

-- STATS maxD --

min ESS = 59.0356060109559

max BMK = 0.149546853680869

max MCSE = 8.60837379658245

all stationary: FALSE

burn: 0

max rel.err.: 2.27022402932644

-- STATS 2D --

min ESS = 3740.90728775771

max BMK = 0.0538874257251102

max MCSE = 1.72404458295895

all stationary: FALSE

burn: 0

max rel.err.: 1.77087323189382

-- STATS 1D --

min ESS = 3482.65451511638

max BMK = 0.0547149703547297

max MCSE = 2.02415992436305

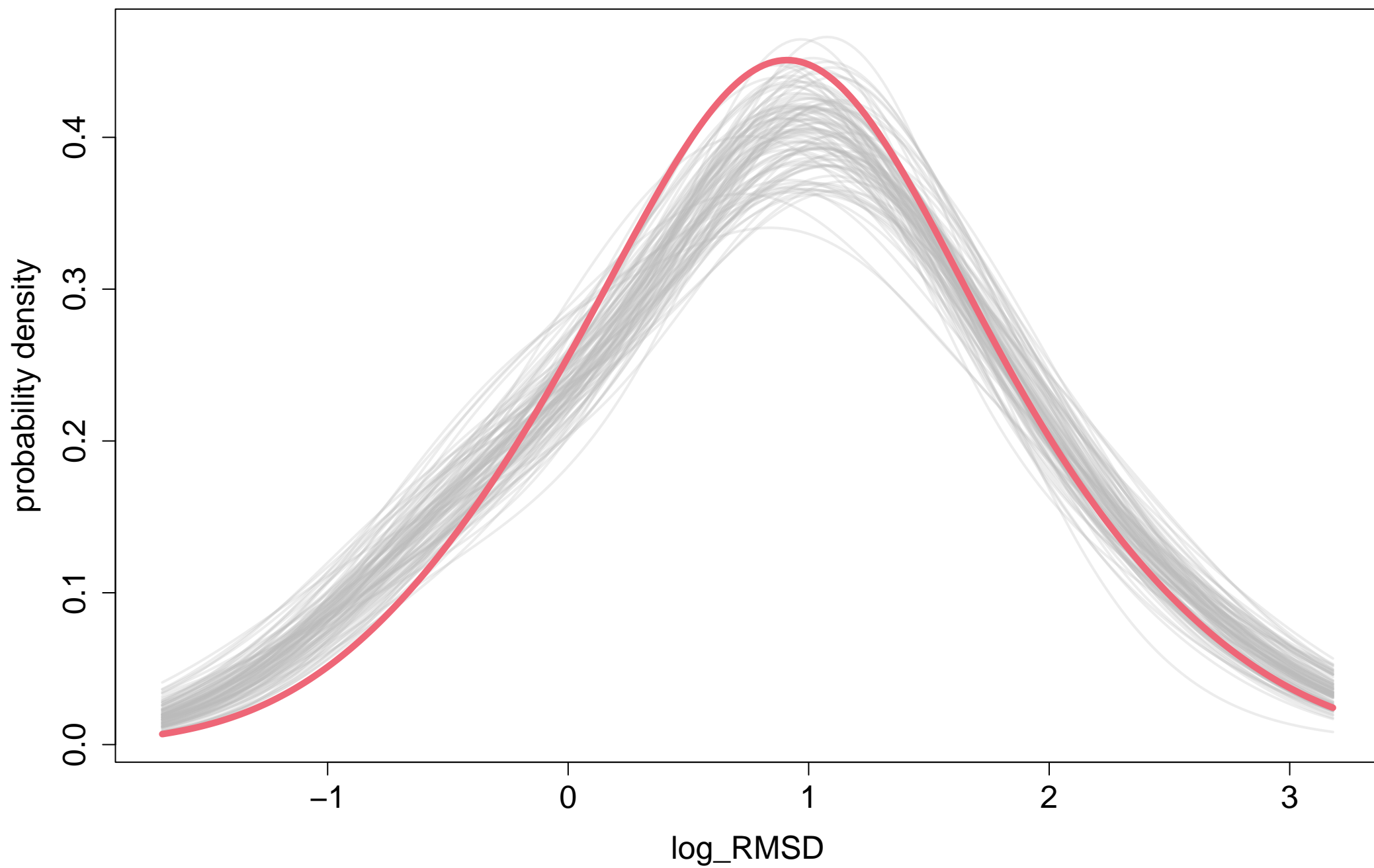
all stationary: TRUE

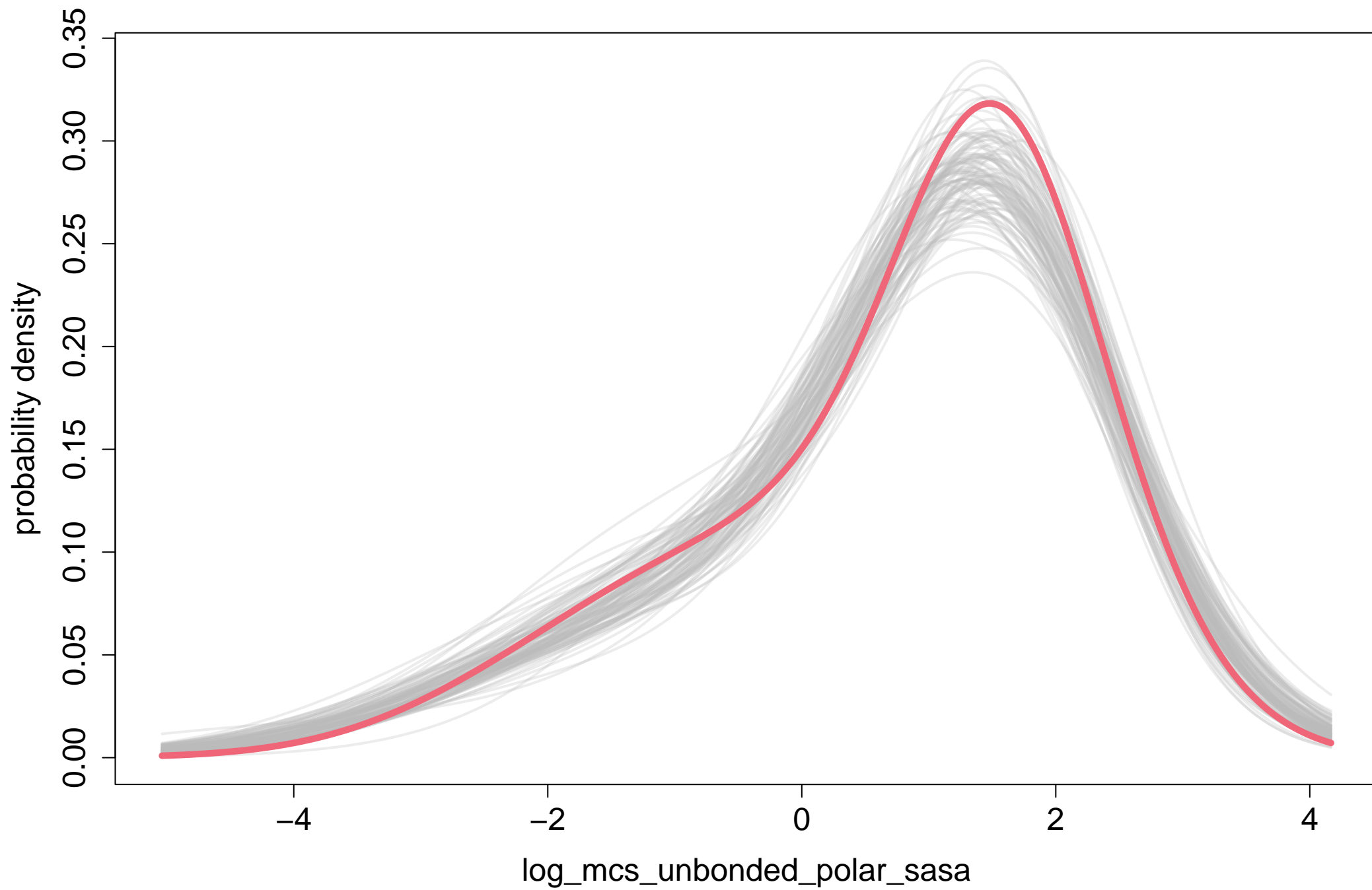
burn: 0

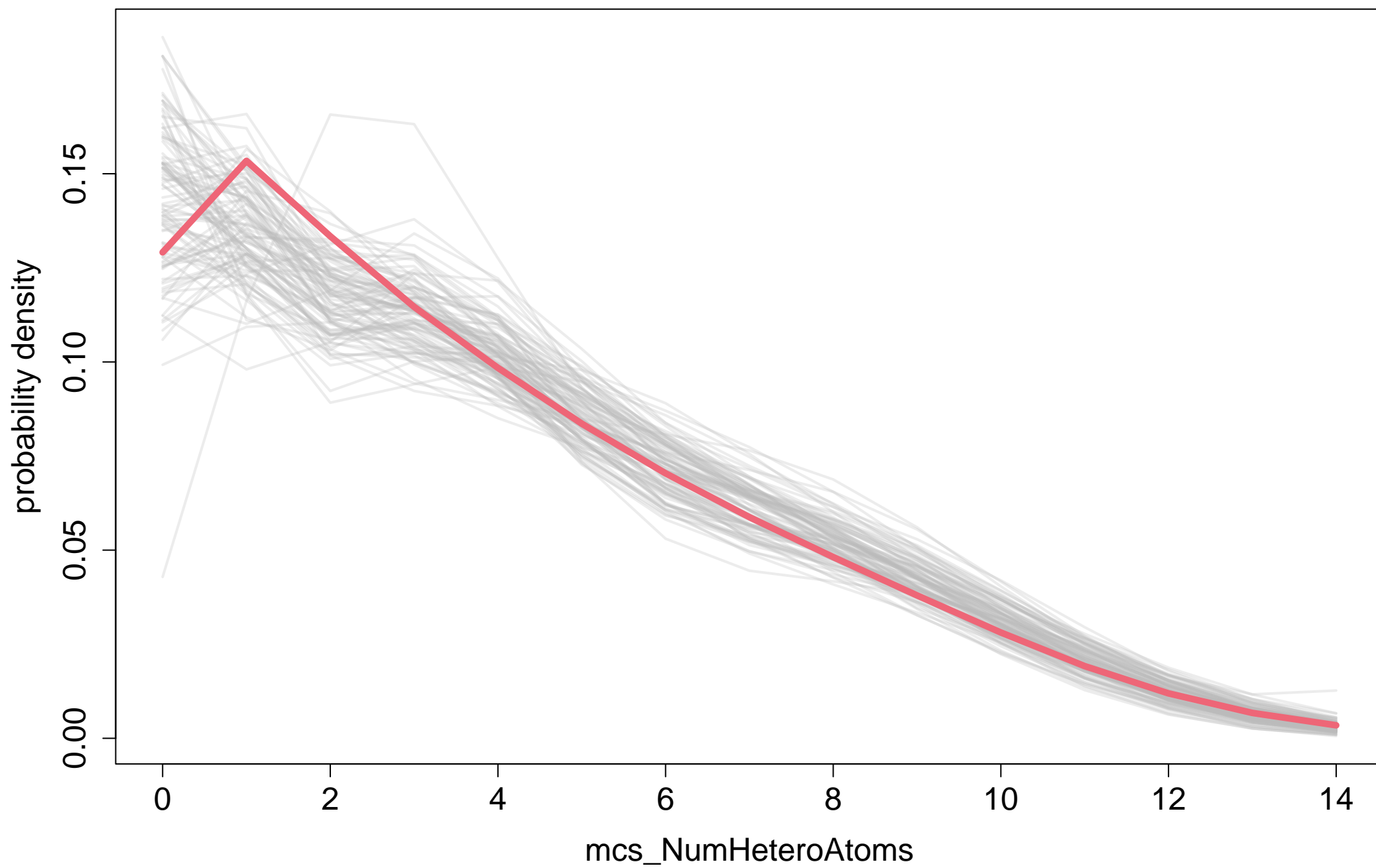
max rel.err.: 2.2264650759255

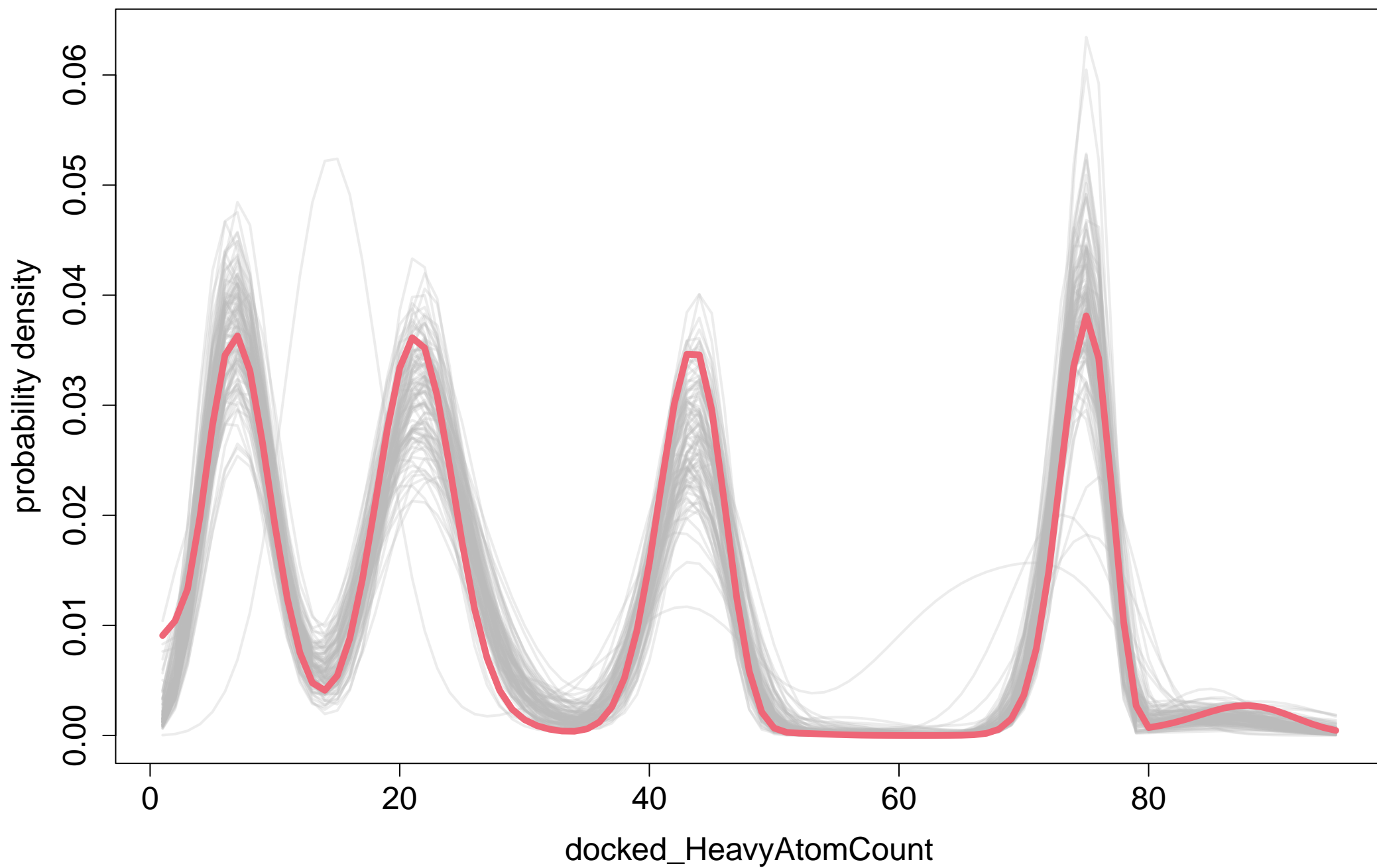
Occupied clusters: 11 of 16

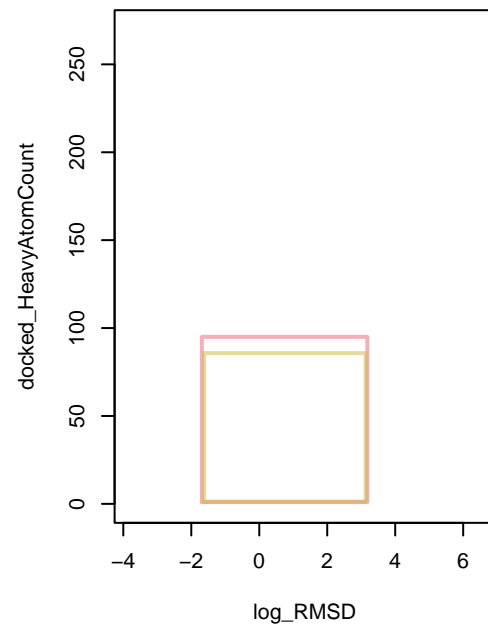
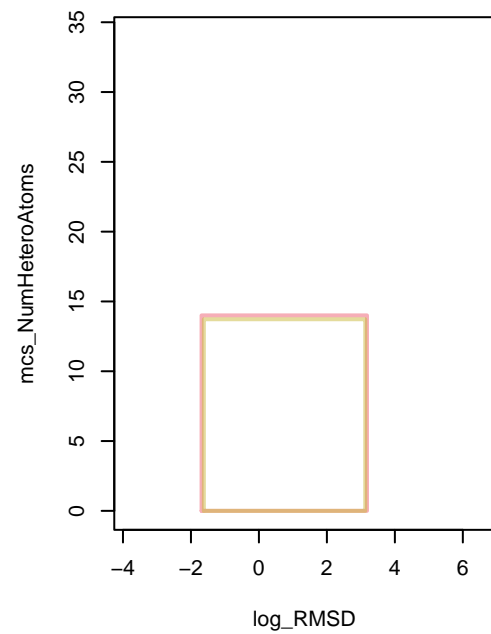
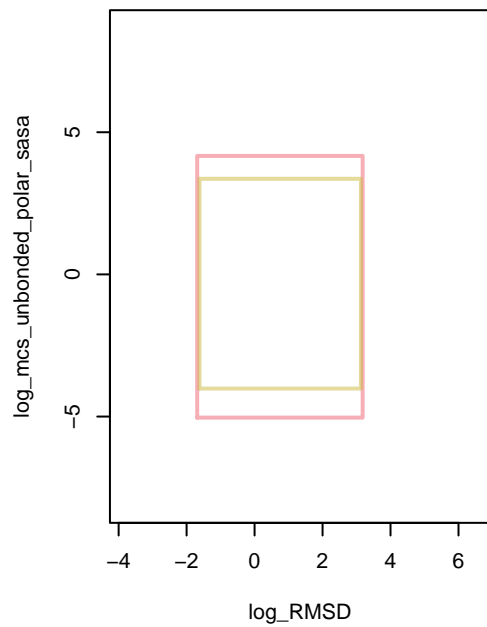
LL: -2160 +- 10.9



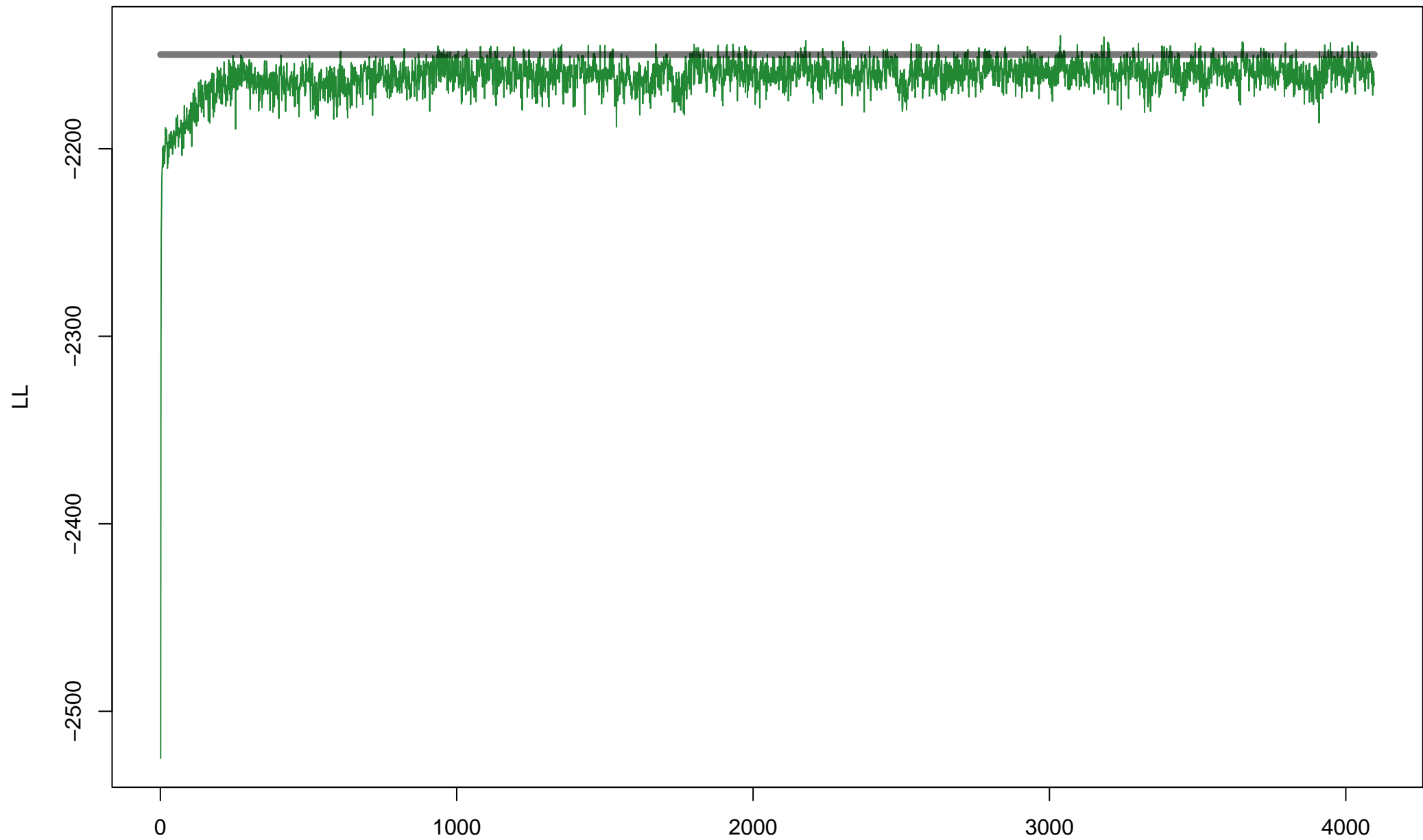






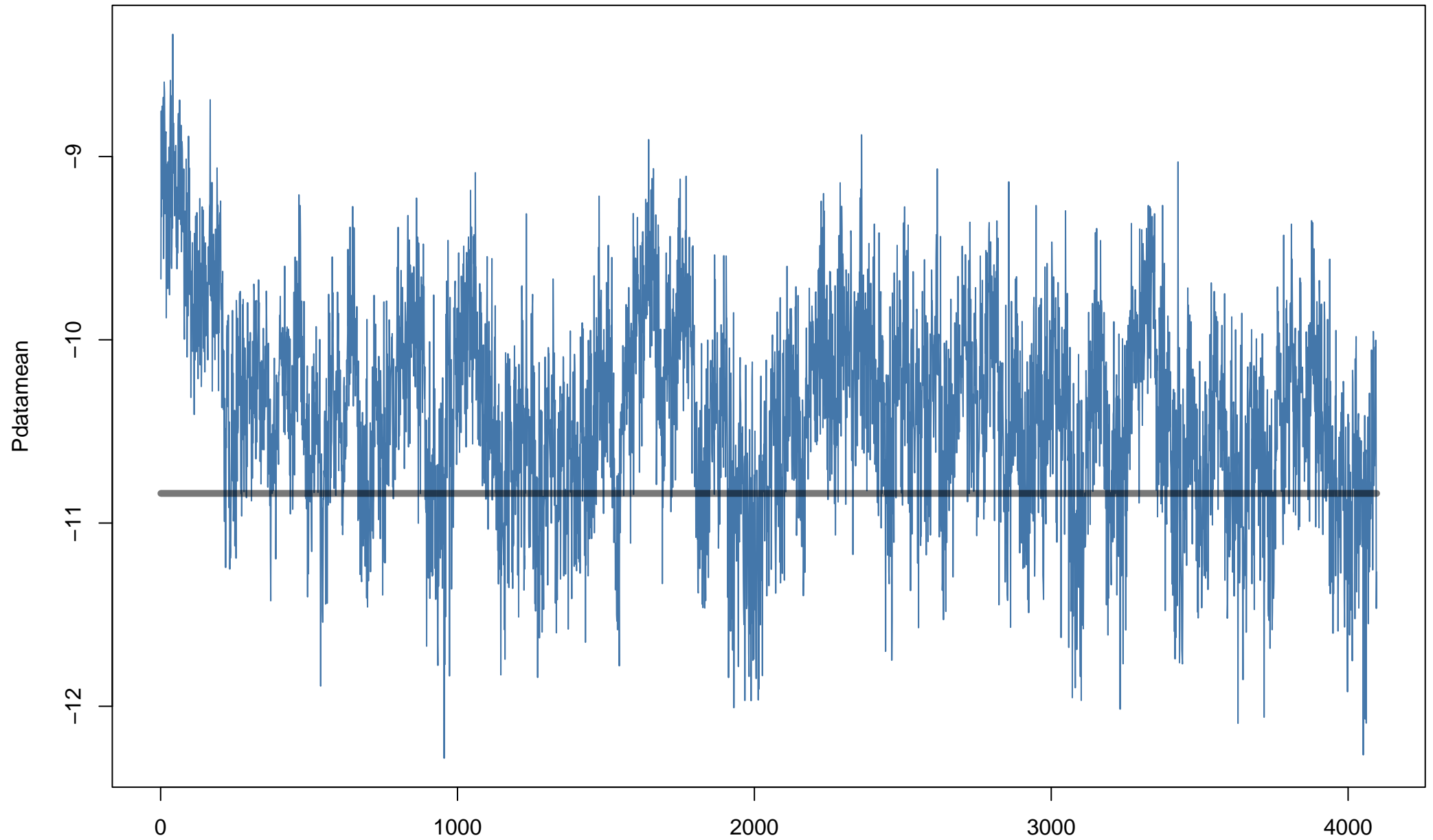


LL

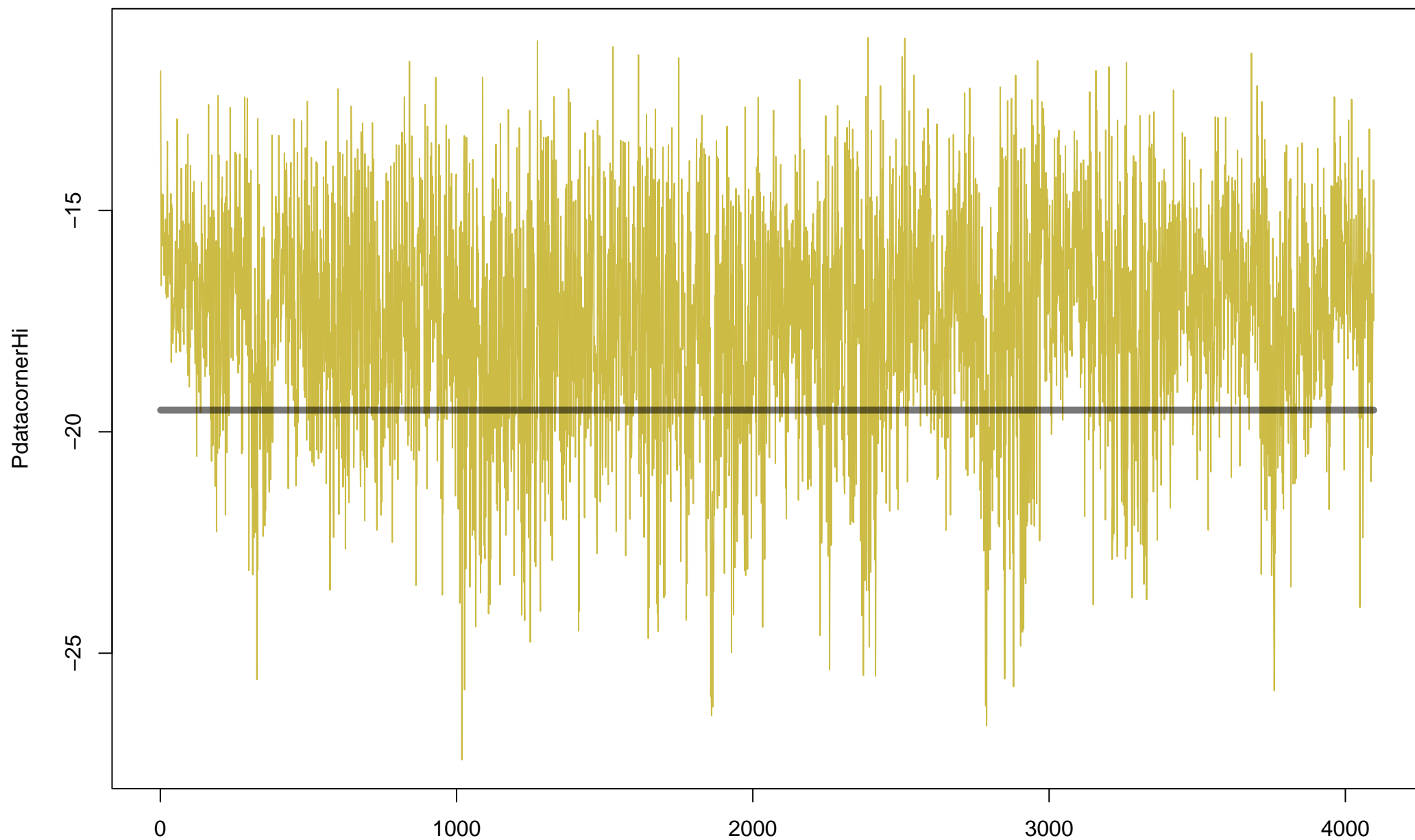


Pdatamean

ESS = 59 | BMK = 0.114 | MCSE(6.27) = 8.61 | stat: FALSE | burn: 0 | rel.err: 0.749

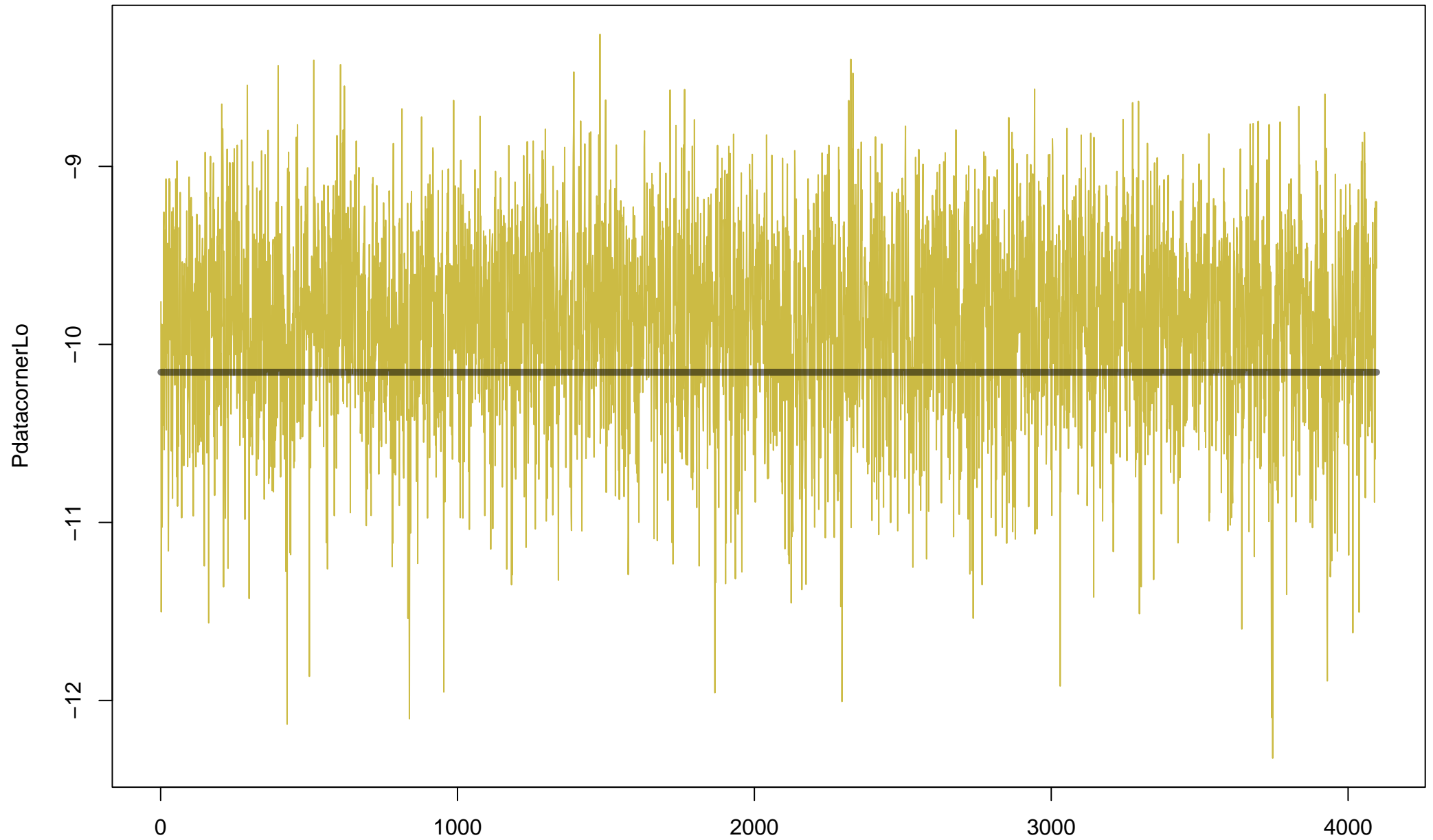


PdatacornerHi
ESS = 3400 | BMK = 0.123 | MCSE(6.27) = 1.8 | stat: TRUE | burn: 0 | rel.err: 0.286

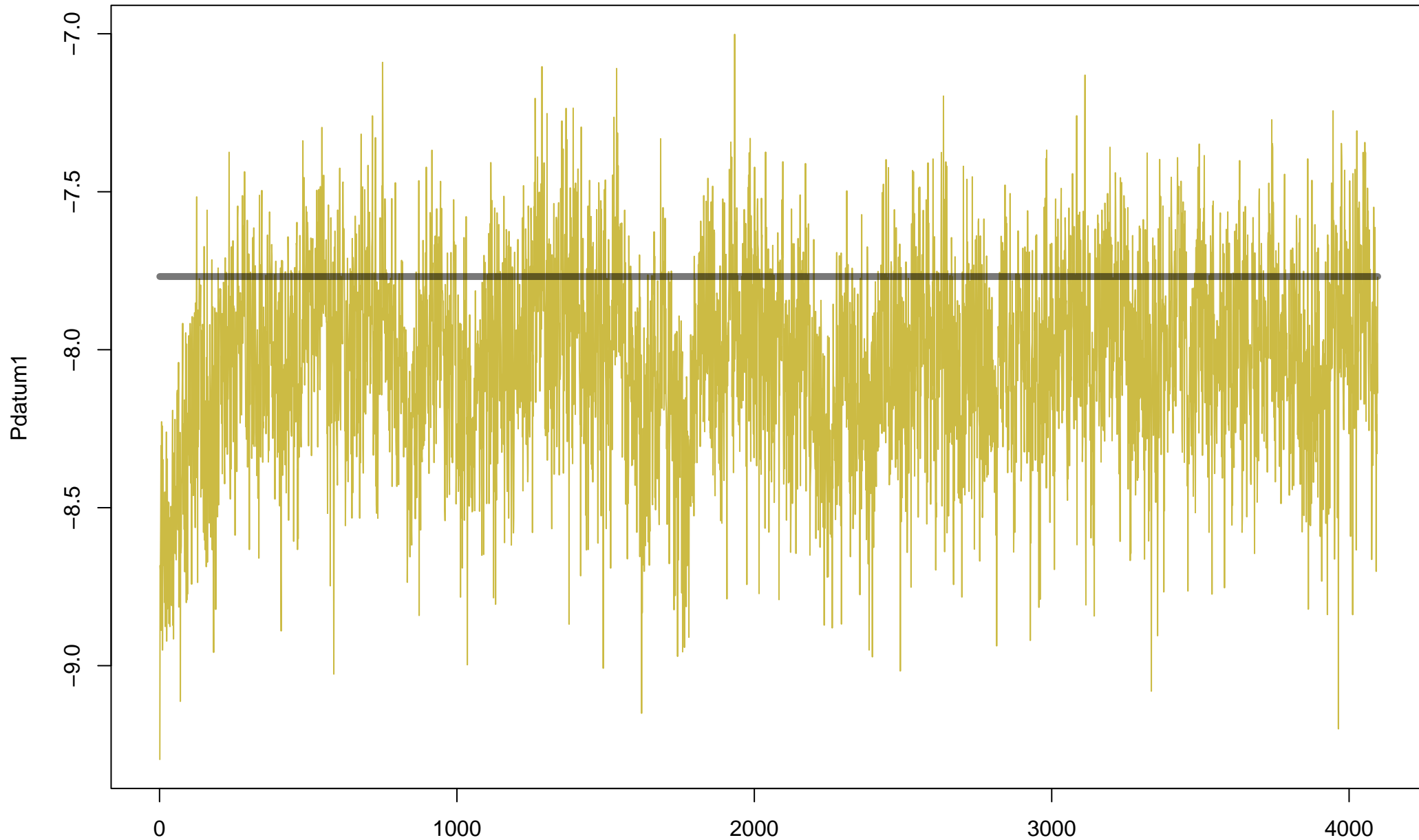


PdatacornerLo

ESS = 3490 | BMK = 0.0373 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0 | rel.err: 0.649

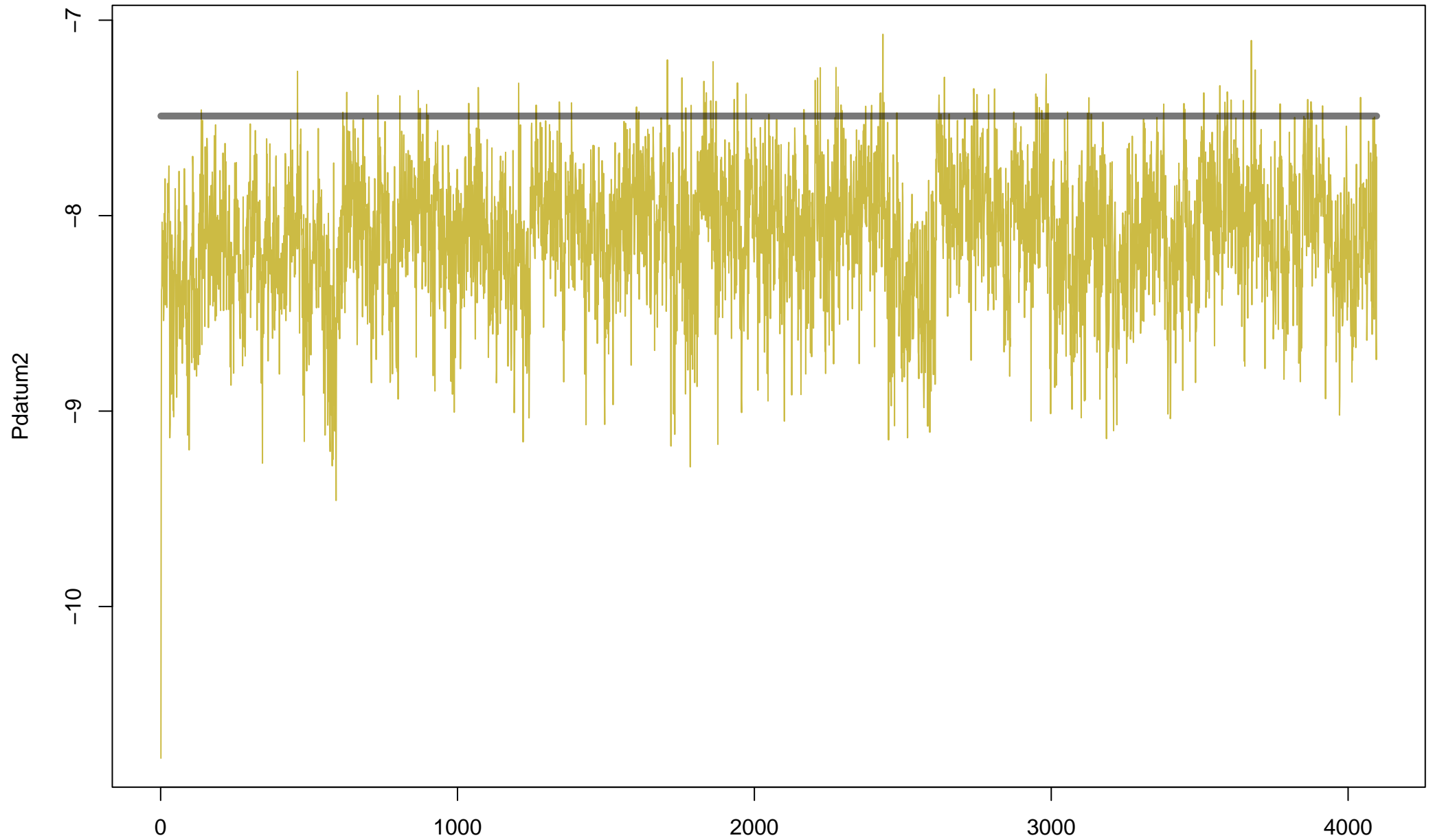


Pdatum1
ESS = 305 | BMK = 0.0599 | MCSE(6.27) = 4.9 | stat: FALSE | burn: 0 | rel.err: -0.808



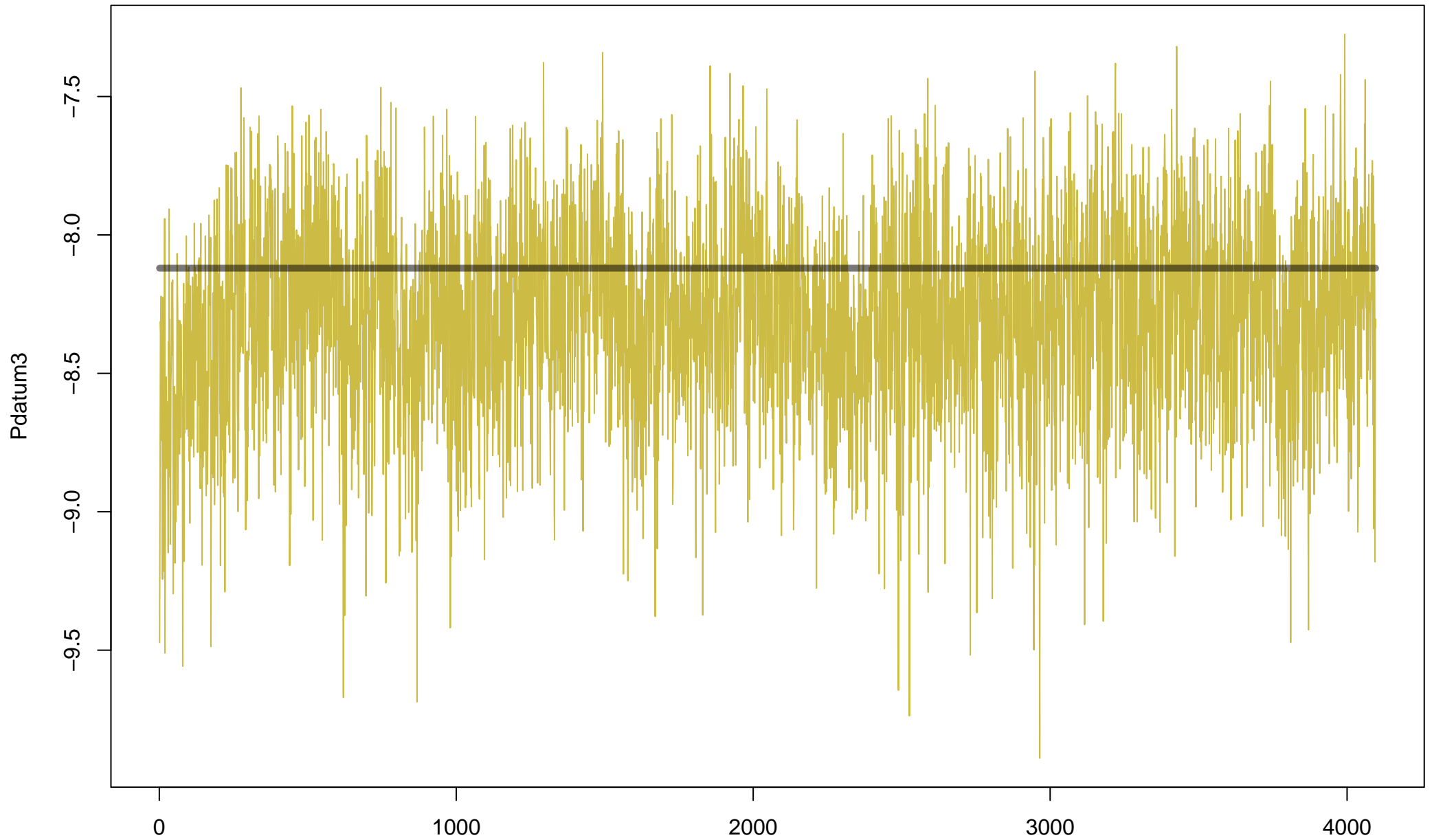
Pdatum2

ESS = 417 | BMK = 0.0618 | MCSE(6.27) = 4.58 | stat: FALSE | burn: 0 | rel.err: -2.27

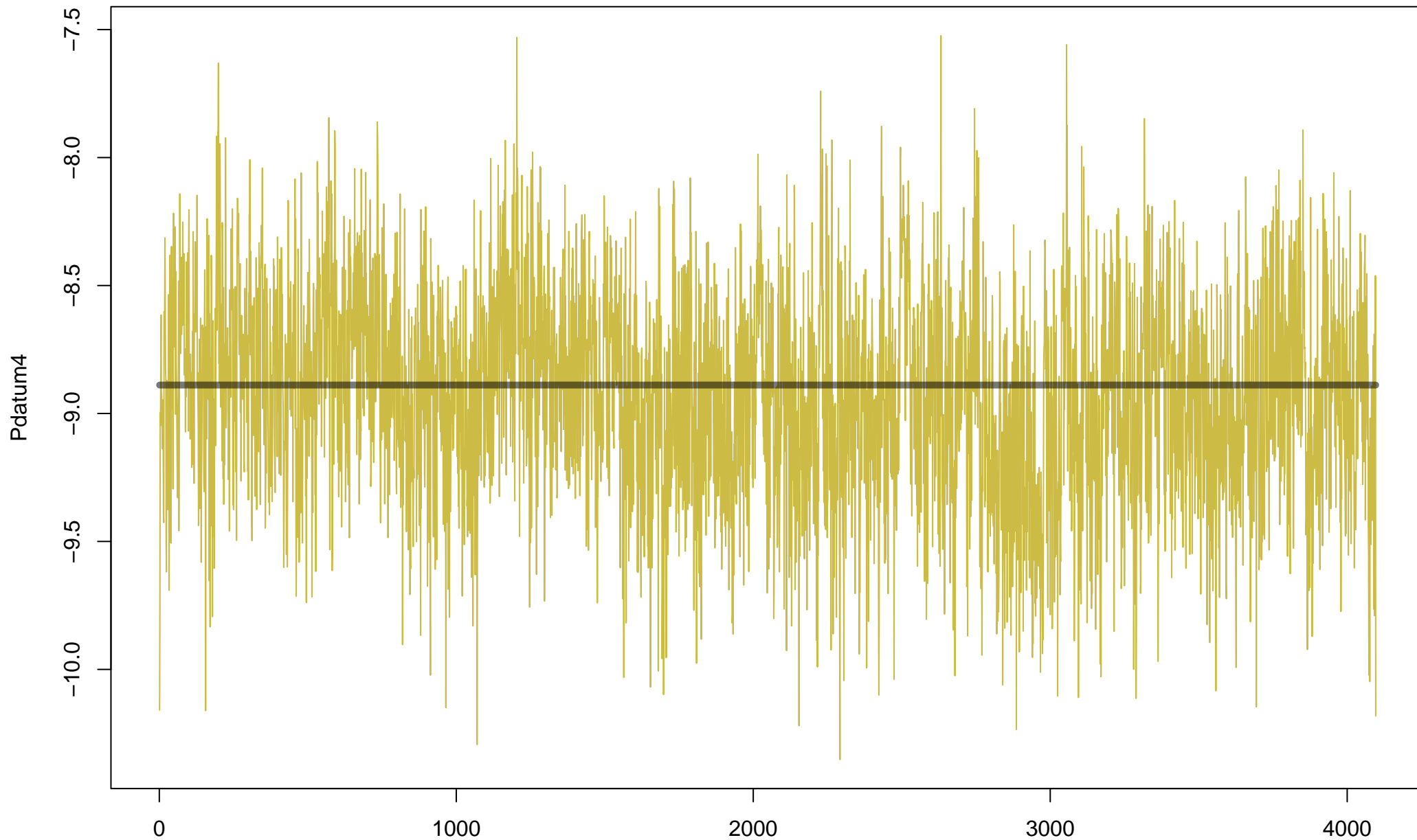


Pdatum3

ESS = 543 | BMK = 0.0218 | MCSE(6.27) = 3.35 | stat: FALSE | burn: 0 | rel.err: -0.378

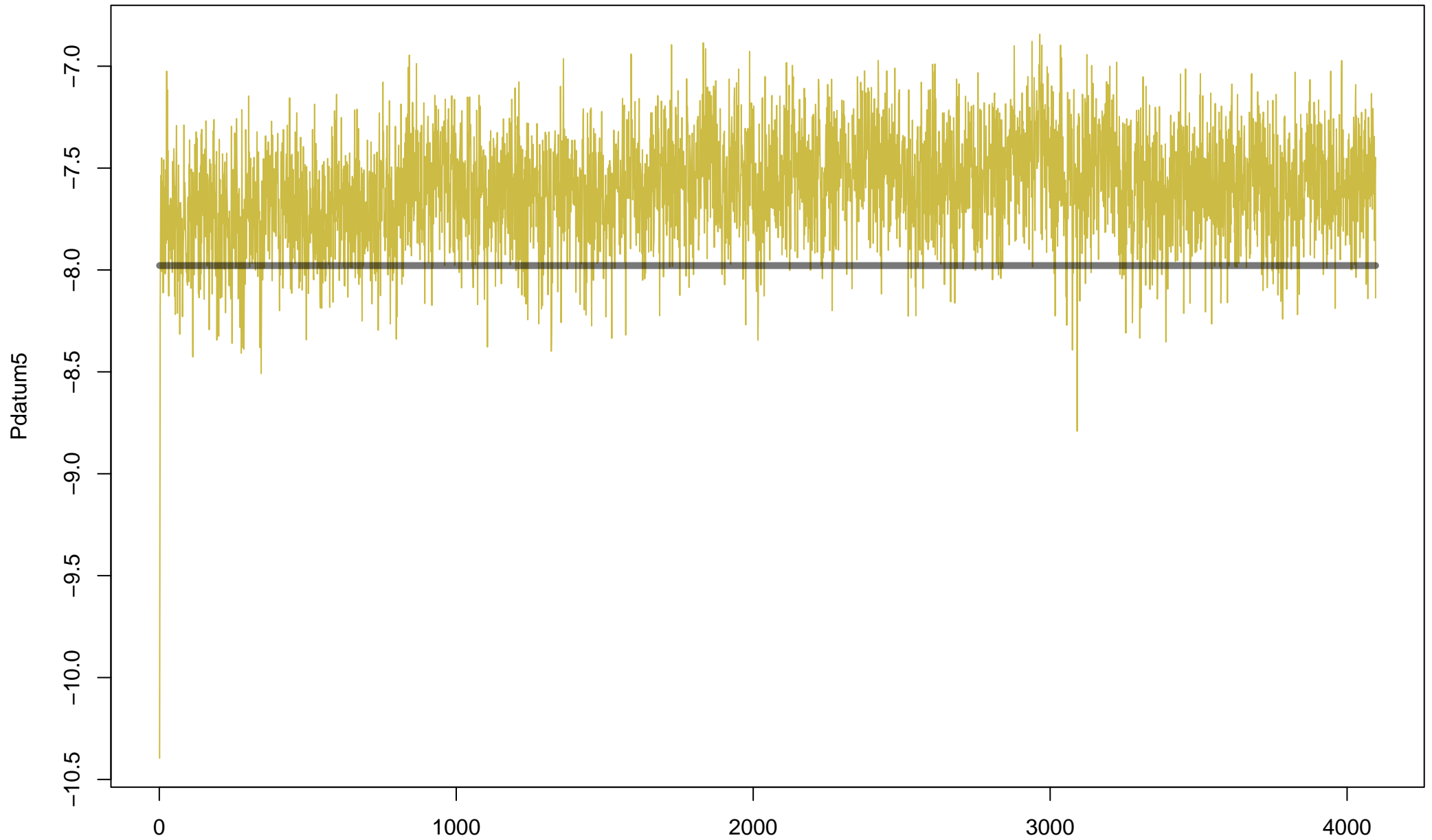


Pdatum4
ESS = 625 | BMK = 0.115 | MCSE(6.27) = 4.3 | stat: FALSE | burn: 0 | rel.err: 0.102



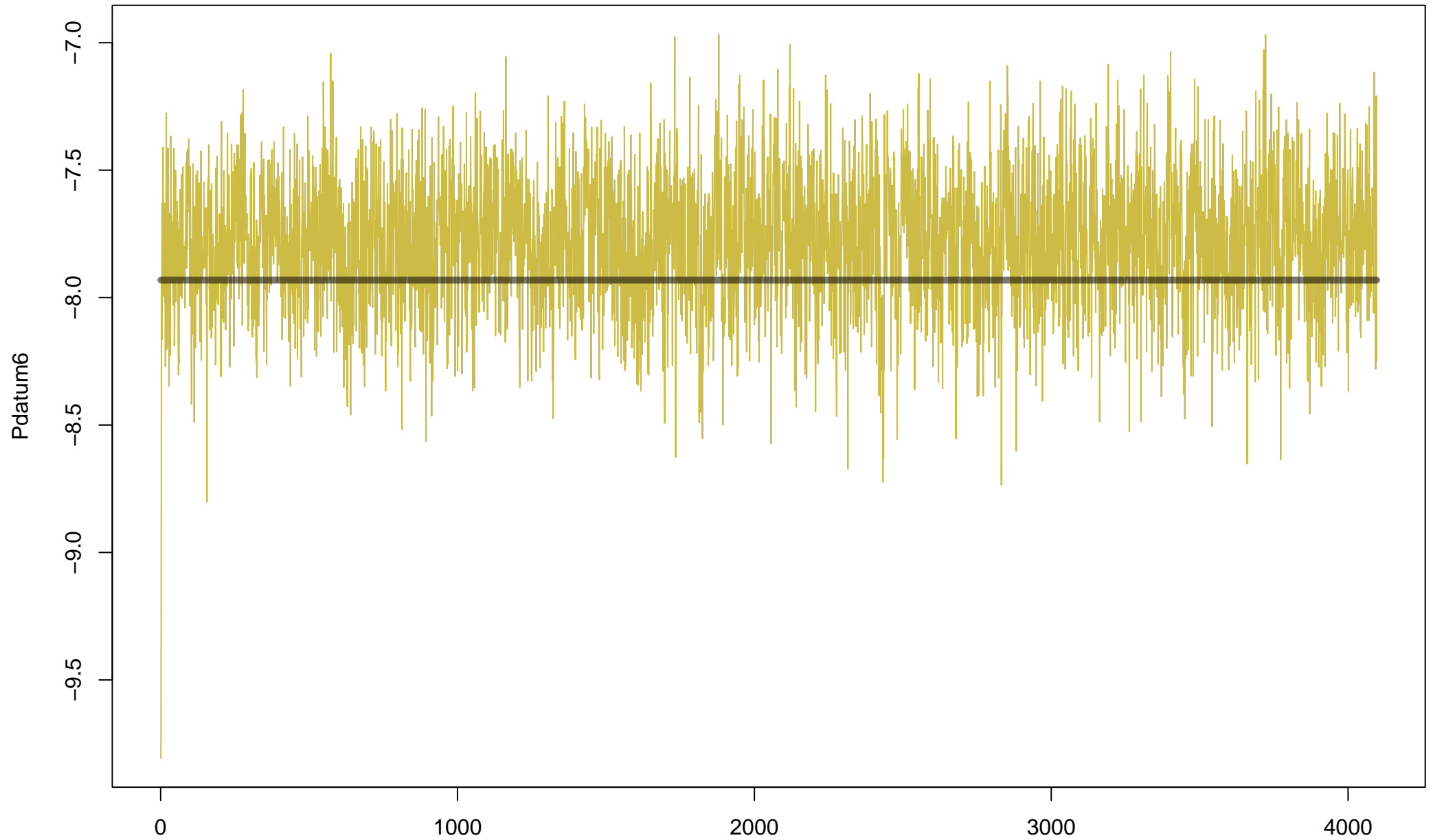
Pdatum5

ESS = 226 | BMK = 0.15 | MCSE(6.27) = 4.47 | stat: FALSE | burn: 0 | rel.err: 1.33



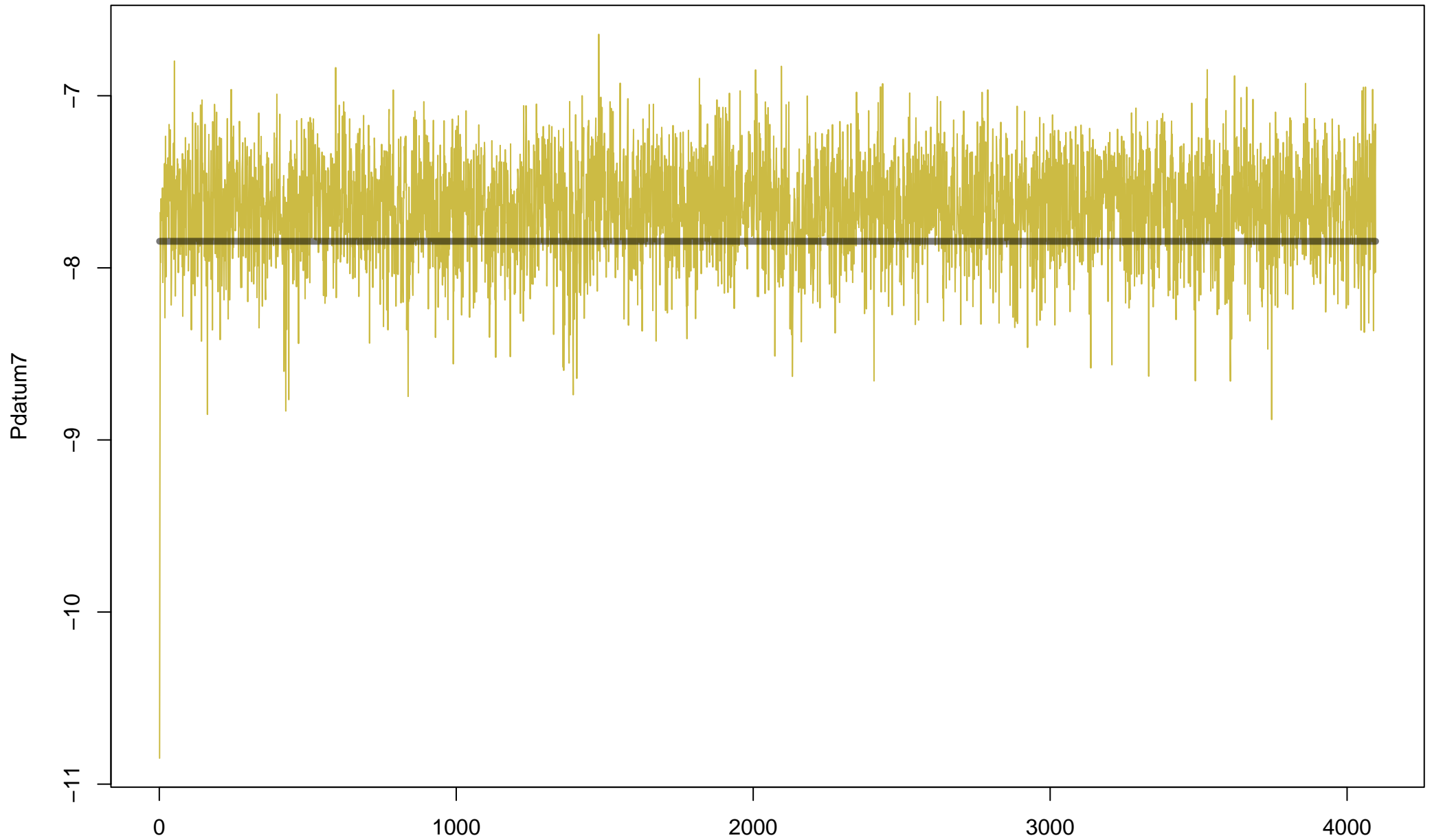
Pdatum6

ESS = 1600 | BMK = 0.0529 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0 | rel.err: 0.648

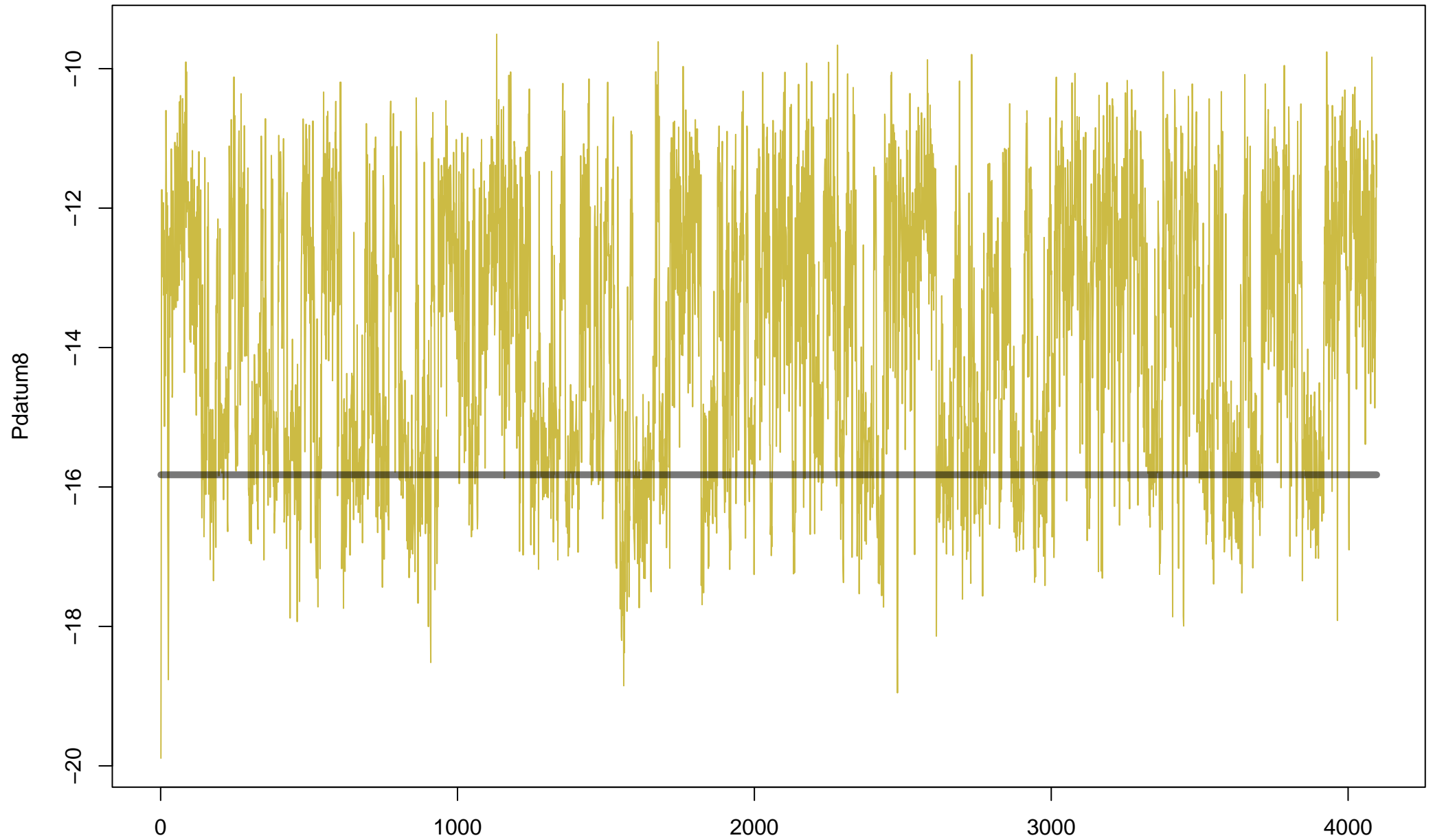


Pdatum7

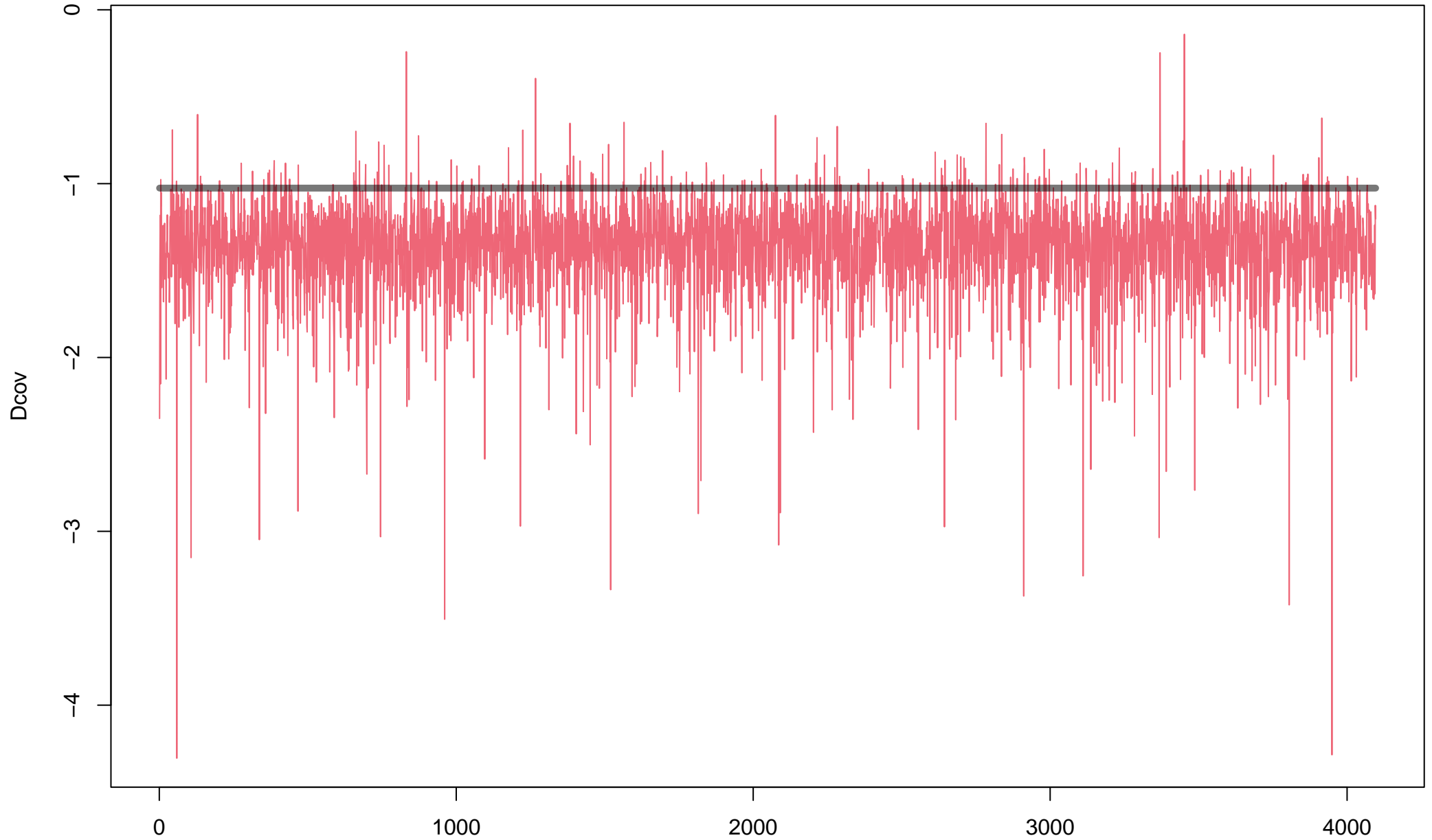
ESS = 2520 | BMK = 0.044 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0 | rel.err: 0.73



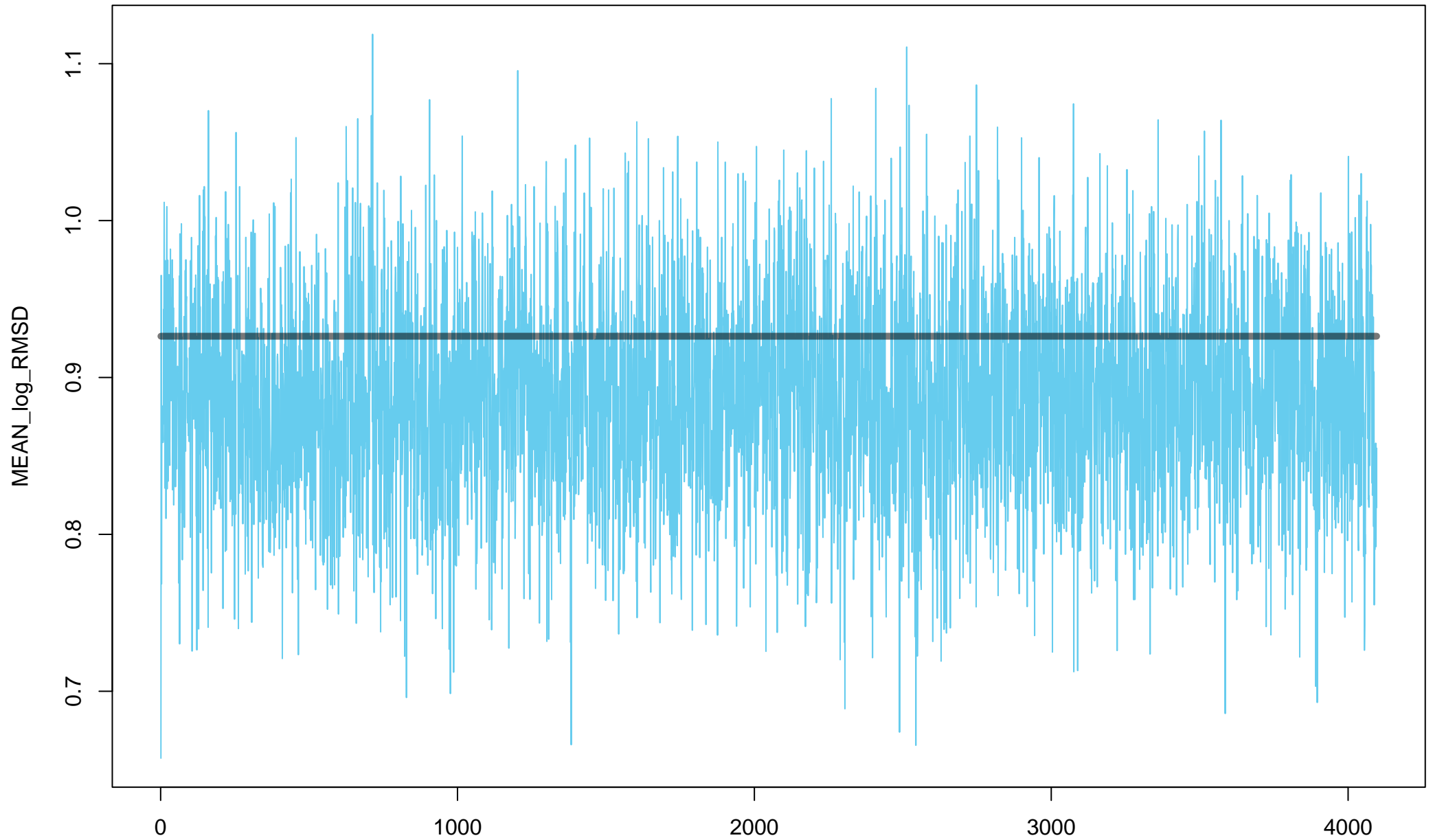
Pdatum8
ESS = 526 | BMK = 0.0943 | MCSE(6.27) = 3.81 | stat: TRUE | burn: 0 | rel.err: 0.559



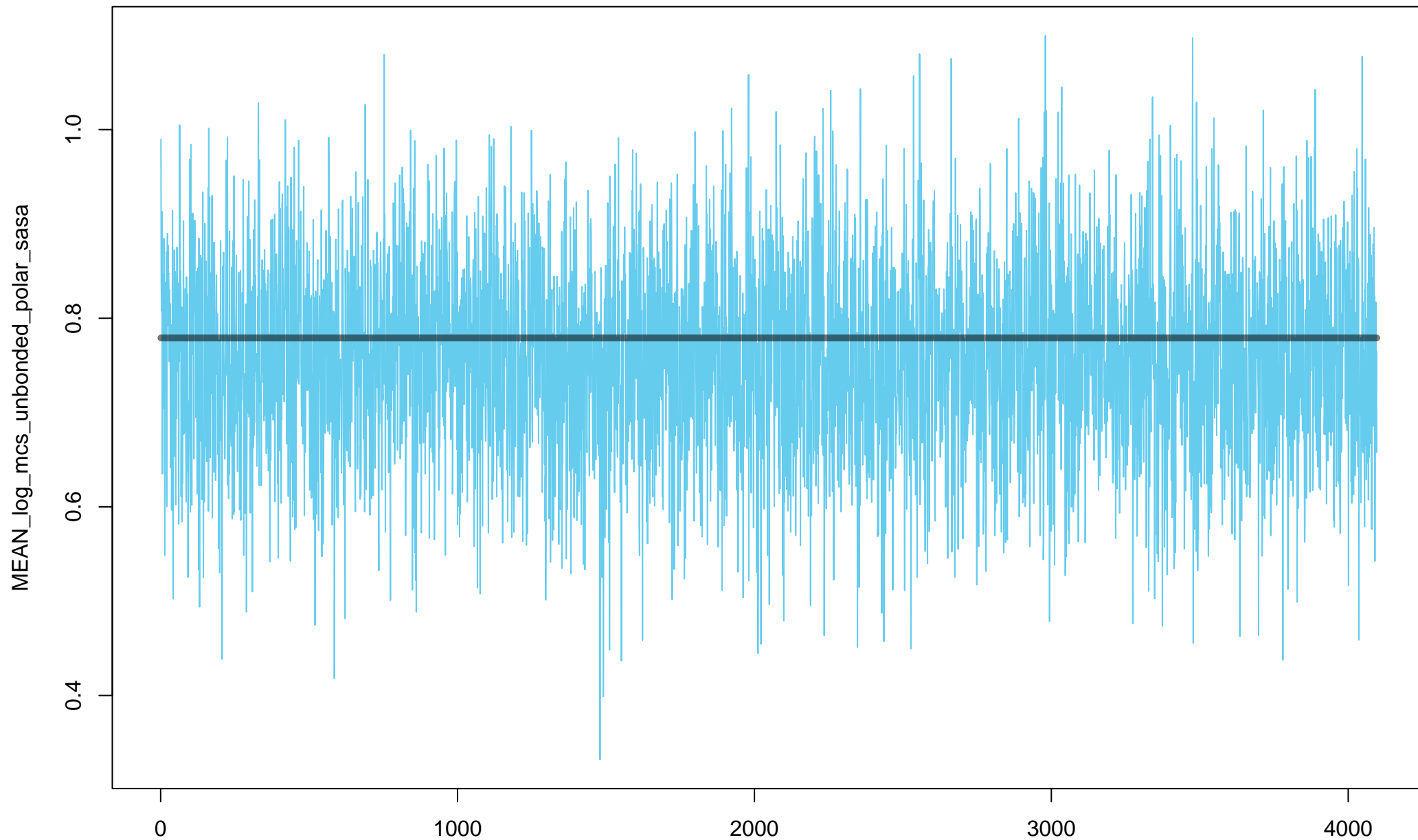
Dcov
ESS = 3810 | BMK = 0.0449 | MCSE(6.27) = 1.53 | stat: TRUE | burn: 0 | rel.err: 1.43



MEAN_log_RMSD
ESS = 3800 | BMK = 0.0292 | MCSE(6.27) = 1.56 | stat: TRUE | burn: 0 | rel.err: -0.602

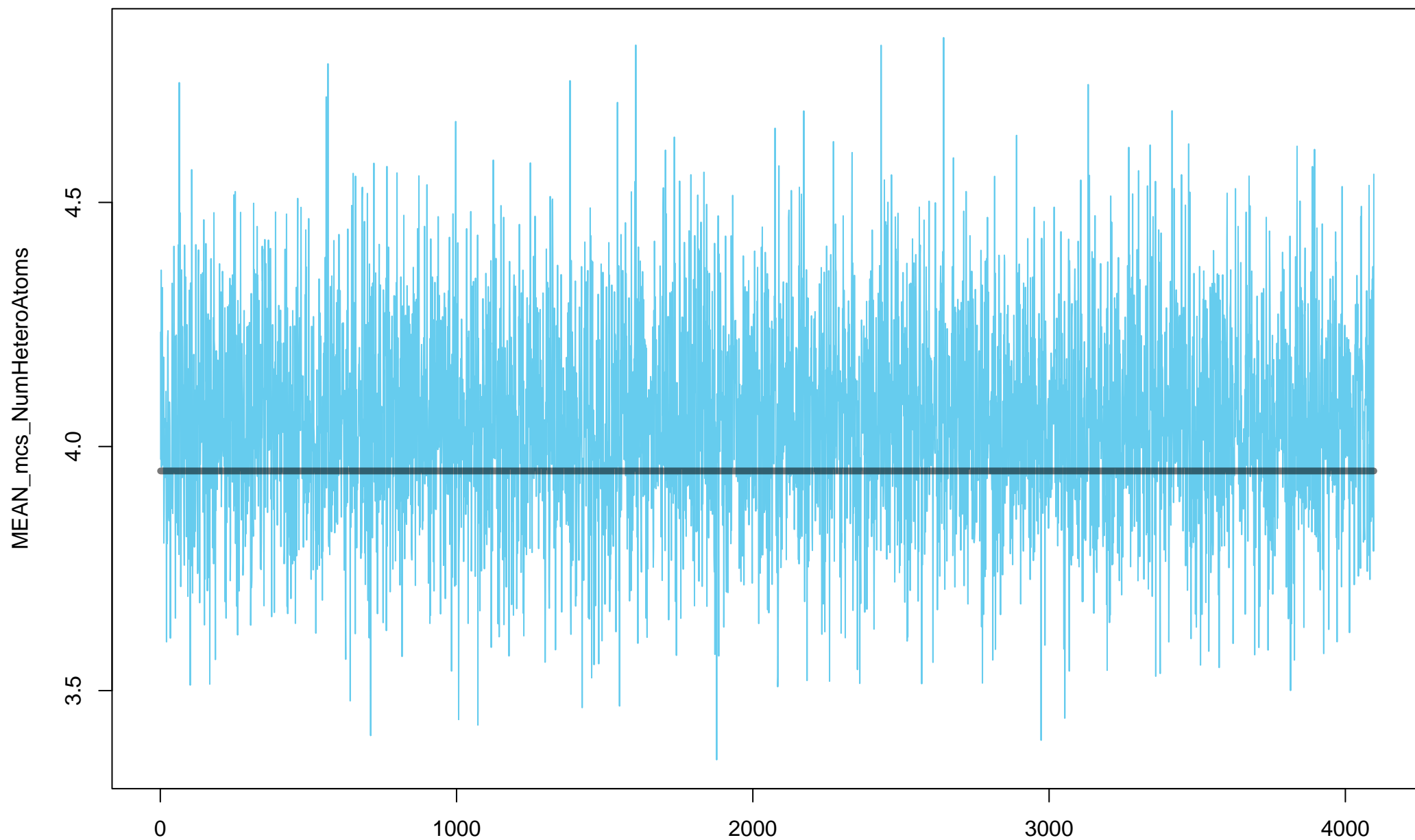


MEAN_log_mcs_unbonded_polar_sasa
ESS = 3910 | BMK = 0.0389 | MCSE(6.27) = 1.44 | stat: TRUE | burn: 0 | rel.err: -0.221

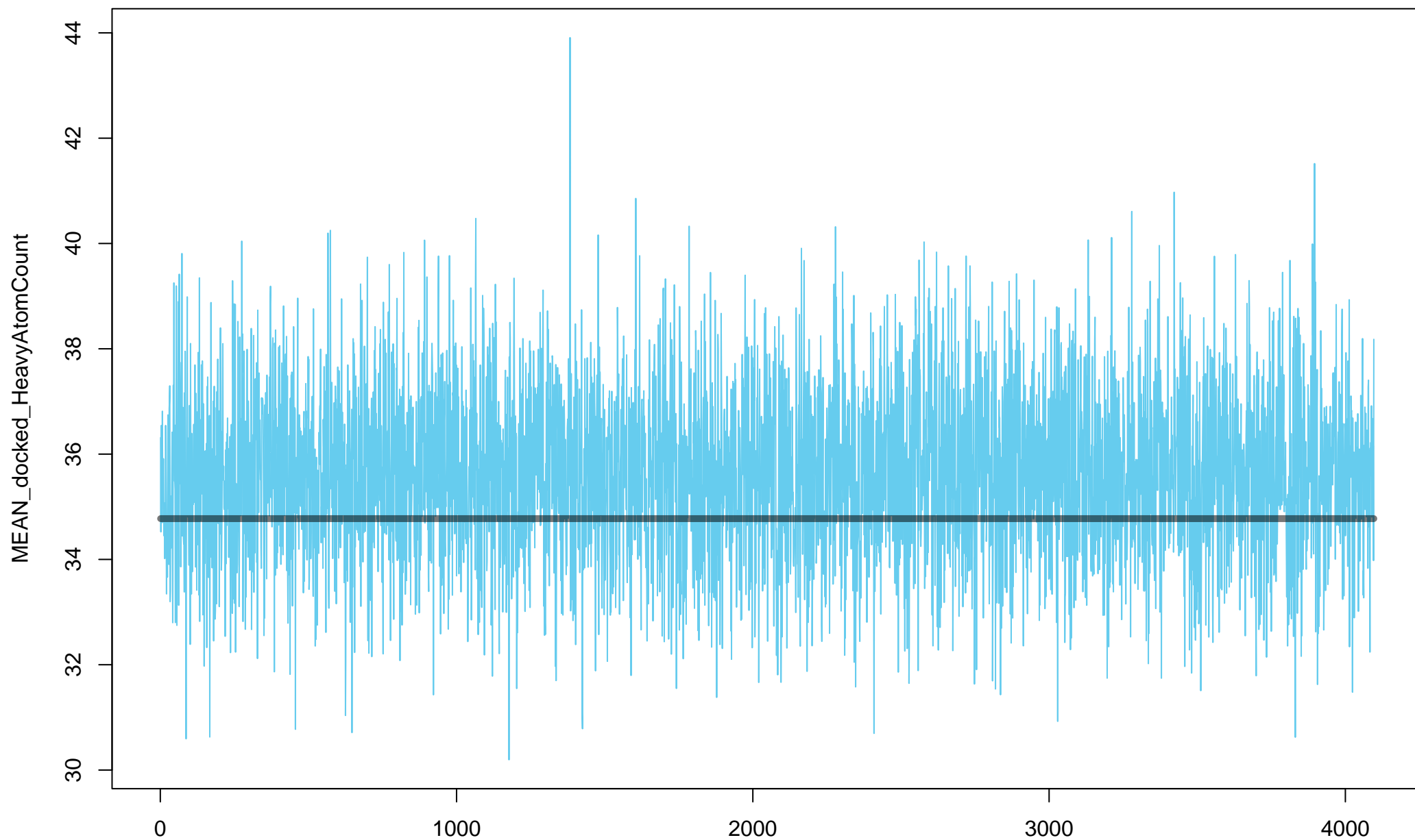


MEAN_mcs_NumHeteroAtoms

ESS = 4100 | BMK = 0.0363 | MCSE(6.27) = 1.47 | stat: TRUE | burn: 0 | rel.err: 0.502

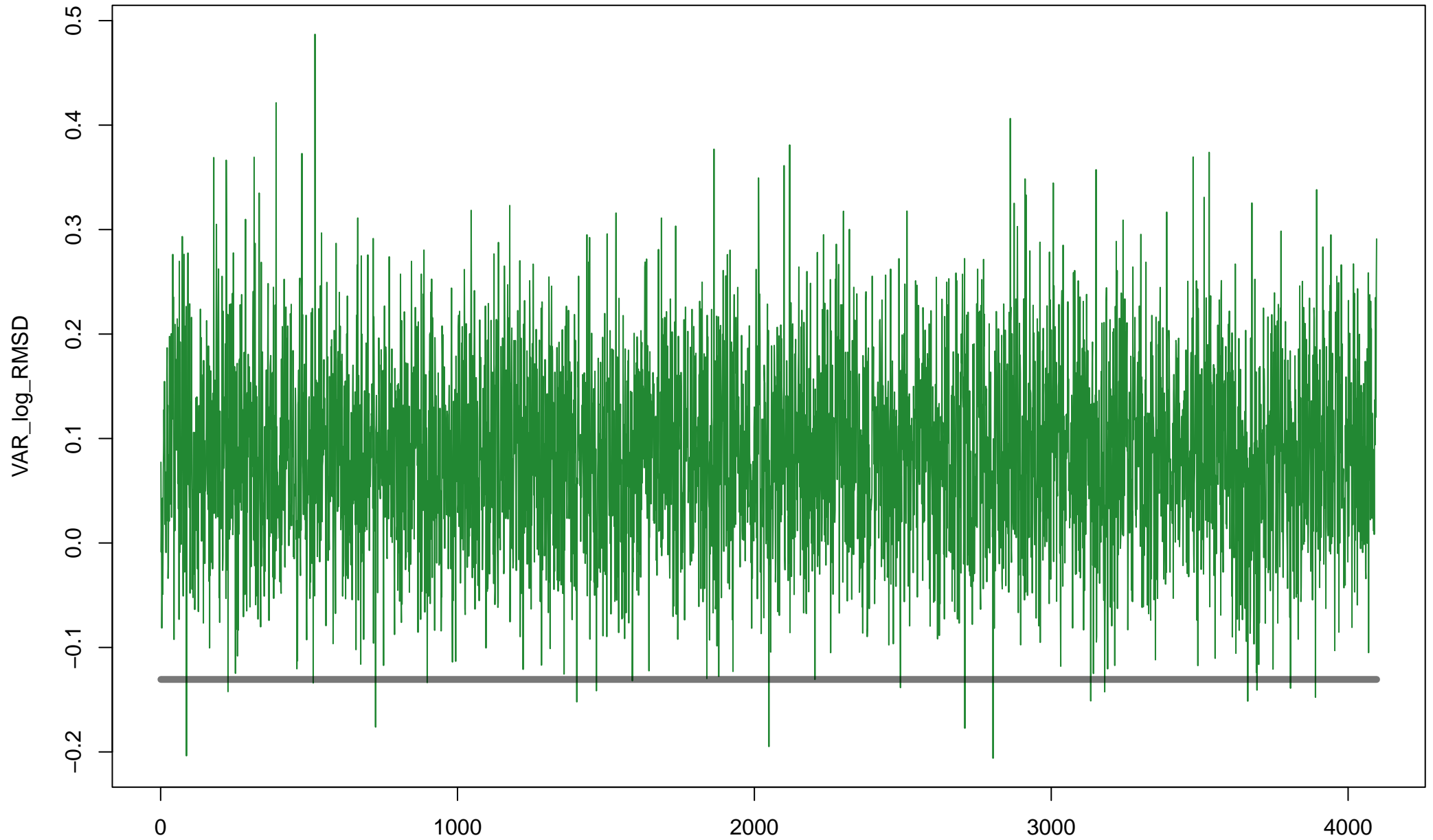


MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0309 | MCSE(6.27) = 1.43 | stat: TRUE | burn: 0 | rel.err: 0.53

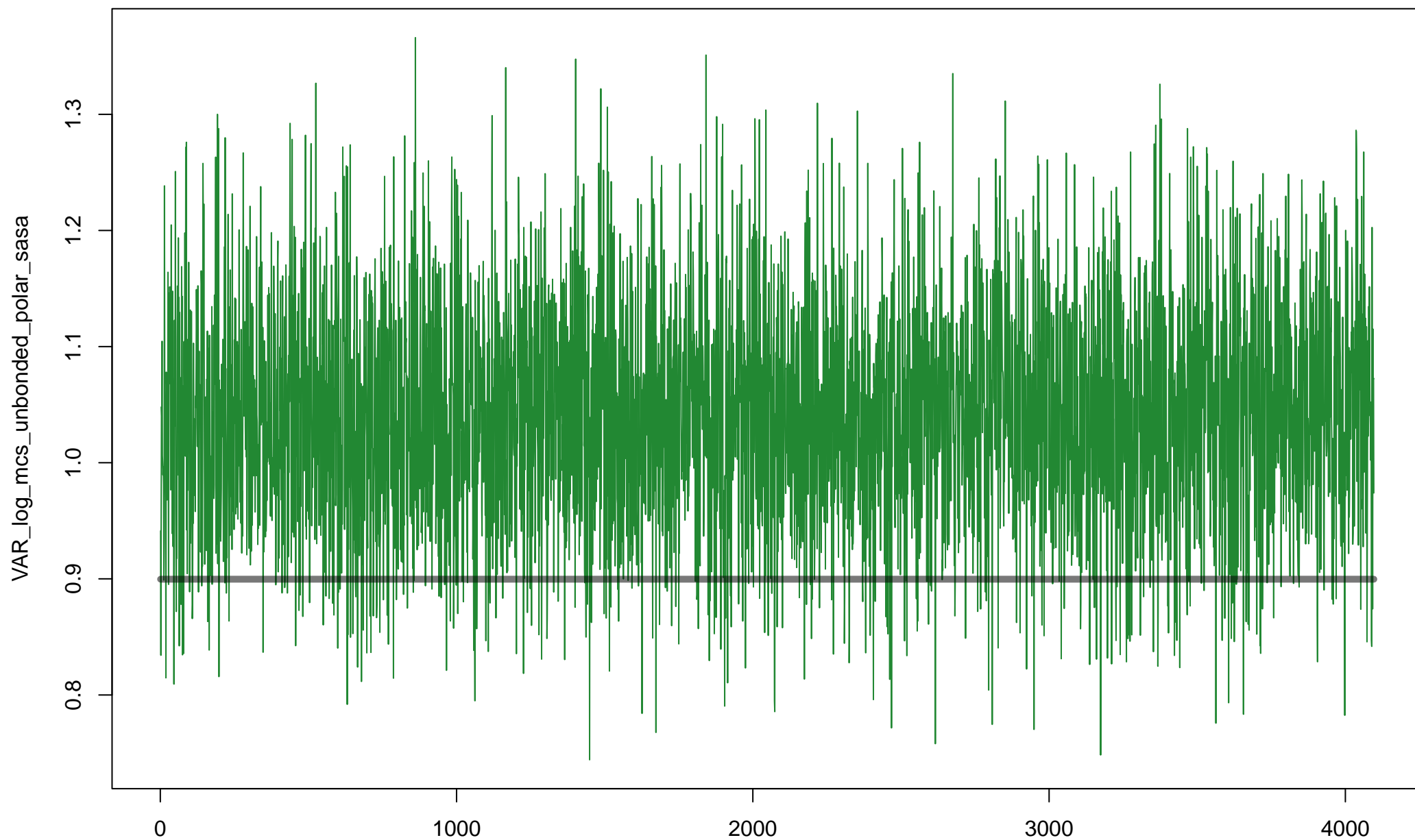


VAR_log_RMSD

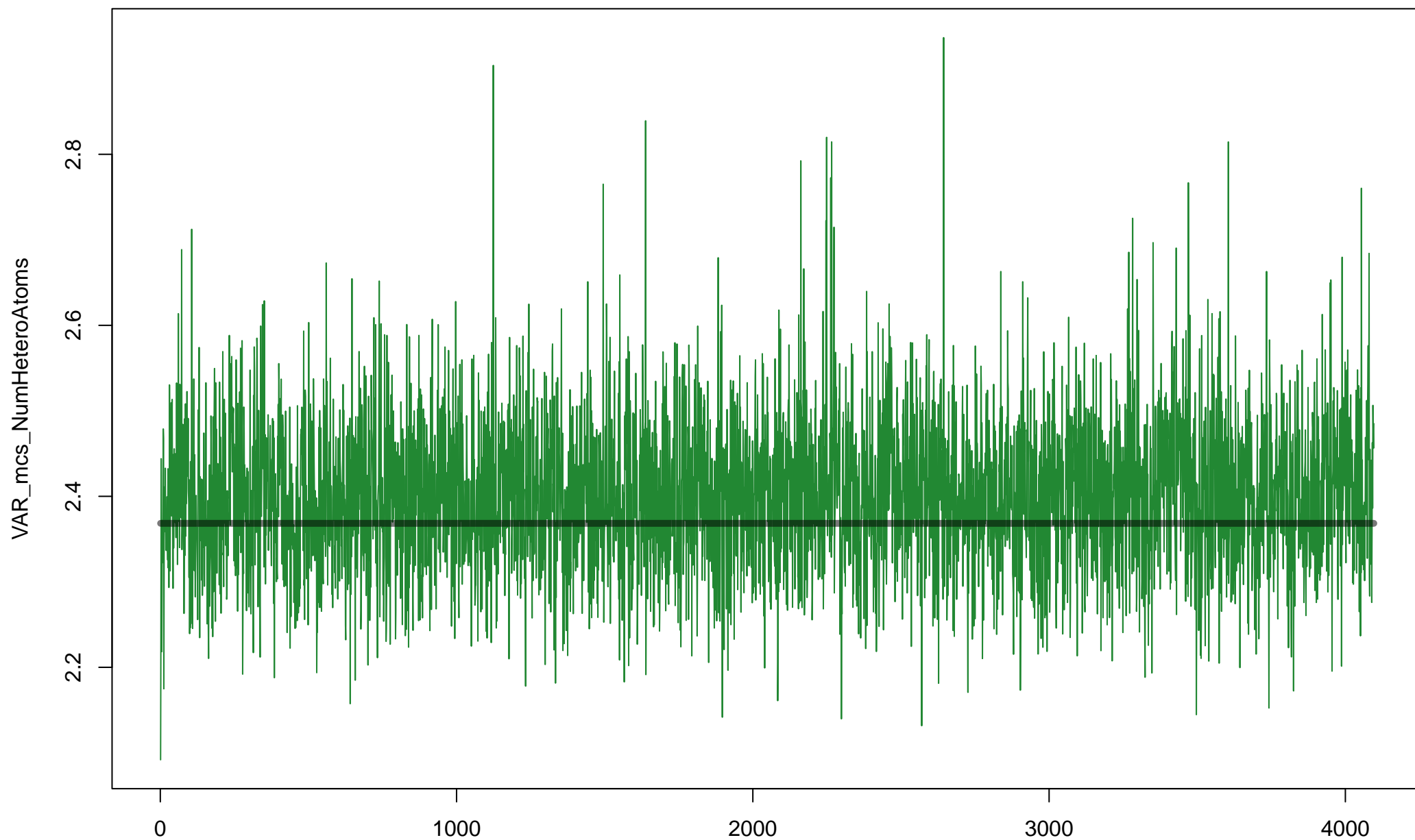
ESS = 4100 | BMK = 0.0294 | MCSE(6.27) = 1.43 | stat: TRUE | burn: 0 | rel.err: 2.23



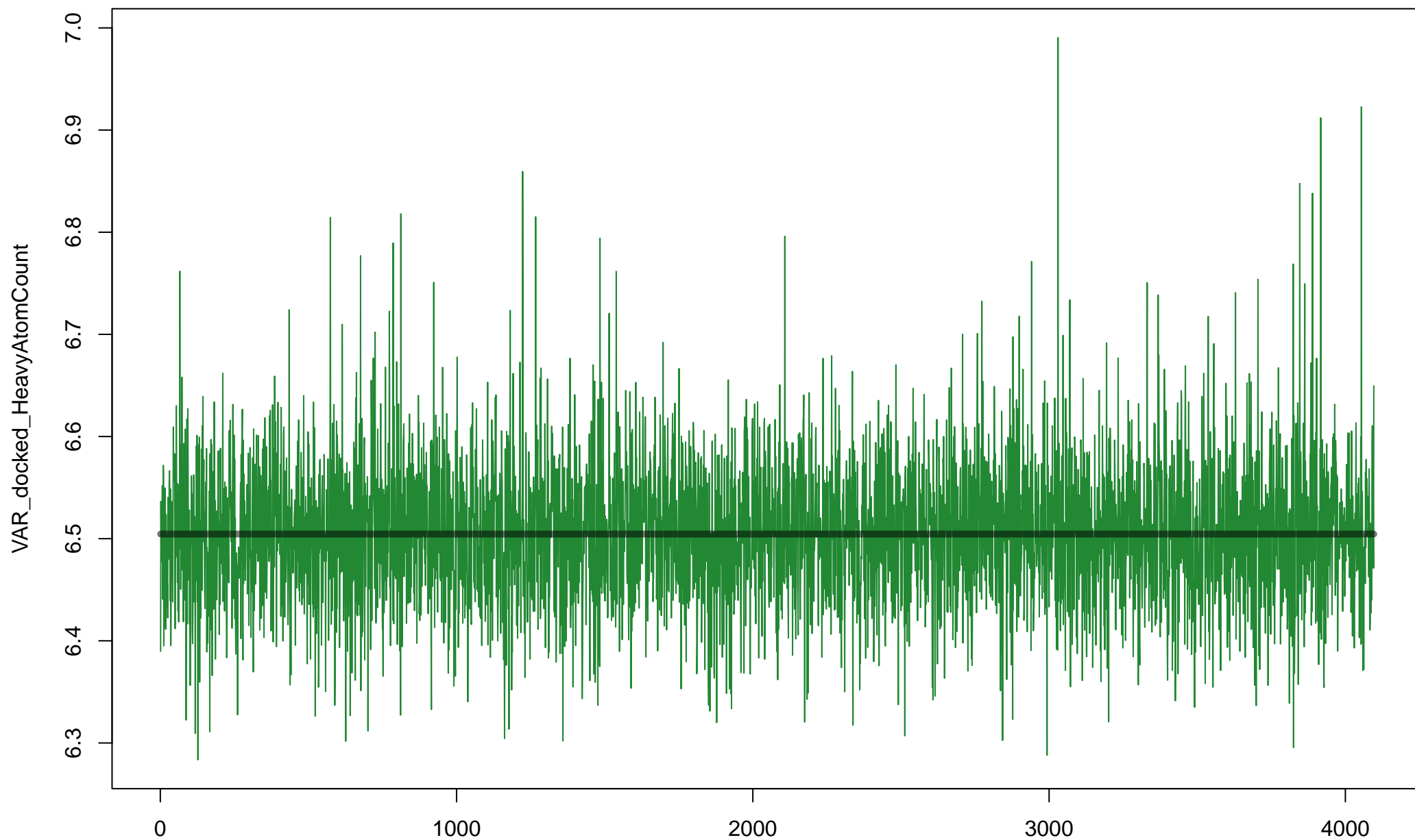
VAR_log_mcs_unbonded_polar_sasa
ESS = 3880 | BMK = 0.0442 | MCSE(6.27) = 1.47 | stat: TRUE | burn: 0 | rel.err: 1.4



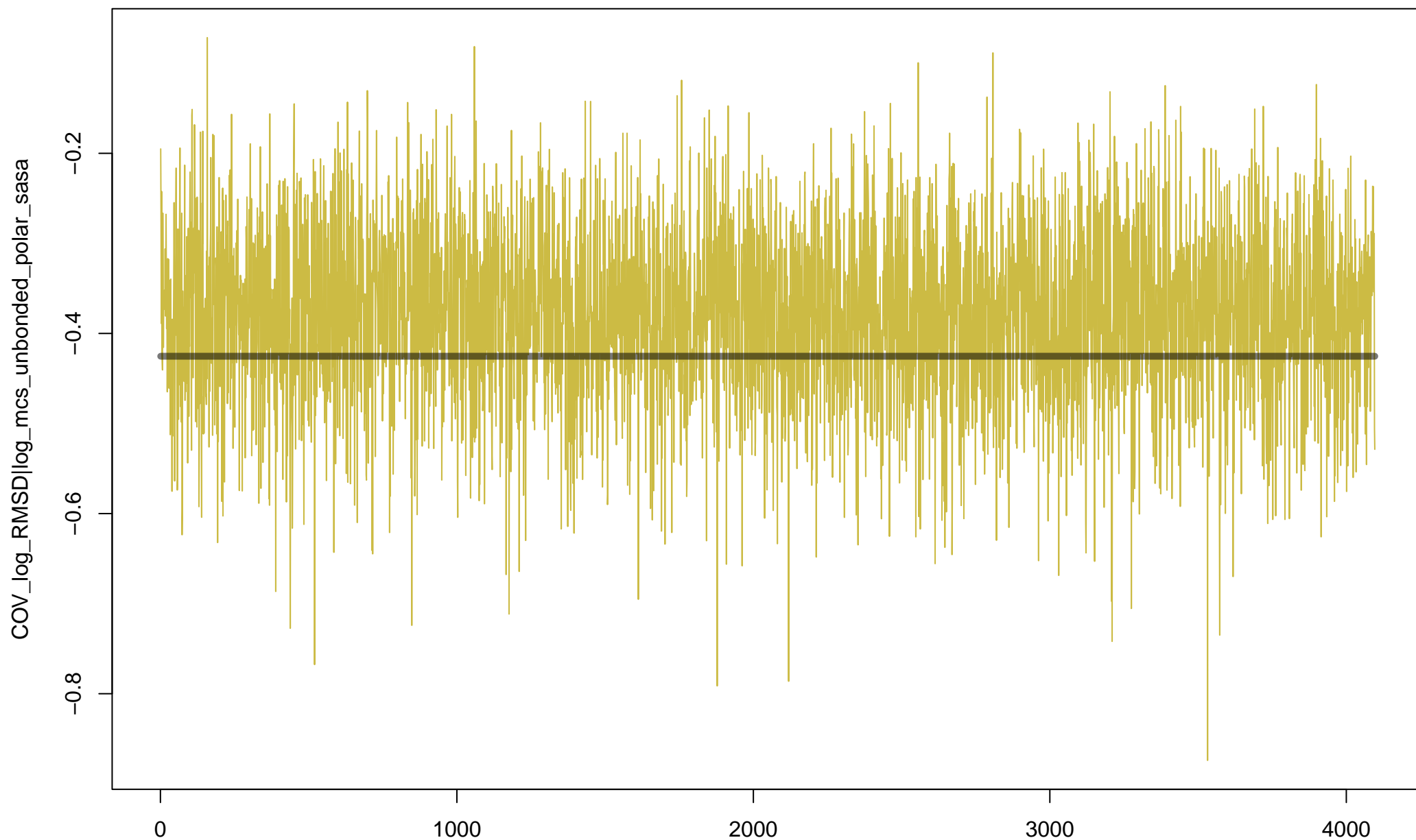
VAR_mcs_NumHeteroAtoms
ESS = 3480 | BMK = 0.0547 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0 | rel.err: 0.4



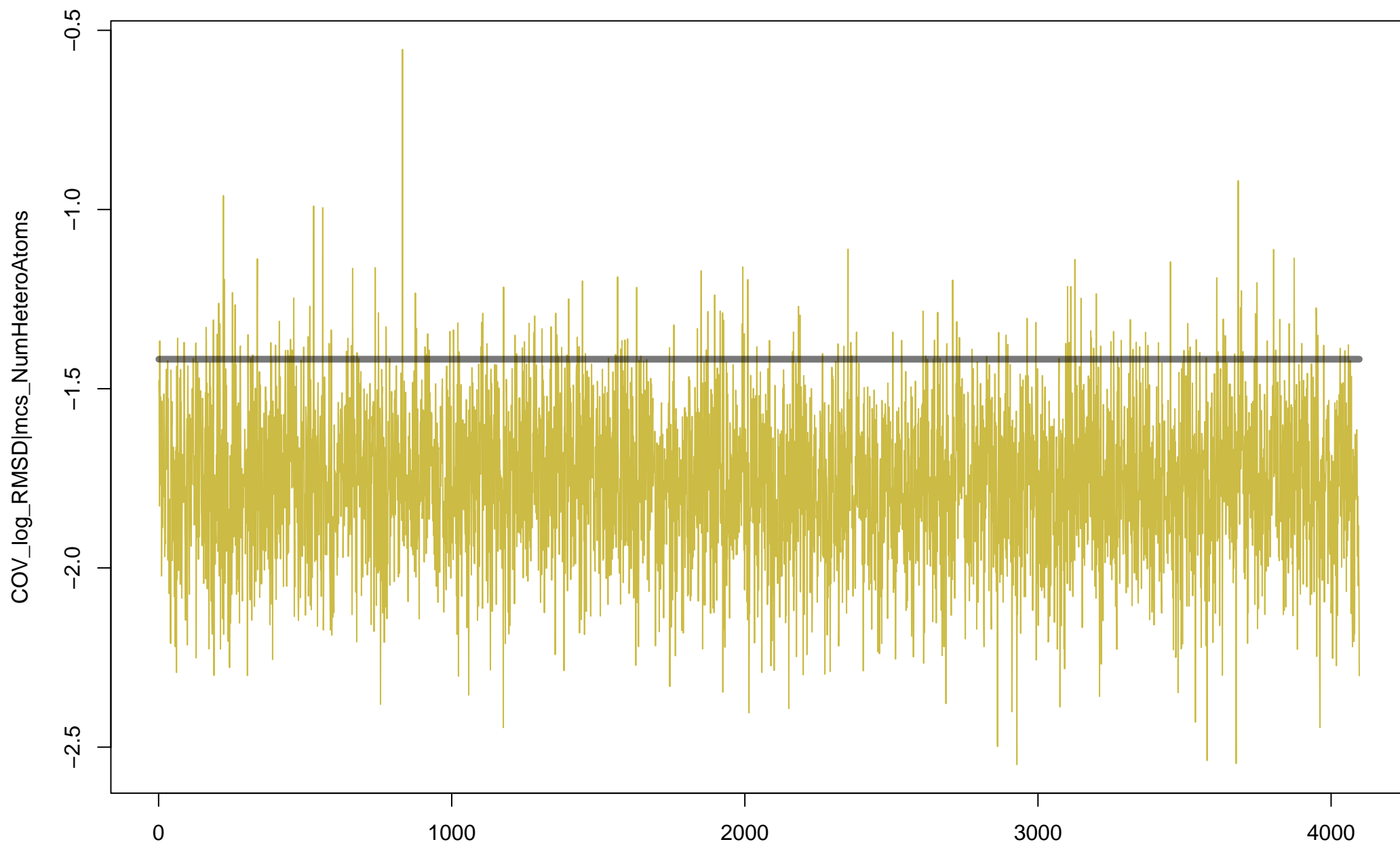
VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0429 | MCSE(6.27) = 1.57 | stat: TRUE | burn: 0 | rel.err: 0.0652



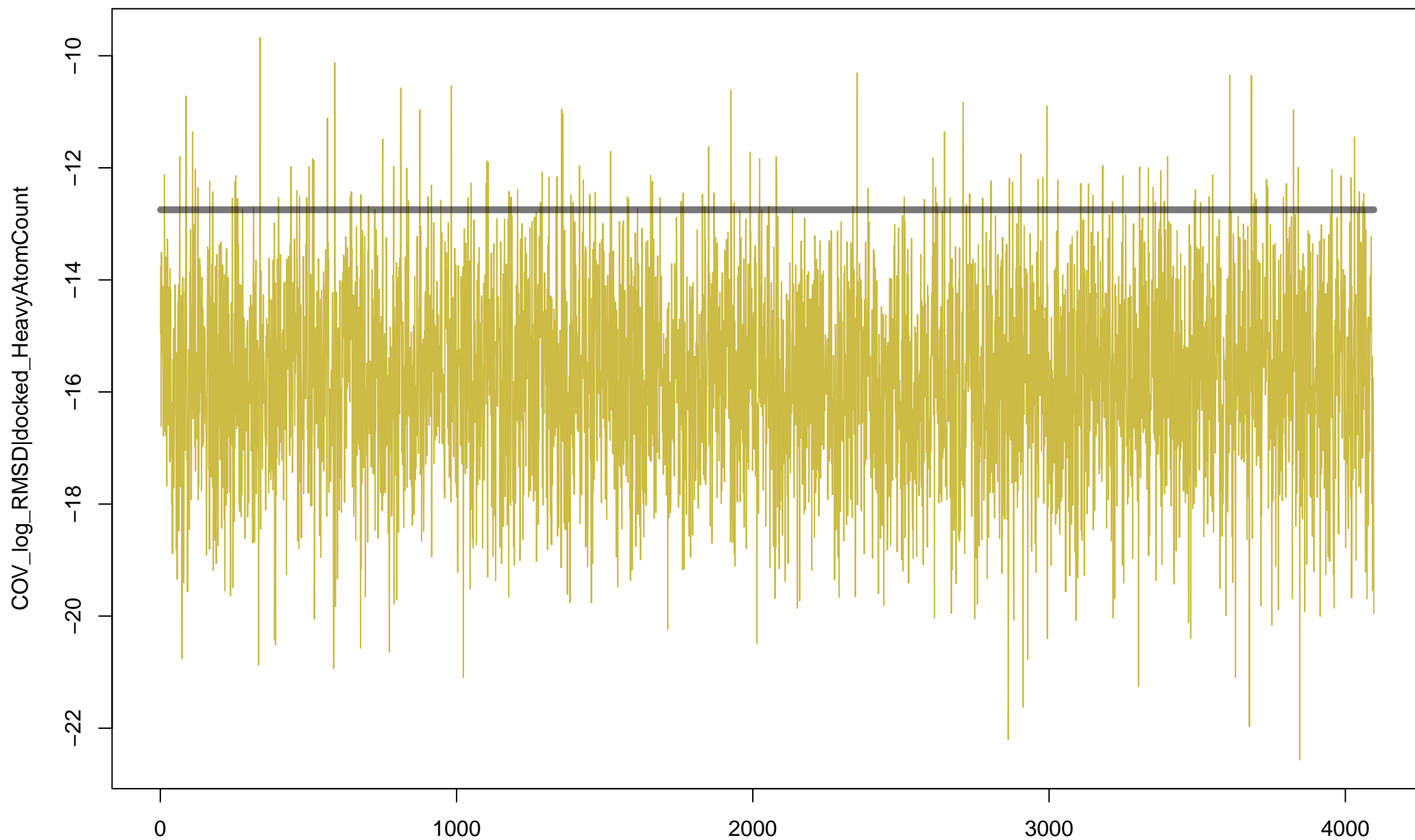
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3740 | BMK = 0.0332 | MCSE(6.27) = 1.54 | stat: TRUE | burn: 0 | rel.err: 0.473



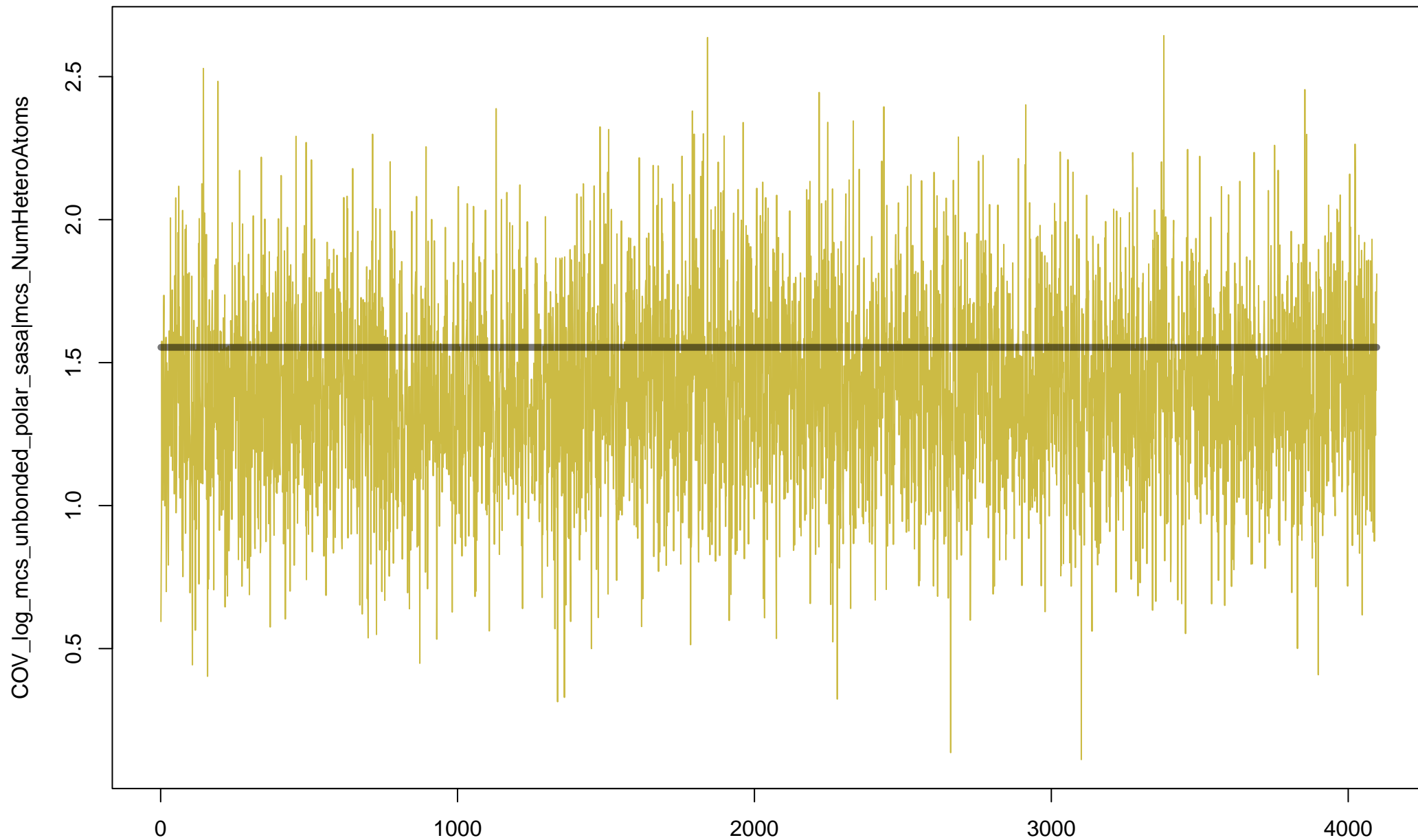
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 3880 | BMK = 0.0539 | MCSE(6.27) = 1.72 | stat: TRUE | burn: 0 | rel.err: -1.61



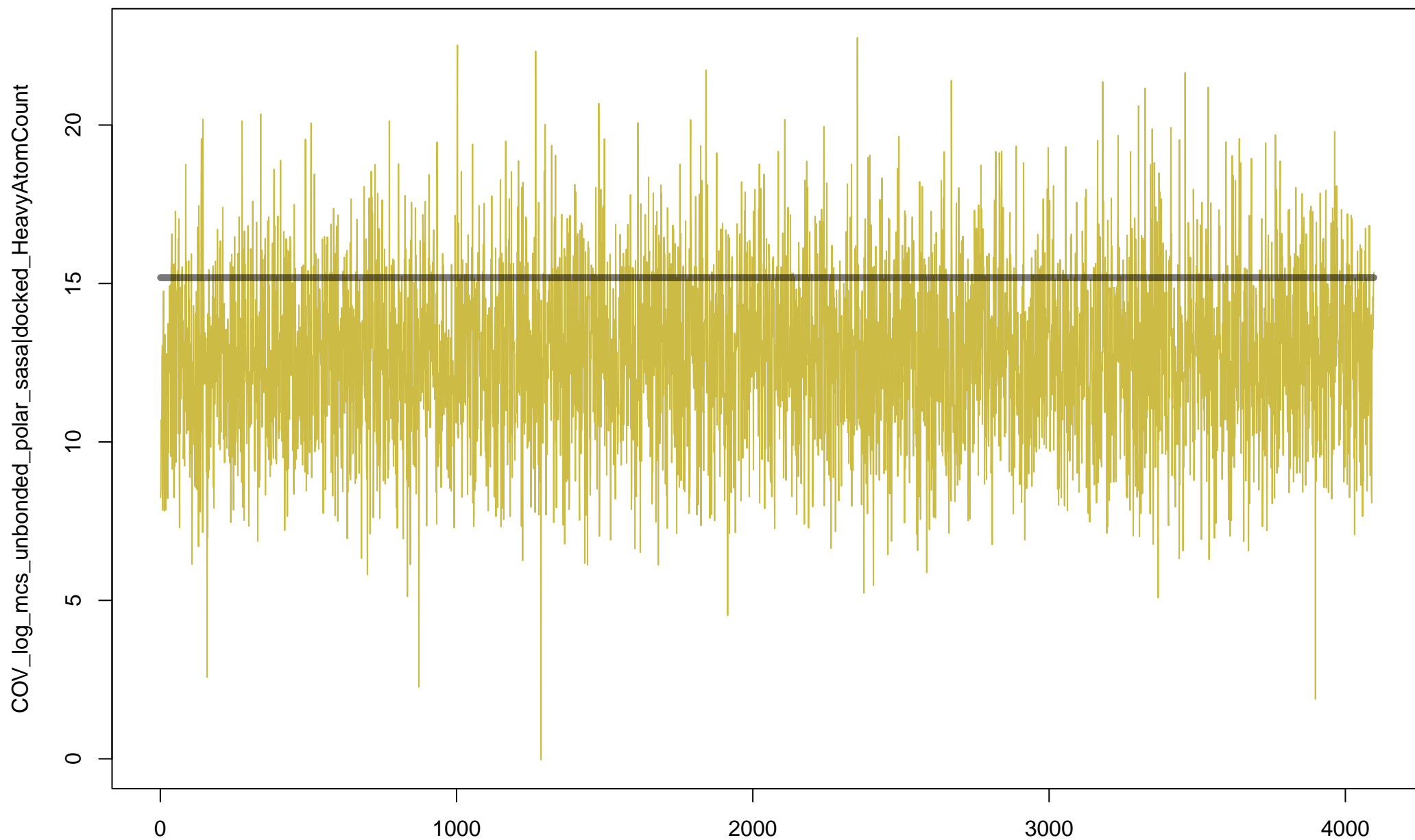
COV_log_RMSD|docked_HeavyAtomCount
ESS = 3890 | BMK = 0.0431 | MCSE(6.27) = 1.3 | stat: TRUE | burn: 0 | rel.err: -1.77



COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0402 | MCSE(6.27) = 1.52 | stat: FALSE | burn: 0 | rel.err: -0.469



COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0287 | MCSE(6.27) = 1.37 | stat: FALSE | burn: 0 | rel.err: -0.924



COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0348 | MCSE(6.27) = 1.5 | stat: TRUE | burn: 0 | rel.err: 0.478

