



# Full wwPDB NMR Structure Validation Report ⓘ

Aug 27, 2020 – 01:58 PM BST

PDB ID : 6TWE  
Title : Cu(I) NMR solution structure of the chitin-active lytic polysaccharide monooxygenase BILPMO10A  
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Deposited on : 2020-01-13

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

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<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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
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 : 2.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

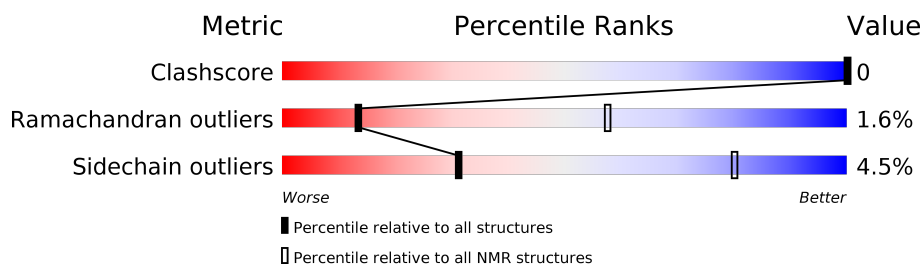
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 82%.

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



Metric	Whole archive (#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	172	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:13, A:29-A:39, A:57-A:172 (140)	1.19	2

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 4 clusters. No single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2635 atoms, of which 1275 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative chitin binding protein.

Mol	Chain	Residues	Atoms						Trace
1	A	172	Total	C	H	N	O	S	0
			2634	869	1275	234	252	4	

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

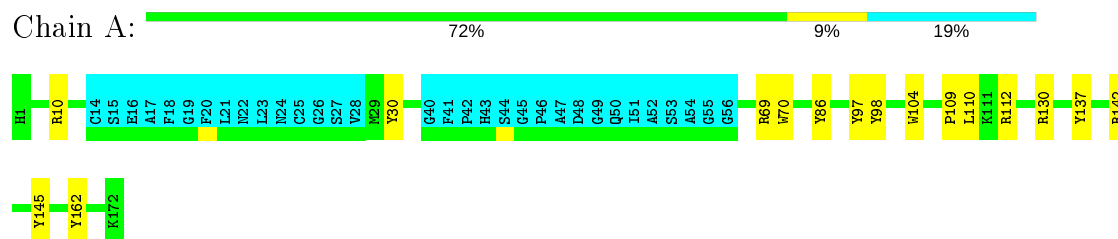
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

## 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: Putative chitin binding protein

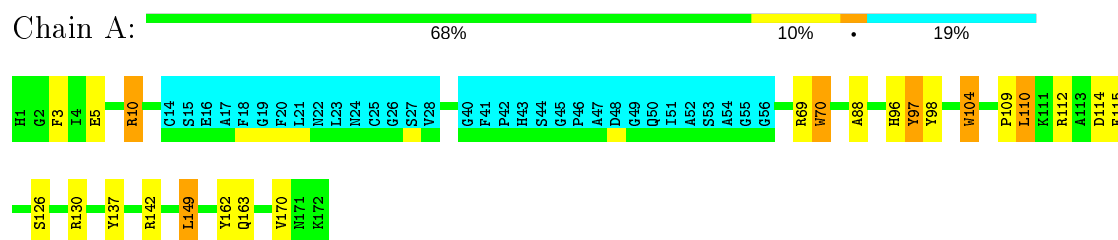


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

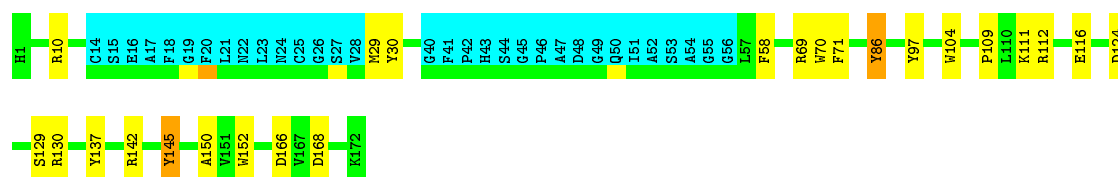
- Molecule 1: Putative chitin binding protein



#### 4.2.2 Score per residue for model 2 (medoid)

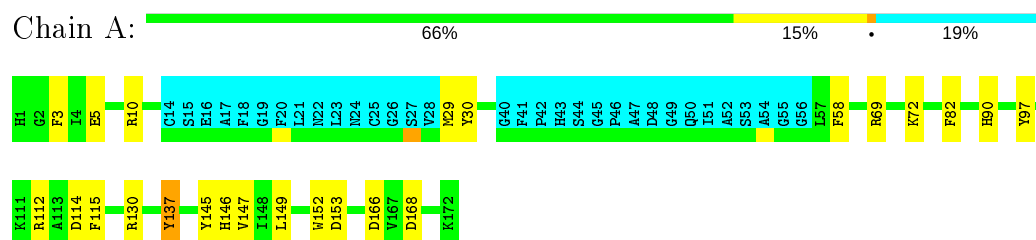
- Molecule 1: Putative chitin binding protein





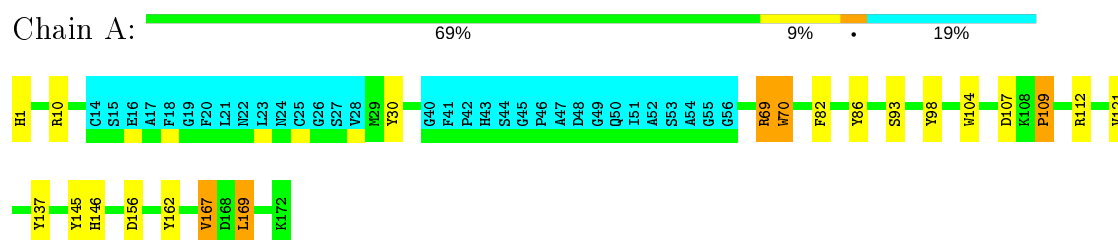
#### 4.2.3 Score per residue for model 3

- Molecule 1: Putative chitin binding protein



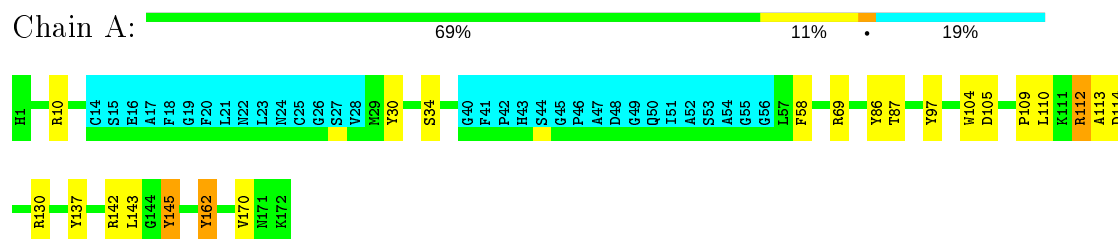
#### 4.2.4 Score per residue for model 4

- Molecule 1: Putative chitin binding protein



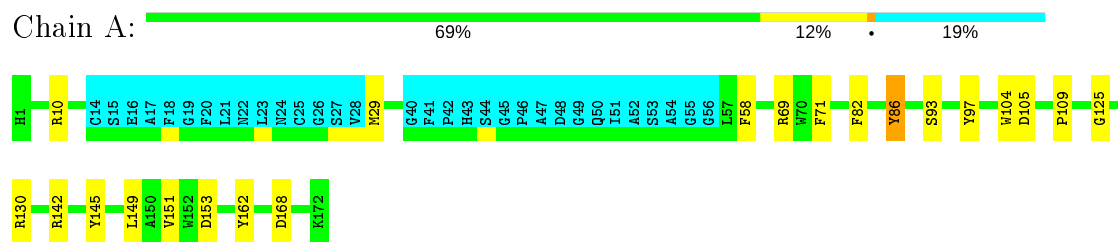
#### 4.2.5 Score per residue for model 5

- Molecule 1: Putative chitin binding protein



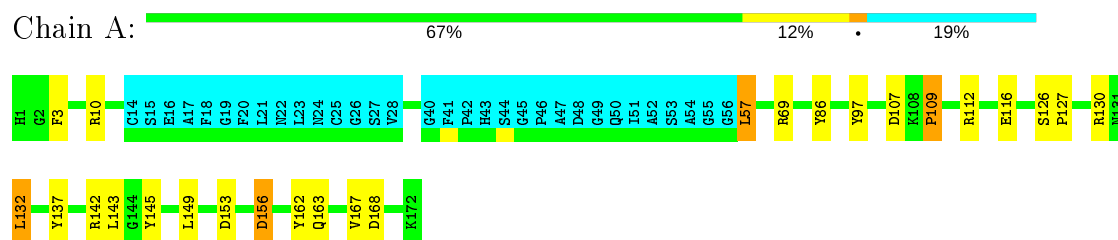
#### 4.2.6 Score per residue for model 6

- Molecule 1: Putative chitin binding protein



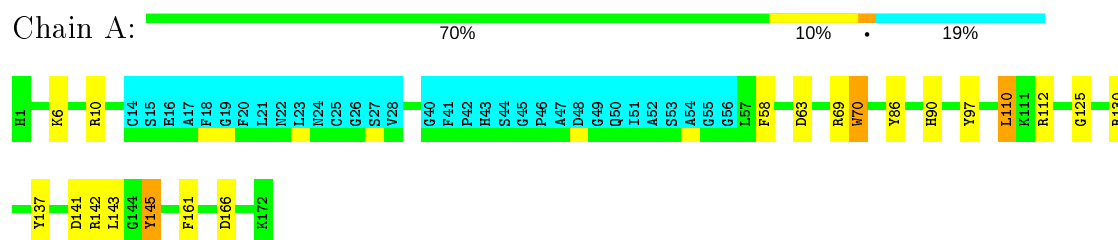
#### 4.2.7 Score per residue for model 7

- Molecule 1: Putative chitin binding protein



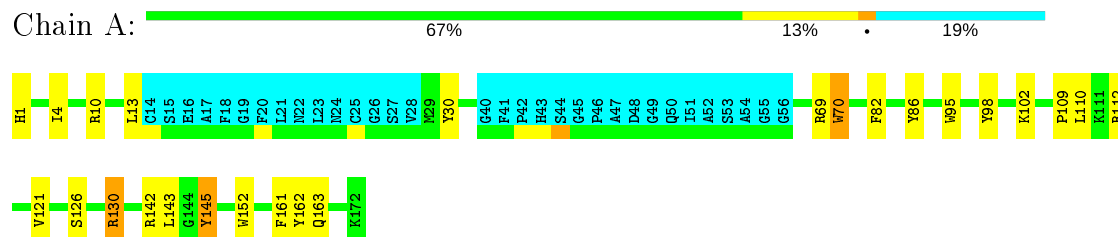
#### 4.2.8 Score per residue for model 8

- Molecule 1: Putative chitin binding protein



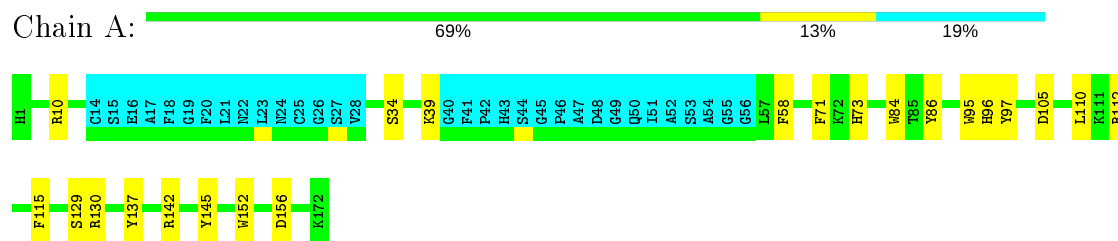
#### 4.2.9 Score per residue for model 9

- Molecule 1: Putative chitin binding protein



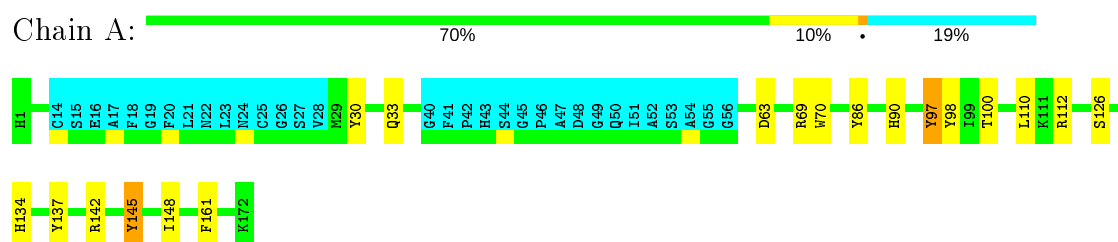
### 4.2.10 Score per residue for model 10

- Molecule 1: Putative chitin binding protein



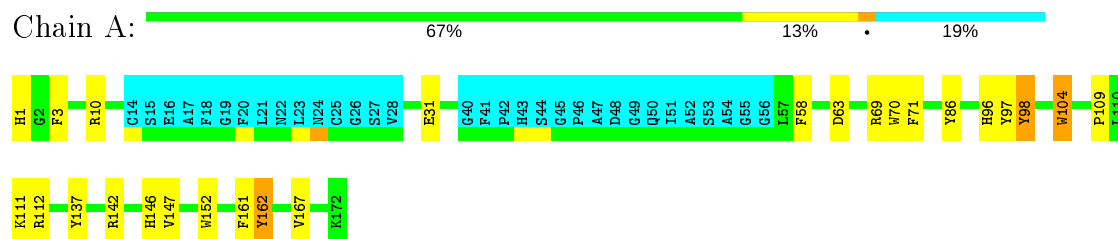
### 4.2.11 Score per residue for model 11

- Molecule 1: Putative chitin binding protein



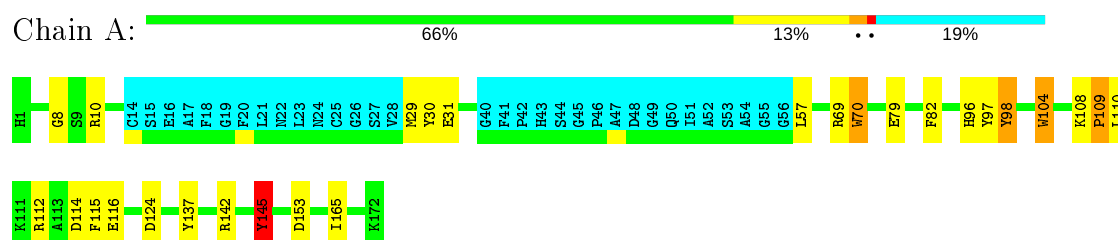
### 4.2.12 Score per residue for model 12

- Molecule 1: Putative chitin binding protein



### 4.2.13 Score per residue for model 13

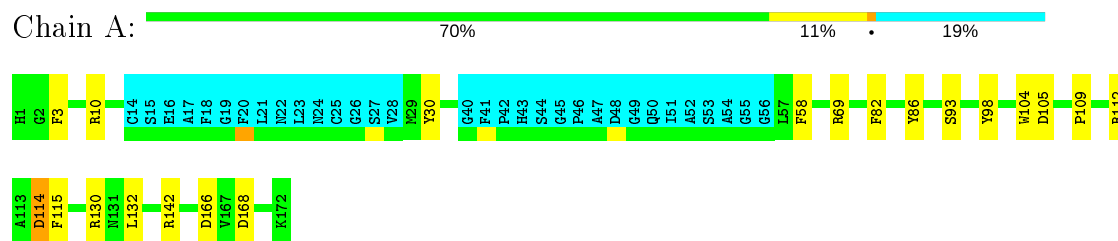
- Molecule 1: Putative chitin binding protein





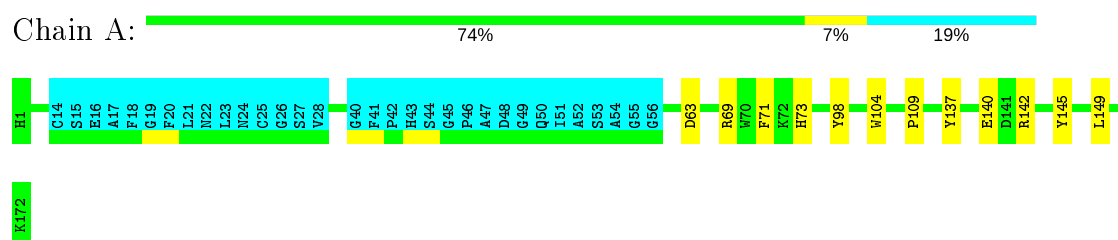
### 4.2.14 Score per residue for model 14

- Molecule 1: Putative chitin binding protein



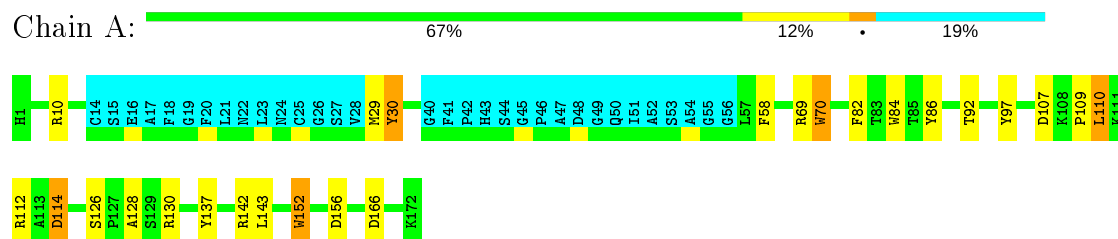
### 4.2.15 Score per residue for model 15

- Molecule 1: Putative chitin binding protein



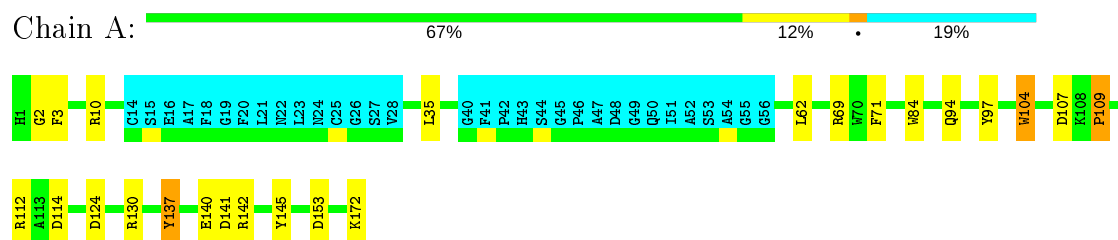
### 4.2.16 Score per residue for model 16

- Molecule 1: Putative chitin binding protein



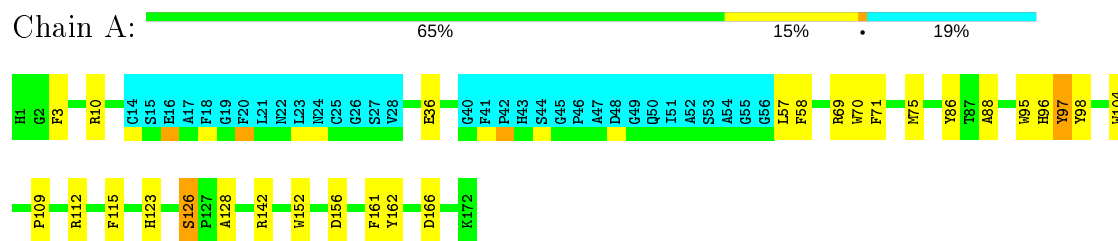
### 4.2.17 Score per residue for model 17

- Molecule 1: Putative chitin binding protein



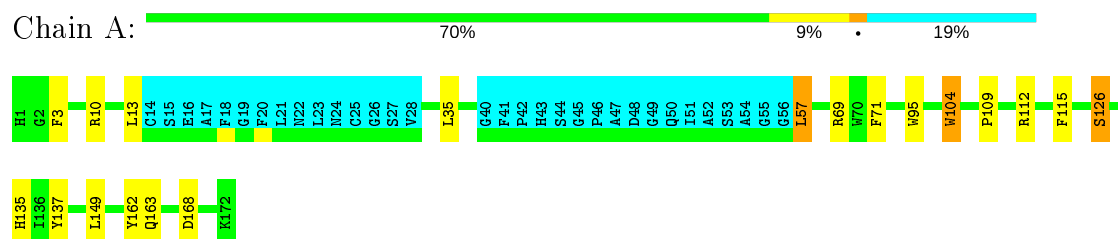
### 4.2.18 Score per residue for model 18

- Molecule 1: Putative chitin binding protein



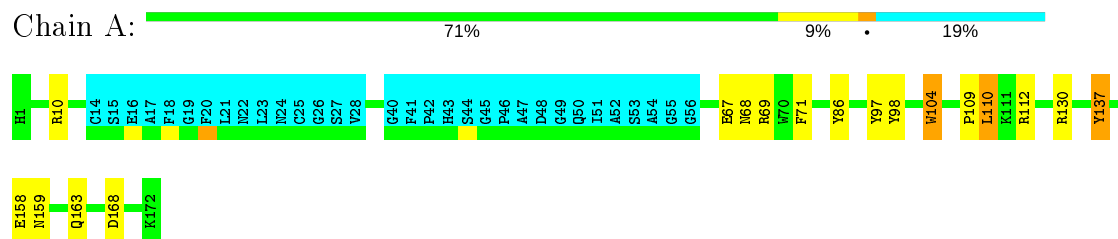
### 4.2.19 Score per residue for model 19

- Molecule 1: Putative chitin binding protein



### 4.2.20 Score per residue for model 20

- Molecule 1: Putative chitin binding protein



## 5 Refinement protocol and experimental data overview

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

Of the 200 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	3.97
YASARA	refinement	14.6.23

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	1921
Number of shifts mapped to atoms	1921
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CU1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.40±0.03	6±2/1184 ( 0.5± 0.2%)	1.61±0.05	16±4/1610 ( 1.0± 0.3%)
All	All	1.40	115/23680 ( 0.5%)	1.61	315/32200 ( 1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.1±0.2	1.8±1.2
All	All	1	35

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	79	GLU	CD-OE1	8.91	1.35	1.25	13	1
1	A	145	TYR	CD1-CE1	8.29	1.51	1.39	2	2
1	A	162	TYR	CD2-CE2	8.00	1.51	1.39	4	2
1	A	137	TYR	CE1-CZ	7.24	1.48	1.38	3	2
1	A	162	TYR	CD1-CE1	7.17	1.50	1.39	9	2
1	A	86	TYR	CG-CD1	7.16	1.48	1.39	2	4
1	A	86	TYR	CD2-CE2	7.00	1.49	1.39	14	2
1	A	104	TRP	CG-CD1	6.96	1.46	1.36	12	1
1	A	98	TYR	CD2-CE2	6.80	1.49	1.39	13	3
1	A	30	TYR	CG-CD2	6.79	1.48	1.39	4	2
1	A	97	TYR	CD2-CE2	6.60	1.49	1.39	18	3
1	A	30	TYR	CG-CD1	6.59	1.47	1.39	14	3
1	A	58	PHE	CE2-CZ	6.52	1.49	1.37	10	2
1	A	137	TYR	CD1-CE1	6.52	1.49	1.39	20	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	97	TYR	CD1-CE1	6.50	1.49	1.39	2	2
1	A	3	PHE	CD1-CE1	6.48	1.52	1.39	7	1
1	A	70	TRP	CE3-CZ3	6.45	1.49	1.38	9	2
1	A	115	PHE	CE1-CZ	6.42	1.49	1.37	1	2
1	A	145	TYR	CD2-CE2	6.41	1.49	1.39	17	1
1	A	82	PHE	CE1-CZ	6.40	1.49	1.37	4	2
1	A	98	TYR	CG-CD2	6.37	1.47	1.39	11	1
1	A	137	TYR	CD2-CE2	6.37	1.49	1.39	20	2
1	A	97	TYR	CG-CD1	-6.29	1.30	1.39	13	1
1	A	69	ARG	CZ-NH1	-6.28	1.24	1.33	8	2
1	A	95	TRP	CG-CD1	-6.26	1.27	1.36	19	1
1	A	98	TYR	CD1-CE1	6.23	1.48	1.39	11	2
1	A	58	PHE	CE1-CZ	6.20	1.49	1.37	16	2
1	A	97	TYR	CE2-CZ	6.20	1.46	1.38	3	2
1	A	3	PHE	CE1-CZ	6.13	1.49	1.37	1	2
1	A	152	TRP	CE3-CZ3	6.10	1.48	1.38	16	1
1	A	86	TYR	CD1-CE1	6.09	1.48	1.39	20	1
1	A	93	SER	CB-OG	-6.07	1.34	1.42	6	1
1	A	104	TRP	CE3-CZ3	6.04	1.48	1.38	19	3
1	A	86	TYR	CE2-CZ	6.02	1.46	1.38	12	2
1	A	116	GLU	CD-OE2	6.01	1.32	1.25	13	1
1	A	116	GLU	CG-CD	6.00	1.60	1.51	2	1
1	A	137	TYR	CG-CD2	5.91	1.46	1.39	2	1
1	A	115	PHE	CE2-CZ	5.81	1.48	1.37	19	2
1	A	86	TYR	CG-CD2	5.81	1.46	1.39	5	2
1	A	140	GLU	CG-CD	5.79	1.60	1.51	17	1
1	A	86	TYR	CE1-CZ	5.76	1.46	1.38	16	1
1	A	71	PHE	CD1-CE1	5.74	1.50	1.39	15	2
1	A	145	TYR	CE1-CZ	5.73	1.46	1.38	17	1
1	A	71	PHE	CE2-CZ	5.73	1.48	1.37	17	3
1	A	70	TRP	CD2-CE2	5.69	1.48	1.41	13	1
1	A	130	ARG	CZ-NH1	-5.68	1.25	1.33	14	1
1	A	1	HIS	N-CA	5.64	1.57	1.46	4	1
1	A	115	PHE	CG-CD1	5.63	1.47	1.38	13	1
1	A	98	TYR	CE2-CZ	5.56	1.45	1.38	4	1
1	A	82	PHE	CE2-CZ	5.54	1.47	1.37	14	1
1	A	161	PHE	CE1-CZ	5.41	1.47	1.37	9	1
1	A	71	PHE	CE1-CZ	5.40	1.47	1.37	19	2
1	A	112	ARG	CZ-NH1	-5.37	1.26	1.33	9	1
1	A	71	PHE	CD2-CE2	5.30	1.49	1.39	12	2
1	A	161	PHE	CG-CD2	5.29	1.46	1.38	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	3	PHE	CE2-CZ	5.28	1.47	1.37	17	2
1	A	36	GLU	CD-OE2	-5.28	1.19	1.25	18	1
1	A	70	TRP	CZ3-CH2	5.27	1.48	1.40	1	2
1	A	137	TYR	CB-CG	-5.25	1.43	1.51	16	2
1	A	82	PHE	CG-CD1	5.23	1.46	1.38	3	2
1	A	69	ARG	CZ-NH2	-5.21	1.26	1.33	16	1
1	A	84	TRP	CB-CG	5.21	1.59	1.50	10	1
1	A	31	GLU	CD-OE2	5.20	1.31	1.25	13	1
1	A	170	VAL	CB-CG1	5.19	1.63	1.52	5	1
1	A	167	VAL	CA-CB	5.17	1.65	1.54	4	1
1	A	71	PHE	CG-CD2	5.17	1.46	1.38	20	1
1	A	145	TYR	CG-CD1	5.13	1.45	1.39	17	1
1	A	86	TYR	CB-CG	-5.11	1.44	1.51	9	1
1	A	58	PHE	CD2-CE2	5.08	1.49	1.39	3	1
1	A	5	GLU	CD-OE1	-5.08	1.20	1.25	1	1
1	A	31	GLU	CB-CG	5.04	1.61	1.52	12	1
1	A	121	VAL	CA-CB	5.03	1.65	1.54	9	1
1	A	170	VAL	CA-CB	5.01	1.65	1.54	1	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	10	ARG	NE-CZ-NH1	20.11	130.35	120.30	6	11
1	A	69	ARG	NE-CZ-NH1	16.48	128.54	120.30	13	13
1	A	112	ARG	NE-CZ-NH1	-16.04	112.28	120.30	19	15
1	A	112	ARG	NE-CZ-NH2	15.89	128.24	120.30	19	13
1	A	130	ARG	NE-CZ-NH1	14.90	127.75	120.30	20	8
1	A	142	ARG	NE-CZ-NH2	13.66	127.13	120.30	15	14
1	A	142	ARG	NE-CZ-NH1	13.51	127.06	120.30	18	10
1	A	10	ARG	NE-CZ-NH2	12.72	126.66	120.30	17	16
1	A	69	ARG	NE-CZ-NH2	12.51	126.55	120.30	9	11
1	A	130	ARG	NE-CZ-NH2	-11.58	114.51	120.30	9	12
1	A	105	ASP	CB-CG-OD2	-10.60	108.76	118.30	5	3
1	A	105	ASP	CB-CG-OD1	9.81	127.13	118.30	5	3
1	A	86	TYR	CB-CG-CD2	-9.78	115.13	121.00	12	2
1	A	124	ASP	CB-CG-OD2	8.83	126.25	118.30	17	1
1	A	166	ASP	CB-CG-OD1	8.67	126.11	118.30	14	4
1	A	145	TYR	CB-CG-CD2	8.47	126.08	121.00	5	3
1	A	58	PHE	CB-CG-CD2	-8.46	114.88	120.80	2	6
1	A	82	PHE	CB-CG-CD1	-8.33	114.97	120.80	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	162	TYR	CB-CG-CD2	-7.95	116.23	121.00	18	2
1	A	114	ASP	CB-CG-OD1	7.93	125.44	118.30	16	5
1	A	161	PHE	CB-CG-CD1	-7.84	115.31	120.80	18	2
1	A	168	ASP	CB-CG-OD1	-7.75	111.33	118.30	6	4
1	A	86	TYR	CB-CG-CD1	-7.70	116.38	121.00	6	6
1	A	124	ASP	CB-CG-OD1	-7.66	111.40	118.30	17	2
1	A	115	PHE	CB-CG-CD2	-7.61	115.47	120.80	18	2
1	A	63	ASP	CB-CG-OD2	7.49	125.04	118.30	11	2
1	A	58	PHE	CB-CG-CD1	-7.32	115.68	120.80	5	3
1	A	161	PHE	CB-CG-CD2	7.30	125.91	120.80	11	2
1	A	97	TYR	CB-CG-CD2	-7.28	116.63	121.00	5	2
1	A	143	LEU	CA-CB-CG	7.25	131.97	115.30	5	5
1	A	137	TYR	CB-CG-CD1	-7.20	116.68	121.00	1	3
1	A	125	GLY	N-CA-C	-7.16	95.21	113.10	8	1
1	A	153	ASP	CB-CG-OD1	7.10	124.69	118.30	13	4
1	A	168	ASP	CB-CG-OD2	7.09	124.68	118.30	6	4
1	A	111	LYS	CD-CE-NZ	-6.99	95.63	111.70	12	1
1	A	126	SER	N-CA-CB	-6.87	100.20	110.50	18	1
1	A	166	ASP	CB-CG-OD2	6.86	124.47	118.30	18	4
1	A	97	TYR	CD1-CE1-CZ	6.82	125.94	119.80	1	1
1	A	137	TYR	CB-CG-CD2	6.80	125.08	121.00	1	3
1	A	153	ASP	CB-CG-OD2	6.77	124.39	118.30	3	2
1	A	69	ARG	CA-C-N	-6.72	102.42	117.20	15	4
1	A	148	ILE	N-CA-C	-6.62	93.13	111.00	11	1
1	A	107	ASP	CB-CG-OD1	6.60	124.24	118.30	17	1
1	A	130	ARG	NH1-CZ-NH2	-6.58	112.16	119.40	16	1
1	A	162	TYR	CB-CG-CD1	-6.47	117.12	121.00	6	5
1	A	141	ASP	CB-CG-OD1	6.47	124.12	118.30	17	2
1	A	10	ARG	NH1-CZ-NH2	-6.40	112.36	119.40	6	2
1	A	149	LEU	CA-CB-CG	6.38	129.99	115.30	1	4
1	A	98	TYR	CD1-CE1-CZ	6.28	125.45	119.80	12	1
1	A	57	LEU	CA-CB-CG	6.27	129.72	115.30	7	2
1	A	30	TYR	CB-CG-CD1	6.23	124.74	121.00	5	3
1	A	156	ASP	CB-CG-OD2	6.19	123.87	118.30	16	4
1	A	30	TYR	CB-CG-CD2	-6.17	117.30	121.00	16	1
1	A	109	PRO	N-CA-C	6.10	127.97	112.10	17	1
1	A	98	TYR	CB-CG-CD2	-6.10	117.34	121.00	11	2
1	A	3	PHE	CB-CG-CD1	6.08	125.06	120.80	3	2
1	A	98	TYR	CG-CD2-CE2	-6.07	116.44	121.30	1	1
1	A	3	PHE	CB-CG-CD2	-6.05	116.57	120.80	14	2
1	A	110	LEU	CA-CB-CG	6.05	129.21	115.30	20	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	112	ARG	NH1-CZ-NH2	-6.04	112.76	119.40	12	2
1	A	104	TRP	CD1-CG-CD2	-6.03	101.47	106.30	20	2
1	A	62	LEU	CB-CG-CD1	6.01	121.22	111.00	17	1
1	A	137	TYR	CZ-CE2-CD2	-6.00	114.40	119.80	15	1
1	A	82	PHE	CB-CG-CD2	-5.95	116.63	120.80	16	2
1	A	145	TYR	CZ-CE2-CD2	-5.94	114.45	119.80	13	1
1	A	172	LYS	CD-CE-NZ	5.93	125.33	111.70	17	1
1	A	97	TYR	CG-CD2-CE2	-5.92	116.56	121.30	5	2
1	A	63	ASP	CB-CG-OD1	5.92	123.63	118.30	15	2
1	A	126	SER	C-N-CD	5.91	140.81	128.40	9	2
1	A	69	ARG	CD-NE-CZ	5.85	131.79	123.60	8	3
1	A	98	TYR	CB-CG-CD1	-5.84	117.50	121.00	14	2
1	A	132	LEU	CA-CB-CG	5.79	128.62	115.30	7	1
1	A	97	TYR	CZ-CE2-CD2	-5.79	114.59	119.80	17	1
1	A	145	TYR	CB-CG-CD1	-5.78	117.53	121.00	5	2
1	A	107	ASP	CB-CG-OD2	5.76	123.49	118.30	7	3
1	A	13	LEU	CB-CG-CD2	-5.72	101.27	111.00	9	1
1	A	69	ARG	NH1-CZ-NH2	-5.71	113.12	119.40	17	1
1	A	104	TRP	CH2-CZ2-CE2	5.66	123.06	117.40	19	1
1	A	97	TYR	CB-CG-CD1	-5.61	117.64	121.00	3	1
1	A	114	ASP	CB-CG-OD2	-5.60	113.26	118.30	5	3
1	A	130	ARG	CD-NE-CZ	5.57	131.39	123.60	16	1
1	A	75	MET	CG-SD-CE	5.53	109.04	100.20	18	1
1	A	88	ALA	N-CA-C	-5.49	96.18	111.00	18	1
1	A	168	ASP	N-CA-C	-5.45	96.28	111.00	14	1
1	A	110	LEU	O-C-N	-5.43	114.00	122.70	1	1
1	A	110	LEU	CB-CG-CD2	5.42	120.21	111.00	1	2
1	A	72	LYS	CD-CE-NZ	5.41	124.14	111.70	3	1
1	A	95	TRP	CD1-CG-CD2	-5.41	101.97	106.30	9	1
1	A	110	LEU	N-CA-C	5.39	125.56	111.00	16	1
1	A	87	THR	CA-CB-CG2	5.38	119.94	112.40	5	1
1	A	135	HIS	CB-CA-C	-5.36	99.69	110.40	19	1
1	A	142	ARG	NH1-CZ-NH2	-5.35	113.51	119.40	18	1
1	A	104	TRP	CD1-NE1-CE2	-5.34	104.20	109.00	3	1
1	A	98	TYR	CZ-CE2-CD2	5.34	124.60	119.80	9	1
1	A	169	LEU	CA-CB-CG	5.28	127.44	115.30	4	1
1	A	86	TYR	N-CA-C	-5.27	96.77	111.00	16	1
1	A	90	HIS	N-CA-CB	5.25	120.04	110.60	3	1
1	A	98	TYR	CG-CD1-CE1	-5.24	117.11	121.30	12	1
1	A	109	PRO	CA-N-CD	-5.24	104.16	111.50	17	1
1	A	129	SER	N-CA-CB	-5.20	102.70	110.50	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	104	TRP	CA-CB-CG	5.17	123.52	113.70	1	1
1	A	30	TYR	CD1-CE1-CZ	-5.15	115.16	119.80	2	1
1	A	57	LEU	CB-CA-C	-5.14	100.44	110.20	18	1
1	A	96	HIS	CB-CA-C	-5.09	100.21	110.40	18	1
1	A	150	ALA	N-CA-C	-5.08	97.28	111.00	2	1
1	A	147	VAL	CG1-CB-CG2	-5.08	102.77	110.90	3	1
1	A	151	VAL	CB-CA-C	-5.07	101.78	111.40	6	1
1	A	110	LEU	CB-CG-CD1	5.07	119.61	111.00	11	1
1	A	71	PHE	CB-CG-CD2	-5.04	117.28	120.80	2	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	90	HIS	CA	1

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	137	TYR	Sidechain	6
1	A	145	TYR	Sidechain	4
1	A	97	TYR	Sidechain	3
1	A	98	TYR	Sidechain	3
1	A	70	TRP	Peptide	2
1	A	57	LEU	Peptide	2
1	A	162	TYR	Sidechain	2
1	A	30	TYR	Sidechain	2
1	A	86	TYR	Sidechain	2
1	A	116	GLU	Mainchain	1
1	A	67	GLU	Mainchain	1
1	A	108	LYS	Peptide	1
1	A	93	SER	Mainchain	1
1	A	88	ALA	Mainchain	1
1	A	112	ARG	Sidechain	1
1	A	94	GLN	Peptide	1
1	A	104	TRP	Peptide	1
1	A	10	ARG	Sidechain	1

## 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1145	1086	1089	0±0
All	All	22920	21720	21780	2

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:HIS:CE1	1:A:161:PHE:CZ	0.44	3.06	12	1
1:A:95:TRP:CZ3	1:A:123:HIS:CD2	0.43	3.06	18	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	138/172 (80%)	128±2 (93±2%)	8±2 (6±2%)	2±1 (2±1%)	13	57
All	All	2760/3440 (80%)	2555 (93%)	161 (6%)	44 (2%)	13	57

All 17 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	109	PRO	17
1	A	110	LEU	5
1	A	70	TRP	4
1	A	29	MET	3
1	A	128	ALA	2
1	A	69	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	130	ARG	1
1	A	8	GLY	1
1	A	114	ASP	1
1	A	125	GLY	1
1	A	127	PRO	1
1	A	113	ALA	1
1	A	102	LYS	1
1	A	2	GLY	1
1	A	6	LYS	1
1	A	126	SER	1
1	A	35	LEU	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	120/141 (85%)	115±2 (96±2%)	5±2 (4±2%)	31	80
All	All	2400/2820 (85%)	2292 (96%)	108 (4%)	31	80

All 46 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	104	TRP	13
1	A	145	TYR	9
1	A	152	TRP	7
1	A	163	GLN	5
1	A	70	TRP	5
1	A	126	SER	5
1	A	97	TYR	4
1	A	96	HIS	4
1	A	110	LEU	3
1	A	167	VAL	3
1	A	149	LEU	3
1	A	109	PRO	3
1	A	146	HIS	3
1	A	34	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	132	LEU	2
1	A	29	MET	2
1	A	73	HIS	2
1	A	156	ASP	2
1	A	84	TRP	2
1	A	114	ASP	2
1	A	90	HIS	2
1	A	13	LEU	1
1	A	95	TRP	1
1	A	147	VAL	1
1	A	165	ILE	1
1	A	4	ILE	1
1	A	159	ASN	1
1	A	10	ARG	1
1	A	57	LEU	1
1	A	134	HIS	1
1	A	33	GLN	1
1	A	111	LYS	1
1	A	68	ASN	1
1	A	169	LEU	1
1	A	129	SER	1
1	A	124	ASP	1
1	A	158	GLU	1
1	A	1	HIS	1
1	A	140	GLU	1
1	A	100	THR	1
1	A	121	VAL	1
1	A	92	THR	1
1	A	35	LEU	1
1	A	93	SER	1
1	A	39	LYS	1
1	A	5	GLU	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](#)

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

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 83% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1921
Number of shifts mapped to atoms	1921
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	15

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	172	$-0.02 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	155	$-0.08 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	171	$0.65 \pm 0.17$	Should be applied
$^{15}\text{N}$	161	$-0.89 \pm 0.35$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1450 atoms were assigned a chemical shift out of a possible 1759. 17 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	681/684 (100%)	271/272 (100%)	279/280 (100%)	131/132 (99%)
Sidechain	685/843 (81%)	417/497 (84%)	260/312 (83%)	8/34 (24%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	84/232 (36%)	61/124 (49%)	18/95 (19%)	5/13 (38%)
Overall	1450/1759 (82%)	749/893 (84%)	557/687 (81%)	144/179 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1727 atoms were assigned a chemical shift out of a possible 2073. 19 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	837/840 (100%)	333/334 (100%)	343/344 (100%)	161/162 (99%)
Sidechain	794/967 (82%)	482/571 (84%)	301/359 (84%)	11/37 (30%)
Aromatic	96/266 (36%)	71/143 (50%)	20/109 (18%)	5/14 (36%)
Overall	1727/2073 (83%)	886/1048 (85%)	664/812 (82%)	177/213 (83%)

#### 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	42	PRO	CD	41.90	55.31 – 45.41	-8.5
1	A	109	PRO	CD	42.70	55.31 – 45.41	-7.7
1	A	4	ILE	HG13	-1.44	3.26 – -0.84	-6.5
1	A	100	THR	HG22	-0.30	2.29 – -0.01	-6.3
1	A	100	THR	HG21	-0.30	2.29 – -0.01	-6.3
1	A	100	THR	HG23	-0.30	2.29 – -0.01	-6.3
1	A	149	LEU	HD21	-0.78	2.14 – -0.66	-5.4
1	A	149	LEU	HD23	-0.78	2.14 – -0.66	-5.4
1	A	149	LEU	HD22	-0.78	2.14 – -0.66	-5.4
1	A	62	LEU	HD21	-0.77	2.14 – -0.66	-5.4
1	A	62	LEU	HD22	-0.77	2.14 – -0.66	-5.4
1	A	62	LEU	HD23	-0.77	2.14 – -0.66	-5.4
1	A	92	THR	HG21	-0.09	2.29 – -0.01	-5.3
1	A	92	THR	HG22	-0.09	2.29 – -0.01	-5.3
1	A	92	THR	HG23	-0.09	2.29 – -0.01	-5.3

#### 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:

