Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information
Adsorption of Lysozyme Into a Charged Confining Pore

Daniel L. Z. Caetano,[ab] Ralf Metzler,[c] Andrey G. Cherstvy,[cd] and Sidney J. de Carvalho[e]

[a] *Institute of Chemistry, State University of Campinas (UNICAMP), Campinas, Brazil.*

[b] *Center for Computational Engineering and Sciences, State University of Campinas (UNICAMP), Campinas, Brazil.*

[c] *Institute for Physics & Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany.*

[d] *Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany.*

[e] *Department of Physics, São Paulo State University (UNESP) Institute of Biosciences, Humanities and Exact Sciences São José do Rio Preto, Brazil. E-mail: sidney.carvalho@unesp.br*

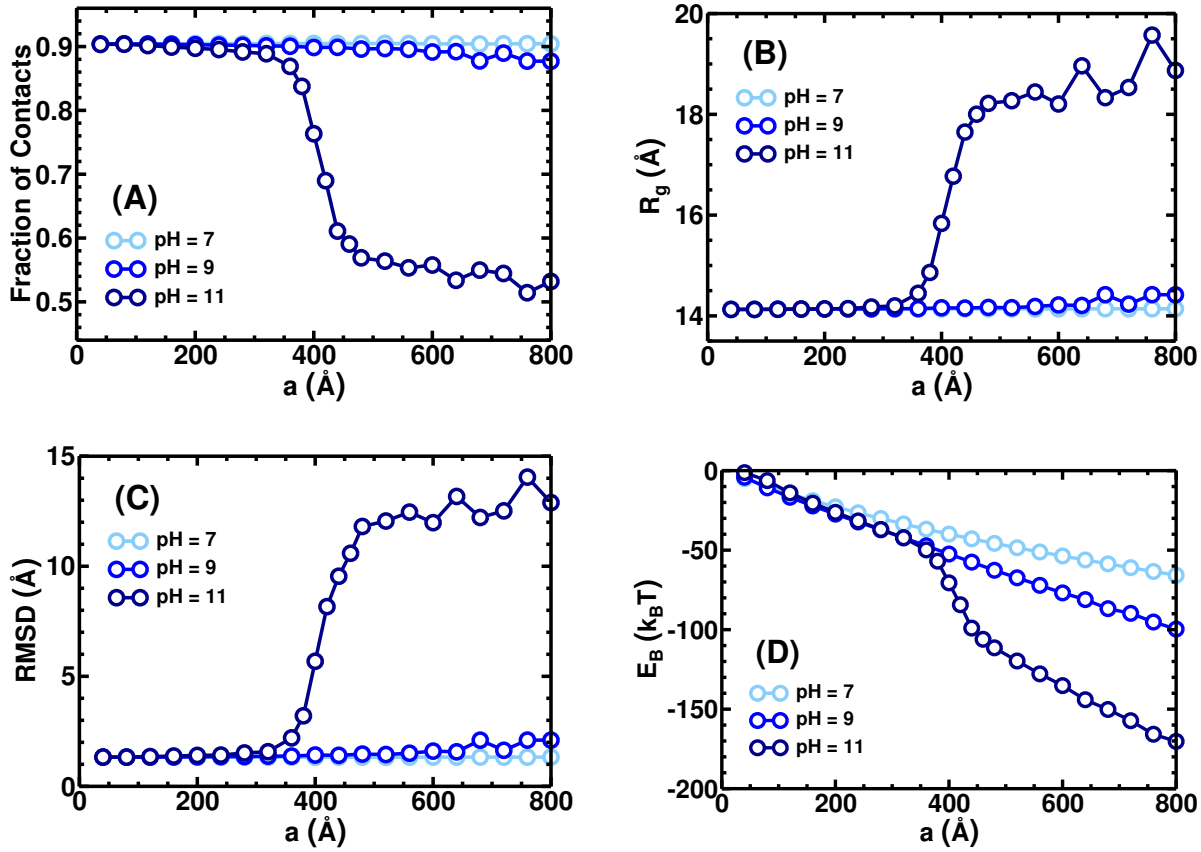

Figure S1: (A) Fraction of native contacts, (B) Mean radius of gyration, R_g, (C) Root-mean-square deviation, RMSD, and (D) Mean binding energy, E_B, of a single HEWL protein into a negatively charged pore as a function of the pore radius a for pH = 7 (light blue circles), pH = 9 (blue circles), and pH = 11 (dark blue circles). The salt concentration is 0.001 M. RMSD was calculated using the trajectories generated by the Monte Carlo simulations and the Python program overlap.py[1].

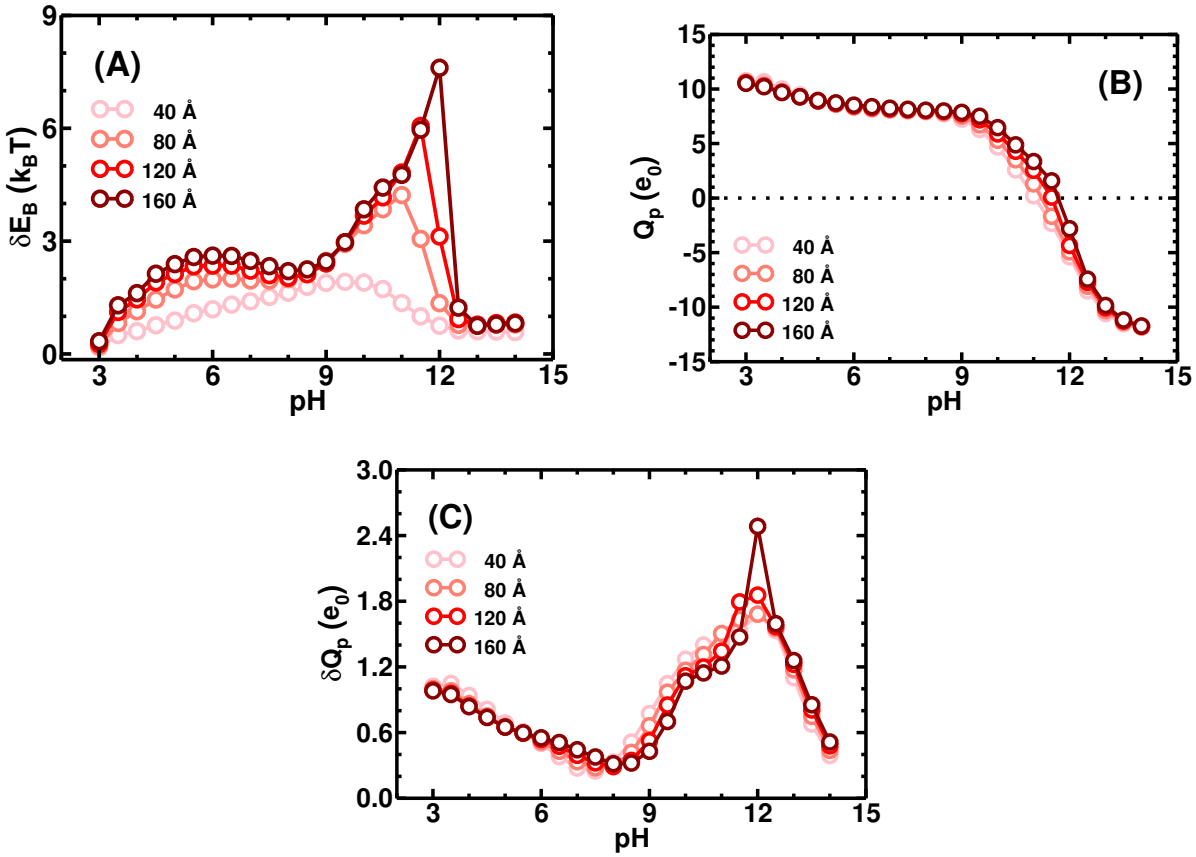

Figure S2: (A) Fluctuations of binding energy, δE_B, (B) Net charge, Q_p (in units of elementary charge e_0), and (C) Fluctuations of net charge, δQ_p, of a single HEWL protein into a negatively charged pore as a function of pH for pore radius $a = 40$ Å (pink circles), 80 Å (light red circles), 120 Å (red circles) and 160 Å (dark red circles). The salt concentration is 0.001 M.

Table S1: Hill coefficient n for all HEWL's basic residues at low salt concentration (0.001 M).

Residue	n				
	Free	$a = 160$ Å	$a = 120$ Å	$a = 80$ Å	$a = 40$ Å
LYS1	0.68 ± 0.01	2.2 ± 0.1	1.8 ± 0.1	1.33 ± 0.04	1.06 ± 0.01
ARG5	0.52 ± 0.01	1.32 ± 0.06	1.17 ± 0.04	1.07 ± 0.01	1.02 ± 0.01
LYS13	0.57 ± 0.01	1.03 ± 0.02	1.01 ± 0.02	0.99 ± 0.01	0.97 ± 0.01
ARG14	0.55 ± 0.01	1.08 ± 0.02	1.02 ± 0.01	0.99 ± 0.01	0.98 ± 0.01
HIS15	0.93 ± 0.01	0.46 ± 0.01	0.52 ± 0.01	0.60 ± 0.01	0.72 ± 0.01
ARG21	0.60 ± 0.01	1.04 ± 0.01	1.04 ± 0.01	1.04 ± 0.01	1.04 ± 0.01
LYS33	0.56 ± 0.01	2.2 ± 0.2	1.8 ± 0.1	1.28 ± 0.04	1.03 ± 0.01
ARG45	0.61 ± 0.01	1.19 ± 0.04	1.10 ± 0.03	1.04 ± 0.01	1.02 ± 0.01
ARG61	0.50 ± 0.01	1.02 ± 0.02	0.97 ± 0.01	0.94 ± 0.01	0.97 ± 0.01
ARG68	0.63 ± 0.01	1.08 ± 0.02	1.02 ± 0.01	0.99 ± 0.01	0.99 ± 0.01
ARG73	0.59 ± 0.01	0.97 ± 0.01	0.94 ± 0.01	0.93 ± 0.01	0.96 ± 0.01
LYS96	0.44 ± 0.01	0.91 ± 0.03	0.89 ± 0.02	0.85 ± 0.01	0.85 ± 0.01
LYS97	0.49 ± 0.01	0.95 ± 0.03	0.92 ± 0.02	0.87 ± 0.01	0.87 ± 0.01
ARG112	0.50 ± 0.01	1.28 ± 0.05	1.10 ± 0.03	0.97 ± 0.01	0.94 ± 0.01
ARG114	0.50 ± 0.01	1.39 ± 0.06	1.18 ± 0.05	1.01 ± 0.02	0.95 ± 0.01
LYS116	0.63 ± 0.01	1.1 ± 0.1	0.99 ± 0.06	0.99 ± 0.02	0.96 ± 0.01
ARG125	0.58 ± 0.01	1.55 ± 0.07	1.29 ± 0.06	1.11 ± 0.02	1.02 ± 0.01
ARG128	0.61 ± 0.01	1.53 ± 0.07	1.27 ± 0.05	1.10 ± 0.01	1.02 ± 0.01

Table S2: Hill coefficient n for all HEWL's basic residues at high salt concentration (0.200 M).

Residue	n				
	Free	$a = 160$ Å	$a = 120$ Å	$a = 80$ Å	$a = 40$ Å
LYS1	0.96 ± 0.01	1.06 ± 0.01	1.04 ± 0.01	1.02 ± 0.01	1.01 ± 0.01
ARG5	0.90 ± 0.01	0.98 ± 0.01	0.99 ± 0.01	0.99 ± 0.01	1.00 ± 0.01
LYS13	0.87 ± 0.01	0.95 ± 0.01	0.95 ± 0.01	0.95 ± 0.01	0.96 ± 0.01
ARG14	0.89 ± 0.01	0.95 ± 0.01	0.96 ± 0.01	0.96 ± 0.01	0.98 ± 0.01
HIS15	0.99 ± 0.01	0.97 ± 0.01	0.96 ± 0.01	0.95 ± 0.01	0.93 ± 0.01
ARG21	0.96 ± 0.01	1.00 ± 0.01	1.01 ± 0.01	1.02 ± 0.01	1.03 ± 0.01
LYS33	0.91 ± 0.01	1.02 ± 0.01	1.01 ± 0.01	1.00 ± 0.01	1.00 ± 0.01
ARG45	0.94 ± 0.01	1.00 ± 0.01	1.00 ± 0.01	1.01 ± 0.01	1.01 ± 0.01
ARG61	0.86 ± 0.01	0.92 ± 0.01	0.93 ± 0.01	0.95 ± 0.01	0.97 ± 0.01
ARG68	0.93 ± 0.01	0.97 ± 0.01	0.97 ± 0.01	0.98 ± 0.01	0.99 ± 0.01
ARG73	0.89 ± 0.01	0.93 ± 0.01	0.94 ± 0.01	0.95 ± 0.01	0.97 ± 0.01
LYS96	0.74 ± 0.01	0.81 ± 0.01	0.82 ± 0.01	0.83 ± 0.01	0.86 ± 0.01
LYS97	0.77 ± 0.01	0.83 ± 0.01	0.84 ± 0.01	0.85 ± 0.01	0.88 ± 0.01
ARG112	0.84 ± 0.01	0.91 ± 0.01	0.91 ± 0.01	0.92 ± 0.01	0.94 ± 0.01
ARG114	0.85 ± 0.01	0.92 ± 0.01	0.92 ± 0.01	0.93 ± 0.01	0.95 ± 0.01
LYS116	0.90 ± 0.01	0.96 ± 0.01	0.96 ± 0.01	0.95 ± 0.01	0.96 ± 0.01
ARG125	0.90 ± 0.01	0.99 ± 0.01	0.99 ± 0.01	0.99 ± 0.01	1.00 ± 0.01
ARG128	0.91 ± 0.01	0.99 ± 0.01	0.99 ± 0.01	0.99 ± 0.01	1.00 ± 0.01

References

[1] H. H. Chuang, *Align2mole*, `https://github.com/HHChuang/align2mole`, 2019.