Supporting Information for Influenza A M2 Inhibitor Binding Understood through Mechanisms of Excess Proton Stabilization and Channel Dynamics

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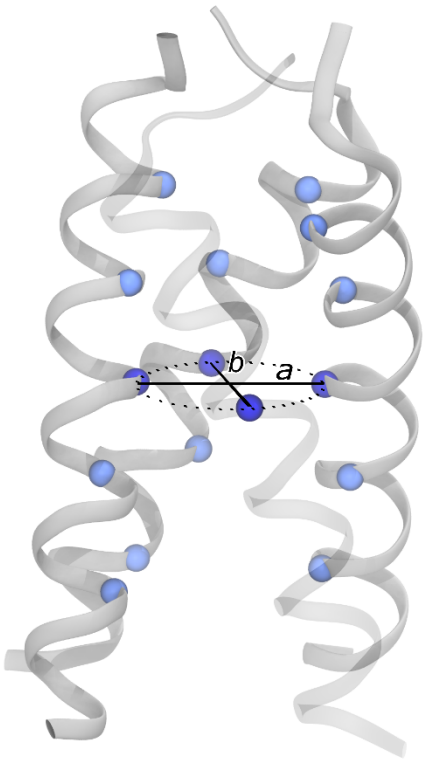

SI Figure 1. A schematic of eccentricity calculations, with pore-lining alpha-carbons shown as blue spheres. Dark blue spheres are Gly34 alpha-carbons. The major and minor axes of the oval are defined by the distances between alpha-carbons on opposing helices, indicated as lines *a* and *b*.

SI Table 1. Eccentricity values of the pore at each of the pore-lining residues, calculated using alpha-carbon positions as described in the text. Eccentricity was calculated for proton positions in the top [1]half of the channel, CEC_z = [-18.0,-1.0] Å.

Residue	Average ***e*** over all CEC_z	Max value of ***e*** and position	Min value of ***e*** and position	Difference between max and min values	RMSD
Val27	0.34	0.43 CEC_z = -4.0 Å	0.27 CEC_z = -17.5 Å	0.16	0.13
Ser31	0.29	0.41 CEC_z = -10.0 Å	0.25 CEC_z = -2.5 Å	0.16	0.13
Gly34	0.38	0.57 CEC_z = -16.5 Å	0.28 CEC_z = -6.0 Å	0.29	0.17
His37	0.42	0.65 CEC_z = -16.5 Å	0.30 CEC_z = -9.0 Å	0.35	0.18
Trp41	0.40	0.60 CEC_z = -16.0 Å	0.27 CEC_z = -4.0 Å	0.33	0.17

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