



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 17, 2018 – 02:18 pm GMT

PDB ID : 1W2B
Title : Trigger Factor ribosome binding domain in complex with 50S
Authors : Ferbitz, L.; Maier, T.; Patzelt, H.; Bukau, B.; Deuerling, E.; Ban, N.
Deposited on : 2004-07-01
Resolution : 3.50 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

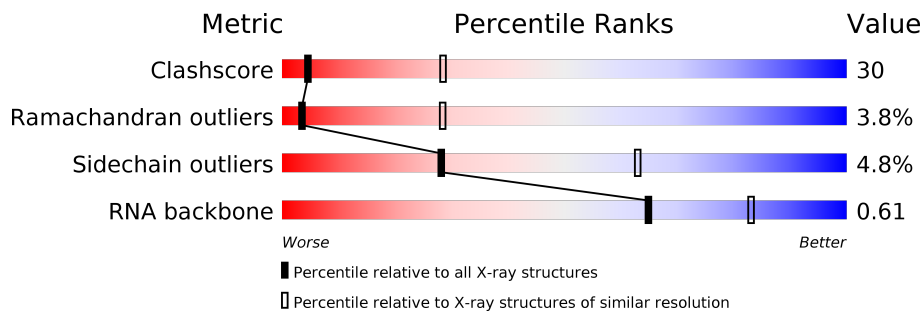
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	122078	1485 (3.60-3.40)
Ramachandran outliers	120005	1446 (3.60-3.40)
Sidechain outliers	119972	1447 (3.60-3.40)
RNA backbone	2633	1052 (4.10-2.90)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2922	
2	1	48	
3	2	92	
4	5	144	
5	9	122	
6	A	239	

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Mol	Chain	Length	Quality of chain
7	B	337	
8	C	246	
9	D	176	
10	E	177	
11	F	119	
12	G	348	
13	H	167	
14	I	145	
15	J	132	
16	K	164	
17	L	194	
18	M	186	
19	N	115	
20	O	148	
21	P	95	
22	Q	154	
23	R	84	
24	S	119	
25	T	66	
26	U	70	
27	V	154	
28	W	91	
29	X	240	
30	Y	73	
31	Z	56	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	I	202	-	-	X	-
35	CL	L	202	-	-	X	-
35	CL	P	102	-	-	X	-
35	CL	X	301	-	-	X	-

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 98859 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	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L44E LA, HLA, RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 4 is a protein called TRIGGER FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	5	35	Total	C	N	O	S	0	0	0
			273	173	52	47	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	A	238	Total	C	N	O	S	0	0	1
			1755	1072	353	325	5			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PHE	conflict	UNP P20279

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L5P HMAL5, HL13, RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	141	Total	C	N	O	S	0	0	1
			1095	685	196	210	4			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	E	173	Total	C	N	O	S	0	0	1
			1358	840	225	289	4			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	G	30	Total	C	N	O	S	0	0	1
			241	149	40	51	1			

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	I	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	K	146	Total	C	N	O	S	0	0	1
			1115	668	223	224				

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	M	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	N	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	O	144	Total	C	N	O	0	0	1
			1134	680	231	223			

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	P	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Q	151	Total	C	N	O	S	0	0	1
			1150	713	210	223	4			

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	R	84	Total	C	N	O	S	0	0	0
			664	405	114	142	3			

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	S	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	T	54	Total	C	N	O	S	0	0	1
			411	244	76	86	5			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	U	66	Total	C	N	O	S	0	0	1
			500	304	95	100	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	V	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	W	83	Total	C	N	O	S	0	0	1
			655	402	130	122	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	143	Total	C	N	O	S	0	0	1
			1131	686	229	216				

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	Z	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	105	Total	Mg	0	0
			105	105		
32	J	1	Total	Mg	0	0
			1	1		
32	B	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	3	Total 3	Mg 3	0	0
32	X	1	Total 1	Mg 1	0	0
32	2	1	Total 1	Mg 1	0	0
32	9	2	Total 2	Mg 2	0	0
32	S	1	Total 1	Mg 1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	2	Total 2	K 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	74	Total 74	Na 74	0	0
34	P	1	Total 1	Na 1	0	0
34	Q	2	Total 2	Na 2	0	0
34	K	1	Total 1	Na 1	0	0
34	I	1	Total 1	Na 1	0	0
34	C	1	Total 1	Na 1	0	0
34	A	1	Total 1	Na 1	0	0
34	R	1	Total 1	Na 1	0	0
34	9	2	Total 2	Na 2	0	0
34	L	1	Total 1	Na 1	0	0
34	S	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	7	Total 7	Cl 7	0	0
35	P	1	Total 1	Cl 1	0	0
35	J	1	Total 1	Cl 1	0	0
35	Q	1	Total 1	Cl 1	0	0
35	K	2	Total 2	Cl 2	0	0
35	B	1	Total 1	Cl 1	0	0
35	I	3	Total 3	Cl 3	0	0
35	A	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	X	1	Total 1	Cl 1	0	0
35	2	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	2	1	Total 1	Cd 1	0	0
36	Y	1	Total 1	Cd 1	0	0
36	T	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	N	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5875	Total 5875	O 5875	0	0
37	1	49	Total 49	O 49	0	0
37	2	69	Total 69	O 69	0	0
37	9	153	Total 153	O 153	0	0
37	A	135	Total 135	O 135	0	0
37	B	156	Total 156	O 156	0	0
37	C	169	Total 169	O 169	0	0
37	D	52	Total 52	O 52	0	0
37	E	41	Total 41	O 41	0	0
37	F	30	Total 30	O 30	0	0
37	G	20	Total 20	O 20	0	0
37	H	80	Total 80	O 80	0	0
37	I	52	Total 52	O 52	0	0
37	J	61	Total 61	O 61	0	0
37	K	98	Total 98	O 98	0	0
37	L	155	Total 155	O 155	0	0
37	M	60	Total 60	O 60	0	0
37	N	38	Total 38	O 38	0	0
37	O	67	Total 67	O 67	0	0
37	P	53	Total 53	O 53	0	0
37	Q	83	Total 83	O 83	0	0
37	R	32	Total 32	O 32	0	0

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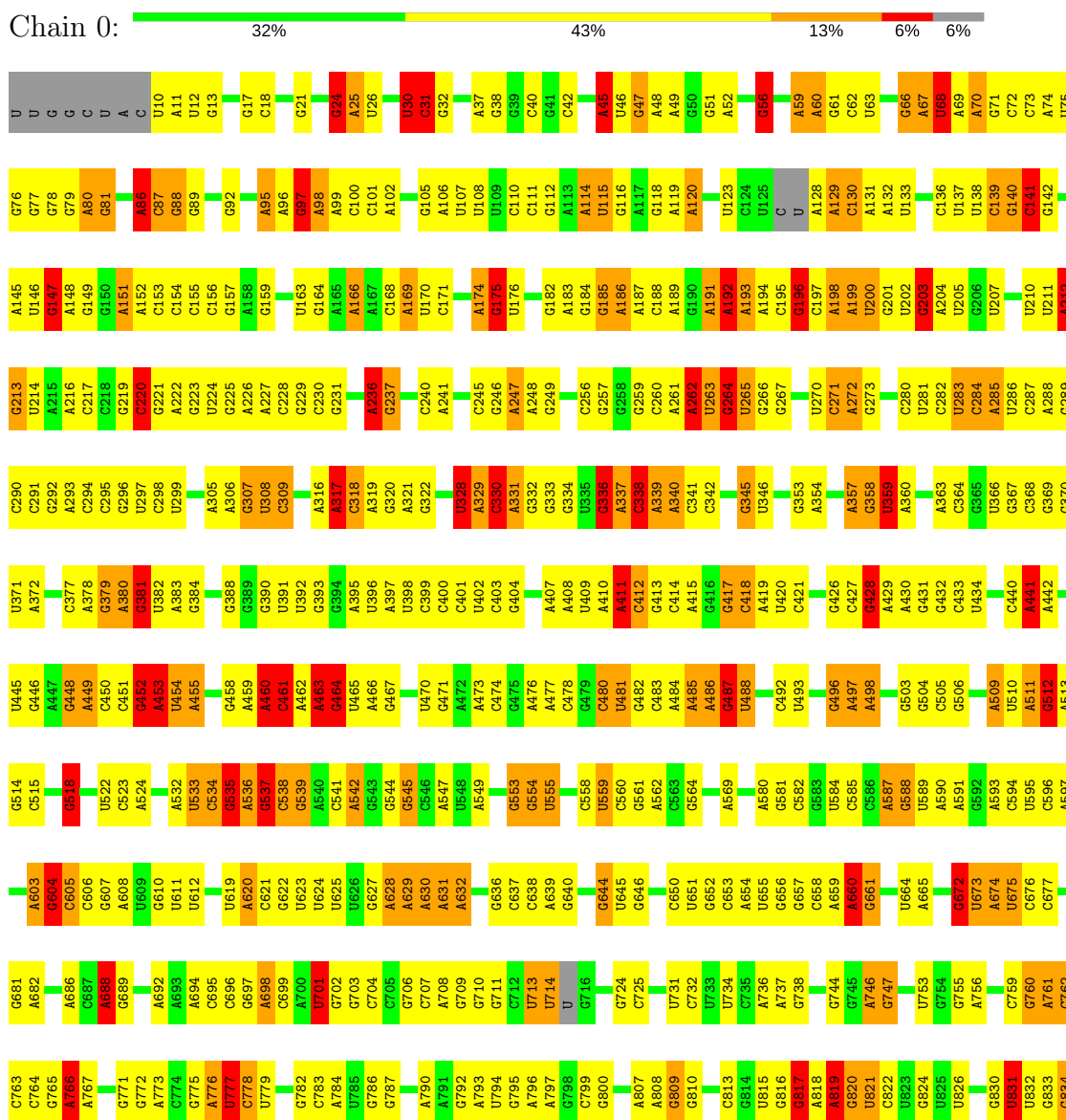
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	S	36	Total 36	O 36	0	0
37	T	25	Total 25	O 25	0	0
37	U	11	Total 11	O 11	0	0
37	V	69	Total 69	O 69	0	0
37	W	26	Total 26	O 26	0	0
37	X	107	Total 107	O 107	0	0
37	Y	35	Total 35	O 35	0	0
37	Z	50	Total 50	O 50	0	0

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 the various outlier classes 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.

Note EDS was not executed.

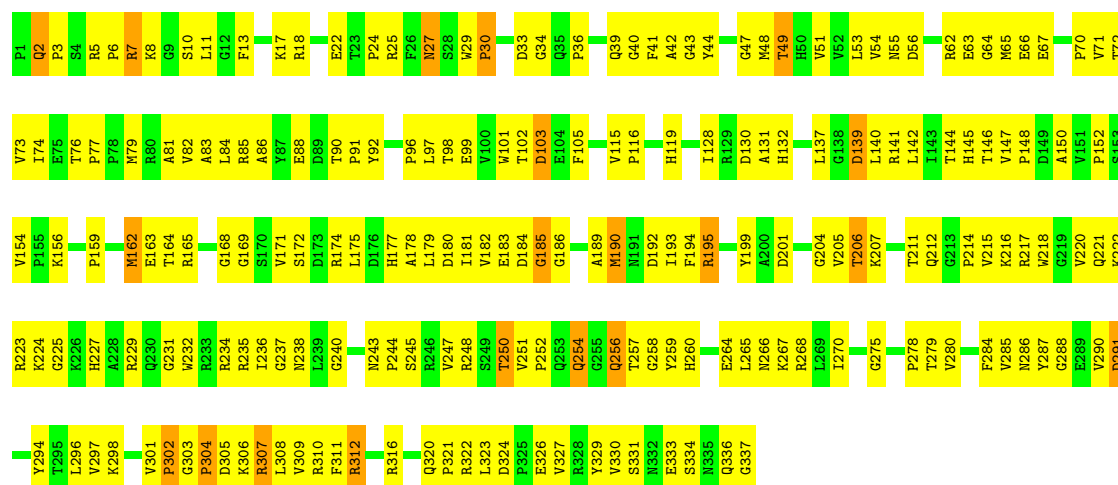
• Molecule 1: 23S rRNA



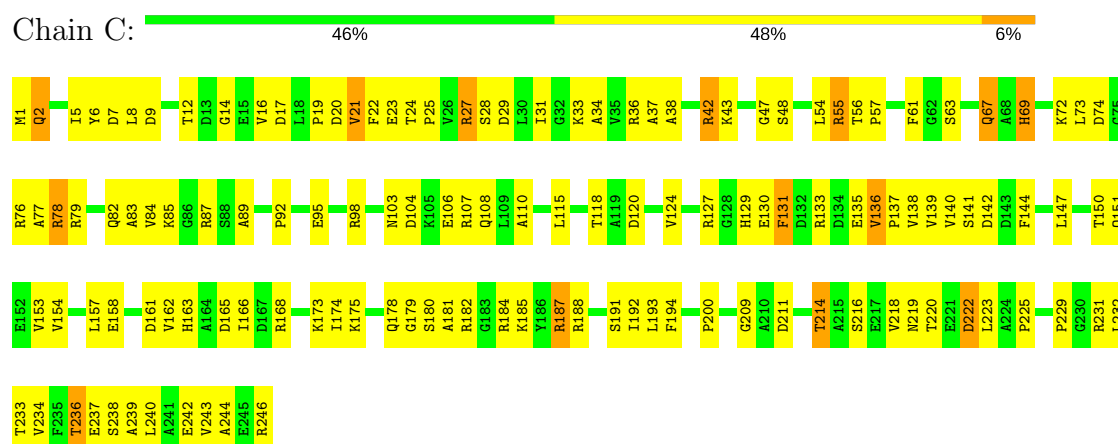
A1910	A1845	U1770	U1696	A1630	A1559	A1471	G1401	C1332	C1262	C1186	A1114	G1038	U903	U835
A1919	A1846	U1771	G1697	A1630	U	C1472	C1404	U1333	G1265	U1187	U1115	G1039	U904	G836
C1920	A1847	G1772	C1700	C1633	U1561	U1473	A1405	C1334	U1266	A1188	U1116	U1040	C905	U837
A1921	G1848	G1773	U1702	G1634	C1562	G1474	A1406	C1335	C1267	A1189	A1117	U1041	C906	U840
A1922	G1849	A1775	G1703	U1635	G1563	G1475	A1407	U1336	C1268	A1190	G1119	C1042	C907	A841
G1923	U1850	A1776	G1703	G1636	C1564	U1476	U1408	U1338	G1269	A1192	U1120	C1043	A908	A841
A1924	G1851	G1777	G1703	A1637	C1565	U1477	G1409	U1339	G1270	A1193	G1121	C1044	U909	C842
G1925	A1852	A1778	C1708	A1641	U1566	U1478	G1409	G1340	A1271	A1194	U1122	G1045	C910	A843
G1929	C1853	A1779	G1709	A1642	U1567	A1482	U1412	G1341	A1272	A1194	U1122	G1046	G911	A844
A1930	G1854	A1780	A1710	C1643	U1568	C1483	A1413	C1342	C1272	G1195	A1123	C1061	U919	U845
A1931	G1855	A1712	C1643	G1646	C1570	G1484	A1414	C1343	C1273	G1197	U1125	G1052	C920	A846
G1932	A1857	G1713	G1646	G1647	G1571	U1485	G1415	U1344	U1278	C1201	U1126	G1053	G921	C847
C1936	A1858	C1786	G1647	G1648	A1572	G1486	G1416	U1347	U1279	A1202	C1127	G1054	A922	C848
G1937	A1859	C1787	G1648	G1649	A1573	U1488	U1418	A1348	G1283	U1205	U1128	G1055	A923	C849
G1938	U1860	G1718	G1649	C1650	C1574	A1489	U1419	A1349	G1284	U1206	U1129	U1056	C923	U850
U1939	C1861	G1789	G1719	C1651	C1575	G1490	U1422	G1351	U1287	A1207	U1130	A1057	C926	C853
G1940	C1862	C1790	G1720	C1652	C1576	G1491	U1423	A1352	A1288	C1208	G1131	G1058	C927	C854
A1941	C1863	G1792	C1721	C1653	C1577	A1492	A1424	C1353	C1289	U1209	A1132	G1059	C931	U855
C1942	A1866	G1795	U1722	C1654	A1580	A1493	G1425	C1354	C1290	G1210	A1133	C1060	U932	C856
C1943	G1867	U1723	G1723	G1655	U1583	A1494	G1426	A1355	G1291	G1211	G1135	C1061	U933	U857
C1944	G1868	G1725	G1725	G1656	C1584	G1496	A1427	A1356	U1292	C1212	U1136	C1062	C934	U858
C1946	A1869	G1726	G1726	A1657	C1585	G1497	U1430	A1357	G1293	C1213	G1137	U1066	C935	C859
C1947	U1870	G1727	G1727	A1658	C1586	U1498	G1431	U1358	U1294	G1214	G1138	A1067	U860	U861
C1948	U1871	C1730	C1730	A1661	A1590	U1500	U1432	U1359	A1295	A1215	C1148	C1068	C888	A867
C1949	C1872	C1731	C1731	C1662	A1591	A1501	A1433	C1360	G1296	A1216	U1149	C1069	G940	C868
C1950	G1873	A1804	G1805	C1663	U1592	A1502	U1434	C1361	U1297	U1297	U1150	A1070	G941	C869
C1951	U1874	G1806	G1807	C1664	C1593	U1503	A1435	C1362	U1298	C1229	G1151	A1072	U942	C870
C1952	A1875	G1808	G1809	C1665	C1594	A1504	U1436	C1363	U1299	A1230	C1152	A1073	G943	C871
C1953	A1876	U1810	G1810	C1666	U1595	A1505	G1437	U1364	G1302	A1231	C1153	G1076	G944	U872
C1954	G1877	A1737	U1737	A1667	U1596	U1506	U1438	A1365	G1303	A1232	G1154	C1080	U945	A875
C1955	U1878	U1741	U1741	U1668	A1597	C1507	U1439	A1366	U1304	A1233	G1155	A1081	U946	A876
C1956	C1880	A1813	G1813	G1672	U1598	G1600	A1440	A1367	C1305	U1234	C1156	A1082	U947	C877
C1957	A1881	G1814	G1814	G1673	U1599	U1600	A1441	A1371	G1306	G1235	G1157	A1083	G948	C878
C1958	C1882	A1815	A1815	C1674	C1601	G1601	G1443	G1373	U1307	U1237	G1158	A1084	C881	C881
C1959	U1883	C1816	C1816	C1675	A1602	A1603	G1444	A1374	A1308	C1238	G1159	C1085	G953	A882
C1960	G1884	U1817	U1817	G1676	G1604	G1604	U1446	A1375	U1309	G1239	G1160	A1086	U954	U883
C1961	A1885	C1818	C1818	G1677	G1605	G1605	U1447	C1377	G1310	G1240	A1161	A1087	A955	C884
C1962	U1886	G1819	G1819	U1677	G1606	A1606	A1448	G1378	G1311	G1241	G1162	G1087	G956	C885
C1963	U1887	G1820	G1820	A1678	A1606	A1606	G1449	A1379	G1312	A1242	U1164	A1088	A957	C886
C1964	U1888	C1751	C1751	C1679	C1609	G1609	U1450	U1380	A1313	C1243	G1165	G1089	G958	C887
C1965	A1968	G1752	G1752	C1680	G1610	U1523	C1451	A1381	U1314	U1244	A1166	U1096	C959	C888
C1966	U1969	C1753	C1753	G1681	G1610	U1524	G1452	G1382	G1315	C1245	G1167	A1096	G960	U889
C1967	C1893	A1829	A1829	A1682	U1525	G1525	G1453	A1386	G1316	A1246	C1168	A1097	A961	C890
C1968	U1894	G1830	C1830	G1683	A1526	A1526	G1454	G1387	A1317	A1247	U1169	A1098	C962	C891
C1969	C1895	U1831	U1831	A1684	A1616	A1616	U1457	G1388	A1318	A1248	G1172	G1099	C963	C892
C1970	U1896	G1832	G1832	A1685	C1617	A1528	A1458	U1389	G1320	U1249	G1173	G1100	G964	C893
C1971	A1900	U1833	U1833	C1686	G1618	U1529	A1459	G1390	A1321	C1250	A1174	C1104	U1028	C894
C1972	G1901	C1834	C1834	G1687	G1619	G1532	U1460	A1392	G1325	C1251	A1175	C1105	U1029	A894
C1973	U1902	A1835	A1835	G1688	C1620	U1533	U1461	A1393	G1326	A1252	G1176	A1106	C1030	A895
C1974	G1903	G1837	G1837	A1689	G1621	C1534	A1462	A1394	U1327	C1253	U1180	A1107	G1031	C896
C1975	U1904	C1762	C1762	C1690	G1622	A1463	U1463	C1394	G1328	C1254	U1181	G1108	A1032	A897
C1976	A1905	C1763	C1763	A1691	C1623	G1543	U1467	C1397	A1328	G1257	C1182	U1109	C1033	C898
C1977	C1982	U1766	U1766	C1692	A1624	U1544	G1468	C1398	A1329	U1260	G1183	G1110	G1034	C899
C1978	U1983	A1841	A1841	G1693	U1625	C1545	U1469	A1399	A1330	G1260	C1184	U1111	G1035	U900
C1979	A1984	C1840	C1840	G1694	A1626	C1546	A1470	A1400	A1331	U1185	U1185	C	G1036	G901
C1980	U1985	A1842	A1842	G1695	G1627	C1553							C	G902



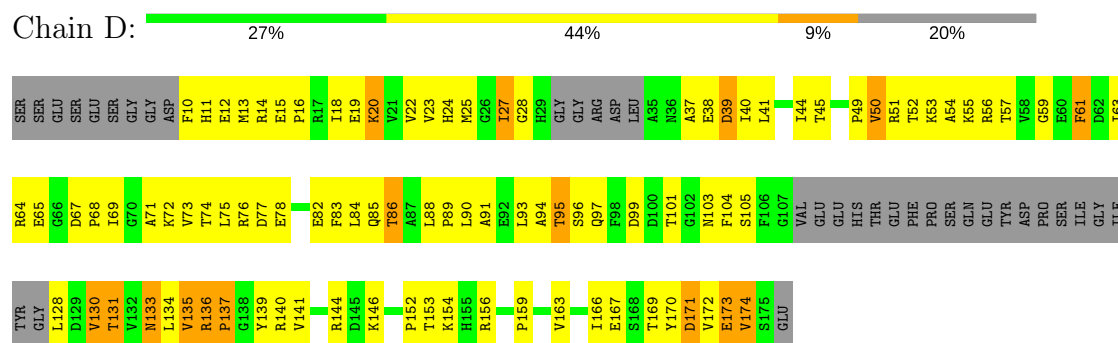
Chain B: 39% 55% 6%



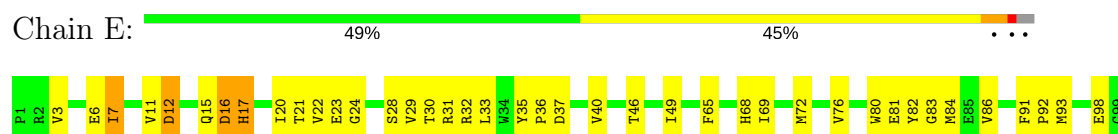
• Molecule 8: 50S RIBOSOMAL PROTEIN L4P



• Molecule 9: 50S RIBOSOMAL PROTEIN L5P HMA5, HL13, RIBOSOMAL PROTEIN L5



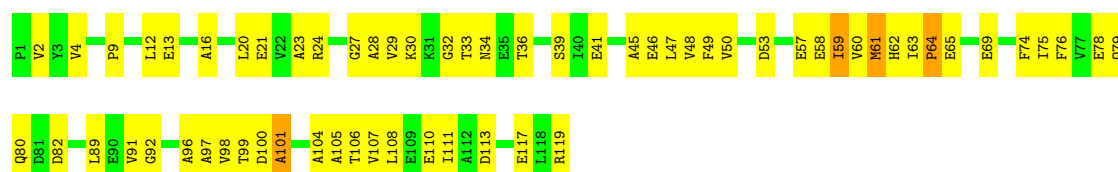
• Molecule 10: 50S RIBOSOMAL PROTEIN L6P





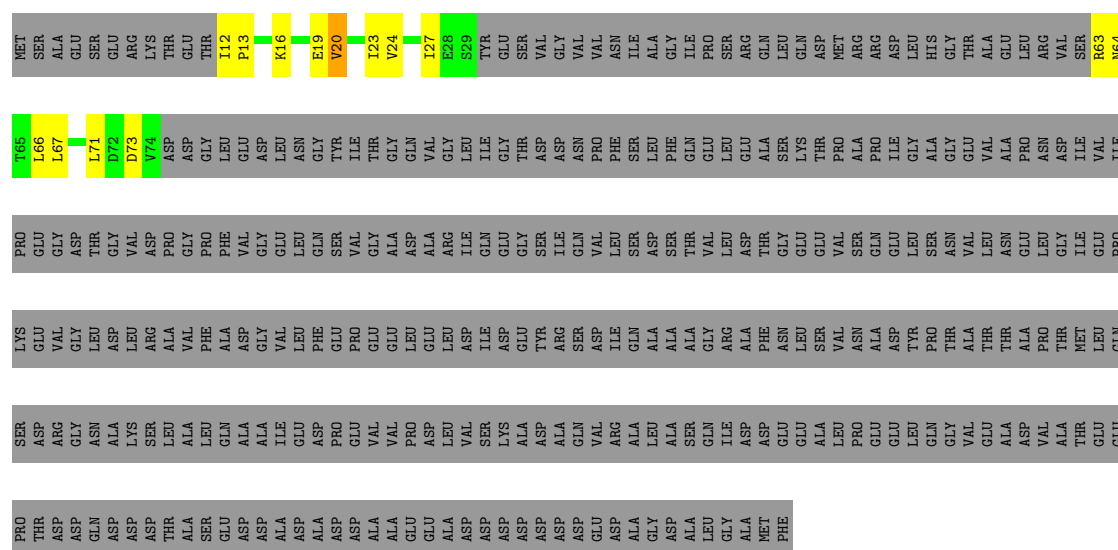
• Molecule 11: 50S RIBOSOMAL PROTEIN L7AE

Chain F: 47% 50%



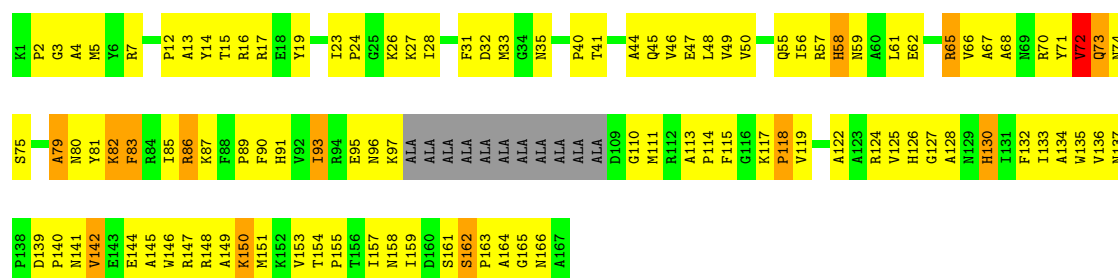
• Molecule 12: 50S RIBOSOMAL PROTEIN L10E

Chain G: 5% 91%

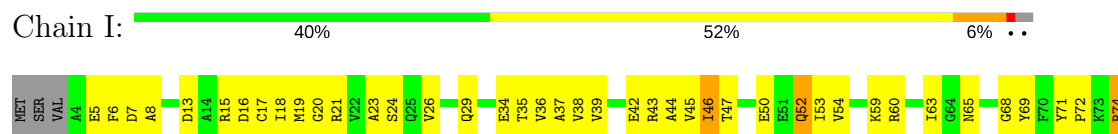


• Molecule 13: 50S RIBOSOMAL PROTEIN L10E

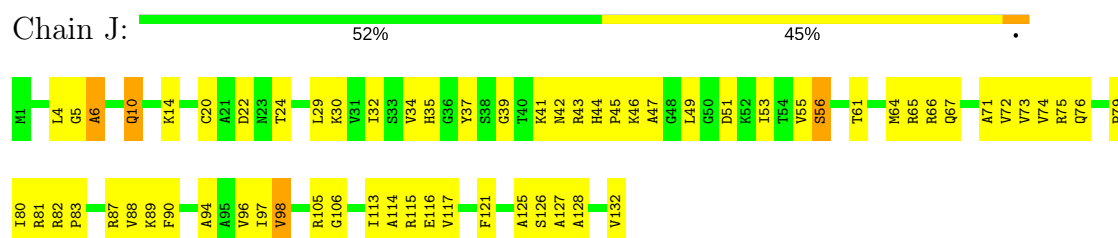
Chain H: 29% 56% 8% 7%



• Molecule 14: 50S RIBOSOMAL PROTEIN L13P



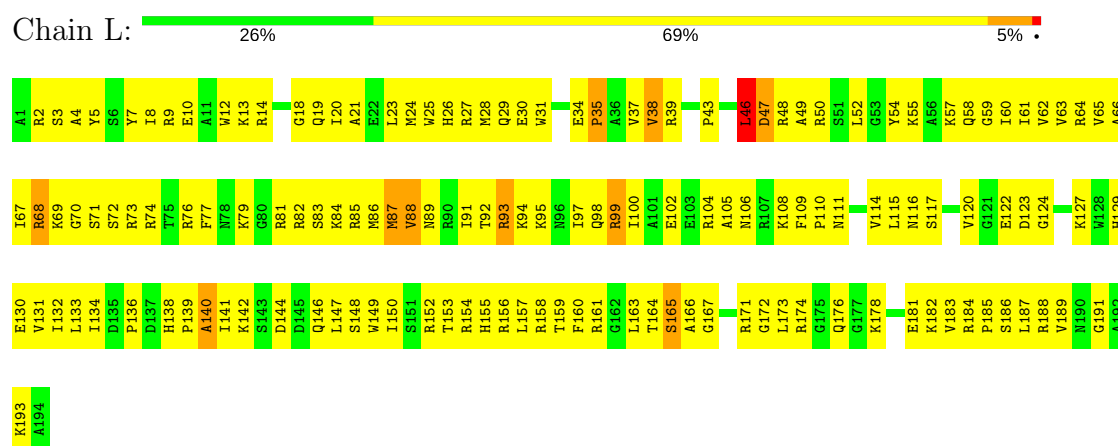
• Molecule 15: 50S RIBOSOMAL PROTEIN L14P



• Molecule 16: 50S RIBOSOMAL PROTEIN L15P

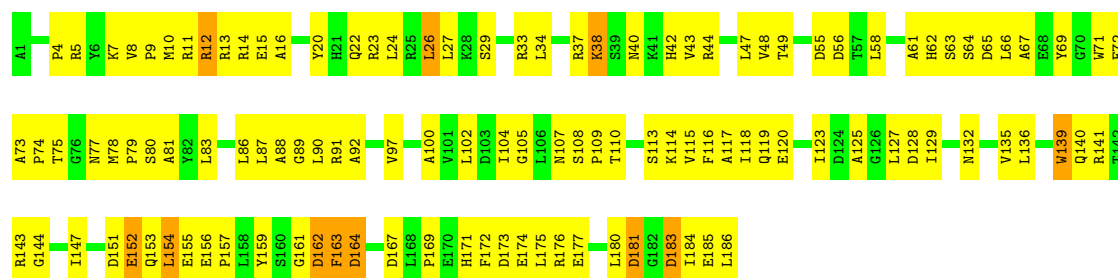


• Molecule 17: 50S RIBOSOMAL PROTEIN L15E



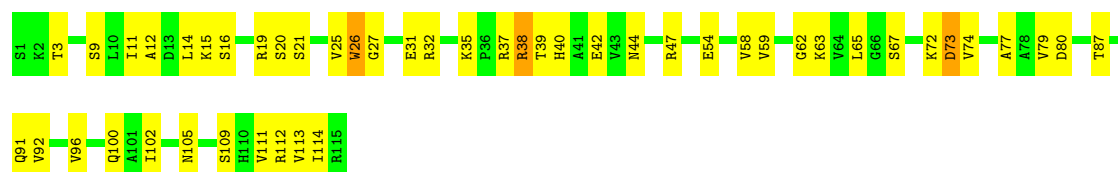
• Molecule 18: 50S RIBOSOMAL PROTEIN L18P





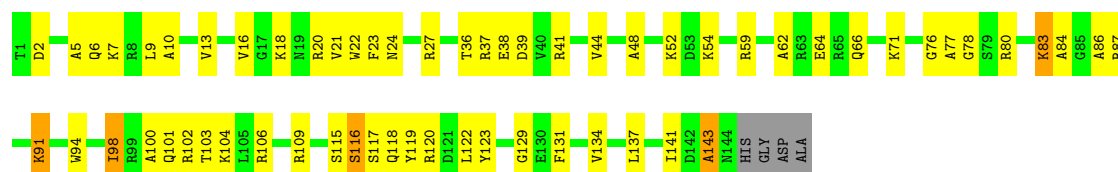
• Molecule 19: 50S RIBOSOMAL PROTEIN L18E

Chain N: 58% 39%



• Molecule 20: 50S RIBOSOMAL PROTEIN L19E

Chain O: 56% 38%



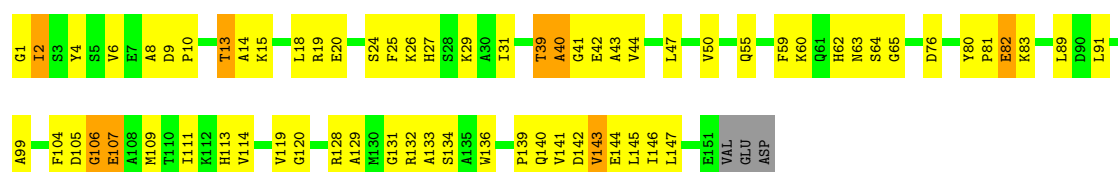
• Molecule 21: 50S RIBOSOMAL PROTEIN L21E

Chain P: 48% 46%

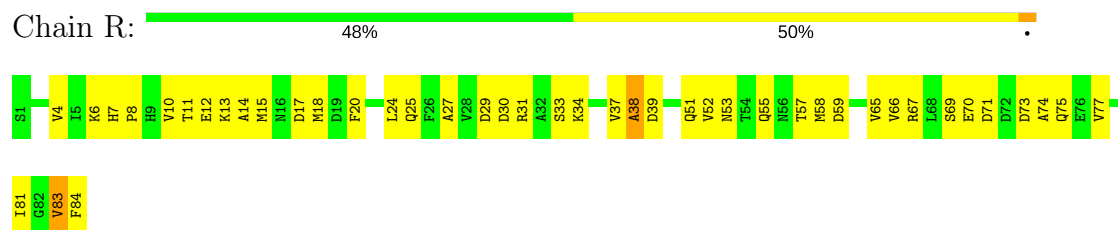


• Molecule 22: 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22

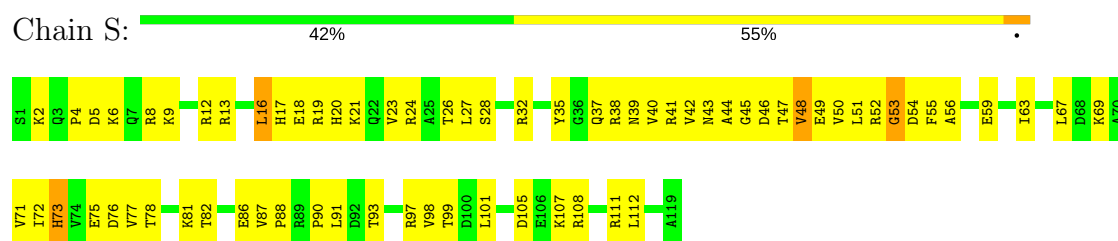
Chain Q: 54% 39% 5%



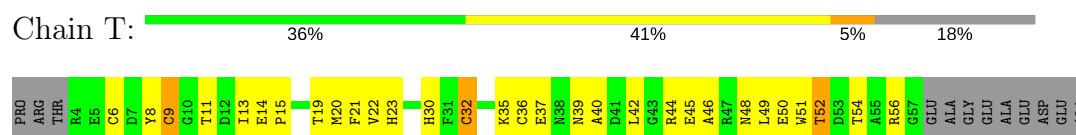
• Molecule 23: 50S RIBOSOMAL PROTEIN L23P



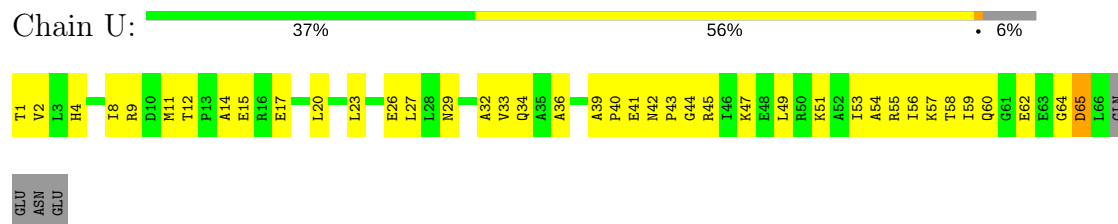
• Molecule 24: RIBOSOMAL PROTEIN L24



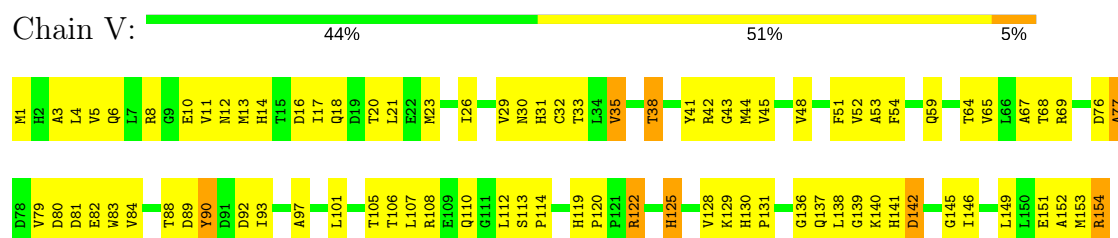
• Molecule 25: 50S RIBOSOMAL PROTEIN L24P



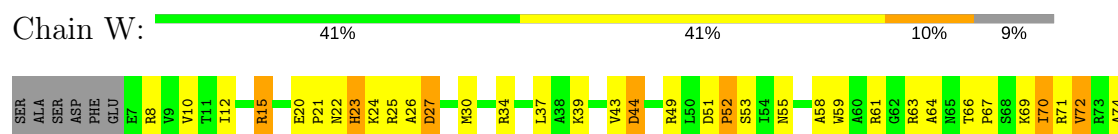
• Molecule 26: 50S RIBOSOMAL PROTEIN L24E

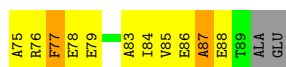


• Molecule 27: 50S RIBOSOMAL PROTEIN L30P

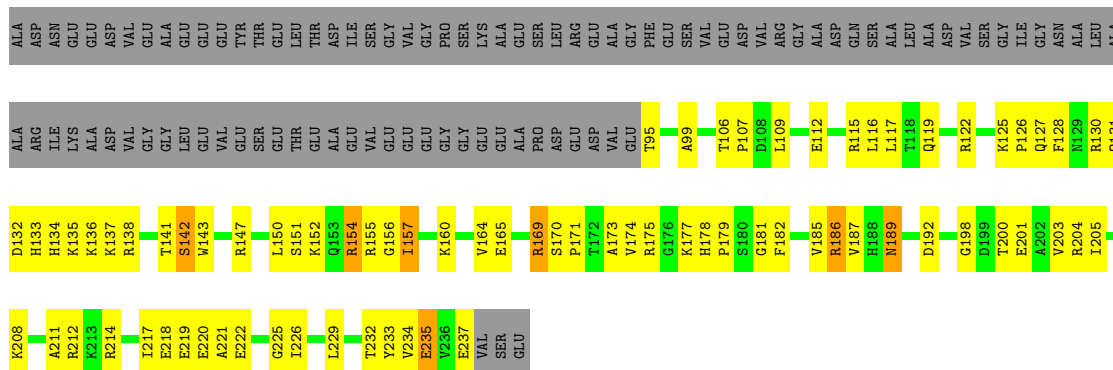
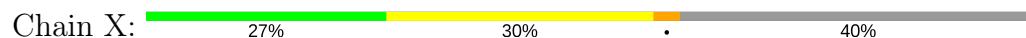


• Molecule 28: 50S RIBOSOMAL PROTEIN L31E

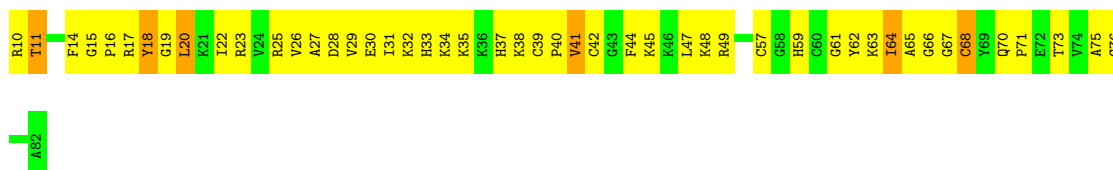




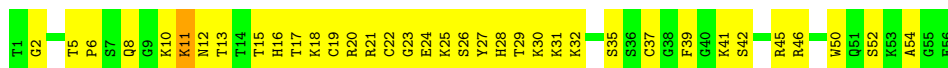
● Molecule 29: 50S RIBOSOMAL PROTEIN L32E



• Molecule 30: 50S RIBOSOMAL PROTEIN L37AE



- Molecule 31: RIBOSOMAL PROTEIN L37E



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	210.75Å 298.87Å 574.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50	Depositor
% Data completeness (in resolution range)	80.3 (30.00-3.50)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	98859	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

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: NA, MG, CD, K, CL

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	0.49	0/66076	0.85	218/103052 (0.2%)
2	1	0.34	0/399	0.56	0/527
3	2	0.34	0/771	0.55	0/1024
4	5	0.38	0/275	0.77	0/366
5	9	0.44	0/2905	0.84	11/4528 (0.2%)
6	A	0.36	0/1788	0.65	0/2411
7	B	0.36	0/2690	0.65	0/3652
8	C	0.37	0/1884	0.62	0/2551
9	D	0.35	0/1112	0.59	0/1500
10	E	0.38	0/1383	0.63	0/1882
11	F	0.35	0/897	0.59	0/1219
12	G	0.41	0/242	0.53	0/326
13	H	0.38	0/1247	0.68	0/1686
14	I	0.37	0/1136	0.63	0/1530
15	J	0.39	0/1004	0.68	0/1351
16	K	0.34	0/1127	0.64	0/1506
17	L	0.40	0/1634	0.66	0/2180
18	M	0.32	0/1474	0.66	0/1999
19	N	0.35	0/874	0.65	0/1181
20	O	0.37	0/1144	0.55	0/1523
21	P	0.37	0/749	0.67	0/1005
22	Q	0.41	0/1173	0.63	0/1580
23	R	0.53	0/672	0.69	0/906
24	S	0.34	0/958	0.65	0/1289
25	T	0.40	0/418	0.57	0/564
26	U	0.36	0/503	0.59	0/677
27	V	0.37	0/1219	0.64	0/1655
28	W	0.37	0/665	0.61	0/897
29	X	0.38	0/1147	0.65	0/1538
30	Y	0.34	0/576	0.58	0/763
31	Z	0.40	0/438	0.63	0/578
All	All	0.45	0/98580	0.80	229/147446 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	65
5	9	0	4
27	V	0	1
All	All	0	70

There are no bond length outliers.

The worst 5 of 229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	535	G	N9-C1'-C2'	10.05	127.07	114.00
1	0	537	G	N9-C1'-C2'	9.91	126.88	114.00
1	0	1235	G	O4'-C1'-N9	8.50	115.00	108.20
1	0	1702	U	N1-C1'-C2'	8.48	125.03	114.00
1	0	337	A	N9-C1'-C2'	8.44	124.97	114.00

There are no chirality outliers.

5 of 70 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	203	G	Sidechain
1	0	224	U	Sidechain
1	0	30	U	Sidechain
1	0	68	U	Sidechain
1	0	86	A	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	59017	0	29808	2081	0
2	1	394	0	406	38	0
3	2	755	0	732	81	0
4	5	273	0	296	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	9	2600	0	1326	119	0
6	A	1755	0	1763	185	0
7	B	2625	0	2533	240	0
8	C	1859	0	1816	166	0
9	D	1095	0	1085	125	0
10	E	1358	0	1266	95	0
11	F	886	0	854	75	0
12	G	241	0	231	20	0
13	H	1216	0	1215	169	0
14	I	1120	0	1098	92	0
15	J	994	0	1027	82	0
16	K	1115	0	1072	91	0
17	L	1606	0	1676	241	0
18	M	1445	0	1401	149	0
19	N	865	0	873	52	0
20	O	1134	0	1127	65	0
21	P	735	0	729	49	0
22	Q	1150	0	1122	76	0
23	R	664	0	626	50	0
24	S	950	0	924	80	0
25	T	411	0	368	35	0
26	U	500	0	511	45	0
27	V	1196	0	1137	120	0
28	W	655	0	653	55	0
29	X	1131	0	1133	100	0
30	Y	564	0	601	85	0
31	Z	431	0	426	45	0
32	0	105	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	3	0	0	0	0
32	B	3	0	0	0	0
32	J	1	0	0	0	0
32	S	1	0	0	0	0
32	X	1	0	0	0	0
33	0	2	0	0	0	0
34	0	74	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	I	1	0	0	0	0
34	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	L	1	0	0	0	0
34	P	1	0	0	0	0
34	Q	2	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	7	0	0	2	0
35	2	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	I	3	0	0	3	0
35	J	1	0	0	0	0
35	K	2	0	0	0	0
35	L	1	0	0	2	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	P	1	0	0	2	0
35	Q	1	0	0	0	0
35	X	1	0	0	2	0
36	2	1	0	0	0	0
36	N	1	0	0	0	0
36	T	1	0	0	0	0
36	Y	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5875	0	0	346	0
37	1	49	0	0	8	0
37	2	69	0	0	7	0
37	9	153	0	0	16	0
37	A	135	0	0	29	0
37	B	156	0	0	31	0
37	C	169	0	0	43	0
37	D	52	0	0	15	0
37	E	41	0	0	8	0
37	F	30	0	0	6	0
37	G	20	0	0	3	0
37	H	80	0	0	19	0
37	I	52	0	0	4	0
37	J	61	0	0	18	0
37	K	98	0	0	23	0
37	L	155	0	0	34	0
37	M	60	0	0	18	0
37	N	38	0	0	5	0
37	O	67	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	P	53	0	0	6	0
37	Q	83	0	0	6	0
37	R	32	0	0	6	0
37	S	36	0	0	4	0
37	T	25	0	0	6	0
37	U	11	0	0	2	0
37	V	69	0	0	10	0
37	W	26	0	0	6	0
37	X	107	0	0	13	0
37	Y	35	0	0	10	0
37	Z	50	0	0	2	0
All	All	98859	0	59835	4534	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 30.

The worst 5 of 4534 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)
1:0:156:C:H5''	17:L:171:ARG:HD3	1.28	1.14
3:2:46:ILE:HG21	17:L:87:MET:HG2	1.24	1.14
26:U:12:THR:HG22	26:U:15:GLU:HG3	1.28	1.14
11:F:91:VAL:HG12	11:F:92:GLY:H	1.09	1.13
5:9:6:C:H5''	18:M:37:ARG:HH12	1.08	1.11

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
2	1	42/48 (88%)	37 (88%)	5 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	90/92 (98%)	82 (91%)	5 (6%)	3 (3%)	4	32
4	5	33/144 (23%)	24 (73%)	9 (27%)	0	100	100
6	A	236/239 (99%)	197 (84%)	27 (11%)	12 (5%)	2	21
7	B	335/337 (99%)	281 (84%)	40 (12%)	14 (4%)	3	26
8	C	244/246 (99%)	201 (82%)	37 (15%)	6 (2%)	6	37
9	D	135/176 (77%)	90 (67%)	31 (23%)	14 (10%)	0	7
10	E	171/177 (97%)	147 (86%)	21 (12%)	3 (2%)	9	44
11	F	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	4	31
12	G	26/348 (8%)	23 (88%)	2 (8%)	1 (4%)	3	28
13	H	152/167 (91%)	123 (81%)	21 (14%)	8 (5%)	2	20
14	I	140/145 (97%)	117 (84%)	17 (12%)	6 (4%)	3	25
15	J	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	11	48
16	K	142/164 (87%)	116 (82%)	20 (14%)	6 (4%)	3	26
17	L	192/194 (99%)	144 (75%)	40 (21%)	8 (4%)	3	26
18	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	3	28
19	N	113/115 (98%)	92 (81%)	17 (15%)	4 (4%)	4	31
20	O	142/148 (96%)	126 (89%)	12 (8%)	4 (3%)	5	35
21	P	93/95 (98%)	72 (77%)	16 (17%)	5 (5%)	2	20
22	Q	149/154 (97%)	127 (85%)	18 (12%)	4 (3%)	5	36
23	R	82/84 (98%)	68 (83%)	9 (11%)	5 (6%)	1	17
24	S	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	6	36
25	T	52/66 (79%)	49 (94%)	3 (6%)	0	100	100
26	U	64/70 (91%)	49 (77%)	13 (20%)	2 (3%)	4	33
27	V	152/154 (99%)	132 (87%)	19 (12%)	1 (1%)	24	65
28	W	81/91 (89%)	65 (80%)	11 (14%)	5 (6%)	1	17
29	X	141/240 (59%)	126 (89%)	12 (8%)	3 (2%)	8	41
30	Y	71/73 (97%)	59 (83%)	7 (10%)	5 (7%)	1	14
31	Z	54/56 (96%)	43 (80%)	7 (13%)	4 (7%)	1	12
All	All	3680/4379 (84%)	3056 (83%)	485 (13%)	139 (4%)	3	28

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	D	20	LYS
9	D	93	LEU
9	D	95	THR
9	D	144	ARG
9	D	173	GLU

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	
2	1	42/44 (96%)	40 (95%)	2 (5%)	28	63
3	2	79/79 (100%)	75 (95%)	4 (5%)	26	61
4	5	29/122 (24%)	26 (90%)	3 (10%)	8	33
6	A	179/181 (99%)	167 (93%)	12 (7%)	18	52
7	B	282/282 (100%)	268 (95%)	14 (5%)	27	61
8	C	193/193 (100%)	181 (94%)	12 (6%)	20	55
9	D	117/147 (80%)	109 (93%)	8 (7%)	17	52
10	E	152/155 (98%)	147 (97%)	5 (3%)	41	72
11	F	92/92 (100%)	91 (99%)	1 (1%)	76	89
12	G	27/283 (10%)	27 (100%)	0	100	100
13	H	122/122 (100%)	111 (91%)	11 (9%)	10	39
14	I	118/121 (98%)	111 (94%)	7 (6%)	21	57
15	J	106/106 (100%)	102 (96%)	4 (4%)	36	69
16	K	112/126 (89%)	106 (95%)	6 (5%)	24	59
17	L	166/166 (100%)	160 (96%)	6 (4%)	38	70
18	M	149/149 (100%)	142 (95%)	7 (5%)	29	63
19	N	93/93 (100%)	90 (97%)	3 (3%)	42	73
20	O	113/116 (97%)	109 (96%)	4 (4%)	39	71
21	P	79/79 (100%)	74 (94%)	5 (6%)	20	55
22	Q	117/121 (97%)	113 (97%)	4 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	R	73/73 (100%)	72 (99%)	1 (1%)	69	87
24	S	105/105 (100%)	101 (96%)	4 (4%)	36	69
25	T	44/52 (85%)	41 (93%)	3 (7%)	17	52
26	U	51/56 (91%)	51 (100%)	0	100	100
27	V	130/130 (100%)	124 (95%)	6 (5%)	29	64
28	W	66/73 (90%)	61 (92%)	5 (8%)	14	47
29	X	120/195 (62%)	115 (96%)	5 (4%)	32	66
30	Y	56/56 (100%)	51 (91%)	5 (9%)	11	40
31	Z	46/46 (100%)	46 (100%)	0	100	100
All	All	3058/3563 (86%)	2911 (95%)	147 (5%)	28	63

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	H	86	ARG
15	J	98	VAL
28	W	51	ASP
13	H	126	HIS
14	I	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
14	I	107	ASN
17	L	58	GLN
29	X	119	GLN
15	J	10	GLN
16	K	42	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	542 (19%)	360 (13%)
5	9	121/122 (99%)	27 (22%)	14 (11%)
All	All	2866/3044 (94%)	569 (19%)	374 (13%)

5 of 569 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	24	G
1	0	25	A
1	0	31	C
1	0	32	G
1	0	46	U

5 of 374 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1354	G
1	0	1563	G
1	0	2791	U
1	0	1370	G
1	0	1430	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 232 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.