



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1UWO  
Title : CALCIUM FORM OF HUMAN S100B, NMR, 20 STRUCTURES  
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Deposited on : 1997-12-05

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
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

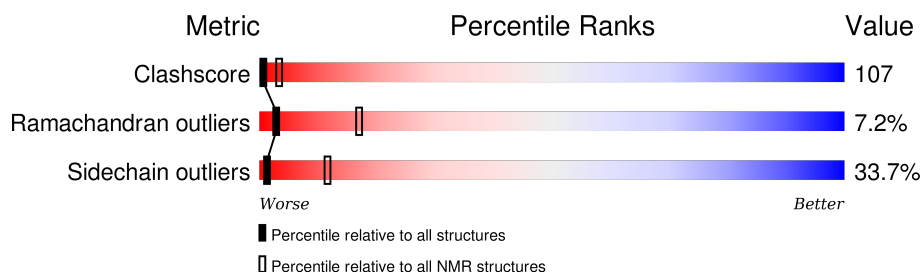
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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  $\geq 3$ , 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	91	
1	B	91	

## 2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 18 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:1-A:41, A:47-A:87, B:1-B:41, B:47-B:87 (164)	0.67	18

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 3 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2876 atoms, of which 1394 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S100B.

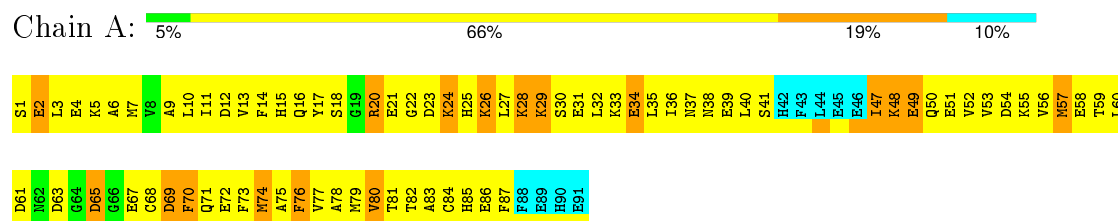
Mol	Chain	Residues	Atoms						Trace
1	A	91	Total	C	H	N	O	S	0
			1438	465	697	118	152	6	
1	B	91	Total	C	H	N	O	S	0
			1438	465	697	118	152	6	

## 4 Residue-property plots [i](#)

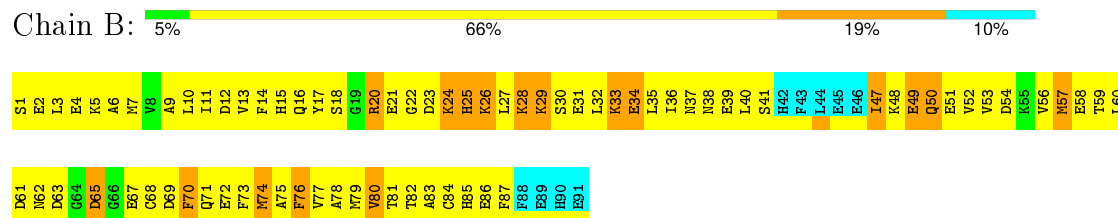
### 4.1 Average score per residue in the NMR ensemble

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: S100B



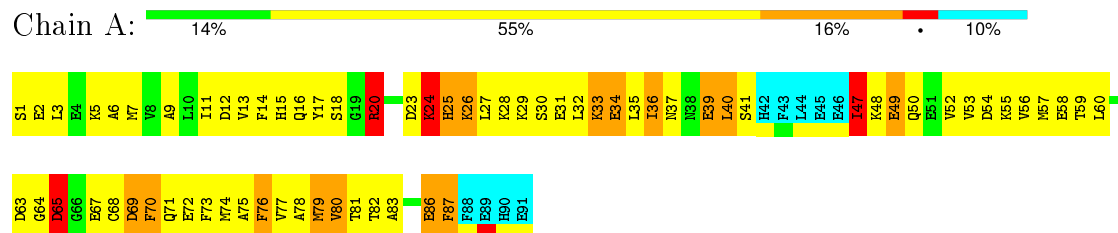
- Molecule 1: S100B



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

The representative model is number 18. Colouring as in section 4.1 above.

- Molecule 1: S100B



- Molecule 1: S100B

D61	N62	D63	G64	D65	G66	E67	C68	D69	F70	Q71	E72	F73	M74	A75	F76	V77	M79	V80	T81	T82	A83	C84	H85	E86	F87	F88	E89	H90	E91
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## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *HYBRID DISTANCE GEOMETRY AND SIMULATED ANNEALING*.

Of the 30 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATIONS*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	

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 5377, BMRB entry 5206
Number of chemical shift lists	3
Total number of shifts	4144
Number of shifts mapped to atoms	4010
Number of unparsed shifts	0
Number of shifts with mapping errors	134
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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.

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	0.9±0.2
1	B	0.0±0.0	1.0±0.0
All	All	0	39

There are no bond-length outliers.

There are no bond-angle outliers.

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	B	20	ARG	Sidechain	20
1	A	20	ARG	Sidechain	19

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	654	633	633	155±16
1	B	654	633	633	159±12
All	All	26160	25314	25320	5522

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 107.

5 of 2423 unique clashes are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:LEU:HD22	1:B:60:LEU:HD12	1.15	1.15	19	3
1:A:75:ALA:HB2	1:B:75:ALA:HB2	1.13	1.16	9	11
1:B:36:ILE:HD12	1:B:53:VAL:HG22	1.09	1.23	11	3
1:A:47:ILE:HD12	1:A:53:VAL:HG23	1.06	1.24	10	3
1:B:17:TYR:CE2	1:B:35:LEU:HD23	1.06	1.86	3	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	81/91 (89%)	58±3 (71±4%)	17±3 (22±3%)	6±2 (7±2%)	3	17
1	B	81/91 (89%)	55±4 (68±4%)	20±3 (25±4%)	6±1 (7±2%)	3	17
All	All	3240/3640 (89%)	2257 (70%)	749 (23%)	234 (7%)	3	17

5 of 39 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	65	ASP	20
1	A	65	ASP	20
1	A	29	LYS	16
1	B	29	LYS	13
1	B	47	ILE	12

### 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	73/82 (89%)	49±3 (68±4%)	24±3 (32±4%)	1	13
1	B	73/82 (89%)	48±4 (65±5%)	26±4 (35±5%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2920/3280 (89%)	1936 (66%)	984 (34%)	<b>1</b> <b>11</b>

5 of 135 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	B	80	VAL	20
1	B	70	PHE	19
1	A	34	GLU	19
1	A	80	VAL	19
1	A	70	PHE	18

### 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

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 88% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5206

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	1896
Number of shifts mapped to atoms	1880
Number of unparsed shifts	0
Number of shifts with mapping errors	16
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. First 5 (of 16) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	1	MET	HG3	2.35	0.02	1
A	1	MET	HG2	2.58	0.02	1
A	1	MET	HB2	2.2	0.02	1
B	1	MET	CG	32.2	0.05	1
B	1	MET	C	175.85	0.05	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	174	$-0.55 \pm 0.19$	Should be applied
$^{13}\text{C}_\beta$	170	$0.29 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	148	$-0.22 \pm 0.07$	None needed ( $< 0.5$ ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{15}\text{N}$	174	0.30 $\pm$ 0.30	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 76%, i.e. 1518 atoms were assigned a chemical shift out of a possible 2000. 28 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	750/820 (91%)	306/328 (93%)	288/328 (88%)	156/164 (95%)
Sidechain	750/1032 (73%)	438/598 (73%)	300/400 (75%)	12/34 (35%)
Aromatic	18/148 (12%)	18/82 (22%)	0/60 (0%)	0/6 (0%)
Overall	1518/2000 (76%)	762/1008 (76%)	588/788 (75%)	168/204 (82%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

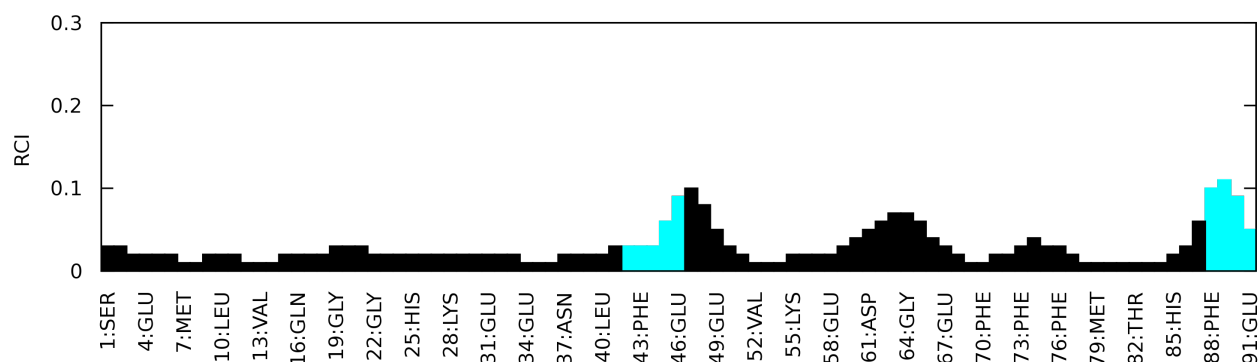
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	18	SER	HB3	2.27	5.25 – 2.45	-5.6
1	B	18	SER	HB3	2.27	5.25 – 2.45	-5.6

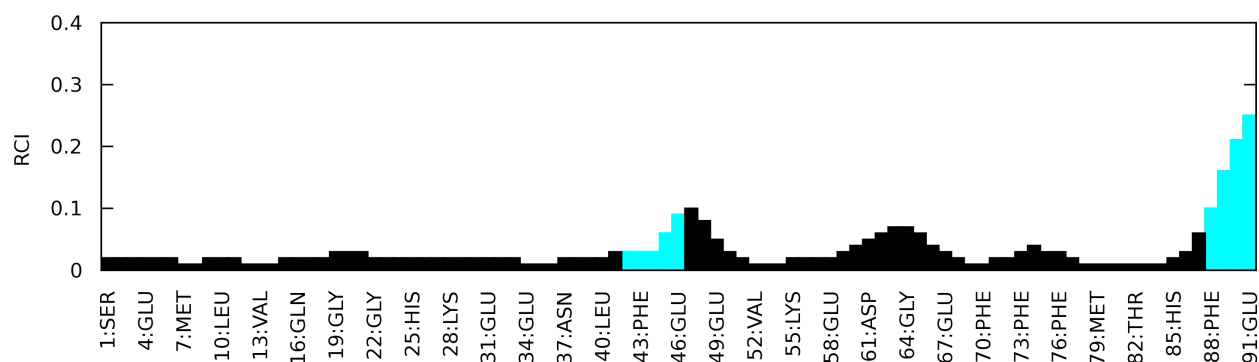
### 7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:



## 7.2 Chemical shift list 2

File name: BMRB entry 5377

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

### 7.2.1 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	2130
Number of shifts mapped to atoms	2130
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

### 7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	182	$-0.66 \pm 0.09$	Should be applied
$^{13}\text{C}_\beta$	174	$0.32 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	160	$-0.48 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	178	$-0.11 \pm 0.20$	None needed ( $< 0.5$ ppm)

### 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 88%, i.e. 1764 atoms were assigned a chemical shift out of a possible 2000. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	792/820 (97%)	324/328 (99%)	308/328 (94%)	160/164 (98%)
Sidechain	886/1032 (86%)	542/598 (91%)	332/400 (83%)	12/34 (35%)
Aromatic	86/148 (58%)	46/82 (56%)	40/60 (67%)	0/6 (0%)
Overall	1764/2000 (88%)	912/1008 (90%)	680/788 (86%)	172/204 (84%)

### 7.2.4 Statistically unusual chemical shifts [i](#)

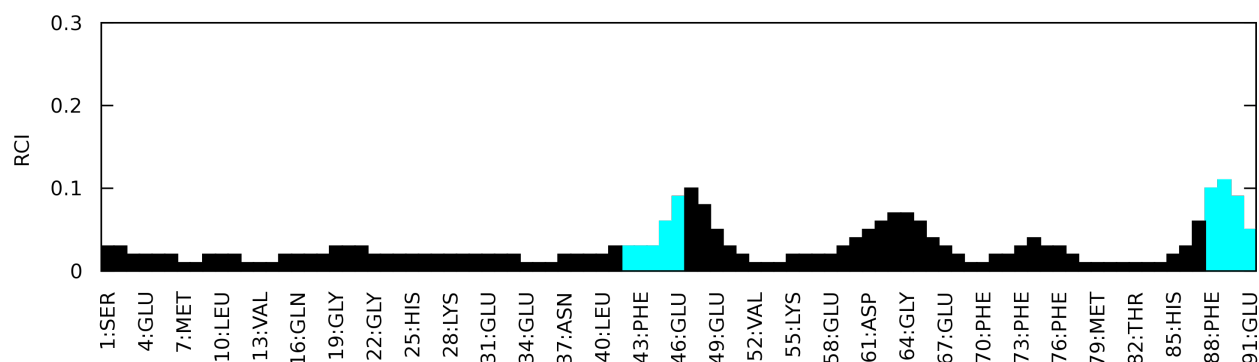
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	18	SER	HB2	2.21	5.18 – 2.58	-6.4
1	B	18	SER	HB2	2.21	5.18 – 2.58	-6.4

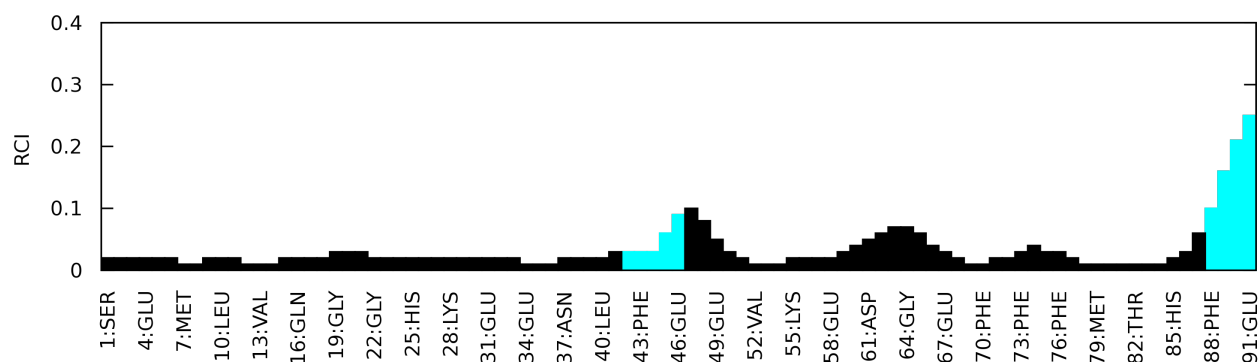
### 7.2.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:



## 7.3 Chemical shift list 3

File name: BMRB entry 5377

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.3.1 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	118
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	118
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.

- Chain not found in structure. First 5 (of 118) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	13	SER	H	8.09	0.01	1
UNMAPPED	3	ARG	HA	4.42	0.01	1
UNMAPPED	9	ASN	CB	42.48	0.2	1
UNMAPPED	10	LYS	HD3	1.65	0.01	1
UNMAPPED	11	ILE	H	7.48	0.01	1

### 7.3.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, <i>ppm</i>	Suggested action
$^{13}\text{C}_\alpha$	4	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	4	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	0	—	—

### 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2000. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/820 (0%)	0/328 (0%)	0/328 (0%)	0/164 (0%)
Sidechain	0/1032 (0%)	0/598 (0%)	0/400 (0%)	0/34 (0%)
Aromatic	0/148 (0%)	0/82 (0%)	0/60 (0%)	0/6 (0%)
Overall	0/2000 (0%)	0/1008 (0%)	0/788 (0%)	0/204 (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, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
???	UNMAPPED	12	LEU	CD2	12.95	32.60 – 15.60	-6.6



### 7.3.5 Random Coil Index (RCI) plots

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.