

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	5HQQ
Title	:	DNA duplex containing a ribonolactone lesion
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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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)	
NmrClust : Kelley et al. (1996)	
$\operatorname{MolProbity}$: 4.02b-467	
Mogul : 1.8.5 (274361), CSD as541be (2020)	
$ \begin{tabular}{lllllllllllllllllllllllllllllllllll$	h 2019)
$RCI : v_1n_11_5_13_A (Berjanski et al., 2005)$	
PANAV : Wang et al. (2010)	
${ m ShiftChecker}$: 2.11	
Ideal geometry (proteins) : Engh & Huber (2001)	
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)	
Validation Pipeline (wwPDB-VP) : 2.11	

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION \ NMR$

The overall completeness of chemical shifts assignment is 42%.

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	Percen	tile Ranks	Value
Clashscore			1
	Worse		Better
	Percentile relative to all structure	2S	
	Percentile relative to all NMR stru	ictures	
	Whole archive	NMR archive	

Metric	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f NMR} { m archive} \ (\#{ m Entries})$
Clashscore	158937	12864

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 <=5%

Mol	Chain	Length		Quality of chain			
1	А	11	9%	36%	55%		
2	В	11	9%	9%	82%		



2 Ensemble composition and analysis (i)

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 (i)

There are 2 unique types of molecules in this entry. The entry contains 680 atoms, of which 241 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues		Atoms			Trace		
1	Λ	11	Total	С	Η	Ν	Ο	Р	0
		326	99	118	35	64	10	0	

• Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*(8OG)P*TP*GP*GP*GP*AP*GP *CP*G)-3').

Mol	Chain	Residues			Atom	.s			Trace
9	D	11	Total	С	Η	Ν	Ο	Р	0
	D	11	354	108	123	48	65	10	0



')

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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*GP*CP*TP*CP*(RIB)P*CP*AP*CP*GP*C)-3')

Chain A:	9%	36%	55%	
C1 C3 C3 C3 C5 C7 A8	610 611 611			
• Molecule	2: DNA (5'-D	(*GP*CP*(8OG)P*7	TP*GP*GP*GP*AP*GP*CP*G)-3')
Chain B:	9% 9%		82%	
812 013 014 016 016 017 018 018 018	320			

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*GP*CP*TP*CP*(RIB)P*CP*AP*CP*GP*C)-3')

Chain A:	9%	45%		45%
C1 C2 C5 C5 C7 A8 C7 A8	<mark>610</mark> 611			
• Molecule	2: DNA	. (5'-D(*GP*CP*(800	G)P*TP*GP*GP	*GP*AP*GP*CP*G)-3
Chain B:	9%	18%	55%	18%
612 C13 T15 614 616 617 618 A19	620 621 622			



4.2.2 Score per residue for model 2

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

Chain A:	9%	27%	64%
8 2 2 3 2 3 3 3 3 3 3 3 5 3 5 3 5 3 5 5 5 5	610 611		
• Molecule	e 2: DNA	(5'-D(*GP*))	CP*(8OG)P*TP*GP*GP*GP*AP*GP*CP*G)-3')
Chain B:	9% 9	%	82%
612 013 013 014 014 016 016 016 016 018	620 621 622		
4.2.3 So	core per	residue for	model 3
• Molecule	e 1: DNA	A (5'-D(*CP*	GP*CP*TP*CP*(RIB)P*CP*AP*CP*GP*C)-3')
Chain A:	9%	36%	55%

• Molecule 2: DNA (5'-D(*GP*CP*(8OG)P*TP*GP*GP*GP*AP*GP*CP*G)-3')

Chain B: 9%	27%	64%
612 C13 C13 C13 616 616 617 618 618 620 620 622		

4.2.4 Score per residue for model 4

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

Chain A: 9%	45%	45%	
C1 C2 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3			
• Molecule 2: DNA (5'-D(*GP*CP*(80G)P	*TP*GP*GP*GP*AP*C	GP*CP*G)-3')
Chain B: 9% 9%	7	3%	9%



4.2.5 Score per residue for model 5

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

Chain A:	9%	45%	36%	9%
C 1 C 2 C 2 C 2 C 2 C 2 C 2 C 2 C 2 C 2 C 2	C9 C11 C11			
• Molecule	2: DNA (5'-D(*0	GP*CP*(8OG)P*TP*GP*(GP*GP*AP*G	P*CP*G)-3')
Chain B:	9%	45%	45%	
G12 C13 C13 G16 G16 G17 G17 A19	620 621 622			

4.2.6 Score per residue for model 6

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

Chain A: 9%	73%	18%
01 02 05 05 05 05 05 05 01 011		

• Molecule 2: DNA (5'-D(*GP*CP*(8OG)P*TP*GP*GP*GP*AP*GP*CP*G)-3')

Chain B: [•]	9%	18%	73%
612 C13 C13 C13 G14 G14 G17 G18 G18	620 622 622		

4.2.7 Score per residue for model 7

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

Chain A:	9%	27%	64%	
C1 C3 C5 C5 C5 C7 A8	C9 610 C11			
• Molecule	2: DNA (5	C-D(*GP*CP*(80G)	P*TP*GP*GP*GP*AP*	GP*CP*G)-3')
Chain B:	9%	55%	36%	
612 C13 115 616 617 618 618	620 C21 622			



4.2.8 Score per residue for model 8

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

Chain A: 9% s	9%	82%	
C1 C3 C3 C5 C5 C5 C4 C1 C1 C1 C1 C1 C1 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2			
• Molecule 2: DN	A $(5'-D(*GP*C))$	P*(8OG)P*TP*GP*GP*GP*A	.P*GP*CP*G)-3')
Chain B: 9%	36%	55%	
612 013 014 016 016 016 018 019 020 021 021 022			
4.2.9 Score pe	r residue for n	nodel 9	
• Molecule 1: DN	A $(5'-D(*CP*G))$	P*CP*TP*CP*(RIB)P*CP*AI	▷*CP*GP*C)-3')
Chain A: 9%	27%	64%	
C1 C1 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1			
• Molecule 2: DN	A $(5'-D(*GP*C))$	P*(8OG)P*TP*GP*GP*GP*A	.P*GP*CP*G)-3')
Chain B: 9%	18%	64%	9%
612 013 014 014 017 016 017 018 018 018 018 019 021 021 022			
4.2.10 Score p	er residue for	model 10	
• Molecule 1: DN	A $(5'-D(*CP*G))$	P*CP*TP*CP*(RIB)P*CP*AI	D*CP*GP*C)-3')
Chain A: 9%	36%	55%	
C1 C2 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3			

• Molecule 2: DNA (5'-D(*GP*CP*(8OG)P*TP*GP*GP*GP*AP*GP*CP*G)-3')

Chain B: 9%	36%	55%	-
612 613 614 616 616 616 617 618 618 618 618 620 621 622			



5 Refinement protocol and experimental data overview (i)

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

Of the 10 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Amber	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	187
Number of shifts mapped to atoms	187
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	А	208	118	101	0 ± 1
2	В	231	123	115	1±1
All	All	4390	2410	2236	8

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 1.

All unique clashes are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
2:B:12:DG:C4	2:B:13:DC:C5	0.47	3.03	1	3
2:B:20:DG:C5	2:B:21:DC:C5	0.44	3.05	4	1
2:B:19:DA:C6	2:B:20:DG:C6	0.43	3.07	6	1
1:A:10:DG:C6	1:A:11:DC:C4	0.42	3.07	5	1
1:A:10:DG:C5	1:A:11:DC:C5	0.42	3.07	5	1
2:B:17:DG:C6	2:B:18:DG:C6	0.41	3.08	1	1

5.2 Torsion angles (i)

5.2.1 Protein backbone (i)

There are no protein molecules in this entry.

5.2.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.2.3 RNA (i)

There are no RNA molecules in this entry. MODRES-GEOMETRY INFOmissingINFO

5.3 Carbohydrates (i)

There are no carbohydrates in this entry.

5.4 Ligand geometry (i)

There are no ligands in this entry.

5.5 Other polymers (i)

There are no such molecules in this entry.

5.6 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 42% for the well-defined parts and 42% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: chemshifts_ribonoG14_new3.txt

6.1.1 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	187
Number of shifts mapped to atoms	187
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

6.1.2 Chemical shift referencing (i)

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

6.1.3 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 42%, i.e. 170 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	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	0/0~(-%)	0/0~(-%)	$0/0 \ (\%)$	0/0 (-%)
Sidechain	0/0~(-%)	0/0~(-%)	$0/0 \ (\%)$	$0/0 \ (-\%)$
Aromatic	0/0~(-%)	0/0~(-%)	$0/0 \ (\%)$	0/0 (-%)
Overall	170/404~(42%)	170/244~(70%)	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 42%, i.e. 170 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	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	0/0~(-%)	0/0~(-%)	0/0 (%)	$0/0 \ (\%)$
Sidechain	0/0~(-%)	$0/0 \ (-\%)$	0/0 (%)	$0/0 \ (-\%)$
Aromatic	0/0~(-%)	0/0~(-%)	0/0 (%)	$0/0 \ (\%)$
Overall	170/404~(42%)	170/244~(70%)	0/132~(0%)	0/28~(0%)

6.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.1.5 Random Coil Index (RCI) plots (i)

No random coil index (RCI) plot could be generated from the current chemical shift list (chemshifts_ribonoG14 RCI is only applicable to proteins.

