Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1IDG
Title	:	THE NMR SOLUTION STRUCTURE OF THE COMPLEX FORMED BETWEEN ALPHA-BUNGAROTOXIN AND AN 18MER COGNATE PEPTIDE
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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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

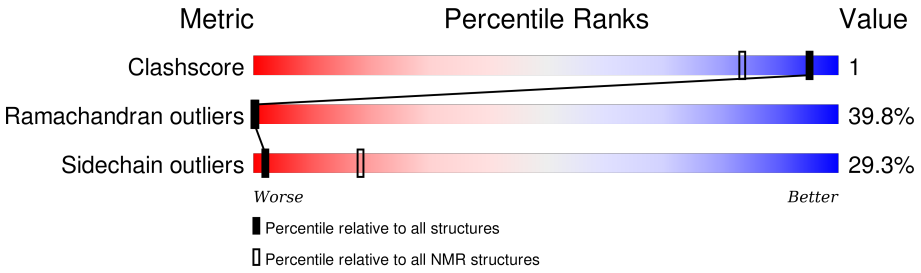
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	38% 32% 20% 9%
2	B	19	5% 26% 47% 16% 5%

2 Ensemble composition and analysis

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

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:

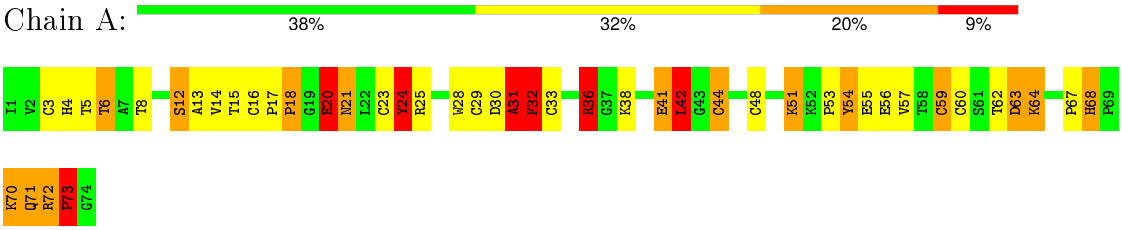
Chain	Residue	Modelled	Actual	Comment	Reference
B	199	HSL	-	cloning artifact	UNP P02710

4 Residue-property plots (i)

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:



- Molecule 2: ACETYLCHOLINE RECEPTOR PROTEIN, ALPHA CHAIN

Chain B:

5 Refinement protocol and experimental data overview

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

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
CNSsolve	refinement	1.0

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	1.31	3/565 (0.5%)	2.61	27/767 (3.5%)
2	B	1.26	0/175 (0.0%)	2.45	17/241 (7.1%)
All	All	1.30	3/740 (0.4%)	2.57	44/1008 (4.4%)

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	2	25
2	B	1	10
All	All	3	35

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	ARG	C-N	7.73	1.49	1.34
1	A	20	GLU	CA-C	5.77	1.68	1.52
1	A	72	ARG	CA-C	5.71	1.67	1.52

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	20	GLU	N-CA-C	-23.39	47.85	111.00
1	A	73	PRO	N-CA-C	-23.31	51.50	112.10
1	A	72	ARG	N-CA-C	-22.62	49.92	111.00
1	A	32	PHE	N-CA-C	-21.36	53.34	111.00
1	A	73	PRO	CA-N-CD	-16.37	88.58	111.50
1	A	73	PRO	N-CA-CB	14.97	121.27	103.30
1	A	73	PRO	N-CD-CG	9.55	117.53	103.20
1	A	72	ARG	N-CA-CB	9.19	127.14	110.60
1	A	32	PHE	CB-CA-C	8.26	126.91	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	20	GLU	CA-C-N	-8.19	99.17	117.20
1	A	25	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	36	ARG	NE-CZ-NH1	7.86	124.23	120.30
2	B	184	TRP	N-CA-CB	7.86	124.74	110.60
2	B	182	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	B	196	THR	CA-CB-CG2	7.59	123.03	112.40
1	A	32	PHE	CA-C-O	-7.51	104.33	120.10
2	B	188	VAL	CA-CB-CG2	7.40	122.00	110.90
1	A	73	PRO	O-C-N	-7.05	111.22	123.20
2	B	188	VAL	O-C-N	-6.94	111.59	122.70
2	B	187	TRP	CA-C-N	6.94	132.47	117.20
2	B	188	VAL	CB-CA-C	6.78	124.28	111.40
2	B	187	TRP	CB-CA-C	6.64	123.69	110.40
1	A	72	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	32	PHE	CA-C-N	-6.46	103.00	117.20
2	B	187	TRP	O-C-N	-6.43	112.42	122.70
1	A	32	PHE	O-C-N	-6.12	112.91	122.70
2	B	190	TYR	CA-CB-CG	5.97	124.75	113.40
2	B	188	VAL	CA-C-N	5.93	130.25	117.20
1	A	31	ALA	CA-C-O	-5.76	108.00	120.10
2	B	189	TYR	N-CA-CB	5.72	120.90	110.60
2	B	184	TRP	CD1-NE1-CE2	-5.72	103.86	109.00
2	B	186	HIS	CB-CA-C	5.68	121.75	110.40
2	B	187	TRP	CD1-NE1-CE2	-5.67	103.90	109.00
1	A	28	TRP	CD1-NE1-CE2	-5.63	103.93	109.00
1	A	4	HIS	CA-CB-CG	5.60	123.12	113.60
1	A	73	PRO	CA-C-N	5.54	127.27	116.20
1	A	25	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	B	195	ASP	CA-C-N	5.47	129.24	117.20
1	A	72	ARG	CB-CA-C	5.34	121.09	110.40
1	A	71	GLN	N-CA-C	5.32	125.38	111.00
1	A	31	ALA	CB-CA-C	5.28	118.02	110.10
1	A	24	TYR	N-CA-CB	-5.27	101.11	110.60
2	B	195	ASP	O-C-N	-5.17	114.43	122.70
1	A	36	ARG	NE-CZ-NH2	-5.15	117.73	120.30

All chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms
1	A	6	THR	CB
1	A	11	ILE	CB
2	B	196	THR	CB

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	54	TYR	Sidechain
2	B	181	TYR	Sidechain,Peptide
1	A	32	PHE	Mainchain,Peptide
2	B	186	HIS	Peptide
2	B	194	PRO	Peptide
1	A	21	ASN	Peptide
1	A	55	GLU	Peptide
1	A	16	CYS	Peptide
2	B	197	PRO	Peptide
2	B	184	TRP	Peptide
2	B	198	TYR	Sidechain
1	A	73	PRO	Mainchain,Peptide
1	A	5	THR	Peptide
1	A	72	ARG	Sidechain,Mainchain,Peptide
1	A	68	HIS	Peptide
1	A	18	PRO	Peptide
1	A	6	THR	Peptide
1	A	24	TYR	Sidechain
1	A	13	ALA	Peptide
2	B	189	TYR	Sidechain
2	B	190	TYR	Sidechain,Peptide
1	A	36	ARG	Sidechain
1	A	63	ASP	Peptide
1	A	70	LYS	Peptide
1	A	8	THR	Peptide
1	A	31	ALA	Mainchain,Peptide
1	A	20	GLU	Mainchain,Peptide

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	551	534	532	1
2	B	165	144	140	1
All	All	716	678	672	2

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 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:183:GLY:H	2:B:184:TRP:HB3	0.46	1.70
1:A:23:CYS:SG	1:A:42:LEU:HD13	0.41	2.56

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	72/74 (97%)	30 (42%)	16 (22%)	26 (36%)	0 0
2	B	16/19 (84%)	3 (19%)	4 (25%)	9 (56%)	0 0
All	All	88/93 (95%)	33 (38%)	20 (23%)	35 (40%)	0 0

All 35 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	42	LEU
2	B	188	VAL
1	A	33	CYS
1	A	73	PRO
1	A	14	VAL
1	A	15	THR
1	A	6	THR
1	A	53	PRO
1	A	20	GLU
1	A	48	CYS
1	A	67	PRO
1	A	68	HIS
1	A	62	THR
2	B	191	THR
1	A	44	CYS
1	A	31	ALA
1	A	56	GLU
1	A	24	TYR

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Mol	Chain	Res	Type
1	A	17	PRO
1	A	32	PHE
1	A	64	LYS
2	B	197	PRO
1	A	12	SER
1	A	51	LYS
1	A	71	GLN
2	B	194	PRO
2	B	184	TRP
2	B	185	LYS
2	B	189	TYR
1	A	18	PRO
1	A	59	CYS
2	B	182	ARG
1	A	41	GLU
2	B	183	GLY
1	A	21	ASN

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	65/65 (100%)	48 (74%)	17 (26%)	3 24
2	B	17/17 (100%)	10 (59%)	7 (41%)	0 4
All	All	82/82 (100%)	58 (71%)	24 (29%)	2 18

All 24 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	42	LEU
1	A	70	LYS
1	A	63	ASP
1	A	30	ASP
1	A	60	CYS
2	B	184	TRP
2	B	196	THR

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Mol	Chain	Res	Type
1	A	38	LYS
1	A	36	ARG
1	A	29	CYS
1	A	3	CYS
1	A	44	CYS
2	B	191	THR
2	B	190	TYR
1	A	64	LYS
2	B	193	CYS
1	A	12	SER
1	A	51	LYS
1	A	54	TYR
2	B	185	LYS
1	A	57	VAL
2	B	189	TYR
1	A	59	CYS
1	A	41	GLU

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