



Full wwPDB NMR Structure Validation Report ⓘ

Nov 23, 2017 – 05:57 AM EST

PDB ID : 2SH1
Title : SOLUTION STRUCTURE OF NEUROTOXIN I FROM THE SEA ANEMONE STICHODACTYLA HELIANTHUS. A NUCLEAR MAGNETIC RESONANCE, DISTANCE GEOMETRY AND RESTRAINED MOLECULAR DYNAMICS STUDY
Authors : Fogh, R.H.; Norton, R.S.
Deposited on : unknown

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20030345
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

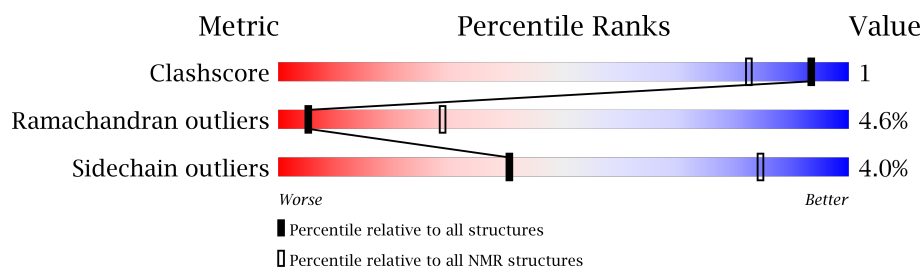
1 Overall quality at a glance

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	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	48	

2 Ensemble composition and analysis

This entry contains 8 models. Model 1 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:6, A:17-A:46 (36)	0.63	1

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	1, 4, 5, 6, 8
2	2, 3, 7

3 Entry composition [i](#)

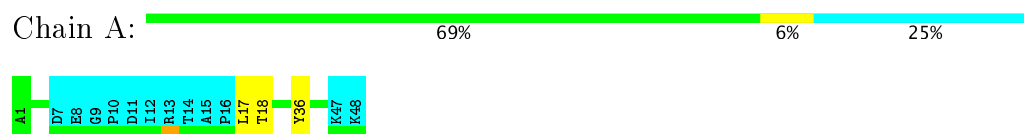
There is only 1 type of molecule in this entry. The entry contains 439 atoms, of which 84 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NEUROTOXIN I.

Mol	Chain	Residues	Atoms						Trace
1	A	48	Total	C	H	N	O	S	0
			439	216	84	61	72	6	

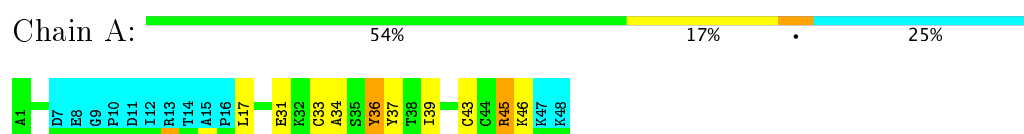
4.2.3 Score per residue for model 3

- Molecule 1: NEUROTOXIN I



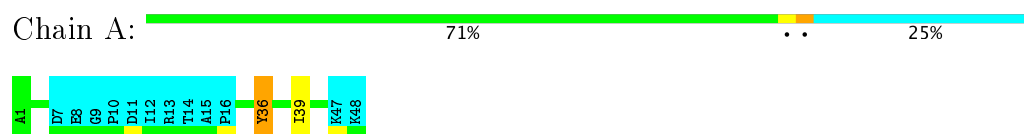
4.2.4 Score per residue for model 4

- Molecule 1: NEUROTOXIN I



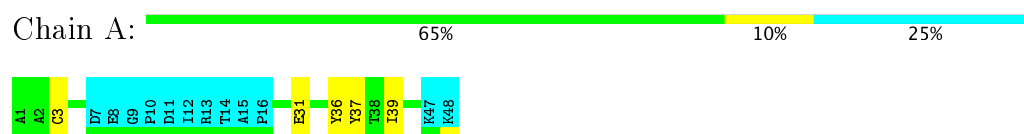
4.2.5 Score per residue for model 5

- Molecule 1: NEUROTOXIN I



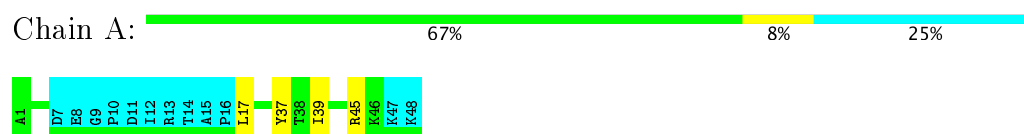
4.2.6 Score per residue for model 6

- Molecule 1: NEUROTOXIN I



4.2.7 Score per residue for model 7

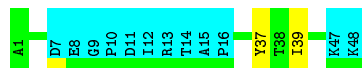
- Molecule 1: NEUROTOXIN I



4.2.8 Score per residue for model 8

- Molecule 1: NEUROTOXIN I

Chain A:  71% 25%



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 8 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DISMAN	refinement	
DISGEO	refinement	
GROMOS-87	refinement	

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

6.1 Standard geometry

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±0.02	0±0/266 (0.0±0.0%)	1.24±0.03	1±1/360 (0.3±0.2%)
All	All	0.60	0/2128 (0.0%)	1.24	8/2880 (0.3%)

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±0.5
All	All	0	8

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	45	ARG	NE-CZ-NH1	6.25	123.42	120.30	4	3
1	A	37	TYR	CB-CG-CD2	-5.68	117.59	121.00	1	2
1	A	36	TYR	CB-CG-CD2	-5.47	117.72	121.00	4	3

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	36	TYR	Sidechain	4
1	A	37	TYR	Sidechain	4

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	262	62	248	1±1
All	All	2096	496	1984	6

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	Total
1:A:30:TRP:HB3	1:A:44:CYS:SG	0.54	2.42	2	1
1:A:34:ALA:HB3	1:A:43:CYS:HB3	0.51	1.83	4	2
1:A:39:ILE:HG23	1:A:40:ILE:H	0.46	1.68	1	1
1:A:45:ARG:CZ	1:A:46:LYS:H	0.45	2.24	4	1
1:A:34:ALA:HB3	1:A:43:CYS:HB2	0.40	1.92	1	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	Percentiles	
1	A	35/48 (73%)	27±1 (78±4%)	6±1 (17±4%)	2±1 (5±2%)	5	29
All	All	280/384 (73%)	219 (78%)	48 (17%)	13 (5%)	5	29

All 5 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	39	ILE	6
1	A	17	LEU	3
1	A	18	THR	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	32	LYS	1
1	A	24	GLY	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	28/38 (74%)	27±1 (96±5%)	1±1 (4±5%)	40	84
All	All	224/304 (74%)	215 (96%)	9 (4%)	40	84

All 6 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	37	TYR	3
1	A	31	GLU	2
1	A	3	CYS	1
1	A	17	LEU	1
1	A	45	ARG	1
1	A	33	CYS	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 carbohydrates 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