Full wwPDB NMR Structure Validation Report (i)

Oct 16, 2021 – 08:34 PM EDT

PDB ID	:	1QXQ
Title	:	STRUCTURE OF AN INDOLICIDIN PEPTIDE DERIVATIVE WITH HIGHER CHARGE
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Deposited on	:	2003-09-08

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
https://www.wwpdb.org/validation/2017/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:

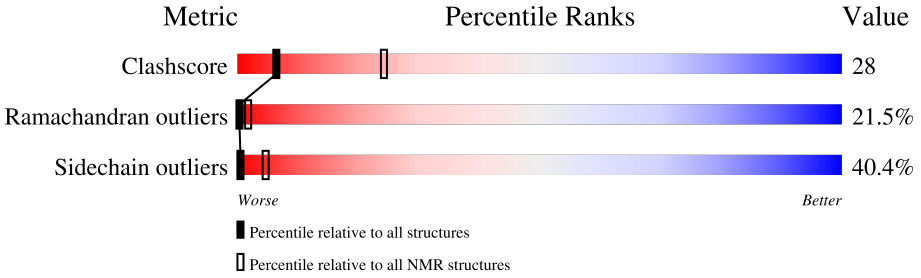
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 (i)

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 mutation	UNP P33046
A	13	LYS	GLY	engineered mutation	UNP P33046

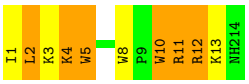
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: 29% 29% 43%



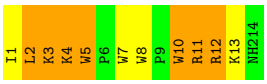
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: INDOLICIDIN DERIVATIVE

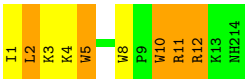
Chain A: 21% 29% 50%



4.2.2 Score per residue for model 2

• Molecule 1: INDOLICIDIN DERIVATIVE

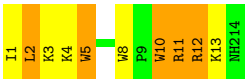
Chain A: 36% 29% 36%



4.2.3 Score per residue for model 3

- Molecule 1: INDOLICIDIN DERIVATIVE

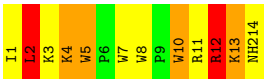
Chain A: 29% 36% 36%



4.2.4 Score per residue for model 4

- Molecule 1: INDOLICIDIN DERIVATIVE

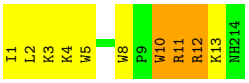
Chain A: 14% 43% 29% 14%



4.2.5 Score per residue for model 5

- Molecule 1: INDOLICIDIN DERIVATIVE

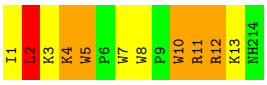
Chain A: 29% 50% 21%



4.2.6 Score per residue for model 6

- Molecule 1: INDOLICIDIN DERIVATIVE

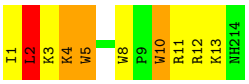
Chain A: 21% 36% 36% 7%



4.2.7 Score per residue for model 7

- Molecule 1: INDOLICIDIN DERIVATIVE

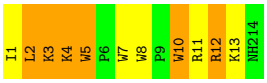
Chain A: 29% 43% 21% 7%



4.2.8 Score per residue for model 8

- Molecule 1: INDOLICIDIN DERIVATIVE

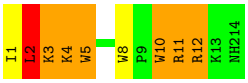
Chain A: 21% 36% 43%



4.2.9 Score per residue for model 9

- Molecule 1: INDOLICIDIN DERIVATIVE

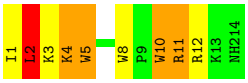
Chain A: 36% 14% 43% 7%



4.2.10 Score per residue for model 10

- Molecule 1: INDOLICIDIN DERIVATIVE

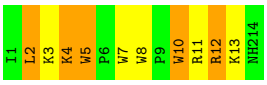
Chain A: 36% 29% 29% 7%



4.2.11 Score per residue for model 11

- Molecule 1: INDOLICIDIN DERIVATIVE

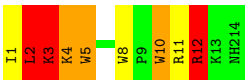
Chain A: 29% 36% 36%



4.2.12 Score per residue for model 12

- Molecule 1: INDOLICIDIN DERIVATIVE

Chain A: 36% 21% 21% 21%



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

No chemical shift data was provided.

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	11	ARG	Sidechain	12
1	A	12	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.

All 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	2
1:A:8:TRP:CD1	1:A:10:TRP:HB2	0.55	2.37	4	12
1:A:12:ARG:O	1:A:13:LYS:CG	0.53	2.56	4	1
1:A:3:LYS:O	1:A:4:LYS:C	0.50	2.50	5	4
1:A:8:TRP:NE1	1:A:10:TRP:HB2	0.50	2.22	5	12
1:A:1:ILE:O	1:A:2:LEU:CB	0.50	2.60	1	10
1:A:1:ILE:HG22	1:A:2:LEU:N	0.49	2.22	12	2
1:A:8:TRP:CD1	1:A:10:TRP:CB	0.49	2.96	2	11
1:A:1:ILE:CG2	1:A:2:LEU:N	0.48	2.76	5	2
1:A:8:TRP:NE1	1:A:10:TRP:CB	0.48	2.77	10	12
1:A:4:LYS:O	1:A:5:TRP:O	0.48	2.32	9	11
1:A:1:ILE:O	1:A:2:LEU:CD1	0.47	2.59	6	1
1:A:12:ARG:O	1:A:14:NH2:N	0.47	2.47	4	1
1:A:4:LYS:O	1:A:4:LYS:HG2	0.46	2.11	10	1
1:A:1:ILE:N	1:A:5:TRP:CE2	0.46	2.84	10	1
1:A:1:ILE:O	1:A:2:LEU:HD23	0.46	2.10	9	1
1:A:12:ARG:O	1:A:13:LYS:HG2	0.46	2.11	4	1
1:A:12:ARG:O	1:A:13:LYS:C	0.43	2.55	4	1
1:A:1:ILE:HG13	1:A:2:LEU:N	0.43	2.28	10	1
1:A:2:LEU:O	1:A:3:LYS:HB2	0.41	2.16	4	3
1:A:4:LYS:O	1:A:5:TRP:C	0.41	2.58	8	1
1:A:2:LEU:O	1:A:3:LYS:CB	0.41	2.67	5	1
1:A:1:ILE:O	1:A:2:LEU:HB2	0.40	2.16	2	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

All 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
1	A	13	LYS	7
1	A	3	LYS	5
1	A	7	TRP	5

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 monosaccharides 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