wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1HAJ
Title	:	A beta-Hairpin Structure in a 13-mer Peptide that Binds a-Bungarotoxin with High Affinity and Neutralizes its Toxicity
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Deposited on	:	2001-04-05

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
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:

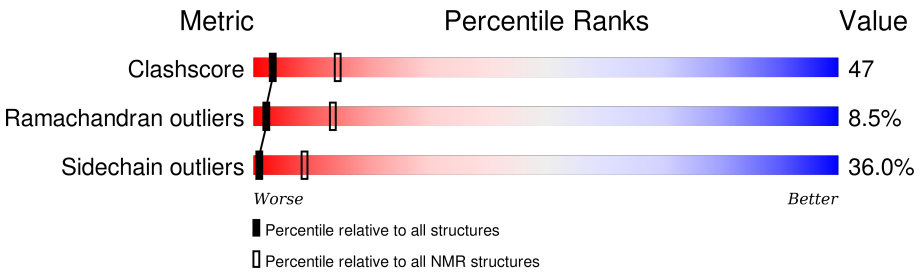
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	74	18% 51% 15% • 15%
2	B	13	31% 54% 15%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:48, A:56-A:70, B:75-B:87 (76)	0.40	10

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 1 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 7, 8, 10
Single-model clusters	2; 3; 6; 9

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1310 atoms, of which 637 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ALPHA-BUNGAROTOXIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	74	1085	338	534	97	105	11	0

- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	13	225	80	103	17	25	0

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: ALPHA-BUNGAROTOXIN

Chain A: 18% 51% 15% • 15%

I1 V2 C3 H4 T5 T6 A7 T8 S9 P10 I11 V14 T15 C16 P17 P18 G19 E20 N21 L22 C23 Y24 R25 K26 M27 W28 C29 D30 A31 F32 C33 S34 S35 R36 G37 K38 V39 V40 E41 L42 G43 A46 T47 C48 P49 S50 K51 K52 P53 Y54 E55 E56 V57 T58 C59 C60 S61 T62

D63 K64 C65 N66 P67 H68 P69 K70 Q71 R72 P73 G74

- Molecule 2: PEPTIDE

Chain B: 31% 54% 15%

W75 R76 Y77 Y78 E79 S80 S81 L82 E83 P84 Y85 P86 D87

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

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: ALPHA-BUNGAROTOXIN

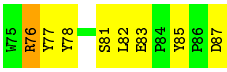
Chain A: 20% 42% 19% • 15%

I1 V2 C3 H4 T5 T6 A7 T8 S9 P10 I11 V14 T15 G19 E20 N21 L22 C23 Y24 R25 K26 M27 W28 C29 D30 A31 F32 C33 S34 S35 R36 G37 K38 V39 V40 E41 L42 G43 A46 T47 C48 P49 S50 K51 K52 P53 Y54 E55 E56 V57 T58 C59 C60 S61 T62 D63 K64

C65 N66 P67 H68 P69 K70 Q71 R72 P73 G74

- Molecule 2: PEPTIDE

Chain B: 38% 54% 8%


W75
R76
Y77
Y78
S81
L82
E83
F84
Y85
F86
D87

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DISTANCE GEOMETRY, DYNAMICAL SIMULATED ANNEALING*.

Of the ? calculated structures, 10 were deposited, based on the following criterion: *NO RESTRAINT VIOLATION*.

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

Software name	Classification	Version
CNS	refinement	0.9
XWINNMR	structure solution	
AURELIA	structure solution	
CNS	structure solution	

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)

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

There are no bond-length outliers.

There are no bond-angle outliers.

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	460	443	441	49±8
2	B	122	103	100	9±4
All	All	5820	5460	5410	530

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 47.

5 of 223 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ASP:O	1:A:32:PHE:N	0.97	1.97	7	10
1:A:6:THR:HG23	1:A:42:LEU:HD23	0.97	1.35	3	1
1:A:30:ASP:HB3	1:A:39:VAL:HG23	0.92	1.37	3	1
1:A:30:ASP:HB3	2:B:78:TYR:CD2	0.90	2.01	9	1
1:A:40:VAL:HG11	1:A:68:HIS:CD2	0.89	2.02	3	8

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	62/74 (84%)	47±2 (75±2%)	9±1 (15±2%)	6±2 (10±3%)	2 11
2	B	11/13 (85%)	11±1 (95±5%)	0±0 (4±4%)	0±0 (1±3%)	26 73
All	All	730/870 (84%)	573 (78%)	95 (13%)	62 (8%)	2 13

5 of 14 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	ALA	10
1	A	32	PHE	10
1	A	33	CYS	9
1	A	36	ARG	8
1	A	19	GLY	5

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	55/65 (85%)	35±3 (64±6%)	20±3 (36±6%)	1 9
2	B	13/13 (100%)	8±1 (62±9%)	5±1 (38±9%)	1 7
All	All	680/780 (87%)	435 (64%)	245 (36%)	1 9

5 of 48 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)
2	B	81	SER	10
1	A	5	THR	10
1	A	32	PHE	10
1	A	8	THR	10
1	A	9	SER	10

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