



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1D76 / pdb\_00001d76  
Title : CRYSTAL AND MOLECULAR STRUCTURE OF A DNA FRAGMENT CONTAINING A 2-AMINO ADENINE MODIFICATION: THE RELATIONSHIP BETWEEN CONFORMATION, PACKING, AND HYDRATION IN Z-DNA HEXAMERS  
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Deposited on : 1992-05-19  
Resolution : 1.30 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](mailto: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>.

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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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49



## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 324 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 DNA chain called DNA (5'-D(\*CP\*GP\*UP\*(1AP)P\*CP\*G)-3').

| Mol | Chain | Residues | Atoms        |         |         |         |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|--------|---------|---------|-------|
|     |       |          | Total        | C       | N       | O       | P      |         |         |       |
| 1   | A     | 6        | Total<br>120 | C<br>57 | N<br>24 | O<br>34 | P<br>5 | 0       | 0       | 0     |
| 1   | B     | 6        | Total<br>120 | C<br>57 | N<br>24 | O<br>34 | P<br>5 | 0       | 0       | 0     |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 2   | A     | 38       | Total<br>38 | O<br>38 | 0       | 0       |
| 2   | B     | 46       | Total<br>46 | O<br>46 | 0       | 0       |

### 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 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.

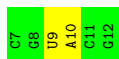
- Molecule 1: DNA (5'-D(\*CP\*GP\*UP\*(1AP)P\*CP\*G)-3')

Chain A: 



- Molecule 1: DNA (5'-D(\*CP\*GP\*UP\*(1AP)P\*CP\*G)-3')

Chain B: 



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 17.94Å 31.28Å 44.70Å<br>90.00° 90.00° 90.00°                | Depositor        |
| Resolution (Å)  | 8.00 – 1.30<br>8.00 – 1.30                                  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (8.00-1.30)<br>90.0 (8.00-1.30)             | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.00 (at 1.02Å)   | Xtrriage         |
| Refinement program  | NUCLSQ  | Depositor        |
| R, $R_{free}$   | 0.138 , (Not available)<br>0.161 , (Not available)          | Depositor<br>DCC |
| $R_{free}$ test set   | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 7.2   | Xtrriage         |
| Anisotropy  | 0.121   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 57.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.33$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.98  | EDS              |
| Total number of atoms   | 324   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 11.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5552e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: 1AP

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   | A     | 1.39         | 1/108 (0.9%) | 1.91        | 5/162 (3.1%)  |
| 1   | B     | 1.14         | 0/108        | 2.03        | 6/162 (3.7%)  |
| All | All   | 1.27         | 1/216 (0.5%) | 1.97        | 11/324 (3.4%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 2   | DG   | O3'-P | 6.80 | 1.63        | 1.56     |

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 9   | DU   | C2-N3-C4 | -9.27 | 121.44      | 127.00   |
| 1   | B     | 9   | DU   | N3-C4-C5 | 8.00  | 119.40      | 114.60   |
| 1   | A     | 3   | DU   | C2-N3-C4 | -7.31 | 122.61      | 127.00   |
| 1   | A     | 3   | DU   | N3-C4-C5 | 7.25  | 118.95      | 114.60   |
| 1   | B     | 9   | DU   | N1-C2-N3 | 6.07  | 118.54      | 114.90   |

There are no chirality outliers.

There are no planarity outliers.

### 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   | A     | 120   | 0        | 68       | 2       | 0            |
| 1   | B     | 120   | 0        | 68       | 0       | 0            |
| 2   | A     | 38    | 0        | 0        | 1       | 0            |
| 2   | B     | 46    | 0        | 0        | 0       | 0            |
| All | All   | 324   | 0        | 136      | 2       | 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 5.

All (2) 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:A:3:DU:OP2 | 2:A:75:HOH:O | 2.18                     | 0.55              |
| 1:A:6:DG:N3  | 1:A:6:DG:H2' | 2.31                     | 0.45              |

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](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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 |
| 1   | 1AP  | A     | 4   | 1    | 21,24,25     | 1.21 | 3 (14%)  | 30,35,38    | 1.41 | 3 (10%)  |
| 1   | 1AP  | B     | 10  | 1    | 21,24,25     | 0.87 | 0        | 30,35,38    | 1.61 | 3 (10%)  |

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   | 1AP  | A     | 4   | 1    | -       | 0/7/21/22 | 0/3/3/3 |
| 1   | 1AP  | B     | 10  | 1    | -       | 0/7/21/22 | 0/3/3/3 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 4   | 1AP  | C6-N1   | 3.21  | 1.39        | 1.35     |
| 1   | A     | 4   | 1AP  | C4-N3   | 2.09  | 1.36        | 1.34     |
| 1   | A     | 4   | 1AP  | O4'-C4' | -2.02 | 1.40        | 1.45     |

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

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 10  | 1AP  | C2-N1-C6 | 5.83  | 124.27      | 117.28   |
| 1   | B     | 10  | 1AP  | C5-C6-N1 | -3.60 | 113.30      | 118.90   |
| 1   | A     | 4   | 1AP  | C2-N1-C6 | 3.55  | 121.54      | 117.28   |
| 1   | B     | 10  | 1AP  | N6-C6-N1 | 3.46  | 121.69      | 117.03   |
| 1   | A     | 4   | 1AP  | C5-C6-N1 | -2.76 | 114.61      | 118.90   |

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

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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed   | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------|--------|-----------|-----------------------|-------|
| 1   | A     | 4/6 (66%)  | -1.28  | 0 100 100 | 5, 6, 6, 7            | 0     |
| 1   | B     | 4/6 (66%)  | -1.25  | 0 100 100 | 6, 6, 7, 7            | 0     |
| All | All   | 8/12 (66%) | -1.26  | 0 100 100 | 5, 6, 7, 7            | 0     |

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 1   | 1AP  | A     | 4   | 22/23 | 0.97 | 0.04 | 2,6,11,16                  | 0     |
| 1   | 1AP  | B     | 10  | 22/23 | 0.98 | 0.03 | 4,7,8,13                   | 0     |

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.