



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 23, 2024 – 07:21 AM EDT

PDB ID : 6PVR  
BMRB ID : 30645  
Title : Influenza B M2 Proton Channel in the Closed State - SSNMR Structure at pH 7.5  
Authors : Mandala, V.S.; Loftis, A.R.; Shcherbakov, A.S.; Pentelute, B.L.; Hong, M.  
Deposited on : 2019-07-21

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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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) 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) : 2.37.1

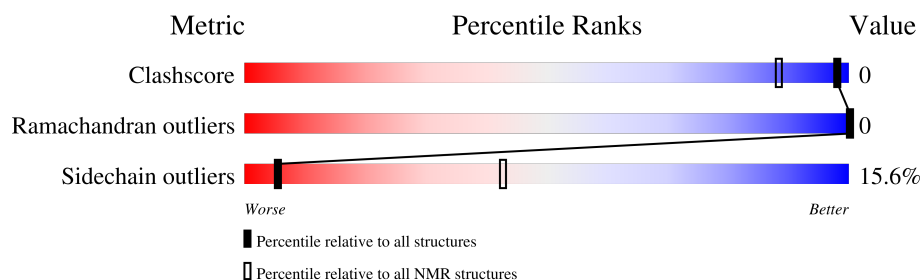
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 10%.

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	51	<div> <div>41%</div> <div>6%</div> <div>18%</div> <div>35%</div> </div>
1	B	51	<div> <div>41%</div> <div>•</div> <div>20%</div> <div>35%</div> </div>
1	C	51	<div> <div>41%</div> <div>6%</div> <div>18%</div> <div>35%</div> </div>
1	D	51	<div> <div>41%</div> <div>•</div> <div>20%</div> <div>35%</div> </div>

## 2 Ensemble composition and analysis

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: *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:5-A:28, B:6-B:28, C:5-C:28, D:6-D:28 (94)	0.49	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 and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 6, 7, 8, 10
2	3, 9
Single-model clusters	5

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2212 atoms, of which 1120 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BM2 protein.

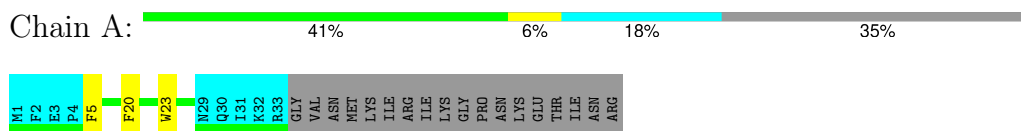
Mol	Chain	Residues	Atoms						Trace
1	A	33	Total	C	H	N	O	S	0
			553	183	280	45	42	3	
1	B	33	Total	C	H	N	O	S	0
			553	183	280	45	42	3	
1	C	33	Total	C	H	N	O	S	0
			553	183	280	45	42	3	
1	D	33	Total	C	H	N	O	S	0
			553	183	280	45	42	3	

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

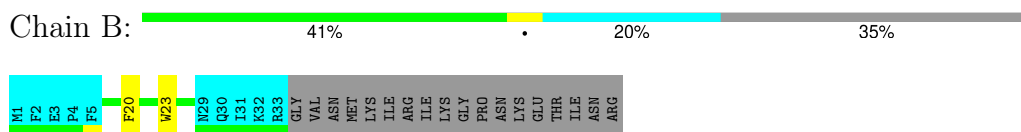
### 4.1 Average score per residue in the NMR ensemble

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.

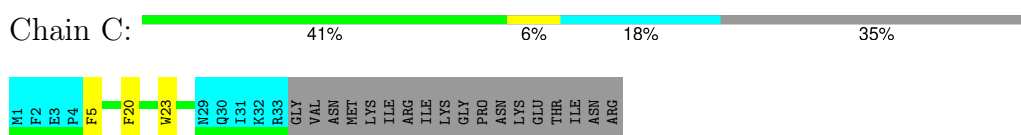
- Molecule 1: BM2 protein



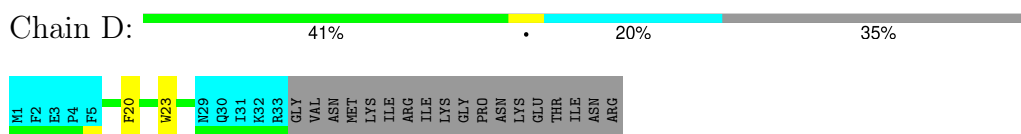
- Molecule 1: BM2 protein



- Molecule 1: BM2 protein



- Molecule 1: BM2 protein

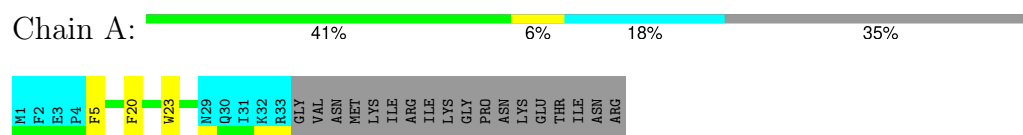


### 4.2 Scores per residue for each member of the ensemble

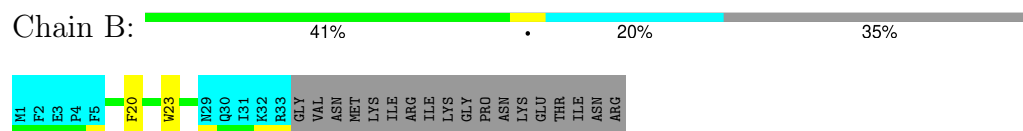
Colouring as in section [4.1](#) above.

### 4.2.1 Score per residue for model 1

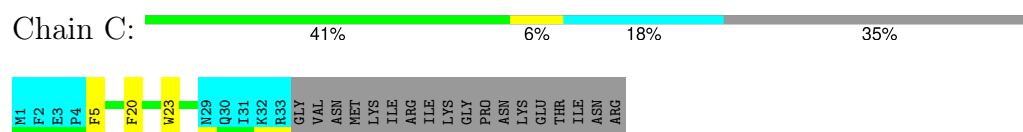
#### • Molecule 1: BM2 protein



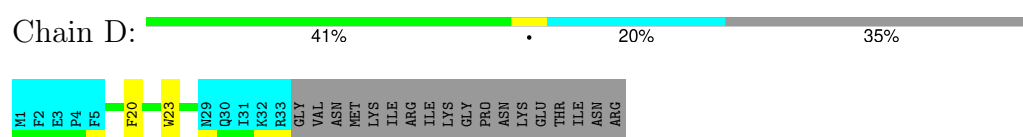
#### • Molecule 1: BM2 protein



#### • Molecule 1: BM2 protein

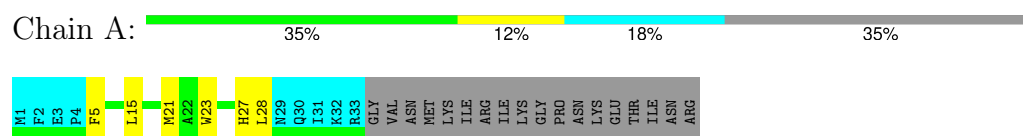


#### • Molecule 1: BM2 protein

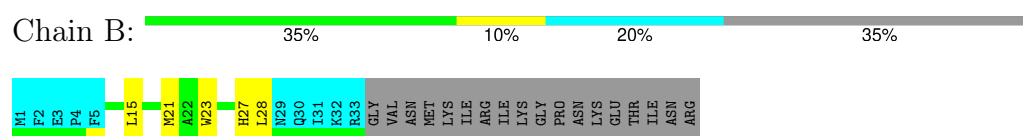


### 4.2.2 Score per residue for model 2

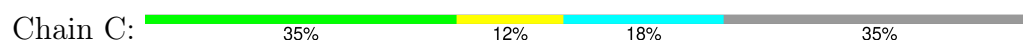
#### • Molecule 1: BM2 protein

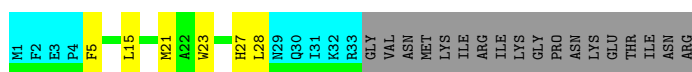


#### • Molecule 1: BM2 protein

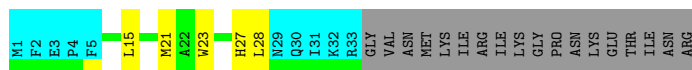
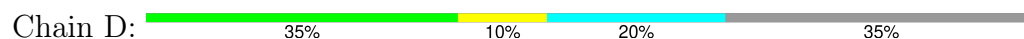


#### • Molecule 1: BM2 protein



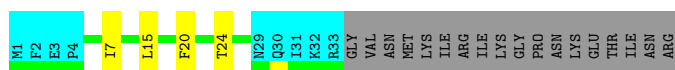
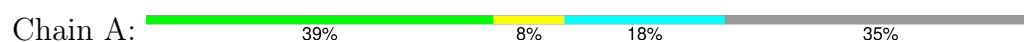


- Molecule 1: BM2 protein

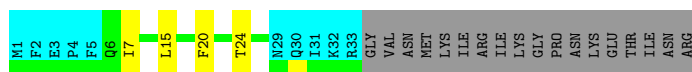
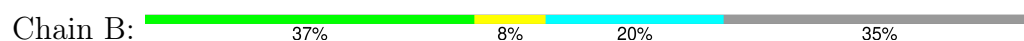


#### 4.2.3 Score per residue for model 3

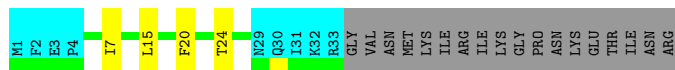
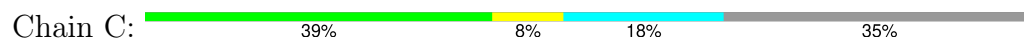
- Molecule 1: BM2 protein



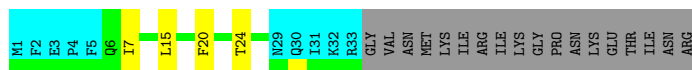
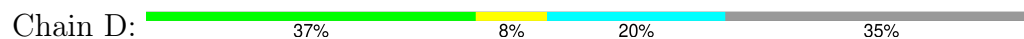
- Molecule 1: BM2 protein



- Molecule 1: BM2 protein

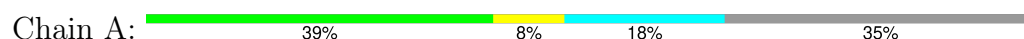


- Molecule 1: BM2 protein

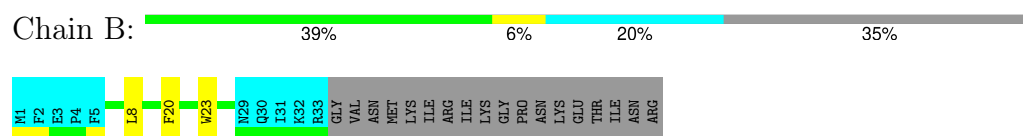


#### 4.2.4 Score per residue for model 4

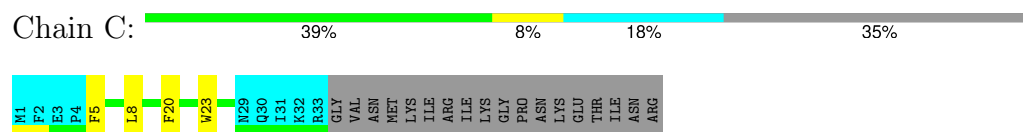
- Molecule 1: BM2 protein



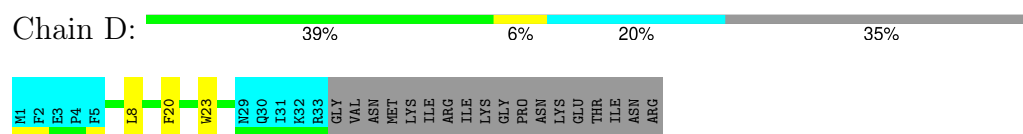
- Molecule 1: BM2 protein



- Molecule 1: BM2 protein

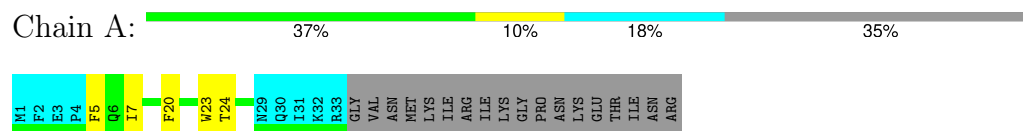


- Molecule 1: BM2 protein

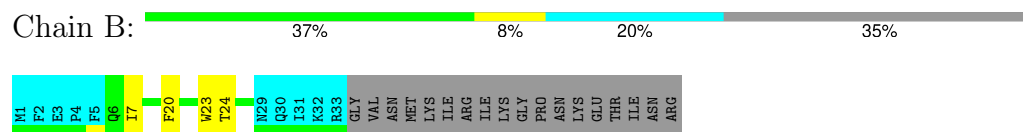


#### 4.2.5 Score per residue for model 5

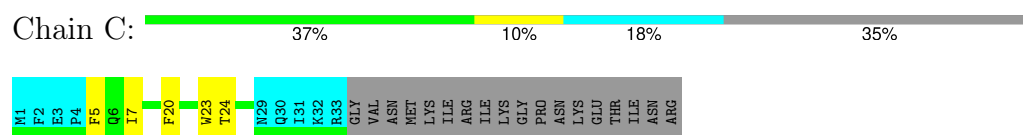
- Molecule 1: BM2 protein



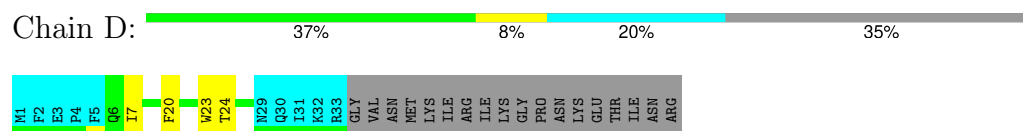
- Molecule 1: BM2 protein



- Molecule 1: BM2 protein



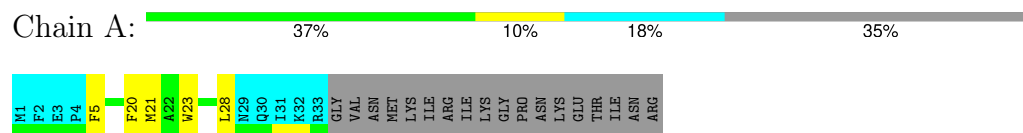
- Molecule 1: BM2 protein



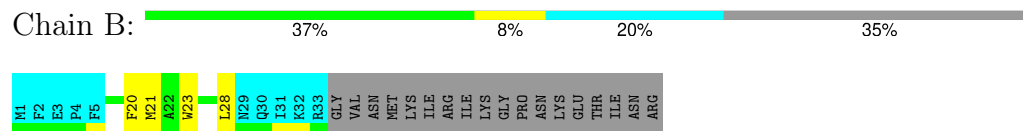


#### 4.2.6 Score per residue for model 6 (medoid)

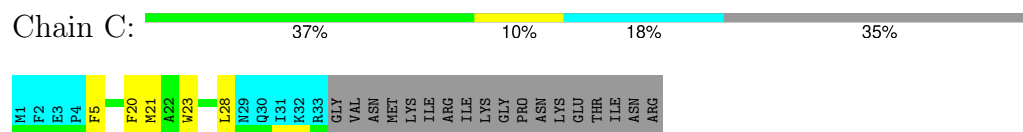
- Molecule 1: BM2 protein



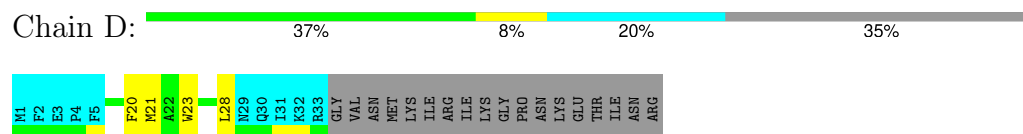
- Molecule 1: BM2 protein



- Molecule 1: BM2 protein

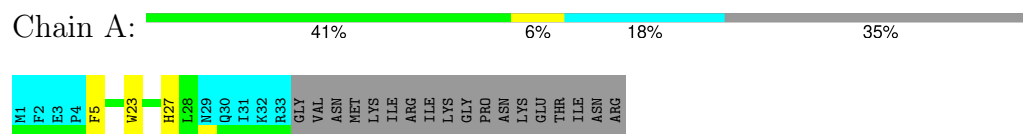


- Molecule 1: BM2 protein

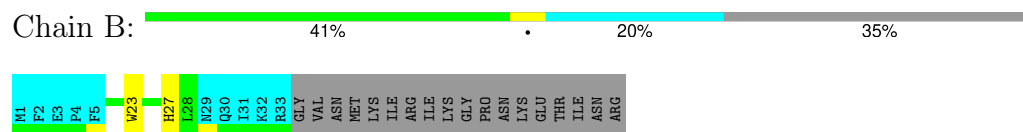


#### 4.2.7 Score per residue for model 7

- Molecule 1: BM2 protein



- Molecule 1: BM2 protein



- Molecule 1: BM2 protein



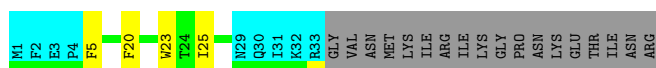
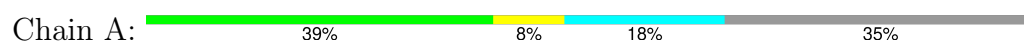


- Molecule 1: BM2 protein

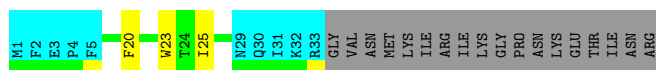
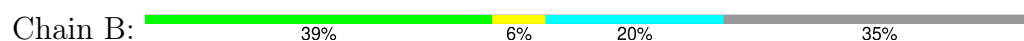


#### 4.2.8 Score per residue for model 8

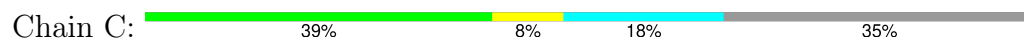
- Molecule 1: BM2 protein



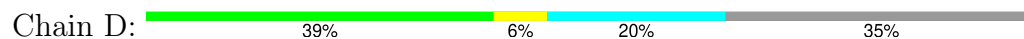
- Molecule 1: BM2 protein



- Molecule 1: BM2 protein

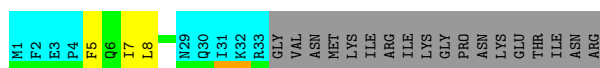


- Molecule 1: BM2 protein

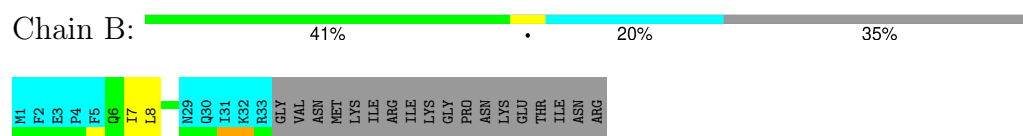


#### 4.2.9 Score per residue for model 9

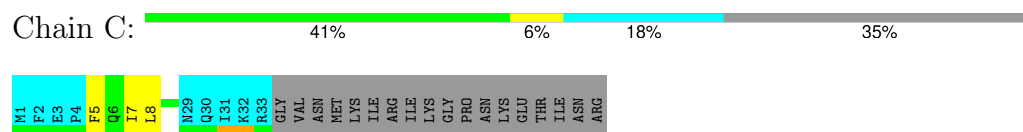
- Molecule 1: BM2 protein



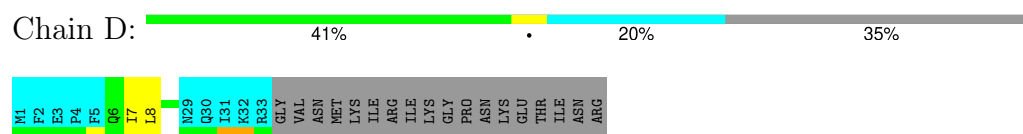
- Molecule 1: BM2 protein



- Molecule 1: BM2 protein

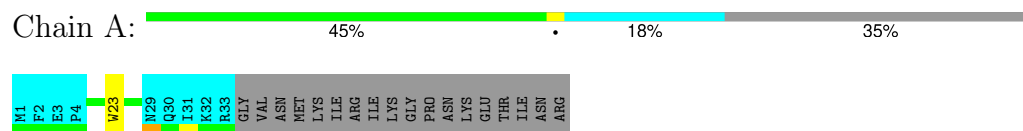


- Molecule 1: BM2 protein

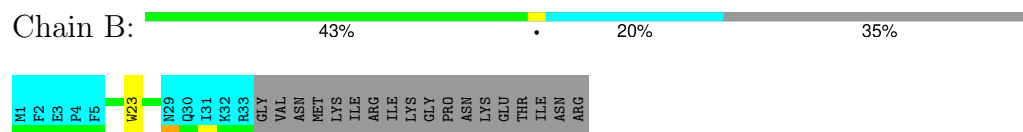


#### 4.2.10 Score per residue for model 10

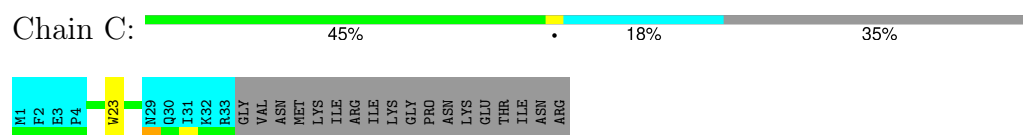
- Molecule 1: BM2 protein



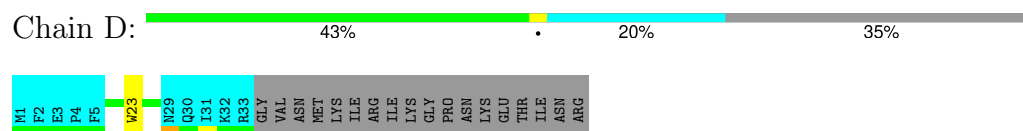
- Molecule 1: BM2 protein



- Molecule 1: BM2 protein



- Molecule 1: BM2 protein



## 5 Refinement protocol and experimental data overview

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

Of the 120 calculated structures, 10 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
X-PLOR NIH	refinement	2.47
X-PLOR NIH	structure calculation	2.47

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	198
Number of shifts mapped to atoms	161
Number of unparsed shifts	0
Number of shifts with mapping errors	37
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	10%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 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	A	193	196	196	0±0
1	B	182	187	187	0±0
1	C	193	196	196	0±0
1	D	182	187	187	0±0
All	All	7500	7660	7660	4

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	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:20:PHE:O	1:D:24:THR:HG23	0.58	1.99	3	1
1:B:20:PHE:O	1:B:24:THR:HG23	0.58	1.99	3	1
1:C:20:PHE:O	1:C:24:THR:HG23	0.58	1.98	3	1
1:A:20:PHE:O	1:A:24:THR:HG23	0.57	1.99	3	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	24/51 (47%)	24±1 (99±3%)	0±1 (1±3%)	0±0 (0±0%)	100	100
1	B	23/51 (45%)	23±1 (99±3%)	0±1 (1±3%)	0±0 (0±0%)	100	100
1	C	24/51 (47%)	24±1 (99±3%)	0±1 (1±3%)	0±0 (0±0%)	100	100
1	D	23/51 (45%)	23±1 (99±3%)	0±1 (1±3%)	0±0 (0±0%)	100	100
All	All	940/2040 (46%)	929 (99%)	11 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 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	21/46 (46%)	17±1 (83±7%)	4±1 (17±7%)	5	40
1	B	20/46 (43%)	17±1 (86±6%)	3±1 (14±6%)	6	46
1	C	21/46 (46%)	17±1 (83±7%)	4±1 (17±7%)	5	40
1	D	20/46 (43%)	17±1 (86±6%)	3±1 (14±6%)	6	46
All	All	820/1840 (45%)	692 (84%)	128 (16%)	5	43

All 42 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	5	PHE	8
1	A	23	TRP	8
1	B	23	TRP	8
1	C	5	PHE	8
1	C	23	TRP	8
1	D	23	TRP	8
1	A	20	PHE	5
1	B	20	PHE	5
1	C	20	PHE	5
1	D	20	PHE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	7	ILE	3
1	B	7	ILE	3
1	C	7	ILE	3
1	D	7	ILE	3
1	A	15	LEU	2
1	A	21	MET	2
1	A	27	HIS	2
1	A	28	LEU	2
1	B	15	LEU	2
1	B	21	MET	2
1	B	27	HIS	2
1	B	28	LEU	2
1	C	15	LEU	2
1	C	21	MET	2
1	C	27	HIS	2
1	C	28	LEU	2
1	D	15	LEU	2
1	D	21	MET	2
1	D	27	HIS	2
1	D	28	LEU	2
1	A	8	LEU	2
1	B	8	LEU	2
1	C	8	LEU	2
1	D	8	LEU	2
1	A	24	THR	1
1	B	24	THR	1
1	C	24	THR	1
1	D	24	THR	1
1	A	25	ILE	1
1	B	25	ILE	1
1	C	25	ILE	1
1	D	25	ILE	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 10% for the well-defined parts and 8% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *BM2-pH75-CS-nmrStarv2.txt*

#### 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	198
Number of shifts mapped to atoms	161
Number of unparsed shifts	0
Number of shifts with mapping errors	37
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 37 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	34	GLY	CA	44.4	.	.
1	A	34	GLY	C	172.9	.	.
1	A	35	VAL	CA	59.7	.	.
1	A	35	VAL	CB	30.7	.	.
1	A	35	VAL	CG1	19.6	.	.
1	A	35	VAL	CG2	19.6	.	.
1	A	43	GLY	CA	42.7	.	.
1	A	43	GLY	C	169.8	.	.
1	A	44	PRO	CA	61.0	.	.
1	A	44	PRO	CB	30.5	.	.
1	A	44	PRO	C	174.4	.	.
1	A	44	PRO	CG	25.3	.	.
1	A	44	PRO	CD	48.3	.	.
1	A	45	ASN	CA	51.5	.	.

*Continued on next page...*

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	ASN	CB	37.1	.	.
1	A	46	LYS	CA	54.6	.	.
1	A	46	LYS	CB	31.1	.	.
1	A	46	LYS	CG	22.9	.	.
1	A	46	LYS	CD	27.3	.	.
1	A	46	LYS	CE	40.2	.	.
1	A	47	ASP	CA	54.8	.	.
1	A	47	ASP	CB	28.5	.	.
1	A	47	ASP	CG	34.5	.	.
1	A	48	THR	CA	60.2	.	.
1	A	48	THR	CB	67.9	.	.
1	A	48	THR	CG2	19.9	.	.
1	A	49	ILE	CA	59.2	.	.
1	A	49	ILE	CB	37.0	.	.
1	A	49	ILE	CG1	25.4	.	.
1	A	49	ILE	CG2	15.7	.	.
1	A	49	ILE	CD1	11.2	.	.
1	A	50	ASN	CA	51.4	.	.
1	A	50	ASN	CB	37.1	.	.
1	A	51	ARG	CA	55.6	.	.
1	A	51	ARG	CB	29.8	.	.
1	A	51	ARG	CG	25.4	.	.
1	A	51	ARG	CD	41.7	.	.

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	40	$0.43 \pm 0.77$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	38	$2.50 \pm 0.23$	Should be checked
$^{13}\text{C}'$	27	$1.09 \pm 0.40$	Should be applied
$^{15}\text{N}$	25	$-0.42 \pm 0.81$	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 10%, i.e. 129 atoms were assigned a chemical shift out of a possible 1344. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	67/474 (14%)	0/192 (0%)	45/188 (24%)	22/94 (23%)
Sidechain	48/666 (7%)	0/456 (0%)	48/206 (23%)	0/4 (0%)
Aromatic	14/204 (7%)	0/106 (0%)	13/86 (15%)	1/12 (8%)
Overall	129/1344 (10%)	0/754 (0%)	106/480 (22%)	23/110 (21%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 155 atoms were assigned a chemical shift out of a possible 1952. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	77/656 (12%)	0/264 (0%)	53/264 (20%)	24/128 (19%)
Sidechain	64/1032 (6%)	0/688 (0%)	63/316 (20%)	1/28 (4%)
Aromatic	14/264 (5%)	0/136 (0%)	13/116 (11%)	1/12 (8%)
Overall	155/1952 (8%)	0/1088 (0%)	129/696 (19%)	26/168 (15%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

#### 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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	47	ASP	CG	34.50	149.18 – 208.82	-24.2
1	A	47	ASP	CB	28.50	32.98 – 48.76	-7.8

#### 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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

