

Supporting Information for:

Structural Insights into Binding of Remdesivir Triphosphate within the Replication-Transcription Complex of SARS-CoV-2

Jimin Wang^{1,*}, Yuanjun Shi², Krystle Reiss², Federica Maschietto², Elias Lolis³, William H. Konigsberg¹, George P. Lisi⁴, Victor S. Batista^{2,*}

¹*Department of Molecular Biophysics and Biochemistry, Yale University, New Haven, CT 06520-8114.*

²*Department of Chemistry, Yale University, New Haven, CT 06520-8499.* ³*Department of Pharmacology, Yale University, New Haven, CT 06520-8066.* ⁴*Department of Molecular and Cell Biology and Biochemistry, Brown University, Providence, RI 02912.*

Supporting information contains the refined PDB coordinates of the equilibrated ATP-bound complex against MD-derived ESP maps.