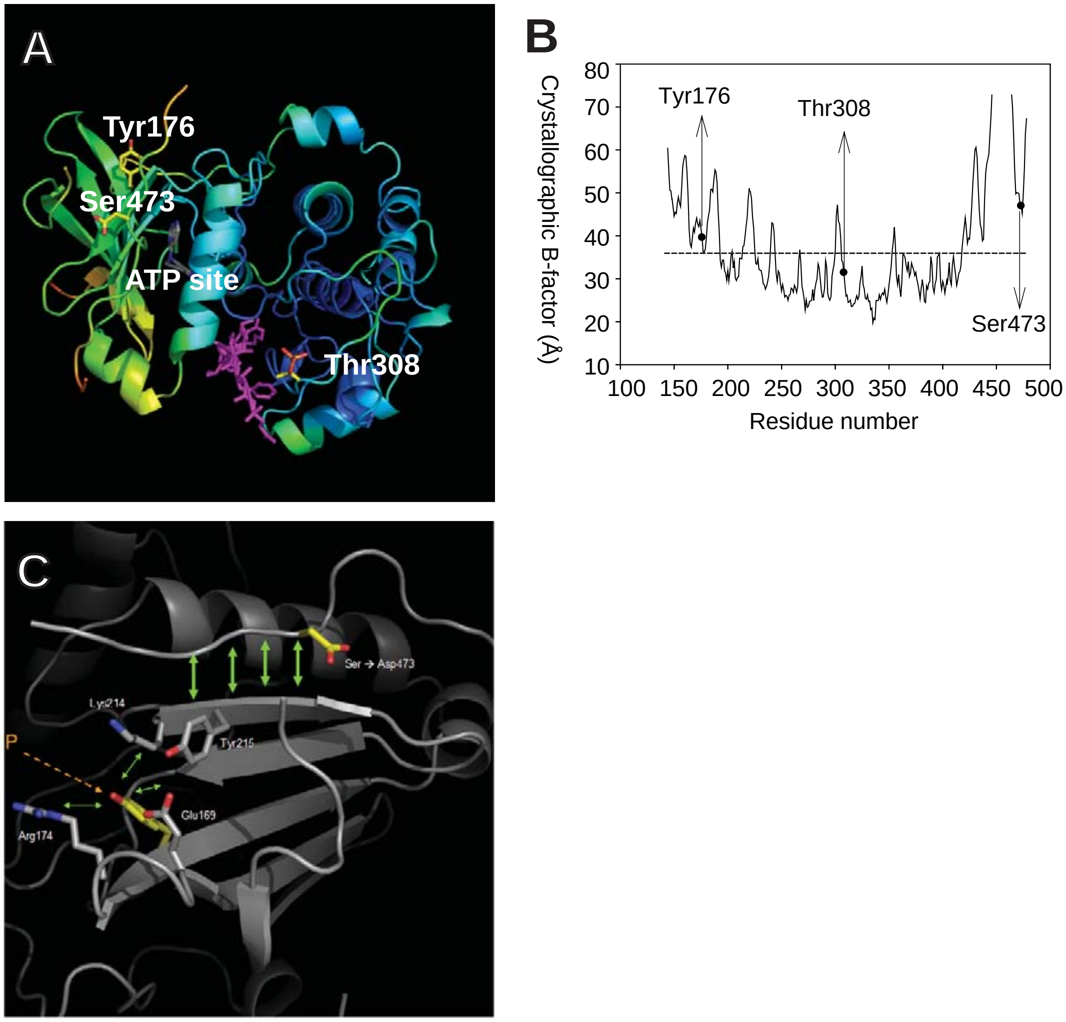

Fig. S3. AKT Tyr176-phosphorylation affects the loop harboring Ser473. (*A*) Residues Tyr176 and Ser473 are located in regions with increased conformational flexibility. The backbone of AKT1 is color-traced according to crystallographic B-factors from blue (20Å, less flexible) to red (76Å, highly flexible). (*B*) B-factor plot of all C-alpha atoms. The average main chain B-factor is 36Å (dashed horizontal line). (*C*) AKT Tyr176-phosphorylation induces substantial conformational changes of residues in its vicinity. Electrostatic interactions could be established with Arg174 and/or Lys214 while electrostatic repulsion and/or steric hindrance (due to the bulky phosphate group) may affect Glu169 and Tyr215. This could lead to a shift of the β-strand flanking the c-terminal portion of the loop harboring Ser473, in turn causing structural alterations of this residue.