



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2LNY
Title : ShB peptide structure bound to negatively charged lipid-bilayer after Molecular Dynamics refinement
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Deposited on : 2012-01-06

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

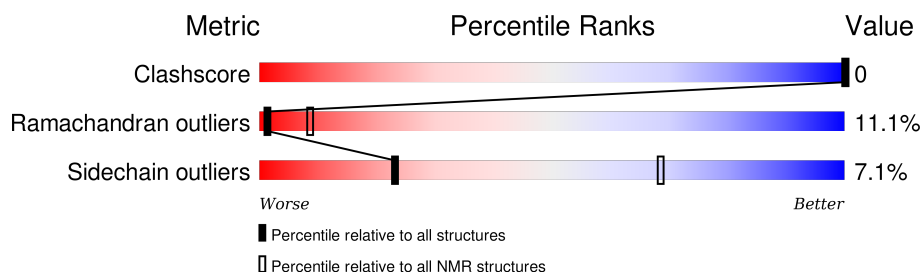
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 21%.

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 ≥ 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	20	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 207 atoms, of which 51 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ShB peptide.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	20	207	95	51	32	28	1	0

4 Residue-property plots

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: ShB peptide

Chain A:  70% 30%



5 Refinement protocol and experimental data overview

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

Of the 1 calculated structures, 1 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
GROMOS	refinement	53a6
CNS	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)	2lny_cs.str
Number of chemical shift lists	1
Total number of shifts	54
Number of shifts mapped to atoms	54
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	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.

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	0.60	0/157 (0.0%)	2.50	8/205 (3.9%)
All	All	0.60	0/157 (0.0%)	2.50	8/205 (3.9%)

There are no bond-length outliers.

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	TYR	CB-CG-CD2	-13.62	112.83	121.00
1	A	14	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	A	8	TYR	CG-CD2-CE2	-9.48	113.72	121.30
1	A	14	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	8	TYR	CZ-CE2-CD2	6.74	125.87	119.80
1	A	8	TYR	CG-CD1-CE1	-6.49	116.11	121.30
1	A	8	TYR	CD1-CG-CD2	6.37	124.91	117.90
1	A	17	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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	156	51	160	-

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	18/20 (90%)	9 (50%)	7 (39%)	2 (11%)	1	9
All	All	18/20 (90%)	9 (50%)	7 (39%)	2 (11%)	1	9

All 2 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	6	GLY
1	A	19	LYS

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	14/14 (100%)	13 (93%)	1 (7%)	23	68
All	All	14/14 (100%)	13 (93%)	1 (7%)	23	68

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

Mol	Chain	Res	Type
1	A	10	LEU

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 21% for the well-defined parts and 21% for the entire structure.

7.1 Chemical shift list 1

File name: 2lny_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	54
Number of shifts mapped to atoms	54
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	12	-0.10 ± 0.42	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	9	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	11	1.77 ± 0.69	Should be applied
^{15}N	11	4.23 ± 2.33	None needed (imprecise)

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 21%, i.e. 54 atoms were assigned a chemical shift out of a possible 253. 2 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	34/100 (34%)	0/40 (0%)	23/40 (58%)	11/20 (55%)
Sidechain	20/137 (15%)	0/81 (0%)	20/46 (43%)	0/10 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/16 (0%)	0/8 (0%)	0/6 (0%)	0/2 (0%)
Overall	54/253 (21%)	0/129 (0%)	43/92 (47%)	11/32 (34%)

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 21%, i.e. 54 atoms were assigned a chemical shift out of a possible 253. 2 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	34/100 (34%)	0/40 (0%)	23/40 (58%)	11/20 (55%)
Sidechain	20/137 (15%)	0/81 (0%)	20/46 (43%)	0/10 (0%)
Aromatic	0/16 (0%)	0/8 (0%)	0/6 (0%)	0/2 (0%)
Overall	54/253 (21%)	0/129 (0%)	43/92 (47%)	11/32 (34%)

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 ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

