wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1JRU
Title	:	NMR STRUCTURE OF THE UBX DOMAIN FROM P47 (ENERGY MINIMISED AVERAGE)
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Deposited on	:	2001-08-15

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
http://wwpdb.org/validation/2016/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:

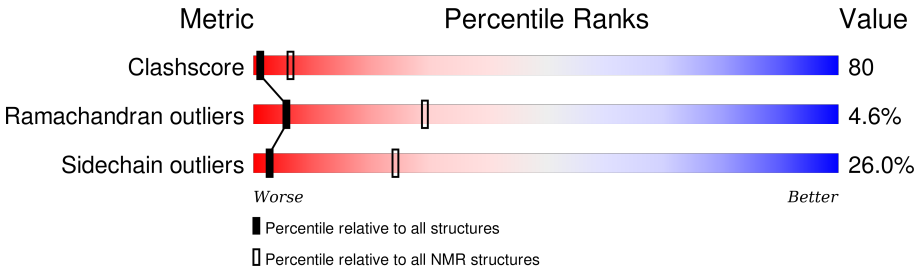
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 74%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	Quality of chain
1	A	89	21% 56% 21% .

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 is only 1 type of molecule in this entry. The entry contains 1414 atoms, of which 719 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called p47 protein.

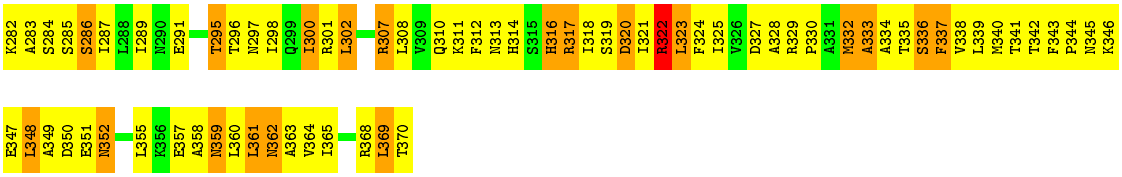
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1414	435	719	126	132	2	0

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: p47 protein

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing.*

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	3.853
X-PLOR	refinement	3.853

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 5155, BMRB entry 5874, BMRB entry 5876
Number of chemical shift lists	3
Total number of shifts	3998
Number of shifts mapped to atoms	1821
Number of unparsed shifts	0
Number of shifts with mapping errors	2177
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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

6 Model quality

6.1 Standard geometry

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	5
All	All	0	5

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	317	ARG	Sidechain
1	A	322	ARG	Sidechain
1	A	368	ARG	Sidechain
1	A	307	ARG	Sidechain
1	A	301	ARG	Sidechain

6.2 Too-close contacts

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	A	695	719	716	113
All	All	695	719	716	113

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 80.

5 of 113 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:302:LEU:HD12	1:A:369:LEU:HD23	0.97	1.33
1:A:314:HIS:CD2	1:A:361:LEU:HD11	0.81	2.11
1:A:295:THR:HG22	1:A:313:ASN:HA	0.76	1.55
1:A:332:MET:SD	1:A:369:LEU:HD21	0.75	2.22
1:A:339:LEU:HD12	1:A:340:MET:N	0.72	1.99

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	87/89 (98%)	67 (77%)	16 (18%)	4 (5%)	5 29
All	All	87/89 (98%)	67 (77%)	16 (18%)	4 (5%)	5 29

All 4 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	352	ASN
1	A	348	LEU
1	A	361	LEU
1	A	333	ALA

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	77/77 (100%)	57 (74%)	20 (26%)	3 24
All	All	77/77 (100%)	57 (74%)	20 (26%)	3 24

5 of 20 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	359	ASN
1	A	332	MET
1	A	345	ASN
1	A	286	SER
1	A	335	THR

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 74% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5155

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	867
Number of shifts mapped to atoms	867
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	88	0.49 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	86	0.87 ± 0.16	Should be applied
$^{13}C'$	0	—	—
^{15}N	86	-0.01 ± 0.30	None needed (< 0.5 ppm)

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 66%, i.e. 730 atoms were assigned a chemical shift out of a possible 1108. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	348/439 (79%)	174/175 (99%)	88/178 (49%)	86/86 (100%)
Sidechain	361/619 (58%)	275/359 (77%)	86/227 (38%)	0/33 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	21/50 (42%)	21/28 (75%)	0/20 (0%)	0/2 (0%)
Overall	730/1108 (66%)	470/562 (84%)	174/425 (41%)	86/121 (71%)

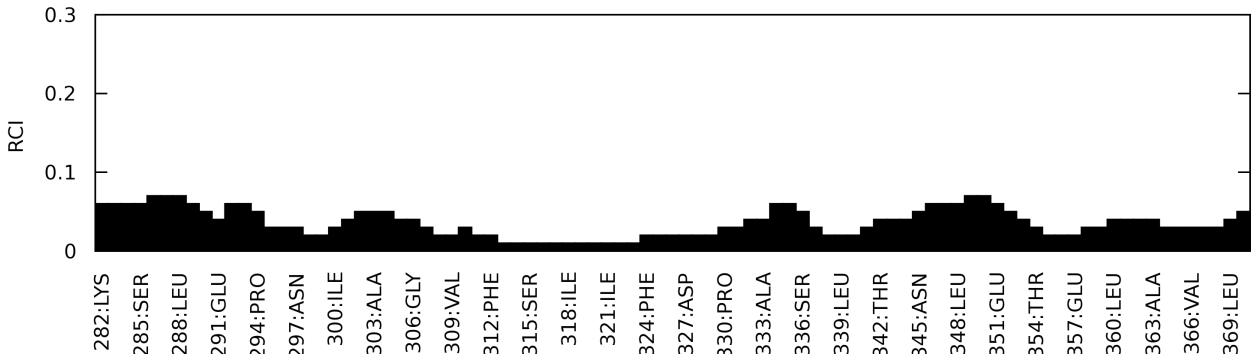
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

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 5874

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

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	1181
Number of shifts mapped to atoms	0
Number of unparsed shifts	0

Number of shifts with mapping errors	1181
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

- Chain not found in structure. First 5 (of 1181) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	54	SER	HB2	3.866	0.05	1
UNMAPPED	30	ALA	HB3	1.48	0.05	1
UNMAPPED	27	LEU	N	120.609	0.05	1
UNMAPPED	64	GLY	H	8.392	0.05	1
UNMAPPED	159	ALA	HB1	1.346	0.05	1

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	125	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	111	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	46	0.00 ± 0.00	None needed (< 0.5 ppm)
^{15}N	134	0.00 ± 0.00	None needed (< 0.5 ppm)

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1108. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/439 (0%)	0/175 (0%)	0/178 (0%)	0/86 (0%)
Sidechain	0/619 (0%)	0/359 (0%)	0/227 (0%)	0/33 (0%)
Aromatic	0/50 (0%)	0/28 (0%)	0/20 (0%)	0/2 (0%)
Overall	0/1108 (0%)	0/562 (0%)	0/425 (0%)	0/121 (0%)

7.2.4 Statistically unusual chemical shifts

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
???	UNMAPPED	10	ARG	NE	110.88	92.63 – 76.73	16.5
???	UNMAPPED	27	LEU	HB2	-0.43	3.32 – -0.08	-6.0
???	UNMAPPED	16	THR	HG21	-0.15	2.29 – -0.01	-5.6
???	UNMAPPED	16	THR	HG22	-0.15	2.29 – -0.01	-5.6
???	UNMAPPED	16	THR	HG23	-0.15	2.29 – -0.01	-5.6

7.2.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.

7.3 Chemical shift list 3

File name: BMRB entry 5876

Chemical shift list name: *assigned_chem_shift_list_1*

7.3.1 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	1950
Number of shifts mapped to atoms	954
Number of unparsed shifts	0
Number of shifts with mapping errors	996
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

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

- Residue not found in structure. First 5 (of 996) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	68	HIS	HB2	1.775	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	8	GLN	HB3	2.016	0.05	1
A	10	VAL	HB	1.857	0.05	1
A	22	SER	CB	67.864	0.05	1
A	74	VAL	HB	1.444	0.05	1

7.3.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	192	-0.57 ± 0.13	Should be applied
$^{13}C_{\beta}$	177	-0.44 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	187	1.21 ± 0.21	Should be applied
^{15}N	170	0.46 ± 0.34	None needed (< 0.5 ppm)

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 74%, i.e. 817 atoms were assigned a chemical shift out of a possible 1108. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	431/439 (98%)	173/175 (99%)	174/178 (98%)	84/86 (98%)
Sidechain	365/619 (59%)	279/359 (78%)	86/227 (38%)	0/33 (0%)
Aromatic	21/50 (42%)	21/28 (75%)	0/20 (0%)	0/2 (0%)
Overall	817/1108 (74%)	473/562 (84%)	260/425 (61%)	84/121 (69%)

7.3.4 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	20	GLY	C	115.14	183.33 – 164.53	-31.3
1	A	53	ARG	NE	118.75	92.63 – 76.73	21.4
1	A	69	ARG	NE	117.49	92.63 – 76.73	20.6
1	A	44	ARG	NE	117.21	92.63 – 76.73	20.5
1	A	45	ARG	NE	116.80	92.63 – 76.73	20.2

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	54	ARG	NE	116.31	92.63 – 76.73	19.9
1	A	29	ARG	NE	115.35	92.63 – 76.73	19.3
1	A	317	ARG	HD2	1.20	4.27 – 1.97	-8.4
1	A	317	ARG	HD3	1.20	4.36 – 1.86	-7.6
1	A	29	ARG	HB2	-0.24	3.15 – 0.45	-7.6
1	A	322	ARG	HD2	1.43	4.27 – 1.97	-7.3
1	A	322	ARG	HD3	1.43	4.36 – 1.86	-6.7
1	A	28	LEU	HB2	-0.64	3.32 – -0.08	-6.7

7.3.5 Random Coil Index (RCI) plots

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: