



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:40 pm GMT

PDB ID : 1R7C
Title : NMR structure of the membrane anchor domain (1-31) of the nonstructural protein 5A (NS5A) of hepatitis C virus (Minimized average structure, Sample in 50% tfe)
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Deposited on : 2003-10-21

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.

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

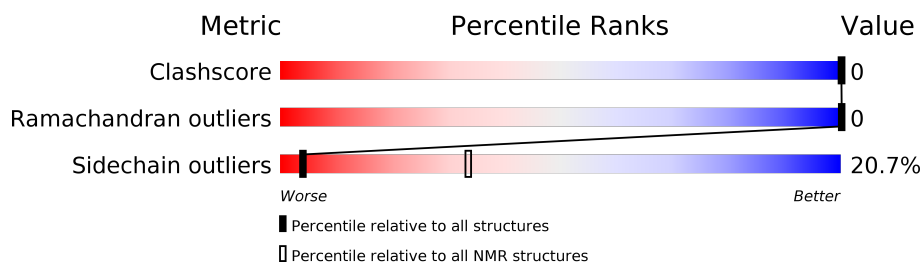
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	31	 77% 23%

2 Ensemble composition and analysis ⓘ

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 532 atoms, of which 266 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms						Trace
1	A	31	Total	C	H	N	O	S	0
			532	177	266	42	45	2	

4 Residue-property plots [i](#)

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: Genome polyprotein

Chain A:  77% 23%



5 Refinement protocol and experimental data overview

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

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	structure solution	3.85
X-PLOR	refinement	3.85

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 5978
Number of chemical shift lists	3
Total number of shifts	939
Number of shifts mapped to atoms	939
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

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.

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	1
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	6	ARG	Sidechain

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	266	266	266	-

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 [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	
1	A	29/31 (94%)	28 (97%)	1 (3%)	0 (0%)	100	100
All	All	29/31 (94%)	28 (97%)	1 (3%)	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	A	29/29 (100%)	23 (79%)	6 (21%)	4	33
All	All	29/29 (100%)	23 (79%)	6 (21%)	4	33

All 6 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	4	TRP
1	A	27	LEU
1	A	30	GLN
1	A	3	SER
1	A	19	PHE
1	A	23	LEU

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 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 78% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5978

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	375
Number of shifts mapped to atoms	375
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	31	-1.41 ± 0.25	Should be applied
$^{13}\text{C}_\beta$	30	-0.40 ± 0.28	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

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 78%, i.e. 323 atoms were assigned a chemical shift out of a possible 415. 2 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	91/153 (59%)	60/61 (98%)	31/62 (50%)	0/30 (0%)
Sidechain	179/205 (87%)	116/121 (96%)	63/77 (82%)	0/7 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	53/57 (93%)	29/29 (100%)	24/24 (100%)	0/4 (0%)
Overall	323/415 (78%)	205/211 (97%)	118/163 (72%)	0/41 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 323 atoms were assigned a chemical shift out of a possible 415. 2 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	91/153 (59%)	60/61 (98%)	31/62 (50%)	0/30 (0%)
Sidechain	179/205 (87%)	116/121 (96%)	63/77 (82%)	0/7 (0%)
Aromatic	53/57 (93%)	29/29 (100%)	24/24 (100%)	0/4 (0%)
Overall	323/415 (78%)	205/211 (97%)	118/163 (72%)	0/41 (0%)

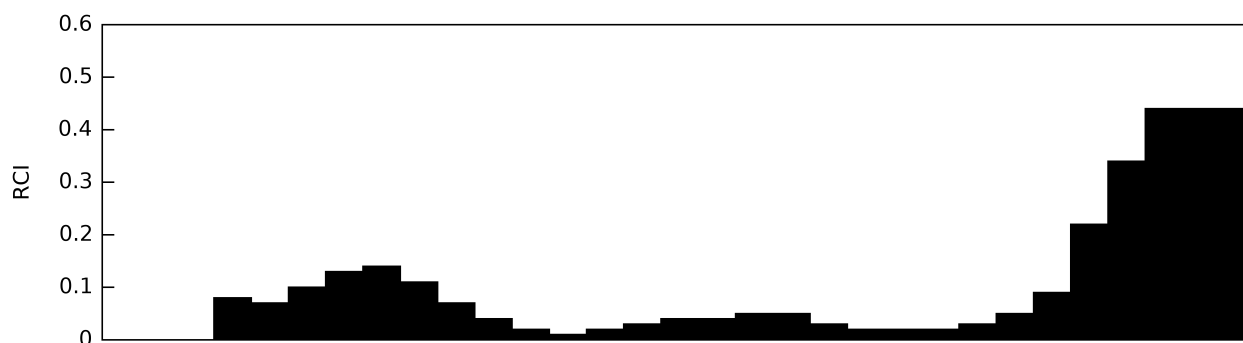
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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 5978

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	344
Number of shifts mapped to atoms	344
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	31	-0.85 ± 1.36	None needed (imprecise)
$^{13}\text{C}_\beta$	29	0.53 ± 0.58	None needed (imprecise)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

7.2.3 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 71%, i.e. 295 atoms were assigned a chemical shift out of a possible 415. 1 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	88/153 (58%)	57/61 (93%)	31/62 (50%)	0/30 (0%)
Sidechain	162/205 (79%)	114/121 (94%)	48/77 (62%)	0/7 (0%)
Aromatic	45/57 (79%)	25/29 (86%)	20/24 (83%)	0/4 (0%)
Overall	295/415 (71%)	196/211 (93%)	99/163 (61%)	0/41 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 295 atoms were assigned a chemical shift out of a possible 415. 1 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	88/153 (58%)	57/61 (93%)	31/62 (50%)	0/30 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	162/205 (79%)	114/121 (94%)	48/77 (62%)	0/7 (0%)
Aromatic	45/57 (79%)	25/29 (86%)	20/24 (83%)	0/4 (0%)
Overall	295/415 (71%)	196/211 (93%)	99/163 (61%)	0/41 (0%)

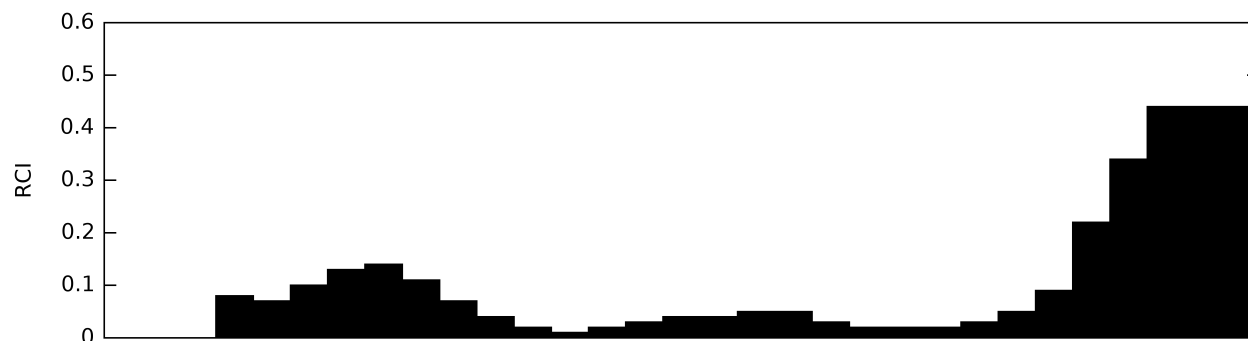
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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:



7.3 Chemical shift list 3

File name: BMRB entry 5978

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 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	220
Number of shifts mapped to atoms	220

Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.3.2 Chemical shift referencing [i](#)

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

7.3.3 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 44%, i.e. 183 atoms were assigned a chemical shift out of a possible 415. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	53/153 (35%)	53/61 (87%)	0/62 (0%)	0/30 (0%)
Sidechain	110/205 (54%)	110/121 (91%)	0/77 (0%)	0/7 (0%)
Aromatic	20/57 (35%)	20/29 (69%)	0/24 (0%)	0/4 (0%)
Overall	183/415 (44%)	183/211 (87%)	0/163 (0%)	0/41 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 183 atoms were assigned a chemical shift out of a possible 415. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	53/153 (35%)	53/61 (87%)	0/62 (0%)	0/30 (0%)
Sidechain	110/205 (54%)	110/121 (91%)	0/77 (0%)	0/7 (0%)
Aromatic	20/57 (35%)	20/29 (69%)	0/24 (0%)	0/4 (0%)
Overall	183/415 (44%)	183/211 (87%)	0/163 (0%)	0/41 (0%)

7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.3.5 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:

