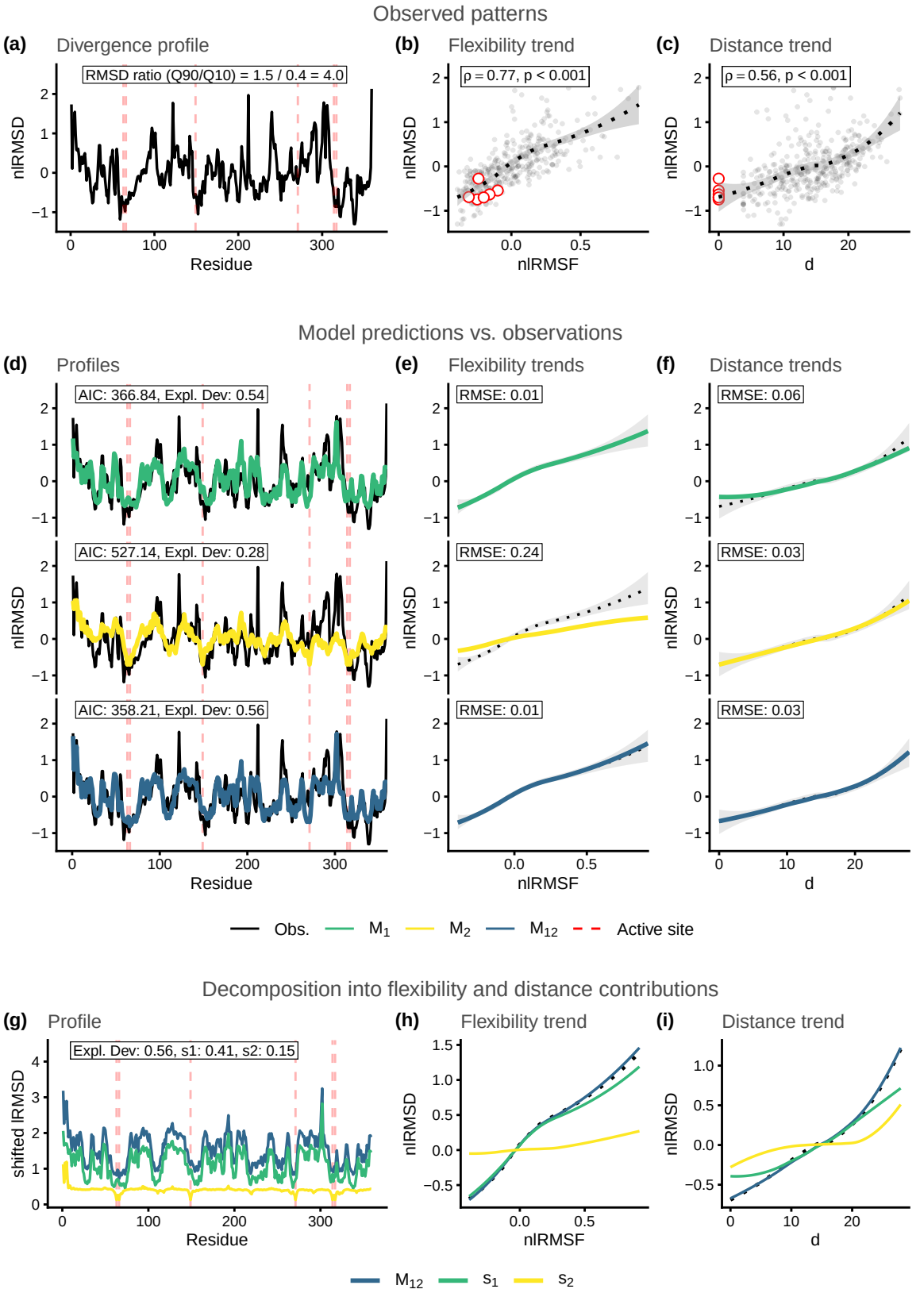
Observed patterns
(a)
Divergence profile
RMSD ratio (Q90/Q10) = 1.5 / 0.4 = 4.0
nlRMSD
Residue
(b)
Flexibility trend
ρ = 0.77, p < 0.001
nlRMSD
nlRMSF
(c)
Distance trend
ρ = 0.56, p < 0.001
nlRMSD
d
Model predictions vs. observations
(d)
Profiles
AIC: 366.84, Expl. Dev: 0.54
AIC: 527.14, Expl. Dev: 0.28
AIC: 358.21, Expl. Dev: 0.56
nlRMSD
Residue
(e)
Flexibility trends
RMSE: 0.01
RMSE: 0.24
RMSE: 0.01
nlRMSD
nlRMSF
(f)
Distance trends
RMSE: 0.06
RMSE: 0.03
RMSE: 0.03
nlRMSD
d
Obs.
M1
M2
M12
Active site
Decomposition into flexibility and distance contributions
(g)
Profile
Expl. Dev: 0.56, s1: 0.41, s2: 0.15
shifted lRMSD
Residue
(h)
Flexibility trend
nlRMSD
nlRMSF
(i)
Distance trend
nlRMSD
d
M12
s1
s2