Full wwPDB NMR Structure Validation Report (i)

Feb 15, 2022 – 09:24 AM EST

PDB ID	:	1KJ6
Title	:	Solution Structure of Human beta-Defensin 3
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Deposited on	:	2001-12-04

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:

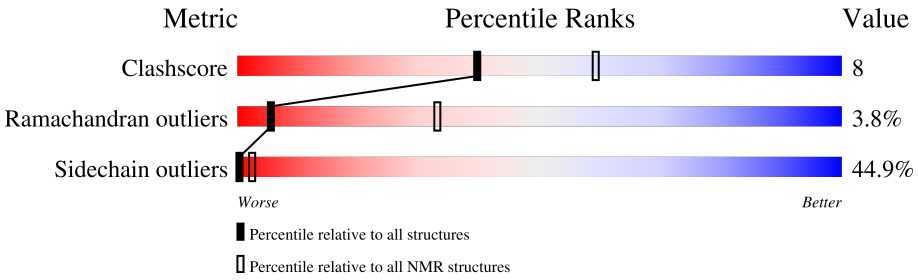
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	45	42% 38% 7% 13%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:6-A:44 (39)	0.41	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 3 clusters and 7 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 738 atoms, of which 382 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta-defensin 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	45	738	216	382	75	59	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, 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: Beta-defensin 3

Chain A: 42% 38% 7% 13%

G1 I2 I3 N4 T5 L6 Y9 Y10 C11 R12 Y13 R14 G15 L21 S22 C23 E27 E28 Q29 I30 R38 K39 C40 C41 R42 R43 K44 K45

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 (medoid)

• Molecule 1: Beta-defensin 3

Chain A: 40% 42% • 13%

G1 I2 I3 N4 T5 K8 Y9 Y10 R14 A19 V20 L21 S22 C23 E27 E28 Q29 I30 C33 S34 T35 R36 G37 R38 K39 C40 C41 R42 R43 K44 K45

4.2.2 Score per residue for model 2

• Molecule 1: Beta-defensin 3

Chain A: 40% 38% 9% 13%

G1 I2 I3 N4 T5 Y10 C11 R12 V13 R14 G15 G16 L21 S22 C23 E27 E28 Q29 I30 S34 R38 K39 C40 C41 R42 R43 K44 K45

4.2.3 Score per residue for model 3

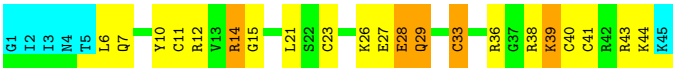
- Molecule 1: Beta-defensin 3

Chain A: 47% 33% 7% 13%

4.2.4 Score per residue for model 4

- Molecule 1: Beta-defensin 3

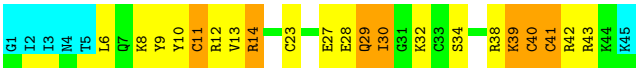
Chain A: 40% 36% 11% 13%



4.2.5 Score per residue for model 5

- Molecule 1: Beta-defensin 3

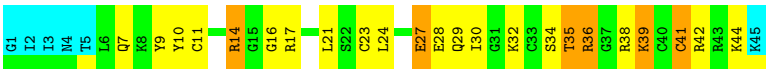
Chain A: 40% 31% 16% 13%



4.2.6 Score per residue for model 6

- Molecule 1: Beta-defensin 3

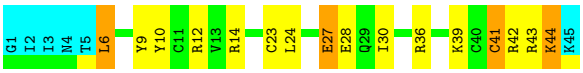
Chain A: 36% 38% 13% 13%



4.2.7 Score per residue for model 7

- Molecule 1: Beta-defensin 3

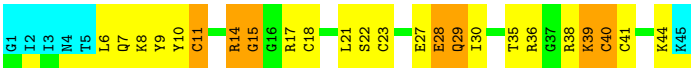
Chain A: 51% 27% 9% 13%



4.2.8 Score per residue for model 8

- Molecule 1: Beta-defensin 3

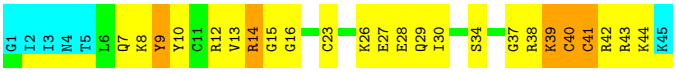
Chain A: 33% 38% 16% 13%



4.2.9 Score per residue for model 9

- Molecule 1: Beta-defensin 3

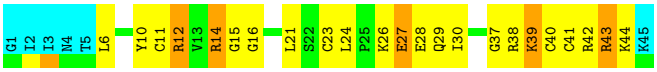
Chain A: 33% 42% 11% 13%



4.2.10 Score per residue for model 10

- Molecule 1: Beta-defensin 3

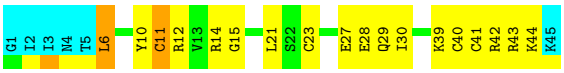
Chain A: 36% 40% 11% 13%



4.2.11 Score per residue for model 11

- Molecule 1: Beta-defensin 3

Chain A: 47% 36% • 13%



4.2.12 Score per residue for model 12

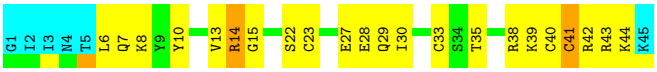
- Molecule 1: Beta-defensin 3

Chain A: 38% 40% 9% 13%

4.2.13 Score per residue for model 13

- Molecule 1: Beta-defensin 3

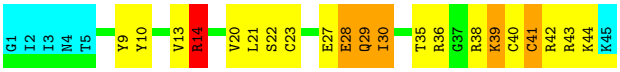
Chain A: 38% 44% • 13%



4.2.14 Score per residue for model 14

- Molecule 1: Beta-defensin 3

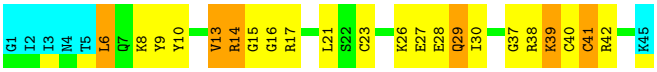
Chain A: 40% 33% 11% • 13%



4.2.15 Score per residue for model 15

- Molecule 1: Beta-defensin 3

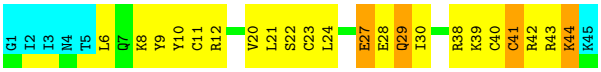
Chain A: 38% 36% 13% 13%



4.2.16 Score per residue for model 16

- Molecule 1: Beta-defensin 3

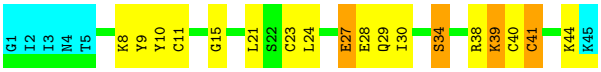
Chain A: 38% 40% 9% 13%



4.2.17 Score per residue for model 17

- Molecule 1: Beta-defensin 3

Chain A: 47% 31% 9% 13%



4.2.18 Score per residue for model 18

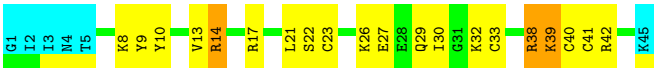
- Molecule 1: Beta-defensin 3

Chain A: 51% 29% 7% 13%

4.2.19 Score per residue for model 19

- Molecule 1: Beta-defensin 3

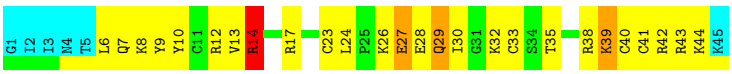
Chain A: 42% 38% 7% 13%



4.2.20 Score per residue for model 20

- Molecule 1: Beta-defensin 3

Chain A: 29% 49% 7% • 13%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Distance geometry, Simulated Annealing, Molecular Dynamics.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	refinement	1.0
ARIA	refinement	1.0

No chemical shift data was provided.

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	311	329	329	5±1
All	All	6220	6580	6580	98

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:VAL:HG23	1:A:14:ARG:HG2	0.70	1.64	2	5
1:A:11:CYS:HA	1:A:15:GLY:HA3	0.56	1.76	10	2
1:A:29:GLN:HA	1:A:40:CYS:O	0.53	2.03	10	17
1:A:28:GLU:O	1:A:41:CYS:HA	0.53	2.03	8	19
1:A:13:VAL:HG12	1:A:14:ARG:HG2	0.53	1.81	15	1
1:A:38:ARG:C	1:A:39:LYS:HG3	0.51	2.25	18	11
1:A:11:CYS:SG	1:A:15:GLY:HA3	0.51	2.46	4	3
1:A:13:VAL:HG23	1:A:14:ARG:HG3	0.50	1.82	14	2
1:A:15:GLY:HA2	1:A:30:ILE:HD12	0.49	1.85	12	1
1:A:44:LYS:H	1:A:44:LYS:HE2	0.49	1.68	7	1
1:A:13:VAL:HG23	1:A:14:ARG:CG	0.48	2.38	13	2
1:A:27:GLU:HB3	1:A:43:ARG:N	0.48	2.24	10	2
1:A:28:GLU:HG3	1:A:29:GLN:N	0.48	2.24	11	2
1:A:34:SER:HB3	1:A:38:ARG:HE	0.48	1.68	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ARG:O	1:A:39:LYS:HG3	0.47	2.09	15	10
1:A:24:LEU:HB2	1:A:27:GLU:CG	0.46	2.40	16	6
1:A:11:CYS:HB2	1:A:30:ILE:HG13	0.46	1.87	5	1
1:A:6:LEU:O	1:A:6:LEU:HD12	0.45	2.10	15	1
1:A:28:GLU:OE2	1:A:30:ILE:HG23	0.44	2.12	14	1
1:A:11:CYS:O	1:A:15:GLY:HA3	0.44	2.12	17	1
1:A:27:GLU:HB3	1:A:43:ARG:HA	0.43	1.89	12	1
1:A:20:VAL:O	1:A:38:ARG:HG2	0.43	2.14	14	1
1:A:27:GLU:HB2	1:A:41:CYS:HB3	0.42	1.90	6	1
1:A:19:ALA:O	1:A:38:ARG:HG2	0.41	2.15	1	1
1:A:12:ARG:O	1:A:12:ARG:HG3	0.41	2.15	10	1
1:A:27:GLU:HA	1:A:44:LYS:HG3	0.41	1.92	16	1
1:A:24:LEU:HB2	1:A:27:GLU:HG3	0.40	1.94	20	1
1:A:9:TYR:O	1:A:12:ARG:HB3	0.40	2.16	9	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	39/45 (87%)	30±2 (76±5%)	8±2 (20±5%)	2±1 (4±3%)	5 33
All	All	780/900 (87%)	596 (76%)	154 (20%)	30 (4%)	5 33

All 9 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	14	ARG	8
1	A	16	GLY	6
1	A	15	GLY	4
1	A	37	GLY	4
1	A	35	THR	2
1	A	36	ARG	2
1	A	6	LEU	2
1	A	33	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	34	SER	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	34/39 (87%)	19±3 (55±7%)	15±3 (45±7%)	0 2
All	All	680/780 (87%)	375 (55%)	305 (45%)	0 2

All 32 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	TYR	20
1	A	23	CYS	20
1	A	27	GLU	20
1	A	30	ILE	19
1	A	39	LYS	17
1	A	14	ARG	16
1	A	44	LYS	16
1	A	42	ARG	15
1	A	9	TYR	13
1	A	21	LEU	13
1	A	43	ARG	13
1	A	41	CYS	13
1	A	6	LEU	12
1	A	8	LYS	10
1	A	29	GLN	10
1	A	12	ARG	9
1	A	22	SER	7
1	A	26	LYS	7
1	A	36	ARG	6
1	A	34	SER	6
1	A	7	GLN	6
1	A	33	CYS	5
1	A	11	CYS	5
1	A	32	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	17	ARG	5
1	A	35	THR	5
1	A	28	GLU	4
1	A	40	CYS	3
1	A	18	CYS	2
1	A	13	VAL	1
1	A	20	VAL	1
1	A	38	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 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