



wwPDB X-ray Structure Validation Summary Report

Sep 15, 2014 – 02:34 PM EDT

PDB ID : 1VW0
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U in the Absence of Paromomycin
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-27
Resolution : 3.92 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

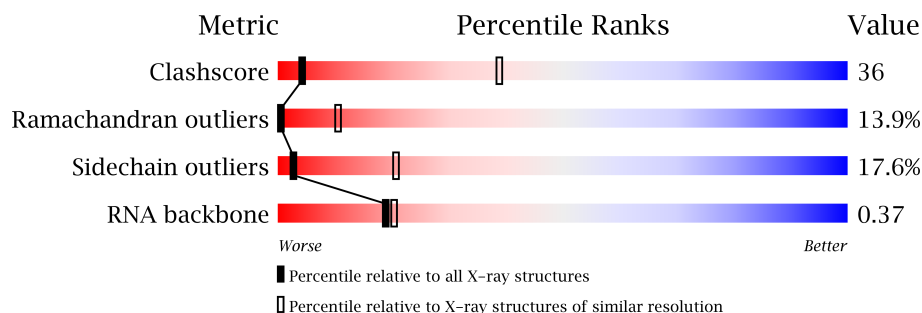
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.92 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	79885	1180 (4.34-3.50)
Ramachandran outliers	78287	1124 (4.34-3.50)
Sidechain outliers	78261	1112 (4.34-3.50)
RNA backbone	1838	1018 (5.00-2.80)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2916	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	
13	R	118	
14	S	112	

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Mol	Chain	Length	Quality of chain
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	
32	a	3	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92289 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- 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	I	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	N	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	O	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	P	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	Q	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	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	S	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	T	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	U	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	V	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	W	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	X	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	Y	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	Z	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	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	2	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	3	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	71	Total	C	N	O	S	0	0	0
			581	364	108	104	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	49	Total	C	N	O	S	0	0	0
			424	264	87	69	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	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	a	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	P	1	Total	Mg	0	0
			1	1		
33	Q	1	Total	Mg	0	0
			1	1		
33	E	1	Total	Mg	0	0
			1	1		
33	B	3	Total	Mg	0	0
			3	3		
33	7	1	Total	Mg	0	0
			1	1		
33	A	269	Total	Mg	0	0
			269	269		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	5	1	Total	Mg	0	0
			1	1		

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	9	1	Total	Zn	0	0
			1	1		

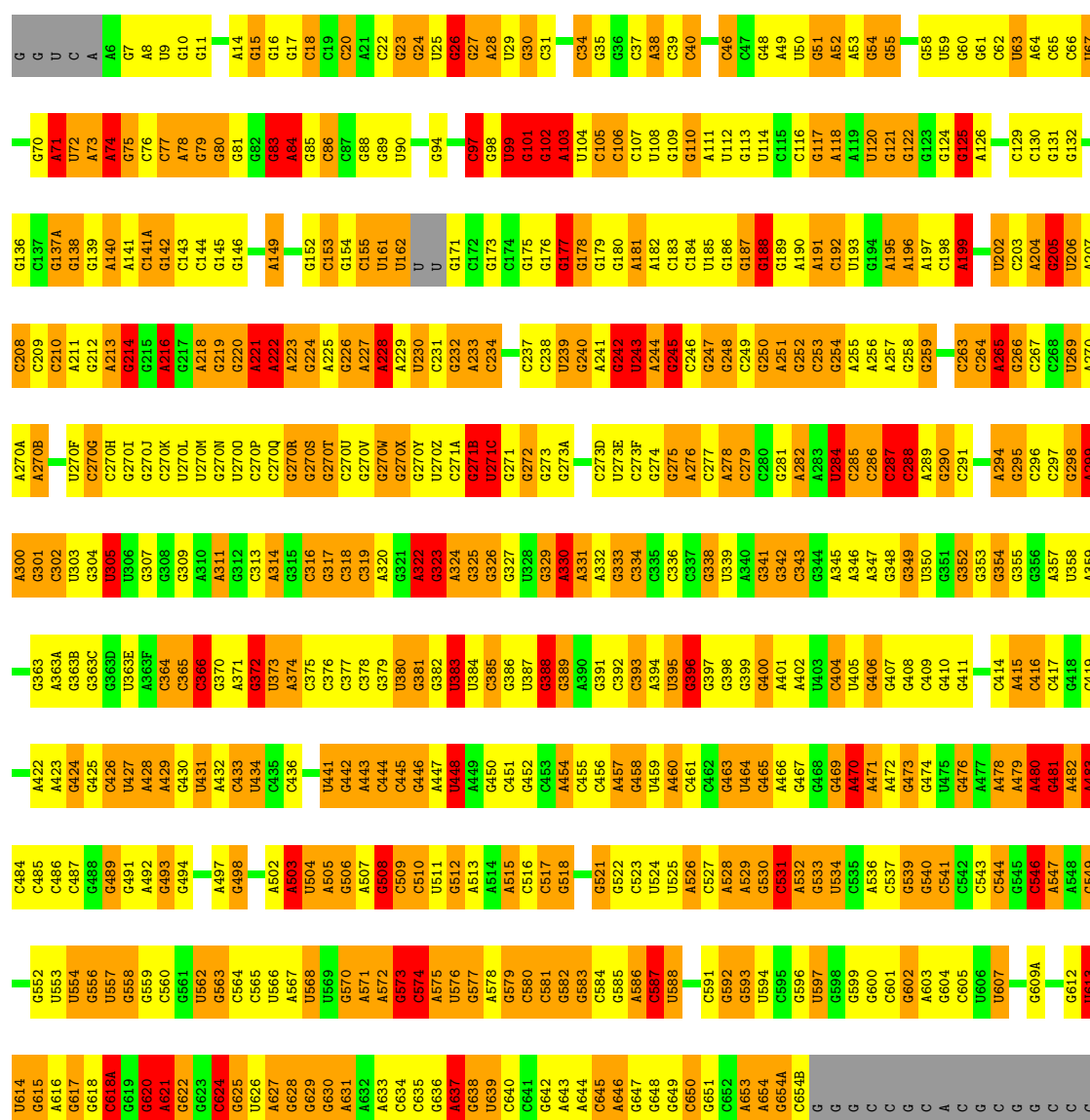
3 Residue-property plots

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.

Note EDS was not executed.

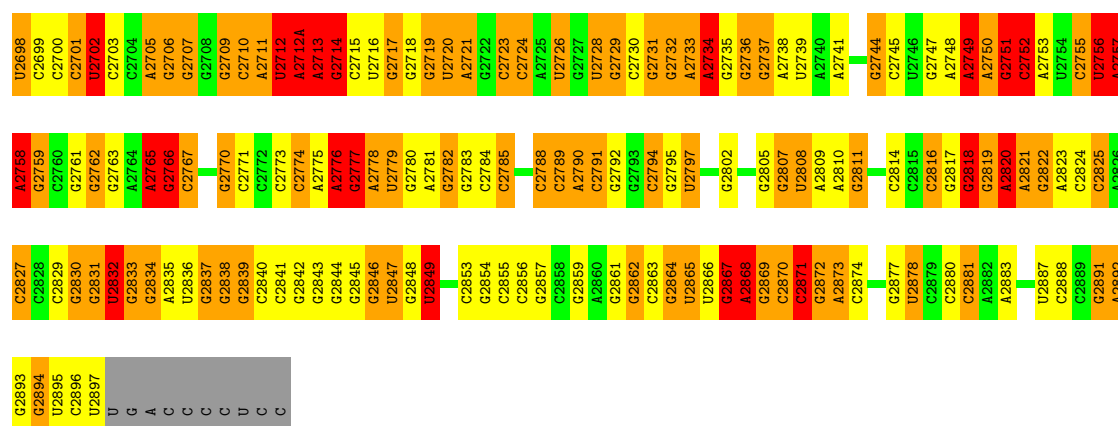
• Molecule 1: 23S rRNA

Chain A:



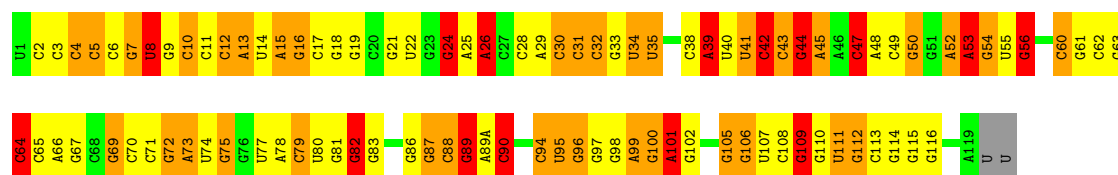
A1586	A1587	A1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1600	A1601	A1602	A1603	A1604	A1605	A1606	A1607	A1608	A1609	A1610	A1611	A1612	A1613	A1614	A1615	A1616	A1617	A1618	A1619	A1620	A1621	A1622	A1623	A1624	A1625	A1626	A1627	A1628	A1629	A1630	A1631	A1632	A1633	A1634	A1635	A1636	A1637	A1638	A1639	A1640	A1641	A1642	A1646	A1647																																																																																																																																																																																																																																																																																																																																																																																			
G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575	G1576	G1577	G1578	G1579	G1580	G1581	G1585	G1647																																																																																																																																																																																																																																																																																																																																																																																		
A1457	A1458	A1459	A1460	A1461	A1464	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1477	A1478	A1479	A1480	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	G1521																																																																																																																																																																																																																																																																																																																																																																																			
C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1453	C1454	C1456																																																																																																																																																																																																																																																																																																																																																																																			
G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1397																																																																																																																																																																																																																																																																																																																																																																																	
G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1336	G1337																																																																																																																																																																																																																																																																																																																																																																																	
C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1230	C1231	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1276	C1277																																																																																																																																																																																																																																																																																																																																																																																			
C1152	C1153	G1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165	C1166	C1169	C1170	C1171	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1185	C1186	C1187	C1188	C1189	C1190	C1191	C1192	C1193	C1194	C1195	C1196	C1197	C1198	C1199	C1200	C1201	C1202	C1203	C1204	C1205	C1206	C1207	C1208	C1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	C1217	C1218	C1219	C1220	C1221	C1222	C1223	C1224	C1225	C1226	C1227	C1228	C1229	C1230	C1231	C1232	C1233	C1234	C1235	C1236	C1237	C1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1248	C1249	C1250	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1258	C1259	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379	C1380	C1381	C1382	C1383	C1384	C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1585
A1088	G1089	U1090	A1091	G1092	A1093	U1094	A1095	A1096	U1097	A1098	G1099	A1100	U1101	A1102	A1103	C1104	U1105	G1106	C1109	G1110	A1111	G1112	U1113	G1114	G1115	C1119	G1122	C1123	G1124	C1125	G1126	A1127	A1128	A1129	U1130	G1131	A1132	U1133	G1135	C1136	G1137	G1138	G1139	C1140	U1141	C1142	U1143	A1144	G1145	C1146	C1147	A1148	G1149	C1150	G1151																																																																																																																																																																																																																																																																																																																																																																																				
A1021	G1022	U1023	C1024	A1025	G1026	A1027	A1028	A1029	G1030	C1031	G1032	A1033	U1034	U1035	G1036	G1042	U1043	G1044	A1045	A1046	G1047	A1048	U1049	C1050	G1051	G1052	A1053	G1054	U1055	G1056	A1057	G1058	C1059	U1060	C1061	G1062	G1063	G1064	U1065	U1066	A1067	G1068	A1069	A1070	C1071	C1076	A1077	U1078	C1079	G1080	U1081	G1082	C1083	A1084	U1085	A1086	G1087																																																																																																																																																																																																																																																																																																																																																																																		
C898	A899	A900	C899	A901	C902	C903	C904	U905	G906	U907	C908	G909	A910	A911	U912	U913	C914	G915	G916	A917	A918	G919	C920	U921	U922	A923	C924	C925	A926	U927	C928	G929	C930	C931	C932	A933	G934	C935	C936	U937	G938	G939	G940	G941	G942	U943	G944	A945	G946	G947	G948	C949	G950	C951	G952	A953	G954	C955	G956	A957	U958	A959	A960																																																																																																																																																																																																																																																																																																																																																																												
G836	C837	C838	U839	C839	C840	A841	G842	G843	G844	C845	G846	U847	G848	A849	C850	U851	G852	C853	G854	G855	C856	C857	U858	G859	U860	A861	G862	C863	U864	C864	A865	G866	C867	G868	A869	C870	U871	C871	C872	A873	C873	C874	C875	U876	A877	C878	A878	G881	A882	C883	G884	C885	U886	A887	C888	G889	A890	C891	G892	U893	C894	A895	G896	C897	A898	A899	A900																																																																																																																																																																																																																																																																																																																																																																								
G775	G776	A777	U778	C779	A780	G781	A782	A783	G784	C785	U786	G787	A788	C789	G790	C791	G792	A793	C794	C795	C796	C797	G798	G799	A800	G801	A802	C803	U804	C805	C806	U807	G808	C809	U810	U811	C812	U813	C814	C815	G818	A819	A820	U821	C822	G823	A824	C825	U826	U827	C828	U829	G830	C831	G832	U833	C834	A835																																																																																																																																																																																																																																																																																																																																																																																	
G713	U714	G715	A716	G717	A718	C721	A722	G723	U724	G725	C726	A727	G728	C729	U730	C731	G732	C733	G734	C735	C736	C737	G738	A800	G801	A802	C803	U804	C805	C806	U807	G808	C809	U810	U811	C812	U813	C814	C815	G818	A819	A820	U821	C822	G823	A824	C825	U826	U827	C828	U829	G830	C831	G832	U833	C834	A835																																																																																																																																																																																																																																																																																																																																																																																		
G854S	C854T	A854U	A854V	A855	G856	U857	C858	C859	G860	C861	G862	G863	C864	C865	G866	U867	G868	G869	A870	C871	C872	C873	G874	A875	A876	C877	C878	C879	G880	G881	G882	C883	G884	U885	C886	C887	C888	C889	C890	C891	C892	C893	U894	G895	C896	G897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1																																																																																																																																																																																																																																											





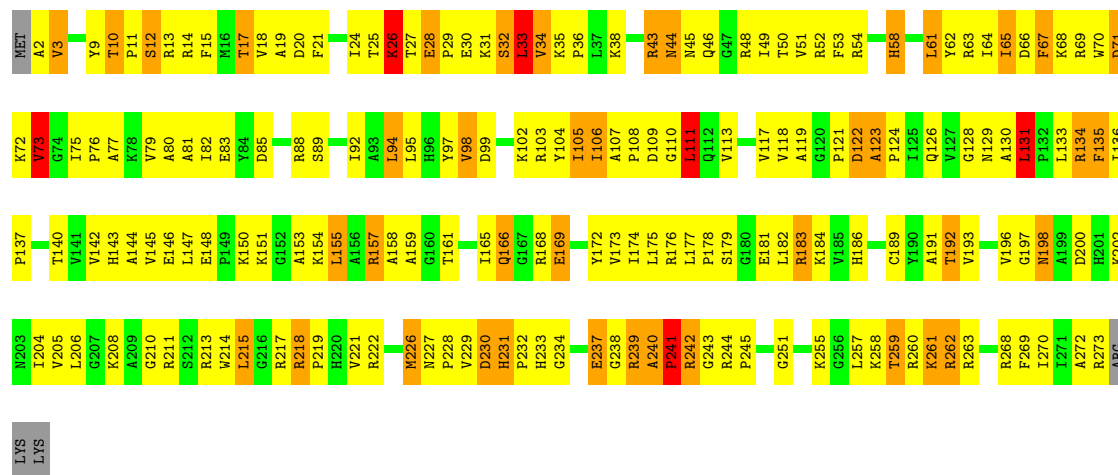
• Molecule 2: 5S rRNA

Chain B:



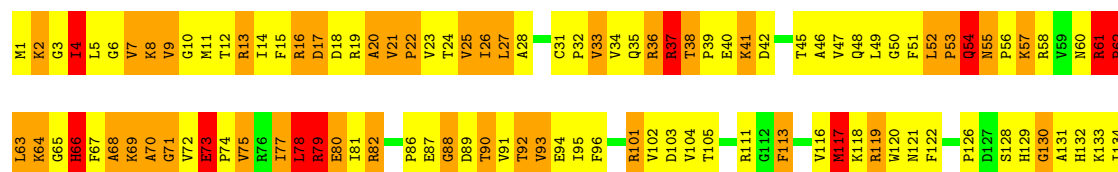
• Molecule 3: 50S ribosomal protein L2

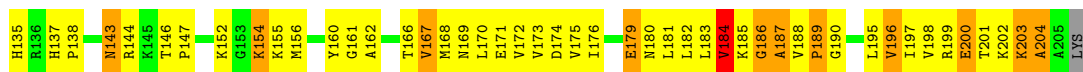
Chain D:



• Molecule 4: 50S ribosomal protein L3

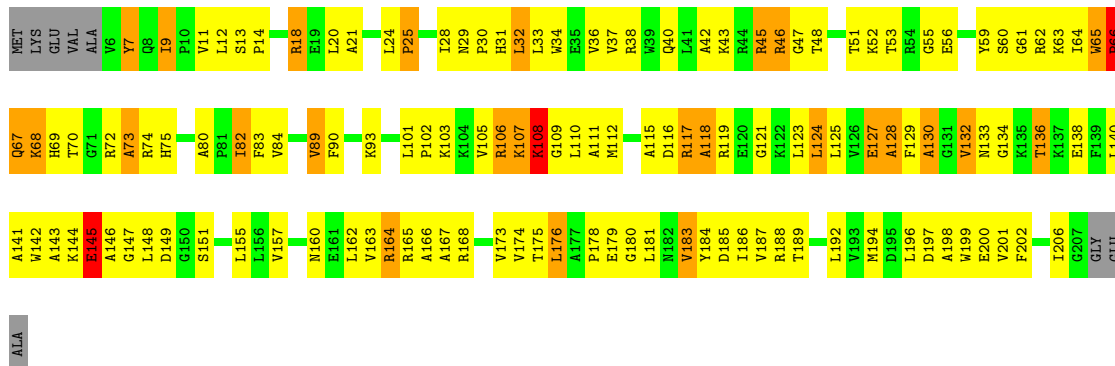
Chain E:





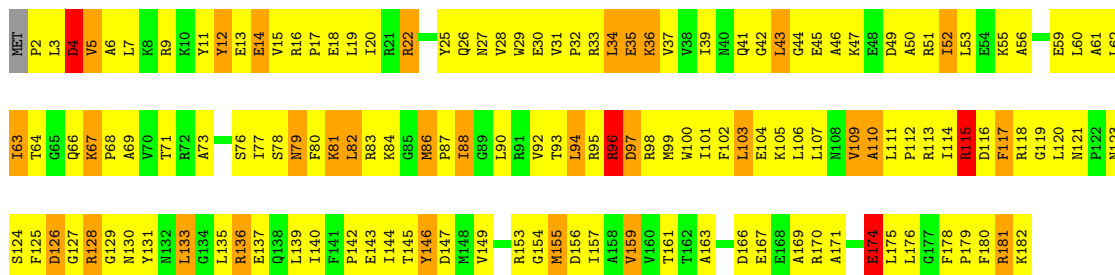
• Molecule 5: 50S ribosomal protein L4

Chain F:



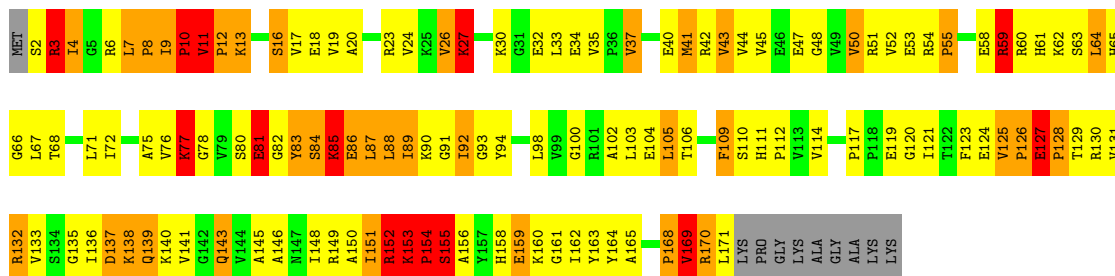
• Molecule 6: 50S ribosomal protein L5

Chain G:



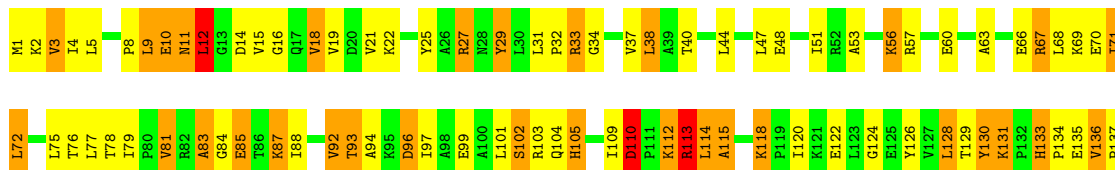
• Molecule 7: 50S ribosomal protein L6

Chain H:



• Molecule 8: 50S ribosomal protein L9

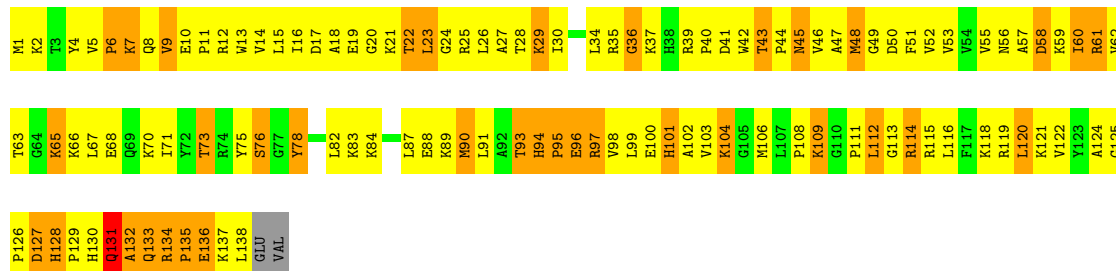
Chain I:





- Molecule 9: 50S ribosomal protein L13

Chain N:



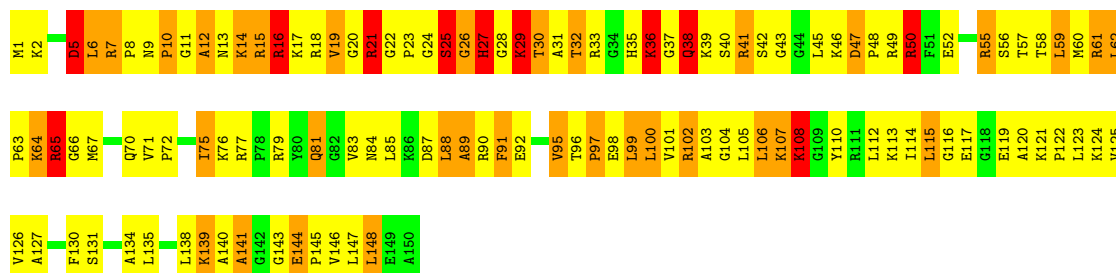
- Molecule 10: 50S ribosomal protein L14

Chain O:



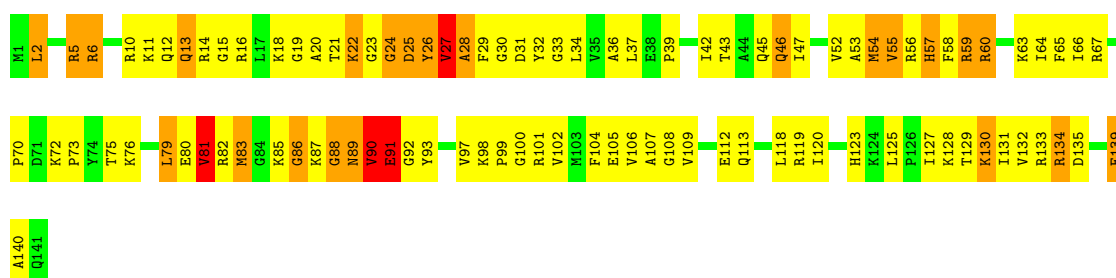
- Molecule 11: 50S ribosomal protein L15

Chain P:



- Molecule 12: 50S ribosomal protein L16

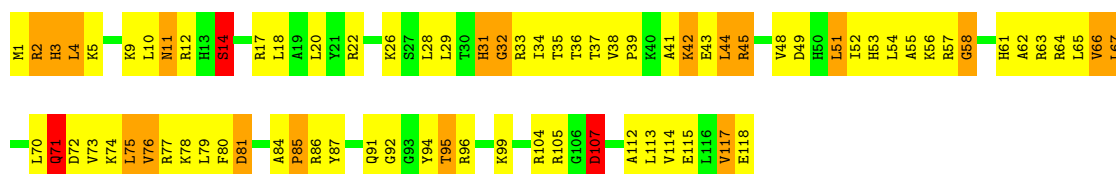
Chain Q:



- Molecule 13: 50S ribosomal protein L17

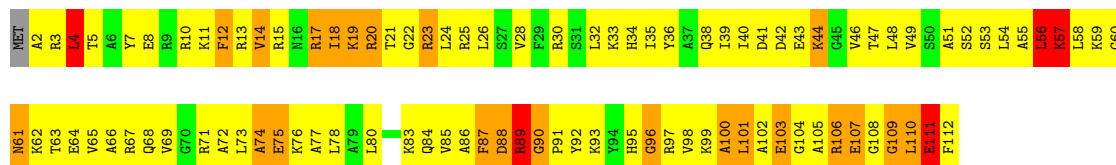
Chain R:





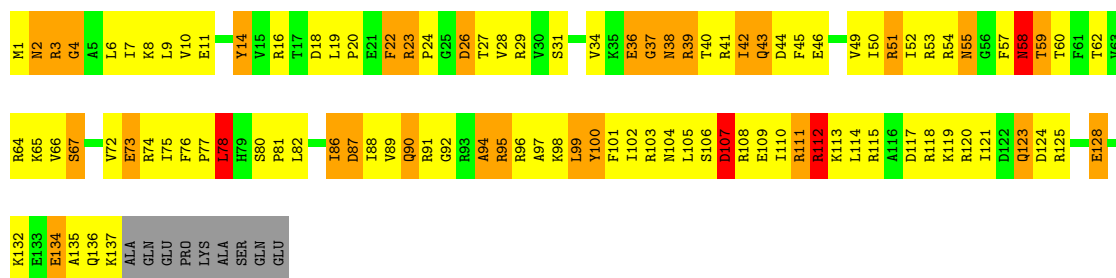
• Molecule 14: 50S ribosomal protein L18

Chain S:



• Molecule 15: 50S ribosomal protein L19

Chain T:



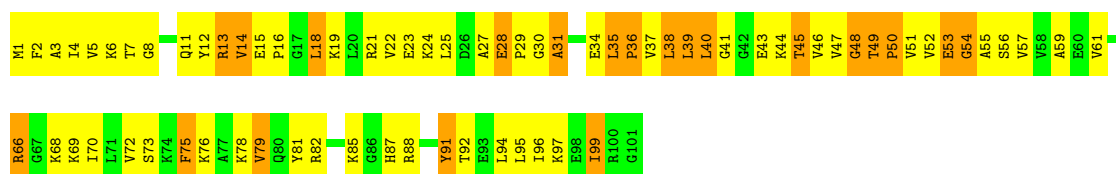
• Molecule 16: 50S ribosomal protein L20

Chain U:



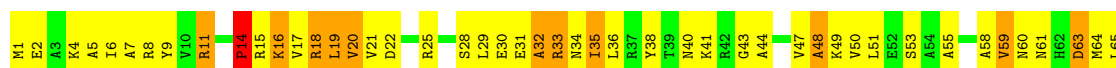
• Molecule 17: 50S ribosomal protein L21

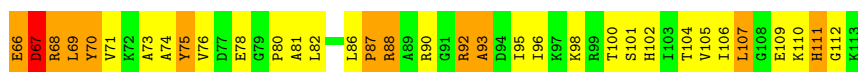
Chain V:



• Molecule 18: 50S ribosomal protein L22

Chain W:





- Molecule 19: 50S ribosomal protein L23

Chain X:



- Molecule 20: 50S ribosomal protein L24

Chain Y:



- Molecule 21: 50S ribosomal protein L25

Chain Z:



- Molecule 22: 50S ribosomal protein L27

Chain 0:



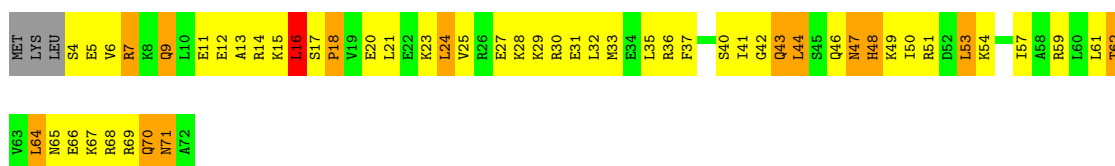
- Molecule 23: 50S ribosomal protein L28

Chain 1:



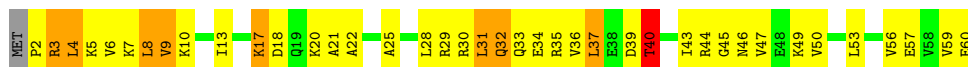
- Molecule 24: 50S ribosomal protein L29

Chain 2:



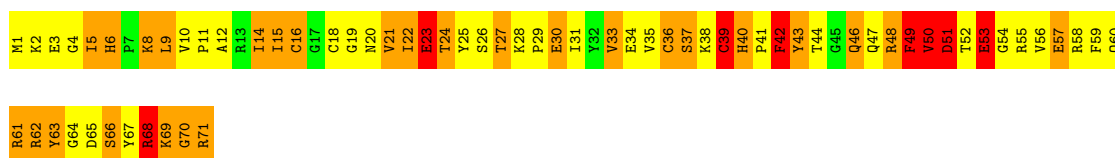
- Molecule 25: 50S ribosomal protein L30

Chain 3:



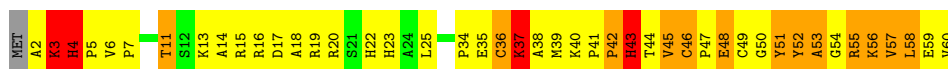
- Molecule 26: 50S ribosomal protein L31

Chain 4:



- Molecule 27: 50S ribosomal protein L32

Chain 5:



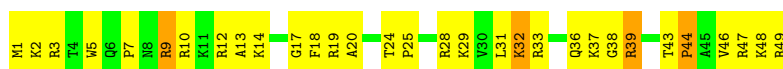
- Molecule 28: 50S ribosomal protein L33

Chain 6:



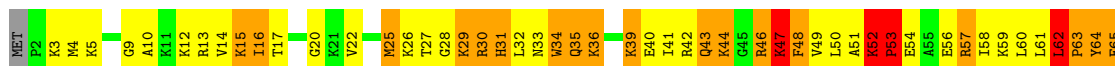
- Molecule 29: 50S ribosomal protein L34

Chain 7:



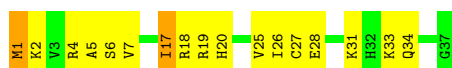
- Molecule 30: 50S ribosomal protein L35

Chain 8:



- Molecule 31: 50S ribosomal protein L36

Chain 9:



- Molecule 32: tRNA acceptor end mimic

Chain a: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.38Å 451.02Å 621.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.77 – 3.92	Depositor
% Data completeness (in resolution range)	99.7 (34.77-3.92)	Depositor
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92289	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: ZN, MG, PPU

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	1.19	254/69543 (0.4%)	1.98	3497/108563 (3.2%)
2	B	0.86	1/2878 (0.0%)	1.72	76/4490 (1.7%)
3	D	0.56	1/2165 (0.0%)	0.90	4/2919 (0.1%)
4	E	0.52	0/1601	0.91	2/2160 (0.1%)
5	F	0.50	0/1620	0.76	0/2194
6	G	0.40	0/1499	0.66	0/2016
7	H	0.45	0/1332	0.85	4/1802 (0.2%)
8	I	0.44	0/1151	0.76	0/1558
9	N	0.46	0/1131	0.78	1/1525 (0.1%)
10	O	0.53	0/943	0.71	0/1269
11	P	0.49	0/1162	0.95	3/1544 (0.2%)
12	Q	0.54	0/1143	0.90	3/1527 (0.2%)
13	R	0.45	0/982	0.80	1/1312 (0.1%)
14	S	0.45	0/892	0.82	1/1187 (0.1%)
15	T	0.47	0/1155	0.73	2/1542 (0.1%)
16	U	0.48	0/982	0.78	0/1306
17	V	0.47	0/790	0.82	0/1057
18	W	0.45	0/911	0.75	0/1220
19	X	0.56	0/739	0.77	0/993
20	Y	0.52	0/798	0.80	0/1064
21	Z	0.43	0/1493	0.70	0/2026
22	0	0.55	0/657	0.80	1/874 (0.1%)
23	1	0.49	0/770	0.85	1/1022 (0.1%)
24	2	0.51	0/583	0.83	1/771 (0.1%)
25	3	0.43	0/474	0.71	0/635
26	4	0.38	0/594	0.78	1/795 (0.1%)
27	5	0.51	0/473	0.74	0/639
28	6	0.42	0/431	0.76	0/575
29	7	0.56	0/438	0.76	0/575
30	8	0.62	0/525	0.93	1/691 (0.1%)
31	9	0.37	0/310	0.61	0/407
32	a	0.79	0/40	1.81	1/60 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
All	All	1.04	256/100205 (0.3%)	1.75	3600/150318 (2.4%)

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
21	Z	0	1

The worst 5 of 256 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	783	A	N7-C5	-11.18	1.32	1.39
1	A	793	A	N7-C5	-10.74	1.32	1.39
1	A	783	A	C5-C6	-10.48	1.31	1.41
1	A	1378	A	N9-C4	-10.25	1.31	1.37
1	A	793	A	N9-C4	-10.17	1.31	1.37

The worst 5 of 3600 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	761	A	N1-C6-N6	19.13	130.07	118.60
1	A	783	A	N1-C6-N6	16.68	128.61	118.60
1	A	783	A	C6-C5-N7	-15.94	121.15	132.30
1	A	450	G	C5-C6-N1	-15.52	103.74	111.50
1	A	783	A	C5-N7-C8	-14.97	96.41	103.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	Z	181	GLU	Peptide

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	62091	0	31293	1975	0
2	B	2573	0	1306	103	0
3	D	2115	0	2195	322	0
4	E	1568	0	1634	263	0
5	F	1585	0	1632	178	0
6	G	1474	0	1535	192	0
7	H	1307	0	1382	228	0
8	I	1136	0	1223	69	0
9	N	1104	0	1180	189	0
10	O	933	0	996	124	0
11	P	1145	0	1228	244	0
12	Q	1122	0	1178	165	0
13	R	968	0	1033	117	0
14	S	882	0	943	159	0
15	T	1141	0	1202	151	0
16	U	964	0	1022	142	0
17	V	779	0	852	131	0
18	W	900	0	964	108	0
19	X	725	0	778	74	0
20	Y	785	0	878	160	0
21	Z	1461	0	1493	86	0
22	0	648	0	672	50	0
23	1	763	0	848	142	0
24	2	581	0	629	78	0
25	3	469	0	518	46	0
26	4	581	0	574	133	0
27	5	459	0	480	76	0
28	6	424	0	450	97	0
29	7	430	0	480	40	0
30	8	517	0	582	105	0
31	9	307	0	336	24	0
32	a	74	0	51	0	0
33	5	1	0	0	0	0
33	7	1	0	0	0	0
33	A	269	0	0	1	0
33	B	3	0	0	0	0
33	E	1	0	0	0	0
33	P	1	0	0	0	0
33	Q	1	0	0	0	0
34	9	1	0	0	0	0
All	All	92289	0	61567	5449	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 36.

The worst 5 of 5449 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	1.52
23:1:81:LYS:NZ	23:1:81:LYS:HA	1.42	1.34
23:1:81:LYS:HE2	23:1:81:LYS:N	1.50	1.26
7:H:127:GLU:HG2	7:H:128:PRO:CD	1.70	1.21
7:H:127:GLU:CB	7:H:128:PRO:HD3	1.69	1.20

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%)	204 (76%)	47 (17%)	19 (7%)	2	33
4	E	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	3
5	F	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	20
6	G	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	15
7	H	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	2
8	I	144/148 (97%)	93 (65%)	30 (21%)	21 (15%)	0	9
9	N	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	7
10	O	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	30
11	P	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	3
12	Q	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	20
13	R	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	14
14	S	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	6
15	T	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	9
16	U	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	V	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	20
18	W	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	13
19	X	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	40
20	Y	100/110 (91%)	57 (57%)	16 (16%)	27 (27%)	0	1
21	Z	181/206 (88%)	128 (71%)	36 (20%)	17 (9%)	1	23
22	0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	3	43
23	1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	15
24	2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	11
25	3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	41
26	4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
27	5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	2
28	6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	1
29	7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	36
30	8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	5
31	9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3379/3526 (96%)	2262 (67%)	648 (19%)	469 (14%)	0	10

5 of 469 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	26	LYS
3	D	28	GLU
3	D	123	ALA
3	D	231	HIS
4	E	4	ILE

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%)	178 (83%)	36 (17%)	3	24
4	E	165/166 (99%)	127 (77%)	38 (23%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	161/166 (97%)	140 (87%)	21 (13%)	6	38
6	G	155/156 (99%)	130 (84%)	25 (16%)	3	27
7	H	142/148 (96%)	114 (80%)	28 (20%)	2	15
8	I	122/124 (98%)	92 (75%)	30 (25%)	1	8
9	N	117/119 (98%)	98 (84%)	19 (16%)	3	26
10	O	100/100 (100%)	90 (90%)	10 (10%)	11	52
11	P	116/116 (100%)	89 (77%)	27 (23%)	1	9
12	Q	111/111 (100%)	93 (84%)	18 (16%)	3	26
13	R	101/101 (100%)	84 (83%)	17 (17%)	3	24
14	S	87/88 (99%)	74 (85%)	13 (15%)	4	30
15	T	120/127 (94%)	97 (81%)	23 (19%)	2	16
16	U	93/94 (99%)	80 (86%)	13 (14%)	5	34
17	V	82/82 (100%)	71 (87%)	11 (13%)	6	36
18	W	92/92 (100%)	77 (84%)	15 (16%)	3	26
19	X	74/78 (95%)	63 (85%)	11 (15%)	4	30
20	Y	85/91 (93%)	70 (82%)	15 (18%)	3	21
21	Z	162/179 (90%)	131 (81%)	31 (19%)	2	16
22	0	65/67 (97%)	58 (89%)	7 (11%)	9	48
23	1	82/83 (99%)	67 (82%)	15 (18%)	2	18
24	2	64/67 (96%)	57 (89%)	7 (11%)	9	47
25	3	51/52 (98%)	40 (78%)	11 (22%)	1	11
26	4	63/63 (100%)	44 (70%)	19 (30%)	0	5
27	5	51/52 (98%)	39 (76%)	12 (24%)	1	9
28	6	48/52 (92%)	38 (79%)	10 (21%)	2	13
29	7	42/42 (100%)	39 (93%)	3 (7%)	21	68
30	8	54/55 (98%)	39 (72%)	15 (28%)	0	6
31	9	34/34 (100%)	32 (94%)	2 (6%)	28	75
All	All	2853/2923 (98%)	2351 (82%)	502 (18%)	3	21

5 of 502 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	88	LEU

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Mol	Chain	Res	Type
14	S	111	GLU
27	5	11	THR
11	P	146	VAL
13	R	37	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
11	P	84	ASN
16	U	49	HIS
25	3	19	GLN
15	T	55	ASN
16	U	94	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2880/2916 (98%)	865 (30%)	93 (3%)
2	B	119/122 (97%)	42 (35%)	2 (1%)
32	a	1/3 (33%)	0	0
All	All	3000/3041 (98%)	907 (30%)	95 (3%)

5 of 907 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	14	A
1	A	15	G
1	A	26	G
1	A	34	C

5 of 95 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1109	C
1	A	1558	A
1	A	2751	G
1	A	1130	U
1	A	1210	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
32	PPU	a	76	1,32	38,40,41	2.42	8 (21%)	54,57,60	2.60	14 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PPU	a	76	1,32	-	0/26/43/44	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	76	PPU	O-C	9.16	1.41	1.23
32	a	76	PPU	C9-N6	-5.37	1.32	1.45
32	a	76	PPU	C-N3'	5.36	1.46	1.34
32	a	76	PPU	C10-N6	-5.15	1.32	1.45
32	a	76	PPU	C4-N9	-3.09	1.33	1.37

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	76	PPU	N3-C2-N1	-8.54	121.38	128.89
32	a	76	PPU	C3'-N3'-C	-8.16	110.20	123.19
32	a	76	PPU	C5-C4-N3	-6.27	119.87	125.98
32	a	76	PPU	C2'-C1'-N9	-5.49	98.40	113.35
32	a	76	PPU	C2'-C3'-N3'	5.17	125.07	113.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 278 ligands modelled in this entry, 278 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.

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.