



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2KD9 / pdb_00002kd9
Title : Solution Structure of DNA Containing Alpha-OH-PdG: the Mutagenic Adduct
Produced by Acrolein
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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
Mogul : 2022.3.0, CSD as543be (2022)
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 26 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

There are 2 unique types of molecules in this entry. The entry contains 703 atoms, of which 254 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*CP*GP*TP*AP*CP*(63G)P*CP*AP*TP*GP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|-----|-----|----|----|-------|---|
| | | | Total | C | H | N | O | | P |
| 1 | A | 11 | 354 | 109 | 129 | 41 | 65 | 10 | 0 |

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*AP*TP*GP*CP*GP*TP*AP*CP*G)-3'.

| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|-----|-----|----|----|-------|---|
| | | | Total | C | H | N | O | | P |
| 2 | B | 11 | 349 | 107 | 125 | 43 | 64 | 10 | 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'-D(*CP*GP*TP*AP*CP*(63G)P*CP*AP*TP*GP*C)-3'

Chain A:  91% 9%



- Molecule 2: 5'-D(*GP*CP*AP*TP*GP*CP*GP*TP*AP*CP*G)-3'

Chain B:  100%

There are no outlier residues in this chain.

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'-D(*CP*GP*TP*AP*CP*(63G)P*CP*AP*TP*GP*C)-3'

Chain A:  91% 9%



- Molecule 2: 5'-D(*GP*CP*AP*TP*GP*CP*GP*TP*AP*CP*G)-3'

Chain B:  100%

There are no outlier residues in this chain.

5 Refinement protocol and experimental data overview

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

Of the 25 calculated structures, 26 were deposited, based on the following criterion: *all calculated structures submitted*.

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

| Software name | Classification | Version |
|---------------|-----------------------|---------|
| Insight II | geometry optimization | |
| Chimera | geometry optimization | |
| X-PLOR NIH | refinement | |
| X-PLOR NIH | structure solution | |

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 63G

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 | 0.49±0.01 | 0±0/221 (0.0± 0.0%) | 1.20±0.03 | 0±0/336 (0.0± 0.1%) |
| 2 | B | 0.53±0.01 | 0±0/251 (0.0± 0.0%) | 1.22±0.04 | 0±1/386 (0.1± 0.2%) |
| All | All | 0.51 | 0/12272 (0.0%) | 1.21 | 9/18772 (0.0%) |

There are no bond-length outliers.

5 of 6 unique angle 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(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 2 | B | 1 | DG | P-O3'-C3' | 6.21 | 129.51 | 120.20 | 6 | 3 |
| 2 | B | 5 | DG | P-O3'-C3' | 5.90 | 129.05 | 120.20 | 6 | 1 |
| 2 | B | 5 | DG | C2'-C3'-O3' | 5.79 | 120.19 | 111.50 | 11 | 1 |
| 1 | A | 5 | DC | C4'-C3'-O3' | 5.74 | 118.61 | 110.00 | 15 | 2 |
| 2 | B | 7 | DG | P-O3'-C3' | 5.17 | 127.95 | 120.20 | 21 | 1 |

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 | 225 | 129 | 129 | 1±1 |
| 2 | B | 224 | 125 | 125 | 0±0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All | 11674 | 6604 | 6604 | 33 |

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 2.

5 of 8 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:6:63G:N3 | 1:A:6:63G:H2' | 0.58 | 2.13 | 2 | 19 |
| 1:A:6:63G:H1' | 1:A:7:DC:O4' | 0.55 | 2.02 | 16 | 2 |
| 1:A:6:63G:H4' | 1:A:7:DC:OP1 | 0.52 | 2.03 | 15 | 5 |
| 1:A:6:63G:N3 | 1:A:6:63G:H5'' | 0.47 | 2.25 | 12 | 1 |
| 2:B:1:DG:C2 | 2:B:2:DC:C2 | 0.46 | 3.03 | 17 | 3 |

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](#)

There are no RNA molecules in this entry.

6.4 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 for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|-----------|-------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 1 | 63G | A | 6 | 1 | 26,29,30 | 1.22±0.08 | 3±0 (11±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|-----------|------------|
| | | | | | Counts | RMSZ | #Z>2 |
| 1 | 63G | A | 6 | 1 | 33,43,46 | 1.47±0.05 | 3±1 (9±1%) |

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 |
|-----|------|-------|-----|------|---------|-------------|-----------|
| 1 | 63G | A | 6 | 1 | - | 0±0,7,30,31 | 0±0,4,4,4 |

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 | 6 | 63G | C2-N2 | 5.11 | 1.39 | 1.35 | 6 | 26 |
| 1 | A | 6 | 63G | C12-N1 | 3.22 | 1.42 | 1.47 | 4 | 26 |
| 1 | A | 6 | 63G | C10-N2 | 3.08 | 1.40 | 1.45 | 3 | 26 |

5 of 8 unique angle 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(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 6 | 63G | C11-C12-N1 | 5.70 | 122.32 | 110.84 | 2 | 26 |
| 1 | A | 6 | 63G | C2-N1-C6 | 4.27 | 124.01 | 121.15 | 23 | 26 |
| 1 | A | 6 | 63G | C12-N1-C6 | 2.63 | 119.86 | 115.87 | 23 | 18 |
| 1 | A | 6 | 63G | O4'-C1'-N9 | 2.50 | 103.43 | 107.86 | 15 | 3 |
| 1 | A | 6 | 63G | O3'-C3'-C2' | 2.36 | 119.08 | 110.88 | 19 | 1 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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