



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 08:24 PM GMT

PDB ID : 2O45
Title : Structure of the 23S rRNA of the large ribosomal subunit from *Deinococcus Radiodurans* in complex with the macrolide RU-69874
Authors : Baram, D.; Pyetan, E.; 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

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

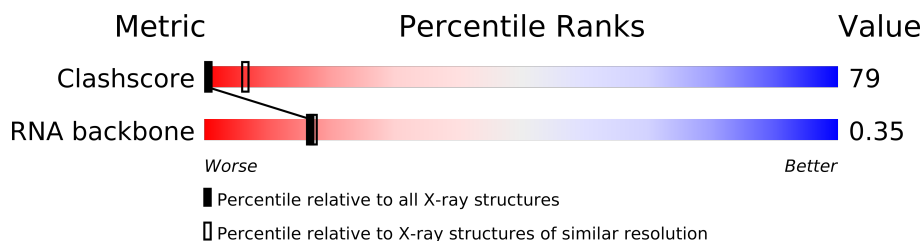
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.60 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 ≥ 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

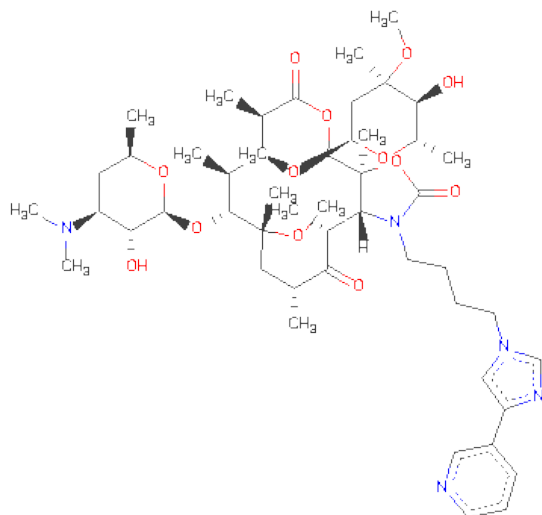
There are 2 unique types of molecules in this entry. The entry contains 59428 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (3AS,4R,7R,8S,9S,10R,11R,13R,15R,15AR)-4-ETHYL-11-METHOXY-3A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-1-[4-(4-PYRIDIN-3-YL-1H-IMIDAZOL-1-YL)BUTYL]-10-{[3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSYL]OXY}TETRADECAHYDRO-2H-OXACYCLOTETRADECINO[4,3-D][1,3]OXAZOL-8-YL2,6-DIDEOXY-3-C-METHYL-3-O-METHYL-ALPHA-L-RIBO-HEXOPYRANOSIDE (three-letter code: RU6) (formula: C₅₁H₈₁N₅O₁₃).



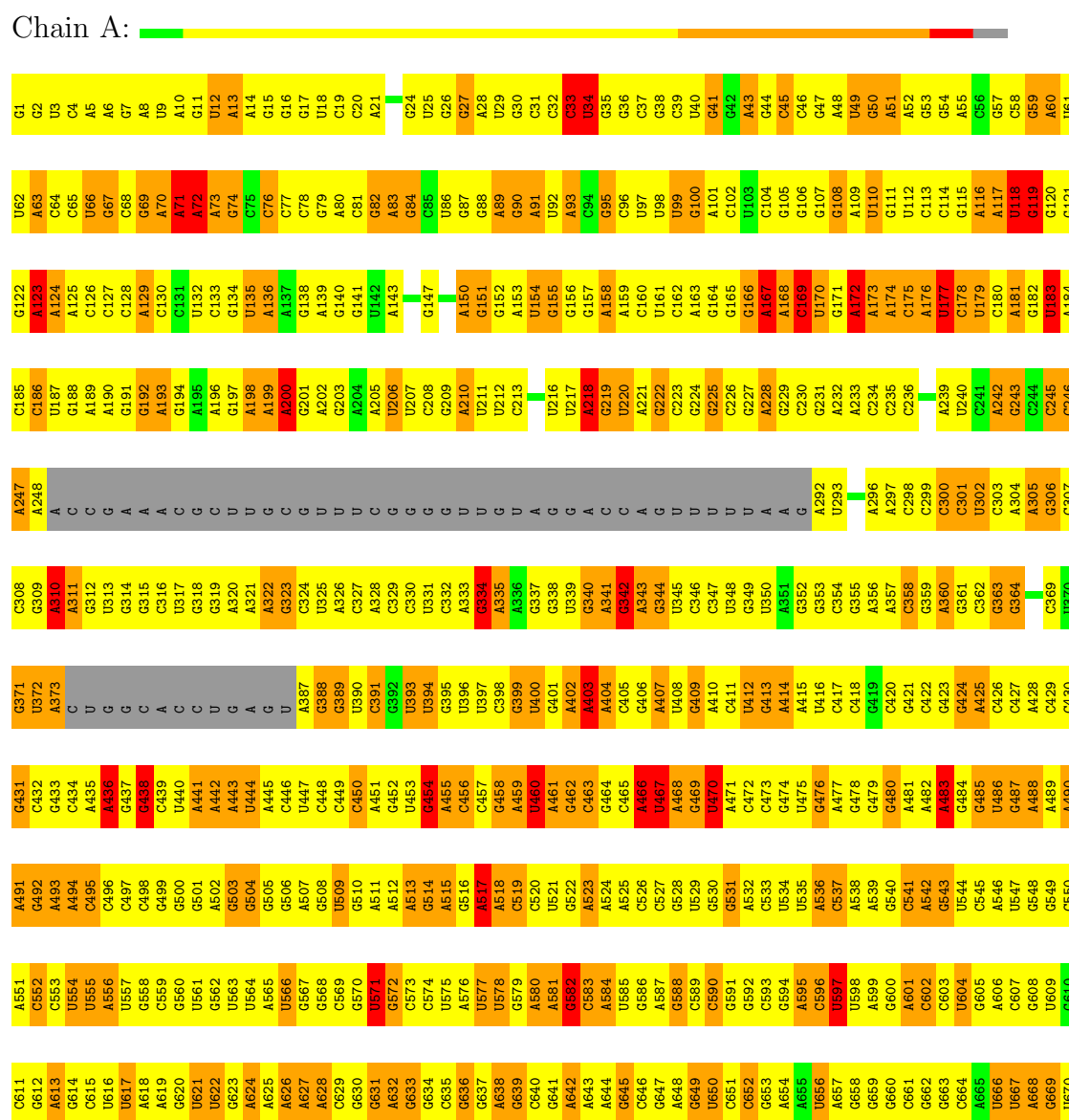
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	69	51	5	13	0	0

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



G1577	A1457	G1337	U1276	G1216	G1155	C1094	G1033	U973	A913	C851	G791	A731	A671
U1578	A1458	G1338	G1277	U1217	U1156	A1095	U1034	U974	C914	U852	U792	G732	C672
G1579	U1459	U1339	A1278	C1218	G1157	A1096	G1035	C975	C915	G853	U793	G733	G673
C1580	G1460	G1340	G1279	C1219	A1158	A1097	G1036	C976	C916	G854	A794	G734	U674
C1581	G1461	G1341	U1280	G1220	U1159	G1098	U1037	G977	U917	G855	A795	G735	C675
C1582	G1462	U1342	A1281	C1221	U1160	A1099	U1038	G978	U918	A856	A796	G736	G676
A1583	G1463	C1343	A1282	G1222	U1161	G1100	A1039	G979	U919	U857	A797	C737	G677
G1584	C1464	G1344	C1283	G1223	A1162	U1101	A1040	G980	G920	G858	G798	G738	G678
A1585	A1405	G1345	G1284	C1224	C1163	G1102	G1041	C981	A921	U859	G799	G739	G679
U1586	A1406	C1346	A1285	C1225	C1164	C1103	A1042	C982	A922	U860	U800	U740	U680
A1587	G1407	C1347	U1286	A1226	G1165	G1104	A1043	G983	A923	G861	A801	G741	A681
C1588	U1408	C1348	A1287	G1227	A1166	U1105	U1044	A984	C924	A862	A802	G742	G682
G1589	A1409	U1349	U1288	G1228	A1167	A1106	G1045	G985	U925	C863	C803	A743	A683
C1590	U1410	G1350	A1289	C1229	G1168	A1107	U1046	A986	C926	G867	C804	C744	C684
U1591	G1471	G1351	A1290	C1230	C1169	U1108	G1047	G987	C927	U868	G805	C745	U685
U1592	C1412	G1352	G1291	A1231	U1170	U1109	U1048	G988	C928	U869	A807	C746	C686
G1593	U1413	A1353	A1292	U1232	A1171	G1110	C1049	G989	A929	C870	A808	A747	G687
U1594	G1414	A1354	A1293	C1234	U1172	C1111	A1233	A990	A930	G871	C908	A748	A688
C1595	A1415	G1355	G1294	C1235	G1173	U1112	U1053	A991	G931	U871	C909	C749	A689
A1596	A1416	U1356	U1295	G1236	A1174	C1113	G1054	A992	G932	U872	U810	G750	A690
U1597	G1477	U1357	G1296	G1237	A1175	U1114	U1055	A993	G933	G873	G811	C751	C691
A1598	U1478	C1358	A1297	G1238	U1176	C1115	A1056	A994	G934	A874	A812	G752	C692
G1599	G1479	G1359	U1298	A1239	U1177	U1116	U1057	A995	C935	G875	A813	U753	A693
U1600	U1480	G1360	A1299	G1240	G1178	G1117	A1058	C996	A936	A876	G814	G754	G694
U1601	U1481	G1361	A1300	A1241	U1179	G1118	U1059	C997	C937	G877	A815	C755	G695
G1602	U1482	A1362	U1301	G1242	A1180	C1121	A1060	C998	G938	C878	U816	C756	U696
A1603	G1483	C1363	A1242	A1243	U1181	G1122	U1061	A999	C939	A879	A817	U757	G697
U1604	U1484	U1424	U1302	G1244	U1182	A1123	G1062	U1000	G940	C880	C818	U758	A698
A1605	G1485	U1365	U1304	U1244	C1183	G1124	U1063	A1001	U941	U881	C819	C759	G699
C1606	A1486	U1366	C1305	G1245	C1185	U1125	C1064	U1002	U942	C882	U820	U760	C700
U1607	C1487	U1367	U1306	G1246	G1186	G1126	U1065	C1003	U943	A883	A821	A761	U701
U1608	G1488	G1368	U1307	U1247	A1187	A1127	U1066	U1004	A944	C884	G822	A762	A702
G1609	U1489	G1369	U1308	G1248	U1188	C1127	U1067	U1005	G945	A885	U823	A763	A703
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A1611	G1491	G1371	A1310	U1251	C1190	U1130	A1069	C947	C948	G887	C825	C765	C705
U1612	G1492	A1372	C1311	G1252	G1191	U1131	G1070	U1009	G949	C888	U826	A766	A706
G1613	A1493	G1373	G1312	C1253	A1192	C1132	U1071	U1010	G950	C889	C827	G767	U707
C1614	G1494	C1374	U1313	G1254	G1193	G1133	U1072	A1011	G951	U890	C828	C768	G708
A1615	G1495	C1375	A1314	U1255	U1194	C1134	G1073	A1012	A952	G	C830	U770	A710
C1616	U1496	G1376	A1315	C1256	U1195	G1135	U1074	G1013	G953	G	A832	G771	C711
G1617	G1497	G1377	G1316	C1257	U1196	C1136	C1075	G1014	U954	G	A833	G772	A712
U1618	U1498	A1378	G1317	U1257	C1197	A1137	U1076	U1015	G955	G	A834	G773	G713
G1619	A1499	C1379	A1318	A1258	U1198	A1138	U1077	C1016	A956	G	A834	A774	G714
C1620	U1500	G1380	C1319	A1259	U1199	A1139	A1078	C1017	G957	C	U835	U775	U715
C1621	C1501	G1381	A1320	A1260	G1200	A1140	G1079	C1018	G958	C	U836	G776	U716
G1622	G1502	C1382	G1321	G1261	G1201	U1141	A1080	U1019	C959	U	U837	A777	G717
C1623	G1503	G1383	G1322	U1262	U1202	G1142	A1081	A1020	U960	A	A838	U778	A718
A1624	U1504	C1384	G1323	G1263	A1203	U1143	G1082	A1021	G961	C	U839	U779	A719
G1625	U1505	A1445	G1324	C1264	G1204	U1144	C1083	A1022	C962	C	U840	U780	A720
A1626	C1506	U1386	G1325	G1265	G1205	G1145	A1084	U1023	G963	A	G841	G781	C721
C1627	A1507	G1387	U1326	G1266	G1206	C1146	G1085	U1024	A964	G	A842	U782	C722
G1628	U1508	C1388	U1327	A1267	G1207	G1147	C1086	A1025	G965	C	G843	U783	C723
A1629	A1509	G1389	U1330	U1268	A1208	G1148	C1087	U1026	A966	U	G844	U784	C724
U1630	G1510	C1390	G1331	C1270	C1210	G1149	A1088	G1027	G967	U	U845	U785	C725
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A1632	U1512	G1392	G1333	G1272	U1212	U1151	C1090	C1029	U969	C	C847	A787	U727
C1633	U1513	G1393	G1334	G1273	U1213	C1152	U1091	U1030	A970	C	A848	G788	G728
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G1635	U1515	G1395	A1336	G1275	C1215	U1154	U1093	A1032	C972	A912	C850	A790	C730
C1636	A1516	C1396	G1336	A1275	A1215	A1154	U1093						

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U2542	A2482	C2422	G2362	G2302	C2242	A2182	G2122	C2061	G2001	C1941	G1880	U1819	C1758	C1698	G1638
A2543	U2483	G2423	G2363	G2303	C2243	A2183	G2123	U2062	A2002	C1942	U1881	G1820	C1759	C1699	U1639
U2544	G2484	C2424	G2364	G2304	C2244	C2184	C2124	A2063	A2003	A1943	U1882	A1821	G1760	C1700	C1640
U2545	U2485	G2425	G2365	C2305	A2245	G2185	C2125	U2064	U2004	C1944	A1883	C1822		C1701	C1641
G2546	C2486	G2426	U2366	A2306	A2246	G2186	U	A2065	U2005	C1945	A1884	G1823	G1763	C1702	G1642
G2547	G2487	A2427	G2367	A2307	A2247	A2187	U	U2066	G2006	U1946	C1885	C1824	A1764	C1703	A1643
G2548	G2488	U2428	G2368	A2308	A2248	A2188	U	G2067	G2007	G1947	G1886	C1825	C1765	G1704	A1644
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C2551	A2491	C2431	A2371	U2311	U2251	A2191	U	G2070	G2010	C1950	U1889	C1828	U1768	U1707	U1647
C2552	G2492	A2432	A2372	A2312	U2252	U2192	G2132	G2071	U2011	G1951	G1890	C1829	U1769	C1708	C1648
G2553	G2493	G2433	C2373	G2313	A2253	C2193	G2133	C2072	A2012	A1952	C1891	C1830	U1770	U1709	A1649
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G2555	G2495	G2435	G2375	A2315	G2255	C2195	G2135	U2074	A2014	A1954	G1893	G1832	C1772	U1711	U1651
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U2563	G2503	C2443	C2383	U2323	C2263	G2203	G	C2082	C2022	C1962	U1901	G1841	A1780	G1719	G1659
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U2567	U2507	G2447	U2387	U2327	A2267	G2207	C	U2086	C2026	C1966	U1906	A1845	C1784	U1723	C1663
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G2571	G2511	G2451	A2391	A2331	C2271	U2211	G	C2091	U2030	G1970	A1910	G1849	C1788	C1727	A1667
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A2573	G2513	C2453	C2393	U2333	C2273	G2213	A	G2093	G2032	C1972	G1912	A1851	U1790	A1729	A1669
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G2576	U2516	U2456	C2396	G2336	C2276	G2216	A	U2096	G2035	G1975	U1915	G1854	A1793	U1732	A1672
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G2578	U2518	U2458	U2398	C2338	A2278	G2218	C2157	G	A2037	C1977	C1917	U1856	C1795	G1734	C1674
A2579	C2519	C2459	C2399	A2339	G2279	U2219	C2158	G	C2038	U1978	A1918	G1857	A1796	G1735	C1675
G2580	U2520	G2460	G2400	C2340	A2280	A2220	A2159	A	G2039	C1979	A1919	C1858	C1797	G1736	U1676
U2581	A2521	G2461	A2401	G2341	C2281	G2221	C2161	U	A2040	A1980	A1920	A1859	G1797	G1737	U1677
G2582	G2522	C2462	U2402	U2342	G2282	U2222	C2162	A	A2041	A1981	A1921	A1860	A1799	G1738	G1678
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G2584	U2524	G2464	A2404	G2344	U2284	U2224	G2164	G2104	A2043	G1983	U1923	C1862	C1801	G1740	U1680
C2585	U2525	G2465	A2405	A2345	U2285	G2225	A2165	U2105	G2044	A1984	C1924	U1863	A1802	G1741	A1681
U2586	U2526	G2466	C2406	G2346	G2286	A2226	G2166	G2106	A2045	G1985	C1925	G1864	U1803	G1742	A1682
G2587	G2527	A2467	G2407	C2347	G2287	C2227	A2167	U2107	C2046	G1986	U1926	C1865	U1804	C1743	G1683
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U2590	C2530	U2470	U2410	G2350	A2290	G2230	C2170	G2110	C2049	C1989	U1929	A1868	A1807	C1746	A1686
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A2593	U2533	G2473	G2413	G2353	G2293	C2233	G2173	U	G2052	G1992	G1932	G1871	U1810	G1749	U1689
U2594	U2534	G2474	A2414	G2354	U2294	G2234	G2174	G	G2053	G1993	G1933	A1872	A1811	A1750	U1690
C2595	G2535	C2475	G2415	A2355	G2295	G2235	A2175	C	A2054	U1994	U1934	G1873	U1812	A1751	G1691
G2596	G2536	U2476	U2416	A2356	U2296	G2236	U2176	G	G2055	G1995	A1935	G1874	U1813	U1752	G1692
C2597	C2537	G2477	U2417	A2357	G2297	G2237	U2177	A2117	C2056	A1996	A1936	C1875	G1814	A1753	A1693
G2598	C2538	C2478	A2418	C2358	U2298	G2238	U2178	A2118	U2057	A1997	G1937	C1876	G1815	G1754	A1694
U2599	U2539	U2479	C2419	U2359	A2299	G2239	C2179	A2119	G2058	A1998	U1938	C1877	G1816	G1755	U1695
A2600	U2540	C2480	C2420	C2360	G2300	C2240	U2180	C2120	U2059	U1999	U1939	C1878	U1817	C1756	C1696

U2841	G2781	A2721	G2661	C2601
C2842	G2782	C2722	C2662	G2602
A2843	U2783	G2723	U2663	G2603
G2844	A2784	G2724	G2664	G2604
C2845	A2785	U2725	G2665	C2605
G2846	G2786	U2726	U2666	G2606
G2847	A2787	G2727	C2667	C2607
A2848	C2788	A2728	U2668	A2608
C2849	U2789	A2729	C2669	G2609
U2850	C2790	A2730	C2670	G2610
G2851	G2791	G2731	C2671	A2611
G2852	C2792	C2732	U2672	G2612
U2853	G2793	A2733	G2673	A2613
G2854	G2794	U2734	C2674	A2614
C2855	A2795	C2735	U2675	U2615
U2856	A2796	U2736	G2676	U2616
C2857	G2797	A2737	U2677	G2617
A2858	U2798	A2738	C2678	A2618
U2859	G2799	G2739	G2679	G2619
C2860	C2800	C2740	U2680	G2620
A2861	A2801	G2741	A2681	G2621
G2862	C2802	G2742	C2682	G2622
U2863	C2803	G2743	C2683	A2623
C2864	G2804	A2744	A2684	G2624
G2865	G2805	A2745	A2685	U2625
A2866	G2806	G2746	C2686	U2626
G2867	U2807	C2747	G2687	G2627
G2868	G2808	C2748	G2688	C2628
U2869	A2809	A2749	C2689	U2629
C2870	C2810	G2750	A2690	C2630
U2871	G2811	C2751	C2691	C2631
U2872	A2812	C2752	A2692	U2632
G2873	G2813	C2753	U2693	A2633
A2874	G2814	C2754	G2694	G2634
C2875	C2815	A2755	C2695	U2635
C2876	C2816	A2756	A2696	A2636
A2877	A2817	G2757	G2697	C2637
C	G2818	A2758	G2698	G2638
U	G2819	U2759	G2699	A2639
C	G2820	G2760	U2700	G2640
	G2821	A2761	A2701	A2641
	U2822	G2762	G2702	G2642
	G2823	U2763	C2703	G2643
	C2824	U2764	U2704	A2644
	A2825	C2765	A2705	C2645
	G2826	U2766	U2706	G2646
	G2827	C2767	G2707	G2647
	C2828	C2768	U2708	G2648
	A2829	C2769	C2709	A2649
	U2830	A2770	C2710	G2650
	A2831	C2771	G2711	U2651
	G2832	U2772	G2712	G2652
	C2833	G2773	A2713	A2653
	A2834	U2774	A2714	A2654
	A2835	U	C2715	C2655
	U2836	U	G2716	G2656
	G2837	A	G2717	G2657
	U2838	U2778	A2718	A2658
	G2839	C2779	U2719	C2659
	U2840	U2780	A2720	C2660

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, α , β , γ	170.01Å 411.48Å 697.62Å 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}	0.18	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.283 , 0.364	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59428	wwPDB-VP
Average B, all atoms (Å ²)	81.0	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: RU6

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	9/66467 (0.0%)	0.88	121/103673 (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	4	204

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	803	C	C3'-O3'	7.88	1.53	1.42
1	A	2589	C	C3'-C2'	-6.84	1.45	1.52
1	A	700	C	N1-C2	6.48	1.46	1.40
1	A	803	C	C3'-C2'	6.40	1.59	1.52
1	A	788	G	N9-C4	6.20	1.43	1.38

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2810	A	N9-C1'-C2'	14.02	132.22	114.00
1	A	2589	C	O4'-C1'-N1	12.82	118.46	108.20
1	A	985	G	N9-C1'-C2'	11.79	129.33	114.00
1	A	2588	U	O3'-P-O5'	10.97	124.85	104.00
1	A	1692	C	N1-C1'-C2'	10.55	127.72	114.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	765	C	C1'
1	A	1139	A	C1'
1	A	1685	A	C1'
1	A	2810	A	C1'

5 of 204 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	C	Sidechain
1	A	34	U	Sidechain
1	A	66	U	Sidechain
1	A	67	G	Sidechain
1	A	71	A	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	6937	0
2	A	69	0	80	8	0
All	All	59428	0	29997	6939	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 79.

The worst 5 of 6939 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2426:G:C4'	1:A:2427:A:H5''	1.53	1.35
1:A:2426:G:H4'	1:A:2427:A:C5'	1.57	1.34
1:A:968:C:N4	1:A:970:A:H1'	1.51	1.26
1:A:43:A:N6	1:A:446:C:H42	1.38	1.20
1:A:1733:U:H5'	1:A:1734:C:C5	1.78	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%)	853 (30%)	190 (6%)

5 of 853 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	A	13	A
1	A	27	G
1	A	33	C
1	A	43	A

5 of 190 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1301	U
1	A	1634	A
1	A	2633	A
1	A	1324	G
1	A	1410	U

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 ⓘ

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$
2	RU6	A	2881	-	74,74,74	2.33	28 (37%)	111,111,111	2.89	39 (35%)

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
2	RU6	A	2881	-	-	1/80/134/134	0/4/6/6

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	RU6	C40-N2	7.36	1.57	1.46
2	A	2881	RU6	C4-C5	5.52	1.67	1.55
2	A	2881	RU6	C10-C9	-5.45	1.43	1.52
2	A	2881	RU6	C46-C45	5.38	1.57	1.48
2	A	2881	RU6	O13-C39	4.70	1.43	1.35

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	RU6	C40-N2-C39	-12.42	106.17	122.24
2	A	2881	RU6	O13-C39-N2	-11.89	100.40	109.80
2	A	2881	RU6	C10-C11-N2	8.25	127.03	112.50
2	A	2881	RU6	O13-C12-C11	-6.89	95.70	103.28
2	A	2881	RU6	C6-C7-C8	6.33	126.61	115.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2881	RU6	C20-O5-C16-C17

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.