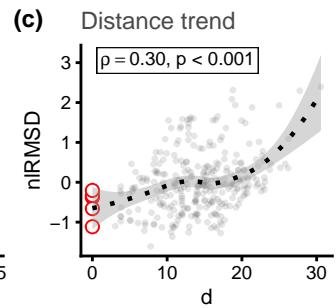
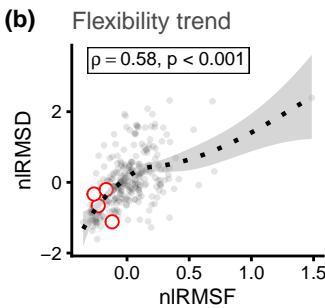
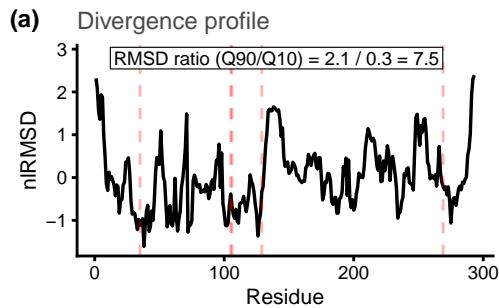
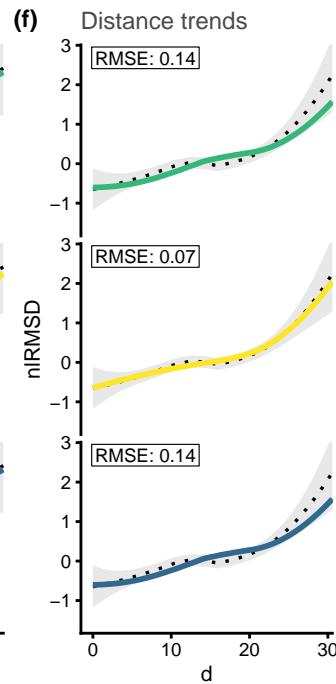
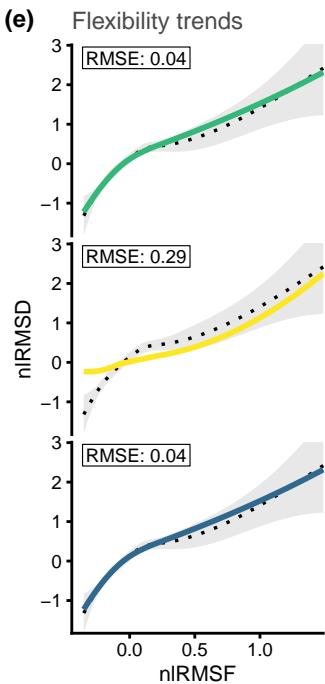
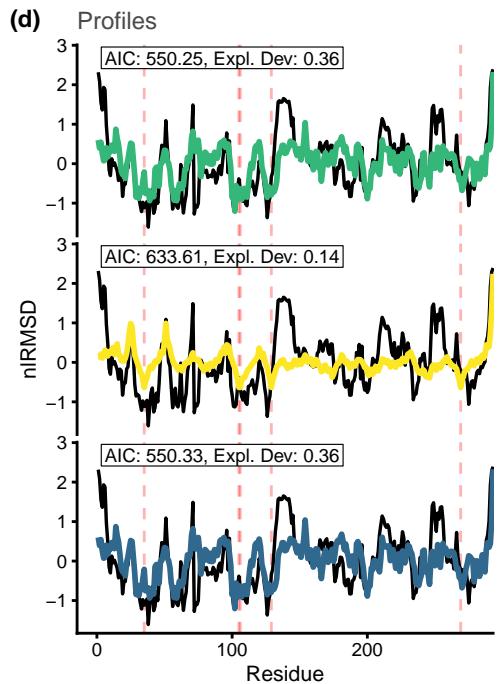


### Observed patterns

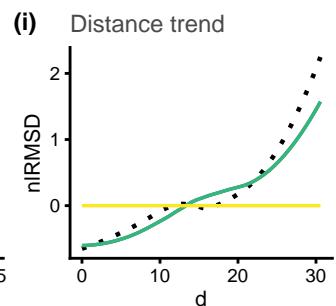
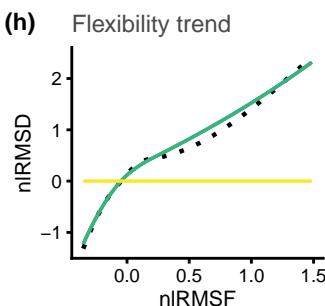


### Model predictions vs. observations



— Obs. — M<sub>1</sub> — M<sub>2</sub> — M<sub>12</sub> - - Active site

### Decomposition into flexibility and distance contributions



— M<sub>12</sub> — S<sub>1</sub> — S<sub>2</sub>