



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:08 PM UTC

PDB ID : 2O43 / pdb_00002o43
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 : 4-5-2 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

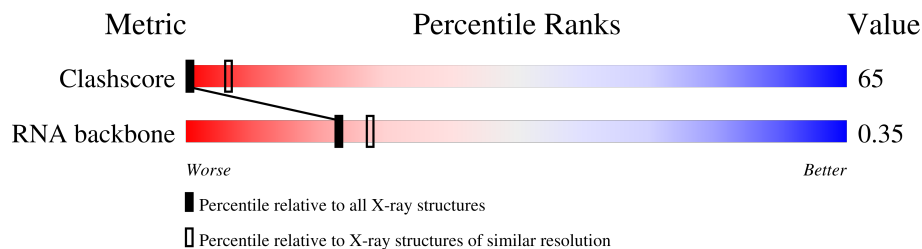
1 Overall quality at a glance

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	8% 57% 24% 7% .

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](#)

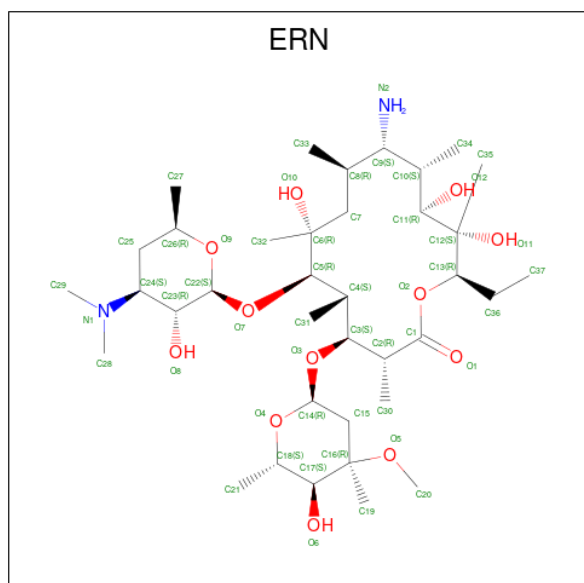
There are 2 unique types of molecules in this entry. The entry contains 59410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

- 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 (CCD ID: ERN) (formula: C₃₇H₇₀N₂O₁₂).



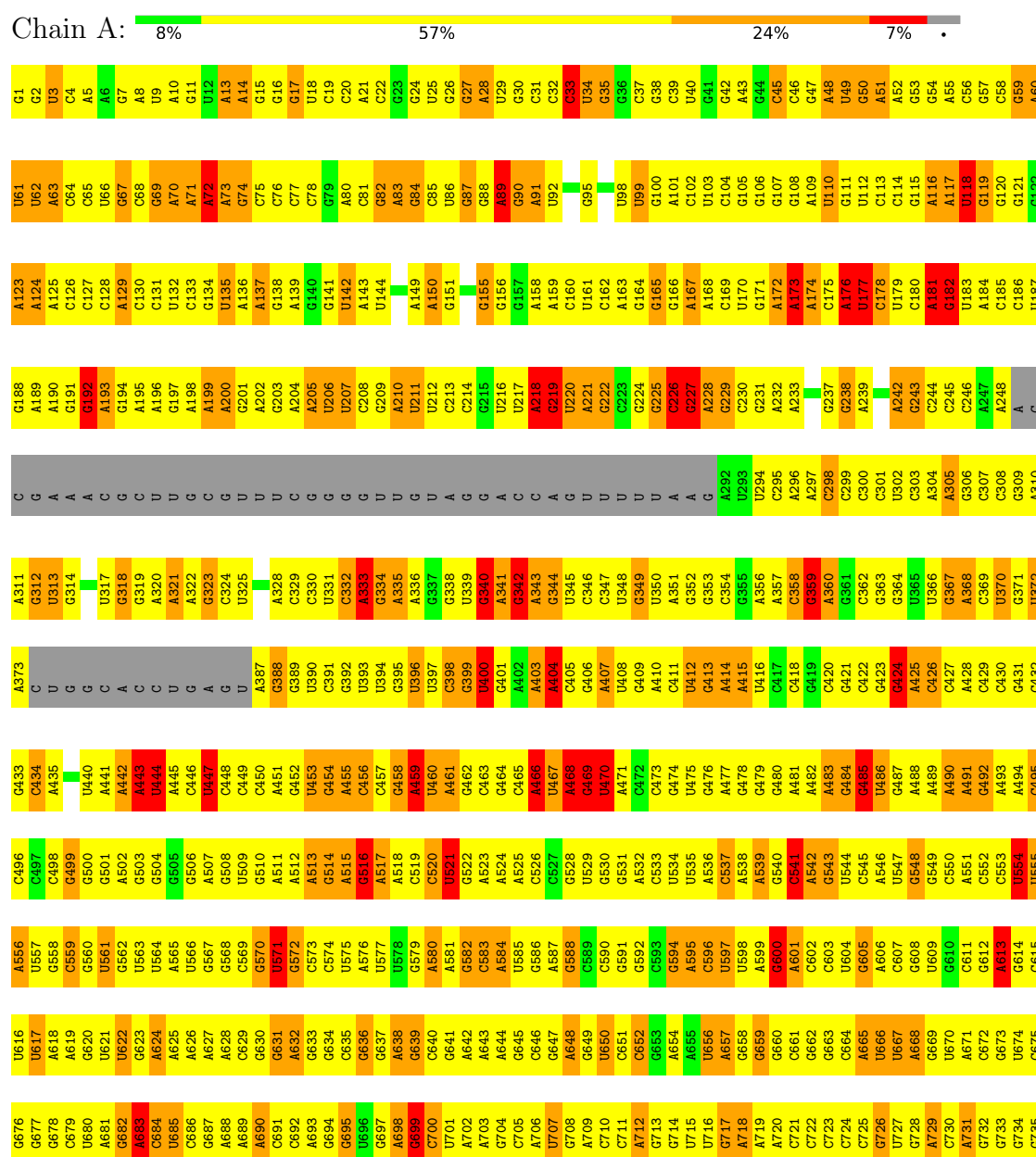
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			51	37	2	12		

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



A1596	U1475	G1414	G1352	A1288	A1227	A1166	C1103	G1041	G980	U919	G858	A796	G736
A1597	C1476	C1415	A1353	A1289	G1228	A1167	G1104	A1042	C981	A922	U859	A797	G737
C1598	C1477	A1416	A1354	A1290	C1229	G1168	G1105	A1043	C982	U860	C982	G798	G738
G1599	U1478	C1417	A1355	G1291	A1230	C1169	A1106	U1044	G983	A923	U861	C799	G739
C1540	U1479	C1418	G1356	A1292	A1231	U1170	A1107	G1045	A984	C924	A862	U800	A740
G1541	G1480	G1419	U1357	A1293	U1232	A1171	U1108	U1046	G985	U925	C863	A801	G741
G1542	U1481	A1420	C1358	G1294	A1233	U1172	A1109	G1047	A986	C926	C864	A802	G742
G1543	U1482	U1421	G1359	U1421	C1234	G1173	G1110	C803	C987	C927	A865	C803	G743
A1604	G1483	C1422	G1360	U1298	G1235	G1174	C1111	C1049	G988	G928	U866	C804	C744
A1605	G1484	A1423	G1361	A1299	G1236	A1175	U1112			A929	G867	G805	C745
C1546	U1485	U1424	A1362	A1300	G1237	U1176	C1113	G1053	A991	A930	U868	A806	G746
U1547	A1486	G1425	C1363	U1301	A1238	U1177	A1114	C1054	A992	G831	C869	A807	A747
C1548	C1487	U1426	C1364	C1302	A1239	C1178	C1115	A1055	C993	G932	C870	A808	A748
G1609	C1488	G1427	U1365	U1303	G1240	A1179	U1116	U1056	A994	G933	U871	C808	C749
C1550	A1489	C1428	A1366	U1304	G1241	A1180	G1117	A1057	A995	G934	G872	U810	C750
U1551	U1490	A1429	A1367	C1305	A1242	U1181	G1118	G1058	C996	C935	U873	G811	
C1612	C1491	G1430	G1368	U1306	G1243	U1182	U1119	A1059	C997	A936	A874	G812	G752
G1613	A1492	U1431		G1309	U1244	C1183	C1120	C1060	C998	C937	G875	A813	U753
C1614	G1495	A1432	G1371	C1310	G1245	G1184	G1121	A1061	C999	G938	A876	G814	G754
C1615	A1496	A1433	A1372	C1310	G1246	C1185	A1122	G1062	G1000	C939	G877	A815	C755
C1616	G1497	G1435	G1373	C1311	U1247	G1186	G1123	C1063	C999	G940	C878	U816	C756
U1618	G1498	A1436	G1374	G1312	G1248	A1187	U1124	C1064	A1001	U941	A879	A817	U757
C1558	G1498	G1437	C1375	U1313	G1249	A1188	G1125	A1065	C1002	U942	C880	G818	G758
A1619	A1499	A1437	C1376	A1314	A1250	G1189	A1126	G1066	C1003	U943	U881	C819	C759
C1560	U1500	G1438	C1377	A1315	G1251	C1190	C1127	G1067	U1005	A944	C882	U820	C760
A1621	C1501	A1439	A1378	A1316	C1252	G1191	A1128	G1068	C1006	U945	A883	A821	G761
G1622	G1502	G1440	A1379	G1317	C1253	A1192	A1129	G1069	U1007	U946	C884	G822	A762
U1563	C1503	A1441	C1380	A1318	G1254	G1193	U1130	C947	G1008	U947	A885	U823	A763
A1624	G1504	C1442	G1381	C1319	A1255	U1194	G1131	U1071	C948	U948	A886	U824	A764
A1625	U1505	G1443	C1382	A1320	C1256	U1195	C1132	U1072	U1010	G949	C887	C825	C765
C1626	C1506	C1444	C1383		U1257	G1196		G1073	A1011	G950	G888	U826	C766
C1627	A1507	U1445	G1384	G1323	G1258	U1197	C1135	G1074	A1012	G951	C889	C827	A767
C1628	G1508	U1446	A1385	G1324	A1259	C1198	G1136	C1075	G1013	G952	U890	C828	G768
G1629	A1509		A1386	U1325	A1260	U1199	A1137	U1076	G1014	A953	C829	U769	
C1630	U1510	G1449	G1387	U1326	G1261	G1200	A1138	U1077	U1015	U954	G	C830	U770
C1631	A1511	G1450	C1388	C1327	U1262	G1201	A1139	A1078	C1016	G955	G	G831	C771
A1632	C1512	C1451	C1389	C1328	G1263	U1202	A1140	G1079	C1017	A956	G	A832	G772
C1633	U1513	U1452	A1390	U1329	C1264	A1203	U1141	A1080	C1018	G957	G	A833	G773
A1634	C1514	A1453	A1391	G1330	G1265	G1204	G1142	A1081	U1019	G958	G	A834	A774
G1635	U1515	U1454	U1392	U1454	A1266	G1205	C1145	G1082	A1020	C959	C	U835	U775
C1636	G1516	C1455	G1393	G1332	C1267	C1206	G1146	C1083	A1021	U960	C	G836	G776
C1637	C1517	C1456	C1394	G1333	U1268		G1147	A1084	A1022	G961	U	U837	A777
	U1518	A1457	A1395	G1334	G1269	G1209	G1147	G1085	U1023	G962	A	A838	G778
C1640	G1519	U1458	C1396	A1335	C1270	C1210	G1148	C1086	C1024	G963	C	U839	U779
C1641	U1520	U1459	A1397	G1336	C1271	G1211	C1087	A1025	A964	C	C	U840	U780
G1642	U1521	G1460	G1398	G1337	G1272	U1212	U1151	U1026	G965	A	A	G841	G781
C1643	C1522	C1461	C1399	G1338	G1273	U1213	C1152	C1027	G966	C	G	A842	U782
A1644	A1523	C1462	A1400	C1339	C1274	C1214	A1153	G1028	C967	C	C	G843	G783
U1645	C1524	G1463	G1401	U1340	A1275	A1215	C1091	C1090	C1029	G968	U	G844	G784
G1646	A1525	A1464	G1402	C1341		C1216	A1154	U1092	U1030	U969	U	U845	U785
U1647	U1526	G1465	U1403	U1342		U1217	U1156	U1093	C1031	A970	A	A846	U786
C1648	G1527	C1466	C1404	U1343	A1278	C1218	G1157	C1094	A1032	A971	C	A847	U787
A1649	A1528	U1467		C1344	U1280	C1219	A1158	A1095	G1033	G972	C	A848	G788
C1650	C1529	A1468	G1407	G1345	A1281	G1220	U1159	A1096	U1034	U973	A911	G849	G789
U1651	U1530	U1469	A1408	C1346	A1282	C1221	C1160	A1097	G1035	U974	C	C850	A790
C1652	C1531	G1470	U1409	C1347	C1283	G1222	U1161	G1098	A913	C975	A913	C851	G791
A1653	U1532	G1471	U1410	A1348	G1284	G1223	A1162	A1099	U1037	C976		U852	U792
C1654	G1533	C1472	C1411	A1349	A1285	A1224	C1163	G1100	U1038	G977	U916	C853	G793
C1655	U1534	U1473	C1412	U1350	U1286	G1225	C1164	U1101	U1039	U978	U917	A794	A795
U1656	C1535	C1474	U1413	G1351	A1287	A1226	C1165	C1102	A918	A979		U957	A796

G2511	G2451	A2390	G2328	A2267	C2205	C	G2084	U2024	G1963	C1903	G1842	A1780	G1719	A1657
A2512	U2452	A2391	C2329	G2268	G2206	A	G2085	A2025	A1964	G1904	U1843	C1781	G1720	A1658
A2513	C2453	G2392	G2330	G2269	G2207	C	U2086	C2026	U1965	G1905	C1844	G1721	G1721	G1659
G2514	C2454	G2393	A2331	U2270	U2208	A	U2087	C2027	C1966	U1906	A1845	G1722	G1722	G1660
U2515	A2455	G2394	G2332	C2271	G2209	G	U2088	C2028	U1967	C1907	A1846	U1723	U1723	C1661
U2516	U2456	C2395	A2333	A2272	C	G	C2089	G2029	U1968	C1908	G1847	A1785	G1724	
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C2518	U2458	A2397	U2335	C2274	G2213	G	C2091	A2031	C	A1910	G1849	U1787	G1726	G1665
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A2521	G2461	G2400	C2338	A2277	G2215	A	C2094	A2034	U1974	G1913	G1852	G1790	A1728	A1667
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G2529	G2469	G2408	C2347	U2285	U2224	C2162	A	A2042	A1982	A1921	A1860	A1799	G1737	U1676
C2530	U2470	A2409	A2348	G2286	U2225	U2163	G2103	A2043	G1983	U1922	G1861	A1800	U1738	C1677
U2531	U2471	U2410	G2349	G2287	A2226	G2164	G2104	G2044	A1984	U1923	C1862	C1801	G1739	G1678
G2532	G2472	A2411	G2350	A2288	U2227	A2165	U2105	A2045	G1985	C1924	G1863	A1802	G1740	U1679
U2533	G2473	A2412	G2351	G2289	U2228	G2166	G2106	C2046	G1986	C1925	U1864	G1803	G1741	U1680
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G2536	A2476	U2416	G2354	C2292	G2231	A2169	A2109	C2049	C1989	G1928	A1867	G1806	C1745	G1683
C2537	C2477	U2417	A2355	G2293	G2232	C2170	G2110	G2050	U1990	C1929	A1868	A1807	C1746	G1684
C2538	C2478	A2418	G2356	U2294	U2233	U2171	C	U2051	C1991	C1930	A1869	A1808	G1747	A1685
C2539	U2479	C2419	A2357	G2295	G2234	U2172	C	G2052	G1992	G1931	U1870	G1809	U1748	A1686
A2540	C2480	C2420	C2358	U2296	G2235	G2173	U	G2053	G1993	G1932	G1871	U1810	G1749	C1687
C2541	G2481	C2421	U2359	G2297	U2236	G2174	C	A2054	U1994	G1933	A1872	A1811	A1750	U1688
U2542	A2482	C2422	C2360	U2298	U2237	C2175	C	G2055	G1995	U1934	A1873	U1812	A1751	U1689
A2543	U2483	G2423	G2361	A2299	G2238	U2176	G	C2056	A1996	A1935	G1874	U1813	U1752	U1690
A2544	G2484	G2424	G2362	C2300	C2239	U2177	A2117	U2057	A1997	U1938	C1875	G1814	G1754	C1692
A2545	U2485	G2425	G2363	A2301	C2240	C2179	A2119	U2059	A1998	G1937	C1876	G1815	G1755	C1693
G2546	C2486	G2426	C2364	C2302	U2241	G2174	C2120	A2060	U1999	U1939	C1877	G1816	G1756	A1694
C2547	G2487	A2427	U2365	C2303	C2242	G2175	U2121	C2061	G2001	C1940	G1878	U1817	C1757	U1695
G2548	C2488	U2428	U2366	C	C2243	A2181	G2122	C2062	G2002	C1941	G1880	U1819	C1758	C1696
G2549	A2489	A2429	A2367	A2306	C2244	A2182	C2123	U2063	A2002	G1942	U1881	G1820	U1759	U1697
C2550	U2490	A2430	G2368	A2307	A2245	C2183	G2124	A2063	A2003	A1943	G1882	A1821	G1760	C1698
A2551	C2491	C2431	U2369	A2308	A2246	C2184	C2125	U2064	U2004	C1944	A1883	C1824	G1761	A1699
C2552	G2492	A2432	C2370	G2309	A2247	U2185	C2126	A2065	U2005	C1945	A1884	C1825	G1762	C1700
G2553	U2493	G2433	A2371	C2310	A2248	G2186	U	U2067	G2006	U1946	C1885	C1826	G1763	C1701
C2554	C2494	G2434	A2372	U2311	C	C2187	U2134	U2074	G2007	A1952	C1891	G1832	U1770	
G2555	G2495	C2435	C2373	A2312	U2251	A2189	U	C2068	C2008	A1953	C1892	U1833	A1771	U1710
A2556	C2496	U2436	C	G2313	A2252	A2190	U	C2069	C2009	G1947	G1886	U1826	A1764	G1704
G2557	A2497	G2437	U2376	A2314	A2253	A2191	G	U2070	U2010	C1948	G1887	C1827	C1765	G1705
C2558	U2498	A2438	U2377	G2315	G2254	U2192	C	G2071	G2010	A1949	C1888	C1828	U1766	U1706
U2559	C2499	U2439	G2378	G2316	G2255	C2193	G2132	C2072	A2012	G1951	G1889	C1829	G1767	A1706
G2560	C2500	C2440	G2379	G2317	G2256	A2194	G2133	A2073	A2013	A1952	G1890	C1830	U1768	U1707
G2561	U2501	U2441	U2380	U2318	A2257	C2195	U2135	U2074	A2014	A1953	C1891	G1831	U1769	C1708
G2562	G2502	C2442	A2381	G2319	G2258	C2196	G2136	U2075	G2015	A1954	C1892	U1832	U1770	U1709
U2563	C2503	C2443	C2382	C2320	G2259	U2197	G2137	G2076	A2016	G1955	G1896	U1834	A1771	U1710
U2564	G2504	C2444	C2383	C2321	C2260	U2198	G2138	G2077	U2017	G1956	A1896	C1835	C1772	C1711
C2565	G2505	C2445	U2384	U2322	G2261	C2199	U2139	A2078	G2018	G1957	C1897	C1836	G1712	G1713
A2566	C2506	C2446	U2385	U2323	C2262	G2200	G2139	G2079	C2019	G1958	U1898	G1837	A1774	G1714
G2567	U2507	G2447	G2386	G2324	C2263	G2201	G2140	U2080	G2020	U1959	A1899	G1838	A1775	A1714
A2568	G2508	U2448	U2387	G2325	C2264	G2202	A	U2081	G2021	A1960	U1900	G1839	A1776	A1715
C2569	A2569	C2449	C2388	A2326	C2265	G2203	G	C2082	C2022	A1961	A1899	A1840	A1777	G1716
G2570	A2510	A2450	G2389	A2266	A2266	A2204	G	G2083	C2023	C1962	A1902	G1841	C1779	A1718

U	C	G2819	G2819	G2756	G2684	G2634	G2571
		C2820	G2757	G2757	C2695	U2635	U2572
		G2821	A2758	A2696	A2697	A2636	C2573
		U2822	U2759	G2697	G2698	C2637	U2574
		C2823	G2760	G2699	G2639	U2575	U2576
		A2824	A2761	U2700	G2640	A2577	A2577
		A2825	G2762	A2701	A2641	G2578	G2578
		C2826	U2763	G2702	A2579	A2580	C2580
		G2827	U2764	C2703	G2643	A2581	A2581
		C2828	C2765	U2704	A2644	A2582	A2582
		A2829	U2766	A2705	C2645	U2583	U2583
		U2830	C2767	A2706	C2646	U2584	U2584
		A2831	C2768	G2707	G2647	C2585	C2585
		G2832	C2769	U2708	G2648	C2586	C2586
		C2833	A2770	C2709	A2649	G2587	G2587
		A2834	C2771	G2710	G2650	U2588	U2588
		A2835	U2836	C2711	U2651	C2589	C2589
		U2836	U2774	G2712	G2652	U2590	U2590
		C2837	U	A2713	A2653	C2591	C2591
		U2838	U	A2714	G2654	U2592	U2592
		G2839	A	C2715	G2655	A2593	A2593
		U2840	C2778	G2716	G2656	U2594	U2594
		U2841	C2779	G2717	G2657	C2595	C2595
		C2842	A2780	U2718	A2658	C2596	C2596
		A2843	G2781	U2719	C2659	C2597	C2597
		G2844	G2782	A2720	C2660	U2599	U2599
		C2845	U2783	A2721	C2661		
		G2846	A2784	C2722	U2662		
		A2847	A2785	C2725	U2663		
		G2848	G2786	U2726	G2664		
		C2849	A2787	G2727	G2665		
		U2850	C2788	A2728	U2666		
		U2851	U2789	A2729	C2667		
		G2852	G2793	A2730	U2668		
		U2853	G2794	G2731	C2669		
		C2854	A2795	C2732	G2670		
		U2855	A2796	A2733	C2671		
		U2856	G2797	U2734	C2672		
		A2857	A2798	C2735	U2673		
		U2858	C2799	U2736	C2674		
		U2859	C2800	A2737	U2675		
		C2860	A2801	A2738	U2676		
		A2861	C2802	G2739	U2677		
		G2862	C2803	C2740	C2678		
		U2863	G2804	G2741	G2679		
		C2864	G2805	G2742	U2680		
		G2865	G2806	G2743	A2681		
		A2866	U2807	A2744	C2682		
		G2867	U2808	A2745	C2683		
		C2868	A2809	G2746	A2684		
		U2869	C2810	C2747	U2685		
		C2870	G2811	A2748	C2686		
		U2871	A2812	A2749	G2687		
		U2872	G2813	G2750	C2688		
		G2873	G2814	C2751	U2689		
		A2874	C2815	C2752	A2690		
		C2875	C2816	C2753	C2691		
		U2876	A2817	C2754	U2692		
		A2877	G2818	A2755	U2693		
		C					

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	170.44Å 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

5.1 Standard geometry

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	0.49	6/66467 (0.0%)	0.90	221/103673 (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	1	183

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2484	G	O3'-P	7.01	1.71	1.61
1	A	2041	A	C5'-C4'	6.18	1.60	1.51
1	A	803	C	C1'-N1	5.94	1.56	1.47
1	A	803	C	C3'-O3'	5.38	1.51	1.43
1	A	2042	A	O5'-C5'	5.34	1.50	1.42

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	803	C	N1-C1'-C2'	23.69	149.53	114.00
1	A	2041	A	O5'-C5'-C4'	11.22	128.33	111.50
1	A	788	G	N9-C1'-C2'	11.04	128.56	112.00
1	A	2483	U	O3'-P-O5'	10.69	120.03	104.00
1	A	985	G	N9-C1'-C2'	10.68	128.02	112.00

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	5718	0
2	A	51	0	70	41	0
All	All	59410	0	29987	5742	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 5742 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%)	765 (27%)	199 (7%)

5 of 765 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 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	ERN	A	2881	-	51,53,53	4.73	35 (68%)	77,82,82	3.93	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	-	-	31/72/107/107	0/2/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	ERN	C10-C11	14.23	1.76	1.55
2	A	2881	ERN	C7-C8	11.42	1.70	1.54
2	A	2881	ERN	C6-C5	11.00	1.76	1.55
2	A	2881	ERN	C4-C5	10.42	1.80	1.54
2	A	2881	ERN	C12-C13	7.26	1.67	1.55

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	14.31	142.12	111.53
2	A	2881	ERN	C13-O2-C1	11.72	138.67	118.20
2	A	2881	ERN	O1-C1-C2	-10.63	96.46	124.11
2	A	2881	ERN	C33-C8-C7	-8.36	93.45	112.45
2	A	2881	ERN	C7-C6-C5	8.30	126.12	110.38

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

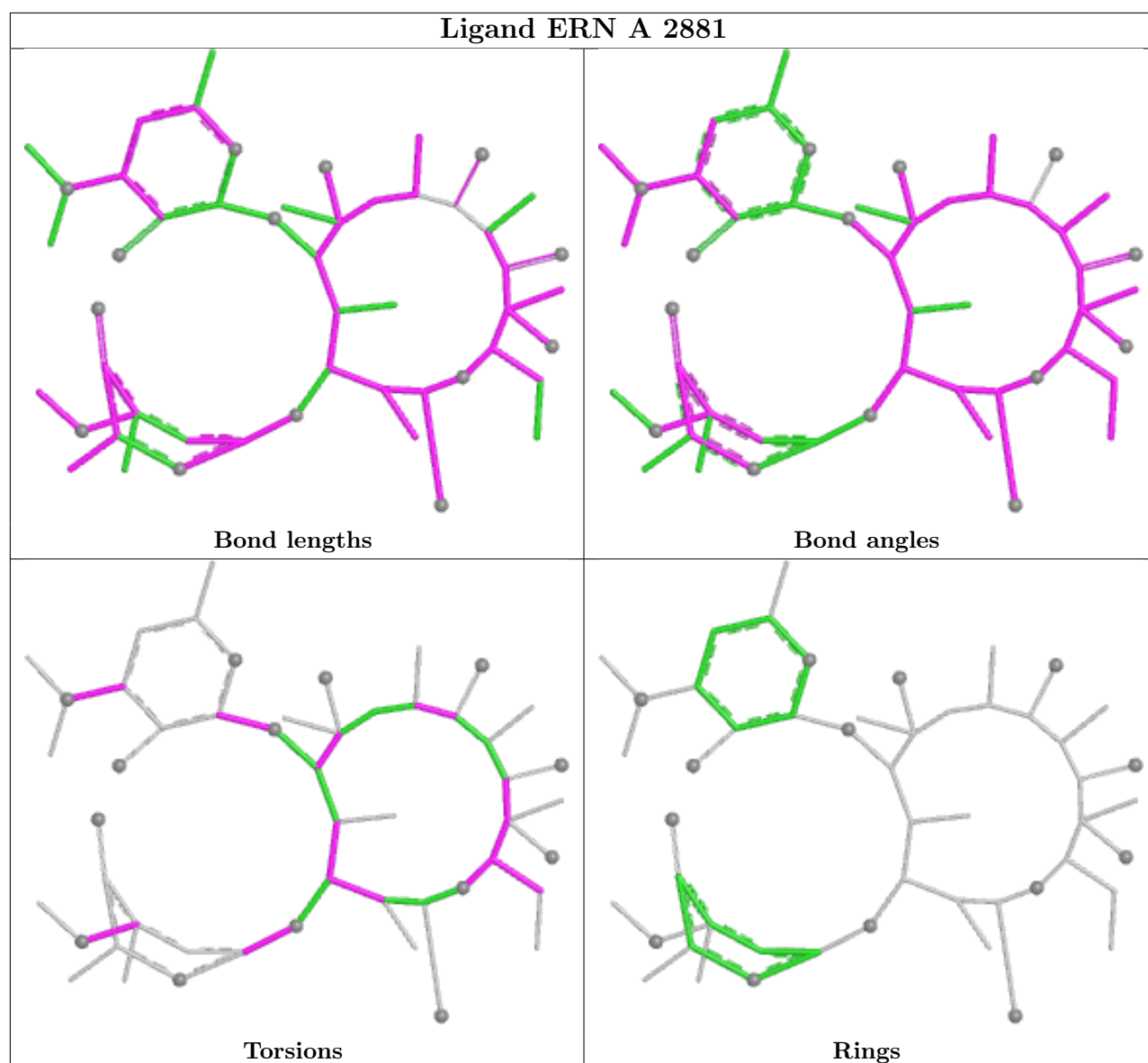
Mol	Chain	Res	Type	Atoms
2	A	2881	ERN	O12-C11-C12-O11
2	A	2881	ERN	C10-C11-C12-C35
2	A	2881	ERN	C10-C11-C12-C13
2	A	2881	ERN	C11-C12-C13-O2
2	A	2881	ERN	C11-C12-C13-C36

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

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.