



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:39 am GMT

PDB ID : 3JQ4  
Title : The structure of the complex of the large ribosomal subunit from *D. Radiodurans* with the antibiotic lankacidin  
Authors : Auerbach-Nevo, T.; Mermershtain, I.; Davidovich, C.; Bashan, A.; Rozenberg, H.; Yonath, A.  
Deposited on : 2009-09-06  
Resolution : 3.52 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

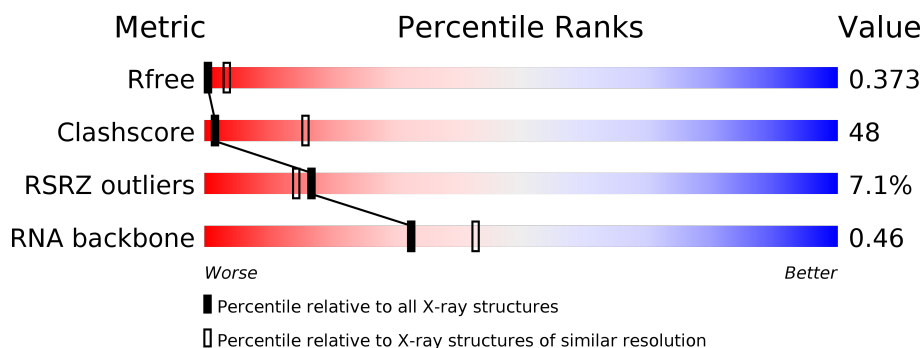
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.52 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))
$R_{free}$	100719	1239 (3.64-3.40)
Clashscore	112137	1007 (3.62-3.42)
RSRZ outliers	101464	1270 (3.64-3.40)
RNA backbone	2435	1027 (4.18-2.86)

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.

Mol	Chain	Length	Quality of chain
1	A	2880	
2	B	118	

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
3	LC2	A	2881	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 61885 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.

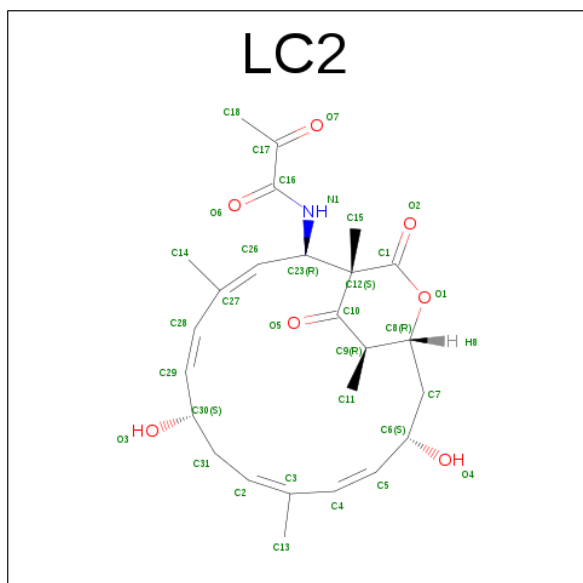
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2765	Total	C	N	O	P	0	0	0
			59336	26469	10944	19159	2764			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	118	Total	C	N	O	P	0	0	0
			2516	1124	464	811	117			

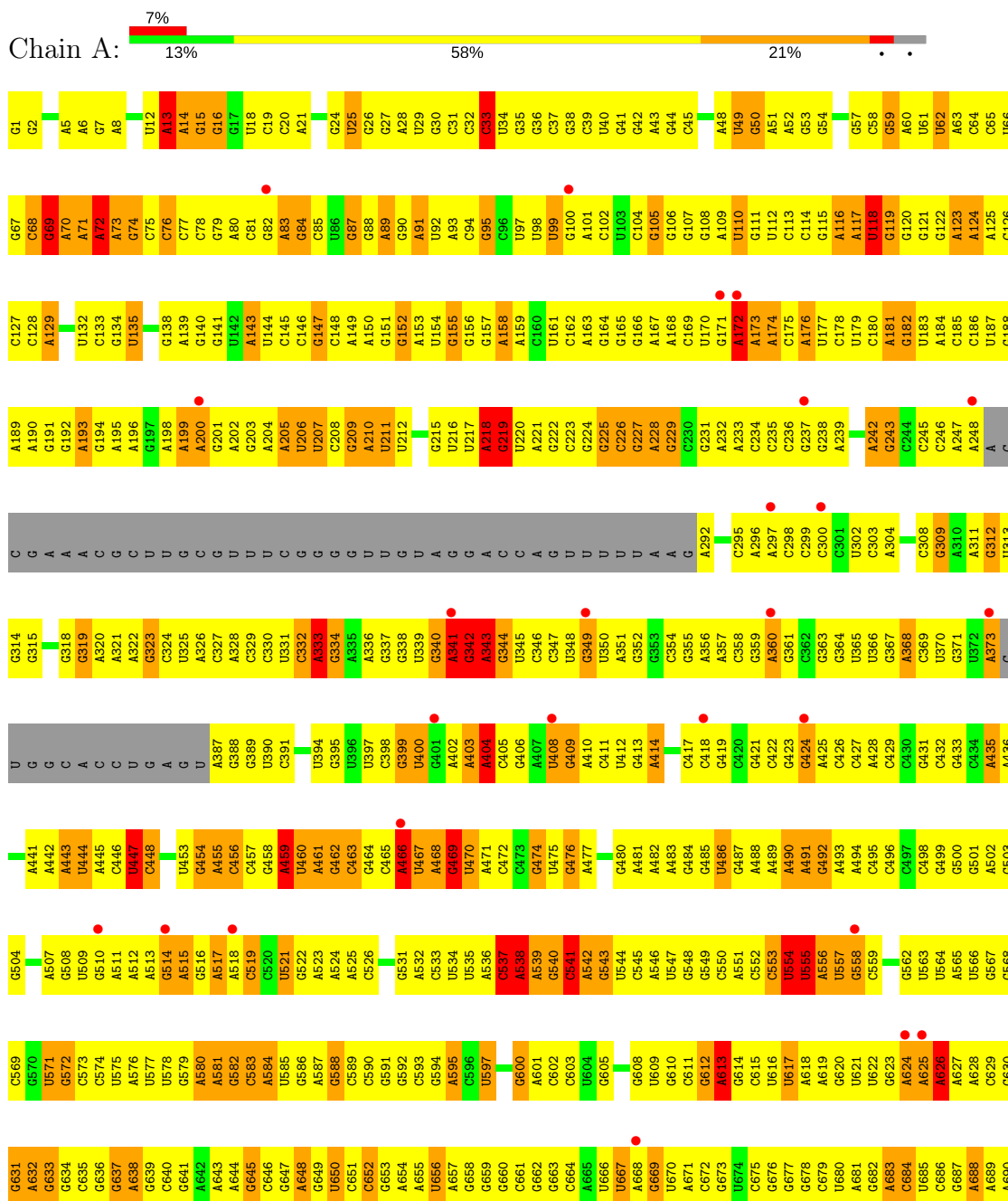
- Molecule 3 is N-[(1S,2R,3E,5E,7S,9E,11E,13S,15R,19R)-7,13-DIHYDROXY-1,4,10,19-TETRAMETHYL-17,18-DIOXO-16-OXABICYCLO[13.2.2]NONADECA-3,5,9,11-TETRAEN-2-YL]-2-OXOPROPANAMIDE (three-letter code: LC2) (formula: C<sub>25</sub>H<sub>33</sub>NO<sub>7</sub>).



### 3 Residue-property plots

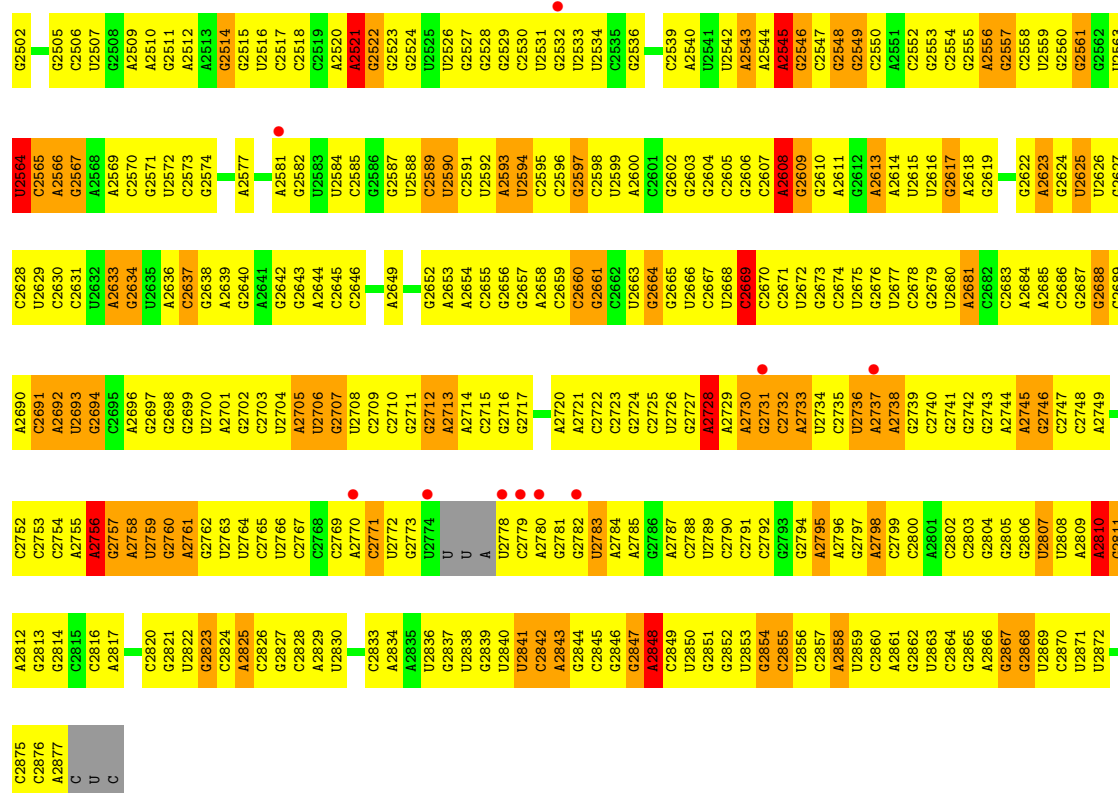
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 23S ribosomal RNA

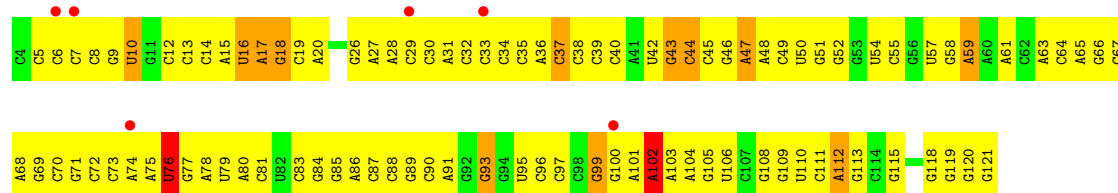


A1561	G1438	C1501	G1309	G1249	A1187	A1126	C1083	C998	C937	G875	G814	U763	C891
G1562	G1439	G1502	C1310	A1250	A1188	A1127	C1084	A999	G938	A876	A815	G764	C892
U1563	G1440	G1503	G1311	G1251	G1189	A1128	A1085	A999	G939	C877	A816	G765	A693
U1564	A1441	G1504	G1312	C1252	C1190	U1129	G1066	A1000	G940	C878	U817	C756	G694
G1565	C1442	U1505	G1313	C1253	G1191	G1131	G1067	A1001	U941	C879	G818	U767	G695
G1566	G1443	U1506	A1314	C1254	A1192	G1132	A1068	C1002	U942	C880	C819	G768	U696
A1567	C1444	G1507	G1315	A1255	G1193	G1133	G1069	C1003	U943	U881	U820	C769	G697
A1568	A1445	G1508	G1316	C1256	U1194	C1134	U1072	U1005	A944	C882	A821	C770	A698
A1569	U1446	G1509	G1317	U1257	U1195	C1135	U1073	U1006	G945	G883	G822	G699	G699
G1570	A1447	A1510	A1318	G1258	U1197	G1136	G1074	A1007	U946	C884	U823	A762	C700
A1571	C1382	A1511	G1383	A1259	U1197	A1137	G1075	G1008	C947	A885	U824	A763	U701
C1572	G1384	U1512	G1385	A1260	U1198	A1138	C1076	C1009	A886	A764	C825	A702	A703
G1573	C1385	U1513	G1322	G1261	U1199	A1139	U1076	U1010	G948	G887	U826	G766	A703
U1574	A1386	C1514	G1323	U1262	G1200	A1140	U1077	A1011	G950	A766	C827	A766	G704
U1575	G1387	U1515	G1324	G1263	G1201	U1141	A1078	A1012	G951	A767	C828	G767	C705
G1576	C1388	A1516	U1325	C1264	U1202	G1142	G1079	G1013	A952	U768	C829	U768	A706
G1577	C1389	U1517	G1327	G1265	A1203	A1143	A1080	G1014	C953	U769	C830	U769	G707
U1578	G1390	G1518	C1328	G1266	G1204	U1144	A1081	U1015	U954	U770	G831	U770	G708
G1579	A1457	U1519	U1329	A1267	G1205	G1145	G1082	C1016	G955	G771	A832	G771	A709
G1580	U1391	G1520	G1330	U1268	G1206	G1146	C1083	C1017	A956	G772	A833	G772	C710
U1521	U1393	U1521	G1331	G1269	G1206	G1147	C1084	C1018	A957	U773	A834	U773	C711
A1582	G1394	A1522	G1332	C1270	C1210	G1148	G1085	U1019	A964	U774	U835	U774	A712
A1583	C1395	A1523	G1333	C1271	G1211	G1149	C1086	A1020	C959	U775	G836	U775	G713
C1524	C1396	C1524	A1334	G1272	U1212	C1150	C1087	A1021	U960	U776	U837	U776	G714
A1585	G1397	A1525	A1335	G1273	U1213	U1151	C1088	A1022	G961	A777	U838	A777	U715
A1586	G1398	U1526	G1336	C1274	U1214	C1152	C1089	U1023	C962	G778	U839	G778	U716
G1587	U1465	G1527	G1337	A1275	C1215	A1153	C1090	G1024	G963	U779	U840	U779	G717
A1588	A1400	A1528	U1338	G1276	A1215	A1154	C1091	A1025	A964	U780	G841	U780	A718
G1589	U1467	C1529	U1339	G1277	G1216	G1155	U1092	U1026	C965	U781	A842	U781	A719
C1590	A1468	U1530	C1340	A1278	U1217	U1156	U1093	A1027	A966	U782	G843	U782	A720
U1591	U1469	C1531	G1341	G1279	C1218	G1157	C1094	G1028	G967	G783	G844	G783	C721
U1592	C1404	A1532	U1342	U1280	C1219	A1158	A1095	C1029	C968	U784	U845	C722	C722
C1593	G1471	G1533	C1343	A1281	G1220	U1159	A1096	U1030	A969	U786	A846	C723	C723
U1594	A1472	A1534	G1344	A1282	C1221	C1160	A1097	C1031	A970	G	A847	C724	C724
C1595	U1473	C1535	G1345	C1283	G1222	U1161	G1098	A1032	A971	G	A848	C725	C725
A1596	A1474	U1536	C1346	G1284	G1223	A1162	A1099	G1033	C972	A790	G849	G726	G726
U1597	U1475	U1537	G1347	A1285	A1224	C1163	G1100	U1034	U973	A791	C950	U727	U727
A1598	G1476	U1538	C1348	U1286	G1225	C1164	U1101	G1035	U974	U792	C951	G728	G728
G1599	C1477	U1539	A1349	A1287	A1226	G1165	G1102	G1036	C975	U793	U852	A730	C730
U1600	G1480	C1540	G1352	A1288	U1229	A1166	C1103	U1037	C976	A795	G854	A795	A731
G1541	C1417	G1541	A1353	A1289	C1230	A1167	G1104	U1038	C977	A796	A856	A796	G734
G1542	U1481	G1542	A1354	A1290	C1231	G1168	U1105	A1039	U978	G798	G857	G798	G735
G1543	C1418	G1543	A1355	G1291	A1231	C1169	U1106	A1040	U979	C799	U858	C737	G737
A1544	G1419	G1544	A1356	A1292	U1232	U1170	A1107	G1041	C980	U800	U859	G738	G738
G1545	A1420	G1545	G1356	A1293	A1233	A1171	U1108	U1044	C981	A801	G861	G739	G739
C1546	U1421	U1546	U1357	G1294	C1234	U1172	A1109	G1045	A921	A802	A862	A740	A740
U1547	C1422	U1547	C1358	U1295	C1235	G1173	G1110	U1046	A922	C803	C963	G741	G741
G1548	A1423	G1548	G1359	G1296	G1236	G1174	C1111	U1047	A984	C804	C964	G742	G742
U1549	G1360	C1549	G1360	A1297	G1237	A1175	C1112	G1047	U925	G805	A865	A743	A743
A1601	G1427	U1550	G1361	G1298	A1238	U1176	C1113	C1052	C926	A806	G866	G746	G746
U1611	G1428	U1551	A1362	A1299	A1239	U1177	A1114	G1053	C927	A807	G867	G747	G747
C1552	A1429	U1552	C1363	A1300	G1240	C1178	C1115	C1054	C928	C808	C809	A747	A747
G1553	C1364	G1553	G1364	U1301	G1241	A1179	U1119	A1055	A929	U810	U811	C749	C749
C1554	U1430	G1554	A1365	A1302	A1242	A1180	G1120	U1056	A930	U812	U812	G751	G751
A1555	G1431	U1555	A1366	G1303	G1243	C1181	G1121	A1057	G931	C870	C870	A748	A748
G1556	A1432	U1556	A1367	U1304	U1244	U1182	G1122	G1058	G932	U871	U871	C750	C750
G1557	G1433	G1557	G1368	C1305	G1245	C1183	A1122	G1058	A994	U872	U872	G751	G751
U1558	U1434	U1558	G1369	U1306	G1246	G1184	U1123	A1061	C935	U873	U873	G752	G752
G1559	G1435	U1559	U1370	U1307	U1247	C1185	U1124	G1062	A936	A813	A813		
A1602	U1500	U1560	G1371	C1308	G1248	G1186	G1125						

C2435	A2371	G2304	U2241	U2180	C2120	U2058	A1998	U1938	U1870	G1809	A1746	A1681	G1621
U2436	G2375	C2305	C2242	A2181	U2121	U2059	U1999	U1939	G1871	U1810	G1747	A1682	G1622
G2437	G2376	A2307	C2243	A2182	G2122	A2060	U2000	C1940	A1872	A1811	U1748	G1683	A1623
A2438	U2377	G2306	C2244	U2185	G2123	C2061	A2002	C1941	U1873	A1812	U1749	A1684	A1624
G2439	G2378	A2308	A2245	G2186	C2125	U2064	A2003	A1943	U1881	A1814	A1750	A1685	A1625
U2440	G2379	G2309	A2246	A2187	U	A2065	U2004	C1944	G1882	G1815	U1752	C1687	C1627
C2442	U2380	G2310	A2247	A2188	U	G2066	U2005	C1945	A1883	G1816	U1753	C1688	C1628
G2447	A2381	U2312	U2249	A2189	U	U2067	G2006	U1946	A1884	U1817	G1754	U1689	G1629
A2448	C2382	G2313	G2250	A2190	G	C2068	G2007	G1947	C1885	G1818	G1755	A1690	A1630
G2449	C2383	A2314	U2251	A2191	U	U2069	C2008	G1948	G1886	G1819	C1756	G1691	G1631
A2450	G2384	G2315	A2252	U2192	G	G2070	U2009	A1949	G1887	G1820	C1692	A1692	A1632
G2451	U2385	A2316	C2253	C2193	G2132	G2071	G2010	C1950	G1888	A1821	C1693	A1693	A1633
U2452	G2386	G2317	G2254	A2194	G2133	C2072	U2011	G1951	G1889	C1822	G1760	A1694	A1634
C2453	U2387	U2295	G2255	U2196	U2134	A2073	A2012	A1952	C1892	G1823	G1761	U1695	G1635
G2454	G2388	C2315	G2256	U2197	U2135	U2074	A2013	A1953	G1893	C1824	C1762	C1696	G1636
A2455	U2389	U2297	U2257	U2198	G2136	U2075	G2014	A1954	U1894	G1825	A1763	U1697	U1637
U2456	A2390	G2318	C2258	U2199	U2137	G2076	A2015	G1955	U1895	U1826	G1764	C1698	G1638
A2457	G2391	U2319	G2261	C2199	U2138	U2076	A2016	G1956	A1895	G1827	C1765	U1699	U1639
G2460	G2392	G2320	C2262	G2200	G2139	A2079	U2017	C1957	A1896	C1828	U1766	C1700	C1640
G2461	U2393	G2321	G2263	G2201	G2140	U2080	U2018	G1958	C1897	G1829	G1767	A1705	G1645
C2462	G2394	C2322	C2264	G2202	A	U2081	C2019	U1959	U1898	C1830	U1768	A1706	G1646
G2463	C2395	G2323	A2265	G2203	G	C2082	G2020	A1960	A1899	G1831	U1769	A1707	U1647
U2464	G2396	U2324	A2266	A2204	G	G2083	G2021	U1961	U1900	G1832	U1770	U1710	A1649
G2465	A2397	G2330	A2267	C2205	C	G2084	C2022	C1962	A1901	U1833	A1771	G1712	A1650
C2466	U2398	A2331	G2268	G2206	A	G2085	C2023	G1963	A1902	G1834	C1772	G1713	G1651
G2469	G2400	A2337	G2269	G2207	A	U2086	U2024	A1964	C1903	G1837	C1773	A1714	G1652
U2470	A2401	U2402	U2270	U2208	C	U2087	A2025	U1965	G1904	U1843	A1774	A1715	C1653
U2471	C2403	G2404	C2271	G2209	G	U2088	C2026	G1966	G1905	G1838	A1775	G1716	A1654
U2472	G2405	U2342	C2272	U2211	U	U2090	C2027	U1967	U1906	G1839	A1776	A1717	C1655
G2473	A2406	G2344	C2273	U2212	U	C2091	G2028	G1968	C1907	U1840	A1777	A1718	U1656
C2474	A2407	G2345	U2274	G2213	A	U2092	G2029	G1969	U1908	G1841	U1778	G1719	A1657
A2475	G2408	A2346	A2275	G2214	A	C2093	U2030	C1970	U1909	G1842	C1781	A1785	A1658
C2476	U2409	G2347	A2276	G2215	U	G2094	A2031	C1971	A1910	U1843	A1782	U1723	G1659
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G2478	A2411	G2349	U2278	G2217	A	U2096	C2033	C1973	G1912	A1845	C1784	C1725	C1661
C2479	A2412	G2350	C2281	G2218	C2157	A2097	G2035	G1975	U1914	G1847	G1790	C1726	G1662
U2480	A2413	G2351	U2219	A2220	C2158	G	G2036	U1976	A1915	U1848	G1791	C1727	C1663
G2481	U2414	G2352	G2221	G2221	A2159	G	A2037	C1977	G1916	U1849	C1792	A1728	G1664
U2482	A2415	A2353	U2222	G2221	C2160	A	C2038	U1978	G1917	G1850	A1793	C1731	C1665
G2483	U2416	G2354	U2223	U2224	C2161	U	G2039	C1979	A1918	A1851	A1794	U1732	A1667
U2484	A2417	G2355	G2225	G2225	U2163	A	A2040	A1980	U1919	G1852	C1795	U1733	G1668
C2485	C2418	A2356	U2226	G2226	G2164	G2103	A2041	A1981	A1920	C1853	C1796	C1734	A1669
G2486	C2419	G2357	A2227	G2227	A2165	U2105	A2042	G1982	A1921	G1854	C1797	G1735	G1670
U2487	C2420	A2358	U2228	G2228	G2166	G2106	A2043	G1983	U1922	G1855	A1800	C1736	A1671
C2488	G2421	G2359	U2229	G2229	A2167	G2107	G2044	A1984	U1923	U1856	C1801	G1737	A1672
U2489	U2422	U2359	U2291	G2230	A2168	G2108	A2045	G1985	C1924	G1857	A1802	U1738	C1673
C2490	G2423	C2360	G2292	G2231	A2169	A2109	C2047	G1986	C1925	C1858	G1803	G1739	C1674
U2491	G2424	G2361	G2293	G2232	C2170	G2110	C2048	G1987	U1926	A1859	U1798	G1735	C1675
G2492	G2425	G2362	G2294	G2233	U2171	C	C2049	A1988	U1927	A1860	A1799	C1736	A1676
U2493	U2426	C2363	G2295	G2234	U2172	U	G2050	A1989	G1928	G1861	A1800	G1737	A1677
G2494	A2427	G2364	G2296	G2235	C2173	C	U2051	U1990	U1929	C1862	C1801	U1738	C1678
C2495	U2428	U2365	G2236	G2236	G2174	G	G2052	G1992	G1931	G1864	A1802	G1739	C1679
U2496	A2429	U2366	G2237	G2237	A2175	C	G2053	G1993	G1932	G1865	U1804	G1740	C1675
G2497	C2430	A2367	G2238	G2238	U2176	G	A2054	U1994	U1934	G1866	U1805	G1741	C1676
U2498	U2431	G2368	A2301	G2239	U2177	A2117	A2055	G1995	A1935	A1867	G1806	G1742	C1677
C2499	G2432	U2369	G2302	G2240	U2178	A2118	C2056	A1996	U1936	A1868	A1807	G1743	G1678
U2500	U2434	G2370	C2303	C2240	C2179	A2119	U2057	A1997	G1937	A1869	C1808	G1744	U1679
G2501													U1680



## • Molecule 2: 5S ribosomal RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.80Å 410.30Å 694.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.52 39.85 – 3.52	Depositor EDS
% Data completeness (in resolution range)	89.8 (8.00-3.52) 91.4 (39.85-3.52)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.268 , 0.325 0.349 , 0.373	Depositor DCC
$R_{free}$ test set	13440 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	106.6	Xtriage
Anisotropy	0.863	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	61885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 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: LC2

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	3/66440 (0.0%)	0.82	93/103628 (0.1%)
2	B	0.39	0/2813	0.73	1/4384 (0.0%)
All	All	0.56	3/69253 (0.0%)	0.81	94/108012 (0.1%)

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	0	124
2	B	0	1
All	All	0	125

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	700	C	N1-C2	9.73	1.49	1.40
1	A	538	A	C5-C6	-5.98	1.35	1.41
1	A	462	G	C6-O6	5.16	1.28	1.24

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	985	G	N9-C1'-C2'	12.36	130.07	114.00
1	A	1337	G	N9-C1'-C2'	9.78	126.71	114.00
1	A	1279	G	N9-C1'-C2'	9.59	126.47	114.00
1	A	1474	A	N9-C1'-C2'	9.59	126.46	114.00
1	A	2608	A	N9-C1'-C2'	8.85	125.51	114.00

There are no chirality outliers.

5 of 125 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	G	Sidechain
1	A	16	G	Sidechain
1	A	172	A	Sidechain
1	A	25	U	Sidechain
1	A	33	C	Sidechain

## 5.2 Too-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 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	59336	0	29907	4296	0
2	B	2516	0	1286	150	0
3	A	33	0	33	1	0
All	All	61885	0	31226	4443	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 48.

The worst 5 of 4443 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:614:G:N2	1:A:634:G:H22	1.28	1.29
1:A:2194:A:H2'	1:A:2195:C:H5''	1.25	1.18
1:A:2691:C:C2'	1:A:2692:A:H5''	1.79	1.11
1:A:2198:U:H3'	1:A:2199:C:H4'	1.14	1.10
1:A:918:A:H2'	1:A:919:U:H5''	1.33	1.10

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein molecules in this entry.

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

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2755/2880 (95%)	675 (24%)	0
2	B	117/118 (99%)	17 (14%)	0
All	All	2872/2998 (95%)	692 (24%)	0

5 of 692 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	45	C
1	A	49	U
1	A	50	G

There are no RNA pucker outliers to report.

## 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](#)

1 ligand is modelled in this entry.

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	$\# Z  > 2$
3	LC2	A	2881	-	30,34,34	1.96	6 (20%)	25,49,49	1.35	2 (8%)

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
3	LC2	A	2881	-	-	0/31/61/61	0/0/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2881	LC2	O7-C17	-2.25	1.18	1.23
3	A	2881	LC2	C2-C3	2.13	1.40	1.33
3	A	2881	LC2	C23-N1	3.29	1.52	1.46
3	A	2881	LC2	C12-C23	4.01	1.63	1.56
3	A	2881	LC2	C13-C3	4.56	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2881	LC2	O5-C10-C12	-2.27	117.75	121.93
3	A	2881	LC2	O7-C17-C18	4.82	130.58	119.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2881	LC2	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2765/2880 (96%)	0.43	200 (7%) 16 14	37, 107, 200, 200	0
2	B	118/118 (100%)	0.24	6 (5%) 29 23	100, 143, 183, 200	0
All	All	2883/2998 (96%)	0.42	206 (7%) 17 14	37, 108, 200, 200	0

The worst 5 of 206 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	G	11.4
1	A	1922	U	9.3
1	A	2125	C	9.2
1	A	1955	G	8.5
1	A	2174	G	8.5

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LC2	A	2881	33/33	0.89	0.37	2.49	88,88,88,88	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.