



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:51 PM GMT

PDB ID : 4G5W  
Title : Crystal Structure of the 70S ribosome with tigecycline. This entry contains the 50S subunit of molecule B.  
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.  
Deposited on : 2012-07-18  
Resolution : 3.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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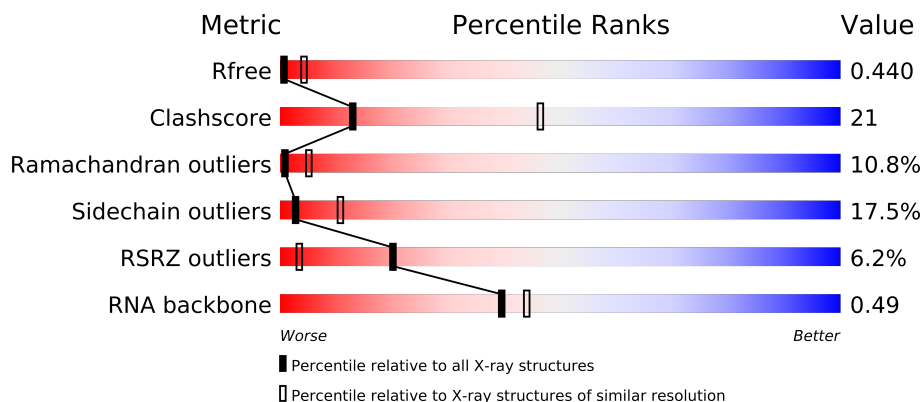
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.10 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.




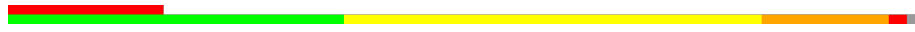

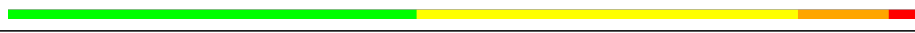
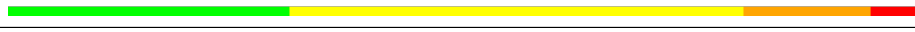



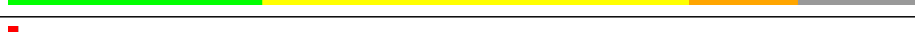

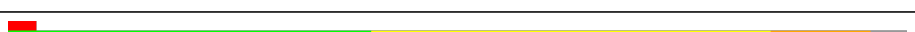
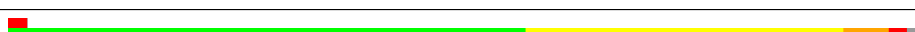




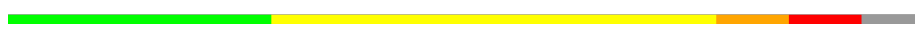

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2912	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	K	148	
9	M	140	
10	N	122	
11	O	150	
12	P	141	

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Mol	Chain	Length	Quality of chain
13	0	118	
14	Q	112	
15	R	146	
16	1	118	
17	2	101	
18	S	113	
19	T	96	
20	U	110	
21	V	206	
22	3	85	
23	Z	98	
24	W	72	
25	X	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 92006 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2906	Total	C	N	O	P	0	0	0
			62587	27857	11709	20116	2905			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	U	-	INSERTION	GB AP008226.1
A	654A	A	G	CONFLICT	GB AP008226.1
A	654E	C	G	CONFLICT	GB AP008226.1
A	654P	G	C	CONFLICT	GB AP008226.1
A	654T	A	C	CONFLICT	GB AP008226.1
A	1058	U	G	CONFLICT	GB AP008226.1
A	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	M	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	O	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Q	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	R	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	T	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	U	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	X	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

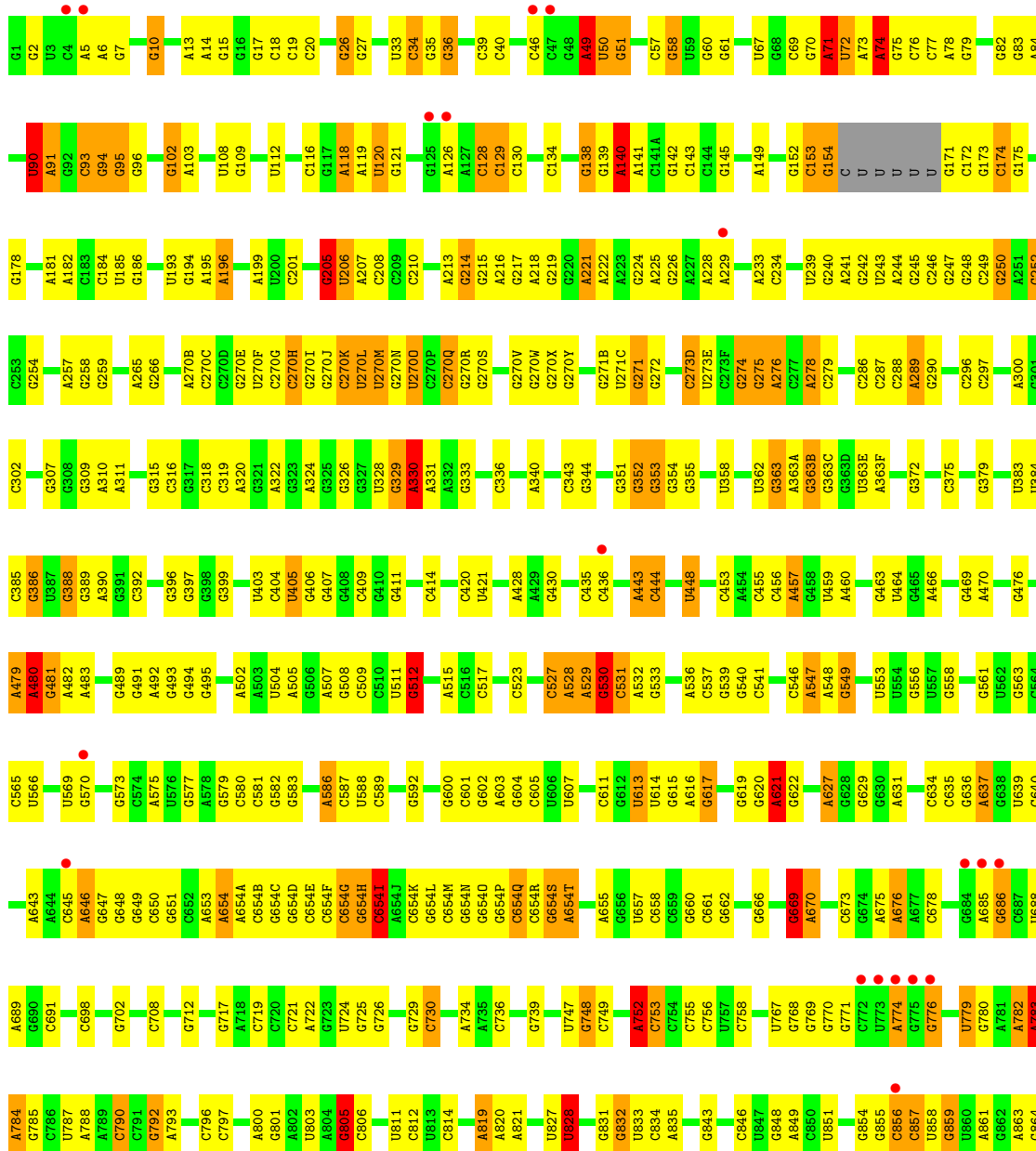


### 3 Residue-property plots

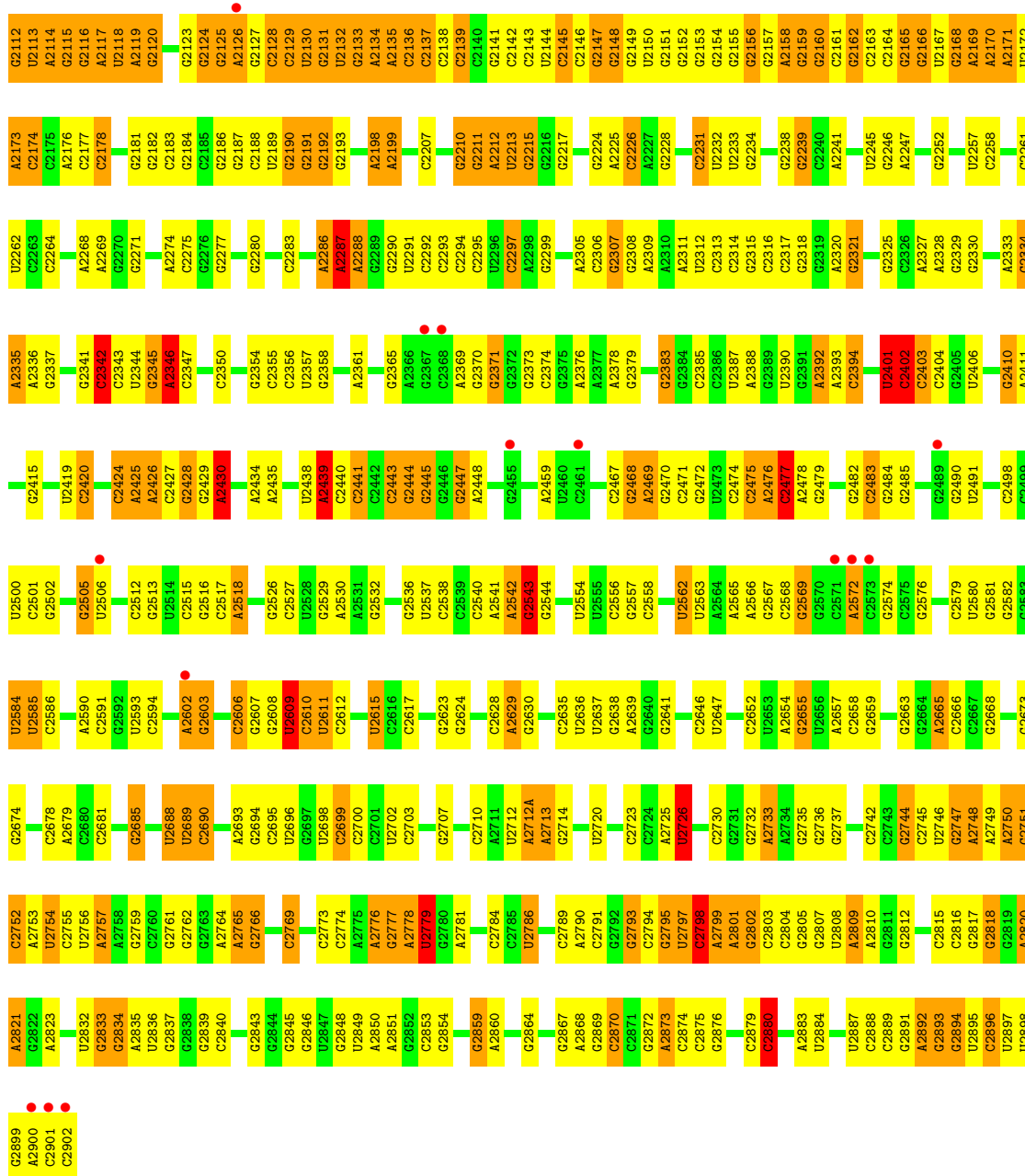
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $RSRZ > 2$ ). 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.

#### • Molecule 1: 23S ribosomal RNA

Chain A: 

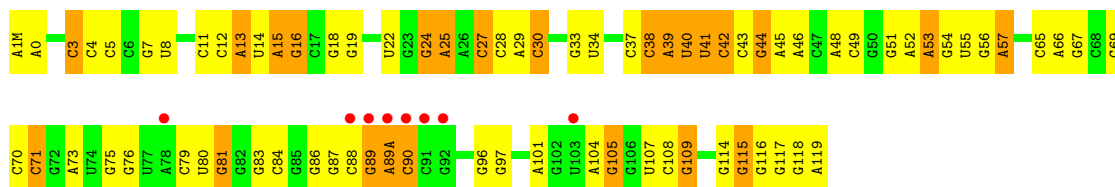


A2033	G1935	U1834	G1743	G1627	C1550	A1472	U1397	G1299	G1269	G1136	C1072	U1011	G932	C865
C2036	A1936	G1635	G1763	G1628	C1556	G1473	C1403	U1300	A1210	G1137	A1073	U1012	A933	A866
C2040	G1950	G1839	C1754	U1629	C1557	C1474	A1301	A1301	G1212	G1138	G1074	C1013	G934	G869
U2041	U1951	G1755	A1755	G1638	A1558	C1476	U1405	G1309	U1219	G1140	C1075	U1014	C935	G871
A2042	A1952	U1757	G1756	C1640	G1559	A1477	U1406	U1313	A1220	U1141	A1076	G1015	G938	U870
C2043	U1955	G1758	G1758	G1645	G1560	G1479	C1407	U1314	G1223	U1142	C1078	G1017	A872	A872
G2046	U1956	A1847	C1761	G1646	C1564	G1483	C1409	A1321	C1225	A1142A	A1080	U1019	A941	G873
G2049	C1962	G1848	A1762	G1647	C1565	G1484	G1410	A1322	G1224	A1143	U1081	A1020	G942	U877
G2052	U1963	G1763	G1763	C1648	A1566	G1486	A1412	U1323	C1225	C1145	U1082	A1021	U943	A878
C2053	G1964	U1851	G1764	G1651	A1567	G1487	G1414	G1324	G1228	G1149	U1083	G1022	A945	G879
G2055	C1965	C1852	G1764	G1652	G1568	G1488	G1415	G1325	C1230	C1150	A1085	U1023	A946	G881
A2054	A1966	A1853	G1771	G1653	A1569	G1489	U1415	U1326	G1236	G1151	A1086	G1024	G947	G882
C2055	C1967	A1570	A1773	A1654	A1570	G1490	G1416	C1327	G1236	A1155	U1087	U1025	G948	G883
G2056	A1970	U1576	U1779	G1655	U1576	G1491	C1417	U1328	G1236	A1156	A1088	A1027	G954	C884
A2059	A1971	C1577	A1780	A1656	C1577	G1492	A1419	G1330	U1240	G1157	U1089	A1028	G955	C885
A2060	A1972	U1578	A1781	C1657	U1578	C1493	U1420	A1331	G1248	C1158	U1090	A1029	G956	C886
C2060	U1971	U1579	A1782	C1658	U1579	A1496	G1424	G1338	G1248	G1169	A1091	G1030	A957	A887
A2062	C1982	C1582	A1784	G1660	G1582	U1497	G1424	G1339	A1247	C1161	U1092	U1033	U958	C888
C2065	G1989	A1583	A1785	G1666	A1583	C1505	A1427	A1342	C1251	G1163	A1098	G1034	A960	C889
C2066	C1990	C1585	A1786	U1671	C1585	A1507	C1428	A1349	G1251	G1165	U1099	G1035	A961	A890
U2067	U1991	A1587	A1787	C1672	A1587	A1508	A1434	U1352	A1253	C1162	C1100	U1036	G962	G892
C2068	G1989	G1888	A1788	G1673	G1588	C1509	G1436	G1352	A1253	G1169	U1101	G1037	G963	C893
G2069	C1992	C1870	A1789	G1674	C1589	A1510	G1437	G1356	U1255	G1170	C1102	U1038	U964	C894
C2070	U1993	G1885	A1791	C1675	U1590	A1511	C1437	U1357	G1256	A1171	A1103	G1039	C964	C895
C2075	C1994	A1886	A1791	G1678	G1591	G1512	G1441	G1366	C1257	G1173	C1104	C1040	G974	C896
U2079	U1995	C1886	A1791	U1678	C1592	U1516	G1442	U1368	G1257	G1175	U1105	G1041	C975	C897
C2080	C1996	C1887	A1791	U1688	G1593	U1517	G1442	A1359	A1262	A1174	G1106	G1042	C976	A899
A2082	C1999	A1889	A1791	A1689	G1595	C1518	A1444A	A1360	G1266	U1177	U1107	G1043	G975	A900
C2083	C2006	C1894	G1801	G1695	U1596	U1519	G1447	C1363	A1269	C1178	G1110	C1048	A883	A901
G2084	G2007	C1895	A1802	G1696	A1597	U1520	G1448	C1364	A1289	C1179	A1111	A1050	A984	A901
C2085	C2008	U1898	U1805	G1697	C1596	G1521	G1449	A1365	G1270	C1180	G1112	C1051	C985	C902
U2086	G2009	G1899	C1806	G1698	C1600	G1525	G1449A	G1368	G1271	C1181	U1113	C1052	C985	C903
C2093	G2012	A1900	G1907	G1699	G1601	G1526	C1450	U1372	U1273	A1182	U1114	C1053	A988	C904
G2094	A2013	U1901	U1808	A1700	A1602	G1527	C1451	G1368	A1274	G1183	G1115	A1054	A989	A910
C2095	A2014	C1902	A1809	A1701	A1603	A1528	C1453	U1372	A1275	G1184	C1116	G1055	A990	A911
U2096	A2015	A1810	C1607	U1716	C1607	C1533	U1454	A1379	A1276	C1185	G1117	G1056	C912	C912
C2097	U2016	A1811	A1608	G1717	A1608	G1534	G1455	G1380	G1277	G1186	C1118	A1057	G993	U913
U2098	G2017	A1812	A1609	G1718	A1609	U1535	C1458	G1381	A1278	G1187	C1119	U1058	C994	C914
C2100	A2019	G1814	A1610	G1725	A1610	A1536	G1459	U1384	G1279	U1188	G1122	G1062	C995	C915
G2101	A2020	A1815	C1611	G1726	A1537	C1537	A1460	A1384	G1280	G1190	G1123	U1061	A996	A917
U2102	A1913	G1816	G1611	U1727	C1537	G1538	G1461	G1385	A1286	G1191	C1124	G1062	G997	A918
C2103	C1914	G1817	A1614	G1728	A1614	G1539	C1462	G1386	A1287	G1192	G1125	U1063	C998	G919
G2104	U1915	A1818	C1615	U1729	A1615	G1540	C1463	G1389	U1288	C1201	A1126	C1064	U999	G920
C2105	A1916	A1819	A1616	U1730	A1616	C1541	C1464	G1389	U1288	G1202	A1127	U1065	A1000	G921
G2106	U1917	U1820	C1617	G1731	A1617	U1541	G1465	A1392	U1292	G1203	A1128	U1066	A1001	U922
C2107	U2027	A1817	A1618	G1732	A1618	G1542	G1466	A1392	U1292	G1203	A1129	A1067	C1005	C923
C2108	G2029	G1823	G1622	C1735	A1543	A1543	C1467	A1393	C1293	A1204	U1130	G1068	C1006	A926
U2109	A2030	G1930	G1622	C1741	A1544	C1544	G1470	A1394	C1293	U1205	G1131	A1069	C1007	G928
G2111	G2032	U1931	A1545	C1742	A1545A	A1545A	A1471	A1396	U1295	C1208	C1135	A1070	A1010	G929



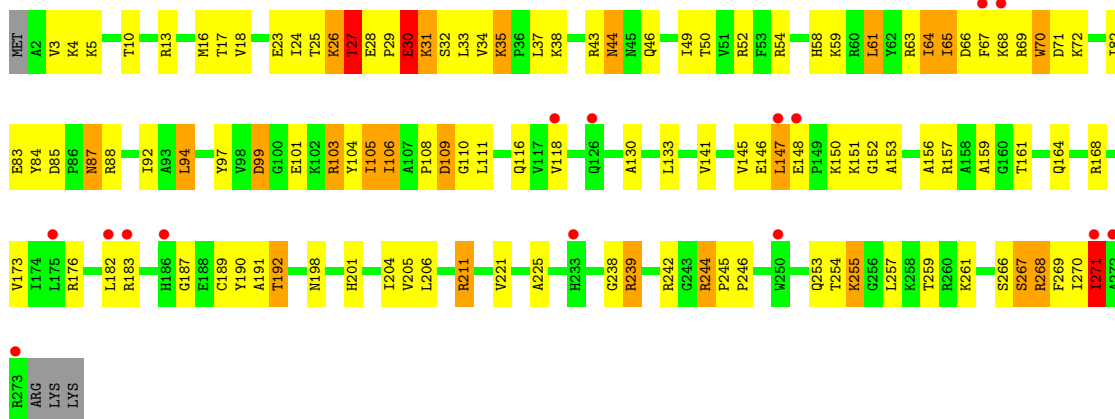
## • Molecule 2: 5S RIBOSOMAL RNA

Chain B:



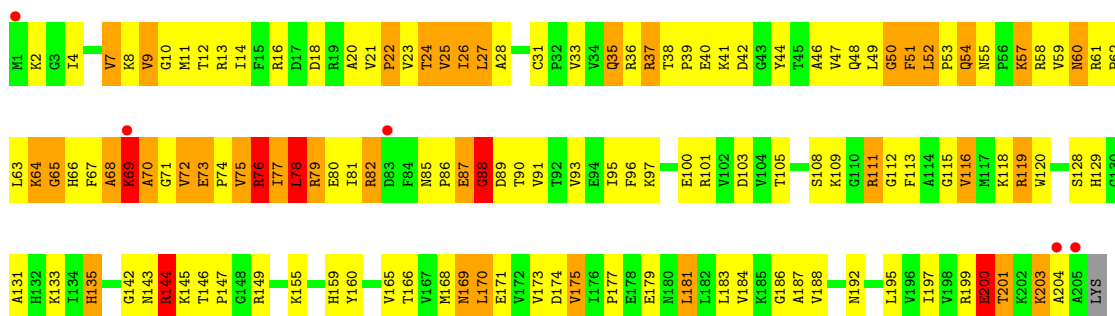
## • Molecule 3: 50S ribosomal protein L2

Chain D:



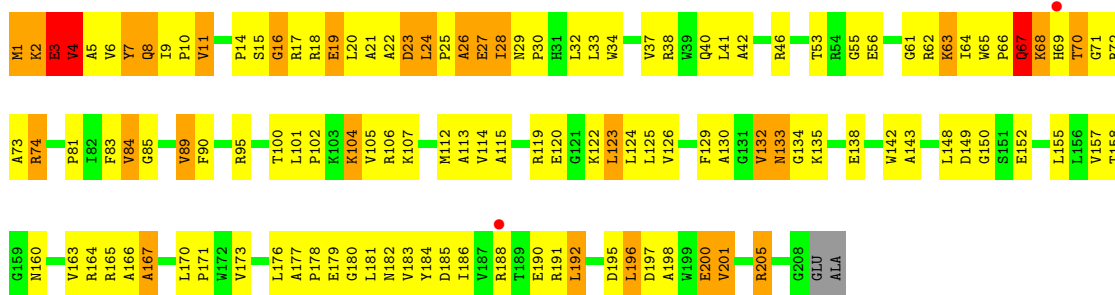
• Molecule 4: 50S ribosomal protein L3

Chain E:



• Molecule 5: 50S ribosomal protein L4

Chain F:



• Molecule 6: 50S ribosomal protein L5

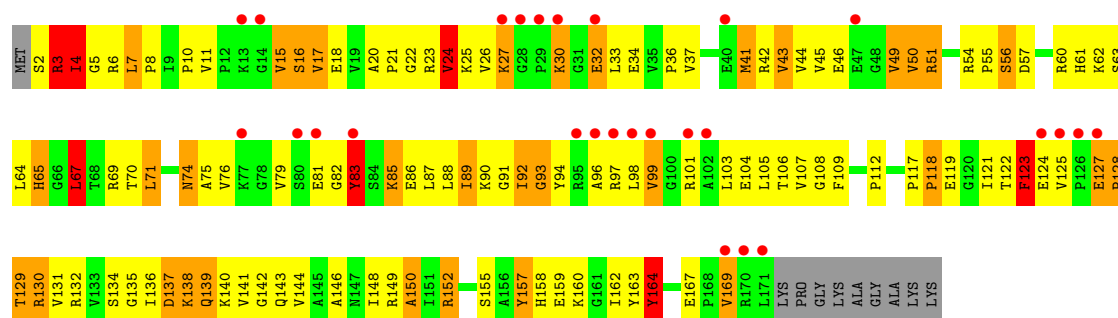
Chain G:





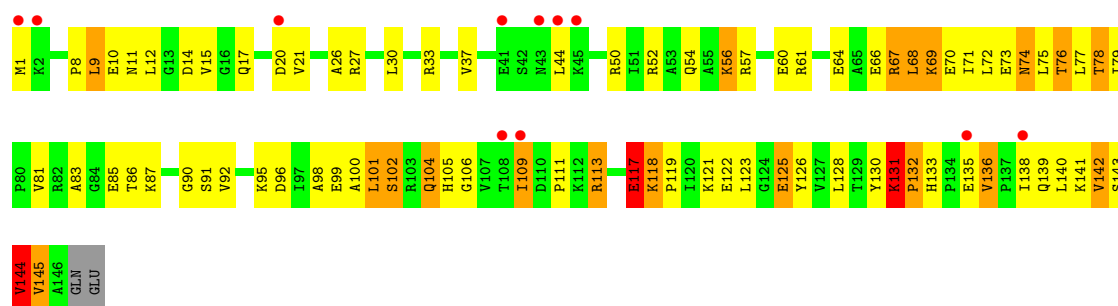
• Molecule 7: 50S ribosomal protein L6

Chain H:



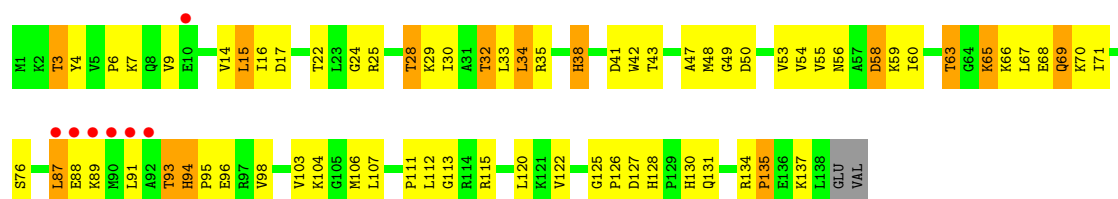
• Molecule 8: 50S ribosomal protein L9

Chain K:



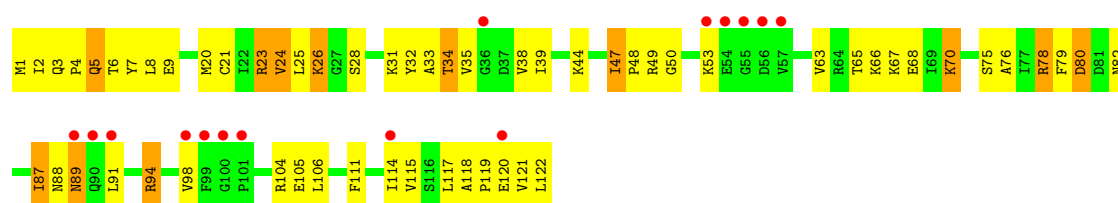
• Molecule 9: 50S ribosomal protein L13

Chain M:



• Molecule 10: 50S ribosomal protein L14

Chain N:



• Molecule 11: 50S ribosomal protein L15

Category	Item	Value
L	L138	0.00
	L139	0.00
	A140	0.00
	A141	0.00
	G142	0.00
	G143	0.00
	E144	0.00
	P145	0.00
	V146	0.00
	L147	0.00
L	L148	0.00
	E149	0.00
	A150	0.00
V	V71	0.00
	P72	0.00
	G73	0.00
	E74	0.00
	R77	0.00
	P78	0.00
	R79	0.00
	Y80	0.00
	Q81	0.00
	G82	0.00
V	V83	0.00
	N84	0.00
	L85	0.00
K	K86	0.00
	L87	0.00
	L88	0.00
A	A89	0.00
	R90	0.00
	F91	0.00
G	G92	0.00
	E93	0.00
	G94	0.00
E	E94	0.00
	Y95	0.00
	T96	0.00
P	P97	0.00
	E98	0.00
	L99	0.00
L	L100	0.00
	V101	0.00
	A102	0.00
R	R103	0.00
	G104	0.00
	L105	0.00
L	L106	0.00
	K107	0.00
	K108	0.00
G	G109	0.00
	Y110	0.00
	R111	0.00
L	L112	0.00
	K113	0.00
	L114	0.00
L	L115	0.00
	G116	0.00
	E117	0.00
G	G118	0.00
	E119	0.00
	A120	0.00
K	K121	0.00
	P122	0.00
	L123	0.00
K	K124	0.00
	V125	0.00
	V126	0.00
H	A127	0.00
	H128	0.00
	S133	0.00
R	R1	0.00
	R2	0.00
	L3	0.00
	S4	0.00
	D5	0.00
	L6	0.00
	R7	0.00
	P8	0.00
	N9	0.00
	P10	0.00
G11	0.00	
R	A12	0.00
	N13	0.00
	K14	0.00
R	R15	0.00
	R18	0.00
	R21	0.00
G	G22	0.00
	P23	0.00
	G24	0.00
S	S25	0.00
	K29	0.00
	T30	0.00
H	H35	0.00
	K36	0.00
	G37	0.00
R	R41	0.00
	S42	0.00
	L45	0.00
K	K46	0.00
	D47	0.00
	P48	0.00
R	R49	0.00
	R50	0.00
	F51	0.00
E	E52	0.00
	G53	0.00
	G54	0.00
R	R55	0.00
	S56	0.00
	T57	0.00
T	T58	0.00
	L59	0.00
	M60	0.00
R	R61	0.00
	L62	0.00
	P63	0.00
K	K64	0.00
	R65	0.00
	G66	0.00
H	M67	0.00
	Q68	0.00
	G69	0.00
S	S70	0.00

- 
- Figure 1 displays four heatmaps (A, B, C, D) showing the distribution of 70 amino acids (K72, P73, Y74, T75, K76, G77, F78, L79, M83, K87, G88, N89, Y90, E91, G92, K93, R101, V102, M103, F104, E105, V106, A107, T110, E111, E112, Q113, E116, A117, L118, R119, G122, I123, K124, K128, T129, K130, I131, V132, R133, R134, A136, D138, E139, A140, Q141) across four protein families (A, B, C, D). The color scale ranges from 0 (white) to 1 (dark red). The diagonal elements are all 1.0. The off-diagonal elements show varying degrees of similarity between amino acids. The distribution of similarity is generally higher in family A and lower in family D.

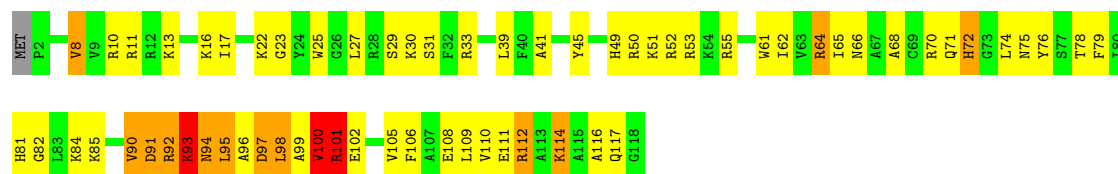
- 
- Figure 1: A 2D heatmap visualization of the protein-protein interaction network. The x-axis and y-axis both list 40 proteins, grouped into 10 sets of 4. The color scale ranges from grey (MET) to red (L44). The diagonal is grey, indicating self-interactions. The heatmap shows a complex network of interactions, with a dense cluster of red and orange colors in the upper right quadrant, indicating strong interactions between proteins in that region.

- [illegible]

- |  |     |     |     |     |     |     |     |     |     |     |     |     |  |     |     |     |     |     |     |     |     |     |      |      |     |      |      |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |      |      |      |     |      |     |     |     |     |     |     |     |     |     |     |     |     |
|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|------|------|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--|------|------|------|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|  | M1  | N2  | R3  | G4  | A5  | L6  | I7  | K8  | B9  | V10 | E11 | S12 |  | R16 | T17 | D18 | L19 | P20 | E21 | F22 | R23 | P24 |      | G25  | D26 | T27  |      | V30 |      | E36  | G37  | N38  |      | R41  |      | F45  |      | V49  | I50  | R51  | I52  |      | N55  |  | T59  | G60  | F61  | T62 | V63  | R64 | G65 | V66 | S67 | Y68 |     | V72 | E73 | R74 | I75 | F76 | P77 |
|  | S80 | P81 | L82 | I83 | G84 | K85 | L86 | B87 | D88 | V89 | Q90 | R91 |  | G92 | R93 | A94 | R95 | R96 | A97 | K98 | L99 |     | D107 | R108 |     | R111 | R112 |     | R115 | A116 | D117 | R118 | K119 | R120 | I121 | D122 | Q123 | D124 | R125 | A126 | A127 | E128 | R129 |  | K132 | E133 | E134 |     | K137 | GLN | ALA | GLU | PRO | LYS | ALA | SER | GLN | GLU |     |     |     |

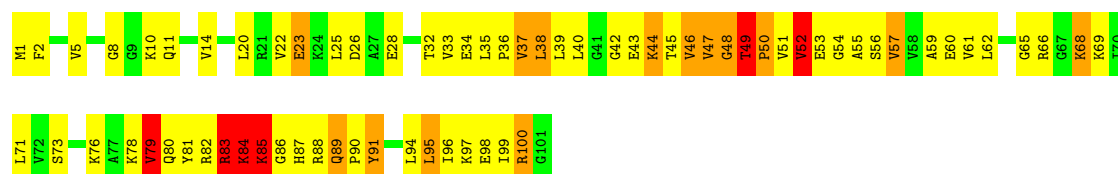
- Molecule 16: 50S ribosomal protein L20

Chain 1:



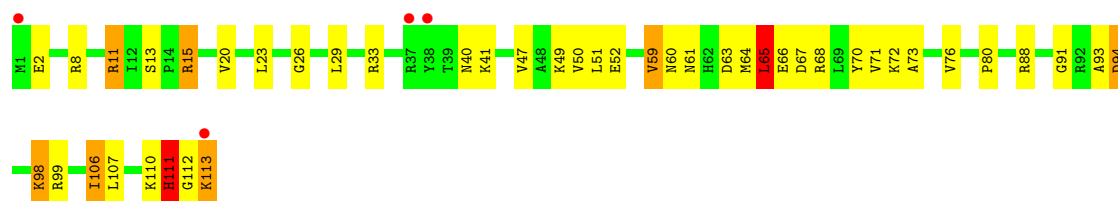
- Molecule 17: 50S ribosomal protein L21

Chain 2:



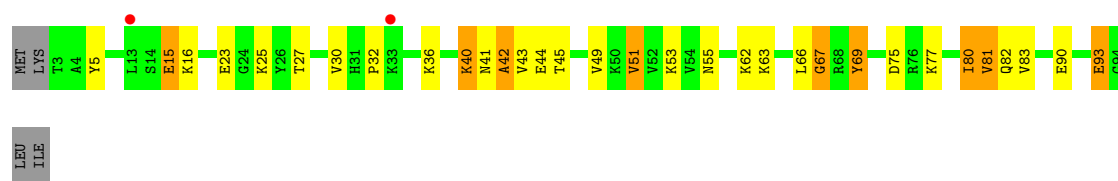
- Molecule 18: 50S ribosomal protein L22

Chain S:



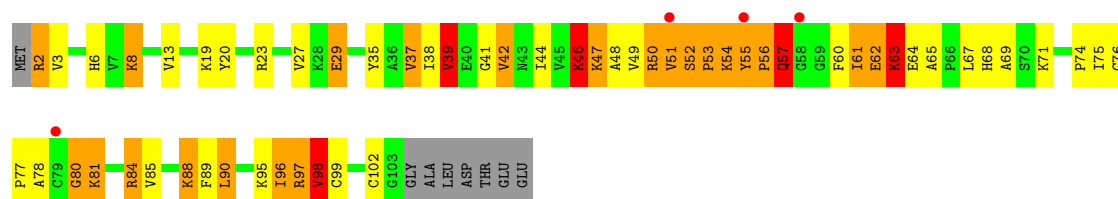
- Molecule 19: 50S ribosomal protein L23

Chain T:



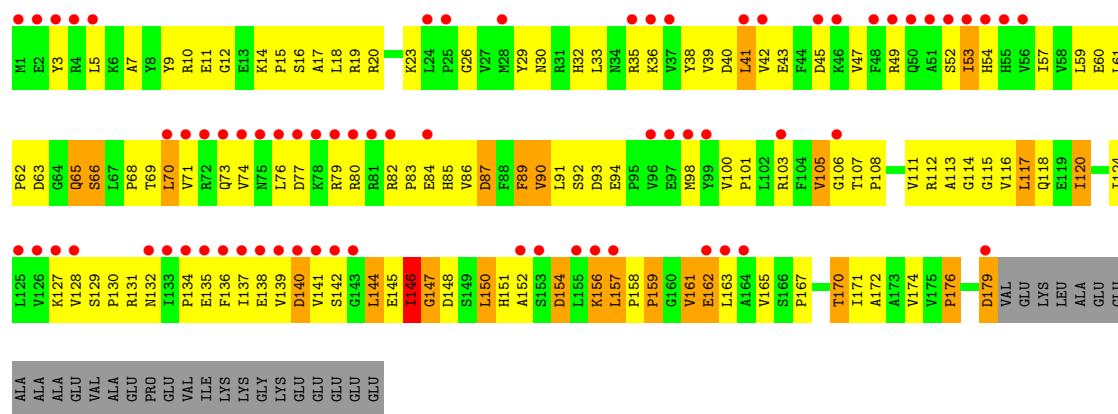
- Molecule 20: 50S ribosomal protein L24

Chain U:



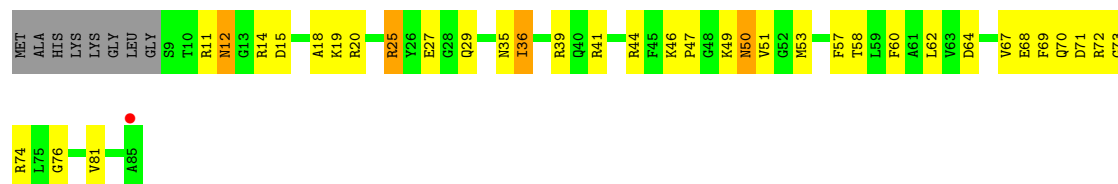
- Molecule 21: 50S ribosomal protein L25

Chain V:



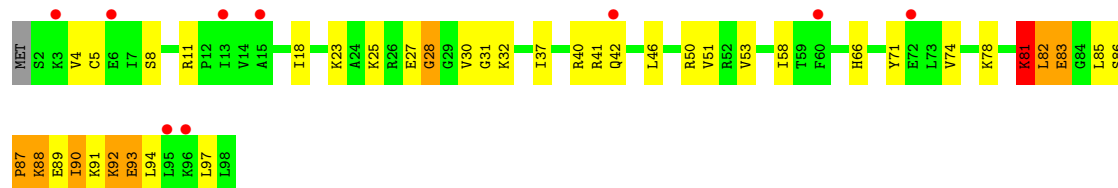
• Molecule 22: 50S ribosomal protein L27

Chain 3:



• Molecule 23: 50S ribosomal protein L28

Chain Z:



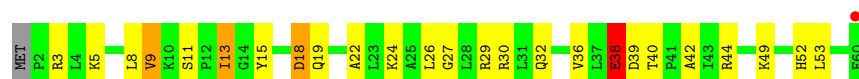
• Molecule 24: 50S ribosomal protein L29

Chain W:



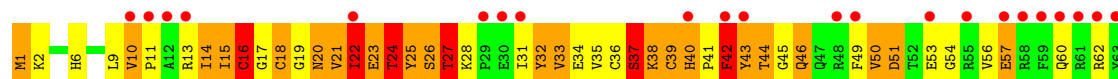
• Molecule 25: 50S ribosomal protein L30

Chain X:



• Molecule 26: 50S ribosomal protein L31

Chain 4:





GLY  
ASP  
SER  
TYR  
ARG  
LYS  
GLY  
ARG

- Molecule 27: 50S ribosomal protein L32

Chain 5: 

MET A2 K3 H4 P5 V6 P7 K10 R15 R16 D17 A18 R19 H23 A24 L25 T29 C33 P34 E35 C36 K37 V45 C46 P47 E48 C49 G50 Y51 R55 K56 V57 L58 E59 V60

- Molecule 28: 50S ribosomal protein L33

Chain 6: 

MET ALA SER GLU VAL ARG ILE LYS L9 L10 L11 E12 C13 T14 E15 C16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 Y39 C40 P41 V42 C43 R44 K45 H46 T47 V48 H49 R50 E51 V52 K53 ILE

- Molecule 29: 50S ribosomal protein L34

Chain 7: 

K1 T4 W5 Q6 P7 R8 R9 R10 K11 K14 T15 F18 R19 A20 R21 R22 R23 T24 K32 K33 R34 R35 R36 R37 R38 R39 W40 R41 L42 T43 P44 A45 V46 R47 R48 R49

- Molecule 30: 50S ribosomal protein L35

Chain 8: 

MET P2 K3 M4 K5 T6 H7 K8 R13 I16 V22 V23 A24 M25 T27 G28 K29 R30 R31 R32 R33 R34 Q35 K36 S37 G38 K39 E40 I41 Q42 Q43 K44 K47 F48 V49 L50 A51 K52 P53 E54 A55 E56 R57 I58 K59 L60 L61 L62 PRO TYR GLU

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.06Å 450.27Å 616.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.59 – 3.10 254.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (153.59-3.10) 93.4 (254.47-3.10)	Depositor EDS
$R_{merge}$	0.47	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_987)	Depositor
R, $R_{free}$	0.213 , 0.269 0.430 , 0.440	Depositor DCC
$R_{free}$ test set	921 reflections (0.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.8	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1045188 reflections	Xtriage
$F_o, F_c$ correlation	0.67	EDS
Total number of atoms	92006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	A	0.61	4/70100 (0.0%)	1.09	282/109435 (0.3%)
2	B	0.55	0/2928	0.99	3/4568 (0.1%)
3	D	0.57	1/2165 (0.0%)	0.70	0/2919
4	E	0.50	0/1601	0.67	1/2160 (0.0%)
5	F	0.44	0/1662	0.64	0/2249
6	G	0.36	0/1499	0.59	0/2016
7	H	0.34	0/1332	0.70	1/1802 (0.1%)
8	K	0.40	0/1151	0.63	1/1558 (0.1%)
9	M	0.39	0/1131	0.58	0/1525
10	N	0.46	0/943	0.61	0/1269
11	O	0.42	0/1162	0.71	0/1544
12	P	0.45	0/1143	0.63	0/1527
13	0	0.46	0/974	0.63	0/1302
14	Q	0.44	0/892	0.73	1/1187 (0.1%)
15	R	0.43	0/1155	0.60	0/1542
16	1	0.42	0/982	0.64	0/1306
17	2	0.42	0/790	0.69	1/1057 (0.1%)
18	S	0.47	0/911	0.59	0/1220
19	T	0.55	0/739	0.64	0/993
20	U	0.50	0/798	0.69	1/1064 (0.1%)
21	V	0.37	0/1460	0.67	1/1982 (0.1%)
22	3	0.46	0/621	0.61	0/827
23	Z	0.49	0/770	0.68	0/1022
24	W	0.48	0/583	0.71	1/771 (0.1%)
25	X	0.40	0/474	0.56	0/635
26	4	0.44	0/527	0.69	0/709
27	5	0.45	0/473	0.67	0/639
28	6	0.52	0/396	0.68	0/529
29	7	0.54	0/438	0.65	0/575
30	8	0.61	0/494	0.93	1/649 (0.2%)
All	All	0.57	5/100294 (0.0%)	1.00	294/150581 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2430	A	N9-C4	-5.89	1.34	1.37
1	A	2518	A	N9-C4	-5.88	1.34	1.37
1	A	2443	C	N1-C6	-5.46	1.33	1.37
1	A	1992	G	N9-C4	5.06	1.42	1.38
3	D	30	GLU	CG-CD	5.02	1.59	1.51

The worst 5 of 294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2401	U	C5-C6-N1	10.78	128.09	122.70
1	A	1786	A	C5-N7-C8	-10.44	98.68	103.90
1	A	1786	A	N7-C8-N9	10.20	118.90	113.80
1	A	2447	G	N1-C6-O6	9.54	125.62	119.90
1	A	2401	U	C5-C4-O4	-9.33	120.30	125.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62587	0	31554	1344	0
2	B	2617	0	1328	85	0
3	D	2115	0	2195	141	0
4	E	1568	0	1634	207	0
5	F	1627	0	1680	130	0
6	G	1474	0	1535	101	0
7	H	1307	0	1382	122	0
8	K	1136	0	1223	44	0
9	M	1104	0	1180	50	0
10	N	933	0	996	41	0
11	O	1145	0	1228	155	0
12	P	1122	0	1179	59	0
13	0	960	0	1021	37	0
14	Q	882	0	943	72	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	R	1141	0	1202	62	0
16	1	964	0	1022	69	0
17	2	779	0	852	89	0
18	S	900	0	964	27	0
19	T	725	0	778	20	0
20	U	785	0	878	57	0
21	V	1428	0	1454	87	0
22	3	613	0	633	35	0
23	Z	763	0	848	34	0
24	W	581	0	629	30	0
25	X	469	0	518	19	0
26	4	515	0	510	71	0
27	5	459	0	480	24	0
28	6	389	0	404	76	0
29	7	430	0	480	13	0
30	8	488	0	560	71	0
All	All	92006	0	61290	2906	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

The worst 5 of 2906 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:127:GLU:CG	7:H:128:PRO:HD3	1.36	1.54
4:E:11:MET:SD	4:E:24:THR:HG22	1.47	1.52
17:2:49:THR:HB	17:2:50:PRO:CD	1.45	1.47
3:D:34:VAL:HG22	3:D:35:LYS:CE	1.44	1.46
11:O:71:VAL:CG1	11:O:72:PRO:HD3	1.44	1.45

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	270/276 (98%)	217 (80%)	40 (15%)	13 (5%)	4	23
4	E	203/206 (98%)	133 (66%)	33 (16%)	37 (18%)	0	0
5	F	206/210 (98%)	151 (73%)	29 (14%)	26 (13%)	0	3
6	G	179/182 (98%)	121 (68%)	38 (21%)	20 (11%)	1	5
7	H	168/180 (93%)	92 (55%)	45 (27%)	31 (18%)	0	0
8	K	144/148 (97%)	104 (72%)	28 (19%)	12 (8%)	1	9
9	M	136/140 (97%)	110 (81%)	22 (16%)	4 (3%)	7	38
10	N	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	9	42
11	O	148/150 (99%)	83 (56%)	44 (30%)	21 (14%)	0	2
12	P	139/141 (99%)	105 (76%)	19 (14%)	15 (11%)	1	5
13	O	115/118 (98%)	99 (86%)	13 (11%)	3 (3%)	8	41
14	Q	109/112 (97%)	78 (72%)	20 (18%)	11 (10%)	1	6
15	R	135/146 (92%)	110 (82%)	19 (14%)	6 (4%)	4	25
16	1	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	11
17	2	99/101 (98%)	73 (74%)	12 (12%)	14 (14%)	0	2
18	S	111/113 (98%)	98 (88%)	8 (7%)	5 (4%)	4	24
19	T	90/96 (94%)	69 (77%)	13 (14%)	8 (9%)	1	8
20	U	100/110 (91%)	53 (53%)	22 (22%)	25 (25%)	0	0
21	V	177/206 (86%)	111 (63%)	35 (20%)	31 (18%)	0	0
22	3	75/85 (88%)	66 (88%)	7 (9%)	2 (3%)	8	39
23	Z	95/98 (97%)	71 (75%)	14 (15%)	10 (10%)	1	5
24	W	67/72 (93%)	53 (79%)	6 (9%)	8 (12%)	1	4
25	X	57/60 (95%)	49 (86%)	5 (9%)	3 (5%)	3	21
26	4	61/71 (86%)	25 (41%)	18 (30%)	18 (30%)	0	0
27	5	57/60 (95%)	46 (81%)	7 (12%)	4 (7%)	2	13
28	6	43/54 (80%)	19 (44%)	13 (30%)	11 (26%)	0	0
29	7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
30	8	59/65 (91%)	42 (71%)	8 (14%)	9 (15%)	0	1
All	All	3325/3489 (95%)	2414 (73%)	552 (17%)	359 (11%)	1	5

5 of 359 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	26	LYS
3	D	32	SER
3	D	267	SER
4	E	25	VAL
4	E	27	LEU

### 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	
3	D	214/218 (98%)	183 (86%)	31 (14%)	5	18
4	E	165/166 (99%)	143 (87%)	22 (13%)	6	22
5	F	165/166 (99%)	138 (84%)	27 (16%)	3	12
6	G	155/156 (99%)	132 (85%)	23 (15%)	4	17
7	H	142/148 (96%)	109 (77%)	33 (23%)	1	5
8	K	122/124 (98%)	92 (75%)	30 (25%)	1	3
9	M	117/119 (98%)	96 (82%)	21 (18%)	2	10
10	N	100/100 (100%)	87 (87%)	13 (13%)	6	23
11	O	116/116 (100%)	84 (72%)	32 (28%)	0	1
12	P	111/111 (100%)	94 (85%)	17 (15%)	4	15
13	0	100/101 (99%)	89 (89%)	11 (11%)	9	34
14	Q	87/88 (99%)	69 (79%)	18 (21%)	2	8
15	R	120/127 (94%)	98 (82%)	22 (18%)	2	10
16	1	93/94 (99%)	79 (85%)	14 (15%)	4	16
17	2	82/82 (100%)	62 (76%)	20 (24%)	1	4
18	S	92/92 (100%)	75 (82%)	17 (18%)	2	9
19	T	74/78 (95%)	66 (89%)	8 (11%)	9	34
20	U	85/91 (93%)	59 (69%)	26 (31%)	0	1
21	V	158/179 (88%)	136 (86%)	22 (14%)	5	21
22	3	62/67 (92%)	58 (94%)	4 (6%)	24	65
23	Z	82/83 (99%)	76 (93%)	6 (7%)	20	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	W	64/67 (96%)	61 (95%)	3 (5%)	36	78
25	X	51/52 (98%)	43 (84%)	8 (16%)	4	14
26	4	57/63 (90%)	36 (63%)	21 (37%)	0	0
27	5	51/52 (98%)	43 (84%)	8 (16%)	4	14
28	6	44/52 (85%)	31 (70%)	13 (30%)	0	1
29	7	42/42 (100%)	33 (79%)	9 (21%)	1	7
30	8	51/55 (93%)	41 (80%)	10 (20%)	2	8
All	All	2802/2889 (97%)	2313 (82%)	489 (18%)	3	11

5 of 489 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	O	98	GLU
14	Q	89	ARG
27	5	29	THR
11	O	138	LEU
12	P	138	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
12	P	45	GLN
16	1	49	HIS
22	3	35	ASN
10	N	3	GLN
11	O	68	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2904/2912 (99%)	645 (22%)	39 (1%)
2	B	121/122 (99%)	32 (26%)	0
All	All	3025/3034 (99%)	677 (22%)	39 (1%)

5 of 677 RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	A	10	G
1	A	14	A
1	A	15	G
1	A	34	C
1	A	36	G

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1427	A
1	A	1819	A
1	A	2776	A
1	A	1460	A
1	A	1558	A

## 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 ⓘ

There are no ligands in this entry.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2906/2912 (99%)	-0.34	63 (2%) 59 11	60, 90, 232, 251	0
2	B	122/122 (100%)	0.02	8 (6%) 18 3	91, 127, 154, 200	0
3	D	272/276 (98%)	0.28	15 (5%) 24 4	58, 81, 99, 122	0
4	E	205/206 (99%)	-0.05	5 (2%) 56 9	60, 97, 142, 165	0
5	F	208/210 (99%)	-0.21	2 (0%) 79 23	66, 102, 156, 182	0
6	G	181/182 (99%)	0.10	14 (7%) 13 2	117, 141, 165, 177	0
7	H	170/180 (94%)	0.55	27 (15%) 3 1	146, 200, 223, 235	0
8	K	146/148 (98%)	0.40	11 (7%) 14 2	88, 132, 151, 159	0
9	M	138/140 (98%)	-0.04	7 (5%) 27 4	80, 107, 137, 157	0
10	N	122/122 (100%)	0.79	15 (12%) 5 1	70, 91, 109, 116	0
11	O	150/150 (100%)	0.58	24 (16%) 3 1	66, 105, 140, 179	0
12	P	141/141 (100%)	0.66	17 (12%) 5 1	80, 106, 130, 152	0
13	0	117/118 (99%)	0.19	6 (5%) 27 4	71, 89, 108, 119	0
14	Q	111/112 (99%)	0.69	19 (17%) 2 0	98, 121, 142, 151	0
15	R	137/146 (93%)	-0.03	2 (1%) 70 16	80, 99, 159, 185	0
16	1	117/118 (99%)	-0.52	0 100 100	72, 101, 136, 155	0
17	2	101/101 (100%)	-0.45	0 100 100	71, 123, 139, 148	0
18	S	113/113 (100%)	-0.03	4 (3%) 42 6	68, 83, 113, 161	0
19	T	92/96 (95%)	-0.03	2 (2%) 59 11	77, 94, 118, 128	0
20	U	102/110 (92%)	0.22	4 (3%) 37 5	93, 118, 160, 182	0
21	V	179/206 (86%)	1.74	69 (38%) 1 0	118, 157, 213, 219	0
22	3	77/85 (90%)	0.07	1 (1%) 74 19	74, 95, 111, 151	0
23	Z	97/98 (98%)	0.58	9 (9%) 9 2	67, 91, 135, 157	0
24	W	69/72 (95%)	-0.11	2 (2%) 49 7	90, 112, 133, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	59/60 (98%)	0.17	1 (1%) 67 15	79, 102, 145, 162	0
26	4	63/71 (88%)	1.64	22 (34%) 1 0	154, 187, 197, 205	0
27	5	59/60 (98%)	0.14	3 (5%) 27 4	68, 91, 178, 192	0
28	6	45/54 (83%)	2.43	27 (60%) 0 0	138, 164, 181, 183	0
29	7	49/49 (100%)	2.15	21 (42%) 1 0	63, 70, 107, 130	0
30	8	61/65 (93%)	-0.48	0 100 100	73, 87, 106, 121	0
All	All	6409/6523 (98%)	0.02	400 (6%) 20 3	58, 98, 202, 251	0

The worst 5 of 400 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1535	U	15.7
11	O	149	GLU	11.4
1	A	1052	C	11.0
29	7	47	ARG	9.6
11	O	92	GLU	9.6

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.