



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 08:24 PM GMT

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)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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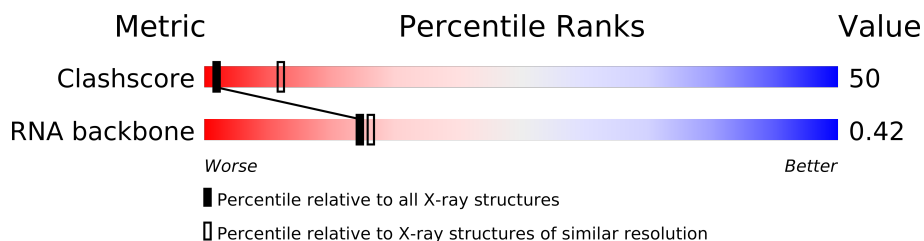
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 Å.

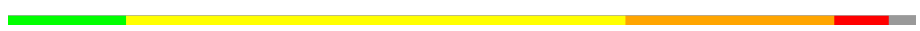
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1696 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	

## 2 Entry composition i

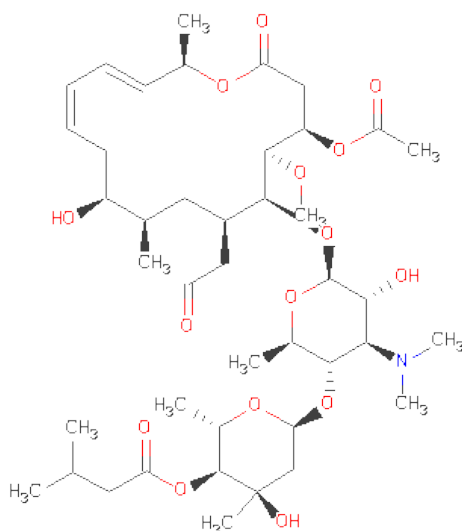
There are 2 unique types of molecules in this entry. The entry contains 59417 atoms, of which 0 are hydrogen and 0 are deuterium.

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)OXACYCLOHEXADEC-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

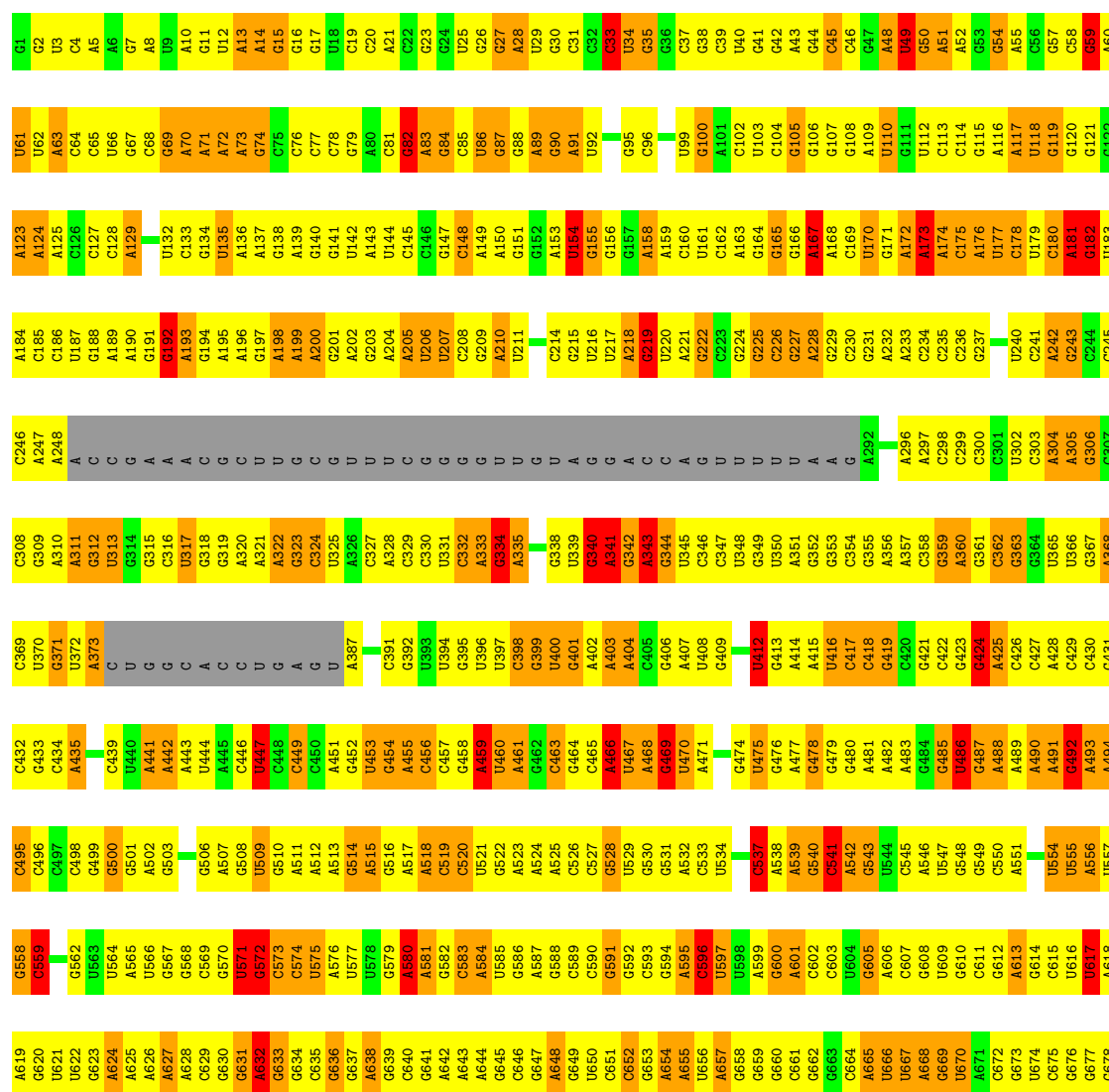
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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

Chain A: 



U1601	G1541	G1479	C1418	G1352	A1292	C1169	U1108	G1047	A984	A923	C863	A802	G741	C679
G1602	G1542	G1480	G1419	A1353	A1293	U1170	A1109	U1048	G986	G924	C864	C803	G742	U680
A1603	G1543	U1481	A1420	A1354	G1294	A1171	C1110	C1049	A986	U925	A865	C804	A743	A681
A1604	A1544	U1482	A1421	A1355	U1295	U1172	C1111	G1050	G987	C926	U866	C805	C744	G682
A1605	G1545	G1483	C1422	G1356	G1296	U1173	C1112	G1051	G988	C927	U867	A806	C745	A683
C1606	G1546	G1484	A1423	U1357	A1297	G1174	C1113	C1052	G989	G928	U868	A807	C746	G684
A1607	U1547	U1485	U1424	C1358	G1298	A1175	A1114	G1053	G990	A929	C869	C808	A747	U685
U1608	U1548	U1486	G1425	G1361	A1299	U1176	C1115	C1054	A992	A930	C870	C809	A748	C686
G1609	C1549	C1487	U1426	G1362	A1300	U1177	U1116	A1055	C993	G931	U871	U810	C749	G687
A1610	U1550	G1488	G1427	A1362	U1301	C1178	G1117	U1056	A994	G932	G872	G811	C750	A688
U1611	U1551	C1489	G1428	C1363	C1302	A1179	G1118	A1057	A995	G933	U873	G812	C751	A689
C1612	C1552	A1490	A1429	G1364	U1303	G1243	U1119	G1058	C996	G934	A874	A813	U752	A690
C1620	G1553	G1491	G1430	U1365	U1304	C1181	C1120	A1059	C997	C935	G875	G814	U753	C691
C1621	G1554	A1492	U1431	A1366	C1305	U1182	G1121	C1060	G1000	A936	A876	A815	C754	C692
C1622	A1555	A1493	A1432	A1367	U1306	C1183	A1122	A1061	C1001	C937	C877	U816	C755	A693
C1623	A1556	G1494	G1433	G1368	U1307	G1184	G1123	G1062	C1002	G938	C878	G817	U757	G694
C1624	G1557	G1495	U1434	G1369	C1308	U1185	U1124	C1063	C1003	G939	A879	G818	C756	A695
C1625	C1558	G1496	G1435	U1370	G1309	G1186	G1125	C1064	A1004	G940	C880	C819	U757	C695
C1626	G1559	C1497	A1436	G1371	C1310	A1187	A1126	A1065	U1005	U941	U881	C819	U758	A696
C1627	A1560	G1498	A1437	A1372	G1311	A1188		G1066	C1006	U942	C882	G822	C759	A698
C1628	A1561	G1499	G1438	G1373	G1312	G1189	A1129	G1067	C1007	U943	A883	U823	U760	C700
C1629	U1562	U1500	G1439	G1374	U1313	C1253	U1130	A1068	U1008	A944	C884	U824	A762	U701
A1625	G1563	C1501	G1440	C1375	A1314	G1191	G1131	G1069	C1009	G945	A885	C825	A763	A702
A1626	U1564	G1502	A1441	G1376	A1315	A1192	C1132	G1070	U1010	U946	A886	U826	A764	G704
C1627	G1565	G1503	A1442	G1377	G1316	G1193	G1133	U1071	A1011	C947	G887	C827	C765	C705
C1631	G1566	G1504	G1443	A1378	G1317	U1194	C1134	U1072	A1012	C948	C888	C828	A766	A706
C1632	A1567	U1505	C1444	C1379	A1318	U1195	C1135	G1073	G1013	G949	C889	C829	C767	U707
C1633	A1568	U1506	G1445	C1380	G1319	G1196	G1136	G1074	U1014	G950	U890	C830	U768	G708
A1634	A1569	A1507	C1446	G1381	A1320	U1197	A1137	C1075	U1015	G951	A891	G831	C769	A709
C1635	C1570	G1508	U1447	G1382	G1321	C1198	A1138	U1076	C1016	A952	G	A832	C770	C710
C1636	G1571	A1509	C1449	C1383	G1322	U1199	A1139	U1077	C1017	G953	G	A833	G772	G711
C1638	U1572	A1510	A1448	G1384	G1323	G1200	U1140	A1078	C1018	U954	G	A834	G773	A712
U1639	G1573	A1511	C1451	C1385	G1324	G1201	U1141	G1079	U1019	G955	G	U835	A774	G713
C1640	A1574	U1512	A1452	A1386	U1325	U1202	G1142	A1080	A1021	G956	G	G836	U775	G714
C1641	C1575	U1513	A1453	G1387	U1326	A1203	G1143	A1081	A1022	C957	C	U837	G776	U715
G1642	G1576	C1514	U1454	G1388	C1327	G1204	U1144	G1082	A1023	G958	C	U838	A777	U716
A1643	G1577	U1515	C1455	C1389	G1328	G1205	G1145	C1083	U1024	C959	U	U839	G778	G717
G1644	U1578	A1516	G1456	G1390	U1329	G1206	G1146	A1084	G1024	U960	A	U840	U779	A718
U1645	G1579		A1457	A1391	G1330	G1207	G1147	C1085	G1025	G963	C	G841	U780	A719
G1646	U1580	G1520	A1458	U1392	G1331	U1208	G1148	C1086	U1026	C964	C	A842	U781	A720
U1647	C1581	U1521	U1459	G1393	G1332	A1209	G1149	C1087	C1027	A964	A	G843	U782	G721
C1648	A1582	C1522	G1460	G1394	G1333	G1210	C1150	A1088	G1028	G965	G	G844	G783	C722
A1649	A1583	A1523	C1461	G1395	A1334	G1211	U1151	C1089	C1029	A966	C	U845	U784	C723
U1650	C1584	C1524	C1462	A1397	G1335	U1212	G1152	C1090	U1030	G967	U	A846	U785	C724
U1651	A1585	A1525	A1463	G1398	G1336	U1213	A1153	C1091	C1031	C968	U	C847	U786	C725
G1652	A1586	U1526	A1464	G1402	G1337	U1214	A1154	U1093	A1032	U969	A	A848	A787	G726
C1653	A1587	G1527	G1465	U1403	G1338	C1215	G1155	A1094	G1033	A970	C	G849	G788	U727
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C1655	G1589	U1529	U1467	G1407	C1340	U1217	G1157	A1096	G1035	C972	A911	C851	A790	A729
U1656	C1590	U1530	A1468	G1408	G1341	C1218	U1158	A1097	G1036	U973	A912	U852	G791	C730
A1657	U1591	U1531	U1469	U1409	U1342	G1219	U1159	G1098	U1037	U974	C913	C853	U792	A731
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G1659	C1593	G1533	G1471	C1344	G1344		U1161	G1100	A1039	C976	C915	C855	U794	G733
C1660	U1594	A1534	C1472	C1411	G1345	U1284	A1162	U1101	A1040	C977	U916	A856	A795	G734
C1661	A1595	C1535	A1473	C1412	C1346	U1285	C1163	G1102	G1041	U978	U917	U857	A796	G735
G1662	A1596	G1536	U1474	U1413	C1347	G1225	C1164	C1103	G1042	A979	A918	G858	A797	G736
C1663	A1597	U1537	U1475	G1414	G1348	A1226	G1165	G1104	A1043	G980	U919	U859	G798	C737
G1664	C1598	A1538	C1476	G1415	A1349	A1227	A1166	U1105	U1044	C981	G920	U860	C799	G738
C1665	U1599	U1539	G1477	A1416	G1350	A1228	A1167	A1106	G1045	C982	A921	G861	U800	G739
G1666	U1600	C1540	U1478	C1417	G1351	C1229	G1168	A1107	U1046	G983	A922	A862	A801	A740

A2613	G2548	U2483	C2422	A2357	G2297	G2234	U2171	C	A1984	A1920	U1856	C1794	G1730	A1667
A2614	G2549	G2484	G2423	C2358	U2298	G2235	U2172	C	G1985	A1921	G1857	C1795	C1731	G1668
U2615	C2550	U2485	G2424	U2359	A2299	U2236	G2173	G	G1986	U1922	G1858	A1796	U1732	A1669
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G2617	C2552	G2487	G2426	G2361	A2301	G2238	A2176	C	A2054	A1988	A1860	G1798	G1734	A1671
A2618	G2553	G2488	A2427	G2362	G2302	G2239	U2175	G	G1989	C1925	G1861	A1799	G1735	A1672
G2619	C2554		U2428	G2363	C2303	C2240	U2177	C	C2056	U1926	C1862	A1800	C1736	C1673
G2620	G2555	C2491	A2429	C2364	G2304	U2241	U2178	A2117	C1991	U1927	U1863	A1801	G1737	C1674
G2621	A2556	G2492		U2365	C2305	C2242	C2179	A2118	G1992	G1864	U1864	A1802	U1738	C1675
G2622	G2557	U2493	A2432	U2366	A2306	C2243	U2180	A2119	G1993	U1928	G1865	G1803	G1739	U1676
A2623	C2558	C2494	G2433	A2367	A2307	C2244	A2181	C2120	U1994	U1929	G1866		G1740	C1677
G2624	G2495	G2495	G2434	G2368	A2308	A2245		G2122	G1995	G1995	A1867	A1807	G1741	G1678
U2625	C2496		G2435	U2369	G2309	A2246	C2184	G2123	C2062	U1996	A1868	C1808	G1742	U1679
U2626	A2497	G2497	U2436	G2370	G2310	A2247	U2185	C2124	U2062	A1869	U1870	C1743	U1680	
G2627	G2562	U2498	G2437	A2371	U2311	A2248	U2186	C2125	A2063	A1936	U1871	U1810	G1744	A1681
G2628	U2499	A2372	A2438	A2372	G2312	U2249	A2187	U	U2067	U1937	U1998	A1811	C1745	A1682
U2629	C2500	C2373	G2439	C2373	G2313	U2249	A2188	U	C2068	U1938	A1872	A1812	U1746	G1683
C2630	G2501		G2440	G2374	G2314	U2251	A2189	U	G2009	U1939	A1873	U1813	G1747	G1684
C2631	G2502		U2441	G2375	G2315		A2190	U	U2069	C1940	A1874	A1814	U1748	A1685
U2632	G2503	G2376	C2442		A2316		A2191	G	G2070	U1941	G1875	G1815	U1749	A1686
A2633	G2504		C2443	G2386	G2317		U2192	G	U2071	A1943	C1876	G1816	U1750	C1687
G2634	U2505	A2381	C2443	U2387	U2318		C2193	G2132	C2072	C1944		U1817	A1751	U1688
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G2637	U2507	G2384	G2446	G2390	G2321		U2196	U2135	U2074	U1947	A1884	G1820	G1754	G1691
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A2639	G2511	A2448	A2448	G2386	U2322		U2198		U2009		G1887	C1822	C1756	A1693
G2640	U2512	C2449	A2450	U2387	G2323		C2199	U2137	G2010	A1949	G1886	G1823	C1757	A1694
A2641	G2513	A2450	G2451	G2388	G2324		G2200	U2138	U2011	C1950	G1887	G1824	U1758	U1695
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G2646	U2518	C2393	A2455	U2393	G2329		C2205	C	G2083	G1955	C1892	C1829	A1764	A1699
G2647	U2519	G2394	U2456	G2394	G2330		C2206	A	G2084	U2017	G1893	C1830	C1765	C1701
G2648	U2520	C2396	U2457	G2396	A2331		C2207	A	G2085	C1957	U1894	G1831	U1766	G1702
A2649	C2585	A2397	U2458	U2397	A2332		U2208	C	U2086	G1968	A1896	G1832	G1767	
G2650	G2586	U2398	C2459	U2398	G2333		G2209	G	U2087	U1969	C1897	U1833		U1705
U2651	G2587	C2399	G2460	U2399	C2334		C2210	G	U2088	A1960	C1897	U1833	U1770	A1706
G2652	U2588		C2461		U2335		U2211	G	C2089	A1961	U1898	G1835	C1772	C1708
A2653	C2589	U2402	G2463	U2402	G2336		U2212	G	U2090	C1962	A1899	C1836	C1773	U1709
G2654	U2590	C2403	G2464	C2403	A2337		G2213	A	C2091	G1963	U1900	G1837	U1774	U1710
G2655	C2591	A2404	G2465	A2404	A2338			A	U2092	A1964	A1901	G1838	A1775	G1711
G2656	U2592	A2405	G2466	A2405	A2339		G2217	A	G2093	U1965	C1903	A1839	A1776	G1712
G2657	U2593	C2406	A2467	C2406	G2340		G2218	U	C2094	G1968	G1904	A1840	A1777	G1713
A2658	G2594	G2407	G2468	G2407	G2341		G2219	A	A2034	G1969	G1905	G1841	A1778	A1714
G2659	U2595	U2532	G2469	U2532	U2342		A2220	C2157	G2035	G1970	U1906	G1842	U1779	G1715
C2660	C2596	G2533	G2469	G2408	G2343		G2221	C2158	A2037	C1971	C1907	G1843	A1780	G1716
G2661	U2597	U2534	U2470	A2409	G2344		U2222	A2159	C2038	G1972	C1908	C1844	C1781	A1717
C2662	G2597	G2535	U2471	U2410	A2345		U2223	U	G2039	U1973	U1909	A1845	A1782	
	U2598	G2536	U2472	A2411	G2346		U2224	C2160	A	U1974	A1910	A1846		G1721
G2665	A2600	C2537	G2473	U2412	C2347		G2225	C2162	A	G1975	A1911	G1847	C1786	G1722
U2666	G2601	A2413	G2474	A2413	A2348		A2226	G2103	A2041	U1976	A1912	U1848	U1787	U1723
C2667		U2414	C2475	G2349	G2349		C2227	G2104	A2042	C1977	G1913	G1849	G1788	G1724
U2668	G2606	A2476	A2476	G2350	A2289		U2228	A2165	G2044	U1978	U1914	G1850	C1789	G1725
C2669	C2607	U2417	G2478	G2351	U2291		G2228	G2106	A2045	G1979	A1915	A1851	G1790	C1726
U2670	G2608	U2416	U2479	G2352	C2293		G2230	A2167	C2046	A1980	G1916	G1852	C1791	C1727
G2671	C2609	A2418	C2480	G2353	U2294		G2231	A2168	C2047	A1981	C1917	G1853	C1792	A1728
U2672	G2610	U2545	G2481	A2354	U2295		G2232	A2169	C2048	G1982	G1918	G1854	C1793	C1729
G2673		C2547	A2482	G2421	U2296		G2233	C2170	C2049	G1983	A1919			

A2858	A2796	U2736	C2674
U2859	G2797	A2737	U2675
A2860	A2798	A2738	
A2861	C2799	G2739	G2679
G2862	C2800	G2740	U2680
U2863	A2801	G2741	A2681
C2864	C2802	G2742	C2682
	C2803	G2743	C2683
G2865	G2804	G2744	A2684
A2866	G2805	A2745	A2685
A2867	G2806	G2746	C2686
G2868	U2807	G2747	G2687
	U2808	C2748	G2688
U2872	A2809	A2749	C2689
G2873	A2810	G2750	A2690
A2874	G2811	C2751	C2691
C2875	A2812	G2752	A2692
C2876	G2813	C2753	U2693
A2877	G2814	C2754	G2694
C	C2815	A2755	C2695
U	C2816	A2756	A2696
C	A2817	G2757	G2697
	G2818	A2758	G2698
	G2819	U2759	G2699
	C2820	G2760	U2700
	G2821	A2761	A2701
	U2822	G2762	G2702
	G2823	U2763	C2703
	C2824	U2764	U2704
	A2825	C2765	A2705
	C2826	U2766	U2706
	G2827	G2767	G2707
	C2828	G2768	U2708
	U2829	C2769	C2709
	A2830	A2770	C2710
	G2831	C2771	G2711
	C2832	U2772	G2712
	C2833	G2773	A2713
	A2834	U2774	A2714
	A2835	U	C2715
	U2836	U	G2716
	G2837	A	G2717
	U2838	U2778	A2718
	G2839	C2779	U2719
	U2840	A2780	A2720
	C2841	G2781	A2721
	A2843	G2782	C2722
	G2844	U2783	C2723
	C2845	A2784	G2724
	G2846	A2785	C2725
	G2847	G2786	U2726
	A2848	A2787	G2727
	C2849	C2788	A2728
		U2789	A2729
		C2790	A2730
		G2791	G2731
		C2792	A2732
		G2793	A2733
		U2794	U2734
		A2795	C2735

## 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, $\alpha$ , $\beta$ , $\gamma$	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 ⓘ

### 5.1 Standard geometry ⓘ

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 50.

The worst 5 of 4365 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

### 5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

### 5.3.3 RNA ⓘ

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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

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	2.72	16 (26%)	85,85,85	1.99	25 (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	-	-	0/65/104/104	0/2/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	JOS	C8-C9	9.72	1.61	1.53
2	A	2881	JOS	C2A-C3A	8.63	1.70	1.53
2	A	2881	JOS	O4B-C4B	5.97	1.56	1.45
2	A	2881	JOS	C10-C11	-5.63	1.30	1.50
2	A	2881	JOS	C4A-C5A	4.83	1.61	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	JOS	C9-C10-C11	6.35	123.26	112.69
2	A	2881	JOS	C15-O2-C1	5.46	125.74	116.56
2	A	2881	JOS	O6-C17-C18	4.61	119.80	111.12
2	A	2881	JOS	O1B-C4A-C5A	4.21	117.65	106.75
2	A	2881	JOS	C10-C9-C8	-3.93	108.63	113.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.