



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 07:46 am BST

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.; Schlutzen, F.; Harms, J.M.; Berisio, R.; Bartels, H.; Hansen, H.A.; Yonath, A.
Deposited on : 2003-01-02
Resolution : 3.50 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)
Xtriage (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)	:	2.11

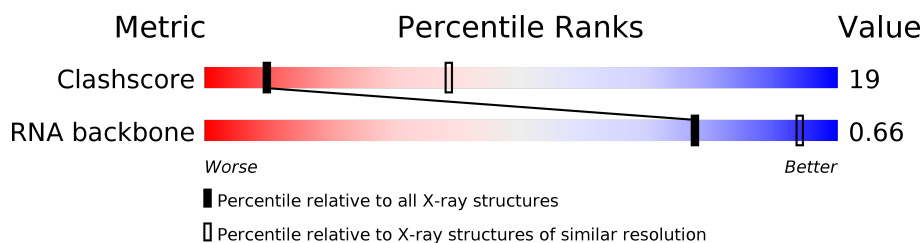
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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 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	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
1	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

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

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

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

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

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

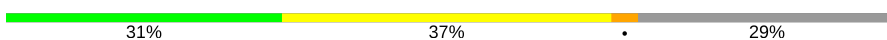
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	T	223	Total	C	0	0	223
			223	223			

U1819	G1859	A1587	G1508	A1441	U1357	A1288	C1214	U1141	U1044		A	A838	G776
G1820	G1660		A1509	C1442	C1358	A1289	U1217	G1142	G1045	U978	C	U839	A777
A1821	G1661	U1591	A1510	G1443	G1359	A1290	C1218	U1143	U1046	A979	C	U840	G778
C1822	G1662		A1511	G1444	G1360	G1291	C1219	U1144	G1047	C981		G841	U779
	G1663	C1593	U1512	A1445	U1365	A1292	C1220	G1145	C1052	U916		G842	U780
C1825	G1664	U1594	U1513	U1446	A1366	A1293	G1221	G1146	G1053	U917		G843	G781
U1826	G1665	A1595	C1514	U1447	U1367		G1222	G1147	G1054	U918		G844	U782
	G1666	A1596	U1515	A1448	G1368	G1288	C1223	G1148	G1055	U919		U845	G783
C1829	G1667	A1597	A1516	C1449			G1224	G1149	U1056	U919		U846	U784
G1830	G1668	C1598	C1517	G1450	G1373	U1301	A1224	G1150	G1057	G920		U847	U785
G1831	G1669	C1599	C1518	C1451	G1374		G1225	U1151	U1057	G921		U848	U786
	G1670	U1600	G1519	U1452	G1377	U1307	A1226	U1154	G1058	G922		U849	U787
C1835	A1671	U1601	G1520		C1308	C1308	A1227	A1154		A991		C853	G788
C1836	A1672	G1602		C1455	C1380	G1309		G1155	A1065	U925		G854	G789
G1837		A1603	C1524	A1456	G1381	C1310	A1231	U1156	U1066	C926		G855	A790
G1838	C1677	A1604		A1457	G1382		U1232	A995	G1067	C927		A856	G791
A1839	G1678		G1527	A1458	C1311	G1312	C1233	A1162	C996	G928		U857	U792
A1840	G1679	A1605	C1528	U1459	A1386	U1313	G1234	C1163	G1069	G929		G858	G793
	U1680	U1607	C1529		G1387	A1314	C1235	C1164	G1070	A930		U859	A794
C1841	U1681	A1608	U1530	A1463	G1388	A1315		G1165		G931		U860	A795
	A1881	U1609	C1531	A1464	C1389	G1316	A1242	A1166	G1073	G932		A796	
G1850	U1766	A1610	G1532	G1465	G1390	G1317	G1243	A1167	G1074	G933		A797	
A1851	G1683	U1611	G1533	G1466	A1391	A1318		C1168	C1075	C1002		C864	G798
	G1684	G1612	U1539	U1467	U1392	G1319	G1248	C1169	U1076	C935		A865	C799
G1855	A1685	G1613	U1540	U1468	G1393	A1320	A1250	U1172		A936		U800	
U1856	C1687	C1614	C1540	U1469			A1251	G1173	A1081	U1005		U868	
G1857		G1615	G1541	G1470	A1397	G1323	C1251	G1173		C939		C869	C803
A1858	G1691	A1616	G1542	G1471	G1398	G1324	C1252	U1177	A1084	C1006		C870	C804
U1859	C1692	G1617	G1543	U1472	C1399	U1325	G1253	U1178	G1085	C1008		G871	G805
G1861	U1618	U1614	A1544	C1473	U1326	U1326	G1254	C1178	G1086	U942		A806	A806
C1862	C1696	A1619	G1545	U1474	G1402	C1327		A1179	G1087	U943		A807	A807
		U1620	U1403	U1475	U1403	G1328	U1257	A1180	A1088	A944		C808	C808
C1865	C1703	G1621	C1552		G1407	U1329	G1258	C1181	C809	G945		A874	
G1866	G1704	G1622		U1478	G1407	G1330	C1259	U1182	G1090	C1016		A875	U810
G1871	C1708	C1623	G1557	G1479	U1410	G1331	A1260	U1183	C1091	C1017		A876	G811
	U1709	A1624	C1558	G1480	C1411	G1332	G1261	G1184	U1092	C1018		A877	G812
G1880	U1710	A1625	A1561	U1481	G1414	G1333	G1262	C1185	U1093	G951		A878	A813
U1881	C1711	A1626	G1562	U1482	G1415	A1334	G1263	G1186		A952		A879	G814
A1883	G1712	C1627		A1486	C1415	A1335	C1264	A1187	G1098	G953		C880	G814
C1884	A1714	G1628	G1566	C1487	C1416	G1336	G1265	A1188	A1099	U954		G887	A815
C1885	A1715	A1632	A1568	G1488	C1417	G1337	G1266	G1189	G1100	G955		A817	U816
G1886	G1716	C1633		U1489	C1418	G1338	A1267	C1190	A956	C889		G889	G818
G1887	A1717	A1634	G1571	U1490	G1419	U1339	G1268	G1191	A1114	G957		U890	C819
C1888		G1635	C1572	C1491		G1340	G1269	A1192		G958		A891	U820
G1890	G1722		G1573	A1492	U1424	G1341	C1270	G1193	C1120	C959		G	A821
	U1723	A1643	A1574	G1493	G1425	C1342	G1271	U1194	G1121	U960		G	U823
A1802	C1724	G1644	C1575	G1495	U1426	C1344	G1272	U1195	A1122	G961		G	U824
			G1576	G1496	G1428	G1346	G1273	G1196	U1030			G	C825
G1893	C1727		G1577	C1497	A1429	C1347	A1275	U1197	G1127	A964		C	U826
U1894	A1728	U1648	U1578	G1498	G1430	C1348	A1278	G1200	A1129	A966		C	C827
A1896	C1729		G1579	A1499	U1431	A1349	G1279	U1199	U1130	G967		U	C828
	U1810	G1652	C1580	U1500	G1432	G1350	U1280	G1203	G1131	U969		A	C829
A1899	C1731	C1653	C1581	C1501	U1433	G1351	A1281	G1204	G1132	C		C	C830
U1900	U1812	A1654	A1582	G1502	U1434	G1352		G1205	G1133	A970		C	G831
	A1813	C1655	A1583	G1503	G1435	A1353	G1284		U1037	A971		A	A832
U1906	G1814	U1656	G1584	A1504	A1436	A1354	A1285	C1210	U1038	C972		G	A833
C1907		A1657	A1585	U1505	A1437	A1355	U1286	G1211	A1039	U973		C	A834
C1908		A1658	A1586			G1356	A1287		G1041	U974		U	
									A1140	C975			U837

A2861	U2778	G2621	G2553	G2484	C2420	G2353	U2270	C2199	U	G2050	C1979	U1909
G2862	G2782	G2622	G2554	U2485	C2421	A2356	C2271	C2199	U	U2051	A1980	A1940
U2863	U2783	G2624	G2555	G2486	G2422	A2357	A2272	G2201	G	G2052	A1981	A1911
G2867	A2784	U2625	G2556	G2492	G2424	C2358	C2274	C2205	G	G2055	G1985	G1912
U2871	A2785	G2628	U2559	G2493	G2426	G2361	U2275	C2206	G	G2056	G1986	G1913
U2872	G2786	U2629	G2560	U2493	A2427	G2362	C2276	C2206	G	U2057	G1986	A1915
G2873	A2787	G2630	G2562	G2494	A2428	G2363	A2277	U2211	G	U2058	G1993	G1916
G2874	G2794	A2633	U2563	G2496	A2429	G2364	G2279	U2212	G	U2059	G1994	G1917
C2875	G2795	G2634	U2564	C2497	A2430	U2365	U2285	U2213	G	A2060	U1995	G1918
G2876	A2796	U2635	C2565	U2498	C2431	U2366	U2286	G2214	G	U2062	A1996	A1919
A2877	G2797	A2636	A2566	A2432	A2433	A2367	C2287	G2217	G	G2140	A1997	A1920
C	A2798	A2639	C2570	G2434	G2433	G2368	A2287	G2217	A	U2069	U1922	U1921
U	C2799	G2640	G2571	G2501	C2435	U2369	A2288	G2218	G	G2070	U1923	U1922
C	C2800	A2641	U2572	G2502	U2436	C2370	U2219	U2219	G	U2071	A2002	U1924
	A2801	G2642	C2573	G2504	G2437	A2371	C2292	A2220	C	U2075	A2003	G1925
	G2805	G2643	G2574	G2505	G2438	C2373	G2293	U2222	A	G2077	U2005	U1927
	G2806		U2575	G2508	U2439	G2376	U2298	U2223	C	G2078	G2006	G1928
	G2807	G2646	G2576	A2509	C2440	G2377	A2299	U2224	G	A2079	G2007	U1929
	U2808	U2651	A2577	A2510	C2441	G2378	C2300	U2225	G	U2080	C2008	C1930
	A2809	G2652	A2578	G2511	C2442	G2379	A2301	A2226	U	U2081	U2009	U2009
	A2810	G2653	A2579	G2512	C2443	U2380	G2302	U2227	G	C2082	G2010	G2010
	G2811		A2580	A2513	G2444	A2381	A2307	U2228	A	C2083	U2011	U2011
	A2812	A2658	G2582	G2514	A2445	C2382	A2308	G2229	A	G2084	A2012	A2012
		C2659	G2583	G2515	A2446	C2383	A2309		A	U2085	A2013	A2013
		G2660	G2584	U2516	A2447	G2384	G2310		U	G2086	A2014	A2014
		G2661	G2585	U2517	A2448	A2385	U2311		A	G2087	G2015	G2015
		U2666	G2586	C2517	G2449	U2386	U2312		A	G2088	A2016	A2016
		U2667	G2587	A2521	C2454	G2389	G2313		C	G2089	U2017	U2017
		U2668	U2588	G2522	A2455	A2390	A2314		C	G2090	C2018	C2018
		C2669	C2589	G2523	A2456	A2391	A2315		C	G2091	C2019	C2019
		G2670	U2590	G2524	A2457	G2392	C2240		G	A2097	G2020	G2020
		G2671	C2591	G2525	U2458	G2393	U2241		G	A	G2021	G2021
		U2674	U2592	U2526	C2459	G2394	C2242		U	A	C2022	C2022
		U2675	U2593	G2527	C2460	G2395	C2243		A	A	A1954	A1954
		G2676	U2594	G2528		G2396	C2244		A	A	G1955	G1955
		U2677	C2595	G2529	G2463	A2397	A2245		A	A	G1956	G1956
		G2678	G2596	G2530	G2464	U2398	A2246		G	G2103	C1957	C1957
		G2679	C2597	G2531	G2465	U2399	A2247		G	G2106	G1958	G1958
		C2681	U2598	U2533	G2466	A2401	C2248		G	G2107	G2028	G2028
		C2682	A2600	U2534	G2467	U2402	U2249		G	G2107	A1961	A1961
		G2683	C2601	G2535	G2468	C2403	C2250		G	G2110	C1962	C1962
		C2686	G2602	G2536	G2469	A2404	C2321		C	G2111	G1963	G1963
		G2687	G2603	C2537	U2470	A2405	U2180		C	G2112	A1964	A1964
		C2688	G2604	C2538	U2471	C2406	A2181		U	G2113	U1965	U1965
		C2689	C2605	A2540	U2472	G2407	A2182		G	G2114	G2035	G2035
		A2690	G2606	U2541	G2473	G2408	U2185		C	G2115	G2036	G2036
		A2691	C2607	A2542	G2474	A2409	G2186		G	A2117	A2037	A2037
		U2692	G2608	A2543	G2475	C2410	G2187		G	G2116	G2038	G2038
		G2693	G2609	G2544	C2476	U2411	A2191		G	G2117	G2039	G2039
		G2694	U2615	G2545	A2477	A2412	U2192		G	G2118	A2043	A2043
		C2695	U2616	G2546	C2478	A2413	C2193		G	G2119	G2044	G2044
		G2698	U2617	G2547	U2479	A2414	C2194		G	G2120	U1974	U1974
		G2699	A2618	G2548	C2480	A2415	C2195		G	G2121	C1975	C1975
		U2700	G2619	A2551	A2481	U2417	U2196		G	G2122	G2047	G2047
			G2620	G2552	U2483	C2419	U2197		G	G2123	C2048	C2048
							U2198		G	G2124	U1978	U1978

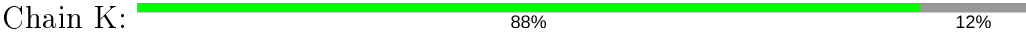
• Molecule 2: tRNA acceptor stem mimic

Chain 5:





- Molecule 3: 50S ribosomal protein L16



- Molecule 4: GENERAL STRESS PROTEIN CTC



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	169.90 Å 409.90 Å 695.90 Å 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.	Xtriage
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	1263	G
1	0	1495	G
1	0	2564	U
1	0	1278	A
1	0	1313	U

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

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 carbohydrates 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.