



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:05 am BST

PDB ID : 2N1L  
Title : Solution structure of the BCOR PUFD  
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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

<https://www.wwpdb.org/validation/2017/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  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

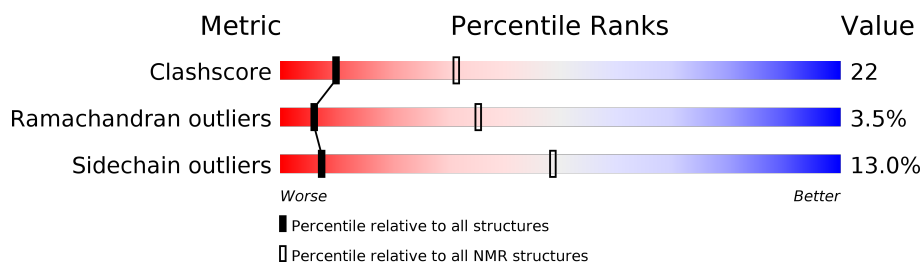
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 99%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	115	

## 2 Ensemble composition and analysis ⓘ

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1838 atoms, of which 911 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BCL-6 corepressor.

Mol	Chain	Residues	Atoms						Trace
1	A	115	Total	C	H	N	O	S	0
			1838	597	911	146	183	1	

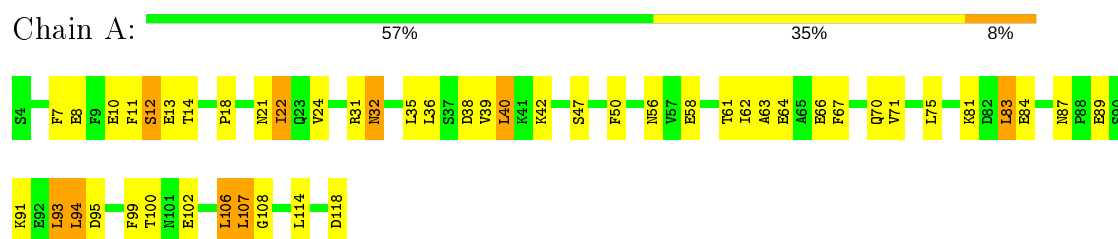
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	CYS	CONFLICT	UNP Q6W2J9
A	52	SER	CYS	CONFLICT	UNP Q6W2J9
A	79	SER	CYS	CONFLICT	UNP Q6W2J9

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

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: BCL-6 corepressor



## 5 Refinement protocol and experimental data overview

Of the 10 calculated structures, 1 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
ARIA	structure solution	
ARIA	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1652
Number of shifts mapped to atoms	1652
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	99%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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 ⓘ

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	927	911	909	40
All	All	927	911	909	40

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 22.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:94:LEU:HD22	1:A:94:LEU:N	0.67	2.04
1:A:106:LEU:HD23	1:A:118:ASP:H	0.66	1.50
1:A:62:ILE:O	1:A:94:LEU:HD23	0.64	1.92
1:A:107:LEU:HD13	1:A:108:GLY:N	0.62	2.09
1:A:21:ASN:HB3	1:A:32:ASN:ND2	0.60	2.10
1:A:22:ILE:N	1:A:22:ILE:HD12	0.60	2.11
1:A:36:LEU:HB3	1:A:95:ASP:CB	0.58	2.29
1:A:67:PHE:O	1:A:71:VAL:HG23	0.57	2.00
1:A:94:LEU:CD2	1:A:94:LEU:N	0.57	2.68
1:A:7:PHE:CD1	1:A:100:THR:HA	0.55	2.37
1:A:62:ILE:HD13	1:A:66:GLU:HB2	0.54	1.78
1:A:36:LEU:HB3	1:A:95:ASP:HB3	0.53	1.78
1:A:7:PHE:O	1:A:8:GLU:HG2	0.53	2.03
1:A:63:ALA:O	1:A:66:GLU:HB2	0.51	2.06
1:A:36:LEU:O	1:A:40:LEU:HB2	0.51	2.06

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:12:SER:O	1:A:14:THR:HG23	0.49	2.07
1:A:21:ASN:ND2	1:A:22:ILE:H	0.49	2.05
1:A:87:ASN:OD1	1:A:89:GLU:HG2	0.49	2.08
1:A:81:LYS:HA	1:A:81:LYS:HE2	0.49	1.84
1:A:62:ILE:HD12	1:A:94:LEU:CD2	0.49	2.37
1:A:91:LYS:C	1:A:93:LEU:H	0.48	2.12
1:A:24:VAL:HG11	1:A:31:ARG:HB2	0.48	1.85
1:A:24:VAL:HG11	1:A:31:ARG:CD	0.48	2.39
1:A:102:GLU:O	1:A:106:LEU:HB2	0.47	2.09
1:A:24:VAL:HG11	1:A:31:ARG:HD3	0.47	1.87
1:A:40:LEU:HD21	1:A:50:PHE:HB2	0.47	1.86
1:A:36:LEU:HA	1:A:39:VAL:CG2	0.46	2.40
1:A:36:LEU:HA	1:A:39:VAL:HG22	0.46	1.87
1:A:39:VAL:O	1:A:42:LYS:HB2	0.43	2.13
1:A:35:LEU:HA	1:A:95:ASP:O	0.43	2.13
1:A:38:ASP:O	1:A:42:LYS:HG3	0.43	2.13
1:A:12:SER:C	1:A:14:THR:HG23	0.42	2.35
1:A:81:LYS:C	1:A:83:LEU:N	0.42	2.73
1:A:40:LEU:CD1	1:A:47:SER:HA	0.42	2.45
1:A:8:GLU:HG3	1:A:10:GLU:H	0.41	1.75
1:A:62:ILE:HD11	1:A:67:PHE:HB2	0.41	1.89
1:A:64:GLU:HA	1:A:94:LEU:HD21	0.41	1.92
1:A:63:ALA:HA	1:A:93:LEU:CD2	0.41	2.46
1:A:81:LYS:O	1:A:84:GLU:HG3	0.41	2.14
1:A:71:VAL:O	1:A:75:LEU:HG	0.41	2.16

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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	113/115 (98%)	89 (79%)	20 (18%)	4 (4%)	6	35
All	All	113/115 (98%)	89 (79%)	20 (18%)	4 (4%)	6	35

All 4 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.



Mol	Chain	Res	Type
1	A	93	LEU
1	A	13	GLU
1	A	11	PHE
1	A	18	PRO

### 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	108/108 (100%)	94 (87%)	14 (13%)	7	48
All	All	108/108 (100%)	94 (87%)	14 (13%)	7	48

All 14 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	40	LEU
1	A	114	LEU
1	A	83	LEU
1	A	32	ASN
1	A	94	LEU
1	A	61	THR
1	A	56	ASN
1	A	58	GLU
1	A	22	ILE
1	A	107	LEU
1	A	99	PHE
1	A	70	GLN
1	A	106	LEU
1	A	12	SER

### 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 99% for the well-defined parts and 99% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

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	1652
Number of shifts mapped to atoms	1652
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	414

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	115	$0.00 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	113	$-0.11 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	115	$0.03 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	115	$0.24 \pm 0.27$	None needed ( $< 0.5$ ppm)

#### 7.1.3 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 99%, i.e. 1428 atoms were assigned a chemical shift out of a possible 1439. 25 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	562/563 (100%)	223/224 (100%)	230/230 (100%)	109/109 (100%)
Sidechain	738/747 (99%)	433/438 (99%)	278/282 (99%)	27/27 (100%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	128/129 (99%)	68/69 (99%)	56/56 (100%)	4/4 (100%)
Overall	1428/1439 (99%)	724/731 (99%)	564/568 (99%)	140/140 (100%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 99%, i.e. 1428 atoms were assigned a chemical shift out of a possible 1439. 25 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	562/563 (100%)	223/224 (100%)	230/230 (100%)	109/109 (100%)
Sidechain	738/747 (99%)	433/438 (99%)	278/282 (99%)	27/27 (100%)
Aromatic	128/129 (99%)	68/69 (99%)	56/56 (100%)	4/4 (100%)
Overall	1428/1439 (99%)	724/731 (99%)	564/568 (99%)	140/140 (100%)

#### 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	42	LYS	HE3	1000.00	3.86 – 1.96	5247.8
1	A	41	LYS	HE3	1000.00	3.86 – 1.96	5247.8
1	A	44	LYS	HE3	1000.00	3.86 – 1.96	5247.8
1	A	44	LYS	HE2	1000.00	3.87 – 1.97	5247.8
1	A	41	LYS	HE2	1000.00	3.87 – 1.97	5247.8
1	A	92	GLU	HG3	1000.00	3.31 – 1.21	4751.1
1	A	98	GLU	HG3	1000.00	3.31 – 1.21	4751.1
1	A	13	GLU	HG3	1000.00	3.31 – 1.21	4751.1
1	A	10	GLU	HG3	1000.00	3.31 – 1.21	4751.1
1	A	10	GLU	HG2	1000.00	3.33 – 1.23	4751.0
1	A	98	GLU	HG2	1000.00	3.33 – 1.23	4751.0
1	A	92	GLU	HG2	1000.00	3.33 – 1.23	4751.0
1	A	41	LYS	HD3	1000.00	2.75 – 0.45	4340.9
1	A	44	LYS	HD3	1000.00	2.75 – 0.45	4340.9
1	A	42	LYS	HD3	1000.00	2.75 – 0.45	4340.9
1	A	44	LYS	HD2	1000.00	2.76 – 0.46	4340.8
1	A	41	LYS	HD2	1000.00	2.76 – 0.46	4340.8
1	A	42	LYS	HD2	1000.00	2.76 – 0.46	4340.8
1	A	51	ARG	HD2	1000.00	4.27 – 1.97	4334.3
1	A	68	TYR	HE1	1000.00	7.86 – 5.56	4318.6
1	A	20	TYR	HE2	1000.00	7.86 – 5.56	4318.6
1	A	68	TYR	HE2	1000.00	7.86 – 5.56	4318.6

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	20	TYR	HE1	1000.00	7.86 – 5.56	4318.6
1	A	51	ARG	HD3	1000.00	4.36 – 1.86	3987.6
1	A	42	LYS	HG2	1000.00	2.67 – 0.07	3840.9
1	A	41	LYS	HG2	1000.00	2.67 – 0.07	3840.9
1	A	44	LYS	HG2	1000.00	2.67 – 0.07	3840.9
1	A	90	SER	HB2	1000.00	5.18 – 2.58	3831.2
1	A	80	SER	HB2	1000.00	5.18 – 2.58	3831.2
1	A	110	SER	HB2	1000.00	5.18 – 2.58	3831.2
1	A	79	SER	HB2	1000.00	5.18 – 2.58	3831.2
1	A	47	SER	HB2	1000.00	5.18 – 2.58	3831.2
1	A	78	SER	HB2	1000.00	5.18 – 2.58	3831.2
1	A	48	ARG	HG2	1000.00	2.92 – 0.22	3697.9
1	A	104	GLN	HG2	1000.00	3.67 – 0.97	3695.1
1	A	76	LEU	HD22	1000.00	2.14 – -0.66	3568.8
1	A	76	LEU	HD23	1000.00	2.14 – -0.66	3568.8
1	A	76	LEU	HD21	1000.00	2.14 – -0.66	3568.8
1	A	76	LEU	HD13	1000.00	2.16 – -0.64	3568.7
1	A	76	LEU	HD12	1000.00	2.16 – -0.64	3568.7
1	A	75	LEU	HD11	1000.00	2.16 – -0.64	3568.7
1	A	76	LEU	HD11	1000.00	2.16 – -0.64	3568.7
1	A	75	LEU	HD12	1000.00	2.16 – -0.64	3568.7
1	A	75	LEU	HD13	1000.00	2.16 – -0.64	3568.7
1	A	42	LYS	HG3	1000.00	2.76 – -0.04	3566.6
1	A	44	LYS	HG3	1000.00	2.76 – -0.04	3566.6
1	A	41	LYS	HG3	1000.00	2.76 – -0.04	3566.6
1	A	110	SER	HB3	1000.00	5.25 – 2.45	3557.7
1	A	80	SER	HB3	1000.00	5.25 – 2.45	3557.7
1	A	47	SER	HB3	1000.00	5.25 – 2.45	3557.7
1	A	78	SER	HB3	1000.00	5.25 – 2.45	3557.7
1	A	79	SER	HB3	1000.00	5.25 – 2.45	3557.7
1	A	90	SER	HB3	1000.00	5.25 – 2.45	3557.7
1	A	48	ARG	HG3	1000.00	3.00 – 0.10	3442.9
1	A	51	ARG	HG3	1000.00	3.00 – 0.10	3442.9
1	A	28	GLN	HG3	1000.00	3.75 – 0.85	3440.3
1	A	104	GLN	HG3	1000.00	3.75 – 0.85	3440.3
1	A	20	TYR	HD1	1000.00	8.44 – 5.44	3310.2
1	A	20	TYR	HD2	1000.00	8.44 – 5.44	3310.2
1	A	50	PHE	HD1	1000.00	8.56 – 5.56	3309.8
1	A	11	PHE	HD1	1000.00	8.56 – 5.56	3309.8
1	A	50	PHE	HD2	1000.00	8.56 – 5.56	3309.8
1	A	77	PHE	HD1	1000.00	8.56 – 5.56	3309.8
1	A	67	PHE	HD2	1000.00	8.56 – 5.56	3309.8

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	9	PHE	HD1	1000.00	8.56 – 5.56	3309.8
1	A	9	PHE	HD2	1000.00	8.56 – 5.56	3309.8
1	A	7	PHE	HD2	1000.00	8.56 – 5.56	3309.8
1	A	11	PHE	HD2	1000.00	8.56 – 5.56	3309.8
1	A	7	PHE	HD1	1000.00	8.56 – 5.56	3309.8
1	A	77	PHE	HD2	1000.00	8.56 – 5.56	3309.8
1	A	67	PHE	HD1	1000.00	8.56 – 5.56	3309.8
1	A	116	PRO	HG2	1000.00	3.48 – 0.38	3219.6
1	A	18	PRO	HG2	1000.00	3.48 – 0.38	3219.6
1	A	30	PRO	HG2	1000.00	3.48 – 0.38	3219.6
1	A	101	ASN	HB2	1000.00	4.36 – 1.26	3216.7
1	A	7	PHE	HE2	1000.00	8.69 – 5.49	3102.8
1	A	11	PHE	HE1	1000.00	8.69 – 5.49	3102.8
1	A	77	PHE	HE2	1000.00	8.69 – 5.49	3102.8
1	A	67	PHE	HE2	1000.00	8.69 – 5.49	3102.8
1	A	50	PHE	HE2	1000.00	8.69 – 5.49	3102.8
1	A	99	PHE	HE2	1000.00	8.69 – 5.49	3102.8
1	A	9	PHE	HE1	1000.00	8.69 – 5.49	3102.8
1	A	50	PHE	HE1	1000.00	8.69 – 5.49	3102.8
1	A	11	PHE	HE2	1000.00	8.69 – 5.49	3102.8
1	A	77	PHE	HE1	1000.00	8.69 – 5.49	3102.8
1	A	67	PHE	HE1	1000.00	8.69 – 5.49	3102.8
1	A	99	PHE	HE1	1000.00	8.69 – 5.49	3102.8
1	A	7	PHE	HE1	1000.00	8.69 – 5.49	3102.8
1	A	9	PHE	HE2	1000.00	8.69 – 5.49	3102.8
1	A	113	TRP	HZ2	1000.00	8.89 – 5.69	3102.2
1	A	33	TRP	HZ2	1000.00	8.89 – 5.69	3102.2
1	A	35	LEU	HG	1000.00	3.16 – -0.14	3025.7
1	A	107	LEU	HG	1000.00	3.16 – -0.14	3025.7
1	A	75	LEU	HG	1000.00	3.16 – -0.14	3025.7
1	A	93	LEU	HG	1000.00	3.16 – -0.14	3025.7
1	A	114	LEU	HG	1000.00	3.16 – -0.14	3025.7
1	A	16	LEU	HG	1000.00	3.16 – -0.14	3025.7
1	A	76	LEU	HG	1000.00	3.16 – -0.14	3025.7
1	A	15	PRO	HG3	1000.00	3.56 – 0.26	3024.5
1	A	30	PRO	HG3	1000.00	3.56 – 0.26	3024.5
1	A	18	PRO	HG3	1000.00	3.56 – 0.26	3024.5
1	A	116	PRO	HG3	1000.00	3.56 – 0.26	3024.5
1	A	101	ASN	HB3	1000.00	4.41 – 1.11	3021.9
1	A	45	MET	HG2	1000.00	4.23 – 0.63	2771.0
1	A	115	HIS	HB2	1000.00	4.91 – 1.31	2769.1
1	A	30	PRO	HD2	1000.00	5.45 – 1.85	2767.6

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	113	TRP	HD1	1000.00	8.95 – 5.35	2757.9
1	A	33	TRP	HD1	1000.00	8.95 – 5.35	2757.9
1	A	77	PHE	HB2	1000.00	4.85 – 1.15	2694.6
1	A	101	ASN	HA	1000.00	6.52 – 2.82	2690.1
1	A	45	MET	HG3	1000.00	4.30 – 0.50	2625.3
1	A	77	PHE	HB3	1000.00	4.85 – 1.05	2623.8
1	A	30	PRO	HD3	1000.00	5.52 – 1.72	2622.1
1	A	115	HIS	HB3	1000.00	5.00 – 1.10	2556.3
1	A	113	TRP	HH2	1000.00	8.94 – 5.04	2546.2
1	A	33	TRP	HH2	1000.00	8.94 – 5.04	2546.2
1	A	69	ARG	HH22	1000.00	8.76 – 4.76	2483.1
1	A	51	ARG	HH22	1000.00	8.76 – 4.76	2483.1
1	A	31	ARG	HH22	1000.00	8.76 – 4.76	2483.1
1	A	48	ARG	HH22	1000.00	8.76 – 4.76	2483.1
1	A	113	TRP	HZ3	1000.00	8.87 – 4.87	2482.8
1	A	33	TRP	HZ3	1000.00	8.87 – 4.87	2482.8
1	A	33	TRP	HE3	1000.00	9.33 – 5.33	2481.7
1	A	113	TRP	HE3	1000.00	9.33 – 5.33	2481.7
1	A	80	SER	HA	1000.00	6.53 – 2.43	2428.1
1	A	47	SER	HA	1000.00	6.53 – 2.43	2428.1
1	A	78	SER	HA	1000.00	6.53 – 2.43	2428.1
1	A	110	SER	HA	1000.00	6.53 – 2.43	2428.1
1	A	79	SER	HA	1000.00	6.53 – 2.43	2428.1
1	A	51	ARG	HH12	1000.00	8.94 – 4.74	2364.7
1	A	69	ARG	HH12	1000.00	8.94 – 4.74	2364.7
1	A	48	ARG	HH12	1000.00	8.94 – 4.74	2364.7
1	A	31	ARG	HH12	1000.00	8.94 – 4.74	2364.7
1	A	50	PHE	HZ	1000.00	9.11 – 4.91	2364.3
1	A	99	PHE	HZ	1000.00	9.11 – 4.91	2364.3
1	A	7	PHE	HZ	1000.00	9.11 – 4.91	2364.3
1	A	67	PHE	HZ	1000.00	9.11 – 4.91	2364.3
1	A	77	PHE	HZ	1000.00	9.11 – 4.91	2364.3
1	A	9	PHE	HZ	1000.00	9.11 – 4.91	2364.3
1	A	11	PHE	HZ	1000.00	9.11 – 4.91	2364.3
1	A	54	PHE	HZ	1000.00	9.11 – 4.91	2364.3
1	A	86	PHE	HZ	1000.00	9.11 – 4.91	2364.3
1	A	115	HIS	HA	1000.00	6.81 – 2.41	2262.2
1	A	48	ARG	HH21	1000.00	9.06 – 4.56	2207.1
1	A	69	ARG	HH21	1000.00	9.06 – 4.56	2207.1
1	A	31	ARG	HH21	1000.00	9.06 – 4.56	2207.1
1	A	51	ARG	HH21	1000.00	9.06 – 4.56	2207.1
1	A	104	GLN	HE22	1000.00	9.27 – 4.77	2206.6

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	115	HIS	HD2	1000.00	9.28 – 4.78	2206.6
1	A	69	ARG	HH11	1000.00	9.21 – 4.61	2158.9
1	A	48	ARG	HH11	1000.00	9.21 – 4.61	2158.9
1	A	31	ARG	HH11	1000.00	9.21 – 4.61	2158.9
1	A	51	ARG	HH11	1000.00	9.21 – 4.61	2158.9
1	A	45	MET	HE1	1000.00	4.28 – -0.52	2079.4
1	A	45	MET	HE2	1000.00	4.28 – -0.52	2079.4
1	A	45	MET	HE3	1000.00	4.28 – -0.52	2079.4
1	A	87	ASN	HD21	1000.00	9.74 – 4.94	2068.0
1	A	101	ASN	HD21	1000.00	9.74 – 4.94	2068.0
1	A	101	ASN	HD22	1000.00	9.59 – 4.69	2026.2
1	A	87	ASN	HD22	1000.00	9.59 – 4.69	2026.2
1	A	115	HIS	HE1	1000.00	10.53 – 5.43	1945.1
1	A	113	TRP	HE1	1000.00	12.85 – 7.35	1799.8
1	A	33	TRP	HE1	1000.00	12.85 – 7.35	1799.8
1	A	79	SER	H	1000.00	11.23 – 5.33	1680.9
1	A	110	SER	H	1000.00	11.23 – 5.33	1680.9
1	A	80	SER	H	1000.00	11.23 – 5.33	1680.9
1	A	4	SER	H1	1000.00	11.23 – 5.33	1680.9
1	A	78	SER	H	999.99	11.23 – 5.33	1680.9
1	A	47	SER	H	999.99	11.23 – 5.33	1680.9
1	A	102	GLU	H	1000.00	11.34 – 5.34	1652.8
1	A	91	LYS	H	1000.00	11.24 – 5.14	1625.9
1	A	81	LYS	H	1000.00	11.24 – 5.14	1625.9
1	A	48	ARG	H	1000.00	11.29 – 5.19	1625.8
1	A	69	ARG	HE	1000.00	10.48 – 4.28	1601.0
1	A	48	ARG	HE	1000.00	10.48 – 4.28	1601.0
1	A	51	ARG	HE	1000.00	10.48 – 4.28	1601.0
1	A	31	ARG	HE	1000.00	10.48 – 4.28	1601.0
1	A	101	ASN	H	1000.00	11.45 – 5.25	1599.4
1	A	42	LYS	HZ2	1000.00	10.62 – 4.22	1550.9
1	A	81	LYS	HZ1	1000.00	10.62 – 4.22	1550.9
1	A	42	LYS	HZ3	1000.00	10.62 – 4.22	1550.9
1	A	41	LYS	HZ1	1000.00	10.62 – 4.22	1550.9
1	A	44	LYS	HZ1	1000.00	10.62 – 4.22	1550.9
1	A	91	LYS	HZ2	1000.00	10.62 – 4.22	1550.9
1	A	81	LYS	HZ3	1000.00	10.62 – 4.22	1550.9
1	A	42	LYS	HZ1	1000.00	10.62 – 4.22	1550.9
1	A	44	LYS	HZ2	1000.00	10.62 – 4.22	1550.9
1	A	91	LYS	HZ3	1000.00	10.62 – 4.22	1550.9
1	A	41	LYS	HZ3	1000.00	10.62 – 4.22	1550.9
1	A	81	LYS	HZ2	1000.00	10.62 – 4.22	1550.9

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	44	LYS	HZ3	1000.00	10.62 – 4.22	1550.9
1	A	41	LYS	HZ2	1000.00	10.62 – 4.22	1550.9
1	A	91	LYS	HZ1	1000.00	10.62 – 4.22	1550.9
1	A	26	VAL	H	1000.00	11.69 – 4.89	1458.4
1	A	111	VAL	H	1000.00	11.69 – 4.89	1458.4
1	A	80	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	52	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	46	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	25	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	47	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	37	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	90	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	110	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	78	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	12	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	79	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	117	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	72	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	109	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	19	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	4	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	74	SER	HG	1000.00	10.51 – 0.11	956.4
1	A	40	LEU	CG	1000.00	32.55 – 21.05	846.3
1	A	75	LEU	CG	1000.00	32.55 – 21.05	846.3
1	A	34	LEU	CG	1000.00	32.55 – 21.05	846.3
1	A	107	LEU	CG	1000.00	32.55 – 21.05	846.3
1	A	43	LEU	CG	1000.00	32.55 – 21.05	846.3
1	A	44	LYS	CD	1000.00	34.86 – 23.06	822.9
1	A	86	PHE	CD2	1000.00	137.34 – 125.84	755.1
1	A	99	PHE	CD2	1000.00	137.34 – 125.84	755.1
1	A	9	PHE	CD2	1000.00	137.34 – 125.84	755.1
1	A	50	PHE	CD2	1000.00	137.34 – 125.84	755.1
1	A	67	PHE	CD2	1000.00	137.34 – 125.84	755.1
1	A	7	PHE	CD2	1000.00	137.34 – 125.84	755.1
1	A	54	PHE	CD2	1000.00	137.34 – 125.84	755.1
1	A	77	PHE	CD2	1000.00	137.34 – 125.84	755.1
1	A	11	PHE	CD2	1000.00	137.34 – 125.84	755.1
1	A	9	PHE	CE2	1000.00	136.81 – 124.71	718.4
1	A	11	PHE	CE2	1000.00	136.81 – 124.71	718.4
1	A	50	PHE	CE2	1000.00	136.81 – 124.71	718.4
1	A	7	PHE	CE2	1000.00	136.81 – 124.71	718.4
1	A	67	PHE	CE2	1000.00	136.81 – 124.71	718.4

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	54	PHE	CE2	1000.00	136.81 – 124.71	718.4
1	A	77	PHE	CE2	1000.00	136.81 – 124.71	718.4
1	A	99	PHE	CE2	1000.00	136.81 – 124.71	718.4
1	A	86	PHE	CE2	1000.00	136.81 – 124.71	718.4
1	A	11	PHE	CD1	1000.00	137.63 – 125.43	711.9
1	A	50	PHE	CD1	1000.00	137.63 – 125.43	711.9
1	A	7	PHE	CD1	1000.00	137.63 – 125.43	711.9
1	A	99	PHE	CD1	1000.00	137.63 – 125.43	711.9
1	A	86	PHE	CD1	1000.00	137.63 – 125.43	711.9
1	A	67	PHE	CD1	1000.00	137.63 – 125.43	711.9
1	A	9	PHE	CD1	1000.00	137.63 – 125.43	711.9
1	A	77	PHE	CD1	1000.00	137.63 – 125.43	711.9
1	A	54	PHE	CD1	1000.00	137.63 – 125.43	711.9
1	A	20	TYR	CE1	1000.00	124.14 – 111.74	711.3
1	A	68	TYR	CE1	1000.00	124.14 – 111.74	711.3
1	A	20	TYR	HH	1000.00	16.26 – 2.26	707.7
1	A	68	TYR	HH	1000.00	16.26 – 2.26	707.7
1	A	100	THR	HG1	1000.00	12.31 – -2.09	690.9
1	A	14	THR	HG1	1000.00	12.31 – -2.09	690.9
1	A	105	THR	HG1	1000.00	12.31 – -2.09	690.9
1	A	61	THR	HG1	1000.00	12.31 – -2.09	690.9
1	A	68	TYR	CD1	1000.00	139.11 – 126.41	682.9
1	A	20	TYR	CD1	1000.00	139.11 – 126.41	682.9
1	A	68	TYR	CE2	1000.00	124.68 – 111.18	653.4
1	A	20	TYR	CE2	1000.00	124.68 – 111.18	653.4
1	A	47	SER	CB	1000.00	71.24 – 56.34	628.3
1	A	79	SER	CB	1000.00	71.24 – 56.34	628.3
1	A	110	SER	CB	1000.00	71.24 – 56.34	628.3
1	A	80	SER	CB	1000.00	71.24 – 56.34	628.3
1	A	78	SER	CB	1000.00	71.24 – 56.34	628.3
1	A	113	TRP	CD2	1000.00	134.55 – 120.45	618.8
1	A	33	TRP	CD2	1000.00	134.55 – 120.45	618.8
1	A	17	LEU	CD1	1000.00	32.77 – 16.57	602.1
1	A	67	PHE	CE1	1000.00	137.92 – 123.42	599.5
1	A	77	PHE	CE1	1000.00	137.92 – 123.42	599.5
1	A	50	PHE	CE1	1000.00	137.92 – 123.42	599.5
1	A	54	PHE	CE1	1000.00	137.92 – 123.42	599.5
1	A	86	PHE	CE1	1000.00	137.92 – 123.42	599.5
1	A	7	PHE	CE1	1000.00	137.92 – 123.42	599.5
1	A	9	PHE	CE1	1000.00	137.92 – 123.42	599.5
1	A	11	PHE	CE1	1000.00	137.92 – 123.42	599.5
1	A	99	PHE	CE1	1000.00	137.92 – 123.42	599.5

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	23	GLN	CD	1000.00	186.62 – 172.72	590.2
1	A	28	GLN	CD	1000.00	186.62 – 172.72	590.2
1	A	70	GLN	CD	1000.00	186.62 – 172.72	590.2
1	A	104	GLN	CD	1000.00	186.62 – 172.72	590.2
1	A	56	ASN	CG	1000.00	183.77 – 169.77	588.0
1	A	32	ASN	CG	1000.00	183.77 – 169.77	588.0
1	A	21	ASN	CG	1000.00	183.77 – 169.77	588.0
1	A	53	ASN	CG	1000.00	183.77 – 169.77	588.0
1	A	101	ASN	CG	1000.00	183.77 – 169.77	588.0
1	A	87	ASN	CG	1000.00	183.77 – 169.77	588.0
1	A	113	TRP	CZ2	1000.00	121.76 – 106.66	586.6
1	A	33	TRP	CZ2	1000.00	121.76 – 106.66	586.6
1	A	20	TYR	CD2	1000.00	140.11 – 125.31	586.0
1	A	68	TYR	CD2	1000.00	140.11 – 125.31	586.0
1	A	31	ARG	NE	1000.00	92.63 – 76.73	575.7
1	A	48	ARG	NE	1000.00	92.63 – 76.73	575.7
1	A	69	ARG	NE	1000.00	92.63 – 76.73	575.7
1	A	51	ARG	NE	1000.00	92.63 – 76.73	575.7
1	A	17	LEU	CD2	1000.00	32.60 – 15.60	574.1
1	A	101	ASN	CB	1000.00	47.13 – 30.23	568.8
1	A	113	TRP	CZ3	1000.00	129.20 – 113.60	563.2
1	A	33	TRP	CZ3	1000.00	129.20 – 113.60	563.2
1	A	99	PHE	CZ	1000.00	137.04 – 121.44	558.2
1	A	7	PHE	CZ	1000.00	137.04 – 121.44	558.2
1	A	67	PHE	CZ	1000.00	137.04 – 121.44	558.2
1	A	9	PHE	CZ	1000.00	137.04 – 121.44	558.2
1	A	11	PHE	CZ	1000.00	137.04 – 121.44	558.2
1	A	86	PHE	CZ	1000.00	137.04 – 121.44	558.2
1	A	50	PHE	CZ	1000.00	137.04 – 121.44	558.2
1	A	54	PHE	CZ	1000.00	137.04 – 121.44	558.2
1	A	77	PHE	CZ	1000.00	137.04 – 121.44	558.2
1	A	33	TRP	CG	1000.00	118.98 – 101.98	523.2
1	A	113	TRP	CG	1000.00	118.98 – 101.98	523.2
1	A	113	TRP	CE3	1000.00	129.06 – 111.96	514.3
1	A	33	TRP	CE3	1000.00	129.06 – 111.96	514.3
1	A	45	MET	CE	1000.00	26.97 – 7.37	501.4
1	A	101	ASN	CA	1000.00	63.05 – 44.05	498.1
1	A	104	GLN	NE2	1000.00	120.91 – 102.81	490.7
1	A	113	TRP	CH2	1000.00	133.06 – 114.56	473.6
1	A	33	TRP	CH2	1000.00	133.06 – 114.56	473.6
1	A	90	SER	C	1000.00	183.48 – 165.88	468.9
1	A	12	SER	C	1000.00	183.48 – 165.88	468.9

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	79	SER	C	1000.00	183.48 – 165.88	468.9
1	A	80	SER	C	1000.00	183.48 – 165.88	468.9
1	A	110	SER	C	1000.00	183.48 – 165.88	468.9
1	A	47	SER	C	1000.00	183.48 – 165.88	468.9
1	A	25	SER	C	1000.00	183.48 – 165.88	468.9
1	A	78	SER	C	1000.00	183.48 – 165.88	468.9
1	A	100	THR	C	1000.00	183.43 – 165.73	466.3
1	A	118	ASP	C	1000.00	185.29 – 167.59	465.3
1	A	101	ASN	C	1000.00	184.41 – 166.21	453.1
1	A	33	TRP	CD1	1000.00	136.18 – 116.78	450.3
1	A	113	TRP	CD1	1000.00	136.18 – 116.78	450.3
1	A	47	SER	CA	1000.00	69.25 – 48.25	448.2
1	A	78	SER	CA	1000.00	69.25 – 48.25	448.2
1	A	80	SER	CA	1000.00	69.25 – 48.25	448.2
1	A	110	SER	CA	1000.00	69.25 – 48.25	448.2
1	A	79	SER	CA	1000.00	69.25 – 48.25	448.2
1	A	33	TRP	NE1	1000.00	139.19 – 119.59	444.2
1	A	113	TRP	NE1	1000.00	139.19 – 119.59	444.2
1	A	95	ASP	CG	1000.00	188.49 – 169.99	443.7
1	A	5	ASP	CG	1000.00	188.49 – 169.99	443.7
1	A	38	ASP	CG	1000.00	188.49 – 169.99	443.7
1	A	82	ASP	CG	1000.00	188.49 – 169.99	443.7
1	A	118	ASP	CG	1000.00	188.49 – 169.99	443.7
1	A	54	PHE	C	1000.00	185.43 – 165.53	414.3
1	A	115	HIS	C	1000.00	185.27 – 165.27	412.4
1	A	17	LEU	C	1000.00	187.06 – 166.96	409.4
1	A	84	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	89	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	92	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	112	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	58	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	10	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	8	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	13	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	102	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	66	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	98	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	64	GLU	CD	1000.00	192.68 – 172.48	404.7
1	A	68	TYR	CZ	1000.00	167.04 – 146.14	403.5
1	A	20	TYR	CZ	1000.00	167.04 – 146.14	403.5
1	A	87	ASN	ND2	1000.00	124.24 – 101.34	387.4
1	A	101	ASN	ND2	1000.00	124.24 – 101.34	387.4

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	21	ASN	ND2	1000.00	124.24 – 101.34	387.4
1	A	9	PHE	CG	1000.00	149.69 – 126.69	374.7
1	A	77	PHE	CG	1000.00	149.69 – 126.69	374.7
1	A	50	PHE	CG	1000.00	149.69 – 126.69	374.7
1	A	54	PHE	CG	1000.00	149.69 – 126.69	374.7
1	A	99	PHE	CG	1000.00	149.69 – 126.69	374.7
1	A	67	PHE	CG	1000.00	149.69 – 126.69	374.7
1	A	7	PHE	CG	1000.00	149.69 – 126.69	374.7
1	A	86	PHE	CG	1000.00	149.69 – 126.69	374.7
1	A	11	PHE	CG	1000.00	149.69 – 126.69	374.7
1	A	115	HIS	HD1	1000.00	22.55 – -4.85	361.7
1	A	115	HIS	CE1	1000.00	149.70 – 125.30	353.5
1	A	68	TYR	CG	1000.00	141.74 – 116.84	349.7
1	A	20	TYR	CG	999.99	141.74 – 116.84	349.7
1	A	41	LYS	NZ	1000.00	49.86 – 18.16	304.7
1	A	44	LYS	NZ	1000.00	49.86 – 18.16	304.7
1	A	42	LYS	NZ	1000.00	49.86 – 18.16	304.7
1	A	91	LYS	NZ	1000.00	49.86 – 18.16	304.7
1	A	81	LYS	NZ	1000.00	49.86 – 18.16	304.7
1	A	31	ARG	NH2	1000.00	91.01 – 55.81	263.2
1	A	51	ARG	NH2	1000.00	91.01 – 55.81	263.2
1	A	48	ARG	NH2	1000.00	91.01 – 55.81	263.2
1	A	69	ARG	NH2	1000.00	91.01 – 55.81	263.2
1	A	115	HIS	CG	1000.00	148.11 – 114.61	259.3
1	A	115	HIS	CD2	1000.00	137.40 – 103.40	258.7
1	A	31	ARG	CZ	1000.00	176.59 – 143.59	254.5
1	A	51	ARG	CZ	1000.00	176.59 – 143.59	254.5
1	A	69	ARG	CZ	1000.00	176.59 – 143.59	254.5
1	A	48	ARG	CZ	1000.00	176.59 – 143.59	254.5
1	A	102	GLU	N	1000.00	138.24 – 103.14	250.5
1	A	80	SER	N	1000.00	134.24 – 98.34	246.2
1	A	79	SER	N	1000.00	134.24 – 98.34	246.2
1	A	110	SER	N	1000.00	134.24 – 98.34	246.2
1	A	4	SER	N	1000.00	134.24 – 98.34	246.2
1	A	78	SER	N	999.99	134.24 – 98.34	246.2
1	A	47	SER	N	999.99	134.24 – 98.34	246.2
1	A	48	ARG	N	1000.00	139.40 – 102.20	236.3
1	A	91	LYS	N	1000.00	140.01 – 102.11	231.9
1	A	81	LYS	N	1000.00	140.01 – 102.11	231.9
1	A	69	ARG	NH1	1000.00	94.37 – 52.87	223.2
1	A	31	ARG	NH1	1000.00	94.37 – 52.87	223.2
1	A	48	ARG	NH1	1000.00	94.37 – 52.87	223.2

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	51	ARG	NH1	1000.00	94.37 – 52.87	223.2
1	A	101	ASN	N	1000.00	139.12 – 98.82	218.6
1	A	26	VAL	N	1000.00	144.09 – 98.19	191.5
1	A	111	VAL	N	1000.00	144.09 – 98.19	191.5
1	A	88	PRO	N	1000.00	167.35 – 100.35	129.3
1	A	18	PRO	N	1000.00	167.35 – 100.35	129.3
1	A	55	PRO	N	1000.00	167.35 – 100.35	129.3
1	A	30	PRO	N	1000.00	167.35 – 100.35	129.3
1	A	116	PRO	N	1000.00	167.35 – 100.35	129.3
1	A	15	PRO	N	1000.00	167.35 – 100.35	129.3
1	A	113	TRP	CE2	1000.00	173.31 – 104.01	124.3
1	A	33	TRP	CE2	1000.00	173.31 – 104.01	124.3
1	A	115	HIS	NE2	1000.00	255.67 – 109.17	55.8
1	A	115	HIS	ND1	1000.00	286.54 – 104.24	44.1

### 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:

