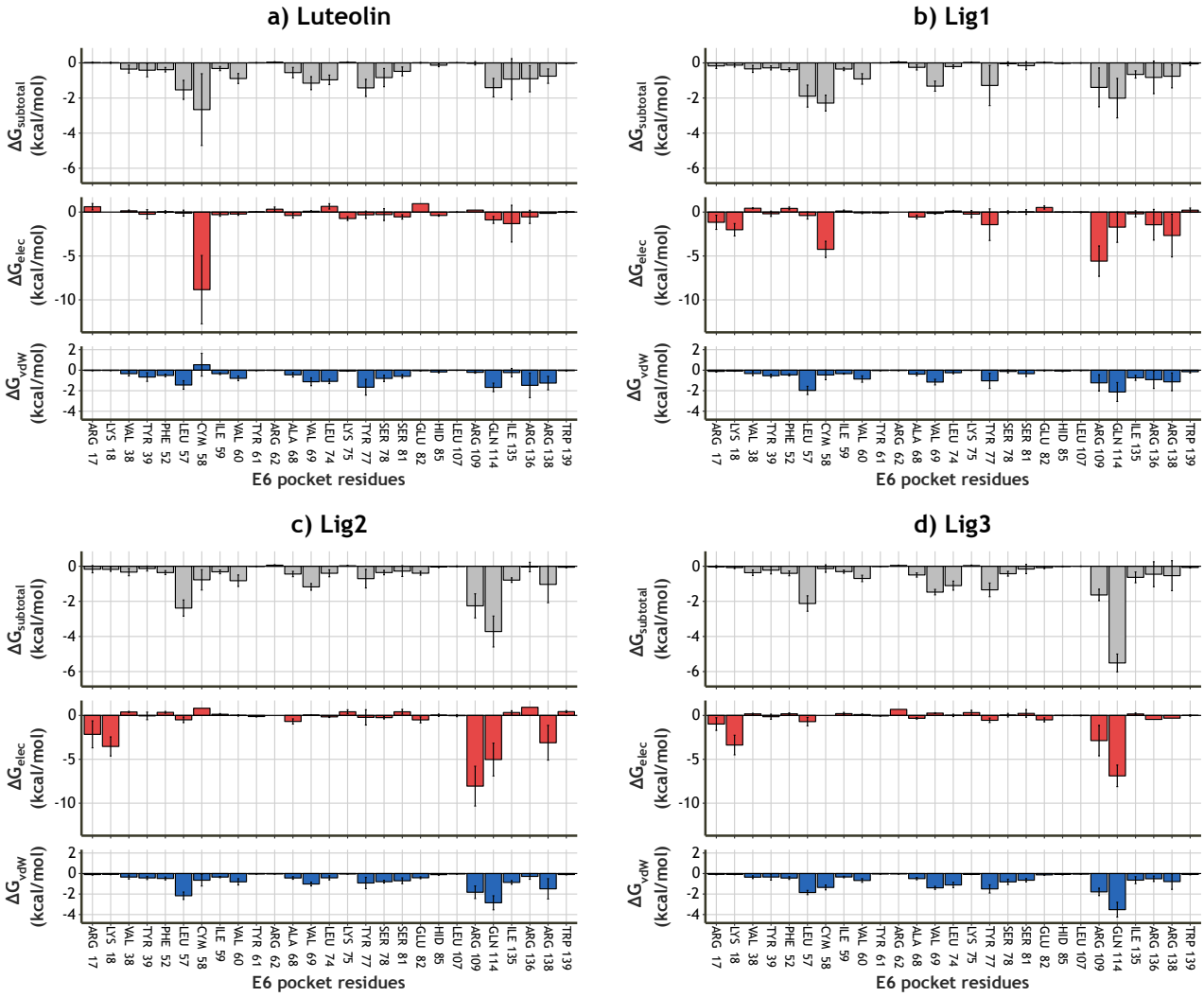

Figure S12: MM/GBSA binding free energy (BFE) decomposition per residue of each of the four E6-lig systems. BFE contribution of each E6 pocket residue ($\Delta G_{subtotal}$) to the E6-ligand interaction. Electrostatic interaction energies (ΔG_{ele}) and van der Waals interaction energies (ΔG_{vdW}) are also presented. **a)** [E6+luteolin]-hx, **b)** [E6+lig1]-hx, **c)** [E6+lig2]-hx, and **d)** [E6+lig3]-hx.