



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2023 – 12:17 PM EDT

PDB ID : 1NJP
Title : The crystal structure of the 50S Large ribosomal subunit from *Deinococcus radiodurans* complexed with a tRNA acceptor stem mimic (ASM)
Authors : Bashan, A.; Agmon, I.; Zarivatch, R.; Schluenzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.
Deposited on : 2003-01-02
Resolution : 3.50 Å(reported)

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A user guide is available at

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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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**
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) : 2.35

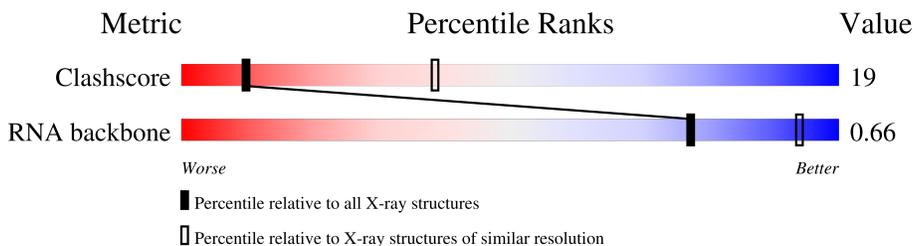
1 Overall quality at a glance

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	141614	1036 (3.58-3.42)
RNA backbone	3102	1002 (4.00-3.00)

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 of 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	0	2880	
2	5	35	
3	K	141	
4	T	237	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 60249 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is a RNA chain called tRNA acceptor stem mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	5	25	543	249	97	173	24	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
3	K	124	124	124	0	0	124

- Molecule 4 is a protein called GENERAL STRESS PROTEIN CTC.

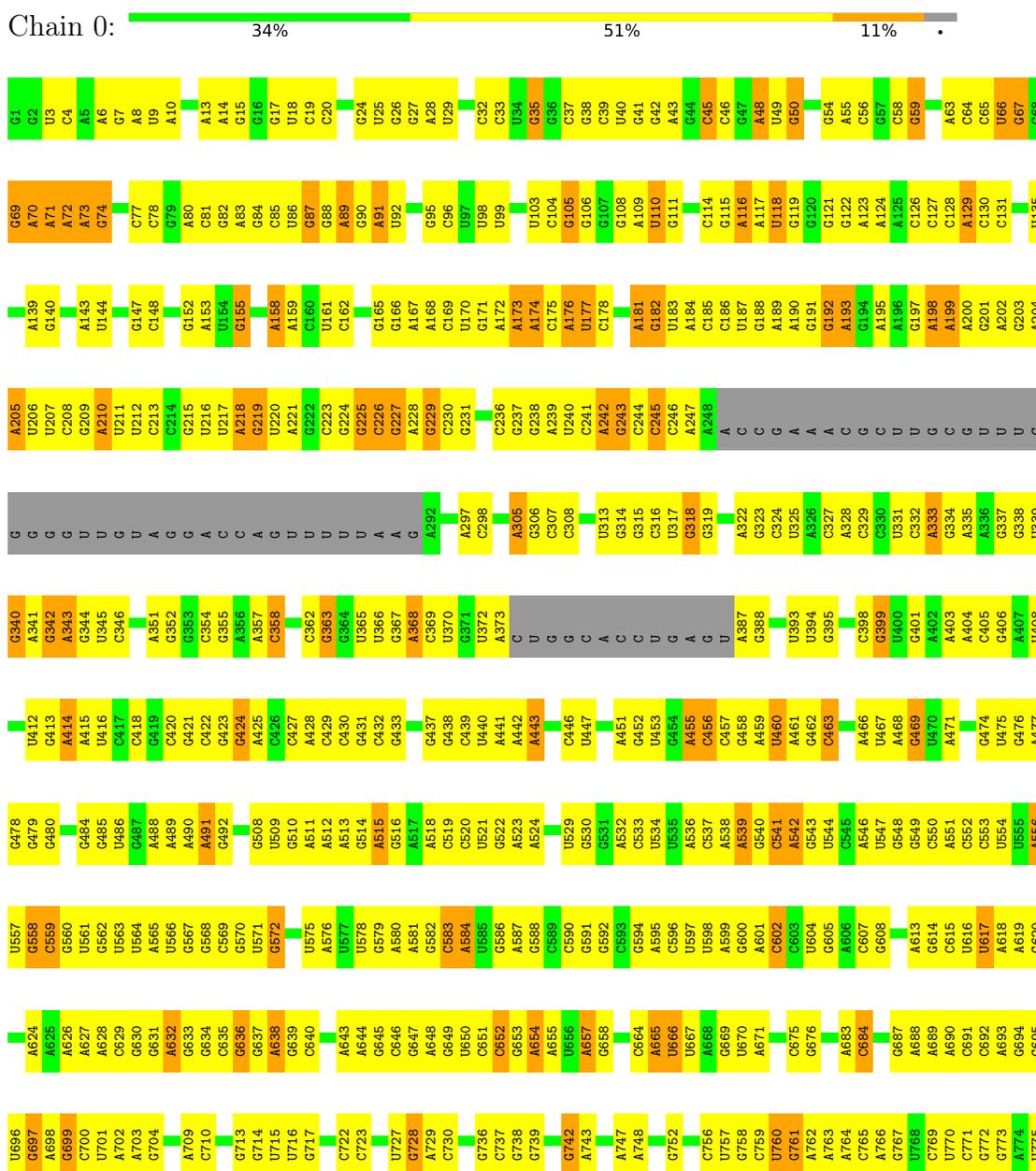
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
4	T	223	223	223	0	0	223

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 ribosomal RNA



G176	A838	A	U1044	U1141	C1214	A1288	H1357	A1441	G1508	A1587	G1659	G1742	U1819
A177	U839	C	G1045	G1142	U1217	A1289	C1358	C1442	A1509	U1591	G1660	G1743	G1820
G178	U840	C	U1046	A1143	C1218	A1290	G1359	G1443	A1510	U1592	C1661	C1744	A1821
U179	G841	C	G1047	A1144	C1219	G1291	C1360	C1444	A1511	C1593	G1662	C1745	C1822
G181	A842	U916	C1052	G1145	C1220	A1292	U1365	U1445	A1512	C1594	G1663	U1746	C1825
U182	G844	U917	G1053	G1146	C1221	A1293	A1366	U1446	U1513	C1595	C1664	C1747	U1826
G183	U845	U918	U1054	G1147	G1222	G1288	A1367	A1447	C1514	A1596	C1665	U1748	U1826
U184	A846	U919	A1055	G1148	G1223	U1301	G1368	A1448	A1515	A1597	G1666	G1749	C1829
U185	U847	U920	U1056	G1149	A1224	U1302	G1373	A1449	C1517	A1598	A1667	A1750	C1830
U186	U847	A921	G987	A1150	G1225	U1303	U1377	C1450	C1518	G1599	A1668	A1751	G1831
G187	U852	A922	U1057	U1151	A1226	U1304	G1377	U1452	G1519	U1600	G1670	G1754	C1835
G188	G853	U925	G1058	A1154	A1227	C1307	U1307	U1453	G1520	U1601	A1671	G1755	C1836
G189	G854	U926	U1059	G1155	U1227	G1308	C1308	C1455	C1524	G1602	A1672	G1760	C1836
A190	G855	C926	A1065	G1156	A1231	G1381	G1381	C1456	U1524	A1603	A1672	G1761	G1837
U191	G856	C927	G1066	U1156	U1232	G1382	G1382	A1457	G1527	A1604	C1677	C1762	G1838
U192	A856	U928	G1067	A1162	U1233	G1383	G1383	U1458	G1528	A1605	G1678	C1763	A1839
G193	G857	A929	C996	A1163	C1234	U1386	A1386	U1459	C1529	A1606	U1679	G1764	A1840
U194	G858	U930	G997	C1163	C1235	U1387	U1387	A1460	C1530	U1607	U1680	A1764	G1841
A195	G859	A931	C998	C1164	U1235	A1314	G1388	A1461	U1530	U1608	A1881	C1765	C1841
U196	U860	G931	U999	G1165	A1242	A1315	C1388	A1462	U1531	U1609	A1882	G1766	G1850
A197	G861	G932	G1000	A1166	G1243	U1316	C1389	A1463	C1532	G1610	A1883	U1766	G1850
G198	C864	G933	A1001	A1167	U1243	G1317	G1390	A1464	A1532	G1611	G1684	G1767	A1851
C199	A865	U934	C1002	G1168	G1244	A1318	A1391	G1465	G1533	U1612	U1685	U1770	G1855
U800	G865	C935	C1003	C1169	C1245	C1319	U1392	G1466	G1533	G1613	A1686	A1771	G1855
	U868	A936	A1004	C1169	G1248	A1320	U1393	U1468	U1539	G1614	U1469	U1771	G1857
	C868	U1005	U1081	U1172	A1250	G1323	A1397	U1470	G1541	G1615	G1470	A1774	C1858
	C869	C1006	A1084	G1173	G1251	G1324	G1398	G1471	G1542	C1616	G1471	A1775	C1858
	C870	A1007	U1085	U1177	C1252	U1325	G1399	G1472	G1543	U1617	C1692	A1776	A1860
	U871	C1008	C1086	C1178	G1254	U1326	C1399	C1473	A1544	U1618	U1692	A1777	G1861
	G872	G1009	G1087	A1179	G1254	U1327	G1402	U1474	G1545	U1619	C1696	U1778	C1862
	A873	U943	U943	U1019	U1257	C1328	U1403	U1475	G1552	C1696	C1703	U1778	C1862
	C808	G944	G1014	A1180	G1258	G1328	U1403	U1475	C1552	C1696	C1703	U1778	C1862
	C809	G945	U1015	C1181	G1259	U1329	G1407	U1478	C1557	G1621	G1704	A1780	C1865
	U810	U949	U1016	U1182	G1260	G1330	G1407	U1479	G1557	G1622	G1704	A1780	C1866
	G811	G950	C1017	C1183	A1260	G1331	G1407	U1480	C1558	C1623	C1708	A1785	G1871
	G812	G951	U1018	G1184	G1261	G1332	U1410	U1481	C1558	C1624	C1709	C1786	G1871
	A813	G951	U1019	G1185	U1262	G1333	C1411	U1482	A1561	U1626	U1710	U1787	G1880
	G814	A952	A1020	G1186	G1263	A1334	C1411	U1482	G1562	C1627	C1711	C1788	U1881
	A815	G953	A1021	A1187	C1264	A1335	G1414	A1486	G1566	C1628	G1712	U1789	U1882
	U816	U954	A1022	A1188	G1265	U1336	C1415	A1487	G1567	C1629	G1713	C1790	A1883
	A817	G955	U1023	G1189	U1266	G1337	C1416	A1488	A1567	G1629	A1714	C1791	A1884
	G888	U956	G1024	C1190	C1267	G1338	C1417	G1489	A1568	A1632	A1715	C1792	C1885
	C889	G957	A1025	G1191	U1268	U1339	C1418	U1490	A1568	C1633	G1716	A1793	C1886
	U890	C958	U1026	G1192	G1269	C1340	G1419	U1491	G1571	A1634	G1717	A1794	G1886
	A891	G	C1027	A1193	C1270	G1341	U1424	C1491	C1572	A1634	A1717	A1799	G1887
	G	U960	U1028	G1194	G1271	U1342	G1425	A1492	C1573	G1635	G1722	A1799	C1888
	G	G961	G1029	A1122	G1272	C1343	U1426	A1493	A1574	A1643	U1723	A1800	C1889
	C	A964	U1030	G1127	G1273	C1344	G1427	G1494	A1575	U1644	U1724	C1801	G1890
	C	G965	A1032	U1128	C1274	G1345	G1428	G1495	C1575	G1644	C1724	A1802	G1890
	U	G966	G1033	A1129	A1275	U1346	G1429	G1496	G1576	C1648	G1727	A1807	G1893
	C	G967	U1034	U1130	A1278	C1347	A1429	C1497	G1577	C1648	C1727	A1807	U1894
	A	C968	G1035	U1131	G1279	C1348	G1430	G1498	U1578	U1651	A1728	C1808	A1895
	C	C969	U1036	A1131	U1280	A1349	U1431	G1499	U1579	G1652	C1729	G1809	A1896
	C	A970	G1037	G1132	U1281	G1350	G1432	U1500	C1580	U1653	C1730	U1810	C1899
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	C	C972	U1039	G1133	G1205	G1352	U1434	G1502	A1582	U1655	U1732	U1812	U1900
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	C	U974	G1040	A1138	C1210	A1354	G1436	U1504	G1584	U1656	U1733	G1814	C1907
	U	U974	A1041	A1139	G1211	A1355	G1437	U1505	A1586	A1658	C1736	G1814	C1908
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A1910	A1980	U2051	G2421	A2356	U2485	C2554	G2622	G2782	G2862	A1910	A1980	U2051	G2421	A2356	U2485	C2554	G2622	G2782	G2862
A1911	A1981	G2052	G2422	A2357	C2486	G2555	A2623	U2783	U2863	A1911	A1981	G2052	G2422	A2357	C2486	G2555	A2623	U2783	U2863
G1912	C1982	G2055	G2423	A2358	C2491	C2558	U2624	U2705	G2867	G1912	C1982	G2055	G2423	A2358	C2491	C2558	U2624	U2705	G2867
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A1914	G1986	G2057	G2425	G2361	U2493	G2560	C2628	U2708	G2786	A1914	G1986	G2057	G2425	G2361	U2493	G2560	C2628	U2708	G2786
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A1920	A1996	U2062	A2432	U2366	U2498	C2565	A2636	A2713	G2797	A1920	A1996	U2062	A2432	U2366	U2498	C2565	A2636	A2713	G2797
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C1924	A2002	G2070	G2434	U2369	U2501	C2571	G2640	A2718	C2799	C1924	A2002	G2070	G2434	U2369	U2501	C2571	G2640	A2718	C2799
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C1930	U2008	A2079	A2448	C2382	G2508	G2576	C2645	G2728	U2807	C1930	U2008	A2079	A2448	C2382	G2508	G2576	C2645	G2728	U2807
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U1932	U2010	U2081	C2444	U2384	A2510	C2578	U2651	A2729	U2809	U1932	U2010	U2081	C2444	U2384	A2510	C2578	U2651	A2729	U2809
U2011	U2011	C2082	C2445	U2385	G2511	A2579	G2652	A2730	A2810	U2011	U2011	C2082	C2445	U2385	G2511	A2579	G2652	A2730	A2810
A2012	A2012	G2083	C2446	U2386	A2512	C2580	A2658	G2731	G2811	A2012	A2012	G2083	C2446	U2386	A2512	C2580	A2658	G2731	G2811
A2013	A2013	G2084	G2447	U2387	A2513	A2581	C2659	G2732	A2812	A2013	A2013	G2084	G2447	U2387	A2513	A2581	C2659	G2732	A2812
A2014	A2014	U2086	A2448	C2388	G2514	G2582	C2660	G2733	C2815	A2014	A2014	U2086	A2448	C2388	G2514	G2582	C2660	G2733	C2815
A2015	A2015	G2093	G2450	U2389	U2515	C2586	G2661	U2736	C2816	A2015	A2015	G2093	G2450	U2389	U2515	C2586	G2661	U2736	C2816
G2016	G2016	C2094	A2451	U2390	G2516	C2587	U2666	A2737	G2821	G2016	G2016	C2094	A2451	U2390	G2516	C2587	U2666	A2737	G2821
C2017	C2017	G2095	C2452	U2391	U2517	C2588	G2667	G2740	U2822	C2017	C2017	G2095	C2452	U2391	U2517	C2588	G2667	G2740	U2822
G2018	G2018	U2096	U2453	U2392	G2518	C2589	C2668	G2741	U2823	G2018	G2018	U2096	U2453	U2392	G2518	C2589	C2668	G2741	U2823
C2019	C2019	U2097	U2454	U2393	U2519	U2590	G2669	G2742	C2824	C2019	C2019	U2097	U2454	U2393	U2519	U2590	G2669	G2742	C2824
G2020	G2020	G	U2455	U2394	G2520	C2591	C2670	G2743	A2825	G2020	G2020	G	U2455	U2394	G2520	C2591	C2670	G2743	A2825
G2021	G2021	G	U2456	U2395	U2521	C2592	U2671	G2744	C2826	G2021	G2021	G	U2456	U2395	U2521	C2592	U2671	G2744	C2826
C2022	C2022	A	U2457	U2396	U2522	C2593	U2672	G2745	U2830	C2022	C2022	A	U2457	U2396	U2522	C2593	U2672	G2745	U2830
A1954	A1954	U	C2458	U2397	U2523	U2594	U2673	A2746	A2831	A1954	A1954	U	C2458	U2397	U2523	U2594	U2673	A2746	A2831
G1955	G1955	A	U2459	U2398	U2524	C2595	U2674	G2747	G2832	G1955	G1955	A	U2459	U2398	U2524	C2595	U2674	G2747	G2832
G1956	G1956	U	C2460	U2399	U2525	C2596	U2675	G2748	U2833	G1956	G1956	U	C2460	U2399	U2525	C2596	U2675	G2748	U2833
C1957	C1957	A	G2463	U2400	U2526	C2597	U2676	G2749	U2834	C1957	C1957	A	G2463	U2400	U2526	C2597	U2676	G2749	U2834
G1958	G1958	G	G2464	U2401	U2527	C2598	U2677	G2750	G2835	G1958	G1958	G	G2464	U2401	U2527	C2598	U2677	G2750	G2835
A1961	A1961	G2106	U2465	U2402	U2533	U2599	U2678	G2751	U2836	A1961	A1961	G2106	U2465	U2402	U2533	U2599	U2678	G2751	U2836
C1962	C1962	G2107	U2466	U2403	U2534	C2600	U2679	G2752	G2837	C1962	C1962	G2107	U2466	U2403	U2534	C2600	U2679	G2752	G2837
G1963	G1963	G2110	U2467	U2404	U2535	C2601	U2680	G2753	U2838	G1963	G1963	G2110	U2467	U2404	U2535	C2601	U2680	G2753	U2838
U1964	U1964	C	U2468	U2405	U2536	G2602	U2681	G2754	C2841	U1964	U1964	C	U2468	U2405	U2536	G2602	U2681	G2754	C2841
U1965	U1965	C	U2469	U2406	U2537	G2603	U2682	G2755	C2842	U1965	U1965	C	U2469	U2406	U2537	G2603	U2682	G2755	C2842
U1966	U1966	U	U2470	U2407	U2538	G2604	U2683	G2756	U2843	U1966	U1966	U	U2470	U2407	U2538	G2604	U2683	G2756	U2843
U1967	U1967	U	U2471	U2408	U2539	C2605	U2684	G2757	G2844	U1967	U1967	U	U2471	U2408	U2539	C2605	U2684	G2757	G2844
G1968	G1968	C	G2472	U2409	U2540	G2606	U2685	G2758	U2845	G1968	G1968	C	G2472	U2409	U2540	G2606	U2685	G2758	U2845
G1969	G1969	G	G2473	U2410	U2541	C2607	U2686	G2759	U2846	G1969	G1969	G	G2473	U2410	U2541	C2607	U2686	G2759	U2846
G1970	G1970	A2117	G2474	U2411	U2542	A2608	U2687	A2761	U2847	G1970	G1970	A2117	G2474	U2411	U2542	A2608	U2687	A2761	U2847
C1971	C1971	A2118	G2475	U2412	U2543	G2609	U2688	G2762	U2848	C1971	C1971	A2118	G2475	U2412	U2543	G2609	U2688	G2762	U2848
G1972	G1972	A2119	U2476	A2412	U2544	U2610	U2689	G2763	U2849	G1972	G1972	A2119	U2476	A2412	U2544	U2610	U2689	G2763	U2849
C1973	C1973	C2120	U2477	A2413	U2545	G2611	U2690	G2764	U2850	C1973	C1973	C2120	U2477	A2413	U2545	G2611	U2690	G2764	U2850
U1974	U1974	U2121	U2478	A2414	U2546	U2612	U2691	G2765	U2851	U1974	U1974	U2121	U2478	A2414	U2546	U2612	U2691	G2765	U2851
G1975	G1975	C	U2178	U2415	U2547	C2613	U2692	G2766	U2852	G1975	G1975	C	U2178	U2415	U2547	C2613	U2692	G2766	U2852
U1976	U1976	U	C2179	U2416	U2548	G2614	U2693	G2767	U2853	U1976	U1976	U	C2179	U2416	U2548	G2614	U2693	G2767	U2853
C1977	C1977	C	U2179	U2416	U2548	G2614	U2693	G2767	U2854	C1977	C1977	C	U2179	U2416	U2548	G2614	U2693	G2767	U2854
U1978	U1978	U	U2198	U2417	U2549	C2615	U2694	G2768	U2855	U1978	U1978	U	U2198	U2417	U2549	C2615	U2694	G2768	U2855
		U	U2199	U2418	U2550	C2616	U2695	G2769	U2856			U	U2199	U2418	U2550	C2616	U2695	G2769	U2856
		U	U2199	U2418	U2550	C2616	U2695	G2769	U2856			U	U2199	U2418	U2550	C2616	U2695	G2769	U2856
		U	U2199	U2418	U2550	C2616	U2695	G2769	U2856			U	U2199	U2418	U2550	C2616	U2695	G2769	U2856

● Molecule 2: tRNA acceptor stem mimic





- Molecule 3: 50S ribosomal protein L16

Chain K: 88% 12%



- Molecule 4: GENERAL STRESS PROTEIN CTC

Chain T: 94% 6%



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	169.90Å 409.90Å 695.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	60249	wwPDB-VP
Average B, all atoms (Å ²)	81.0	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: PPU

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	0	0.14	0/66467	0.63	0/103673
2	5	0.15	0/563	0.63	0/873
All	All	0.14	0/67030	0.63	0/104546

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	873	U	Sidechain

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	0	59359	0	29917	1724	0
2	5	543	0	290	11	0
3	K	124	0	0	0	0
4	T	223	0	0	0	0
All	All	60249	0	30207	1731	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 19.

The worst 5 of 1731 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)
1:0:940:G:H3'	1:0:941:U:H5''	1.22	1.14
1:0:1141:U:H3	1:0:2008:C:H5''	1.20	1.04
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.01
1:0:2548:G:H2'	1:0:2549:G:H5''	1.44	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.21	0.99

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	0	2757/2880 (95%)	413 (14%)	44 (1%)
2	5	22/35 (62%)	2 (9%)	0
All	All	2779/2915 (95%)	415 (14%)	44 (1%)

5 of 415 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	G
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1807	A
1	0	2245	A
1	0	1820	G
1	0	2093	G
1	0	2377	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PPU	5	35	2	32,40,41	2.78	7 (21%)	33,57,60	1.01	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PPU	5	35	2	-	1/21/43/44	0/4/4/4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	C-N3'	12.42	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.87	1.28	1.42
2	5	35	PPU	C6-N1	3.91	1.38	1.33
2	5	35	PPU	CE1-CZ	3.69	1.46	1.38
2	5	35	PPU	CE2-CZ	2.73	1.44	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	CM-OC-CZ	2.87	123.75	117.51
2	5	35	PPU	C9-N6-C6	2.30	126.49	119.51
2	5	35	PPU	C-CA-N	2.21	117.94	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5	35	PPU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.