wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 11:13 AM EDT

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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

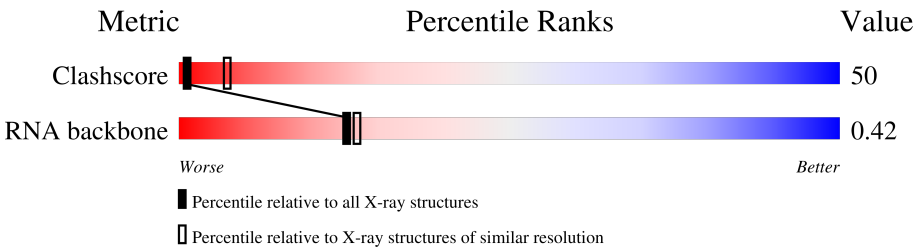
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	13% 55% 23% 6% •

2 Entry composition (i)

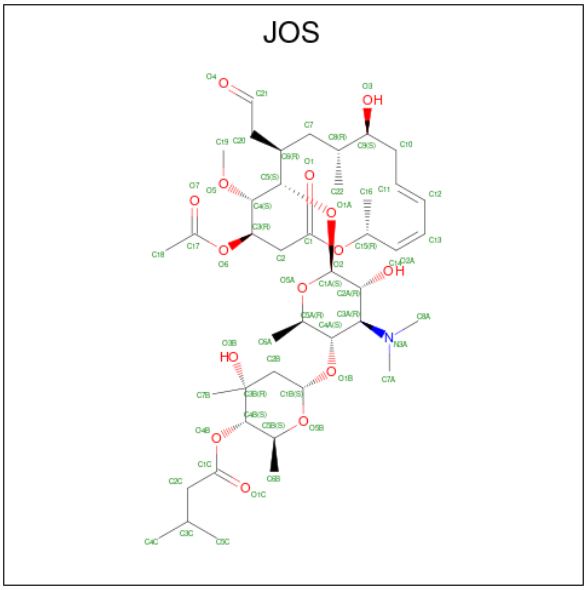
There are 2 unique types of molecules in this entry. The entry contains 59417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_{42}H_{69}NO_{15}$).



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

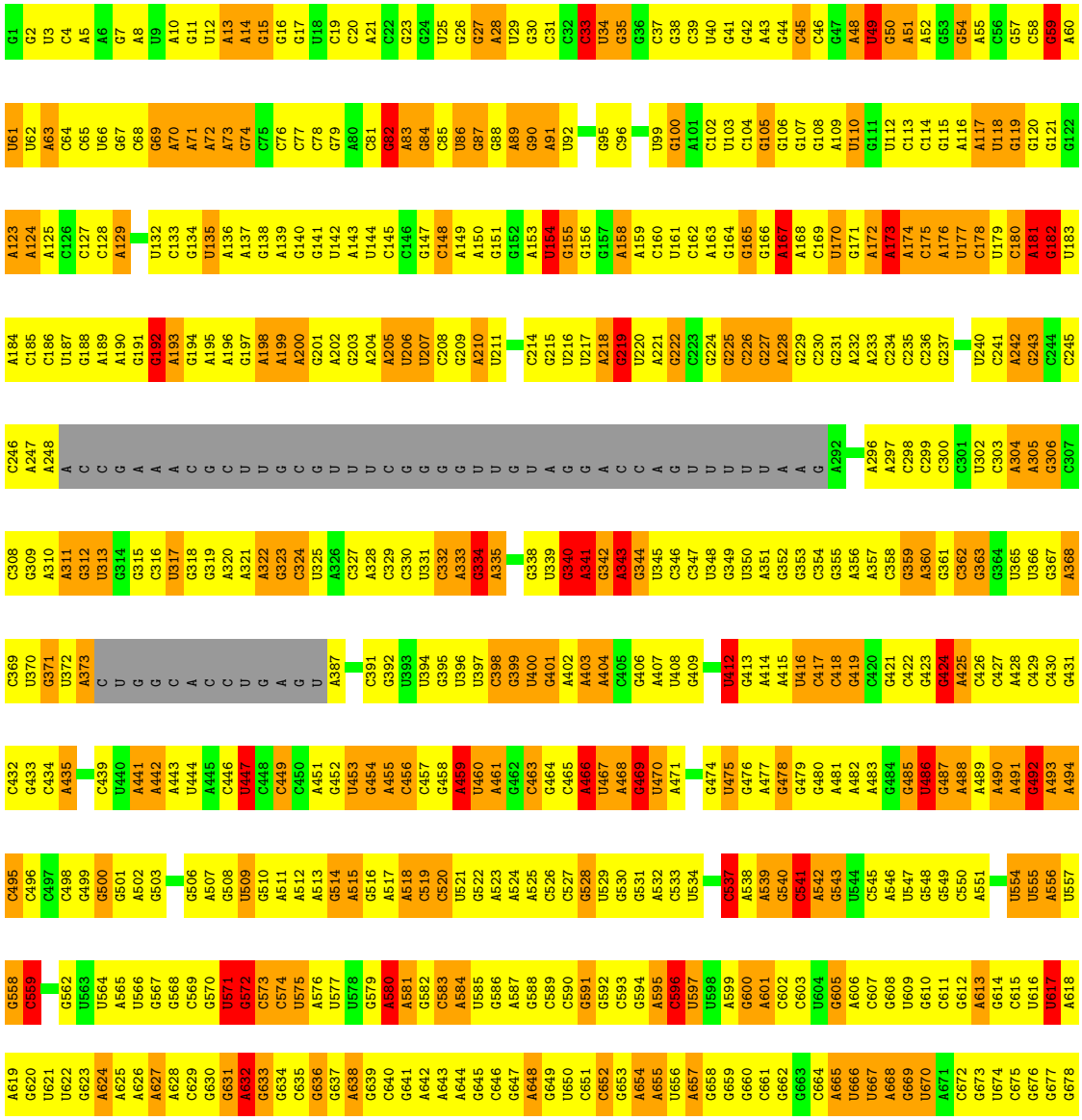
3 Residue-property plots (i)

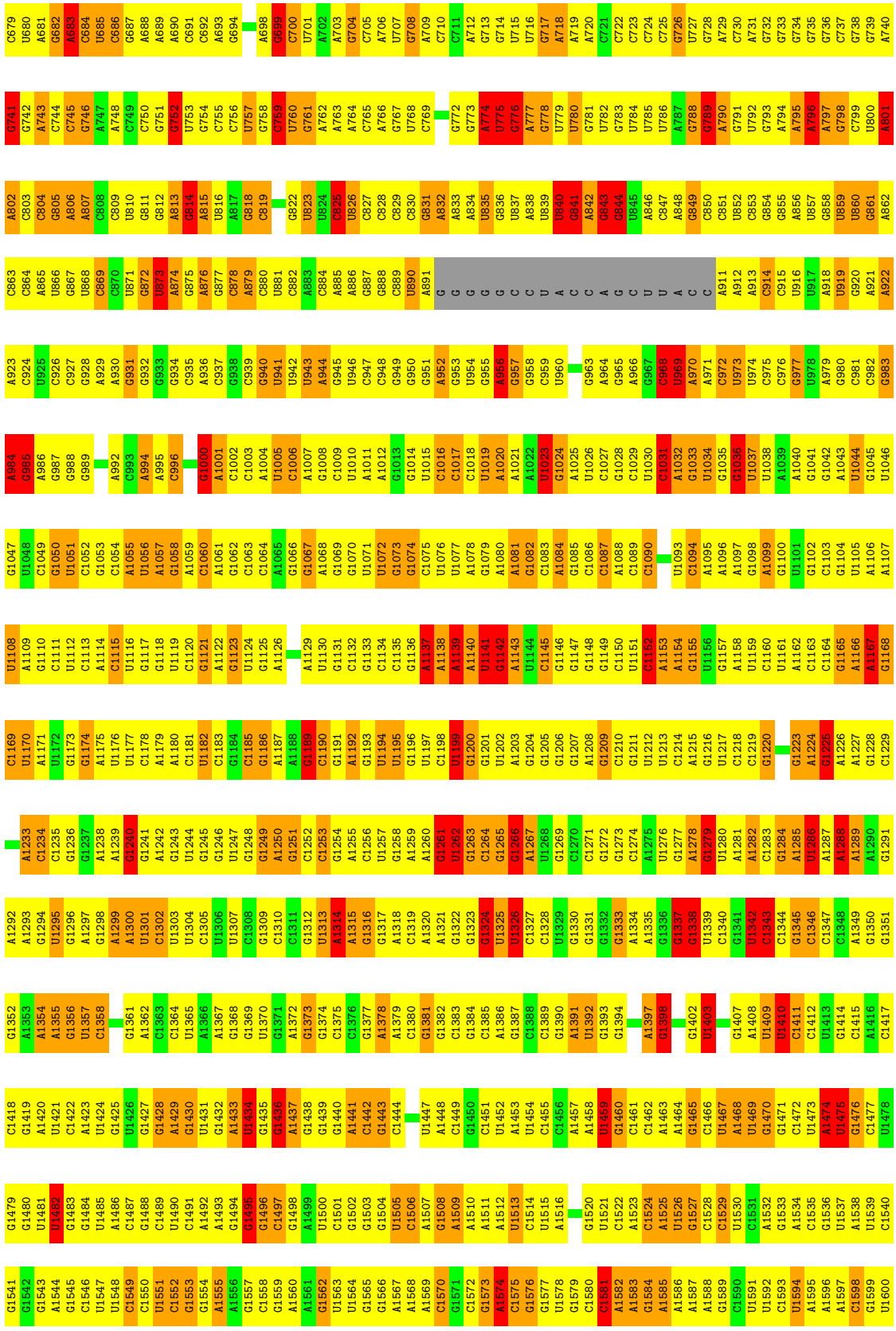
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

Chain A: 13% 55% 23% 6% •





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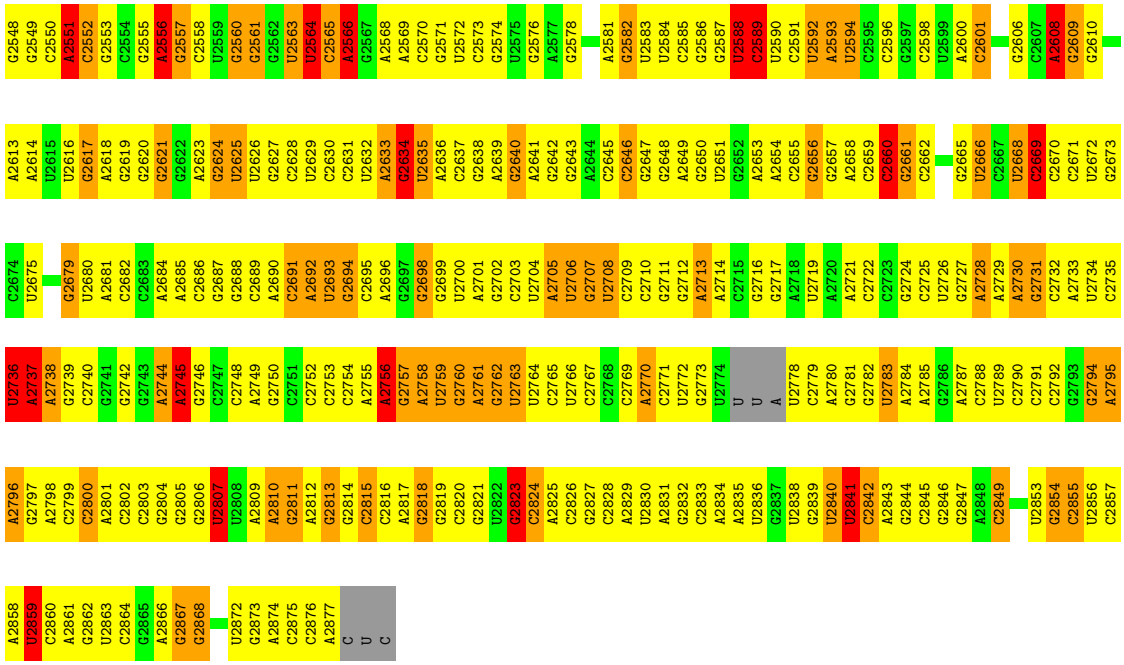
C2422 G2423 G2424 G2425 G2426 A2427 U2428 A2429 A2432 G2433 G2434 C2435 U2436 G2437 A2438 U2439 C2440 U2441 C2442 C2443 C2444 C2445 C2446 G2447 A2448 G2449 A2450 G2451 U2452 C2453 C2454 A2455 U2456 A2457 U2458 C2459 G2460 G2461 C2462 G2463 G2464 G2465 C2466 A2467 G2468 G2469 U2470 U2471 U2472 G2473 G2474 C2475 A2476 C2477 C2478 U2479 C2480 G2481 A2482
A2357 C2358 U2359 C2360 G2361 G2362 G2363 C2364 U2365 U2366 A2367 G2368 U2369 G2370 A2371 A2372 C2373 G2376 A2381 C2382 C2383 G2384 U2385 G2386 U2387 G2388 G2389 A2390 A2391 G2392 G2393 G2394 C2395 C2396 A2397 U2398 C2399 U2402 C2403 A2404 A2405 C2406 G2407 G2408 A2409 U2410 A2411 A2412 A2413 A2414 G2415 U2416 U2417 A2418 C2419 C2420 C2421
G2297 U2298 A2299 G2300 A2301 G2302 C2303 C2240 U2241 C2305 A2306 A2307 A2308 G2309 G2310 U2311 A2312 G2313 A2314 A2315 G2316 G2317 U2318 G2319 G2320 C2321 U2322 U2323 G2324 A2325 C2326 U2327 G2328 C2329 G2330 A2331 G2332 A2333 C2334 U2335 G2336 A2337 A2338 A2339 C2340 G2341 U2342 C2343 G2344 A2345 G2346 C2347 A2348 A2349 G2350 G2351 A2352 G2353 G2354 A2355 A2356
G2234 G2235 U2236 C2237 G2238 C2239 C2240 U2241 C2242 C2243 C2244 A2245 A2246 A2247 A2248 U2249 G2250 U2251 C2254 G2255 G2259 C2260 G2261 C2262 C2263 C2264 A2265 A2266 A2267 G2268 G2269 U2270 C2271 A2272 C2273 C2274 U2275 C2276 A2277 A2278 G2279 A2280 C2281 G2282 G2283 U2284 U2285 G2286 G2287 A2288 A2289 A2290 U2291 C2292 G2293 U2294 C2295 U2296
U2171 U2172 G2173 G2174 A2175 U2176 U2177 U2178 C2179 U2180 A2181 C2184 U2185 G2186 A2187 A2188 A2189 A2190 A2191 U2192 C2193 A2194 C2195 U2196 U2197 U2198 C2199 A2200 G2201 G2202 G2203 A2204 C2205 C2206 G2207 U2208 C2209 C2210 U2211 U2212 G2213 G2217 G2218 U2219 A2220 G2221 U2222 U2223 U2224 G2225 A2226 C2227 U2228 G2229 G2230 G2231 G2232 C2233
C A U G C C G A2117 A2118 A2119 C2120 U2121 G2122 G2123 C2124 C2125 U U U U G G G G2132 G2133 U2134 C2135 G2136 G2137 U2138 G2139 G2140 A A G G C A A C G G G U G G A A U A C2157 C2158 A2159 C2160 C2161 C2162 U2163 G2164 A2165 G2166 A2167 A2168 A2169 G2170
G2050 U2051 G2052 G2053 A2054 G2055 C2056 U2057 U2058 U2059 A2060 C2061 U2062 A2063 U2064 U2067 C2068 U2069 G2070 G2071 G2072 A2073 U2074 U2075 G2076 G2077 G2078 A2079 U2080 U2081 C2082 G2083 G2084 G2085 U2086 U2087 U2088 C2089 U2090 U2091 U2092 G2093 C2094 G2095 U2096 A2097 G G G A U A G2103 G2104 U2105 G2106 G2107 G2108 A2109 G2110
A1984 G1985 G1986 G1987 A1988 C1989 U1990 C1991 G1992 G1993 U1994 G1995 A1996 A1997 A1998 U1999 U2000 G2001 A2002 A2003 U2004 U2005 G2006 G2007 C2008 U2009 G2010 U2011 G2012 A2013 A2014 G2015 A2016 U2017 G2018 C2019 G2020 G2021 C2022 C2023 U2024 A2025 C2026 A2034 G2035 G2036 A2037 C2038 G2039 A2040 A2041 A2042 A2043 G2044 A2045 C2046 C2047 C2048 C2049
A1920 A1921 U1922 U1923 C1924 C1925 U1926 U1927 G1928 U1929 C1930 A1935 A1936 G1937 U1938 U1939 C1940 C1941 G1942 A1943 C1944 C1945 U1946 G1947 C1948 A1949 C1950 G1951 A1952 A1953 A1954 G1955 G1956 C1957 G1958 U1959 A1960 A1961 C1962 G1963 A1964 U1965 G1968 G1969 G1970 C1971 G1972 C1973 U1974 G1975 U1976 C1977 U1978 C1979 A1980 A1981 C1982 G1983
U1856 G1857 C1858 A1859 A1860 G1861 C1862 U1863 G1864 C1865 G1866 A1867 A1868 A1869 U1870 G1871 A1872 A1873 G1874 C1875 C1876 G1882 A1883 A1884 C1885 G1886 G1887 C1888 G1889 G1890 C1891 C1892 G1893 U1894 A1895 A1896 C1897 U1898 A1899 C1900 A1901 A1902 C1903 G1904 G1905 U1906 C1907 C1908 U1909 A1910 A1911 G1912 G1913 U1914 A1915 G1916 C1917 G1918 A1919
A1794 C1795 A1796 C1797 G1798 A1799 A1800 C1801 A1802 G1803 A1807 C1808 G1809 U1810 A1811 U1812 A1813 G1814 G1815 G1816 U1817 G1818 U1819 G1820 A1821 C1822 G1823 C1824 C1825 G1826 U1827 C1828 G1829 C1830 G1831 U1832 G1833 G1834 C1835 C1836 G1837 G1838 A1839 A1840 G1841 G1842 U1843 C1844 A1845 A1846 G1847 U1848 G1849 U1850 A1851 G1852 C1853 G1854 G1855
G1730 C1731 U1732 U1733 C1734 G1735 C1736 G1737 U1738 G1739 G1740 G1741 G1742 C1743 G1744 C1745 A1746 G1747 U1748 G1749 A1750 A1751 U1752 A1753 G1754 G1755 C1756 C1757 C1758 G1761 C1762 G1763 A1764 C1765 U1766 G1767 U1770 A1771 C1772 C1773 A1774 A1775 A1776 A1777 U1778 C1779 A1780 C1781 A1782 C1786 U1787 C1788 U1789 G1790 C1791 C1792 A1793
A1667 G1668 A1669 G1670 A1671 A1672 C1673 C1674 C1675 U1676 C1677 G1678 U1679 U1680 A1681 A1682 G1683 G1684 A1685 A1686 C1687 U1688 U1689 U1690 G1691 C1692 A1693 A1694 U1695 C1696 U1697 C1698 A1699 C1700 C1701 C1702 U1705 A1706 A1707 C1708 U1709 U1710 C1711 G1712 G1713 A1714 A1715 G1716 A1717 G1721 G1722 U1723 C1724 C1725 C1726 C1727 A1728 C1729
U1601 G1602 A1603 A1604 A1605 C1606 A1607 U1608 G1609 A1610 U1611 C1614 U1618 A1619 C1620 C1621 G1622 C1623 A1624 A1625 A1626 C1627 C1631 A1632 C1633 A1634 G1635 G1638 U1639 C1640 C1641 G1642 A1643 G1644 U1645 G1646 U1647 C1648 A1649 A1650 U1651 G1652 C1653 A1654 C1655 U1656 A1657 A1658 G1659 G1660 C1661 G1662 C1663 G1664 C1665 G1666


G2548 G2549 C2550 A2551 C2552 G2553 C2554 G2555 A2556 G2557 C2558 U2559 G2560 G2561 G2562 U2563 U2564 C2565 A2566 G2567 A2568 A2569 C2570 G2571 U2572 C2573 G2574 U2575 G2576 A2577 G2578 A2581 G2582 U2583 U2584 C2585 G2586 G2587 U2588 C2589 U2590 C2591 U2592 A2593 U2594 C2595 C2596 G2597 C2598 U2599 A2600 C2601 G2606 C2607 A2608 G2609 G2610
A2613 A2614 U2615 U2616 G2617 A2618 G2619 G2620 G2621 G2622 A2623 G2624 U2625 U2626 G2627 C2628 U2629 C2630 C2631 U2632 A2633 G2634 U2635 A2636 C2637 G2638 A2639 G2640 A2641 G2642 G2643 A2644 C2645 C2646 G2647 G2648 A2649 G2650 U2651 G2652 A2653 A2654 C2655 G2656 G2657 A2658 C2659 C2660 G2661 C2662 G2665 U2666 C2667 U2668 C2669 C2670 C2671 U2672 G2673
C2674 U2675 G2679 U2680 A2681 C2682 C2683 A2684 A2685 C2686 G2687 G2688 C2689 A2690 C2691 A2692 U2693 G2694 C2695 A2696 G2697 G2698 G2699 U2700 A2701 G2702 C2703 U2704 A2705 U2706 G2707 U2708 C2709 C2710 G2711 G2712 A2713 A2714 C2715 G2716 G2717 A2718 U2719 A2720 A2721 C2722 C2723 G2724 C2725 U2726 G2727 A2728 A2729 A2730 G2731 C2732 A2733 U2734 C2735
U2736 A2737 A2738 G2739 C2740 G2741 G2742 G2743 A2744 A2745 G2746 C2747 C2748 A2749 G2750 C2751 C2752 C2753 C2754 A2755 A2756 G2757 A2758 U2759 G2760 A2761 G2762 U2763 U2764 C2765 U2766 C2767 C2768 C2769 A2770 C2771 U2772 G2773 U2774 U U A U2778 C2779 A2780 G2781 G2782 U2783 A2784 A2785 G2786 A2787 C2788 U2789 C2790 C2791 C2792 G2793 G2794 A2795
A2796 G2797 A2798 C2799 C2800 A2801 C2802 C2803 C2804 G2805 G2806 U2807 U2808 A2809 A2810 G2811 A2812 G2813 G2814 C2815 C2816 A2817 G2818 G2819 C2820 G2821 U2822 G2823 C2824 A2825 C2826 G2827 C2828 A2829 U2830 A2831 G2832 C2833 A2834 A2835 U2836 G2837 U2838 G2839 U2840 U2841 C2842 A2843 G2844 C2845 G2846 G2847 A2848 C2849 U2853 G2854 C2855 U2856 C2857
A2858 U2859 C2860 A2861 G2862 U2863 C2864 G2865 A2866 G2867 G2868 U2872 G2873 A2874 C2875 C2876 A2877 C U C

4 Data and refinement statistics (i)

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	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^2)	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(^{o})	Ideal(^{o})
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 (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	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	1333	G
1	A	2823	G
1	A	1710	U
1	A	2760	G
1	A	2521	A

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 (i)

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(^{o})	Ideal(^{o})
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:

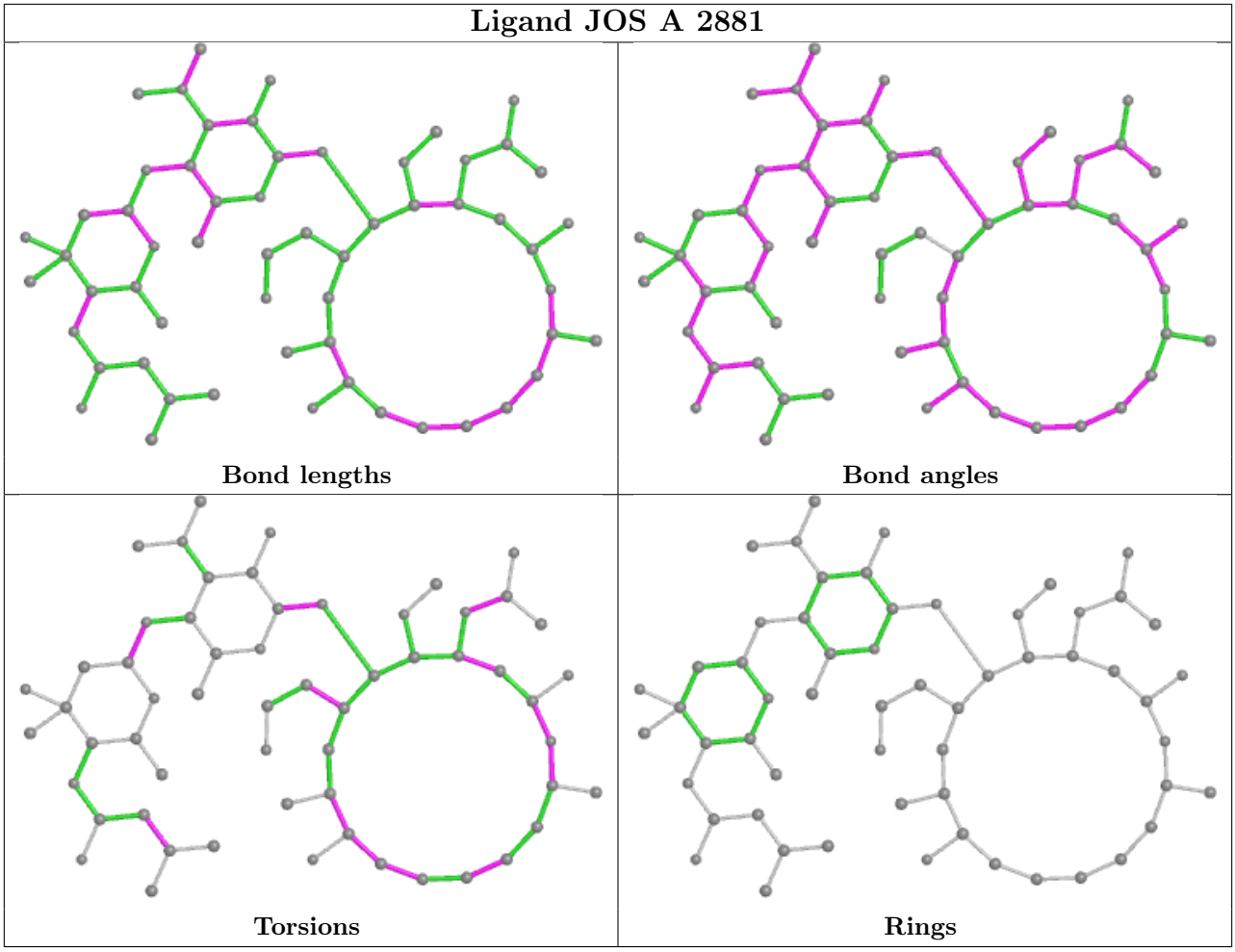
Mol	Chain	Res	Type	Atoms
2	A	2881	JOS	C11-C10-C9-C8
2	A	2881	JOS	C11-C10-C9-O3
2	A	2881	JOS	C11-C12-C13-C14
2	A	2881	JOS	C1-C2-C3-C4
2	A	2881	JOS	C18-C17-O6-C3

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 then 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.