



Activation of kainate receptor GluK2–Neto2 complex

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Supplementary Table 1. Cryo-EM data collection, refinement and validation statistics.

Structure	GluK2 _{Apo-asm} Composite	GluK2 _{Apo-asm} ATD	GluK2 _{Apo-asm} LBD-TMD	GluK2 _{Apo-2fold} Composite	GluK2 _{Apo-2fold} ATD	GluK2 _{Apo-2fold} LBD-TMD
PDB code	9N4L	-	-	9N4M	-	-
EMDB code	EMD-48897	EMD-48878	EMD-48879	EMD-48890	EMD-48880	EMD-48881
Data collection and processing						
Magnification	105000	105000	105000	105000	105000	105000
Voltage (kV)	300	300	300	300	300	300
Electron exposure (e ⁻ Å ⁻²)	50	50	50	50	50	50
Defocus range (µm)	-1 to -2	-1 to -2	-1 to -2	-1 to -2	-1 to -2	-1 to -2
Reported pixel size (Å)	0.82	0.82	0.82	0.82	0.82	0.82
Processing software	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4
Symmetry imposed	-	C1	C1	-	C2	C2
Initial particles images (no.)	-	627,603	627,603	-	627,603	627,603
Final particle images (no.)	-	157,657	150,109	-	81,205	119,953
Map resolution (Å)	-	3.48	4.24	-	3.72	3.77
FSC threshold	-	0.143	0.143	-	0.143	0.143
Map resolution range (Å)	-	1.99 - 7.04	2.55 - 10.82	-	2.20 - 7.73	2.50 - 8.59
Refinement						
Initial models used (PDB code)	-	8FWT	8FWS	-	8FWT	8FWS
Model resolution	-	3.48	4.24	-	3.72	3.77
Map sharpening B factor (Å ²)	-	-119.6	-163.2	-	-141.0	-134.9
B factors (Å²)						
Protein	51.51	-	-	102.66	-	-
Ligands	38.01	-	-	25.49	-	-
R.m.s. deviations						
Bond lengths (Å)	0.006	-	-	0.008	-	-
Bond angles (°)	1.289	-	-	1.435	-	-
Model composition						
Non-hydrogen atoms	27183	-	-	28054	-	-
Protein residues	3354	-	-	3360	-	-
Ligands						
2J9 (BPAM344)	-	-	-	-	-	-
BMA	3	-	-	2	-	-
NAG	34	-	-	38	-	-
POV	-	-	-	16	-	-
MAN	6	-	-	4	-	-
KA (agonist)	-	-	-	-	-	-
Validation						
MolProbity score	1.88	-	-	1.94	-	-
Clash score, all atoms	4.94	-	-	5.11	-	-
CC (mask)	0.71	-	-	0.73	-	-
CC (box)	0.68	-	-	0.64	-	-
CC (peaks)	0.52	-	-	0.55	-	-
CC (volume)	0.67	-	-	0.70	-	-
Q-score	3.35	-	-	0.39	-	-
EMRinger Score	1.86	-	-	1.69	-	-
3DFSC sphericity score	0.95	-	-	0.98	-	-
Poor rotamers (%)	0.58	-	-	0.21	-	-
Ramachandran plot						
Favored (%)	86.84	-	-	84.70	-	-
Allowed (%)	12.77	-	-	14.95	-	-
Disallowed (%)	0.39	-	-	0.36	-	-

Structure	GluK2 _{KA-BPAM} Composite	GluK2 _{KA-BPAM} ATD	GluK2 _{KA-BPAM} LBD-TMD	GluK2-0xNeto2 _{Apo} composite	GluK2-0xNeto2 _{Apo} ATD	GluK2-0xNeto2 _{Apo} LBD-TMD
PDB code	9N4N	-	-	9N4O	-	-
EMDB code	EMD-48899	EMD-48882	EMD-48884	EMD-48900	EMD-48885	EMD-48886
Data collection and processing						
Magnification	105000	105000	105000	105000	105000	105000
Voltage (kV)	300	300	300	300	300	300
Electron exposure (e ⁻ Å ⁻²)	58.2	58.2	58.2	58.8	58.8	58.8
Defocus range (µm)	-1 to -2	-1 to -2	-1 to -2	-1 to -2	-1 to -2	-1 to -2
Reported pixel size (Å)	0.83	0.83	0.83	0.83	0.83	0.83
Processing software	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4
Symmetry imposed	-	C2	C2	-	C1	C1
Initial particles images (no.)	-	222,226	222,226	-	585,167	585,167
Final particle images (no.)	-	93,649	151,189	-	139,000	139,000
Map resolution (Å)	-	3.32	3.22	-	3.48	3.60
FSC threshold	-	0.143	0.143	-	0.143	0.143
Map resolution range (Å)	-	2.90 - 8.99	2.11 - 7.44	-	2.24 - 5.69	2.90 - 7.71
Refinement						
Initial models used (PDB code)	-	8FWT	9B35	-	8FWT	8FWS
Model resolution	-	3.32	3.22	-	3.48	3.60
Map sharpening B factor (Å ²)	-	-114.7	-97.8	-	-107.6	-108.4
B factors (Å²)						
Protein	48.45	-	-	91.71	-	-
Ligands	23.84	-	-	39.38	-	-
R.m.s. deviations						
Bond lengths (Å)	0.012	-	-	0.008	-	-
Bond angles (°)	1.642	-	-	1.372	-	-
Model composition						
Non-hydrogen atoms	28384	-	-	27503	-	-
Protein residues	3368	-	-	3272	-	-
Ligands						
2J9 (BPAM344)	4	-	-	-	-	-
BMA	8	-	-	7	-	-
NAG	38	-	-	48	-	-
POV	16	-	-	15	-	-
MAN	8	-	-	6	-	-
KA (agonist)	4	-	-	-	-	-
Validation						
MolProbity score	1.81	-	-	1.72	-	-
Clash score, all atoms	3.93	-	-	3.71	-	-
CC (mask)	0.77	-	-	0.72	-	-
CC (box)	0.67	-	-	0.63	-	-
CC (peaks)	0.63	-	-	0.50	-	-
CC (volume)	0.74	-	-	0.69	-	-
Q-score	0.47	-	-	0.35	-	-
EMRinger Score	3.43	-	-	2.20	-	-
3DFSC sphericity score	0.95	-	-	0.97	-	-
Poor rotamers (%)	0.48	-	-	0.56	-	-
Ramachandran plot						
Favored (%)	86.52	-	-	89.68	-	-
Allowed (%)	12.95	-	-	9.87	-	-
Disallowed (%)	0.54	-	-	0.46	-	-

Structure	GluK2-1xNeto2 _{Apo} composite	GluK2-1xNeto2 _{Apo} ATD	GluK2-1xNeto2 _{Apo} LBD-TMD	GluK2-2xNeto2 _{Apo} composite	GluK2-2xNeto2 _{Apo} ATD	GluK2-2xNeto2 _{Apo} LBD-TMD
PDB code	9N4P	-	-	9N4Q	-	-
EMDB code	EMD-48901	EMD-48887	EMD-48888	EMD-48902	EMD-48889	EMD-48890
Data collection and processing						
Magnification	105000	105000	105000	105000	105000	105000
Voltage (kV)	300	300	300	300	300	300
Electron exposure (e ⁻ Å ⁻²)	58.8	58.8	58.8	58.8	58.8	58.8
Defocus range (µm)	-1 to -2	-1 to -2	-1 to -2	-1 to -2	-1 to -2	-1 to -2
Reported pixel size (Å)	0.83	0.83	0.83	0.83	0.83	0.83
Processing software	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4
Symmetry imposed	-	C1	C1	-	C1	C1
Initial particles images (no.)	-	585,167	585,167	-	585,167	585,167
Final particle images (no.)	-	62,000	101,000	-	112,000	112,000
Map resolution (Å)	-	3.58	3.69	-	3.43	3.48
FSC threshold	-	0.143	0.143	0.143	0.143	0.143
Map resolution range (Å)	-	2.30 - 6.47	2.39 - 7.20	-	2.02 - 5.31	2.5 - 20.29
Refinement						
Initial models used (PDB code)	-	8FWT,7F57	8FWS,7F57	-	8FWT,7F57	8FWS,7F57
Model resolution	-	3.58	3.69	-	3.43	3.48
Map sharpening B factor (Å ²)	-	-101.7	-98.8	-	-98.1	-85.4
B factors (Å²)						
Protein	95.87	-	-	91.65	-	-
Ligands	90.34	-	-	46.65	-	-
R.m.s. deviations						
Bond lengths (Å)	0.010	-	-	0.008	-	-
Bond angles (°)	1.419	-	-	1.330	-	-
Model composition						
Non-hydrogen atoms	30797	-	-	33333	-	-
Protein residues	3680	-	-	3998	-	-
Ligands						
2J9 (BPAM344)	-	-	-	-	-	-
BMA	7	-	-	9	-	-
NAG	48	-	-	49	-	-
POV	15	-	-	15	-	-
MAN	10	-	-	8	-	-
KA (agonist)	-	-	-	-	-	-
Validation						
MolProbity score	1.81	-	-	1.72	-	-
Clash score, all atoms	4.10	-	-	3.82	-	-
CC (mask)	0.76	-	-	0.78	-	-
CC (box)	0.65	-	-	0.66	-	-
CC (peaks)	0.53	-	-	0.55	-	-
CC (volume)	0.73	-	-	0.76	-	-
Q-score	0.38	-	-	0.42	-	-
EMRinger Score	2.06	-	-	3.04	-	-
3DFSC sphericity score	0.96	-	-	0.97	-	-
Poor rotamers (%)	0.53	-	-	0.43	-	-
Ramachandran plot						
Favored (%)	87.16	-	-	90.04	-	-
Allowed (%)	12.16	-	-	9.56	-	-
Disallowed (%)	0.68	-	-	0.40	-	-

Structure	GluK2- 0xNeto2 _{KA-BPAM} composite	GluK2- 0xNeto2 _{KA-BPAM} ATD	GluK2- 0xNeto2 _{KA-BPAM} LBD-TMD	GluK2- 1xNeto2 _{KA-BPAM} composite	GluK2- 1xNeto2 _{KA-BPAM} ATD	GluK2- 1xNeto2 _{KA-BPAM} LBD-TMD
PDB code	9N4R	-	-	9N4S	-	-
EMDB code	EMD-48903	EMD-48891	EMD-48892	EMD-48904	EMD-48893	EMD-48894
Data collection and processing						
Magnification	105000	105000	105000	105000	105000	105000
Voltage (kV)	300	300	300	300	300	300
Electron exposure (e ⁻ Å ⁻²)	58.8	58.8	58.8	58.8	58.8	58.8
Defocus range (µm)	-1 to -2	-1 to -2	-1 to -2	-1 to -2	-1 to -2	-1 to -2
Reported pixel size (Å)	0.825	0.825	0.825	0.825	0.825	0.825
Processing software	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4
Symmetry imposed	-	C2	C2	-	C1	C1
Initial particles images (no.)	-	647,799	647,799	-	647,799	647,799
Final particle images (no.)	-	55,383	144,141	-	113,543	194,105
Map resolution (Å)	-	3.74	3.42	-	3.34	3.31
FSC threshold	-	0.143	0.143	-	0.143	0.143
Map resolution range (Å)	-	2.17 - 10.76	2.27 - 8.37	-	2.94 - 18.71	2.78 - 9.99
Refinement						
Initial models used (PDB code)	-	8FWT	9B35	-	8FWT, 7F57	9B35, 7F57
Model resolution	-	3.74	3.42	-	3.34	3.31
Map sharpening B factor (Å ²)	-	-141.0	-111.2	-	-112.7	-105.0
B factors (Å²)						
Protein	101.99	-	-	93.60	-	-
Ligands	28.30	-	-	30.17	-	-
R.m.s. deviations						
Bond lengths (Å)	0.011	-	-	0.012	-	-
Bond angles (°)	1.632	-	-	1.584	-	-
Model composition						
Non-hydrogen atoms	28356	-	-	31000	-	-
Protein residues	3368	-	-	3687	-	-
Ligands						
2J9 (BPAM344)	4	-	-	4	-	-
BMA	8	-	-	10	-	-
NAG	36	-	-	39	-	-
POV	16	-	-	17	-	-
MAN	8	-	-	8	-	-
KA (agonist)	4	-	-	4	-	-
Validation						
MolProbity score	1.83	-	-	1.77	-	-
Clash score, all atoms	1.83	-	-	4.24	-	-
CC (mask)	0.76	-	-	0.77	-	-
CC (box)	0.71	-	-	0.66	-	-
CC (peaks)	0.62	-	-	0.58	-	-
CC (volume)	0.73	-	-	0.74	-	-
Q-score	0.16	-	-	0.43	-	-
EMRinger Score	2.80	-	-	3.20	-	-
3DFSC sphericity score	0.75	-	-	0.95	-	-
Poor rotamers (%)	0.27	-	-	0.09	-	-
Ramachandran plot						
Favored (%)	87.35	-	-	89.44	-	-
Allowed (%)	12.05	-	-	10.20	-	-
Disallowed (%)	0.60	-	-	0.35	-	-

Structure	GluK2-2xNeto2 _{KA-BPAM} composite	GluK2-2xNeto2 _{KA-BPAM} ATD	GluK2-2xNeto2 _{KA-BPAM} LBD-TMD
PDB code	9N4T	-	-
EMDB code	EMD-48905	EMD-48895	EMD-48896
Data collection and processing			
Magnification	105000	105000	105000
Voltage (kV)	300	300	300
Electron exposure (e ⁻ Å ⁻²)	58.8	58.8	58.8
Defocus range (µm)	-1 to -2	-1 to -2	-1 to -2
Reported pixel size (Å)	0.825	0.825	0.825
Processing software	CryoSPARCv4	CryoSPARCv4	CryoSPARCv4
Symmetry imposed	-	C2	C2
Initial particles images (no.)	-	647,799	647,799
Final particle images (no.)	-	116,689	193,705
Map resolution (Å)	-	3.21	3.22
FSC threshold	-	0.143	0.143
Map resolution range (Å)	-	2.01 - 5.80	2.02 - 7.77
Refinement			
Initial models used (PDB code)	-	8FWT, 7F57	9B35, 7F57
Model resolution	-	3.21	3.22
Map sharpening B factor (Å ²)	-	-117.3	-114.1
B factors (Å²)			
Protein	85.45	-	-
Ligands	41.70	-	-
R.m.s. deviations			
Bond lengths (Å)	0.010	-	-
Bond angles (°)	1.556	-	-
Model composition			
Non-hydrogen atoms	33572	-	-
Protein residues	4006	-	-
Ligands			
2J9 (BPAM344)	4	-	-
BMA	8	-	-
NAG	40	-	-
POV	18	-	-
MAN	8	-	-
KA (agonist)	4	-	-
Validation			
MolProbity score	1.86	-	-
Clash score, all atoms	5.81	-	-
CC (mask)	0.73	-	-
CC (box)	0.64	-	-
CC (peaks)	0.57	-	-
CC (volume)	0.71	-	-
Q-score	0.45	-	-
EMRinger Score	3.12	-	-
3DFSC sphericity score	0.75	-	-
Poor rotamers (%)	0.57	-	-
Ramachandran plot			
Favored (%)	88.50	-	-
Allowed (%)	10.63	-	-
Disallowed (%)	0.88	-	-