

-- STATS maxD --

min ESS = 72.715010157334

max BMK = 0.156577326860884

max MCSE = 8.29583058884191

all stationary: FALSE

burn: 0

max rel.err.: 1.90431697302769

-- STATS 2D --

min ESS = 1763.02594861723

max BMK = 0.0507193100666302

max MCSE = 2.64178509081982

all stationary: TRUE

burn: 0

max rel.err.: 1.82353853672523

-- STATS 1D --

min ESS = 1912.57339908587

max BMK = 0.0689855413413962

max MCSE = 2.93365272702607

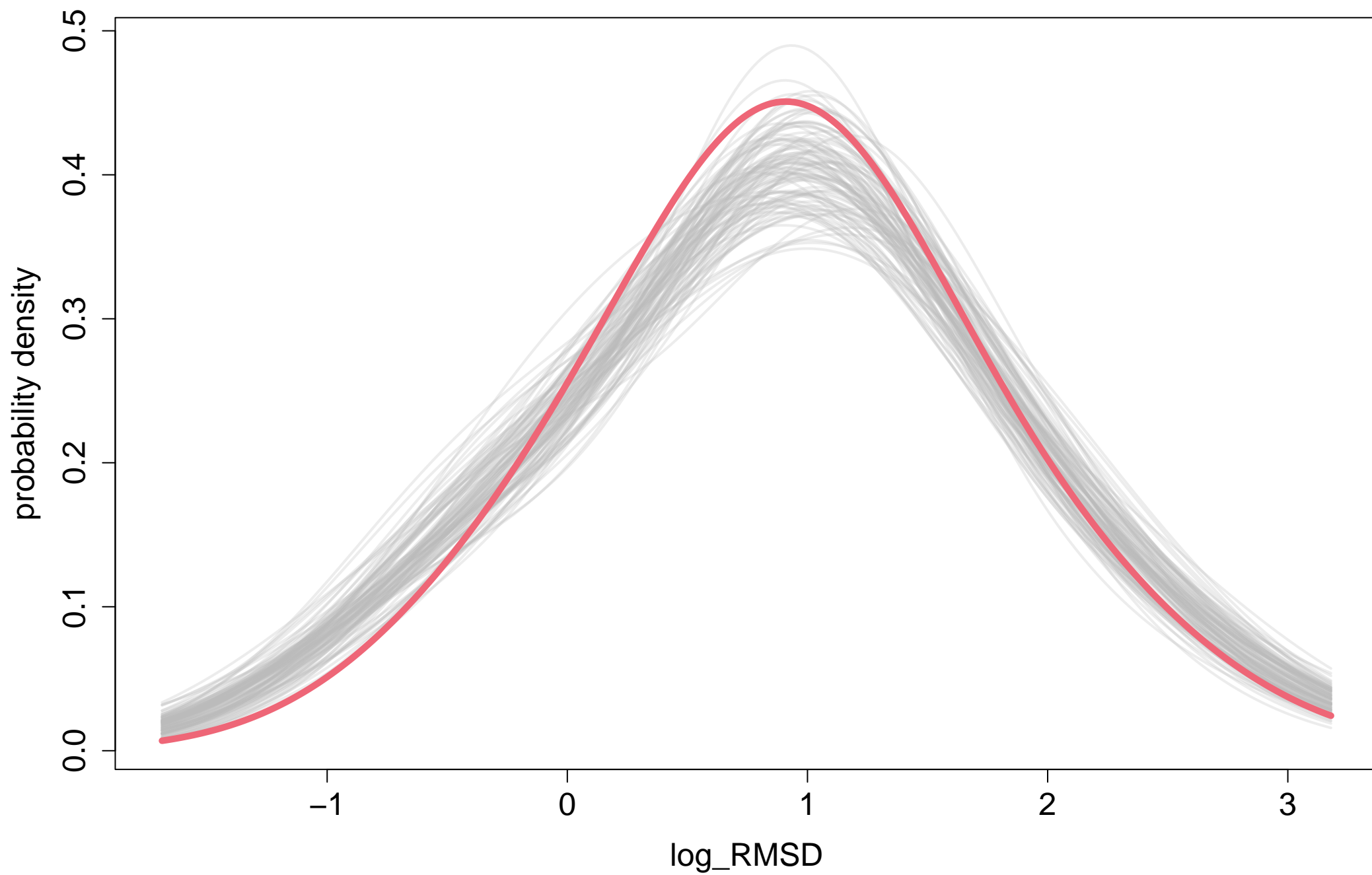
all stationary: FALSE

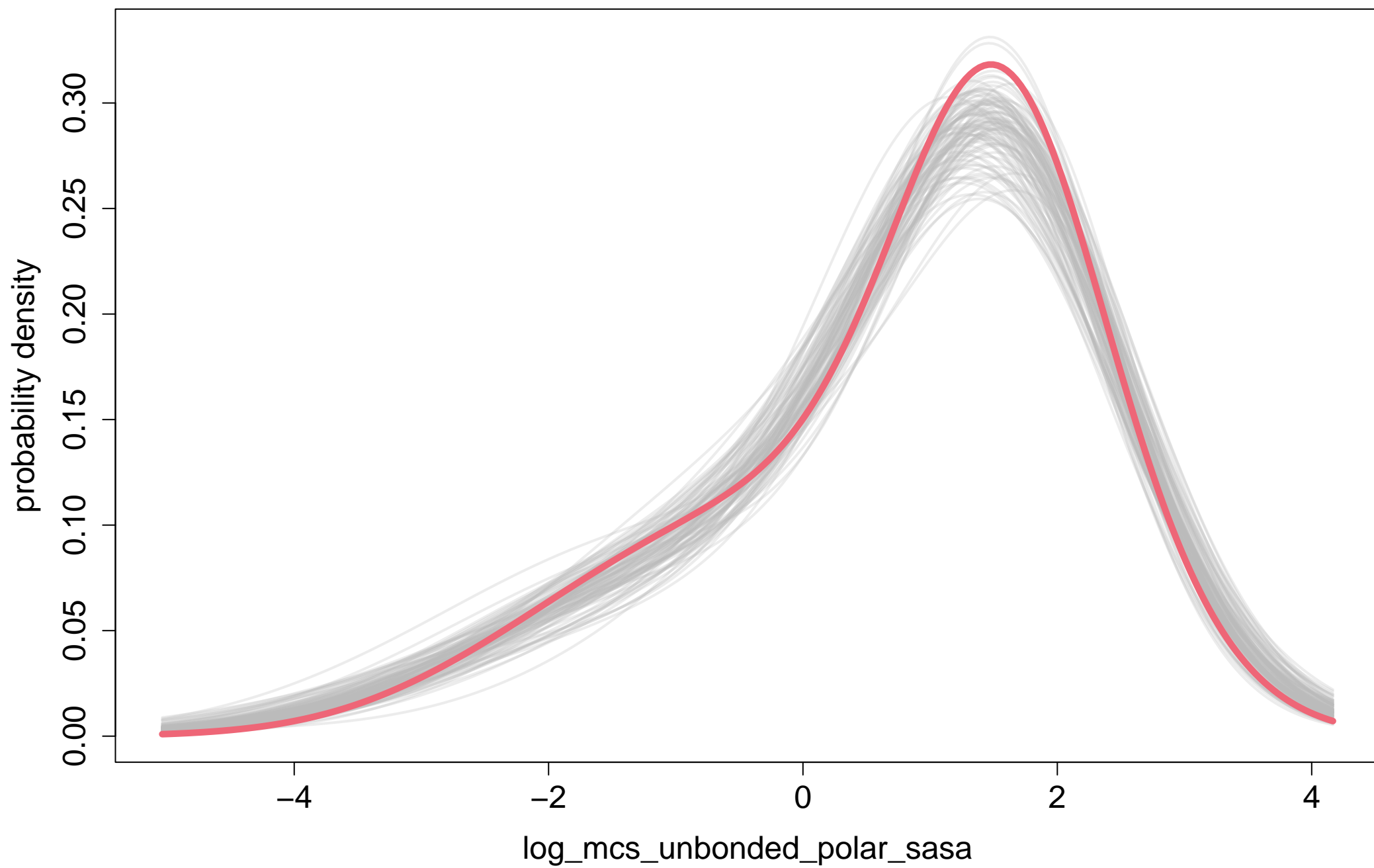
burn: 0

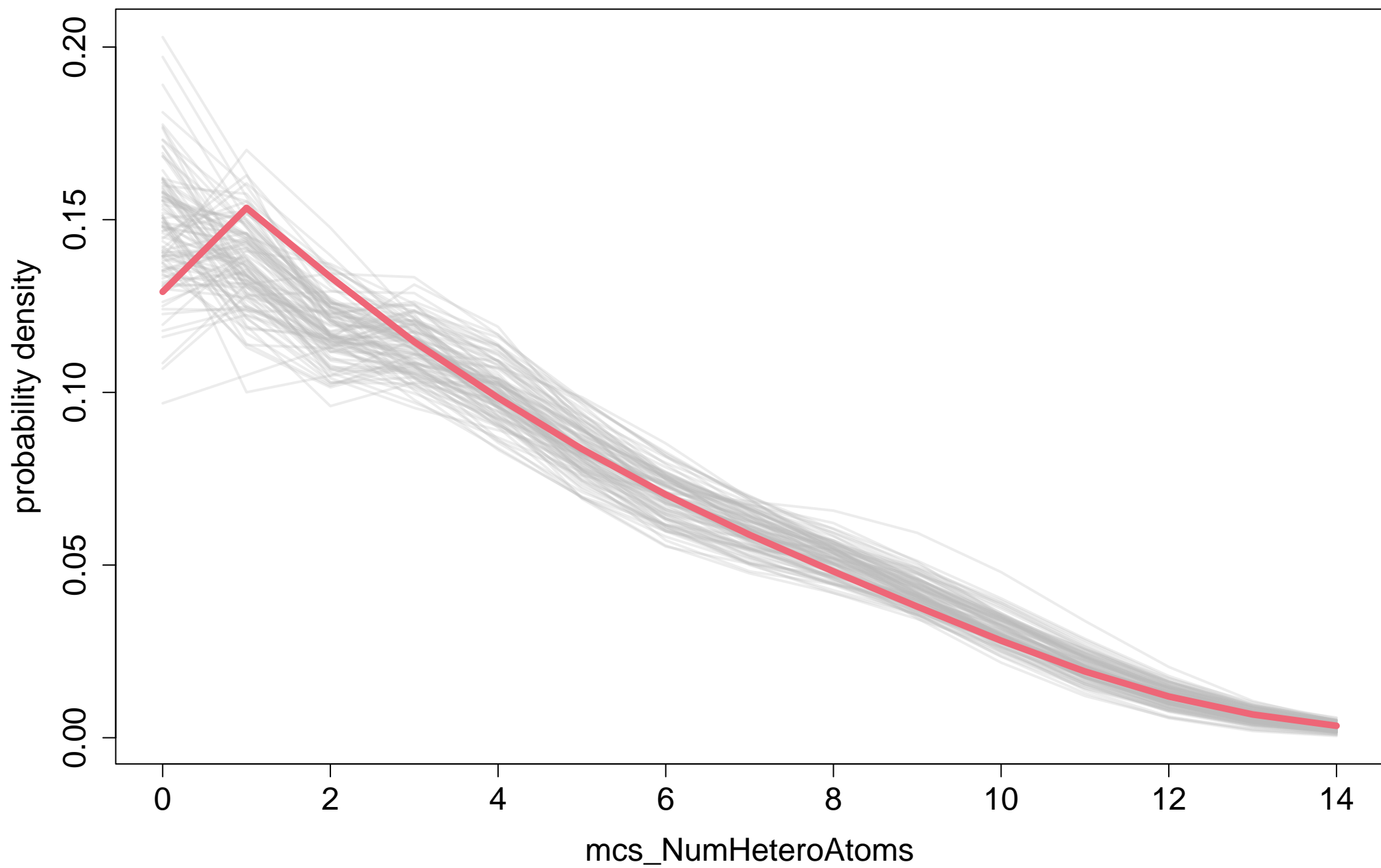
max rel.err.: 2.30366767538934

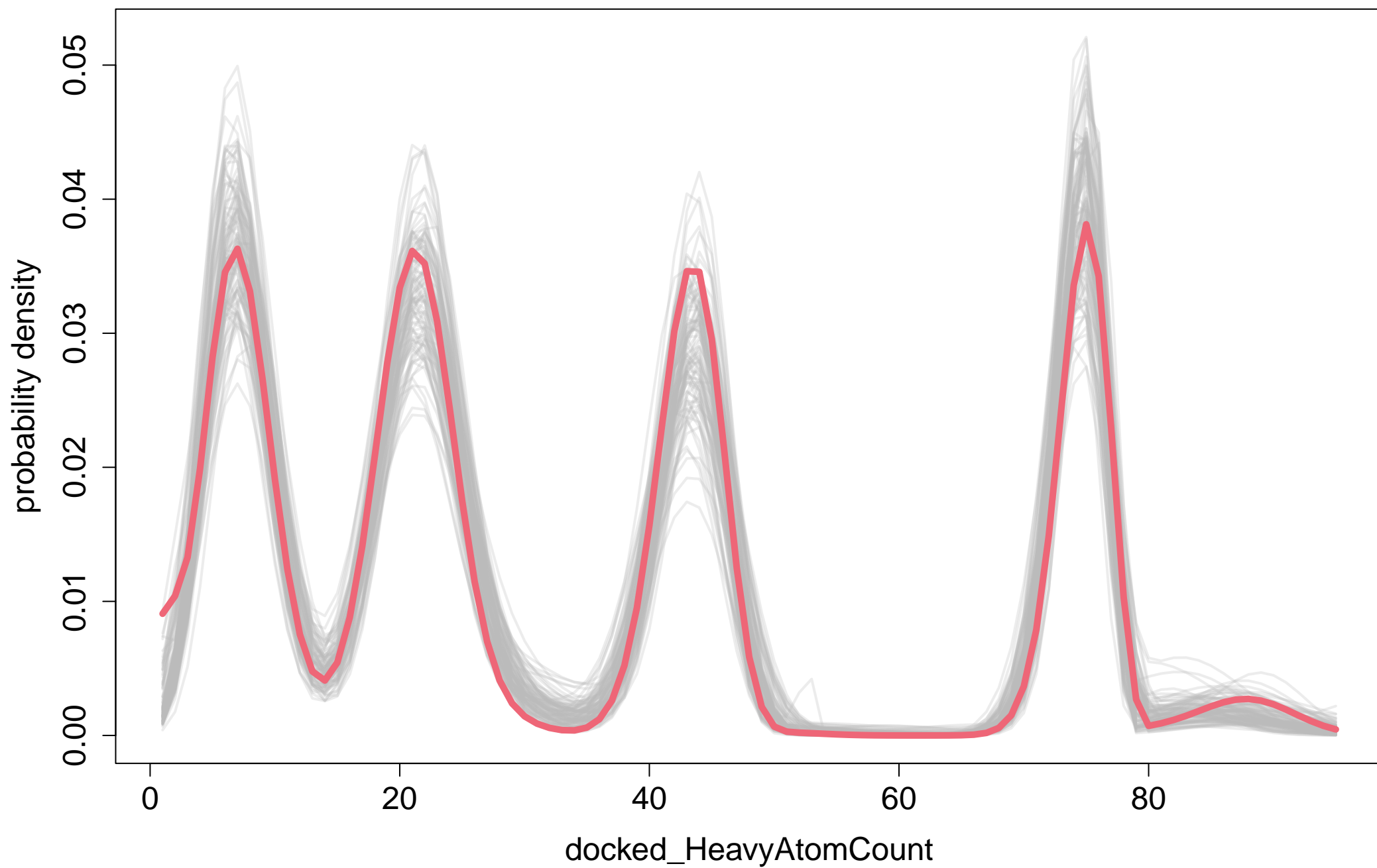
Occupied clusters: 9 of 16

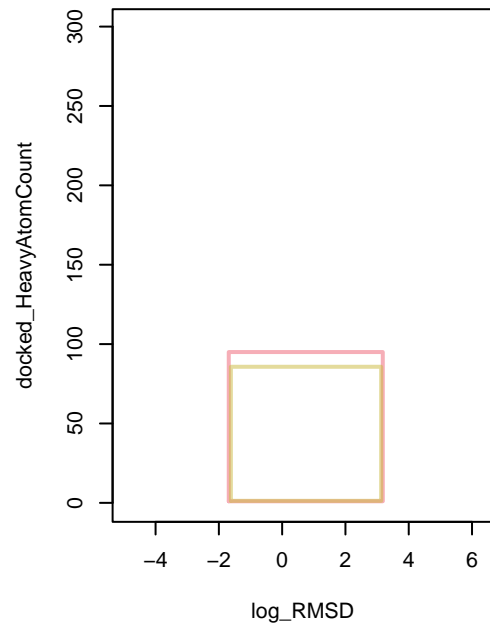
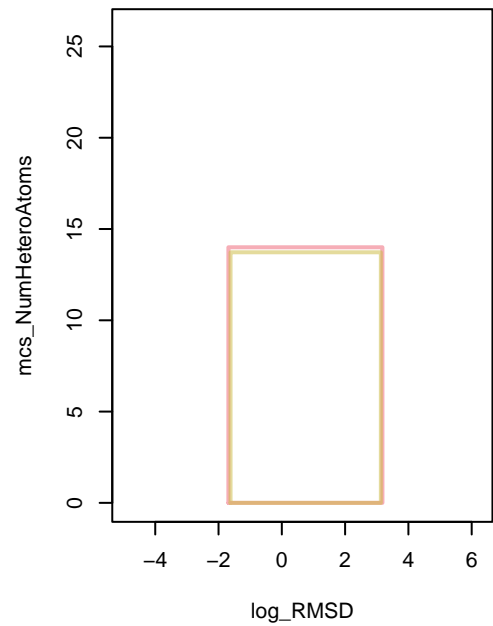
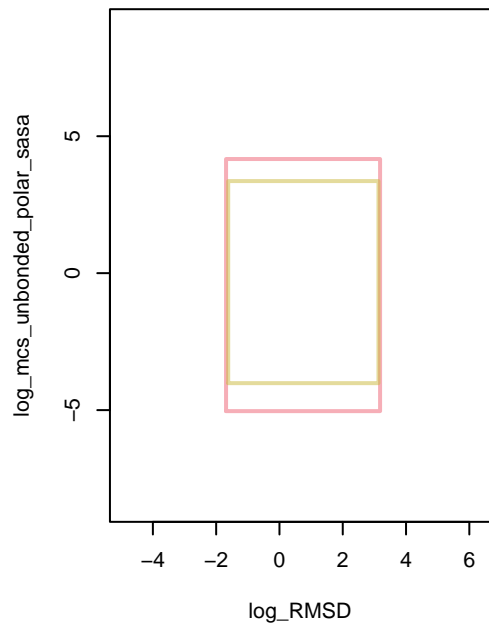
LL: -2158.63846224364 sd: 6.77428632652494



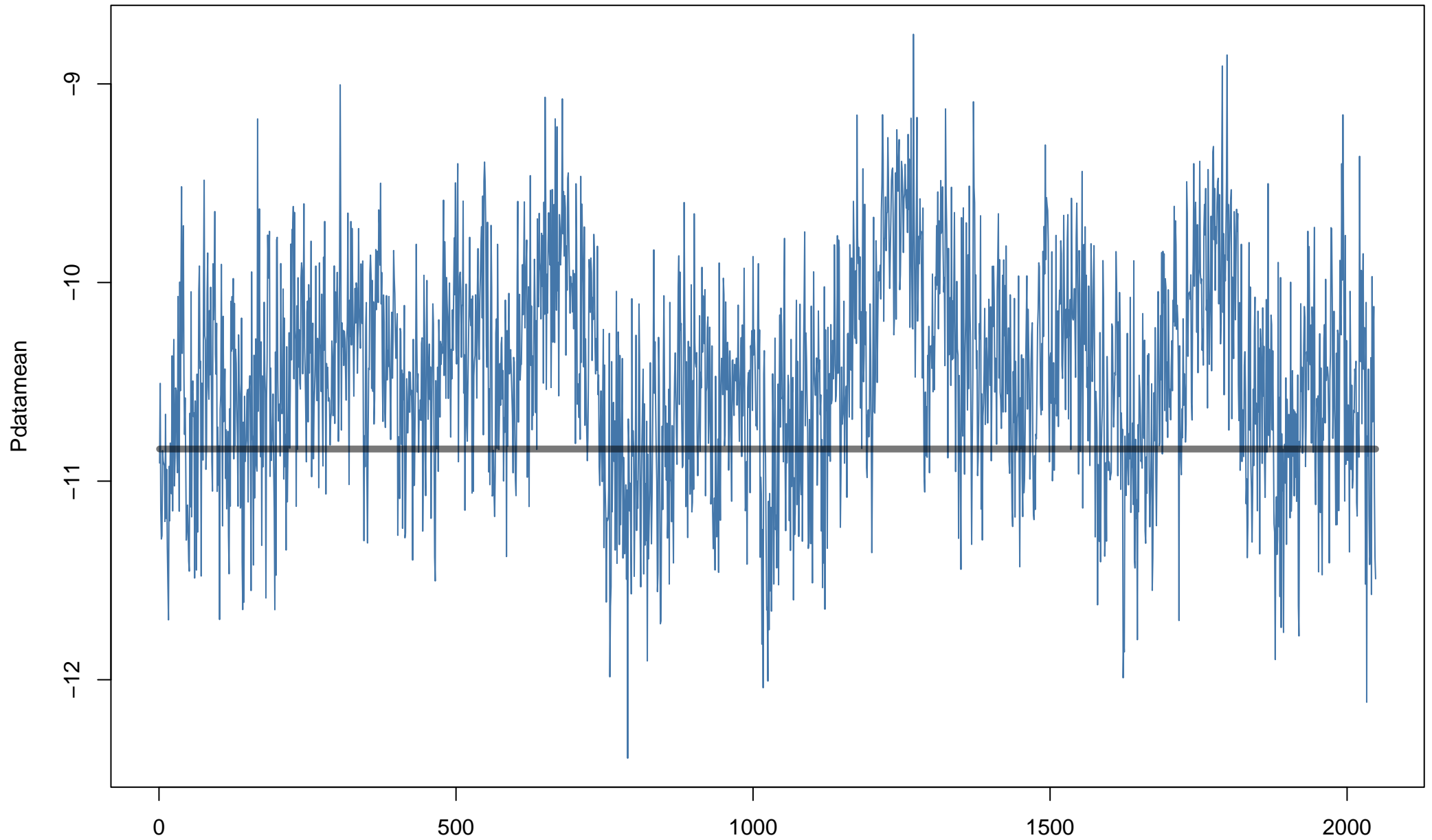




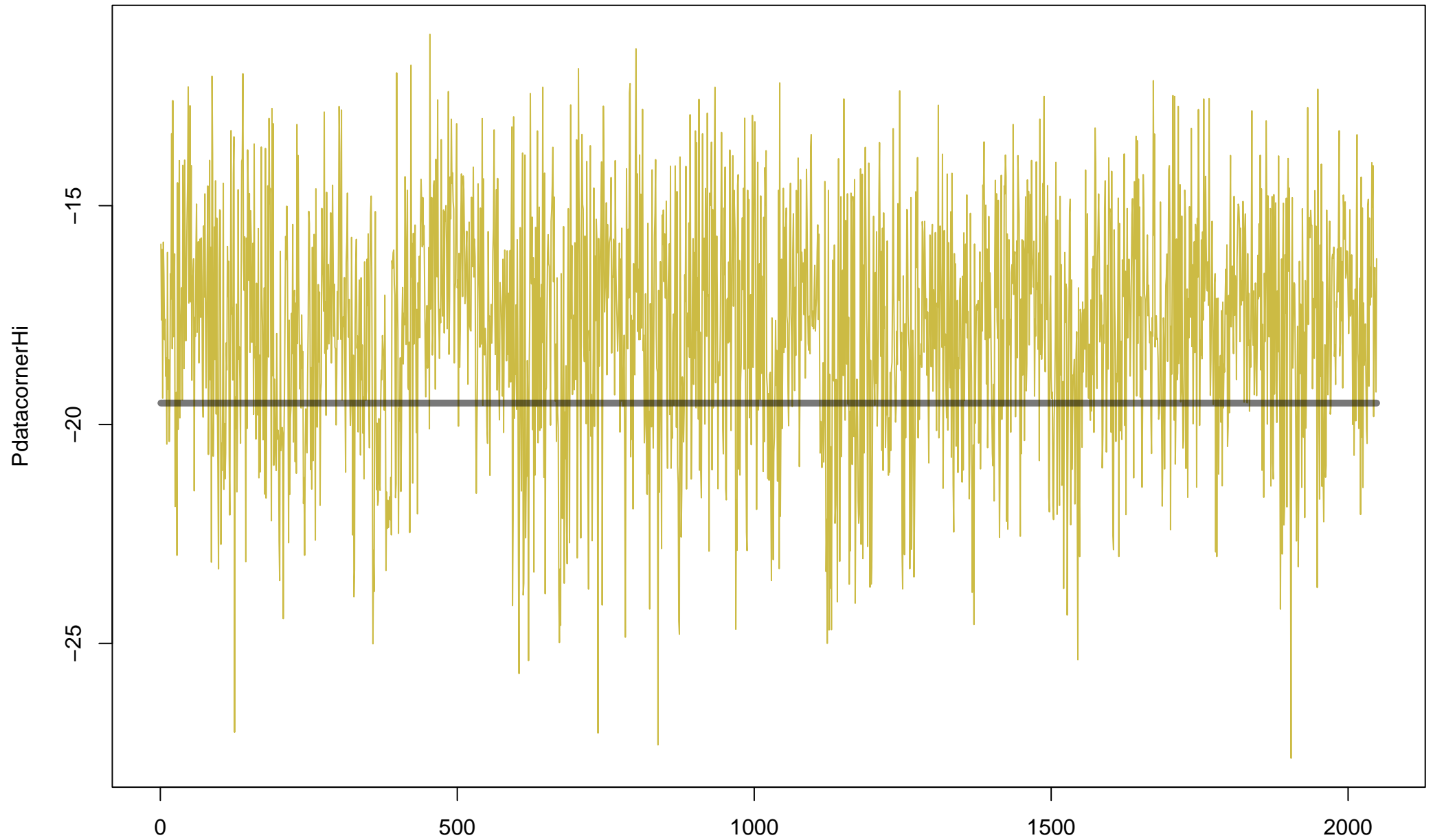




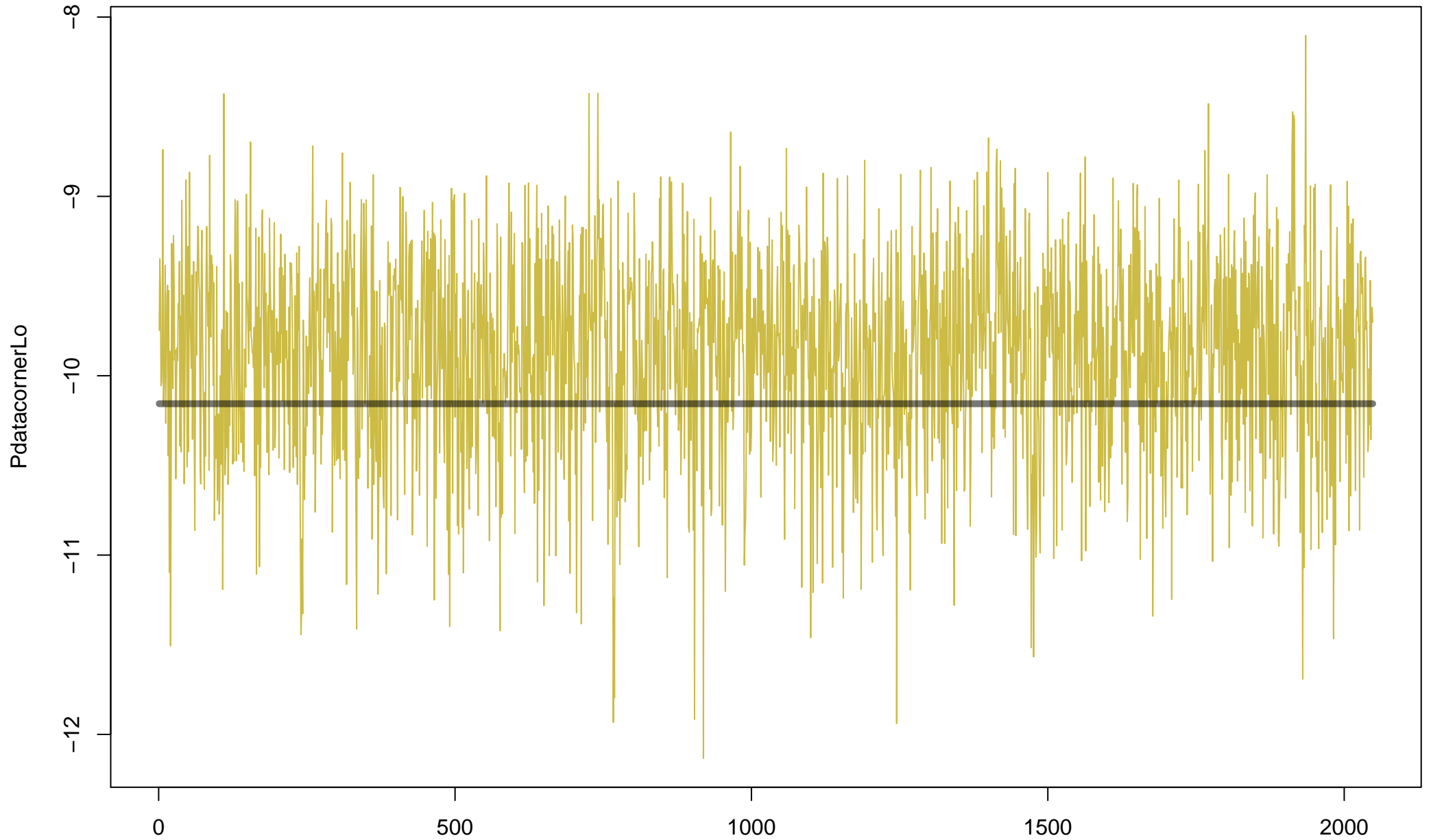
Pdatamean
ESS = 72.7 | BMK = 0.101 | MCSE(6.27) = 8.3 | stat: FALSE | burn: 0 | rel.err: 0.734



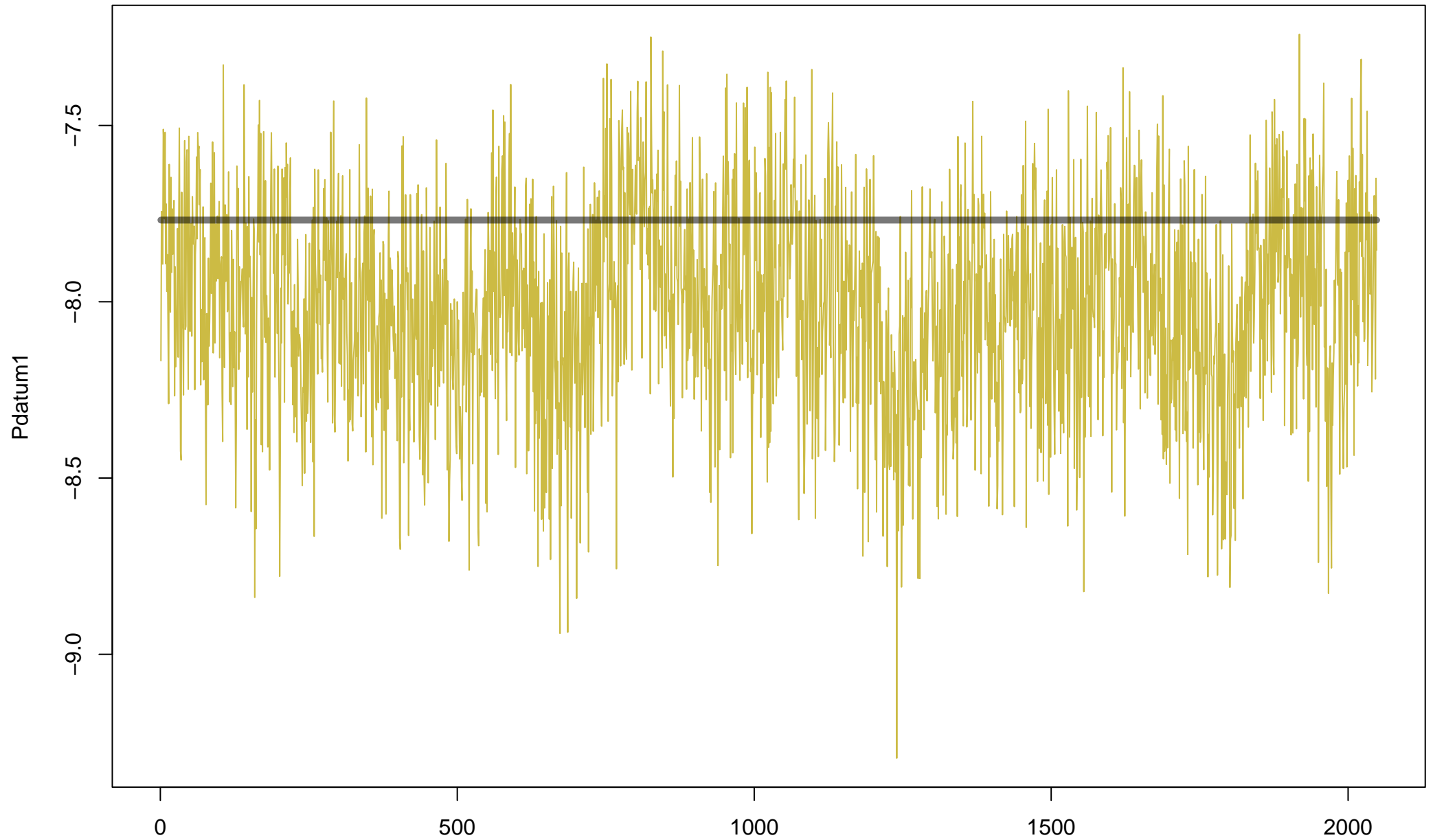
PdatacornerHi
ESS = 2050 | BMK = 0.157 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0 | rel.err: 0.288



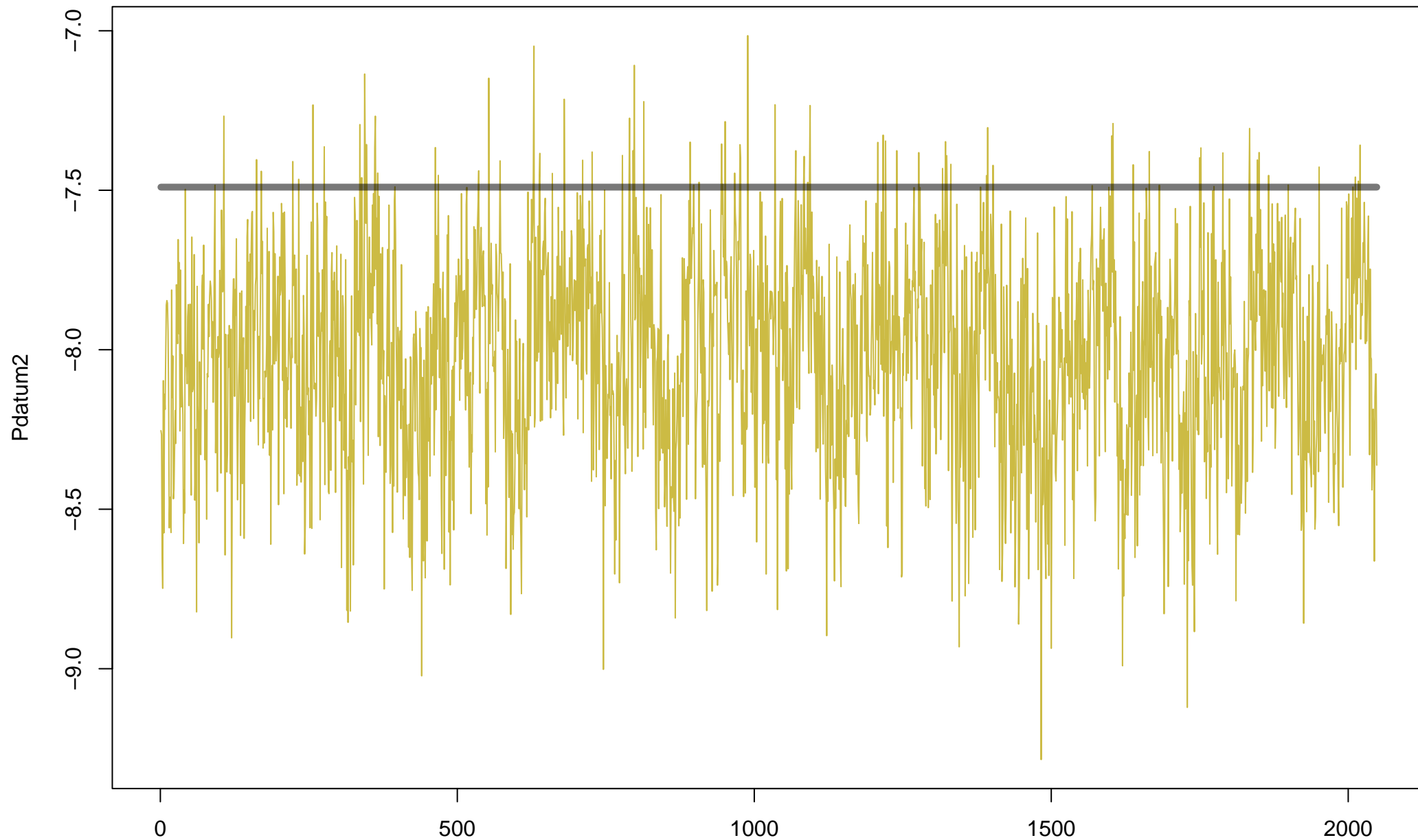
PdatacornerLo
ESS = 1390 | BMK = 0.0608 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | rel.err: 0.638



Pdatum1
ESS = 154 | BMK = 0.0432 | MCSE(6.27) = 5.84 | stat: FALSE | burn: 0 | rel.err: -0.792

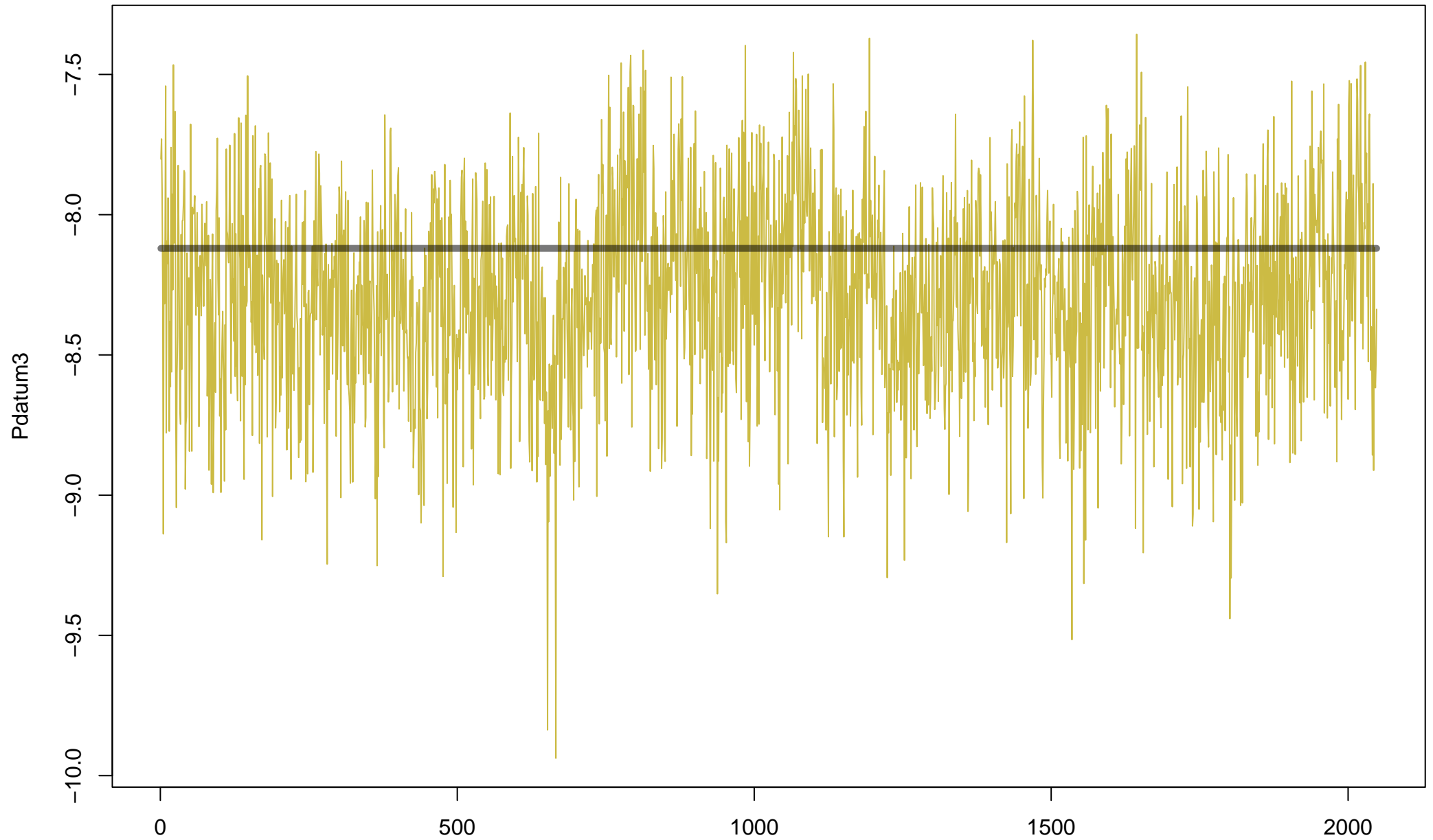


Pdatum2
ESS = 309 | BMK = 0.0526 | MCSE(6.27) = 4.55 | stat: TRUE | burn: 0 | rel.err: -1.9

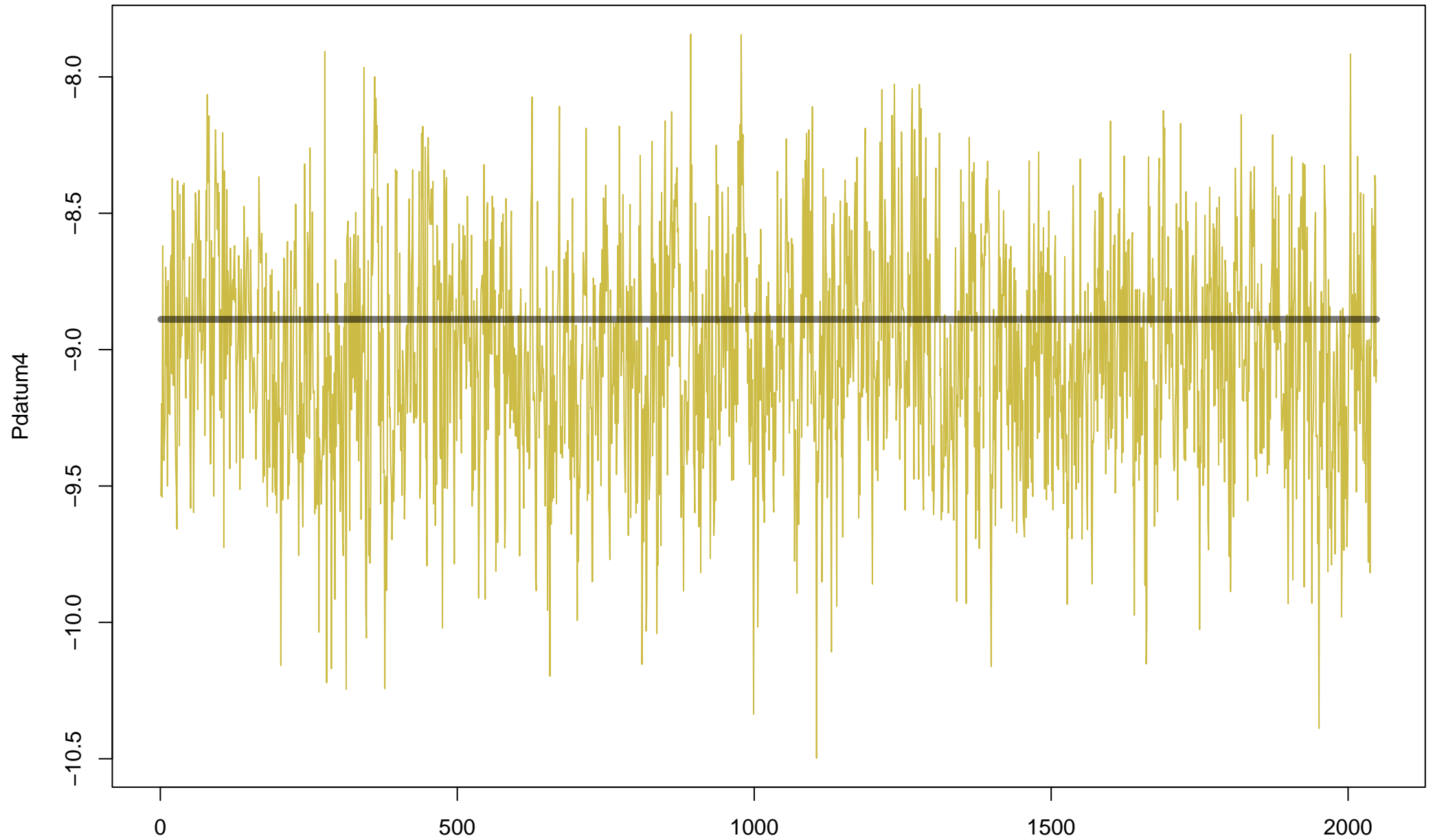


Pdatum3

ESS = 261 | BMK = 0.0283 | MCSE(6.27) = 5.01 | stat: TRUE | burn: 0 | rel.err: -0.324

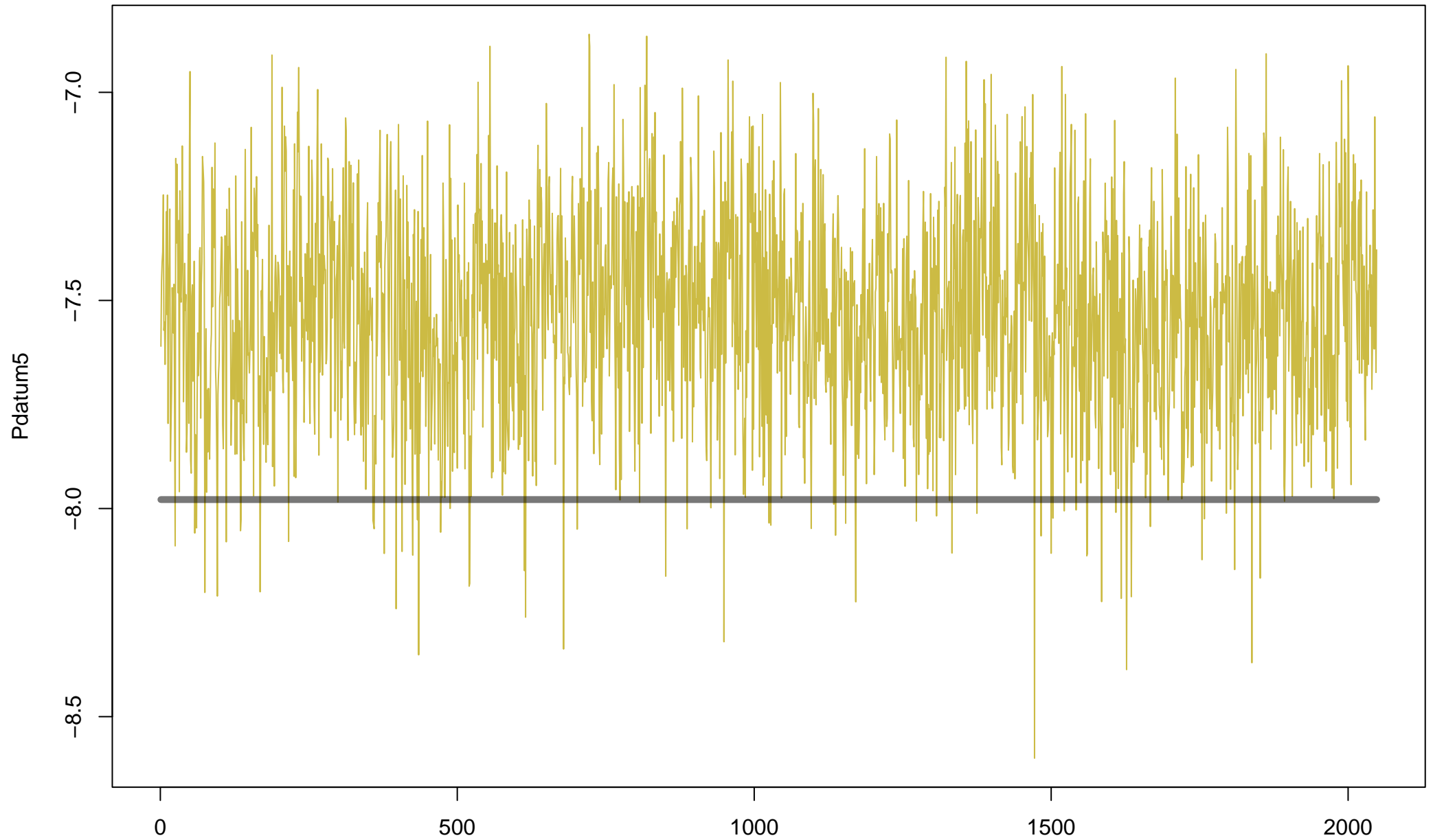


Pdatum4
ESS = 748 | BMK = 0.04 | MCSE(6.27) = 3.85 | stat: TRUE | burn: 0 | rel.err: -0.12

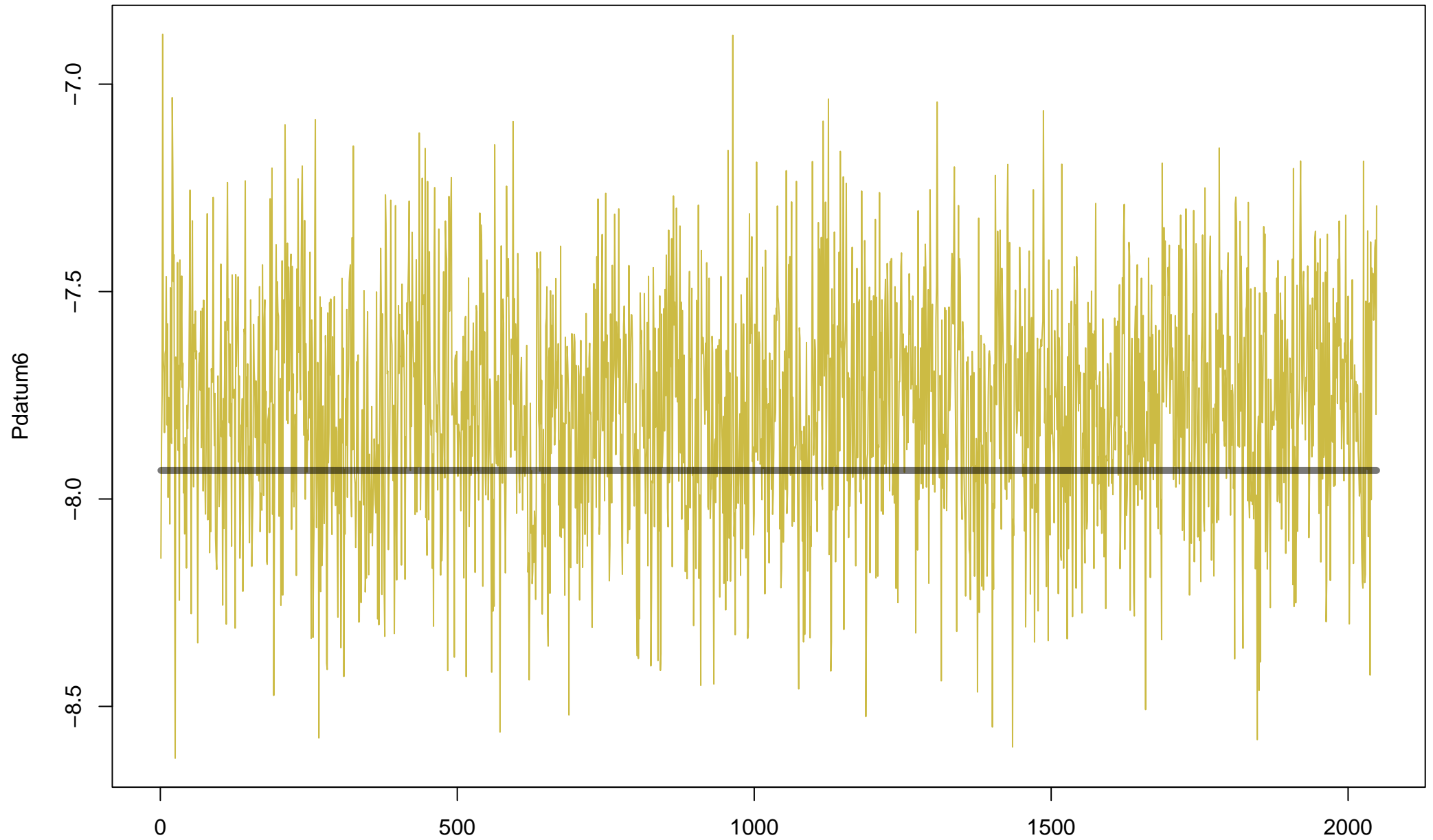


Pdatum5

ESS = 1000 | BMK = 0.0625 | MCSE(6.27) = 3.69 | stat: TRUE | burn: 0 | rel.err: 1.54

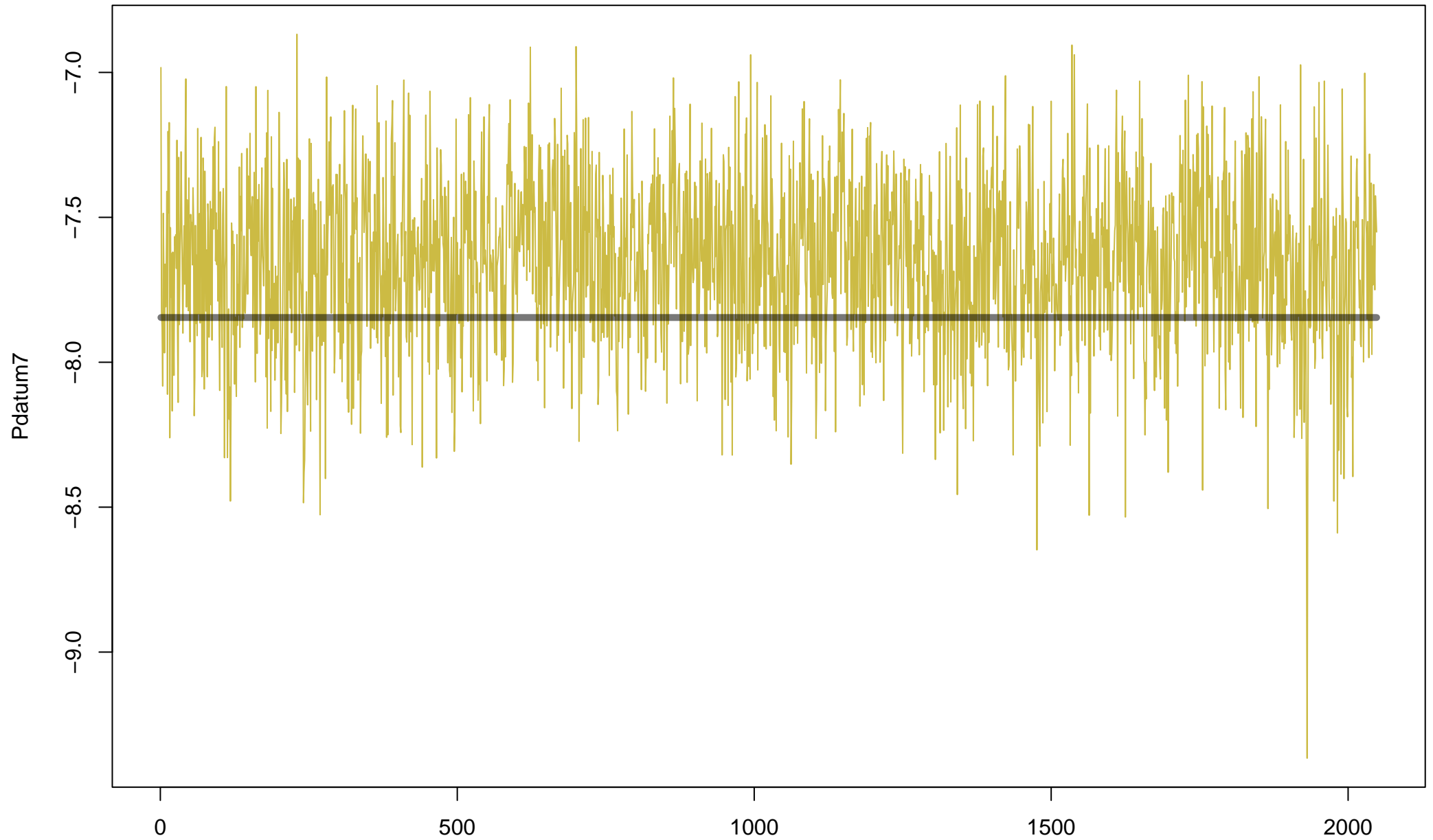


Pdatum6
ESS = 1070 | BMK = 0.048 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: 0.62

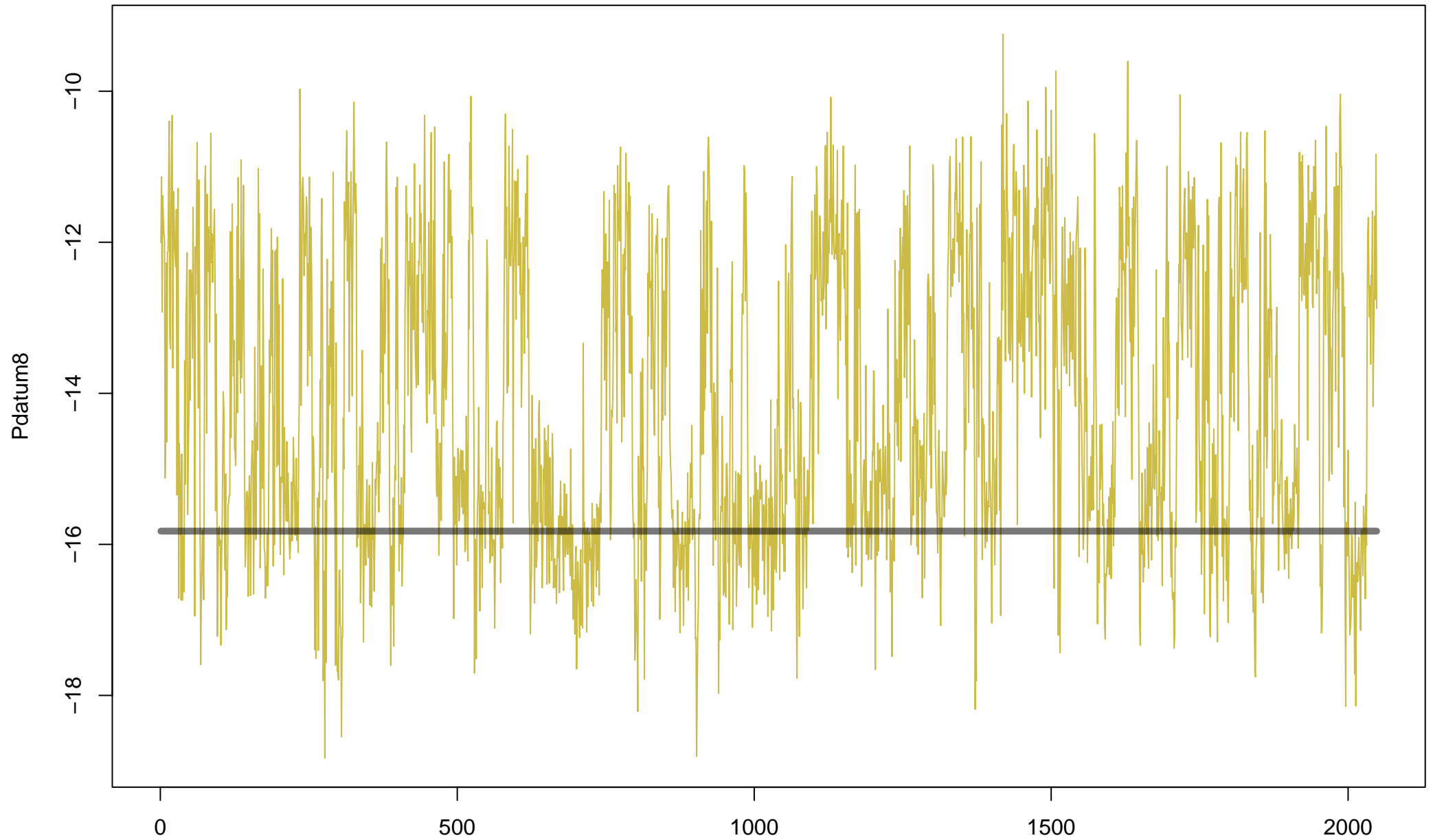


Pdatum7

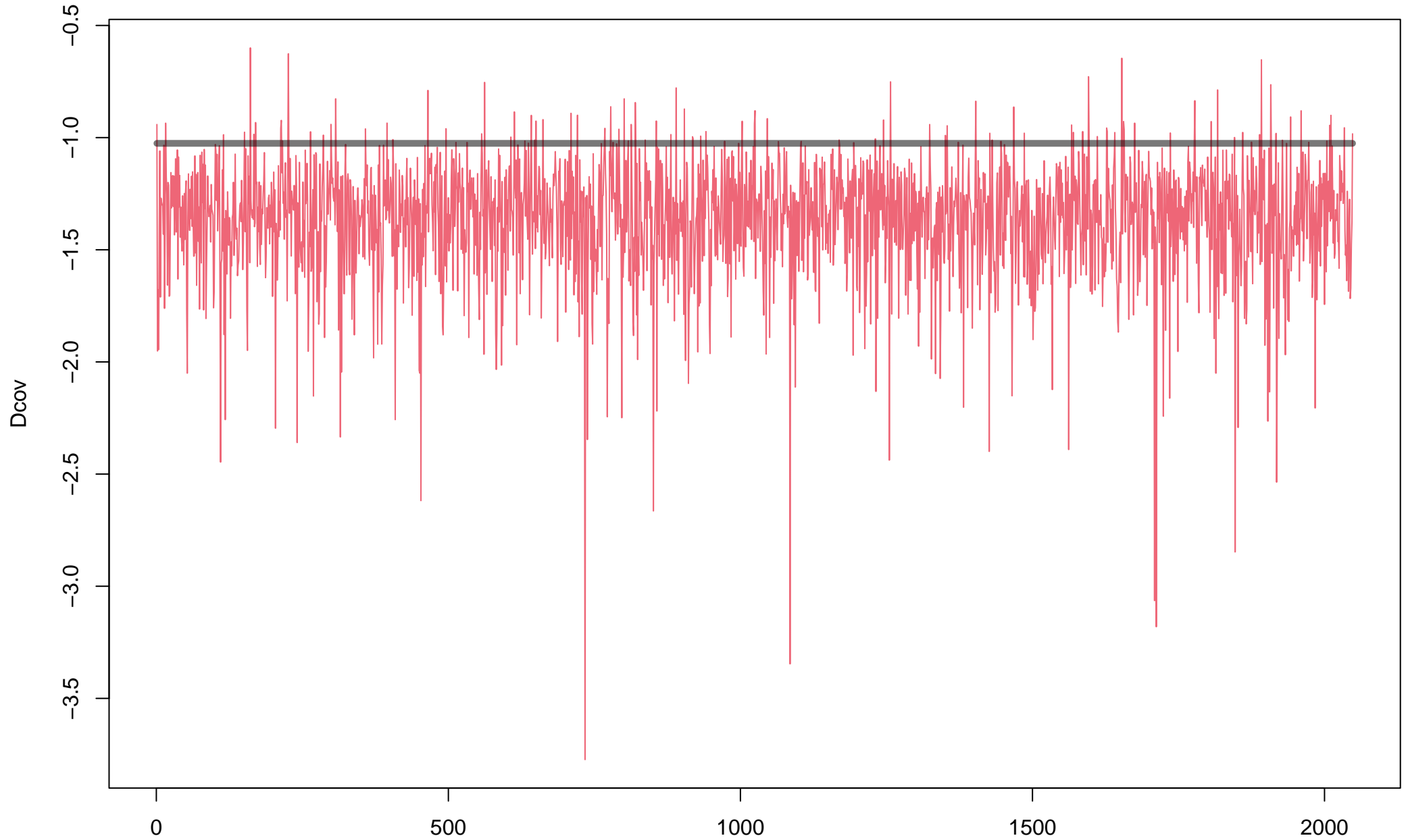
ESS = 1310 | BMK = 0.0411 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | rel.err: 0.729



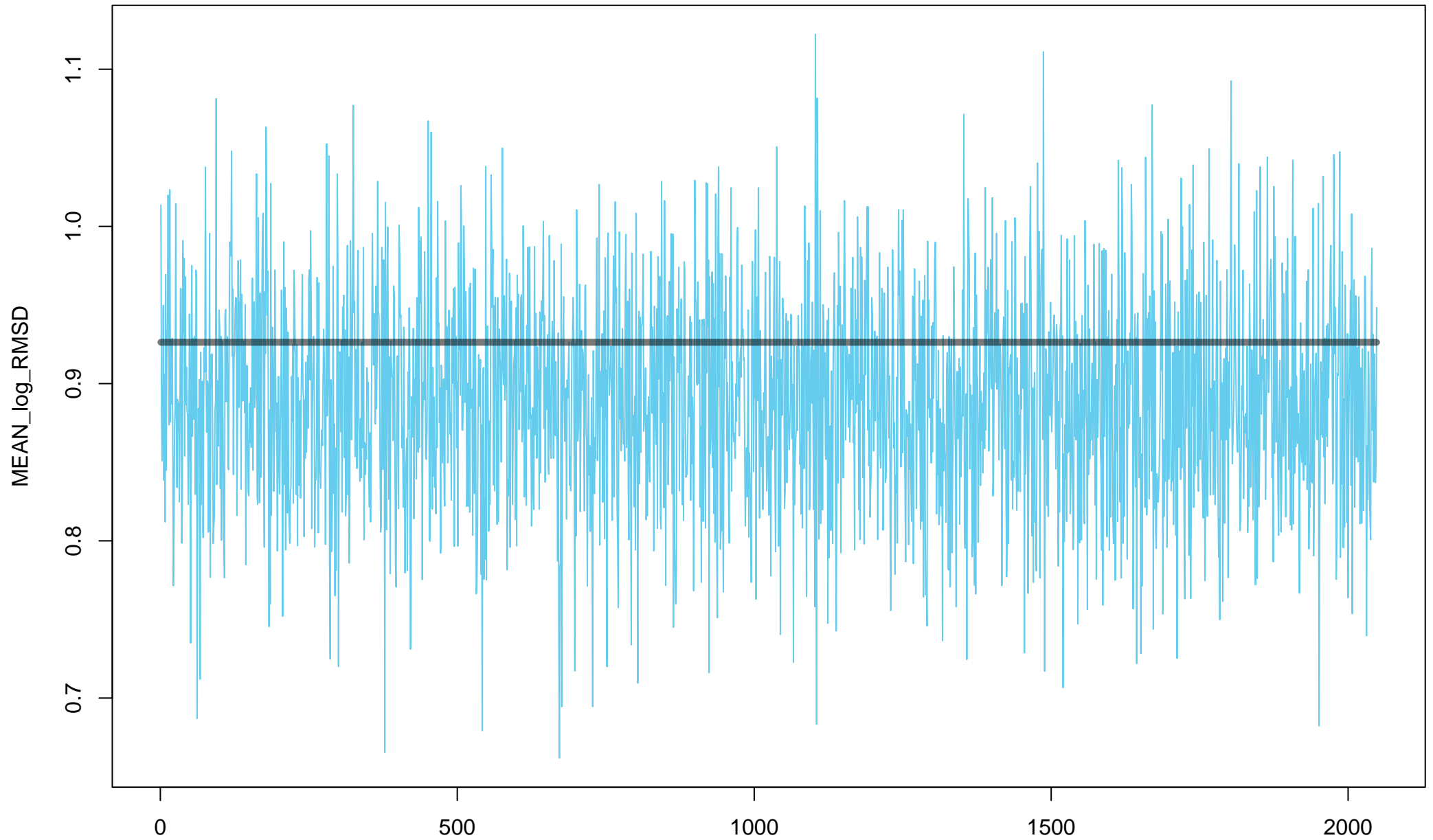
Pdatum8
ESS = 364 | BMK = 0.137 | MCSE(6.27) = 4.62 | stat: TRUE | burn: 0 | rel.err: 0.5



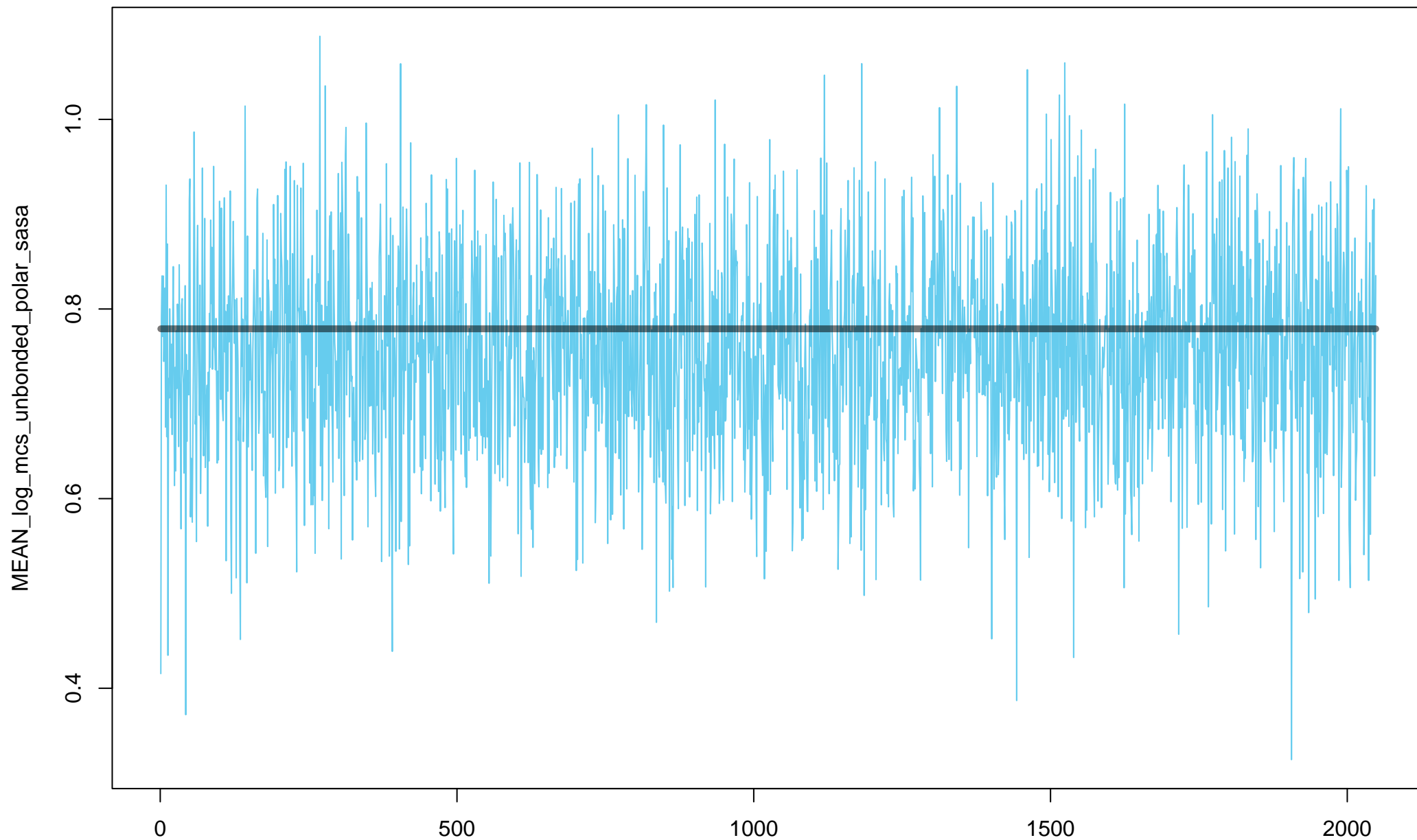
Dcov
ESS = 2050 | BMK = 0.0697 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0 | rel.err: 1.48



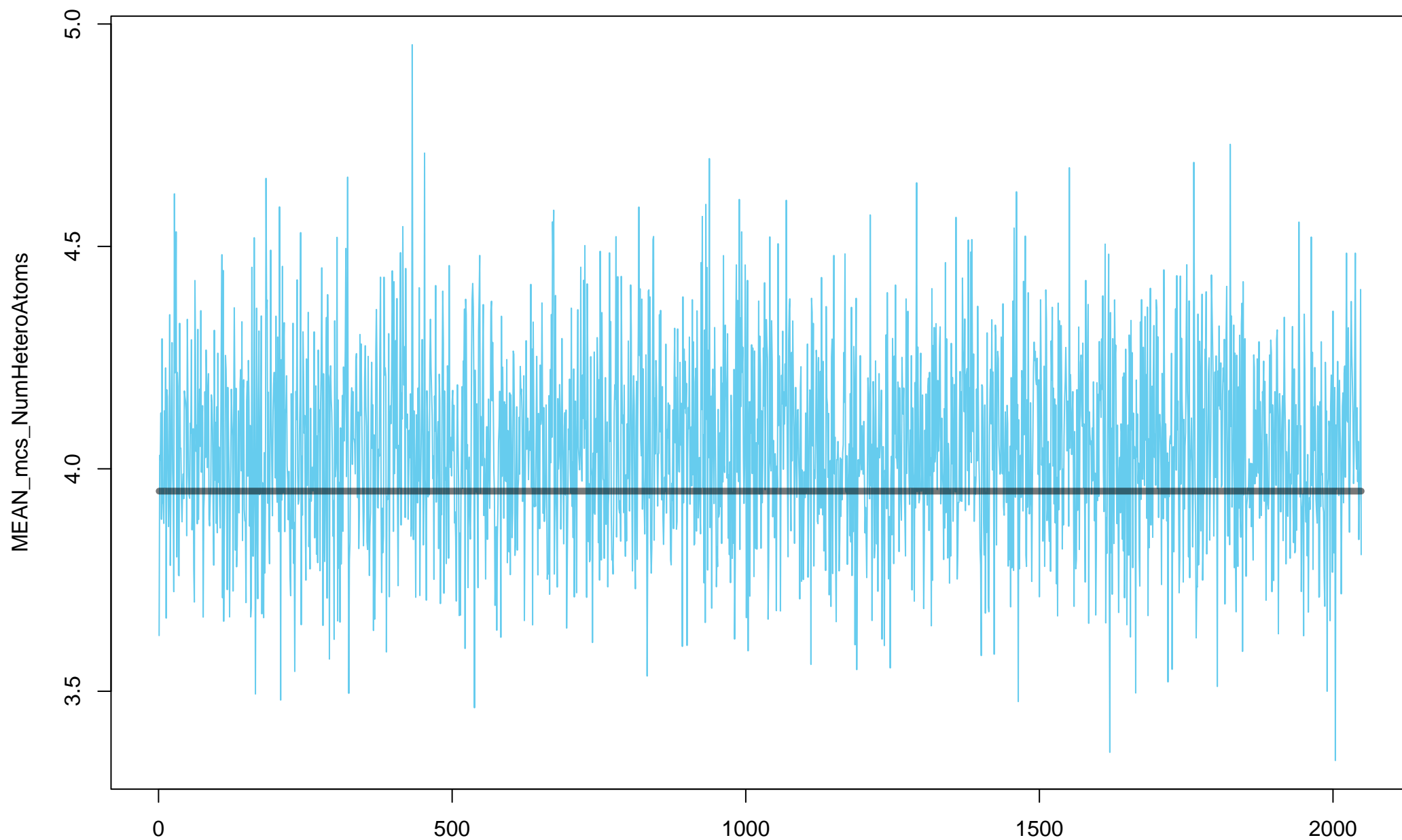
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 1.9 | stat: TRUE | burn: 0 | rel.err: -0.548



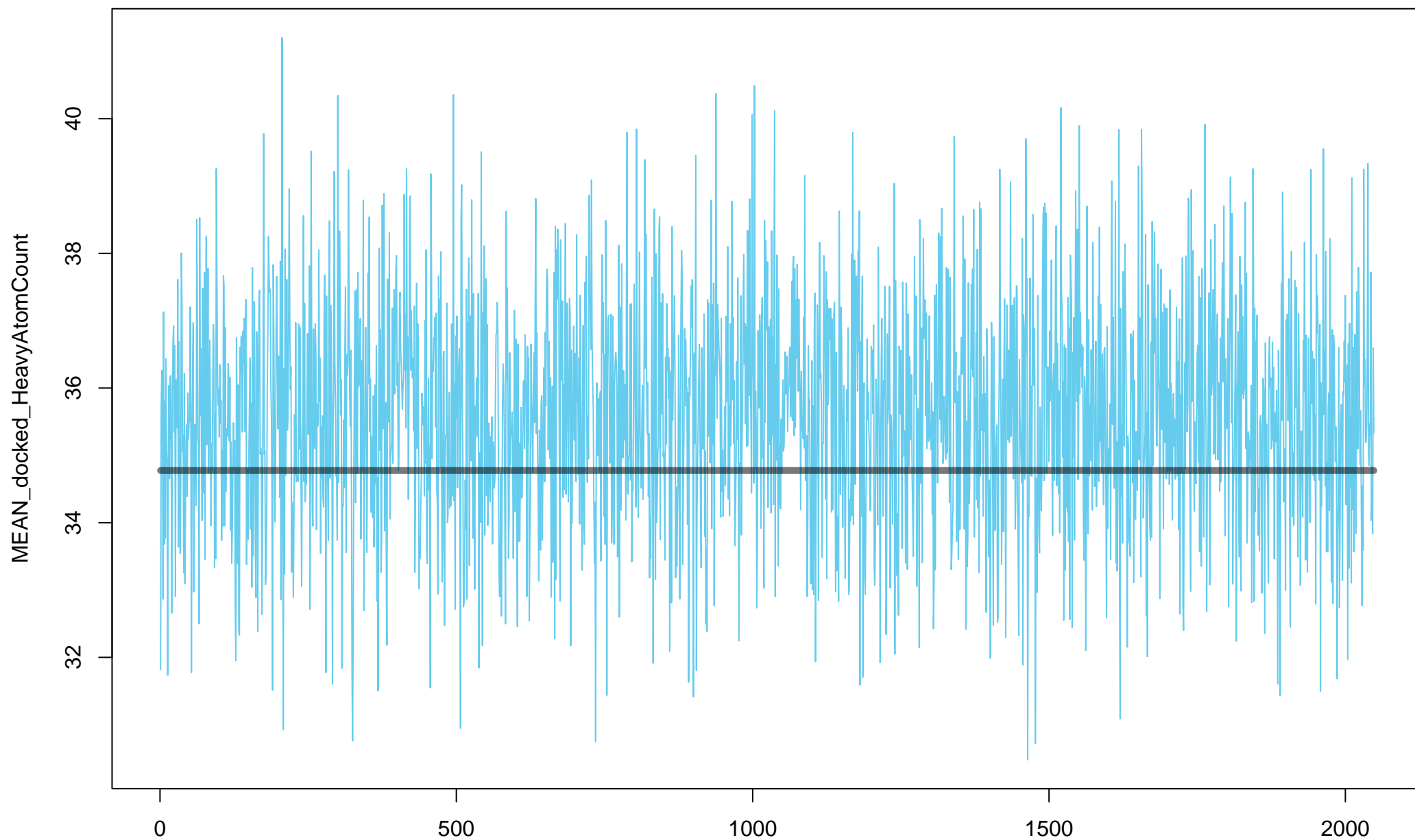
MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0359 | MCSE(6.27) = 2.1 | stat: FALSE | burn: 0 | rel.err: -0.231



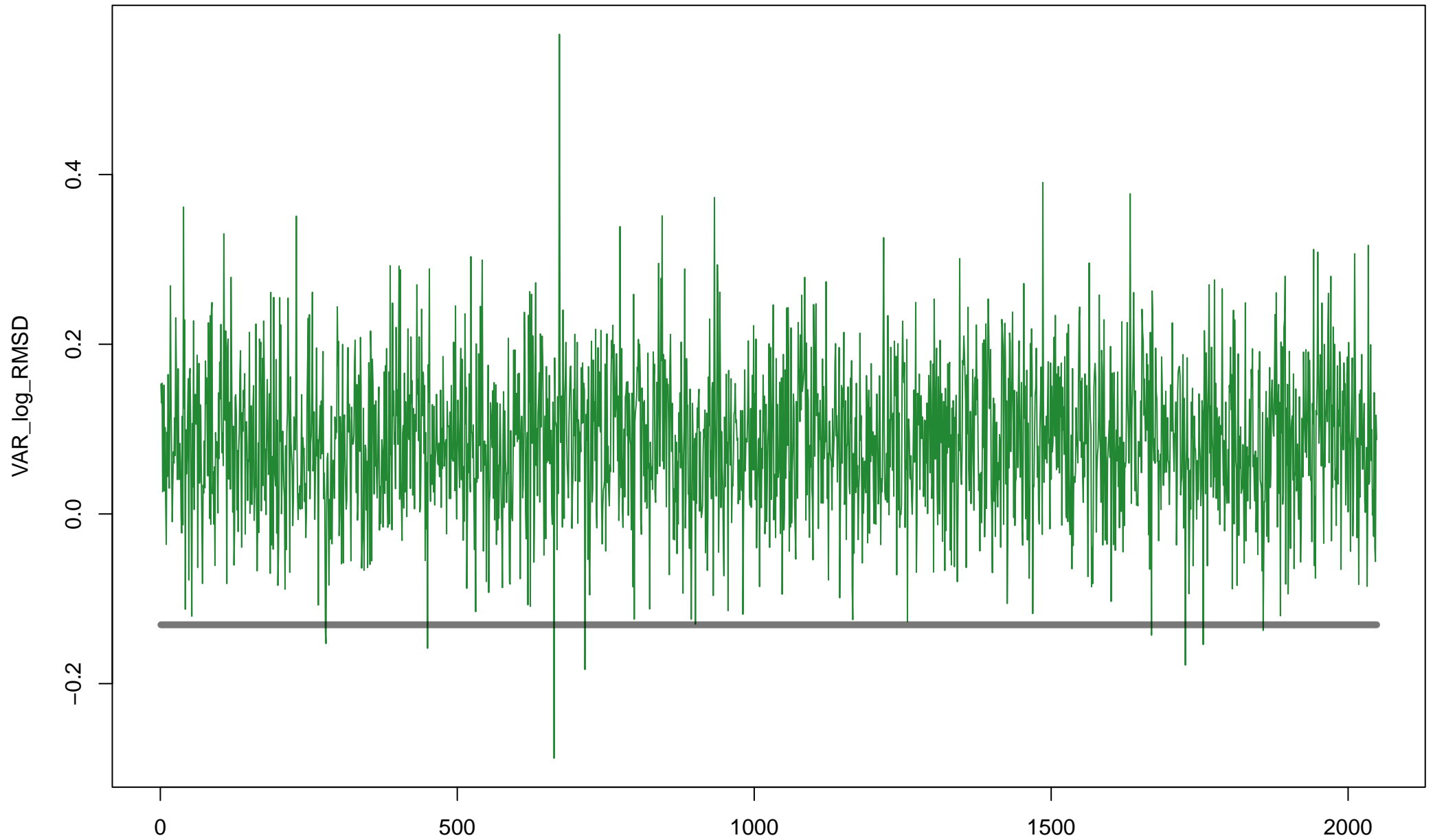
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0466 | MCSE(6.27) = 2 | stat: TRUE | burn: 0 | rel.err: 0.48



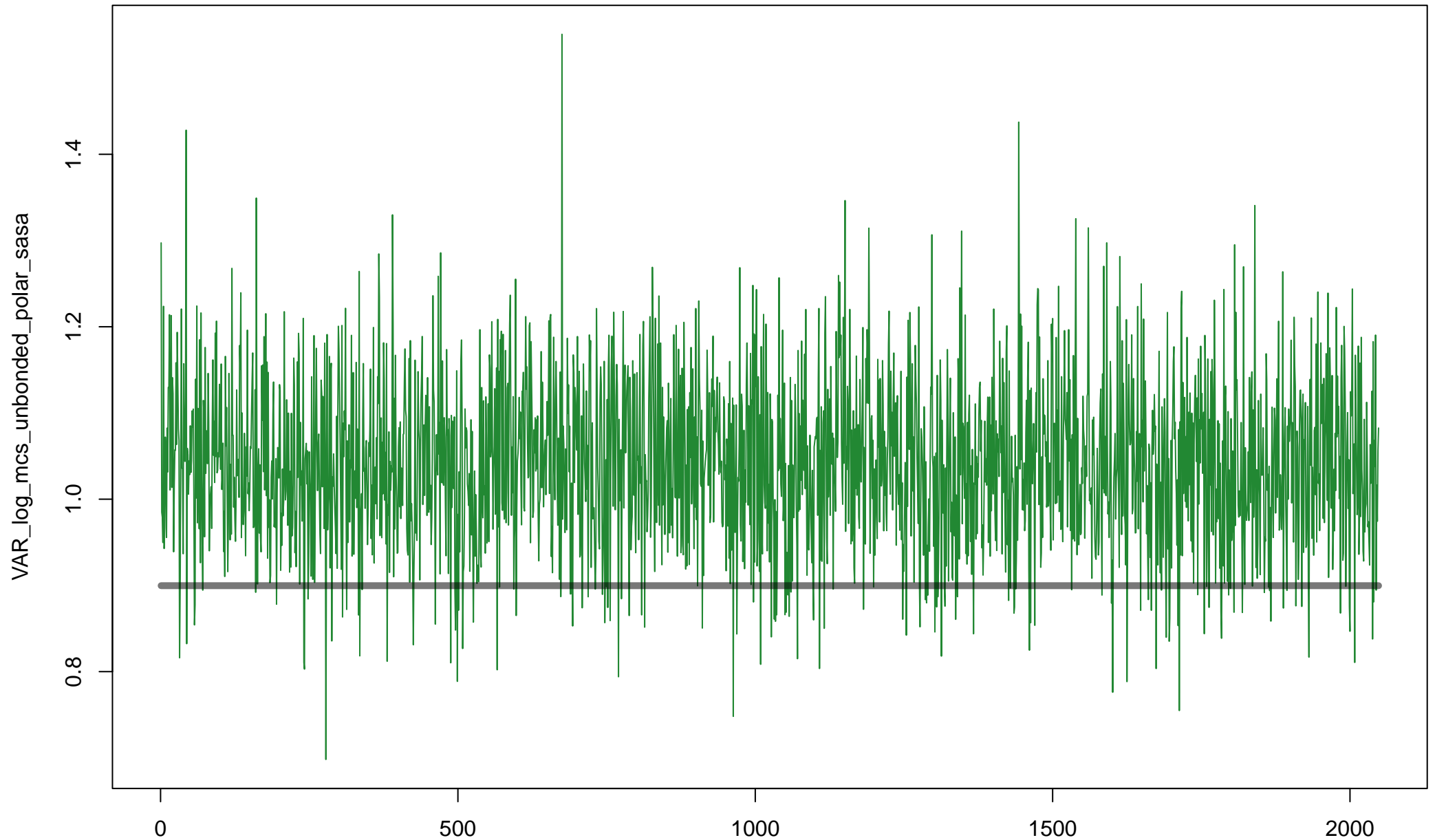
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0294 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | rel.err: 0.499



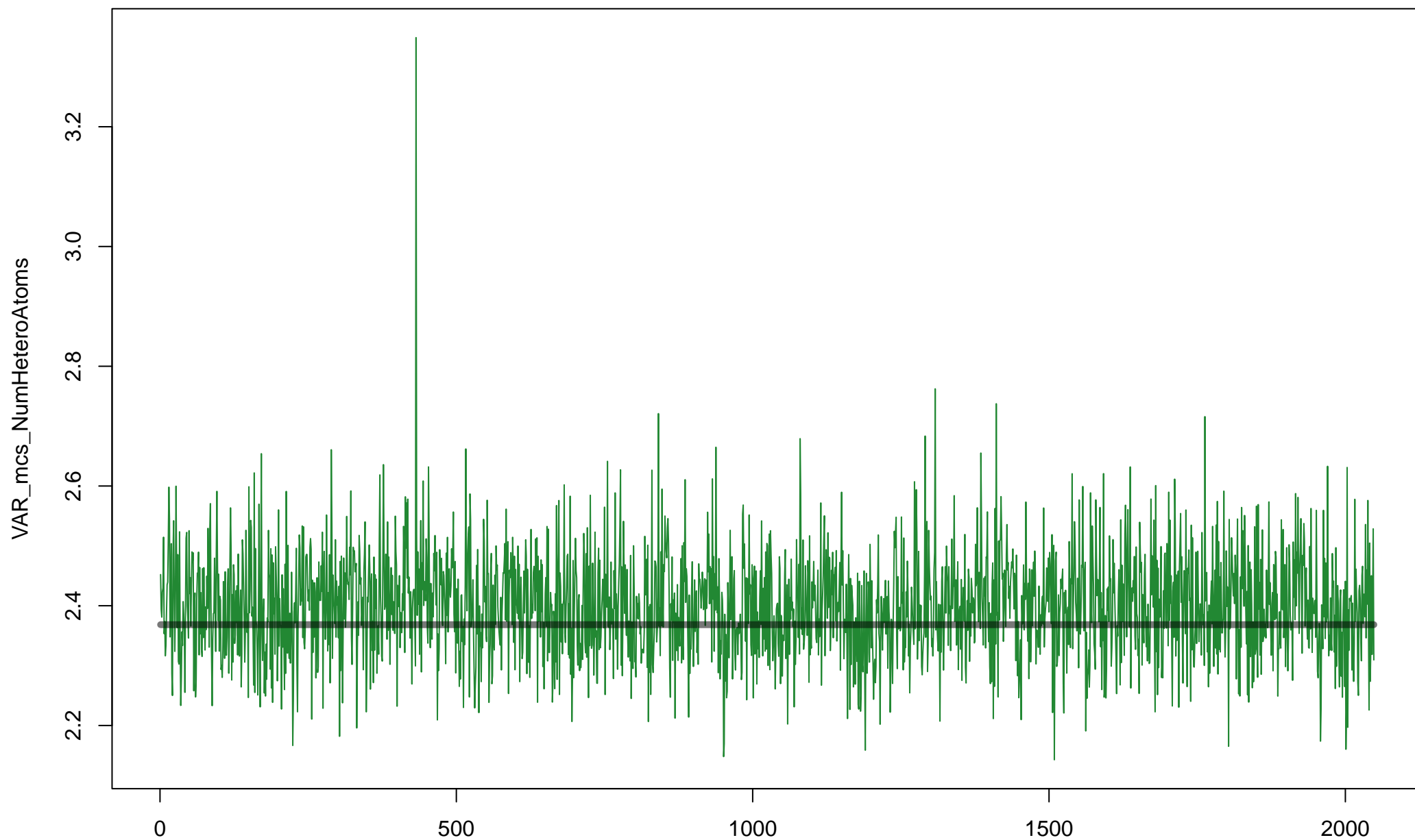
VAR_log_RMSD
ESS = 1910 | BMK = 0.0479 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0 | rel.err: 2.3



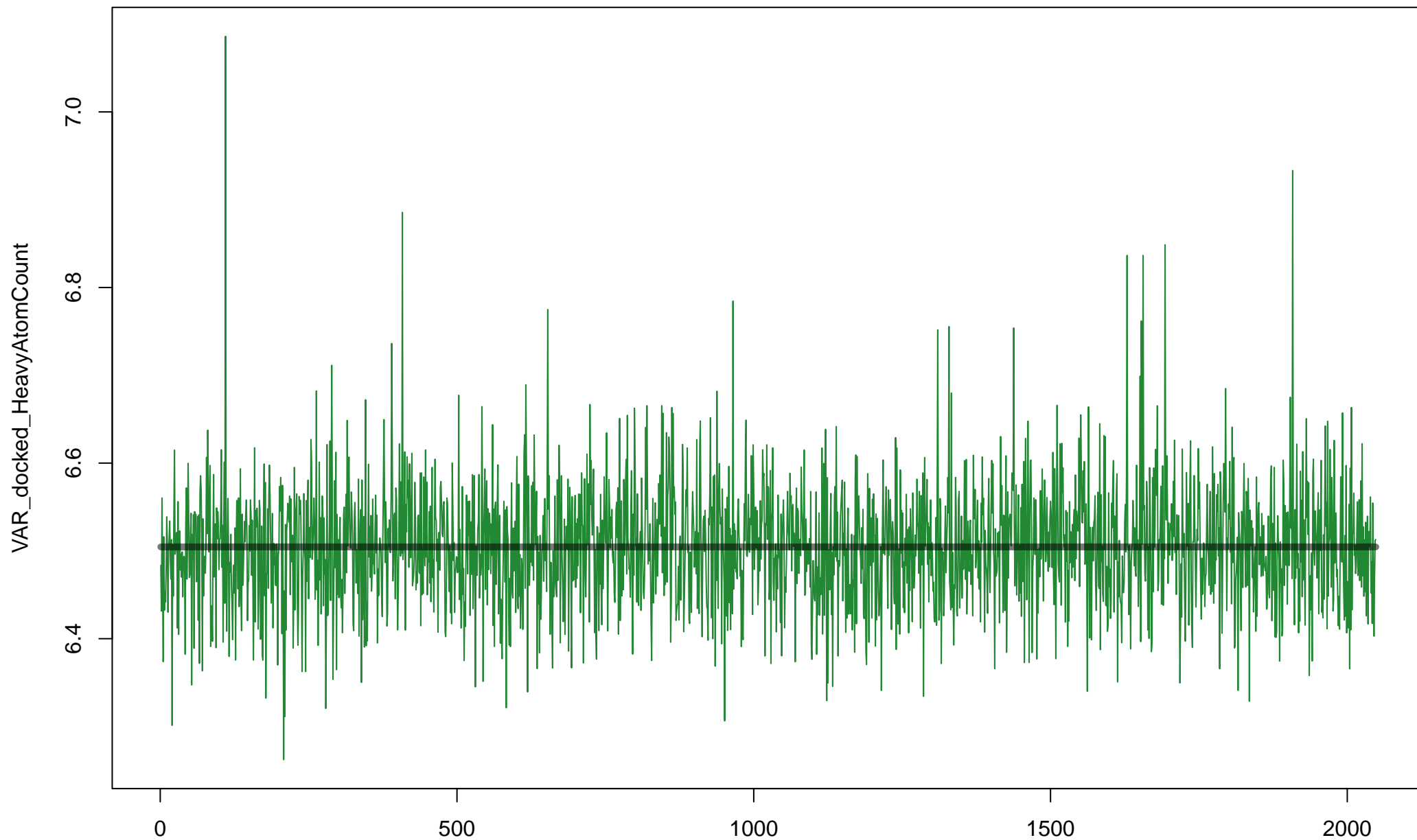
VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0563 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | rel.err: 1.38



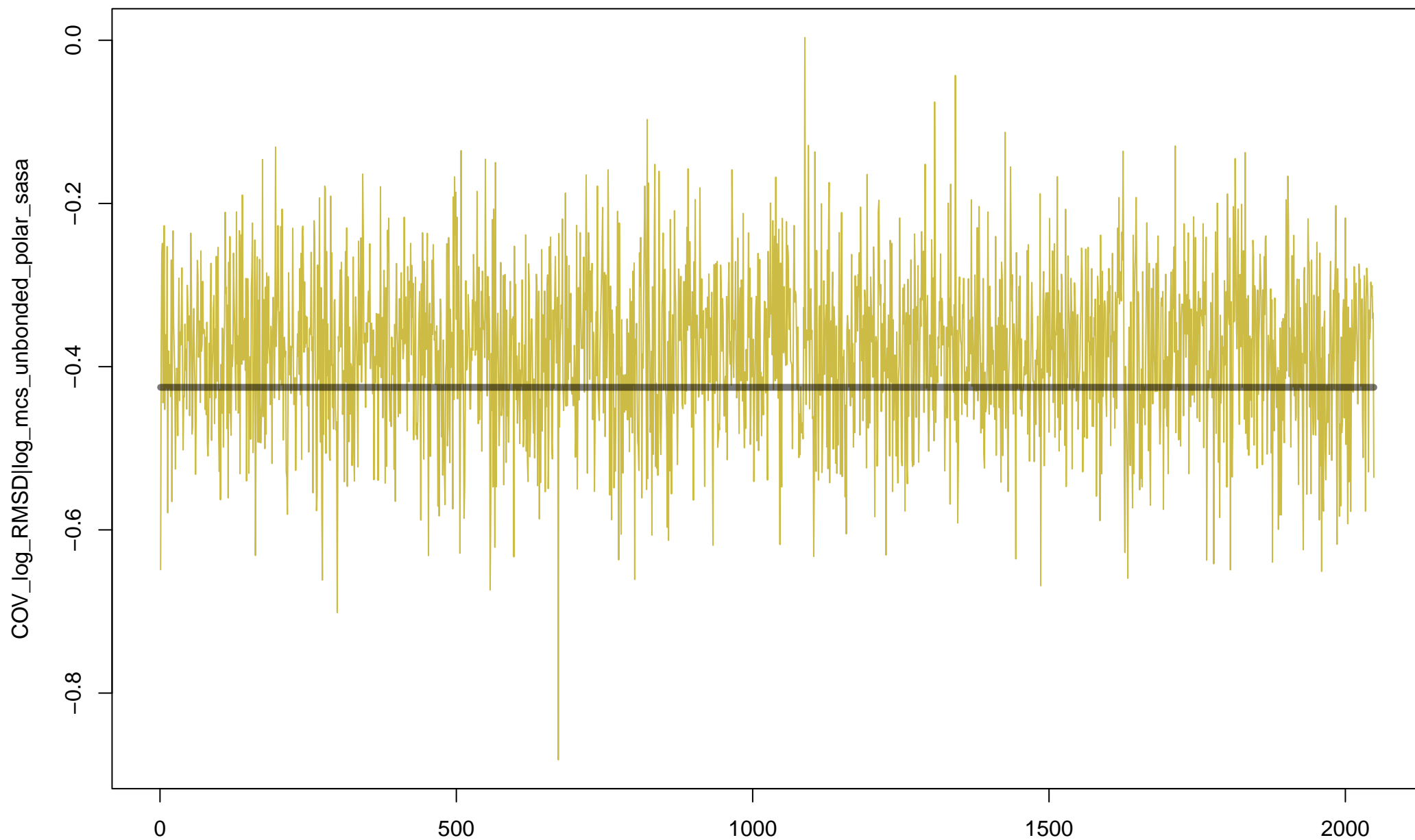
VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0463 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | rel.err: 0.374



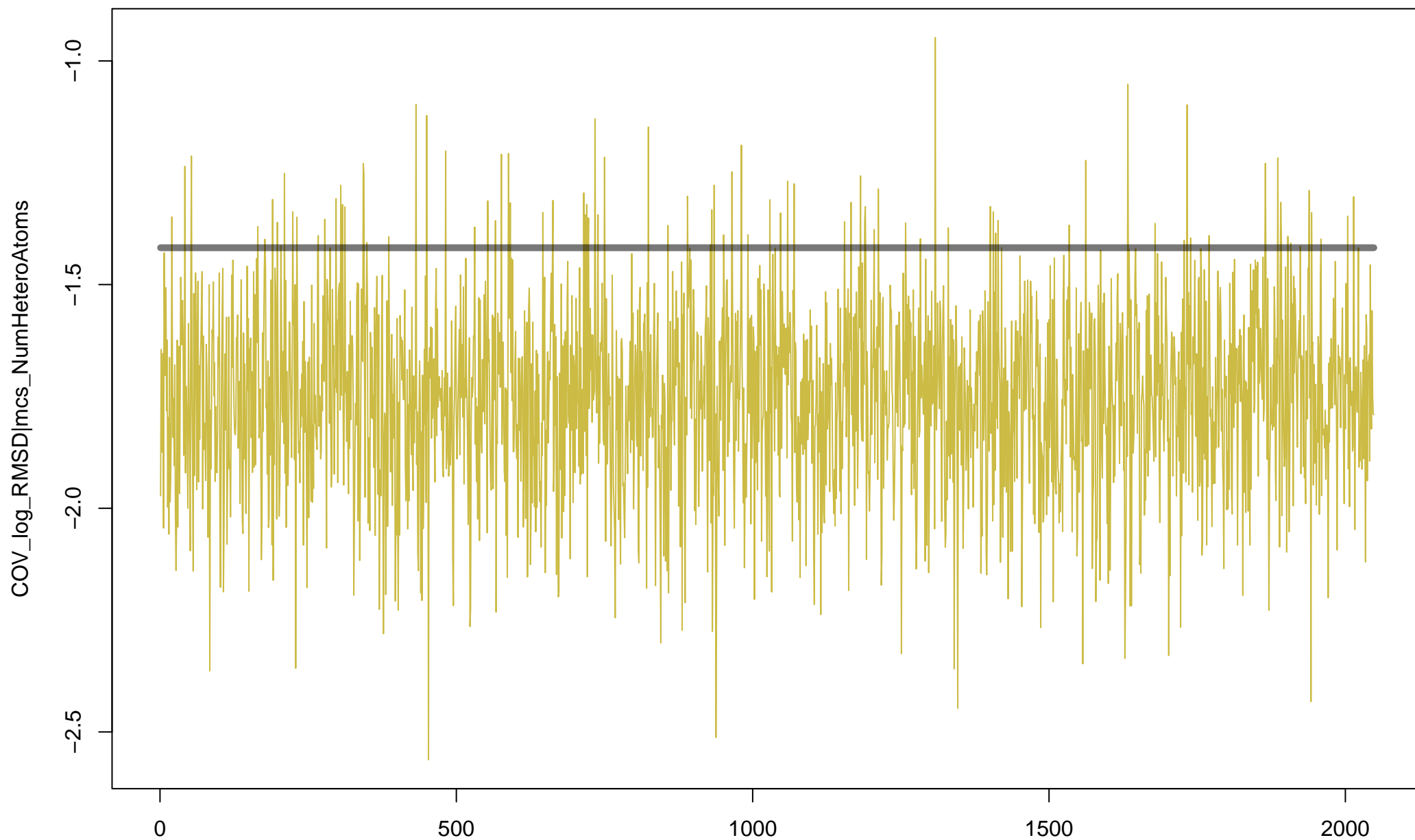
VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.069 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | rel.err: 0.0489



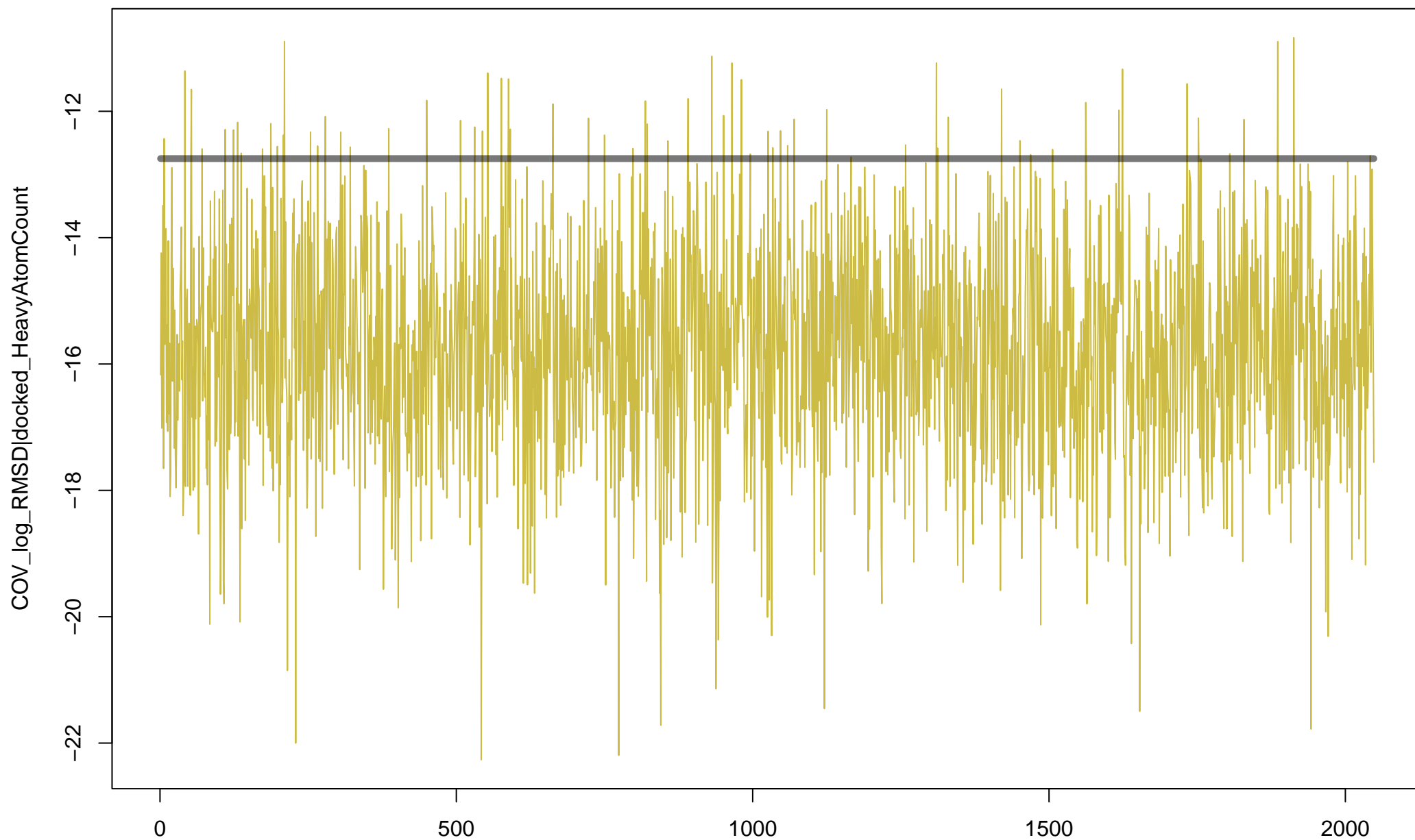
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0465 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0 | rel.err: 0.453



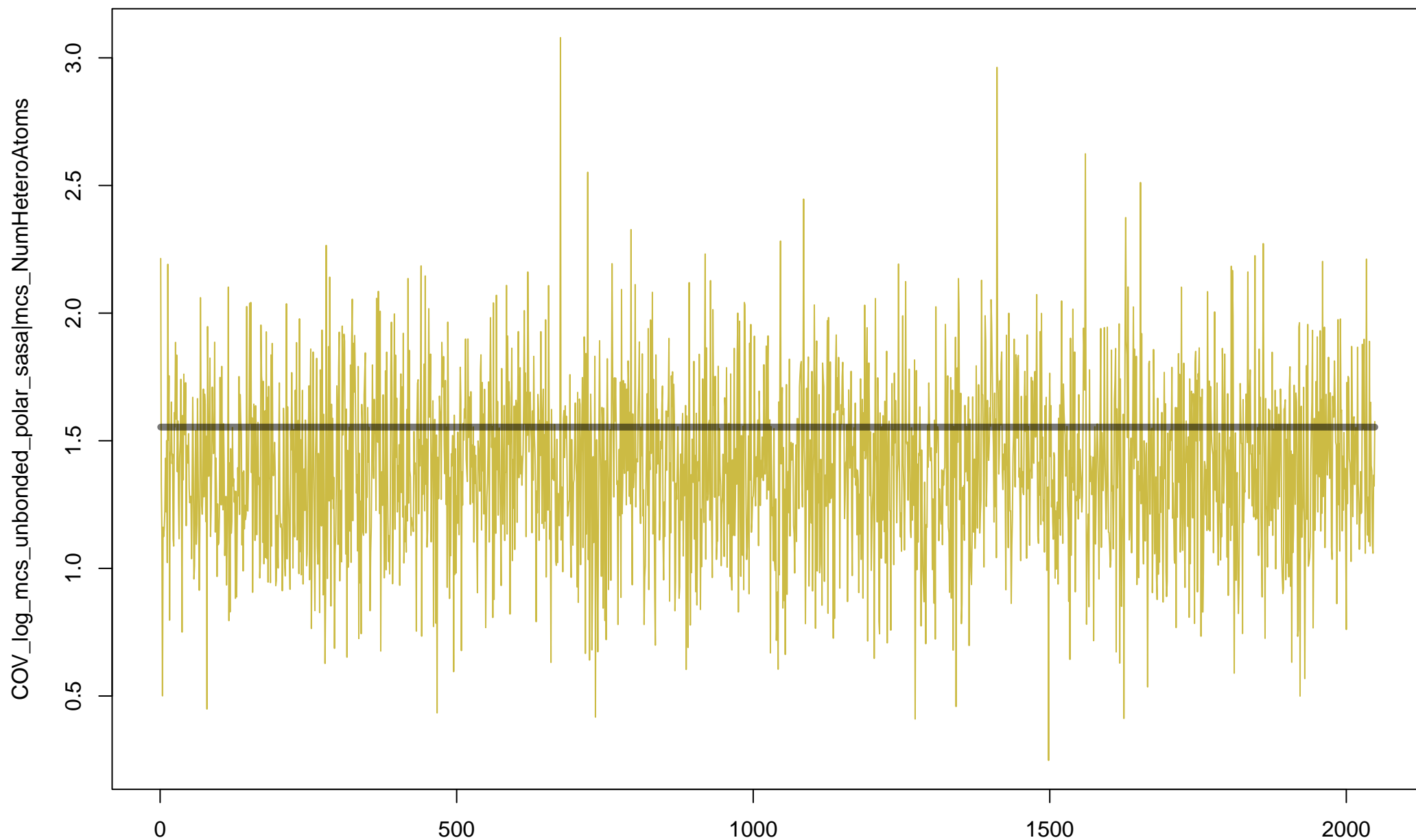
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1760 | BMK = 0.0507 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | rel.err: -1.64



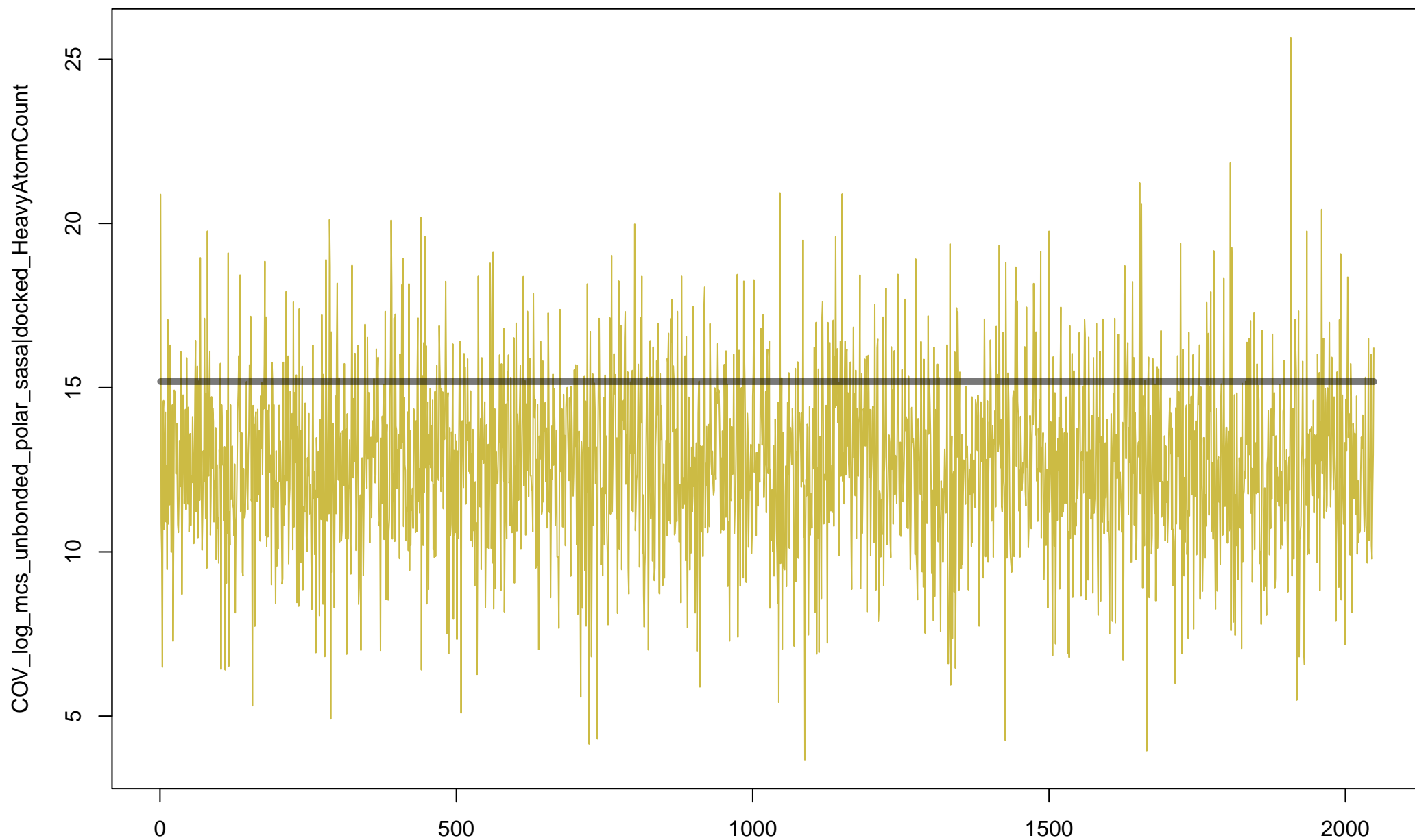
COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0362 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0 | rel.err: -1.82



COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.03 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: -0.472



COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0434 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | rel.err: -0.941



COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0501 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | rel.err: 0.508

