



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:12 PM UTC

PDB ID : 1NJO / pdb_00001njo
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.; Schlutzen, 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

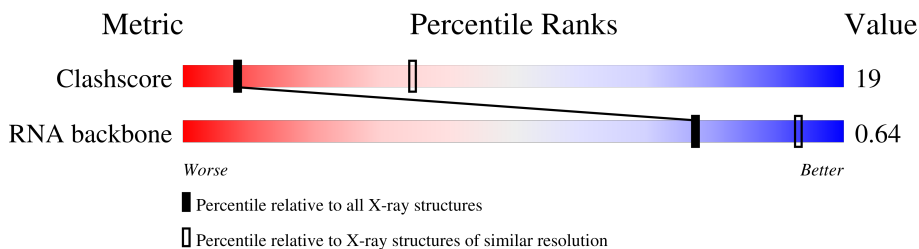
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

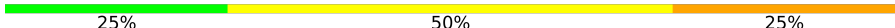
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1171 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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	 34% 51% 11% .
2	5	4	 25% 50% 25%

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
1	0	2766	Total	C	N	O	P	0	0	0
			59359	26479	10949	19166	2765			

- Molecule 2 is a RNA chain called RNA ACC(Puromycin).

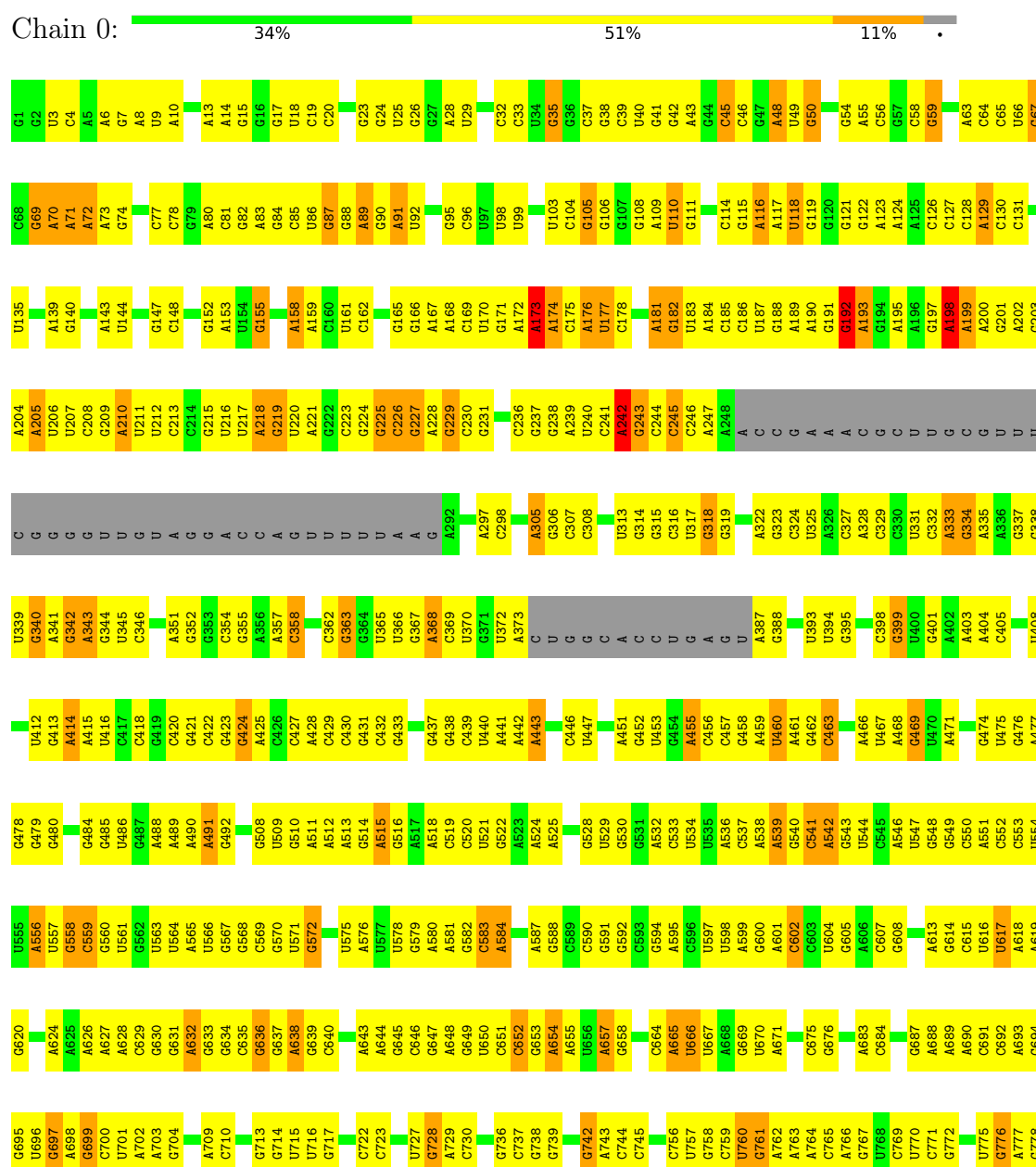
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	5	4	Total	C	N	O	P	0	0	0
			96	50	18	25	3			

3 Residue-property plots

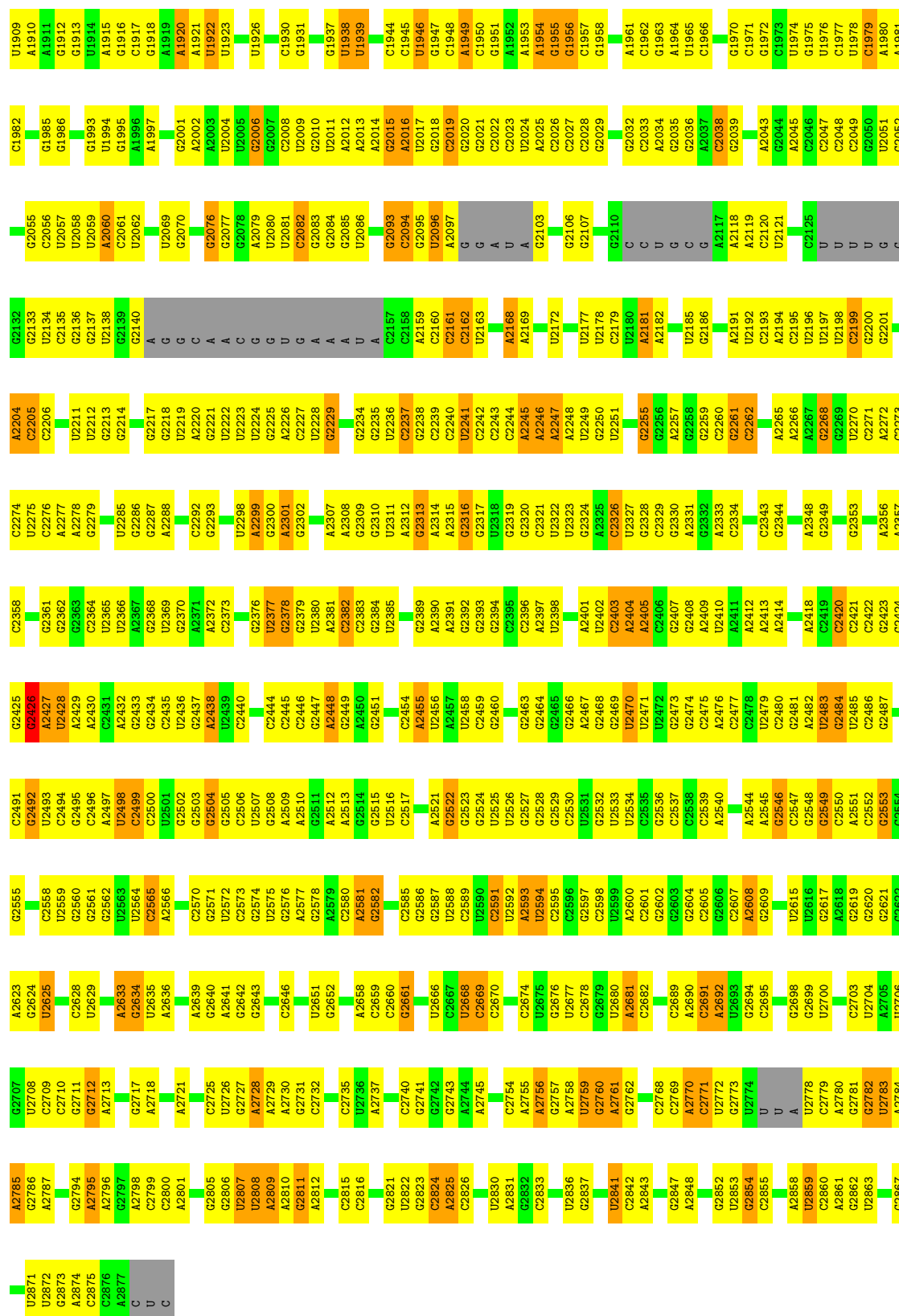
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



G1818	U1782	G1855	A1582	G1436	U1357	A1290	C1218	U1144	G1047	G980	A911	G841	U179
U1819	U1783	U1656	A1583	A1437	C1358	G1291	C1219	C1145	C1052	C981	U916	A842	U780
G1820	A1821	A1657	A1584		G1359	A1292	G1220	G1146	C1053	A984	U917	G843	G781
C1822	G1742	A1658	A1585	A1441	A1509	A1293	C1221	G1147	G1054	G985	U918	G844	G782
	G1743	G1659	A1586	A1442	A1510		G1222	G1148	C1055	A986	U919	U845	G783
C1825	G1744	G1660	A1587	G1443	A1511	G1298	G1223	G1149	U1055	G987	G920	U846	G784
	C1745	C1661		C1444	A1367		A1224	C1150	U1056	G988	A921	C847	U785
U1826	A1746	G1662	U1591	A1445	A1368	U1301	G1225	U1151	A1057	G989	A922	U786	U786
	G1747	C1663	U1592	U1446	G1369	C1302	A1226		U1058	A991		U852	A787
C1829	U1748	C1593	A1593	U1447	U1370	C1302	A1226	A1154	A1065	A994	U925	C853	G788
C1830	G1749	C1665	U1514	U1448	G1371	U1303	A1227	U1155	G1066	A995	C926	G854	G789
G1831	A1750	G1666	A1595	C1449	A1372			U1156	G1067	A996	U927	A790	A790
		A1667	A1596	G1450	G1373	U1307	A1231	U1157	A1068	A997	C928	G855	A791
C1835	G1754	G1668	A1597	C1451	G1374	C1308	U1232	U1158	G1069	A998	G929	G856	U792
C1836	G1755	A1669	C1598	U1452		G1389	A1233	A1162	U1070	C997	A929	U857	U792
G1838		G1670	G1599		G1377	C1310	C1234	C1163	G1071	C998	A930	U858	G793
A1839		A1671	U1600	C1455	G1380	G1312	C1235	G1165	G1072	A999	G931	U859	A794
A1840	G1760	U1601	G1602	A1456	G1381	U1313	A1242	A1166	G1073	G1000	G932	A795	A795
G1841	C1762	A1603	A1603	A1457	G1382	A1314	G1243	A1167	G1074	A1001	G933	A796	A796
	G1763	A1604		A1458	G1383	A1315	G1244	A1168	C1075	C1002	G934	A797	A797
	A1764	A1605	C1606	U1459	A1386	G1317	U1244	G1169	U1076	C1003		C864	G798
G1850	C1765	U1607	A1607	A1463	G1387	A1318	G1245			C935		A865	G799
A1851	U1766	U1608	G1609	A1464	G1388	G1319		U1172	A1081	A1004	A936	U868	U800
		A1680		A1465	G1389	C1320	G1248	G1173		C1006	C939	C869	C803
G1855	U1770	A1681	A1681	A1466	G1390	A1321	G1249	G1174	A1084	A1007	G940	C870	C804
U1856	A1771	G1682	U1611	U1467	U1392	G1323	G1251	U1177	G1085	C1008	U941	G805	G805
C1857		G1683	C1610	A1468	G1393	G1324	C1252	C1178	C1086	C1009	U942	A806	A806
G1858	A1774	A1684	U1612	A1469	U1397	U1325		A1179	C1087		U943	U872	A807
A1859	A1775	A1685	C1613	G1470	G1398	U1326	G1258	C1181	U1088	A1180	G944	A874	C808
A1860	A1776	A1686	G1614	G1471	G1399	C1327	A1259	U1182	C1089	C1016		G875	C809
G1861	A1777	C1687	C1615	A1472	C1399	G1328	G1260	G1183	G1090	C1017	G949	A876	U810
C1862	U1778		C1616	U1473	U1403	U1329	G1261	G1184	U1092	C1018		G877	G811
	C1779	G1691	G1617	A1474	G1402	G1330	G1262	C1185	U1093	U1019	G951	C878	G812
C1865	A1780	C1692	U1618	U1475	U1403	G1332	G1263	G1186	A1021	A1020	A952	A879	A813
G1866			A1619	U1478	G1407	G1333	C1264	A1187	G1098	A1022	G953	C880	G814
			G1620	G1479		A1334	G1265	A1188	A1099	U1023	U954	G867	U816
G1871			C1621	G1480	U1410	G1335	G1266	G1189	G1100	A1025	G955	G888	A817
			G1622	U1481	C1411	G1336	A1267	C1190		G1024	A956	C889	G818
G1880			C1623	U1482		G1337	G1268	A1192	A1114	A1026	G957	U890	C819
U1881			A1624		G1414	G1338	G1269	G1193	C1120	C1027	C959	U820	U820
G1882			A1625		A1415	U1339	G1270	U1194	G1121	G1028	U960	A821	A821
A1883			C1626	A1486	A1416	G1340	C1271	U1195	A1122	C1029	G961	G822	G822
A1884			G1627	C1487	A1417	G1341	G1272	G1196		U1030		U824	U824
C1885			C1628	G1488	C1418	U1342	G1273	U1197	C1127	C1031	A964	C825	C825
G1886			G1629	G1489	G1419	C1343	C1274	C1198	U1129	A1032	G965	U826	U826
G1887				U1490	G1419	C1344	A1275	U1199	G1131	G1033	G967	C827	C827
C1888			A1632	C1491	U1424	G1345		G1200	G1132	G1035	C968	C828	C828
G1889			C1633	A1492	G1425	G1346	A1278		C1133	G1036	U969	C829	C829
G1890			A1634	A1493	G1426	C1347	G1279	A1203	G1133	U1037	C970	C830	C830
			G1635	G1494	U1427	C1348	U1280	G1204	G1133	G1038	A971	G831	G831
A1895				G1495	G1428	A1349	A1281	G1205	A1137	U1038	C972	A832	A832
A1896			A1643	G1496	A1429	G1350			A1138	A1039	U973	A833	A833
A1899			C1644	C1497	U1431	G1351	G1284	G1210	A1139	A1040	U974	C834	C834
U1900			G1645	G1498	U1431	G1352	G1285	G1211	A1140	G1041	C975		
A1901			C1648	U1499	U1432	A1353	U1286	G1214	U1141	U1045	U978	U837	U837
			U1651	U1500	G1432	A1354	A1287		G1142	G1046	U978	A838	A838
U1906			C1651	U1501	U1433	A1355	A1288	G1214	A1143	U1046	U978	U839	U839
C1907			G1579	G1502	U1434	A1356	A1289					C	U840
C1908			C1581	G1503	G1435	G1356		U1217				C	U840



● Molecule 2: RNA ACC(Puromycin)

Chain 5: 25% 50% 25%



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 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.	Xtriage
Total number of atoms	59455	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.25	0/66467	0.50	5/103673 (0.0%)
2	5	0.32	0/65	0.47	0/99
All	All	0.25	0/66532	0.50	5/103772 (0.0%)

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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	0	2426	G	C2'-C3'-O3'	6.06	118.60	109.50
1	0	192	G	C2'-C3'-O3'	5.92	118.38	109.50
1	0	242	A	C2'-C3'-O3'	5.76	118.14	109.50
1	0	198	A	C2'-C3'-O3'	5.26	117.39	109.50
1	0	173	A	C2'-C3'-O3'	5.18	117.27	109.50

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	1725	0
2	5	96	0	62	1	0
All	All	59455	0	29979	1725	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 1725 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%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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
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 ⓘ

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	37,40,41	2.64	7 (18%)	47,57,60	0.98	4 (8%)

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	-	1/25/43/44	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'	12.78	1.61	1.34
2	5	35	PPU	OC-CM	-5.33	1.27	1.42
2	5	35	PPU	CE1-CZ	3.98	1.46	1.38
2	5	35	PPU	CD2-CG	2.85	1.44	1.38
2	5	35	PPU	CE2-CZ	2.81	1.44	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	C2-N1-C6	3.32	119.95	111.83
2	5	35	PPU	CM-OC-CZ	3.03	123.99	117.50
2	5	35	PPU	C9-N6-C6	2.27	126.28	120.52
2	5	35	PPU	C-CA-N	2.24	117.83	109.37

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 oligosaccharides 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 ⓘ

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.