



wwPDB NMR Structure Validation Summary Report ⓘ

Feb 12, 2017 – 07:41 pm GMT

PDB ID : 1RGO
Title : Structural Basis for Recognition of the mRNA Class II AU-Rich Element by the Tandem Zinc Finger Domain of TIS11d
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Deposited on : 2003-11-12

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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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

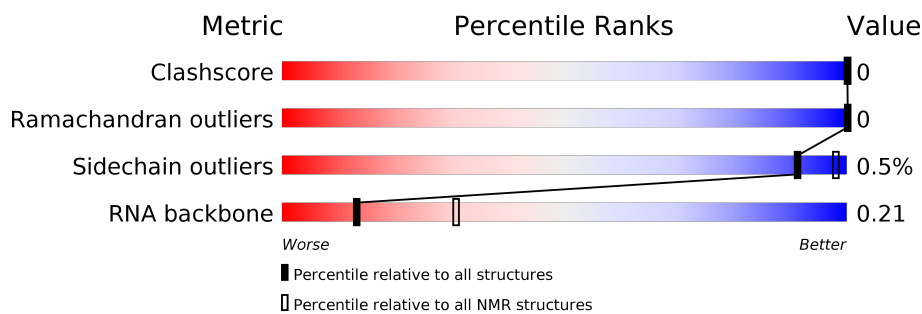
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 72%.

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
RNA backbone	3398	623

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	D	9	<div> <div>33%</div> <div>44%</div> <div>22%</div> </div>
2	A	70	<div> <div>63%</div> <div>•</div> <div>33%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:155-A:179 (25)	0.08	3
2	A:195-A:216 (22)	0.07	10

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1402 atoms, of which 637 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (5'-R(*UP*UP*AP*UP*UP*UP*AP*UP*U)-3').

Mol	Chain	Residues	Atoms						Trace
1	D	9	Total	C	H	N	O	P	0
			274	83	93	24	66	8	

- Molecule 2 is a protein called Butyrate response factor 2.

Mol	Chain	Residues	Atoms						Trace
2	A	70	Total	C	H	N	O	S	0
			1126	367	544	107	102	6	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

4 Residue-property plots [i](#)

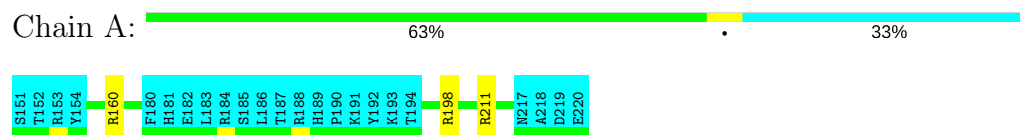
4.1 Average score per residue in the NMR ensemble

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: RNA (5'-R(*UP*UP*AP*UP*UP*UP*AP*UP*U)-3')



- Molecule 2: Butyrate response factor 2



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

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: RNA (5'-R(*UP*UP*AP*UP*UP*UP*AP*UP*U)-3')



- Molecule 2: Butyrate response factor 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *Individual zinc finger domains were created in DYANA and docked to UAUU (finger I) and UUAUU (finger II) using five rounds of simulated annealing in AMBER using distance and torsional restraints. Finger I/UAUU and Finger II/UUAUU complexes were connected to form TZF/UUAUUUAUU complexes and refined in AMBER with residual dipolar coupling restraints added. Calculations were then switched from in vacuo to Generalized Born continuum solvent model and one additional round of simulated annealing was performed..*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
AMBER	structure solution	8
AMBER	refinement	8

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 6005
Number of chemical shift lists	2
Total number of shifts	835
Number of shifts mapped to atoms	835
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

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

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	D	1.33±0.01	0±0/200 (0.0±0.0%)	2.11±0.04	8±1/308 (2.5±0.3%)
2	A	0.85±0.01	0±0/395 (0.0±0.0%)	1.09±0.01	2±1/531 (0.4±0.1%)
All	All	1.04	0/11900 (0.0%)	1.55	199/16780 (1.2%)

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	D	0.0±0.0	2.0±1.0
2	A	0.0±0.0	0.1±0.2
All	All	0	42

There are no bond-length outliers.

5 of 21 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(°)	Ideal(°)	Models	
								Worst	Total
1	D	3	A	N1-C6-N6	-9.65	112.81	118.60	15	20
1	D	2	U	O4'-C1'-N1	8.56	115.05	108.20	15	8
1	D	7	A	N1-C6-N6	-8.35	113.59	118.60	14	20
1	D	7	A	C5-C6-N1	8.17	121.78	117.70	13	20
2	A	198	ARG	NE-CZ-NH1	8.09	124.34	120.30	9	14

There are no chirality outliers.

5 of 7 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	D	7	A	Sidechain	17
1	D	6	U	Sidechain	10
1	D	3	A	Sidechain	5
1	D	2	U	Sidechain	5
1	D	5	U	Sidechain	3

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	11280	8840	8860	-

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	
2	A	47/70 (67%)	45±0 (96±1%)	2±0 (4±1%)	0±0 (0±0%)	100	100
All	All	940/1400 (67%)	907 (96%)	33 (4%)	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	
2	A	41/63 (65%)	41±0 (100±1%)	0±0 (0±1%)	91	98
All	All	820/1260 (65%)	816 (100%)	4 (0%)	91	98

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
2	A	211	ARG	4

6.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	D	8/9 (89%)	3±1 (31±17%)	0±0 (0±0%)	0.21±0.07
All	All	160/180 (89%)	50 (31%)	0 (0%)	0.21

The overall RNA backbone suiteness is 0.21.

5 of 8 unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	D	2	U	13
1	D	6	U	12
1	D	3	A	8
1	D	5	U	7
1	D	4	U	6

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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 72% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6005

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	812
Number of shifts mapped to atoms	812
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	68	-0.46 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	63	0.45 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}'$	62	-0.37 ± 0.39	None needed (< 0.5 ppm)
^{15}N	62	-2.08 ± 0.79	Should be applied

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 69%, i.e. 517 atoms were assigned a chemical shift out of a possible 748. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	225/229 (98%)	91/91 (100%)	90/94 (96%)	44/44 (100%)
Sidechain	235/273 (86%)	150/166 (90%)	81/94 (86%)	4/13 (31%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	57/89 (64%)	32/49 (65%)	25/36 (69%)	0/4 (0%)
Overall	517/748 (69%)	273/391 (70%)	196/287 (68%)	48/70 (69%)

7.1.4 Statistically unusual chemical shifts [i](#)

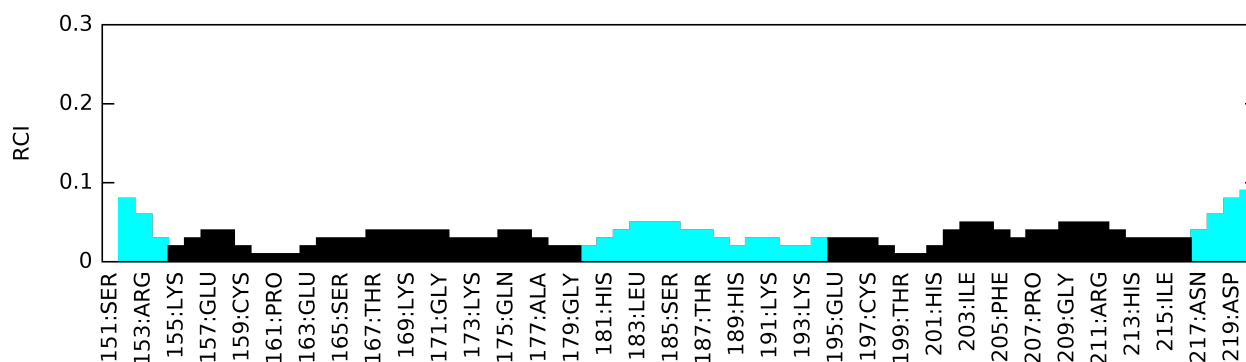
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	211	ARG	NE	117.18	92.63 – 76.73	20.4
1	A	184	ARG	NE	116.67	92.63 – 76.73	20.1
1	A	188	ARG	NE	115.77	92.63 – 76.73	19.6
1	A	153	ARG	NE	115.59	92.63 – 76.73	19.4
1	A	160	ARG	NE	114.40	92.63 – 76.73	18.7
1	A	198	ARG	NE	114.00	92.63 – 76.73	18.4
1	A	191	LYS	H	0.32	11.24 – 5.14	-12.9
1	A	156	THR	CG2	29.87	27.15 – 15.95	7.4
1	A	155	LYS	HG2	-0.47	2.67 – 0.07	-7.1
1	A	193	LYS	HG2	-0.35	2.67 – 0.07	-6.6
1	A	155	LYS	HG3	-0.28	2.76 – -0.04	-5.9
1	A	188	ARG	HD2	1.82	4.27 – 1.97	-5.6
1	A	178	HIS	HB3	0.96	5.00 – 1.10	-5.4
1	A	198	ARG	H	11.33	11.29 – 5.19	5.1

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 6005

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	23
Number of shifts mapped to atoms	23
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](#)

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 3%, i.e. 19 atoms were assigned a chemical shift out of a possible 748. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/229 (0%)	0/91 (0%)	0/94 (0%)	0/44 (0%)
Sidechain	0/273 (0%)	0/166 (0%)	0/94 (0%)	0/13 (0%)
Aromatic	0/89 (0%)	0/49 (0%)	0/36 (0%)	0/4 (0%)

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	Total	¹H	¹³C	¹⁵N
Overall	19/748 (3%)	19/391 (5%)	0/287 (0%)	0/70 (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](#)

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.