



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2023 – 07:27 AM EDT

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.

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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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

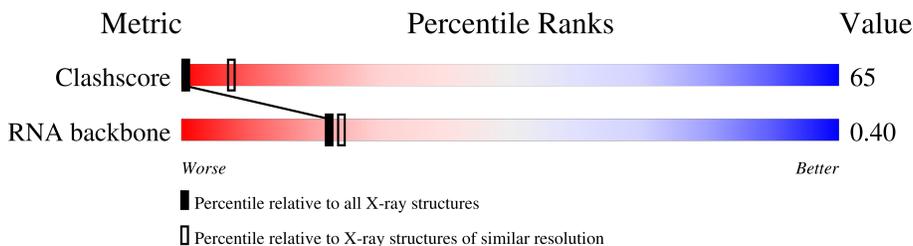
1 Overall quality at a glance

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	141614	1353 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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	8% 58% 25% 5%

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	X	-

2 Entry composition [i](#)

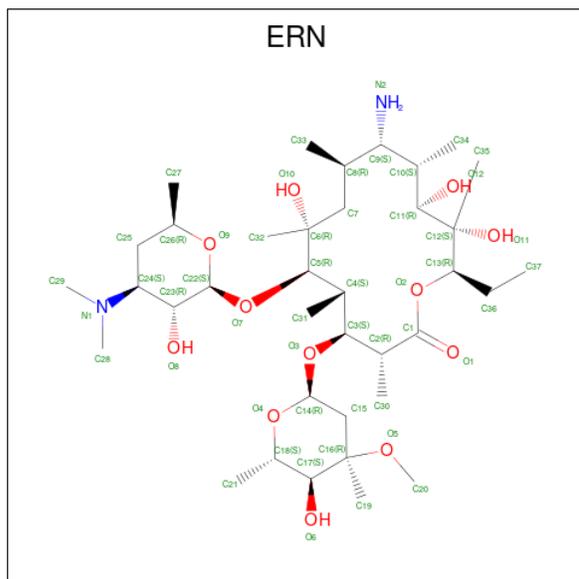
There are 2 unique types of molecules in this entry. The entry contains 59410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-HEXAMETHYLOXACYCLOTETRADECAN-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	A1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	U1656																					
U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596																					
G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474																						
G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1407	G1408	G1409	G1410	G1411	G1412	G1413																					
U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535																				
G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226
A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1351	A1352	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287														
A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287																				
A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226																						
C1103	C1104	C1105	C1106	C1107	C1108	C1109	C1110	C1111	C1112	C1113	C1114	C1115	C1116	C1117	C1118	C1119	C1120	C1121	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1129	C1130	C1131	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139	C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	C1164	C1165																		
G1041	G1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102																			
U919	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979																						
G858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920																		
U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856																				
G736	C737	G738	G739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795																					

A2512	U2452	A2391	C2329	A2267	C2205	G2084	U2024	G1963	C1903	G1842	A1780	G1719	A1657
A2513	C2453	G2392	G2350	G2268	G2206	G2085	A2025	A1964	G1904	U1843	C1781	G1720	A1658
G2514	G2454	G2393	A2331	G2269	G2207	U2086	C2026	U1965	G1905	C1844	A1782	G1721	G1659
G2515	A2455	G2394	G2332	U2270	C2208	U2087	C2027	U1966	U1906	A1845	G1722	G1722	G1660
U2516	G2456	C2395	A2333	C2271	G2209	U2088	G2028	U1967	C1907	A1846	A1785	U1723	C1661
C2517	A2457	C2396	G2334	A2272	G	C2089	C2029	U1968	C1908	G1847	A1786	C1724	G1664
C2518	U2458	A2397	U2335	C2273	U	U2090	U2030	G1969	U1909	U1787	C1725	C1725	C1665
C2519	C2459	C2398	A2336	U2274	G	C2091	A2031	U1970	A1910	C1788	C1726	G1726	G1666
A2520	G2460	C2399	A2337	C2275	U	U2092	G2032	G	A1911	U1789	U1789	C1727	C1667
A2521	G2461	C2400	C2338	C2276	A	G2093	C2033	C1973	G1912	A1851	A1728	A1728	A1667
G2522	G2462	A2401	A2339	A2277	A	C2094	A2034	U1974	G1913	G1852	C1791	C1729	G1668
G2523	G2463	G2402	C2340	G2278	A	G2095	G2035	G1975	G1914	G1853	G1792	G1730	A1669
G2524	G2464	C2403	C2340	G2279	U	U2096	G2036	U1976	A1915	G1854	A1793	C1731	G1670
U2525	G2465	A2404	C2343	A2280	C2187	A2097	A2037	C1977	G1916	G1855	A1794	U1732	A1671
U2526	G2466	A2405	G2344	A2220	C2188	G	C2038	U1978	C1917	U1856	C1795	U1733	A1672
G2527	A2467	C2406	A2345	G2221	A	G	G2039	C1979	G1918	U1857	A1796	C1734	A1673
G2528	G2468	G2407	G2346	U2222	C2189	A	C2040	U1980	A1919	C1858	C1797	G1735	C1674
G2529	G2469	G2408	C2347	U2223	C2190	U	A2041	A1981	A1920	A1859	G1798	G1736	G1675
G2530	U2470	A2409	A2348	U2224	C2191	A	A2042	U1982	A1921	A1860	A1799	G1737	U1676
U2531	U2471	U2410	G2349	G2225	U2163	G2103	C2043	C1983	U1922	A1800	A1800	U1738	C1677
U2532	U2472	A2411	G2350	G2226	G2164	G2104	G2044	A1984	U1923	C1861	C1801	G1739	G1678
U2533	G2473	A2412	A2351	U2227	G2165	U2105	A2045	G1985	C1924	A1863	A1802	G1740	U1679
U2534	G2474	G	A2352	U2228	G2166	G2106	C2046	G1986	C1925	U1864	G1803	G1741	U1680
G2535	C2475	G2415	A2353	U2229	A2167	G2107	C2047	G1987	C1926	G1865	U1804	U1681	A1681
G2536	A2476	U2416	G2354	G2230	A2168	G2108	C2048	A1988	U1927	G1866	G1805	G1744	A1682
C2537	C2477	U2417	A2355	G2231	A2169	A2109	C2049	C1989	G1928	A1867	G1806	C1745	G1683
C2538	C2478	A2418	A2356	G2232	C2170	G2110	G2050	U1990	U1929	A1868	A1807	A1746	G1684
C2539	U2479	C2419	A2357	G2233	C2171	C	U2051	C1991	C1930	A1869	C1808	G1747	A1685
U2540	C2480	G2420	C2358	G2234	U2172	C	G2052	G1992	G1931	A1870	U1748	U1748	A1686
U2541	G2481	C2421	U2359	G2235	G2173	U	G2053	G1993	G1932	G1871	G1809	G1749	C1687
U2542	A2482	C2422	G2360	U2236	C2174	C	A2054	U1994	G1933	A1872	A1811	A1750	U1688
U2543	U2483	G2423	G2361	G2237	A2175	G	C2055	C1995	U1934	A1873	U1812	A1751	U1689
A2544	G2484	G2424	G2362	G2238	U2176	C	C2056	A1996	A1935	G1874	A1813	U1752	U1690
A2545	U2485	G2425	G2363	C2239	U2177	A2117	U2057	A1997	A1936	C1875	A1814	U1753	C1691
C2546	C2486	A2426	G2364	C2240	C2179	A2118	U2058	A1998	G1937	C1876	G1815	G1754	G1692
G2547	G2487	U2427	U2365	U2241	C2179	A2119	U2059	U1999	U1938	C1877	G1816	G1755	A1693
G2548	G2488	U2428	U2366	C2242	U2180	C2120	A2060	U2000	U1939	C1878	U1817	G1756	A1694
G2549	C2489	A2429	A2367	C2243	A2181	U2121	C2061	G2001	C1940	G1879	G1818	C1757	U1695
C2550	U2490	A2430	G2368	C2244	A2182	G2122	U2062	C2008	C1941	G1880	U1819	C1758	U1696
C2551	C2491	C2431	U2369	A2245	C2183	G2123	A2063	A2003	G1942	U1881	G1820	A1769	U1697
C2552	G2492	A2432	G2370	A2246	C2184	C2124	U2064	U2004	A1943	G1882	G1760	G1760	C1698
C2553	U2493	G2433	A2371	A2247	U2185	C2125	A2065	U2005	C1944	A1883	G1761	G1761	A1699
C2554	G2494	G2434	A2372	A2248	G2186	U	G2066	G2006	U1945	A1884	C1762	C1762	C1700
G2555	G2495	C2435	C2373	U2251	A2189	U	U2067	G2007	U1946	C1825	C1824	G1763	C1701
A2556	C2496	U2436	G	U2252	A2190	U	C2068	C2008	G1947	G1826	U1826	A1764	G1704
G2557	A2497	G2437	G2376	A2253	A2190	U	U2069	U2009	C1948	G1827	G1827	C1765	G1704
C2558	U2498	A2438	U2377	A2254	A2191	G	U2070	G2010	A1949	C1828	U1766	C1765	U1705
U2559	C2499	G2439	G2378	G2255	U2192	C	G2071	U2011	A1950	G1888	G1767	C1772	U1706
G2560	C2500	C2440	G2379	G2256	C2193	G2132	C2072	A2012	G1951	G1890	C1830	G1768	A1707
G2561	U2501	U2441	U2380	G2257	A2194	G2133	A2073	A2013	A1952	C1891	G1831	U1769	C1708
G2562	G2502	C2442	A2381	A2258	C2195	U2134	U2074	A2014	A1953	C1892	G1832	U1770	U1709
U2563	G2503	C2443	C2382	G2259	U2196	C2135	U2075	G2015	A1954	G	U1833	A1771	U1710
G2564	G2504	C2444	G2383	C2260	U2197	G2136	G2076	A2016	G1955	A1895	U1834	C1772	U1711
G2565	G2505	C2445	G2384	G2261	U2198	G2137	G2077	A2017	G1956	A1896	C1835	C1773	G1712
A2566	C2506	C2446	U2385	G2262	C2199	U2138	G2078	G2018	C1957	C1897	C1836	A1774	G1713
G2567	U2507	G2447	G2386	C2263	G2200	U2139	A2079	G2019	G1958	C1837	G1837	A1775	A1714
A2568	G2508	A2448	U2387	C2264	G2201	G2140	U2080	G2020	U1959	A1899	G1838	A1776	A1715
A2569	A2509	G2449	G2388	C2265	G2202	A	C2081	G2021	A1960	U1900	A1839	A1777	G1716
C2570	U2510	U2327	G2389	A2266	G2203	G	C2082	C2022	A1961	U1901	A1840	A1778	G1717
G2571	G2511	A2267	A2390	A2266	A2204	C	G2083	C2023	C1962	A1902	G1841	C1779	A1718

C	C2820	G2757	C2695	U2635	U2572
	G2821	A2758	A2696	A2636	C2573
	U2822	U2759	G2697	G2637	G2608
	G2823	G2760	G2698	G2638	G2609
	C2824	A2761	G2699	A2639	G2610
	A2825	G2762	U2700	G2640	A2611
	C2826	U2763	A2701	A2641	G2612
	G2827	U2764	G2702	G2642	A2613
	C2828	C2765	C2703	G2643	A2614
	A2829	U2766	U2704	G2644	U2615
	U2830	C2767	A2705	A2644	G2616
	A2831	U2768	U2706	C2645	G2617
	G2832	C2769	G2707	G2646	A2618
	C2833	A2770	U2708	U2647	G2619
	A2834	C2771	C2709	G2648	G2620
	U2835	G2772	G2710	A2649	A2621
	U2836	U2773	G2711	G2650	G2622
	G2837	U	G2712	U2651	U2623
	U2838	U	A2713	G2652	G2624
	G2839	A	A2714	A2653	U2625
	U2840	U2778	C2715	G2654	A2626
	U2841	C2779	G2716	C2655	G2627
	C2842	A2780	G2717	G2656	G2628
	A2843	G2781	U2720	U2657	U2629
	G2844	G2782	A2721	A2658	C2630
	C2845	U2783	C2722	C2659	G2631
	G2846	A2784	U2725	G2660	U2632
	U2847	A2785	U2726	G2661	A2633
	C2848	G2786	G2727	U2662	G2634
	U2849	A2787	U2728	U2663	
	G2850	C2788	A2729	G2664	G2604
	C2851	U2789	A2730	G2665	G2605
	G2852	G2793	U2731	U2666	G2606
	U2853	G2794	G2732	C2667	C2607
	G2854	A2795	U2733	U2668	A2608
	C2855	U2796	U2734	G2669	G2609
	U2856	G2797	C2735	G2670	G2610
	C2857	A2798	U2736	C2671	A2611
	A2858	C2799	A2737	U2672	G2612
	U2859	G2800	U2738	G2673	A2613
	C2860	A2801	A2739	G2674	A2614
	G2861	C2802	G2740	U2675	U2615
	U2862	G2803	G2741	G2676	G2616
	C2863	G2804	G2742	U2677	G2617
	G2864	G2805	A2743	G2678	A2618
	A2865	G2806	U2744	G2679	G2619
	U2866	U2807	A2745	U2680	G2620
	G2867	U2808	G2746	A2681	G2621
	U2868	A2809	C2747	C2682	G2622
	U2869	U2810	U2748	C2683	A2623
	C2870	G2811	A2749	A2684	G2624
	U2871	A2812	G2750	A2685	U2625
	U2872	G2813	C2751	G2686	U2626
	G2873	G2814	U2752	G2687	G2627
	A2874	U2815	C2753	G2688	C2628
	C2875	G2816	U2754	C2689	U2629
	C2876	A2817	A2755	A2690	C2630
	A2877	G2818	G2819	G2691	C2631
	C	U		U2692	U2632
	U			A2693	A2633
				G2694	G2634

4 Data and refinement statistics

Xtrriage (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	170.44Å 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.	Xtrriage
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 [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	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	1698	C
1	A	2093	G
1	A	1733	U
1	A	1953	A
1	A	2261	G

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 monosaccharides 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	4.69	36 (69%)	77,82,82	3.83	35 (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	-	-	29/72/107/107	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	C10-C11	13.83	1.76	1.55
2	A	2881	ERN	C7-C8	11.42	1.70	1.54
2	A	2881	ERN	C6-C5	10.55	1.76	1.55
2	A	2881	ERN	C4-C5	10.53	1.80	1.55
2	A	2881	ERN	C8-C9	7.28	1.70	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	ERN	O2-C1-C2	13.92	142.12	111.56
2	A	2881	ERN	C13-O2-C1	11.53	138.67	118.18
2	A	2881	ERN	O1-C1-C2	-10.33	96.46	124.08
2	A	2881	ERN	C33-C8-C7	-8.36	93.45	112.45
2	A	2881	ERN	C7-C6-C5	8.01	126.12	110.48

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

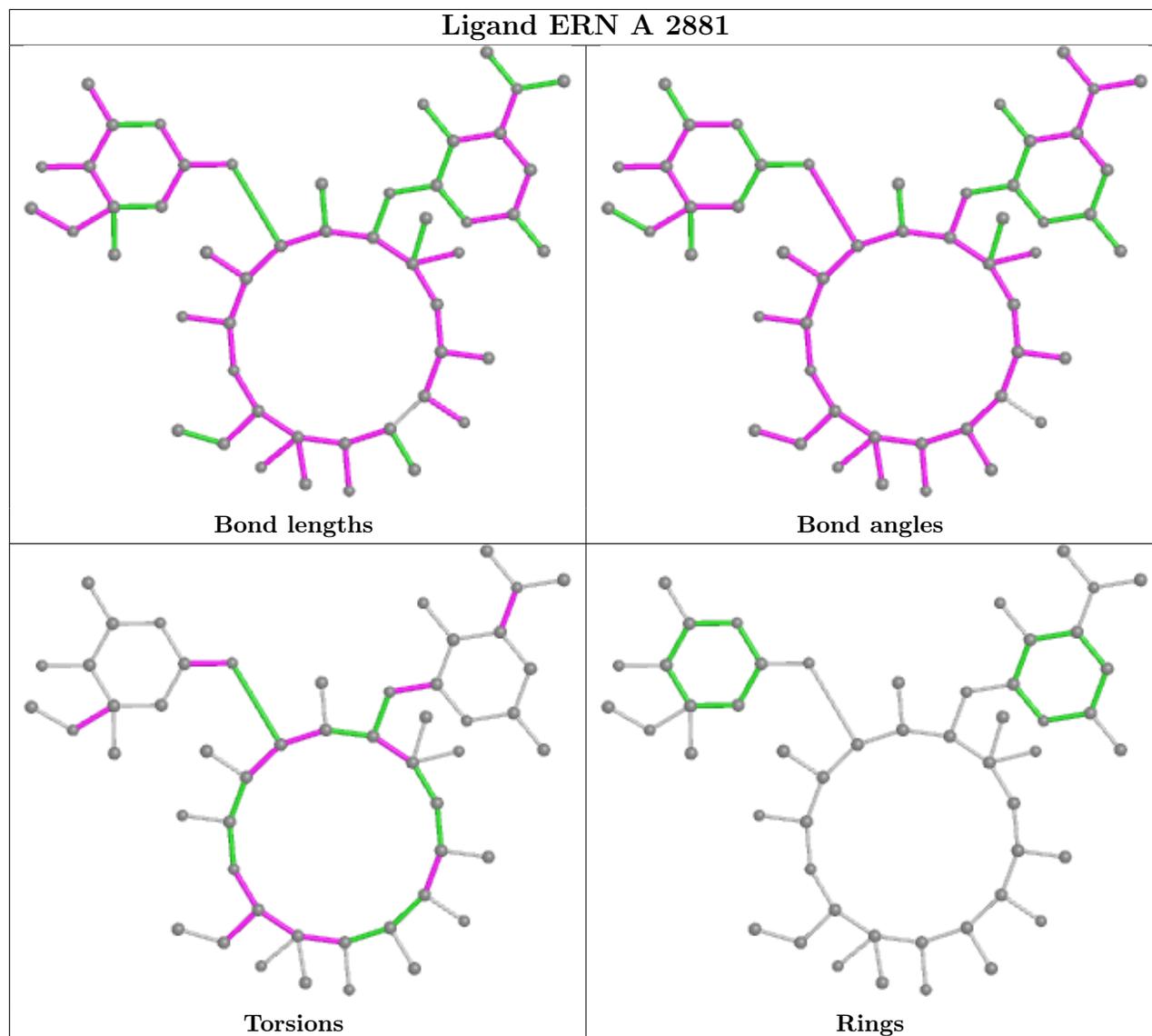
Mol	Chain	Res	Type	Atoms
2	A	2881	ERN	O12-C11-C12-O11
2	A	2881	ERN	C10-C11-C12-C35
2	A	2881	ERN	C10-C11-C12-C13
2	A	2881	ERN	C11-C12-C13-O2
2	A	2881	ERN	C11-C12-C13-C36

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.