

Full wwPDB NMR Structure Validation Report (i)

Jun 10, 2021 - 01:05 PM BST

:	6ZOP
:	Structure of the cysteine-rich domain of PiggyMac, a domesticated PiggyBac
	transposase involved in programmed genome rearrangements
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:	2020-07-07
	:

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:

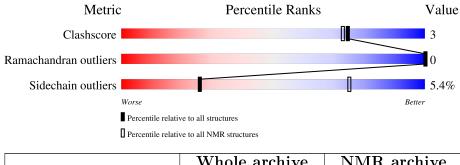
$\operatorname{MolProbity}$:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v $1n_11_5_13_A$ (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
${ m ShiftChecker}$:	2.20
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

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 84%.

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	Whole archive	NMR archive
Methe	$(\# { m Entries})$	$(\# { m Entries})$
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	Qual	ity of chain	
1	٨	0.4			
	А	84	57%	•	39%



2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues					
Well-defined core Residue range (total) Backbone RMSD (Å) Medoid model					
1	A:17-A:67 (51)	0.34	1		

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 9 single-model clusters were found.

Cluster number	Models
1	10, 13
2	1, 4
3	2, 6
Single-model clusters	3; 5; 7; 8; 9; 11; 12; 14; 15



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1329 atoms, of which 653 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called DDE_Tnp_1_7 domain-containing protein.

Mol	Chain	Residues			Aton	ıs			Trace
1	Λ	Q /	Total	С	Η	Ν	Ο	S	0
	A	04	1327	427	653	111	129	7	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0DFJ7
А	2	PRO	-	expression tag	UNP A0DFJ7
A	3	LEU	-	expression tag	UNP A0DFJ7
А	4	GLY	-	expression tag	UNP A0DFJ7
A	5	SER	-	expression tag	UNP A0DFJ7
A	6	PRO	-	expression tag	UNP A0DFJ7
A	7	GLU	_	expression tag	UNP A0DFJ7

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms
2	А	2	Total Zn 2 2



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: DDE_Tnp_1_7 domain-containing protein

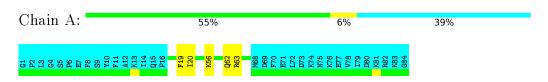
Chain A:	57%	•	39%
61 22 22 64 25 25 25 25 25 26 25 21 11 21 24 21 25 21 25 21 21 25 21 21 25 21 21 21 21 21 21 21 21 21 21 21 21 21	F19 120 K56 M68 M68 F70 D69 T72 T72 K74 W75	K76 E77 179 D80 K81 K83 G84 G84	

4.2 Scores per residue for each member of the ensemble

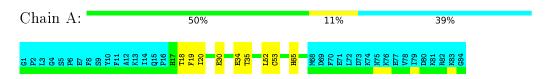
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: DDE_Tnp_1_7 domain-containing protein



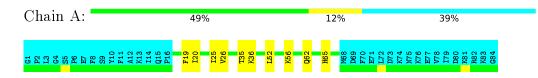
4.2.2 Score per residue for model 2





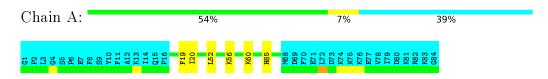
4.2.3 Score per residue for model 3

• Molecule 1: DDE_Tnp_1_7 domain-containing protein



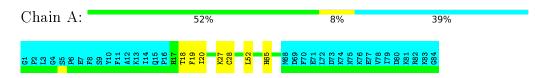
4.2.4 Score per residue for model 4

• Molecule 1: DDE_Tnp_1_7 domain-containing protein



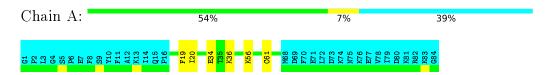
4.2.5 Score per residue for model 5

• Molecule 1: DDE_Tnp_1_7 domain-containing protein

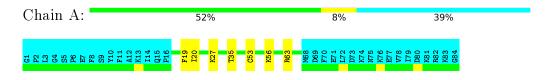


4.2.6 Score per residue for model 6

• Molecule 1: DDE_Tnp_1_7 domain-containing protein



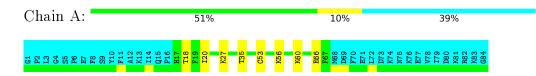
4.2.7 Score per residue for model 7





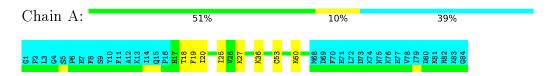
4.2.8 Score per residue for model 8

• Molecule 1: DDE_Tnp_1_7 domain-containing protein



4.2.9 Score per residue for model 9

• Molecule 1: DDE_Tnp_1_7 domain-containing protein



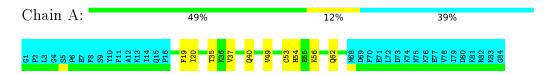
4.2.10 Score per residue for model 10

• Molecule 1: DDE_Tnp_1_7 domain-containing protein

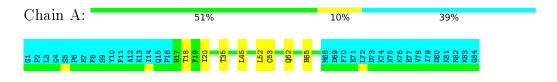
Chain A:		57%	•	39%
년 12 2 13 2 13 2 13 2 13 2 13 2 13 2 13	7 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	M68 M68 M68 M68 M68 M77 M75 M75 M75 M75 M75 M75 M75 M78 M78 M78 M78 M78 M78 M78 M78 M78 M78	R82 684 684	

4.2.11 Score per residue for model 11

• Molecule 1: DDE_Tnp_1_7 domain-containing protein



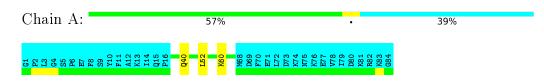
4.2.12 Score per residue for model 12





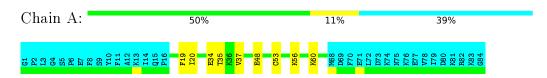
4.2.13 Score per residue for model 13

• Molecule 1: DDE_Tnp_1_7 domain-containing protein



4.2.14 Score per residue for model 14

• Molecule 1: DDE_Tnp_1_7 domain-containing protein



4.2.15 Score per residue for model 15

Chain A:	54%	7%	39%	
61 12 13 14 14 14 14 11 11 14 11 14 11 14 11 14 11 14 11 14 14	125 134 135 135 152 152 152 152 152 152	M68 170 172 172 173 173 173 173 173 173 173 173 173	179 1280 1881 1883 1883 1883 1884	



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: distance geometry.

Of the 200 calculated structures, 15 were deposited, based on the following criterion: target function.

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

Software name	Classification	Version
CYANA	structure calculation	

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	918
Number of shifts mapped to atoms	917
Number of unparsed shifts	1
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%



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: ZN

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	408	388	388	3 ± 1
All	All	6150	5820	5820	38

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 3.

Models Atom-1 Atom-2 Clash(Å) Distance(Å) Worst Total 1:A:25:ILE:HD13 1:A:36:LYS:HB3 0.631.71151 1:A:19:PHE:O 1:A:20:ILE:HD13 0.601.957 10 $\mathbf{2}$ 1:A:52:LEU:HD21 1:A:65:HIS:HB2 0.581.7621:A:18:THR:HG22 1:A:20:ILE:HD11 0.551.7756 1:A:35:THR:HG21 1:A:53:CYS:HA 1.798 50.5551:A:52:LEU:HD11 1:A:65:HIS:ND1 2.210.504 1:A:52:LEU:HD11 1:A:65:HIS:CD2 0.492.42151 1:A:37:VAL:HG21 1:A:54:HIS:HB3 0.471.86 11 1 1:A:25:ILE:HD13 1:A:36:LYS:HG2 0.461.87 3 1 3 1:A:26:VAL:HG22 1:A:35:THR:O 2.111 0.451:A:18:THR:CG2 1:A:20:ILE:HD11 0.452.418 1 1:A:37:VAL:HG11 1:A:56:LYS:HE3 1.8914 0.441

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:52:LEU:HD11	1:A:65:HIS:HD2	0.43	1.74	15	1
1:A:25:ILE:HD13	1:A:36:LYS:CG	0.42	2.44	9	1
1:A:35:THR:HG21	1:A:53:CYS:SG	0.41	2.55	2	1
1:A:49:VAL:HG13	1:A:49:VAL:O	0.40	2.17	11	1

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6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	А	51/84~(61%)	$46 \pm 1 \ (90 \pm 2\%)$	$5\pm1 (10\pm2\%)$	0±0 (0±0%)	100	100
All	All	765/1260~(61%)	691 (90%)	74 (10%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	47/76~(62%)	$44 \pm 1 \ (95 \pm 2\%)$	$3\pm1~(5\pm2\%)$	26 75
All	All	705/1140~(62%)	667~(95%)	38~(5%)	26 75

All 16 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	А	56	LYS	8
1	А	60	LYS	5
1	А	62	GLN	4
1	А	34	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	А	27	LYS	4
1	А	63	ARG	2
1	А	40	GLN	2
1	А	30	GLU	1
1	А	28	CYS	1
1	А	36	LYS	1
1	А	61	CYS	1
1	А	66	GLU	1
1	А	53	CYS	1
1	А	45	LEU	1
1	А	52	LEU	1
1	А	48	GLU	1

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6.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 84% for the well-defined parts and 80% 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	918
Number of shifts mapped to atoms	917
Number of unparsed shifts	1
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

• Chemical shift has been reported more than once. The only occurrence is reported below.

Shift ID	Chain	Pog	Tuno	Atom Shift Data Value Uncertainty Ambiguit			a
		nes	Type Atom	Value	Uncertainty	Ambiguity	
321	А	32	GLY	HA2	3.526	0.001	?

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\bf Correction}\pm{\bf precision},ppm$	Suggested action
$^{13}C_{\alpha}$	83	0.20 ± 0.31	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	78	0.18 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	79	0.28 ± 0.31	None needed (< 0.5 ppm)
¹⁵ N	78	-0.06 ± 0.50	None needed (< 0.5 ppm)



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 84%, i.e. 528 atoms were assigned a chemical shift out of a possible 627. 3 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	15 N
Backbone	245/255~(96%)	98/102~(96%)	98/102~(96%)	49/51~(96%)
Sidechain	251/315~(80%)	154/184~(84%)	97/120~(81%)	0/11~(0%)
Aromatic	32/57~(56%)	23/32~(72%)	9/22~(41%)	0/3~(0%)
Overall	528/627~(84%)	275/318~(86%)	204/244~(84%)	49/65~(75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 839 atoms were assigned a chemical shift out of a possible 1051. 6 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	15 N
Backbone	394/414~(95%)	154/165~(93%)	162/168~(96%)	78/81~(96%)
Sidechain	393/545~(72%)	229/322~(71%)	164/202~(81%)	0/21~(0%)
Aromatic	52/92~(57%)	39/51~(76%)	13/38~(34%)	0/3~(0%)
Overall	839/1051~(80%)	422/538~(78%)	339/408~(83%)	78/105 (74%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



