Supplementary Material

Investigation of the dynamics of the viral immediate-early protein 1 in different conformations and oligomerization states

Joachim D. Stump, Heinrich Sticht

Bioinformatik, Institut für Biochemie, Friedrich-Alexander-Universität, Erlangen-Nürnberg,
Fahrstraße 17, D-91054 Erlangen, Germany

Figure S1. Backbone RMSD of IE1 monomers IE_{as}A (black), IE_{1as}B (red), and IE_{1sy}C (green). For RMSD calculation the following crystal structure served as reference: A) IE_{1as}A, B) IE_{1as}B, and C) IE_{1sy}C.

Figure S2. Conformational stability of the IE1 dimers. For clarity, overlay of snapshots taken every 10 ns from the dimer simulation are shown separately for the individual chains of the IE1_{as} dimer (A, B) and of the IE1_{sy} dimer (C, D). Snapshots are color coded according to time from red to blue.

Figure S3. Correlation analysis of the subunits constituting the IE1 dimers. Correlation (red) and anti-correlation (blue) of C_{α} atoms is color coded and shown for the individual chains forming the IE1_{as} dimer (A, B) and the IE1_{sy} dimer (C, D).