



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:49 am BST

PDB ID : 2O44  
Title : Structure of 23S rRNA of the large ribosomal subunit from *Deinococcus radiodurans* in complex with the macrolide josamycin  
Authors : Pyetan, E.; Daram, D.; Auerbach-Nevo, T.; Yonath, A.  
Deposited on : 2006-12-03  
Resolution : 3.30 Å(reported)

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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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (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) : 2.11

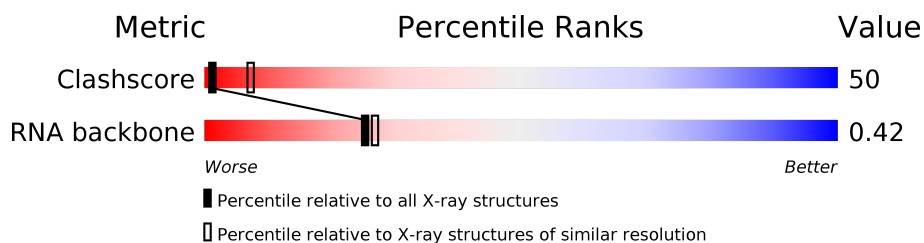
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1205 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	

## 2 Entry composition [i](#)

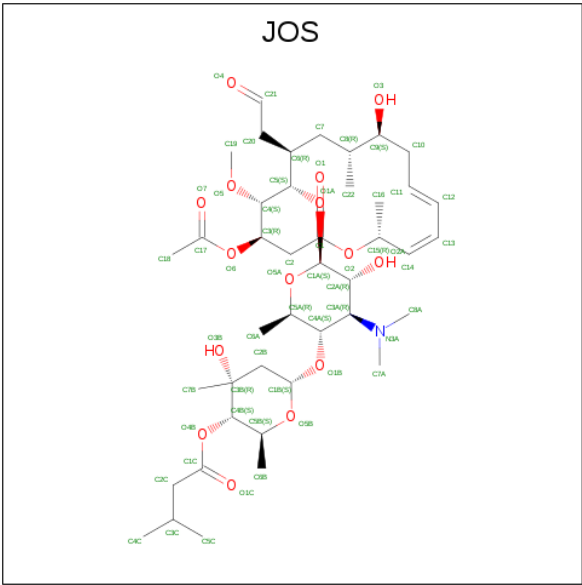
There are 2 unique types of molecules in this entry. The entry contains 59417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (2S,3S,4R,6S)-6-([(2R,3S,4R,5R,6S)-6-([(4R,5S,6S,7R,9R,10S,12E,14Z,16R)-4-(ACETYLOXY)-10-HYDROXY-5-METHOXY-9,16-DIMETHYL-2-OXO-7-(2-OXOETHYL)OXACYCLOHEXADECA-12,14-DIEN-6-YL]OXY}-4-(DIMETHYLAMINO)-5-HYDROXY-2-METHYLTETRAHYDRO-2H-PYRAN-3-YL]OXY}-4-HYDROXY-2,4-DIMETHYLTETRAHYDRO-2H-PYRAN-3-YL 3-METHYLBUTANOATE (three-letter code: JOS) (formula: C<sub>42</sub>H<sub>69</sub>NO<sub>15</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	58	42	1	15	0	0



G1541	G1479	G1352	A1292	C1169	U1108	G1047	A984	A923	C863	A802	G741	C679
G1542	G1480	A1353	A1293	U1170	A1109	U1048	G985	C924	C864	C803	G742	U680
G1543	A1420	A1354	G1294	A1171	G1110	C1049	A986	U925	A865	C804	A881	A681
A1544	U1481	A1355	U1295	U1172	C1111	C1050	G987	G926	U866	G805	C743	G682
G1545	C1422	G1356	G1296	G1173	C1112	U1051	G988	C927	U868	A806	G745	A683
G1546	A1423	U1357	A1297	G1174	C1113	C1052	G989	G928	U868	A807	G746	G684
U1547	U1485	C1358	G1298	A1175	A1114	G1053	A992	A929	C869	C808	A747	U885
U1548	U1486	A1359	G1299	U1176	C1115	C1054	G993	A930	C870	C809	A748	C886
U1549	U1425	G1361	A1300	U1177	U1116	A1055	C993	G931	U871	U810	G749	G687
C1550	G1427	A1362	U1301	C1178	G1117	U1056	A994	G932	U872	G811	C750	A688
U1551	G1428	C1363	C1302	A1179	G1118	A1057	A995	G933	G873	G812	G751	A689
C1552	A1429	G1364	U1303	G1180	U1119	G1058	C996	G934	A874	A813	G752	A690
G1553	G1430	U1365	U1304	C1181	C1120	A1059	G1000	C935	G875	G814	U753	C691
G1554	U1431	A1366	C1305	U1182	G1121	C1060	A1001	A936	A876	A815	G754	C692
A1555	G1432	A1367	U1306	C1183	A1122	A1061	A1002	C937	G877	U816	C755	A693
A1556	A1433	G1368	U1307	G1184	G1123	G1062	C1003	G938	C878	A817	C756	G694
G1557	U1434	G1369	C1308	C1185	U1124	C1063	A1004	C939	A879	G818	U757	G695
C1558	G1435	U1370	G1309	G1186	G1125	A1064	C1005	G940	C880	C819	G758	A698
G1559	G1436	G1371	C1310	A1187	A1126	A1065	U1006	U941	U881	G822	G759	G699
G1560	A1437	A1372	G1311	U1188	A1129	G1066	C1006	U942	C882	U823	U760	C700
A1561	G1438	G1373	C1312	U1189	U1130	G1067	A1007	U943	U824	G824	U761	C701
G1562	G1439	G1374	U1313	C1190	U1131	A1068	G1008	U944	C884	U825	A762	A702
U1563	G1440	C1375	A1314	G1191	G1131	G1069	A885	G945	C885	C826	A763	A703
U1564	A1441	G1376	A1315	A1192	G1132	U1070	U1010	U946	A886	U826	A764	G704
G1565	G1442	G1377	G1316	G1193	G1133	G1071	A1011	C947	G887	C827	G765	C705
G1566	G1443	A1378	G1317	U1194	C1134	U1072	A1012	C948	C888	C828	A766	A706
A1567	A1444	A1379	A1318	U1195	G1135	G1073	G1013	G949	C889	C829	G767	U707
A1568	C1380	G1381	C1319	U1196	G1136	G1074	A1014	G950	U890	C830	U768	G708
A1569	G1382	A1382	A1320	U1197	A1137	C1075	U1015	G951	G831	G831	C769	A709
A1570	G1383	G1383	G1322	C1198	A1138	U1076	A1016	A952	A832	A832	G772	G711
A1511	A1448	G1384	A1321	U1199	A1139	U1077	C1017	G953	A833	A833	A773	A712
A1512	C1451	C1385	G1324	G1200	A1140	A1078	U1018	U954	U834	U834	G774	G713
A1574	U1452	A1386	G1325	U1201	U1141	G1079	A1019	G955	U835	U835	U775	G714
A1453	G1387	G1387	U1326	A1202	G1142	A1080	A1020	A956	G836	U836	G776	U715
U1454	U1454	C1388	C1327	G1204	U1144	G1082	A1021	G958	A838	U837	A777	U716
C1455	C1455	G1389	G1328	G1205	G1145	C1083	U1022	C959	U839	U839	G778	G717
G1456	G1456	G1390	U1329	G1206	G1146	A1084	G1024	U960	U840	U840	U779	A718
A1457	A1457	A1391	G1330	G1207	G1147	G1085	A1025	G963	G841	G841	U780	A719
A1458	A1458	U1392	C1331	A1208	G1148	C1086	U1026	G964	A842	A842	U781	A720
A1461	G1460	G1393	G1332	G1209	G1149	C1087	C1027	A964	G843	G843	G782	C721
C1462	C1461	G1394	G1333	C1210	C1150	A1088	G1028	G965	G844	G844	G783	G722
A1463	C1462	A1397	A1335	G1211	U1151	C1089	U1029	A966	U845	U845	U784	C723
A1464	A1463	G1398	G1336	U1212	C1152	C1090	C1030	G967	A846	A846	U785	C724
G1465	G1465	G1398	U1337	U1213	A1153	C1091	C1031	C968	C847	C847	U786	C725
C1466	C1466	G1402	G1338	C1214	A1154	U1093	A1032	U969	A848	A848	A787	G726
U1467	U1467	U1403	U1339	A1215	G1155	C1094	G1033	A970	C849	C849	G788	U727
A1468	A1468	G1407	C1340	G1216	U1156	A1095	U1034	A971	C850	C850	G789	G728
U1469	U1469	A1408	C1341	U1217	G1157	A1096	G1035	G972	C851	C851	A790	A729
G1470	G1470	A1409	U1342	C1218	U1158	A1097	G1036	U973	U852	U852	G791	C730
C1471	C1471	U1410	G1343	C1219	C1159	G1098	U1037	U974	C853	C853	U792	A731
C1472	C1472	C1411	C1344	G1223	U1161	A1099	A1039	C975	G854	G854	G793	G732
U1473	U1473	C1412	A1345	A1224	A1162	U1101	G1100	C976	C915	C915	G794	G733
A1474	A1474	U1413	C1346	G1225	C1163	G1102	A1041	G977	U916	A856	A795	G734
U1475	U1475	G1414	G1348	A1226	C1164	G1103	G1042	U978	U917	U857	A796	G735
C1476	C1476	A1415	A1349	A1227	G1165	C1104	A1043	G980	U919	U859	A797	G736
G1477	G1477	A1416	U1350	A1166	U1166	U1105	U1044	C981	U919	U860	G798	C737
A1580	C1540	C1417	G1351	C1228	A1167	A1106	G1045	C982	U920	U861	G799	G738
				C1229	A1168	A1107	U1046	G983	A922	A862	A801	A740

U2463	G2297	A2357	G2297	G2284	U2171	C	G2050	A1984	A1920	U1856	A1794	G1730	A1667	U1601
G2484	U2298	C2358	U2298	G2285	U2172	C	U2051	G1985	A1921	G1957	C1795	C1731	G1668	G1602
G2485	G2299	U2359	G2299	U2236	G2173	G	G2052	G1986	U1922	C1858	A1796	U1732	A1669	A1603
G2486	G2300	C2360	G2300	G2237	G2174	G	G2053	G1987	U1923	G1859	C1797	U1733	G1670	A1604
G2487	G2301	G2361	G2301	G2238	A2175	G	A2054	A1988	C1924	A1860	G1798	G1734	A1671	A1605
G2488	G2302	G2362	G2302	G2239	U2176	C	G2055	G1989	C1925	G1861	A1799	G1735	A1672	C1606
	G2303	G2363	G2303	G2240	U2177	G	C2056	G1990	U1926	C1862	A1800	C1736	C1673	A1607
	G2304	G2364	G2304	U2241	A2117	A	U2057	G1991	U1927	U1863	C1801	G1737	C1674	U1608
	G2305	U2365	G2305	U2242	A2118	A	U2058	G1992	U1928	U1864	A1802	G1738	C1675	G1609
	A2306	U2366	G2306	C2243	C2120	C	U2059	G1993	U1929	C1865	G1803	G1739	U1676	A1610
	A2307	U2367	G2307	C2244	U2121	C	A2060	U1994	U1930	G1866	G1803	G1740	C1677	U1611
	A2308	U2368	G2308	A2245	G2122	G	U2061	G1995	A1935	A1867	A1807	G1741	G1678	
	A2309	U2369	G2309	A2246	U2062	G	U2062	A1996	A1936	A1868	C1808	G1742	U1679	C1614
	G2310	G2370	G2310	A2247	G2123	C	A2063	A1997	A1937	A1869	U1680	C1743	U1680	
	G2311	A2371	U2311	A2248	C2124	C	U2064	A1998	U1938	U1870	A1618	G1744	A1681	U1618
	G2312	C2372	A2312	U2249	U	G	U2065	A1999	U1939	G1871	A1619	C1745	A1682	A1619
	G2313	C2373	G2313	G2250	U	U	U2066	G2001	C1940	A1872	G1632	G1746	G1633	C1620
	A2314	U2374	G2314	U2251	U	U	U2067	G2002	C1941	A1873	G1633	G1747	G1634	C1621
	A2315	G2376	G2315	U2252	U	G	G2070	G2003	C1942	G1874	A1685	U1748	A1685	G1622
	G2316		G2316	G2284	G	G	G2071	A2004	G1943	C1875	A1686	G1749	A1686	C1623
	G2317	A2381	U2317	G2285	U	U	U2072	G2005	C1944		U1688	A1750	C1627	A1624
	U2318	C2382	G2318		U	U	A2073	G2006	C1945	G1876	U1689	U1752	A1626	A1625
	G2319	G2383	G2319	G2259	A2194	C	G2073	G2007	C1946	A1883	U1690	G1753	A1627	C1627
	G2320	U2384	G2320	G2260	C2195	U	U2074	G2008	U1947	A1884	G1691	G1754		
	G2321	G2385	G2321	G2261	U2196	U	U2075	C2009	C1948	C1885	C1692	G1755	C1692	C1631
	U2322	U2386	U2322	C2282	U2197	U	G2076	G2010	C1949	G1886	A1693	C1756	A1693	A1632
	U2323	U2387	U2323	C2283	U2198	G	G2077	G2011	C1950	G1887	A1694	C1757	A1694	C1633
	U2324	C2388	U2324	C2284	C2199	U	U2078	G2012	C1951	G1888	U1695	C1758	A1695	A1634
	G2325	G2389	A2325	G2265	G2200	G	A2079	A2013	G1952	C1889	G1696		A1696	A1635
	G2326	A2390	G2326	A2266	G2201	A	U2080	A2014	A1953	G1890	U1697	G1761	U1705	
	U2327	U2391	U2327	A2267	G2202	A	U2081	G2015	A1954	C1891	G1698	C1762	G1698	G1638
	G2328	G2392	G2328	G2268	G2203	G	G2082	G2016	A1955	C1892	A1699	C1763	C1700	C1640
	G2329	G2393	G2329	G2269	A2404	C	G2083	A2017	G1956	G1893	C1701	C1764	C1701	C1641
	G2330	C2394	G2330	U2270	C2205	C	G2084	G2018	C1957	U1894	G1702	U1766	G1702	
	A2331	G2395	A2331	C2271	G2206	A	G2085	G2019	G1958	A1895				
	G2332	C2396	G2332	A2272	G2207	C	U2086	G2020	U1959	A1896	G1832	G1767		A1642
	A2333	U2397	G2333	C2273	U2208	G	U2087	G2021	A1960	C1897	U1833			A1643
	G2334	U2398	G2334	C2274	G2209	G	U2088	G2022	A1961	U1898	A1839	A1775	A1710	A1649
	U2335	C2399	U2335	U2275	C2210	G	C2089	C2023	G1962	A1899	A1839	A1776	G1712	U1651
	G2336		G2336	C2276	U2211	U	U2090	C2024	G1963	U1900	A1840	A1777	G1713	U1652
	A2337		A2337	A2277	U2212	G	C2091	U2024	A1964	U1901	G1837	A1778	A1714	C1653
	G2338		G2338	A2278	U2213	A	U2092	A2025	U1965	G1902	A1838	C1779	A1715	A1654
	A2339		A2339	G2279	G2214	A	G2093	C2026		G1903	A1902	A1774	G1716	C1655
	G2340		G2340	A2280	G2217	A	C2094		G1968	A1904	A1839	A1775	A1717	U1656
	G2341		G2341	C2281	G2218	U	G2095	A2034	G1969	G1904	A1840	A1776	A1717	A1657
	U2342		U2342	G2282	U2219	A	U2096	G2035	G1970	U1905	G1841	A1777	G1712	A1658
	G2343		G2343	U2283	U2220	C	A2097	G2036	G1971	U1906	G1842	A1778	G1722	G1659
	U2344		U2344	U2284	G2221	C	G	A2037	G1972	U1907	G1843	C1779	U1787	U1723
	A2345		A2345	U2285	U2222	G	G	C2038	U1973	C1908	U1844	A1774	G1788	G1660
	G2346		G2346	G2286	U2223	A	A	G2039	G1974	U1909	A1845	A1782	C1789	C1661
	G2347		G2347	G2287	U2224	C	U	A2040	U1975	A1910	A1846		C1725	G1662
	A2348		A2348	A2288	G2225	C	A	A2041	G1976	A1911	G1847		C1726	C1663
	G2349		G2349	A2289	A2226	U	G2103	A2042	U1976	G1912	U1848	C1786	A1727	C1664
	U2350		U2350	A2290	G2227	C	G2104	A2043	C1977	G1913	G1849	U1787	C1728	C1665
	G2351		G2351	U2291	U2228	C	U2105	G2044	U1978	U1914	A1851	C1788	C1729	A1728
	U2352		U2352	G2229	U2229	C	G2106	A2045	G1979	A1915	G1852	G1789	C1730	G1666
	G2353		G2353	G2230	G2230	C	G2107	C2046	A1980	G1916	C1853	C1791	C1729	C1667
	U2354		U2354	G2231	G2231	C	A2108	C2047	A1981	C1917	G1854	C1792	C1730	C1668
	G2355		G2355	G2232	U2232	C	A2109	C2048	C1982	C1918	A1727	A1793	C1731	C1669
	A2356		A2356	U2296	G2233	C	G2110	C2049	G1983	A1919	G1855		C1732	C1670

A2858	A2796	U2736	C2674	A2613	G2548
U2859	G2797	A2737	U2675	G2549	C2550
C2860	A2798	A2738	G2679	U2615	A2551
A2861	C2799	G2739	U2680	U2616	C2552
G2862	C2800	C2740	A2681	A2618	G2553
U2863	A2801	G2741	C2682	G2619	U2554
C2864	C2802	G2742	C2683	G2620	C2555
G2865	C2803	G2743	A2694	G2621	A2556
A2866	G2804	A2744	A2685	G2622	C2557
G2867	G2805	G2745	C2686	A2623	C2558
G2868	G2806	G2746	G2687	G2624	U2559
	U2807	C2747	G2688	U2625	G2560
	U2808	C2748	C2689	U2626	G2561
	A2809	A2749	A2690	G2627	G2562
G2872	A2810	G2750	C2691	U2628	U2563
A2874	G2811	C2751	A2692	U2629	U2564
C2875	A2812	C2752	U2693	C2630	C2565
G2876	G2813	C2753	U2694	C2631	A2566
A2877	G2814	C2754	C2695	U2632	G2567
C	C2815	A2755	A2696	A2633	A2568
U	C2816	U2756	G2697	G2634	A2569
C	A2817	G2757	G2698	U2635	C2570
	G2818	A2758	G2699	A2636	G2571
	G2819	U2759	U2700	C2637	U2572
	C2820	G2760	A2701	G2638	C2573
	G2821	A2761	G2702	A2639	G2574
	U2822	G2762	C2703	U2575	U2576
	C2823	U2763	U2704	A2641	G2577
	A2824	U2764	U2705	G2642	G2578
	C2825	C2765	U2706	G2643	
	G2826	U2766	G2707	A2644	
	G2827	C2767	U2708	C2645	A2581
	C2828	G2768	C2709	G2646	G2582
	A2829	C2769	C2710	U2583	U2584
	U2830	A2770	G2711	G2648	C2585
	A2831	C2771	G2712	A2649	G2586
	G2832	U2772	A2713	G2650	G2587
	C2833	G2773	A2714	U2651	U2588
	A2834	U2774	C2715	G2652	C2589
	A2835	U	G2716	A2653	C2590
	U2836	A	G2717	C2655	C2591
	G2837	U2778	A2718	U2592	U2593
	U2838	C2779	U2719	U2594	C2595
	G2839	A2780	A2720	G2656	G2596
	U2840	G2781	C2721	G2657	G2597
	C2841	G2782	C2722	A2658	C2598
	A2842	U2783	C2723	C2659	U2599
	G2843	A2784	G2724	G2660	A2600
	C2844	A2785	U2725	G2661	C2601
	G2845	G2786	U2726	C2662	
	U2846	A2787	G2727	G2665	
	G2847	C2788	A2728	U2666	
	A2848	U2789	U2729	C2667	G2606
	C2849	C2790	A2730	U2668	C2607
		G2791	G2731	C2669	A2608
		C2792	C2732	C2670	G2609
		G2793	U2733	U2671	G2610
		U2794	U2734	G2672	
		A2795	C2735	G2673	

## 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, $\alpha$ , $\beta$ , $\gamma$	172.80Å 411.48Å 697.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.282 , 0.331	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	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: JOS

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	4/66467 (0.0%)	0.85	130/103673 (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	200

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1711	C	N1-C2	6.95	1.47	1.40
1	A	528	G	C5-C6	-6.20	1.36	1.42
1	A	2566	A	C5-C6	-5.34	1.36	1.41
1	A	475	U	N1-C2	-5.10	1.33	1.38

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2044	G	N9-C1'-C2'	11.61	129.09	114.00
1	A	2237	C	N1-C1'-C2'	9.82	126.77	114.00
1	A	2045	A	N9-C1'-C2'	9.68	126.58	114.00
1	A	219	G	N9-C1'-C2'	9.26	126.04	114.00
1	A	841	G	N9-C1'-C2'	9.26	126.04	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	541	C	C1'

5 of 200 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	U	Sidechain
1	A	49	U	Sidechain
1	A	54	G	Sidechain
1	A	59	G	Sidechain
1	A	86	U	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	29916	4363	0
2	A	58	0	68	7	0
All	All	59417	0	29984	4365	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 50.

The worst 5 of 4365 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:1435:G:C2	1:A:1436:G:H1'	1.70	1.25
1:A:2094:C:N4	1:A:2162:C:H42	1.40	1.19
1:A:793:G:H21	1:A:796:A:N6	1.41	1.17
1:A:1463:A:H1'	1:A:1543:G:N2	1.59	1.17
1:A:2498:U:H4'	1:A:2499:C:OP1	1.40	1.14

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%)	718 (26%)	224 (8%)

5 of 718 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	23	G
1	A	28	A
1	A	33	C

5 of 224 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1264	C
1	A	1442	C
1	A	2593	A
1	A	1278	A
1	A	1324	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 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	JOS	A	2881	-	60,60,60	2.64	17 (28%)	71,85,85	1.86	21 (29%)

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	JOS	A	2881	-	-	20/65/104/104	0/2/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	JOS	C2A-C3A	10.07	1.70	1.53
2	A	2881	JOS	C10-C11	-6.25	1.30	1.50
2	A	2881	JOS	O4B-C4B	6.13	1.56	1.45
2	A	2881	JOS	C8-C9	5.30	1.61	1.53
2	A	2881	JOS	C4A-C5A	5.05	1.61	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	JOS	O6-C17-C18	4.74	119.80	111.09
2	A	2881	JOS	O1B-C4A-C5A	4.17	117.65	106.79
2	A	2881	JOS	O2-C1-C2	3.97	118.76	111.46
2	A	2881	JOS	O3-C9-C10	-3.83	100.87	109.08
2	A	2881	JOS	C10-C11-C12	-3.70	120.64	125.41

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

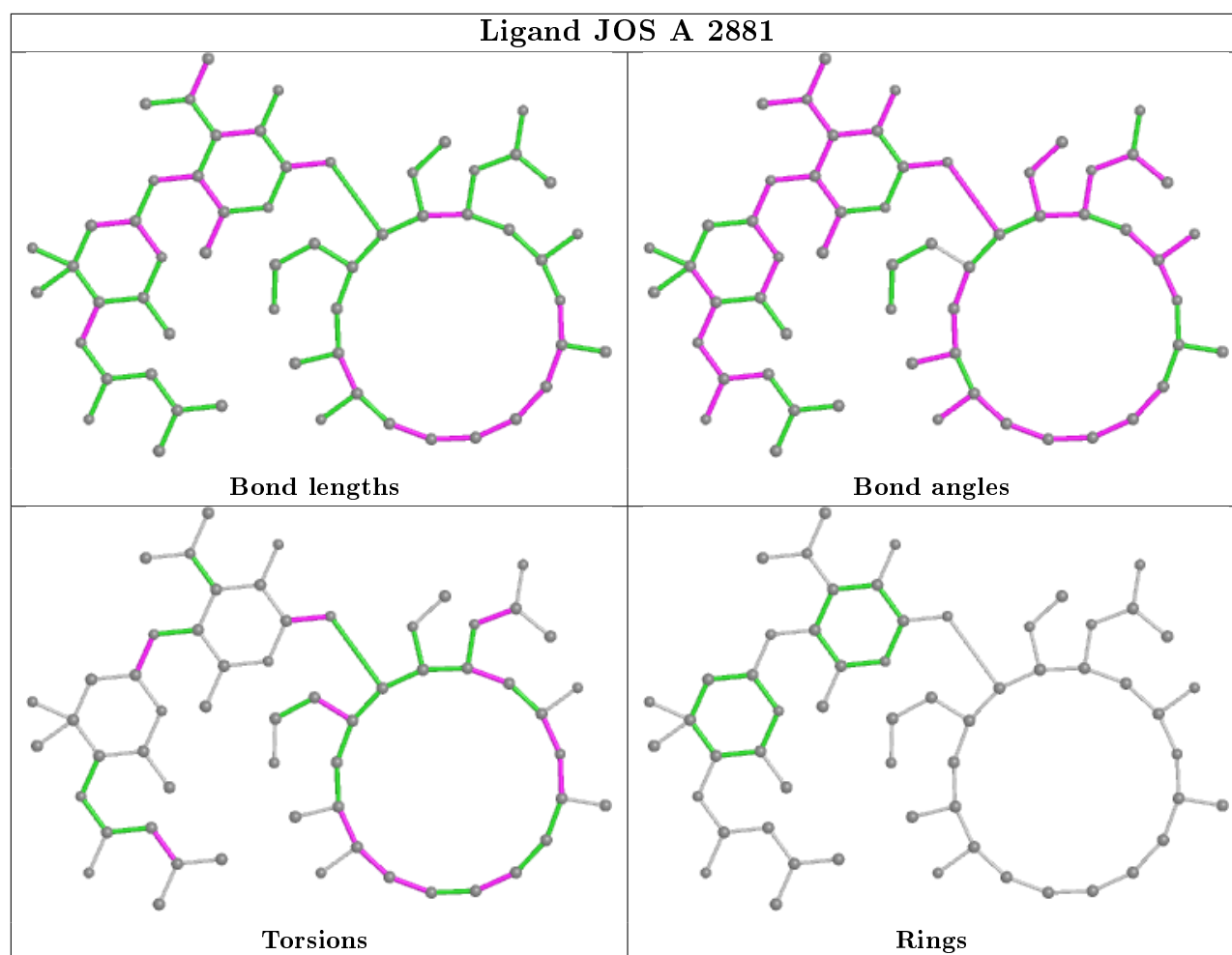
Mol	Chain	Res	Type	Atoms
2	A	2881	JOS	C11-C10-C9-C8
2	A	2881	JOS	C11-C10-C9-O3
2	A	2881	JOS	C11-C12-C13-C14
2	A	2881	JOS	C1-C2-C3-C4
2	A	2881	JOS	C18-C17-O6-C3

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2881	JOS	7	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.