

Supplementary Materials

The Recognition Pathway of the SARS-CoV-2 Spike Receptor-Binding Domain to Human Angiotensin-Converting Enzyme 2

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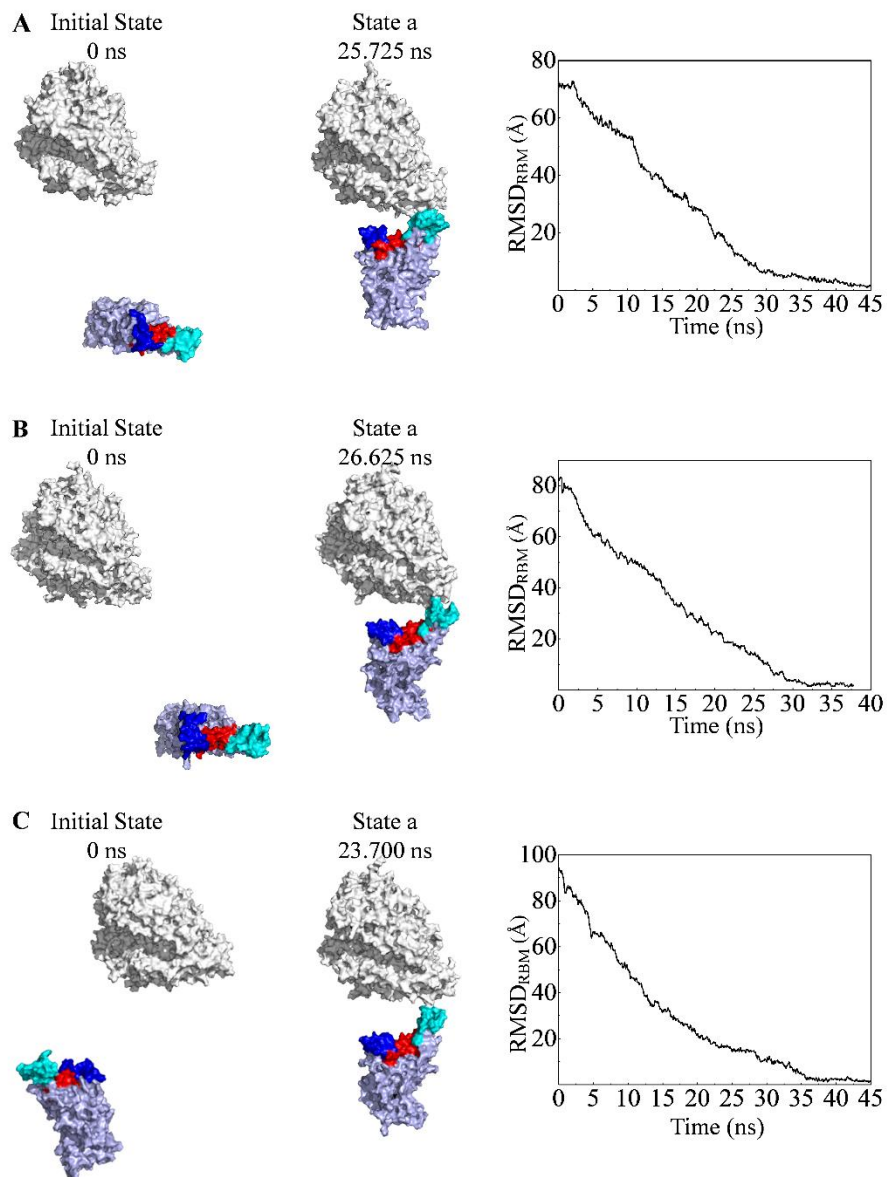


Figure S1. The initial state, State a and the time-dependent RMSD_{RBM} of the Su-GaMD simulations from three different starting points for the recognition process of RBD_{WT} to ACE2.

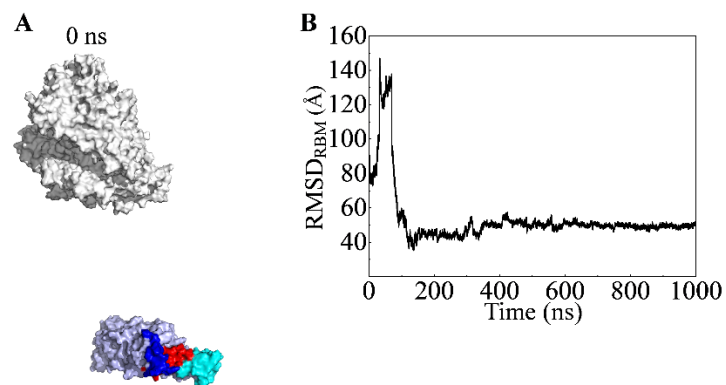


Figure S2. (A) The starting point (which is the same as in Figure 2A) and (B) the time-dependent RMSD_{RBM} of the 1000-ns cMD simulation for the recognition process of RBD_{WT} to ACE2.

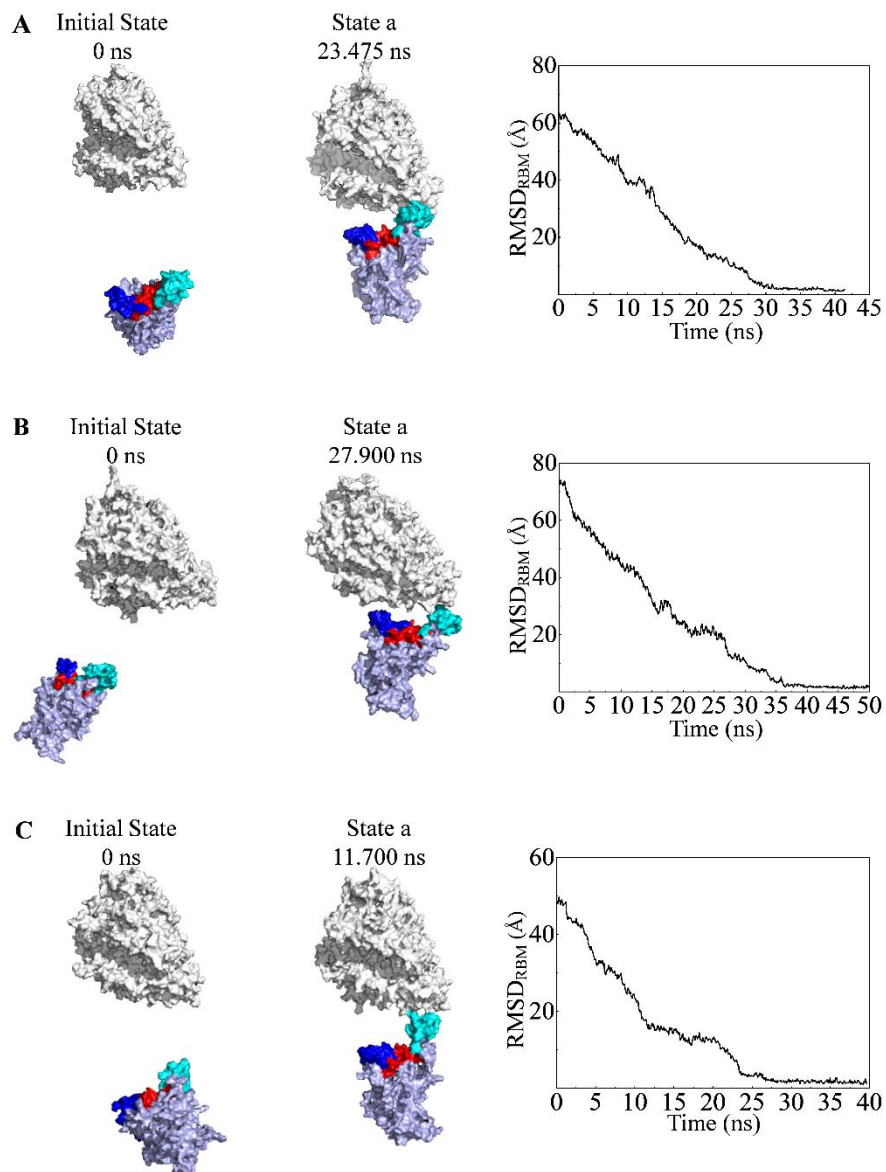


Figure S3. The initial state, State a and the time-dependent RMSD_{RBM} of the Su-GaMD simulations from three different starting points for the recognition process of $\text{RBD}_{\text{Delta}}$ to ACE2.

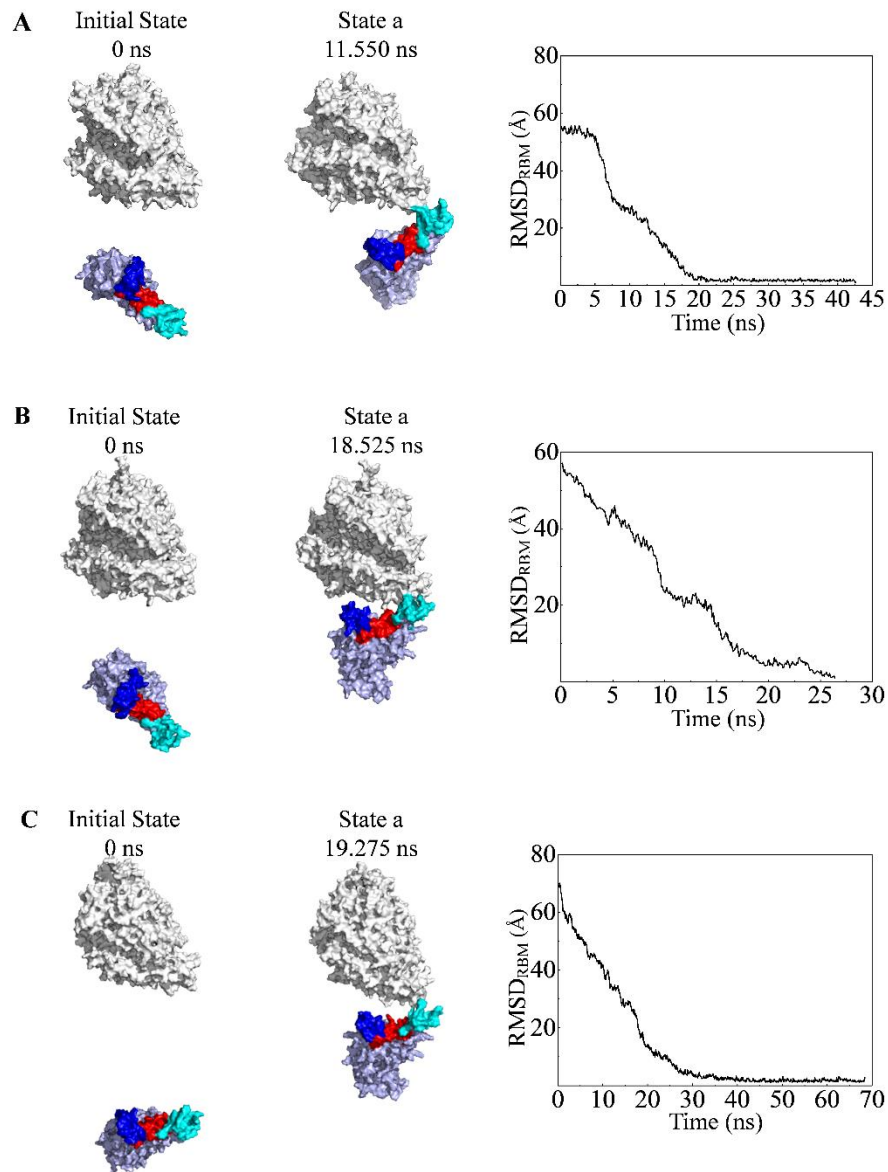


Figure S4. The initial state, State a and the time-dependent RMSD_{RBM} of the Su-GaMD simulations from three different starting points for the recognition process of RBD_{OmicronBA.2} to ACE2.

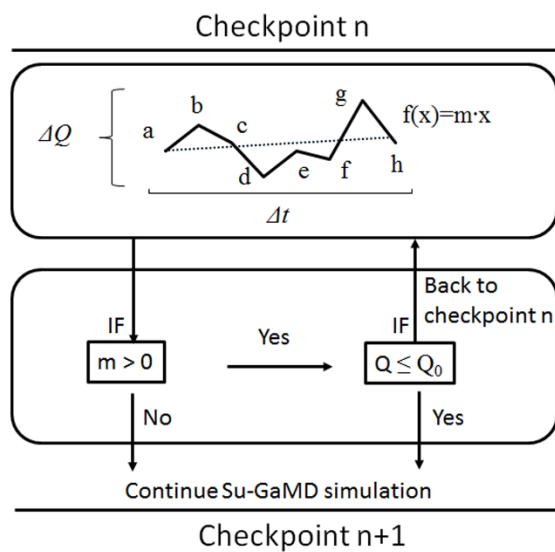


Figure S5. Workflow of the Su-GaMD simulation.