



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1MIS / pdb\_00001mis  
Title : STRUCTURE OF RNA (5'-R(GP\*CP\*GP\*GP\*AP\*CP\*GP\*C)-3') ANTI-PARALLEL RNA DUPLEX WITH TANDEM G:A MISMATCHES, NMR, MINIMIZED AVERAGE STRUCTURE  
Authors : Wu, M.; Turner, D.H.  
Deposited on : 1997-03-26

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49



## 2 Ensemble composition and analysis

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 522 atoms, of which 180 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (5'-R(\*GP\*CP\*GP\*GP\*AP\*CP\*GP\*C)-3').

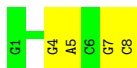
| Mol | Chain | Residues | Atoms |    |    |    |    | Trace |   |
|-----|-------|----------|-------|----|----|----|----|-------|---|
|     |       |          | Total | C  | H  | N  | O  |       | P |
| 1   | A     | 8        | 261   | 77 | 90 | 34 | 53 | 7     | 0 |
| 1   | B     | 8        | 261   | 77 | 90 | 34 | 53 | 7     | 0 |

## 4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: RNA (5'-R(\*GP\*CP\*GP\*GP\*AP\*CP\*GP\*C)-3')

Chain A:  50% 50%



- Molecule 1: RNA (5'-R(\*GP\*CP\*GP\*GP\*AP\*CP\*GP\*C)-3')

Chain B:  75% 25%



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 1 were deposited, based on the following criterion: *MINIMIZED AVERAGE : STRUCTURE*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name               | Classification | Version |
|-----------------------------|----------------|---------|
| DISCOVER, AMBER FORCE FIELD | refinement     | FIELD   |

No chemical shift data was provided.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 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 each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 171   | 90       | 90       | 2       |
| 1   | B     | 171   | 90       | 90       | 1       |
| All | All   | 342   | 180      | 180      | 3       |

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 6.

All clashes are listed below, sorted by their clash magnitude.

| Atom-1      | Atom-2      | Clash(Å) | Distance(Å) |
|-------------|-------------|----------|-------------|
| 1:B:12:G:C5 | 1:B:13:A:C8 | 0.48     | 3.01        |
| 1:A:4:G:C5  | 1:A:5:A:C8  | 0.48     | 3.02        |
| 1:A:7:G:C6  | 1:A:8:C:C4  | 0.41     | 3.09        |

### 6.3 Torsion angles [i](#)

#### 6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

#### 6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 6.3.3 RNA [i](#)

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers | Suiteness |
|-----|-------|-------------|-------------------|-----------------|-----------|
| 1   | A     | 7/8 (88%)   | 0 (0%)            | 0 (0%)          | 0.75      |
| 1   | B     | 7/8 (88%)   | 0 (0%)            | 0 (0%)          | 0.76      |
| All | All   | 14/16 (88%) | 0 (0%)            | 0 (0%)          | 0.76      |

The overall RNA backbone suiteness is 0.76.

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided