36%)	34 (32%)	35 (32%)	0	0
23	Y	178/206 (86%)	85 (48%)	50 (28%)	43 (24%)	0	2
24	Z	83/85 (98%)	48 (58%)	20 (24%)	15 (18%)	0	6
25	1	65/67 (97%)	30 (46%)	20 (31%)	15 (23%)	0	3
26	2	57/60 (95%)	33 (58%)	12 (21%)	12 (21%)	0	4
27	3	69/71 (97%)	20 (29%)	23 (33%)	26 (38%)	0	0
28	4	55/60 (92%)	14 (26%)	22 (40%)	19 (34%)	0	0
29	5	47/54 (87%)	15 (32%)	8 (17%)	24 (51%)	0	0
30	6	47/49 (96%)	18 (38%)	14 (30%)	15 (32%)	0	0
31	7	62/65 (95%)	23 (37%)	18 (29%)	21 (34%)	0	0
32	8	35/37 (95%)	21 (60%)	6 (17%)	8 (23%)	0	3
All	All	3632/3799 (96%)	1681 (46%)	940 (26%)	1011 (28%)	0	1

5 of 1011 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	22	ILE
3	C	35	ALA
3	C	41	VAL
3	C	52	ARG
3	C	62	VAL

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	
3	C	180/181 (99%)	145 (81%)	35 (19%)	2	16
4	D	215/218 (99%)	146 (68%)	69 (32%)	0	4
5	E	166/166 (100%)	95 (57%)	71 (43%)	0	1
6	F	164/166 (99%)	106 (65%)	58 (35%)	0	2
7	G	156/156 (100%)	113 (72%)	43 (28%)	0	6
8	H	143/148 (97%)	91 (64%)	52 (36%)	0	2
9	K	124/124 (100%)	88 (71%)	36 (29%)	0	5
10	L	105/111 (95%)	86 (82%)	19 (18%)	2	19
11	M	118/119 (99%)	82 (70%)	36 (30%)	0	5
12	N	100/100 (100%)	60 (60%)	40 (40%)	0	1
13	O	111/116 (96%)	66 (60%)	45 (40%)	0	1
14	P	106/111 (96%)	68 (64%)	38 (36%)	0	2
15	Q	100/101 (99%)	73 (73%)	27 (27%)	1	6
16	R	87/88 (99%)	61 (70%)	26 (30%)	0	5
17	S	105/127 (83%)	65 (62%)	40 (38%)	0	1
18	T	93/94 (99%)	61 (66%)	32 (34%)	0	3
19	U	82/82 (100%)	55 (67%)	27 (33%)	0	3
20	V	90/92 (98%)	56 (62%)	34 (38%)	0	1
21	W	76/78 (97%)	59 (78%)	17 (22%)	1	11
22	X	91/91 (100%)	71 (78%)	20 (22%)	1	11
23	Y	159/179 (89%)	107 (67%)	52 (33%)	0	4
24	Z	67/67 (100%)	49 (73%)	18 (27%)	1	7
25	1	62/62 (100%)	49 (79%)	13 (21%)	1	12
26	2	51/52 (98%)	37 (72%)	14 (28%)	0	6
27	3	63/63 (100%)	42 (67%)	21 (33%)	0	3
28	4	50/52 (96%)	33 (66%)	17 (34%)	0	3
29	5	48/52 (92%)	32 (67%)	16 (33%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	6	42/42 (100%)	29 (69%)	13 (31%)	0	4
31	7	54/55 (98%)	39 (72%)	15 (28%)	0	6
32	8	34/34 (100%)	25 (74%)	9 (26%)	1	7
All	All	3042/3127 (97%)	2089 (69%)	953 (31%)	0	4

5 of 953 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	N	34	THR
14	P	112	GLU
27	3	59	PHE
12	N	67	LYS
13	O	88	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	13	ASN
17	S	38	ASN
29	5	20	ASN
13	O	128	HIS
14	P	113	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2888/2916 (99%)	1218 (42%)	265 (9%)
2	B	122/123 (99%)	49 (40%)	4 (3%)
All	All	3010/3039 (99%)	1267 (42%)	269 (8%)

5 of 1267 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	U
1	A	13	A
1	A	14	A
1	A	15	G
1	A	23	G

5 of 269 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1253	A
1	A	1647	G
1	A	2655	G
1	A	1310	G
1	A	1428	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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	2889/2916 (99%)	-0.18	104 (3%) 41 36	63, 155, 266, 322	0
2	B	123/123 (100%)	-0.09	8 (6%) 18 22	146, 209, 257, 291	0
3	C	228/229 (99%)	-0.31	0 100 100	220, 256, 308, 312	0
4	D	272/276 (98%)	-0.39	1 (0%) 90 83	80, 125, 153, 198	0
5	E	206/206 (100%)	-0.34	1 (0%) 88 79	69, 117, 172, 224	0
6	F	208/210 (99%)	-0.12	18 (8%) 10 16	111, 179, 215, 231	0
7	G	182/182 (100%)	0.14	19 (10%) 7 13	160, 198, 226, 240	0
8	H	174/180 (96%)	-0.05	6 (3%) 43 38	146, 186, 216, 238	0
9	K	148/148 (100%)	-0.35	0 100 100	135, 161, 188, 190	0
10	L	138/147 (93%)	0.01	6 (4%) 34 31	277, 307, 330, 334	0
11	M	139/140 (99%)	-0.14	2 (1%) 72 59	107, 133, 167, 183	0
12	N	122/122 (100%)	0.93	25 (20%) 1 4	78, 106, 140, 154	0
13	O	145/150 (96%)	-0.34	1 (0%) 84 74	106, 190, 227, 239	0
14	P	136/141 (96%)	-0.45	0 100 100	109, 141, 173, 186	0
15	Q	117/118 (99%)	0.25	3 (2%) 53 44	91, 124, 157, 173	0
16	R	110/112 (98%)	0.54	11 (10%) 8 13	152, 183, 210, 248	0
17	S	117/146 (80%)	0.38	8 (6%) 17 21	83, 127, 165, 184	0
18	T	117/118 (99%)	0.01	0 100 100	100, 138, 152, 158	0
19	U	101/101 (100%)	0.34	4 (3%) 36 33	104, 160, 186, 197	0
20	V	110/113 (97%)	1.92	45 (40%) 1 3	110, 143, 179, 195	0
21	W	94/96 (97%)	1.14	24 (25%) 1 4	153, 170, 232, 237	0
22	X	110/110 (100%)	0.57	10 (9%) 9 15	157, 199, 247, 273	0
23	Y	180/206 (87%)	-0.46	0 100 100	142, 190, 211, 226	0
24	Z	85/85 (100%)	0.58	10 (11%) 5 11	139, 166, 181, 197	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	1	67/67 (100%)	0.11	4 (5%) 21 24	172, 186, 199, 209	0
26	2	59/60 (98%)	0.53	4 (6%) 17 21	127, 163, 188, 202	0
27	3	71/71 (100%)	0.27	3 (4%) 35 32	127, 160, 176, 185	0
28	4	57/60 (95%)	0.30	2 (3%) 42 37	96, 147, 217, 241	0
29	5	49/54 (90%)	-0.01	1 (2%) 62 50	141, 163, 183, 198	0
30	6	49/49 (100%)	0.64	2 (4%) 35 33	87, 145, 164, 188	0
31	7	64/65 (98%)	0.38	2 (3%) 47 40	113, 131, 153, 165	0
32	8	37/37 (100%)	-0.51	0 100 100	146, 157, 169, 172	0
All	All	6704/6838 (98%)	-0.03	324 (4%) 29 28	63, 160, 275, 334	0

The worst 5 of 324 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1537	C	10.6
1	A	1536	A	9.8
1	A	1535	U	7.8
7	G	79	ASN	7.6
20	V	83	LYS	7.3

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.