

# Full wwPDB NMR Structure Validation Report (i)

# Apr 21, 2024 – 10:11 AM EDT

PDB ID	:	2MOF
BMRB ID	:	19941
Title	:	Structural insights of TM domain of LAMP-2A in DPC micelles
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Deposited on	:	2014-04-25

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:

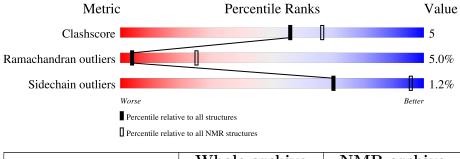
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson 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 is 92%.

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f NMR} \; { m archive} \ (\#{ m Entries})$
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	42	40%	5%	55%



# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 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:380-A:398 (19)	0.29	17	

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 5 clusters and 1 single-model cluster was found.

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



# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 640 atoms, of which 321 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Lysosome-associated membrane glycoprotein 2.

Mol	Chain	Residues		At	oms			Trace
1	۸	49	Total	С	Η	Ν	0	0
	1 A	42	640	212	321	51	56	0



# 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: Lysosome-associated membrane glycoprotein 2

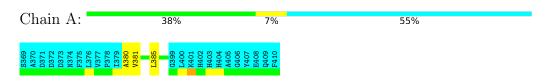


# 4.2 Scores per residue for each member of the ensemble

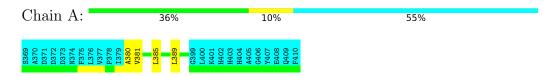
Colouring as in section 4.1 above.

## 4.2.1 Score per residue for model 1

 $\bullet$  Molecule 1: Lysosome-associated membrane glycoprotein 2



## 4.2.2 Score per residue for model 2





#### 4.2.3 Score per residue for model 3

• Molecule 1: Lysosome-associated membrane glycoprotein 2



#### 4.2.4 Score per residue for model 4

• Molecule 1: Lysosome-associated membrane glycoprotein 2

Chain A:	36%	7% •	55%
8369 8371 0371 0373 0373 1375 1375 1375 1376 1376 1376 1379 1379 1379 1379 1379 1379 1379	L385 L385 L389 L400 K401 H402 H403 H404 A406	6406 74407 74403 74409 7410	

### 4.2.5 Score per residue for model 5

• Molecule 1: Lysosome-associated membrane glycoprotein 2

Chain A:	33%	12%	55%	
S369 A370 D371 D372 D372 D373 N374 F375	8 33 33 33 33 33 33 33 33 33 33 33 33 33	G399 K401 H402 H403 A405 G406 G406 G406 F410 F410		

## 4.2.6 Score per residue for model 6

• Molecule 1: Lysosome-associated membrane glycoprotein 2

Chain A: 38% 7% 55%

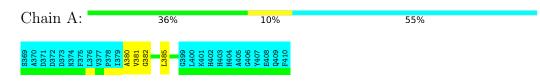
## 4.2.7 Score per residue for model 7

Chain A:	36%	10%	55%
S369 8370 8371 8372 8372 8374 8375 8376 8376 8376 8377 8377 8377 8377 8378 8381 8380 8381	L385 L389 C399 L400 K401	H402 H403 H406 A405 G406 F407 F407 F410	



#### 4.2.8 Score per residue for model 8

• Molecule 1: Lysosome-associated membrane glycoprotein 2



#### 4.2.9 Score per residue for model 9

• Molecule 1: Lysosome-associated membrane glycoprotein 2

Chain A:	40%	5%	55%	
S369 A370 D371 D372 D373 A375 F375 L376 L376 F375 F375 F375 F376 F377 F378 F378 F378 F378 F378 F378 F378	63399 1.400 1.400 1.401 1.402 1.403 1.403 1.405 6.405 6.405 7.407	E408 (1409 F410		

### 4.2.10 Score per residue for model 10

 $\bullet$  Molecule 1: Lysosome-associated membrane glycoprotein 2

Chain A:	38%	7%	55%	
8369 A370 D371 D372 B372 F375 F375 L376 L376 L376 L376 L376 L376 L376 A380 A380	8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	A405 G406 F407 E408 Q409 F410		

## 4.2.11 Score per residue for model 11

• Molecule 1: Lysosome-associated membrane glycoprotein 2

Chain A:	33%	12%	55%	
S369 A370 D371 D372 D373 F375 F375 L376 V377 P378 T379	<u> </u>	6339 K401 H402 H403 A405 6406 6406 6406 6406 F410 F410		

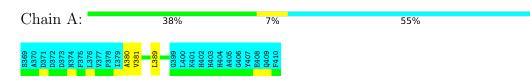
#### 4.2.12 Score per residue for model 12

Chain A:	45%	55%
8369 8370 8370 8371 8372 8375 8375 8375 8375 8375 8376 8376 8376 1376 8377 8377	G399 1400 1401 1402 1404 1404 1404 1405 1406 1406 1406 1409 1409 17407	



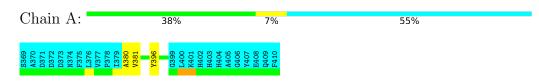
#### 4.2.13 Score per residue for model 13

• Molecule 1: Lysosome-associated membrane glycoprotein 2



#### 4.2.14 Score per residue for model 14

• Molecule 1: Lysosome-associated membrane glycoprotein 2



## 4.2.15 Score per residue for model 15

 $\bullet$  Molecule 1: Lysosome-associated membrane glycoprotein 2

Chain A:	36%	10%	55%	
8369 A370 D371 D373 D373 L376 F375 F375 F376 F376 F376 F378 A380 V381	G382 (382 (382 (399 (400) (4401 (4401) (4402)	H403 H404 A405 G406 E408 Q409 F410		

## 4.2.16 Score per residue for model 16

 $\bullet$  Molecule 1: Lysosome-associated membrane glycoprotein 2

Chain A: 38% 7% 55%

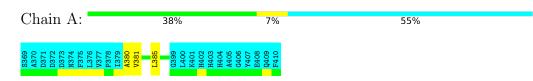
## 4.2.17 Score per residue for model 17 (medoid)

Chain A:	38%	7%	55%
8389 8370 8371 8372 8372 8373 1374 1375 1375 1375 1376 1378 1378 1378 1378 1378 1378 1378 1378	G 399 F 400 F 400	<mark>41</mark>	



## 4.2.18 Score per residue for model 18

• Molecule 1: Lysosome-associated membrane glycoprotein 2



#### 4.2.19 Score per residue for model 19

• Molecule 1: Lysosome-associated membrane glycoprotein 2

Chain A:	36%	10%	55%
S369 A370 D371 D372 D372 D373 F375 F375 F375 F375 F375 F376 F376 F376 F376 F376 F376 F376 F376	L385 L389 C399 L400 H403 H403 H403	4405 7406 6406 6403 6409 7409 7410	

### 4.2.20 Score per residue for model 20

7º	%
	F410



# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, torsion angle dynamics.* 

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
X-PLOR NIH	structure solution	
X-PLOR NIH	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	431
Number of shifts mapped to atoms	431
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%



# 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	133	153	153	2±1
All	All	2660	3060	3060	30

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 5.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Moo	dels
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:385:LEU:HD23	1:A:385:LEU:O	0.56	2.00	19	10
1:A:389:LEU:O	1:A:389:LEU:HD23	0.55	2.02	11	7
1:A:381:VAL:HG13	1:A:382:GLY:N	0.53	2.19	3	7
1:A:381:VAL:CG1	1:A:382:GLY:N	0.48	2.77	11	6

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

# 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	P	erce	entiles
1	А	19/42~(45%)	$18\pm0$ (95 $\pm1\%$ )	0±0 (0±0%)	$1\pm0~(5\pm1\%)$		4	25
All	All	380/840~(45%)	361 (95%)	0 (0%)	19 (5%)		4	25

All 1 unique Ramachandran outliers are listed below.

Μ	ol	Chain	Res	Type	Models (Total)
]	1	А	380	ALA	19

#### 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	А	12/31~(39%)	$12\pm0$ (99 $\pm3\%$ )	0±0 (1±3%)	70 96
All	All	240/620~(39%)	237~(99%)	3 (1%)	70 96

All 1 unique residues with a non-rotameric sidechain are listed below.

Mol	Chain	Res	Type	Models (Total)
1	А	389	LEU	3

#### 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)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 76% for the entire structure.

# 7.1 Chemical shift list 1

File name: working\_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	431
Number of shifts mapped to atoms	431
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

## 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\rm Correction}\pm{\rm precision},ppm$	Suggested action
$^{13}C_{\alpha}$	41	$-0.48 \pm 0.24$	None needed ( $< 0.5$ ppm)
$^{13}C_{\beta}$	34	$0.26 \pm 0.21$	None needed ( $< 0.5$ ppm)
$^{13}C'$	33	$0.04 \pm 0.16$	None needed ( $< 0.5$ ppm)
<sup>15</sup> N	37	$0.86 \pm 0.19$	Should be applied

## 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 92%, i.e. 241 atoms were assigned a chemical shift out of a possible 263. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	91/97~(94%)	37/40~(92%)	36/38~(95%)	18/19~(95%)
Sidechain	140/147~(95%)	98/103~(95%)	42/44~(95%)	0/0 (%)

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	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}$ N
Aromatic	10/19~(53%)	5/9~(56%)	5/10~(50%)	0/0 (%)
Overall	241/263~(92%)	140/152~(92%)	83/92~(90%)	18/19~(95%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 431 atoms were assigned a chemical shift out of a possible 567. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}$ N
Backbone	188/212~(89%)	77/87~(89%)	74/84~(88%)	37/41 (90%)
Sidechain	215/283~(76%)	143/191~(75%)	72/89~(81%)	0/3~(0%)
Aromatic	28/72~(39%)	15/35~(43%)	13/31~(42%)	0/6~(0%)
Overall	431/567~(76%)	235/313~(75%)	159/204~(78%)	37/50~(74%)

## 7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

# 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:

