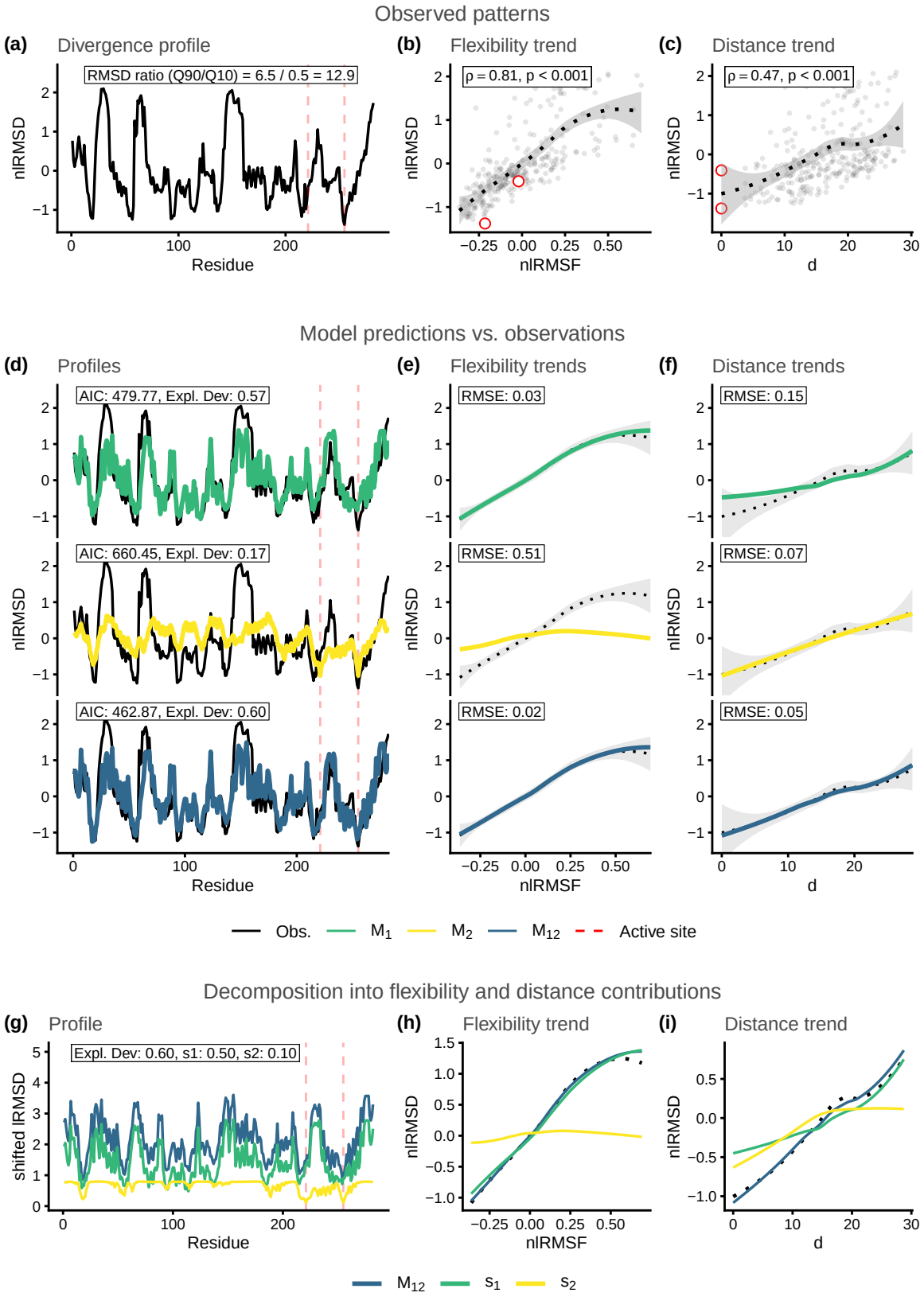
Observed patterns
(a)
Divergence profile
RMSD ratio (Q90/Q10) = 6.5 / 0.5 = 12.9
nlRMSD
Residue
(b)
Flexibility trend
ρ = 0.81, p < 0.001
nlRMSD
nlRMSF
(c)
Distance trend
ρ = 0.47, p < 0.001
nlRMSD
d
Model predictions vs. observations
(d)
Profiles
AIC: 479.77, Expl. Dev: 0.57
AIC: 660.45, Expl. Dev: 0.17
AIC: 462.87, Expl. Dev: 0.60
nlRMSD
Residue
(e)
Flexibility trends
RMSE: 0.03
RMSE: 0.51
RMSE: 0.02
nlRMSD
nlRMSF
(f)
Distance trends
RMSE: 0.15
RMSE: 0.07
RMSE: 0.05
nlRMSD
d
Obs.
M1
M2
M12
Active site
Decomposition into flexibility and distance contributions
(g)
Profile
Expl. Dev: 0.60, s1: 0.50, s2: 0.10
shifted lRMSD
Residue
(h)
Flexibility trend
nlRMSD
nlRMSF
(i)
Distance trend
nlRMSD
d
M12
s1
s2