



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:29 am 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

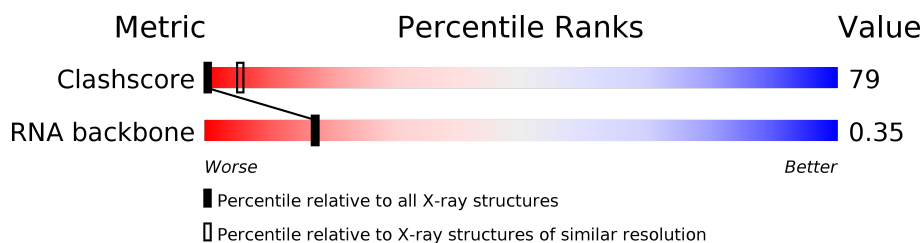
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	112137	1036 (3.70-3.50)
RNA backbone	2435	1002 (4.30-2.90)

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. 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	

2 Entry composition ⓘ

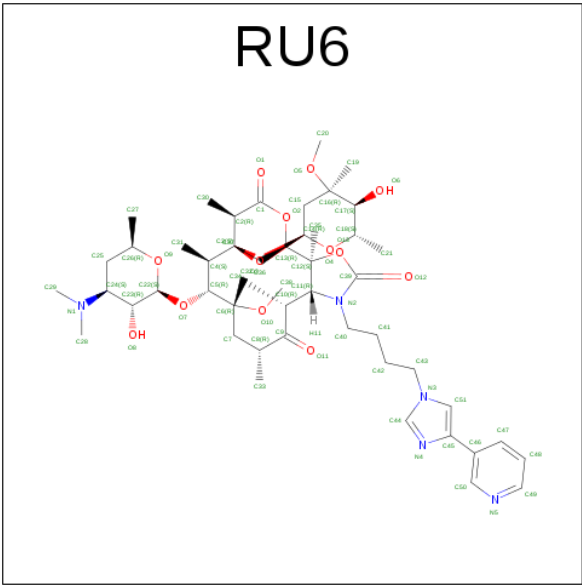
There are 2 unique types of molecules in this entry. The entry contains 59428 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			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-YL 2,6-DIDEOXY-3-C-METHYL-3-O-METHYL-ALPHA-L-RIBO-HEXOPYRANOSIDE (three-letter code: RU6) (formula: C₅₁H₈₁N₅O₁₃).



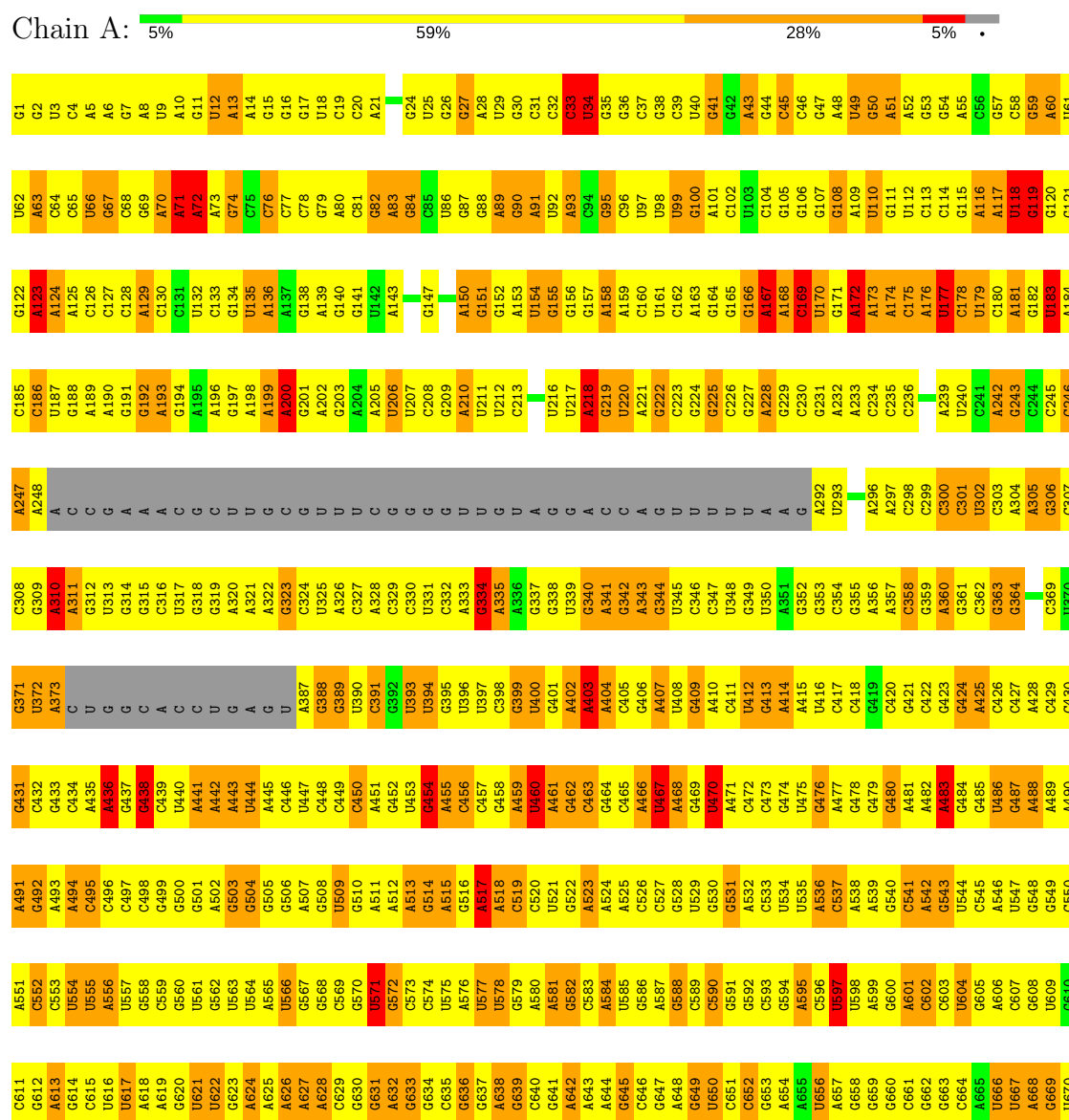
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	69	51	5	13	0	0

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 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.

Note EDS was not executed.

• Molecule 1: 23S rRNA





U2541	G2481	C2421	G2361	A2301	U2241	A2181	U2121	A2060	U2000	C1940	G1879	G1818	C1757	U1697	U1637
U2542	A2482	C2422	G2362	G2302	C2242	A2182	G2122	C2061	G2001	C1941	G1880	U1819	C1758	C1698	G1638
A2543	U2483	G2423	G2363	G2303	C2243	C2183	G2123	A2062	A2002	C1942	U1881	G1820	C1759	C1699	U1639
U2544	G2484	C2424	G2364	G2304	C2244	C2184	C2124	A2063	A2003	C1943	G1882	G1821	G1760	C1700	C1640
U2545	U2485	G2425	G2365	C2305	A2245	G2185	C2125	U2064	U2004	C1944	G1883	G1822		C1701	C1641
G2546	C2486	U2426	U2366	A2306	A2246	G2186	U	A2065	U2005	C1945	A1884	G1823	G1763	C1702	G1642
G2547	G2487	A2427	A2367	A2307	A2247	A2187	U	G2066	G2006	U1946	G1885	C1824	A1764	C1703	A1643
G2548	G2488	U2428	G2368	A2308	A2248	A2188	U	G2067	G2007	C1947	G1886	G1825	C1765	G1704	A1644
G2549	A2489	G2429	U2369	G2309	U2249	A2189	U	C2068	C2008	C1948	G1887	U1826	U1766	U1705	U1645
C2550	U2490	G2430	G2370	G2310	G2250	A2190	G	U2069	U2009	A1949	C1888	G1827	G1767	A1706	G1646
A2551	C2431	U2431	A2371	U2311	U2251	A2191	U	G2070	G2010	C1950	G1889	C1828	U1768	U1707	U1647
C2552	G2492	A2432	A2372	A2312	A2252	U2192	G2132	G2071	U2011	G1951	G1890	G1829	U1769	G1708	C1648
G2553	U2493	G2433	C2373	G2313	A2253	C2193	G2133	G2072	A2012	A1952	C1891	C1830	U1770	U1709	A1649
C2554	C2494	G2434	C2374	A2314	C2254	A2194	U2134	A2073	A2013	A1953	C1892	G1831	A1771	U1710	A1650
G2555	G2495	U2435	G2375	A2315	G2255	C2195	G2135	U2074	A2014	A1954	G1893	G1832	C1772	U1711	U1651
A2556	U2496	G2436	G2376	G2316	G2256	C2196	G2136	U2075	G2015	G1955	U1894	U1833	C1773	G1712	G1652
C2557	G2497	U2437	U2377	G2317	A2257	U2197	G2137	G2076	A2016	G1956	A1895	G1834	A1774	G1713	C1653
U2558	U2498	A2438	G2378	U2318	G2258	U2198	U2138	G2077	U2017	C1957	A1896	G1835	A1775	A1714	A1654
C2559	G2499	U2439	G2379	G2319	G2259	C2199	G2139	G2078	G2018	G1958	C1897	G1836	A1776	A1715	C1655
G2560	C2500	C2440	U2380	G2320	C2260	G2200	G2140	G2079	C2019	U1959	U1898	G1837	A1777	G1716	U1656
U2561	U2501	U2441	A2381	C2321	G2261	G2201	A	U2080	C2020	A1960	U1899		U1778	A1717	A1657
G2562	G2502	C2442	C2382	U2322	C2262	G2202	G	U2081	G2021	A1961	U1900	G1840	C1779	G1718	A1658
U2563	G2503	C2443	C2383	U2323	C2263	G2203	G	C2082	C2022	C1962	A1901	G1841	U1780	G1719	G1659
U2564	G2504	C2444	G2384	G2324	C2264	A2204	C	G2083	C2023	G1963		G1842	C1781	G1720	G1660
C2565	U2505	C2445	U2385	A2325	A2265	G2205	A	G2084	U2024	A1964	G1904	U1843	A1782	G1721	C1661
A2566	C2506	G2446	G2386	C2326	A2266	C2206	A	G2085	A2025	U1965	G1905	C1844	G1783	G1722	G1662
U2567	U2507	G2447	U2387	U2327	A2267	G2207	C	U2086	C2026	C1966	U1906	A1845	C1784	U1723	C1663
A2568	G2508	U2448	G2388	G2328	G2268	U2208	G	U2087	C2027	U1967	C1907	A1846	U1785	C1724	G1664
U2569	A2509	G2449	G2389	C2329	G2269	G2209	U		C2028	G1968	C1908	G1847	C1786	G1725	C1665
C2570	U2510	G2450	A2390	G2330	U2270	G2210	G	G2091	G2029	G1969	U1909	U1848	U1787	C1726	G1666
U2571	G2511	U2451	A2391	A2331	C2271	U2211	G	C2092	U2030	G1970	A1910	G1849	C1788	G1727	A1667
U2572	A2512	U2452	G2392	G2332	A2272	U2212	A	U2093	A2031	C1971	A1911	G1850	U1789	A1728	G1668
G2573	U2513	C2453	G2393	C2333	C2273	G2213	A	G2094	A2032	C1972	G1912	A1851	U1790	C1729	A1669
U2574	G2514	U2454	G2394	U2334	C2274	G2214	A	C2095	C2033	C1973	G1913	G1852	C1791	G1730	G1670
G2575	A2515	A2455	C2395	U2335	U2275	G2215	U	U2096	A2034	U1974	U1914	G1853	C1792	C1731	A1671
U2576	U2516	U2456	C2396	G2336	C2276	G2216	A	U2097	G2035	G1975	A1915	G1854	U1793	U1732	A1672
U2577	C2517	A2457	A2397	A2337	A2277	G2217	C2157	A2097	G2036	U1976	G1916	G1855	A1794	U1733	C1673
G2578	U2458	U2457	U2398	C2338	A2278	G2218	C2158	G	A2037	C1977	C1917	U1856	C1795	G1734	C1674
A2579	C2459	G2460	C2399	A2339	G2279	U2219	A2159	G	C2038	U1978	G1918	G1857	A1796	G1735	C1675
C2580	U2520	G2461	G2400	C2340	A2280	A2220	C2160	A	G2039	C1979	A1919	C1858	C1797	C1736	U1676
U2581	A2521	U2462	A2401	G2341	C2281	G2221	C2161	U	A2040	A1980	A1920	A1859	G1798	G1737	U1677
G2582	G2522	C2463	U2402	U2342	G2282	U2222	C2162	A	A2041	A1981	A1921	A1860	A1799	G1738	G1678
U2583	G2523	G2464	C2403	G2343	U2283	U2223	U2163		A2042	C1982	U1922	G1861	A1800	G1739	U1679
C2584	U2524	G2465	A2404	G2344	U2284	U2224	G2164	G2103	A2043	G1983	U1923	C1862	C1801	G1740	U1680
U2585	U2525	A2466	A2405	A2345	U2285	G2225	A2165	U2104	G2044	A1984	C1924	U1863	A1802	G1741	A1681
G2586	G2466	G2346	G2406	G2346	G2286	A2226	G2166	U2105	A2045	G1985	C1925	G1864	G1803	G1742	A1682
U2587	U2467	C2347	G2407	C2347	G2287	G2227	A2167	G2107	C2046	G1986	U1926	G1865	U1804	C1743	G1683
U2588	G2528	A2348	G2408	G2348	A2288	U2228	A2168	G2108	C2047	G1987	U1927	G1866	G1805	G1744	G1684
C2589	G2529	G2469	A2409	G2349	A2289	U2229	A2169	A2109	C2048	A1988	G1928	A1867	G1806	C1745	A1685
U2590	U2470	G2350	U2410	G2350	A2290	G2230	C2170	G2110	C2049	C1989	U1929	A1868	A1807	G1746	A1686
C2591	U2471	G2351	A2411	G2351	U2291	G2231	U2171	C	G2050	C1990	C1930	A1869	C1808	G1747	C1687
U2592	A2472	A2352	A2412	A2352	C2292	G2232	U2172	C	U2051	C1991	G1931	A1870	C1809	U1748	U1688
A2593	G2473	G2353	G2413	G2353	G2293	G2233	G2173	U	G2052	G1992	G1932	U1871	U1810	G1749	U1689
U2594	U2534	G2474	A2414	G2354	U2294	G2234	G2174	G	G2053	G1993	G1933	A1872	A1811	A1750	C1690
C2595	G2475	A2355	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	C2477	U2477	U2417	A2357	G2297	G2237	U2177	A2117	C2056	A1996	A1936	C1875	G1814	A1753	A1693
U2598	G2478	C2358	A2418	G2358	U2298	G2238	U2178	A2118	U2057	A1997	G1937	C1876	G1815	G1754	A1694
U2599	U2479	U2359	C2419	G2359	A2299	G2239	C2179	A2119	U2058	U1998	U1938	C1877	G1816	G1755	U1695
A2600	G2480	C2360	C2420	G2360	G2300	C2240	U2180	C2120	U2059	U1999	U1939	C1878	U1817	C1756	C1696

U2841	G2781	A2721	G2661	G2601
C2842	G2782	C2722	C2662	G2602
A2843	U2783	G2723	U2663	G2603
G2844	A2784	C2724	G2664	G2604
C2845	A2785	U2725	G2665	C2605
G2846	G2786	U2726	U2666	G2606
A2847	A2787	G2727	C2667	C2607
U2848	C2788	A2728	U2668	A2608
C2849	U2789	A2729	C2669	G2609
U2850	C2790	A2730	C2670	G2610
G2851	G2791	G2731	C2671	A2611
C2852	G2792	C2732	U2672	G2612
U2853	G2793	A2733	G2673	A2613
G2854	G2794	U2734	C2674	A2614
C2855	A2795	C2735	U2675	U2615
U2856	U2796	C2736	G2676	C2616
C2857	G2797	A2737	U2677	G2617
A2858	A2798	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
U2868	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	C2693	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	C2717	G2657
	U2838	U2778	A2718	A2658
	G2839	C2779	U2719	C2659
	U2840	A2780	A2720	C2660

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 [i](#)

5.1 Standard geometry [i](#)

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 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	59359	0	29917	6937	0
2	A	69	0	80	8	0
All	All	59428	0	29997	6939	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 79.

The worst 5 of 6939 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: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 [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	2757/2880 (95%)	853 (30%)	0

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

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	$\# Z > 2$
2	RU6	A	2881	-	72,74,74	2.47	27 (37%)	102,111,111	2.76	35 (34%)

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	0/6/6/6

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	RU6	C10-C9	-5.87	1.43	1.52
2	A	2881	RU6	O11-C9	-3.46	1.15	1.21
2	A	2881	RU6	C2-C1	-3.09	1.44	1.51
2	A	2881	RU6	C2-C3	-2.64	1.48	1.55
2	A	2881	RU6	O7-C22	-2.03	1.36	1.41

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	RU6	C40-N2-C39	-12.74	106.17	122.31
2	A	2881	RU6	O13-C39-N2	-11.44	100.40	109.78
2	A	2881	RU6	C25-C24-C23	-5.27	102.63	110.07
2	A	2881	RU6	C42-C43-N3	-5.05	97.94	111.67
2	A	2881	RU6	O5-C16-C15	-4.95	104.68	112.95

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.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2881	RU6	8	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.