



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:28 am 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 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

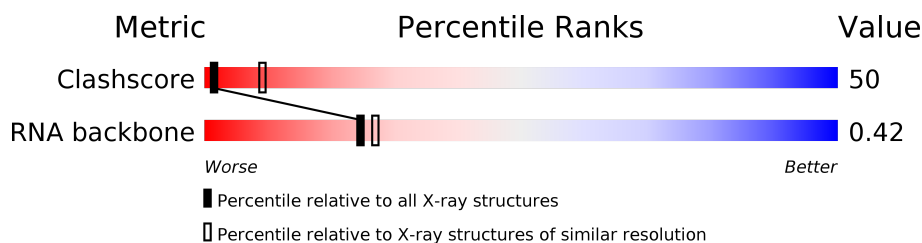
1 Overall quality at a glance

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	112137	1100 (3.36-3.24)
RNA backbone	2435	1111 (3.80-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2880	

2 Entry composition ⓘ

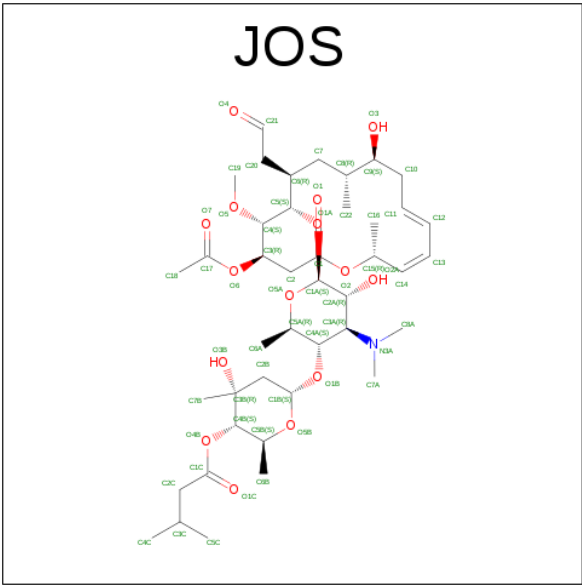
There are 2 unique types of molecules in this entry. The entry contains 59417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C₄₂H₆₉NO₁₅).



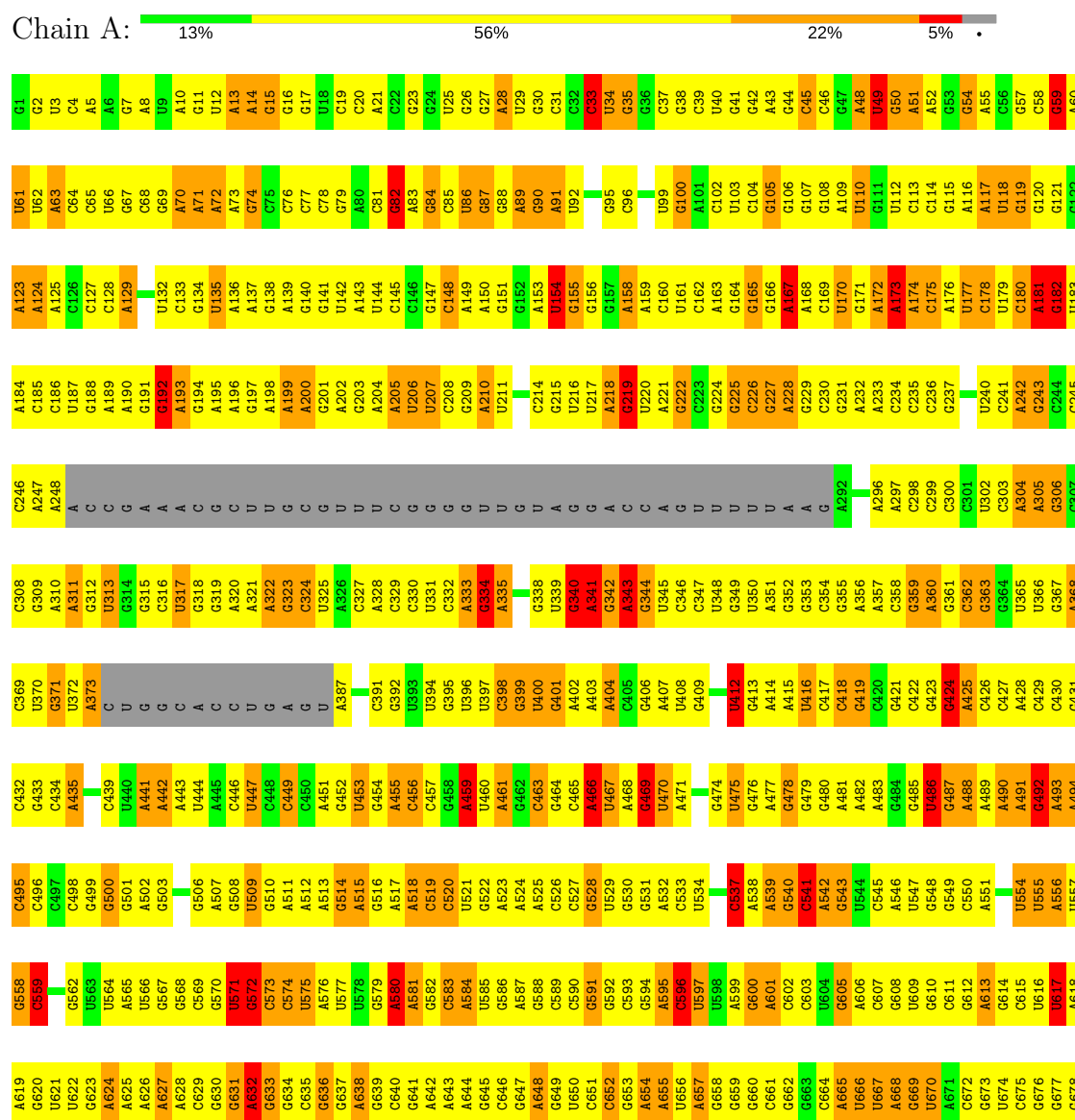
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	58	42	1	15	0	0

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 the various outlier classes 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





A2614	G2549	G2484	G2423	C2358	U2298	G2235	U2172	C	U2051	G1985	A1921	G1857	G1795	G1731	G1668
U2615	C2550	U2485	G2424	U2359	A2299	U2236	G2173	U	G2052	G1986	U1922	C1858	A1796	U1732	A1669
G2617	A2551	C2487	G2425	C2360	G2301	G2237	G2174	C	G2053	G1987	U1923	A1860	G1798	U1733	A1670
G2618	C2552	G2488	G2426	G2361	A2300	G2238	A175	G	A2054	A1988	C1924	A1861	C1799	C1734	A1671
G2619	G2553	G2489	A2427	G2362	G2302	C2239	U2176	G	G2055	C1989	C1925	G1861	A1799	G1735	A1672
G2620	C2554	G2490	U2428	G2363	C2303	C2240	U2177	A2117	G2056	U1990	U1926	C1862	A1800	C1736	C1673
G2621	G2555	G2491	A2429	C2364	G2304	U2241	U2178	A2118	U2057	C1991	U1927	U1863	C1801	G1737	G1674
G2622	A2556	G2492	G2432	U2365	C2305	G2242	C2179	A2119	U2058	G1992	G1928	G1864	A1802	U1738	C1675
G2623	C2557	U2493	G2433	U2366	A2306	C2243	U2180	C2120	U2059	G1993	U1929	G1865	A1803	U1739	U1676
G2624	G2558	G2494	G2434	A2367	A2307	C2244	A2181	U2121	A2060	U1994	A1930	G1866	G1740	G1677	C1677
U2625	U2559	G2495	G2434	G2368	A2308	A2245	G2122	G2122	C2061	A1967	A1867	A1867	G1741	G1678	U1679
G2626	G2560	C2496	U2435	U2369	G2309	A2246	U2185	G2123	U2062	A1996	A1868	A1868	G1742	U1680	U1680
G2627	G2561	A2497	U2436	G2370	G2310	A2247	U2186	C2124	A2063	A1997	A1869	A1869	C1743	U1681	A1681
G2628	G2562	U2498	G2437	A2371	U2311	A2248	G2187	C2125	U2064	A1998	G1937	U1870	G1744	U1682	A1682
U2629	U2563	C2499	A2438	C2372	G2312	U2249	A2187	U	U2067	U1999	U1938	G1871	A1811	G1745	A1683
G2630	U2564	C2500	G2439	C2373	G2313	U2250	A2188	U	U2068	U2000	U1939	A1872	A1812	A1746	G1683
C2631	C2565	G2501	G2440	G2374	A2314	U2251	A2189	U	C2069	G2001	U1940	A1873	A1813	G1747	A1684
G2632	A2566	U2502	U2441	G2375	A2315	G2252	A2190	U	U2070	A2002	C1941	G1874	G1814	U1748	A1685
U2633	G2567	G2503	C2442	U2376	G2316	G2253	A2191	G	G2070	A2003	G1942	C1875	G1815	G1749	A1686
A2634	A2568	G2504	C2443	A2381	G2317	G2254	U2192	G	G2071	U2004	A1943	C1876	G1816	A1750	C1687
G2635	A2569	G2505	C2444	C2382	U2318	G2255	C2193	U2132	C2072	U2005	C1944	G1882	U1817	A1751	U1688
U2636	U2570	C2506	G2445	C2383	G2319	G2256	A2194	U2133	A2073	G2006	C1945	A1882	G1818	U1752	U1689
A2637	G2571	U2507	C2446	G2384	G2320	U2257	C2195	U2134	U2074	G2007	U1946	A1883	U1819	A1753	U1690
G2638	U2572	G2508	G2447	U2385	C2321	G2258	U2196	G2135	G2075	C2008	G1947	A1884	G1820	G1754	G1691
G2639	C2573	G2509	A2448	G2386	U2322	G2259	U2197	U2136	G2076	U2009	C1948	C1885	A1821	G1755	G1692
A2640	G2574	G2511	G2449	U2387	U2323	C2260	U2198	G2137	G2077	G2010	A1949	G1886	C1822	G1756	A1693
G2641	U2575	A2512	A2450	G2388	G2324	C2261	C2199	U2138	G2078	U2011	C1950	G1887	G1823	C1757	A1694
U2642	G2576	U2513	G2451	C2389	A2325	C2262	A2199	U2139	A2079	G2012	G1951	A1888	G1824	U1758	U1695
G2643	A2577	G2514	U2452	G2390	G2326	C2263	A2199	G2140	U2080	A2013	A1952	G1889	C1825	G1761	C1696
G2644	G2578	U2515	C2453	A2391	U2327	G2264	U2199	A	U2081	A2014	A1953	G1890	G1826	U1697	U1697
A2645	G2581	U2516	C2454	G2392	G2328	U2275	G2203	G	G2082	G2015	A1954	C1891	G1827	C1762	C1698
G2646	A2582	C2517	U2455	G2393	C2329	C2276	G2204	G	G2083	A2016	G1955	A1892	C1828	G1763	A1699
G2647	U2583	G2518	A2456	C2394	G2330	C2277	C2205	C	G2084	U2017	G1956	A1893	C1829	A1764	G1700
G2648	U2584	C2519	G2457	G2395	A2331	C2278	C2206	A	G2085	G2018	C1957	A1894	G1830	C1759	C1701
A2649	G2585	A2520	U2458	C2396	G2332	C2279	G2207	A	U2086	C2019	G1958	A1895	G1831	U1766	U1696
G2650	G2586	A2521	C2459	A2397	A2333	C2274	U2208	C	U2087	G2020	U1959	A1896	G1832	G1767	G1702
U2651	G2587	G2522	G2460	U2398	G2334	C2274	G2209	G	U2088	G2021	A1960	C1897	U1833	U1770	U1705
G2652	G2588	G2523	G2461	C2399	U2335	U2275	C2210	G	G2089	C2022	A1961	U1898	G1834	G1711	G1711
A2653	C2589	U2526	C2462	U2402	G2336	C2276	U2211	U	U2090	C2023	G1962	A1899	C1835	A1706	A1706
G2654	U2590	G2527	G2463	C2403	A2337	C2277	U2212	G	C2091	U2024	G1963	U1900	C1836	A1771	A1707
G2655	C2591	G2528	G2464	A2404	G2338	C2278	G2213	A	U2092	A2025	A1964	A1901	G1837	C1772	C1708
G2656	U2592	U2530	A2465	A2405	A2339	C2279	U2214	A	U2093	C2026	U1965	G1838	G1773	C1773	U1709
G2657	G2593	U2531	G2466	G2406	G2340	C2280	G2215	A	G2094	C2027	A1966	C1902	U1774	U1710	U1710
A2658	U2594	G2532	G2467	C2407	G2341	C2281	U2216	U	G2095	A2040	G1967	A1839	A1775	G1712	G1712
G2659	C2595	U2533	G2468	G2408	U2342	C2282	G2217	A	U2096	G2034	G1968	A1840	A1776	G1713	G1713
C2660	G2596	G2534	U2470	A2409	G2343	G2283	A2220	C2157	U2097	G2035	G1969	G1905	A1777	G1714	A1714
G2661	U2597	U2535	G2471	U2410	G2344	U2284	G2221	C2158	G	G2036	G1970	U1906	U1778	C1779	A1715
C2662	G2598	G2536	U2472	A2411	A2345	U2285	U2222	A2159	G	A2037	C1971	C1907	C1779	G1716	G1716
G2663	U2599	G2537	G2473	G2412	G2346	G2286	U2223	C2160	A	G2038	G1972	C1908	A1780	A1717	A1717
A2664	A2600	C2538	G2474	A2413	C2347	G2287	U2224	C2161	U	G2039	C1973	U1909	C1844	C1781	A1717
U2665	G2601	U2539	G2475	A2414	U2348	G2288	G2225	C2162	A	A2040	U1974	A1910	A1846	A1782	G1721
G2666	U2602	G2540	A2476	A2415	A2349	A2289	A2226	U2163	A2041	A2041	U1976	A1911	G1847	G1786	G1722
U2667	G2606	U2542	C2477	G2416	G2350	C2290	G2227	U2164	G2103	A2042	U1976	G1912	U1848	U1723	U1722
C2668	A2607	A2543	G2478	U2417	G2351	U2291	U2228	A2165	G2104	A2043	C1977	G1913	G1849	U1787	U1723
G2669	G2608	G2544	U2479	U2418	A2352	C2292	G2229	C2166	U2105	G2044	C1978	U1914	G1850	G1788	G1724
C2670	U2609	A2545	G2480	A2419	G2353	G2293	G2230	A2167	G2106	A2045	C1979	A1915	A1851	C1725	C1725
G2671	G2610	U2546	C2481	C2419	G2354	U2294	G2231	A2168	G2107	C2046	A1980	G1916	G1852	U1790	G1726
U2672	G2613	G2547	A2482	C2420	A2355	U2295	G2232	A2169	A2109	C2047	A1981	C1917	C1853	C1791	C1727
G2673	A2613	U2548	U2483	C2422	C2356	C2296	G2233	A2170	G2110	C2048	C1982	G1918	G1854	A1792	A1728
C2674					A2357	G2297	G2234	U2171	C	G2050	A1984	A1920	G1855	A1793	G1730

U2858	G2797	A2737	U2675
C2860	A2798	A2738	
A2861	G2799	G2739	G2679
G2862	C2800	C2740	U2680
U2863	A2801	G2741	A2681
C2864	C2802	G2742	C2682
G2865	C2803	G2743	C2683
A2866	G2804	A2744	A2684
G2867	G2805	A2745	A2685
G2868	G2806	G2746	C2686
	U2807	C2747	G2687
	G2808	C2748	G2688
G2872	A2809	A2749	C2689
G2873	A2810	G2750	A2690
A2874	G2811	C2751	C2691
C2875	A2812	C2752	A2692
G2876	G2813	G2753	U2693
A2877	G2814	C2754	G2694
C	C2815	A2755	C2695
U	G2816	A2756	A2696
C	A2817	G2757	G2697
	G2818	A2758	G2698
	G2819	U2759	G2699
	C2820	G2760	U2700
	G2821	A2761	A2701
	U2822	G2762	G2702
	G2823	U2763	G2703
	C2824	U2764	U2704
	A2825	C2765	A2705
	C2826	U2766	U2706
	G2827	C2767	G2707
	C2828	G2768	U2708
	A2829	C2769	C2709
	U2830	A2770	C2710
	A2831	C2771	G2711
	G2832	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
	U2841	G2781	A2721
	C2842	G2782	C2722
	A2843	U2783	C2723
	G2844	A2784	G2724
	C2845	A2785	C2725
	G2846	G2786	U2726
	G2847	A2787	G2727
	A2848	C2788	A2728
	C2849	U2789	A2729
		C2790	A2730
	U2853	C2791	G2731
	G2854	C2792	C2732
	C2855	G2793	A2733
	U2856	G2794	U2734
	C2857	A2795	C2735
	A2858	A2796	U2736

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	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(°)	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%)	0

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

There are no RNA pucker outliers to report.

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 [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	-	59,60,60	2.82	16 (27%)	70,85,85	1.93	21 (30%)

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	C10-C11	-6.01	1.30	1.50
2	A	2881	JOS	C13-C12	-3.76	1.33	1.44
2	A	2881	JOS	C6A-C5A	-3.42	1.43	1.51
2	A	2881	JOS	C2B-C1B	2.10	1.56	1.51
2	A	2881	JOS	C8A-N3A	2.14	1.54	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2881	JOS	O3-C9-C10	-3.84	100.87	108.92
2	A	2881	JOS	C10-C11-C12	-3.44	120.64	125.40
2	A	2881	JOS	C4A-C3A-N3A	-3.16	103.98	111.70
2	A	2881	JOS	C19-O5-C4	-3.06	106.16	114.54
2	A	2881	JOS	C22-C8-C7	-2.90	106.20	110.70

There are no chirality outliers.

There are no torsion outliers.

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

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.