



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:32 PM GMT

PDB ID : 4TLL  
Title : Crystal structure of GluN1/GluN2B NMDA receptor, structure 1  
Authors : Gouaux, E.; Lee, C.-H.; Lu, W.  
Deposited on : 2014-05-30  
Resolution : 3.59 Å(reported)

This is a wwPDB X-ray 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

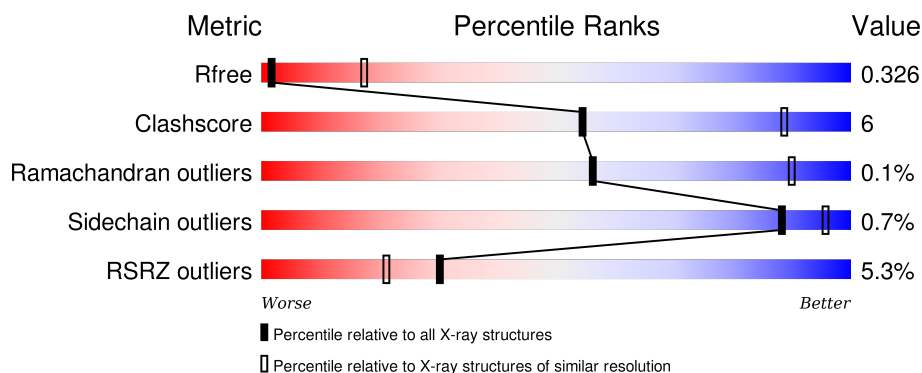
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.59 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	823	<div> <div>9%</div> <div>78% 15% 7%</div> </div>
1	C	823	<div> <div>9%</div> <div>81% 6% 13%</div> </div>
2	B	824	<div> <div>5%</div> <div>77% 12% 10%</div> </div>
2	D	824	<div> <div>4%</div> <div>85% 7% 8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	JEG	D	902	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18759 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 receptor subunit GluN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	767	Total	C	N	O	S	0	0	0
			5208	3300	915	969	24			
1	C	719	Total	C	N	O	S	0	0	0
			4193	2583	787	808	15			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	CYS	engineered mutation	UNP C0KD18
A	51	PHE	LYS	engineered mutation	UNP C0KD18
A	52	PHE	ARG	engineered mutation	UNP C0KD18
A	300	GLN	ASN	engineered mutation	UNP C0KD18
A	350	GLN	ASN	engineered mutation	UNP C0KD18
A	368	ASP	ASN	engineered mutation	UNP C0KD18
A	440	ASP	ASN	engineered mutation	UNP C0KD18
A	469	ASP	ASN	engineered mutation	UNP C0KD18
A	493	ALA	LYS	engineered mutation	UNP C0KD18
A	494	ALA	LYS	engineered mutation	UNP C0KD18
A	495	ALA	GLU	engineered mutation	UNP C0KD18
A	602	ARG	GLY	engineered mutation	UNP C0KD18
A	609	LEU	ILE	engineered mutation	UNP C0KD18
A	648	ARG	ASP	engineered mutation	UNP C0KD18
A	761	GLU	ASN	engineered mutation	UNP C0KD18
A	829	SER	-	insertion	UNP C0KD18
A	830	ARG	-	insertion	UNP C0KD18
A	831	ALA	-	insertion	UNP C0KD18
A	832	GLU	-	insertion	UNP C0KD18
A	833	ALA	-	insertion	UNP C0KD18
A	834	LYS	-	insertion	UNP C0KD18
A	835	ARG	-	insertion	UNP C0KD18
A	836	MET	-	insertion	UNP C0KD18
A	837	LYS	-	insertion	UNP C0KD18
A	838	GLY	-	expression tag	UNP C0KD18

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Chain	Residue	Modelled	Actual	Comment	Reference
A	839	LEU	-	expression tag	UNP C0KD18
A	840	GLU	-	expression tag	UNP C0KD18
A	841	VAL	-	expression tag	UNP C0KD18
A	842	LEU	-	expression tag	UNP C0KD18
A	843	PHE	-	expression tag	UNP C0KD18
A	844	GLN	-	expression tag	UNP C0KD18
C	22	ALA	CYS	engineered mutation	UNP C0KD18
C	51	PHE	LYS	engineered mutation	UNP C0KD18
C	52	PHE	ARG	engineered mutation	UNP C0KD18
C	300	GLN	ASN	engineered mutation	UNP C0KD18
C	350	GLN	ASN	engineered mutation	UNP C0KD18
C	368	ASP	ASN	engineered mutation	UNP C0KD18
C	440	ASP	ASN	engineered mutation	UNP C0KD18
C	469	ASP	ASN	engineered mutation	UNP C0KD18
C	493	ALA	LYS	engineered mutation	UNP C0KD18
C	494	ALA	LYS	engineered mutation	UNP C0KD18
C	495	ALA	GLU	engineered mutation	UNP C0KD18
C	602	ARG	GLY	engineered mutation	UNP C0KD18
C	609	LEU	ILE	engineered mutation	UNP C0KD18
C	648	ARG	ASP	engineered mutation	UNP C0KD18
C	761	GLU	ASN	engineered mutation	UNP C0KD18
C	829	SER	-	insertion	UNP C0KD18
C	830	ARG	-	insertion	UNP C0KD18
C	831	ALA	-	insertion	UNP C0KD18
C	832	GLU	-	insertion	UNP C0KD18
C	833	ALA	-	insertion	UNP C0KD18
C	834	LYS	-	insertion	UNP C0KD18
C	835	ARG	-	insertion	UNP C0KD18
C	836	MET	-	insertion	UNP C0KD18
C	837	LYS	-	insertion	UNP C0KD18
C	838	GLY	-	expression tag	UNP C0KD18
C	839	LEU	-	expression tag	UNP C0KD18
C	840	GLU	-	expression tag	UNP C0KD18
C	841	VAL	-	expression tag	UNP C0KD18
C	842	LEU	-	expression tag	UNP C0KD18
C	843	PHE	-	expression tag	UNP C0KD18
C	844	GLN	-	expression tag	UNP C0KD18

- Molecule 2 is a protein called receptor subunit GluN2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	738	Total	C	N	O	S	0	0	0
			4669	2924	812	910	23			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	757	Total	C	N	O	S	0	0	0
			4565	2856	808	882	19			

There are 58 discrepancies between the modelled and reference sequences:

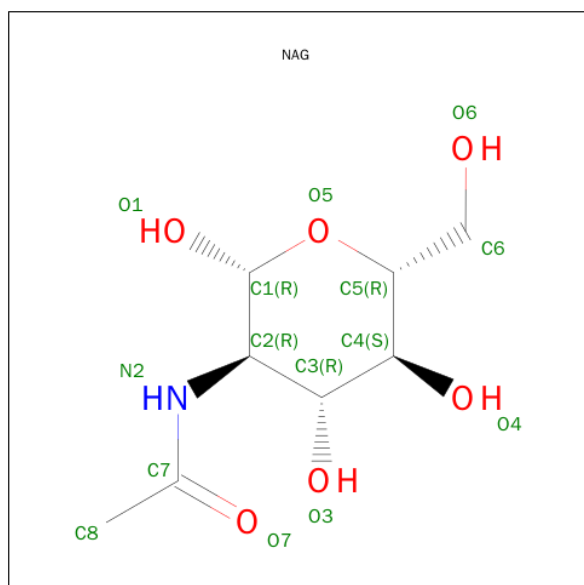
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	MET	engineered mutation	UNP A7XY94
B	21	ARG	GLY	engineered mutation	UNP A7XY94
B	22	ALA	CYS	engineered mutation	UNP A7XY94
B	64	GLU	ALA	engineered mutation	UNP A7XY94
B	69	GLN	ASN	engineered mutation	UNP A7XY94
B	216	CYS	LYS	engineered mutation	UNP A7XY94
B	343	ASP	ASN	engineered mutation	UNP A7XY94
B	486	VAL	THR	engineered mutation	UNP A7XY94
B	601	LEU	VAL	engineered mutation	UNP A7XY94
B	640	ARG	GLU	engineered mutation	UNP A7XY94
B	641	ARG	GLU	engineered mutation	UNP A7XY94
B	826	TYR	-	insertion	UNP A7XY94
B	827	LYS	-	insertion	UNP A7XY94
B	828	SER	-	insertion	UNP A7XY94
B	829	ARG	-	insertion	UNP A7XY94
B	830	ALA	-	insertion	UNP A7XY94
B	831	GLU	-	insertion	UNP A7XY94
B	832	ALA	-	insertion	UNP A7XY94
B	833	LYS	-	insertion	UNP A7XY94
B	834	ARG	-	insertion	UNP A7XY94
B	835	MET	-	insertion	UNP A7XY94
B	836	LYS	-	insertion	UNP A7XY94
B	837	GLY	-	expression tag	UNP A7XY94
B	838	LEU	-	expression tag	UNP A7XY94
B	839	GLU	-	expression tag	UNP A7XY94
B	840	VAL	-	expression tag	UNP A7XY94
B	841	LEU	-	expression tag	UNP A7XY94
B	842	PHE	-	expression tag	UNP A7XY94
B	843	GLN	-	expression tag	UNP A7XY94
D	20	SER	MET	engineered mutation	UNP A7XY94
D	21	ARG	GLY	engineered mutation	UNP A7XY94
D	22	ALA	CYS	engineered mutation	UNP A7XY94
D	64	GLU	ALA	engineered mutation	UNP A7XY94
D	69	GLN	ASN	engineered mutation	UNP A7XY94
D	216	CYS	LYS	engineered mutation	UNP A7XY94
D	343	ASP	ASN	engineered mutation	UNP A7XY94

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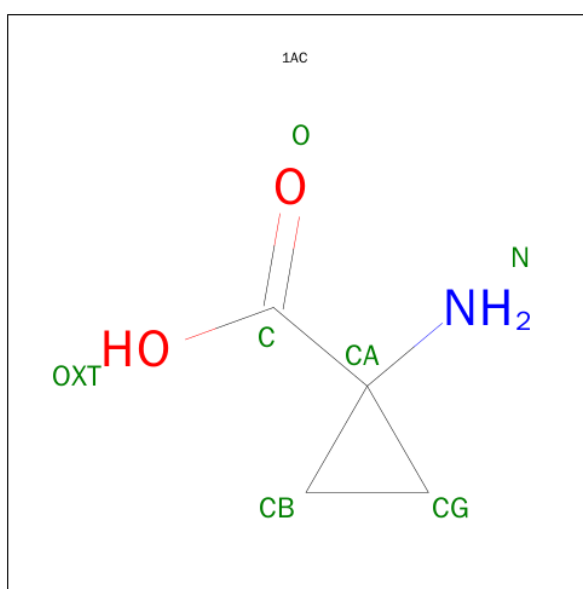
Chain	Residue	Modelled	Actual	Comment	Reference
D	486	VAL	THR	engineered mutation	UNP A7XY94
D	601	LEU	VAL	engineered mutation	UNP A7XY94
D	640	ARG	GLU	engineered mutation	UNP A7XY94
D	641	ARG	GLU	engineered mutation	UNP A7XY94
D	826	TYR	-	insertion	UNP A7XY94
D	827	LYS	-	insertion	UNP A7XY94
D	828	SER	-	insertion	UNP A7XY94
D	829	ARG	-	insertion	UNP A7XY94
D	830	ALA	-	insertion	UNP A7XY94
D	831	GLU	-	insertion	UNP A7XY94
D	832	ALA	-	insertion	UNP A7XY94
D	833	LYS	-	insertion	UNP A7XY94
D	834	ARG	-	insertion	UNP A7XY94
D	835	MET	-	insertion	UNP A7XY94
D	836	LYS	-	insertion	UNP A7XY94
D	837	GLY	-	expression tag	UNP A7XY94
D	838	LEU	-	expression tag	UNP A7XY94
D	839	GLU	-	expression tag	UNP A7XY94
D	840	VAL	-	expression tag	UNP A7XY94
D	841	LEU	-	expression tag	UNP A7XY94
D	842	PHE	-	expression tag	UNP A7XY94
D	843	GLN	-	expression tag	UNP A7XY94

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

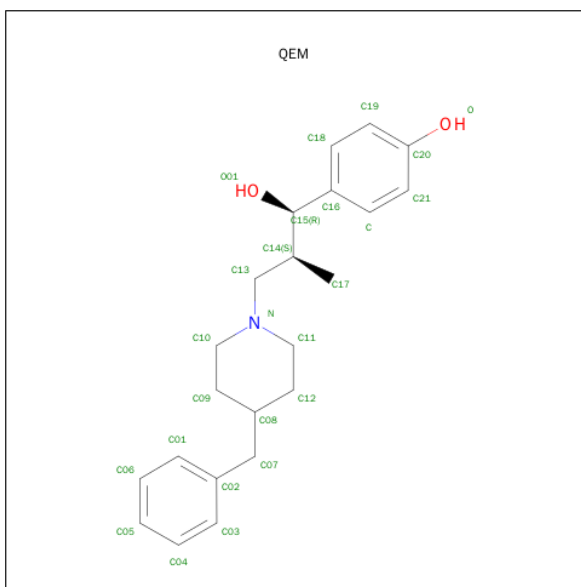
- Molecule 4 is 1-AMINOCYCLOPROPANECARBOXYLIC ACID (three-letter code: 1AC) (formula: C<sub>4</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	4	1	2		

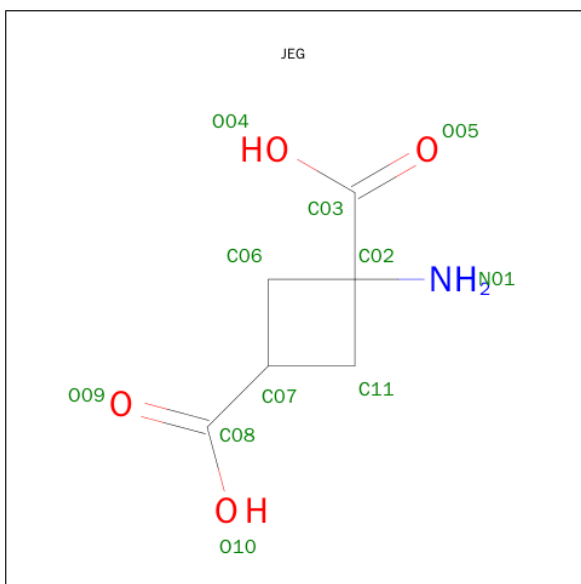
- Molecule 5 is 4-[(1R,2S)-3-(4-benzylpiperidin-1-yl)-1-hydroxy-2-methylpropyl]phenol (three-letter code: QEM) (formula: C<sub>22</sub>H<sub>29</sub>NO<sub>2</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			25	22	1	2		
5	D	1	Total	C	N	O	0	0
			25	22	1	2		

- Molecule 6 is trans-1-aminocyclobutane-1,3-dicarboxylic acid (three-letter code: JEG) (formula:  $C_4H_7NO_4$ ).

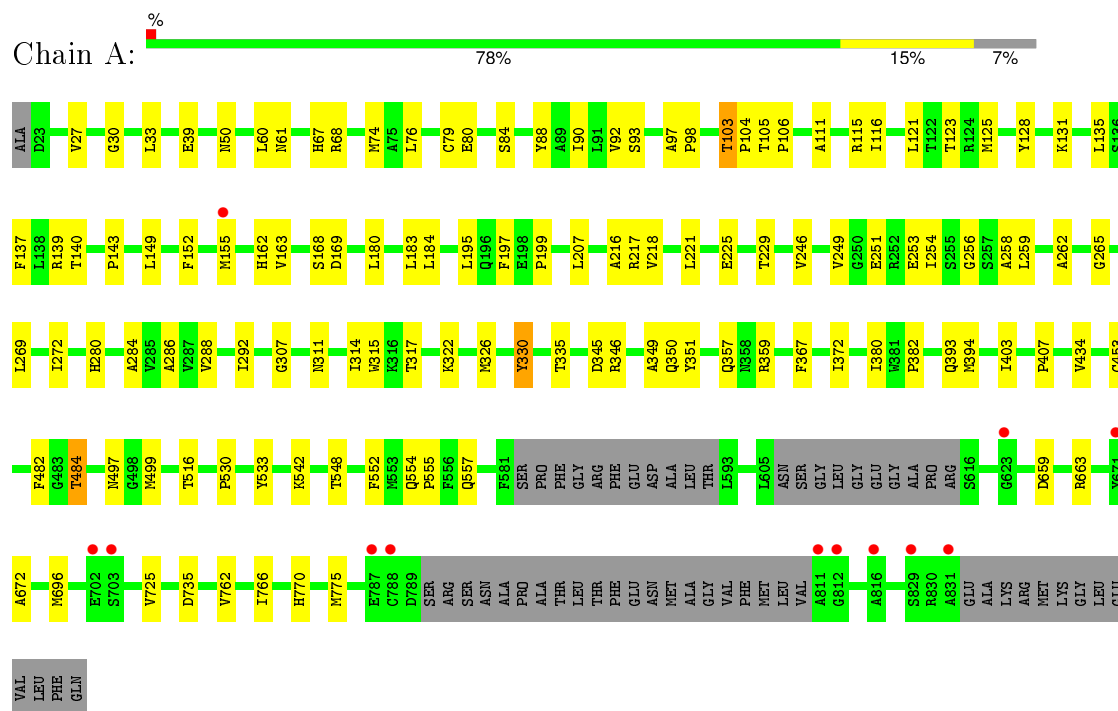


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			11	6	1	4		

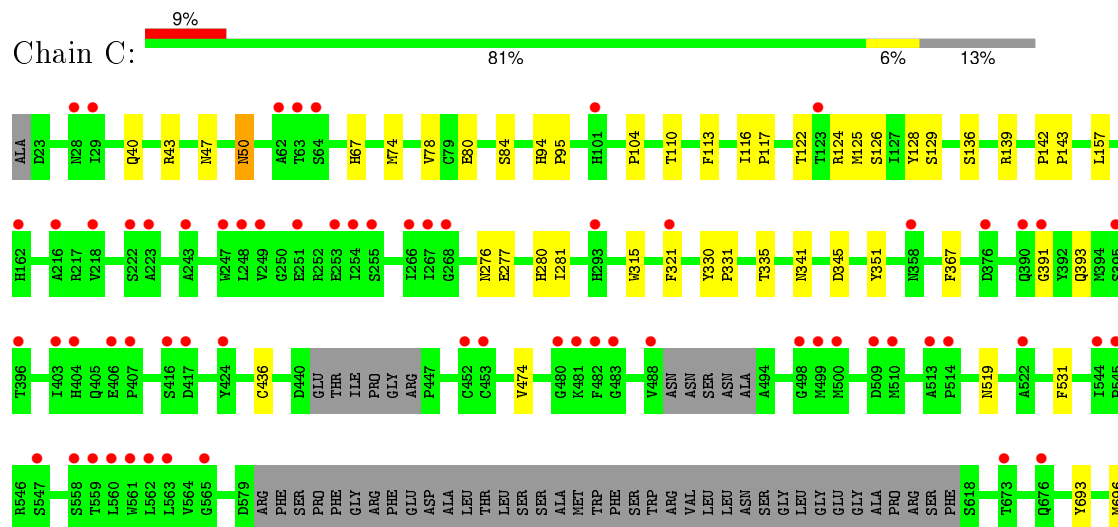
### 3 Residue-property plots

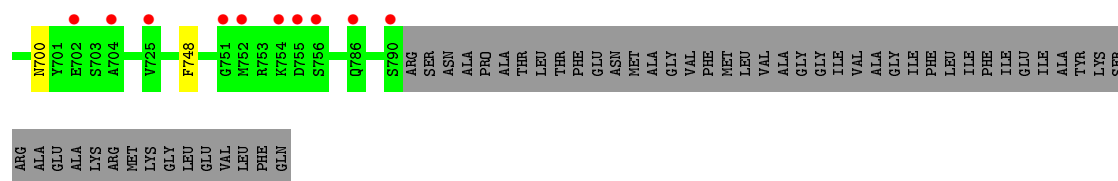
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: receptor subunit GluN1

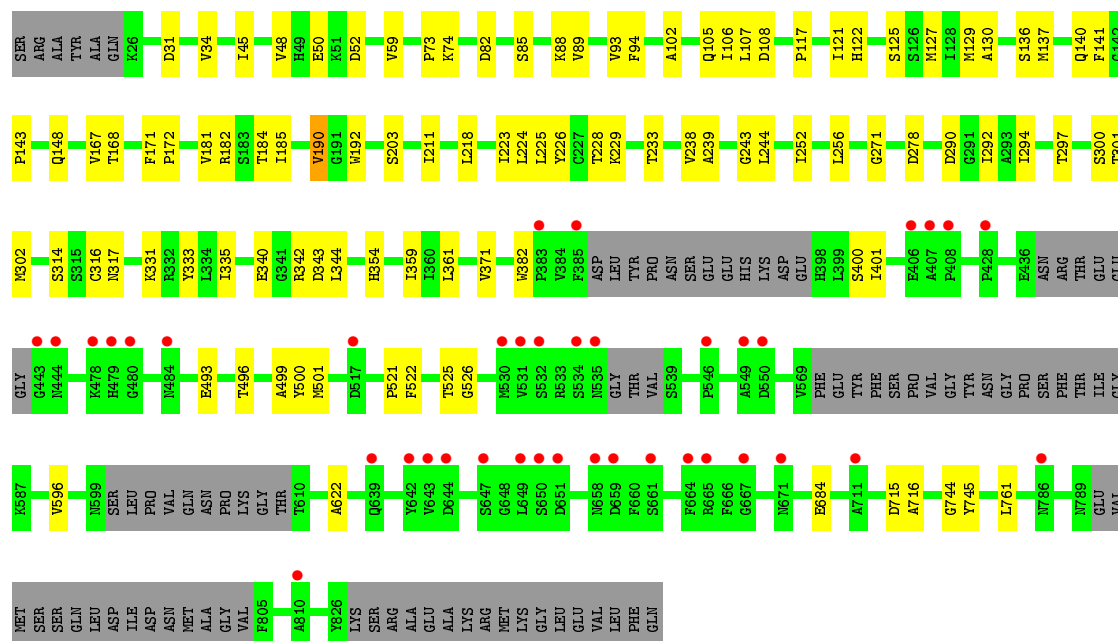
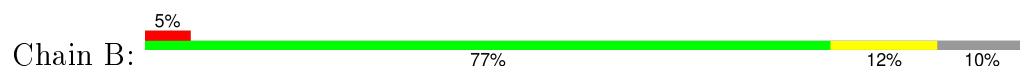


#### • Molecule 1: receptor subunit GluN1

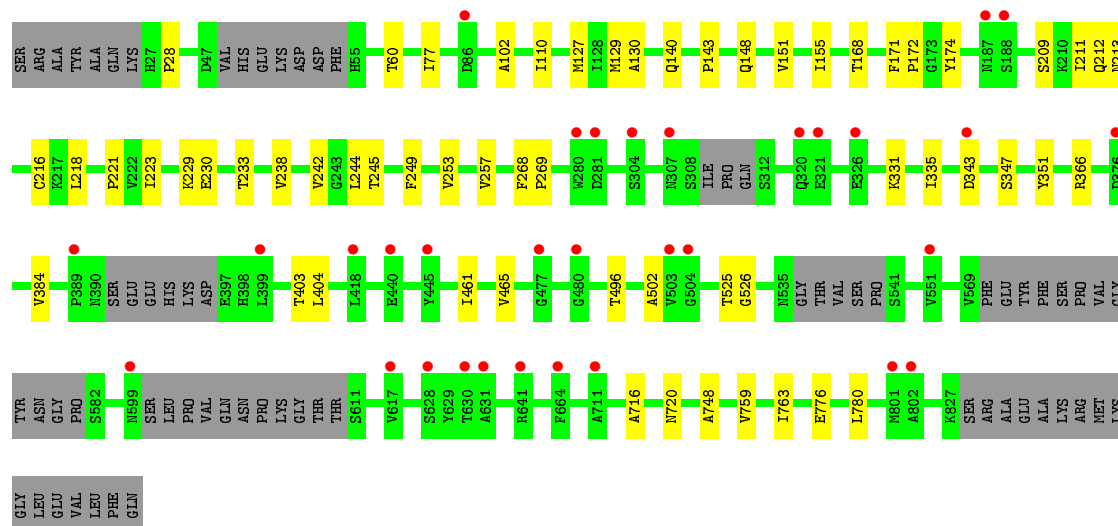
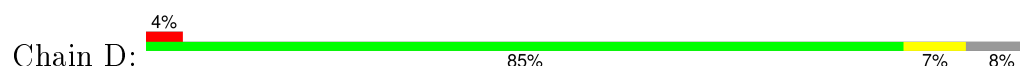




• Molecule 2: receptor subunit GluN2B



• Molecule 2: receptor subunit GluN2B



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.46 Å   117.26 Å   218.76 Å 90.00°   106.70°   90.00°	Depositor
Resolution (Å)	48.08 – 3.59 48.08 – 3.50	Depositor EDS
% Data completeness (in resolution range)	93.2 (48.08-3.59) 88.6 (48.08-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 3.48 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.266 , 0.305 0.298 , 0.326	Depositor DCC
$R_{free}$ test set	2655 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	88.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.15 , 143.1	EDS
Estimated twinning fraction	0.099 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.110 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 54732 reflections	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	18759	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	196.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QEM, NAG, 1AC, JEG

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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/5317	0.47	0/7290
1	C	0.22	0/4265	0.44	0/5906
2	B	0.24	0/4743	0.47	0/6531
2	D	0.23	0/4638	0.44	0/6405
All	All	0.23	0/18963	0.46	0/26132

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	5208	0	4360	84	0
1	C	4193	0	2746	31	0
2	B	4669	0	3509	64	0
2	D	4565	0	3142	34	0
3	A	42	0	39	0	0
3	B	14	0	13	1	0
4	A	7	0	6	1	0
5	B	25	0	29	1	0
5	D	25	0	29	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	11	0	6	0	0
All	All	18759	0	13879	209	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 6.

The worst 5 of 209 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)
1:A:125:MET:O	1:A:139:ARG:NH2	2.09	0.85
1:A:79:CYS:SG	2:B:74:LYS:HB2	2.20	0.81
2:D:502:ALA:HB3	2:D:748:ALA:HB3	1.65	0.77
2:D:143:PRO:HG2	2:D:148:GLN:HE21	1.54	0.71
2:B:290:ASP:OD1	2:B:342:ARG:NH2	2.16	0.70

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 X-ray entries followed by that with respect to entries of similar resolution.

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	759/823 (92%)	732 (96%)	27 (4%)	0	100	100
1	C	711/823 (86%)	686 (96%)	25 (4%)	0	100	100
2	B	724/824 (88%)	690 (95%)	33 (5%)	1 (0%)	56	90
2	D	743/824 (90%)	703 (95%)	39 (5%)	1 (0%)	56	90
All	All	2937/3294 (89%)	2811 (96%)	124 (4%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	48	VAL

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Mol	Chain	Res	Type
2	D	384	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	410/705 (58%)	407 (99%)	3 (1%)	88	96
1	C	191/705 (27%)	190 (100%)	1 (0%)	92	97
2	B	308/724 (42%)	305 (99%)	3 (1%)	82	93
2	D	241/724 (33%)	240 (100%)	1 (0%)	93	98
All	All	1150/2858 (40%)	1142 (99%)	8 (1%)	88	96

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	184	THR
2	D	496	THR
2	B	382	TRP
1	A	484	THR
2	B	190	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	280	HIS
2	D	148	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	901	1	14,14,15	0.22	0	15,19,21	0.24	0
3	NAG	A	902	1	14,14,15	0.70	1 (7%)	15,19,21	1.13	1 (6%)
3	NAG	A	903	1	14,14,15	0.31	0	15,19,21	0.30	0
4	1AC	A	904	-	3,7,7	3.12	2 (66%)	3,11,11	4.99	3 (100%)
5	QEM	B	901	-	26,27,27	0.82	0	34,36,36	1.24	4 (11%)
3	NAG	B	902	2	14,14,15	0.30	0	15,19,21	0.31	0
5	QEM	D	901	-	26,27,27	0.85	1 (3%)	34,36,36	1.17	4 (11%)
6	JEG	D	902	-	2,11,11	3.68	2 (100%)	4,17,17	3.40	2 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	901	1	-	0/6/23/26	0/1/1/1
3	NAG	A	902	1	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1	-	0/6/23/26	0/1/1/1
4	1AC	A	904	-	-	0/0/10/10	0/0/1/1
5	QEM	B	901	-	-	0/16/26/26	0/3/3/3
3	NAG	B	902	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	QEM	D	901	-	-	0/16/26/26	0/3/3/3
6	JEG	D	902	-	-	0/0/20/20	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	1AC	CG-CA	-3.79	1.48	1.51
6	D	902	JEG	C11-C07	-3.78	1.50	1.54
4	A	904	1AC	CB-CA	-3.78	1.48	1.51
6	D	902	JEG	C06-C07	-3.58	1.50	1.54
5	D	901	QEM	C12-C08	-2.12	1.46	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	1AC	C-CA-N	-7.62	104.67	116.73
6	D	902	JEG	C11-C07-C08	-3.98	113.64	120.15
4	A	904	1AC	CG-CB-CA	-2.89	59.09	60.39
4	A	904	1AC	CB-CG-CA	-2.88	59.10	60.39
5	D	901	QEM	C14-C13-N	-2.81	109.33	115.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	904	1AC	1	0
5	B	901	QEM	1	0
3	B	902	NAG	1	0
5	D	901	QEM	3	0

## 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	767/823 (93%)	-0.37	12 (1%) 74 61	39, 141, 337, 448	0
1	C	719/823 (87%)	0.16	75 (10%) 8 6	120, 244, 345, 411	0
2	B	738/824 (89%)	-0.12	39 (5%) 30 21	55, 210, 392, 457	0
2	D	757/824 (91%)	-0.08	32 (4%) 40 28	95, 212, 312, 376	0
All	All	2981/3294 (90%)	-0.11	158 (5%) 30 21	39, 206, 356, 457	0

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	480	GLY	12.1
1	C	482	PHE	8.7
2	D	504	GLY	8.3
1	C	755	ASP	8.2
2	B	479	HIS	7.9

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	JEG	D	902	11/11	0.82	0.44	1.90	106,204,205,205	0
3	NAG	A	901	14/15	0.93	0.23	1.39	103,112,122,128	0
5	QEM	D	901	25/25	0.92	0.31	0.84	88,112,139,147	0
4	1AC	A	904	7/7	0.90	0.19	-0.32	128,137,163,166	0
5	QEM	B	901	25/25	0.97	0.18	-0.87	0,38,59,61	0
3	NAG	A	902	14/15	0.90	0.16	-	114,141,154,164	0
3	NAG	A	903	14/15	0.90	0.14	-	103,119,125,127	0
3	NAG	B	902	14/15	0.85	0.32	-	115,129,138,149	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.