



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 27, 2020 – 05:47 pm BST

PDB ID : 1JZX  
Title : Structural Basis for the Interaction of Antibiotics with the Peptidyl Transferase Center in Eubacteria  
Authors : Schluenzen, F.; Zarivach, R.; Harms, J.; Bashan, A.; Tocilj, A.; Albrecht, R.; Yonath, A.; Franceschi, F.  
Deposited on : 2001-09-17  
Resolution : 3.10 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](mailto: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.

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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)  
Xtrriage (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

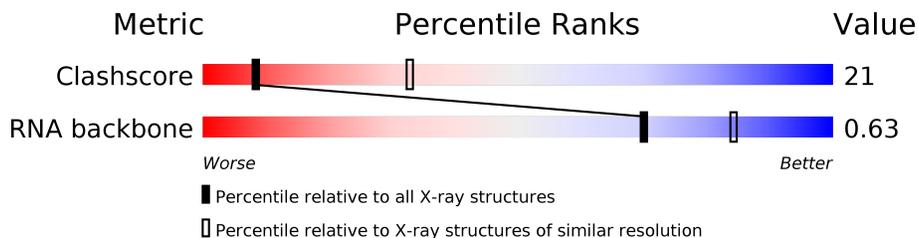
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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  $\geq 3$ , 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	K	205	
3	L	134	
4	M	60	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 59946 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	2774	59532	26556	10982	19221	2773	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1526	U	Y	SEE REMARK 999	GB 15805042

- Molecule 2 is a protein called Ribosomal Protein L4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
2	K	197	197	197	0	0	197

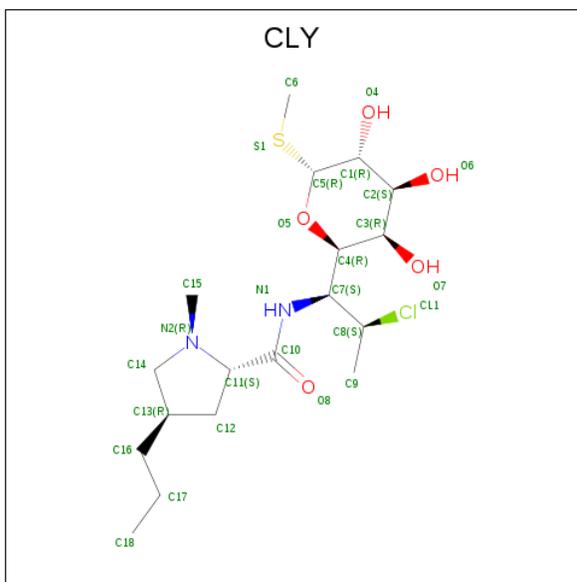
- Molecule 3 is a protein called Ribosomal Protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
3	L	130	130	130	0	0	130

- Molecule 4 is a protein called Ribosomal Protein L32.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
4	M	58	58	58	0	0	58

- Molecule 5 is CLINDAMYCIN (three-letter code: CLY) (formula: C<sub>18</sub>H<sub>33</sub>ClN<sub>2</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
5	A	1	27	18	1	2	5	1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

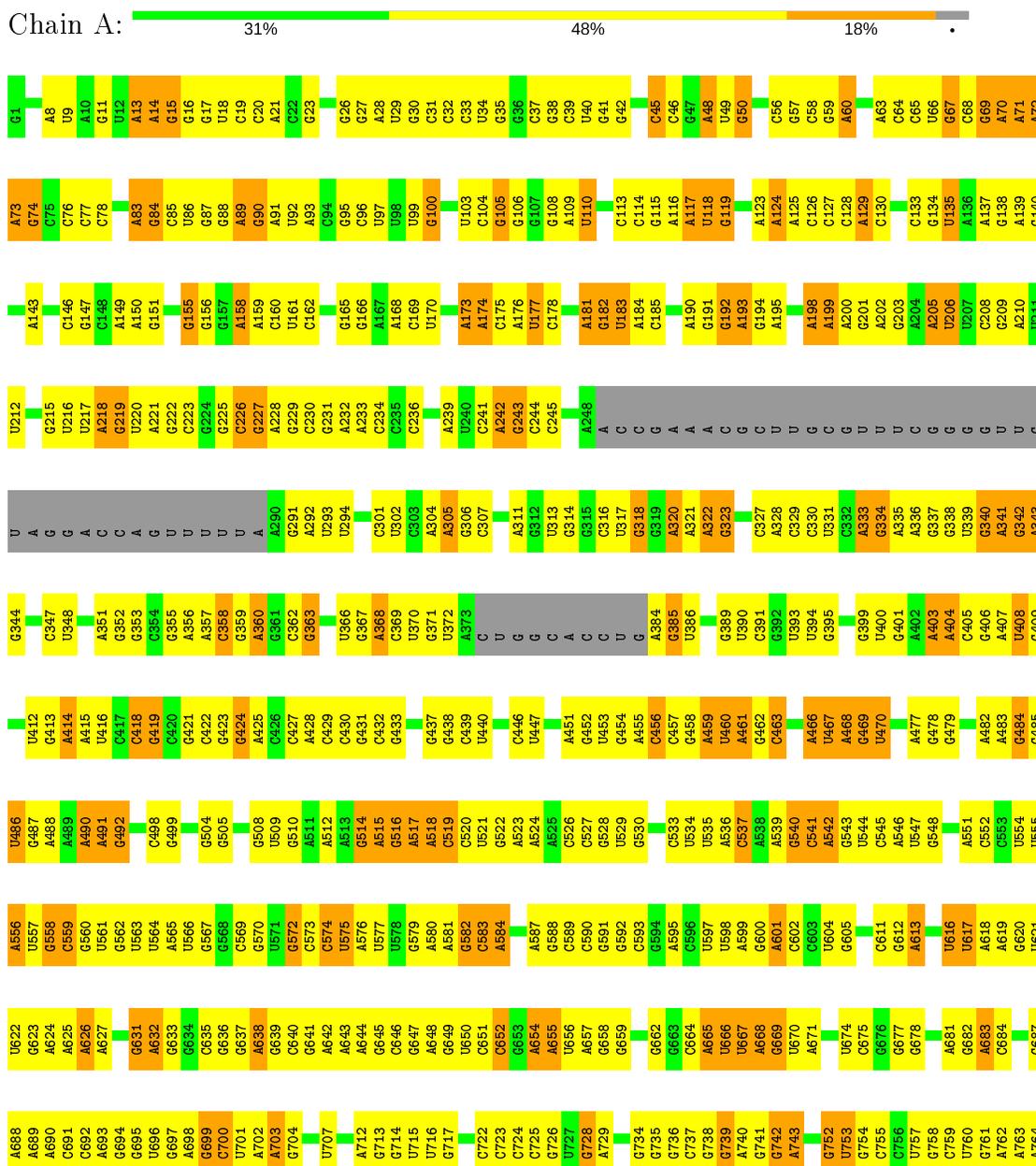
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	2	2	2	0	0

### 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



A1753	G1683	U1611	U1539	U1403	G1285	G1118	G1047	U974	G	A833	C765
G1754	U1612	U1613	C1540	C1494	G1286	U1119	U1048	C975	C	A838	A766
A1685	G1613	C1614	G1541	A1405	A1287	C1120	C1049	C976	U	U839	G767
C1756	A1686				U1288	G1121		G977	U	U839	U768
C1757	U1547	U1409	U1481	U1410	G1289	A1122	C1054	U978	A	G840	G773
C1758	U1481	U1411	U1482	C1411	G1290	G1123	A1055	A979	C909	G841	A774
U1689	C1549	C1412	G1483	C1412	C1271	U1194	U1056	G980	C910	A842	U775
G1690	U1551	C1415	G1484	C1415	G1272	U1195	A1057	G981	A911	G843	G776
G1691	C1552	C1416	U1485	U1416	G1273	U1197	A1059	G982	A912	G844	G777
A1692	G1553	C1417	U1486	A1417	A1274	U1199	C1060	A984	A913	C850	A778
A1693	G1554	C1417	C1487	C1417	A1275	U1199	G1060	A984	A913	C850	A778
A1694	A1555		G1488		U1276	G1200	A1061	G985	A918	C851	U784
U1697	A1556	A1420	G1489	A1420	A1278	G1201			U919	C852	U785
C1698	G1557	U1421	U1490	U1421	G1279	U1202	A1065	A994	A922	C853	U786
A1699	C1558	U1422			G1279	A1203	A1066	A995	A922	G854	U786
C1700	U1559	U1424	A1493	A1424	A1280	G1204	G1067	C996	A923	G854	U786
C1703	A1560	G1425	A1493	G1425	A1281	G1205	A1068	C997	C924	G855	U787
G1704	A1561	U1426	G1495	U1426	A1282		G1069	C998	C925	A856	G788
A1707	G1562	G1427	G1496	G1427	C1283	G1209	G1070	A999	U925	U857	G789
C1708	U1563	G1428	C1497	G1428	G1284	C1210	U1071	A999	C926	G858	A790
U1709	U1564	A1429	G1498	A1429	A1286	G1211	U1072	A1001	C927	U859	G791
U1710	A1565	G1430	A1499	G1430	A1287	U1141	G1073	C1002	A929	G861	A794
C1711	G1571	U1431	U1500	U1431	A1288	U1141	G1074	C1003	A930	A862	A795
G1712	G1572	A1432	G1501	G1432	A1289	A1143	C1075	U1005	G931	C863	A796
G1713	G1573	A1433	G1502	A1433	A1290	U1144		A1006	G932	C864	A797
A1714	A1574	U1434	G1503	U1434	A1291	G1145		C1006	G933	A865	G798
A1715	C1575	G1435	G1504	G1435	G1292	G1146		G1008	G934	U866	C799
A1716	G1576	G1436	U1505	G1436	A1292			A1007	U800	U800	U800
A1717	G1579	U1438	C1506	A1438	A1293	G1149		C937	A801	U868	A801
G1722	C1580	G1439	A1507	G1439	G1298	C1150		A1012	A802	C869	A802
A1723	U1581	U1440	U1508	U1440	A1298	U1151		G1013	C803	C870	C803
C1724	A1582	A1441	A1509	A1441	A1300	C1152		C1014	C804	U871	C804
G1725	G1584	C1442	A1510	C1442	A1301	A1153		C1016	G805	G872	G805
C1726	A1585	U1443	U1511	U1443	U1301	G1155		C1016	A806	U873	A806
C1727	A1588	C1444	U1512	C1444	A1302	G1155		U1019	C808	G875	C808
A1728	U1588	A1445	U1513	A1445	U1306	C1160		A1020	U810	A876	C809
C1729	G1589	U1446	C1514	U1446	U1307	U1161		A1021	G811	G877	U810
G1730	C1590	U1447	U1515	U1447	C1308	A1162		A1022	G812	C878	G811
U1733	U1592	G1450	G1519	G1450	C1309	C1163		G1024	A813	C880	A813
C1734	C1593	U1451	U1520	U1451	G1311	G1164		G1028	G814	A866	G814
G1735	U1594	A1452	C1522	A1452	U1312	C1166		C1029	U816	C887	U816
A1807	C1666	A1453	A1523	A1453	U1313	A1167		U1030	A817	G888	A817
C1808	A1667	C1456	C1524	C1456	A1314	G1168		C1031	G818	C889	G818
G1809	G1668	A1457	U1526	A1457	A1315	C1169		A956	C819	U890	C819
U1810	A1669	U1458	G1527	U1458	G1316	U1170		G1032	U820	A891	U820
A1811	G1736	A1459	C1528	U1459	C1316	U1171		G1033	A821	G892	A821
U1812	C1737	G1460	C1529	G1460	G1319	G1172		G1035	G822	G	G822
A1813	U1670	U1459	U1528	U1459	A1320	U1173		G1036	U823	G	U823
G1742	A1672	G1460	C1529	G1460	A1321	G1174		G1037	U824	G	U824
C1743	C1673	U1459	U1530	U1459	G1322	A1175		A1038	C825	G	U824
G1744	U1674	G1465	U1531	G1465	G1323	U1176		A1039	U826	C	C825
A1745	C1675	A1602	A1532	A1602	G1324	U1177		A1040	C827	U	U826
A1746	U1675	A1603	G1533	A1603	U1325	C1178		G1041	C828	U	C827
G1747	G1677	U1467	A1534	U1467	A1326	C1178		U1044	C829	A	C828
U1748	A1678	U1468	G1535	U1468	C1327	G1183		U1044	C830	C	G829
G1749	U1679	G1468	U1536	U1468	U1328	U1187		G1046	G831	C	C830
A1750	U1680	G1470	G1537	G1470	C1329	A1187		U1046	A832	A	A832
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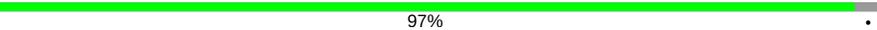
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A2761	G2762	G2763	A2764	A2765	G2766	G2767	A2768	A2769	A2770	A2771	A2772	A2773	A2774	A2775	A2776	A2777	A2778	A2779	A2780	A2781	A2782	A2783	A2784	A2785	A2786	A2787	A2788	A2789	A2790	A2791	A2792	A2793	A2794	A2795	A2796	A2797	A2798	A2799	A2800	A2801	A2802	A2803	A2804	A2805	A2806	A2807	A2808	A2809	A2810	A2811	A2812	A2813	A2814	A2815	A2816	A2817	A2818	A2819	A2820	A2821	A2822	A2823	A2824	A2825	A2826	A2827	A2828	A2829	A2830	A2831	A2832	A2833	A2834	A2835	A2836	A2837	A2838	A2839	A2840	A2841	A2842	A2843	A2844	A2845	A2846	A2847	A2848	A2849	A2850	A2851	A2852	A2853	A2854	A2855																																																																																																																																																																																																																																																																																																																																																																																													
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U2629	C2630	A2633	A2634	U2635	A2636	A2641	A2642	A2643	A2644	A2645	A2646	A2653	A2654	A2658	A2659	A2660	A2661	A2662	A2663	A2664	A2665	A2666	A2667	A2668	A2669	A2670	A2671	A2672	A2673	A2674	A2675	A2676	A2677	A2678	A2679	A2680	A2681	A2686	A2687	A2688	A2689	A2690	A2691	A2692	A2693	A2694	A2695	A2696	A2697	A2698	A2699	A2700	A2701	A2702	A2703	A2704	A2705	A2706	A2707	A2708	A2709	A2710	A2711	A2712	A2713	A2714	A2715	A2716	A2717	A2718	A2719	A2720	A2721	A2722	A2723	A2724	A2725	A2726	A2727	A2728	A2729	A2730	A2731	A2732	A2733	A2734	A2735	A2736	A2737	A2738	A2739	A2740	A2741	A2742	A2743	A2744	A2745	A2756	A2757	A2758	A2759	A2760	A2761	A2766	A2767	A2768	A2769	A2770	A2771	A2772	A2773	A2774	A2775	A2776	A2777	A2778	A2779	A2780	A2781	A2782	A2783	A2784	A2785	A2786	A2787	A2788	A2789	A2790	A2791	A2792	A2793	A2794	A2795	A2796	A2797	A2798	A2799	A2800	A2801	A2802	A2803	A2804	A2805	A2806	A2807	A2808	A2809	A2810	A2811	A2812	A2813	A2814	A2815	A2816	A2817	A2818	A2819	A2820	A2821	A2822	A2823	A2824	A2825	A2826	A2827	A2828	A2829	A2830	A2831	A2832	A2833	A2834	A2835	A2836	A2837	A2838	A2839	A2840	A2841	A2842	A2843	A2844	A2845	A2846	A2847	A2848	A2849	A2850	A2851	A2852	A2853	A2854	A2855																																																																																																																																																																																																																																																																																										
A2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	A2432	C2433	C2434	G2437	A2438	U2439	C2440	C2441	C2442	C2443	C2444	C2445	C2446	C2449	A2450	C2454	A2455	U2456	U2457	U2458	U2459	U2460	U2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	C2475	A2476	C2477	C2478	U2479	C2480	G2481	A2482	U2483	U2484	U2485	U2486	U2487	U2488	U2489	U2490	U2491	U2492	U2493	U2494	U2495	U2496	U2497	U2498	U2499	U2500	U2501	G2502	G2503	G2504	G2505	G2506	U2507	G2508	A2509	A2510	G2515	U2516	C2517	C2518	C2519	C2520	A2521	G2522	G2523	G2524	U2525	U2526	G2527	G2528	G2529	C2530	U2531	G2532	U2533	U2534	C2539	A2540	A2544	A2545	G2546	C2547	G2548	G2549	C2550	A2551	C2552	G2553	C2554	U2555	C2556	C2557	C2558	C2559	C2560	C2561	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585	C2586	C2587	C2588	C2589	C2590	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598	C2599	C2600	C2601	C2602	C2603	G2604	C2605	C2606	C2607	A2608	C2609	C2610	A2613	A2614	U2615	U2616	G2620	G2621	G2622	A2623	G2624	U2625	U2626	G2627	C2628	C2629	C2630	C2631	C2632	C2633	C2634	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649	C2650	C2651	C2652	C2653	C2654	C2655																																																																																																																																																																																																																																																																										
A2337	C2338	A2348	A2349	A2350	A2355	A2356	A2357	C2358	G2361	G2362	G2363	C2364	U2365	U2366	G2367	G2368	U2369	G2370	A2371	A2372	C2373	C2374	C2375	G2376	G2377	G2378	G2379	U2380	C2381	C2382	U2385	A2390	A2391	G2392	G2393	G2394	C2395	C2396	A2397	U2398	C2399	C2403	A2404	A2405	G2406	U2407	U2408	A2409	U2410	U2416	U2417	U2418	U2419	U2420	U2421	U2422	U2423	U2424	U2425	U2426	U2427	U2428	U2429	U2430	U2431	U2432	U2433	U2434	U2435	U2436	U2437	U2438	U2439	U2440	U2441	U2442	U2443	U2444	U2445	U2446	U2447	U2448	U2449	U2450	U2451	U2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	U2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	U2472	U2473	U2474	U2475	U2476	U2477	U2478	U2479	U2480	U2481	U2482	U2483	U2484	U2485	U2486	U2487	U2488	U2489	U2490	U2491	U2492	U2493	U2494	U2495	U2496	U2497	U2498	U2499	U2500	U2501	U2502	U2503	U2504	U2505	U2506	U2507	U2508	U2509	U2510	U2511	U2512	U2513	U2514	U2515	U2516	U2517	U2518	U2519	U2520	U2521	U2522	U2523	U2524	U2525	U2526	U2527	U2528	U2529	U2530	U2531	U2532	U2533	U2534	U2535	U2536	U2537	U2538	U2539	U2540	U2541	U2542	U2543	U2544	U2545	U2546	U2547	U2548	U2549	U2550	U2551	U2552	U2553	U2554	U2555	U2556	U2557	U2558	U2559	U2560	U2561	U2562	U2563	U2564	U2565	U2566	U2567	U2568	U2569	U2570	U2571	U2572	U2573	U2574	U2575	U2576	U2577	U2578	U2579	U2580	U2581	U2582	U2583	U2584	U2585	U2586	U2587	U2588	U2589	U2590	U2591	U2592	U2593	U2594	U2595	U2596	U2597	U2598	U2599	U2600	U2601	U2602	U2603	U2604	U2605	U2606	U2607	U2608	U2609	U2610	U2611	U2612	U2613	U2614	U2615	U2616	U2617	U2618	U2619	U2620	U2621	U2622	U2623	U2624	U2625	U2626	U2627	U2628	U2629	U2630	U2631	U2632	U2633	U2634	U2635	U2636	U2637	U2638	U2639	U2640	U2641	U2642	U2643	U2644	U2645	U2646	U2647	U2648	U2649	U2650	U2651	U2652	U2653	U2654	U2655	U2656	U2657	U2658	U2659	U2660	U2661	U2662	U2663	U2664	U2665	U2666	U2667	U2668	U2669	U2670	U2671	U2672	U2673	U2674	U2675	U2676	U2677	U2678	U2679	U2680	U2681	U2682	U2683	U2684	U2685	U2686	U2687	U2688	U2689	U2690	U2691	U2692	U2693	U2694	U2695	U2696	U2697	U2698	U2699	U2700	U2701	U2702	U2703	U2704	U2705	U2706	U2707	U2708	U2709	U2710	U2711	U2712	U2713	U2714	U2715	U2716	U2717	U2718	U2719	U2720	U2721	U2722	U2723	U2724	U2725	U2726	U2727	U2728	U2729	U2730	U2731	U2732	U2733	U2734	U2735	U2736	U2737	U2738	U2739	U2740	U2741	U2742	U2743	U2744	U2745	U2756	U2757	U2758	U2759	U2760	U2761	U2766	U2767	U2768	U2769	U2770	U2771	U2772	U2773	U2774	U2775	U2776	U2777	U2778	U2779	U2780	U2781	U2782	U2783	U2784	U2785	U2786	U2787	U2788	U2789	U2790	U2791	U2792	U2793	U2794	U2795	U2796	U2797	U2798	U2799	U2800	U2801	U2802	U2803	U2804	U2805	U2806	U2807	U2808	U2809	U2810	U2811	U2812	U2813	U2814	U2815	U2816	U2817	U2818	U2819	U2820	U2821	U2822	U2823	U2824	U2825	U2826	U2827	U2828	U2829	U2830	U2831	U2832	U2833	U2834	U2835	U2836	U2837	U2838	U2839	U2840	U2841	U2842	U2843	U2844	U2845	U2846	U2847	U2848	U2849	U2850	U2851	U2852	U2853	U2854	U2855
G1826	G1827	C1828	G1829	G1830	G1831	G1834	G1835	G1836	A1840	A1851	G1854	G1855	U1856	G1857	A1857	G1871	C1876	C1877	G1878	G1879	G1880	U1881	G1882	A1883	C1884	C1885	G1886	G1887	C1888	G1889	C1890	C1891	U1894	A1895	A1896	C1897	U1898	A1899	U1900	A1901	G1905	U1906	C1907	G1908	U1909	A1910	A1911	G1912	G1913	U1914	A1915	G1916	G1917	G1918	G1919	A1920	A1921	U1922	U1923	U1924	C1925	U1926	U1927	G1928	U1929	C1930	G1931	G1937	U1938	U1939	U1942	G1943	C1944	C1945	U1946	G1947	G1948	A1949	G1950	G1951	A1952	A1953	A1954	G1955	G1956	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	G2010	U2011	A2012	A2013	A2014	G2015	A2016	U2017	U2018	C2019	C2022	C2023	U2024	A2025	C2026	G2029	U2030	A2031	G2032	A2033	G2034	G2035	C2038	A2041	A2042	A2043	G2044	A2045	C2048	C2049	G2050	G2051	G2052	A2053	A2054	G2055	A2056	A2057	A2058	A2059	A2060																																																																																																																																																																																																																																																																																																																																																					

- Molecule 2: Ribosomal Protein L4

Chain K:  96%

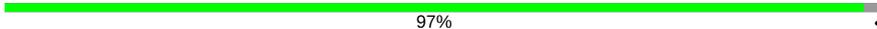


- Molecule 3: Ribosomal Protein L22

Chain L:  97%



- Molecule 4: Ribosomal Protein L32

Chain M:  97%



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	170.30Å 410.10Å 697.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, $R_{free}$	0.268 , 0.303	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	59946	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	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: MG, CLY

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	0.23	0/66661	0.66	2/103976 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	777	A	C2'-C3'-O3'	5.46	122.43	113.70
1	A	1746	A	C2'-C3'-O3'	5.25	122.09	113.70

There are no chirality outliers.

There are no planarity outliers.

### 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	59532	0	30004	1876	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	27	0	32	2	0
6	A	2	0	0	0	0
All	All	59946	0	30036	1876	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 21.

The worst 5 of 1876 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:1747:G:H4'	1:A:1749:G:H1'	1.29	1.14
1:A:2668:U:H4'	1:A:2669:C:H5'	1.32	1.12
1:A:940:G:H3'	1:A:941:U:H5''	1.34	1.09
1:A:367:G:H2'	1:A:368:A:H5''	1.34	1.08
1:A:1199:U:H3'	1:A:1200:G:H5''	1.35	1.07

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

#### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2765/2880 (96%)	556 (20%)	144 (5%)

5 of 556 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	23	G
1	A	45	C

5 of 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1279	G
1	A	1575	C
1	A	2633	A
1	A	1301	U
1	A	1355	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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$
5	CLY	A	2881	-	25,28,28	1.76	6 (24%)	29,40,40	1.28	3 (10%)

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
5	CLY	A	2881	-	-	4/21/53/53	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	CLY	C7-N1	4.62	1.53	1.45
5	A	2881	CLY	C12-C11	-3.02	1.48	1.53
5	A	2881	CLY	C10-N1	2.89	1.40	1.34
5	A	2881	CLY	C4-C7	2.77	1.56	1.53
5	A	2881	CLY	O5-C4	2.27	1.47	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	CLY	C11-C10-N1	-3.01	109.89	116.58
5	A	2881	CLY	O8-C10-N1	2.68	127.89	122.93
5	A	2881	CLY	C12-C11-C10	2.37	116.05	111.32

There are no chirality outliers.

All (4) torsion outliers are listed below:

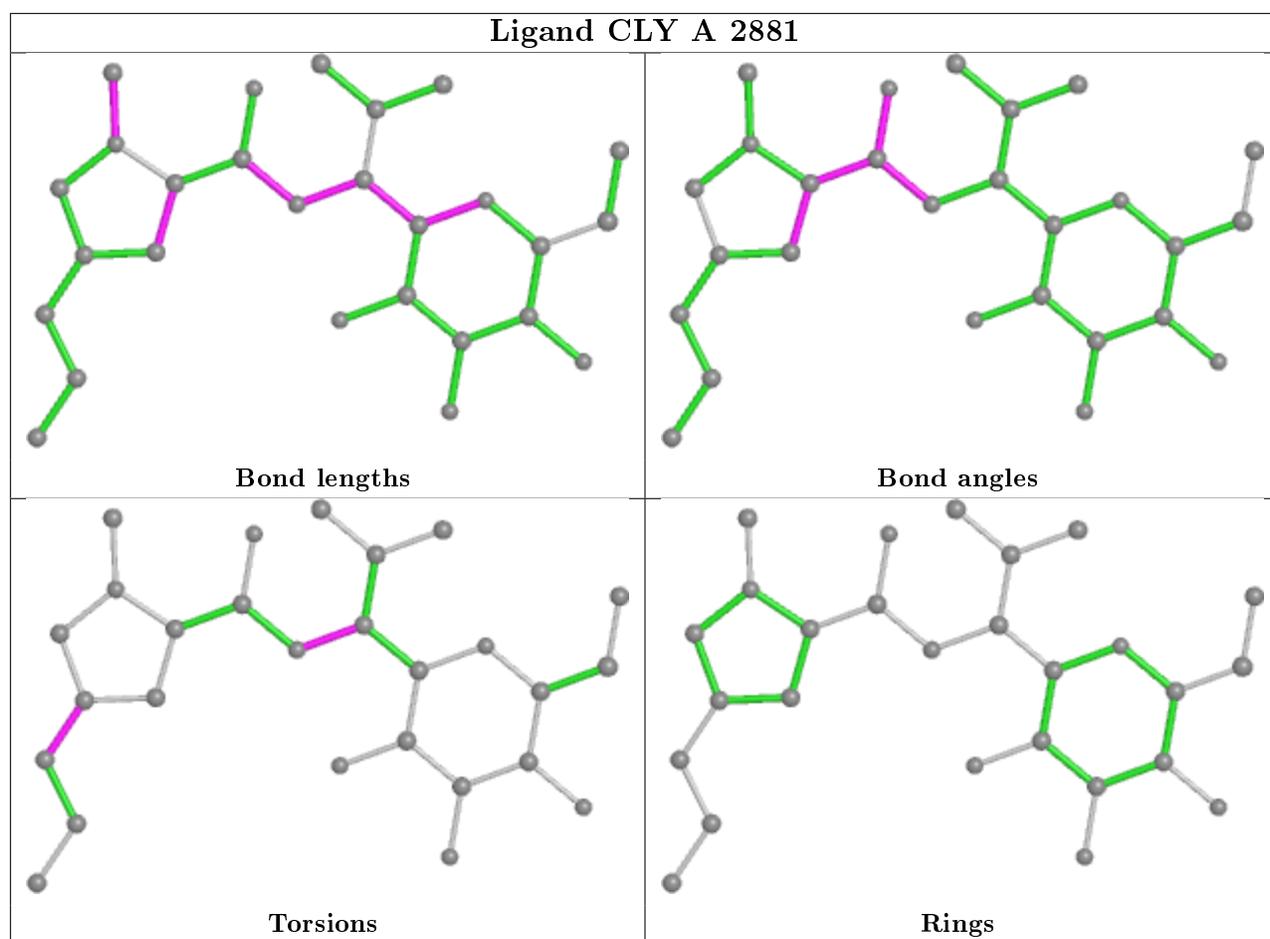
Mol	Chain	Res	Type	Atoms
5	A	2881	CLY	C8-C7-N1-C10
5	A	2881	CLY	C12-C13-C16-C17
5	A	2881	CLY	C14-C13-C16-C17
5	A	2881	CLY	C4-C7-N1-C10

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	CLY	2	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.