

Full wwPDB NMR Structure Validation Report (i)

Oct 23, 2021 – 05:33 PM EDT

PDB ID	:	1BJC
Title	:	SOLUTION NMR STRUCTURE OF AMYLOID BETA[F16], RESIDUES 1-
		28, 15 STRUCTURES
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Deposited on	:	1998-06-23

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:

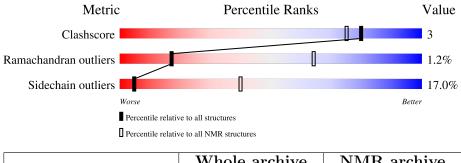
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	${f NMR} { m archive} \ (\#{ m Entries})$
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	А	28	36%	•	61%	



2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 5 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:15-A:25 (11)	0.44	5		

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 3 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 436 atoms, of which 202 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called AMYLOID BETA-PEPTIDE.

Mol	Chain	Residues		At	oms			Trace
1	٨	28	Total	С	Η	Ν	0	0
	А	20	436	148	202	40	46	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	PHE	LYS	engineered mutation	UNP P05067



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: AMYLOID BETA-PEPTIDE

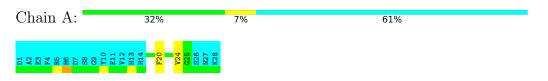


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: AMYLOID BETA-PEPTIDE



4.2.2 Score per residue for model 2

Chain A:	18%	21%	61%
D1 A2 R5 R5 B7 S8 C9 G9	410 411 413 414 415 415	F20 F20 D23 C25 C25 C25 C25 C25 K28 K28	



4.2.3 Score per residue for model 3

• Molecule 1: AMYLOID BETA-PEPTIDE

Chain A:	39%	61%
D1 A2 E3 F74 H6 D7 S8 S8 S8 C9 C9 E11	V 12 H14 S26 S26 K28 K28	

4.2.4 Score per residue for model 4

• Molecule 1: AMYLOID BETA-PEPTIDE

Chain A:	32%	7%	61%	
D1 A2 E3 F4 H6 D7	58 69 710 711 111 112 117 526 526 526 526 526 527 527 527 527 526 527 526 526 526 526 526 526 526 526 526 526			

- 4.2.5 Score per residue for model 5 (medoid)
- Molecule 1: AMYLOID BETA-PEPTIDE

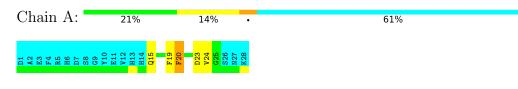
Chain A:	29%	11%	61%
D1 E3 F4 H6 C9 C9 C9 C9	日 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	N27 K28	

4.2.6 Score per residue for model 6

• Molecule 1: AMYLOID BETA-PEPTIDE



4.2.7 Score per residue for model 7





4.2.8 Score per residue for model 8

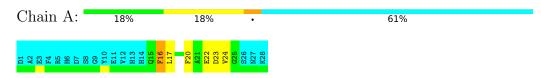
• Molecule 1: AMYLOID BETA-PEPTIDE

Chain A:	32%	7%	61%	
D1 A2 E3 F4 F4 F4 F4 F4 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3	V12 H14 F19 F20 S26 N27	K28		
4.2.9 Score	per residu	e for model 9)	
• Molecule 1: A	AMYLOID	BETA-PEPTID)E	
Chain A:	32%	7%	61%	
D1 A2 E3 F4 F4 F4 H6 D7 S8 S8 C10 C10	V12 H14 H14 E22 S26 S26 N27	K28		
4.2.10 Score	e per resid	ue for model	10	

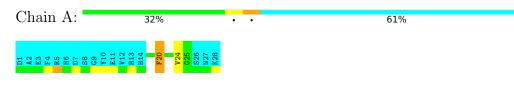
• Molecule 1: AMYLOID BETA-PEPTIDE

Chain A:	32%	7%	61%
D1 A2 A2 A2 A2 A2 A2 A2 A2 A2 A2 A2 A2 A2	E22 625 826 N27 K28		

4.2.11 Score per residue for model 11



- 4.2.12 Score per residue for model 12
- Molecule 1: AMYLOID BETA-PEPTIDE





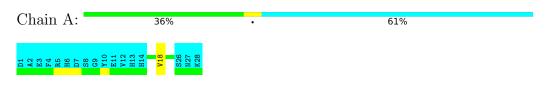
4.2.13 Score per residue for model 13

• Molecule 1: AMYLOID BETA-PEPTIDE



4.2.14 Score per residue for model 14

• Molecule 1: AMYLOID BETA-PEPTIDE



4.2.15 Score per residue for model 15

Chain A:	32%	7%	61%
D1 A2 F3 F4 F4 F5 F4 F5 F3 C9 C9 C9 C9	E11 V12 H13 H14 Q15 P16 D23 S26	N27	



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *SIMULATED ANNEALING USING NOE DISTANCE CONSTRAINTS*.

Of the 50 calculated structures, 15 were deposited, based on the following criterion: LOW ENERGY, LOW VIOLATIONS.

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

Software name	Classification	Version
XPLOR	refinement	
X-PLOR	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	В	ond lengths	Bond angles		
WOI Chai	Ullalli	RMSZ	$\#Z{>}5$	RMSZ	#Z>5	
1	А	$1.10 {\pm} 0.02$	$0{\pm}0/93~(~0.0{\pm}~0.0\%)$	1.03 ± 0.07	$0\pm 0/126~(~0.1\pm~0.2\%)$	
All	All	1.10	0/1395~(~0.0%)	1.03	1/1890 (0.1%)	

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$	Moo Worst	
				Worst	Total				
1	А	16	PHE	N-CA-C	-5.38	96.47	111.00	11	1

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	А	90	82	82	0 ± 1
All	All	1350	1230	1230	7

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
		()	()	Worst	Total
1:A:20:PHE:O	1:A:24:VAL:HG23	0.72	1.85	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models		
	Atom-2		Distance(A)	Worst	Total	
1:A:17:LEU:HD12	1:A:17:LEU:H	0.44	1.72	4	1	
1:A:16:PHE:O	1:A:17:LEU:CB	0.43	2.66	11	1	

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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	А	11/28~(39%)	8 ± 1 (76±11%)	2 ± 1 ($22\pm12\%$)	0±0 (1±3%)	17 64	
All	All	165/420~(39%)	126 (76%)	37 (22%)	2(1%)	17 64	

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	А	25	GLY	2

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	9/24~(38%)	7 ± 1 (83 $\pm13\%$)	$2\pm1 (17\pm13\%)$		5	40
All	All	135/360~(38%)	112 (83%)	23 (17%)		5	40

All 7 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	А	15	GLN	5
1	А	22	GLU	5
1	А	23	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	А	20	PHE	3
1	А	16	PHE	2
1	А	19	PHE	2
1	А	18	VAL	1

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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

