



Figure S15: MM/GBSA binding free energy (BFE) decomposition per residue of each of the four [E6+lig]-hx systems, evaluating E6-hx interaction. BFE contribution of each E6 pocket residue ($\Delta G_{subtotal}$) to the E6-*LxxLL* interaction. Electrostatic interaction energies (ΔG_{elec}) and van der Waals interaction energies (ΔG_{vdW}) are also presented. **a)** E6-hx system, **b)** [E6]-hx system, **c)** [E6+luteolin]-hx, **d)** [E6+lig1]-hx, **e)** [E6+lig2]-hx, and **f)** [E6+lig3]-hx.