

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	8B9R
BMRB ID	:	34763
Title	:	Molecular structure of Cu(II)-bound amyloid-beta monomer implicated in in-
		hibition of peptide self-assembly in Alzheimer's disease
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Deposited on	:	2022-10-06

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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

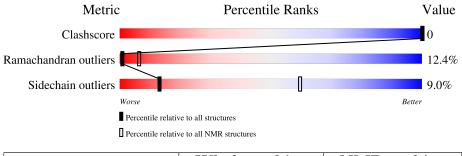
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.31.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 is 30%.

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f NMR} \ {f archive} \ (\#{f Entries})$
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	40	50%	8%	42%		



2 Ensemble composition and analysis (i)

This entry contains 5 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (7) was below the domain threshold value (8).

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 4, 5
2	1, 3



3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 367 atoms, of which 169 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Amyloid-beta A4 protein.

Mol	Chain	Residues	Atoms				Trace	
1	А	23	Total	С	Н	Ν	0	0
			366	125	169	34	38	Ū

• Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms
2	А	1	Total Cu 1 1



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 A4 protein

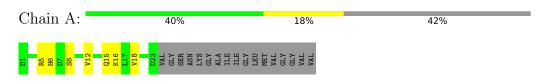


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

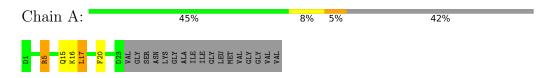
4.2.1 Score per residue for model 1

• Molecule 1: Amyloid-beta A4 protein



4.2.2 Score per residue for model 2

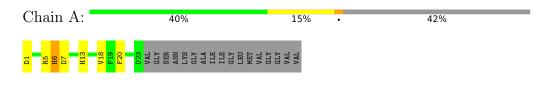
• Molecule 1: Amyloid-beta A4 protein





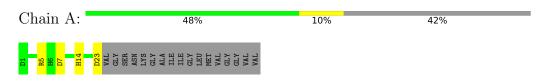
4.2.3 Score per residue for model 3

• Molecule 1: Amyloid-beta A4 protein



4.2.4 Score per residue for model 4

• Molecule 1: Amyloid-beta A4 protein



4.2.5 Score per residue for model 5

• Molecule 1: Amyloid-beta A4 protein

Chain	A:	45%	8%	5%	42%
D1 R5 H6	V12 H13 H14	23 VAL VAL GLY GLY ALA ALA ALA ALA TLE CLY CLY GLY GLY VAL VAL VAL			



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 5 calculated structures, 5 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
Amber	refinement	
CYANA	structure calculation	3.98.13

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	161
Number of shifts mapped to atoms	161
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	30%



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: CU

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 Chair		E	Sond lengths	Bond angles		
	Chain	RMSZ	$\#Z{>}5$	RMSZ	$\#Z{>}5$	
1	А	$0.84{\pm}0.02$	$0{\pm}0/203$ ($0.0{\pm}$ $0.0\%)$	1.22 ± 0.06	$1{\pm}0/272~(~0.4{\pm}~0.0\%)$	
All	All	0.84	0/1015~(~0.0%)	1.22	5/1360~(~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	А	$0.0{\pm}0.0$	$1.4{\pm}1.5$
All	All	0	7

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$\operatorname{Ideal}(^{o})$	Moo Worst	d els Total
1	А	5	ARG	NE-CZ-NH1	5.97	123.29	120.30	1	5

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	А	1	ASP	Peptide,Mainchain	2
1	А	6	HIS	Sidechain	1
1	А	13	HIS	Peptide	1
1	А	5	ARG	Peptide	1
1	А	14	HIS	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
All	All	990	845	850	-

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is -.

There are no clashes.

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	21/40~(52%)	$11 \pm 1 (54 \pm 5\%)$	$7 \pm 1 (33 \pm 5\%)$	$3\pm1~(12\pm5\%)$	1 6
All	All	105/200~(52%)	57 (54%)	35~(33%)	13 (12%)	1 6

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	А	12	VAL	2
1	А	18	VAL	2
1	А	20	PHE	2
1	А	6	HIS	2
1	А	8	SER	1
1	А	15	GLN	1
1	А	16	LYS	1
1	А	17	LEU	1
1	А	7	ASP	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	Perce	entiles
1	А	20/31~(65%)	18 ± 0 (91 $\pm2\%$)	2 ± 0 (9 $\pm2\%$)	13	60
All	All	100/155~(65%)	91 (91%)	9 (9%)	13	60

All 9 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	1
1	А	16	LYS	1
1	А	5	ARG	1
1	А	17	LEU	1
1	А	6	HIS	1
1	А	7	ASP	1
1	А	14	HIS	1
1	А	23	ASP	1
1	А	12	VAL	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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.



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)

The completeness of assignment taking into account all chemical shift lists is 30% for the well-defined parts and 30% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	161
Number of shifts mapped to atoms	161
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\rm Correction}\pm{\rm precision},ppm$	Suggested action
$^{13}C_{\alpha}$	27	-0.18 ± 0.31	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	21		None (insufficient data)
$^{13}C'$	36	-0.25 ± 0.15	None needed (< 0.5 ppm)
¹⁵ N	36	-1.39 ± 0.40	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 30%, i.e. 87 atoms were assigned a chemical shift out of a possible 294. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	70/115 (61%)	17/46~(37%)	34/46~(74%)	19/23~(83%)
Sidechain	15/123~(12%)	0/72~(0%)	14/46~(30%)	1/5~(20%)

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	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$				
Aromatic	2/56~(4%)	0/31~(0%)	2/22~(9%)	0/3~(0%)				
Overall	87/294 (30%)	17/149~(11%)	50/114 (44%)	20/31~(65%				

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 87 atoms were assigned a chemical shift out of a possible 294. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	15 N
Backbone	70/115 (61%)	17/46~(37%)	34/46~(74%)	19/23~(83%)
Sidechain	15/123~(12%)	0/72~(0%)	14/46~(30%)	1/5~(20%)
Aromatic	2/56~(4%)	0/31~(0%)	2/22~(9%)	0/3~(0%)
Overall	87/294~(30%)	17/149~(11%)	50/114 (44%)	20/31~(65%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (1)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

