

Full wwPDB NMR Structure Validation Report (i)

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PDB ID : 2NPV

Title: Structure and dynamics of surfactin studied by NMR in micellar media

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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)

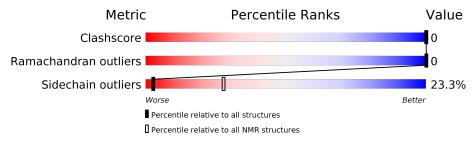
Validation Pipeline (wwPDB-VP) : 2.13.1

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 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$ m 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 >=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	7	86%	14%		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Dog	Total mo	dels with violations
WIOI	Chain	Compound	nes	Chirality	Geometry
2	A	BFC	1	8	-



2 Ensemble composition and analysis (i)

This entry contains 24 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (5) was below the domain threshold value (8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust



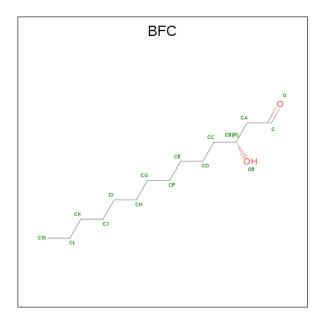
3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 163 atoms, of which 91 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called ELLVDLL.

Mol	Chain	Residues		Trace				
1	Λ	7	Total	С	Н	N	О	0
1	A	(121	38	65	7	11	U

• Molecule 2 is (R)-3-HYDROXYTETRADECANAL (three-letter code: BFC) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			
9	Λ	1	Total	С	Н	О
2	А	1	42	14	26	2



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: ELLVDLL

Chain A: 86% 14%

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: ELLVDLL

Chain A: 86% 14%



4.2.2 Score per residue for model 2

• Molecule 1: ELLVDLL

Chain A: 86% 14%





4.2.3 Score p	er residue	for	model	3
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Chain A:

There are no outlier residues in this chain.

4.2.4 Score per residue for model 4

• Molecule 1: ELLVDLL

Chain A: 57% 43%



4.2.5 Score per residue for model 5

• Molecule 1: ELLVDLL

Chain A: 71% 29%



4.2.6 Score per residue for model 6

• Molecule 1: ELLVDLL

Chain A: 71% 29%



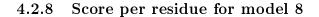
4.2.7 Score per residue for model 7

• Molecule 1: ELLVDLL

Chain A: 86% 14%







Chain A: 86% 14%



4.2.9 Score per residue for model 9

• Molecule 1: ELLVDLL

Chain A: 71% 29%



4.2.10 Score per residue for model 10

• Molecule 1: ELLVDLL

Chain A: 71% 29%



4.2.11 Score per residue for model 11

• Molecule 1: ELLVDLL

Chain A: 71% 29%



4.2.12 Score per residue for model 12

• Molecule 1: ELLVDLL

Chain A: 57% 43%





4.2.13 Score per residu	ue for	model	13
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Chain A: 57% 43%



4.2.14 Score per residue for model 14

• Molecule 1: ELLVDLL

Chain A:

There are no outlier residues in this chain.

4.2.15 Score per residue for model 15

• Molecule 1: ELLVDLL

Chain A:

There are no outlier residues in this chain.

4.2.16 Score per residue for model 16

• Molecule 1: ELLVDLL

Chain A: 86% 14%



4.2.17 Score per residue for model 17

• Molecule 1: ELLVDLL

Chain A: 100%

There are no outlier residues in this chain.



4.2.18 Score per residue for model 18	
• Molecule 1: ELLVDLL	
Chain A: 100% There are no outlier residues in this chain.	
4.2.19 Score per residue for model 19	
• Molecule 1: ELLVDLL	
Chain A: 71%	29%
4.2.20 Score per residue for model 20	
• Molecule 1: ELLVDLL	
Chain A: 71%	29%
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4.2.21 Score per residue for model 21	

Chain A:

There are no outlier residues in this chain.

4.2.22 Score per residue for model 22

• Molecule 1: ELLVDLL

Chain A: 71% 29%





4.2.23 Score per residue for model 23

• Molecule 1: ELLVDLL

Chain A:

There are no outlier residues in this chain.

4.2.24 Score per residue for model 24

• Molecule 1: ELLVDLL

Chain A: 71% 29%





5 Refinement protocol and experimental data overview (i)



The models were refined using the following method: distance geometry, simulated annealing.

Of the 50 calculated structures, 24 were deposited, based on the following criterion: structures with the least restraint violations, structures with the lowest energy.

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

Software name	Classification	Version	
CHARMM	${ m refinement}$	22	

No chemical shift data was provided. 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: BFC, DLE

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	В	ond lengths	Bond angles		
WIOI		RMSZ	#Z>5	RMSZ	#Z>5	
1	A	0.84 ± 0.02	$0\pm0/37~(~0.0\pm~0.0\%)$	1.17 ± 0.08	$0\pm0/46~(~0.4\pm~0.8\%)$	
All	All	0.84	0/888~(~0.0%)	1.17	4/1104 (0.4%)	

There are no bond-length outliers.

All unique angle outliers are listed below.

Mal	Chain	Dog	Tuna	Atoms	7	$Observed(^o)$	Ideal(0)	Mod	lels
10101	Chain	nes	туре	Atoms	Z	Observed(')	Ideal(*)	Worst	Total
1	A	2	GLU	N-CA-C	-5.96	94.91	111.00	12	4

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
All	All	1728	2184	2070	_

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	Perce	\mathbf{ntiles}
1	A	3/7 (43%)	2±0 (78±16%)	1±0 (22±16%)	0±0 (0±0%)	100	100
All	All	72/168 (43%)	56 (78%)	16 (22%)	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 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	Analysed Rotameric		Percentiles		
1	A	5/5 (100%)	4±1 (77±18%)	1±1 (23±18%)	3	28	
All	All	120/120 (100%)	92 (77%)	28 (23%)	3	28	

All 3 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	${f Res}$	Type	Models (Total)
1	A	6	ASP	13
1	A	8	LEU	8
1	A	3	LEU	7

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.



There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

1 ligand is 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	Tuno	Chain	Pos	Link		Bond leng	${ m ths}$
WIOI	Type	Chain	res	LIIIK	Counts	RMSZ	#Z>2
2	BFC	A	1	1	15,15,15	0.81 ± 0.00	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.

Mol	Tuno	Chain	Pos	Link		Bond ang	les
WIOI	туре	Chain	res	LIIIK	Counts	RMSZ	#Z>2
2	BFC	A	1	1	15,15,15	0.82 ± 0.00	0±0 (0±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.



\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BFC	A	1	1	-	$0\pm0,14,14,14$	-

There are no bond-length outliers.

There are no bond-angle outliers.

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	Α	1	BFC	СВ	8

There are no torsion outliers.

There are no ring outliers.

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

