

The Molecular Mechanism of Temperature-dependent p53C Phase Separation Accelerated by Oncogenic Mutations: Insights from All-atom and Coarse-grained Molecular Dynamics Simulations

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The authors declare no competing financial interest.

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This material contains eleven supplemental figures.

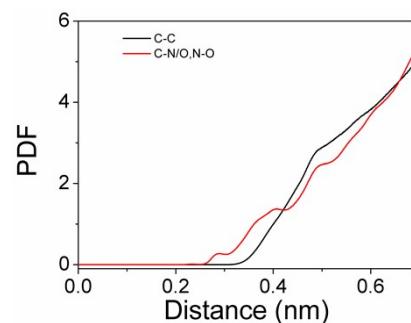


Figure S1, The PDF of distance among heavy atoms.

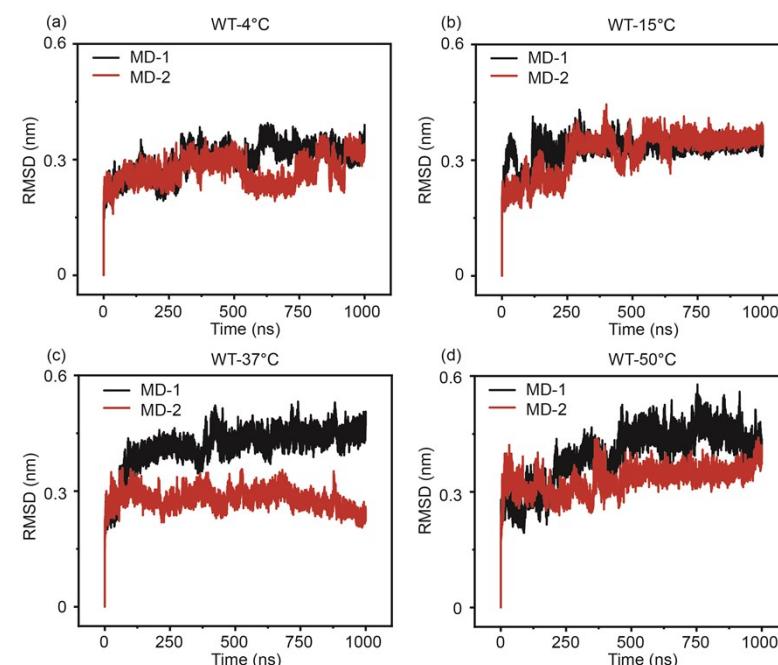


Figure S2. Time evolution of backbone root-mean-square-deviation (RMSD) for WT.

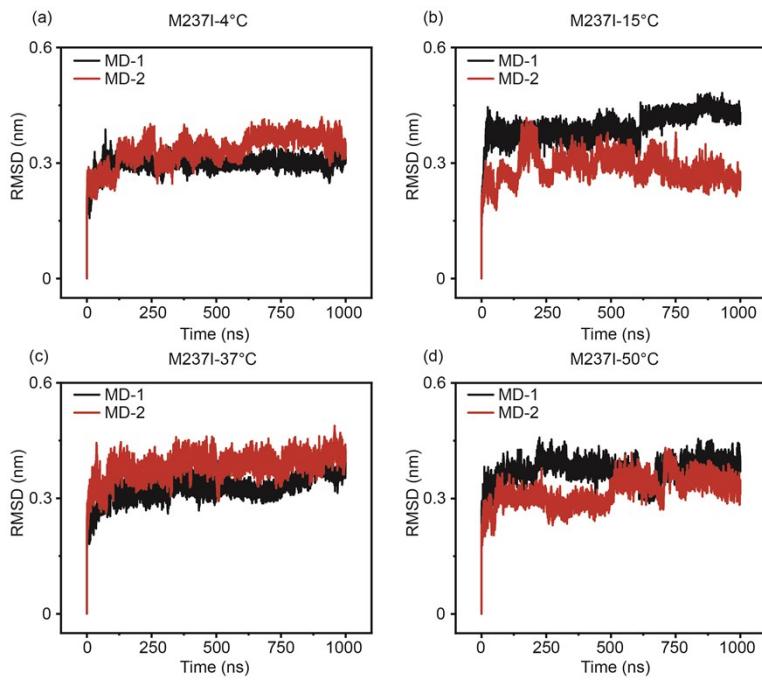


Figure S3. Time evolution of backbone root-mean-square-deviation (RMSD) for M237I.

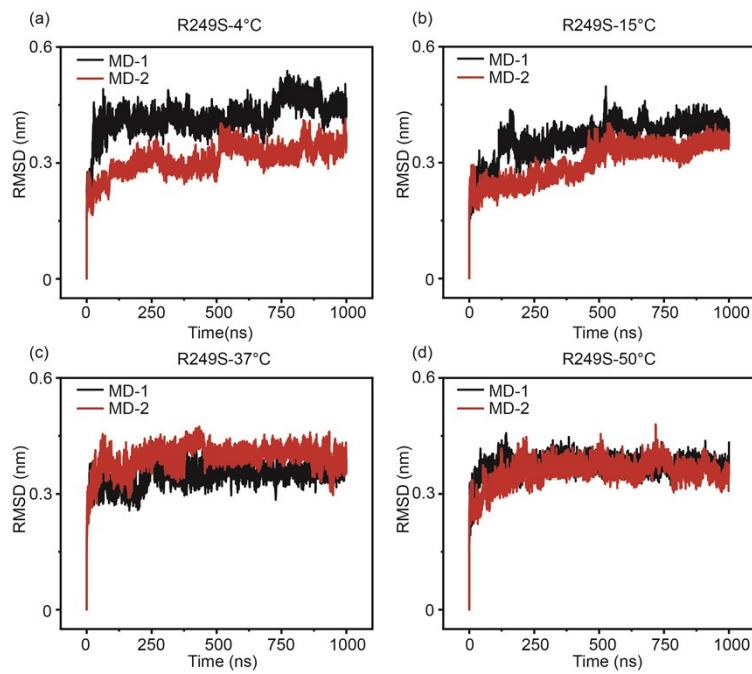


Figure S4. Time evolution of backbone root-mean-square-deviation (RMSD) for R249S.

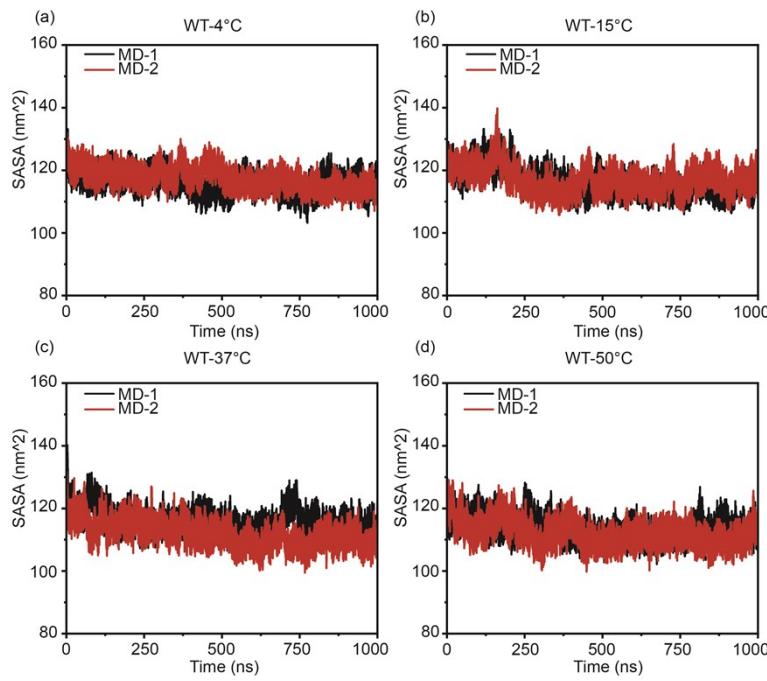


Figure S5. Time evolution of protein solvent-accessible surface area (SASA) for WT.

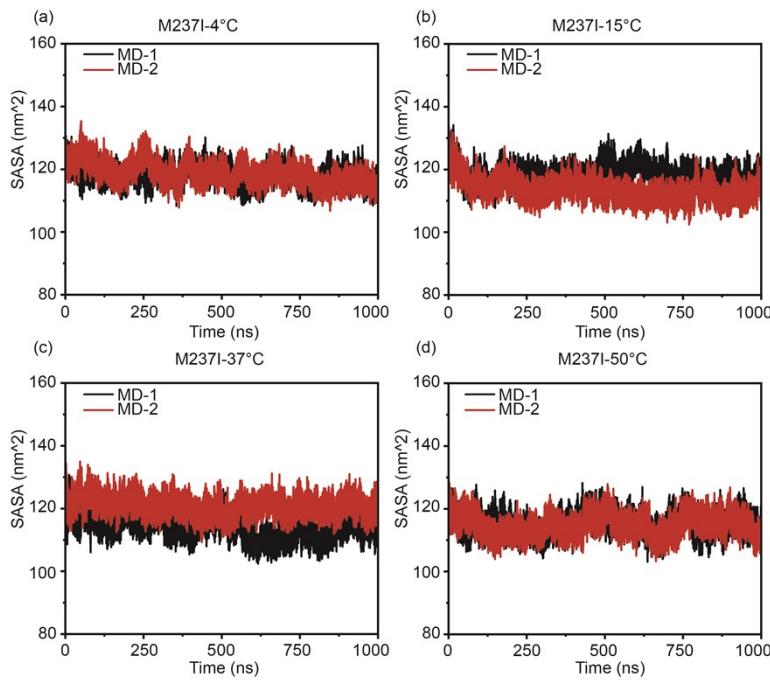


Figure S6. Time evolution of protein solvent-accessible surface area (SASA) for M237I.

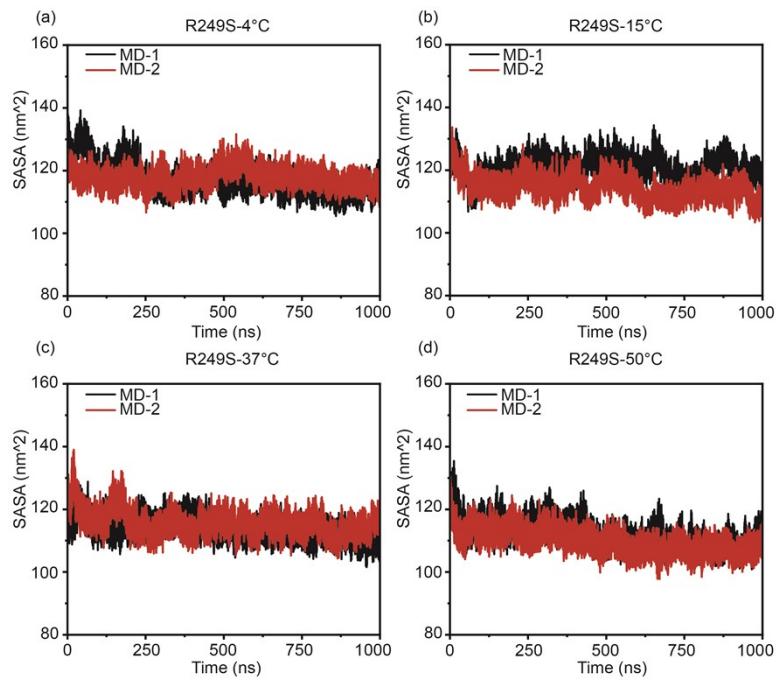


Figure S7. Time evolution of protein solvent-accessible surface area (SASA) for R249S.

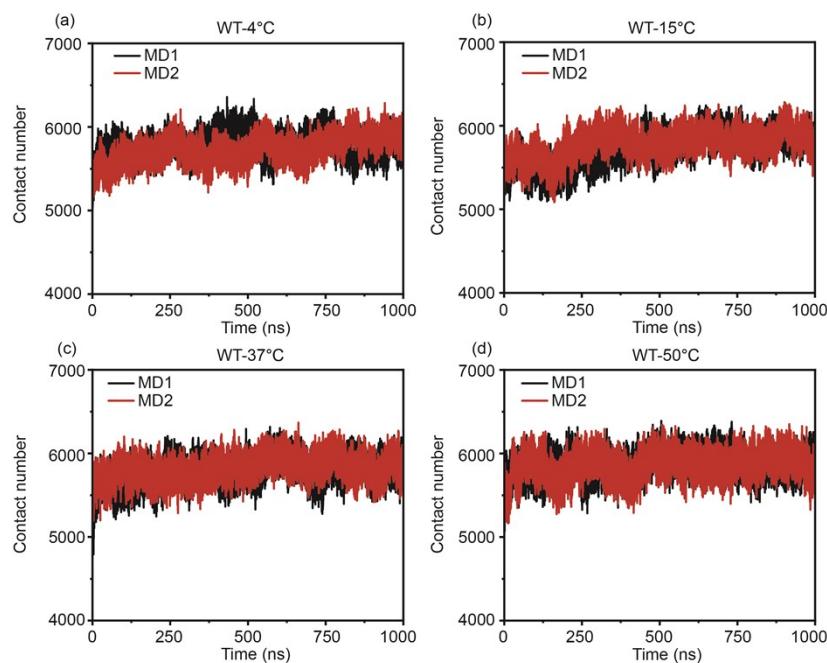


Figure S8. Time evolution of total residue-residue contact number for WT.

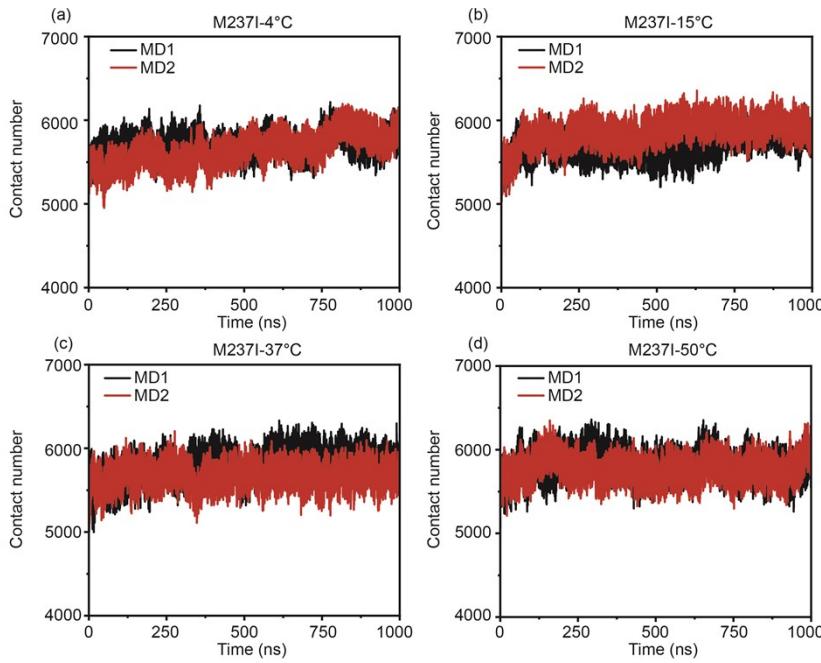


Figure S9. Time evolution of total residue-residue contact number for M237I.

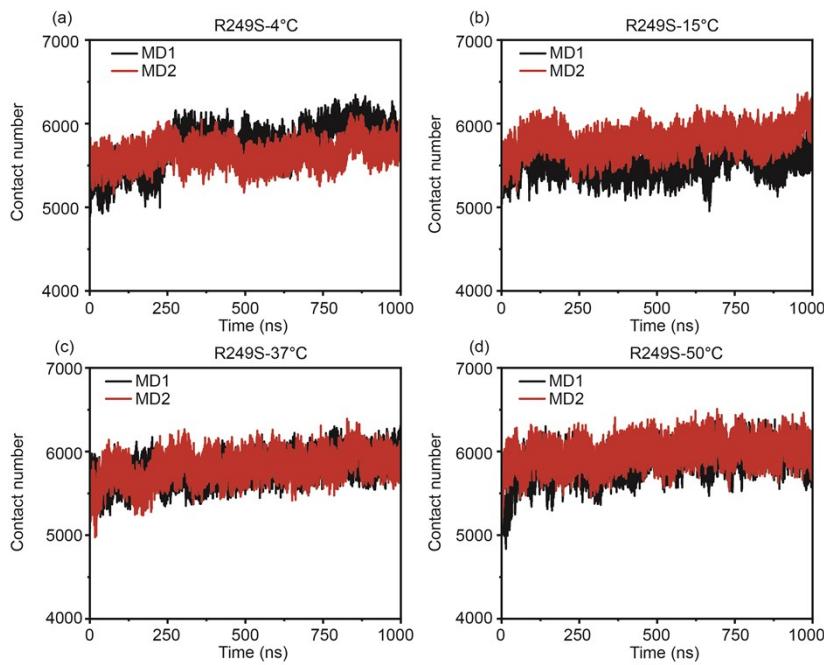


Figure S10. Time evolution of total residue-residue contact number for R249S.

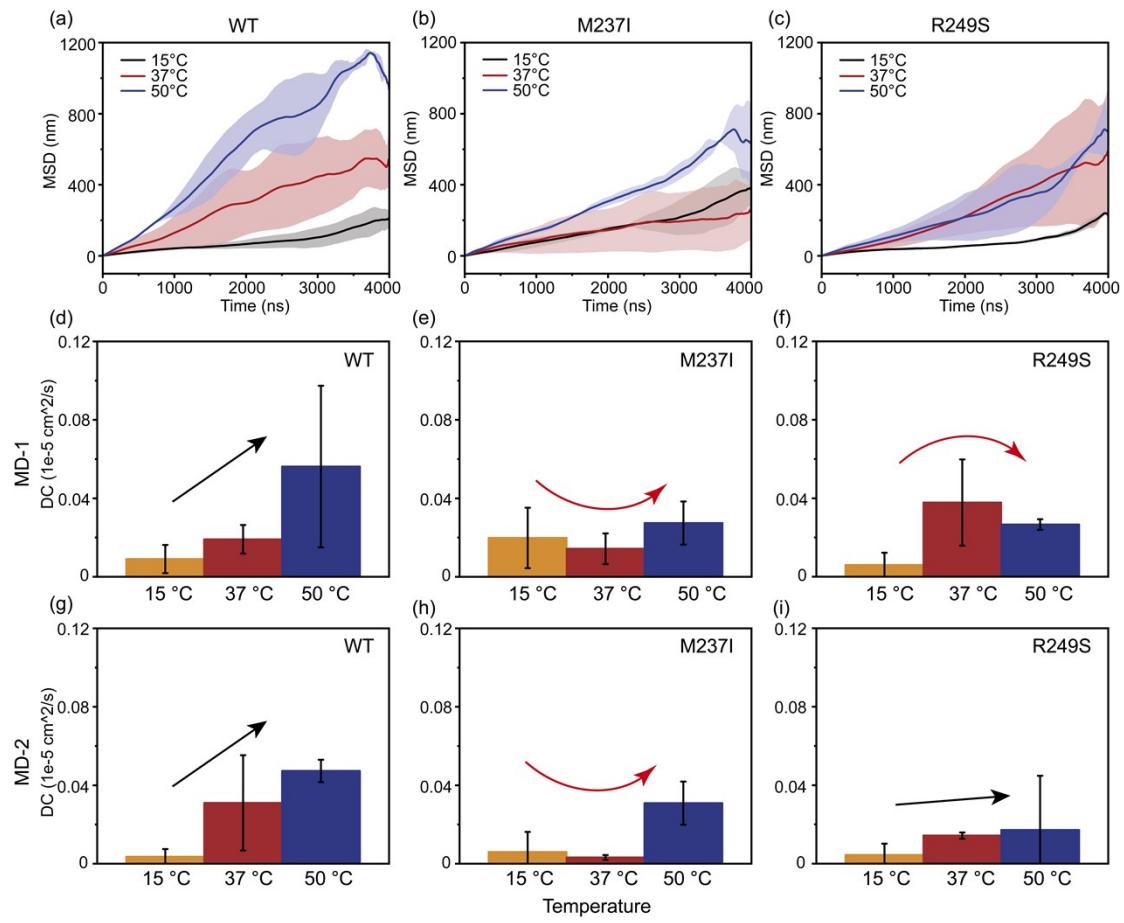


Figure S11. Time evolution of the total mean-square displacement (MSD) of the proteins in the (a) wild-type (WT), (b) M237I, and (c) R249S systems; and the diffusion coefficients (DC) derived from two independent molecular dynamics (MD) groups for the three systems (d–i), as obtained from coarse-grained (CG) simulations.