



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:04 am BST

PDB ID : 2MYJ
Title : Solution structure of a bacterial chaperone
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Deposited on : 2015-01-27

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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

2 Ensemble composition and analysis i

This entry contains 20 models. Model 8 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:3-A:29, A:47-A:73, B:82-B:108, B:126-B:152 (108)	0.26	8

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2502 atoms, of which 1232 are hydrogens and 0 are deuteriums.

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

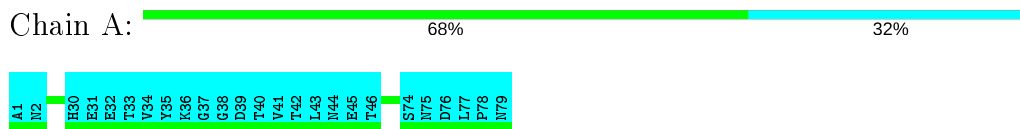
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	79	1251	400	616	103	127	5	0
1	B	79	1251	400	616	103	127	5	0

4 Residue-property plots

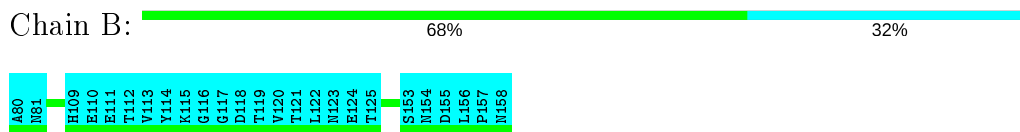
4.1 Average score per residue in the NMR ensemble

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 HdeB



- Molecule 1: Acid stress chaperone HdeB

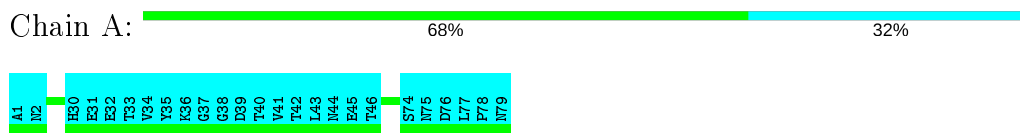


4.2 Scores per residue for each member of the ensemble

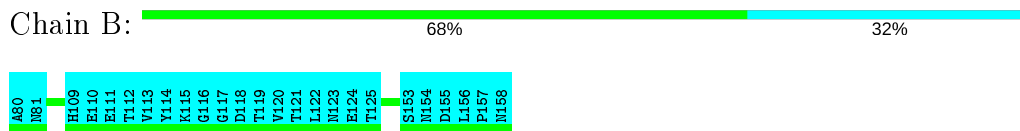
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Acid stress chaperone HdeB

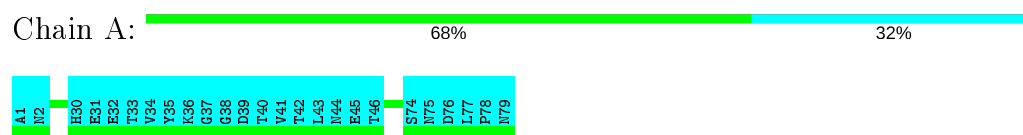


- Molecule 1: Acid stress chaperone HdeB

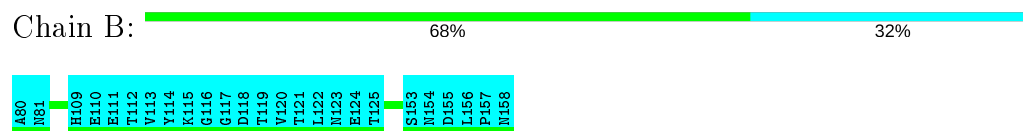


4.2.2 Score per residue for model 2

- Molecule 1: Acid stress chaperone HdeB

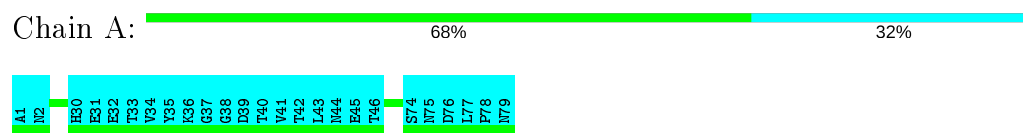


- Molecule 1: Acid stress chaperone HdeB

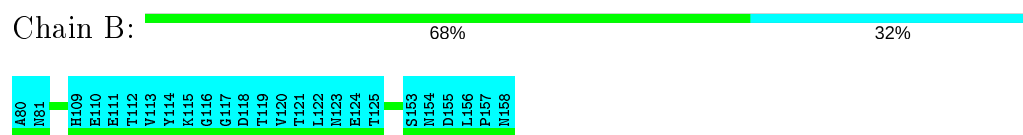


4.2.3 Score per residue for model 3

- Molecule 1: Acid stress chaperone HdeB

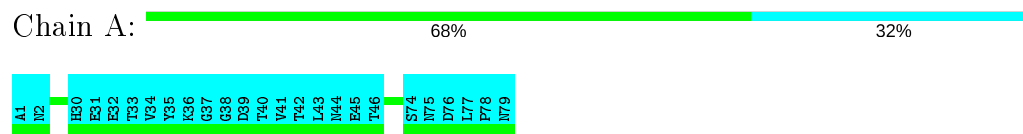


- Molecule 1: Acid stress chaperone HdeB

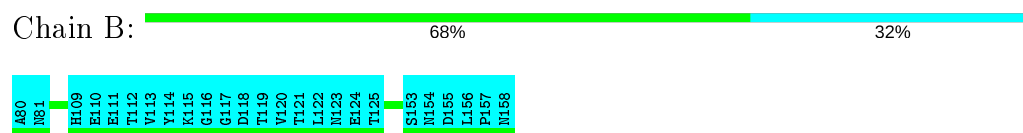


4.2.4 Score per residue for model 4

- Molecule 1: Acid stress chaperone HdeB

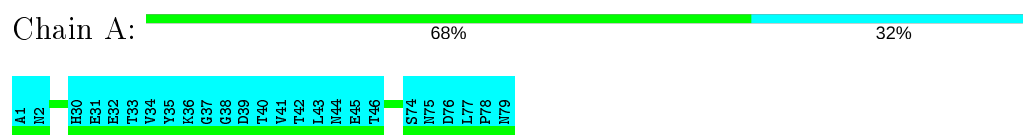


- Molecule 1: Acid stress chaperone HdeB

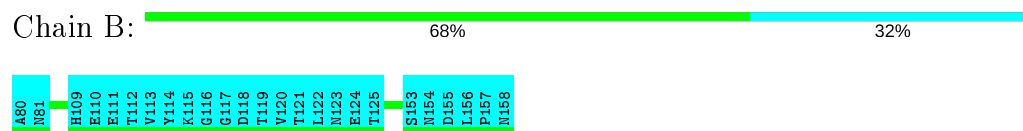


4.2.5 Score per residue for model 5

- Molecule 1: Acid stress chaperone HdeB

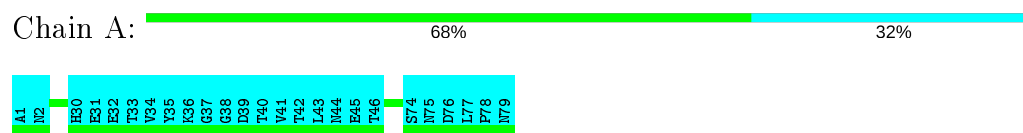


- Molecule 1: Acid stress chaperone HdeB

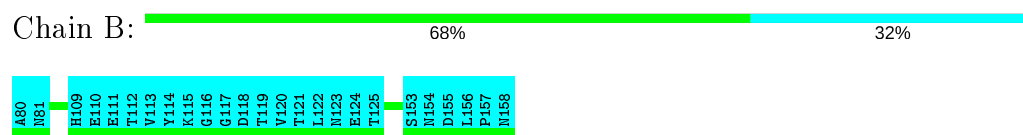


4.2.6 Score per residue for model 6

- Molecule 1: Acid stress chaperone HdeB

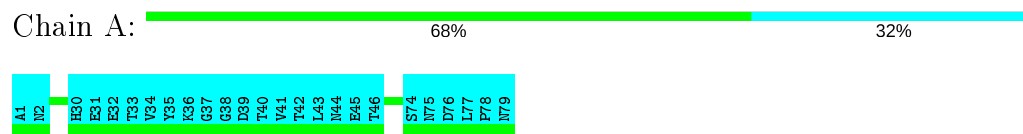


- Molecule 1: Acid stress chaperone HdeB

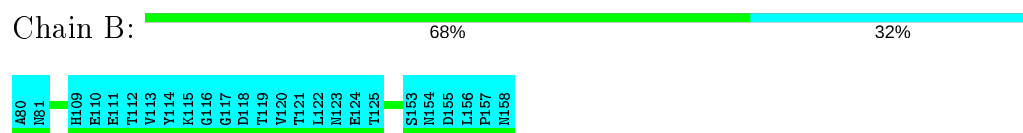


4.2.7 Score per residue for model 7

- Molecule 1: Acid stress chaperone HdeB

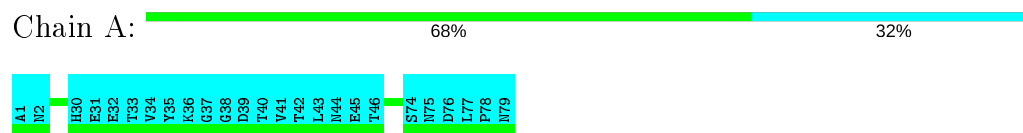


- Molecule 1: Acid stress chaperone HdeB

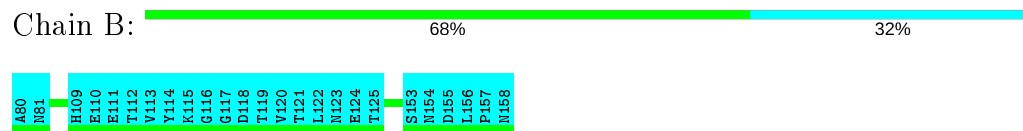


4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Acid stress chaperone HdeB

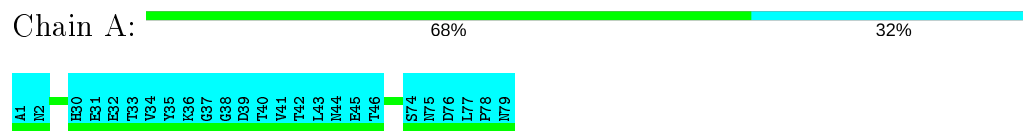


- Molecule 1: Acid stress chaperone HdeB

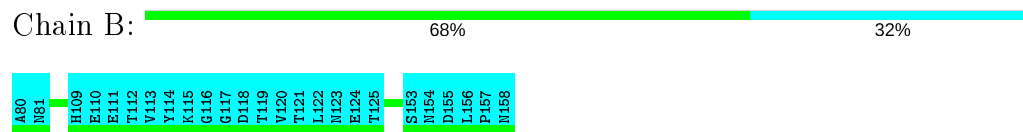


4.2.9 Score per residue for model 9

- Molecule 1: Acid stress chaperone HdeB

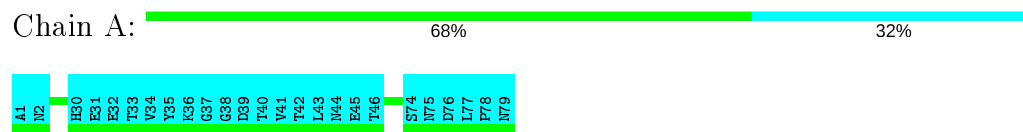


- Molecule 1: Acid stress chaperone HdeB

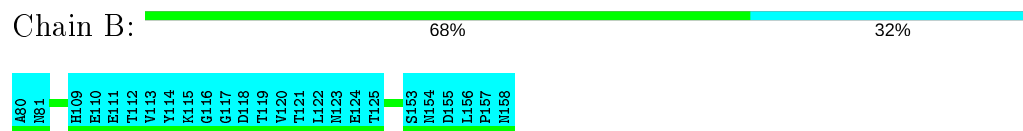


4.2.10 Score per residue for model 10

- Molecule 1: Acid stress chaperone HdeB

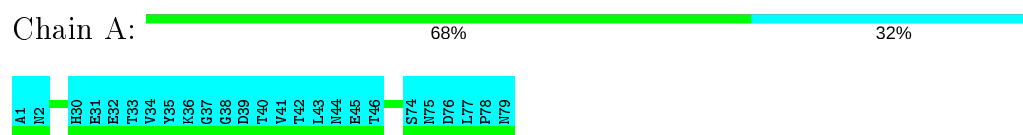


- Molecule 1: Acid stress chaperone HdeB

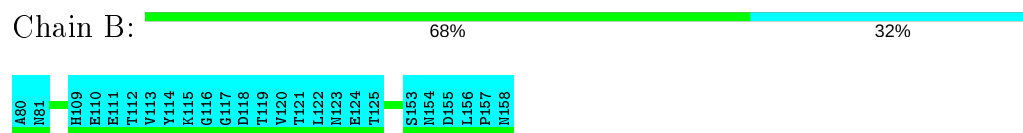


4.2.11 Score per residue for model 11

- Molecule 1: Acid stress chaperone HdeB

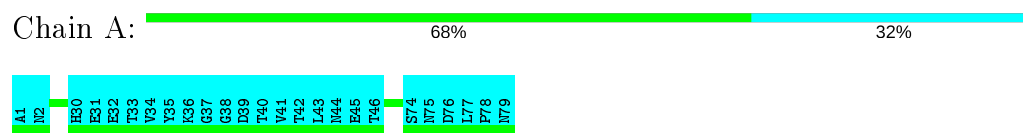


- Molecule 1: Acid stress chaperone HdeB

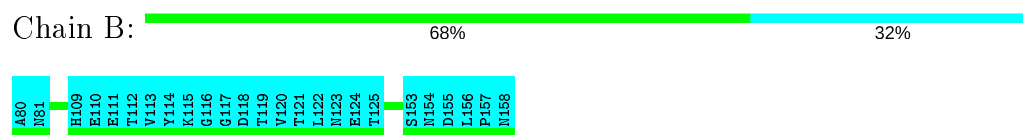


4.2.12 Score per residue for model 12

- Molecule 1: Acid stress chaperone HdeB

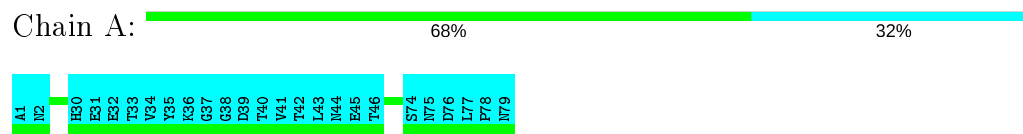


- Molecule 1: Acid stress chaperone HdeB

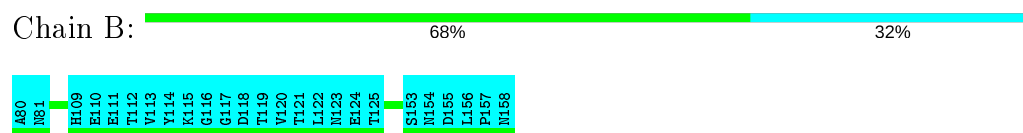


4.2.13 Score per residue for model 13

- Molecule 1: Acid stress chaperone HdeB

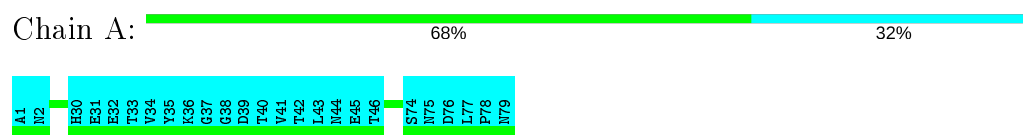


- Molecule 1: Acid stress chaperone HdeB

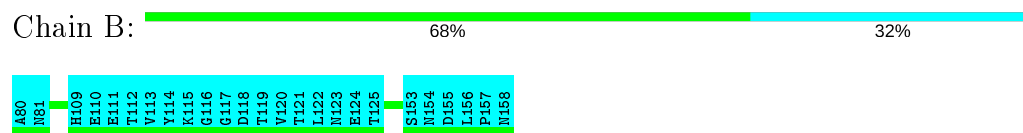


4.2.14 Score per residue for model 14

- Molecule 1: Acid stress chaperone HdeB

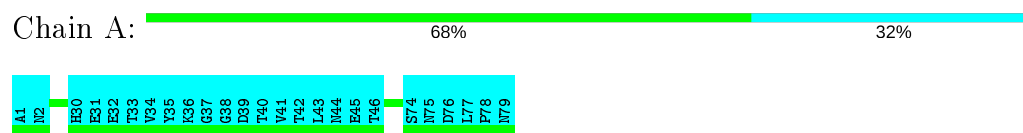


- Molecule 1: Acid stress chaperone HdeB

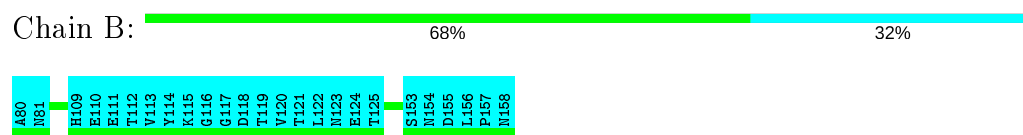


4.2.15 Score per residue for model 15

- Molecule 1: Acid stress chaperone HdeB

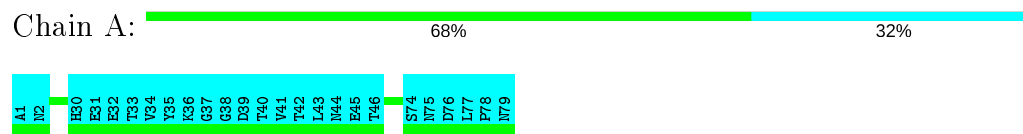


- Molecule 1: Acid stress chaperone HdeB

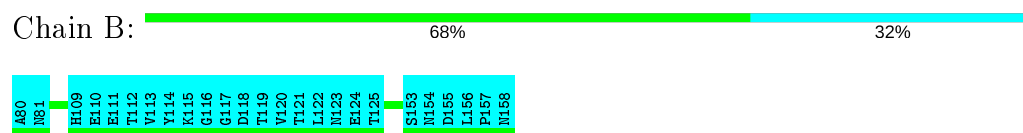


4.2.16 Score per residue for model 16

- Molecule 1: Acid stress chaperone HdeB

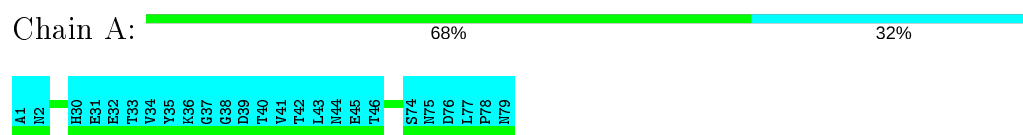


- Molecule 1: Acid stress chaperone HdeB

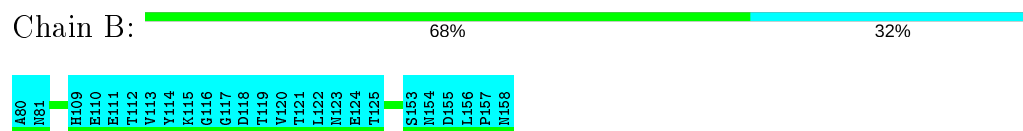


4.2.17 Score per residue for model 17

- Molecule 1: Acid stress chaperone HdeB

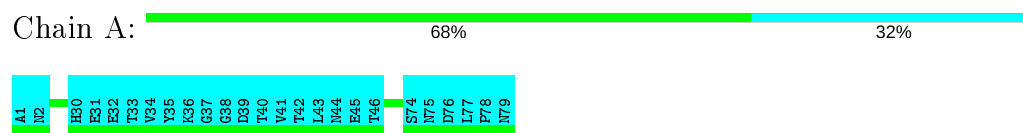


- Molecule 1: Acid stress chaperone HdeB

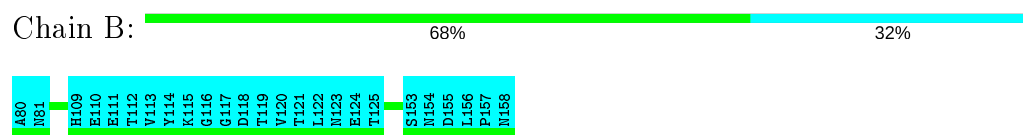


4.2.18 Score per residue for model 18

- Molecule 1: Acid stress chaperone HdeB

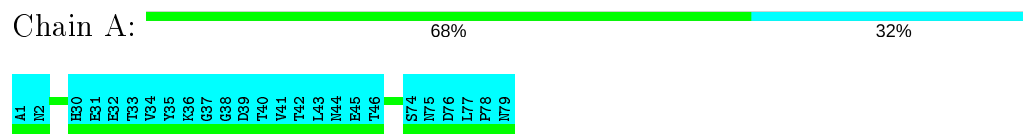


- Molecule 1: Acid stress chaperone HdeB

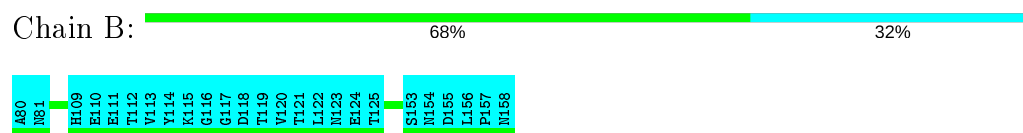


4.2.19 Score per residue for model 19

- Molecule 1: Acid stress chaperone HdeB



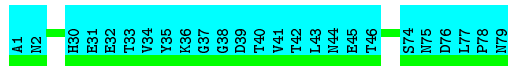
- Molecule 1: Acid stress chaperone HdeB



4.2.20 Score per residue for model 20

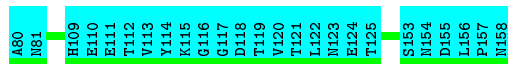
- Molecule 1: Acid stress chaperone HdeB

Chain A:  68% 32%



- Molecule 1: Acid stress chaperone HdeB

Chain B:  68% 32%



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
CYANA	structure solution	
AMBER	refinement	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	945
Number of shifts mapped to atoms	945
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

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](#)

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 [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
All	All	17760	17760	0	-

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 -.

There are no clashes.

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	0	-	-	-	-
1	B	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	0	-	-	-
1	B	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates 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 44% for the well-defined parts and 44% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	945
Number of shifts mapped to atoms	945
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

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
$^{13}\text{C}_\alpha$	79	-0.67 ± 0.33	Should be applied
$^{13}\text{C}_\beta$	77	0.07 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}'$	69	-0.29 ± 0.13	None needed (< 0.5 ppm)
^{15}N	73	0.15 ± 0.54	None needed (< 0.5 ppm)

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 44%, i.e. 618 atoms were assigned a chemical shift out of a possible 1396. 4 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	257/524 (49%)	104/208 (50%)	103/216 (48%)	50/100 (50%)
Sidechain	324/756 (43%)	197/448 (44%)	119/278 (43%)	8/30 (27%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	37/116 (32%)	19/60 (32%)	16/52 (31%)	2/4 (50%)
Overall	618/1396 (44%)	320/716 (45%)	238/546 (44%)	60/134 (45%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 849 atoms were assigned a chemical shift out of a possible 1944. 8 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	373/770 (48%)	152/306 (50%)	148/316 (47%)	73/148 (49%)
Sidechain	431/1028 (42%)	260/602 (43%)	160/386 (41%)	11/40 (28%)
Aromatic	45/146 (31%)	23/76 (30%)	20/64 (31%)	2/6 (33%)
Overall	849/1944 (44%)	435/984 (44%)	328/766 (43%)	86/194 (44%)

7.1.4 Statistically unusual chemical shifts [i](#)

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	26	TRP	CE3	135.20	129.06 – 111.96	8.6

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

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:

