



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:30 PM BST

PDB ID : 1ZAC  
Title : N-DOMAIN OF TROPONIN C FROM CHICKEN SKELETAL MUSCLE,  
NMR, MINIMIZED AVERAGE STRUCTURE  
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Deposited on : 1998-04-07

This is a Full wwPDB NMR Structure Validation 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

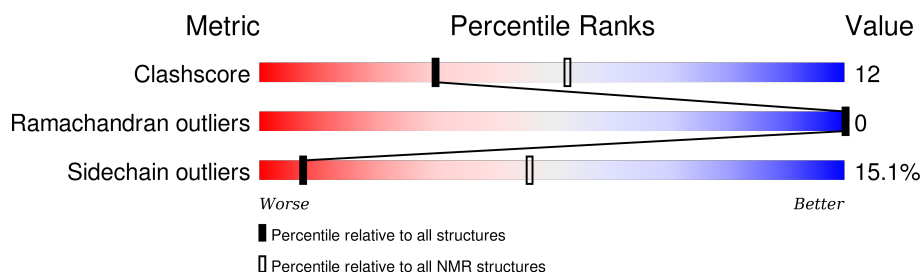
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 71%.

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	90	<div> <div style="width: 68%; background-color: green;"></div> <div style="width: 28%; background-color: yellow;"></div> <div style="width: 4%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: cyan;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>68% 28% .</div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

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

There is only 1 type of molecule in this entry. The entry contains 1347 atoms, of which 654 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TROPONIN-C.

Mol	Chain	Residues	Atoms						Trace
1	A	90	Total	C	H	N	O	S	0
			1347	426	654	108	151	8	

## 4 Residue-property plots

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: TROPONIN-C

Chain A:  68% 28% .



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISGEO,SA*.

Of the 100 calculated structures, 1 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
NMRPIPE	structure solution	
PIPP	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 4232
Number of chemical shift lists	2
Total number of shifts	1213
Number of shifts mapped to atoms	1213
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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	3
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	11	ARG	Sidechain
1	A	84	ARG	Sidechain
1	A	47	ARG	Sidechain

### 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	693	654	654	16
All	All	693	654	654	16

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:11:ARG:HG2	1:A:79:LEU:HD13	0.66	1.68

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:77:GLU:O	1:A:80:VAL:HG22	0.52	2.04
1:A:13:PHE:CD1	1:A:83:VAL:HG22	0.50	2.41
1:A:22:PHE:CD1	1:A:49:LEU:HD22	0.49	2.41
1:A:22:PHE:HB3	1:A:82:MET:HE1	0.49	1.83
1:A:11:ARG:CG	1:A:79:LEU:HD13	0.49	2.36
1:A:10:ALA:O	1:A:83:VAL:HG21	0.48	2.08
1:A:10:ALA:CB	1:A:80:VAL:HG12	0.46	2.41
1:A:11:ARG:HA	1:A:79:LEU:HD22	0.46	1.86
1:A:78:PHE:CE2	1:A:82:MET:SD	0.45	3.09
1:A:22:PHE:HB3	1:A:82:MET:CE	0.43	2.43
1:A:14:LEU:HD22	1:A:18:MET:HG2	0.43	1.91
1:A:29:PHE:CB	1:A:41:GLU:HG2	0.43	2.44
1:A:62:ILE:O	1:A:66:ASP:HB2	0.42	2.14
1:A:25:ALA:HB3	1:A:49:LEU:HD21	0.42	1.92
1:A:73:ILE:CG1	1:A:78:PHE:HB2	0.41	2.44

## 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	88/90 (98%)	87 (99%)	1 (1%)	0 (0%)	100	100
All	All	88/90 (98%)	87 (99%)	1 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	73/73 (100%)	62 (85%)	11 (15%)	7	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	73/73 (100%)	62 (85%)	11 (15%)	7	46

All 11 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	29	PHE
1	A	64	GLU
1	A	81	MET
1	A	48	MET
1	A	18	MET
1	A	51	GLN
1	A	6	GLN
1	A	30	ASP
1	A	86	MET
1	A	66	ASP
1	A	57	GLU

### 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 71% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 4232

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	360
Number of shifts mapped to atoms	360
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	87	$-0.36 \pm 0.24$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	88	$-0.07 \pm 0.28$	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 34%, i.e. 353 atoms were assigned a chemical shift out of a possible 1043. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	353/448 (79%)	178/179 (99%)	87/180 (48%)	88/89 (99%)
Sidechain	0/541 (0%)	0/313 (0%)	0/210 (0%)	0/18 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/54 (0%)	0/30 (0%)	0/24 (0%)	0/0 (—%)
Overall	353/1043 (34%)	178/522 (34%)	87/414 (21%)	88/107 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 34%, i.e. 353 atoms were assigned a chemical shift out of a possible 1043. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	353/448 (79%)	178/179 (99%)	87/180 (48%)	88/89 (99%)
Sidechain	0/541 (0%)	0/313 (0%)	0/210 (0%)	0/18 (0%)
Aromatic	0/54 (0%)	0/30 (0%)	0/24 (0%)	0/0 (—%)
Overall	353/1043 (34%)	178/522 (34%)	87/414 (21%)	88/107 (82%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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	12	ALA	CA	67.10	63.07 – 43.27	7.0

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

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 4232

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

### 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	853
Number of shifts mapped to atoms	853
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	137

### 7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	90	$-11.34 \pm 0.39$	Should be applied
$^{13}\text{C}_\beta$	82	$-10.78 \pm 0.09$	Should be applied
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	88	$-0.28 \pm 0.22$	None needed ( $< 0.5$ ppm)

### 7.2.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 71%, i.e. 745 atoms were assigned a chemical shift out of a possible 1043. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	356/448 (79%)	178/179 (99%)	90/180 (50%)	88/89 (99%)
Sidechain	363/541 (67%)	273/313 (87%)	82/210 (39%)	8/18 (44%)
Aromatic	26/54 (48%)	26/30 (87%)	0/24 (0%)	0/0 (—%)
Overall	745/1043 (71%)	477/522 (91%)	172/414 (42%)	96/107 (90%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 745 atoms were assigned a chemical shift out of a possible 1043. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	356/448 (79%)	178/179 (99%)	90/180 (50%)	88/89 (99%)
Sidechain	363/541 (67%)	273/313 (87%)	82/210 (39%)	8/18 (44%)
Aromatic	26/54 (48%)	26/30 (87%)	0/24 (0%)	0/0 (—%)
Overall	745/1043 (71%)	477/522 (91%)	172/414 (42%)	96/107 (90%)

### 7.2.4 Statistically unusual chemical shifts ⓘ

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	90	ALA	CB	99.00	28.03 – 9.93	44.2
1	A	52	ASN	CB	99.00	47.13 – 30.23	35.7
1	A	52	ASN	CA	99.00	63.05 – 44.05	23.9
1	A	90	ALA	CA	99.00	63.07 – 43.27	23.1
1	A	11	ARG	NE	113.90	92.63 – 76.73	18.4
1	A	47	ARG	NE	113.50	92.63 – 76.73	18.1
1	A	84	ARG	NE	112.20	92.63 – 76.73	17.3
1	A	12	ALA	CA	78.10	63.07 – 43.27	12.6
1	A	60	ALA	CB	41.60	28.03 – 9.93	12.5
1	A	4	THR	CB	51.11	78.10 – 61.30	-11.1
1	A	43	GLY	CA	58.98	51.81 – 38.91	10.6
1	A	8	ALA	CA	72.76	63.07 – 43.27	9.9
1	A	69	GLY	CA	58.00	51.81 – 38.91	9.8
1	A	33	GLY	CA	57.82	51.81 – 38.91	9.7
1	A	1	ALA	CB	36.13	28.03 – 9.93	9.5
1	A	20	ALA	CA	71.14	63.07 – 43.27	9.1
1	A	50	GLY	CA	56.94	51.81 – 38.91	9.0
1	A	71	GLY	CA	56.84	51.81 – 38.91	8.9
1	A	53	PRO	CB	42.43	37.79 – 25.89	8.9
1	A	34	GLY	CA	56.81	51.81 – 38.91	8.9
1	A	35	GLY	CA	56.52	51.81 – 38.91	8.7
1	A	36	ASP	CB	54.62	49.06 – 32.66	8.4
1	A	15	SER	CA	76.07	69.25 – 48.25	8.2
1	A	1	ALA	CA	68.71	63.07 – 43.27	7.8
1	A	2	SER	CA	75.18	69.25 – 48.25	7.8
1	A	70	SER	CA	74.88	69.25 – 48.25	7.7
1	A	38	SER	CA	74.86	69.25 – 48.25	7.7
1	A	74	ASP	CB	53.42	49.06 – 32.66	7.7
1	A	54	THR	CA	82.16	75.37 – 49.07	7.6
1	A	46	MET	CA	72.49	67.38 – 44.88	7.3
1	A	14	LEU	CB	55.77	51.69 – 32.89	7.2

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	73	ILE	CB	53.20	48.82 – 28.42	7.1
1	A	37	ILE	CB	53.00	48.82 – 28.42	7.0
1	A	32	ASP	CB	52.23	49.06 – 32.66	6.9
1	A	89	ASP	CB	52.12	49.06 – 32.66	6.9
1	A	10	ALA	CA	66.70	63.07 – 43.27	6.8
1	A	59	ASP	CA	68.47	64.88 – 44.48	6.8
1	A	56	GLU	CA	71.52	67.86 – 46.86	6.7
1	A	17	GLU	CB	41.38	38.65 – 21.35	6.6
1	A	17	GLU	CA	71.12	67.86 – 46.86	6.6
1	A	5	ASP	CA	67.98	64.88 – 44.48	6.5
1	A	60	ALA	CA	66.03	63.07 – 43.27	6.5
1	A	16	GLU	CA	70.99	67.86 – 46.86	6.5
1	A	53	PRO	CA	73.44	71.13 – 55.53	6.5
1	A	27	ASP	CA	67.89	64.88 – 44.48	6.5
1	A	64	GLU	CB	41.20	38.65 – 21.35	6.5
1	A	88	GLU	CB	41.12	38.65 – 21.35	6.4
1	A	51	GLN	CB	40.98	38.36 – 19.96	6.4
1	A	55	LYS	CA	71.10	67.97 – 45.97	6.4
1	A	87	LYS	CB	44.21	41.68 – 23.88	6.4
1	A	68	ASP	CB	51.39	49.06 – 32.66	6.4
1	A	66	ASP	CB	51.38	49.06 – 32.66	6.4
1	A	25	ALA	CA	65.87	63.07 – 43.27	6.4
1	A	79	LEU	CA	69.38	66.36 – 44.96	6.4
1	A	42	LEU	CA	69.37	66.36 – 44.96	6.4
1	A	24	ALA	CA	65.85	63.07 – 43.27	6.4
1	A	77	GLU	CB	41.05	38.65 – 21.35	6.4
1	A	31	ALA	CA	65.77	63.07 – 43.27	6.4
1	A	67	GLU	CB	40.99	38.65 – 21.35	6.4
1	A	21	GLU	CA	70.59	67.86 – 46.86	6.3
1	A	57	GLU	CB	40.87	38.65 – 21.35	6.3
1	A	27	ASP	CB	51.14	49.06 – 32.66	6.3
1	A	30	ASP	CB	50.99	49.06 – 32.66	6.2
1	A	48	MET	CA	70.02	67.38 – 44.88	6.2
1	A	25	ALA	CB	30.14	28.03 – 9.93	6.2
1	A	63	GLU	CB	40.66	38.65 – 21.35	6.2
1	A	31	ALA	CB	30.12	28.03 – 9.93	6.2
1	A	9	GLU	CB	40.62	38.65 – 21.35	6.1
1	A	67	GLU	CA	70.25	67.86 – 46.86	6.1
1	A	58	LEU	CA	68.79	66.36 – 44.96	6.1
1	A	5	ASP	CB	50.92	49.06 – 32.66	6.1
1	A	7	GLN	CA	69.63	67.31 – 45.91	6.1
1	A	65	VAL	CB	43.68	41.76 – 23.66	6.1

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	19	ILE	CA	77.93	75.08 – 48.18	6.1
1	A	21	GLU	CB	40.46	38.65 – 21.35	6.0
1	A	84	ARG	CA	70.69	68.35 – 45.25	6.0
1	A	18	MET	CA	69.64	67.38 – 44.88	6.0
1	A	6	GLN	CA	69.43	67.31 – 45.91	6.0
1	A	59	ASP	CB	50.67	49.06 – 32.66	6.0
1	A	77	GLU	CA	69.92	67.86 – 46.86	6.0
1	A	9	GLU	CA	69.91	67.86 – 46.86	6.0
1	A	57	GLU	CA	69.90	67.86 – 46.86	6.0
1	A	63	GLU	CA	69.89	67.86 – 46.86	6.0
1	A	16	GLU	CB	40.31	38.65 – 21.35	6.0
1	A	42	LEU	CB	53.48	51.69 – 32.89	6.0
1	A	26	PHE	CA	73.43	70.99 – 45.29	5.9
1	A	23	LYS	CB	43.35	41.68 – 23.88	5.9
1	A	76	GLU	CA	69.81	67.86 – 46.86	5.9
1	A	55	LYS	CB	43.29	41.68 – 23.88	5.9
1	A	11	ARG	CA	70.42	68.35 – 45.25	5.9
1	A	40	LYS	CB	43.26	41.68 – 23.88	5.9
1	A	49	LEU	CB	53.29	51.69 – 32.89	5.9
1	A	64	GLU	CA	69.64	67.86 – 46.86	5.8
1	A	41	GLU	CB	40.06	38.65 – 21.35	5.8
1	A	26	PHE	CB	52.04	50.37 – 29.47	5.8
1	A	62	ILE	CA	77.22	75.08 – 48.18	5.8
1	A	81	MET	CA	69.13	67.38 – 44.88	5.8
1	A	28	MET	CA	69.11	67.38 – 44.88	5.8
1	A	12	ALA	CB	29.42	28.03 – 9.93	5.8
1	A	23	LYS	CA	69.65	67.97 – 45.97	5.8
1	A	44	THR	CB	79.38	78.10 – 61.30	5.8
1	A	86	MET	CB	45.88	44.20 – 21.80	5.8
1	A	86	MET	CA	69.05	67.38 – 44.88	5.7
1	A	11	ARG	CB	41.16	39.81 – 21.51	5.7
1	A	84	ARG	CB	41.12	39.81 – 21.51	5.7
1	A	13	PHE	CB	51.86	50.37 – 29.47	5.7
1	A	56	GLU	CB	39.78	38.65 – 21.35	5.7
1	A	44	THR	CA	77.08	75.37 – 49.07	5.7
1	A	40	LYS	CA	69.39	67.97 – 45.97	5.6
1	A	10	ALA	CB	29.18	28.03 – 9.93	5.6
1	A	85	GLN	CB	39.45	38.36 – 19.96	5.6
1	A	85	GLN	CA	68.43	67.31 – 45.91	5.5
1	A	83	VAL	CA	78.44	76.93 – 48.03	5.5
1	A	61	ILE	CA	76.45	75.08 – 48.18	5.5
1	A	80	VAL	CB	42.66	41.76 – 23.66	5.5

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	58	LEU	CB	52.61	51.69 – 32.89	5.5
1	A	75	PHE	CA	72.23	70.99 – 45.29	5.5
1	A	76	GLU	CB	39.48	38.65 – 21.35	5.5
1	A	61	ILE	CB	49.73	48.82 – 28.42	5.4
1	A	45	VAL	CB	42.54	41.76 – 23.66	5.4
1	A	8	ALA	CB	28.81	28.03 – 9.93	5.4
1	A	20	ALA	CB	28.75	28.03 – 9.93	5.4
1	A	87	LYS	CA	68.84	67.97 – 45.97	5.4
1	A	79	LEU	CB	52.42	51.69 – 32.89	5.4
1	A	24	ALA	CB	28.73	28.03 – 9.93	5.4
1	A	83	VAL	CB	42.30	41.76 – 23.66	5.3
1	A	39	THR	CA	76.09	75.37 – 49.07	5.3
1	A	89	ASP	CA	65.31	64.88 – 44.48	5.2
1	A	70	SER	CB	71.51	71.24 – 56.34	5.2
1	A	39	THR	CB	78.39	78.10 – 61.30	5.2
1	A	7	GLN	CB	38.53	38.36 – 19.96	5.1
1	A	47	ARG	CB	39.96	39.81 – 21.51	5.1
1	A	3	MET	CA	67.54	67.38 – 44.88	5.1
1	A	6	GLN	CB	38.49	38.36 – 19.96	5.1
1	A	62	ILE	CB	48.96	48.82 – 28.42	5.1
1	A	45	VAL	CA	77.12	76.93 – 48.03	5.1
1	A	19	ILE	CB	48.90	48.82 – 28.42	5.0

### 7.2.5 Random Coil Index (RCI) plots

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:

