



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:25 PM UTC

PDB ID : 2IRO / pdb_00002iro
Title : The NMR Structures of (rGCUGAGGCU)2 and (rGCGGAUGCUC)2
Authors : Tolbert, B.S.
Deposited on : 2006-10-16

This is a wwPDB NMR 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/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>.

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 15 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 588 atoms, of which 198 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(P*GP*CP*GP*GP*AP*UP*GP*CP*U)-3'.

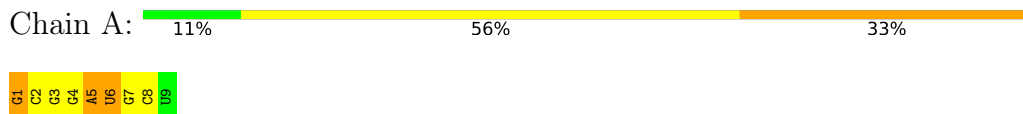
| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|----|----|----|----|-------|---|
| | | | Total | C | H | N | O | | P |
| 1 | A | 9 | 294 | 86 | 99 | 35 | 65 | 9 | 0 |
| 1 | B | 9 | 294 | 86 | 99 | 35 | 65 | 9 | 0 |

4 Residue-property plots

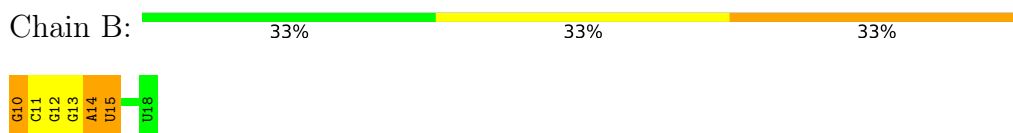
4.1 Average score per residue in the NMR ensemble

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: 5'-R(P*GP*CP*GP*GP*AP*UP*GP*CP*U)-3'



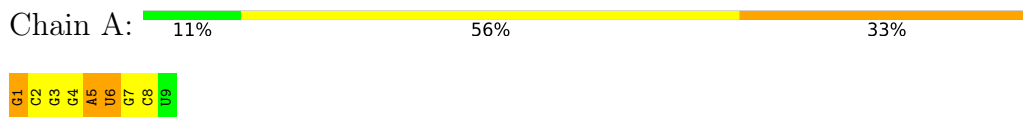
- Molecule 1: 5'-R(P*GP*CP*GP*GP*AP*UP*GP*CP*U)-3'



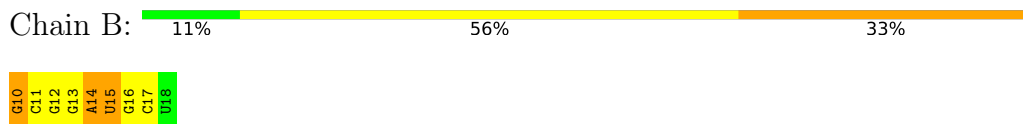
4.2 Residue scores for the representative (author defined) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: 5'-R(P*GP*CP*GP*GP*AP*UP*GP*CP*U)-3'



- Molecule 1: 5'-R(P*GP*CP*GP*GP*AP*UP*GP*CP*U)-3'



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing and restrained molecular dynamics*.

Of the 30 calculated structures, 15 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| CNS | structure solution | 1.1 |
| CNS | refinement | 1.1 |

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 (average) 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 | A | 0.46±0.00 | 1±0/217 (0.5± 0.0%) | 0.50±0.02 | 0±0/335 (0.0± 0.0%) |
| 1 | B | 0.45±0.00 | 1±0/217 (0.5± 0.0%) | 0.47±0.02 | 0±0/335 (0.0± 0.0%) |
| All | All | 0.46 | 30/6510 (0.5%) | 0.48 | 0/10050 (0.0%) |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Models | |
|-----|-------|-----|------|-------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 1 | G | OP3-P | 5.66 | 1.59 | 1.48 | 8 | 15 |
| 1 | B | 10 | G | OP3-P | 5.65 | 1.59 | 1.48 | 2 | 15 |

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 | 195 | 99 | 98 | 11±2 |
| 1 | B | 195 | 99 | 98 | 10±2 |
| All | All | 5850 | 2970 | 2940 | 207 |

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 24.

5 of 36 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|--------------|--------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:5:A:H2' | 1:A:6:U:O4' | 0.82 | 1.74 | 4 | 7 |
| 1:A:4:G:C6 | 1:B:13:G:C6 | 0.73 | 2.77 | 5 | 15 |
| 1:B:14:A:O2' | 1:B:15:U:H5' | 0.70 | 1.86 | 7 | 9 |
| 1:A:5:A:C6 | 1:B:14:A:C8 | 0.67 | 2.83 | 6 | 15 |
| 1:A:1:G:OP3 | 1:A:1:G:H3' | 0.65 | 1.91 | 9 | 1 |

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 | 8/9 (89%) | 2±0 (25±0%) | 0±0 (0±0%) | 0.58±0.00 |
| 1 | B | 8/9 (89%) | 2±0 (25±0%) | 0±0 (0±0%) | 0.57±0.00 |
| All | All | 240/270 (89%) | 60 (25%) | 0 (0%) | 0.58 |

The overall RNA backbone suiteness is 0.54.

All unique RNA backbone outliers are listed below:

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 5 | A | 15 |
| 1 | A | 6 | U | 15 |
| 1 | B | 14 | A | 15 |
| 1 | B | 15 | U | 15 |

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