

# Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2L2M
Title	:	Solution structure of the second dsRBD of HYL1
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This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $SOLUTION\ NMR$ 

The overall completeness of chemical shifts assignment was not calculated.

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	2	Percentile Ranks	Value
Clashscore			0
Ramachandran outliers			0
Sidechain outliers			0
	Worse		Better
	Percentile relative to all	structures	
	Percentile relative to all	NMR structures	
		x71 1 1 •	

Metric	Whole archive (#Entries)	${f NMR} \ { m archive} \ (\#{ m Entries})$
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 >=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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	77	84%	6%	9%



## 2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 6 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:101-A:165 (65)	0.76	6			

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, 2, 3, 4, 5, 6, 7, 9
2	8, 10



## 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1099 atoms, of which 561 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Hyponastic leave 1.

Mol	Chain	Residues	Atoms				Trace		
1	Δ	70	Total	С	Η	Ν	0	S	0
	А	A 70	1099	339	561	93	102	4	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	94	GLY	-	expression tag	UNP 004492
A	95	HIS	-	expression tag	UNP 004492
А	96	MET	-	expression tag	UNP 004492



# 4 Residue-property plots (i)

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

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

• Molecule 1: Hyponastic leave 1

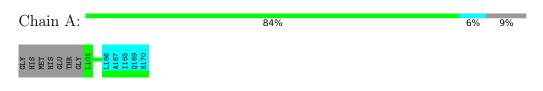
Chain A:	84%	6%	9%
GLY HIS MET MET MET HIS GLU GLU CLI CLI GLO CLI GLO CLI GLO CLI GLO CLI GLO CLI CLI CLI CLI CLI CLI CLI CLI CLI CLI			

### 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: Hyponastic leave 1



#### 4.2.2 Score per residue for model 2

• Molecule 1: Hyponastic leave 1

Chain A: 84% 6% 9%



#### 4.2.3 Score per residue for model 3

• Molecule 1: Hyponastic leave 1

Chain A:	84%	6%	9%
GLY MET MET MET MET HIS GLU CLU CLU CLU CLU CLU CLU CLU CLU CLU C			

#### 4.2.4 Score per residue for model 4

• Molecule 1: Hyponastic leave 1

Chain A:	84%	6%	9%
GLY HIS MET MET MET HIR GLU CLU CLU L101 L106 L166 L166 L166 L168 L168 R168 R168 R168 R168 R168 R168 R168			

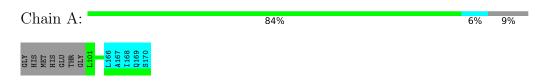
#### 4.2.5 Score per residue for model 5

• Molecule 1: Hyponastic leave 1

Chain A:	84%	6%	9%
GLY MMET MMET MMET GLU GLU GLU LLIOL LLIOL L166 A167 S170 S170			

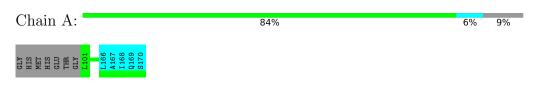
#### 4.2.6 Score per residue for model 6 (medoid)

• Molecule 1: Hyponastic leave 1



#### 4.2.7 Score per residue for model 7

• Molecule 1: Hyponastic leave 1





#### 4.2.8 Score per residue for model 8

• Molecule 1: Hyponastic leave 1

Chain A:	84%	6%	9%
GLY HIS MET MET MET HIS GLU CLU CLY	11 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		

#### 4.2.9 Score per residue for model 9

• Molecule 1: Hyponastic leave 1

Chain A:	84%	6%	9%
GLY HET MET MET GLU GLU GLY GLY GLY 1166 9166 9168 9168 9170			

#### 4.2.10 Score per residue for model 10

• Molecule 1: Hyponastic leave 1

Chain A:		82%	•	•	6%	9%	-
GLY HIS MET MET HIS GLY GLY L101 L106 L106 P118	40000						



## 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: rosetta full atom relaxation.

Of the 1000 calculated structures, 10 were deposited, based on the following criterion: target function.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.



# 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
1	А	502	521	520	0±0
All	All	5020	5210	5200	1

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	om-1 Atom-2		Distance(Å)	Models	
Atom-1	Atom-2	Clash(Å)	Distance(A)	Worst	Total
1:A:106:LEU:HB3	1:A:118:PRO:HG2	0.52	1.81	10	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	А	64/77~(83%)	$64\pm0$ (100 $\pm1\%$ )	0±0 (0±1%)	0±0 (0±0%)	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	640/770~(83%)	638~(100%)	2~(0%)	0~(0%)	100 100

There are no Ramachandran outliers.

#### 6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers Percentile		entiles
1	А	53/62~(85%)	53±0 (100±0%)	0±0 (0±0%)	100	100
All	All	530/620~(85%)	530 (100%)	0 (0%)	100	100

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 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)

No chemical shift data were provided

