

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	7KUB
Title	:	Au1 Domain of VEGF Readthrough Element
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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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.28.1
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 is 15%.

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	Metric Percentile Ranks			
Clashscore			1	
RNA backbone			0.93	
Worse			Better	
Percer	ntile relative to all structures			
Percer	tile relative to all NMR structures			
Matuia	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	
1	А	60	92%	8%



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 is only 1 type of molecule in this entry. The entry contains 1924 atoms, of which 650 are hydrogens and 0 are deuteriums.

• Molecule 1 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues		Atoms					
1	Λ	60	Total	С	Н	Ν	0	Р	0
	А	60	1924	570	650	230	415	59	0



4 Residue-property plots (i)

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: RNA (60-MER)

Ch	ain	А	: •			92%	8%
C43	A65 G66	C 89	A90	Tep	G102		

4.2 Scores per residue for each member of the ensemble

92%

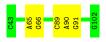
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: RNA (60-MER)

Chain A:

8%



4.2.2 Score per residue for model 2

• Molecule 1: RNA (60-MER)

Chain A: 90% 7% •



4.2.3 Score per residue for model 3

• Molecule 1: RNA (60-MER)

Chain A: 90% 8% •

4.2.4 Score per residue for model 4

• Molecule 1: RNA (60-MER)

Chain A: 92% 8%

4.2.5 Score per residue for model 5

• Molecule 1: RNA (60-MER)

Chain A: 90% 8% •

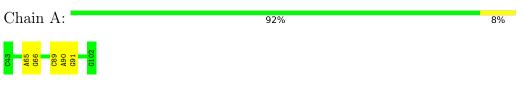
4.2.6 Score per residue for model 6

• Molecule 1: RNA (60-MER)

Chain A: 92% 8%

4.2.7 Score per residue for model 7

• Molecule 1: RNA (60-MER)





4.2.8 Score per residue for model 8

• Molecule 1: RNA (60-MER)

Chain A: 92% 8%

4.2.9 Score per residue for model 9

• Molecule 1: RNA (60-MER)

Chain A: 92% 8%

4.2.10 Score per residue for model 10

• Molecule 1: RNA (60-MER)

Chain A: 92% 8%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 100 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
CYANA	structure calculation	
X-PLOR NIH	refinement	

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	180
Number of shifts mapped to atoms	180
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	15%



6 Model quality (i)

6.1 Standard geometry (i)

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	I	Bond lengths	Bond angles		
		RMSZ	$\#Z{>}5$	RMSZ	#Z>5	
1	А	$0.36 {\pm} 0.01$	$0{\pm}0/1423~(~0.0{\pm}~0.0\%)$	$0.72 {\pm} 0.01$	$1{\pm}1/2216~(~0.0{\pm}~0.0\%)$	
All	All	0.36	0/14230 ($0.0%$)	0.72	9/22160~(~0.0%)	

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	7	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$	Models	
			туре				Ideal()	Worst	Total
1	А	90	A	C1'-O4'-C4'	-6.43	104.76	109.90	2	1
1	А	89	С	C1'-O4'-C4'	-6.34	104.83	109.90	8	8

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
1	А	1274	650	652	2 ± 1
All	All	12740	6500	6520	16

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	
1:A:89:C:O	2 1:A:89:C:O4'	0.46	2.34	3	2	
1:A:56:A:N	6 1:A:91:G:C6	0.43	2.86	5	3	
1:A:65:A:C	5 1:A:66:G:C6	0.43	3.07	4	10	
1:A:89:C:C	2 1:A:89:C:O5'	0.42	2.73	3	1	

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)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	А	59/60~(98%)	2±0 (3±0%)	$0\pm0~(0\pm0\%)$	$0.93 {\pm} 0.00$
All	All	590/600~(98%)	20 (3%)	0 (0%)	0.93

The overall RNA backbone suiteness is 0.93.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	А	90	A	10
1	А	91	G	10

There are no RNA pucker outliers to report.

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 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 15% for the well-defined parts and 15% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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

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 15%, i.e. 170 atoms were assigned a chemical shift out of a possible 1137. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
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	170/1137~(15%)	170/657~(26%)	0/403~(0%)	0/77~(0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 170 atoms were assigned a chemical shift out of a possible 1137. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



	Total	$^{1}\mathbf{H}$	$^{13}\mathbf{C}$	$^{15}\mathbf{N}$
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	170/1137~(15%)	170/657~(26%)	0/403~(0%)	0/77~(0%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	А	75	G	H8	5.55	9.29 - 5.89	-6.0

7.1.5 Random Coil Index (RCI) plots (i)

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

