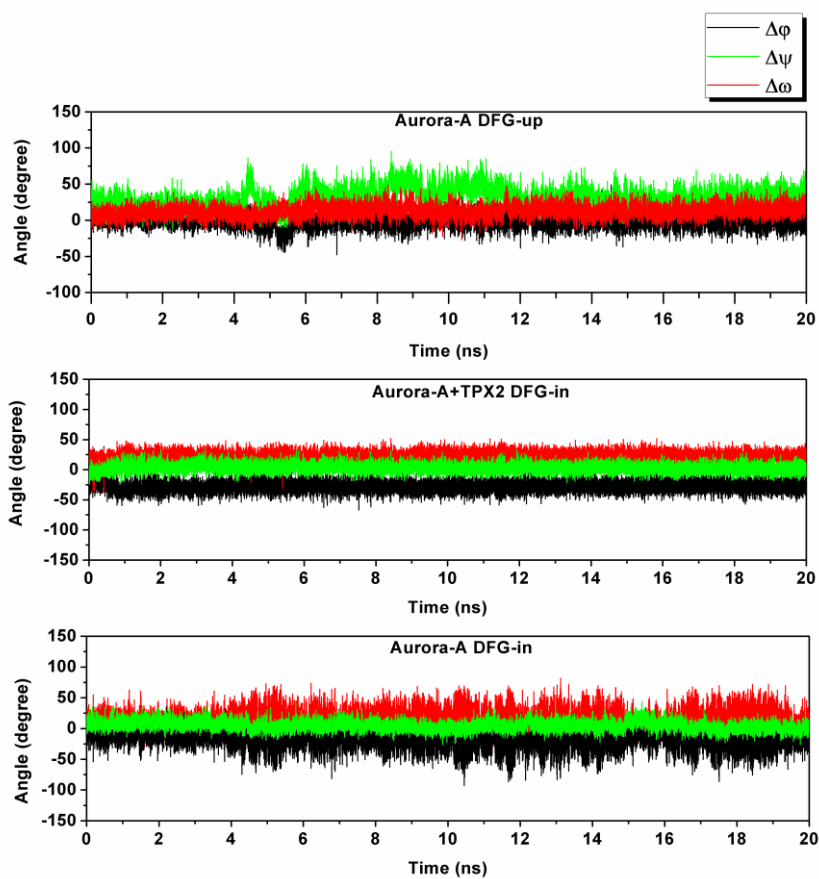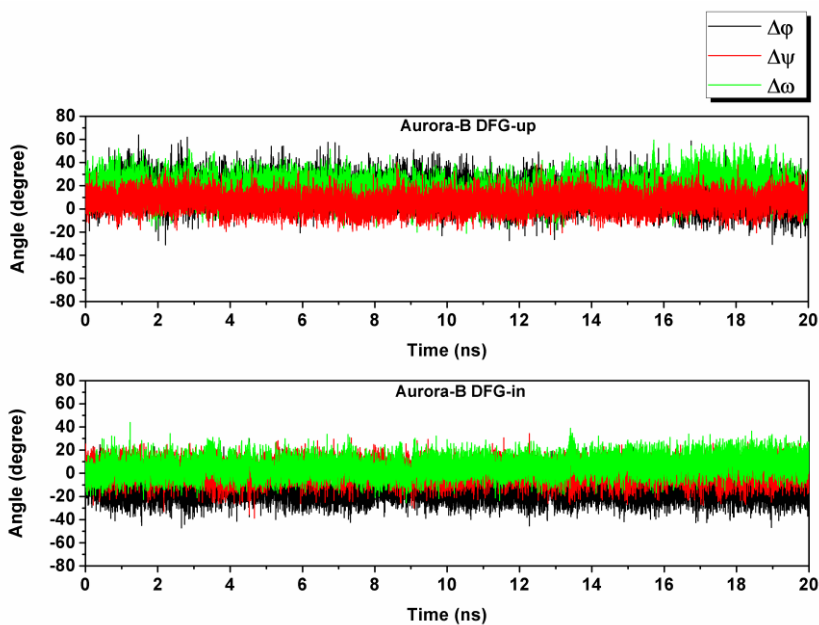Figure S1. Sequence alignment of human Aurora-A, human Aurora-B and *Xenopus laevis* Aurora-B protein kinases. The four residues of the active site that are not identical between Aurora-A and –B are enclosed in the red boxes.
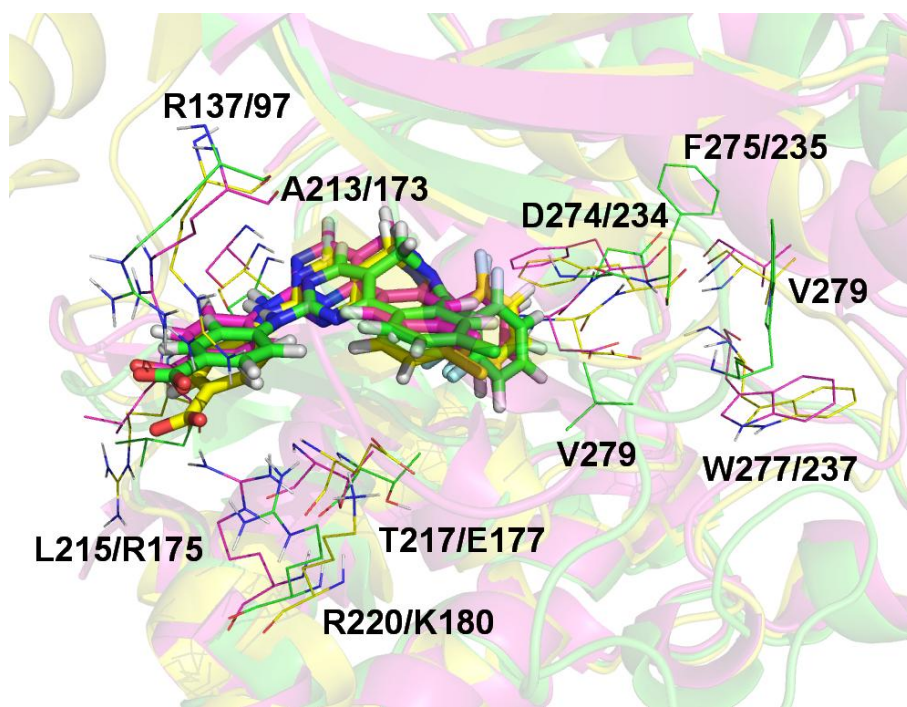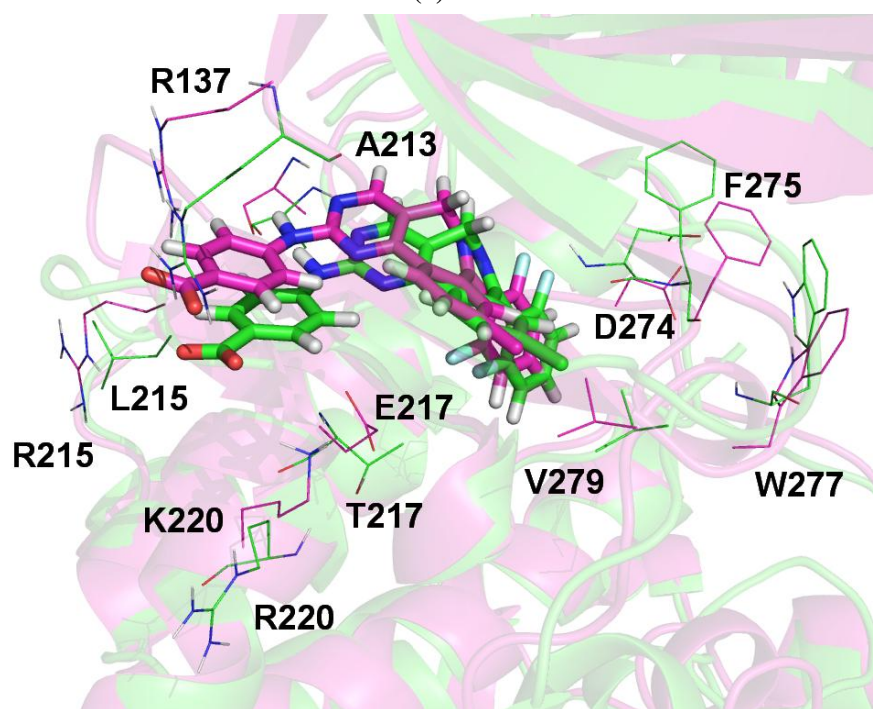
(a)

(b)

Figure S2. The differences $\Delta\varphi$, $\Delta\psi$ and $\Delta\omega$ between the values of MD and crystal structure for 20 ns simulation.

(a)

(b)

Figure S3. (a) Superposition of the DFG-up forms of Aurora-A and -B (b) Superposition of the DFG-up form of Aurora-A with the DFG-in forms of Aurora-A and −B for the average structures obtained from MD simulation.