



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 12:52 PM EDT

PDB ID : 4UQQ
EMDB ID: : EMD-2685
Title : Electron density map of GluK2 desensitized state in complex with 2S,4R-4-methylglutamate
Authors : Meyerson, J.R.; Kumar, J.; Chittori, S.; Rao, P.; Pierson, J.; Bartesaghi, A.; Mayer, M.L.; Subramaniam, S.
Deposited on : unknown
Resolution : 7.60 Å(reported)
Based on PDB ID : 3G3F, 3H6G, 3KG2

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

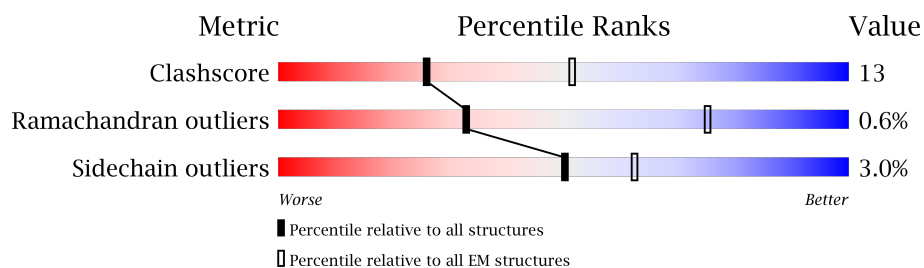
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 ≥ 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	882	
1	B	882	
1	C	882	
1	D	882	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22081 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, KAINATE 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	693	Total	C	N	O	S	0	0
			5523	3545	922	1025	31		
1	B	688	Total	C	N	O	S	0	0
			5498	3530	918	1020	30		
1	C	693	Total	C	N	O	S	0	0
			5523	3545	922	1025	31		
1	D	688	Total	C	N	O	S	0	0
			5497	3529	918	1020	30		

There are 36 discrepancies between the modelled and reference sequences:

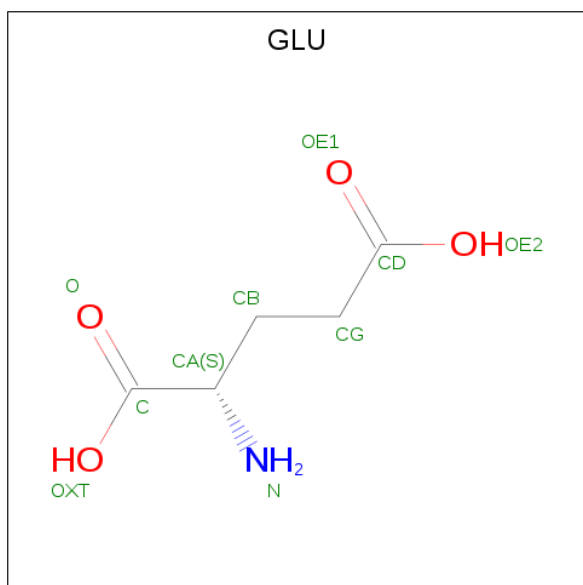
Chain	Residue	Modelled	Actual	Comment	Reference
A	878	GLY	-	expression tag	UNP P42260
A	879	LEU	-	expression tag	UNP P42260
A	880	VAL	-	expression tag	UNP P42260
A	881	PRO	-	expression tag	UNP P42260
A	882	ARG	-	expression tag	UNP P42260
A	536	VAL	ILE	variant	UNP P42260
A	540	CYS	TYR	variant	UNP P42260
A	545	VAL	CYS	engineered mutation	UNP P42260
A	564	SER	CYS	engineered mutation	UNP P42260
B	878	GLY	-	expression tag	UNP P42260
B	879	LEU	-	expression tag	UNP P42260
B	880	VAL	-	expression tag	UNP P42260
B	881	PRO	-	expression tag	UNP P42260
B	882	ARG	-	expression tag	UNP P42260
B	536	VAL	ILE	variant	UNP P42260
B	540	CYS	TYR	variant	UNP P42260
B	545	VAL	CYS	engineered mutation	UNP P42260
B	564	SER	CYS	engineered mutation	UNP P42260
C	878	GLY	-	expression tag	UNP P42260
C	879	LEU	-	expression tag	UNP P42260
C	880	VAL	-	expression tag	UNP P42260
C	881	PRO	-	expression tag	UNP P42260

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Chain	Residue	Modelled	Actual	Comment	Reference
C	882	ARG	-	expression tag	UNP P42260
C	536	VAL	ILE	variant	UNP P42260
C	540	CYS	TYR	variant	UNP P42260
C	545	VAL	CYS	engineered mutation	UNP P42260
C	564	SER	CYS	engineered mutation	UNP P42260
D	878	GLY	-	expression tag	UNP P42260
D	879	LEU	-	expression tag	UNP P42260
D	880	VAL	-	expression tag	UNP P42260
D	881	PRO	-	expression tag	UNP P42260
D	882	ARG	-	expression tag	UNP P42260
D	536	VAL	ILE	variant	UNP P42260
D	540	CYS	TYR	variant	UNP P42260
D	545	VAL	CYS	engineered mutation	UNP P42260
D	564	SER	CYS	engineered mutation	UNP P42260

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).

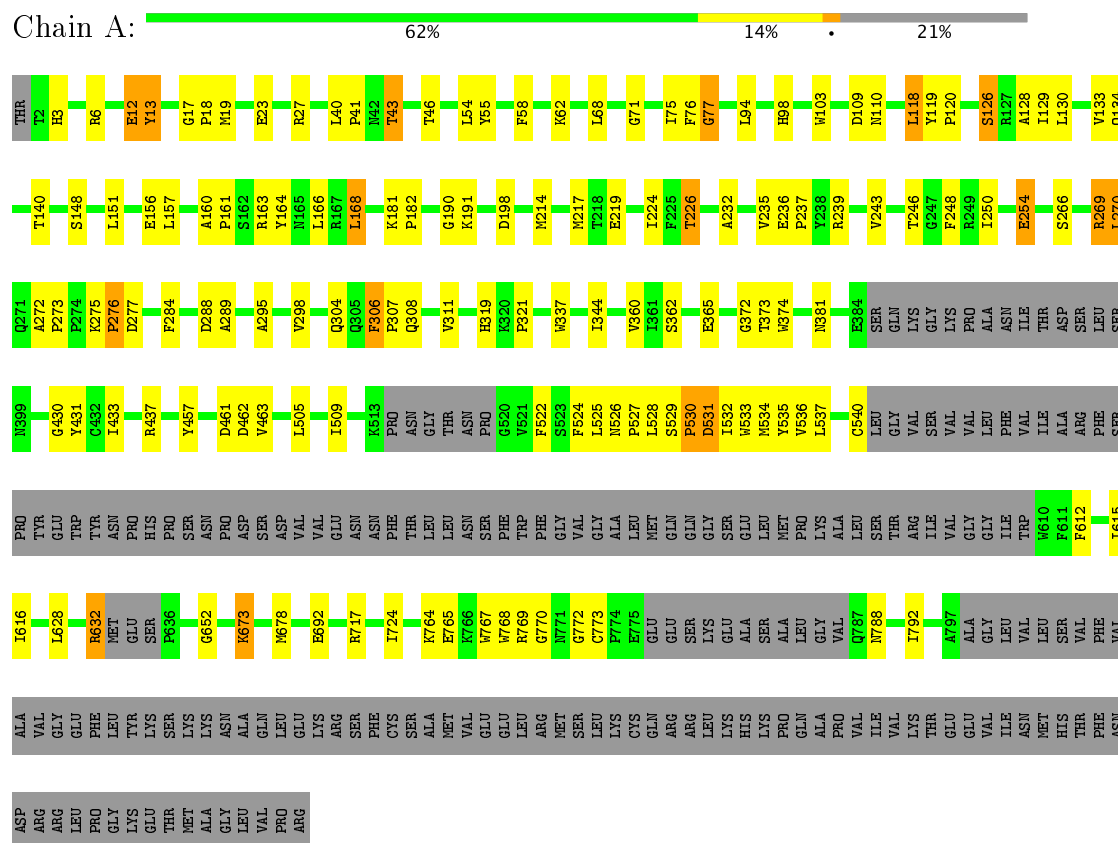


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			10	5	1	4	
2	B	1	Total	C	N	O	0
			10	5	1	4	
2	C	1	Total	C	N	O	0
			10	5	1	4	
2	D	1	Total	C	N	O	0
			10	5	1	4	

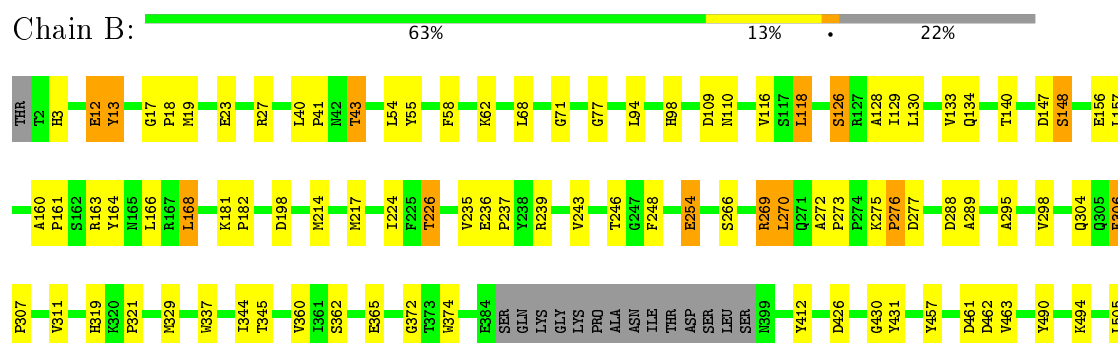
3 Residue-property plots

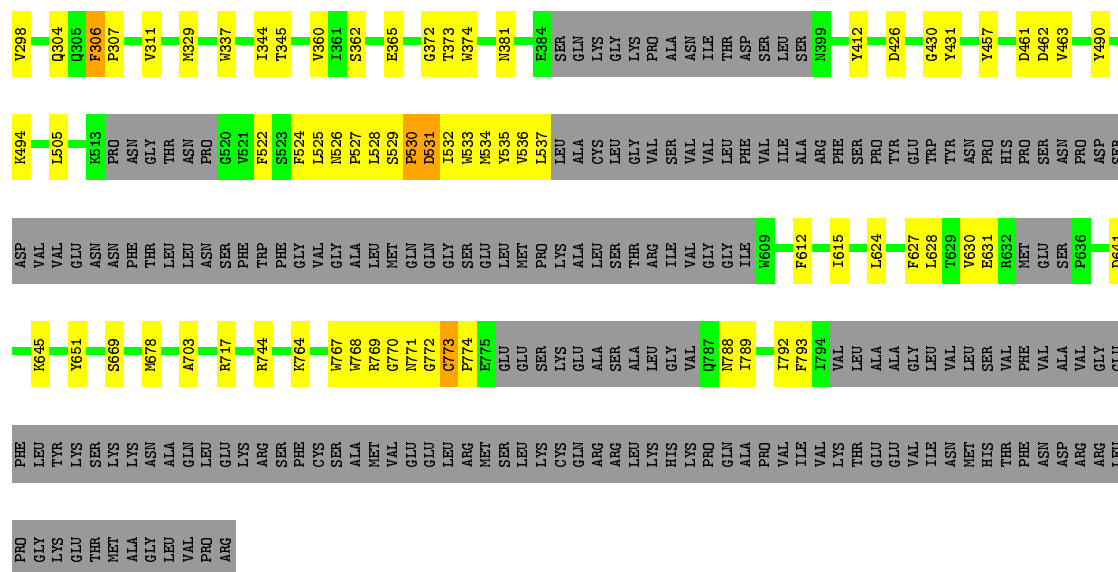
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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, KAINATE 2



• Molecule 1: GLUTAMATE RECEPTOR IONOTROPIC, KAINATE 2





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	21360	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON II (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	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.56	2/5642 (0.0%)	0.68	5/7628 (0.1%)
1	B	0.59	1/5619 (0.0%)	0.70	4/7597 (0.1%)
1	C	0.56	2/5642 (0.0%)	0.69	5/7628 (0.1%)
1	D	0.59	1/5617 (0.0%)	0.70	4/7593 (0.1%)
All	All	0.58	6/22520 (0.0%)	0.69	18/30446 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	TYR	CE2-CZ	-6.43	1.30	1.38
1	D	457	TYR	CE2-CZ	-6.41	1.30	1.38
1	C	692	GLU	CB-CG	5.71	1.63	1.52
1	A	692	GLU	CB-CG	5.69	1.62	1.52
1	A	457	TYR	CE2-CZ	-5.23	1.31	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	632	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	A	632	ARG	NE-CZ-NH2	-12.54	114.03	120.30
1	C	632	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	A	632	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	C	530	PRO	CA-N-CD	-8.46	99.65	111.50

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	5523	0	5507	156	0
1	B	5498	0	5471	153	0
1	C	5523	0	5507	150	0
1	D	5497	0	5467	148	0
2	A	10	0	5	0	0
2	B	10	0	5	0	0
2	C	10	0	5	0	0
2	D	10	0	5	0	0
All	All	22081	0	21972	563	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 13.

The worst 5 of 563 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:764:LYS:O	1:A:768:TRP:HB2	1.39	1.19
1:A:530:PRO:HD2	1:A:531:ASP:H	1.05	1.14
1:C:530:PRO:HD2	1:C:531:ASP:H	1.06	1.12
1:C:764:LYS:O	1:C:768:TRP:HB2	1.47	1.12
1:B:530:PRO:HD2	1:B:531:ASP:H	1.06	1.11

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	Percentiles
1	A	681/882 (77%)	647 (95%)	30 (4%)	4 (1%)	28 71
1	B	676/882 (77%)	643 (95%)	30 (4%)	3 (0%)	38 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	681/882 (77%)	645 (95%)	31 (5%)	5 (1%)	25 68
1	D	676/882 (77%)	642 (95%)	30 (4%)	4 (1%)	28 71
All	All	2714/3528 (77%)	2577 (95%)	121 (4%)	16 (1%)	33 71

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	771	ASN
1	A	276	PRO
1	A	773	CYS
1	B	276	PRO
1	B	773	CYS

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 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	604/769 (78%)	586 (97%)	18 (3%)	46 72
1	B	601/769 (78%)	583 (97%)	18 (3%)	46 72
1	C	604/769 (78%)	585 (97%)	19 (3%)	45 71
1	D	601/769 (78%)	583 (97%)	18 (3%)	46 72
All	All	2410/3076 (78%)	2337 (97%)	73 (3%)	50 72

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	462	ASP
1	C	126	SER
1	D	275	LYS
1	C	13	TYR
1	C	163	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	304	GLN
1	B	623	ASN
1	D	106	GLN
1	B	110	ASN
1	C	304	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	GLU	A	999	-	1,9,9	0.02	0	1,11,11	0.61	0
2	GLU	B	999	-	1,9,9	0.38	0	1,11,11	1.12	0
2	GLU	C	999	-	1,9,9	0.03	0	1,11,11	0.64	0
2	GLU	D	999	-	1,9,9	0.38	0	1,11,11	1.13	0

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
2	GLU	A	999	-	-	0/3/9/9	0/0/0/0
2	GLU	B	999	-	-	0/3/9/9	0/0/0/0
2	GLU	C	999	-	-	0/3/9/9	0/0/0/0
2	GLU	D	999	-	-	0/3/9/9	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.