

Conformational Dynamics of Herpesviral NEC Proteins in Different Oligomerization States

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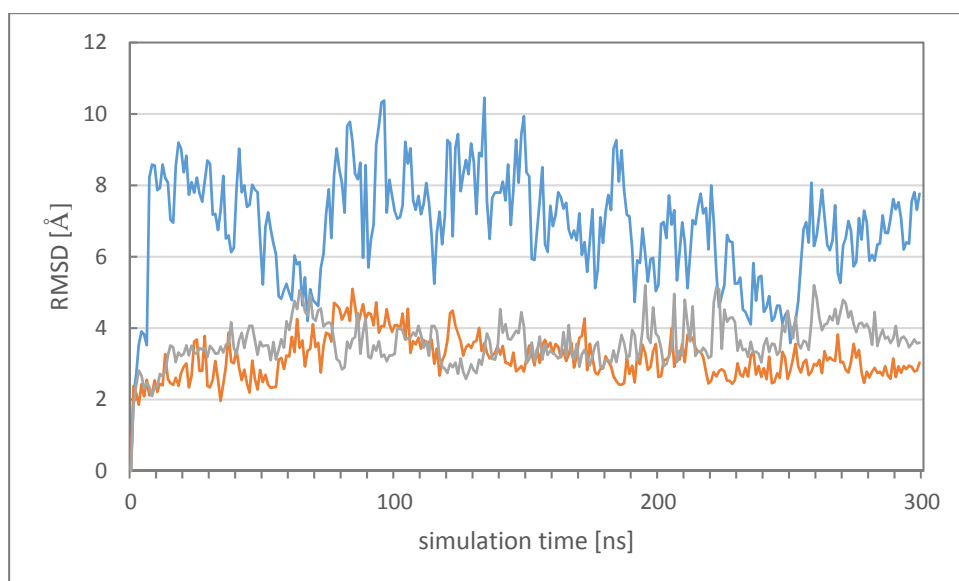


Figure S1. Plot of the RMSD of the HCMV NEC (blue), the HSV-1 NEC (orange), and the PRV NEC (grey), of run2 of the heterodimer simulations.

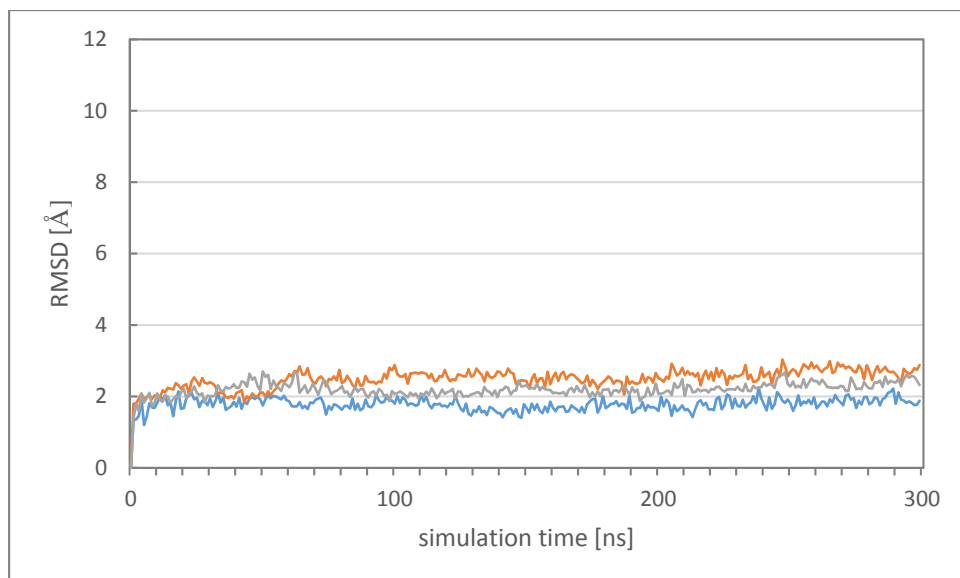


Figure S2. Plot of the RMSD of the pUL53 (pUL31) subdomains of HCMV (blue), HSV-1 (orange), and PRV (grey), of run2 of the heterodimer simulations.

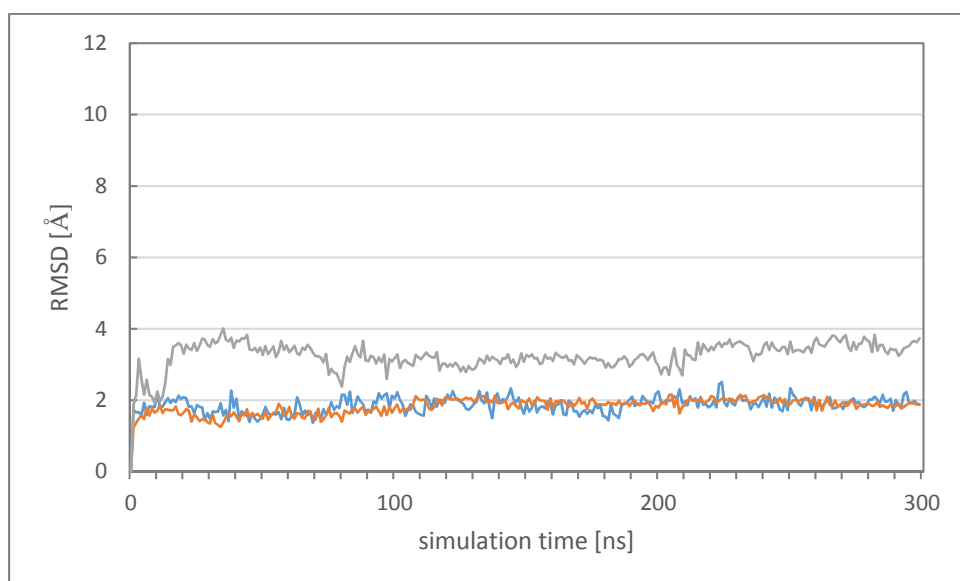


Figure S3. Plot of the RMSD of the pUL50 (pUL34) subdomains of HCMV (blue), HSV-1 (orange), and PRV (grey), of run2 of the heterodimer simulations.

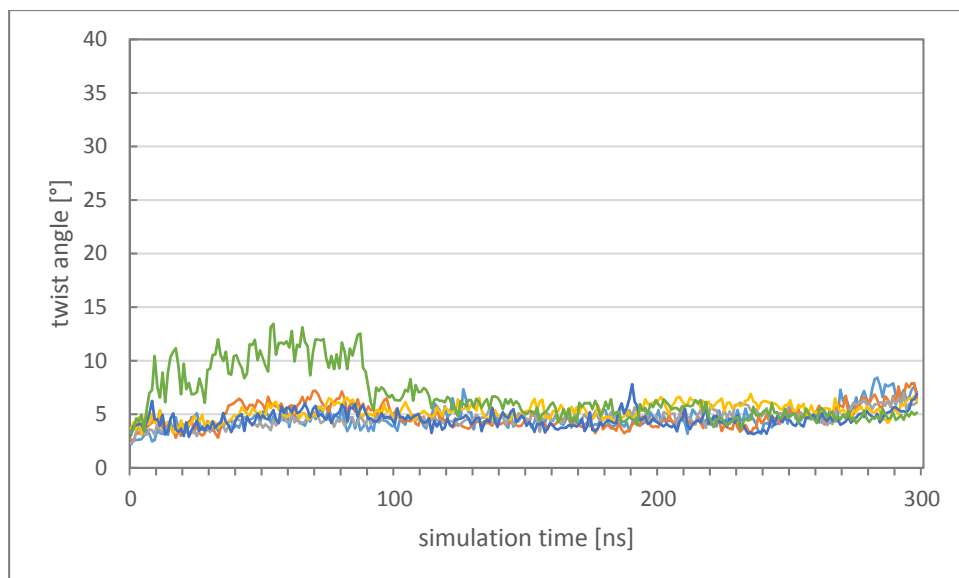


Figure S4. Twist angle of HCMV Hexagon simulation run2; the different colours mark the individual heterodimers.

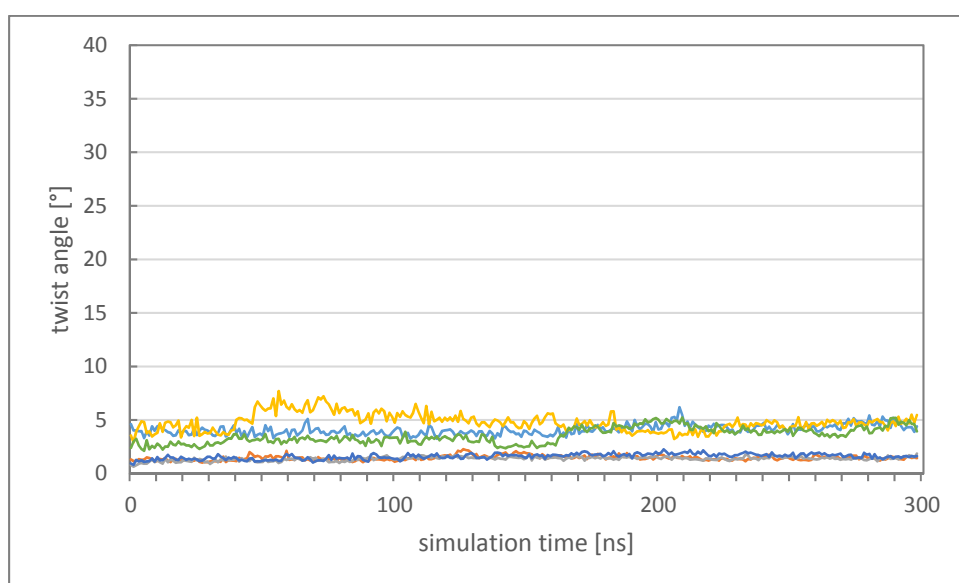


Figure S5. Twist angle of HSV-1 Hexagon simulation run2; the different colours mark the individual heterodimers.

Movie M1. The twisting of the HCMV NEC subdomains illustrated by a video containing simulation frames arranged in a fashion that displays a continuous twist. In the video the twisting is played forwards and backwards, so it can be watched in a loop.

Movie M2. This video shows the first 120 ns of run1 of the HCMV Hexagon simulation. All chains are coloured individually. Top-view on the pUL53 side with the pUL50 subdomains partially concealed.

Movie M3. This video shows the first 120 ns of run1 of the HSV-1 Hexagon simulation. All chains are coloured individually. Top-view on the pUL31 side with the pUL34 subdomains partially concealed.