



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1IDH  
Title : THE NMR SOLUTION STRUCTURE OF THE COMPLEX FORMED BETWEEN ALPHA-BUNGAROTOXIN AND AN 18MER COGNATE PEPTIDE  
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We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

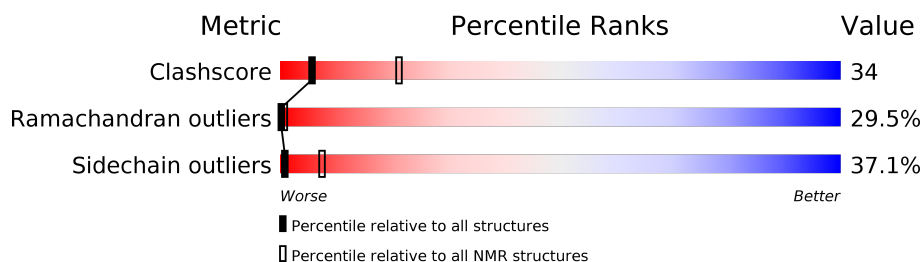
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 33%.

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  $\geq 3$ , 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	74	 . 59% 14% 24%
2	B	19	 26% 11% 58% 5%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 8 as representative, based on the following criterion: *it is the lowest potential energy structure of the ensemble*.

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:8, A:17-A:38, A:43-A:54, A:58-A:71, B:192-B:198 (63)	1.59	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 6 clusters and 3 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1394 atoms, of which 678 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ALPHA-BUNGAROTOXIN.

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

- Molecule 2 is a protein called ACETYLCHOLINE RECEPTOR PROTEIN, ALPHA CHAIN.

Mol	Chain	Residues	Atoms						Trace
2	B	18	Total	C	H	N	O	S	0
			309	111	144	26	26	2	

There is a discrepancy between the modelled and reference sequences:

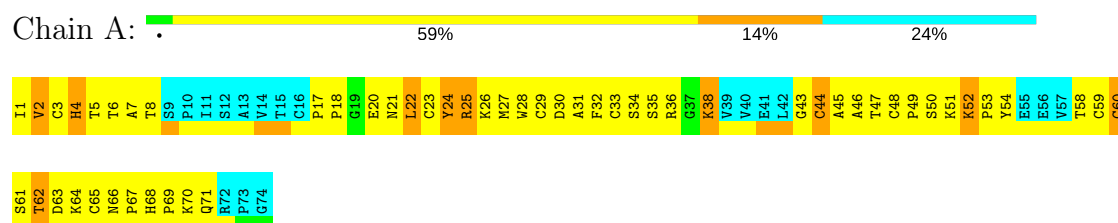
Chain	Residue	Modelled	Actual	Comment	Reference
B	199	HSL	-	cloning artifact	UNP P02710

## 4 Residue-property plots [i](#)

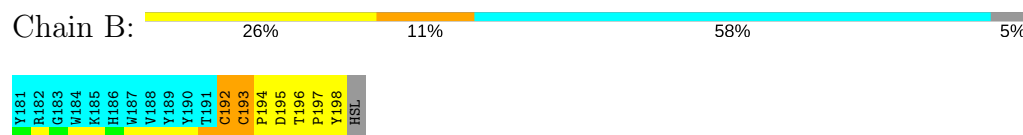
### 4.1 Average score per residue in the NMR ensemble

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



#### • Molecule 2: ACETYLCHOLINE RECEPTOR PROTEIN, ALPHA CHAIN



Y181	R182	G183	W184	K185	H186	W187	Y188	Y189	Y190	T191	C192	C193	P194	D195	T196	P197	Y198	HSL
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## 5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *The submitted conformer models are the 20 structures with the lowest energy from 120 acceptable structures which were from 300 total calculated structures and had no restraint violations. The best representative conformer is the lowest potential energy structure of the ensemble..*

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

Software name	Classification	Version
CNSsolve	refinement	1.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 5025
Number of chemical shift lists	2
Total number of shifts	370
Number of shifts mapped to atoms	370
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	33%

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	420	402	400	26±6
2	B	53	42	42	6±1
All	All	9460	8880	8840	618

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 34.

5 of 370 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:HD12	1:A:48:CYS:CB	0.86	2.00	9	1
1:A:22:LEU:HD23	1:A:61:SER:CB	0.84	2.03	1	1
1:A:46:ALA:O	1:A:47:THR:HG22	0.80	1.76	20	1
1:A:24:TYR:CD1	1:A:45:ALA:HB2	0.79	2.12	10	5
1:A:1:ILE:HG22	1:A:22:LEU:HD11	0.79	1.54	19	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	55/74 (74%)	20±3 (36±5%)	19±3 (35±6%)	16±3 (30±6%)	0	1
2	B	6/19 (32%)	1±1 (23±14%)	3±1 (48±18%)	2±1 (29±13%)	0	1
All	All	1220/1860 (66%)	421 (35%)	439 (36%)	360 (30%)	0	1

5 of 58 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	44	CYS	15
1	A	43	GLY	13
1	A	53	PRO	12
1	A	62	THR	12
1	A	24	TYR	10

### 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	49/65 (75%)	31±2 (63±4%)	18±2 (37±4%)	1	7
2	B	7/17 (41%)	5±1 (64±10%)	3±1 (36±10%)	1	9
All	All	1120/1640 (68%)	705 (63%)	415 (37%)	1	7

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	193	CYS	20
1	A	54	TYR	20
1	A	38	LYS	20
2	B	192	CYS	20
1	A	52	LYS	16

### 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

The completeness of assignment taking into account all chemical shift lists is 33% for the well-defined parts and 33% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5025

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	298
Number of shifts mapped to atoms	298
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 30%, i.e. 217 atoms were assigned a chemical shift out of a possible 723. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	102/299 (34%)	102/118 (86%)	0/126 (0%)	0/55 (0%)
Sidechain	109/363 (30%)	109/222 (49%)	0/126 (0%)	0/15 (0%)
Aromatic	6/61 (10%)	6/31 (19%)	0/25 (0%)	0/5 (0%)
Overall	217/723 (30%)	217/371 (58%)	0/277 (0%)	0/75 (0%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

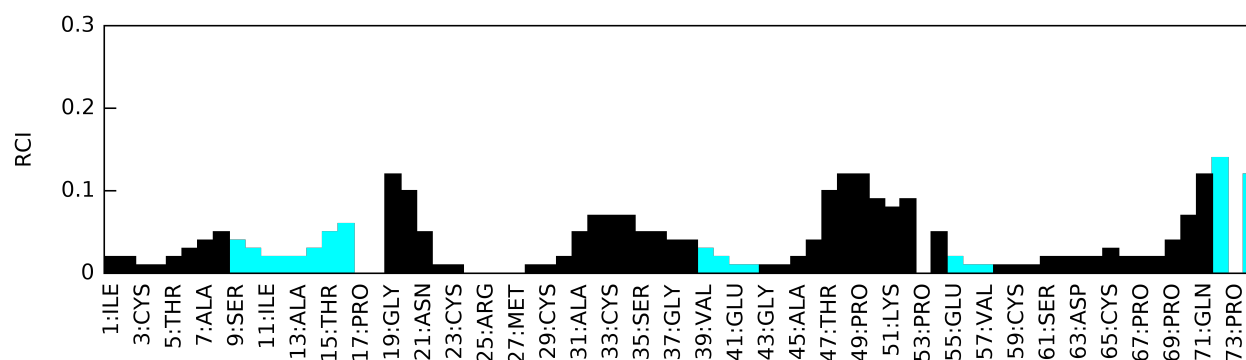
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	39	VAL	HB	0.22	3.59 – 0.39	-5.5

### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



## 7.2 Chemical shift list 2

File name: BMRB entry 5025

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.2.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	72
Number of shifts mapped to atoms	72
Number of unparsed shifts	0
Number of shifts with mapping errors	0

Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

### 7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

### 7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 24 atoms were assigned a chemical shift out of a possible 723. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	15/299 (5%)	10/118 (8%)	0/126 (0%)	5/55 (9%)
Sidechain	9/363 (2%)	9/222 (4%)	0/126 (0%)	0/15 (0%)
Aromatic	0/61 (0%)	0/31 (0%)	0/25 (0%)	0/5 (0%)
Overall	24/723 (3%)	19/371 (5%)	0/277 (0%)	5/75 (7%)

### 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:

