Supporting Information

Armel and Leinwand 10.1073/pnas.0900107106

SI Text

The change in mean residue ellipticity, θ, as a function of temperature was modeled using a nonlinear least squares algorithm assuming the 2-state transition of a monomer from a folded to an unfolded state with a change in heat capacity, ΔCp, between the folded and unfolded forms.

The fraction folded at any temperature is

$$f_{\mathrm{F(t)}} = (\theta_t - \theta_{\mathrm{U}})/(\theta_F - \theta_{\mathrm{U}}),$$

where θ_{t} is the observed ellipticity at a given temperature, θ_{F} is the ellipticity of fully folded protein, and θ_{U} is the ellipticity of unfolded protein. The fraction of folded protein, $f_{\mathrm{F(t)}}$, was used to determine ΔG, with pretransition and posttransition baseline corrections applied that are assumed to be linearly dependent on temperature,

$$f_{\mathrm{F}(t)} = y \times ((\theta_{\mathrm{F}} + (\theta_{\mathrm{F},1} \times t)) - (\theta_{\mathrm{U}} + (\theta_{\mathrm{U},1} \times t))) + (\theta_{\mathrm{U}} + (\theta_{\mathrm{U},1} \times t)),$$

where $\theta_{\mathrm{F},1}$ is the linear correction of the mean residue ellipticity of the folded protein as a function of temperature, $\theta_{\mathrm{U},1}$ is the linear correction of the mean residue ellipticity of the unfolded protein as a function of temperature, t is the observed temperature and

$$y = \exp[(-\Delta \mathrm{G}/Rt)]/[1 + \exp(-\Delta \mathrm{G}/Rt)].$$

ΔG is the Gibbs free energy of folding, which is given by the Gibbs-Helmholtz equation,

$$\Delta \mathrm{G} = \Delta \mathrm{H}(1 - t/T_m) + \Delta Cp(t - T_m) - t \times \ln(t/T_m),$$

where ΔH is the enthalpy of unfolding, T_{m} is the temperature midpoint of the melting transition, and ΔCp is the change in heat capacity associated with unfolding. These thermodynamic parameters were fit using the program Kaleidagraph, and the entropy, ΔS, was calculated at the T_{m} (where $K = 1$) using

$$\Delta S = \Delta \mathrm{H}/T_m.$$

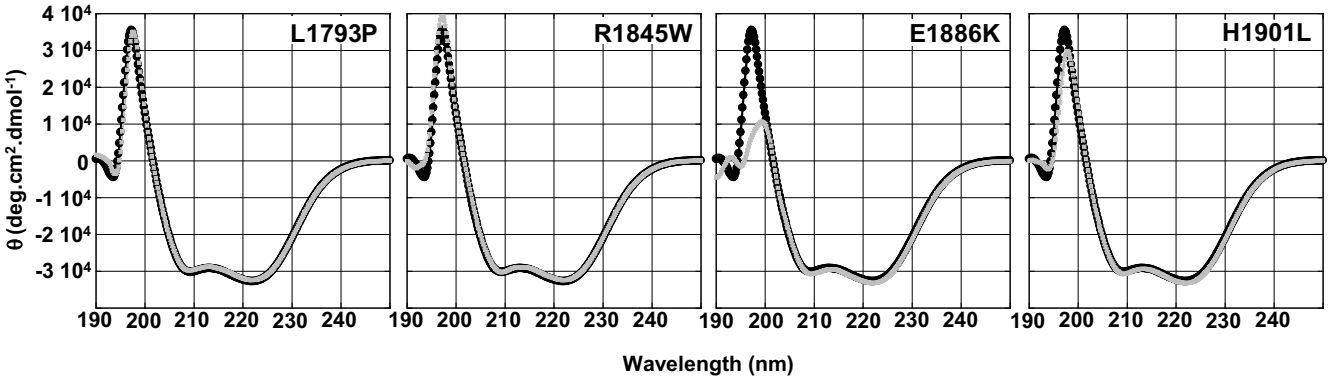

Fig. S1. Mutations associated with MSM do not alter the secondary structure of the protein. Far-UV CD spectra for wild type (black) and mutant (gray) LMM were determined in high salt buffer (300 mM NaCl, 10 mM TES, 3.5 mM EDTA, 1 mM TCEP, pH 7.3) at 4 °C. Under these conditions, wild type, L1793P, R1845W, E1886K, and H1901L LMM all display canonical α-helical spectra, with characteristic minima at 208 nm and 222 nm.

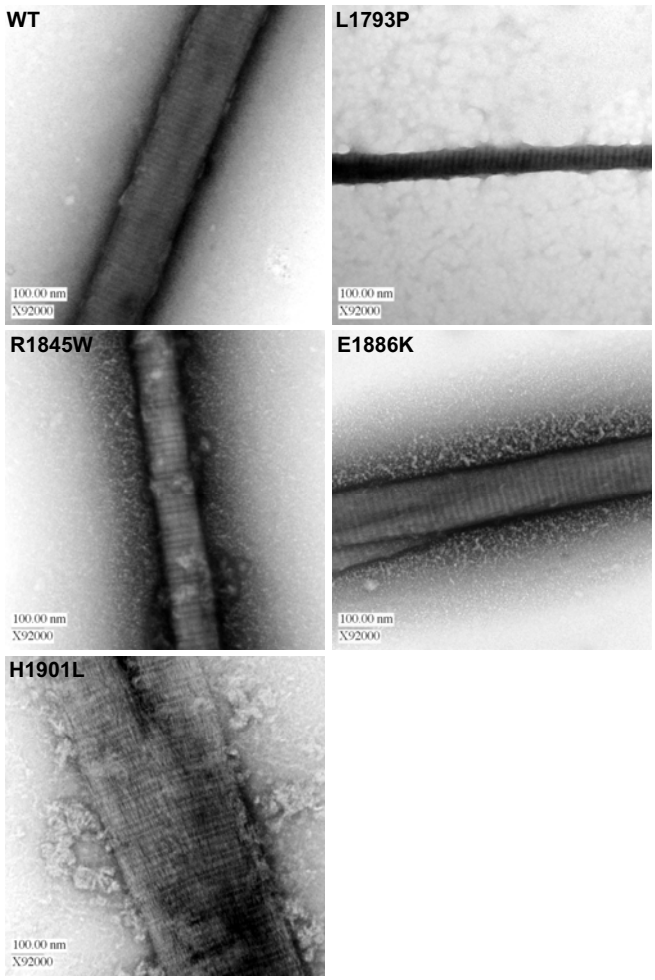

Fig. S2. Paracrystals formed by mutant LMM are morphologically indistinguishable from those formed by WT protein. WT and mutant LMM were each dialyzed from high salt buffer to low salt buffer to induce paracrystal formation. Electron micrographs were then recorded at a magnification of ×92,000, and image manipulation software was used to determine measurements of paracrystal periodicity.

Table S1. LMM paracrystal parameters

	Striations, nm	±	*n*
Wild type	14.0	0.44	20
L1793P	13.6	0.54	24
R1845W	14.2	0.51	40
E1886K	14.4	0.55	44
H1901L	14.6	0.31	28