Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2MKN
BMRB ID	:	17679
Title	:	Structural Characterization of Interactions between the Double-Stranded RNA-Binding Zinc Finger Protein JAZ and dsRNA
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Deposited on	:	2014-02-10

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

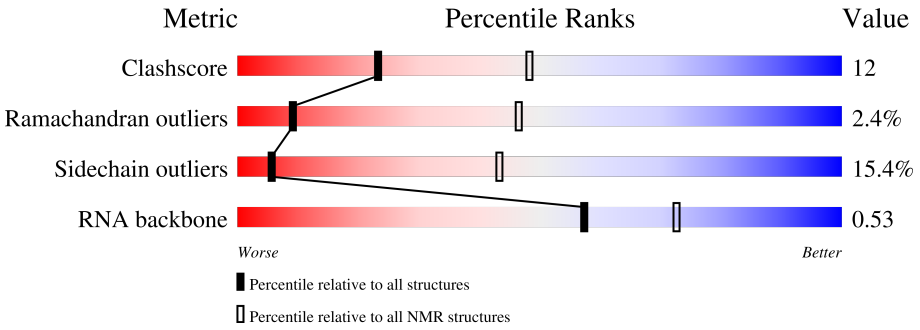
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 12%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428
RNA backbone	4643	676

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	60	47% 27% 27%
2	B	19	42% 53% 5%
3	C	19	53% 42% 5%

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

There are 4 unique types of molecules in this entry. The entry contains 1681 atoms, of which 508 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger protein 346.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	44	454	228	92	69	61	4	0

- Molecule 2 is a RNA chain called RNA (5'-R(*GP*CP*CP*GP*UP*GP*GP*UP*CP*UP*GP*GP*UP*GP*GP*CP*CP*GP*G)-3').

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	19	613	181	206	73	135	18	0

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
3	C	19	613	180	210	75	129	19	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

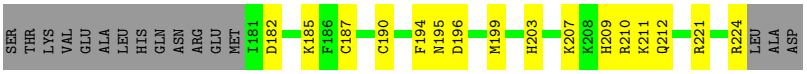
Mol	Chain	Residues	Atoms	
			Total	Zn
4	A	1	1	1

4 Residue-property plots (i)

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.

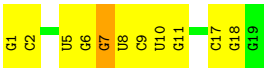
• Molecule 1: Zinc finger protein 346

Chain A:



• Molecule 2: RNA (5'-R(*GP*CP*CP*GP*UP*GP*GP*UP*CP*UP*GP*GP*UP*GP*GP*CP*CP*GP*G)-3')

Chain B:



• Molecule 3: RNA (5'-R(P*CP*CP*GP*GP*CP*CP*AP*CP*CP*AP*GP*AP*CP*CP*AP*CP*GP*GP*C)-3')

Chain C:

5 Refinement protocol and experimental data overview

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

Of the 100 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
Amber	refinement	
CYANA	structure solution	
TALOS	geometry optimization	
HADDOCK	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	223
Number of shifts mapped to atoms	169
Number of unparsed shifts	0
Number of shifts with mapping errors	54
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	12%

6 Model quality

6.1 Standard geometry

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

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	362	92	364	11
2	B	407	206	207	12
3	C	403	210	210	7
4	A	1	0	0	1
All	All	1173	508	781	24

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:190:CYS:HG	4:A:301:ZN:ZN	0.87	0.67
1:A:211:LYS:HB3	2:B:5:U:H5"	0.81	1.50
3:C:26:A:H2'	3:C:27:C:C6	0.66	2.26
2:B:7:G:H2'	2:B:8:U:C6	0.58	2.33
1:A:196:ASP:HB2	1:A:199:MET:HB2	0.56	1.78
1:A:212:GLN:NE2	2:B:6:G:H5"	0.54	2.16
3:C:28:C:H2'	3:C:29:A:C8	0.52	2.40
1:A:187:CYS:SG	1:A:190:CYS:SG	0.51	3.08
2:B:10:U:H2'	2:B:11:G:C8	0.50	2.41
2:B:6:G:O2'	2:B:7:G:H5'	0.49	2.07

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:1:G:H2'	2:B:2:C:C6	0.47	2.44
1:A:187:CYS:HB2	1:A:194:PHE:CE2	0.47	2.44
2:B:8:U:H2'	2:B:9:C:C6	0.47	2.44
2:B:5:U:O2'	2:B:6:G:H5'	0.47	2.10
1:A:211:LYS:CB	2:B:5:U:H5"	0.47	2.32
2:B:6:G:H2'	2:B:7:G:C8	0.46	2.46
1:A:203:HIS:HA	3:C:26:A:H5'	0.45	1.89
3:C:26:A:O2'	3:C:27:C:H5'	0.45	2.11
2:B:17:C:H2'	2:B:18:G:C8	0.44	2.47
1:A:211:LYS:HB3	2:B:5:U:C5'	0.43	2.34
1:A:203:HIS:HA	3:C:26:A:C5'	0.42	2.45
1:A:185:LYS:HB2	1:A:194:PHE:HB2	0.42	1.90
3:C:30:G:H2'	3:C:31:A:C8	0.41	2.49
3:C:25:C:H2'	3:C:26:A:C8	0.40	2.52

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	42/60 (70%)	39 (93%)	2 (5%)	1 (2%)	9	46
All	All	42/60 (70%)	39 (93%)	2 (5%)	1 (2%)	9	46

All 1 Ramachandran outliers are listed below.

Mol	Chain	Res	Type
1	A	209	HIS

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	39/53 (74%)	33 (85%)	6 (15%)	6 43
All	All	39/53 (74%)	33 (85%)	6 (15%)	6 43

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	182	ASP
1	A	195	ASN
1	A	207	LYS
1	A	210	ARG
1	A	221	ARG
1	A	224	ARG

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	18/19 (95%)	1 (6%)	0 (0%)	0.59
3	C	18/19 (95%)	3 (17%)	0 (0%)	0.47
All	All	36/38 (95%)	4 (11%)	0 (0%)	0.53

The overall RNA backbone suiteness is 0.53.

All RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	7	G
3	C	22	G
3	C	23	G
3	C	27	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 monosaccharides in this entry.

6.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 12% for the well-defined parts and 12% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	223
Number of shifts mapped to atoms	169
Number of unparsed shifts	0
Number of shifts with mapping errors	54
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 54 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	168	SER	CA	61.981	.	1
1	A	169	THR	C	174.284	.	1
1	A	169	THR	CA	61.864	.	1
1	A	170	LYS	H	8.296	.	1
1	A	170	LYS	C	176.283	.	1
1	A	170	LYS	CA	56.318	.	1
1	A	170	LYS	N	124.627	.	1
1	A	171	VAL	H	8.136	.	1
1	A	171	VAL	C	176.101	.	1
1	A	171	VAL	CA	62.503	.	1
1	A	171	VAL	N	122.74	.	1
1	A	172	GLU	H	8.358	.	1
1	A	172	GLU	C	176.029	.	1
1	A	172	GLU	CA	56.398	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	172	GLU	N	125.282	.	1
1	A	173	ALA	H	8.152	.	1
1	A	173	ALA	C	177.482	.	1
1	A	173	ALA	CA	52.368	.	1
1	A	173	ALA	N	125.145	.	1
1	A	174	LEU	H	7.983	.	1
1	A	174	LEU	C	177.337	.	1
1	A	174	LEU	CA	55.28	.	1
1	A	174	LEU	N	120.83	.	1
1	A	175	HIS	H	8.047	.	1
1	A	175	HIS	CA	56.078	.	1
1	A	175	HIS	N	119.523	.	1
1	A	176	GLN	C	175.447	.	1
1	A	176	GLN	CA	55.764	.	1
1	A	177	ASN	H	8.429	.	1
1	A	177	ASN	C	175.193	.	1
1	A	177	ASN	CA	53.206	.	1
1	A	177	ASN	N	119.812	.	1
1	A	178	ARG	H	8.175	.	1
1	A	178	ARG	C	176.065	.	1
1	A	178	ARG	CA	56.238	.	1
1	A	178	ARG	N	121.48	.	1
1	A	179	GLU	H	8.45	.	1
1	A	179	GLU	C	176.144	.	1
1	A	179	GLU	CA	56.573	.	1
1	A	179	GLU	N	121.16	.	1
1	A	180	MET	H	8.253	.	1
1	A	180	MET	C	175.667	.	1
1	A	180	MET	CA	55.178	.	1
1	A	180	MET	N	120.949	.	1
1	A	225	LEU	H	8.363	.	1
1	A	225	LEU	C	176.683	.	1
1	A	225	LEU	CA	54.824	.	1
1	A	225	LEU	N	123.604	.	1
1	A	226	ALA	H	8.182	.	1
1	A	226	ALA	C	176.79	.	1
1	A	226	ALA	CA	52.1	.	1
1	A	226	ALA	N	124.798	.	1
1	A	227	ASP	H	7.895	.	1
1	A	227	ASP	N	125.54	.	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	59	-0.11 ± 0.21	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	54	-0.14 ± 0.14	None needed (< 0.5 ppm)
^{15}N	55	-0.34 ± 0.33	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 12%, i.e. 169 atoms were assigned a chemical shift out of a possible 1359. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	169/218 (78%)	42/88 (48%)	85/88 (97%)	42/42 (100%)
Sidechain	0/352 (0%)	0/226 (0%)	0/107 (0%)	0/19 (0%)
Aromatic	0/60 (0%)	0/30 (0%)	0/26 (0%)	0/4 (0%)
Sugar	0/418 (0%)	0/228 (0%)	0/190 (0%)	0/0 (—%)
Base	0/311 (0%)	0/197 (0%)	0/61 (0%)	0/53 (0%)
Overall	169/1359 (12%)	42/769 (5%)	85/472 (18%)	42/118 (36%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 169 atoms were assigned a chemical shift out of a possible 1359. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	169/218 (78%)	42/88 (48%)	85/88 (97%)	42/42 (100%)
Sidechain	0/352 (0%)	0/226 (0%)	0/107 (0%)	0/19 (0%)
Aromatic	0/60 (0%)	0/30 (0%)	0/26 (0%)	0/4 (0%)
Sugar	0/418 (0%)	0/228 (0%)	0/190 (0%)	0/0 (—%)
Base	0/311 (0%)	0/197 (0%)	0/61 (0%)	0/53 (0%)
Overall	169/1359 (12%)	42/769 (5%)	85/472 (18%)	42/118 (36%)

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: