



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 02:00 AM UTC

PDB ID : 2O45 / pdb_00002o45
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

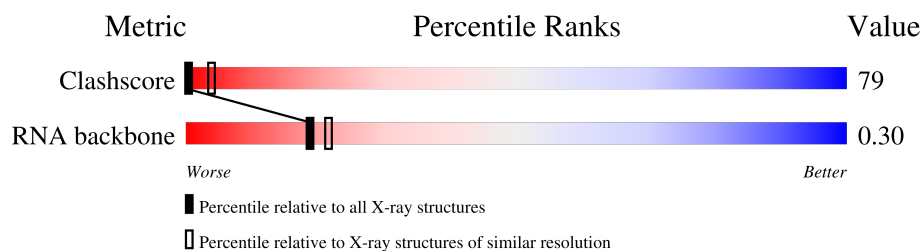
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

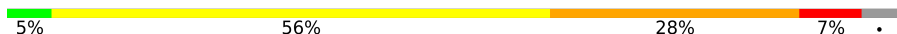
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1827 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	 5% 56% 28% 7% .

2 Entry composition ⓘ

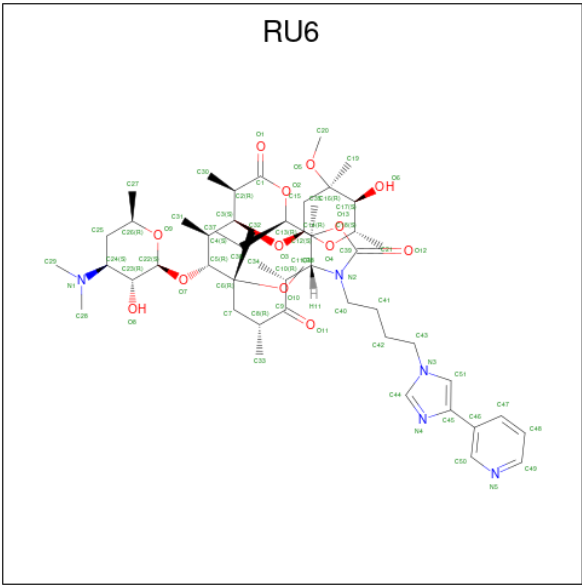
There are 2 unique types of molecules in this entry. The entry contains 59428 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: RU6) (formula: C₅₁H₈₁N₅O₁₃).



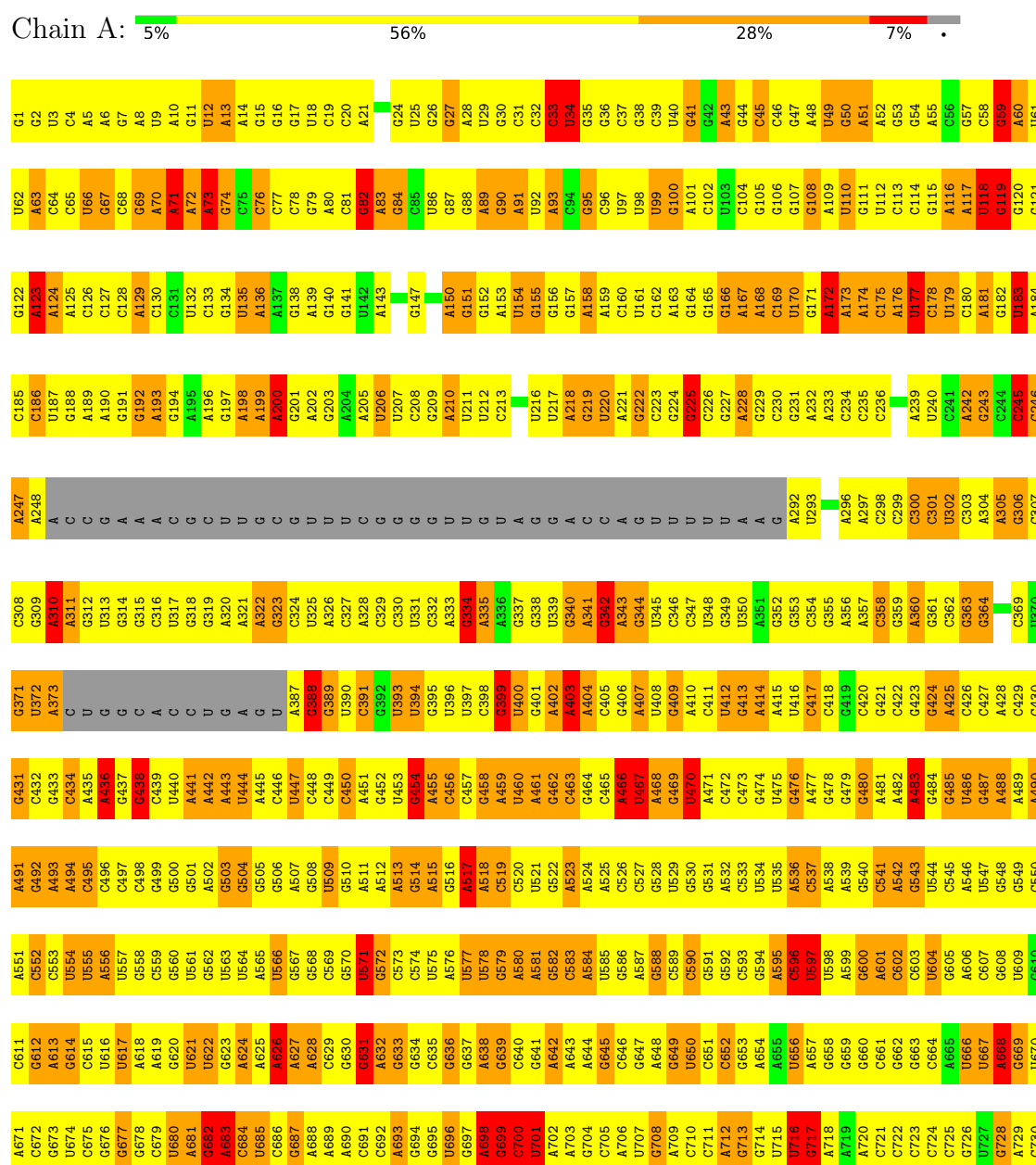
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	69	51	5	13	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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



U1697	C1698	G1637	G1577	G1517	A1457	G1337	U1276	G1216	G1155	C1094	G1033	U973	A913	C851	G791	A731
G1638	G1578	G1458	G1458	C1518	A1458	G1338	G1277	U1217	U1156	A1095	U1034	U974	C914	U852	U792	G732
G1639	G1579	G1459	G1459	G1519	A1459	G1339	A1278	C1218	G1157	A1096	G1035	C975	C915	C853	U793	G733
C1700	C1580	G1460	A1400	G1520	G1460	C1340	G1279	C1219	G1158	A1097	G1036	C976	U916	G854	A794	G734
C1701	C1641	C1461	G1401	U1521	C1461	G1341	U1280	G1220	U1159	G1098	U1037	G977	U917	G855	A795	G735
C1702	C1582	C1462	G1402	C1522	C1462	G1342	A1281	C1221	C1160	A1099	U1038	U978	A918	A856	A796	G736
C1703	A1583	A1463	U1403	A1523	A1463	C1343	C1282	G1222	U1161	G1100	A1039	A979	U919	U857	A797	C737
C1704	G1584	A1464	G1404	C1524	A1464	C1344	C1283	G1223	A1162	U1101	A1040	G980	G920	G858	G738	G738
U1705	A1585	G1465	A1405	A1525	G1465	G1345	G1284	A1224	C1163	G1102	G1041	C981	A921	U859	G739	G739
A1706	A1586	A1466	G1406	C1526	A1466	C1346	A1285	G1225	C1164	C1103	G1042	C982	A922	U860	U800	A740
A1707	A1587	U1467	G1407	G1527	U1467	C1347	U1286	A1226	G1165	G1104	A1043	G983	A923	G861	A801	G741
C1708	A1588	A1468	A1408	C1528	A1468	C1348	A1287	G1227	A1166	U1105	U1044	A884	G924	A862	A802	G742
U1709	C1589	U1469	U1409	C1529	U1469	C1349	A1288	G1228	A1167	A1106	G1045	G985	U925	G863	C803	A743
U1710	C1590	U1470	U1410	U1530	G1470	G1350	A1289	C1229	G1168	A1107	U1046	A866	C926	G867	C804	C744
C1711	U1591	C1471	C1411	C1531	G1471	G1351	A1290	C1230	C1169	U1108	G1047	G987	C927	U868	G805	C745
C1712	U1592	C1472	C1412	A1532	G1472	G1352	G1291	C1231	U1170	A1109	U1048	G988	G928	U868	A806	C746
C1713	C1593	G1473	U1413	G1533	U1473	A1353	A1292	U1232	A1171	G1110	U1049	G989	A929	C869	A807	A747
A1714	U1594	A1474	G1414	A1534	A1474	A1354	A1293	A1233	U1172	A990	C870	A930	G931	U871	C808	A748
A1715	A1595	U1475	C1415	C1535	U1475	A1355	G1294	C1234	G1173	A991	C871	A931	G932	C872	C809	C749
A1716	A1596	G1476	A1416	G1536	G1476	G1356	U1295	C1235	G1174	A992	C873	A932	G933	U873	U810	C750
C1717	C1597	C1477	C1417	U1537	G1477	U1357	U1296	G1236	A1175	C993	C874	C933	G934	C875	G811	G751
A1718	A1598	U1478	C1418	A1538	U1478	C1358	A1297	G1237	U1176	A994	A1055	A934	G935	A874	A812	G752
C1719	C1599	G1479	G1419	U1539	G1479	G1359	A1298	A1238	U1177	U1116	U1056	A935	C935	G875	A813	U753
C1720	G1600	G1480	A1420	C1540	G1480	G1360	A1299	G1239	C1178	G1117	A1057	C936	A936	A876	G814	G754
G1721	U1601	U1481	U1421	G1541	U1481	G1361	A1300	G1240	A1179	G1118	G1058	C937	C937	G877	A815	C755
C1722	G1602	U1482	C1422	G1542	U1482	A1362	U1301	G1241	A1180	C998	A1059	C938	G938	C878	U816	C756
U1723	A1603	G1483	A1423	G1543	G1483	C1363	C1302	A1242	C1181	A999	C1060	C939	G939	A879	A817	G757
C1724	A1604	A1484	U1424	A1544	G1484	C1364	U1303	G1243	U1182	C1000	A1061	G940	C940	C880	G818	G758
C1725	A1605	U1485	G1425	G1545	U1485	U1365	U1304	U1244	G1183	A1001	G1062	U941	U941	U881	C819	C759
C1726	A1606	A1486	U1426	G1546	A1486	A1366	C1305	G1245	C1185	C1002	C1063	C1002	U942	C882	U820	U760
C1727	A1607	C1487	G1427	U1547	C1487	G1367	U1306	G1246	G1125	C1064	C1064	U943	U943	A883	A821	G761
A1728	G1608	G1488	G1428	U1548	G1488	G1368	U1307	U1247	A1187	A1004	A1065	A1004	A944	C884	G822	A762
C1729	G1609	C1489	A1429	U1549	G1489	G1369	C1308	G1248	A1188	C1005	G1066	U945	G945	A885	U823	A763
G1730	A1610	U1490	U1430	C1550	U1490	C1370	G1309	G1249	G1189	C1006	A1067	C1006	U946	A886	U824	A764
C1731	U1611	A1491	U1431	U1551	G1491	C1371	C1310	A1250	C1190	A1007	A1068	C948	C947	C887	C825	A765
U1732	C1612	A1492	G1432	C1552	A1492	C1372	C1311	G1251	G1191	G1008	G1069	C949	G949	C888	U826	A766
U1733	G1613	A1493	A1433	G1553	A1493	G1373	G1312	C1252	A1192	C1009	G1070	C950	G950	C889	C827	G767
C1734	C1614	G1494	U1434	G1554	G1494	C1374	U1313	C1253	G1193	U1010	U1071	C951	C951	U890	C828	U768
C1735	C1615	G1495	G1435	A1555	G1495	U1375	U1194	G1254	U1194	A1011	U1072	A952	A952	A891	C829	C769
C1736	U1616	A1496	G1436	A1556	G1496	C1376	U1195	A1255	G1196	A1012	G1073	C953	C953	C	C830	U770
C1737	C1617	C1497	A1437	G1557	C1497	C1377	G1316	C1256	G1197	G1013	G1074	U954	U954	C	A832	C771
U1738	G1618	C1498	G1438	C1558	G1498	A1378	G1317	C1257	U1197	G1014	C1075	U954	U954	C	A833	C772
G1739	U1619	A1499	A1439	G1559	A1499	C1379	A1318	G1258	C1198	U1015	U1076	C955	C955	G	A834	C773
C1740	C1620	U1500	G1440	A1560	A1500	C1380	C1319	A1259	U1199	A1016	U1077	C956	C956	C	U835	A774
G1741	A1621	C1501	A1441	A1561	C1501	G1381	A1320	A1260	G1200	C1017	A1078	C957	C957	C	U836	U775
C1742	G1622	G1502	C1442	G1562	G1502	C1382	A1321	G1261	G1201	C1018	G1079	C958	C958	C	A842	G776
C1743	G1623	G1503	G1443	U1563	G1503	C1383	G1322	U1262	U1202	U1019	A1080	C959	C959	U	U837	A777
C1744	A1624	G1504	C1444	U1564	G1504	C1384	G1323	G1263	A1203	A1020	A1081	U960	U960	A	A838	C778
C1745	A1625	U1505	A1445	G1565	U1505	C1385	G1324	C1264	A1143	G1204	G1082	C961	C961	C	U839	U779
A1746	A1626	C1506	U1446	G1566	C1506	A1386	U1325	G1265	U1144	A1022	C1083	C962	C962	C	U840	U780
G1747	C1627	A1507	U1447	A1567	A1507	G1387	U1326	G1266	G1206	G1023	A1084	C963	C963	A	G841	G781
U1748	C1628	A1508	A1448	U1568	A1508	C1388	U1327	A1267	G1207	U1024	A964	G964	A964	G	A842	U782
C1749	U1629	A1509	A1449	A1569	A1509	C1389	G1329	U1268	A1268	A1025	C1085	C965	C965	C	G843	G783
A1750	U1630	A1510	G1450	C1570	A1510	G1390	G1330	G1269	G1148	U1026	C1086	A966	A966	U	G844	U784
A1751	G1631	A1511	C1451	G1571	A1511	A1391	G1331	C1270	G1149	C1027	A1088	C967	C967	U	U845	U785
U1752	C1632	U1512	U1452	C1572	U1512	U1392	G1332	C1271	G1211	G1028	C1089	C968	C968	A	A846	U786
A1753	C1633	U1513	A1453	G1573	U1513	G1393	G1333	G1272	U1212	C1029	C1090	C969	C969	C	C847	A787
C1754	A1634	U1514	U1454	C1574	U1514	G1394	A1334	G1273	U1213	U1030	U1091	C970	A970	C	A848	G788
G1755	C1635	U1515	A1455	C1575	U1515	A1395	A1335	G1274	C1152	C1032	U1092	U1030	A971	C	G849	G789
C1756	G1636	G1516	C1456	G1576	A1516	C1396	G1336	A1275	A1215	A1032	U1093	A1032	C972	A912	C850	A790

G26861	G26862	G26863	G26864	G26865	G26866	G26867	G26868	G26869	G26870	G26871	G26872	G26873	G26874	G26875	G26876	G26877	G26878	G26879	G26880	G26881	G26882	G26883	G26884	G26885	G26886	G26887	G26888	G26889	G26890	G26891	G26892	G26893	G26894	G26895	G26896	G26897	G26898	G26899	G26900	G26901	G26902	G26903	G26904	G26905	G26906	G26907	G26908	G26909	G26910	G26911	G26912	G26913	G26914	G26915	G26916	G26917	G26918	G26919	G26920	
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A2181	G2182	G2183	G2184	U2185	G2186	U2187	A2188	A2189	G2190	A2191	U2192	G2193	A2194	G2195	U2196	U2197	U2198	G2199	G2200	G2201	G2202	G2203	A2204	G2205	A2206	G2207	U2208	G2209	G2210	U2211	U2212	G2213	G2214	G2215	G2216	G2217	G2218	U2219	A2220	G2221	U2222	U2223	U2224	G2225	A2226	G2227	U2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	U2236	G2237	G2238	G2239	G2240	
U2121	G2122	G2123	G2124	G2125	U	U	U	U	G	U	G2132	G2133	U2134	G2135	G2136	G2137	U2138	G2139	G2140	A	G	G	C	A	A	C	U	U	U	G	U2091	U2092	A	G2093	G2094	G2095	U2096	G	G	A	U	U	A	G2103	G2104	U2105	G2106	G2107	G2108	A2109	G2110	C	C	U	G	G	A2117	A2118	A2119	G2120
A2060	G2061	U2062	A2063	U2064	A2065	G2066	U2067	G2068	U2069	G2070	G2071	G2072	U2073	U2074	U2075	G2076	G2077	A2078	U2079	U2080	U2081	G2082	G2083	G2084	G2085	U2086	U2087	U	U	U	G	U2092	A	G2093	G	G	A	U	U	A	G2103	G2104	U2105	G2106	G2107	G2108	A2109	G2110	C	C	U	G	G	A2117	A2118	A2119	G2120			
U2000	G2001	A2002	U2003	U2004	U2005	G2006	G2007	G2008	U2009	G2010	U2011	A2012	A2013	A2014	G2015	U2016	G2017	G2018	G2019	G2020	G2021	G2022	G2023	U2024	A2025	G2026	G2027	G2028	G2029	U2030	A2031	G2032	G2033	G2034	G2035	G2036	A2037	G2038	A2039	G2040	A2041	A2042	A2043	G2044	G2045	G2046	G2047	G2048	G2049	G2050	U2051	G2052	G2053	A2054	G2055	G2056	U2057	U2058	U2059	
C1940	C1941	G1942	A1943	C1944	G1945	U1946	G1947	G1948	A1949	G1950	G1951	A1952	A1953	G1954	G1955	G1956	G1957	U1958	U1959	A1960	A1961	G1962	G1963	A1964	U1965	G1966	U1967	G1968	G1969	G1970	C1971	G1972	U1973	U1974	G1975	U1976	C1977	G1978	A1979	A1980	A1981	G1982	G1983	G1984	G1985	G1986	G1987	A1988	C1989	U1990	G1991	G1992	G1993	U1994	G1995	A1996	A1997	A1998	U1999	
G1879	G1880	U1881	G1882	A1883	G1884	A1885	G1886	G1887	G1888	G1889	G1890	C1891	G1892	G1893	U1894	G1895	G1896	C1897	U1898	A1899	U1900	A1901	U	G1904	G1905	U1906	U1907	G1908	U1909	U1910	A1911	G1912	G1913	U1914	A1915	G1916	G1917	G1918	A1919	A1920	A1921	U1922	U1923	C1924	G1925	U1926	U1927	G1928	U1929	G1930	G1931	G1932	G1933	U1934	A1935	A1936	U1937	U1938	U1939	
G1818	U1819	G1820	C1821	G1822	G1823	G1824	G1825	U1826	G1827	C1828	G1829	C1830	G1831	G1832	U1833	A1834	G1835	G1836	G1837	U1838	A1839	A1840	G1841	G1842	U1843	G1844	A1845	A1846	G1847	U1848	G1849	G1850	A1851	G1852	C1853	G1854	G1855	G1856	G1857	C1858	A1859	A1860	G1861	C1862	G1863	G1864	C1865	G1866	A1867	A1868	C1869	U1870	G1871	A1872	U1873	G1874	C1875	G1876	C1877	G1878
C1767	C1768	G1769	U	G1763	G1764	A1765	C1766	U1767	G1768	U1769	U1770	A1771	C1772	U1773	A1774	A1775	A1776	A1777	U1778	U1779	C1780	C1781	G1782	U1783	G1784	A1785	A1786	G1787	U1788	U1789	U1790	C1791	C1792	U1793	U1794	A1795	A1796	C1797	G1798	A1799	A1800	C1801	A1802	G1803	U1804	G1805	G1806	A1807	C1808	G1809	U1810	A1811	U1812	A1813	G1814	G1815	C1816	C1817	G1818	

A2721	G2781	U2841
C2722	G2782	C2842
C2723	U2783	A2843
G2724	A2784	G2844
C2725	G2785	C2845
U2726	G2786	G2846
G2727	A2787	G2847
A2728	C2788	A2848
A2729	U2789	C2849
A2730	C2790	U2850
G2731	C2791	G2851
C2732	C2792	G2852
G2733	G2793	U2853
U2734	G2794	G2854
C2735	A2795	C2855
U2736	A2796	U2856
A2737	G2797	C2857
A2738	A2798	A2858
G2739	C2799	U2859
C2740	C2800	C2860
G2741	A2801	A2861
G2742	C2802	G2862
G2743	C2803	U2863
A2744	G2804	C2864
A2745	G2805	G2865
G2746	G2806	A2866
C2747	U2807	G2867
G2748	U2808	G2868
A2749	A2809	U2869
G2750	A2810	C2870
C2751	G2811	U2871
C2752	A2812	U2872
G2753	C2813	G2873
C2754	G2814	A2874
A2755	C2815	C2875
A2756	C2816	C2876
G2757	A2817	A2877
A2758	G2818	C
U2759	G2819	U
G2760	C2820	C
A2761	G2821	
C2762	U2822	
U2763	G2823	
U2764	C2824	
C2765	A2825	
U2766	C2826	
C2767	G2827	
C2768	C2828	
C2769	A2829	
A2770	U2830	
C2771	A2831	
U2772	G2832	
G2773	C2833	
U2774	A2834	
U	A2835	
U	U2836	
A	G2837	
U2778	U2838	
C2779	G2839	
A2780	U2840	

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

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	0.50	3/66467 (0.0%)	0.92	220/103673 (0.2%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	803	C	C3'-O3'	7.36	1.53	1.42
1	A	2589	C	C3'-O3'	5.48	1.50	1.42
1	A	2589	C	C3'-C2'	-5.02	1.45	1.52

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2588	U	O3'-P-O5'	13.90	124.85	104.00
1	A	2810	A	N9-C1'-C2'	12.15	132.22	114.00
1	A	803	C	P-O5'-C5'	-10.79	104.71	120.90
1	A	985	G	N9-C1'-C2'	10.22	129.33	114.00
1	A	1249	G	C2'-C3'-O3'	10.14	124.70	109.50

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	765	C	C1'

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Mol	Chain	Res	Type	Atom
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	6917	0
2	A	69	0	80	8	0
All	All	59428	0	29997	6919	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 6919 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	2758/2880 (95%)	857 (31%)	190 (6%)

5 of 857 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	1723	U
1	A	2204	A
1	A	1775	A
1	A	1947	G
1	A	2323	U

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 oligosaccharides 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	-	72,74,74	2.60	27 (37%)	102,111,111	2.77	38 (37%)

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	-	-	13/80/134/134	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	C40-N2	6.96	1.57	1.46
2	A	2881	RU6	C46-C45	6.59	1.57	1.47
2	A	2881	RU6	C10-C9	-5.93	1.43	1.52
2	A	2881	RU6	C47-C46	5.47	1.47	1.39
2	A	2881	RU6	C4-C5	5.22	1.67	1.54

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	RU6	O13-C39-N2	-11.89	100.40	109.86
2	A	2881	RU6	O13-C12-C11	-7.44	95.70	103.28
2	A	2881	RU6	N3-C44-N4	-6.69	107.01	112.35
2	A	2881	RU6	O12-C39-N2	6.63	136.85	128.08
2	A	2881	RU6	C6-C7-C8	6.45	126.61	116.10

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

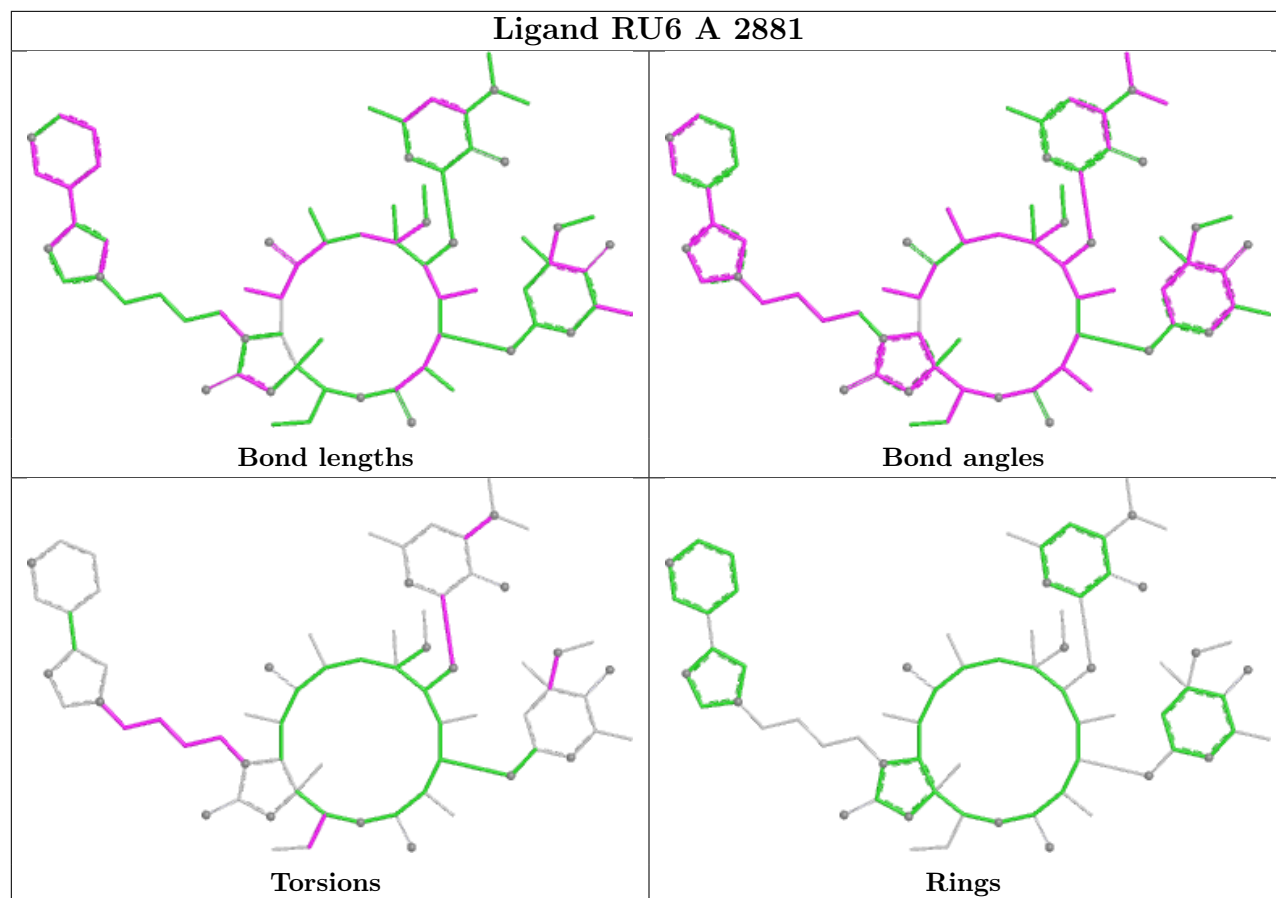
Mol	Chain	Res	Type	Atoms
2	A	2881	RU6	C17-C16-O5-C20
2	A	2881	RU6	C41-C40-N2-C11
2	A	2881	RU6	C40-C41-C42-C43
2	A	2881	RU6	C41-C42-C43-N3
2	A	2881	RU6	N2-C40-C41-C42

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.