



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:09 AM BST

PDB ID : 2RQ5  
Title : Solution structure of the AT-rich interaction domain (ARID) of Junji/JARID2  
Authors : Kusunoki, H.; Kohno, T.  
Deposited on : 2009-02-06

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.

---

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

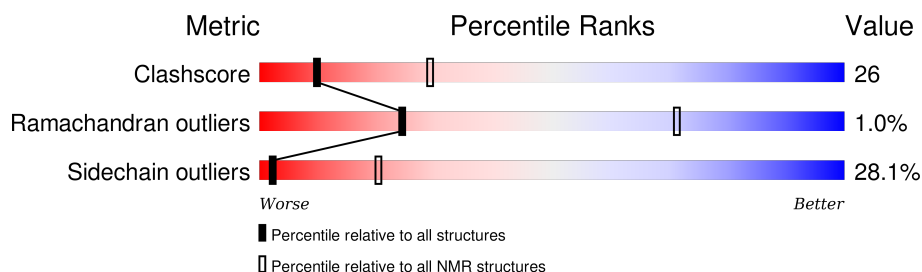
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

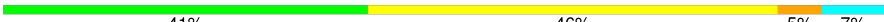
The overall completeness of chemical shifts assignment was not calculated.

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	121	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:619-A:730 (112)	0.29	20

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 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1985 atoms, of which 1010 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein Jumonji.

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1985	615	1010	174	177	9	

There are 5 discrepancies between the modelled and reference sequences:

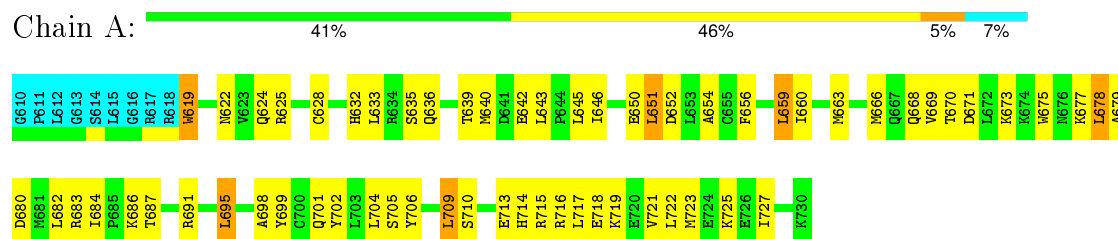
Chain	Residue	Modelled	Actual	Comment	Reference
A	610	GLY	-	EXPRESSION TAG	UNP Q62315
A	611	PRO	-	EXPRESSION TAG	UNP Q62315
A	612	LEU	-	EXPRESSION TAG	UNP Q62315
A	613	GLY	-	EXPRESSION TAG	UNP Q62315
A	614	SER	-	EXPRESSION TAG	UNP Q62315

## 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: Protein Jumonji

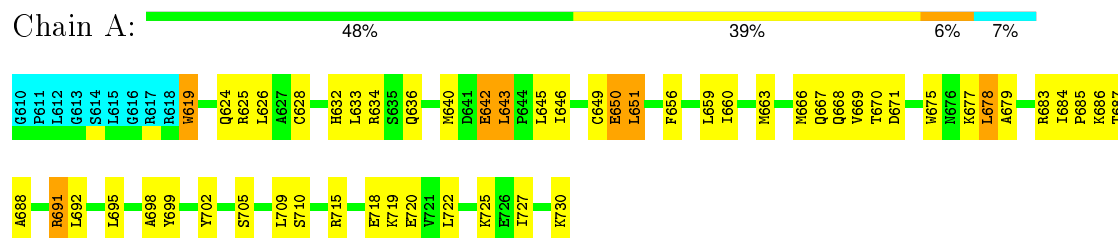


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

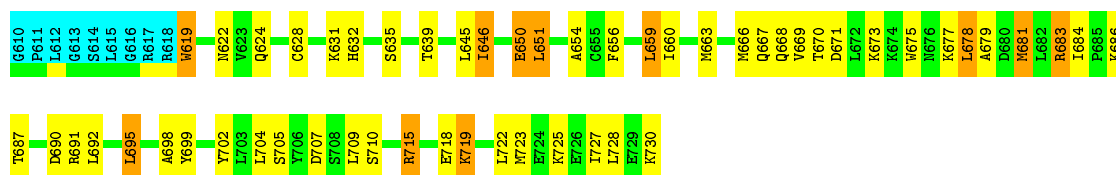
- Molecule 1: Protein Jumonji



#### 4.2.2 Score per residue for model 2

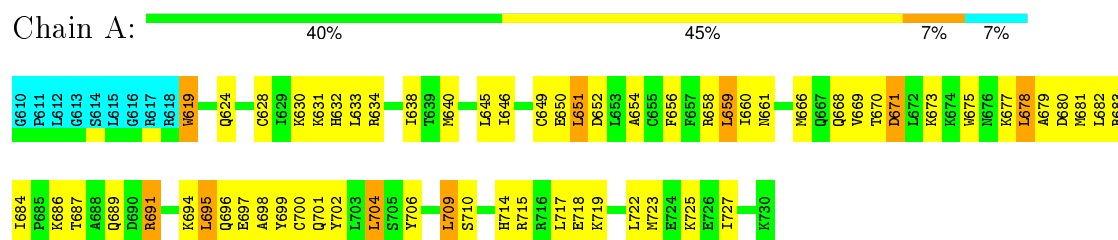
- Molecule 1: Protein Jumonji





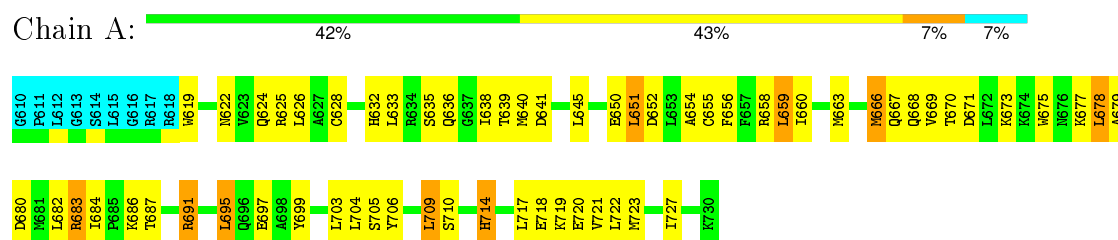
### 4.2.3 Score per residue for model 3

- Molecule 1: Protein Jumonji



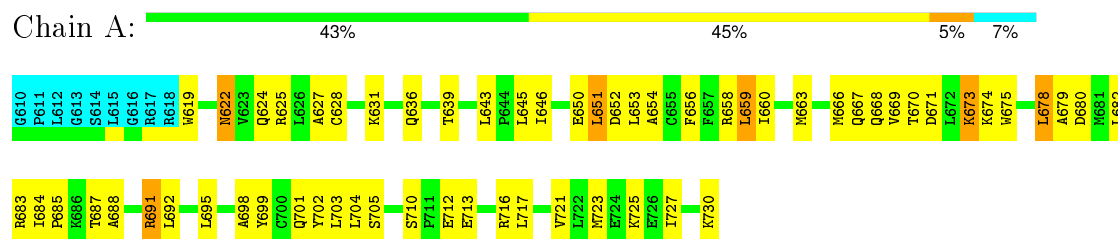
### 4.2.4 Score per residue for model 4

- Molecule 1: Protein Jumonji



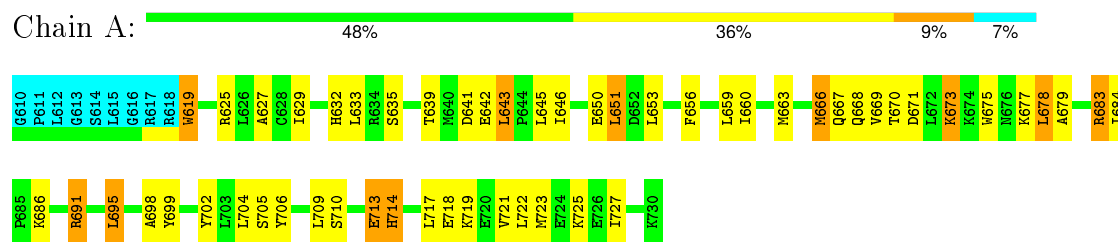
### 4.2.5 Score per residue for model 5

- Molecule 1: Protein Jumonji



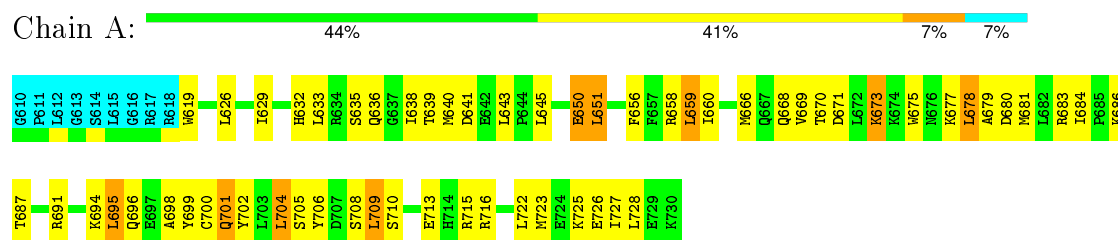
### 4.2.6 Score per residue for model 6

- Molecule 1: Protein Jumonji



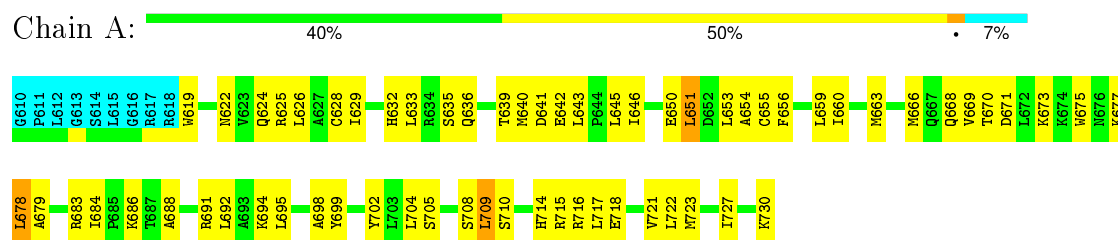
#### 4.2.7 Score per residue for model 7

- Molecule 1: Protein Jumonji



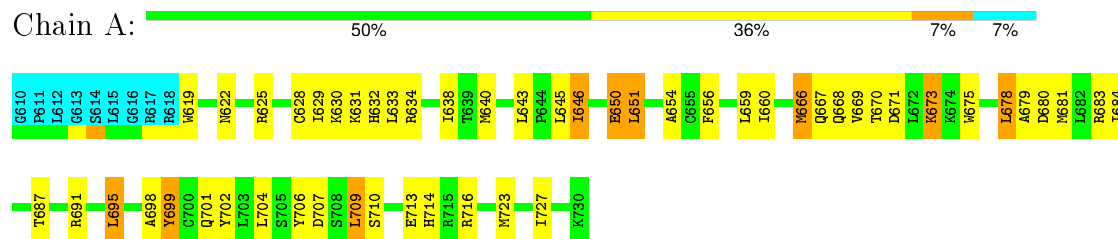
#### 4.2.8 Score per residue for model 8

- Molecule 1: Protein Jumonji



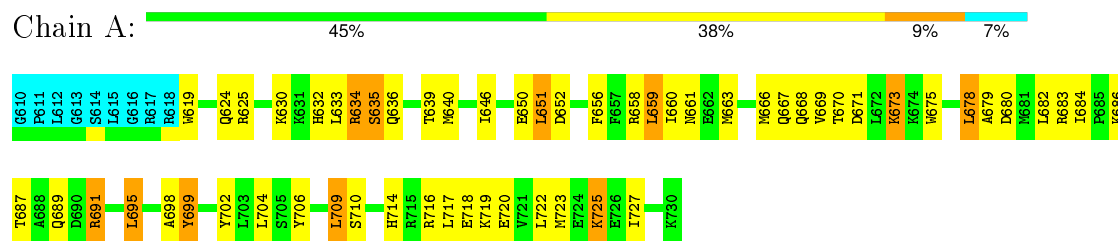
#### 4.2.9 Score per residue for model 9

- Molecule 1: Protein Jumonji



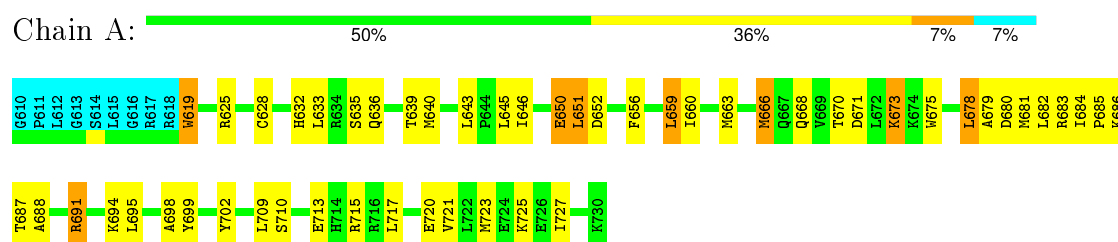
### 4.2.10 Score per residue for model 10

- Molecule 1: Protein Jumonji



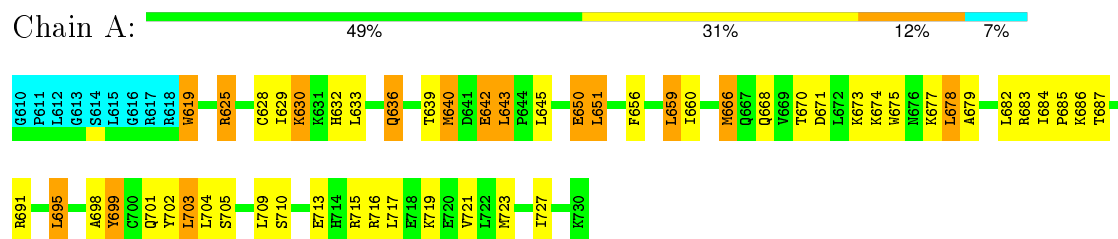
### 4.2.11 Score per residue for model 11

- Molecule 1: Protein Jumonji



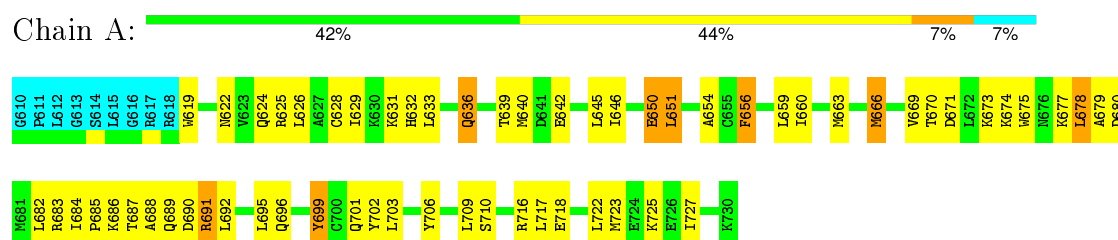
### 4.2.12 Score per residue for model 12

- Molecule 1: Protein Jumonji



### 4.2.13 Score per residue for model 13

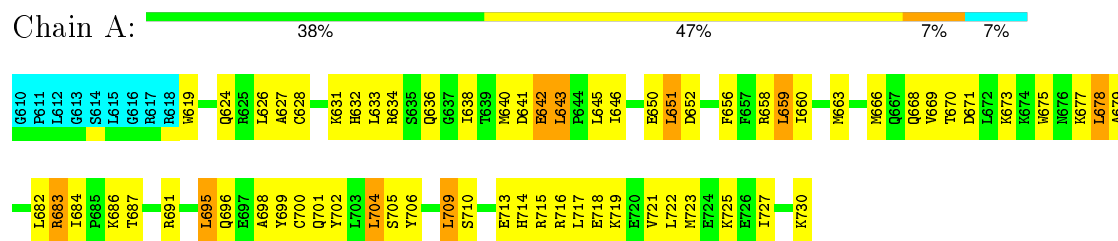
- Molecule 1: Protein Jumonji





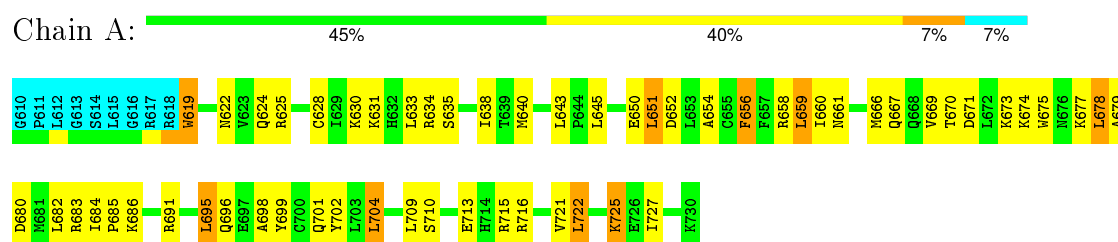
#### 4.2.14 Score per residue for model 14

- Molecule 1: Protein Jumonji



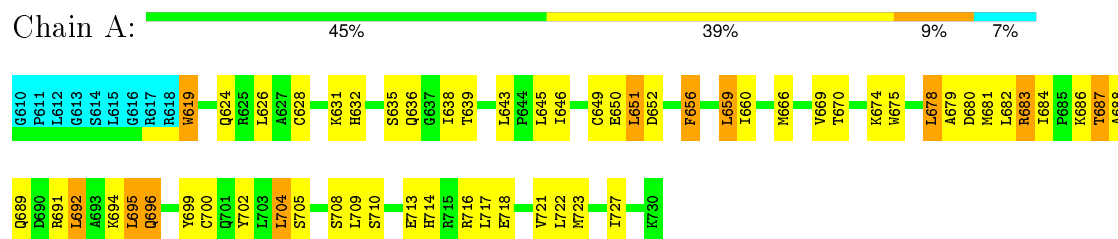
#### 4.2.15 Score per residue for model 15

- Molecule 1: Protein Jumonji



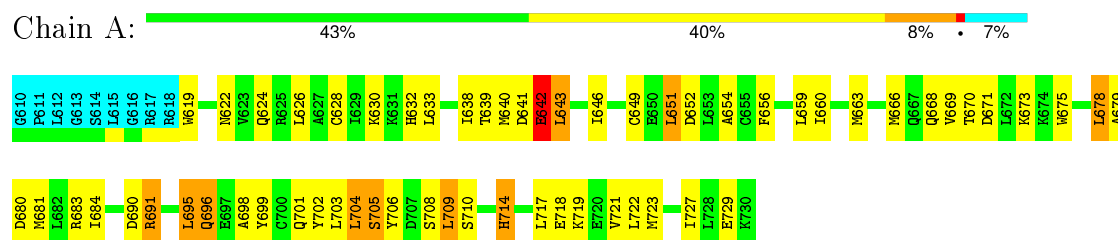
#### 4.2.16 Score per residue for model 16

- Molecule 1: Protein Jumonji



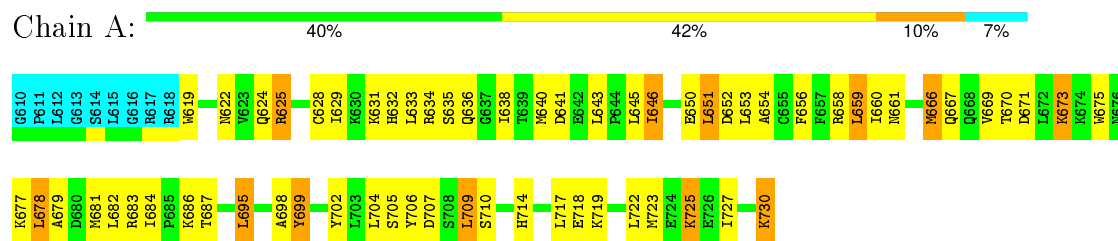
#### 4.2.17 Score per residue for model 17

- Molecule 1: Protein Jumonji



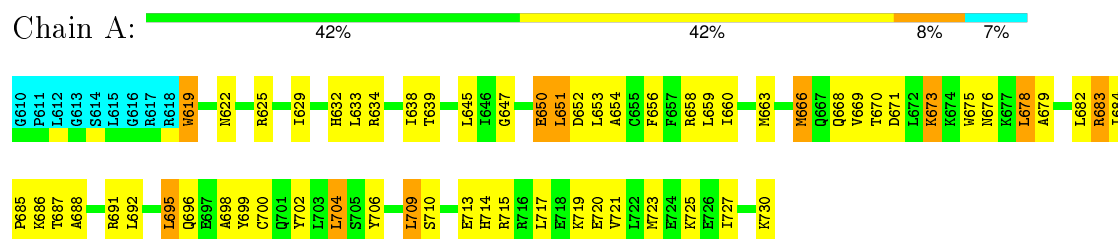
### 4.2.18 Score per residue for model 18

- Molecule 1: Protein Jumonji



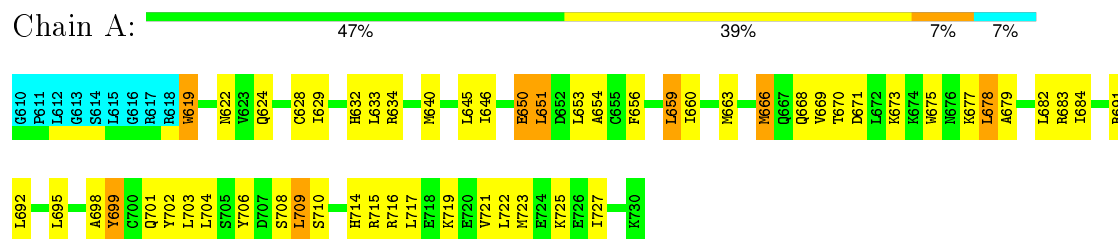
### 4.2.19 Score per residue for model 19

- Molecule 1: Protein Jumonji



### 4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: Protein Jumonji



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 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	1.1

No chemical shift data was provided. 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	912	939	937	47±5
All	All	18240	18780	18740	947

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:675:TRP:CZ3	1:A:695:LEU:HD11	1.03	1.88	9	19
1:A:675:TRP:CE3	1:A:678:LEU:HD21	0.97	1.95	1	20
1:A:675:TRP:CE3	1:A:695:LEU:HD11	0.87	2.04	18	20
1:A:632:HIS:CE1	1:A:709:LEU:HD11	0.81	2.09	13	4
1:A:632:HIS:CE1	1:A:709:LEU:HD21	0.78	2.13	1	4
1:A:675:TRP:CE3	1:A:695:LEU:HD21	0.78	2.13	9	19
1:A:678:LEU:HD23	1:A:679:ALA:N	0.78	1.94	8	20
1:A:675:TRP:HA	1:A:678:LEU:HD22	0.78	1.56	20	20
1:A:659:LEU:HD13	1:A:682:LEU:CD2	0.74	2.13	15	6
1:A:626:LEU:HD13	1:A:626:LEU:O	0.72	1.84	7	2
1:A:659:LEU:HD22	1:A:682:LEU:HD23	0.71	1.60	5	3
1:A:683:ARG:C	1:A:684:ILE:HD12	0.70	2.06	19	20
1:A:659:LEU:HD22	1:A:682:LEU:CD2	0.70	2.16	5	3
1:A:642:GLU:O	1:A:643:LEU:HD12	0.68	1.88	17	5

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:666:MET:O	1:A:670:THR:HG22	0.68	1.89	16	16
1:A:675:TRP:CE3	1:A:678:LEU:CD2	0.68	2.77	15	20
1:A:646:ILE:HD11	1:A:695:LEU:HA	0.67	1.67	2	14
1:A:633:LEU:HD13	1:A:640:MET:SD	0.65	2.31	13	12
1:A:659:LEU:HD13	1:A:682:LEU:HD21	0.65	1.69	12	6
1:A:660:ILE:HD11	1:A:675:TRP:CH2	0.65	2.26	18	7
1:A:723:MET:O	1:A:727:ILE:HD12	0.63	1.93	6	15
1:A:692:LEU:O	1:A:695:LEU:HD23	0.63	1.93	16	1
1:A:691:ARG:HG3	1:A:692:LEU:HD22	0.63	1.70	13	4
1:A:709:LEU:HD22	1:A:713:GLU:CB	0.63	2.23	15	1
1:A:709:LEU:HD13	1:A:713:GLU:OE1	0.62	1.94	16	1
1:A:660:ILE:HG23	1:A:669:VAL:HG21	0.62	1.69	3	17
1:A:709:LEU:HD22	1:A:713:GLU:CD	0.61	2.14	6	1
1:A:709:LEU:HD13	1:A:713:GLU:CD	0.61	2.15	16	1
1:A:660:ILE:HG21	1:A:666:MET:HG2	0.60	1.74	4	8
1:A:688:ALA:HB3	1:A:691:ARG:HG2	0.60	1.73	13	5
1:A:709:LEU:HD22	1:A:713:GLU:OE1	0.60	1.96	6	1
1:A:632:HIS:NE2	1:A:709:LEU:HD11	0.60	2.11	16	3
1:A:626:LEU:O	1:A:626:LEU:HD13	0.60	1.97	13	1
1:A:632:HIS:HB2	1:A:717:LEU:HD13	0.60	1.73	18	8
1:A:675:TRP:CE3	1:A:695:LEU:CD1	0.60	2.84	16	14
1:A:624:GLN:CG	1:A:722:LEU:HD11	0.60	2.26	13	9
1:A:622:ASN:O	1:A:654:ALA:HB2	0.59	1.97	20	11
1:A:675:TRP:HE3	1:A:678:LEU:HD21	0.59	1.55	12	17
1:A:727:ILE:HG22	1:A:727:ILE:O	0.59	1.97	1	12
1:A:638:ILE:N	1:A:638:ILE:HD12	0.59	2.13	3	1
1:A:727:ILE:O	1:A:727:ILE:HG22	0.59	1.98	4	8
1:A:705:SER:O	1:A:709:LEU:HD13	0.58	1.99	4	4
1:A:636:GLN:OE1	1:A:709:LEU:HD11	0.57	1.98	12	1
1:A:638:ILE:HD12	1:A:638:ILE:N	0.57	2.13	14	4
1:A:722:LEU:HD13	1:A:725:LYS:HE2	0.57	1.75	15	2
1:A:651:LEU:HD22	1:A:651:LEU:C	0.57	2.20	14	12
1:A:706:TYR:O	1:A:709:LEU:HD22	0.56	2.01	9	7
1:A:675:TRP:HB3	1:A:695:LEU:HD11	0.56	1.78	16	1
1:A:659:LEU:HD21	1:A:681:MET:HE2	0.56	1.77	7	1
1:A:727:ILE:HG23	1:A:730:LYS:HE3	0.56	1.78	8	1
1:A:659:LEU:HD11	1:A:681:MET:CE	0.56	2.31	2	2
1:A:651:LEU:C	1:A:651:LEU:HD22	0.55	2.21	7	8
1:A:709:LEU:HD23	1:A:709:LEU:O	0.55	2.00	20	3
1:A:718:GLU:HG2	1:A:722:LEU:HD22	0.55	1.78	2	6
1:A:669:VAL:HG11	1:A:678:LEU:HD13	0.55	1.78	7	5

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:709:LEU:O	1:A:709:LEU:HD23	0.55	2.01	3	3
1:A:669:VAL:HG12	1:A:675:TRP:CD1	0.55	2.37	16	1
1:A:676:ASN:CG	1:A:692:LEU:HD11	0.55	2.22	19	1
1:A:632:HIS:ND1	1:A:709:LEU:HD11	0.55	2.17	11	2
1:A:678:LEU:HD23	1:A:679:ALA:H	0.54	1.62	6	19
1:A:709:LEU:C	1:A:709:LEU:HD23	0.54	2.22	20	3
1:A:699:TYR:HB2	1:A:703:LEU:HD12	0.54	1.78	4	1
1:A:718:GLU:HG3	1:A:722:LEU:HD13	0.54	1.78	6	8
1:A:679:ALA:O	1:A:684:ILE:HD13	0.54	2.03	16	14
1:A:629:ILE:HG21	1:A:653:LEU:HD23	0.54	1.78	18	5
1:A:632:HIS:CG	1:A:709:LEU:HD11	0.54	2.38	11	3
1:A:691:ARG:HG2	1:A:692:LEU:HD22	0.53	1.80	2	2
1:A:691:ARG:CG	1:A:692:LEU:HD22	0.53	2.33	20	2
1:A:627:ALA:HB1	1:A:721:VAL:HG11	0.53	1.80	14	3
1:A:660:ILE:HD12	1:A:703:LEU:CD2	0.53	2.33	13	3
1:A:709:LEU:HD21	1:A:714:HIS:CD2	0.53	2.39	14	4
1:A:684:ILE:HG23	1:A:685:PRO:HD2	0.53	1.81	13	7
1:A:675:TRP:O	1:A:678:LEU:HD23	0.53	2.04	6	19
1:A:626:LEU:HD23	1:A:626:LEU:O	0.53	2.04	8	4
1:A:717:LEU:O	1:A:721:VAL:HG23	0.52	2.05	19	8
1:A:684:ILE:HG23	1:A:691:ARG:NE	0.52	2.19	4	1
1:A:633:LEU:HD21	1:A:702:TYR:CD2	0.52	2.38	13	3
1:A:675:TRP:CZ2	1:A:699:TYR:CD2	0.52	2.98	20	13
1:A:626:LEU:O	1:A:626:LEU:HD23	0.51	2.05	1	1
1:A:624:GLN:HG2	1:A:722:LEU:HD11	0.51	1.82	13	5
1:A:709:LEU:HD23	1:A:709:LEU:C	0.51	2.25	14	4
1:A:670:THR:HG23	1:A:671:ASP:OD1	0.51	2.05	3	1
1:A:645:LEU:HD12	1:A:650:GLU:HA	0.51	1.82	9	18
1:A:660:ILE:HD12	1:A:703:LEU:HD22	0.51	1.83	12	1
1:A:660:ILE:CD1	1:A:703:LEU:HD13	0.51	2.35	5	1
1:A:699:TYR:CE2	1:A:704:LEU:HD23	0.50	2.41	7	4
1:A:675:TRP:HE3	1:A:695:LEU:HD21	0.50	1.64	6	16
1:A:632:HIS:CD2	1:A:633:LEU:N	0.50	2.80	14	2
1:A:713:GLU:OE1	1:A:717:LEU:HD12	0.50	2.06	16	1
1:A:660:ILE:HG21	1:A:666:MET:SD	0.50	2.47	14	6
1:A:696:GLN:O	1:A:699:TYR:CD1	0.50	2.64	16	5
1:A:706:TYR:CE2	1:A:714:HIS:CE1	0.50	2.99	17	4
1:A:713:GLU:O	1:A:717:LEU:HD12	0.49	2.07	19	4
1:A:632:HIS:CD2	1:A:709:LEU:HD11	0.49	2.42	1	3
1:A:706:TYR:CZ	1:A:714:HIS:CE1	0.49	3.00	20	2
1:A:660:ILE:HD12	1:A:703:LEU:HD13	0.49	1.83	5	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:651:LEU:CD2	1:A:653:LEU:HD12	0.49	2.38	5	2
1:A:619:TRP:CZ2	1:A:721:VAL:HG12	0.49	2.42	11	6
1:A:706:TYR:CE1	1:A:714:HIS:CD2	0.48	3.01	10	1
1:A:629:ILE:HG22	1:A:633:LEU:CD1	0.48	2.38	7	2
1:A:638:ILE:HG21	1:A:702:TYR:CZ	0.48	2.44	15	4
1:A:676:ASN:OD1	1:A:692:LEU:HD11	0.48	2.09	19	1
1:A:688:ALA:CB	1:A:691:ARG:NE	0.48	2.77	11	2
1:A:688:ALA:O	1:A:691:ARG:HG2	0.47	2.09	1	3
1:A:666:MET:HE2	1:A:699:TYR:CE2	0.47	2.44	7	5
1:A:629:ILE:HG22	1:A:633:LEU:HD11	0.47	1.87	13	3
1:A:659:LEU:HD22	1:A:678:LEU:O	0.47	2.10	15	2
1:A:709:LEU:HD11	1:A:713:GLU:HB2	0.47	1.87	19	3
1:A:666:MET:HE3	1:A:666:MET:HA	0.47	1.86	13	2
1:A:670:THR:HG23	1:A:671:ASP:N	0.47	2.24	5	18
1:A:625:ARG:O	1:A:629:ILE:HD12	0.47	2.10	18	2
1:A:669:VAL:CG1	1:A:678:LEU:HD13	0.46	2.40	7	5
1:A:624:GLN:HG3	1:A:722:LEU:HD11	0.46	1.85	3	1
1:A:626:LEU:HD13	1:A:626:LEU:C	0.46	2.30	16	2
1:A:684:ILE:HD12	1:A:684:ILE:N	0.46	2.26	16	7
1:A:638:ILE:HG21	1:A:702:TYR:CE2	0.46	2.45	3	2
1:A:718:GLU:HG3	1:A:722:LEU:HD23	0.46	1.86	10	3
1:A:651:LEU:O	1:A:651:LEU:HD22	0.46	2.09	19	10
1:A:718:GLU:CG	1:A:722:LEU:HD22	0.46	2.41	16	2
1:A:626:LEU:C	1:A:626:LEU:HD13	0.46	2.31	13	1
1:A:638:ILE:HD11	1:A:701:GLN:OE1	0.46	2.10	7	1
1:A:675:TRP:HE3	1:A:695:LEU:HD11	0.46	1.71	16	1
1:A:633:LEU:CD2	1:A:702:TYR:CD2	0.46	2.99	20	4
1:A:679:ALA:HB3	1:A:691:ARG:NH2	0.46	2.25	10	1
1:A:632:HIS:CE1	1:A:636:GLN:CG	0.45	2.99	11	6
1:A:642:GLU:HB3	1:A:643:LEU:HD23	0.45	1.87	8	1
1:A:699:TYR:CE2	1:A:704:LEU:CD2	0.45	2.99	16	4
1:A:651:LEU:HD21	1:A:653:LEU:HD12	0.45	1.86	5	1
1:A:659:LEU:HD21	1:A:681:MET:CE	0.45	2.40	16	1
1:A:632:HIS:CE1	1:A:709:LEU:CD1	0.45	2.99	9	5
1:A:666:MET:HA	1:A:666:MET:HE3	0.45	1.87	18	1
1:A:619:TRP:CE2	1:A:725:LYS:CD	0.45	2.99	1	3
1:A:686:LYS:NZ	1:A:687:THR:HG23	0.45	2.26	16	1
1:A:709:LEU:HD22	1:A:713:GLU:HB3	0.45	1.86	15	1
1:A:700:CYS:HA	1:A:704:LEU:HD23	0.45	1.88	14	1
1:A:698:ALA:O	1:A:702:TYR:CD1	0.45	2.70	3	17
1:A:651:LEU:HD22	1:A:651:LEU:O	0.45	2.11	12	9

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:630:LYS:HB3	1:A:640:MET:HE1	0.45	1.87	12	1
1:A:723:MET:HB2	1:A:727:ILE:HD13	0.45	1.89	10	3
1:A:667:GLN:O	1:A:671:ASP:CB	0.45	2.65	5	9
1:A:706:TYR:CE2	1:A:714:HIS:NE2	0.45	2.84	4	1
1:A:660:ILE:HG23	1:A:669:VAL:CG2	0.45	2.40	3	2
1:A:643:LEU:HD23	1:A:643:LEU:N	0.45	2.27	8	1
1:A:684:ILE:N	1:A:684:ILE:HD12	0.45	2.27	12	5
1:A:660:ILE:HD13	1:A:666:MET:SD	0.44	2.52	14	3
1:A:709:LEU:HD13	1:A:709:LEU:H	0.44	1.72	18	4
1:A:666:MET:HE2	1:A:699:TYR:CE1	0.44	2.47	3	4
1:A:633:LEU:HD23	1:A:638:ILE:HD13	0.44	1.88	19	1
1:A:675:TRP:CZ2	1:A:699:TYR:CG	0.44	3.06	5	4
1:A:656:PHE:CD1	1:A:682:LEU:CD1	0.44	3.00	15	1
1:A:659:LEU:HD12	1:A:678:LEU:HB2	0.44	1.89	4	1
1:A:660:ILE:CG2	1:A:666:MET:HA	0.44	2.43	19	4
1:A:624:GLN:CG	1:A:722:LEU:HD21	0.44	2.43	10	2
1:A:692:LEU:H	1:A:692:LEU:HD22	0.43	1.73	16	1
1:A:656:PHE:CD2	1:A:682:LEU:CD1	0.43	3.01	13	2
1:A:675:TRP:CD2	1:A:695:LEU:HD21	0.43	2.48	9	2
1:A:632:HIS:HB3	1:A:717:LEU:HD13	0.43	1.88	14	2
1:A:678:LEU:O	1:A:682:LEU:HD23	0.43	2.13	18	2
1:A:691:ARG:O	1:A:695:LEU:HB3	0.43	2.14	8	2
1:A:695:LEU:HD23	1:A:696:GLN:N	0.43	2.29	16	1
1:A:684:ILE:HG23	1:A:691:ARG:CD	0.43	2.44	3	1
1:A:696:GLN:O	1:A:699:TYR:CD2	0.43	2.71	3	2
1:A:682:LEU:O	1:A:683:ARG:HB2	0.43	2.13	19	7
1:A:659:LEU:HD11	1:A:681:MET:HE1	0.43	1.90	7	1
1:A:692:LEU:O	1:A:695:LEU:CD2	0.43	2.66	16	1
1:A:619:TRP:HZ2	1:A:721:VAL:HG12	0.43	1.73	11	3
1:A:666:MET:HE2	1:A:699:TYR:CZ	0.43	2.49	14	4
1:A:683:ARG:O	1:A:684:ILE:HD12	0.43	2.14	7	1
1:A:638:ILE:N	1:A:638:ILE:CD1	0.43	2.82	3	2
1:A:691:ARG:HH22	1:A:695:LEU:HD22	0.42	1.73	6	1
1:A:632:HIS:HE1	1:A:709:LEU:HD21	0.42	1.69	11	1
1:A:706:TYR:HA	1:A:709:LEU:HD12	0.42	1.91	13	1
1:A:646:ILE:HD11	1:A:695:LEU:CA	0.42	2.42	2	2
1:A:727:ILE:HG23	1:A:730:LYS:NZ	0.42	2.28	18	1
1:A:706:TYR:CD1	1:A:709:LEU:HD12	0.42	2.50	6	1
1:A:669:VAL:HG12	1:A:675:TRP:NE1	0.42	2.30	18	3
1:A:727:ILE:CG2	1:A:727:ILE:O	0.42	2.68	1	2
1:A:638:ILE:CD1	1:A:638:ILE:N	0.42	2.82	18	3

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:659:LEU:HD13	1:A:682:LEU:HD23	0.42	1.90	10	1
1:A:684:ILE:CG1	1:A:691:ARG:NH2	0.42	2.83	17	2
1:A:646:ILE:HG22	1:A:651:LEU:HB3	0.42	1.90	2	5
1:A:709:LEU:HD21	1:A:714:HIS:HD2	0.42	1.75	20	1
1:A:666:MET:SD	1:A:699:TYR:CE1	0.42	3.13	18	2
1:A:619:TRP:CE2	1:A:725:LYS:HD3	0.41	2.50	1	2
1:A:699:TYR:CE1	1:A:704:LEU:CD2	0.41	3.02	3	2
1:A:624:GLN:HG2	1:A:722:LEU:HD21	0.41	1.92	15	2
1:A:675:TRP:O	1:A:679:ALA:CB	0.41	2.68	16	1
1:A:670:THR:CG2	1:A:671:ASP:N	0.41	2.84	13	2
1:A:675:TRP:CZ2	1:A:699:TYR:CD1	0.41	3.08	7	1
1:A:627:ALA:CB	1:A:721:VAL:HG11	0.41	2.45	14	1
1:A:722:LEU:HD13	1:A:725:LYS:NZ	0.41	2.29	18	1
1:A:652:ASP:OD1	1:A:654:ALA:HB3	0.41	2.15	3	1
1:A:727:ILE:O	1:A:727:ILE:CG2	0.41	2.68	4	2
1:A:634:ARG:HG3	1:A:635:SER:N	0.41	2.30	10	1
1:A:706:TYR:CZ	1:A:714:HIS:NE2	0.41	2.89	3	1
1:A:651:LEU:HD13	1:A:651:LEU:H	0.41	1.76	8	3
1:A:688:ALA:HB3	1:A:691:ARG:CG	0.41	2.45	16	1
1:A:633:LEU:HD13	1:A:640:MET:CE	0.41	2.45	13	1
1:A:626:LEU:HD23	1:A:626:LEU:C	0.41	2.36	14	1
1:A:715:ARG:O	1:A:719:LYS:CG	0.41	2.68	2	1
1:A:709:LEU:CD1	1:A:713:GLU:HB2	0.41	2.46	9	2
1:A:647:GLY:O	1:A:691:ARG:NH1	0.41	2.54	19	1
1:A:651:LEU:H	1:A:651:LEU:HD13	0.41	1.75	7	3
1:A:699:TYR:CE1	1:A:704:LEU:HD23	0.41	2.51	8	2
1:A:679:ALA:CB	1:A:691:ARG:NH2	0.41	2.84	10	1
1:A:684:ILE:HG22	1:A:691:ARG:HD2	0.41	1.91	13	1
1:A:619:TRP:NE1	1:A:725:LYS:CD	0.41	2.84	2	1
1:A:700:CYS:O	1:A:704:LEU:HB2	0.40	2.16	7	3
1:A:713:GLU:HG3	1:A:717:LEU:HD12	0.40	1.92	6	1
1:A:666:MET:HE3	1:A:699:TYR:CZ	0.40	2.52	11	1
1:A:656:PHE:CE2	1:A:682:LEU:HG	0.40	2.51	16	1
1:A:728:LEU:HD23	1:A:728:LEU:O	0.40	2.16	7	1
1:A:633:LEU:HD12	1:A:640:MET:CE	0.40	2.46	17	1
1:A:704:LEU:O	1:A:708:SER:CB	0.40	2.70	20	1
1:A:619:TRP:CE2	1:A:725:LYS:HD2	0.40	2.52	2	1
1:A:666:MET:HE1	1:A:699:TYR:CZ	0.40	2.51	12	1
1:A:632:HIS:CE1	1:A:636:GLN:NE2	0.40	2.89	13	1
1:A:722:LEU:O	1:A:725:LYS:CG	0.40	2.70	6	1
1:A:660:ILE:HD11	1:A:675:TRP:HH2	0.40	1.77	11	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:716:ARG:CG	1:A:717:LEU:N	0.40	2.85	14	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	111/121 (92%)	102±1 (92±1%)	8±1 (7±1%)	1±1 (1±0%)	24	71
All	All	2220/2420 (92%)	2043 (92%)	155 (7%)	22 (1%)	24	71

All 3 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	673	LYS	17
1	A	642	GLU	4
1	A	619	TRP	1

### 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	100/106 (94%)	72±3 (72±3%)	28±3 (28±3%)	2	20
All	All	2000/2120 (94%)	1439 (72%)	561 (28%)	2	20

All 68 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	656	PHE	20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	659	LEU	20
1	A	678	LEU	20
1	A	619	TRP	20
1	A	710	SER	20
1	A	651	LEU	20
1	A	628	CYS	16
1	A	668	GLN	16
1	A	704	LEU	15
1	A	686	LYS	15
1	A	687	THR	15
1	A	691	ARG	14
1	A	695	LEU	14
1	A	625	ARG	13
1	A	639	THR	13
1	A	677	LYS	13
1	A	663	MET	13
1	A	719	LYS	12
1	A	643	LEU	12
1	A	709	LEU	11
1	A	666	MET	11
1	A	680	ASP	11
1	A	715	ARG	11
1	A	650	GLU	10
1	A	635	SER	10
1	A	716	ARG	10
1	A	725	LYS	10
1	A	652	ASP	10
1	A	701	GLN	10
1	A	631	LYS	9
1	A	658	ARG	9
1	A	705	SER	9
1	A	634	ARG	9
1	A	673	LYS	9
1	A	641	ASP	7
1	A	730	LYS	6
1	A	699	TYR	6
1	A	636	GLN	6
1	A	683	ARG	6
1	A	630	LYS	6
1	A	714	HIS	5
1	A	720	GLU	5
1	A	694	LYS	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	674	LYS	5
1	A	681	MET	5
1	A	649	CYS	4
1	A	708	SER	4
1	A	646	ILE	4
1	A	661	ASN	4
1	A	689	GLN	4
1	A	696	GLN	3
1	A	690	ASP	3
1	A	707	ASP	3
1	A	655	CYS	2
1	A	640	MET	2
1	A	642	GLU	2
1	A	722	LEU	2
1	A	697	GLU	2
1	A	671	ASP	1
1	A	624	GLN	1
1	A	726	GLU	1
1	A	712	GLU	1
1	A	622	ASN	1
1	A	703	LEU	1
1	A	700	CYS	1
1	A	692	LEU	1
1	A	713	GLU	1
1	A	728	LEU	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided