



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 09:12 AM GMT

PDB ID : 2QP1  
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with spectinomycin and neomycin. This file contains the 50S subunit of the second 70S ribosome, with neomycin bound. The entire crystal structure contains two 70S ribosomes.  
Authors : Borovinskaya, M.A.; Shoji, S.; Holton, J.M.; Fredrick, K.; Cate, J.H.D.  
Deposited on : 2007-07-21  
Resolution : 3.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

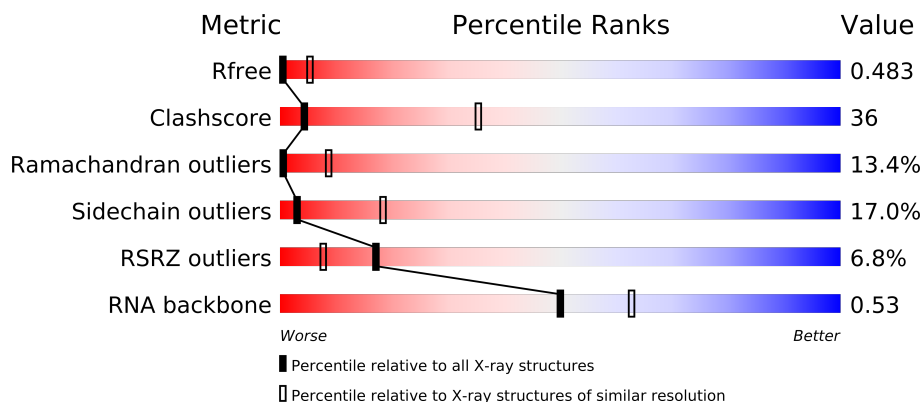
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	120	
2	B	2904	
3	I	141	
4	C	272	
5	D	209	
6	K	123	
7	P	114	
8	E	201	
9	Y	58	
10	0	56	
11	4	38	
12	1	54	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
13	3	64	
14	V	94	
15	2	46	
16	L	144	
17	M	136	
18	X	63	
19	H	149	
20	J	142	
21	N	127	
22	O	117	
23	Q	117	
24	S	110	
25	U	103	
26	F	178	
27	G	176	
28	R	103	
29	T	100	
30	Z	78	
31	W	84	

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	NMY	B	3521	-	X
33	MG	B	2919	-	X
33	MG	B	2933	-	X
33	MG	B	2938	-	X
33	MG	B	2939	-	X
33	MG	B	2952	-	X
33	MG	B	2962	-	X
33	MG	B	2963	-	X
33	MG	B	2964	-	X
33	MG	B	2970	-	X
33	MG	B	2987	-	X
33	MG	B	2994	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 90305 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 5S rRNA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	U	-	INSERTION	GB 85674274

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2903	U	-	INSERTION	GB 85674274
B	2904	U	-	INSERTION	GB 85674274

- Molecule 3 is a protein called 50S ribosomal protein L11.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

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

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

- Molecule 6 is a protein called 50S ribosomal protein L14.

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

- Molecule 7 is a protein called 50S ribosomal protein L19.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L30.

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

- Molecule 10 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 11 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 12 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	1	50	Total	C	N	O			
			409	263	75	71	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	3	64	Total	C	N	O	S			
			504	323	105	74	2	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L25.

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

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	46	Total	C	N	O	S			
			377	228	90	57	2	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	143	Total	C	N	O	S			
			1045	649	206	189	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L29.

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

- Molecule 19 is a protein called 50S ribosomal protein L9.

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

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	J	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	O	116	Total	C	N	O	S	0	0	0
			892	552	178	162				

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- 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 L24.

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

- Molecule 26 is a protein called 50S ribosomal protein L5.

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

- Molecule 27 is a protein called 50S ribosomal protein L6.

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

- Molecule 28 is a protein called 50S ribosomal protein L21.

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

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 30 is a protein called 50S ribosomal protein L28.

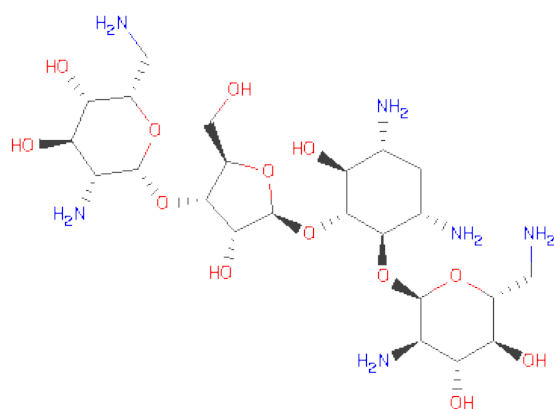
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Z	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	W	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 32 is NEOMYCIN (three-letter code: NMY) (formula: C<sub>23</sub>H<sub>46</sub>N<sub>6</sub>O<sub>13</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	N	O	0	0
			42	23	6	13		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	111	Total	Mg	0	0
			111	111		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	4	1	Total	Zn	0	0
			1	1		

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	504	Total	O	0	0
			504	504		
35	C	4	Total	O	0	0
			4	4		
35	D	1	Total	O	0	0
			1	1		
35	E	1	Total	O	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

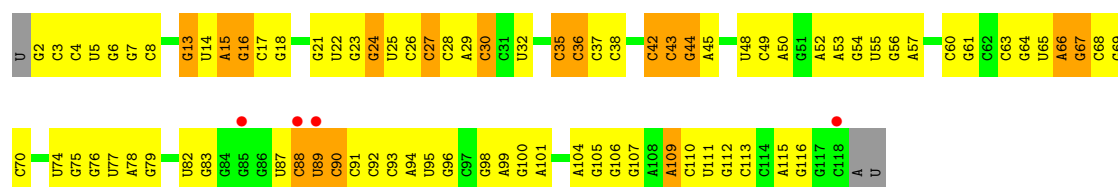
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	L	1	Total	O	0	0
			1	1		
35	R	1	Total	O	0	0
			1	1		

### 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.

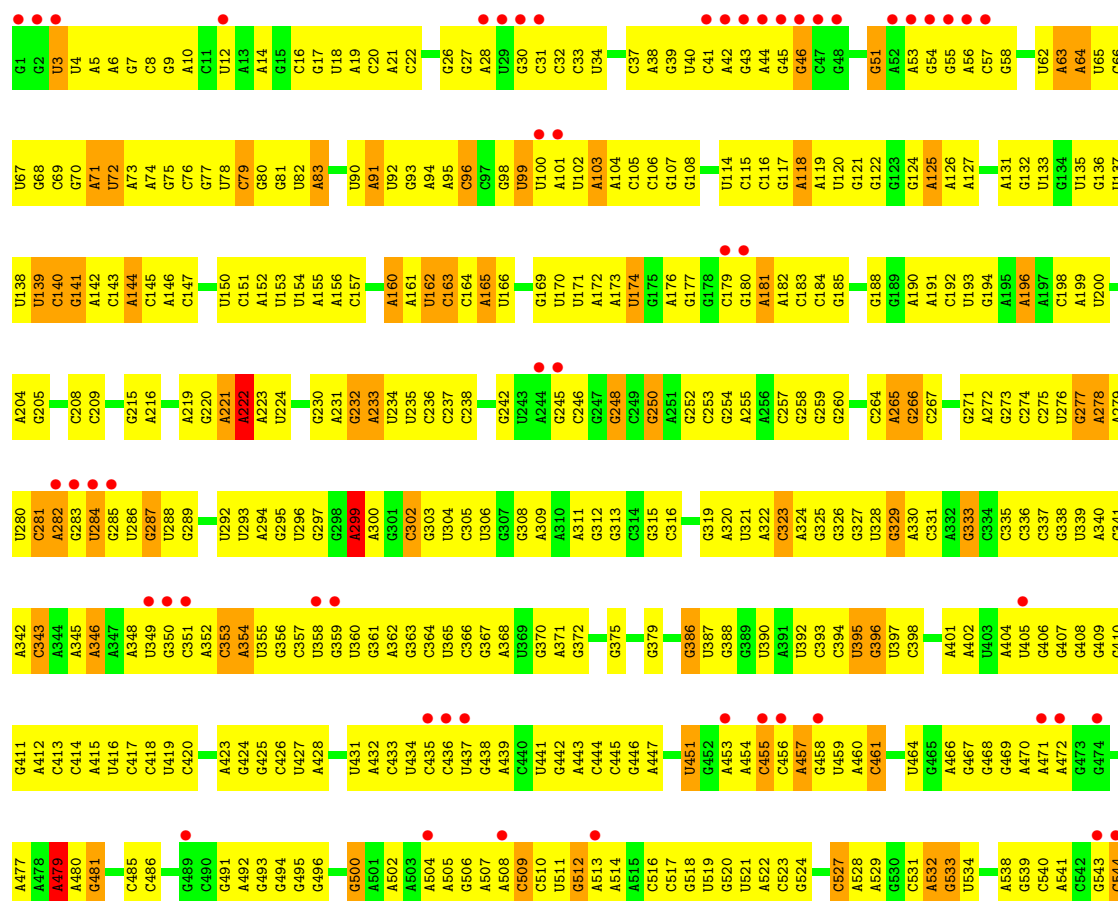
#### • Molecule 1: 5S rRNA

Chain A: 



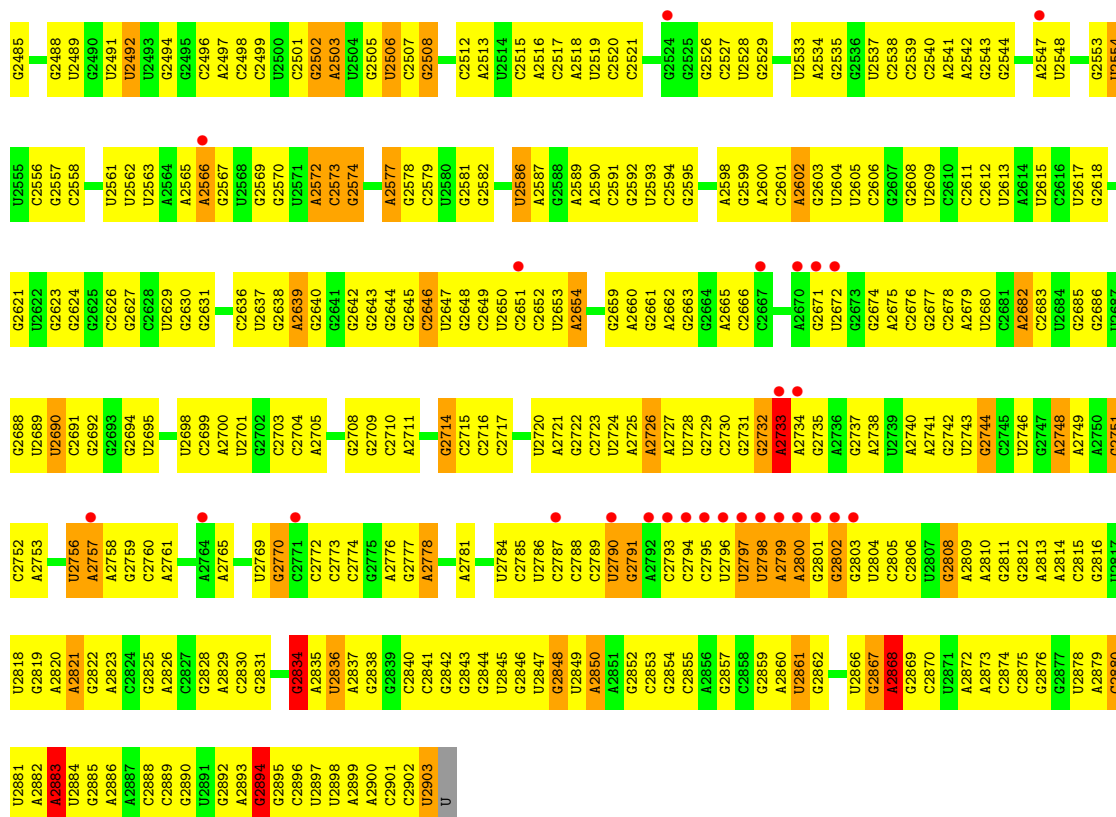
#### • Molecule 2: 23S rRNA

Chain B: 



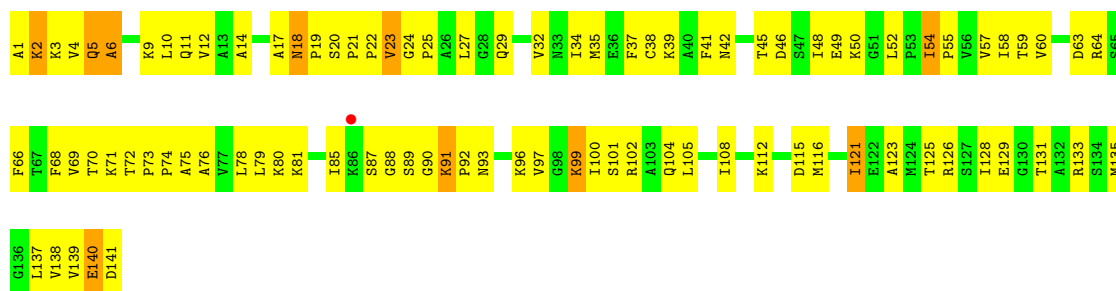
U1486	G1424	G1358	G1293	U1222	A1156	G1087	G1016	G952	C	A825	G674	A608	U545
U1487	G1425	A1359	C1297	G1223	U1159	C1092	U1017	U956	C	U827	A675	A609	U546
C1488	G1426	G1360	C1298	G1228	G1160	G1093	U1018	U955	G	U827	C679	C611	G547
C1489	A1427	A1361	G1299	G1229	G1161	U1094	U1019	G956	A	U828	G745	C610	G548
A1490	C1428	C1362	G1300	A1230	G1163	U1094	A1021	U958	C	U828	G746	G612	G549
G1491	G1429	G1363	G1300	U1231	G1164	U1094	G1022	U959	U	G831	G681	A613	C550
G1492	G1430	A1365	A1301	U1231	A1166	U1097	U1022	A959	U	U832	G682	A614	G551
C1493	A1431	G1368	A1302	G1236	G1166	A1098	U1023	A960	A	A833	U683	U615	U552
A1495	G1432	G1371	C1306	G1237	G1167	G1099	G1024	C961	C	G834	U684	A616	G553
A1496	A1434	G1372	A1307	G1238	G1168	C1100	G1025	U962	C898	G835	U685	U617	U554
		U1372	G1308	U1240	A1169	U1101	G1026	G963	A899	U886	U686		G555
	C1437	U1373	G1309	G1241	C1170	C1102	A1027	C964	A900	G836	C687	G620	
G1500	U1438	G1374	G1310	A1241	G1171	A1103	A1028	U967	C901	G837	U688	A621	C557
G1501	A1439	U1375	G1311	U1242	C1172	A1103	A1029	C968	C902	C838	A689	G622	U558
A1502	U1440	C1376	U1312	C1243	U1173	C1104	C1030	G969	C903	G839	G690	G623	G559
A1503	G1441	G1377	U1313	A1244	U1174	U1105	G1031	U970	G904	C840	C691	C624	C560
U1504	U1442	A1378	C1314	G1245	A1175	G1106	A1032	G971	G908	U842	C692	G561	G561
U1505	U1443	U1379	U1315	G1245	U1176	U1107	U1033	A972	C908	G843	A693	U562	U562
U1506	G1444	G1380	U1316	G1248	U1177	U1108	G1034	A973	A909	U844	U694	A563	C564
C1507		G1381	G1317	U1249	C1178	C1109	G1037	A974	A910	A845	G695	G630	C565
A1508	C1447	G1382	U1318	U1250	G1179	G1110	G1038	A975	A911	U846	G696	A631	C566
A1509	G1448	A1383	C1319	C1251	U1180	G1111	A1039		A912	U847	G697	A632	U566
G1510	G1449	A1384	U1320	A1253	U1181	G1112	G1040	G978	U913	C948	U698	A633	
G1511	A1450	A1385	A1321	G1252	U1182	U1113	A1041	G979	G914	A849	G770	A699	C634
C1512	G1451	C1386	A1322	G1253	U1183	G1115	G1042	A980	C915	U850	G771	G635	G570
U1513	G1452	G1387	C1323	G1256	U1184	G1116	C1043	A981	A917	C852	U702	G636	U571
G1514	A1453	G1388	G1324	C1257	U1185	C1117	U1044	C982	A918	C853	G774	A637	A572
A1515	C1454	G1389	U1325	U1258	G1186	C1118	G1045	A983	U919	C854	G775	U703	U573
G1516	G1455	U1390	U1326	G1259	G1187	U1119	A1046	A984	A920	G855	G776	G704	A574
U1517	U1456	U1391	A1327	A1260	U1188	U1119	G1047	C985	C921	G856	G777	C640	A575
C1518	U1457	A1328	A1328	C1261	U1189	G1125	U1048	C986	C922	G857	G778	U641	U576
G1519	U1458	A1395	U1329	U1266	G1190	A1126	C1049	C987	G923	G858	U779	U642	G577
	U1459	U1396	C1330	U1267	G1191	G1127	U1050	A988	G924	G859	G780	A643	U580
A1526	C1461	U1397	G1331	U1268	G1192	A1129	G1051	A989	A925		G781	C645	C581
G1527	C1462	C1399	G1334	A1269	G1193	U1132	C1052	A990	G926	G862	A782	U646	A582
	C1463	U1400	C1335	C1270	G1195	A1194	A1057	C991	A927	A863	A783	G647	G583
G1530	G1464	G1401	A1336	A1271	C1196	U1058	U1058	C992	A928	G864	G784	G648	C584
C1531	U1465	U1402	G1337	A1272	G1197	G1059	U1059	G993	U929	C865	G785	G649	G585
A1532	U1466	A1403	G1338	U1273	U1198	G1136	U1060	C994	G930	A866	G786	A715	A586
U1533	G1467	C1404	G1339	A1274	U1199	G1137	U1061	C995	U931	C867	C787	G650	C587
U1534	U1468	U1405	U1340	A1275	C1200	G1138	G1062	A996	U932	U870	A718	U653	U588
A1535	A1469	U1406	G1341	A1276	U1201	G1139	G1063	G997	A933	U871	C719	A654	U589
C1536	A1470	G1407	A1342	G1277	G1202	C1140	C1064	C998	U934	U872	U720	A655	A590
G1537	G1471	G1408	G1343	C1278	U1203	U1141	U1065	U999	C935	C873	A721	G656	U591
	C1472	U1409	U1344	G1279	A1204	A1142	U1065	A1000	A936	G874	A722	U657	A592
U1540	U1473	G1410	C1345	G1280	A1205	A1143	A1070	A1001	C937	G875	C723	U658	U593
C1541	U1474	U1411	G1346	G1281	G1206	A1144		C876	G938	C876	U724	G659	U594
U1542	G1475	U1412	A1347	U1282	G1206	U1145	U1076	A877		A878	G725	C660	C595
G1543	U1476	A1413	C1348	U1283	G1210	C1146	C1076	G805		G	G726	A661	U596
A1544	G1477	G1416	C1349	A1284	C1211	A1147	A1077	A878		G	A727	G664	G597
U1545	G1478	C1417	C1350	A1285	G1212	U1148	U1078	G		G	G728	U665	U598
G1546	G1479	U1351	C1351	A1286	G1212	G1149	A1079	G		G	G729	U666	A599
U1547	A1480	U1352	U1352	A1287	G1216	U1150	A1080	U1009		G	A730	A666	G600
A1548	U1481	A1419	A1353	G1288	U1217	A1151	U1081	A1010		C	C731	G669	A603
U1549	G1482	A1420	A1354	G1289	G1218	C1152	U1083	G1011		C	G738	A670	G604
C1550	U1483	G1421	G1355	C1290	U1219	C1153	A1084	U1012		A	A739	C671	G605
	U1484	G1422	G1356	C1291	G1220	A1014	A1085	C1013		U	C817	C672	U606
A1551	U1485	G1423	C1357	G1292	C1221	A1155	A1086	U1015		C	U741	C673	U607

U2419	G2355	U2291	G2223	G	A2101	C2036	A1966	U1888	U1820	U1768	U1889	U1820	U1888	U1820	U1888	A1552
C2420	U2356	U2292	G2224	A	G2102	A2037	C1967	A1898	A1821	U1769	A1889	A1821	C1967	A1821	A1889	A1553
G2421	G2357	G2293	A2225	C	C2103	G2038	G1968	U1899	G1822	A1759	G1968	G1822	G1968	G1822	A1759	U1554
C2422	A2358	G2294	C2226	C	C2104	U2039	A1969	A1900	G1823	C1760	A1900	G1823	A1900	G1823	C1760	G1555
U2423	G2359	G2295	A2227	U	U2105	G2040	A1970	A1901	G1824	C1761	A1901	G1824	A1901	G1824	C1761	C1558
C2424	G2360	U2296	G2228	U	U2106	U2041	U1971	G1902	G1825	G1762	G1902	G1825	G1902	G1825	G1762	U1559
A2425	G2361	A2297	U2229	G	G2107	A2042	G1972	G1903	G1826	G1763	G1903	G1826	G1903	G1826	G1763	G1560
A2426	C2362	A2298	U2230	A	A2108	C2043	G1973	G1904	U1827	U1764	G1904	U1827	G1904	U1827	U1764	G1561
G2427	G2363	U2299	U2231	A	U2109	C2044	C1974	G1905	G1828	G1765	G1905	G1828	G1905	G1828	G1765	U1562
C2428	G2364	C2300	U2232	U	G2110			G1906	A1829	G1766	G1906	A1829	G1906	A1829	G1766	C1564
G2429	G2365	U2233	U2233	U				G1907	G1830	U1767	G1907	G1830	G1907	G1830	U1767	C1565
A2430	A2366	U2302	G2234	A				U1978	C1831	G1768	U1978	C1831	U1978	C1831	G1768	G1568
U2431	G2367	G2303	G2235	C	U			G1908	G1832	U1771	G1908	G1832	G1908	G1832	U1771	U1569
G2432	C2368	G2304	U2236	C	G			A1981		U1772	A1981		A1981		U1772	A1570
A2433	A2369	U2305	G2237	A	G			G1984	C1836	A1773	G1984	C1836	G1984	C1836	A1773	A1571
A2434	G2370	C2306	G2238	C	G			C1985	G1842	U1777	C1985	G1842	C1985	G1842	U1777	A1572
A2435	G2371	G2307	U2239	C	A			G1986	G1843	A1778	G1986	G1843	G1986	G1843	A1778	U1576
G2436	U2372	G2308	U2240	U	U2179	A2061		U1911	C1844	A1779	U1911	C1844	U1911	C1844	A1779	C1577
G2437	G2373	A2309	A2241	U	G	G2062		A1912	G1845	C1774	A1912	G1845	A1912	G1845	C1774	U1578
U2438	C2374	C2310	G2242	A		C2063		U1913	G1846	U1781	U1913	G1846	U1913	G1846	U1781	A1579
A2439	G2375	A2311	U2243	G	G	C2064		U1914	A1848	U1782	U1914	A1848	U1914	A1848	U1782	A1580
G2440	A2376	U2312	U2244	U	U2180	C2065		U1915	G1849	U1783	U1915	G1849	U1915	G1849	U1783	G1581
U2441	A2377	G2315	U2245	G	U2181	G2066		U1916	G1850	U1784	U1916	G1850	U1916	G1850	U1784	C1582
C2442	A2378	G2316	G2246	G	G	A2062		U1917	G1851	A1785	U1917	G1851	U1917	G1851	A1785	U1583
C2443	G2379		A2247	U	U2182	C2067		U1918	G1852	U1786	U1918	G1852	U1918	G1852	U1786	U1584
G2444	C2380		C2248	A	U2183	G2068		U1919	A1853	U1787	U1919	A1853	U1919	A1853	U1787	C1585
G2445	A2381	G2319	U2249	G	U2184	G2069		U1920	G1854	U1788	U1920	G1854	U1920	G1854	U1788	A1586
G2446	G2382	U2320	G2250	G	U2185	A2070		U1921	G1857	U1789	U1921	G1857	U1921	G1857	U1789	G1587
G2447	C2383	U2321	G2251	U	U2186	C2072		U1922	A1858	C1790	U1922	A1858	U1922	A1858	C1790	U1588
A2448	U2384	A2322	G2252	C	U2187	C2073		U1923	G1859	U1791	U1923	G1859	U1923	G1859	U1791	U1589
U2449	C2385	G2323	G2253	U	U2188	C2074		U1924	G1860	U1792	U1924	G1860	U1924	G1860	U1792	A1591
A2450	A2386	U2324	U2254	U	U2189	G2075		U1925	U1864	C1793	U1925	U1864	U1925	U1864	C1793	C1592
	U2387	G2325	U2255	U	U2190	U2076		U1926	U1865	C1794	U1926	U1865	U1926	U1865	C1794	U1593
G2454	A2388	A2328	C2256	U	G2133	A2077		U1927	G1866	U1795	U1927	G1866	U1927	G1866	U1795	U1594
G2455	G2389	U2329	U2257	U	A2134	C2072		U1928	U1867	U1796	U1928	U1867	U1928	U1867	U1796	C1595
C2456	U2390	U2330	C2258	U	C2135	G2073		U1929	G1868	U1797	U1929	G1868	U1929	G1868	U1797	A1596
U2457	G2391	G2330	C2261	U	U2136	U2074		U1930	U1869	U1798	U1930	U1869	U1930	U1869	U1798	A1597
G2458	A2392	G2331	U2262	U	U2137	U2075		U1931	G1870	C1800	U1931	G1870	U1931	G1870	C1800	U1598
A2459	U2393	C2332	C2263	U	G2138	U2076		U1932	U1871	A1801	U1932	U1871	U1932	U1871	A1801	U1599
U2460	C2394	U2333	U2264	U	U2139	A2077		U1933	A1872	A1802	U1933	A1872	U1933	A1872	A1802	C1600
A2461	G2395	U2334	U2265	U	G2140	C2078		U1934	G1873	C1803	U1934	G1873	U1934	G1873	C1803	A1603
C2462	U2396	A2335	A2266	U	G2141	U2079		U1935	U1874	U1809	U1935	U1874	U1935	U1874	U1809	G1606
C2463	G2396	G2336	A2267	U	A2142	A2080		U1936	G1875	A1810	U1936	G1875	U1936	G1875	A1810	C1607
		G2337	A2268	U	G2143	U2081		U1937	U1879	U1811	U1937	U1879	U1937	U1879	U1811	A1608
C2466	U2401	C2338	G2269	U	G2144	A2082		U1938	U1880	A1812	U1938	U1880	U1938	U1880	A1812	A1609
C2467	U2402	A2339	A2270	U	C2145	U2085		U1939	U1881	G1813	U1939	U1881	U1939	U1881	G1813	A1610
A2468		A2340	G2271	U	C2146	G2086		U1940	U1882	U1814	U1940	U1882	U1940	U1882	U1814	G1613
A2469	G2405	G2341	U2272	U	G2147	G2087		U1941	U1883	U1815	U1941	U1883	U1941	U1883	U1815	A1616
G2470	A2406	C2342	A2273	U	G2148	A2088		U1942	U1884	C1816	U1942	U1884	U1942	U1884	C1816	C1617
A2471		U2343		U	C2149	C2089		U1943	U1885	G1817	U1943	U1885	U1943	U1885	G1817	A1618
G2472	G2409	U2344	G2276	U	U2151	U2092		U1944	U1886	U1818	U1944	U1886	U1944	U1886	U1818	G1619
U2473	G2410	A2345	G2277	U	C2152	G2093		U1945	U1889	A1819	U1945	U1889	U1945	U1889	A1819	
U2474	A2411	A2346	U2278	U	C2153	A2094		U1946	U1890	U1819	U1946	U1890	U1946	U1890	U1819	
C2475	A2412	C2347	G2282	U	A2154	A2095		U1947	U1891	U1819	U1947	U1891	U1947	U1891	U1819	
A2476	G2413	U2348	C2283	U		A2096		U1948	U1892	U1819	U1948	U1892	U1948	U1892	U1819	
U2477		C2350	C2284	U	G2157	C2096		U1949	U1893	U1819	U1949	U1893	U1949	U1893	U1819	
	G2415	G2351	G2286	U	A	A2097		U1950	U1894	U1819	U1950	U1894	U1950	U1894	U1819	
A2482	C2416	A2352	A2287	U	C	U2098		U1951	U1895	U1819	U1951	U1895	U1951	U1895	U1819	
C2483	G2417	G2353	C2287	U	G	U2099		U1952	U1896	U1819	U1952	U1896	U1952	U1896	U1819	
G2484	C2418	C2354	G2290	U	C	G2100		U1953	U1897	U1819	U1953	U1897	U1953	U1897	U1819	



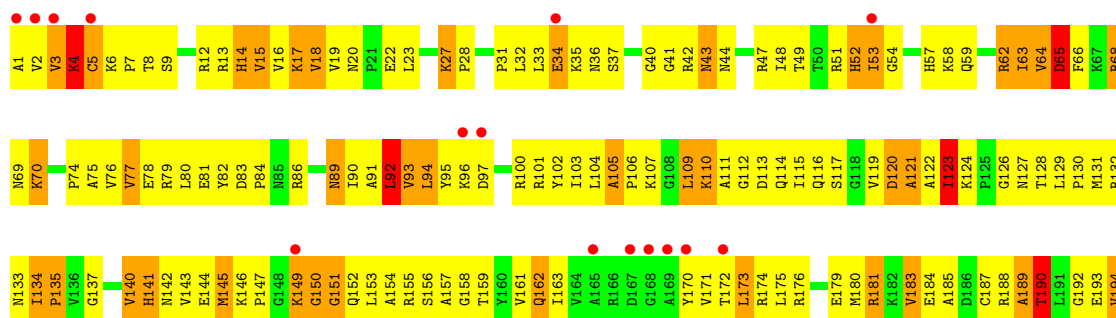
• Molecule 3: 50S ribosomal protein L11

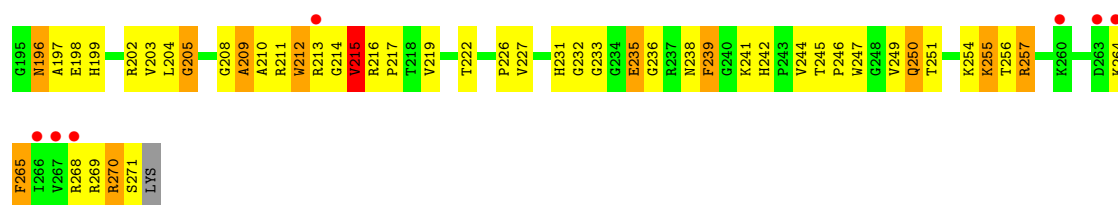
Chain I:



• Molecule 4: 50S ribosomal protein L2

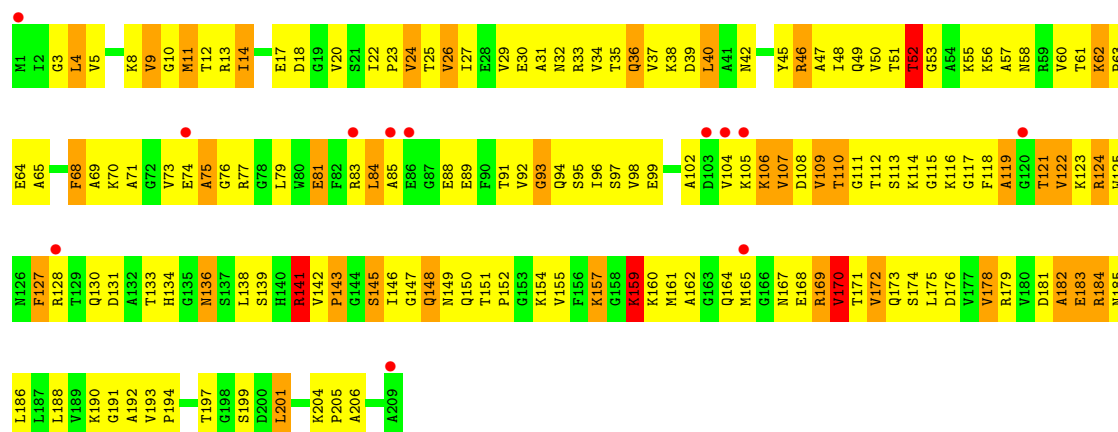
Chain C:





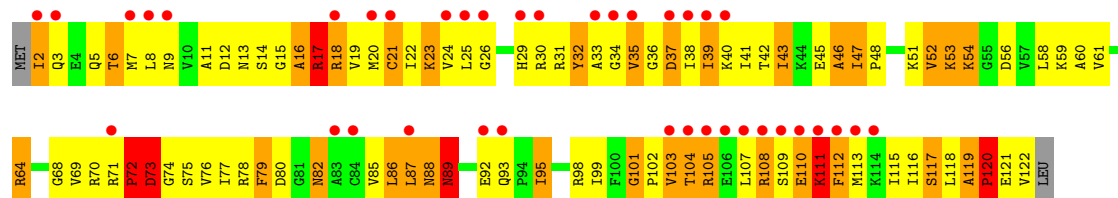
• Molecule 5: 50S ribosomal protein L3

Chain D:



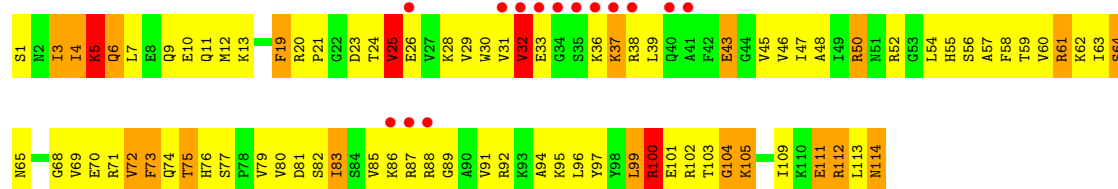
• Molecule 6: 50S ribosomal protein L14

Chain K:



• Molecule 7: 50S ribosomal protein L19

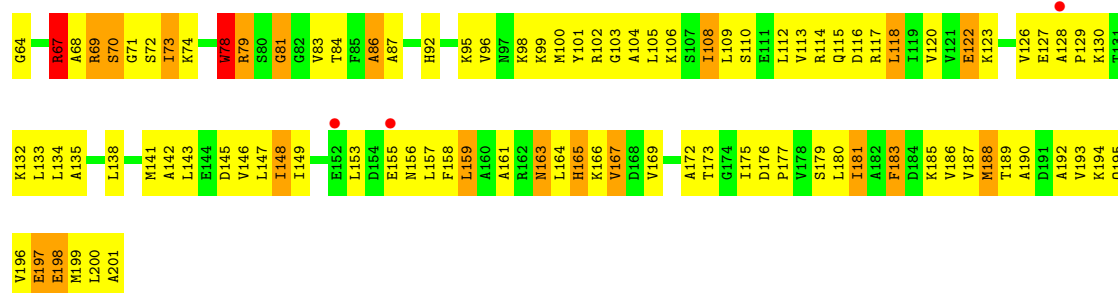
Chain P:



• Molecule 8: 50S ribosomal protein L4

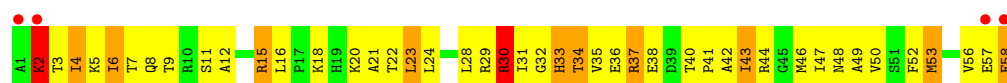
Chain E:





- Molecule 9: 50S ribosomal protein L30

Chain Y:



- Molecule 10: 50S ribosomal protein L32

Chain 0:



- Molecule 11: 50S ribosomal protein L36

Chain 4:



- Molecule 12: 50S ribosomal protein L33

Chain 1:



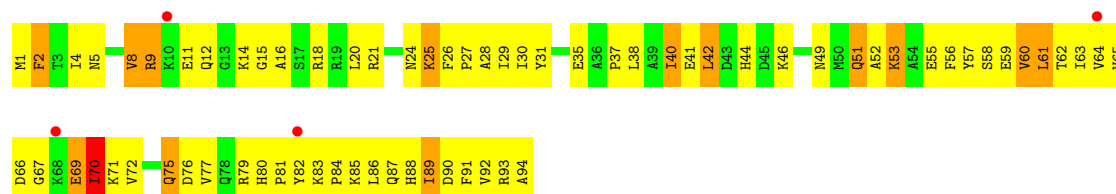
- Molecule 13: 50S ribosomal protein L35

Chain 3:



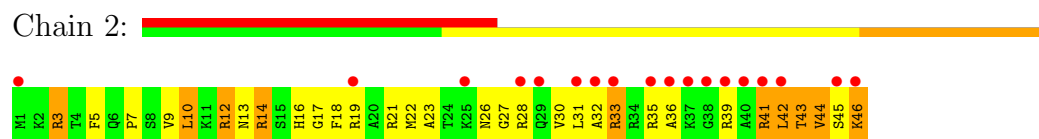
- Molecule 14: 50S ribosomal protein L25

Chain V:

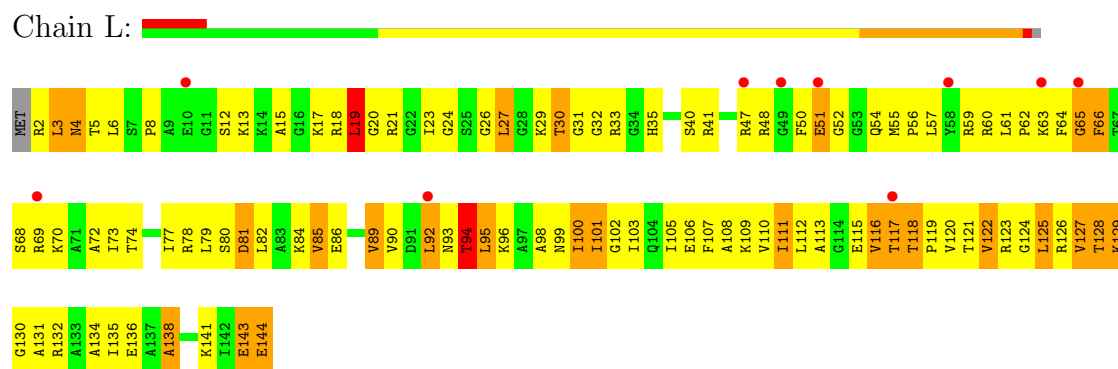




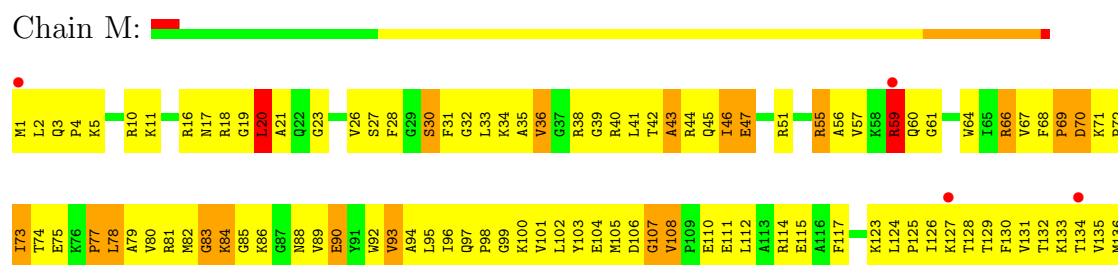
- Molecule 15: 50S ribosomal protein L34



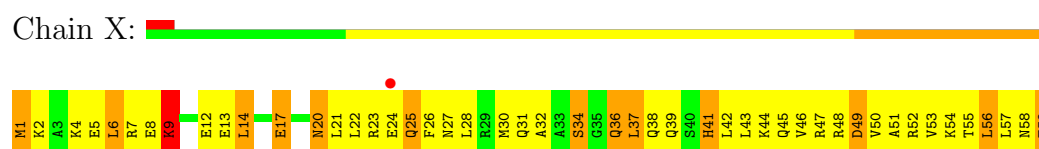
- Molecule 16: 50S ribosomal protein L15



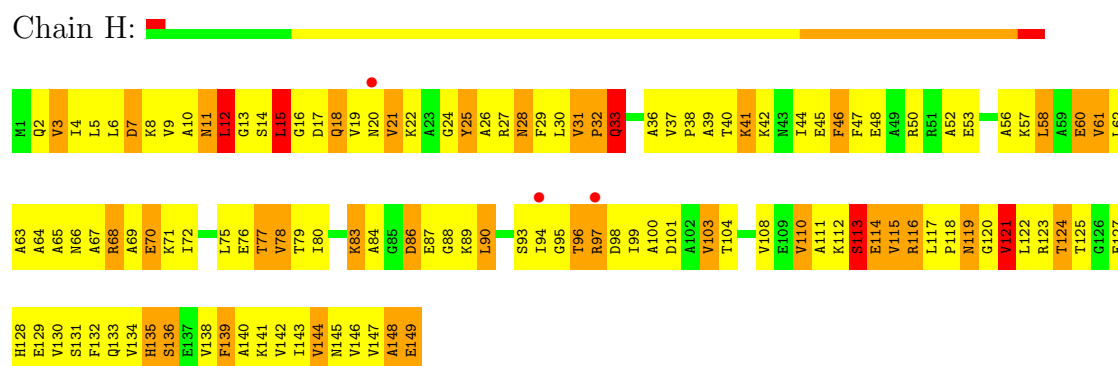
- Molecule 17: 50S ribosomal protein L16



- Molecule 18: 50S ribosomal protein L29

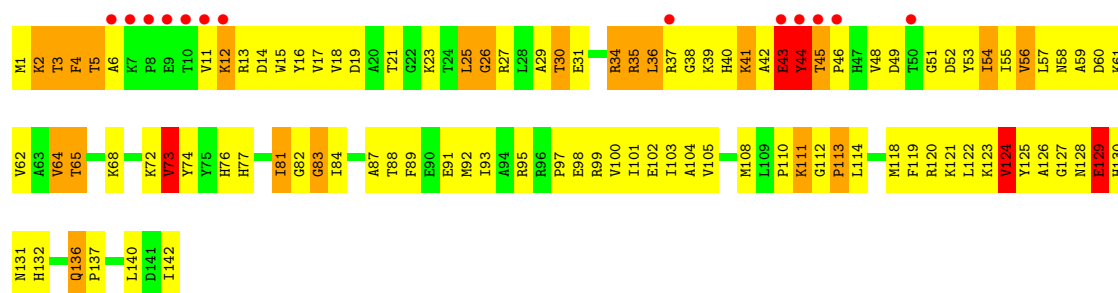


- Molecule 19: 50S ribosomal protein L9



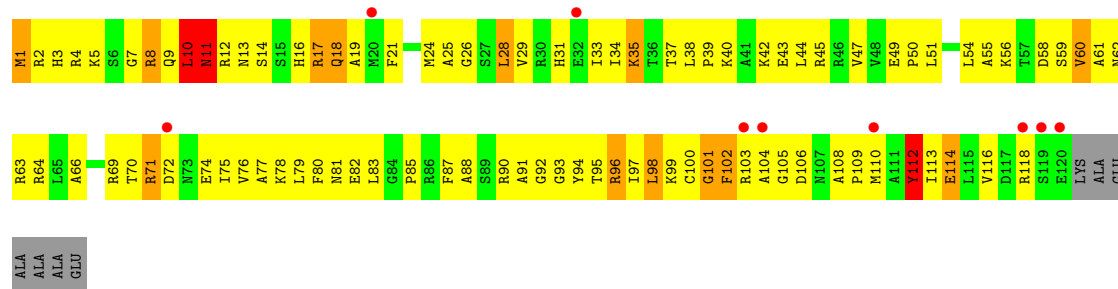
- Molecule 20: 50S ribosomal protein L13





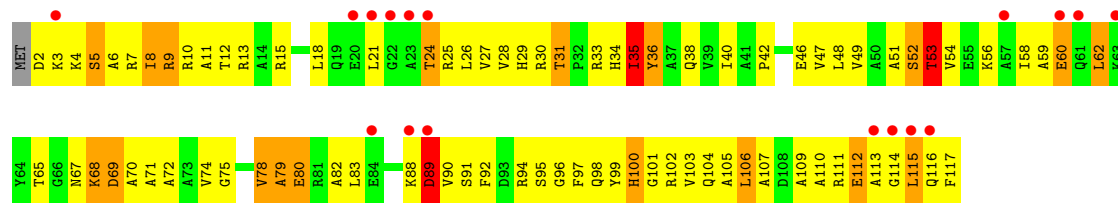
- Molecule 21: 50S ribosomal protein L17

Chain N:



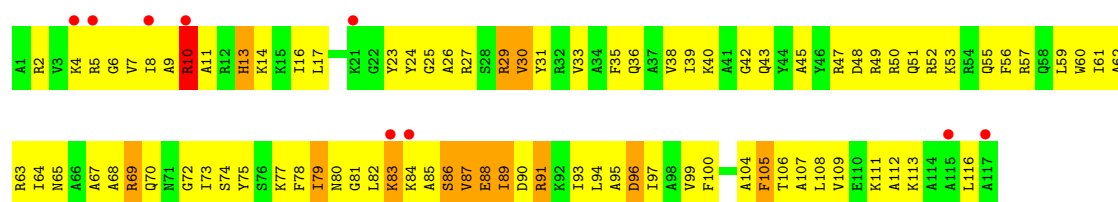
- Molecule 22: 50S ribosomal protein L18

Chain O:



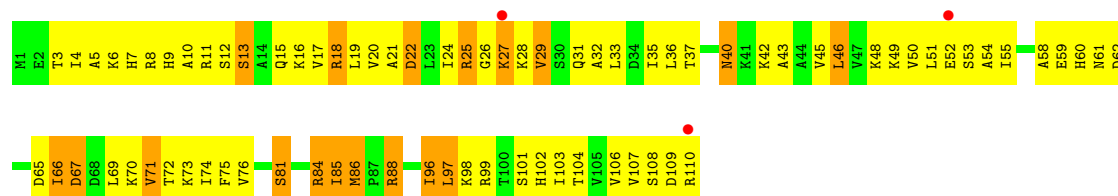
- Molecule 23: 50S ribosomal protein L20

Chain Q:



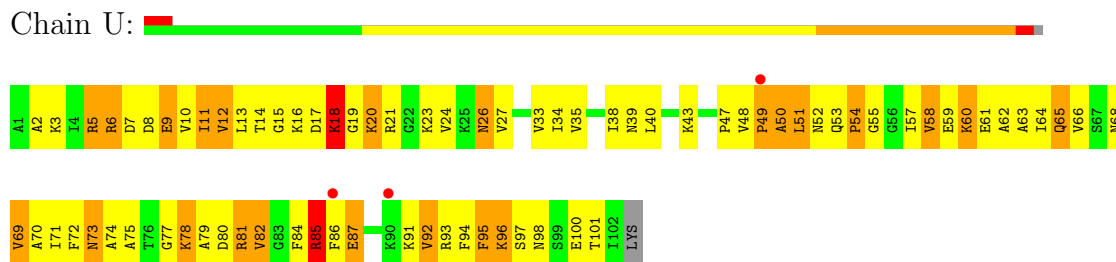
- Molecule 24: 50S ribosomal protein L22

Chain S:



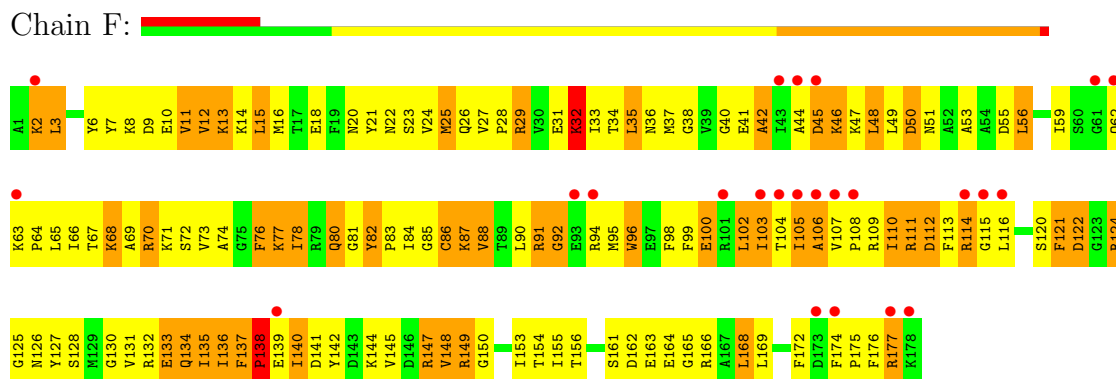
- Molecule 25: 50S ribosomal protein L24

Chain U:



- Molecule 26: 50S ribosomal protein L5

Chain F:



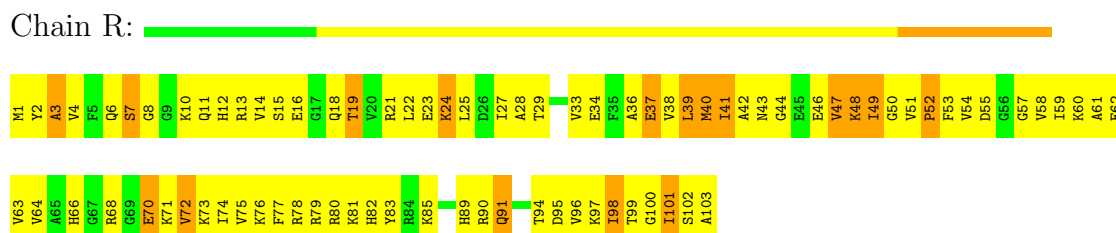
- Molecule 27: 50S ribosomal protein L6

Chain G:



- Molecule 28: 50S ribosomal protein L21

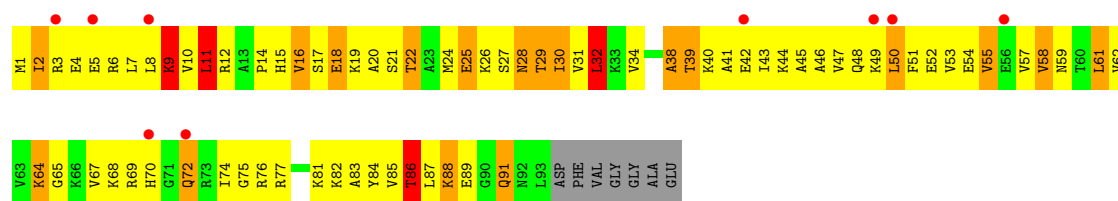
Chain R:



- Molecule 29: 50S ribosomal protein L23

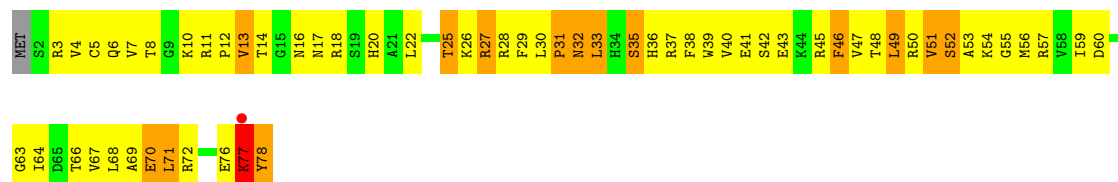
Chain T:





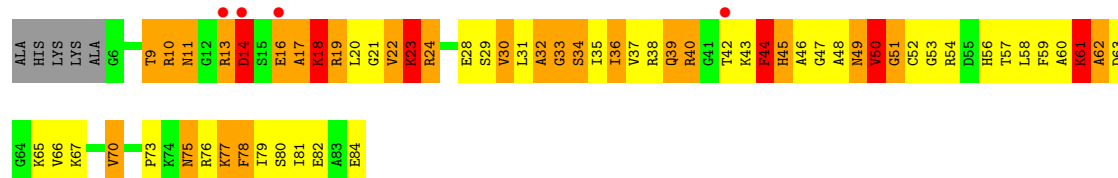
• Molecule 30: 50S ribosomal protein L28

Chain Z:



• Molecule 31: 50S ribosomal protein L27

Chain W:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.50 182.94 – 3.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.50) 73.0 (182.94-3.53)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.264 , 0.306 0.473 , 0.483	Depositor DCC
$R_{free}$ test set	25267 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	132.6	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 22.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 521228 reflections	Xtriage
$F_o, F_c$ correlation	0.67	EDS
Total number of atoms	90305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.25	0/2803	0.74	0/4371
2	B	0.28	6/68314 (0.0%)	0.77	41/106569 (0.0%)
3	I	0.25	0/1046	0.47	0/1410
4	C	0.22	0/2121	0.47	0/2852
5	D	0.24	0/1586	0.47	0/2134
6	K	0.23	0/939	0.52	0/1258
7	P	0.24	0/929	0.49	0/1242
8	E	0.24	0/1571	0.49	0/2113
9	Y	0.24	0/453	0.48	0/605
10	O	0.22	0/450	0.51	0/599
11	4	0.23	0/303	0.44	0/397
12	1	0.27	0/416	0.47	0/554
13	3	0.24	0/513	0.47	0/676
14	V	0.25	0/766	0.43	0/1025
15	2	0.26	0/380	0.47	0/498
16	L	0.23	0/1054	0.47	0/1403
17	M	0.25	0/1093	0.47	0/1460
18	X	0.24	0/510	0.52	0/677
19	H	0.25	0/1122	0.46	0/1515
20	J	0.23	0/1152	0.47	0/1551
21	N	0.24	0/973	0.49	0/1301
22	O	0.23	0/902	0.47	0/1209
23	Q	0.25	0/960	0.46	0/1278
24	S	0.21	0/864	0.50	0/1156
25	U	0.25	0/787	0.45	0/1051
26	F	0.25	0/1444	0.50	0/1937
27	G	0.23	0/1343	0.46	0/1816
28	R	0.25	0/829	0.46	0/1107
29	T	0.22	0/744	0.51	0/994
30	Z	0.25	0/635	0.48	0/848
31	W	0.27	0/603	0.48	0/797
All	All	0.27	6/97605 (0.0%)	0.71	41/146403 (0.0%)

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
2	B	0	43

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1086	A	C5-C6	-15.80	1.26	1.41
2	B	1088	A	C6-N1	-10.48	1.28	1.35
2	B	1060	U	C2-N3	7.81	1.43	1.37
2	B	1086	A	N3-C4	-7.68	1.30	1.34
2	B	1086	A	N7-C5	-6.09	1.35	1.39

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2204	G	O5'-P-OP1	-29.68	75.09	110.70
2	B	2791	G	O5'-P-OP2	-27.53	77.67	110.70
2	B	2791	G	O5'-P-OP1	17.94	132.23	110.70
2	B	2204	G	O5'-P-OP2	17.65	131.88	110.70
2	B	2790	U	OP2-P-O3'	14.62	137.37	105.20

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	221	A	Sidechain
2	B	222	A	Sidechain
2	B	232	G	Sidechain
2	B	299	A	Sidechain
2	B	51	G	Sidechain

## 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	2507	0	1270	107	0
2	B	60995	0	30678	2309	0
3	I	1032	0	1088	176	0
4	C	2082	0	2157	218	0
5	D	1565	0	1616	207	0
6	K	930	0	1000	135	0
7	P	917	0	965	114	0
8	E	1552	0	1619	183	0
9	Y	449	0	491	57	0
10	0	444	0	461	40	0
11	4	302	0	340	39	0
12	1	409	0	440	38	0
13	3	504	0	574	44	0
14	V	753	0	780	100	0
15	2	377	0	418	45	0
16	L	1045	0	1117	153	0
17	M	1074	0	1157	115	0
18	X	509	0	543	67	0
19	H	1111	0	1148	179	0
20	J	1129	0	1162	127	0
21	N	960	0	1000	114	0
22	O	892	0	923	102	0
23	Q	947	0	1022	143	0
24	S	857	0	922	92	0
25	U	779	0	834	111	0
26	F	1420	0	1460	213	0
27	G	1323	0	1374	178	0
28	R	816	0	839	105	0
29	T	738	0	807	116	0
30	Z	625	0	652	67	0
31	W	596	0	610	127	0
32	B	42	0	46	1	0
33	B	111	0	0	0	0
34	4	1	0	0	0	0
35	B	504	0	0	14	0
35	C	4	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
35	L	1	0	0	0	0
35	R	1	0	0	0	0
All	All	90305	0	59513	5347	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 5347 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1099:G:H8	3:I:3:LYS:N	1.32	1.27
2:B:1098:A:H3'	3:I:3:LYS:HA	1.32	1.08
2:B:704:G:H2'	2:B:726:G:H22	1.21	1.05
29:T:29:THR:HA	29:T:86:THR:HA	1.37	1.05
9:Y:12:ALA:HA	9:Y:15:ARG:HD3	1.37	1.05

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	I	139/141 (99%)	115 (83%)	19 (14%)	5 (4%)	5	49
4	C	269/272 (99%)	162 (60%)	61 (23%)	46 (17%)	0	4
5	D	207/209 (99%)	118 (57%)	58 (28%)	31 (15%)	0	6
6	K	119/123 (97%)	69 (58%)	29 (24%)	21 (18%)	0	4
7	P	112/114 (98%)	66 (59%)	29 (26%)	17 (15%)	0	6
8	E	199/201 (99%)	124 (62%)	48 (24%)	27 (14%)	0	8
9	Y	56/58 (97%)	40 (71%)	11 (20%)	5 (9%)	1	18
10	0	54/56 (96%)	36 (67%)	12 (22%)	6 (11%)	1	13
11	4	36/38 (95%)	21 (58%)	8 (22%)	7 (19%)	0	3
12	1	48/54 (89%)	35 (73%)	9 (19%)	4 (8%)	1	20
13	3	62/64 (97%)	39 (63%)	18 (29%)	5 (8%)	1	21
14	V	92/94 (98%)	59 (64%)	23 (25%)	10 (11%)	1	13
15	2	44/46 (96%)	24 (54%)	16 (36%)	4 (9%)	1	18
16	L	141/144 (98%)	78 (55%)	42 (30%)	21 (15%)	0	6
17	M	134/136 (98%)	91 (68%)	26 (19%)	17 (13%)	0	10

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	X	61/63 (97%)	35 (57%)	22 (36%)	4 (7%)	2	28
19	H	147/149 (99%)	86 (58%)	38 (26%)	23 (16%)	0	5
20	J	140/142 (99%)	88 (63%)	32 (23%)	20 (14%)	0	7
21	N	118/127 (93%)	74 (63%)	32 (27%)	12 (10%)	1	14
22	O	114/117 (97%)	79 (69%)	25 (22%)	10 (9%)	1	19
23	Q	115/117 (98%)	75 (65%)	33 (29%)	7 (6%)	2	30
24	S	108/110 (98%)	67 (62%)	28 (26%)	13 (12%)	1	11
25	U	100/103 (97%)	54 (54%)	31 (31%)	15 (15%)	0	6
26	F	176/178 (99%)	102 (58%)	48 (27%)	26 (15%)	0	6
27	G	174/176 (99%)	110 (63%)	40 (23%)	24 (14%)	0	8
28	R	101/103 (98%)	59 (58%)	31 (31%)	11 (11%)	1	13
29	T	91/100 (91%)	47 (52%)	27 (30%)	17 (19%)	0	3
30	Z	75/78 (96%)	48 (64%)	19 (25%)	8 (11%)	1	13
31	W	77/84 (92%)	26 (34%)	25 (32%)	26 (34%)	0	0
All	All	3309/3397 (97%)	2027 (61%)	840 (25%)	442 (13%)	0	9

5 of 442 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	5	GLN
3	I	18	ASN
4	C	15	VAL
4	C	18	VAL
4	C	53	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	I	109/109 (100%)	103 (94%)	6 (6%)	30	77
4	C	216/217 (100%)	184 (85%)	32 (15%)	4	26
5	D	164/164 (100%)	136 (83%)	28 (17%)	3	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	K	102/104 (98%)	73 (72%)	29 (28%)	0	4
7	P	99/99 (100%)	83 (84%)	16 (16%)	3	21
8	E	165/165 (100%)	145 (88%)	20 (12%)	7	36
9	Y	48/48 (100%)	37 (77%)	11 (23%)	1	7
10	O	47/47 (100%)	38 (81%)	9 (19%)	2	13
11	4	34/34 (100%)	31 (91%)	3 (9%)	14	57
12	1	45/48 (94%)	35 (78%)	10 (22%)	1	8
13	3	51/51 (100%)	48 (94%)	3 (6%)	28	75
14	V	78/78 (100%)	65 (83%)	13 (17%)	3	19
15	2	38/38 (100%)	28 (74%)	10 (26%)	1	5
16	L	102/103 (99%)	85 (83%)	17 (17%)	3	19
17	M	109/109 (100%)	93 (85%)	16 (15%)	4	26
18	X	55/55 (100%)	43 (78%)	12 (22%)	1	8
19	H	114/114 (100%)	87 (76%)	27 (24%)	1	7
20	J	116/116 (100%)	100 (86%)	16 (14%)	5	29
21	N	100/103 (97%)	85 (85%)	15 (15%)	4	26
22	O	86/87 (99%)	67 (78%)	19 (22%)	1	8
23	Q	89/89 (100%)	77 (86%)	12 (14%)	6	30
24	S	93/93 (100%)	83 (89%)	10 (11%)	9	44
25	U	83/84 (99%)	68 (82%)	15 (18%)	2	15
26	F	149/149 (100%)	112 (75%)	37 (25%)	1	6
27	G	137/137 (100%)	113 (82%)	24 (18%)	3	17
28	R	84/84 (100%)	72 (86%)	12 (14%)	5	28
29	T	80/84 (95%)	66 (82%)	14 (18%)	3	17
30	Z	67/68 (98%)	56 (84%)	11 (16%)	3	20
31	W	59/62 (95%)	44 (75%)	15 (25%)	1	5
All	All	2719/2739 (99%)	2257 (83%)	462 (17%)	3	18

5 of 462 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	M	5	LYS
19	H	129	GLU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
29	T	11	LEU
17	M	70	ASP
18	X	59	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
16	L	4	ASN
18	X	45	GLN
29	T	92	ASN
16	L	35	HIS
17	M	17	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	20 (17%)	1 (0%)
2	B	2838/2904 (97%)	437 (15%)	20 (0%)
All	All	2954/3024 (97%)	457 (15%)	21 (0%)

5 of 457 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	G
1	A	15	A
1	A	16	G
1	A	24	G
1	A	25	U

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1607	C
2	B	2133	G
2	B	2732	G
2	B	1301	A
2	B	2756	U

## 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 113 ligands modelled in this entry, 112 are monoatomic - leaving 1 for Mogul analysis.

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	NMY	B	3521	-	45,45,45	2.22	14 (31%)	67,67,67	1.29	7 (10%)

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	NMY	B	3521	-	-	0/18/94/94	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	3521	NMY	C8-C7	6.15	1.57	1.52
32	B	3521	NMY	C8-C9	5.93	1.56	1.52
32	B	3521	NMY	O22-C18	4.58	1.53	1.41
32	B	3521	NMY	C3-C2	4.37	1.59	1.53
32	B	3521	NMY	O5-C1	3.52	1.50	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	3521	NMY	O11-C13-O16	4.51	115.82	111.51
32	B	3521	NMY	O22-C22-C23	3.91	111.77	106.97
32	B	3521	NMY	O18-C18-C19	3.04	114.10	108.09
32	B	3521	NMY	O5-C5-C6	3.00	110.66	106.97
32	B	3521	NMY	C18-O22-C22	2.83	119.23	113.73

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	117/120 (97%)	-0.02	4 (3%) 43 19	36, 86, 127, 180	0
2	B	2841/2904 (97%)	-0.04	168 (5%) 22 9	5, 48, 146, 180	0
3	I	141/141 (100%)	-0.38	1 (0%) 84 56	91, 179, 180, 180	0
4	C	271/272 (99%)	0.27	22 (8%) 12 6	5, 40, 100, 146	0
5	D	209/209 (100%)	0.19	12 (5%) 23 10	5, 49, 129, 180	0
6	K	121/123 (98%)	1.70	38 (31%) 1 1	5, 41, 118, 180	0
7	P	114/114 (100%)	0.49	14 (12%) 5 3	5, 49, 103, 145	0
8	E	201/201 (100%)	-0.10	9 (4%) 32 14	5, 70, 144, 180	0
9	Y	58/58 (100%)	0.32	4 (6%) 17 7	5, 66, 116, 142	0
10	0	56/56 (100%)	0.00	3 (5%) 25 10	12, 58, 116, 165	0
11	4	38/38 (100%)	-0.14	0 100 100	7, 60, 114, 135	0
12	1	50/54 (92%)	0.33	5 (10%) 8 5	20, 69, 142, 157	0
13	3	64/64 (100%)	0.82	12 (18%) 2 2	5, 42, 88, 133	0
14	V	94/94 (100%)	0.13	4 (4%) 34 14	9, 96, 151, 169	0
15	2	46/46 (100%)	1.77	18 (39%) 1 1	11, 43, 103, 159	0
16	L	143/144 (99%)	0.16	10 (6%) 16 7	5, 56, 119, 164	0
17	M	136/136 (100%)	0.05	4 (2%) 49 23	7, 60, 116, 137	0
18	X	63/63 (100%)	-0.17	2 (3%) 45 21	38, 106, 178, 180	0
19	H	149/149 (100%)	-0.19	3 (2%) 62 30	11, 112, 162, 180	0
20	J	142/142 (100%)	0.22	13 (9%) 9 5	5, 59, 125, 180	0
21	N	120/127 (94%)	0.22	9 (7%) 14 7	5, 43, 103, 180	0
22	O	116/117 (99%)	0.52	17 (14%) 3 3	32, 85, 152, 180	0
23	Q	117/117 (100%)	0.27	9 (7%) 13 7	5, 52, 112, 161	0
24	S	110/110 (100%)	0.11	3 (2%) 52 24	5, 52, 131, 180	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	U	102/103 (99%)	-0.09	3 (2%) 49 23	22, 97, 158, 180	0
26	F	178/178 (100%)	0.55	24 (13%) 4 3	33, 110, 176, 180	0
27	G	176/176 (100%)	0.18	13 (7%) 14 7	26, 98, 169, 180	0
28	R	103/103 (100%)	-0.18	0 100 100	13, 79, 144, 180	0
29	T	93/100 (93%)	0.39	9 (9%) 8 5	13, 79, 154, 180	0
30	Z	77/78 (98%)	-0.13	1 (1%) 74 40	5, 47, 124, 144	0
31	W	79/84 (94%)	0.12	4 (5%) 27 11	9, 77, 144, 164	0
All	All	6325/6421 (98%)	0.10	438 (6%) 17 7	5, 59, 155, 180	0

The worst 5 of 438 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	645	C	12.6
6	K	110	GLU	11.5
2	B	1459	G	10.5
2	B	284	U	10.4
6	K	111	LYS	10.4

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
33	MG	B	2962	1/1	0.94	52.13	180,180,180,180	0

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	NMY	B	3521	42/42	0.43	12.43	68,68,68,68	42
33	MG	B	2987	1/1	0.36	8.54	109,109,109,109	0
33	MG	B	2933	1/1	0.22	8.20	81,81,81,81	0
33	MG	B	2970	1/1	0.33	5.16	137,137,137,137	0
33	MG	B	2938	1/1	0.42	4.41	80,80,80,80	0
33	MG	B	2963	1/1	0.24	4.10	96,96,96,96	0
33	MG	B	2952	1/1	0.45	4.02	66,66,66,66	0
33	MG	B	2964	1/1	0.20	3.62	117,117,117,117	0
33	MG	B	2939	1/1	0.67	2.93	85,85,85,85	0
33	MG	B	2919	1/1	0.19	2.26	53,53,53,53	0
33	MG	B	2981	1/1	0.19	1.91	24,24,24,24	0
33	MG	B	2911	1/1	0.15	1.68	41,41,41,41	0
33	MG	B	2973	1/1	0.27	1.65	38,38,38,38	0
33	MG	B	2957	1/1	0.19	1.41	80,80,80,80	0
33	MG	B	3005	1/1	0.18	1.18	6,6,6,6	0
33	MG	B	2932	1/1	0.28	0.94	30,30,30,30	0
33	MG	B	2951	1/1	0.23	0.27	14,14,14,14	0
33	MG	B	2980	1/1	0.13	0.25	28,28,28,28	0
33	MG	B	2994	1/1	0.50	0.17	55,55,55,55	0
33	MG	B	2936	1/1	0.25	0.07	82,82,82,82	0
33	MG	B	2927	1/1	0.21	0.02	32,32,32,32	0
33	MG	B	2907	1/1	0.20	-0.01	41,41,41,41	0
33	MG	B	2945	1/1	0.27	-0.10	17,17,17,17	0
33	MG	B	2982	1/1	0.16	-0.21	80,80,80,80	0
33	MG	B	2999	1/1	0.19	-0.24	115,115,115,115	0
33	MG	B	2930	1/1	0.14	-0.27	72,72,72,72	0
33	MG	B	2965	1/1	0.16	-0.33	75,75,75,75	0
33	MG	B	2989	1/1	0.16	-0.33	41,41,41,41	0
33	MG	B	2991	1/1	0.13	-0.38	37,37,37,37	0
33	MG	B	2915	1/1	0.12	-0.40	32,32,32,32	0
33	MG	B	3015	1/1	0.12	-0.46	87,87,87,87	0
33	MG	B	2916	1/1	0.17	-0.47	12,12,12,12	0
33	MG	B	2928	1/1	0.13	-0.49	47,47,47,47	0
33	MG	B	2941	1/1	0.14	-0.51	10,10,10,10	0
33	MG	B	3011	1/1	0.21	-0.55	27,27,27,27	0
33	MG	B	2949	1/1	0.12	-0.68	104,104,104,104	0
33	MG	B	2988	1/1	0.14	-0.75	12,12,12,12	0
33	MG	B	2956	1/1	0.41	-0.80	90,90,90,90	0
33	MG	B	3004	1/1	0.11	-0.82	20,20,20,20	0
33	MG	B	2913	1/1	0.15	-0.89	8,8,8,8	0
33	MG	B	3012	1/1	0.11	-0.90	33,33,33,33	0
33	MG	B	2959	1/1	0.20	-0.92	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	2996	1/1	0.08	-1.00	98,98,98,98	0
33	MG	B	2925	1/1	0.12	-1.01	5,5,5,5	0
33	MG	B	3010	1/1	0.12	-1.02	20,20,20,20	0
33	MG	B	2924	1/1	0.16	-1.10	5,5,5,5	0
33	MG	B	2974	1/1	0.14	-1.11	93,93,93,93	0
33	MG	B	2950	1/1	0.13	-1.13	27,27,27,27	0
33	MG	B	3013	1/1	0.16	-1.14	17,17,17,17	0
33	MG	B	2998	1/1	0.10	-1.14	39,39,39,39	0
33	MG	B	2948	1/1	0.28	-1.19	32,32,32,32	0
33	MG	B	2942	1/1	0.07	-1.21	19,19,19,19	0
33	MG	B	3014	1/1	0.07	-1.25	36,36,36,36	0
33	MG	B	2918	1/1	0.09	-1.30	37,37,37,37	0
33	MG	B	2969	1/1	0.08	-1.37	32,32,32,32	0
33	MG	B	2923	1/1	0.10	-1.37	6,6,6,6	0
33	MG	B	2908	1/1	0.09	-1.41	23,23,23,23	0
33	MG	B	2967	1/1	0.09	-1.46	34,34,34,34	0
33	MG	B	2954	1/1	0.06	-1.47	67,67,67,67	0
33	MG	B	3000	1/1	0.09	-1.53	12,12,12,12	0
33	MG	B	2976	1/1	0.16	-1.61	62,62,62,62	0
33	MG	B	2926	1/1	0.10	-1.64	7,7,7,7	0
33	MG	B	2910	1/1	0.08	-1.83	9,9,9,9	0
33	MG	B	2985	1/1	0.21	-1.84	9,9,9,9	0
34	ZN	4	624	1/1	0.06	-1.91	40,40,40,40	0
33	MG	B	2978	1/1	0.14	-1.98	58,58,58,58	0
33	MG	B	2984	1/1	0.08	-2.02	35,35,35,35	0
33	MG	B	2972	1/1	0.14	-2.02	8,8,8,8	0
33	MG	B	2937	1/1	0.04	-2.08	5,5,5,5	0
33	MG	B	3003	1/1	0.07	-2.10	6,6,6,6	0
33	MG	B	2979	1/1	0.07	-2.26	22,22,22,22	0
33	MG	B	2905	1/1	0.09	-2.29	5,5,5,5	0
33	MG	B	2968	1/1	0.06	-2.33	20,20,20,20	0
33	MG	B	2931	1/1	0.08	-2.35	17,17,17,17	0
33	MG	B	2955	1/1	0.07	-2.39	40,40,40,40	0
33	MG	B	2971	1/1	0.11	-2.69	36,36,36,36	0
33	MG	B	2922	1/1	0.12	-2.75	25,25,25,25	0
33	MG	B	2909	1/1	0.09	-2.78	13,13,13,13	0
33	MG	B	2944	1/1	0.09	-2.82	9,9,9,9	0
33	MG	B	2961	1/1	0.06	-2.88	39,39,39,39	0
33	MG	B	2940	1/1	0.07	-2.90	23,23,23,23	0
33	MG	B	2943	1/1	0.05	-2.91	78,78,78,78	0
33	MG	B	2986	1/1	0.06	-2.91	37,37,37,37	0
33	MG	B	2946	1/1	0.07	-3.02	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	B	2977	1/1	0.12	-3.09	29,29,29,29	0
33	MG	B	2934	1/1	0.03	-3.13	21,21,21,21	0
33	MG	B	2997	1/1	0.10	-3.20	5,5,5,5	0
33	MG	B	2914	1/1	0.26	-3.22	9,9,9,9	0
33	MG	B	2960	1/1	0.08	-3.22	11,11,11,11	0
33	MG	B	2958	1/1	0.06	-3.31	22,22,22,22	0
33	MG	B	3002	1/1	0.03	-3.32	9,9,9,9	0
33	MG	B	2993	1/1	0.09	-3.43	99,99,99,99	0
33	MG	B	3007	1/1	0.07	-3.45	31,31,31,31	0
33	MG	B	2906	1/1	0.09	-3.47	21,21,21,21	0
33	MG	B	2929	1/1	0.07	-3.52	16,16,16,16	0
33	MG	B	3006	1/1	0.04	-3.59	14,14,14,14	0
33	MG	B	2990	1/1	0.06	-3.67	11,11,11,11	0
33	MG	B	3008	1/1	0.07	-3.88	41,41,41,41	0
33	MG	B	3001	1/1	0.04	-4.06	41,41,41,41	0
33	MG	B	2917	1/1	0.07	-4.18	80,80,80,80	0
33	MG	B	2992	1/1	0.05	-4.42	13,13,13,13	0
33	MG	B	3009	1/1	0.16	-4.53	53,53,53,53	0
33	MG	B	2983	1/1	0.06	-4.81	46,46,46,46	0
33	MG	B	2935	1/1	0.09	-5.74	5,5,5,5	0
33	MG	B	2921	1/1	0.09	-6.42	5,5,5,5	0
33	MG	B	2920	1/1	0.05	-6.70	29,29,29,29	0
33	MG	B	2975	1/1	0.19	-6.72	36,36,36,36	0
33	MG	B	2947	1/1	0.04	-7.65	11,11,11,11	0
33	MG	B	2966	1/1	0.05	-7.76	50,50,50,50	0
33	MG	B	2995	1/1	0.03	-8.37	12,12,12,12	0
33	MG	B	2953	1/1	0.06	-9.15	6,6,6,6	0
33	MG	B	2912	1/1	0.12	-12.55	49,49,49,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.