

Supplementary information for:

Electric-field Driven Translocation of ssDNA Through Hydrophobic Nanopores.

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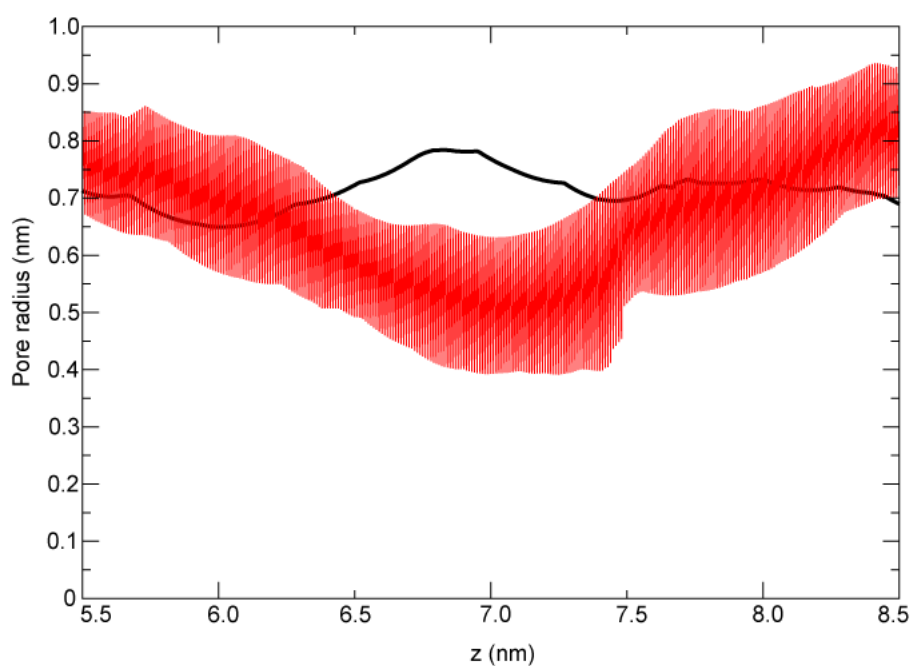


Figure S1: pore radius profile during a simulation of 20 ns duration, under an applied electric field of 0.2 Vnm^{-1} in the absence of DNA (red) and the pore radius of a single snapshot of the reference pore, in which the constriction region residues are replaced by glycine residues (black).

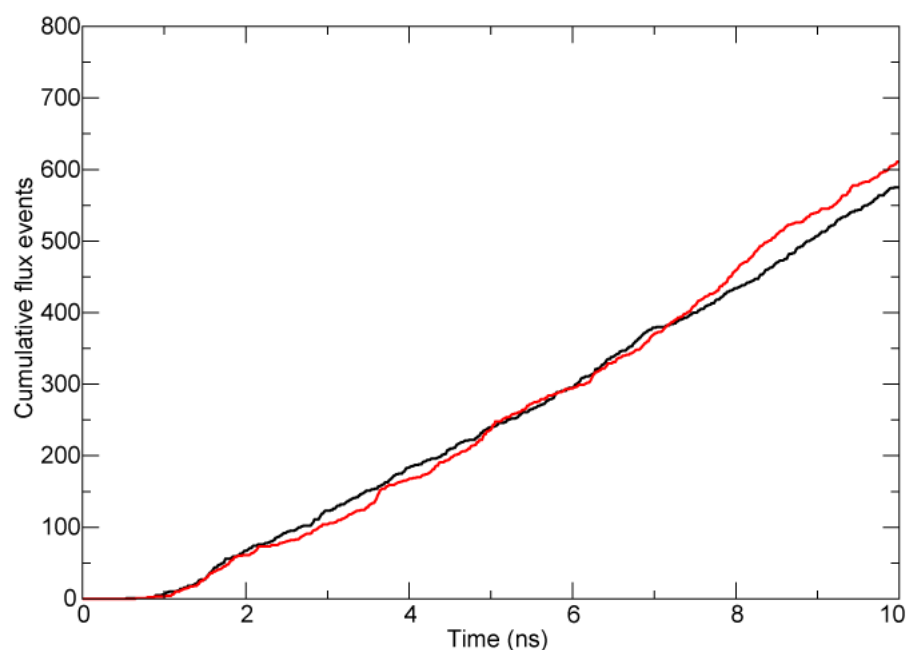


Figure S2: Cumulative water flux for the original (black) and TYR-mutant (red) hourglass pores under a 0.2 Vnm^{-1} electric field and in the absence of DNA. Flux events were counted by defining rings of residues at the pore entrance and exit, and only once a water molecule had passed through both rings was it counted.

Table S1 Table 1 A summary of the DNA translocation behavior as a function of its starting position relative to the entrance of the pore. The values in parenthesis correspond to simulations with a field strength of 0.1 Vnm^{-1} , with all others at 0.2 Vnm^{-1} .

Initial DNA location		Final DNA location (number of simulations)		
		DNA at entrance	DNA at constriction	Translocation through pore
Hour glass pores TRP	Threaded through pore constriction	0	(3)	3
	At pore entrance	5 (2)	3 (1)	3
Hour glass pore TYR	Threaded through pore constriction	0	0	6
	At pore entrance	3	3	4
Reference pores	Threaded through pore entrance	(3)	N/A	6
	At pore entrance	-	N/A	-

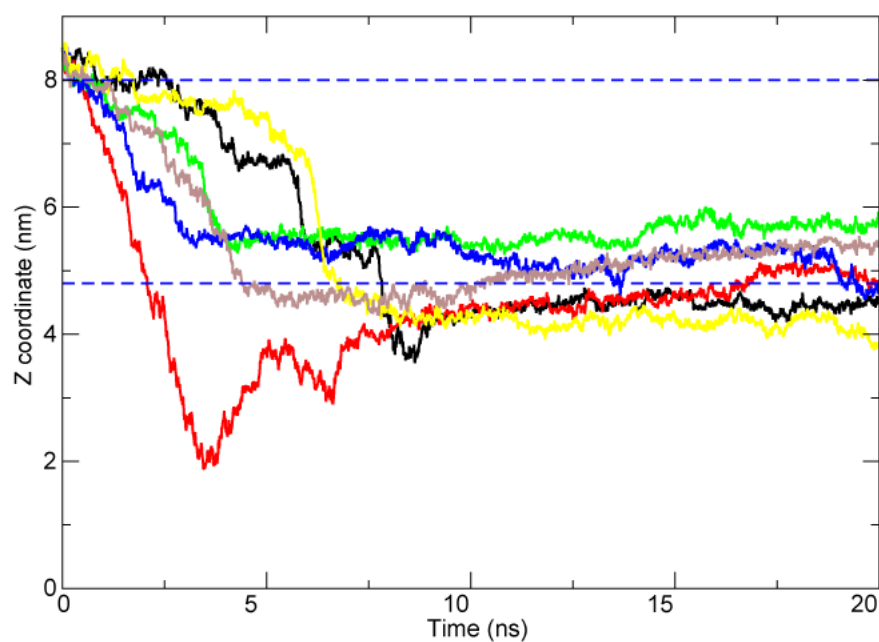


Figure S3: The z-coordinate of the leading nucleotide as a function of time for all simulations of ssDNA translocation through the GAGGGAG pore. The z coordinates of the pore entrance (top) and exit (bottom) are marked with dashed blue lines. Translocation was observed in under 10 ns in all cases, with any interruptions corresponding to a new nucleotide coming into contact with the pore entrance.

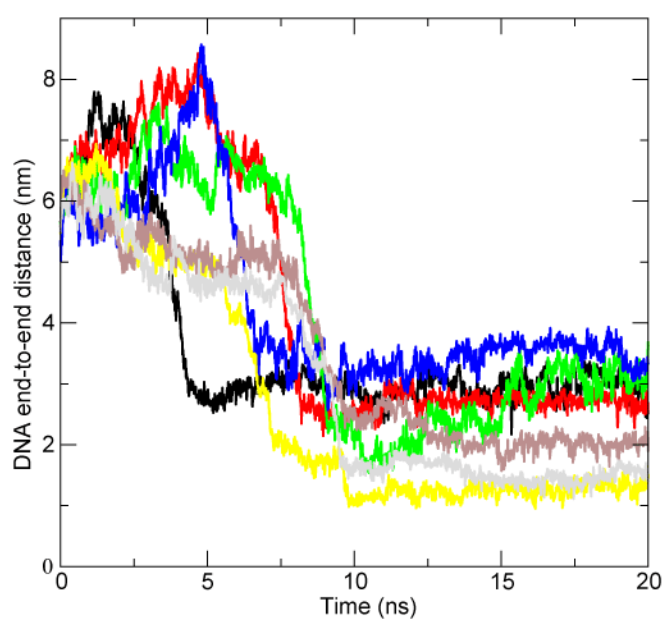


Figure S4: DNA end-to-end distances as a function of time for all simulations in which DNA was initially placed at the pore entrance and in which full translocation was observed. In all cases, the initial (mostly linear) conformation was either maintained or extended during translocation. Rapid folding/coiling was observed immediately following translocation in all cases.

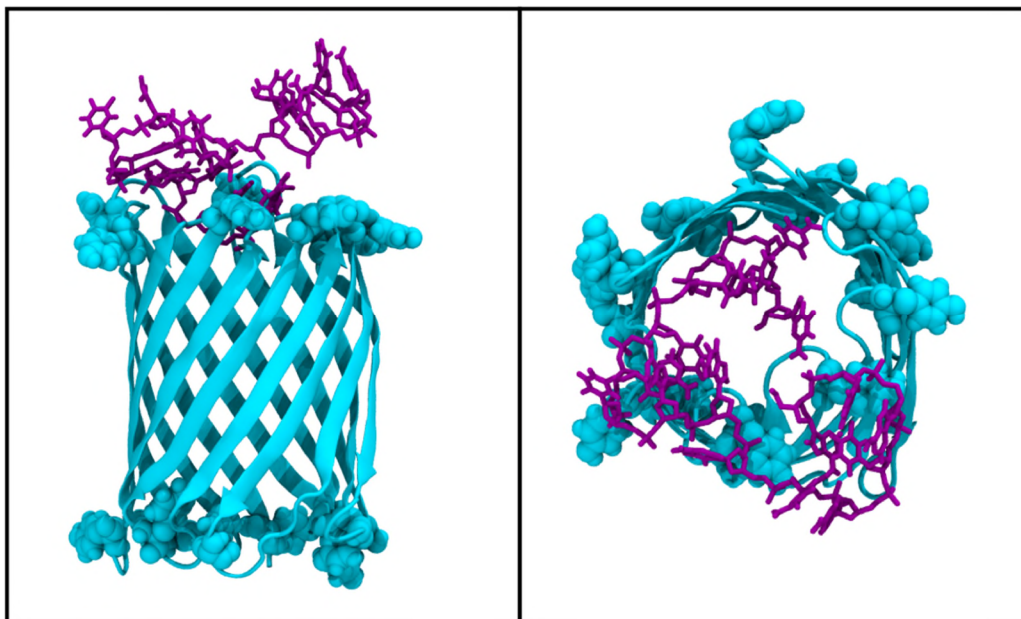


Figure S5: In the absence of an electric field, ssDNA was observed to coil around the entrance to the pore, interacting with at the aromatic residues at the pore mouth. The DNA did not translocate through the pore when we did not apply an external electric field.