



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:07 PM GMT

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
<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

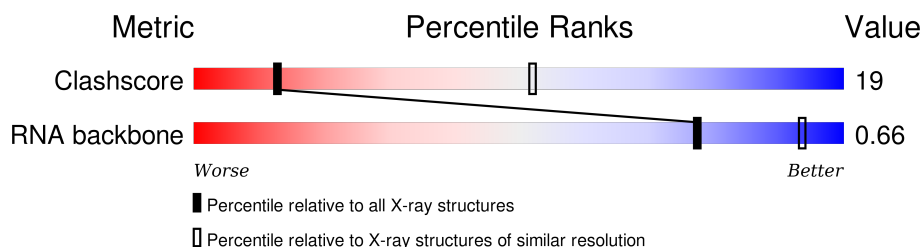
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

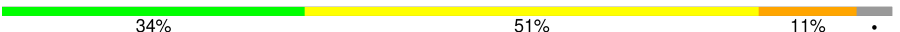
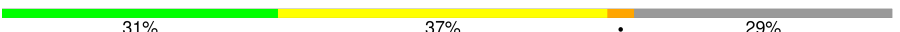


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	0	2880	 34% 51% 11% •
2	5	35	 31% 37% • 29%
3	K	141	 88% 12%
4	T	237	 94% 6%

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.

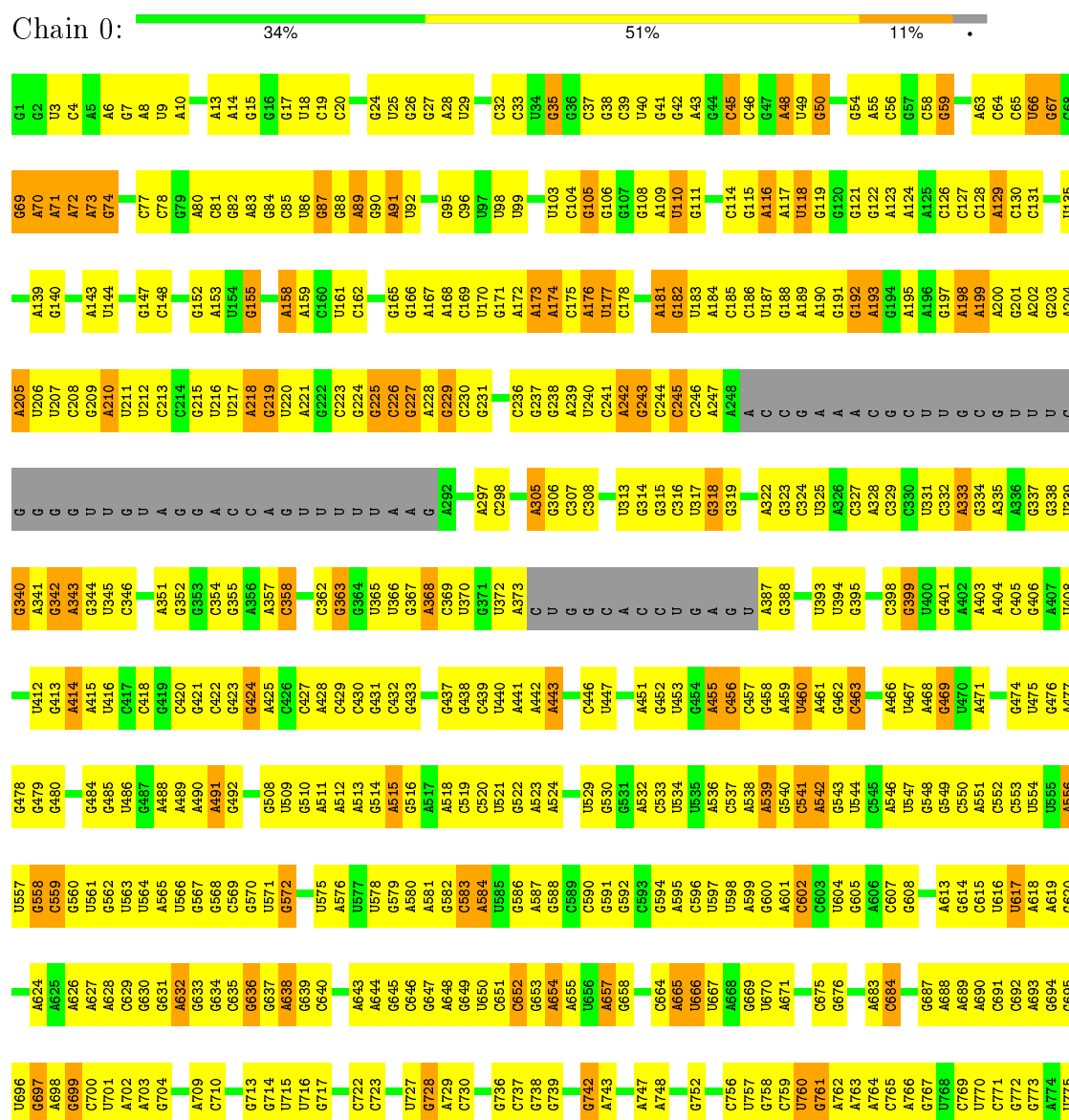
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	T	223	Total	C	0	0	223
			223	223			

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 ($RSRZ > 2$). 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 ribosomal RNA



U1909	U1819	G1659	A1587	G1508	A1441	U1357	A1288	G1214	U1441	U1044	U978	A	A838	G776
A1940	G1820	G1660	U1591	A1509	C1442	C1358	A1289	U1217	G1442	G1044	U979	C	U839	A777
A1911	A1821	C1661	U1592	A1510	G1443	G1359	A1290	U1218	A1443	U1046	A979	C	U840	A778
G1913	C1822	G1662	U1593	A1511	G1444	G1360	A1291	C1219	U1444	G1047	C981		G841	U779
U1914	C1825	C1663	U1594	A1512	A1445	U1365	A1292	C1218	G1445	C1052	U916		A842	U780
A1915	U1826	G1664	A1595	U1513	U1446	U1366	A1293	G1220	G1446	G1053	U917		G843	G781
G1916	C1827	C1665	A1596	C1514	U1447	A1367	G1298	C1221	G1447	C1054	U918		G844	U782
C1829	U1917	G1666	A1597	U1515	U1448	G1368		G1222	G1448	U1055	U919		U845	G783
G1918	C1830	A1667	A1598	U1516	C1449	U1369		G1223	G1449	C1056	U920		A846	U784
A1919	G1831	G1668	C1599	C1517	U1450	G1370		A1224	C1150	U1056	U921		C847	U785
		A1669	G1599	C1518	U1451	G1371		G1225	C1151	A1057	U922		U852	U786
A1920	C1835	G1670	U1600	G1519	U1452	G1372		A1226	A1154	G1058	U923		G853	A787
A1921	U1922	A1671	G1601	G1520		U1307	C1308	A1227	A1155		U924		G854	G788
C1836	C1837	A1672	G1602		C1455	C1380	G1309		U1156	A1065	U925		G855	G789
U1923	G1837		A1603	C1524	A1456	G1381		A1231	U1157	G1066	U926		G856	A790
G1924	C1838	C1677	A1604		A1457	G1382	U1231	U1232		G1067	U927		A857	G791
C1925	A1839	G1678	A1605	G1527	A1458	U1383	A1233	A1234	A1162	A1068	U928		U857	U792
A1926	A1840	C1679	C1606	U1528	U1459	A1386	U1313	C1234	C1163	G1069	U929		G858	G793
U1927	G1841	U1680	A1607	C1529		G1387	A1314	C1235	C1164	G1070	U930		U859	A794
G1928	C1842	A1681	U1608	U1530	A1463	C1388	A1315		G1165		U931		U860	A795
U1929	G1850	U1766	A1682	C1531	A1464	U1389	G1316	A1242	A1166	G1073	U932		G861	A796
C1930	A1851	G1683	A1610	U1532	C1465	G1390	A1317	G1243	A1167	G1074	U933			A797
G1931		G1684	U1611	G1533	C1466	A1391	A1318		G1168	C1075	U934		C864	G798
		A1685	U1612	U1539	U1467	U1392	C1319	G1248	C1169	U1076	U935		A865	C799
G1937	U1855	A1686	G1613	U1540	U1468	G1393	A1320	U1249		A1081	U936		U868	U800
U1938	G1856	C1687	C1614		U1469			A1250	U1172		U1005		C869	C803
U1939	C1857		G1615	G1541	G1470	A1397	G1323	G1251	G1173		C1006		C870	C804
	A1774	G1691	A1616	U1542	C1471	G1398	G1324	C1252		A1084	A1007		U871	A805
U1946	A1859	C1692	C1617	G1543	C1472	C1399	U1325	G1253	U1177	G1085	U941		G872	A806
G1947	A1860	G1693	U1618	A1544	U1473		U1326	G1254	C1178	G1086	U942		U873	A807
C1948	C1862	C1696	A1619	G1545	U1474	G1402	C1327		A1179	C1087	U943		C874	C808
A1949		C1703	G1620	C1552	U1475	U1403	G1328	U1257	A1180	A1088	U944		A875	C809
C1950	G1865	G1704	C1621		U1478	G1407	U1329	G1258	C1181	C1089			A876	U810
G1951	G1866	C1705	G1622	G1557	C1479		G1330	A1259	U1182	C1090	U949		G877	G811
A1953	C1871	G1706	C1623	C1558	U1480	U1410	G1331	G1261	C1183	C1091	U950		C878	G812
A1954	U1854	U1709	A1625		U1481	C1411	G1332	U1262	G1184	U1092	U951		A879	A813
G1955	G1860	U1710	A1626	A1561	U1482		G1333	G1263	C1185	U1093	U952		C880	G814
U1956	U1851	C1711	G1627	G1562		G1414	A1334		A1186		A1030			
G1957	G1862	G1712	C1628		A1486	C1415	A1335	C1264	A1187	G1098	A1021		G887	A815
G1958	A1883	G1713	G1629	G1566	C1487	A1416	G1336	G1265	A1188	A1099	A1022		G888	U816
	C1884	A1714	G1629	A1567	C1488	G1417	G1337	G1266	G1189	U1023	U954		C889	A817
A1961	C1885	A1715	A1632	A1568	U1489	C1418	U1339	U1267	C1190	G1024	U955		U890	G818
C1962	G1866	G1716	C1633		U1490	G1419	G1340	U1268	G1191	A1114	A1025		A891	C819
G1963	C1867	A1717	A1634	G1571	C1491		G1341	G1269	A1192	U1026	G957			U820
A1964	U1867	G1722	G1635	C1572	A1492	U1424	U1342	C1270	G1193	C1027	C959		G	A821
U1965	G1889	U1723	A1643	G1573	A1493	G1425	C1343	C1271	U1194	G1028	U960		G	G822
G1966	C1890	C1724	G1644	A1574	U1494	U1426	G1344	G1272	U1195	C1029	U961		G	U823
U1967	C1893	G1725		C1575	G1495	G1427	G1345	G1273	G1196	U1030			G	U824
G1968	U1894	C1727	C1648	G1576	U1496	G1428	C1346	A1275	U1197	C1031	A964		C	C825
C1969	A1895	A1728	U1651	G1577	C1497	A1429	C1347		U1199	G1032	U965		C	U826
A1970	G1896	C1808	U1652	U1578	G1498	G1430	C1348	A1278	G1200	A1033	U966		U	C827
G1971	U1810	C1729	G1653	G1579	A1499	U1431	A1349	G1279		U1034	C967		A	C828
C1972	A1811	G1730	C1654	C1580	U1500	G1432	G1350	U1280	A1203	G1035	C968		C	A829
U1973	U1812	U1732	A1654	C1581	C1501	U1433	G1351	A1281	G1204	G1132	U969		C	C830
G1974	C1813	U1733	C1655	A1582	G1502	A1434	G1352		G1205	G1133	A970		C	G831
U1975	U1900		U1656	A1583	C1503	G1435	A1353	G1284		A1137	U1038		A	A832
C1976	C1907	G1814	A1657	G1584	G1504	G1436	A1354	U1285	C1210	A1138	A1039		G	A833
U1977	U1908	G1818	U1658	A1585	U1505	A1437	A1355	U1286	G1211	A1139	U973		C	A834
U1978								A1287		A1140	G1041		U	U837

A2861	G2178	G2050	C1979
G2862	G2782	U2051	A1980
U2863	G2783	G2052	A1981
	G2784		C1982
G2867	G2785	G2055	G1985
	G2786	C2056	G1986
U2871	G2787	U2057	
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A2874	G2790	A2060	U1994
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	G2792	C2061	A1996
C2876	G2793	U2062	A1997
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C2799	G2799	G2076	U2004
G2800	G2800	G2077	U2005
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	G2802	U2080	C2008
G2805	G2803	U2081	U2009
U2806	G2804	G2082	G2010
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U2808	G2806	A2012	A2012
A2809	G2807	G2085	A2013
G2810	G2808	U2086	A2014
U2811	G2809		G2015
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C2816	G2813	U2096	C2019
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A2825	G2819		U2025
C2826	G2820		C2026
	G2821		C2027
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	G2826		A2034
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	G2829		A2037
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	G2836		C2046
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	G3218		
	G3219		
	G3220		
	G3221		
	G3222		
	G3223		
	G3224		

Chain K:

88%

12%



● Molecule 4: GENERAL STRESS PROTEIN CTC

Chain T:

94%

6%



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 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	30,40,41	2.74	6 (20%)	37,57,60	1.31	6 (16%)

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	-	0/21/43/44	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	OC-CM	-4.83	1.28	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	35	PPU	CD2-CG	2.60	1.44	1.38
2	5	35	PPU	CE2-CZ	2.70	1.44	1.38
2	5	35	PPU	C6-N1	3.46	1.38	1.34
2	5	35	PPU	CE1-CZ	3.66	1.46	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	35	PPU	C4'-C3'-N3'	-3.66	105.97	113.61
2	5	35	PPU	C1'-N9-C4	-2.17	123.67	126.94
2	5	35	PPU	C-CA-N	2.07	117.94	108.73
2	5	35	PPU	C9-N6-C6	2.23	126.49	119.48
2	5	35	PPU	CM-OC-CZ	2.66	123.75	117.51

There are no chirality outliers.

There are no torsion outliers.

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 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.