SUPPLEMENTARY MATERIAL

Ser170 Controls the Conformational Multiplicity of the Loop 166-175 in Prion Proteins: Implication for Conversion and Species Barrier

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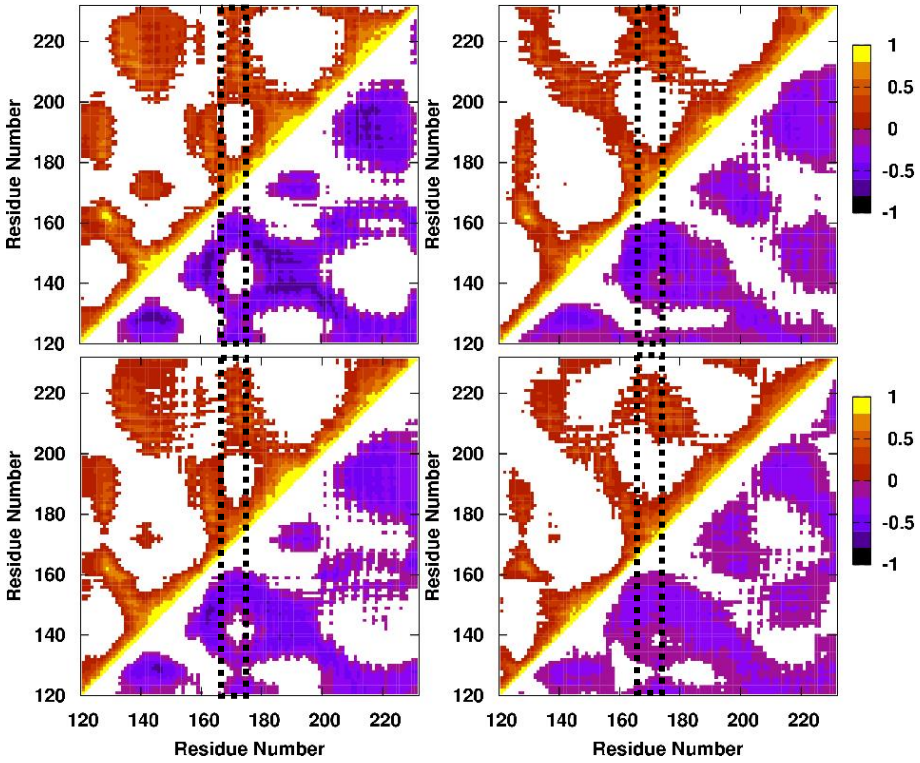

Figure S1 The cross-correlation coefficient C_{ij} between the displacements of C_α atoms i and j is calculated as

$$C_{ij} = \left\langle \Delta \vec{r}_i \, \Delta \vec{r}_j \right\rangle \Big/ \left(\left\langle \Delta r_i^2 \right\rangle \left\langle \Delta r_j^2 \right\rangle \right)^{1/2}$$

where $\Delta \vec{r}_i$ is the displacement of C_α atom i from its average position, and $\langle\ \rangle$ represents an average over a simulation segment. Data were obtained by averaging the C_{ij} over 20 segments of 1 ns each. The last 20 ns of the trajectories mPrP (top) and mPrPmb (bottom) were used for this plott. In each plot, the upper and lower triangles show correlated and anti-correlated displacement, respectively. The dotted rectangle emphasizes L1 residues 166-175.

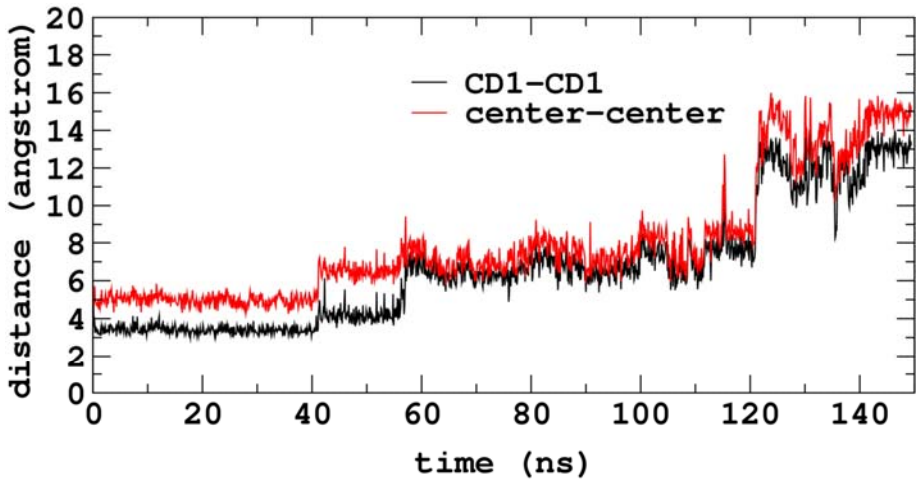

Figure S2 Time evolution (simulation mPrPmb) of the separation of the ring centroids (center-center ≡ R_{cen} in Ref. (1)) and the closest distance (Cδ1-Cδ1 ≡ R_{clo} in Ref. (1)) between Tyr169 and Phe175.

REFERENCE

1. McGaughey, G. B., Gagne, M., and Rappe, A. K. (1998) *The Journal of biological chemistry* **273**(25), 15458-15463