



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2023 – 03:58 PM EDT

PDB ID : 1NJO
Title : The crystal structure of the 50S Large ribosomal subunit from *Deinococcus radiodurans* complexed with a short substrate analog ACCPuromycin (ACCP)
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 : 3.70 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 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

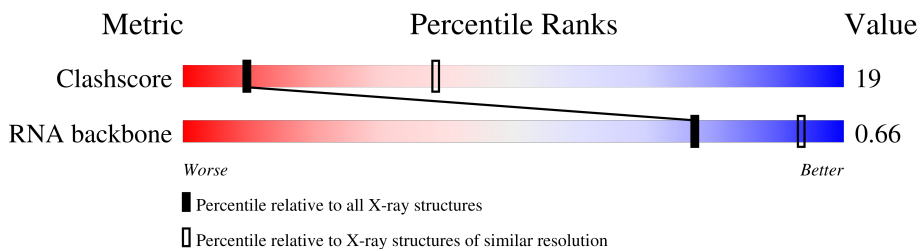
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1027 (3.86-3.54)
RNA backbone	3102	1027 (4.40-3.00)

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	4	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 59455 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.

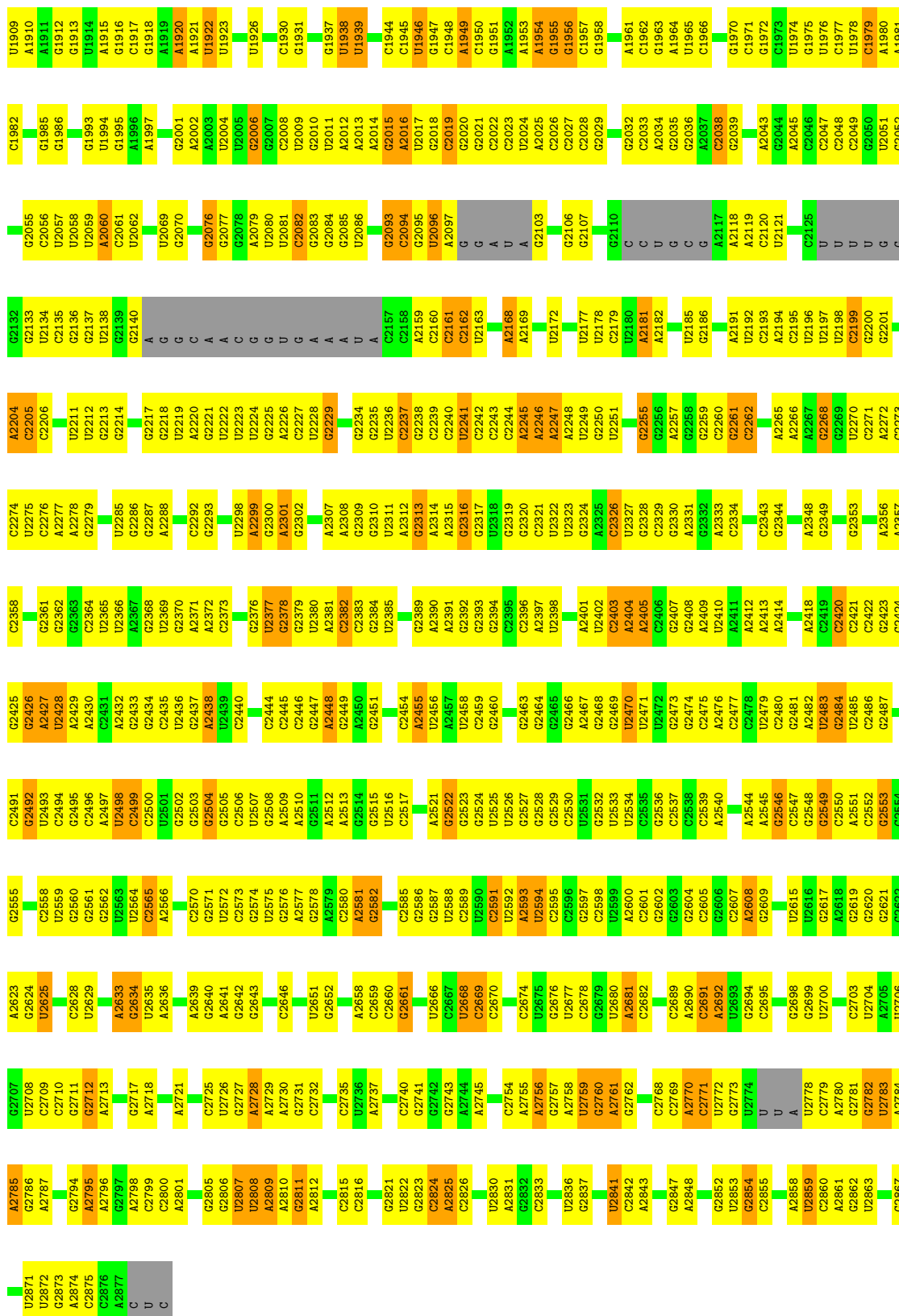
- Molecule 1 is a RNA chain called 23S ribosomal RNA.

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 RNA ACC(Puromycin).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	5	4	96	50	18	25	3	0	0	0

G1818	G1855	G1782	G1655	A1582	G1436	U1357	A1290	U1144	G1047	G980	A911	G841	U779
U1819	U1656	U1783	U1657	A1583	A1437	C1358	G1291	C1145	C1052	C981	U916	A842	U780
G1820	A1657	G1742	G1584	G1584	A1441	G1359	A1292	G1146	G1053	A884	U917	G843	G781
C1822	A1658	G1743	A1585	A1587	C1442	A1365	A1293	G1147	C1054	G985	U918	G844	G782
C1825	G1660	G1744	A1509	A1587	G1443	U1366	G1298	G1148	C1055	A986	U919	A845	G783
U1826	C1661	C1745	A1511	A1587	C1444	A1367	G1298	G1149	U1055	G987	U920	A846	G784
C1829	G1662	A1746	A1512	U1591	A1445	U1301	U1301	C1150	U1056	G988	A921	C847	U785
G1830	C1663	G1747	A1513	U1592	U1446	C1302	C1302	U1151	A1057	U988	A922	U852	U786
C1830	C1664	U1748	C1593	C1593	U1447	C1303	C1303	A1154	A1065	C853	U925	C853	G788
G1831	C1665	A1749	U1514	C1594	U1448	U1370	U1370	U1155	G1066	G854	C926	G854	G789
C1835	G1666	A1750	A1515	A1594	U1449	G1371	U1371	U1156	G1067	G855	C927	G855	A790
C1836	A1667	G1754	A1516	A1595	C1449	A1372	A1372	A1182	A1068	G856	C928	G856	G791
G1836	G1668	G1755	C1517	A1596	G1450	G1373	U1307	C1182	A1069	G857	C929	G857	U792
C1837	A1669	G1756	U1518	A1597	C1451	U1377	U1308	C1183	A1070	G858	C930	G858	G793
G1838	G1670	A1757	G1519	C1598	U1452	G1377	C1310	C1184	G1071	U859	A929	G859	A794
A1840	A1671	C1762	G1520	C1602	C1455	C1380	U1312	C1185	G1072	A1000	G932	U860	A795
G1841	A1672	G1763	C1524	A1603	C1456	G1381	U1313	G1186	G1073	A1001	G933	G861	A796
C1850	U1676	U1676	G1527	A1604	A1457	G1382	U1314	G1187	C1074	A1002	G934	C864	A797
A1851	U1677	U1677	C1528	A1605	U1458	A1386	U1315	G1188	C1075	C1003	G935	A865	G798
G1855	U1678	U1678	C1529	A1606	U1459	C1387	G1316	C1189	U1076	A1004	G936	U868	U800
U1856	U1680	U1680	C1530	A1607	A1463	C1388	U1317	U1172	A1081	A1005	C939	U868	C803
C1857	U1681	U1681	C1531	A1608	A1464	C1389	U1318	G1173	A1084	C1006	G940	C870	C804
C1858	U1682	U1682	C1532	A1609	A1465	U1390	C1319	U1177	G1085	A1007	G941	U871	G805
A1859	U1683	U1683	G1533	A1610	U1467	U1392	A1323	U1178	C1086	C1009	U942	G872	A806
A1860	U1684	U1684	C1534	A1611	A1468	G1393	G1324	C1179	C1087	G1014	U943	U873	A807
G1861	U1685	U1685	C1540	A1612	A1469	U1397	U1325	A1180	A1088	A1180	U944	A874	C808
C1862	U1686	U1686	C1543	A1613	A1470	G1398	U1326	A1181	C1089	G945	U945	A875	C809
C1865	U1687	U1687	G1544	A1614	C1471	U1399	C1327	U1182	C1090	C1016	U946	A876	U810
G1866	U1688	U1688	U1545	A1615	C1472	C1399	C1328	U1183	G1091	C1017	U949	A877	G811
G1871	U1689	U1689	C1546	A1616	U1473	U1402	U1329	G1184	U1092	C1018	U950	C878	G812
U1880	U1692	U1692	U1547	A1617	A1474	U1403	G1330	G1185	U1093	A1019	U951	A879	A813
U1785	U1696	U1696	U1548	A1619	U1475	G1407	U1332	G1186	G1098	A1021	U952	C880	G814
U1787	U1703	U1703	C1552	A1620	U1478	U1410	A1336	C1190	A1099	A1022	U953	G887	U816
C1788	G1704	G1704	C1557	A1621	G1479	C1411	U1337	C1191	G1100	U1023	U954	G888	U817
G1789	C1708	C1708	C1558	A1622	G1480	U1414	G1338	A1192	A1114	A1025	U955	G889	G818
C1791	U1709	U1709	A1561	A1625	U1481	G1415	U1339	A1193	C1120	U1026	U956	U890	C819
A1793	C1711	C1711	C1562	A1626	U1482	A1416	G1340	G1194	G1121	C1027	U957	A891	U820
A1794	G1712	G1712	G1566	A1627	A1486	C1417	C1341	U1195	A1122	C1028	U960	G	G822
A1799	G1713	G1713	A1567	A1628	G1488	C1418	U1342	G1196	G	C1029	U961	G	U824
A1800	A1714	A1714	A1568	A1632	C1489	C1419	C1344	U1197	C1127	U1030	A964	G	C825
C1801	G1716	G1716	A1568	A1633	U1490	G1419	G1345	C1198	G1128	A1032	A965	C	U826
A1802	A1717	A1717	G1571	A1634	A1493	U1424	G1346	C1199	U1130	G1033	A966	C	C827
A1807	G1722	G1722	G1572	A1635	G1494	U1425	C1347	U1200	G1131	G1035	C968	A	C828
C1808	U1723	U1723	G1573	A1643	G1496	U1426	C1348	A1203	G1132	G1036	U969	C	C830
G1809	C1724	C1724	A1574	A1644	U1497	G1427	C1349	G1204	G1133	U1037	A970	C	G831
U1900	G1644	G1644	C1575	A1645	C1497	U1428	A1429	G1205	A1137	A1038	A971	A	A832
A1901	G1648	G1648	G1576	A1646	G1498	U1429	G1350	U1210	A1138	A1039	C972	G	A833
U1812	U1728	U1728	U1578	A1648	U1499	U1430	G1351	G1211	A1139	A1040	U973	C	A834
A1813	C1729	C1729	U1579	A1651	U1500	U1431	G1352	C1214	A1140	G1041	U974	U	U837
C1907	G1730	G1730	U1433	A1654	C1501	G1432	A1353	U1288	G1142	U1044	C975	A	A838
C1908	C1731	C1731	U1434	A1654	G1503	U1433	A1354	A1287	U1441	G1045	U978	C	U839
						G1435	A1355	A1289	A1143	U1046	U979	C	U840



● Molecule 2: RNA ACC(Puromycin)





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 410.40Å 697.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.70	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.283 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	59455	wwPDB-VP
Average B, all atoms (Å ²)	77.0	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	0.21	0/65	0.56	0/99
All	All	0.14	0/66532	0.63	0/103772

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	1732	0
2	5	96	0	62	1	0
All	All	59455	0	29979	1732	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 1732 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	1.05
1:0:1073:G:H2'	1:0:1074:G:H4'	1.40	1.00
1:0:2769:C:H2'	1:0:2867:G:H22	1.21	0.99
1:0:2668:U:H4'	1:0:2669:C:H5'	1.45	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2757/2880 (95%)	411 (14%)	43 (1%)
2	5	2/4 (50%)	2 (100%)	0
All	All	2759/2884 (95%)	413 (14%)	43 (1%)

5 of 413 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	15	G

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

5 of 43 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1820	G
1	0	2261	G
1	0	1938	U
1	0	2161	C
1	0	2404	A

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	2.80	7 (21%)	33,57,60	0.98	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'	12.44	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.93	1.27	1.42
2	5	35	PPU	C6-N1	3.79	1.38	1.33
2	5	35	PPU	CE1-CZ	3.77	1.46	1.38
2	5	35	PPU	CE2-CZ	2.68	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	2.99	123.99	117.51
2	5	35	PPU	C9-N6-C6	2.24	126.28	119.51
2	5	35	PPU	C-CA-N	2.18	117.83	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.