wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1UJR
Title	:	Solution structure of WWE domain in BAB28015
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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:

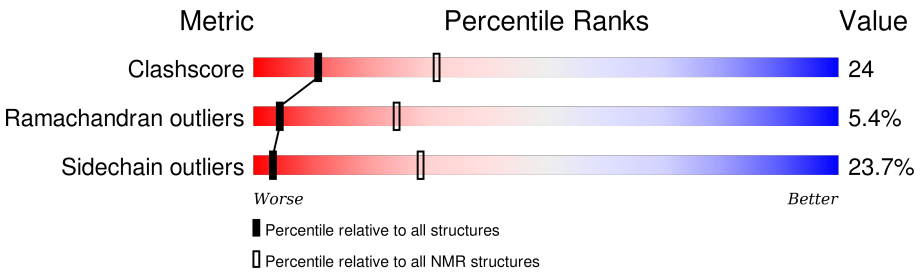
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	110	21% 37% • 39%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:30-A:96 (67)	0.33	4

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 5 single-model clusters were found.

Cluster number	Models
1	5, 6, 11, 13, 14, 17
2	1, 2, 3, 10, 15
3	4, 7, 9, 16
Single-model clusters	8; 12; 18; 19; 20

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1745 atoms, of which 860 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical protein AK012080.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	110	1745	553	860	161	169	2	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	CLONING ARTIFACT	UNP Q9CZW6
A	2	SER	-	CLONING ARTIFACT	UNP Q9CZW6
A	3	SER	-	CLONING ARTIFACT	UNP Q9CZW6
A	4	GLY	-	CLONING ARTIFACT	UNP Q9CZW6
A	5	SER	-	CLONING ARTIFACT	UNP Q9CZW6
A	6	SER	-	CLONING ARTIFACT	UNP Q9CZW6
A	7	GLY	-	CLONING ARTIFACT	UNP Q9CZW6
A	105	SER	-	CLONING ARTIFACT	UNP Q9CZW6
A	106	GLY	-	CLONING ARTIFACT	UNP Q9CZW6
A	107	PRO	-	CLONING ARTIFACT	UNP Q9CZW6
A	108	SER	-	CLONING ARTIFACT	UNP Q9CZW6
A	109	SER	-	CLONING ARTIFACT	UNP Q9CZW6
A	110	GLY	-	CLONING ARTIFACT	UNP Q9CZW6

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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: hypothetical protein AK012080

Chain A: 21% 37% • 39%

P1 S2 S3 G4 S5 S6 G7 F8 L9 D10 K11 P12 T13 L14 L15 S16 P17 E18 E19 L20 K21 A22 A23 S24 R25 G26 N27 G28 E29 Y30 A31 W32 Y33 Y34 E35 G36 R37 W41 Q42 Y43 D44 E45 S48 R49 E50 L51 E52 D53 S56 K59 K60 N61 T62 E63 M64 L65

I66 A67 G68 F69 L70 Y71 V72 A73 D74 L75 E76 N77 M78 V79 Q80 Y81 R82 R83 N84 E85 R89 R90 K91 I96 I97 D98 I99 P100 K101 K102 G103 V104 S105 G106 P107 S108 S109 G110

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: hypothetical protein AK012080

Chain A: 26% 27% 7% 39%

P1 S2 S3 G4 S5 S6 G7 F8 L9 D10 K11 P12 T13 L14 L15 S16 P17 E18 E19 L20 K21 A22 A23 S24 R25 G26 N27 G28 E29 Y30 A31 W32 R37 N38 G39 Y43 D44 E45 R46 T47 S48 R49 E50 L51 E52 D53 A54 F55 S56 K57 G58 K59 K60 N61 M64 L65 I66

A67 G68 Y71 V72 A73 D74 L75 M78 V79 Q80 Y81 R82 R83 N84 E85 H86 K91 R94 D95 I96 I97 D98 I99 P100 K101 K102 G103 V104 S105 G106 P107 S108 S109 G110

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.7
CYANA	refinement	1.0.7

No chemical shift data was provided. 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	A	587	561	561	27±6
All	All	11740	11220	11220	547

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 24.

5 of 221 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:HD13	1:A:70:LEU:HD12	1.05	1.26	16	2
1:A:66:ILE:HD12	1:A:71:TYR:CD2	0.95	1.96	7	6
1:A:64:MET:CE	1:A:73:ALA:HB2	0.88	1.97	11	9
1:A:65:LEU:HD13	1:A:70:LEU:HD22	0.87	1.43	12	7
1:A:32:TRP:CH2	1:A:75:LEU:HD22	0.85	2.05	18	11

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	67/110 (61%)	53±2 (79±3%)	10±2 (16±3%)	4±1 (5±1%)	4 24
All	All	1340/2200 (61%)	1060 (79%)	208 (16%)	72 (5%)	4 24

5 of 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	45	GLU	20
1	A	67	ALA	20
1	A	39	GLY	10
1	A	44	ASP	7
1	A	83	ARG	5

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	58/92 (63%)	44±3 (76±5%)	14±3 (24±5%)	3 28
All	All	1160/1840 (63%)	885 (76%)	275 (24%)	3 28

5 of 39 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	A	64	MET	19
1	A	37	ARG	18
1	A	83	ARG	16
1	A	76	GLU	15
1	A	78	MET	13

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 (i)

No chemical shift data were provided