



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

PDB ID : 1JZZ  
Title : Structural Basis for the Interaction of Antibiotics with the Peptidyl Transferase Center in Eubacteria  
Authors : Schlutzen, F.; Zarivach, R.; Harms, J.; Bashan, A.; Tocilj, A.; Albrecht, R.; Yonath, A.; Franceschi, F.  
Deposited on : 2001-09-17  
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

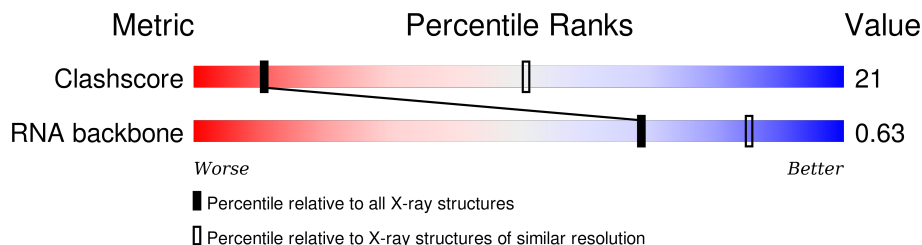
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.



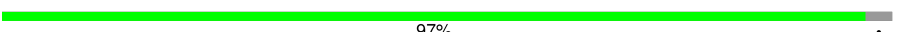
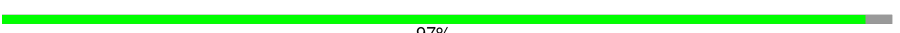
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1458 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	 30% 48% 18% .
2	K	205	 96% .
3	L	134	 97% .
4	M	60	 97% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ROX	A	2881	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59977 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2774	Total	C	N	O	P	0	0	0
			59532	26556	10982	19221	2773			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1526	U	Y	SEE REMARK 999	GB 15805042

- Molecule 2 is a protein called Ribosomal Protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	K	197	Total	C	0	0	197
			197	197			

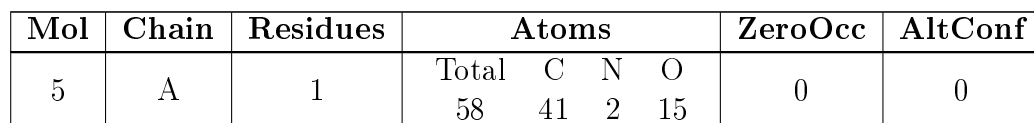
- Molecule 3 is a protein called Ribosomal Protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	L	130	Total	C	0	0	130
			130	130			

- Molecule 4 is a protein called Ribosomal Protein L32.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	M	58	Total	C	0	0	58
			58	58			

- Molecule 5 is ROXITHROMYCIN (three-letter code: ROX) (formula: C<sub>41</sub>H<sub>76</sub>N<sub>2</sub>O<sub>15</sub>).



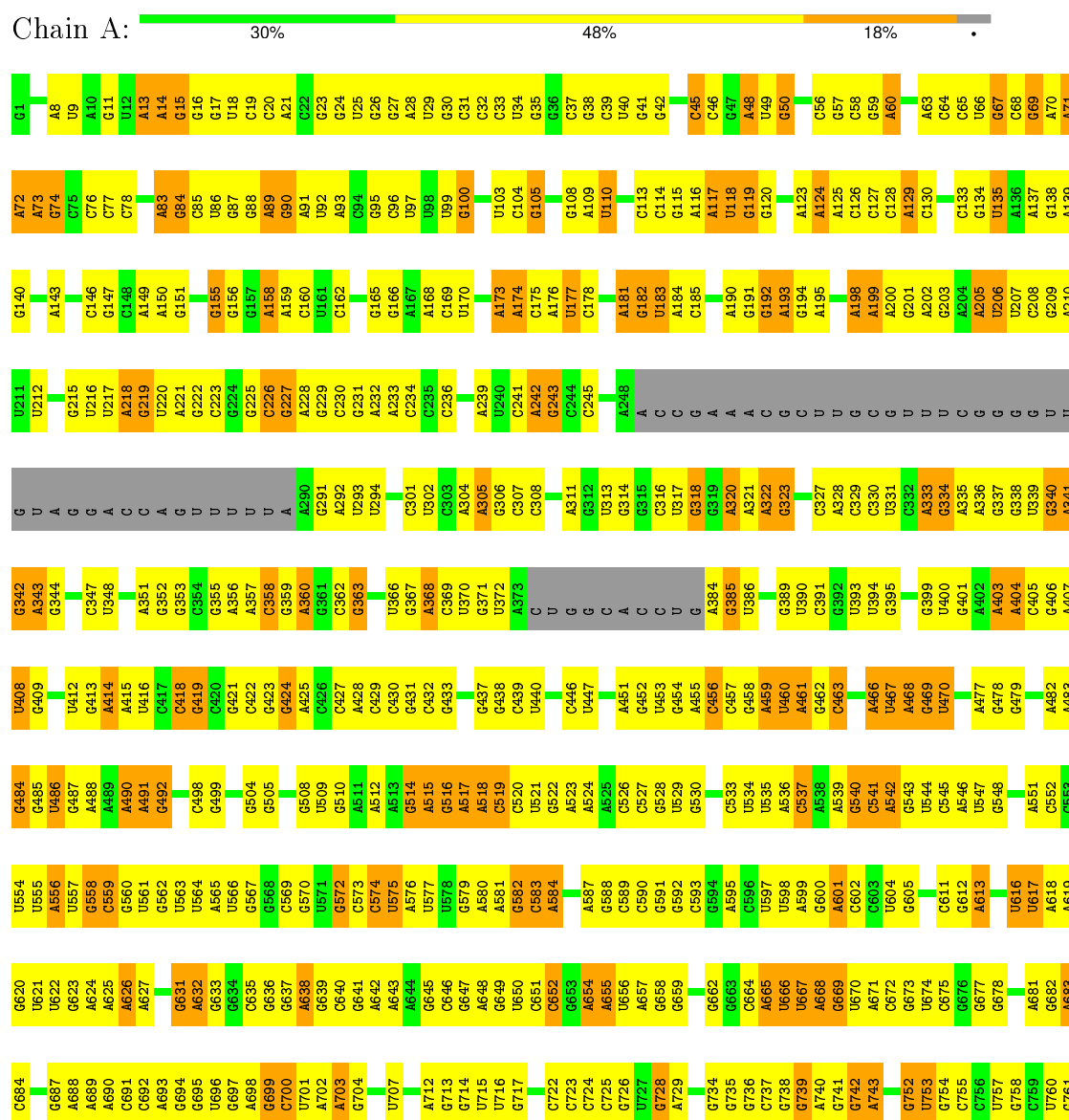
- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 6   | A     | 2        | Total Mg<br>2 2 | 0       | 0       |

### 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 rRNA

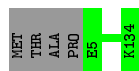


U1819	U1748	U1679	C1606	U1537	U1473	G1401	G1333	G1263	G1186	C1111	U1044	A970	U	C830	A762
G1820	G1749	U1680	A1607	A1538	U1473	G1402	G1333	C1263	A1187	U1112	U1044	A971	A	G831	A763
A1821	A1750	U1681	U1608	U1539	A1474	U1403	A1334	G1265	G1188	C1113	U1045	C972	C	A832	A764
C1822	A1751	A1682	U1611	C1540	U1475	C1404	G1337	G1266	C1190	U1118	U1047	U974	C	A833	C765
C1823	U1752	G1683	U1612	G1542	G1476	A1405	G1338	U1268	C1191	G1119	U1048	C975	A	A766	C766
C1824	G1684	G1684	G1613	G1543	U1481	U1409	U1339	G1269	A1192	G1120	C1049	C976	C	U839	U768
C1825	G1754	A1685	C1614	A1544	U1482	U1410	C1340	C1270	A1193	G1121	U1049	U977	U	U840	U768
U1826	C1756	C1687	U1617	U1548	U1481	U1410	C1341	G1271	U1194	A1122	C1054	U978	U	G841	G773
G1827	U1688	U1688	U1618	U1549	G1483	C1412	U1342	G1272	U1195	G1123	A1055	A979	A	A842	A774
C1828	U1689	U1689	U1619	U1550	U1484	C1412	U1343	G1273	G1196	U1124	U1056	G980	C	G843	U775
C1829	U1690	C1550	U1619	C1550	U1485	C1415	C1344	C1274	U1197	G1125	A1057	C981	C	G844	C776
C1830	U1691	U1551	A1619	U1551	U1486	A1416	C1345	A1275	C1198	A1126	G1058	C982	C	U845	A777
G1831	C1692	C1552	C1623	C1552	C1487	C1417	C1346	U1276	U1199	G1127	A1059	G983	C	A846	G778
G1834	G1763	G1553	A1624	G1553	G1488	U1420	C1347	G1277	U1200	G1128	A1060	A984	C	C850	U784
C1835	A1764	G1554	A1625	G1554	C1489	A1420	C1348	A1278	G1201	A1129	A1061	G985	C	C851	U785
C1836	C1765	A1555	A1626	A1555	U1490	U1421	A1349	G1279	G1202	U1130	U1065	A994	C	U852	U786
U1840	U1766	A1556	C1627	C1557	U1493	U1424	G1350	U1280	G1204	C1134	A1066	A995	C	C853	A787
A1851	U1768	C1558	C1631	C1558	G1494	G1425	G1351	A1281	G1205	C1135	G1067	C996	C	G854	G788
C1854	U1770	G1559	A1632	U1559	G1495	U1426	G1352	A1282	G1209	C1136	A1068	C997	C	G855	G789
G1854	C1771	A1560	C1633	A1560	G1496	G1427	A1354	G1284	C1210	A1137	G1069	C998	C	A856	A790
G1855	A1771	C1703	A1634	A1561	C1497	G1428	A1355	A1285	G1211	A1138	G1070	A999	C	U857	C791
U1856	C1772	G1704	G1635	G1562	G1498	A1429	G1356	U1286	U1212	A1139	U1071	G1000	C	G858	C791
C1857	A1774	U1563	U1640	U1563	A1499	G1430	U1357	A1287	U1213	A1140	U1072	A1001	C	U859	A794
U1875	C1775	U1564	C1641	U1564	U1500	U1431	C1358	A1288	G1214	U1141	G1073	C1002	C	U860	A795
A1867	A1776	G1571	G1642	C1571	C1501	G1432	G1359	A1289	A1215	A1142	G1074	C1003	C	G861	A796
U1877	U1777	C1572	G1645	C1572	G1502	A1433	C1364	A1290	G1216	A1143	G1075	A1004	C	A862	A797
U1878	C1778	U1710	U1645	G1573	G1503	G1434	C1365	A1291	U1217	U1144	U1076	U1005	C	G863	C798
U1879	A1779	G1574	C1648	C1575	U1505	G1436	A1366	A1293	C1218	G1145	A1080	A1007	C	C864	C799
C1881	U1780	C1576	U1651	U1574	C1506	A1437	A1367	A1298	G1220	G1146	U1081	A1008	C	A865	U800
G1882	C1781	G1576	C1651	C1576	U1507	A1438	G1368	G1298	C1221	U1149	G1082	G1008	C	U866	A801
A1883	U1782	U1714	U1652	C1579	A1507	G1439	G1369	A1299	G1222	C1150	C1083	A1012	C	U868	C803
C1884	A1783	G1579	G1652	G1579	G1508	G1440	U1370	A1300	G1223	G1013	U1084	G1013	C	C869	C804
C1885	C1784	C1580	C1653	C1580	A1509	A1441	G1371	U1301	A1224	G1085	G1014	C939	C	C870	C805
U1894	U1785	C1581	A1654	C1581	A1510	A1441	G1372	U1302	C1225	A1153	C1086	U1015	C	U871	A806
A1895	G1803	A1582	C1655	A1582	A1511	G1442	G1373	C1302	A1226	A1154	G1087	C1016	C	G872	A807
C1896	C1786	U1583	U1656	U1583	U1512	G1443	G1374	U1306	A1227	G1155	A1088	U1019	C	U873	C808
C1897	U1787	G1584	C1657	G1584	U1513	C1444	G1377	U1307	A1233	U1161	C1089	U1020	C	A874	C809
A1898	A1788	U1585	U1660	U1585	U1514	A1445	C1380	U1308	C1234	U1162	C1090	A1021	C	G875	U810
C1899	C1789	C1586	C1661	C1586	U1515	U1446	C1381	C1310	C1234	A1163	U1092	A1022	C	G876	C812
C1900	U1790	G1588	G1662	G1588	G1519	G1450	G1382	G1311	G1240	C1164	U1093	U1023	C	C877	A813
A1901	A1791	U1591	C1663	U1591	U1521	C1451	G1383	G1312	G1241	G1165	A1096	G1024	C	A879	C814
U1902	C1801	C1592	C1664	C1592	C1522	U1452	G1384	U1313	U1244	G1166	A1097	C1029	C	C880	A815
C1903	G1803	C1593	C1665	C1593	C1523	A1453	C1385	A1314	G1245	A1167	G1098	U1030	C	A886	A817
A1904	U1733	U1594	G1666	U1594	A1525	C1456	A1366	G1315	G1249	G1168	A1099	C1031	C	G887	C818
C1905	C1734	A1595	U1667	A1595	U1526	A1457	G1387	G1316	U1249	U1170	G1100	C1031	C	G888	C819
A1906	G1735	A1596	C1668	A1596	U1527	A1457	G1387	A1321	A1250	G1171	U1101	A1032	C	C889	U820
C1907	C1736	U1597	G1670	U1597	G1528	U1459	A1391	G1322	G1251	A1171	G1102	G1033	C	U890	A821
U1908	U1737	C1598	A1671	C1598	C1529	G1460	U1392	C1323	C1261	U1172	C1103	U1034	C	A891	G822
C1909	U1738	G1599	C1672	G1599	U1530	G1461	G1393	G1324	C1253	G1173	G1104	G1035	C	G892	U823
A1910	C1742	U1600	C1531	U1600	C1531	G1465	G1394	G1324	C1253	G1174	U1105	U1036	C	G	U824
C1911	C1743	C1673	C1531	C1673	C1531	C1466	G1394	U1326	G1258	A1175	A1106	U1037	C	G	C825
U1912	C1744	C1674	C1532	U1601	A1532	C1466	A1397	U1327	A1259	C1183	U1107	U1038	C	G	U826
C1913	C1745	C1675	C1533	G1602	G1533	U1467	C1398	C1328	A1260	G1184	U1108	A1039	C	G	C827
A1914	C1746	A1603	A1534	A1603	C1534	U1468	C1399	C1328	G1261	C1184	A1109	A1040	C	G	C828
U1915	C1747	C1676	C1535	C1604	C1535	U1469	U1329	G1330	U1262	C1185	G1110	G1041	C	C	C829

U1909	A1984	G2055	A2119	C2183	G2255	C2329	U2416	U2485	C2554	U2626	G2699	U2778	U2853
A1910	G1985	C2056	C2120	U2185	G2256	G2330	U2417	C2486	G2555	G2627	G2699	C2779	G2854
A1911	G1986	U2057	G2121	G2186	G2261	A2337	A2418	G2487	G2556	G2628	A2705	A2780	G2855
G1912	U1987	U2058	G2122	A2189	C2263	C2338	C2419	G2491	G2557	U2629	U2706	G2781	A2858
G1913	A1988	U2059	G2123	A2190	C2264	A2348	C2420	U2493	U2558	A2633	U2708	U2783	A2859
U1914	G1989	A2060	C2125	A2191	C2266	G2349	C2421	C2494	G2560	U2634	C2709	A2784	G2860
A1915	C1989	C2061	U	U2192	A2268	G2350	C2422	C2496	G2561	U2635	G2711	A2785	A2861
A1916	U1994	U2062	U	U2193	A2267	A2355	G2423	C2497	U2564	A2636	G2712	G2786	G2862
G1917	G1995	A2063	U	A2194	G2269	A2356	G2424	U2498	C2565	A2641	A2713	A2787	U2865
A1918	A1996	U2067	U	A2195	U2270	A2357	A2425	C2499	A2566	G2642	G2714	C2788	A2866
A1919	A1997	U2068	U	C2193	C2271	A2358	G2426	C2500	A2567	G2643	A2715	G2789	G2867
A1920	A1998	U2069	G	C2194	C2272	C2359	U2427	C2501	U2568	A2644	G2716	G2790	G2868
A1921	U1999	U2070	U	C2195	C2273	C2360	U2428	U2502	U2569	C2645	A2717	A2791	U2869
A1922	U2000	G2070	G2132	U2196	C2274	G2361	A2429	G2503	U2570	C2646	A2718	A2792	U2870
U1923	U2001	G2071	G2133	U2197	C2275	G2362	U2430	G2504	U2571	A2647	A2719	G2793	U2871
U1924	A2002	C2072	U2138	U2198	C2276	G2363	U2431	G2505	U2572	A2648	A2720	A2794	G2872
C1925	U2003	A2073	U2139	G2200	C2277	G2364	U2432	C2506	A2573	A2649	C2721	G2795	A2873
U1926	U2004	U2074	G2139	G2201	C2278	U2365	U2433	U2507	C2574	A2650	C2722	A2796	G2874
U1927	U2005	U2075	G2140	G2202	C2279	U2366	U2434	A2508	U2575	G2651	C2723	A2797	G2875
U1928	G2006	U2076	A	G2203	C2280	U2367	U2435	A2509	U2576	G2652	C2724	A2798	C2876
U1929	G2007	G2076	G	A2204	G2282	U2368	U2436	C2510	C2577	A2653	C2725	A2799	A2877
U1930	G2008	A2079	G	C2205	U2283	U2369	U2437	C2511	C2578	A2654	C2726	G2800	C
G1931	U2009	U2080	C	G2206	U2284	U2370	U2438	A2512	U2579	G2655	C2727	A2801	U
G1937	U2010	U2081	A	G2207	U2285	U2371	U2439	A2513	C2580	U2656	A2728	G2804	G2805
U1938	U2011	G2082	C	G2208	G2286	U2372	U2440	A2514	C2581	G2657	A2729	G2806	G2806
U1939	A2012	G2083	A	C2210	G2287	U2373	U2441	A2515	C2582	U2658	C2730	G2807	U2807
G1942	A2013	G2084	G	U2211	U2291	U2374	C2442	G2516	U2583	U2659	C2731	G2808	U2808
A1943	G2015	U2086	U	G2212	C2292	U2375	C2443	C2517	U2584	A2660	C2732	G2809	A2809
A1944	A2016	U2087	C	G2213	C2293	C2373	U2444	C2518	U2585	U2661	C2733	G2810	A2810
C1945	U2017	U2088	A	G2217	G2294	C2374	U2445	C2519	U2586	U2662	C2734	G2811	A2811
U1946	G2018	C2088	A	G2218	C2295	U2376	U2446	A2520	C2587	U2663	C2735	G2812	A2812
U1947	C2019	U2090	A	U2219	C2296	U2377	U2447	A2521	U2588	U2664	C2736	G2813	A2813
C1948	C2091	U2092	U	G2225	G2297	U2378	U2448	G2522	U2589	U2665	C2737	G2814	G2814
A1949	G2093	U2093	A	A2226	U2298	U2379	C2454	G2523	U2590	C2666	C2738	G2815	C2815
C1950	C2094	C2094	C2158	C2227	A2299	U2380	U2455	U2524	U2591	U2667	C2739	U2822	U2822
G1951	A2025	G2095	A2159	U2228	G2300	U2381	U2456	U2525	U2592	U2668	C2740	C2823	C2823
A1952	C2026	U2096	C2160	G2229	A2301	C2382	U2457	U2526	U2593	U2669	C2741	C2824	C2824
A1953	G2032	A2097	C2161	U2234	U2306	U2385	U2458	U2527	U2594	U2670	C2742	C2825	C2825
A1954	C2033	G	U2162	G2235	A2307	U2386	U2459	U2528	U2595	U2671	C2743	C2826	C2826
G1955	A2034	U	U2163	U2236	A2308	U2387	U2460	U2529	U2596	U2672	C2744	C2827	C2827
A1964	C2038	A	G2166	G2237	A2312	U2388	U2461	U2530	U2597	U2673	C2745	C2828	C2828
U1965	G2039	G2103	A2167	G2238	G2313	G2392	G2462	U2531	U2598	U2674	C2746	C2829	C2829
C1966	A2040	U2104	A2168	C2239	A2314	G2393	G2463	U2532	U2599	U2675	C2747	C2830	C2830
G1970	A2041	U2105	C2170	U2241	A2315	C2394	U2464	U2533	U2600	U2676	C2748	C2831	C2831
C1971	A2042	G2106	U2171	U2242	A2316	C2395	U2465	U2534	G2601	U2677	C2749	C2832	C2832
G1972	A2043	U2109	U2172	C2243	G2318	U2397	U2466	U2535	G2602	U2678	C2750	C2833	C2833
C1973	G2045	A2109	A2175	U2244	G2319	C2398	U2467	U2536	G2603	U2679	C2751	C2834	C2834
U1974	C2048	C	U2176	A2245	G2320	C2403	U2468	U2537	G2604	U2680	C2752	C2835	C2835
G1975	C2049	U	U2177	A2246	U2321	C2404	U2469	U2538	G2605	U2681	C2753	C2836	C2836
U1976	C2049	C	U2178	A2247	U2322	A2404	U2470	U2539	G2606	U2682	C2754	C2837	C2837
C1977	G2050	U	C2179	U2248	U2323	A2405	U2471	U2540	C2607	U2683	C2755	C2838	C2838
U1978	U2051	C	U2180	U2251	G2324	C2406	U2472	U2541	G2608	U2684	C2756	C2839	C2839
U1979	G2052	G	A2181	A2252	A2325	G2407	U2473	U2542	G2609	U2685	C2757	C2840	C2840
A1980	C2053	A2117	A2182	A2253	U2327	G2408	U2474	U2543	G2610	U2686	C2758	C2841	C2841
	A2054	C2118	C2183	C2254	G2328	U2410	U2475	U2544	G2611	U2687	C2759	C2842	C2842
							U2476	U2545	G2612	U2688	C2760	C2843	C2843
							U2477	U2546	G2613	U2689	C2761	C2844	C2844
							U2478	U2547	G2614	U2690	C2762	C2845	C2845
							U2479	U2548	G2615	U2691	C2763	C2846	C2846
							U2480	U2549	G2616	U2692	C2764	C2847	C2847
							U2481	U2550	G2617	U2693	C2765	C2848	C2848
							U2482	U2551	G2618	U2694	C2766	C2849	C2849
							U2483	U2552	G2619	U2695	C2767	C2850	C2850
							U2484	U2553	G2620	U2696	C2768	C2851	C2851
							U2485	U2554	G2621	U2697	C2769	C2852	C2852
							U2486	U2555	G2622	U2698	C2770	C2853	C2853
							U2487	U2556	G2623	U2699	C2771	C2854	C2854
							U2488	U2557	G2624	U2700	C2772	C2855	C2855
							U2489	U2558	G2625	U2701	C2773	C2856	C2856
							U2490	U2559	G2626	U2702	C2774	C2857	C2857
							U2491	U2560	G2627	U2703	C2775	C2858	C2858
							U2492	U2561	G2628	U2704	C2776	C2859	C2859
							U2493	U2562	G2629	U2705	C2777	C2860	C2860
							U2494	U2563	G2630	U2706	C2778	C2861	C2861
							U2495	U2564	G2631	U2707	C2779	C2862	C2862
							U2496	U2565	G2632	U2708	C2780	C2863	C2863
							U2497	U2566	G2633	U2709	C2781	C2864	C2864
							U2498	U2567	G2634	U2710	C2782	C2865	C2865
							U2499	U2568	G2635	U2711	C2783	C2866	C2866
							U2500	U2569	G2636	U2712	C2784	C2867	C2867
							U2501	U2570	G2637	U2713	C2785	C2868	C2868
							U2502	U2571	G2638	U2714	C2786	C2869	C2869
							U2503	U2572	G2639	U2715	C2787	C2870	C2870
							U2504	U2573	G2640	U2716	C2788	C2871	C2871
							U2505	U2574	G2641	U2717	C2789	C2872	C2872
							U2506	U2575	G2642	U2718	C2790	C2873	C2873
							U2507	U2576	G2643	U2719	C2791	C2874	C2874
							U2508	U2577	G2644	U2720	C2792	C2875	C2875
							U2509	U2578	G2645	U2721	C2793	C2876	C2876
							U2510	U2579	G2646	U2722	C2794	C2877	C2877
							U2511	U2580	G2647	U2723	C2795	C2878	C2878
							U2512	U2581	G2648	U2724	C2796	C2879	C2879
							U2513	U2582	G2649	U2725	C2797	C2880	C2880
							U2514	U2583	G2650	U2726	C2798	C2881	C2881
							U2515	U2584	G2651	U2727	C2799	C2882	C2882
							U2516	U2585	G2652	U2728	C2800	C2883	C2883
							U2517	U2586	G2653	U2729	C2801	C2884	C2884
							U2518	U2587	G2654	U2730	C2802	C2885	C2885
							U2519	U2588	G2655	U2731	C2803	C2886	C2886
							U2520	U2589	G2656	U2732	C2804	C2887	C2887
							U2521	U2590	G2657	U2733	C2805	C2888	C2888
							U2522	U2591	G2658	U2734	C2806	C2889	C2889
							U2523	U2592	G2659	U2735	C2807	C2890	C2890
							U2524	U2593	G2660	U2736	C2808	C2891	C2891
							U2525	U2594	G2661	U2737			

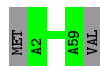
- Molecule 3: Ribosomal Protein L22

Chain L:  97% .



- Molecule 4: Ribosomal Protein L32

Chain M:  97% .





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.40 Å   410.70 Å   694.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.209 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.23	0/66661	0.66	2/103976 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	777	A	C2'-C3'-O3'	5.48	122.47	113.70
1	A	1746	A	C2'-C3'-O3'	5.31	122.19	113.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59532	0	30004	1878	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	58	0	76	22	0
6	A	2	0	0	0	0
All	All	59977	0	30080	1896	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 1896 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1747:G:H4'	1:A:1749:G:H1'	1.31	1.13
1:A:940:G:H3'	1:A:941:U:H5''	1.35	1.09
1:A:367:G:H2'	1:A:368:A:H5''	1.34	1.08
1:A:1199:U:H3'	1:A:1200:G:H5''	1.35	1.07
5:A:2881:ROX:H211	5:A:2881:ROX:H71	1.36	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2765/2880 (96%)	557 (20%)	142 (5%)

5 of 557 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	23	G
1	A	45	C

5 of 142 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1278	A
1	A	1563	U
1	A	2633	A
1	A	1285	A
1	A	1354	A

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	$\# Z  > 2$
5	ROX	A	2881	-	59,60,60	1.48	10 (16%)	84,89,89	3.26	45 (53%)

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
5	ROX	A	2881	-	-	1/79/115/115	1/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	ROX	O2-C13	-3.03	1.40	1.46
5	A	2881	ROX	C10-C9	-2.76	1.50	1.53
5	A	2881	ROX	C19-C16	-2.19	1.47	1.52
5	A	2881	ROX	C2-C1	2.01	1.56	1.51
5	A	2881	ROX	C15-C16	2.08	1.57	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	ROX	O5-C16-C19	-8.13	98.19	110.88
5	A	2881	ROX	C15-C16-C17	-7.66	98.22	107.81
5	A	2881	ROX	C34-C10-C9	-6.83	101.01	110.41
5	A	2881	ROX	O5-C16-C15	-5.35	104.43	113.00
5	A	2881	ROX	C27-C26-C25	-4.89	105.24	113.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	ROX	C20-O5-C16-C17

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	ROX	C14-C15-C16-C17-C18-O4

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	ROX	22	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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.