Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Phosphorylation-dependent conformational changes of arrestin in the rhodopsin-arrestin complex

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Supplementary Table:

Table S1. Pair force distribution in different phosphorylation systems (kJ/mol/nm). A positive value means attraction, while a negative value means repulsion.

	None	Crystal	CLR	All
T336-R172	3.37	558.68	594.77	339.11
S338-K301	1.57	425.39	839.83	432.60
T340-V12	-7.28	-42.39	-10.79	28.97
T342-V12	1.95	3.04	-14.52	18.97
S343-K111	161.22	100.63	793.60	414.81

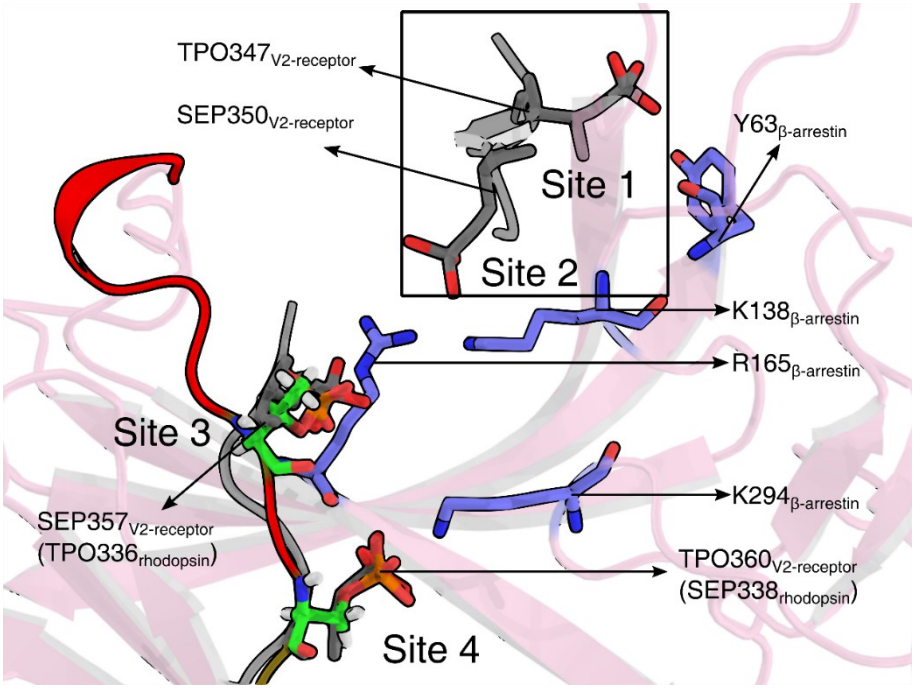

Fig. S1 The interface between the GPCR C-loop and the arrestin N-domain. The C-loop in the V_2-receptor is colored with grey, and the C-loop of the rhodopsin is colored with red. Phosphorylated residues are shown with sticks in grey and green in the V_2-receptor and rhodopsin, respectively. The residues colored in blue represent the sites of interest on arrestin, which may have direct contacts with the phosphorylated residues of GPCRs.

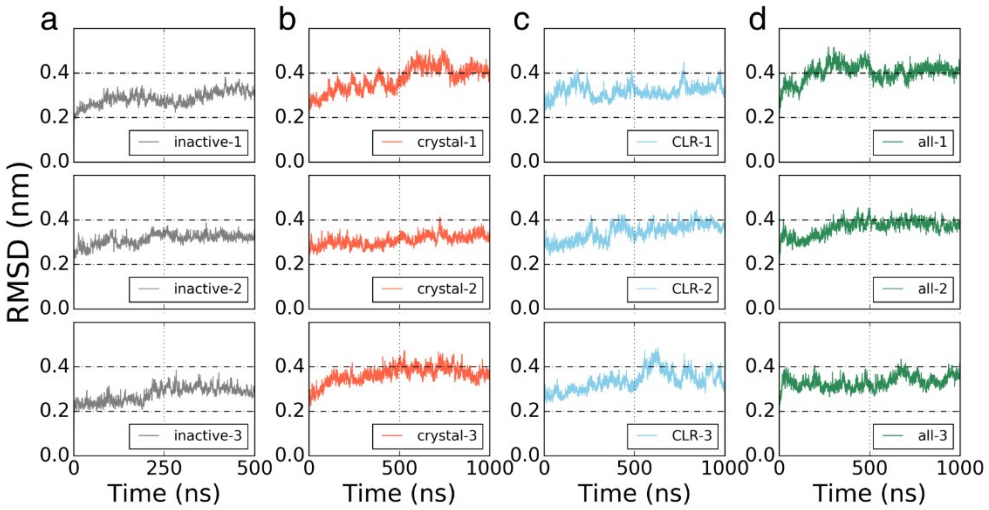

Fig. S2 The root mean squared deviation (RMSD) of all the simulation systems. We ran three repeats for each situation: (a) the inactive systems, (b) the "crystal" systems, (c) the "CLR" systems, and (d) the "all" systems.

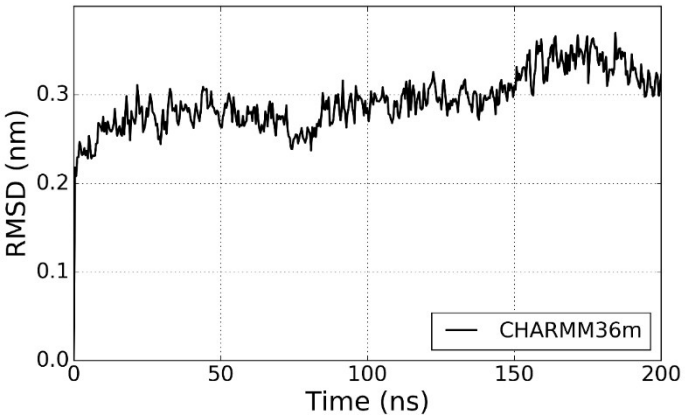

Fig. S3 The root mean squared deviation (RMSD) of the simulation with the CHARMM36m force field.

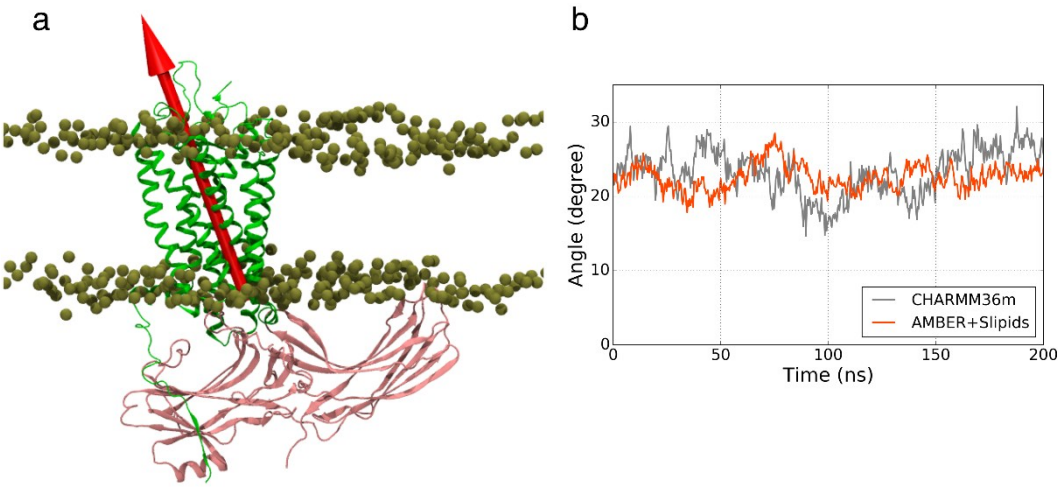

Fig. S4 The angle between the first principal axis of the rhodopsin-arrestin complex and the z-axis, characterizing the orientation of the complex embedded in a bilayer. (a) The side view of the complex and its first principal axis (red arrow). The green and pink cartoon represent rhodopsin and arrestin, respectively. The spheres indicate the phosphorous atoms of the lipid headgroups. (b) The evolution of the orientation angle of the complex in MD simulations with the two force fields.

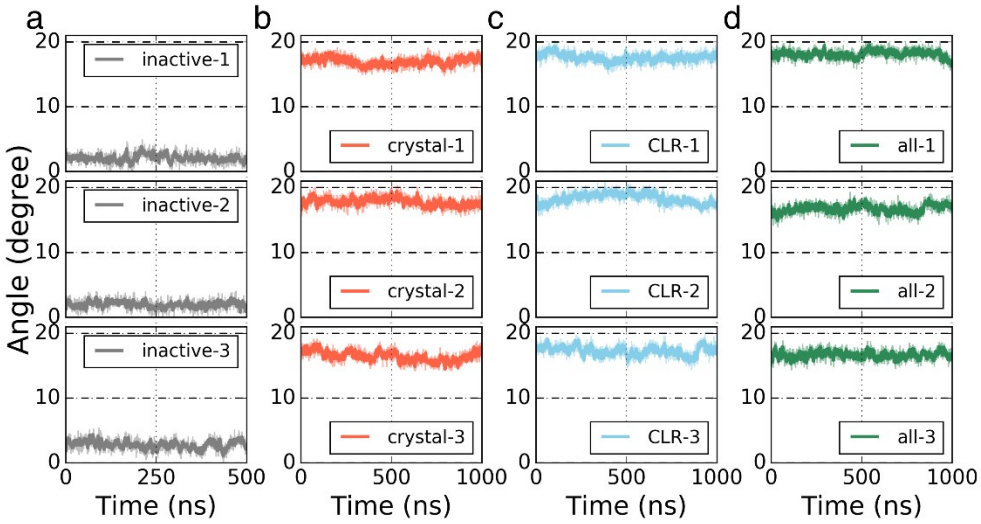

Fig. S5 The inter-domain rotation angle of arrestin, calculated with the method of Latorraca et al. [Ref. 24], for the (a) “inactive” systems; (b) “crystal” systems; (c) “CLR” systems; (d) “all” systems.

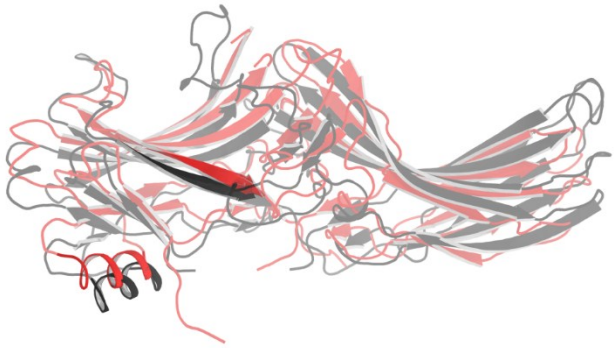

Fig. S6 The overlaid structures of the arrestin from the crystal structure of the Arrestin-Clathrin complex and our simulations. The red cartoon represents the crystal structure of arrestin in the Arrestin-Clathrin complex (PDB ID: 3GD1) [ref. 42], and the black cartoon shows the conformation of arrestin generated from our MD simulation that may be able to bind to clathrin. The α-helix (from $L101_{arrestin}$-$L112_{arrestin}$) and the β-strand (from $S170_{arrestin}$ -$K177_{arrestin}$) in opaque color highlight the deviations, which may be induced by the lacking of C-terminus of the arrestin as well as clathrin in our MD simulations.