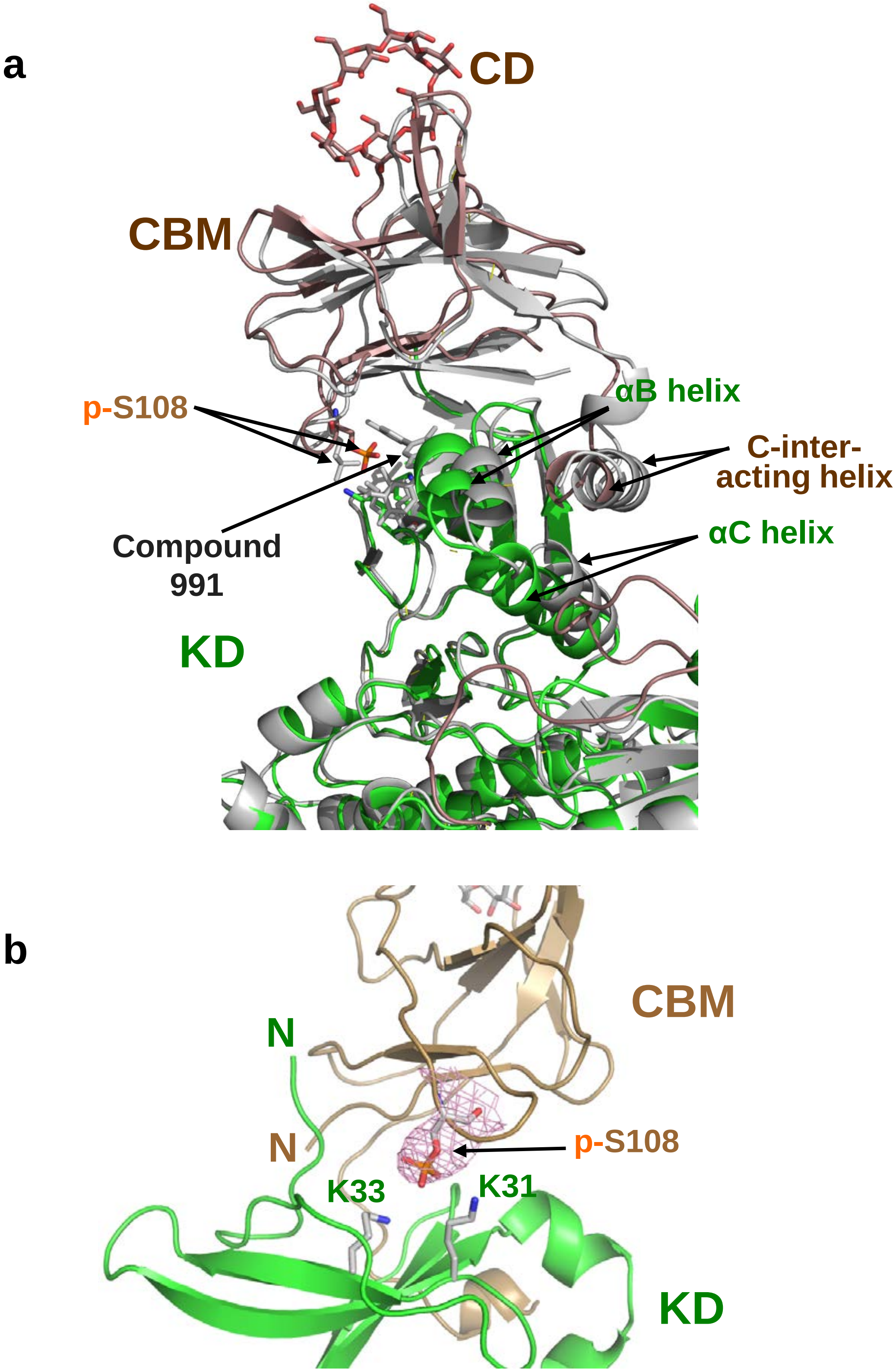

Supplementary Figure 3. Close-up views of the CBM–KD interface and conformation. **(a)** Overlay of the structure of compound 991-bound AMPK (grey, PDB 4CFE) with that of cyclodextrin (CD)-bound AMPK (color). The CBMs and the αB- and αC-helices of the KDs adopt distinctly different conformations in the two structures. Please note that the C-interacting helix in CD-bound CBM is partially disordered and presented here as a single helical turn. **(b)** Close-up of the KD–CBM interface around phospho-serine 108 of the CBM (shown with $2F_o$-F_c electron density map [pink mesh] contoured at 1σ. N: N-terminus of α1 and β2 subunit.