



## wwPDB EM Map/Model Validation Report ⓘ

Jun 9, 2016 – 04:26 PM EDT

PDB ID : 5FXI  
EMDB ID: : 3354  
Title : GluN1b-GluN2B NMDA receptor structure in non-active-2 conformation  
Authors : Tajima, N.; Karakas, E.; Grant, T.; Simorowski, N.; Diaz-Avalos, R.; Grigorieff, N.; Furukawa, H.  
Deposited on : 2016-03-02  
Resolution : 6.40 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

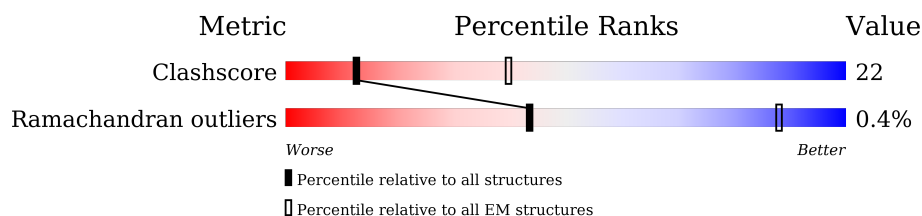
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.40 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 (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	846	
1	C	846	
2	B	827	
2	D	827	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15318 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 N-METHYL-D-ASPARTATE RECEPTOR GLUN1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	784	Total	C	N	O	0	0
			3868	2300	784	784		
1	C	787	Total	C	N	O	0	0
			3881	2307	787	787		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLN	ASN	ENGINEERED MUTATION	UNP P35439
A	260	ASP	ASN	ENGINEERED MUTATION	UNP P35439
A	371	GLN	ASN	ENGINEERED MUTATION	UNP P35439
A	492	GLN	ASN	ENGINEERED MUTATION	UNP P35439
A	512	GLN	ASN	ENGINEERED MUTATION	UNP P35439
A	615	GLN	GLU	ENGINEERED MUTATION	UNP P35439
A	616	SER	GLU	ENGINEERED MUTATION	UNP P35439
A	618	SER	GLU	ENGINEERED MUTATION	UNP P35439
A	619	THR	GLU	ENGINEERED MUTATION	UNP P35439
A	792	GLN	ASN	ENGINEERED MUTATION	UNP P35439
A	831	CYS	PHE	ENGINEERED MUTATION	UNP P35439
A	865	ASN	ARG	ENGINEERED MUTATION	UNP P35439
A	866	GLY	ARG	ENGINEERED MUTATION	UNP P35439
A	867	ALA	LYS	ENGINEERED MUTATION	UNP P35439
C	61	GLN	ASN	ENGINEERED MUTATION	UNP P35439
C	260	ASP	ASN	ENGINEERED MUTATION	UNP P35439
C	371	GLN	ASN	ENGINEERED MUTATION	UNP P35439
C	492	GLN	ASN	ENGINEERED MUTATION	UNP P35439
C	512	GLN	ASN	ENGINEERED MUTATION	UNP P35439
C	615	GLN	GLU	ENGINEERED MUTATION	UNP P35439
C	616	SER	GLU	ENGINEERED MUTATION	UNP P35439
C	618	SER	GLU	ENGINEERED MUTATION	UNP P35439
C	619	THR	GLU	ENGINEERED MUTATION	UNP P35439
C	792	GLN	ASN	ENGINEERED MUTATION	UNP P35439
C	831	CYS	PHE	ENGINEERED MUTATION	UNP P35439
C	865	ASN	ARG	ENGINEERED MUTATION	UNP P35439

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Chain	Residue	Modelled	Actual	Comment	Reference
C	866	GLY	ARG	ENGINEERED MUTATION	UNP P35439
C	867	ALA	LYS	ENGINEERED MUTATION	UNP P35439

- Molecule 2 is a protein called N-METHYL-D-ASPARTATE RECEPTOR GLUN2B.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	770	Total	C	N	O	0	0
			3799	2259	770	770		
2	D	764	Total	C	N	O	0	0
			3770	2242	764	764		

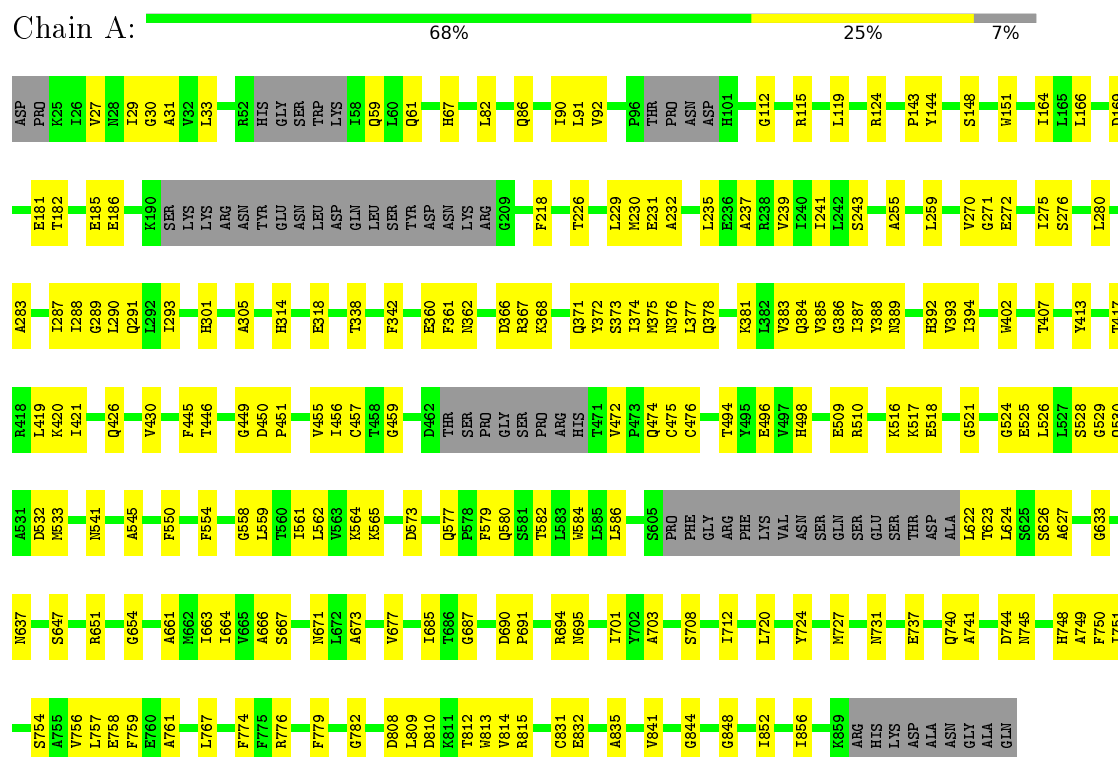
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLY	-	EXPRESSION TAG	UNP Q00960
B	348	ASP	ASN	ENGINEERED MUTATION	UNP Q00960
B	557	CYS	ASP	ENGINEERED MUTATION	UNP Q00960
B	588	SER	CYS	ENGINEERED MUTATION	UNP Q00960
B	838	SER	CYS	ENGINEERED MUTATION	UNP Q00960
B	849	SER	CYS	ENGINEERED MUTATION	UNP Q00960
D	26	GLY	-	EXPRESSION TAG	UNP Q00960
D	348	ASP	ASN	ENGINEERED MUTATION	UNP Q00960
D	557	CYS	ASP	ENGINEERED MUTATION	UNP Q00960
D	588	SER	CYS	ENGINEERED MUTATION	UNP Q00960
D	838	SER	CYS	ENGINEERED MUTATION	UNP Q00960
D	849	SER	CYS	ENGINEERED MUTATION	UNP Q00960

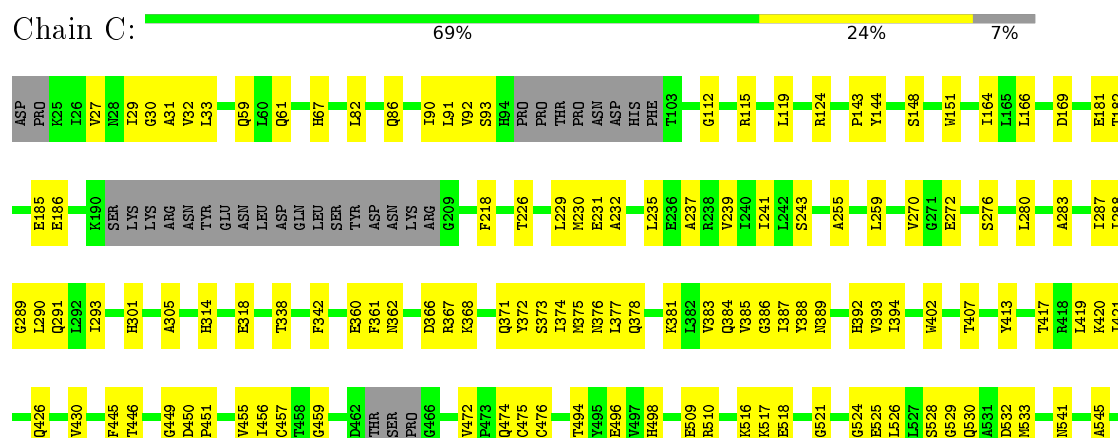
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: N-METHYL-D-ASPARTATE RECEPTOR GLUN1



#### • Molecule 1: N-METHYL-D-ASPARTATE RECEPTOR GLUN1





TRP
GLN
PHE
ARG
HIS
SER
PHE
MET
GLY

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	100	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor



## 5 Model quality

### 5.1 Standard geometry

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	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	A	0.28	0/3862	0.47	0/5366
1	C	0.28	0/3876	0.47	0/5386
2	B	0.27	0/3793	0.45	0/5270
2	D	0.27	0/3764	0.47	1/5230 (0.0%)
All	All	0.28	0/15295	0.46	1/21252 (0.0%)

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 outliers	#Planarity outliers
1	C	0	2
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	547	PRO	N-CA-CB	6.76	111.42	103.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	683	GLU	Peptide
1	C	684	ARG	Peptide
2	D	658	GLU	Peptide
2	D	812	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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	3868	0	1753	138	0
1	C	3881	0	1763	134	0
2	B	3799	0	1696	108	0
2	D	3770	0	1683	106	0
All	All	15318	0	6895	486	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 486 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:PRO:HA	2:B:82:ILE:H	1.38	0.89
1:A:737:GLU:O	1:A:741:ALA:HB2	1.75	0.86
1:C:737:GLU:O	1:C:741:ALA:HB2	1.75	0.86
2:D:78:PRO:HA	2:D:82:ILE:H	1.38	0.84
1:A:623:THR:O	1:A:627:ALA:HB2	1.79	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	Percentiles	
1	A	772/846 (91%)	696 (90%)	74 (10%)	2 (0%)	46	83
1	C	777/846 (92%)	700 (90%)	75 (10%)	2 (0%)	46	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	758/827 (92%)	684 (90%)	70 (9%)	4 (0%)	34 77
2	D	752/827 (91%)	680 (90%)	67 (9%)	5 (1%)	26 71
All	All	3059/3346 (91%)	2760 (90%)	286 (9%)	13 (0%)	43 80

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	490	ILE
2	D	490	ILE
2	D	547	PRO
1	C	685	ILE
1	A	685	ILE

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 carbohydrates 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 ⓘ

There are no chain breaks in this entry.