



# Full wwPDB NMR Structure Validation Report ⓘ

Aug 2, 2022 – 10:13 am BST

PDB ID : 6TV5  
Title : NMR structure of N-terminal domain from *A. argentata* tubuliform spidroin (TuSp) at pH 5.5  
Authors : Fridmanis, J.; Jaudzems, K.  
Deposited on : 2020-01-09

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 ⓘ](#)) 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)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.29
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

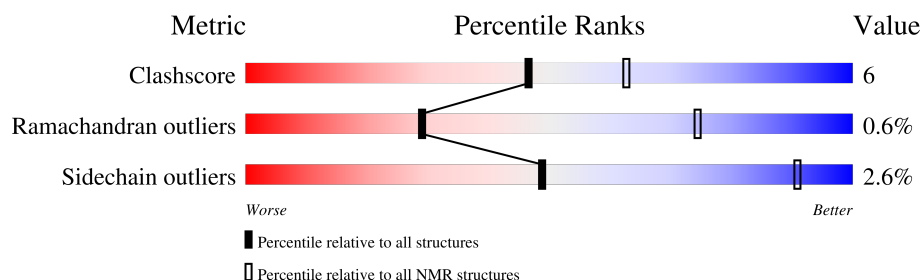
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 47%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	137	 80% 6% 14%
1	B	137	 78% 7% 15%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 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:7-A:55, A:59-A:127, B:208-B:255, B:260-B:327 (234)	0.49	1

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. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3913 atoms, of which 1941 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tubuliform spidroin 1.

Mol	Chain	Residues	Atoms						Trace
1	A	137	Total	C	H	N	O	S	0
			1956	610	970	164	210	2	
1	B	137	Total	C	H	N	O	S	0
			1957	610	971	164	210	2	

There are 2 discrepancies between the modelled and reference sequences:

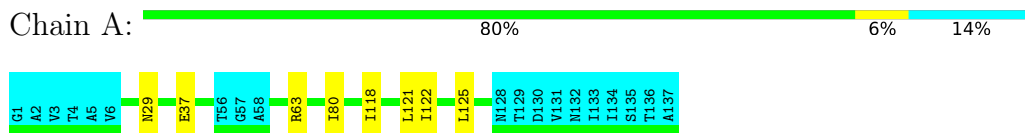
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A2R2YSJ7
B	201	GLY	-	expression tag	UNP A0A2R2YSJ7

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

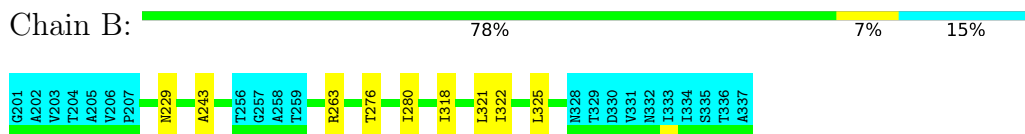
### 4.1 Average score per residue in the NMR ensemble

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: Tubuliform spidroin 1



- Molecule 1: Tubuliform spidroin 1

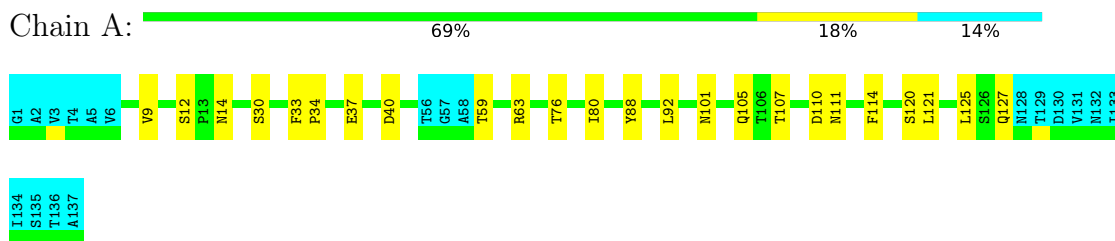


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Tubuliform spidroin 1



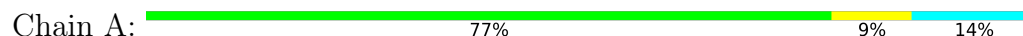
- Molecule 1: Tubuliform spidroin 1





#### 4.2.2 Score per residue for model 2

- Molecule 1: Tubuliform spidroin 1

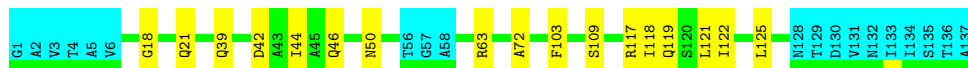


- Molecule 1: Tubuliform spidroin 1



#### 4.2.3 Score per residue for model 3

- Molecule 1: Tubuliform spidroin 1



- Molecule 1: Tubuliform spidroin 1

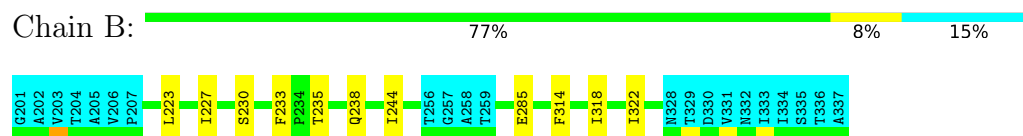


#### 4.2.4 Score per residue for model 4

- Molecule 1: Tubuliform spidroin 1

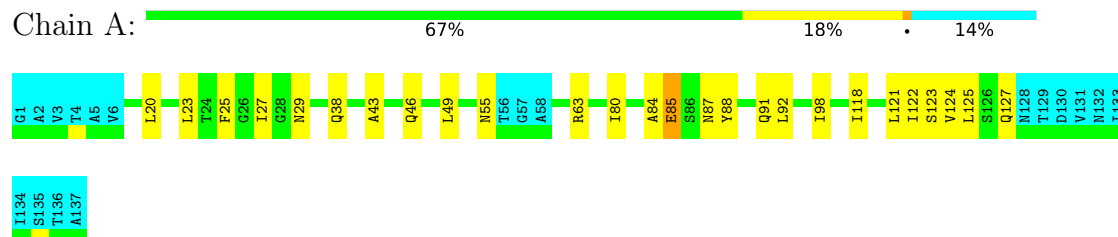


- Molecule 1: Tubuliform spidroin 1

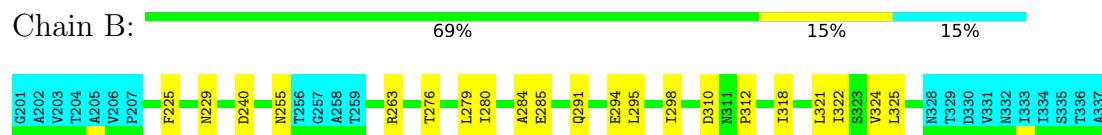


#### 4.2.5 Score per residue for model 5

- Molecule 1: Tubuliform spidroin 1

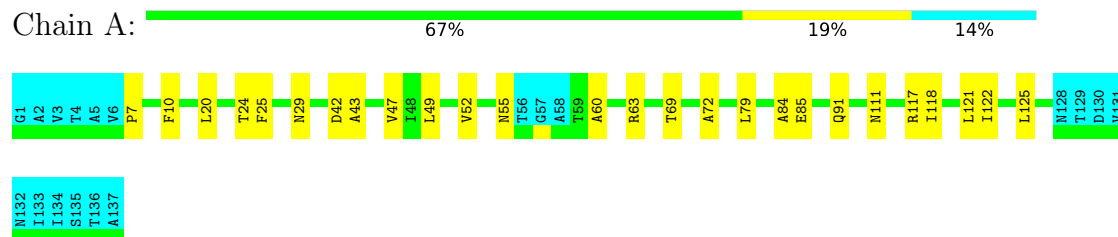


- Molecule 1: Tubuliform spidroin 1

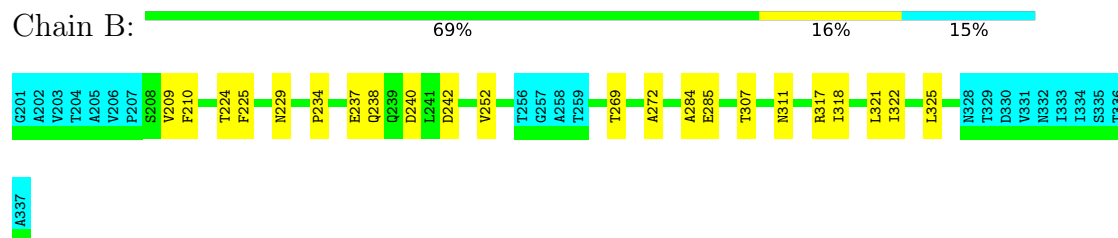


#### 4.2.6 Score per residue for model 6

- Molecule 1: Tubuliform spidroin 1




- Molecule 1: Tubuliform spidroin 1



### 4.2.7 Score per residue for model 7

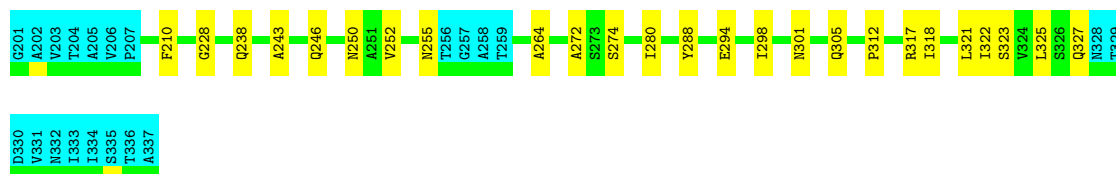
- Molecule 1: Tubuliform spidroin 1

Chain A:  77% 9% 14%



- Molecule 1: Tubuliform spidroin 1

Chain B:  66% 18% 15%



### 4.2.8 Score per residue for model 8

- Molecule 1: Tubuliform spidroin 1

Chain A:  72% 14% 14%



- Molecule 1: Tubuliform spidroin 1

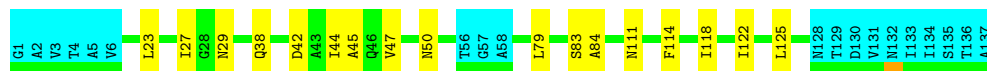
Chain B:  71% 13% 15%



### 4.2.9 Score per residue for model 9

- Molecule 1: Tubuliform spidroin 1

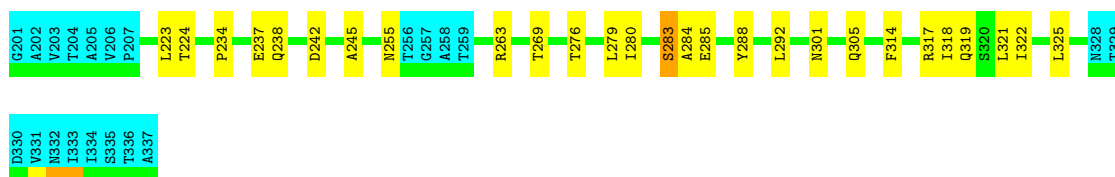
Chain A:  74% 12% 14%



- Molecule 1: Tubuliform spidroin 1

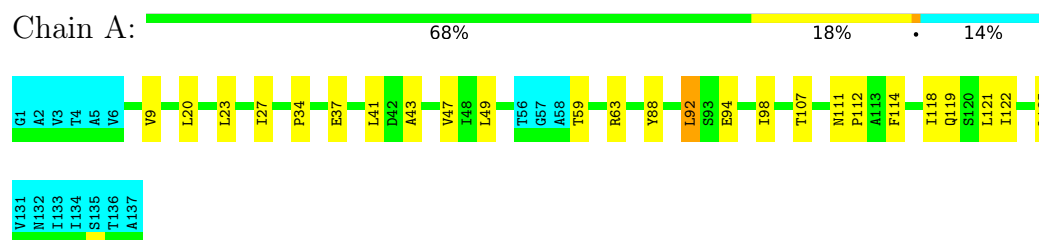
Chain B:  65% 19% 15%



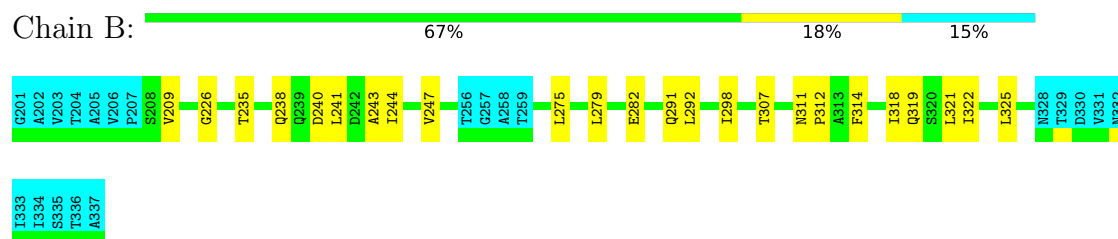


#### 4.2.10 Score per residue for model 10

- Molecule 1: Tubuliform spidroin 1

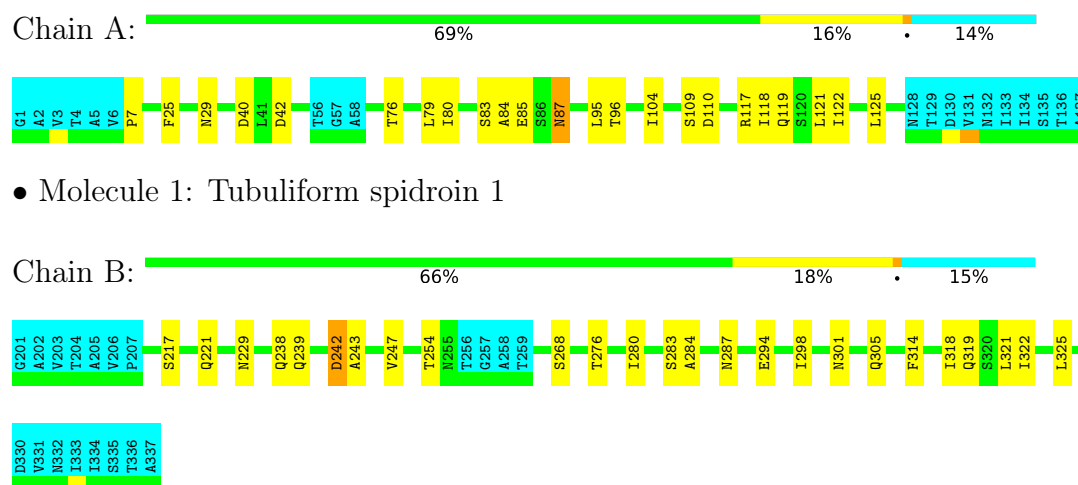


- Molecule 1: Tubuliform spidroin 1



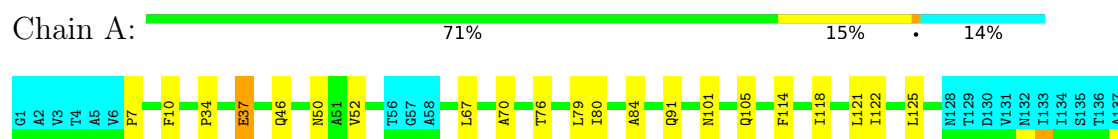
#### 4.2.11 Score per residue for model 11

- Molecule 1: Tubuliform spidroin 1

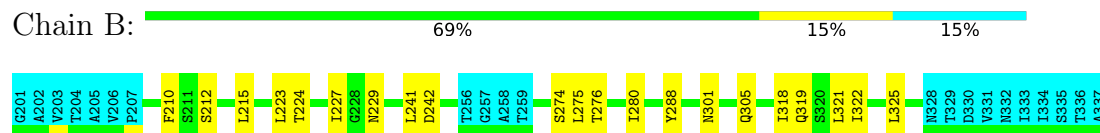


### 4.2.12 Score per residue for model 12

- Molecule 1: Tubuliform spidroin 1

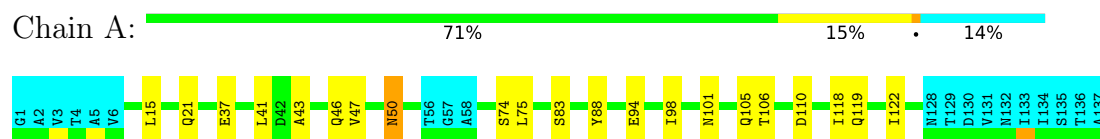


- Molecule 1: Tubuliform spidroin 1

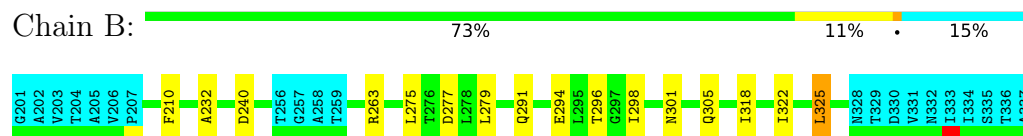


### 4.2.13 Score per residue for model 13

- Molecule 1: Tubuliform spidroin 1

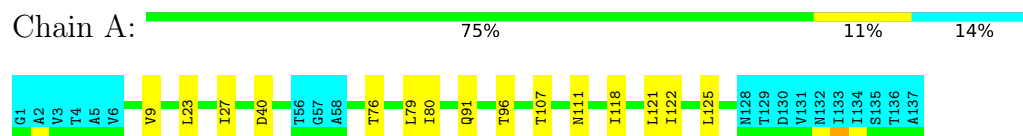


- Molecule 1: Tubuliform spidroin 1

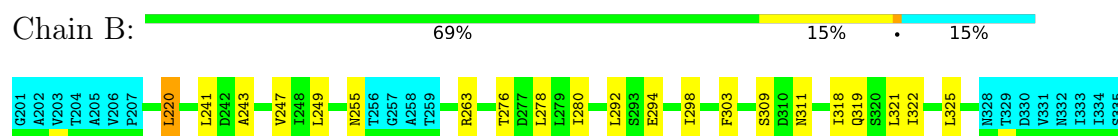


### 4.2.14 Score per residue for model 14

- Molecule 1: Tubuliform spidroin 1



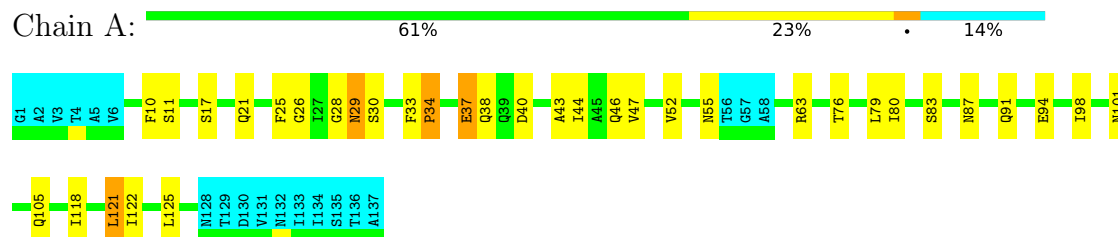
- Molecule 1: Tubuliform spidroin 1



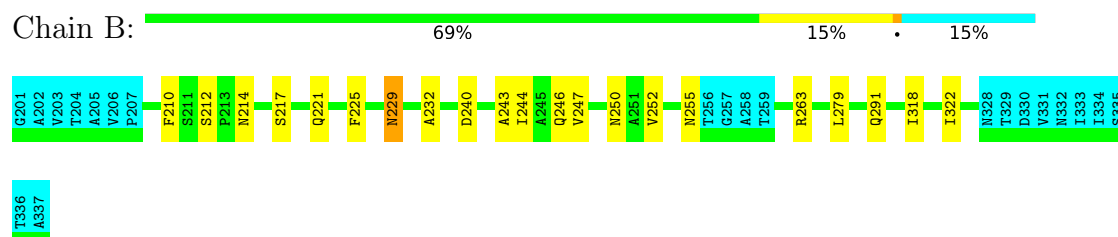
T336  
A337

#### 4.2.15 Score per residue for model 15

- Molecule 1: Tubuliform spidroin 1



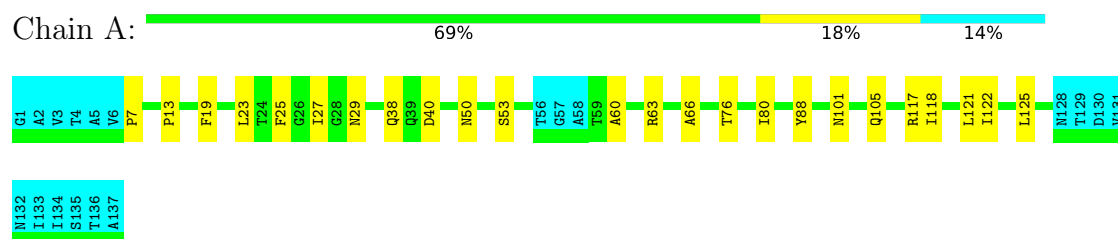
- Molecule 1: Tubuliform spidroin 1



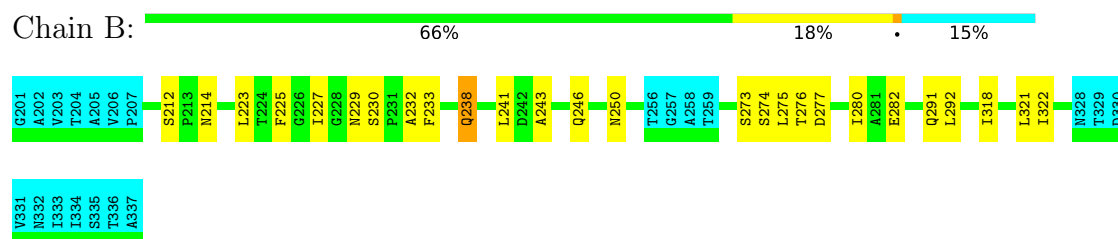
T336  
A337

#### 4.2.16 Score per residue for model 16

- Molecule 1: Tubuliform spidroin 1



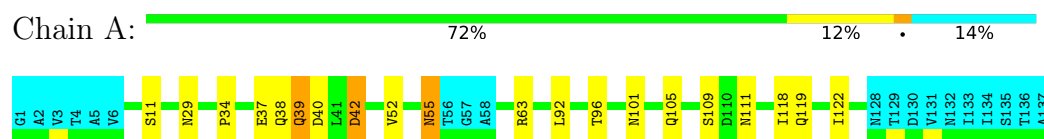
- Molecule 1: Tubuliform spidroin 1



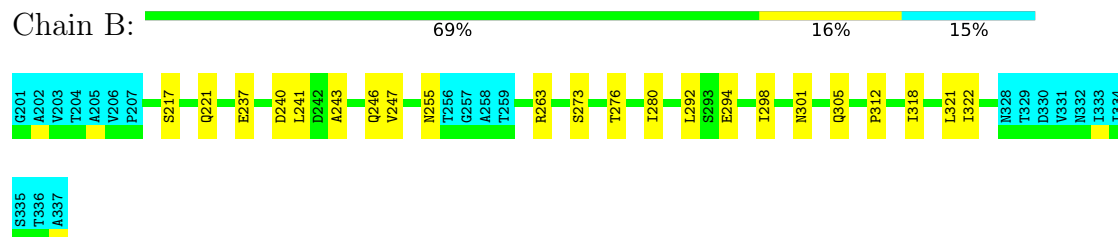
V331  
N332  
I333  
I334  
S335  
T336  
A337

### 4.2.17 Score per residue for model 17

- Molecule 1: Tubuliform spidroin 1

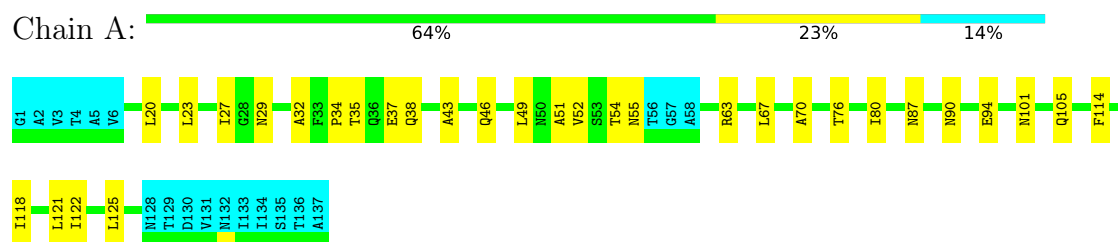


- Molecule 1: Tubuliform spidroin 1

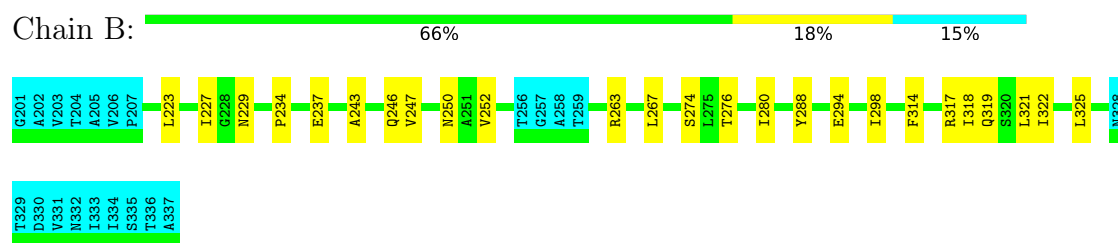


### 4.2.18 Score per residue for model 18

- Molecule 1: Tubuliform spidroin 1



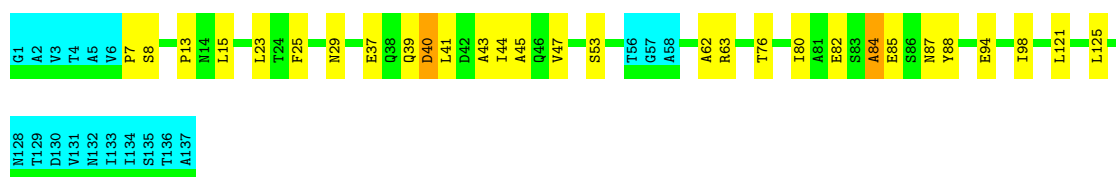
- Molecule 1: Tubuliform spidroin 1



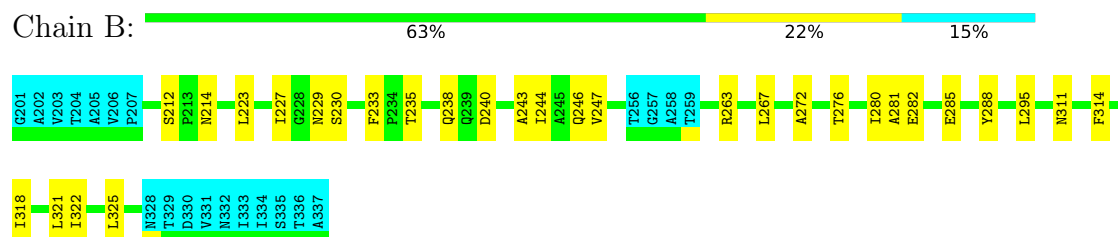
### 4.2.19 Score per residue for model 19

- Molecule 1: Tubuliform spidroin 1



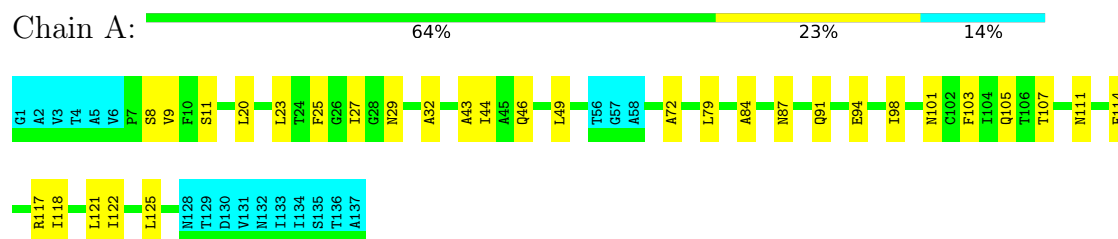


- Molecule 1: Tubuliform spidroin 1

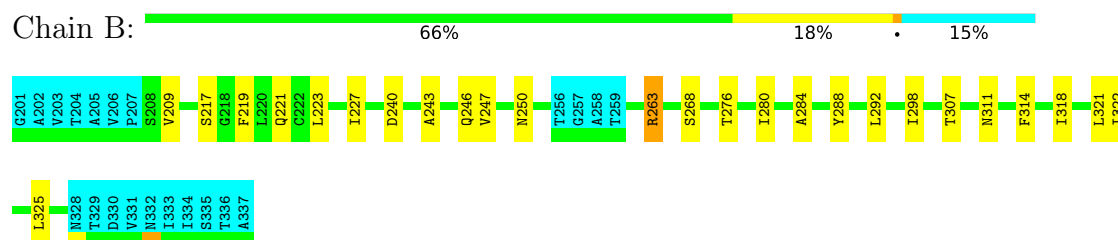


#### 4.2.20 Score per residue for model 20

- Molecule 1: Tubuliform spidroin 1



- Molecule 1: Tubuliform spidroin 1



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	2.1
CNS	refinement	1.3
CANDID	structure calculation	

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	1609
Number of shifts mapped to atoms	1609
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	47%

## 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	863	847	847	12±4
1	B	849	833	833	12±3
All	All	34240	33600	33600	440

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:VAL:HG23	1:A:107:THR:HB	0.72	1.61	20	4
1:A:44:ILE:HD11	1:B:263:ARG:HG3	0.67	1.66	15	3
1:A:34:PRO:HG2	1:A:37:GLU:HG2	0.64	1.69	7	4
1:B:246:GLN:O	1:B:250:ASN:HB2	0.62	1.94	16	7
1:A:41:LEU:HD22	1:A:75:LEU:HD13	0.62	1.70	13	1
1:A:20:LEU:HB2	1:A:49:LEU:HG	0.61	1.71	6	4
1:A:121:LEU:O	1:A:125:LEU:HG	0.60	1.96	19	15
1:A:79:LEU:HD21	1:A:91:GLN:HB2	0.60	1.72	15	4
1:B:292:LEU:HD21	1:B:322:ILE:HD13	0.60	1.73	20	2
1:A:79:LEU:O	1:A:83:SER:HB2	0.60	1.95	11	2
1:A:117:ARG:HH21	1:A:121:LEU:HD21	0.59	1.58	16	1
1:B:272:ALA:HB1	1:B:318:ILE:HG12	0.59	1.75	7	3
1:A:26:GLY:HA3	1:A:98:ILE:HG23	0.58	1.76	15	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:243:ALA:HA	1:B:246:GLN:HE21	0.58	1.58	19	5
1:B:273:SER:HB2	1:B:321:LEU:HD13	0.58	1.75	17	1
1:B:252:VAL:HB	1:B:267:LEU:HD13	0.58	1.75	18	1
1:A:72:ALA:HB1	1:A:118:ILE:HG12	0.57	1.75	6	3
1:B:321:LEU:O	1:B:325:LEU:HG	0.57	1.99	7	13
1:A:63:ARG:HG3	1:B:244:ILE:HD11	0.57	1.77	19	3
1:A:117:ARG:O	1:A:121:LEU:HG	0.57	2.00	16	7
1:B:317:ARG:O	1:B:321:LEU:HG	0.56	2.01	3	3
1:A:125:LEU:HD21	1:B:269:THR:HG21	0.56	1.75	9	1
1:B:244:ILE:HG13	1:B:278:LEU:HD22	0.56	1.77	2	1
1:A:46:GLN:O	1:A:50:ASN:HB2	0.56	2.00	4	5
1:B:301:ASN:O	1:B:305:GLN:HG2	0.56	2.00	9	6
1:A:44:ILE:HD11	1:B:263:ARG:HD3	0.55	1.76	3	1
1:B:318:ILE:O	1:B:322:ILE:HG13	0.55	2.02	8	20
1:A:55:ASN:HA	1:A:63:ARG:HH11	0.55	1.62	18	1
1:B:268:SER:HB2	1:B:314:PHE:HE1	0.55	1.62	20	1
1:A:69:THR:HG21	1:B:325:LEU:HD11	0.54	1.79	6	1
1:A:73:SER:HB2	1:A:121:LEU:HD13	0.54	1.78	8	1
1:A:44:ILE:O	1:A:47:VAL:HG12	0.54	2.03	9	1
1:B:279:LEU:HD11	1:B:291:GLN:HB2	0.54	1.79	2	1
1:B:319:GLN:HA	1:B:322:ILE:HD12	0.53	1.79	14	7
1:B:255:ASN:OD1	1:B:263:ARG:HD2	0.53	2.03	5	4
1:B:209:VAL:HG23	1:B:307:THR:HB	0.53	1.79	20	3
1:B:220:LEU:HG	1:B:249:LEU:HD12	0.53	1.80	14	1
1:A:83:SER:O	1:A:87:ASN:HB3	0.53	2.04	11	2
1:B:241:LEU:HD22	1:B:275:LEU:HD13	0.52	1.82	10	1
1:A:43:ALA:HA	1:A:46:GLN:HE21	0.52	1.64	18	4
1:B:234:PRO:HD2	1:B:237:GLU:HB2	0.52	1.81	9	1
1:B:276:THR:O	1:B:280:ILE:HG13	0.52	2.05	18	14
1:A:55:ASN:OD1	1:A:63:ARG:HD2	0.52	2.04	5	2
1:B:303:PHE:HB3	1:B:309:SER:O	0.52	2.05	3	2
1:A:23:LEU:HD23	1:A:45:ALA:HB1	0.52	1.81	9	2
1:A:28:GLY:HA2	1:A:38:GLN:NE2	0.52	2.20	15	1
1:B:239:GLN:HA	1:B:242:ASP:OD1	0.51	2.05	11	1
1:A:117:ARG:NH2	1:A:121:LEU:HD21	0.51	2.19	16	1
1:B:279:LEU:O	1:B:283:SER:HB2	0.51	2.06	2	2
1:A:7:PRO:HD3	1:A:111:ASN:ND2	0.51	2.21	6	1
1:A:25:PHE:O	1:A:29:ASN:HB3	0.51	2.05	7	2
1:B:280:ILE:HG12	1:B:288:TYR:CD2	0.51	2.40	20	3
1:A:101:ASN:O	1:A:105:GLN:HG2	0.51	2.05	12	10
1:B:314:PHE:O	1:B:318:ILE:HG13	0.51	2.06	4	6

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:PHE:O	1:A:118:ILE:HG13	0.51	2.06	12	3
1:A:111:ASN:ND2	1:A:114:PHE:HB2	0.50	2.21	1	2
1:B:210:PHE:HA	1:B:252:VAL:HG21	0.50	1.82	8	3
1:B:234:PRO:HG2	1:B:237:GLU:HB2	0.50	1.82	6	1
1:A:63:ARG:HD2	1:B:244:ILE:HD11	0.50	1.84	3	2
1:A:70:ALA:HB2	1:B:274:SER:HB2	0.50	1.81	7	2
1:B:223:LEU:O	1:B:227:ILE:HG13	0.50	2.06	16	5
1:B:235:THR:HA	1:B:238:GLN:HB3	0.50	1.83	4	2
1:B:276:THR:HG21	1:B:322:ILE:HG12	0.50	1.83	20	3
1:A:119:GLN:HA	1:A:122:ILE:HD12	0.50	1.84	17	6
1:A:118:ILE:O	1:A:122:ILE:HG13	0.49	2.07	17	16
1:A:7:PRO:HB2	1:A:10:PHE:HD1	0.49	1.67	12	1
1:A:25:PHE:O	1:A:29:ASN:HB2	0.49	2.08	6	6
1:B:280:ILE:HG12	1:B:288:TYR:CD1	0.49	2.43	9	2
1:B:217:SER:O	1:B:221:GLN:HG2	0.49	2.08	20	4
1:A:9:VAL:CG2	1:A:107:THR:HB	0.49	2.35	1	2
1:A:39:GLN:HA	1:A:42:ASP:OD2	0.49	2.07	3	1
1:B:279:LEU:HD21	1:B:291:GLN:HB2	0.49	1.85	10	3
1:A:39:GLN:HA	1:A:42:ASP:OD1	0.49	2.07	17	1
1:A:34:PRO:HG2	1:A:37:GLU:OE1	0.49	2.08	1	1
1:A:76:THR:O	1:A:80:ILE:HG13	0.49	2.08	19	9
1:B:243:ALA:O	1:B:247:VAL:HG23	0.48	2.08	19	8
1:A:52:VAL:O	1:A:55:ASN:HB2	0.48	2.08	17	1
1:B:288:TYR:O	1:B:292:LEU:HG	0.48	2.09	8	1
1:A:52:VAL:HB	1:A:67:LEU:HD13	0.48	1.84	12	2
1:A:70:ALA:HB2	1:B:274:SER:HB3	0.48	1.85	12	2
1:B:228:GLY:HA2	1:B:238:GLN:NE2	0.48	2.24	7	1
1:B:252:VAL:HA	1:B:255:ASN:ND2	0.48	2.23	7	1
1:A:44:ILE:HD11	1:B:263:ARG:HD2	0.47	1.85	2	1
1:B:263:ARG:O	1:B:267:LEU:HG	0.47	2.08	18	2
1:B:243:ALA:O	1:B:246:GLN:HG2	0.47	2.09	3	4
1:A:27:ILE:HA	1:A:98:ILE:HD13	0.47	1.86	5	1
1:A:118:ILE:HG22	1:A:122:ILE:HD11	0.47	1.87	18	2
1:A:92:LEU:HD21	1:A:122:ILE:HD13	0.47	1.86	5	2
1:B:224:THR:HA	1:B:242:ASP:OD2	0.47	2.09	6	1
1:A:63:ARG:HD3	1:B:240:ASP:OD1	0.47	2.09	17	1
1:B:225:PHE:O	1:B:229:ASN:HB2	0.47	2.09	5	4
1:B:323:SER:O	1:B:327:GLN:HG3	0.47	2.10	7	1
1:A:12:SER:HB3	1:A:14:ASN:OD1	0.46	2.09	1	1
1:B:296:THR:HG22	1:B:318:ILE:HD13	0.46	1.85	13	1
1:A:43:ALA:O	1:A:46:GLN:HG2	0.46	2.09	5	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:224:THR:HG22	1:B:242:ASP:HA	0.46	1.87	12	1
1:A:24:THR:HA	1:A:42:ASP:OD2	0.46	2.10	6	1
1:B:224:THR:HA	1:B:242:ASP:OD1	0.46	2.10	9	1
1:A:37:GLU:O	1:A:41:LEU:HG	0.46	2.10	10	2
1:B:226:GLY:HA3	1:B:298:ILE:HG23	0.46	1.88	10	1
1:B:234:PRO:HG2	1:B:237:GLU:OE2	0.46	2.11	18	1
1:A:84:ALA:HB3	1:A:87:ASN:HB3	0.46	1.87	19	1
1:A:80:ILE:HG12	1:A:88:TYR:CD2	0.46	2.46	19	1
1:B:219:PHE:CE1	1:B:223:LEU:HD11	0.46	2.46	20	1
1:A:94:GLU:O	1:A:98:ILE:HG13	0.46	2.11	20	5
1:A:19:PHE:O	1:A:23:LEU:HG	0.45	2.10	16	1
1:A:103:PHE:O	1:A:107:THR:HG22	0.45	2.11	20	1
1:A:120:SER:HB3	1:B:324:VAL:HB	0.45	1.89	1	1
1:A:111:ASN:HD21	1:A:114:PHE:HB2	0.45	1.71	9	1
1:B:283:SER:O	1:B:287:ASN:HB3	0.45	2.12	11	1
1:B:225:PHE:O	1:B:229:ASN:HB3	0.45	2.12	15	1
1:A:34:PRO:HG2	1:A:37:GLU:CD	0.45	2.32	18	1
1:B:311:ASN:ND2	1:B:314:PHE:HB2	0.45	2.26	10	2
1:A:40:ASP:OD2	1:B:263:ARG:HD3	0.45	2.11	17	1
1:A:80:ILE:HG12	1:A:88:TYR:CD1	0.45	2.47	4	4
1:B:280:ILE:HA	1:B:288:TYR:CB	0.45	2.42	7	1
1:B:241:LEU:HD23	1:B:278:LEU:HD23	0.45	1.88	14	1
1:A:104:ILE:HD13	1:A:109:SER:HA	0.45	1.89	11	1
1:B:294:GLU:O	1:B:298:ILE:HG13	0.45	2.11	11	7
1:A:10:PHE:HA	1:A:52:VAL:HG21	0.45	1.88	8	3
1:A:43:ALA:O	1:A:47:VAL:HG23	0.45	2.12	6	6
1:A:32:ALA:HB3	1:A:94:GLU:HG3	0.45	1.90	18	2
1:A:79:LEU:HD11	1:A:91:GLN:HB3	0.45	1.88	20	1
1:A:37:GLU:HG2	1:A:82:GLU:HB3	0.44	1.87	19	1
1:A:34:PRO:HD2	1:A:37:GLU:HB2	0.44	1.87	4	1
1:A:23:LEU:O	1:A:27:ILE:HG13	0.44	2.12	14	6
1:A:30:SER:HB3	1:A:33:PHE:HD1	0.44	1.72	8	1
1:A:59:THR:HG22	1:B:282:GLU:HG3	0.44	1.90	10	1
1:A:27:ILE:HG22	1:A:38:GLN:HG2	0.44	1.88	9	1
1:B:273:SER:HB2	1:B:321:LEU:HD23	0.44	1.88	16	1
1:A:8:SER:HB2	1:A:15:LEU:HD12	0.44	1.88	19	1
1:A:20:LEU:HG	1:A:49:LEU:HD12	0.44	1.89	5	1
1:A:80:ILE:HA	1:A:88:TYR:HB3	0.44	1.89	16	1
1:B:210:PHE:HB3	1:B:264:ALA:HB1	0.44	1.89	7	1
1:B:212:SER:HB3	1:B:214:ASN:OD1	0.44	2.13	16	3
1:A:35:THR:O	1:A:38:GLN:HB3	0.43	2.12	18	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ILE:HA	1:A:88:TYR:CB	0.43	2.43	16	1
1:A:103:PHE:HB3	1:A:109:SER:O	0.43	2.13	3	1
1:A:55:ASN:OD1	1:A:60:ALA:HA	0.43	2.13	6	1
1:A:60:ALA:HA	1:A:63:ARG:HD2	0.43	1.90	16	1
1:A:8:SER:HA	1:A:11:SER:OG	0.43	2.14	20	1
1:B:251:ALA:O	1:B:254:THR:HG22	0.43	2.14	1	1
1:A:63:ARG:HD3	1:B:240:ASP:OD2	0.43	2.14	10	1
1:A:37:GLU:O	1:A:41:LEU:HD13	0.43	2.14	19	1
1:A:88:TYR:O	1:A:92:LEU:HB2	0.42	2.14	10	1
1:B:230:SER:HB2	1:B:233:PHE:HD1	0.42	1.73	4	1
1:A:13:PRO:HB3	1:A:53:SER:HA	0.42	1.90	16	2
1:A:125:LEU:CD2	1:B:269:THR:HG21	0.42	2.43	6	1
1:A:59:THR:O	1:A:63:ARG:HG3	0.42	2.14	1	1
1:A:124:VAL:HG21	1:B:324:VAL:HG21	0.42	1.92	5	1
1:A:123:SER:O	1:A:127:GLN:HG3	0.42	2.15	7	2
1:A:104:ILE:HD13	1:A:109:SER:CA	0.42	2.45	11	1
1:B:241:LEU:HD12	1:B:275:LEU:HD22	0.42	1.91	16	1
1:A:49:LEU:HA	1:A:52:VAL:HG12	0.42	1.90	7	2
1:A:15:LEU:HG	1:A:106:THR:HG22	0.41	1.92	13	1
1:B:255:ASN:HA	1:B:263:ARG:HH21	0.41	1.75	17	1
1:A:21:GLN:OE1	1:A:21:GLN:HA	0.41	2.15	13	1
1:B:232:ALA:HB1	1:B:291:GLN:HG2	0.41	1.91	16	1
1:A:51:ALA:O	1:A:54:THR:HB	0.41	2.15	18	1
1:B:227:ILE:HG22	1:B:238:GLN:HG2	0.41	1.93	2	2
1:B:223:LEU:HD23	1:B:245:ALA:HB1	0.41	1.92	9	1
1:A:83:SER:CB	1:A:88:TYR:HA	0.41	2.45	13	1
1:B:212:SER:HB2	1:B:215:LEU:HB2	0.41	1.93	12	1
1:B:318:ILE:HG22	1:B:322:ILE:HD11	0.41	1.93	2	2
1:A:30:SER:HB2	1:A:33:PHE:CD2	0.41	2.51	15	1
1:B:317:ARG:NE	1:B:317:ARG:HA	0.41	2.30	3	1
1:B:230:SER:HB3	1:B:233:PHE:HD1	0.41	1.76	16	1
1:B:232:ALA:O	1:B:291:GLN:HG2	0.41	2.15	13	2
1:A:17:SER:O	1:A:21:GLN:HG2	0.41	2.16	15	2
1:A:18:GLY:O	1:A:21:GLN:HG2	0.41	2.16	3	1
1:A:27:ILE:HG22	1:A:38:GLN:HG3	0.41	1.92	4	2
1:B:268:SER:HB2	1:B:314:PHE:CD1	0.41	2.51	11	1
1:A:34:PRO:HD2	1:A:37:GLU:CD	0.41	2.37	15	1
1:B:275:LEU:O	1:B:279:LEU:HB2	0.41	2.16	13	1
1:B:277:ASP:HA	1:B:325:LEU:CD1	0.41	2.46	13	1
1:A:66:ALA:HB1	1:B:274:SER:OG	0.41	2.15	16	1
1:B:237:GLU:O	1:B:241:LEU:HG	0.41	2.16	17	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:235:THR:HA	1:B:238:GLN:HE21	0.41	1.76	19	1
1:B:227:ILE:HA	1:B:298:ILE:HD13	0.41	1.92	20	1
1:B:230:SER:HB2	1:B:233:PHE:HD2	0.41	1.76	19	1
1:A:30:SER:HB2	1:A:33:PHE:HD1	0.40	1.75	1	1
1:B:274:SER:HA	1:B:277:ASP:OD2	0.40	2.16	16	1
1:B:285:GLU:H	1:B:285:GLU:CD	0.40	2.19	4	1
1:B:241:LEU:HD12	1:B:275:LEU:HD12	0.40	1.92	12	1
1:A:62:ALA:HB2	1:B:282:GLU:HG2	0.40	1.93	19	1
1:B:277:ASP:HA	1:B:325:LEU:HD11	0.40	1.93	13	1
1:B:271:LEU:O	1:B:275:LEU:HD23	0.40	2.17	3	1

## 6.3 Torsion angles

### 6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	118/137 (86%)	113±2 (96±2%)	4±2 (3±2%)	1±1 (1±1%)	24	71
1	B	116/137 (85%)	112±2 (96±1%)	4±2 (3±1%)	1±1 (0±1%)	32	76
All	All	4680/5480 (85%)	4506 (96%)	145 (3%)	29 (1%)	29	74

All 11 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	84	ALA	7
1	B	284	ALA	5
1	B	311	ASN	4
1	A	7	PRO	4
1	A	111	ASN	2
1	A	11	SER	2
1	A	85	GLU	1
1	A	29	ASN	1
1	B	254	THR	1
1	A	34	PRO	1
1	B	281	ALA	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	99/112 (88%)	96±2 (97±2%)	3±2 (3±2%)	46	90
1	B	97/112 (87%)	95±1 (98±1%)	2±1 (2±1%)	51	92
All	All	3920/4480 (88%)	3819 (97%)	101 (3%)	49	91

All 40 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	B	240	ASP	8
1	A	40	ASP	7
1	B	229	ASN	6
1	B	292	LEU	6
1	A	85	GLU	5
1	A	92	LEU	4
1	A	87	ASN	4
1	B	285	GLU	4
1	B	238	GLN	4
1	A	29	ASN	4
1	A	110	ASP	3
1	A	42	ASP	3
1	A	50	ASN	3
1	A	96	THR	3
1	B	220	LEU	2
1	A	91	GLN	2
1	B	295	LEU	2
1	B	311	ASN	2
1	B	317	ARG	2
1	A	37	GLU	2
1	B	263	ARG	2
1	A	111	ASN	2
1	A	55	ASN	2
1	A	38	GLN	2
1	A	39	GLN	2
1	A	127	GLN	1
1	B	237	GLU	1
1	A	94	GLU	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	B	279	LEU	1
1	A	79	LEU	1
1	B	291	GLN	1
1	B	283	SER	1
1	A	95	LEU	1
1	B	242	ASP	1
1	A	74	SER	1
1	B	325	LEU	1
1	A	121	LEU	1
1	B	282	GLU	1
1	A	90	ASN	1
1	B	250	ASN	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 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

The completeness of assignment taking into account all chemical shift lists is 47% for the well-defined parts and 46% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `starch_output`

#### 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	1609
Number of shifts mapped to atoms	1609
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

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	137	$-0.77 \pm 0.09$	Should be applied
$^{13}\text{C}_\beta$	130	$-0.05 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	104	$0.01 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	131	$0.38 \pm 0.23$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 47%, i.e. 1214 atoms were assigned a chemical shift out of a possible 2609. 20 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	548/1152 (48%)	231/459 (50%)	204/468 (44%)	113/225 (50%)
Sidechain	619/1333 (46%)	376/772 (49%)	220/511 (43%)	23/50 (46%)

*Continued on next page...*

Continued from previous page...

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	47/124 (38%)	33/68 (49%)	14/56 (25%)	0/0 (—%)
Overall	1214/2609 (47%)	640/1299 (49%)	438/1035 (42%)	136/275 (49%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 1376 atoms were assigned a chemical shift out of a possible 2982. 23 out of 46 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	640/1350 (47%)	268/538 (50%)	241/548 (44%)	131/264 (50%)
Sidechain	689/1508 (46%)	415/866 (48%)	249/588 (42%)	25/54 (46%)
Aromatic	47/124 (38%)	33/68 (49%)	14/56 (25%)	0/0 (—%)
Overall	1376/2982 (46%)	716/1472 (49%)	504/1192 (42%)	156/318 (49%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

