wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1HP2
Title	:	SOLUTION STRUCTURE OF A TOXIN FROM THE SCORPION TITYUS SERRULATUS (TSTX-K ALPHA) DETERMINED BY NMR.
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This is a wwPDB NMR Structure Validation Summary 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 (i)) were used in the production of this report:

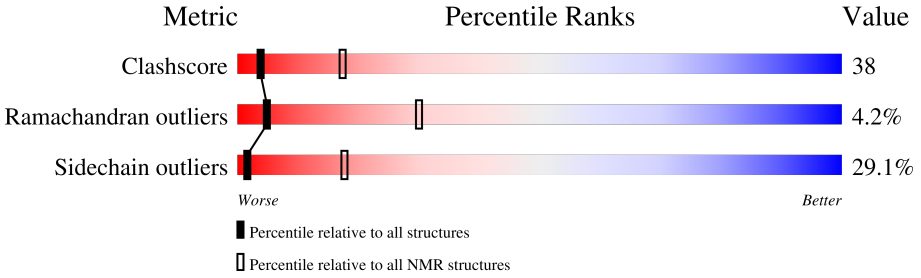
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	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	37	30% 57% 8% 5%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 25 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:3-A:37 (35)	0.38	25

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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 551 atoms, of which 281 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TITYUSTOXIN K ALPHA.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	37	551	168	281	49	46	7	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: TITYUSTOXIN K ALPHA

Chain A: 30% 57% 8% 5%

V1 F2 I3 N4 A5 K6 C7 R8 G9 S10 P11 E12 C13 L14 P15 K18 I21 G22 K23 A24 A25 G26 K27 C28 M29 N30 G31 K32 C33 K34 P37

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 25. Colouring as in section 4.1 above.

• Molecule 1: TITYUSTOXIN K ALPHA

Chain A: 22% 49% 24% 5%

V1 F2 I3 N4 A5 K6 C7 R8 G9 S10 P11 E12 C13 L14 P15 K16 C17 K18 E19 A20 I21 G22 K23 G26 K27 C28 M29 N30 G31 K32 C33 K34 C35 Y36 P37

5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 30 were deposited, based on the following criterion: *structures with acceptable covalent geometry,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
X-PLOR	refinement	3.851
X-PLOR	structure solution	3.851

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±0.0
All	All	0	30

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	8	ARG	Sidechain	30

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	252	261	261	19±5
All	All	7560	7830	7830	583

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 38.

5 of 158 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:CYS:O	1:A:21:ILE:HG22	0.91	1.62	2	8
1:A:21:ILE:HD11	1:A:37:PRO:O	0.83	1.74	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:LEU:HD12	1:A:24:ALA:HB1	0.69	1.62	2	3
1:A:21:ILE:HD13	1:A:35:CYS:HB3	0.66	1.67	11	1
1:A:10:SER:N	1:A:11:PRO:CD	0.63	2.61	24	30

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	34/37 (92%)	29±2 (85±6%)	4±1 (10±4%)	1±1 (4±4%)	5 30
All	All	1020/1110 (92%)	871 (85%)	106 (10%)	43 (4%)	5 30

5 of 8 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	6	LYS	12
1	A	10	SER	9
1	A	9	GLY	8
1	A	5	ALA	6
1	A	7	CYS	4

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	27/29 (93%)	19±2 (71±6%)	8±2 (29±6%)	1 18
All	All	810/870 (93%)	574 (71%)	236 (29%)	1 18

5 of 22 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	10	SER	30
1	A	14	LEU	19
1	A	13	CYS	17
1	A	29	MET	17
1	A	23	LYS	17

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)

No chemical shift data were provided