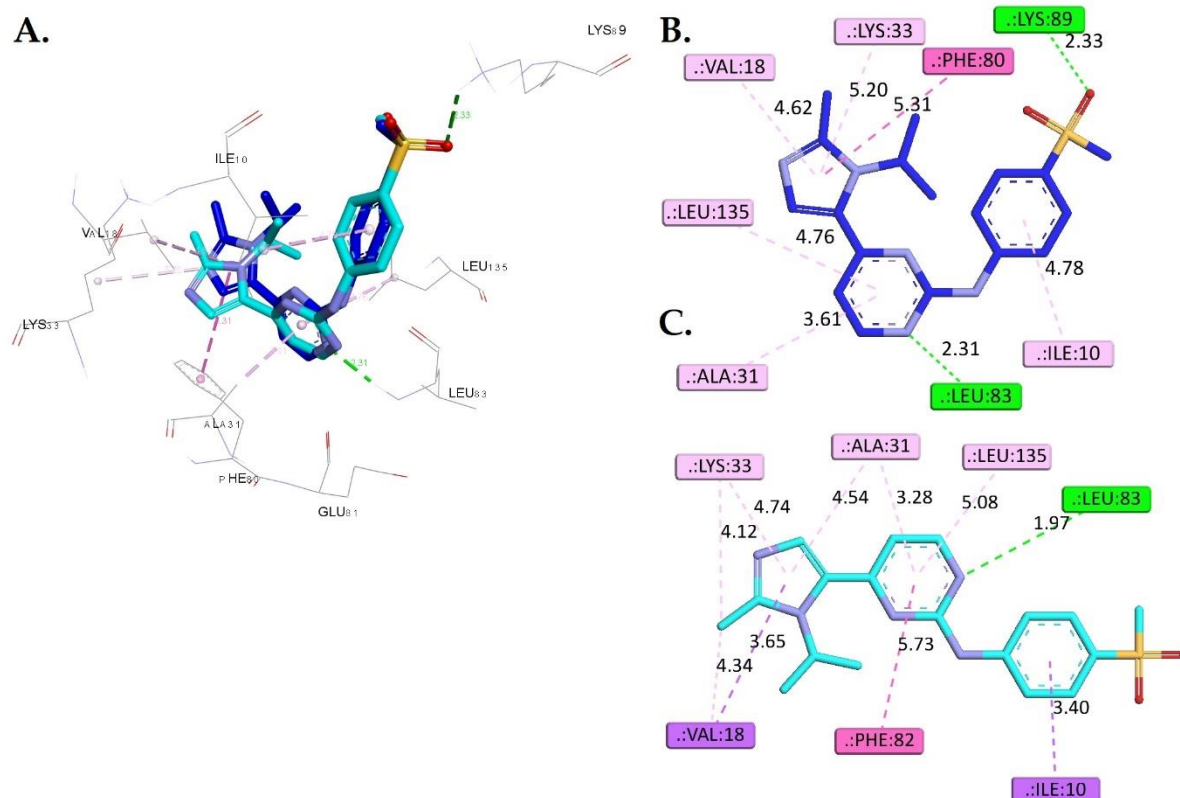


# Supplementary material



**Figure S1.** (A) Superimposition and (B) 2D interaction analysis of the original co-crystallized ligand AZD5438 (depicted in blue for carbon (C), red for oxygen (O), navy for nitrogen (N), and orange for sulphur (S)). (C) Re-docked ligand (depicted in cyan for carbon (C), red for oxygen (O), navy for nitrogen (N), and orange for sulphur (S)) in the crystal structure of human CDK1/CKS2 complex with AZD5438 (PDB ID: 6GU7). The root mean square deviation between the original co-crystallized ligand of AZD5438 and re-docked ligand was 0.92 Å.