wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2ERR
Title	:	NMR Structure of the RNA Binding Domain of Human Fox-1 in Complex with UGCAUGU
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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:

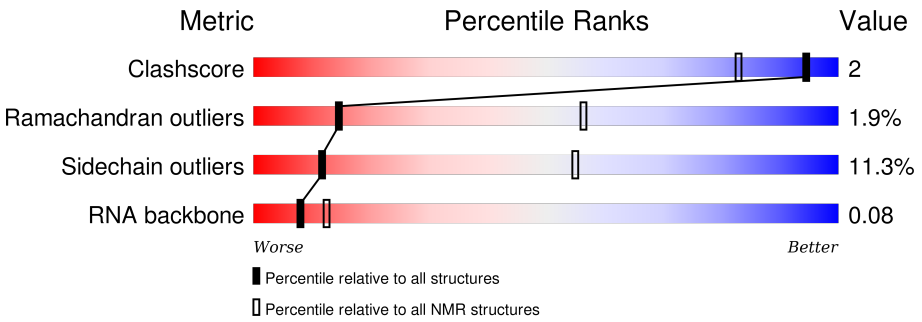
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 is 71%.

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
RNA backbone	3027	600

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	B	7	43% 43% 14%
2	A	109	55% 15% • 10% 19%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:116-A:192 (77)	0.27	7

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 7, 11, 13, 14, 15, 16, 17, 18, 19, 21, 22, 24, 25, 28
2	6, 8, 10, 20, 30
3	5, 9, 12
4	23, 26
Single-model clusters	27; 29

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1636 atoms, of which 780 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called UGCAUGU.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	7	221	66	76	24	49	6	0

- Molecule 2 is a protein called Ataxin-2-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	88	1415	443	704	135	131	2	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	EXPRESSION TAG	UNP Q9NWB1
A	89	GLY	-	EXPRESSION TAG	UNP Q9NWB1
A	90	SER	-	EXPRESSION TAG	UNP Q9NWB1
A	91	SER	-	EXPRESSION TAG	UNP Q9NWB1
A	92	HIS	-	EXPRESSION TAG	UNP Q9NWB1
A	93	HIS	-	EXPRESSION TAG	UNP Q9NWB1
A	94	HIS	-	EXPRESSION TAG	UNP Q9NWB1
A	95	HIS	-	EXPRESSION TAG	UNP Q9NWB1
A	96	HIS	-	EXPRESSION TAG	UNP Q9NWB1
A	97	HIS	-	EXPRESSION TAG	UNP Q9NWB1
A	98	SER	-	EXPRESSION TAG	UNP Q9NWB1
A	99	SER	-	EXPRESSION TAG	UNP Q9NWB1
A	100	GLY	-	EXPRESSION TAG	UNP Q9NWB1
A	101	LEU	-	EXPRESSION TAG	UNP Q9NWB1
A	102	VAL	-	EXPRESSION TAG	UNP Q9NWB1
A	103	PRO	-	EXPRESSION TAG	UNP Q9NWB1
A	104	ARG	-	EXPRESSION TAG	UNP Q9NWB1
A	105	GLY	-	EXPRESSION TAG	UNP Q9NWB1
A	106	SER	-	EXPRESSION TAG	UNP Q9NWB1
A	107	HIS	-	EXPRESSION TAG	UNP Q9NWB1
A	108	MET	-	EXPRESSION TAG	UNP Q9NWB1

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: UGCAUGU

Chain B: 43% 43% 14%

U197 G198 C199 A200 U201 G202 U203

- Molecule 2: Ataxin-2-binding protein 1

Chain A: 55% 15% • 10% 19%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET N109 T110 E111 N112 K113 S114 Q115 P116 K117 R118 R127 I143 I149 F150 K156 F160 V161 T162 F163 E164 N165 R173 H177 R184 V188 A193 R194 V195 M196

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

The representative model is number 7. Colouring as in section 4.1 above.

- Molecule 1: UGCAUGU

Chain B: 43% 43% 14%

U197 G198 C199 A200 U201 G202 U203

- Molecule 2: Ataxin-2-binding protein 1

Chain A: 54% 15% • 10% 19%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET N109 T110 E111 N112 K113 S114 Q115 P116 K117 R118 S122 R127 D130 R134 I149 F150 K156 F160 V161 T162 F163 E164 N165 R173 H177 V188 A193 R194

V195 M196

5 Refinement protocol and experimental data overview (i)

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

Of the 30 calculated structures, 30 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
CYANA	structure solution	2.0
AMBER	refinement	7.0

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 6895
Number of chemical shift lists	2
Total number of shifts	882
Number of shifts mapped to atoms	882
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	B	1.40±0.03	0±0/161 (0.0±0.1%)	2.29±0.04	11±2/249 (4.2±0.8%)
2	A	0.73±0.01	0±0/636 (0.0±0.0%)	1.28±0.03	6±2/852 (0.6±0.2%)
All	All	0.91	1/23910 (0.0%)	1.56	481/33030 (1.5%)

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	B	0.0±0.0	1.8±1.0
2	A	0.0±0.0	4.0±1.4
All	All	0	173

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	202	G	C2-N2	-5.27	1.29	1.34	15	1

5 of 50 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	173	ARG	NE-CZ-NH1	9.68	125.14	120.30	1	22
1	B	202	G	O4'-C1'-N9	8.65	115.12	108.20	11	28
2	A	118	ARG	NE-CZ-NH1	8.43	124.52	120.30	3	16
1	B	200	A	N1-C6-N6	-8.38	113.57	118.60	5	12
1	B	200	A	C5-C6-N1	8.15	121.78	117.70	25	30

There are no chirality outliers.

5 of 17 unique planar outliers are listed below. They are sorted by the frequency of occurrence in

the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	A	162	THR	Peptide	27
2	A	163	PHE	Peptide	20
2	A	117	LYS	Peptide	20
2	A	164	GLU	Peptide	20
2	A	118	ARG	Peptide	19

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	145	76	76	0±1
2	A	623	617	617	2±1
All	All	23040	20790	20788	66

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 2.

5 of 14 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:149:ILE:HG22	2:A:156:LYS:CE	0.72	2.15	10	9
2:A:149:ILE:HG22	2:A:156:LYS:HE2	0.69	1.63	10	1
2:A:149:ILE:HG22	2:A:156:LYS:HE3	0.66	1.67	14	16
2:A:143:ILE:HD12	2:A:143:ILE:H	0.64	1.53	11	11
2:A:143:ILE:H	2:A:143:ILE:HD12	0.54	1.62	16	6

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	77/109 (71%)	67±2 (88±3%)	8±2 (10±2%)	1±1 (2±2%)	14 56
All	All	2310/3270 (71%)	2024 (88%)	242 (10%)	44 (2%)	14 56

5 of 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	117	LYS	11
2	A	182	GLU	5
2	A	150	PHE	3
2	A	127	ARG	3
2	A	126	PHE	3

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	66/94 (70%)	59±2 (89±3%)	7±2 (11±3%)	12 55
All	All	1980/2820 (70%)	1756 (89%)	224 (11%)	12 55

5 of 33 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)
2	A	177	HIS	29
2	A	188	VAL	25
2	A	160	PHE	24
2	A	184	ARG	17
2	A	165	ASN	17

6.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	B	7/7 (100%)	3±1 (40±9%)	1±1 (20±14%)	0.08±0.04
All	All	192/210 (91%)	85 (44%)	41 (21%)	0.08

The overall RNA backbone suiteness is 0.08.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	199	C	30
1	B	203	U	30
1	B	198	G	17
1	B	201	U	8

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	B	199	C	16
1	B	197	U	12
1	B	198	G	11
1	B	200	A	2

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)

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6895

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

7.1.1 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	829
Number of shifts mapped to atoms	829
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	78	0.55 ± 0.27	None needed (imprecise)
$^{13}C_{\beta}$	70	0.79 ± 0.17	Should be applied
$^{13}C'$	0	—	—
^{15}N	77	0.26 ± 0.56	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 67%, i.e. 753 atoms were assigned a chemical shift out of a possible 1131. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	300/379 (79%)	150/151 (99%)	76/154 (49%)	74/74 (100%)
Sidechain	413/537 (77%)	257/316 (81%)	149/185 (81%)	7/36 (19%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	40/86 (47%)	40/48 (83%)	0/36 (0%)	0/2 (0%)
Overall	753/1131 (67%)	447/588 (76%)	225/422 (53%)	81/121 (67%)

7.1.4 Statistically unusual chemical shifts (i)

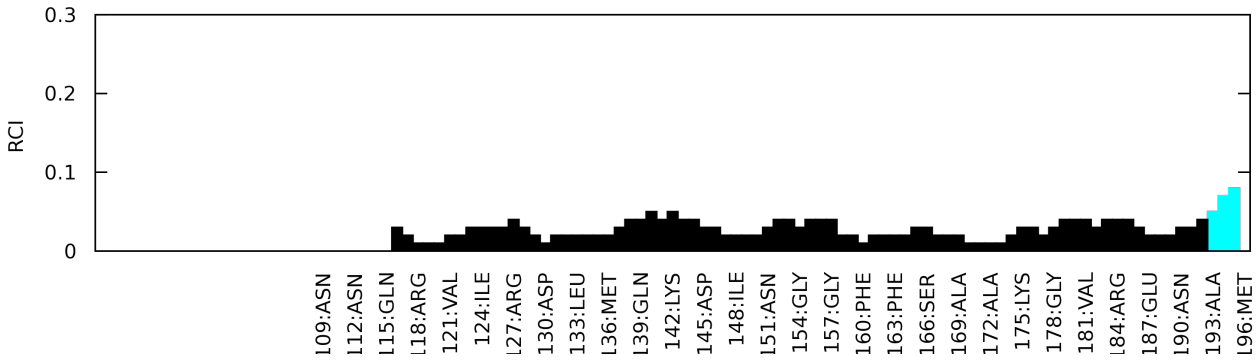
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	132	ASP	HB2	0.92	4.07 – 1.37	-6.7
1	A	125	PRO	HD2	1.70	5.45 – 1.85	-5.4

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 6895

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	53
Number of shifts mapped to atoms	53
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.2.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough 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 4%, i.e. 50 atoms were assigned a chemical shift out of a possible 1131. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	0/379 (0%)	0/151 (0%)	0/154 (0%)	0/74 (0%)
Sidechain	0/537 (0%)	0/316 (0%)	0/185 (0%)	0/36 (0%)
Aromatic	0/86 (0%)	0/48 (0%)	0/36 (0%)	0/2 (0%)
Overall	50/1131 (4%)	50/588 (9%)	0/422 (0%)	0/121 (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, *ppm***	**Expected range, *ppm***	**Z-score**
2	B	199	C	H3'	3.25	5.20 – 3.60	-7.2

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.