



S1 Fig. (left) The structure of the co-crystallized abacavir-peptide-MHC molecule (PDB ID: 3UPR): abacavir shown in green and peptide (HSITYLLPV) shown in red; (right) structure of the acyclovir-peptide-MHC molecule predicted by molecular docking studies (GOLD 5.2) acyclovir shown in blue and peptide (HSITYLLPV) shown in red.

Figure prepared by using PyMOL (The PyMOL Molecular Graphics System, Version 1.5.0.4 Schrödinger, LLC.).

doi:10.1371/journal.pone.0124878.s001