

Supporting Information for

Piece of the Puzzle: Remdesivir disassemble the multimeric SARS-CoV-2 RNA-dependent RNA Polymerase Non-Structural Proteins (RdRp-NSPs) complex

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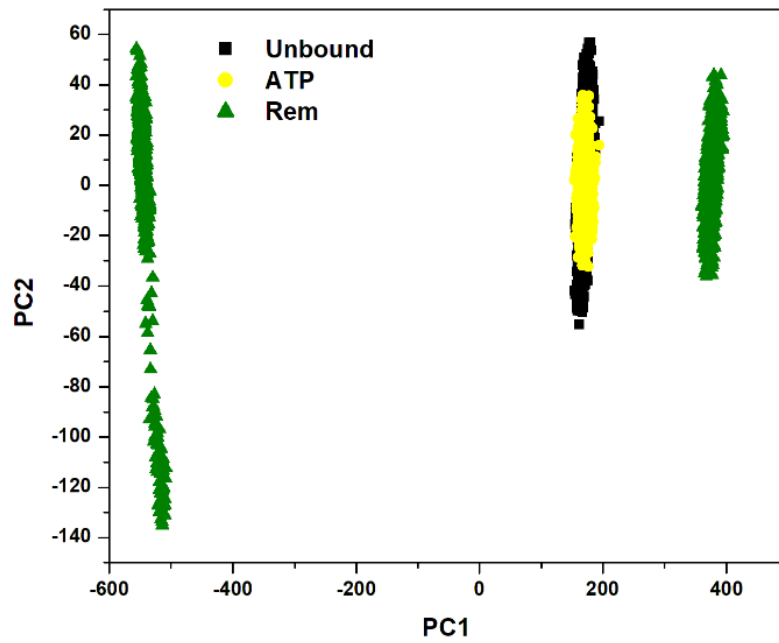
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Supplementary Table 1: Mean values for estimated structural stabilities using the finally equilibrated (FE) time-frames

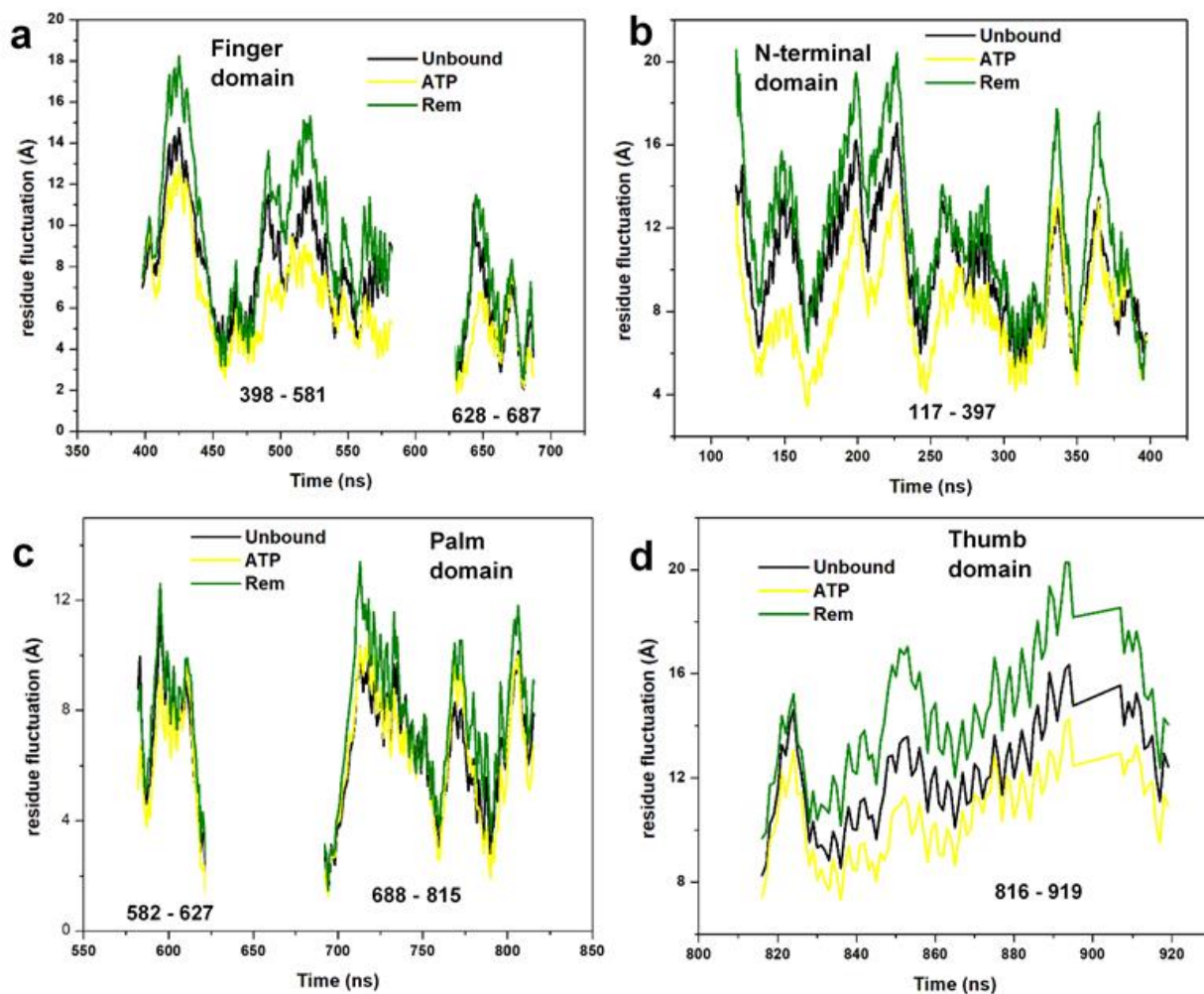
Whole structure			
SARS-CoV-2 RdRp-NSP	Unbound	ATP-bound	<i>Rem-P₃</i> -bound
FE-RMSD (Å)	6.8 ± 0.02	1.8 ± 0.3	12.6 ± 0.02
FE-RMSF (Å)	11.8 ± 0.2	8.4 ± 0.1	13.9 ± 0.3
Active site motions			
FE-RMSD (Å)	1.3 ± 0.4	1.4 ± 0.4	1.6 ± 0.4
FE-RoG (Å)	32.9 ± 0.2	32.8 ± 0.1	33.2 ± 0.2
Ligand motions			
FE-RMSD (Å)	----	1.5 ± 0.8	3.5 ± 0.5

Supplementary Table 2. RMSF estimations of per-residual fluctuations across the NSP12 subdomains and attached NSP7 and 8 subunits.

FE-RMSF (Å)			
Structural components	Unbound	ATP	Rem
NSP12			
<i>N-terminal</i>	10.1 ± 2.6	8.1 ± 2.3	11.9 ± 3.5
<i>Finger</i>	7.5 ± 2.7	6.1 ± 2.4	9.0 ± 3.6
<i>Thumb</i>	12.2 ± 1.9	10.6 ± 1.6	14.5 ± 2.4
<i>Palm</i>	6.4 ± 2.2	6.1 ± 2.4	7.5 ± 2.3
NSP7	12.2 ± 1.9	9.9 ± 2.1	14.2 ± 2.6
NSP8	34.1 ± 1.5	13.3 ± 2.0	41.6 ± 1.6
NSP8_{II} (<i>subunit II</i>)	11.3 ± 1.5	10.2 ± 1.5	11.7 ± 1.4



Supplementary Figure S1. Principal component plot showing projection of the RdRp-NSP complex in the unbound (black), ATP-bound (yellow) and *Rem-P₃*-bound states.



Supplementary Figure S2. RMSF plot showing residual fluctuations across the NSP12 subdomains in the unbound (black), ATP-bound (yellow) and *Rem-P₃*-bound states. A. NSP12-finger domain B. NSP12 N-terminal domain C. NSP12-Palm domain D. NSP12-Thumb domain.