



wwPDB EM Map/Model Validation Report ⓘ

Sep 27, 2016 – 09:31 PM EDT

PDB ID : 5KUH
EMDB ID: : EMD-8290
Title : GluK2EM with LY466195
Authors : Meyerson, J.R.; Chittori, S.; Merk, A.; Rao, P.; Han, T.H.; Serpe, M.; Mayer, M.L.; Subramaniam, S.
Deposited on : 2016-07-13
Resolution : 11.60 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
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-20027939

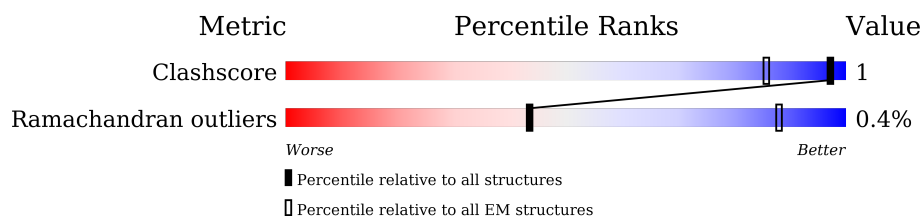
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.60 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	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 ≥ 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	757	
1	B	757	
1	C	757	
1	D	757	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12648 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	636	Total	C	N	O	0	0
			3138	1866	636	636		
1	B	636	Total	C	N	O	0	0
			3138	1866	636	636		
1	C	636	Total	C	N	O	0	0
			3138	1866	636	636		
1	D	636	Total	C	N	O	0	0
			3138	1866	636	636		

There are 24 discrepancies between the modelled and reference sequences:

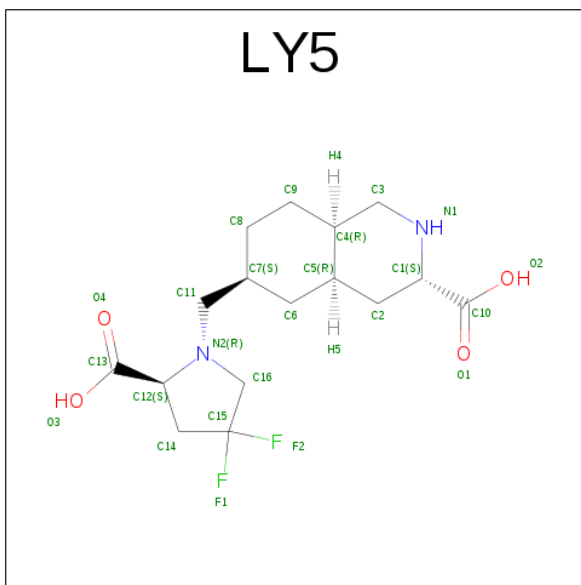
Chain	Residue	Modelled	Actual	Comment	Reference
A	487	THR	ALA	engineered mutation	UNP P42260
A	516	GLY	-	linker	UNP P42260
A	517	THR	-	linker	UNP P42260
A	658	SER	ALA	engineered mutation	UNP P42260
A	690	SER	ASN	engineered mutation	UNP P42260
A	704	LEU	PHE	engineered mutation	UNP P42260
B	487	THR	ALA	engineered mutation	UNP P42260
B	516	GLY	-	linker	UNP P42260
B	517	THR	-	linker	UNP P42260
B	658	SER	ALA	engineered mutation	UNP P42260
B	690	SER	ASN	engineered mutation	UNP P42260
B	704	LEU	PHE	engineered mutation	UNP P42260
C	487	THR	ALA	engineered mutation	UNP P42260
C	516	GLY	-	linker	UNP P42260
C	517	THR	-	linker	UNP P42260
C	658	SER	ALA	engineered mutation	UNP P42260
C	690	SER	ASN	engineered mutation	UNP P42260
C	704	LEU	PHE	engineered mutation	UNP P42260
D	487	THR	ALA	engineered mutation	UNP P42260
D	516	GLY	-	linker	UNP P42260
D	517	THR	-	linker	UNP P42260
D	658	SER	ALA	engineered mutation	UNP P42260

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Chain	Residue	Modelled	Actual	Comment	Reference
D	690	SER	ASN	engineered mutation	UNP P42260
D	704	LEU	PHE	engineered mutation	UNP P42260

- Molecule 2 is (3S,4aR,6S,8aR)-6-{[(2S)-2-carboxy-4,4-difluoropyrrolidin-1-yl]methyl}decahydroisoquinoline-3-carboxylic acid (three-letter code: LY5) (formula: C₁₆H₂₄F₂N₂O₄).




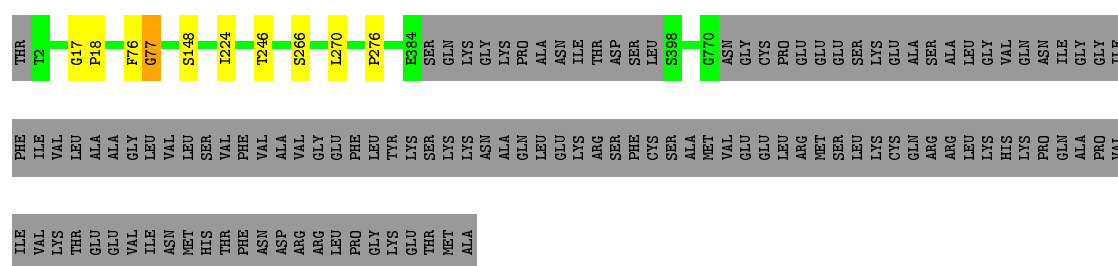
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 24	C 16	F 2	N 2	O 4	0
2	B	1	Total 24	C 16	F 2	N 2	O 4	0
2	C	1	Total 24	C 16	F 2	N 2	O 4	0
2	D	1	Total 24	C 16	F 2	N 2	O 4	0

3 Residue-property plots [i](#)


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.

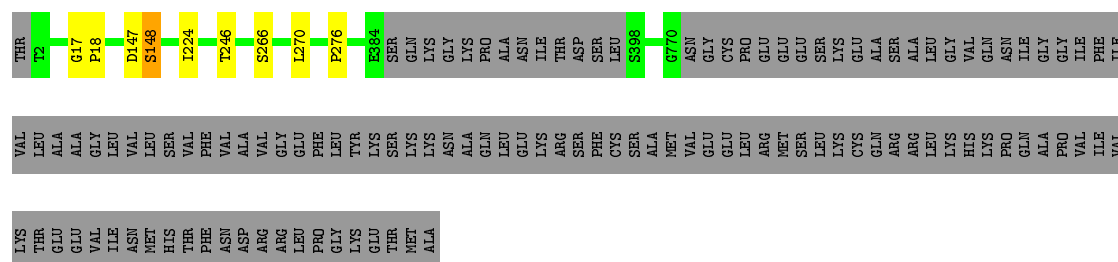
- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain A: 




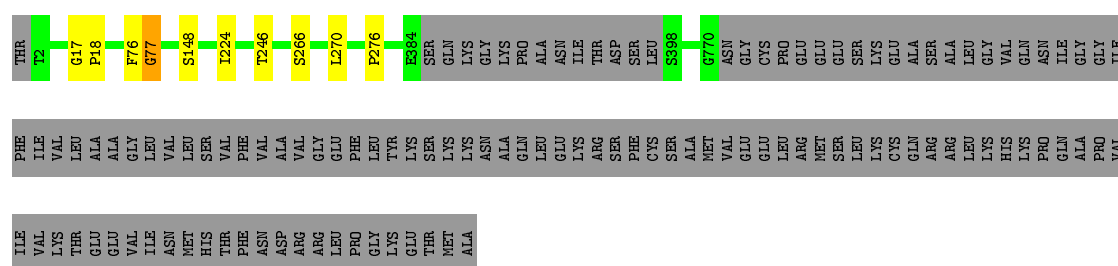
- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain B: 




- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain C: 



- Molecule 1: Glutamate receptor ionotropic, kainate 2

Chain D: 

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

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	31000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

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: LY5

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	0.43	0/3136	0.57	0/4362
1	B	0.43	0/3136	0.58	0/4362
1	C	0.43	0/3136	0.58	0/4362
1	D	0.43	0/3136	0.58	0/4362
All	All	0.43	0/12544	0.58	0/17448

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	3138	0	1398	4	0
1	B	3138	0	1398	4	0
1	C	3138	0	1398	4	0
1	D	3138	0	1398	4	0
2	A	24	0	22	0	0
2	B	24	0	22	0	0
2	C	24	0	22	0	0
2	D	24	0	22	0	0
All	All	12648	0	5680	16	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 1.

All (16) 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:76:PHE:O	1:C:77:GLY:O	2.32	0.48
1:A:76:PHE:O	1:A:77:GLY:O	2.32	0.48
1:B:17:GLY:HA2	1:B:18:PRO:O	2.16	0.46
1:A:17:GLY:HA2	1:A:18:PRO:O	2.16	0.45
1:D:17:GLY:HA2	1:D:18:PRO:O	2.16	0.45
1:C:17:GLY:HA2	1:C:18:PRO:O	2.16	0.45
1:B:266:SER:O	1:B:270:LEU:CB	2.65	0.44
1:D:266:SER:O	1:D:270:LEU:CB	2.65	0.44
1:D:224:ILE:HA	1:D:246:THR:O	2.19	0.43
1:A:224:ILE:HA	1:A:246:THR:O	2.19	0.43
1:C:224:ILE:HA	1:C:246:THR:O	2.19	0.42
1:B:224:ILE:HA	1:B:246:THR:O	2.19	0.42
1:C:266:SER:O	1:C:270:LEU:CB	2.67	0.42
1:A:266:SER:O	1:A:270:LEU:CB	2.67	0.42
1:B:147:ASP:O	1:B:148:SER:C	2.59	0.41
1:D:147:ASP:O	1:D:148:SER:C	2.59	0.41

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	632/757 (84%)	601 (95%)	28 (4%)	3 (0%)	34	77
1	B	632/757 (84%)	603 (95%)	27 (4%)	2 (0%)	46	83
1	C	632/757 (84%)	601 (95%)	28 (4%)	3 (0%)	34	77
1	D	632/757 (84%)	603 (95%)	27 (4%)	2 (0%)	46	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2528/3028 (84%)	2408 (95%)	110 (4%)	10 (0%)	43 80

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	PRO
1	B	276	PRO
1	C	276	PRO
1	D	276	PRO
1	A	77	GLY
1	A	148	SER
1	B	148	SER
1	C	77	GLY
1	C	148	SER
1	D	148	SER

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](#)

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	LY5	A	901	-	14,26,26	2.46	4 (28%)	20,39,39	2.16	8 (40%)
2	LY5	B	901	-	14,26,26	2.45	3 (21%)	20,39,39	2.16	8 (40%)
2	LY5	C	901	-	14,26,26	2.46	3 (21%)	20,39,39	2.15	8 (40%)
2	LY5	D	901	-	14,26,26	2.46	3 (21%)	20,39,39	2.16	8 (40%)

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	LY5	A	901	-	-	0/4/48/48	0/3/3/3
2	LY5	B	901	-	-	0/4/48/48	0/3/3/3
2	LY5	C	901	-	-	0/4/48/48	0/3/3/3
2	LY5	D	901	-	-	0/4/48/48	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	LY5	F2-C15	-7.93	1.28	1.38
2	C	901	LY5	F2-C15	-7.93	1.28	1.38
2	B	901	LY5	F2-C15	-7.90	1.28	1.38
2	D	901	LY5	F2-C15	-7.90	1.28	1.38
2	B	901	LY5	F1-C15	-3.11	1.34	1.38
2	D	901	LY5	F1-C15	-3.06	1.34	1.38
2	C	901	LY5	F1-C15	-3.05	1.34	1.38
2	A	901	LY5	F1-C15	-3.05	1.34	1.38
2	A	901	LY5	C14-C12	-2.00	1.51	1.54
2	B	901	LY5	C2-C1	2.07	1.55	1.53
2	A	901	LY5	C2-C1	2.11	1.55	1.53
2	C	901	LY5	C2-C1	2.11	1.55	1.53
2	D	901	LY5	C2-C1	2.18	1.55	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	LY5	C6-C5-C4	-4.43	103.33	110.59
2	B	901	LY5	C6-C5-C4	-4.43	103.33	110.59
2	A	901	LY5	C6-C5-C4	-4.42	103.36	110.59
2	C	901	LY5	C6-C5-C4	-4.41	103.36	110.59
2	A	901	LY5	C8-C9-C4	-2.81	105.47	112.25
2	D	901	LY5	C8-C9-C4	-2.80	105.50	112.25
2	B	901	LY5	C8-C9-C4	-2.79	105.52	112.25
2	C	901	LY5	C8-C9-C4	-2.79	105.53	112.25
2	C	901	LY5	C5-C2-C1	2.15	115.17	111.54
2	D	901	LY5	C5-C2-C1	2.17	115.19	111.54
2	A	901	LY5	C5-C2-C1	2.18	115.21	111.54
2	B	901	LY5	C5-C2-C1	2.18	115.21	111.54
2	B	901	LY5	F1-C15-C14	2.30	117.82	112.17
2	D	901	LY5	F1-C15-C14	2.30	117.83	112.17
2	A	901	LY5	F1-C15-C14	2.32	117.87	112.17
2	C	901	LY5	F1-C15-C14	2.33	117.90	112.17
2	C	901	LY5	C9-C4-C3	2.64	115.66	112.03
2	A	901	LY5	C9-C4-C3	2.64	115.67	112.03
2	D	901	LY5	C9-C4-C3	2.64	115.67	112.03
2	B	901	LY5	C9-C4-C3	2.65	115.68	112.03
2	C	901	LY5	C9-C4-C5	2.73	117.94	110.21
2	A	901	LY5	C9-C4-C5	2.73	117.95	110.21
2	B	901	LY5	C9-C4-C5	2.75	117.99	110.21
2	D	901	LY5	C9-C4-C5	2.76	118.01	110.21
2	C	901	LY5	C6-C7-C8	2.94	114.29	109.12
2	D	901	LY5	C6-C7-C8	2.95	114.30	109.12
2	B	901	LY5	C6-C7-C8	2.97	114.33	109.12
2	A	901	LY5	C6-C7-C8	2.98	114.36	109.12
2	B	901	LY5	C3-C4-C5	4.30	115.81	107.93
2	C	901	LY5	C3-C4-C5	4.31	115.83	107.93
2	D	901	LY5	C3-C4-C5	4.31	115.83	107.93
2	A	901	LY5	C3-C4-C5	4.33	115.87	107.93

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.