



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:01 PM BST

PDB ID : 3BBX
EMDB ID: : EMD-1455
Title : The Hsp15 protein fitted into the low resolution Cryo-EM map of the 50S.nc-tRNA.Hsp15 complex
Authors : Jiang, L.; Abrahams, J.P.
Deposited on : 2007-11-11
Resolution : 10.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

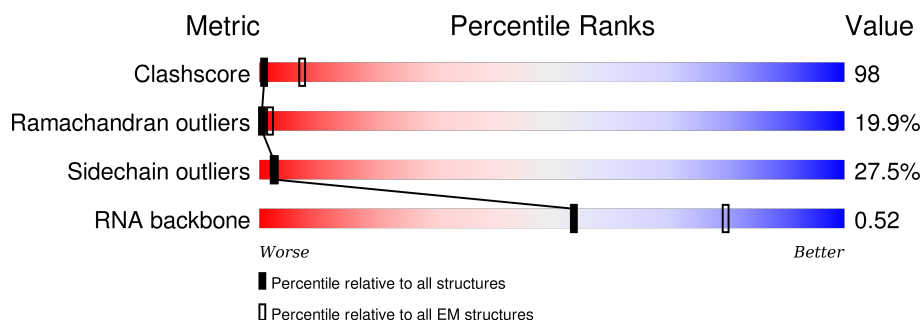
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




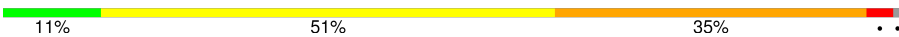



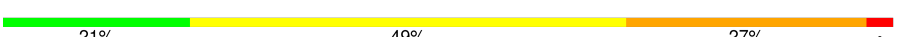
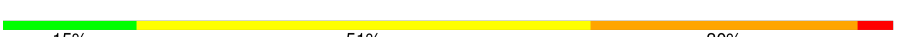

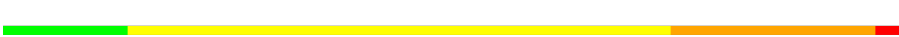

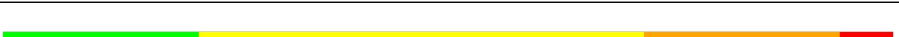
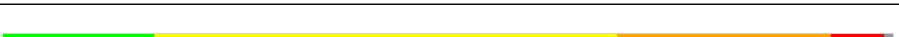

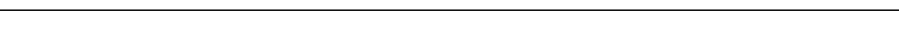
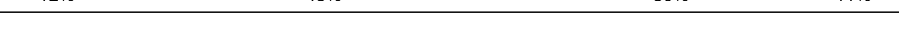
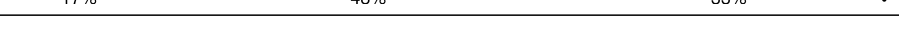
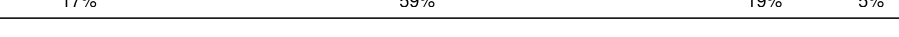





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	120	22% 63% 13% .
2	B	2904	20% 66% 13% .
3	V	94	27% 56% 16% .
4	C	273	13% 41% 37% 8% .
5	D	209	10% 53% 33% .
6	E	201	12% 55% 28% 5%
7	F	178	19% 52% 27% .
8	G	176	24% 57% 16% .

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Mol	Chain	Length	Quality of chain
9	H	149	
10	J	142	
11	K	123	
12	L	144	
13	M	136	
14	N	127	
15	O	117	
16	P	114	
17	Q	117	
18	R	103	
19	S	110	
20	T	100	
21	U	103	
22	W	84	
23	X	63	
24	Y	58	
25	Z	70	
26	0	56	
27	1	54	
28	2	46	
29	3	64	
30	4	38	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 89335 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	117	Total	C	N	O	P	0	0
			2507	1116	459	815	117		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2902	Total	C	N	O	P	0	61
			61056	27210	11229	19715	2902		

- Molecule 3 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	267	Total	C	N	O	S	0	0
			2053	1271	416	359	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	140	Total	C	N	O	S	0	0
			1112	704	210	194	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	121	Total	C	N	O	S	0	0
			930	582	179	164	5		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			777	491	145	139	2		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	84	Total	C	N	O	S	0
			634	391	129	113	1	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	63	Total	C	N	O	S	0
			509	313	99	95	2	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	58	Total	C	N	O	S	0
			449	281	87	79	2	0

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Z	70	Total	C	N	O	S	0
			549	339	104	100	6	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	0	56	Total	C	N	O	S	0
			444	269	94	80	1	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	1	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	Q	2	Total	Mg	0
			2	2	
31	E	3	Total	Mg	0
			3	3	
31	B	92	Total	Mg	0
			92	92	
31	C	1	Total	Mg	0
			1	1	
31	T	2	Total	Mg	0
			2	2	
31	U	1	Total	Mg	0
			1	1	
31	2	3	Total	Mg	0
			3	3	
31	L	4	Total	Mg	0
			4	4	
31	S	2	Total	Mg	0
			2	2	

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
32	B	443	Total	O	0
			443	443	

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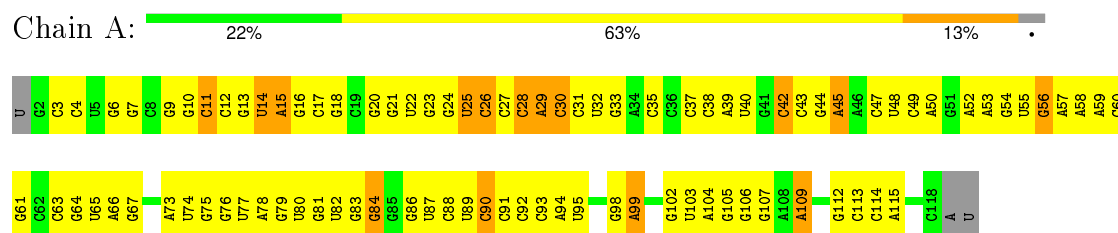
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Mol	Chain	Residues	Atoms		AltConf
32	C	1	Total 1	O 1	0
32	D	1	Total 1	O 1	0
32	E	18	Total 18	O 18	0
32	L	8	Total 8	O 8	0
32	Q	7	Total 7	O 7	0
32	S	7	Total 7	O 7	0
32	T	5	Total 5	O 5	0
32	U	5	Total 5	O 5	0
32	2	11	Total 11	O 11	0

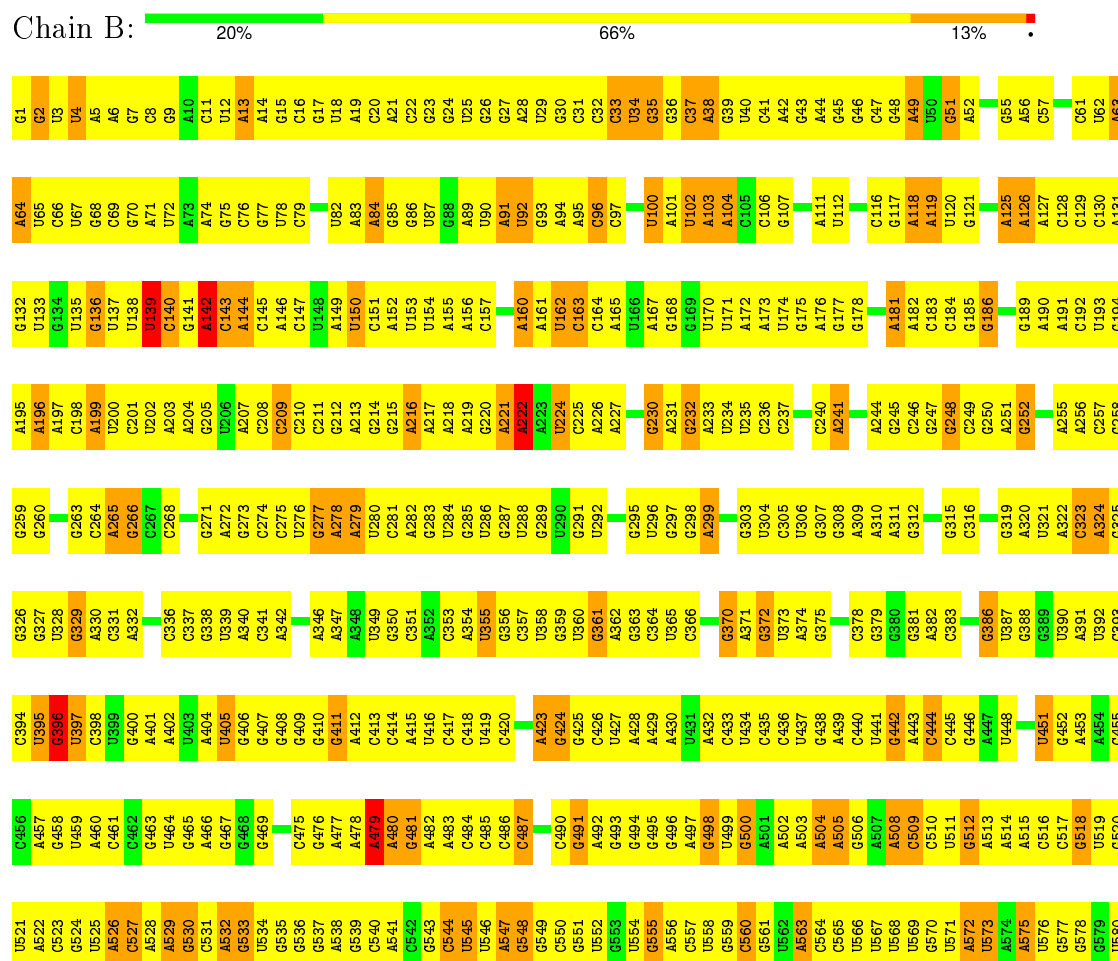
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

• Molecule 1: 5S ribosomal RNA

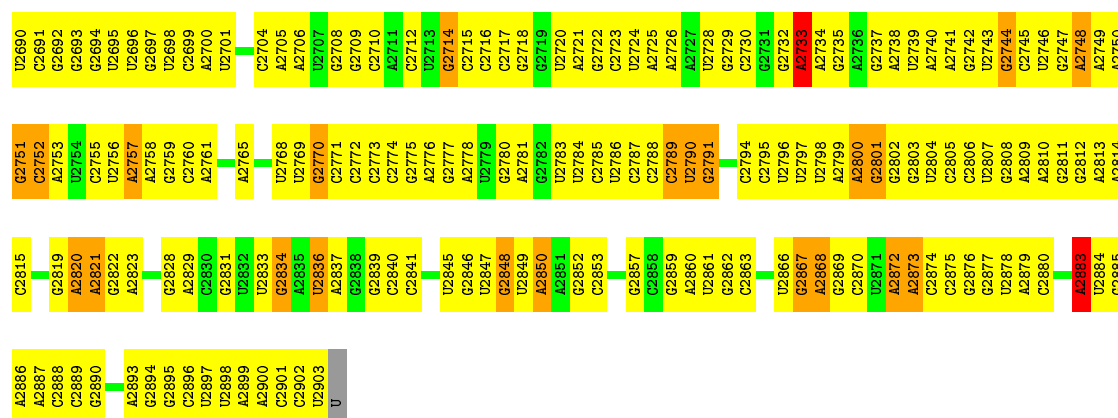


• Molecule 2: 23S ribosomal RNA

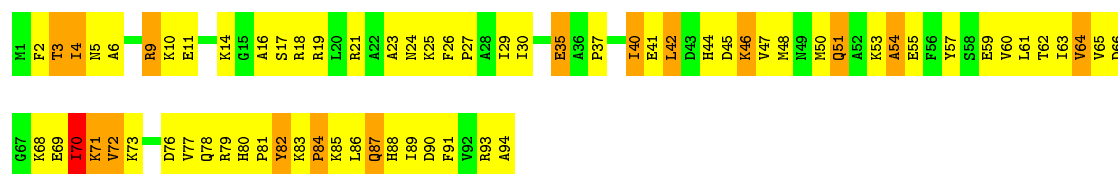


C1493	C1494	C1495	C1496	G1501	C1502	A1503	C1504	C1428	A1365	C1298	G1238	U1173	A1111	C1043	G978	A918	A844	A781	U709	A644	C581	
A1494	A1495	A1496	A1497	G1501	C1502	A1503	C1504	G1429	A1366	G1299	G1239	U1174	A1112	C1044	A979	U919	A845	A782	U710	A645	C582	
A1498	A1499	A1500	A1501	G1501	C1502	A1503	C1504	G1430	A1367	G1300	U1240	A1175	U1113	C1045	A980	A920	U846	A783	G711	U646	C583	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1431	A1368	A1301	U1241	A1176	U1114	A1046	A981	C921	U847	G784	G712		C584	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1432	A1369	A1302	U1242	G1177	G1115	A1047	A982	C922	C848	G785	G713	G649	C585	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1433	A1370	A1303	U1243	G1178	G1116	A1048	A983	C923	C849	G786		C650	C586	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1434	A1371	A1304	U1244	G1179	C1117	A1049	A984	C924	U850	C787		C651	C587	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	C1437	A1372	C1305	U1245	G1180	C1118	A1050	C985	A925	C851	A788	A716	U651	C588	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1438	A1373	G1311	U1246	U1181	U1119	A1051	C986	G926	U852	A789	C717	U652	C589	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1439	A1374	G1312	U1247	U1182	G1120	C1052	C987	A927	C853	U790	C719	U653	C590	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1440	A1375	G1313	U1248	U1183	G1121	C1053	A988	A928	C854	C791	U720	A654	C591	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1441	A1376	U1313	U1249	U1184	G1122	A1054	G989	U929	G855	A792	A721	A655	C592	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1442	A1377	C1314	U1250	U1185	G1123	A1055	A990	G930	G856	A793	A722	U656	C593	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1443	A1378	C1315	C1251		G1124	G1056	C991	U931	G857	A794		U657	C594	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1444	A1379	U1316	U1252	U1188	G1125	A1057	C992	U932	G858	C795	A726	U658	C595	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1445	A1380	U1317	A1253	U1189	G1126		C993	A933	C859	A727	A727	U659	C596	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1446	A1381	U1318	A1254	U1190	A1127	U1060	C994	U934	U860	G728	G728	A661	C597	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1447	A1382	U1319	U1255	G1191	G1128	U1061	C995	U935	A861	G729	G729	A662	C598	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1448	A1383	C1320	U1256	G1192	A1129	U1062	A996	A936	G862	G730	A730	G663	C599	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1449	A1384	A1321	U1257	G1193	U1130	U1063	C997	C937	A863	A800		G664	C600	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1450	A1385	A1322	U1258	A1194	G1131	C1064	C998	G938	G864	G801	C732	U665	C601	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1451	A1386	C1323	U1259	G1195	U1132	U1065	C999	G939	C865	A802	C733	U666	C602	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1452	A1387	G1324	U1260	G1196	A1133	U1066	A1000	G940	U803	A734	A734	U667	C603	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1453	A1388	U1325	U1261	G1197	A1134	U1068	A1001	A941	G869	A804	A735	U668	C604	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1454	A1389	U1326	U1262	U1198	C1135	A1069	A1002	G942	U870	G805	C736	U669	C605	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1455	A1390	U1327	U1263	U1199	G1136	A1070		G943	U871	C806	C737	U670	C606	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1456	A1391	A1328	A1264	U1200	G1137	U1071	C1005	A945	U872	U807	G738		C607	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1457	A1392	U1329	A1265	U1201	G1138	C1072	C1006	A946	C873	G808		C672	C611	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1458	A1393	G1330	U1266	U1202	G1139	C1073	C1007	C946	G874	G809	U741	U674	C612	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1459	A1394	G1331	U1267	U1203	G1140	U1076	A1008	A947	U810	U840	A742	G674	C613	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1460	A1395	G1332	U1268	U1204	U1141	U1077	A1009	C948	C876	U811	A743	A614	C614	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1461	A1396	G1333	U1269	U1205	A1142	U1078	A1010	C949	A877	C812	U744	U615	C615	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1462	A1397	G1334	U1270	U1206	A1143	U1079	A1011	G950	A878	U813	U745	C616	C616	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1463	A1398	U1335	U1271	U1207	A1144	U1080	C1012	C951	C879	C814	U746	U617	C617	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1464	A1399	A1336	U1272	U1208	A1145	U1081	C1013	G952	G880	C815	U747	U618	C618	
C1501	C1502	A1503	C1504	G1501	C1502	A1503	C1504	A1465	A1400	G1337	U1273	U1209		U1082	A1014	G953	G881	C816	A748	G619	C619	
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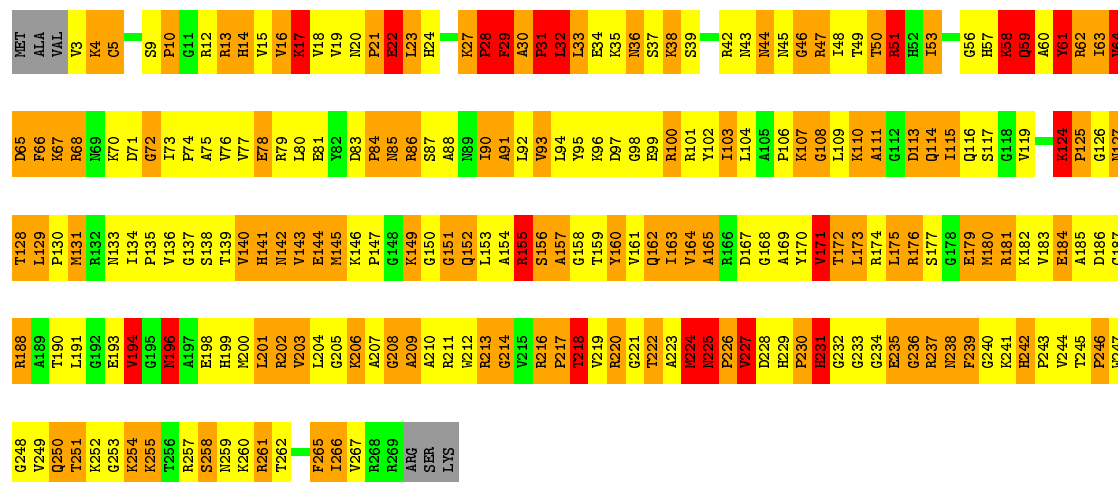
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G2631	G2370	C2506	C2306	G2246	A2184	C2078	U2017	U1956	G1817	G1817	G1755	U1693	
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C2649	U2586	G2325	G2325	U2265	A2205	C2097	C2036	C1975	G1839	G1776	G1776	U1714	
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				A2284	U2224	C2143	C2055	C1994	G1933	G1863		G1733	
				G2285	A2225	G2144	G2056	U1995	C1934	U1864		G1734	
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				A2288	G2228	A2147	A2060	A1998	G1867	G1867		G1737	
				G2289	U2229	G2148	G2061	C1999	C1868	C1800		G1738	
				C2290	G2230	U2149	A2062	C2000	G1869	A1801		C1739	
				U2291	U2231	C2150	C2063	C2001	A1802	G1740		G1740	
				U2292	C2232	U2151	C2064	G2002	A1803	C1741		G1741	
				G2293	U2233	C2152	C2065	A2003	A1804	C1804		U1742	
				C2294	G2234	C2153	C2066	G2004	A1805			G1743	
				U2295	G2235	A2154	G2067	A2005	C1873	C1873		U1744	
				U2296	U2236	U2155	U2068	C2006	G1806	G1806		G1682	
				A2297	G2237	G2156	G2069	U2007	G1807	G1807		G1683	
				A2298	G2238		A2070	C2008	A1808	A1746		G1684	
				G2299	G2239	A2071	A2071	C2009	A1809	A1877		U1747	
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				C2301	A2241	C2073	G2074	G2012	G1811	C1879		A1749	
				C2302	G2242	U2180	U2074	A2013	U1812	G1812		G1750	
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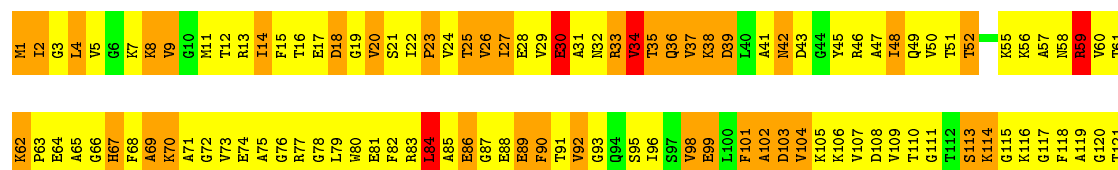
• Molecule 3: 50S ribosomal protein L25

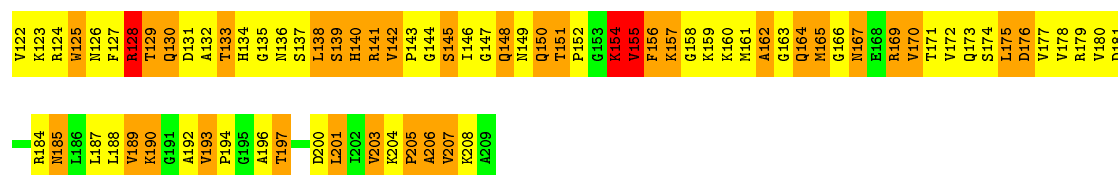


• Molecule 4: 50S ribosomal protein L2



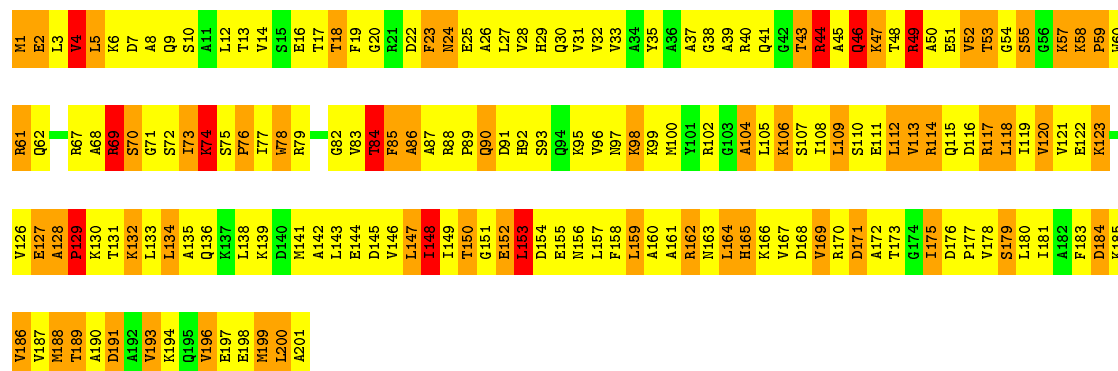
• Molecule 5: 50S ribosomal protein L3





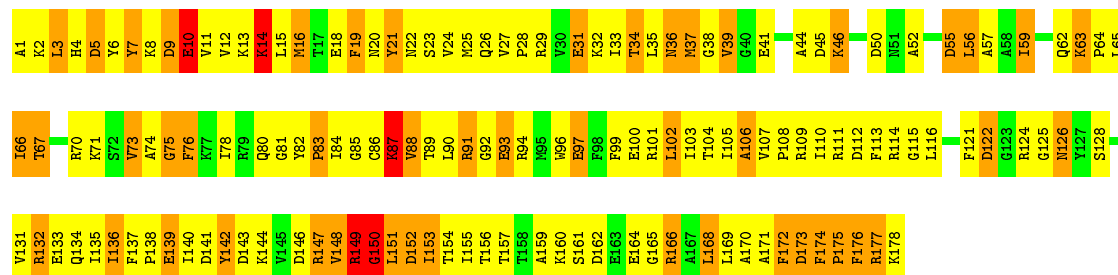
• Molecule 6: 50S ribosomal protein L4

Chain E: 12% 55% 28% 5%



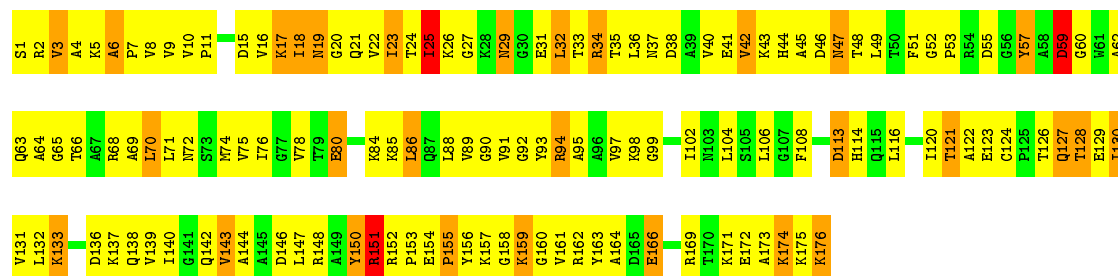
• Molecule 7: 50S ribosomal protein L5

Chain F: 19% 52% 27%



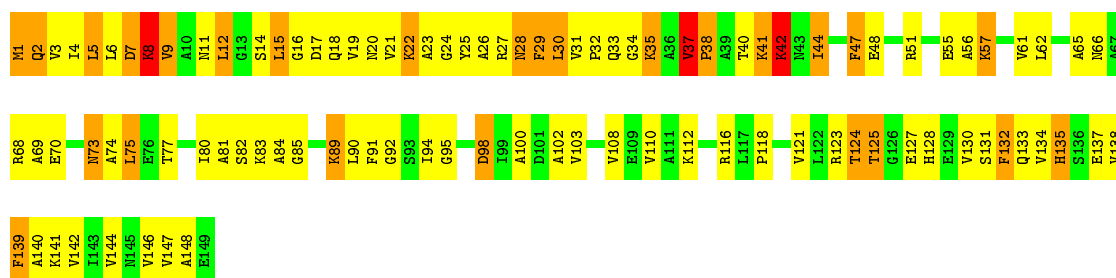
• Molecule 8: 50S ribosomal protein L6

Chain G: 24% 57% 16%



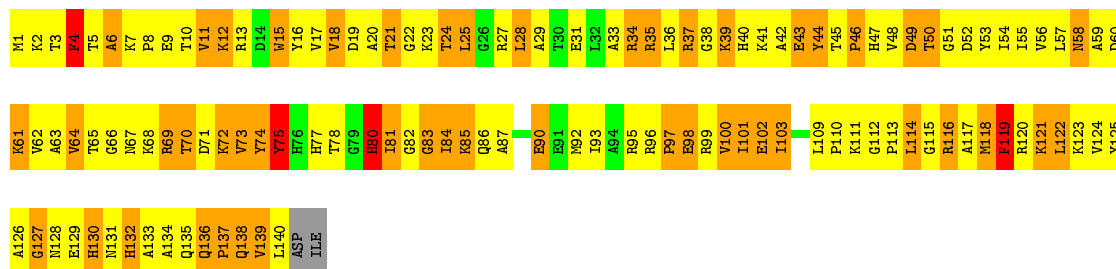
• Molecule 9: 50S ribosomal protein L9

Chain H: 34% 47% 17%



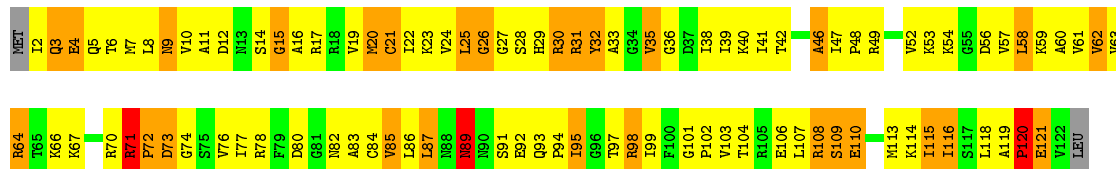
• Molecule 10: 50S ribosomal protein L13

Chain J: 11% 51% 35%



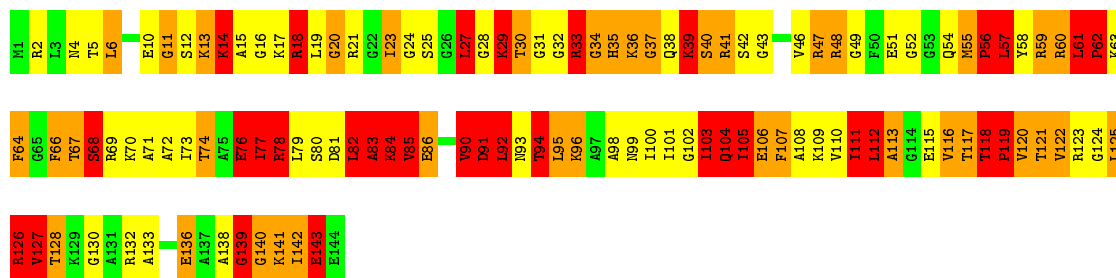
• Molecule 11: 50S ribosomal protein L14

Chain K: 20% 53% 23%



• Molecule 12: 50S ribosomal protein L15

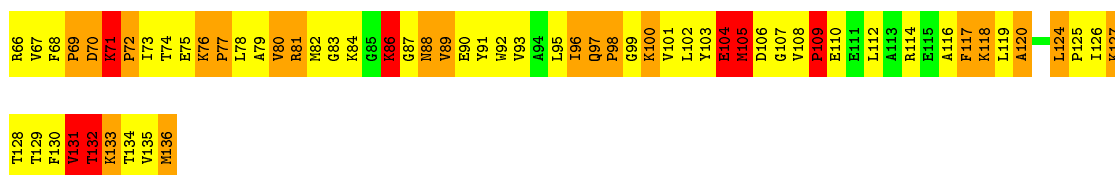
Chain L: 17% 34% 26% 23%



• Molecule 13: 50S ribosomal protein L16

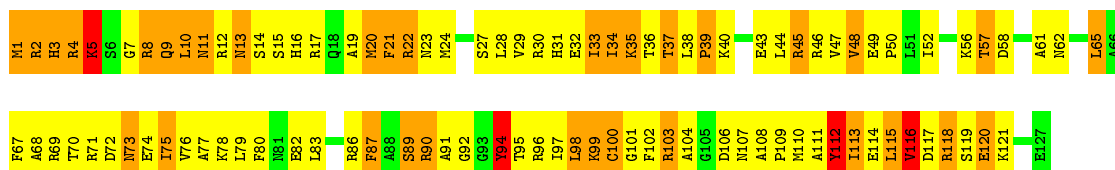
Chain M: 15% 50% 24% 12%





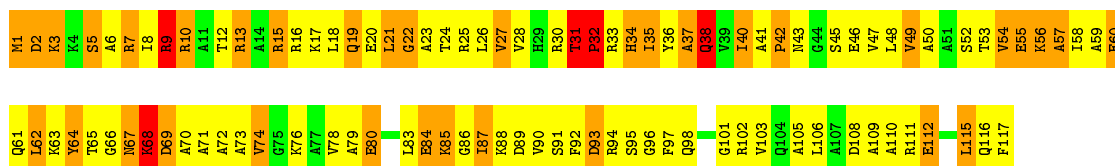
• Molecule 14: 50S ribosomal protein L17

Chain N: 21% 49% 27%



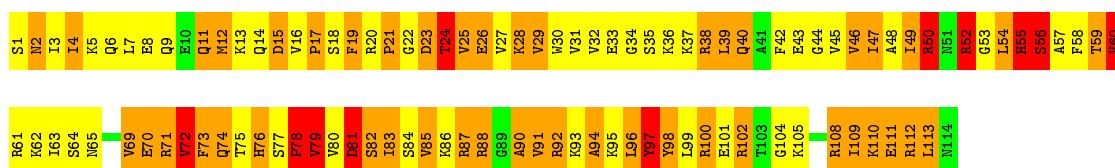
• Molecule 15: 50S ribosomal protein L18

Chain O: 15% 51% 30%



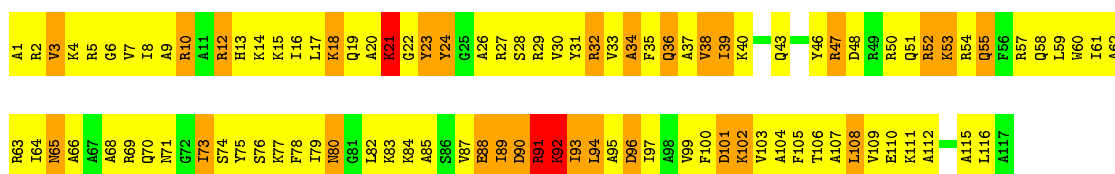
• Molecule 16: 50S ribosomal protein L19

Chain P: 10% 40% 40% 10%



• Molecule 17: 50S ribosomal protein L20

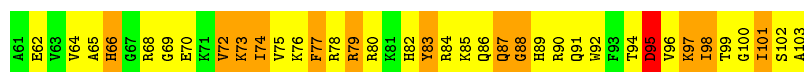
Chain Q: 14% 61% 23%



• Molecule 18: 50S ribosomal protein L21

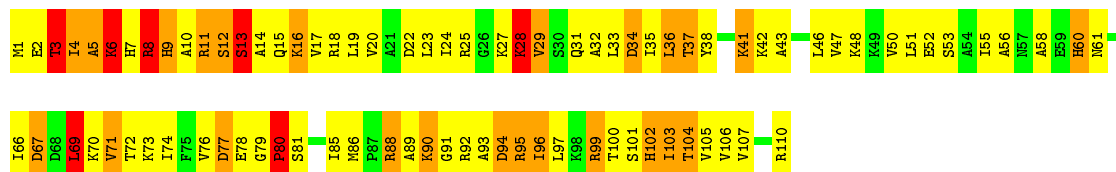
Chain R: 13% 52% 31%





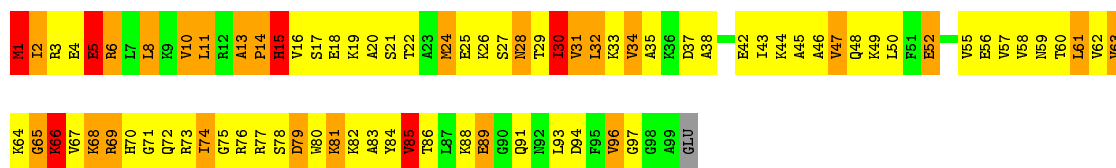
• Molecule 19: 50S ribosomal protein L22

Chain S: 22% 50% 22% 6%



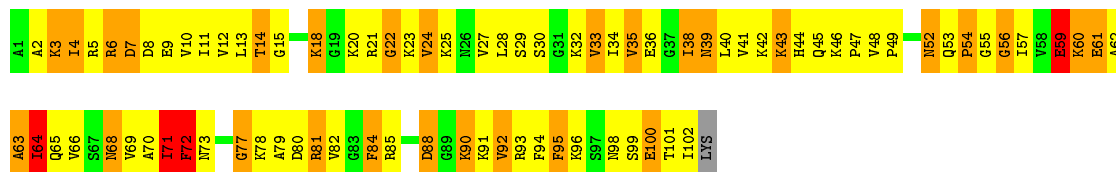
• Molecule 20: 50S ribosomal protein L23

Chain T: 17% 52% 24% 6%



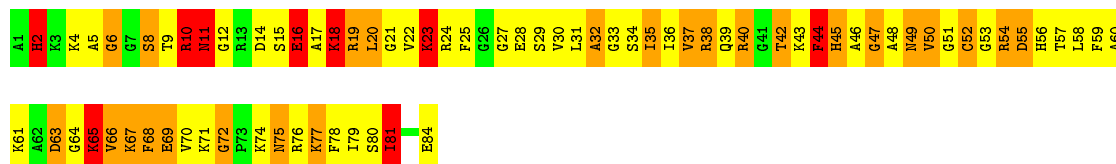
• Molecule 21: 50S ribosomal protein L24

Chain U: 18% 50% 27% 6%



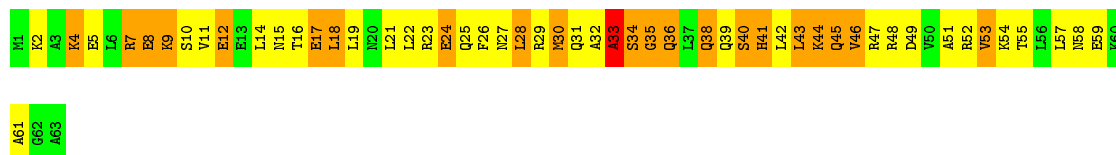
• Molecule 22: 50S ribosomal protein L27

Chain W: 12% 48% 30% 11%

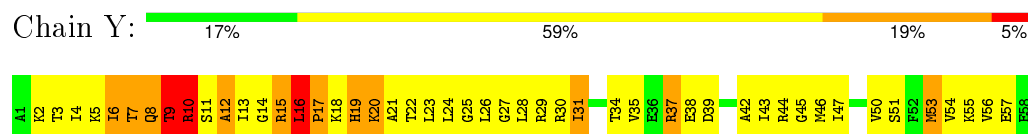


• Molecule 23: 50S ribosomal protein L29

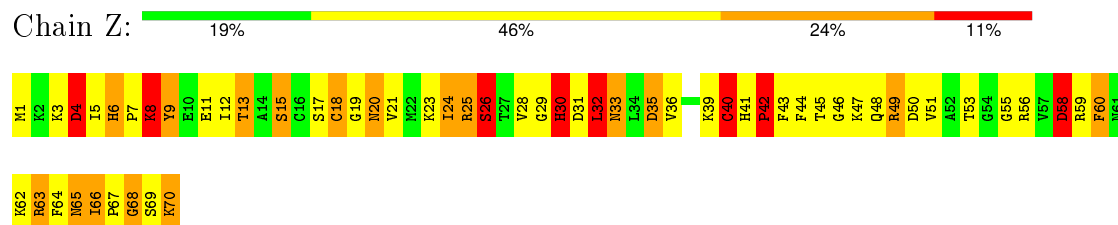
Chain X: 17% 48% 33% 6%



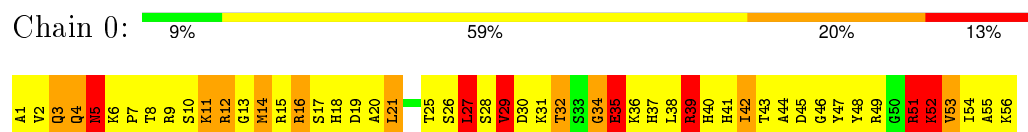
- Molecule 24: 50S ribosomal protein L30



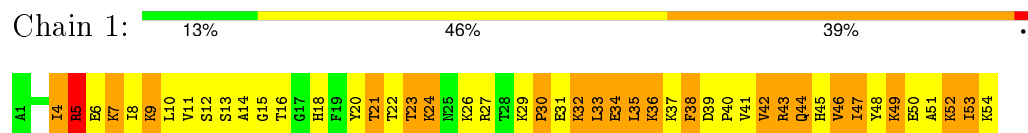
- Molecule 25: 50S ribosomal protein L31



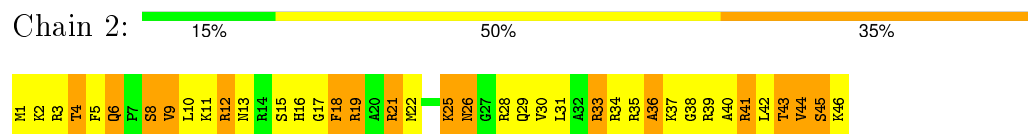
- Molecule 26: 50S ribosomal protein L32



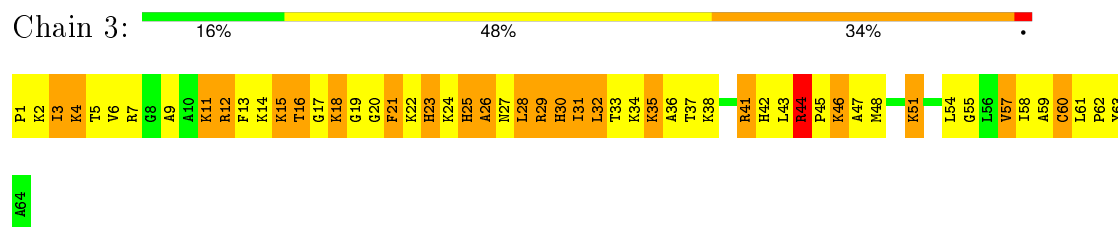
- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



M1	K2	V3	R4	A5	S6	V7	K8	K9	I10	C11	R12	M13	C14	K15	I16	V17	K18	R19	I20	G21	V22	I23	R24	V25	I26	C27	S28	A29	E30	P31	K32	H33	K34	Q35	R36	Q37	G38
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4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction of each particle	Depositor
Microscope	FEI Tecnai F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	3.5	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO-163 film	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.29	0/2801	0.75	0/4363
10	J	0.41	1/1135 (0.1%)	0.72	3/1529 (0.2%)
11	K	0.35	0/939	1.00	2/1258 (0.2%)
12	L	0.70	0/1062	1.60	30/1413 (2.1%)
13	M	0.48	0/1093	1.03	8/1460 (0.5%)
14	N	0.38	0/1021	0.92	7/1364 (0.5%)
15	O	0.30	0/910	0.67	0/1219
16	P	0.55	0/929	1.40	16/1242 (1.3%)
17	Q	0.41	0/960	0.86	2/1278 (0.2%)
18	R	1.06	6/829 (0.7%)	1.42	14/1107 (1.3%)
19	S	0.28	0/864	0.69	1/1156 (0.1%)
2	B	0.45	23/68281 (0.0%)	0.93	94/106437 (0.1%)
20	T	0.39	0/784	0.78	4/1048 (0.4%)
21	U	0.33	0/787	0.74	0/1051
22	W	0.37	0/642	0.96	5/848 (0.6%)
23	X	0.30	0/510	0.80	1/677 (0.1%)
24	Y	0.31	0/453	0.64	0/605
25	Z	0.48	0/559	1.04	5/745 (0.7%)
26	0	0.53	1/450 (0.2%)	1.15	7/599 (1.2%)
27	1	0.36	0/448	0.71	0/594
28	2	0.33	0/380	0.64	0/498
29	3	0.48	0/513	0.96	1/676 (0.1%)
3	V	0.31	0/766	0.53	0/1025
30	4	0.40	0/303	0.73	0/397
4	C	0.40	0/2092	0.88	7/2813 (0.2%)
5	D	0.40	0/1586	0.80	2/2134 (0.1%)
6	E	0.45	1/1571 (0.1%)	0.88	6/2113 (0.3%)
7	F	0.34	0/1444	0.87	5/1937 (0.3%)
8	G	0.31	0/1343	0.70	0/1816
9	H	1.99	0/1121	0.83	1/1512 (0.1%)
All	All	0.49	32/96576 (0.0%)	0.92	221/144914 (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
10	J	0	2
12	L	0	1
16	P	0	1
17	Q	0	1
18	R	0	1
2	B	0	61
4	C	0	3
All	All	0	70

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2789	C	O3'-P	44.85	2.15	1.61
2	B	2390	U	O3'-P	-27.39	1.28	1.61
2	B	2626	C	O3'-P	23.56	1.89	1.61
2	B	2582	G	O3'-P	21.37	1.86	1.61
2	B	1417	C	O3'-P	-19.51	1.37	1.61

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1250	G	P-O3'-C3'	-66.83	39.50	119.70
2	B	2582	G	P-O3'-C3'	-54.08	54.80	119.70
2	B	1250	G	O3'-P-O5'	-47.15	14.41	104.00
2	B	1417	C	O3'-P-O5'	-41.83	24.52	104.00
2	B	1580	A	O3'-P-O5'	-38.06	31.68	104.00

There are no chirality outliers.

5 of 70 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	136	G	Sidechain
2	B	139	U	Sidechain
2	B	142	A	Sidechain
2	B	143	C	Sidechain
2	B	51	G	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	A	2507	0	1261	547	0
2	B	61056	0	30280	9648	0
3	V	753	0	777	235	0
4	C	2053	0	2111	760	0
5	D	1565	0	1597	807	0
6	E	1552	0	1611	578	0
7	F	1420	0	1451	471	0
8	G	1323	0	1367	217	0
9	H	1111	0	1146	140	0
10	J	1112	0	1141	313	0
11	K	930	0	997	291	0
12	L	1053	0	1114	673	0
13	M	1074	0	1136	507	0
14	N	1008	0	1040	285	0
15	O	900	0	927	259	0
16	P	917	0	958	316	0
17	Q	947	0	1016	425	0
18	R	816	0	830	336	0
19	S	857	0	915	293	0
20	T	777	0	832	278	0
21	U	779	0	832	210	0
22	W	634	0	654	294	0
23	X	509	0	528	238	0
24	Y	449	0	487	170	0
25	Z	549	0	546	175	0
26	0	444	0	444	324	0
27	1	441	0	485	153	0
28	2	377	0	408	327	0
29	3	504	0	563	259	0
30	4	302	0	336	147	0
31	2	3	0	0	0	0
31	B	92	0	0	0	0
31	C	1	0	0	0	0
31	E	3	0	0	0	0
31	L	4	0	0	0	0
31	Q	2	0	0	0	0
31	S	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	T	2	0	0	0	0
31	U	1	0	0	0	0
32	2	11	0	0	8	0
32	B	443	0	0	273	0
32	C	1	0	0	1	0
32	D	1	0	0	0	0
32	E	18	0	0	5	0
32	L	8	0	0	7	0
32	Q	7	0	0	2	0
32	S	7	0	0	0	0
32	T	5	0	0	16	0
32	U	5	0	0	6	0
All	All	89335	0	57790	14330	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 98.

The worst 5 of 14330 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)
2:B:1417:C:C5	2:B:1418:G:C5	1.77	1.72
2:B:827:U:P	2:B:2446:G:H5'	1.30	1.69
2:B:5:A:C2	2:B:2899:A:C5	1.79	1.68
1:A:57:A:C4	7:F:12:VAL:HG13	1.19	1.68
2:B:2848:G:C8	16:P:96:LEU:HD23	1.24	1.67

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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V	92/94 (98%)	62 (67%)	21 (23%)	9 (10%)	1	14
4	C	265/273 (97%)	103 (39%)	82 (31%)	80 (30%)	0	0
5	D	207/209 (99%)	90 (44%)	69 (33%)	48 (23%)	0	2
6	E	199/201 (99%)	99 (50%)	60 (30%)	40 (20%)	0	3
7	F	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	3
8	G	174/176 (99%)	118 (68%)	39 (22%)	17 (10%)	1	14
9	H	145/149 (97%)	86 (59%)	43 (30%)	16 (11%)	0	11
10	J	138/142 (97%)	69 (50%)	40 (29%)	29 (21%)	0	3
11	K	119/123 (97%)	71 (60%)	32 (27%)	16 (13%)	0	7
12	L	142/144 (99%)	60 (42%)	40 (28%)	42 (30%)	0	0
13	M	134/136 (98%)	69 (52%)	37 (28%)	28 (21%)	0	3
14	N	125/127 (98%)	73 (58%)	35 (28%)	17 (14%)	0	7
15	O	115/117 (98%)	64 (56%)	26 (23%)	25 (22%)	0	2
16	P	112/114 (98%)	39 (35%)	36 (32%)	37 (33%)	0	0
17	Q	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	1	12
18	R	101/103 (98%)	44 (44%)	31 (31%)	26 (26%)	0	1
19	S	108/110 (98%)	63 (58%)	27 (25%)	18 (17%)	0	5
20	T	97/100 (97%)	42 (43%)	40 (41%)	15 (16%)	0	5
21	U	100/103 (97%)	33 (33%)	46 (46%)	21 (21%)	0	3
22	W	82/84 (98%)	29 (35%)	26 (32%)	27 (33%)	0	0
23	X	61/63 (97%)	28 (46%)	21 (34%)	12 (20%)	0	3
24	Y	56/58 (97%)	29 (52%)	17 (30%)	10 (18%)	0	4
25	Z	68/70 (97%)	29 (43%)	26 (38%)	13 (19%)	0	3
26	0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	5
27	1	52/54 (96%)	19 (36%)	23 (44%)	10 (19%)	0	3
28	2	44/46 (96%)	23 (52%)	14 (32%)	7 (16%)	0	5
29	3	62/64 (97%)	30 (48%)	25 (40%)	7 (11%)	0	10
30	4	36/38 (95%)	18 (50%)	9 (25%)	9 (25%)	0	2
All	All	3179/3249 (98%)	1596 (50%)	950 (30%)	633 (20%)	0	3

5 of 633 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	21	PRO
4	C	22	GLU
4	C	28	PRO
4	C	29	PHE
4	C	31	PRO

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 PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	V	78/78 (100%)	66 (85%)	12 (15%)	3	22
4	C	213/218 (98%)	144 (68%)	69 (32%)	0	2
5	D	164/164 (100%)	112 (68%)	52 (32%)	0	2
6	E	165/165 (100%)	115 (70%)	50 (30%)	0	3
7	F	149/149 (100%)	118 (79%)	31 (21%)	1	10
8	G	137/137 (100%)	105 (77%)	32 (23%)	1	7
9	H	114/114 (100%)	83 (73%)	31 (27%)	0	4
10	J	114/116 (98%)	84 (74%)	30 (26%)	0	5
11	K	102/104 (98%)	78 (76%)	24 (24%)	1	7
12	L	103/103 (100%)	61 (59%)	42 (41%)	0	0
13	M	109/109 (100%)	77 (71%)	32 (29%)	0	3
14	N	103/103 (100%)	78 (76%)	25 (24%)	1	6
15	O	87/87 (100%)	58 (67%)	29 (33%)	0	2
16	P	99/99 (100%)	77 (78%)	22 (22%)	1	9
17	Q	89/89 (100%)	66 (74%)	23 (26%)	0	5
18	R	84/84 (100%)	68 (81%)	16 (19%)	2	13
19	S	93/93 (100%)	72 (77%)	21 (23%)	1	8
20	T	83/84 (99%)	60 (72%)	23 (28%)	0	4
21	U	83/84 (99%)	62 (75%)	21 (25%)	1	6
22	W	62/62 (100%)	46 (74%)	16 (26%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	X	55/55 (100%)	40 (73%)	15 (27%)	0	4
24	Y	48/48 (100%)	36 (75%)	12 (25%)	1	6
25	Z	62/62 (100%)	44 (71%)	18 (29%)	0	3
26	0	47/47 (100%)	31 (66%)	16 (34%)	0	2
27	1	48/48 (100%)	33 (69%)	15 (31%)	0	2
28	2	38/38 (100%)	27 (71%)	11 (29%)	0	3
29	3	51/51 (100%)	33 (65%)	18 (35%)	0	1
30	4	34/34 (100%)	21 (62%)	13 (38%)	0	1
All	All	2614/2625 (100%)	1895 (72%)	719 (28%)	2	4

5 of 719 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	98	ARG
13	M	132	THR
27	1	6	GLU
12	L	18	ARG
12	L	115	GLU

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

Mol	Chain	Res	Type
10	J	135	GLN
14	N	9	GLN
25	Z	65	ASN
10	J	136	GLN
11	K	88	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	114/120 (95%)	22 (19%)	0
2	B	2805/2904 (96%)	445 (15%)	20 (0%)
All	All	2919/3024 (96%)	467 (15%)	20 (0%)

5 of 467 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	C
1	A	12	C
1	A	13	G
1	A	14	U
1	A	15	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1250	G
2	B	1301	A
2	B	2336	A
2	B	1210	G
2	B	1236	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 110 ligands modelled in this entry, 110 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.