

# Computational study of helicase from SARS-CoV-2 in RNA-free and engaged form

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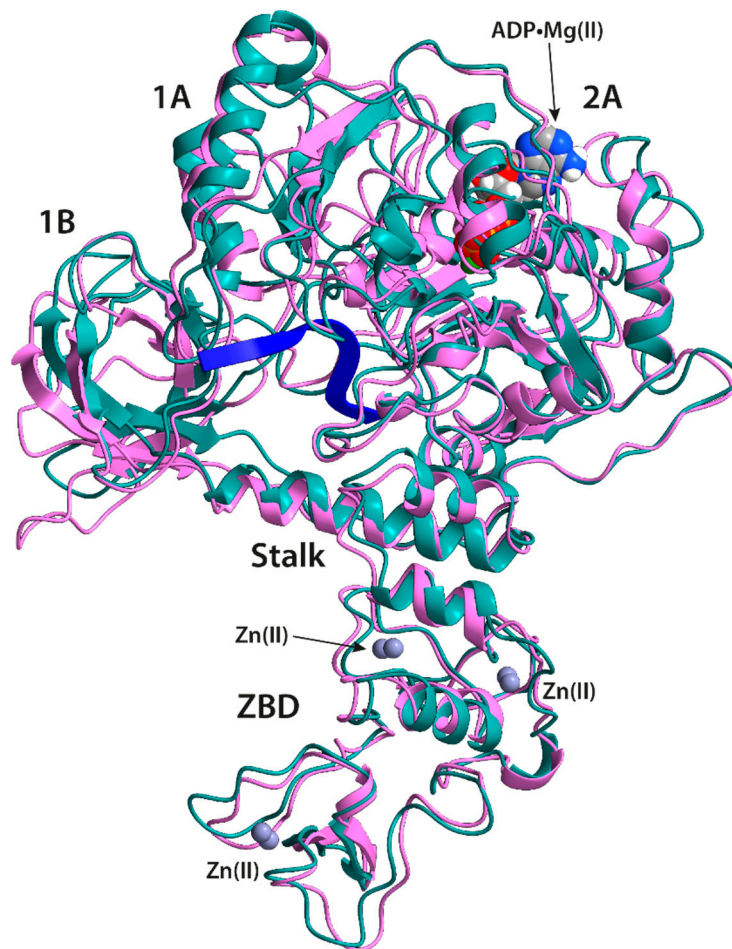
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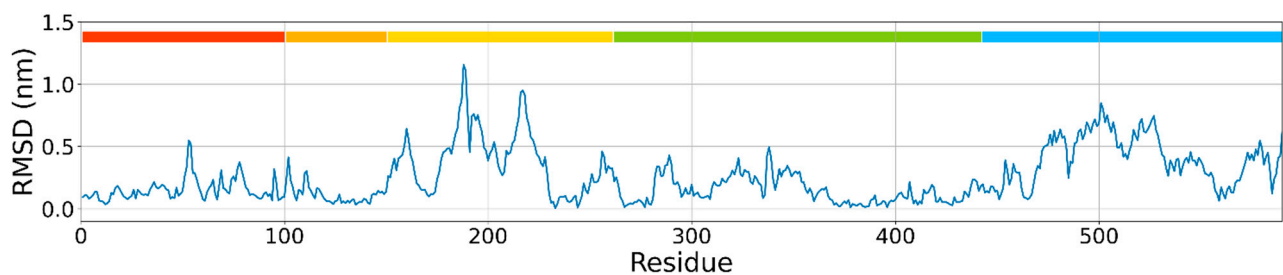
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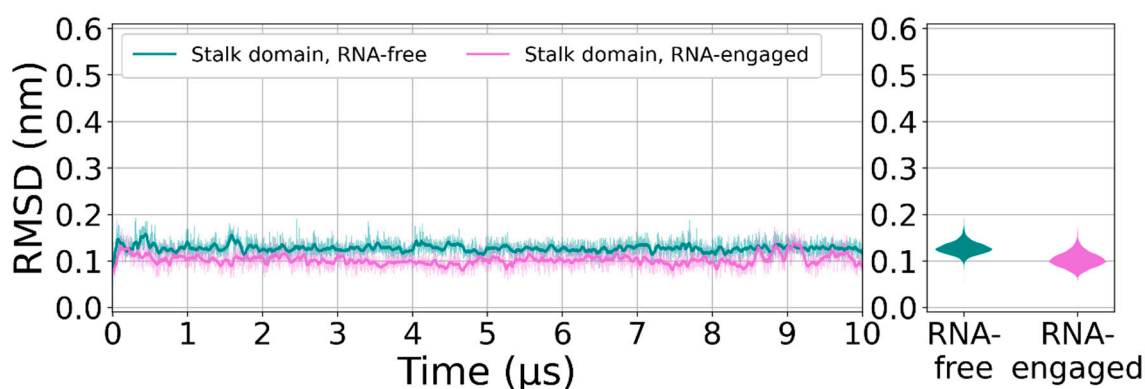
## SUPPLEMENTARY INFORMATION



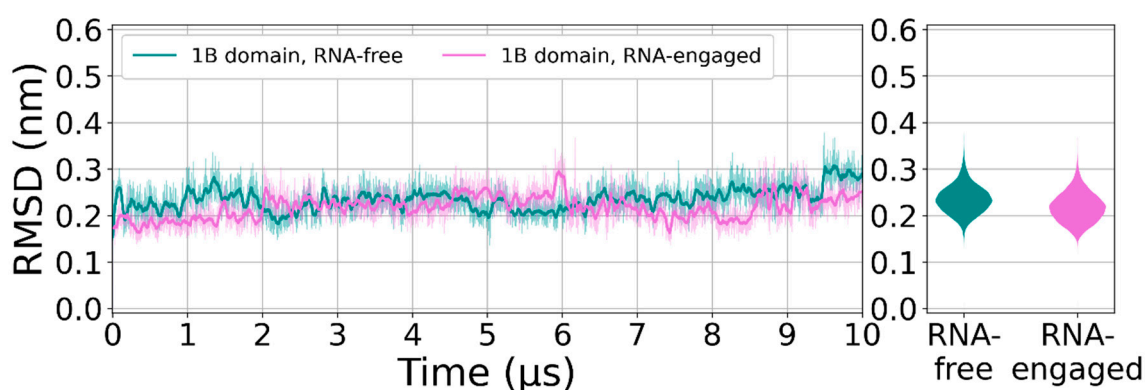
**Figure S1.** Superimposition of NSP13 initial structures in the RNA-free (dark cyan ribbons) and RNA-engaged (orchid ribbons) form. The RNA fragment is reported as a blue ribbon. The Zn(II) and Mg(II) ions as well as the ADP molecule are reported as spheres colored according to the atom type.



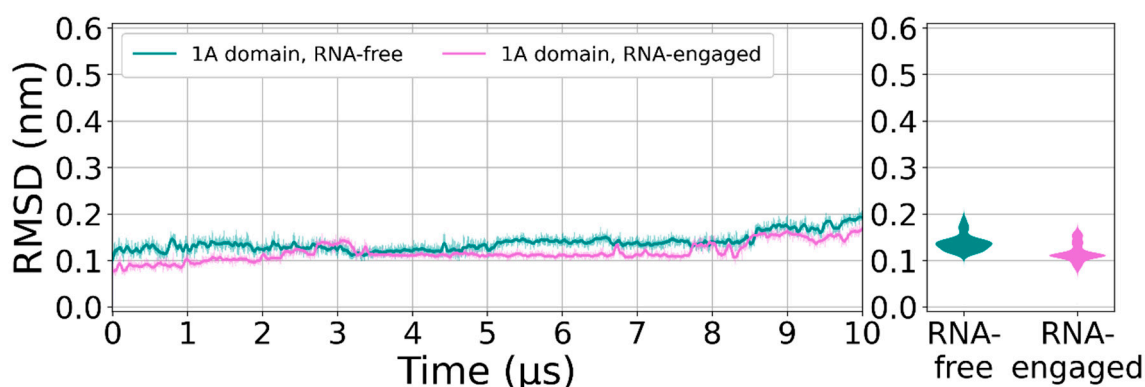
**Figure S2.** Calculated per residue Cα root mean square deviations (RMSD) of NSP13 between the RNA-free and RNA-engaged initial structures. The horizontal bars report the position of each domain in the sequence and are colored according to the domain coloration in Figure 1C.



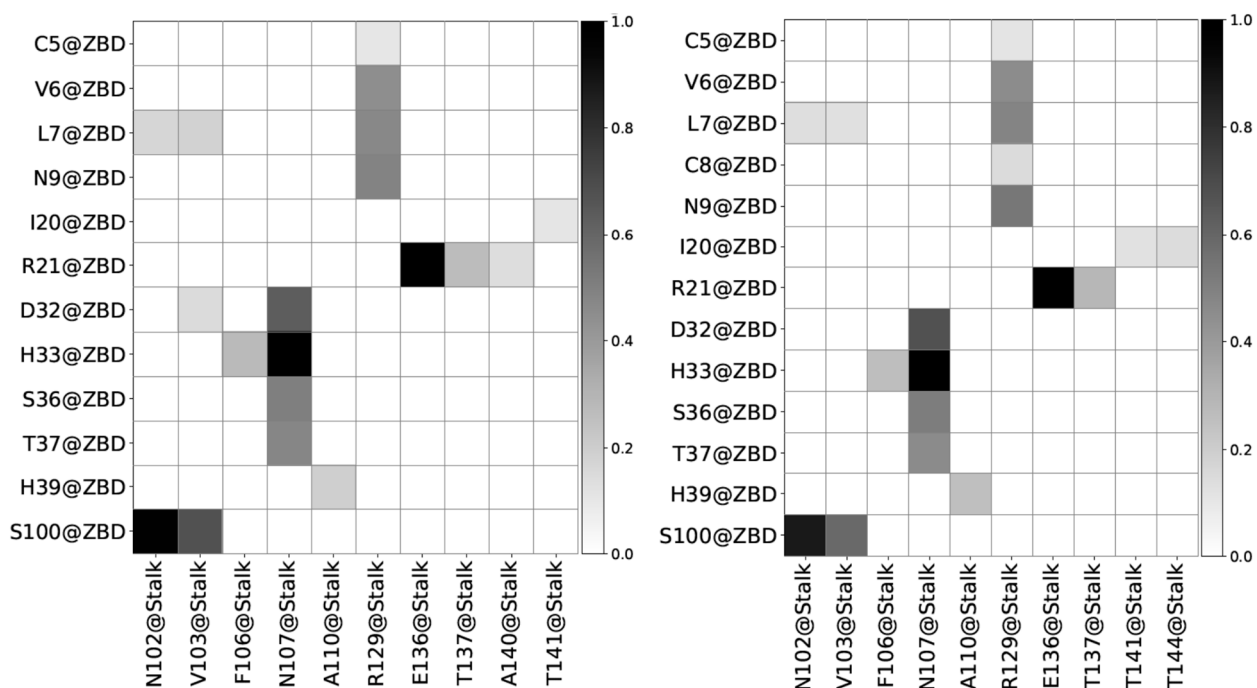
**Figure S3.** Calculated root mean square deviations (RMSD) of Stalk domain from the initial structures plotted as a function of the simulation time. RMSD values for Stalk domain in the RNA-free and in the RNA-engaged form are in dark cyan and orchid, respectively. The bold lines are obtained by applying a Savitzky-Golay filter in order to cut-off the noise. In the right panel, the violin representation of the RMSD distribution is provided.



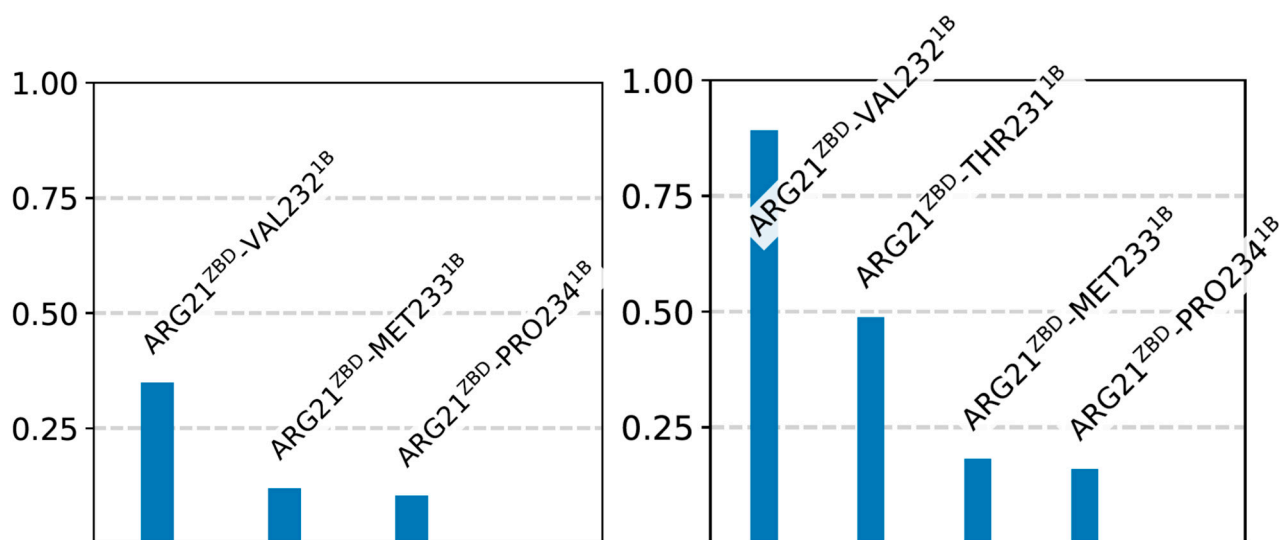
**Figure S4.** Calculated root mean square deviations (RMSD) of 1B domain from the initial structures plotted as a function of the simulation time. RMSD values for 1B domain in the RNA-free and in the RNA-engaged form are in dark cyan and orchid, respectively. The bold lines are obtained by applying a Savitzky-Golay filter in order to cut-off the noise. In the right panel, the violin representation of the RMSD distribution is provided.



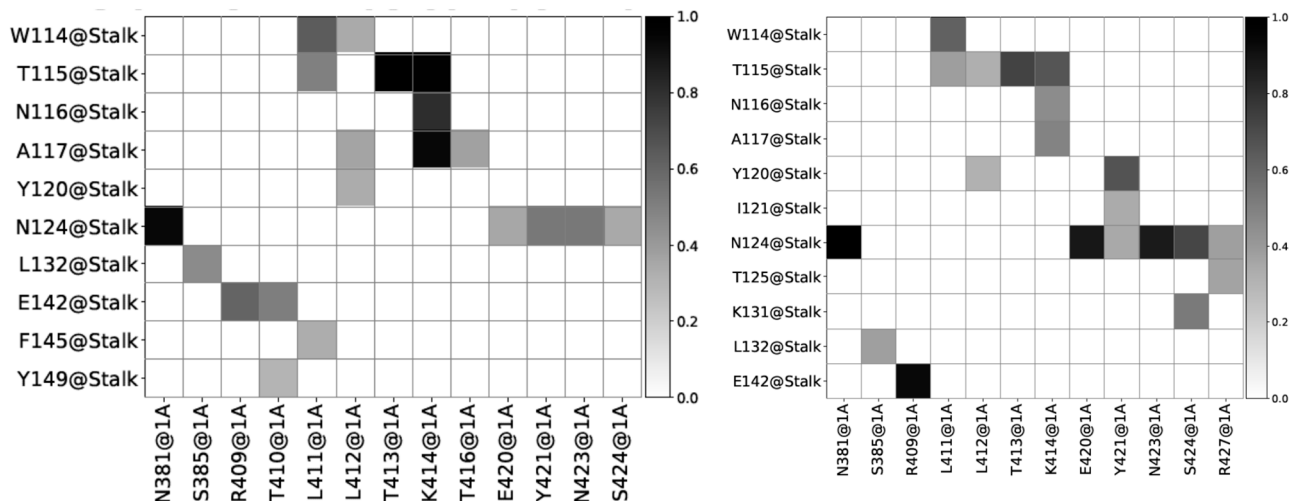
**Figure S5.** Calculated root mean square deviations (RMSD) of 1A domain from the initial structures plotted as a function of the simulation time. RMSD values for 1A domain in the RNA-free and in the RNA-engaged form are in dark cyan and orchid, respectively. The bold lines are obtained by applying a Savitzky-Golay filter in order to cut-off the noise. In the right panel, the violin representation of the RMSD distribution is provided.



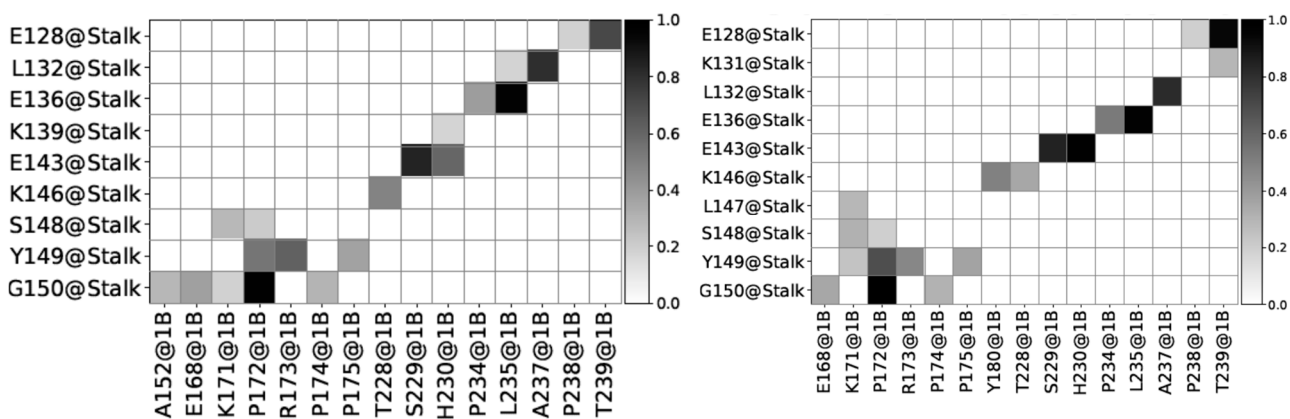
**Figure S6.** Plot of the interface contact matrix between domains ZBD and Stalk in the RNA-free (left panel) and RNA-engaged (right panel) nsp13. Contacts are colored from white to black if they are observed in the 0% or 100% of the simulation time, respectively.



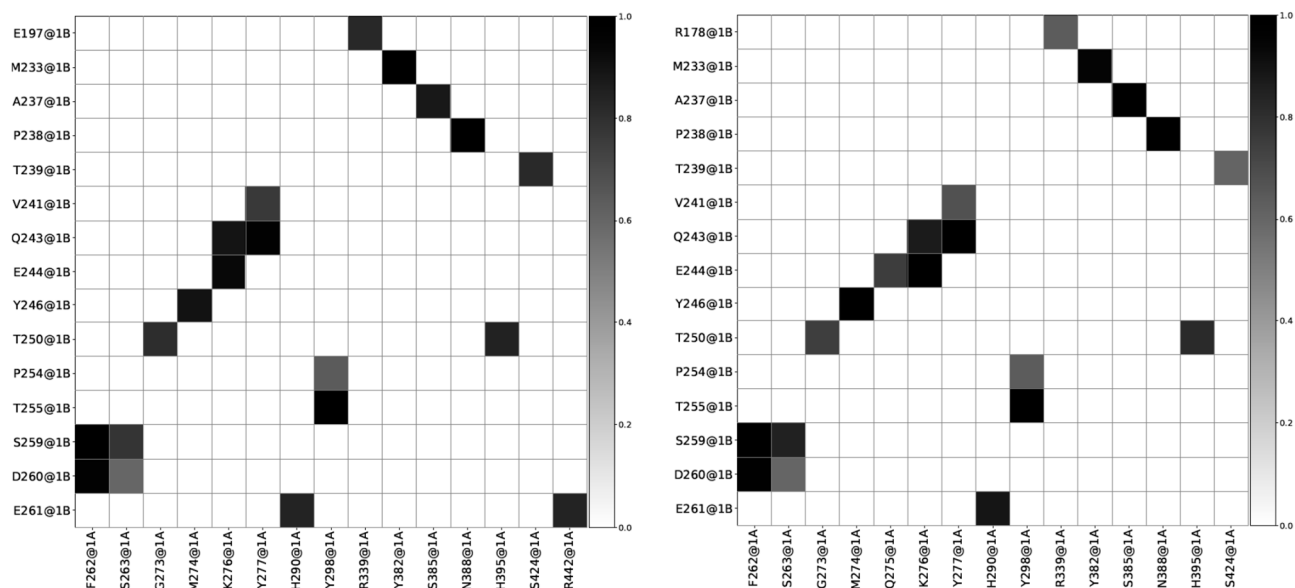
**Figure S7.** Contact frequencies between domains ZBD and 1B in the RNA-free (left panel) and RNA-engaged (right panel) nsp13. Bar heights are proportional to the relative contact time observed during the simulations.



**Figure S8.** Plot of the interface contact matrix between domains Stalk and 1A in the RNA-free (left panel) and RNA-engaged (right panel) nspl3. Contacts are colored from white to black if they are observed in the 0% or 100% of the simulation time, respectively.



**Figure S9.** Plot of the interface contact matrix between domains Stalk and 1B in the RNA-free (left panel) and RNA-engaged (right panel) nspl3. Contacts are colored from white to black if they are observed in the 0% or 100% of the simulation time, respectively.



**Figure S10.** Plot of the interface contact matrix between domains 1A and 1B in the RNA-free (left panel) and RNA-engaged (right panel) nsP13. Contacts are colored from white to black if they are observed in the 0% or 100% of the simulation time, respectively.