



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:08 PM GMT

PDB ID : 1NJO  
Title : The crystal structure of the 50S Large ribosomal subunit from *Deinococcus radiodurans* complexed with a short substrate analog ACCPuromycin (ACCP)  
Authors : Bashan, A.; Agmon, I.; Zarivatch, R.; Schlutzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.  
Deposited on : 2003-01-02  
Resolution : 3.70 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

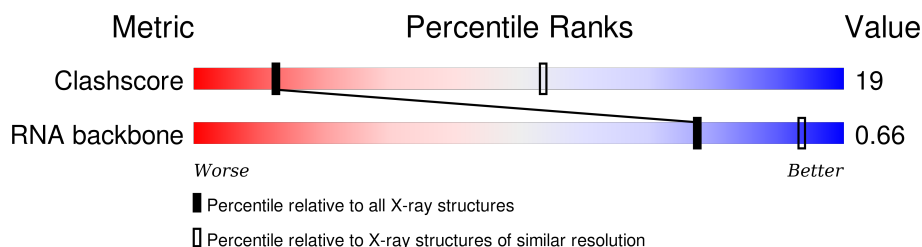
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 Å.

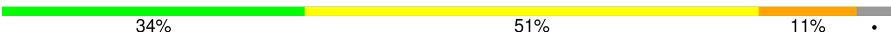

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1224 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

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	0	2880	
2	5	4	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 59455 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	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

- Molecule 2 is a RNA chain called RNA ACC(Puromycin).

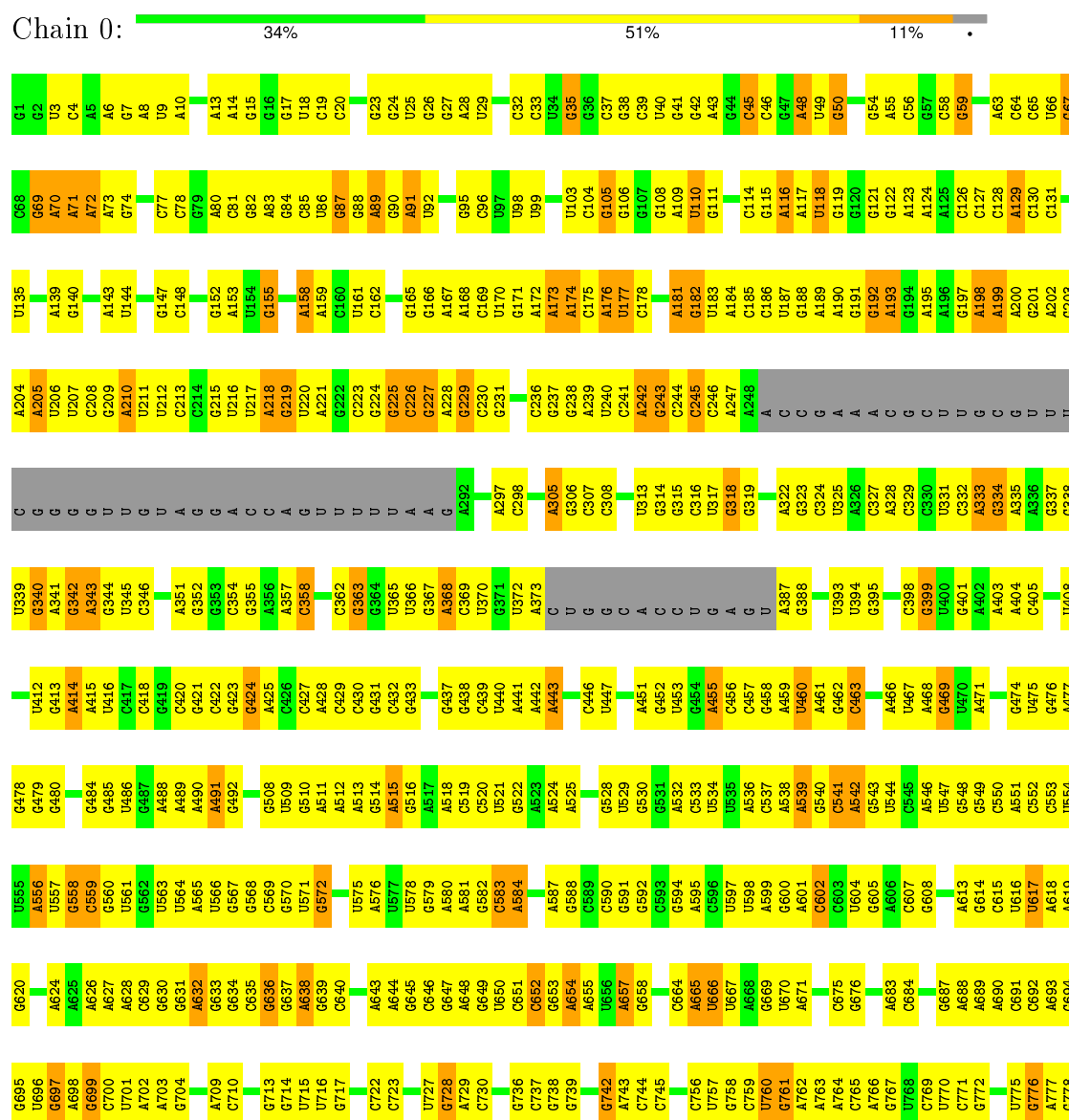
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	5	4	Total	C	N	O	P	0	0	0
			96	50	18	25	3			

### 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 ribosomal RNA



U1909	G1818	U1732	C1655	A1582	G1504	G1436	U1357	A1290	C1218	U1144	G1047	G980	A911	G841	U779
A1940	U1819	U1733	U1656	A1583	U1505	A1437	C1358	G1291	C1219	C1445	C1052	C981	U916	A842	U780
A1911	G1820	A1657	A1657	G1584	G1508	A1441	G1359	A1292	G1220	G1146	C1052	A984	U917	G843	G781
G1912	A1821	G1742	A1658	A1585	A1509	A1442	G1365	A1293	G1221	G1147	G1053	A985	U918	G844	U782
G1913	C1822	C1743	G1659	A1586	A1510	C1443	A1366	G1298	G1222	G1148	C1054	G985	U919	U845	G783
U1914	C1825	C1744	G1660	A1587	A1511	G1444	A1367	U1301	G1223	G1149	A1055	A986	U920	A846	U784
A1915	U1826	C1745	C1661	U1591	A1512	A1445	A1368	U1302	A1224	C1150	U1056	G987	G920	C847	U785
G1916	U1826	A1746	G1662	U1592	U1513	A1446	G1369	C1302	G1225	U1151	A1057	G988	A921	U852	U786
C1917	U1826	G1747	C1663	U1593	C1514	A1447	G1370	C1302	A1226	U1152	A1058	A991	A922	U852	U787
C1829	G1830	U1748	C1664	A1594	U1515	A1448	G1371	U1303	A1227	U1154	A1059	A992	U925	G853	G788
G1831	U1831	A1750	G1665	A1595	C1516	C1449	G1372	U1307	A1231	G1155	A1060	A993	U926	G854	G789
C1835	C1835	G1754	G1666	A1596	C1517	G1450	G1373	C1308	U1232	U1156	G1066	A994	G926	G855	A790
C1836	C1837	G1755	A1667	A1597	C1518	C1451	G1374	U1309	A1233	A1162	A1068	G996	G928	G856	G791
U1922	C1837	U1756	A1668	A1598	G1519	U1452	G1375	C1310	C1234	C1163	G1069	G997	A929	U857	U792
U1923	U1600	U1757	G1670	C1599	G1520	U1453	G1376	C1311	C1235	G1165	G1070	C998	A930	U858	G793
U1926	A1671	A1672	A1671	U1601	C1524	C1455	C1380	U1312	A1242	A1166	G1073	A999	G931	U859	A794
C1838	G1760	U1673	U1672	U1602	G1527	C1456	C1381	G1313	U1243	A1167	G1074	A1001	G932	G861	A796
A1840	C1762	U1674	U1673	A1603	G1528	A1457	G1382	A1314	G1244	A1168	C1075	A1002	G933	U862	A797
G1841	G1763	A1764	U1677	A1604	C1529	U1458	A1386	A1315	U1245	G1169	C1076	C1003	G934	C864	G798
C1841	U1765	U1766	U1678	A1605	U1530	C1466	G1387	G1316	G1248	U1172	A1081	A1004	G935	A865	U800
U1937	U1680	U1681	U1680	A1606	U1531	A1463	C1388	G1317	G1249	U1173	G1084	U1005	G936	U868	C803
U1938	A1681	A1682	A1681	U1607	C1532	G1465	C1389	C1319	U1250	G1174	A1085	C1006	G937	C869	C804
U1939	U1682	U1683	U1682	A1608	G1533	C1466	A1390	A1320	G1251	U1175	G1086	C1007	G938	C870	C805
C1944	U1684	U1684	U1684	U1609	U1534	C1467	U1392	A1321	G1252	U1176	C1087	C1008	G939	U871	G806
C1945	U1685	U1685	U1685	A1610	U1535	U1468	C1393	G1323	C1253	A1177	C1088	C1009	G940	G872	A807
U1946	C1858	A1774	G1677	U1611	C1540	U1469	U1394	U1324	C1254	A1178	C1089	U1014	G941	U873	C808
C1947	A1859	A1775	U1678	U1612	C1541	C1470	A1395	U1325	U1257	A1179	C1090	U1015	G942	A874	C809
A1948	A1860	A1776	U1679	U1613	G1542	C1471	G1396	G1326	G1258	C1181	C1091	C1016	G943	G875	U810
C1949	G1861	A1777	C1687	C1614	G1543	C1472	C1397	U1327	A1259	U1182	G1092	C1017	G944	A876	U811
C1950	C1862	U1778	C1687	C1615	A1544	C1473	C1398	G1328	U1260	U1183	G1093	C1018	G945	C877	G812
G1951	U1865	C1779	G1691	C1616	U1545	U1474	C1399	U1329	G1261	C1184	U1093	C1019	G950	C878	G813
A1952	C1865	A1780	C1692	U1617	C1546	U1475	U1402	G1330	U1262	C1185	U1094	C1020	G951	A879	A814
A1953	G1866	U1785	U1696	U1618	U1547	U1476	U1403	G1331	G1263	G1186	G1095	A1021	G952	C880	G815
A1954	U1871	C1786	C1696	A1619	U1548	U1477	G1407	G1332	G1264	A1187	G1096	A1022	G953	G887	U816
G1955	U1872	U1787	C1703	C1620	U1549	U1478	U1408	G1333	C1265	A1188	A1097	U1023	G954	A817	G818
G1956	G1880	C1788	G1704	G1622	C1552	G1479	U1410	A1334	G1266	A1189	G1100	U1024	G955	G888	C819
C1957	U1881	U1789	G1705	C1623	G1557	C1480	C1411	G1335	A1267	C1190	A1114	A1025	G956	C889	U820
G1958	G1882	C1790	C1624	A1624	C1558	U1482	C1412	G1336	U1268	A1191	A1115	G1026	G957	A891	G822
A1961	A1883	C1791	A1625	A1625	A1561	A1486	G1414	G1337	G1269	G1193	C1120	U1027	G958	G	U823
C1962	A1884	C1792	A1626	A1626	G1562	C1487	C1415	G1338	C1270	U1194	G1121	C1028	G959	G	A821
G1963	C1885	A1793	C1627	C1627	G1562	C1488	A1416	U1339	C1271	U1195	A1122	C1029	U960	G	G823
A1964	G1886	C1711	C1628	C1628	G1566	G1489	C1417	G1340	C1272	U1196	A1123	U1030	U961	G	U824
U1965	C1887	G1712	G1629	G1629	G1566	U1490	G1419	U1342	G1273	U1197	C1127	U1031	A964	G	C825
C1966	C1888	G1713	G1630	G1630	A1567	C1491	G1419	C1343	C1274	U1198	G1128	A1032	G965	C	U826
G1970	G1889	A1714	A1632	A1632	A1568	C1492	U1424	C1344	A1275	U1199	A1129	G1033	A966	C	C827
C1971	U1890	G1715	C1633	C1633	A1568	U1493	G1425	G1345	G1276	G1200	U1130	G1034	G967	U	C828
G1972	A1895	A1717	A1634	A1634	G1571	C1494	U1426	G1346	A1278	A1203	U1131	G1035	C968	A	C829
C1973	A1896	G1722	C1572	C1572	C1572	G1495	U1426	C1347	U1279	A1204	C1132	G1036	U969	C	C830
U1974	C1808	U1723	G1573	G1573	G1573	U1496	G1427	C1348	U1280	G1205	G1133	U1037	A970	C	G831
G1975	A1899	C1724	A1574	A1574	A1574	G1496	G1428	C1349	A1281	U1038	A1137	U1038	A971	A	A832
U1976	U1810	C1724	C1575	C1575	C1575	C1497	A1429	G1350	U1282	A1039	A1138	A1040	C972	G	A833
A1901	U1811	C1727	G1576	G1576	G1576	G1498	G1430	G1351	G1284	G1210	A1139	G1041	U973	C	A834
U1978	U1812	A1728	C1648	C1648	C1648	U1499	U1431	G1352	U1285	G1211	A1140	U1042	U974	U	U837
C1979	U1813	U1729	U1651	U1651	U1651	U1500	G1432	A1353	U1286	U1214	U1141	U1043	C975	A	A838
A1980	C1907	G1730	C1729	C1729	C1729	U1501	U1433	A1354	A1287	G1142	U1044	U1044	U978	C	U839
A1981	C1908	C1731	C1731	C1731	C1731	G1503	G1435	A1356	A1289	A1143	U1045	U1046	A979	C	U840

G1982	G2055	G2133	A2204	C2274	C2358	G2425	C2491	G2555	A2623	G2707	A2785	U2871	C1982
G1985	G2056	G2134	C2205	U2275	G2361	G2426	G2492	G2558	G2624	U2708	G2786	U2872	G2055
G1986	U2057	C2135	G2206	A2277	G2362	A2427	U2493	U2559	U2625	C2709	A2787	U2873	G2056
G1993	U2058	G2136	U2211	G2278	G2363	U2428	G2494	G2560	C2628	C2710	G2794	A2874	U2057
U1994	U2059	G2137	U2212	G2279	G2364	A2429	G2495	G2561	G2629	G2711	A2795	A2875	U2058
G1996	A2060	U2138	G2213	U2285	U2365	C2431	A2497	G2562	U2630	G2712	A2796	A2876	A2060
A1997	U2062	G2139	G2214	U2286	A2367	A2432	U2498	U2563	A2633	A2713	G2797	A2877	U2062
G2001	G2069	A	G2217	G2286	G2368	G2433	C2499	U2564	G2634	G2717	A2798	C	U2069
A2002	G2070	G	G2218	A2287	U2369	G2434	C2500	C2565	U2635	A2718	C2799	U	G2070
A2003	G2076	C	A2219	A2288	U2370	G2435	U2501	A2566	A2636	A2721	A2801	C	G2076
U2004	G2077	A	G2220	G2292	A2371	U2436	G2502	G2567	A2639	A2722	G2805	G	G2077
U2005	G2078	C	G2221	G2293	C2372	A2437	G2503	G2568	G2640	C2725	U2806	U	G2078
G2006	U2079	A	U2222	U2298	C2373	C2439	G2504	G2569	A2641	U2726	U2807	C	U2079
G2007	U2080	G	U2223	U2299	G2376	G2444	G2505	G2570	G2642	U2727	G2808	U	G2080
C2008	U2081	G	G2224	A2300	U2377	U2445	U2506	U2571	G2643	A2728	U2809	U	U2081
U2009	G2082	U	G2225	A2301	G2378	C2446	A2509	G2572	C2646	U2729	A2810	U	U2082
U2010	U2083	G	A2226	G2302	U2380	U2447	U2510	A2577	U2647	G2730	G2811	U	G2083
U2011	G2084	A	U2228	A2307	A2381	A2448	A2512	U2578	G2652	C2731	A2812	U	G2084
A2012	U2085	A	G2229	G2308	C2382	G2449	A2513	C2580	A2658	C2732	C2815	U	U2085
A2013	U2086	U	G2230	G2309	U2383	A2450	G2514	A2581	C2659	U2733	C2816	U	A2013
A2014	G2088	A	G2231	U2310	G2384	G2451	G2515	G2582	C2660	A2737	U2821	U	A2014
G2015	G2089	C2157	U2232	U2311	U2385	C2454	C2516	C2583	G2661	C2740	U2822	U	G2015
A2016	G2094	C2158	U2233	A2312	G2388	A2455	U2517	G2586	U2662	G2741	U2823	U	A2016
U2017	G2095	C2159	G2237	G2313	U2389	U2456	A2521	G2587	G2666	A2742	C2824	U	U2017
G2018	U2096	C2160	U2238	A2314	A2390	A2457	G2522	U2588	C2667	G2743	U2825	U	G2018
C2019	U2097	C2161	C2240	A2315	A2391	U2458	G2523	C2589	U2668	A2744	C2826	U	C2019
G2020	G	U2162	U2241	G2316	G2392	C2459	U2524	U2590	C2669	A2745	U2830	U	G2020
G2021	A	U2163	C2242	G2317	G2393	U2460	G2525	C2591	C2670	C2746	U2831	U	G2021
C2022	G	C2243	C2243	U2318	G2394	G2461	U2526	U2592	C2671	C2747	A2832	U	C2022
C2023	U	A2168	A2244	G2319	C2395	G2462	G2527	A2593	U2674	A2748	C2833	U	C2023
U2024	A	A2169	A2245	G2320	C2396	U2463	G2528	U2594	G2675	A2749	U2836	U	U2024
A2025	G2103	G2103	A2246	C2321	A2397	G2464	G2529	C2595	U2676	G2750	U2837	U	A2025
C2026	G2106	G2106	A2247	U2322	U2398	G2465	G2530	C2596	U2677	G2751	U2838	U	C2026
C2027	G2107	G2107	U2248	U2323	G2399	G2466	U2531	G2597	C2678	A2752	U2839	U	C2027
G2028	G2110	G2110	U2249	G2324	A2401	U2467	U2532	C2598	U2679	C2753	U2840	U	G2028
G2029	C	C	G2250	A2325	U2402	G2468	G2533	C2599	G2680	C2754	U2841	U	C
G2032	U	U	U2251	C2326	C2403	U2469	U2534	U2599	A2681	C2755	C2842	U	U
A2033	G	A2181	G2255	U2327	A2404	U2470	U2535	A2600	C2682	U2756	A2843	U	A2033
A2034	G	A2182	G2256	C2328	C2405	U2471	G2536	C2601	C2683	U2757	U2844	U	A2034
G2035	C	A2185	A2257	G2329	G2406	U2472	C2537	G2602	C2684	C2758	G2847	U	G2035
G2036	G	U2185	G2258	G2330	G2407	G2473	C2538	G2603	U2689	A2770	A2848	U	G2036
A2037	G	U2186	G2259	A2331	A2408	U2474	C2539	C2604	C2690	C2771	U2849	U	A2037
C2038	A2117	G	C2260	G2332	A2409	C2475	A2540	C2605	A2691	U2772	U2852	U	C2038
G2039	A2118	A2118	C2261	A2333	U2410	A2476	G2541	G2606	U2692	G2773	U2853	U	A2117
A2043	A2119	A2119	G2262	C2334	U2411	C2477	U2542	A2607	G2694	U2774	G2854	U	A2118
G2044	C2120	C2120	G2263	G2343	A2412	U2478	A2544	G2608	C2695	U	C2855	U	A2119
A2045	U2121	U2121	A2265	G2344	A2413	U2479	G2545	G2609	U2698	A	U2856	U	C2120
C2046	C2125	C2125	A2266	A2348	A2414	C2480	G2546	U2615	G2699	U2778	A2858	U	C2125
C2047	U	U	A2267	A2349	A2418	G2481	C2547	U2616	U2700	C2779	C2860	U	U
C2048	U2198	U2198	G2268	G2349	C2419	A2482	G2548	U2617	U2701	A2780	A2861	U	U2198
G2049	U2199	U2199	U2270	G2353	C2420	U2483	C2549	A2618	C2703	G2781	G2862	U	U2199
U2051	G	G	C2271	A2356	C2421	U2484	A2551	G2619	U2704	U2782	U2863	U	U2199
G2052	U2201	U2201	A2272	A2357	C2422	G2485	C2552	G2620	A2705	U2783	U2864	U	U2201
			A2273	G2357	G2424	G2487	C2554	G2622	U2706	A2784	G2867	U	G

• Molecule 2: RNA ACC(Puromycin)

Chain 5:

50%

25%

25%

A32  
C33  
C34  
A35

## 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, $\alpha$ , $\beta$ , $\gamma$	169.90 Å   410.40 Å   697.10 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	15.00 – 3.70	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.283 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	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: PPU

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	0	0.14	0/66467	0.63	0/103673
2	5	0.21	0/65	0.56	0/99
All	All	0.14	0/66532	0.63	0/103772

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	0	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	873	U	Sidechain

### 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	0	59359	0	29917	1732	0
2	5	96	0	62	1	0
All	All	59455	0	29979	1732	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 19.

The worst 5 of 1732 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)
1:0:940:G:H3'	1:0:941:U:H5''	1.22	1.14
1:0:1141:U:H3	1:0:2008:C:H5''	1.20	1.05
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.21	0.99
1:0:2668:U:H4'	1:0:2669:C:H5'	1.45	0.97

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	0	2757/2880 (95%)	411 (14%)	43 (1%)
2	5	2/4 (50%)	2 (100%)	0
All	All	2759/2884 (95%)	413 (14%)	43 (1%)

5 of 413 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	G

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Mol	Chain	Res	Type
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1278	A
1	0	1518	C
1	0	2668	U
1	0	1279	G
1	0	1313	U

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

1 non-standard protein/DNA/RNA residue 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	PPU	5	35	2	30,40,41	2.76	6 (20%)	37,57,60	1.26	5 (13%)

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	PPU	5	35	2	-	0/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.89	1.27	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	CE2-CZ	2.66	1.44	1.38
2	5	35	PPU	CD2-CG	2.70	1.44	1.38
2	5	35	PPU	C6-N1	3.32	1.38	1.34
2	5	35	PPU	CE1-CZ	3.74	1.46	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	C4'-C3'-N3'	-3.05	107.25	113.61
2	5	35	PPU	C-CA-N	2.04	117.83	108.73
2	5	35	PPU	C9-N6-C6	2.16	126.28	119.48
2	5	35	PPU	CM-OC-CZ	2.77	123.99	117.51
2	5	35	PPU	C2-N1-C6	4.00	119.95	111.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.