Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2K1I
Title	:	Synthesis, Structure and Activities of an Oral Mucosal Alpha-Defensin from Rhesus Macaque
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Deposited on	:	2008-03-05

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:

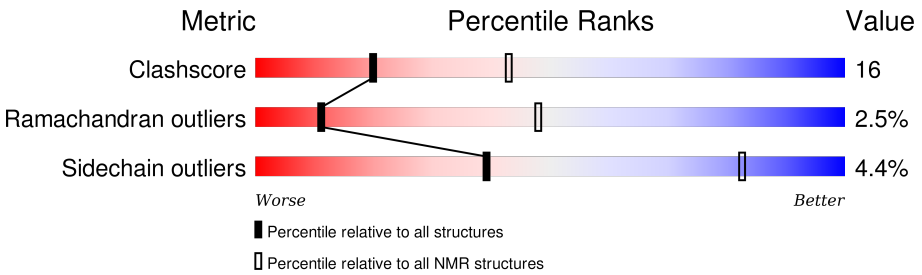
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	32	59% 31% 9%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:4-A:32 (29)	0.29	3

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 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 8, 9
2	7, 10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 509 atoms, of which 253 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mucosal Alpha-Defensin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	32	509	145	253	61	44	6	0

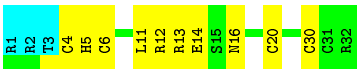
4 Residue-property plots (i)

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: Mucosal Alpha-Defensin

Chain A: 59% 31% 9%



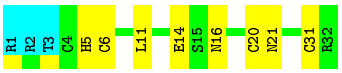
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Mucosal Alpha-Defensin

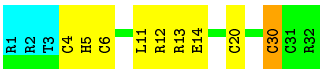
Chain A: 66% 25% 9%



4.2.2 Score per residue for model 2

- Molecule 1: Mucosal Alpha-Defensin

Chain A: 63% 25% • 9%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Mucosal Alpha-Defensin

Chain A: 59% 28% • 9%

R1 R2 T3 C4 H5 C6 L11 R12 R13 E14 C20 F27 C30 C31 R32

4.2.4 Score per residue for model 4

- Molecule 1: Mucosal Alpha-Defensin

Chain A: 78% 13% 9%

R1 R2 T3 C4 L11 N16 C20 R32

4.2.5 Score per residue for model 5

- Molecule 1: Mucosal Alpha-Defensin

Chain A: 50% 41% 9%

R1 R2 T3 C4 H5 C6 L11 R12 R13 N16 C20 N21 I22 R25 I26 F27 S28 L29 C30 C31 R32

4.2.6 Score per residue for model 6

- Molecule 1: Mucosal Alpha-Defensin

Chain A: 66% 25% 9%

R1 R2 T3 C4 H5 C6 L11 E14 S17 G18 S19 C20 R32

4.2.7 Score per residue for model 7

- Molecule 1: Mucosal Alpha-Defensin

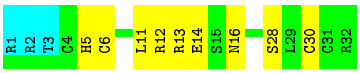
Chain A: 56% 34% 9%

R1 R2 T3 C4 H5 C6 L11 R12 R13 C20 I26 F27 C30 C31 R32

4.2.8 Score per residue for model 8

- Molecule 1: Mucosal Alpha-Defensin

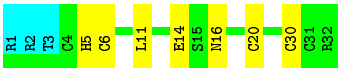
Chain A: 63% 28% 9%



4.2.9 Score per residue for model 9

- Molecule 1: Mucosal Alpha-Defensin

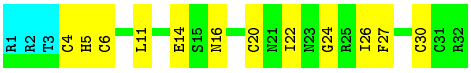
Chain A: 69% 22% 9%



4.2.10 Score per residue for model 10

- Molecule 1: Mucosal Alpha-Defensin

Chain A: 53% 38% 9%



5 Refinement protocol and experimental data overview (i)

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

Of the 60 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations, strutures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.18

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	227	218	217	7±2
All	All	2270	2180	2170	72

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 16.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:N	1:A:11:LEU:HD22	0.61	2.09	3	3
1:A:5:HIS:CG	1:A:6:CYS:N	0.61	2.69	10	8
1:A:5:HIS:CG	1:A:6:CYS:H	0.58	2.16	10	3
1:A:11:LEU:N	1:A:11:LEU:HD12	0.56	2.15	1	2
1:A:11:LEU:HD12	1:A:11:LEU:N	0.56	2.16	10	5
1:A:11:LEU:N	1:A:11:LEU:CD2	0.56	2.69	3	3
1:A:14:GLU:N	1:A:14:GLU:OE1	0.55	2.39	9	6
1:A:16:ASN:ND2	1:A:28:SER:OG	0.53	2.41	5	2
1:A:4:CYS:SG	1:A:30:CYS:O	0.53	2.67	10	3
1:A:14:GLU:OE1	1:A:14:GLU:N	0.52	2.42	6	1
1:A:11:LEU:N	1:A:11:LEU:CD1	0.51	2.74	10	4
1:A:20:CYS:SG	1:A:27:PHE:O	0.51	2.68	7	2
1:A:5:HIS:ND1	1:A:6:CYS:N	0.51	2.59	2	3
1:A:5:HIS:CD2	1:A:6:CYS:N	0.50	2.80	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:C	1:A:13:ARG:H	0.49	2.09	8	5
1:A:5:HIS:CD2	1:A:6:CYS:O	0.49	2.65	10	1
1:A:5:HIS:CD2	1:A:6:CYS:H	0.49	2.25	10	1
1:A:11:LEU:O	1:A:13:ARG:N	0.47	2.48	2	4
1:A:11:LEU:CD1	1:A:11:LEU:N	0.45	2.79	9	2
1:A:20:CYS:O	1:A:27:PHE:O	0.44	2.35	5	2
1:A:16:ASN:O	1:A:16:ASN:OD1	0.43	2.36	1	2
1:A:4:CYS:SG	1:A:30:CYS:C	0.43	2.96	2	1
1:A:16:ASN:OD1	1:A:16:ASN:O	0.42	2.36	4	2
1:A:21:ASN:O	1:A:21:ASN:OD1	0.42	2.37	1	1
1:A:20:CYS:SG	1:A:22:ILE:CD1	0.41	3.09	5	1
1:A:4:CYS:N	1:A:31:CYS:SG	0.41	2.93	7	1
1:A:22:ILE:C	1:A:24:GLY:N	0.41	2.74	10	1
1:A:17:SER:OG	1:A:18:GLY:N	0.40	2.55	6	1
1:A:11:LEU:C	1:A:13:ARG:N	0.40	2.75	8	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	28/32 (88%)	26±1 (93±3%)	1±1 (4±2%)	1±1 (2±2%)	11	48
All	All	280/320 (88%)	261 (93%)	12 (4%)	7 (2%)	11	48

All 2 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	12	ARG	5
1	A	26	ILE	2

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	27/30 (90%)	26±1 (96±2%)	1±1 (4±2%)	39	82
All	All	270/300 (90%)	258 (96%)	12 (4%)	39	82

All 3 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	30	CYS	6
1	A	20	CYS	5
1	A	25	ARG	1

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