



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:51 PM BST

PDB ID : 1ZRP  
Title : SOLUTION-STATE STRUCTURE BY NMR OF ZINC-SUBSTITUTED RUBREDOXIN FROM THE MARINE HYPERTHERMOPHILIC ARCHAE-BACTERIUM PYROCOCCLUS FURIOSUS  
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Deposited on : 1992-07-10

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

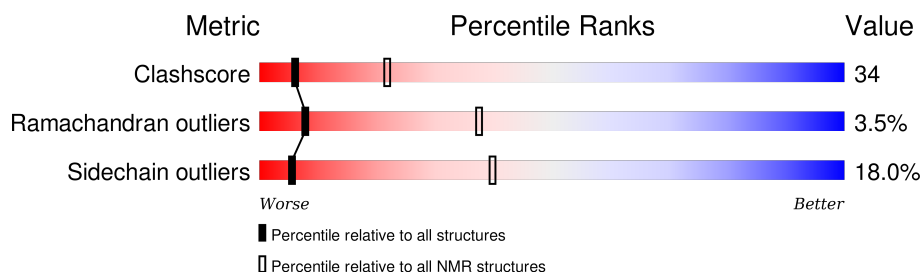
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 97%.

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	53	

## 2 Ensemble composition and analysis

This entry contains 40 models. Model 9 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:50 (50)	0.23	9

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 6 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 7, 8, 9, 10, 13, 14, 15, 16, 17, 18, 21, 23, 24, 25, 27, 28, 35, 36, 39, 40
2	32, 34, 37
3	12, 26
4	30, 33
5	2, 3
6	31, 38
Single-model clusters	11; 19; 20; 22; 29

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 789 atoms, of which 375 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RUBREDOXIN.

Mol	Chain	Residues	Atoms						Trace
1	A	53	Total	C	H	N	O	S	0
			788	262	375	61	86	4	

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

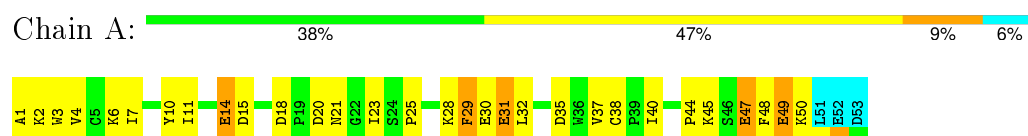
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

## 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: RUBREDOXIN

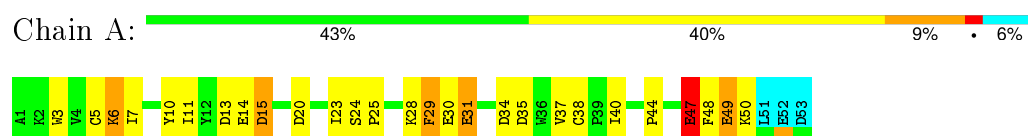


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

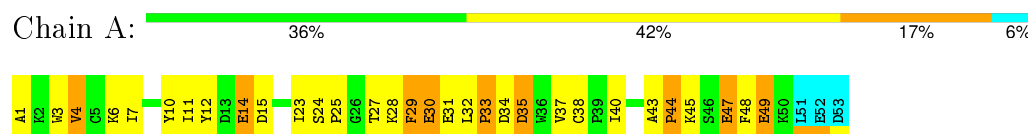
#### 4.2.1 Score per residue for model 1

- Molecule 1: RUBREDOXIN



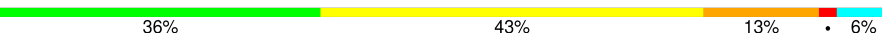
#### 4.2.2 Score per residue for model 2

- Molecule 1: RUBREDOXIN



### 4.2.3 Score per residue for model 3

- Molecule 1: RUBREDOXIN

Chain A:  36% 43% 13% • 6%



### 4.2.4 Score per residue for model 4

- Molecule 1: RUBREDOXIN

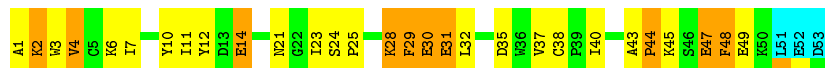
Chain A:  36% 45% 11% • 6%



### 4.2.5 Score per residue for model 5

- Molecule 1: RUBREDOXIN

Chain A:  40% 36% 19% • 6%



### 4.2.6 Score per residue for model 6

- Molecule 1: RUBREDOXIN

Chain A:  40% 43% 9% • 6%



### 4.2.7 Score per residue for model 7

- Molecule 1: RUBREDOXIN

Chain A:  42% 38% 15% • 6%



### 4.2.8 Score per residue for model 8

- Molecule 1: RUBREDOXIN

Chain A:  43% 36% 13% • 6%



### 4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: RUBREDOXIN

Chain A:  36% 49% 6% • 6%



### 4.2.10 Score per residue for model 10

- Molecule 1: RUBREDOXIN

Chain A:  28% 57% 9% 6%



### 4.2.11 Score per residue for model 11

- Molecule 1: RUBREDOXIN

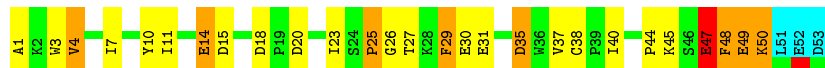
Chain A:  49% 30% 15% 6%



### 4.2.12 Score per residue for model 12

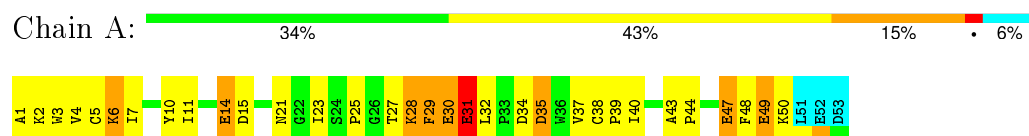
- Molecule 1: RUBREDOXIN

Chain A:  43% 34% 15% • 6%



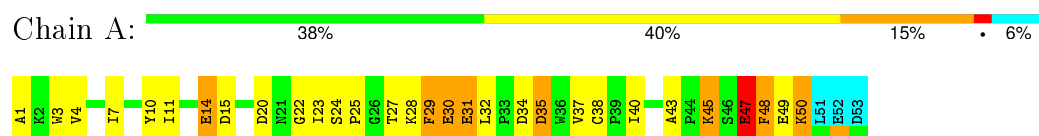
### 4.2.13 Score per residue for model 13

- Molecule 1: RUBREDOXIN



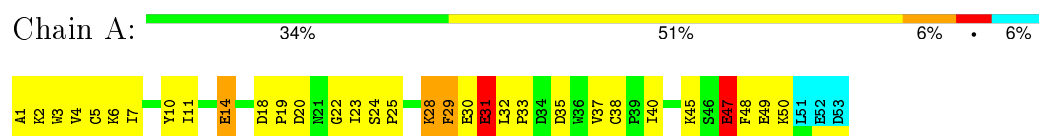
### 4.2.14 Score per residue for model 14

- Molecule 1: RUBREDOXIN



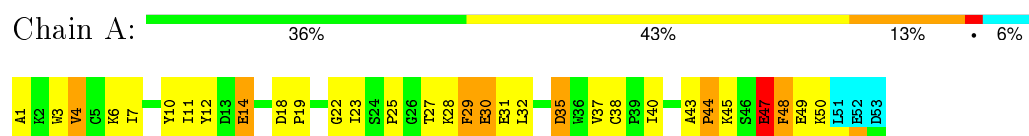
### 4.2.15 Score per residue for model 15

- Molecule 1: RUBREDOXIN



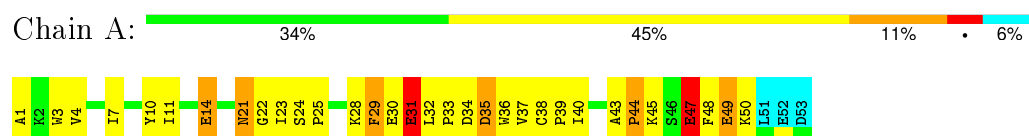
### 4.2.16 Score per residue for model 16

- Molecule 1: RUBREDOXIN



### 4.2.17 Score per residue for model 17

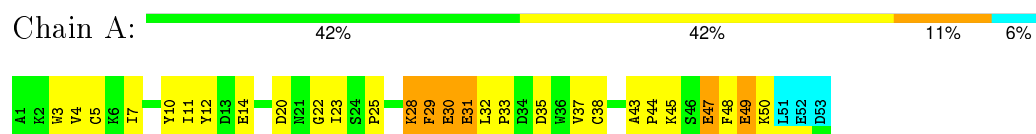
- Molecule 1: RUBREDOXIN





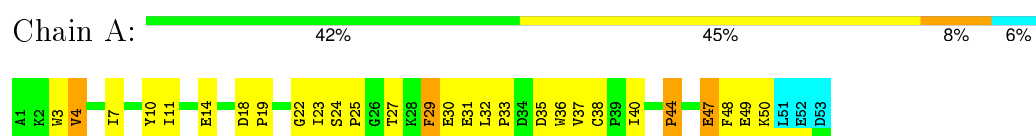
#### 4.2.18 Score per residue for model 18

- Molecule 1: RUBREDOXIN



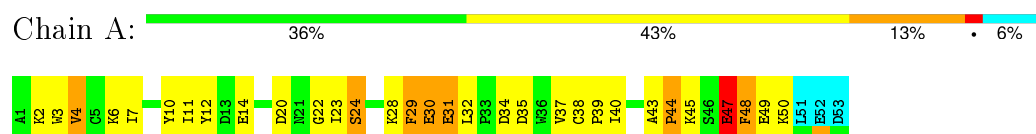
#### 4.2.19 Score per residue for model 19

- Molecule 1: RUBREDOXIN



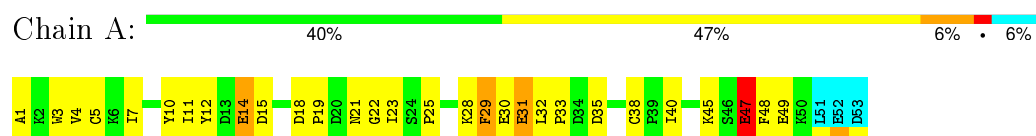
#### 4.2.20 Score per residue for model 20

- Molecule 1: RUBREDOXIN



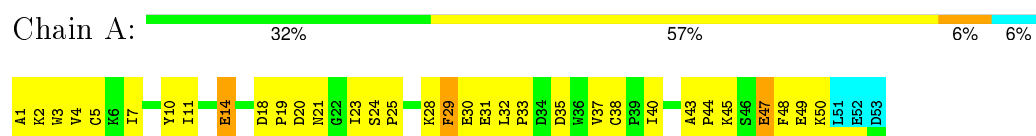
#### 4.2.21 Score per residue for model 21

- Molecule 1: RUBREDOXIN



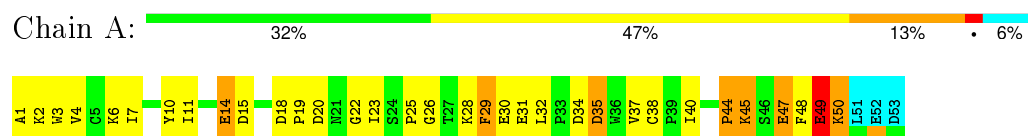
#### 4.2.22 Score per residue for model 22

- Molecule 1: RUBREDOXIN



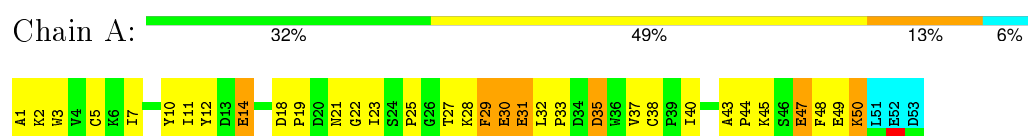
### 4.2.23 Score per residue for model 23

- Molecule 1: RUBREDOXIN



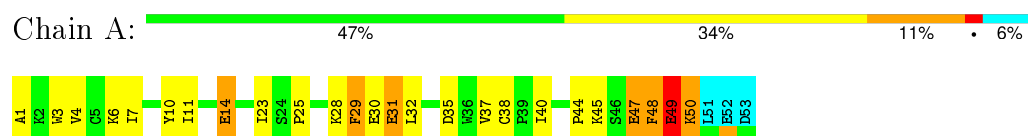
### 4.2.24 Score per residue for model 24

- Molecule 1: RUBREDOXIN



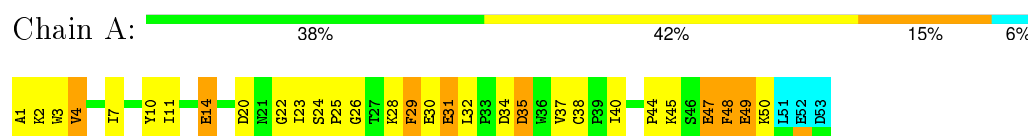
### 4.2.25 Score per residue for model 25

- Molecule 1: RUBREDOXIN



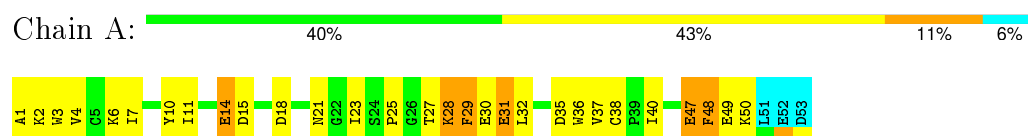
### 4.2.26 Score per residue for model 26

- Molecule 1: RUBREDOXIN



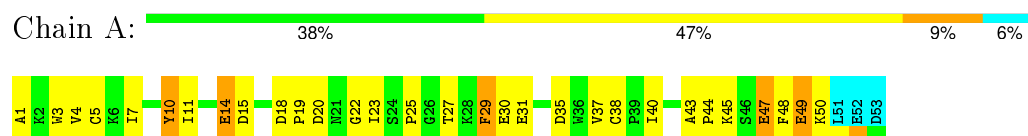
### 4.2.27 Score per residue for model 27

- Molecule 1: RUBREDOXIN



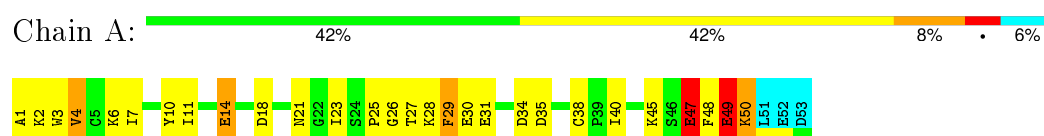
### 4.2.28 Score per residue for model 28

- Molecule 1: RUBREDOXIN



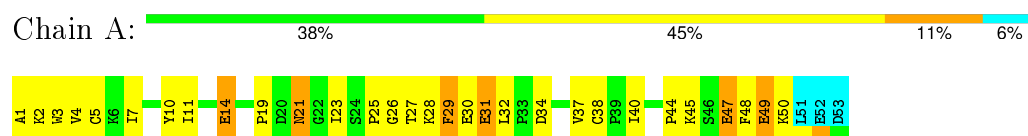
### 4.2.29 Score per residue for model 29

- Molecule 1: RUBREDOXIN



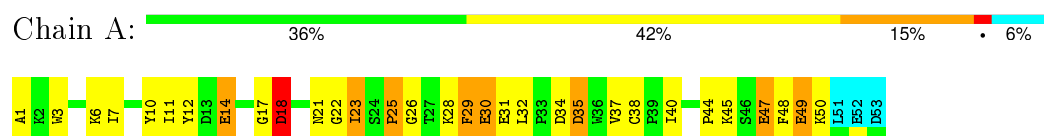
### 4.2.30 Score per residue for model 30

- Molecule 1: RUBREDOXIN



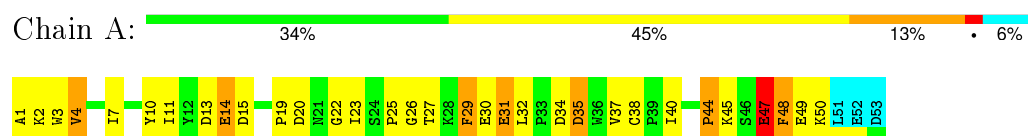
### 4.2.31 Score per residue for model 31

- Molecule 1: RUBREDOXIN



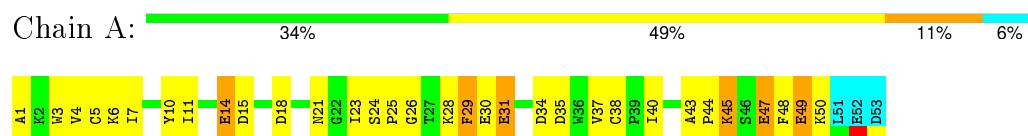
### 4.2.32 Score per residue for model 32

- Molecule 1: RUBREDOXIN



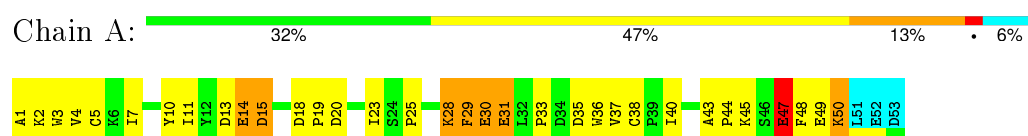
### 4.2.33 Score per residue for model 33

- Molecule 1: RUBREDOXIN



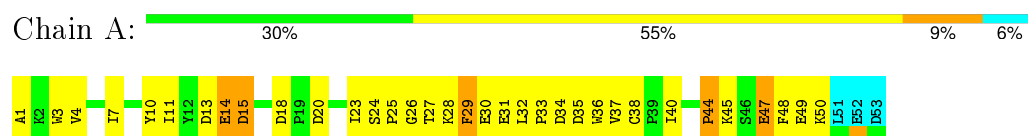
### 4.2.34 Score per residue for model 34

- Molecule 1: RUBREDOXIN



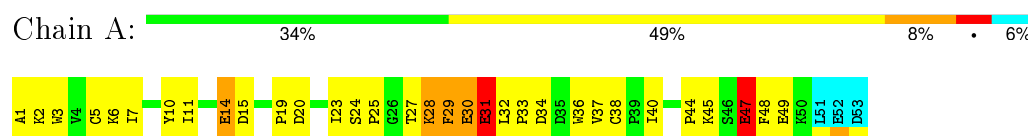
### 4.2.35 Score per residue for model 35

- Molecule 1: RUBREDOXIN



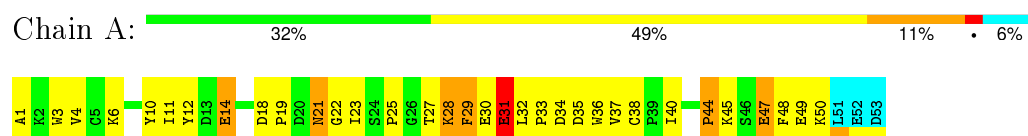
### 4.2.36 Score per residue for model 36

- Molecule 1: RUBREDOXIN



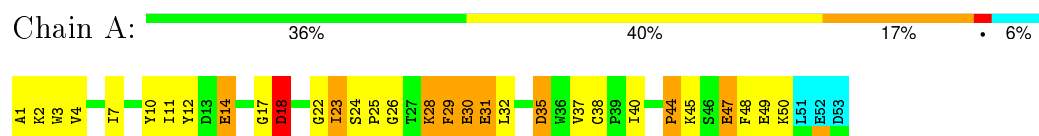
### 4.2.37 Score per residue for model 37

- Molecule 1: RUBREDOXIN



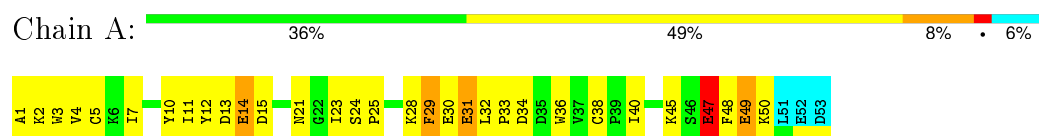
#### 4.2.38 Score per residue for model 38

- Molecule 1: RUBREDOXIN



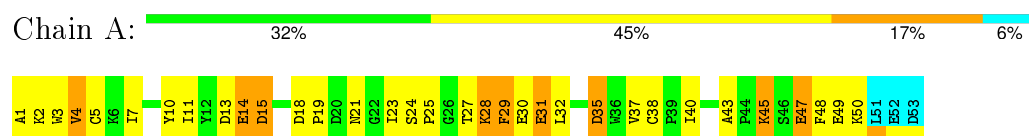
#### 4.2.39 Score per residue for model 39

- Molecule 1: RUBREDOXIN



#### 4.2.40 Score per residue for model 40

- Molecule 1: RUBREDOXIN



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 40 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DSPACE	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 5601
Number of chemical shift lists	3
Total number of shifts	1239
Number of shifts mapped to atoms	660
Number of unparsed shifts	0
Number of shifts with mapping errors	579
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	97%

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

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.83±0.00	5±0/400 (1.2±0.0%)	1.12±0.00	7±0/545 (1.3±0.0%)
All	All	0.83	200/16000 (1.2%)	1.12	280/21800 (1.3%)

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	2.3±1.0
All	All	0	91

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	30	GLU	CB-CG	-5.28	1.42	1.52	32	40
1	A	49	GLU	CB-CG	-5.25	1.42	1.52	32	40
1	A	47	GLU	CB-CG	-5.24	1.42	1.52	14	40
1	A	14	GLU	CB-CG	-5.24	1.42	1.52	20	40
1	A	31	GLU	CB-CG	-5.23	1.42	1.52	14	40

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	29	PHE	CB-CG-CD1	-5.83	116.72	120.80	30	40
1	A	48	PHE	CB-CG-CD2	-5.51	116.94	120.80	3	40
1	A	31	GLU	CA-CB-CG	5.31	125.08	113.40	28	40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	GLU	CA-CB-CG	5.17	124.77	113.40	14	40
1	A	49	GLU	CA-CB-CG	5.17	124.77	113.40	24	40
1	A	14	GLU	CA-CB-CG	5.14	124.71	113.40	36	40
1	A	30	GLU	CA-CB-CG	5.08	124.58	113.40	35	40

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	38	CYS	Mainchain	40
1	A	4	VAL	Mainchain	12
1	A	5	CYS	Mainchain	11
1	A	15	ASP	Mainchain	9
1	A	13	ASP	Mainchain	6
1	A	48	PHE	Mainchain	5
1	A	23	ILE	Mainchain	2
1	A	18	ASP	Sidechain	2
1	A	24	SER	Mainchain	1
1	A	45	LYS	Mainchain	1
1	A	25	PRO	Mainchain	1
1	A	10	TYR	Mainchain	1

## 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	387	354	354	25±4
All	All	15520	14160	14160	1001

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 34.

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



Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:ILE:HD11	1:A:47:GLU:HB3	0.82	1.51	24	18
1:A:7:ILE:HD11	1:A:47:GLU:CB	0.80	2.04	22	20
1:A:27:THR:HG21	1:A:32:LEU:HD23	0.80	1.52	30	2
1:A:17:GLY:HA2	1:A:23:ILE:HG22	0.76	1.57	38	2
1:A:4:VAL:HG23	1:A:11:ILE:CD1	0.76	2.10	26	13
1:A:4:VAL:HG23	1:A:11:ILE:HG13	0.74	1.58	40	10
1:A:7:ILE:HD13	1:A:47:GLU:HB3	0.73	1.59	16	12
1:A:1:ALA:HB3	1:A:14:GLU:OE2	0.73	1.84	22	28
1:A:35:ASP:O	1:A:37:VAL:HG13	0.73	1.83	5	29
1:A:7:ILE:HD11	1:A:47:GLU:HB2	0.72	1.59	13	5
1:A:37:VAL:HG12	1:A:44:PRO:HA	0.72	1.62	24	26
1:A:10:TYR:O	1:A:11:ILE:HD13	0.72	1.83	18	11
1:A:7:ILE:HD13	1:A:43:ALA:CB	0.70	2.16	13	9
1:A:22:GLY:C	1:A:23:ILE:HD12	0.68	2.09	3	19
1:A:10:TYR:HB2	1:A:40:ILE:HD13	0.65	1.69	9	8
1:A:27:THR:CG2	1:A:32:LEU:HD23	0.65	2.22	30	2
1:A:7:ILE:HD11	1:A:47:GLU:HG3	0.64	1.68	34	2
1:A:1:ALA:HB3	1:A:14:GLU:CD	0.64	2.13	34	8
1:A:28:LYS:O	1:A:32:LEU:HG	0.63	1.92	26	21
1:A:7:ILE:HD11	1:A:47:GLU:CG	0.62	2.24	24	3
1:A:10:TYR:C	1:A:11:ILE:HD13	0.62	2.15	30	12
1:A:40:ILE:HD12	1:A:40:ILE:N	0.61	2.11	7	15
1:A:7:ILE:N	1:A:7:ILE:HD12	0.61	2.11	30	12
1:A:40:ILE:N	1:A:40:ILE:HD12	0.61	2.11	11	16
1:A:18:ASP:HB3	1:A:23:ILE:HD13	0.60	1.72	29	6
1:A:23:ILE:N	1:A:23:ILE:HD12	0.60	2.12	21	17
1:A:23:ILE:HD12	1:A:23:ILE:N	0.60	2.12	24	18
1:A:7:ILE:HD12	1:A:7:ILE:N	0.59	2.12	15	9
1:A:1:ALA:HB3	1:A:14:GLU:OE1	0.59	1.97	16	2
1:A:37:VAL:HG12	1:A:44:PRO:CA	0.59	2.25	4	21
1:A:23:ILE:HG23	1:A:27:THR:HB	0.58	1.74	2	14
1:A:10:TYR:CG	1:A:40:ILE:HD13	0.58	2.34	1	34
1:A:12:TYR:CE2	1:A:32:LEU:HD11	0.57	2.34	37	7
1:A:18:ASP:CG	1:A:23:ILE:HD13	0.57	2.20	31	2
1:A:17:GLY:CA	1:A:23:ILE:HG22	0.57	2.29	38	2
1:A:7:ILE:CD1	1:A:47:GLU:HB3	0.56	2.30	17	12
1:A:10:TYR:CB	1:A:40:ILE:HD13	0.56	2.31	12	8
1:A:28:LYS:HB3	1:A:31:GLU:HB2	0.56	1.76	34	4
1:A:37:VAL:HG12	1:A:44:PRO:CB	0.54	2.32	10	15
1:A:11:ILE:HD12	1:A:11:ILE:N	0.53	2.18	37	5
1:A:4:VAL:HG23	1:A:11:ILE:HD13	0.53	1.80	28	6
1:A:4:VAL:HG12	1:A:49:GLU:O	0.52	2.04	33	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HG22	1:A:12:TYR:H	0.52	1.64	7	3
1:A:5:CYS:SG	1:A:7:ILE:HD12	0.52	2.45	24	6
1:A:3:TRP:O	1:A:11:ILE:HG23	0.52	2.04	31	13
1:A:18:ASP:OD2	1:A:23:ILE:HD13	0.52	2.04	22	1
1:A:18:ASP:N	1:A:19:PRO:HD3	0.50	2.21	16	11
1:A:4:VAL:HG23	1:A:10:TYR:O	0.50	2.06	34	9
1:A:4:VAL:HG23	1:A:11:ILE:HD12	0.50	1.83	16	4
1:A:3:TRP:CE2	1:A:29:PHE:CG	0.50	3.00	29	35
1:A:3:TRP:CZ3	1:A:29:PHE:CE2	0.50	3.00	17	5
1:A:3:TRP:CD2	1:A:29:PHE:CG	0.50	3.00	30	14
1:A:10:TYR:CG	1:A:11:ILE:N	0.50	2.80	36	28
1:A:3:TRP:CD2	1:A:29:PHE:CD1	0.50	3.00	5	25
1:A:3:TRP:CG	1:A:29:PHE:CD1	0.49	3.00	6	20
1:A:3:TRP:CE3	1:A:29:PHE:CZ	0.49	3.00	12	3
1:A:49:GLU:HG3	1:A:50:LYS:N	0.49	2.23	11	2
1:A:10:TYR:C	1:A:11:ILE:HD12	0.49	2.28	9	10
1:A:29:PHE:O	1:A:32:LEU:HD12	0.49	2.07	37	4
1:A:43:ALA:HB1	1:A:47:GLU:HG2	0.49	1.85	3	2
1:A:11:ILE:N	1:A:11:ILE:HD12	0.49	2.23	38	1
1:A:3:TRP:CD1	1:A:29:PHE:CD1	0.49	3.01	2	1
1:A:29:PHE:CZ	1:A:45:LYS:HG3	0.49	2.43	30	2
1:A:3:TRP:CZ3	1:A:50:LYS:HG2	0.48	2.43	34	2
1:A:33:PRO:HD2	1:A:36:TRP:CD1	0.48	2.43	19	4
1:A:28:LYS:CB	1:A:31:GLU:HB2	0.48	2.37	34	5
1:A:45:LYS:HD2	1:A:45:LYS:N	0.48	2.23	23	1
1:A:21:ASN:C	1:A:23:ILE:HD12	0.48	2.29	10	5
1:A:4:VAL:HG13	1:A:49:GLU:HB3	0.48	1.85	18	2
1:A:37:VAL:HG12	1:A:44:PRO:HB3	0.47	1.84	25	8
1:A:17:GLY:N	1:A:25:PRO:HA	0.47	2.25	38	2
1:A:33:PRO:HB2	1:A:36:TRP:N	0.47	2.23	37	5
1:A:28:LYS:HB2	1:A:31:GLU:HB2	0.47	1.87	30	5
1:A:3:TRP:CE2	1:A:29:PHE:HB2	0.47	2.45	1	6
1:A:37:VAL:HA	1:A:44:PRO:HA	0.47	1.87	36	28
1:A:18:ASP:N	1:A:23:ILE:HB	0.46	2.25	38	2
1:A:11:ILE:HG22	1:A:12:TYR:N	0.46	2.25	7	4
1:A:28:LYS:CG	1:A:31:GLU:HB3	0.46	2.40	18	1
1:A:3:TRP:NE1	1:A:29:PHE:HB2	0.46	2.26	38	28
1:A:3:TRP:CH2	1:A:29:PHE:CD2	0.46	3.03	16	3
1:A:3:TRP:CZ2	1:A:29:PHE:CG	0.46	3.04	16	1
1:A:7:ILE:CD1	1:A:47:GLU:HB2	0.45	2.41	29	1
1:A:3:TRP:CE3	1:A:29:PHE:CE2	0.45	3.04	30	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:TYR:CG	1:A:40:ILE:CD1	0.45	3.00	16	29
1:A:7:ILE:CD1	1:A:7:ILE:N	0.45	2.80	5	3
1:A:29:PHE:CE2	1:A:45:LYS:HD3	0.45	2.46	33	1
1:A:29:PHE:CZ	1:A:45:LYS:CG	0.45	3.00	14	4
1:A:18:ASP:N	1:A:19:PRO:CD	0.45	2.80	19	10
1:A:40:ILE:CD1	1:A:40:ILE:N	0.45	2.80	29	15
1:A:50:LYS:HD3	1:A:50:LYS:H	0.45	1.70	25	1
1:A:7:ILE:N	1:A:7:ILE:CD1	0.45	2.80	36	13
1:A:3:TRP:NE1	1:A:29:PHE:CB	0.45	2.80	30	1
1:A:23:ILE:CD1	1:A:23:ILE:N	0.45	2.80	21	10
1:A:3:TRP:CD2	1:A:29:PHE:CD2	0.45	3.05	30	1
1:A:43:ALA:HB1	1:A:47:GLU:CG	0.45	2.42	14	8
1:A:3:TRP:CE2	1:A:50:LYS:CG	0.45	3.00	20	1
1:A:40:ILE:N	1:A:40:ILE:CD1	0.44	2.80	14	6
1:A:3:TRP:CE2	1:A:29:PHE:CB	0.44	3.01	13	4
1:A:29:PHE:CE2	1:A:45:LYS:CD	0.44	3.00	33	1
1:A:29:PHE:CZ	1:A:45:LYS:CD	0.44	3.00	33	1
1:A:23:ILE:N	1:A:23:ILE:CD1	0.44	2.80	17	8
1:A:45:LYS:HD2	1:A:45:LYS:H	0.44	1.73	23	1
1:A:3:TRP:CD1	1:A:29:PHE:HB2	0.44	2.48	30	1
1:A:23:ILE:HG12	1:A:32:LEU:HD22	0.44	1.90	3	2
1:A:3:TRP:CZ3	1:A:50:LYS:CG	0.44	3.00	1	2
1:A:28:LYS:HG3	1:A:31:GLU:CB	0.44	2.42	18	1
1:A:28:LYS:HB2	1:A:31:GLU:HB3	0.44	1.89	27	2
1:A:29:PHE:CZ	1:A:45:LYS:HG2	0.44	2.47	34	2
1:A:28:LYS:CB	1:A:31:GLU:HB3	0.44	2.42	27	1
1:A:6:LYS:HG2	1:A:49:GLU:HB2	0.44	1.90	1	1
1:A:3:TRP:CH2	1:A:50:LYS:HG2	0.43	2.48	14	2
1:A:23:ILE:HG23	1:A:27:THR:CB	0.43	2.44	12	3
1:A:3:TRP:CE2	1:A:50:LYS:HB3	0.43	2.48	29	1
1:A:21:ASN:N	1:A:21:ASN:ND2	0.43	2.66	30	1
1:A:28:LYS:HD3	1:A:31:GLU:HG3	0.43	1.91	5	1
1:A:28:LYS:CG	1:A:31:GLU:HB2	0.43	2.42	11	1
1:A:10:TYR:CD1	1:A:40:ILE:HD11	0.43	2.47	35	1
1:A:21:ASN:HB2	1:A:23:ILE:HD13	0.43	1.90	31	1
1:A:1:ALA:O	1:A:14:GLU:HB2	0.43	2.13	39	2
1:A:21:ASN:ND2	1:A:39:PRO:HG3	0.43	2.29	17	1
1:A:12:TYR:CZ	1:A:32:LEU:HD21	0.43	2.49	18	2
1:A:50:LYS:HB2	1:A:50:LYS:NZ	0.42	2.29	24	1
1:A:28:LYS:HB2	1:A:31:GLU:CB	0.42	2.44	36	2
1:A:29:PHE:CE2	1:A:45:LYS:HD2	0.42	2.49	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:TRP:CH2	1:A:48:PHE:CE2	0.42	3.07	27	1
1:A:33:PRO:HG2	1:A:36:TRP:CD1	0.42	2.50	17	1
1:A:32:LEU:HB3	1:A:33:PRO:HD2	0.42	1.92	17	14
1:A:29:PHE:CZ	1:A:48:PHE:HB2	0.42	2.50	20	2
1:A:29:PHE:CZ	1:A:45:LYS:HB2	0.42	2.50	40	2
1:A:7:ILE:HD11	1:A:47:GLU:HG2	0.41	1.92	24	1
1:A:36:TRP:CZ3	1:A:48:PHE:CE2	0.41	3.08	27	1
1:A:43:ALA:HB1	1:A:47:GLU:HG3	0.41	1.92	7	1
1:A:21:ASN:HB2	1:A:23:ILE:CD1	0.41	2.45	39	1
1:A:3:TRP:CH2	1:A:50:LYS:HG3	0.41	2.49	20	1
1:A:7:ILE:CD1	1:A:47:GLU:HG3	0.41	2.45	3	1
1:A:4:VAL:HG13	1:A:49:GLU:HG3	0.41	1.91	23	1
1:A:37:VAL:CG1	1:A:44:PRO:HA	0.41	2.46	32	6
1:A:18:ASP:HB3	1:A:23:ILE:HB	0.41	1.93	34	3
1:A:49:GLU:CG	1:A:50:LYS:N	0.41	2.84	11	1
1:A:6:LYS:CG	1:A:49:GLU:HG2	0.41	2.45	13	1
1:A:7:ILE:CG1	1:A:47:GLU:HB3	0.41	2.46	38	1
1:A:28:LYS:HB3	1:A:31:GLU:CB	0.40	2.46	34	1
1:A:21:ASN:ND2	1:A:21:ASN:N	0.40	2.69	6	1
1:A:3:TRP:CE2	1:A:29:PHE:CD2	0.40	3.08	30	1
1:A:3:TRP:CE3	1:A:50:LYS:HB3	0.40	2.52	23	1
1:A:7:ILE:CD1	1:A:43:ALA:CB	0.40	3.00	24	1
1:A:23:ILE:HG12	1:A:32:LEU:CD2	0.40	2.47	2	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	49/53 (92%)	41±1 (84±2%)	6±1 (13±3%)	2±1 (3±2%)	8	37
All	All	1960/2120 (92%)	1644 (84%)	248 (13%)	68 (3%)	8	37

All 5 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	25	PRO	37
1	A	44	PRO	14
1	A	26	GLY	11
1	A	15	ASP	5
1	A	49	GLU	1

### 6.3.2 Protein sidechains ⓘ

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	42/45 (93%)	34±2 (82±5%)	8±2 (18±5%)	5	40
All	All	1680/1800 (93%)	1378 (82%)	302 (18%)	5	40

All 21 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	45	LYS	31
1	A	50	LYS	30
1	A	35	ASP	23
1	A	6	LYS	22
1	A	2	LYS	21
1	A	20	ASP	20
1	A	28	LYS	19
1	A	47	GLU	19
1	A	31	GLU	18
1	A	34	ASP	18
1	A	30	GLU	18
1	A	24	SER	18
1	A	21	ASN	12
1	A	49	GLU	12
1	A	15	ASP	11
1	A	19	PRO	3
1	A	39	PRO	2
1	A	18	ASP	2
1	A	48	PHE	1
1	A	33	PRO	1
1	A	25	PRO	1

### 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 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 97% for the well-defined parts and 97% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5601

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	677
Number of shifts mapped to atoms	660
Number of unparsed shifts	0
Number of shifts with mapping errors	17
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- Residue not found in structure. All 17 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1	FME	CN	167.25	0.1	1
A	1	FME	N	129.2	0.05	1
A	1	FME	HB3	2.0	0.01	2
A	1	FME	CB	33.1	0.1	1
A	1	FME	HCN	8.19	0.01	1
A	1	FME	H	8.59	0.01	1
A	1	FME	CE	17.18	0.1	1
A	1	FME	C	174.97	0.05	1
A	1	FME	HG3	2.48	0.01	2
A	1	FME	HA	4.7	0.01	1
A	1	FME	HG2	2.77	0.01	2
A	1	FME	CG	33.26	0.1	1
A	1	FME	HE3	2.07	0.01	1
A	1	FME	HE2	2.07	0.01	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1	FME	HB2	2.46	0.01	2
A	1	FME	CA	53.33	0.1	1
A	1	FME	HE1	2.07	0.01	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
$^{13}\text{C}_\alpha$	54	$0.47 \pm 0.20$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	49	$0.85 \pm 0.30$	Should be applied
$^{13}\text{C}'$	54	$-0.06 \pm 0.29$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	54	$-1.65 \pm 0.53$	Should be applied

### 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 97%, i.e. 561 atoms were assigned a chemical shift out of a possible 577. 1 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	240/240 (100%)	95/95 (100%)	100/100 (100%)	45/45 (100%)
Sidechain	271/279 (97%)	165/166 (99%)	105/107 (98%)	1/6 (17%)
Aromatic	50/58 (86%)	30/30 (100%)	18/26 (69%)	2/2 (100%)
Overall	561/577 (97%)	290/291 (100%)	223/233 (96%)	48/53 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 97%, i.e. 595 atoms were assigned a chemical shift out of a possible 612. 1 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	255/255 (100%)	101/101 (100%)	106/106 (100%)	48/48 (100%)
Sidechain	290/299 (97%)	176/177 (99%)	113/116 (97%)	1/6 (17%)
Aromatic	50/58 (86%)	30/30 (100%)	18/26 (69%)	2/2 (100%)
Overall	595/612 (97%)	307/308 (100%)	237/248 (96%)	51/56 (91%)



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

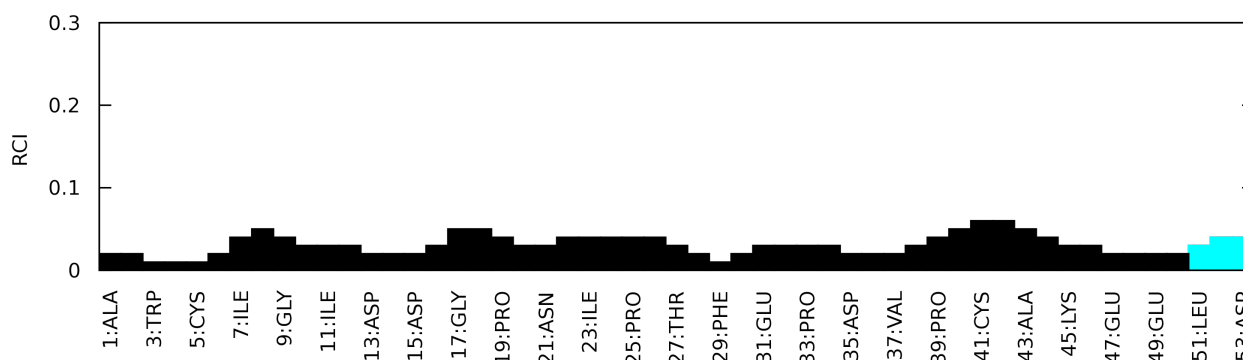
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	32	LEU	HD13	-1.76	2.16 – -0.64	-9.0
1	A	32	LEU	HD11	-1.76	2.16 – -0.64	-9.0
1	A	32	LEU	HD12	-1.76	2.16 – -0.64	-9.0
1	A	50	LYS	HB3	0.01	3.10 – 0.40	-6.4

### 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 5601

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

### 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	281
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Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	281
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 281 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	45	PRO	CA	61.48	-1.0	1
UNMAPPED	38	VAL	H	6.17	-1.0	1
UNMAPPED	10	GLY	N	113.6	-1.0	1
UNMAPPED	8	ILE	H	9.08	-1.0	1
UNMAPPED	12	ILE	CB	38.78	-1.0	1
UNMAPPED	15	GLU	C	177.73	-1.0	1
UNMAPPED	43	GLY	N	112.97	-1.0	1
UNMAPPED	21	ASP	C	177.04	-1.0	1
UNMAPPED	48	GLU	HB3	2.0	-1.0	2
UNMAPPED	42	CYS	CB	32.53	-1.0	1
UNMAPPED	37	TRP	CB	29.22	-1.0	1
UNMAPPED	12	ILE	N	126.19	-1.0	1
UNMAPPED	24	ILE	CA	57.37	-1.0	1
UNMAPPED	7	LYS	CB	31.53	-1.0	1
UNMAPPED	37	TRP	CA	59.71	-1.0	1
UNMAPPED	6	CYS	H	9.23	-1.0	1
UNMAPPED	4	TRP	HE1	9.95	-1.0	5
UNMAPPED	52	LEU	H	8.636	-1.0	5
UNMAPPED	7	LYS	CA	58.43	-1.0	1
UNMAPPED	37	TRP	N	123.42	-1.0	1
UNMAPPED	4	TRP	CB	31.55	-1.0	1
UNMAPPED	5	VAL	H	9.74	-1.0	1
UNMAPPED	53	GLU	HB2	2.12	-1.0	2
UNMAPPED	48	GLU	C	173.75	-1.0	1
UNMAPPED	36	ASP	C	175.57	-1.0	1
UNMAPPED	16	ASP	N	114.14	-1.0	1
UNMAPPED	50	GLU	CA	53.36	-1.0	1
UNMAPPED	47	SER	H	7.91	-1.0	1
UNMAPPED	16	ASP	CA	56.33	-1.0	5
UNMAPPED	12	ILE	HG23	0.65	-1.0	1
UNMAPPED	11	TYR	H	9.38	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	19	ASP	H	8.26	-1.0	1
UNMAPPED	29	LYS	H	8.65	-1.0	5
UNMAPPED	2	ALA	HB3	1.46	-1.0	1
UNMAPPED	38	VAL	CA	56.6	-1.0	1
UNMAPPED	15	GLU	CB	30.38	-1.0	5
UNMAPPED	2	ALA	N	125.82	-1.0	1
UNMAPPED	15	GLU	CA	58.13	-1.0	5
UNMAPPED	2	ALA	CA	51.38	-1.0	5
UNMAPPED	20	PRO	C	180.06	-1.0	1
UNMAPPED	26	PRO	CA	63.79	-1.0	1
UNMAPPED	39	CYS	CA	56.69	-1.0	1
UNMAPPED	14	ASP	C	176.79	-1.0	5
UNMAPPED	31	GLU	CA	58.44	-1.0	5
UNMAPPED	54	ASP	H	7.92	-1.0	5
UNMAPPED	52	LEU	N	128.92	-1.0	5
UNMAPPED	30	PHE	H	10.01	-1.0	5
UNMAPPED	36	ASP	N	114.26	-1.0	1
UNMAPPED	49	PHE	C	177.09	-1.0	1
UNMAPPED	29	LYS	HG2	1.41	-1.0	2
UNMAPPED	36	ASP	CA	51.96	-1.0	1
UNMAPPED	12	ILE	HB	1.46	-1.0	1
UNMAPPED	36	ASP	CB	39.09	-1.0	1
UNMAPPED	32	GLU	H	7.41	-1.0	1
UNMAPPED	12	ILE	HA	4.76	-1.0	1
UNMAPPED	22	ASN	HD21	9.36	-1.0	2
UNMAPPED	35	ASP	H	8.71	-1.0	1
UNMAPPED	23	GLY	H	7.76	-1.0	1
UNMAPPED	24	ILE	H	7.6	-1.0	1
UNMAPPED	34	PRO	C	177.03	-1.0	1
UNMAPPED	18	GLY	C	173.27	-1.0	1
UNMAPPED	28	THR	N	117.54	-1.0	5
UNMAPPED	42	CYS	CA	58.42	-1.0	1
UNMAPPED	50	GLU	H	9.09	-1.0	1
UNMAPPED	27	GLY	CA	44.8	-1.0	5
UNMAPPED	2	ALA	C	175.84	-1.0	1
UNMAPPED	20	PRO	CA	64.99	-1.0	1
UNMAPPED	18	GLY	HA3	3.58	-1.0	2
UNMAPPED	52	LEU	C	176.71	-1.0	5
UNMAPPED	20	PRO	CB	31.53	-1.0	1
UNMAPPED	32	GLU	C	176.76	-1.0	1
UNMAPPED	45	PRO	CB	32.31	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	14	ASP	CA	51.05	-1.0	5
UNMAPPED	43	GLY	C	173.26	-1.0	1
UNMAPPED	17	ALA	HA	4.34	-1.0	5
UNMAPPED	13	TYR	H	9.71	-1.0	5
UNMAPPED	49	PHE	H	7.75	-1.0	1
UNMAPPED	47	SER	N	110.12	-1.0	1
UNMAPPED	17	ALA	HB2	1.48	-1.0	5
UNMAPPED	53	GLU	N	121.99	-1.0	5
UNMAPPED	40	PRO	C	176.18	-1.0	1
UNMAPPED	10	GLY	C	173.99	-1.0	1
UNMAPPED	42	CYS	N	121.29	-1.0	1
UNMAPPED	33	LEU	CB	39.29	-1.0	1
UNMAPPED	53	GLU	CB	30.72	-1.0	5
UNMAPPED	41	ILE	H	8.72	-1.0	1
UNMAPPED	23	GLY	C	173.8	-1.0	1
UNMAPPED	33	LEU	CA	52.85	-1.0	1
UNMAPPED	35	ASP	CA	56.42	-1.0	1
UNMAPPED	44	ALA	N	128.76	-1.0	1
UNMAPPED	33	LEU	N	122.86	-1.0	1
UNMAPPED	35	ASP	C	176.47	-1.0	1
UNMAPPED	14	ASP	H	8.58	-1.0	1
UNMAPPED	28	THR	H	7.25	-1.0	5
UNMAPPED	4	TRP	C	173.9	-1.0	1
UNMAPPED	44	ALA	CA	50.75	-1.0	1
UNMAPPED	17	ALA	H	7.29	-1.0	5
UNMAPPED	30	PHE	C	178.78	-1.0	5
UNMAPPED	27	GLY	C	175.0	-1.0	5
UNMAPPED	42	CYS	H	8.83	-1.0	1
UNMAPPED	54	ASP	HA	4.29	-1.0	5
UNMAPPED	32	GLU	N	116.37	-1.0	1
UNMAPPED	32	GLU	CA	54.69	-1.0	1
UNMAPPED	35	ASP	N	120.66	-1.0	1
UNMAPPED	3	LYS	C	174.69	-1.0	5
UNMAPPED	31	GLU	H	9.59	-1.0	5
UNMAPPED	28	THR	CB	67.81	-1.0	5
UNMAPPED	38	VAL	CB	34.74	-1.0	1
UNMAPPED	28	THR	CA	63.21	-1.0	5
UNMAPPED	8	ILE	C	178.36	-1.0	1
UNMAPPED	2	ALA	HA	4.64	-1.0	1
UNMAPPED	40	PRO	CA	63.07	-1.0	1
UNMAPPED	47	SER	C	175.85	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	38	VAL	C	172.11	-1.0	1
UNMAPPED	46	LYS	CB	32.31	-1.0	5
UNMAPPED	16	ASP	CB	40.02	-1.0	5
UNMAPPED	21	ASP	H	9.21	-1.0	1
UNMAPPED	50	GLU	CB	33.27	-1.0	1
UNMAPPED	24	ILE	C	176.47	-1.0	1
UNMAPPED	13	TYR	N	127.85	-1.0	5
UNMAPPED	49	PHE	N	118.8	-1.0	1
UNMAPPED	9	CYS	H	9.32	-1.0	1
UNMAPPED	30	PHE	CB	37.91	-1.0	5
UNMAPPED	13	TYR	CA	57.34	-1.0	1
UNMAPPED	46	LYS	H	8.45	-1.0	5
UNMAPPED	30	PHE	CA	60.74	-1.0	5
UNMAPPED	18	GLY	N	103.8	-1.0	5
UNMAPPED	30	PHE	N	126.02	-1.0	5
UNMAPPED	2	ALA	CB	21.74	-1.0	5
UNMAPPED	41	ILE	N	122.03	-1.0	1
UNMAPPED	51	LYS	N	127.34	-1.0	5
UNMAPPED	19	ASP	HB3	2.98	-1.0	2
UNMAPPED	3	LYS	H	8.3	-1.0	5
UNMAPPED	41	ILE	CA	60.47	-1.0	1
UNMAPPED	54	ASP	HB2	2.627	-1.0	5
UNMAPPED	18	GLY	HA2	3.98	-1.0	2
UNMAPPED	54	ASP	CB	42.01	-1.0	5
UNMAPPED	10	GLY	H	8.04	-1.0	1
UNMAPPED	37	TRP	C	174.9	-1.0	1
UNMAPPED	39	CYS	N	121.69	-1.0	1
UNMAPPED	43	GLY	CA	45.38	-1.0	1
UNMAPPED	17	ALA	N	120.46	-1.0	5
UNMAPPED	8	ILE	CA	61.75	-1.0	1
UNMAPPED	25	SER	H	8.65	-1.0	1
UNMAPPED	8	ILE	CB	34.84	-1.0	1
UNMAPPED	12	ILE	H	7.03	-1.0	1
UNMAPPED	21	ASP	CA	56.48	-1.0	1
UNMAPPED	38	VAL	N	117.29	-1.0	1
UNMAPPED	53	GLU	C	174.78	-1.0	5
UNMAPPED	41	ILE	C	178.12	-1.0	1
UNMAPPED	14	ASP	N	129.92	-1.0	1
UNMAPPED	37	TRP	H	7.61	-1.0	1
UNMAPPED	7	LYS	H	9.07	-1.0	1
UNMAPPED	6	CYS	CB	30.39	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	5	VAL	CA	58.12	-1.0	1
UNMAPPED	14	ASP	CB	41.96	-1.0	5
UNMAPPED	4	TRP	H	9.51	-1.0	5
UNMAPPED	48	GLU	HA	4.76	-1.0	1
UNMAPPED	5	VAL	CB	35.48	-1.0	1
UNMAPPED	37	TRP	NE1	129.74	-1.0	1
UNMAPPED	25	SER	N	125.04	-1.0	1
UNMAPPED	12	ILE	C	175.11	-1.0	1
UNMAPPED	11	TYR	N	128.36	-1.0	1
UNMAPPED	19	ASP	N	116.85	-1.0	1
UNMAPPED	25	SER	CA	57.27	-1.0	1
UNMAPPED	27	GLY	N	113.79	-1.0	1
UNMAPPED	11	TYR	CA	59.81	-1.0	1
UNMAPPED	29	LYS	CA	55.53	-1.0	5
UNMAPPED	11	TYR	CB	39.64	-1.0	1
UNMAPPED	19	ASP	CB	40.14	-1.0	1
UNMAPPED	51	LYS	CB	30.87	-1.0	1
UNMAPPED	29	LYS	CB	31.61	-1.0	5
UNMAPPED	9	CYS	CA	58.44	-1.0	1
UNMAPPED	17	ALA	HB1	1.48	-1.0	5
UNMAPPED	48	GLU	N	121.31	-1.0	1
UNMAPPED	47	SER	CB	61.81	-1.0	1
UNMAPPED	15	GLU	H	8.24	-1.0	5
UNMAPPED	44	ALA	H	9.14	-1.0	1
UNMAPPED	4	TRP	NE1	129.2	-1.0	5
UNMAPPED	46	LYS	C	178.27	-1.0	1
UNMAPPED	48	GLU	HB2	2.58	-1.0	2
UNMAPPED	48	GLU	CB	27.67	-1.0	1
UNMAPPED	31	GLU	N	114.98	-1.0	5
UNMAPPED	31	GLU	C	176.82	-1.0	1
UNMAPPED	31	GLU	CB	28.23	-1.0	5
UNMAPPED	3	LYS	HB2	1.63	-1.0	5
UNMAPPED	44	ALA	CB	19.03	-1.0	1
UNMAPPED	39	CYS	H	8.97	-1.0	1
UNMAPPED	10	GLY	CA	45.33	-1.0	1
UNMAPPED	52	LEU	CB	42.41	-1.0	5
UNMAPPED	5	VAL	C	172.81	-1.0	1
UNMAPPED	7	LYS	C	176.43	-1.0	1
UNMAPPED	22	ASN	CA	52.03	-1.0	1
UNMAPPED	18	GLY	CA	44.36	-1.0	1
UNMAPPED	22	ASN	HD22	6.98	-1.0	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	29	LYS	HA	4.22	-1.0	5
UNMAPPED	51	LYS	CA	56.8	-1.0	1
UNMAPPED	22	ASN	H	7.67	-1.0	1
UNMAPPED	12	ILE	CA	58.63	-1.0	1
UNMAPPED	23	GLY	N	106.03	-1.0	1
UNMAPPED	24	ILE	N	121.84	-1.0	1
UNMAPPED	36	ASP	H	8.18	-1.0	1
UNMAPPED	32	GLU	CB	29.4	-1.0	1
UNMAPPED	23	GLY	CA	45.57	-1.0	1
UNMAPPED	7	LYS	N	131.28	-1.0	1
UNMAPPED	35	ASP	CB	39.93	-1.0	1
UNMAPPED	24	ILE	CB	35.46	-1.0	1
UNMAPPED	4	TRP	N	124.22	-1.0	5
UNMAPPED	9	CYS	C	177.64	-1.0	1
UNMAPPED	4	TRP	CA	55.16	-1.0	1
UNMAPPED	40	PRO	CB	31.66	-1.0	1
UNMAPPED	46	LYS	CA	60.01	-1.0	5
UNMAPPED	17	ALA	C	179.93	-1.0	5
UNMAPPED	46	LYS	N	117.88	-1.0	5
UNMAPPED	27	GLY	H	8.22	-1.0	1
UNMAPPED	26	PRO	C	176.69	-1.0	1
UNMAPPED	12	ILE	HG21	0.65	-1.0	1
UNMAPPED	50	GLU	N	120.12	-1.0	1
UNMAPPED	51	LYS	C	176.65	-1.0	1
UNMAPPED	22	ASN	ND2	119.63	-1.0	1
UNMAPPED	12	ILE	HG22	0.65	-1.0	1
UNMAPPED	42	CYS	C	177.64	-1.0	1
UNMAPPED	2	ALA	HB1	1.46	-1.0	1
UNMAPPED	13	TYR	CB	38.67	-1.0	1
UNMAPPED	49	PHE	CB	42.34	-1.0	1
UNMAPPED	2	ALA	HB2	1.46	-1.0	1
UNMAPPED	15	GLU	N	124.68	-1.0	5
UNMAPPED	49	PHE	CA	56.21	-1.0	1
UNMAPPED	28	THR	HB	3.93	-1.0	5
UNMAPPED	43	GLY	H	7.89	-1.0	1
UNMAPPED	37	TRP	HE1	10.6	-1.0	1
UNMAPPED	33	LEU	H	6.82	-1.0	1
UNMAPPED	4	TRP	HA	4.98	-1.0	5
UNMAPPED	53	GLU	H	8.15	-1.0	5
UNMAPPED	41	ILE	CB	34.89	-1.0	1
UNMAPPED	48	GLU	H	8.42	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	34	PRO	CB	32.02	-1.0	1
UNMAPPED	53	GLU	CA	55.57	-1.0	5
UNMAPPED	54	ASP	N	126.99	-1.0	5
UNMAPPED	53	GLU	HB3	1.82	-1.0	5
UNMAPPED	25	SER	CB	61.71	-1.0	1
UNMAPPED	26	PRO	CB	31.2	-1.0	1
UNMAPPED	17	ALA	CB	19.76	-1.0	5
UNMAPPED	54	ASP	CA	55.62	-1.0	5
UNMAPPED	17	ALA	CA	52.01	-1.0	5
UNMAPPED	51	LYS	H	8.3	-1.0	5
UNMAPPED	8	ILE	N	122.14	-1.0	1
UNMAPPED	53	GLU	HA	4.29	-1.0	1
UNMAPPED	47	SER	CA	59.66	-1.0	1
UNMAPPED	6	CYS	CA	59.24	-1.0	1
UNMAPPED	45	PRO	C	177.12	-1.0	5
UNMAPPED	22	ASN	C	175.19	-1.0	1
UNMAPPED	6	CYS	N	131.23	-1.0	1
UNMAPPED	5	VAL	N	123.28	-1.0	1
UNMAPPED	3	LYS	HA	5.47	-1.0	5
UNMAPPED	21	ASP	N	120.46	-1.0	1
UNMAPPED	52	LEU	CA	54.55	-1.0	5
UNMAPPED	16	ASP	H	8.0	-1.0	1
UNMAPPED	19	ASP	HA	5.16	-1.0	1
UNMAPPED	50	GLU	C	174.1	-1.0	1
UNMAPPED	22	ASN	N	114.94	-1.0	1
UNMAPPED	21	ASP	CB	39.6	-1.0	1
UNMAPPED	6	CYS	C	178.85	-1.0	1
UNMAPPED	19	ASP	CA	52.24	-1.0	1
UNMAPPED	39	CYS	CB	30.75	-1.0	1
UNMAPPED	9	CYS	CB	33.17	-1.0	1
UNMAPPED	18	GLY	H	8.12	-1.0	5
UNMAPPED	22	ASN	CB	38.87	-1.0	1
UNMAPPED	29	LYS	N	130.03	-1.0	1
UNMAPPED	17	ALA	HB3	1.48	-1.0	5
UNMAPPED	48	GLU	CA	54.73	-1.0	1
UNMAPPED	9	CYS	N	122.15	-1.0	1
UNMAPPED	2	ALA	H	8.92	-1.0	1
UNMAPPED	34	PRO	CA	62.12	-1.0	1
UNMAPPED	3	LYS	CB	35.93	-1.0	5
UNMAPPED	16	ASP	C	177.23	-1.0	5
UNMAPPED	11	TYR	C	173.08	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	3	LYS	CA	54.61	-1.0	5
UNMAPPED	28	THR	C	174.48	-1.0	1
UNMAPPED	29	LYS	C	177.2	-1.0	5
UNMAPPED	3	LYS	N	118.71	-1.0	5

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	53	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	48	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	46	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{15}\text{N}$	48	0.00 $\pm$ 0.00	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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 577. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/240 (0%)	0/95 (0%)	0/100 (0%)	0/45 (0%)
Sidechain	0/279 (0%)	0/166 (0%)	0/107 (0%)	0/6 (0%)
Aromatic	0/58 (0%)	0/30 (0%)	0/26 (0%)	0/2 (0%)
Overall	0/577 (0%)	0/291 (0%)	0/233 (0%)	0/53 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 612. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	0/255 (0%)	0/101 (0%)	0/106 (0%)	0/48 (0%)
Sidechain	0/299 (0%)	0/177 (0%)	0/116 (0%)	0/6 (0%)
Aromatic	0/58 (0%)	0/30 (0%)	0/26 (0%)	0/2 (0%)
Overall	0/612 (0%)	0/308 (0%)	0/248 (0%)	0/56 (0%)

## 7.2.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

## 7.2.5 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.

## 7.3 Chemical shift list 3

File name: BMRB entry 5601

Chemical shift list name: *assigned\_chem\_shift\_list\_3*

### 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	281
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	281
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- Chain not found in structure. All 281 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	12	TYR	CA	57.34	-1.0	1
UNMAPPED	21	ASN	H	7.67	-1.0	1
UNMAPPED	47	GLU	HA	4.76	-1.0	1
UNMAPPED	12	TYR	N	127.38	-1.0	5
UNMAPPED	35	ASP	N	114.26	-1.0	1
UNMAPPED	30	GLU	H	9.39	-1.0	5
UNMAPPED	19	PRO	CA	64.99	-1.0	1
UNMAPPED	45	LYS	C	178.27	-1.0	1
UNMAPPED	38	CYS	H	8.97	-1.0	1
UNMAPPED	19	PRO	CB	31.53	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	8	CYS	N	122.15	-1.0	1
UNMAPPED	10	TYR	C	173.08	-1.0	1
UNMAPPED	35	ASP	H	8.18	-1.0	1
UNMAPPED	16	ALA	HB3	1.47	-1.0	5
UNMAPPED	48	PHE	C	177.09	-1.0	1
UNMAPPED	17	GLY	H	8.3	-1.0	5
UNMAPPED	16	ALA	N	120.14	-1.0	5
UNMAPPED	51	LEU	CB	42.54	-1.0	5
UNMAPPED	9	GLY	N	113.47	-1.0	1
UNMAPPED	40	ILE	CB	34.89	-1.0	1
UNMAPPED	47	GLU	H	8.42	-1.0	1
UNMAPPED	2	LYS	HB2	1.54	-1.0	5
UNMAPPED	43	ALA	CA	50.75	-1.0	1
UNMAPPED	39	PRO	CB	31.66	-1.0	1
UNMAPPED	43	ALA	CB	19.03	-1.0	1
UNMAPPED	6	LYS	CA	58.43	-1.0	1
UNMAPPED	4	VAL	N	123.28	-1.0	1
UNMAPPED	3	TRP	C	173.9	-1.0	1
UNMAPPED	48	PHE	CA	56.21	-1.0	1
UNMAPPED	42	GLY	C	173.26	-1.0	1
UNMAPPED	4	VAL	CB	35.48	-1.0	1
UNMAPPED	34	ASP	CB	39.93	-1.0	1
UNMAPPED	52	GLU	H	8.05	-1.0	5
UNMAPPED	1	ALA	H	8.92	-1.0	1
UNMAPPED	1	ALA	HA	4.64	-1.0	1
UNMAPPED	27	THR	H	7.1	-1.0	5
UNMAPPED	47	GLU	C	173.75	-1.0	1
UNMAPPED	2	LYS	H	8.67	-1.0	5
UNMAPPED	49	GLU	H	9.09	-1.0	1
UNMAPPED	3	TRP	N	123.55	-1.0	5
UNMAPPED	26	GLY	C	174.36	-1.0	5
UNMAPPED	31	GLU	CA	54.69	-1.0	1
UNMAPPED	52	GLU	HB2	2.12	-1.0	2
UNMAPPED	3	TRP	CB	31.55	-1.0	1
UNMAPPED	11	ILE	CA	58.63	-1.0	1
UNMAPPED	21	ASN	CA	52.03	-1.0	1
UNMAPPED	39	PRO	C	176.18	-1.0	1
UNMAPPED	46	SER	N	110.12	-1.0	1
UNMAPPED	14	GLU	H	8.42	-1.0	5
UNMAPPED	29	PHE	N	125.97	-1.0	5
UNMAPPED	2	LYS	C	174.46	-1.0	5

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	5	CYS	H	9.23	-1.0	1
UNMAPPED	53	ASP	HA	4.33	-1.0	5
UNMAPPED	20	ASP	C	177.04	-1.0	1
UNMAPPED	28	LYS	N	130.03	-1.0	1
UNMAPPED	16	ALA	CB	19.7	-1.0	5
UNMAPPED	32	LEU	H	6.82	-1.0	1
UNMAPPED	46	SER	CA	59.66	-1.0	1
UNMAPPED	47	GLU	HB3	2.0	-1.0	2
UNMAPPED	15	ASP	CA	56.8	-1.0	5
UNMAPPED	28	LYS	CB	31.77	-1.0	5
UNMAPPED	3	TRP	HA	4.98	-1.0	5
UNMAPPED	47	GLU	N	121.31	-1.0	1
UNMAPPED	18	ASP	HA	5.16	-1.0	1
UNMAPPED	47	GLU	CA	54.73	-1.0	1
UNMAPPED	45	LYS	CB	32.21	-1.0	5
UNMAPPED	52	GLU	HA	4.29	-1.0	1
UNMAPPED	31	GLU	N	116.37	-1.0	1
UNMAPPED	24	SER	CB	61.71	-1.0	1
UNMAPPED	5	CYS	C	178.85	-1.0	1
UNMAPPED	24	SER	CA	57.27	-1.0	1
UNMAPPED	16	ALA	HB2	1.47	-1.0	5
UNMAPPED	44	PRO	CB	32.31	-1.0	1
UNMAPPED	33	PRO	CA	62.12	-1.0	1
UNMAPPED	24	SER	N	125.04	-1.0	1
UNMAPPED	29	PHE	CB	37.95	-1.0	5
UNMAPPED	28	LYS	HG2	1.41	-1.0	2
UNMAPPED	3	TRP	HE1	9.74	-1.0	5
UNMAPPED	40	ILE	N	122.03	-1.0	1
UNMAPPED	28	LYS	HA	4.27	-1.0	5
UNMAPPED	2	LYS	N	117.83	-1.0	5
UNMAPPED	17	GLY	HA3	3.58	-1.0	2
UNMAPPED	9	GLY	C	173.99	-1.0	1
UNMAPPED	2	LYS	CA	54.46	-1.0	5
UNMAPPED	18	ASP	HB3	2.98	-1.0	2
UNMAPPED	7	ILE	C	178.36	-1.0	1
UNMAPPED	10	TYR	CB	39.64	-1.0	1
UNMAPPED	38	CYS	N	121.69	-1.0	1
UNMAPPED	18	ASP	N	116.85	-1.0	1
UNMAPPED	13	ASP	CB	41.75	-1.0	5
UNMAPPED	35	ASP	C	175.57	-1.0	1
UNMAPPED	44	PRO	C	177.16	-1.0	5

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	15	ASP	C	177.59	-1.0	5
UNMAPPED	17	GLY	N	104.26	-1.0	5
UNMAPPED	13	ASP	CA	50.97	-1.0	5
UNMAPPED	11	ILE	H	7.03	-1.0	1
UNMAPPED	36	TRP	HE1	10.46	-1.0	1
UNMAPPED	52	GLU	C	174.82	-1.0	5
UNMAPPED	28	LYS	CA	55.81	-1.0	5
UNMAPPED	23	ILE	H	7.6	-1.0	1
UNMAPPED	5	CYS	N	131.23	-1.0	1
UNMAPPED	14	GLU	CA	58.37	-1.0	5
UNMAPPED	22	GLY	C	173.8	-1.0	1
UNMAPPED	37	VAL	C	172.11	-1.0	1
UNMAPPED	48	PHE	N	118.8	-1.0	1
UNMAPPED	5	CYS	CA	59.24	-1.0	1
UNMAPPED	8	CYS	CB	33.17	-1.0	1
UNMAPPED	32	LEU	N	122.86	-1.0	1
UNMAPPED	33	PRO	C	177.03	-1.0	1
UNMAPPED	8	CYS	CA	58.44	-1.0	1
UNMAPPED	32	LEU	CA	52.85	-1.0	1
UNMAPPED	40	ILE	C	178.12	-1.0	1
UNMAPPED	15	ASP	H	8.0	-1.0	1
UNMAPPED	15	ASP	N	114.14	-1.0	1
UNMAPPED	11	ILE	HA	4.76	-1.0	1
UNMAPPED	50	LYS	H	8.31	-1.0	5
UNMAPPED	7	ILE	H	9.08	-1.0	1
UNMAPPED	11	ILE	HB	1.46	-1.0	1
UNMAPPED	23	ILE	C	176.47	-1.0	1
UNMAPPED	1	ALA	HB3	1.46	-1.0	1
UNMAPPED	51	LEU	CA	54.41	-1.0	5
UNMAPPED	6	LYS	CB	31.53	-1.0	1
UNMAPPED	43	ALA	N	128.76	-1.0	1
UNMAPPED	30	GLU	C	176.82	-1.0	1
UNMAPPED	6	LYS	N	131.28	-1.0	1
UNMAPPED	50	LYS	N	127.52	-1.0	5
UNMAPPED	4	VAL	CA	58.12	-1.0	1
UNMAPPED	52	GLU	CA	55.47	-1.0	5
UNMAPPED	53	ASP	H	8.01	-1.0	5
UNMAPPED	49	GLU	C	174.1	-1.0	1
UNMAPPED	16	ALA	HA	4.29	-1.0	5
UNMAPPED	26	GLY	N	113.79	-1.0	1
UNMAPPED	25	PRO	C	176.69	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	18	ASP	H	8.26	-1.0	1
UNMAPPED	9	GLY	CA	45.33	-1.0	1
UNMAPPED	17	GLY	C	173.27	-1.0	1
UNMAPPED	12	TYR	H	9.7	-1.0	5
UNMAPPED	36	TRP	CA	59.71	-1.0	1
UNMAPPED	3	TRP	CA	55.16	-1.0	1
UNMAPPED	21	ASN	HD22	6.98	-1.0	2
UNMAPPED	42	GLY	CA	45.38	-1.0	1
UNMAPPED	21	ASN	CB	38.87	-1.0	1
UNMAPPED	21	ASN	HD21	9.36	-1.0	2
UNMAPPED	42	GLY	N	112.97	-1.0	1
UNMAPPED	27	THR	C	174.48	-1.0	1
UNMAPPED	23	ILE	N	121.84	-1.0	1
UNMAPPED	39	PRO	CA	63.07	-1.0	1
UNMAPPED	21	ASN	N	114.94	-1.0	1
UNMAPPED	23	ILE	CA	57.37	-1.0	1
UNMAPPED	53	ASP	HB2	2.47	-1.0	5
UNMAPPED	38	CYS	CB	30.75	-1.0	1
UNMAPPED	16	ALA	H	7.22	-1.0	5
UNMAPPED	25	PRO	CB	31.2	-1.0	1
UNMAPPED	29	PHE	CA	60.65	-1.0	5
UNMAPPED	31	GLU	CB	29.4	-1.0	1
UNMAPPED	41	CYS	CA	58.42	-1.0	1
UNMAPPED	11	ILE	C	175.33	-1.0	1
UNMAPPED	51	LEU	H	8.76	-1.0	5
UNMAPPED	31	GLU	H	7.41	-1.0	1
UNMAPPED	47	GLU	CB	27.67	-1.0	1
UNMAPPED	41	CYS	CB	32.53	-1.0	1
UNMAPPED	21	ASN	C	175.19	-1.0	1
UNMAPPED	28	LYS	C	177.4	-1.0	5
UNMAPPED	26	GLY	H	8.22	-1.0	1
UNMAPPED	43	ALA	H	9.14	-1.0	1
UNMAPPED	41	CYS	H	8.83	-1.0	1
UNMAPPED	20	ASP	CA	56.48	-1.0	1
UNMAPPED	37	VAL	CB	34.74	-1.0	1
UNMAPPED	46	SER	CB	61.81	-1.0	1
UNMAPPED	20	ASP	CB	39.6	-1.0	1
UNMAPPED	46	SER	H	7.91	-1.0	1
UNMAPPED	27	THR	N	117.1	-1.0	5
UNMAPPED	41	CYS	N	121.29	-1.0	1
UNMAPPED	4	VAL	H	9.74	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	34	ASP	H	8.71	-1.0	1
UNMAPPED	27	THR	CA	62.52	-1.0	5
UNMAPPED	52	GLU	CB	30.84	-1.0	5
UNMAPPED	1	ALA	CB	19.94	-1.0	5
UNMAPPED	19	PRO	C	180.06	-1.0	1
UNMAPPED	27	THR	CB	68.01	-1.0	5
UNMAPPED	11	ILE	HG23	0.65	-1.0	1
UNMAPPED	36	TRP	NE1	129.59	-1.0	1
UNMAPPED	31	GLU	C	176.76	-1.0	1
UNMAPPED	10	TYR	CA	59.81	-1.0	1
UNMAPPED	20	ASP	N	120.46	-1.0	1
UNMAPPED	10	TYR	N	128.36	-1.0	1
UNMAPPED	3	TRP	H	9.42	-1.0	5
UNMAPPED	38	CYS	CA	56.69	-1.0	1
UNMAPPED	48	PHE	CB	42.34	-1.0	1
UNMAPPED	42	GLY	H	7.89	-1.0	1
UNMAPPED	21	ASN	ND2	119.63	-1.0	1
UNMAPPED	33	PRO	CB	32.02	-1.0	1
UNMAPPED	14	GLU	CB	30.1	-1.0	5
UNMAPPED	50	LYS	C	176.65	-1.0	1
UNMAPPED	5	CYS	CB	30.39	-1.0	1
UNMAPPED	16	ALA	HB1	1.47	-1.0	5
UNMAPPED	16	ALA	CA	52.02	-1.0	5
UNMAPPED	35	ASP	CB	39.09	-1.0	1
UNMAPPED	14	GLU	N	124.46	-1.0	5
UNMAPPED	29	PHE	H	9.85	-1.0	5
UNMAPPED	32	LEU	CB	39.29	-1.0	1
UNMAPPED	27	THR	HB	4.04	-1.0	5
UNMAPPED	35	ASP	CA	51.96	-1.0	1
UNMAPPED	51	LEU	N	129.56	-1.0	5
UNMAPPED	50	LYS	CA	56.8	-1.0	1
UNMAPPED	28	LYS	H	8.76	-1.0	5
UNMAPPED	50	LYS	CB	30.87	-1.0	1
UNMAPPED	45	LYS	H	8.51	-1.0	5
UNMAPPED	1	ALA	HB2	1.46	-1.0	1
UNMAPPED	22	GLY	CA	45.57	-1.0	1
UNMAPPED	24	SER	H	8.65	-1.0	1
UNMAPPED	1	ALA	HB1	1.46	-1.0	1
UNMAPPED	26	GLY	CA	45.14	-1.0	5
UNMAPPED	22	GLY	N	106.03	-1.0	1
UNMAPPED	20	ASP	H	9.21	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	40	ILE	H	8.72	-1.0	1
UNMAPPED	8	CYS	C	178.011	-1.0	1
UNMAPPED	34	ASP	N	120.66	-1.0	1
UNMAPPED	48	PHE	H	7.75	-1.0	1
UNMAPPED	49	GLU	CA	53.34	-1.0	1
UNMAPPED	34	ASP	CA	56.42	-1.0	1
UNMAPPED	40	ILE	CA	60.47	-1.0	1
UNMAPPED	1	ALA	N	125.82	-1.0	1
UNMAPPED	10	TYR	H	9.38	-1.0	1
UNMAPPED	30	GLU	N	114.68	-1.0	5
UNMAPPED	11	ILE	N	126.19	-1.0	1
UNMAPPED	2	LYS	HA	5.58	-1.0	5
UNMAPPED	2	LYS	CB	35.81	-1.0	5
UNMAPPED	36	TRP	CB	29.22	-1.0	1
UNMAPPED	13	ASP	H	8.58	-1.0	1
UNMAPPED	46	SER	C	175.85	-1.0	1
UNMAPPED	30	GLU	CB	28.13	-1.0	5
UNMAPPED	11	ILE	CB	38.78	-1.0	1
UNMAPPED	4	VAL	C	172.81	-1.0	1
UNMAPPED	37	VAL	N	117.29	-1.0	1
UNMAPPED	49	GLU	CB	33.22	-1.0	1
UNMAPPED	1	ALA	C	175.84	-1.0	1
UNMAPPED	37	VAL	CA	56.6	-1.0	1
UNMAPPED	23	ILE	CB	35.46	-1.0	1
UNMAPPED	53	ASP	CB	41.7	-1.0	5
UNMAPPED	37	VAL	H	6.17	-1.0	1
UNMAPPED	25	PRO	CA	63.79	-1.0	1
UNMAPPED	8	CYS	H	9.32	-1.0	1
UNMAPPED	17	GLY	CA	44.36	-1.0	1
UNMAPPED	36	TRP	C	174.9	-1.0	1
UNMAPPED	16	ALA	C	179.79	-1.0	5
UNMAPPED	47	GLU	HB2	2.58	-1.0	2
UNMAPPED	15	ASP	CB	40.55	-1.0	5
UNMAPPED	34	ASP	C	176.47	-1.0	1
UNMAPPED	9	GLY	H	8.04	-1.0	1
UNMAPPED	45	LYS	N	117.57	-1.0	5
UNMAPPED	36	TRP	N	123.42	-1.0	1
UNMAPPED	7	ILE	CB	34.84	-1.0	1
UNMAPPED	45	LYS	CA	60.03	-1.0	5
UNMAPPED	6	LYS	C	176.43	-1.0	1
UNMAPPED	7	ILE	CA	61.75	-1.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	22	GLY	H	7.76	-1.0	1
UNMAPPED	6	LYS	H	9.07	-1.0	1
UNMAPPED	7	ILE	N	122.14	-1.0	1
UNMAPPED	29	PHE	C	178.77	-1.0	5
UNMAPPED	44	PRO	CA	61.48	-1.0	1
UNMAPPED	3	TRP	NE1	130.68	-1.0	5
UNMAPPED	13	ASP	C	176.47	-1.0	5
UNMAPPED	36	TRP	H	7.61	-1.0	1
UNMAPPED	52	GLU	HB3	1.88	-1.0	5
UNMAPPED	1	ALA	CA	51.13	-1.0	5
UNMAPPED	30	GLU	CA	58.27	-1.0	5
UNMAPPED	51	LEU	C	176.65	-1.0	5
UNMAPPED	52	GLU	N	120.8	-1.0	5
UNMAPPED	11	ILE	HG22	0.65	-1.0	1
UNMAPPED	53	ASP	CA	55.47	-1.0	5
UNMAPPED	14	GLU	C	177.73	-1.0	1
UNMAPPED	17	GLY	HA2	3.98	-1.0	2
UNMAPPED	18	ASP	CA	52.24	-1.0	1
UNMAPPED	11	ILE	HG21	0.65	-1.0	1
UNMAPPED	53	ASP	N	127.23	-1.0	5
UNMAPPED	49	GLU	N	120.12	-1.0	1
UNMAPPED	18	ASP	CB	40.14	-1.0	1
UNMAPPED	13	ASP	N	129.92	-1.0	1
UNMAPPED	12	TYR	CB	38.67	-1.0	1
UNMAPPED	41	CYS	C	177.64	-1.0	1

### 7.3.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	53	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	48	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	46	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{15}\text{N}$	48	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)

### 7.3.3 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 577. 0 out of 3 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	0/240 (0%)	0/95 (0%)	0/100 (0%)	0/45 (0%)
Sidechain	0/279 (0%)	0/166 (0%)	0/107 (0%)	0/6 (0%)
Aromatic	0/58 (0%)	0/30 (0%)	0/26 (0%)	0/2 (0%)
Overall	0/577 (0%)	0/291 (0%)	0/233 (0%)	0/53 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 612. 0 out of 4 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	0/255 (0%)	0/101 (0%)	0/106 (0%)	0/48 (0%)
Sidechain	0/299 (0%)	0/177 (0%)	0/116 (0%)	0/6 (0%)
Aromatic	0/58 (0%)	0/30 (0%)	0/26 (0%)	0/2 (0%)
Overall	0/612 (0%)	0/308 (0%)	0/248 (0%)	0/56 (0%)

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

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned\_chem\_shift\_list\_3). RCI is only applicable to proteins.