

Supplementary information, Figure S2 Crystallographically related dimer of BRI1-KD-BIM and the active site interactions of BRI1-KD and BAK1-KD. Related to Figure 2.

(A) Ribbon diagram representation of BRI1-KD-BIM dimer within one asymmetric unit. For Molecule A, the N-lobe, C-lobe and the activation segment of BRI1 are colored in light orange, forest, and violet, respectively, and the BIM peptide is colored in blue. For Molecule B, BRI1-KD and BKI1-BIM are colored in sky blue and salmon, respectively. The color scheme for Molecule A is used in the following supplemental figures unless specifically mentioned.

(B) The two molecules within one asymmetric unit share almost the same overall architecture. Molecule A and Molecule B are superimposed and shown as ribbon.

(C) The $F_o - F_c$ omit map of BKI1-BIM. The map is contoured at 2.0 σ and shown in mesh, and the residues of BKI1-BIM are shown as blue sticks.

(D) Structure-based sequence alignment of BRI1-KD and BAK1-KD. The code following each protein name is the corresponding UniProt identifier. The alignment includes secondary structure assignments of BRI1-KD (pale green) and BAK1-KD (light blue). Residues of BRI1-KD recognizing BKI1-BIM are indicated by orange triangles, and the observed phosphorylated residues are indicated by cyan asterisks. The activation segments of BRI1-KD and BAK1-KD are boxed in magenta. Residues determining the recognition specificity of BKI1 by BRI1 are boxed in deep blue.

(E) BRI1-KD shares similar overall architecture with BAK1-KD. BAK1-KD is superimposed with BRI1-KD and shown as slate ribbon.

(F) Comparison of the active site interactions of BRI1-KD and BAK1-KD. The color scheme of BRI1-KD and BAK1-KD follows that in Figure 2B. AMP-PNP and interacting residues are shown as magenta sticks. In BRI1-KD, the adenine ring of AMP-PNP binds to the hinge region via one hydrogen bond with the backbone carbonyl of Glu957, and both the P-loop and DFG motif contribute to the stabilization of the bound AMP-PNP by interacting with its phosphate groups.