Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 05:17 PM BST

PDB ID	:	1SXM
Title	:	SCORPION TOXIN (NOXIUSTOXIN) WITH HIGH AFFINITY FOR VOLTAGE DEPENDENT POTASSIUM CHANNEL AND LOW AFFINITY FOR CALCIUM DEPENDENT POTASSIUM CHANNEL (NMR AT 20 DEGREES, PH3.5, 39 STRUCTURES)
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Deposited on	:	1995-09-07

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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

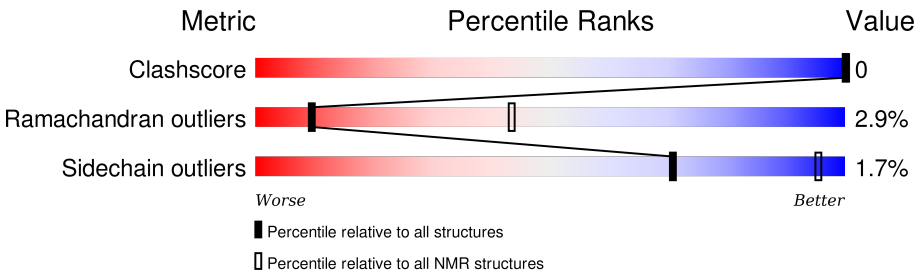
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	40	88% • 10%

2 Ensemble composition and analysis (i)

This entry contains 39 models. Model 4 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:2-A:37 (36)	0.14	4

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 12 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 15, 17, 22
2	23, 26, 29, 35, 38
3	28, 33
4	24, 32
5	25, 37
Single-model clusters	14; 16; 18; 19; 20; 21; 27; 30; 31; 34; 36; 39

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 580 atoms, of which 293 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NOXIUSTOXIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	40	580	174	293	52	54	7	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	TYR	THR	CONFLICT	UNP P08815

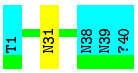
4 Residue-property plots (i)

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: NOXIUSTOXIN

Chain A:



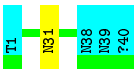
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: NOXIUSTOXIN

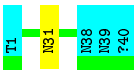
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: NOXIUSTOXIN

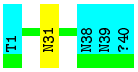
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: NOXIUSTOXIN

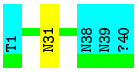
Chain A: 88% • 10%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: NOXIUSTOXIN

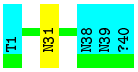
Chain A: 88% • 10%



4.2.5 Score per residue for model 5

- Molecule 1: NOXIUSTOXIN

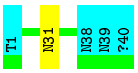
Chain A: 88% • 10%



4.2.6 Score per residue for model 6

- Molecule 1: NOXIUSTOXIN

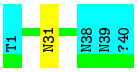
Chain A: 88% • 10%



4.2.7 Score per residue for model 7

- Molecule 1: NOXIUSTOXIN

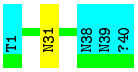
Chain A: 88% • 10%



4.2.8 Score per residue for model 8

- Molecule 1: NOXIUSTOXIN

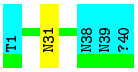
Chain A: 88% • 10%



4.2.9 Score per residue for model 9

- Molecule 1: NOXIUSTOXIN

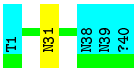
Chain A: 88% • 10%



4.2.10 Score per residue for model 10

- Molecule 1: NOXIUSTOXIN

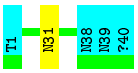
Chain A: 88% • 10%



4.2.11 Score per residue for model 11

- Molecule 1: NOXIUSTOXIN

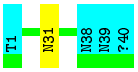
Chain A: 88% • 10%



4.2.12 Score per residue for model 12

- Molecule 1: NOXIUSTOXIN

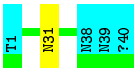
Chain A: 88% • 10%



4.2.13 Score per residue for model 13

- Molecule 1: NOXIUSTOXIN

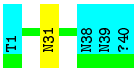
Chain A: 88% • 10%



4.2.14 Score per residue for model 14

- Molecule 1: NOXIUSTOXIN

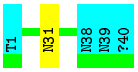
Chain A: 88% • 10%



4.2.15 Score per residue for model 15

- Molecule 1: NOXIUSTOXIN

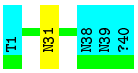
Chain A: 88% • 10%



4.2.16 Score per residue for model 16

- Molecule 1: NOXIUSTOXIN

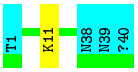
Chain A: 88% • 10%



4.2.17 Score per residue for model 17

- Molecule 1: NOXIUSTOXIN

Chain A: 88% • 10%



4.2.18 Score per residue for model 18

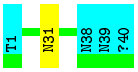
- Molecule 1: NOXIUSTOXIN

Chain A: 83% 8% 10%

4.2.19 Score per residue for model 19

- Molecule 1: NOXIUSTOXIN

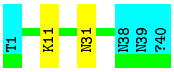
Chain A: 88% • 10%



4.2.20 Score per residue for model 20

- Molecule 1: NOXIUSTOXIN

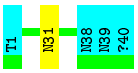
Chain A: 85% 5% 10%



4.2.21 Score per residue for model 21

- Molecule 1: NOXIUSTOXIN

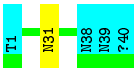
Chain A: 88% • 10%



4.2.22 Score per residue for model 22

- Molecule 1: NOXIUSTOXIN

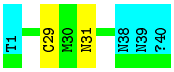
Chain A: 88% • 10%



4.2.23 Score per residue for model 23

- Molecule 1: NOXIUSTOXIN

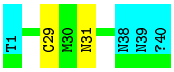
Chain A: 85% 5% 10%



4.2.24 Score per residue for model 24

- Molecule 1: NOXIUSTOXIN

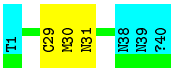
Chain A: 85% 5% 10%



4.2.25 Score per residue for model 25

- Molecule 1: NOXIUSTOXIN

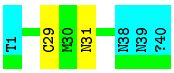
Chain A: 83% 8% 10%



4.2.26 Score per residue for model 26

- Molecule 1: NOXIUSTOXIN

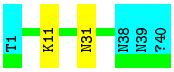
Chain A: 85% 5% 10%



4.2.27 Score per residue for model 27

- Molecule 1: NOXIUSTOXIN

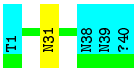
Chain A: 85% 5% 10%



4.2.28 Score per residue for model 28

- Molecule 1: NOXIUSTOXIN

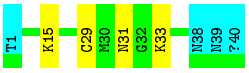
Chain A: 88% • 10%



4.2.29 Score per residue for model 29

- Molecule 1: NOXIUSTOXIN

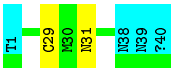
Chain A: 80% 10% 10%



4.2.30 Score per residue for model 30

- Molecule 1: NOXIUSTOXIN

Chain A: 85% 5% 10%



4.2.31 Score per residue for model 31

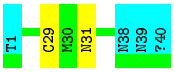
- Molecule 1: NOXIUSTOXIN

Chain A: 83% 8% 10%

4.2.32 Score per residue for model 32

- Molecule 1: NOXIUSTOXIN

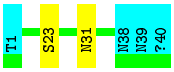
Chain A: 85% 5% 10%



4.2.33 Score per residue for model 33

- Molecule 1: NOXIUSTOXIN

Chain A: 85% 5% 10%



4.2.34 Score per residue for model 34

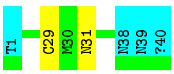
- Molecule 1: NOXIUSTOXIN

Chain A: 88% • 10%

4.2.35 Score per residue for model 35

- Molecule 1: NOXIUSTOXIN

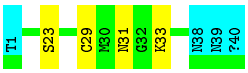
Chain A: 85% 5% 10%



4.2.36 Score per residue for model 36

- Molecule 1: NOXIUSTOXIN

Chain A: 80% 10% 10%



4.2.37 Score per residue for model 37

- Molecule 1: NOXIUSTOXIN

Chain A: 83% 8% 10%

4.2.38 Score per residue for model 38

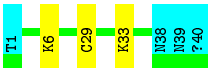
- Molecule 1: NOXIUSTOXIN

Chain A:

4.2.39 Score per residue for model 39

- Molecule 1: NOXIUSTOXIN

Chain A:



5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 39 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

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: NH2

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	0.88±0.01	0±0/267 (0.0±0.0%)	1.13±0.03	0±0/355 (0.0±0.1%)
All	All	0.88	0/10413 (0.0%)	1.13	4/13845 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	30	MET	C-N-CA	5.40	135.19	121.70	25	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	10257	10530	10530	-

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	36/40 (90%)	24±1 (67±4%)	11±1 (30±4%)	1±0 (3±1%)	9 43
All	All	1404/1560 (90%)	940 (67%)	423 (30%)	41 (3%)	9 43

All 4 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	31	ASN	37
1	A	23	SER	2
1	A	27	ALA	1
1	A	6	LYS	1

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	31/34 (91%)	30±1 (98±2%)	1±1 (2±2%)	71 95
All	All	1209/1326 (91%)	1188 (98%)	21 (2%)	71 95

All 5 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	29	CYS	12
1	A	11	LYS	4
1	A	33	LYS	3
1	A	15	LYS	1
1	A	6	LYS	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 (i)

No chemical shift data were provided