Table S1. Summary of predicted hydrogen bond energies and inter-atomic distances in Kv7.2–GMPI(4,5)P_2 complexes I

Kv7.2–GMPI(4,5)P_2 interactions							
Hydrogen bond		Interaction		Hydrogen bond		Interaction	
Atom 1 (WT)	Atom 2 (ligand)	Energy (kJ/mol)	Length (Å)	Atom 1 (KRR-EEE)	Atom 2 (ligand)	Energy (kJ/mol)	Length (Å)
R461(Nα)	InsP1	−0.41	3.52	R463(NH2)	InsP4	−2.27	2.93
R461(NH1)	InsP1	−2.49	2.60	R463(NH1)	InsP4	−0.52	3.50
R461(NH2)	InsP1	−0.45	3.34	R463(NH1)	InsP5	−2.5	2.60
R463(NH2)	InsP4	−1.47	2.80				
R463(NH2)	InsP4	−0.12	3.30				
R463(Nε)	InsP4	−0.64	2.50				
R459(NH2)	InsP5	−2.5	2.60				
S460(Oγ)	InsP5	−2.5	2.85				
R463(Nε)	InsP5	−1.67	2.95				
R463(NH1)	InsP5	−0.09	3.58				
R463(NH1)	InsP5	−2.5	2.60				
S460(Oγ)	InsC2	−2.5	2.69				
R461(Nα)	InsC2	−0.37	3.01				
R461(Oα)	InsC2	−2.5	2.69				

Shown are the predicted hydrogen bonds between the indicated atom of the wild-type and KRR-EEE Kv7.2 channel and the indicated atom of GMPI(4,5)P_2.

Table S2. Summary of predicted hydrogen bonds energies and inter-atomic distances in Kv7.2– GPMI-P_2 complexes II

Kv7.2–GMPI(4,5)P_2 interactions															
Hydrogen bond		Interaction		Hydrogen bond		Interaction		Hydrogen bond		Interaction		Hydrogen bond		Interaction	
Atom 1 (R463Q)	Atom 2 (ligand)	Energy (kJ/mol)	Length (Å)	Atom 1 (R463E)	Atom 2 (ligand)	Energy (kJ/mol)	Length (Å)	Atom 1 (R467Q)	Atom 2 (ligand)	Energy (kJ/mol)	Length (Å)	Atom 1 (R467E)	Atom 2 (ligand)	Energy (kJ/mol)	Length (Å)
R459 (NH1)	InsP1	−2.5	2.61	S460 (Oγ)	InsP1	−2.5	2.80	R461 (Nε)	InsP1	−0.31	3.52	R461 (NH2)	InsP4	−1.19	2.54
R461 (NH1)	InsP4	−2.5	2.79	R434 (NH1)	InsP4	−2.5	2.96	R463 (NH2)	InsP4	−1.30	3.02	R461 (NH1)	InsP4	−2.03	2.54
R461 (Nε)	InsP5	−0.90	2.80	R435 (NH2)	InsP4	−1.38	2.84	R463 (NH1)	InsP4	−2.5	2.62	R463 (NH2)	InsP4	−0.64	2.38
R461 (NH1)	InsP5	−2.5	3.08	R461 (NH2)	InsP4	−1.61	2.77	R461 (NH2)	InsP5	−2.01	3.18	R463 (NH2)	InsP4	−1.04	3.23
R461 (NH1)	InsP5	−0.61	2.81	R461 (NH1)	InsP4	−2.49	2.60	R463 (NH1)	InsP5	−2.5	2.70	R434 (NH2)	InsP5	−0.04	2.82
				R434 (NH1)	InsP5	−1.73	3.25	R463 (NH1)	InsP5	−0.84	3.02	R434 (NH2)	InsP5	−0.47	3.33
				R434 (NH2)	InsP5	−1.33	2.94	R463 (NH2)	InsP5	−0.38	3.35	R435 (Nα)	InsP5	−2.5	2.81
				V433 (Oα)	InsC2	−2.5	2.70	S460 (Oγ)	InsC3	−1.70	2.50	R463 (Nε)	InsP5	−1.66	3.23
				S460 (Oγ)	InsC2	−2.5	2.70					V433 (Oα)	InsC2	−1.72	3.26
				R435 (Nα)	InsC3	−0.41	3.36					S460 (Oγ)	InsC3	−2.5	2.76
				R461 (Nα)	InsC3	−2.23	3.15					R461 (Nα)	InsC3	−1.33	3.29
												R461 (Oα)	InsC3	−2.13	2.56
												R461 (NH1)	InsC3	−2.5	3.06
												R434 (NH2)	InsC6	−2.5	2.62

Shown are the predicted hydrogen bonds between the indicated atom of the R463Q, R463E, R467Q, or R467E Kv7.2 channel and the indicated atom of GMPI(4,5)P_2.

Table S3. Summary of predicted hydrogen bond energies and inter-atomic distances in Kv7.3–GMPI(4,5)P_2 complexes

Kv7.3–GMPI(4,5)P_2 interactions							
Hydrogen bond		Interaction		Hydrogen bond		Interaction	
Atom 1 (WT)	Atom 2 (ligand)	Energy (kJ/mol)	Length (Å)	Atom 1 (KKR-EEE)	Atom 2 (ligand)	Energy (kJ/mol)	Length (Å)
R434(NH2)	InsP1	−1.25	2.58	R436(NH1)	InsP5	−2.50	2.76
R434(NH2)	InsP5	−1.29	3.00	R436(NH2)	InsP5	−2.50	2.73
R434(NH1)	InsP5	−2.50	3.10	R436(NH2)	InsP4	−1.29	2.60
K432(Nε)	InsP5	−0.86	3.43	T437(Oα)	InsC3	−1.61	2.49
K406(Nε)	InsP5	−2.45	2.59	T437(Nα)	InsC3	−0.70	2.60
R436(NH1)	InsP5	−1.17	2.44	T437(Oγ)	InsC3	−2.50	3.02
K406(Nε)	InsP4	−2.49	2.60	R436(NH1)	InsC2	−1.05	3.39
R436(NH1)	InsP4	−2.33	3.13				
R436(NH1)	InsC2	−2.50	2.83				
R436(NH2)	InsC2	−1.86	2.77				

Shown are the predicted hydrogen bonds between the indicated atom of the wild-type or KKR-EEE Kv7.3 channel and the indicated atom of GMPI(4,5)P_2.