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Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 09:28 pm GMT

PDB ID : 2DD2
Title : An alternating sheared AA pair in 5'GGUGAAGGCU/3'PCCGAAGCCG: I.
The major conformation with A6/A15/A16 stack
Authors : Chen, G.; Kennedy, S.D.; Krugh, T.R.; Turner, D.H.
Deposited on : 2006-01-19

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
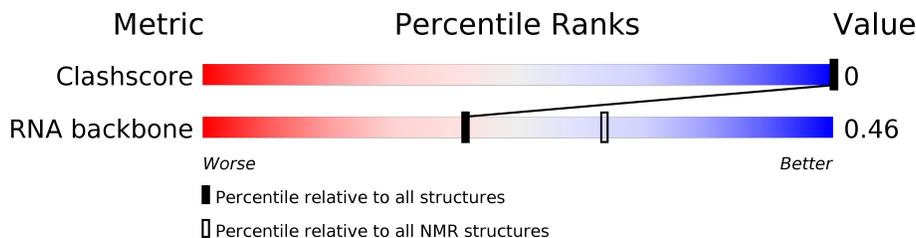with specific help available everywhere you see the ⓘ symbol.

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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.

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 Ranks	Value
Clashscore		0
RNA backbone		0.46

Worse ... *Better*

▌ Percentile relative to all structures
⫿ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
RNA backbone	3398	623

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	A	10	50% 50%
2	B	10	50% 50%

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2 Ensemble composition and analysis ⓘ

This entry contains 27 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 648 atoms, of which 221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'.

Mol	Chain	Residues	Atoms						Trace
1	A	10	Total	C	H	N	O	P	0
			326	97	110	42	68	9	

- Molecule 2 is a RNA chain called 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'.

Mol	Chain	Residues	Atoms						Trace
2	B	10	Total	C	H	N	O	P	0
			322	96	111	41	65	9	

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: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

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'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.2 Score per residue for model 2

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

50% 40% 10%

G1 G2 U3 G4 A5 A6 G7 G8 C9 U10

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

40% 40% 20%

G11 C12 C13 G14 A15 A16 C19 A20

4.2.3 Score per residue for model 3

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

50% 40% 10%

G1 G2 U3 G4 A5 A6 G7 G8 C9 U10

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

50% 50%

G11 C12 C13 G17 C18 C19 A20

4.2.4 Score per residue for model 4

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

40% 50% 10%

G1 G2 U3 G4 A5 C9 U10

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

70% 30%

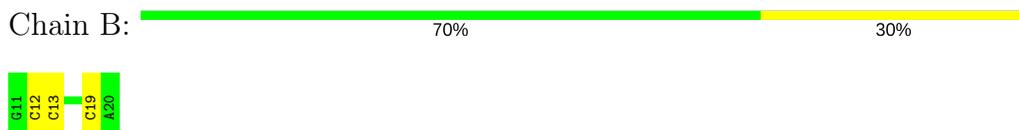G11 C12 C13 C19 A20

4.2.5 Score per residue for model 5

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.6 Score per residue for model 6

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.7 Score per residue for model 7

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.8 Score per residue for model 8

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

G1 G2 U3 G4 A5 C9 U10

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

G11 C12 C13 G14 A15 A16 G17 C18 C19 A20

4.2.9 Score per residue for model 9

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

G1 G2 U3 G4 A5 A6 G7 G8 C9 U10

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

G11 C12 C13 C18 C19 A20

4.2.10 Score per residue for model 10

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

G1 G2 U3 G4 A5 C9 U10

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

G11 C12 C13 G14 C18 C19 A20

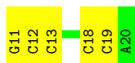### 4.2.11   Score per residue for model 11

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.12   Score per residue for model 12

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.13   Score per residue for model 13

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.14 Score per residue for model 14

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.15 Score per residue for model 15
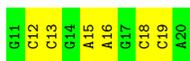
• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.16 Score per residue for model 16

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'
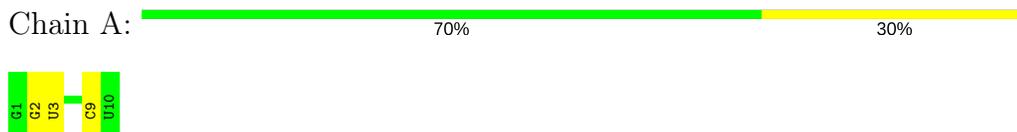
Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.17 Score per residue for model 17

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

70%   30%

G1 G2 U3 C9 U10

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

40%   60%

G11 C12 C13 G14 A15 A16 G17 C18 C19 A20

4.2.18 Score per residue for model 18

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

40%   50%   10%

G1 G2 U3 G4 A5 A6 G7 G8 C9 U10

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

60%   40%

G11 C12 C13 C18 C19 A20

4.2.19 Score per residue for model 19

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

30%   60%   10%

G1 G2 U3 G4 A5 A6 G7 G8 C9 U10

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

50%   40%   10%

G11 C12 C13 G14 A15 A16 C19 A20

4.2.20 Score per residue for model 20

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'
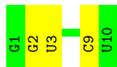
Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.21 Score per residue for model 21

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.22 Score per residue for model 22

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.23 Score per residue for model 23

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:

4.2.24 Score per residue for model 24

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'
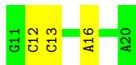
Chain B:

4.2.25 Score per residue for model 25

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:
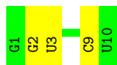
4.2.26 Score per residue for model 26

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'
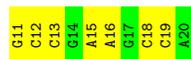
Chain B:

4.2.27 Score per residue for model 27

• Molecule 1: 5'-R(*GP*GP*UP*GP*AP*AP*GP*GP*CP*U)-3'

Chain A:

• Molecule 2: 5'-R(*GP*CP*CP*GP*AP*AP*GP*CP*CP*(P5P))-3'

Chain B:
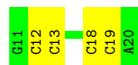
5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *distance geometry, simulated annealing, molecular dynamics.*

Of the 40 calculated structures, 27 were deposited, based on the following criterion: *structures with the lowest energy, structures with the least restraint violations.*

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

Software name	Classification	Version
DISCOVER	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: P5P

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	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.14±0.01	0±0/242 (0.0±0.0%)	1.79±0.02	4±1/377 (1.1±0.2%)
2	B	1.13±0.01	0±0/212 (0.0±0.0%)	1.72±0.02	3±1/329 (1.1±0.2%)
All	All	1.13	0/12258 (0.0%)	1.76	202/19062 (1.1%)

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
1	A	0.0±0.0	0.6±0.6
2	B	0.0±0.0	1.2±1.1
All	All	0	47

There are no bond-length outliers.

All 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(^{o})	Ideal(^{o})	Models Worst	Total
1	A	3	U	O4'-C1'-N1	7.91	114.53	108.20	11	27
2	B	13	C	O4'-C1'-N1	7.30	114.04	108.20	9	27
1	A	7	G	O4'-C1'-N9	7.20	113.96	108.20	3	9
1	A	9	C	O4'-C1'-N1	6.87	113.70	108.20	19	27
2	B	14	G	P-O3'-C3'	6.34	127.31	119.70	22	3
1	A	5	A	O4'-C1'-N9	6.30	113.24	108.20	10	1
2	B	12	C	O4'-C1'-N1	6.24	113.19	108.20	19	27
2	B	19	C	O4'-C1'-N1	6.06	113.05	108.20	25	22
1	A	2	G	O4'-C1'-N9	6.04	113.03	108.20	5	27
1	A	4	G	P-O3'-C3'	6.03	126.93	119.70	11	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models Worst	Models Total
1	A	10	U	O4'-C1'-N1	5.74	112.79	108.20	12	11
2	B	14	G	O4'-C1'-N9	5.53	112.62	108.20	16	1
2	B	16	A	O4'-C1'-N9	5.43	112.55	108.20	14	1
2	B	18	C	O4'-C1'-N1	5.38	112.50	108.20	3	11
2	B	13	C	N1-C2-O2	5.09	121.95	118.90	12	1
2	B	14	G	N9-C1'-C2'	-5.07	106.42	112.00	10	1
1	A	4	G	O4'-C1'-N9	5.00	112.20	108.20	18	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	5	A	Sidechain	14
2	B	15	A	Sidechain	13
2	B	16	A	Sidechain	11
2	B	11	G	Sidechain	5
2	B	19	C	Sidechain	1
1	A	4	G	Sidechain	1
2	B	18	C	Sidechain	1
2	B	14	G	Sidechain	1

6.2 Too-close contacts ⓘ

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	11529	5967	5967	-

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 ⓘ

6.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

6.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	9/10 (90%)	1±1 (9±7%)	0±0 (0±0%)	0.39±0.04
2	B	8/10 (80%)	1±1 (11±9%)	0±0 (0±0%)	0.55±0.06
All	All	459/540 (85%)	46 (10%)	0 (0%)	0.46

The overall RNA backbone suiteness is 0.46.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	16	A	14
1	A	6	A	10
2	B	15	A	8
1	A	7	G	6
1	A	5	A	6
2	B	17	G	1
2	B	14	G	1

There are no RNA pucker outliers to report.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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.

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Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	P5P	B	20	2	16,23,24	1.03±0.01	0±0 (0±0%)

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.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	P5P	B	20	2	14,33,36	0.80±0.02	0±0 (0±0%)

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
2	P5P	B	20	2	-	0±0,3,25,26	0±0,3,3,3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

No chemical shift data were provided