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Supplemental Information

**Molecular Mechanisms of the R61T Mutation in Apolipoprotein E4: A
Dynamic Rescue**

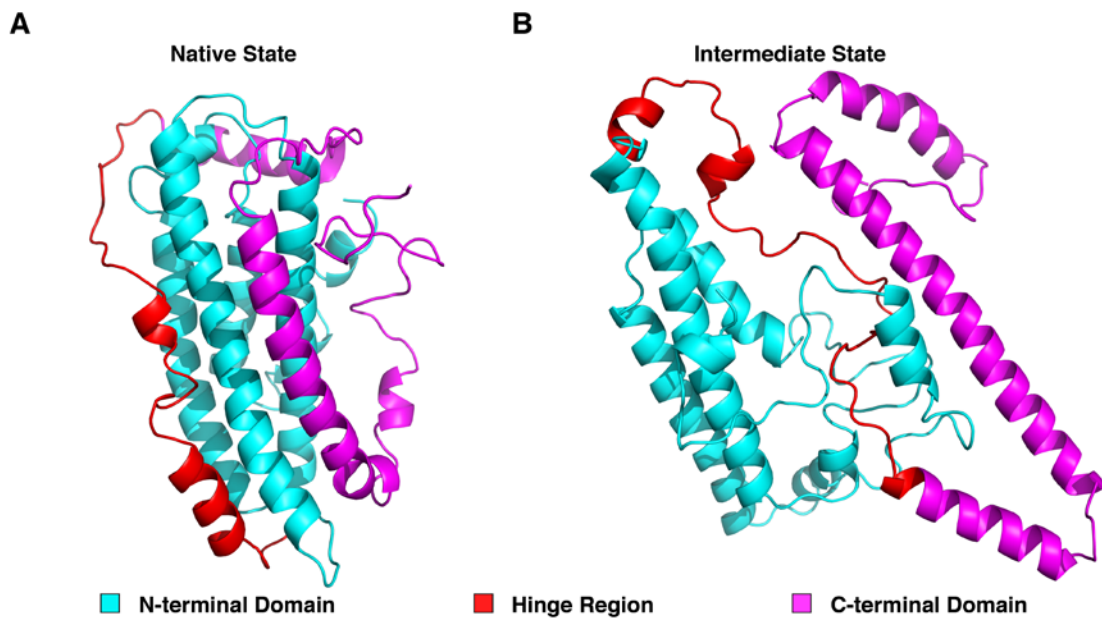
Benfeard Williams, II, Marino Convertino, Jhuma Das, and Nikolay V. Dokholyan

Supporting materials for

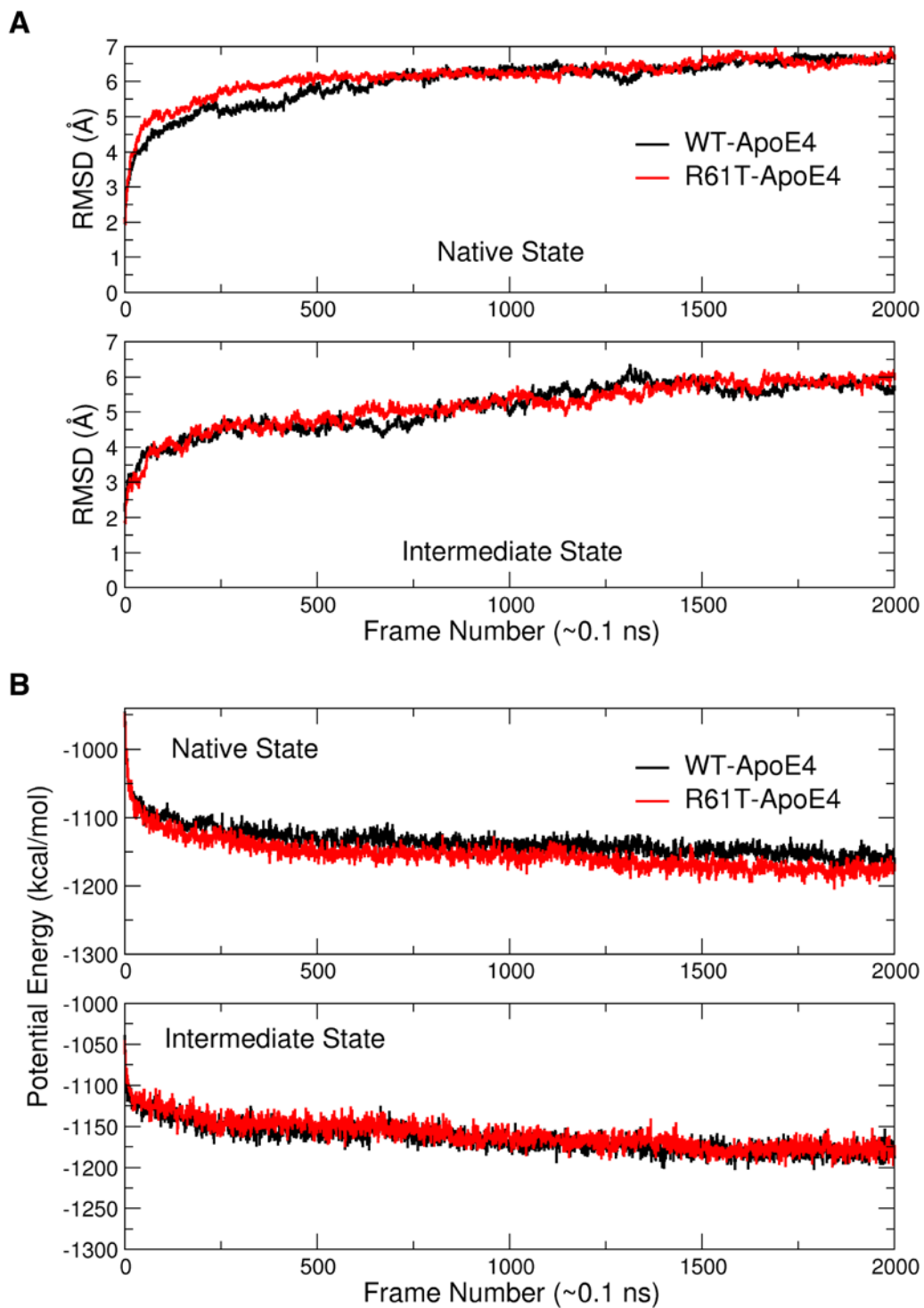
Molecular Mechanisms of the R61T Mutation in Apolipoprotein E4: A Dynamic Rescue

B. Williams, M. Convertino, J. Das, and N. V. Dokholyan[†]

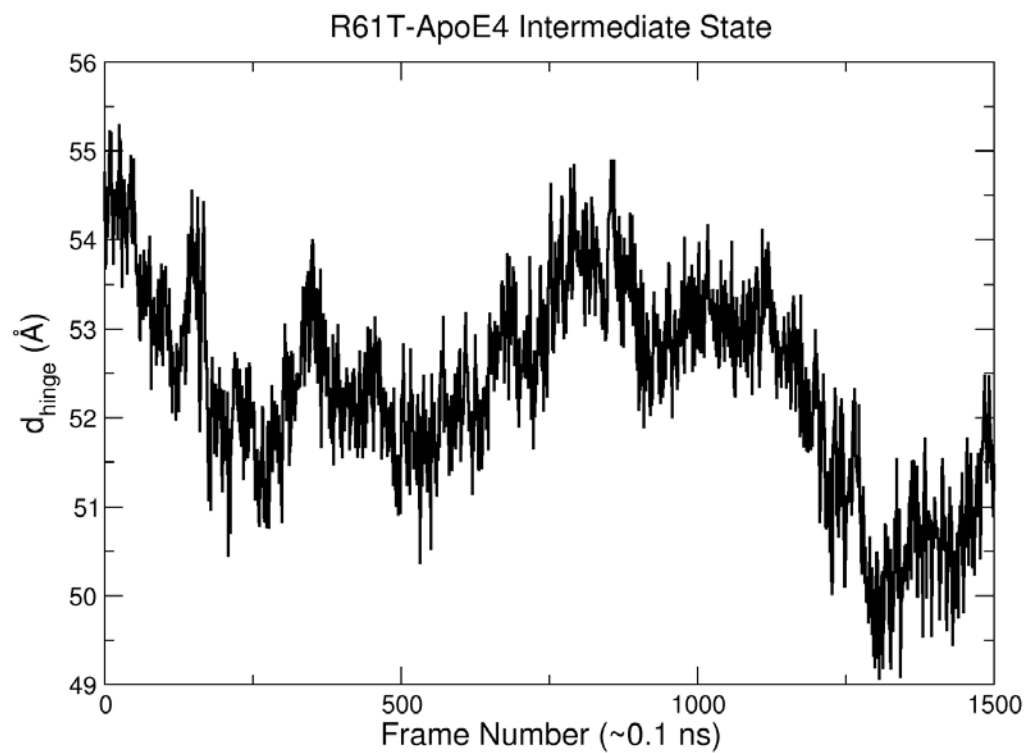
[†]To whom correspondence should be addressed: dokh@unc.edu



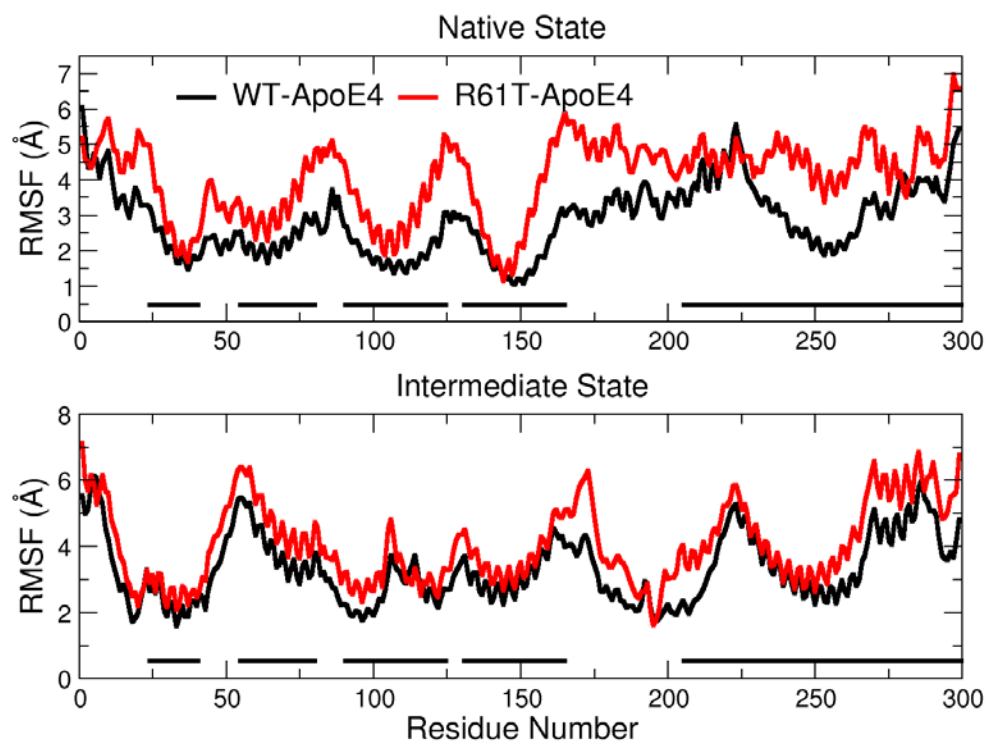
S1 Figure. Representative structures of the native and intermediate state conformations. The N-terminal domain, hinge region and C-terminal domain are shown in cyan, red and magenta cartoon, respectively.



S2 Figure. Time series of the (A) RMSD and (B) potential energy for WT- and R61T-ApoE4 systems from DMD simulations.



S3 Figure. End-to-end distance of the hinge region (d_{hinge}) for R61T-ApoE4 in the intermediate state conformation.



S4 Figure. Root mean square fluctuation (RMSF) for WT- and R61T-ApoE4 systems. Black bars represent the four N-terminal helices (H1-H4) and the C-terminal domain.