



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:37 AM UTC

PDB ID : 1I5V / pdb_00001i5v
Title : SOLUTION STRUCTURE OF 2-(PYRIDO[1,2-E]PURIN-4-YL)AMINO-ETHANOL INTERCALATED IN THE DNA DUPLEX D(CGATCG)₂
Authors : Favier, A.; Blackledge, M.; Simorre, J.P.; Marion, D.; Debouisy, J.C.
Deposited on : 2001-03-01

This is a Full wwPDB NMR Structure Validation 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	:	FAILED
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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis ⓘ

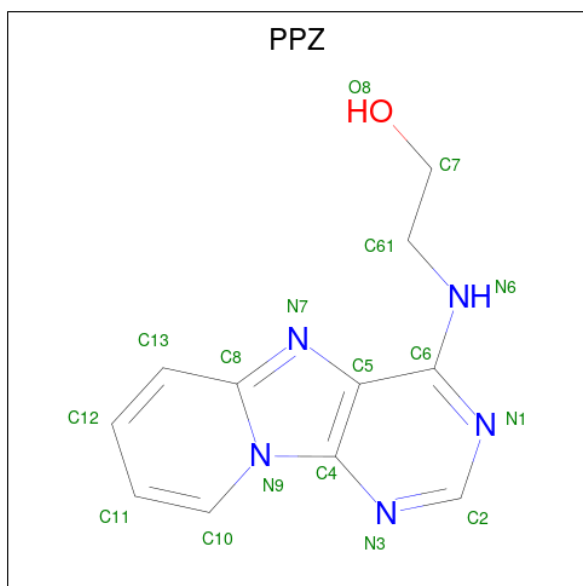
This entry contains 22 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

There are 2 unique types of molecules in this entry. The entry contains 432 atoms, of which 158 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	6	Total 188	C 58	H 68	N 23	O 34	P 5	0
1	B	6	Total 188	C 58	H 68	N 23	O 34	P 5	0

- Molecule 2 is 2-(PYRIDO[1,2-E]PURIN-4-YL)AMINO-ETHANOL (CCD ID: PPZ) (formula: $C_{11}H_{11}N_5O$).



Mol	Chain	Residues	Atoms				
2	A	1	Total 28	C 11	H 11	N 5	O 1
2	B	1	Total 28	C 11	H 11	N 5	O 1

4 Residue-property plots [i](#)

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*AP*TP*CP*G)-3'

Chain A:  67% 33%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  50% 50%



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

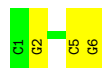
- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

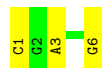
Chain B:  50% 50%



4.2.2 Score per residue for model 2

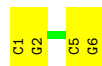
- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

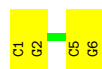
Chain B:  33% 67%



4.2.3 Score per residue for model 3

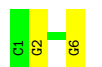
- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  33% 67%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

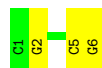
Chain B:  67% 33%



4.2.4 Score per residue for model 4

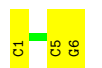
- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  50% 50%



4.2.5 Score per residue for model 5

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  50% 50%



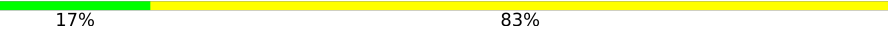
4.2.6 Score per residue for model 6

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  67% 33%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  17% 83%



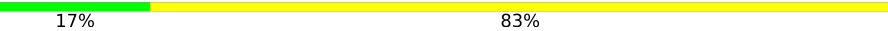
4.2.7 Score per residue for model 7

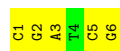
- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

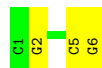
Chain B:  17% 83%



4.2.8 Score per residue for model 8

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  83% 17%



4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  67% 33%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  67% 33%



4.2.10 Score per residue for model 10

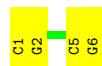
- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  67% 33%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  33% 67%



4.2.11 Score per residue for model 11

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  67% 33%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  50% 50%



4.2.12 Score per residue for model 12

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  67% 33%



4.2.13 Score per residue for model 13

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

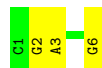
Chain B:  50% 50%



4.2.14 Score per residue for model 14

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  83% 17%



4.2.15 Score per residue for model 15

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  67% 33%



4.2.16 Score per residue for model 16

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  83% 17%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

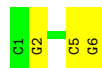
Chain B:  67% 33%



4.2.17 Score per residue for model 17

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  67% 33%



4.2.18 Score per residue for model 18

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  67% 33%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  67% 33%



4.2.19 Score per residue for model 19

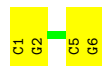
- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  83% 17%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  33% 67%



4.2.20 Score per residue for model 20

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  50% 50%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

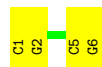
Chain B:  50% 50%



4.2.21 Score per residue for model 21

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  33% 67%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  83% 17%



4.2.22 Score per residue for model 22

- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain A:  67% 33%



- Molecule 1: 5'-D(*CP*GP*AP*TP*CP*G)-3'

Chain B:  67% 33%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 22 were deposited, based on the following criterion: *The submitted conformer models are the 22 structures with the lowest experimental energy*.

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

Software name	Classification	Version
Discover	structure solution	
Discover	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

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

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided