



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 06:32 pm BST

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](mailto: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.

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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  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

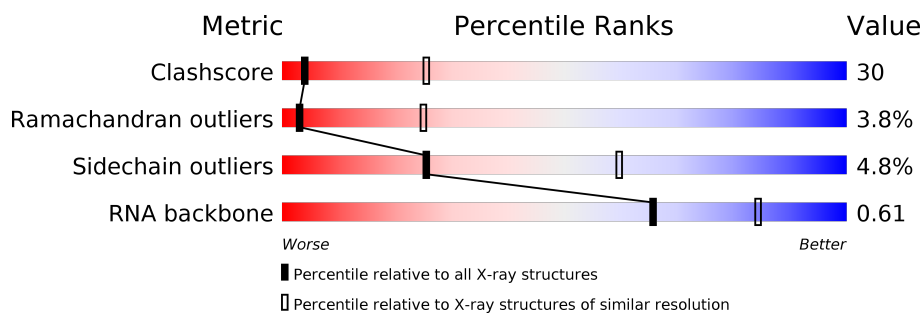
# 1 Overall quality at a glance

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	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

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	
7	B	337	

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Mol	Chain	Length	Quality of chain
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 crite-

ria:

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

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



A1845	U1770	U1696	A1630	A1569	A1471	G1401	C1332	C1262	C1186	A1114	G1038	G	U903	U835
A1846	U1771	G1697	A1630	U	C1472	C1404	U1333	G	U1187	U1115	G1039	C	U904	G836
A1847	C1772	C1700	C1633	U1561	U1473	U1405	C1334	G1285	A1188	U1116	U1041	C	C905	U837
A1848	G1773	C1700	C1633	U1561	U1473	U1405	C1334	U1266	A1189	U1117	U1042	U	C906	U840
G1849	G1774	U1702	G1634	G1562	G1475	A1407	C1336	C1267	A1189	A1118	C1043	C	A907	U841
U1850	A1775	G1703	G1635	G1563	G1476	A1407	A1337	C1268	A1191	G1119	G1064	C	A908	A841
G1851	A1776	G1703	G1636	C1564	C1477	U1408	U1338	G1269	A1192	U1120	G1064	G	U909	C842
A1852	G1777	C1565	A1637	G1565	U1478	G1409	C1339	U1270	A1193	U1121	G1045	A	C910	A843
A1853	A1778	C1566	C1637	C1566	A1482	G1409	G1340	A1271	A1194	G1122	G1046	G	G911	A844
C1854	A1779	A1567	A1641	A1567	A1483	U1412	A1341	C1272	G1195	A1123	C1051	A	U919	U845
G1855	A1780	A1568	A1642	A1568	A1413	A1413	C1342	C1273	C1196	A1124	G1052	G	G920	A846
G1856	A1781	G1484	C1643	G1484	A1414	A1414	C1343	A1278	G1197	U1125	G1053	G	G921	C847
A1857	A1712	A1485	C1643	G1415	A1415	G1415	C1343	U1279	G1197	C1126	G1054	A	G922	C848
A1858	G1713	A1486	G1646	G1571	A1486	G1416	U1346	U1279	G1197	C1127	G1055	G	A922	C849
C1859	A1717	A1487	G1647	A1572	A1487	G1417	U1347	U1283	C1201	U1128	G1056	U	A923	U850
U1860	C1787	A1573	G1648	A1573	U1488	U1418	A1348	G1283	A1202	U1129	G1057	C	G924	
U1861	U1788	G1649	G1649	A1574	G1489	U1419	A1348	G1284	U1205	U1130	A1058	G	G925	
A1861	G1719	C1574	C1650	C1575	G1490	U1419	G1351	U1284	U1206	G1131	G1059	G	A926	
C1862	C1720	C1575	C1651	C1575	G1491	U1422	G1352	A1287	A1207	A1132	C1060	C	C931	
G1863	C1721	C1575	C1652	C1575	A1492	C1423	C1353	U1288	C1208	A1133	C1061	A	C932	
A1866	C1722	C1575	C1653	C1575	A1493	A1424	G1354	U1289	C1209	G1134	C1062	C	G933	
G1867	G1723	C1575	C1654	C1575	A1494	G1425	A1355	G1290	G1210	U1135	C934	C	C934	
G1868	U1724	U1654	G1654	U1654	C1495	G1426	A1356	A1291	G1211	U1136	U1066	A	G935	
A1869	G1725	G1655	G1655	U1583	C1496	A1427	A1357	G1292	C1212	G1137	A1067	C	U936	
A1870	C1726	C1584	A1656	C1584	G1496	A1427	A1358	U1293	C1213	G1138	C1068	U	A861	
C1871	G1727	A1657	A1657	C1589	G1497	G1430	U1359	A1294	G1214	C1138	C1069	U	G938	
U1871	C1727	A1658	A1658	A1590	U1500	C1431	C1360	G1295	G1216	C1148	A1070	U	A939	
C1872	G1730	A1661	A1661	A1591	A1501	U1432	C1361	U1296	C1149	U1149	C1004	U	G940	
U1873	C1731	C1662	C1662	A1592	A1502	U1432	C1361	U1297	G1216	A1150	C1005	U	G941	
G1874	C1732	G1663	G1663	C1593	U1503	U1435	C1366	U1298	C1229	G1151	A1006	U	U942	
A1875	C1735	A1664	A1664	C1594	U1504	U1435	C1366	G1299	A1230	A1152	A1007	U	A943	
C1876	U1736	G1665	G1665	G1595	U1505	G1438	U1368	U1299	A1231	C1153	C1008	U	U944	
G1877	A1737	U1666	C1666	U1596	U1506	C1439	A1369	G1299	A1232	A1154	G1009	U	G945	
U1878	A1737	A1667	A1667	A1597	C1507	G1440	G1370	U1304	U1233	G1155	U1009	U	U946	
G1879	U1741	G1668	U1668	A1598	G1510	U1442	A1372	U1305	A1234	C1156	C1080	U	U947	
C1880	A1742	U1668	U1668	U1599	U1511	G1443	G1373	U1306	G1235	G1157	A1081	U	G948	
A1881	G1745	G1672	G1672	G1600	U1511	G1443	G1373	U1306	A1236	A1158	A1082	U	C952	
C1882	A1746	C1673	C1673	G1601	C1512	G1444	C1374	A1307	U1237	G1159	C1083	U	G953	
G1883	U1746	C1674	C1674	C1602	C1513	G1445	A1375	A1308	C1238	G1160	C1084	U	U954	
U1884	A1747	C1675	C1675	A1603	C1514	U1446	G1376	U1309	G1239	A1161	A1085	U	A955	
A1885	U1748	G1676	G1676	G1604	A1515	U1447	C1377	G1310	G1241	G1162	A1086	U	C956	
C1886	U1749	U1677	U1677	G1605	C1516	A1448	G1378	G1311	G1241	G1163	G1087	U	G957	
U1890	G1750	A1678	A1678	A1606	C1516	G1449	A1379	G1312	C1242	U1164	A1088	U	A957	
C1891	G1751	C1679	C1679	A1609	A1522	C1450	U1380	A1313	C1243	U1165	G1089	U	G958	
G1892	U1752	C1680	C1680	C1609	G1523	C1451	A1381	U1314	U1244	A1166	A1096	U	G959	
A1893	C1753	G1681	G1681	G1610	U1524	G1452	G1382	G1315	C1245	G1167	C1024	U	U960	
C1894	A1754	A1682	A1682	G1610	G1525	G1452	G1382	G1316	A1246	C1168	G1025	U	G961	
A1895	A1755	G1683	G1683	A1615	A1526	G1453	G1386	A1317	A1247	U1169	A1098	U	C962	
G1896	G1756	A1684	A1684	A1616	A1527	U1457	G1387	A1318	A1248	G1170	G1099	U	G963	
C1897	U1757	C1685	C1685	C1617	U1528	A1458	U1388	G1319	U1249	G1172	G1100	U	G964	
U1898	U1758	A1686	A1686	G1618	A1528	A1459	G1389	U1320	C1250	A1173	U1026	U	G965	
A1899	A1759	C1687	C1687	G1619	G1532	G1460	G1392	A1321	C1251	A1174	U1027	U	G966	
G1900	C1760	G1688	G1688	A1620	A1533	U1461	A1393	G1325	A1252	G1175	U1030	U	A969	
U1901	U1761	A1689	A1689	C1621	C1534	C1462	A1394	G1326	C1253	G1176	A1106	U	U970	
G1902	C1762	G1690	G1690	G1622	C1534	A1463	C1394	G1327	C1254	U1180	A1107	U	G971	
U1903	C1763	C1691	C1691	C1623	G1543	A1463	C1394	G1327	C1254	A1181	A1108	U	G972	
A1904	U1766	C1692	C1692	A1624	U1544	C1467	C1397	A1328	C1257	U1182	U1109	U	G973	
U1905	C1766	A1693	A1693	U1625	C1545	G1468	G1398	A1329	C1260	C1183	G1034	U	G974	
C1906	U1769	G1694	G1694	A1626	C1545	C1469	A1399	A1330	G1261	C1184	U1110	U	G975	
U1909	C1769	G1695	G1695	C1627	C1553	A1470	C1400	A1331	A1261	U1185	G1037	C	G976	

• Molecule 2: 50S RIBOSOMAL PROTEIN L39E

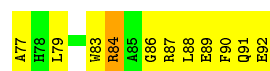


Chain 1:  38% 56% . .



- Molecule 3: 50S RIBOSOMAL PROTEIN L44E LA, HLA, RIBOSOMAL PROTEIN L44E

Chain 2:  39% 57% .



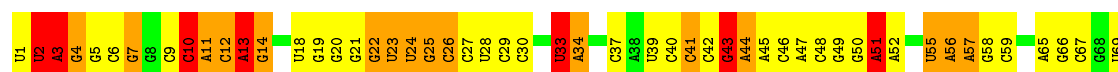
- Molecule 4: TRIGGER FACTOR

Chain 5:  9% 14% . 76%



- Molecule 5: 5S rRNA

Chain 9: 



- Molecule 6: 50S RIBOSOMAL PROTEIN L2P

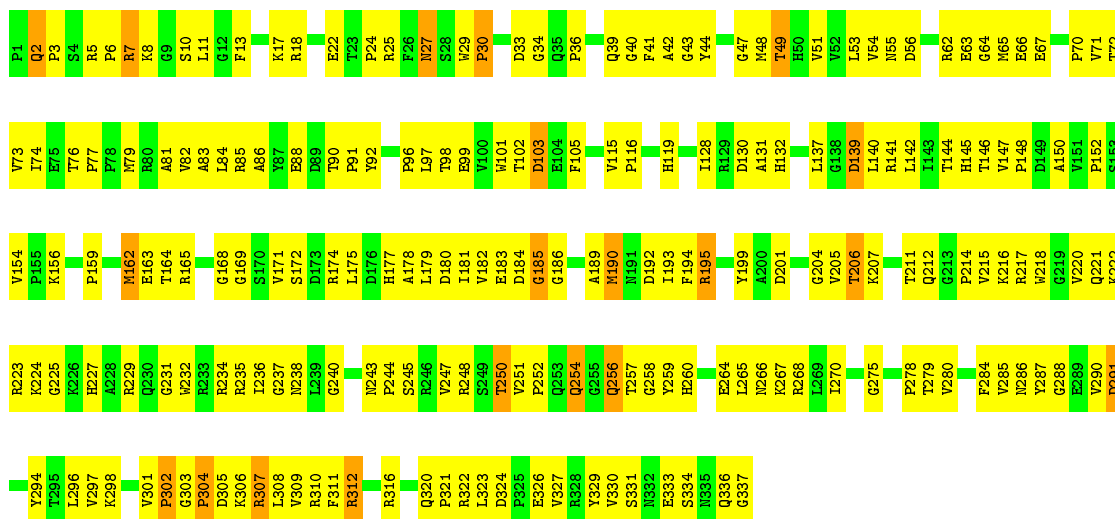
Chain A:  41% 51% 8%





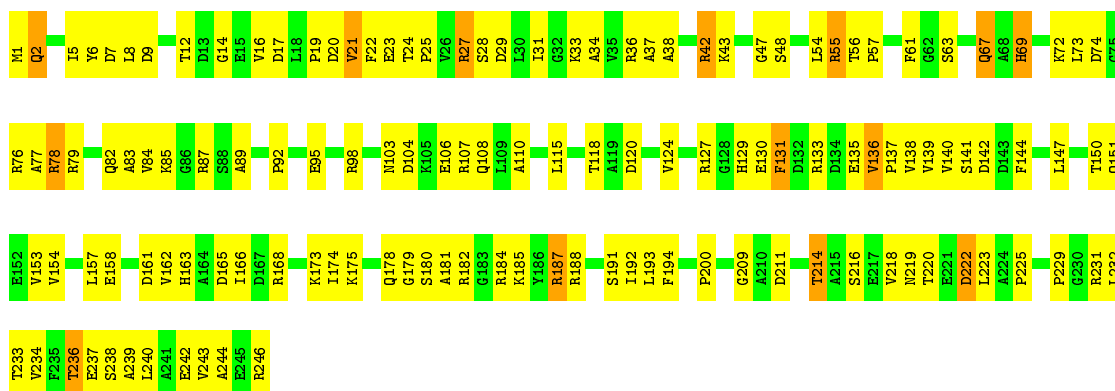
• Molecule 7: 50S RIBOSOMAL PROTEIN L3P

Chain B: 39% 55% 6%



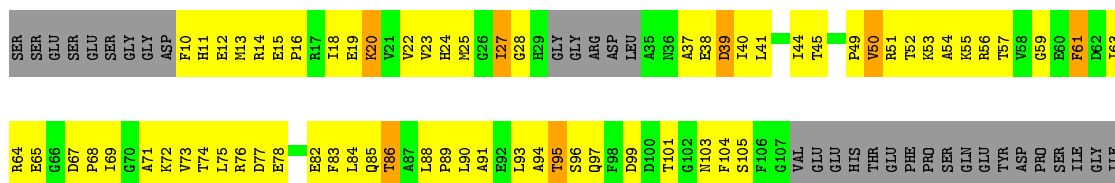
• Molecule 8: 50S RIBOSOMAL PROTEIN L4P

Chain C: 46% 48% 6%



• Molecule 9: 50S RIBOSOMAL PROTEIN L5P HMAL5, HL13, RIBOSOMAL PROTEIN L5

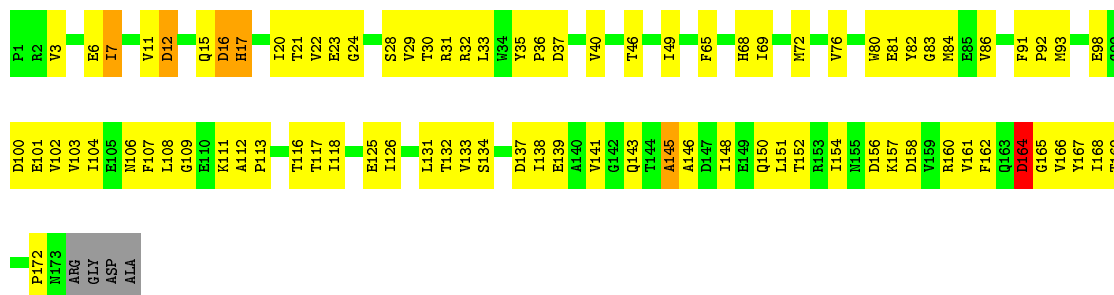
Chain D: 27% 44% 9% 20%





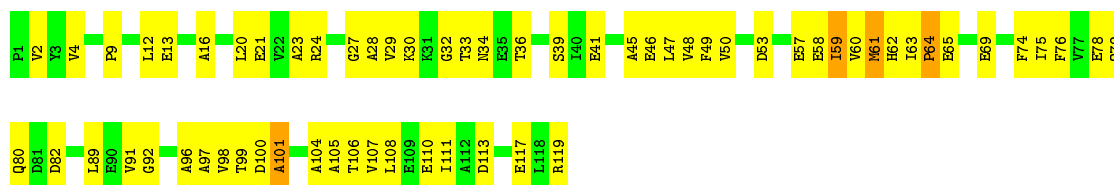
- Molecule 10: 50S RIBOSOMAL PROTEIN L6P

Chain E:  49% 45% ..



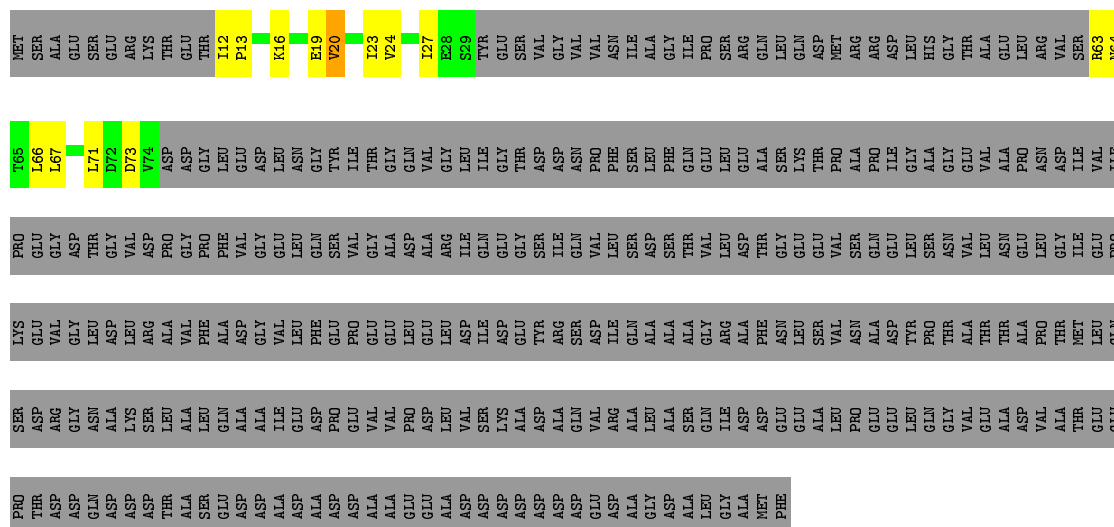
- Molecule 11: 50S RIBOSOMAL PROTEIN L7AE

Chain F:  47% 50%



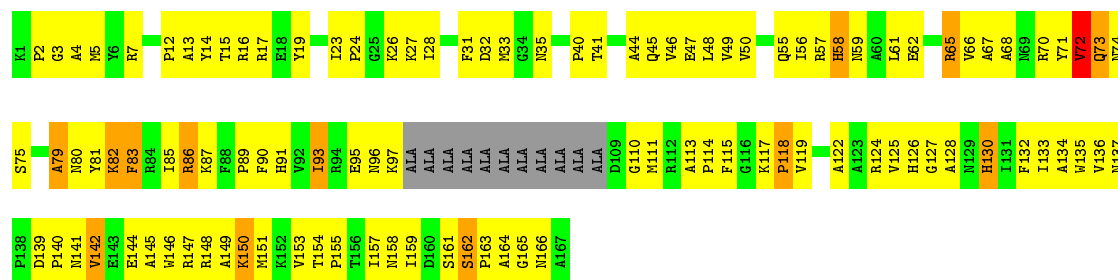
- Molecule 12: 50S RIBOSOMAL PROTEIN L10E

Chain G:  5% 91%



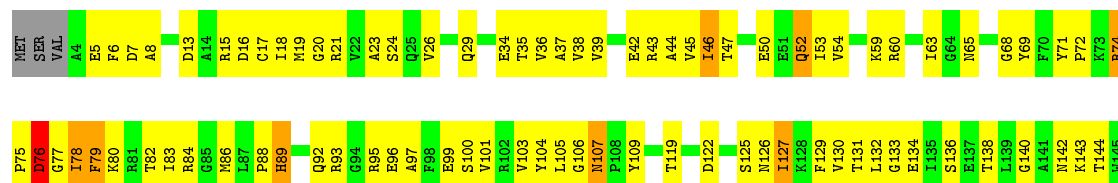
• Molecule 13: 50S RIBOSOMAL PROTEIN L10E

Chain H:  29% 56% 8% 7%



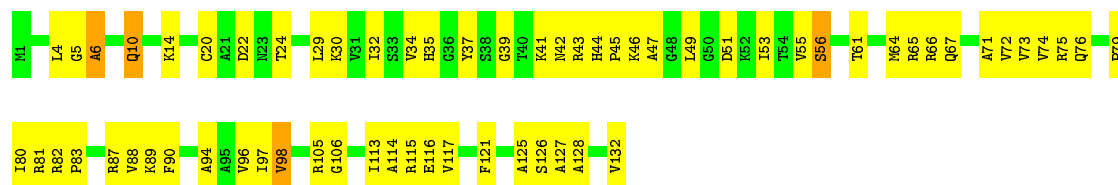
• Molecule 14: 50S RIBOSOMAL PROTEIN L13P

Chain I: 40% 52% 6% ..



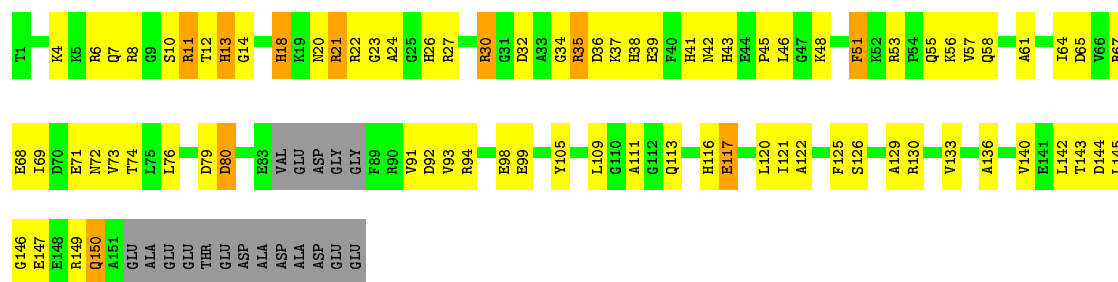
• Molecule 15: 50S RIBOSOMAL PROTEIN L14P

Chain J: 52% 45% .



• Molecule 16: 50S RIBOSOMAL PROTEIN L15P

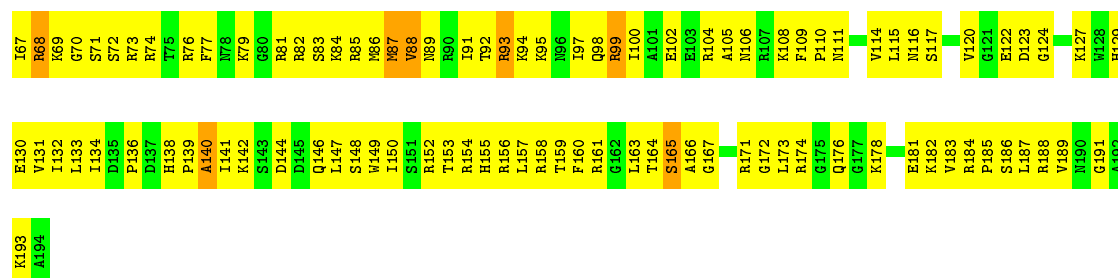
Chain K: 40% 43% 6% 11%



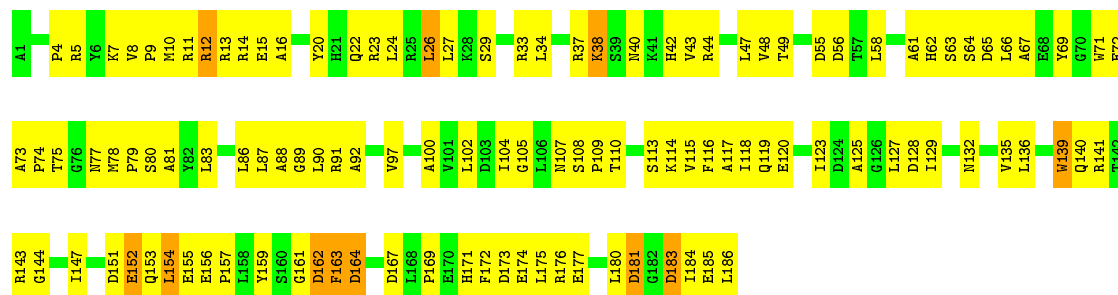
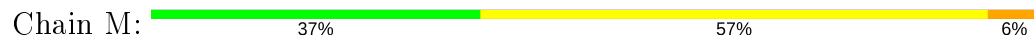
• Molecule 17: 50S RIBOSOMAL PROTEIN L15E

Chain L: 26% 69% 5% .

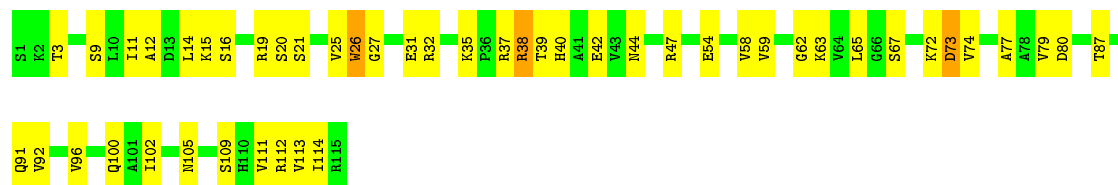




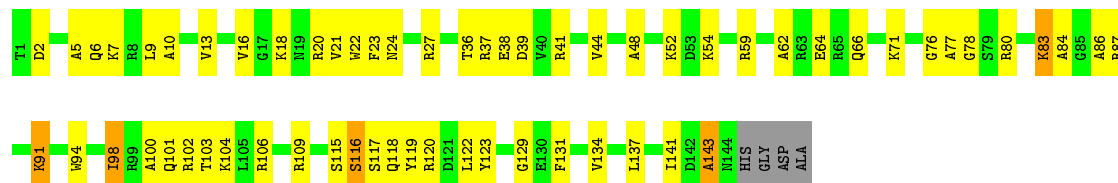
• Molecule 18: 50S RIBOSOMAL PROTEIN L18P



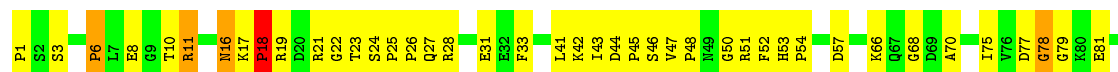
• Molecule 19: 50S RIBOSOMAL PROTEIN L18E



• Molecule 20: 50S RIBOSOMAL PROTEIN L19E



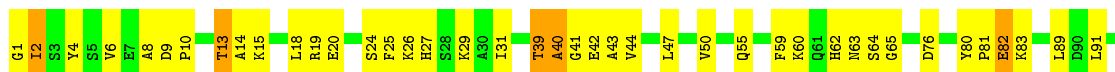
• Molecule 21: 50S RIBOSOMAL PROTEIN L21E





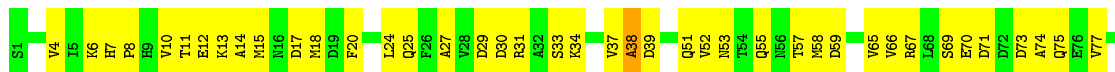
- Molecule 22: 50S RIBOSOMAL PROTEIN L22P HMA122, HL23, RIBOSOMAL PROTEIN L22

Chain Q: 54% 39% 5%



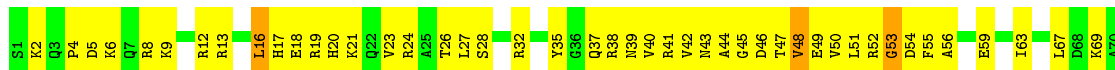
- Molecule 23: 50S RIBOSOMAL PROTEIN L23P

Chain R: 48% 50%



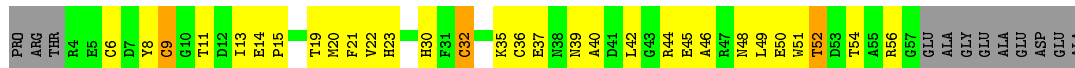
- Molecule 24: RIBOSOMAL PROTEIN L24

Chain S: 42% 55%



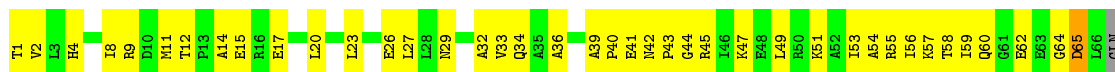
- Molecule 25: 50S RIBOSOMAL PROTEIN L24P

Chain T: 36% 41% 5% 18%

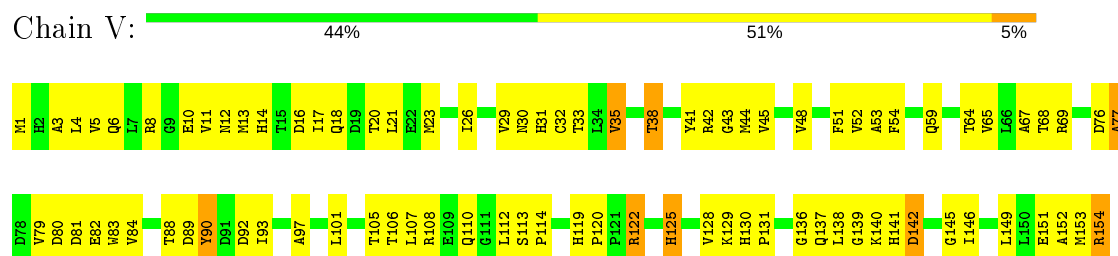


- Molecule 26: 50S RIBOSOMAL PROTEIN L24E

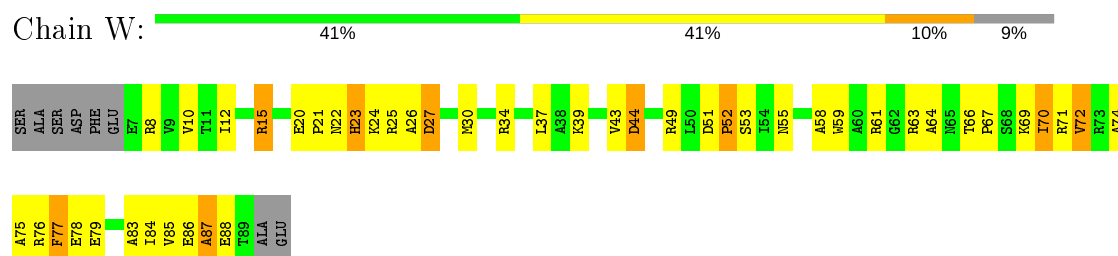
Chain U: 37% 56% 6%



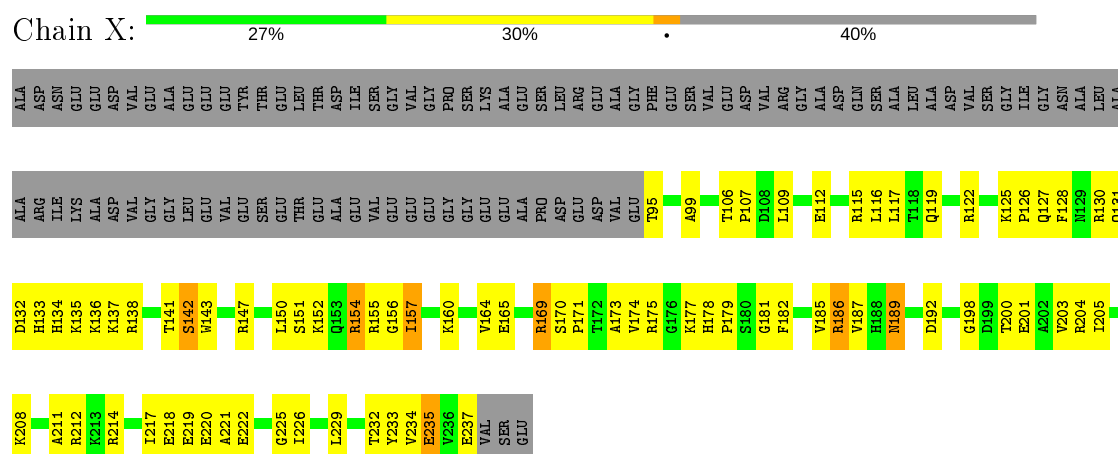
- Molecule 27: 50S RIBOSOMAL PROTEIN L30P



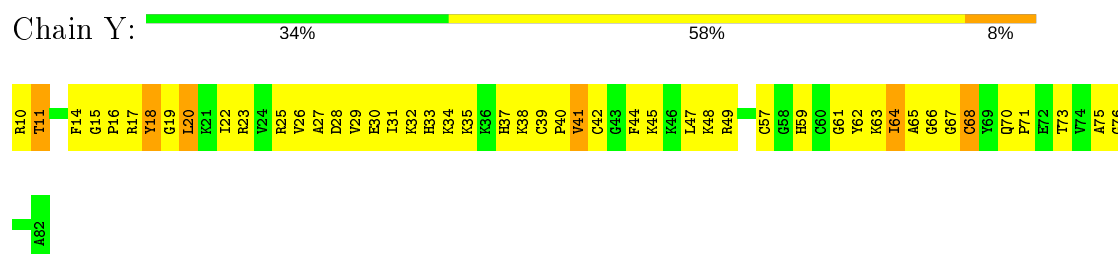
- Molecule 28: 50S RIBOSOMAL PROTEIN L31E



- Molecule 29: 50S RIBOSOMAL PROTEIN L32E

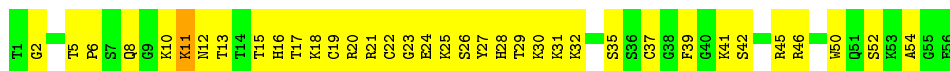


- Molecule 30: 50S RIBOSOMAL PROTEIN L37AE



- 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	41.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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 [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	28
4	5	33/144 (23%)	24 (73%)	9 (27%)	0	100	100
6	A	236/239 (99%)	197 (84%)	27 (11%)	12 (5%)	2	19
7	B	335/337 (99%)	281 (84%)	40 (12%)	14 (4%)	3	23
8	C	244/246 (99%)	201 (82%)	37 (15%)	6 (2%)	5	34
9	D	135/176 (77%)	90 (67%)	31 (23%)	14 (10%)	0	7
10	E	171/177 (97%)	147 (86%)	21 (12%)	3 (2%)	8	41
11	F	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	3	28
12	G	26/348 (8%)	23 (88%)	2 (8%)	1 (4%)	3	25
13	H	152/167 (91%)	123 (81%)	21 (14%)	8 (5%)	2	17
14	I	140/145 (97%)	117 (84%)	17 (12%)	6 (4%)	2	22
15	J	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	10	45
16	K	142/164 (87%)	116 (82%)	20 (14%)	6 (4%)	3	23
17	L	192/194 (99%)	144 (75%)	40 (21%)	8 (4%)	3	23
18	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	3	25
19	N	113/115 (98%)	92 (81%)	17 (15%)	4 (4%)	3	27
20	O	142/148 (96%)	126 (89%)	12 (8%)	4 (3%)	5	32
21	P	93/95 (98%)	72 (77%)	16 (17%)	5 (5%)	2	17
22	Q	149/154 (97%)	127 (85%)	18 (12%)	4 (3%)	5	33
23	R	82/84 (98%)	68 (83%)	9 (11%)	5 (6%)	1	15
24	S	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	5	33
25	T	52/66 (79%)	49 (94%)	3 (6%)	0	100	100
26	U	64/70 (91%)	49 (77%)	13 (20%)	2 (3%)	4	30
27	V	152/154 (99%)	132 (87%)	19 (12%)	1 (1%)	22	61
28	W	81/91 (89%)	65 (80%)	11 (14%)	5 (6%)	1	15
29	X	141/240 (59%)	126 (89%)	12 (8%)	3 (2%)	7	38
30	Y	71/73 (97%)	59 (83%)	7 (10%)	5 (7%)	1	12
31	Z	54/56 (96%)	43 (80%)	7 (13%)	4 (7%)	1	11
All	All	3680/4379 (84%)	3056 (83%)	485 (13%)	139 (4%)	3	25

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%)	25	60
3	2	79/79 (100%)	75 (95%)	4 (5%)	24	57
4	5	29/122 (24%)	26 (90%)	3 (10%)	7	32
6	A	179/181 (99%)	167 (93%)	12 (7%)	16	48
7	B	282/282 (100%)	268 (95%)	14 (5%)	24	58
8	C	193/193 (100%)	181 (94%)	12 (6%)	18	51
9	D	117/147 (80%)	109 (93%)	8 (7%)	16	48
10	E	152/155 (98%)	147 (97%)	5 (3%)	38	68
11	F	92/92 (100%)	91 (99%)	1 (1%)	73	88
12	G	27/283 (10%)	27 (100%)	0	100	100
13	H	122/122 (100%)	111 (91%)	11 (9%)	9	37
14	I	118/121 (98%)	111 (94%)	7 (6%)	19	53
15	J	106/106 (100%)	102 (96%)	4 (4%)	33	65
16	K	112/126 (89%)	106 (95%)	6 (5%)	22	55
17	L	166/166 (100%)	160 (96%)	6 (4%)	35	66
18	M	149/149 (100%)	142 (95%)	7 (5%)	26	60
19	N	93/93 (100%)	90 (97%)	3 (3%)	39	69
20	O	113/116 (97%)	109 (96%)	4 (4%)	36	67
21	P	79/79 (100%)	74 (94%)	5 (6%)	18	51
22	Q	117/121 (97%)	113 (97%)	4 (3%)	37	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	R	73/73 (100%)	72 (99%)	1 (1%)	67	85
24	S	105/105 (100%)	101 (96%)	4 (4%)	33	65
25	T	44/52 (85%)	41 (93%)	3 (7%)	16	48
26	U	51/56 (91%)	51 (100%)	0	100	100
27	V	130/130 (100%)	124 (95%)	6 (5%)	27	61
28	W	66/73 (90%)	61 (92%)	5 (8%)	13	43
29	X	120/195 (62%)	115 (96%)	5 (4%)	30	63
30	Y	56/56 (100%)	51 (91%)	5 (9%)	9	37
31	Z	46/46 (100%)	46 (100%)	0	100	100
All	All	3058/3563 (86%)	2911 (95%)	147 (5%)	25	60

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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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 ⓘ

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.