



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:07 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : trunk26865

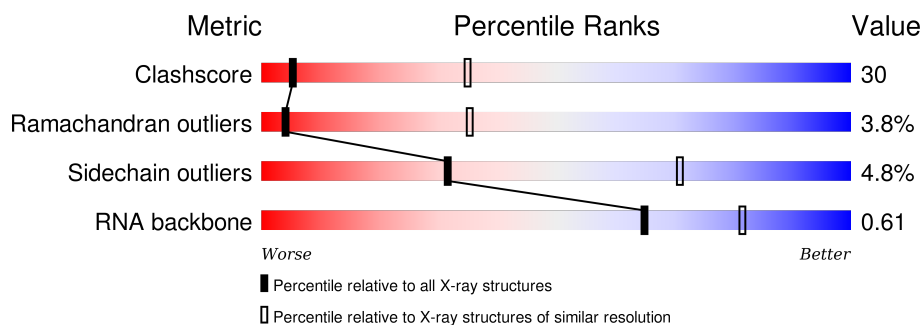
# 1 Overall quality at a glance

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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)



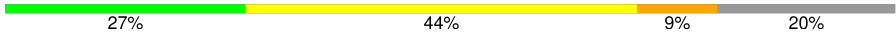

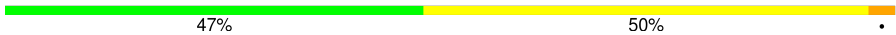

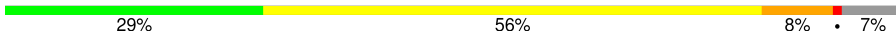
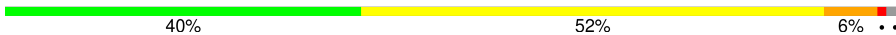

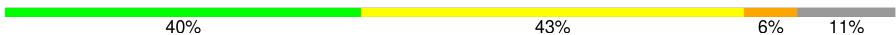
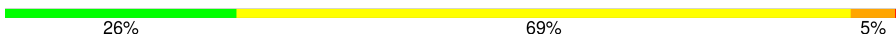
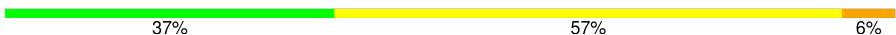













The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	I	1147	-	-	X	-
35	CL	L	1196	-	-	X	-
35	CL	P	1097	-	-	X	-
35	CL	X	1237	-	-	X	-

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 98859 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

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

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

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

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

- Molecule 4 is a protein called TRIGGER FACTOR.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L24.

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

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

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

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



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

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

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

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

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

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

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

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

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

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L37E.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	62	Total	Mg	0	0
			62	62		
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	1	Total 1	Mg 1	0	0
32	9	1	Total 1	Mg 1	0	0
32	3	49	Total 49	Mg 49	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	56	Total 56	Na 56	0	0
34	P	1	Total 1	Na 1	0	0
34	Q	2	Total 2	Na 2	0	0
34	H	2	Total 2	Na 2	0	0
34	B	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	S	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	1	Total 1	Na 1	0	0
34	L	1	Total 1	Na 1	0	0
34	3	17	Total 17	Na 17	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	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	I	3	Total 3	Cl 3	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	3	2	Total 2	Cl 2	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	5944	Total 5944	O 5944	0	0
37	1	49	Total 49	O 49	0	0
37	2	66	Total 66	O 66	0	0
37	9	153	Total 153	O 153	0	0
37	A	132	Total 132	O 132	0	0
37	B	145	Total 145	O 145	0	0
37	C	160	Total 160	O 160	0	0
37	D	52	Total 52	O 52	0	0
37	E	41	Total 41	O 41	0	0
37	F	29	Total 29	O 29	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	91	Total 91	O 91	0	0
37	L	148	Total 148	O 148	0	0
37	M	59	Total 59	O 59	0	0
37	N	35	Total 35	O 35	0	0
37	O	64	Total 64	O 64	0	0
37	P	52	Total 52	O 52	0	0
37	Q	80	Total 80	O 80	0	0
37	R	29	Total 29	O 29	0	0

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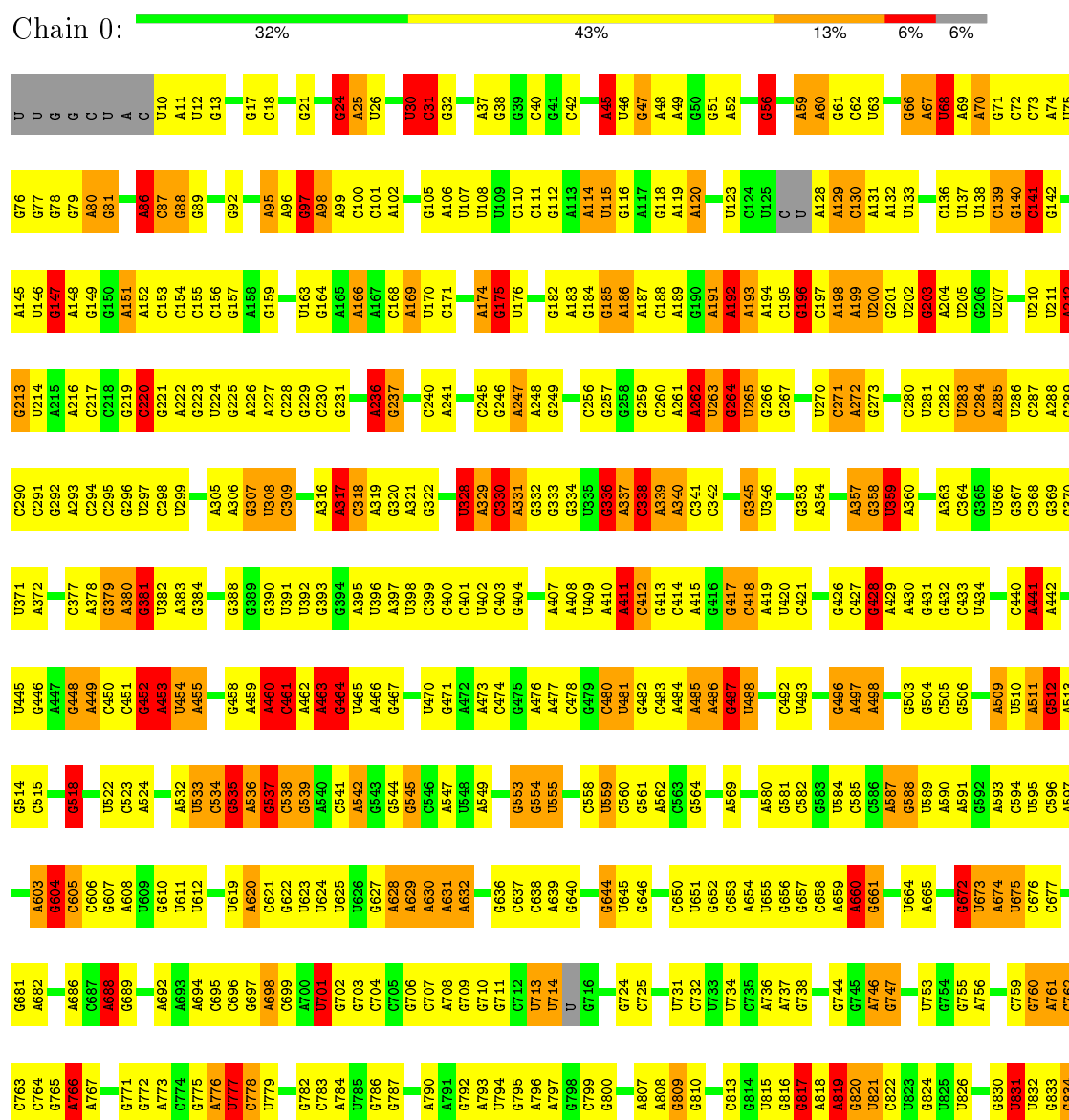
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	S	31	Total 31	O 31	0	0
37	T	25	Total 25	O 25	0	0
37	U	11	Total 11	O 11	0	0
37	V	69	Total 69	O 69	0	0
37	W	26	Total 26	O 26	0	0
37	X	101	Total 101	O 101	0	0
37	Y	35	Total 35	O 35	0	0
37	Z	47	Total 47	O 47	0	0

### 3 Residue-property plots

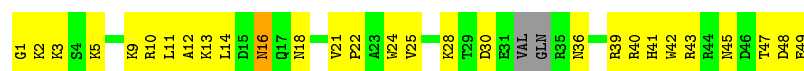
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: 23S rRNA

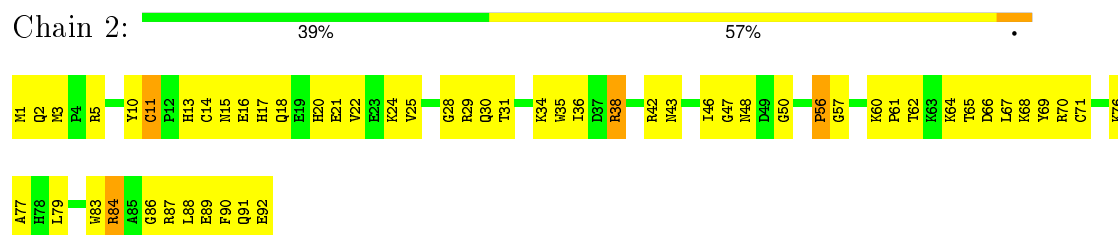


A1910	A1845	U1770	U1696	A1630	A1559	A1471	C1332	C1262	C1186	A1114	G1038	G	U903	U835
A1919	A1846	U1771	G1697	A1630	U	C1472	U1333	G1265	U1187	U1115	G1039	C	U904	G836
C1920	A1847	C1772	C1700	C1633	A1561	U1473	C1334	U1266	A1188	U1116	U1041	C	C905	U837
A1921	A1848	G1773	A1701	G1634	C1562	C1474	C1335	C1267	A1189	A1117	U1042	U	C906	U840
A1922	G1849	A1775	U1702	U1635	G1563	A1476	U1336	C1268	A1190	C1118	C1043	C	A907	A841
G1923	U1850	A1776	G1703	G1636	C1564	C1477	U1338	G1269	A1191	G1119	G1044	G	A908	A842
A1924	G1851	G1777	C1708	A1637	C1565	U1478	G1339	U1270	A1192	U1120	C1045	A	U909	C842
G1925	A1852	A1778	C1566	U1641	C1566	U1479	U1340	A1271	A1193	G1122	G1046	G	C910	A843
G1929	C1853	A1779	A1567	A1642	A1567	A1482	G1341	A1272	A1194	U1121	U1047	A	G911	A844
A1930	G1854	A1780	A1568	A1643	C1568	C1483	C1342	C1273	G1195	A1123	C1051	A	U919	U845
A1931	C1855	A1711	C1643	U1646	G1484	A1413	C1343	C1274	G1196	A1124	G1052	A	C920	A846
G1932	A1857	G1712	U1647	G1648	G1485	A1414	C1344	U1275	G1197	U1125	G1053	A	C921	C847
C1936	A1858	G1713	G1646	G1647	A1486	A1415	U1346	A1278	G1197	C1128	G1054	G	A922	C848
U1937	C1859	A1717	G1648	G1649	A1487	A1416	U1347	U1279	C1201	C1127	U1065	G	A923	C849
G1938	U1860	G1718	A1653	G1654	U1488	A1417	A1348	G1283	A1202	U1128	G1056	U	C924	U850
U1939	G1861	U1788	G1723	G1655	G1489	A1418	U1349	G1284	U1205	C1129	U1057	C	G925	C853
C1940	C1862	C1790	G1724	G1656	G1490	U1419	G1351	U1287	U1206	U1130	G1058	G	A926	U855
A1941	G1863	U1791	C1721	C1657	G1491	U1422	A1352	U1288	A1207	A1132	G1059	C	C931	U856
C1943	A1866	G1795	U1722	C1658	A1492	A1423	C1353	U1289	C1208	A1133	C1060	A	U932	G856
C1946	G1867	A1796	G1723	G1659	C1493	A1424	G1354	C1290	G1210	U1134	C1061	C	U933	U858
G1950	G1868	U1797	G1724	G1660	C1494	G1425	A1355	G1291	G1211	U1135	U1066	A	C934	C859
G1951	A1869	G1725	G1725	A1656	G1495	C1426	A1356	G1292	C1212	G1137	C1067	C999	G935	U860
U	C1870	G1726	A1657	A1658	G1496	A1427	A1357	U1293	C1213	G1138	C1068	U1001	U	A861
A	U1871	G1727	A1659	A1660	G1497	U1430	U1358	U1294	G1214	C1148	C1069	C1002	C938	A867
U	C1872	G1730	A1661	A1662	U1500	C1431	U1359	G1295	A1215	U1149	G1070	U1003	A939	C868
A	G1873	C1731	C1663	C1664	A1501	U1432	C1360	U1296	A1216	U1149	A1071	C1004	G940	U868
A	U1874	G1805	G1665	G1666	A1502	A1433	C1361	U1297	G1217	A1150	G1072	U1005	G941	C869
A	A1875	G1735	G1665	G1666	U1503	U1434	C1362	U1298	C1218	G1151	A1073	A1006	U942	C870
C	C1876	A1736	G1667	G1668	U1504	U1435	U1366	G1299	U1231	A1152	G1076	A1007	A943	C871
U	U1877	A1737	A1667	A1668	U1505	U1436	U1367	G1300	A1232	C1153	G1077	U1008	G944	U872
U	G1878	U1741	U1668	U1669	C1507	U1437	A1369	G1302	U1233	C1154	C1080	U1009	U945	A875
G	C1880	A1742	U1669	U1670	U1508	U1438	U1370	C1303	U1234	G1155	A1081	U947	C946	A876
A	A1881	G1745	G1672	G1673	G1600	U1439	A1372	C1305	U1235	C1157	A1082	U948	G948	C877
C	C1882	A1746	C1674	C1675	G1601	U1440	A1373	U1306	G1236	G1158	A1083	U1013	A1014	C878
C	U1883	A1747	C1676	C1677	C1602	G1441	C1374	U1307	U1237	G1159	C1084	C1015	C1016	C881
U1964	A1884	U1748	G1676	G1677	A1603	U1442	A1375	U1308	C1238	G1160	C1085	U1017	U1018	A882
U1967	A1885	U1749	G1677	G1678	G1604	U1443	C1376	U1309	G1239	A1161	C1086	U1019	A1018	U883
U1968	U1886	C1820	C1756	C1679	G1605	U1444	G1377	U1310	G1240	G1162	G1087	C1019	G956	C884
A1969	U1890	G1827	G1751	C1680	A1606	U1445	A1378	G1312	A1242	U1163	A1088	A1020	A957	C885
C1893	C1893	G1828	C1753	A1681	C1609	U1446	U1380	G1313	C1243	A1165	G1089	G1021	G958	C886
C1894	A1894	A1829	A1754	A1682	G1610	U1447	A1381	U1314	U1244	A1166	U1096	A1022	C959	C887
A1895	C1895	C1830	A1755	G1683	U1615	U1448	G1382	G1315	C1245	G1167	C1097	C1023	G960	U888
G1898	C1898	U1831	G1756	A1684	A1616	U1449	U1386	G1316	A1246	C1168	A1098	G1024	A961	C889
C1899	U1900	G1832	U1757	A1685	C1617	A1458	U1388	A1317	A1247	U1169	C1099	C1025	C962	C890
A1900	G1901	U1833	U1758	C1686	U1618	A1459	U1389	G1318	A1248	U1172	G1100	G1026	C963	C891
G1902	C1902	C1834	G1760	C1687	G1619	U1460	C1392	G1319	C1250	A1173	C1104	U1028	G	C892
U1903	G1903	A1835	U1761	G1688	C1620	U1461	A1393	G1320	C1251	A1174	C1105	U1029	U	C893
A1904	U1904	G1837	C1762	C1690	A1621	C1462	A1394	U1321	A1252	G1175	A1106	U1030	G969	A894
U1905	C1905	C1763	G1763	C1691	C1622	A1463	C1394	G1325	C1253	U1180	A1107	G1031	U970	A895
C1982	U1906	U1766	U1766	C1692	A1624	C1467	C1397	G1326	C1254	U1181	U1108	C1032	G	C896
C1983	C1983	A1840	U1625	A1693	U1625	G1468	G1398	A1328	G1257	C1182	U1109	G1034	U	C898
U1984	U1984	C1841	A1626	G1694	C1626	C1469	A1399	A1330	G1260	C1183	G1110	C1035	U	C899
A1909	A1909	A1842	G1627	G1695	C1553	U1544	C1400	A1331	A1261	U1185	U1111	G1036	C	G901

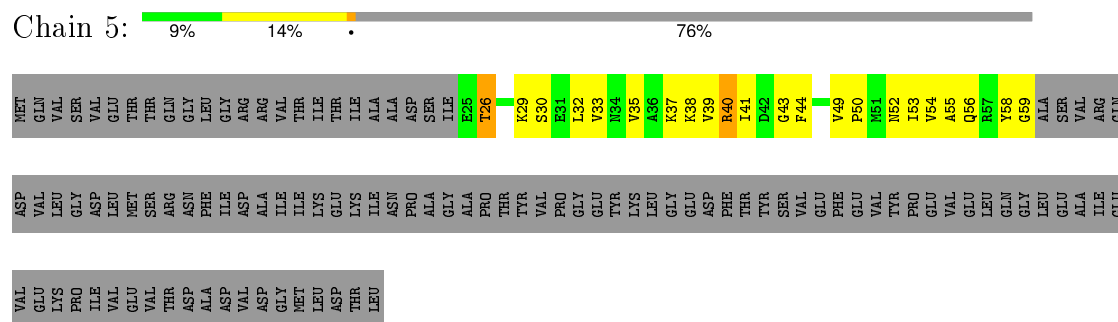




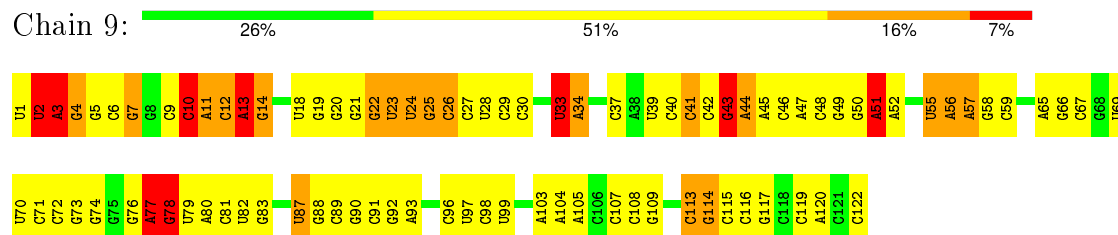
• Molecule 3: 50S RIBOSOMAL PROTEIN L44E LA, HLA, RIBOSOMAL PROTEIN L44E



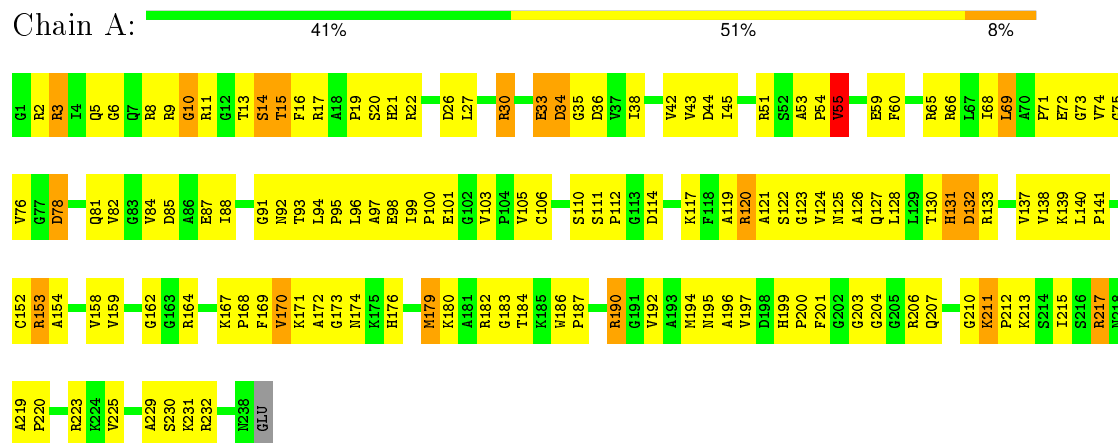
• Molecule 4: TRIGGER FACTOR



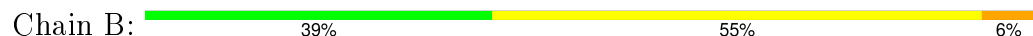
• Molecule 5: 5S RRNA

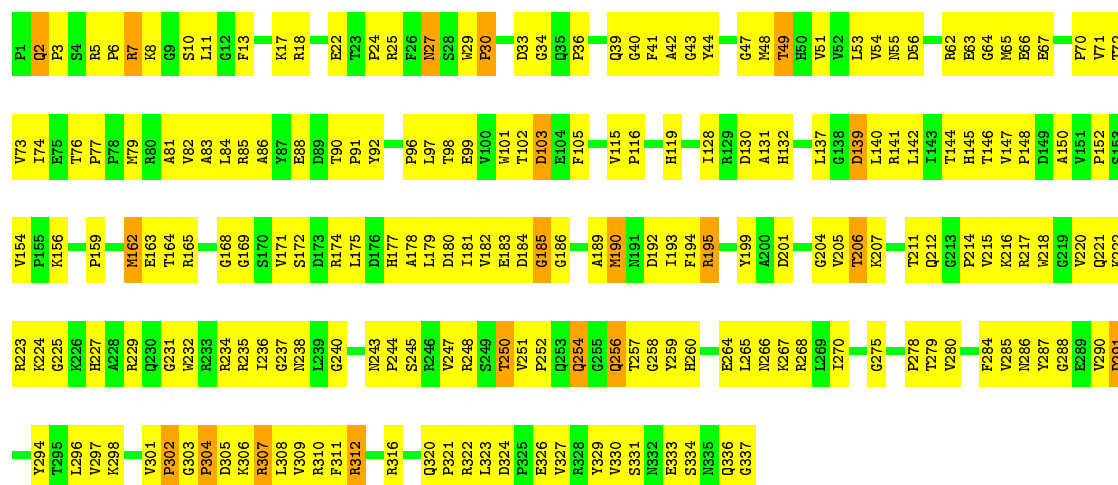


• Molecule 6: 50S RIBOSOMAL PROTEIN L2P

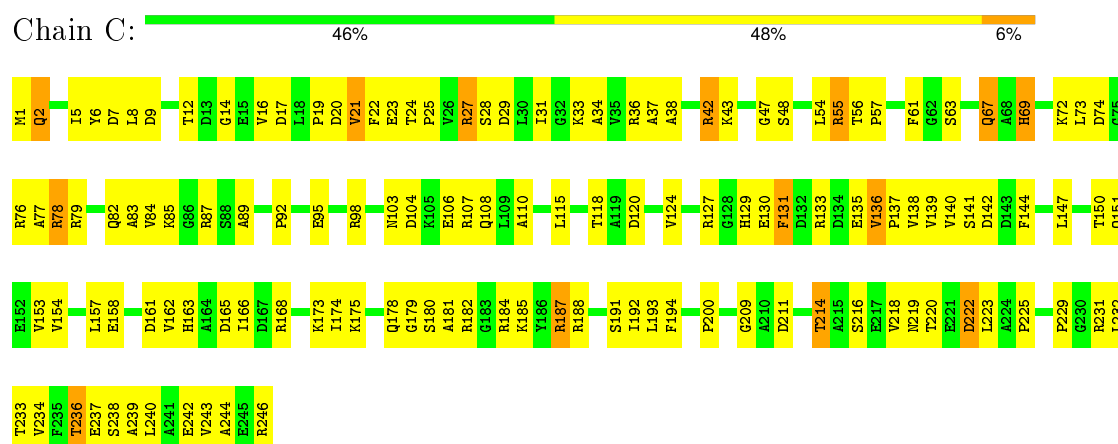


• Molecule 7: 50S RIBOSOMAL PROTEIN L3P

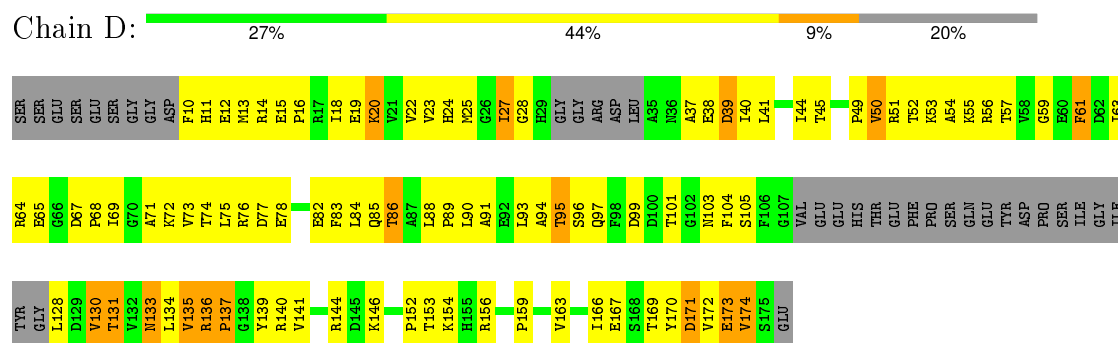




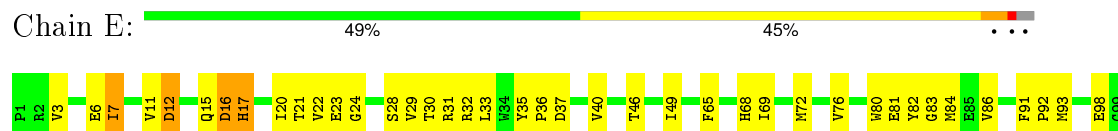
• Molecule 8: 50S RIBOSOMAL PROTEIN L4P



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



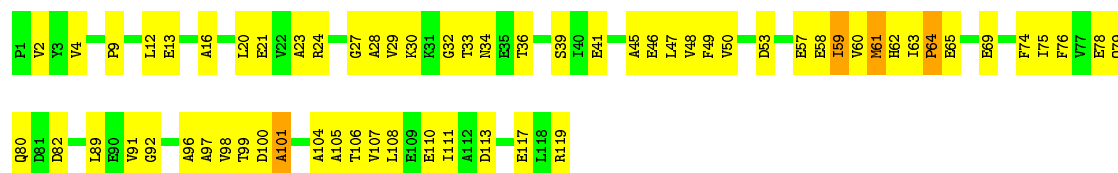
• Molecule 10: 50S RIBOSOMAL PROTEIN L6P





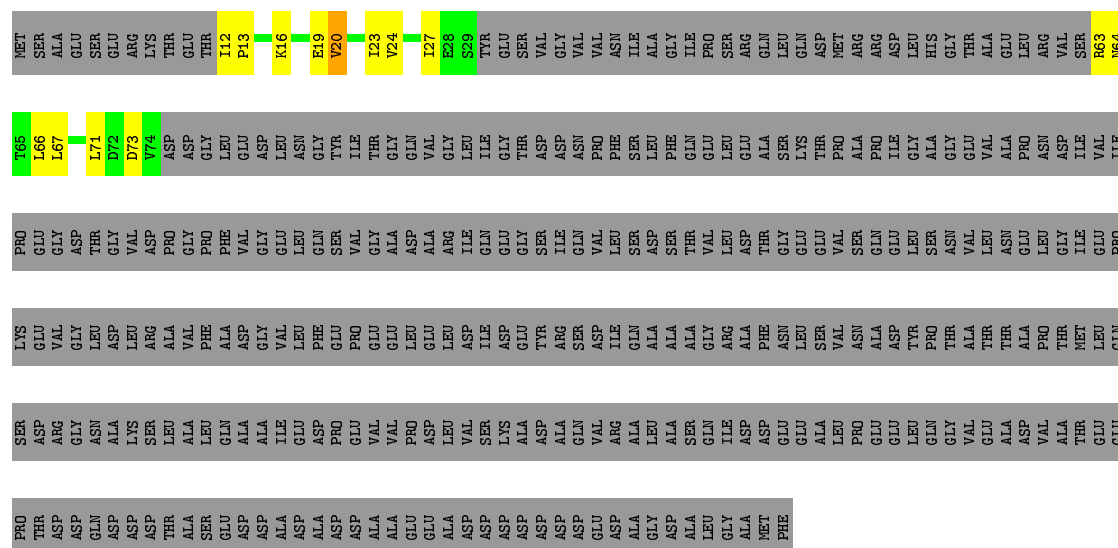
- Molecule 11: 50S RIBOSOMAL PROTEIN L7AE

Chain F: 47% 50%



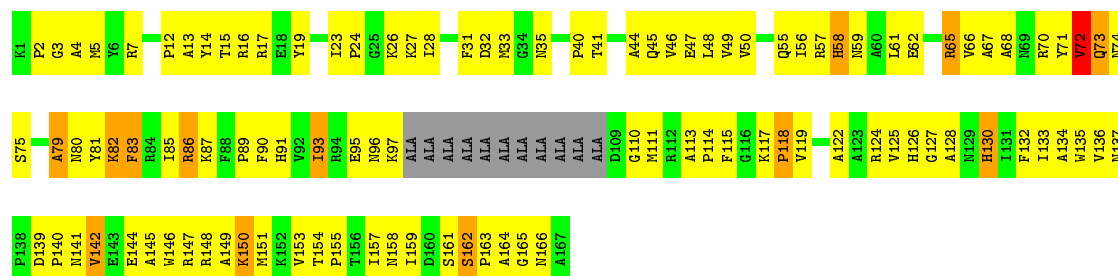
- Molecule 12: 50S RIBOSOMAL PROTEIN L10E

Chain G: 5% 91%

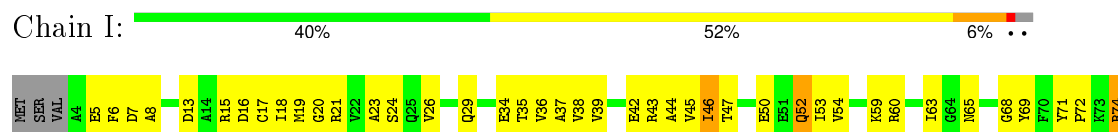


- Molecule 13: 50S RIBOSOMAL PROTEIN L10E

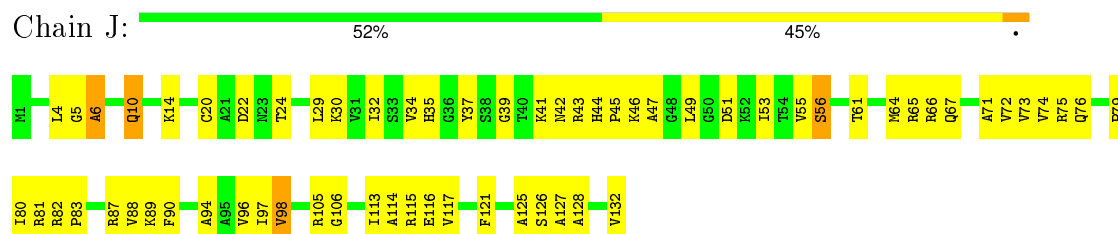
Chain H: 29% 56% 8% 7%



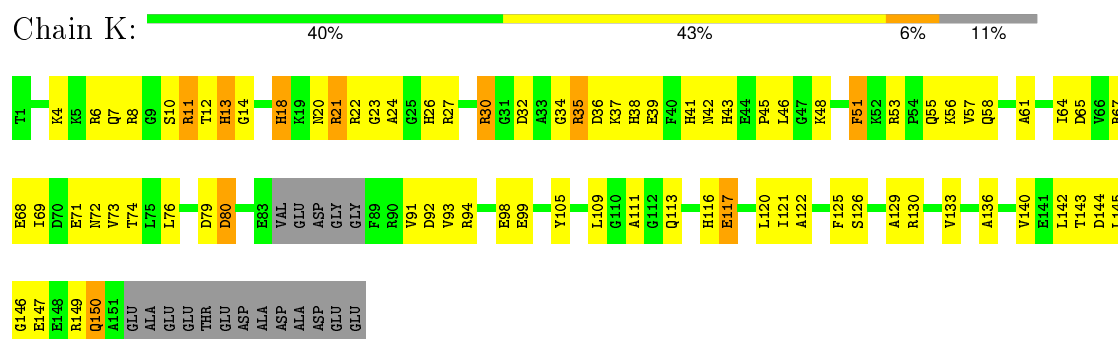
- Molecule 14: 50S RIBOSOMAL PROTEIN L13P



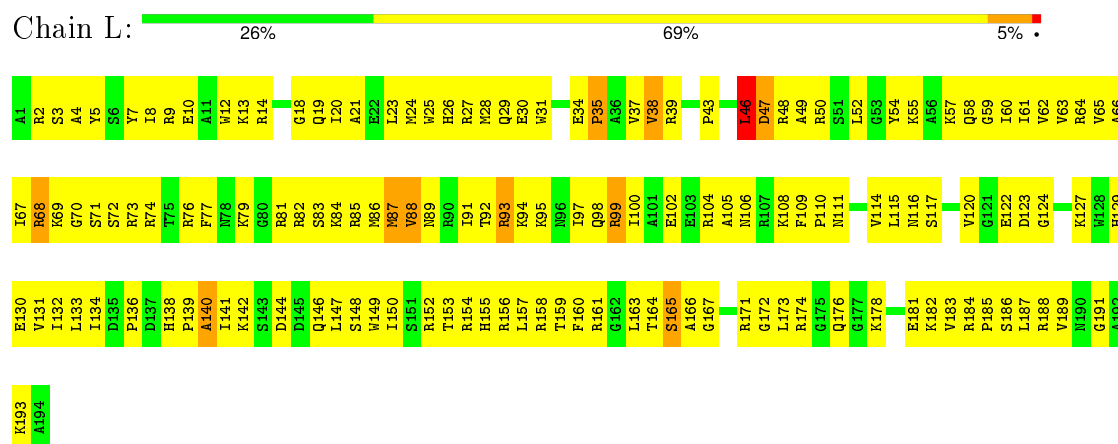
• Molecule 15: 50S RIBOSOMAL PROTEIN L14P



• Molecule 16: 50S RIBOSOMAL PROTEIN L15P

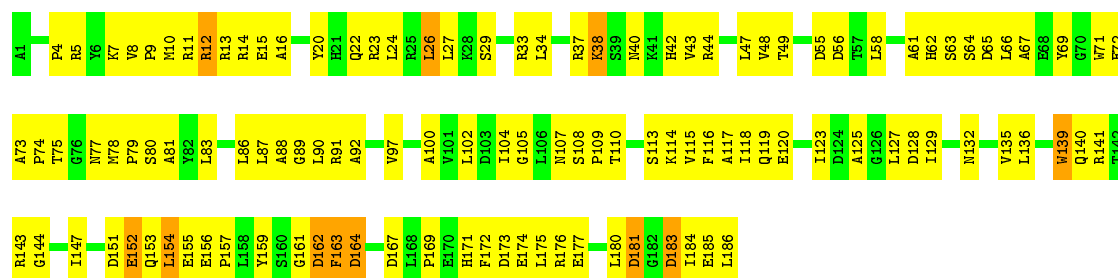


• Molecule 17: 50S RIBOSOMAL PROTEIN L15E



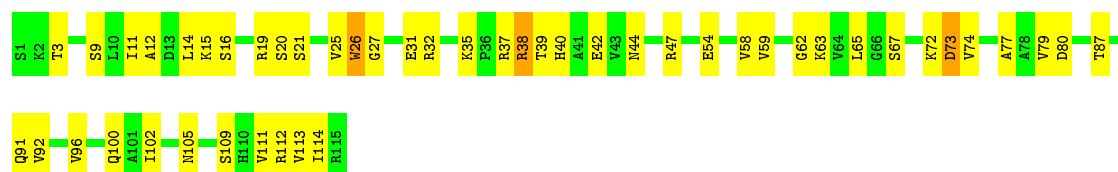
• Molecule 18: 50S RIBOSOMAL PROTEIN L18P





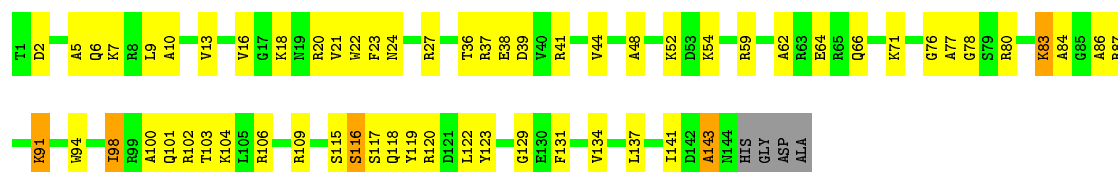
• Molecule 19: 50S RIBOSOMAL PROTEIN L18E

Chain N: 58% 39%



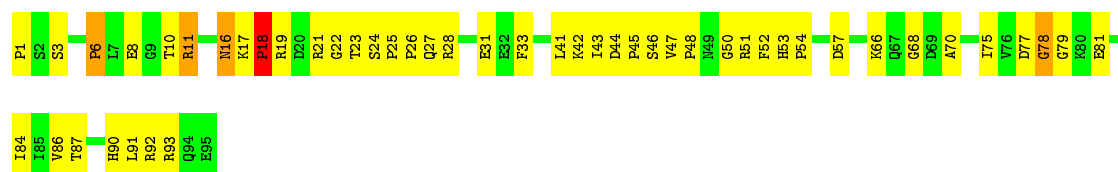
• Molecule 20: 50S RIBOSOMAL PROTEIN L19E

Chain O: 56% 38%



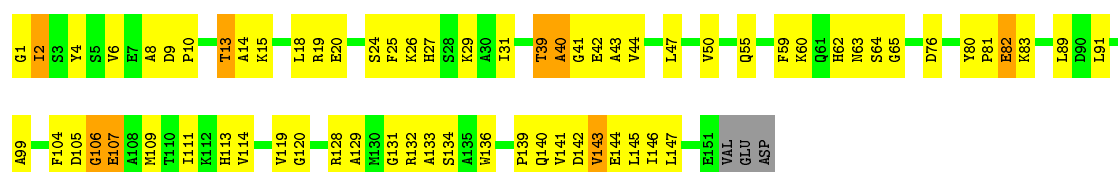
• Molecule 21: 50S RIBOSOMAL PROTEIN L21E

Chain P: 48% 46%

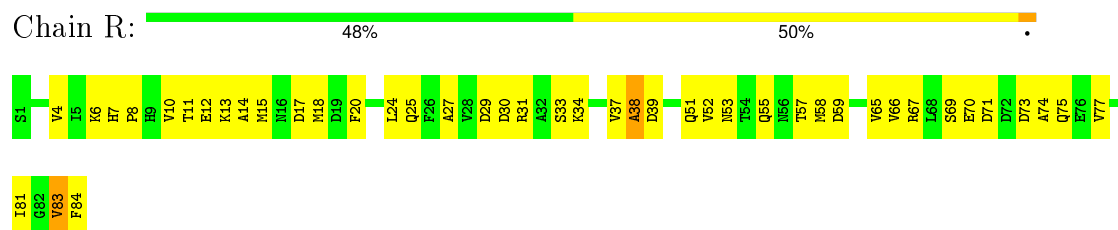


• Molecule 22: 50S RIBOSOMAL PROTEIN L22P HMAL22, HL23, RIBOSOMAL PROTEIN L22

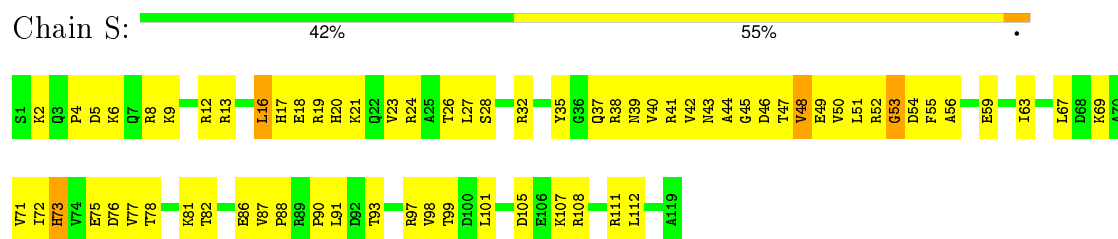
Chain Q: 54% 39% 5%



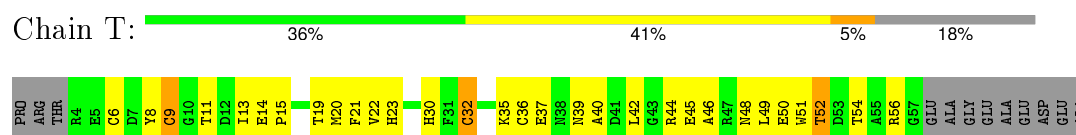
• Molecule 23: 50S RIBOSOMAL PROTEIN L23P



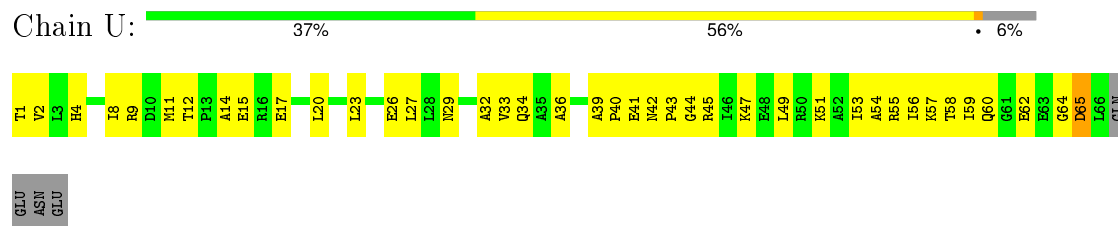
- Molecule 24: RIBOSOMAL PROTEIN L24



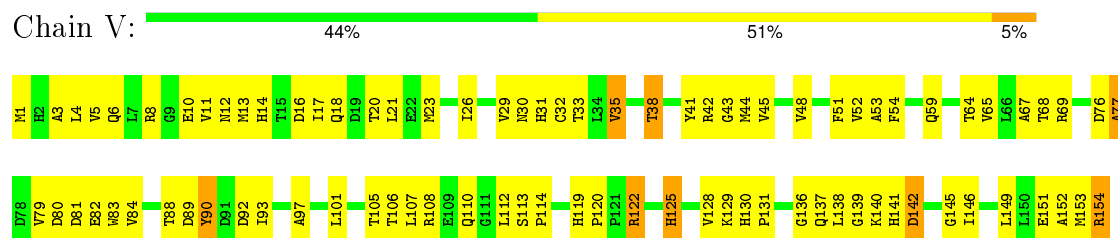
- Molecule 25: 50S RIBOSOMAL PROTEIN L24P



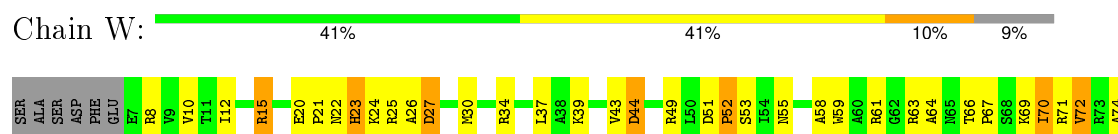
- Molecule 26: 50S RIBOSOMAL PROTEIN L24E

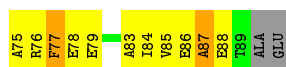


- Molecule 27: 50S RIBOSOMAL PROTEIN L30P



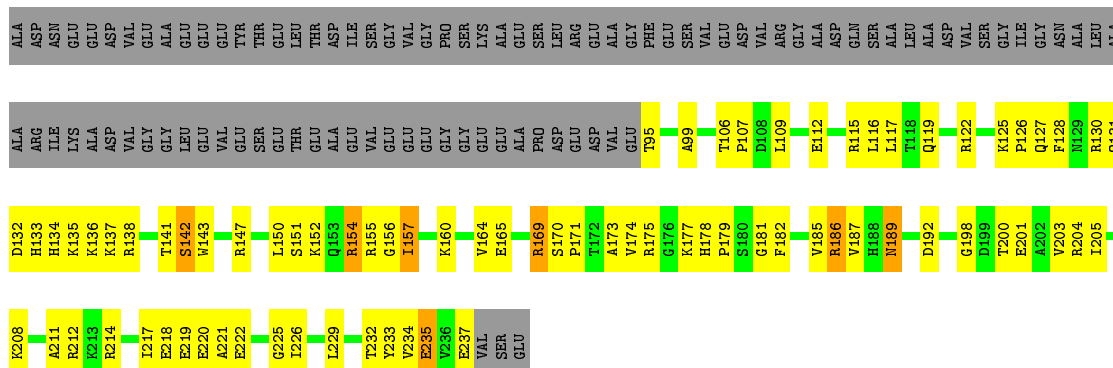
- Molecule 28: 50S RIBOSOMAL PROTEIN L31E





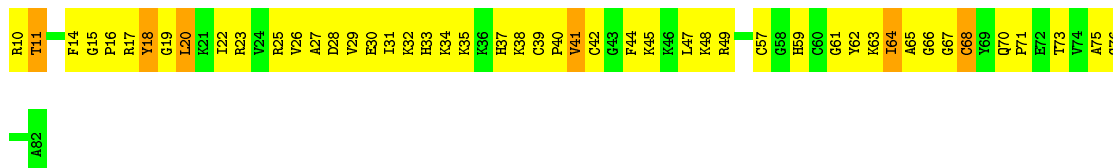
• Molecule 29: 50S RIBOSOMAL PROTEIN L32E

Chain X: 27% 30% 40%



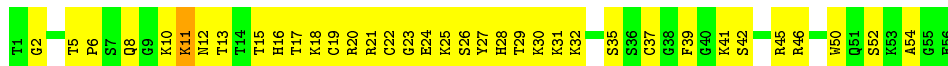
• Molecule 30: 50S RIBOSOMAL PROTEIN L37AE

Chain Y: 34% 58% 8%



• Molecule 31: RIBOSOMAL PROTEIN L37E

Chain Z: 36% 63% 1%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	62	0	0	0	0
32	3	49	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	3	0	0	0	0
32	J	1	0	0	0	0
33	0	2	0	0	0	0
34	0	56	0	0	0	0
34	3	17	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	H	2	0	0	0	0
34	I	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	3	2	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	1	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	5944	0	0	351	0
37	1	49	0	0	8	0
37	2	66	0	0	8	0
37	9	153	0	0	16	0
37	A	132	0	0	28	0
37	B	145	0	0	30	0
37	C	160	0	0	42	0
37	D	52	0	0	15	0
37	E	41	0	0	8	0
37	F	29	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	91	0	0	23	0
37	L	148	0	0	33	0
37	M	59	0	0	17	0
37	N	35	0	0	5	0
37	O	64	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	P	52	0	0	6	0
37	Q	80	0	0	6	0
37	R	29	0	0	6	0
37	S	31	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	101	0	0	13	0
37	Y	35	0	0	10	0
37	Z	47	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	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	90/92 (98%)	82 (91%)	5 (6%)	3 (3%)	5	39
4	5	33/144 (23%)	24 (73%)	9 (27%)	0	100	100
6	A	236/239 (99%)	197 (84%)	27 (11%)	12 (5%)	2	26
7	B	335/337 (99%)	281 (84%)	40 (12%)	14 (4%)	3	32
8	C	244/246 (99%)	201 (82%)	37 (15%)	6 (2%)	7	46
9	D	135/176 (77%)	90 (67%)	31 (23%)	14 (10%)	1	8
10	E	171/177 (97%)	147 (86%)	21 (12%)	3 (2%)	11	53
11	F	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	5	39
12	G	26/348 (8%)	23 (88%)	2 (8%)	1 (4%)	4	35
13	H	152/167 (91%)	123 (81%)	21 (14%)	8 (5%)	2	25
14	I	140/145 (97%)	117 (84%)	17 (12%)	6 (4%)	3	31
15	J	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	13	56
16	K	142/164 (87%)	116 (82%)	20 (14%)	6 (4%)	3	32
17	L	192/194 (99%)	144 (75%)	40 (21%)	8 (4%)	3	32
18	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	4	35
19	N	113/115 (98%)	92 (81%)	17 (15%)	4 (4%)	4	38
20	O	142/148 (96%)	126 (89%)	12 (8%)	4 (3%)	6	43
21	P	93/95 (98%)	72 (77%)	16 (17%)	5 (5%)	2	25
22	Q	149/154 (97%)	127 (85%)	18 (12%)	4 (3%)	6	44
23	R	82/84 (98%)	68 (83%)	9 (11%)	5 (6%)	2	21
24	S	117/119 (98%)	101 (86%)	13 (11%)	3 (3%)	7	45
25	T	52/66 (79%)	49 (94%)	3 (6%)	0	100	100
26	U	64/70 (91%)	49 (77%)	13 (20%)	2 (3%)	5	41
27	V	152/154 (99%)	132 (87%)	19 (12%)	1 (1%)	26	72
28	W	81/91 (89%)	65 (80%)	11 (14%)	5 (6%)	2	21
29	X	141/240 (59%)	126 (89%)	12 (8%)	3 (2%)	9	50
30	Y	71/73 (97%)	59 (83%)	7 (10%)	5 (7%)	1	18
31	Z	54/56 (96%)	43 (80%)	7 (13%)	4 (7%)	1	16
All	All	3680/4379 (84%)	3056 (83%)	485 (13%)	139 (4%)	4	35

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%)	31	71
3	2	79/79 (100%)	75 (95%)	4 (5%)	29	69
4	5	29/122 (24%)	26 (90%)	3 (10%)	9	40
6	A	179/181 (99%)	167 (93%)	12 (7%)	20	61
7	B	282/282 (100%)	268 (95%)	14 (5%)	30	69
8	C	193/193 (100%)	181 (94%)	12 (6%)	23	63
9	D	117/147 (80%)	109 (93%)	8 (7%)	20	60
10	E	152/155 (98%)	147 (97%)	5 (3%)	45	79
11	F	92/92 (100%)	91 (99%)	1 (1%)	80	92
12	G	27/283 (10%)	27 (100%)	0	100	100
13	H	122/122 (100%)	111 (91%)	11 (9%)	12	46
14	I	118/121 (98%)	111 (94%)	7 (6%)	24	65
15	J	106/106 (100%)	102 (96%)	4 (4%)	40	76
16	K	112/126 (89%)	106 (95%)	6 (5%)	27	67
17	L	166/166 (100%)	160 (96%)	6 (4%)	42	77
18	M	149/149 (100%)	142 (95%)	7 (5%)	32	72
19	N	93/93 (100%)	90 (97%)	3 (3%)	46	80
20	O	113/116 (97%)	109 (96%)	4 (4%)	43	78
21	P	79/79 (100%)	74 (94%)	5 (6%)	22	63
22	Q	117/121 (97%)	113 (97%)	4 (3%)	44	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	R	73/73 (100%)	72 (99%)	1 (1%)	74	91
24	S	105/105 (100%)	101 (96%)	4 (4%)	40	76
25	T	44/52 (85%)	41 (93%)	3 (7%)	20	60
26	U	51/56 (91%)	51 (100%)	0	100	100
27	V	130/130 (100%)	124 (95%)	6 (5%)	33	72
28	W	66/73 (90%)	61 (92%)	5 (8%)	16	55
29	X	120/195 (62%)	115 (96%)	5 (4%)	36	74
30	Y	56/56 (100%)	51 (91%)	5 (9%)	12	47
31	Z	46/46 (100%)	46 (100%)	0	100	100
All	All	3058/3563 (86%)	2911 (95%)	147 (5%)	31	71

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.