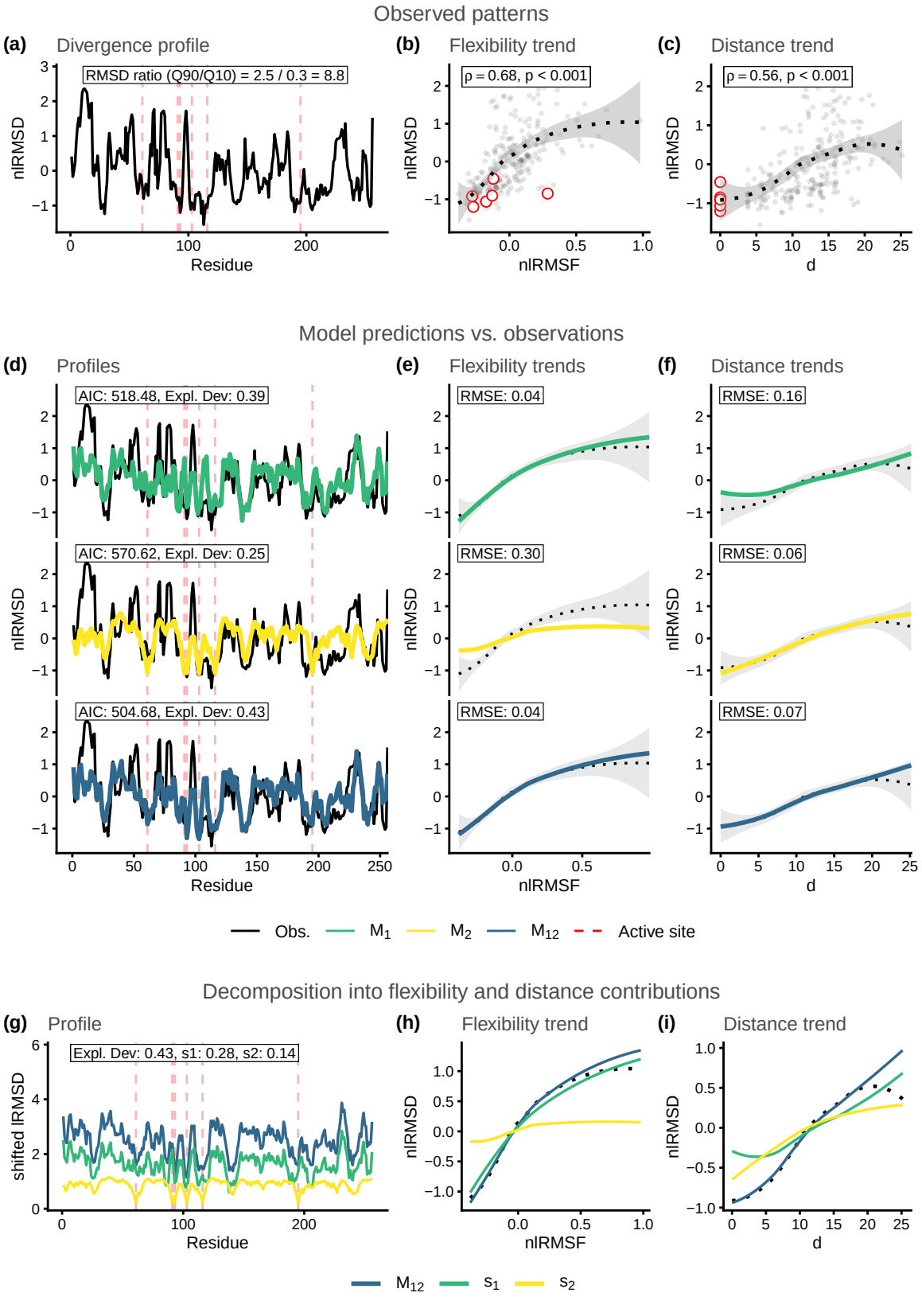
Observed patterns
(a)
Divergence profile
RMSD ratio (Q90/Q10) = 2.5 / 0.3 = 8.8
nlRMSD
Residue
(b)
Flexibility trend
ρ = 0.68, p < 0.001
nlRMSD
nlRMSF
(c)
Distance trend
ρ = 0.56, p < 0.001
nlRMSD
d
Model predictions vs. observations
(d)
Profiles
AIC: 518.48, Expl. Dev: 0.39
AIC: 570.62, Expl. Dev: 0.25
AIC: 504.68, Expl. Dev: 0.43
nlRMSD
Residue
(e)
Flexibility trends
RMSE: 0.04
RMSE: 0.30
RMSE: 0.04
nlRMSD
nlRMSF
(f)
Distance trends
RMSE: 0.16
RMSE: 0.06
RMSE: 0.07
nlRMSD
d
Obs.
M1
M2
M12
Active site
Decomposition into flexibility and distance contributions
(g)
Profile
Expl. Dev: 0.43, s1: 0.28, s2: 0.14
shifted lRMSD
Residue
(h)
Flexibility trend
nlRMSD
nlRMSF
(i)
Distance trend
nlRMSD
d
M12
s1
s2