Observed patterns

(a) Divergence profile

RMSD ratio (Q90/Q10) = 2.6 / 0.4 = 6.3
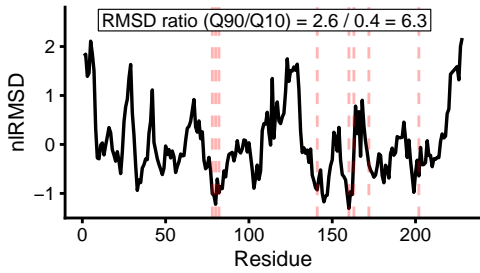
(b) Flexibility trend

$\rho = 0.71$, $p < 0.001$

(c) Distance trend

$\rho = 0.64$, $p < 0.001$
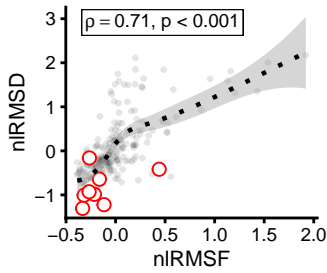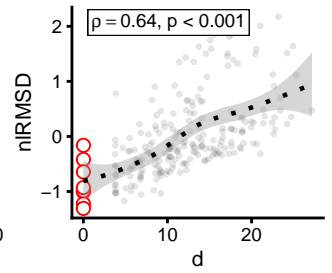
Model predictions vs. observations

(d) Profiles

AIC: 335.58, Expl. Dev: 0.51

AIC: 395.83, Expl. Dev: 0.35

AIC: 286.06, Expl. Dev: 0.61

(e) Flexibility trends

RMSE: 0.08

RMSE: 0.32

RMSE: 0.06

(f) Distance trends

RMSE: 0.21

RMSE: 0.06

RMSE: 0.04
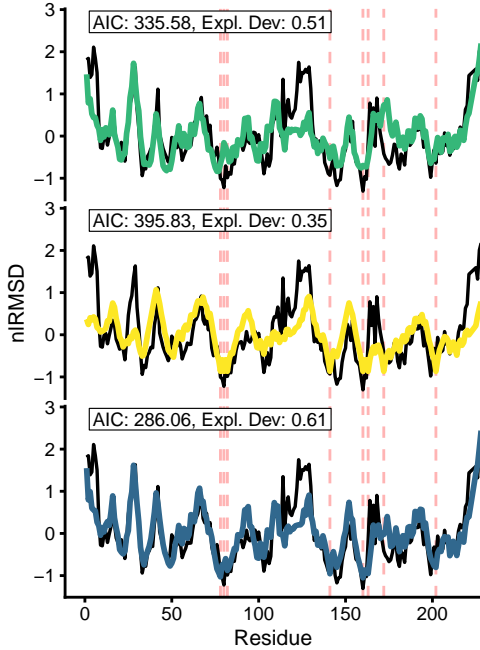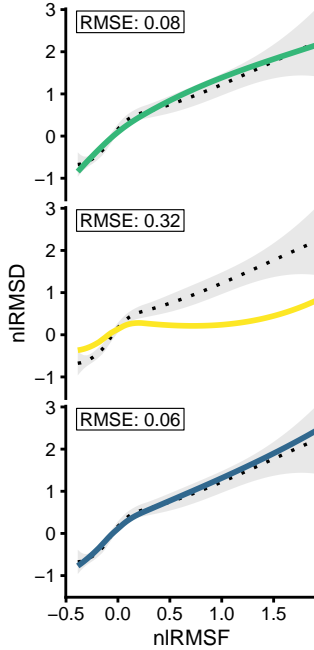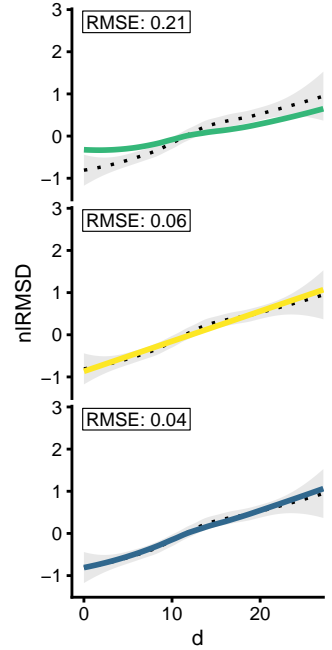
— Obs. — M_1 — M_2 — M_{12} – – Active site

Decomposition into flexibility and distance contributions

(g) Profile

Expl. Dev: 0.61, s1: 0.38, s2: 0.22
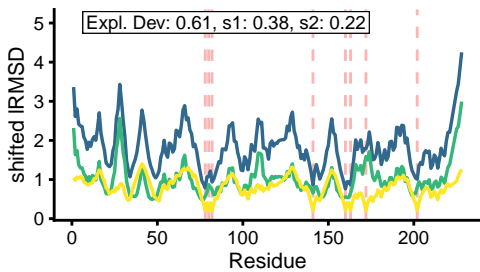
(h) Flexibility trend
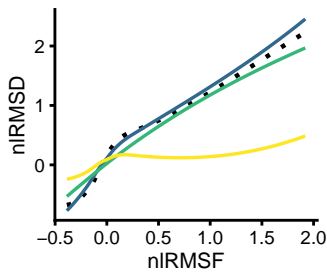
(i) Distance trend

— M_{12} — s_1 — s_2