Activation of the West Nile virus NS3 protease: Molecular dynamics evidence for a conformational selection mechanism

SUPPLEMENTARY MATERIAL

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(Dated: December 17, 2008)

Keywords: protein simulations; conformational selection; flaviviral protease; West Nile virus; Dengue virus; oxyanion hole

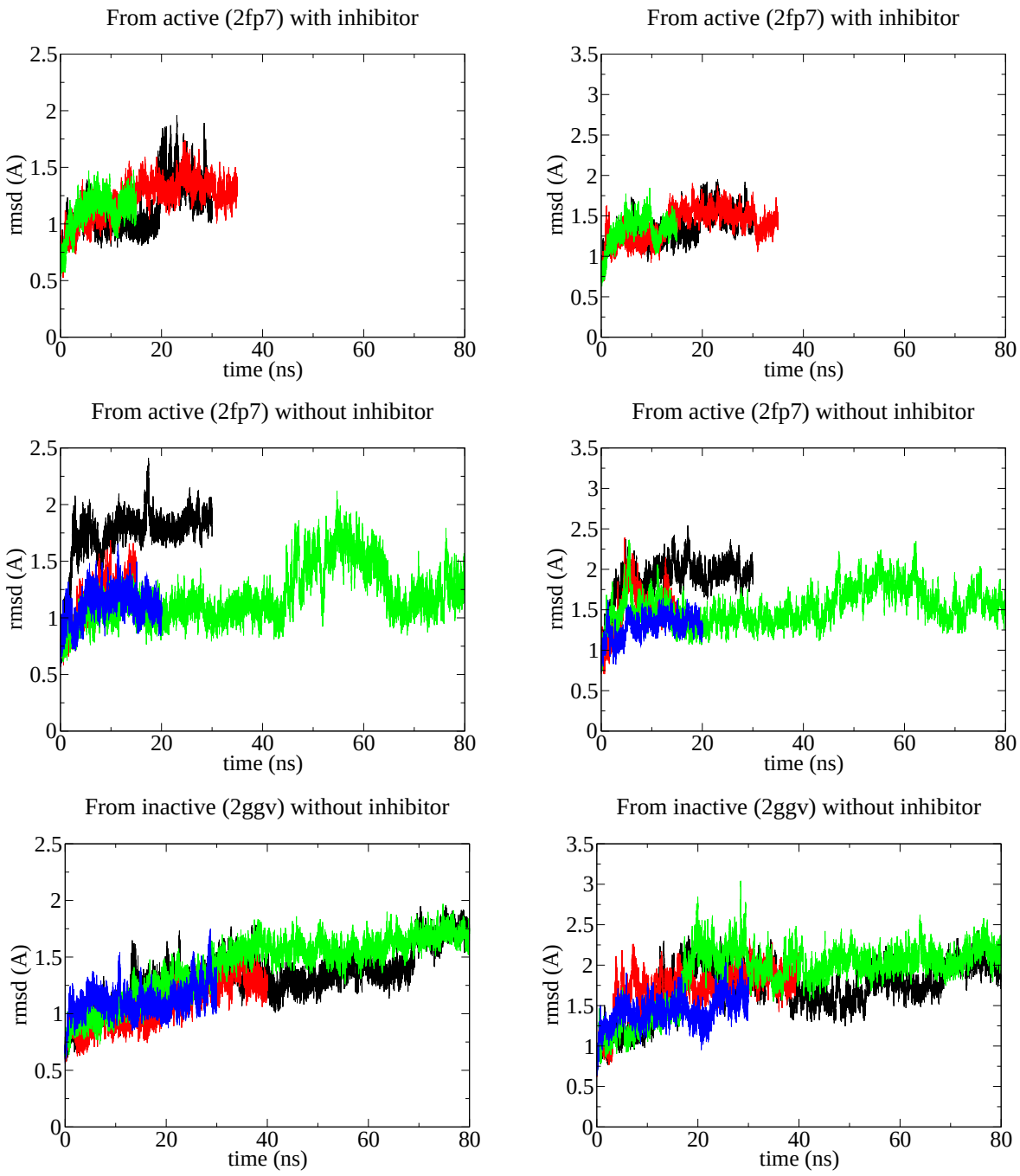

FIG. S1: Time series of C_α RMSD of NS3pro (left) and NS2B-NS3pro (right). All C_α atoms of NS3pro were used to calculate the RMSD values except for the residues 28-32, which are missing in the 2fp7 structure, and the loops B2B-C2 and E2B-F2 which are flexible.

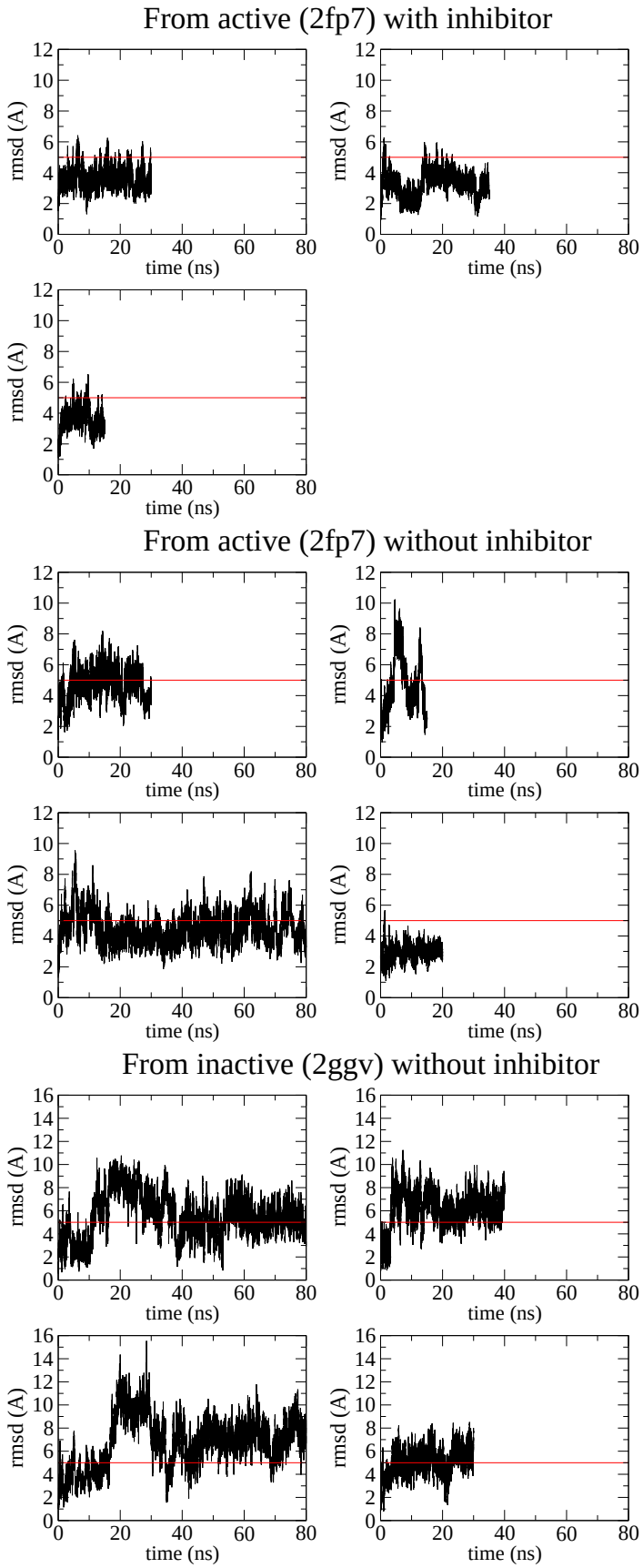

FIG. S2: RMSD of the β2-β3 loop of NS2B from the initial snapshot upon optimal overlap of NS3pro C_α atoms. The red horizontal line is shown to emphasize that the value of the RMSD is almost always smaller than 5 Å in the runs started from the active conformation (top and middle), and larger than 5 Å in the runs started from the inactive conformation (bottom). Note the different y-axis range in the four time series in the bottom (from inactive).

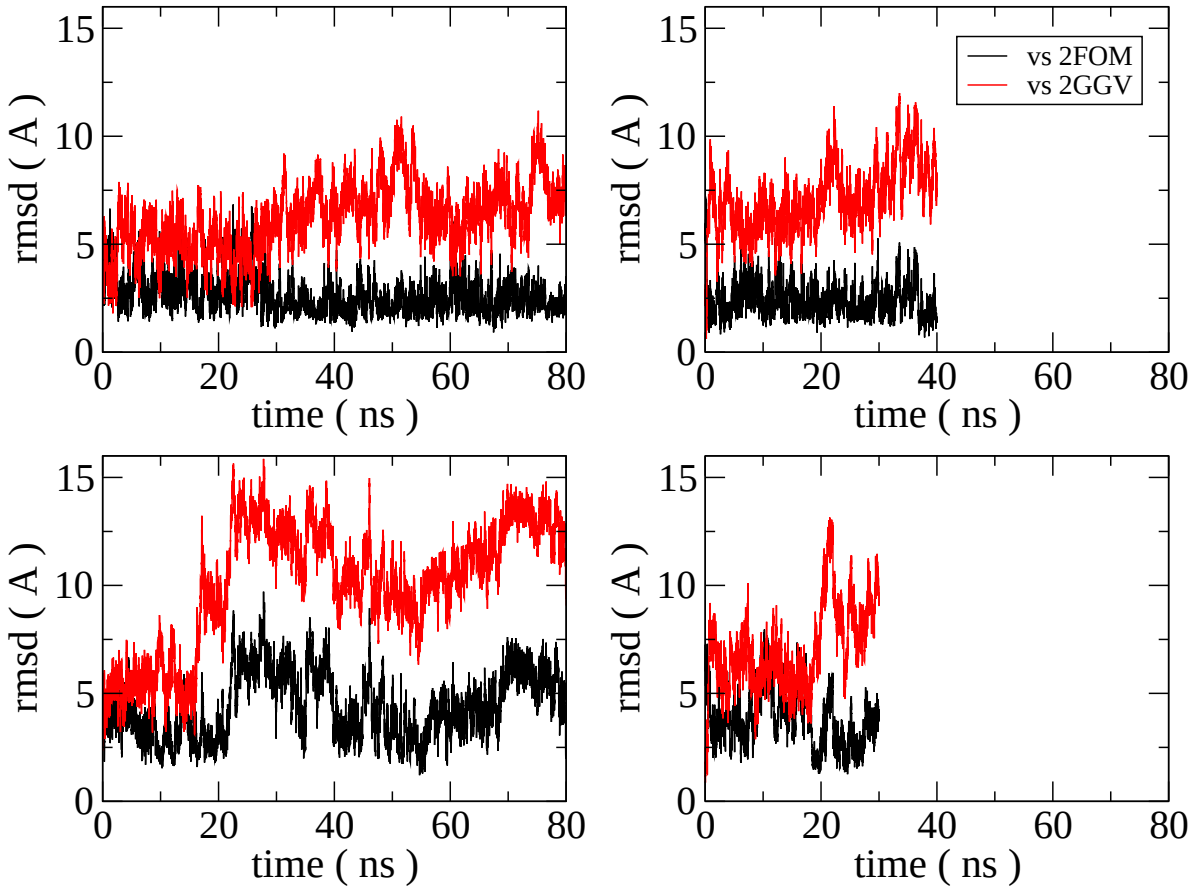

FIG. S3: Displacement of the E2B-F2 loop of NS3pro towards the orientation as in the X-ray structure of the Dengue NS2B-NS3pro complex (2fom) during the MD runs started from the inactive conformation (2ggv).

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