

Abstract Submitted
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Computational assessment of the stiffness of the Gram-negative bacterial cell wall SANDHYA SINHA, YAO ZHAO, K.C. HUANG — The bacterial cytoplasm exists in a state of constant metabolic activity, leading to a turgor pressure across the membrane that measures an atmosphere or more. For most bacteria, the peptidoglycan cell wall bears this stress and is also a primary determinant of the cell's shape. In this work, we investigate how the elastic properties of Gram-negative cell walls emerge from the molecular organization of the peptidoglycan network by studying the structure of a mechanical model of the cell wall under the computational application of several types of strain. Experimental evidence has suggested that the Young's modulus of the cell wall increases nonlinearly with the turgor pressure. We have conducted simulations to determine what intrinsic physical characteristics of the molecular components of the cell wall, including bending, tension, and anisotropy, are necessary and sufficient for recapitulating the nonlinear rise in stiffness. Furthermore, we have modeled the effect of missing springs on the elastic response of the cell-wall network to bridge the gap between molecular organization and a continuum model of cell-wall elasticity.

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