



# wwPDB NMR Structure Validation Summary Report ⓘ

Mar 24, 2026 – 09:08 AM UTC

PDB ID : 8F4V / pdb\_00008f4v  
BMRB ID : 31058  
Title : Alpha7 nicotinic acetylcholine receptor intracellular and transmembrane domains bound to ivermectin in a desensitized state  
Authors : Bondarenko, V.; Chen, Q.; Tang, P.  
Deposited on : 2022-11-11

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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)  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 12%.

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 15 models. Model 11 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:209-A:472, B:209-B:472, C:209-C:472, D:209-D:472, E:209-E:472 (1320)	1.87	11

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21090 atoms, of which 10680 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Neuronal acetylcholine receptor subunit alpha-7.

Mol	Chain	Residues	Atoms						Trace
1	A	264	Total	C	H	N	O	S	0
			4082	1300	2062	340	359	21	
1	B	264	Total	C	H	N	O	S	0
			4082	1300	2062	340	359	21	
1	C	264	Total	C	H	N	O	S	0
			4082	1300	2062	340	359	21	
1	D	264	Total	C	H	N	O	S	0
			4082	1300	2062	340	359	21	
1	E	264	Total	C	H	N	O	S	0
			4082	1300	2062	340	359	21	

There are 50 discrepancies between the modelled and reference sequences:

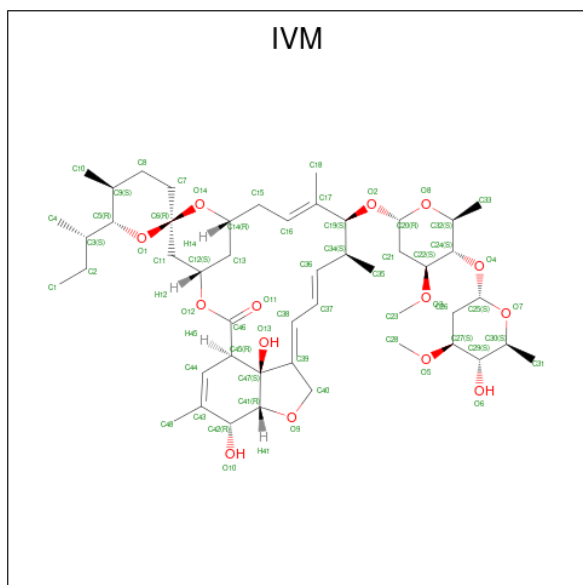
Chain	Residue	Modelled	Actual	Comment	Reference
A	203	SER	-	expression tag	UNP P36544
A	204	ASN	-	expression tag	UNP P36544
A	205	ALA	-	expression tag	UNP P36544
A	206	GLU	-	expression tag	UNP P36544
A	207	GLU	-	expression tag	UNP P36544
A	208	GLU	-	expression tag	UNP P36544
A	263	SER	ALA	engineered mutation	UNP P36544
A	268	SER	VAL	engineered mutation	UNP P36544
A	270	SER	LEU	engineered mutation	UNP P36544
A	474	GLU	ALA	engineered mutation	UNP P36544
B	203	SER	-	expression tag	UNP P36544
B	204	ASN	-	expression tag	UNP P36544
B	205	ALA	-	expression tag	UNP P36544
B	206	GLU	-	expression tag	UNP P36544
B	207	GLU	-	expression tag	UNP P36544
B	208	GLU	-	expression tag	UNP P36544
B	263	SER	ALA	engineered mutation	UNP P36544
B	268	SER	VAL	engineered mutation	UNP P36544
B	270	SER	LEU	engineered mutation	UNP P36544
B	474	GLU	ALA	engineered mutation	UNP P36544
C	203	SER	-	expression tag	UNP P36544
C	204	ASN	-	expression tag	UNP P36544
C	205	ALA	-	expression tag	UNP P36544

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Chain	Residue	Modelled	Actual	Comment	Reference
C	206	GLU	-	expression tag	UNP P36544
C	207	GLU	-	expression tag	UNP P36544
C	208	GLU	-	expression tag	UNP P36544
C	263	SER	ALA	engineered mutation	UNP P36544
C	268	SER	VAL	engineered mutation	UNP P36544
C	270	SER	LEU	engineered mutation	UNP P36544
C	474	GLU	ALA	engineered mutation	UNP P36544
D	203	SER	-	expression tag	UNP P36544
D	204	ASN	-	expression tag	UNP P36544
D	205	ALA	-	expression tag	UNP P36544
D	206	GLU	-	expression tag	UNP P36544
D	207	GLU	-	expression tag	UNP P36544
D	208	GLU	-	expression tag	UNP P36544
D	263	SER	ALA	engineered mutation	UNP P36544
D	268	SER	VAL	engineered mutation	UNP P36544
D	270	SER	LEU	engineered mutation	UNP P36544
D	474	GLU	ALA	engineered mutation	UNP P36544
E	203	SER	-	expression tag	UNP P36544
E	204	ASN	-	expression tag	UNP P36544
E	205	ALA	-	expression tag	UNP P36544
E	206	GLU	-	expression tag	UNP P36544
E	207	GLU	-	expression tag	UNP P36544
E	208	GLU	-	expression tag	UNP P36544
E	263	SER	ALA	engineered mutation	UNP P36544
E	268	SER	VAL	engineered mutation	UNP P36544
E	270	SER	LEU	engineered mutation	UNP P36544
E	474	GLU	ALA	engineered mutation	UNP P36544

- Molecule 2 is (2aE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17aR,20R,20aR,20bS)-6'-[(2S)-butan-2-yl]-20,20b-dihydroxy-5',6,8,19-tetramethyl-17-oxo-3',4',5',6,6',10,11,14,15,17,17a,20,20a,20b-tetradecahydro-2H,7H-spiro[11,15-methanofuro[4,3,2-pq][2,6]benzodioxacy clooctadecine-13,2'-pyran]-7-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl-alpha-L-arabino-hexopyranosyl)-3-O-methyl-alpha-L-arabino-hexopyranoside (CCD ID: IVM) (formula: C<sub>48</sub>H<sub>74</sub>O<sub>14</sub>) (labeled as "Ligand of Interest" by depositor).



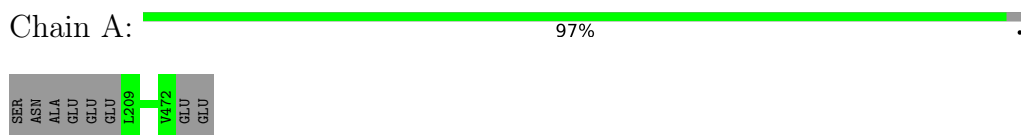
Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	A	1	Total	C	H	O
			136	48	74	14
2	A	1	Total	C	H	O
			136	48	74	14
2	B	1	Total	C	H	O
			136	48	74	14
2	C	1	Total	C	H	O
			136	48	74	14
2	D	1	Total	C	H	O
			136	48	74	14

## 4 Residue-property plots [i](#)

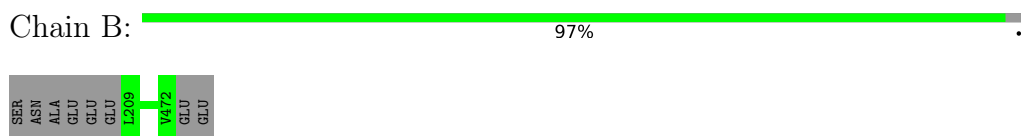
### 4.1 Average score per residue in the NMR ensemble

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.

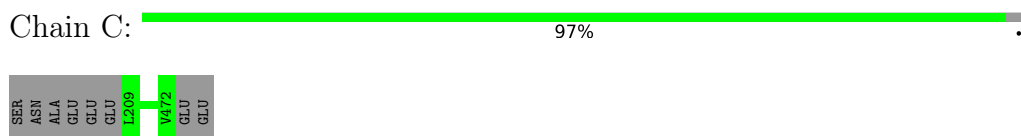
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



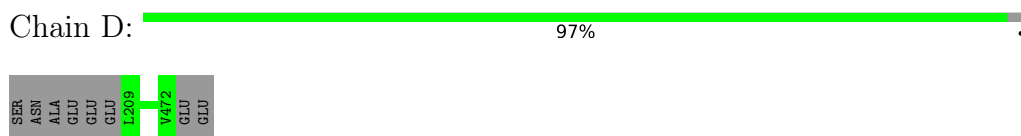
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



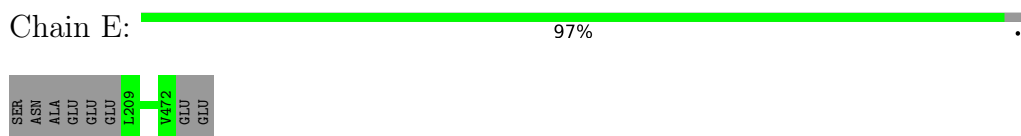
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7



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- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

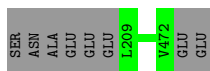


## 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 11. Colouring as in section 4.1 above.

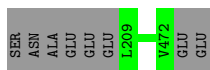
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain A:  97%



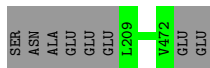
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain B:  97%



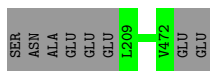
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain C:  97%



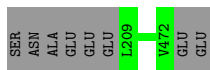
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain D:  97%



- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7

Chain E:  97%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *na, na*.

Of the 1000 calculated structures, 15 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
CS-ROSETTA	structure calculation	3.17
Rosetta	structure calculation	3.7
Rosetta	refinement	3.7
MolProbity	refinement	

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	2107
Number of shifts mapped to atoms	2107
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	12%

## 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 12% for the well-defined parts and 12% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: starch\_output

#### 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	2107
Number of shifts mapped to atoms	2107
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	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	259	$-0.51 \pm 0.07$	Should be checked
$^{13}\text{C}_\beta$	170	$0.24 \pm 0.02$	None needed (< 0.5 ppm)
$^{13}\text{C}'$	200	$-0.09 \pm 0.08$	None needed (< 0.5 ppm)
$^{15}\text{N}$	231	$0.33 \pm 0.13$	None needed (< 0.5 ppm)

#### 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 12%, i.e. 2107 atoms were assigned a chemical shift out of a possible 17880. 0 out of 285 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	1155/6505 (18%)	465/2635 (18%)	459/2640 (17%)	231/1230 (19%)
Sidechain	904/10045 (9%)	612/6665 (9%)	288/3100 (9%)	4/280 (1%)

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	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Aromatic	48/1330 (4%)	27/650 (4%)	17/580 (3%)	4/100 (4%)
Overall	2107/17880 (12%)	1104/9950 (11%)	764/6320 (12%)	239/1610 (15%)

#### 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:

