

AqpM 2F2B AqpZ:1RC2 A chain , b-Aqp1:1J4N , h-Aqp4 3GD8 ,GlpF:1LDI

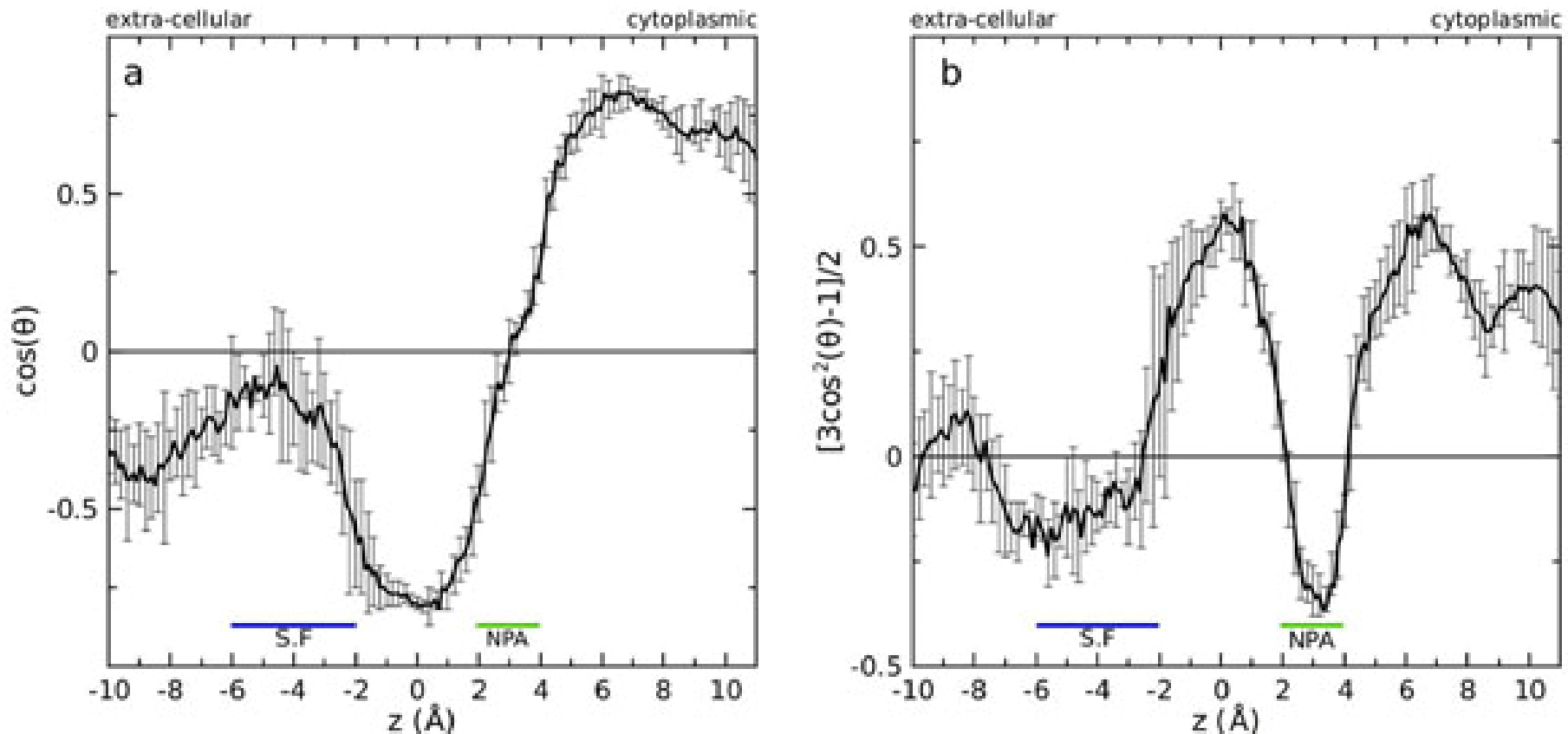


Figure 6 Water orientation inside the constriction region of the AqpM channel. (a) Order parameter $p_1(z) = \langle \cos(\theta)_z \rangle$. (b) Order parameter $p_2(z) = 0.5 \langle 3\cos^2(\theta)_z - 1 \rangle$. θ is the angle between the unit vector, approximately aligned along the **channel axis/membrane normal**, \mathbf{n}_z , and the **Water dipole vector**. Both parameters were measured for each **AqpM monomer** from 10000 snapshots separated by 2 ps taken from the 20 ns simulation. The **black** continuous line in each panel represents the average over the 10,000 snapshots and over the four monomers. The error bars represent the standard deviation from the average.