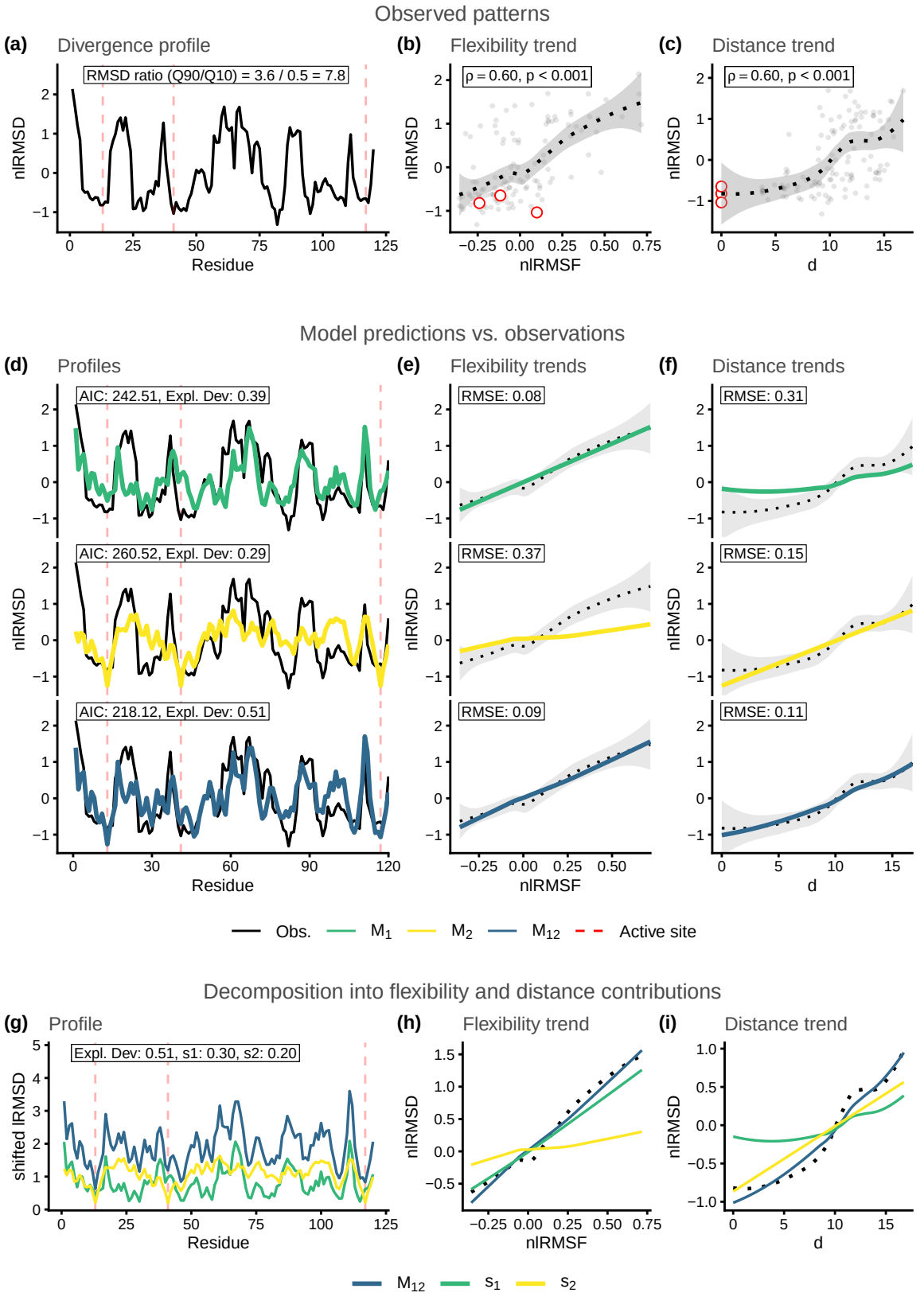
Observed patterns
(a)
Divergence profile
RMSD ratio (Q90/Q10) = 3.6 / 0.5 = 7.8
nlRMSD
Residue
(b)
Flexibility trend
ρ = 0.60, p < 0.001
nlRMSD
nlRMSF
(c)
Distance trend
ρ = 0.60, p < 0.001
nlRMSD
d
Model predictions vs. observations
(d)
Profiles
AIC: 242.51, Expl. Dev: 0.39
AIC: 260.52, Expl. Dev: 0.29
AIC: 218.12, Expl. Dev: 0.51
nlRMSD
Residue
(e)
Flexibility trends
RMSE: 0.08
RMSE: 0.37
RMSE: 0.09
nlRMSD
nlRMSF
(f)
Distance trends
RMSE: 0.31
RMSE: 0.15
RMSE: 0.11
nlRMSD
d
Obs.
M1
M2
M12
Active site
Decomposition into flexibility and distance contributions
(g)
Profile
Expl. Dev: 0.51, s1: 0.30, s2: 0.20
shifted lRMSD
Residue
(h)
Flexibility trend
nlRMSD
nlRMSF
(i)
Distance trend
nlRMSD
d
M12
s1
s2