



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:04 AM BST

PDB ID : 2MWM  
Title : NMR structure of the protein YP\_193882.1 from *Lactobacillus acidophilus* NCFM in presence of FMN  
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Deposited on : 2014-11-13

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  
<http://wwpdb.org/validation/2016/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  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

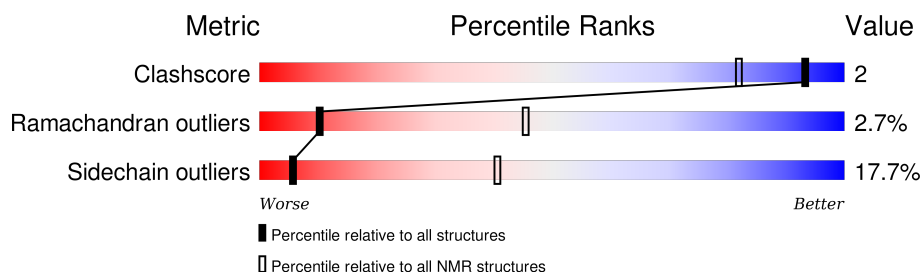
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	151	 86% 11% ••

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:4-A:151 (148)	0.51	1

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 7 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2174 atoms, of which 972 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative trp repressor binding protein.

Mol	Chain	Residues	Atoms						Trace
1	A	151	Total	C	H	N	O	S	0
			2174	764	972	193	241	4	

There is a discrepancy between the modelled and reference sequences:

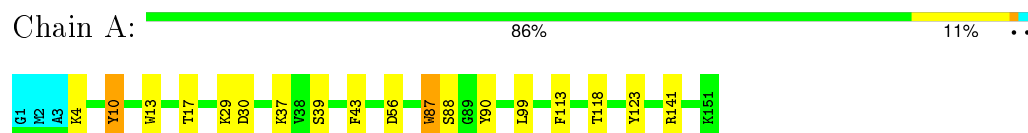
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q5FKC3

## 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: Putative trp repressor binding protein

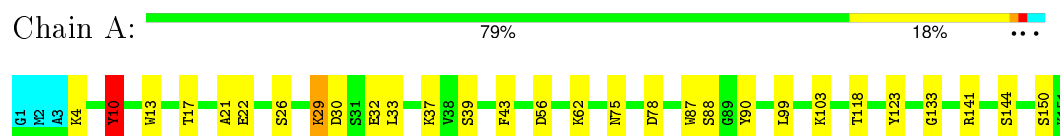


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

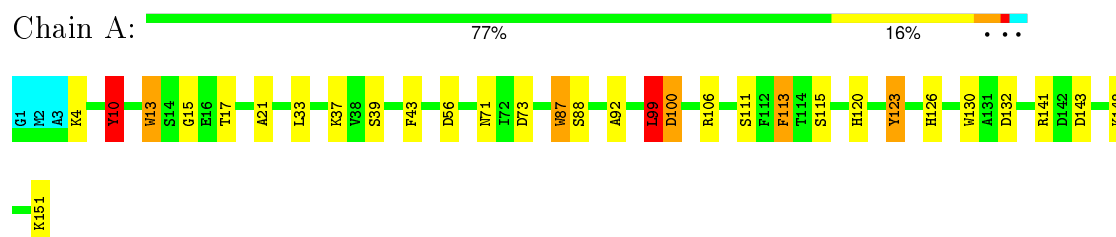
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Putative trp repressor binding protein



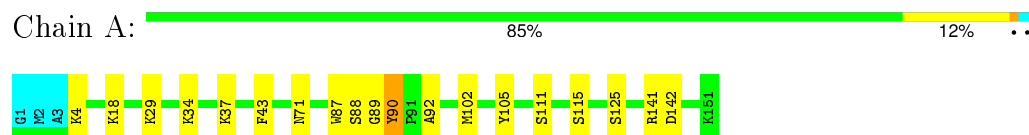
#### 4.2.2 Score per residue for model 2

- Molecule 1: Putative trp repressor binding protein



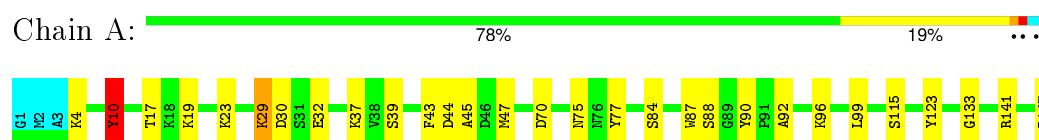
### 4.2.3 Score per residue for model 3

- Molecule 1: Putative trp repressor binding protein



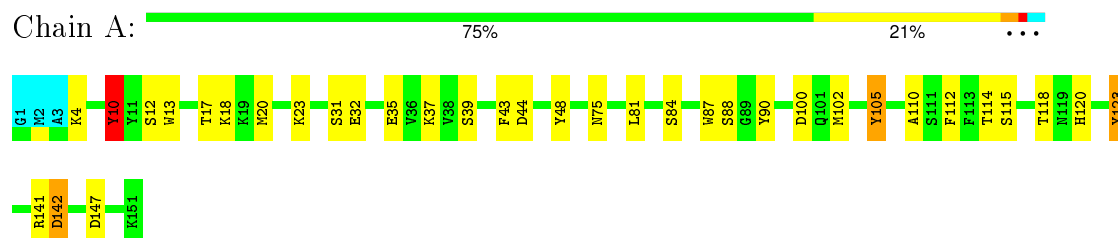
### 4.2.4 Score per residue for model 4

- Molecule 1: Putative trp repressor binding protein



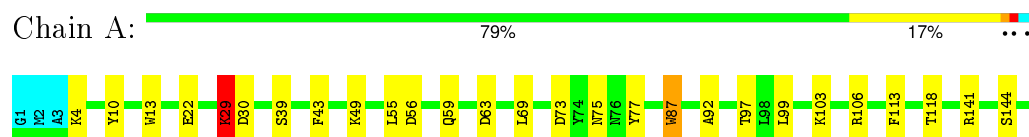
### 4.2.5 Score per residue for model 5

- Molecule 1: Putative trp repressor binding protein



### 4.2.6 Score per residue for model 6

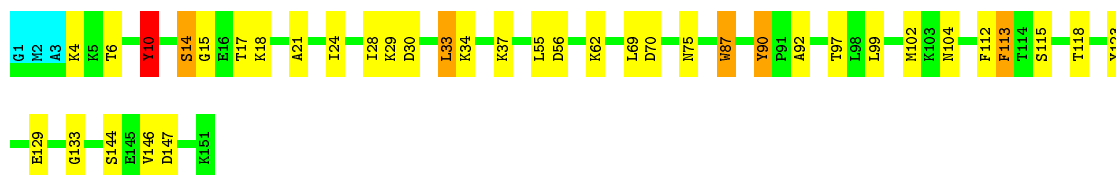
- Molecule 1: Putative trp repressor binding protein



### 4.2.7 Score per residue for model 7

- Molecule 1: Putative trp repressor binding protein





#### 4.2.8 Score per residue for model 8

- Molecule 1: Putative trp repressor binding protein

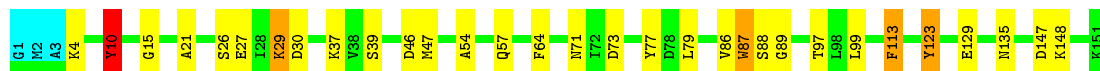
Chain A: 84% 13% ..



#### 4.2.9 Score per residue for model 9

- Molecule 1: Putative trp repressor binding protein

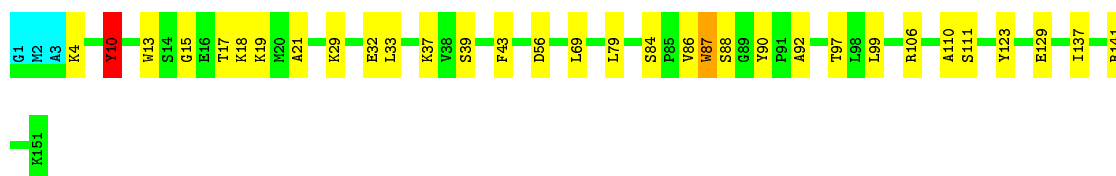
Chain A: 77% 17% ...



#### 4.2.10 Score per residue for model 10

- Molecule 1: Putative trp repressor binding protein

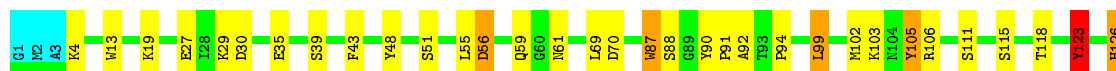
Chain A: 77% 20% ...



#### 4.2.11 Score per residue for model 11

- Molecule 1: Putative trp repressor binding protein

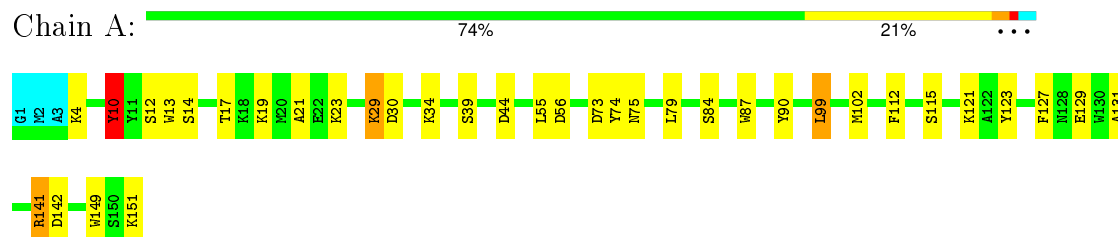
Chain A: 72% 21% ...





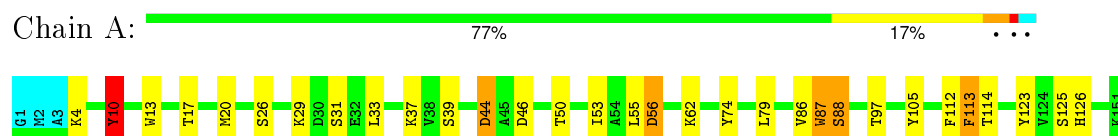
#### 4.2.12 Score per residue for model 12

- Molecule 1: Putative trp repressor binding protein



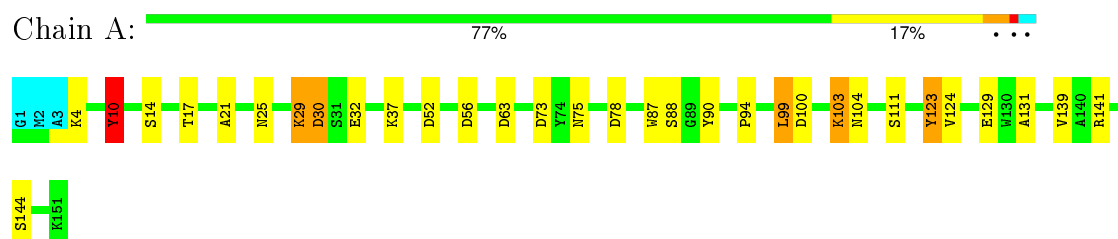
#### 4.2.13 Score per residue for model 13

- Molecule 1: Putative trp repressor binding protein



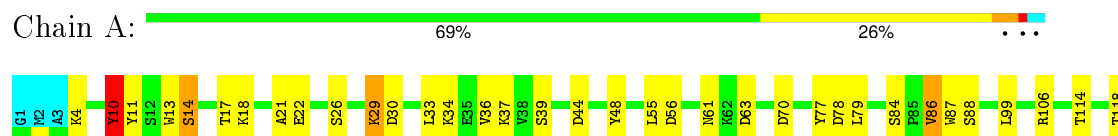
#### 4.2.14 Score per residue for model 14

- Molecule 1: Putative trp repressor binding protein



#### 4.2.15 Score per residue for model 15

- Molecule 1: Putative trp repressor binding protein



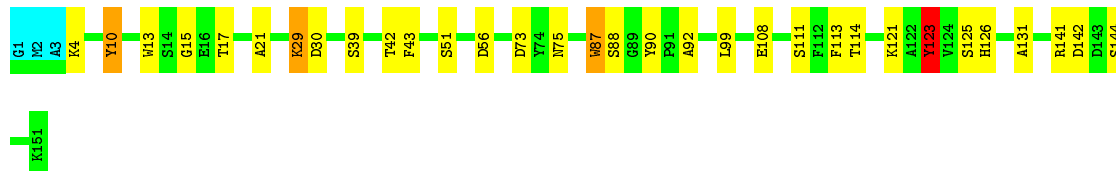




#### 4.2.16 Score per residue for model 16

- Molecule 1: Putative trp repressor binding protein

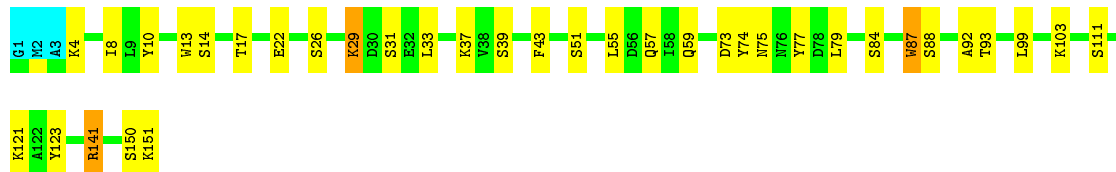
Chain A: 77% 19% ...



#### 4.2.17 Score per residue for model 17

- Molecule 1: Putative trp repressor binding protein

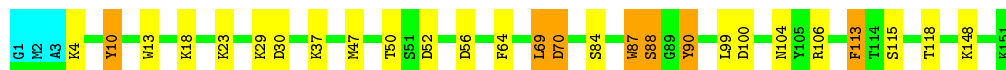
Chain A: 74% 22% ..



#### 4.2.18 Score per residue for model 18

- Molecule 1: Putative trp repressor binding protein

Chain A: 80% 13% 5% .



#### 4.2.19 Score per residue for model 19

- Molecule 1: Putative trp repressor binding protein

Chain A: 76% 19% ...





4.2.20 Score per residue for model 20

- Molecule 1: Putative trp repressor binding protein



## 5 Refinement protocol and experimental data overview

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

Of the 80 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	refinement	3.0
CYANA	structure solution	3.0
OPAL	geometry optimization	

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)	2mwm_cs.str
Number of chemical shift lists	1
Total number of shifts	1792
Number of shifts mapped to atoms	1792
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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

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	0.63±0.01	0±0/1211 (0.0±0.0%)	1.08±0.03	2±1/1638 (0.1±0.1%)
All	All	0.63	0/24220 (0.0%)	1.08	42/32760 (0.1%)

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	0.0±0.0	2.0±1.0
All	All	0	40

There are no bond-length outliers.

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	86	VAL	CA-CB-CG2	8.48	123.61	110.90	13	2
1	A	10	TYR	CB-CG-CD2	-8.20	116.08	121.00	9	12
1	A	141	ARG	CD-NE-CZ	6.99	133.38	123.60	12	1
1	A	56	ASP	CB-CG-OD1	-6.95	112.05	118.30	7	5
1	A	113	PHE	CB-CG-CD2	-6.29	116.40	120.80	7	4
1	A	86	VAL	CG1-CB-CG2	6.27	120.94	110.90	9	2
1	A	20	MET	CG-SD-CE	-6.27	90.17	100.20	5	1
1	A	141	ARG	NE-CZ-NH2	-6.23	117.19	120.30	15	2
1	A	123	TYR	CB-CG-CD2	-6.06	117.36	121.00	11	4
1	A	113	PHE	CB-CG-CD1	5.97	124.98	120.80	19	1
1	A	141	ARG	NE-CZ-NH1	5.94	123.27	120.30	12	1
1	A	142	ASP	CB-CG-OD1	5.63	123.37	118.30	5	1
1	A	27	GLU	CA-CB-CG	5.59	125.70	113.40	9	1
1	A	118	THR	CA-CB-CG2	-5.17	105.16	112.40	20	1
1	A	10	TYR	CB-CG-CD1	5.09	124.06	121.00	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	106	ARG	NE-CZ-NH2	-5.09	117.75	120.30	10	1
1	A	99	LEU	CB-CG-CD1	5.08	119.63	111.00	2	1
1	A	144	SER	N-CA-CB	-5.04	102.93	110.50	19	1

There are no chirality outliers.

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	10	TYR	Sidechain	10
1	A	77	TYR	Sidechain	6
1	A	123	TYR	Sidechain	6
1	A	90	TYR	Sidechain	5
1	A	48	TYR	Sidechain	5
1	A	74	TYR	Sidechain	2
1	A	141	ARG	Sidechain	2
1	A	106	ARG	Sidechain	2
1	A	113	PHE	Sidechain	1
1	A	105	TYR	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	1185	957	1145	4±2
All	All	23700	19140	22900	81

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:TYR:CE2	1:A:21:ALA:HB2	0.71	2.20	10	8
1:A:86:VAL:HG11	1:A:123:TYR:CZ	0.66	2.26	15	3
1:A:55:LEU:HD11	1:A:59:GLN:HE21	0.63	1.53	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:TRP:CE3	1:A:92:ALA:HB2	0.62	2.29	19	9
1:A:43:PHE:CE2	1:A:92:ALA:HB1	0.62	2.29	17	4
1:A:113:PHE:CE2	1:A:123:TYR:CE1	0.62	2.87	16	1
1:A:99:LEU:HD22	1:A:131:ALA:HA	0.61	1.71	12	3
1:A:43:PHE:CZ	1:A:92:ALA:HB1	0.60	2.31	4	1
1:A:54:ALA:HB2	1:A:87:TRP:CZ3	0.60	2.30	9	1
1:A:105:TYR:CD1	1:A:134:LEU:HD22	0.56	2.35	19	1
1:A:6:THR:HG21	1:A:28:ILE:HG21	0.56	1.76	7	1
1:A:43:PHE:CD2	1:A:92:ALA:HB1	0.55	2.37	19	1
1:A:124:VAL:HG13	1:A:139:VAL:HG13	0.53	1.79	14	1
1:A:11:TYR:HB2	1:A:36:VAL:CG1	0.53	2.34	15	1
1:A:100:ASP:O	1:A:103:LYS:HE3	0.53	2.04	14	1
1:A:24:ILE:HG23	1:A:146:VAL:HG21	0.52	1.81	7	1
1:A:55:LEU:HD11	1:A:59:GLN:NE2	0.51	2.20	11	3
1:A:113:PHE:CD2	1:A:123:TYR:CD2	0.49	3.01	9	1
1:A:38:VAL:HG21	1:A:43:PHE:CZ	0.47	2.44	20	1
1:A:29:LYS:HE3	1:A:29:LYS:HA	0.47	1.86	6	1
1:A:81:LEU:HD23	1:A:110:ALA:HB3	0.47	1.86	5	1
1:A:8:ILE:HG23	1:A:10:TYR:CZ	0.47	2.45	17	1
1:A:10:TYR:CE2	1:A:21:ALA:HA	0.46	2.45	20	1
1:A:21:ALA:HB1	1:A:33:LEU:HD21	0.46	1.87	7	2
1:A:90:TYR:HA	1:A:126:HIS:CE1	0.46	2.46	11	1
1:A:86:VAL:HG11	1:A:123:TYR:CE1	0.46	2.46	10	1
1:A:43:PHE:CD1	1:A:92:ALA:HB1	0.46	2.46	11	2
1:A:113:PHE:CD2	1:A:123:TYR:CG	0.45	3.04	13	1
1:A:90:TYR:CD1	1:A:126:HIS:CE1	0.45	3.05	16	1
1:A:99:LEU:HD13	1:A:100:ASP:N	0.45	2.27	2	1
1:A:43:PHE:CE1	1:A:92:ALA:HB1	0.44	2.47	6	1
1:A:123:TYR:HA	1:A:126:HIS:CE1	0.44	2.48	11	1
1:A:74:TYR:CD2	1:A:102:MET:HB3	0.44	2.48	12	1
1:A:11:TYR:HB2	1:A:36:VAL:HG12	0.44	1.90	15	1
1:A:10:TYR:CE2	1:A:21:ALA:CB	0.43	3.01	16	1
1:A:126:HIS:CE1	1:A:130:TRP:HE1	0.43	2.32	2	1
1:A:10:TYR:CE2	1:A:21:ALA:HB1	0.43	2.48	16	1
1:A:110:ALA:HB2	1:A:137:ILE:HG13	0.43	1.91	10	1
1:A:91:PRO:HD2	1:A:126:HIS:HE2	0.43	1.73	11	1
1:A:120:HIS:HA	1:A:123:TYR:CD2	0.42	2.49	2	1
1:A:55:LEU:CD1	1:A:59:GLN:HE21	0.42	2.27	6	1
1:A:105:TYR:CE1	1:A:134:LEU:HD23	0.42	2.49	11	1
1:A:46:ASP:CG	1:A:47:MET:H	0.42	2.17	20	1
1:A:50:THR:HB	1:A:87:TRP:CZ2	0.42	2.50	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:LEU:HD12	1:A:99:LEU:C	0.42	2.33	8	1
1:A:50:THR:HG21	1:A:87:TRP:HE1	0.42	1.75	13	1
1:A:10:TYR:CZ	1:A:21:ALA:HB2	0.41	2.50	15	1
1:A:44:ASP:OD2	1:A:53:ILE:HD11	0.41	2.16	13	1
1:A:69:LEU:HD13	1:A:70:ASP:H	0.41	1.75	18	1
1:A:112:PHE:CE1	1:A:149:TRP:CE3	0.40	3.09	12	1
1:A:126:HIS:C	1:A:126:HIS:CD2	0.40	2.93	11	1
1:A:42:THR:HG22	1:A:43:PHE:CE2	0.40	2.52	16	1
1:A:87:TRP:CZ3	1:A:92:ALA:HB2	0.40	2.52	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	A	147/151 (97%)	124±3 (84±2%)	19±3 (13±2%)	4±1 (3±1%)	10	45
All	All	2940/3020 (97%)	2474 (84%)	386 (13%)	80 (3%)	10	45

All 18 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	88	SER	16
1	A	29	LYS	14
1	A	13	TRP	11
1	A	30	ASP	10
1	A	15	GLY	6
1	A	133	GLY	3
1	A	94	PRO	3
1	A	142	ASP	3
1	A	14	SER	2
1	A	39	SER	2
1	A	89	GLY	2
1	A	31	SER	2
1	A	45	ALA	1

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Mol	Chain	Res	Type	Models (Total)
1	A	131	ALA	1
1	A	20	MET	1
1	A	103	LYS	1
1	A	47	MET	1
1	A	106	ARG	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	130/131 (99%)	107±4 (82±3%)	23±4 (18±3%)	6	41
All	All	2600/2620 (99%)	2141 (82%)	459 (18%)	6	41

All 84 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	4	LYS	20
1	A	87	TRP	19
1	A	141	ARG	15
1	A	37	LYS	15
1	A	99	LEU	15
1	A	17	THR	14
1	A	10	TYR	14
1	A	39	SER	14
1	A	29	LYS	13
1	A	56	ASP	10
1	A	75	ASN	10
1	A	115	SER	10
1	A	118	THR	9
1	A	90	TYR	9
1	A	111	SER	9
1	A	18	LYS	8
1	A	73	ASP	8
1	A	79	LEU	8
1	A	84	SER	8
1	A	129	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	113	PHE	7
1	A	70	ASP	7
1	A	33	LEU	7
1	A	144	SER	7
1	A	148	LYS	7
1	A	123	TYR	7
1	A	14	SER	6
1	A	147	ASP	6
1	A	32	GLU	6
1	A	97	THR	6
1	A	43	PHE	5
1	A	114	THR	5
1	A	26	SER	5
1	A	44	ASP	5
1	A	105	TYR	5
1	A	19	LYS	5
1	A	69	LEU	5
1	A	103	LYS	5
1	A	102	MET	5
1	A	88	SER	5
1	A	23	LYS	5
1	A	150	SER	5
1	A	22	GLU	4
1	A	151	LYS	4
1	A	55	LEU	4
1	A	62	LYS	4
1	A	125	SER	4
1	A	34	LYS	4
1	A	121	LYS	4
1	A	112	PHE	4
1	A	63	ASP	3
1	A	78	ASP	3
1	A	106	ARG	3
1	A	100	ASP	3
1	A	51	SER	3
1	A	35	GLU	3
1	A	46	ASP	3
1	A	104	ASN	3
1	A	64	PHE	3
1	A	47	MET	3
1	A	71	ASN	3
1	A	31	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	132	ASP	2
1	A	12	SER	2
1	A	61	ASN	2
1	A	30	ASP	2
1	A	57	GLN	2
1	A	126	HIS	2
1	A	52	ASP	2
1	A	13	TRP	2
1	A	127	PHE	1
1	A	142	ASP	1
1	A	135	ASN	1
1	A	120	HIS	1
1	A	16	GLU	1
1	A	134	LEU	1
1	A	145	GLU	1
1	A	93	THR	1
1	A	143	ASP	1
1	A	108	GLU	1
1	A	96	LYS	1
1	A	25	ASN	1
1	A	49	LYS	1
1	A	27	GLU	1

### 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

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 89% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2mwm\_cs.str

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	1792
Number of shifts mapped to atoms	1792
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	23

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	148	$2.56 \pm 0.22$	Should be applied
$^{13}\text{C}_\beta$	140	$2.87 \pm 0.14$	Should be applied
$^{13}\text{C}'$	127	$2.68 \pm 0.22$	Should be applied
$^{15}\text{N}$	144	$0.09 \pm 0.40$	None needed ( $< 0.5$ ppm)

#### 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 90%, i.e. 1622 atoms were assigned a chemical shift out of a possible 1806. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	707/732 (97%)	290/292 (99%)	274/296 (93%)	143/144 (99%)
Sidechain	809/903 (90%)	504/527 (96%)	292/342 (85%)	13/34 (38%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	106/171 (62%)	53/89 (60%)	49/76 (64%)	4/6 (67%)
Overall	1622/1806 (90%)	847/908 (93%)	615/714 (86%)	160/184 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1628 atoms were assigned a chemical shift out of a possible 1831. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	711/747 (95%)	292/298 (98%)	275/302 (91%)	144/147 (98%)
Sidechain	811/913 (89%)	505/533 (95%)	293/346 (85%)	13/34 (38%)
Aromatic	106/171 (62%)	53/89 (60%)	49/76 (64%)	4/6 (67%)
Overall	1628/1831 (89%)	850/920 (92%)	617/724 (85%)	161/187 (86%)

#### 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	96	LYS	HB3	-0.72	3.10 – 0.40	-9.1
1	A	96	LYS	HD3	-0.36	2.75 – 0.45	-8.5
1	A	145	GLU	HB3	0.17	3.10 – 0.90	-8.3
1	A	96	LYS	HG2	-0.71	2.67 – 0.07	-8.0
1	A	10	TYR	CD1	122.95	139.11 – 126.41	-7.7
1	A	96	LYS	HD2	-0.05	2.76 – 0.46	-7.2
1	A	110	ALA	HB2	-0.44	2.61 – 0.11	-7.2
1	A	110	ALA	HB3	-0.44	2.61 – 0.11	-7.2
1	A	110	ALA	HB1	-0.44	2.61 – 0.11	-7.2
1	A	96	LYS	HG3	-0.44	2.76 – -0.04	-6.4
1	A	50	THR	HG21	-0.24	2.29 – -0.01	-6.0
1	A	50	THR	HG22	-0.24	2.29 – -0.01	-6.0
1	A	50	THR	HG23	-0.24	2.29 – -0.01	-6.0
1	A	92	ALA	HB1	-0.12	2.61 – 0.11	-5.9
1	A	92	ALA	HB2	-0.12	2.61 – 0.11	-5.9
1	A	92	ALA	HB3	-0.12	2.61 – 0.11	-5.9
1	A	57	GLN	HB2	0.60	3.30 – 0.80	-5.8
1	A	111	SER	HB3	2.29	5.25 – 2.45	-5.6
1	A	7	LEU	HB2	-0.24	3.32 – -0.08	-5.5
1	A	96	LYS	HE3	1.87	3.86 – 1.96	-5.5
1	A	83	GLY	HA3	1.83	5.80 – 2.00	-5.4
1	A	16	GLU	H	11.55	11.34 – 5.34	5.4

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	111	SER	HB2	2.58	5.18 – 2.58	-5.0

### 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:

