Supporting information for article “Theoretical studies of Leu-Pro-Arg-Asp-Ala pentapeptide (LPRDA) binding to Sortase A of Staphylococcus aureus”

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LPRDA-SrtA MD with 3 replicas for 10 ns

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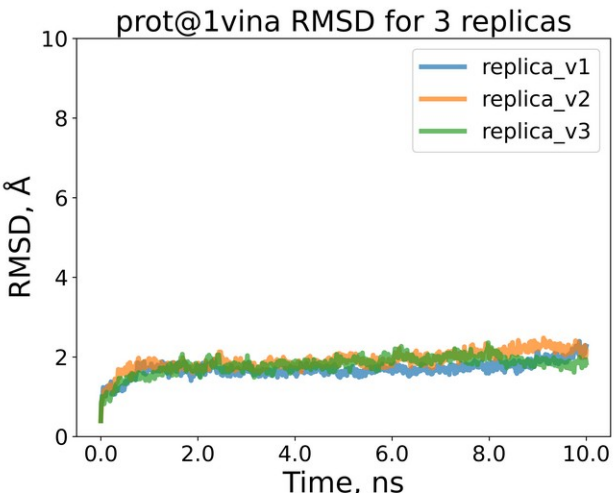
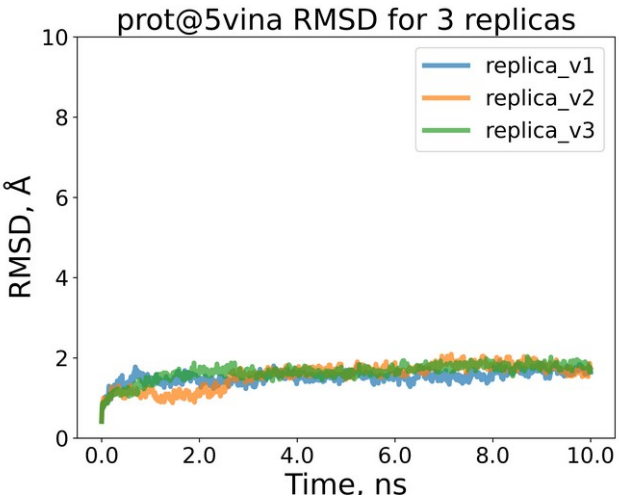
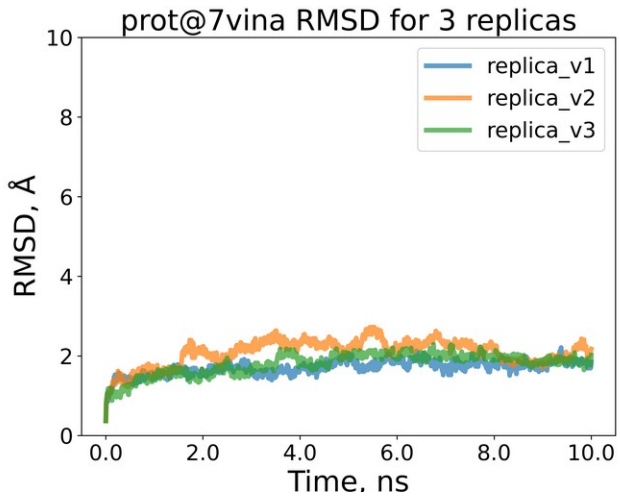
Table S1. RMSD values of the SrtA protein (C-alpha atoms) in LPRDA-SrtA complex.



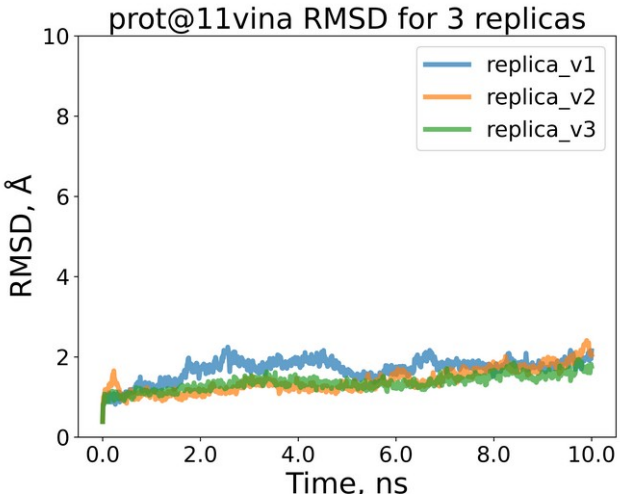
ADV #1, E = -7.3 kcal/mol



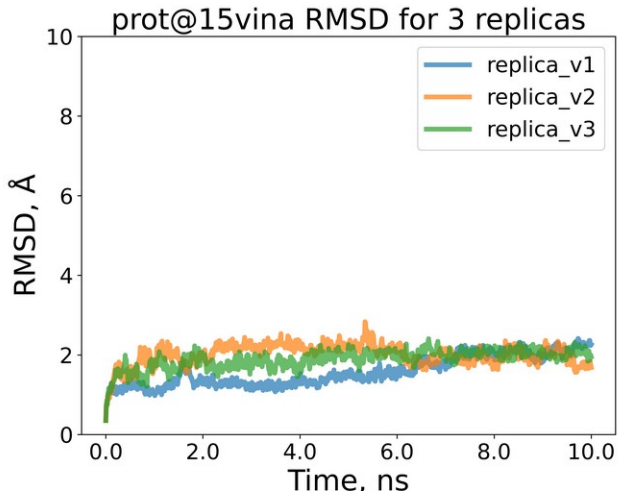
ADV #5, E = -7.0 kcal/mol



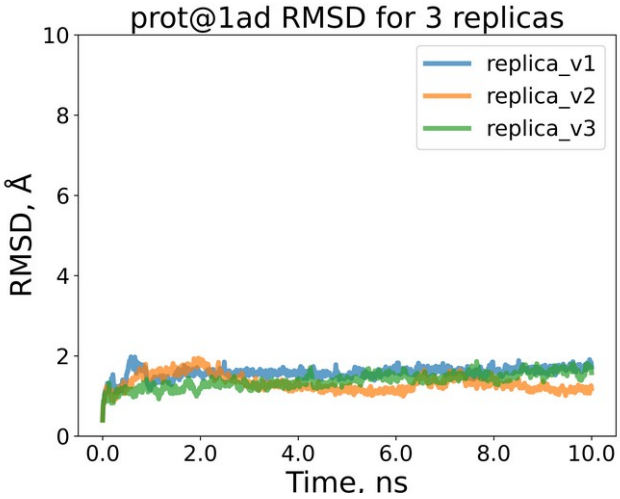
ADV #7, E = -6.9 kcal/mol



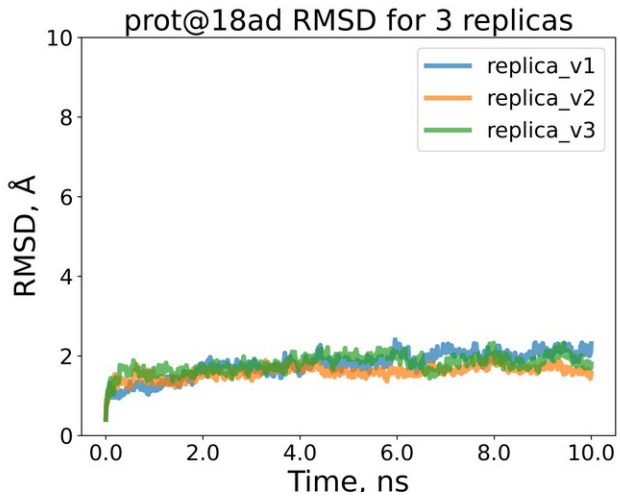
ADV #11, E = -6.8 kcal/mol



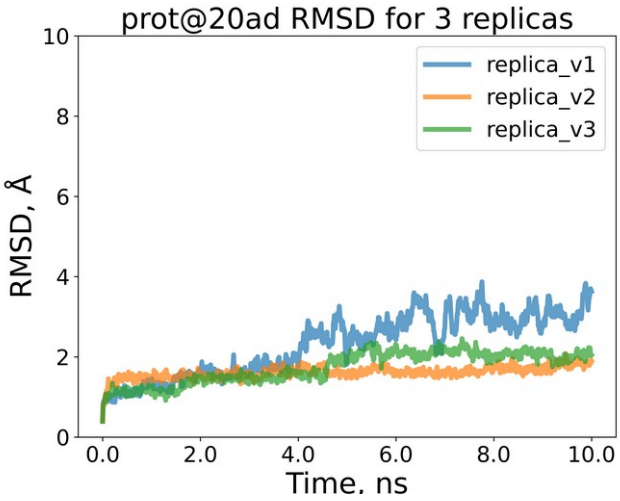
ADV #15, E = -6.6 kcal/mol



AD #1, E = -7.94 kcal/mol



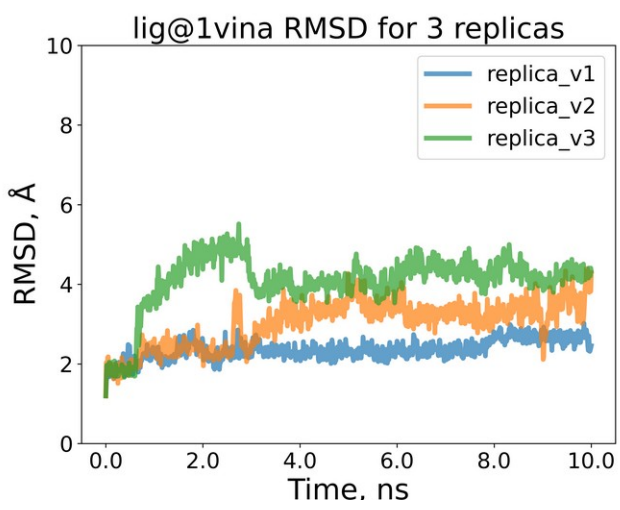
AD #18, E = -5.83 kcal/mol



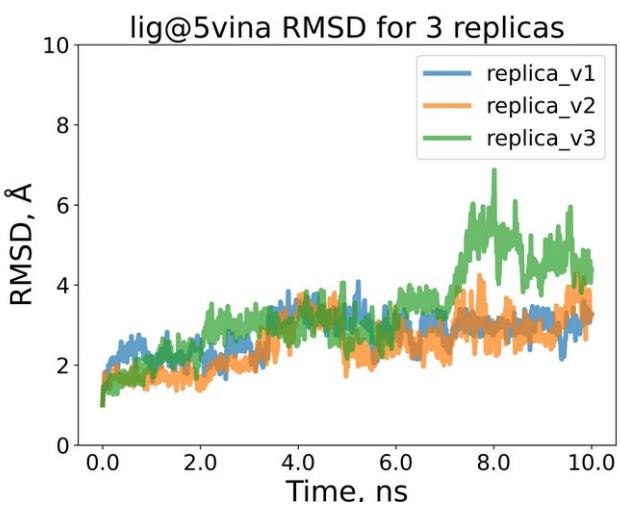
AD #20, E = -5.75 kcal/mol

Ligand

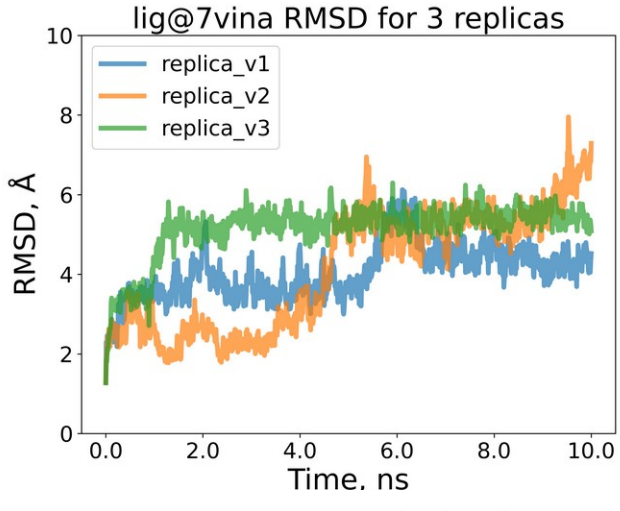
Table S2. RMSD values of LPRDA in LPRDA-SrtA complex.



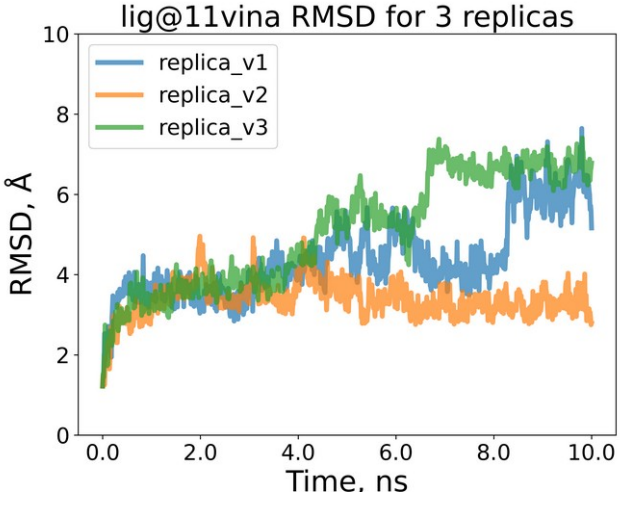
ADV #1, E = -7.3 kcal/mol



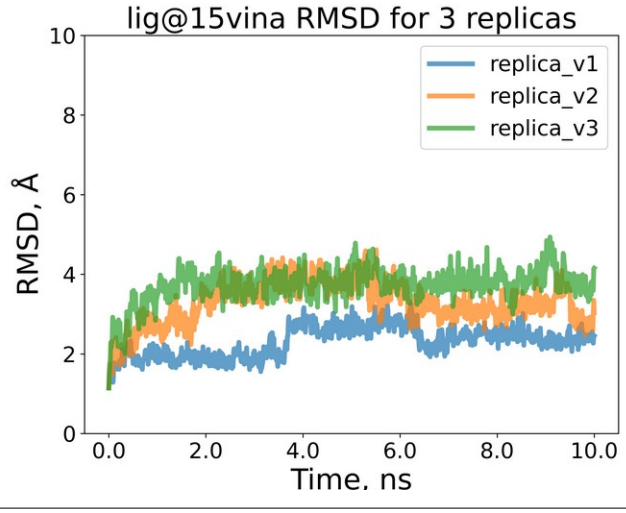
ADV #5, E = -7.0 kcal/mol

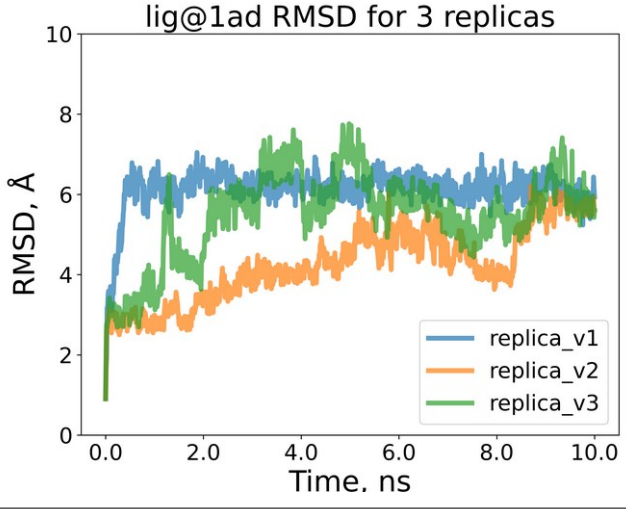


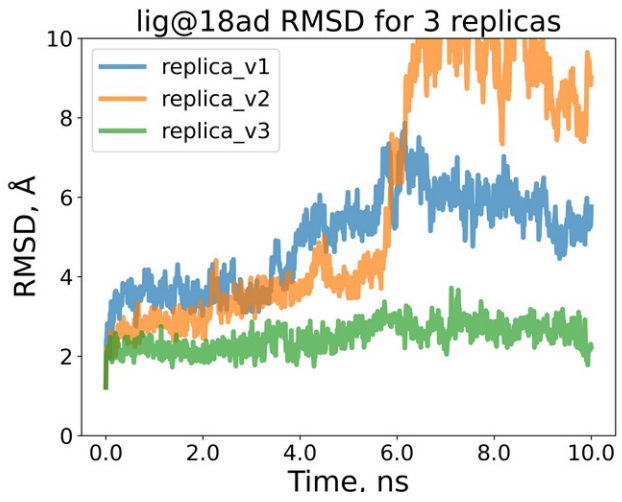
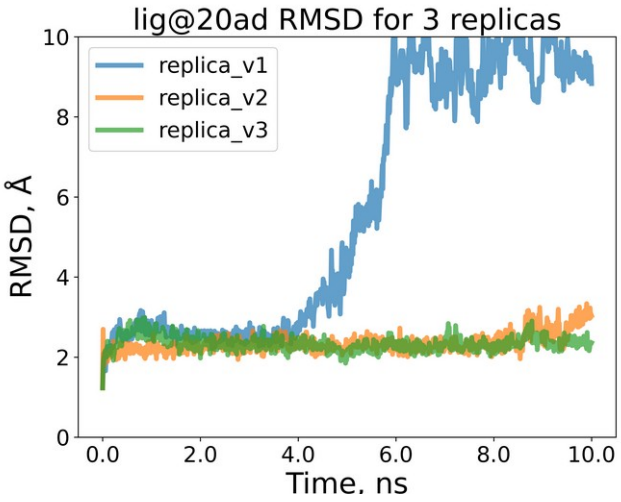
ADV #7, E = -6.9 kcal/mol



ADV #11, E = -6.8 kcal/mol

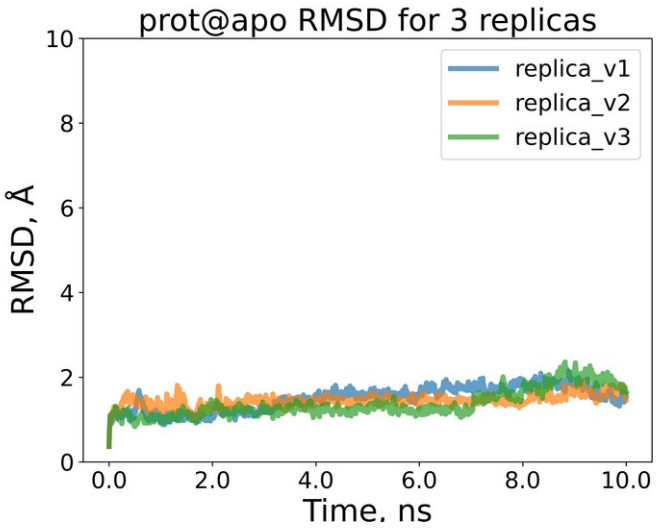




ADV #15, E = -6.6 kcal/mol	AD #1, E = -7.94 kcal/mol
 AD #18, E = -5.83 kcal/mol	 AD #20, E = -5.75 kcal/mol

SrtA (apo form) MD for 10 ns

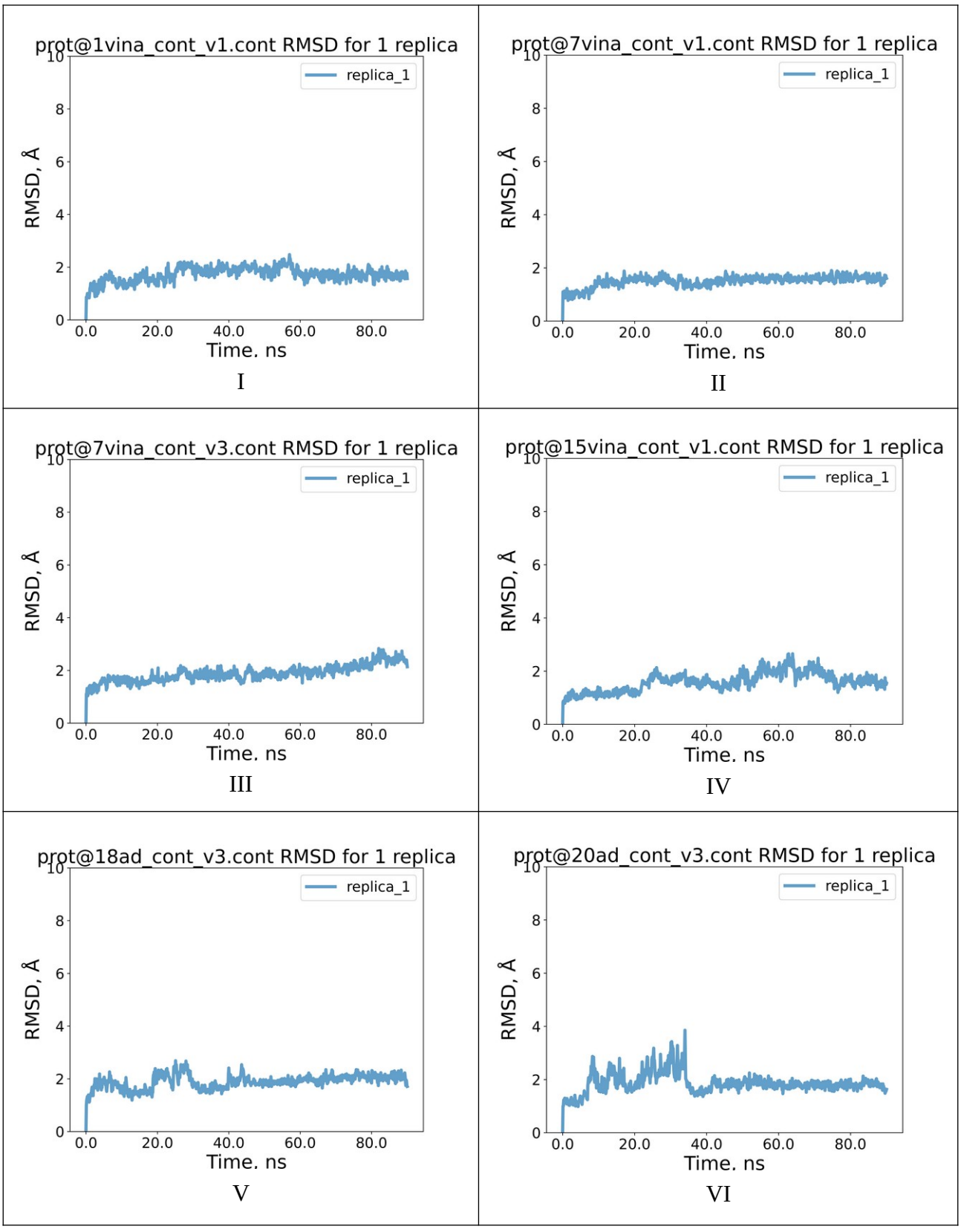
Figure S1. RMSD of the apo form of SrtA during the 10 ns MD simulation.



LPRDA-SrtA complex MD for 90 ns (continuation)

Receptor

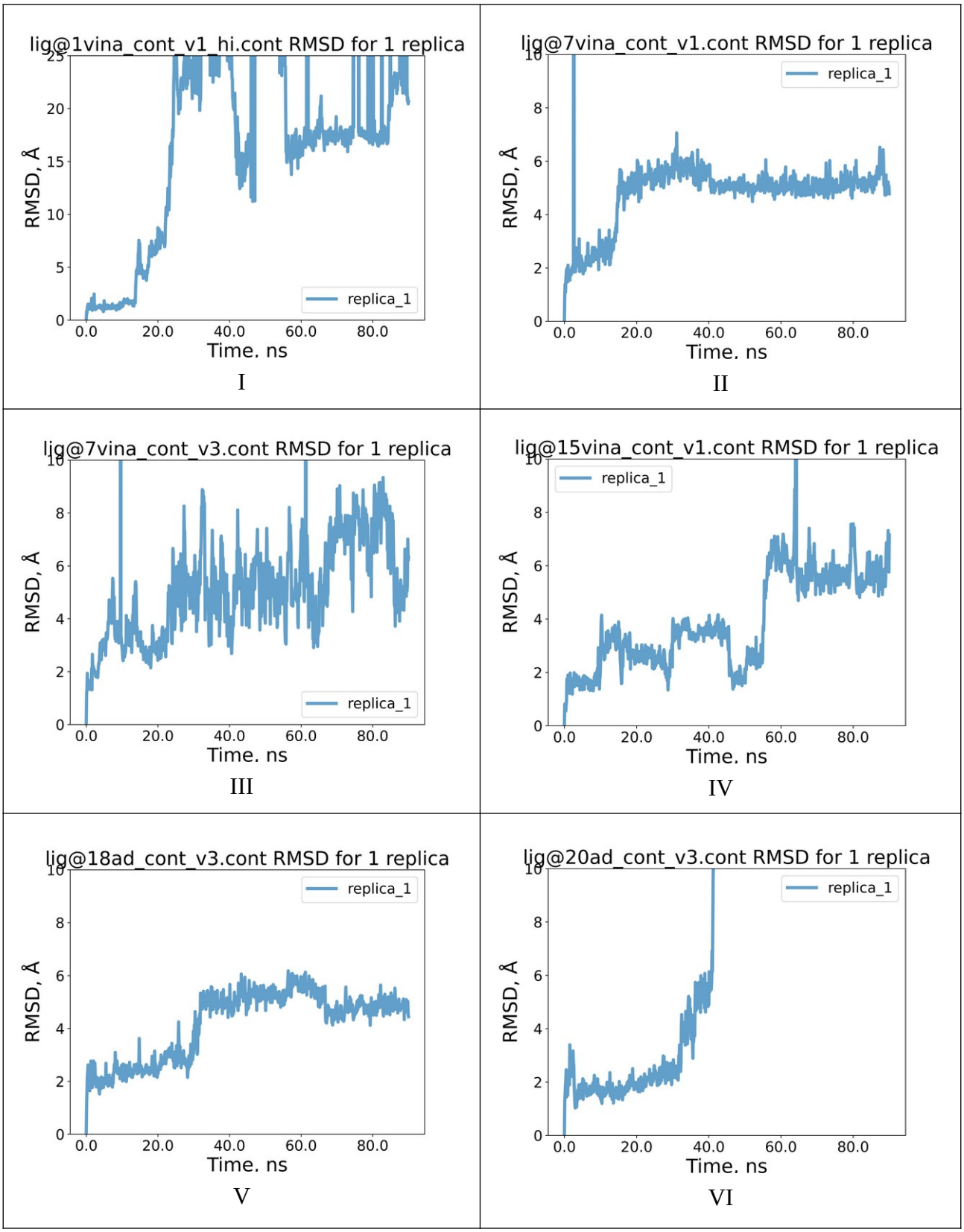
Table S3. SrtA (C-alpha atoms) RMSD for the continued MD (for another 90 ns) for the selected LPRDA-SrtA complexes. I. ADV #1 (repl.1), II. ADV #7 (repl. 1), III. ADV #7 (repl.3), IV. ADV #15 (repl.1), V. AD #18 (repl.3), VI. AD #20 (repl.3). The starting geometry for each complex was taken from the final geometries of the respective 10 ns MD trajectories.



Ligand

Table S4. LPRDA RMSD for the continued MD (for another 90 ns) for the selected LPRDA-SrtA complexes. I. ADV #1 (repl.1), II. ADV #7 (repl. 1), III. ADV #7 (repl.3), IV. ADV #15 (repl.1), V.

AD #18 (repl.3), VI. AD #20 (repl.3). The starting geometry for each complex was taken from the final geometries of the respective 10 ns MD trajectories.



RMSF analysis

LPRDA-SrtA complex MD for 90 ns (continuation)

Receptor

Table S5. RMSF values obtained for the SrtA receptor from 90 ns MD simulation of 6 different LPRDA-SrtA complexes. RMSF values are obtained for C-alpha atoms.