

-- STATS maxD --

min ESS = 95.9749749444298

max BMK = 0.173343251062206

max MCSE = 6.89425998401094

all stationary: FALSE

burn: 0

max rel.err.: 2.04888005235629

-- STATS 2D --

min ESS = 3413.66922085327

max BMK = 0.0504041078095835

max MCSE = 1.91737733339328

all stationary: TRUE

burn: 0

max rel.err.: 1.74487514641305

-- STATS 1D --

min ESS = 2434.01977320669

max BMK = 0.0534821556088849

max MCSE = 2.02909131381374

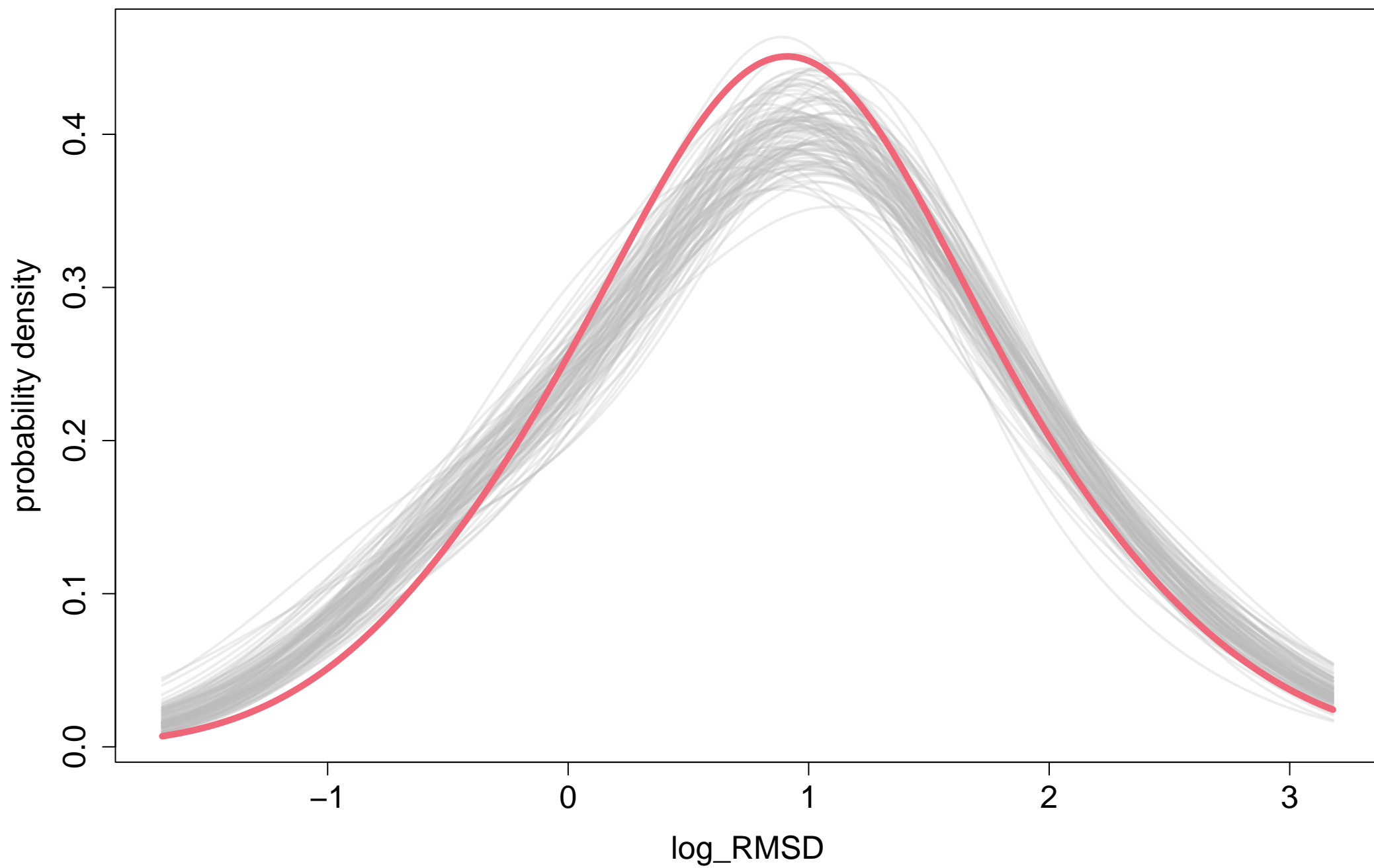
all stationary: FALSE

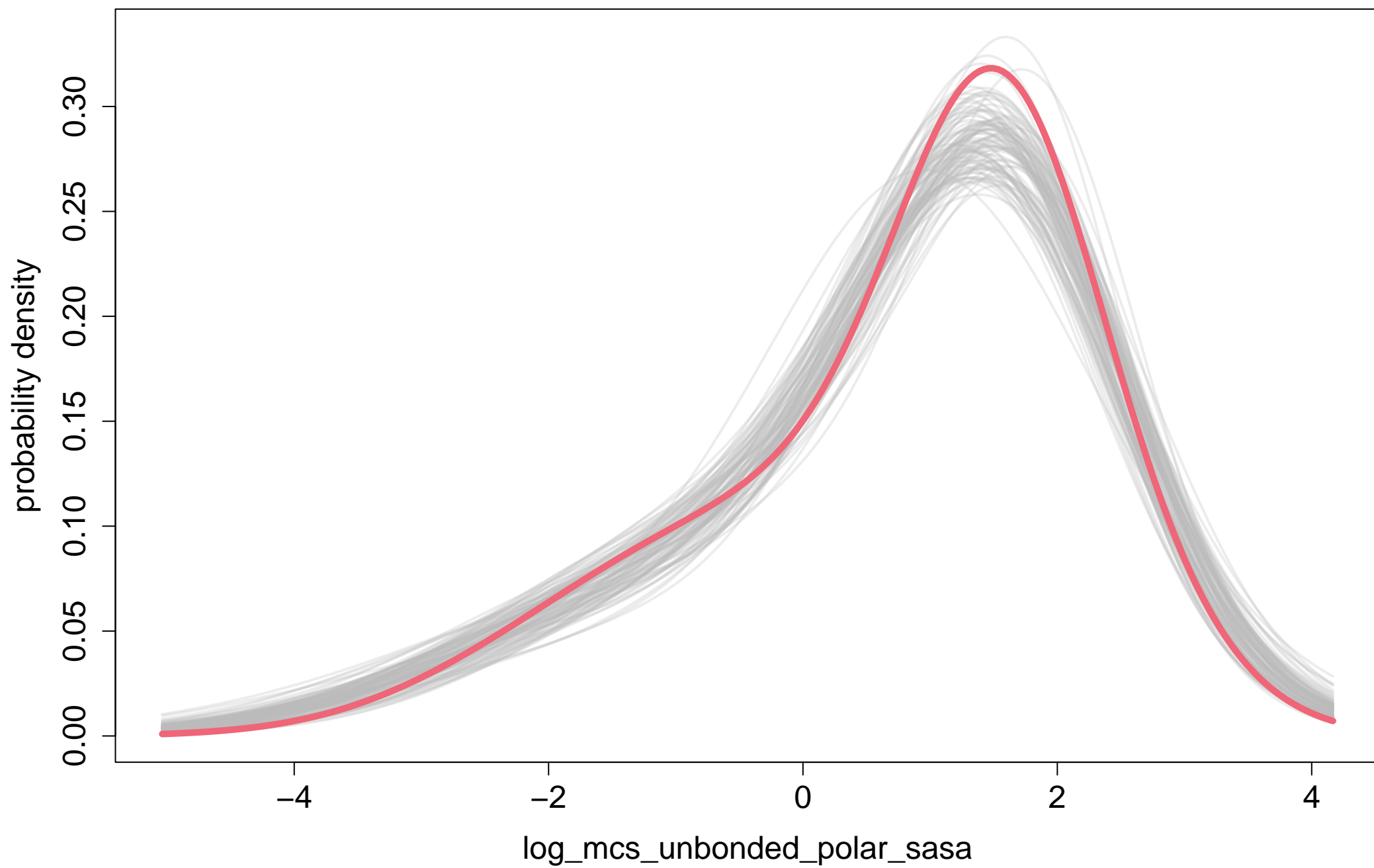
burn: 0

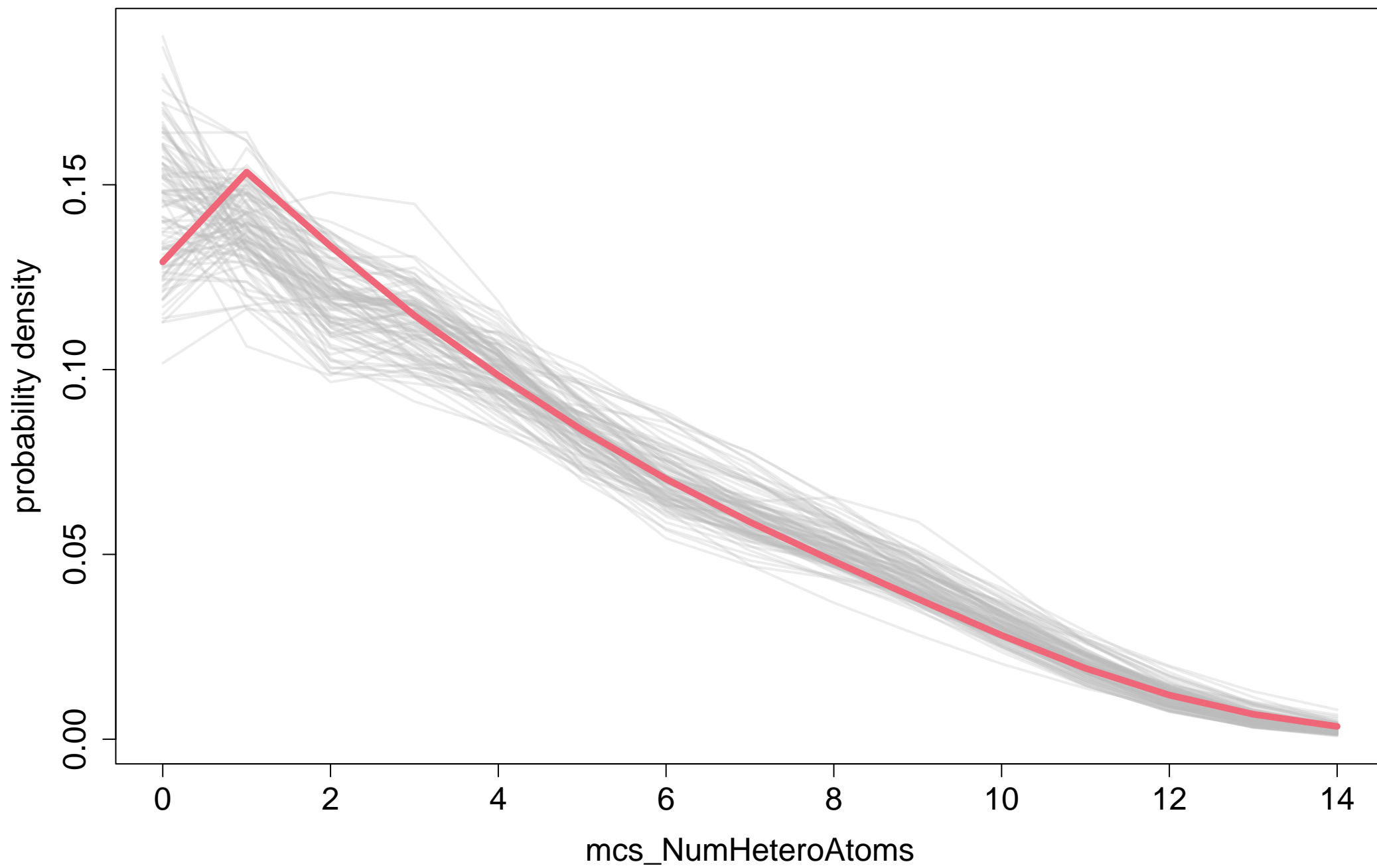
max rel.err.: 2.26006885070676

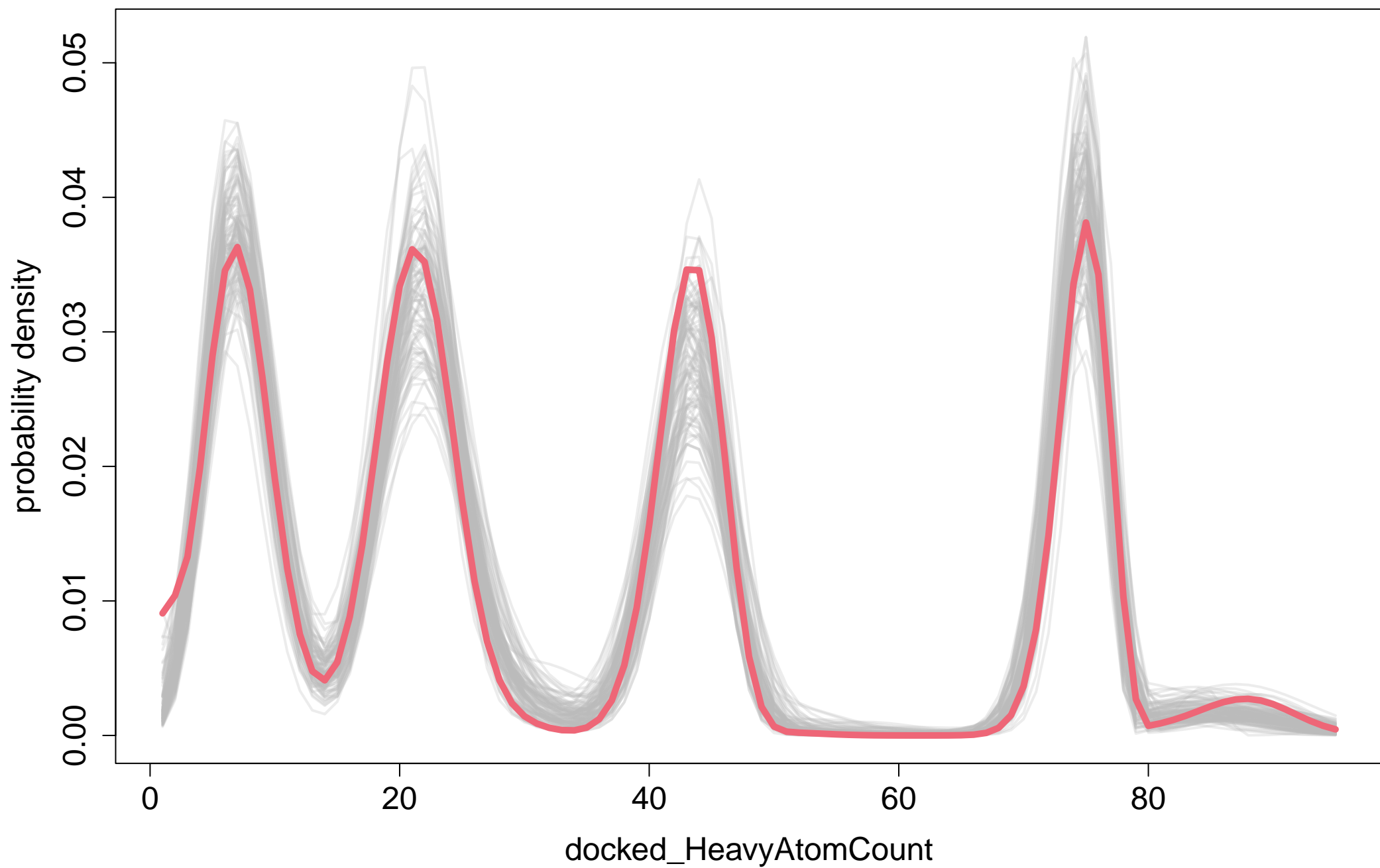
Occupied clusters: 9 of 16

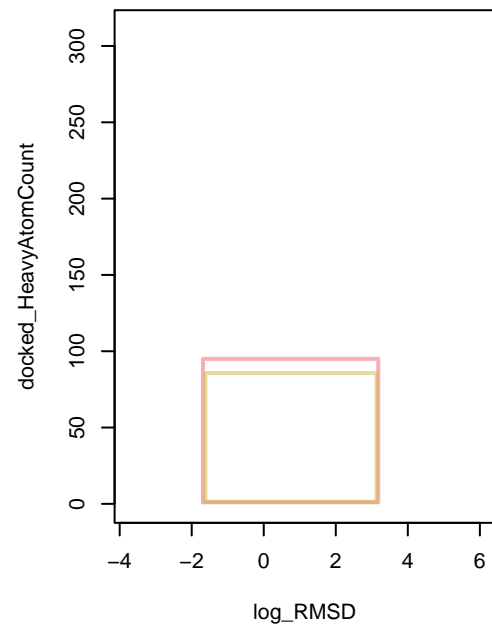
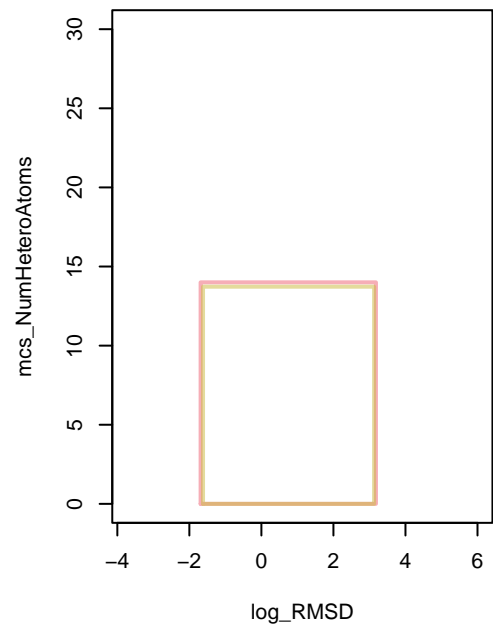
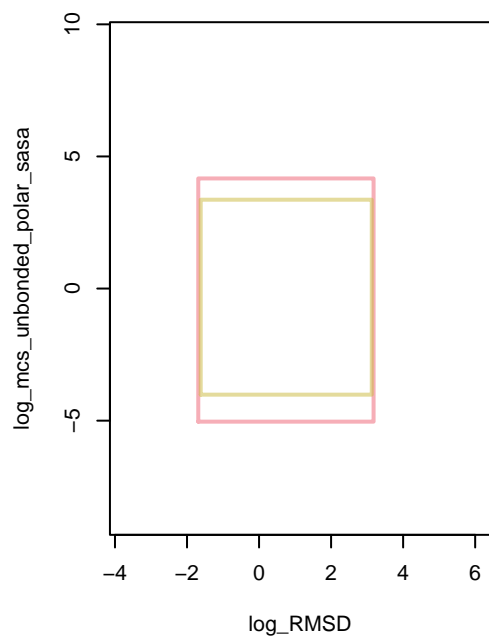
LL: -2160 +- 6.76



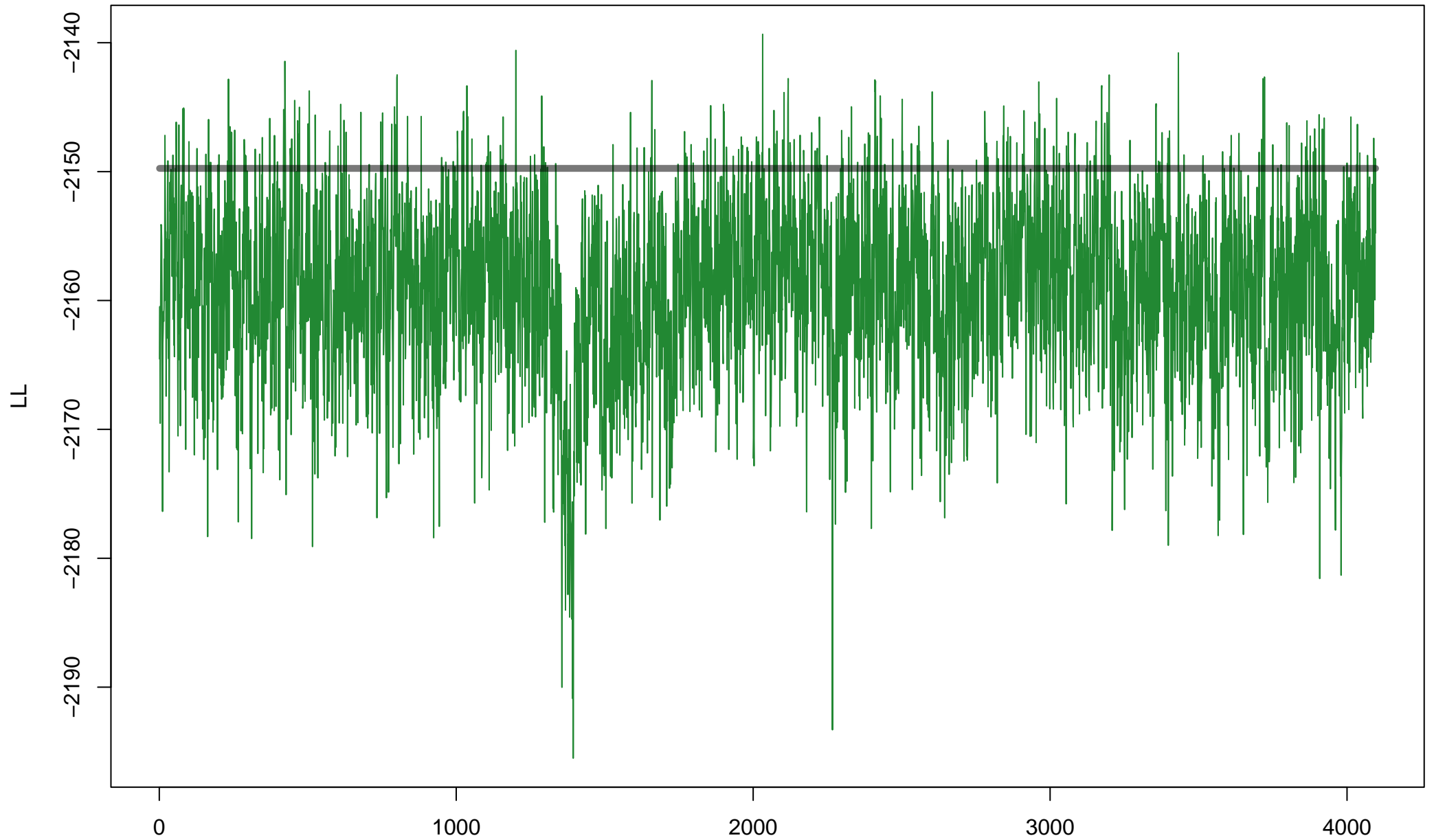




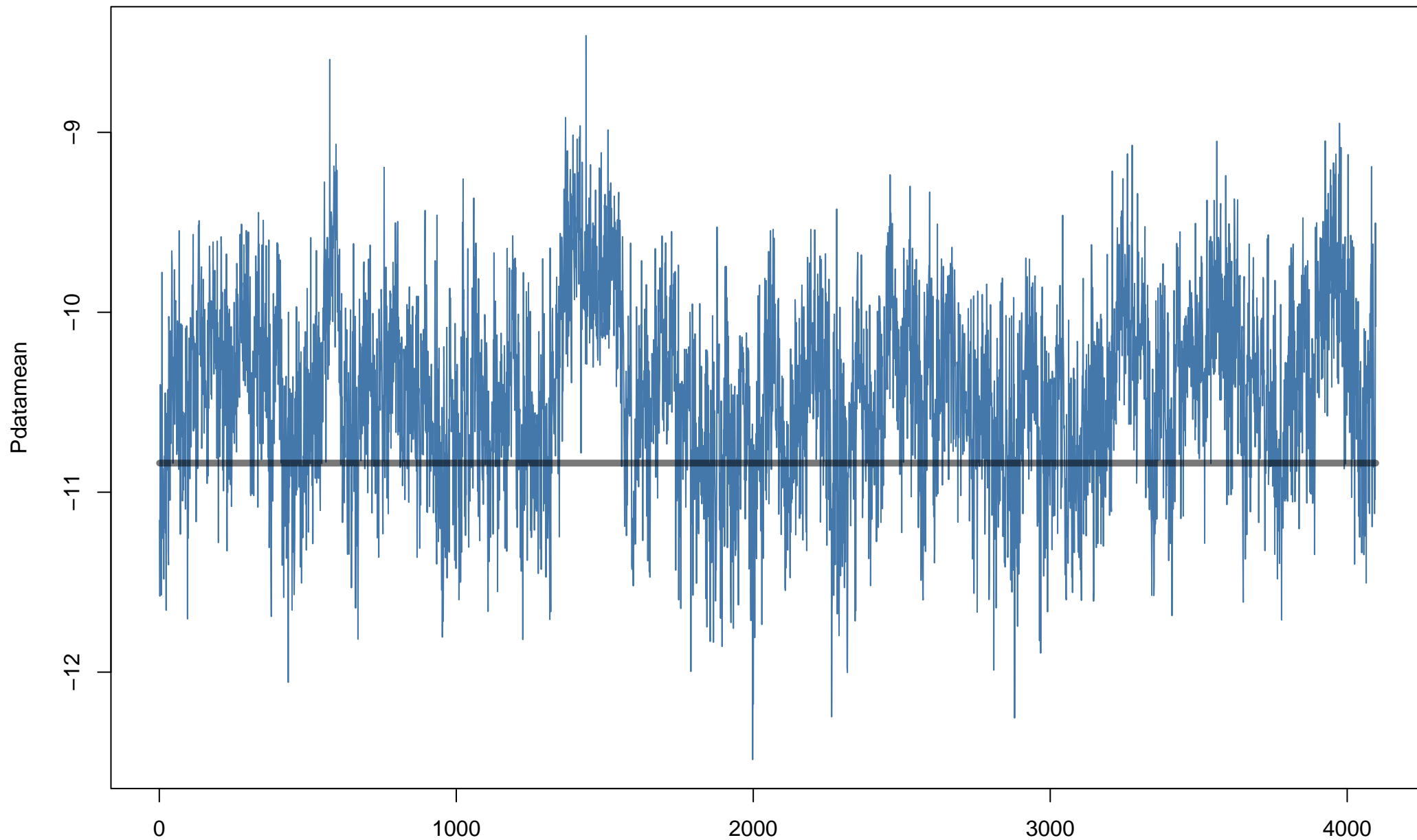




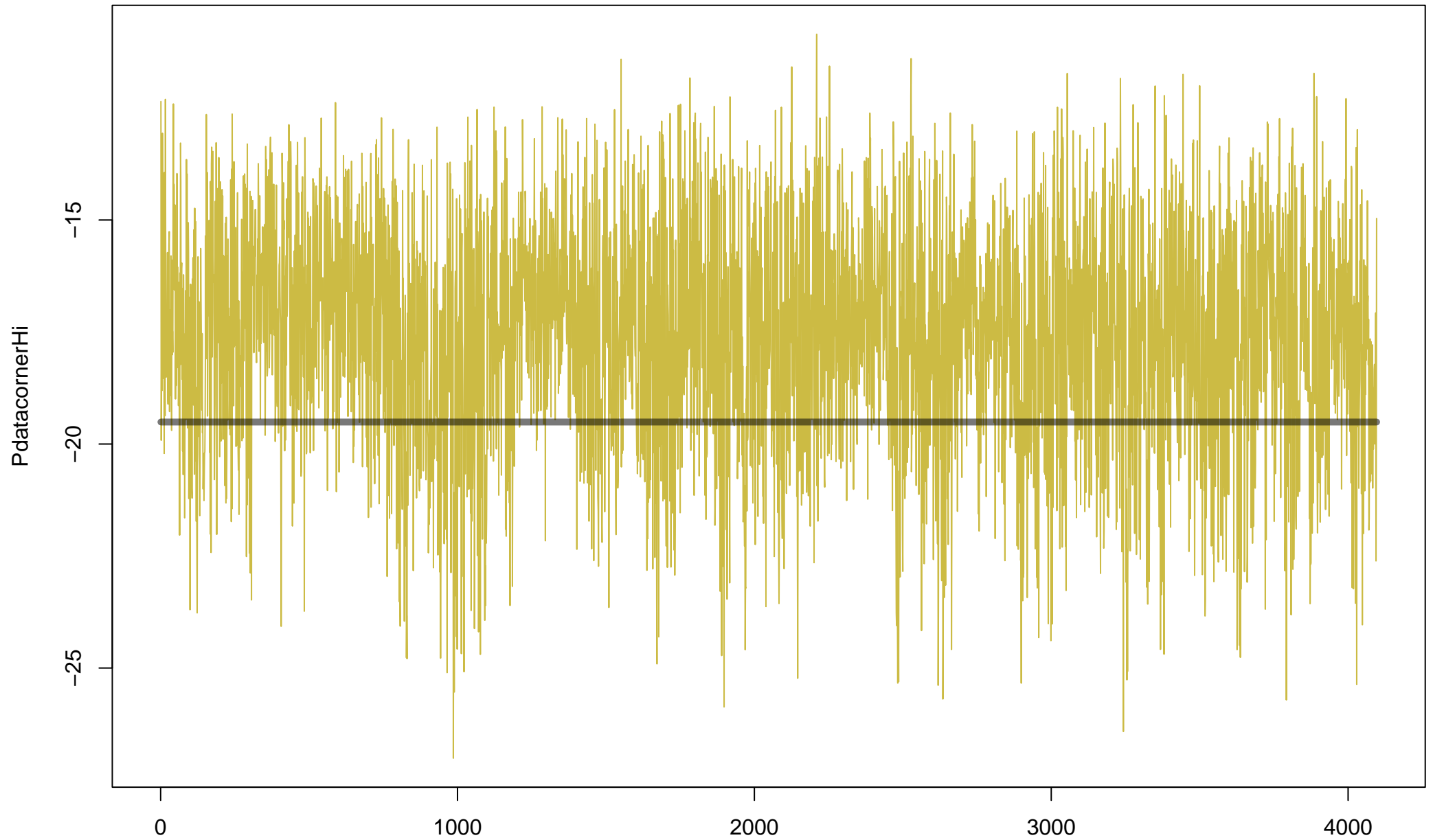
LL



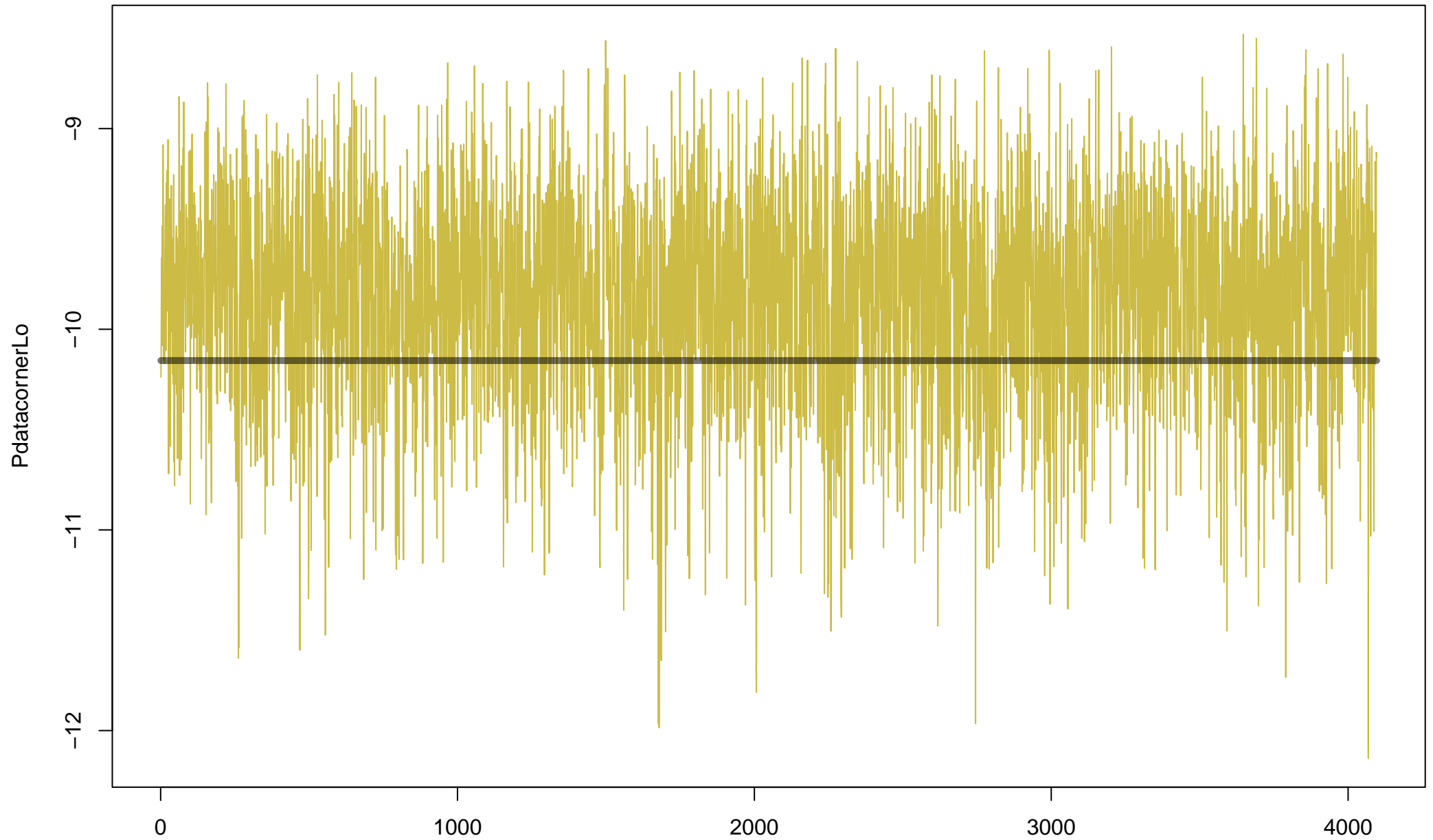
Pdatamean
ESS = 96 | BMK = 0.0508 | MCSE(6.27) = 6.89 | stat: TRUE | burn: 0 | rel.err: 0.759



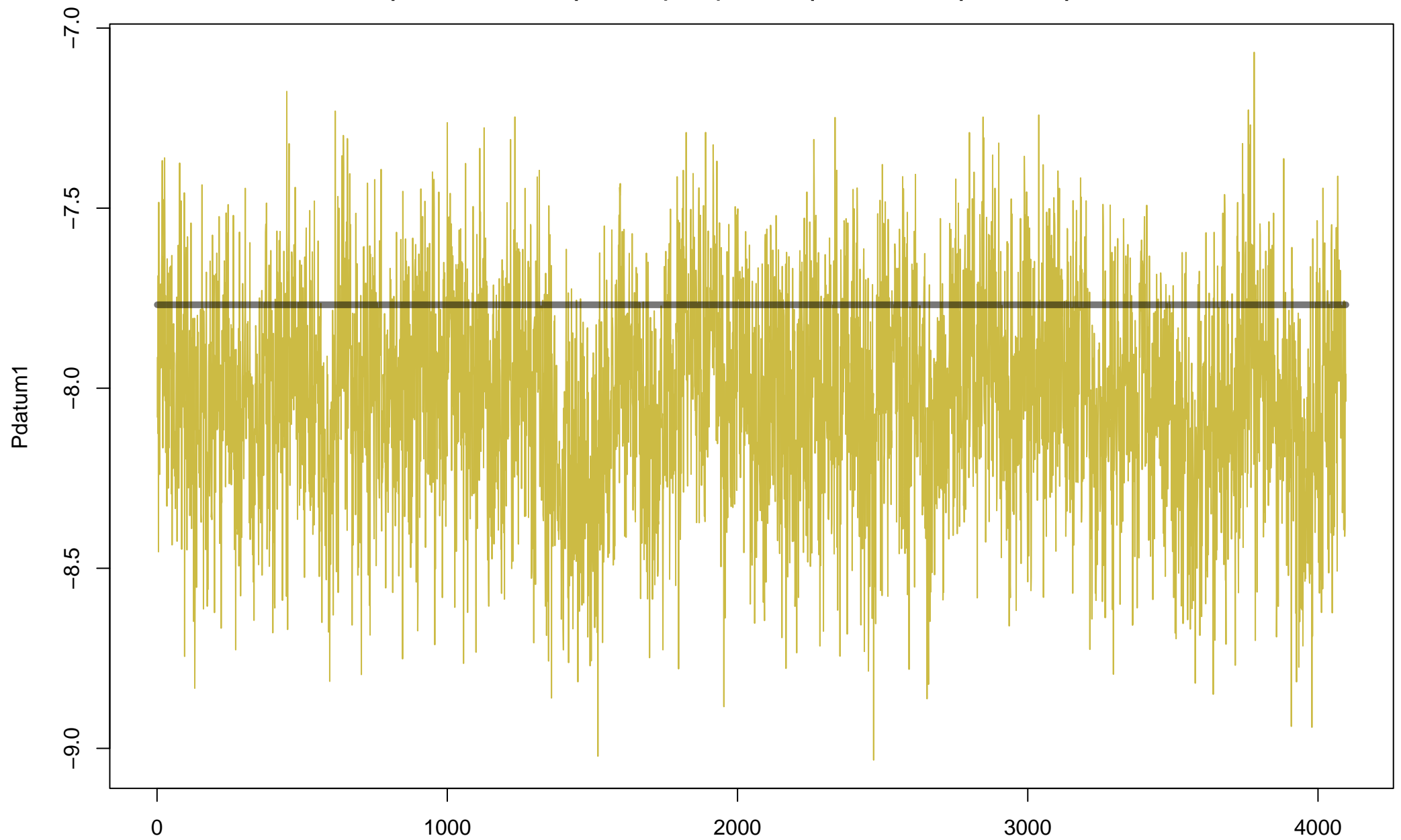
PdatacornerHi
ESS = 3720 | BMK = 0.122 | MCSE(6.27) = 1.7 | stat: TRUE | burn: 0 | rel.err: 0.3



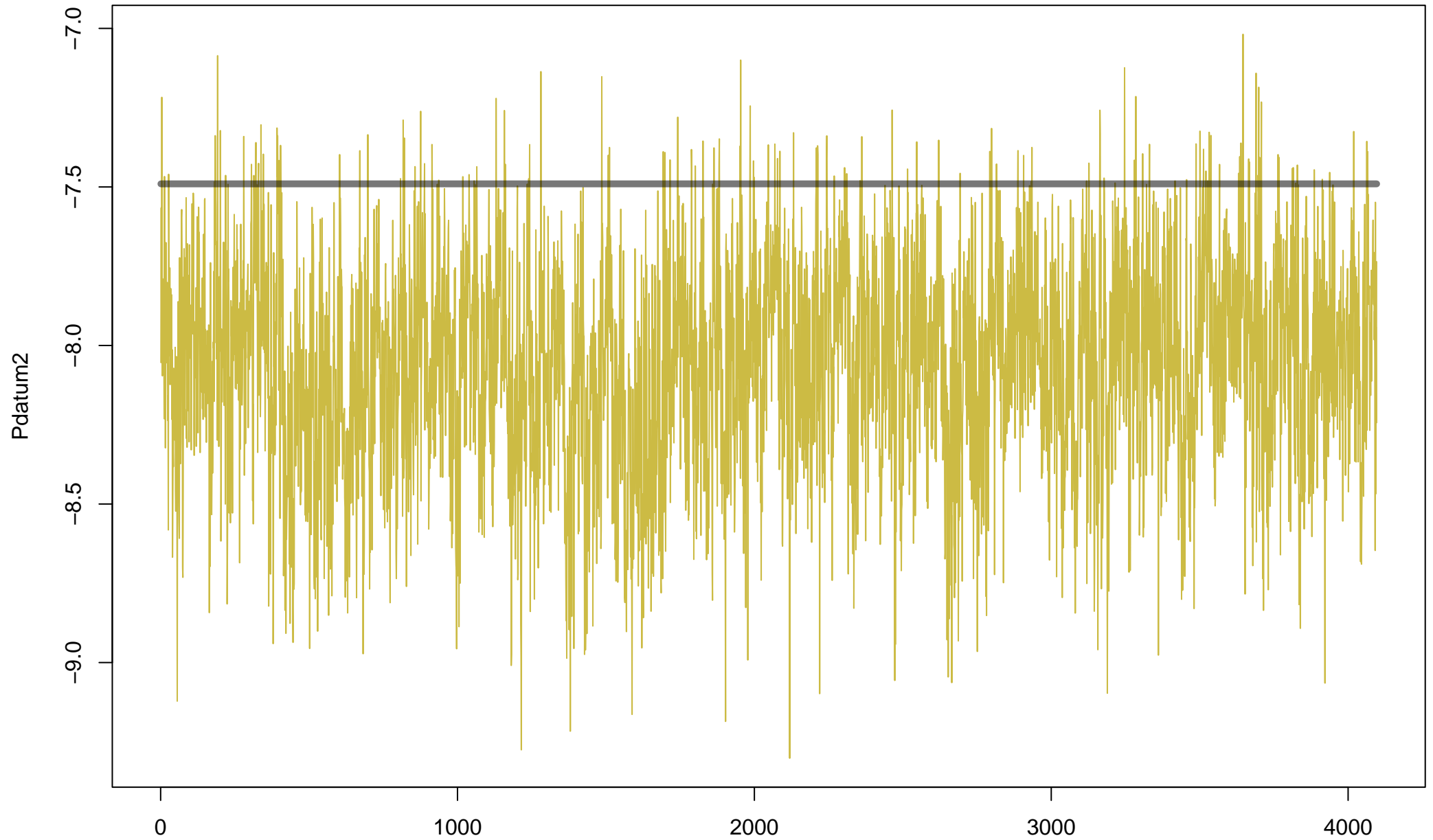
PdatacornerLo
ESS = 3100 | BMK = 0.043 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0 | rel.err: 0.709



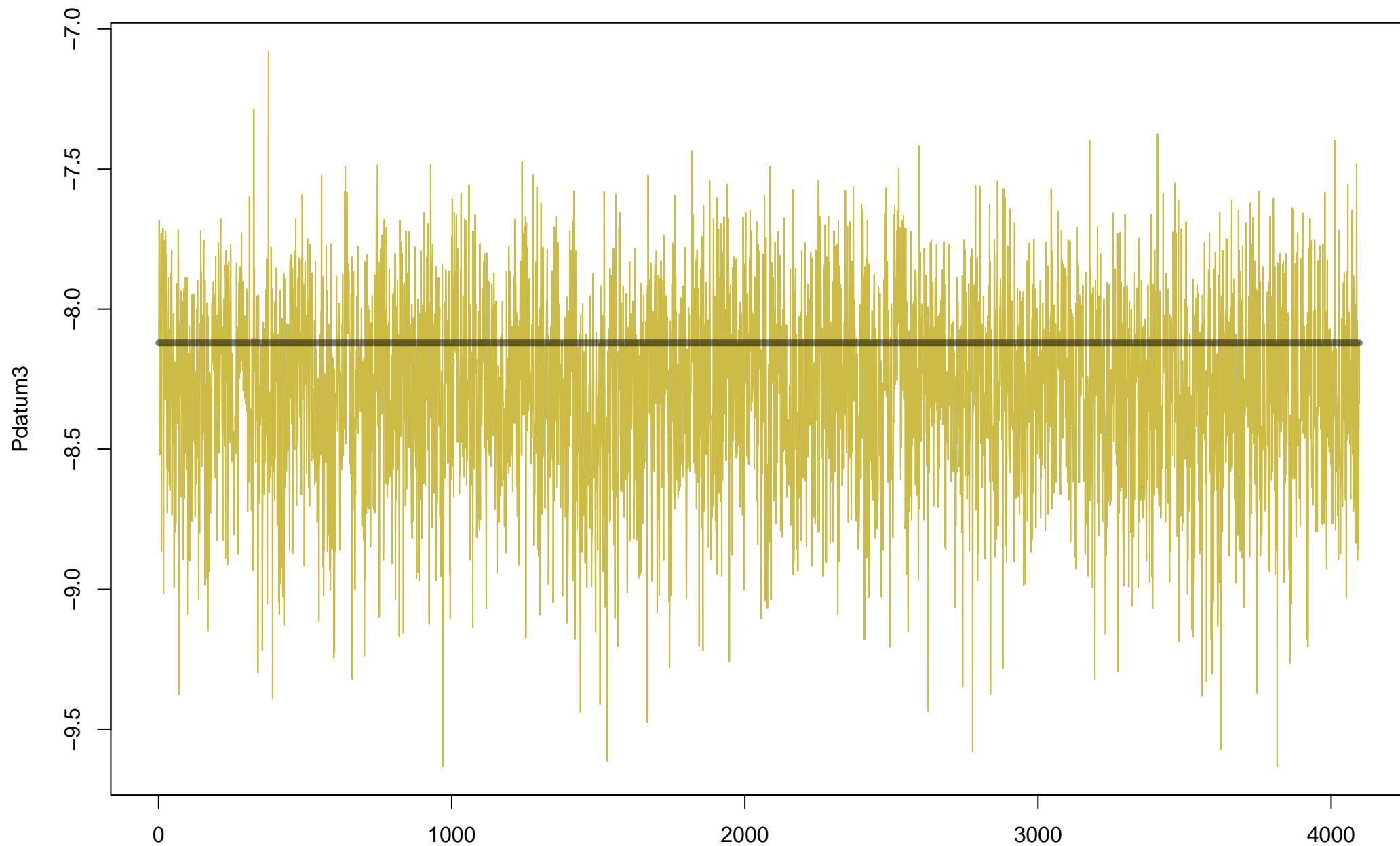
Pdatum1
ESS = 641 | BMK = 0.0347 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0 | rel.err: -0.827



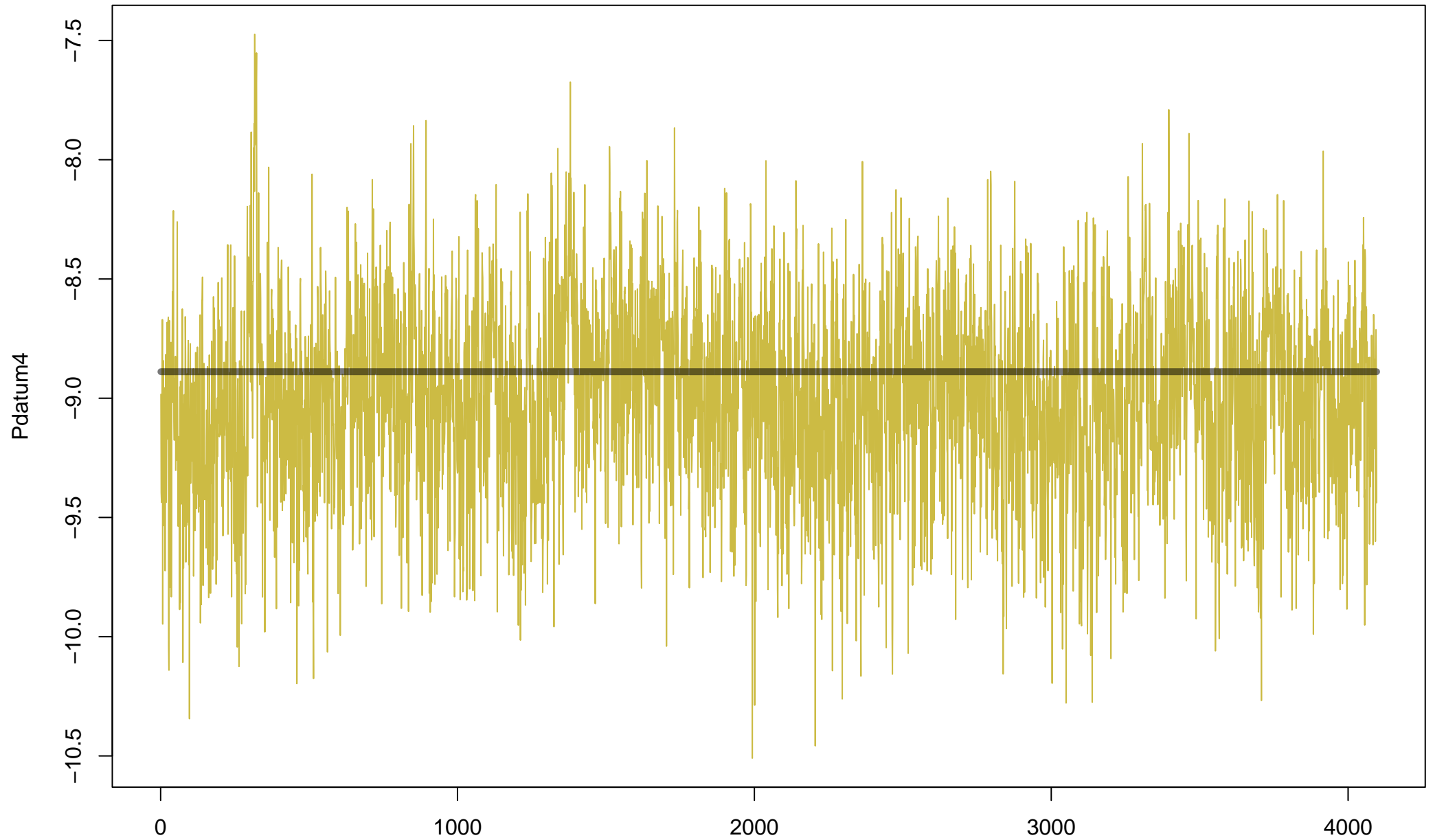
Pdatum2
ESS = 673 | BMK = 0.0933 | MCSE(6.27) = 3.81 | stat: TRUE | burn: 0 | rel.err: -2.05



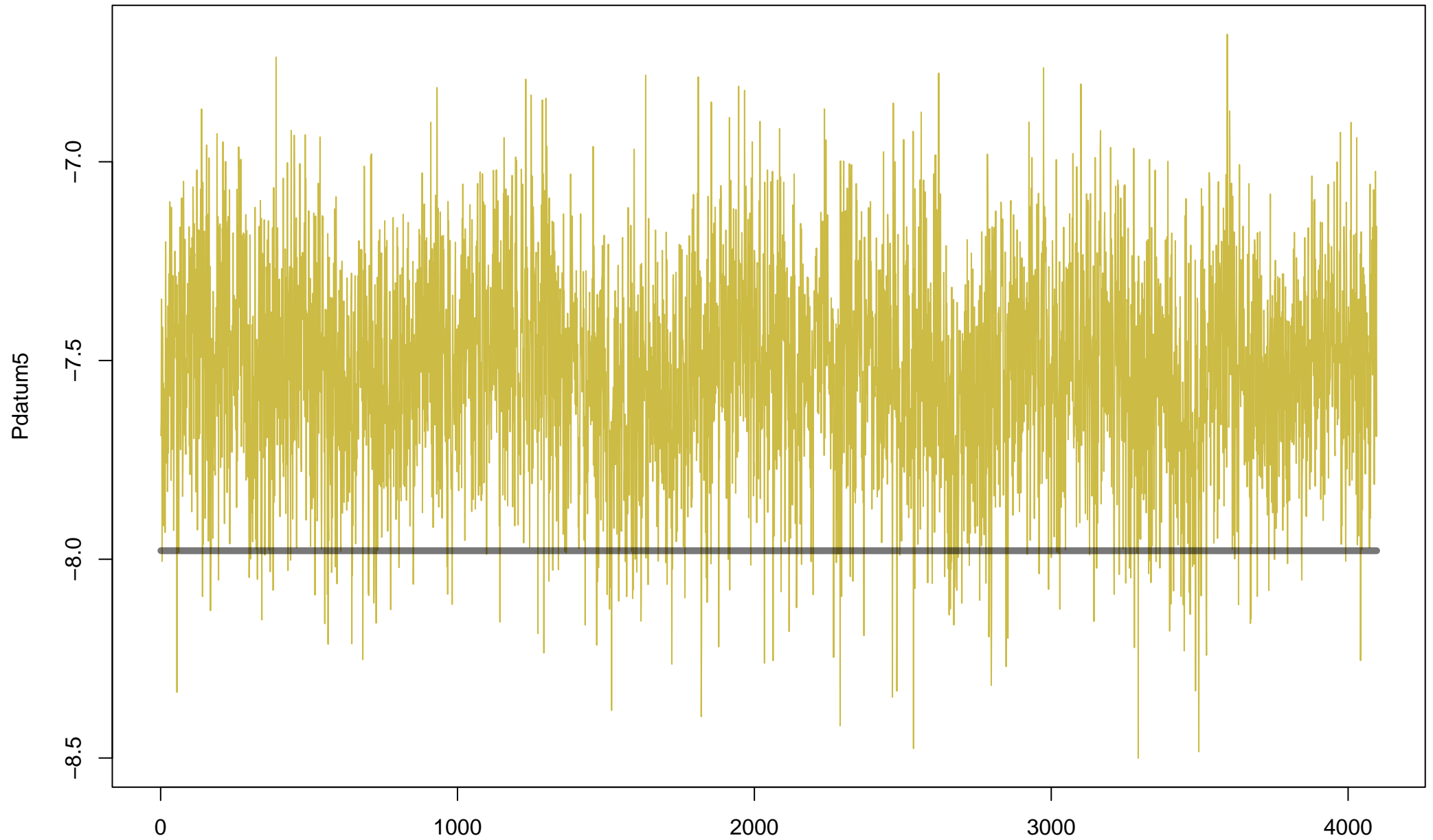
Pdatum3
ESS = 2230 | BMK = 0.0383 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0 | rel.err: -0.365



Pdatum4
ESS = 833 | BMK = 0.061 | MCSE(6.27) = 3.72 | stat: TRUE | burn: 0 | rel.err: -0.096

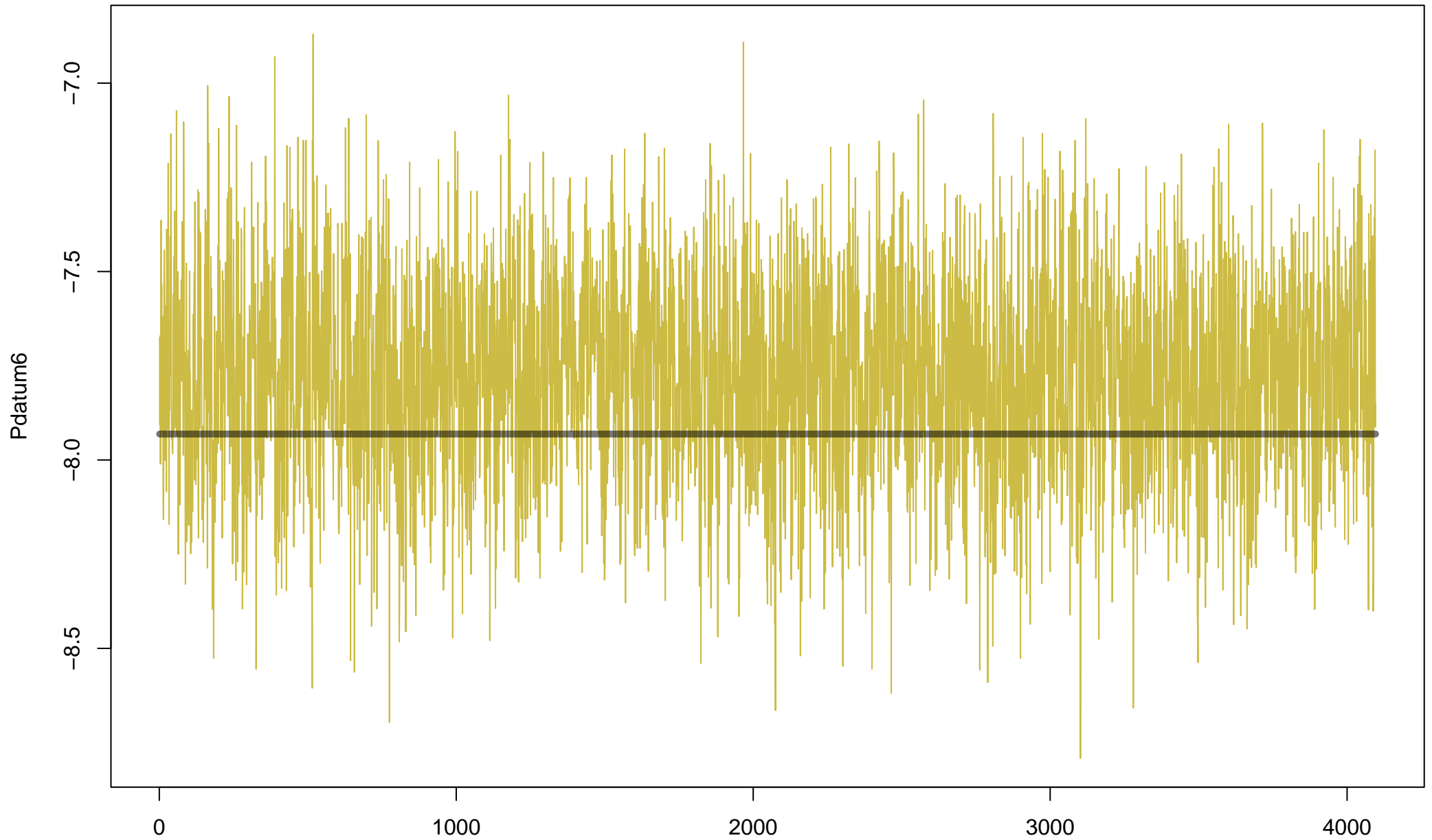


Pdatum5
ESS = 1000 | BMK = 0.0392 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | rel.err: 1.51



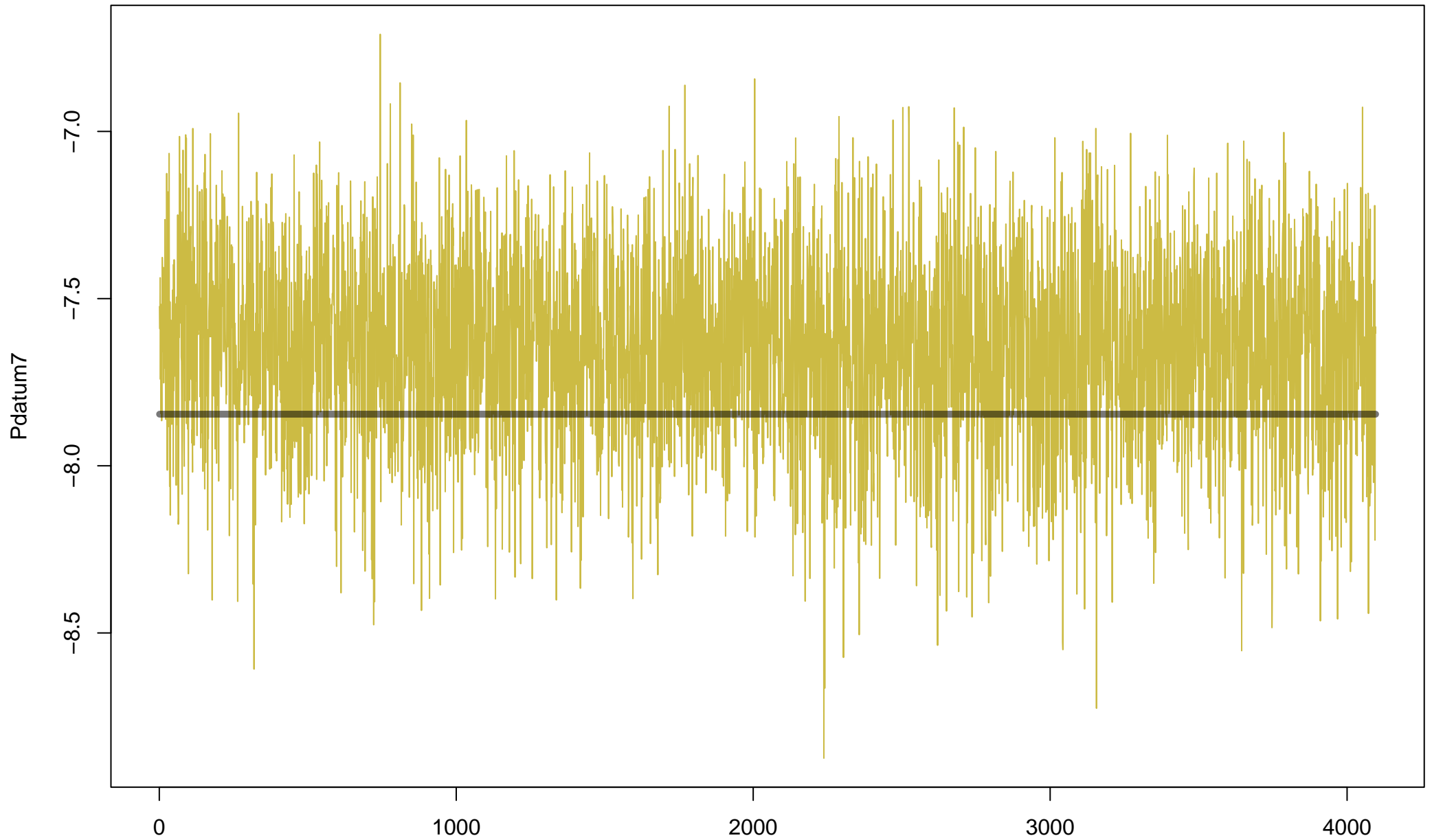
Pdatum6

ESS = 2380 | BMK = 0.0374 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0 | rel.err: 0.643



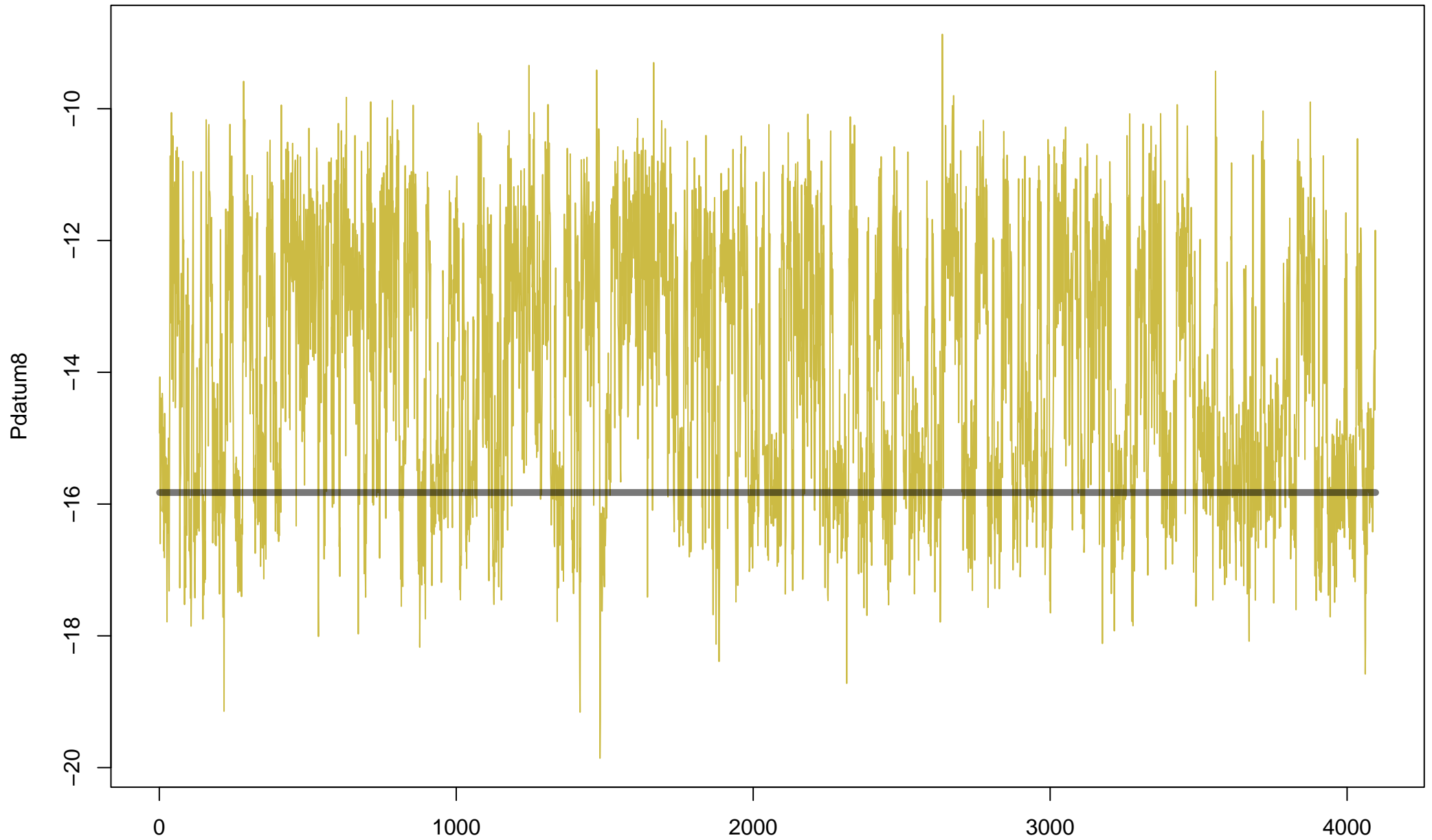
Pdatum7

ESS = 3680 | BMK = 0.0565 | MCSE(6.27) = 1.88 | stat: FALSE | burn: 0 | rel.err: 0.759



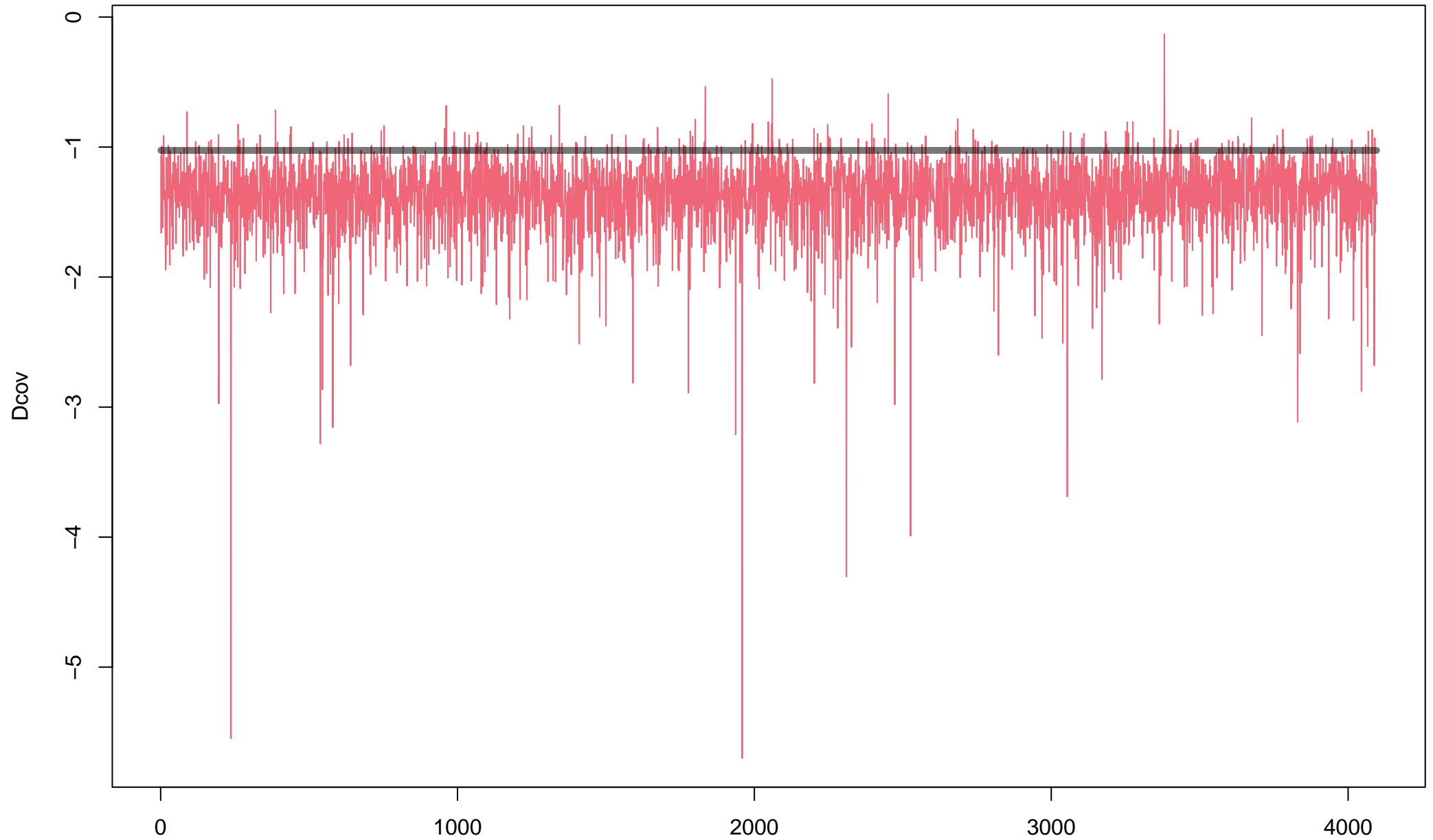
Pdatum8

ESS = 845 | BMK = 0.173 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0 | rel.err: 0.516

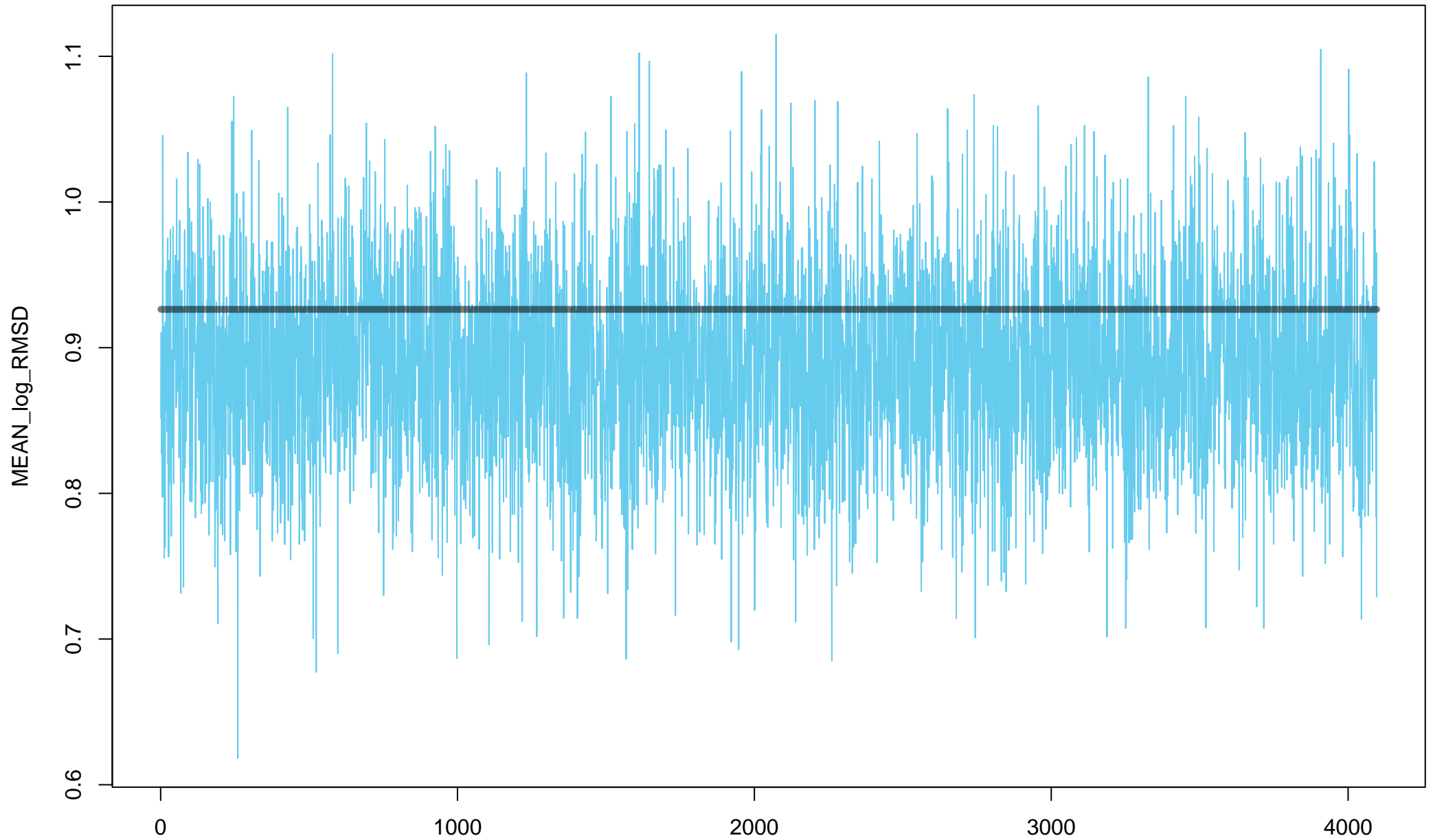


Dcov

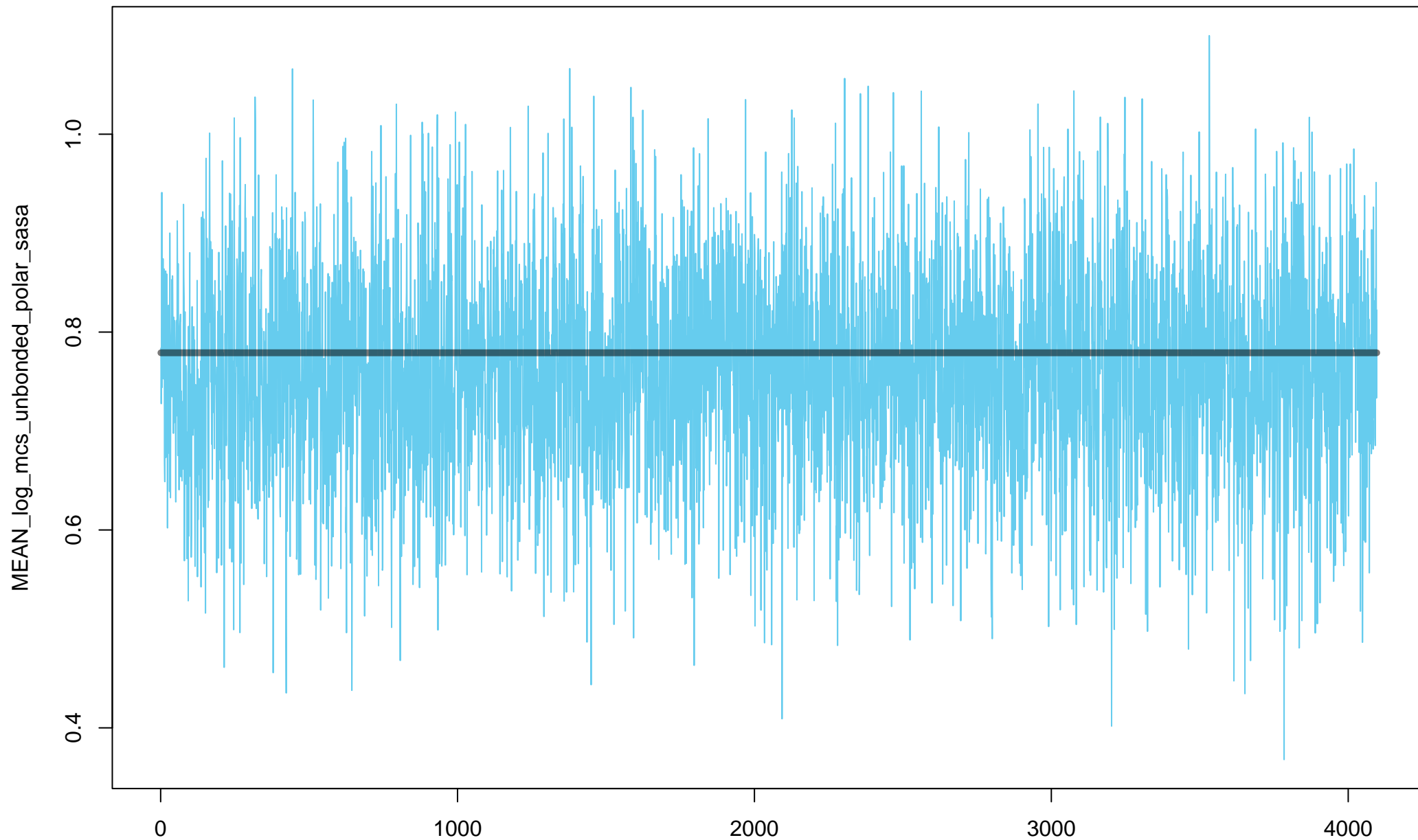
ESS = 3280 | BMK = 0.0562 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0 | rel.err: 1.5



MEAN_log_RMSD
ESS = 4100 | BMK = 0.0279 | MCSE(6.27) = 1.61 | stat: TRUE | burn: 0 | rel.err: -0.583

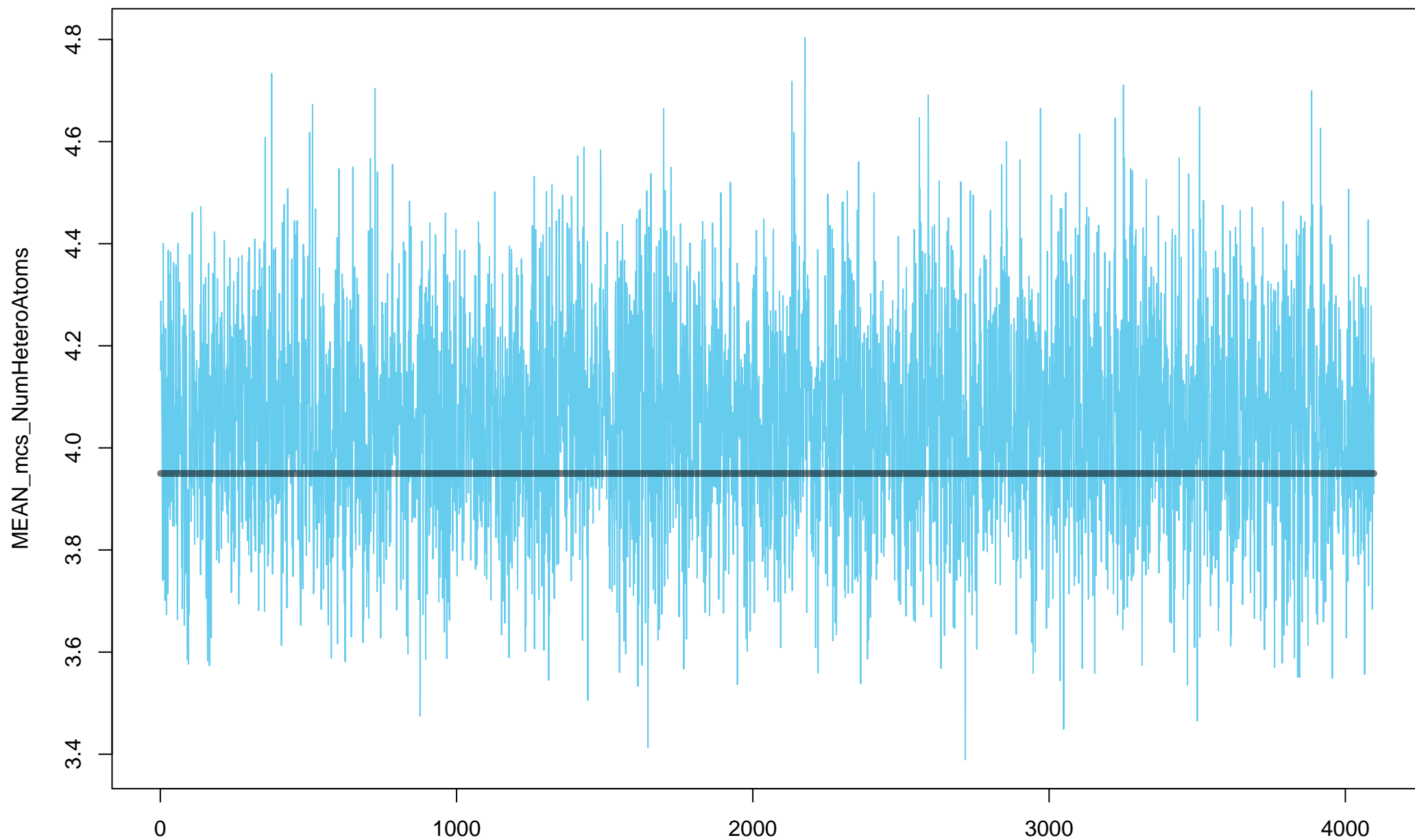


MEAN_log_mcs_unbonded_polar_sasa
ESS = 3850 | BMK = 0.0353 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: -0.185

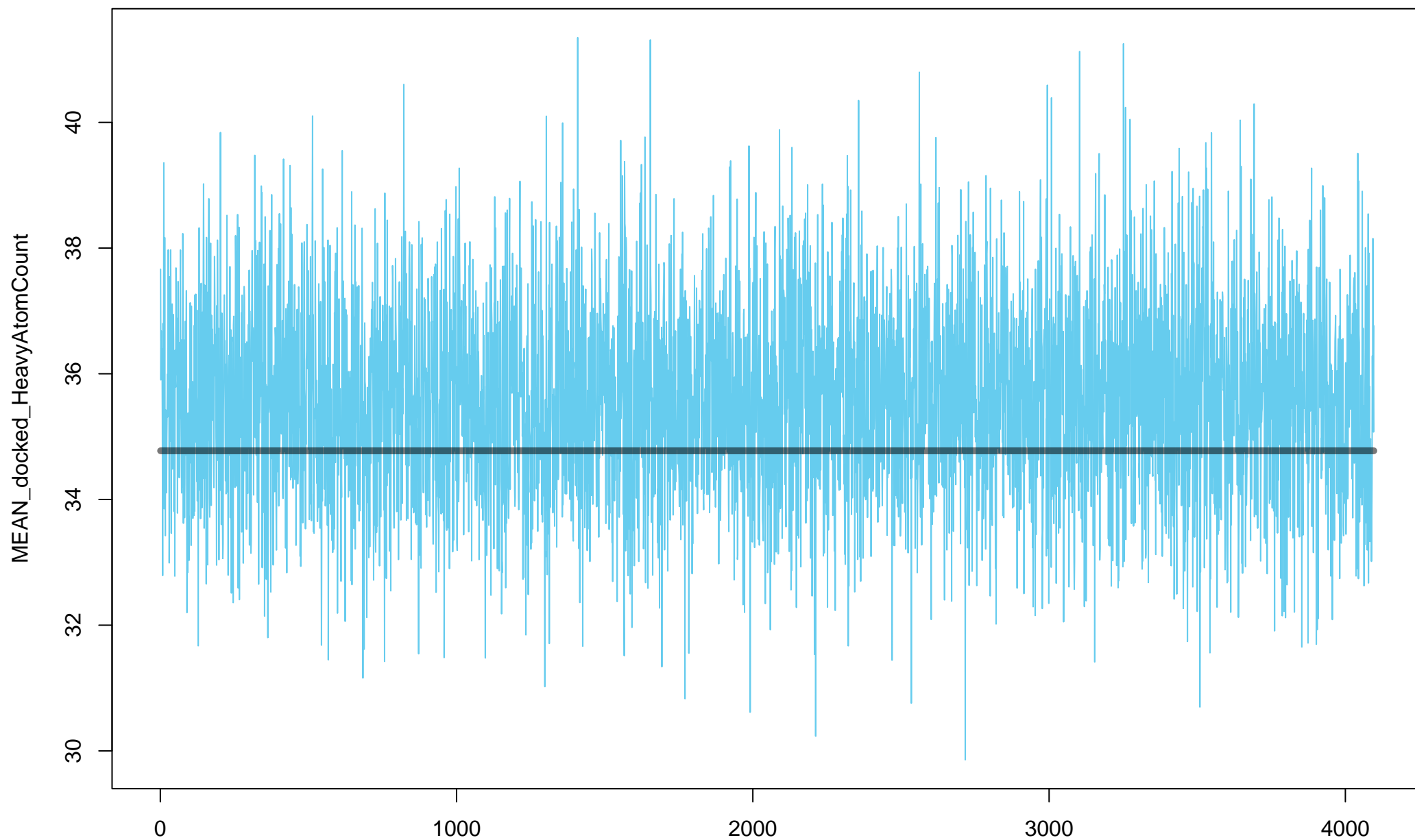


MEAN_mcs_NumHeteroAtoms

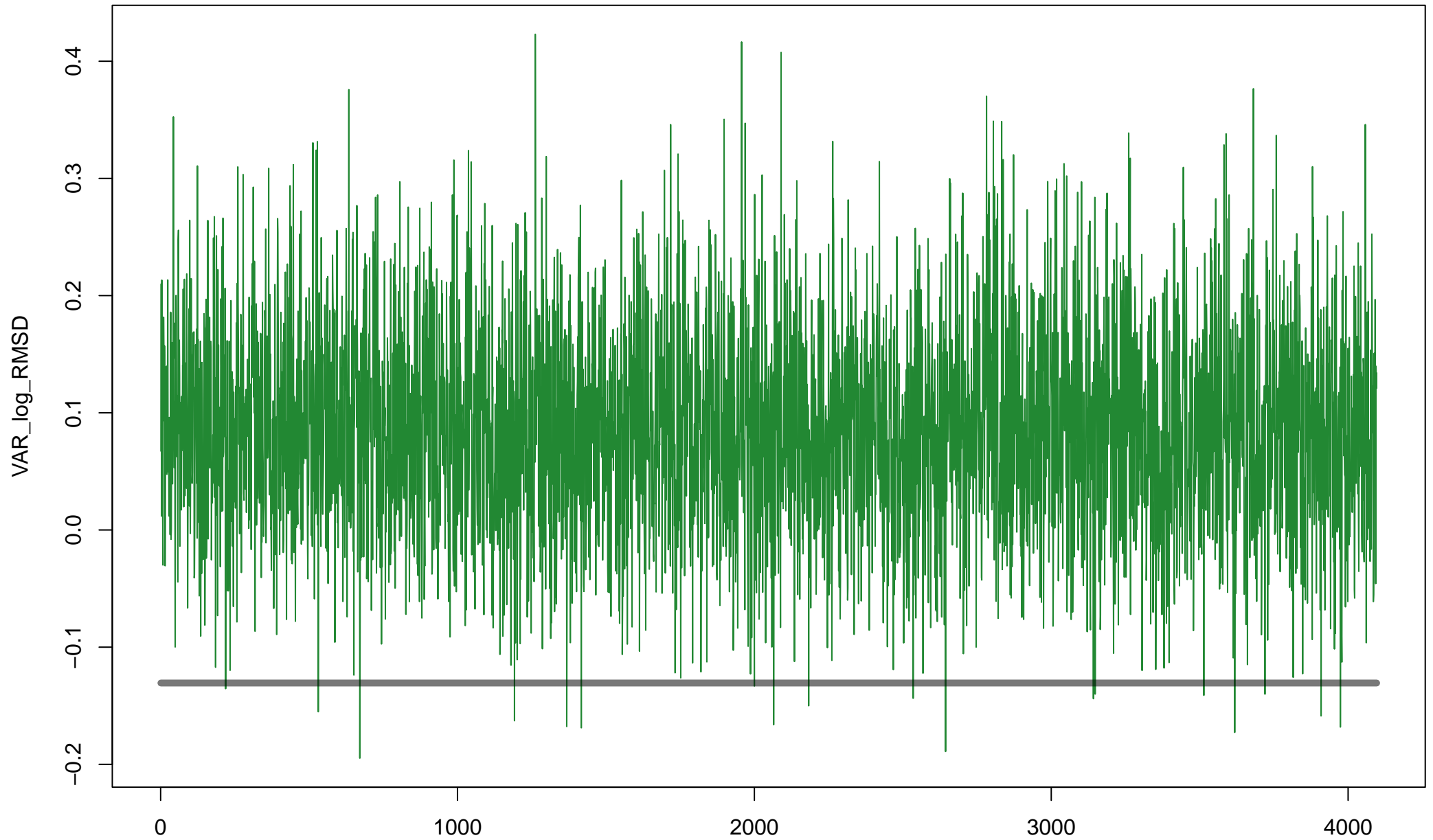
ESS = 4100 | BMK = 0.0223 | MCSE(6.27) = 1.49 | stat: TRUE | burn: 0 | rel.err: 0.493



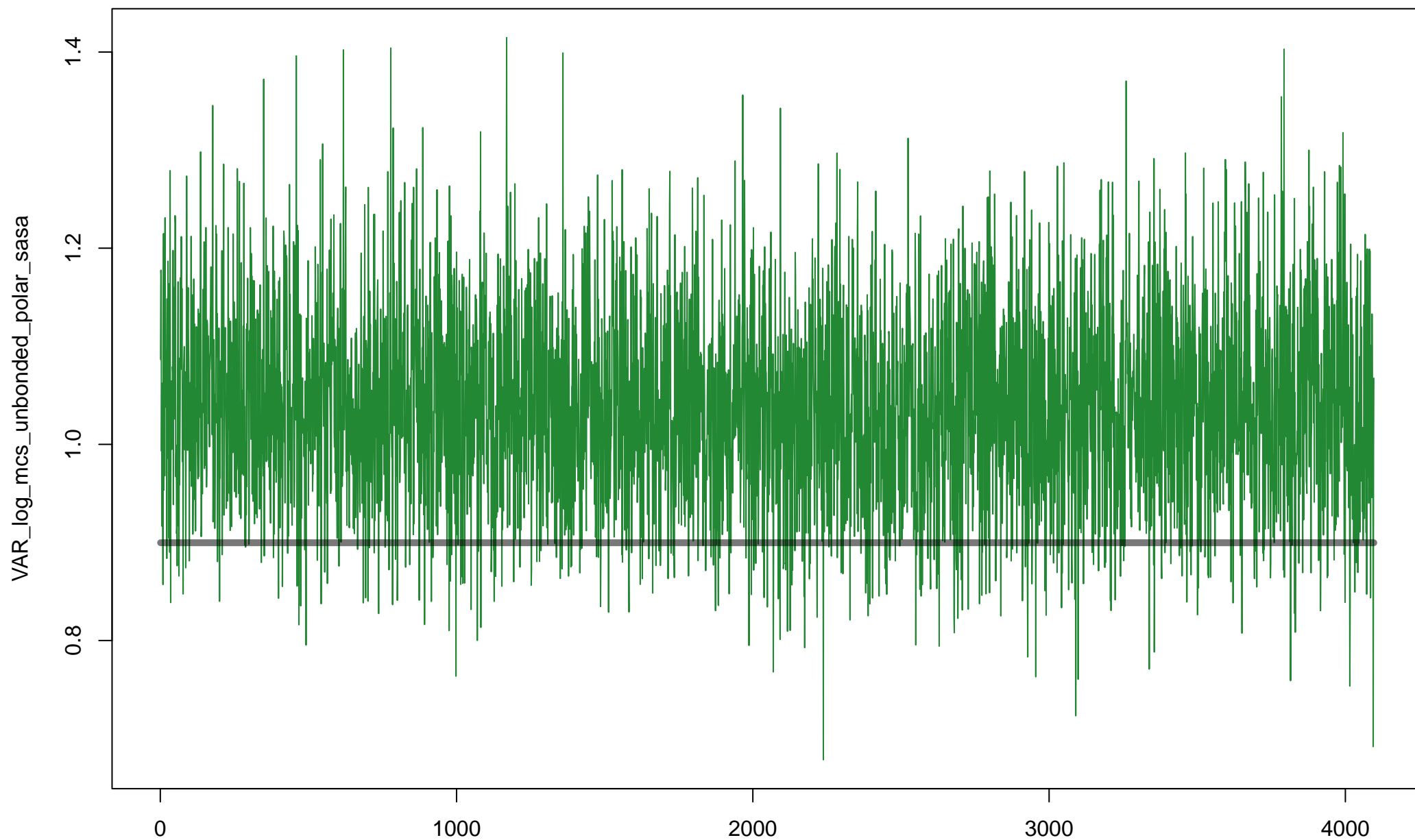
MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0409 | MCSE(6.27) = 1.33 | stat: TRUE | burn: 0 | rel.err: 0.521



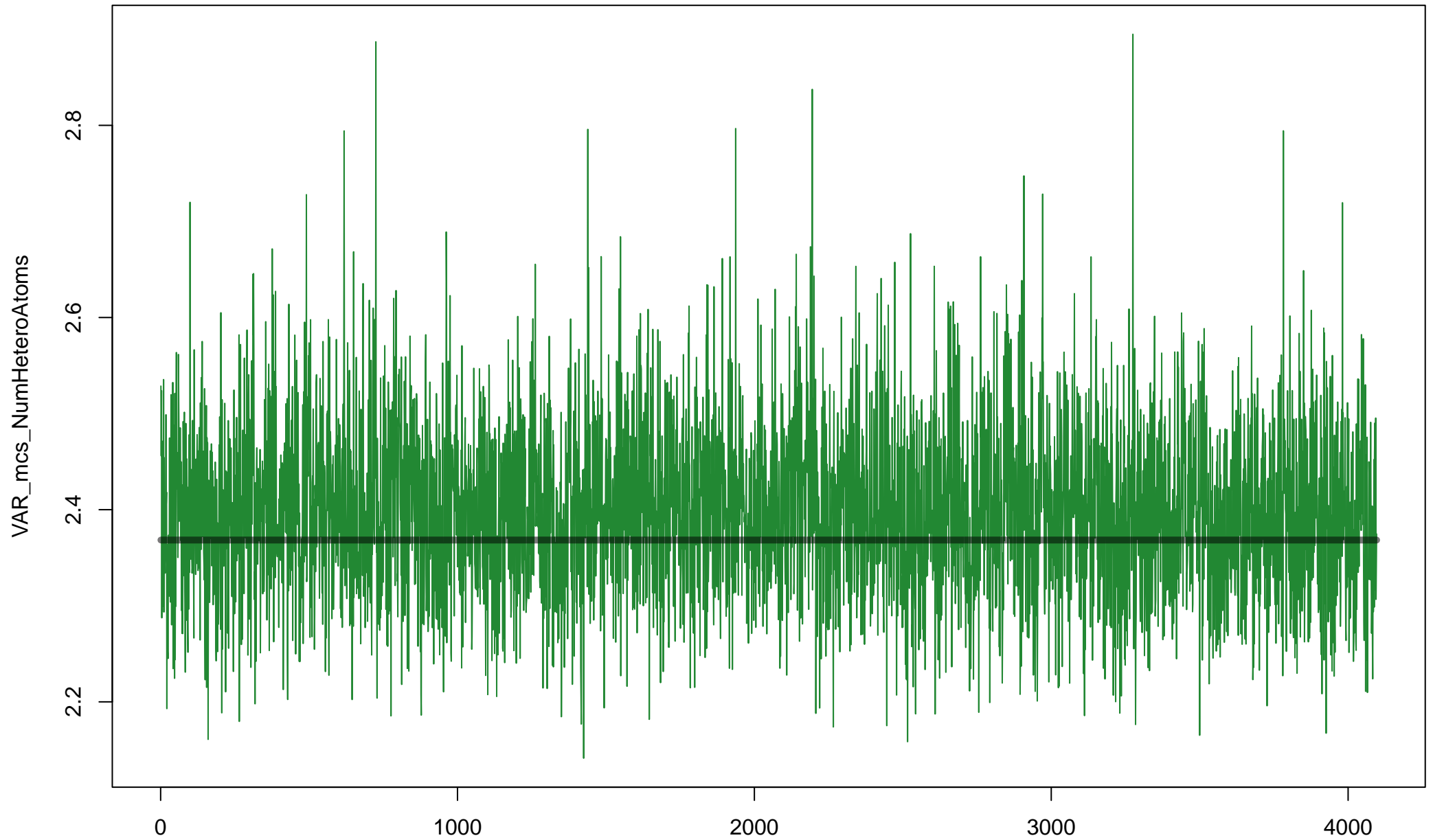
VAR_log_RMSD
ESS = 3910 | BMK = 0.0305 | MCSE(6.27) = 1.7 | stat: TRUE | burn: 0 | rel.err: 2.26



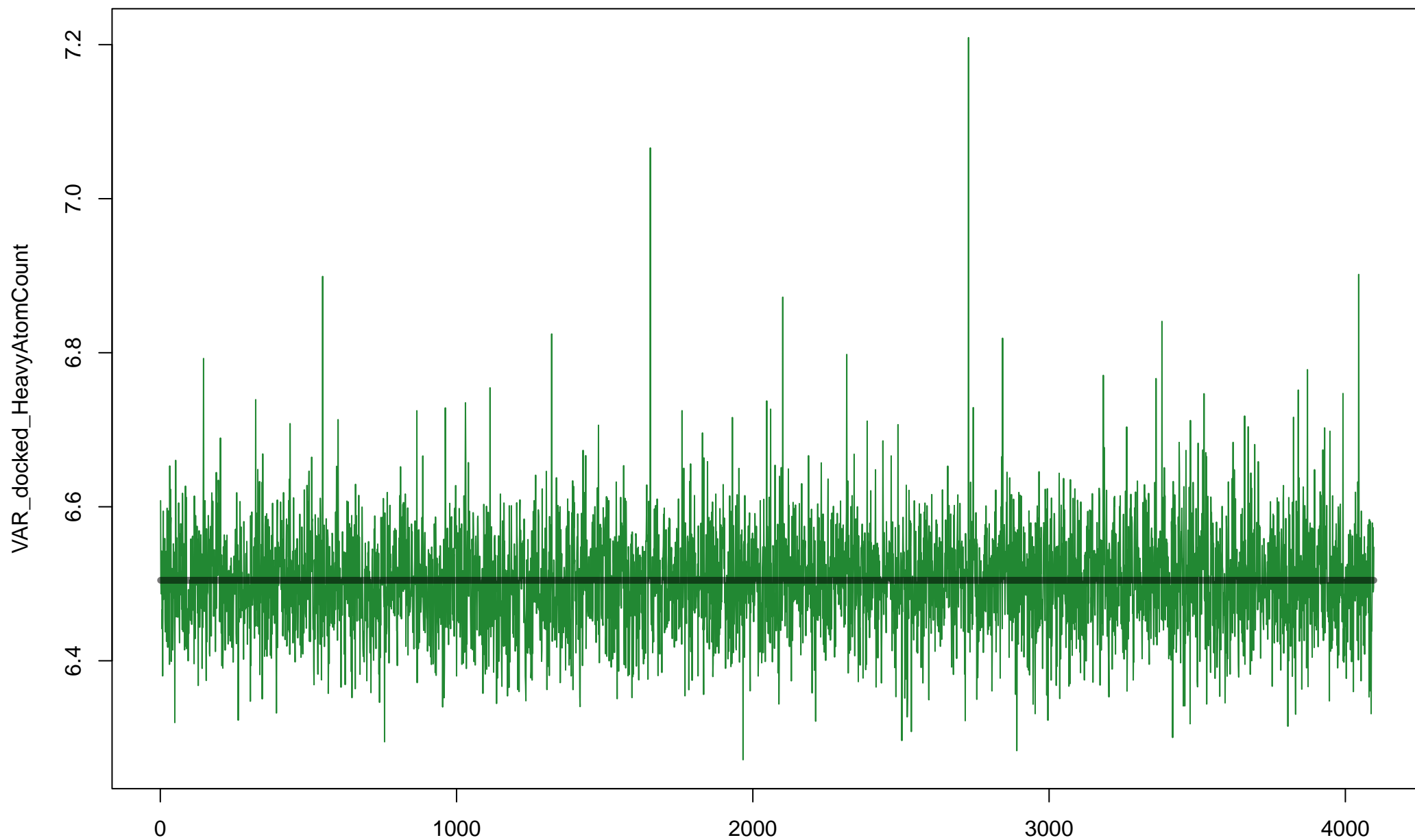
VAR_log_mcs_unbonded_polar_sasa
ESS = 3620 | BMK = 0.0517 | MCSE(6.27) = 1.71 | stat: FALSE | burn: 0 | rel.err: 1.35



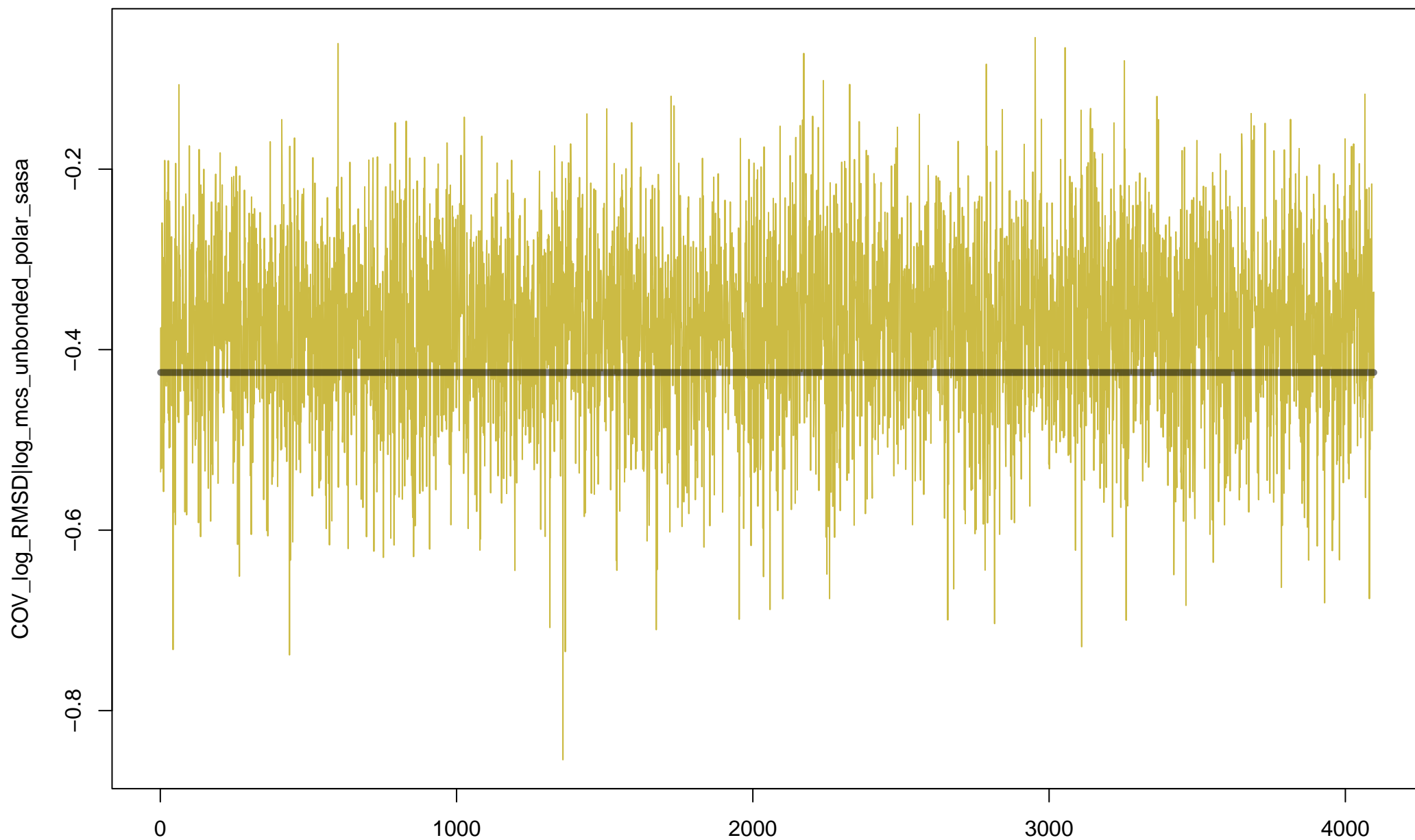
VAR_mcs_NumHeteroAtoms
ESS = 2430 | BMK = 0.036 | MCSE(6.27) = 2.03 | stat: TRUE | burn: 0 | rel.err: 0.373



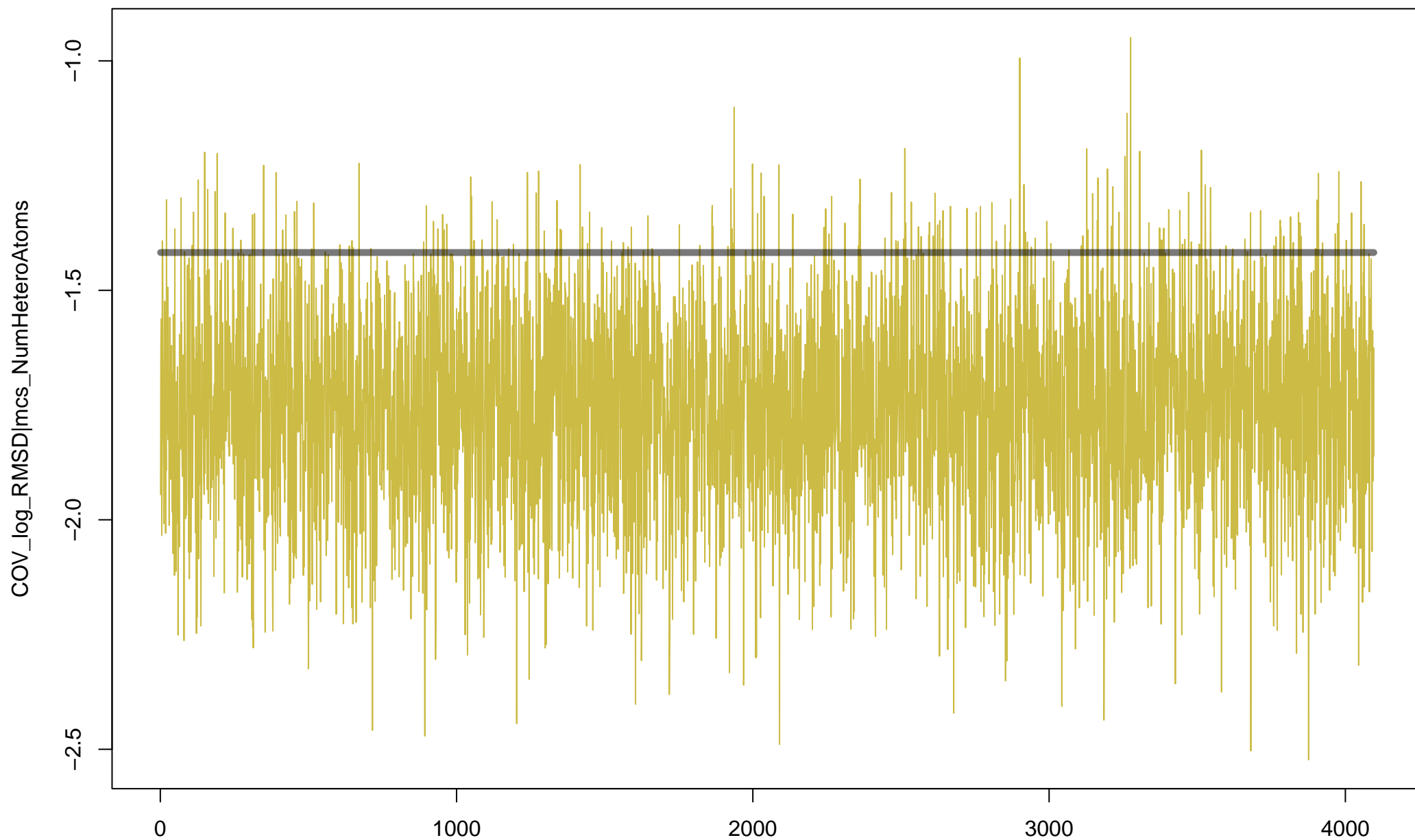
VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0535 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: 0.0303



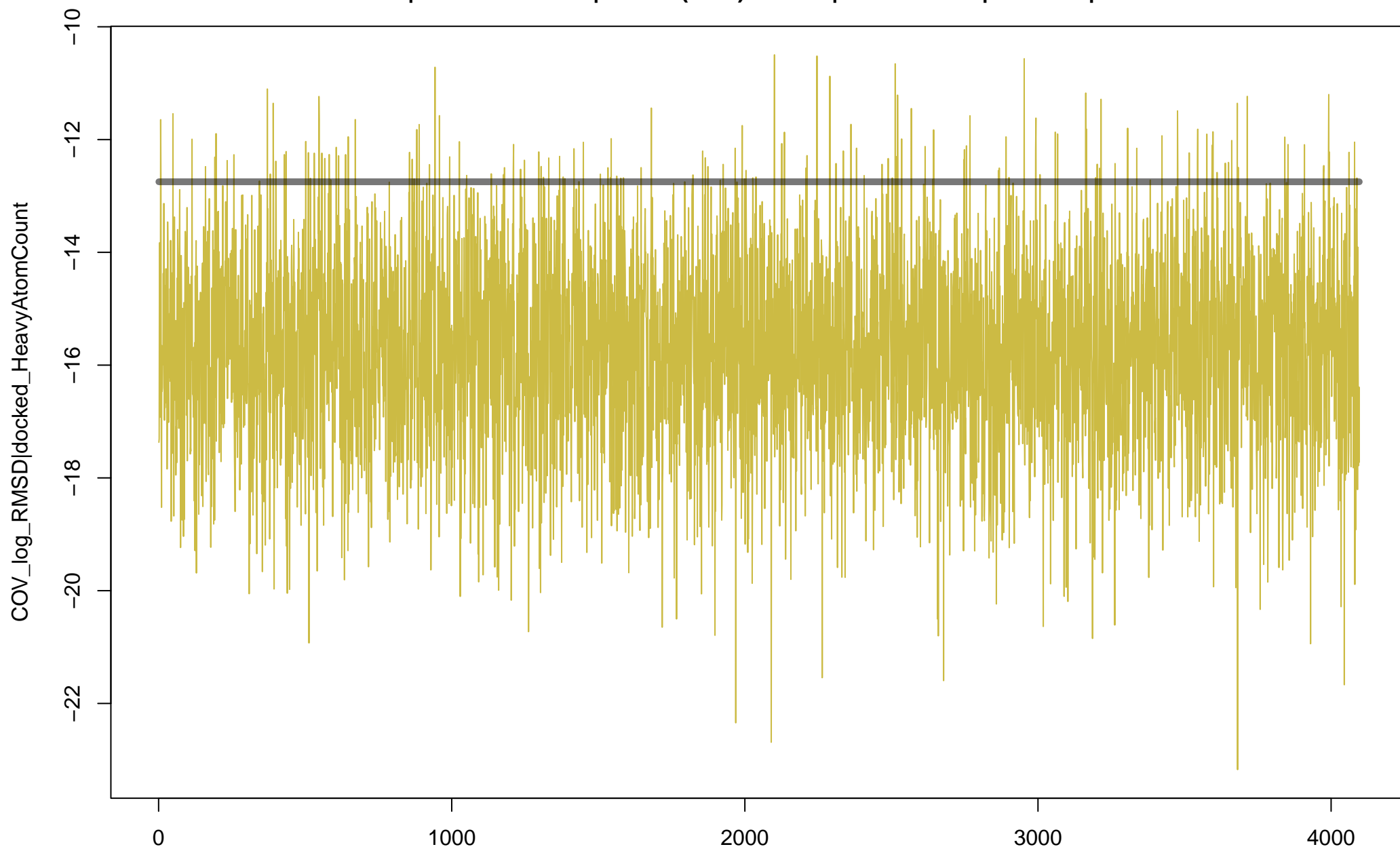
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3880 | BMK = 0.049 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0 | rel.err: 0.485



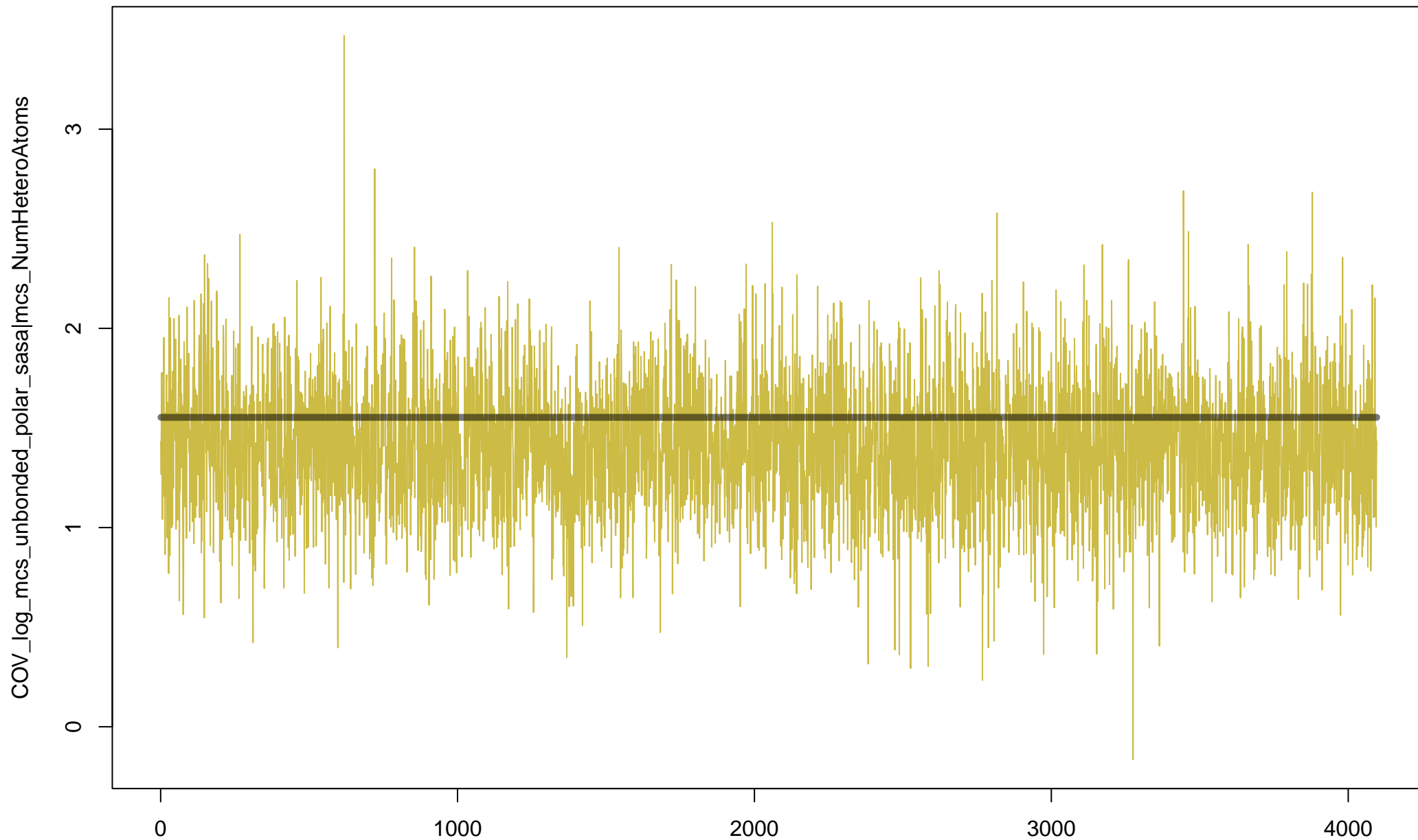
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 3890 | BMK = 0.0349 | MCSE(6.27) = 1.52 | stat: TRUE | burn: 0 | rel.err: -1.62



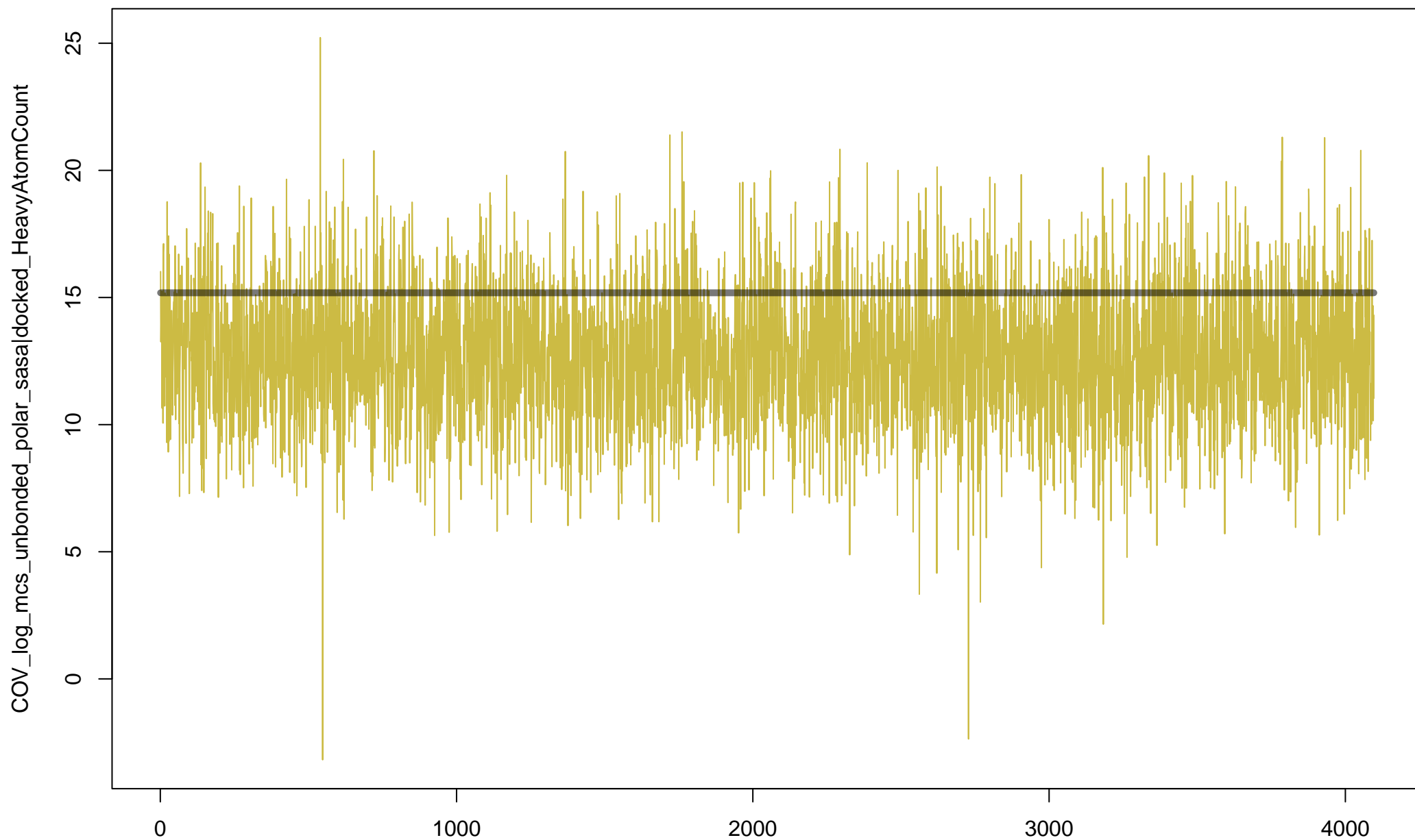
COV_log_RMSD|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0422 | MCSE(6.27) = 1.56 | stat: TRUE | burn: 0 | rel.err: -1.74



COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 3410 | BMK = 0.0496 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0 | rel.err: -0.456



COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0504 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: -0.93



COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 3880 | BMK = 0.0396 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0 | rel.err: 0.45

