



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 08:52 am BST

PDB ID : 5WYO  
Title : Solution structure of E.coli HdeA  
Authors : Yang, C.; Hu, Y.; Jin, C.  
Deposited on : 2017-01-14

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 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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

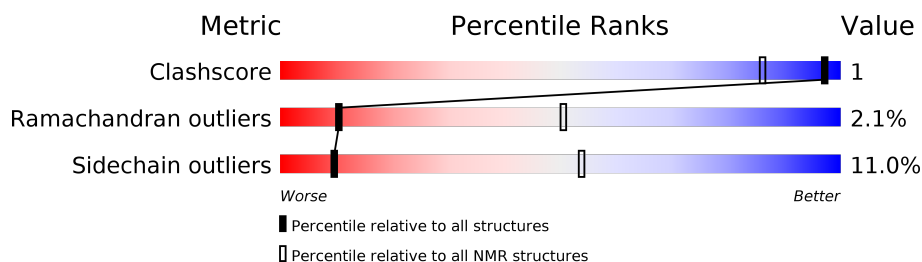
# 1 Overall quality at a glance

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	89	 75% 8% 17%
1	B	89	 75% 9% 16%

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:12-A:85, B:101-B:175 (149)	0.43	18

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2704 atoms, of which 1336 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Acid stress chaperone HdeA.

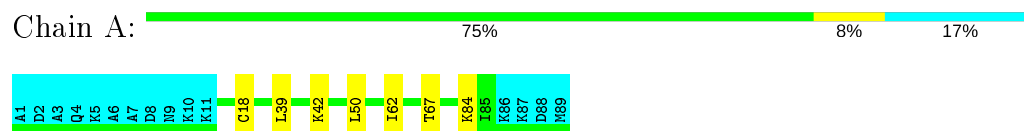
Mol	Chain	Residues	Atoms						Trace
1	A	89	Total	C	H	N	O	S	0
			1352	427	668	114	140	3	
1	B	89	Total	C	H	N	O	S	0
			1352	427	668	114	140	3	

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

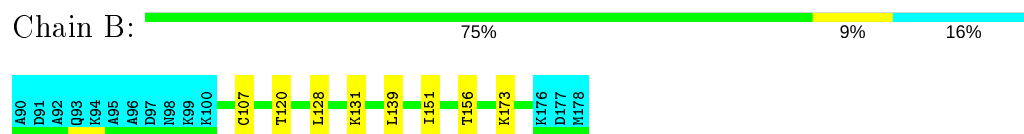
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Acid stress chaperone HdeA



- Molecule 1: Acid stress chaperone HdeA

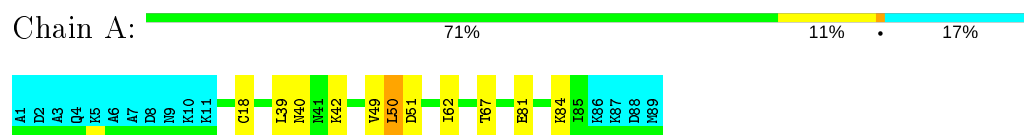


### 4.2 Scores per residue for each member of the ensemble

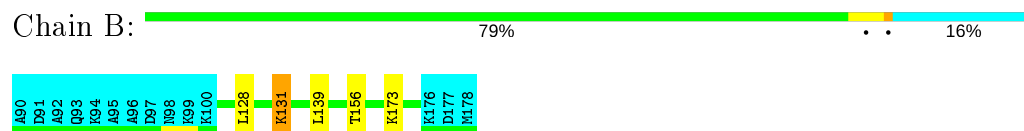
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Acid stress chaperone HdeA

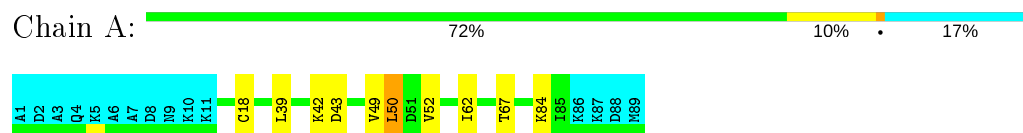


- Molecule 1: Acid stress chaperone HdeA

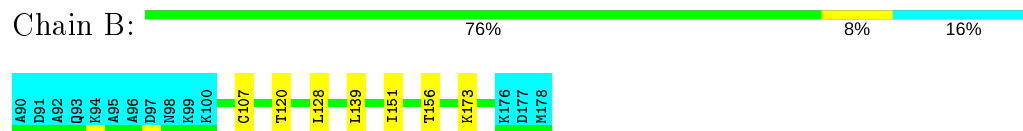


### 4.2.2 Score per residue for model 2

- Molecule 1: Acid stress chaperone HdeA

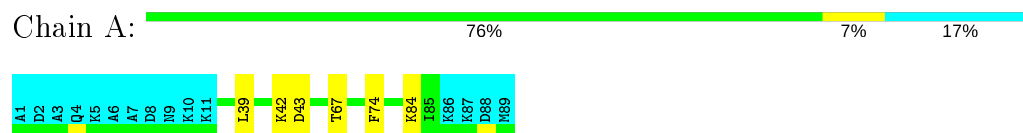


- Molecule 1: Acid stress chaperone HdeA

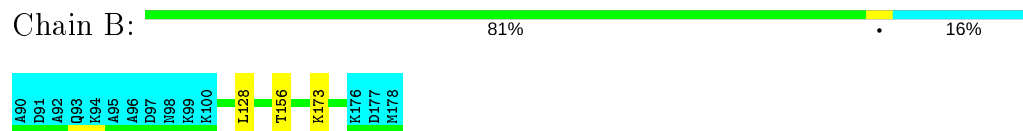


### 4.2.5 Score per residue for model 5

- Molecule 1: Acid stress chaperone HdeA

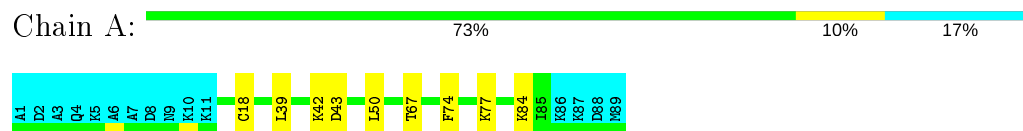


- Molecule 1: Acid stress chaperone HdeA

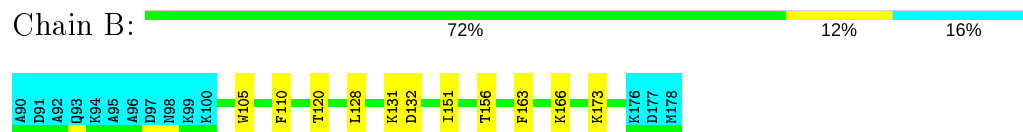


### 4.2.6 Score per residue for model 6

- Molecule 1: Acid stress chaperone HdeA

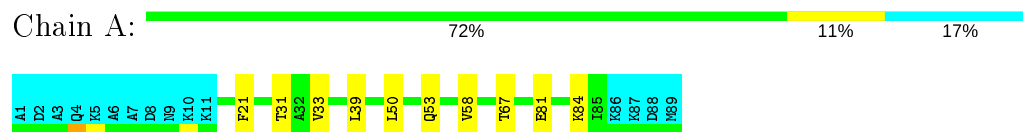


- Molecule 1: Acid stress chaperone HdeA

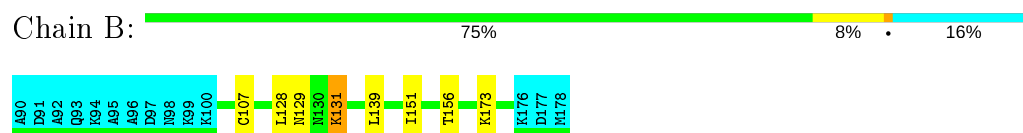


### 4.2.7 Score per residue for model 7

- Molecule 1: Acid stress chaperone HdeA

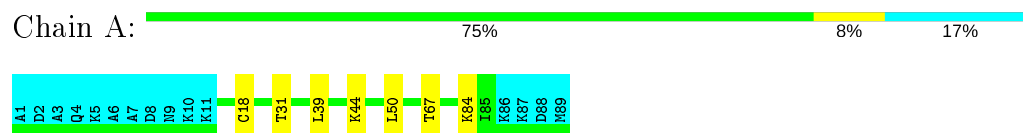


- Molecule 1: Acid stress chaperone HdeA

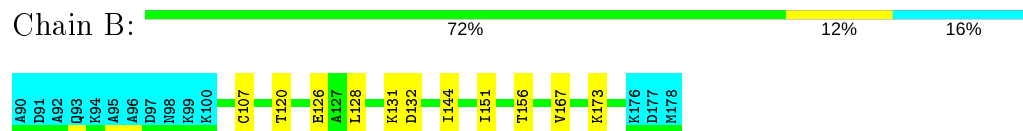


### 4.2.8 Score per residue for model 8

- Molecule 1: Acid stress chaperone HdeA

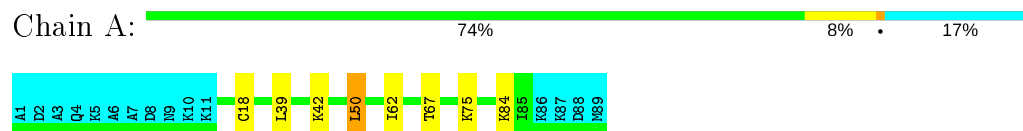


- Molecule 1: Acid stress chaperone HdeA

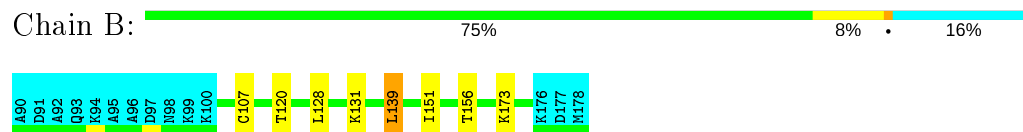


### 4.2.9 Score per residue for model 9

- Molecule 1: Acid stress chaperone HdeA

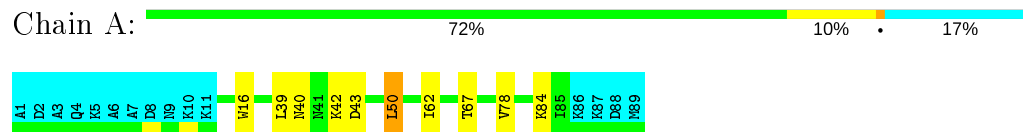


- Molecule 1: Acid stress chaperone HdeA

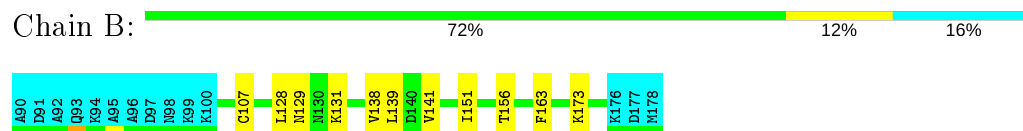


### 4.2.10 Score per residue for model 10

- Molecule 1: Acid stress chaperone HdeA



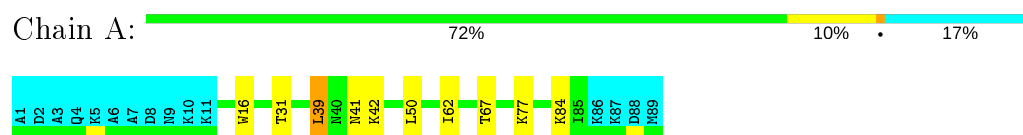
- Molecule 1: Acid stress chaperone HdeA



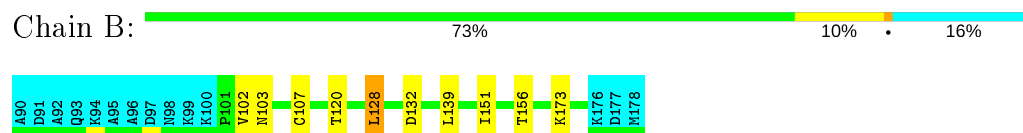


#### 4.2.11 Score per residue for model 11

- Molecule 1: Acid stress chaperone HdeA

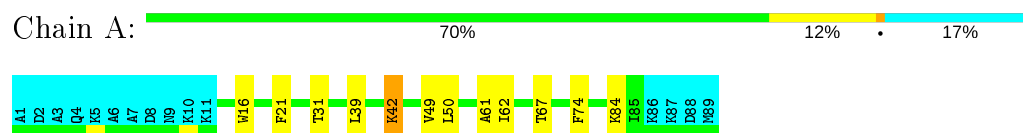


- Molecule 1: Acid stress chaperone HdeA

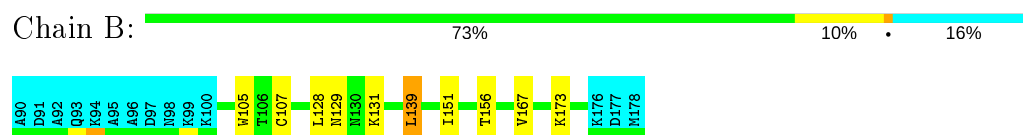


#### 4.2.12 Score per residue for model 12

- Molecule 1: Acid stress chaperone HdeA

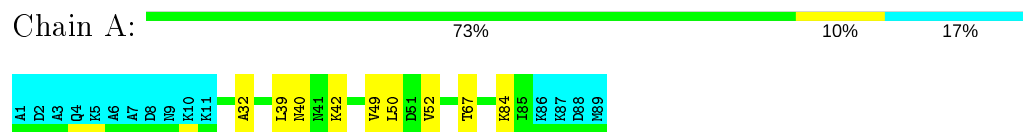


- Molecule 1: Acid stress chaperone HdeA

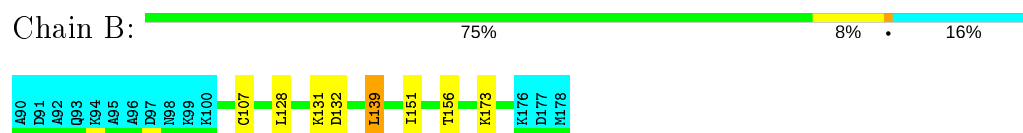


#### 4.2.13 Score per residue for model 13

- Molecule 1: Acid stress chaperone HdeA

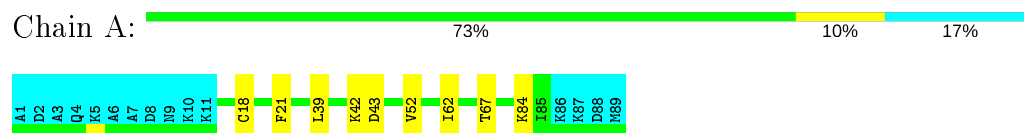


- Molecule 1: Acid stress chaperone HdeA

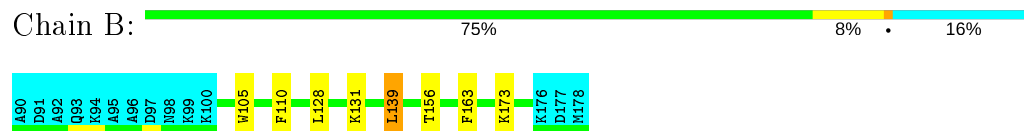


#### 4.2.14 Score per residue for model 14

- Molecule 1: Acid stress chaperone HdeA

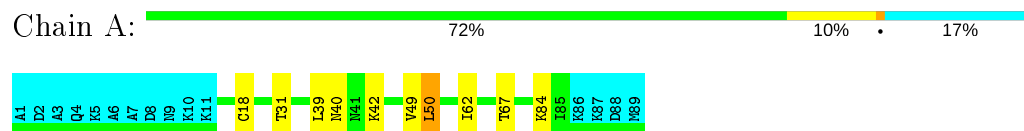


- Molecule 1: Acid stress chaperone HdeA

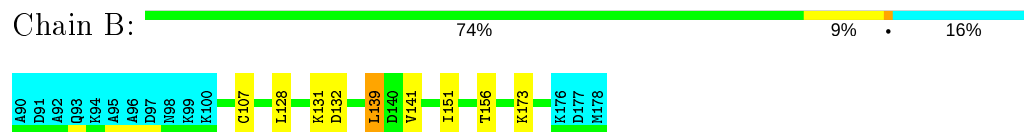


#### 4.2.15 Score per residue for model 15

- Molecule 1: Acid stress chaperone HdeA

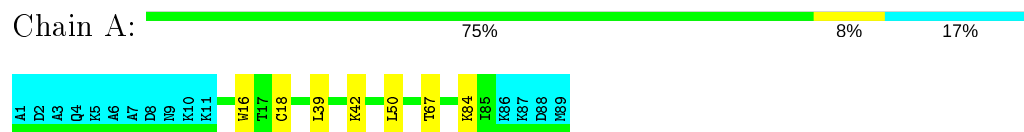


- Molecule 1: Acid stress chaperone HdeA

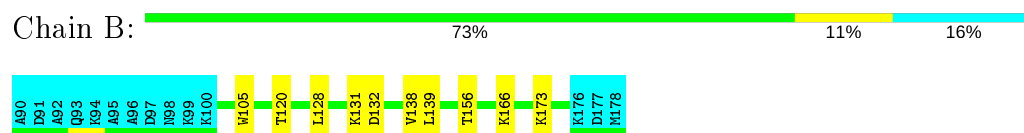


#### 4.2.16 Score per residue for model 16

- Molecule 1: Acid stress chaperone HdeA

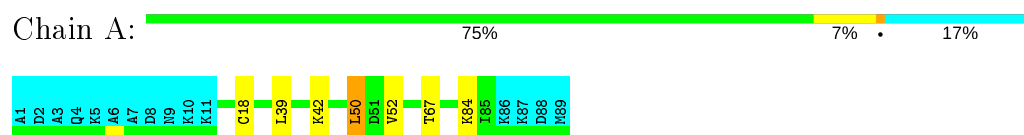


- Molecule 1: Acid stress chaperone HdeA

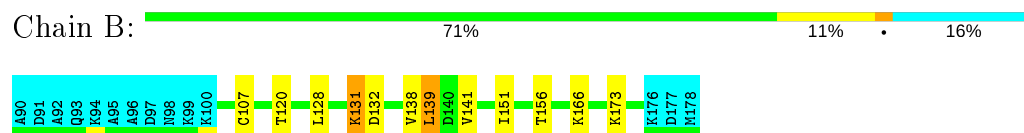


### 4.2.17 Score per residue for model 17

- Molecule 1: Acid stress chaperone HdeA

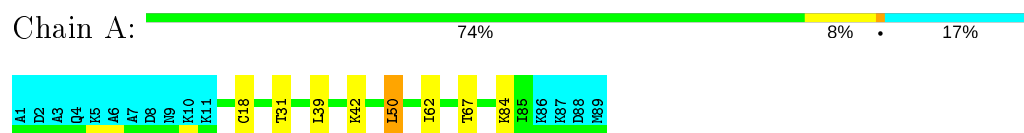


- Molecule 1: Acid stress chaperone HdeA

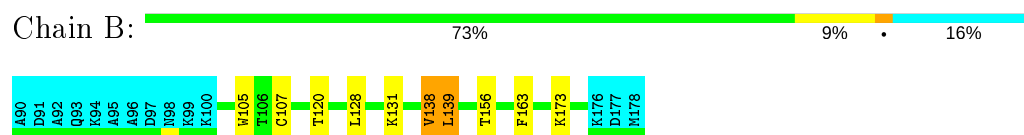


### 4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Acid stress chaperone HdeA

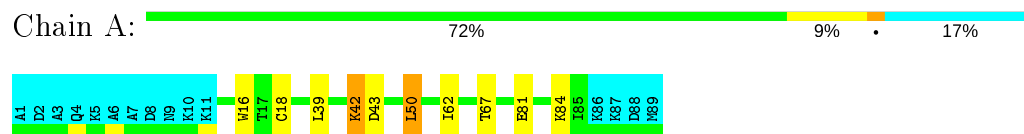


- Molecule 1: Acid stress chaperone HdeA

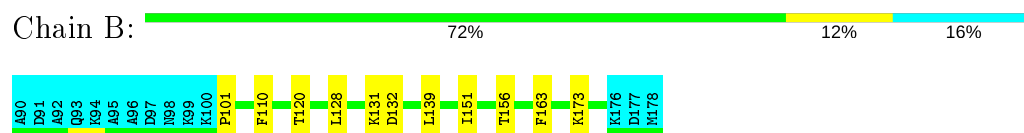


### 4.2.19 Score per residue for model 19

- Molecule 1: Acid stress chaperone HdeA



- Molecule 1: Acid stress chaperone HdeA



#### 4.2.20 Score per residue for model 20

- Molecule 1: Acid stress chaperone HdeA

Chain A: 74% 7% 17%



- Molecule 1: Acid stress chaperone HdeA

Chain B: 73% 9% 16%



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
AMBER	refinement	
CYANA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	984
Number of shifts mapped to atoms	984
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%

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

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 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	569	546	546	1±1
1	B	578	559	559	1±1
All	All	22940	22100	22100	27

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LEU:HD21	1:B:120:THR:HG22	0.70	1.63	20	11
1:A:31:THR:HG22	1:B:139:LEU:HD21	0.62	1.71	3	6
1:A:32:ALA:HB2	1:B:139:LEU:HD12	0.51	1.82	13	1
1:A:33:VAL:HG21	1:A:58:VAL:HG11	0.46	1.87	7	1
1:B:110:PHE:CD1	1:B:163:PHE:CE1	0.46	3.03	14	2
1:A:31:THR:HG21	1:B:144:ILE:HD13	0.44	1.88	8	1
1:A:50:LEU:HD13	1:A:51:ASP:H	0.42	1.75	1	1
1:A:21:PHE:CD2	1:A:74:PHE:CE1	0.42	3.07	12	1
1:B:110:PHE:CD2	1:B:163:PHE:CE2	0.42	3.07	6	2
1:A:39:LEU:HD13	1:B:128:LEU:HD13	0.41	1.92	11	1

## 5.2 Torsion angles [i](#)

### 5.2.1 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	74/89 (83%)	68±2 (92±2%)	5±2 (7±2%)	1±1 (2±1%)	11	53
1	B	75/89 (84%)	67±2 (89±3%)	6±2 (8±3%)	2±1 (2±1%)	9	48
All	All	2980/3560 (84%)	2696 (90%)	221 (7%)	63 (2%)	10	50

All 14 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	132	ASP	10
1	A	50	LEU	10
1	B	139	LEU	10
1	B	131	LYS	10
1	A	43	ASP	7
1	A	42	LYS	7
1	B	101	PRO	2
1	B	102	VAL	1
1	A	74	PHE	1
1	B	163	PHE	1
1	A	13	VAL	1
1	A	44	LYS	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	75	LYS	1
1	B	133	LYS	1

### 5.2.2 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	62/73 (85%)	55±2 (89±3%)	7±2 (11±3%)	9	53
1	B	63/73 (86%)	56±2 (89±2%)	7±2 (11±2%)	10	54
All	All	2500/2920 (86%)	2226 (89%)	274 (11%)	10	54

All 39 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	128	LEU	20
1	A	39	LEU	20
1	A	84	LYS	20
1	B	173	LYS	20
1	B	156	THR	20
1	A	67	THR	20
1	B	151	ILE	15
1	A	42	LYS	14
1	A	18	CYS	13
1	B	107	CYS	13
1	A	62	ILE	12
1	B	131	LYS	12
1	B	139	LEU	7
1	A	50	LEU	7
1	A	49	VAL	6
1	A	16	TRP	6
1	B	105	TRP	6
1	A	40	ASN	4
1	B	138	VAL	4
1	A	52	VAL	4
1	A	77	LYS	3
1	A	81	GLU	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	B	129	ASN	3
1	B	166	LYS	3
1	B	141	VAL	3
1	A	21	PHE	2
1	B	167	VAL	2
1	A	41	ASN	1
1	B	164	LYS	1
1	B	103	ASN	1
1	B	124	PHE	1
1	A	53	GLN	1
1	B	142	GLN	1
1	B	170	GLU	1
1	A	78	VAL	1
1	A	74	PHE	1
1	B	126	GLU	1
1	B	163	PHE	1
1	A	58	VAL	1

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.5 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.6 Other polymers [i](#)

There are no such molecules in this entry.



## 5.7 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 42% for the well-defined parts and 42% for the entire structure.

### 6.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: ppm.str

#### 6.1.1 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	984
Number of shifts mapped to atoms	984
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	89	$-0.54 \pm 0.07$	Should be applied
$^{13}\text{C}_\beta$	86	$0.62 \pm 0.12$	Should be applied
$^{13}\text{C}'$	81	$-0.30 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	84	$-0.58 \pm 0.43$	None needed (imprecise)

#### 6.1.3 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 42%, i.e. 734 atoms were assigned a chemical shift out of a possible 1746. 9 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	356/729 (49%)	144/290 (50%)	142/298 (48%)	70/141 (50%)
Sidechain	378/897 (42%)	230/518 (44%)	142/346 (41%)	6/33 (18%)

*Continued on next page...*

Continued from previous page...

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/120 (0%)	0/64 (0%)	0/52 (0%)	0/4 (0%)
Overall	734/1746 (42%)	374/872 (43%)	284/696 (41%)	76/178 (43%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 42%, i.e. 883 atoms were assigned a chemical shift out of a possible 2098. 9 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	426/874 (49%)	172/348 (49%)	170/356 (48%)	84/170 (49%)
Sidechain	457/1104 (41%)	279/640 (44%)	170/418 (41%)	8/46 (17%)
Aromatic	0/120 (0%)	0/64 (0%)	0/52 (0%)	0/4 (0%)
Overall	883/2098 (42%)	451/1052 (43%)	340/826 (41%)	92/220 (42%)

#### 6.1.4 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	20	ASP	HB2	1.29	4.07 – 1.37	-5.3

#### 6.1.5 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:

