



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:34 AM GMT

PDB ID : 2QBK
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin and ribosome recycling factor (RRF). This file contains the 50S subunit of the second 70S ribosome, with gentamicin and RRF bound. The entire crystal structure contains two 70S ribosomes and is described in remark 400.
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-17
Resolution : 4.00 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>

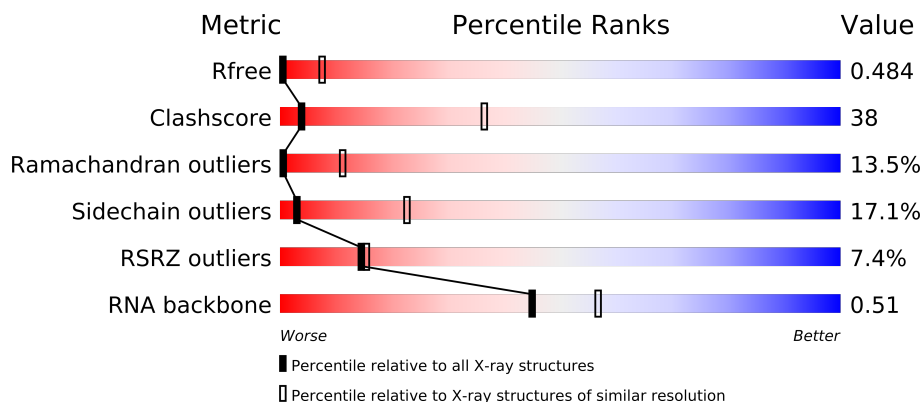
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.00 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	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)
RNA backbone	1838	1018 (5.00-2.80)

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

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	

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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	
32	6	185	

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

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	B	2932	-	X
33	MG	B	2938	-	X
33	MG	B	2939	-	X
33	MG	B	2952	-	X
33	MG	B	2956	-	X
33	MG	B	2964	-	X
33	MG	B	2994	-	X
33	MG	B	2999	-	X
33	MG	B	3005	-	X
33	MG	B	3010	-	X
34	LLL	B	3016	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 91772 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			

- 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			

- 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	0	0	0
			409	263	75	71			

- 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	0	0	0
			504	323	105	74	2			

- 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	0	0	0
			753	479	137	134	3			

- 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	0	0	0
			377	228	90	57	2			

- 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	0	0	0
			1045	649	206	189	1			

- 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	0	0	0
			1074	686	205	177	6			

- 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	0	0	0
			509	313	99	95	2			

- 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		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		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		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			

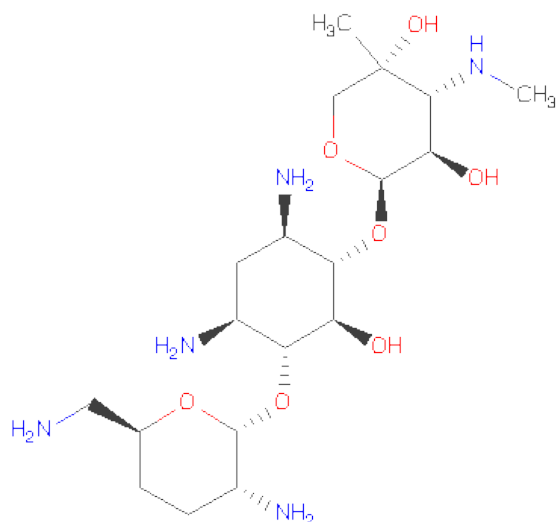
- Molecule 32 is a protein called 50S ribosomal protein RRF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- 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 (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	4	1	Total	Zn	0	0
			1	1		

- Molecule 36 is water.

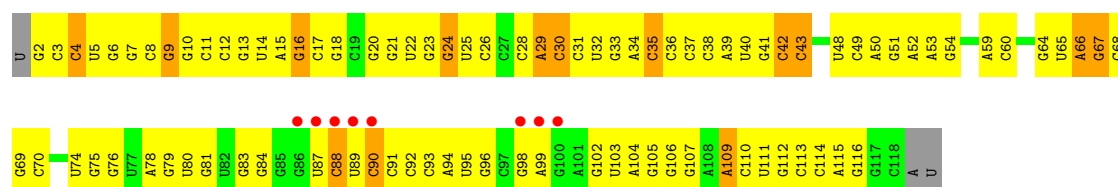
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	B	499	Total	O	0	0
			499	499		
36	C	6	Total	O	0	0
			6	6		
36	E	3	Total	O	0	0
			3	3		
36	L	2	Total	O	0	0
			2	2		
36	R	1	Total	O	0	0
			1	1		
36	T	1	Total	O	0	0
			1	1		

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

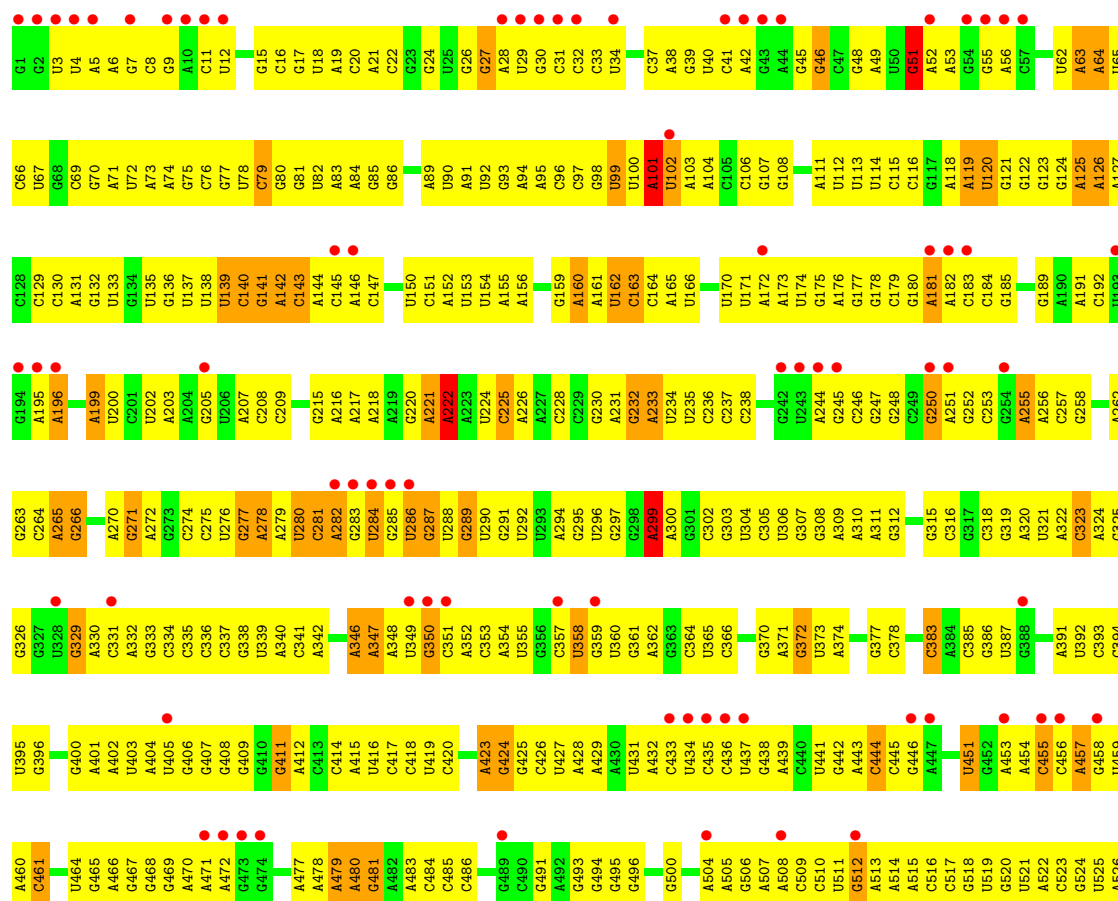
• Molecule 1: 5S rRNA

Chain A: 



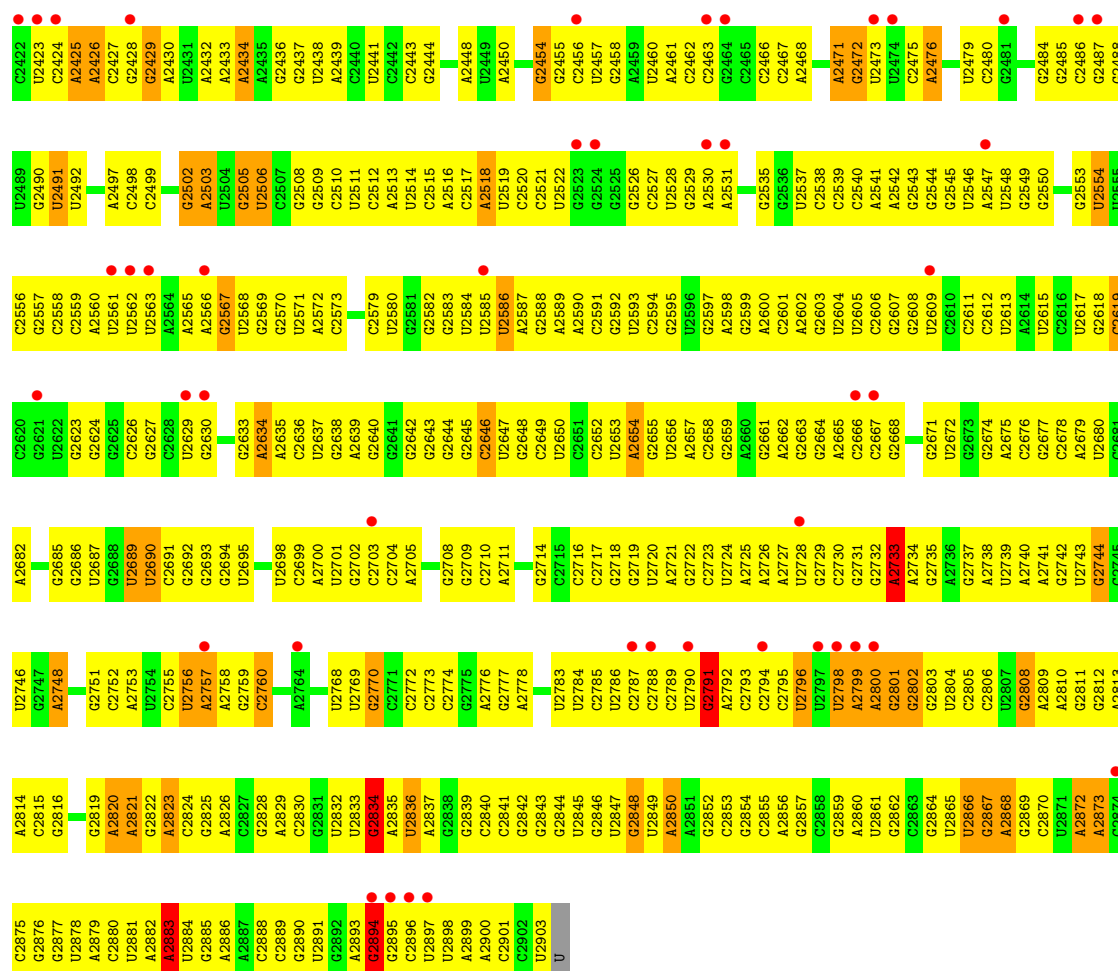
• Molecule 2: 23S rRNA

Chain B: 



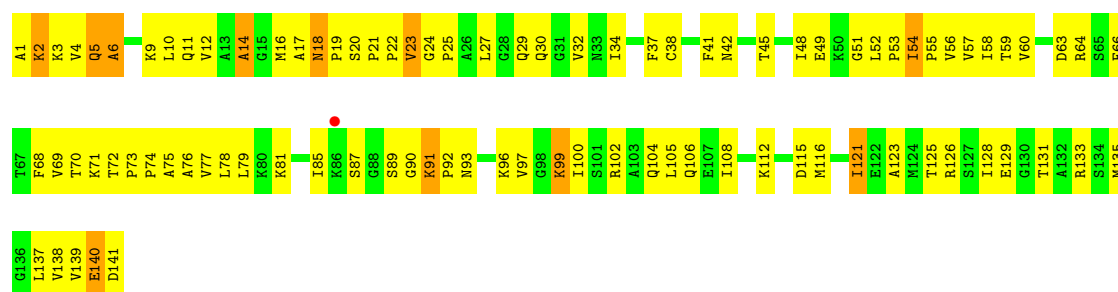
U1440	A1378	G1310	A1244	U1180	G1116	G1047	A980	A917	U850	A782	G713	U562	A590	C527
G1441	U1379	G1310	G1245	U1181	G1117	A1048	A981	A918	C551	A783	U714	U653	U591	A528
U1442	G1380	U1316	A1246	G1182	C1117	C1049	C982	A919	U852	G784	A715	A854	A592	A529
U1443	U1443	U1317	A1247	G1183	C1118	A1050	A983	U919	C953	G785	A716	A855	U593	G530
G1444	G1382	U1318	G1248	U1184	G1119	G1051	A984	A920	C854	C786	C717	G856	U594	C531
G1445	A1383	U1318	U1249	G1185	G1120	C1052	C985	C921	G855	C787	A718	U657	C595	A532
G1446	A1384	C1319	G1250	G1186	C1121	C1053	C986	C922	G856	A788	C719	U658	U596	G533
C1447	A1385	C1320	C1251	G1187	G1122	A1054	C987	A925	G857	A789	U720	G859	G597	U534
G1448	G1386	A1321	G1252	U1188	C1123	G1055	A989	G926	G858	A790	U721	C860	U598	G538
C1451	A1387	C1322	A1253	A1189	G1124	G1056	C991	G927	U860	C795	A722	A861	A599	G539
A1452	G1388	C1323	G1254	G1190	G1125	A1057	C992	U928	G861	C796	G725	G664	G600	A539
A1453	U1389	G1324	U1255	G1191	A1126	U1058	C993	U929	G862	G797	G726	U665	C601	C540
C1454	U1390	U1325	G1256	G1192	A1127	C1059	C994	G930	A863	G798	A727	A866	A603	A541
U1455	U1391	U1326	C1257	G1193	G1131	U1060	C995	U931	G864	G799	G728	U667	G604	C542
G1456	A1392	A1327	U1258	A1194	U1132	U1061	C996	U932	G865	A800	G729	A868	G605	C543
A1457	A1393	U1328	G1259	G1195	A1133	G1062	A996	U933	C965	G798	G730	G669	U606	C544
U1458	U1394	U1329	A1260	C1196	A1134	G1063	C997	U934	A866	G799	A731	A670	U607	U545
U1459	A1395	C1330	C1261	G1197	C1135	C1064	C998	U935	G869	C805	C732	C671	A608	U546
G1459	U1396	G1331	U1262	U1198	G1136	U1065	U999	C936	G870	C806	C733	C672	A609	A547
U1460	U1397	G1332	U1263	U1199	G1137	U1066	A1000	A936	U870	C807	C734	C673	G610	G548
C1461	C1398	G1333	A1264	C1200	G1138	G1068	A1001	C937	U871	U807	C735	C674	C611	C550
C1462	U1399	G1334	U1265	U1201	G1139	A1069	G1002	G938	U872	U808	C736	C675	G612	G551
C1463	U1400	C1335	G1266	G1202	C1140	A1070	G1007	G939	U873	U809	C737	C676	C613	U552
G1464	A1401	A1336	U1267	U1203	U1141	C1076	A941	G940	G874	U811	U740	A677	A614	G553
G1465	U1402	G1337	A1268	A1204	A1142	A1077	A942	G942	C875	C812	U741	A678	A615	U554
U1466	A1403	G1338	A1269	A1205	A1143	A1078	G943	G943	C876	U813	A742	C678	U616	U555
U1467	A1404	G1339	C1270	G1206	A1144	A1079	A944	A944	A877	C814	A743	C679	A616	G556
U1468	U1405	U1340	G1271	C1207	A1145	A1080	U1011	U1012	A878	C815	U744	C680	A556	A556
A1469	A1406	G1341	A1272	C1208	C1146	U1081	C1013	A945	G	C816	U745	G681	G620	C557
A1470	G1407	G1341	U1273	U1209	U1147	U1082	A1014	C946	G	C817	U746	G682	A621	U558
G1471	A1408	C1345	A1274	G1210	U1148	U1083	A1015	A947	G	C818	U747	U683	G622	G559
G1472	C1346	C1346	A1275	C1211	G1149	A1084	G1016	C948	G	A819	C748	G684	G623	C560
G1473	A1473	A1347	U1276	G1212	C1150	A1085	G1017	G949	G	A820	A753	U685	C624	G561
U1474	U1412	C1348	G1277	A1213	A1151	A1086	U1018	G950	U	G821	U754	C687	A563	U562
G1475	A1413	C1349	C1278	G1214	C1152	A1087	G1019	C951	C	A822	U755	U688	C564	C564
U1476	C1350	C1350	G1279	G1215	C1153	A1088	A1020	G952	A	C823	U756	U689	A626	U565
A1477	C1351	C1351	G1280	U1216	C1154	A1089	A1021	G953	U	U824	A757	G690	A627	U566
C1477	U1352	U1352	G1281	U1217	G1157	A1090	G1022	G954	C	A825	C757	C691	G630	U567
G1478	A1417	A1353	U1282	G1218	C1158	A1091	U1023	U955	C	U826	C758	C692	A631	U568
G1479	G1418	A1354	U1283	U1219	U1159	C1092	G1024	G956	C	U827	C759	C693	A632	U569
A1480	A1419	A1354	G1283	G1220	C1160	C1093	G1025	C957	G	U828	G760	U694	A633	G570
U1481	A1420	G1355	C1284	G1221	C1161	U1094	A1026	U958	A	G831	A764	G695	C634	U571
G1482	G1421	G1356	A1285	C1222	C1162	U1095	G1027	A959	C	U832	C765	G696	C635	A572
G1483	G1422	C1357	G1286	U1222	G1163	A1096	A1028	A960	U	A833	C766	G697	C636	U573
U1484	G1423	G1358	G1287	G1223	G1164	U1097	A1029	C961	C	A834	U767	C698	A637	A574
U1485	G1424	C1358	C1288	U1224	C1165	A1098	G1030	G962	A	G835	C768	C699	A638	A575
U1486	G1425	C1361	C1289	G1225	A1166	U1099	G1031	U963	C	G836	G769	G700	U639	U576
U1487	G1426	C1362	C1290	G1226	G1167	C1100	A1032	C964	C	C837	U769	G701	C640	G577
C1488	A1427	A1365	G1291	U1227	C1168	U1096	A1033	G965	C	C838	G770	U702	U641	U580
C1489	C1428	C1365	G1292	U1228	A1169	U1097	G1034	G966	U	U839	G771	U703	U642	C581
A1490	G1429	U1365	U1293	U1231	C1170	A1103	G1036	U967	C	C840	G772	U704	A643	C582
G1491	G1430	G1368	C1295	G1236	C1171	C1104	A1039	C968	C	G841	C773	A705	A644	G583
G1492	A1431	G1369	G1296	G1237	C1172	U1105	A1040	G969	G	U842	G774	A706	C645	C584
C1493	C1432	C1370	C1297	A1237	U1173	G1106	G1041	U970	A	A845	G775	G708	U646	G585
A1494	A1433	G1371	G1298	G1238	U1174	G1107	G1042	A971	C	U846	G776	U709	G647	U586
A1495	U1372	U1372	G1299	G1239	U1175	U1108	G1043	A972	A	U847	G777	U710	G648	A588
A1496	G1435	G1300	G1300	G1239	U1176	G1109	C1043	A973	A	U848	G778	U711	G649	C587
U1497	G1436	A1301	A1301	U1240	U1177	G1110	C1044	G974	C	C912	G780	G712	C650	U589
C1501	U1437	A1302	A1302	A1241	G1177	A1111	C1045	A974	C	U849	G781	G713	C651	
A1502	A1439	G1309	C1243	C1243	G1179	G1112	A1046	A979	U					

U2356	G2295	G2048	C1974	C1905	C1843	C1774	C1704	A1635	C1565	A1503
G2357	U2296	G2049	A1977	G1906	C1844	U1775	A1705	U1636	A1566	A1504
A2358	A2297	G2050	G1983	C1907	G1845	G1776	C1708	C1637	G1567	U1506
C2359	U2232	A2051	G1984	C1908	A1846	U1777	C1709	C1638	G1568	C1507
G2360	G2234	A2052	G1985	C1909	A1847	U1778	G1710	A1640	C1569	A1508
C2361	C2235	G2053	C1986	G1910	A1848	U1779	A1711	A1570	U1570	C1509
C2362	U2236	A2054	C1987	U1911	G1849	A1783	U1712	A1571	A1571	G1510
G2363	G2237	G2055	A1987	A1912	A1853	U1784	U1713	A1572	G1511	G1511
G2238	G2238	G2056	G1988	A1913	A1854	A1785	U1714	G1573	U1512	C1512
U2180	A2060	G2061	G1991	U1914	A1855	A1786	U1715	C1574	U1513	U1513
U2181	G2062	G2062	U1992	U1915	A1856	A1787	U1716	C1575	G1514	G1514
U2182	C2063	C2063	U1993	A1916	G1857	C1788	U1717	C1576	U1576	C1576
A2183	G2064	C2064	U1994	U1917	A1858	A1789	G1718	C1577	G1515	G1515
A2184	G2065	C2065	U1995	A1918	A1859	C1790	G1719	U1578	U1578	G1516
U2185	C2066	C2066	U1996	U1923	G1860	C1791	U1720	A1579	C1517	C1517
U2186	G2067	C2067	C1996	C1924	G1861	G1792	U1721	A1580	G1518	G1518
U2187	G2068	C2068	C1997	C1925	G1862	G1793	A1722	C1582	U1520	G1519
U2188	U2069	C2069	A1998	U1926	G1863	A1794	G1723	A1583	G1521	G1521
G2190	C2070	A2070	C2001	A1927	A1864	C1795	U1726	U1584	A1522	U1522
A2191	C2071	A2071	U2007	A1928	A1865	U1796	C1727	C1585	U1523	U1523
U2192	C2072	C2072	C2008	G1929	A1866	G1797	C1728	A1586	G1524	A1524
G2193	G2073	C2073	C2009	U1931	G1867	U1798	U1729	A1590	C1526	C1526
U2194	U2074	C2074	A2008	G1932	G1868	G1799	U1730	A1591	G1527	G1527
U2195	U2075	C2075	G2010	U1933	C1869	C1800	G1731	C1592	A1528	A1528
C2196	U2076	U2076	G2011	C1934	C1870	A1801	C1732	A1593	G1529	G1529
G2233	A2077	A2077	C2012	U1935	A1871	A1802	G1733	A1594	C1530	C1530
A2198	G2078	C2078	A2013	G1936	G1872	C1803	G1734	C1595	C1533	C1533
A2199	U2079	C2079	A2014	A1937	G1873	C1804	A1735	A1596	U1534	U1534
C2200	A2080	C2080	A2015	A1938	G1874	A1805	G1736	A1597	A1535	A1535
U2201	U2081	C2081	U2016	U1939	G1875	C1806	U1737	A1598	C1536	C1536
U2202	A2082	C2082	U2019	U1940	A1876	G1807	G1738	C1600	U1539	U1539
U2203	G2083	C2083	A2020	C1941	G1877	U1812	U1739	A1603	G1540	G1540
G2204	C2084	C2084	C2021	C1942	A1878	G1813	G1740	C1604	C1541	C1541
C2205	U2085	C2085	U2022	U1943	C1881	G1814	G1741	C1605	U1542	U1542
C2206	U2086	C2086	U2023	G1945	U1882	A1815	G1743	C1606	G1943	G1943
C2207	G2087	C2087	C2024	U1946	U1883	G1816	A1744	C1607	A1544	A1544
C2208	A2088	C2088	G2025	C1947	G1884	G1817	A1745	A1608	A1545	A1545
G2209	A2090	C2090	U2026	G1948	A1885	U1818	U1746	A1609	G1546	G1546
U2210	C2091	C2091	G2027	U1949	A1886	A1819	G1681	A1610	C1547	C1547
A2211	U2092	C2092	U2028	U1955	C1887	U1820	G1682	C1611	A1548	A1548
U2212	G2093	C2093	G2029	U1956	A1888	A1821	U1683	G1612	A1549	A1549
C2214	A2094	C2094	A2030	U1957	A1889	C1822	G1684	C1613	C1550	C1550
C2215	A2095	C2095	A2031	C1957	A1890	G1823	A1759	A1614	A1551	A1551
G2216	C2096	C2096	G2032	C1958	G1891	G1824	C1760	C1615	A1552	A1552
G2217	A2097	C2097	A2033	G1959	C1892	U1825	C1761	U1688	U1553	U1553
G2218	U2098	C2098	U2034	U1963	C1893	G1826	A1762	A1616	U1554	U1554
U2219	C2099	C2099	G2035	U1964	A1894	U1827	G1763	C1617	G1555	G1555
U2220	G2100	C2100	C2036	G1965	C1895	G1828	C1764	A1690	C1556	C1556
G2221	A2101	C2101	A2037	C1966	G1896	A1829	U1765	G1620	C1557	C1557
C2222	G2102	C2102	G2038	A1966	G1897	C1830	G1766	U1692	U1558	U1558
G2223	C2103	C2103	U2039	C1967	A1898	G1831	G1767	G1623	C1559	C1559
G2224	C2104	C2104	G2040	G1968	A1899	C1832	G1768	U1624	U1560	U1560
C2225	U2105	C2105	U2041	A1969	A1900	C1833	U1769	G1628	C1561	C1561
G2226	U2106	C2106	A2042	A1970	A1901	U1834	G1770	G1629	U1562	U1562
A2227	G2107	C2107	C2043	U1971	G1902	U1841	C1771	A1700	U1563	U1563
G2228	A2108	C2108	U2043	G1972	G1903	A1772	A1772	G1633	A1634	A1634
U2229	U2109	C2109	C2047	G1973	G1904	G1842	A1773			
G2230	U2231	A	A							
U2232	U2232	U	U							
U2233	U2233	G	G							
G2234	U2234	A	A							
U2235	G2235	C	C							
U2236	U2236	C	C							
G2237	G2237	A	A							
G2238	G2238	C	C							
U2239	U2239	C	C							
U2240	U2240	U2180	C2179							
A2241	U2241	U2181	U2180							
G2242	U2242	U2182	U2181							
U2243	U2243	A2183	U2182							
U2244	U2244	A2184	A2183							
U2245	U2245	U2185	A2184							
G2246	U2246	U2186	U2185							
A2247	U2247	U2187	U2186							
C2248	U2248	U2188	U2187							
U2249	U2249	U2189	U2188							
G2250	U2250	G2190	U2189							
G2253	U2253	A2191	G2190							
U2257	U2257	U2192	A2191							
C2258	U2258	G2193	U2192							
C2259	U2259	U2194	U2193							
C2260	U2260	U2195	U2194							
C2261	U2261	C2196	U2195							
U2262	U2262	U2197	U2196							
C2263	U2263	A2198	U2197							
C2264	U2264	U2199	A2198							
U2265	U2265	C2200	U2199							
A2266	U2266	U2201	C2200							
A2267	U2267	U2202	U2201							
A2268	U2268	U2203	U2202							
C2269	U2269	G2204	U2203							
A2270	U2270	A2205	G2204							
G2271	U2271	C2206	C2205							
U2272	U2272	C2207	U2206							
A2273	U2273	C2208	U2207							
G2276	U2276	U2210	C2208							
G2277	U2277	A2212	U2210							
G2279	U2279	U2213	A2212							
G2280	U2280	C2214	U2213							
A2281	U2281	C2215	C2214							
G2282	U2282	G2216	C2215							
C2283	U2283	G2217	G2216							
A2284	U2284	U2218	G2217							
C2285	U2285	U2219	U2218							
U2286	U2286	U2220	U2219							
A2287	U2287	G2221	U2220							
U2288	U2288	C2222	G2221							
G2289	U2289	C2223	C2222							
C2290	U2290	G2224	G2223							
A2291	U2291	C2225	G2224							
U2292	U2292	U2226	C2225							
G2293	U2293	A2227	U2226							
C2294	U2294	G2228	U2227							
G2356	U2356	U2357	U2356							
A2357	U2357	A2358	U2357							
C2358	U2358	U2359	A2358							
G2359	U2359	U2360	U2359							
C2360	U2360	U2361	U2360							
U2361	U2361	U2362	U2361							
C2362	U2362	U2363	U2362							
G2363	U2363	U2364	U2363							
A2364	U2364	U2365	U2364							
C2365	U2365	U2366	U2365							
G2366	U2366	U2367	U2366							
C2367	U2367	U2368	U2367							
A2368	U2368	U2369	U2368							
G2369	U2369	U2370	U2369							
C2370	U2370	U2371	U2370							
G2373	U2373	U2374	U2373							
C2374	U2374	U2375	U2374							
A2375	U2375	U2376	U2375							
G2376	U2376	U2377	U2376							
C2377	U2377	U2378	U2377							
A2378	U2378	U2379	U2378							
G2379	U2379	U2380	U2379							
C2380	U2380	U2381	U2380							
A2381	U2381	U2382	U2381							
G2382	U2382	U2383	U2382							
C2383	U2383	U2384	U2383							
A2384	U2384	U2385	U2384							
G2385	U2385	U2386	U2385							
C2386	U2386	U2387	U2386							
A2387	U2387	U2388	U2387							
G2388	U2388	U2389	U2388							
C2389	U2389	U2390	U2389							
A2390	U2390	U2391	U2390							
G2391	U2391	U2392	U2391							



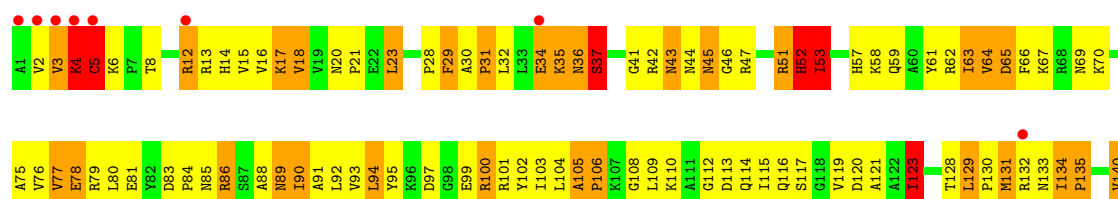
• Molecule 3: 50S ribosomal protein L11

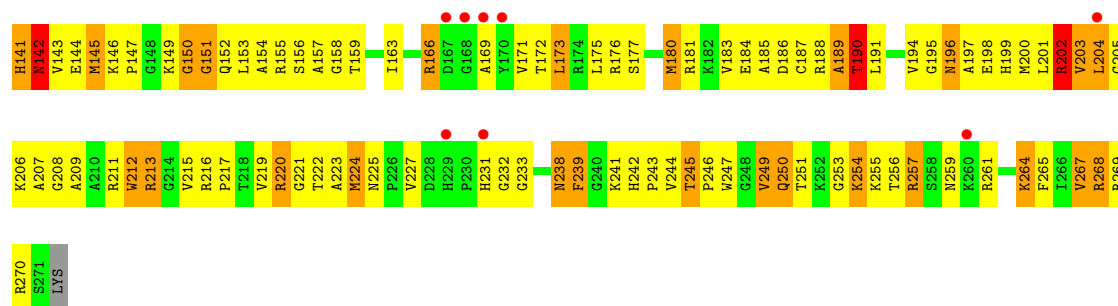
Chain I:



• Molecule 4: 50S ribosomal protein L2

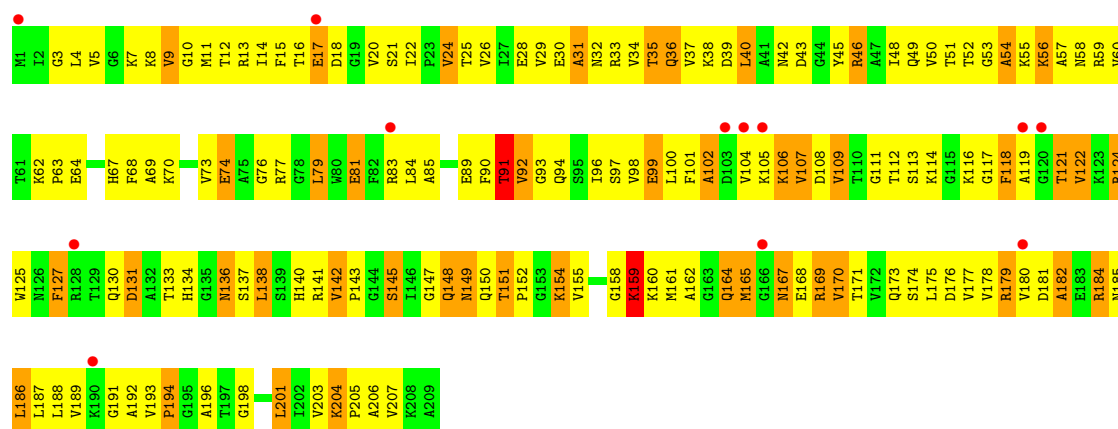
Chain C:





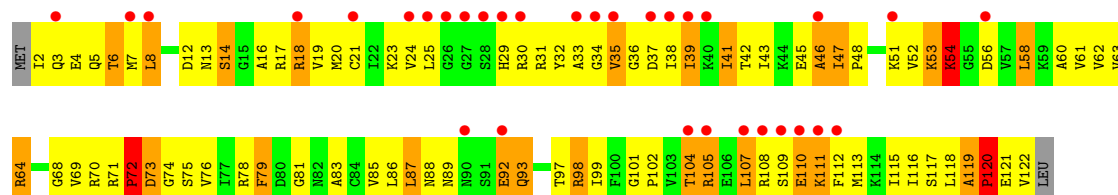
• Molecule 5: 50S ribosomal protein L3

Chain D:



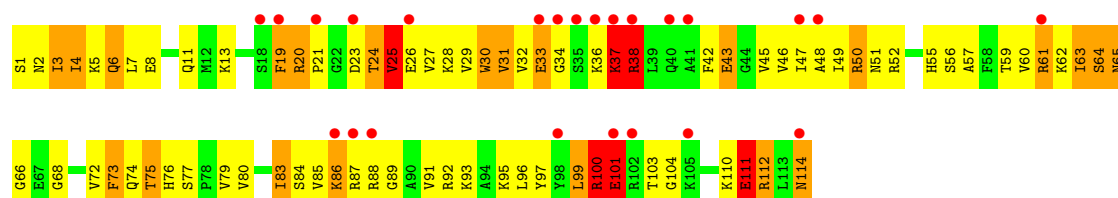
• Molecule 6: 50S ribosomal protein L14

Chain K:



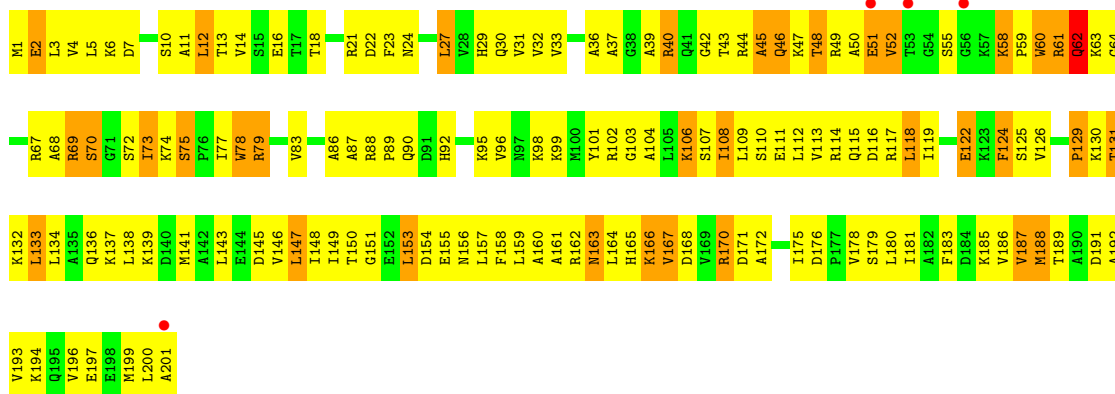
• Molecule 7: 50S ribosomal protein L19

Chain P:



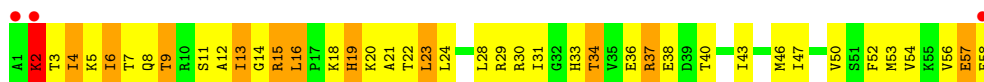
• Molecule 8: 50S ribosomal protein L4

Chain E:



- Molecule 9: 50S ribosomal protein L30

Chain Y:



- Molecule 10: 50S ribosomal protein L32

Chain 0:



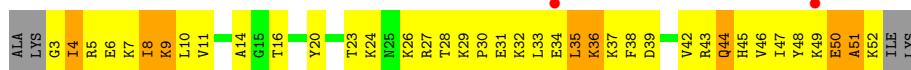
- Molecule 11: 50S ribosomal protein L36

Chain 4:



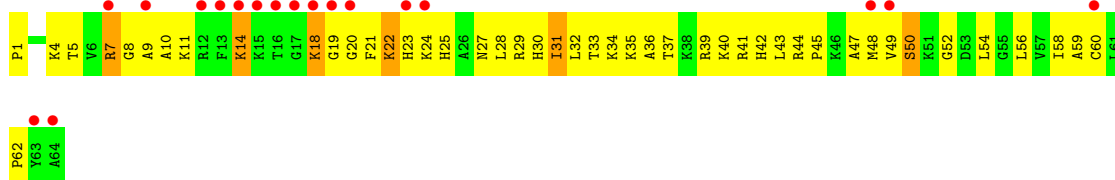
- Molecule 12: 50S ribosomal protein L33

Chain 1:



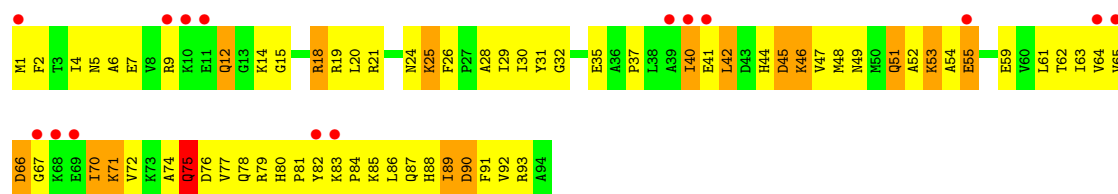
- Molecule 13: 50S ribosomal protein L35

Chain 3:



- Molecule 14: 50S ribosomal protein L25

Chain V:



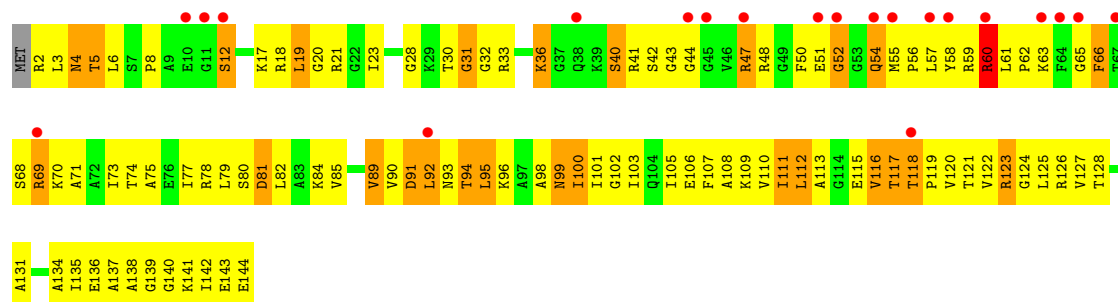
- Molecule 15: 50S ribosomal protein L34

Chain 2:



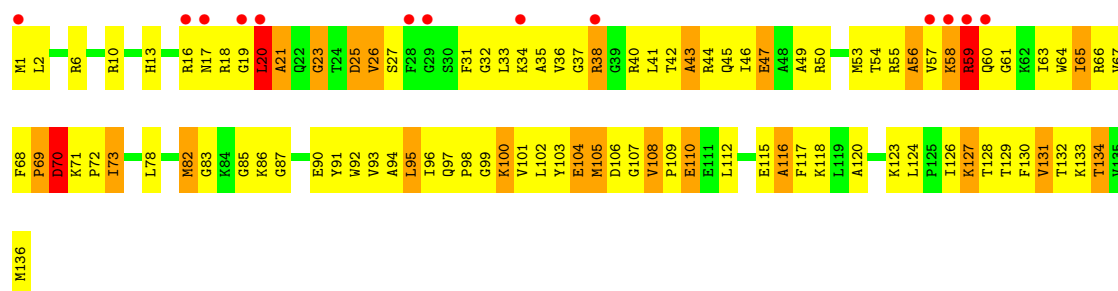
- Molecule 16: 50S ribosomal protein L15

Chain L:



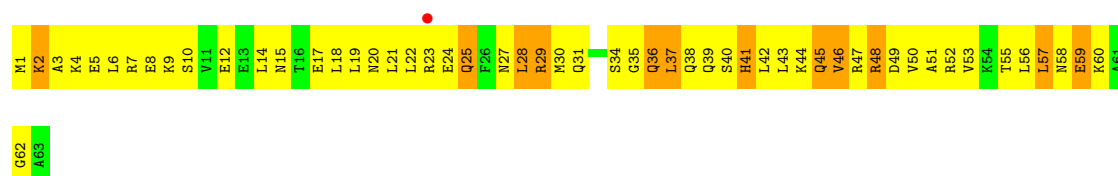
- Molecule 17: 50S ribosomal protein L16

Chain M:



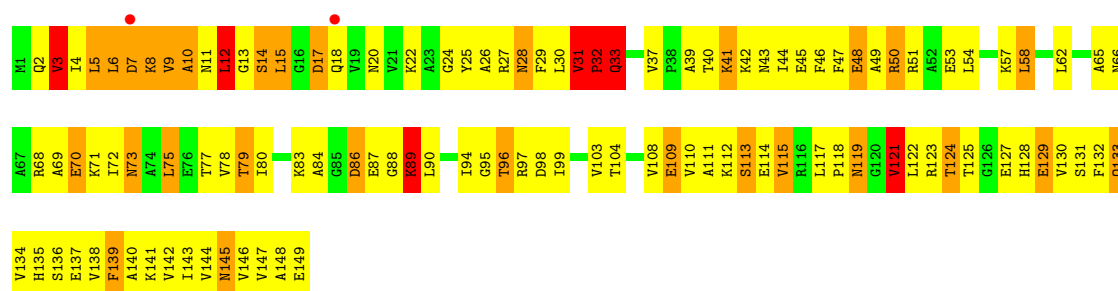
- Molecule 18: 50S ribosomal protein L29

Chain X:



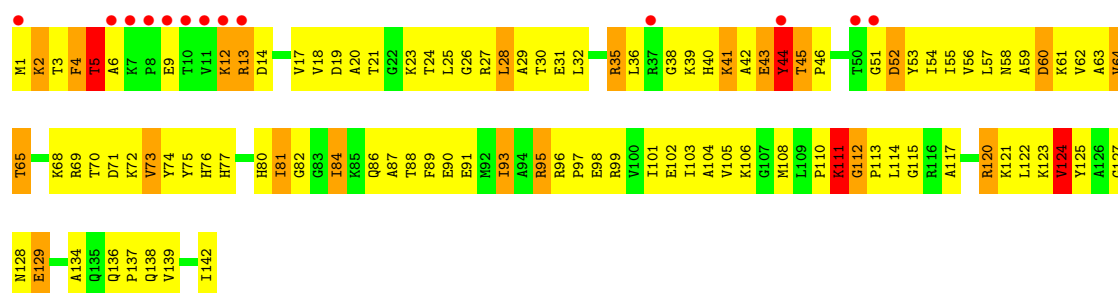
- Molecule 19: 50S ribosomal protein L9

Chain H:



• Molecule 20: 50S ribosomal protein L13

Chain J:



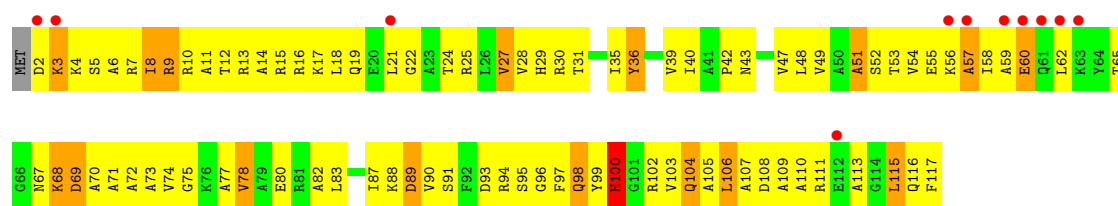
• Molecule 21: 50S ribosomal protein L17

Chain N:



• Molecule 22: 50S ribosomal protein L18

Chain O:



• Molecule 23: 50S ribosomal protein L20

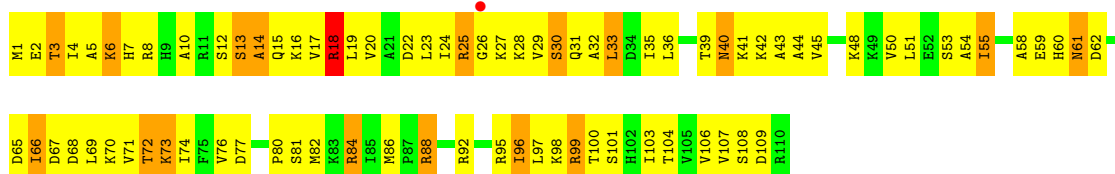
Chain Q:





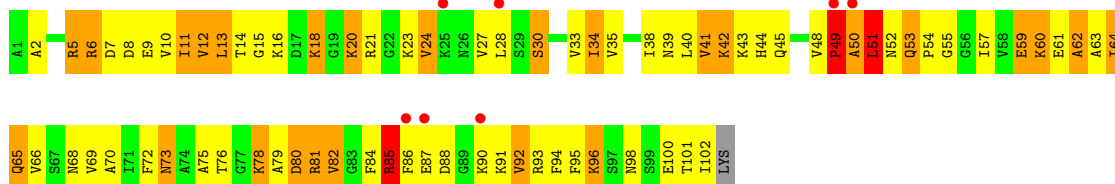
• Molecule 24: 50S ribosomal protein L22

Chain S:



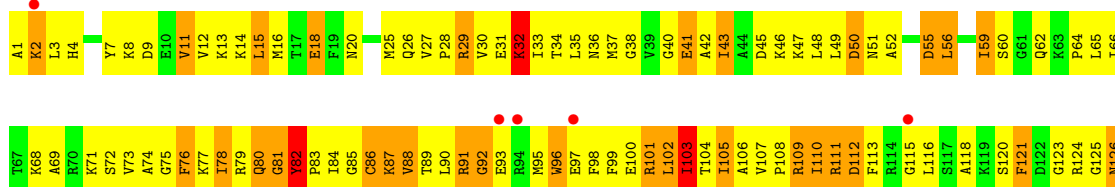
• Molecule 25: 50S ribosomal protein L24

Chain U:



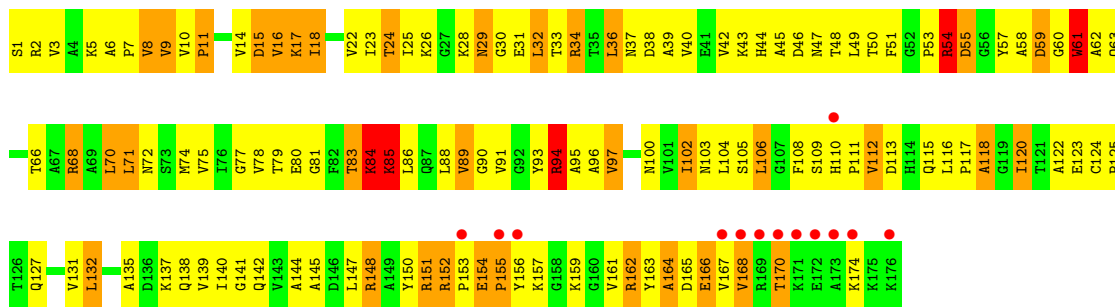
• Molecule 26: 50S ribosomal protein L5

Chain F:

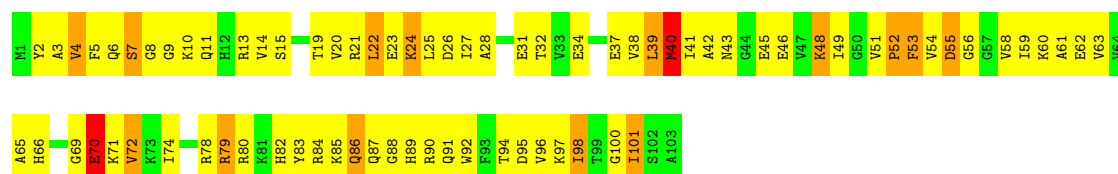


• Molecule 27: 50S ribosomal protein L6

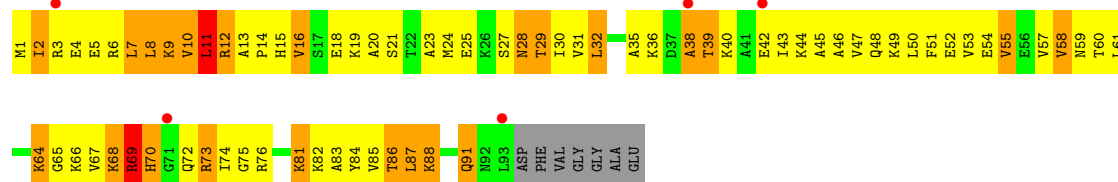
Chain G:



• Molecule 28: 50S ribosomal protein L21

Chain R: 

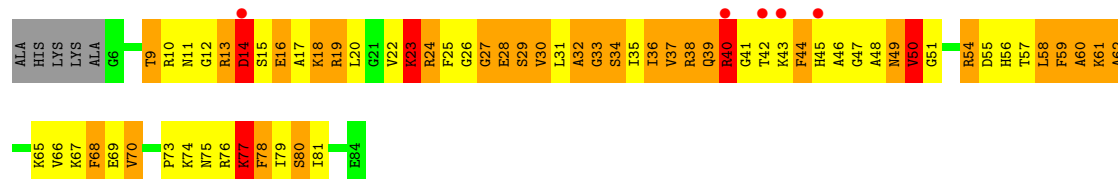
- Molecule 29: 50S ribosomal protein L23

Chain T: 

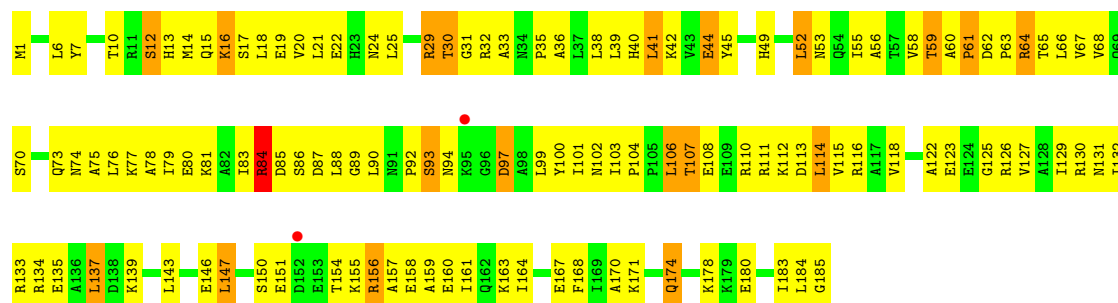
- Molecule 30: 50S ribosomal protein L28

Chain Z: 

- Molecule 31: 50S ribosomal protein L27

Chain W: 

- Molecule 32: 50S ribosomal protein RRF

Chain 6: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.54Å 378.89Å 736.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 138.07 – 4.15	Depositor EDS
% Data completeness (in resolution range)	87.4 (40.00-4.00) 87.4 (138.07-4.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 4.15Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.305 0.474 , 0.484	Depositor DCC
R_{free} test set	18864 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	133.1	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 9.6	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 382905 reflections	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	91772	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: ZN, MG, LLL

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	0.28	0/2803	0.76	0/4371
2	B	0.30	6/68314 (0.0%)	0.79	48/106569 (0.0%)
3	I	0.25	0/1046	0.48	0/1410
4	C	0.22	0/2121	0.48	0/2852
5	D	0.24	0/1586	0.49	0/2134
6	K	0.24	0/939	0.55	0/1258
7	P	0.24	0/929	0.51	0/1242
8	E	0.24	0/1571	0.51	0/2113
9	Y	0.23	0/453	0.49	0/605
10	O	0.23	0/450	0.55	0/599
11	4	0.23	0/303	0.47	0/397
12	1	0.27	0/416	0.49	0/554
13	3	0.24	0/513	0.48	0/676
14	V	0.25	0/766	0.43	0/1025
15	2	0.25	0/380	0.48	0/498
16	L	0.23	0/1054	0.48	0/1403
17	M	0.25	0/1093	0.48	0/1460
18	X	0.24	0/510	0.53	0/677
19	H	0.25	0/1122	0.48	0/1515
20	J	0.23	0/1152	0.48	0/1551
21	N	0.24	0/973	0.51	0/1301
22	O	0.23	0/902	0.49	0/1209
23	Q	0.26	0/960	0.49	0/1278
24	S	0.22	0/864	0.52	0/1156
25	U	0.25	0/787	0.47	0/1051
26	F	0.26	0/1444	0.52	0/1937
27	G	0.23	0/1343	0.47	0/1816
28	R	0.25	0/829	0.50	0/1107
29	T	0.22	0/744	0.55	0/994
30	Z	0.25	0/635	0.52	0/848
31	W	0.28	0/603	0.51	0/797
32	6	0.30	0/1497	0.58	1/2017 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.29	6/99102 (0.0%)	0.73	49/148420 (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	47

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	-16.53	1.26	1.41
2	B	1088	A	C6-N1	-10.57	1.28	1.35
2	B	1060	U	C2-N3	7.78	1.43	1.37
2	B	1086	A	N7-C5	-6.75	1.35	1.39
2	B	2318	G	O3'-P	-6.33	1.53	1.61

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2204	G	O5'-P-OP1	-29.74	75.02	110.70
2	B	2791	G	O5'-P-OP2	-27.84	77.29	110.70
2	B	2791	G	O5'-P-OP1	17.87	132.15	110.70
2	B	2204	G	O5'-P-OP2	17.66	131.89	110.70
2	B	2790	U	OP2-P-O3'	14.53	137.17	105.20

There are no chirality outliers.

5 of 47 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	108	0
2	B	60995	0	30678	2536	0
3	I	1032	0	1088	181	0
4	C	2082	0	2157	241	0
5	D	1565	0	1616	216	0
6	K	930	0	1000	122	0
7	P	917	0	965	106	0
8	E	1552	0	1619	181	0
9	Y	449	0	491	55	0
10	0	444	0	461	47	0
11	4	302	0	340	44	0
12	1	409	0	440	54	0
13	3	504	0	574	48	0
14	V	753	0	780	102	0
15	2	377	0	418	38	0
16	L	1045	0	1117	153	0
17	M	1074	0	1157	121	0
18	X	509	0	543	60	0
19	H	1111	0	1148	158	0
20	J	1129	0	1162	137	0
21	N	960	0	1000	129	0
22	O	892	0	923	96	0
23	Q	947	0	1022	178	0
24	S	857	0	922	101	0
25	U	779	0	834	109	0
26	F	1420	0	1460	212	0
27	G	1323	0	1374	195	0
28	R	816	0	839	128	0
29	T	738	0	807	120	0
30	Z	625	0	652	82	0
31	W	596	0	610	126	0
32	6	1478	0	1526	148	0
33	B	111	0	0	0	0
34	B	31	0	39	0	0
35	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	B	499	0	0	7	0
36	C	6	0	0	0	0
36	E	3	0	0	0	0
36	L	2	0	0	0	0
36	R	1	0	0	0	0
36	T	1	0	0	0	0
All	All	91772	0	61032	5785	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 38.

The worst 5 of 5785 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	1.36	1.20
4:C:144:GLU:HA	4:C:151:GLY:HA2	1.33	1.11
16:L:143:GLU:HG2	16:L:144:GLU:H	1.10	1.10
19:H:31:VAL:HB	19:H:32:PRO:HD2	1.23	1.10
2:B:1099:G:C8	3:I:3:LYS:N	2.20	1.09

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%)	114 (82%)	20 (14%)	5 (4%)	5	54
4	C	269/272 (99%)	155 (58%)	65 (24%)	49 (18%)	0	5
5	D	207/209 (99%)	124 (60%)	51 (25%)	32 (16%)	0	8
6	K	119/123 (97%)	78 (66%)	24 (20%)	17 (14%)	0	10
7	P	112/114 (98%)	61 (54%)	34 (30%)	17 (15%)	0	8
8	E	199/201 (99%)	125 (63%)	51 (26%)	23 (12%)	1	15
9	Y	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	0	54/56 (96%)	39 (72%)	8 (15%)	7 (13%)	0	12
11	4	36/38 (95%)	16 (44%)	10 (28%)	10 (28%)	0	1
12	1	48/54 (89%)	36 (75%)	8 (17%)	4 (8%)	1	27
13	3	62/64 (97%)	34 (55%)	22 (36%)	6 (10%)	1	21
14	V	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	2	36
15	2	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	1	24
16	L	141/144 (98%)	89 (63%)	32 (23%)	20 (14%)	0	10
17	M	134/136 (98%)	83 (62%)	31 (23%)	20 (15%)	0	8
18	X	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	12
19	H	147/149 (99%)	91 (62%)	33 (22%)	23 (16%)	0	7
20	J	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	11
21	N	118/127 (93%)	77 (65%)	28 (24%)	13 (11%)	1	16
22	O	114/117 (97%)	75 (66%)	27 (24%)	12 (10%)	1	18
23	Q	115/117 (98%)	75 (65%)	29 (25%)	11 (10%)	1	21
24	S	108/110 (98%)	66 (61%)	31 (29%)	11 (10%)	1	19
25	U	100/103 (97%)	59 (59%)	22 (22%)	19 (19%)	0	4
26	F	176/178 (99%)	105 (60%)	42 (24%)	29 (16%)	0	7
27	G	174/176 (99%)	101 (58%)	41 (24%)	32 (18%)	0	5
28	R	101/103 (98%)	74 (73%)	18 (18%)	9 (9%)	1	25
29	T	91/100 (91%)	46 (50%)	27 (30%)	18 (20%)	0	4
30	Z	75/78 (96%)	50 (67%)	13 (17%)	12 (16%)	0	7
31	W	77/84 (92%)	28 (36%)	24 (31%)	25 (32%)	0	0
32	6	183/185 (99%)	152 (83%)	24 (13%)	7 (4%)	5	52
All	All	3492/3582 (98%)	2205 (63%)	814 (23%)	473 (14%)	0	11

5 of 473 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	5	GLN
3	I	18	ASN
4	C	51	ARG
4	C	59	GLN
4	C	77	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	
3	I	109/109 (100%)	103 (94%)	6 (6%)	30	78
4	C	216/217 (100%)	176 (82%)	40 (18%)	2	18
5	D	164/164 (100%)	134 (82%)	30 (18%)	2	18
6	K	102/104 (98%)	81 (79%)	21 (21%)	2	13
7	P	99/99 (100%)	80 (81%)	19 (19%)	2	16
8	E	165/165 (100%)	142 (86%)	23 (14%)	5	34
9	Y	48/48 (100%)	38 (79%)	10 (21%)	2	13
10	0	47/47 (100%)	38 (81%)	9 (19%)	2	16
11	4	34/34 (100%)	29 (85%)	5 (15%)	4	31
12	1	45/48 (94%)	41 (91%)	4 (9%)	14	58
13	3	51/51 (100%)	46 (90%)	5 (10%)	12	52
14	V	78/78 (100%)	64 (82%)	14 (18%)	2	19
15	2	38/38 (100%)	28 (74%)	10 (26%)	1	7
16	L	102/103 (99%)	91 (89%)	11 (11%)	9	48
17	M	109/109 (100%)	87 (80%)	22 (20%)	2	14
18	X	55/55 (100%)	46 (84%)	9 (16%)	3	25
19	H	114/114 (100%)	89 (78%)	25 (22%)	1	11
20	J	116/116 (100%)	100 (86%)	16 (14%)	5	34
21	N	100/103 (97%)	84 (84%)	16 (16%)	3	27
22	O	86/87 (99%)	72 (84%)	14 (16%)	3	26
23	Q	89/89 (100%)	79 (89%)	10 (11%)	9	45
24	S	93/93 (100%)	77 (83%)	16 (17%)	3	22
25	U	83/84 (99%)	65 (78%)	18 (22%)	1	11
26	F	149/149 (100%)	117 (78%)	32 (22%)	1	11
27	G	137/137 (100%)	112 (82%)	25 (18%)	2	18
28	R	84/84 (100%)	70 (83%)	14 (17%)	3	24
29	T	80/84 (95%)	64 (80%)	16 (20%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	Z	67/68 (98%)	56 (84%)	11 (16%)	3	25
31	W	59/62 (95%)	42 (71%)	17 (29%)	0	5
32	6	157/157 (100%)	134 (85%)	23 (15%)	5	31
All	All	2876/2896 (99%)	2385 (83%)	491 (17%)	3	22

5 of 491 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	M	104	GLU
20	J	111	LYS
31	W	16	GLU
17	M	131	VAL
19	H	70	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
16	L	104	GLN
19	H	20	ASN
31	W	39	GLN
17	M	17	ASN
18	X	25	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	16 (13%)	0
2	B	2837/2904 (97%)	435 (15%)	22 (0%)
All	All	2953/3024 (97%)	451 (15%)	22 (0%)

5 of 451 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	C
1	A	9	G
1	A	16	G
1	A	24	G
1	A	26	C

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1210	G
2	B	1911	U
2	B	2832	U
2	B	1301	A
2	B	1419	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
34	LLL	B	3016	-	33,33,33	3.21	14 (42%)	49,49,49	1.55	5 (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
34	LLL	B	3016	-	-	0/12/65/65	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	3016	LLL	C22-C32	9.11	1.59	1.52
34	B	3016	LLL	C22-C12	7.55	1.58	1.52
34	B	3016	LLL	O53-C53	6.05	1.52	1.43
34	B	3016	LLL	C43-C33	4.98	1.63	1.54
34	B	3016	LLL	C42-C32	4.58	1.59	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	3016	LLL	C93-N33-C33	6.38	117.48	113.85
34	B	3016	LLL	C53-O53-C13	4.47	117.59	111.22
34	B	3016	LLL	C83-C43-C33	2.62	116.51	112.15
34	B	3016	LLL	C11-O51-C51	2.56	115.78	113.19
34	B	3016	LLL	O43-C43-C83	-2.51	102.54	108.08

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	A	117/120 (97%)	0.28	8 (6%) 17 17	36, 88, 148, 180	0
2	B	2841/2904 (97%)	0.33	234 (8%) 12 13	5, 46, 154, 180	0
3	I	141/141 (100%)	-0.41	1 (0%) 84 73	63, 162, 180, 180	0
4	C	271/272 (99%)	0.28	16 (5%) 22 20	5, 38, 99, 145	0
5	D	209/209 (100%)	0.40	12 (5%) 23 21	5, 51, 131, 180	0
6	K	121/123 (98%)	1.36	32 (26%) 1 3	5, 42, 103, 180	0
7	P	114/114 (100%)	1.05	24 (21%) 1 3	5, 52, 119, 161	0
8	E	201/201 (100%)	0.00	4 (1%) 62 48	5, 66, 138, 180	0
9	Y	58/58 (100%)	0.35	3 (5%) 26 23	10, 66, 149, 158	0
10	0	56/56 (100%)	0.11	2 (3%) 41 33	9, 54, 119, 180	0
11	4	38/38 (100%)	0.81	6 (15%) 3 5	17, 62, 132, 171	0
12	1	50/54 (92%)	0.14	2 (4%) 36 30	24, 73, 125, 155	0
13	3	64/64 (100%)	1.47	18 (28%) 1 2	6, 49, 107, 180	0
14	V	94/94 (100%)	0.65	15 (15%) 3 5	27, 94, 160, 180	0
15	2	46/46 (100%)	0.41	0 100 100	7, 43, 103, 180	0
16	L	143/144 (99%)	0.63	21 (14%) 3 5	5, 61, 128, 162	0
17	M	136/136 (100%)	0.65	13 (9%) 8 11	5, 63, 134, 171	0
18	X	63/63 (100%)	-0.13	1 (1%) 68 54	38, 94, 166, 180	0
19	H	149/149 (100%)	-0.20	2 (1%) 74 59	5, 109, 171, 180	0
20	J	142/142 (100%)	0.34	13 (9%) 9 12	5, 65, 128, 180	0
21	N	120/127 (94%)	-0.11	3 (2%) 54 43	5, 44, 116, 141	0
22	O	116/117 (99%)	0.42	11 (9%) 8 11	5, 93, 156, 180	0
23	Q	117/117 (100%)	0.22	5 (4%) 34 28	5, 50, 131, 156	0
24	S	110/110 (100%)	-0.04	1 (0%) 81 68	5, 50, 120, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	U	102/103 (99%)	0.16	7 (6%) 17 17	26, 93, 154, 180	0
26	F	178/178 (100%)	0.06	7 (3%) 37 31	22, 106, 175, 180	0
27	G	176/176 (100%)	0.17	13 (7%) 14 15	32, 104, 164, 180	0
28	R	103/103 (100%)	-0.23	0 100 100	5, 85, 144, 180	0
29	T	93/100 (93%)	0.42	5 (5%) 25 22	15, 79, 167, 180	0
30	Z	77/78 (98%)	-0.10	0 100 100	5, 56, 101, 131	0
31	W	79/84 (94%)	0.46	5 (6%) 19 19	5, 79, 143, 180	0
32	6	185/185 (100%)	0.09	2 (1%) 77 63	5, 104, 180, 180	0
All	All	6510/6606 (98%)	0.30	486 (7%) 14 15	5, 59, 160, 180	0

The worst 5 of 486 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	645	C	10.7
2	B	31	C	8.4
2	B	2799	A	8.3
27	G	172	GLU	8.3
9	Y	1	ALA	8.0

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(\AA^2)	Q<0.9
33	MG	B	3010	1/1	0.64	23.32	64,64,64,64	0
33	MG	B	2939	1/1	2.40	11.54	75,75,75,75	0
34	LLL	B	3016	31/31	0.26	8.23	121,121,121,121	0
33	MG	B	2938	1/1	0.37	6.65	69,69,69,69	0
33	MG	B	2964	1/1	0.15	6.60	104,104,104,104	0
33	MG	B	2999	1/1	0.32	5.46	88,88,88,88	0
33	MG	B	2952	1/1	0.44	4.77	34,34,34,34	0
33	MG	B	2994	1/1	1.84	4.58	64,64,64,64	0
33	MG	B	2956	1/1	0.79	4.19	113,113,113,113	0
33	MG	B	2932	1/1	0.83	3.98	58,58,58,58	0
33	MG	B	3005	1/1	0.31	3.06	25,25,25,25	0
33	MG	B	2981	1/1	0.16	1.88	15,15,15,15	0
33	MG	B	2983	1/1	0.20	1.33	34,34,34,34	0
33	MG	B	2930	1/1	0.28	1.14	54,54,54,54	0
33	MG	B	2923	1/1	0.26	0.98	5,5,5,5	0
33	MG	B	2936	1/1	0.28	0.97	51,51,51,51	0
33	MG	B	3000	1/1	0.19	0.93	20,20,20,20	0
33	MG	B	2963	1/1	0.20	0.79	166,166,166,166	0
33	MG	B	2984	1/1	0.28	0.63	5,5,5,5	0
33	MG	B	2974	1/1	0.38	0.60	38,38,38,38	0
33	MG	B	3011	1/1	0.35	0.51	11,11,11,11	0
33	MG	B	2926	1/1	0.15	0.46	71,71,71,71	0
33	MG	B	3003	1/1	0.25	0.00	5,5,5,5	0
33	MG	B	2927	1/1	0.18	0.00	17,17,17,17	0
33	MG	B	2980	1/1	0.17	-0.06	104,104,104,104	0
33	MG	B	2933	1/1	0.26	-0.09	59,59,59,59	0
33	MG	B	2973	1/1	0.28	-0.17	14,14,14,14	0
33	MG	B	2965	1/1	0.18	-0.22	69,69,69,69	0
33	MG	B	2946	1/1	0.15	-0.26	23,23,23,23	0
33	MG	B	2961	1/1	0.14	-0.28	77,77,77,77	0
33	MG	B	2996	1/1	0.19	-0.37	56,56,56,56	0
33	MG	B	2948	1/1	0.25	-0.49	21,21,21,21	0
33	MG	B	2998	1/1	0.20	-0.52	55,55,55,55	0
33	MG	B	3004	1/1	0.16	-0.60	46,46,46,46	0
33	MG	B	2982	1/1	0.15	-0.64	32,32,32,32	0
33	MG	B	3015	1/1	0.17	-0.69	32,32,32,32	0
33	MG	B	2918	1/1	0.16	-0.77	43,43,43,43	0
33	MG	B	2960	1/1	0.21	-0.91	12,12,12,12	0
33	MG	B	2977	1/1	0.22	-0.92	67,67,67,67	0
33	MG	B	2979	1/1	0.15	-0.94	35,35,35,35	0
33	MG	B	2922	1/1	0.20	-0.94	22,22,22,22	0
33	MG	B	3007	1/1	0.21	-1.00	42,42,42,42	0
33	MG	B	3008	1/1	0.24	-1.00	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	2976	1/1	0.26	-1.01	54,54,54,54	0
33	MG	B	2931	1/1	0.17	-1.03	28,28,28,28	0
33	MG	B	3014	1/1	0.13	-1.10	38,38,38,38	0
33	MG	B	2920	1/1	0.30	-1.12	25,25,25,25	0
33	MG	B	3006	1/1	0.18	-1.16	22,22,22,22	0
33	MG	B	2972	1/1	0.18	-1.25	22,22,22,22	0
33	MG	B	2907	1/1	0.16	-1.30	33,33,33,33	0
33	MG	B	2988	1/1	0.13	-1.31	16,16,16,16	0
33	MG	B	2928	1/1	0.12	-1.33	45,45,45,45	0
33	MG	B	2905	1/1	0.13	-1.33	6,6,6,6	0
33	MG	B	2910	1/1	0.14	-1.38	15,15,15,15	0
33	MG	B	2957	1/1	0.16	-1.39	80,80,80,80	0
33	MG	B	2969	1/1	0.21	-1.44	45,45,45,45	0
33	MG	B	2959	1/1	0.18	-1.47	41,41,41,41	0
33	MG	B	2985	1/1	0.25	-1.47	19,19,19,19	0
33	MG	B	2942	1/1	0.11	-1.47	37,37,37,37	0
35	ZN	4	624	1/1	0.06	-1.48	45,45,45,45	0
33	MG	B	2911	1/1	0.11	-1.53	13,13,13,13	0
33	MG	B	2908	1/1	0.13	-1.53	69,69,69,69	0
33	MG	B	2919	1/1	0.13	-1.60	24,24,24,24	0
33	MG	B	2945	1/1	0.20	-1.62	34,34,34,34	0
33	MG	B	2986	1/1	0.10	-1.77	57,57,57,57	0
33	MG	B	2950	1/1	0.09	-1.79	11,11,11,11	0
33	MG	B	2925	1/1	0.09	-1.81	51,51,51,51	0
33	MG	B	2914	1/1	0.17	-1.86	16,16,16,16	0
33	MG	B	2987	1/1	0.16	-1.87	83,83,83,83	0
33	MG	B	2967	1/1	0.13	-1.88	19,19,19,19	0
33	MG	B	2929	1/1	0.13	-2.03	42,42,42,42	0
33	MG	B	2913	1/1	0.09	-2.04	18,18,18,18	0
33	MG	B	2943	1/1	0.09	-2.12	69,69,69,69	0
33	MG	B	2997	1/1	0.12	-2.20	10,10,10,10	0
33	MG	B	2944	1/1	0.09	-2.25	18,18,18,18	0
33	MG	B	2968	1/1	0.12	-2.28	19,19,19,19	0
33	MG	B	2937	1/1	0.07	-2.30	43,43,43,43	0
33	MG	B	2955	1/1	0.04	-2.35	32,32,32,32	0
33	MG	B	3002	1/1	0.10	-2.36	28,28,28,28	0
33	MG	B	2916	1/1	0.15	-2.36	12,12,12,12	0
33	MG	B	2906	1/1	0.07	-2.42	6,6,6,6	0
33	MG	B	2975	1/1	0.21	-2.46	37,37,37,37	0
33	MG	B	2993	1/1	0.07	-2.52	61,61,61,61	0
33	MG	B	2954	1/1	0.07	-2.54	123,123,123,123	0
33	MG	B	2962	1/1	0.16	-2.58	162,162,162,162	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	2917	1/1	0.16	-2.75	41,41,41,41	0
33	MG	B	2991	1/1	0.10	-2.80	75,75,75,75	0
33	MG	B	2978	1/1	0.15	-2.82	17,17,17,17	0
33	MG	B	2947	1/1	0.10	-2.90	32,32,32,32	0
33	MG	B	3001	1/1	0.11	-2.91	64,64,64,64	0
33	MG	B	2951	1/1	0.22	-2.97	19,19,19,19	0
33	MG	B	2934	1/1	0.14	-3.06	10,10,10,10	0
33	MG	B	2971	1/1	0.16	-3.12	16,16,16,16	0
33	MG	B	2989	1/1	0.08	-3.14	49,49,49,49	0
33	MG	B	2940	1/1	0.08	-3.23	20,20,20,20	0
33	MG	B	2992	1/1	0.09	-3.40	46,46,46,46	0
33	MG	B	2909	1/1	0.12	-3.50	45,45,45,45	0
33	MG	B	3013	1/1	0.07	-3.64	83,83,83,83	0
33	MG	B	2921	1/1	0.07	-3.81	5,5,5,5	0
33	MG	B	2941	1/1	0.07	-3.83	54,54,54,54	0
33	MG	B	3009	1/1	0.17	-3.89	30,30,30,30	0
33	MG	B	2924	1/1	0.10	-3.97	13,13,13,13	0
33	MG	B	2958	1/1	0.07	-4.03	29,29,29,29	0
33	MG	B	2953	1/1	0.07	-4.11	9,9,9,9	0
33	MG	B	2949	1/1	0.11	-4.14	68,68,68,68	0
33	MG	B	2995	1/1	0.08	-4.43	5,5,5,5	0
33	MG	B	2915	1/1	0.09	-5.06	33,33,33,33	0
33	MG	B	3012	1/1	0.09	-5.33	5,5,5,5	0
33	MG	B	2935	1/1	0.17	-5.53	24,24,24,24	0
33	MG	B	2966	1/1	0.07	-6.77	67,67,67,67	0
33	MG	B	2990	1/1	0.07	-9.09	52,52,52,52	0
33	MG	B	2912	1/1	0.08	-15.96	17,17,17,17	0
33	MG	B	2970	1/1	0.59	-	158,158,158,158	0

6.5 Other polymers ⓘ

There are no such residues in this entry.