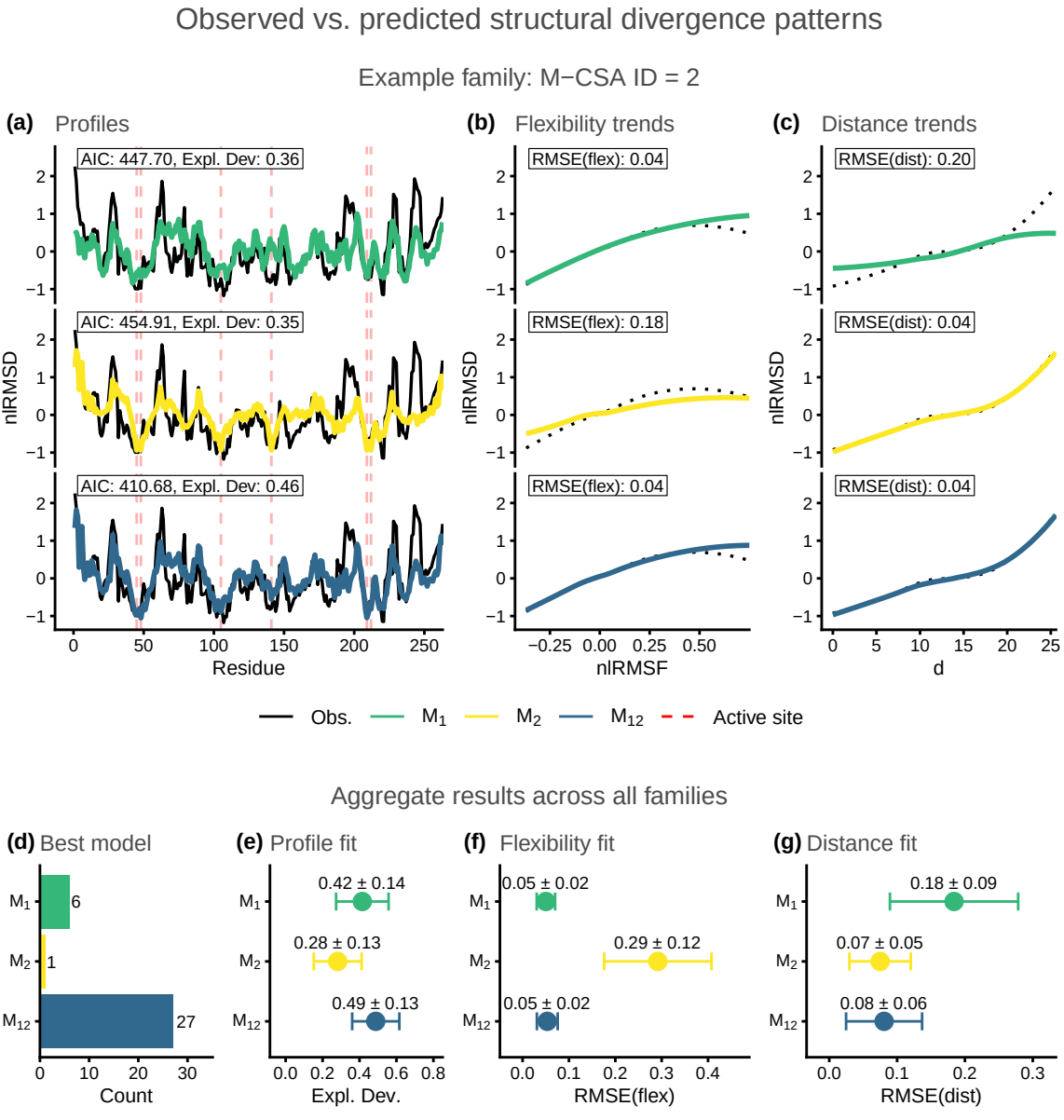
Observed vs. predicted structural divergence patterns
Example family: M−CSA ID = 2
(a) Profiles
(b) Flexibility trends
(c) Distance trends
AIC: 447.70, Expl. Dev: 0.36
AIC: 454.91, Expl. Dev: 0.35
AIC: 410.68, Expl. Dev: 0.46
RMSE(flex): 0.04
RMSE(flex): 0.18
RMSE(flex): 0.04
RMSE(dist): 0.20
RMSE(dist): 0.04
RMSE(dist): 0.04
nlRMSD
Residue
nlRMSF
d
Obs.
M1
M2
M12
Active site
Aggregate results across all families
(d) Best model
(e) Profile fit
(f) Flexibility fit
(g) Distance fit
Count
Expl. Dev.
RMSE(flex)
RMSE(dist)
0.42 ± 0.14
0.28 ± 0.13
0.49 ± 0.13
0.05 ± 0.02
0.29 ± 0.12
0.05 ± 0.02
0.18 ± 0.09
0.07 ± 0.05
0.08 ± 0.06