Supplementary Materials

Large Subunit of the Human Herpes Simplex Virus Terminase as a Promising Target in Design of Anti-Herpesvirus Agents

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Molecular Docking

Table S1. Molecular docking results

| Site	ID complex	Pose	Docking score	E-model	IFD score	$\Delta G_{MM\text{-}BSGA}$ (kcal/mol)	H-bond	Other interactions	Clash
ATP domain	**1**–ATP-D	5	−8.9 (Δ = 2.7)	−91.04	−2739.8 (Δ = 3.3)	−61.1	R260 R261 G263 K264 S385	W266 – π-π H194 – π-π	None
Central channel	**1**–CC	9	−3.3 (Δ = 1.0)	-36.71	−2732.7 (Δ = 3.2)	−32.8	H316	H316 – π-π	H316 D315
Loop 339–350	**1**–loop1 **1**–loop2	5 6	−8.3 −7.7	−79.4 −65.0	−2737.8 −2741.4	−56.3 −58.2	G347 E367 H340 N341 E320	F350 - π-π none	I345 T368 T333 T321 none

RMSD = 0.526 Å
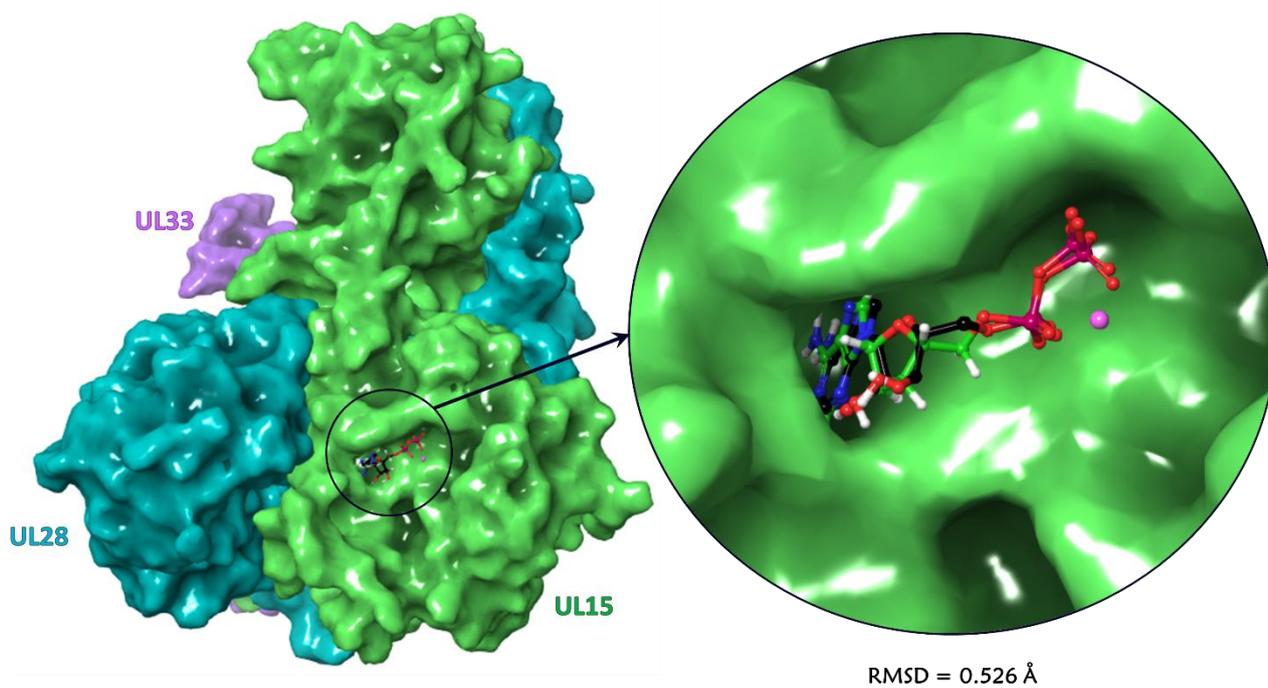
Figure S1. Molecular re-docking procedure. The green molecule corresponds to the geometric parameters obtained as a result of molecular docking. The black molecule corresponds to PDB code 6M5V.

Molecular Dynamics
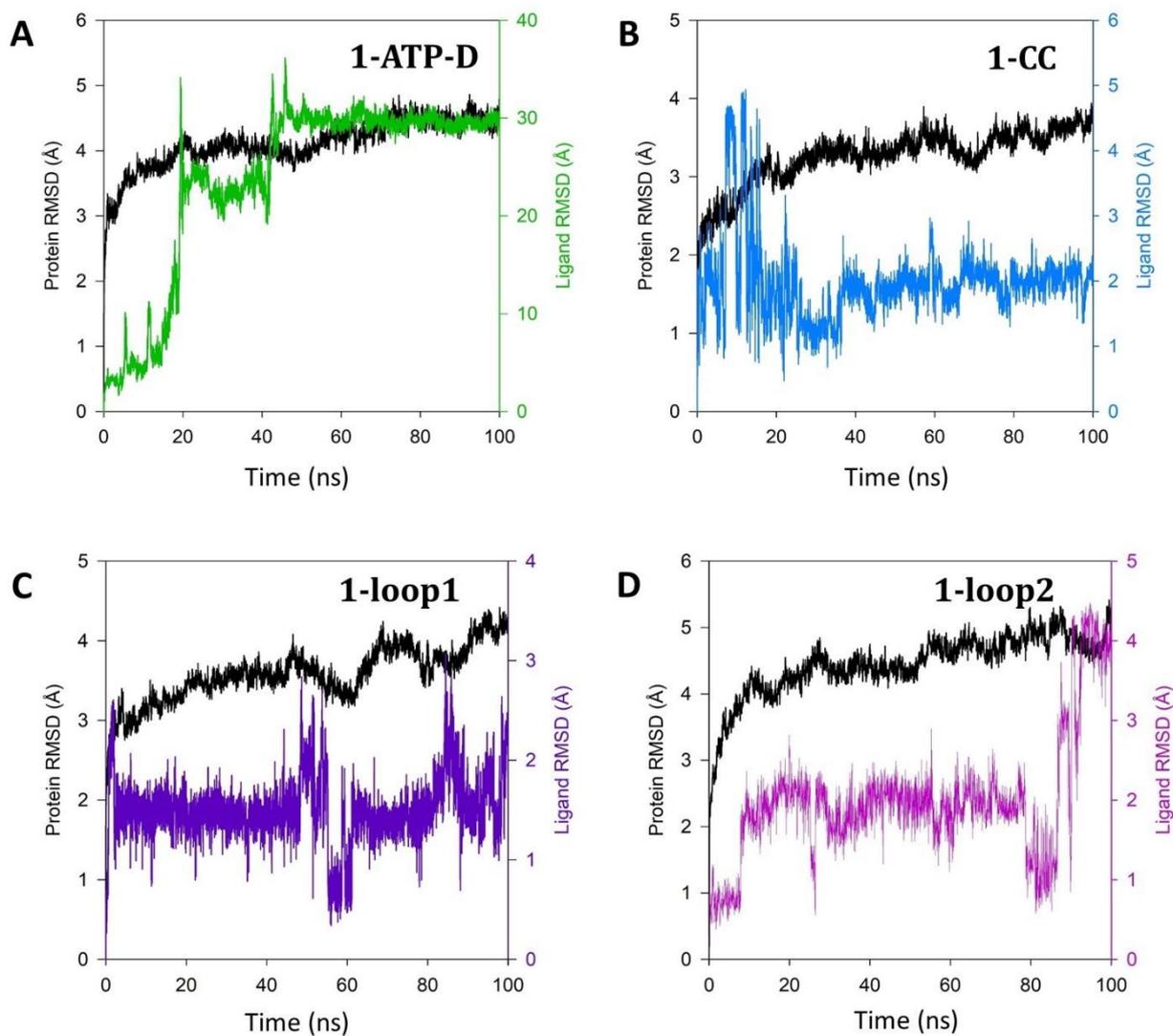
Figure S2. Protein–ligand root-mean-square deviation (RMSD): **A**, RMSD of the ligand and protein atoms in **1**–ATP-D complex; **B**, RMSD the ligand and protein atoms in **1**–CC complex; **C**, RMSD of the ligand and protein atoms in **1**–loop1 complex; **D**, RMSD of the ligand and protein atoms in **1**–loop2 complex.
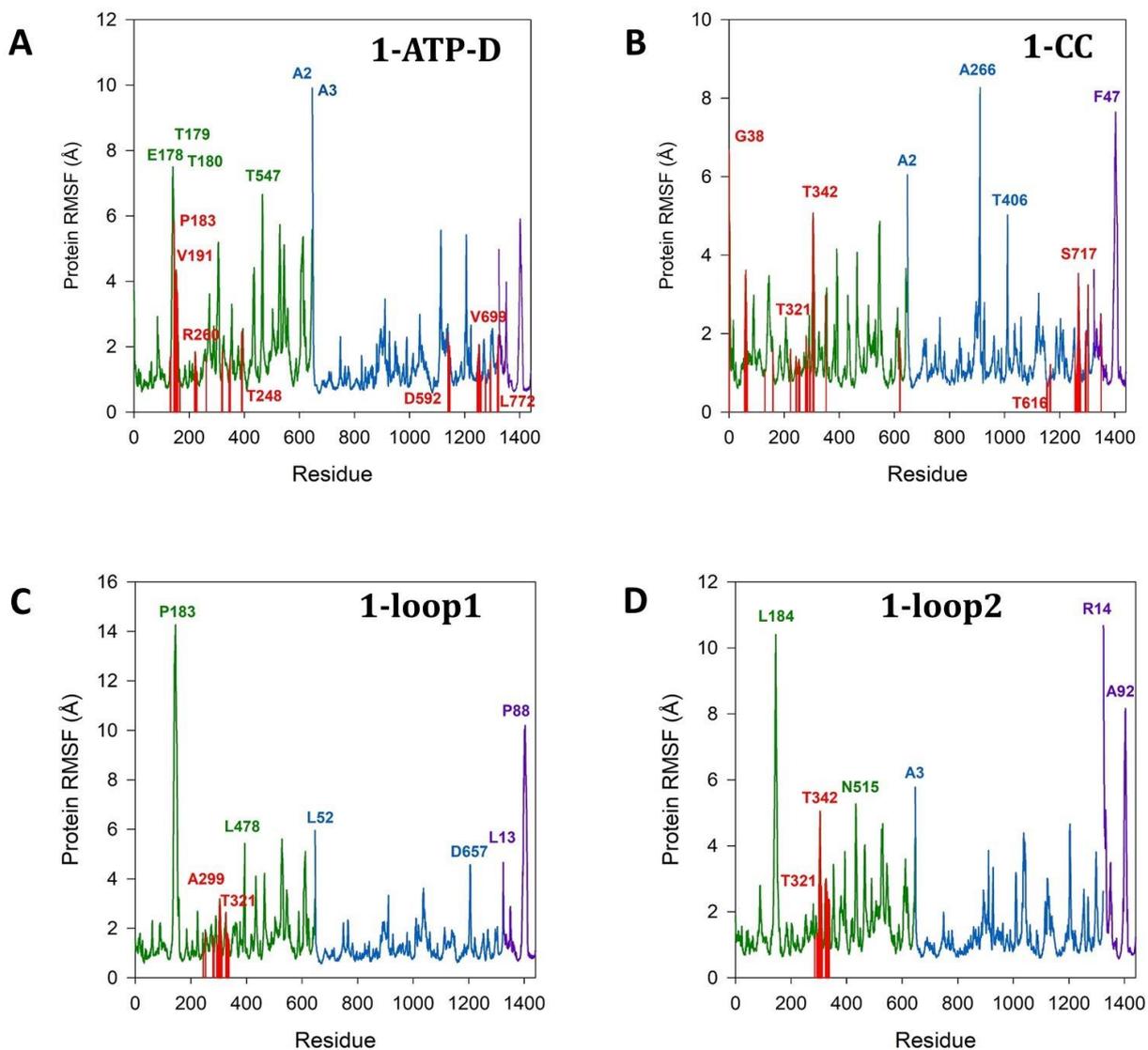
Figure S3. Protein root-mean-square fluctuations (RMSF): **A**, RMSF of the ligand and protein atoms in **1**–ATP-D complex; **B**, RMSF of the ligand and protein atoms in **1**–CC complex; **C**, RMSF of the ligand and protein atoms in **1**–loop1 complex; **D**, RMSF of the ligand and protein atoms in **1**–loop2 complex. Green plot corresponds to subunit UL15; blue, UL28; violet, UL33. Peaks indicate areas of the protein that fluctuate the most during the simulation. Protein residues that interact with the ligand are marked with red-colored vertical bars.
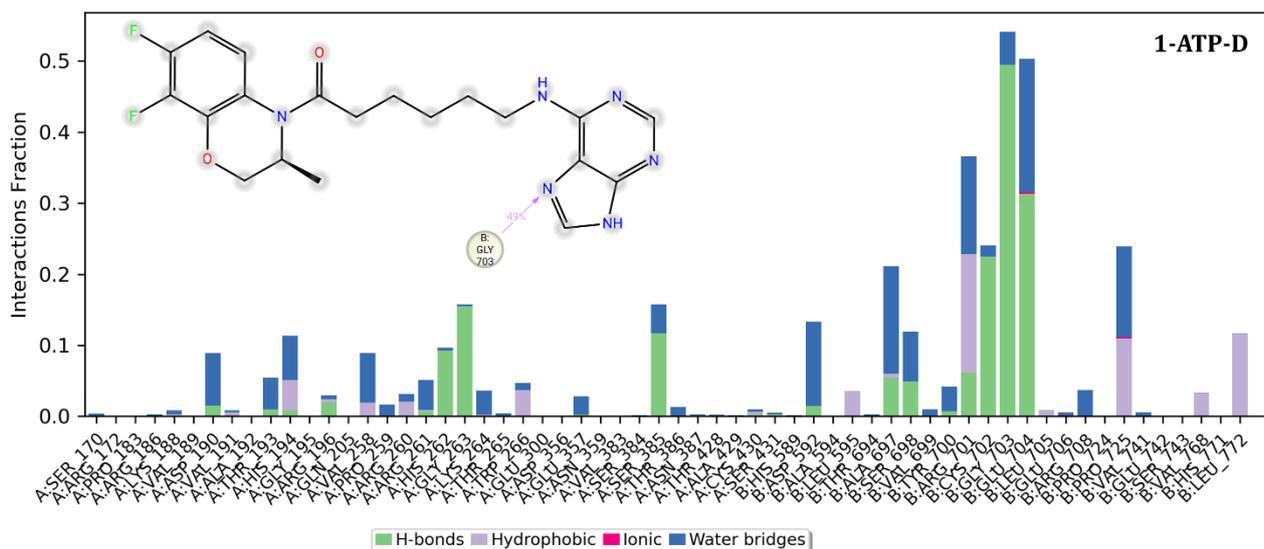
Figure S4. Protein–ligand contacts between atoms of ligand and protein in **1**–ATP-D complex.
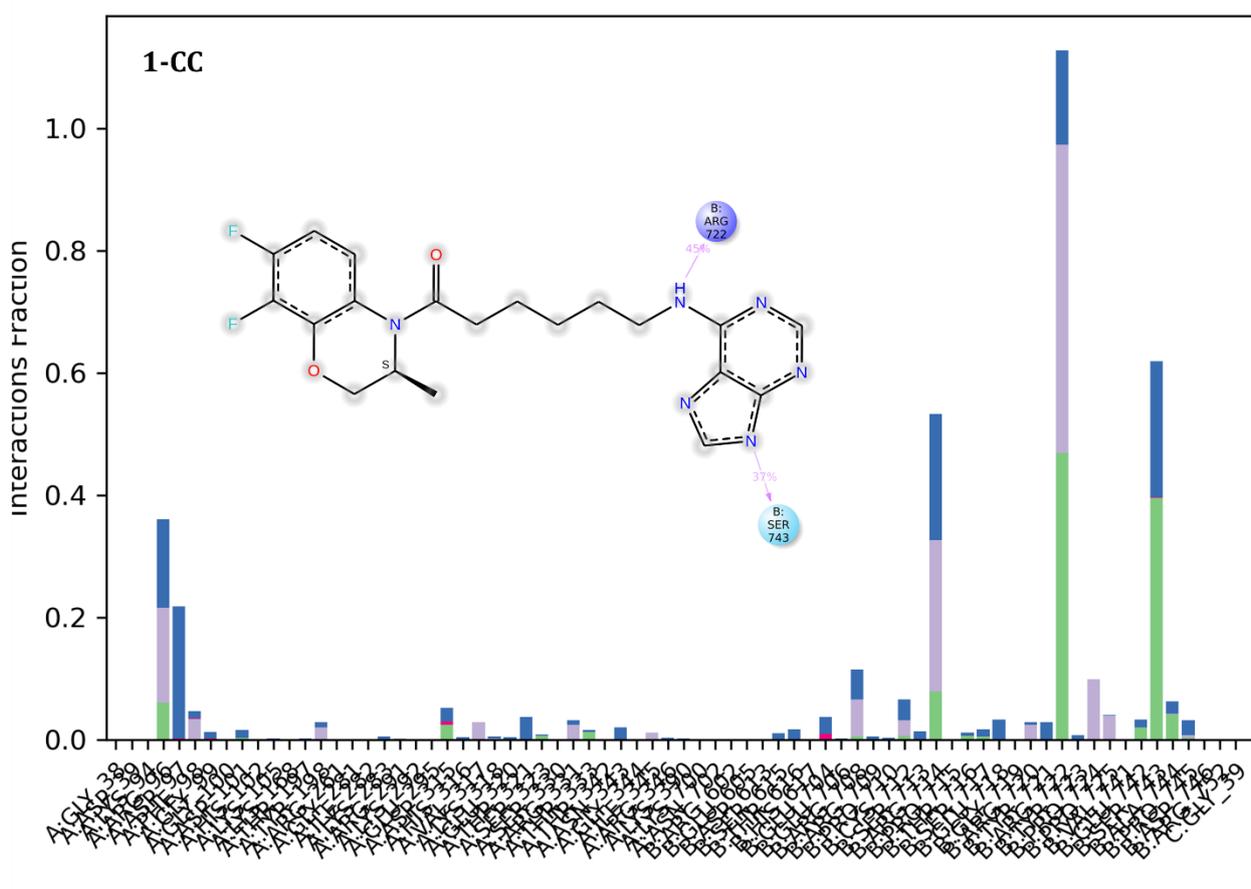
Figure S5. Protein–ligand contacts between atoms of ligand and protein in **1**–CC complex.
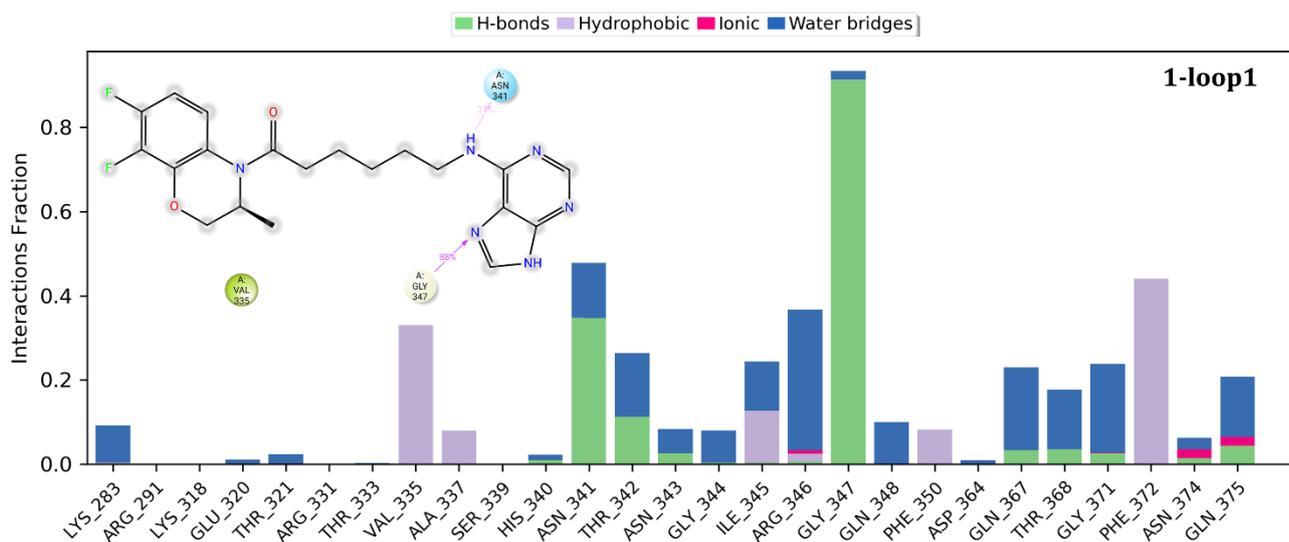
Figure S6. Protein–ligand contacts between atoms of ligand and protein in **1**–loop1 complex.
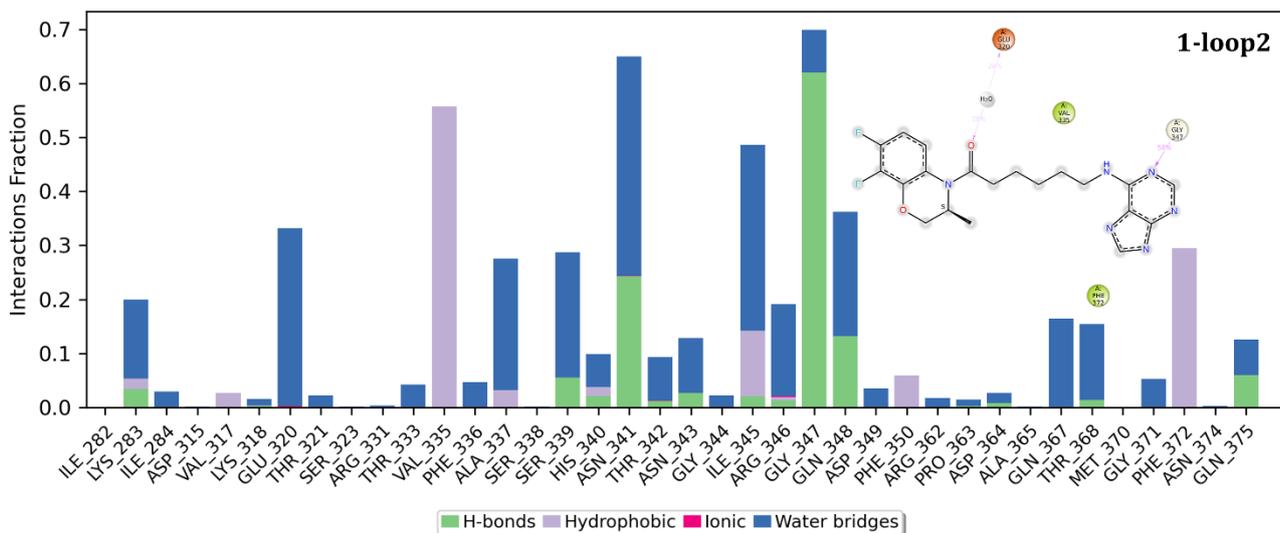
Figure S7. Protein–ligand contacts between atoms of ligand and protein in **1**–loop2 complex.