wwPDB X-ray Structure Validation Summary Report (i)

Sep 2, 2023 – 06:03 PM EDT

PDB ID	:	3QLV
Title	:	Crystal structure of the GluK2/GluK5 (GluR6/KA2) ATD tetramer assembly
Authors	:	Kumar, J.; Mayer, M.L.
Deposited on	:	2011-02-03
Resolution	:	3.94 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

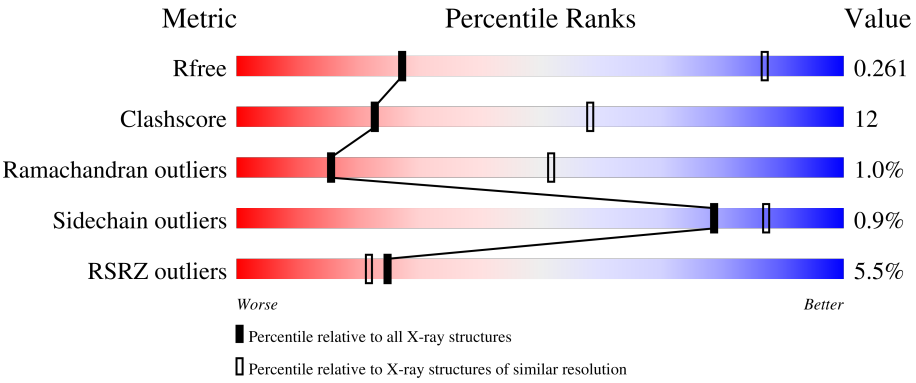
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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}	130704	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)

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 of the lower 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	4% 73% 21% • 6%
1	B	393	3% 72% 21% • 6%
1	E	393	5% 69% 24% • 6%
1	G	393	5% 70% 23% • 6%
1	I	393	13% 73% 21% • 6%

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Mol	Chain	Length	Quality of chain
2	C	395	2% 71% 26%
2	D	395	3% 69% 27%
2	F	395	4% 70% 26%
2	H	395	3% 71% 25%
2	J	395	10% 71% 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 59281 atoms, of which 29647 are hydrogens and 0 are deuteriums.

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 Glutamate receptor, ionotropic kainate 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	371	Total	C	H	N	O	S	0	0	0
			5804	1821	2911	501	553	18			
1	B	371	Total	C	H	N	O	S	0	0	0
			5804	1821	2911	501	553	18			
1	E	371	Total	C	H	N	O	S	0	0	0
			5792	1818	2902	501	553	18			
1	G	371	Total	C	H	N	O	S	0	0	0
			5804	1821	2911	501	553	18			
1	I	371	Total	C	H	N	O	S	0	0	0
			5792	1818	2902	501	553	18			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	LEU	-	expression tag	UNP Q63273
A	389	GLU	-	expression tag	UNP Q63273
A	390	LEU	-	expression tag	UNP Q63273
A	391	VAL	-	expression tag	UNP Q63273
A	392	PRO	-	expression tag	UNP Q63273
A	393	ARG	-	expression tag	UNP Q63273
B	388	LEU	-	expression tag	UNP Q63273
B	389	GLU	-	expression tag	UNP Q63273
B	390	LEU	-	expression tag	UNP Q63273
B	391	VAL	-	expression tag	UNP Q63273
B	392	PRO	-	expression tag	UNP Q63273
B	393	ARG	-	expression tag	UNP Q63273
E	388	LEU	-	expression tag	UNP Q63273
E	389	GLU	-	expression tag	UNP Q63273
E	390	LEU	-	expression tag	UNP Q63273
E	391	VAL	-	expression tag	UNP Q63273
E	392	PRO	-	expression tag	UNP Q63273
E	393	ARG	-	expression tag	UNP Q63273
G	388	LEU	-	expression tag	UNP Q63273

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Chain	Residue	Modelled	Actual	Comment	Reference
G	389	GLU	-	expression tag	UNP Q63273
G	390	LEU	-	expression tag	UNP Q63273
G	391	VAL	-	expression tag	UNP Q63273
G	392	PRO	-	expression tag	UNP Q63273
G	393	ARG	-	expression tag	UNP Q63273
I	388	LEU	-	expression tag	UNP Q63273
I	389	GLU	-	expression tag	UNP Q63273
I	390	LEU	-	expression tag	UNP Q63273
I	391	VAL	-	expression tag	UNP Q63273
I	392	PRO	-	expression tag	UNP Q63273
I	393	ARG	-	expression tag	UNP Q63273

- Molecule 2 is a protein called Glutamate receptor, ionotropic kainate 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	381	Total	C	H	N	O	S	0	0	0
			6057	1938	3022	517	563	17			
2	D	381	Total	C	H	N	O	S	0	0	0
			6057	1938	3022	517	563	17			
2	F	381	Total	C	H	N	O	S	0	0	0
			6057	1938	3022	517	563	17			
2	H	381	Total	C	H	N	O	S	0	0	0
			6057	1938	3022	517	563	17			
2	J	381	Total	C	H	N	O	S	0	0	0
			6057	1938	3022	517	563	17			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	390	LEU	-	expression tag	UNP P42260
C	391	GLU	-	expression tag	UNP P42260
C	392	LEU	-	expression tag	UNP P42260
C	393	VAL	-	expression tag	UNP P42260
C	394	PRO	-	expression tag	UNP P42260
C	395	ARG	-	expression tag	UNP P42260
D	390	LEU	-	expression tag	UNP P42260
D	391	GLU	-	expression tag	UNP P42260
D	392	LEU	-	expression tag	UNP P42260
D	393	VAL	-	expression tag	UNP P42260
D	394	PRO	-	expression tag	UNP P42260
D	395	ARG	-	expression tag	UNP P42260
F	390	LEU	-	expression tag	UNP P42260

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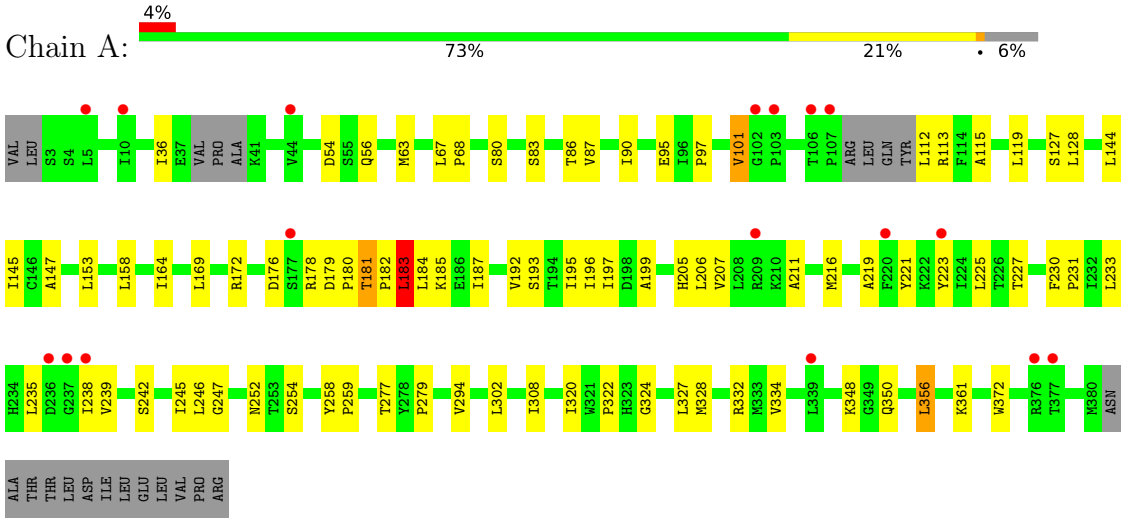
Chain	Residue	Modelled	Actual	Comment	Reference
F	391	GLU	-	expression tag	UNP P42260
F	392	LEU	-	expression tag	UNP P42260
F	393	VAL	-	expression tag	UNP P42260
F	394	PRO	-	expression tag	UNP P42260
F	395	ARG	-	expression tag	UNP P42260
H	390	LEU	-	expression tag	UNP P42260
H	391	GLU	-	expression tag	UNP P42260
H	392	LEU	-	expression tag	UNP P42260
H	393	VAL	-	expression tag	UNP P42260
H	394	PRO	-	expression tag	UNP P42260
H	395	ARG	-	expression tag	UNP P42260
J	390	LEU	-	expression tag	UNP P42260
J	391	GLU	-	expression tag	UNP P42260
J	392	LEU	-	expression tag	UNP P42260
J	393	VAL	-	expression tag	UNP P42260
J	394	PRO	-	expression tag	UNP P42260
J	395	ARG	-	expression tag	UNP P42260

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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.

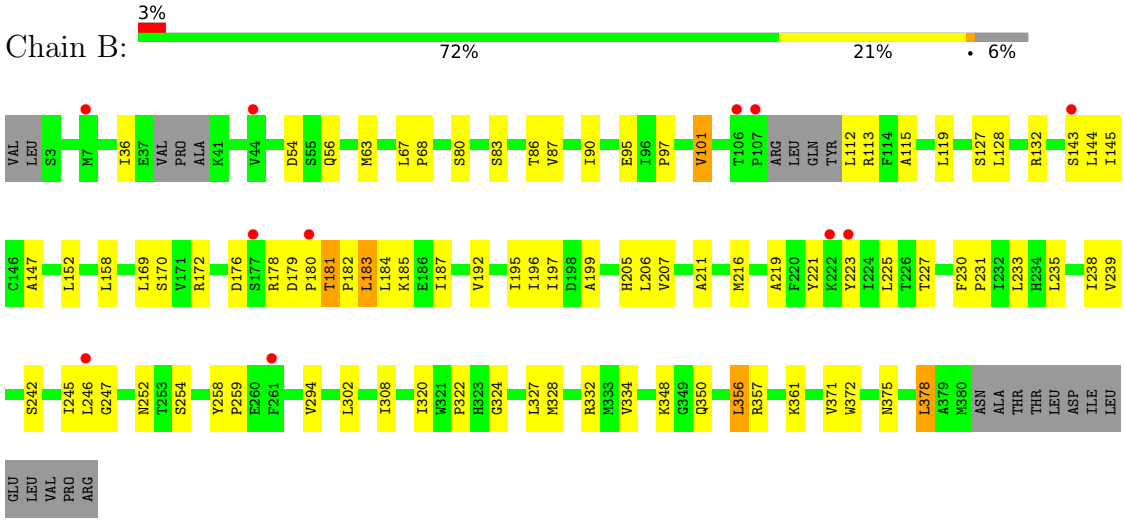
• Molecule 1: Glutamate receptor, ionotropic kainate 5

Chain A:



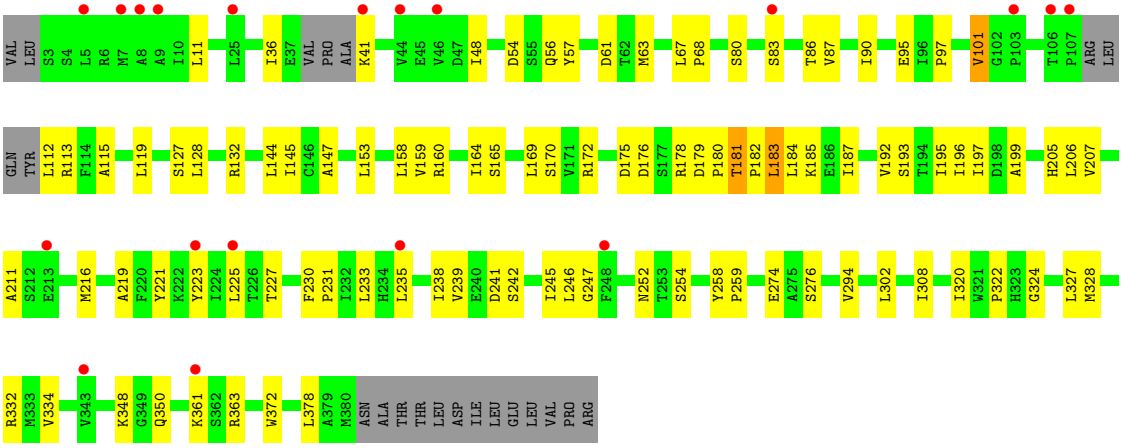
• Molecule 1: Glutamate receptor, ionotropic kainate 5

Chain B:



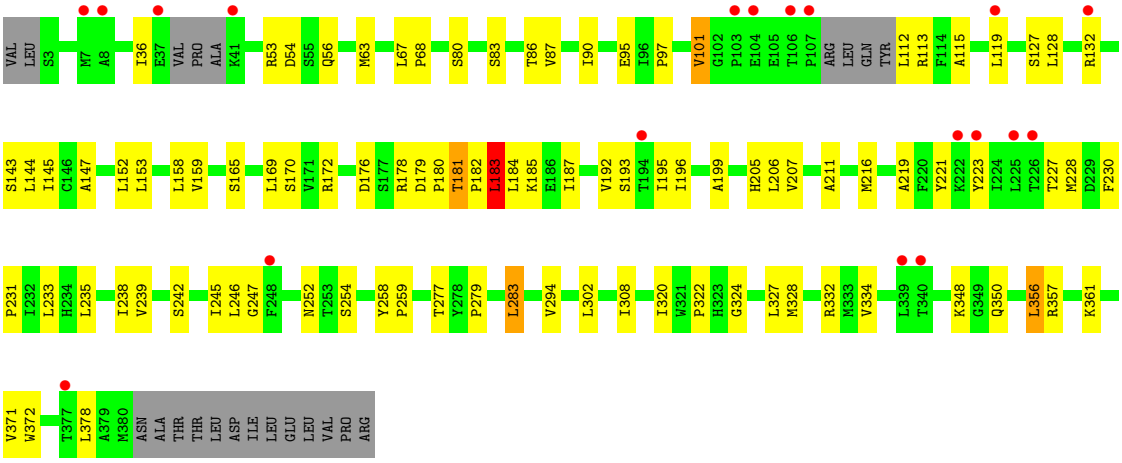
• Molecule 1: Glutamate receptor, ionotropic kainate 5

Chain E:



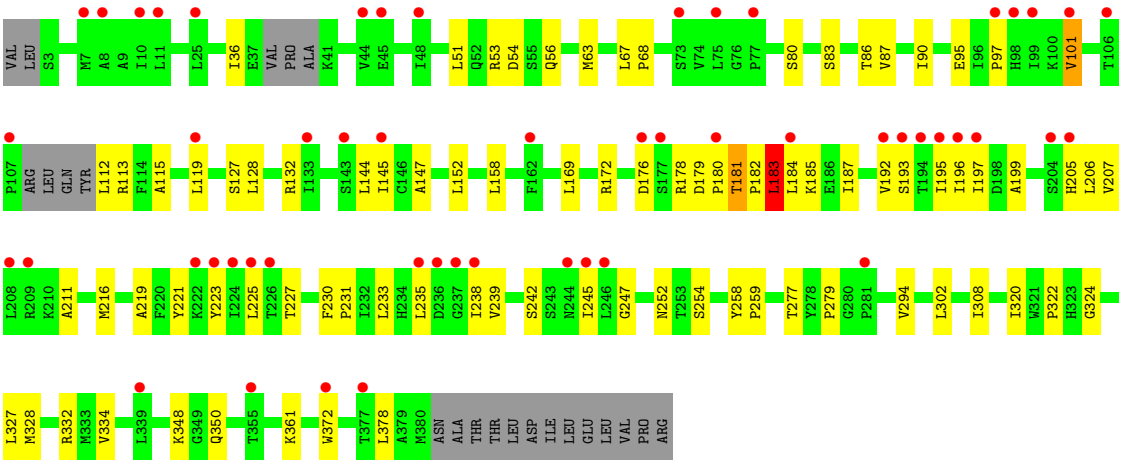
• Molecule 1: Glutamate receptor, ionotropic kainate 5

Chain G:



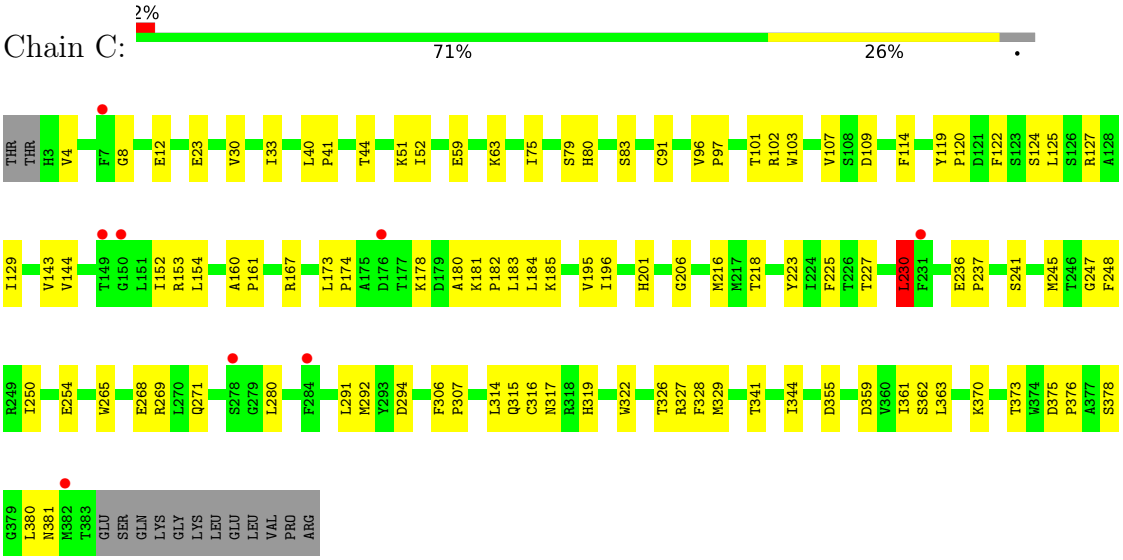
• Molecule 1: Glutamate receptor, ionotropic kainate 5

Chain I:



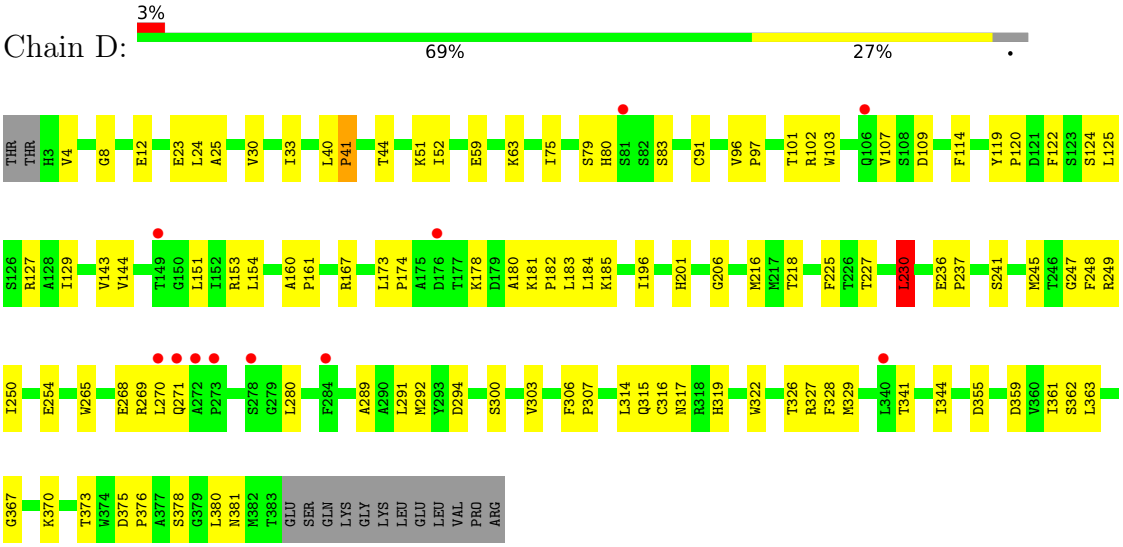
• Molecule 2: Glutamate receptor, ionotropic kainate 2

Chain C:



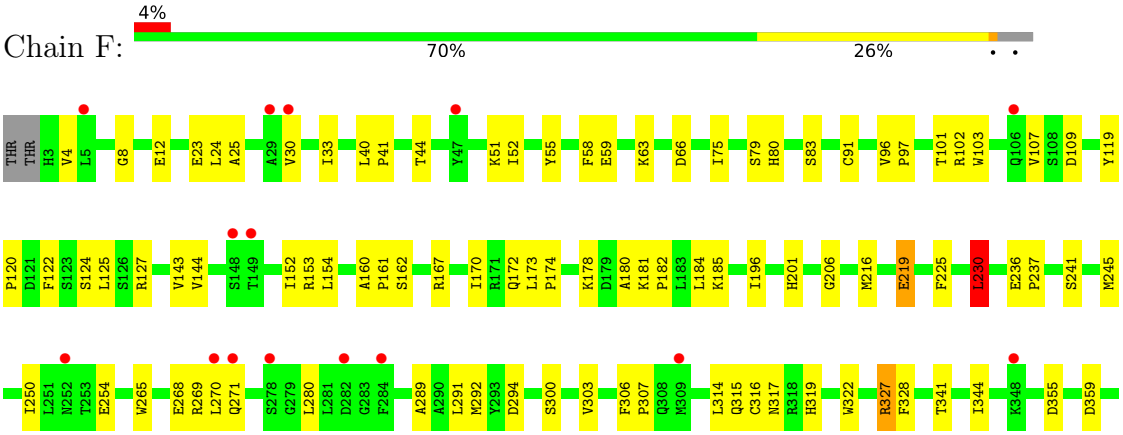
• Molecule 2: Glutamate receptor, ionotropic kainate 2

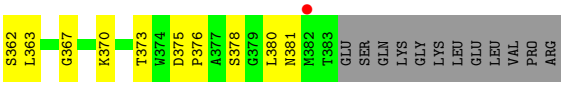
Chain D:



• Molecule 2: Glutamate receptor, ionotropic kainate 2

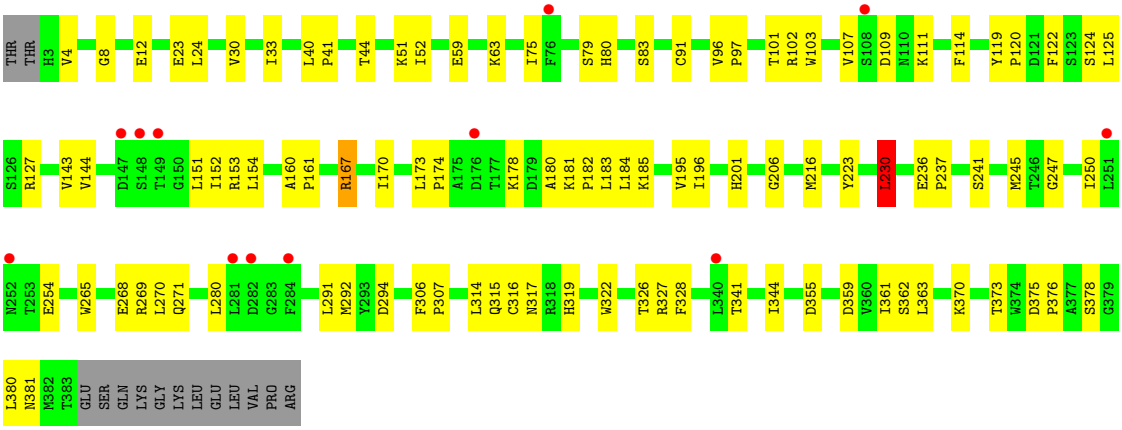
Chain F:





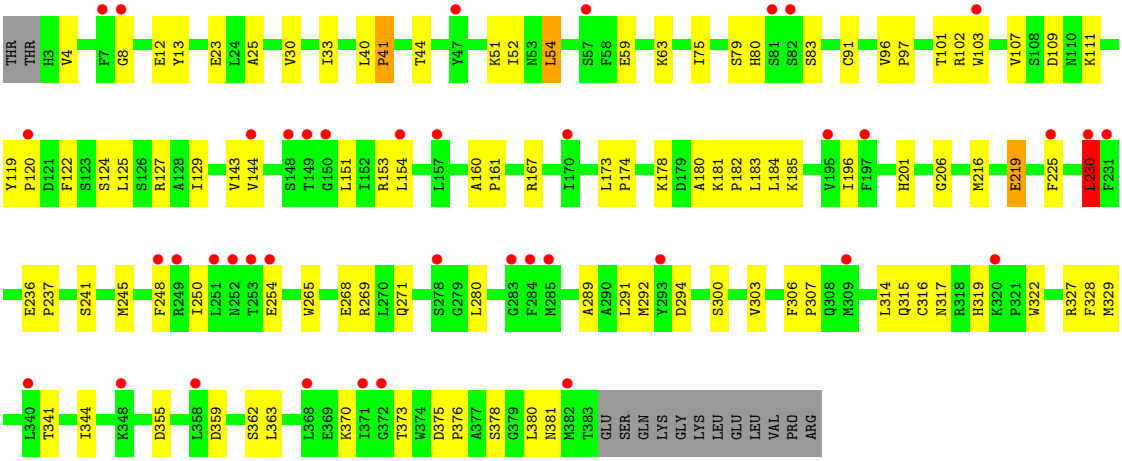
• Molecule 2: Glutamate receptor, ionotropic kainate 2

Chain H:



• Molecule 2: Glutamate receptor, ionotropic kainate 2

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	366.55Å 109.18Å 155.47Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	48.95 – 3.94 48.95 – 3.94	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.95-3.94) 93.7 (48.95-3.94)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.264 , 0.280 0.247 , 0.261	Depositor DCC
R_{free} test set	2595 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	128.5	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 100.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	59281	wwPDB-VP
Average B, all atoms (Å^2)	186.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.25	0/2944	0.40	2/3985 (0.1%)
1	B	0.26	1/2944 (0.0%)	0.39	2/3985 (0.1%)
1	E	0.22	0/2941	0.37	0/3981
1	G	0.26	0/2944	0.39	2/3985 (0.1%)
1	I	0.21	0/2941	0.37	0/3981
2	C	0.24	0/3105	0.40	1/4204 (0.0%)
2	D	0.25	0/3105	0.41	1/4204 (0.0%)
2	F	0.26	0/3105	0.43	3/4204 (0.1%)
2	H	0.25	0/3105	0.40	1/4204 (0.0%)
2	J	0.26	0/3105	0.43	5/4204 (0.1%)
All	All	0.25	1/30239 (0.0%)	0.40	17/40937 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	LEU	CG-CD2	5.04	1.70	1.51

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	230	LEU	CB-CG-CD1	6.14	121.43	111.00
2	C	230	LEU	CB-CG-CD1	6.12	121.40	111.00
2	D	230	LEU	CB-CG-CD1	6.11	121.39	111.00
1	G	356	LEU	CB-CG-CD1	5.78	120.83	111.00
1	B	356	LEU	CB-CG-CD1	5.78	120.82	111.00

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	2893	2911	2903	65	0
1	B	2893	2911	2903	64	0
1	E	2890	2902	2894	78	0
1	G	2893	2911	2903	72	0
1	I	2890	2902	2894	61	0
2	C	3035	3022	3012	69	0
2	D	3035	3022	3012	81	0
2	F	3035	3022	3012	78	1
2	H	3035	3022	3012	75	0
2	J	3035	3022	3012	64	1
All	All	29634	29647	29557	682	1

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 682 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)
2:D:359:ASP:HB3	2:D:370:LYS:HE2	1.47	0.95
2:D:359:ASP:CB	2:D:370:LYS:HE2	2.06	0.84
2:D:230:LEU:HD23	2:D:247:GLY:HA3	1.61	0.82
2:H:230:LEU:HD23	2:H:247:GLY:HA3	1.62	0.82
2:C:230:LEU:HD23	2:C:247:GLY:HA3	1.62	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:66:ASP:OD2	2:J:13:TYR:OH[1_545]	2.16	0.04

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 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	365/393 (93%)	314 (86%)	45 (12%)	6 (2%)	9	44
1	B	365/393 (93%)	313 (86%)	46 (13%)	6 (2%)	9	44
1	E	365/393 (93%)	314 (86%)	46 (13%)	5 (1%)	11	45
1	G	365/393 (93%)	313 (86%)	46 (13%)	6 (2%)	9	44
1	I	365/393 (93%)	313 (86%)	46 (13%)	6 (2%)	9	44
2	C	379/395 (96%)	332 (88%)	46 (12%)	1 (0%)	41	74
2	D	379/395 (96%)	330 (87%)	47 (12%)	2 (0%)	29	66
2	F	379/395 (96%)	330 (87%)	48 (13%)	1 (0%)	41	74
2	H	379/395 (96%)	332 (88%)	46 (12%)	1 (0%)	41	74
2	J	379/395 (96%)	332 (88%)	45 (12%)	2 (0%)	29	66
All	All	3720/3940 (94%)	3223 (87%)	461 (12%)	36 (1%)	15	52

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	B	36	ILE
2	C	241	SER
2	D	241	SER
1	E	36	ILE

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 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	326/346 (94%)	325 (100%)	1 (0%)	92	95
1	B	326/346 (94%)	324 (99%)	2 (1%)	86	91
1	E	325/346 (94%)	323 (99%)	2 (1%)	86	91
1	G	326/346 (94%)	323 (99%)	3 (1%)	78	87
1	I	325/346 (94%)	322 (99%)	3 (1%)	78	87
2	C	333/346 (96%)	330 (99%)	3 (1%)	78	87
2	D	333/346 (96%)	330 (99%)	3 (1%)	78	87
2	F	333/346 (96%)	328 (98%)	5 (2%)	65	79
2	H	333/346 (96%)	330 (99%)	3 (1%)	78	87
2	J	333/346 (96%)	328 (98%)	5 (2%)	65	79
All	All	3293/3460 (95%)	3263 (99%)	30 (1%)	78	87

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	230	LEU
2	J	167	ARG
1	G	283	LEU
2	J	230	LEU
1	I	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	350	GLN
1	I	123	ASN
1	G	353	ASN
2	H	304	GLN
1	I	350	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 monosaccharides 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.

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^{th} 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^2)	Q<0.9
1	A	371/393 (94%)	0.26	17 (4%)	32	27	92, 163, 252, 346	0
1	B	371/393 (94%)	0.21	11 (2%)	50	39	85, 155, 235, 320	0
1	E	371/393 (94%)	0.33	19 (5%)	28	24	96, 173, 256, 367	0
1	G	371/393 (94%)	0.31	19 (5%)	28	24	91, 178, 256, 340	0
1	I	371/393 (94%)	0.72	53 (14%)	2	3	134, 242, 336, 425	0
2	C	381/395 (96%)	0.13	8 (2%)	63	54	90, 152, 223, 374	0
2	D	381/395 (96%)	0.19	11 (2%)	51	41	89, 148, 215, 304	0
2	F	381/395 (96%)	0.31	16 (4%)	36	30	97, 162, 247, 387	0
2	H	381/395 (96%)	0.24	12 (3%)	49	38	100, 156, 228, 368	0
2	J	381/395 (96%)	0.50	40 (10%)	6	6	141, 232, 301, 386	0
All	All	3760/3940 (95%)	0.32	206 (5%)	25	22	85, 172, 278, 425	0

The worst 5 of 206 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	223	TYR	15.4
1	E	107	PRO	7.6
1	I	236	ASP	7.4
1	I	224	ILE	7.1
1	I	225	LEU	7.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.