



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:06 AM GMT

PDB ID : 1N8R
Title : Structure of large ribosomal subunit in complex with virginiamycin M
Authors : Hansen, J.L.; Moore, P.B.; Steitz, T.A.
Deposited on : 2002-11-21
Resolution : 3.00 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>

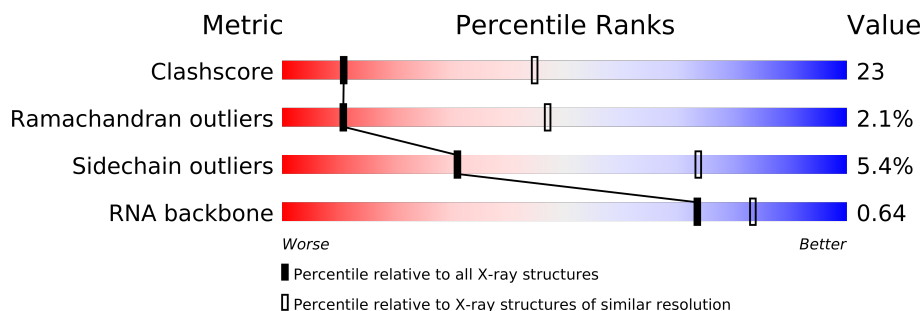
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2922	
2	B	122	
3	C	239	
4	D	337	
5	E	246	
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	

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Mol	Chain	Length	Quality of chain
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98569 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 5 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 7 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 14 is a protein called 50S ribosomal protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called 50S ribosomal protein L18E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O	0	0	0
			864	529	161	174			

- Molecule 17 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O	0	0	0
			1133	680	230	223			

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O		0	0	0
			949	568	180	201				

- Molecule 22 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 25 is a protein called 50S ribosomal protein L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 26 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 27 is a protein called 50S ribosomal protein L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

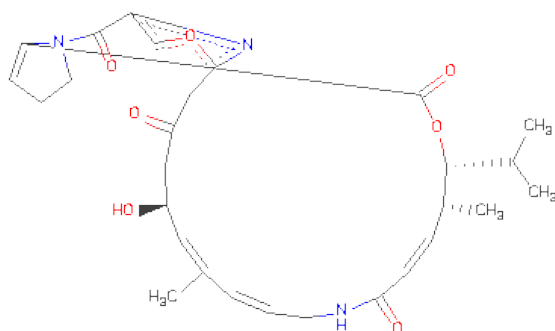
- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is VIRGINIAMYCIN M1 (three-letter code: VIR) (formula: $C_{28}H_{35}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			38	28	3	7		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	D	1	Total Mg 1 1	0	0
32	B	1	Total Mg 1 1	0	0
32	C	2	Total Mg 2 2	0	0
32	Z	1	Total Mg 1 1	0	0
32	A	109	Total Mg 109 109	0	0
32	4	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total K 1 1	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	U	1	Total 1	Na 1	0	0
34	4	1	Total 1	Na 1	0	0
34	R	1	Total 1	Na 1	0	0
34	S	2	Total 2	Na 2	0	0
34	M	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	P	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	C	1	Total 1	Cl 1	0	0
35	Z	2	Total 2	Cl 2	0	0
35	A	8	Total 8	Cl 8	0	0
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	P	1	Total Cd 1 1	0	0
36	2	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	4	1	Total Cd 1 1	0	0
36	V	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	5881	Total O 5881 5881	0	0
37	B	146	Total O 146 146	0	0
37	C	135	Total O 135 135	0	0
37	D	141	Total O 141 141	0	0
37	E	178	Total O 178 178	0	0
37	F	49	Total O 49 49	0	0
37	G	43	Total O 43 43	0	0
37	H	30	Total O 30 30	0	0
37	I	21	Total O 21 21	0	0
37	J	76	Total O 76 76	0	0
37	K	55	Total O 55 55	0	0
37	L	64	Total O 64 64	0	0
37	M	85	Total O 85 85	0	0
37	N	141	Total O 141 141	0	0
37	O	67	Total O 67 67	0	0

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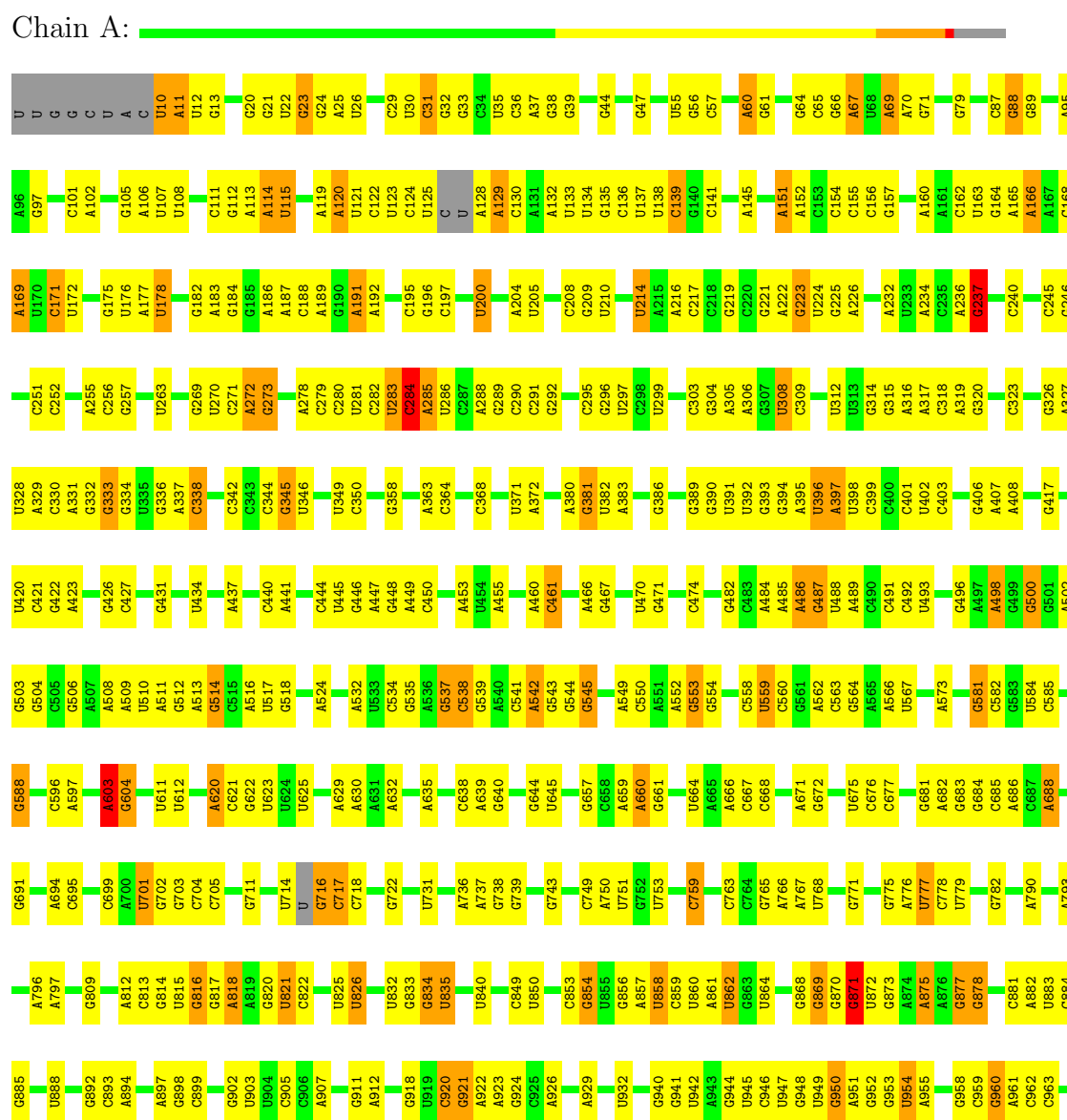
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	P	45	Total 45	O 45	0	0
37	Q	72	Total 72	O 72	0	0
37	R	57	Total 57	O 57	0	0
37	S	87	Total 87	O 87	0	0
37	T	34	Total 34	O 34	0	0
37	U	33	Total 33	O 33	0	0
37	V	27	Total 27	O 27	0	0
37	W	16	Total 16	O 16	0	0
37	X	68	Total 68	O 68	0	0
37	Y	27	Total 27	O 27	0	0
37	Z	100	Total 100	O 100	0	0
37	1	35	Total 35	O 35	0	0
37	2	57	Total 57	O 57	0	0
37	3	40	Total 40	O 40	0	0
37	4	72	Total 72	O 72	0	0

3 Residue-property plots

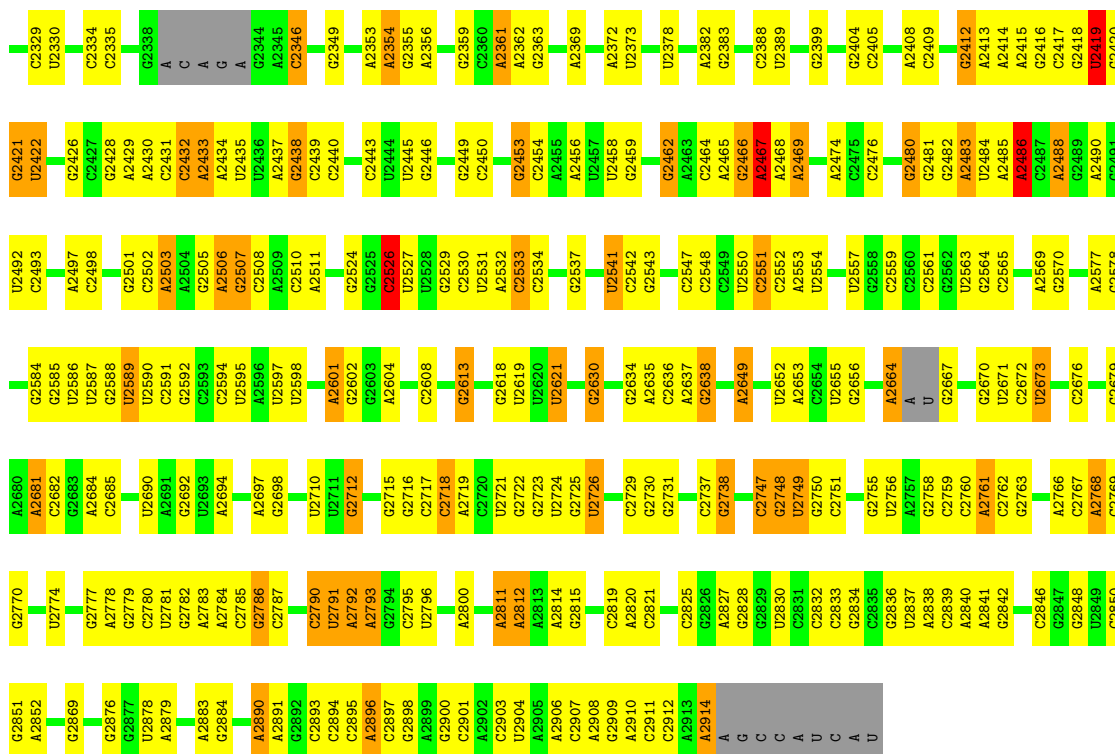
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 23S ribosomal RNA

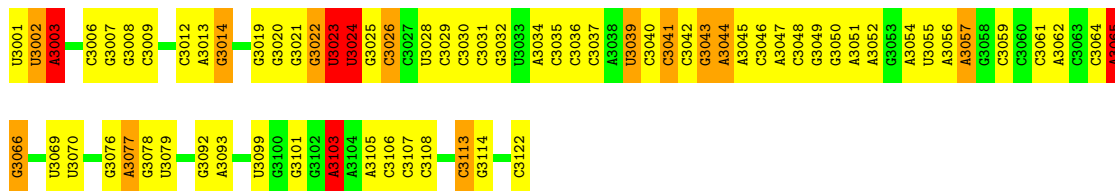


C2243	C2249	G2121	C2029	A1859	C1768	A1603	C1516	G1416	C1228	G1052	U970
G2250	G2251	A2123	U2032	U1860	C1686	G1604	U1517	G1417	C1229	G1053	G
A2252	G2257	C2126	G2033	C1861	G1687	A1606	G1523	U1418	U1143	G1054	U
A2255	A2258	U2127	C2034	C1862	G1688	A1607	U1524	U1419	G1151	G1055	G
A2256	A2258	G2128	C2035	C1863	C1692	G1609	G1525	C1421	G1158	A1057	U
G2257	A2258	U2133	A2038	A1865	G1699	G1610	A1526	U1422	G1159	A1058	C
G2262	G2263	U2134	A2039	G1866	C1700	C1613	A1527	C1423	G1160	G1059	G
A2264	U2265	A2135	G2040	C1867	U1702	A1615	A1528	A1424	A1161	C1060	C
A2266	G2267	G2136	G2041	A1868	U1706	A1616	U1531	U1436	G1162	C1061	C
G2270	G2271	A	G2063	C1872	G1706	C1617	U1531	A1437	G1163	U1062	U
G2272	U2276	C	A2064	U1874	A1710	U1625	G1536	G1441	A1166	G1063	C
U2277	U2278	U	A2065	G1875	A1711	U1626	C1536	U1442	A1067	A1067	C
U2278	G2279	G	U2063	U1878	A1712	A1627	G1543	A1443	C1068	C1068	A
G2280	U2281	C	U2064	G1879	G1713	G1627	U1544	A1444	C1069	C1069	G
U2282	G2283	C	G2068	C1880	A1796	C1633	C1545	G1445	G1072	A1073	G
G2289	U2290	A	U2072	A1881	U1797	G1634	G1546	U1445	G1074	G1075	A
A2291	G2292	G	G2073	C1882	C1798	U1635	U1547	C1450	C1172	G1075	G
G2293	G2294	U	A2074	U1883	U1799	G1636	C1557	C1451	C1174	C1080	U
U2299	A2300	C	A2081	A1885	G1805	A1637	C1558	G1452	C1175	A1081	C
A2301	G2302	C	G2082	U1887	G1806	C1641	U1559	U1454	C1176	A1082	G
G2303	U2304	G	A2082	C1888	C1810	A1642	U1561	U1454	A1177		C
G2308	A2309	A	U2083	G1889	U1813	C1643	C1562	U1461	U1180	A1086	A
G2310	G2311	C	C2092	C1894	G1818	U1732	C1563	C1462	A1181	G1087	G
G2312	C2313	U	G2093	A1895	G1819	A1733	C1564	A1463	A1182	A1088	A
G2314	G2315	C	G2094	U1896	G1820	C1734	C1565	U1471	C1183	U1095	U
G2316	G2317	A	A2095	C1897	C1826	A1736	C1566	C1472	U1185		U
U2320	U2321	C	G2097	G1898	G1827	G1651	C1567	C1473	C1186	A1098	U
U2322	G2323	G	U2004	C1899	G1828	A1653	C1570	U1474	U1187	G1099	U
U2324	U2325	U	G2100	U1902	A1829	C1654	G1571	C1477	A1188	U1109	U
U2326	U2327	C	A2101	G1903	G1834	G1655	A1572	U1478	A1189	G1110	U
U2328	U2329	A	G2102	A1904	U1835	A1656	C1573	U1479	A1191		U
U2330	U2331	C	A2103	A1909	U1836	A1657	C1574	C1483	A1192	U1116	U
U2332	U2333	U	C2105	U1916	U1837	A1658	C1579	U1484	A1193	A1117	U
U2334	U2335	C	C2106	G1917	U1838	A1659	A1580	U1485	G1119	G1118	U
U2336	U2337	A	G2110	U1918	U1839	A1660	U1583	A1494	G1120	U1120	U
U2338	U2339	C	G2111	U1919	U1840	A1661	U1586	C1495	C1201	U1122	U
U2340	U2341	G	C2112	U1920	U1841	A1662	G1587	G1496	U1205	A1123	U
U2342	U2343	U	U2012	C1921	U1842	A1663	U1588	G1497	U1206	A1124	U
U2344	U2345	C	U2013	A1922	U1843	A1664	G1589	U1499	U1207	U1125	U
U2346	U2347	A	G2113	U1923	U1844	A1665	G1592	U1500	C1208	C1126	U
U2348	U2349	C	G2114	U1924	U1845	A1666	C1593	U1503	C1209	U1127	U
U2350	U2351	U	C2115	U1925	U1846	A1667	C1594	A1504	G1210	U1128	U
U2352	U2353	C	U2116	U1926	U1847	A1668	C1595	U1505	G1211	U1129	U
U2354	U2355	G	U2117	U1927	U1848	A1669	G1596	U1506	C1212	U1130	U
U2356	U2357	A	U2118	U1928	U1849	A1670	A1597	U1507	C1213	U1131	U
U2358	U2359	C	U2119	U1929	U1850	A1671	A1598	U1508	G1214	A1132	U
U2360	U2361	U	U2120	U1930	U1851	A1672	A1599	U1509	A1133	U1029	U
U2362	U2363	C	U2121	U1931	U1852	A1673	A1601	G1512	G1215	C1134	U
U2364	U2365	A	U2122	U1932	U1853	A1674	G1602	C1513	G1216	G1135	U
U2366	U2367	C	U2123	U1933	U1854	A1675	G1603	U1514	G1226	U1136	U
U2368	U2369	U	U2124	U1934	U1855	A1676	A1681	A1414	G1137	G1137	U
U2370	U2371	C	U2125	U1935	U1856	A1677	A1682	A1415			U
U2372	U2373	A	U2126	U1936	U1857	A1678	A1683	A1416			U
U2374	U2375	C	U2127	U1937	U1858	A1679	A1684	A1417			U
U2376	U2377	G	U2128	U1938	U1859	A1680	A1685	A1418			U
U2378	U2379	U	U2129	U1939	U1860	A1681	A1686	A1419			U
U2380	U2381	C	U2130	U1940	U1861	A1682	A1687	A1420			U
U2382	U2383	A	U2131	U1941	U1862	A1683	A1688	A1421			U
U2384	U2385	C	U2132	U1942	U1863	A1684	A1689	A1422			U
U2386	U2387	U	U2133	U1943	U1864	A1685	A1690	A1423			U
U2388	U2389	C	U2134	U1944	U1865	A1686	A1691	A1424			U
U2390	U2391	A	U2135	U1945	U1866	A1687	A1692	A1425			U
U2392	U2393	U	U2136	U1946	U1867	A1688	A1693	A1426			U
U2394	U2395	C	U2137	U1947	U1868	A1689	A1694	A1427			U
U2396	U2397	A	U2138	U1948	U1869	A1690	A1695	A1428			U
U2398	U2399	U	U2139	U1949	U1870	A1691	A1696	A1429			U
U2400	U2401	C	U2140	U1950	U1871	A1692	A1697	A1430			U
U2402	U2403	A	U2141	U1951	U1872	A1693	A1698	A1431			U
U2404	U2405	C	U2142	U1952	U1873	A1694	A1699	A1432			U
U2406	U2407	U	U2143	U1953	U1874	A1695	A1700	A1433			U
U2408	U2409	C	U2144	U1954	U1875	A1696	A1701	A1434			U
U2410	U2411	A	U2145	U1955	U1876	A1697	A1702	A1435			U
U2412	U2413	C	U2146	U1956	U1877	A1698	A1703	A1436			U
U2414	U2415	U	U2147	U1957	U1878	A1699	A1704	A1437			U
U2416	U2417	C	U2148	U1958	U1879	A1700	A1705	A1438			U
U2418	U2419	A	U2149	U1959	U1880	A1701	A1706	A1439			U
U2420	U2421	C	U2150	U1960	U1881	A1702	A1707	A1440			U
U2422	U2423	U	U2151	U1961	U1882	A1703	A1708	A1441			U
U2424	U2425	C	U2152	U1962	U1883	A1704	A1709	A1442			U
U2426	U2427	A	U2153	U1963	U1884	A1705	A1710	A1443			U
U2428	U2429	C	U2154	U1964	U1885	A1706	A1711	A1444			U
U2430	U2431	U	U2155	U1965	U1886	A1707	A1712	A1445			U
U2432	U2433	C	U2156	U1966	U1887	A1708	A1713	A1446			U
U2434	U2435	A	U2157	U1967	U1888	A1709	A1714	A1447			U
U2436	U2437	C	U2158	U1968	U1889	A1710	A1715	A1448			U
U2438	U2439	U	U2159	U1969	U1890	A1711	A1716	A1449			U
U2440	U2441	C	U2160	U1970	U1891	A1712	A1717	A1450			U
U2442	U2443	A	U2161	U1971	U1892	A1713	A1718	A1451			U
U2444	U2445	C	U2162	U1972	U1893	A1714	A1719	A1452			U
U2446	U2447	U	U2163	U1973	U1894	A1715	A1720	A1453			U
U2448	U2449	C	U2164	U1974	U1895	A1716	A1721	A1454			U
U2450	U2451	A	U2165	U1975	U1896	A1717	A1722	A1455			U
U2452	U2453	C	U2166	U1976	U1897	A1718	A1723	A1456			U
U2454	U2455	U	U2167	U1977	U1898	A1719	A1724	A1457			U
U2456	U2457	C	U2168	U1978	U1899	A1720	A1725	A1458			U
U2458	U2459	A	U2169	U1979	U1900	A1721	A1726	A1459			U
U2460	U2461	C	U2170	U1980	U1901	A1722	A1727	A1460			U
U2462	U2463	U	U2171	U1981	U1902	A1723	A1728	A1461			U
U2464	U2465	C	U2172	U1982	U1903	A1724	A1729	A1462			U
U2466	U2467	A	U2173	U1983	U1904	A1725	A1730	A1463			U
U2468	U2469	C	U2174	U1984	U1905	A1726	A1731	A1464			U
U2470	U2471	U	U2175	U1985	U1906	A1727	A1732	A1465			U
U2472	U2473	C	U2176	U1986	U1907	A1728	A1733	A1466			U
U2474	U2475	A	U2177	U1987	U1908	A1729	A1734	A1467			U
U2476	U2477	C	U2178	U1988	U1909	A1730	A1735	A1468			U
U2478	U2479	U	U2179	U1989	U1910	A1731	A1736	A1469			U
U2480	U2481	C	U2180	U1990	U1911	A1732	A1737	A1470			U
U2482	U2483	A	U2181	U1991	U1912	A1733	A1738	A1471			U
U2484	U2485	C	U2182	U1992	U1913	A1734	A1739	A1472			U
U2486	U2487	U	U2183	U1993	U1914	A1735	A1740	A1473			U
U2488	U2489	C	U2184	U1994	U1915	A1736	A1741	A1474			U
U2490	U2491	A	U2185	U1995	U1916	A1737	A1742	A1475			U
U2492	U2493	C	U2186	U1996	U1917	A1738	A1743	A1476			U
U2494	U2495	U	U2187	U1997	U1918	A1739	A1744	A1477			U
U2496	U2497	C	U2188	U1998	U1919	A1740	A1745	A1478			U
U2498	U2499	A	U2189	U1999							



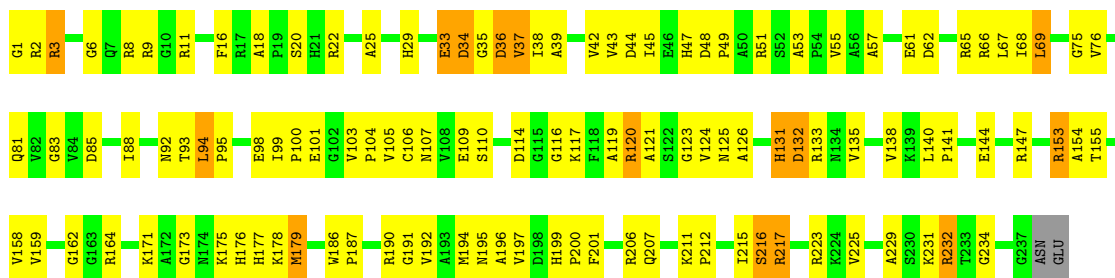
• Molecule 2: 5S ribosomal RNA

Chain B:



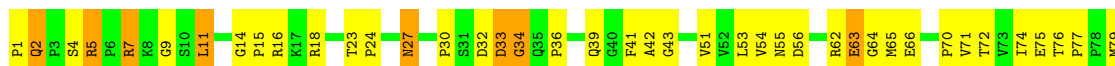
• Molecule 3: 50S ribosomal protein L2P

Chain C:



• Molecule 4: 50S ribosomal protein L3P

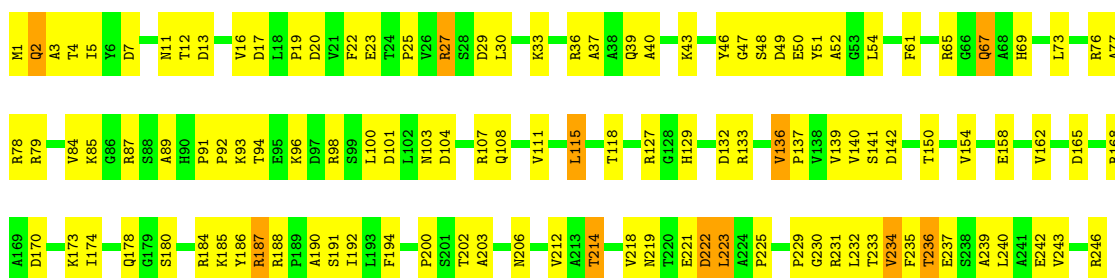
Chain D:





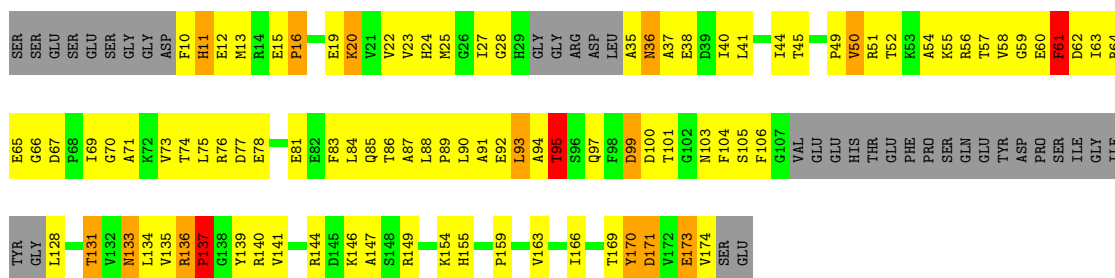
• Molecule 5: 50S ribosomal protein L4E

Chain E:



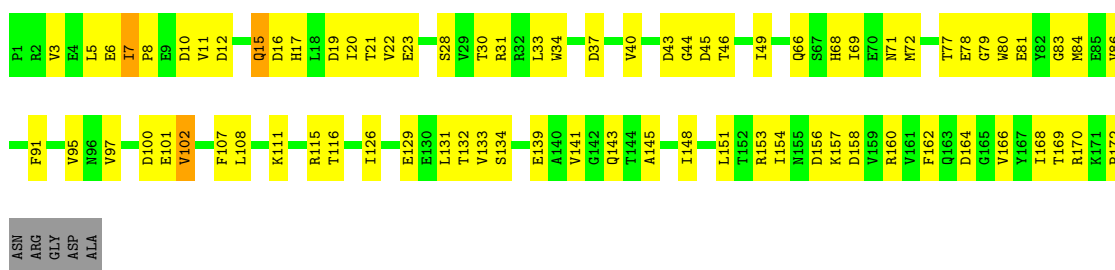
• Molecule 6: 50S ribosomal protein L5P

Chain F:



• Molecule 7: 50S ribosomal protein L6P

Chain G:



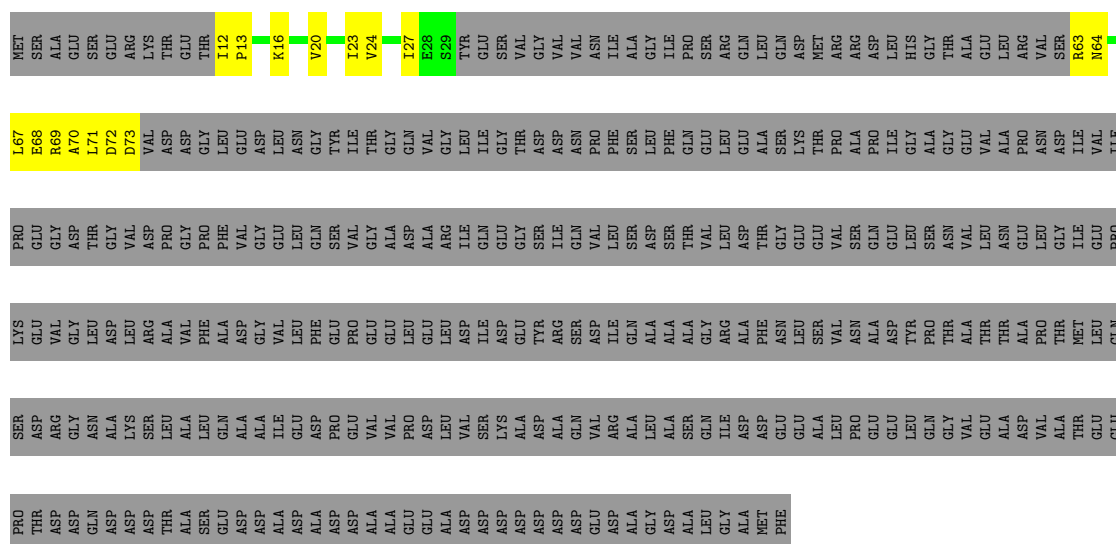
• Molecule 8: 50S ribosomal protein L7Ae

Chain H:



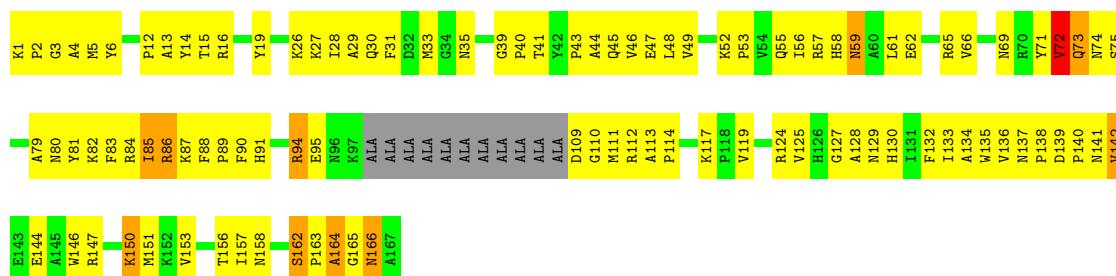
• Molecule 9: Acidic ribosomal protein P0 homolog

Chain I:



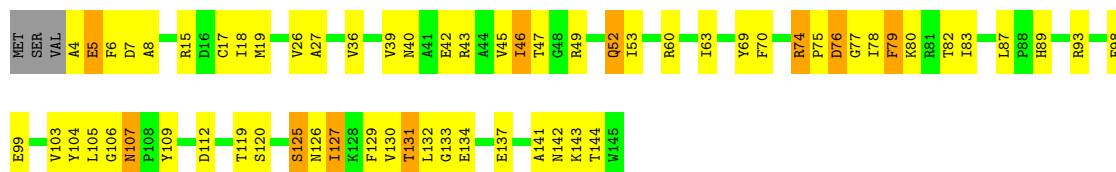
• Molecule 10: 50S ribosomal protein L10e

Chain J:



• Molecule 11: 50S ribosomal protein L13P

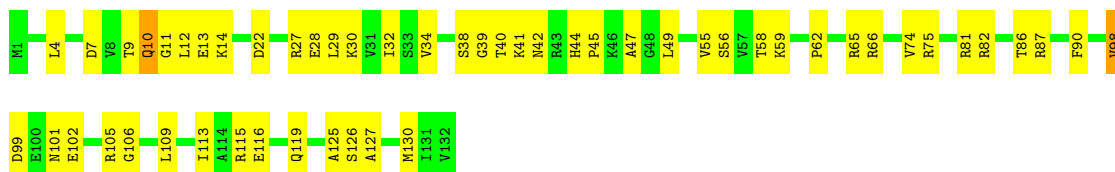
Chain K:



• Molecule 12: 50S ribosomal protein L14P

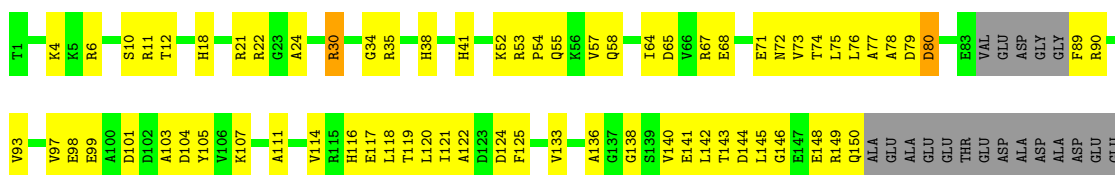
Chain L:





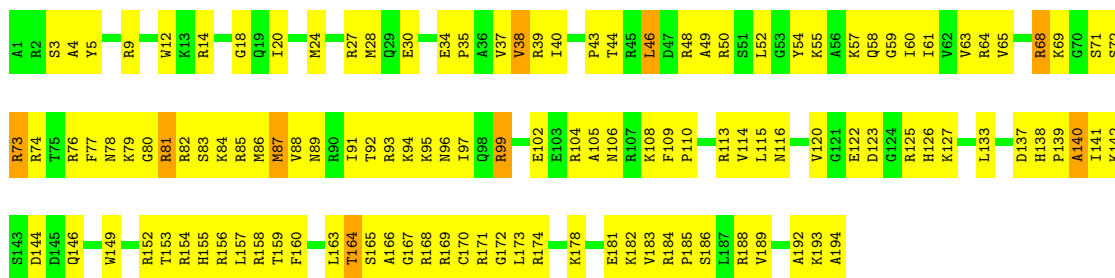
• Molecule 13: 50S ribosomal protein L15P

Chain M:



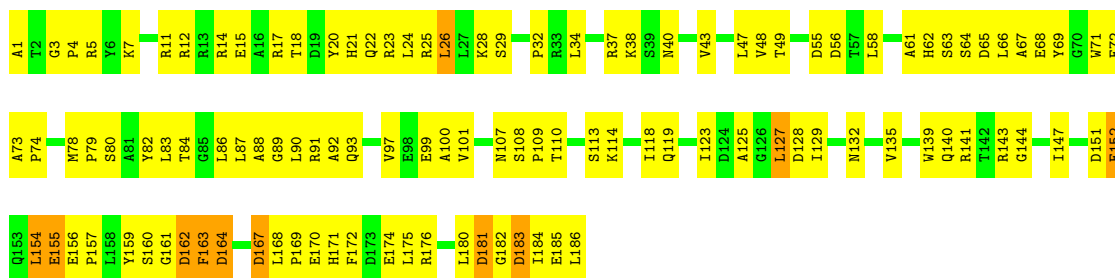
• Molecule 14: 50S ribosomal protein L15E

Chain N:



• Molecule 15: 50S ribosomal protein L18P

Chain O:



• Molecule 16: 50S ribosomal protein L18E

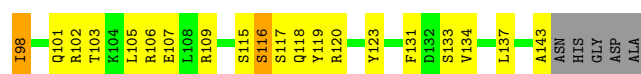
Chain P:



• Molecule 17: 50S ribosomal protein L19E

Chain Q:





- Molecule 18: 50S ribosomal protein L21e

Chain R:



- Molecule 19: 50S ribosomal protein L22P

Chain S:



- Molecule 20: 50S ribosomal protein L23P

Chain T:



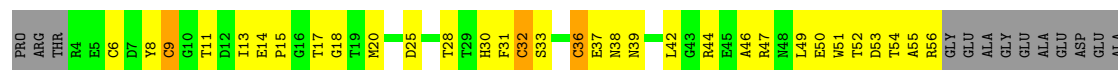
- Molecule 21: 50S ribosomal protein L24P

Chain U:



- Molecule 22: 50S ribosomal protein L24E

Chain V:



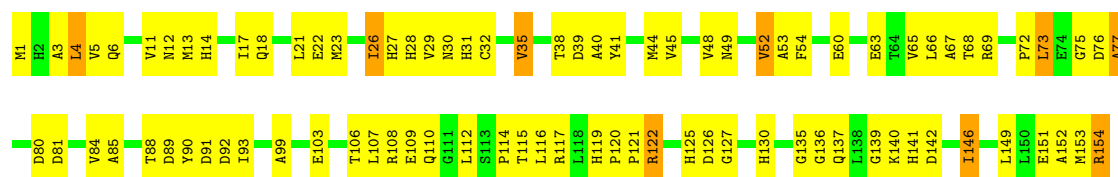
- Molecule 23: 50S ribosomal protein L29P

Chain W:



- Molecule 24: 50S ribosomal protein L30P

Chain X:



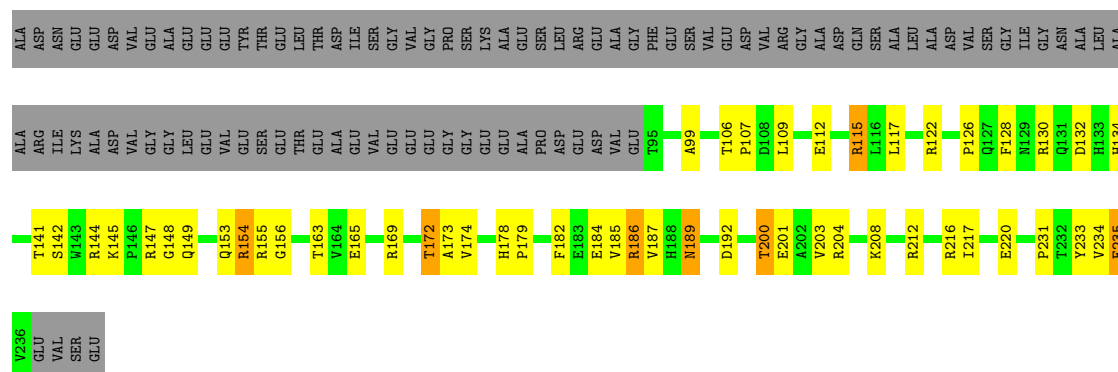
• Molecule 25: 50S ribosomal protein L31E

Chain Y:



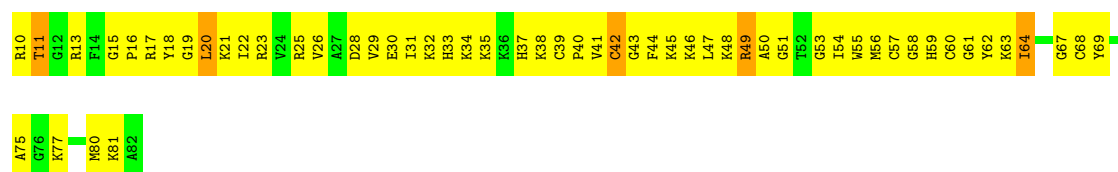
• Molecule 26: 50S ribosomal protein L32E

Chain Z:



• Molecule 27: 50S ribosomal protein L37AE

Chain 1:



• Molecule 28: 50S ribosomal protein L37e

Chain 2:



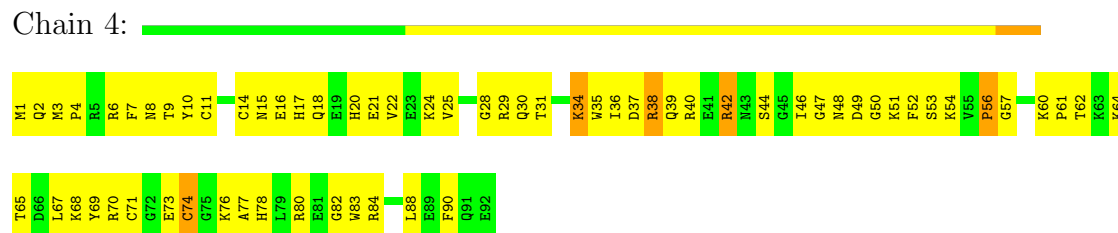
• Molecule 29: 50S ribosomal protein L39e

Chain 3:



- Molecule 30: 50S ribosomal protein L44E

Chain 4:



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	94.6 (20.00-3.00)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	98569	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, CD, VIR

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	0.57	9/66076 (0.0%)	0.76	37/103052 (0.0%)
2	B	0.81	10/2905 (0.3%)	0.91	17/4528 (0.4%)
3	C	0.44	0/1787	0.75	0/2409
4	D	0.41	0/2689	0.71	0/3652
5	E	0.48	0/1883	0.74	0/2551
6	F	0.40	0/1111	0.64	0/1498
7	G	0.44	0/1382	0.66	0/1880
8	H	0.40	0/896	0.63	0/1219
9	I	0.33	0/241	0.53	0/324
10	J	0.46	0/1246	0.83	2/1686 (0.1%)
11	K	0.46	0/1135	0.70	0/1530
12	L	0.43	0/1003	0.75	0/1351
13	M	0.42	0/1126	0.75	0/1504
14	N	0.63	0/1633	0.86	1/2180 (0.0%)
15	O	0.42	0/1473	0.71	0/1999
16	P	0.45	0/873	0.71	0/1181
17	Q	0.44	0/1143	0.64	0/1521
18	R	0.45	0/748	0.79	0/1005
19	S	0.45	0/1172	0.76	0/1578
20	T	0.41	0/648	0.65	0/875
21	U	0.38	0/957	0.70	0/1289
22	V	0.82	0/417	0.81	1/562 (0.2%)
23	W	0.40	0/502	0.61	0/675
24	X	0.50	0/1218	0.73	0/1655
25	Y	0.44	0/664	0.70	0/895
26	Z	0.46	0/1146	0.72	0/1536
27	1	0.77	0/575	0.82	0/763
28	2	0.54	0/437	0.78	0/578
29	3	0.42	0/398	0.63	0/527
30	4	0.98	0/771	0.81	0/1024
All	All	0.56	19/98255 (0.0%)	0.76	58/147027 (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
1	A	1	157
2	B	0	4
All	All	1	161

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2488	A	O5'-C5'	-8.71	1.28	1.42
2	B	3025	G	C2'-O2'	-7.62	1.31	1.41
2	B	3003	A	O5'-C5'	7.52	1.56	1.44
2	B	3024	U	O5'-C5'	7.15	1.55	1.44
2	B	3023	U	C4'-O4'	7.08	1.54	1.45

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP2-P-O3'	-18.66	64.14	105.20
1	A	1164	U	OP1-P-O3'	-18.19	65.19	105.20
1	A	1979	G	C2'-C3'-O3'	9.72	130.90	109.50
1	A	1563	G	C2'-C3'-O3'	9.58	130.58	109.50
1	A	1165	G	O5'-P-OP1	-8.38	98.16	105.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 161 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	U	Sidechain
1	A	23	G	Sidechain
1	A	26	U	Sidechain
1	A	32	G	Sidechain
1	A	33	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	59017	0	29801	1306	0
2	B	2600	0	1326	85	0
3	C	1754	0	1763	144	0
4	D	2624	0	2533	195	0
5	E	1858	0	1816	146	0
6	F	1094	0	1085	135	0
7	G	1357	0	1266	79	0
8	H	885	0	854	73	0
9	I	240	0	231	23	0
10	J	1215	0	1215	168	0
11	K	1119	0	1098	70	0
12	L	993	0	1027	60	0
13	M	1114	0	1072	79	0
14	N	1605	0	1676	212	0
15	O	1444	0	1401	152	0
16	P	864	0	873	29	0
17	Q	1133	0	1127	68	0
18	R	734	0	729	27	0
19	S	1149	0	1122	68	0
20	T	641	0	605	26	0
21	U	949	0	923	52	0
22	V	410	0	368	48	0
23	W	499	0	511	30	0
24	X	1195	0	1137	115	0
25	Y	654	0	653	48	0
26	Z	1130	0	1133	62	0
27	1	563	0	601	83	0
28	2	430	0	426	30	0
29	3	393	0	406	22	0
30	4	755	0	732	89	0
31	A	38	0	34	3	0
32	4	1	0	0	0	0
32	A	109	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	D	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	1	0	0	0	0
34	4	1	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	2	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	1	0
35	A	8	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	2	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	2	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	35	0	0	15	0
37	2	57	0	0	1	0
37	3	40	0	0	6	0
37	4	72	0	0	11	0
37	A	5881	0	0	302	0
37	B	146	0	0	21	0
37	C	135	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	D	141	0	0	33	0
37	E	178	0	0	46	0
37	F	49	0	0	17	0
37	G	43	0	0	10	0
37	H	30	0	0	11	0
37	I	21	0	0	7	0
37	J	76	0	0	23	0
37	K	55	0	0	6	0
37	L	64	0	0	16	0
37	M	85	0	0	21	0
37	N	141	0	0	35	0
37	O	67	0	0	20	0
37	P	45	0	0	10	0
37	Q	72	0	0	10	0
37	R	57	0	0	3	0
37	S	87	0	0	10	0
37	T	34	0	0	5	0
37	U	33	0	0	6	0
37	V	27	0	0	6	0
37	W	16	0	0	2	0
37	X	68	0	0	11	0
37	Y	27	0	0	5	0
37	Z	100	0	0	14	0
All	All	98569	0	59544	3401	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 23.

The worst 5 of 3401 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.52	1.20
10:J:165:GLY:HA3	37:J:8397:HOH:O	1.39	1.18
27:1:39:CYS:SG	27:1:47:LEU:HD21	1.84	1.17
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.25	1.15
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.31	1.11

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	C	235/239 (98%)	200 (85%)	29 (12%)	6 (3%)	8	39
4	D	335/337 (99%)	302 (90%)	22 (7%)	11 (3%)	6	32
5	E	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	1	5
7	G	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	33	81
8	H	117/119 (98%)	104 (89%)	10 (8%)	3 (3%)	8	39
9	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	5	25
10	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	6	32
11	K	140/145 (97%)	127 (91%)	8 (6%)	5 (4%)	5	29
12	L	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	15	58
13	M	141/164 (86%)	120 (85%)	20 (14%)	1 (1%)	30	78
14	N	192/194 (99%)	165 (86%)	24 (12%)	3 (2%)	14	56
15	O	184/186 (99%)	164 (89%)	12 (6%)	8 (4%)	4	23
16	P	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	30	78
18	R	93/95 (98%)	86 (92%)	3 (3%)	4 (4%)	4	23
19	S	148/154 (96%)	134 (90%)	13 (9%)	1 (1%)	30	78
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
21	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
22	V	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	6	33
24	X	152/154 (99%)	142 (93%)	8 (5%)	2 (1%)	18	62
25	Y	80/91 (88%)	71 (89%)	5 (6%)	4 (5%)	3	19
26	Z	140/240 (58%)	133 (95%)	7 (5%)	0	100	100
27	1	71/73 (97%)	61 (86%)	7 (10%)	3 (4%)	4	24
28	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	3	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
30	4	90/92 (98%)	83 (92%)	5 (6%)	2 (2%)	10	45
All	All	3633/4235 (86%)	3265 (90%)	291 (8%)	77 (2%)	11	47

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	101	ALA

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	C	179/181 (99%)	166 (93%)	13 (7%)	20	59
4	D	282/282 (100%)	264 (94%)	18 (6%)	25	66
5	E	193/193 (100%)	178 (92%)	15 (8%)	18	55
6	F	117/147 (80%)	106 (91%)	11 (9%)	13	44
7	G	152/155 (98%)	148 (97%)	4 (3%)	59	91
8	H	92/92 (100%)	91 (99%)	1 (1%)	84	97
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	14	47
11	K	118/121 (98%)	107 (91%)	11 (9%)	13	45
12	L	106/106 (100%)	102 (96%)	4 (4%)	44	85
13	M	112/126 (89%)	108 (96%)	4 (4%)	47	86
14	N	166/166 (100%)	158 (95%)	8 (5%)	35	79
15	O	149/149 (100%)	144 (97%)	5 (3%)	49	88
16	P	93/93 (100%)	91 (98%)	2 (2%)	64	93
17	Q	113/116 (97%)	109 (96%)	4 (4%)	48	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	79/79 (100%)	75 (95%)	4 (5%)	33	76
19	S	117/121 (97%)	113 (97%)	4 (3%)	49	88
20	T	71/73 (97%)	69 (97%)	2 (3%)	56	91
21	U	105/105 (100%)	102 (97%)	3 (3%)	55	90
22	V	44/52 (85%)	42 (96%)	2 (4%)	38	81
23	W	51/56 (91%)	51 (100%)	0	100	100
24	X	130/130 (100%)	121 (93%)	9 (7%)	22	62
25	Y	66/73 (90%)	61 (92%)	5 (8%)	19	57
26	Z	120/195 (62%)	110 (92%)	10 (8%)	16	52
27	1	56/56 (100%)	49 (88%)	7 (12%)	7	28
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	61	92
30	4	79/79 (100%)	73 (92%)	6 (8%)	19	57
All	All	3027/3441 (88%)	2863 (95%)	164 (5%)	31	74

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	52	GLN
13	M	117	GLU
27	1	32	LYS
11	K	76	ASP
11	K	131	THR

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

Mol	Chain	Res	Type
13	M	116	HIS
18	R	40	HIS
29	3	18	ASN
14	N	58	GLN
15	O	153	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	248 (9%)	38 (1%)
2	B	121/122 (99%)	14 (11%)	4 (3%)
All	All	2868/3044 (94%)	262 (9%)	42 (1%)

5 of 262 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1352	A
1	A	1667	A
2	B	3023	U
1	A	1377	C
1	A	1474	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 232 ligands modelled in this entry, 231 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
31	VIR	A	9403	-	40,40,40	2.27	19 (47%)	53,55,55	2.17	16 (30%)

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
31	VIR	A	9403	-	-	0/46/58/58	0/0/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9403	VIR	C28-C29	-6.28	1.15	1.32
31	A	9403	VIR	C26-N25	3.86	1.40	1.34
31	A	9403	VIR	C10-N9	-3.72	1.26	1.36
31	A	9403	VIR	C4-N5	3.63	1.53	1.47
31	A	9403	VIR	C28-C26	3.46	1.55	1.48

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9403	VIR	O27-C26-C28	6.61	135.79	123.13
31	A	9403	VIR	C4-N5-C6	5.14	126.88	118.92
31	A	9403	VIR	C28-C26-N25	-5.02	103.44	114.66
31	A	9403	VIR	C8-N9-C10	-4.72	104.76	107.50
31	A	9403	VIR	C8-C6-N5	-3.69	110.64	118.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.