How does temperature affect the dynamics of SARS-CoV-2 M proteins? Insights from Molecular Dynamics Simulations

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Table S1. Details of systems analyzed in this study using all-atom and coarse-grained molecular dynamics simulations

Serial No.	System	No. of M protein	Temperature (in degree Celcius)	Simulation Time
1	All atom	2	10	500ns
2	All atom	2	20	500ns
3	All atom	2	30	500ns
4	All atom	2	40	500ns
5	All atom	2	50	500ns
6	Coarse Grained	16	10	500ns
7	Coarse Grained	16	20	500ns
8	Coarse Grained	16	30	500ns
9	Coarse Grained	16	40	500ns
10	Coarse Grained	16	50	500ns
11	Coarse Grained	128	30	200ns
12	Coarse Grained	128	40	200ns

Table S2. Total number of atoms in all-atom and coarse-grained systems

Serial No.	System	No. of M Proteins	No. of DPPC lipids	No. of DPPG lipids	No. of solvent (water)
1	All atom	2	210	90	29273
2	Coarse Grained	16	3423	1467	112172
3	Coarse Grained	128	14791	6339	493141

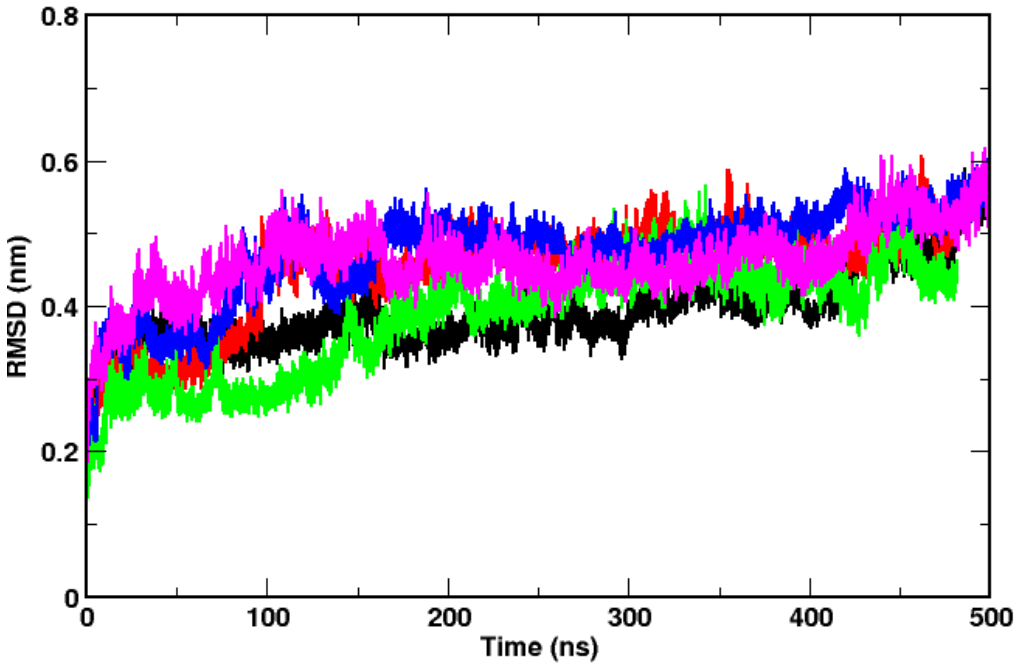

Figure S1. RMSD of the full M protein dimer in atomistic simulations at 10˚C (black), 20 ˚C (red), 30 ˚C (green), 40 ˚C (blue) and 50 ˚C (magenta) over the full simulation trajectory (500 ns).

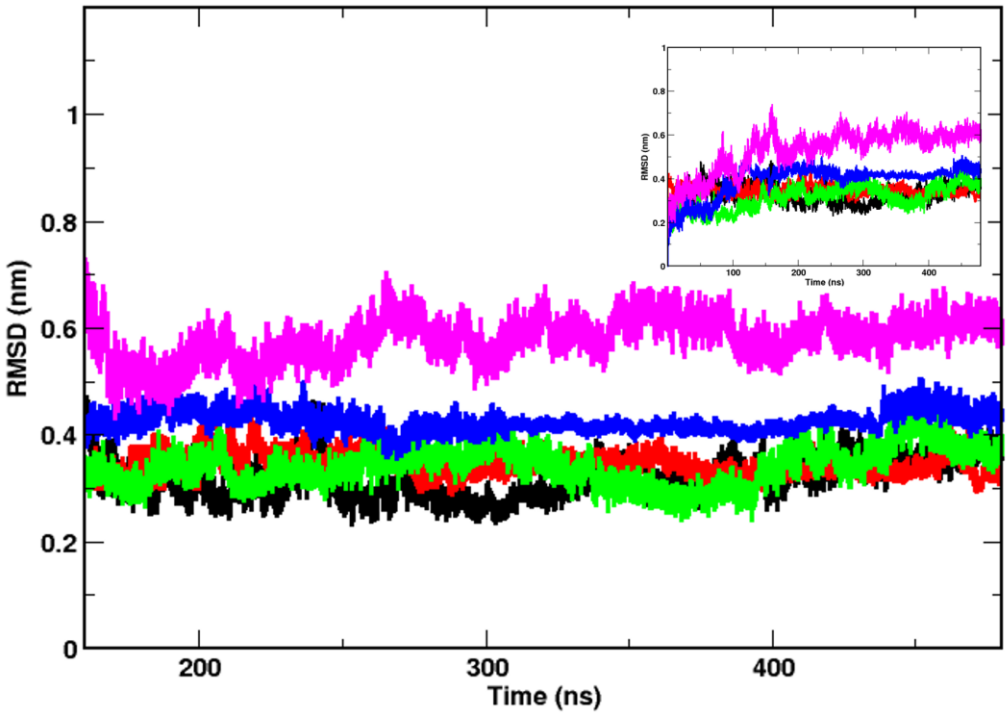

Figure S2. RMSD of the M protein dimer in atomistic simulations, using only the CA atoms and excluding 10 residues at each terminal, at 10˚C (black), 20 ˚C (red), 30 ˚C (green), 40 ˚C (blue) and 50 ˚C (magenta) from 160ns to 500ns indicating equilibration. Inset shows the RMSD over the full trajectory of length 500ns, where the initial increase indicates relxation of the system.

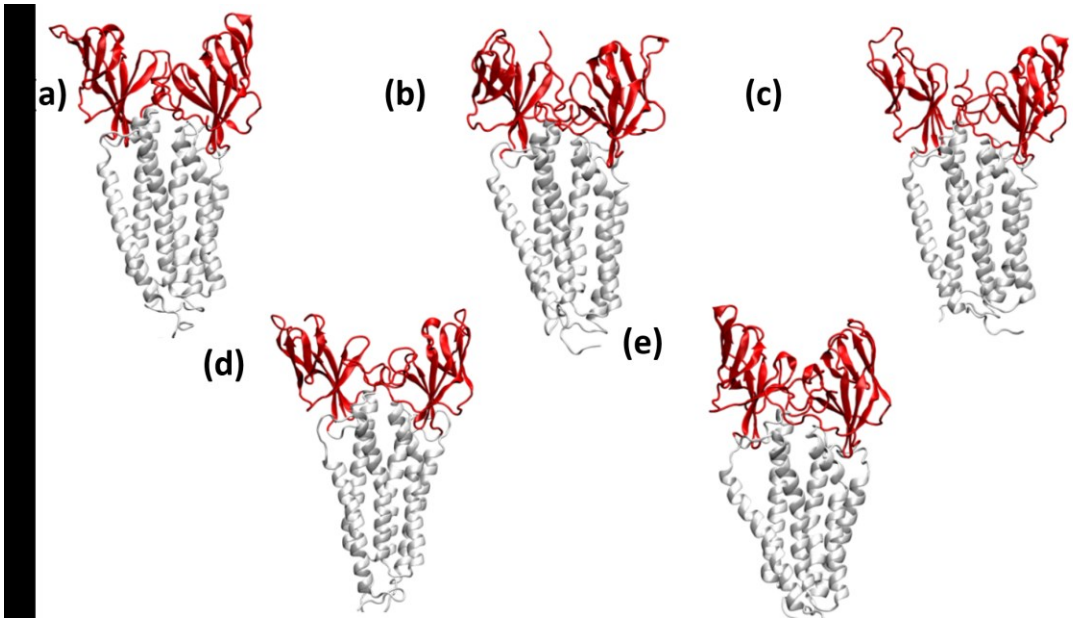

Figure S3. Lowest energy conformers obtained from the PCA distribution (Figure 4 in the manuscript). The extrinsic domains are highlighted in red to indicate the differences at (a)10, (b) 20, (c) 30, (d) 40 and (e) 50℃. The flaps of the extrinsic domain can be seen to be more open at 30 and 40℃, while relatively confined at 10 and 20℃ and very close to each other at 50℃.

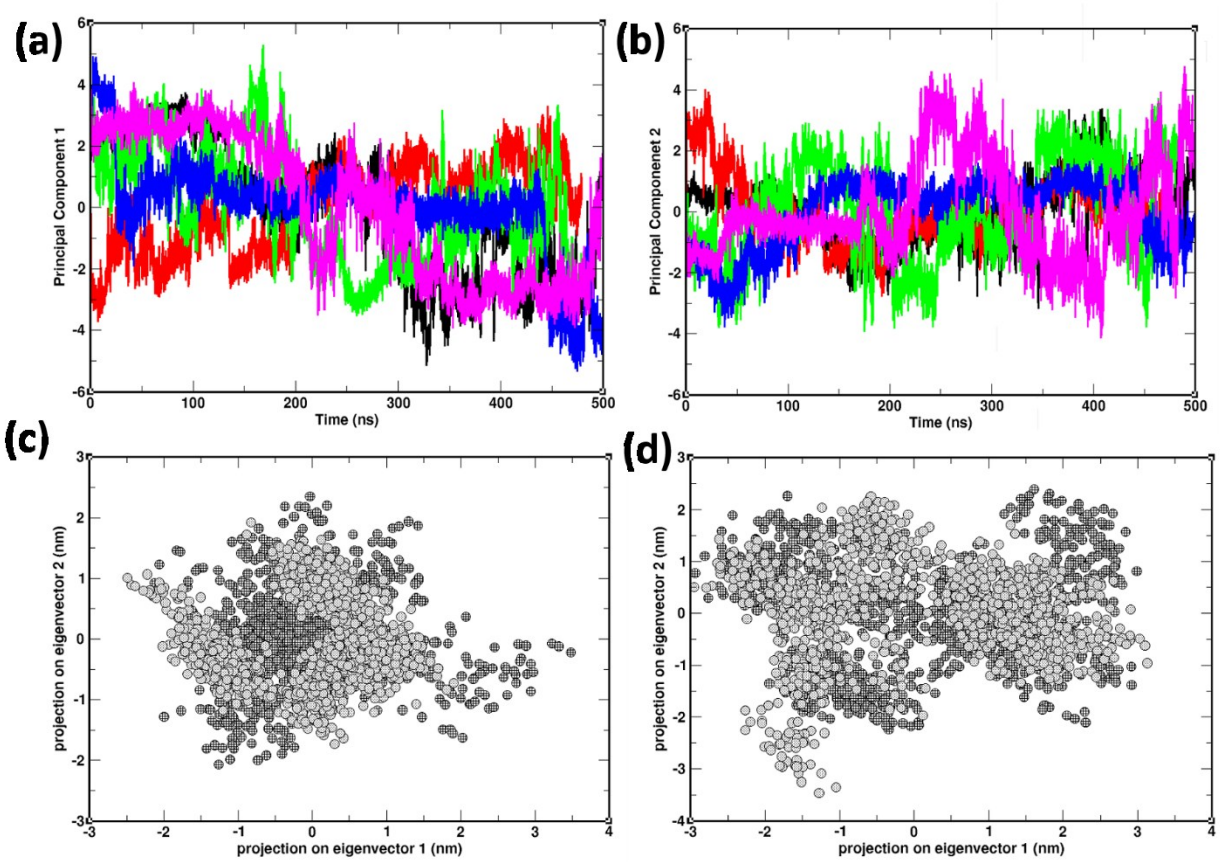

Figure S4. Time evolution of the (a) first and (b) second principal component at 10 ˚C (in black), 20 ˚C (in red), 30 ˚C (in green), 40 ˚C(in blue) and 50 ˚C (in magenta). The PCs were very stable at 40 ˚C. PCA distribution along the first and second eigenvectors taken at different time intervals during the last 50ns of the simulation to showing similarity of dynamics and energies for (c) 10˚C and (d) 50˚C. The average delta G was 7.55±0.86 kcal/mol and 6.69±0.34 kcal/mol respectively.

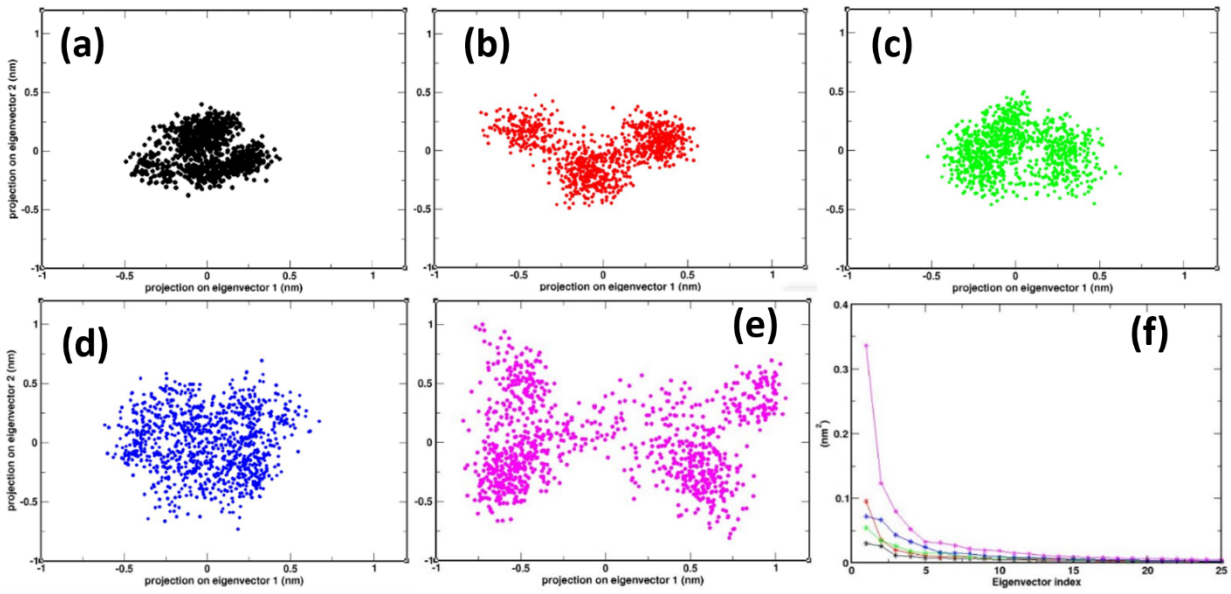

Figure S5. PCA distribution of the intrinsic domain of the M-protein along the first and second eigenvectors at 10 (black), 20 (red), 30 (green), 40 (blue) and 50 (magenta) ℃ (a-e) indicating how temperature directly impacts the dynamics of the intrinsic domain. (f) Eigenvalues corresponding to the eigenvectors show that the first few eigenvectors are sufficient to capture the dynamics of the systems. The average PCA calculated during the last 50ns window for Figure S5 were done considering two separate 10ns windows with 1000 frames.

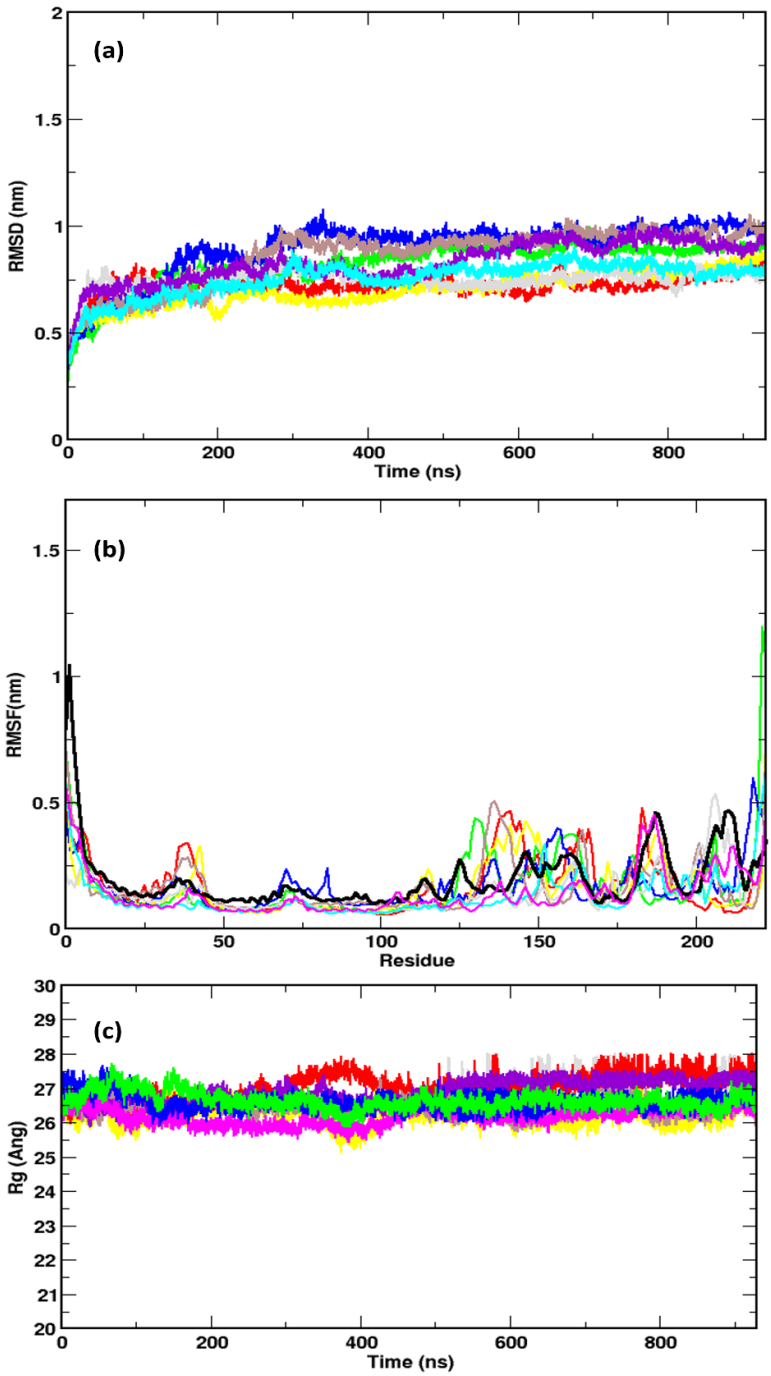

Figure S6. (a) RMSD of individual M protein dimers at 30 ˚C in CG 128-mer system (b) Comparative RMSF of M protein monomers at 30 ˚C in CG (in different colors) with atomistic simulation of M protein at 30 ˚C (in black). (c) Radius of gyration of individual M protein dimers in CG simulations. For clarity, data for only 8 M protein has been shown.