Full wwPDB NMR Structure Validation Report (i)

Oct 17, 2023 – 10:09 PM JST

PDB ID	:	6IZG
BMRB ID	:	36226
Title	:	Solution structure of Ufm1 protein from Trypanosoma brucei
Authors	:	Diwu, Y.; Tu, X.
Deposited on	:	2018-12-19

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
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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:

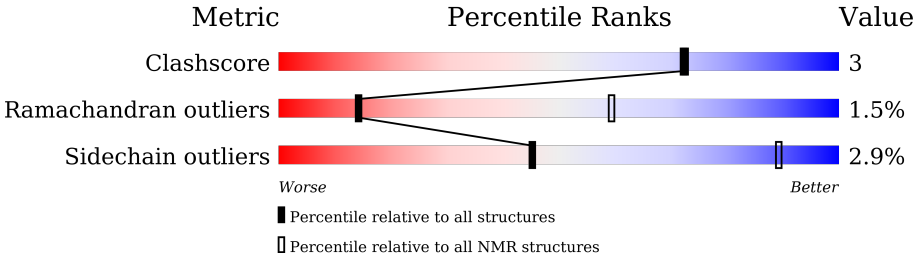
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 43%.

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

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	95	74% 8% 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 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:13-A:90 (78)	0.70	5

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1432 atoms, of which 717 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ubiquitin-fold modifier 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1432	445	717	128	139	3	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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: Ubiquitin-fold modifier 1

Chain A: 74% 8% 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 A35 A38 P39 L40 A60 T63 G68 P71 I89 P90 R91 D92 R93 V94 G95

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Ubiquitin-fold modifier 1

Chain A: 76% 6% 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 A35 A38 P39 L40 A60 P71 I89 P90 R91 D92 R93 V94 G95

4.2.2 Score per residue for model 2

• Molecule 1: Ubiquitin-fold modifier 1

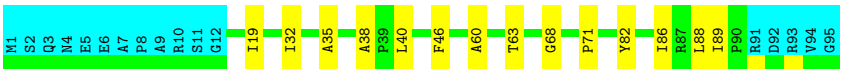
Chain A: 67% 15% 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 V15 I19 I20 L21 E24 A35 A38 P39 L40 A60 T63 G68 P71 A75 I86 I89 P90 R91 D92 R93 V94 G95

4.2.3 Score per residue for model 3

- Molecule 1: Ubiquitin-fold modifier 1

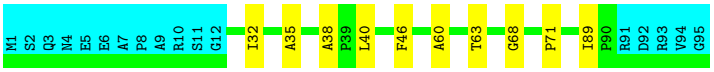
Chain A: 67% 15% 18%



4.2.4 Score per residue for model 4

- Molecule 1: Ubiquitin-fold modifier 1

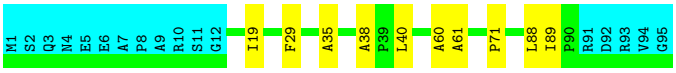
Chain A: 72% 11% 18%



4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Ubiquitin-fold modifier 1

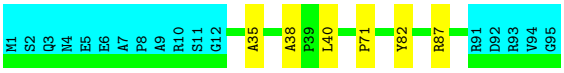
Chain A: 72% 11% 18%



4.2.6 Score per residue for model 6

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 76% 6% 18%



4.2.7 Score per residue for model 7

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 69% 11% • 18%

4.2.8 Score per residue for model 8

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 72% 11% 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 A35 A38 P39 L40 A60 T63 G68 I69 N70 P71 A72 Q73 I89 P90 R91 D92 R93 V94 G95

4.2.9 Score per residue for model 9

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 71% 12% 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 I32 A35 A38 P39 L40 F46 A60 T63 G68 P71 I89 P90 R91 D92 R93 V94 G95

4.2.10 Score per residue for model 10

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 80% • 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 L40 P71 R91 D92 R93 V94 G95

4.2.11 Score per residue for model 11

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 67% 15% 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 I19 I32 A35 A38 P39 L40 F46 A60 T63 K64 P71 Y82 I86 R87 L88 I89 P90 R91 D92 R93 V94 G95

4.2.12 Score per residue for model 12

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 78% • 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 I32 L40 F46 P71 R91 D92 R93 V94 G95

4.2.13 Score per residue for model 13

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 73% 8% • 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 F29 A60 T63 G68 P71 V78 Y82 I86 I89 P90 R91 D92 R93 V94 G95

4.2.14 Score per residue for model 14

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 71% 12% 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 A35 A38 P39 L40 S58 M59 A60 T63 G68 P71 L88 I89 P90 R91 D92 R93 V94 G95

4.2.15 Score per residue for model 15

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 68% 14% 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 R18 I19 F29 R30 V31 L40 A61 T62 T63 K64 G68 P71 Y82 R87 L88 R91 D92 R93 V94 G95

4.2.16 Score per residue for model 16

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 74% 8% 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 A35 A38 P39 L40 T63 G68 P71 Y82 I86 R91 D92 R93 V94 G95

4.2.17 Score per residue for model 17

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 71% 11% • 18%

M1 S2 Q3 N4 E5 E6 A7 P8 A9 R10 S11 G12 L21 I32 L40 F46 F51 A60 T63 G68 P71 E85 I89 P90 R91 D92 R93 V94 G95

4.2.18 Score per residue for model 18

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 69% 13% 18%

4.2.19 Score per residue for model 19

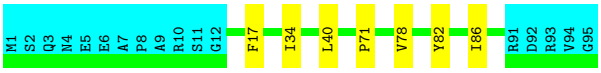
- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 65% 16% • 18%

4.2.20 Score per residue for model 20

- Molecule 1: Ubiquitin-fold modifier 1

Chain A: 75% 7% 18%



5 Refinement protocol and experimental data overview (i)

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

Of the 500 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
X-PLOR NIH	refinement	
CYANA	structure calculation	

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	522
Number of shifts mapped to atoms	522
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	43%

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	586	595	597	4±2
All	All	11720	11900	11940	81

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ILE:HG21	1:A:88:LEU:HD12	0.76	1.57	15	3
1:A:63:THR:HG23	1:A:68:GLY:HA3	0.71	1.60	2	12
1:A:35:ALA:HB3	1:A:38:ALA:HB2	0.66	1.66	2	12
1:A:60:ALA:HB3	1:A:89:ILE:O	0.58	1.98	2	14
1:A:61:ALA:HB2	1:A:88:LEU:CD2	0.57	2.29	5	1
1:A:58:SER:O	1:A:88:LEU:HD11	0.57	1.99	14	1
1:A:19:ILE:HG21	1:A:88:LEU:CD1	0.57	2.30	11	1
1:A:61:ALA:HB2	1:A:88:LEU:HD23	0.53	1.80	5	1
1:A:82:TYR:CE2	1:A:86:ILE:HD12	0.53	2.39	3	2
1:A:63:THR:HG21	1:A:82:TYR:CD2	0.52	2.40	15	2
1:A:61:ALA:HB3	1:A:68:GLY:O	0.51	2.05	15	1
1:A:40:LEU:HD21	1:A:73:GLN:O	0.50	2.06	19	1
1:A:21:LEU:HD23	1:A:24:GLU:HB2	0.49	1.84	2	1
1:A:32:ILE:HG22	1:A:46:PHE:HB3	0.48	1.86	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:VAL:HG13	1:A:82:TYR:CE1	0.48	2.44	13	1
1:A:18:ARG:HG2	1:A:31:VAL:HG22	0.48	1.84	15	1
1:A:68:GLY:O	1:A:86:ILE:HD11	0.47	2.10	16	1
1:A:19:ILE:HG22	1:A:86:ILE:CG2	0.47	2.39	2	1
1:A:74:THR:HG23	1:A:75:ALA:N	0.47	2.25	19	1
1:A:63:THR:HG23	1:A:68:GLY:CA	0.47	2.39	15	1
1:A:74:THR:HG23	1:A:76:GLY:H	0.46	1.71	19	1
1:A:82:TYR:CD1	1:A:86:ILE:HD12	0.45	2.45	11	1
1:A:22:THR:HB	1:A:87:ARG:HE	0.44	1.72	7	1
1:A:17:PHE:CZ	1:A:78:VAL:HG12	0.44	2.47	20	1
1:A:82:TYR:CD2	1:A:86:ILE:HD13	0.44	2.48	13	1
1:A:82:TYR:CG	1:A:86:ILE:HD12	0.44	2.48	16	2
1:A:32:ILE:HG22	1:A:46:PHE:CB	0.43	2.43	3	4
1:A:32:ILE:HG23	1:A:46:PHE:CD1	0.43	2.48	11	1
1:A:15:VAL:HG21	1:A:75:ALA:HB1	0.43	1.91	2	1
1:A:40:LEU:HD13	1:A:73:GLN:CB	0.42	2.43	8	1
1:A:21:LEU:HD11	1:A:51:PHE:CZ	0.42	2.50	17	1
1:A:17:PHE:CE1	1:A:78:VAL:HG12	0.41	2.49	20	1
1:A:19:ILE:HG23	1:A:88:LEU:HD23	0.41	1.91	7	1
1:A:19:ILE:HG21	1:A:88:LEU:HD11	0.41	1.92	3	1
1:A:18:ARG:H	1:A:84:GLN:CB	0.40	2.29	19	1

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	78/95 (82%)	70±1 (90±2%)	6±1 (8±2%)	1±0 (2±1%)	14	59
All	All	1560/1900 (82%)	1409 (90%)	127 (8%)	24 (2%)	14	59

All 4 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	71	PRO	20

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Mol	Chain	Res	Type	Models (Total)
1	A	90	PRO	2
1	A	29	PHE	1
1	A	85	GLU	1

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	60/74 (81%)	58±1 (97±2%)	2±1 (3±2%)	45 89
All	All	1200/1480 (81%)	1165 (97%)	35 (3%)	45 89

All 13 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	40	LEU	17
1	A	87	ARG	3
1	A	64	LYS	3
1	A	29	PHE	2
1	A	82	TYR	2
1	A	88	LEU	1
1	A	70	ASN	1
1	A	21	LEU	1
1	A	19	ILE	1
1	A	50	GLU	1
1	A	69	ILE	1
1	A	74	THR	1
1	A	34	ILE	1

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 monosaccharides 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 43% for the well-defined parts and 41% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *shifts1.txt*

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	522
Number of shifts mapped to atoms	522
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	93	-0.14 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	85	0.11 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	83	-0.09 ± 0.18	None needed (< 0.5 ppm)
^{15}N	86	0.23 ± 0.34	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 43%, i.e. 444 atoms were assigned a chemical shift out of a possible 1041. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	287/388 (74%)	66/158 (42%)	148/156 (95%)	73/74 (99%)
Sidechain	157/594 (26%)	22/390 (6%)	135/181 (75%)	0/23 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/59 (0%)	0/29 (0%)	0/30 (0%)	0/0 (—%)
Overall	444/1041 (43%)	88/577 (15%)	283/367 (77%)	73/97 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 522 atoms were assigned a chemical shift out of a possible 1258. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	339/473 (72%)	77/193 (40%)	176/190 (93%)	86/90 (96%)
Sidechain	183/726 (25%)	23/473 (5%)	160/219 (73%)	0/34 (0%)
Aromatic	0/59 (0%)	0/29 (0%)	0/30 (0%)	0/0 (—%)
Overall	522/1258 (41%)	100/695 (14%)	336/439 (77%)	86/124 (69%)

7.1.4 Statistically unusual chemical shifts (i)

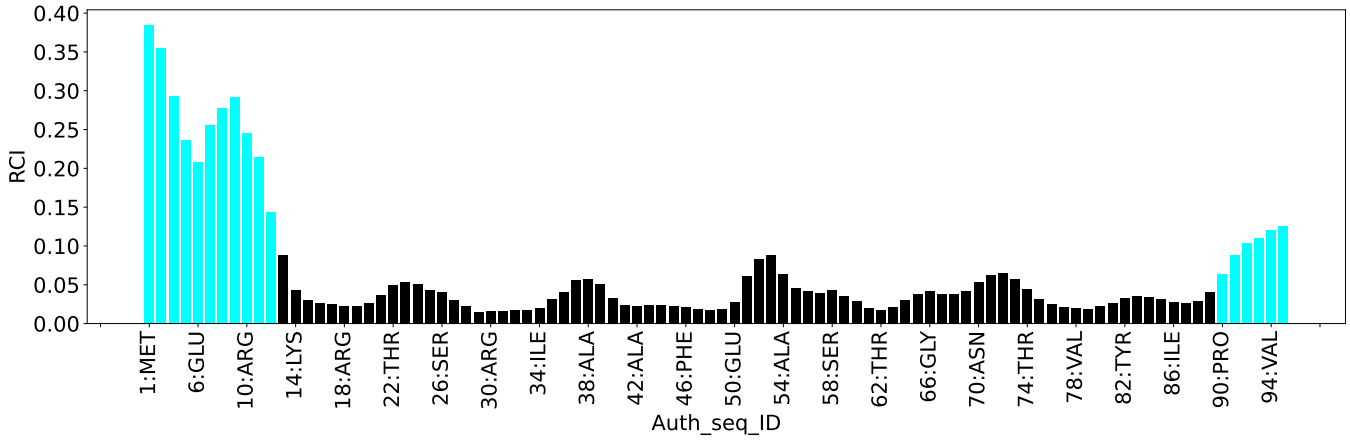
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	32	ILE	CG2	24.63	10.93 – 24.12	5.4
1	A	53	ILE	CG2	24.63	10.93 – 24.12	5.4
1	A	19	ILE	CG1	18.94	19.24 – 36.26	-5.2
1	A	20	ILE	CG1	18.94	19.24 – 36.26	-5.2
1	A	32	ILE	CG1	18.94	19.24 – 36.26	-5.2
1	A	34	ILE	CG1	18.94	19.24 – 36.26	-5.2
1	A	53	ILE	CG1	18.94	19.24 – 36.26	-5.2
1	A	69	ILE	CG1	18.94	19.24 – 36.26	-5.2
1	A	86	ILE	CG1	18.94	19.24 – 36.26	-5.2

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:


RCI
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1:MET
6:GLU
10:ARG
14:LYS
18:ARG
22:THR
26:SER
30:ARG
34:ILE
38:ALA
42:ALA
46:PHE
50:GLU
54:ALA
58:SER
62:THR
66:GLY
70:ASN
74:THR
78:VAL
82:TYR
86:ILE
90:PRO
94:VAL
Auth_seq_ID