

-- STATS maxD --

min ESS = 250.909406083443

max BMK = 0.120804602809065

max MCSE = 5.98071593525619

all stationary: FALSE

burn: 0

max rel.err.: 2.2867384996089

-- STATS 2D --

min ESS = 2981.12873895593

max BMK = 0.0516940201027788

max MCSE = 1.98077931955124

all stationary: TRUE

burn: 0

max rel.err.: 1.77076088980509

-- STATS 1D --

min ESS = 2117.04998502932

max BMK = 0.0520421920542695

max MCSE = 2.30573732918091

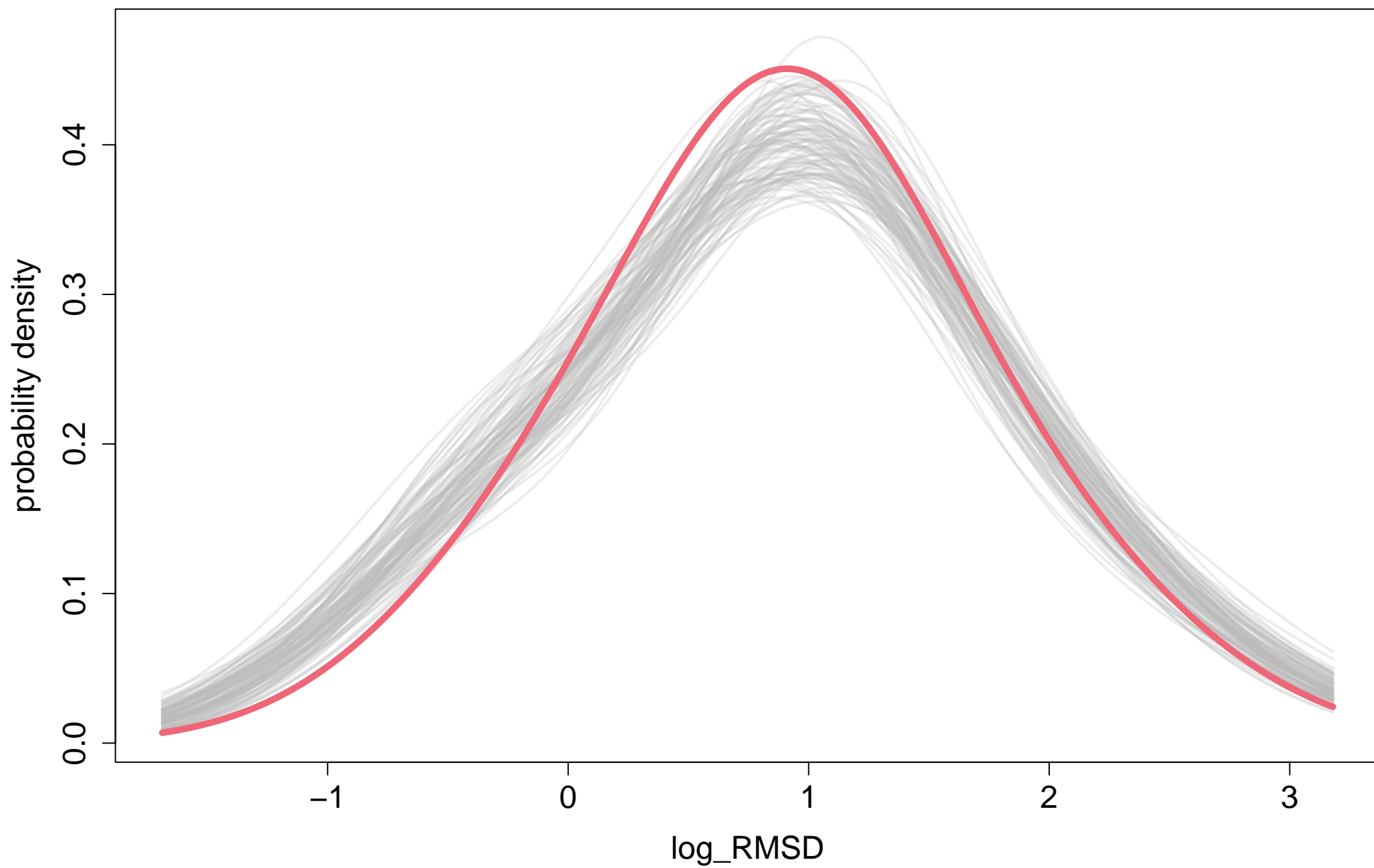
all stationary: FALSE

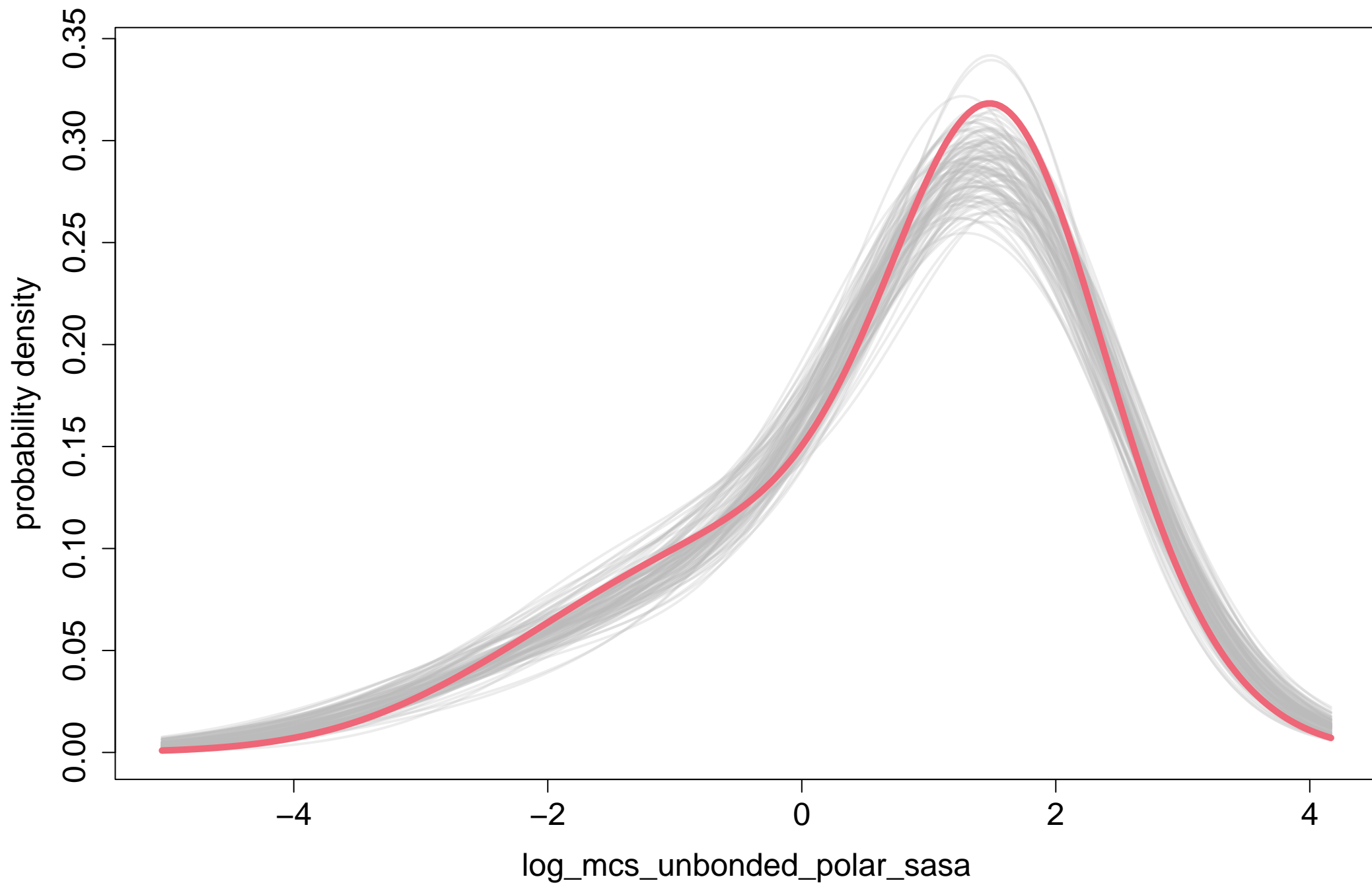
burn: 0

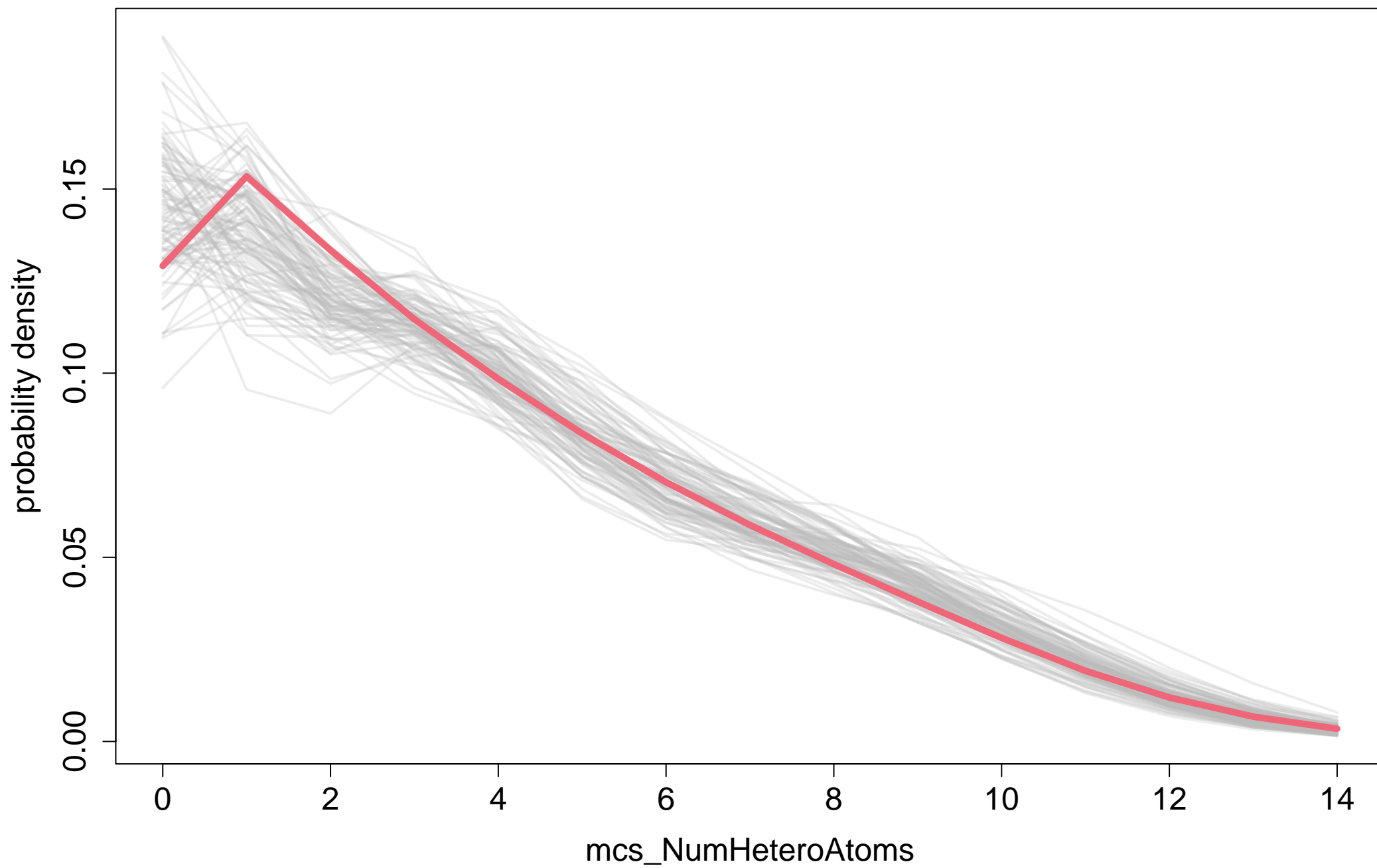
max rel.err.: 2.27829101738397

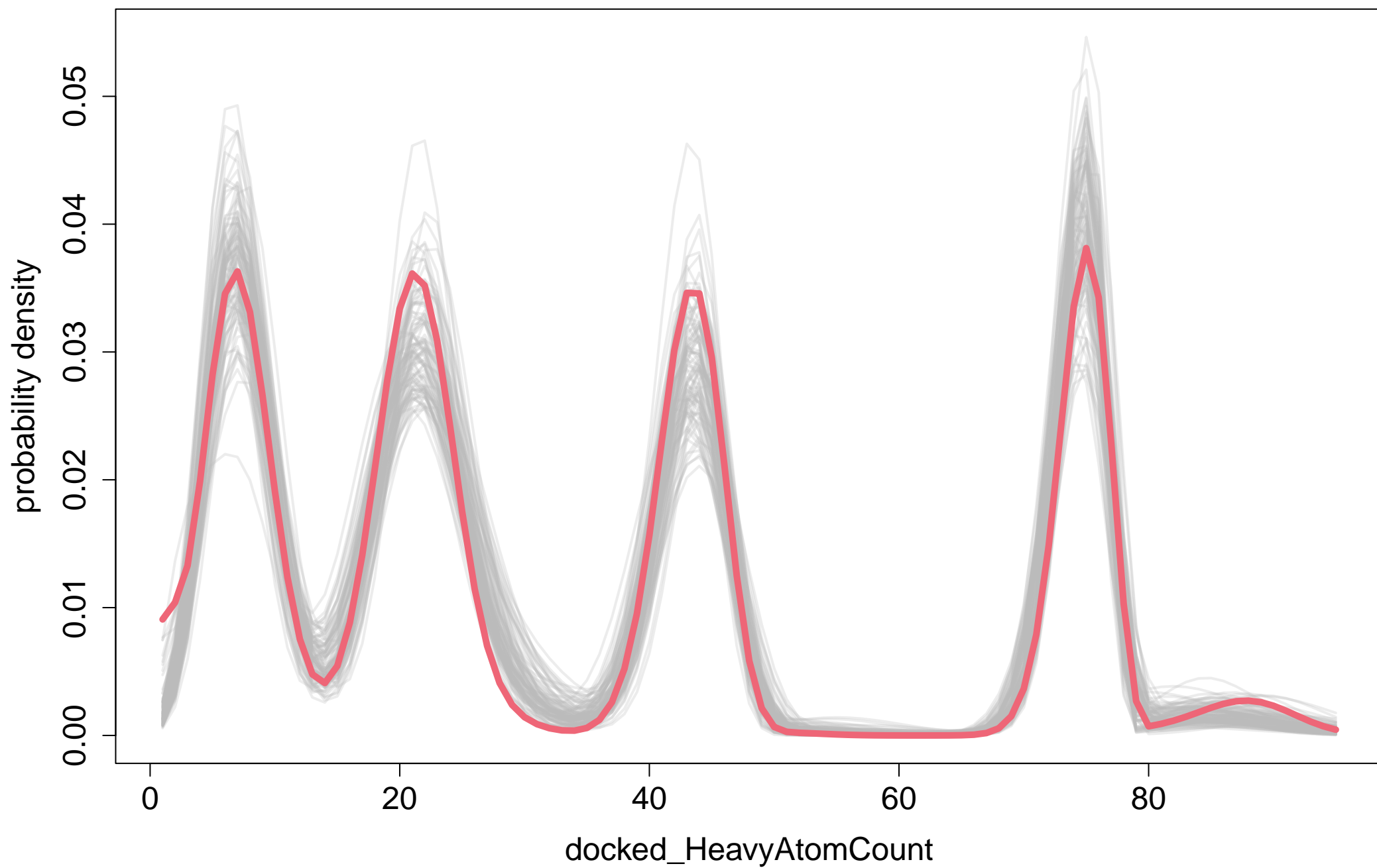
Occupied clusters: 9 of 16

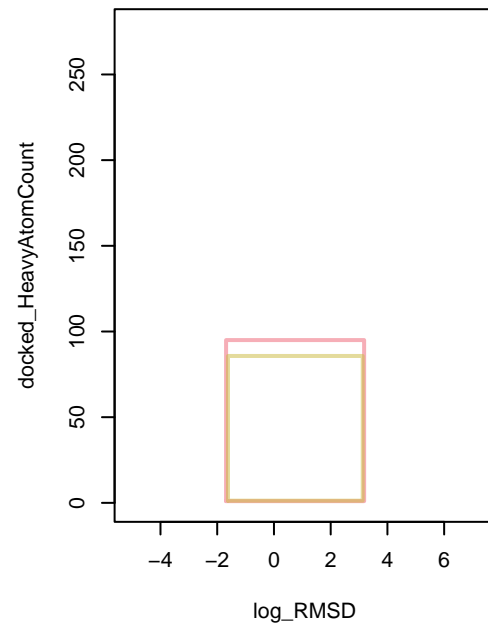
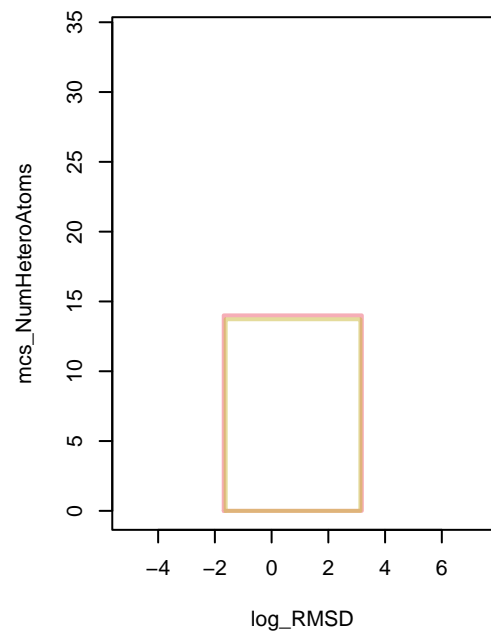
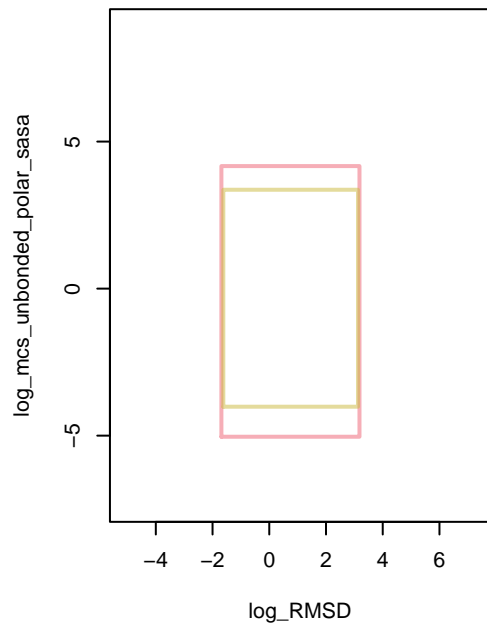
LL: -2160 +- 6.84



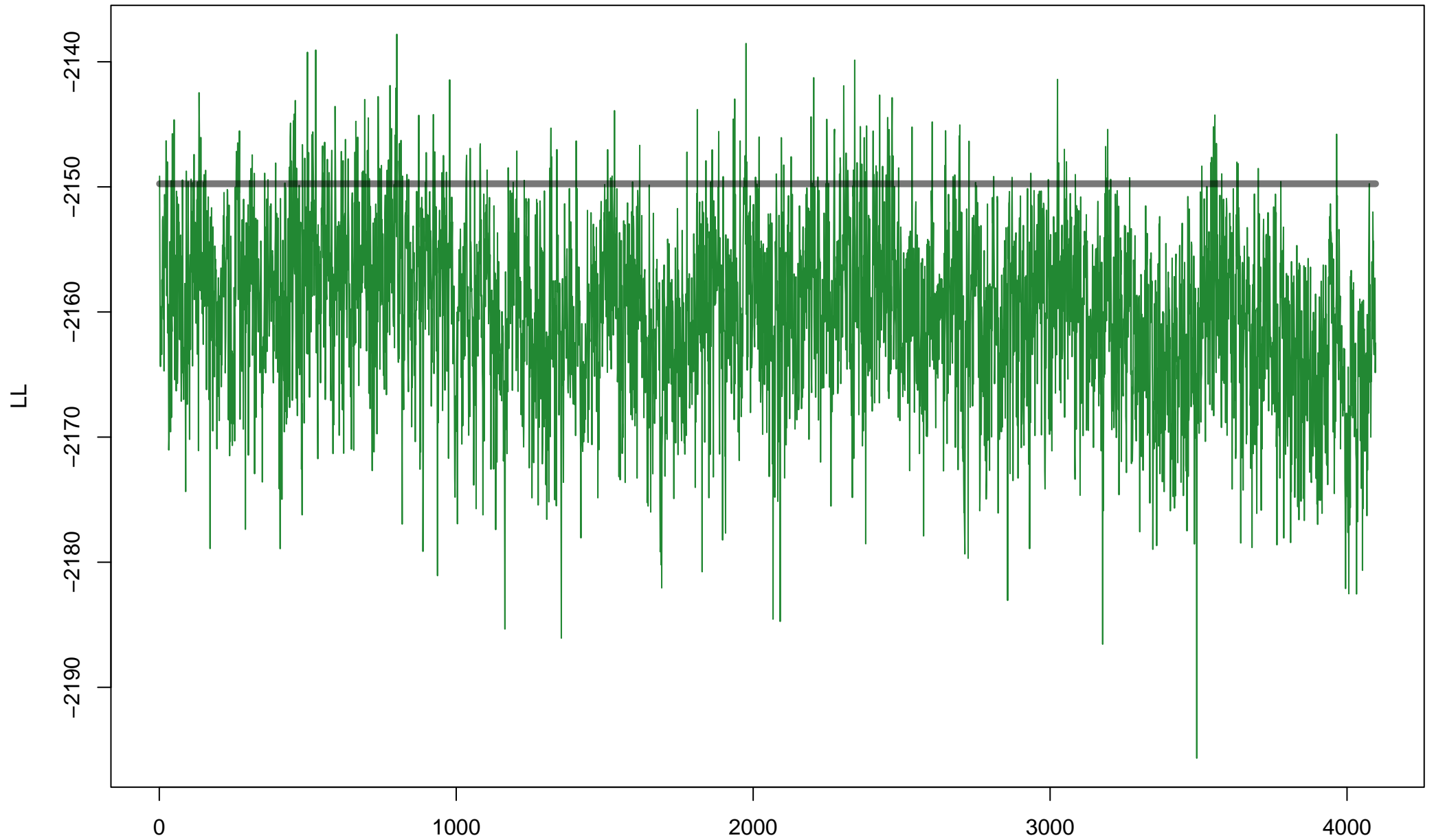




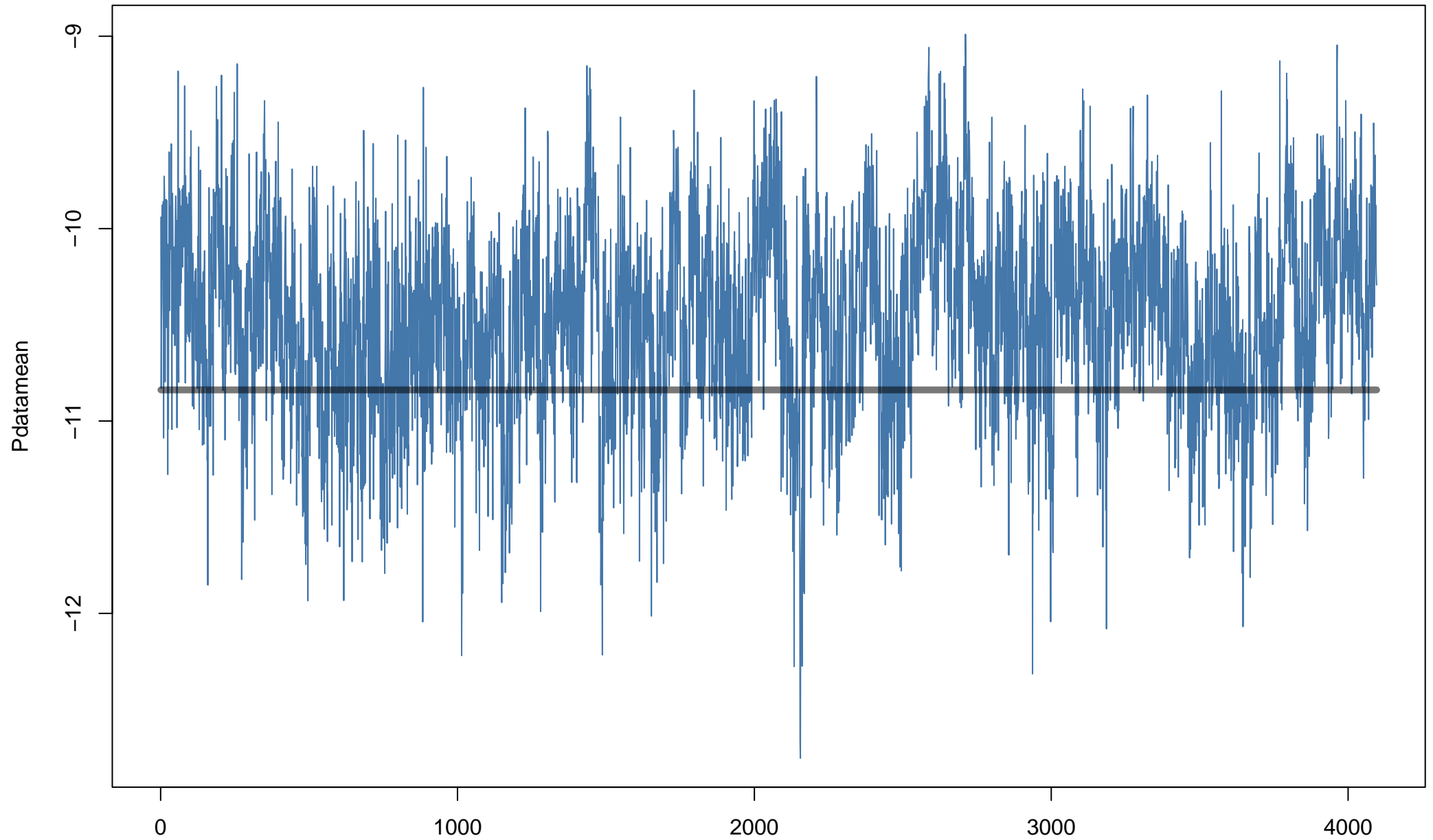




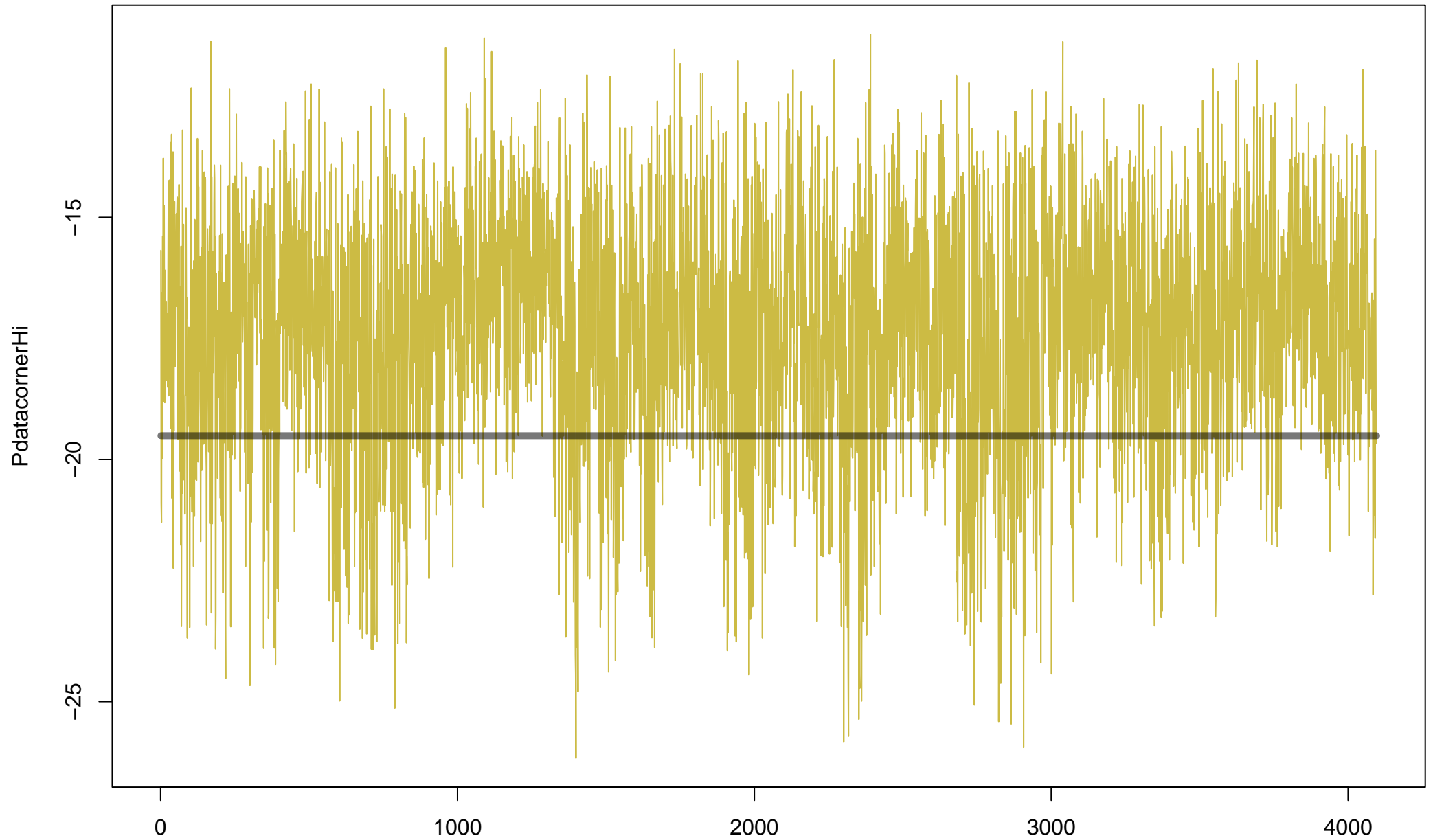
LL



Pdatamean
ESS = 251 | BMK = 0.0705 | MCSE(6.27) = 5.98 | stat: TRUE | burn: 0 | rel.err: 0.769

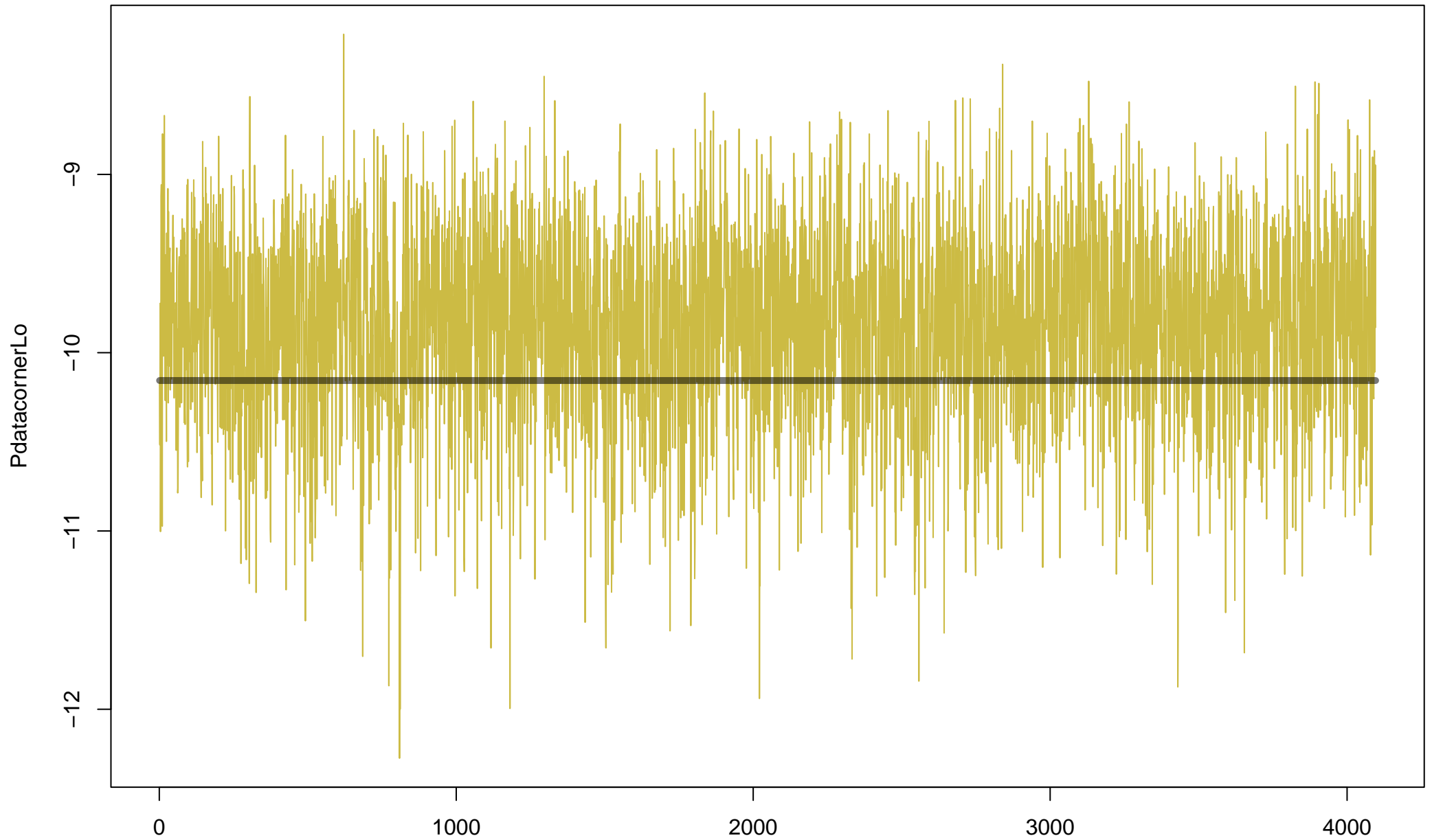


PdatacornerHi
ESS = 4100 | BMK = 0.121 | MCSE(6.27) = 1.73 | stat: TRUE | burn: 0 | rel.err: 0.314

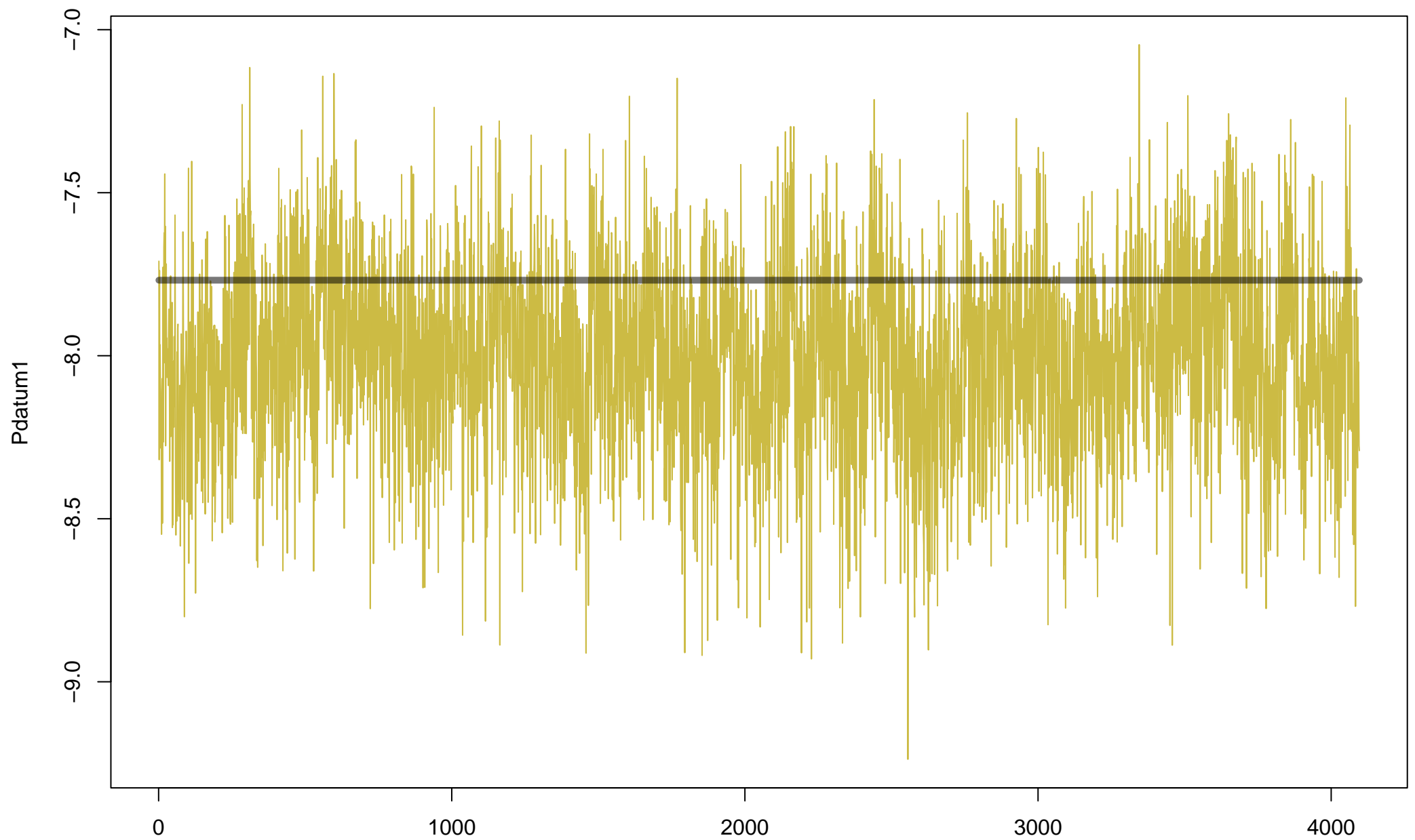


PdatacornerLo

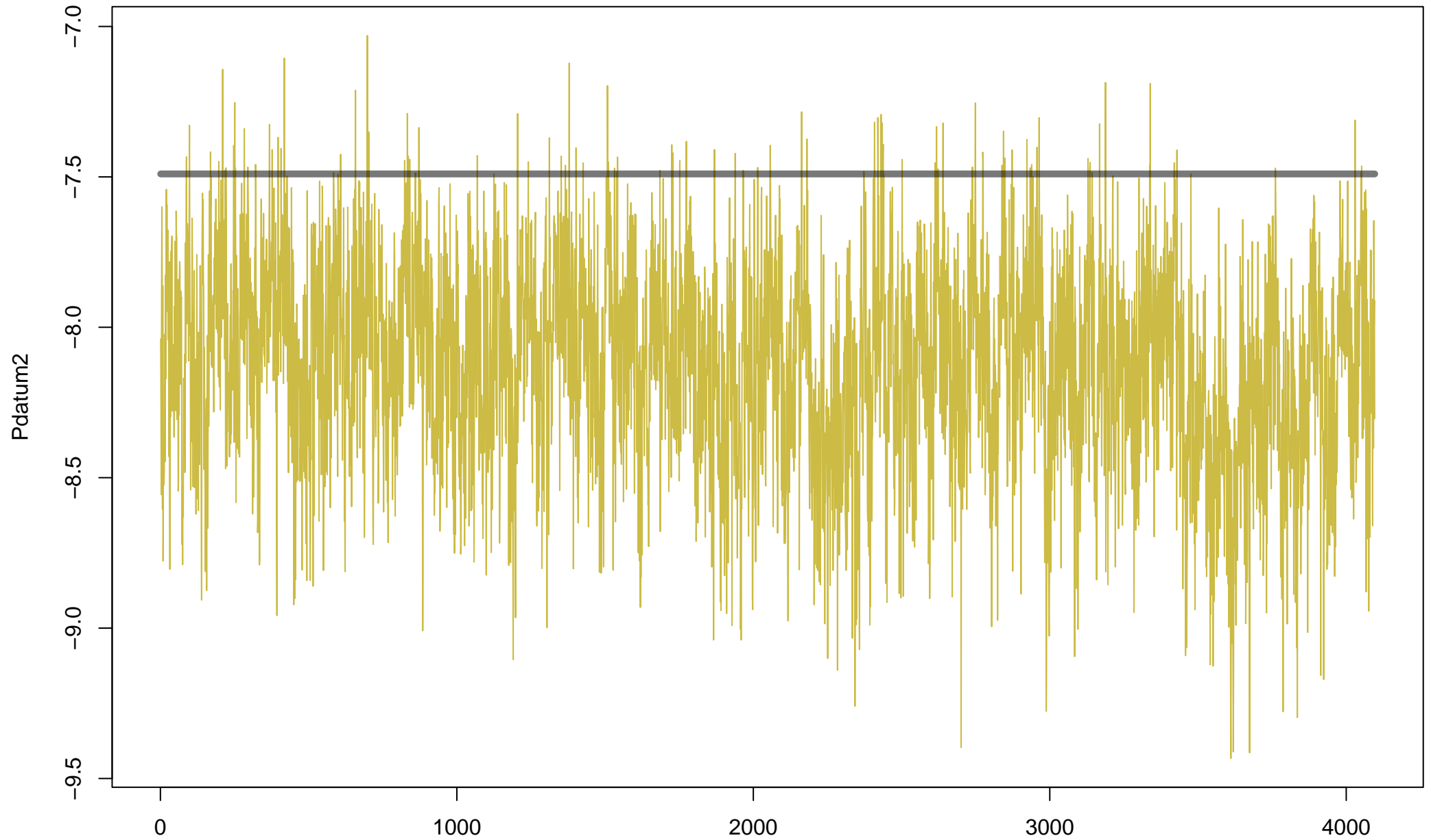
ESS = 3420 | BMK = 0.0421 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | rel.err: 0.669



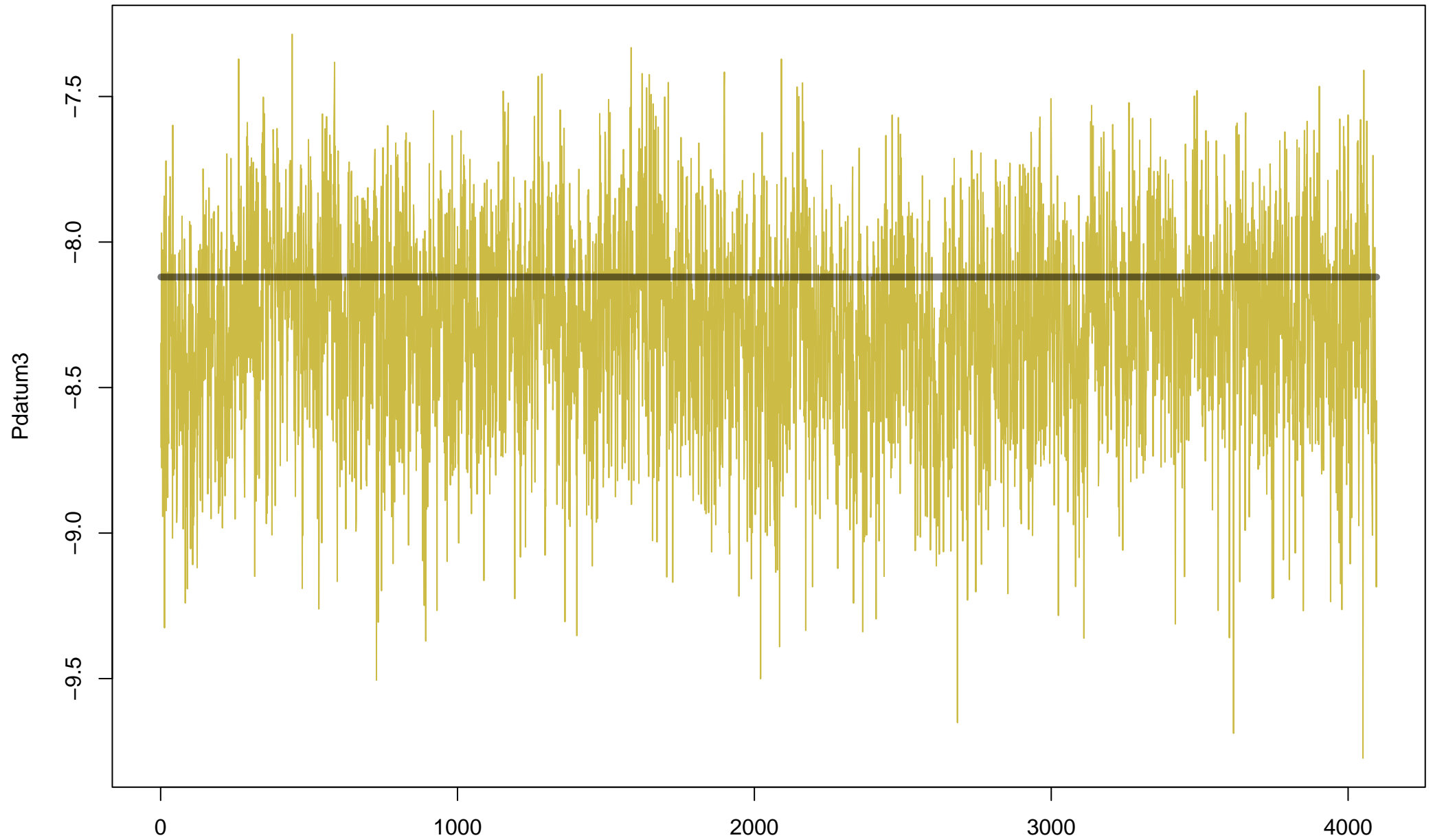
Pdatum1
ESS = 519 | BMK = 0.053 | MCSE(6.27) = 3.92 | stat: TRUE | burn: 0 | rel.err: -0.781



Pdatum2
ESS = 481 | BMK = 0.111 | MCSE(6.27) = 4.63 | stat: FALSE | burn: 0 | rel.err: -2.29

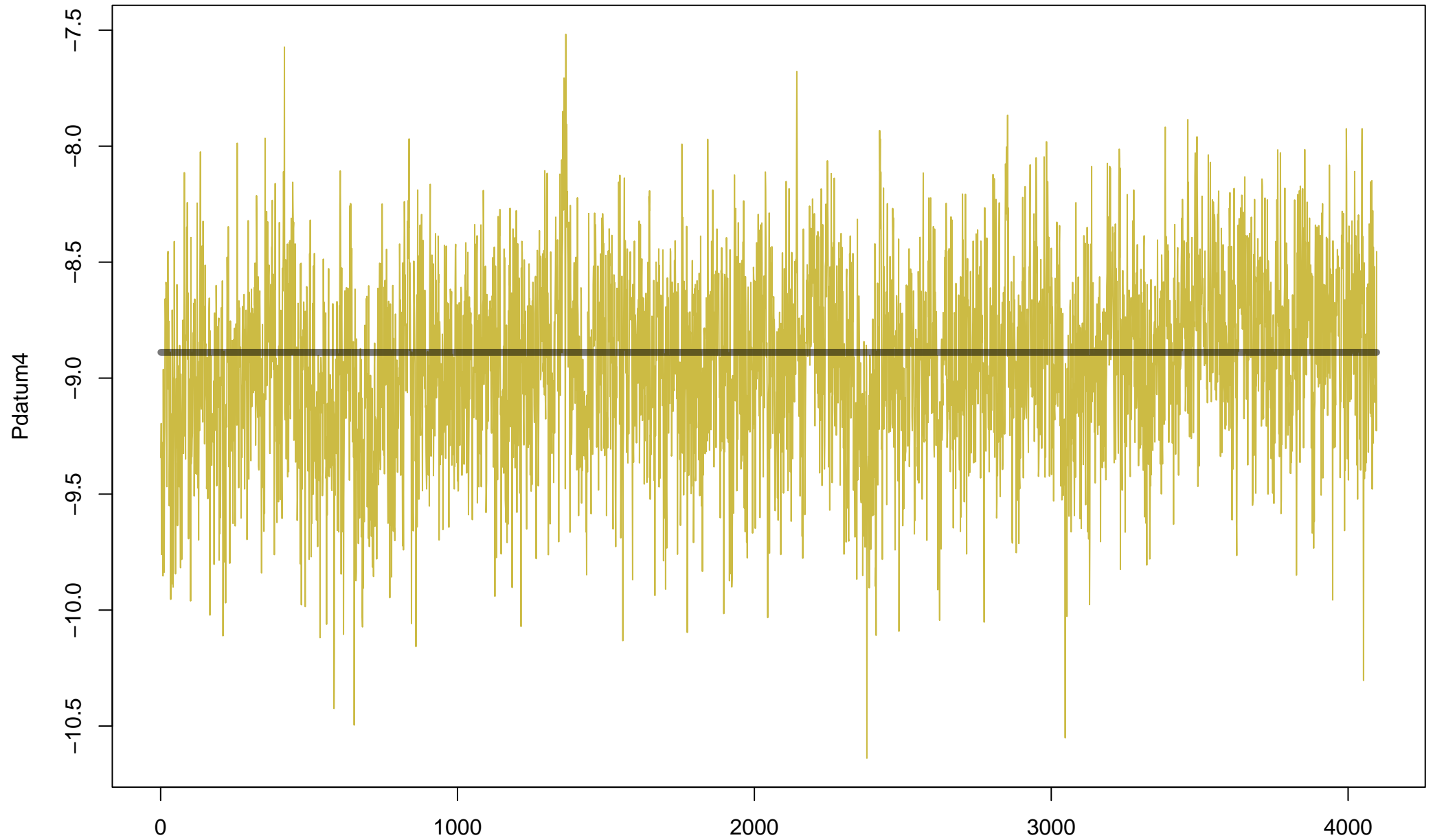


Pdatum3
ESS = 676 | BMK = 0.047 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | rel.err: -0.338



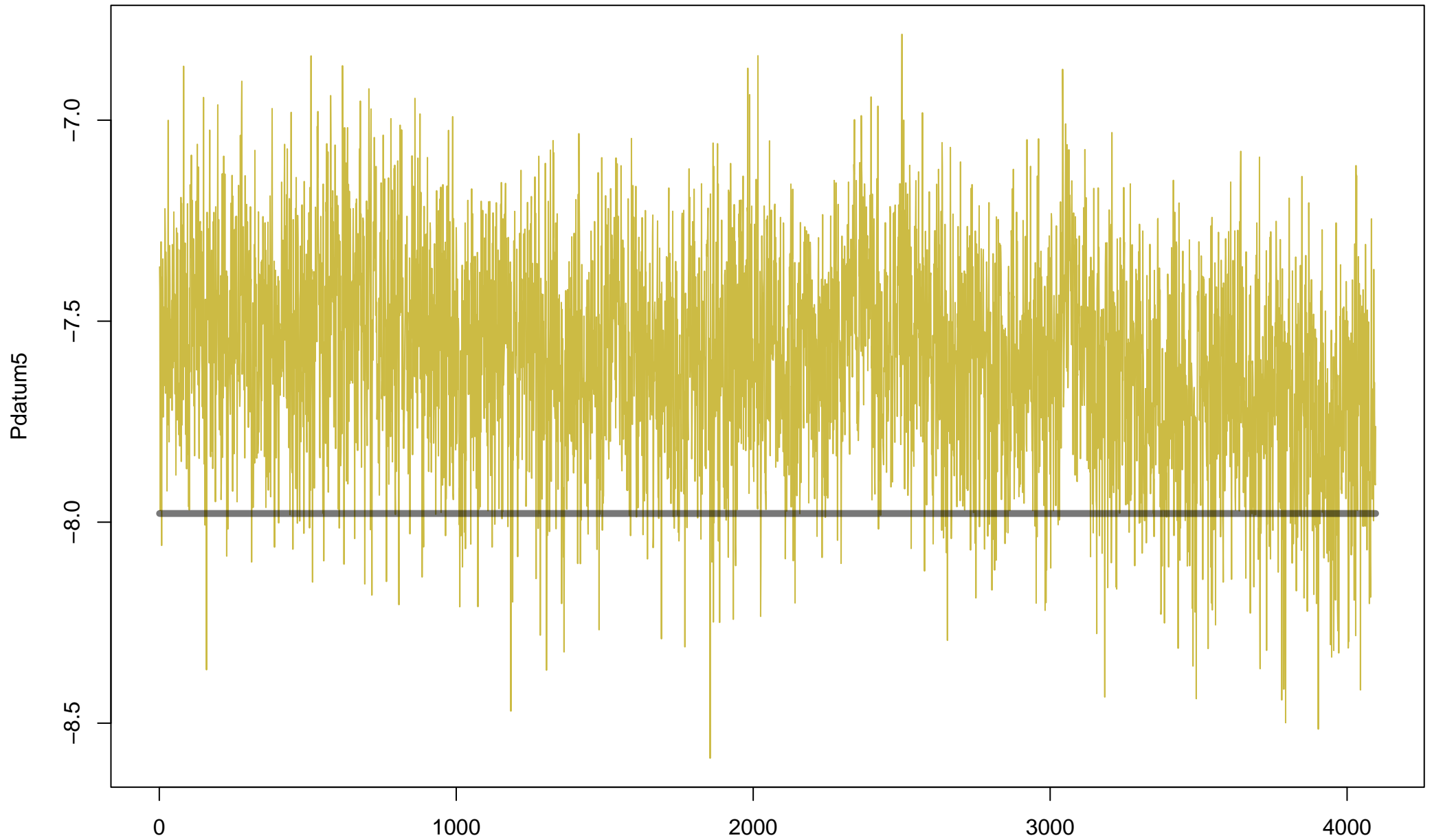
Pdatum4

ESS = 749 | BMK = 0.1 | MCSE(6.27) = 3.96 | stat: FALSE | burn: 0 | rel.err: 0.0799



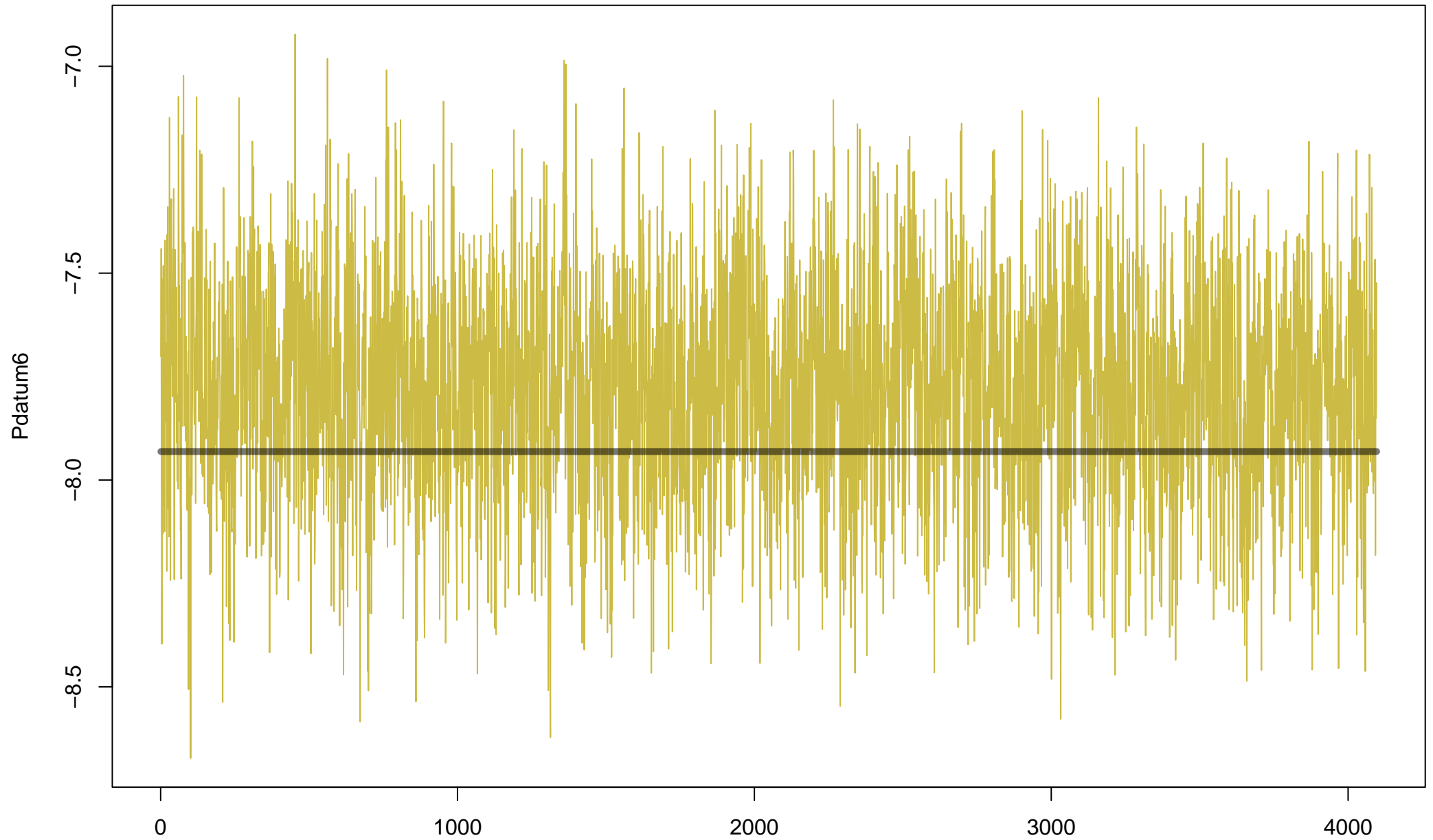
Pdatum5

ESS = 310 | BMK = 0.107 | MCSE(6.27) = 4.03 | stat: FALSE | burn: 0 | rel.err: 1.35



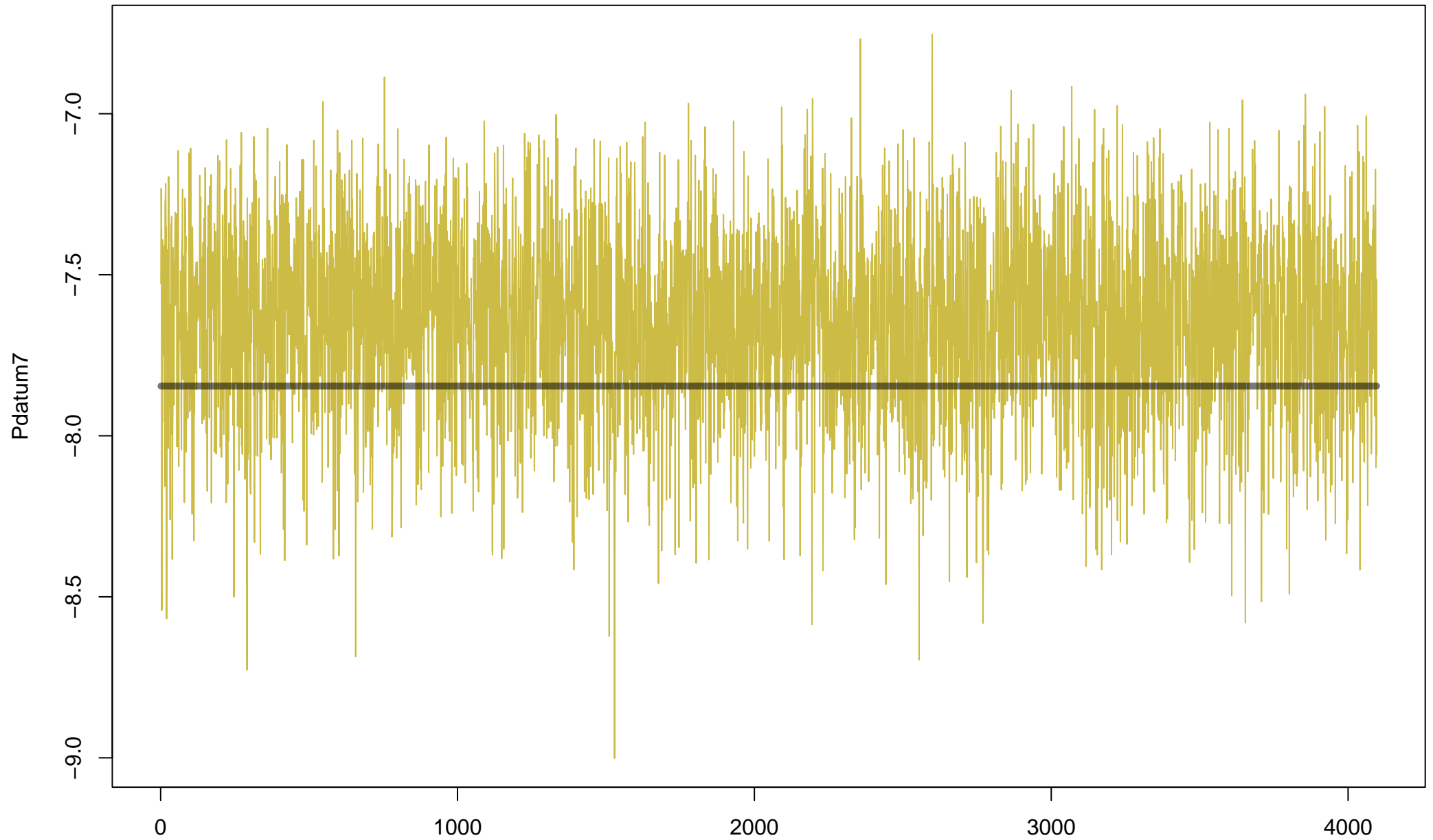
Pdatum6

ESS = 1820 | BMK = 0.0513 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0 | rel.err: 0.653

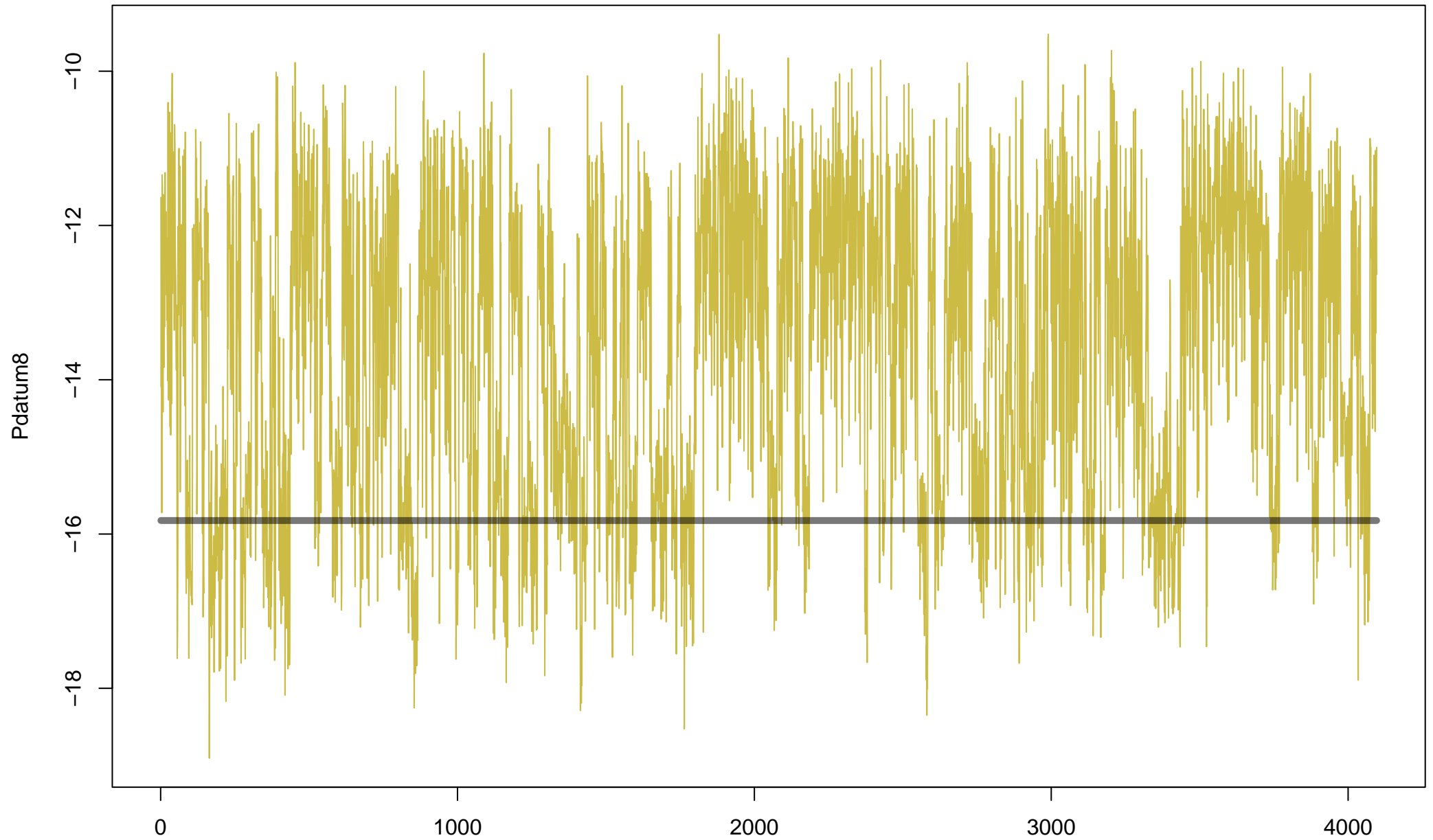


Pdatum7

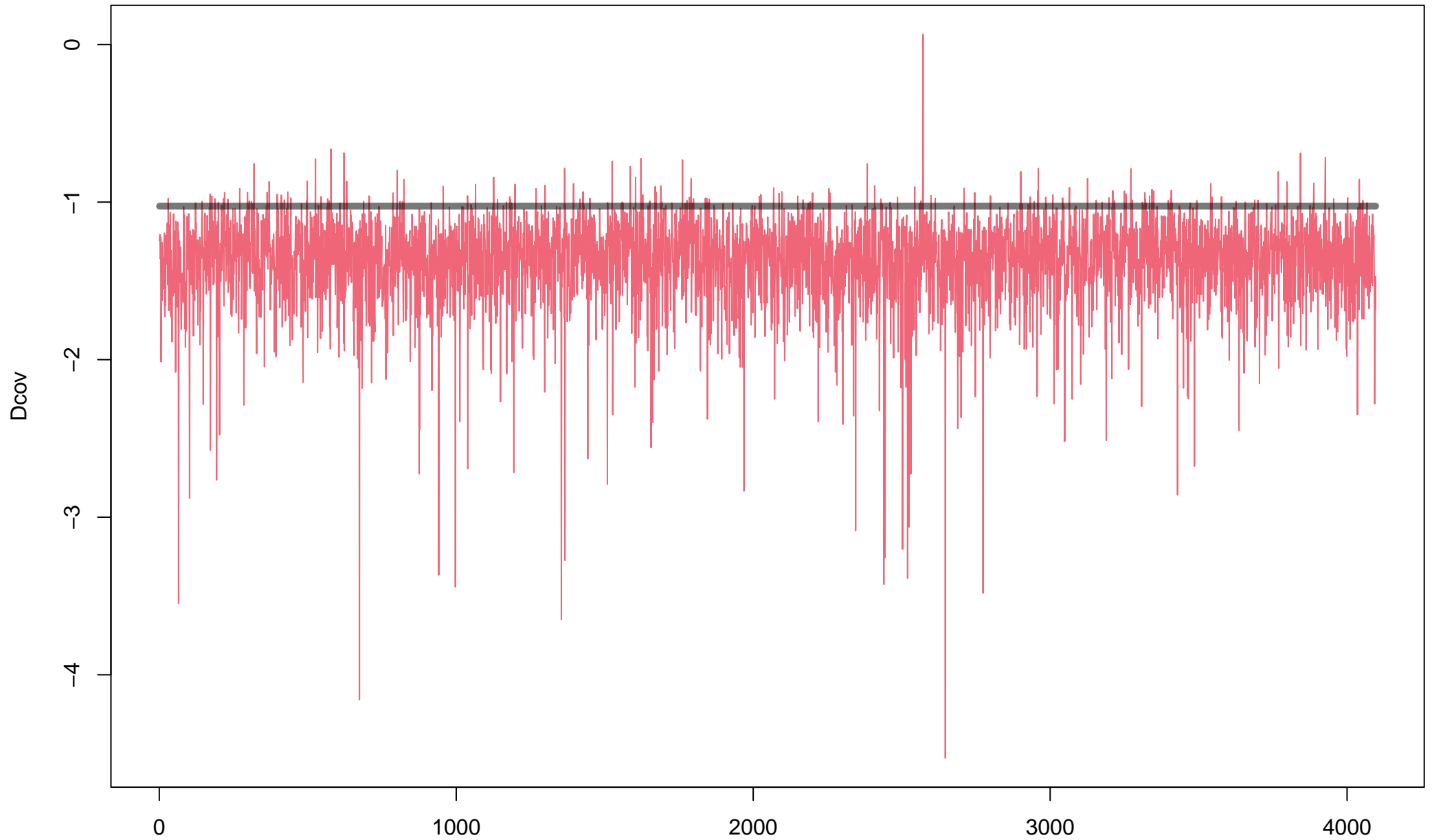
ESS = 4100 | BMK = 0.0368 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0 | rel.err: 0.764



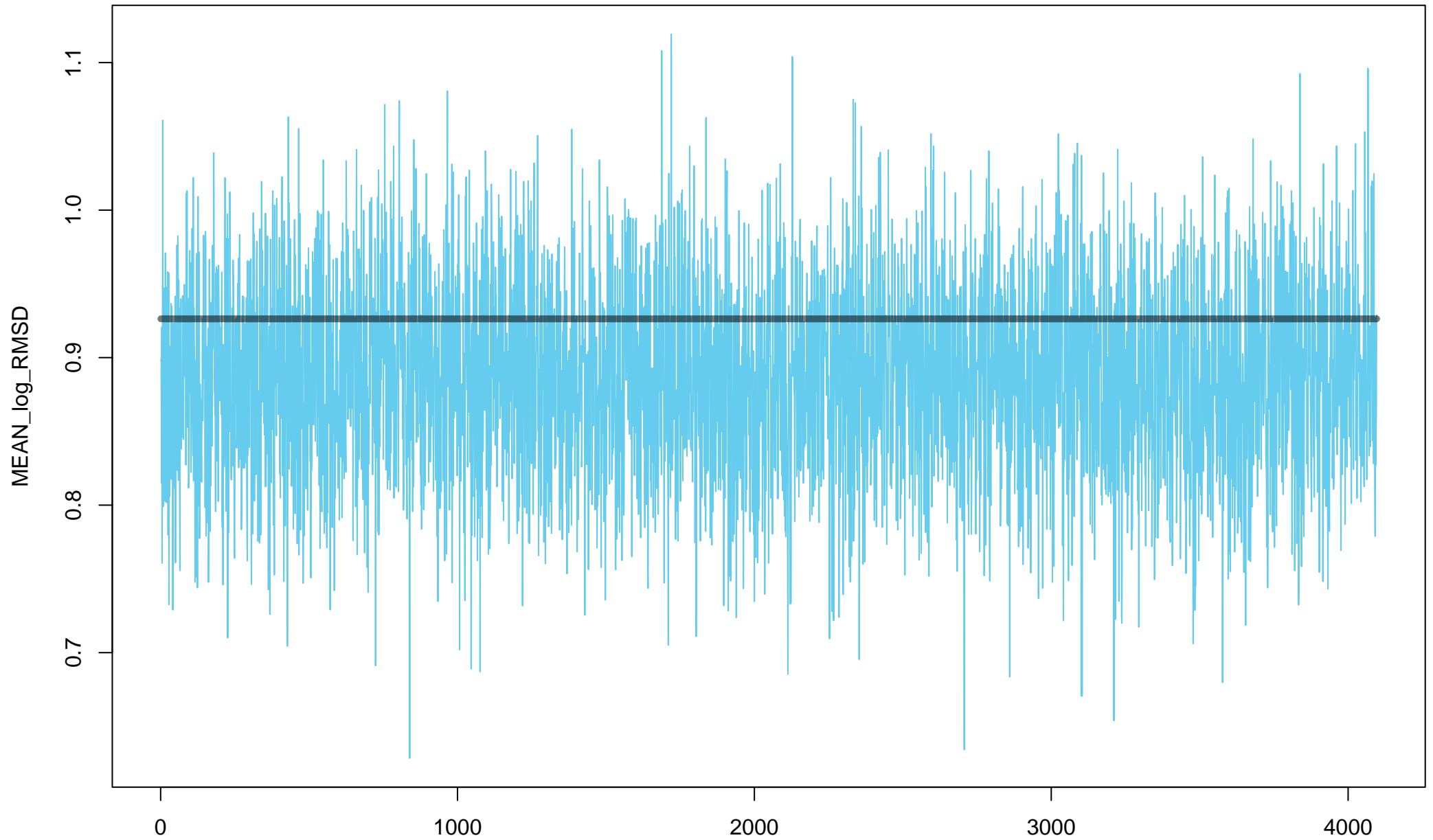
Pdatum8
ESS = 515 | BMK = 0.101 | MCSE(6.27) = 4.32 | stat: FALSE | burn: 0 | rel.err: 0.609



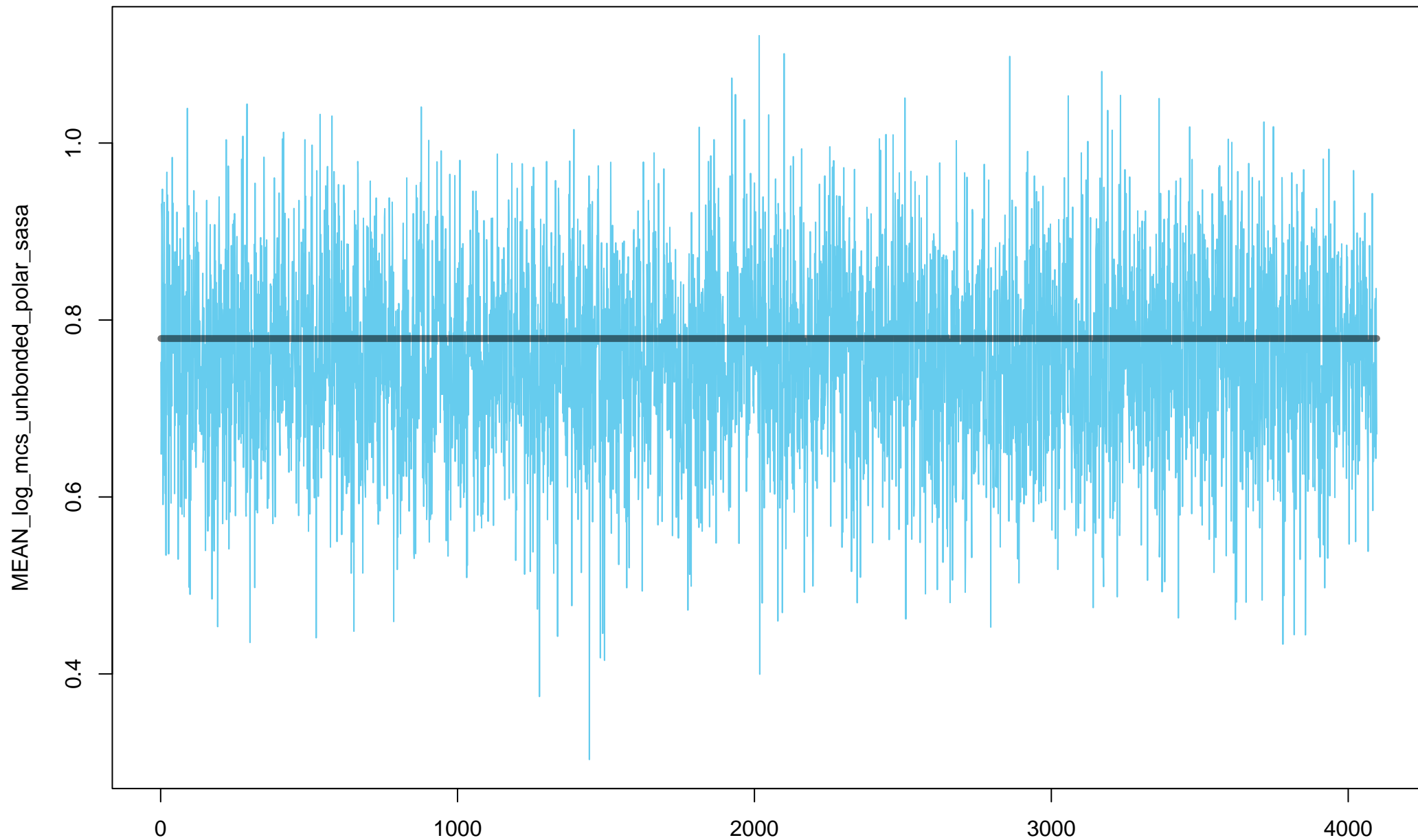
Dcov
ESS = 3610 | BMK = 0.039 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: 1.53



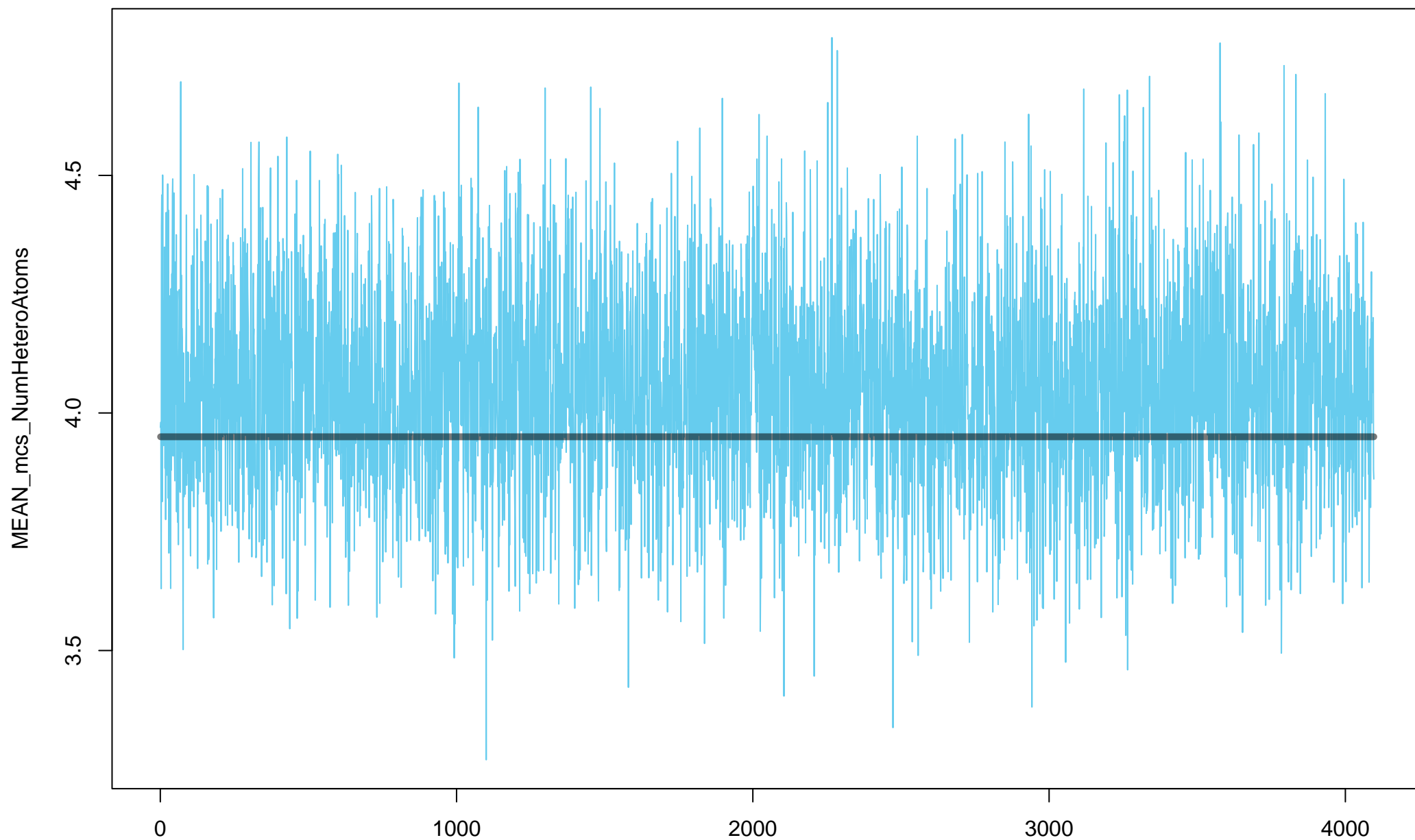
MEAN_log_RMSD
ESS = 3870 | BMK = 0.0347 | MCSE(6.27) = 1.51 | stat: TRUE | burn: 0 | rel.err: -0.605



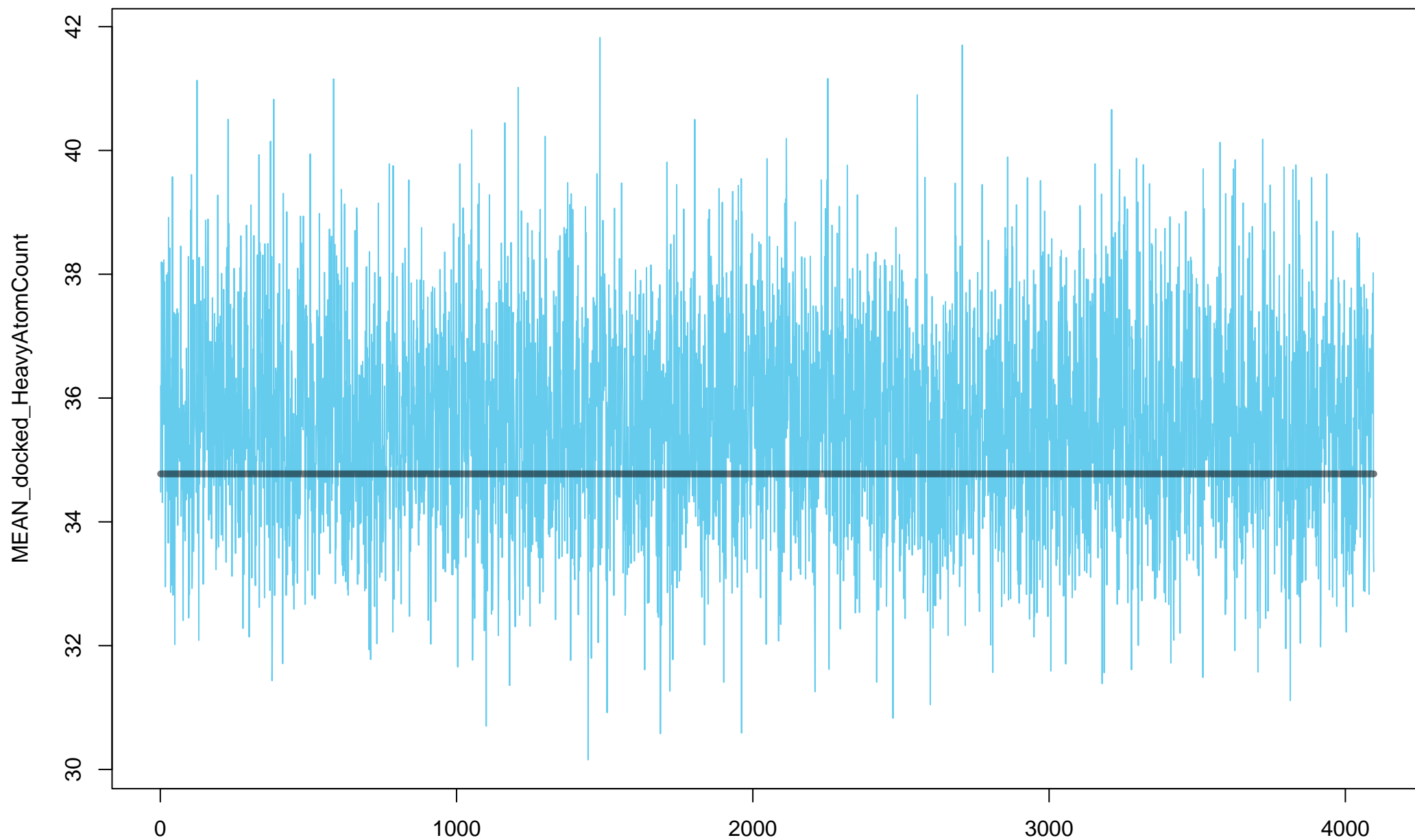
MEAN_log_mcs_unbonded_polar_sasa
ESS = 3360 | BMK = 0.0307 | MCSE(6.27) = 1.84 | stat: TRUE | burn: 0 | rel.err: -0.206



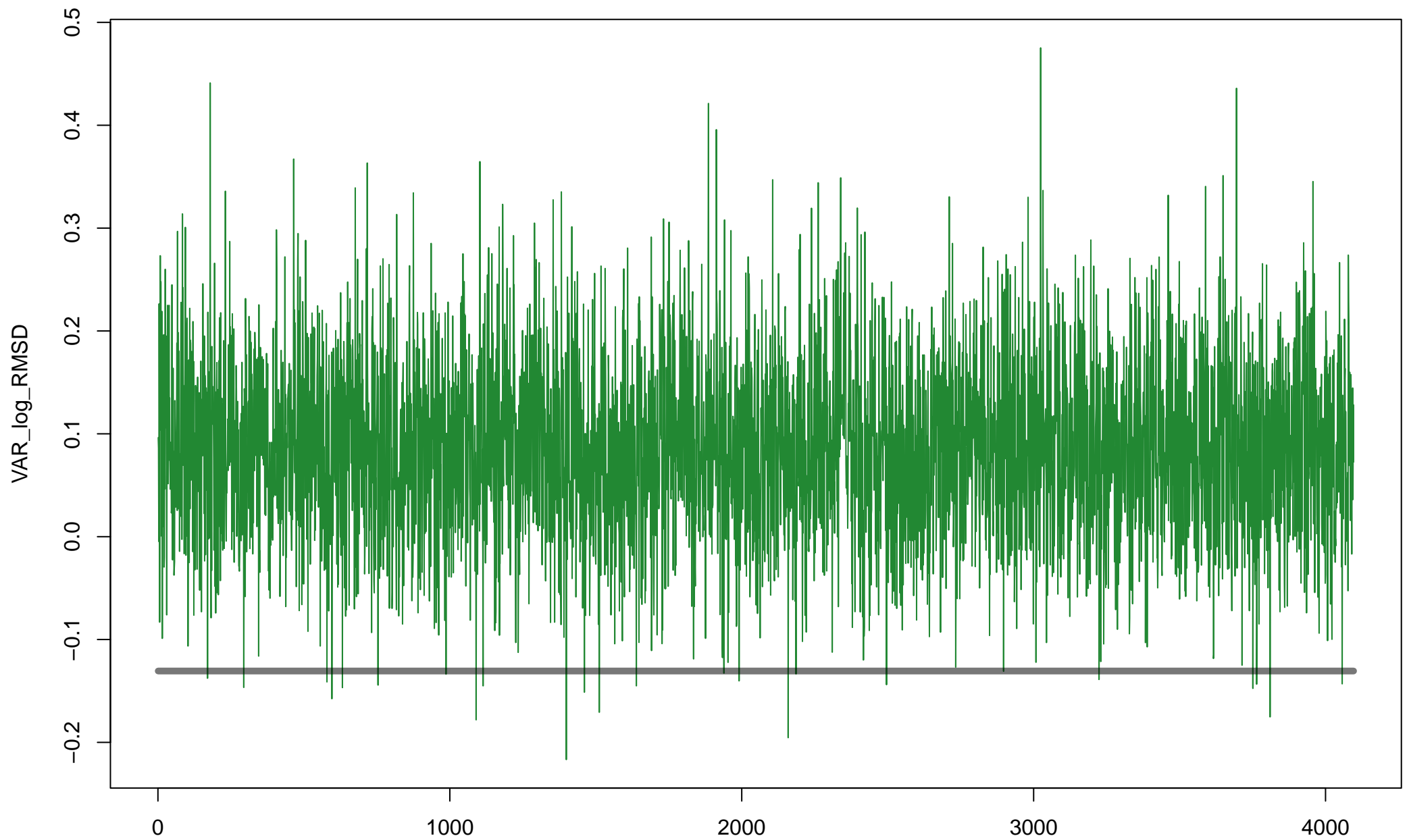
MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0453 | MCSE(6.27) = 1.49 | stat: TRUE | burn: 0 | rel.err: 0.49



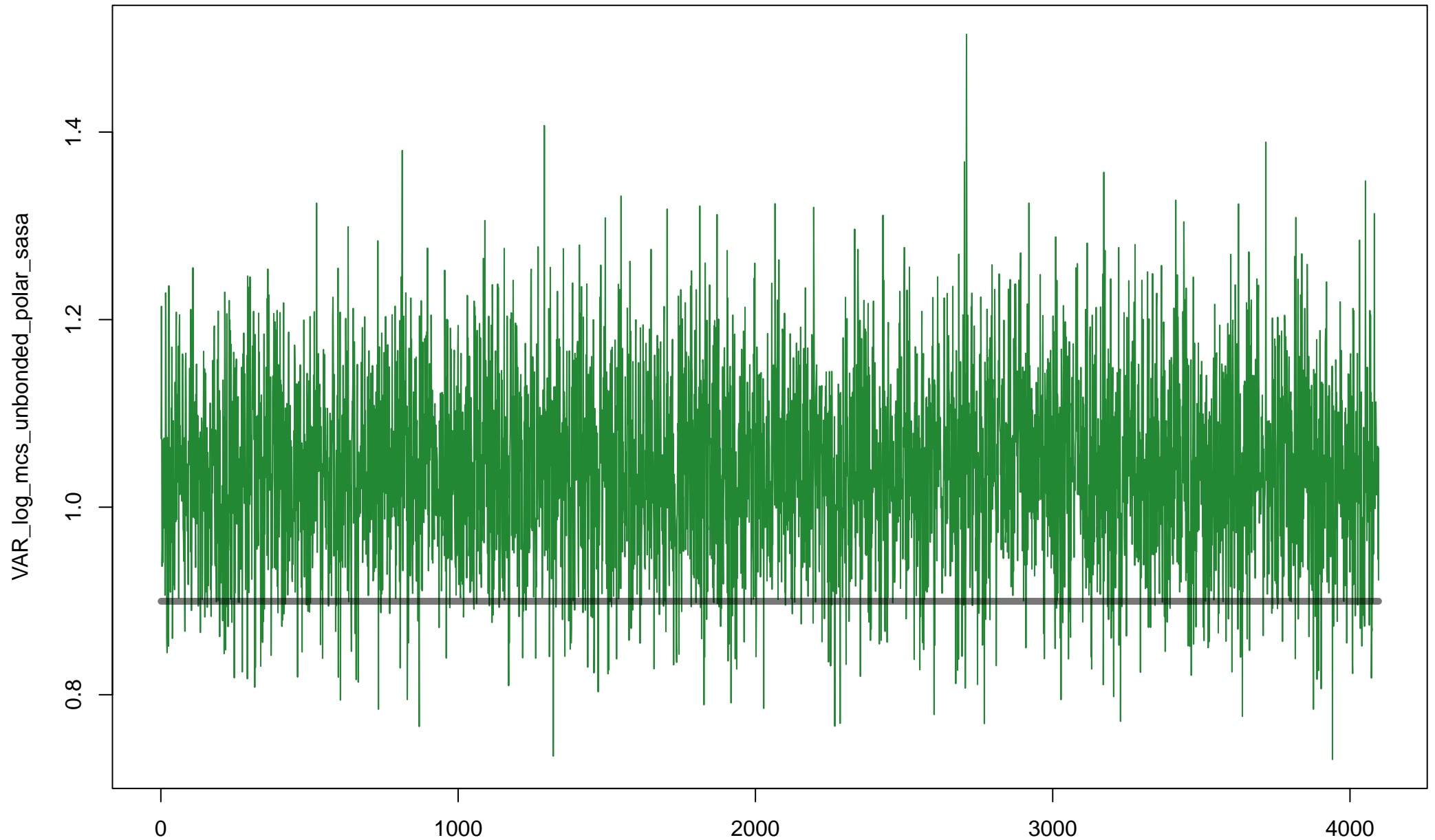
MEAN_docked_HeavyAtomCount
ESS = 3890 | BMK = 0.0294 | MCSE(6.27) = 1.62 | stat: FALSE | burn: 0 | rel.err: 0.524



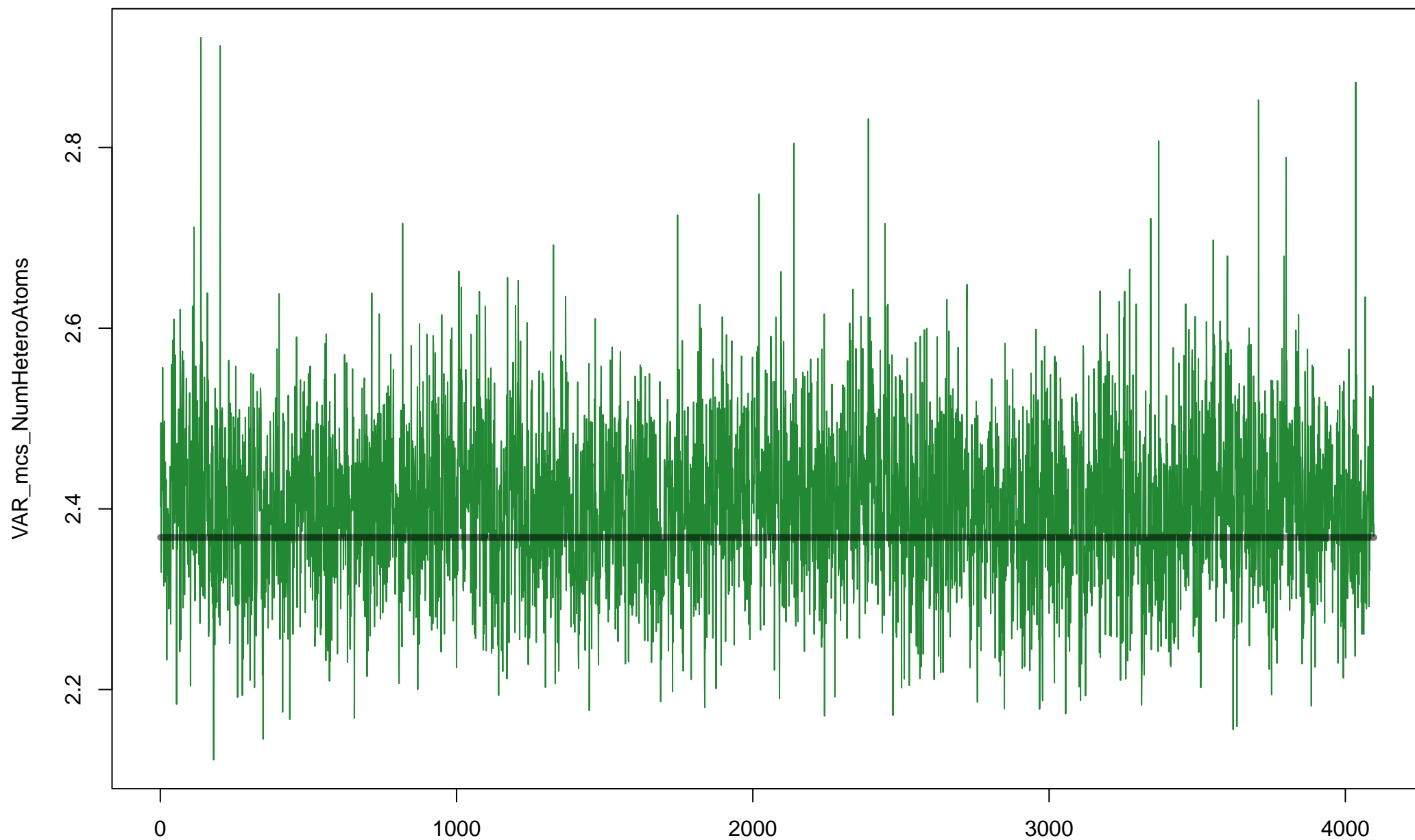
VAR_log_RMSD
ESS = 4100 | BMK = 0.0348 | MCSE(6.27) = 1.77 | stat: TRUE | burn: 0 | rel.err: 2.28



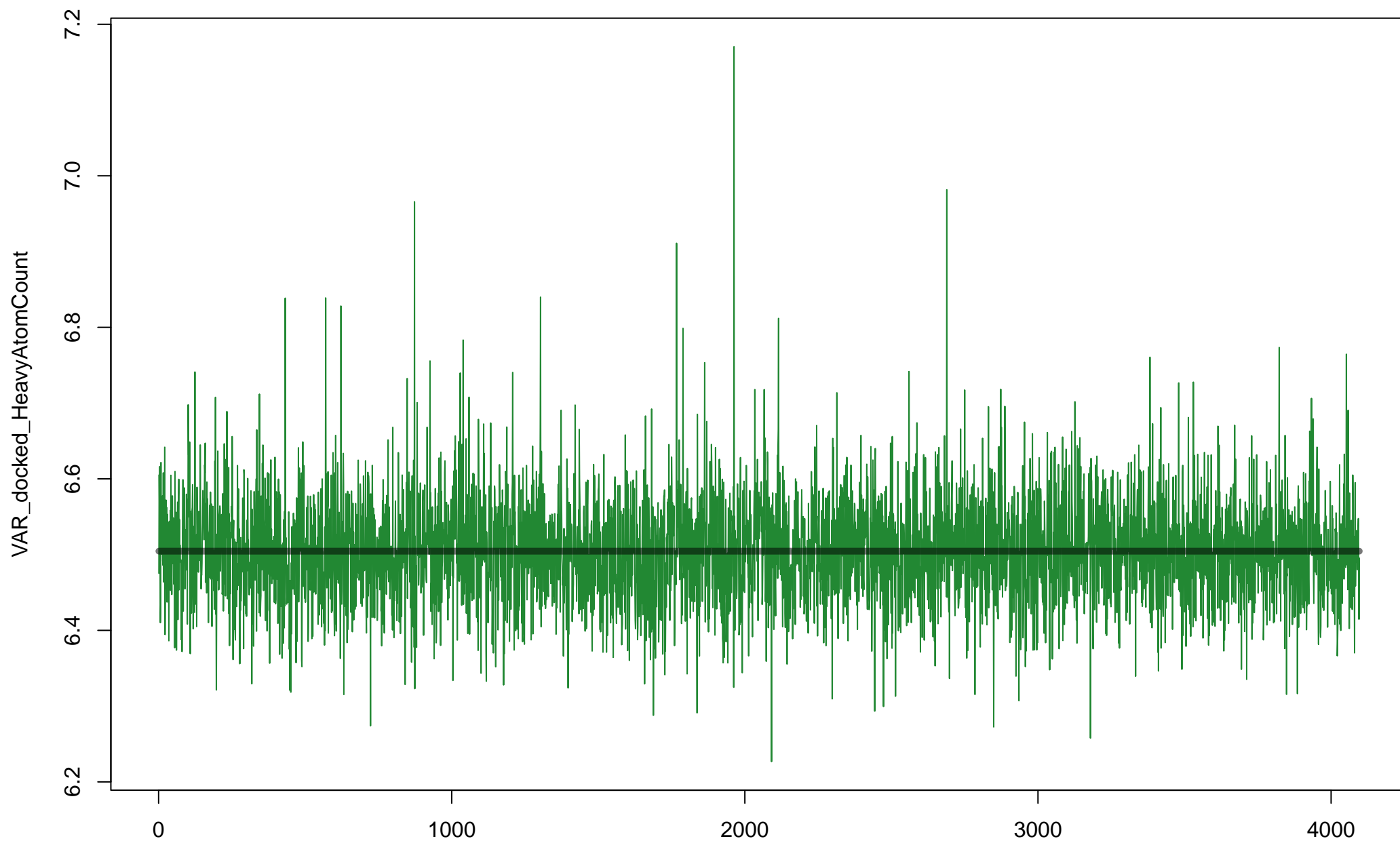
VAR_log_mcs_unbonded_polar_sasa
ESS = 3850 | BMK = 0.0385 | MCSE(6.27) = 1.51 | stat: TRUE | burn: 0 | rel.err: 1.37



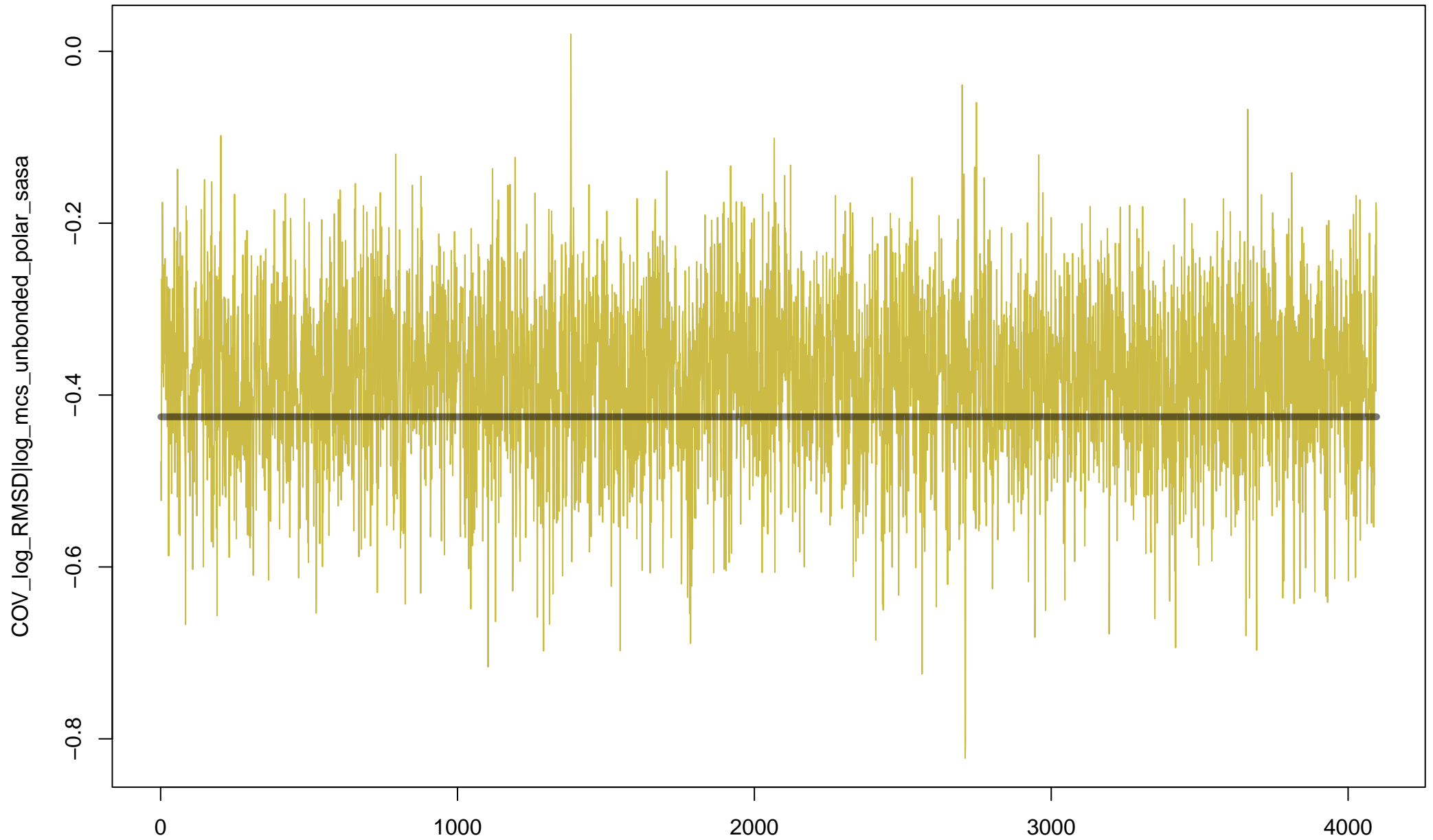
VAR_mcs_NumHeteroAtoms
ESS = 2120 | BMK = 0.0468 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0 | rel.err: 0.433



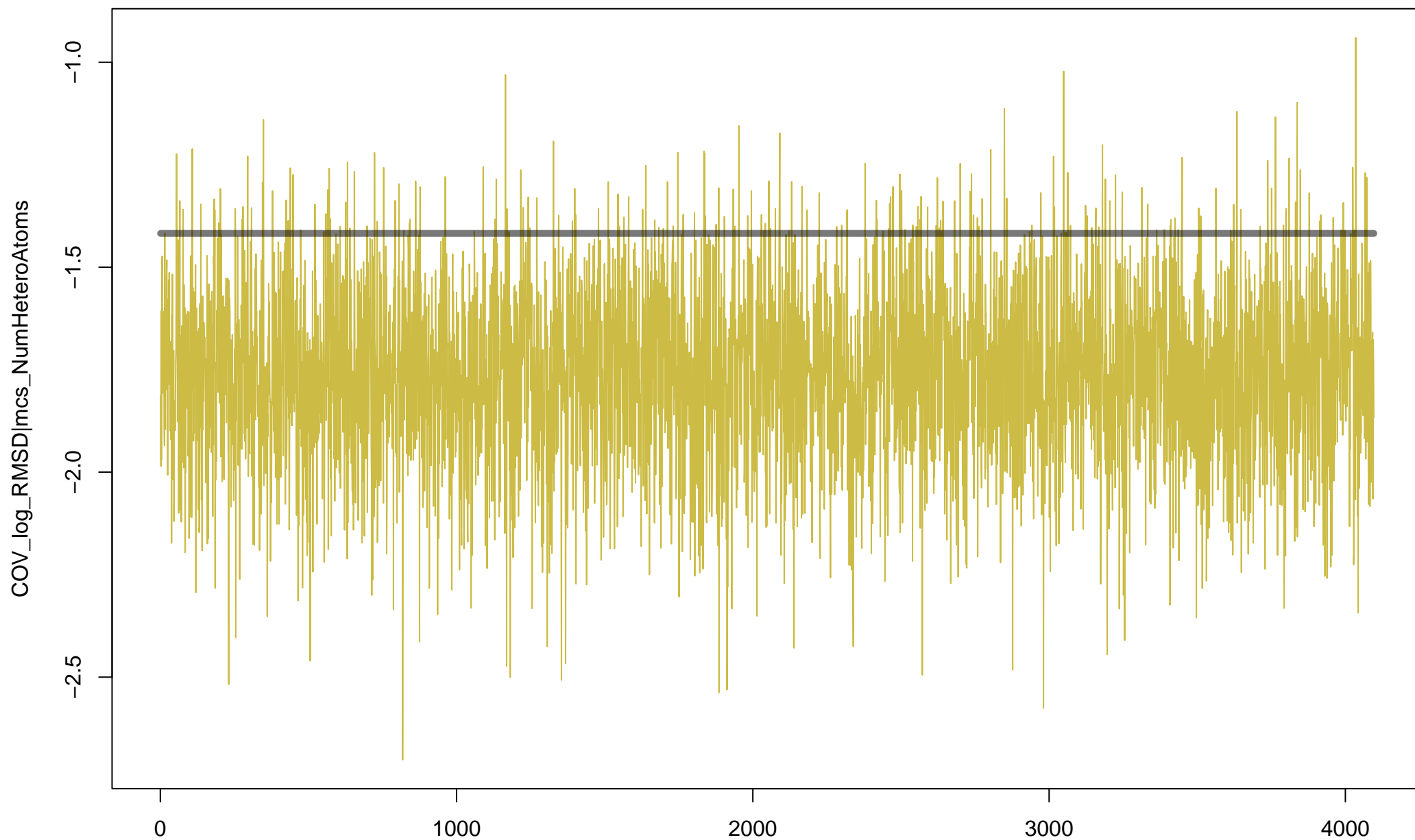
VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.052 | MCSE(6.27) = 1.58 | stat: TRUE | burn: 0 | rel.err: 0.0559



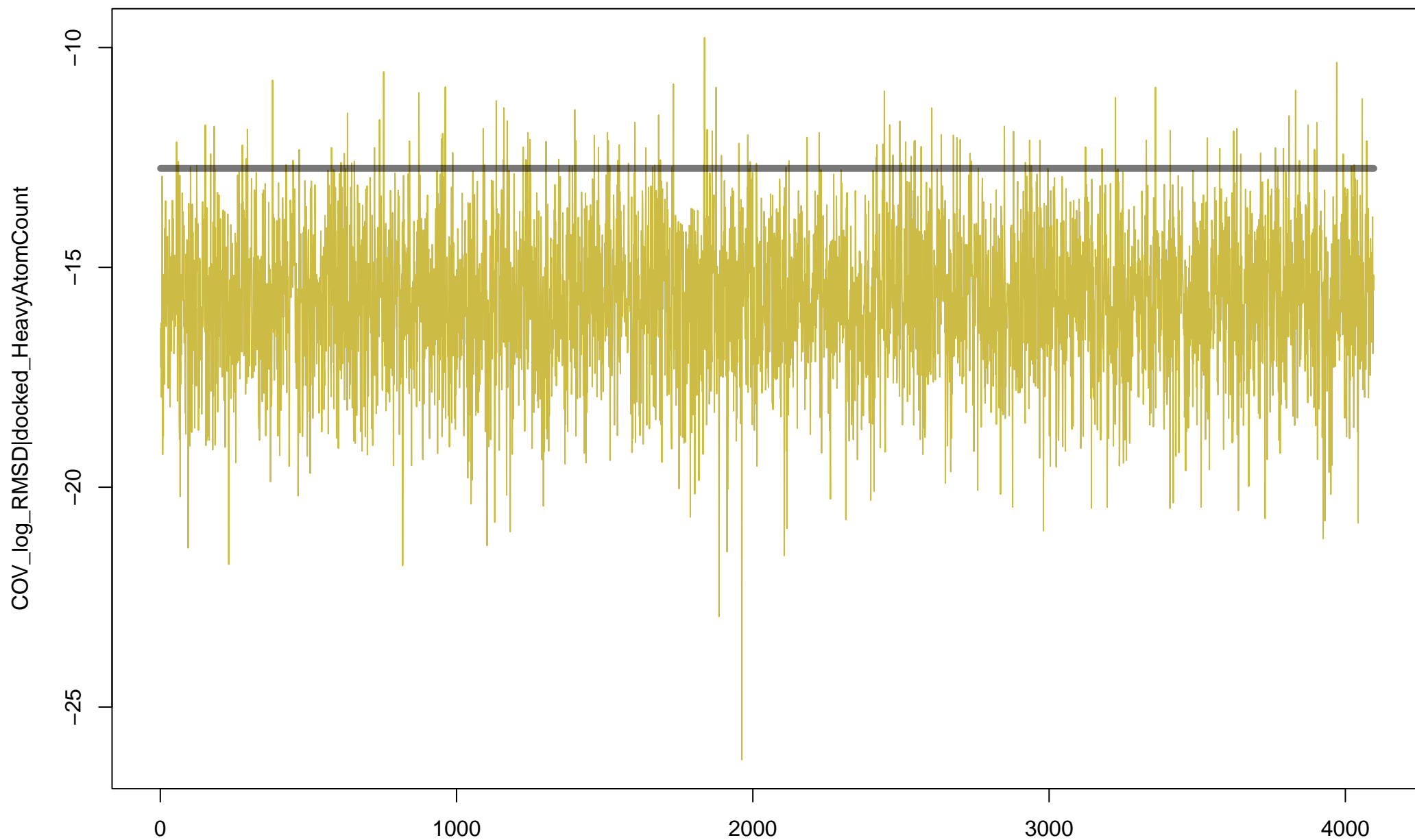
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3430 | BMK = 0.0412 | MCSE(6.27) = 1.83 | stat: TRUE | burn: 0 | rel.err: 0.47



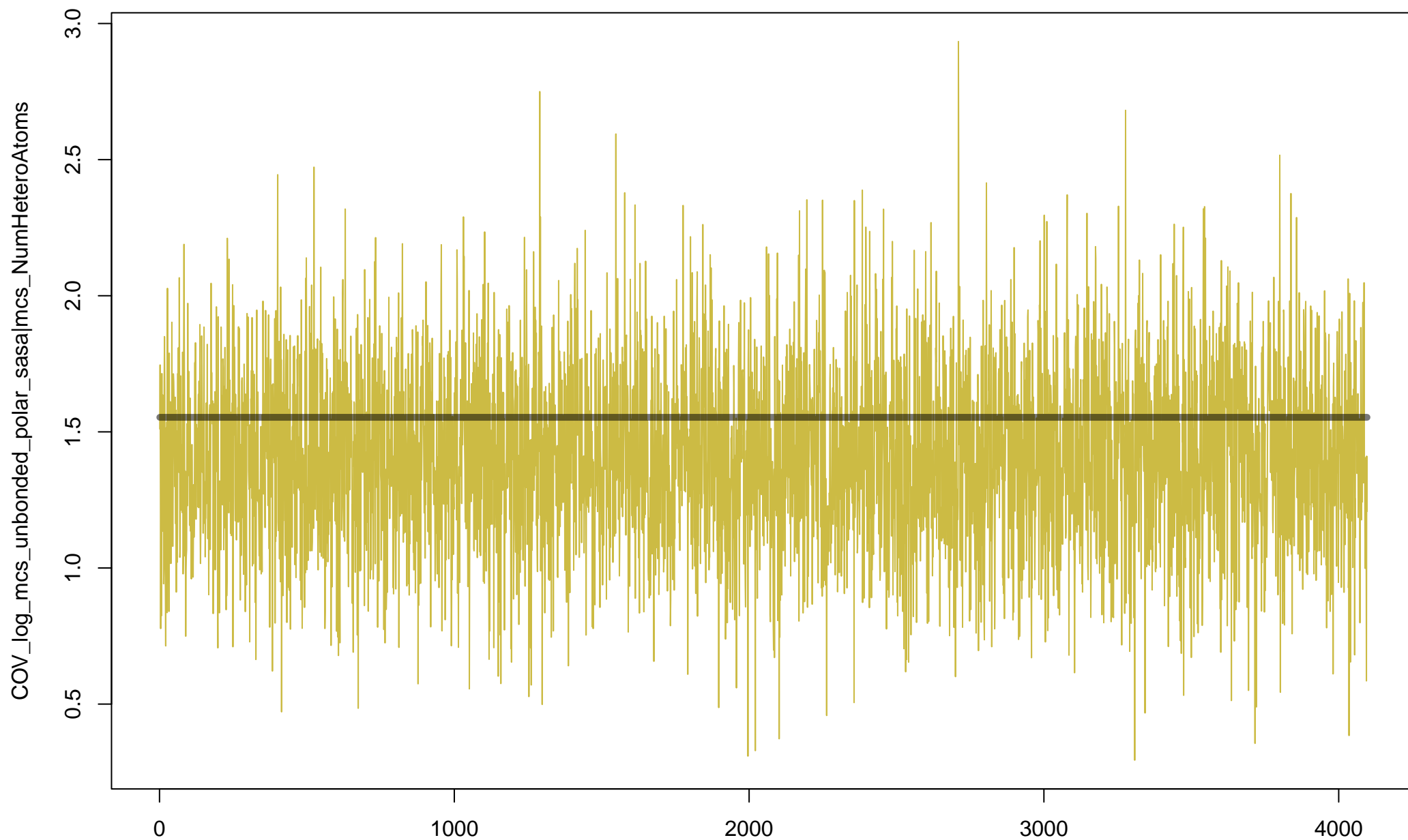
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 3350 | BMK = 0.0352 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0 | rel.err: -1.59



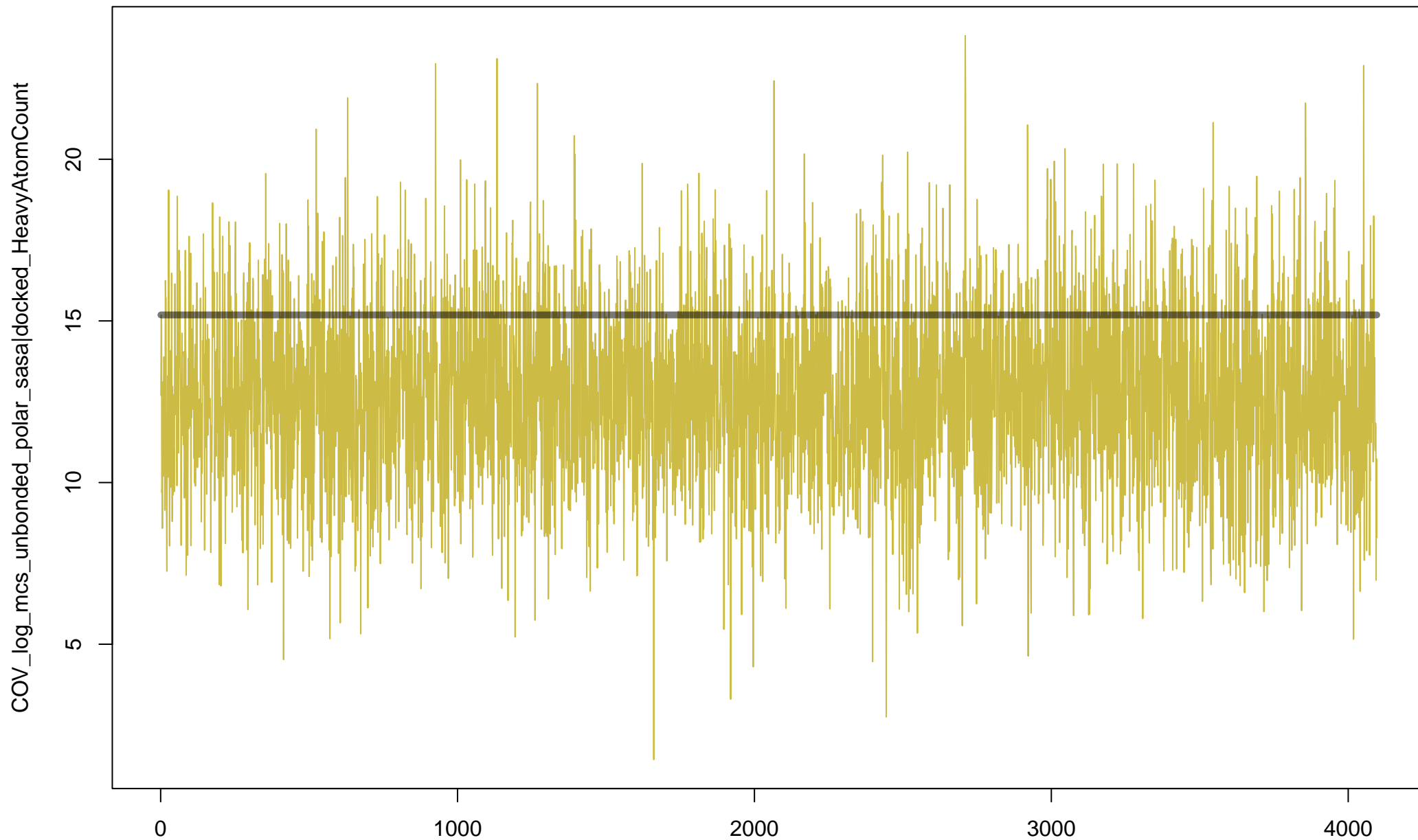
COV_log_RMSD|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0517 | MCSE(6.27) = 1.66 | stat: TRUE | burn: 0 | rel.err: -1.77



COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0372 | MCSE(6.27) = 1.38 | stat: TRUE | burn: 0 | rel.err: -0.453



COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 3890 | BMK = 0.0297 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0 | rel.err: -0.935



COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2980 | BMK = 0.0458 | MCSE(6.27) = 1.73 | stat: TRUE | burn: 0 | rel.err: 0.455

