Full wwPDB NMR Structure Validation Report (i)

Feb 12, 2022 – 07:17 PM EST

PDB ID	:	1GIO
Title	:	NMR SOLUTION STRUCTURE OF BOVINE ANGIOGENIN, 10 STRUCTURES
Authors	:	Lequin, O.; Albaret, C.; Bontems, F.; Spik, G.; Lallemand, J.Y.
Deposited on	:	1996-04-12

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:

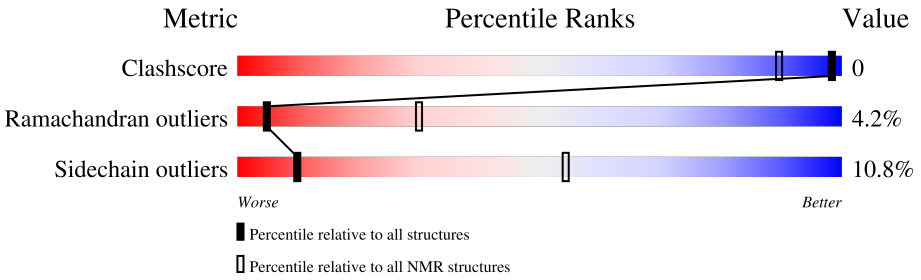
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	125	78% 6% • 15%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 2 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:7-A:84, A:93-A:120 (106)	0.42	2

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 and 2 single-model clusters were found.

Cluster number	Models
1	2, 3, 7, 8, 9, 10
2	4, 6
Single-model clusters	1; 5

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2007 atoms, of which 983 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ANGIOGENIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	125	2007	631	983	197	188	8	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: ANGIOGENIN

Chain A: 78% 6% • 15%

A1 Q2 D3 D4 Y5 R6 Y7 M30 R43 F46 D60 R61 N62 I72 K85 G86 G87 S88 S89 R90 P91 P92 L112 I121 T122 P123 R124 H125

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: ANGIOGENIN

Chain A: 71% 10% • 15%

A1 Q2 D3 D4 Y5 R6 Y7 A17 G21 D24 M30 M31 K32 L36 T37 R38 P39 D42 F46 E59 D60 Y66 D69 K85 G86 G87 S88 S89 R90 P91 P92 Y95 D100 I121 T122 P123 R124 H125

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: ANGIOGENIN

Chain A: 74% 10% • 15%

A1 Q2 D3 D4 Y5 R6 Y7 P19 Y26 M30 M31 R43 F46 I54 D60 R61 N62 G63 Q64 F65 Y66 R67 K85 G86 G87 S88 S89 R90 P91 P92 G111 I121 T122 P123 R124 H125

4.2.3 Score per residue for model 3

- Molecule 1: ANGIOGENIN

Chain A: 75% 8% • 15%

A1 Q2 D3 D4 Y5 R6 M30 R34 R43 N44 T45 F46 D60 R67 I72 E76 K85 G86 G87 S88 S89 R90 P91 P92 C93 R94 Y95 L112 I121 T122 P123 R124 H125

4.2.4 Score per residue for model 4

- Molecule 1: ANGIOGENIN

Chain A: 67% 17% • 15%

A1 Q2 D3 D4 Y5 R6 Q13 P19 R22 M30 M31 K32 R35 L36 T37 C40 F46 D53 I54 K55 D60 I72 I79 K85 G86 G87 S88 S89 R90 P91 P92 C93 R94 Y95 D100 S101 R102 L112 D117 E118 I121 T122 P123 R124

H125

4.2.5 Score per residue for model 5

- Molecule 1: ANGIOGENIN

Chain A: 70% 12% • • 15%

A1 Q2 D3 D4 Y5 R6 Y7 F28 L36 P39 C40 K41 D42 R43 F46 I54 D60 R61 N62 R67 L70 R71 I72 I79 K85 G86 G87 S88 S89 R90 P91 P92 V105 V106 L112 F120 I121 T122 P123 R124 H125

4.2.6 Score per residue for model 6

- Molecule 1: ANGIOGENIN

Chain A: 70% 12% • 15%

A1 Q2 D3 D4 Y5 R6 Y7 L11 R22 T37 R38 D42 R43 F46 D53 D60 R61 N62 I72 E76 K85 G86 G87 S88 S89 R90 P91 P92 C93 R94 Y95 V105 L112 D117 E118 I121 T122 P123 R124 H125

4.2.7 Score per residue for model 7

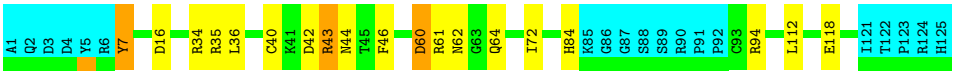
- Molecule 1: ANGIOGENIN

Chain A: 69% 15% • 15%

4.2.8 Score per residue for model 8

- Molecule 1: ANGIOGENIN

Chain A:



4.2.9 Score per residue for model 9

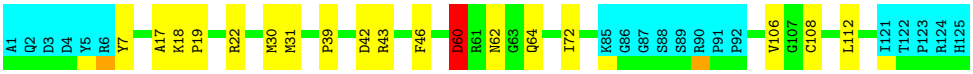
- Molecule 1: ANGIOGENIN

Chain A:

4.2.10 Score per residue for model 10

- Molecule 1: ANGIOGENIN

Chain A:



5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 10 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
DIANA	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	1.01±0.01	0±0/893 (0.0± 0.0%)	1.27±0.03	5±2/1199 (0.4± 0.2%)
All	All	1.01	0/8930 (0.0%)	1.27	49/11990 (0.4%)

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	0.0±0.0	1.0±0.6
All	All	0	10

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	95	TYR	CB-CG-CD2	-9.74	115.16	121.00	3	1
1	A	7	TYR	CA-CB-CG	8.46	129.48	113.40	10	1
1	A	46	PHE	CB-CG-CD2	-8.40	114.92	120.80	10	10
1	A	66	TYR	CB-CG-CD2	-7.86	116.29	121.00	2	2
1	A	46	PHE	CB-CG-CD1	7.74	126.22	120.80	10	8
1	A	7	TYR	CB-CG-CD2	-7.73	116.36	121.00	5	4
1	A	95	TYR	CB-CG-CD1	7.45	125.47	121.00	3	1
1	A	7	TYR	CB-CG-CD1	6.66	124.99	121.00	5	3
1	A	17	ALA	N-CA-CB	6.29	118.91	110.10	1	1
1	A	28	PHE	CB-CG-CD2	-6.15	116.50	120.80	5	2
1	A	28	PHE	CB-CG-CD1	6.05	125.04	120.80	5	1
1	A	95	TYR	N-CA-CB	5.87	121.16	110.60	3	1
1	A	66	TYR	CB-CG-CD1	5.85	124.51	121.00	2	2
1	A	60	ASP	N-CA-CB	5.77	120.98	110.60	10	7
1	A	105	VAL	CG1-CB-CG2	5.76	120.11	110.90	6	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	43	ARG	N-CA-CB	5.56	120.62	110.60	5	2
1	A	55	LYS	CA-CB-CG	5.55	125.60	113.40	4	1
1	A	21	GLY	N-CA-C	-5.00	100.59	113.10	1	1

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	62	ASN	Peptide	6
1	A	95	TYR	Sidechain	2
1	A	26	TYR	Sidechain	1
1	A	35	ARG	Peptide	1

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	873	837	837	0±0
All	All	8730	8370	8370	3

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:VAL:HG23	1:A:117:ASP:HB2	0.56	1.77	7	1
1:A:40:CYS:SG	1:A:84:HIS:CD2	0.56	2.99	8	1
1:A:7:TYR:CE2	1:A:112:LEU:HD22	0.42	2.49	6	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	106/125 (85%)	84±2 (79±2%)	18±2 (17±2%)	4±2 (4±1%)	5 30
All	All	1060/1250 (85%)	839 (79%)	176 (17%)	45 (4%)	5 30

All 22 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	60	ASP	10
1	A	39	PRO	4
1	A	19	PRO	4
1	A	64	GLN	4
1	A	94	ARG	3
1	A	17	ALA	2
1	A	67	ARG	2
1	A	95	TYR	2
1	A	24	ASP	1
1	A	59	GLU	1
1	A	69	ASP	1
1	A	111	GLY	1
1	A	40	CYS	1
1	A	102	ARG	1
1	A	43	ARG	1
1	A	120	PHE	1
1	A	38	ARG	1
1	A	41	LYS	1
1	A	68	GLY	1
1	A	34	ARG	1
1	A	50	ASN	1
1	A	18	LYS	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	96/112 (86%)	86±3 (89±4%)	10±3 (11±4%)	10 54
All	All	960/1120 (86%)	856 (89%)	104 (11%)	10 54

All 38 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	43	ARG	8
1	A	72	ILE	8
1	A	112	LEU	8
1	A	7	TYR	6
1	A	30	MET	6
1	A	42	ASP	5
1	A	118	GLU	5
1	A	36	LEU	4
1	A	31	MET	4
1	A	37	THR	3
1	A	54	ILE	3
1	A	22	ARG	3
1	A	24	ASP	2
1	A	32	LYS	2
1	A	60	ASP	2
1	A	100	ASP	2
1	A	34	ARG	2
1	A	44	ASN	2
1	A	76	GLU	2
1	A	53	ASP	2
1	A	79	ILE	2
1	A	94	ARG	2
1	A	117	ASP	2
1	A	105	VAL	2
1	A	106	VAL	2
1	A	11	LEU	2
1	A	61	ARG	2
1	A	67	ARG	1
1	A	13	GLN	1
1	A	35	ARG	1
1	A	55	LYS	1
1	A	41	LYS	1
1	A	70	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	38	ARG	1
1	A	16	ASP	1
1	A	103	VAL	1
1	A	104	ILE	1
1	A	108	CYS	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