

-- STATS maxD --

min ESS = 150.72830372962

max BMK = 0.121974207818285

max MCSE = 6.3636927648822

all stationary: FALSE

burn: 0

max rel.err.: 2.02805057894253

-- STATS 1D --

min ESS = 2891.60839920263

max BMK = 0.0471694665376879

max MCSE = 1.92560215858908

all stationary: FALSE

burn: 0

max rel.err.: 2.37649752198555

-- STATS 2D --

min ESS = 3590.35841527093

max BMK = 0.0471908875138518

max MCSE = 1.82772960271314

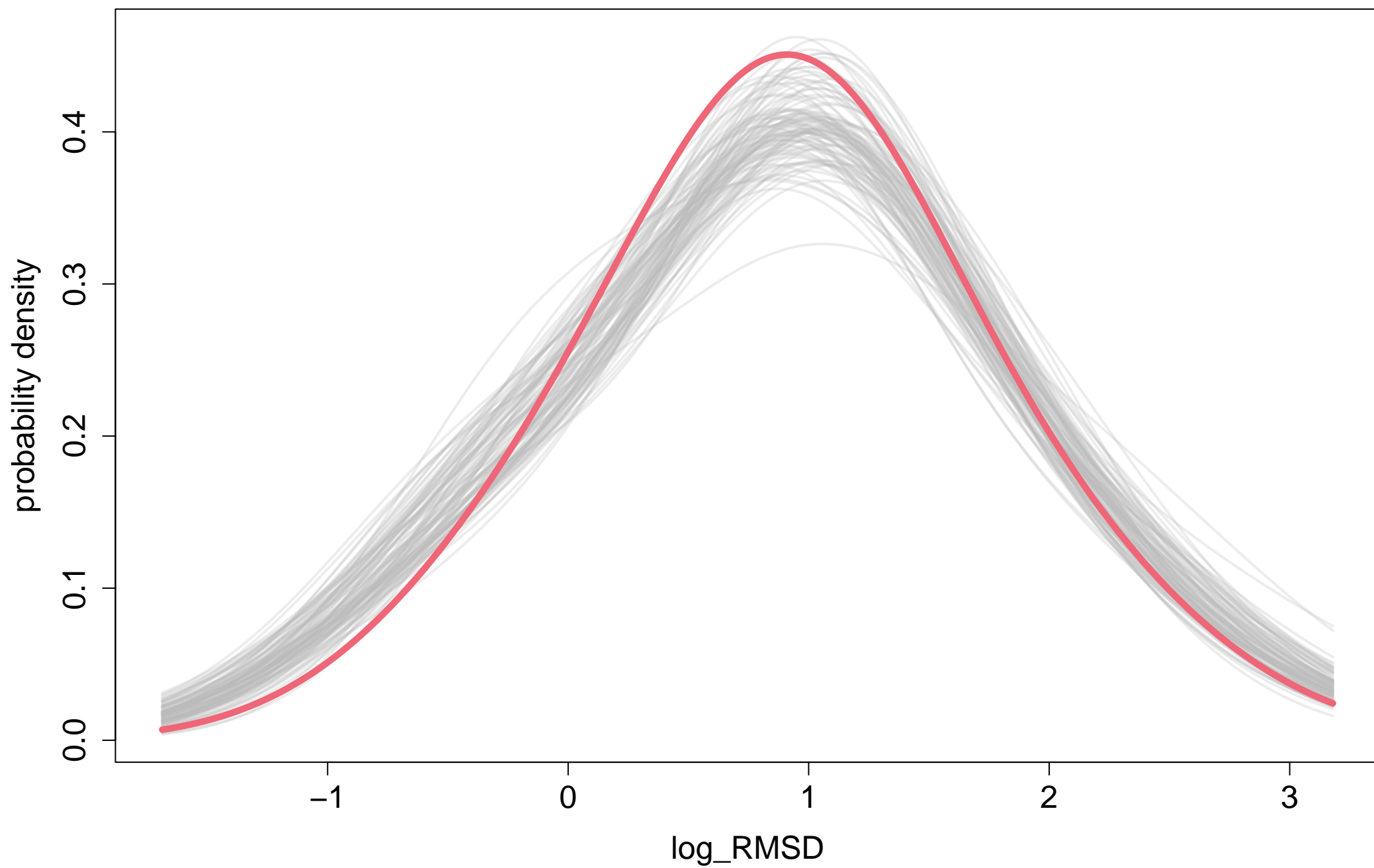
all stationary: TRUE

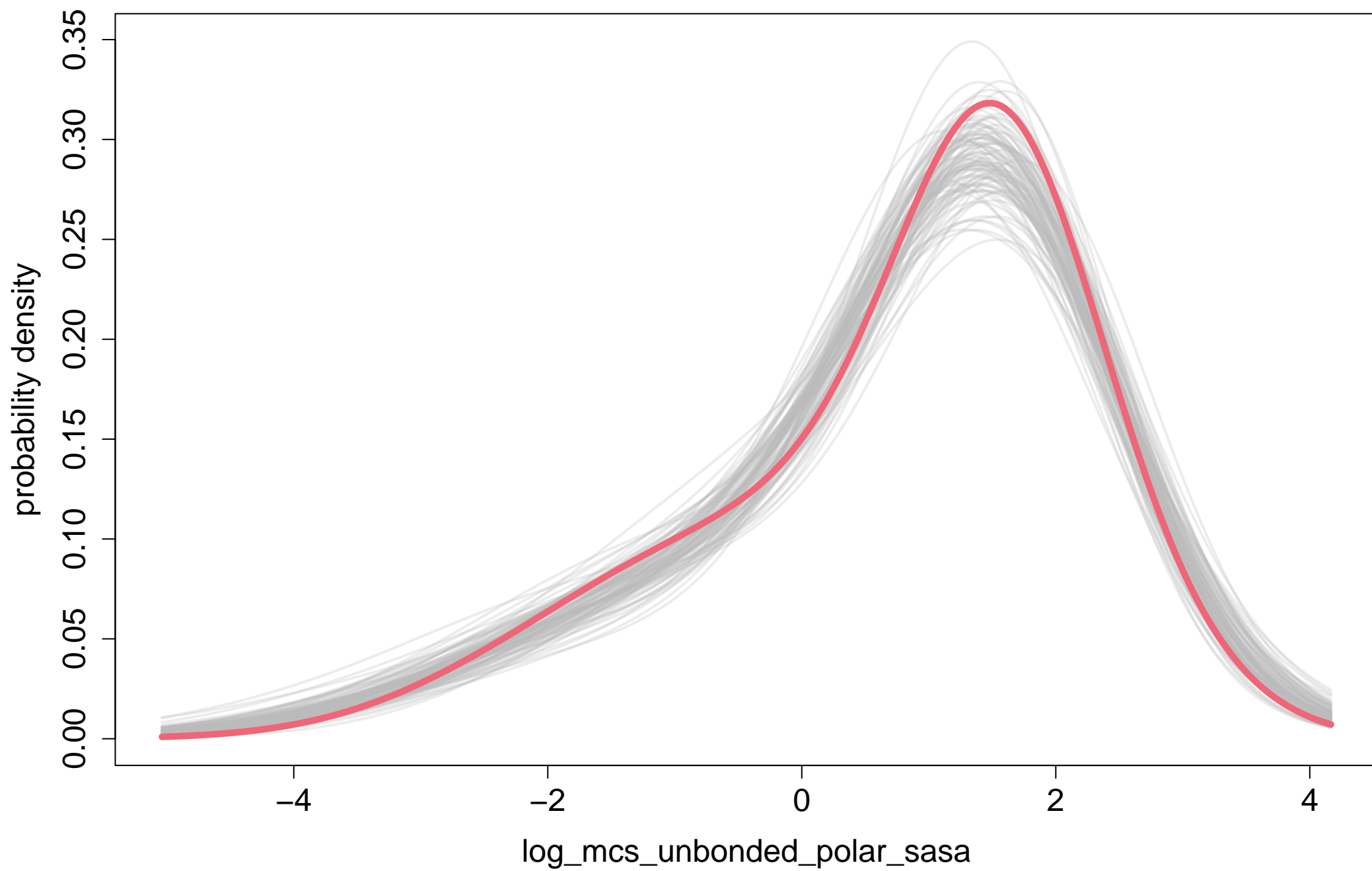
burn: 0

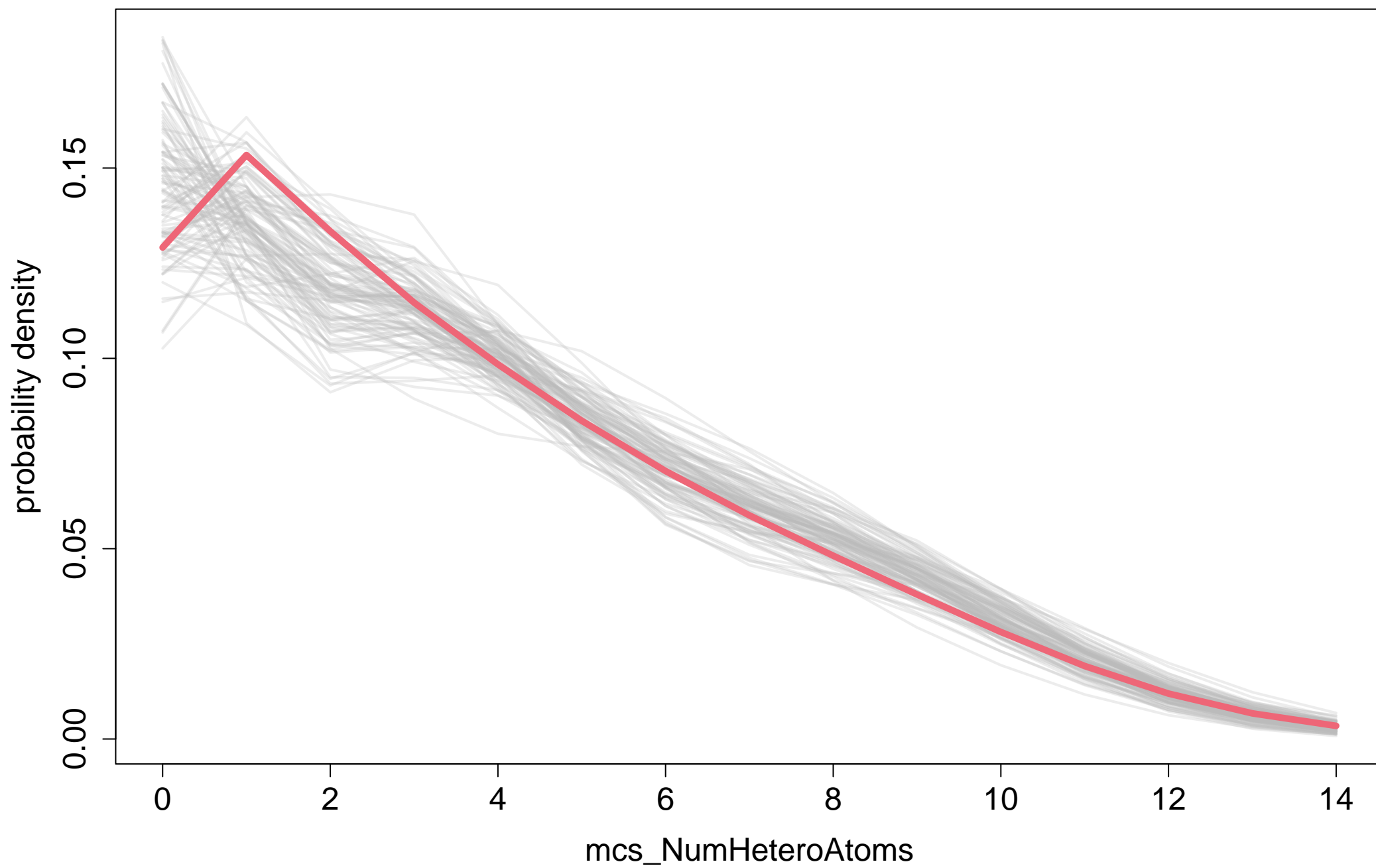
max rel.err.: 1.82258592492123

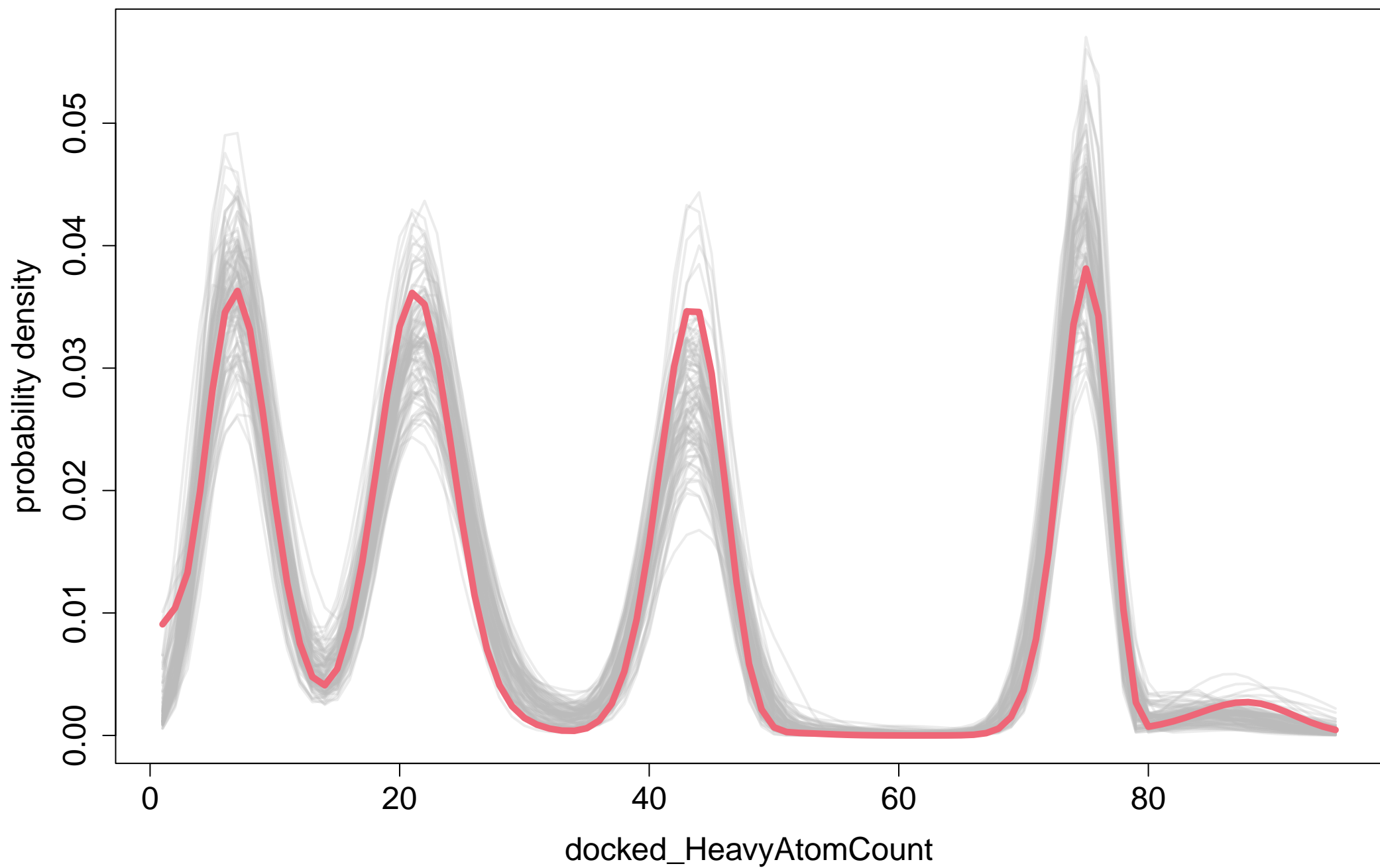
Occupied clusters: 10 of 16

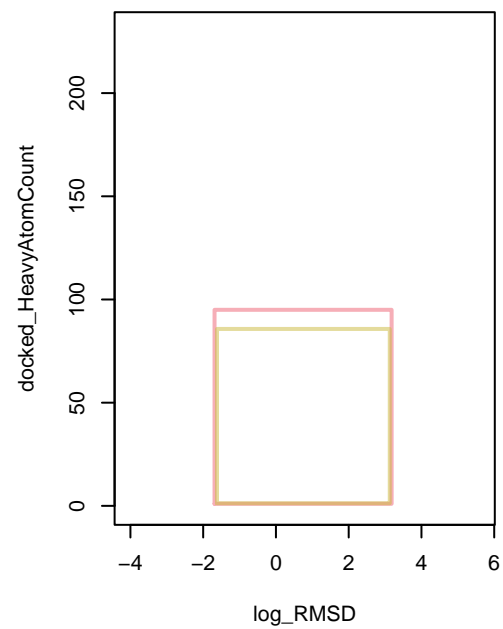
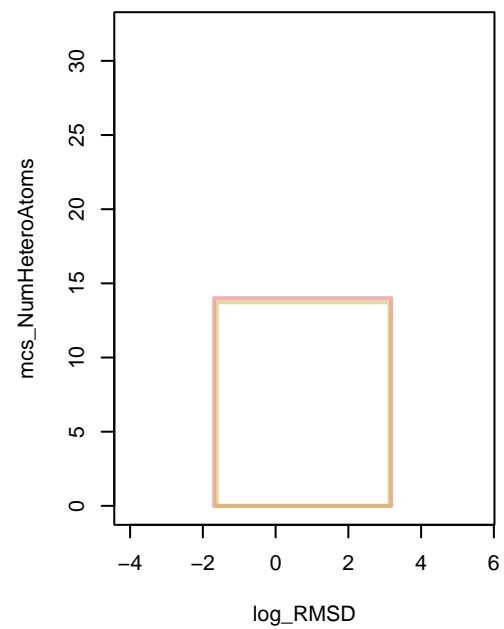
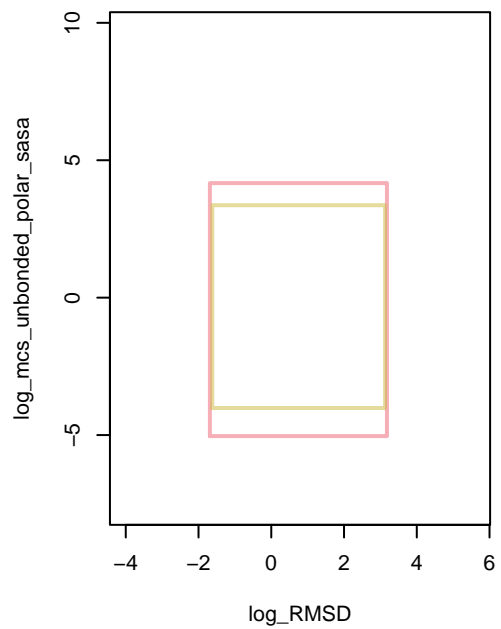
LL: -2160 +- 6.66



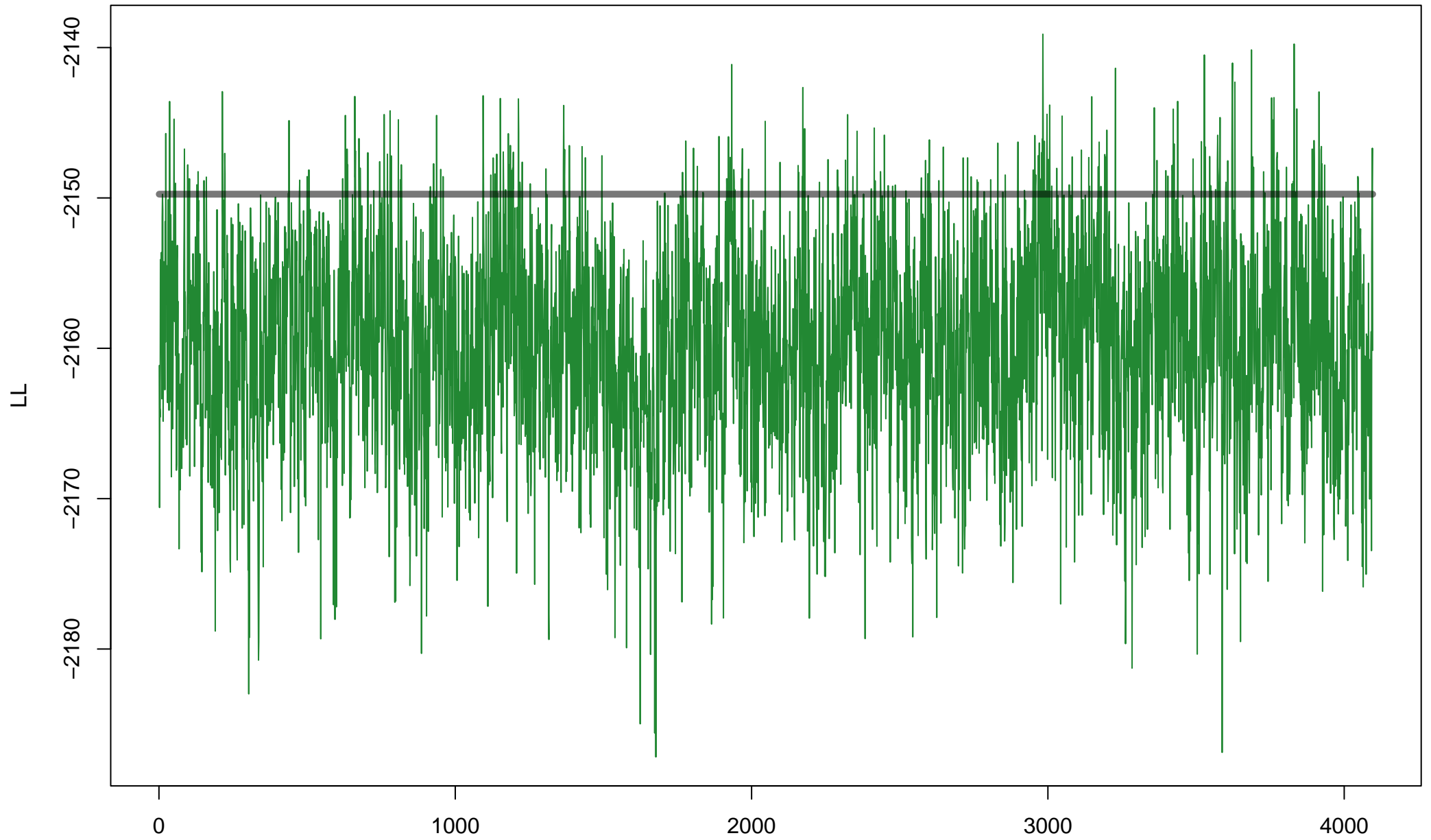




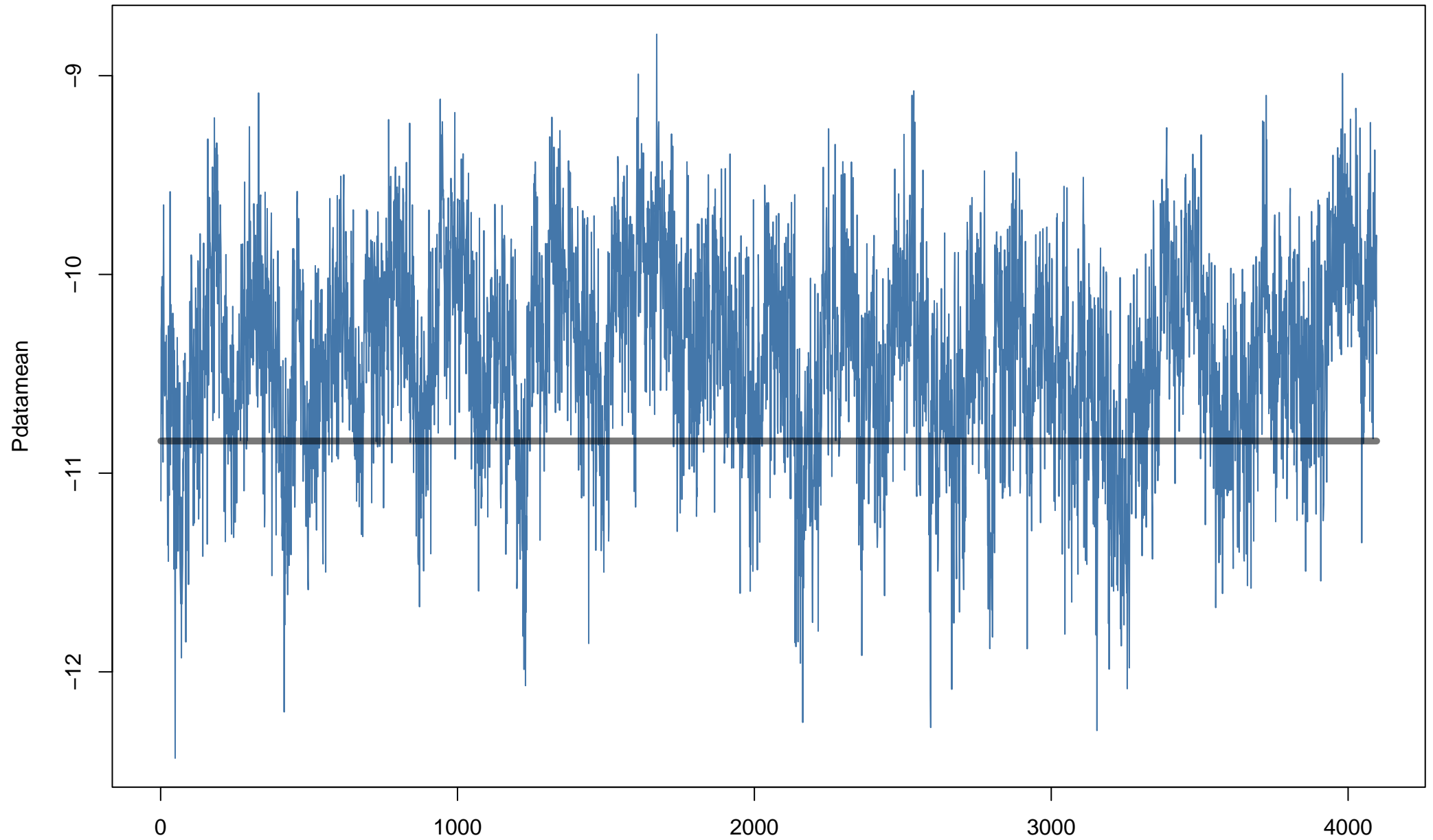




LL

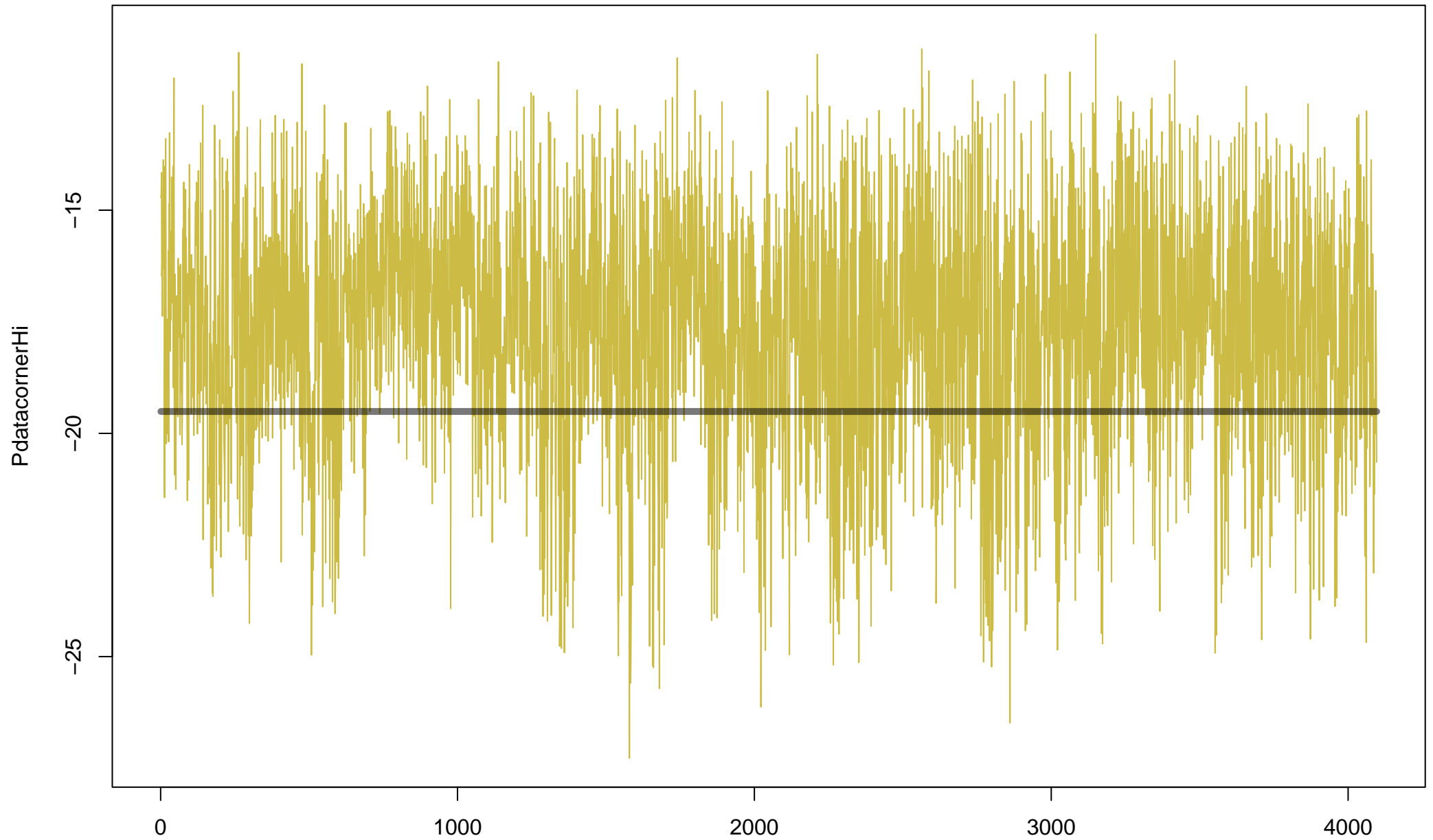


Pdatamean
ESS = 151 | BMK = 0.0766 | MCSE(6.27) = 6.36 | stat: TRUE | burn: 0 | rel.err: 0.852



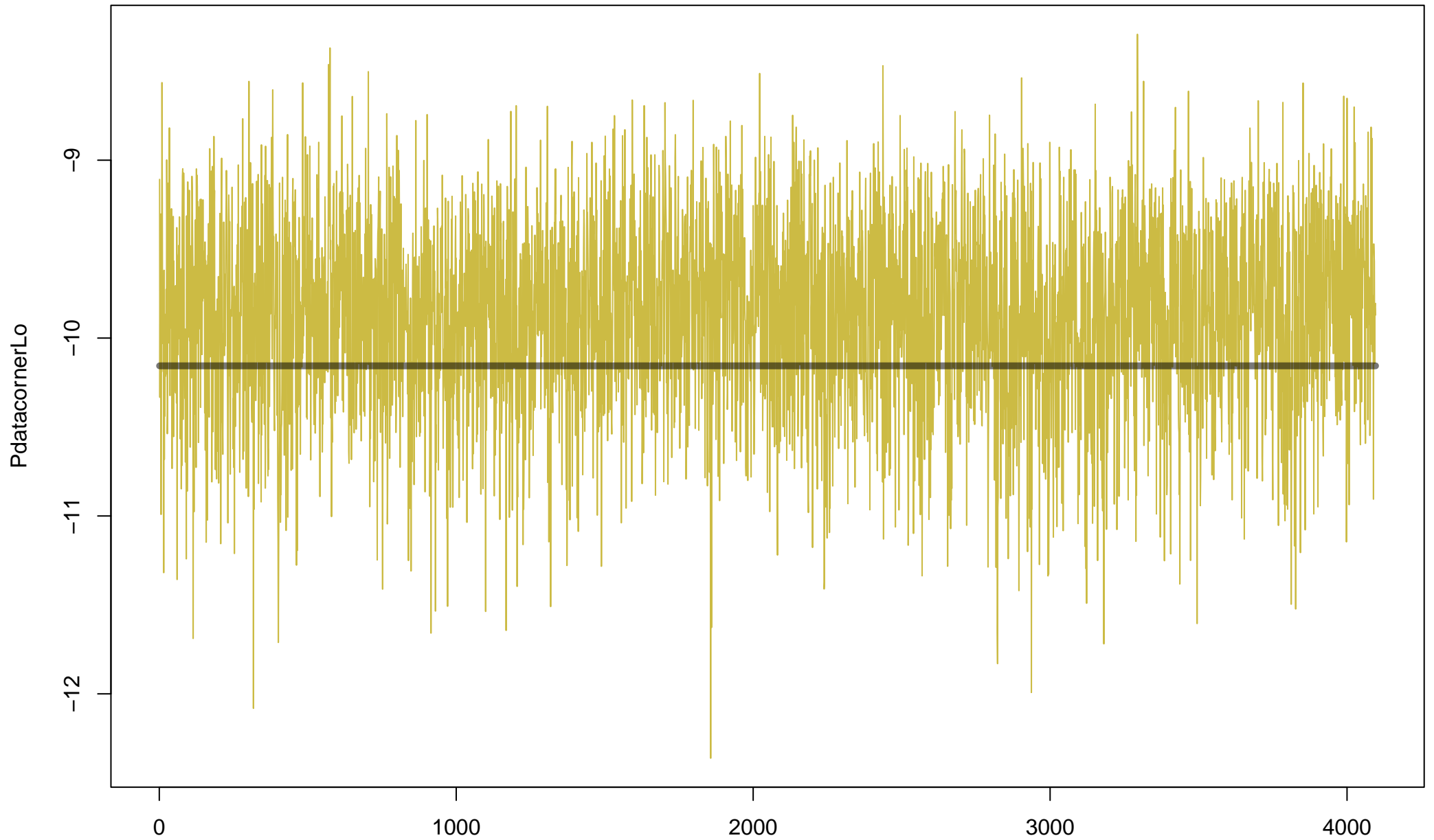
PdatacornerHi

ESS = 4100 | BMK = 0.122 | MCSE(6.27) = 1.53 | stat: TRUE | burn: 0 | rel.err: 0.304

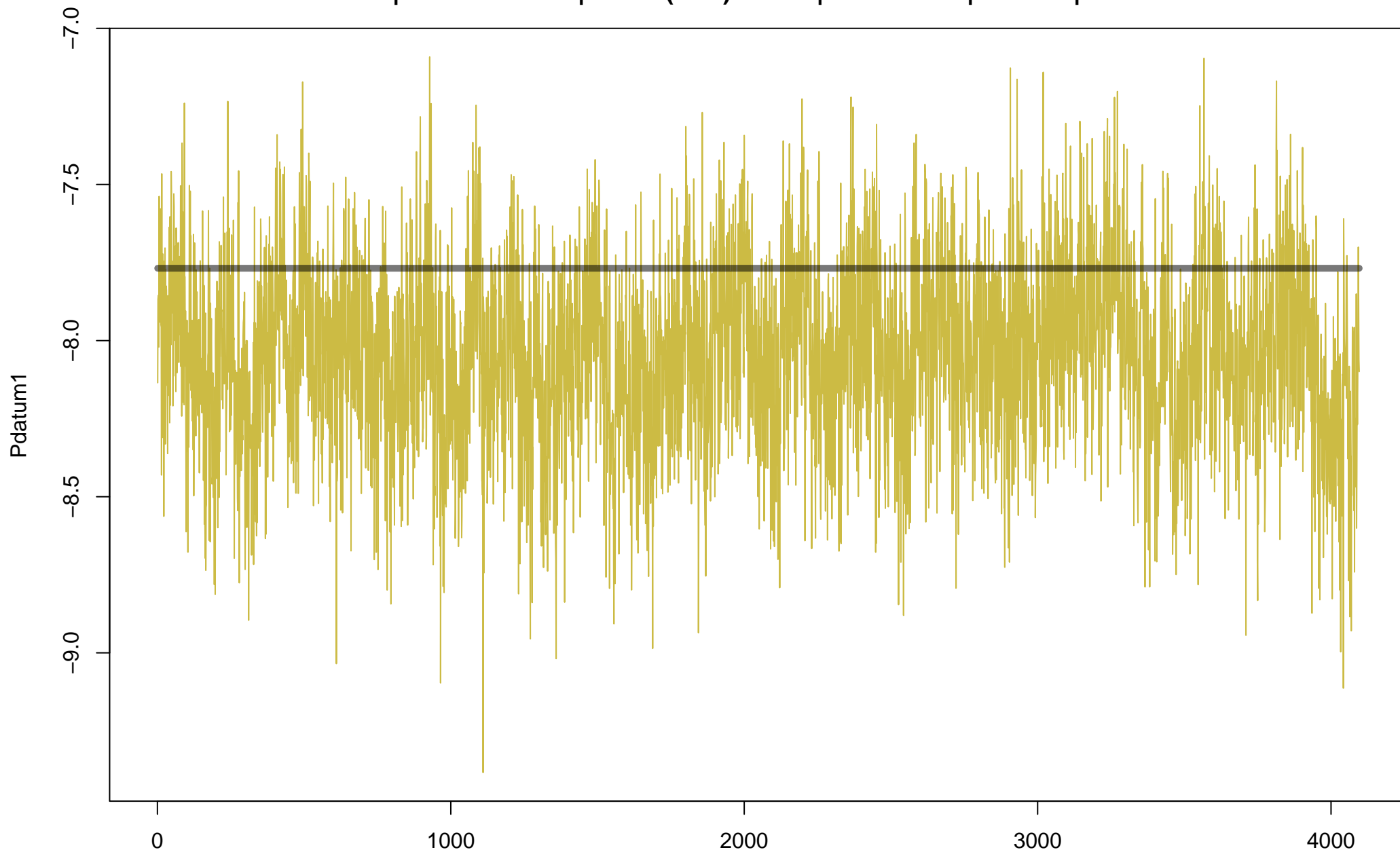


PdatacornerLo

ESS = 2840 | BMK = 0.0316 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0 | rel.err: 0.657

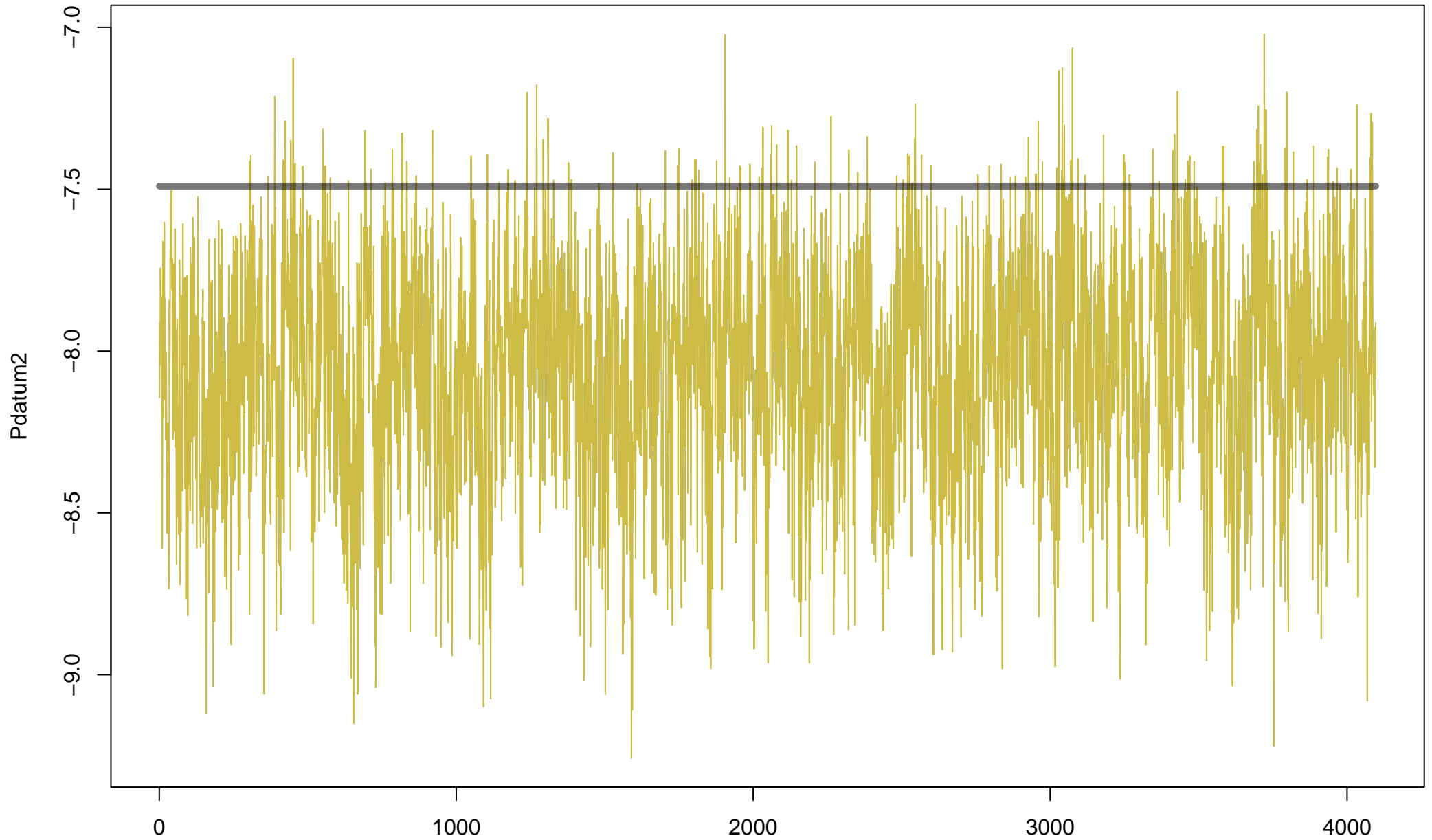


Pdatum1
ESS = 406 | BMK = 0.0473 | MCSE(6.27) = 4.25 | stat: TRUE | burn: 0 | rel.err: -0.873



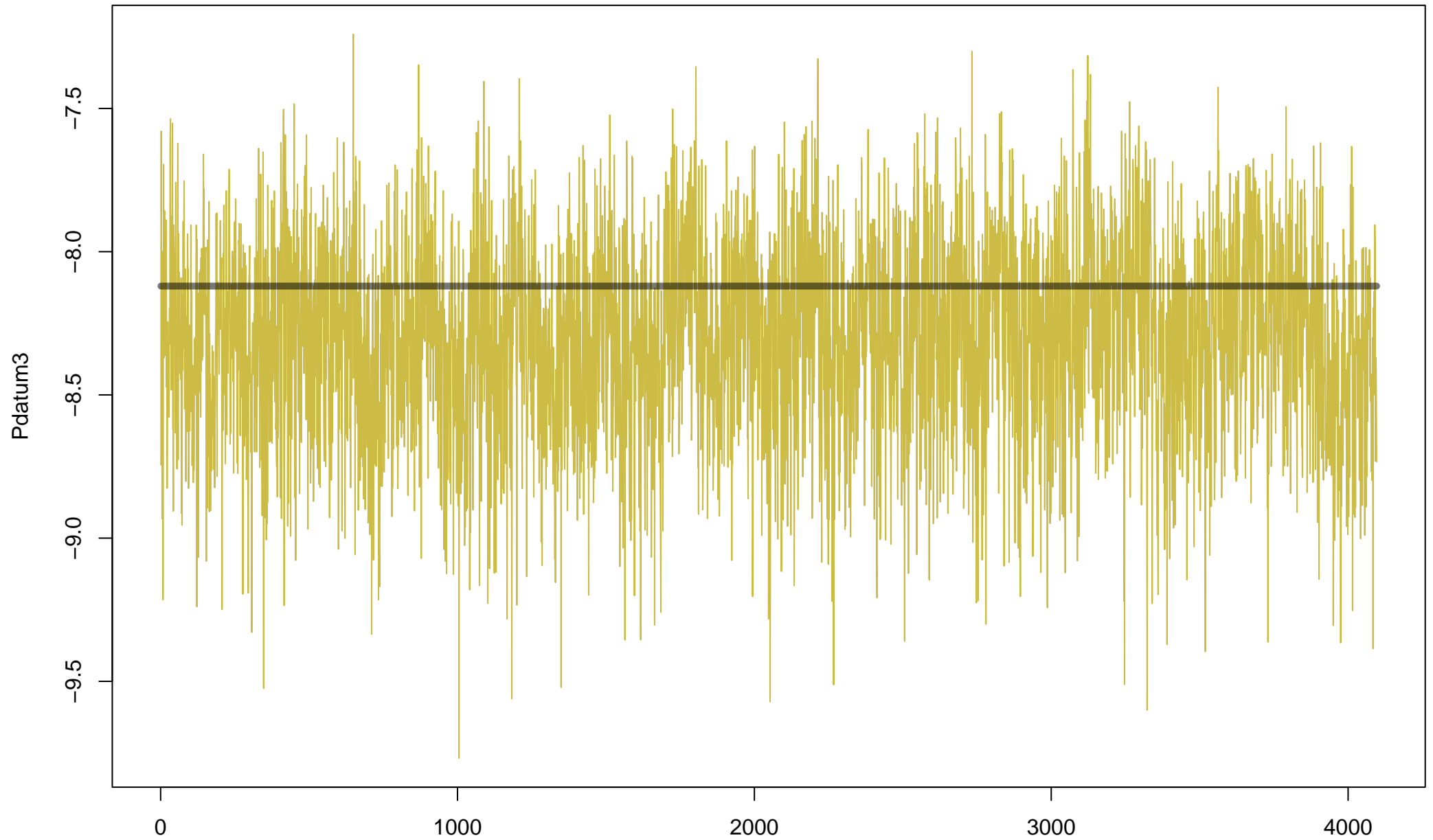
Pdatum2

ESS = 819 | BMK = 0.0436 | MCSE(6.27) = 3.66 | stat: FALSE | burn: 0 | rel.err: -2.03



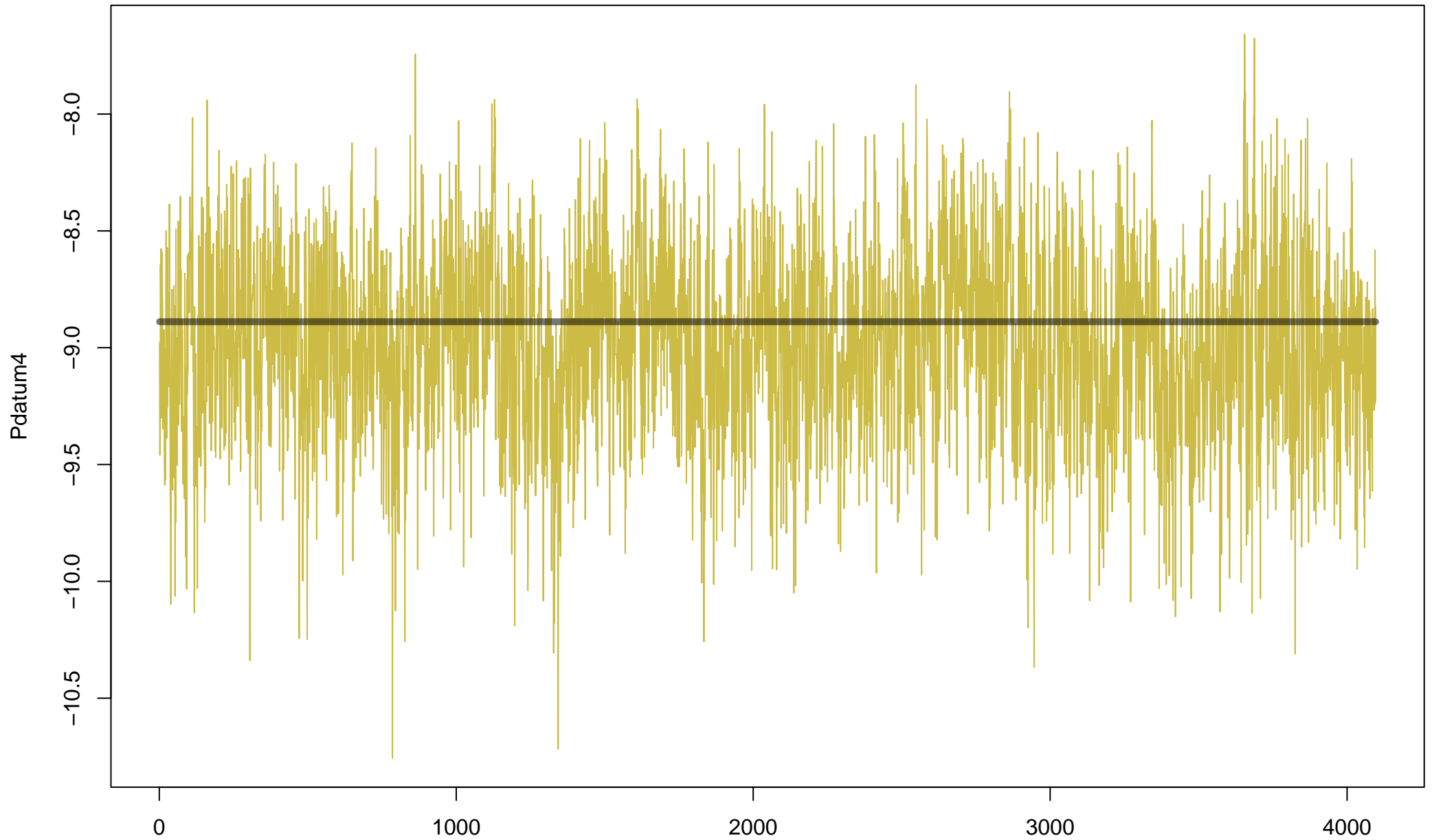
Pdatum3

ESS = 676 | BMK = 0.0406 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | rel.err: -0.386

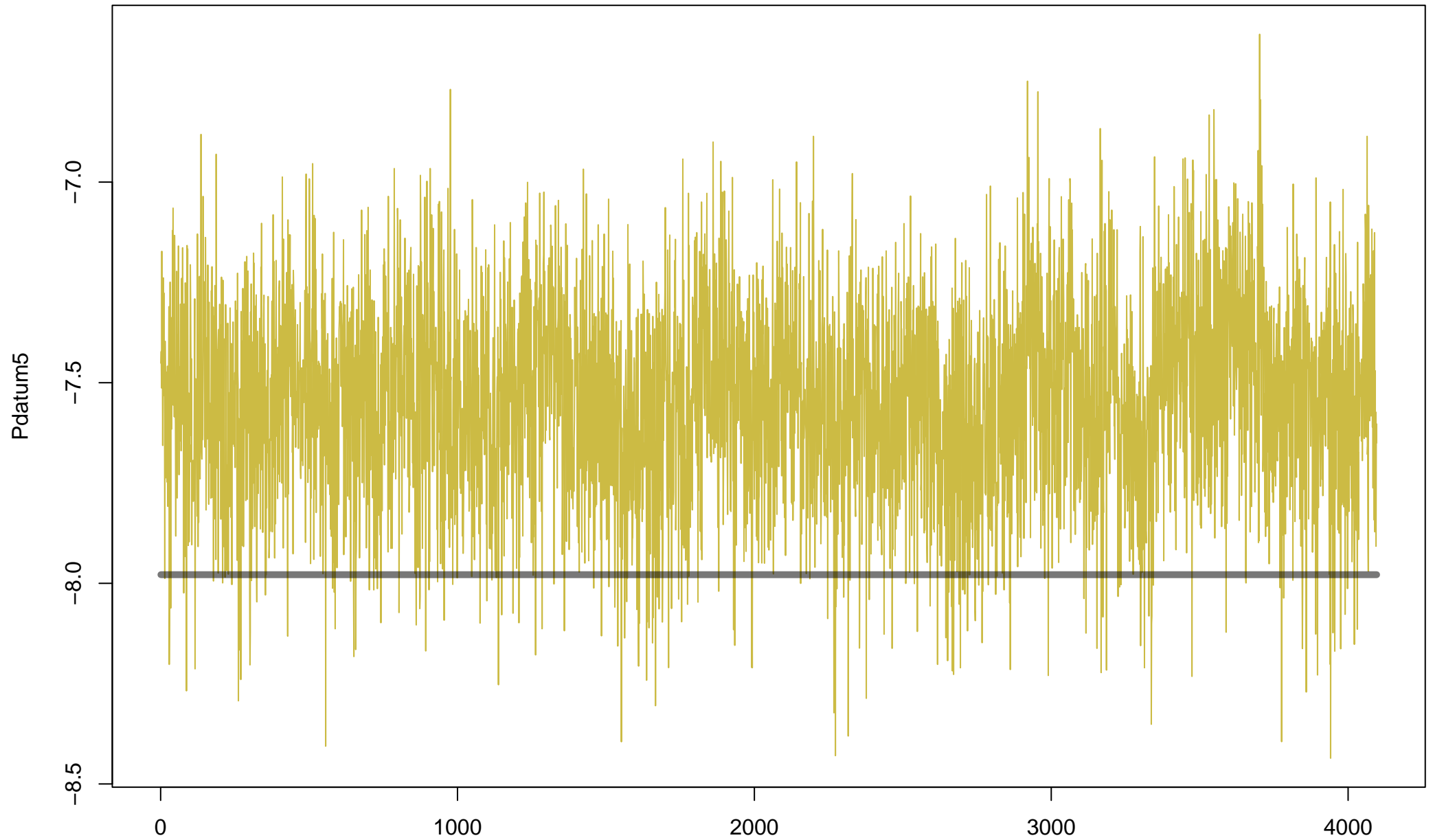


Pdatum4

ESS = 1010 | BMK = 0.0415 | MCSE(6.27) = 3.69 | stat: TRUE | burn: 0 | rel.err: -0.0579

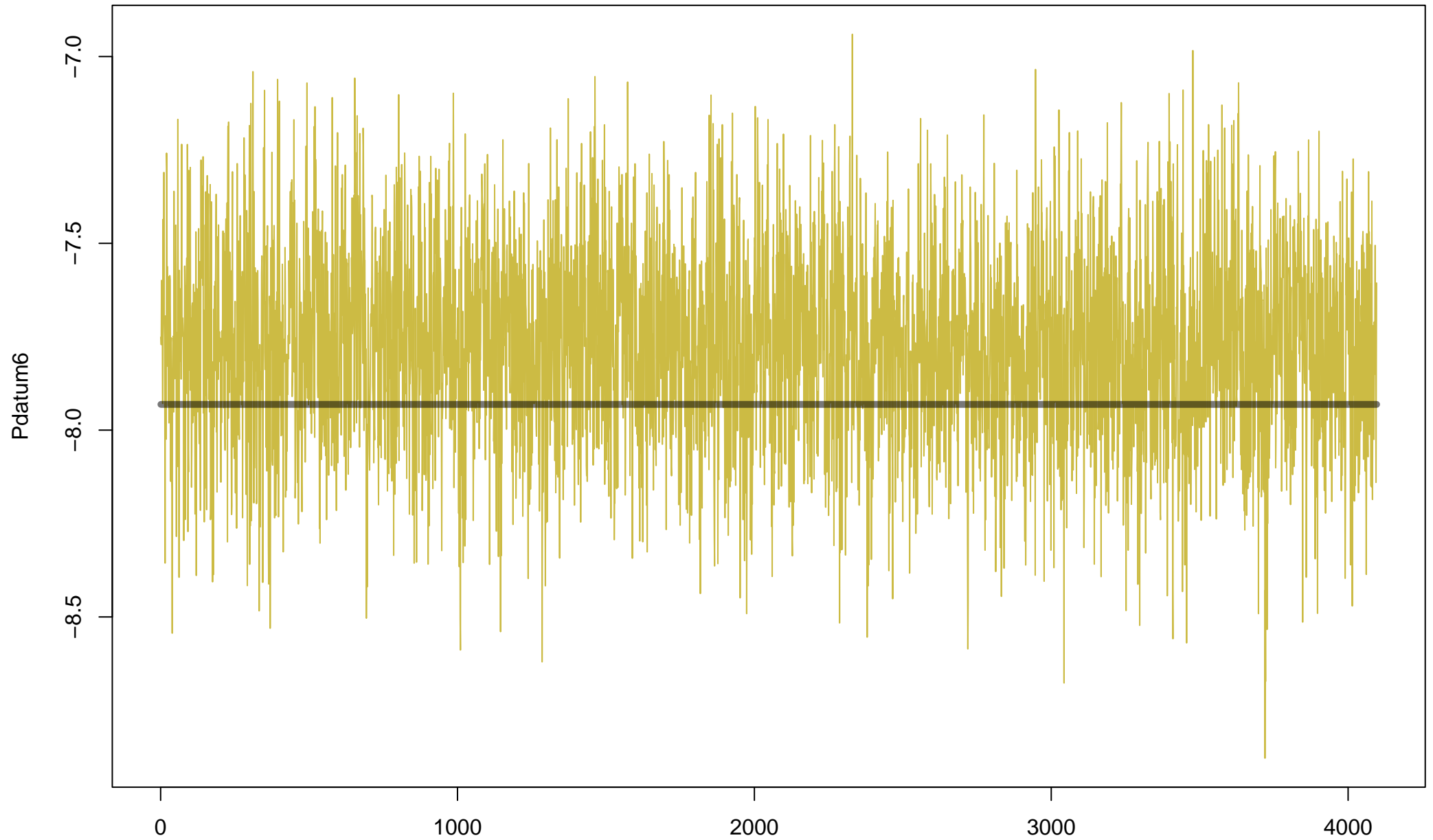


Pdatum5
ESS = 480 | BMK = 0.0367 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | rel.err: 1.5



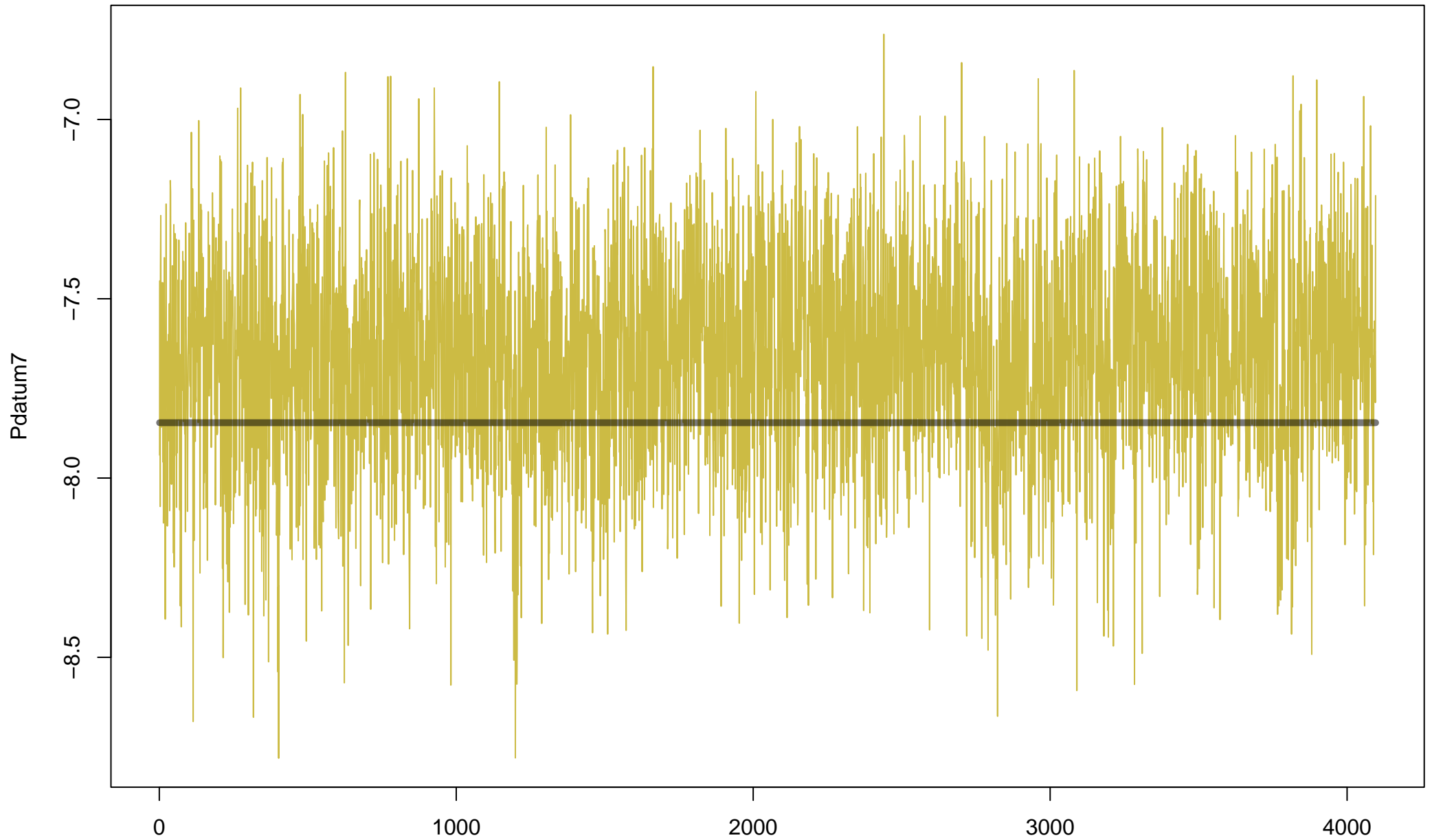
Pdatum6

ESS = 2600 | BMK = 0.0505 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0 | rel.err: 0.653

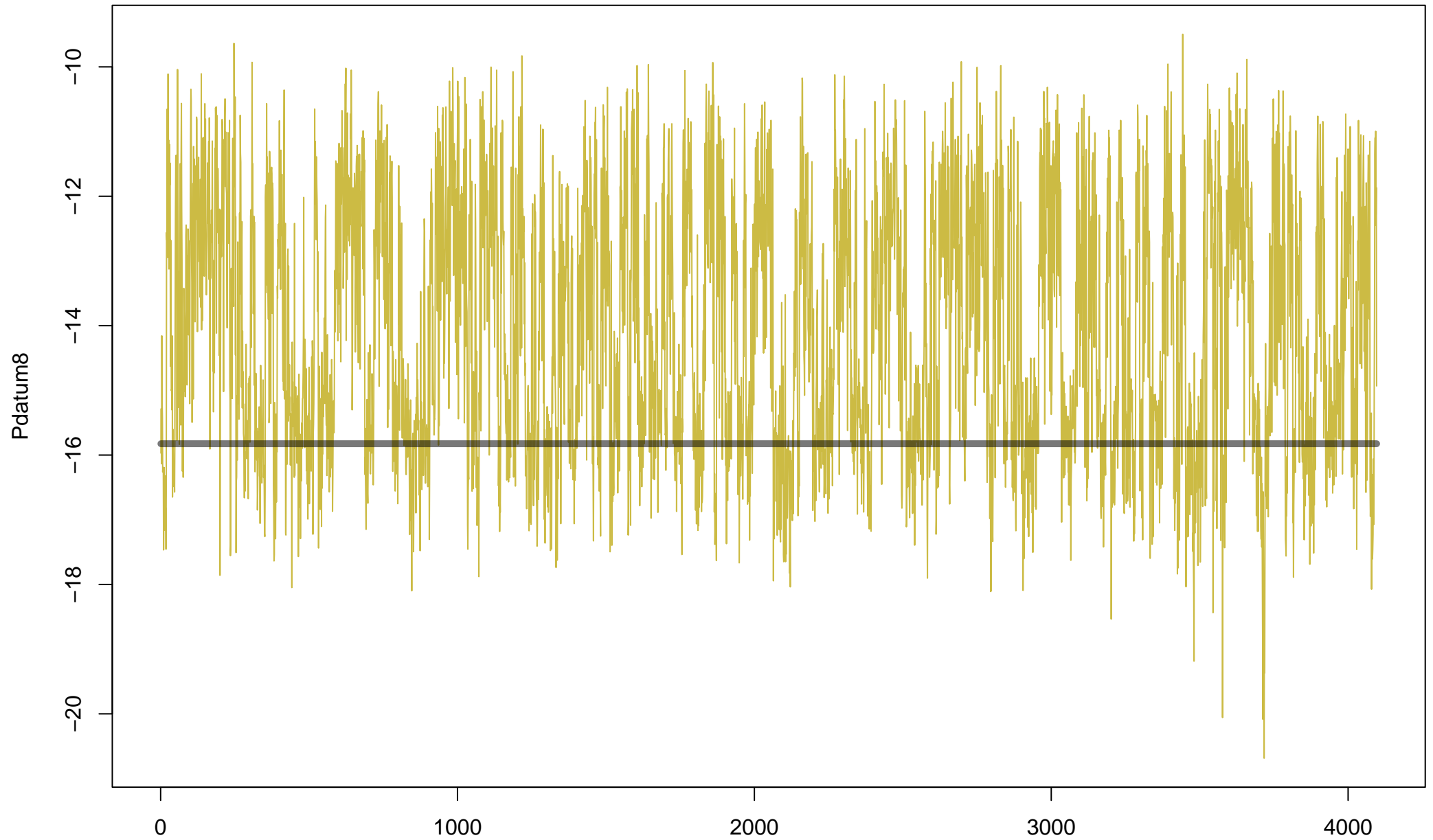


Pdatum7

ESS = 2670 | BMK = 0.0442 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0 | rel.err: 0.695

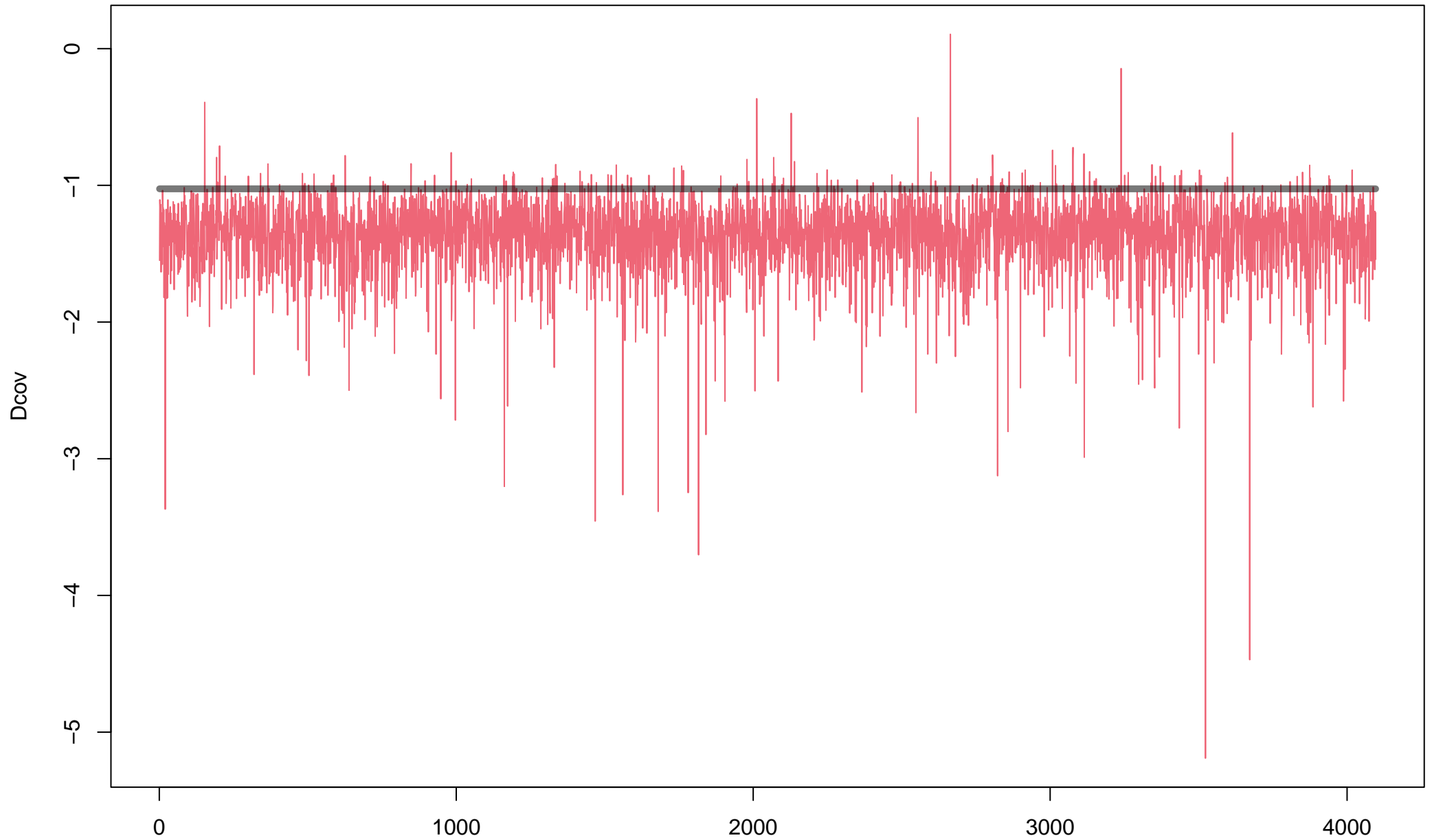


Pdatum8
ESS = 692 | BMK = 0.0739 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0 | rel.err: 0.539



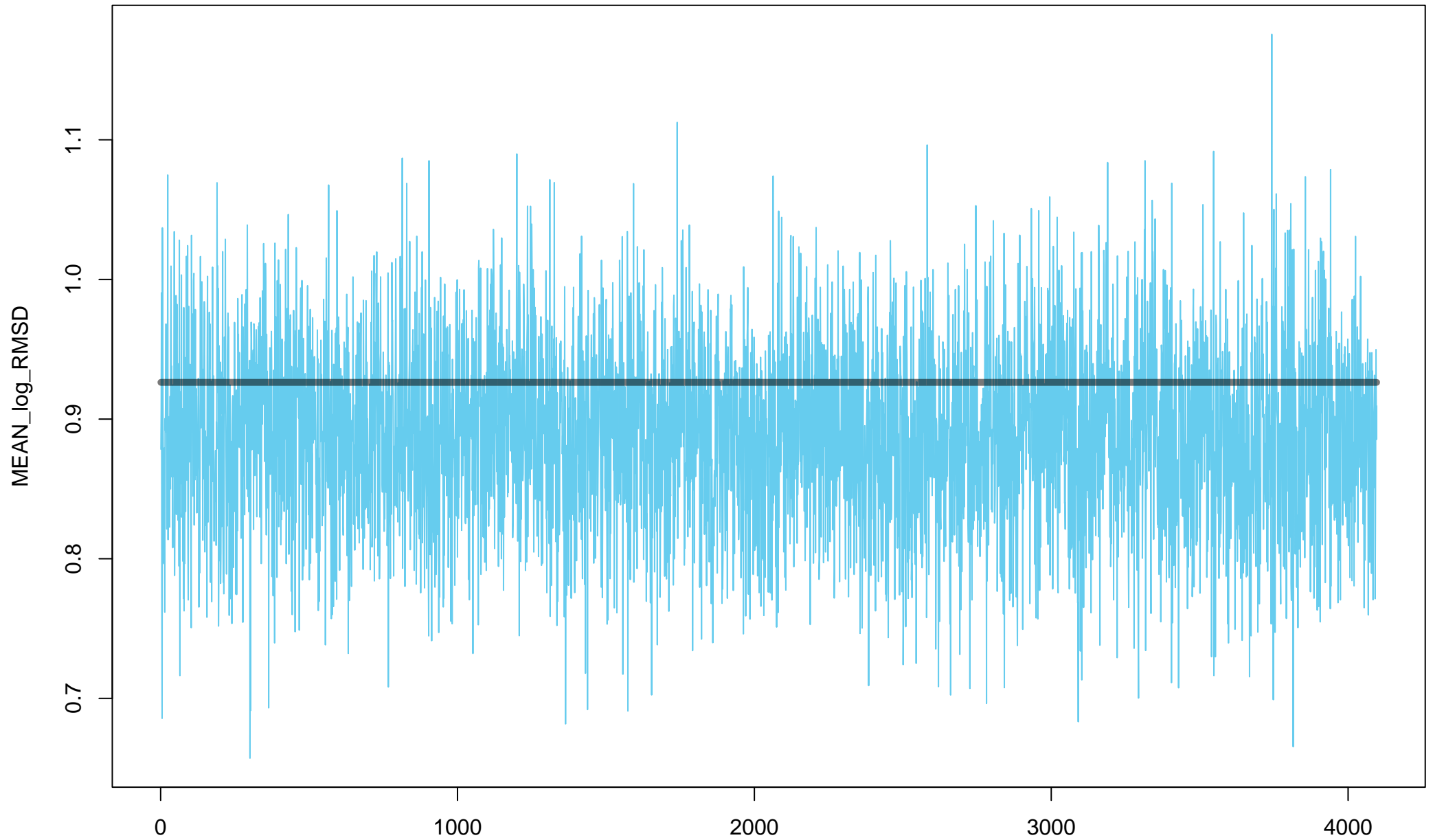
Dcov

ESS = 3730 | BMK = 0.0694 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0 | rel.err: 1.42

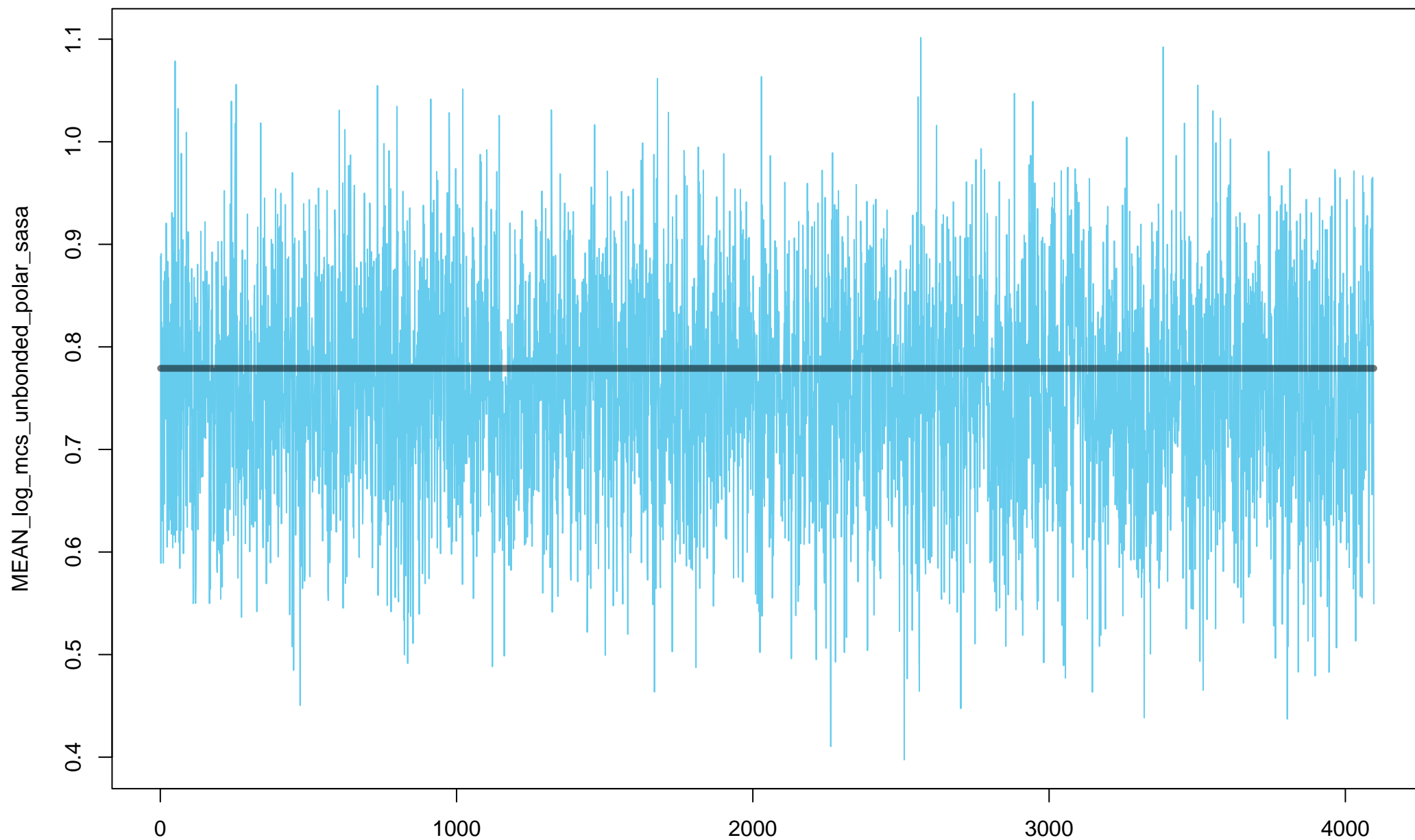


MEAN_log_RMSD

ESS = 4100 | BMK = 0.0371 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0 | rel.err: -0.572

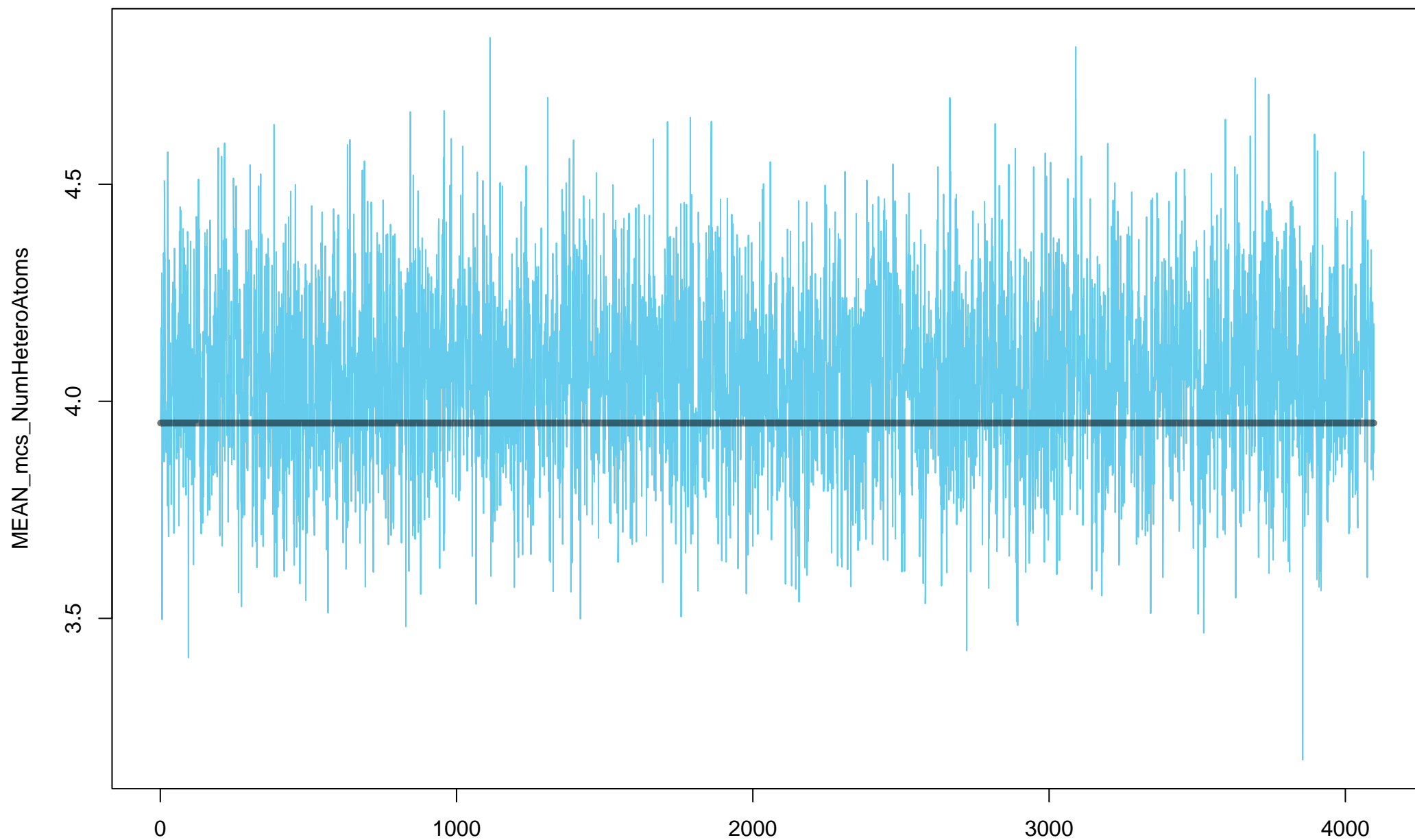


MEAN_log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.0455 | MCSE(6.27) = 1.58 | stat: TRUE | burn: 0 | rel.err: -0.198

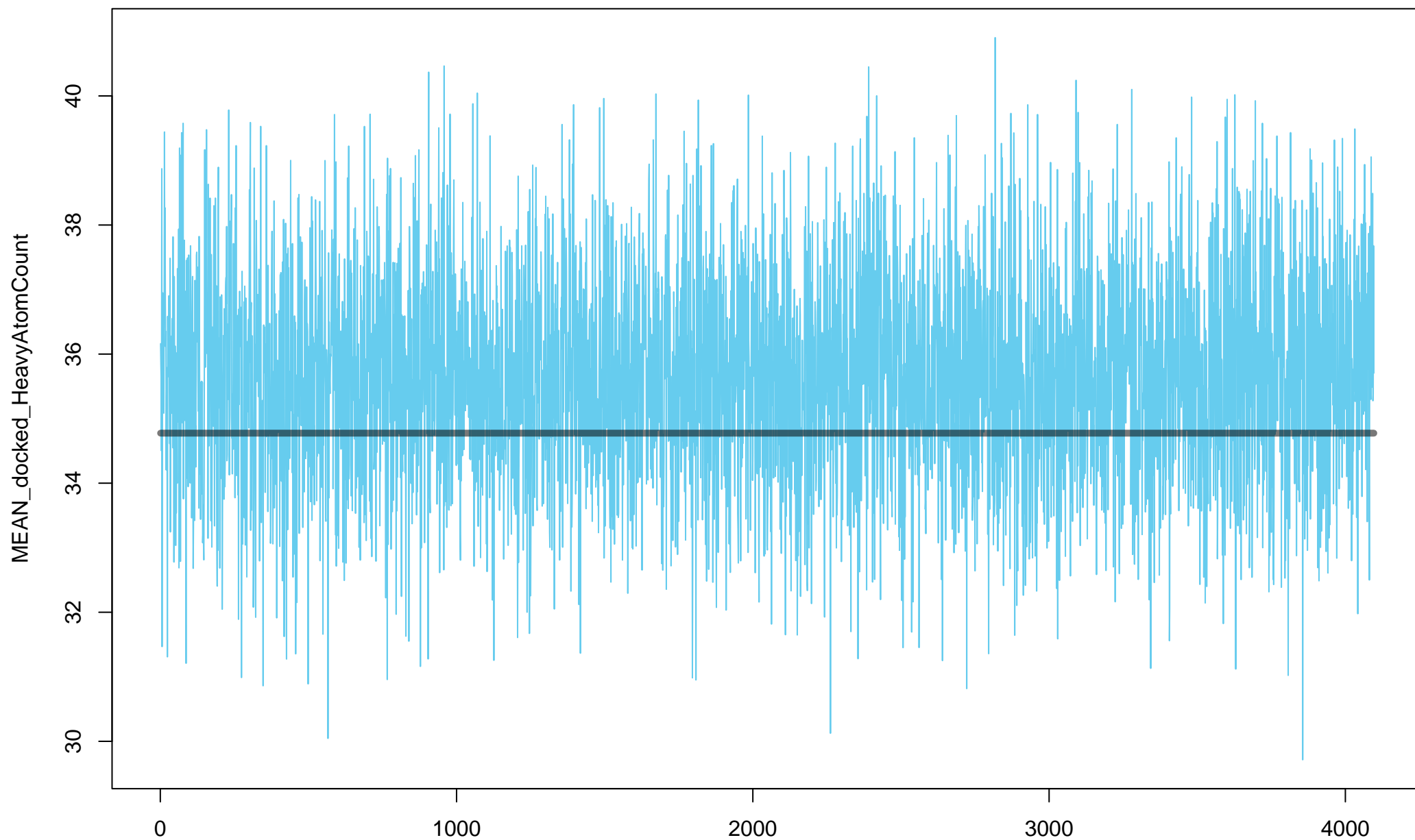


MEAN_mcs_NumHeteroAtoms

ESS = 4100 | BMK = 0.0248 | MCSE(6.27) = 1.74 | stat: TRUE | burn: 0 | rel.err: 0.513

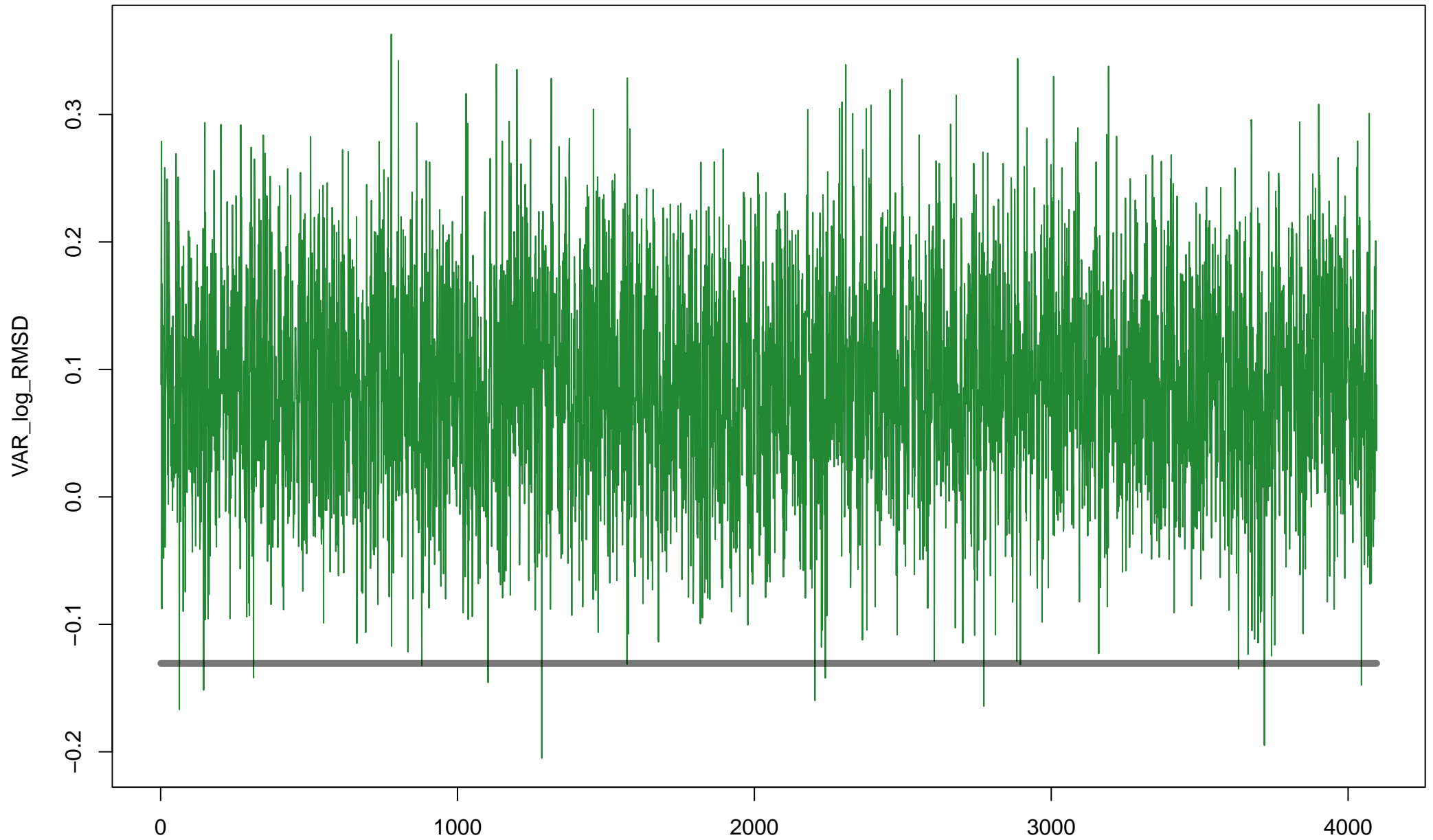


MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0306 | MCSE(6.27) = 1.59 | stat: TRUE | burn: 0 | rel.err: 0.533

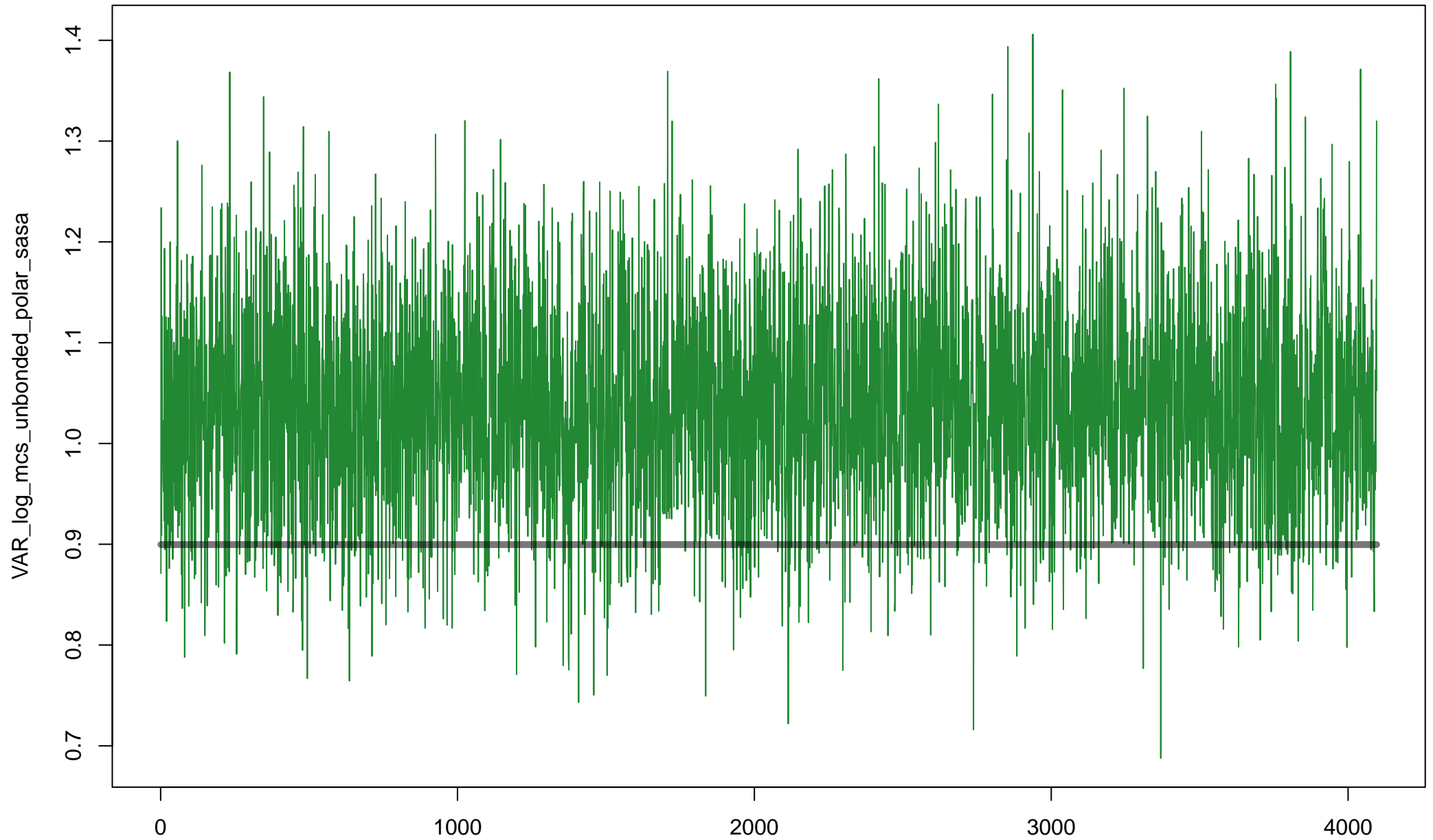


VAR_log_RMSD

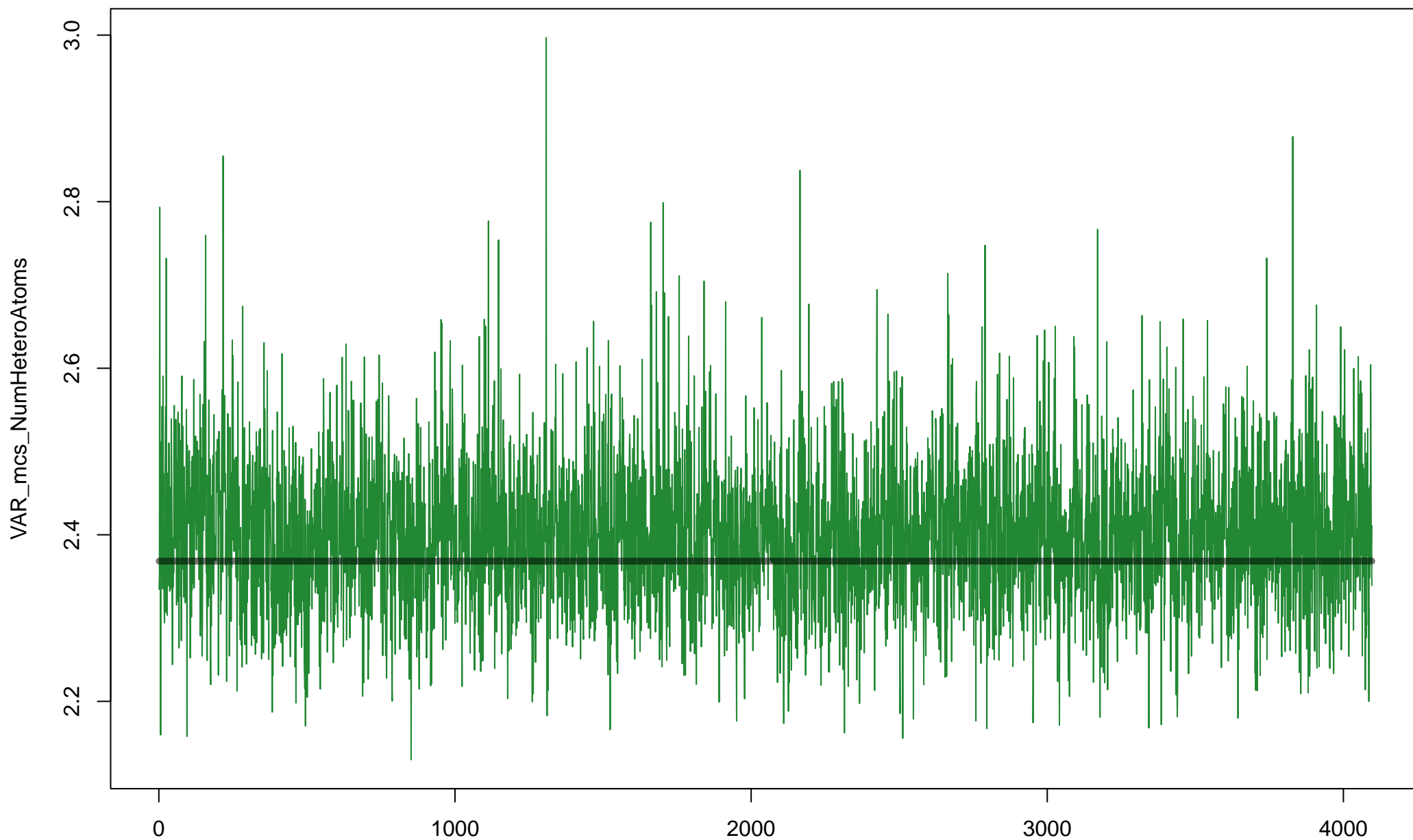
ESS = 4100 | BMK = 0.0405 | MCSE(6.27) = 1.45 | stat: TRUE | burn: 0 | rel.err: 2.38



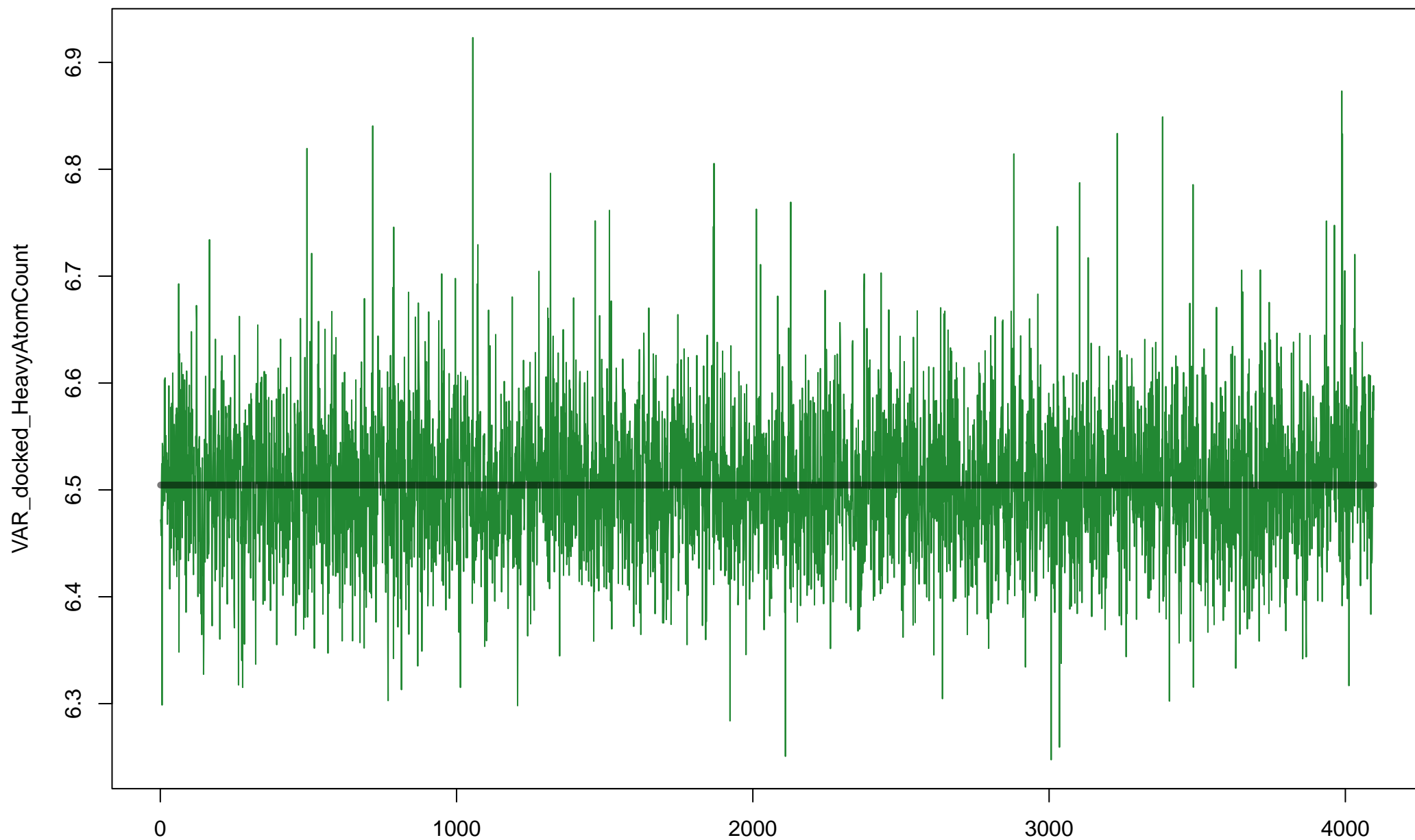
VAR_log_mcs_unbonded_polar_sasa
ESS = 3690 | BMK = 0.0472 | MCSE(6.27) = 1.64 | stat: TRUE | burn: 0 | rel.err: 1.34



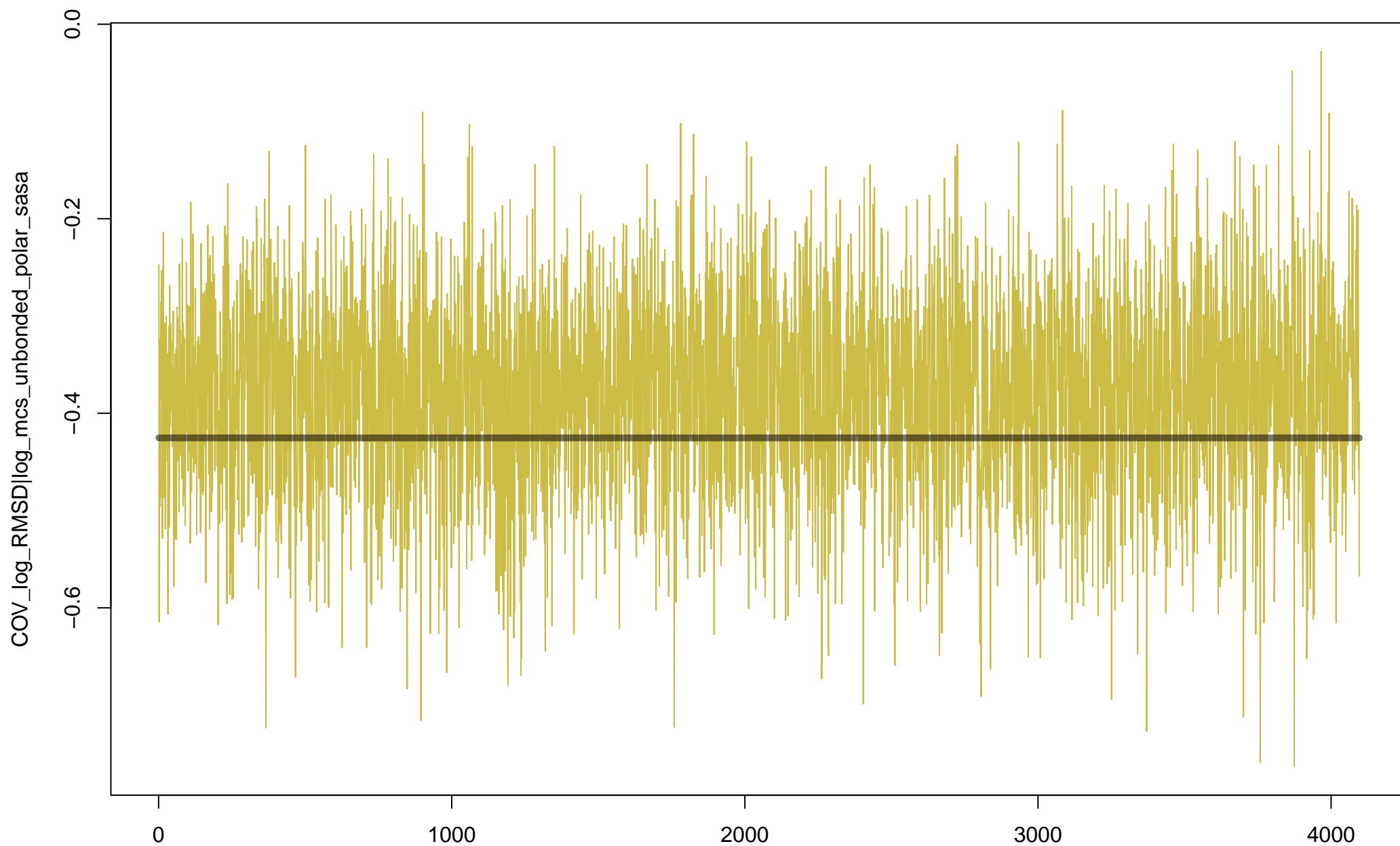
VAR_mcs_NumHeteroAtoms
ESS = 2890 | BMK = 0.0391 | MCSE(6.27) = 1.93 | stat: FALSE | burn: 0 | rel.err: 0.401



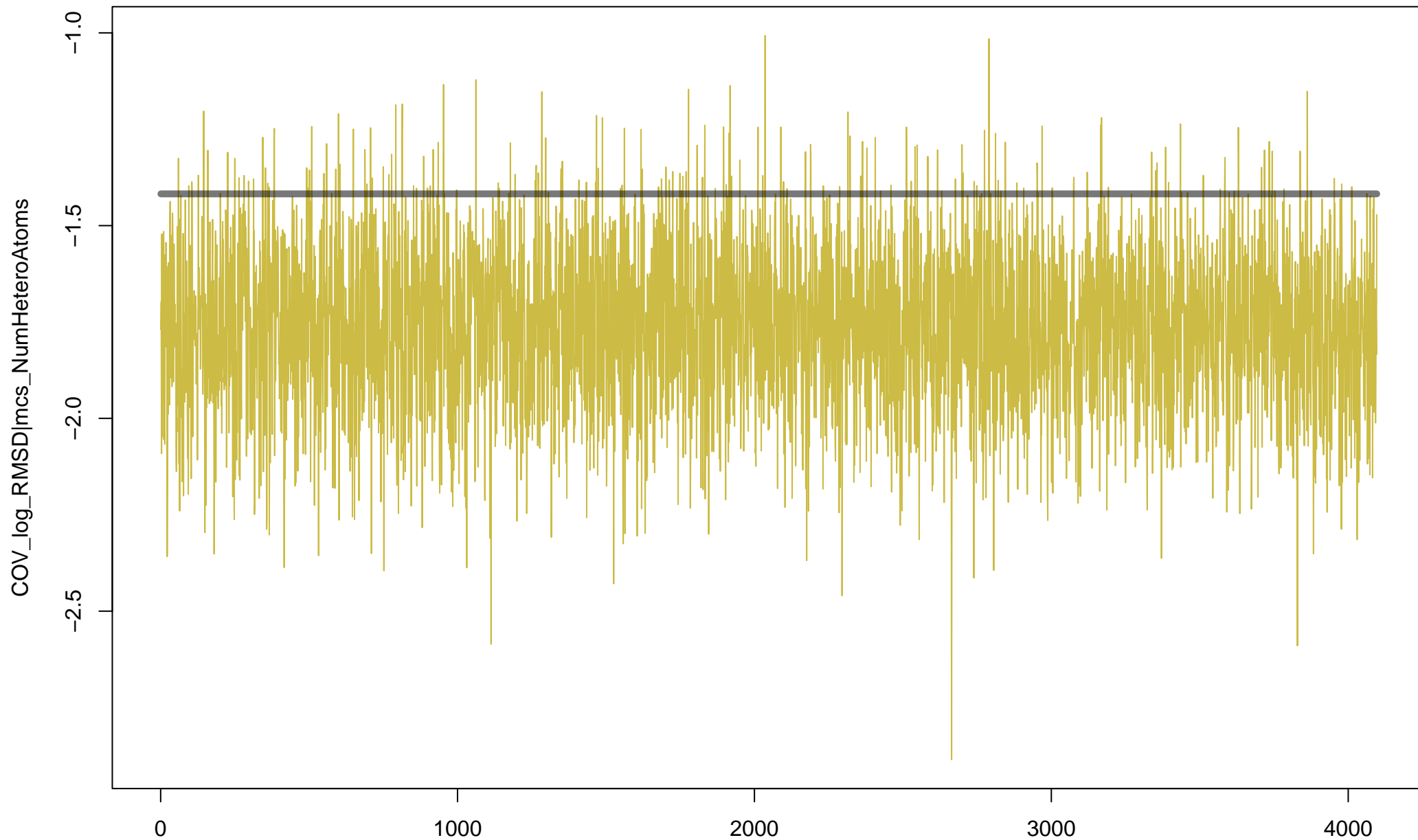
VAR_docked_HeavyAtomCount
ESS = 3690 | BMK = 0.0438 | MCSE(6.27) = 1.8 | stat: TRUE | burn: 0 | rel.err: 0.0628



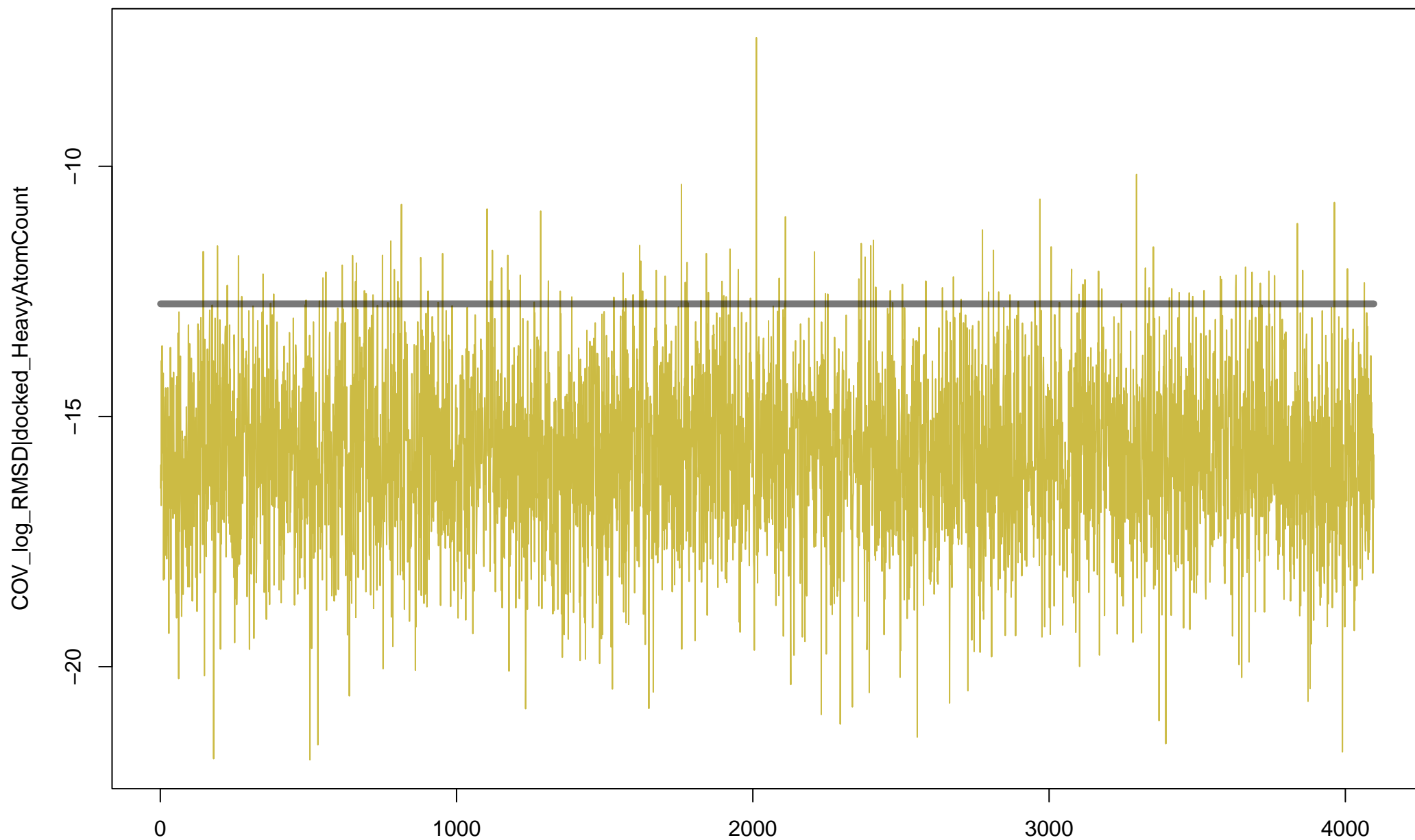
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3640 | BMK = 0.0312 | MCSE(6.27) = 1.83 | stat: TRUE | burn: 0 | rel.err: 0.469



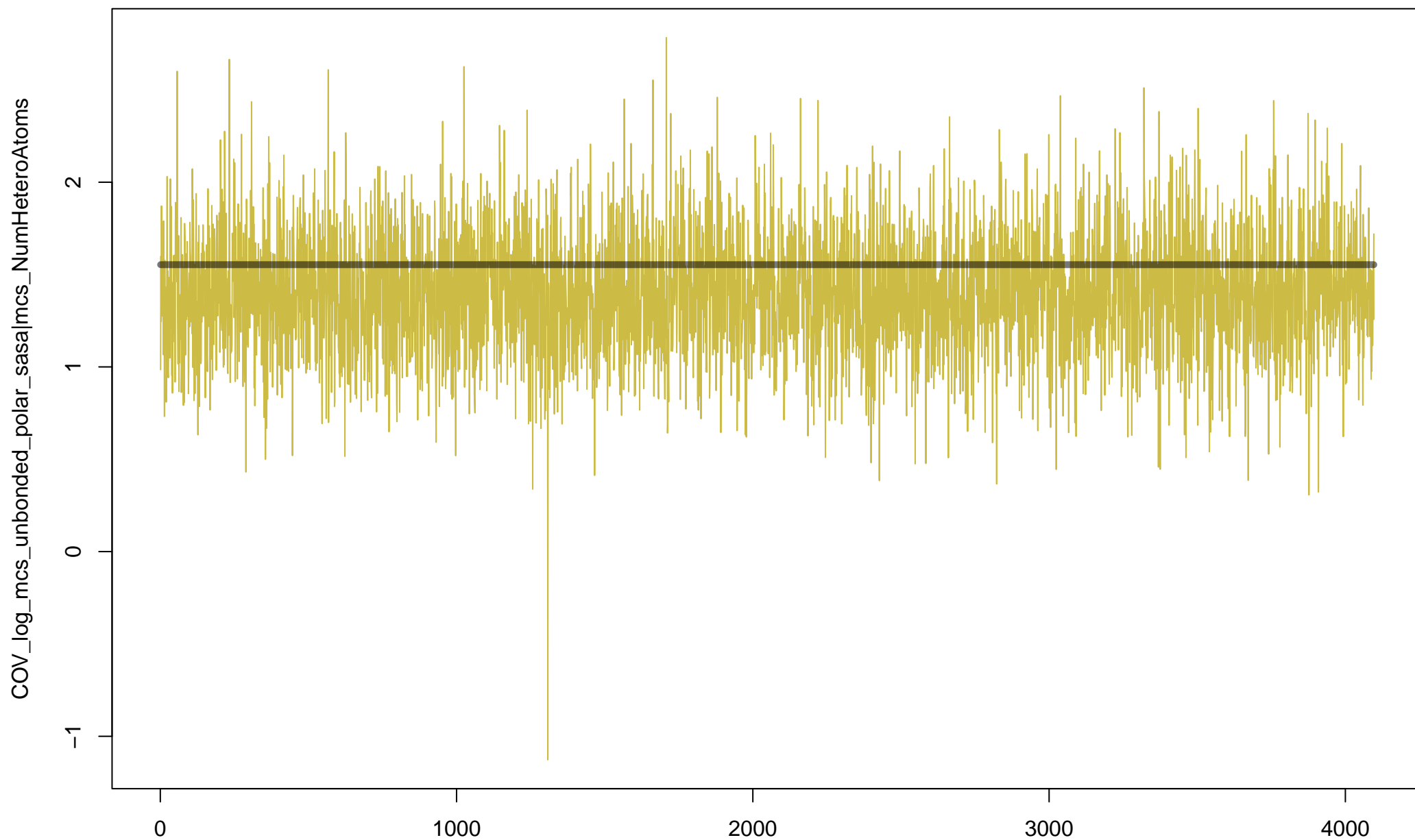
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 3590 | BMK = 0.0472 | MCSE(6.27) = 1.52 | stat: TRUE | burn: 0 | rel.err: -1.65



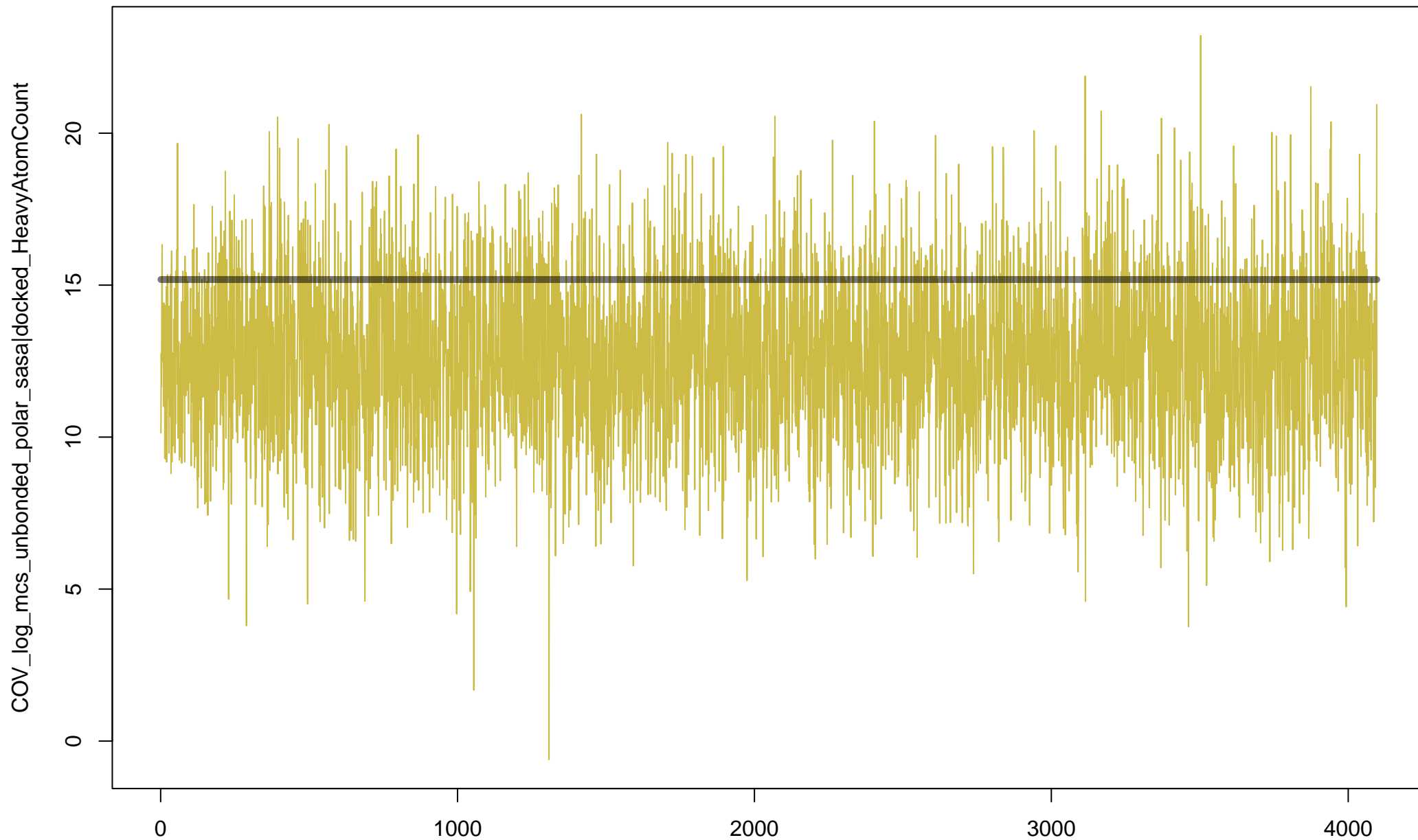
COV_log_RMSD|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0316 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: -1.82



COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 3770 | BMK = 0.0468 | MCSE(6.27) = 1.73 | stat: TRUE | burn: 0 | rel.err: -0.475



COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 3820 | BMK = 0.043 | MCSE(6.27) = 1.75 | stat: TRUE | burn: 0 | rel.err: -0.961



COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0352 | MCSE(6.27) = 1.48 | stat: TRUE | burn: 0 | rel.err: 0.513

