



wwPDB EM Model Validation Summary Report ⓘ

Feb 25, 2020 – 12:27 PM EST

PDB ID : 6L6F
EMDB ID : EMD-0839
Title : GluK3 receptor complex with UBP301
Authors : Kumar, J.; Kumari, J.; Burada, A.P.
Deposited on : 2019-10-28
Resolution : 10.60 Å (reported)
Based on initial model : 6JFY

This is a wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

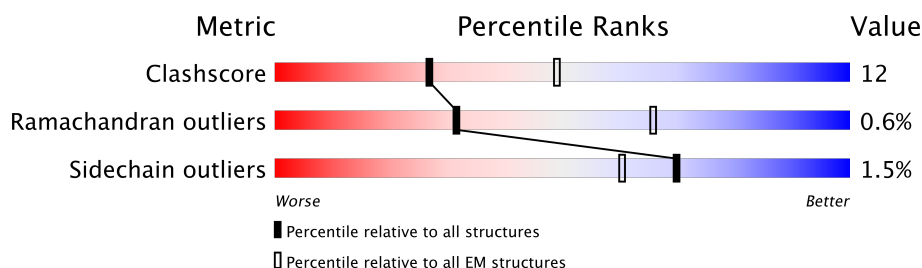
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.60 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. 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 respectively. 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	832	
1	B	832	
1	C	832	
1	D	832	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22836 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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	715	Total	C	N	O	S	0	0
			5710	3672	970	1038	30		
1	B	715	Total	C	N	O	S	0	0
			5710	3672	970	1038	30		
1	C	715	Total	C	N	O	S	0	0
			5706	3670	970	1036	30		
1	D	715	Total	C	N	O	S	0	0
			5710	3672	970	1038	30		

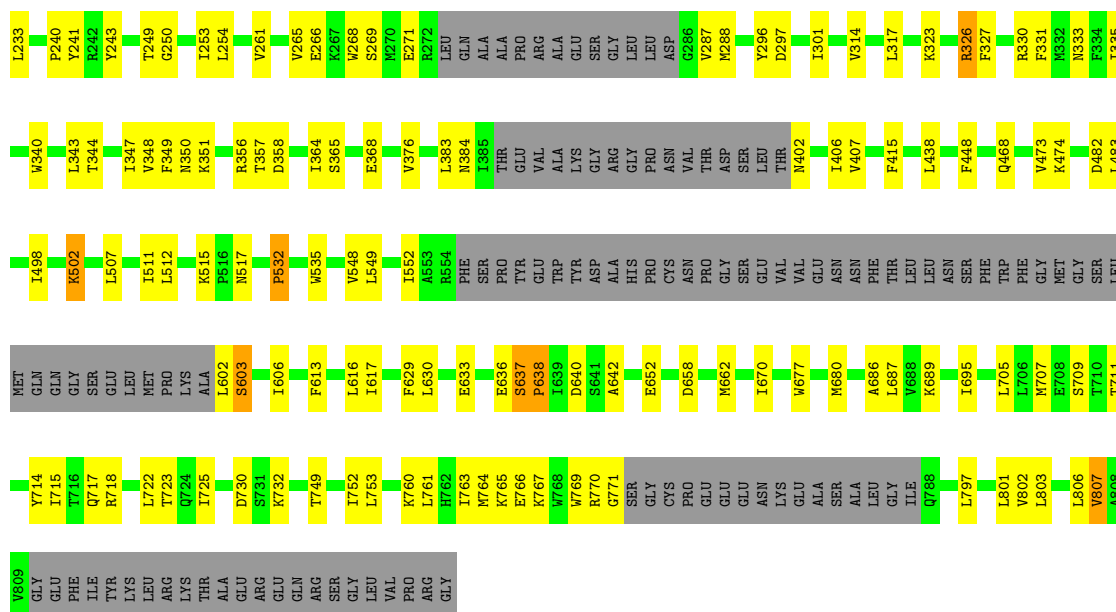
There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	THR	CYS	engineered mutation	UNP G3V9I2
A	305	THR	CYS	engineered mutation	UNP G3V9I2
A	547	VAL	CYS	engineered mutation	UNP G3V9I2
A	825	ARG	-	expression tag	UNP G3V9I2
A	826	SER	-	expression tag	UNP G3V9I2
A	827	GLY	-	expression tag	UNP G3V9I2
A	828	LEU	-	expression tag	UNP G3V9I2
A	829	VAL	-	expression tag	UNP G3V9I2
A	830	PRO	-	expression tag	UNP G3V9I2
A	831	ARG	-	expression tag	UNP G3V9I2
A	832	GLY	-	expression tag	UNP G3V9I2
B	86	THR	CYS	engineered mutation	UNP G3V9I2
B	305	THR	CYS	engineered mutation	UNP G3V9I2
B	547	VAL	CYS	engineered mutation	UNP G3V9I2
B	825	ARG	-	expression tag	UNP G3V9I2
B	826	SER	-	expression tag	UNP G3V9I2
B	827	GLY	-	expression tag	UNP G3V9I2
B	828	LEU	-	expression tag	UNP G3V9I2
B	829	VAL	-	expression tag	UNP G3V9I2
B	830	PRO	-	expression tag	UNP G3V9I2
B	831	ARG	-	expression tag	UNP G3V9I2
B	832	GLY	-	expression tag	UNP G3V9I2

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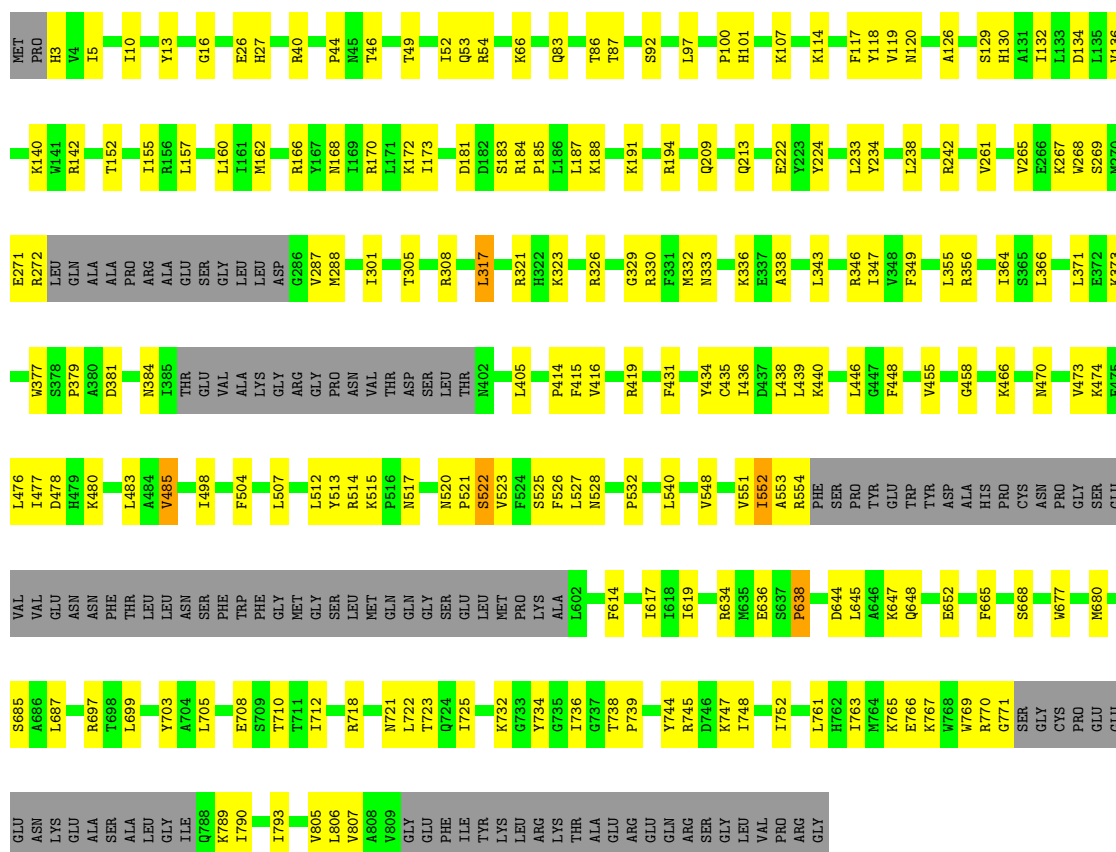
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Chain	Residue	Modelled	Actual	Comment	Reference
C	86	THR	CYS	engineered mutation	UNP G3V9I2
C	305	THR	CYS	engineered mutation	UNP G3V9I2
C	547	VAL	CYS	engineered mutation	UNP G3V9I2
C	825	ARG	-	expression tag	UNP G3V9I2
C	826	SER	-	expression tag	UNP G3V9I2
C	827	GLY	-	expression tag	UNP G3V9I2
C	828	LEU	-	expression tag	UNP G3V9I2
C	829	VAL	-	expression tag	UNP G3V9I2
C	830	PRO	-	expression tag	UNP G3V9I2
C	831	ARG	-	expression tag	UNP G3V9I2
C	832	GLY	-	expression tag	UNP G3V9I2
D	86	THR	CYS	engineered mutation	UNP G3V9I2
D	305	THR	CYS	engineered mutation	UNP G3V9I2
D	547	VAL	CYS	engineered mutation	UNP G3V9I2
D	825	ARG	-	expression tag	UNP G3V9I2
D	826	SER	-	expression tag	UNP G3V9I2
D	827	GLY	-	expression tag	UNP G3V9I2
D	828	LEU	-	expression tag	UNP G3V9I2
D	829	VAL	-	expression tag	UNP G3V9I2
D	830	PRO	-	expression tag	UNP G3V9I2
D	831	ARG	-	expression tag	UNP G3V9I2
D	832	GLY	-	expression tag	UNP G3V9I2



- Molecule 1: Glutamate receptor ionotropic, kainate 3

Chain C: 62% 23% 14%



- Molecule 1: Glutamate receptor ionotropic, kainate 3

Chain D: 66% 19% 14%

MET	P185	Y304	THR	N523	T604	I752	PRO
PRO	L186	T305	H402	F524	R605	L753	ARG
H3	L187	R308	I406	L527	I606	Q754	GLY
G8	E189	S316	Y407	P632	G609	L755	
A24	R192	R321	F415	N533	F613	D759	
H27	F196	A324	V416	I534	F629	K764	
A28	R197	W325	G427	W535	E766	K765	
A33	F200	R326	R430	N554	E633	E767	
N34	H204	F327	Y434	PHE	P638	W768	
I35	H209	G328	C435	SER	I639	W769	
N39	I210	N332	C439	PRO	D640	K770	
L42	L211	I335	L439	TYR	D643	G771	
L48	K212	Q339	L446	TRP	D646	GLY	
D61	E222	R346	I452	ASP	A646	CYS	
I52	H225	I347	R453	ALA	K650	PRO	
Q53	F226	Y348	Q463	HIS	K657	GLU	
F57	L233	F349	W469	PRO	M662	ASN	
H58	D239	N350	E475	GLY	T672	LYS	
D59	E239	L355	I476	SER	M676	ALA	
K65	R242	D360	L477	GLU	S685	LEU	
Q70	Y243	L361	K480	VAL	K689	TLE	
I78	N247	I364	A481	ASN	G694	Q768	
T87	R252	E368	D482	PHE	I695	W802	
V119	V265	G370	V485	LEU	N696	N805	
L133	W268	G375	T489	ASN	R697	L806	
D134	R272	W376	I490	SER	T698	W807	
L135	LEU	W377	T491	PHE	L699	A608	
W141	GLN	L383	E495	TRP	L705	GLY	
V146	ALA	N384	K496	GLY	I715	PHE	
D150	ALA	I385	A497	MET	R718	TLE	
S151	ARG	THR	R502	GLY	N719	TYR	
T152	ALA	VAL	L507	SER	L722	LYS	
G153	GLU	ALA	G508	MET	I729	ARG	
R156	SER	LYS	W509	GLN	Y734	THR	
R166	GLY	ARG	I510	GLY	G735	ALA	
ASP	LEU	GLY	L512	LEU	W736	GLU	
L171	ASP	ASN	N514	MET	K747	GLN	
S183	G286	VAL	T519	PRO	I750	ARG	
R194	V287	THR	N520	LYS	A751	SER	
	K288	ASP	P521	ALA		GLY	
	S303	LEU	S522	L602		LEU	
				S603		VAL	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16.73	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/5834	0.64	0/7896
1	B	0.33	0/5834	0.69	8/7896 (0.1%)
1	C	0.33	0/5830	0.65	2/7891 (0.0%)
1	D	0.32	0/5834	0.63	1/7896 (0.0%)
All	All	0.33	0/23332	0.65	11/31579 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	LEU	CA-CB-CG	7.14	131.71	115.30
1	B	201	ASP	CB-CG-OD1	6.97	124.57	118.30
1	B	730	ASP	CB-CG-OD2	6.95	124.55	118.30
1	C	540	LEU	CA-CB-CG	6.59	130.45	115.30
1	B	51	ASP	CB-CG-OD1	5.89	123.61	118.30

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	5710	0	5741	140	0
1	B	5710	0	5741	159	0
1	C	5706	0	5736	145	0
1	D	5710	0	5741	121	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	22836	0	22959	546	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 12.

The worst 5 of 546 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:548:VAL:CG1	1:C:552:ILE:HD11	1.35	1.54
1:C:548:VAL:HG12	1:C:552:ILE:CD1	1.46	1.45
1:B:803:LEU:O	1:B:807:VAL:CG1	1.67	1.42
1:C:268:TRP:CZ2	1:C:272:ARG:C	1.96	1.39
1:C:718:ARG:HG2	1:C:771:GLY:C	1.44	1.37

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	705/832 (85%)	650 (92%)	54 (8%)	1 (0%)	53	88
1	B	705/832 (85%)	652 (92%)	47 (7%)	6 (1%)	19	61
1	C	705/832 (85%)	652 (92%)	46 (6%)	7 (1%)	17	60
1	D	705/832 (85%)	656 (93%)	47 (7%)	2 (0%)	43	81
All	All	2820/3328 (85%)	2610 (93%)	194 (7%)	16 (1%)	31	70

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	637	SER
1	B	638	PRO

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Mol	Chain	Res	Type
1	D	807	VAL
1	B	351	LYS
1	B	517	ASN

5.3.2 Protein sidechains [i](#)

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	619/715 (87%)	608 (98%)	11 (2%)	62	82
1	B	619/715 (87%)	613 (99%)	6 (1%)	78	89
1	C	618/715 (86%)	609 (98%)	9 (2%)	67	85
1	D	619/715 (87%)	609 (98%)	10 (2%)	65	84
All	All	2475/2860 (86%)	2439 (98%)	36 (2%)	70	85

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	807	VAL
1	C	326	ARG
1	D	603	SER
1	C	173	ILE
1	C	522	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	B	255	ASN
1	D	225	HIS
1	B	225	HIS
1	A	300	HIS

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](#)

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](#)

There are no chain breaks in this entry.