



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 10, 2023 – 12:25 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 types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtrriage (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) : 2.36

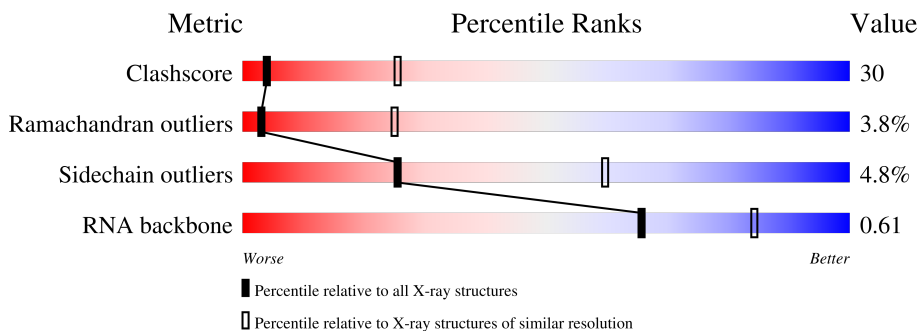
1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	32% 43% 13% 6% 6%
2	1	48	38% 56% . .
3	2	92	39% 57% .
4	5	144	9% 14% . 76%
5	9	122	26% 51% 16% 7%
6	A	239	41% 51% 8%

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Mol	Chain	Length	Quality of chain
7	B	337	39% 55% 6%
8	C	246	46% 48% 6%
9	D	176	27% 44% 9% 20%
10	E	177	49% 45% ...
11	F	119	47% 50% .
12	G	348	5% . 91%
13	H	167	29% 56% 8% . 7%
14	I	145	40% 52% 6% ..
15	J	132	52% 45% .
16	K	164	40% 43% 6% 11%
17	L	194	26% 69% 5% .
18	M	186	37% 57% 6%
19	N	115	58% 39% .
20	O	148	56% 38% ..
21	P	95	48% 46% ..
22	Q	154	54% 39% 5% .
23	R	84	48% 50% .
24	S	119	42% 55% .
25	T	66	36% 41% 5% 18%
26	U	70	37% 56% . 6%
27	V	154	44% 51% 5%
28	W	91	41% 41% 10% 9%
29	X	240	27% 30% . 40%
30	Y	73	34% 58% 8%
31	Z	56	36% 62% .

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
			Total	C	N	O	P			
1	0	2754	59017	26346	10878	19048	2745	0	0	0

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

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

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

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

- Molecule 4 is a protein called TRIGGER FACTOR.

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
8	C	246	1859	1131	344	383	1	0	0	0

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

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

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

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

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

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

- 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	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
			Total	C	N	O			
19	N	115	865	529	161	175	0	0	0

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

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

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

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

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

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

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

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L37E.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	105	Total Mg 105 105	0	0
32	2	1	Total Mg 1 1	0	0
32	9	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	3	Total Mg 3 3	0	0
32	B	3	Total Mg 3 3	0	0
32	J	1	Total Mg 1 1	0	0
32	S	1	Total Mg 1 1	0	0
32	X	1	Total Mg 1 1	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	2	1	Total Cd 1 1	0	0
36	N	1	Total Cd 1 1	0	0
36	T	1	Total Cd 1 1	0	0
36	Y	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 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 O 36 36	0	0
37	T	25	Total O 25 25	0	0
37	U	11	Total O 11 11	0	0
37	V	69	Total O 69 69	0	0
37	W	26	Total O 26 26	0	0
37	X	107	Total O 107 107	0	0
37	Y	35	Total O 35 35	0	0
37	Z	50	Total O 50 50	0	0

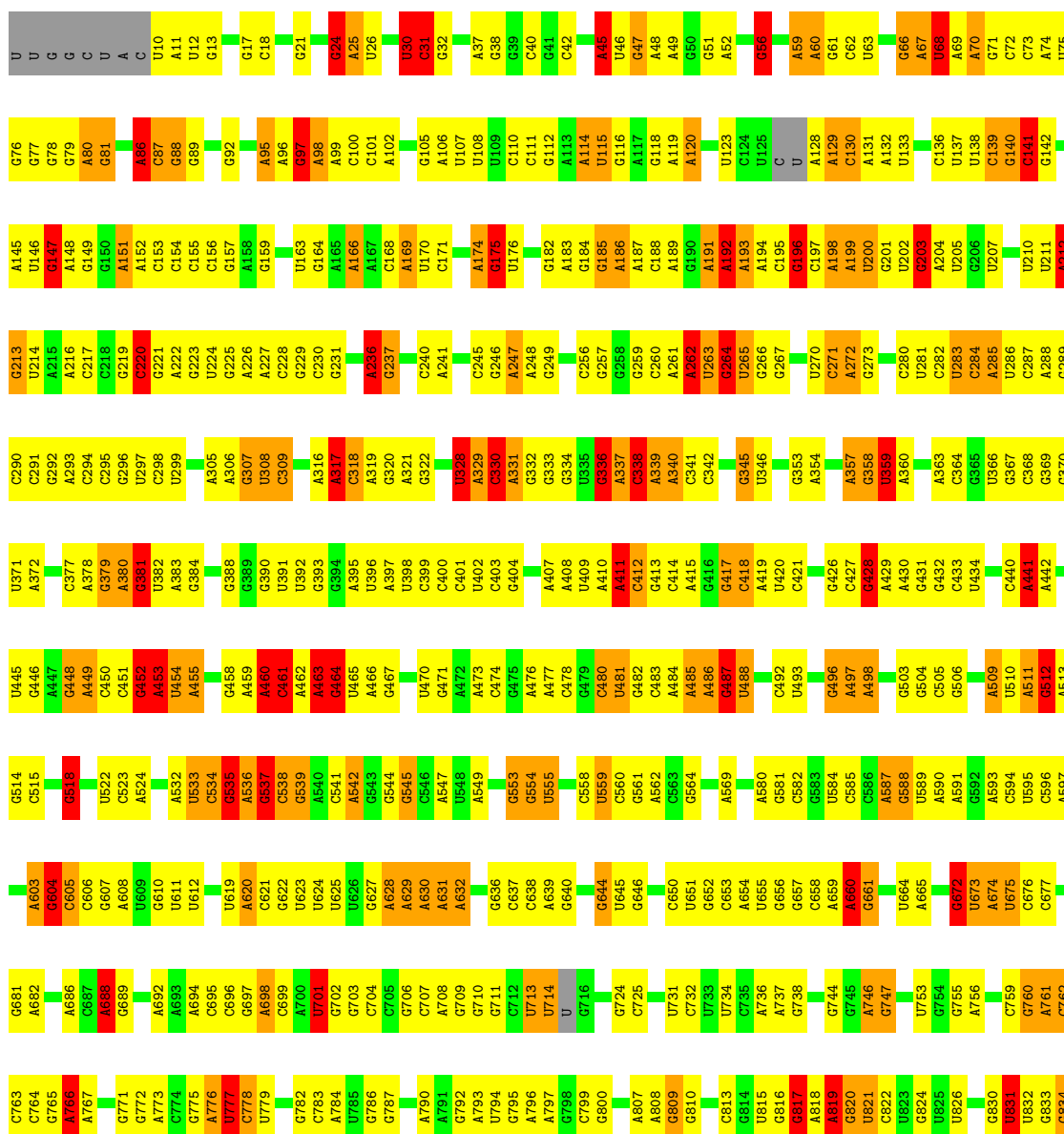
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

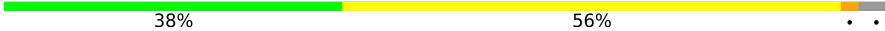
Note EDS was not executed.

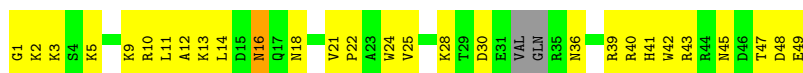
- Molecule 1: 23S rRNA

Chain 0: 



A1845	A1846	A1847	A1848	G1849	U1850	A1851	A1852	A1853	C1854	G1855	A1856	A1857	A1858	A1859	U1860	A1861	C1862	G1863	A1866	A1867	A1868	A1869	C1870	A1871	A1872	A1873	A1874	A1875	C1876	A1877	A1878	C1880	A1881	A1882	U1883	A1884	A1885	A1886	U1890	C1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	U1902	U1903	A1904	U1905	C1906	A1909																																																												
U1770	U1771	C1772	G1773	G1774	A1775	A1776	G1777	C1778	A1779	A1783	U1784	G1785	C1786	A1787	A1788	U1789	C1790	U1791	C1792	G1795	A1796	A1797	C1798	C1803	A1804	G1805	A1806	A1807	A1808	C1809	C1810	A1811	G1812	U1813	G1814	A1815	C1816	U1817	C1818	U1819	G1820	G1827	G1828	A1829	C1830	G1831	C1832	U1833	C1834	U1835	A1836	U1837	U1838	A1839	A1840	C1841	A1842																																																									
U1696	G1697	C1700	A1701	A1702	G1703	C1708	A1709	A1710	A1711	A1712	G1713	A1717	U1718	U1719	U1720	C1721	C1722	A1723	U1724	U1725	A1726	G1727	C1730	C1731	A1735	A1736	A1737	U1741	A1742	G1745	A1746	U1747	U1748	U1749	U1750	G1751	G1752	A1754	A1755	G1756	U1757	U1758	A1759	U1760	U1761	C1762	C1763	A1682	A1693	U1766	C1769																																																															
A1630	C1633	U1634	G1635	G1636	A1637	A1641	A1642	C1643	G1646	G1647	U1648	U1649	C1650	C1651	C1652	A1653	U1654	U1655	A1656	A1657	A1658	A1661	C1662	C1663	A1664	G1665	A1666	A1667	U1668	U1672	U1673	C1674	C1675	U1676	A1677	A1678	C1679	C1680	G1681	A1682	U1683	A1684	C1685	C1686	C1687	G1688	U1689	A1690	A1691	C1692	A1693	C1694	C1695																																																													
A1471	C1472	U1473	C1474	A1475	A1476	C1477	U1478	A1482	A1483	G1484	A1485	A1486	A1487	U1488	U1489	G1490	G1491	A1492	A1493	A1494	A1495	A1496	G1497	U1500	A1501	U1502	A1503	U1504	U1505	U1506	C1507	G1510	U1511	U1512	C1513	A1514	A1515	C1516	A1522	G1523	U1524	A1525	A1526	A1527	A1528	G1532	A1533	C1534	G1543	U1544	C1545	C1553																																																														
G1401	C1405	U1406	A1407	A1408	G1409	U1412	A1413	A1414	G1415	G1416	G1417	U1418	U1419	U1422	C1423	A1424	G1425	A1426	A1427	U1430	C1431	A1432	A1433	A1434	U1435	G1438	C1439	U1440	G1441	A1442	G1443	G1444	U1445	U1446	A1447	U1448	G1449	C1450	C1451	G1452	G1453	A1457	A1458	A1459	G1460	U1461	A1462	A1463	C1467	U1468	A1469	A1470																																																														
C1332	U1333	C1334	C1335	U1336	A1337	U1338	G1339	U1340	A1341	C1342	C1343	U1346	U1347	A1348	G1351	A1352	C1353	G1354	A1355	A1356	A1357	U1358	U1359	C1360	A1361	C1366	A1367	U1368	A1369	U1370	U1371	A1372	U1373	C1374	A1375	G1376	C1377	U1378	A1379	U1380	A1381	G1382	G1386	U1387	U1388	G1389	A1392	A1393	C1394	C1397	U1398	A1399	C1400																																																													
C1282	U1283	G1284	A1287	C1288	U1289	A1290	A1291	C1292	U1293	A1294	G1295	A1296	U1297	U1298	G1299	G1302	U1303	U1304	U1305	U1306	A1307	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	A1321	U1325	G1326	U1327	A1328	A1329	A1331	A1332	G1335	C1336	C1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400								
C1186	U1187	A1188	U1189	A1190	A1191	U1192	A1193	A1194	G1195	C1196	G1197	C1201	A1202	U1205	A1207	C1208	C1209	G1210	U1211	C1212	C1213	G1214	A1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	C1250	C1251	C1252	C1253	C1254	C1257	G1260	A1261																																																	
A1114	U1115	A1116	U1117	A1118	G1119	U1120	A1121	U1122	A1123	A1124	U1125	U1126	U1127	U1128	U1129	G1131	A1132	A1133	U1134	U1135	U1136	G1137	U1138	C1148	U1149	G1150	A1151	A1152	C1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	G1165	A1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1180	U1181	U1182	U1183	U1184	U1185																																																									
G1038	U1039	A1040	U1041	U1042	C1043	G1044	U1045	A1046	C1051	U1052	G1053	G1054	U1055	U1056	A1057	U1058	G1059	C1060	C1061	U1066	A1067	C1068	C1069	A1070	U1071	U1072	A1073	U1076	U1077	C1080	A1081	A1082	C1083	G1084	C1085	A1086	U1087	A1088	G1089	U1096	A1097	A1098	U1099	G1100	C1104	C1105	A1106	A1107	A1108	A1109	U1110	U1111																																																														
U903	G904	C905	U906	A907	U908	U909	C910	G911	U919	A920	G921	C922	U923	U924	C925	A926	C931	U932	C933	U934	G935	C938	A939	G940	G941	U942	A943	U944	U945	U946	U947	G948	G952	G953	U954	A955	U956	A957	G958	C959	G960	U961	C962	C963	G964	G968	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037
U835	G836	U837	U840	A841	C842	A843	A844	U845	A846	C847	C848	C849	U850	U851	U852	U853	U854	U855	U856	A857	U858	C859	U860	A861	A867	G868	G869	G870	G871	U872	A875	A876	G877	G878	C881	A882	U883	U884	C885	U886	G887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911																																																	

Chain 1:  38% 56%



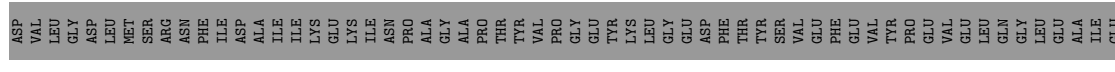
- Molecule 3: 50S RIBOSOMAL PROTEIN L44E LA, HLA, RIBOSOMAL PROTEIN L44E

Chain 2:  39% 57%



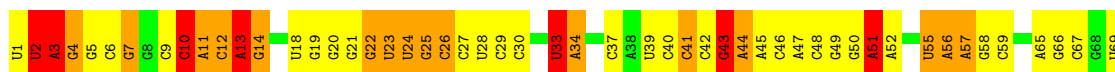
- Molecule 4: TRIGGER FACTOR

Chain 5:  9% 14% 76%



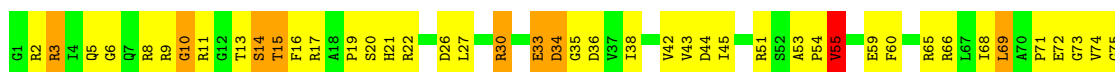
- Molecule 5: 5S RRNA

Chain 9:  26% 51% 16% 7%



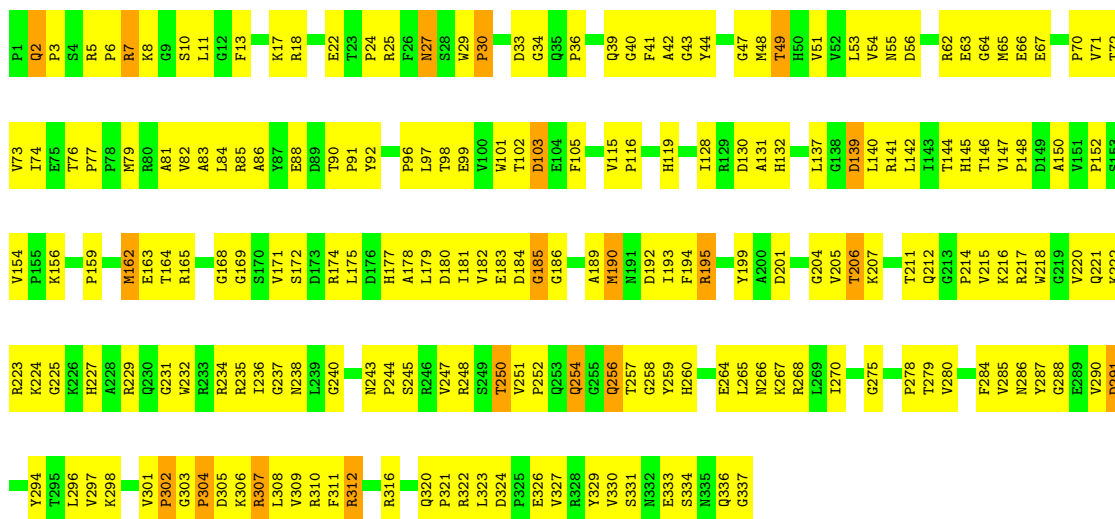
- Molecule 6: 50S RIBOSOMAL PROTEIN L2P

Chain A:  41% 51% 8%

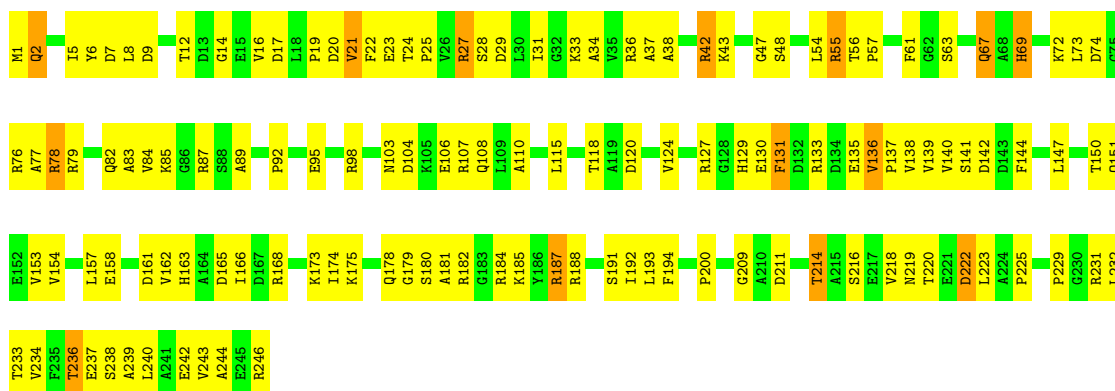




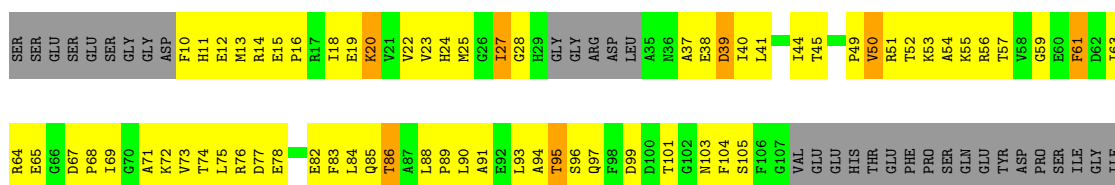
● Molecule 7: 50S RIBOSOMAL PROTEIN L3P

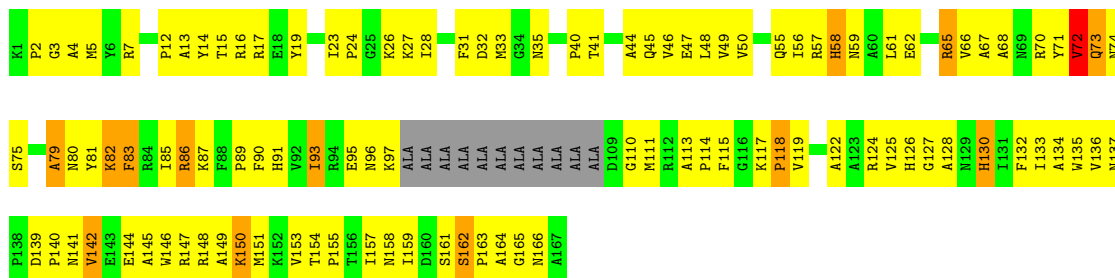


● Molecule 8: 50S RIBOSOMAL PROTEIN L4P



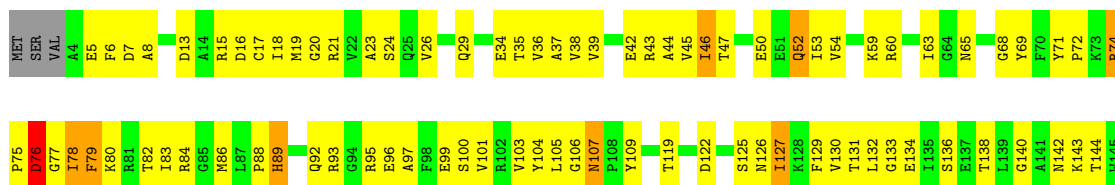
● Molecule 9: 50S RIBOSOMAL PROTEIN L5P HMA15, HL13, RIBOSOMAL PROTEIN L5





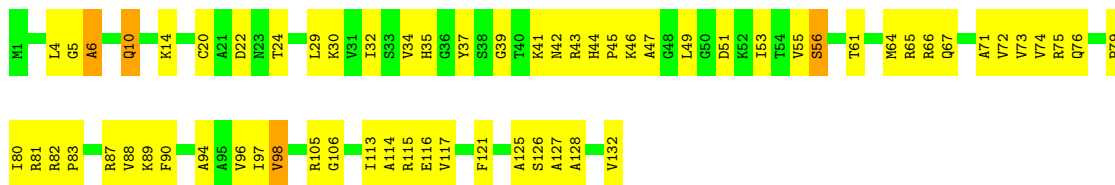
- Molecule 14: 50S RIBOSOMAL PROTEIN L13P

Chain I: 40% 52% 6% ..



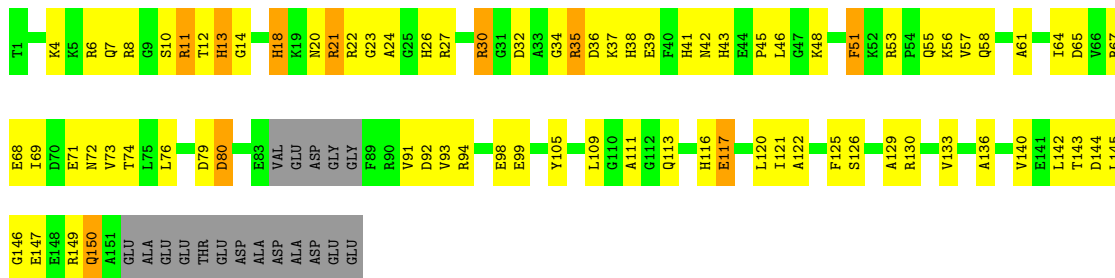
- Molecule 15: 50S RIBOSOMAL PROTEIN L14P

Chain J: 52% 45% .



- Molecule 16: 50S RIBOSOMAL PROTEIN L15P

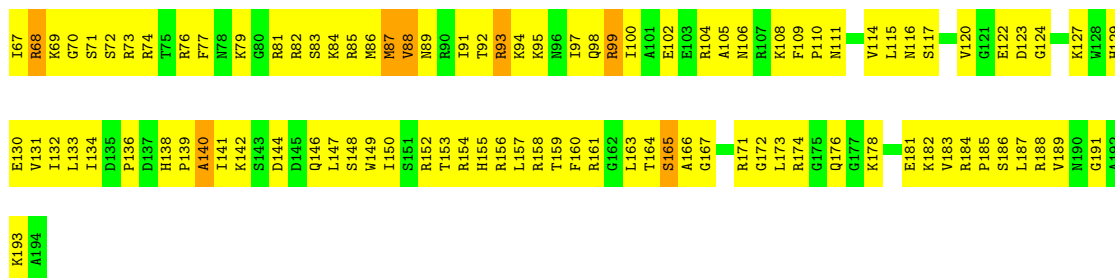
Chain K: 40% 43% 6% 11%



- Molecule 17: 50S RIBOSOMAL PROTEIN L15E

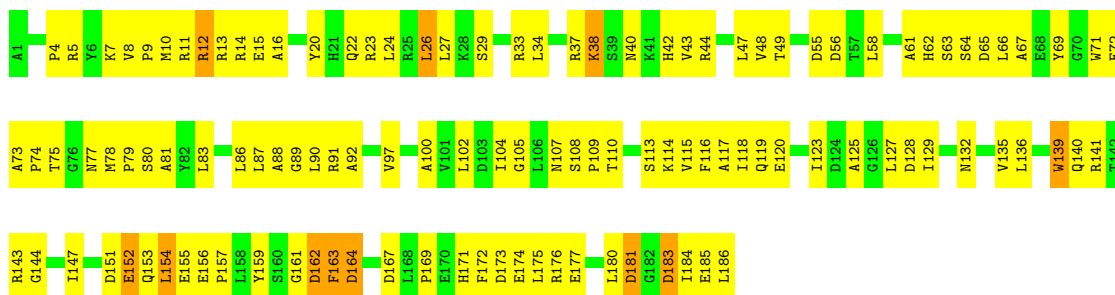
Chain L: 26% 69% 5% .





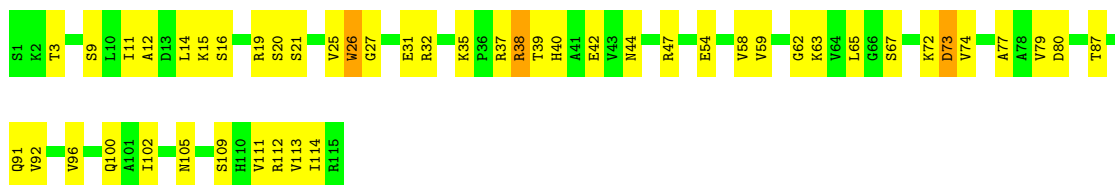
- Molecule 18: 50S RIBOSOMAL PROTEIN L18P

Chain M: 37% 57% 6%



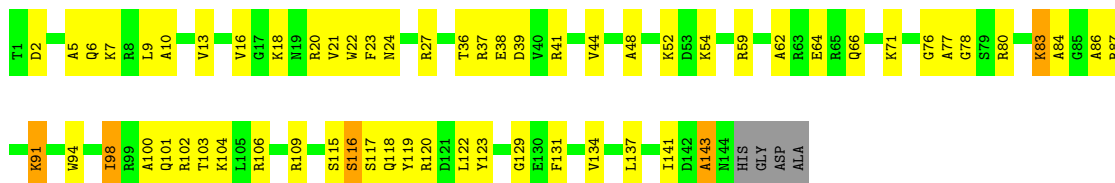
- Molecule 19: 50S RIBOSOMAL PROTEIN L18E

Chain N: 58% 39% 3%



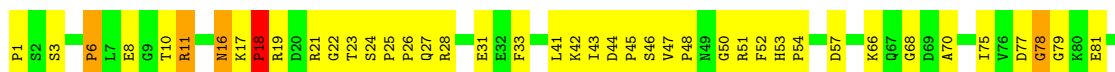
- Molecule 20: 50S RIBOSOMAL PROTEIN L19E

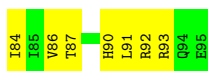
Chain O: 56% 38% 6%



- Molecule 21: 50S RIBOSOMAL PROTEIN L21E

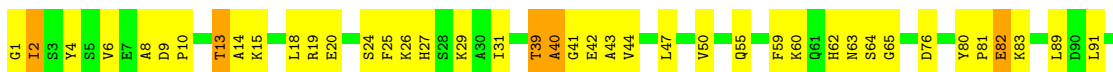
Chain P: 48% 46% 6%





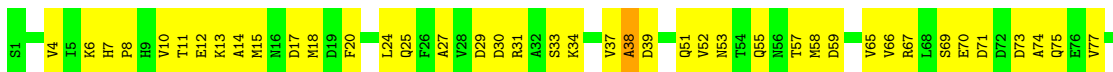
- Molecule 22: 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22

Chain Q: 54% 39% 5%



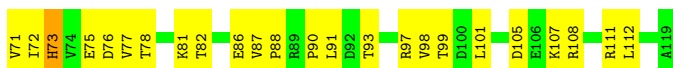
- Molecule 23: 50S RIBOSOMAL PROTEIN L23P

Chain R: 48% 50%



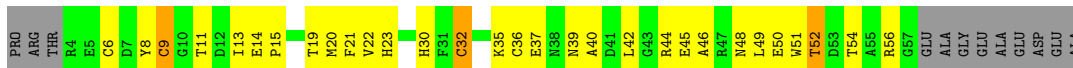
- Molecule 24: RIBOSOMAL PROTEIN L24

Chain S: 42% 55%



- Molecule 25: 50S RIBOSOMAL PROTEIN L24P

Chain T: 36% 41% 5% 18%



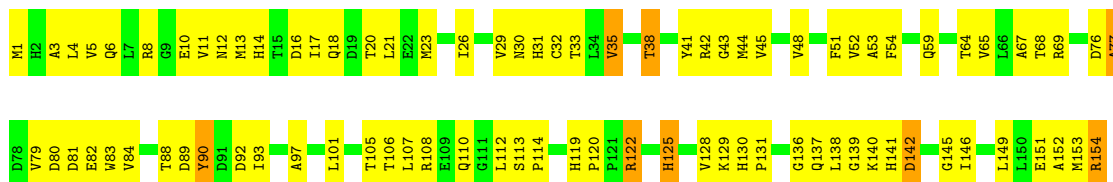
- Molecule 26: 50S RIBOSOMAL PROTEIN L24E

Chain U: 37% 56% 6%



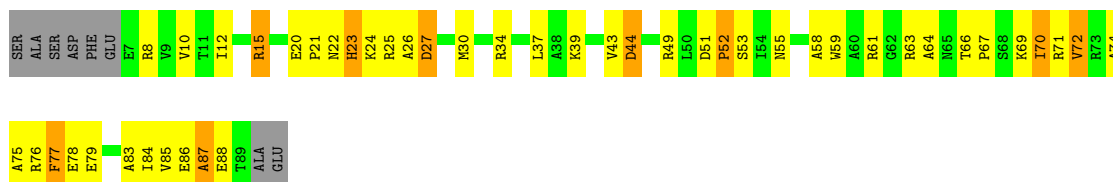
- Molecule 27: 50S RIBOSOMAL PROTEIN L30P

Chain V: 44% 51% 5%



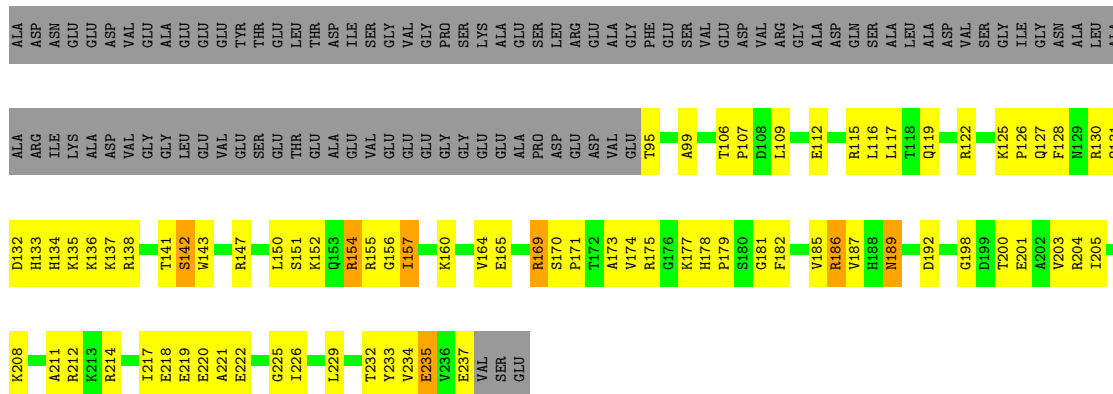
- Molecule 28: 50S RIBOSOMAL PROTEIN L31E

Chain W: 41% 41% 10% 9%



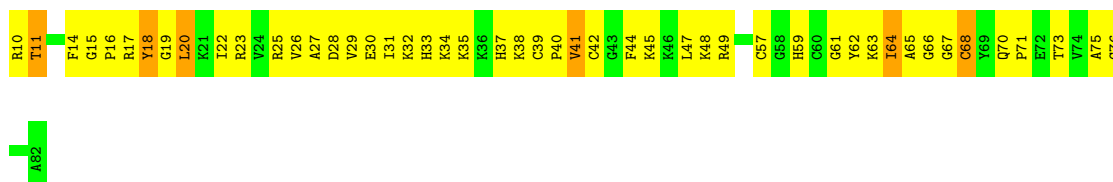
- Molecule 29: 50S RIBOSOMAL PROTEIN L32E

Chain X: 27% 30% 40%



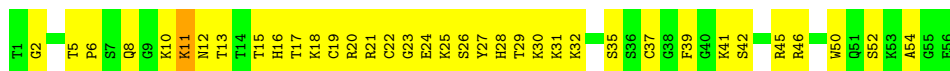
- Molecule 30: 50S RIBOSOMAL PROTEIN L37AE

Chain Y: 34% 58% 8%



- Molecule 31: RIBOSOMAL PROTEIN L37E

Chain Z: 36% 62%



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
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: MG, CL, NA, CD, K

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 [i](#)

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 [i](#)

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
22	Q	39	THR
30	Y	28	ASP
24	S	5	ASP
27	V	142	ASP
9	D	50	VAL

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

Mol	Chain	Res	Type
19	N	105	ASN
26	U	60	GLN
20	O	66	GLN
22	Q	113	HIS
27	V	110	GLN

5.3.3 RNA [i](#)

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	1722	U
1	0	2282	U
1	0	1771	U
1	0	1977	U
1	0	2370	A

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.