Supporting Information

Conformational modifications of gB from Herpes simplex virus type 1 analyzed by synthetic peptides

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Supporting Information Contents:

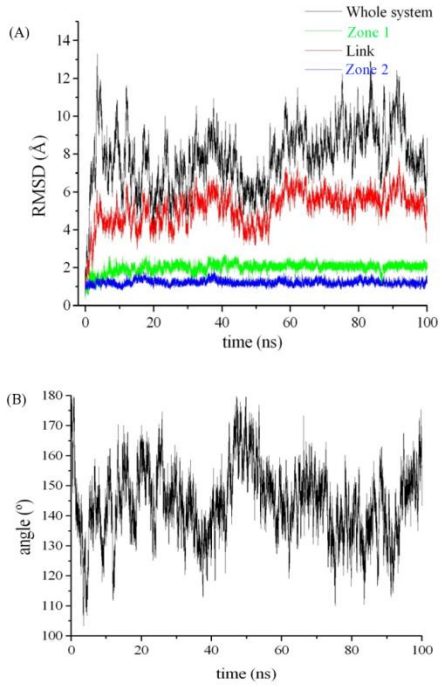

Figure S1. (A) RMSD values computed for the entire molecule and for individual zones with the OPLS force field. (B) Analysis of the bending angle throughout the MD simulations using the OPLS force field. The bending angle is defined as the angle generated by the centres of mass of the Zone 1, Zone 2 and Link regions.

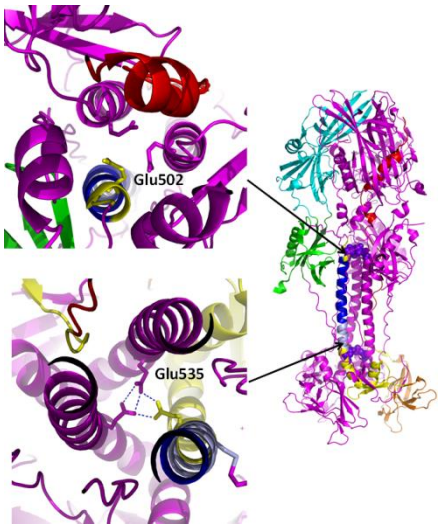

Figure S2. Cartoon representation of gB post-fusion structure. The two insets show the two patches of Glu residues at the two extremities of the central coiled coil.

Table S1. Pka values calculated using the software PropKa 3.1 and the PDB structure 2gum.

Residue (chain)	**pK_a**	**% Burial**	**H-bonding interactions (chain)**	**Coulombic interactions (chain)**
Glu 535 (A)	5.85	100	Glu 535 (B)	
Glu 535 (B)	10.59	100	Glu 535 (C)	Glu 535 A
Glu 535 (C)	15.16	100	Glu 535 (B)	Glu 535 B
Glu 502 (A)	6.87	100	Ser 500 (C)	Arg 505 B
Glu 502 (B)	9.54	100		Arg 505 C
Glu 502 (C)	8.27	100	Ser 500 (B)	Arg 505 A