



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 02:33 pm BST

PDB ID : 2O43
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.

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 ⓘ symbol.

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

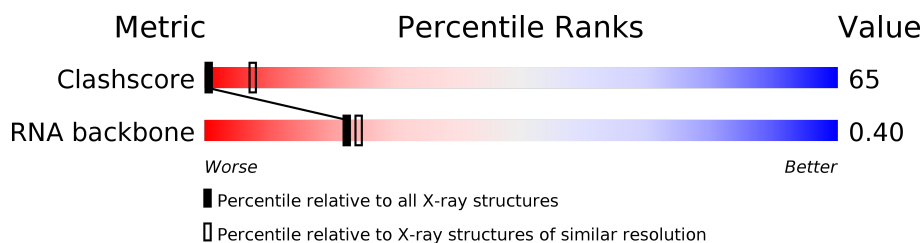
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	141614	1353 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 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	

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](#)

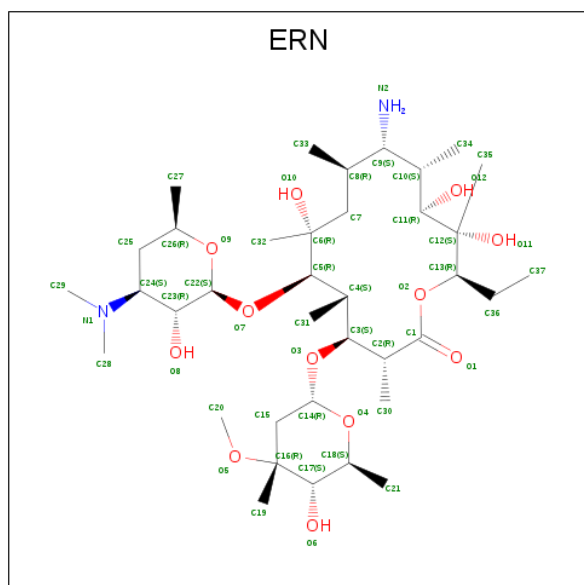
There are 2 unique types of molecules in this entry. The entry contains 59410 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- 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-HEXAMETHYLOXA CYCLOTETRADECAN-2-ONE (three-letter code: ERN) (formula: C₃₇H₇₀N₂O₁₂).



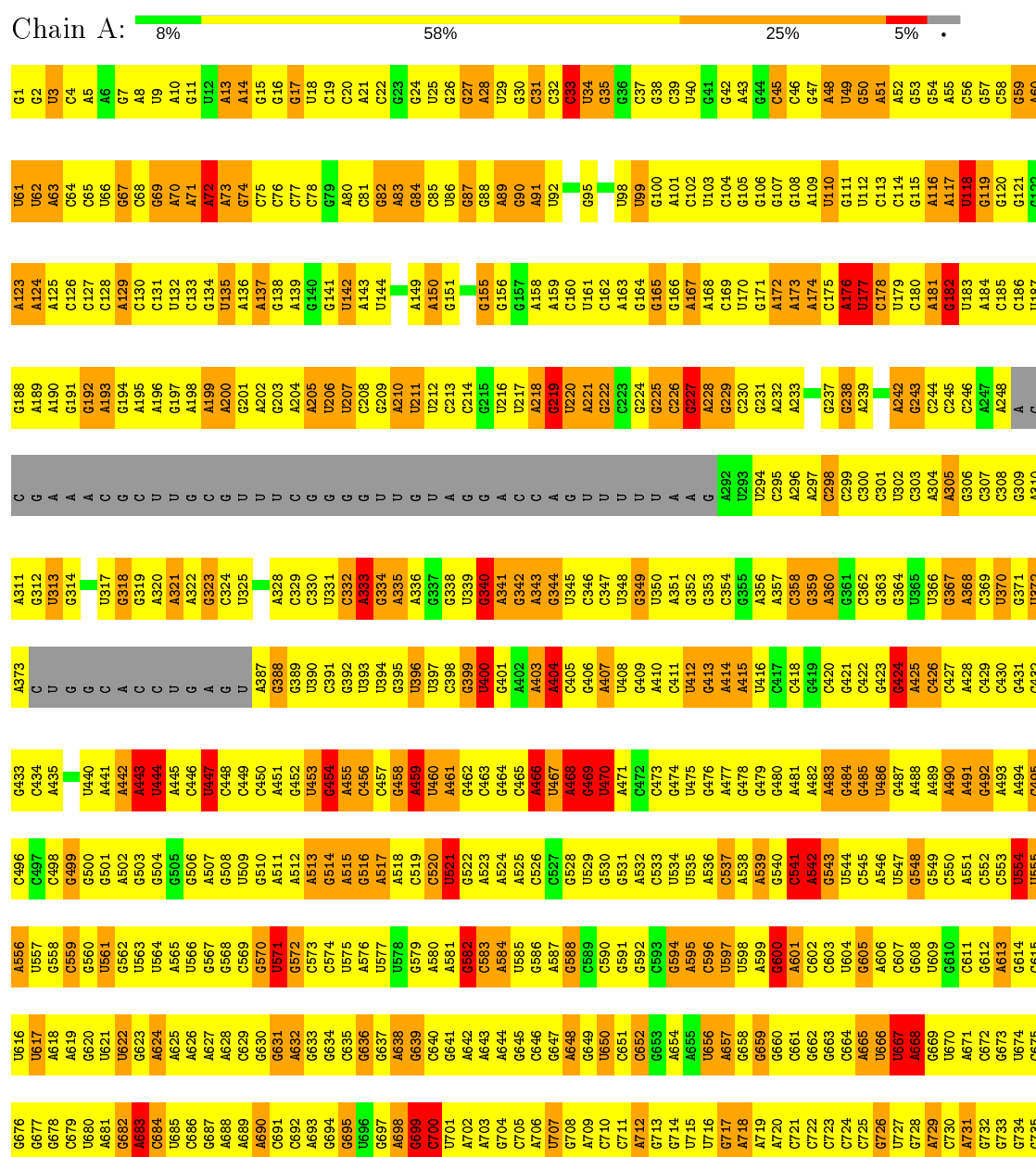
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	51	37	2	12	0	0

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. 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





A2512	U2452	A2391	G2329	A2267	G2205	G	G2084	U2024	G1963	C1903	G1842	A1780	G1719	A1657
A2513	C2453	G2392	G2330	G2268	G2206	A	G2085	A2025	A1964	G1904	U1843	C1781	G1720	A1658
G2514	A2454	G2393	A2331	G2207	G2207	A	U2086	C2026	U1965	G1905	C1844	A1782	G1721	G1659
G2515	A2455	G2394	G2332	U2270	U2208	C	U2087	C2027	C1966	U1906	A1845	G1722	G1722	G1660
U2516	U2456	C2395	A2333	C2271	G2209	G	U2088	G2028	U1967	C1907	A1846	A1785	U1723	C1661
C2517	A2457	G2396	G2334	A2272	G2212	G	C2089	C2029	U1968	C1908	G1847	A1786	G1724	G1664
C2518	U2458	A2397	U2335	C2273	G2213	U	U2090	U2030	G1969	U1909	U1787	U1787	G1725	G1665
A2519	C2459	C2398	G2336	C2274	G2214	G	C2091	U2030	G1970	A1910	U1788	C1726	G1726	C1666
A2520	G2460	C2399	A2337	U2275	G2215	A	U2092	G2032	A1911	A1911	G1849	C1727	C1727	A1667
A2521	G2461	G2400	G2338	C2276	G2216	A	G2093	C2033	C1973	G1912	G1850	A1789	A1728	A1668
A2522	C2462	A2401	C2339	A2277	G2217	A	C2094	A2034	U1974	G1913	A1851	C1790	G1729	A1669
G2523	G2463	U2402	A2340	G2278	G2217	U	G2095	G2035	G1975	U1914	C1853	C1792	G1730	A1670
G2524	G2464	C2403	G2341	G2279	G2218	A	U2096	G2036	U1976	A1915	G1854	A1793	G1731	A1671
U2525	G2465	A2404	G2342	A2280	U2219	C2157	A2097	A2037	C1977	G1916	G1855	A1794	U1732	A1672
U2526	G2466	A2405	G2343	C2281	A2220	G	G	C2038	U1978	C1917	U1856	C1795	U1733	A1673
G2527	A2467	C2406	A2344	G2282	A2221	C2158	G	C2039	C1979	G1918	G1857	A1796	C1734	C1673
G2528	G2468	G2407	G2345	G2283	U2222	A	A	A2040	A1980	A1919	C1858	C1797	G1735	C1674
G2529	G2469	G2408	G2346	U2284	U2223	C2160	U	A2041	A1981	A1920	A1859	G1798	G1736	C1675
G2530	U2470	A2409	C2347	U2285	U2224	C2162	A	A2042	C1982	A1921	A1860	A1799	G1737	U1676
U2531	U2471	G2410	G2348	G2286	G2225	C2163	G2103	G2043	C1983	U1922	G1861	A1800	U1738	C1677
U2532	A2472	A2411	G2349	G2287	A2226	G2164	G2104	A2044	A1984	U1923	G1862	C1801	G1739	C1678
U2533	G2473	A2412	G2350	A2288	C2227	A2165	U2105	C2045	G1985	C1924	U1863	A1802	G1740	U1679
U2534	G2474	G	A2351	A2289	U2228	G2166	G2106	C2046	G1986	C1925	G1864	G1803	G1741	U1680
C2535	C2475	G2415	G2352	A2290	G2229	A2167	G2107	C2047	G1987	U1926	G1865	U1804	G1744	A1681
G2536	A2476	U2416	G2353	U2291	G2230	A2168	G2108	C2048	A1988	U1927	G1866	G1805	G1745	A1682
C2537	C2477	U2417	A2354	C2292	G2231	A2169	A2109	C2049	C1989	G1928	A1867	G1806	C1745	G1683
C2538	C2478	A2418	G2355	G2293	G2232	C2170	G2110	G2050	U1990	U1929	A1868	A1807	A1746	G1684
G2539	U2479	C2419	A2357	U2294	C2233	C2171	C	U2051	C1991	C1930	A1869	C1808	G1747	A1685
A2540	C2480	C2420	G2358	C2295	G2234	G2173	C	G2052	G1992	G1931	U1870	G1809	U1748	A1686
U2541	G2481	C2421	U2359	G2296	G2235	G2173	U	G2053	G1993	G1932	G1871	G1810	G1749	C1687
U2542	A2482	C2422	C2360	G2297	U2236	G2174	C	A2054	U1994	G1933	A1872	A1811	A1750	U1688
A2543	U2483	G2423	G2361	U2298	G2237	A2175	C	G2055	G1995	U1934	A1873	U1812	A1751	U1689
G2484	G2484	G2424	G2362	A2299	C2238	U2176	G	C2056	A1996	U1935	G1874	U1813	A1752	U1690
U2485	U2485	G2425	G2363	A2301	C2239	U2177	A2117	U2057	A1997	G1937	C1875	G1814	G1753	C1691
C2546	C2486	G2426	G2364	G2302	C2240	U2178	A2118	U2058	A1998	G1937	C1876	G1815	G1754	C1692
C2547	G2487	A2427	U2365	G2302	U2241	C2179	A2119	U2059	U1999	U1938	C1877	G1816	G1755	A1693
G2548	G2488	U2428	U2366	A2306	C2242	U2180	C2120	A2060	U2000	U1939	C1878	U1817	G1756	A1694
G2549	C2489	A2429	A2367	A2307	C2243	A2181	U2121	C2061	G2001	C1940	G1879	G1818	C1757	U1695
C2550	U2490	A2430	G2368	A2307	C2244	A2182	G2122	U2062	A2002	C1941	G1880	U1819	C1758	U1696
A2551	C2491	C2431	U2369	A2308	A2245	C2183	G2123	A2063	A2003	G1942	U1881	G1820	A1759	U1697
C2552	G2492	A2432	G2370	G2309	A2246	C2184	C2124	U2064	U2004	A1943	G1882	A1821	G1760	C1698
G2553	U2493	G2433	A2371	G2310	A2247	U2185	C2125	A2065	U2005	C1944	A1883	G1761	G1761	A1699
C2554	C2494	G2434	A2372	U2311	A2248	G2186	U	G2066	G2006	U1945	A1884	C1824	C1762	C1700
G2555	G2495	C2435	C2373	A2312	A2249	G	U	U2067	G2007	U1946	C1885	C1825	G1763	C1701
A2556	C2496	U2436	G	G2313	U2251	A2189	U	C2068	C2008	G1947	G1886	U1826	G1764	G1704
G2557	A2497	G2437	G2376	A2314	A2252	A2190	U	C2069	U2009	C1948	G1887	G1827	C1765	G1705
C2558	U2498	A2438	U2377	A2315	A2253	A2191	G	G2070	G2010	C1949	C1888	U1705	U1766	U1706
U2559	C2499	U2439	G2378	G2316	C2254	U2192	G	G2071	G2011	C1950	G1889	C1829	G1767	A1707
G2560	C2500	C2440	G2379	G2317	G2255	C2193	G2132	C2072	A2012	G1951	G1890	G1830	U1768	A1707
C2561	U2501	U2441	U2380	U2318	G2256	C2194	G2133	A2073	A2013	A1952	C1891	G1831	U1769	C1708
G2562	G2502	C2442	A2381	G2319	A2257	C2195	U2134	U2074	A2014	A1953	C1892	G1832	U1770	U1709
U2563	C2503	G2443	C2382	G2320	G2258	U2196	C2135	U2075	G2015	U1954	G	U1833	A1771	U1710
U2564	U2504	C2444	C2383	C2321	G2259	U2197	G2136	G2076	A2016	G1955	G1896	G1834	C1772	U1710
C2565	G2505	C2445	G2384	U2322	C2260	U2198	G2137	G2077	U2017	G1956	A1896	C1835	C1773	G1712
A2566	C2506	G2446	U2385	U2323	G2261	C2199	U2138	G2078	G2018	C1957	C1897	C1836	A1774	G1713
G2567	U2507	G2447	G2386	C2324	C2262	G2200	U2139	A2079	C2019	G1958	U1898	G1837	A1775	A1714
A2568	G2508	A2448	U2387	A2325	C2263	G2201	G2140	U2080	G2020	U1959	A1899	G1838	A1776	A1715
A2569	A2509	G2449	G2388	C2326	C2264	G2202	A	U2081	G2021	A1960	U1900	A1839	A1777	G1716
C2570	U2510	A2450	G2389	C2327	A2265	G2203	G	C2082	C2022	A1961	A1901	A1840	U1778	A1717
G2571	G2511	G2451	A2390	A2328	A2266	A2204	G	G2083	C2023	C1962	A1902	G1841	C1779	A1718

C	C2820	G2757	C2695	U2635	U2572
	G2821	A2758	A2696	A2636	C2573
	U2822	U2759	G2697	G2637	G2574
	G2823	G2760	G2698	G2638	U2575
	C2824	A2761	G2699	A2639	G2576
	A2825	G2762	U2700	G2640	A2577
	C2826	U2763	A2701	A2641	G2578
	G2827	U2764	G2702	G2642	A2579
	C2828	C2765	C2703	G2643	C2580
	A2829	U2766	U2704	A2644	A2581
	U2830	C2767	A2705	C2645	G2582
	A2831	G2768	U2706	C2646	U2583
	G2832	C2769	G2707	G2647	U2584
	C2833	A2770	U2708	G2648	C2585
	A2834	C2771	C2709	A2649	G2586
	A2835	U2772	C2710	G2650	G2587
	U2836	U2773	G2711	U2651	U2588
	G2837	U	G2712	G2652	C2589
	U2838	U	A2713	A2653	U2590
	G2839	A	A2714	A2654	C2591
	U2840	U2776	C2715	C2655	U2592
	U2841	C2779	G2716	G2656	A2593
	C2842	A2780	G2717	G2657	U2594
	A2843	G2781	U2720	A2658	C2595
	G2844	G2782	A2721	C2659	C2596
	C2845	U2783	G2722	C2660	G2597
	U2846	A2784	U2725	G2661	U2598
	G2847	A2785	U2726	C2662	U2599
	A2848	G2786	G2727	U2663	G2604
	C2849	A2787	U2728	G2664	C2605
	U2850	C2788	A2729	G2665	G2606
	G2851	U2789	A2730	C2666	C2607
	G2852	U2800	G2731	U2668	A2608
	U2853	G2793	G2732	C2669	G2609
	C2854	G2794	A2733	C2670	G2610
	C2855	A2795	U2734	G2671	A2611
	U2856	G2796	C2735	U2672	G2612
	C2857	A2797	U2736	G2673	A2613
	A2858	C2799	A2737	C2674	A2614
	U2859	U2800	A2738	U2675	U2615
	C2860	A2801	G2739	G2676	U2616
	G2861	C2802	C2740	U2677	G2617
	U2862	G2803	G2741	C2678	A2618
	U2863	G2804	G2742	G2679	G2619
	C2864	G2805	G2743	U2680	G2620
	G2865	U2806	A2744	A2681	G2621
	A2866	G2807	U2745	C2682	G2622
	U2867	U2808	G2746	C2683	A2623
	G2868	A2809	C2747	A2684	G2624
	U2869	A2810	G2748	A2685	U2625
	C2870	G2811	A2749	C2686	U2626
	U2871	A2812	G2750	G2687	G2627
	U2872	G2813	C2751	G2688	C2628
	G2873	G2814	G2752	C2689	U2629
	A2874	C2815	C2753	A2690	C2630
	C2875	G2816	A2754	C2691	C2631
	C2876	A2817	U2755	A2692	U2632
	A2877	G2818	G2756	U2693	A2633
	C	G2819		G2694	G2634
	U				

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 [i](#)

5.1 Standard geometry [i](#)

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	0.67	17/66467 (0.0%)	0.86	140/103673 (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	183

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2484	G	O3'-P	8.76	1.71	1.61
1	A	788	G	N9-C4	8.06	1.44	1.38
1	A	2041	A	C8-N7	-7.66	1.26	1.31
1	A	2041	A	C5'-C4'	7.64	1.60	1.51
1	A	2042	A	P-O5'	7.49	1.67	1.59

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	803	C	N1-C1'-C2'	27.33	149.53	114.00
1	A	2041	A	P-O3'-C3'	13.45	135.84	119.70
1	A	803	C	C3'-C2'-C1'	12.56	111.55	101.50
1	A	788	G	N9-C1'-C2'	11.20	128.56	114.00
1	A	985	G	N9-C1'-C2'	10.78	128.02	114.00

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	5720	0
2	A	51	0	70	41	0
All	All	59410	0	29987	5744	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 5744 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%)	762 (27%)	199 (7%)

5 of 762 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	1325	U
1	A	1684	G
1	A	2593	A
1	A	1337	G
1	A	1442	C

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	ERN	A	2881	-	52,53,53	4.69	36 (69%)	77,82,82	3.83	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	-	-	29/72/107/107	0/2/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2881	ERN	C10-C11	13.83	1.76	1.55
2	A	2881	ERN	C7-C8	11.42	1.70	1.54
2	A	2881	ERN	C6-C5	10.55	1.76	1.55
2	A	2881	ERN	C4-C5	10.53	1.80	1.55
2	A	2881	ERN	C8-C9	7.28	1.70	1.54

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	13.92	142.12	111.56
2	A	2881	ERN	C13-O2-C1	11.53	138.67	118.18
2	A	2881	ERN	O1-C1-C2	-10.33	96.46	124.08
2	A	2881	ERN	C33-C8-C7	-8.36	93.45	112.45
2	A	2881	ERN	C7-C6-C5	8.01	126.12	110.48

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

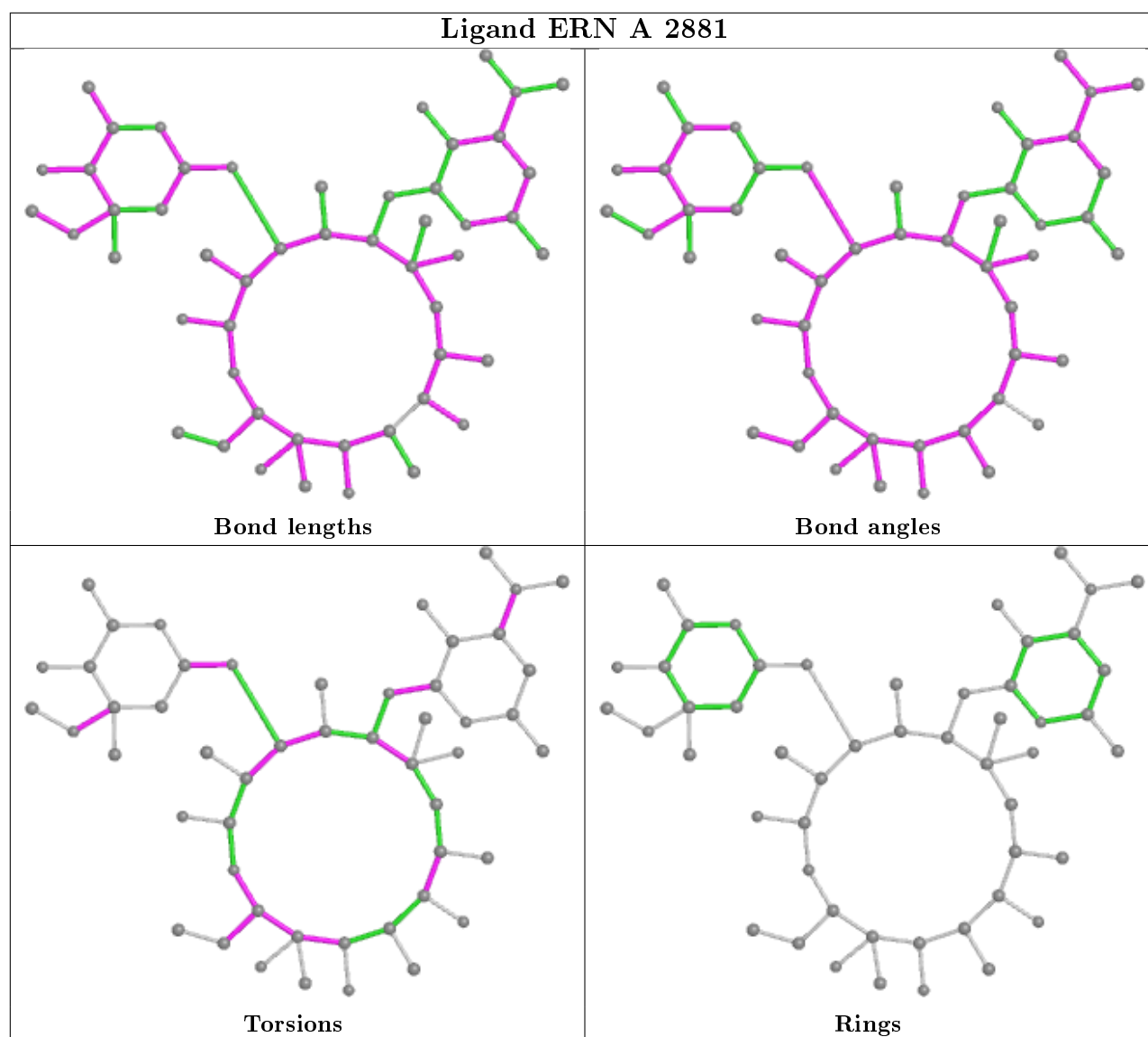
Mol	Chain	Res	Type	Atoms
2	A	2881	ERN	O12-C11-C12-O11
2	A	2881	ERN	C10-C11-C12-C35
2	A	2881	ERN	C10-C11-C12-C13
2	A	2881	ERN	C11-C12-C13-O2
2	A	2881	ERN	C11-C12-C13-C36

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.