



Figure S14: MM/GBSA binding free energy (BFE) decomposition per residue of each of the four [E6+lig]-hx systems, evaluating E6-ligand interaction. BFE contribution of each E6 pocket residue ($\Delta G_{subtotal}$) to the E6-ligand interaction. Electrostatic interaction energies (ΔG_{elec}) 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.