

## wwPDB NMR Structure Validation Summary Report (i)

#### Nov 5, 2023 – 10:43 AM EST

:	176D
:	NMR SOLUTION STRUCTURE OF A PEPTIDE NUCLEIC ACID COM-
	PLEXED WITH RNA
:	Brown, S.C.; Veal, J.M.
:	1994-05-17
	:

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 (i) 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 (1)) were used in the production of this report:

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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)	:	2.36

RNA backbone

# 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 was not calculated.

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	Percentile	Value	
Clashscore			0
RNA backbone			0.65
Worse			Better
Percer	ntile relative to all structures		
Percer	ntile relative to all NMR structures		
D.C. taria	Whole archive	NMR archive	
Metric	(# Entries)	(# Entries)	
Clashscore	158937	12864	

4643

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%

676

Mol	Chain	Length	Quality of chain				
2	В	6	17%	33%	50%		



## 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.

ENTRY-COMPOSITION INFOmissingINFO



# 3 Residue-property plots (i)

### 3.1 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 2: RNA (5'-R(P\*GP\*AP\*GP\*UP\*UP\*C)-3')

Chain B:	17%	33%	50%
67 A8 69 U10 C12			

### 3.2 Residue scores for the first model from the NMR ensemble

No representative models were identified. Colouring as in section 3.1 above.

• Molecule 2: RNA (5'-R(P\*GP\*AP\*GP\*UP\*UP\*C)-3')

Chain B:	33%	33%	33%
G7 A8 G9 U10 C12			



## 4 Refinement protocol and experimental data overview (i)

The models were refined using the following method:  $DISTANCE \ GEOMETRY, \ SIMULATED \ ANNEALING.$ 

Of the ? calculated structures, 10 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	3.10

No chemical shift data was provided.



# 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: CPN, APN, TPN, GPN

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	B	ond lengths	Bond angles		
	Chain	RMSZ	$\#Z{>}5$	RMSZ	$\#Z{>}5$	
1	А	$0.00 {\pm} 0.00$	-	$0.00 {\pm} 0.00$	-	
2	В	$1.55 {\pm} 0.04$	$1{\pm}1/143~(~0.5{\pm}~0.4\%)$	$1.94{\pm}0.05$	$4{\pm}1/219~(~1.9{\pm}~0.4\%)$	
All	All	1.55	7/1430~(~0.5%)	1.94	41/2190 ( 1.9%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
2	В	$0.0{\pm}0.0$	$2.5{\pm}1.0$
All	All	0	25

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Moo Worst	dels Total
						. ,		worst	Total
2	В	9	G	C5-C6	5.51	1.47	1.42	2	1
2	В	8	А	N3-C4	5.50	1.38	1.34	7	6

5 of 10 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms Z		Observed(°)	Ideal(°)	Moo	dels
	Unain	nes	Type	Atoms		Z Observeu()	Ideal()	Worst	Total
2	В	10	U	O4'-C1'-N1	7.22	113.97	108.20	1	10
2	В	11	U	O4'-C1'-N1	6.72	113.58	108.20	4	10
2	В	9	G	O4'-C1'-N9	6.20	113.16	108.20	2	8
2	В	7	G	N3-C4-C5	-5.98	125.61	128.60	2	7
2	В	9	G	N9-C4-C5	5.97	107.79	105.40	7	1



There are no chirality outliers.

5 of 6 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	В	10	U	Sidechain	9
2	В	8	А	Sidechain	8
2	В	12	С	Sidechain	3
2	В	7	G	Sidechain	2
2	В	9	G	Sidechain	2

### 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 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	2460	1470	1140	-

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.

#### 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)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	В	5/6~(83%)	0±0 (8±10%)	0±0 (0±0%)	$0.65 {\pm} 0.15$
All	All	50/60~(83%)	4 (8%)	0 (0%)	0.65



176D

The overall RNA backbone suiteness is 0.65.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	В	9	G	4

There are no RNA pucker outliers to report.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link		Bond len	$\mathbf{gths}$
10101	туре	Chain	nes	LIIIK	Counts	RMSZ	#Z>2
1	$\operatorname{CPN}$	А	6	2,1	$19,\!19,\!19$	$1.05 {\pm} 0.06$	$1\pm0 (5\pm0\%)$
1	TPN	А	5	2,1	19,19,20	$1.06 {\pm} 0.05$	$2\pm0$ (10 $\pm0\%$ )
1	$\operatorname{CPN}$	А	4	2,1	18,18,19	$1.06{\pm}0.07$	$1\pm0 (5\pm0\%)$
1	APN	А	3	2,1	18,21,22	$0.91{\pm}0.04$	$1\pm0 (5\pm1\%)$
1	GPN	А	1	2,1	18,22,23	$1.12{\pm}0.02$	1±0 (6±1%)
1	APN	А	2	2,1	18,21,22	$0.93{\pm}0.02$	$1\pm0 (5\pm0\%)$

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mal	Turne	Chain	Dec	Tink		Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	#Z>2
1	CPN	А	6	2,1	$24,\!25,\!25$	$1.31{\pm}0.10$	$2\pm1 (9\pm3\%)$
1	TPN	А	5	2,1	$23,\!25,\!27$	$1.98{\pm}0.18$	$7 \pm 1 (28 \pm 5\%)$
1	CPN	А	4	2,1	20,23,25	$2.26 \pm 0.48$	4±1 (20±3%)



Mol	I Type Chain Res Link Bond angles				gles		
INIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	#Z>2
1	APN	А	3	2,1	15,28,30	$1.85 {\pm} 0.17$	$4\pm1~(24\pm5\%)$
1	GPN	А	1	2,1	17,30,32	$1.47{\pm}0.22$	3±1 (18±8%)
1	APN	А	2	2,1	15,28,30	$1.71 {\pm} 0.16$	$3\pm1(20\pm4\%)$

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	CPN	А	6	2,1	-	$0\pm0,\!15,\!15,\!15$	$0\pm 0,1,1,1$
1	CPN	А	4	2,1	-	$0\pm0,13,14,15$	$0\pm 0,1,1,1$
1	APN	А	3	2,1	-	$0\pm0,13,14,15$	$0\pm 0,2,2,2$
1	GPN	А	1	2,1	-	$0\pm0,13,14,15$	$0\pm0,2,2,2$
1	APN	А	2	2,1	-	$0\pm0,13,14,15$	$0\pm 0,2,2,2$
1	TPN	А	5	2,1	-	$0\pm0,13,14,15$	$0\pm 0,1,1,1$

5 of 9 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Turne	Atoma	Z	Observed(Å)	Ideal(Å)	Moo	lels
	Unam	nes	Type	Atoms		Observed(A)	Ideal(A)	Worst	Total
1	А	4	CPN	C8'-N1	3.61	1.50	1.46	8	10
1	А	6	CPN	C8'-N1	2.97	1.50	1.46	10	9
1	А	5	TPN	C8'-N1	2.88	1.49	1.46	5	10
1	А	1	GPN	C8-N7	2.63	1.30	1.35	4	10
1	А	5	TPN	C2-N1	2.46	1.41	1.37	5	10

5 of 37 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoma	Z	Observed(°)	$Ideal(^{o})$	Models	
	Unam	nes	туре	Atoms	2	Observed()	Ideal()	Worst	Total
1	А	4	CPN	C7'-C8'-N1	13.76	123.15	110.99	7	10
1	А	3	APN	C7'-C8'-N9	6.14	118.08	110.76	4	10
1	А	2	APN	C7'-C8'-N9	5.65	117.49	110.76	4	10
1	А	5	TPN	C7'-C8'-N1	5.49	115.84	110.99	5	8
1	А	1	GPN	C7'-C8'-N9	5.11	116.85	110.76	10	8

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

6 such molecules are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link		Bond len	gths
10101	Type	Chain	nes	LIIIK	Counts	RMSZ	#Z>2
1	CPN	А	6	2,1	$19,\!19,\!19$	$1.05 {\pm} 0.06$	$1\pm0 (5\pm0\%)$
1	TPN	А	5	2,1	19,19,20	$1.06 {\pm} 0.05$	2±0 (10±0%)
1	CPN	А	4	2,1	18,18,19	$1.06 {\pm} 0.07$	$1\pm0 (5\pm0\%)$
1	APN	А	3	2,1	18,21,22	$0.91{\pm}0.04$	$1\pm0(5\pm1\%)$
1	GPN	А	1	2,1	18,22,23	$1.12{\pm}0.02$	$1\pm0$ (6±1%)
1	APN	А	2	2,1	18,21,22	$0.93{\pm}0.02$	$1\pm0(5\pm0\%)$

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mal	Type	Chain	Dog	Link		Bond ang	gles
Mol	Type	Ullaili	nes		Counts	RMSZ	#Z>2
1	CPN	А	6	2,1	24,25,25	$1.31{\pm}0.10$	$2\pm1 (9\pm3\%)$



Mol	Type	Chain	Res	Link		Bond ang	gles
IVIOI	Type	Ullalli	nes		Counts	RMSZ	#Z>2
1	TPN	А	5	2,1	$23,\!25,\!27$	$1.98{\pm}0.18$	7±1 (28±5%)
1	CPN	А	4	2,1	20,23,25	$2.26 \pm 0.48$	4±1 (20±3%)
1	APN	А	3	2,1	15,28,30	$1.85 {\pm} 0.17$	$4\pm1~(24\pm5\%)$
1	GPN	А	1	2,1	17,30,32	$1.47 {\pm} 0.22$	$3\pm1$ (18 $\pm8\%$ )
1	APN	А	2	2,1	15,28,30	$1.71 {\pm} 0.16$	$3\pm1(20\pm4\%)$

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	CPN	А	6	2,1	-	$0\pm0,\!15,\!15,\!15$	$0\pm 0,1,1,1$
1	CPN	А	4	2,1	-	$0\pm0,13,14,15$	$0\pm 0,1,1,1$
1	APN	А	3	2,1	-	$0\pm0,13,14,15$	$0\pm0,2,2,2$
1	GPN	А	1	2,1	-	$0\pm0,13,14,15$	$0\pm 0,2,2,2$
1	APN	А	2	2,1	-	$0\pm0,13,14,15$	$0\pm0,2,2,2$
1	TPN	А	5	2,1	-	$0\pm0,13,14,15$	$0\pm 0,1,1,1$

5 of 9 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$	Models	
								Worst	Total
1	А	4	CPN	C8'-N1	3.61	1.50	1.46	8	10
1	А	6	CPN	C8'-N1	2.97	1.50	1.46	10	9
1	А	5	TPN	C8'-N1	2.88	1.49	1.46	5	10
1	А	1	GPN	C8-N7	2.63	1.30	1.35	4	10
1	А	5	TPN	C2-N1	2.46	1.41	1.37	5	10

5 of 37 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$Observed(^{o})$	$\mathrm{Ideal}(^{o})$	Models	
								Worst	Total
1	А	4	CPN	C7'-C8'-N1	13.76	123.15	110.99	7	10
1	А	3	APN	C7'-C8'-N9	6.14	118.08	110.76	4	10
1	А	2	APN	C7'-C8'-N9	5.65	117.49	110.76	4	10
1	А	5	TPN	C7'-C8'-N1	5.49	115.84	110.99	5	8
1	А	1	GPN	C7'-C8'-N9	5.11	116.85	110.76	10	8



There are no chirality outliers. There are no torsion outliers.

There are no ring outliers.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Chemical shift validation (i)

No chemical shift data were provided

