



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 12:16 am BST

PDB ID : 1JZZ
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 : 3.80 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)
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

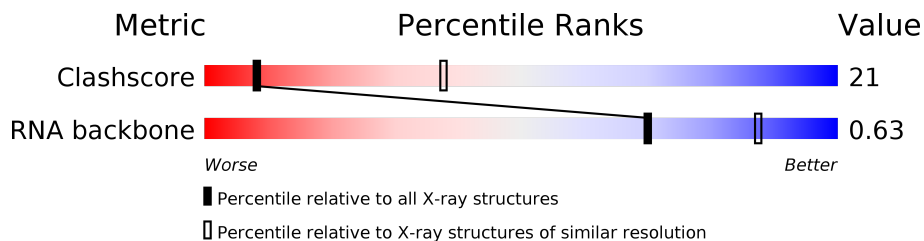
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

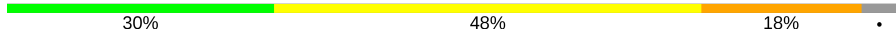


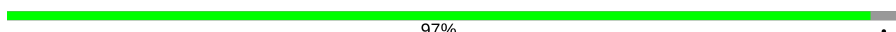
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1288 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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	
2	K	205	
3	L	134	
4	M	60	

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
5	ROX	A	2881	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59977 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

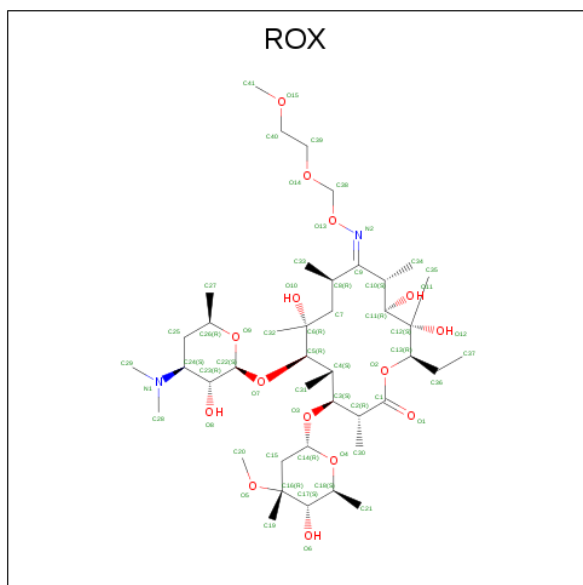
- Molecule 3 is a protein called Ribosomal Protein L22.

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 ROXITHROMYCIN (three-letter code: ROX) (formula: C₄₁H₇₆N₂O₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	58	41	2	15	0	0

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

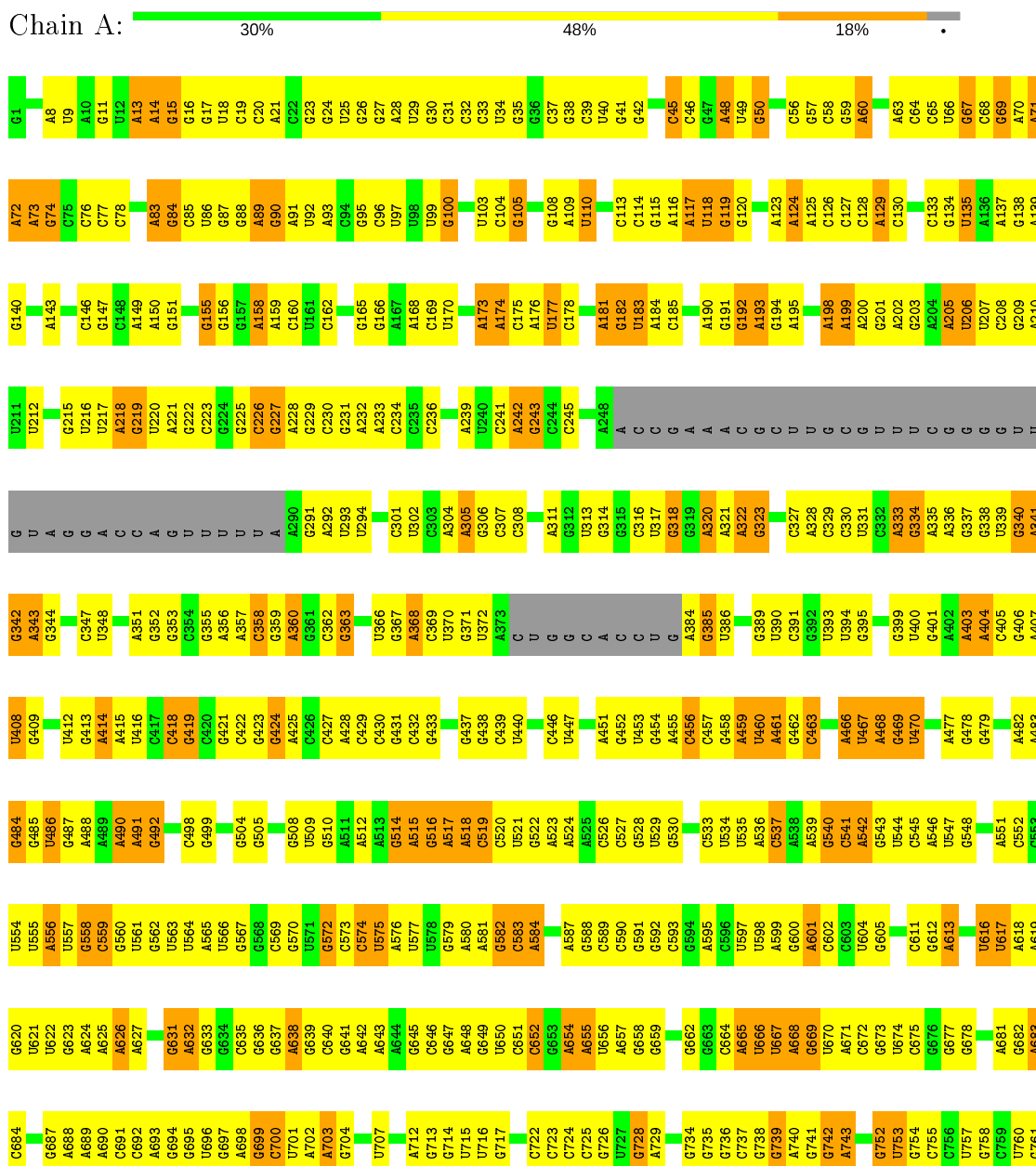
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	2	2	2	0	0

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

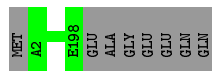


U1748	U1679	G1606	U1537	G1401	G1333	G1283	C1111	A970	U	C830	A762
G1749	U1680	A1607	A1538	G1402	G1402	C1284	U1112	A971	A	G831	A763
A1750	U1681	A1474	U1539	U1403	A1334	G1285	C1113	A972	A	A832	A764
A1751	A1682	U1475	C1540	U1404	G1337	G1286	G1118	U973	C	A833	C765
U1752	G1683	G1476	G1541	A1405	G1338	A1287	G1119	U974	C	A834	A766
G1684	G1542	G1480	U1409	U1406	U1339	U1288	G1120	C975	A	A838	G767
A1685	G1543	U1481	U1410	U1407	G1340	G1271	G1121	C976	C	U839	U768
G1686	A1544	U1482	C1412	C1412	G1341	U1194	G1122	U978	U	U840	G773
U1537	U1548	G1483	C1412	C1412	U1342	U1195	G1123	A979	A	A842	A774
A1538	U1549	G1484	C1413	C1413	C1343	U1196	U1124	G980	C909	G843	U775
G1539	C1550	U1485	C1415	C1415	G1344	U1197	G1125	C981	C910	G844	G776
U1540	U1551	U1486	A1416	A1416	G1345	A1275	A1126	C982	A911	U845	A777
C1552	C1552	C1487	C1417	C1417	C1346	U1276	C1127	G983	A912	A846	G778
G1553	G1553	G1488	A1420	A1420	C1347	A1277	G1128	A984	A913	C850	U784
A1554	U1490	U1489	U1421	U1421	U1348	A1278	A1129	A985	A918	C851	U785
A1555	U1491	U1490	G1425	G1425	G1350	U1280	U1130	A994	A919	U852	U786
A1556	A1556	A1493	U1426	U1426	G1351	A1281	C1134	A995	U919	C853	A787
G1557	C1557	G1494	U1427	U1427	G1352	A1282	C1135	A996	A922	G854	G788
C1558	G1558	G1495	G1428	G1428	A1353	G1283	G1136	C997	A923	G855	G789
G1559	G1559	G1496	G1429	G1429	A1354	G1284	A1137	C998	U925	A856	A790
U1560	A1560	C1497	G1430	G1430	A1355	A1285	A1138	A999	U926	U857	G791
A1561	A1561	G1498	A1429	A1429	G1356	U1286	A1139	G1000	C926	G858	U794
U1562	U1562	A1499	G1431	G1431	U1357	A1287	A1140	A1001	C927	U859	A795
U1563	U1563	U1500	U1432	U1432	C1358	A1288	U1141	C1002	G928	U860	A796
U1564	U1564	G1501	G1432	G1432	G1359	A1289	G1142	C1003	A929	G861	A797
G1571	G1571	U1502	A1433	A1433	C1364	A1290	A1143	A1004	A930	A862	C803
C1572	A1572	G1503	U1434	U1434	U1365	U1292	U1144	U1005	A931	C863	C804
G1573	G1573	U1504	G1435	G1435	U1366	A1293	C1145	G1006	G932	C864	G798
A1574	A1574	U1505	G1436	G1436	A1367	A1293	C1146	A1007	G933	A865	U800
C1575	C1575	U1506	A1437	A1437	G1367	A1294	G1147	G1008	G934	U866	A801
G1576	G1576	A1507	G1438	G1438	G1368	G1288	G1149	C1008	U942	G867	A802
U1577	U1577	G1508	G1439	G1439	A1369	A1299	C1150	A1012	U943	U873	C808
C1578	C1578	A1509	A1440	A1440	U1370	A1300	U1151	A1013	U944	G875	U810
A1580	C1580	U1510	A1441	A1441	G1371	U1301	C1152	A1022	A944	A876	G811
C1581	A1581	A1511	G1442	G1442	A1372	C1302	C1153	U1023	C948	G877	G812
A1582	A1582	A1512	G1443	G1443	G1373	C1302	C1154	G1024	C949	C878	A813
A1583	A1583	U1513	C1444	C1444	G1374	U1307	G1155	A1096	G950	A879	G814
C1584	C1584	C1514	A1446	A1446	G1377	U1307	G1156	A1097	G951	C880	A815
A1585	A1585	U1515	U1447	U1447	G1380	C1308	C1160	A1098	A952	U816	U816
U1586	U1586	G1519	G1450	G1450	G1381	C1309	U1161	A1099	A953	A886	A817
A1588	G1589	G1520	C1451	C1451	G1382	C1310	A1162	U1030	U954	G887	G818
G1589	C1590	U1521	U1452	U1452	G1383	C1311	C1163	C1031	G955	G888	C819
U1591	U1591	C1522	A1453	A1453	C1384	A1314	C1164	A1032	A956	C889	U820
C1592	C1593	C1524	C1456	C1456	C1385	A1315	G1165	G1033	G957	U890	A821
U1593	U1593	U1526	A1457	A1457	G1386	A1316	A1167	A1034	G958	A881	G822
A1595	A1595	G1527	A1458	A1458	G1387	G1316	C1169	G1035	C959	G892	U823
A1596	A1596	C1528	U1459	U1459	A1391	G1322	U1170	G1036	U960	G	U824
A1597	A1597	U1529	G1460	G1460	U1392	A1323	A1171	A1037	G	G	C825
C1598	C1598	U1530	C1461	C1461	G1393	G1324	U1172	U1038	A964	G	U826
U1599	U1599	U1531	C1462	C1462	G1394	G1325	G1173	A1039	C968	G	C827
G1600	G1600	C1532	G1465	G1465	G1394	G1326	G1174	U1039	U969	C	C828
A1601	A1601	A1532	C1466	C1466	A1397	C1327	A1175	U1037	U969	C	C829
G1602	G1602	G1533	U1467	U1467	G1398	C1328	C1183	U1038	U969	C	C829
A1603	A1603	A1534	U1468	U1468	G1399	C1329	G1184	A1039	U969	C	C829
U1604	U1604	C1535	U1469	U1469	A1400	G1330	C1185	G1041	U969	C	C829
G1605	G1605	G1536	G1470	G1470							

U1819	U1909	A1984	G2055	A2119	G2184	G2255	C2329	U2416	U2485	C2554	U2626	G2699	U2778	U2853
G1820	A1910	G1985	C2056	C2120	U2185	G2286	G2330	U2417	C2486	G2585	G2627	C2779	C2779	G2854
A1851	A1911	G1987	U2057	U2121	G2186	G2287	A2337	A2418	G2487	G2586	G2628	A2705	A2780	C2855
G1822	G1912	G1987	G2122	U2058	A2189	G2281	C2338	C2420	C2491	G2587	U2629	U2706	G2781	A2856
G1823	G1913	A1988	G2123	U2059	A2190	C2263	C2338	C2421	U2492	C2588	C2630	U2707	G2782	A2857
G1824	A1914	C1989	A2060	C2063	A2191	C2264	A2348	C2422	U2493	G2589	A2633	U2708	G2783	C2860
C1825	A1915	C1989	C2063	U	U2192	A2285	G2349	C2423	G2494	G2590	G2634	C2709	A2784	A2861
U1826	G1916	U1994	A2062	U	U2193	A2286	G2350	G2424	C2495	C2591	A2635	G2710	A2785	G2862
G1827	G1917	G1995	A2063	U	A2194	G2267	A2355	G2425	U2496	C2592	A2636	G2711	A2786	G2863
C1828	A1918	A1996	U2067	U	A2195	A2268	A2356	G2426	U2497	U2593	A2641	A2712	A2787	G2864
A1829	A1919	A1997	U2068	U	C2196	G2269	A2357	G2427	C2498	C2594	G2642	G2713	A2788	A2865
C1830	A1920	A1998	C2069	G	C2197	U2270	A2358	A2428	C2500	G2595	A2643	A2714	C2789	G2866
G1831	A1921	U1999	U2070	G	U2198	C2271	C2359	A2429	U2501	C2596	A2644	A2715	C2790	G2867
U1834	U1922	U2000	G2071	G2132	U2199	A2272	U2359	A2430	G2502	C2597	A2645	A2716	A2791	G2868
C1835	U1923	A2002	A2072	G2133	G2200	C2273	G2360	A2431	G2503	U2598	A2646	G2717	C2792	G2869
C1836	A1924	A2003	A2073	U2138	G2201	C2274	G2361	A2432	G2504	G2599	A2647	A2718	G2793	G2870
U1925	U1925	U2004	U2074	G2139	G2202	U2275	G2362	A2433	G2505	U2600	A2648	A2719	A2794	G2871
U1927	U1927	U2005	U2075	G2140	G2203	C2276	C2363	G2434	C2506	C2580	A2653	G2720	A2795	G2872
G1928	G1928	G2006	G2076	A	A2204	G2282	C2364	G2435	C2507	C2581	A2654	C2721	A2796	C2873
U1929	U1929	G2007	A2079	G	C2205	G2283	U2365	G2436	U2507	A2581	G2657	U2722	A2797	C2874
A1930	A1930	C2008	U2080	G	C2206	G2284	U2366	A2437	A2508	A2582	G2658	C2723	A2798	C2875
G1931	G1931	C2009	U2081	C	G2207	U2285	U2367	A2438	A2509	G2583	A2659	A2724	A2799	C2876
U1855	U2010	G2010	G2082	A	U2286	U2286	U2368	U2439	A2510	G2584	C2660	A2725	A2800	C2877
U1856	U2011	G2011	C2083	A	G2208	G2286	U2369	U2441	A2511	U2585	G2661	A2726	A2801	C
G1857	A2012	A2012	G2083	C	C2210	G2287	G2370	C2442	G2515	C2586	G2662	A2727	A2802	U
A1867	A2013	A2013	G2084	G	U2211	U2291	A2371	C2443	U2516	C2587	C2663	C2728	A2803	C
G1942	A2015	G2015	G2085	G	U2212	U2291	A2372	C2444	C2517	U2588	G2664	A2729	A2804	C
A1943	G2016	G2016	U2086	U	G2213	G2292	A2373	C2445	C2518	U2589	G2665	A2730	A2805	C
G1944	U2017	U2017	U2087	U	G2214	G2293	C2374	C2446	C2519	U2590	G2666	A2731	A2806	C
C1945	G2018	G2018	U2088	A	G2215	U2294	G2375	G2447	A2520	C2591	U2666	U2732	G2811	C
U1946	G2019	G2019	G2089	A	G2216	C2285	G2376	G2448	A2521	U2592	G2667	A2733	A2812	C
G1947	C2022	C2022	U2090	A	U2219	U2297	U2377	A2450	G2522	A2593	U2668	A2734	A2813	C
A1948	C2023	C2023	U2091	U	G2225	G2297	G2378	C2451	G2523	U2594	G2669	A2735	A2814	C
A1949	U2024	U2024	U2092	A	A2226	A2298	U2379	C2452	G2524	C2595	C2670	C2736	A2815	C
C1950	A2025	A2025	C2094	C2157	C2227	A2300	U2380	U2455	U2525	U2596	U2671	A2737	U2822	C
G1951	G2026	G2026	G2095	C2158	U2228	A2301	C2382	A2456	G2526	C2597	U2672	G2738	G2823	C
A1952	C2026	C2026	U2096	C2159	G2229	A2306	U2385	U2457	U2527	U2600	G2673	A2739	G2824	C
A1953	G2032	G2032	G	C2160	G2234	A2307	A2390	G2466	G2528	A2608	U2674	A2740	A2825	C
A1954	C2033	C2033	G	C2161	G2235	A2308	A2391	G2467	G2529	A2609	U2675	A2741	A2826	C
G1955	A2034	A2034	A	U2163	U2236	G2312	C2392	A2468	G2530	G2610	G2676	G2742	A2827	C
G1956	G	G	U	G2166	G2237	G2313	C2393	G2469	U2531	C2604	U2677	G2743	A2828	C
A1964	C2038	C2038	A	A2167	U2238	G2314	G2394	G2470	U2532	C2605	G2678	A2744	A2829	C
U1965	A2039	A2039	G	G2168	G2239	A2315	G2395	U2471	U2533	C2606	U2679	A2745	A2830	C
G1970	A2040	A2040	G2103	A2169	C2239	A2316	G2396	U2472	U2534	C2607	U2680	G2746	A2831	C
A1895	A2041	A2041	U2104	C2170	C2240	G2317	G2397	U2473	U2535	A2608	G2686	U2747	A2832	C
A1896	A2042	A2042	U2105	U2171	C2241	G2318	G2398	U2474	U2536	G2609	G2687	U2748	A2833	C
C1897	A2043	A2043	G2106	U2172	C2242	G2319	U2398	U2475	U2537	G2610	G2688	U2749	A2834	C
U1898	G2044	G2044	A2109	A2175	C2243	G2320	C2399	C2476	A2543	U2611	C2689	U2750	A2835	C
A1899	A2045	A2045	C	U2176	C2244	G2321	C2403	A2477	A2544	U2612	G2690	U2751	A2836	C
U1900	C2048	C2048	U	U2177	A2245	C2321	A2404	C2478	A2545	U2613	A2614	U2752	A2837	C
A1901	C2049	C2049	C	U2178	A2246	C2322	A2405	C2479	A2546	U2614	A2615	U2753	A2838	C
G1977	G2050	G2050	U	C2179	A2247	U2323	A2406	U2480	A2547	U2615	A2616	U2754	A2839	C
U1976	U2051	U2051	C	C2179	A2248	G2324	A2407	G2481	A2548	U2616	A2617	U2755	A2840	C
G1975	U2052	U2052	C	U2180	U2251	A2325	G2407	G2482	A2549	G2621	G2622	U2756	A2841	C
U1973	G2053	G2053	U	A2181	A2252	U2326	G2408	U2483	A2550	G2622	A2623	U2757	A2842	C
A1979	U2054	U2054	G	A2182	A2253	C2327	G2409	U2483	A2551	G2623	G2624	U2758	A2843	C
G1972	A2117	A2117	A2118	C2183	C2254	G2328	U2410	G2484	G2553	U2625	G2626	U2759	A2844	C

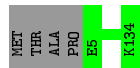
- Molecule 2: Ribosomal Protein L4

Chain K:  96%



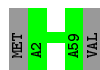
- Molecule 3: Ribosomal Protein L22

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, α , β , γ	170.40Å 410.70Å 694.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.209 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	59977	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: ROX, MG

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'	5.48	122.47	113.70
1	A	1746	A	C2'-C3'-O3'	5.31	122.19	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	1878	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	58	0	76	22	0
6	A	2	0	0	0	0
All	All	59977	0	30080	1896	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 1896 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'	1.31	1.13
1:A:940:G:H3'	1:A:941:U:H5''	1.35	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
5:A:2881:ROX:H211	5:A:2881:ROX:H71	1.36	1.06

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%)	557 (20%)	142 (5%)

5 of 557 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 142 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1278	A
1	A	1563	U
1	A	2633	A
1	A	1285	A
1	A	1354	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	ROX	A	2881	-	60,60,60	1.54	12 (20%)	84,89,89	3.12	44 (52%)

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	ROX	A	2881	-	-	11/80/115/115	1/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	ROX	C7-C8	4.75	1.60	1.54
5	A	2881	ROX	C7-C6	3.29	1.60	1.54
5	A	2881	ROX	O2-C13	-3.22	1.40	1.46
5	A	2881	ROX	C35-C12	3.02	1.58	1.52
5	A	2881	ROX	C10-C9	-2.96	1.50	1.53

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	ROX	O5-C16-C19	-7.64	98.19	110.92
5	A	2881	ROX	C34-C10-C9	-7.44	101.01	110.50
5	A	2881	ROX	O3-C3-C4	7.23	116.94	108.22
5	A	2881	ROX	C33-C8-C7	7.06	122.80	109.81
5	A	2881	ROX	C19-C16-C17	6.66	124.86	111.24

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	ROX	C17-C16-O5-C20
5	A	2881	ROX	O4-C14-O3-C3
5	A	2881	ROX	C1-C2-C3-O3
5	A	2881	ROX	O13-C38-O14-C39
5	A	2881	ROX	C1-C2-C3-C4

All (1) ring outliers are listed below:

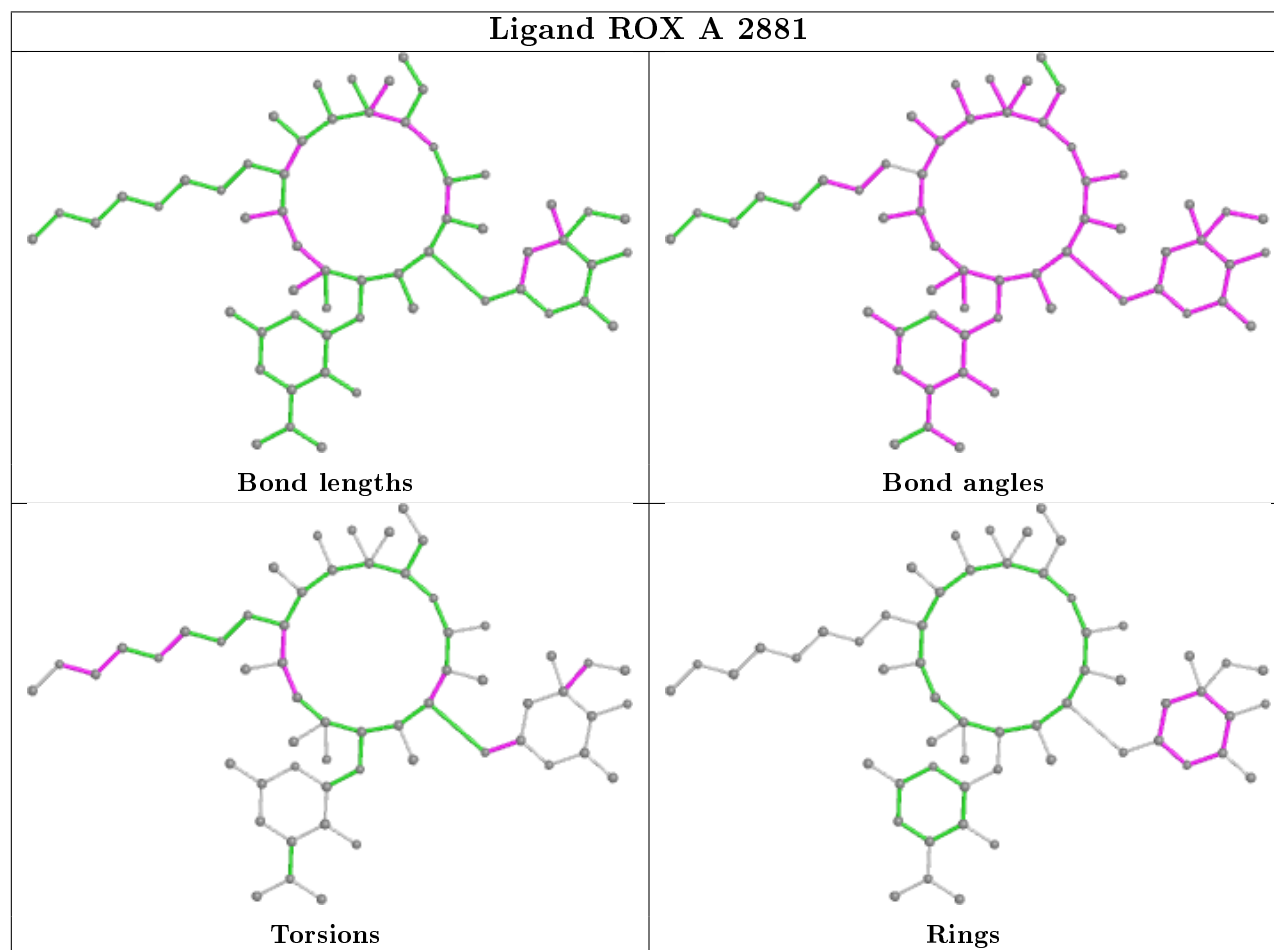
Mol	Chain	Res	Type	Atoms
5	A	2881	ROX	C14-C15-C16-C17-C18-O4

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	ROX	22	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.