Biophysical Journal, Volume *116*

Supplemental Information

Molecular Features of the Zn^{2+} Binding Site in the Prion Protein Probed by ^{113}Cd NMR

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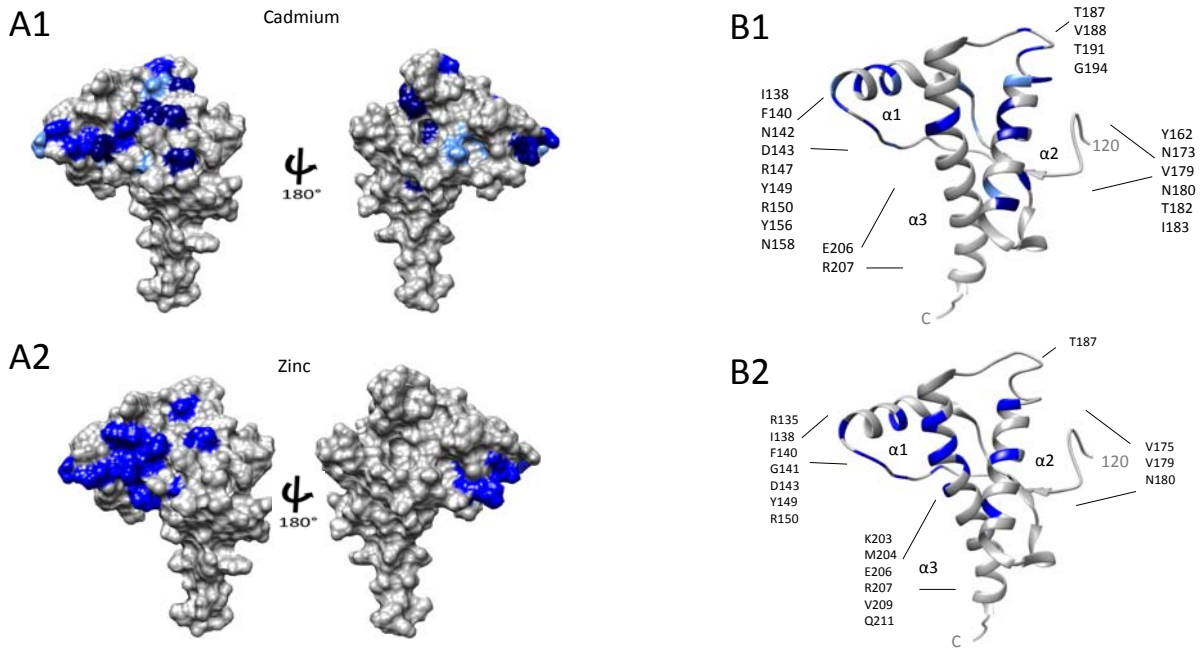

Figure S1 Zn^{2+} and Cd^{2+} Promoted *cis* Interaction Wild-Type MoPrP is Localized to the Same C-terminal Surface. Both samples were run with 300μM protein in a buffer containing 10mM MES (Sigma), 10% D_2O, at pH 7.0 for solubility purposes. Subsequent to the addition of 500μM $ZnCl_2$ or 1mM $CdCl_2$, the pH was measured and adjusted, if necessary. Residues that are broadened (dark blue), broadened+shifted (medium blue), and shifted (light blue) in the presence of the respective metal ion are indicated in the surface diagrams, A1 and A2, and ribbon diagrams, B1 and B2. Coordinates for the C-terminal PrP^C structure are from PDB:1XYX.

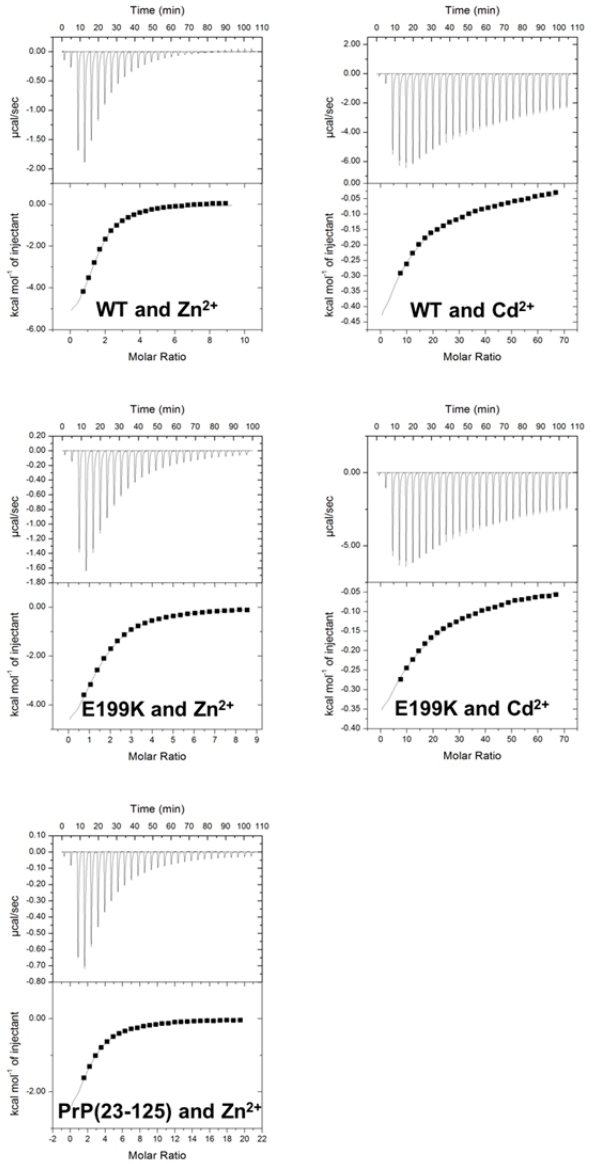

Figure S2 Raw isotherms of either Zn^{2+} or Cd^{2+} ITC titrations into different PrP^{C}variants: Zinc Chloride (2 mM) or Cadmium Chloride (20 mM) was titrated into PrP^{C}variants. Each figure contains the raw ITC data (top panel) and the integrated raw data (bottom panel). Zinc chloride was titrated into WT, E199K, and PrP(23-125) at pH 7.4 in 50 mM MOPS buffer. Cadmium chloride was titrated into WT and E199K at pH 6.0 in 10 mM MES buffer. The integrated raw ITC data shown for cadmium chloride have been background subtracted due to high heats of dilution. Calculated Kd values are reported in Table 2.