

**Supplemental information for ‘Characterization of  
the Water Defect at the HIV-1 gp41 Membrane  
Spanning Domain in Bilayers With and Without  
Cholesterol using Molecular Simulations’**

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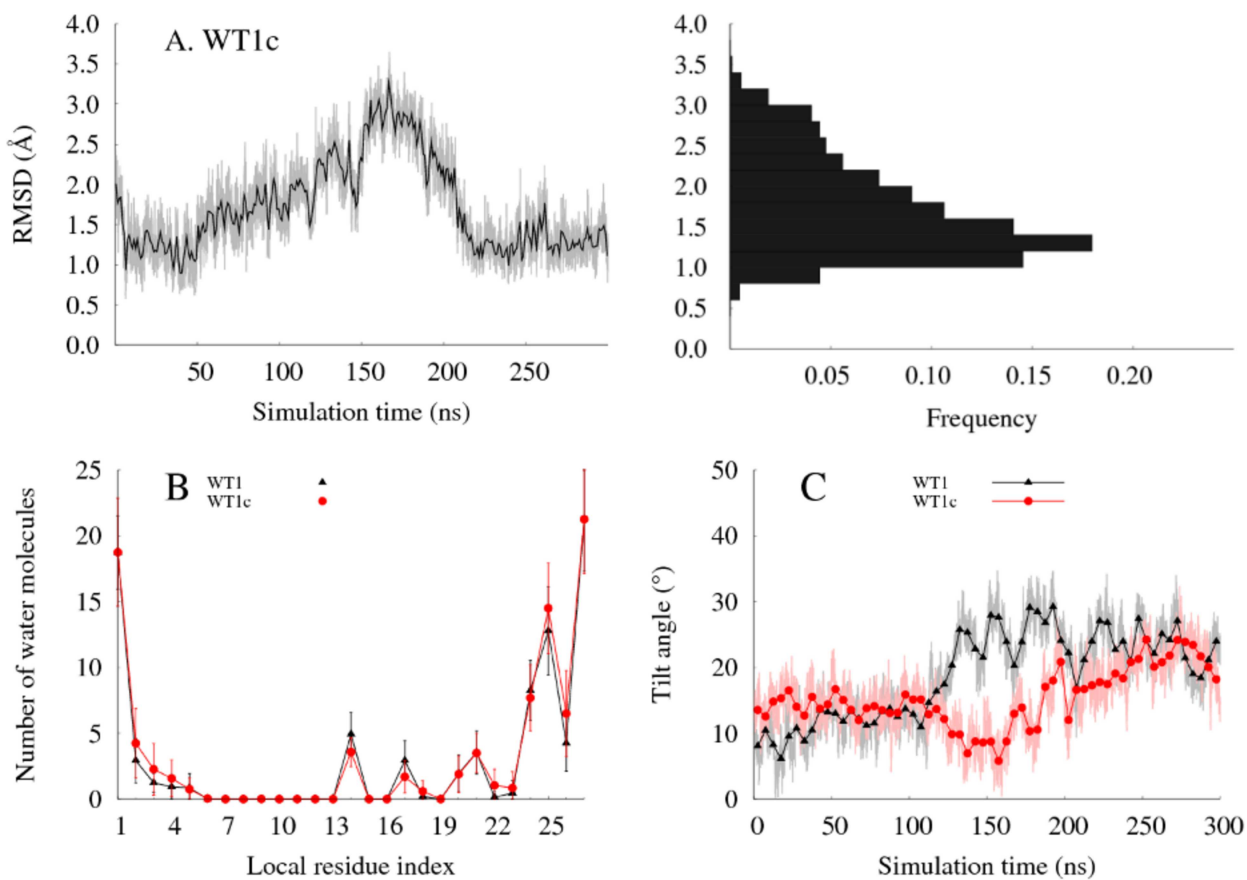


Figure 1: Comparison of WT systems run with more aggressive (WT1) and less aggressive (WT1c) configuration parameters (see Methods). (A) Collective variable (RMSD of backbone compared to perfect helix) in Å vs simulation time in ns and histogram of RMSD vs frequency for equilibrium MD of WT1c. Compare to Figure 2A for WT1. (B) Number of water molecules within 4 Å of protein vs amino acid that each water molecule is uniquely attributed to during equilibrium MD for WT1 and WT1c systems. All statistics are from the last 100 ns of each trajectory and error bars represent standard deviation. (C) Tilt angle in degrees vs simulation time in ns for WT1 and WT1c systems.

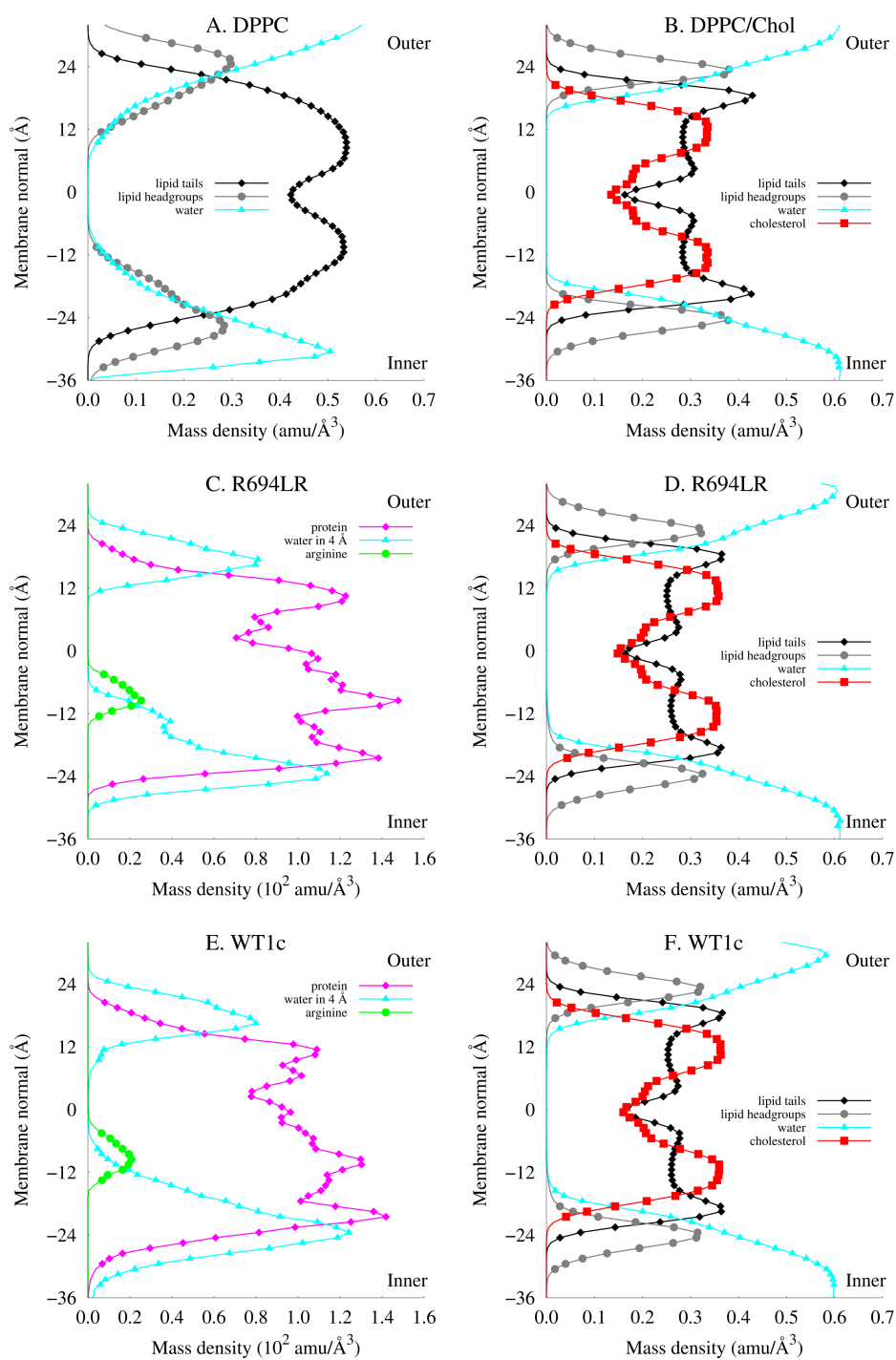


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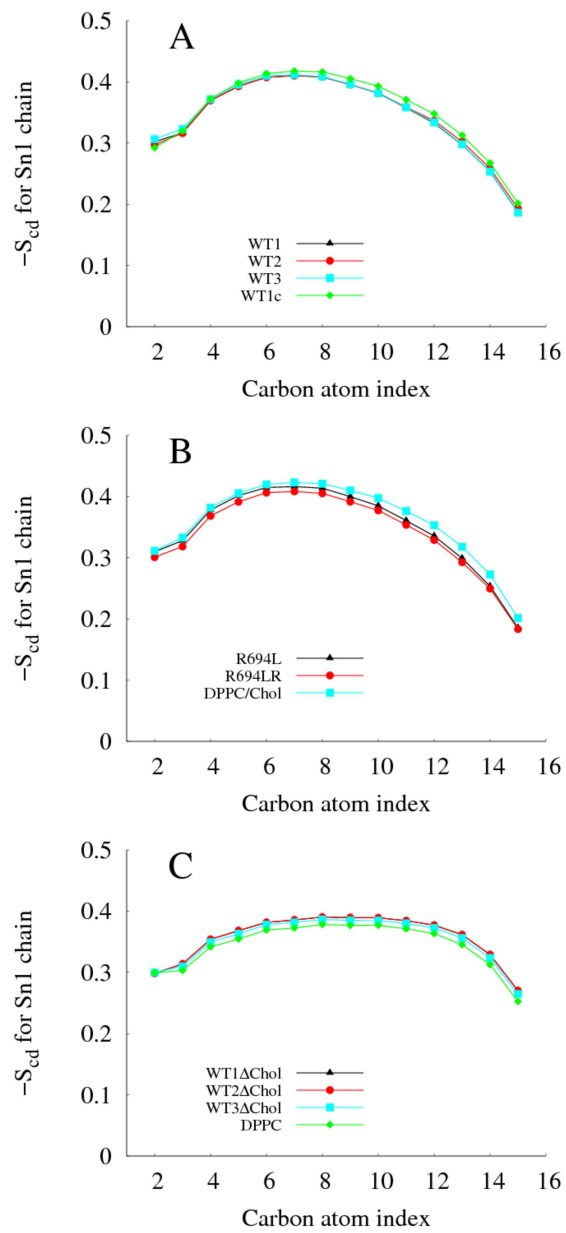


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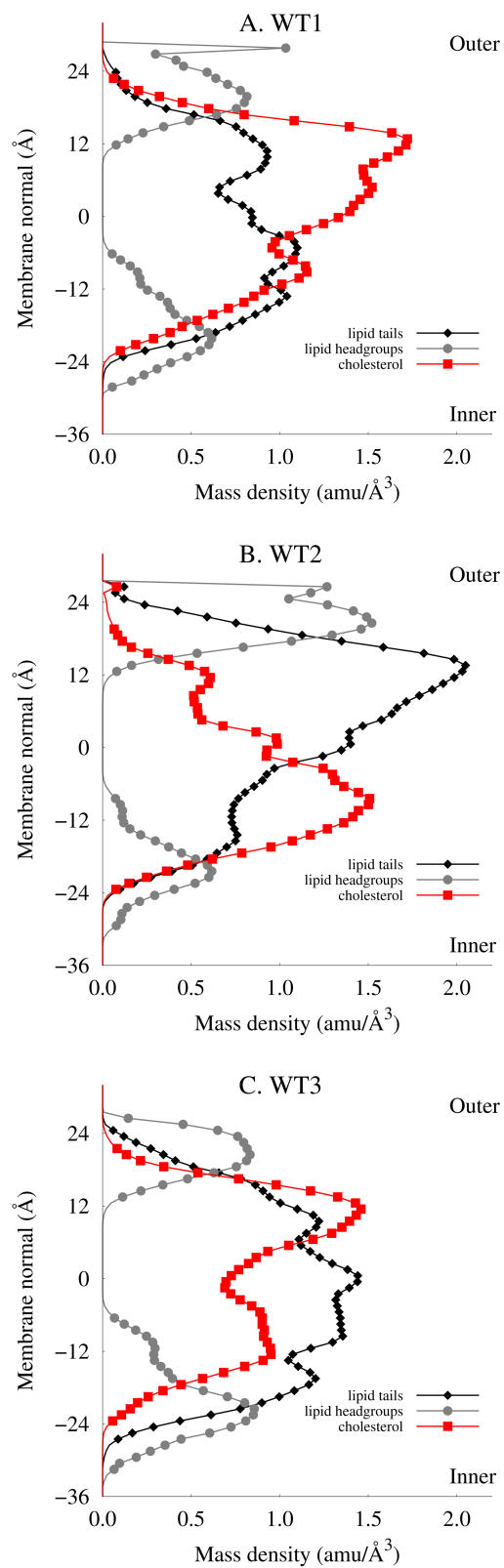


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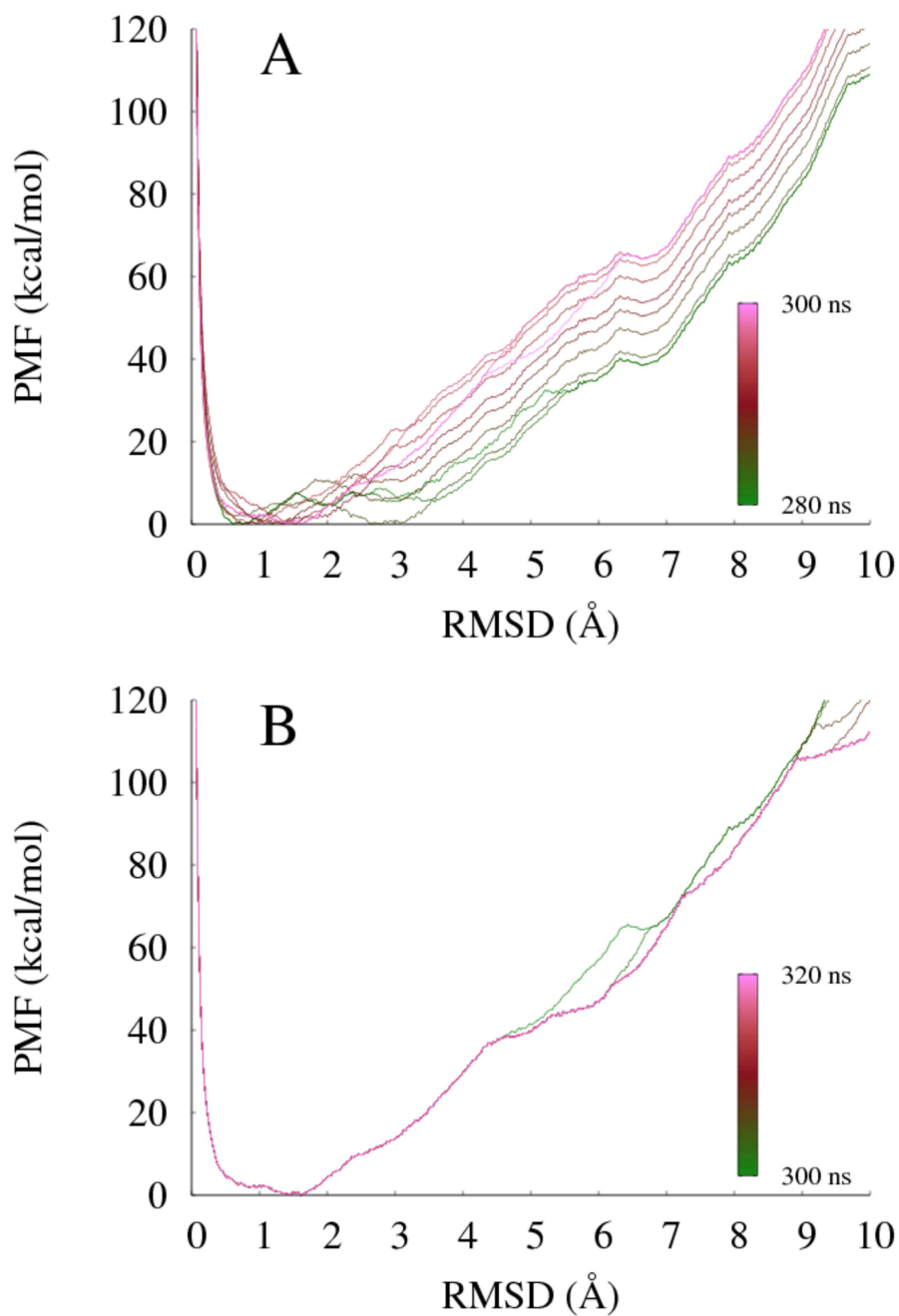


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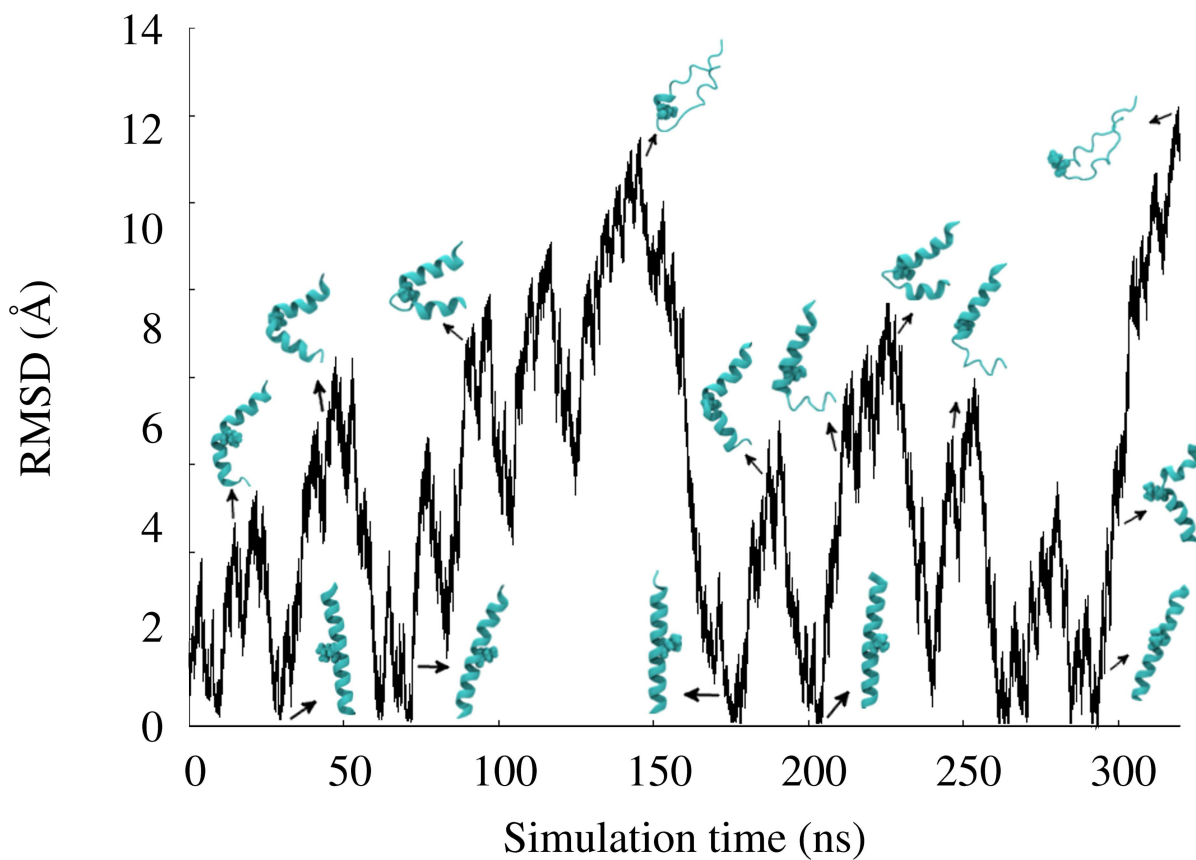


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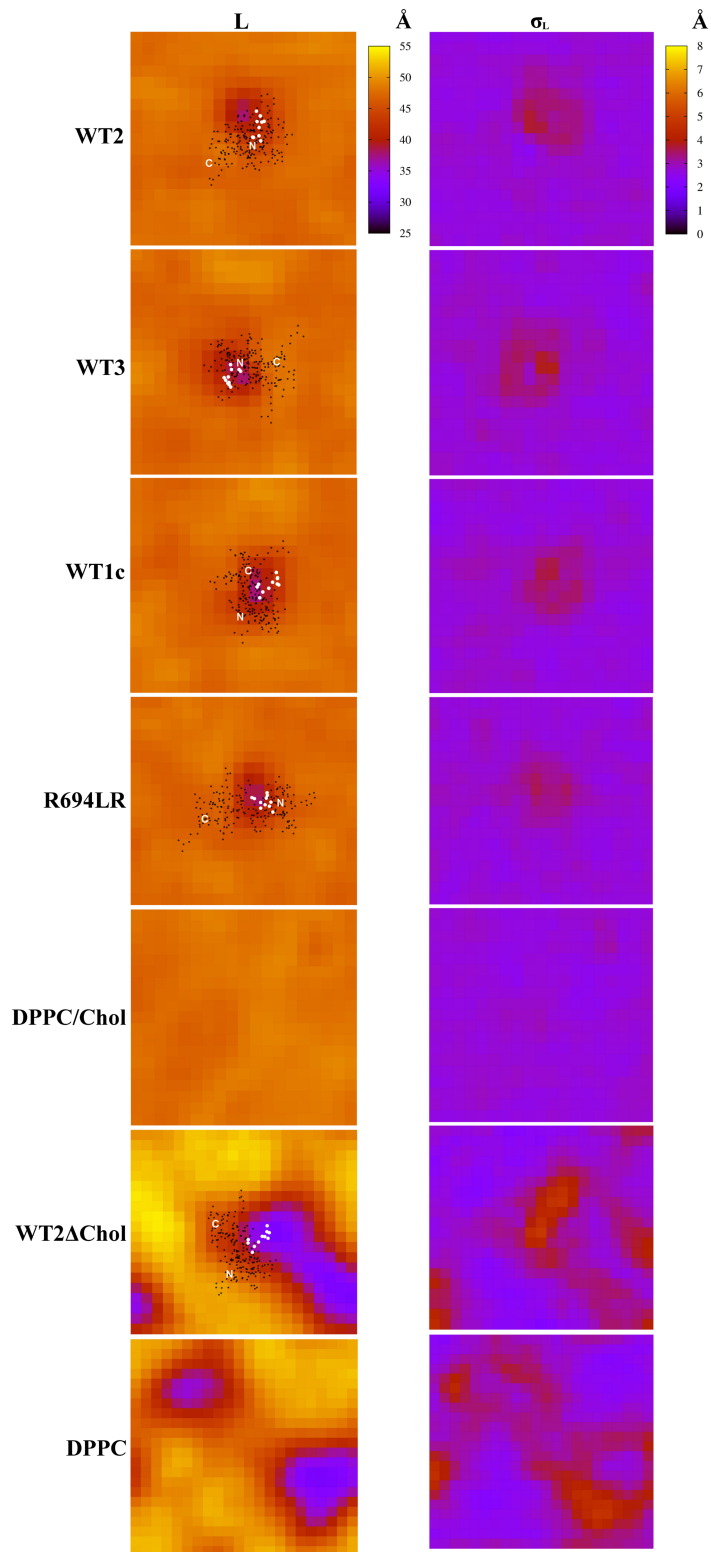


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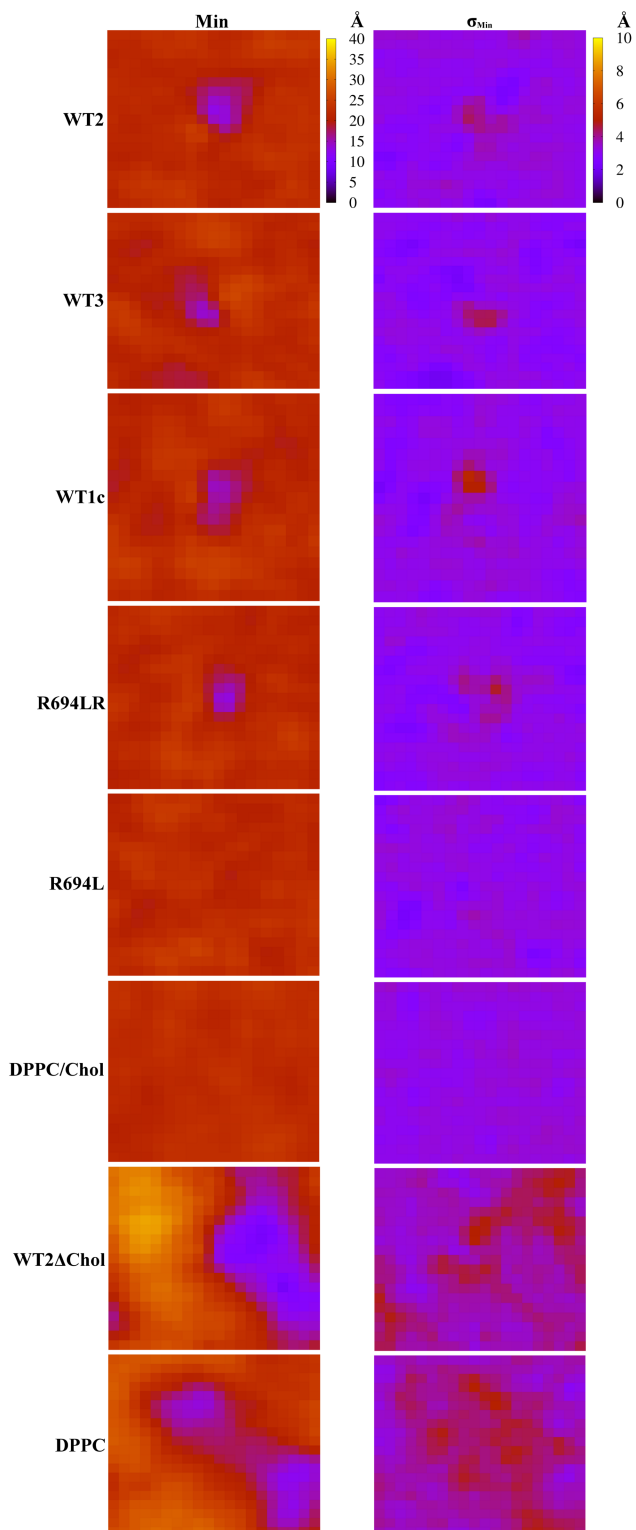


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