wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 30, 2017 – 08:55 PM EDT

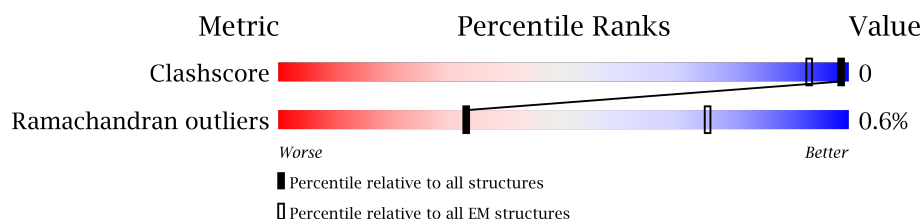|		
PDB ID	:	5IDF
EMDB ID:	:	EMD-8091
Title	:	Cryo-EM structure of GluA2/3 AMPA receptor heterotetramer (model II)
Authors	:	Herguedas, B.; Garcia-Nafria, J.; Fernandez-Leiro, R.; Greger, I.H.
Deposited on	:	unknown
Resolution	:	10.31 Å(reported)
Based on PDB ID	:	3KG2, 1FTO, 3UA8, 3HSY, 3O21

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 10.31 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	Percentile Ranks	Value
Clashscore		0
Ramachandran outliers		0.6%

Worse — *Better*

▌ Percentile relative to all structures

⧠ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	872	84% • 15%
1	C	872	84% • 15%
2	B	874	84% 16%
2	D	874	84% 16%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11786 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 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	741	Total 2963	C 1482	N 741	O 740	0	0
1	C	738	Total 2951	C 1476	N 738	O 737	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	VAL	-	expression tag	UNP P19491
A	-8	GLU	-	expression tag	UNP P19491
A	-7	GLN	-	expression tag	UNP P19491
A	-6	LYS	-	expression tag	UNP P19491
A	-5	LEU	-	expression tag	UNP P19491
A	-4	ILE	-	expression tag	UNP P19491
A	-3	SER	-	expression tag	UNP P19491
A	-2	GLU	-	expression tag	UNP P19491
A	-1	GLU	-	expression tag	UNP P19491
A	0	ASP	-	expression tag	UNP P19491
A	1	LEU	-	expression tag	UNP P19491
A	292	CYS	ASN	engineered mutation	UNP P19491
C	-9	VAL	-	expression tag	UNP P19491
C	-8	GLU	-	expression tag	UNP P19491
C	-7	GLN	-	expression tag	UNP P19491
C	-6	LYS	-	expression tag	UNP P19491
C	-5	LEU	-	expression tag	UNP P19491
C	-4	ILE	-	expression tag	UNP P19491
C	-3	SER	-	expression tag	UNP P19491
C	-2	GLU	-	expression tag	UNP P19491
C	-1	GLU	-	expression tag	UNP P19491
C	0	ASP	-	expression tag	UNP P19491
C	1	LEU	-	expression tag	UNP P19491
C	292	CYS	ASN	engineered mutation	UNP P19491

- Molecule 2 is a protein called Glutamate receptor 3.

| Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	734	Total 2936	C 1468	N 734	O 734	0	0
2	D	734	Total 2936	C 1468	N 734	O 734	0	0

There are 22 discrepancies between the modelled and reference sequences:

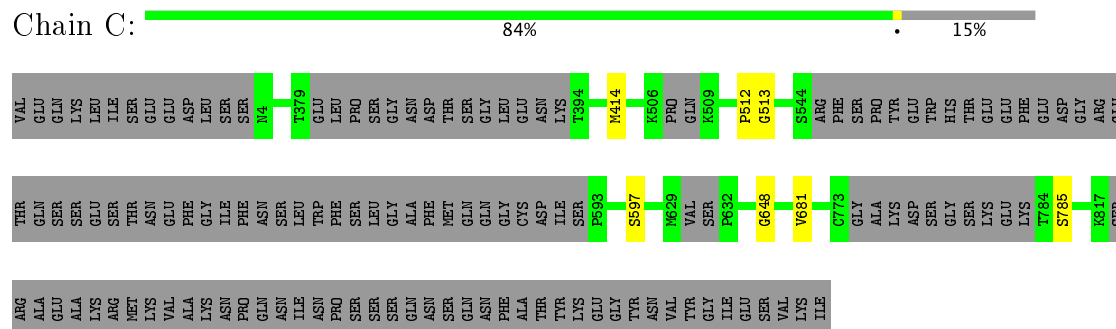| Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLY	-	expression tag	UNP P19492
B	-6	ASP	-	expression tag	UNP P19492
B	-5	TYR	-	expression tag	UNP P19492
B	-4	LYS	-	expression tag	UNP P19492
B	-3	ASP	-	expression tag	UNP P19492
B	-2	ASP	-	expression tag	UNP P19492
B	-1	ASP	-	expression tag	UNP P19492
B	0	ASP	-	expression tag	UNP P19492
B	1	LYS	-	expression tag	UNP P19492
B	265	CYS	ARG	engineered mutation	UNP P19492
B	439	GLY	ARG	engineered mutation	UNP P19492
D	-7	GLY	-	expression tag	UNP P19492
D	-6	ASP	-	expression tag	UNP P19492
D	-5	TYR	-	expression tag	UNP P19492
D	-4	LYS	-	expression tag	UNP P19492
D	-3	ASP	-	expression tag	UNP P19492
D	-2	ASP	-	expression tag	UNP P19492
D	-1	ASP	-	expression tag	UNP P19492
D	0	ASP	-	expression tag	UNP P19492
D	1	LYS	-	expression tag	UNP P19492
D	265	CYS	ARG	engineered mutation	UNP P19492
D	439	GLY	ARG	engineered mutation	UNP P19492

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 2
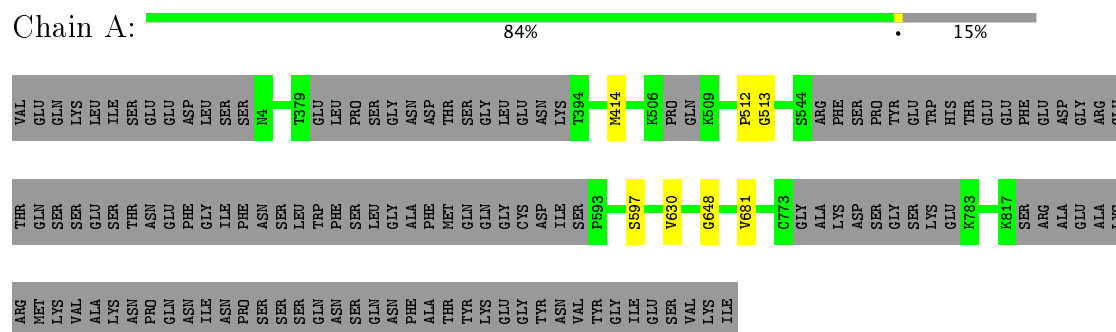
- Molecule 1: Glutamate receptor 2

- Molecule 2: Glutamate receptor 3
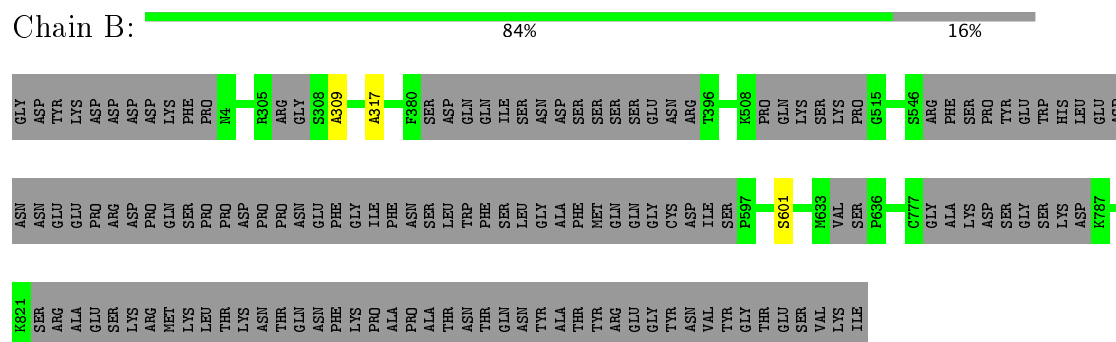
- Molecule 2: Glutamate receptor 3

Chain D:

84%   16%

GLY ASP TYR LYS ASP ASP ASP LYS PHE PRO N4 R305 ARG GLY S308 A309 A317 F380 SER ASP GLN GLN ILE SER ASN ASP SER SER SER GLU ASN ARG T396 K507 LYS PRO GLN LYS SER LYS P512 G515 S546 ARG PHE SER PRO TYR GLU TRP HIS LEU GLU

ASP ASN ASN GLU GLU PRO ARG ASP PRO GLN SER PRO PRO ASP PRO PRO ASN GLU PHE GLY ILE PHE ASN SER LEU TRP PHE SER LEU GLY ALA PHE MET GLN GLN GLY CYS ASP ILE SER P597 S601 M633 VAL P636 C777 GLY ALA LYS ASP SER GLY SER LYS ASP K787

K821 SER ARG ALA GLU SER LYS ARG MET LYS LEU THR LYS ASN THR GLN ASN PHE LYS PRO ALA PRO ALA THR ASN THR GLN ASN TYR ALA THR TYR ARG GLU GLY TYR ASN VAL TYR GLY THR GLU SER VAL LYS ILE

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	14119	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	28409	Depositor
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	
		RMSZ	#$|Z|$ >2	RMSZ	#$|Z|$ >2
1	A	0.33	0/2957	0.56	0/3686
1	C	0.33	0/2945	0.57	0/3671
2	B	0.37	0/2929	0.49	0/3649
2	D	0.37	0/2929	0.49	0/3649
All	All	0.35	0/11760	0.53	0/14655

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	2963	0	834	1	0
1	C	2951	0	831	1	0
2	B	2936	0	812	0	0
2	D	2936	0	812	0	0
All	All	11786	0	3289	2	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 0.

All (2) 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:C:648:GLY:HA3	1:C:681:VAL:O	2.21	0.40
1:A:648:GLY:HA3	1:A:681:VAL:O	2.21	0.40

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	729/872 (84%)	704 (97%)	20 (3%)	5 (1%)	25	68
1	C	726/872 (83%)	703 (97%)	18 (2%)	5 (1%)	25	68
2	B	720/874 (82%)	695 (96%)	22 (3%)	3 (0%)	38	77
2	D	720/874 (82%)	695 (96%)	21 (3%)	4 (1%)	28	71
All	All	2895/3492 (83%)	2797 (97%)	81 (3%)	17 (1%)	33	71

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	MET
2	B	309	ALA
2	B	317	ALA
1	C	414	MET
2	D	309	ALA

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	631:SER	C	632:PRO	N	6.49