

# wwPDB EM Validation Summary Report (i)

Nov 9, 2022 – 06:20 AM JST

PDB ID : 6IRF

EMDB ID : EMD-9715

Title : Structure of the human GluN1/GluN2A NMDA receptor in the glutamate/gl

ycine-bound state at pH 6.3, Class I

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Deposited on : 2018-11-12

Resolution : 5.10 Å(reported)
Based on initial models : 4PE5, 5TQ0, 5H8F

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

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:

EMDB validation analysis : 0.0.1.dev43

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ: FAILED

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

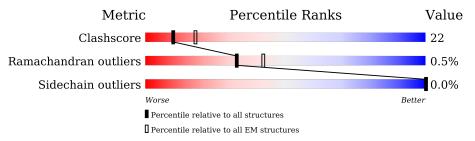
Validation Pipeline (wwPDB-VP) : 2.31.2

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 5.10 Å.

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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	847	63%	29%	• 7%		
1	С	847	62%	30%	• 7%		
2	В	841	63%	26%	11%		
2	D	841	63%	26%	11%		



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23912 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Glutamate receptor ionotropic, NMDA 1.

$\mathbf{Mol}$	Chain	Residues	${f Atoms}$					AltConf	Trace	
1	Δ	787	Total	С	N	О	S	1	0	
1	Λ	101	6168	3931	1070	1132	35	1	U	
1	C	787	Total	С	N	O	S	1	0	
1	C	101	6168	3931	1070	1132	35	1	U	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	ARG	GLY	engineered mutation	UNP Q05586
С	612	ARG	GLY	engineered mutation	UNP Q05586

• Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	В	752	Total 5788	C 3740	N 950	O 1062	S 36	1	0
2	D	752	Total 5788	C 3740	N 950	O 1062	S 36	1	0

There are 4 discrepancies between the modelled and reference sequences:

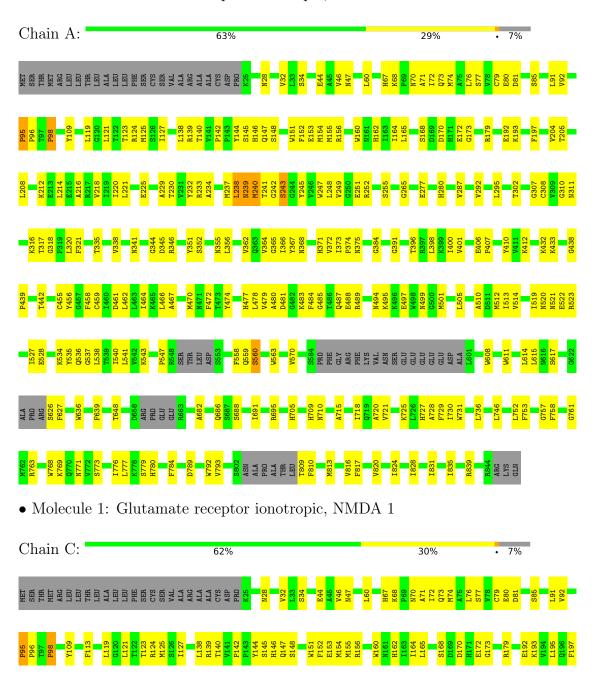
Chain	Residue	Modelled	Actual	Comment	Reference
В	656	ARG	GLU	engineered mutation	UNP Q12879
В	657	ARG	GLU	engineered mutation	UNP Q12879
D	656	ARG	GLU	engineered mutation	UNP Q12879
D	657	ARG	GLU	engineered mutation	UNP Q12879



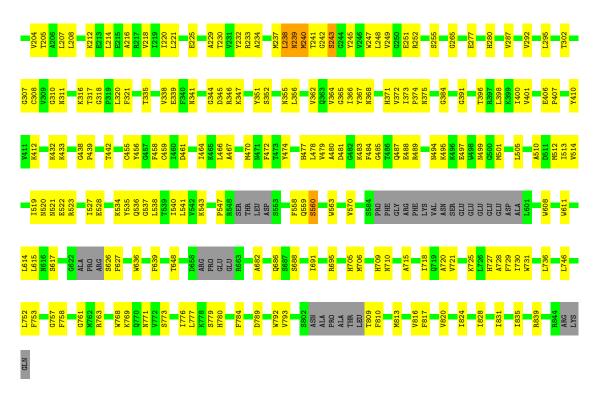
## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

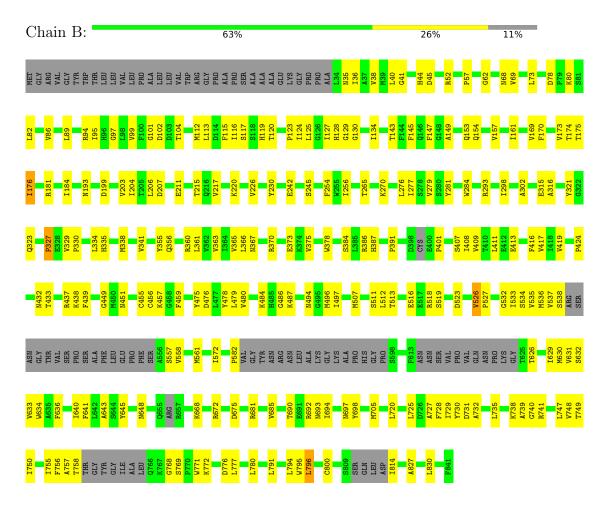
• Molecule 1: Glutamate receptor ionotropic, NMDA 1





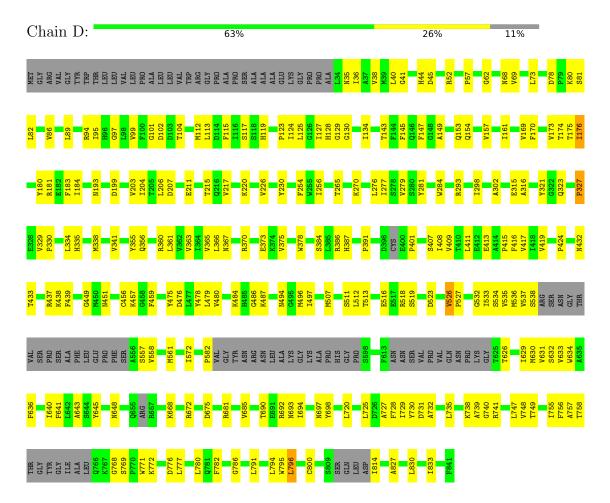


• Molecule 2: Glutamate receptor ionotropic, NMDA 2A





• Molecule 2: Glutamate receptor ionotropic, NMDA 2A





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193878	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality (i)

### 5.1 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 root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.33	0/6297	0.60	6/8519 (0.1%)	
1	С	0.33	0/6297	0.59	5/8519 (0.1%)	
2	В	0.32	0/5918	0.59	9/8033 (0.1%)	
2	D	0.32	0/5918	0.59	9/8033 (0.1%)	
All	All	0.32	0/24430	0.59	$29/33104 \ (0.1\%)$	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	С	0	1
2	В	0	4
2	D	0	4
All	All	0	10

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	С	95	PRO	N-CA-CB	8.20	113.14	103.30
1	A	95	PRO	N-CA-CB	8.20	113.14	103.30
2	D	526	VAL	C-N-CD	7.89	144.97	128.40
2	В	526	VAL	C-N-CD	7.75	144.68	128.40
2	D	327	PRO	N-CA-CB	6.56	111.17	103.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	232	TYR	Mainchain
2	В	170	PHE	Peptide
2	В	44	HIS	Peptide
2	В	62	GLY	Peptide
2	В	796	LEU	Peptide

#### 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6168	0	6120	296	0
1	С	6168	0	6119	307	0
2	В	5788	0	5594	360	0
2	D	5788	0	5594	356	0
All	All	23912	0	23427	1034	0

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 22.

The worst 5 of 1034 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
2:D:537:VAL:CG1	2:D:727:ALA:HB2	1.35	1.52
2:B:537:VAL:CG1	2:B:727:ALA:HB2	1.35	1.51
2:B:537:VAL:HG12	2:B:727:ALA:CB	1.39	1.51
2:D:537:VAL:HG12	2:D:727:ALA:CB	1.39	1.49
2:B:561:MET:HB3	1:C:817:PHE:CZ	1.47	1.49

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 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 EM 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	Perce	ntiles
1	A	776/847 (92%)	702 (90%)	68 (9%)	6 (1%)	19	60
1	С	776/847 (92%)	703 (91%)	67 (9%)	6 (1%)	19	60
2	В	737/841 (88%)	659 (89%)	76 (10%)	2 (0%)	41	76
2	D	737/841 (88%)	659 (89%)	76 (10%)	2 (0%)	41	76
All	All	3026/3376 (90%)	2723 (90%)	287 (10%)	16 (0%)	32	68

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	PRO
1	A	98	PRO
1	A	240	MET
2	В	329	VAL
1	С	95	PRO

#### 5.3.2 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 EM 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	661/731 (90%)	661 (100%)	0	100	100
1	С	661/731 (90%)	660 (100%)	1 (0%)	93	96
2	В	609/729 (84%)	609 (100%)	0	100	100
2	D	609/729 (84%)	609 (100%)	0	100	100
All	All	2540/2920 (87%)	2539 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	243	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36



such sidechains are listed below:

Mol	Chain	Res	Type
2	D	42	HIS
2	D	766	GLN
2	D	96	HIS
2	D	367	ASN
2	В	323	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9715. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections (i)

This section was not generated.

#### 6.2 Central slices (i)

This section was not generated.

#### 6.3 Largest variance slices (i)

This section was not generated.

### 6.4 Orthogonal surface views (i)

This section was not generated.

#### 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

#### 7.1 Map-value distribution (i)

This section was not generated.

### 7.2 Volume estimate versus contour level (i)

This section was not generated.

### 7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



# 9 Map-model fit (i)

This section was not generated.

