



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 7B4Z / pdb_00007b4z
BMRB ID : 34579
Title : Synthetic DNA duplex dodecamer
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Deposited on : 2020-12-03

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 : 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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

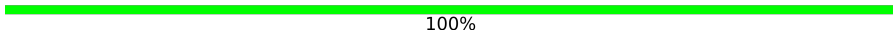
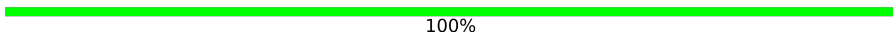
The overall completeness of chemical shifts assignment is 38%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	10	 100%
2	B	10	 100%

2 Ensemble composition and analysis ⓘ

This entry contains 10 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 630 atoms, of which 226 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	10	Total	C	H	N	O	P	0
			312	95	113	37	58	9	

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

Mol	Chain	Residues	Atoms						Trace
2	B	10	Total	C	H	N	O	P	0
			318	97	113	41	58	9	

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

Chain A:  100%

There are no outlier residues in this chain.

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

Chain B:  100%

There are no outlier residues in this chain.

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

Chain A:  100%

There are no outlier residues in this chain.

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

Chain B:  100%

There are no outlier residues in this chain.

4.2.2 Score per residue for model 2

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

Chain A:  100%

There are no outlier residues in this chain.

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

Chain B:  100%

There are no outlier residues in this chain.

4.2.3 Score per residue for model 3

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

Chain A:  100%

There are no outlier residues in this chain.

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

Chain B:  100%

There are no outlier residues in this chain.

4.2.4 Score per residue for model 4

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

Chain A:  100%

There are no outlier residues in this chain.

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

Chain B:  100%

There are no outlier residues in this chain.

4.2.5 Score per residue for model 5

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

Chain A:  100%

There are no outlier residues in this chain.

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

Chain B:  100%

There are no outlier residues in this chain.

4.2.6 Score per residue for model 6

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

Chain A:  100%

There are no outlier residues in this chain.

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

Chain B:  100%

There are no outlier residues in this chain.

4.2.7 Score per residue for model 7

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

Chain A:  100%

There are no outlier residues in this chain.

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

Chain B:  100%

There are no outlier residues in this chain.

4.2.8 Score per residue for model 8

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

Chain A:  100%

There are no outlier residues in this chain.

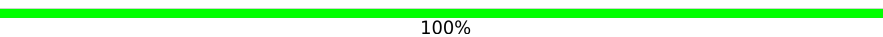
- Molecule 2: DNA (5'-D(*CP*AP*GP*CP*GP*GP*CP*GP*TP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

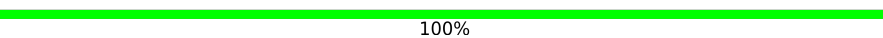
4.2.9 Score per residue for model 9

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

Chain A:  100%

There are no outlier residues in this chain.

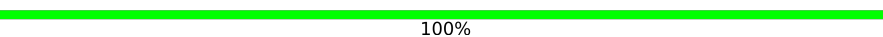
- Molecule 2: DNA (5'-D(*CP*AP*GP*CP*GP*GP*CP*GP*TP*G)-3')

Chain B:  100%

There are no outlier residues in this chain.

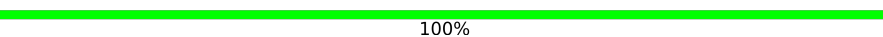
4.2.10 Score per residue for model 10

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

Chain A:  100%

There are no outlier residues in this chain.

- Molecule 2: DNA (5'-D(*CP*AP*GP*CP*GP*GP*CP*GP*TP*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: *molecular dynamics*.

Of the 10 calculated structures, 10 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
Amber	refinement	14
Amber	structure calculation	14

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	265
Number of shifts mapped to atoms	265
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

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
All	All	4040	2260	2260	-

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 -.

There are no clashes.

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](#)

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

The completeness of assignment taking into account all chemical shift lists is 38% for the well-defined parts and 38% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: 15.3_H2O_1-20.txt

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	136
Number of shifts mapped to atoms	136
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 32%, i.e. 130 atoms were assigned a chemical shift out of a possible 404. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	100/240 (42%)	100/140 (71%)	0/100 (0%)	0/0 (—%)
Base	30/164 (18%)	30/104 (29%)	0/32 (0%)	0/28 (0%)
Overall	130/404 (32%)	130/244 (53%)	0/132 (0%)	0/28 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 32%, i.e. 130 atoms were assigned a chemical shift out of a possible 404. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Sugar	100/240 (42%)	100/140 (71%)	0/100 (0%)	0/0 (—%)
Base	30/164 (18%)	30/104 (29%)	0/32 (0%)	0/28 (0%)
Overall	130/404 (32%)	130/244 (53%)	0/132 (0%)	0/28 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins

7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: 33.3_H2O_1-20.txt

7.2.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	129
Number of shifts mapped to atoms	129
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 30%, i.e. 123 atoms were assigned a chemical shift out of a possible 404. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Sugar	69/240 (29%)	69/140 (49%)	0/100 (0%)	0/0 (—%)
Base	54/164 (33%)	54/104 (52%)	0/32 (0%)	0/28 (0%)
Overall	123/404 (30%)	123/244 (50%)	0/132 (0%)	0/28 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 123 atoms were assigned a chemical shift out of a possible 404. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Sugar	69/240 (29%)	69/140 (49%)	0/100 (0%)	0/0 (—%)
Base	54/164 (33%)	54/104 (52%)	0/32 (0%)	0/28 (0%)
Overall	123/404 (30%)	123/244 (50%)	0/132 (0%)	0/28 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots [i](#)

No *random coil index*(RCI) plot could be generated from the current chemical shift list. RCI is only applicable to proteins