



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:06 AM GMT

PDB ID : 2VHN
Title : STRUCTURE OF PDF BINDING HELIX IN COMPLEX WITH THE RIBOSOME. (PART 2 OF 4)
Authors : Bingel-Erlenmeyer, R.; Kohler, R.; Kramer, G.; Sandikci, A.; Antolic, S.; Maier, T.; Schaffitzel, C.; Wiedmann, B.; Bukau, B.; Ban, N.
Deposited on : 2007-11-22
Resolution : 3.74 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>

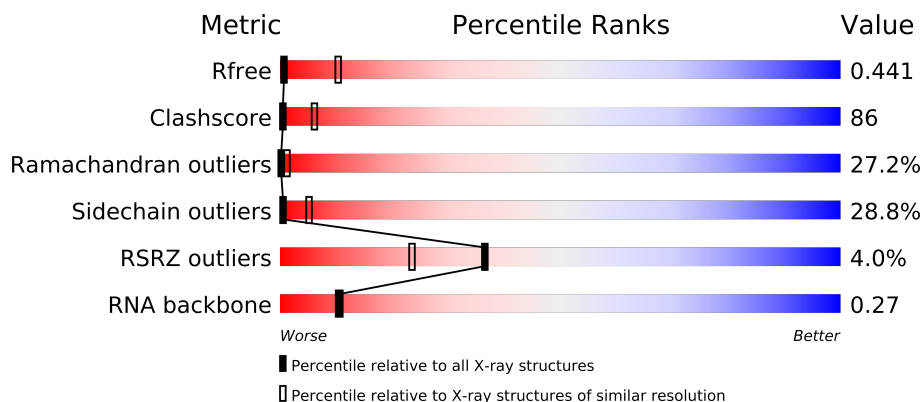
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 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 3.74 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	1103 (4.04-3.40)
Clashscore	79885	1072 (4.00-3.48)
Ramachandran outliers	78287	1023 (4.00-3.48)
Sidechain outliers	78261	1016 (4.00-3.48)
RSRZ outliers	66119	1104 (4.04-3.40)
RNA backbone	1838	1008 (4.52-2.80)

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.

Mol	Chain	Length	Quality of chain
1	0	56	
2	1	54	
3	2	46	
4	3	64	
5	4	38	
6	A	120	
7	B	2904	
8	C	273	
9	D	209	
10	E	201	
11	F	178	
12	G	176	

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Mol	Chain	Length	Quality of chain
13	H	149	
14	I	141	
15	J	142	
16	K	123	
17	L	144	
18	M	136	
19	N	127	
20	O	117	
21	P	114	
22	Q	117	
23	R	103	
24	S	110	
25	T	100	
26	U	103	
27	V	94	
28	W	84	
29	X	63	
30	Y	58	
31	Z	70	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	Z	4001	-	X
32	MG	Z	4012	-	X
32	MG	Z	4013	-	X
32	MG	Z	4027	-	X
32	MG	Z	4028	-	X
32	MG	Z	4031	-	X
32	MG	Z	4038	-	X
32	MG	Z	4039	-	X
32	MG	Z	4040	-	X
32	MG	Z	4051	-	X
32	MG	Z	4059	-	X
32	MG	Z	4063	-	X
32	MG	Z	4065	-	X
32	MG	Z	4069	-	X
32	MG	Z	4074	-	X
32	MG	Z	4076	-	X
32	MG	Z	4078	-	X
32	MG	Z	4079	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	Z	4082	-	X
32	MG	Z	4083	-	X
32	MG	Z	4090	-	X
32	MG	Z	4095	-	X
32	MG	Z	4100	-	X
32	MG	Z	4102	-	X
32	MG	Z	4105	-	X
32	MG	Z	4108	-	X
32	MG	Z	4109	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 90314 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 protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 7 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	B	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	268	Total	C	N	O	S	0	0	1
			2054	1271	417	359	7			

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	J	141	Total	C	N	O	S	0	0	1
			1113	704	211	194	4			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	K	122	Total	C	N	O	S	0	0	1
			931	582	180	164	5			

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	T	100	Total	C	N	O	S	0	0	1
			778	491	146	139	2			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	U	103	Total	C	N	O		0	0	1
			780	492	147	141				

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L31.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	Z	111	Total	Mg	0	0
			111	111		

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	1	Total	O	0	0
			1	1		
33	2	2	Total	O	0	0
			2	2		
33	B	485	Total	O	0	0
			485	485		
33	C	3	Total	O	0	0
			3	3		
33	D	1	Total	O	0	0
			1	1		
33	E	2	Total	O	0	0
			2	2		

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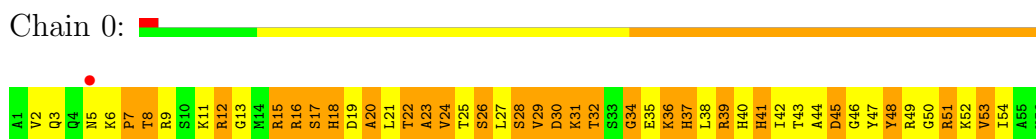
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	J	1	Total 1	O 1	0	0
33	K	1	Total 1	O 1	0	0
33	L	4	Total 4	O 4	0	0
33	N	4	Total 4	O 4	0	0
33	Q	1	Total 1	O 1	0	0
33	T	2	Total 2	O 2	0	0
33	U	1	Total 1	O 1	0	0

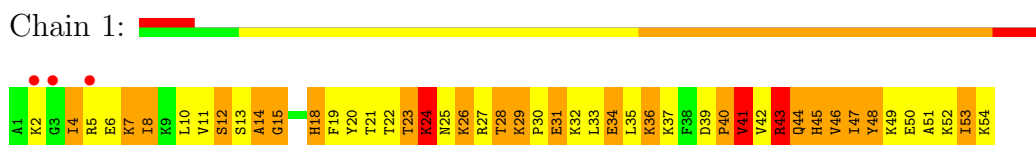
3 Residue-property plots

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 ($RSRZ > 2$). 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.

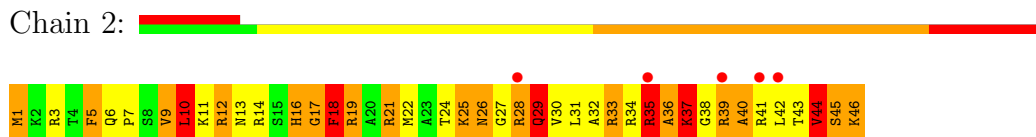
- Molecule 1: 50S RIBOSOMAL PROTEIN L32



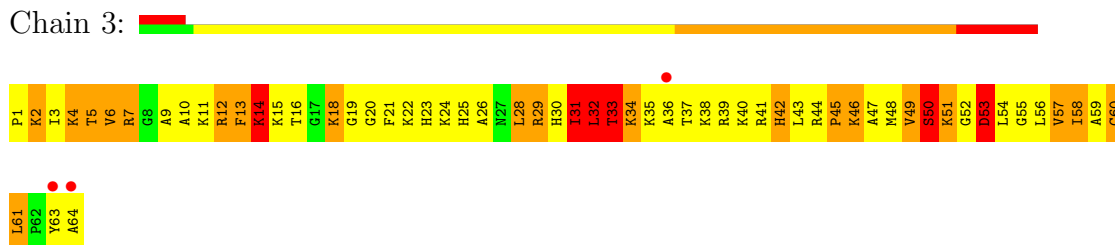
- Molecule 2: 50S RIBOSOMAL PROTEIN L33



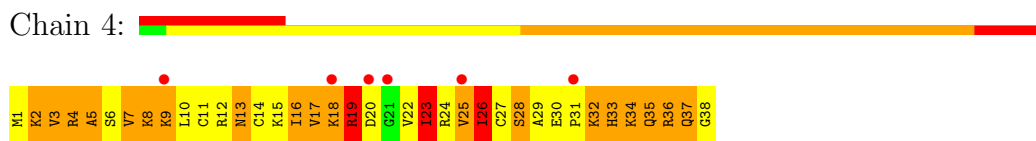
- Molecule 3: 50S RIBOSOMAL PROTEIN L34



- Molecule 4: 50S RIBOSOMAL PROTEIN L35

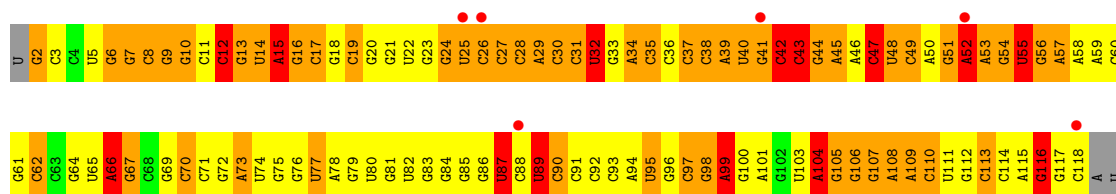


- Molecule 5: 50S RIBOSOMAL PROTEIN L36



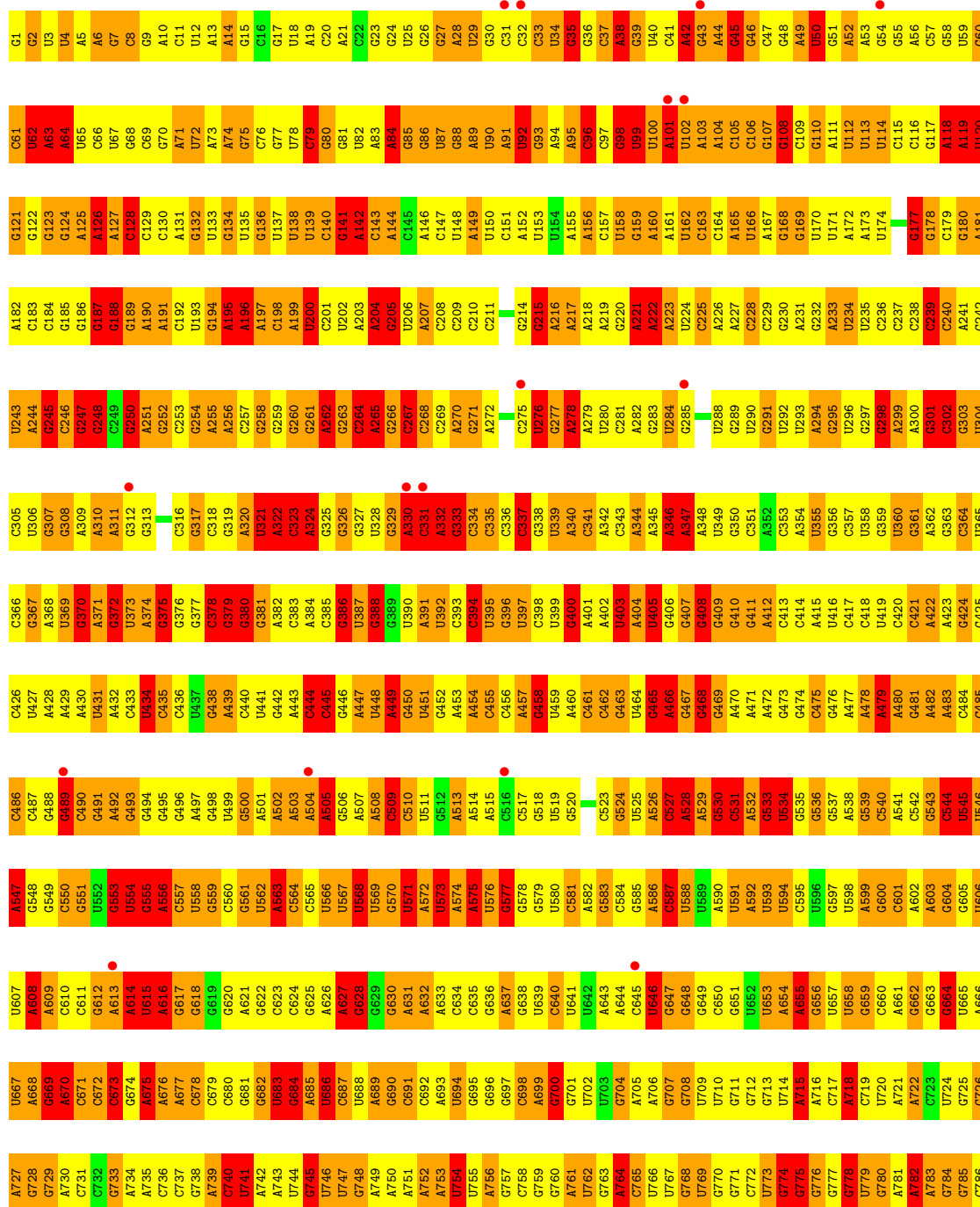
- Molecule 6: 5S RIBOSOMAL RNA





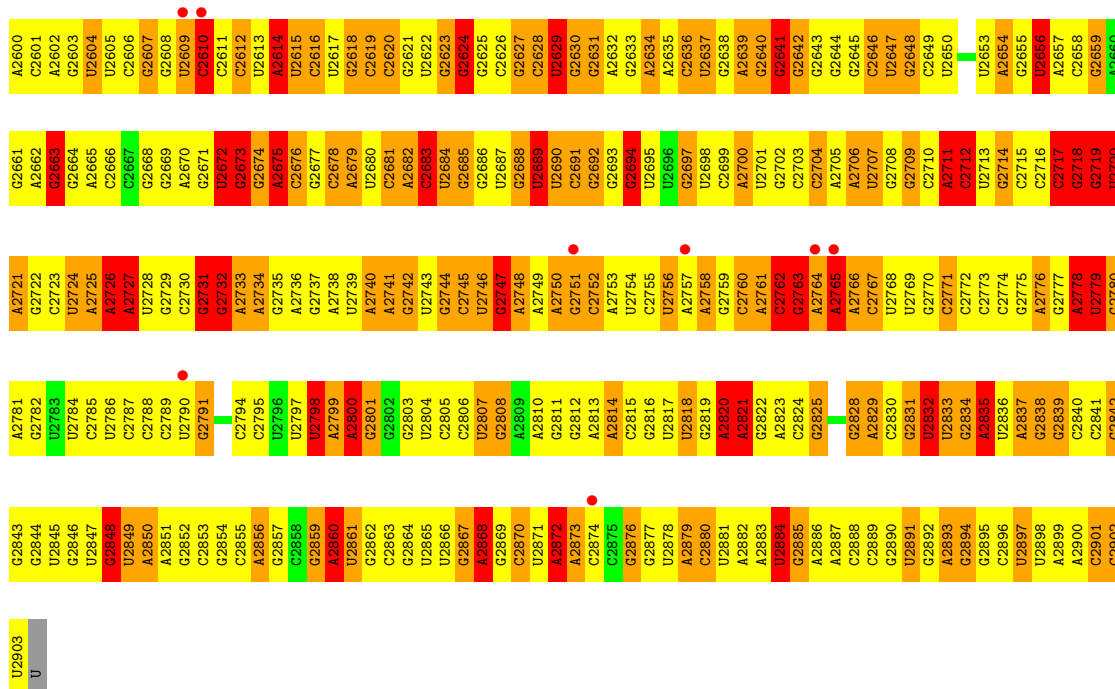
• Molecule 7: 23S RIBOSOMAL RNA

Chain B:



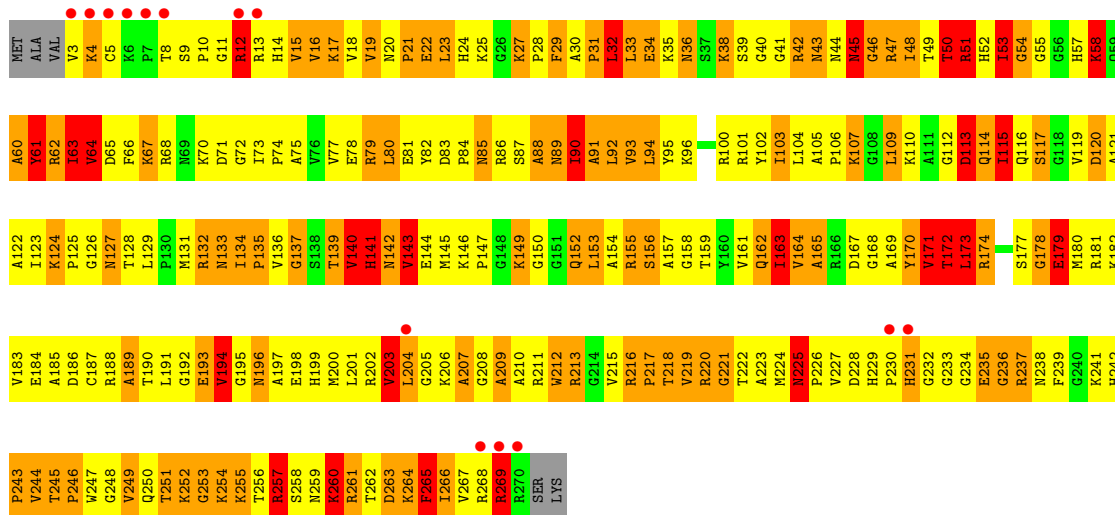
A1634	C1574	G1514	G1450	U1390	C1330	G1270	G1210	G1149	A1088	A1027	U967	G907	U847	C787
A1635	C1575	A1515	C1461	U1391	G1331	G1271	C1211	C1150	A1089	A1028	C968	C908	C848	A788
U1636	U1576	G1516	C1452	A1392	G1332	A1272	G1212	A1151	G1091	A1029	C969	C909	C849	A789
A1637	C1577	G1517	G1453	A1393	G1333	U1273	A1213	C1152	G1092	C1030	U970	A1090	U850	U790
C1638	U1578	C1518	C1454	A1394	G1334	A1274	A1214	C1153	G1093	G1031	C851	C912	C851	C791
C1639	U1579	G1519	G1455	A1395	C1335	A1275	G1215	C1154	G1094	A1032	A972	C912	U852	A792
A1640	A1580	U1520	G1456	U1396	A1336	A1276	G1216	A1155	U1094	U1033	A973	U913	C853	A793
A1641	G1581	G1521	U1457	U1397	G1337	G1277	U1217	A1156	A1095	G1034	G874	C914	C854	A794
G1642	A1522	A1522	U1458	C1398	G1338	C1278	G1218	A1157	A1096	U1035	A975	C915	G855	
G1643	U1583	U1523	G1459	C1399	G1339	G1279	U1219	C1158	U1097	G1036	A976	C916	G856	
G1644	U1584	G1524	U1460	U1400	U1340	G1280	G1220	C1159	A1098	G1037	G977	A917	G857	C797
G1645	C1585	A1525	C1461	G1401	G1341	G1281	C1221	C1160	G1099	G1038	G878	A918	G858	G798
C1646	C1526	C1526	C1462	U1402	A1342	U1282	U1222	C1161	C1100	A1039	A979	U919	G859	G799
U1647	G1587	G1527		A1403	G1343	G1283	G1223	G1162	U1101	A1040	A880	A920	U860	A800
U1648	U1588	A1528	G1465	C1404	G1344	A1284	U1224	G1163	C1102	G1041	A981	C921	A861	G801
G1649	U1589	A1529	U1466	U1405	C1345	A1285	G1225	C1164	A1103	G1042	C982	C922	G862	A802
A1650	A1590	G1530		U1406	G1346	A1286	A1226	A1165	C1104	C1043	A983	G923	A863	U803
G1651	A1591	C1531	A1469	G1407	A1347	A1287	G1227	G1166	U1105	C1044	A984	G924	G864	A804
A1652	C1592	A1532	A1470	G1408	C1348	G1288	G1228	C1167	G1106	C1045	C985	A925	C865	G805
G1653	A1593	G1533	G1471	U1409	C1349	C1289	C1229	G1168	G1107	A1046	C986	G926	A866	C806
A1654	U1594	U1534	G1472	G1410	C1350	C1290	A1230	A1169	U1108	G1047	C987	A927	C867	U807
A1655	C1595	A1535	G1473	U1411	C1351	G1291	U1231	C1170	C1109	A1048	A988	A928	U868	G808
C1656	A1596	C1536	U1474	U1412	U1352	G1292	G1232	G1171	G1110	C1049	G989	U929	U869	G809
U1657	A1597	G1537	G1475	A1413	C1353	C1293	C1233	C1172	A1111	A1050	A990	G930	U870	U810
C1658	A1598	G1538	U1476	A1414	A1354	U1294	U1234	U1173	G1112	G1051	C991	U931	U871	U811
G1659	U1599	U1539	A1477	U1415	G1355	C1295	G1235	U1174	U1113	C1052	C992	U932	U872	C812
G1660	C1600	G1540	G1478	G1416	G1356	G1296	G1236	A1175	C1114	G1053	G993	A933	C873	U813
G1661	G1601	C1541	G1479	C1417	C1357	U1297	A1237	U1176	G1115	A1054	C994	A941	G874	C814
U1662	U1602	U1542	C1480	G1418	G1358	C1298	G1238	G1177	G1116	G1055	C995	C935	C875	C815
G1663	A1603	G1543	U1481	A1419	A1359	G1299	G1239	C1178	C1117	G1056	A996	A936	C876	C816
A1664	C1604	A1544	G1482	A1420	G1360	G1300	U1240	C1179	C1118	A1057	C997	C937	A877	C817
A1665	C1605	A1545	G1483	G1421	G1361	A1301	A1241	U1180	U1119	U1058	C998	G938	A878	G818
G1666	C1606	G1546	U1484	G1422	C1362	A1302	U1242	U1181	G1120	G1059	U999	G939	G	A819
G1667	G1607	C1547	U1485	G1423	G1363	G1303	C1243	G1182	C1121	U1060	A1000	A941	G	A820
A1668	A1608	A1548	U1486	G1424	G1364	A1304	A1244	U1183	G1122	U1061	A1001	G942	G	A821
A1669	A1609	A1549	U1487	G1425	A1365	C1305	G1245	U1184	C1123	G1062	G1002	G943	G	G822
C1670	A1610	C1550	G1488	G1426	A1366	C1306	A1246	G1185	G1124	G1063	G1003	A943	G	C823
U1671	C1611	A1551	C1489	A1427	A1367	A1307	A1247	G1186	G1125	C1064	U1004	C944	U	U824
A1672	G1612	A1552	A1490	C1428	G1368	A1308	G1248	G1187	A1126	U1065	C1005	A945	C	A825
G1673	G1613	A1553	G1491	G1429	G1369	A1309	U1249	U1188	A1127	U1066	C1006	C946	A	U826
G1674	A1614	U1554	G1492	G1430	C1370	G1310	G1250	A1189	G1128	A1067	C1007	A947	U	U827
C1675	C1615	G1555	G1493	A1431	G1371	G1311	C1251	G1190	A1129	G1068	A1008	C948	C	U828
A1676	A1616	C1556	A1494	G1432	U1372	U1312	G1252	G1191	U1130	A1069	A1009	G949	C	A829
A1677	C1617	C1557	A1495	A1433	A1373	U1313	A1253	G1192	G1131	A1070	A1010	G950	C	G830
A1678	A1618	C1558	A1496	A1434	G1374	C1314	A1254	G1193	U1132	G1071	G1011	C951	G	G831
A1679	G1619	U1559	U1497	G1435	U1375	C1315	U1255	A1194	A1133	C1072	U1012	G952	A	U832
U1680	G1620	G1560	C1498	G1436	C1376	U1316	G1256	G1195	A1134	A1073	C	G953	C	A833
G1681	U1621	C1561	C1499	C1437	G1377	G1317	C1257	C1196	C1135	G1074	A1014	G954	U	G834
G1682	G1622	U1562		U1438	A1378	U1318	U1258	G1197	G1136	C1075	U1015	U955	U	C835
U1683	G1623	U1563	A1503	A1439	U1379	C1319	G1259	U1198	G1137	C1076	G1016	G956	A	G836
G1684	U1624	C1564	A1504	U1440	G1380	C1320	A1260	U1199	G1138	A1077	G1017	C957	C	C837
C1685	C1625	C1565	A1505	G1441	G1381	A1321	A1261	U1200	G1139		G898	C958	C838	
G1686	A1626	U1566	U1506	U1442	G1382	A1322	A1262	C1201	C1140	A1080	U1018	U958	C839	
G1687	G1627	G1567	C1507	U1443	A1383	C1323	U1263	U1202	U1141	U1081	A1020	A959	U839	
U1688	G1628	G1568	A1508	G1444	A1384	G1324	A1264	G1203	A1142	U1082	A1021	C961	A900	C840
	U1629	A1569	A1509	G1445	A1385	U1325	A1265	U1204	A1143	U1083	G1022	G962	C901	C841
	A1630	A1570	G1510	C1446	C1386	U1326	G1266	A1205	A1144	A1084	U1023	U963	C903	G843
	G1691		G1511	C1447	A1387	U1327	U1267	G1206		A1085	G1024	C964	G904	A844
U1692	A1631	A1571	C1512	G1448	G1388	A1328	U1268	C1207	A1147	A1086	G1025	C965	A905	A845
U1693	C1633	G1573	U1513	G1449	G1389	U1329	A1269		U1148	G1087	G1026	G966	U906	U846

C2539	U2479	U2419	C2559	U2299	G2239	C2179	A	A2059	C1999	A1877	A1815	A1755	G1895
C2540	C2480	C2420	G2560	C2300	U2240	U2160	G	U1939	G1878	G1878	C1816	G1755	G1896
A2541	G2481	G2421	G2361	C2301	A2241	U2181	G	U1940	C1879	A1757	G1817	G1756	G1897
A2542	A2542	C2422	C2362	U2302	G2242	U2182	U	C1941	A2662	U1758	U1818	U1757	U1698
G2543	C2483	U2423	G2363	G2303	U2243	A2183	G	C1942	C1881	C1881	A1819	U1758	A1699
G2544	C2484	U2424	G2364	G2304	U2244	A2184	G	U1943	U1882	C1760	U1820	C1760	A1700
G2545	A2425	A2425	G2365	U2305	U2245	U2185	G	U1944	U1883	C1761	U1821	C1761	A1701
G2546	A2426	A2426	A2366	C2306	G2246	U2186	G	G1945	G1884	A1762	C1822	A1762	G1702
A2547	G2487	G2427	G2367	G2307	A2247	U2187	G	U1946	A1885	G1763	G1823	G1763	G1703
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G2549	U2489	G2429	A2369	A2309	U2249	U2189	C	G1948	U1887	U1765	U1825	U1765	A1705
G2550	G2490	U2430	G2370	C2310	G2250	G2190	U	G1949	G1888	G1766	G1826	G1766	G1706
G2551	U2491	U2431	G2371	A2311	G2251	A2071	U	G1950	A1889	G1767	U1827	G1767	G1707
U2552	U2492	A2432	U2372	U2312	G2252	U2192	U	U1951	A1890	C1768	G1828	C1768	C1708
G2553	U2493	A2433	G2373	C2313	G2253	U2193	G2183	A1952	G1891	U1769	A1829	U1769	U1709
G2554	G2494	A2434	G2374	A2314	C2254	U2194	A2134	A1953	C1892	G1770	C1830	G1770	G1710
G2555	G2495	A2435	G2375	G2315	G2255	U2195	A2135	G1954	U1956	C1771	G1831	C1771	A1711
G2556	G2496	A2436	A2376	G2316	G2256	C2196	A2136	U1955	C1995	A1772	C1832	A1772	U1712
G2557	A2497	G2437	A2377	A2317	U2257	U2197	U2137	U1956	G1996	C1773	C1833	C1773	A1713
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C2559	A2499	A2439	G2379	G2319	U2259	A2199	U2139	C1958	U1999	U1775	G1835	U1775	G1715
A2560	U2500	C2440	C2380	U2320	C2260	C2200	G2140	A1959	A1999	G1776	C1836	G1776	U1716
U2561	C2501	U2441	A2381	U2321	C2261	G2201	A2141	A1960	A1900	U1777	C1837	U1777	A1717
U2562	G2502	C2442	G2382	A2322	U2262	U2202	A2142	A1961	U1901	U1778	C1838	U1778	G1718
U2563	G2503	C2443	G2383	G2323	C2263	U2203	C2143	C1962	C1902	G1779	G1839	U1779	G1719
A2564	A2503	C2443	U2384	U2324	C2264	G2204	G2144	G1964	G1903	U1780	G1840	U1780	U1720
A2565	U2504	G2444	C2385	G2325	U2265	A2205	C2145	C1965	G1904	U1781	G1841	U1781	G1721
A2566	G2505	G2445	C2386	G2326	U2266	C2206	C2146	A1966	C1905	U1782	G1842	U1782	A1722
G2567	U2506	G2446	A2387	C2327	A2267	C2207	A2147	C1967	G1906	A1783	C1843	A1783	G1723
U2568	G2507	G2447	U2388	A2327	U2267	C2208	G2148	C1968	G1907	G1784	C1844	G1784	G1724
G2569	C2508	A2448	A2389	U2328	G2269	G2209	U2149	A1969	C1908	A1785	G1845	U1785	U1725
G2570	G2509	U2449	G2390	G2330	G2270	U2210	C2150	A1970	C1909	A1786	G1846	A1786	G1726
U2571	C2510	A2450	G2391	G2331	G2271	A2211	U2151	U1971	G1910	U1787	A1847	U1787	C1727
A2572	U2511	A2451	C2392	C2332	U2272	U2212	G2152	G1972	U1911	C1788	G1848	C1788	U1728
C2573	C2512	C2452	U2393	A2333	A2273	U2213	C2153	G1973	A1912	U1789	G1849	U1789	U1729
G2574	A2513	C2453	U2394	U2334	A2274	C2214	A2154	C1974	A1913	C1790	G1850	C1790	G1730
C2575	U2514	G2454	C2395	A2335	C2275	C2215	U2155	G1975	C1914	A1791	G1851	G1791	G1731
G2576	C2515	G2455	G2396	A2336	G2276	G2216	G2156	U1976	U1915	G1792	C1853	G1792	C1732
A2577	A2516	C2456	G2397	G2337	G2277	G2217	A	A1977	U1916	C1793	A1854	C1793	G1733
G2578	C2517	U2457	U2398	C2338	A2278	G2218	G	A1978	U1917	G1794	U1855	A1794	G1734
C2579	A2518	G2458	U2399	C2339	G2279	U2219	C	U1979	A1918	C1795	U1856	C1795	A1735
U2580	U2519	A2459	G2400	A2340	G2280	U2220	C	G1980	A1919	U1796	G1857	U1796	U1736
G2581	C2520	U2460	G2401	G2341	A2281	G2221	C	A1981	G1920	G1797	G1858	G1797	G1737
C2582	U2521	A2461	U2401	C2342	G2282	C2222	A	U1982	C1921	U1798	G1859	U1798	G1738
G2583	G2522	C2462	U2402	U2343	G2283	G2223	G	G1983	G1922	G1799	G1861	G1799	A1739
U2584	G2523	C2463	C2403	U2344	A2284	G2224	C	G1984	U1923	C1800	G1862	C1800	G1740
U2585	G2524	G2464	U2404	G2345	C2285	A2225	C	C1985	C1924	G1801	G1863	G1801	C1741
U2586	G2525	C2465	G2405	G2346	G2286	U2226	U	C1986	C1925	A1802	U1864	A1802	U1742
A2587	G2526	C2466	A2406	A2346	G2287	C2227	U	A1987	U1926	G1803	U1865	G1803	G1743
G2588	C2527	C2467	A2407	U2347	A2287	G2228	U	G1988	U1927	A1804	C1804	A1744	A1744
U2589	U2528	A2468	U2408	U2348	A2288	G2229	G	G1989	A1928	A1805	G1867	A1805	A1745
A2590	G2529	A2469	G2409	G2349	G2290	U2230	A	C1990	G1929	C1806	G1868	C1806	A1746
G2591	A2530	G2470	G2410	C2350	C2291	U2231	A	G1991	G1930	G1807	G1869	G1807	U1747
G2592	A2531	A2471	A2411	G2351	U2291	C2232	U	A2052	U1931	C1808	C1870	A1808	U1748
U2593	G2532	G2472	A2412	A2352	U2292	G2233	U	G1992	U1932	A1809	C1871	A1809	A1749
C2594	G2533	G2473	G2413	G2353	G2293	U2234	C	G1993	A1933	A1810	A1871	A1810	G1750
G2595	U2534	U2474	G2414	C2354	G2294	G2235	C	C1994	G1934	G1811	A1872	G1811	U1751
G2596	C2475	C2475	G2415	G2355	C2295	G2236	C	U1995	C1935	U1812	G1873	G1812	U1752
G2597	G2536	A2476	C2416	U2356	U2296	U2237	A	C1996	A1936	G1813	C1874	G1813	C1752
A2598	U2537	U2477	G2417	G2357	A2297	C2237	C	C1997	A1937	G1814	A1876	G1814	A1754
G2599	C2538	A2478	A2418	A2358	A2298	G2238	C	A1998	U1937				



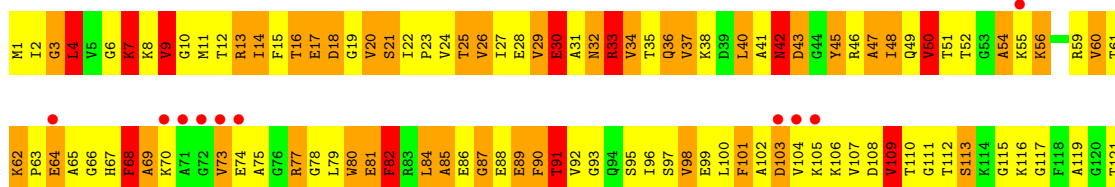
• Molecule 8: 50S RIBOSOMAL PROTEIN L2

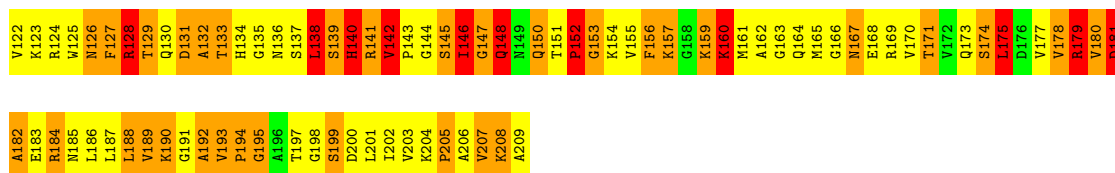
Chain C:



• Molecule 9: 50S RIBOSOMAL PROTEIN L3

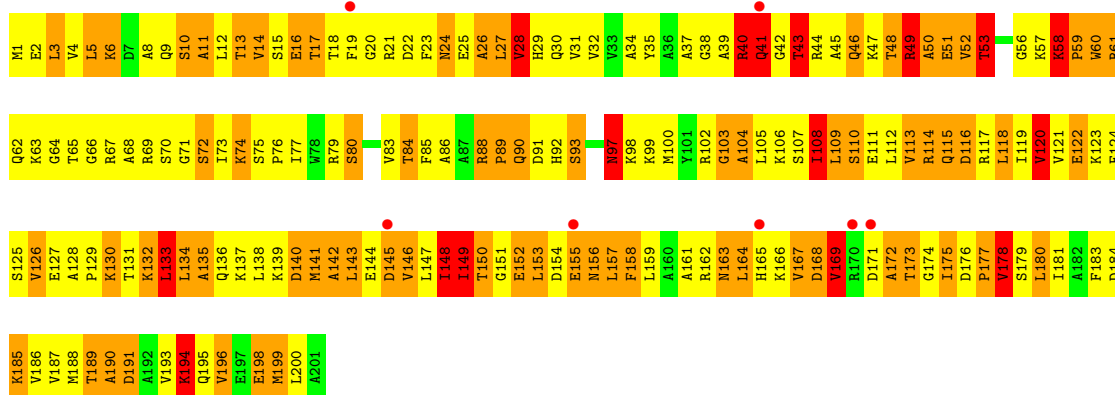
Chain D:





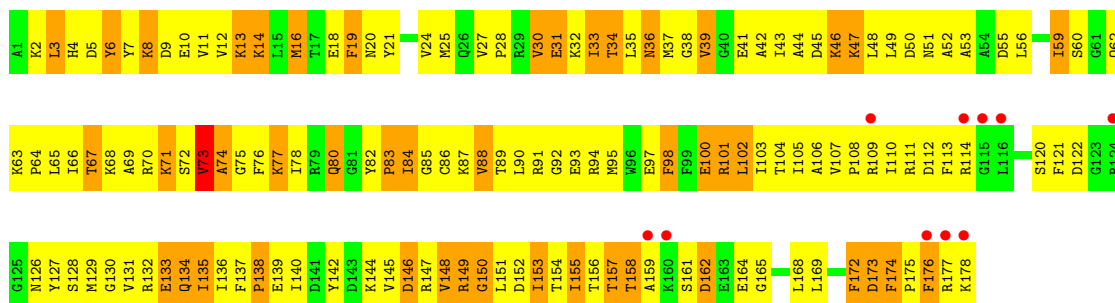
• Molecule 10: 50S RIBOSOMAL PROTEIN L4

Chain E:



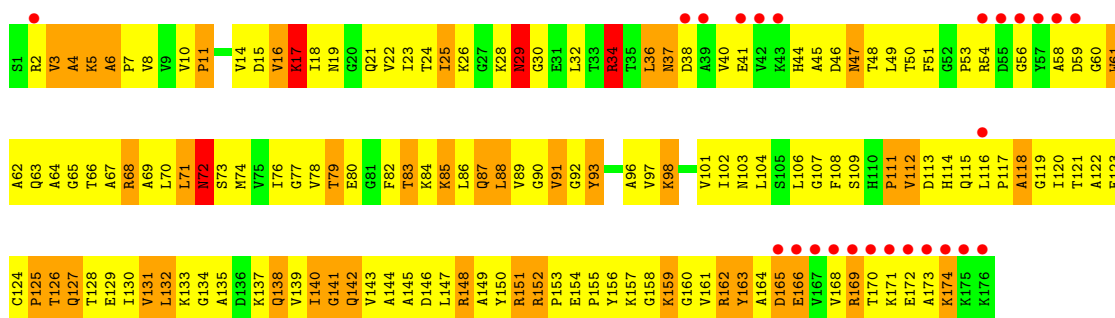
• Molecule 11: 50S RIBOSOMAL PROTEIN L5

Chain F:



• Molecule 12: 50S RIBOSOMAL PROTEIN L6

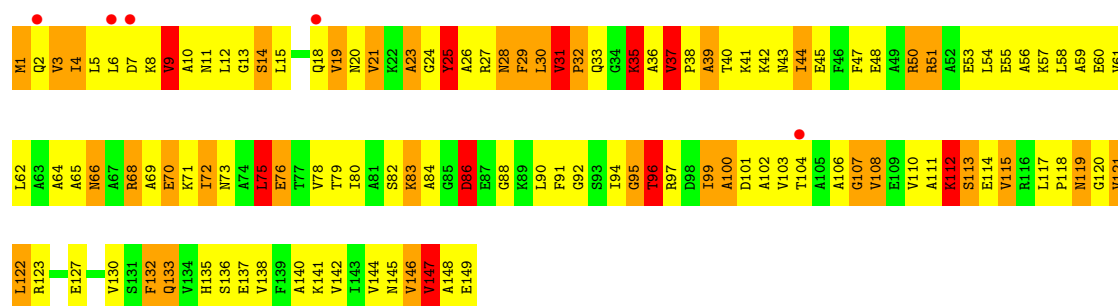
Chain G:



• Molecule 13: 50S RIBOSOMAL PROTEIN L9

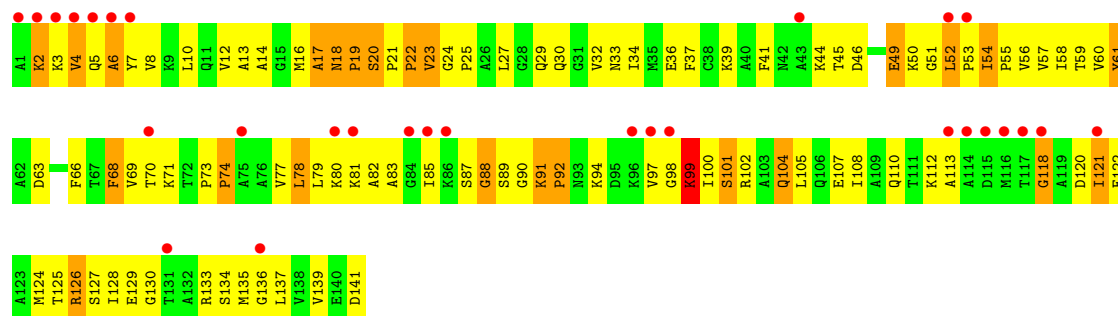
Chain H:





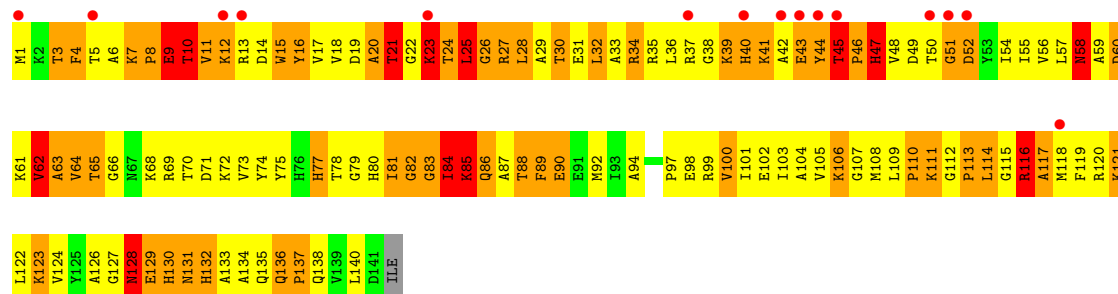
• Molecule 14: 50S RIBOSOMAL PROTEIN L11

Chain I:



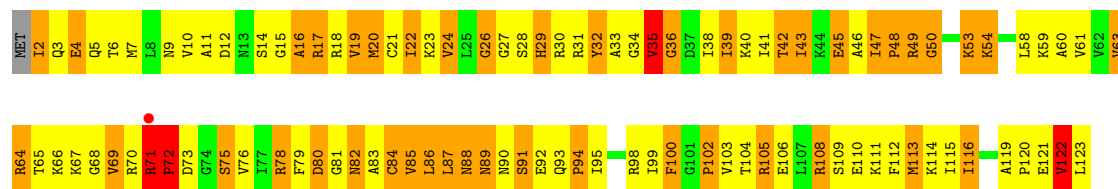
• Molecule 15: 50S RIBOSOMAL PROTEIN L13

Chain J:



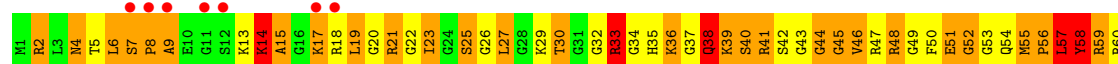
• Molecule 16: 50S RIBOSOMAL PROTEIN L14

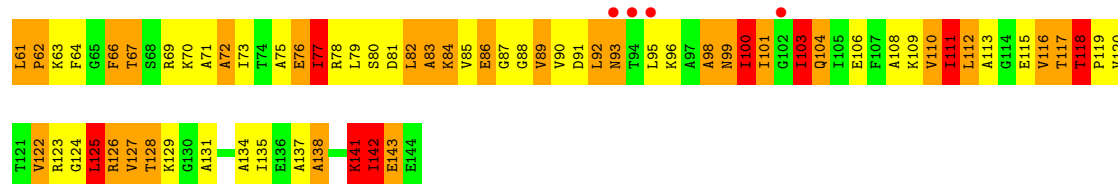
Chain K:



• Molecule 17: 50S RIBOSOMAL PROTEIN L15

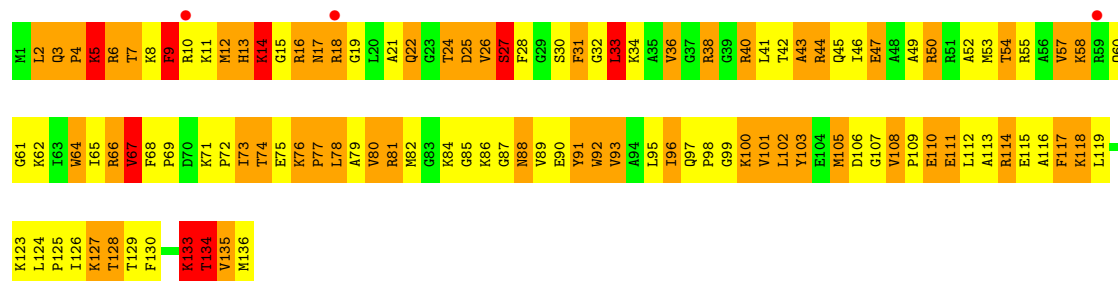
Chain L:





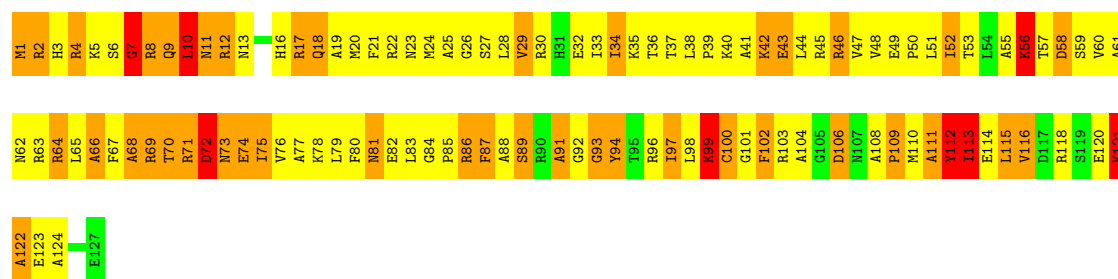
• Molecule 18: 50S RIBOSOMAL PROTEIN L16

Chain M:



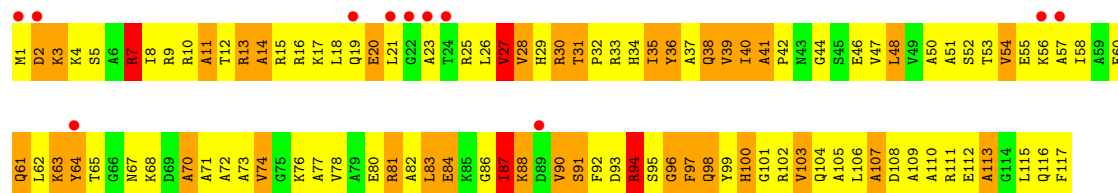
• Molecule 19: 50S RIBOSOMAL PROTEIN L17

Chain N:



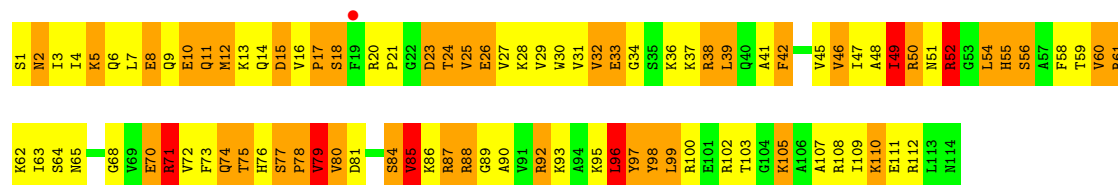
• Molecule 20: 50S RIBOSOMAL PROTEIN L18

Chain O:



• Molecule 21: 50S RIBOSOMAL PROTEIN L19

Chain P:



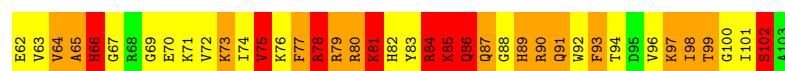
• Molecule 22: 50S RIBOSOMAL PROTEIN L20

Chain Q: 



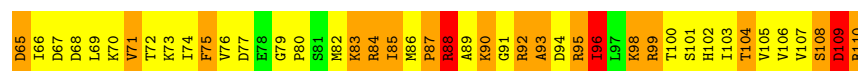
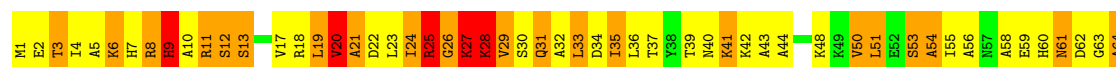
• Molecule 23: 50S RIBOSOMAL PROTEIN L21

Chain R: 



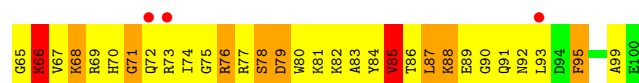
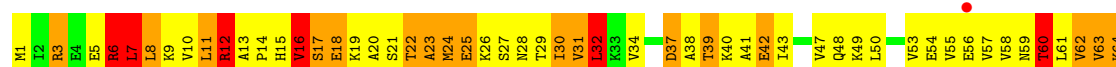
• Molecule 24: 50S RIBOSOMAL PROTEIN L22

Chain S: 



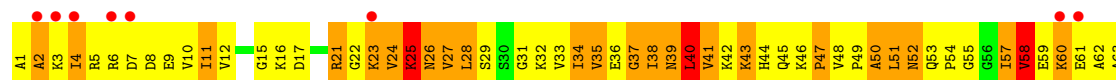
• Molecule 25: 50S RIBOSOMAL PROTEIN L23

Chain T: 



• Molecule 26: 50S RIBOSOMAL PROTEIN L24

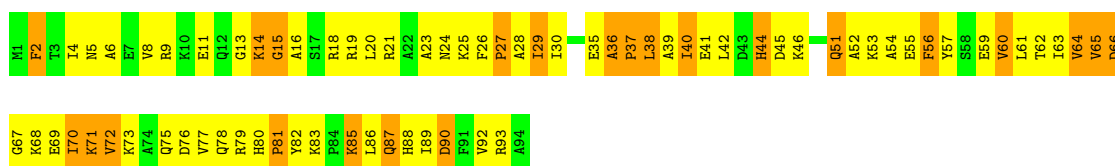
Chain U: 



• Molecule 27: 50S RIBOSOMAL PROTEIN L25

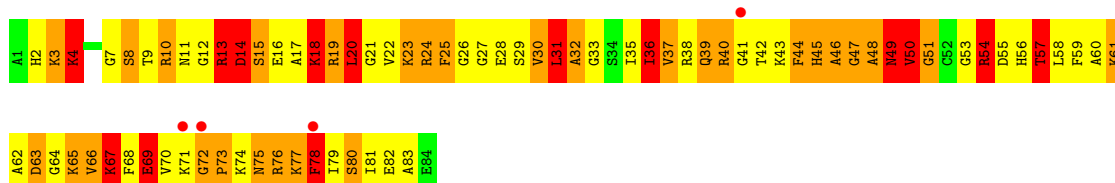
Chain V: 





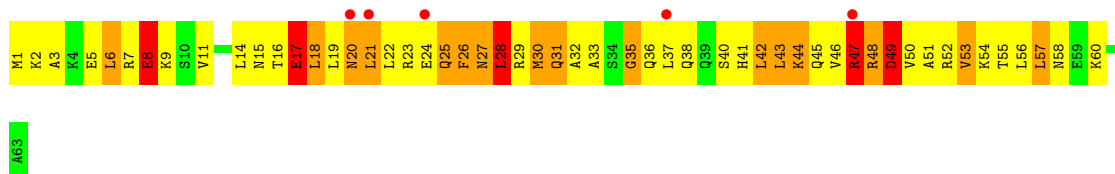
• Molecule 28: 50S RIBOSOMAL PROTEIN L27

Chain W:



• Molecule 29: 50S RIBOSOMAL PROTEIN L29

Chain X:



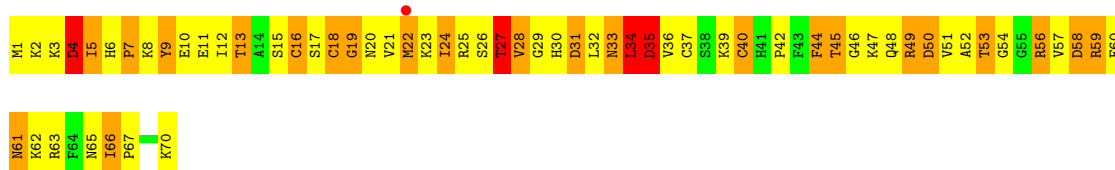
• Molecule 30: 50S RIBOSOMAL PROTEIN L30

Chain Y:



• Molecule 31: 50S RIBOSOMAL PROTEIN L31

Chain Z:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.18Å 380.08Å 736.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.74 49.74 – 3.74	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-3.74) 91.5 (49.74-3.74)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.259 , 0.323 0.422 , 0.441	Depositor DCC
R_{free} test set	5522 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.07 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Outliers	0 of 546832 reflections	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	90314	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.48	0/450	0.78	0/599
2	1	0.46	0/448	0.73	0/594
3	2	0.46	0/380	0.83	1/498 (0.2%)
4	3	0.54	0/513	0.91	0/676
5	4	0.46	0/303	0.78	0/397
6	A	0.79	2/2803 (0.1%)	1.52	47/4371 (1.1%)
7	B	0.90	15/68314 (0.0%)	1.64	1204/106569 (1.1%)
8	C	0.55	0/2093	0.82	1/2815 (0.0%)
9	D	0.51	0/1586	0.77	0/2134
10	E	0.50	0/1571	0.75	0/2113
11	F	0.32	0/1444	0.54	0/1937
12	G	0.37	0/1343	0.62	0/1816
13	H	0.37	0/1122	0.64	0/1515
14	I	0.26	0/1045	0.52	0/1406
15	J	0.50	0/1136	0.75	0/1531
16	K	0.54	0/940	0.72	0/1260
17	L	0.44	0/1062	0.81	0/1413
18	M	0.48	0/1093	0.77	0/1460
19	N	0.49	0/1021	0.73	0/1364
20	O	0.45	0/910	0.77	0/1219
21	P	0.51	0/929	0.81	1/1242 (0.1%)
22	Q	0.53	0/960	0.81	1/1278 (0.1%)
23	R	0.46	0/829	0.75	0/1107
24	S	0.44	0/864	0.82	0/1156
25	T	0.43	0/785	0.69	0/1050
26	U	0.42	0/788	0.69	0/1053
27	V	0.36	0/766	0.52	0/1025
28	W	0.45	0/642	0.78	0/848
29	X	0.40	0/510	0.69	0/677
30	Y	0.34	0/453	0.67	0/605
31	Z	0.68	0/559	0.97	0/745
All	All	0.80	17/97662 (0.0%)	1.47	1255/146473 (0.9%)

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	2
4	3	0	2
10	E	0	3
13	H	0	1
15	J	0	1
17	L	0	1
19	N	0	2
21	P	0	4
23	R	0	1
24	S	0	2
25	T	0	1
29	X	0	1
31	Z	0	1
All	All	0	22

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	301	G	C3'-O3'	7.66	1.52	1.42
6	A	87	U	C1'-N1	7.10	1.59	1.48
7	B	2288	A	C5-C4	6.04	1.43	1.38
7	B	2288	A	N1-C2	-6.02	1.28	1.34
7	B	1440	U	C1'-N1	5.92	1.57	1.48

The worst 5 of 1255 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2288	A	C2-N3-C4	-69.49	75.85	110.60
7	B	2288	A	N1-C2-N3	59.84	159.22	129.30
7	B	2288	A	C6-N1-C2	-58.14	83.72	118.60
7	B	1996	C	C1'-O4'-C4'	-14.20	98.54	109.90
7	B	196	A	C1'-O4'-C4'	-14.15	98.58	109.90

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	26	SER	Peptide

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Mol	Chain	Res	Type	Group
1	0	28	SER	Peptide
4	3	32	LEU	Peptide
4	3	50	SER	Peptide
10	E	27	LEU	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	0	444	0	461	112	0
2	1	441	0	485	89	0
3	2	377	0	418	104	0
4	3	504	0	574	137	0
5	4	302	0	340	99	0
6	A	2507	0	1270	303	0
7	B	60995	0	30678	7134	0
8	C	2054	0	2122	625	0
9	D	1565	0	1616	508	0
10	E	1552	0	1619	401	0
11	F	1420	0	1460	214	0
12	G	1323	0	1374	226	0
13	H	1111	0	1148	191	0
14	I	1032	0	1088	131	0
15	J	1113	0	1147	307	0
16	K	931	0	1000	156	0
17	L	1053	0	1129	336	0
18	M	1074	0	1157	294	0
19	N	1008	0	1045	248	0
20	O	900	0	935	247	0
21	P	917	0	965	240	0
22	Q	947	0	1022	284	0
23	R	816	0	839	308	0
24	S	857	0	922	200	0
25	T	778	0	840	173	0
26	U	780	0	834	172	0
27	V	753	0	780	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	W	634	0	656	226	0
29	X	509	0	543	123	0
30	Y	449	0	491	84	0
31	Z	549	0	552	152	0
32	Z	111	0	0	0	0
33	0	1	0	0	0	0
33	2	2	0	0	0	0
33	B	485	0	0	65	0
33	C	3	0	0	0	0
33	D	1	0	0	0	0
33	E	2	0	0	0	0
33	J	1	0	0	0	0
33	K	1	0	0	0	0
33	L	4	0	0	1	0
33	N	4	0	0	2	0
33	Q	1	0	0	0	0
33	T	2	0	0	0	0
33	U	1	0	0	2	0
All	All	90314	0	59510	12780	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 86.

The worst 5 of 12780 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:B:2822:G:OP2	19:N:2:ARG:HB3	1.29	1.26
1:O:27:LEU:HG	7:B:2886:A:C6	1.77	1.19
22:Q:49:ARG:HG3	23:R:77:PHE:CZ	1.79	1.18
22:Q:39:ILE:O	22:Q:43:GLN:HB3	1.40	1.18
7:B:1813:G:H2'	7:B:1814:G:H5''	1.24	1.17

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	
1	0	54/56 (96%)	24 (44%)	12 (22%)	18 (33%)	0	0
2	1	52/54 (96%)	18 (35%)	12 (23%)	22 (42%)	0	0
3	2	44/46 (96%)	16 (36%)	16 (36%)	12 (27%)	0	1
4	3	62/64 (97%)	29 (47%)	20 (32%)	13 (21%)	0	4
5	4	36/38 (95%)	9 (25%)	16 (44%)	11 (31%)	0	1
8	C	266/273 (97%)	101 (38%)	70 (26%)	95 (36%)	0	0
9	D	207/209 (99%)	72 (35%)	65 (31%)	70 (34%)	0	0
10	E	199/201 (99%)	71 (36%)	63 (32%)	65 (33%)	0	0
11	F	176/178 (99%)	95 (54%)	45 (26%)	36 (20%)	0	4
12	G	174/176 (99%)	89 (51%)	52 (30%)	33 (19%)	0	5
13	H	147/149 (99%)	74 (50%)	39 (26%)	34 (23%)	0	2
14	I	137/141 (97%)	87 (64%)	32 (23%)	18 (13%)	0	13
15	J	139/142 (98%)	57 (41%)	37 (27%)	45 (32%)	0	0
16	K	120/123 (98%)	66 (55%)	29 (24%)	25 (21%)	0	4
17	L	142/144 (99%)	54 (38%)	39 (28%)	49 (34%)	0	0
18	M	134/136 (98%)	55 (41%)	45 (34%)	34 (25%)	0	2
19	N	125/127 (98%)	55 (44%)	44 (35%)	26 (21%)	0	4
20	O	115/117 (98%)	46 (40%)	41 (36%)	28 (24%)	0	2
21	P	112/114 (98%)	48 (43%)	31 (28%)	33 (30%)	0	1
22	Q	115/117 (98%)	57 (50%)	30 (26%)	28 (24%)	0	2
23	R	101/103 (98%)	37 (37%)	23 (23%)	41 (41%)	0	0
24	S	108/110 (98%)	52 (48%)	29 (27%)	27 (25%)	0	2
25	T	98/100 (98%)	42 (43%)	33 (34%)	23 (24%)	0	2
26	U	101/103 (98%)	38 (38%)	31 (31%)	32 (32%)	0	0
27	V	92/94 (98%)	57 (62%)	21 (23%)	14 (15%)	0	8
28	W	82/84 (98%)	17 (21%)	29 (35%)	36 (44%)	0	0
29	X	61/63 (97%)	26 (43%)	22 (36%)	13 (21%)	0	3
30	Y	56/58 (97%)	26 (46%)	19 (34%)	11 (20%)	0	4
31	Z	68/70 (97%)	34 (50%)	21 (31%)	13 (19%)	0	5
All	All	3323/3390 (98%)	1452 (44%)	966 (29%)	905 (27%)	0	1

5 of 905 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	23	ALA
1	0	29	VAL
1	0	30	ASP
1	0	36	LYS
1	0	53	VAL

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	
1	0	47/47 (100%)	39 (83%)	8 (17%)	3	23
2	1	48/48 (100%)	36 (75%)	12 (25%)	1	8
3	2	38/38 (100%)	20 (53%)	18 (47%)	0	0
4	3	51/51 (100%)	30 (59%)	21 (41%)	0	1
5	4	34/34 (100%)	19 (56%)	15 (44%)	0	0
8	C	213/218 (98%)	147 (69%)	66 (31%)	0	5
9	D	164/164 (100%)	111 (68%)	53 (32%)	0	4
10	E	165/165 (100%)	118 (72%)	47 (28%)	0	5
11	F	149/149 (100%)	131 (88%)	18 (12%)	7	42
12	G	137/137 (100%)	106 (77%)	31 (23%)	1	10
13	H	114/114 (100%)	85 (75%)	29 (25%)	1	8
14	I	109/109 (100%)	98 (90%)	11 (10%)	11	52
15	J	114/116 (98%)	76 (67%)	38 (33%)	0	3
16	K	102/104 (98%)	65 (64%)	37 (36%)	0	2
17	L	103/103 (100%)	63 (61%)	40 (39%)	0	1
18	M	109/109 (100%)	66 (61%)	43 (39%)	0	1
19	N	103/103 (100%)	69 (67%)	34 (33%)	0	4
20	O	87/87 (100%)	69 (79%)	18 (21%)	2	13
21	P	99/99 (100%)	81 (82%)	18 (18%)	2	19
22	Q	89/89 (100%)	55 (62%)	34 (38%)	0	1
23	R	84/84 (100%)	52 (62%)	32 (38%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	S	93/93 (100%)	66 (71%)	27 (29%)	0	5
25	T	83/84 (99%)	59 (71%)	24 (29%)	0	5
26	U	83/84 (99%)	63 (76%)	20 (24%)	1	8
27	V	78/78 (100%)	62 (80%)	16 (20%)	2	14
28	W	62/62 (100%)	39 (63%)	23 (37%)	0	2
29	X	55/55 (100%)	38 (69%)	17 (31%)	0	5
30	Y	48/48 (100%)	32 (67%)	16 (33%)	0	3
31	Z	62/62 (100%)	43 (69%)	19 (31%)	0	5
All	All	2723/2734 (100%)	1938 (71%)	785 (29%)	0	5

5 of 785 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	J	85	LYS
17	L	127	VAL
28	W	49	ASN
15	J	130	HIS
16	K	100	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
14	I	30	GLN
17	L	99	ASN
29	X	36	GLN
14	I	110	GLN
16	K	29	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	A	117/120 (97%)	48 (41%)	15 (12%)
7	B	2838/2904 (97%)	1137 (40%)	386 (13%)
All	All	2955/3024 (97%)	1185 (40%)	401 (13%)

5 of 1185 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	3	C
6	A	6	G
6	A	7	G
6	A	8	C
6	A	9	G

5 of 401 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	B	1141	U
7	B	1454	C
7	B	2674	G
7	B	1204	A
7	B	1291	C

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 111 ligands modelled in this entry, 111 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 ⓘ

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, 95th 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 ²)	Q<0.9
1	0	56/56 (100%)	0.13	1 (1%) 65 43	97, 120, 190, 244	0
2	1	54/54 (100%)	0.29	3 (5%) 24 15	92, 113, 223, 254	0
3	2	46/46 (100%)	0.85	5 (10%) 6 7	68, 103, 198, 264	0
4	3	64/64 (100%)	0.32	3 (4%) 30 20	69, 99, 174, 229	0
5	4	38/38 (100%)	0.75	6 (15%) 3 4	124, 144, 238, 298	0
6	A	117/120 (97%)	0.25	6 (5%) 27 17	71, 127, 170, 285	0
7	B	2841/2904 (97%)	0.04	63 (2%) 59 37	41, 89, 202, 421	0
8	C	268/273 (98%)	0.23	14 (5%) 26 17	63, 91, 165, 248	0
9	D	209/209 (100%)	0.18	10 (4%) 29 19	11, 94, 186, 271	0
10	E	201/201 (100%)	0.07	7 (3%) 42 26	88, 117, 224, 290	0
11	F	178/178 (100%)	0.33	10 (5%) 24 15	92, 155, 224, 286	0
12	G	176/176 (100%)	0.55	25 (14%) 3 4	88, 138, 222, 271	0
13	H	149/149 (100%)	0.10	5 (3%) 43 27	107, 147, 233, 274	0
14	I	141/141 (100%)	1.01	29 (20%) 1 2	219, 343, 422, 470	0
15	J	141/142 (99%)	0.54	15 (10%) 7 7	104, 121, 207, 250	0
16	K	122/123 (99%)	-0.02	1 (0%) 83 63	80, 94, 127, 208	0
17	L	144/144 (100%)	0.53	11 (7%) 14 10	83, 128, 275, 315	0
18	M	136/136 (100%)	0.20	3 (2%) 59 37	77, 108, 223, 279	0
19	N	127/127 (100%)	-0.00	0 100 100	58, 78, 155, 257	0
20	O	117/117 (100%)	0.34	11 (9%) 9 8	52, 118, 211, 255	0
21	P	114/114 (100%)	0.09	1 (0%) 81 61	77, 96, 196, 257	0
22	Q	117/117 (100%)	0.17	2 (1%) 67 44	70, 93, 148, 225	0
23	R	103/103 (100%)	-0.05	0 100 100	87, 132, 229, 286	0
24	S	110/110 (100%)	0.01	0 100 100	49, 85, 152, 211	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	T	100/100 (100%)	0.33	4 (4%) 36 23	85, 120, 248, 278	0
26	U	103/103 (100%)	0.48	11 (10%) 6 7	118, 162, 256, 281	0
27	V	94/94 (100%)	-0.14	0 100 100	87, 125, 194, 215	0
28	W	84/84 (100%)	0.51	4 (4%) 29 19	111, 136, 238, 275	0
29	X	63/63 (100%)	0.36	5 (7%) 13 10	86, 150, 233, 320	0
30	Y	58/58 (100%)	0.28	3 (5%) 26 17	126, 138, 240, 249	0
31	Z	70/70 (100%)	0.06	1 (1%) 72 48	70, 91, 169, 255	0
All	All	6341/6414 (98%)	0.17	259 (4%) 36 23	11, 103, 239, 470	0

The worst 5 of 259 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	B	645	C	10.0
14	I	113	ALA	9.1
8	C	270	ARG	8.3
15	J	43	GLU	8.3
17	L	8	PRO	7.7

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	Z	4109	1/1	0.88	91.12	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	Z	4090	1/1	0.45	53.02	42,42,42,42	0
32	MG	Z	4059	1/1	0.67	21.61	78,78,78,78	0
32	MG	Z	4079	1/1	1.10	19.10	55,55,55,55	1
32	MG	Z	4102	1/1	0.32	16.29	8,8,8,8	0
32	MG	Z	4108	1/1	0.34	9.25	22,22,22,22	0
32	MG	Z	4051	1/1	0.29	8.43	43,43,43,43	0
32	MG	Z	4063	1/1	0.59	8.04	63,63,63,63	0
32	MG	Z	4038	1/1	0.49	7.31	27,27,27,27	0
32	MG	Z	4031	1/1	0.36	6.56	52,52,52,52	0
32	MG	Z	4040	1/1	0.25	4.94	19,19,19,19	0
32	MG	Z	4095	1/1	0.38	4.31	38,38,38,38	0
32	MG	Z	4013	1/1	0.23	4.18	33,33,33,33	0
32	MG	Z	4082	1/1	0.34	4.11	9,9,9,9	0
32	MG	Z	4001	1/1	0.30	3.65	54,54,54,54	0
32	MG	Z	4027	1/1	0.37	3.16	46,46,46,46	0
32	MG	Z	4076	1/1	0.24	3.12	76,76,76,76	0
32	MG	Z	4100	1/1	0.26	3.07	43,43,43,43	0
32	MG	Z	4028	1/1	0.36	2.82	39,39,39,39	0
32	MG	Z	4105	1/1	0.37	2.71	6,6,6,6	0
32	MG	Z	4078	1/1	0.46	2.65	54,54,54,54	0
32	MG	Z	4039	1/1	0.37	2.51	46,46,46,46	0
32	MG	Z	4012	1/1	0.22	2.36	14,14,14,14	0
32	MG	Z	4065	1/1	0.34	2.32	45,45,45,45	0
32	MG	Z	4083	1/1	0.28	2.22	24,24,24,24	0
32	MG	Z	4074	1/1	0.51	2.16	61,61,61,61	0
32	MG	Z	4069	1/1	0.27	2.08	33,33,33,33	0
32	MG	Z	4062	1/1	0.29	1.82	11,11,11,11	0
32	MG	Z	4044	1/1	0.24	1.58	67,67,67,67	0
32	MG	Z	4106	1/1	0.29	1.37	20,20,20,20	0
32	MG	Z	4042	1/1	0.23	1.20	69,69,69,69	0
32	MG	Z	4002	1/1	0.30	0.88	8,8,8,8	0
32	MG	Z	4066	1/1	0.29	0.70	9,9,9,9	0
32	MG	Z	4003	1/1	0.28	0.61	9,9,9,9	0
32	MG	Z	4091	1/1	0.18	0.48	7,7,7,7	0
32	MG	Z	4056	1/1	0.25	0.48	7,7,7,7	0
32	MG	Z	4070	1/1	0.21	0.23	52,52,52,52	0
32	MG	Z	4092	1/1	0.20	0.14	3,3,3,3	0
32	MG	Z	4055	1/1	0.24	0.06	8,8,8,8	0
32	MG	Z	4049	1/1	0.15	0.04	45,45,45,45	0
32	MG	Z	4036	1/1	0.20	0.00	10,10,10,10	0
32	MG	Z	4053	1/1	0.21	-0.05	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	Z	4030	1/1	0.20	-0.11	55,55,55,55	0
32	MG	Z	4080	1/1	0.17	-0.30	10,10,10,10	0
32	MG	Z	4019	1/1	0.20	-0.30	8,8,8,8	0
32	MG	Z	4075	1/1	0.17	-0.34	15,15,15,15	0
32	MG	Z	4029	1/1	0.20	-0.34	17,17,17,17	0
32	MG	Z	4058	1/1	0.15	-0.40	12,12,12,12	0
32	MG	Z	4098	1/1	0.17	-0.61	43,43,43,43	0
32	MG	Z	4068	1/1	0.19	-0.69	10,10,10,10	0
32	MG	Z	4096	1/1	0.21	-0.73	89,89,89,89	0
32	MG	Z	4077	1/1	0.16	-0.74	57,57,57,57	0
32	MG	Z	4097	1/1	0.18	-0.82	9,9,9,9	0
32	MG	Z	4046	1/1	0.14	-0.95	10,10,10,10	0
32	MG	Z	4000	1/1	0.13	-0.95	9,9,9,9	0
32	MG	Z	4009	1/1	0.16	-0.98	30,30,30,30	0
32	MG	Z	4043	1/1	0.16	-1.01	83,83,83,83	0
32	MG	Z	4035	1/1	0.16	-1.09	19,19,19,19	0
32	MG	Z	4021	1/1	0.14	-1.13	21,21,21,21	0
32	MG	Z	4064	1/1	0.15	-1.15	26,26,26,26	0
32	MG	Z	4048	1/1	0.09	-1.16	30,30,30,30	1
32	MG	Z	4088	1/1	0.15	-1.21	38,38,38,38	0
32	MG	Z	4057	1/1	0.13	-1.34	31,31,31,31	0
32	MG	Z	4087	1/1	0.12	-1.41	52,52,52,52	0
32	MG	Z	4081	1/1	0.13	-1.43	17,17,17,17	0
32	MG	Z	4085	1/1	0.13	-1.44	17,17,17,17	0
32	MG	Z	4007	1/1	0.17	-1.47	16,16,16,16	0
32	MG	Z	4041	1/1	0.14	-1.47	18,18,18,18	0
32	MG	Z	4067	1/1	0.15	-1.52	59,59,59,59	0
32	MG	Z	4024	1/1	0.13	-1.52	27,27,27,27	0
32	MG	Z	4061	1/1	0.13	-1.63	7,7,7,7	0
32	MG	Z	4026	1/1	0.19	-1.65	40,40,40,40	0
32	MG	Z	4089	1/1	0.12	-1.66	67,67,67,67	0
32	MG	Z	4086	1/1	0.15	-1.69	25,25,25,25	0
32	MG	Z	4033	1/1	0.10	-1.71	7,7,7,7	0
32	MG	Z	4005	1/1	0.15	-1.74	19,19,19,19	0
32	MG	Z	4073	1/1	0.14	-1.75	33,33,33,33	0
32	MG	Z	4050	1/1	0.10	-1.82	12,12,12,12	0
32	MG	Z	4018	1/1	0.12	-1.83	11,11,11,11	0
32	MG	Z	4110	1/1	0.13	-1.97	16,16,16,16	0
32	MG	Z	4017	1/1	0.12	-2.01	25,25,25,25	0
32	MG	Z	4099	1/1	0.09	-2.16	7,7,7,7	0
32	MG	Z	4022	1/1	0.08	-2.42	7,7,7,7	0
32	MG	Z	4011	1/1	0.12	-2.43	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	Z	4060	1/1	0.17	-2.44	31,31,31,31	0
32	MG	Z	4023	1/1	0.12	-2.45	21,21,21,21	0
32	MG	Z	4004	1/1	0.09	-2.47	26,26,26,26	0
32	MG	Z	4032	1/1	0.10	-2.62	33,33,33,33	0
32	MG	Z	4015	1/1	0.08	-2.72	18,18,18,18	0
32	MG	Z	4025	1/1	0.09	-2.74	10,10,10,10	0
32	MG	Z	4047	1/1	0.07	-3.14	4,4,4,4	0
32	MG	Z	4072	1/1	0.07	-3.16	14,14,14,14	0
32	MG	Z	4020	1/1	0.09	-3.20	22,22,22,22	0
32	MG	Z	4008	1/1	0.10	-3.24	13,13,13,13	0
32	MG	Z	4094	1/1	0.08	-3.43	22,22,22,22	0
32	MG	Z	4084	1/1	0.09	-3.88	16,16,16,16	0
32	MG	Z	4016	1/1	0.11	-3.96	13,13,13,13	0
32	MG	Z	4104	1/1	0.18	-4.02	10,10,10,10	0
32	MG	Z	4071	1/1	0.12	-4.29	42,42,42,42	0
32	MG	Z	4034	1/1	0.09	-4.30	20,20,20,20	0
32	MG	Z	4045	1/1	0.06	-4.65	29,29,29,29	0
32	MG	Z	4010	1/1	0.10	-6.38	33,33,33,33	0
32	MG	Z	4052	1/1	0.10	-6.58	5,5,5,5	0
32	MG	Z	4054	1/1	0.07	-6.58	5,5,5,5	0
32	MG	Z	4037	1/1	0.07	-7.14	58,58,58,58	0
32	MG	Z	4006	1/1	0.10	-9.88	25,25,25,25	0
32	MG	Z	4014	1/1	0.07	-34.60	9,9,9,9	0
32	MG	Z	4093	1/1	0.09	-36.33	16,16,16,16	0
32	MG	Z	4101	1/1	0.18	-	43,43,43,43	0
32	MG	Z	4107	1/1	0.32	-	20,20,20,20	0
32	MG	Z	4103	1/1	0.21	-	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.