



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:46 AM 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 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 (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

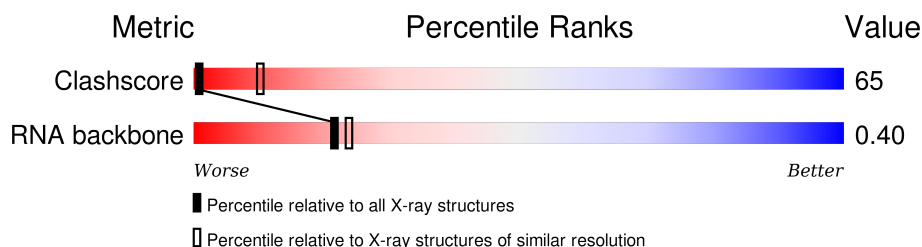
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	102246	1010 (3.74-3.46)
RNA backbone	2183	1058 (4.40-2.80)

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 ≥ 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ERN	A	2881	-	-	X	-

2 Entry composition [i](#)

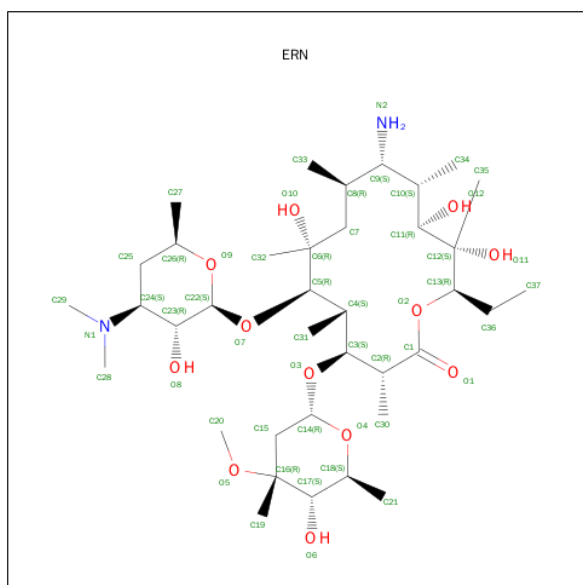
There are 2 unique types of molecules in this entry. The entry contains 59410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (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: C₃₇H₇₀N₂O₁₂).



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

A1596	G1536	U1475	G1414	G1352	A1288	A1227	A1166	C1103	G1041	G980	U919	G858	A796	G736	G676
A1597	U1537	G1476	G1415	A1353	A1289	G1228	A1167	G1104	G1042	C981	A922	U859	A797	C737	G677
A1598	A1538	C1477	A1416	A1354	A1290	C1229	G1168	U1105	A1043	C982	A923	U860	A798	C738	G678
G1599	U1539	U1478	G1417	A1355	G1291	C1230	C1169	A1066	U1044	G983	A924	G861	C799	G739	C679
U1600	U1601	G1479	G1418	G1356	A1292	A1231	A1170	U1107	G1045	A984	C924	A862	U800	A740	U680
G1601	G1541	G1480	G1419	U1357	A1293	U1232	A1171	U1108	U1046	G985	U925	G863	A801	G741	A681
G1602	G1542	U1481	A1420	C1358	G1294	A1233	U1172	A1109	G1047	A986	C926	C864	A802	G742	G682
A1603	G1543	U1482	U1421	G1359	G1298	C1234	G1173	G1110	U1048	A987	C927	A865	C803	A743	A683
A1604	A1544	G1483	G1422	G1360	U1299	C1235	G1174	C1111	U1049	G988	C928	U866	C804	C744	C684
A1605	G1545	G1484	A1423	G1361	A1300	G1236	A1175	U1112	G1053	A991	A929	U867	A805	C745	U685
C1606	U1546	U1485	U1424	A1362	U1301	G1237	U1176	C1113	A1054	A992	A930	U868	A806	G746	C686
A1607	U1547	G1486	G1425	G1363	U1302	A1238	U1177	A1114	C1054	A993	G931	C869	A807	A747	G687
U1608	C1487	C1487	U1426	C1364	C1302	A1239	C1178	C1115	A1055	C993	G932	C870	C808	A748	A688
G1609	C1549	G1488	G1427	U1365	U1303	G1240	A1179	U1116	U1056	A994	G933	U871	C809	C749	A689
U1610	U1550	G1489	G1428	A1366	U1304	G1241	A1180	G1117	A1057	A995	G934	G872	U810	C750	A690
A1611	U1551	U1490	A1429	A1367	C1305	A1242	C1181	G1118	U1058	C996	C935	U873	G811	G751	C691
U1612	C1552	C1491	G1430	G1368	U1306	G1243	U1182	U1119	A1059	C997	A936	A874	G812	G752	C692
G1613	G1553	A1492	G1431	G1369	G1309	U1244	C1183	C1120	C1060	C998	C937	G875	A813	G753	A693
C1614	G1554	G1493	A1432	G1371	G1310	G1245	G1184	G1121	A1061	A999	G938	A876	G814	G754	G694
C1615	A1555	A1494	A1433	A1372	C1310	G1246	C1185	A1122	G1062	G1000	C939	G877	A815	C755	G695
C1616	U1556	G1496	U1434	G1373	C1311	U1247	G1186	G1123	C1063	A1001	G940	C878	U816	G756	G696
G1617	C1497	G1497	G1435	G1374	U1312	G1248	A1187	U1124	A1064	C1002	U941	A879	A817	U757	G697
U1618	C1558	G1498	G1436	C1375	G1313	G1249	A1188	G1125	A1065	C1003	U942	C880	G818	G758	A698
A1619	U1559	A1499	A1437	G1376	A1314	A1250	G1189	A1126	G1066	A1004	U943	U881	C819	G759	G699
C1620	U1560	U1500	G1438	C1377	A1315	G1251	C1190	C1127	G1067	U1005	A944	C882	U820	U760	C700
C1621	A1561	C1501	G1439	A1378	G1316	C1252	G1191	G1128	A1068	C1006	G945	A883	A821	G761	U701
G1622	U1562	G1502	G1440	A1379	G1317	C1253	A1192	G1129	G1069	A1007	U946	C884	G822	A762	A702
C1623	G1563	G1503	A1441	C1380	G1318	G1254	G1193	U1130	G1070	C1008	C947	A885	U823	A763	A703
A1624	U1564	G1504	G1442	G1381	C1319	A1255	U1194	G1131	U1071	C1009	C948	A886	U824	A764	G704
A1625	G1565	U1505	G1443	G1382	U1320	C1256	U1195	C1132	U1072	U1010	G949	G887	C825	C765	C705
A1626	G1566	C1506	C1444	C1383	A1320	U1257	G1196	G1142	G1073	A1011	G950	G888	U826	A766	A706
C1627	A1567	A1507	A1445	G1384	G1323	G1258	U1197	G1135	G1074	A1012	G951	C889	C827	G767	U707
C1628	A1568	G1508	U1446	C1385	G1324	A1259	C1198	G1136	C1075	A1013	A952	U890	C828	G768	G708
G1629	A1569	A1509	C1449	A1386	U1325	A1260	U1199	A1137	U1076	G1014	G953	A891	C829	C769	A709
A1630	C1570	U1510	G1450	G1387	A1326	G1261	G1200	U1138	U1077	U1015	U954	G	C830	U770	C710
C1631	G1571	A1511	G1451	C1388	C1327	U1262	G1201	A1139	A1078	C1016	G955	G	8831	C771	C711
A1632	C1572	A1512	C1451	C1389	G1328	G1263	U1202	A1140	A1079	C1017	A956	G	A832	A712	A712
C1633	G1573	U1513	U1452	G1390	U1329	C1264	A1203	U1141	A1080	C1018	G957	G	A833	G772	G713
A1634	A1574	C1514	A1453	A1391	G1330	G1265	G1204	U1142	A1081	U1019	G958	G	A834	G773	G713
G1635	C1575	U1515	U1454	U1392	G1331	A1266	G1205	G1082	A1082	A1020	C959	C	U835	A774	G714
G1636	G1576	A1516	C1455	G1393	G1332	A1267	G1206	C1083	U1084	A1021	U960	C	U836	A775	U715
U1637	G1577	C1517	C1456	G1394	G1333	U1268	G1206	G1146	G1085	A1022	G961	U	U837	A776	U716
C1638	U1578	G1518	A1457	A1395	G1334	G1269	G1207	G1147	G1086	U1023	C962	A	A838	A777	G717
C1639	G1579	U1519	A1458	C1396	A1335	C1270	G1210	G1148	C1087	U1024	G963	C	U839	G778	A718
C1640	C1580	G1520	U1459	A1397	G1336	C1271	C1217	G1156	G1088	C1031	A970	A	U840	U779	A719
G1641	C1581	U1521	G1460	G1398	G1337	G1272	U1212	G1157	A1089	A1032	A971	C	C841	U780	A720
A1643	A1582	C1522	C1461	C1399	U1338	G1273	U1213	U1151	C1089	U1026	G965	A	A842	C721	C721
G1644	A1583	A1523	C1462	U1339	U1339	C1274	C1214	C1152	C1089	C1027	A966	G	A843	U782	C722
U1645	U1645	C1524	A1463	G1401	C1340	A1275	A1215	A1154	C1090	G1028	G967	C	G843	G783	C723
G1646	A1585	A1525	A1464	G1402	G1341	G1275	G1216	G1155	U1091	C1029	C968	U	U844	G784	C724
U1647	A1586	U1526	G1465	U1403	U1342	A1278	U1217	U1156	U1092	U1030	U969	U	U845	U785	C725
C1648	A1587	G1527	C1466	C1404	U1343	G1279	U1218	G1157	U1093	C1031	A970	A	A846	U786	G726
A1649	U1588	C1528	U1467	G1407	U1280	U1280	C1219	G1157	C1094	A1032	A971	C	C847	A787	U727
A1650	G1589	C1529	A1468	G1345	G1345	A1281	G1220	U1158	A1095	U1033	C972	C	A848	G788	G728
U1651	C1590	U1530	U1469	C1346	C1346	A1282	G1221	C1160	A1096	U1034	U973	A911	G849	G789	A729
G1652	U1531	C1531	G1470	U1409	C1347	C1283	C1222	U1161	A1097	G1035	U974	A912	C850	G790	C730
C1653	U1532	A1532	G1471	U1410	C1348	G1284	G1223	A1162	A1098	G1036	C975	A913	C851	G791	A731
C1654	C1533	U1533	C1472	C1411	A1349	A1285	A1224	A1163	A1099	U1037	G976	U	U852	U792	G732
C1655	U1534	A1534	G1473	C1412	G1350	U1286	A1225	C1163	G1100	U1038	G977	U916	C853	G793	G733
U1656	A1595	C1535	A1474	U1413	G1351	A1287	A1226	G1165	G1102	A1040	A979	A918	U857	A795	G735

U2572	A2512	U2452	C2329	A2267	C2205	G2084	U2024	G1963	G1842	G1780	G1719	A1657
C2573	A2513	C2453	G2330	G2268	C2206	G2085	A2025	A1964	U1843	C1781	G1720	A1658
G2574	G2514	C2454	A2331	G2269	G2207	U2086	C2026	U1965	C1844	A1782	G1721	G1659
U2575	G2515	A2455	G2332	U2270	U2208	U2087	C2027	C1966	A1845	G1722	G1722	G1660
G2576	U2516	C2456	C2333	C2271	G2209	U2088	C2028	U1967	G1846	A1785	U1723	C1661
U2577	C2517	C2457	C2334	A2272	U2212	C2089	G2029	G1968	U1847	G1786	G1724	G1664
G2578	C2518	U2458	U2335	C2273	U2213	U2090	U2030	U1969	U1848	U1787	G1725	G1665
A2579	C2519	C2459	A2337	C2274	G2214	C2091	A2031	G1970	G1849	C1788	C1726	G1666
C2580	A2520	G2460	G2338	U2275	G2215	U2092	G2032	G1971	G1850	U1789	G1727	G1667
A2581	A2521	C2461	C2339	C2276	C2216	G2093	C2033	C1973	A1851	G1790	A1728	A1667
G2582	G2522	U2462	A2339	A2277	A2094	G2094	A2034	U1974	G1852	C1791	G1729	G1668
U2583	G2523	C2463	C2340	G2278	G2217	U2095	G2035	G1975	C1853	C1792	G1730	A1669
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C2585	U2525	G2465	C2342	G2280	U2219	A2097	A2037	C1977	G1855	A1794	U1732	A1671
U2586	G2526	G2466	G2343	C2281	A2220	G	C2038	U1978	U1856	C1795	U1732	A1672
G2587	G2527	A2467	A2345	G2282	G2221	G	C2039	C1979	U1857	C1796	G1733	C1673
U2588	C2528	U2468	G2346	C2283	U2222	U	A2040	A1980	G1858	C1797	G1734	C1674
C2589	G2529	G2469	C2347	U2284	C2223	A	A2041	A1981	A1859	G1798	G1735	C1675
U2590	U2409	U2470	A2348	U2285	U2224	A	A2042	C1982	A1860	A1799	G1737	U1676
C2591	U2531	U2471	G2349	G2286	G2225	G2103	A2043	G1983	G1861	A1800	U1738	C1677
U2592	G2532	A2472	G2350	G2287	A2226	G2104	C2044	U1984	C1862	C1801	U1739	G1678
A2593	U2533	C2473	G2351	A2288	C2227	U2105	A2045	G1985	U1863	A1802	G1740	U1679
U2594	G2534	G2474	A2352	A2289	U2228	G2106	C2046	G1986	G1864	G1803	G1741	U1680
C2595	C2535	C2475	G2353	U2290	G2229	G2107	C2047	G1987	C1865	U1804	G1742	A1681
G2596	G2536	A2476	G2354	U2291	G2230	U2108	C2048	A1988	G1866	G1805	C1744	A1682
C2597	C2537	C2477	A2355	C2292	G2231	A2109	C2049	C1989	A1867	G1806	C1745	G1683
U2598	C2538	C2478	A2356	G2293	G2232	G2110	G2050	U1990	A1868	A1807	G1746	G1684
C2599	G2539	U2479	A2357	U2294	C2233	C	U2051	C1991	A1869	C1808	G1747	A1685
G2600	A2540	C2480	C2358	C2295	G2234	U	G2052	G1992	U1870	G1809	U1748	A1686
U2601	U2541	G2481	U2359	U2296	G2235	G2173	G2053	G1993	G1871	G1810	G1749	C1687
C2602	U2542	A2482	C2360	G2297	U2236	G2174	A2054	U1994	A1872	A1811	U1750	U1688
G2603	A2543	U2483	G2361	U2298	C2237	C	G2055	G1995	A1873	U1812	A1751	U1689
C2607	A2544	G2484	G2362	A2299	G2238	G	C2056	A1996	C1874	A1813	U1752	U1690
U2608	A2545	U2485	G2363	G2300	C2239	A2117	U2057	A1997	C1875	G1814	G1753	G1691
G2609	C2546	G2486	C2364	A2301	U2240	A2118	U2058	A1998	C1876	G1815	G1754	C1692
U2610	C2547	U2487	U2365	G2302	U2241	C2179	U2059	U1999	C1877	G1816	G1755	A1693
A2611	G2548	C2488	U2366	C2303	C2242	U2180	A2060	U2000	C1878	U1817	G1756	A1694
C2612	G2549	C2489	A2367	A2306	C2243	U2121	C2061	G2001	G1879	G1818	C1757	U1695
A2613	C2550	U2490	G2368	A2307	C2244	G2122	U2062	A2002	U1880	U1819	G1758	C1696
G2614	A2551	C2491	U2369	A2308	C2245	G2123	A2063	A2003	U1881	G1820	A1759	U1697
U2615	C2552	U2492	G2370	G2309	A2246	U2064	U2064	U2004	G1882	G1760	C1759	C1698
G2616	G2553	U2493	A2371	G2310	U2247	C2124	A2065	U2005	A1883	G1761	C1761	A1699
C2617	C2554	G2494	A2372	U2311	A2248	C2125	G2066	G2006	A1884	C1762	C1762	C1700
A2618	G2555	U2495	C2373	A2312	U	U	U2067	G2007	C1885	C1824	G1763	C1701
G2619	A2556	C2496	U2374	G2313	U2251	U	C2068	C2008	G1886	U1826	A1764	G1704
C2620	C2557	U2497	A2376	A2314	A2252	U	U2069	C2009	G1887	G1827	C1765	U1705
G2621	U2558	U2498	U2377	A2315	A2253	A2191	G2070	G2010	C1888	C1828	U1766	A1706
C2622	C2559	C2499	G2378	G2316	C2254	U2192	G2071	C1950	C1889	C1829	G1767	A1707
A2623	G2560	U2500	G2379	G2317	G2255	C2193	C2072	A2012	G1890	C1830	U1768	C1708
C2624	C2561	U2501	U2380	U2318	G2256	G2133	A2073	A2013	C1891	G1831	U1769	U1709
U2625	U2562	G2502	A2381	G2319	A2257	U2134	U2074	A2014	C1892	G1832	U1770	U1710
G2626	G2563	C2503	C2382	G2320	C2258	C2195	U2075	G2015	U1893	U1833	A1771	C1711
C2627	U2564	U2504	C2383	C2321	G2259	C2196	G2076	A2016	A1895	G1834	C1772	C1712
G2628	C2565	G2505	G2384	U2322	C2260	U2197	G2077	U2017	A1896	C1835	C1773	G1713
U2629	A2566	C2506	U2385	G2323	C2261	C2198	G2078	C2018	C1897	C1836	A1774	A1714
C2630	G2567	U2507	G2386	U2324	C2262	C2199	A2079	C2019	G1898	G1837	U1775	G1715
G2631	A2568	U2508	U2387	A2325	C2263	G2200	U2080	G2020	A1899	G1838	A1776	A1716
U2632	C2569	G2509	G2388	C2326	C2264	G2201	U2081	G2021	U1900	A1839	U1777	G1717
A2633	U2570	A2510	G2389	U2327	C2265	G2202	C2082	C2022	A1901	A1840	U1778	A1717
C2634	G2571	G2511	A2390	A2328	A2266	A2204	G2083	C2023	A1902	G1841	C1779	A1718

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	C2703	G2643
A2829	U2766	U2704	A2644
U2830	C2767	A2705	C2645
A2831	C2768	U2706	C2646
G2832	G2769	G2707	G2647
C2833	A2770	U2708	G2648
A2834	C2771	C2709	A2649
A2835	U2772	G2710	G2650
U2836	U2773	G2711	U2651
G2837	U2774	G2712	G2652
U2838	U2775	A2713	A2653
G2839	U2776	A2714	A2654
U2840	A2777	C2715	G2655
U2841	U2778	G2716	G2656
C2842	C2779	G2717	G2657
A2843	G2780		A2658
G2844	G2781	A2720	C2659
C2845	G2782	A2721	C2660
G2846	U2783	C2722	G2661
G2847	A2784		C2662
A2848	A2785	C2725	U2663
C2849	G2786	U2726	G2664
U2850	A2787	G2727	G2665
G2851	C2788	G2728	U2666
G2852	U2789	A2729	C2667
U2853		U2730	U2668
G2854	G2793	G2731	C2669
C2855	G2794	C2732	C2670
U2856	A2795	A2733	G2671
C2857	G2796	U2734	U2672
A2858	G2797	C2735	G2673
U2859	A2798	U2736	C2674
C2860	C2799	A2737	U2675
A2861	C2800	A2738	G2676
G2862	A2801	G2739	U2677
U2863	C2802	C2740	C2678
C2864	C2803	G2741	G2679
G2865	G2804	G2742	U2680
A2866	G2805	G2743	A2681
G2867	U2806	A2744	C2682
G2868	U2807	A2745	C2683
U2869	U2808	G2746	A2684
C2870	A2809	C2747	A2685
U2871	G2810	C2748	C2686
U2872	U2811	A2749	G2687
G2873	A2812	G2750	G2688
A2874	G2813	C2751	C2689
G2875	G2814	G2752	A2690
C2876	C2815	C2753	C2691
A2877	C2816	G2754	A2692
C	G2817	U2755	U2693
U	G2818	G2819	G2694

C

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	170.44Å 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 ²)	71.0	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: 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 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	5720	0
2	A	51	0	70	41	0
All	All	59410	0	29987	5744	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 65.

The worst 5 of 5744 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)
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 [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%)	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 [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

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	ERN	A	2881	-	52,53,53	4.54	36 (69%)	75,82,82	4.00	34 (45%)

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	ERN	A	2881	-	-	3/72/107/107	0/2/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	ERN	C7-C6	-2.21	1.50	1.54
2	A	2881	ERN	O10-C6	2.04	1.48	1.44
2	A	2881	ERN	O9-C26	2.06	1.48	1.44
2	A	2881	ERN	O4-C14	2.13	1.47	1.42
2	A	2881	ERN	O3-C14	2.22	1.47	1.41

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	ERN	O1-C1-C2	-11.14	96.46	124.22
2	A	2881	ERN	C35-C12-C11	-8.11	99.79	113.28
2	A	2881	ERN	O10-C6-C5	-7.60	93.26	107.59
2	A	2881	ERN	C33-C8-C7	-7.59	93.45	112.47
2	A	2881	ERN	O5-C16-C15	-5.72	103.83	113.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2881	ERN	C10-C11-C12-C13
2	A	2881	ERN	C20-O5-C16-C17
2	A	2881	ERN	O12-C11-C12-O11

There are no ring outliers.

1 monomer is involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2881	ERN	41	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 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.