

wwPDB NMR Structure Validation Summary Report (i)

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Title	:	Solution structure of AGA modified
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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:

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)	:	2.36.2

Clashscore

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 33%.

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.

Metri	: Р	Percentile Ranks	Value
Clashscore			0
	Worse	Better	
	Percentile relative to all structure	es	
	Percentile relative to all NMR st	tructures	
ЪЛани	Whole arch	ive NMR archiv	/e
Metr	$\mathbf{c} (\# \text{Entries})$	s) (#Entries)	

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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%

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Mol	Chain	Length	Quality of chain					
1	А	10	100%					
2	В	10	10% 90%					



2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 674 atoms, of which 245 are hydrogens and 0 are deuteriums.

• Molecule 1 is a DNA chain called DNA_(5'-D(*CP*TP*AP*AP*(FAG)P*AP*TP*TP*CP *A)-3').

Mol	Chain	Residues	Atoms					Trace	
1	٨	10	Total	С	Η	Ν	Ο	Р	0
	I A	10	355	115	129	37	65	9	0

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

Mol	Chain	Residues	Atoms					Trace	
9 D	10	Total	С	Н	Ν	Ο	Р	0	
	2 B	10	319	99	116	36	59	9	0



4 Residue-property plots (i)

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*TP*AP*AP*(FAG)P*AP*TP*TP*CP*A)-3')

Chain A:	100%
C1 A 2 A 5 A 5 A 5 A 5 A 5 A 5 A 5 A 5 A 5 A 5	A CONTRACTOR OF
• Molecule	2: DNA_(5'-D(*TP*GP*AP*AP*TP*CP*TP*TP*AP*G)-3')
Chain B:	90%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 10 calculated structures, 1 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum*.

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

Software name	Classification	Version
Amber	refinement	12

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	1
Total number of shifts	161
Number of shifts mapped to atoms	160
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	33%



6 Model quality (i)

6.1 Standard geometry (i)

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

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		Bor	nd lengths	Bond angles		
	Chain	RMSZ	#Z > 5	RMSZ	#Z > 5	
1	А	1.73	1/199 ($0.5%)$	2.69	26/302 ($8.6%$)	
2	В	1.69	1/227 ($0.4%)$	2.60	28/349 ($8.0%$)	
All	All	1.71	2/426 ($0.5%)$	2.64	54/651 ($8.3%$)	

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	7	DT	C5-C7	5.48	1.53	1.50
2	В	11	DT	C5-C7	5.38	1.53	1.50

5 of 54 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	10	DA	N1-C6-N6	-10.94	112.03	118.60
2	В	18	DT	O4'-C1'-N1	10.17	115.12	108.00
2	В	13	DA	N1-C6-N6	-9.70	112.78	118.60
2	В	19	DA	N1-C6-N6	-8.39	113.56	118.60
1	А	9	DC	N3-C2-O2	-8.37	116.04	121.90

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	429	245	245	-

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score 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)

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.

Mal	Type	Chain	Dog	Link	Bo	ond leng	ths
	туре	Ullaill	nes		Counts	RMSZ	#Z>2
1	FAG	А	5	1	48,53,54	1.57	5 (10%)

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	Tune	Chain	Ros Link		B	ond ang	gles
	туре		nes	LIIIK	Counts	RMSZ	#Z>2
1	FAG	А	5	1	53,81,84	<mark>3.53</mark>	18 (33%)

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	FAG	А	5	1	-	$0,\!11,\!66,\!67$	0,7,7,7

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	5	FAG	C3-C3A	4.94	1.45	1.52
1	А	5	FAG	O10-C11	4.73	1.31	1.38
1	А	5	FAG	O10-CAA	4.34	1.31	1.38
1	А	5	FAG	C9B-C9A	2.73	1.47	1.50
1	А	5	FAG	C8-N7	2.06	1.40	1.36

5 of 18 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	5	FAG	O4'-C1'-N9	18.50	128.72	110.04
1	А	5	FAG	O7-C8A-N7	9.15	129.28	108.36
1	А	5	FAG	CM-O4-C4B	6.36	127.13	117.53
1	А	5	FAG	O4-C4B-C4A	5.23	123.14	115.85
1	А	5	FAG	O6A-C5M-C9B	4.74	117.27	112.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 33% for the well-defined parts and 33% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: assigned_chem_shift_list_1

7.1.1 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	161
Number of shifts mapped to atoms	160
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

• No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Bos	Typo	Atom		Shift Dat	a
	Ullalli	nes	туре	Atom	Value	Shift Dat Uncertainty	Ambiguity
1	А	5	FAG	H7	3.471		

7.1.2 Chemical shift referencing (i)

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

7.1.3 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 33%, i.e. 122 atoms were assigned a chemical shift out of a possible 368. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Sugar	99/228~(43%)	99/133~(74%)	0/95~(0%)	0/0 (%)
Base	23/140~(16%)	23/83~(28%)	0/36~(0%)	0/21~(0%)
Overall	122/368~(33%)	122/216~(56%)	0/131~(0%)	0/21~(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

