



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 6OC9 / pdb_00006oc9
BMRB ID : 30596
Title : S8 phosphorylated beta amyloid 40 fibrils
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This is a wwPDB NMR Structure Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 2%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 10 models. Model 10 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:8-A:40, B:1-B:40, C:1-C:3, C:17-C:40, D:17-D:40, E:18-E:40, F:9-F:40, G:1-G:40, H:1-H:40, I:1-I:40, J:1-J:40 (339)	3.03	10

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 1 clusters and 2 single-model clusters were found.

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

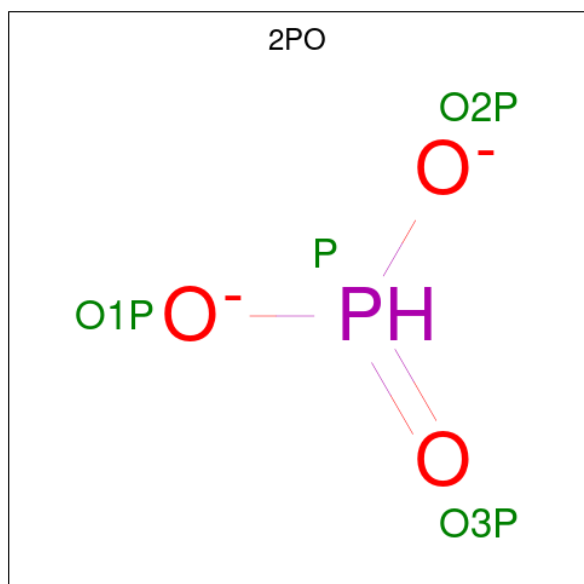
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6010 atoms, of which 2910 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amyloid-beta precursor protein.

Mol	Chain	Residues	Atoms						Trace
1	A	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	B	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	C	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	D	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	E	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	F	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	G	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	H	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	I	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	
1	J	40	Total	C	H	N	O	S	0
			597	194	291	53	58	1	

- Molecule 2 is PHOSPHONATE (CCD ID: 2PO) (formula: HO_3P).



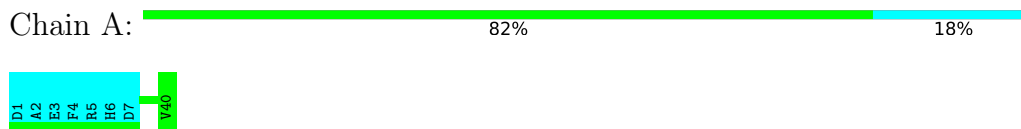
Mol	Chain	Residues	Atoms		
2	A	1	Total	O	P
			4	3	1
2	B	1	Total	O	P
			4	3	1
2	C	1	Total	O	P
			4	3	1
2	D	1	Total	O	P
			4	3	1
2	E	1	Total	O	P
			4	3	1
2	F	1	Total	O	P
			4	3	1
2	G	1	Total	O	P
			4	3	1
2	H	1	Total	O	P
			4	3	1
2	I	1	Total	O	P
			4	3	1
2	J	1	Total	O	P
			4	3	1

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 precursor protein

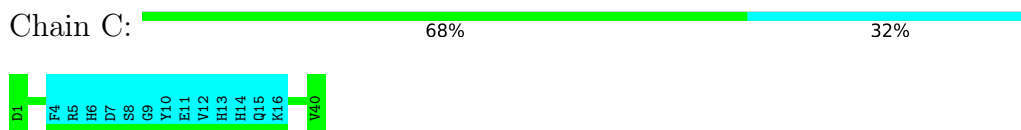


- Molecule 1: Amyloid-beta precursor protein



There are no outlier residues in this chain.

- Molecule 1: Amyloid-beta precursor protein



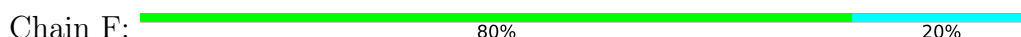
- Molecule 1: Amyloid-beta precursor protein

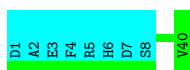


- Molecule 1: Amyloid-beta precursor protein



- Molecule 1: Amyloid-beta precursor protein





- Molecule 1: Amyloid-beta precursor protein

Chain G: 100%

There are no outlier residues in this chain.

- Molecule 1: Amyloid-beta precursor protein

Chain H: 100%

There are no outlier residues in this chain.

- Molecule 1: Amyloid-beta precursor protein

Chain I: 100%

There are no outlier residues in this chain.

- Molecule 1: Amyloid-beta precursor protein

Chain J: 100%

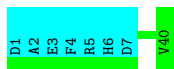
There are no outlier residues in this chain.

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: Amyloid-beta precursor protein

Chain A: 82% 18%



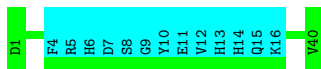
- Molecule 1: Amyloid-beta precursor protein

Chain B: 100%

There are no outlier residues in this chain.

- Molecule 1: Amyloid-beta precursor protein

Chain C: 68% 32%



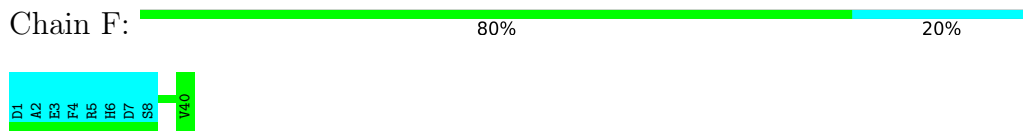
- Molecule 1: Amyloid-beta precursor protein



- Molecule 1: Amyloid-beta precursor protein



- Molecule 1: Amyloid-beta precursor protein



- Molecule 1: Amyloid-beta precursor protein



There are no outlier residues in this chain.

- Molecule 1: Amyloid-beta precursor protein



There are no outlier residues in this chain.

- Molecule 1: Amyloid-beta precursor protein



There are no outlier residues in this chain.

- Molecule 1: Amyloid-beta precursor protein



There are no outlier residues in this chain.

5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 10 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
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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	123
Number of shifts mapped to atoms	123
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	2%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 2% for the well-defined parts and 2% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *NMR-STAR_3.1_for_pABeta_fibrils_new1.txt*

7.1.1 Bookkeeping

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	123
Number of shifts mapped to atoms	123
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	32	1.10 ± 0.56	None needed (imprecise)
$^{13}\text{C}_\beta$	26	0.28 ± 0.51	None needed (< 0.5 ppm)
$^{13}\text{C}'$	32	1.70 ± 0.23	Should be applied
^{15}N	0	—	None (insufficient data)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 2%, i.e. 108 atoms were assigned a chemical shift out of a possible 4376. 0 out of 76 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	56/1752 (3%)	0/735 (0%)	56/678 (8%)	0/339 (0%)
Sidechain	52/2178 (2%)	0/1439 (0%)	52/690 (8%)	0/49 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/446 (0%)	0/229 (0%)	0/198 (0%)	0/19 (0%)
Overall	108/4376 (2%)	0/2403 (0%)	108/1566 (7%)	0/407 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

