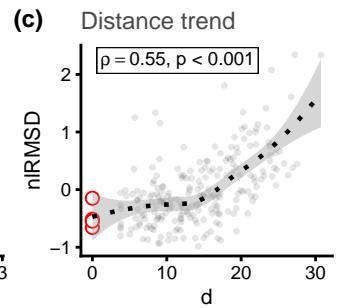
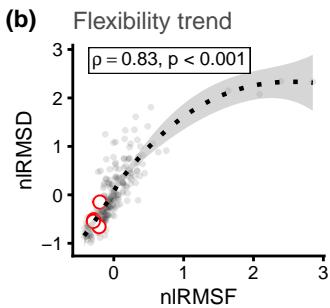
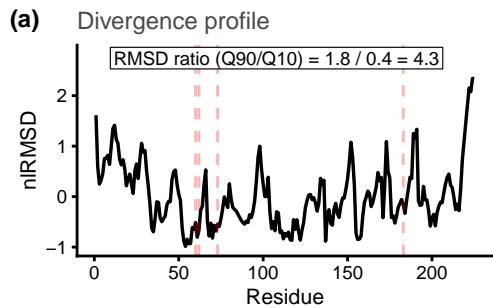
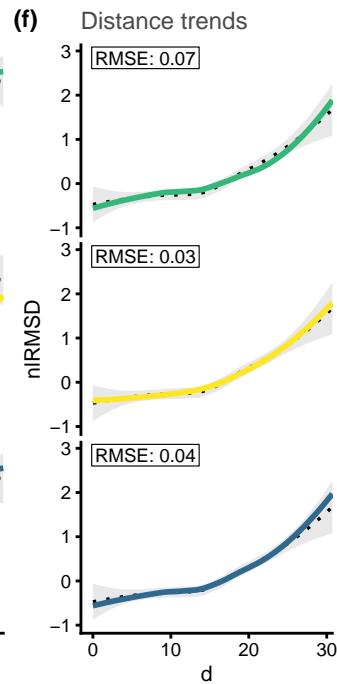
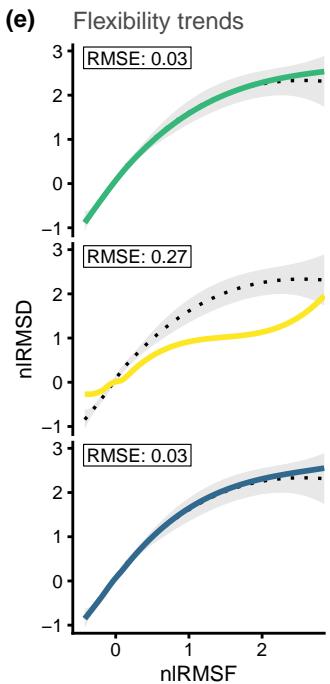
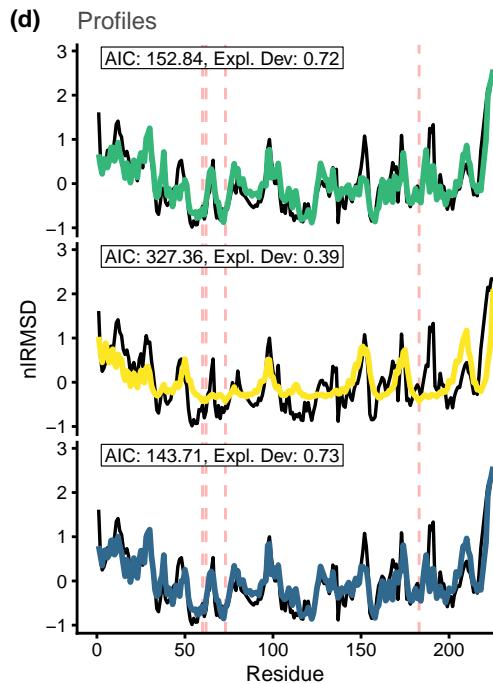


Observed patterns

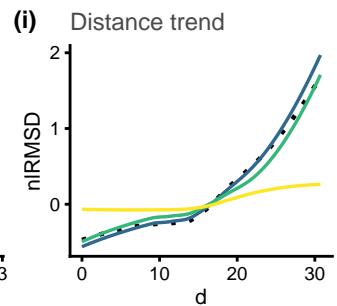
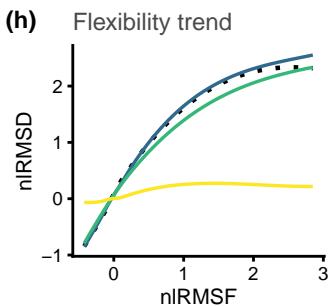
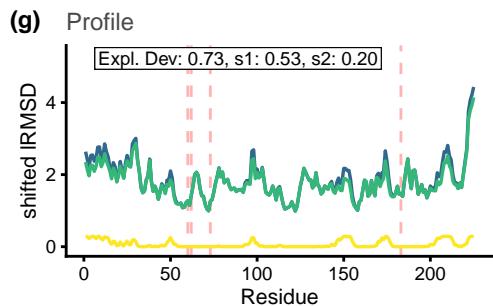


Model predictions vs. observations



— Obs. — M₁ — M₂ — M₁₂ - - Active site

Decomposition into flexibility and distance contributions



— M₁₂ — s₁ — s₂