

# Full wwPDB NMR Structure Validation Report (i)

#### Aug 9, 2020 – 07:18 PM BST

PDB ID : 2YHH

Title: Microvirin:mannobiose complex

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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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

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 : 2.13.1

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

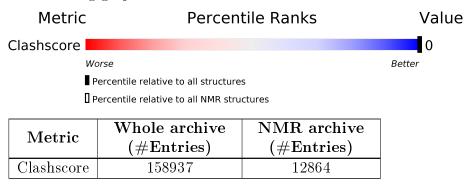
Validation Pipeline (wwPDB-VP) : 2.13.1

## 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 is 62%.

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.



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	A	108	100%		
2	В	2	100%		



# 2 Ensemble composition and analysis (i)

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.



# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1657 atoms, of which 784 are hydrogens and 0 are deuteriums.

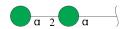
• Molecule 1 is a protein called MANNAN-BINDING LECTIN.

Mol	Chain	Residues		Atoms				Trace	
1	Λ	100	Total	С	Н	N	О	S	0
	A	108	1612	516	762	141	185	8	U

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
Α	64	ARG	HIS	$\operatorname{conflict}$	UNP Q2MDE2	

• Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			Trace	
9	D	9	Total	С	Н	О	0
	В	2	45	12	22	11	U



## 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: MANNAN-BINDING LECTIN						
Chain A:						
77						
961 963 963 964 965 966 966 966 966 966 966 966						
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose						
Chain B:						
MANY MANY MANY MANY MANY MANY MANY MANY						
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: MANNAN-BINDING LECTIN						
Chain A: 100%						
Name						
### Molecule 2: alpha-D-mannopyranose (1-2)-alpha-D-mannopyranose						

● Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose



Chain B:	100%
MAU2 MAU2	
4.2.2 Score per residue for model	. 2
• Molecule 1: MANNAN-BINDING LE	CTIN
Chain A:	100%
### Page 12	E30 E32 E32 E33 E33 E33 E33 E34 E44 E44 E44 E44 E44
961 062 063 165 165 165 165 167 177 177 177 179 179 179 178 179 179 178 178 178 178 178 178 178 178 178 178	190 193 193 193 193 194 198 198 198 198 198 100 100 1107 1107
• Molecule 2: alpha-D-mannopyranose-	(1-2)-alpha-D-mannopyranose
Chain B:	100%
MAN2 MAN2	



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

The models were refined using the following method: TORSION ANGLE, SIMULATED ANNEALING.

Of the 40 calculated structures, 2 were deposited, based on the following criterion: LEAST RE-STRAINT VIOLATION.

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

Software name	Classification	Version
Xplor-NIH	refinement	
X-PLOR	structure solution	

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	840
Number of shifts mapped to atoms	840
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	62%

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: MAN

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	A	0	0	0	0±0
All	All	46	44	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	-	-	-	-
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	-	-	-
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)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Tuna	no Chain Bog		ype Chain Res Li	Link		Bond lengths		
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	#Z>2		
2	MAN	В	1	2	12,12,12	$0.99 \pm 0.00$	0±0 (0±0%)		
2	MAN	В	2	2	11,11,12	$1.14\pm0.00$	0±0 (0±0%)		

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types,



if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mal	Т	Chain	Dag	T in le	Bond angles		
MIOI	Type	Chain	nes	Link	Counts	RMSZ	#Z>2
2	MAN	В	1	2	17,17,17	$1.24 \pm 0.00$	0±0 (0±0%)
2	MAN	В	2	2	15,15,17	$1.93 \pm 0.00$	1±0 (6±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	В	1	2	-	$0\pm0,2,22,22$	$0\pm0,1,1,1$
2	MAN	В	2	2	-	$0\pm0,2,19,22$	$0\pm0,1,1,1$

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$	Moc Worst	
2	В	2	MAN	C1-O5-C5	7.06	121.75	112.19	2	2

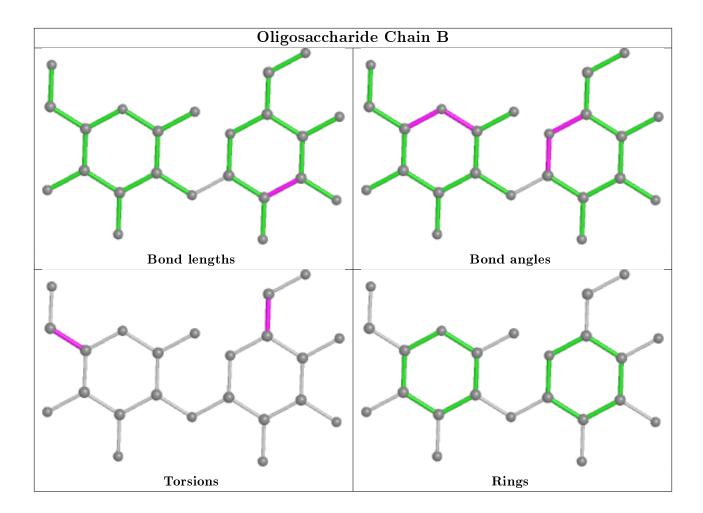
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 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 62% for the well-defined parts and 62% for the entire structure.

#### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: 2yhh

#### 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	840
Number of shifts mapped to atoms	840
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	$\text{Correction} \pm \text{precision}, \textit{ppm}$	Suggested action
$^{13}\mathrm{C}_{\alpha}$	108	$-0.21 \pm 0.16$	None needed ( $< 0.5 \text{ ppm}$ )
$^{13}C_{\beta}$	100	$-0.03 \pm 0.17$	None needed ( $< 0.5 \text{ ppm}$ )
<sup>13</sup> C′	106	$0.34 \pm 0.15$	None needed ( $< 0.5 \text{ ppm}$ )
$^{15}N$	102	$-0.01 \pm 0.64$	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 62%, i.e. 785 atoms were assigned a chemical shift out of a possible 1266. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	517/534 (97%)	201/213 (94%)	214/216 (99%)	102/105 (97%)
Sidechain	235/638 (37%)	51/372 (14%)	168/240 (70%)	16/26 (62%)

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	Total	$^{1}\mathbf{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Aromatic	33/94 (35%)	22/50~(44%)	8/39 (21%)	3/5~(60%)
Overall	785/1266 (62%)	274/635 (43%)	390/495 (79%)	121/136~(89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 62%, i.e. 785 atoms were assigned a chemical shift out of a possible 1266. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	517/534 (97%)	$201/213 \ (94\%)$	$214/216 \ (99\%)$	$102/105 \ (97\%)$
Sidechain	$235/638 \ (37\%)$	51/372 (14%)	$168/240 \ (70\%)$	$16/26 \ (62\%)$
Aromatic	33/94 (35%)	22/50~(44%)	8/39 (21%)	3/5~(60%)
Overall	785/1266 (62%)	$274/635 \ (43\%)$	390/495~(79%)	121/136 (89%)

#### 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.

Mo	l Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	91	GLN	С	77.39	186.20 - 166.50	-50.2

## 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:

