



Full wwPDB NMR Structure Validation Report ⓘ

Feb 16, 2018 – 11:42 am GMT

PDB ID : 1MMC
Title : 1H NMR STUDY OF THE SOLUTION STRUCTURE OF AC-AMP2
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Deposited on : 1995-10-25

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

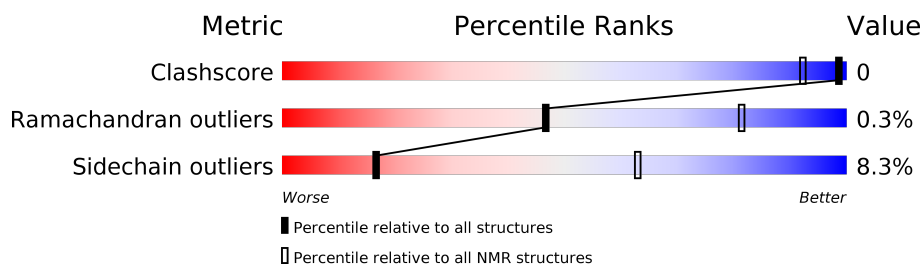
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 47%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	A	30	 80% 17%

2 Ensemble composition and analysis

This entry contains 26 models. Model 19 is the overall representative, medoid model (most similar to other models).

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:4-A:28 (25)	0.29	19

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 423 atoms, of which 206 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ANTIMICROBIAL PEPTIDE 2.

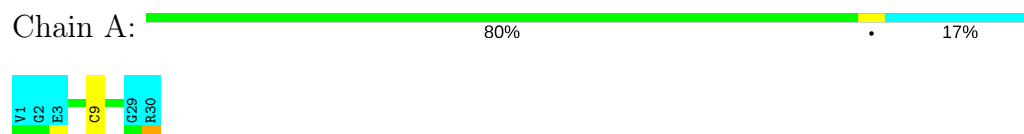
Mol	Chain	Residues	Atoms						Trace
1	A	30	Total	C	H	N	O	S	0
			423	130	206	42	38	7	

4 Residue-property plots

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: ANTIMICROBIAL PEPTIDE 2

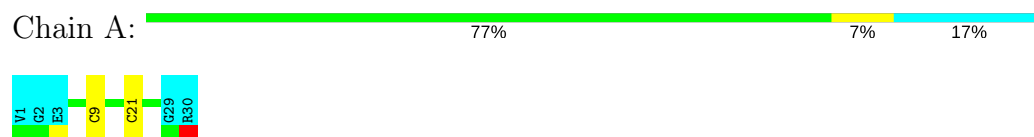


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

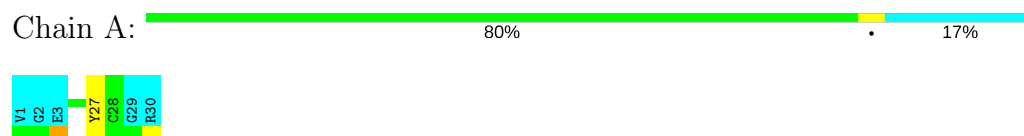
4.2.1 Score per residue for model 1

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



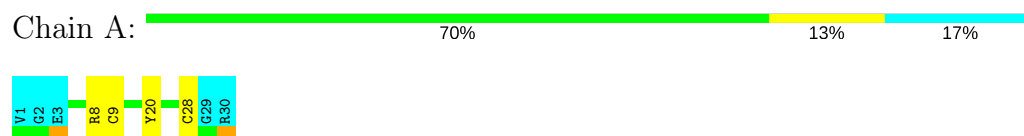
4.2.2 Score per residue for model 2

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



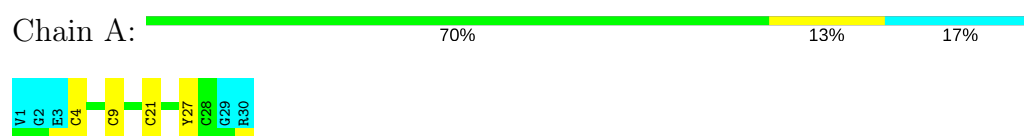
4.2.3 Score per residue for model 3

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



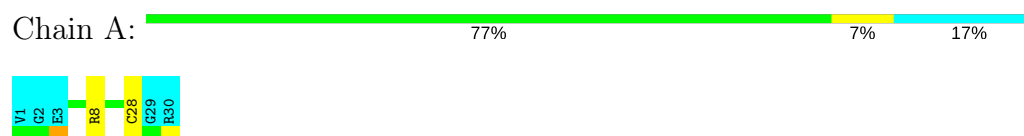
4.2.4 Score per residue for model 4

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



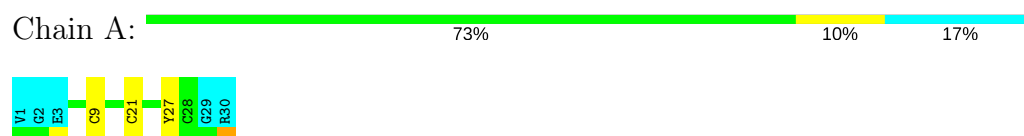
4.2.5 Score per residue for model 5

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



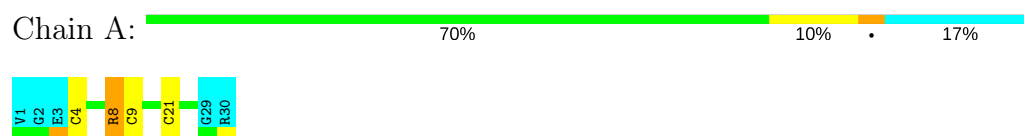
4.2.6 Score per residue for model 6

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



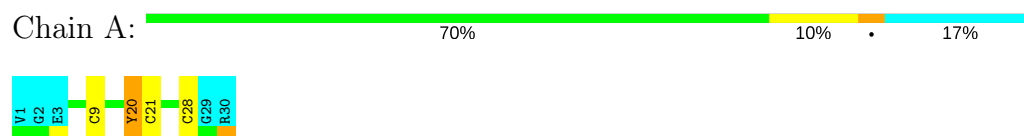
4.2.7 Score per residue for model 7

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



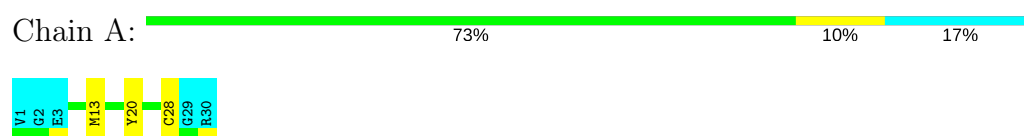
4.2.8 Score per residue for model 8

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



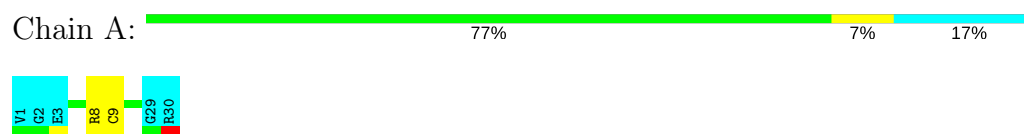
4.2.9 Score per residue for model 9

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



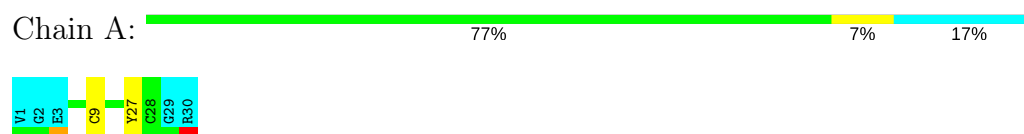
4.2.10 Score per residue for model 10

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



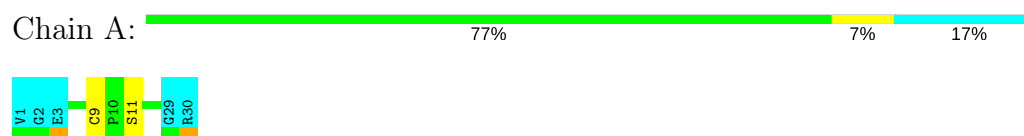
4.2.11 Score per residue for model 11

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



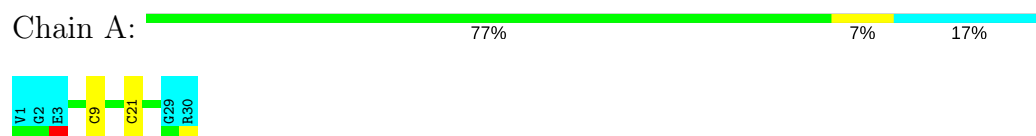
4.2.12 Score per residue for model 12

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



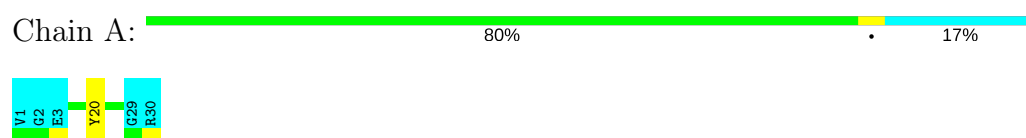
4.2.13 Score per residue for model 13

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



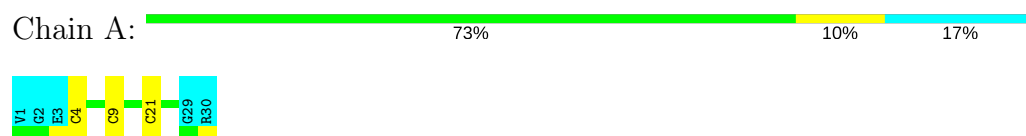
4.2.14 Score per residue for model 14

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



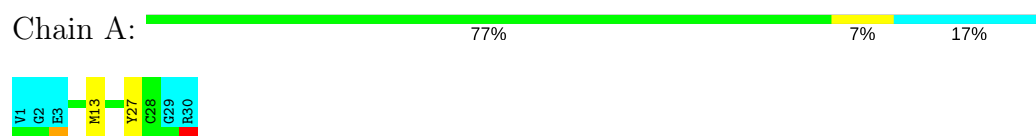
4.2.15 Score per residue for model 15

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



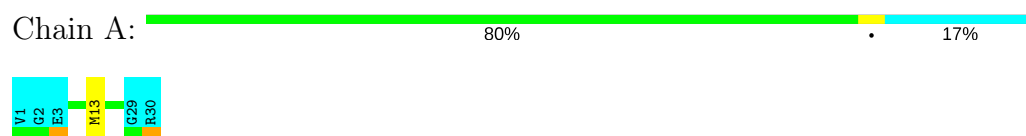
4.2.16 Score per residue for model 16

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



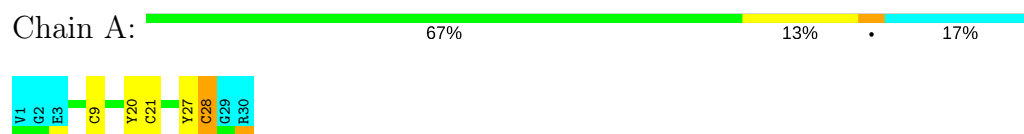
4.2.17 Score per residue for model 17

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



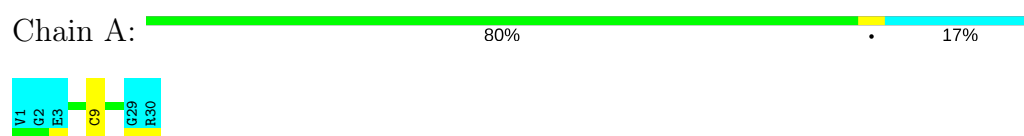
4.2.18 Score per residue for model 18

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



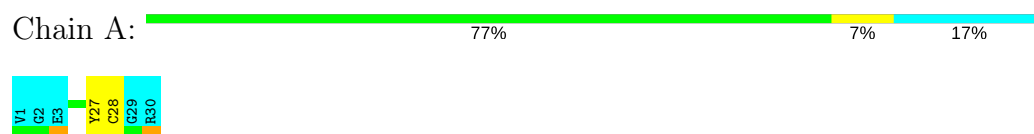
4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



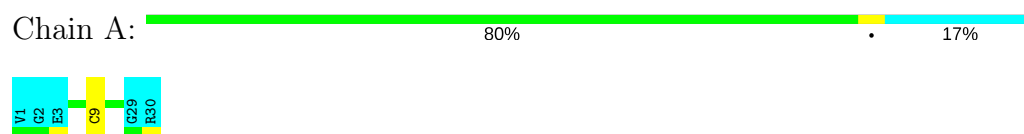
4.2.20 Score per residue for model 20

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



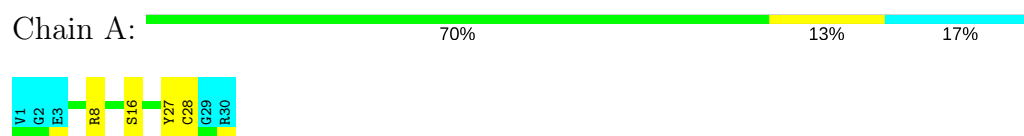
4.2.21 Score per residue for model 21

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



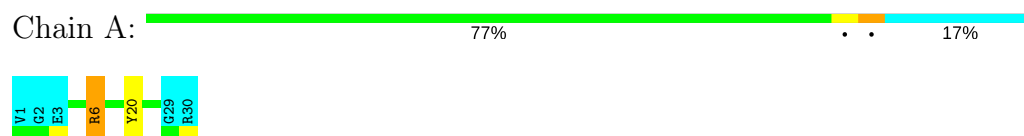
4.2.22 Score per residue for model 22

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



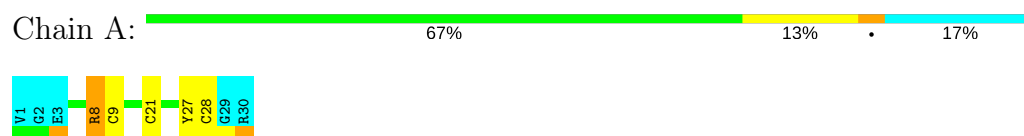
4.2.23 Score per residue for model 23

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



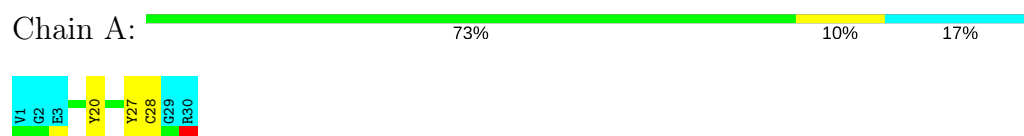
4.2.24 Score per residue for model 24

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



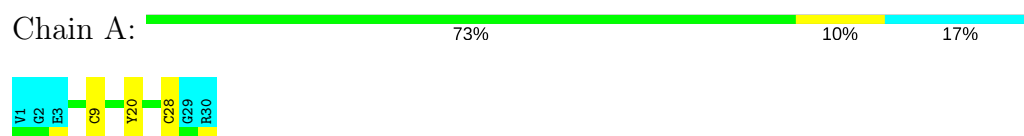
4.2.25 Score per residue for model 25

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



4.2.26 Score per residue for model 26

- Molecule 1: ANTIMICROBIAL PEPTIDE 2



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 26 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DIANA	refinement	
AMBER	refinement	

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 6647, BMRB entry 6639, BMRB entry 6637, 1
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

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	A	0.68±0.01	0±0/186 (0.0±0.0%)	1.04±0.06	0±1/247 (0.1±0.2%)
All	All	0.68	0/4836 (0.0%)	1.05	6/6422 (0.1%)

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	A	0.0±0.0	0.8±0.7
All	All	0	21

There are no bond-length outliers.

All 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	A	20	TYR	CB-CG-CD2	-5.46	117.72	121.00	8	1
1	A	27	TYR	CB-CG-CD2	-5.32	117.81	121.00	20	2
1	A	20	TYR	CB-CG-CD1	-5.16	117.91	121.00	8	1
1	A	6	ARG	NE-CZ-NH2	-5.07	117.77	120.30	23	1
1	A	8	ARG	NE-CZ-NH2	-5.02	117.79	120.30	5	1

There are no chirality outliers.

All 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	A	20	TYR	Sidechain	8
1	A	27	TYR	Sidechain	7
1	A	8	ARG	Sidechain	5

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	6	ARG	Sidechain	1

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	181	168	168	0±0
All	All	4706	4368	4368	1

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:SER:HB3	1:A:27:TYR:CD2	0.41	2.51	22	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	25/30 (83%)	22±1 (87±3%)	3±1 (13±3%)	0±0 (0±1%)	47	81
All	All	650/780 (83%)	563 (87%)	85 (13%)	2 (0%)	47	81

All 2 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	28	CYS	1
1	A	11	SER	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	20/23 (87%)	18±1 (92±6%)	2±1 (8±6%)	17	63
All	All	520/598 (87%)	477 (92%)	43 (8%)	17	63

All 6 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	9	CYS	16
1	A	28	CYS	10
1	A	21	CYS	9
1	A	13	MET	3
1	A	4	CYS	3
1	A	8	ARG	2

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

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 47% for the well-defined parts and 46% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6591

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	148
Number of shifts mapped to atoms	134
Number of unparsed shifts	0
Number of shifts with mapping errors	14
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Residue not found in structure. All 14 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	18	PFF	HD1	7.119	0.02	3
A	20	PFF	HD1	7.113	0.02	3
A	18	PFF	HD2	7.119	0.02	3
A	20	PFF	H	7.52	0.02	1
A	18	PFF	H	7.793	0.02	1
A	18	PFF	HE2	7.078	0.02	3
A	20	PFF	HA	5.004	0.02	1
A	18	PFF	HB2	2.83	0.02	2
A	20	PFF	HB2	3.054	0.02	2
A	20	PFF	HB3	3.498	0.02	2
A	20	PFF	HD2	7.113	0.02	3
A	18	PFF	HA	4.742	0.02	1
A	18	PFF	HE1	7.078	0.02	3
A	18	PFF	HB3	3.576	0.02	2

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 39%, i.e. 111 atoms were assigned a chemical shift out of a possible 283. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	44/121 (36%)	44/48 (92%)	0/50 (0%)	0/23 (0%)
Sidechain	63/137 (46%)	63/86 (73%)	0/42 (0%)	0/9 (0%)
Aromatic	4/25 (16%)	4/13 (31%)	0/12 (0%)	0/0 (—%)
Overall	111/283 (39%)	111/147 (76%)	0/104 (0%)	0/32 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 133 atoms were assigned a chemical shift out of a possible 339. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	53/146 (36%)	53/58 (91%)	0/60 (0%)	0/28 (0%)
Sidechain	76/168 (45%)	76/104 (73%)	0/52 (0%)	0/12 (0%)
Aromatic	4/25 (16%)	4/13 (31%)	0/12 (0%)	0/0 (—%)
Overall	133/339 (39%)	133/175 (76%)	0/124 (0%)	0/40 (0%)

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.

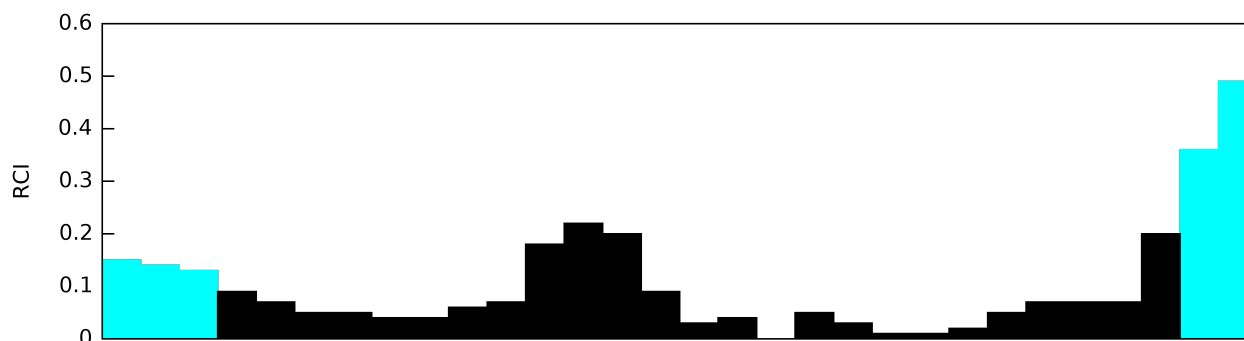
Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	22	GLY	HA3	1.79	5.80 – 2.00	-5.5

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 6637

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	160
Number of shifts mapped to atoms	149
Number of unparsed shifts	0
Number of shifts with mapping errors	11
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- Residue not found in structure. All 11 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	18	NAL	HA	4.87	0.004	1
A	18	NAL	HE2	7.974	0.003	1
A	18	NAL	HB3	3.788	0.003	2
A	18	NAL	HZ1	7.847	0.002	1
A	18	NAL	HD1	7.573	0.003	1
A	18	NAL	H	7.884	0.003	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	18	NAL	HH1	7.546	0.001	1
A	18	NAL	HB2	3.084	0.003	2
A	18	NAL	HH2	7.878	0.004	1
A	18	NAL	HP	7.518	0.001	1
A	18	NAL	HD2	7.432	0.002	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 44%, i.e. 125 atoms were assigned a chemical shift out of a possible 283. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	46/121 (38%)	46/48 (96%)	0/50 (0%)	0/23 (0%)
Sidechain	71/137 (52%)	71/86 (83%)	0/42 (0%)	0/9 (0%)
Aromatic	8/25 (32%)	8/13 (62%)	0/12 (0%)	0/0 (—%)
Overall	125/283 (44%)	125/147 (85%)	0/104 (0%)	0/32 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 148 atoms were assigned a chemical shift out of a possible 339. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	55/146 (38%)	55/58 (95%)	0/60 (0%)	0/28 (0%)
Sidechain	85/168 (51%)	85/104 (82%)	0/52 (0%)	0/12 (0%)
Aromatic	8/25 (32%)	8/13 (62%)	0/12 (0%)	0/0 (—%)
Overall	148/339 (44%)	148/175 (85%)	0/124 (0%)	0/40 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

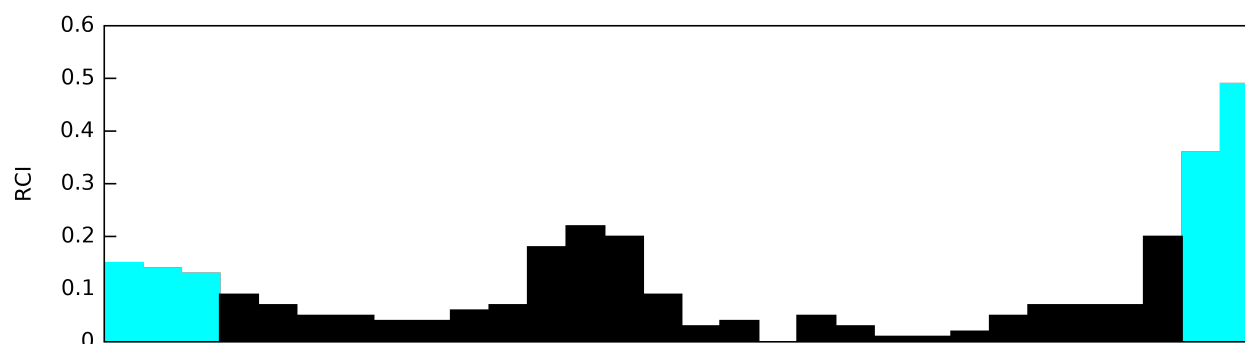
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	17	GLN	HG2	0.46	3.67 – 0.97	-6.9
1	A	22	GLY	HA2	1.83	5.87 – 2.07	-5.6

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 6639

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	152
Number of shifts mapped to atoms	142
Number of unparsed shifts	0
Number of shifts with mapping errors	10
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

file.

- Residue not found in structure. All 10 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	18	TRP	HB2	3.153	0.003	2
A	18	TRP	HE1	10.167	0.001	1
A	18	TRP	HD1	7.255	0.002	1
A	18	TRP	HZ2	7.299	0.004	1
A	18	TRP	H	7.276	0.004	1
A	18	TRP	HB3	3.622	0.004	2
A	18	TRP	HE3	7.644	0.001	2
A	18	TRP	HA	4.802	0.001	1
A	18	TRP	HZ3	7.121	0.0	1
A	18	TRP	HH2	7.041	0.004	1

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 45%, i.e. 128 atoms were assigned a chemical shift out of a possible 283. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	46/121 (38%)	46/48 (96%)	0/50 (0%)	0/23 (0%)
Sidechain	74/137 (54%)	74/86 (86%)	0/42 (0%)	0/9 (0%)
Aromatic	8/25 (32%)	8/13 (62%)	0/12 (0%)	0/0 (—%)
Overall	128/283 (45%)	128/147 (87%)	0/104 (0%)	0/32 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 149 atoms were assigned a chemical shift out of a possible 339. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	55/146 (38%)	55/58 (95%)	0/60 (0%)	0/28 (0%)
Sidechain	86/168 (51%)	86/104 (83%)	0/52 (0%)	0/12 (0%)
Aromatic	8/25 (32%)	8/13 (62%)	0/12 (0%)	0/0 (—%)
Overall	149/339 (44%)	149/175 (85%)	0/124 (0%)	0/40 (0%)

7.3.4 Statistically unusual chemical shifts [i](#)

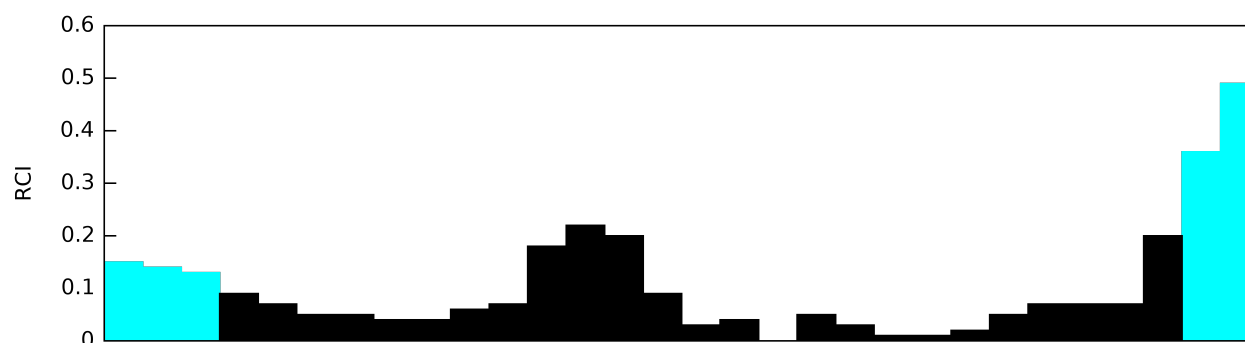
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	22	GLY	HA2	1.87	5.87 – 2.07	-5.5

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 6647

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	160
Number of shifts mapped to atoms	150
Number of unparsed shifts	0
Number of shifts with mapping errors	10

Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- Residue not found in structure. All 10 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	18	TRP	HB2	3.065	0.004	2
A	18	TRP	HE1	10.201	0.002	1
A	18	TRP	HD1	7.171	0.001	1
A	18	TRP	HZ2	7.374	0.001	1
A	18	TRP	H	7.666	0.004	1
A	18	TRP	HB3	3.664	0.004	2
A	18	TRP	HE3	7.572	0.002	1
A	18	TRP	HA	4.721	0.009	1
A	18	TRP	HZ3	7.013	0.001	1
A	18	TRP	HH2	7.147	0.004	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 45%, i.e. 127 atoms were assigned a chemical shift out of a possible 283. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	46/121 (38%)	46/48 (96%)	0/50 (0%)	0/23 (0%)
Sidechain	75/137 (55%)	75/86 (87%)	0/42 (0%)	0/9 (0%)
Aromatic	6/25 (24%)	6/13 (46%)	0/12 (0%)	0/0 (—%)
Overall	127/283 (45%)	127/147 (86%)	0/104 (0%)	0/32 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 150 atoms were assigned a chemical shift out of a possible 339. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	55/146 (38%)	55/58 (95%)	0/60 (0%)	0/28 (0%)
Sidechain	89/168 (53%)	89/104 (86%)	0/52 (0%)	0/12 (0%)
Aromatic	6/25 (24%)	6/13 (46%)	0/12 (0%)	0/0 (—%)
Overall	150/339 (44%)	150/175 (86%)	0/124 (0%)	0/40 (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	22	GLY	HA2	1.74	5.87 – 2.07	-5.9
1	A	17	GLN	HG2	0.78	3.67 – 0.97	-5.7

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:

