

# Full wwPDB NMR Structure Validation Report (i)

Aug 8, 2023 – 03:14 pm BST

PDB ID : 8OS0 BMRB ID : 34808

Title : Solution NMR structure of Notch3 WT TMD Authors : Guschtschin-Schmidt, N.; Muhle-Goll, C.

Deposited on : 2023-04-17

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

wwPDB-RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

 $\begin{array}{ccc} wwPDB\text{-}ShiftChecker &: & v1.2 \\ BMRB \ Restraints \ Analysis &: & v1.2 \\ \end{array}$ 

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

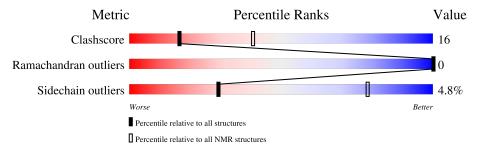
Validation Pipeline (wwPDB-VP) : 2.35

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $SOLUTION\ NMR$ 

The overall completeness of chemical shifts assignment is 82%.

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	NMR archive	
Metric	$(\# \mathrm{Entries})$	$(\# { m Entries})$	
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 >=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 <=5%

Mol	Chain	Length		Quality of chain				
1	A	30	30%	17%	53%			



## 2 Ensemble composition and analysis (i)

This entry contains 40 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: closest to the average.

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 mod				
1	A:1648-A:1661 (14)	0.34	8	

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters. No single-model clusters were found.

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



## 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 510 atoms, of which 288 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Notch 3 extracellular truncation.

Mol	Chain	Residues	Atoms				Trace		
1	Λ	20	Total	С	Н	N	О	S	0
	1 A .	30	510	154	288	36	31	1	U

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1639	LYS	-	expression tag	UNP Q9UM47
A	1640	LYS	-	expression tag	UNP Q9UM47
A	1641	LYS	-	expression tag	UNP Q9UM47
A	1666	LYS	-	expression tag	UNP Q9UM47
A	1667	LYS	-	expression tag	UNP Q9UM47
A	1668	LYS	-	expression tag	UNP Q9UM47



## 4 Residue-property plots (i)

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

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Notch 3 extracellular truncation

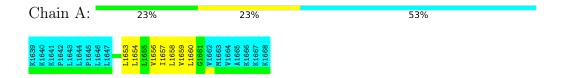


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

• Molecule 1: Notch 3 extracellular truncation



#### 4.2.2 Score per residue for model 2

• Molecule 1: Notch 3 extracellular truncation





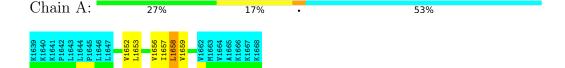
#### 4.2.3 Score per residue for model 3

• Molecule 1: Notch 3 extracellular truncation



#### 4.2.4 Score per residue for model 4

• Molecule 1: Notch 3 extracellular truncation



#### 4.2.5 Score per residue for model 5

• Molecule 1: Notch 3 extracellular truncation



#### 4.2.6 Score per residue for model 6

• Molecule 1: Notch 3 extracellular truncation



## 4.2.7 Score per residue for model 7

• Molecule 1: Notch 3 extracellular truncation





#### 4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: Notch 3 extracellular truncation

Chain A: 33% 13% 53%

KK639
KK640
KK640
KK640
KK641
K642
K1643
K1646
K1646
K1665
K1666
K1666
K1666
K1666
K1666
K1666
K1666
K1666
K1666

### 4.2.9 Score per residue for model 9

• Molecule 1: Notch 3 extracellular truncation

Chain A: 33% 13% 53%

K1639
K1640
K1640
K1640
F1643
F1643
F1645
F1645
F1665
K1666
K1666
K1666
K1666
K1666
K1666
K1666
K1666
K1666

#### 4.2.10 Score per residue for model 10

• Molecule 1: Notch 3 extracellular truncation

Chain A: 30% 17% 53%

K1639
K1640
K1640
L1644
L1644
L1646
L1646
L1653
K1656
K1666
K1666
K1668

#### 4.2.11 Score per residue for model 11

• Molecule 1: Notch 3 extracellular truncation

Chain A: 37% 10% 53%

K1639 K1640 K1641 P1642 L1644 P1646 L1647 L1655 V1652 M1664 M1663 K1666 K1666

#### 4.2.12 Score per residue for model 12

• Molecule 1: Notch 3 extracellular truncation

Chain A: 37% 10% 53%





#### 4.2.13 Score per residue for model 13

• Molecule 1: Notch 3 extracellular truncation

Chain A: 30% 13% • 53%



#### 4.2.14 Score per residue for model 14

• Molecule 1: Notch 3 extracellular truncation

Chain A: 37% 10% 53%



## 4.2.15 Score per residue for model 15

• Molecule 1: Notch 3 extracellular truncation

Chain A: 37% 10% 53%



#### 4.2.16 Score per residue for model 16

• Molecule 1: Notch 3 extracellular truncation

Chain A: 30% 17% 53%



#### 4.2.17 Score per residue for model 17

• Molecule 1: Notch 3 extracellular truncation

Chain A: 30% 13% · 53%





#### 4.2.18 Score per residue for model 18

• Molecule 1: Notch 3 extracellular truncation

Chain A: 37% 10% 53%

KK659
KK640
KK640
KK640
KK640
KK640
KK666
KK666
KK666
KK666
KK666
KK666
KK666
KK666
KK666

#### 4.2.19 Score per residue for model 19

• Molecule 1: Notch 3 extracellular truncation

Chain A: 37% 10% 53%

K1639
K1640
K1641
P1642
L1644
L1646
L1646
L1646
L1647
V1666
V1667
A1665
K1666
K1668

#### 4.2.20 Score per residue for model 20

• Molecule 1: Notch 3 extracellular truncation

Chain A: 30% 17% 53%

KK639
KK641
PK642
PK642
LK643
PK644
PK644
PK645
RK666
KK666
KK666
KK666
KK666
KK666

#### 4.2.21 Score per residue for model 21

• Molecule 1: Notch 3 extracellular truncation

Chain A: 33% 13% 53%

K1638 K1640 K1641 F1642 F1648 F1646 F1646 F1646 F1667 F1667

## 4.2.22 Score per residue for model 22

• Molecule 1: Notch 3 extracellular truncation

Chain A: 33% 13% 53%

K1639
K1640
K1641
P1642
L1643
L1646
L1646
L1657
L1657
L1657
L1657
K1666
K1666
K1666
K1666
K1666
K1666
K1666



#### 4.2.23 Score per residue for model 23

• Molecule 1: Notch 3 extracellular truncation

Chain A: 33% 13% 53%



#### 4.2.24 Score per residue for model 24

• Molecule 1: Notch 3 extracellular truncation

Chain A: 30% 17% 53%

K1639
K1640
K1640
F1642
F1643
F1645
F1646
F1646
F1666
V1665
M1663
M1663
K1666
K1666
K1666
K1666
K1666

#### 4.2.25 Score per residue for model 25

• Molecule 1: Notch 3 extracellular truncation

Chain A: 33% 13% 53%

| K1639 | K1640 | K1660 | K166

#### 4.2.26 Score per residue for model 26

• Molecule 1: Notch 3 extracellular truncation

Chain A: 40% 7% 53%

K1639 K1640 K1641 P1642 L1644 P1645 L1647 L1647 L1647 A1665 K1668 K1668

#### 4.2.27 Score per residue for model 27

• Molecule 1: Notch 3 extracellular truncation

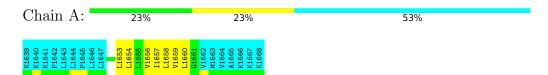
Chain A: 27% 20% 53%

KK6659
KK6656
KK6640
KK6656
LI6643
LI6643
LI6654
LI6655
LI6655
LI6656
LI6656
LI6656
KK666
KK666
KK666
KK666
KK666
KK666
KK666



#### 4.2.28 Score per residue for model 28

• Molecule 1: Notch 3 extracellular truncation



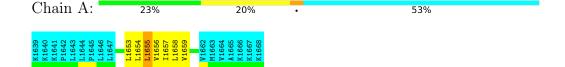
#### 4.2.29 Score per residue for model 29

• Molecule 1: Notch 3 extracellular truncation



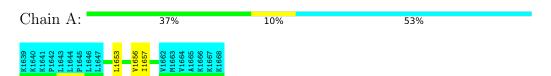
#### 4.2.30 Score per residue for model 30

• Molecule 1: Notch 3 extracellular truncation



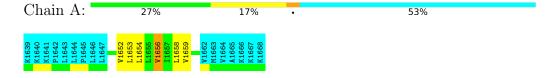
#### 4.2.31 Score per residue for model 31

• Molecule 1: Notch 3 extracellular truncation



#### 4.2.32 Score per residue for model 32

• Molecule 1: Notch 3 extracellular truncation





#### 4.2.33 Score per residue for model 33

• Molecule 1: Notch 3 extracellular truncation

Chain A: 33% 13% 53%



#### 4.2.34 Score per residue for model 34

• Molecule 1: Notch 3 extracellular truncation

Chain A: 27% 20% 53%



#### 4.2.35 Score per residue for model 35

• Molecule 1: Notch 3 extracellular truncation

Chain A: 27% 17% • 53%



#### 4.2.36 Score per residue for model 36

• Molecule 1: Notch 3 extracellular truncation

Chain A: 33% 10% • 53%



#### 4.2.37 Score per residue for model 37

• Molecule 1: Notch 3 extracellular truncation

Chain A: 23% 23% 53%





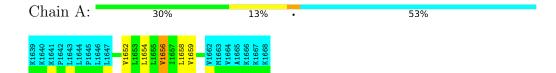
## 4.2.38 Score per residue for model 38

• Molecule 1: Notch 3 extracellular truncation



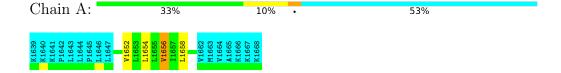
#### 4.2.39 Score per residue for model 39

• Molecule 1: Notch 3 extracellular truncation



#### 4.2.40 Score per residue for model 40

• Molecule 1: Notch 3 extracellular truncation





#### Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: simulated annealing.

Of the 400 calculated structures, 40 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
CNS	refinement	1.2.1
ARIA	structure calculation	2.3.2

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	433
Number of shifts mapped to atoms	433
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%



## 6 Model quality (i)

## 6.1 Standard geometry (i)

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 (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	94	118	118	3±1
All	All	3760	4720	4720	133

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 16.

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

Atom-1	Atom-2	Clash(Å)	$Distance(\mathring{A})$	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:1655:LEU:C	1:A:1655:LEU:HD13	0.56	2.21	35	2
1:A:1656:VAL:HG13	1:A:1657:ILE:N	0.55	2.17	6	31
1:A:1652:VAL:O	1:A:1656:VAL:HG23	0.51	2.06	11	1
1:A:1654:LEU:O	1:A:1658:LEU:HB3	0.48	2.08	7	14
1:A:1653:LEU:HA	1:A:1656:VAL:HG12	0.47	1.87	19	29
1:A:1656:VAL:CG1	1:A:1657:ILE:N	0.47	2.78	26	15
1:A:1656:VAL:HG13	1:A:1657:ILE:HG13	0.45	1.86	1	17
1:A:1657:ILE:HG22	1:A:1658:LEU:N	0.45	2.25	23	7
1:A:1652:VAL:O	1:A:1656:VAL:HG22	0.45	2.11	32	4
1:A:1653:LEU:O	1:A:1657:ILE:HB	0.45	2.12	36	3
1:A:1652:VAL:O	1:A:1656:VAL:HG12	0.44	2.12	4	4
1:A:1660:LEU:O	1:A:1660:LEU:HD23	0.44	2.13	1	1
1:A:1654:LEU:HD12	1:A:1658:LEU:HD22	0.43	1.90	39	1
1:A:1653:LEU:HA	1:A:1657:ILE:HG12	0.43	1.89	14	1



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Atom-1	Atom 2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:1660:LEU:O	1:A:1660:LEU:HD13	0.42	2.14	27	1
1:A:1653:LEU:HA	1:A:1656:VAL:HG23	0.41	1.92	32	2

## 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	Perce	entiles
1	A	14/30 (47%)	13±1 (92±6%)	1±1 (8±6%)	0±0 (0±0%)	100	100
All	All	560/1200 (47%)	514 (92%)	46 (8%)	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	Perce	ntiles
1	A	10/25 (40%)	10±0 (95±5%)	0±0 (5±5%)	29	78
All	All	400/1000 (40%)	381 (95%)	19 (5%)	29	78

All 5 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	1658	LEU	5
1	A	1655	LEU	5
1	A	1656	VAL	4
1	A	1654	LEU	3
1	A	1660	LEU	2



### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 80% for the entire structure.

## 7.1 Chemical shift list 1

File name: working cs.cif

Chemical shift list name: Notch3.str

## 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	433
Number of shifts mapped to atoms	433
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

• Chemical shift has been reported more than once. All 66 occurrences are reported below.

T:-4 ID	Clasia	Das	Т	A 4	Shift Data		a
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	A	1643	LEU	HD12	0.967	•	
1	A	1643	LEU	HD13	0.967	•	
1	A	1643	LEU	HD22	0.906		
1	A	1643	LEU	HD23	0.906	•	•
1	A	1644	LEU	HD12	0.982	•	
1	A	1644	LEU	HD13	0.982	•	
1	A	1644	LEU	HD22	0.919	•	
1	A	1644	LEU	HD23	0.919		
1	A	1646	LEU	HD12	0.968	•	•
1	A	1646	LEU	HD13	0.968		
1	A	1646	LEU	HD22	0.893	•	
1	A	1646	LEU	HD23	0.893	•	
1	A	1647	LEU	HD12	0.919	•	•
1	A	1647	LEU	HD13	0.919	•	
1	A	1647	LEU	HD22	0.877		•



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T : -4 ID	Chair	_		Atom		Shift Dat	a
List ID	Chain	Res	Type		Value	Uncertainty	Ambiguity
1	A	1647	LEU	HD23	0.877	•	
1	A	1648	VAL	HG12	0.940		
1	A	1648	VAL	HG13	0.940	•	
1	A	1648	VAL	HG22	1.007	•	
1	A	1648	VAL	HG23	1.007	•	
1	A	1649	ALA	HB2	1.507	•	
1	A	1649	ALA	HB3	1.507	•	
1	A	1651	ALA	HB2	1.559	•	
1	A	1651	ALA	HB3	1.559	•	
1	A	1652	VAL	HG12	1.056	•	
1	A	1652	VAL	HG13	1.056	•	
1	A	1652	VAL	HG22	0.944	•	
1	A	1652	VAL	HG23	0.944		
1	A	1653	LEU	HD12	0.944		
1	A	1653	LEU	HD13	0.944		
1	A	1653	LEU	HD22	0.902		
1	A	1653	LEU	HD23	0.902	•	
1	A	1654	LEU	HD12	0.936		
1	A	1654	LEU	HD13	0.936	•	
1	A	1654	LEU	HD22	0.898	•	
1	A	1654	LEU	HD23	0.898	•	
1	A	1655	LEU	HD12	0.934	•	
1	A	1655	LEU	HD13	0.934		
1	A	1655	LEU	HD22	0.899	•	
1	A	1655	LEU	HD23	0.899	•	
1	A	1656	VAL	HG12	1.077	•	
1	A	1656	VAL	HG13	1.077	•	
1	A	1656	VAL	HG22	0.937	•	
1	A	1656	VAL	HG23	0.937	•	
1	A	1657	ILE	HD12	0.845	•	
1	A	1657	ILE	HD13	0.845	•	
1	A	1657	ILE	HG22	0.940	•	
1	A	1657	ILE	HG23	0.940	•	
1	A	1658	LEU	HD12	0.888		
1	A	1658	LEU	HD13	0.888	•	
1	A	1659	VAL	HG12	1.080		
1	A	1659	VAL	HG13	1.080		
1	A	1659	VAL	HG22	0.965		
1	A	1659	VAL	HG23	0.965		
1	A	1660	LEU	HD12	0.869		
1	A	1660	LEU	HD13	0.869		



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COMBINE	THOTH.	memors	DULUE.

List ID	Chain	Res	Tuno	Type Atom		Shift Dat	a
LIST ID	Chain	nes	туре	Atom	Value	Uncertainty	Ambiguity
1	A	1662	VAL	HG12	1.096	•	
1	A	1662	VAL	HG13	1.096	•	
1	A	1662	VAL	HG22	0.968	•	
1	A	1662	VAL	HG23	0.968	•	
1	A	1664	VAL	HG12	1.082	•	•
1	A	1664	VAL	HG13	1.082	•	•
1	A	1664	VAL	HG22	0.955	•	•
1	A	1664	VAL	HG23	0.955	•	•
1	A	1665	ALA	HB2	1.549	•	•
1	A	1665	ALA	HB3	1.549	•	

#### 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
$^{13}\mathrm{C}_{\alpha}$	30	$0.12 \pm 0.09$	None needed ( $< 0.5 \text{ ppm}$ )
$^{13}C_{\beta}$	28	$0.81 \pm 0.12$	Should be checked
<sup>13</sup> C′	0		None (insufficient data)
$^{15}N$	28	$0.60 \pm 0.57$	None needed (imprecise)

## 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 82%, i.e. 163 atoms were assigned a chemical shift out of a possible 198. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	57/72 (79%)	29/30 (97%)	$14/28 \ (50\%)$	14/14 (100%)
Sidechain	106/126 (84%)	75/88 (85%)	31/38 (82%)	0/0 (%)
Overall	163/198 (82%)	104/118 (88%)	45/66 (68%)	14/14 (100%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 366 atoms were assigned a chemical shift out of a possible 456. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}{ m C}$	$^{15}{ m N}$
Backbone	116/148 (78%)	58/60 (97%)	30/60~(50%)	28/28 (100%)
Sidechain	250/308 (81%)	169/208 (81%)	81/94 (86%)	0/6 (0%)



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	Total	$^{1}\mathbf{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Overall	366/456 (80%)	227/268 (85%)	111/154 (72%)	28/34 (82%)

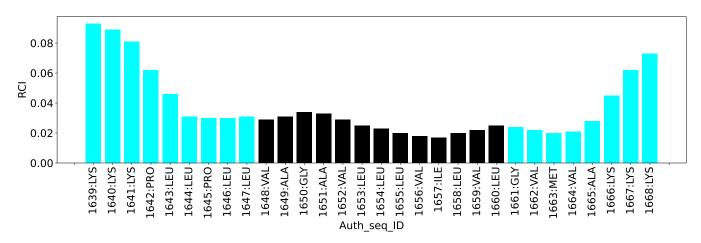
### 7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

### 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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:





# 8 NMR restraints analysis (i)

No restraints data found



# 9 Distance violation analysis (i)

No distance restraints data found



# 10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found

