W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB NMR Structure Validation Summary Report (i)

Apr 26, 2016 – 04:31 PM BST

PDB ID	:	1QXQ
Title	:	STRUCTURE OF AN INDOLICIDIN PEPTIDE DERIVATIVE WITH HIGHER CHARGE
Authors	:	Rozek, A.; Powers, J.P.; Friedrich, C.L.; Hancock, R.E.
Deposited on	:	2003-09-08

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

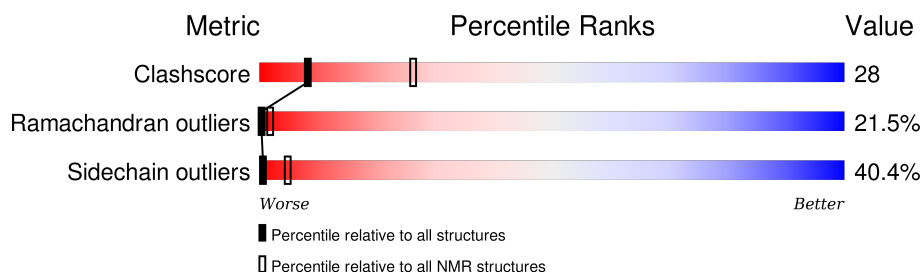|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
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 is 50%.

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	Percentile Ranks	Value
Clashscore		28
Ramachandran outliers		21.5%
Sidechain outliers		40.4%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

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	14	29% 29% 43%

2 Ensemble composition and analysis ⓘ

This entry contains 12 models.

Cyrange was unable to find well-defined residues.

Error message: Only domains with < 8 residues could be identified.

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 281 atoms, of which 145 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INDOLICIDIN DERIVATIVE.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	14	281	96	145	27	13	1

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	DELETION	UNP P33046
A	3	LYS	TRP	ENGINEERED	UNP P33046
A	13	LYS	GLY	ENGINEERED	UNP P33046

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.

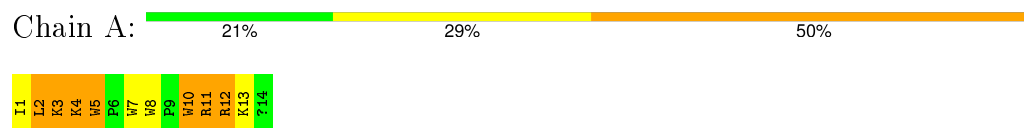• Molecule 1: INDOLICIDIN DERIVATIVE

Chain A:
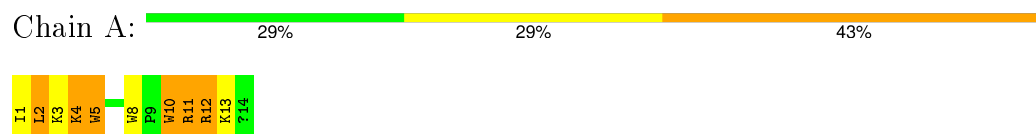
4.2 Residue scores for the representative (author defined) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: INDOLICIDIN DERIVATIVE

Chain A:

5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 12 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	3.851
DGII	structure solution	97.2

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 5938, BMRB entry 5941
Number of chemical shift lists	2
Total number of shifts	265
Number of shifts mapped to atoms	257
Number of unparsed shifts	0
Number of shifts with mapping errors	8
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	50%

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)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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

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	2.0±0.0
All	All	0	24

There are no bond-length outliers.

There are no bond-angle outliers.

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	12	ARG	Sidechain	12
1	A	11	ARG	Sidechain	12

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	136	145	143	8±2
All	All	1632	1740	1716	95

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 28.

5 of 26 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1:ILE:O	1:A:2:LEU:HD12	0.76	1.79	6	1
1:A:1:ILE:C	1:A:2:LEU:HD23	0.69	2.08	9	1
1:A:4:LYS:CG	1:A:4:LYS:O	0.57	2.52	10	1
1:A:8:TRP:CD1	1:A:10:TRP:HB2	0.55	2.36	12	12
1:A:12:ARG:O	1:A:13:LYS:CG	0.53	2.56	4	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	12/14 (86%)	2±1 (18±7%)	7±1 (60±8%)	3±1 (22±6%)	0	2
All	All	144/168 (86%)	26 (18%)	87 (60%)	31 (22%)	0	2

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	5	TRP	12
1	A	2	LEU	10
1	A	3	LYS	7
1	A	13	LYS	1
1	A	12	ARG	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	13/13 (100%)	8±1 (60±10%)	5±1 (40±10%)	0	5
All	All	156/156 (100%)	93 (60%)	63 (40%)	0	5

5 of 8 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	10	TRP	12
1	A	12	ARG	10
1	A	4	LYS	9
1	A	2	LEU	8
1	A	11	ARG	7

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 50% for the well-defined parts and 50% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5938

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	123
Number of shifts mapped to atoms	123
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

7.1.2 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 49%, i.e. 113 atoms were assigned a chemical shift out of a possible 232. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|	Total	^{1}H	^{13}C	^{15}N
Backbone	23/61 (38%)	23/24 (96%)	0/26 (0%)	0/11 (0%)
Sidechain	66/123 (54%)	66/76 (87%)	0/38 (0%)	0/9 (0%)
Aromatic	24/48 (50%)	24/24 (100%)	0/20 (0%)	0/4 (0%)
Overall	113/232 (49%)	113/124 (91%)	0/84 (0%)	0/24 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

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:
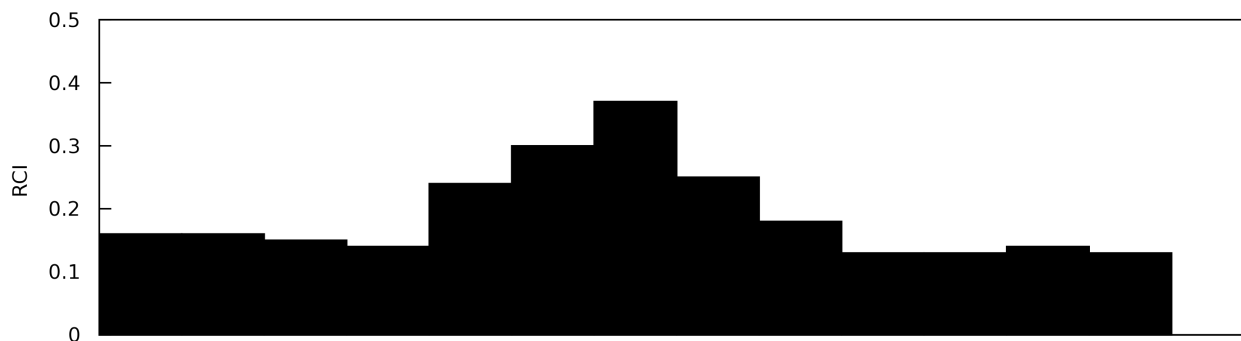
7.2   Chemical shift list 2

File name: BMRB entry 5941

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

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	142
Number of shifts mapped to atoms	134
Number of unparsed shifts	0
Number of shifts with mapping errors	8
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. First 5 (of 8) occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	14	CYS	HB2	3.04	0.01	2
A	2	CYS	HA	4.95	0.01	1
A	14	CYS	HA	4.83	0.01	1
A	14	CYS	H	8.15	0.01	1
A	2	CYS	HB3	3.0	0.01	2

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 50%, i.e. 115 atoms were assigned a chemical shift out of a possible 232. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	23/61 (38%)	23/24 (96%)	0/26 (0%)	0/11 (0%)
Sidechain	68/123 (55%)	68/76 (89%)	0/38 (0%)	0/9 (0%)
Aromatic	24/48 (50%)	24/24 (100%)	0/20 (0%)	0/4 (0%)
Overall	115/232 (50%)	115/124 (93%)	0/84 (0%)	0/24 (0%)

7.2.4 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	9	PRO	HG2	0.28	$3.48 - 0.38$	-5.3

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Random coil index (RCI) for chain A: