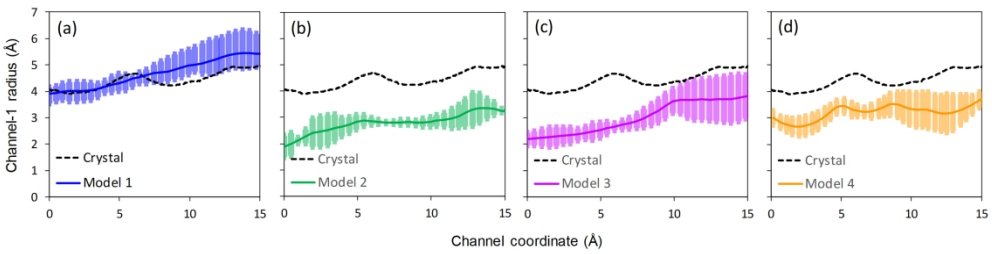
Figure S1. *Pore radius profiles of channel-1 (from the cleft entrance to proximal binding pocket) for monomer II of AcrB at the end of the simulations. (a) Model system 1; (b) Model system 2; (c) Model system 3; and (d) Model system 4. The black dashed lines represent the pore radius profile*

at the initial stage from the original crystal structure (PDB ID: 2DHH). The statistical error bars are calculated based on 100 frames of the last 100 ns simulations and three independent realizations. The channel 1 coordinate is defined from the cleft to S134.

Figure S2. *Pore radius profiles of channel-2 (from the distal binding pocket to the exit gate) for monomer II of AcrB at the end of the simulations. (a) Model system 1; (b) Model system 2; (c) Model system 3; and (d) Model system 4. The black dashed lines represent the pore radius profile at the initial stage from the original crystal structure (PDB ID: 2DHH). The statistical error bars are calculated based on 100 frames of the last 100 ns simulations and three independent realizations. The channel 2 coordinate is defined from S134 to the exit gate.*



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734x190mm (125 x 125 DPI)

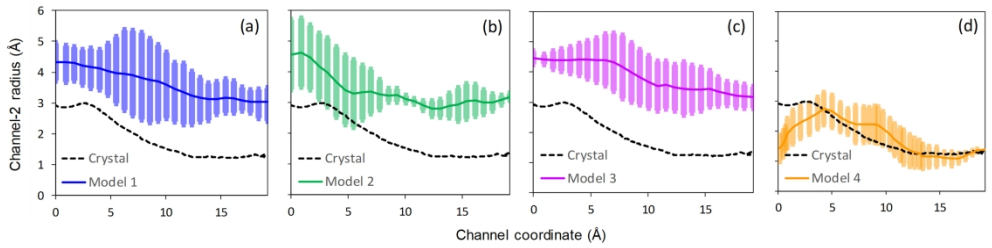

Figure S2. Pore radius profiles of channel-2 (from the distal binding pocket to the exit gate) for monomer II of AcrB at the end of the simulations. (a) Model system 1; (b) Model system 2; (c) Model system 3; and (d) Model system 4. The black dashed lines represent the pore radius profile at the initial stage from the original crystal structure (PDB ID: 2DHH). The statistical error bars are calculated based on 100 frames of the last 100 ns simulations and three independent realizations. The channel 2 coordinate is defined from S134 to the exit gate.

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