



Figure S13: Molecular dynamics of the protein-ligand-*LxxLL* ([E6+lig]-hx) complexes (50ns). a) RMSD values of each of the three ligands comparing with its docked pose. b) RMSD values of the E6 pocket. c) RMSD values of the *LxxLL* motif. d) Distance between the center of mass of E6 protein and the center of mass of the *LxxLL* motif. e) MM/GBSA ΔG_{bind} values (kcal/mol), and f) MM/PBSA ΔG_{bind} values (kcal/mol) between E6-ligand complex and *LxxLL* motif.