



# wwPDB NMR Structure Validation Summary Report ⓘ

Feb 12, 2017 – 09:03 pm GMT

PDB ID : 2B6G  
Title : RNA recognition by the Vts1 SAM domain  
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Deposited on : 2005-10-01

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

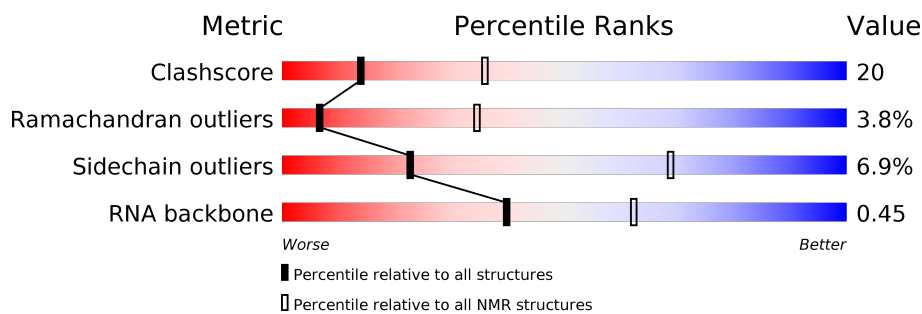
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 65%.

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 (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367
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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	B	19	
2	A	119	

## 2 Ensemble composition and analysis ⓘ

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1969 atoms, of which 906 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	B	19	Total	C	H	N	O	P	0
			608	180	206	70	134	18	

- Molecule 2 is a protein called Vts1p.

Mol	Chain	Residues	Atoms						Trace
2	A	81	Total	C	H	N	O	S	0
			1361	430	700	112	118	1	

There are 2 discrepancies between the modelled and reference sequences:

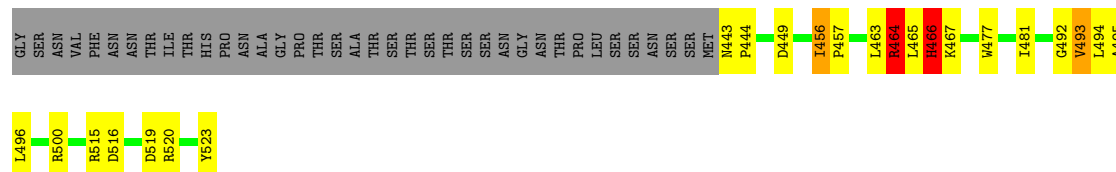
Chain	Residue	Modelled	Actual	Comment	Reference
A	405	GLY	-	CLONING ARTIFACT	GB 6324935
A	406	SER	-	CLONING ARTIFACT	GB 6324935



- Molecule 1: 5'-R(\*GP\*GP\*AP\*GP\*GP\*CP\*UP\*CP\*UP\*GP\*GP\*CP\*AP\*GP\*CP\*UP\*UP\*UP\*C)-3'

G1	C6	U7	C8	U9	G10	G11	C12	A13	G14	C15	U16	U17	U18	C19
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Chain A:  49% 16% .. 32%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the ? calculated structures, 1 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 solution	2.1
XPLOR-NIH	structure solution	2.11.0
XPLOR-NIH	refinement	2.11.0

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)	BMRB entry 6956
Number of chemical shift lists	2
Total number of shifts	1048
Number of shifts mapped to atoms	1015
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	65%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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	B	402	206	206	21
2	A	661	700	699	19
All	All	1063	906	905	39

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 20.

5 of 39 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:11:G:O2'	1:B:12:C:H4'	0.99	1.56
1:B:18:U:O2'	1:B:19:C:H5'	0.68	1.87
1:B:8:C:O2'	1:B:9:U:P	0.67	2.52
2:A:466:HIS:CD2	2:A:466:HIS:N	0.66	2.64
2:A:465:LEU:O	2:A:467:LYS:N	0.66	2.28

### 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	Percentiles	
2	A	79/119 (66%)	73 (92%)	3 (4%)	3 (4%)	7	34
All	All	79/119 (66%)	73 (92%)	3 (4%)	3 (4%)	7	34

All 3 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	A	493	VAL
2	A	466	HIS
2	A	464	ARG

### 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	
2	A	72/105 (69%)	67 (93%)	5 (7%)	23	69
All	All	72/105 (69%)	67 (93%)	5 (7%)	23	69

All 5 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	A	456	ILE
2	A	523	TYR
2	A	466	HIS
2	A	449	ASP
2	A	464	ARG

### 6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	18/19 (95%)	4 (22%)	0 (0%)	0.45
All	All	18/19 (95%)	4 (22%)	0 (0%)	0.45

The overall RNA backbone suiteness is 0.45.

All RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	B	11	G
1	B	9	U
1	B	10	G
1	B	12	C

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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 65% for the well-defined parts and 65% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 6956

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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	1015
Number of shifts mapped to atoms	1015
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	80	$-0.81 \pm 0.18$	Should be applied
$^{13}\text{C}_\beta$	74	$0.21 \pm 0.21$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	72	$2.31 \pm 0.05$	Should be applied
$^{15}\text{N}$	75	$0.60 \pm 0.54$	None needed (imprecise)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 65%, i.e. 924 atoms were assigned a chemical shift out of a possible 1424. 15 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	380/397 (96%)	153/158 (97%)	152/162 (94%)	75/77 (97%)
Sidechain	479/596 (80%)	294/350 (84%)	179/219 (82%)	6/27 (22%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	65/73 (89%)	37/37 (100%)	26/32 (81%)	2/4 (50%)
Overall	924/1424 (65%)	484/751 (64%)	357/539 (66%)	83/134 (62%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

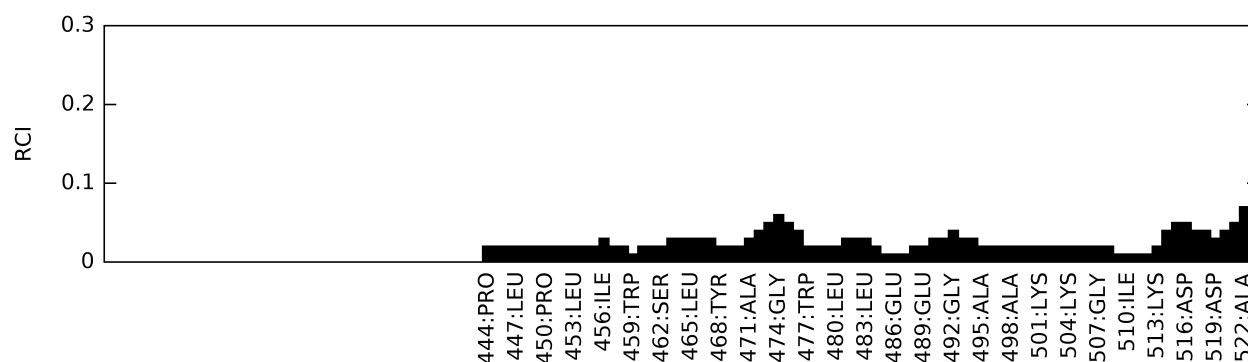
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	467	LYS	HG2	-0.01	2.67 – 0.07	-5.3
1	A	453	LEU	HD12	-0.67	2.16 – -0.64	-5.1
1	A	453	LEU	HD13	-0.67	2.16 – -0.64	-5.1
1	A	453	LEU	HD11	-0.67	2.16 – -0.64	-5.1

#### 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:



## 7.2 Chemical shift list 2

File name: BMRB entry 6956

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.2.1 Bookkeeping

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	33
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Chain not found in structure. First 5 (of 33) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	11	G	H1'	5.83	-1.0	1
UNMAPPED	9	U	H5'	3.75	-1.0	1
UNMAPPED	8	C	H1'	5.8	-1.0	1
UNMAPPED	8	C	H5'	4.09	-1.0	1
UNMAPPED	11	G	H3'	5.08	-1.0	1

### 7.2.2 Chemical shift referencing

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

### 7.2.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1424. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/397 (0%)	0/158 (0%)	0/162 (0%)	0/77 (0%)
Sidechain	0/596 (0%)	0/350 (0%)	0/219 (0%)	0/27 (0%)
Aromatic	0/73 (0%)	0/37 (0%)	0/32 (0%)	0/4 (0%)
Overall	0/1424 (0%)	0/751 (0%)	0/539 (0%)	0/134 (0%)

#### 7.2.4 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, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
???	UNMAPPED	10	G	H4'	3.46	5.12 – 3.72	-6.9

#### 7.2.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned\_chem\_shift\_list\_2). RCI is only applicable to proteins.