

-- STATS maxD --

min ESS = 111.434407355497

max BMK = 0.123309901341177

max MCSE = 6.90640874868653

all stationary: FALSE

burn: 0

max rel.err.: 2.07081951375692

-- STATS 2D --

min ESS = 4064.52517199526

max BMK = 0.0373206921114645

max MCSE = 1.86321031681907

all stationary: TRUE

burn: 0

max rel.err.: 1.78694355188441

-- STATS 1D --

min ESS = 1817.77756973607

max BMK = 0.0449912807155352

max MCSE = 2.55176502996884

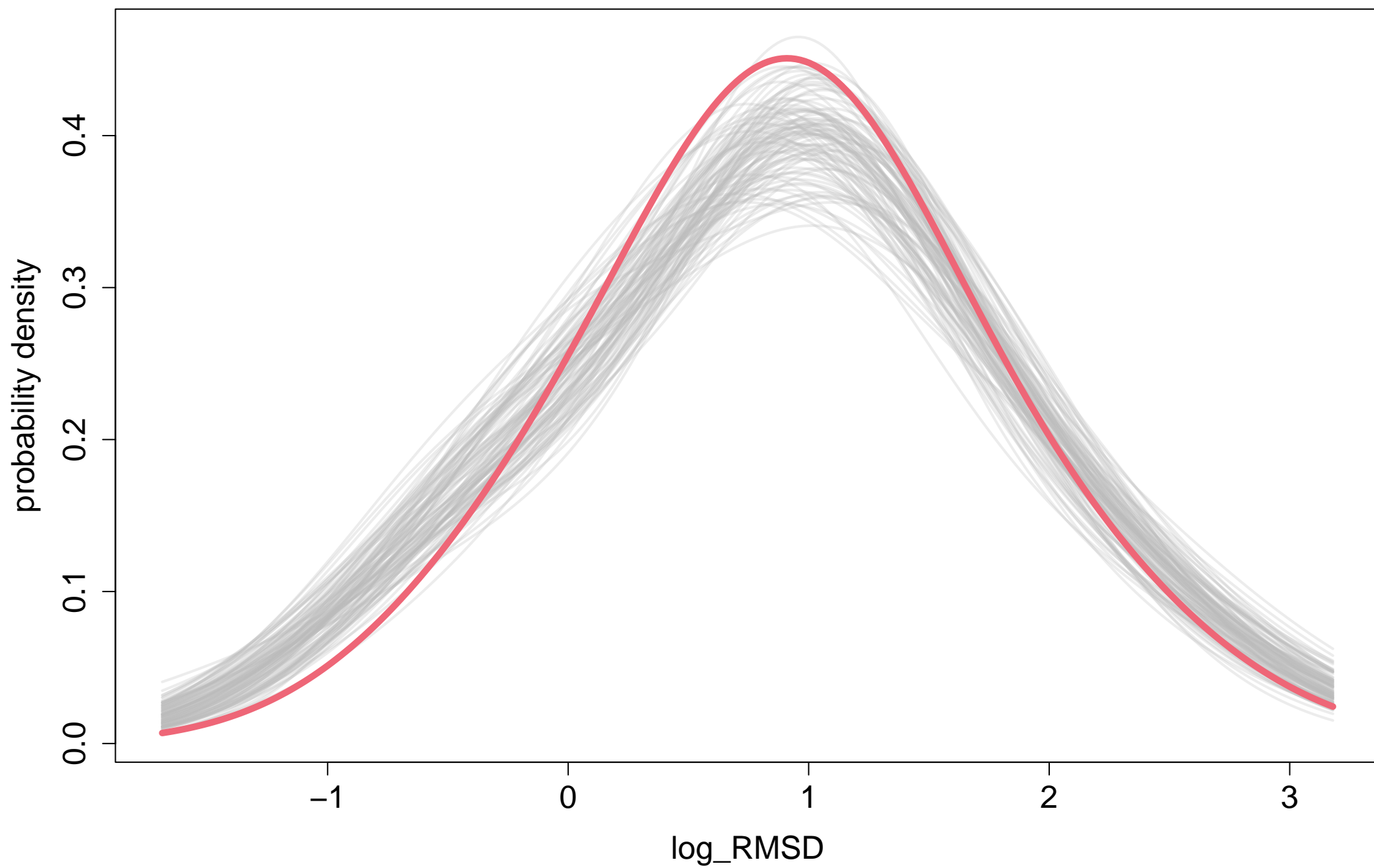
all stationary: TRUE

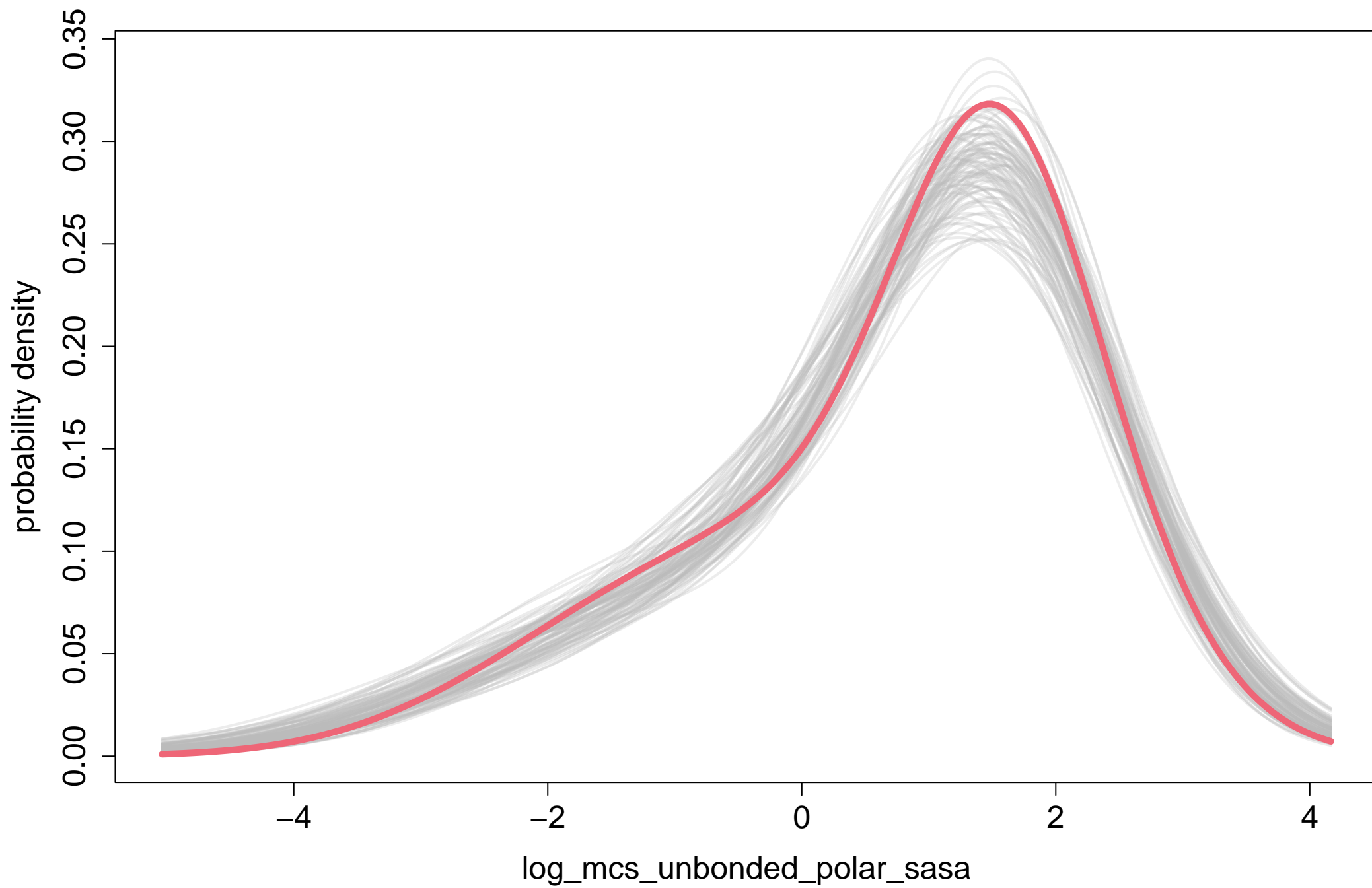
burn: 0

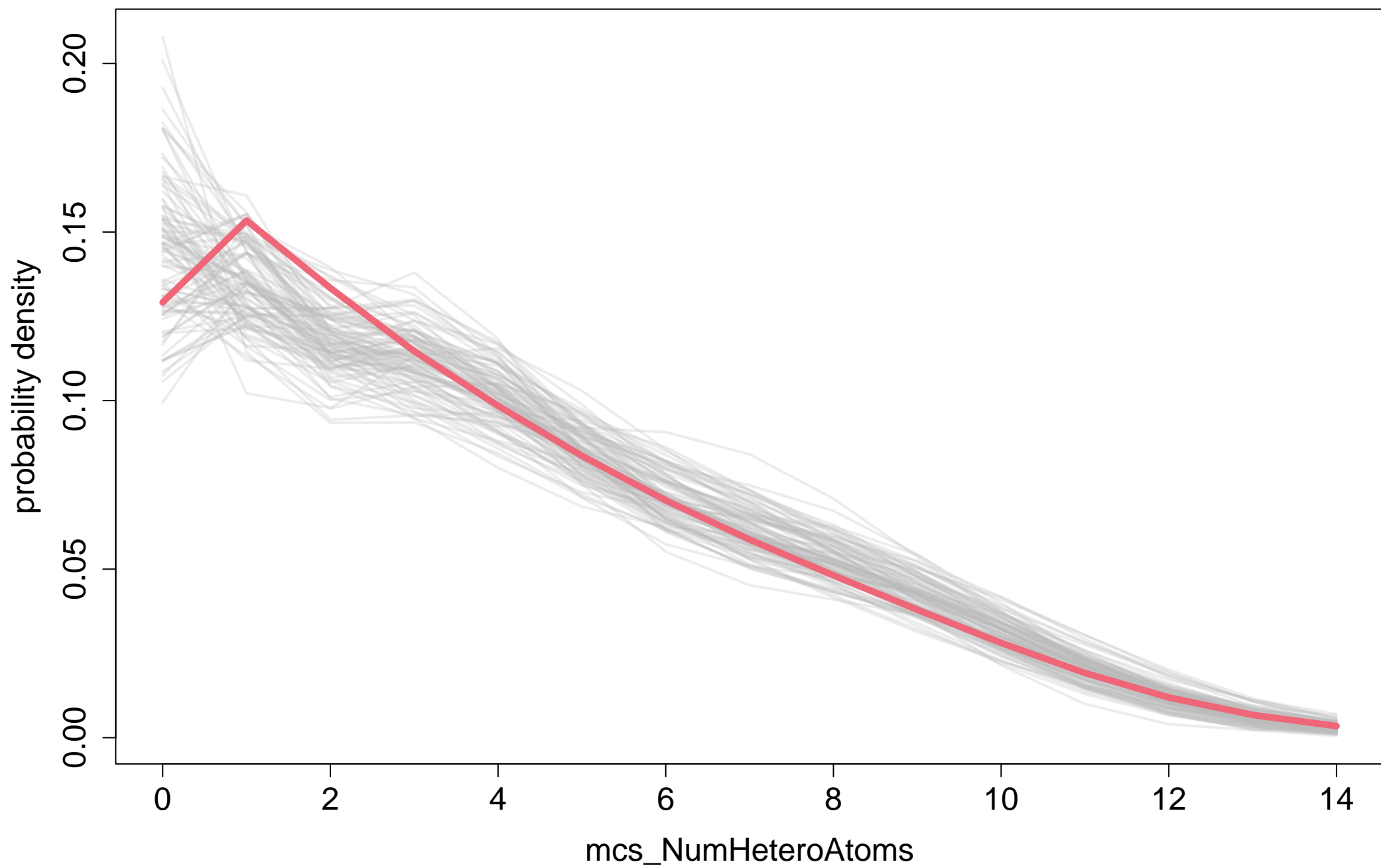
max rel.err.: 2.34394957310721

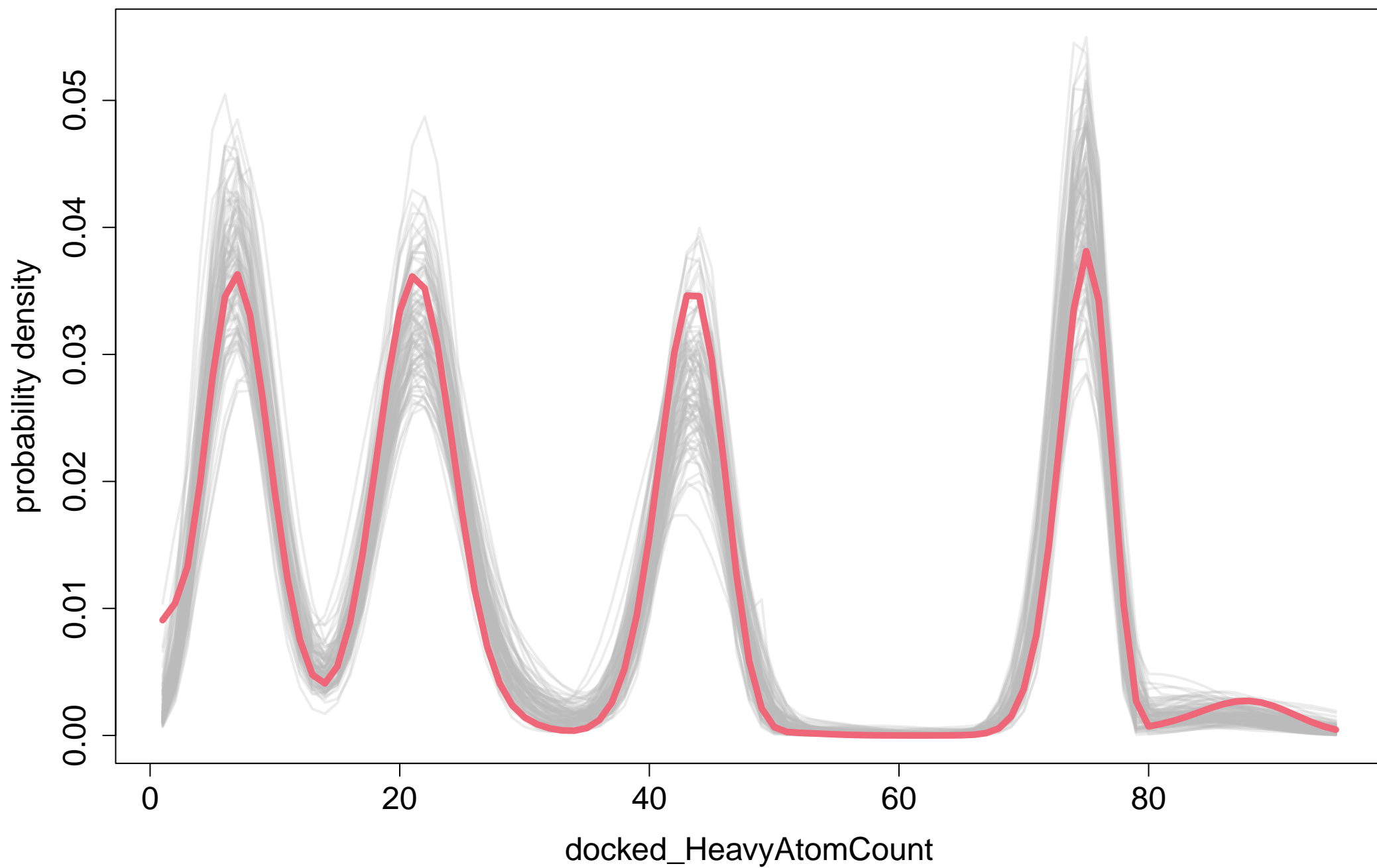
Occupied clusters: 10 of 16

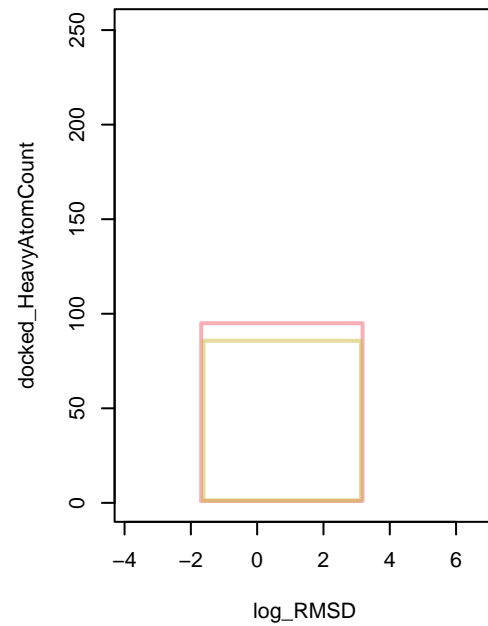
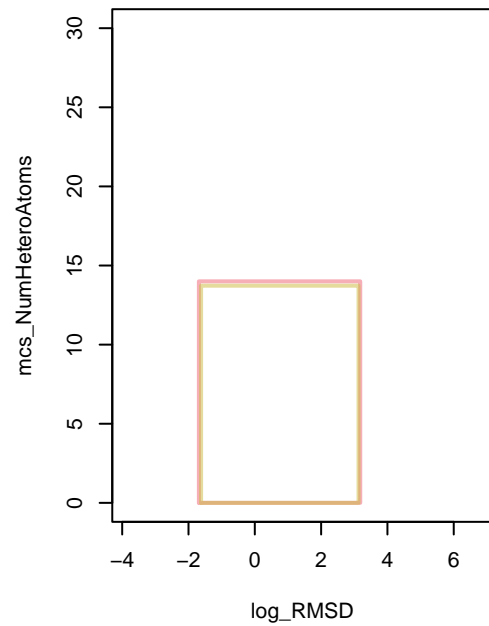
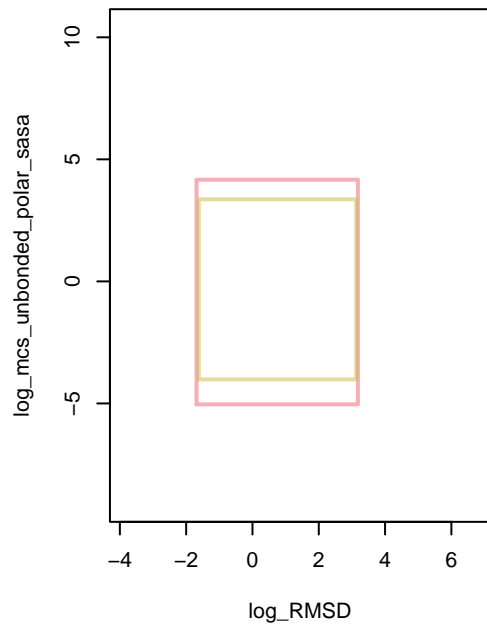
LL: -2160 +- 6.64



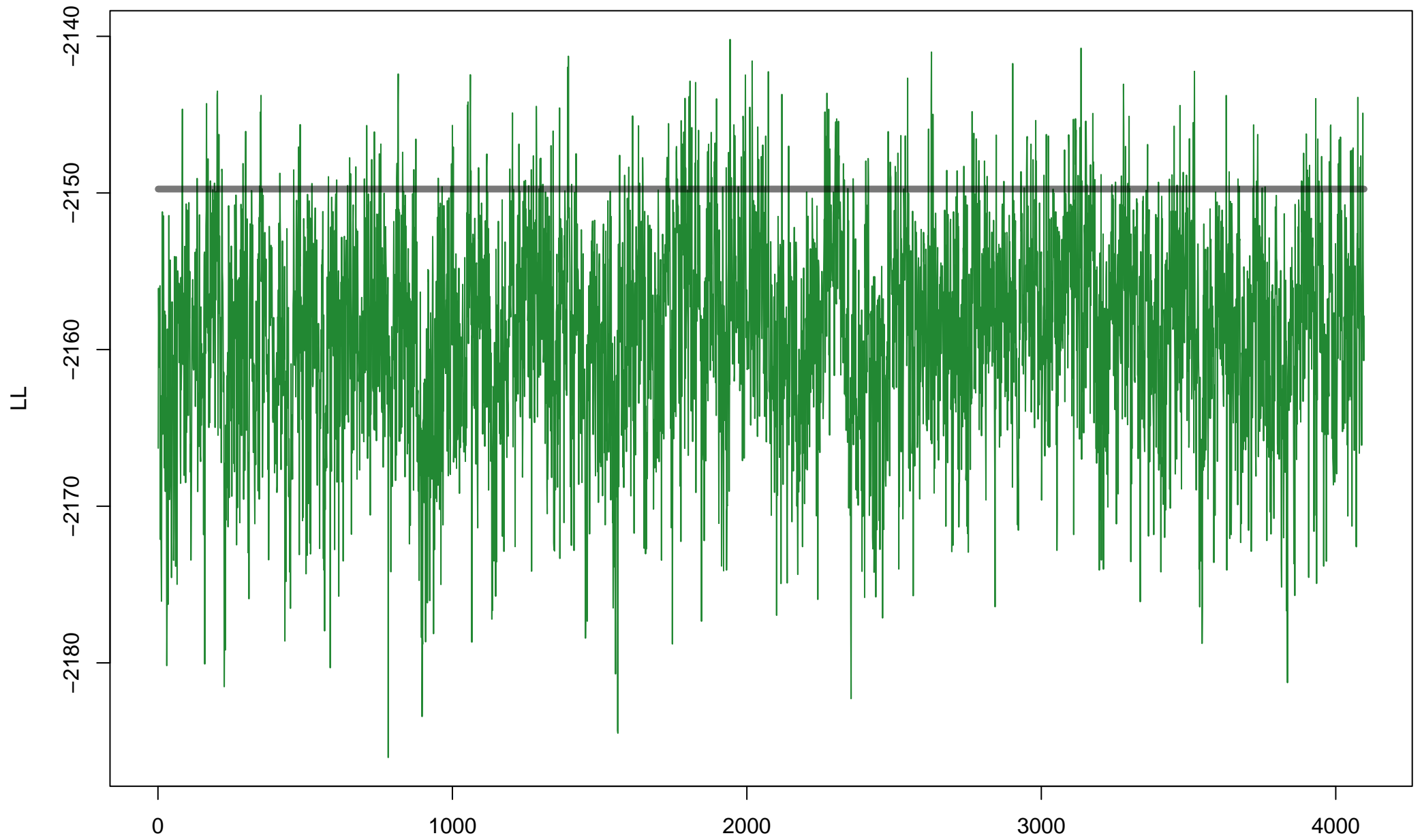






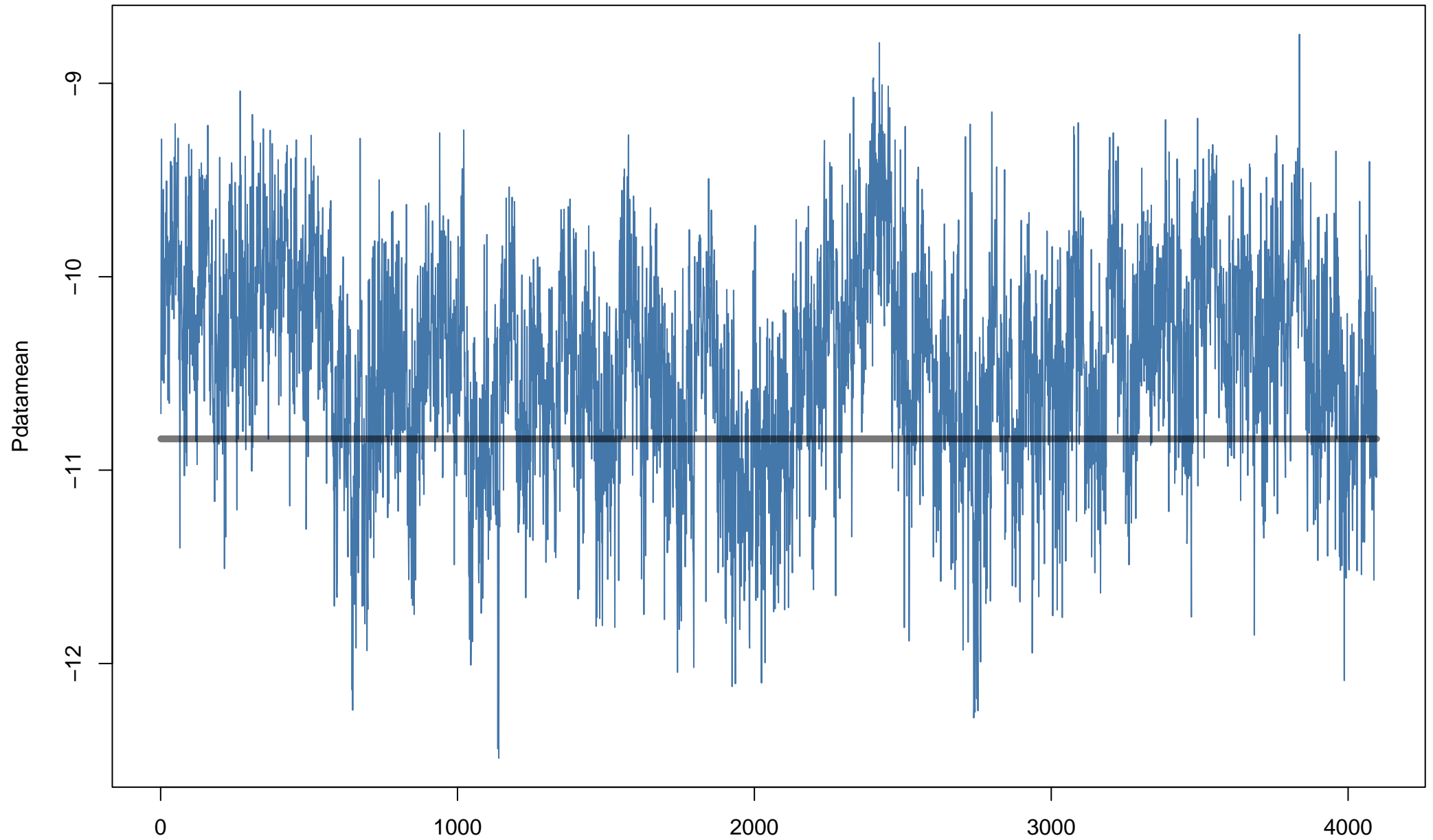


LL

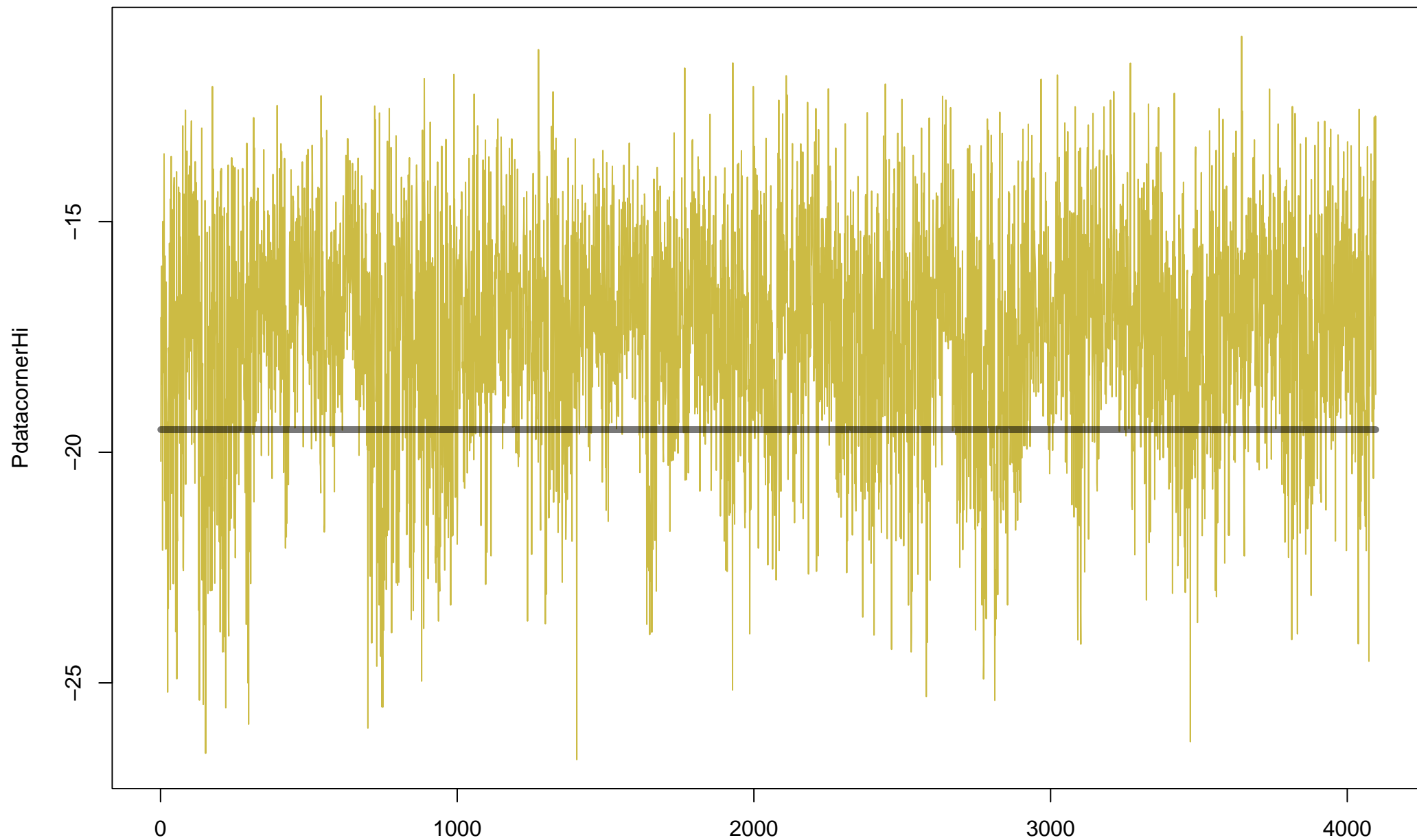


Pdatamean

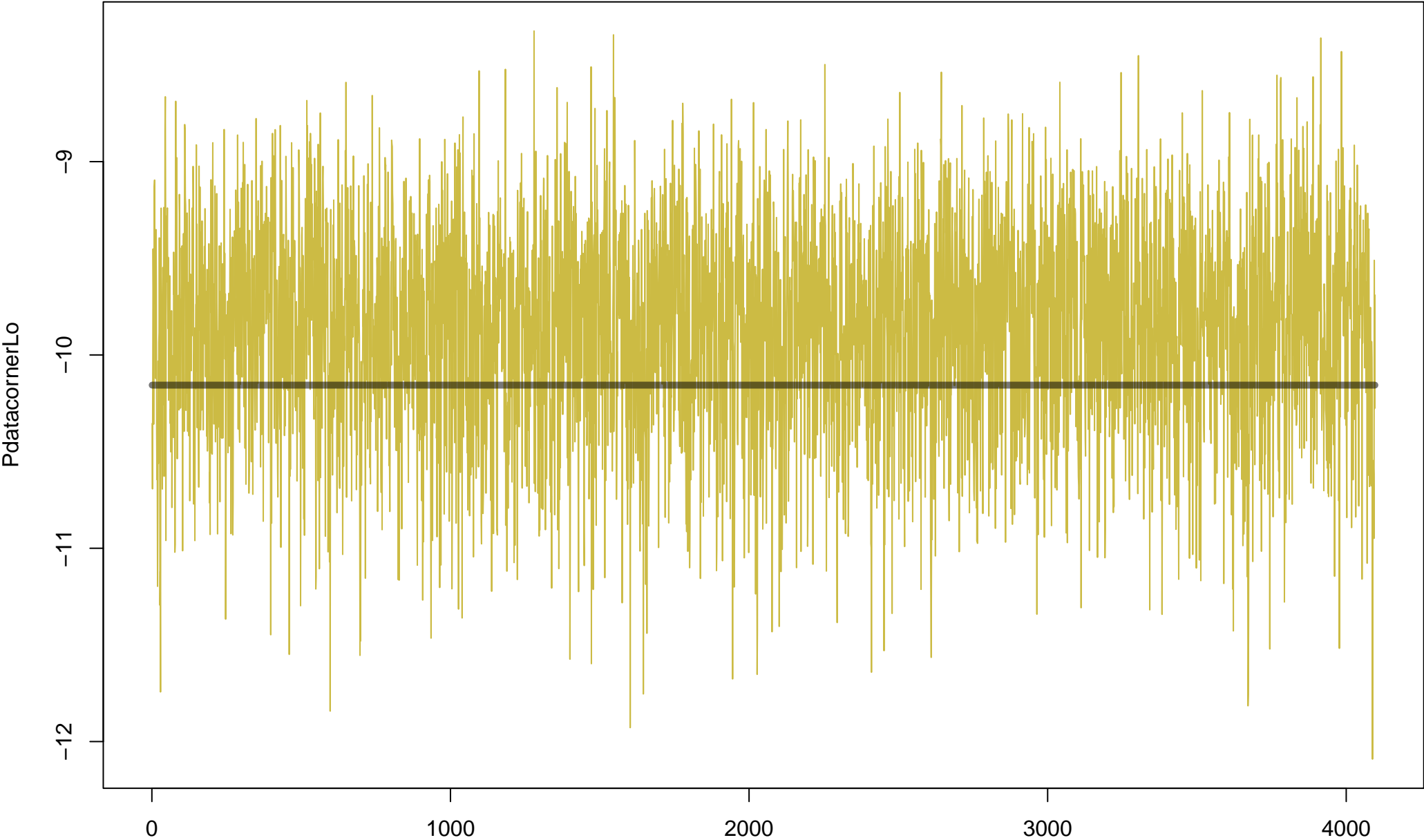
ESS = 111 | BMK = 0.0598 | MCSE(6.27) = 6.91 | stat: FALSE | burn: 0 | rel.err: 0.758



PdatacornerHi
ESS = 4100 | BMK = 0.123 | MCSE(6.27) = 1.4 | stat: TRUE | burn: 0 | rel.err: 0.313

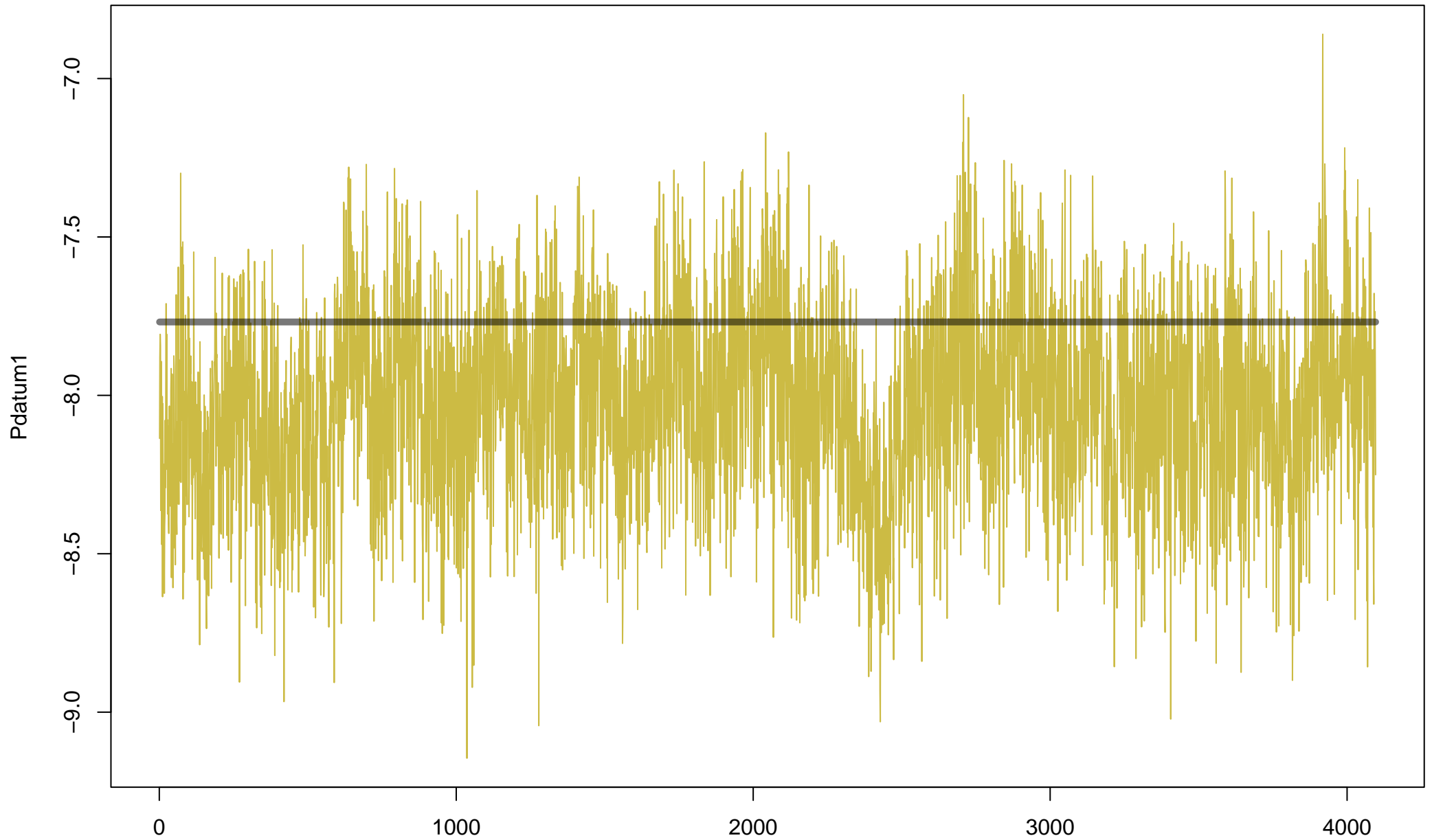


PdatacornerLo
ESS = 2340 | BMK = 0.0387 | MCSE(6.27) = 2 | stat: TRUE | burn: 0 | rel.err: 0.649

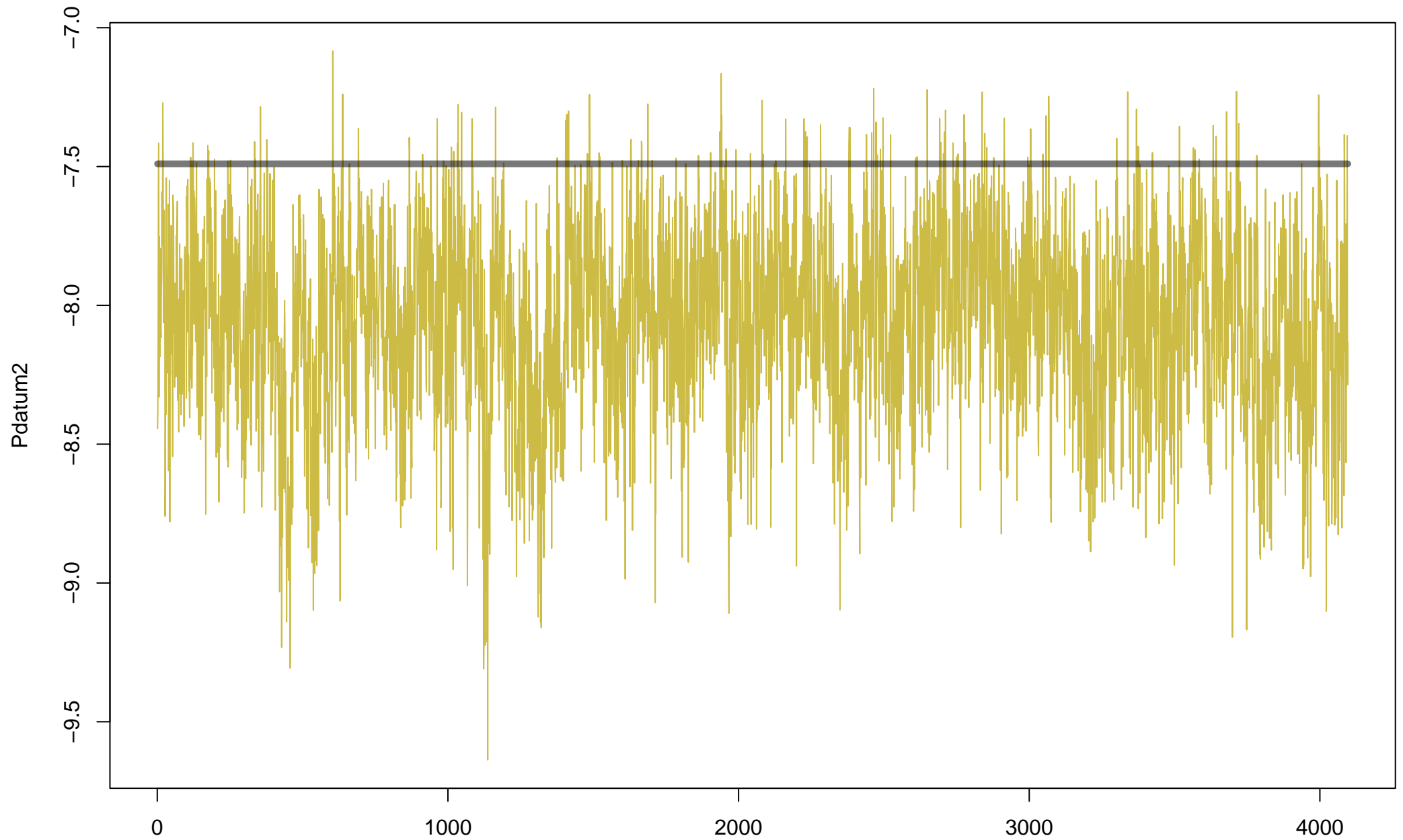


Pdatum1

ESS = 293 | BMK = 0.0381 | MCSE(6.27) = 4.87 | stat: FALSE | burn: 0 | rel.err: -0.79

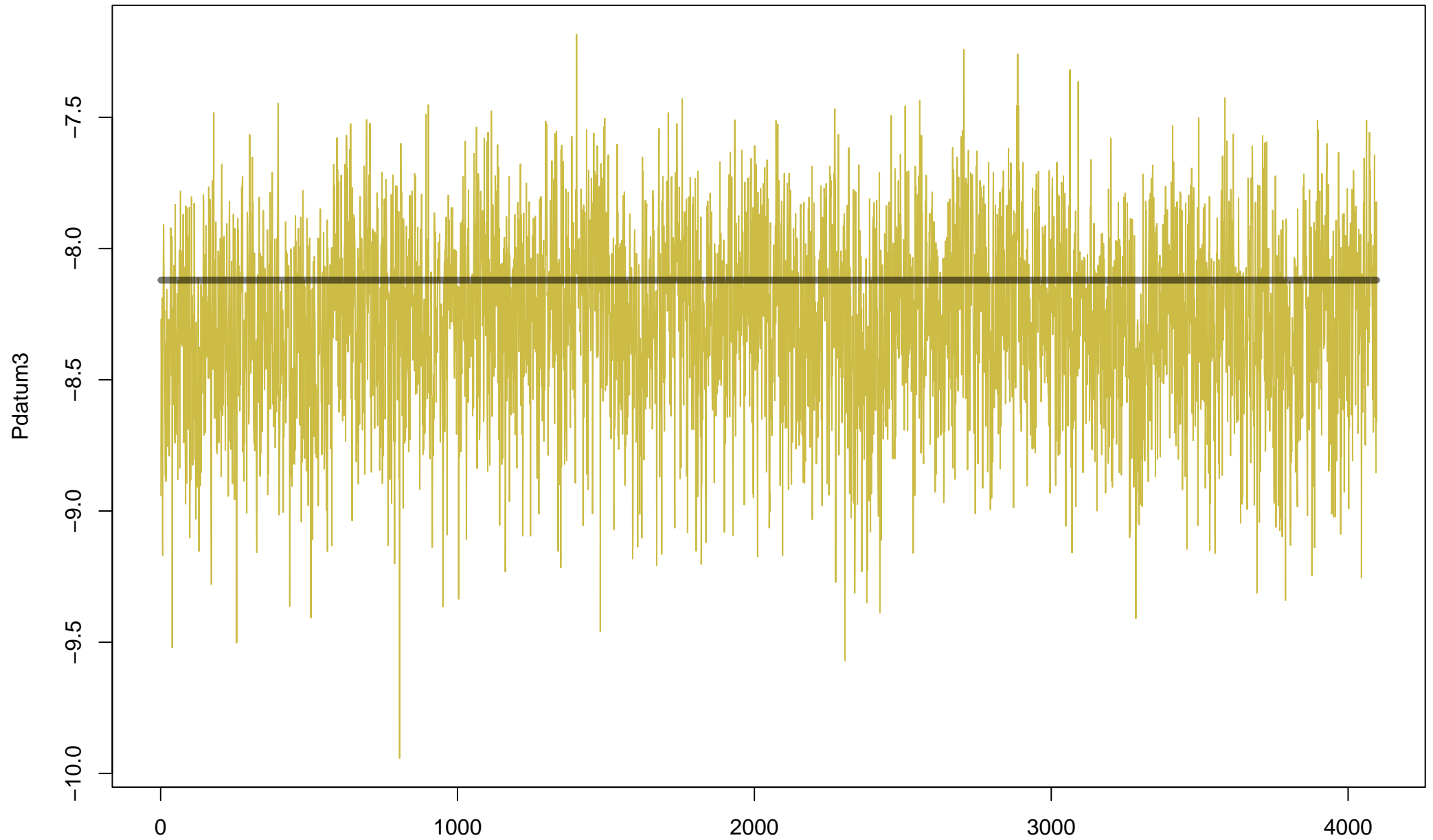


Pdatum2
ESS = 562 | BMK = 0.0526 | MCSE(6.27) = 4.45 | stat: TRUE | burn: 0 | rel.err: -2.07



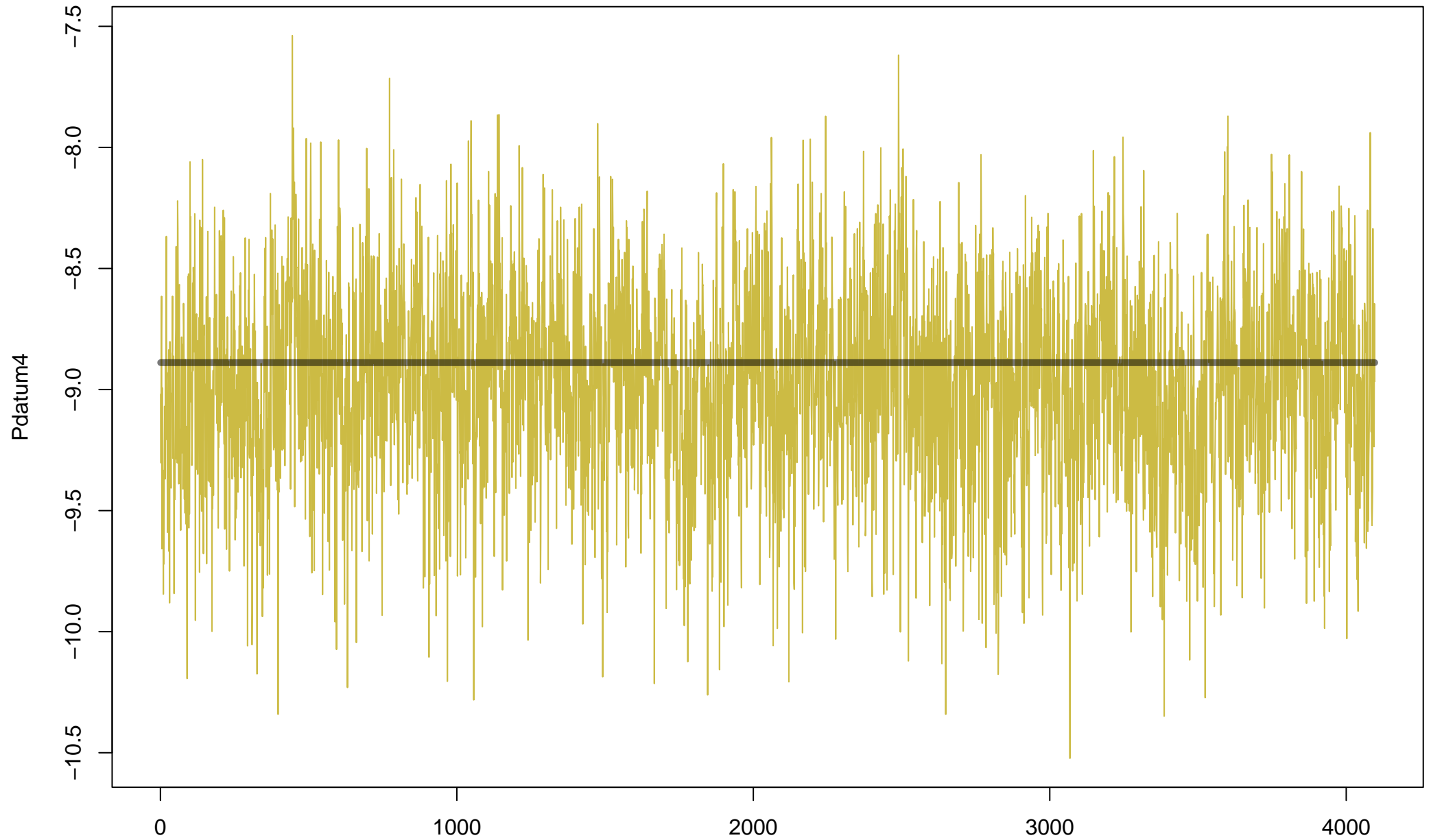
Pdatum3

ESS = 1080 | BMK = 0.036 | MCSE(6.27) = 3.13 | stat: FALSE | burn: 0 | rel.err: -0.31

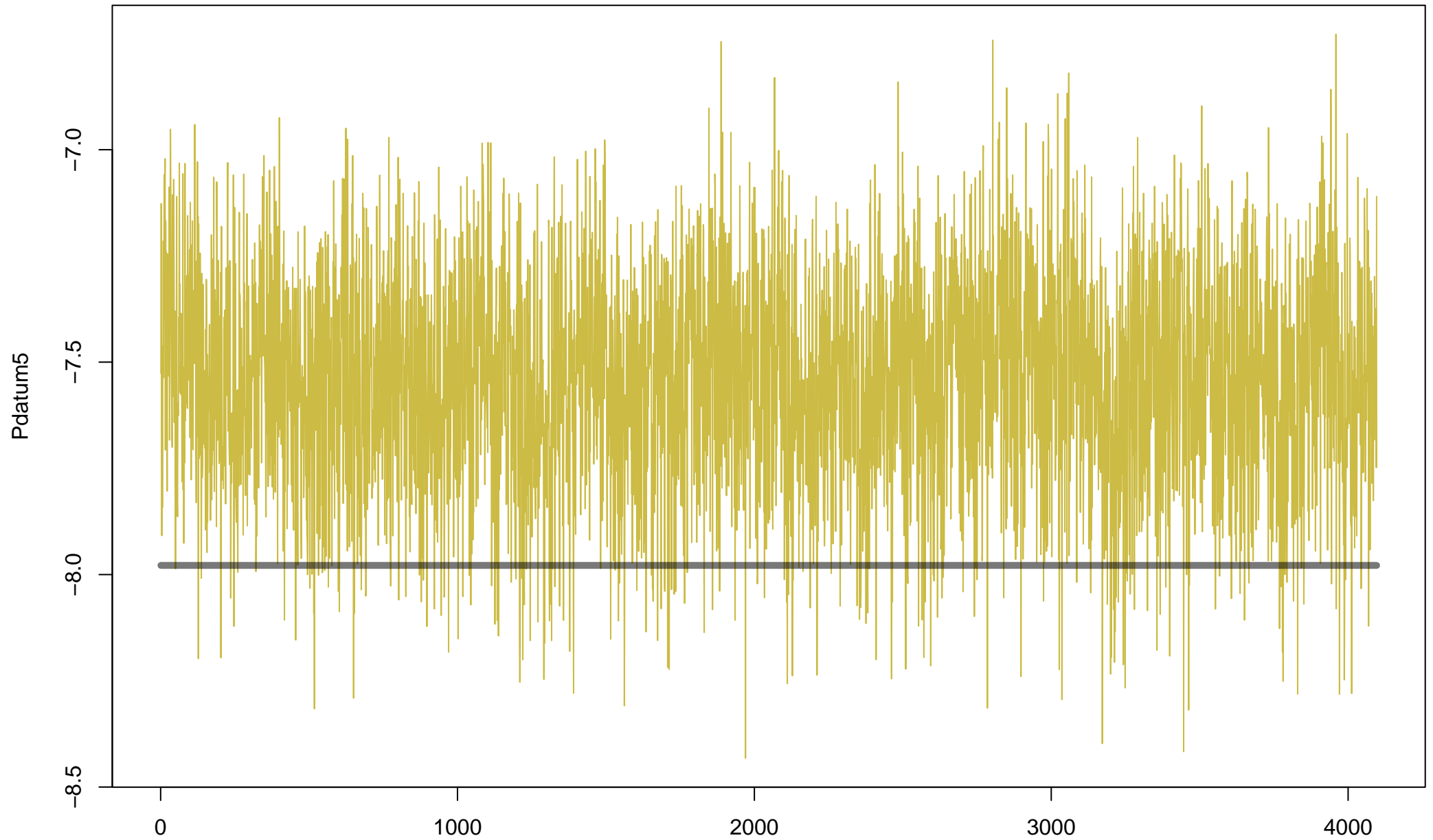


Pdatum4

ESS = 982 | BMK = 0.042 | MCSE(6.27) = 3.29 | stat: FALSE | burn: 0 | rel.err: -0.0192

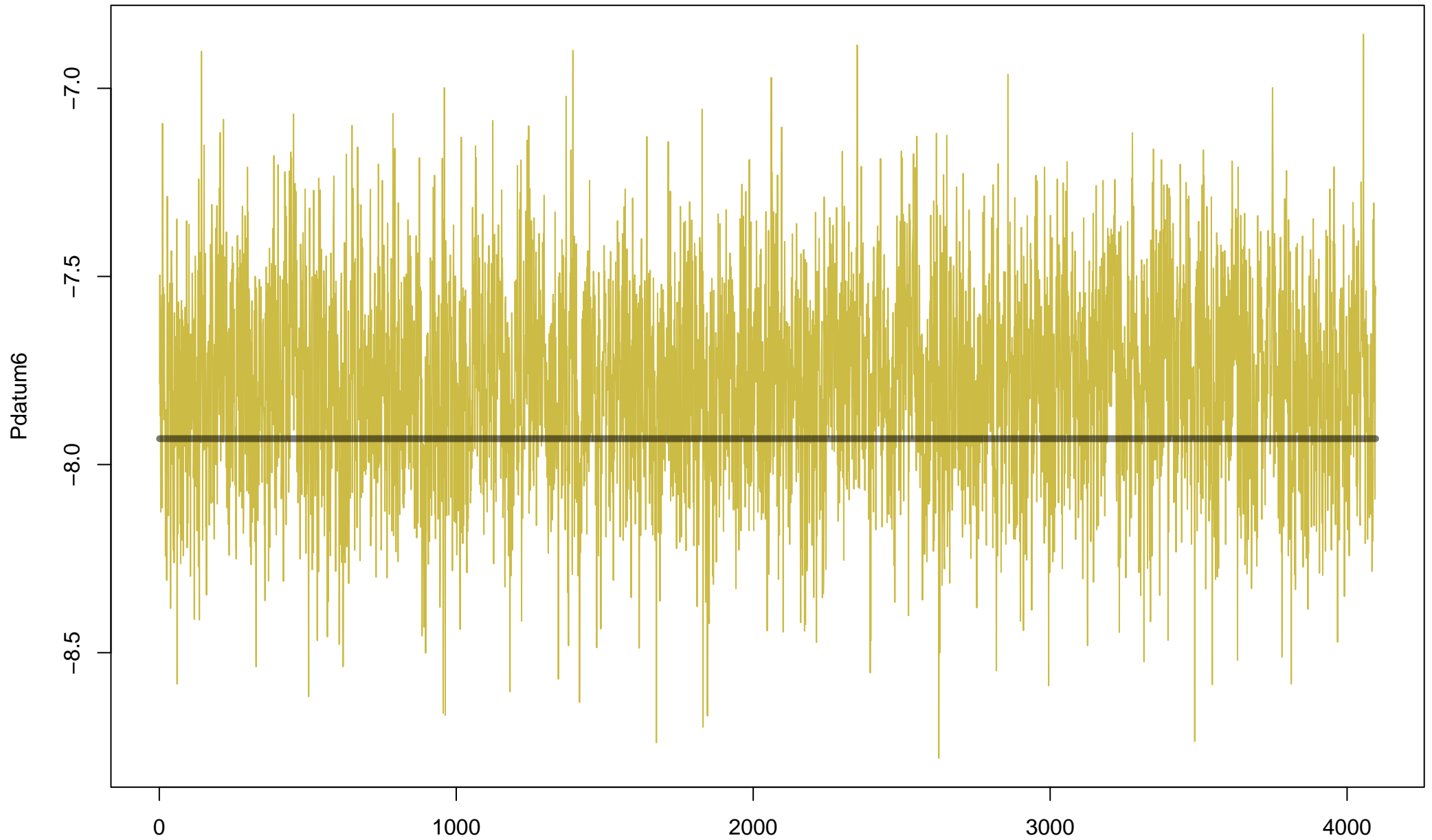


Pdatum5
ESS = 1090 | BMK = 0.0378 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: 1.5



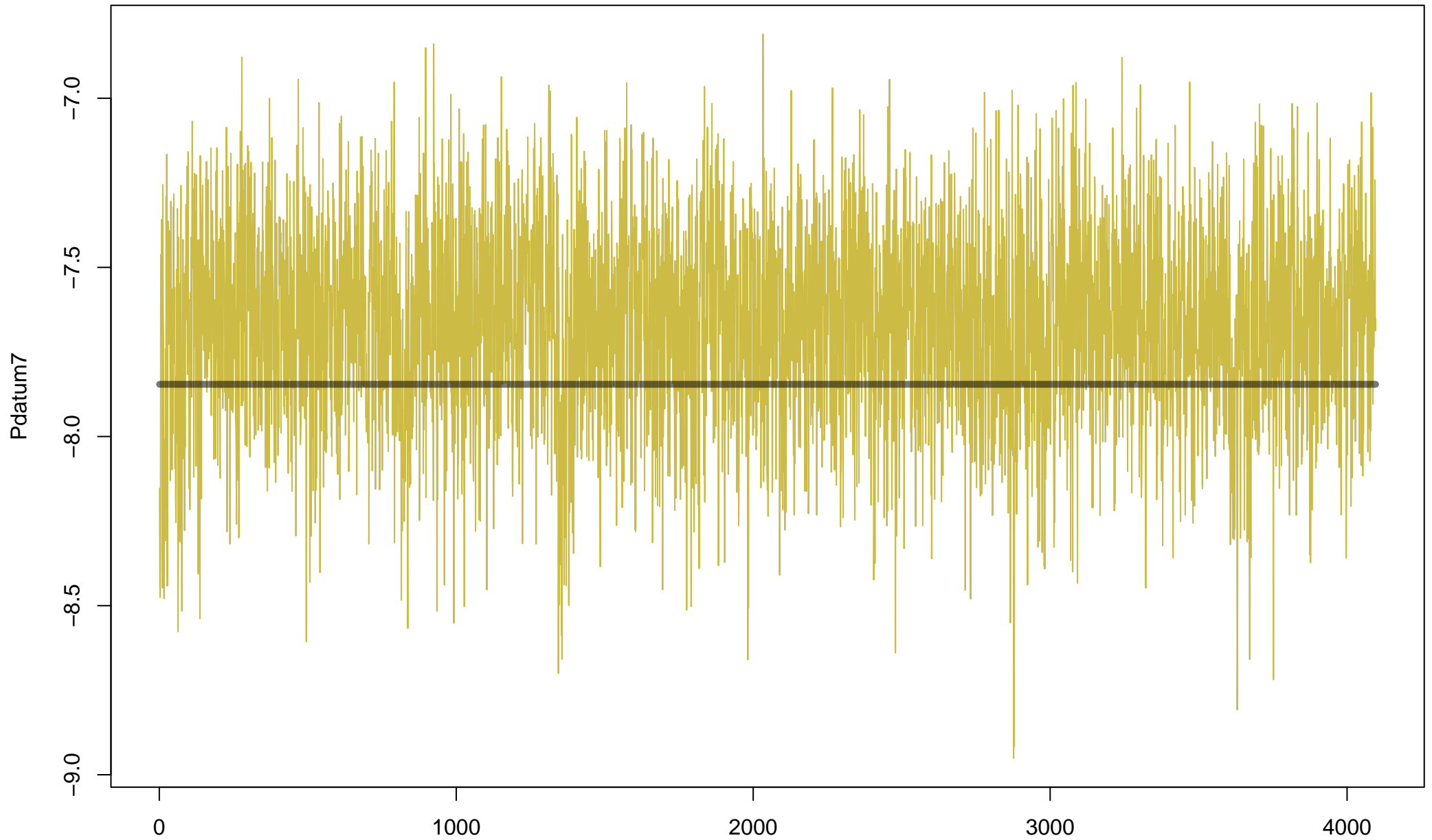
Pdatum6

ESS = 1910 | BMK = 0.0455 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | rel.err: 0.628



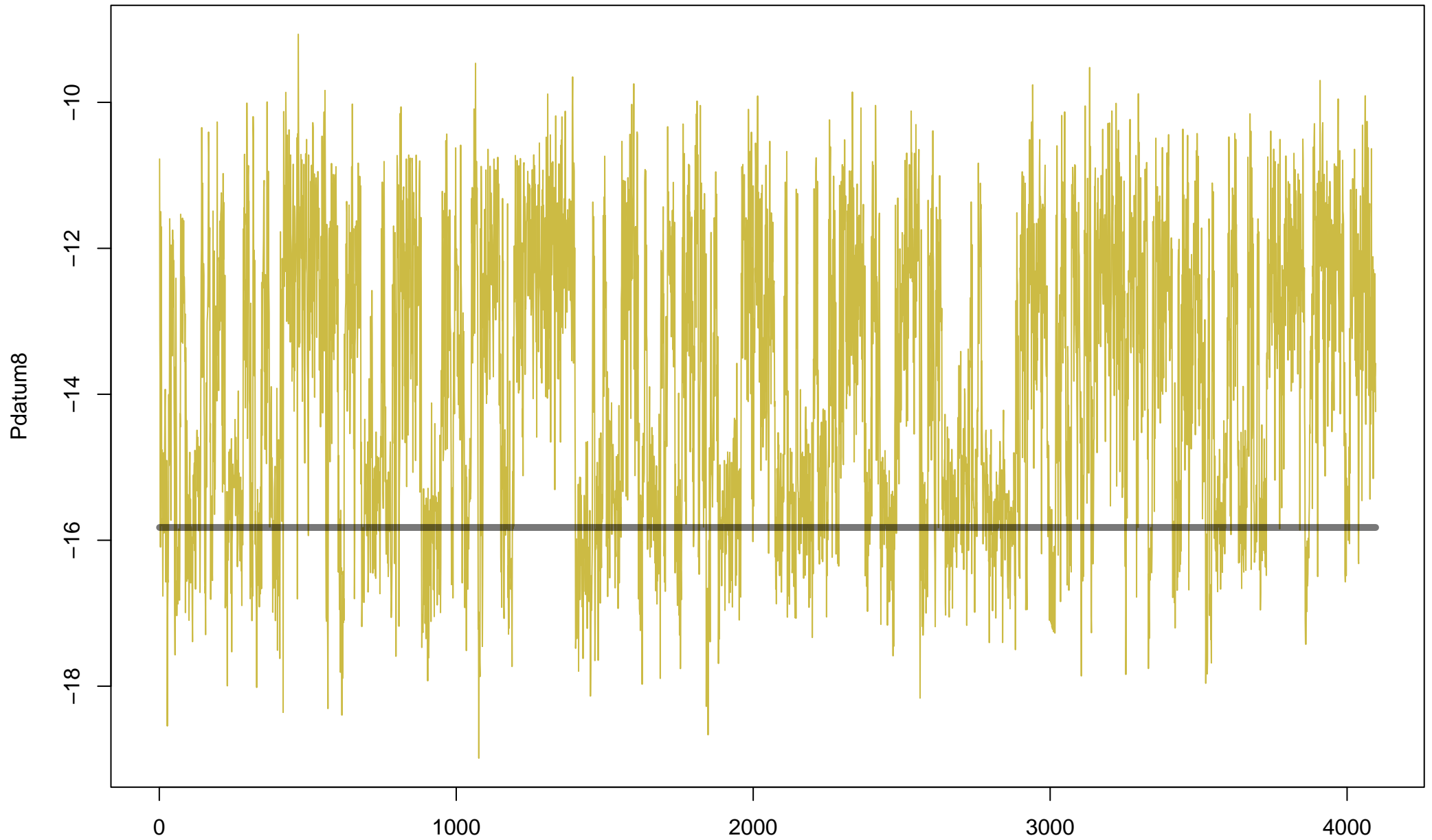
Pdatum7

ESS = 2980 | BMK = 0.0405 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: 0.698



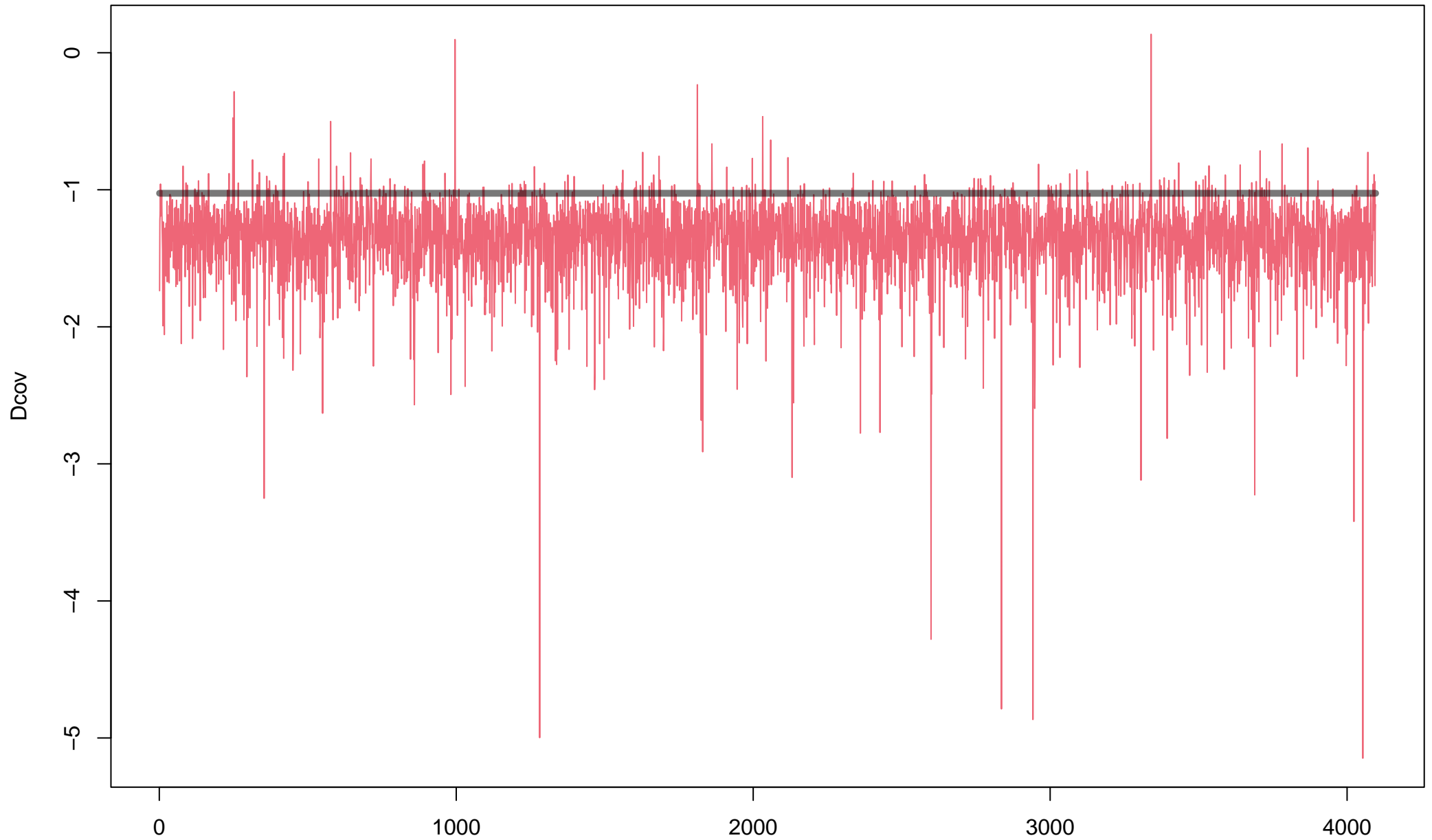
Pdatum8

ESS = 603 | BMK = 0.0545 | MCSE(6.27) = 4.03 | stat: FALSE | burn: 0 | rel.err: 0.551



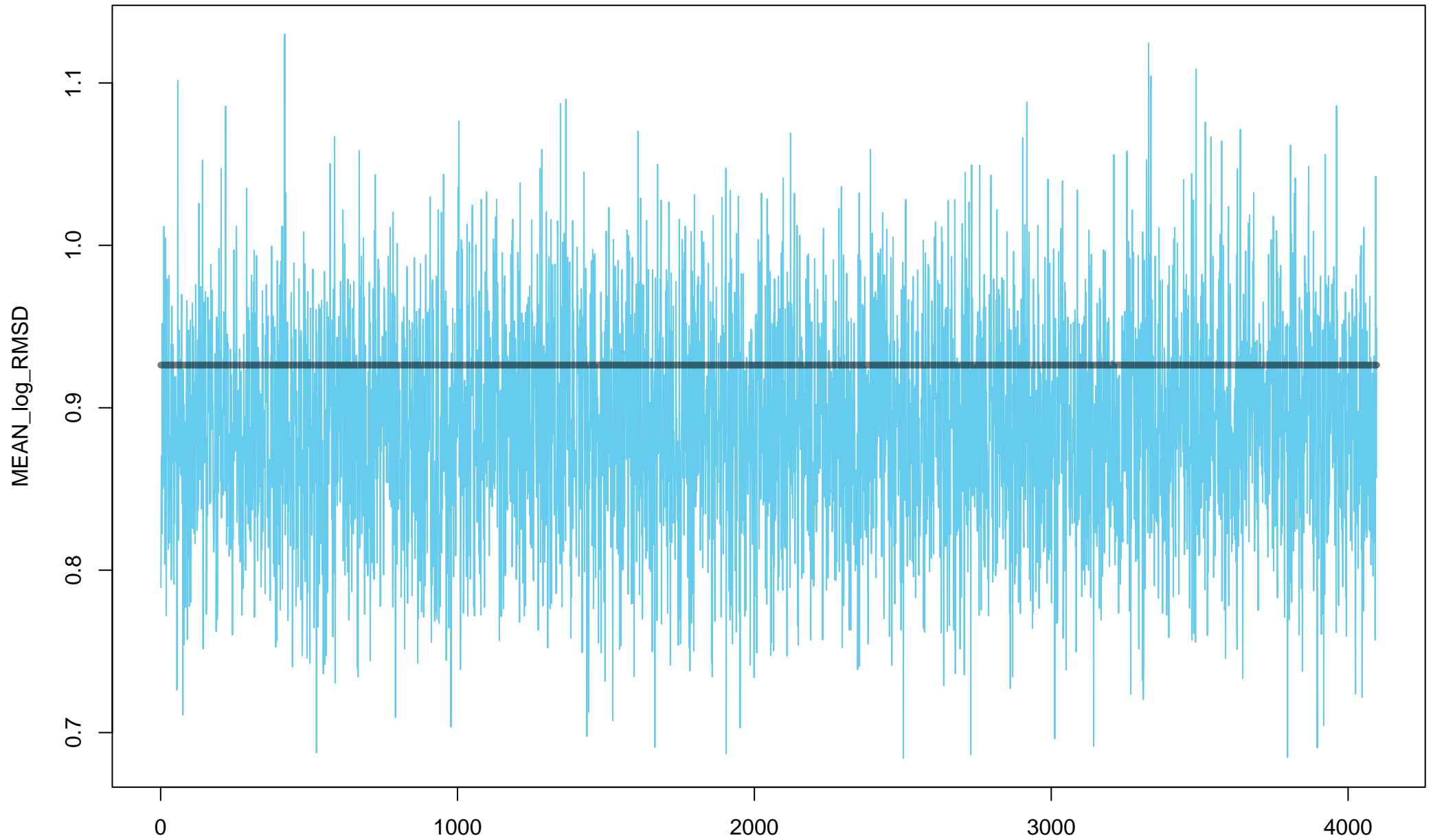
Dcov

ESS = 3310 | BMK = 0.0619 | MCSE(6.27) = 1.8 | stat: TRUE | burn: 0 | rel.err: 1.39

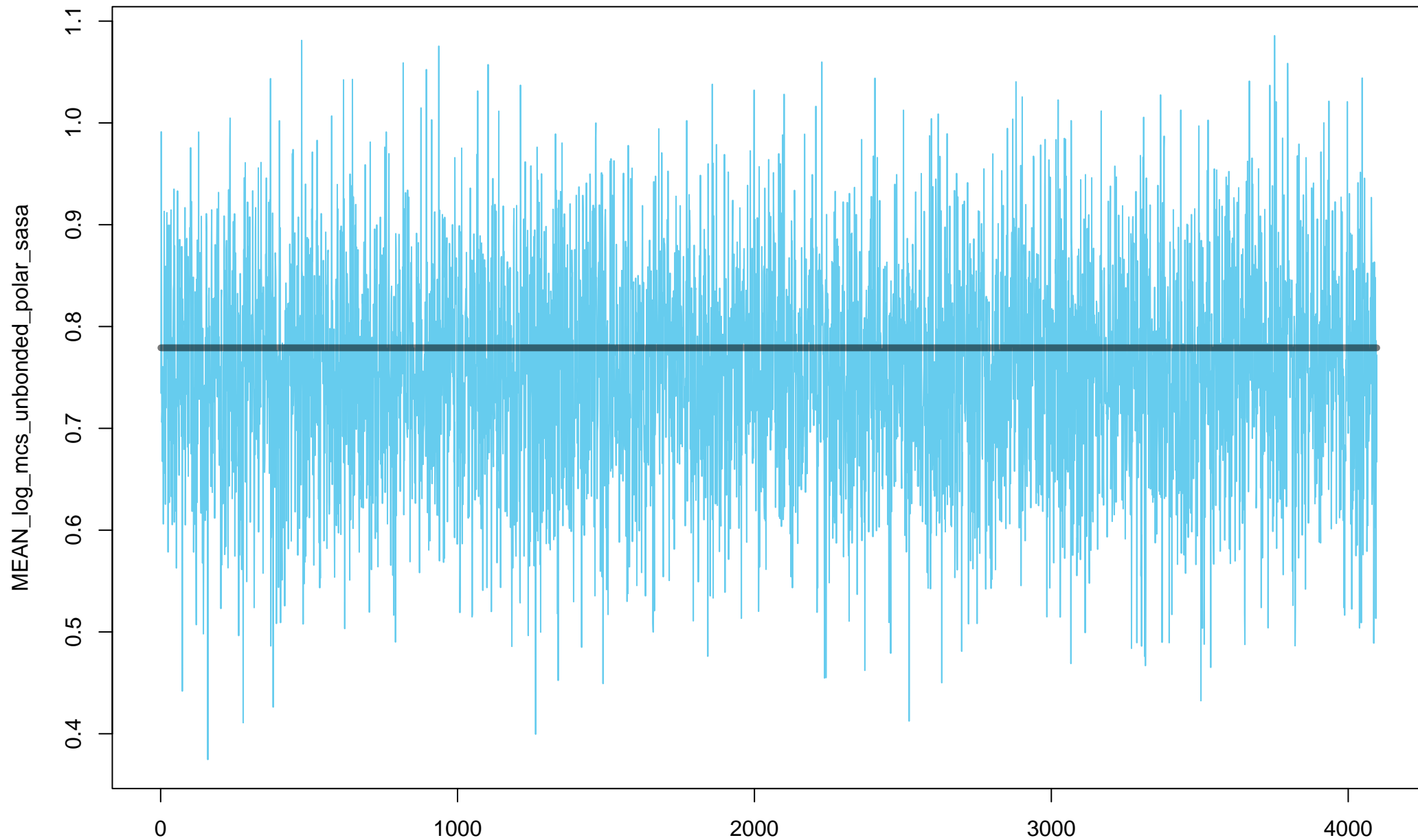


MEAN_log_RMSD

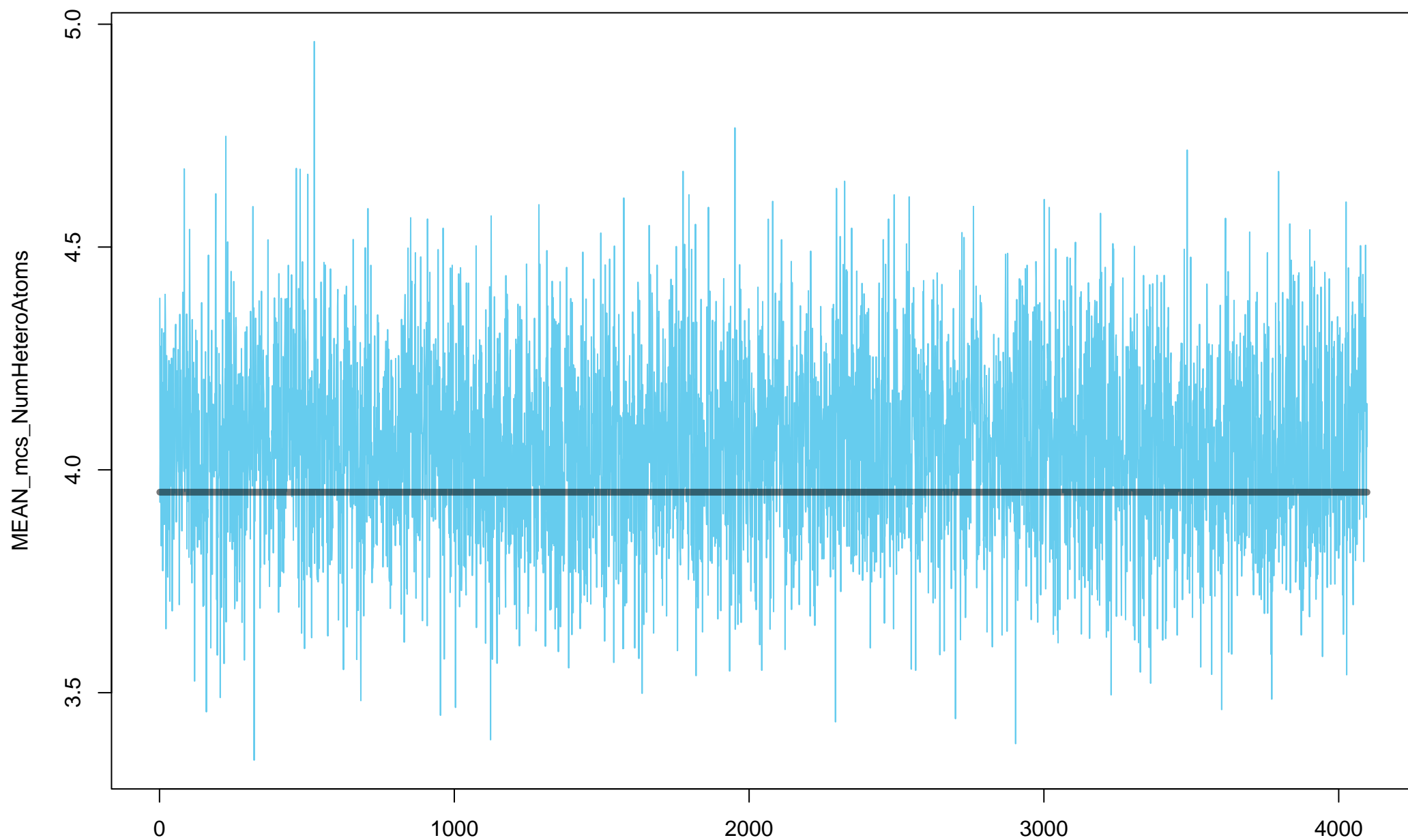
ESS = 4100 | BMK = 0.0348 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: -0.576



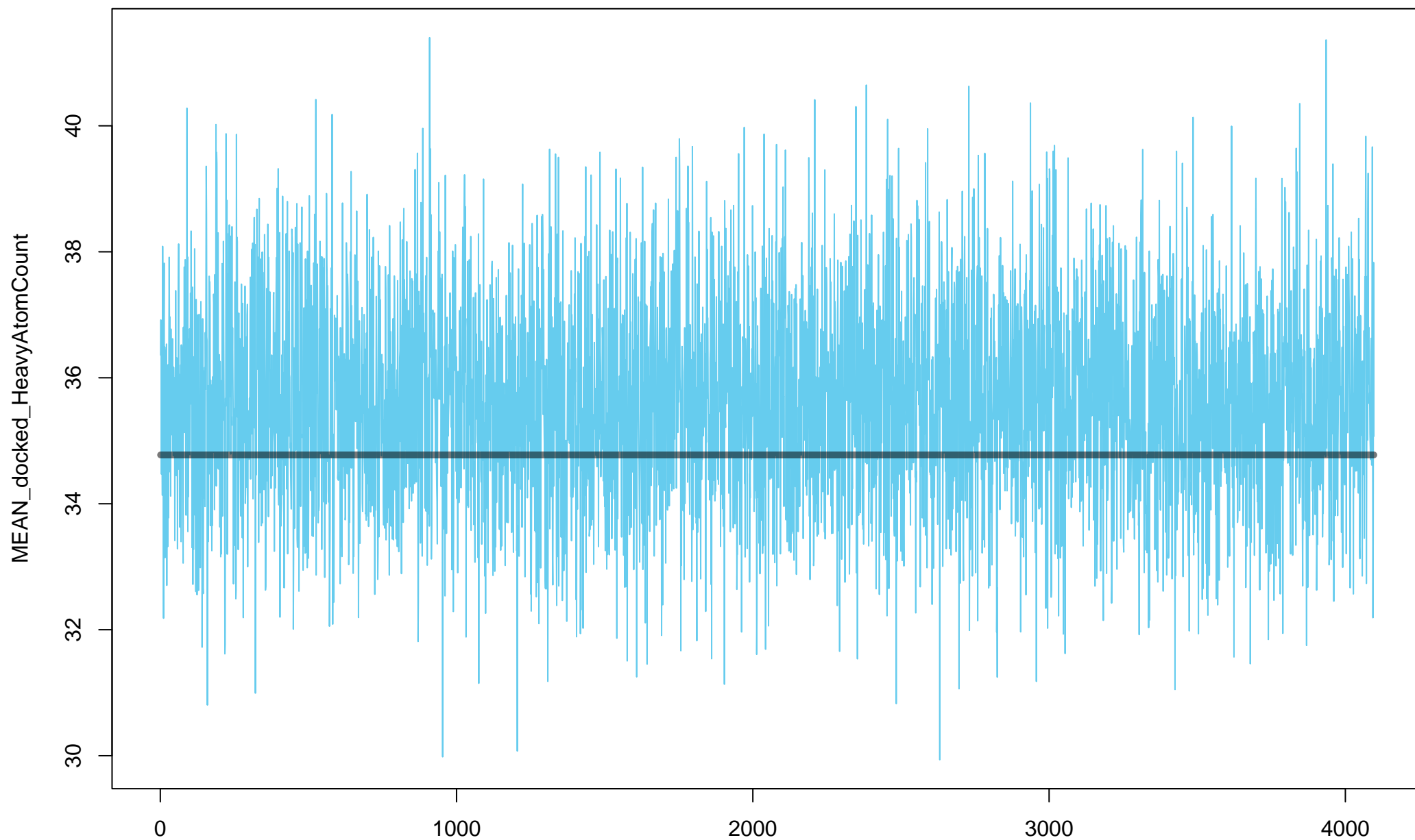
MEAN_log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.0326 | MCSE(6.27) = 1.48 | stat: TRUE | burn: 0 | rel.err: -0.218



MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0283 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: 0.507

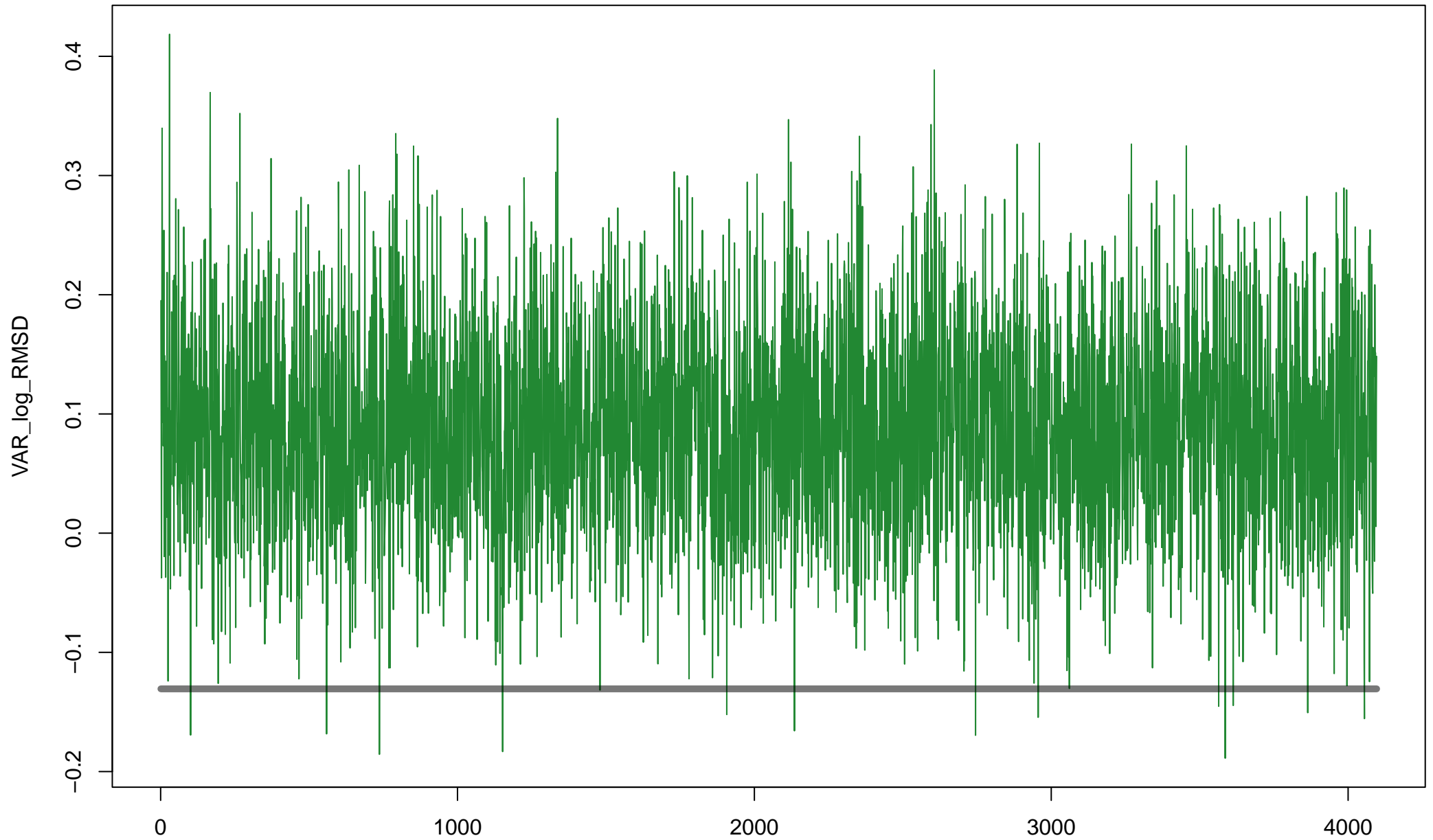


MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0258 | MCSE(6.27) = 1.54 | stat: TRUE | burn: 0 | rel.err: 0.519

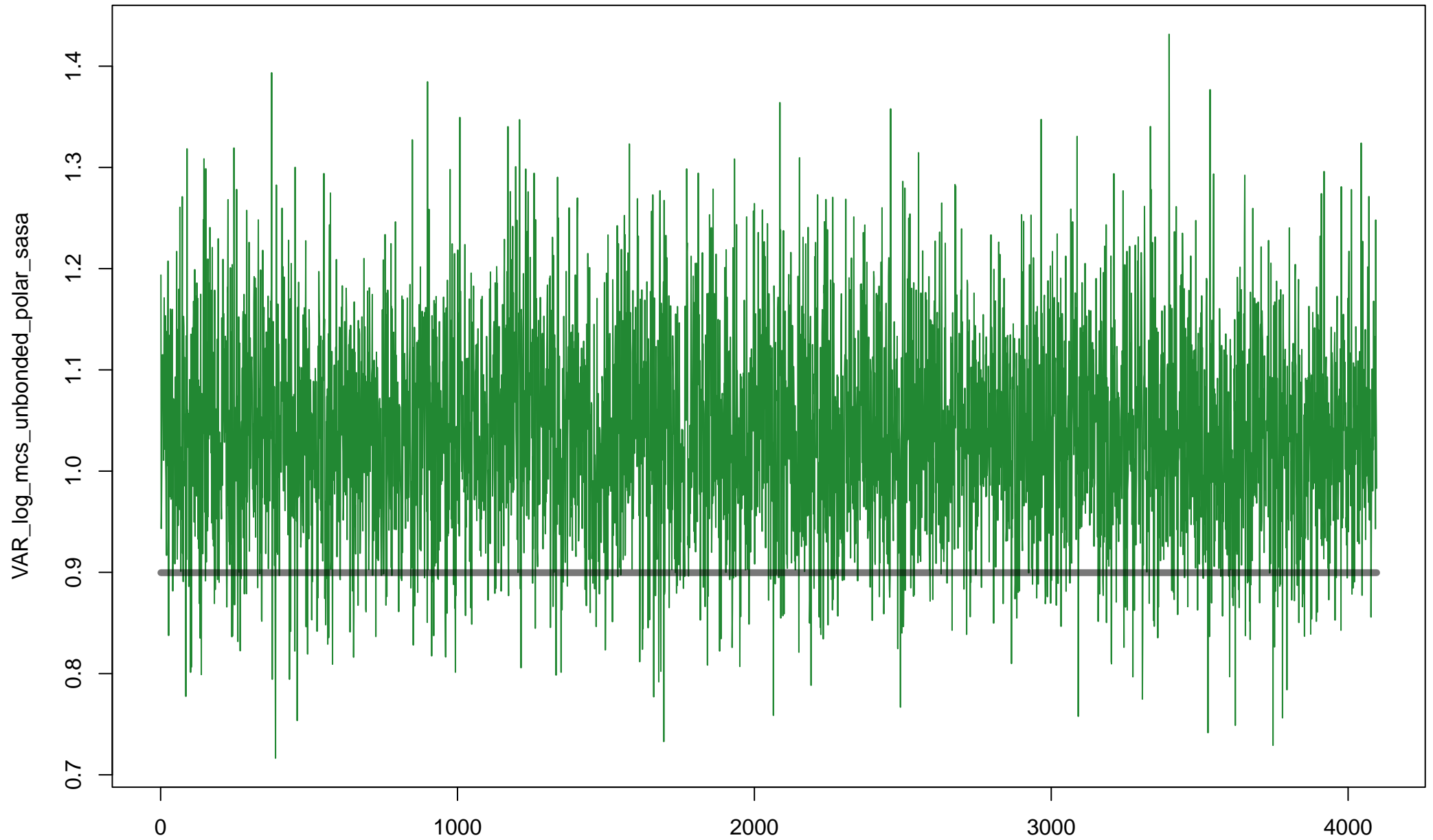


VAR_log_RMSD

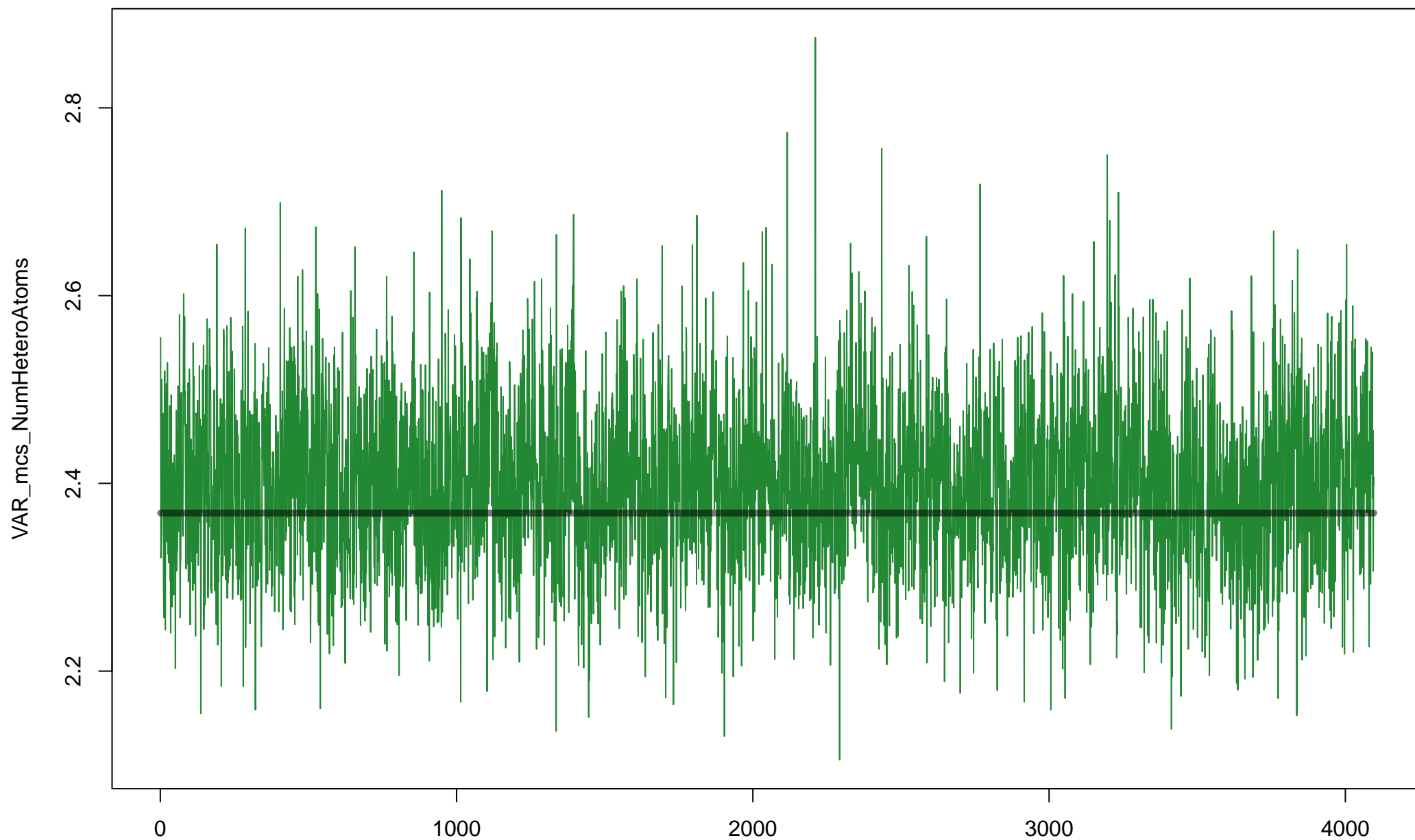
ESS = 3840 | BMK = 0.0254 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0 | rel.err: 2.34



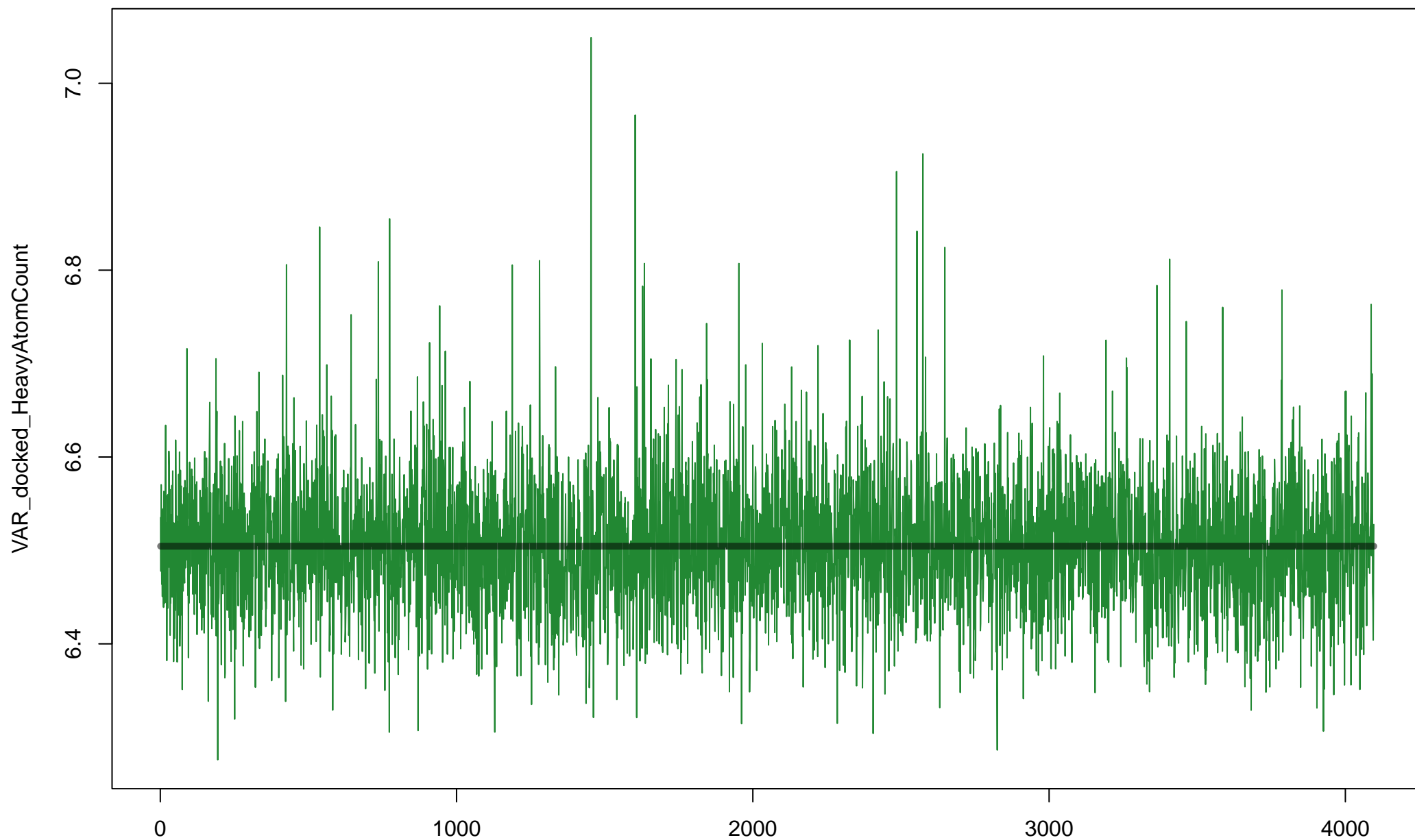
VAR_log_mcs_unbonded_polar_sasa
ESS = 3900 | BMK = 0.0348 | MCSE(6.27) = 1.72 | stat: TRUE | burn: 0 | rel.err: 1.35



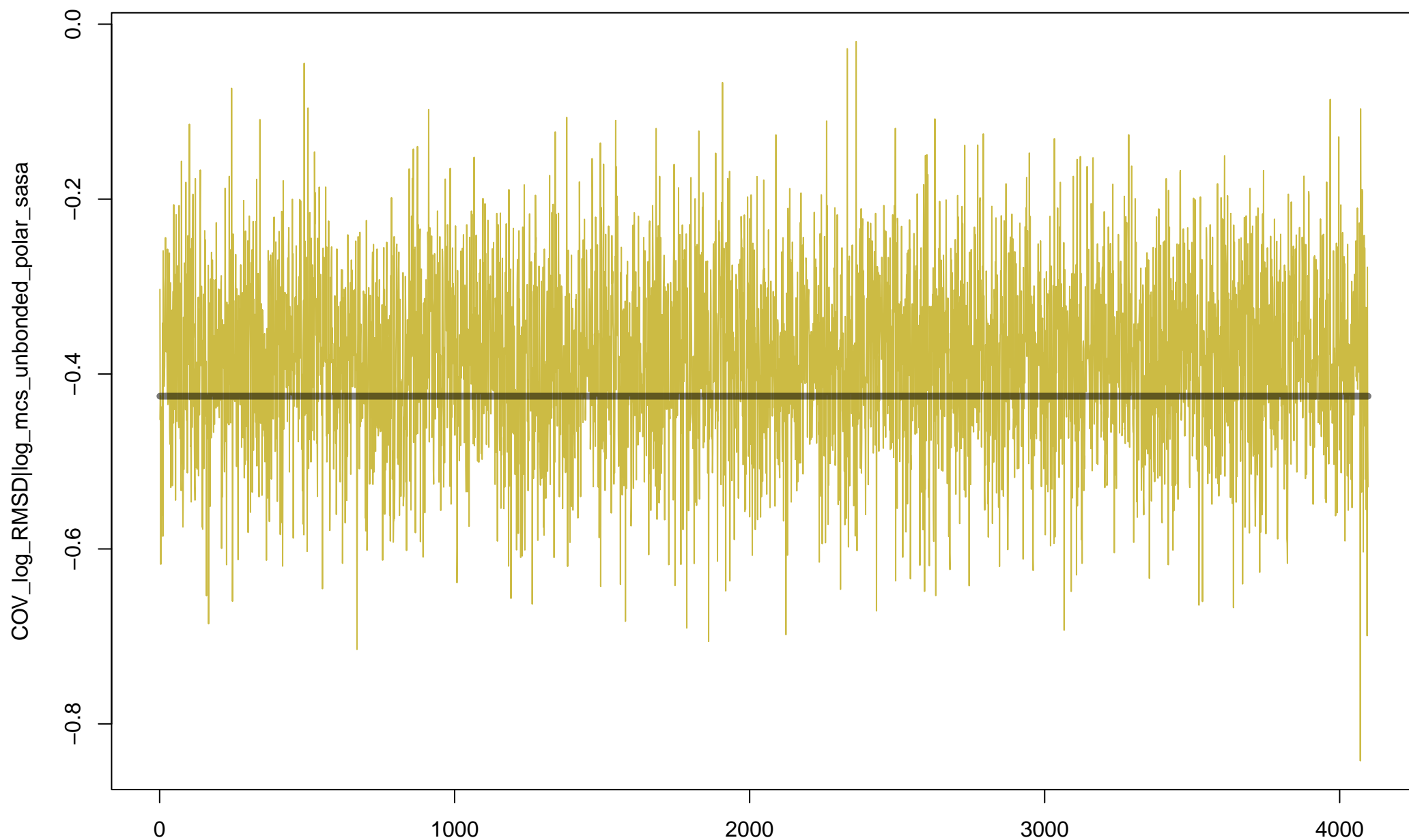
VAR_mcs_NumHeteroAtoms
ESS = 1820 | BMK = 0.0426 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: 0.397



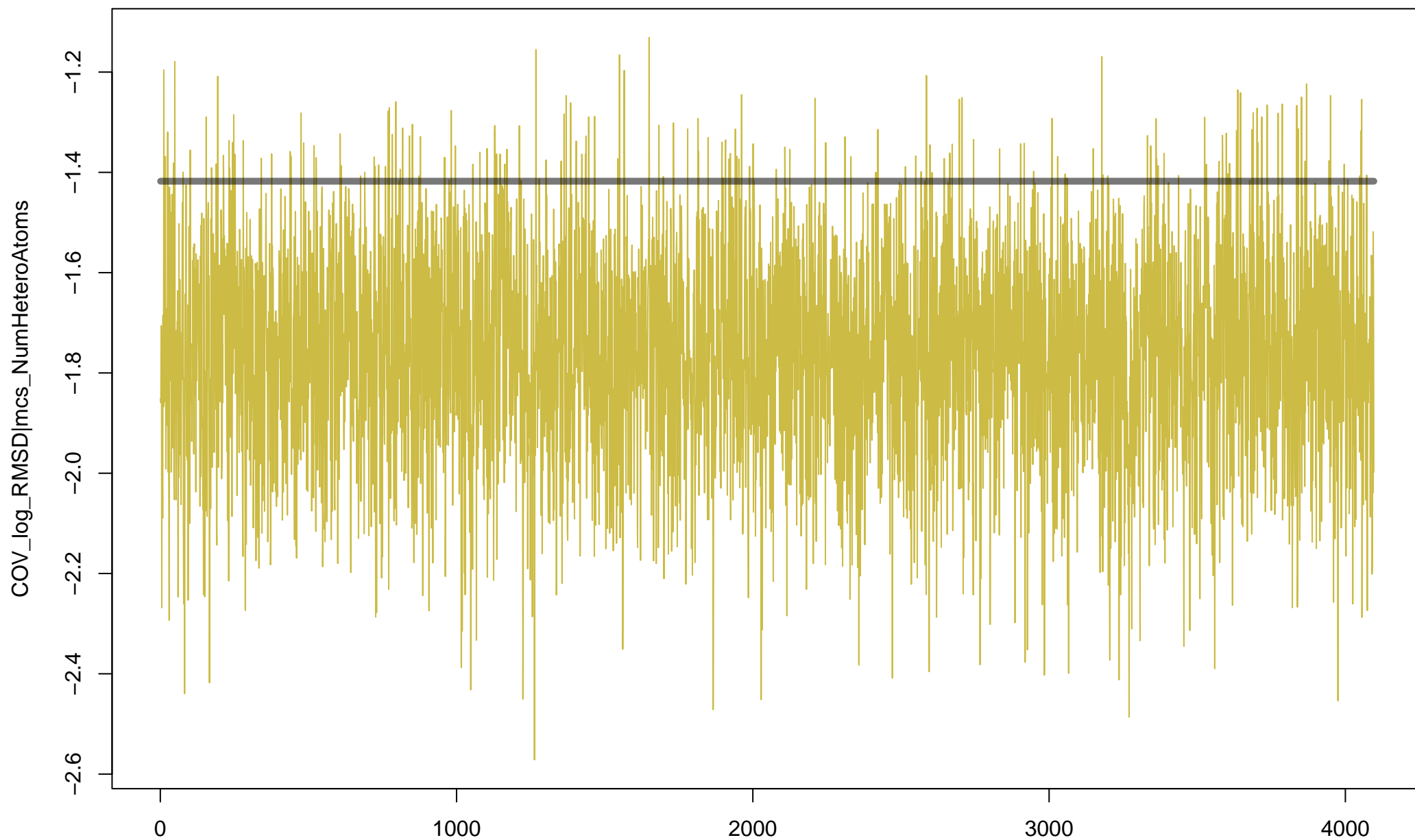
VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.045 | MCSE(6.27) = 1.81 | stat: TRUE | burn: 0 | rel.err: 0.0673



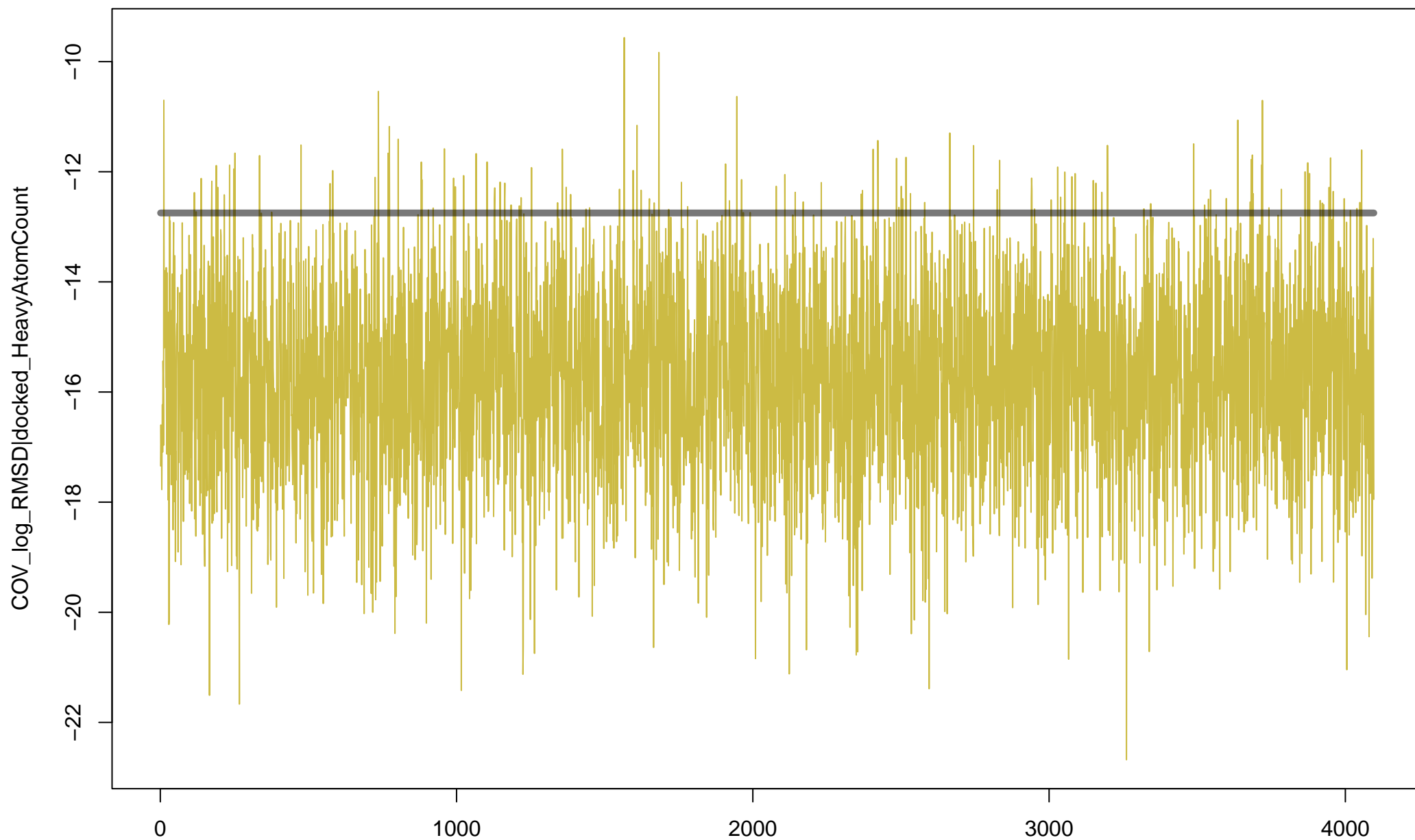
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 4070 | BMK = 0.0247 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.439



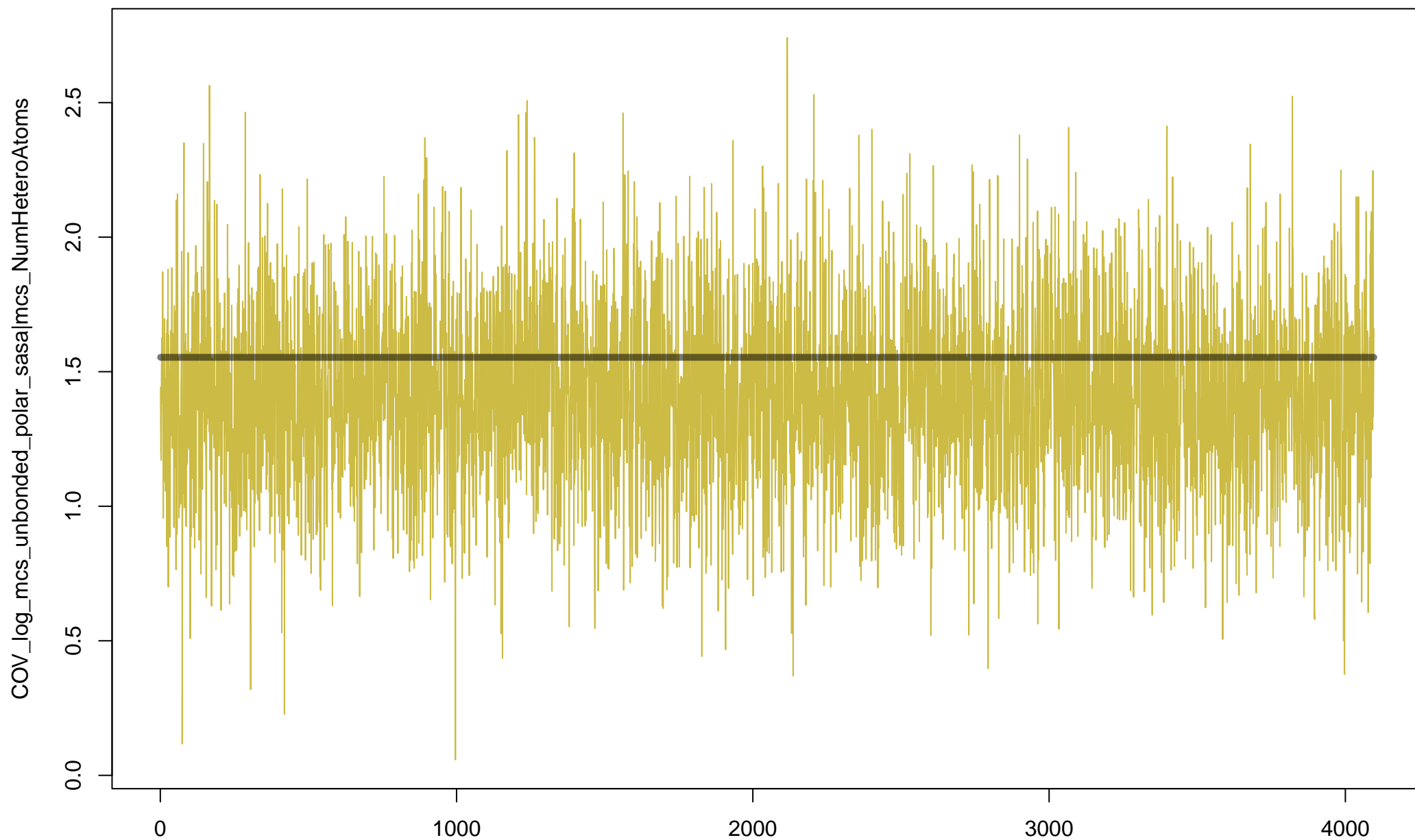
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0373 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0 | rel.err: -1.64



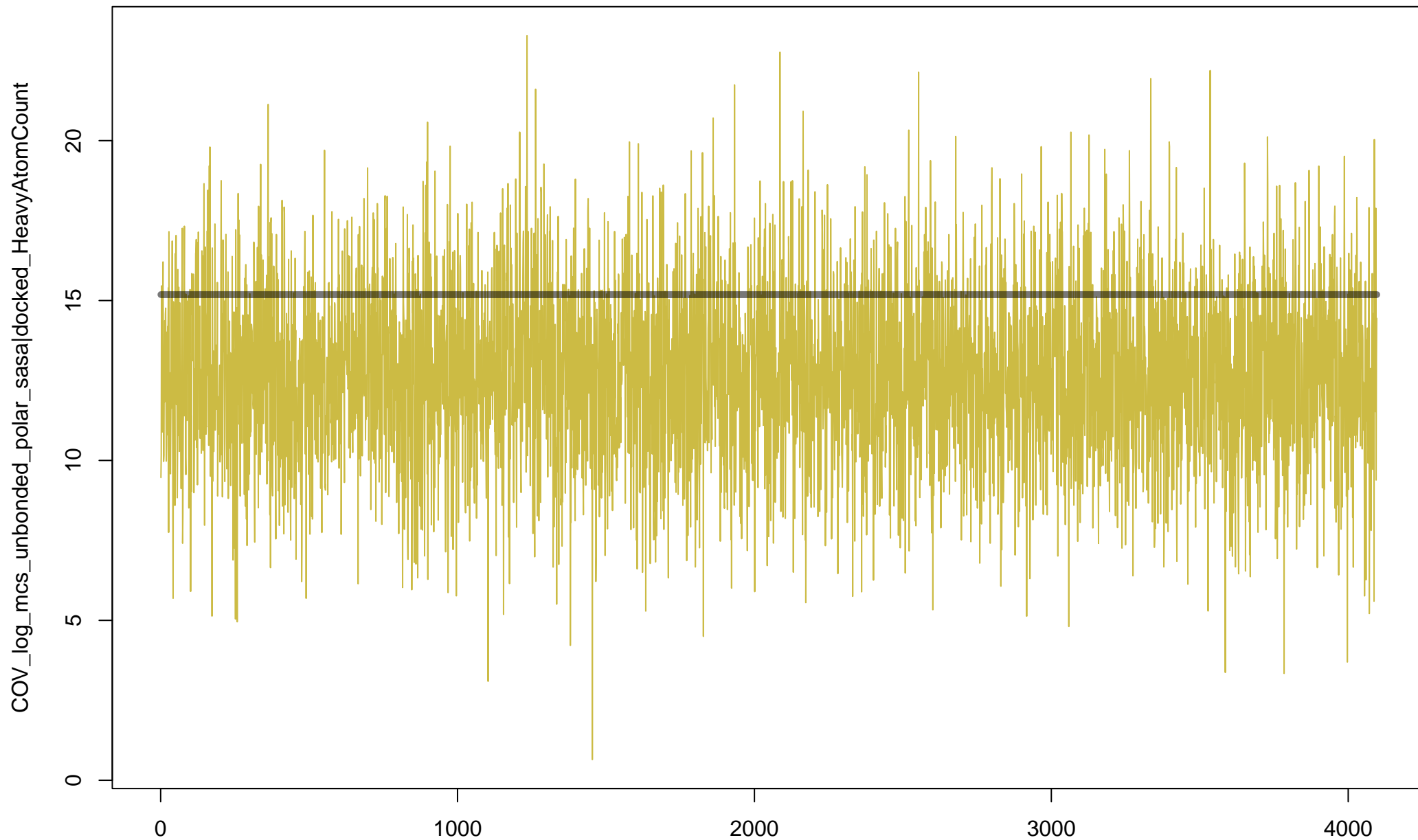
COV_log_RMSD|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0269 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: -1.79



COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 4060 | BMK = 0.0361 | MCSE(6.27) = 1.7 | stat: TRUE | burn: 0 | rel.err: -0.434



COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0243 | MCSE(6.27) = 1.56 | stat: TRUE | burn: 0 | rel.err: -0.926



COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0339 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.472

