



# wwPDB X-ray Structure Validation Summary Report i

Sep 18, 2014 – 09:37 PM EDT

PDB ID : 4TLM  
Title : Crystal structure of GluN1/GluN2B NMDA receptor, structure 2  
Authors : Gouaux, E.; Lee, C.-H.; Lu, W.  
Deposited on : 2014-05-30  
Resolution : 3.77 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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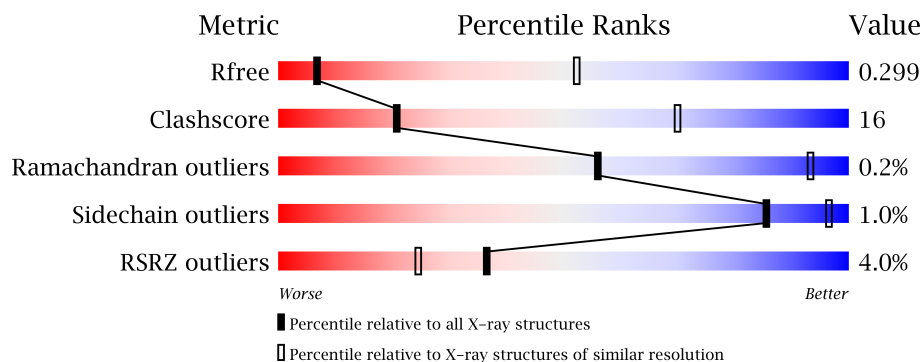
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 3.77 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))
$R_{free}$	66092	1139 (4.16-3.40)
Clashscore	79885	1069 (4.06-3.50)
Ramachandran outliers	78287	1019 (4.06-3.50)
Sidechain outliers	78261	1012 (4.06-3.50)
RSRZ outliers	66119	1140 (4.16-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	823	
1	C	823	
2	B	824	
2	D	824	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	B	901	-	X
5	QEM	C	903	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19547 atoms, of which 0 are hydrogen and 0 are deuterium.

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	796	Total	C	N	O	S	0	0	0
			5383	3411	945	1004	23			
1	C	750	Total	C	N	O	S	0	0	0
			4582	2855	818	893	16			

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	749	Total	C	N	O	S	0	0	0
			4752	2998	811	923	20			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	753	Total	C	N	O	S	0	0	0
			4664	2932	803	914	15			

There are 58 discrepancies between the modelled and reference sequences:

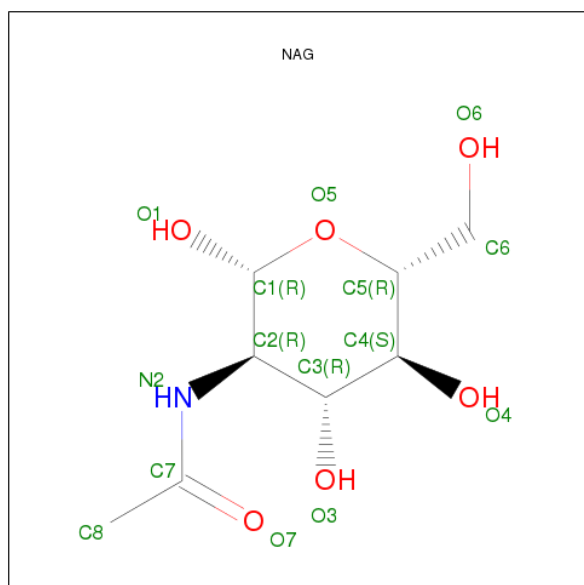
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	SER	MET	engineered mutation	UNP A7XY94
B	21	ARG	GLY	engineered mutation	UNP A7XY94
B	22	ALA	CYS	engineered mutation	UNP A7XY94
B	64	GLU	ALA	engineered mutation	UNP A7XY94
B	69	GLN	ASN	engineered mutation	UNP A7XY94
B	216	CYS	LYS	engineered mutation	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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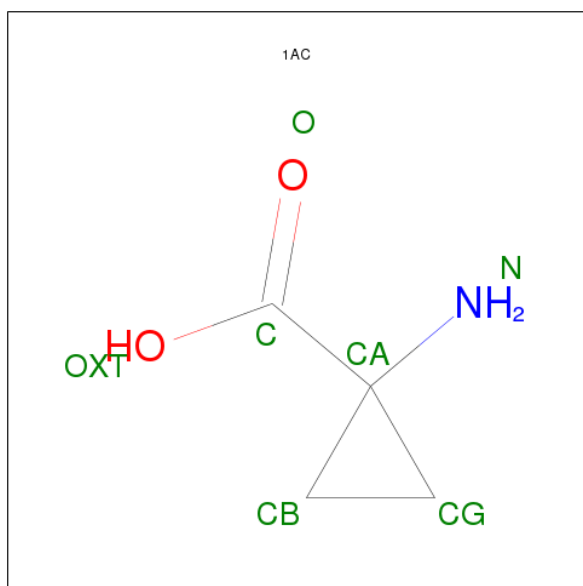
Chain	Residue	Modelled	Actual	Comment	Reference
D	486	VAL	THR	engineered mutation	UNP A7XY94
D	601	LEU	VAL	engineered mutation	UNP A7XY94
D	640	ARG	GLU	engineered mutation	UNP A7XY94
D	641	ARG	GLU	engineered mutation	UNP A7XY94
D	826	TYR	-	insertion	UNP A7XY94
D	827	LYS	-	insertion	UNP A7XY94
D	828	SER	-	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:  $C_8H_{15}NO_6$ ).



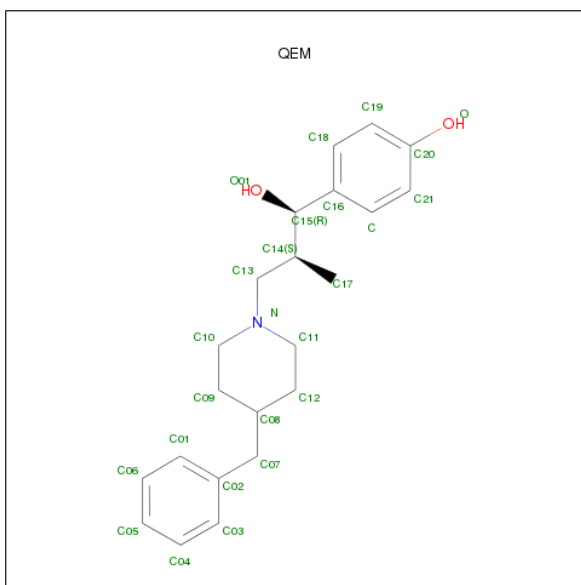
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 1-AMINOCYCLOPROPANECARBOXYLICACID (three-letter code: 1AC) (formula:  $C_4H_7NO_2$ ).



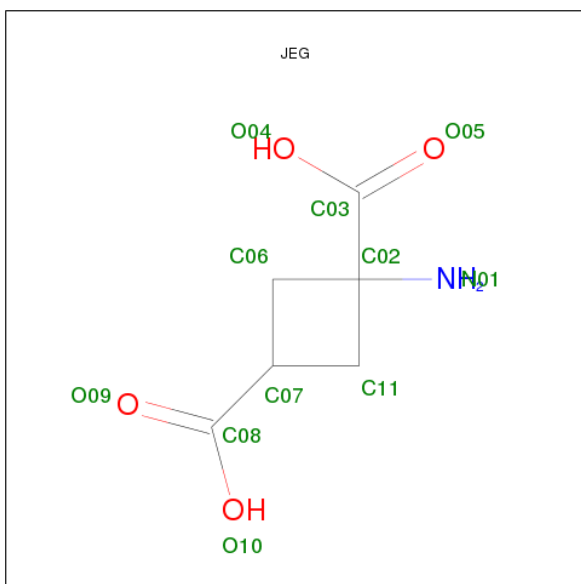
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 5 is 4-[(1R,2S)-3-(4-benzylpiperidin-1-yl)-1-hydroxy-2-methylpropyl]phenol (three-letter code: QEM) (formula:  $C_{22}H_{29}NO_2$ ).



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

- Molecule 6 is trans-1-aminocyclobutane-1,3-dicarboxylicacid (three-letter code: JEG) (formula:  $C_6H_9NO_4$ ).



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

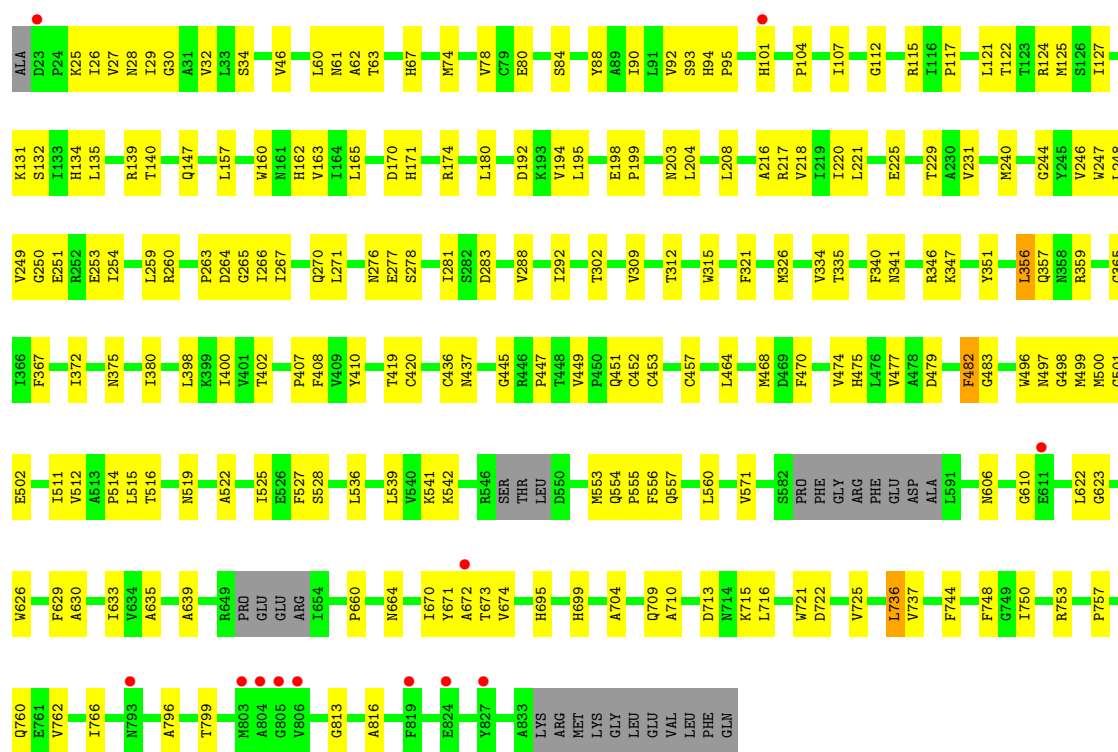


### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

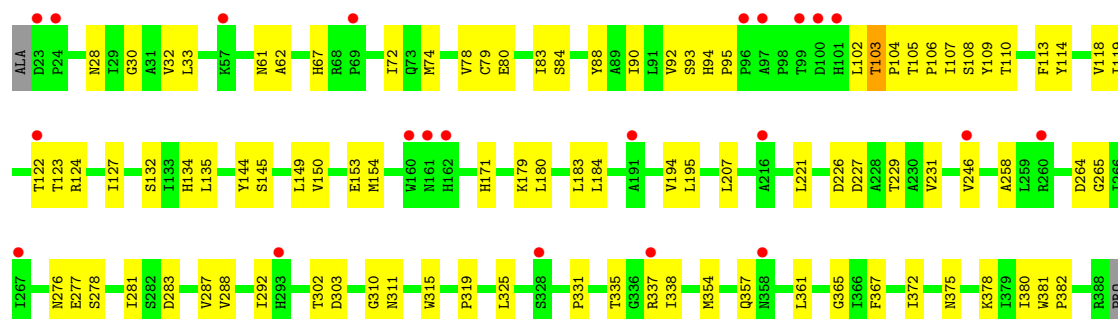
#### • Molecule 1: receptor subunit GluN1

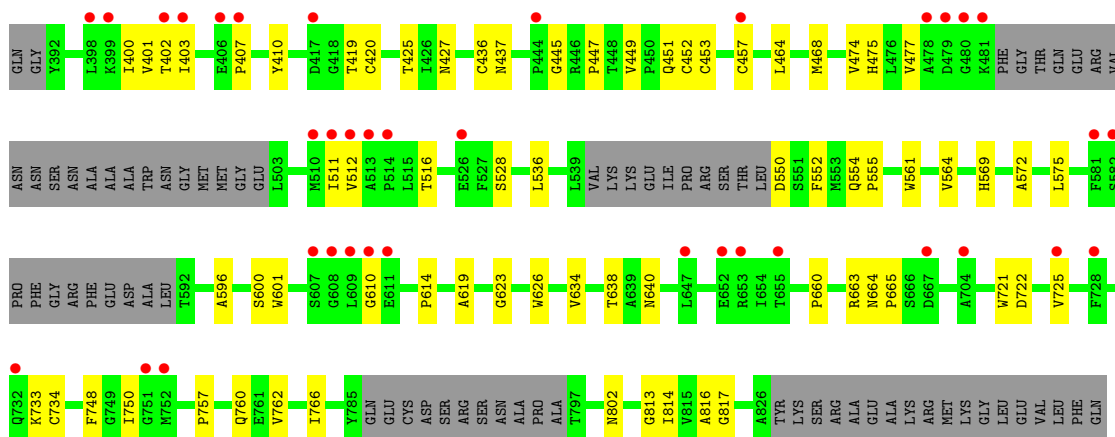
Chain A: 



#### • Molecule 1: receptor subunit GluN1

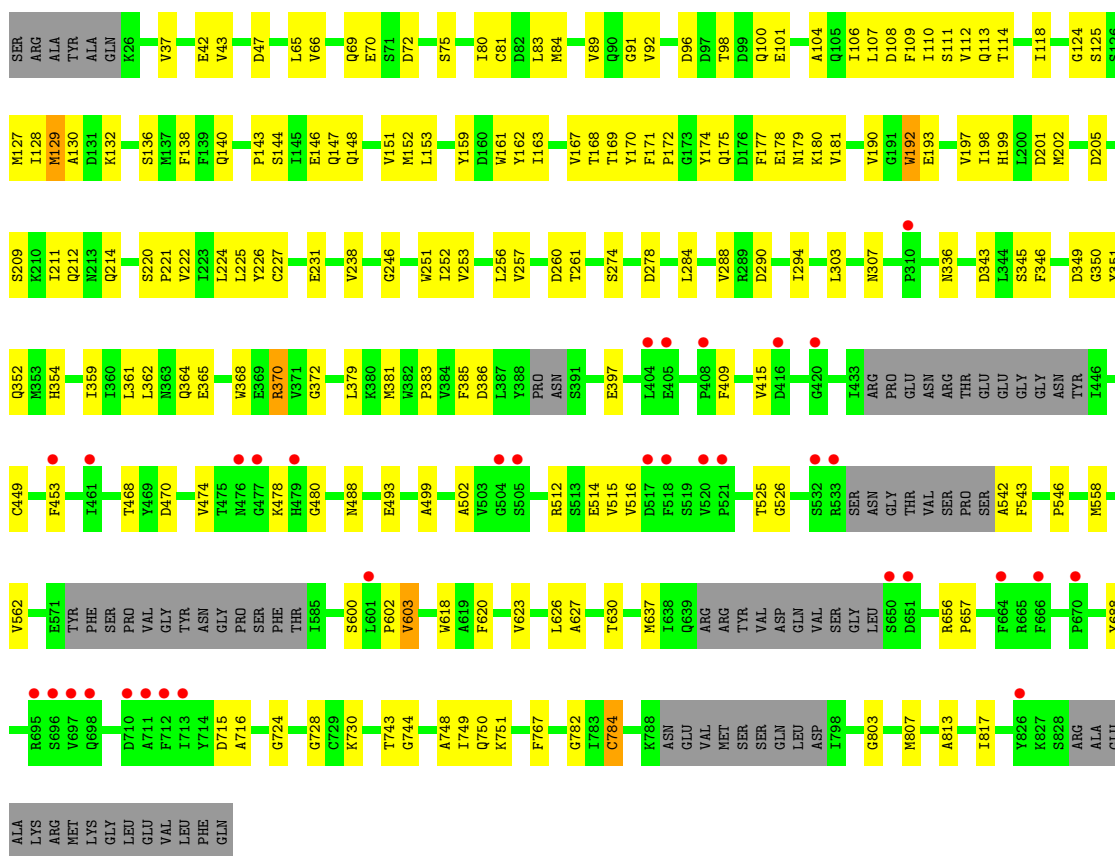
Chain C: 





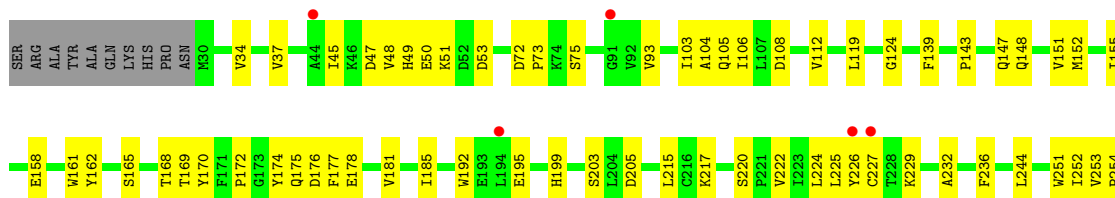
• Molecule 2: receptor subunit GluN2B

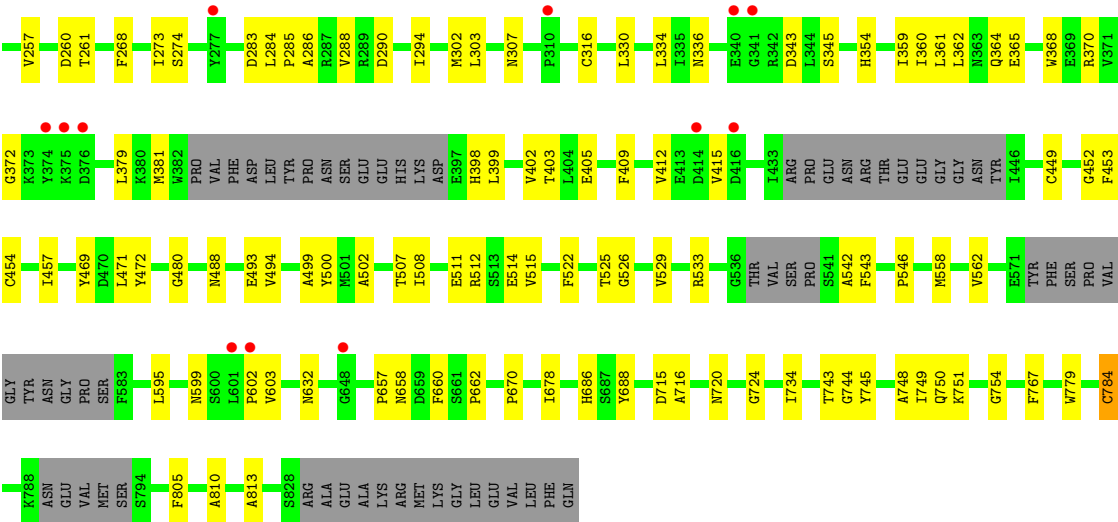
Chain B:



• Molecule 2: receptor subunit GluN2B

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.49Å 118.43Å 226.59Å 90.00° 103.82° 90.00°	Depositor
Resolution (Å)	29.96 – 3.77 44.70 – 3.47	Depositor EDS
% Data completeness (in resolution range)	83.2 (29.96-3.77) 70.8 (44.70-3.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1723)	Depositor
R, $R_{free}$	0.253 , 0.292 0.256 , 0.299	Depositor DCC
$R_{free}$ test set	2207 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 101.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 47943 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	19547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	218.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.32	0/5494	0.60	0/7543
1	C	0.33	1/4653 (0.0%)	0.63	1/6433 (0.0%)
2	B	0.32	0/4832	0.66	3/6668 (0.0%)
2	D	0.34	0/4735	0.64	1/6550 (0.0%)
All	All	0.32	1/19714 (0.0%)	0.63	5/27194 (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	A	0	1
2	B	0	2
2	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	596	ALA	CA-CB	-5.17	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	37	VAL	C-N-CA	-6.66	108.32	122.30
1	C	103	THR	C-N-CD	6.36	141.75	128.40
2	B	42	GLU	N-CA-C	-5.22	96.89	111.00
2	D	37	VAL	C-N-CA	5.12	133.05	122.30
2	B	603	VAL	N-CA-C	5.10	124.78	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	542	LYS	Peptide
2	B	246	GLY	Peptide
2	B	603	VAL	Peptide
2	D	603	VAL	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5383	0	4571	160	0
1	C	4582	0	3453	134	0
2	B	4752	0	3629	150	0
2	D	4664	0	3494	119	0
3	A	42	0	39	6	0
3	B	14	0	13	1	0
3	C	28	0	26	3	0
3	D	14	0	13	1	0
4	A	7	0	6	2	0
5	A	25	0	29	4	0
5	C	25	0	29	14	0
6	D	11	0	0	0	0
All	All	19547	0	15302	544	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 544 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:110:THR:HA	5:C:903:QEM:H03	1.31	1.10
5:C:903:QEM:H10	2:D:105:GLN:OE1	1.67	0.95
1:C:74:MET:HG3	1:C:107:ILE:HD11	1.50	0.94
1:A:610:GLY:HA2	2:B:602:PRO:HB3	1.51	0.93
1:A:276:ASN:HD22	3:A:902:NAG:C1	1.88	0.87

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 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	788/823 (96%)	763 (97%)	24 (3%)	1 (0%)	59	95
1	C	738/823 (90%)	718 (97%)	20 (3%)	0	100	100
2	B	735/824 (89%)	705 (96%)	28 (4%)	2 (0%)	50	91
2	D	741/824 (90%)	712 (96%)	27 (4%)	2 (0%)	50	91
All	All	3002/3294 (91%)	2898 (96%)	99 (3%)	5 (0%)	56	93

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	399	LEU
1	A	799	THR
2	B	397	GLU
2	D	533	ARG
2	B	43	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	434/705 (62%)	428 (99%)	6 (1%)	78	95
1	C	294/705 (42%)	292 (99%)	2 (1%)	91	98
2	B	328/724 (45%)	324 (99%)	4 (1%)	82	96
2	D	307/724 (42%)	305 (99%)	2 (1%)	91	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1363/2858 (48%)	1349 (99%)	14 (1%)	85 96

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	129	MET
2	B	192	TRP
1	C	561	TRP
1	A	736	LEU
1	C	452	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	306	HIS
2	B	681	ASN
2	D	306	HIS
2	B	199	HIS
2	D	479	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

11 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	12,14,15	0.32	0	15,19,21	0.42	0
3	NAG	A	902	-	12,14,15	0.44	0	15,19,21	0.53	0
3	NAG	A	903	-	12,14,15	0.55	0	15,19,21	1.20	2 (13%)
4	1AC	A	904	-	7,7,7	2.63	3 (42%)	11,11,11	5.26	8 (72%)
5	QEM	A	905	-	27,27,27	0.83	1 (3%)	36,36,36	1.23	5 (13%)
3	NAG	B	901	-	12,14,15	0.49	0	15,19,21	0.59	0
3	NAG	C	901	1	12,14,15	0.42	0	15,19,21	0.40	0
3	NAG	C	902	-	12,14,15	0.39	0	15,19,21	0.57	0
5	QEM	C	903	-	27,27,27	0.85	1 (3%)	36,36,36	1.14	3 (8%)
3	NAG	D	901	2	12,14,15	0.33	0	15,19,21	0.44	0
6	JEG	D	902	-	11,11,11	2.45	5 (45%)	15,17,17	7.65	3 (20%)

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	-	-	0/6/23/26	0/1/1/1
3	NAG	A	903	-	-	0/6/23/26	0/1/1/1
4	1AC	A	904	-	-	0/5/10/10	0/0/1/1
5	QEM	A	905	-	-	0/16/26/26	0/3/3/3
3	NAG	B	901	-	-	0/6/23/26	0/1/1/1
3	NAG	C	901	1	-	0/6/23/26	0/1/1/1
3	NAG	C	902	-	-	0/6/23/26	0/1/1/1
5	QEM	C	903	-	-	0/16/26/26	0/3/3/3
3	NAG	D	901	2	-	0/6/23/26	0/1/1/1
6	JEG	D	902	-	-	0/10/20/20	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	1AC	CG-CA	-4.13	1.48	1.51
6	D	902	JEG	C07-C08	-4.13	1.44	1.51
4	A	904	1AC	CB-CA	-3.93	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	902	JEG	C11-C07	-3.79	1.50	1.54
6	D	902	JEG	C06-C07	-3.73	1.50	1.54

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	902	JEG	C03-C02-N01	-28.77	92.00	112.57
4	A	904	1AC	CB-CA-C	9.22	139.23	116.83
4	A	904	1AC	C-CA-N	-7.91	102.33	115.94
4	A	904	1AC	CG-CA-C	7.78	135.72	116.83
4	A	904	1AC	CG-CA-CB	6.47	62.34	59.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	796/823 (96%)	-0.21	12 (1%) 70 48	41, 153, 321, 553	0
1	C	750/823 (91%)	0.25	59 (7%) 13 11	150, 269, 396, 519	0
2	B	749/824 (90%)	0.10	34 (4%) 32 22	63, 240, 383, 454	0
2	D	753/824 (91%)	-0.11	17 (2%) 57 37	109, 220, 338, 497	0
All	All	3048/3294 (92%)	0.01	122 (4%) 36 24	41, 226, 370, 553	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	405	GLU	9.1
2	B	695	ARG	8.3
1	C	407	PRO	7.4
1	C	161	ASN	7.3
1	C	216	ALA	7.3

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	QEM	C	903	25/25	0.51	3.05	74,100,146,157	0
3	NAG	B	901	14/15	0.36	2.14	173,193,216,246	0
3	NAG	C	902	14/15	0.17	1.76	189,204,228,252	0
3	NAG	D	901	14/15	0.49	1.29	324,362,384,386	0
5	QEM	A	905	25/25	0.28	1.16	0,28,59,62	0
4	1AC	A	904	7/7	0.38	0.91	158,161,184,208	0
3	NAG	A	902	14/15	0.21	0.48	126,164,180,199	0
6	JEG	D	902	11/11	0.23	-0.17	167,188,232,237	0
3	NAG	C	901	14/15	0.26	-0.31	160,237,260,283	0
3	NAG	A	903	14/15	0.14	-0.73	99,135,215,230	0
3	NAG	A	901	14/15	0.16	-0.81	130,153,198,212	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.