

Full wwPDB NMR Structure Validation Report (i)

Feb 10, 2022 – 10:41 AM EST

PDB ID : 1EYO

Title : SOLUTION STRUCTURE OF CONOTOXIN TVIIA FROM CONUS

TULIPA

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Deposited on : 2000-05-07

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
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:

Mol Probity : 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 : 2.26

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

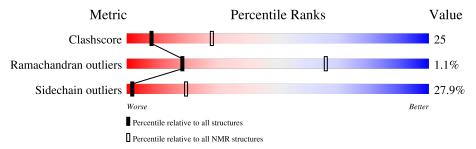
Validation Pipeline (wwPDB-VP) : 2.26

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 $(\# \mathrm{Entries})$	$rac{ m NMR~archive}{ m (\#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	30	30%	33%	10%	27%		



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: fewest violations, lowest energy.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues								
Well-defined core	Well-defined core Residue range (total) Backbone RMSD (Å) Medoid model							
1 A:2-A:9, A:12-A:25 (22) 0.06 12								

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 422 atoms, of which 206 are hydrogens and 0 are deuteriums.

 \bullet Molecule 1 is a protein called CONOTOXIN TVIIA.

Mol	Chain	Residues	Atoms					Trace	
1	Λ	20	Total	С	Н	N	О	S	0
1	A	30	422	125	206	40	43	8	

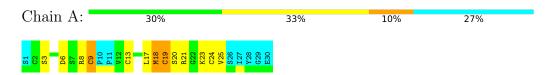


4 Residue-property plots (i)

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.



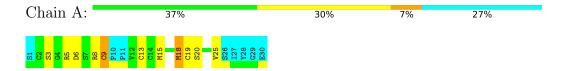


4.2 Scores per residue for each member of the ensemble

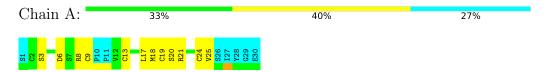
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CONOTOXIN TVIIA



4.2.2 Score per residue for model 2





4.2.3 Score per residue for model 3

• Molecule 1: CONOTOXIN TVIIA



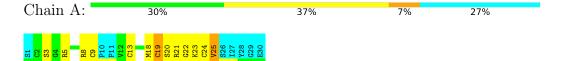
4.2.4 Score per residue for model 4

• Molecule 1: CONOTOXIN TVIIA



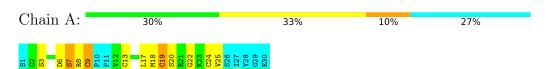
4.2.5 Score per residue for model 5

• Molecule 1: CONOTOXIN TVIIA

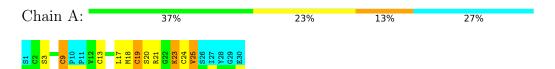


4.2.6 Score per residue for model 6

• Molecule 1: CONOTOXIN TVIIA



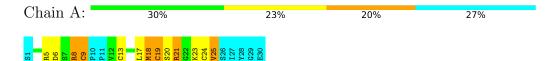
4.2.7 Score per residue for model 7





4.2.8 Score per residue for model 8

• Molecule 1: CONOTOXIN TVIIA



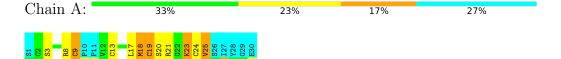
4.2.9 Score per residue for model 9

• Molecule 1: CONOTOXIN TVIIA



4.2.10 Score per residue for model 10

• Molecule 1: CONOTOXIN TVIIA



4.2.11 Score per residue for model 11

• Molecule 1: CONOTOXIN TVIIA



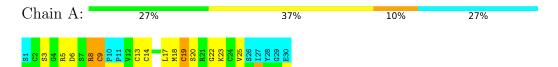
4.2.12 Score per residue for model 12 (medoid)





4.2.13 Score per residue for model 13

• Molecule 1: CONOTOXIN TVIIA



4.2.14 Score per residue for model 14

• Molecule 1: CONOTOXIN TVIIA



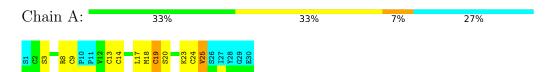
4.2.15 Score per residue for model 15

• Molecule 1: CONOTOXIN TVIIA



4.2.16 Score per residue for model 16

• Molecule 1: CONOTOXIN TVIIA



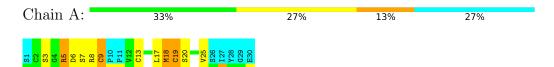
4.2.17 Score per residue for model 17





4.2.18 Score per residue for model 18

• Molecule 1: CONOTOXIN TVIIA



4.2.19 Score per residue for model 19

• Molecule 1: CONOTOXIN TVIIA



4.2.20 Score per residue for model 20





Refinement protocol and experimental data overview (i) 5



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

Of the 50 calculated structures, 20 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	
X-PLOR	refinement	3.1	

No chemical shift data was provided.



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: HYP

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	Sond lengths	I	Bond angles
MIOI	RMSZ		#Z>5	RMSZ	#Z>5
1	A	1.17 ± 0.02	$0\pm0/153~(~0.0\pm~0.0\%)$	1.35 ± 0.04	$1\pm1/199~(~0.6\pm~0.5\%)$
All	All	1.17	0/3060 (0.0%)	1.35	22/3980 (0.6%)

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	${f Chain} oxed{f Res} {f Type} oxed{f Atoms} oxed{f Z} oxed{f Observed} {f (}^o{f)}$		$Ideal(^{o})$	Mod	dels					
MIOI	Chain	nes	Туре	Atoms		$oxed{\mathbf{Z} \operatorname{Observed}(^o)}$		Z Observed(*)		Worst	Total
1	A	5	ARG	NE-CZ-NH2	-8.78	115.91	120.30	11	9		
1	A	8	ARG	NE-CZ-NH2	-6.38	117.11	120.30	5	8		
1	A	21	ARG	NE-CZ-NH2	-5.37	117.62	120.30	8	5		

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
1	A	154	151	151	8±1
All	All	3080	3020	3020	150

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 25.



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

Atom-1	Atom-2	Clash(Å)	$Distance(\mathring{A})$	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:9:CYS:SG	1:A:13:CYS:SG	0.90	2.69	17	20
1:A:9:CYS:CB	1:A:13:CYS:SG	0.72	2.77	4	20
1:A:9:CYS:HB3	1:A:13:CYS:SG	0.64	2.33	4	20
1:A:13:CYS:SG	1:A:18:MET:O	0.60	2.60	1	20
1:A:20:SER:OG	1:A:25:VAL:HG21	0.58	1.98	11	20
1:A:3:SER:OG	1:A:24:CYS:SG	0.54	2.66	4	2
1:A:19:CYS:SG	1:A:23:LYS:N	0.53	2.80	5	12
1:A:17:LEU:HD22	1:A:24:CYS:HB3	0.48	1.86	14	14
1:A:17:LEU:HD23	1:A:25:VAL:C	0.45	2.32	11	3
1:A:9:CYS:O	1:A:19:CYS:SG	0.45	2.74	5	9
1:A:9:CYS:SG	1:A:24:CYS:SG	0.44	3.16	19	2
1:A:19:CYS:SG	1:A:22:GLY:CA	0.43	3.06	5	2
1:A:3:SER:O	1:A:24:CYS:SG	0.43	2.77	19	2
1:A:14:CYS:HB2	1:A:17:LEU:HD12	0.42	1.90	13	2
1:A:7:SER:O	1:A:9:CYS:SG	0.42	2.77	6	1
1:A:5:ARG:HG3	1:A:17:LEU:HD21	0.42	1.91	18	1

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	entiles
1	A	22/30 (73%)	18±1 (82±4%)	4±1 (17±4%)	0±0 (1±2%)	18	66
All	All	440/600 (73%)	359 (82%)	76 (17%)	5 (1%)	18	66

All 2 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	22	GLY	4
1	A	2	CYS	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	19/24 (79%)	14±1 (72±7%)	5±1 (28±7%)	2 19
All	All	380/480 (79%)	274 (72%)	106 (28%)	2 19

All 11 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	19	CYS	20
1	A	9	CYS	16
1	A	3	SER	14
1	A	8	ARG	13
1	A	6	ASP	12
1	A	18	MET	10
1	A	25	VAL	9
1	A	21	ARG	6
1	A	15	MET	2
1	A	7	SER	2
1	A	23	LYS	2

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.

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.



Mal	Tuno	Chain	Peg	Tiple	Bond lengths Counts RMSZ #Z>2			
MIOI	туре	Chain	nes	Lilik	Counts	RMSZ	#Z>2	
1	HYP	A	11	1	6,8,9	0.94 ± 0.01	0±0 (7±8%)	
1	HYP	A	10	1	6,8,9	1.33 ± 0.03	1±0 (16±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.

Mal	Tuno	Chain	Dec	Tiple	$\begin{array}{c c} \textbf{Bond angles} \\ \textbf{Counts} & \textbf{RMSZ} & \#\textbf{Z}{>}2 \end{array}$			
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	#Z>2	
1	HYP	A	11	1	5,10,12	2.41 ± 0.01	$2\pm0 \ (40\pm0\%)$	
1	HYP	A	10	1	5,10,12	2.46 ± 0.03	4±0 (71±9%)	

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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	A	11	1	-	$0\pm0,0,11,13$	$0\pm0,1,1,1$
1	HYP	A	10	1	-	$0\pm0,0,11,13$	$0\pm0,1,1,1$

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

Mol Chain		hain Res		Atoms	\mathbf{z}	$\operatorname{Observed}(\mathring{\mathrm{A}})$	Ideal(Å)	Models	
MIOI	Chain	nes	Type	Atoms		Observed(A)	Ideal(A)	Worst	Total
1	A	10	HYP	CB-CG	2.77	1.57	1.52	17	20
1	A	11	HYP	CB-CG	2.08	1.56	1.52	17	9

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

Mol Chain		ain Res		Atoms	7	$Observed(^o)$	$Ideal(^{o})$	Models	
IVIOI	Chain	nes	Type	Atoms	Z Observed(*)		ideai()	Worst	Total
1	A	11	HYP	CB-CG-CD	4.27	108.49	103.27	5	20
1	A	10	HYP	CB-CG-CD	3.95	108.10	103.27	19	20
1	A	10	HYP	O-C-CA	2.60	117.97	124.78	5	20

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Mal	Mol Chain		Trens	zno Atoma		$Observed(^o)$	$Ideal(^{o})$	Models	
MIOI	Chain	nes	Type	Atoms		Observed(*)	ideai()	Worst	Total
1	A	11	HYP	OD1-CG-CD	2.55	104.78	110.35	7	20
1	A	10	HYP	OD1-CG-CD	2.25	105.42	110.35	11	20
1	A	10	HYP	OD1-CG-CB	2.22	104.55	110.03	6	11

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)

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

