



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:12 PM GMT

PDB ID : 1J5A
Title : STRUCTURAL BASIS FOR THE INTERACTION OF ANTIBIOTICS
WITH THE PEPTIDYL TRANSFERASE CENTER IN EUBACTERIA
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Deposited on : 2002-03-06
Resolution : 3.50 Å(reported)

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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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

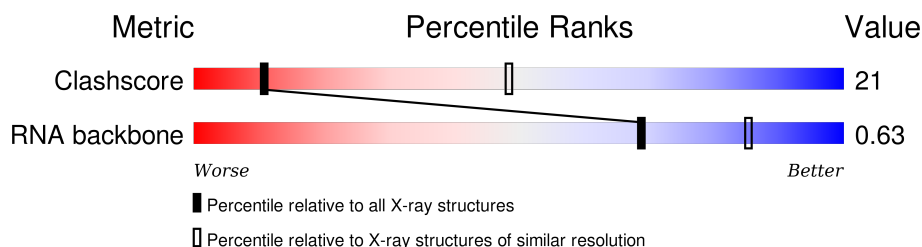
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

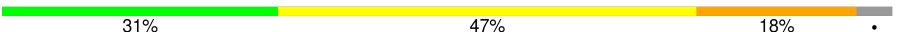

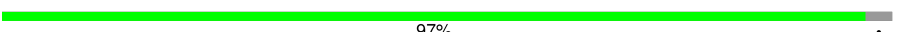
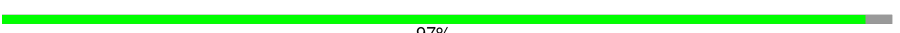
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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	 31% 47% 18% .
2	K	205	 96% .
3	L	134	 97% .
4	M	60	 97% .

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			

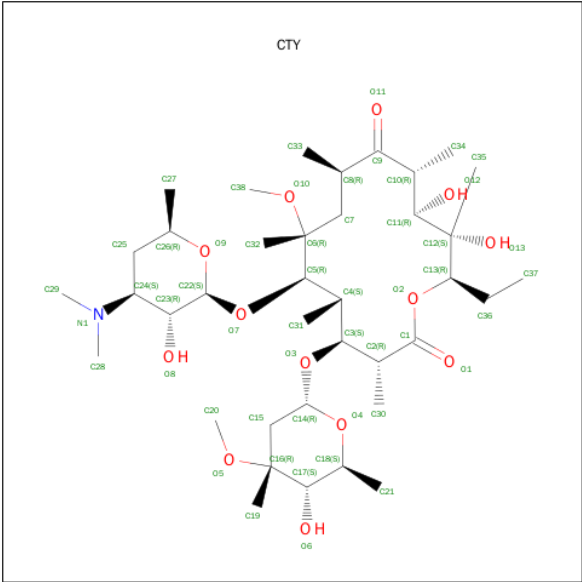
- Molecule 3 is a protein called RIBOSOMAL PROTEIN L22.

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).

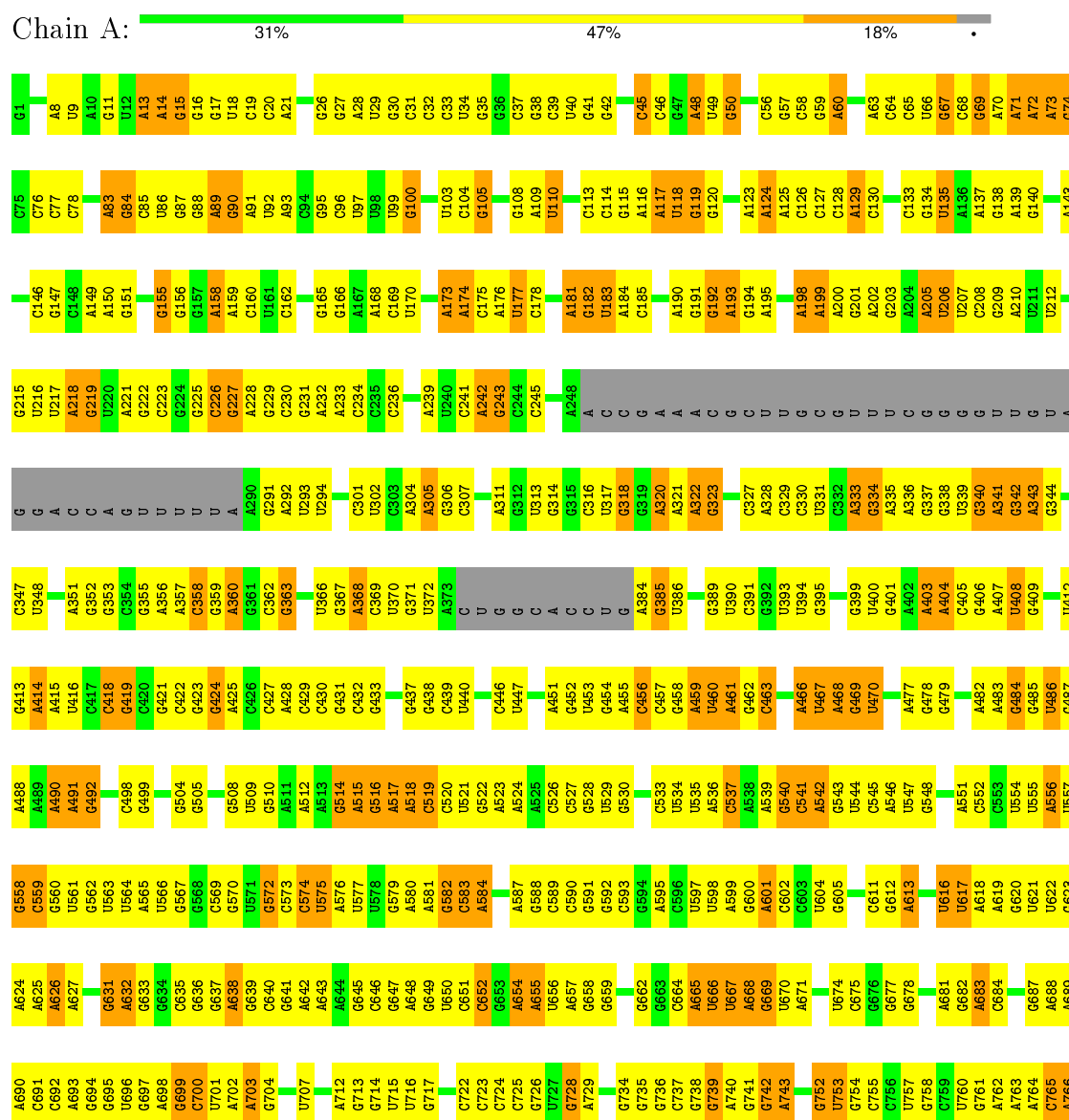
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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 errors 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 ($\text{RSRZ} > 2$). 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



C1824	U1752	G1683	U1612	G1542	G1480	U1409	G1338	G1269	G1193	U1124	A1055	G997	C909	U840	G773
C1825	A1753	G1684	G1613	G1543	U1481	U1410	U1339	C1270	U1194	G1125	U1056	U978	C910	G841	G774
U1826	G1754	A1685	C1614	U1544	U1482	C1411	C1340	C1271	U1195	A1126	G1057	A979	A911	A842	A775
G1827	G1755	A1686	C1615	U1483	G1483	C1412	G1341	G1272	G1196	G1127	G1058	G980	A912	G843	G776
C1828	C1756	U1687	G1616	U1548	G1484	U1413	U1342	G1273	U1197	G1128	A1059	C981	A913	G844	G777
C1829	C1757	U1688	G1617	C1549	U1485	G1414	C1343	C1274	C1198	A1129	C1060	C982	C914	U845	A777
C1830	C1758	U1689	U1618	C1550	U1486	G1415	C1344	U1275	U1199	U1130	A1061	G983	C915	A846	G778
C1831	U1752	U1690	A1619	U1551	A1416	A1416	G1345	A1276	G1200	C1134	A1065	A984	U918	C850	U784
C1832	C1762	C1691	C1552	C1487	C1417	C1417	C1346	G1277	G1201	C1135	G1066	U994	U919	C851	U785
C1833	A1763	C1553	G1553	G1488	U1420	A1420	C1347	A1278	U1202	C1136	G1067	U995	A922	U852	U786
C1836	A1764	G1554	U1490	U1421	U1421	U1421	A1348	G1279	A1203	G1137	G1068	A995	A923	U857	A787
C1837	U1765	A1555	U1491	U1422	U1422	U1422	A1349	U1280	G1204	A1138	G1069	C996	A924	G858	G788
C1840	U1766	A1556	U1492	U1423	U1423	U1423	G1350	A1282	G1205	A1139	G1070	C997	C924	U859	G789
C1841	U1767	C1557	U1493	U1424	U1424	U1424	G1351	A1283	G1209	A1140	U1071	C998	U925	U860	G790
C1842	U1768	C1558	G1494	G1425	G1425	G1425	G1352	C1283	C1210	U1141	U1072	A999	U926	G861	G791
C1843	U1769	C1559	G1495	G1426	G1426	G1426	A1353	G1284	C1211	G1142	G1073	G1000	C927	G862	A794
C1844	U1770	A1560	U1496	G1427	G1427	G1427	A1354	A1285	G1211	A1143	G1074	A1001	G928	A862	A795
C1845	A1771	A1561	C1497	G1428	G1428	G1428	A1355	U1286	U1212	U1144	C1075	C1002	A929	C863	A796
C1855	C1772	U1562	G1498	A1429	A1429	A1429	G1356	A1287	U1213	U1145	U1079	C1003	A930	C864	A797
U1856	C1773	U1563	A1499	G1430	G1430	G1430	U1357	A1288	G1214	G1146	G1079	A1004	A931	C865	A798
G1857	U1774	U1564	U1500	U1431	U1431	U1431	C1358	A1289	G1215	U1150	A1081	U1005	A932	C866	A799
C1867	A1775	G1571	G1502	G1432	G1432	G1432	G1359	A1290	G1216	G1149	A1082	C1006	A933	U868	U800
C1871	A1776	C1572	G1503	U1434	U1434	U1434	C1364	A1292	C1218	U1151	G1082	A1007	A934	C869	A801
C1872	U1777	G1573	G1504	G1435	G1435	G1435	U1365	A1293	C1219	U1152	G1083	G1008	C937	C870	A802
C1873	U1778	A1574	U1505	G1436	G1436	G1436	A1366	G1298	C1221	A1153	G1084	U1012	G938	U871	C803
C1876	A1782	C1575	U1506	U1437	U1437	U1437	U1367	G1299	C1222	A1154	G1085	A1013	G939	U872	C804
C1877	U1787	G1576	A1507	G1438	G1438	G1438	G1368	A1299	G1223	A1155	C1087	G1014	G940	U873	A805
C1878	C1788	U1710	U1508	G1439	G1439	G1439	A1300	U1301	G1224	U1156	A1088	U1015	U941	A874	A806
C1879	A1715	G1579	A1509	G1440	G1440	G1440	U1370	C1302	A1225	C1160	C1089	C1016	U942	G875	A807
C1880	G1716	C1580	A1510	A1441	A1441	A1441	G1371	U1306	A1226	U1161	C1090	U1019	U943	A876	C808
C1881	A1717	C1581	A1511	G1442	G1442	G1442	A1372	U1307	A1227	A1162	C1091	A1020	A944	G877	C809
C1882	C1791	A1582	A1512	G1443	G1443	G1443	G1373	U1308	A1228	C1163	C1092	A1021	G945	C878	U810
A1883	C1792	U1583	C1514	G1444	G1444	G1444	G1374	U1309	A1229	C1164	U1093	A1022	G946	A879	G811
C1884	U1723	G1584	U1514	U1445	U1445	U1445	G1375	C1310	A1233	G1165	U1094	U1023	C948	C880	A812
C1885	C1724	A1585	U1515	U1446	U1446	U1446	G1377	C1311	C1234	A1166	A1096	U1024	G949	C881	A813
C1886	C1725	U1586	U1516	U1447	U1447	U1447	C1380	G1312	G1240	A1167	A1097	G1024	G950	A886	G814
C1887	G1726	A1588	G1519	U1448	U1448	U1448	G1381	U1313	G1241	G1168	G1098	U1030	G951	G887	A815
C1888	U1727	C1589	U1520	C1450	C1450	C1450	G1382	U1314	U1244	G1169	A1099	U1031	G952	G888	U816
C1889	A1728	C1590	U1521	U1451	U1451	U1451	C1383	A1314	G1245	U1170	G1100	A1032	G953	C889	A817
C1890	C1729	U1591	C1522	U1452	U1452	U1452	G1384	A1315	G1246	U1171	U1101	U1033	U954	U890	A818
C1891	G1730	G1664	A1523	U1453	U1453	U1453	C1385	G1316	G1249	U1172	G1102	G1034	G955	A891	C819
C1892	U1733	C1665	C1524	U1454	U1454	U1454	A1386	U1326	U1250	G1173	C1103	U1035	A956	C892	U820
C1893	U1734	G1666	A1525	C1456	C1456	C1456	G1387	A1321	A1251	G1174	G1104	G1036	G957	G	A821
A1895	C1735	U1596	U1526	A1457	A1457	A1457	U1387	G1322	G1251	A1175	U1105	U1037	G958	G	G822
A1896	G1736	C1597	C1528	U1458	U1458	U1458	A1391	C1323	C1252	U1176	A1106	U1038	G959	G	U823
C1897	A1737	U1598	U1529	U1459	U1459	U1459	U1392	G1324	C1253	U1177	A1107	U1039	U960	G	U824
C1898	G1738	G1670	C1530	G1460	G1460	G1460	G1393	U1325	G1254	C1178	U1108	A1039	U961	C	C825
C1899	U1739	U1599	U1530	U1461	U1461	U1461	G1394	U1326	G1255	U1178	A1109	A1040	A964	C	U826
C1900	U1740	C1600	C1531	U1462	U1462	U1462	C1394	C1327	G1256	C1183	G1110	G1041	U962	U	C827
C1901	G1742	U1601	A1532	C1463	C1463	C1463	A1397	C1328	A1259	G1184	C1111	U1044	C968	A	C828
C1902	C1743	G1602	G1533	U1464	U1464	U1464	G1398	G1329	G1261	C1185	U1112	G1045	U969	C	U829
C1903	U1744	A1603	A1534	U1465	U1465	U1465	C1399	U1330	U1262	G1186	C1113	U1046	A970	C	C830
C1904	G1745	U1604	C1535	U1466	U1466	U1466	U1400	G1333	G1263	A1187	G1118	U1047	A971	A	A831
C1905	U1746	C1605	G1536	G1470	G1470	G1470	G1401	U1334	C1264	A1188	U1119	U1048	G972	G	A832
C1906	G1747	C1606	U1537	U1471	U1471	U1471	G1402	A1335	G1265	G1189	U1120	U1049	U973	C	A833
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C1908	U1749	U1608	C1539	U1473	U1473	U1473	U1404	A1337	A1267	G1191	A1123	C1054	C976	A	U835
C1909	A1750	U1609	U1540	U1474	U1474	U1474	C1405	G1337	U1268	A1192	G1123				
C1910	C1751	U1610	U1541	U1475	U1475	U1475									
C1911	U1752	U1611													
C1912															
C1913															

C2860	U2783	U2629	G2557	C2419	C2338	C2262	A2189	G2123	U2059	C1989	U1914
A2861	A2784	C2630	C2558	C2420	A2348	C2263	A2190	C2124	A2060	U1994	A1915
G2862	A2785	C2631	U2559	C2421	G2349	C2264	A2191	C2125	C2061	G1995	G1916
G2865	G2786	A2633	G2560	G2422	G2350	A2265	U2192	U	A2063	G1996	C1917
A2866	A2787	U2635	G2561	G2423	G2355	A2267	A2194	U	U2067	A1997	G1918
G2867	C2788	A2636	U2564	G2425	A2356	G2268	C2195	U	U2068	A1998	A1919
G2868	C2789	A2641	C2565	G2426	A2357	G2269	U2196	G	U2069	A1999	A1920
U2869	G2790	G2642	A2568	U2427	C2358	C2270	U2197	G	U2070	U2000	A1921
C2870	A2791	G2643	U2569	C2428	U2359	C2271	U2198	C2132	G2071	G2001	U1922
U2871	C2792	U2638	G2570	A2429	G2360	C2272	U2199	G2133	G2072	U2002	U1923
A2874	G2793	A2644	C2571	G2430	G2361	C2273	G2200	U2138	C2073	A2003	C1925
C2875	C2794	G2645	U2572	G2431	G2362	C2274	G2201	U2139	U2074	U2005	U1926
C2876	G2795	A2653	U2573	G2432	G2363	U2275	G2202	G2140	U2075	G2006	G1928
A2877	A2801	A2654	A2574	G2433	C2364	C2276	G2203	A	U2076	G2007	U1929
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	A2809	G2588	U2584	C2444	G2370	G2287	C2210	C	G2084	A2013	U1939
	A2810	G2589	U2585	C2445	A2371	U2291	U2211	G	G2085	A2014	
	G2811	C2590	C2586	C2446	A2372	C2292	U2212	U	U2086	G2015	A1942
		G2591	U2587		A2373	G2293	G2213	G	U2087	A2016	A1943
		U2592	U2588		C2374	U2294		A	U2088	U2017	C1944
		G2593	C2589		G2375	U2295	G2217	A	C2089	G2018	A1945
		U2594	U2590		U2376	C2296	U2218	A	U2090	C2019	U1946
		C2595	G2591		G2377	U2297	U2219	U	C2091	G2022	G1947
		U2596	A2592		U2378	G2298	G2225	A	U2092	C2023	C1948
		G2600	G2593		U2379	A2299	A2226	C2157	G2093	U2024	A1949
		C2601	U2594		U2380	G2300	C2227	C2158	C2094	A2025	G1950
		G2602	G2595		A2381	A2301	G2228	C2159	U2095	G2026	A1951
		G2603	C2596		C2382	U2306	G2229	C2160	U2096	G2032	A1952
		U2604	U2597		U2383	A2307	G2234	C2161	G	C2033	A1953
		G2605	C2598		U2384	A2308	G2235	C2162	G	A2034	G1954
		C2606	A2540		A2390		G2236	U2163	A	G2035	G1955
		G2607	U2541		A2391		U2237	G2166	U	A1964	
		U2608	A2542		G2392		G2238	A2167	A	C2038	U1965
		G2609	G2543		G2393		C2239	A2168	G2103	G2039	C1966
		U2610	A2544		G2394		C2240	A2169	G2104	A2040	
		A2613	U2545		C2395		U2241	C2170	U2105	A2041	G1970
		G2614	C2546		G2396		C2242	U2171	G2106	A2042	C1971
		U2615	C2547		U2397		C2243	U2172		G2043	G1972
		G2616	A2548		C2398		C2244	A2175	C	A2045	C1973
		U2617	G2549		U2400		A2245	U2176	G	G2048	U1974
		G2618	U2550		A2401		U2246	U2177	U	C2049	G1975
		C2619	G2551		A2402		U2247	U2178	C	G2050	U1976
		U2620	A2552		A2403		U2248	C2179	G	U2051	C1977
		G2621	U2553		A2404		U2249	C2180	U	C2052	A1980
		C2622	G2554		A2405		U2250	A2181	C	G2053	
		A2623	C2555		A2406		U2251	A2182	G	A2054	A1984
		G2624	U2556		G2407		C2252	C2183	C	G2055	G1985
		U2625	G2557		A2408		A2253	C2184	U	C2056	G1986
		G2626	U2558		A2409		G2254	C2185	G	U2057	U1987
		U2627	C2559		U2410		G2255	C2186		U2058	A1988
		G2628	U2560		U2411		G2256				
			A2556		U2412		A2337				
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					U2445						
					U2446						
					U2447						
					U2448						
					U2449						
					U2450						
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					U2481						
					U2482						
					U2483						
					U2484						
					U2485						
					U2486						
					U2487						
					U2488						
					U2489						

• Molecule 2: RIBOSOMAL PROTEIN L4

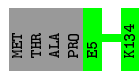
Chain K:

96%



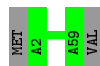
- Molecule 3: RIBOSOMAL PROTEIN L22

Chain L:  97% .



- Molecule 4: RIBOSOMAL PROTEIN L32

Chain M:  97% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90 Å 412.70 Å 697.00 Å 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%)	142 (5%)

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

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	CTY	A	2881	-	54,54,54	1.57	9 (16%)	83,83,83	3.07	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 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2881	CTY	O2-C13	-3.06	1.40	1.46
5	A	2881	CTY	C19-C16	-2.18	1.47	1.52
5	A	2881	CTY	C12-C13	2.03	1.58	1.54
5	A	2881	CTY	C15-C16	2.08	1.57	1.52
5	A	2881	CTY	C33-C8	2.53	1.61	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	-8.12	98.20	110.88
5	A	2881	CTY	C15-C16-C17	-7.65	98.23	107.81
5	A	2881	CTY	O5-C16-C15	-5.35	104.43	113.00
5	A	2881	CTY	C7-C6-C5	-5.19	103.81	110.03
5	A	2881	CTY	C27-C26-C25	-4.88	105.25	113.38

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.