Biophysical Journal, Volume *121*

Supplemental information

Programming xenon diffusion in maltose-binding protein

Zhuangyu Zhao, Nathan A. Rudman, Jiayi He, and Ivan J. Dmochowski

Supporting Information

Programming xenon diffusion in maltose binding protein

Zhuangyu Zhao, Nathan A. Rudman, Jiayi He, and Ivan J. Dmochowski*

Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104–6323, United States.

Table of Contents

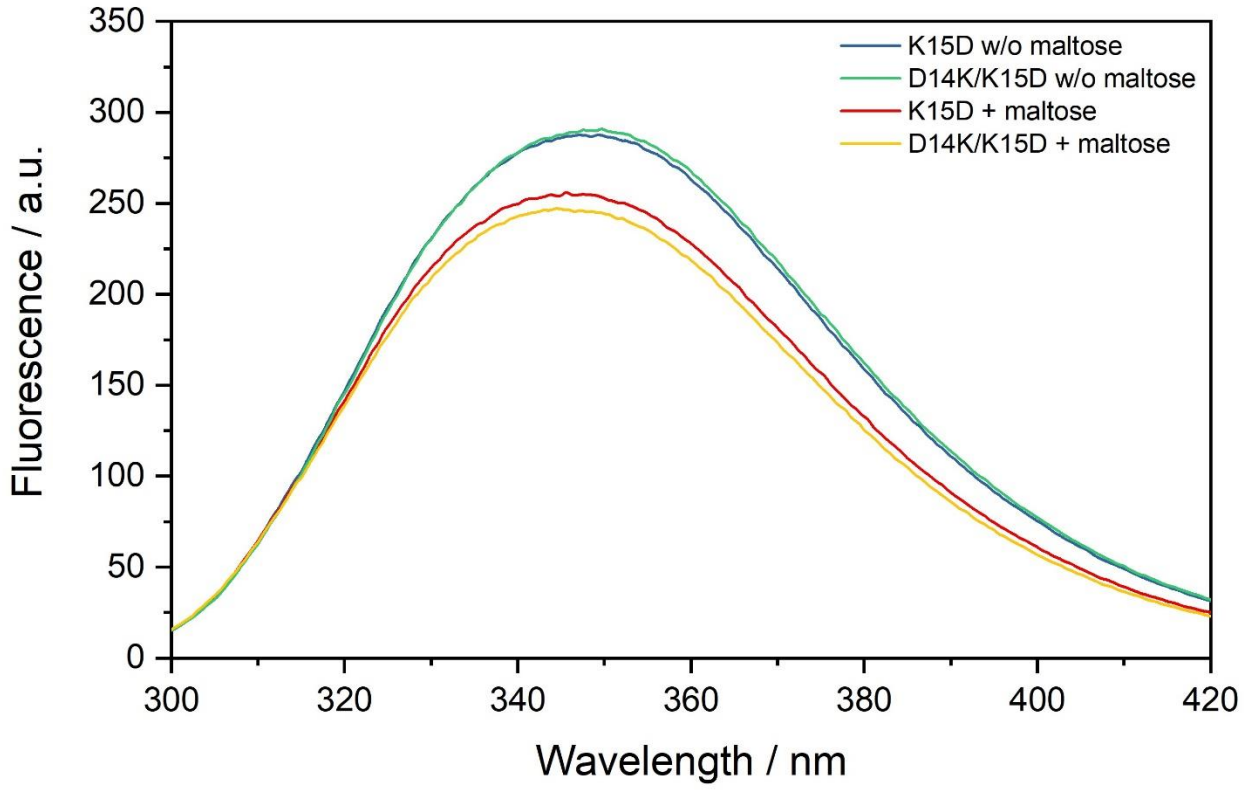

Figure S1. Fluorescence spectra of K15D and D14K/K15D proteins in PBS, pH 7.4. Maltose induces 12% and 15% quenching effect on intrinsic fluorescence of K15D and D14K/K15D, respectively.

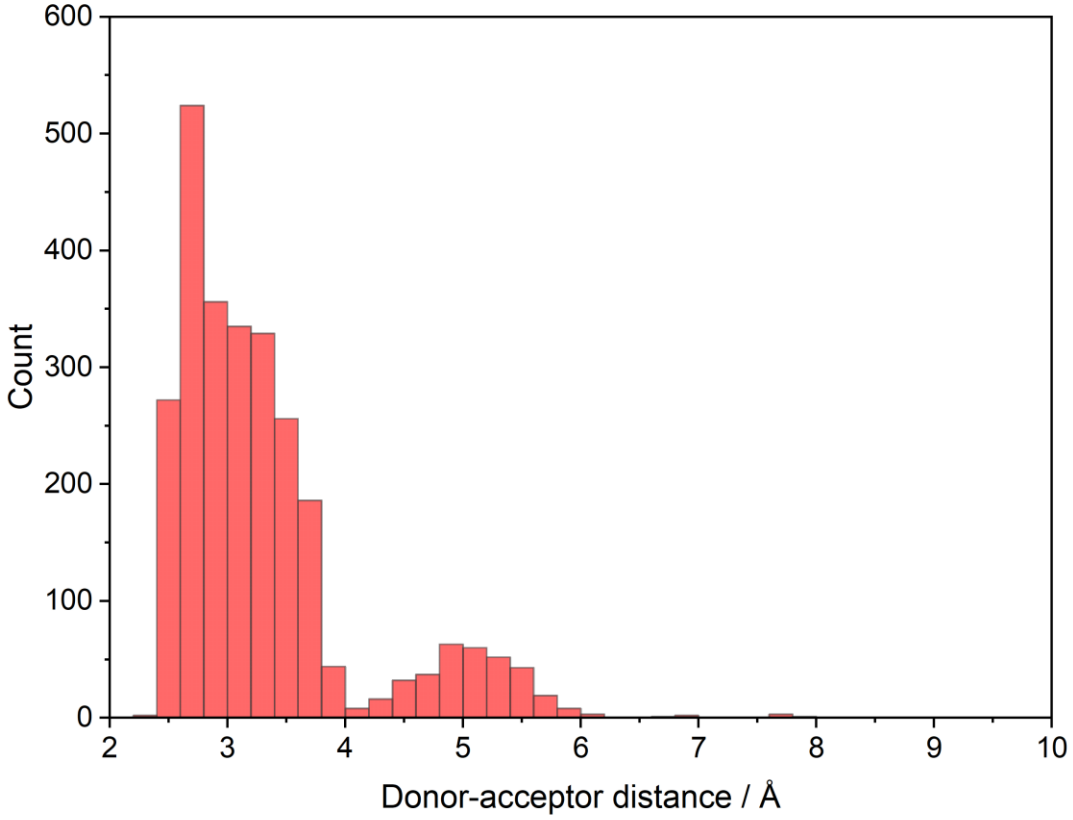

Figure S2. Donor-to-acceptor distance between K14 and E111 in the D14K/K15D protein. Salt bridge is defined to exist when the distance is less than 4 Å.

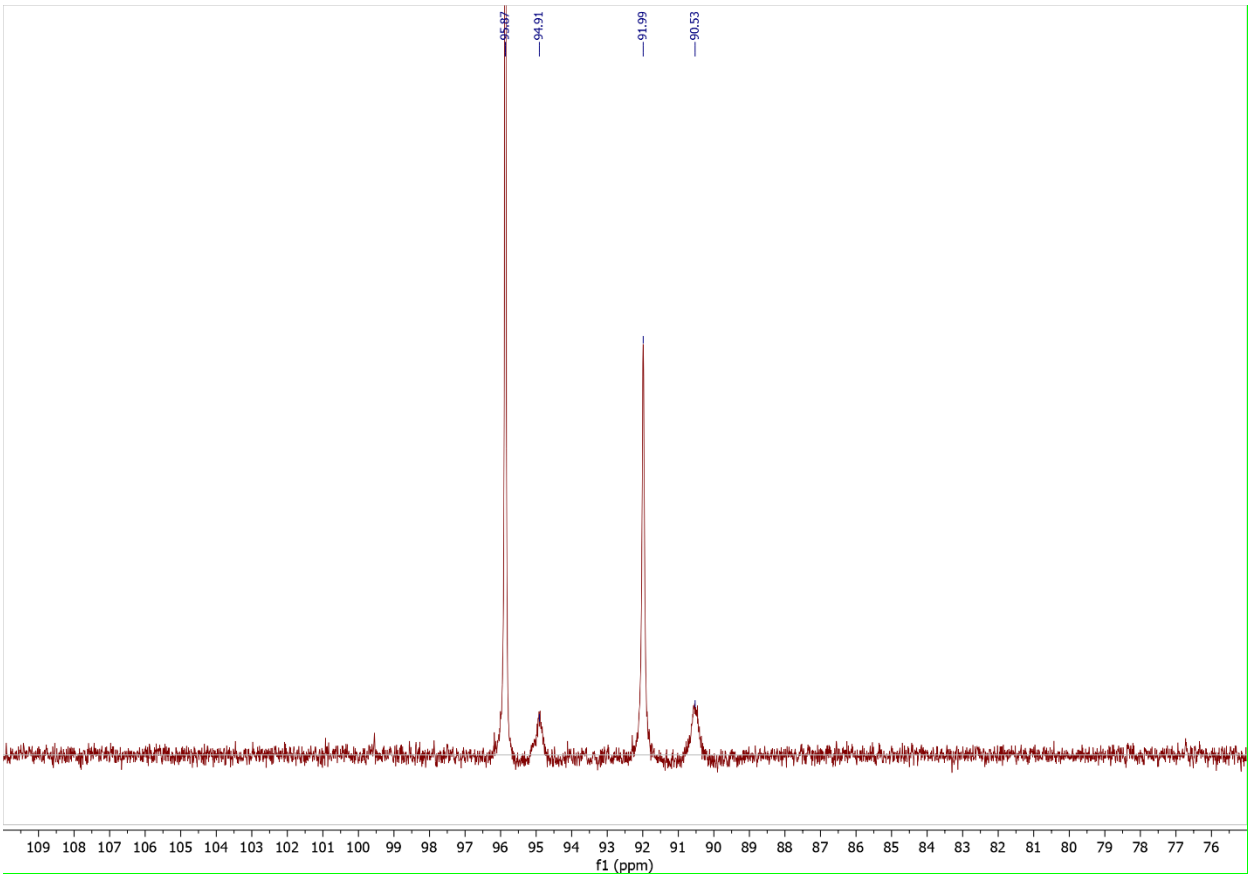

Figure S3. ^{13}C NMR spectrum of 2 mM [1-^{13}C]-maltose and 0.6 mM V23A protein in PBS, pH 7.4. From high frequency to low frequency are free β-maltose (δ = 95.87 ppm), bound β-maltose (δ = 94.91 ppm), free α-maltose (δ = 91.99 ppm), and bound α-maltose (δ = 90.53 ppm). The peak width (FWHM) is 37.8 Hz for bound β-maltose and 37.4 Hz for bound α-maltose.

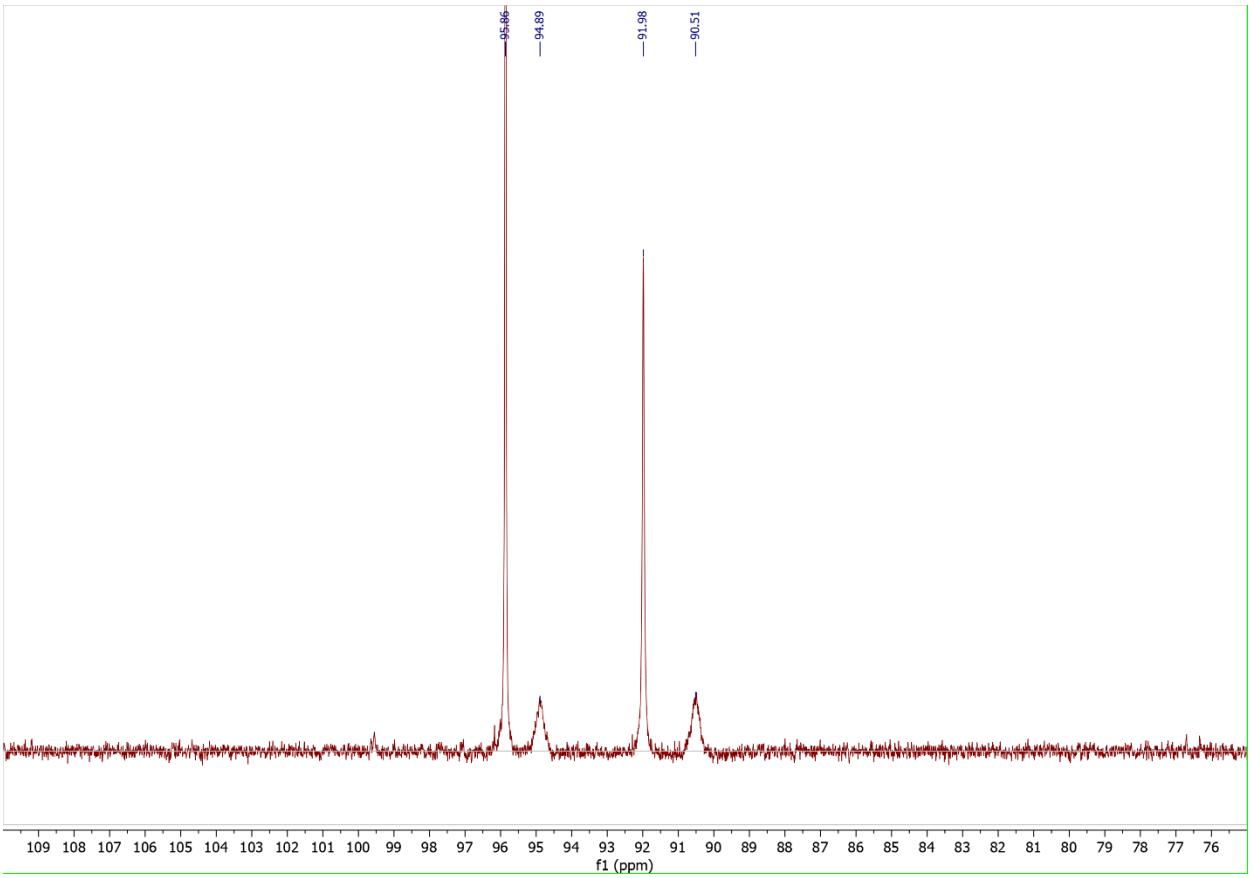

Figure S4. ^{13}C NMR spectrum of 2 mM [1-^{13}C]-maltose and 0.6 mM V23L protein in PBS, pH 7.4. From high frequency to low frequency are free β-maltose (δ = 95.86 ppm), bound β-maltose (δ = 94.89 ppm), free α-maltose (δ = 91.98 ppm), and bound α-maltose (δ = 90.51 ppm). The peak width (FWHM) is 38.0 Hz for bound β-maltose and 39.2 Hz for bound α-maltose.

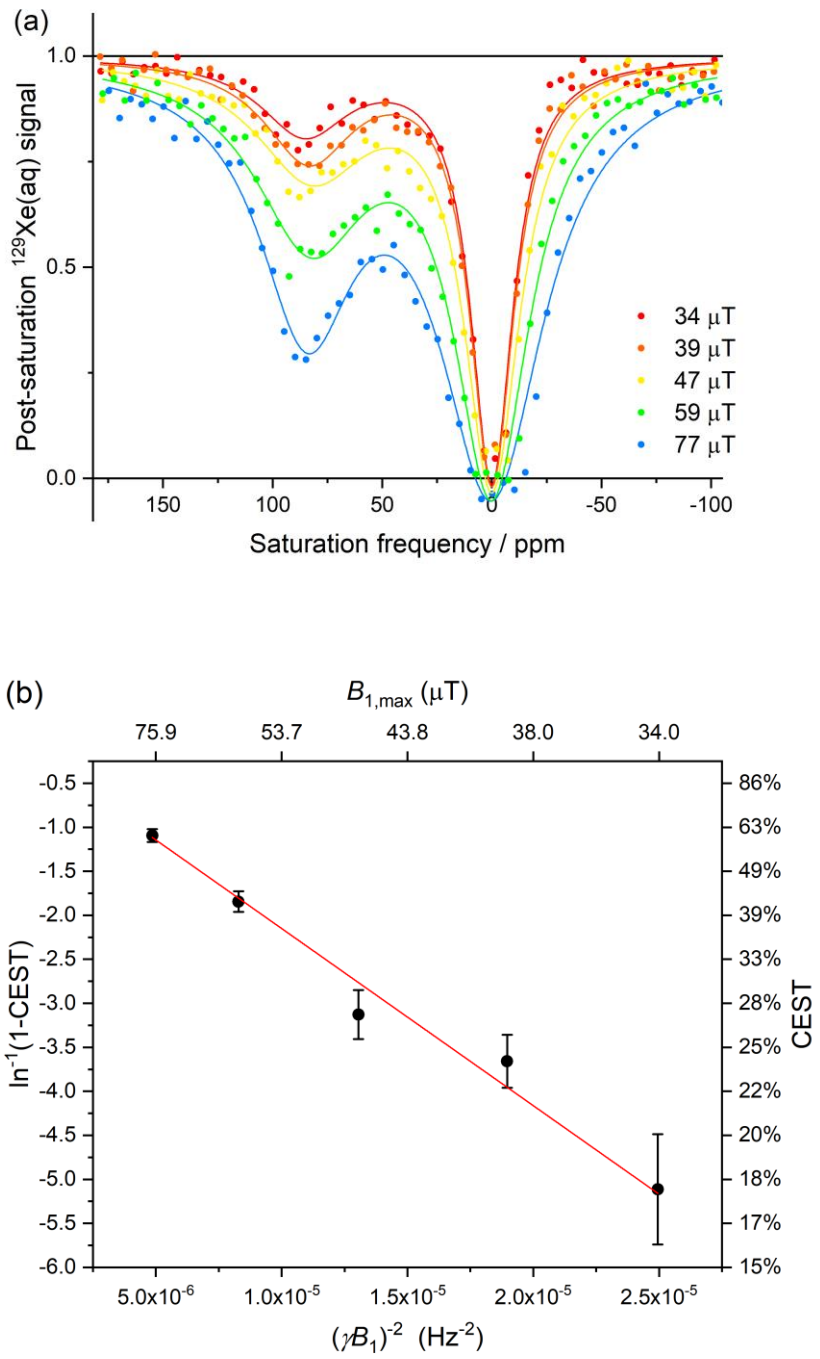

Figure S5. (a) Hyper-CEST z-spectra of V23A using a series of saturation pulse strengths at 300 K. (b) Linear fitting of $\ln^{-1}$(1-CEST) versus $(\gamma B_1)^{-2}$ yields the slope = (-2.0 ± 0.2) × 10^5 s^{-2}, y-intercept = -0.14 ± 0.12, and $k_{off,Xe}$ = (slope/y-intercept)$^{1/2}$ = (1.2 ± 0.5) × 10^3 s^{-1}.

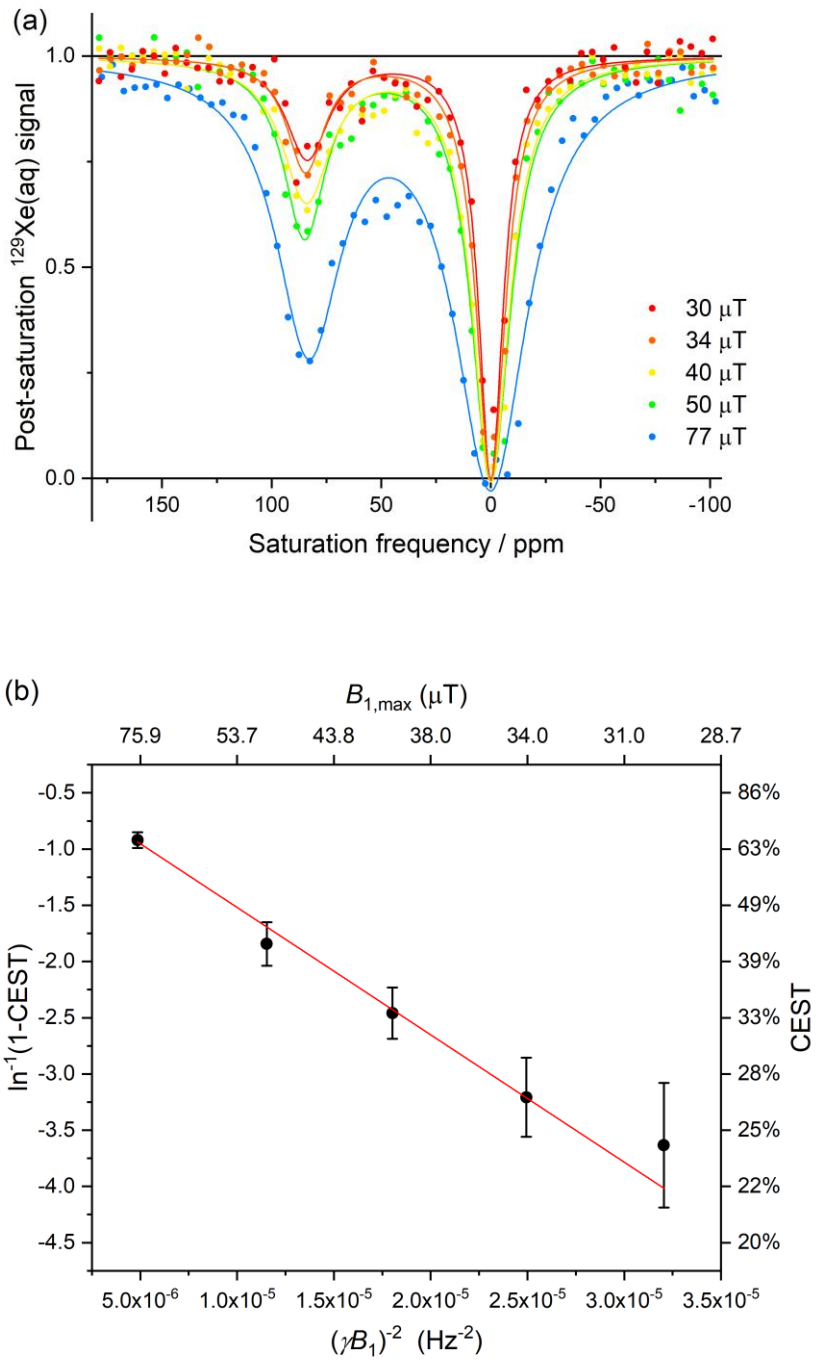

Figure S6. (a) Hyper-CEST z-spectra of V23L using a series of saturation pulse strengths at 300 K. (b) Linear fitting of $\ln^{-1}$(1-CEST) versus $(\gamma B_1)^{-2}$ yields the slope = (-1.1 ± 0.1) × 10^5 s^{-2}, y-intercept = -0.39 ± 0.06, and $k_{off,Xe}$ = (slope/y-intercept)$^{1/2}$ = (5.4 ± 0.3) × 10^2 s^{-1}.

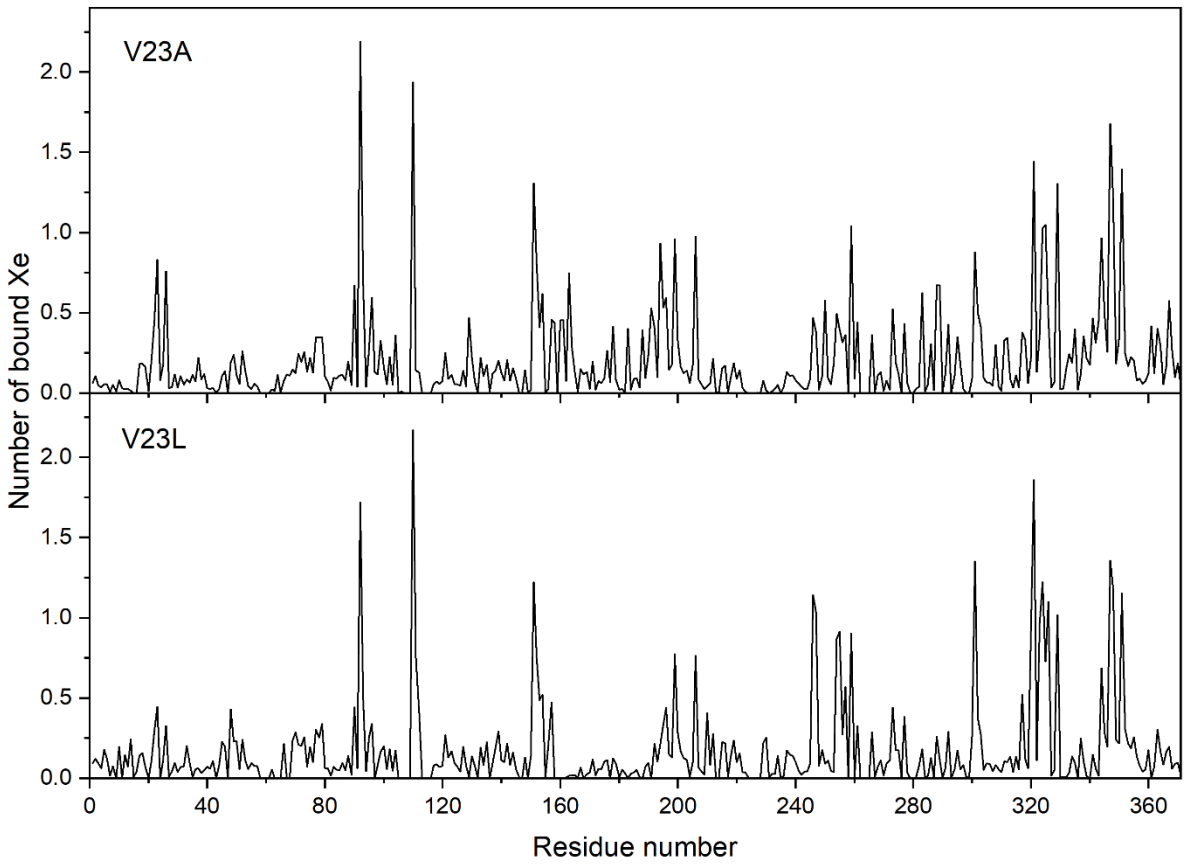

Figure S7. Average number of Xe atoms bound to the surface of V23A (top) and V23L (bottom) during the "Xe flooding" simulations.

Table S1. Oligonucleotide primers used in MBP site-directed mutagenesis.

K15D	Forward primer	5′ – GATTAACGGCGATGATGGCTATAACGGTC – 3′
	Reverse primer	5′ – GACCGTTATAGCCATCATCGCCGTTAATC – 3′
D14K/K15D	Forward primer	5′ – CTGGATTAACGGCAAAGATGGCTATAACGGTC – 3′
	Reverse primer	5′ – GACCGTTATAGCCATCTTTGCCGTTAATCCAG – 3′
V23A	Forward primer	5′ – GTCTCGCTGAAGCTGGTAAGAAATTCGAG – 3′
	Reverse primer	5′ – CTCGAATTTCTTACCAGCTTCAGCGAGAC – 3′
V23L	Forward primer	5′ – GTCTCGCTGAACTGGGTAAGAAATTCGAG – 3′
	Reverse primer	5′ – CTCGAATTTCTTACCCAGTTCAGCGAGAC – 3′