WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Feb 19, 2022 – 08:35 PM EST

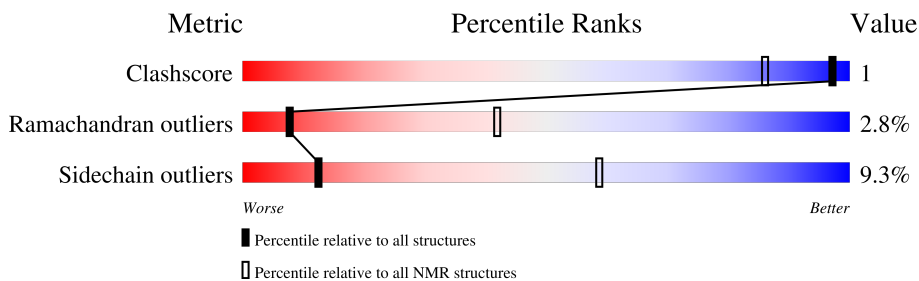|		
PDB ID	:	1TFS
Title	:	NMR AND RESTRAINED MOLECULAR DYNAMICS STUDY OF THE THREE-DIMENSIONAL SOLUTION STRUCTURE OF TOXIN FS2, A SPECIFIC BLOCKER OF THE L-TYPE CALCIUM CHANNEL, ISO-LATED FROM BLACK MAMBA VENOM
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Deposited on	:	1995-01-26

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		1
Ramachandran outliers		2.8%
Sidechain outliers		9.3%

Worse   *Better*

■ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	60	77% 10% 13%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 16 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:1-A:5, A:14-A:60 (52)	0.45	16

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 2 clusters. No single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 952 atoms, of which 467 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TOXIN FS2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	60	952	297	467	91	87	10	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	GLN	conflict	UNP P01414

4 Residue-property plots ⓘ

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.
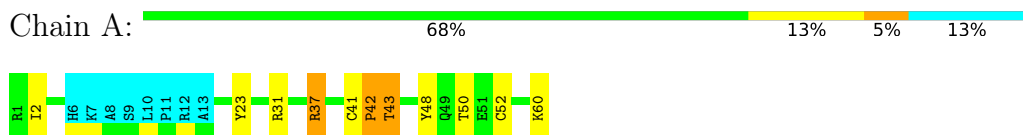
• Molecule 1: TOXIN FS2

Chain A:

77%　　　　10%　　13%

R1　H6 K7 A8 S9 L10 P11 R12 A13　Y23　R31　C41 P42 T43　T50　K60
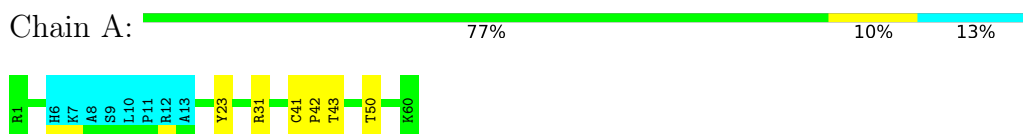
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: TOXIN FS2

Chain A:

68%　　　　13%　5%　13%

R1 I2　H6 K7 A8 S9 L10 P11 R12 A13　Y23　R31　R37　C41 P42 T43　Y48 Q49 T50 E51 C52　K60

4.2.2 Score per residue for model 2

• Molecule 1: TOXIN FS2

Chain A:

73%　　　　13%　　13%

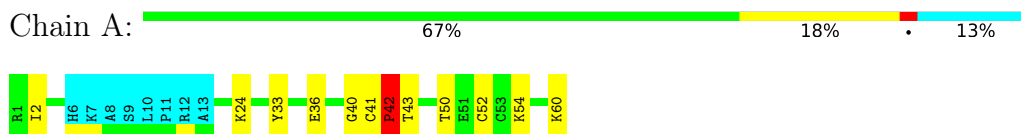R1　Y4 S5 H6 K7 A8 S9 L10 P11 R12 A13　T21　C41 P42 T43　T50　D56 R57 C58 N59 K60
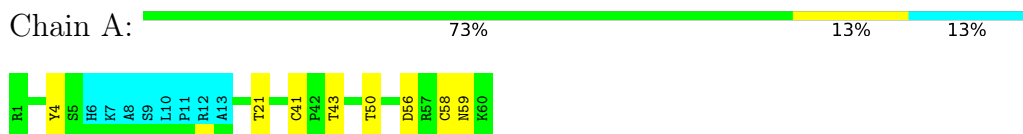
4.2.3 Score per residue for model 3

• Molecule 1: TOXIN FS2

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: TOXIN FS2

Chain A:
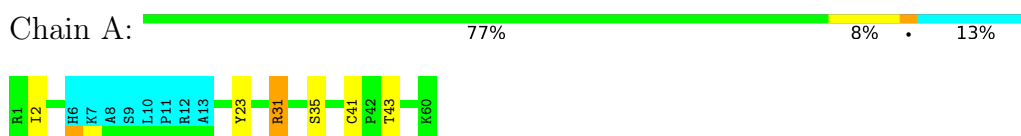
4.2.5 Score per residue for model 5

• Molecule 1: TOXIN FS2

Chain A:
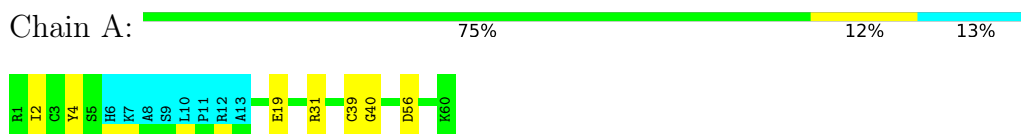
4.2.6 Score per residue for model 6

• Molecule 1: TOXIN FS2

Chain A:
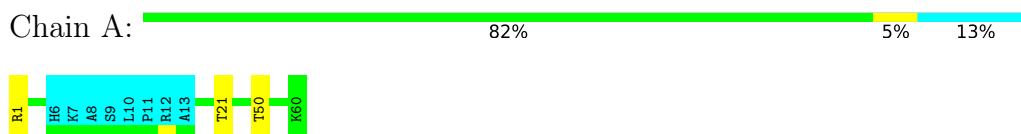
4.2.7 Score per residue for model 7

• Molecule 1: TOXIN FS2

Chain A:
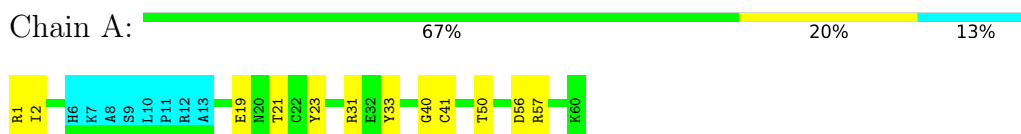
4.2.8 Score per residue for model 8

• Molecule 1: TOXIN FS2

Chain A:
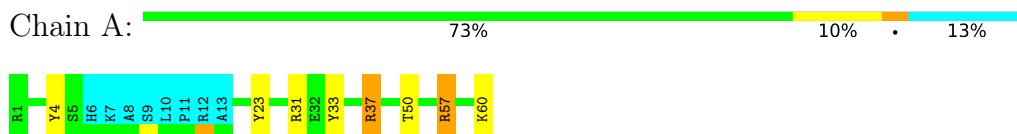
4.2.9 Score per residue for model 9

• Molecule 1: TOXIN FS2

Chain A:
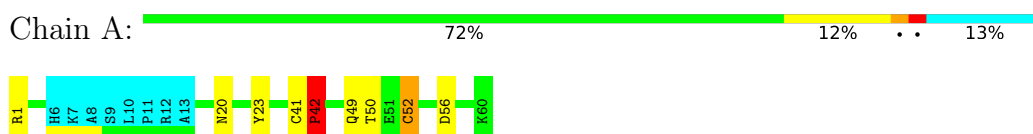
4.2.10 Score per residue for model 10

• Molecule 1: TOXIN FS2

Chain A:
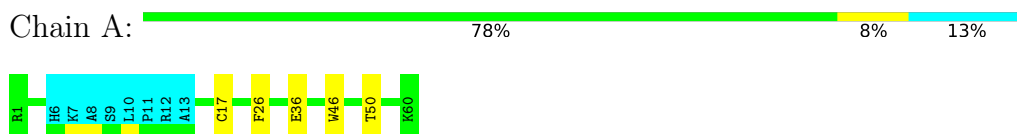
4.2.11 Score per residue for model 11

• Molecule 1: TOXIN FS2

Chain A:
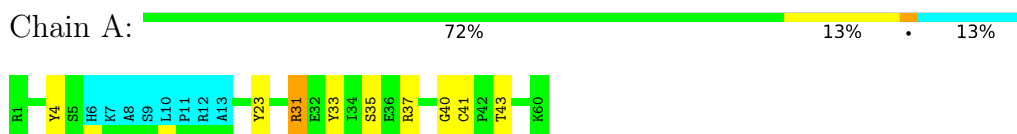
4.2.12 Score per residue for model 12

• Molecule 1: TOXIN FS2

Chain A:
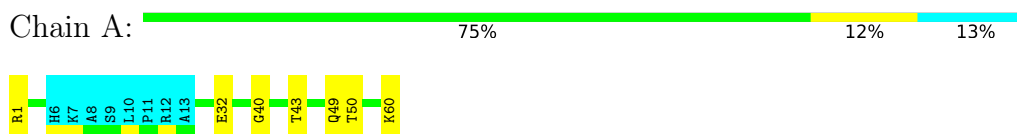
4.2.13 Score per residue for model 13

• Molecule 1: TOXIN FS2

Chain A:
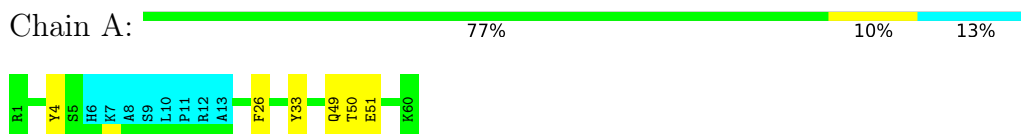
4.2.14 Score per residue for model 14

• Molecule 1: TOXIN FS2

Chain A:
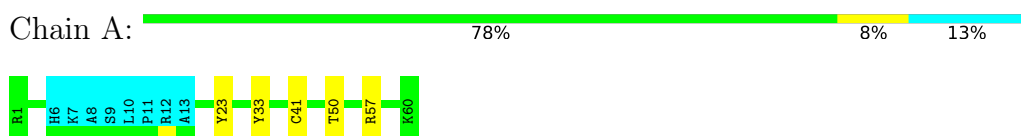
4.2.15 Score per residue for model 15

• Molecule 1: TOXIN FS2

Chain A:
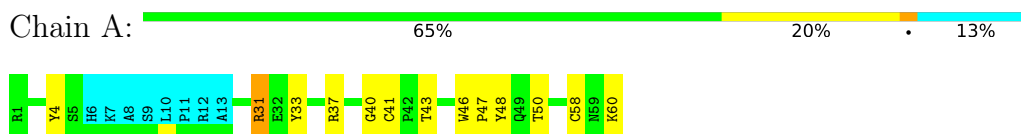
4.2.16 Score per residue for model 16 (medoid)

• Molecule 1: TOXIN FS2

Chain A:
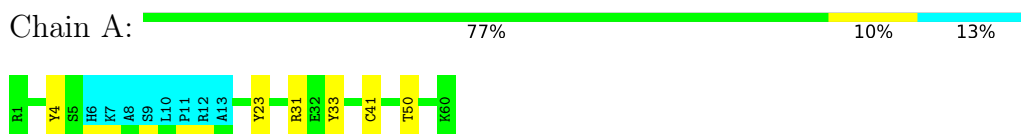
4.2.17 Score per residue for model 17

• Molecule 1: TOXIN FS2

Chain A:
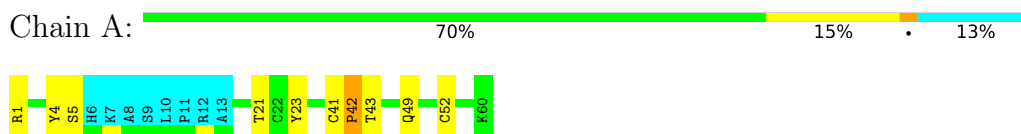
4.2.18 Score per residue for model 18

• Molecule 1: TOXIN FS2

Chain A:
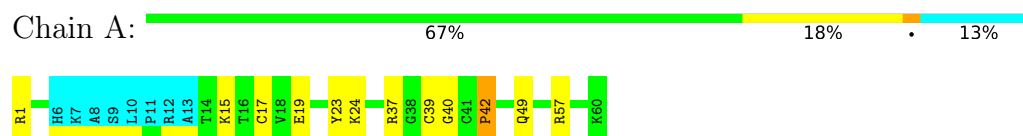
4.2.19 Score per residue for model 19

• Molecule 1: TOXIN FS2

Chain A:
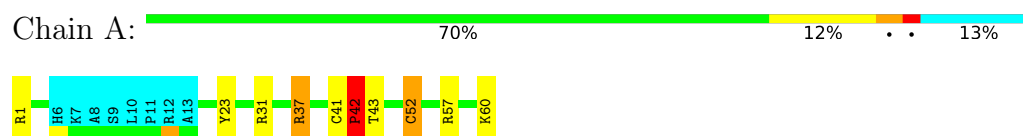
4.2.20 Score per residue for model 20

• Molecule 1: TOXIN FS2

Chain A:
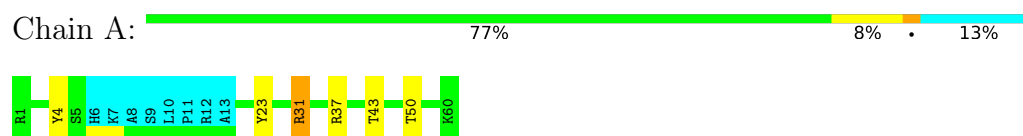
5   Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
Discover	refinement	

No chemical shift data was provided.

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	0.61±0.01	0±0/433 (0.0± 0.0%)	1.07±0.07	1±1/579 (0.2± 0.1%)
All	All	0.61	0/8660 (0.0%)	1.08	21/11580 (0.2%)

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	1.8±1.3
All	All	0	36

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Total
1	A	42	PRO	CA-N-CD	-7.87	100.48	111.50	3	1
1	A	41	CYS	CA-CB-SG	7.86	128.15	114.00	19	4
1	A	37	ARG	NE-CZ-NH2	-6.63	116.98	120.30	8	3
1	A	37	ARG	NE-CZ-NH1	6.58	123.59	120.30	19	3
1	A	31	ARG	NE-CZ-NH2	-6.50	117.05	120.30	11	3
1	A	1	ARG	NE-CZ-NH2	-5.93	117.33	120.30	6	3
1	A	4	TYR	CB-CG-CD2	-5.27	117.84	121.00	16	2
1	A	1	ARG	NE-CZ-NH1	5.23	122.92	120.30	6	1
1	A	31	ARG	NE-CZ-NH1	5.11	122.86	120.30	5	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	23	TYR	Sidechain	12
1	A	33	TYR	Sidechain	8
1	A	4	TYR	Sidechain	7
1	A	31	ARG	Sidechain	3
1	A	37	ARG	Sidechain	3
1	A	48	TYR	Sidechain	2
1	A	1	ARG	Sidechain	1

6.2 Too-close contacts ⓘ

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	424	401	401	0±1
All	All	8480	8020	8020	10

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:42:PRO:HD2	1:A:52:CYS:SG	0.47	2.50	9	4
1:A:42:PRO:CD	1:A:52:CYS:SG	0.45	3.04	19	4
1:A:46:TRP:CD1	1:A:47:PRO:HA	0.42	2.50	15	1
1:A:58:CYS:SG	1:A:59:ASN:N	0.42	2.92	2	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	50/60 (83%)	43±2 (86±4%)	6±2 (12±3%)	1±1 (3±2%)	8	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1000/1200 (83%)	855 (86%)	117 (12%)	28 (3%)	8 42

All 7 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	41	CYS	8
1	A	40	GLY	7
1	A	42	PRO	6
1	A	57	ARG	3
1	A	43	THR	2
1	A	19	GLU	1
1	A	56	ASP	1

6.3.2   Protein sidechains ⓘ

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	48/54 (89%)	44±2 (91±4%)	4±2 (9±4%)	12 59
All	All	960/1080 (89%)	871 (91%)	89 (9%)	12 59

All 28 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	50	THR	14
1	A	43	THR	9
1	A	31	ARG	7
1	A	60	LYS	6
1	A	2	ILE	5
1	A	49	GLN	5
1	A	21	THR	4
1	A	42	PRO	4
1	A	56	ASP	3
1	A	1	ARG	3
1	A	57	ARG	3
1	A	37	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	24	LYS	2
1	A	36	GLU	2
1	A	35	SER	2
1	A	19	GLU	2
1	A	39	CYS	2
1	A	52	CYS	2
1	A	17	CYS	2
1	A	26	PHE	2
1	A	54	LYS	1
1	A	20	ASN	1
1	A	46	TRP	1
1	A	32	GLU	1
1	A	51	GLU	1
1	A	58	CYS	1
1	A	5	SER	1
1	A	15	LYS	1

6.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6   Ligand geometry ⓘ

There are no ligands in this entry.

6.7   Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

No chemical shift data were provided