



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 08:24 PM GMT

PDB ID : 2O43  
Title : Structure of 23S rRNA of the large ribosomal subunit from *Deinococcus radiodurans* in complex with the macrolide erythromycylamine  
Authors : Pyetan, E.; Baram, D.; Auerbach-Nevo, T.; Yonath, A.  
Deposited on : 2006-12-03  
Resolution : 3.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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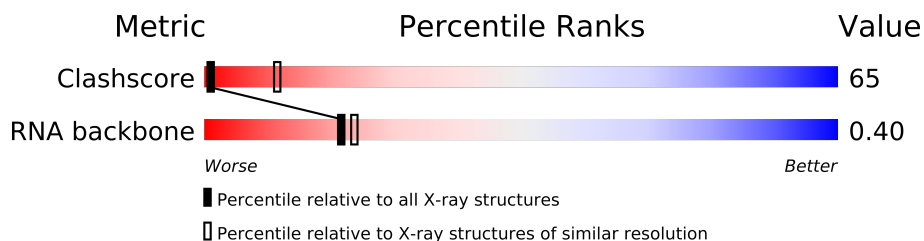
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
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 3.60 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	1155 (3.80-3.40)
RNA backbone	1838	1012 (4.40-2.76)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	

## 2 Entry composition i

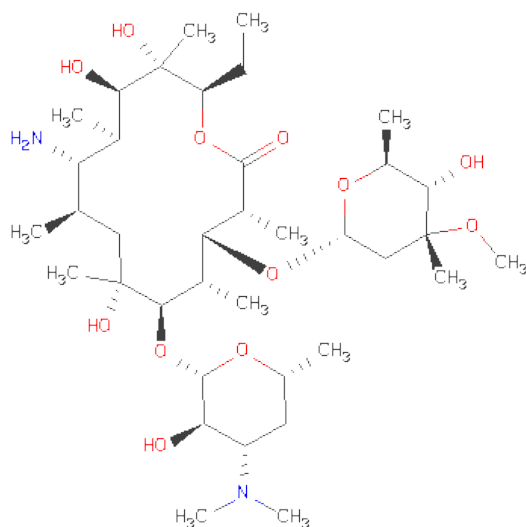
There are 2 unique types of molecules in this entry. The entry contains 59410 atoms, of which 0 are hydrogen and 0 are deuterium.

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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is (3R,4S,5S,6R,7R,9R,10S,11S,12R,13S,14R)-10-AMINO-6-{[(2S,3R,4S,6R)-4-(DIMETHYLAMINO)-3-HYDROXY-6-METHYLTETRAHYDRO-2H-PYRAN-2-YL]OXY}-14-ETHYL-7,12,13-TRIHYDROXY-4-{[(2R,4R,5S,6S)-5-HYDROXY-4-METHOXY-4,6-DIMETHYLTETRAHYDRO-2H-PYRAN-2-YL]OXY}-3,5,7,9,11,13-HEXAMETHYLOXA CYCLOTETRADECAN-2-ONE (three-letter code: ERN) (formula: C<sub>37</sub>H<sub>70</sub>N<sub>2</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	51	37	2	12	0	0

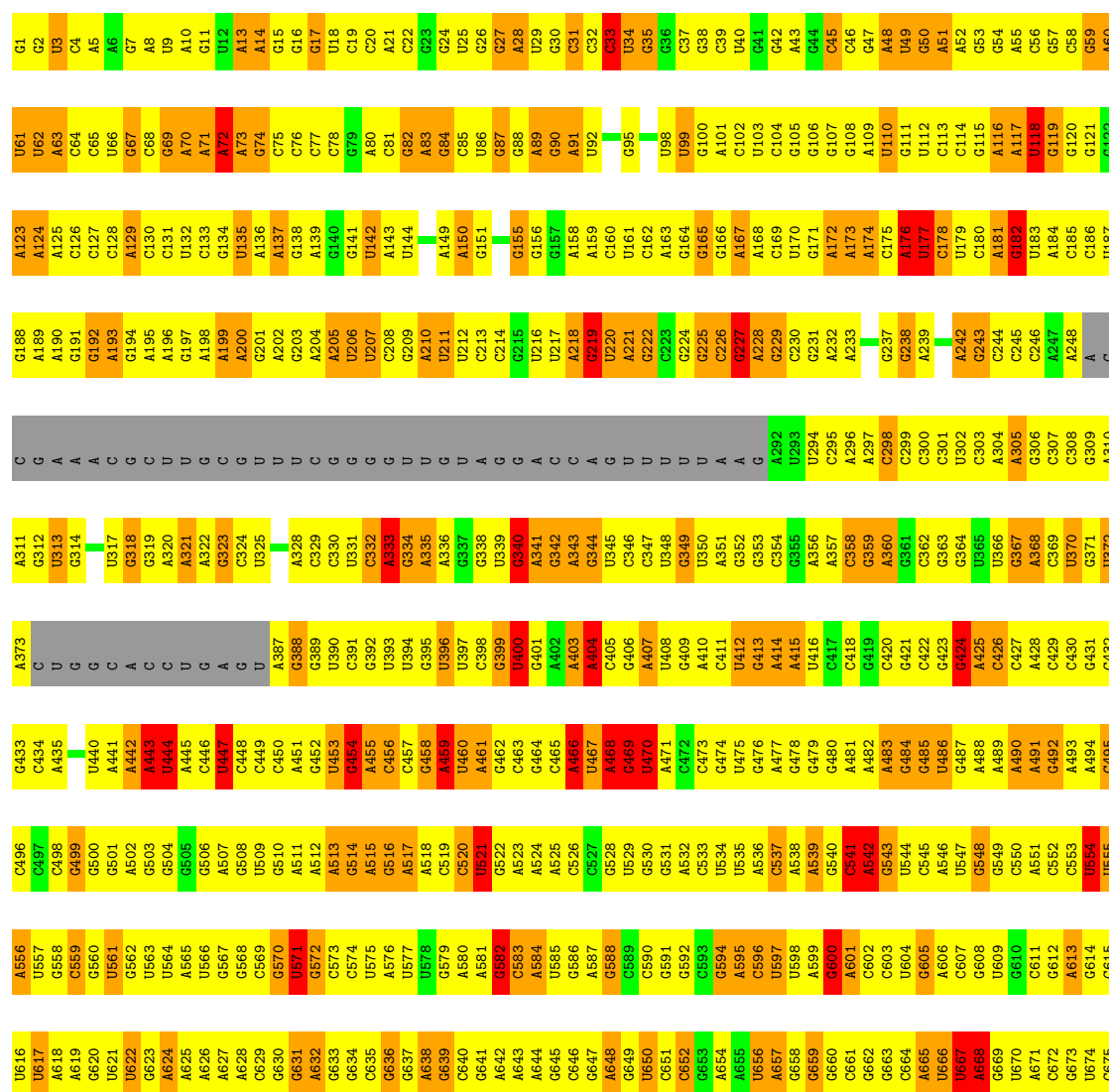
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: 23S rRNA

Chain A: 



A1596	G1536	U1475	G1414	G1352	A1288	A1227	A1166	C1103	G1041	G980	U919	G858	A796	G736	G676
A1597	U1537	G1476	C1415	A1353	A1289	G1228	A1167	G1104	G1042	C981	A922	U859	A797	C737	G677
C1598	A1538	C1477	A1416	A1354	A1290	G1229	G1168	U1105	A1043	C982	A923	U860	C798	G738	G678
G1599	U1539	U1478	C1417	A1355	G1291	C1230	C1169	A1106	U1044	G983	C924	G861	C799	G739	G679
U1600	C1540	G1479	C1418	G1356	A1292	A1231	U1170	A1107	G1045	A984	C925	U862	U800	A740	U680
U1601	A1541	G1480	G1419	U1357	A1293	U1232	U1171	U1108	A1046	G985	U925	G863	A801	G741	A681
G1602	G1542	U1481	A1420	C1358	G1294	A1233	U1172	A1109	G1047	A986	C926	C864	A802	G742	G682
A1603	G1543	U1421	U1421	G1359	G1298	C1234	G1173	G1110	U1048	G987	C927	A865	C803	A743	A683
C1604	A1544	U1422	G1422	G1360	A1299	C1235	G1174	C1111	U1049	G988	C928	U866	C804	C744	A684
A1605	G1545	G1484	A1423	G1361	A1300	G1236	A1175	U1112	G1053	A991	A930	U867	G805	C745	U685
C1606	A1546	U1485	U1424	A1362	A1301	G1237	U1176	C1113	A1054	A992	A931	U868	A806	G746	C686
A1607	U1547	G1486	G1425	C1363	U1302	A1238	U1177	A1114	C1055	A993	G932	C869	A807	A747	G687
U1608	C1487	U1426	U1426	C1364	C1302	A1239	C1178	U1115	A1056	C993	G933	C870	C808	A748	A688
G1609	G1488	G1427	G1427	U1365	U1303	G1240	A1179	U1116	U1056	A994	G934	U871	C809	C749	A689
A1610	U1550	G1428	G1428	U1366	U1304	A1241	A1180	G1117	A1057	A995	G935	U872	U810	C750	A690
U1611	C1551	U1429	A1367	C1367	C1305	A1242	C1181	U1118	G1058	C996	C936	U873	G811	G751	C691
G1612	U1552	G1430	U1430	G1368	U1306	G1243	A1182	U1119	A1059	C997	A936	U874	G812	G752	C692
C1613	G1553	U1431	G1431	G1369	G1309	U1244	C1183	C1120	C1060	C998	C937	G875	G813	U753	A693
G1614	U1554	G1432	G1432	G1371	G1310	G1245	G1184	G1121	A1061	A999	G938	A876	G814	G754	G694
C1615	G1495	A1433	A1433	A1372	C1310	G1246	C1185	G1122	G1062	G1000	C939	C877	A815	C755	G695
U1616	U1496	G1434	G1434	G1373	C1311	U1247	G1186	G1123	C1063	A1001	G940	U878	U816	G756	U696
G1617	C1497	G1435	G1435	G1374	G1312	U1248	A1187	U1124	C1064	C1002	U941	A879	A817	U757	G697
U1618	G1498	G1436	G1436	C1375	U1313	G1249	A1188	G1125	A1065	C1003	U942	C880	G818	U758	A698
A1619	A1499	A1437	A1437	A1376	A1314	A1250	G1189	A1126	G1066	A1004	U943	U881	C819	G759	G699
C1620	U1500	G1438	G1438	G1377	A1315	G1251	C1190	C1127	G1067	U1005	A944	C882	U820	U760	C700
G1621	C1501	G1439	G1439	A1378	G1316	C1252	G1191	G1128	A1068	C1006	G945	A883	A821	G761	U701
C1622	G1502	G1440	G1440	A1379	G1317	C1253	A1192	G1129	G1069	A1007	U946	C884	G822	A762	A702
U1623	U1503	A1441	A1441	C1380	A1318	G1254	G1193	U1130	G1070	G1008	C947	A885	U823	A763	A703
A1624	G1504	G1442	G1442	G1381	C1319	A1255	U1194	G1131	U1071	C1009	G948	A886	U824	G764	G704
G1625	U1505	G1443	G1443	G1382	G1320	C1256	U1195	C1132	U1072	U1010	G950	G887	C825	C765	C705
A1626	C1506	C1444	C1444	C1383	A1320	U1257	G1196	G1135	G1073	A1011	G951	C888	U826	A766	A706
C1627	U1507	A1445	A1445	G1384	G1323	G1258	U1197	G1136	G1074	A1012	G952	C889	C827	G767	U707
G1628	G1508	U1446	U1446	C1385	G1324	G1259	C1198	C1136	C1075	G1013	A952	U890	C828	U768	G708
U1629	A1509	G1449	G1449	A1386	U1325	A1260	A1199	A1137	U1076	G1014	G953	A891	C829	C769	A709
A1630	C1510	G1450	G1450	G1387	A1326	G1261	G1200	U1138	U1077	U1015	U954	C830	G831	U770	C710
C1631	A1511	C1451	C1451	C1388	C1327	U1262	G1201	A1139	A1078	C1016	G955	G	G	C771	C711
U1632	U1512	G1452	G1452	C1389	C1328	G1263	U1202	A1140	U1079	C1017	A956	G	A832	G772	A712
G1633	U1513	U1453	U1453	G1390	U1329	C1264	A1203	U1141	A1080	C1018	G957	G	A833	G773	G713
A1634	C1514	A1454	A1454	A1391	G1330	G1265	G1204	U1142	A1081	U1019	G958	G	A834	A774	G714
G1635	U1515	U1455	U1455	G1392	G1331	A1266	G1205	C1145	C1082	A1020	C959	C	U835	U775	U715
G1636	A1516	C1456	C1456	G1393	G1332	A1267	G1206	G1146	C1083	A1021	U960	C	G836	U776	U716
U1637	G1517	G1457	G1457	G1394	U1333	U1268	G1208	U1147	A1084	C1022	G961	U	U837	A777	G717
C1638	U1518	A1458	A1458	A1395	A1334	G1269	G1209	G1147	G1085	U1023	C962	A	A838	G778	A718
U1639	G1519	U1459	U1459	C1396	G1335	C1270	C1210	G1148	C1086	G1024	G963	C	U839	U779	A719
G1640	U1520	U1460	U1460	A1397	G1336	C1271	G1211	U1151	C1087	A1025	A964	C	U840	U780	A720
C1641	C1521	G1461	G1461	G1398	G1337	G1272	U1212	C1152	A1088	U1026	G965	A	G841	G781	C721
A1642	A1522	C1462	C1462	C1399	G1338	G1273	U1213	C1153	C1089	C1027	A966	G	A842	U782	C722
G1643	U1523	A1463	A1463	A1400	U1339	C1274	C1214	A1153	C1090	G1028	G967	C	G843	G783	C723
U1644	C1524	G1464	G1464	G1401	C1340	A1275	A1215	A1154	C1091	C1029	C968	U	G844	U784	C724
G1645	A1525	A1465	A1465	G1402	G1341	C1276	G1216	G1155	U1092	U1030	U969	U	U845	U785	C725
U1646	U1526	G1466	G1466	U1403	U1342	A1278	U1217	U1156	U1093	C1031	A970	A	A846	U786	G726
C1647	G1527	U1467	U1467	C1404	G1343	G1279	C1218	G1157	C1094	A1032	A971	C	U847	A787	G727
U1648	A1528	A1468	A1468	G1407	G1344	U1280	C1219	C1158	A1095	U1034	C972	C	A848	G788	G728
A1649	C1529	U1469	U1469	C1345	A1281	A1281	G1220	U1159	A1096	U1037	G973	A911	G849	G789	A729
U1650	U1530	G1470	G1470	U1409	C1346	C1282	C1221	C1160	A1097	G1035	U974	C850	A790	U790	C730
G1651	C1531	U1471	U1471	U1410	C1347	C1283	G1222	U1161	G1098	G1036	C975	G851	C850	G791	A731
C1652	A1532	G1472	G1472	U1411	C1348	G1284	G1223	A1162	A1099	U1037	G976	U	U852	U792	G732
U1653	U1533	C1473	C1473	C1411	A1349	A1285	A1224	C1163	A1099	U1038	G977	U	C853	G793	G733
A1654	G1534	U1473	U1473	C1412	A1350	U1286	G1225	C1164	G1100	A1039	U978	U916	A794	G794	G734
C1655	U1535	A1474	A1474	U1413	G1351	A1287	A1226	G1165	G1102	A1040	A979	A918	U857	A795	G735

U2572	A2512	U2452	C2329	A2267	C2205	C	G2084	U2024	G1963	G1842	A1780	G1719	A1657
C2573	A2513	C2453	G2330	G2268	C2206	A	G2085	A2025	A1964	U1843	C1781	G1720	A1658
G2574	G2514	C2454	A2331	G2269	G2207	A	U2086	U1965	U1965	C1844	G1782	G1721	G1659
U2575	G2515	C2455	G2332	U2270	G2208	C	U2087	C2027	C1966	A1845		G1722	G1660
G2576	U2516	C2456	A2333	C2271	G2209	G	U2088	C2028	U1967	U1846	A1785	U1723	G1661
A2577	C2517	C2457	C2334	A2272		G	C2089	G2029	G1968	G1847	C1786	C1724	
G2578	U2518	U2458	U2335	C2273	U2212	U	U2090	U2030	G1969	U1848	U1787	G1725	G1664
A2579	C2519	C2459	G2336	C2274	G2213	G	C2091	A2031	G1970	G1849	C1788		G1665
C2580	A2520	G2460	A2337	U2275	G2214	A	U2092	G2032		U1911	U1789	G1726	G1666
A2581	G2521	C2461	C2338	C2276	C2215	A	G2093	C2033	C1973	A1851	G1790	G1727	G1667
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U2583	G2523	G2463	G2340	A2278	G2217	U	G2095	G2035	G1975	C1853	C1792	G1729	G1668
G2584	U2524	C2464		C2279	G2218	A	U2096	G2036	U1976	G1854	A1793	G1730	A1669
C2585	U2525	G2465	C2343	A2280	U2219	C2157	A2097	A2037	C1977	G1855	A1794	C1731	G1670
U2586	G2526	C2466	G2344	C2281	A2220	C2158	G	A2038	U1978	U1856	C1795	U1732	A1671
G2587	A2527	A2467	A2345	G2282	G2221	A	G	C2039	U1979	G1857	C1796	U1733	A1672
U2588	C2528	C2468	G2346	A2283	U2222	A2159	U	A2040	A1980	U1858	C1797	G1734	C1673
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U2592	G2532	A2472	G2350	G2287	A2226	U2163	G2103	G2044	U1984	C1862	A1801	U1738	C1677
C2593	G2533	G2473	G2351	A2288	U2227	A2165	G2104	A2045	G1985	U1863	A1802	G1739	G1678
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G2596	G2536	A2476	G2354	U2291	G2230	A2168	G2107	C2048	A1988	G1866	G1805	G1744	A1681
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U2598	G2538	C2478	A2356	G2293	G2232	C2170	G2110	G2050	U1990	A1868	A1807	A1746	G1683
G2599	C2539	U2479	A2357	U2294	G2233	U2171	C	U2051	C1991	A1869	A1808	G1747	G1684
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C2602	G2542	A2482	C2360	G2297	U2236	G2174	G	A2054	U1994	A1872	A1811	U1750	C1687
U2603	A2543	U2483	G2361	U2298	C2237	A2175	C	G2055	G1995	A1873	U1812	U1751	U1688
G2604	C2544	C2484	G2362	A2299	G2238	U2176	G	C2056	A1996	G1874	U1813	A1752	U1689
A2605	A2545	U2485	G2363	G2300	C2239	A2177	A2117	U2057	A1997	C1875	G1814	G1753	C1691
U2606	G2546	C2486	C2364	A2301	C2240	U2178	A2118	U2058	A1998	C1876	G1815	G1754	C1692
G2607	C2547	G2487	U2365	G2302	U2241	C2179	A2119	U2059	U1999	C1877	G1816	G1755	A1693
U2608	U2548	U2488	U2366	G2302	C2242	U2180	C2120	A2060	U2000	C1878	U1817	G1756	A1694
C2609	A2549	C2489	A2367	A2306	C2243	A2181	U2121	C2061	G2001	G1879	G1818	C1757	U1695
U2610	G2550	C2490	G2368	A2307	C2244	A2182	G2122	U2062	A2002	U1880	U1819	C1758	C1696
A2611	A2551	C2491	U2369	A2308	C2245	C2183	G2123	A2063	U2003	G1881	G1820	A1759	U1697
G2612	C2552	G2492	C2370	G2309	A2246	C2184	C2124	U2064	U2004	U1882	G1760	C1759	C1698
U2613	G2553	U2493	A2371	C2310	A2247	U2185	C2125	A2065	C1944	A1883	G1761	G1762	A1699
C2614	C2554	C2494	A2372	U2311	A2248	G2186	U	G2066	G2006	A1884	C1824	G1763	C1700
U2615	G2555	C2495	C2373	A2312			U	U2067	G2007	C1885	C1825	U1764	G1701
G2616	A2556	C2496		G2313	U2251	A2189	U	C2068	C2008	G1886	U1826	A1765	
U2617	C2557	A2497	G2376	A2314	A2252	A2190	U	U2069	U2009	G1887	G1827	U1766	G1704
A2618	G2558	U2498	U2377	A2315	A2253	A2191	G	G2070	G2010	C1948	G1828	U1767	U1705
C2619	U2559	C2499	G2378	G2316	C2264	U2192	G	C2071	U2011	C1888	C1829	G1767	A1706
U2620	G2560	C2500	G2379	G2317	G2265	C2193	G2132	C2072	A2012	G1889	C1830	U1768	A1707
C2621	U2561	U2501	U2380	U2318	G2266	A2194	G2133	A2073	U2013	C1891	G1831	U1769	C1708
U2622	C2562	C2442	A2381	G2319	A2257	C2195	U2134	A2074	A2014	C1892	G1832	U1770	U1709
G2623	U2563	G2443	C2382	G2320	G2258	U2196	C2135	U2075	G2015		U1833	U1771	U1710
U2624	C2564	C2444	C2383	C2321	C2259	U2197	G2136	G2076	A2016	A1895	G1834	C1772	C1711
A2625	G2565	G2504	G2384	U2322	C2260	U2198	G2137	G2077	U2017	C1896	C1835	C1773	G1712
C2626	U2566	C2505	U2385	U2323	G2261	C2199	U2138	G2078	C2018	C1897	G1836	A1774	G1713
U2627	G2567	U2507	G2386	G2324	G2262	G2200	G2139	A2079	C2019	G1968	G1837	A1775	A1714
C2628	C2568	A2448	U2387	A2325	C2263	G2201	G2140	U2080	G2020	A1899	G1838	A1776	A1715
U2629	A2569	G2509	G2388	C2326	C2264	G2202	A	U2081	G2021	U1900	A1839	A1777	A1716
G2630	C2570	U2510	U2389	U2327	A2265	G2203	G	C2082	A1961	C2022	A1840	U1778	G1717
C2631	U2571	G2511	A2390	A2266	A2266	A2204		G2083	C2023	A1902	G1841	C1779	A1718

C	C2820	G2757	C2695	U2635
	G2821	A2758	A2696	A2636
	G2822	U2759	G2697	C2637
	G2823	G2760	G2698	G2638
	A2824	A2761	G2699	A2639
	A2825	G2762	U2700	G2640
	C2826	U2763	A2701	A2641
	G2827	U2764	G2702	G2642
	C2828	C2765	G2703	G2643
	A2829	U2766	U2704	A2644
	U2830	C2767	A2705	C2645
	A2831	C2768	U2706	A2646
	G2832	G2769	G2707	G2647
	C2833	A2770	U2708	G2648
	A2834	C2771	C2709	A2649
	A2835		C2710	G2650
	U2836	U2774	G2711	U2651
	G2837	U	G2712	G2652
	U2838	U	A2713	A2653
	G2839	A	A2714	A2654
	U2840	U2776	G2715	C2655
	U2841	C2779	G2716	G2656
	C2842	G2780	G2717	G2657
	A2843	G2781		A2658
	G2844	G2782	A2720	C2659
	C2845	U2783	A2721	C2660
	G2846	A2784	C2722	G2661
	G2847	A2785		C2662
	A2848	G2786	U2725	U2663
	C2849	A2787	U2726	G2664
	U2850	C2788	G2727	G2665
	G2851	U2789	A2728	U2666
	G2852		A2729	C2667
	U2853	G2793	A2730	U2668
	G2854	G2794	G2731	C2669
	U2855	A2795	C2732	C2670
	U2856	A2796	A2733	G2671
	C2857	G2797	U2734	U2672
	A2858	A2798	C2735	G2673
	U2859	C2799	U2736	C2674
	C2860	C2800	A2737	U2675
	A2861	A2801	A2738	G2676
	G2862	C2802	G2739	U2677
	U2863	C2803	C2740	C2678
	C2864	G2804	G2741	G2679
	G2865	G2805	G2742	U2680
	A2866	G2806	G2743	A2681
	G2867	U2807	A2744	C2682
	G2868	U2808	A2745	G2683
	U2869	A2809	G2746	A2684
	C2870	A2810	G2747	A2685
	U2871	G2811	C2748	C2686
	U2872	A2812	A2749	G2687
	G2873	G2813	G2750	G2688
	A2874	G2814	G2751	C2689
	C2875	C2815	C2752	A2690
	C2876	C2816	C2753	C2691
	A2877	A2817	C2754	A2692
	C	G2818	A2755	U2693
	U	G2819	A2756	G2694

## 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, $\alpha$ , $\beta$ , $\gamma$	170.44Å 413.54Å 693.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.60)	Depositor
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.281 , 0.341	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	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: ERN

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	0.67	17/66467 (0.0%)	0.86	140/103673 (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	1	183

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2484	G	O3'-P	8.76	1.71	1.61
1	A	788	G	N9-C4	8.06	1.44	1.38
1	A	2041	A	C8-N7	-7.66	1.26	1.31
1	A	2041	A	C5'-C4'	7.64	1.60	1.51
1	A	2042	A	P-O5'	7.49	1.67	1.59

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	803	C	N1-C1'-C2'	27.33	149.53	114.00
1	A	2041	A	P-O3'-C3'	13.45	135.84	119.70
1	A	803	C	C3'-C2'-C1'	12.56	111.55	101.50
1	A	788	G	N9-C1'-C2'	11.20	128.56	114.00
1	A	985	G	N9-C1'-C2'	10.78	128.02	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	765	C	C1'

5 of 183 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	U	Sidechain
1	A	17	G	Sidechain
1	A	28	A	Sidechain
1	A	33	C	Sidechain
1	A	67	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	59359	0	29917	5720	0
2	A	51	0	70	41	0
All	All	59410	0	29987	5744	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 65.

The worst 5 of 5744 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:2881:ERN:C10	2:A:2881:ERN:C11	1.76	1.63
2:A:2881:ERN:C6	2:A:2881:ERN:C5	1.76	1.59
2:A:2881:ERN:C5	2:A:2881:ERN:C4	1.80	1.57
1:A:2516:U:H2'	1:A:2517:C:C6	1.76	1.20
1:A:795:A:H4'	1:A:796:A:OP1	1.41	1.17

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

### 5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2757/2880 (95%)	762 (27%)	199 (7%)

5 of 762 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	U
1	A	13	A
1	A	14	A
1	A	27	G
1	A	34	U

5 of 199 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1325	U
1	A	1684	G
1	A	2593	A
1	A	1337	G
1	A	1442	C

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

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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.