



# Full wwPDB NMR Structure Validation Report ⓘ

Aug 10, 2021 – 10:08 am BST

PDB ID : 7A0O  
Title : NMR structure of flagelliform spidroin (FlagSp) N-terminal domain from *Trichonephila clavipes* at pH 5.5  
Authors : Sarr, M.; Kitoka, K.; Walsh-White, K.-A.; Kaldmae, M.; Landreh, M.; Rising, A.; Johansson, J.; Jaudzems, K.; Kronqvist, N.  
Deposited on : 2020-08-10

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

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

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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	:	2.23.1
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

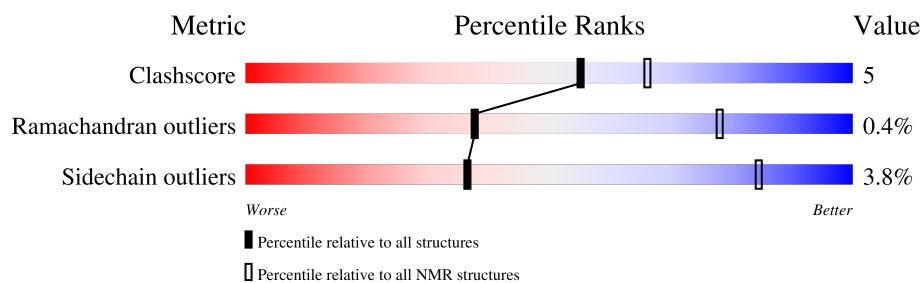
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 42%.

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	135	
1	B	135	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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 model
1	A:13-A:132, B:13-B:132 (240)	0.82	14

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 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3923 atoms, of which 1929 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Flagelliform spidroin variant 1.

Mol	Chain	Residues	Atoms						Trace
1	A	135	Total	C	H	N	O	S	0
			1961	606	964	176	211	4	
1	B	135	Total	C	H	N	O	S	0
			1962	606	965	176	211	4	

There are 16 discrepancies between the modelled and reference sequences:

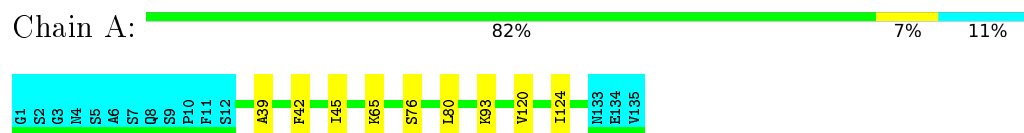
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A2S2B4P9
A	2	SER	-	expression tag	UNP A0A2S2B4P9
A	3	GLY	-	expression tag	UNP A0A2S2B4P9
A	4	ASN	-	expression tag	UNP A0A2S2B4P9
A	5	SER	-	expression tag	UNP A0A2S2B4P9
A	6	ALA	-	expression tag	UNP A0A2S2B4P9
A	7	SER	-	expression tag	UNP A0A2S2B4P9
A	8	GLN	-	expression tag	UNP A0A2S2B4P9
B	1	GLY	-	expression tag	UNP A0A2S2B4P9
B	2	SER	-	expression tag	UNP A0A2S2B4P9
B	3	GLY	-	expression tag	UNP A0A2S2B4P9
B	4	ASN	-	expression tag	UNP A0A2S2B4P9
B	5	SER	-	expression tag	UNP A0A2S2B4P9
B	6	ALA	-	expression tag	UNP A0A2S2B4P9
B	7	SER	-	expression tag	UNP A0A2S2B4P9
B	8	GLN	-	expression tag	UNP A0A2S2B4P9

## 4 Residue-property plots

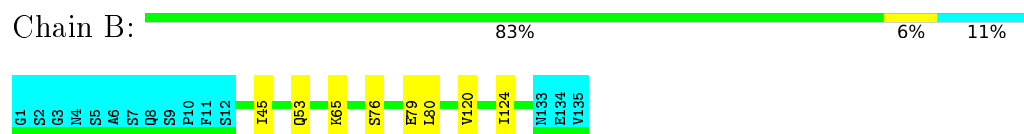
### 4.1 Average score per residue in the NMR ensemble

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: Flagelliform spidroin variant 1



- Molecule 1: Flagelliform spidroin variant 1

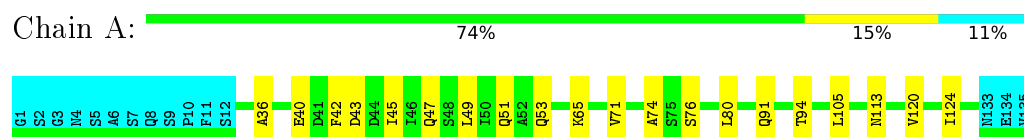


### 4.2 Scores per residue for each member of the ensemble

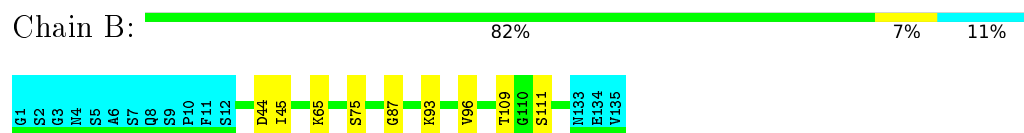
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Flagelliform spidroin variant 1

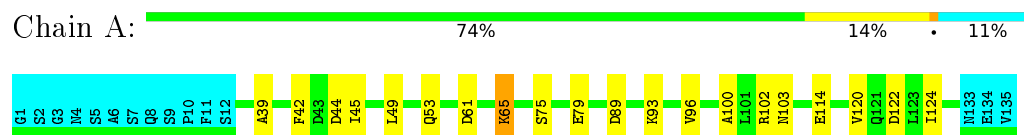


- Molecule 1: Flagelliform spidroin variant 1

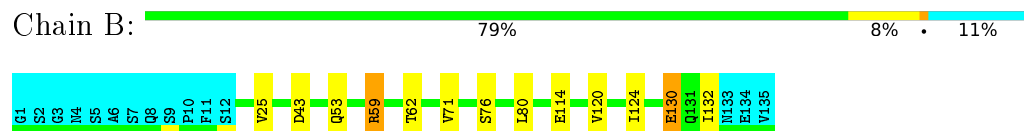


### 4.2.2 Score per residue for model 2

- Molecule 1: Flagelliform spidroin variant 1

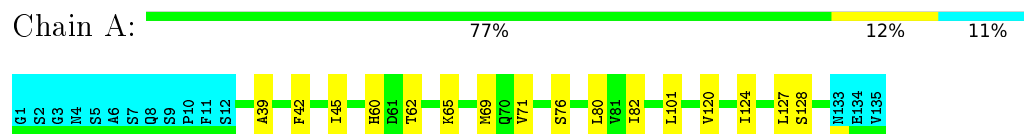


- Molecule 1: Flagelliform spidroin variant 1

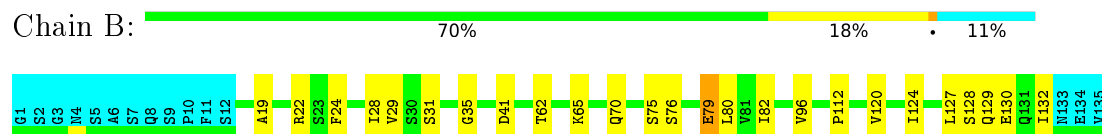


### 4.2.3 Score per residue for model 3

- Molecule 1: Flagelliform spidroin variant 1

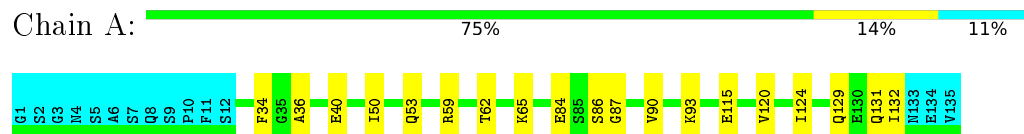


- Molecule 1: Flagelliform spidroin variant 1

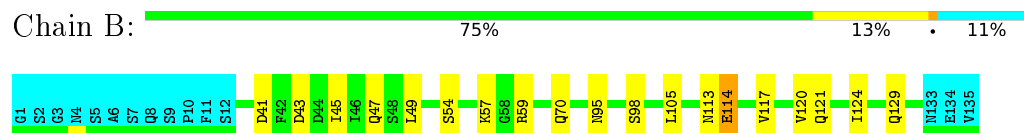


### 4.2.4 Score per residue for model 4

- Molecule 1: Flagelliform spidroin variant 1

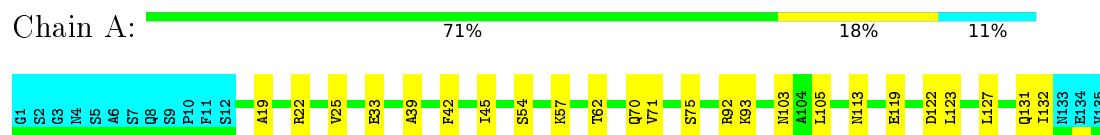


- Molecule 1: Flagelliform spidroin variant 1

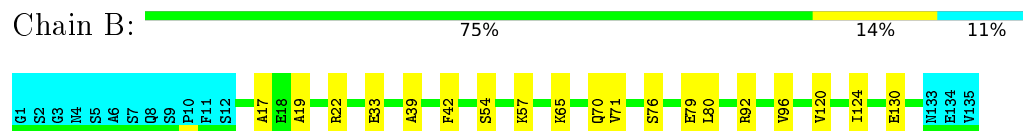


### 4.2.5 Score per residue for model 5

- Molecule 1: Flagelliform spidroin variant 1

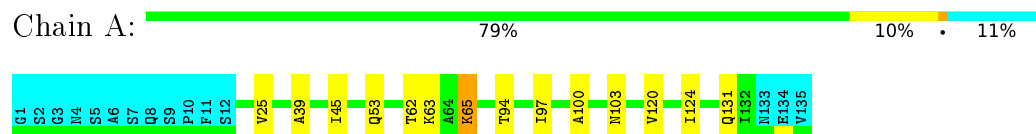


- Molecule 1: Flagelliform spidroin variant 1

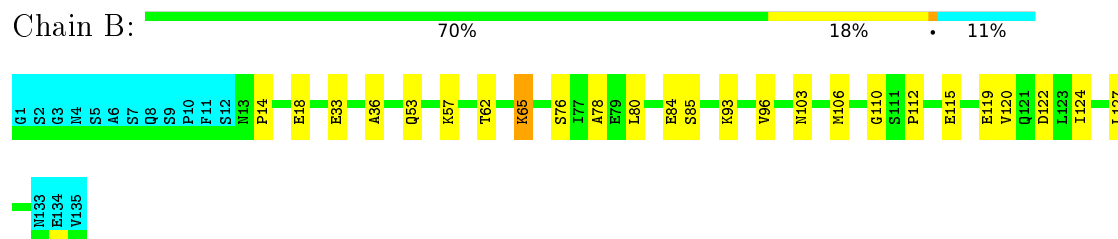


### 4.2.6 Score per residue for model 6

- Molecule 1: Flagelliform spidroin variant 1

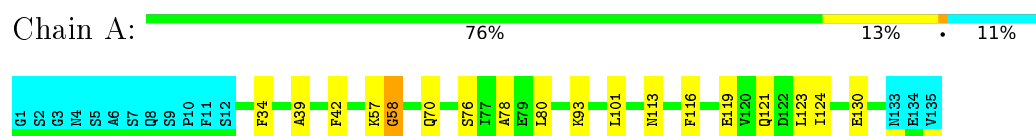


- Molecule 1: Flagelliform spidroin variant 1

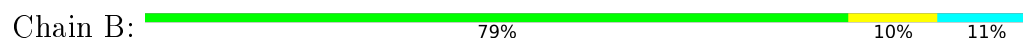


### 4.2.7 Score per residue for model 7

- Molecule 1: Flagelliform spidroin variant 1



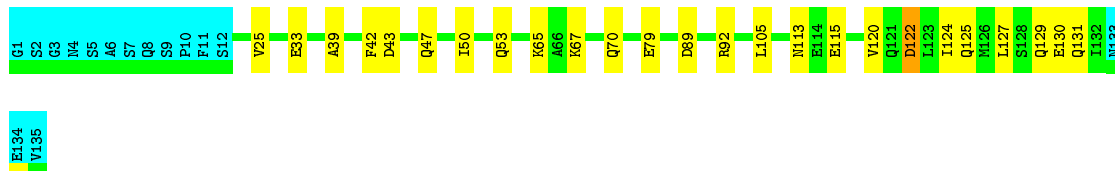
- Molecule 1: Flagelliform spidroin variant 1



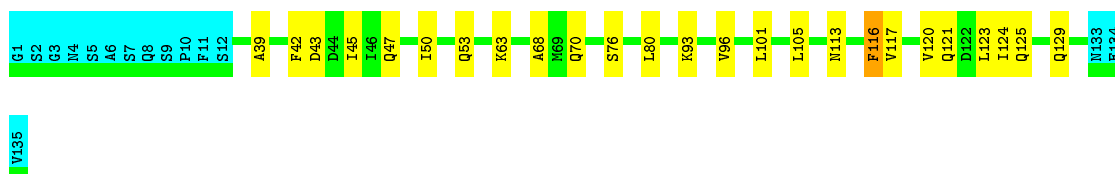


#### 4.2.8 Score per residue for model 8

- Molecule 1: Flagelliform spidroin variant 1



- Molecule 1: Flagelliform spidroin variant 1



#### 4.2.9 Score per residue for model 9

- Molecule 1: Flagelliform spidroin variant 1

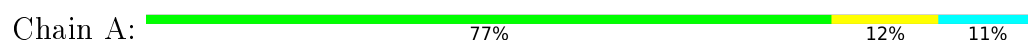


- Molecule 1: Flagelliform spidroin variant 1



#### 4.2.10 Score per residue for model 10

- Molecule 1: Flagelliform spidroin variant 1





- Molecule 1: Flagelliform spidroin variant 1

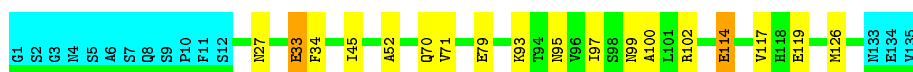
Chain B: 73% 16% 11%



#### 4.2.11 Score per residue for model 11

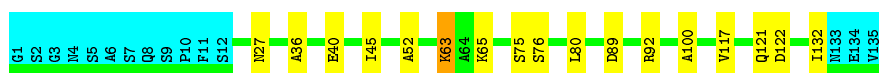
- Molecule 1: Flagelliform spidroin variant 1

Chain A: 76% 12% 11%



- Molecule 1: Flagelliform spidroin variant 1

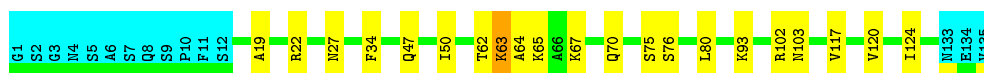
Chain B: 76% 12% 11%



#### 4.2.12 Score per residue for model 12

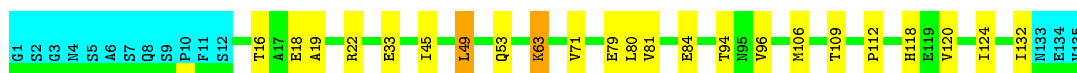
- Molecule 1: Flagelliform spidroin variant 1

Chain A: 73% 15% 11%



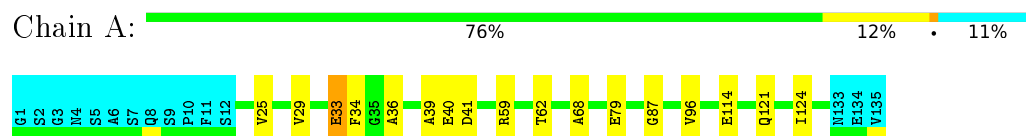
- Molecule 1: Flagelliform spidroin variant 1

Chain B: 72% 16% 11%

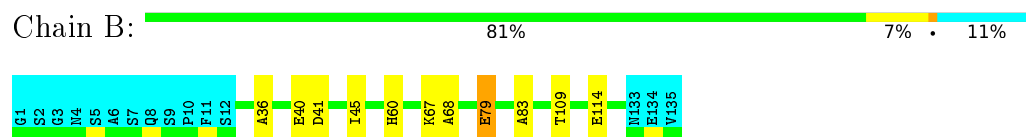


#### 4.2.13 Score per residue for model 13

- Molecule 1: Flagelliform spidroin variant 1

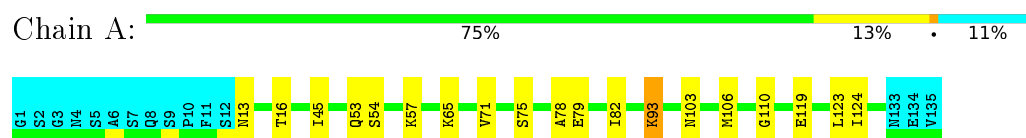


- Molecule 1: Flagelliform spidroin variant 1

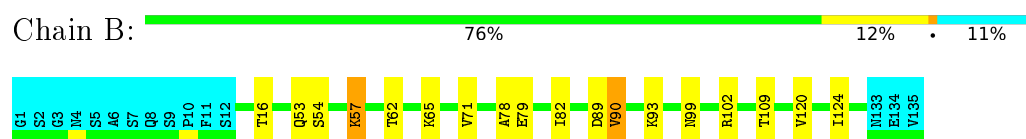


#### 4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Flagelliform spidroin variant 1

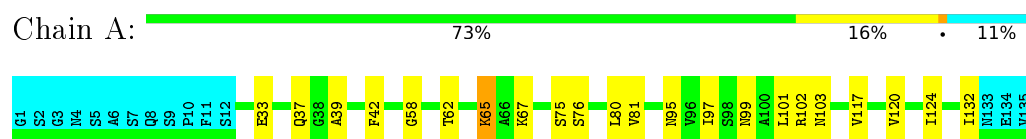


- Molecule 1: Flagelliform spidroin variant 1

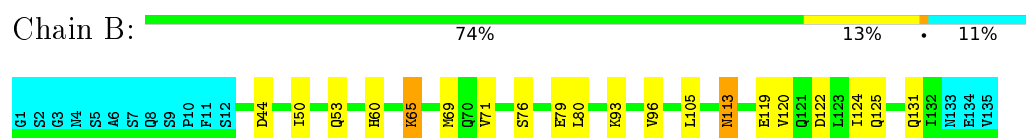


#### 4.2.15 Score per residue for model 15

- Molecule 1: Flagelliform spidroin variant 1

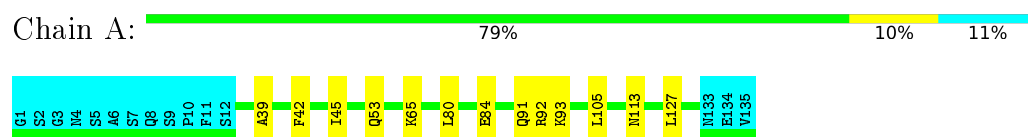


- Molecule 1: Flagelliform spidroin variant 1

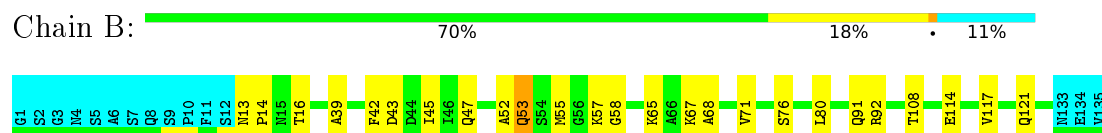


### 4.2.16 Score per residue for model 16

- Molecule 1: Flagelliform spidroin variant 1

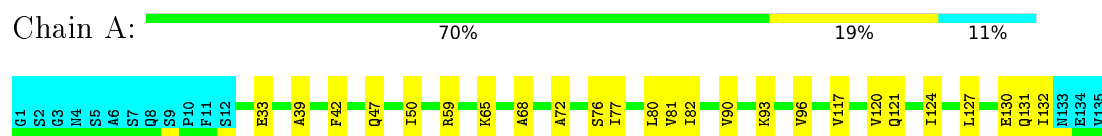


- Molecule 1: Flagelliform spidroin variant 1

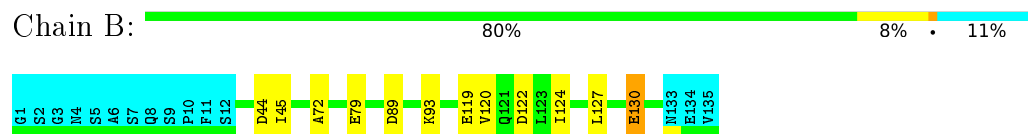


### 4.2.17 Score per residue for model 17

- Molecule 1: Flagelliform spidroin variant 1

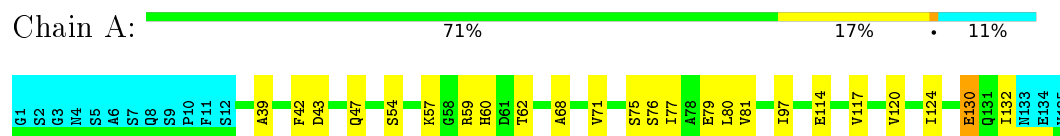


- Molecule 1: Flagelliform spidroin variant 1

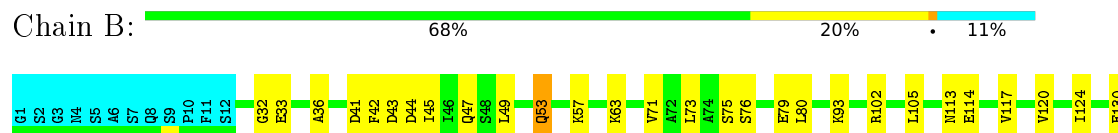


### 4.2.18 Score per residue for model 18

- Molecule 1: Flagelliform spidroin variant 1



- Molecule 1: Flagelliform spidroin variant 1





#### 4.2.19 Score per residue for model 19

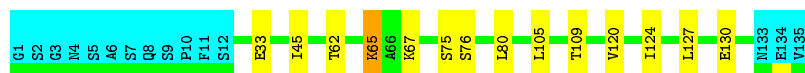
- Molecule 1: Flagelliform spidroin variant 1

Chain A: 73% 13% 11%



- Molecule 1: Flagelliform spidroin variant 1

Chain B: 79% 10% 11%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Flagelliform spidroin variant 1

Chain A: 68% 19% 11%



- Molecule 1: Flagelliform spidroin variant 1

Chain B: 76% 13% 11%



## 5 Refinement protocol and experimental data overview

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

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	1.2

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	1470
Number of shifts mapped to atoms	1470
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	42%

## 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	895	878	878	12±3
1	B	895	878	878	11±3
All	All	35800	35120	35120	379

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LYS:HG2	1:B:45:ILE:HG13	0.78	1.53	19	1
1:B:32:GLY:HA2	1:B:36:ALA:HB2	0.78	1.56	9	2
1:B:54:SER:HA	1:B:57:LYS:HE3	0.77	1.55	4	2
1:A:65:LYS:HG3	1:B:45:ILE:HG12	0.76	1.56	16	3
1:A:54:SER:HA	1:A:57:LYS:HE2	0.76	1.57	9	2
1:A:33:GLU:HG3	1:A:93:LYS:HD2	0.74	1.57	11	1
1:A:105:LEU:HB3	1:A:113:ASN:HB2	0.74	1.58	5	1
1:A:127:LEU:HD22	1:A:132:ILE:HD12	0.74	1.60	5	1
1:B:85:SER:HB2	1:B:93:LYS:HE2	0.73	1.60	6	1
1:B:57:LYS:HA	1:B:65:LYS:HD3	0.72	1.61	9	1
1:A:76:SER:O	1:A:80:LEU:HG	0.67	1.89	7	7
1:A:62:THR:HG21	1:B:41:ASP:HA	0.67	1.65	13	1
1:A:33:GLU:HG3	1:A:96:VAL:HG11	0.67	1.67	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:ASN:HA	1:A:102:ARG:HD2	0.65	1.68	15	1
1:A:65:LYS:HD3	1:B:45:ILE:HG12	0.65	1.68	17	1
1:B:45:ILE:H	1:B:45:ILE:HD12	0.64	1.51	19	2
1:A:67:LYS:HA	1:A:70:GLN:HG2	0.63	1.71	9	1
1:B:16:THR:HG23	1:B:108:THR:HB	0.63	1.70	16	1
1:A:65:LYS:HE3	1:B:44:ASP:HB2	0.62	1.69	15	1
1:B:31:SER:HB3	1:B:96:VAL:HB	0.62	1.70	3	1
1:A:33:GLU:HG2	1:A:96:VAL:HG11	0.62	1.71	13	1
1:A:61:ASP:HB2	1:A:65:LYS:HE2	0.61	1.71	19	1
1:B:63:LYS:HE2	1:B:63:LYS:N	0.61	2.10	12	1
1:A:57:LYS:HA	1:A:65:LYS:HD3	0.61	1.71	14	1
1:A:28:ILE:HG22	1:A:35:GLY:HA2	0.61	1.71	19	1
1:A:45:ILE:H	1:A:45:ILE:HD12	0.61	1.56	19	1
1:B:76:SER:O	1:B:80:LEU:HG	0.61	1.95	19	8
1:B:99:ASN:HA	1:B:102:ARG:HD3	0.60	1.73	14	1
1:A:54:SER:HA	1:A:57:LYS:HG2	0.60	1.71	5	1
1:A:61:ASP:HB2	1:A:65:LYS:CE	0.60	2.26	19	1
1:A:127:LEU:HD21	1:B:123:LEU:HD21	0.60	1.73	8	1
1:A:82:ILE:HG12	1:A:124:ILE:HG23	0.59	1.74	14	1
1:A:42:PHE:CD2	1:A:80:LEU:HG	0.59	2.32	17	3
1:A:89:ASP:HB2	1:A:92:ARG:HD3	0.59	1.72	8	1
1:A:45:ILE:HG12	1:B:65:LYS:HG3	0.59	1.72	20	4
1:B:105:LEU:HD22	1:B:113:ASN:ND2	0.59	2.13	8	1
1:A:100:ALA:HA	1:A:103:ASN:OD1	0.59	1.98	2	2
1:A:34:PHE:HZ	1:A:81:VAL:HA	0.58	1.56	9	1
1:B:42:PHE:CD2	1:B:80:LEU:HG	0.58	2.32	18	1
1:A:122:ASP:HA	1:A:125:GLN:HE21	0.58	1.58	8	1
1:A:132:ILE:HD13	1:B:71:VAL:HG23	0.58	1.74	15	1
1:A:71:VAL:HG22	1:B:75:SER:HB2	0.58	1.75	11	1
1:A:75:SER:HB3	1:B:71:VAL:HG12	0.58	1.75	15	6
1:A:60:HIS:CE1	1:B:44:ASP:HB2	0.58	2.34	18	1
1:B:33:GLU:HG3	1:B:96:VAL:HG21	0.57	1.76	5	3
1:A:44:ASP:OD1	1:B:59:ARG:HG2	0.57	2.00	2	1
1:B:65:LYS:HB3	1:B:65:LYS:HZ3	0.57	1.59	15	1
1:A:59:ARG:HB3	1:B:44:ASP:OD1	0.57	1.99	17	1
1:A:54:SER:HA	1:A:57:LYS:NZ	0.57	2.15	14	1
1:A:61:ASP:HA	1:A:65:LYS:HE2	0.56	1.77	2	1
1:A:19:ALA:HA	1:A:22:ARG:HG2	0.56	1.77	9	3
1:A:52:ALA:HB2	1:B:52:ALA:HB2	0.56	1.76	11	1
1:A:39:ALA:HA	1:A:42:PHE:CD2	0.56	2.36	8	5
1:A:123:LEU:O	1:A:127:LEU:HG	0.56	2.00	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:GLN:HE22	1:B:132:ILE:HG21	0.55	1.61	12	1
1:B:105:LEU:HG	1:B:113:ASN:HB2	0.55	1.79	18	3
1:B:78:ALA:HA	1:B:124:ILE:HG12	0.55	1.78	6	2
1:A:65:LYS:HD2	1:B:44:ASP:HB3	0.55	1.78	1	1
1:B:19:ALA:HA	1:B:22:ARG:HG2	0.54	1.79	12	3
1:A:114:GLU:O	1:A:117:VAL:HG22	0.54	2.02	11	3
1:A:105:LEU:HD21	1:A:113:ASN:HB2	0.54	1.80	8	1
1:A:41:ASP:HA	1:B:60:HIS:CE1	0.54	2.38	13	1
1:B:117:VAL:O	1:B:121:GLN:HG2	0.54	2.02	20	2
1:B:34:PHE:HE1	1:B:97:ILE:HD11	0.54	1.63	10	1
1:A:119:GLU:HG2	1:B:132:ILE:HD12	0.54	1.80	11	1
1:B:129:GLN:HG2	1:B:130:GLU:HG3	0.53	1.81	3	1
1:B:114:GLU:O	1:B:117:VAL:HG22	0.53	2.02	16	2
1:A:54:SER:HA	1:A:57:LYS:HZ3	0.53	1.63	14	1
1:A:120:VAL:O	1:A:124:ILE:HG13	0.53	2.04	19	11
1:A:79:GLU:HG3	1:B:71:VAL:HG21	0.53	1.80	2	2
1:B:63:LYS:N	1:B:63:LYS:HD2	0.53	2.18	9	1
1:B:45:ILE:HD12	1:B:45:ILE:H	0.53	1.64	13	2
1:B:29:VAL:HA	1:B:35:GLY:O	0.53	2.04	3	1
1:A:34:PHE:HD2	1:A:93:LYS:HB3	0.53	1.63	7	1
1:A:93:LYS:HD2	1:A:93:LYS:H	0.53	1.64	16	1
1:B:78:ALA:HB2	1:B:120:VAL:HB	0.53	1.81	14	1
1:A:76:SER:O	1:A:80:LEU:HB2	0.52	2.05	20	1
1:A:45:ILE:CG1	1:B:65:LYS:HA	0.52	2.35	19	1
1:A:93:LYS:HD2	1:A:93:LYS:N	0.52	2.20	16	1
1:A:67:LYS:O	1:A:70:GLN:HG2	0.52	2.04	20	1
1:A:49:LEU:O	1:A:53:GLN:HG3	0.52	2.05	1	2
1:A:91:GLN:HE22	1:A:125:GLN:HA	0.52	1.65	20	1
1:A:45:ILE:HD12	1:A:45:ILE:H	0.51	1.64	2	2
1:B:120:VAL:O	1:B:124:ILE:HG13	0.51	2.05	4	15
1:B:82:ILE:HD12	1:B:127:LEU:HD22	0.51	1.82	3	1
1:B:53:GLN:O	1:B:57:LYS:HE3	0.51	2.06	16	2
1:B:93:LYS:O	1:B:96:VAL:HG12	0.51	2.06	15	4
1:B:25:VAL:HG21	1:B:43:ASP:HB2	0.51	1.82	2	1
1:A:105:LEU:HG	1:A:113:ASN:HB2	0.51	1.83	10	3
1:B:106:MET:HG2	1:B:112:PRO:HA	0.51	1.82	12	1
1:B:76:SER:O	1:B:80:LEU:HB2	0.50	2.06	3	1
1:B:89:ASP:HB2	1:B:92:ARG:HB2	0.50	1.83	11	1
1:A:71:VAL:HG21	1:B:79:GLU:HG2	0.50	1.82	14	1
1:A:74:ALA:O	1:A:120:VAL:HG12	0.50	2.07	1	1
1:B:63:LYS:HD2	1:B:63:LYS:N	0.50	2.21	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:SER:O	1:A:80:LEU:HD13	0.50	2.06	18	3
1:A:39:ALA:HA	1:A:42:PHE:CD1	0.50	2.42	5	5
1:A:65:LYS:O	1:A:69:MET:HG2	0.50	2.07	3	1
1:A:65:LYS:HB3	1:B:45:ILE:HD11	0.50	1.84	12	1
1:A:42:PHE:CD2	1:A:80:LEU:HD22	0.49	2.42	3	1
1:A:71:VAL:HG21	1:B:79:GLU:HG3	0.49	1.84	20	2
1:B:76:SER:O	1:B:80:LEU:HD13	0.49	2.07	10	2
1:A:71:VAL:HG12	1:B:75:SER:HB3	0.49	1.83	1	3
1:B:50:ILE:HA	1:B:53:GLN:HE21	0.49	1.68	15	1
1:A:32:GLY:HA2	1:A:36:ALA:HB2	0.49	1.84	20	1
1:B:59:ARG:HA	1:B:59:ARG:NE	0.49	2.23	4	1
1:A:34:PHE:CZ	1:A:93:LYS:HD3	0.49	2.42	12	1
1:A:57:LYS:HG3	1:A:58:GLY:H	0.49	1.68	7	1
1:A:68:ALA:HB2	1:B:79:GLU:HG2	0.49	1.84	17	1
1:A:13:ASN:HB2	1:A:16:THR:OG1	0.49	2.08	14	1
1:B:49:LEU:HG	1:B:73:LEU:HB2	0.49	1.83	18	1
1:A:65:LYS:HB2	1:A:65:LYS:HZ2	0.48	1.68	6	1
1:A:132:ILE:HD11	1:B:119:GLU:OE1	0.48	2.07	17	1
1:B:43:ASP:O	1:B:47:GLN:HB2	0.48	2.08	18	4
1:B:117:VAL:O	1:B:121:GLN:HG3	0.48	2.09	11	3
1:A:44:ASP:HA	1:B:59:ARG:HD3	0.48	1.85	2	1
1:A:101:LEU:HD11	1:A:116:PHE:CD2	0.48	2.44	10	1
1:A:82:ILE:HD13	1:A:127:LEU:HD22	0.48	1.84	3	1
1:A:45:ILE:HD11	1:B:65:LYS:HA	0.48	1.84	3	2
1:A:45:ILE:HD11	1:B:65:LYS:HG3	0.48	1.85	16	1
1:A:36:ALA:O	1:A:40:GLU:HG3	0.48	2.08	4	2
1:B:43:ASP:O	1:B:47:GLN:HG2	0.48	2.09	8	1
1:A:99:ASN:HA	1:A:102:ARG:CD	0.48	2.37	15	1
1:A:130:GLU:HB3	1:A:132:ILE:HG22	0.48	1.86	18	1
1:B:82:ILE:HD11	1:B:124:ILE:HG23	0.47	1.85	3	1
1:A:25:VAL:HG21	1:A:43:ASP:HB2	0.47	1.86	8	1
1:A:106:MET:HA	1:A:110:GLY:HA2	0.47	1.85	14	1
1:A:33:GLU:CD	1:A:34:PHE:H	0.47	2.12	13	1
1:B:67:LYS:HZ2	1:B:67:LYS:HB2	0.47	1.69	19	1
1:A:121:GLN:HA	1:A:124:ILE:HD12	0.47	1.85	7	2
1:A:79:GLU:HG3	1:B:68:ALA:HA	0.47	1.86	8	2
1:A:82:ILE:HD11	1:A:124:ILE:HG23	0.47	1.86	20	1
1:B:82:ILE:HD11	1:B:124:ILE:HA	0.47	1.85	14	2
1:A:45:ILE:CD1	1:B:65:LYS:HA	0.47	2.38	6	1
1:B:36:ALA:O	1:B:40:GLU:HG2	0.47	2.10	13	1
1:A:43:ASP:O	1:A:47:GLN:HB2	0.47	2.10	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ARG:HB3	1:A:117:VAL:HG21	0.46	1.85	12	1
1:A:62:THR:HB	1:B:41:ASP:OD2	0.46	2.11	18	2
1:B:39:ALA:HA	1:B:42:PHE:CD1	0.46	2.46	16	2
1:B:51:GLN:O	1:B:55:MET:HG2	0.46	2.11	7	1
1:A:47:GLN:HA	1:A:50:ILE:HD12	0.46	1.87	9	3
1:A:102:ARG:O	1:A:102:ARG:HD3	0.46	2.10	19	1
1:A:34:PHE:CZ	1:A:81:VAL:HA	0.46	2.42	9	1
1:B:18:GLU:O	1:B:22:ARG:HG3	0.46	2.11	7	1
1:B:79:GLU:OE2	1:B:83:ALA:HB2	0.46	2.11	13	1
1:A:111:SER:HB2	1:A:113:ASN:OD1	0.46	2.11	20	1
1:B:126:MET:HG3	1:B:127:LEU:N	0.46	2.26	9	1
1:B:63:LYS:HA	1:B:63:LYS:HE3	0.46	1.88	11	1
1:A:29:VAL:HG13	1:A:36:ALA:HB2	0.46	1.88	13	1
1:B:57:LYS:HA	1:B:65:LYS:CD	0.46	2.40	9	1
1:B:39:ALA:HA	1:B:42:PHE:CD2	0.45	2.45	9	3
1:B:105:LEU:HG	1:B:113:ASN:HB3	0.45	1.88	10	1
1:A:59:ARG:HA	1:A:59:ARG:NE	0.45	2.26	4	1
1:A:34:PHE:HE2	1:A:97:ILE:HD11	0.45	1.71	11	1
1:A:50:ILE:O	1:A:53:GLN:HG2	0.45	2.11	8	1
1:A:63:LYS:HA	1:A:63:LYS:CE	0.45	2.41	12	1
1:A:75:SER:HB3	1:B:71:VAL:CG1	0.45	2.42	14	1
1:B:54:SER:HA	1:B:57:LYS:NZ	0.45	2.27	14	1
1:A:59:ARG:NE	1:A:59:ARG:HA	0.45	2.27	18	1
1:A:65:LYS:HB2	1:B:45:ILE:HG12	0.45	1.89	4	1
1:A:82:ILE:HG12	1:A:90:VAL:HG21	0.45	1.89	17	1
1:A:71:VAL:HG22	1:B:75:SER:HB3	0.45	1.88	3	1
1:B:79:GLU:HG2	1:B:127:LEU:HD21	0.45	1.88	3	1
1:B:81:VAL:HG11	1:B:94:THR:HB	0.45	1.89	12	1
1:A:82:ILE:HD11	1:A:124:ILE:HA	0.44	1.89	9	1
1:A:65:LYS:CE	1:B:44:ASP:HB2	0.44	2.41	15	1
1:A:77:ILE:O	1:A:81:VAL:HG23	0.44	2.12	18	2
1:B:14:PRO:O	1:B:18:GLU:HG2	0.44	2.12	6	1
1:B:19:ALA:HA	1:B:22:ARG:HB3	0.44	1.90	3	1
1:B:27:ASN:HD22	1:B:100:ALA:HA	0.44	1.71	11	1
1:B:89:ASP:HB3	1:B:93:LYS:HE2	0.44	1.89	14	1
1:A:94:THR:HA	1:A:97:ILE:HB	0.44	1.89	6	1
1:A:127:LEU:O	1:A:127:LEU:HD13	0.44	2.12	19	1
1:A:93:LYS:HA	1:A:93:LYS:HE2	0.44	1.88	14	1
1:A:89:ASP:O	1:A:93:LYS:HG2	0.44	2.12	2	1
1:B:65:LYS:O	1:B:69:MET:HG2	0.44	2.12	15	1
1:B:127:LEU:O	1:B:127:LEU:HD23	0.44	2.12	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:GLU:OE1	1:A:82:ILE:HB	0.44	2.12	20	1
1:A:45:ILE:CG1	1:B:65:LYS:HG2	0.44	2.43	1	1
1:B:109:THR:HG23	1:B:111:SER:H	0.44	1.73	10	2
1:A:36:ALA:O	1:A:40:GLU:HG2	0.44	2.13	1	1
1:A:33:GLU:HG3	1:A:93:LYS:HE3	0.44	1.90	5	1
1:B:45:ILE:CD1	1:B:80:LEU:HD21	0.43	2.43	11	1
1:A:94:THR:HG22	1:A:121:GLN:HG3	0.43	1.89	20	1
1:A:34:PHE:CD2	1:A:93:LYS:HB3	0.43	2.47	7	1
1:A:78:ALA:HA	1:A:124:ILE:HG12	0.43	1.89	7	1
1:B:57:LYS:HA	1:B:65:LYS:NZ	0.43	2.29	16	1
1:A:42:PHE:CD1	1:A:80:LEU:HG	0.43	2.47	1	1
1:B:36:ALA:O	1:B:40:GLU:HG3	0.43	2.13	11	1
1:A:81:VAL:HG22	1:A:97:ILE:HG13	0.43	1.89	18	2
1:B:50:ILE:O	1:B:53:GLN:HG2	0.43	2.14	7	2
1:B:24:PHE:CE1	1:B:28:ILE:HD11	0.43	2.49	3	1
1:A:25:VAL:HG13	1:A:39:ALA:HB1	0.43	1.90	6	3
1:B:122:ASP:HA	1:B:125:GLN:NE2	0.43	2.29	15	1
1:A:93:LYS:O	1:A:96:VAL:HG12	0.43	2.13	2	1
1:A:70:GLN:HG3	1:A:71:VAL:N	0.43	2.29	9	1
1:A:63:LYS:HA	1:A:63:LYS:HE2	0.43	1.90	12	1
1:A:116:PHE:HA	1:A:119:GLU:HG2	0.43	1.89	7	1
1:B:13:ASN:OD1	1:B:14:PRO:HD2	0.43	2.14	16	1
1:A:62:THR:HB	1:B:41:ASP:OD1	0.43	2.14	4	1
1:B:114:GLU:HA	1:B:117:VAL:HG22	0.43	1.88	4	1
1:A:129:GLN:HG3	1:A:130:GLU:H	0.43	1.73	8	1
1:A:91:GLN:O	1:A:94:THR:HG22	0.42	2.14	1	1
1:A:62:THR:HB	1:B:41:ASP:CG	0.42	2.35	4	1
1:A:129:GLN:HB3	1:A:131:GLN:OE1	0.42	2.13	8	1
1:B:121:GLN:HA	1:B:124:ILE:HD12	0.42	1.91	10	1
1:A:78:ALA:O	1:A:82:ILE:HG13	0.42	2.14	14	1
1:A:34:PHE:CZ	1:A:93:LYS:HG2	0.42	2.49	4	1
1:B:93:LYS:HE2	1:B:93:LYS:HA	0.42	1.91	15	2
1:A:117:VAL:O	1:A:121:GLN:HG3	0.42	2.14	17	1
1:B:74:ALA:O	1:B:120:VAL:HG23	0.42	2.13	10	1
1:A:43:ASP:O	1:A:47:GLN:HG2	0.42	2.14	8	1
1:A:119:GLU:O	1:A:123:LEU:HD13	0.42	2.14	14	2
1:B:116:PHE:O	1:B:120:VAL:HG23	0.42	2.14	8	1
1:B:89:ASP:O	1:B:93:LYS:HG2	0.42	2.15	17	1
1:A:45:ILE:HG13	1:B:65:LYS:HG3	0.42	1.90	10	1
1:A:101:LEU:HD23	1:A:117:VAL:HA	0.42	1.92	15	1
1:A:61:ASP:HA	1:A:65:LYS:CE	0.42	2.45	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:82:ILE:HD13	1:B:128:SER:HB2	0.42	1.91	3	1
1:A:27:ASN:HD22	1:A:100:ALA:HA	0.42	1.74	20	2
1:A:42:PHE:HB3	1:A:80:LEU:HD21	0.42	1.92	20	1
1:A:62:THR:OG1	1:A:65:LYS:HG2	0.42	2.14	6	1
1:B:106:MET:HA	1:B:110:GLY:HA2	0.42	1.92	6	1
1:B:49:LEU:O	1:B:53:GLN:HG3	0.42	2.15	12	1
1:A:121:GLN:O	1:A:124:ILE:HG12	0.41	2.15	9	1
1:A:126:MET:SD	1:B:122:ASP:HB3	0.41	2.55	11	1
1:B:16:THR:CG2	1:B:108:THR:HB	0.41	2.43	16	1
1:B:53:GLN:OE1	1:B:57:LYS:HE2	0.41	2.15	18	1
1:B:132:ILE:HG12	1:B:132:ILE:O	0.41	2.15	3	1
1:B:65:LYS:HZ3	1:B:65:LYS:CB	0.41	2.26	15	1
1:A:45:ILE:HG21	1:B:68:ALA:HB1	0.41	1.91	16	1
1:A:102:ARG:HD3	1:A:114:GLU:OE1	0.41	2.16	2	1
1:A:131:GLN:HG3	1:A:132:ILE:HG13	0.41	1.92	4	1
1:B:99:ASN:HA	1:B:102:ARG:CD	0.41	2.42	14	1
1:B:127:LEU:HD13	1:B:127:LEU:O	0.41	2.15	19	1
1:B:119:GLU:O	1:B:123:LEU:HG	0.41	2.14	20	1
1:B:130:GLU:HB3	1:B:132:ILE:HG22	0.41	1.93	2	1
1:A:64:ALA:HB1	1:B:80:LEU:HD23	0.41	1.91	12	1
1:A:68:ALA:HB1	1:B:45:ILE:HG21	0.41	1.93	13	3
1:A:47:GLN:O	1:A:51:GLN:HG2	0.41	2.16	19	2
1:A:13:ASN:HB2	1:A:16:THR:HB	0.41	1.92	10	1
1:A:127:LEU:HD21	1:B:71:VAL:HG21	0.41	1.91	16	1
1:A:50:ILE:HA	1:A:53:GLN:HE21	0.41	1.75	4	1
1:B:95:ASN:HA	1:B:98:SER:OG	0.41	2.16	4	1
1:A:67:LYS:HB2	1:B:79:GLU:OE2	0.41	2.16	15	1
1:A:65:LYS:HB2	1:A:65:LYS:NZ	0.41	2.30	16	1
1:A:41:ASP:CG	1:B:62:THR:HB	0.41	2.36	19	1
1:A:99:ASN:O	1:A:102:ARG:HG2	0.40	2.17	11	1
1:A:67:LYS:HE3	1:B:79:GLU:OE1	0.40	2.17	12	1
1:A:132:ILE:CD1	1:B:71:VAL:HG23	0.40	2.46	15	1
1:B:105:LEU:HG	1:B:113:ASN:CB	0.40	2.47	15	1
1:A:45:ILE:HG13	1:B:65:LYS:HG2	0.40	1.93	19	1
1:B:121:GLN:O	1:B:125:GLN:HG3	0.40	2.15	8	1
1:A:72:ALA:HA	1:B:72:ALA:HA	0.40	1.93	17	1
1:A:65:LYS:HG3	1:B:45:ILE:HD11	0.40	1.94	1	1
1:B:52:ALA:HA	1:B:55:MET:HG2	0.40	1.94	16	1
1:B:105:LEU:O	1:B:109:THR:HG22	0.40	2.16	19	1
1:A:27:ASN:HD22	1:A:103:ASN:ND2	0.40	2.14	12	1
1:B:62:THR:OG1	1:B:65:LYS:HB2	0.40	2.16	14	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	120/135 (89%)	112±3 (93±2%)	8±2 (6±2%)	0±1 (0±1%)	38	78
1	B	120/135 (89%)	113±2 (94±2%)	6±2 (5±2%)	0±1 (0±0%)	38	78
All	All	4800/5400 (89%)	4502 (94%)	279 (6%)	19 (0%)	38	78

All 18 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	58	GLY	2
1	B	87	GLY	1
1	B	112	PRO	1
1	A	86	SER	1
1	A	87	GLY	1
1	A	90	VAL	1
1	A	131	GLN	1
1	B	36	ALA	1
1	B	116	PHE	1
1	B	88	GLY	1
1	B	57	LYS	1
1	B	90	VAL	1
1	A	37	GLN	1
1	B	60	HIS	1
1	B	58	GLY	1
1	A	33	GLU	1
1	A	35	GLY	1
1	A	38	GLY	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	97/109 (89%)	93±2 (96±2%)	4±2 (4±2%)	35	83
1	B	97/109 (89%)	94±2 (96±2%)	4±2 (4±2%)	38	86
All	All	3880/4360 (89%)	3733 (96%)	147 (4%)	36	84

All 65 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	79	GLU	6
1	B	130	GLU	5
1	B	70	GLN	5
1	A	70	GLN	5
1	A	53	GLN	4
1	A	65	LYS	4
1	B	53	GLN	4
1	B	62	THR	4
1	B	114	GLU	4
1	A	101	LEU	4
1	B	79	GLU	4
1	A	62	THR	4
1	A	33	GLU	4
1	A	114	GLU	4
1	A	122	ASP	3
1	A	92	ARG	3
1	A	103	ASN	3
1	B	65	LYS	3
1	B	84	GLU	3
1	B	63	LYS	3
1	A	93	LYS	3
1	B	33	GLU	3
1	A	84	GLU	2
1	A	115	GLU	2
1	B	49	LEU	2
1	B	129	GLN	2
1	A	119	GLU	2
1	B	92	ARG	2
1	A	63	LYS	2
1	A	131	GLN	2
1	B	103	ASN	2
1	B	119	GLU	2
1	B	122	ASP	2
1	B	127	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	130	GLU	2
1	A	95	ASN	2
1	B	18	GLU	2
1	A	59	ARG	2
1	B	67	LYS	2
1	A	127	LEU	2
1	A	102	ARG	2
1	A	49	LEU	1
1	B	59	ARG	1
1	A	60	HIS	1
1	A	129	GLN	1
1	B	112	PRO	1
1	B	115	GLU	1
1	A	113	ASN	1
1	B	121	GLN	1
1	A	67	LYS	1
1	B	101	LEU	1
1	A	61	ASP	1
1	B	93	LYS	1
1	A	51	GLN	1
1	B	37	GLN	1
1	B	118	HIS	1
1	A	40	GLU	1
1	B	90	VAL	1
1	B	113	ASN	1
1	B	131	GLN	1
1	A	91	GLN	1
1	B	91	GLN	1
1	B	102	ARG	1
1	A	18	GLU	1
1	B	16	THR	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 [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 42% for the well-defined parts and 42% 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 [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	1470
Number of shifts mapped to atoms	1470
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

#### 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
$^{13}\text{C}_\alpha$	135	$-1.12 \pm 0.19$	Should be applied
$^{13}\text{C}_\beta$	125	$-0.40 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	3	—	None (insufficient data)
$^{15}\text{N}$	131	$-1.17 \pm 0.19$	Should be applied

#### 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 42%, i.e. 1166 atoms were assigned a chemical shift out of a possible 2766. 15 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	476/1192 (40%)	238/476 (50%)	120/480 (25%)	118/236 (50%)
Sidechain	647/1456 (44%)	396/846 (47%)	230/542 (42%)	21/68 (31%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	43/118 (36%)	29/66 (44%)	14/48 (29%)	0/4 (0%)
Overall	1166/2766 (42%)	663/1388 (48%)	364/1070 (34%)	139/308 (45%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 42%, i.e. 1294 atoms were assigned a chemical shift out of a possible 3062. 16 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	535/1338 (40%)	266/534 (50%)	138/540 (26%)	131/264 (50%)
Sidechain	709/1588 (45%)	436/926 (47%)	249/588 (42%)	24/74 (32%)
Aromatic	50/136 (37%)	34/76 (45%)	16/56 (29%)	0/4 (0%)
Overall	1294/3062 (42%)	736/1536 (48%)	403/1184 (34%)	155/342 (45%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	10	PRO	HG2	0.18	3.48 – 0.38	-5.6
1	A	28	ILE	HD11	-0.93	2.13 – -0.77	-5.5
1	A	28	ILE	HD12	-0.93	2.13 – -0.77	-5.5
1	A	28	ILE	HD13	-0.93	2.13 – -0.77	-5.5

#### 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:

