Supporting Information for Publication

Modeling and Experiment Reveal Structure and Nanomechanics across the Inverse Temperature Transition in *B. mori* Silk-Elastin-like Protein Polymers

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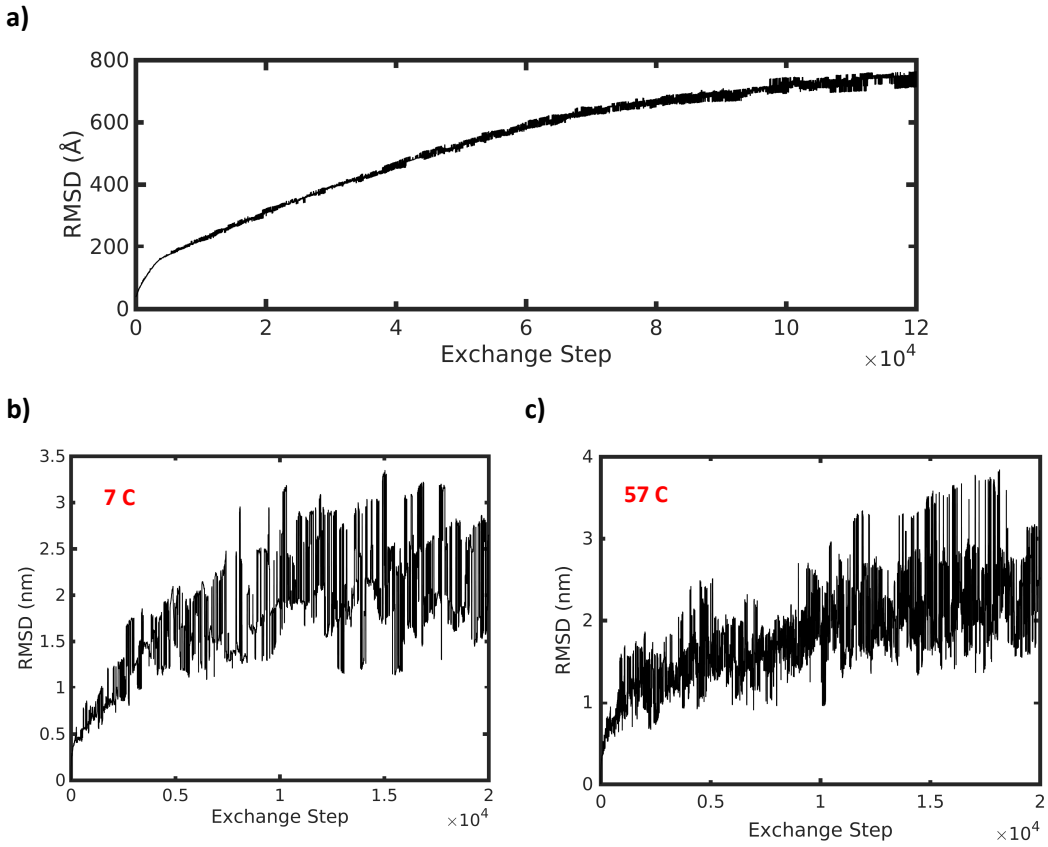
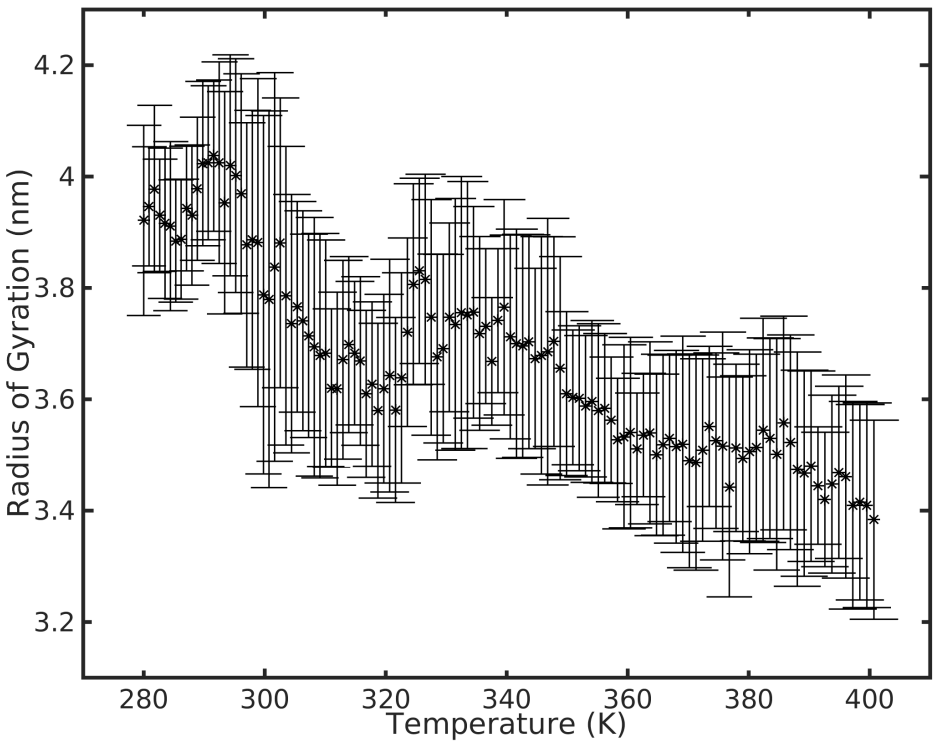
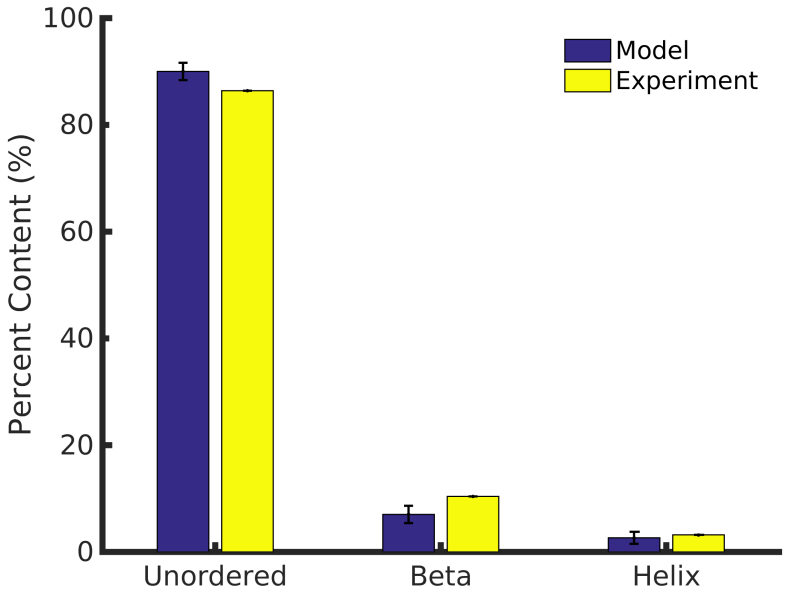


SI Figure 1 | a) Root mean square deviation (RMSD) for implicit solvent Replica Exchange simulation. Replica at 27°C. b) RMSD for explicit solvent Replica Exchange simulation. Replica at 7°C. c) RMSD for explicit solvent Replica Exchange simulation. Replica at 57°C.

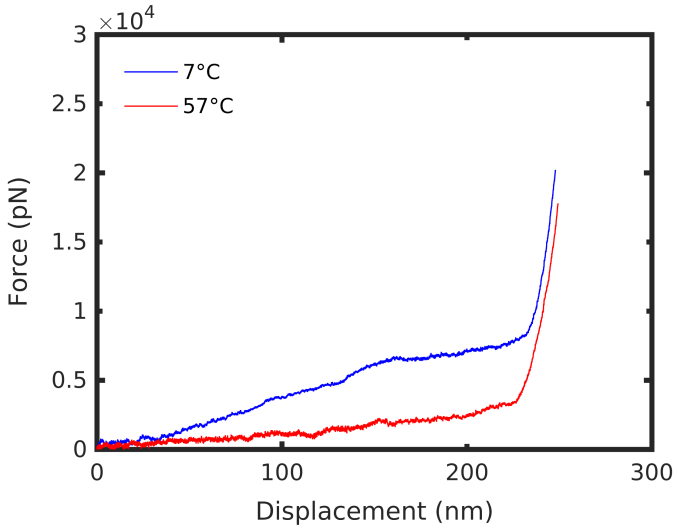


SI Figure 2 | Radius of gyration change with temperature shows a gradual structural transition.

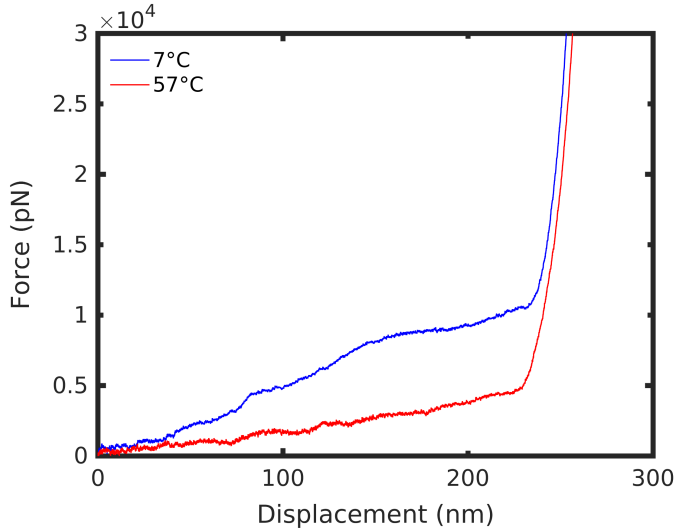


SI Figure 3 | Secondary structure comparison between simulation (derived via the DSSP algorithm) and experiment (CD Spectra) at 7°C. Ordered structure includes beta structure and helices. Unordered structure includes bends, turns and coils.

a)


×10^4
3
2.5
2
1.5
1
0.5
0
7°C
57°C
Force (pN)
0
100
200
300
Displacement (nm)

b)


×10^4
3
2.5
2
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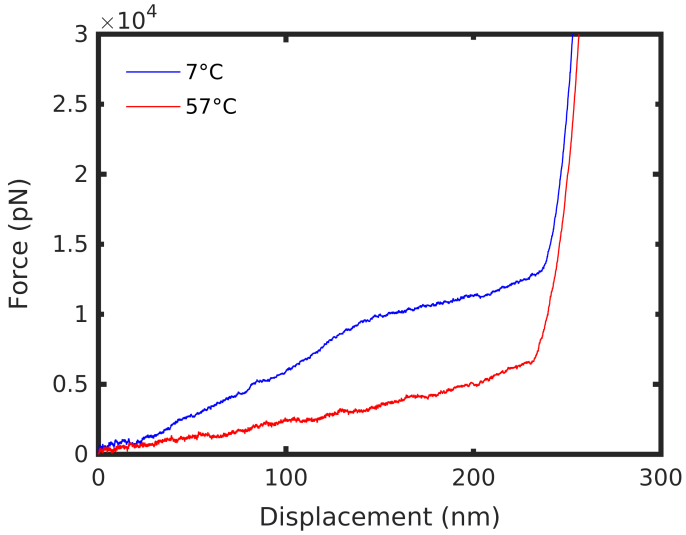
0.5
0
7°C
57°C
Force (pN)
0
100
200
300
Displacement (nm)

c)


×10^4
3
2.5
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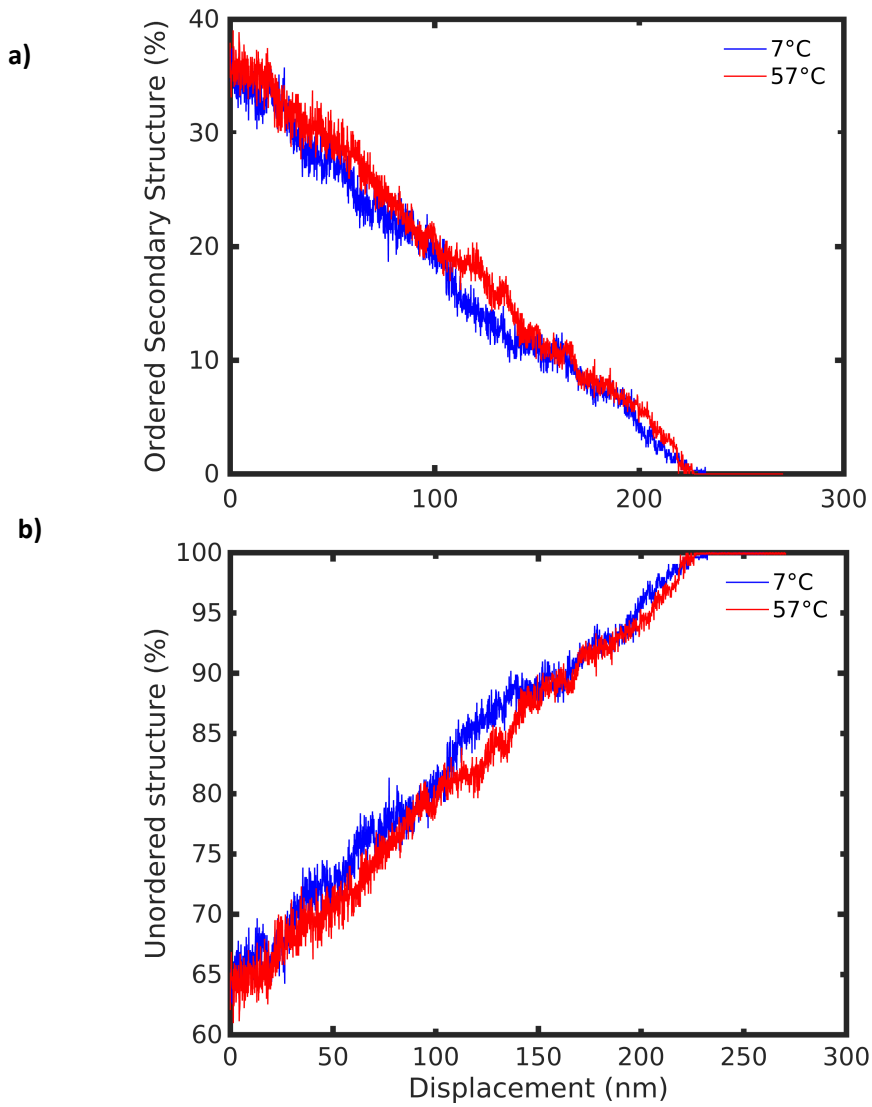
0.5
0
7°C
57°C
Force (pN)
0
100
200
300
Displacement (nm)

SI Figure 4 | Force-displacement curves at 7°C and 57°C for pulling speed a) 20 m/s b) 30 m/s and c) 40 m/s.



SI Figure 5 | Evolution of secondary structure at 7°C and 57°C during SMD pulling. Ordered structure includes beta structure and helices. Unordered structure includes bends, turns and coils.