



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 202D / pdb_0000202d
Title : SOLUTION STRUCTURE OF THE MENOGARIL-DNA COMPLEX
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Deposited on : 1995-03-29

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

<https://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)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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 4 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.

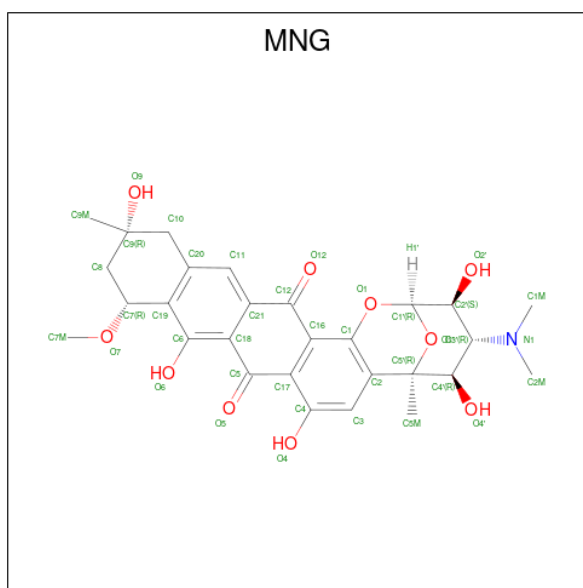
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 646 atoms, of which 246 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		P
1	A	8	253	78	92	30	46	7	0
1	B	8	253	78	92	30	46	7	0

- Molecule 2 is MENOGARIL (CCD ID: MNG) (formula: $C_{28}H_{31}NO_{10}$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	70	28	31	1	10
2	B	1	70	28	31	1	10

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: DNA (5'-D(*GP*AP*CP*AP*TP*GP*TP*C)-3')

Chain A:  100%

There are no outlier residues in this chain.

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

Chain B:  100%

There are no outlier residues in this chain.

4.2 Residue scores for the first model from the NMR ensemble

No representative models were identified. Colouring as in section 4.1 above.

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

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 1: DNA (5'-D(*GP*AP*CP*AP*TP*GP*TP*C)-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: *MOLECULAR DYNAMICS, MATRIX RELAXATION*.

Of the 4 calculated structures, 4 were deposited, based on the following criterion: *all calculated structures submitted*.

The authors did not provide any information on software used for structure solution, optimization or 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](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

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

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6.5 Carbohydrates [i](#)

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6.6 Ligand geometry [i](#)

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6.7 Other polymers [i](#)

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6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided