



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:03 am GMT

PDB ID : 1J5A
Title : STRUCTURAL BASIS FOR THE INTERACTION OF ANTIBIOTICS
WITH THE PEPTIDYL TRANSFERASE CENTER IN EUBACTERIA
Authors : Schlutzen, F.; Zarivach, R.; Harms, J.; Bashan, A.; Tocilj, A.; Albrecht, R.;
Yonath, A.; Franceschi, F.
Deposited on : 2002-03-06
Resolution : 3.50 Å(reported)

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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

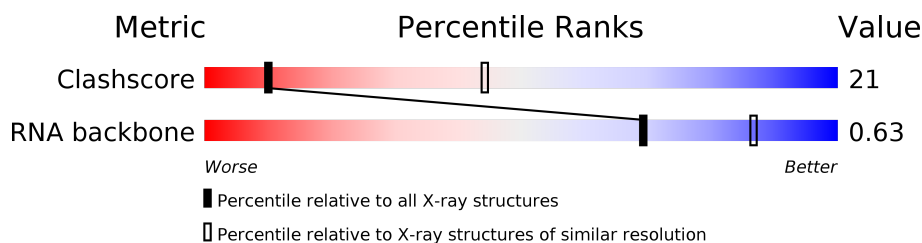
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

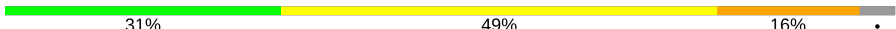

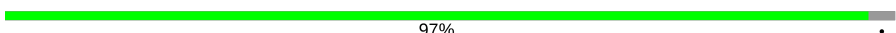

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1322 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

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	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	CTY	A	2881	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59971 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
1	A	2774	Total	C	N	O	P	0	0	0
			59532	26556	10982	19221	2773			

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
2	K	197	Total	C	0	0	197
			197	197			

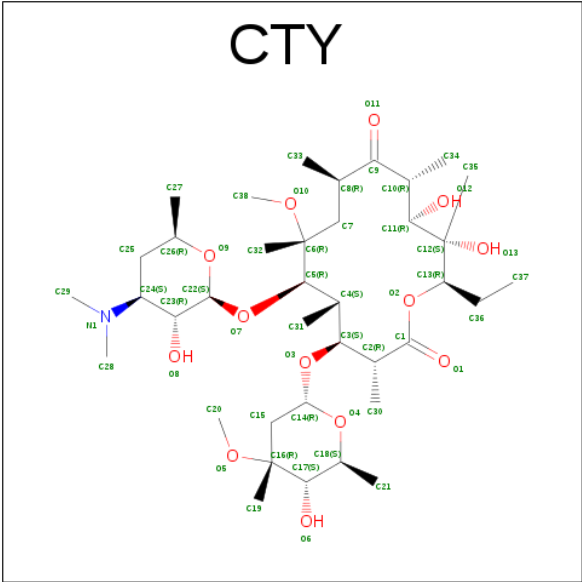
- Molecule 3 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L32.

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

- Molecule 5 is CLARITHROMYCIN (three-letter code: CTY) (formula: C₃₈H₆₉NO₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			52	38	1	13		

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

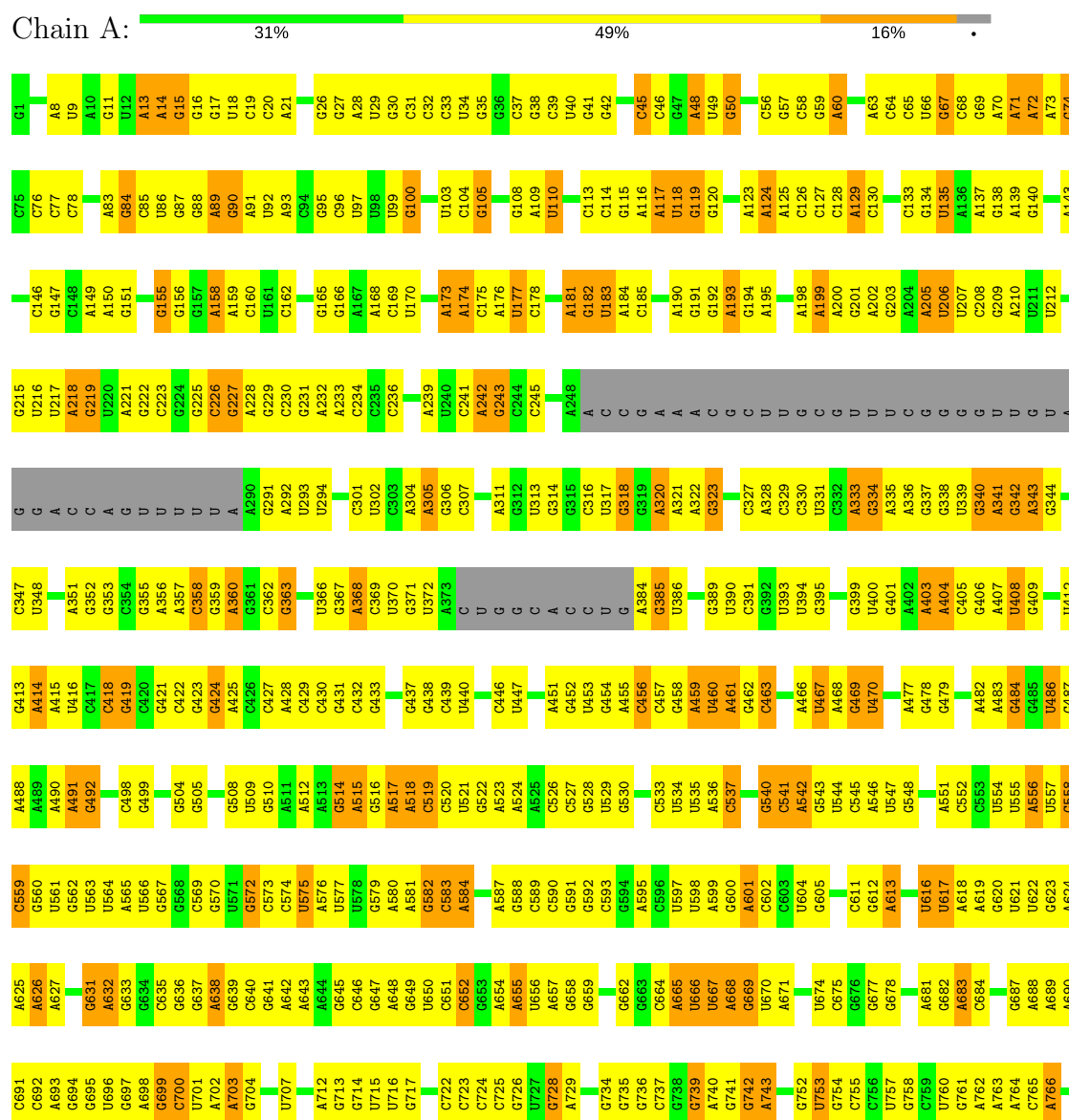
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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

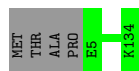


C1825	A1753	G1684	G1613	G1543	G1480	U1409	U1339	C1270	U1194	G1125	U1056	U978	C910	G841	G773
U1826	G1754	A1685	C1614	A1544	U1481	U1410	C1340	C1271	U1195	A1126	A1057	A979	A911	A842	A774
G1827	G1755	A1686	C1615	U1482	U1482	C1411	U1341	G1272	G1196	C1127	G1058	G980	A912	G843	U775
C1828	C1756	C1616	G1483	U1548	G1484	G1483	U1342	G1273	U1197	G1128	A1059	G981	A913	G844	G776
C1829	C1757	U1688	G1617	C1549	U1485	C1415	C1343	C1274	C1198	A1129	C1060	G982	C914	U845	A777
C1830	G1758	U1689	U1618	C1550	U1486	A1416	C1344	A1275	U1199	U1130	A1061	G983	C915	U846	G778
G1831	U1690	U1551	A1619	C1552	A1487	C1417	G1345	G1276	G1200	U1131	A1062	A984		C850	U784
	G1691	C1553		G1488	G1487		G1346	G1277	G1201	C1134	A1065	G985	A918	C851	U785
G1834	C1692	G1554	C1623	U1555	C1489	U1420	C1347	A1278	U1202	C1135	G1066		U919	C852	U786
C1836	A1693	G1554	A1624	G1554	C1489	A1421	C1348	G1279	A1203	A1136	G1067	A994	A922	U852	A787
	A1694	U1555	A1625	U1556	U1490	U1420	A1349	U1280	G1204	A1137	A1068	A995			G788
			A1626			U1424	G1350	A1281	G1205	A1138	G1069	C996	A923	U857	G788
A1840	G1697	G1557	C1627	G1558	A1493	G1425	G1351	A1282	G1209	A1139	G1070	C997	C924	U858	G789
	U1767	C1558		C1559	G1494	U1426	G1352	G1283	G1210	A1140	U1071	C998	U925	U859	A790
A1851	C1699	U1559	A1631	U1560	G1495	G1427	A1353	G1284	C1211	U1141	U1072	A999	U926	U860	G791
	U1769	U1560	A1632	U1561	G1496	G1427	A1354	G1285	G1212	U1142	U1073	A999	C926	U861	
G1854	C1702	G1561	C1633	U1562	G1497	G1428	A1355	A1286	U1212	A1143	G1074	A1001	C927	G861	A794
G1855	G1771	U1563	A1634	G1498	G1498	A1429	G1356	A1287	U1213	A1144	C1075	A1002	A929	C863	A795
U1856	C1773	U1563	G1635	U1563	A1499	G1430	U1357	A1288	C1214	U1145		C1003	A930	C864	A796
G1857	A1774	U1564		U1564	U1500	U1431	G1358	A1289	A1215	G1146		A1004	A931	A865	A797
	A1775		C1640		C1501	G1432	G1359	A1290	G1216		G1079	U1005	G932	U866	G798
A1867	C1776	G1571	G1502	G1572	G1503	A1433	C1364	G1291	U1217	G1149	A1080	A1006	G933	U867	C799
	U1777	G1572	G1503	G1573	G1504	A1434	U1365	A1292	C1218	C1150	A1081	C1006	A1007	U868	U800
G1871	U1778	U1574	G1504	G1575	G1505	G1435	U1366	A1293	C1219	U1151	C1083	A1007	G934	C869	A801
		U1575	U1506	G1576	C1506	A1437	A1367	G1298	C1221	A1153	G1085		C937	C870	A802
C1876	A1782	U1576	C1648		C1507	G1438	G1368	U1299	G1222	A1154	G1086	A1012	G938	U871	G803
C1877		G1577			A1507	G1439	G1369	A1300	G1223	G1155	C1087	G1013	C939	G872	C804
C1878	U1787	U1579	U1651	G1579	G1508	G1439	G1370	A1301	U1224	U1170	A1099	G1014	G940	U873	G805
G1879	C1788	U1580	G1652	C1580	A1510	G1440	U1371	C1302	A1225	C1160	C1088	U1015	U941	A874	A806
C1880	G1716	U1581	U1653	C1581	A1511	G1442	A1372	U1306	A1226	U1161	C1090	C1016	U942	G875	A807
U1881	A1717	U1582	A1654	A1582	A1512	G1443	G1373	U1307	A1227	A1162	C1091	U1019	U943	G876	C808
G1882	C1791	U1583	C1655	U1583	U1513	G1444	G1374	U1308		A1163	U1092	A1020	G944	G877	G809
A1883	C1792	G1584	U1656	G1584	C1514	A1445	U1377	C1309	A1227	C1164	U1093	A1021	G945	C878	U810
C1884	A1794	U1585	U1657	A1585	U1515	U1446		C1310	C1234	A1166		U1022	C948	A879	G811
						U1447	G1377	C1311		A1096	A1096	U1023	G949	C880	G812
C1888	G1798	U1588	G1660	U1588	G1519	U1450	C1380	G1312	G1240	A1167	A1097	G1024	G950	A866	A813
C1889	A1799	G1589	C1661	G1589	G1520	G1450	G1381	G1313	G1241	G1168	G1098		G951	G867	G814
G1890		U1590	U1662	U1590	U1521	C1451	G1382	U1314		C1169	A1099	U1030	G952	G868	A815
C1891	C1801	U1591	C1663	U1591	C1522	U1452	C1383	A1314	U1244	U1170	G1100	G1031	A953	C888	U816
A1892	G1730	C1592	G1664	U1592	A1523	A1453	C1384	A1315	G1245	A1171	U1101	A1032	U954	C889	A817
		C1593	C1665	C1593	C1524		C1385	G1316		U1172	G1102	G1033	G955	U890	G818
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A1895	C1734	U1595	U1667	U1595	U1526	A1457	G1387	A1321	G1250	G1174	G1104	G1035	A957	G892	U820
C1897	G1735	A1596	G1668	A1596	G1527	A1458		G1322	A1251	A1175	U1105	G1036	G958	G	A821
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A1899	G1737	C1598	G1670	C1598	C1529	U1460	U1392	G1324	C1253	U1177	A1107	U1038	U960	G	U823
U1900	U1811	G1599	U1671	U1599	U1530	G1461	G1393	U1325		C1178	U1108	A1039		C	U824
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	A1813	U1601	C1673	U1601	A1532	C1466		U1327	A1259	C1183		G1041		U	U826
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C1907	G1816	U1604	U1676	A1604	C1535	U1469	C1399	G1330	U1262	C1186	C1113	G1045	C830	C	C829
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G2867	C2788	A2713	U2635	G2561	C2494	G2423	G2351	A2266	C2193	U	A2063	A1997	G1918
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U2890	A2812	U2736	U2665	U2589	U2517	C2446	C2374	U2289	U2215	A	U2089	C2019	G1947
U2891	G2813	A2737	U2666	U2590	A2518	G2447	C2375	U2290	G2216	A	U2090	C2020	C1948
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U2894	C2816	C2740	C2669	U2593	U2521	A2450	C2378	U2293	U2219	A	U2093	C2023	G1951
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U2900	C2827	A2746	U2677	U2599	U2527	A2456	U2384	U2299	U2225	U	U2099	C2029	C1965
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U2904	U2831	G2750	U2681	U2603	U2531	C2460	U2388	U2303	G2229	A	U2103	C2033	C1972
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U2906	U2840	C2752	U2683	U2605	U2533	G2462	U2390	U2305	U2231	U	U2105	C2035	U1974
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U2908	C2842	C2754	U2685	U2607	U2535	G2464	U2392	U2307	U2233	U	U2107	C2037	U1976
U2909	A2843	G2755	U2686	U2608	U2536	G2465	U2393	U2308	U2234	C	U2108	C2038	U1977
U2910	C2844	C2756	U2687	U2609	U2537	G2466	U2394	U2309	U2235	U	U2109	C2039	A1984
U2911	G2845	U2757	U2688	U2610	U2538	G2467	U2395	U2310	U2236	C	U2110	C2040	G1985
U2912	U2846	G2758	U2689	U2611	U2539	A2468	U2396	U2311	U2237	U	U2111	C2041	G1986
U2913	C2847	C2759	U2690	U2612	U2540	G2469	U2397	U2312	U2238	C	U2112	C2042	G1987
U2914	A2848	U2760	U2691	U2613	A2541	U2470	U2398	U2313	U2239	U	U2113	C2043	A1988
U2915	C2849	U2761	U2692	U2614	U2542	U2471	U2399	U2314	U2240	C	U2114	C2044	U2059
U2916	G2850	U2762	U2693	U2615	U2543	G2472	U2400	U2315	U2241	U	U2115	C2045	U2060
U2917	U2851	C2763	U2694	U2616	U2544	A2473	U2401	U2316	U2242	C	U2116	C2046	U2061
U2918	A2852	U2764	U2695	U2617	U2545	U2474	U2402	U2317	U2243	U	U2117	C2047	U2062
U2919	G2853	U2765	U2696	U2618	U2546	G2475	U2403	U2318	U2244	C	U2118	C2048	U2063
U2920	U2854	C2766	U2697	U2619	U2547	A2476	U2404	U2319	U2245	U	U2119	C2049	U2064
U2921	C2855	U2767	U2698	U2620	U2548	U2477	U2405	U2320	U2246	C	U2120	C2050	U2065
U2922	A2856	U2768	U2699	U2621	U2549	G2478	U2406	U2321	U2247	U	U2121	C2051	U2066
U2923	U2857	C2769	U2700	U2622	U2550	A2479	U2407	U2322	U2248	C	U2122	C2052	A1989
U2924	G2858	U2770	U2701	U2623	U2551	U2480	U2408	U2323	U2249	U	U2123	C2053	U2067
U2925	C2859	U2771	U2702	U2624	U2552	A2481	U2409	U2324	U2250	C	U2124	C2054	U2068
U2926	A2860	C2772	U2703	U2625	U2553	A2482	U2410	U2325	U2251	U	U2125	C2055	U2069
U2927	U2861	U2773	U2704	U2626	U2554	U2483	U2411	U2326	U2252	C	U2126	C2056	U2070
U2928	C2862	U2774	U2705	U2627	U2555	U2484	U2412	U2327	U2253	U	U2127	C2057	U2071
U2929	A2863	U2775	U2706	U2628	U2556	U2485	U2413	U2328	U2254	C	U2128	C2058	U2072
U2930	U2864	C2776	U2707	U2629	U2557	U2486	U2414	U2329	U2255	U	U2129	C2059	U2073
U2931	C2865	U2777	U2708	U2630	U2558	U2487	U2415	U2330	U2256	C	U2130	C2060	U2074
U2932	A2866	U2778	U2709	U2631	U2559	U2488	U2416	U2331	U2257	U	U2131	C2061	U2075
U2933	U2867	C2779	U2710	U2632	U2560	U2489	U2417	U2332	U2258	C	U2132	C2062	U2076
U2934	G2868	U2780	U2711	U2633	U2561	U2490	U2418	U2333	U2259	U	U2133	C2063	U2077
U2935	C2869	U2781	U2712	U2634	U2562	U2491	U2419	U2334	U2260	C	U2134	C2064	U2078
U2936	A2870	C2782	U2713	U2635	U2563	U2492	U2420	U2335	U2261	U	U2135	C2065	U2079
U2937	U2871	U2783	U2714	U2636	U2564	U2493	U2421	U2336	U2262	C	U2136	C2066	U2080
U2938	C2872	U2784	U2715	U2637	U2565	U2494	U2422	U2337	U2263	U	U2137	C2067	U2081
U2939	A2872	C2785	U2716	U2638	U2566	U2495	U2423	U2338	U2264	C	U2138	C2068	U2082
U2940	U2873	U2786	U2717	U2639	U2567	U2496	U2424	U2339	U2265	U	U2139	C2069	U2083
U2941	C2874	U2787	U2718	U2640	U2568	U2497	U2425	U2340	U2266	C	U2140	C2070	U2084
U2942	A2875	C2788	U2719	U2641	U2569	U2498	U2426	U2341	U2267	U	U2141	C2071	U2085
U2943	U2876	U2789	U2720	U2642	U2570	U2499	U2427	U2342	U2268	C	U2142	C2072	U2086
U2944	C2877	C2790	U2721	U2643	U2571	U2500	U2428	U2343	U2269	U	U2143	C2073	U2087
U2945	A2878	U2791	U2722	U2644	U2572	U2501	U2429	U2344	U2270	C	U2144	C2074	U2088
U2946	U2879	C2792	U2723	U2645	U2573	U2502	U2430	U2345	U2271	U	U2145	C2075	U2089
U2947	G2880	C2793	C2724	U2646	U2574	U2503	U2431	U2346	U2272	C	U2146	C2076	U2090
U2948	A2881	U2725	U2647	U2575	U2575	U2504	U2432	U2347	U2273	U	U2147	C2077	U2091
U2949	C2882	C2726	U2648	U2576	U2576	U2505	U2433	U2348	U2274	C	U2148	C2078	U2092
U2950	U2883	U2727	A2654	U2577	U2577	U2506	U2434	U2349	U2275	U	U2149	C2079	U2093
U2951	G2884	G2728	G2657	U2578	U2578	U2507	U2435	U2350	U2276	C	U2150	C2080	U2094
U2952	A2885	A2729	U2658	A2581	U2579	U2508	U2436	U2351	U2277	U	U2151	C2081	U2095
U2953	G2886	U2730	C2659	U2582	U2580	U2509	U2437	U2352	U2278	C	U2152	C2082	U2096
U2954	U2887	C2731	C2660										

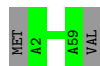
- Molecule 3: RIBOSOMAL PROTEIN L22

Chain L:  97% .



- Molecule 4: RIBOSOMAL PROTEIN L32

Chain M:  97% .



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	169.90Å 412.70Å 697.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.273 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	59971	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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, CTY

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($^{\circ}$)	Ideal($^{\circ}$)
1	A	1746	A	C2'-C3'-O3'	5.89	123.12	113.70
1	A	777	A	C2'-C3'-O3'	5.52	122.53	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	1877	0
2	K	197	0	0	0	0
3	L	130	0	0	0	0
4	M	58	0	0	0	0
5	A	52	0	69	32	0
6	A	2	0	0	0	0
All	All	59971	0	30073	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:2042:A:C2	5:A:2881:CTY:H383	1.63	1.30
1:A:2042:A:N3	5:A:2881:CTY:H383	1.62	1.14
1:A:1747:G:H4'	1:A:1749:G:H1'	1.29	1.12
1:A:940:G:H3'	1:A:941:U:H5''	1.34	1.09
1:A:1199:U:H3'	1:A:1200:G:H5''	1.35	1.08

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%)	555 (20%)	0

5 of 555 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	45	C
1	A	48	A

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](#)

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	CTY	A	2881	-	54,54,54	1.61	10 (18%)	83,83,83	3.01	41 (49%)

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	CTY	A	2881	-	-	1/75/110/110	1/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	CTY	O2-C13	-3.14	1.40	1.46
5	A	2881	CTY	C19-C16	-2.16	1.47	1.52
5	A	2881	CTY	C2-C1	2.00	1.56	1.51
5	A	2881	CTY	C12-C13	2.04	1.58	1.54
5	A	2881	CTY	C15-C16	2.14	1.57	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2881	CTY	O5-C16-C19	-7.30	98.20	110.96
5	A	2881	CTY	C7-C6-C5	-5.13	103.81	110.21
5	A	2881	CTY	O5-C16-C15	-5.10	104.43	112.95
5	A	2881	CTY	C27-C26-C25	-5.08	105.25	113.39
5	A	2881	CTY	C15-C16-C17	-4.99	98.23	107.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2881	CTY	C20-O5-C16-C17

All (1) ring outliers are listed below:

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

1 monomer is involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2881	CTY	32	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.