SELF-ASSEMBLY OF A SIMPLE MEMBRANE PROTEIN: COARSE-GRAINED MOLECULAR DYNAMICS SIMULATIONS OF THE INFLUENZA M2 CHANNEL

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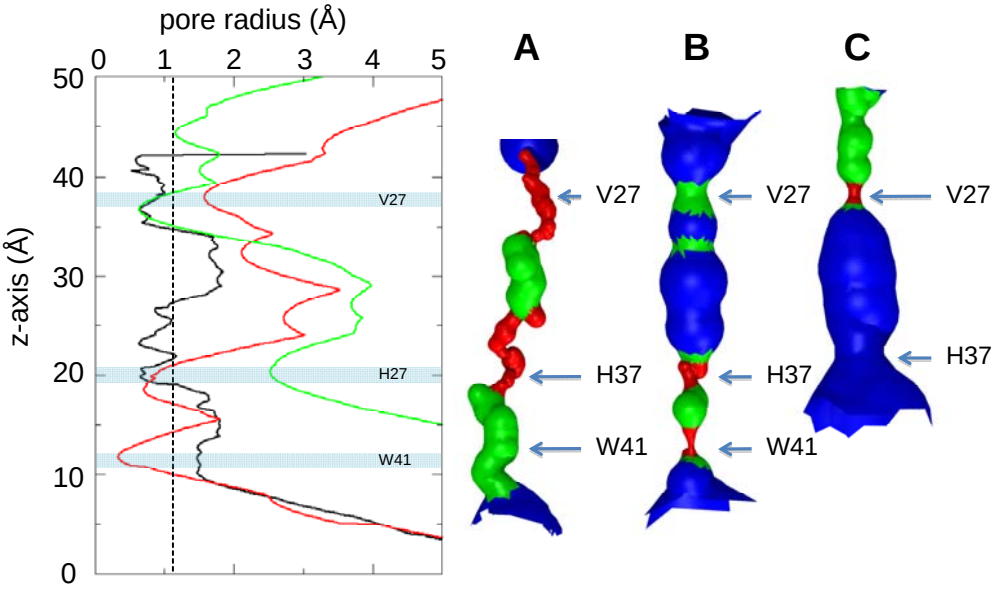
Supplementary Information

Comparison of Pore Radius profiles

The 2D and 3D pore profiles of the three structures (**A** our atomistic model, **B** the NMR structure (1), and **C** the X-ray structure (2)) have been calculated using HOLE (3). The solid black line represents the pore radius profile of our model, the red line represents the radius profile of the NMR structure, and the green line represents the pore radius of the X-ray structure. The dashed black line is the radius of a water molecule. The positions of the key residues involved in gating the pore (i.e. V27, H37, and W41) are indicated. The 'closed' conformation of the channel (represented by the NMR structure) has a constriction at the H37 (and W41) region that is narrow enough to prevent the passage of water molecules. There is also a narrow region in the vicinity of V27, although the pore is still wide enough to allow water through. The 'open' conformation (X-ray structure), despite having a slight narrowing at H37, will still allow water through this region. There is, however, a constriction at V27 that will block water. Our M2 model appears to be closed to a greater extent than the NMR structure, with constrictions at both the C-terminal H37 region (although not at W41) and the N-terminal region. The internal cavity between these two constrictions also appears to be smaller in size. This may be because the CG water particles (representing four water molecules) are not unable to enter the cavity during the tetramer formation. Additional waters are seen to enter the pore during the course of the atomistic simulation, so it is possible that over a longer timescale simulation more water molecules would enter the pore and expand the central cavity.



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