wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1MA2
Title	:	Tachyplesin I Wild type peptide NMR Structure
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Deposited on	:	2002-07-31

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:

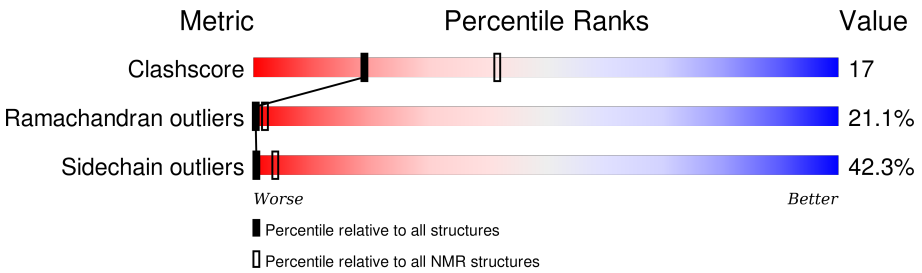
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 45%.

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	17	6% 88% 6%

2 Ensemble composition and analysis (i)

This entry contains 31 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (6) was below the domain threshold value (8).

The models can be grouped into 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 4, 15, 18, 19, 21, 27, 28, 29, 31
2	2, 5, 7, 8, 11, 14, 17, 23, 25, 26
3	6, 10, 24, 30
4	13, 16, 22
5	12, 20
Single-model clusters	9

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 313 atoms, of which 156 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tachyplesin I.

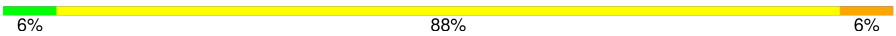
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	17	313	99	156	34	20	4	0

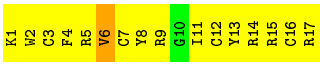
4 Residue-property plots (i)

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: Tachyplesin I

Chain A: 



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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: Tachyplesin I

Chain A:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing with complete cross validation.*

Of the 300 calculated structures, 31 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
CNS	structure solution	1.0
CNS	refinement	1.0

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 5487, BMRB entry 5486, BMRB entry 5489,
Number of chemical shift lists	
Total number of shifts	
Number of shifts mapped to atoms	
Number of unparsed shifts	
Number of shifts with mapping errors	
Number of shifts with mapping warnings	
Assignment completeness (well-defined parts)	

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	157	156	156	5±3
All	All	4867	4836	4836	163

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 17.

5 of 100 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HD13	1:A:12:CYS:N	0.86	1.85	11	10
1:A:11:ILE:HD12	1:A:13:TYR:CE2	0.73	2.18	31	3
1:A:11:ILE:HD12	1:A:13:TYR:CD1	0.72	2.19	23	2
1:A:11:ILE:HD12	1:A:13:TYR:CD2	0.70	2.21	26	5
1:A:5:ARG:O	1:A:6:VAL:HG23	0.69	1.87	10	4

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	15/17 (88%)	7±2 (48±11%)	5±2 (31±10%)	3±1 (21±8%)	0 2
All	All	465/527 (88%)	222 (48%)	145 (31%)	98 (21%)	0 2

5 of 13 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	6	VAL	16
1	A	9	ARG	14
1	A	3	CYS	10
1	A	4	PHE	9
1	A	16	CYS	9

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	16/16 (100%)	9±2 (58±11%)	7±2 (42±11%)	0 4
All	All	496/496 (100%)	286 (58%)	210 (42%)	0 4

5 of 16 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	1	LYS	23
1	A	15	ARG	21
1	A	5	ARG	19
1	A	9	ARG	18
1	A	3	CYS	17

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)

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 45% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5486

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	103
Number of shifts mapped to atoms	103
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

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 44%, i.e. 116 atoms were assigned a chemical shift out of a possible 264. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	33/85 (39%)	33/34 (97%)	0/34 (0%)	0/17 (0%)
Sidechain	65/142 (46%)	65/87 (75%)	0/39 (0%)	0/16 (0%)
Aromatic	18/37 (49%)	18/19 (95%)	0/17 (0%)	0/1 (0%)
Overall	116/264 (44%)	116/140 (83%)	0/90 (0%)	0/34 (0%)

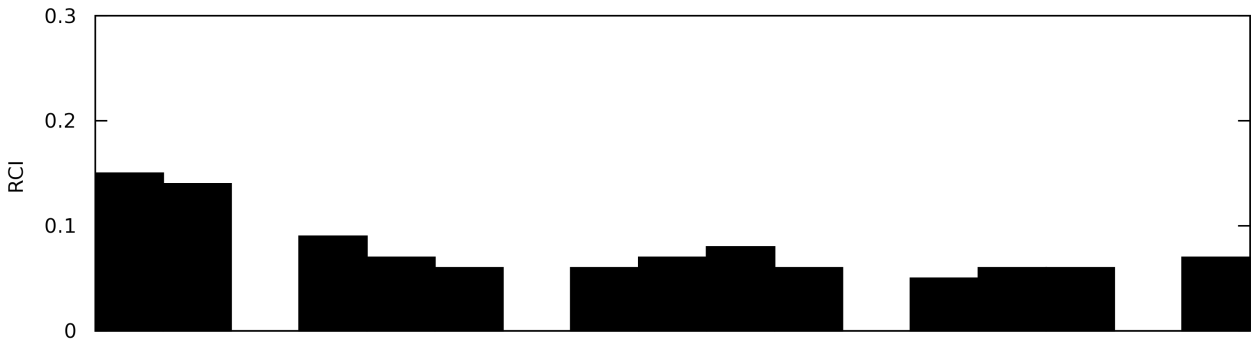
7.1.4 Statistically unusual chemical shifts (i)

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.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5487

Chemical shift list name: *assigned_chem_shift_list_1*

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	100
Number of shifts mapped to atoms	76
Number of unparsed shifts	0
Number of shifts with mapping errors	24
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.

- Residue not found in structure. First 5 (of 24) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	3	TYR	HB3	2.589	0.001	2
A	16	TYR	HE1	6.759	0.001	2
A	12	TYR	HB3	2.735	0.001	2
A	7	TYR	H	8.672	0.001	1
A	3	TYR	HD1	6.558	0.001	2

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 32%, i.e. 84 atoms were assigned a chemical shift out of a possible 264. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	25/85 (29%)	25/34 (74%)	0/34 (0%)	0/17 (0%)
Sidechain	41/142 (29%)	41/87 (47%)	0/39 (0%)	0/16 (0%)
Aromatic	18/37 (49%)	18/19 (95%)	0/17 (0%)	0/1 (0%)
Overall	84/264 (32%)	84/140 (60%)	0/90 (0%)	0/34 (0%)

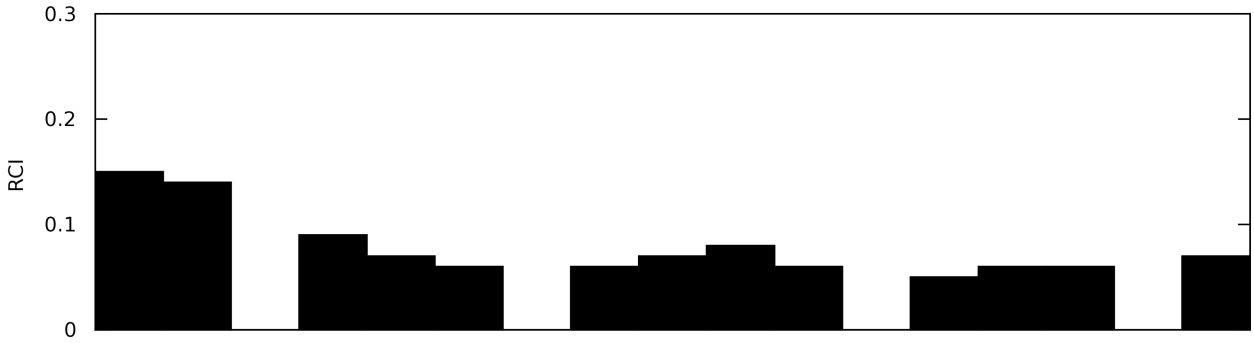
7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots (i)

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:



7.3 Chemical shift list 3

File name: BMRB entry 5488

Chemical shift list name: *assigned_chem_shift_list_1*

7.3.1 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	72
Number of shifts mapped to atoms	58
Number of unparsed shifts	0
Number of shifts with mapping errors	14
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.

- Residue not found in structure. First 5 (of 14) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	12	PHE	H	8.458	0.001	1
A	7	PHE	HB2	2.923	0.001	2
A	3	PHE	HA	4.519	0.001	1
A	3	PHE	H	8.035	0.001	1
A	3	PHE	HB2	2.874	0.001	2

7.3.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.3.3 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 25%, i.e. 66 atoms were assigned a chemical shift out of a possible 264. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	25/85 (29%)	25/34 (74%)	0/34 (0%)	0/17 (0%)
Sidechain	41/142 (29%)	41/87 (47%)	0/39 (0%)	0/16 (0%)
Aromatic	0/37 (0%)	0/19 (0%)	0/17 (0%)	0/1 (0%)
Overall	66/264 (25%)	66/140 (47%)	0/90 (0%)	0/34 (0%)

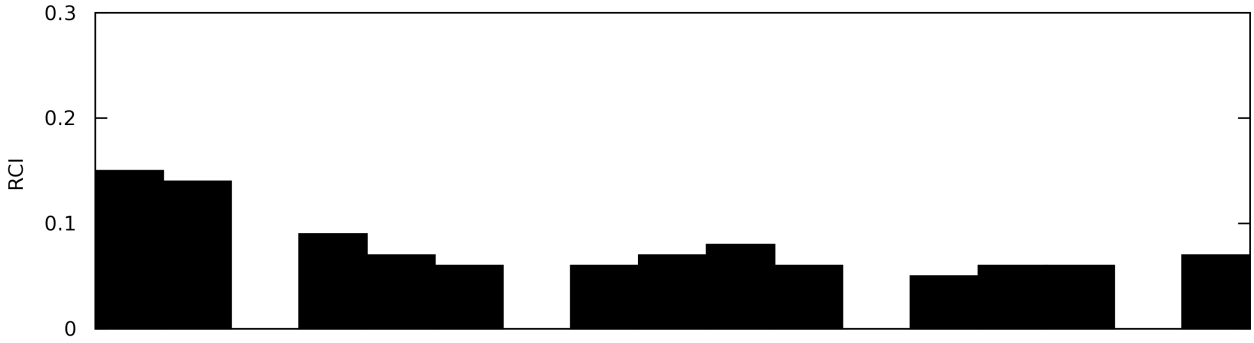
7.3.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.3.5 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:



7.4 Chemical shift list 4

File name: BMRB entry 5489

Chemical shift list name: *assigned_chem_shift_list_1*

7.4.1 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	51
Number of shifts mapped to atoms	42
Number of unparsed shifts	0
Number of shifts with mapping errors	9
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- Residue not found in structure. First 5 (of 9) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	3	ALA	HB3	2.702	0.001	1
A	3	ALA	H	8.158	0.001	1
A	3	ALA	HB2	2.702	0.001	1
A	12	ALA	HA	4.279	0.001	1
A	7	ALA	H	8.522	0.001	1

7.4.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.4.3 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 19%, i.e. 50 atoms were assigned a chemical shift out of a possible 264. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	23/85 (27%)	23/34 (68%)	0/34 (0%)	0/17 (0%)
Sidechain	12/142 (8%)	12/87 (14%)	0/39 (0%)	0/16 (0%)
Aromatic	15/37 (41%)	15/19 (79%)	0/17 (0%)	0/1 (0%)
Overall	50/264 (19%)	50/140 (36%)	0/90 (0%)	0/34 (0%)

7.4.4 Statistically unusual chemical shifts (i)

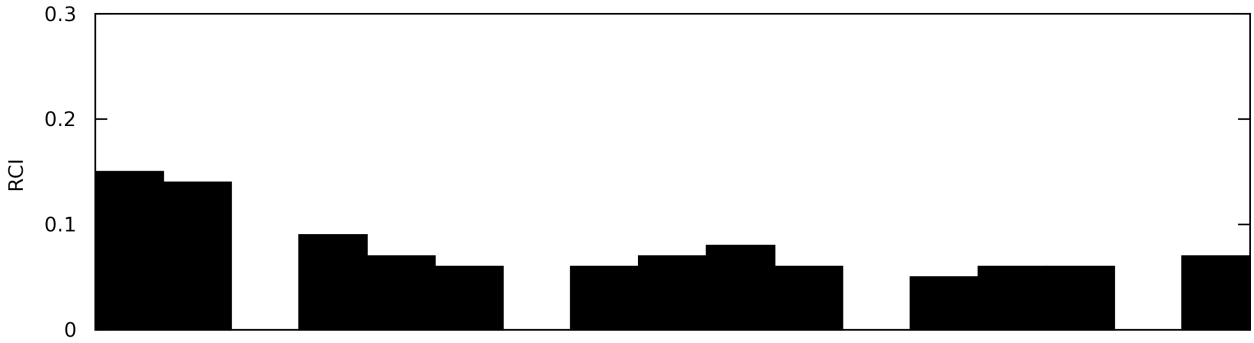
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	3	ALA	HB3	2.70	2.61 – 0.11	5.4
1	A	3	ALA	HB2	2.70	2.61 – 0.11	5.4
1	A	3	ALA	HB1	2.70	2.61 – 0.11	5.4

7.4.5 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:



7.5 Chemical shift list 5

File name: BMRB entry 5486

Chemical shift list name: *assigned_chem_shift_list_2*

7.5.1 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	95
Number of shifts mapped to atoms	95

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

7.5.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.5.3 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 39%, i.e. 104 atoms were assigned a chemical shift out of a possible 264. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	33/85 (39%)	33/34 (97%)	0/34 (0%)	0/17 (0%)
Sidechain	54/142 (38%)	54/87 (62%)	0/39 (0%)	0/16 (0%)
Aromatic	17/37 (46%)	17/19 (89%)	0/17 (0%)	0/1 (0%)
Overall	104/264 (39%)	104/140 (74%)	0/90 (0%)	0/34 (0%)

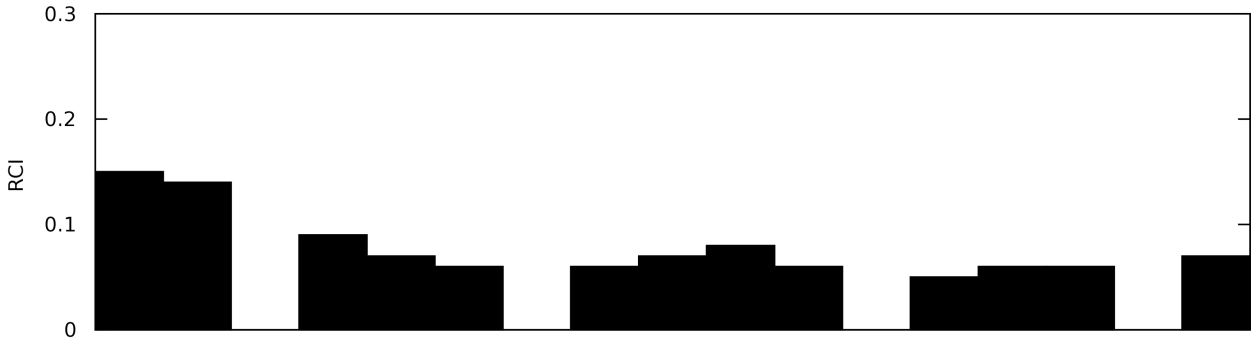
7.5.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.5.5 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:



7.6 Chemical shift list 6

File name: BMRB entry 5487

Chemical shift list name: *assigned_chem_shift_list_2*

7.6.1 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	109
Number of shifts mapped to atoms	86
Number of unparsed shifts	0
Number of shifts with mapping errors	23
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.

- Residue not found in structure. First 5 (of 23) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	3	TYR	HB3	2.885	0.001	2
A	16	TYR	HE1	6.648	0.001	2
A	12	TYR	HB3	3.041	0.001	2
A	7	TYR	H	7.65	0.001	1
A	3	TYR	HD1	6.712	0.001	2

7.6.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

7.6.3 Completeness of resonance assignments (i)

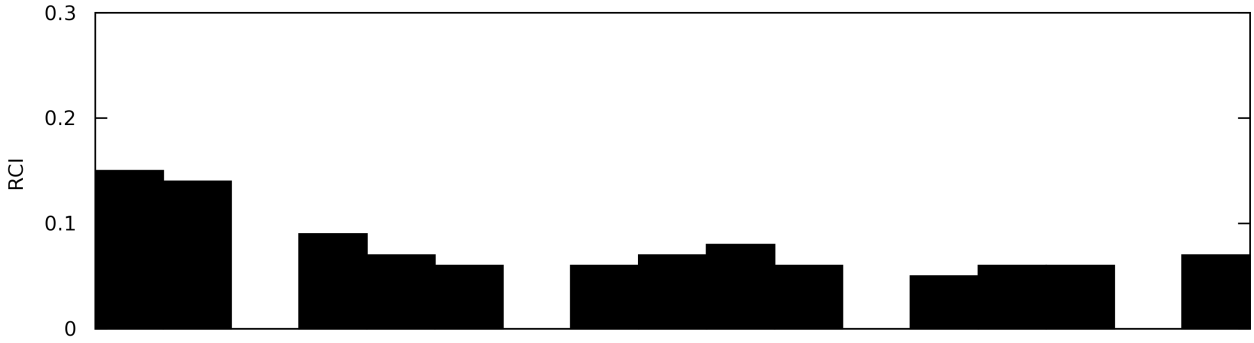
The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 37%, i.e. 98 atoms were assigned a chemical shift out of a possible 264. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	25/85 (29%)	25/34 (74%)	0/34 (0%)	0/17 (0%)
Sidechain	55/142 (39%)	55/87 (63%)	0/39 (0%)	0/16 (0%)
Aromatic	18/37 (49%)	18/19 (95%)	0/17 (0%)	0/1 (0%)
Overall	98/264 (37%)	98/140 (70%)	0/90 (0%)	0/34 (0%)

7.6.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.6.5 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: