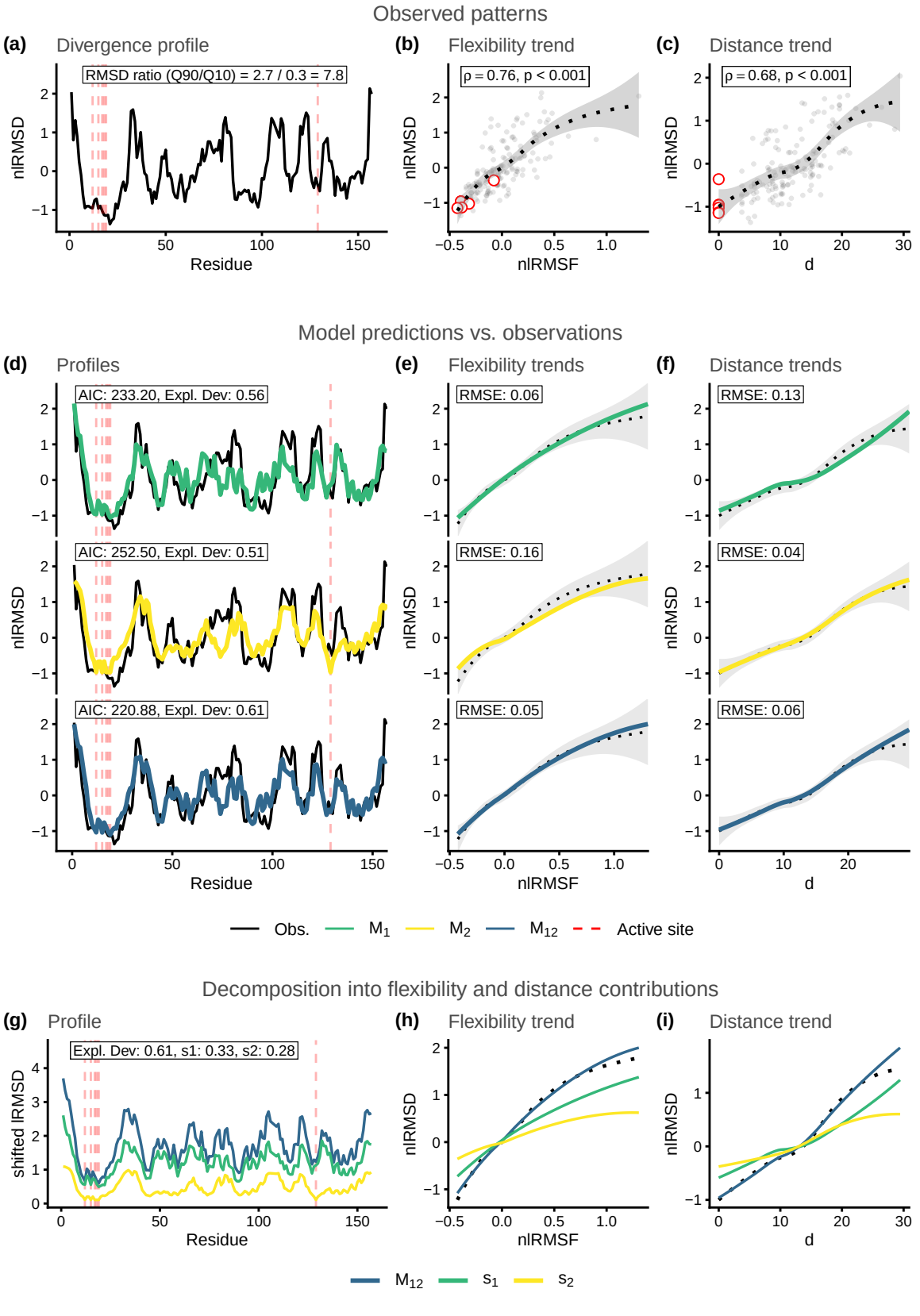
Observed patterns
(a)
Divergence profile
RMSD ratio (Q90/Q10) = 2.7 / 0.3 = 7.8
nlRMSD
Residue
(b)
Flexibility trend
ρ = 0.76, p < 0.001
nlRMSD
nlRMSF
(c)
Distance trend
ρ = 0.68, p < 0.001
nlRMSD
d
Model predictions vs. observations
(d)
Profiles
AIC: 233.20, Expl. Dev: 0.56
AIC: 252.50, Expl. Dev: 0.51
AIC: 220.88, Expl. Dev: 0.61
nlRMSD
Residue
(e)
Flexibility trends
RMSE: 0.06
RMSE: 0.16
RMSE: 0.05
nlRMSD
nlRMSF
(f)
Distance trends
RMSE: 0.13
RMSE: 0.04
RMSE: 0.06
nlRMSD
d
Obs.
M1
M2
M12
Active site
Decomposition into flexibility and distance contributions
(g)
Profile
Expl. Dev: 0.61, s1: 0.33, s2: 0.28
shifted lRMSD
Residue
(h)
Flexibility trend
nlRMSD
nlRMSF
(i)
Distance trend
nlRMSD
d
M12
s1
s2