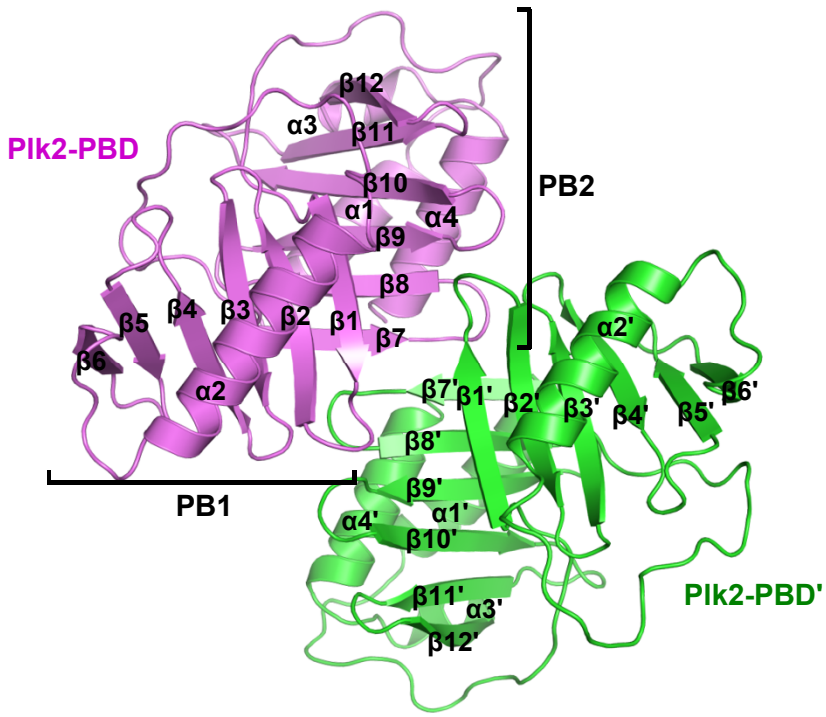

Figure S1. Two Plk2-PBD molecules in the asymmetric unit

The two molecules are represented by different colors (violet and green) with the labels of secondary structures according to the order of their appearance in the primary sequence. Two subdomains (PB1 and PB2) of Plk2-PBD are also indicated.

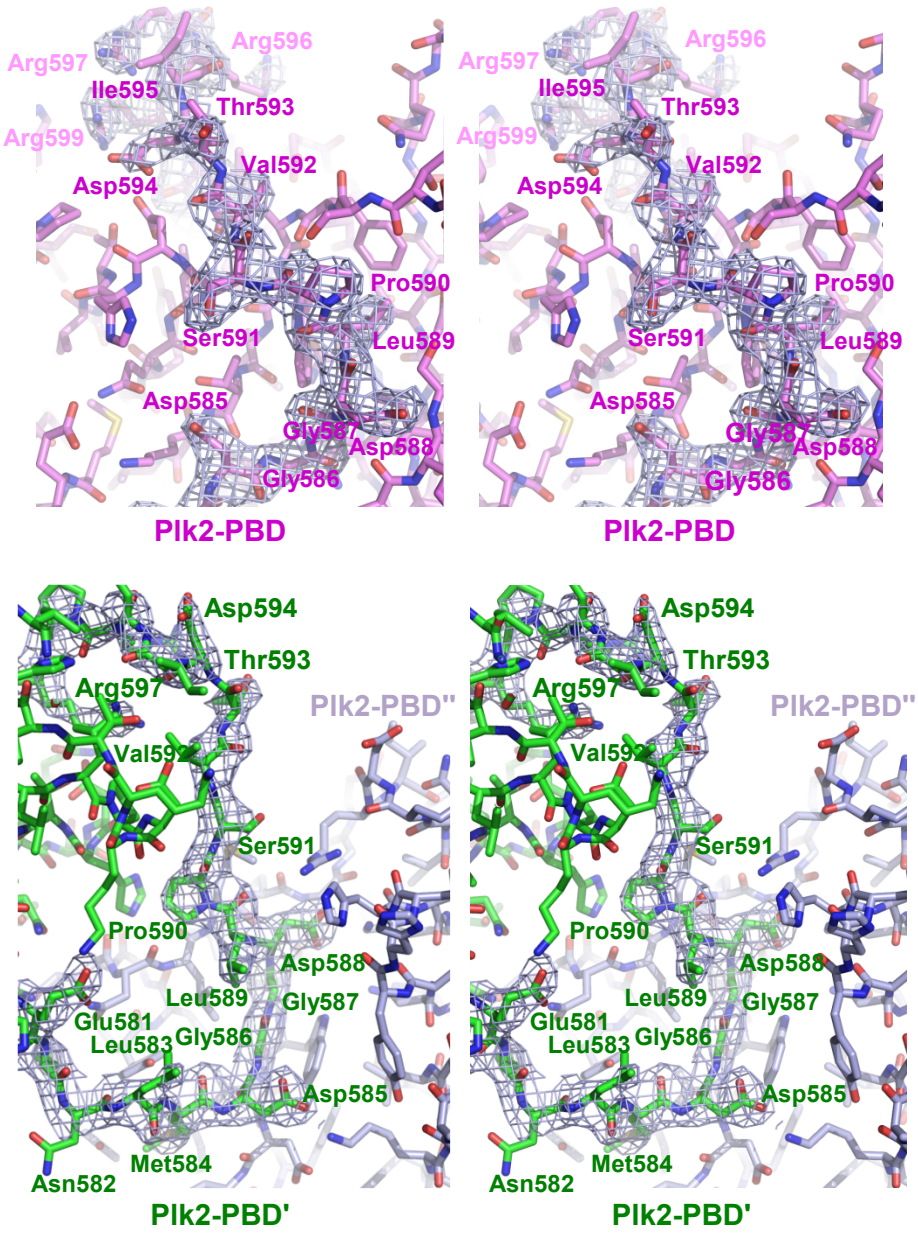

Figure S2. Stereo views of PB1-PB2 loop

Plk2-PBDs are presented in sticks together with the 2Fo-Fc electron density map (contoured at 1.0 σ) covering the PB1-PB2 loop residues which are labeled. Plk2-PBD in violet (top); Plk2-PBD' in green and a symmetry-related molecule Plk2-PBD'' in light purple (bottom).

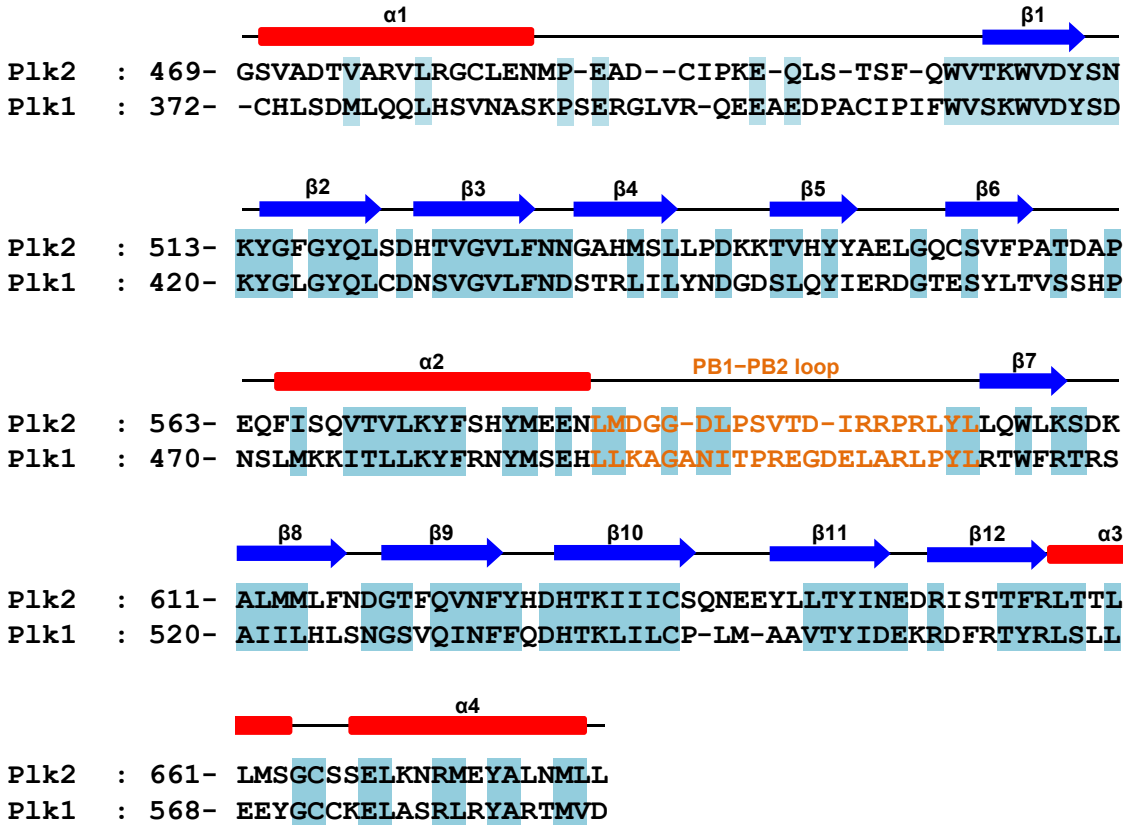

Figure S3. Structure-based sequence alignment

The sequences of Plk2-PBD and Plk1-PBD are aligned based on the structural comparison. The secondary structures of Plk2-PBD are shown together. Aligned residues are shaded cyan. The PB1-PB2 loop residues of Plk2 and Plk1 are presented in orange.

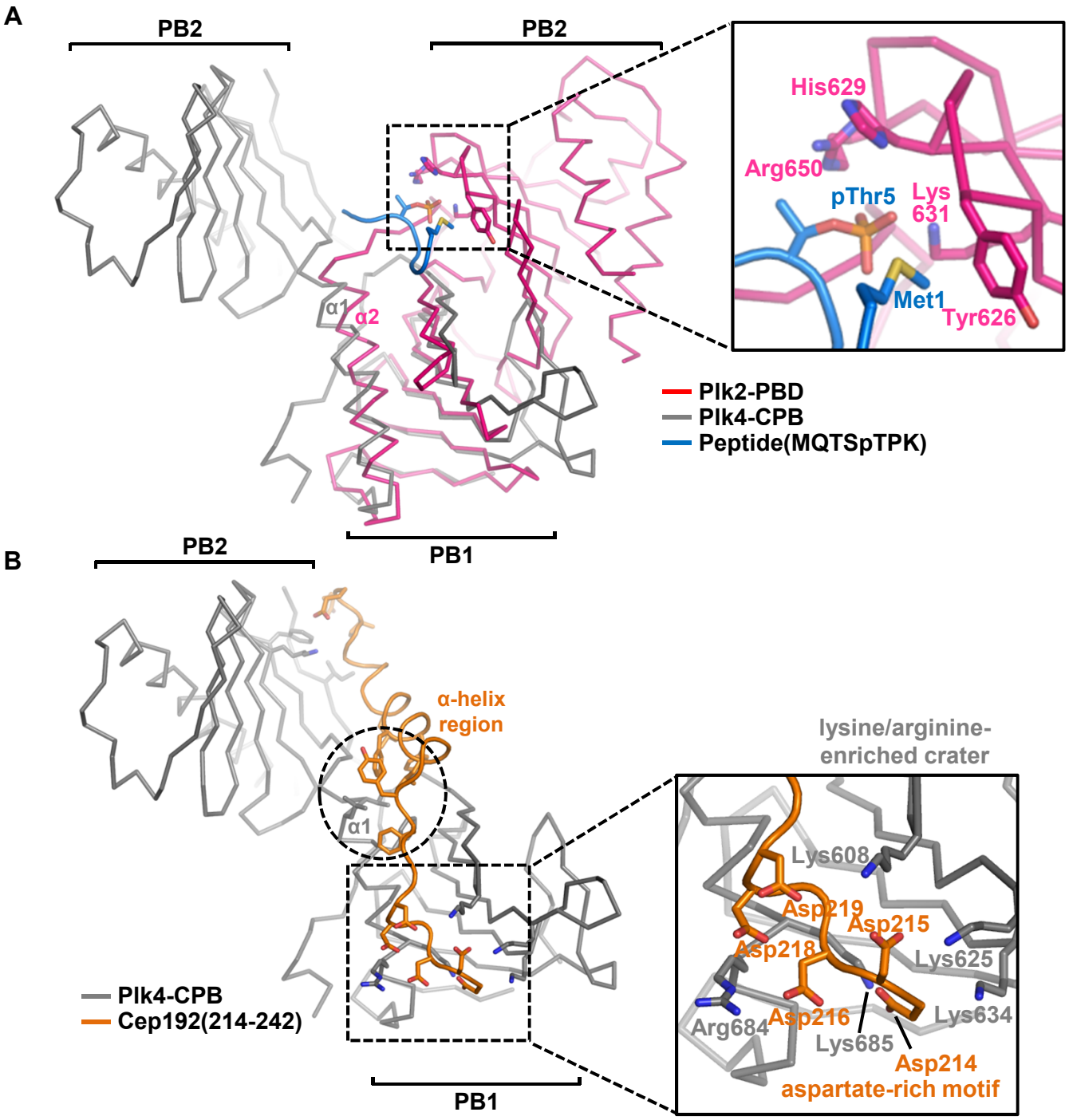

Figure S4. Structural comparison of Plk2-PBD modeled to bind a phosphopeptide with Plk4-CPB in a complex with a Cep192 fragment

Plk2-PBD (violet) and Plk4-CPB (gray) are oriented as in Figure 3(A).

(A) The phosphopeptide MQTSpTPK (skyblue) is bound to Plk2-PBD as modeled in Figure 4(B). Shown with magnification in the box are the interaction of Met1 and pThr5 from the peptide with the PB2 residues from Plk2-PBD.

(B) Complex structure of Plk4-CPB bound to a Cep192 fragment (orange; PDB code 4N7Z). The main residues mediating the complex formation are shown in stick representation. Dashed circle indicates intermolecular contacts between the α-helix region of Cep192 and α1 of Plk4-CPB. Association between the aspartate-rich motif of Cep192 and the lysine/arginine-enriched crater of Plk4-CPB are shown with magnification in the box.