

-- STATS maxD --

min ESS = 164.700795098374

max BMK = 0.132882209928192

max MCSE = 6.04324791073373

all stationary: FALSE

burn: 0

max rel.err.: 2.1814084907434

-- STATS 1D --

min ESS = 2377.82957811721

max BMK = 0.0497333316856198

max MCSE = 2.17210680999155

all stationary: TRUE

burn: 0

max rel.err.: 2.25742741421441

-- STATS 2D --

min ESS = 3744.48718399919

max BMK = 0.0403270016638324

max MCSE = 1.91927233575086

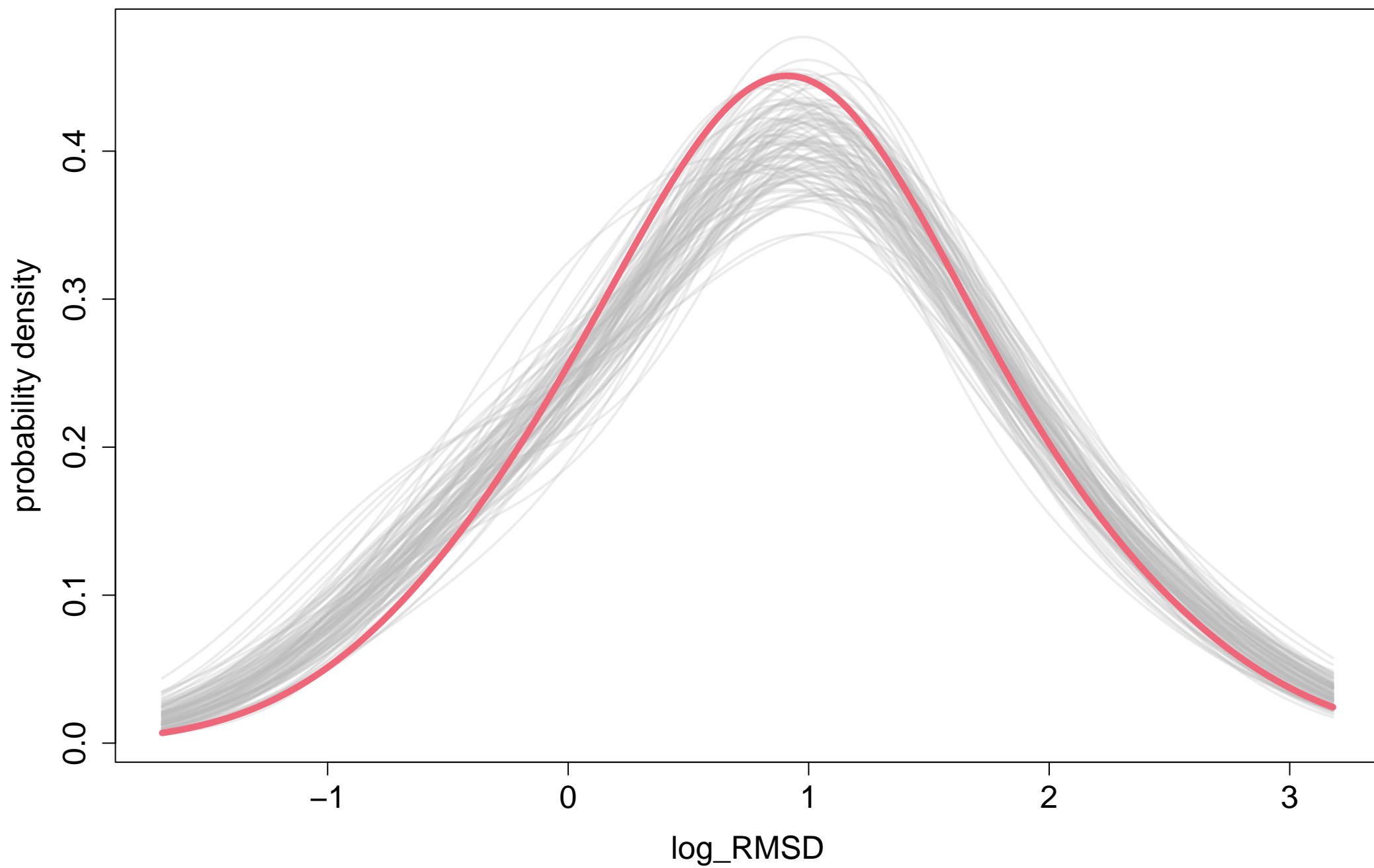
all stationary: FALSE

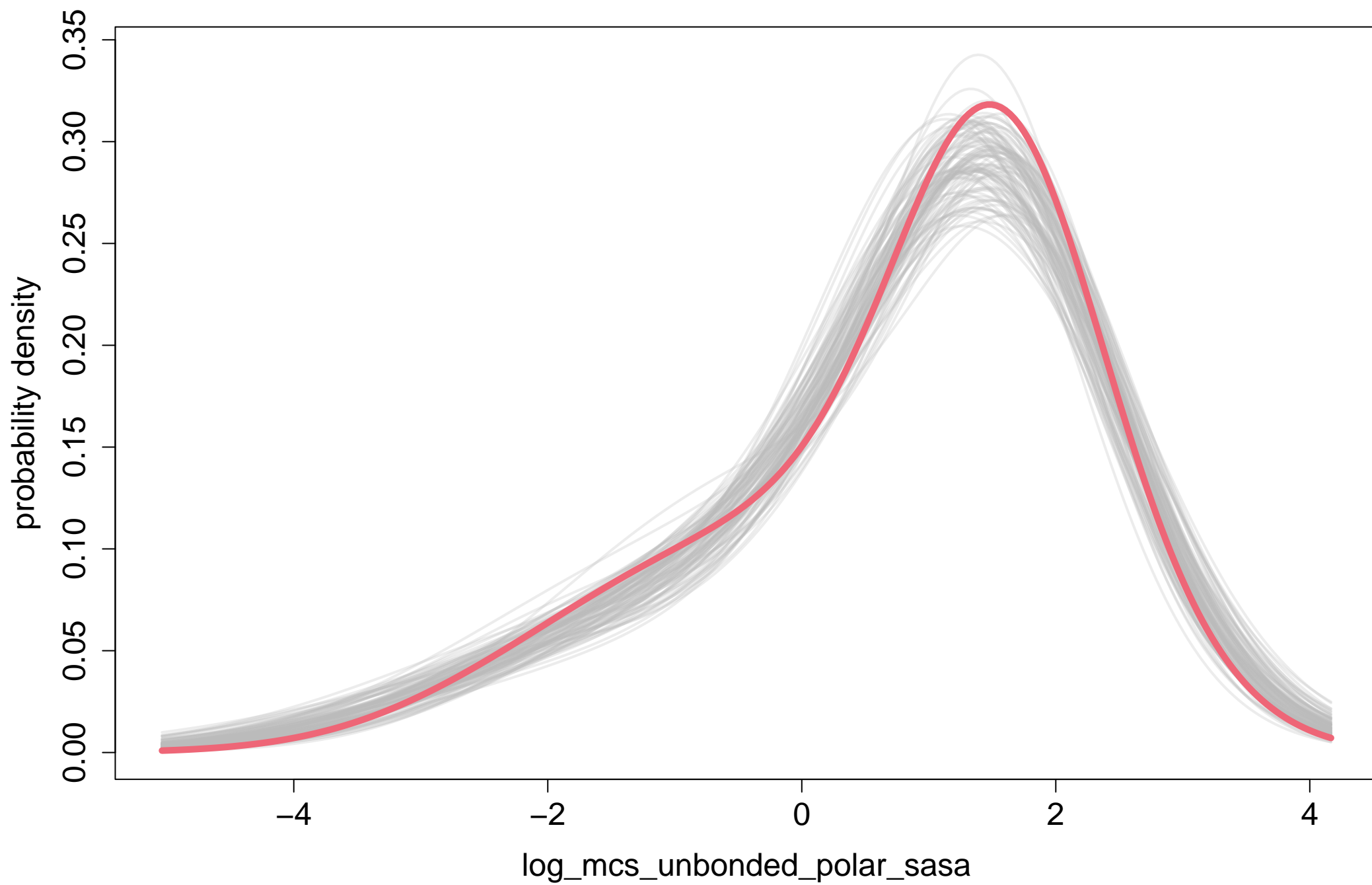
burn: 0

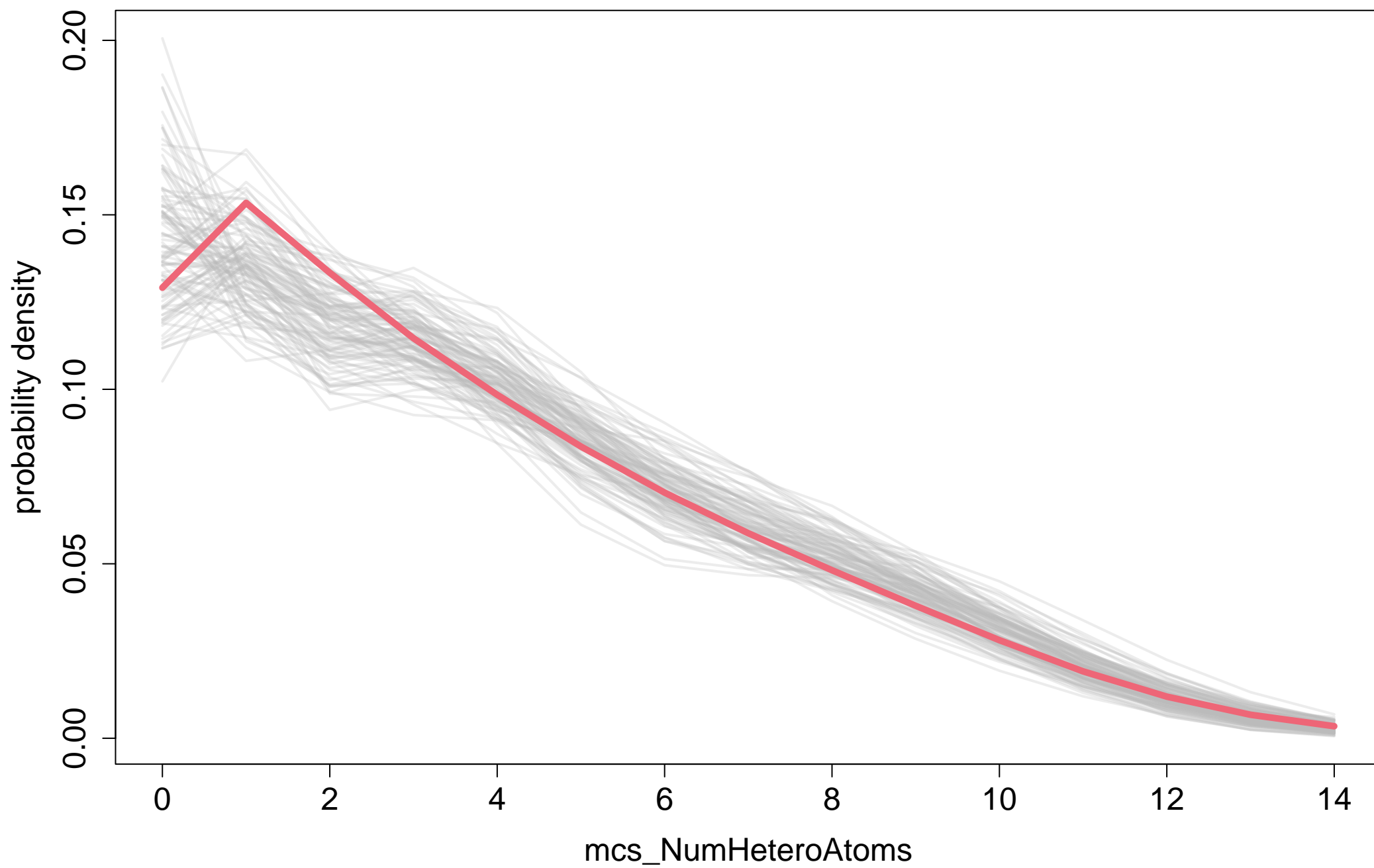
max rel.err.: 1.71197640746945

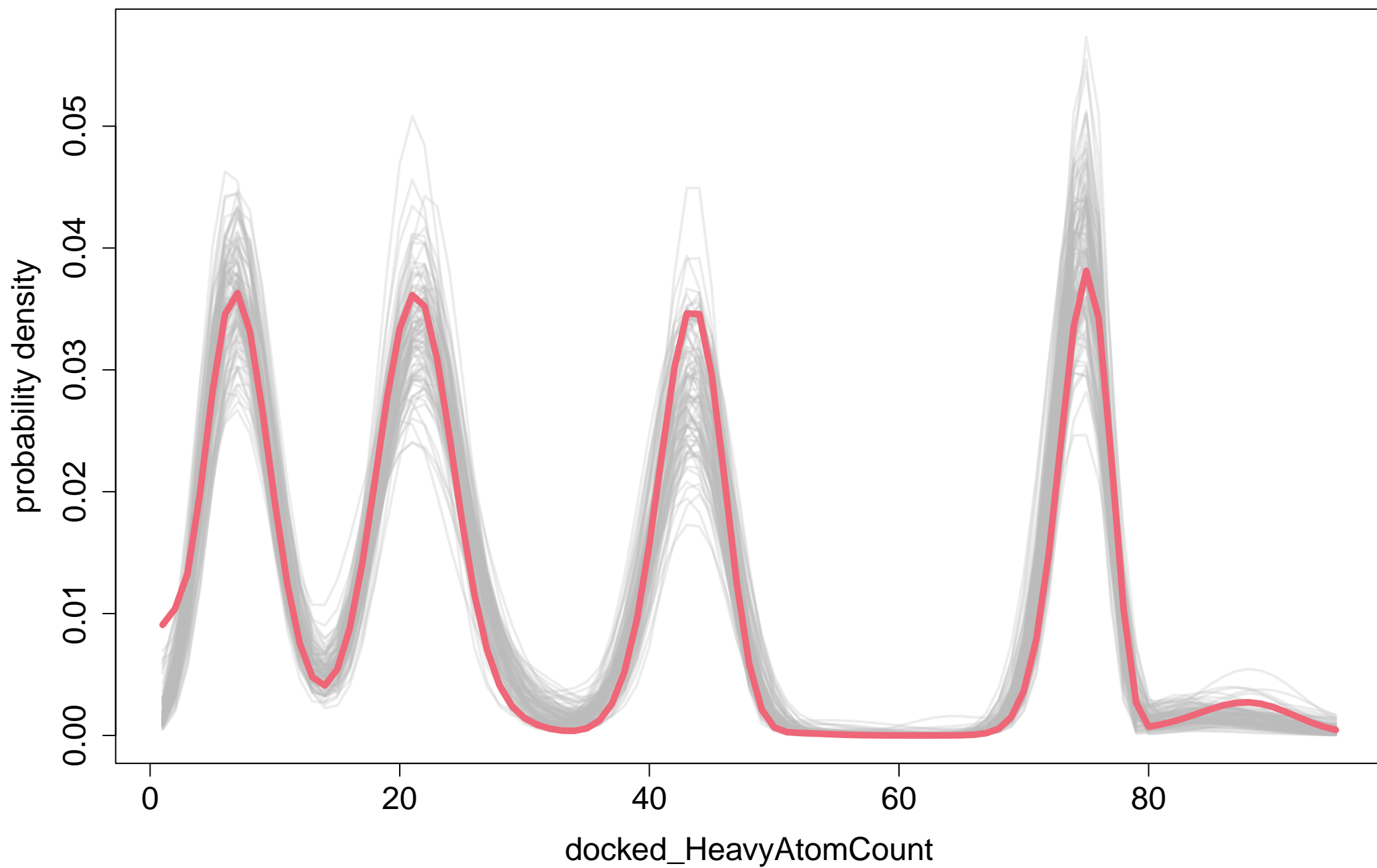
Occupied clusters: 8 of 16

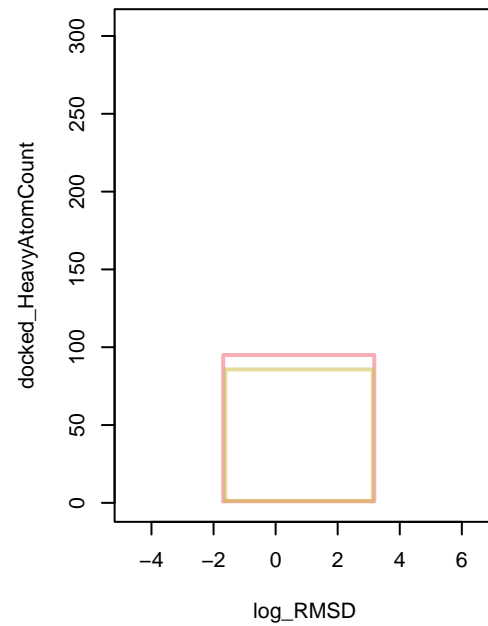
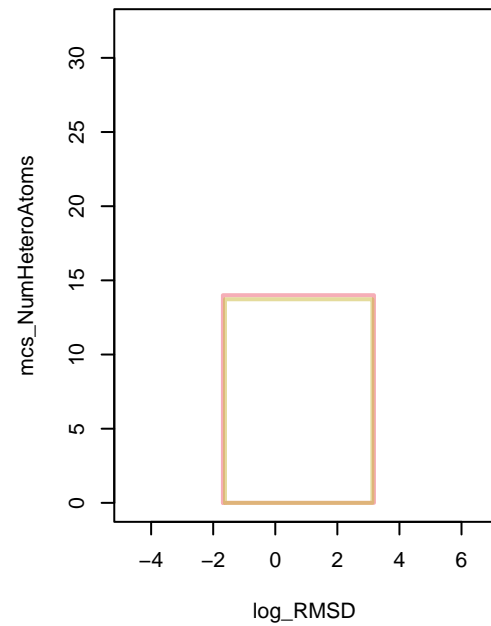
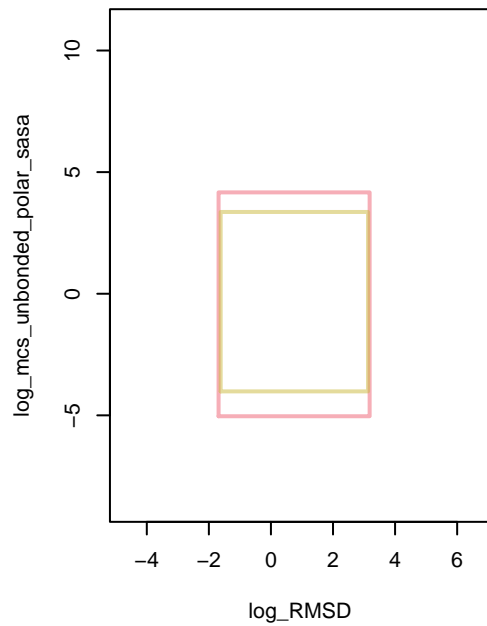
LL: -2160 +- 6.65



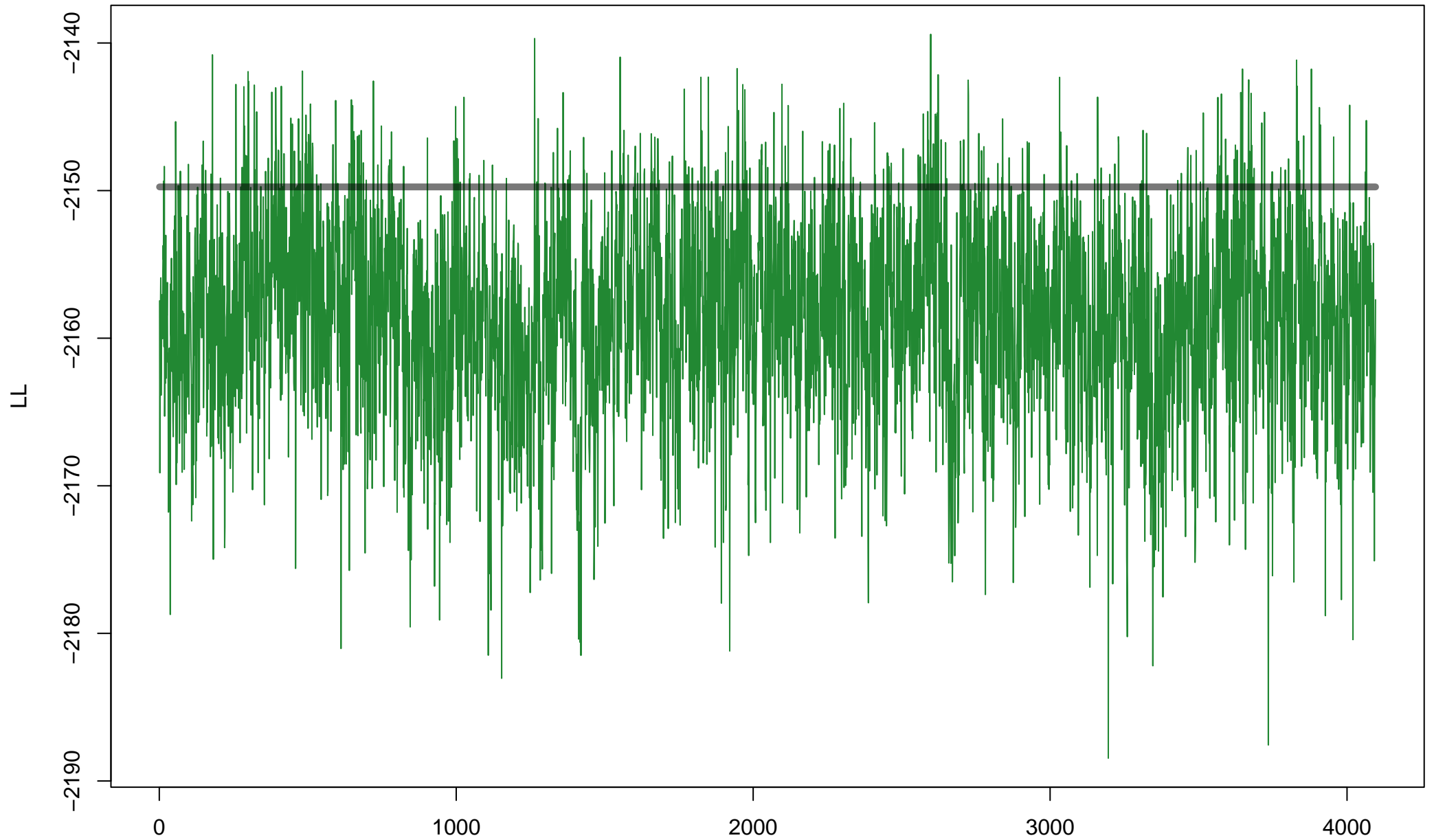




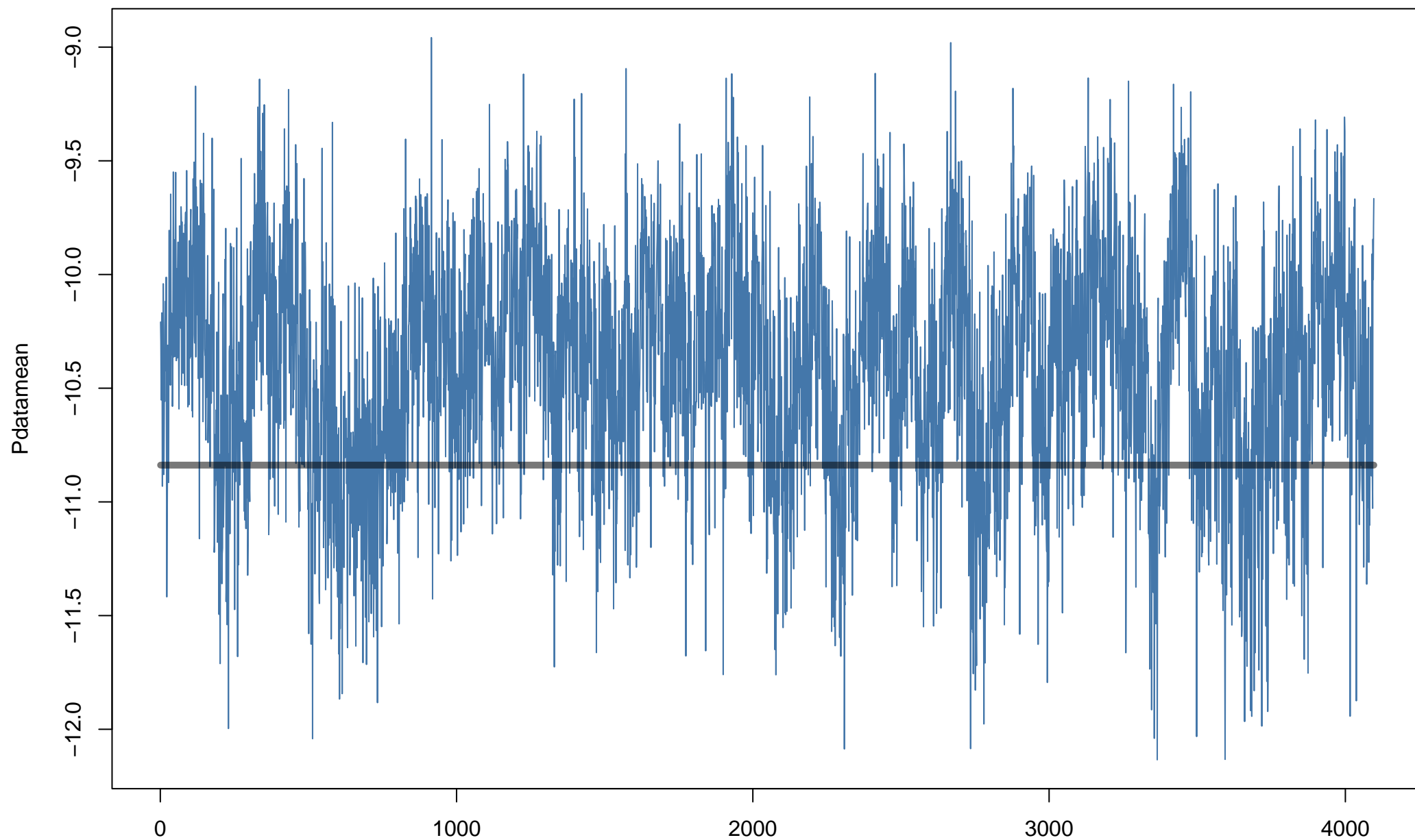




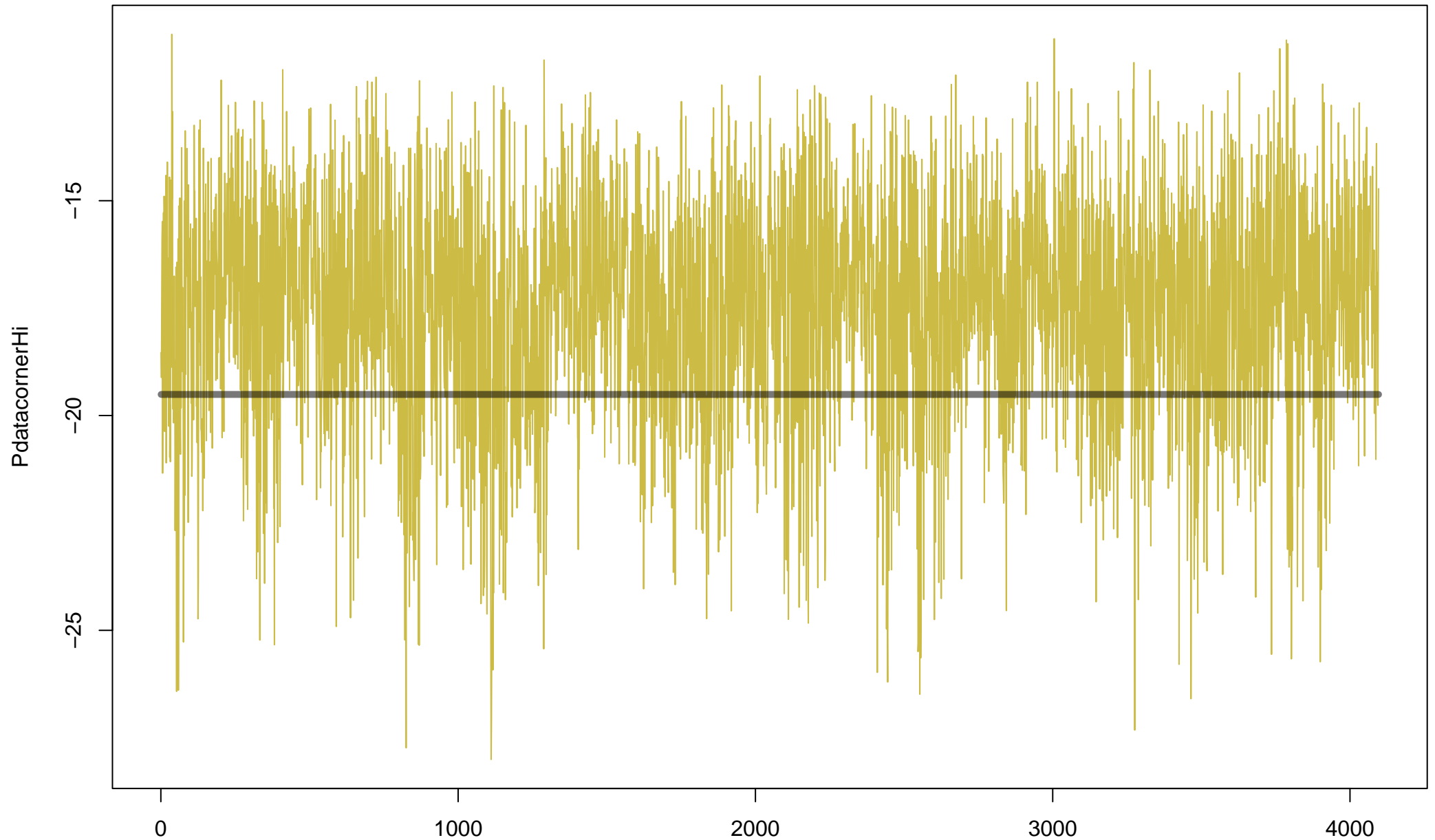
LL



Pdatamean
ESS = 165 | BMK = 0.0613 | MCSE(6.27) = 6.04 | stat: TRUE | burn: 0 | rel.err: 0.86

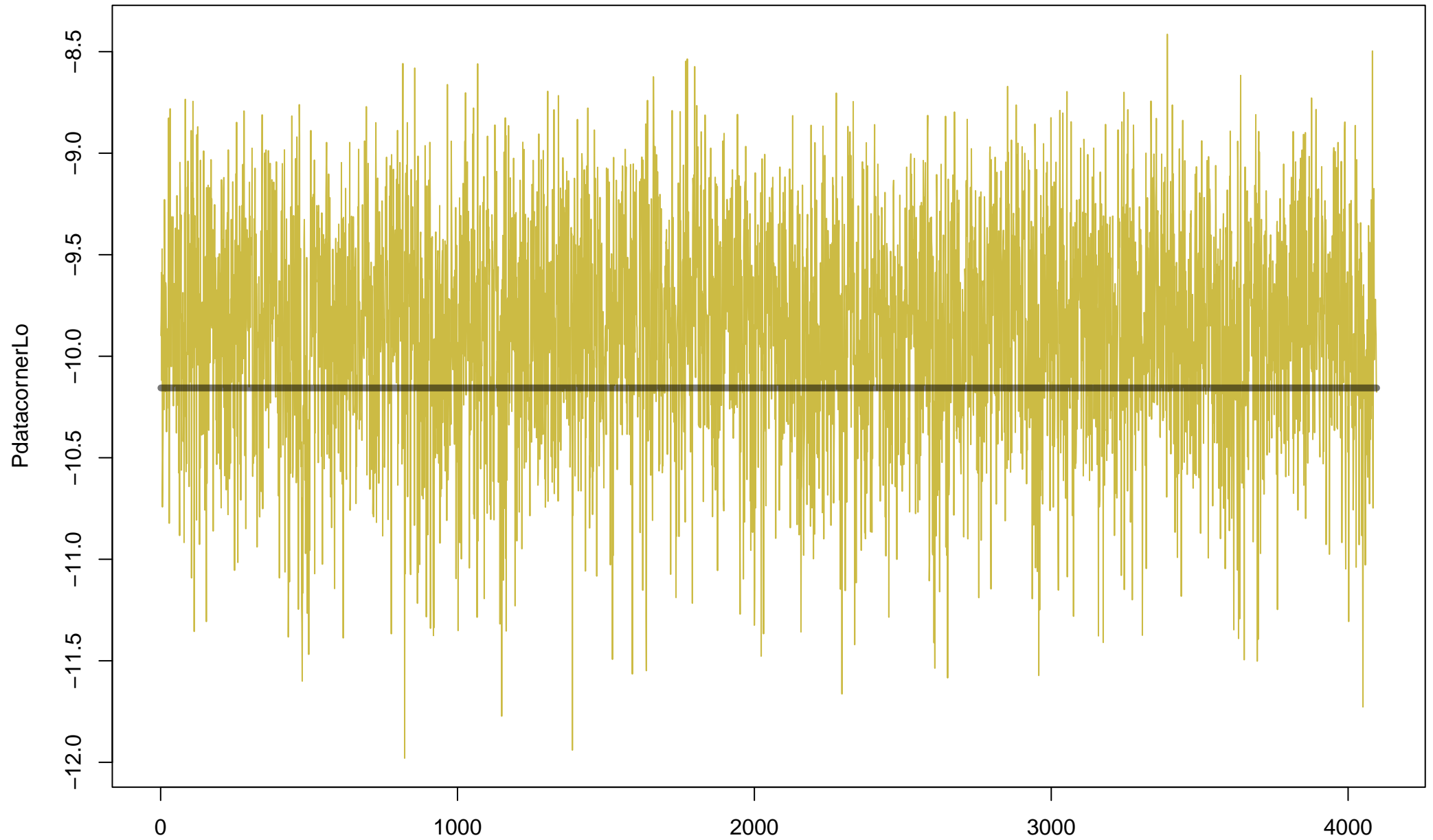


PdatacornerHi
ESS = 2420 | BMK = 0.133 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0 | rel.err: 0.307

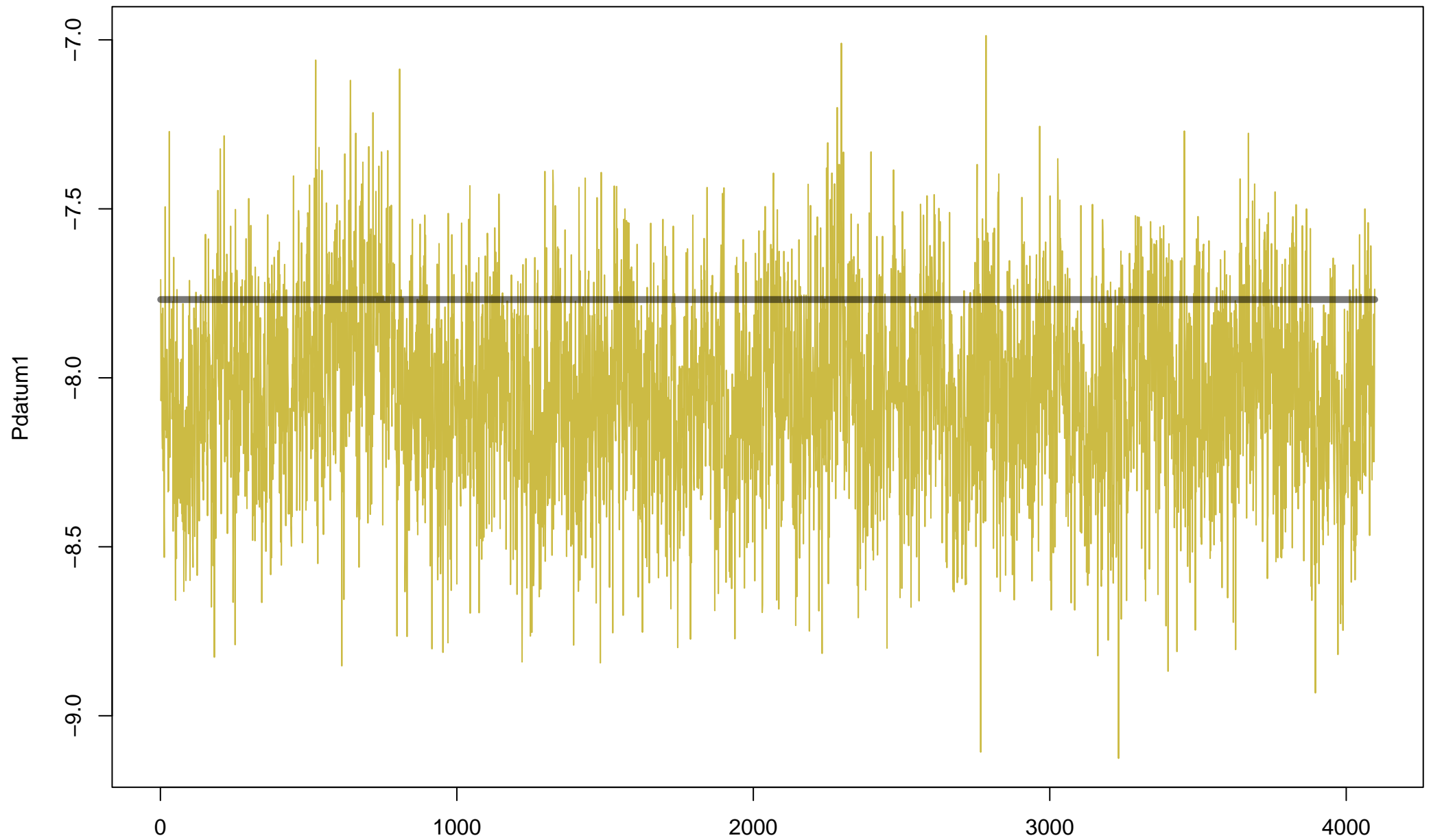


PdatacornerLo

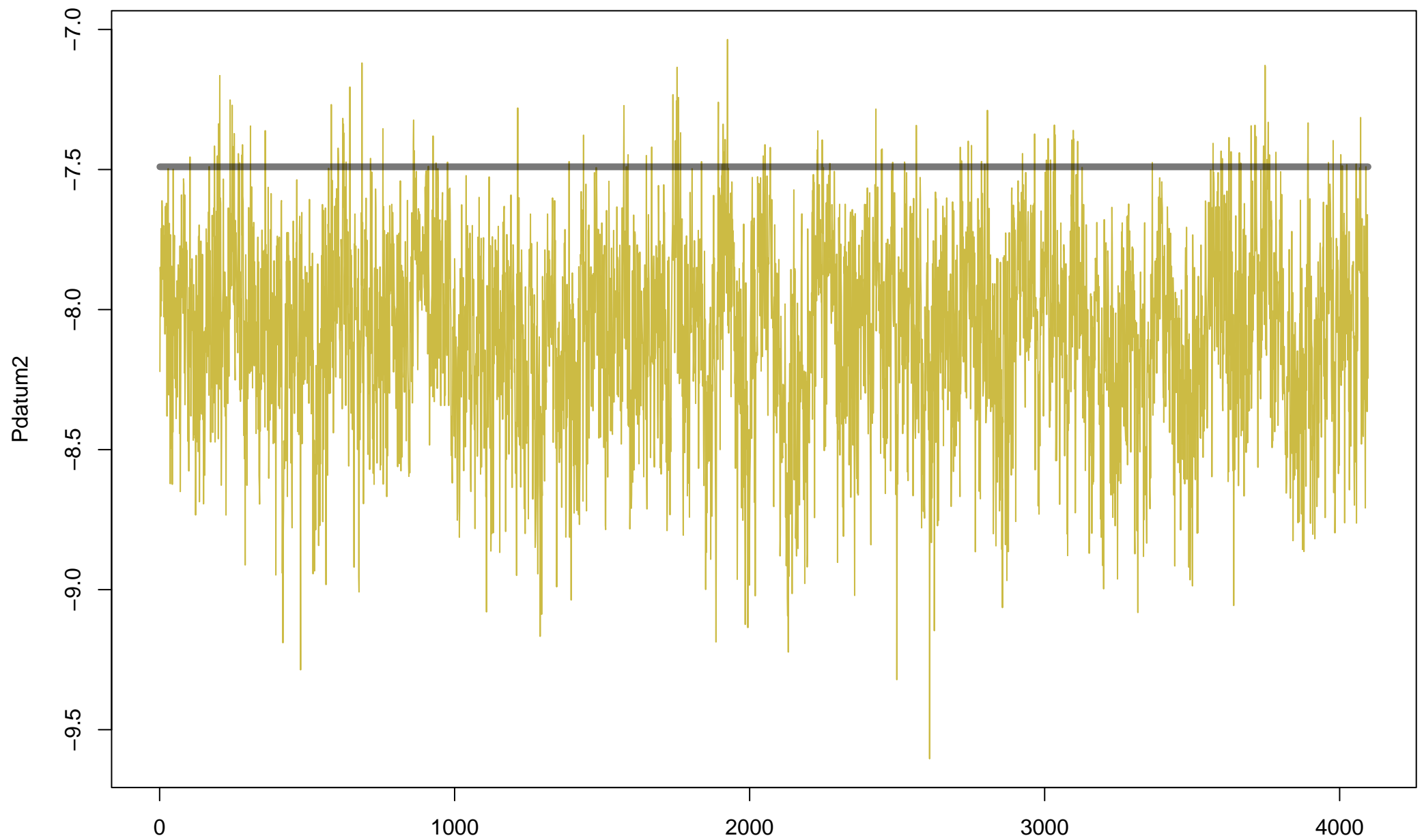
ESS = 2980 | BMK = 0.036 | MCSE(6.27) = 1.81 | stat: TRUE | burn: 0 | rel.err: 0.684



Pdatum1
ESS = 743 | BMK = 0.0414 | MCSE(6.27) = 3.74 | stat: TRUE | burn: 0 | rel.err: -0.933

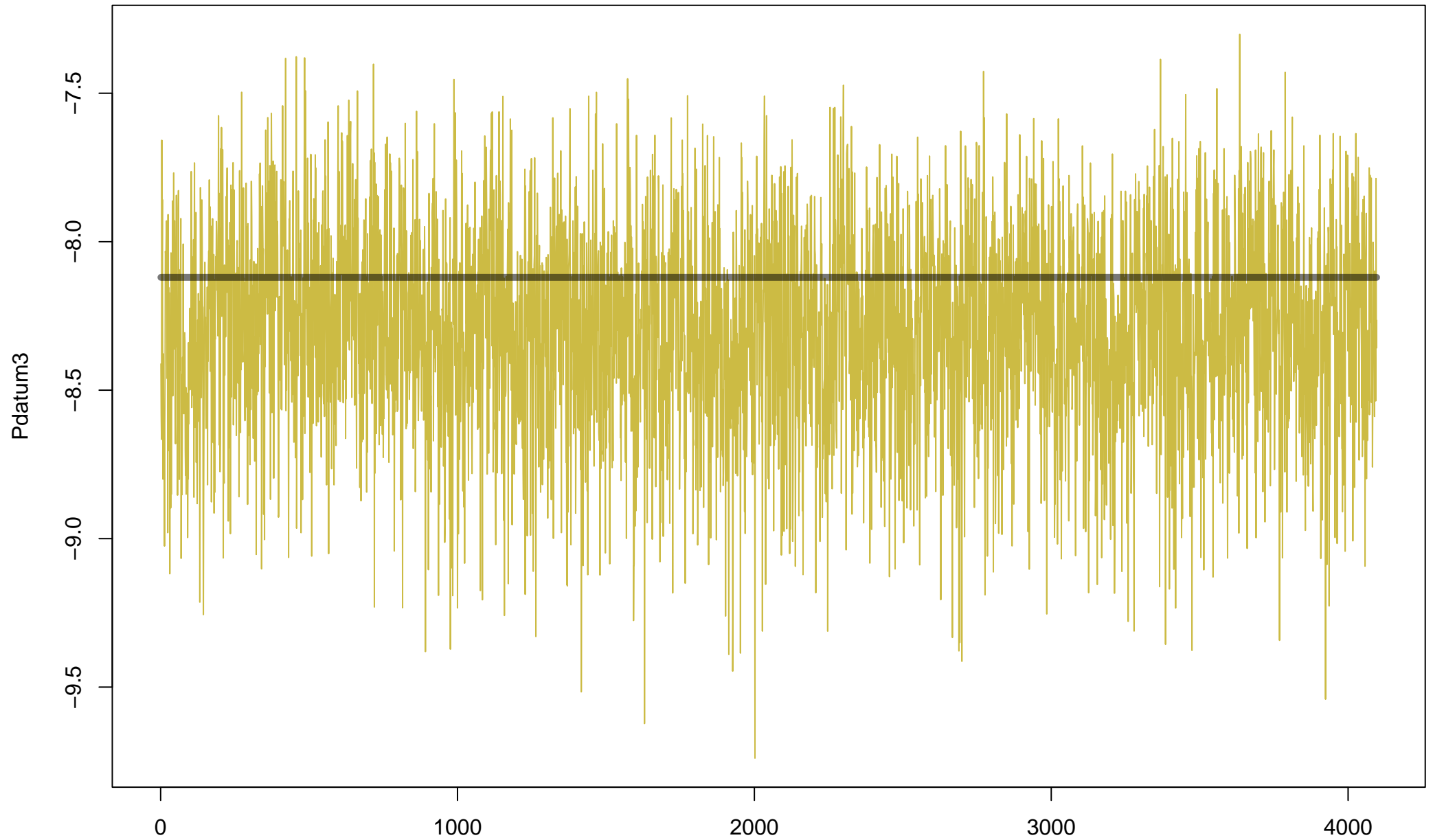


Pdatum2
ESS = 466 | BMK = 0.0406 | MCSE(6.27) = 4.07 | stat: TRUE | burn: 0 | rel.err: -2.18



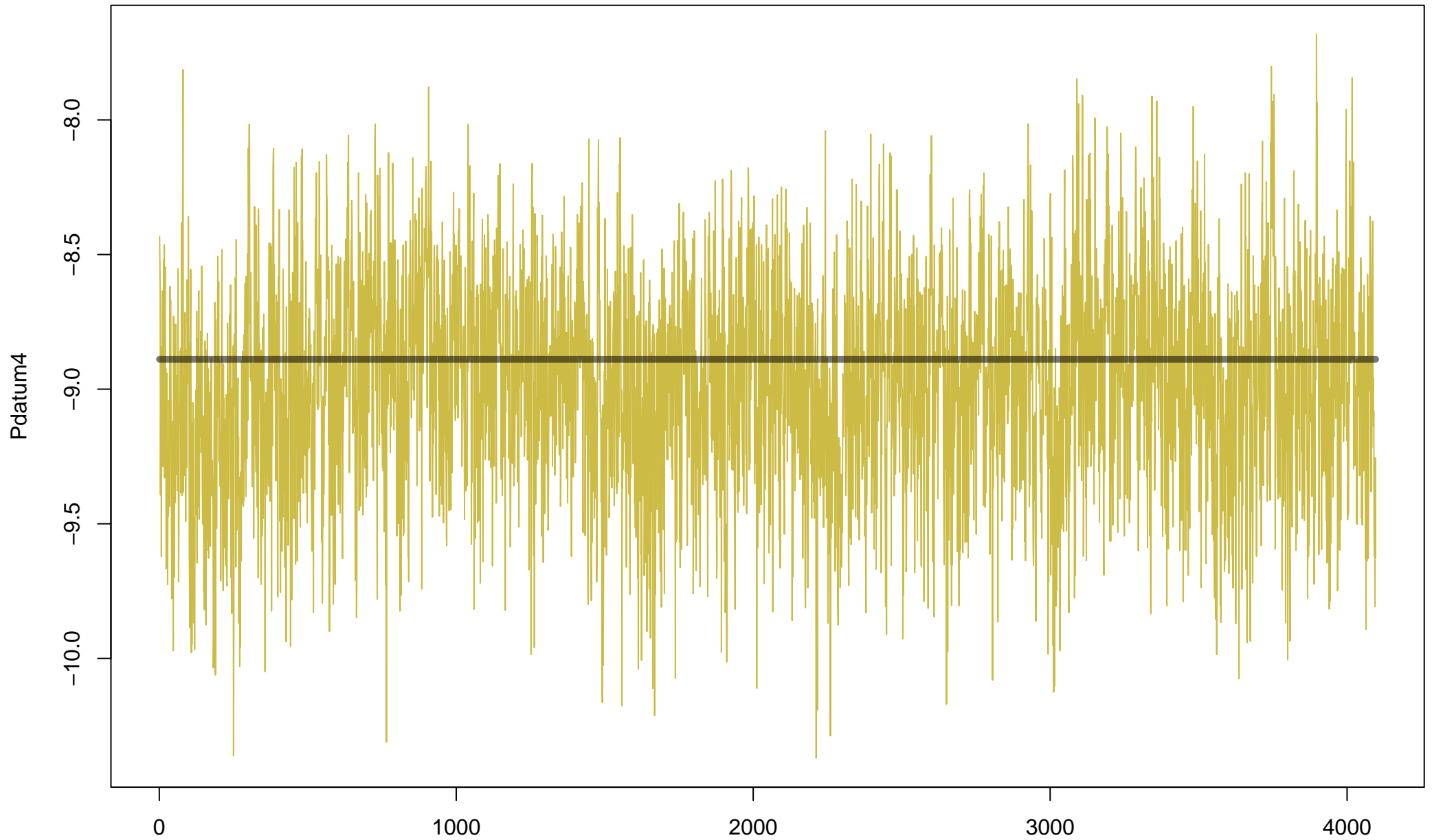
Pdatum3

ESS = 2090 | BMK = 0.0411 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0 | rel.err: -0.379

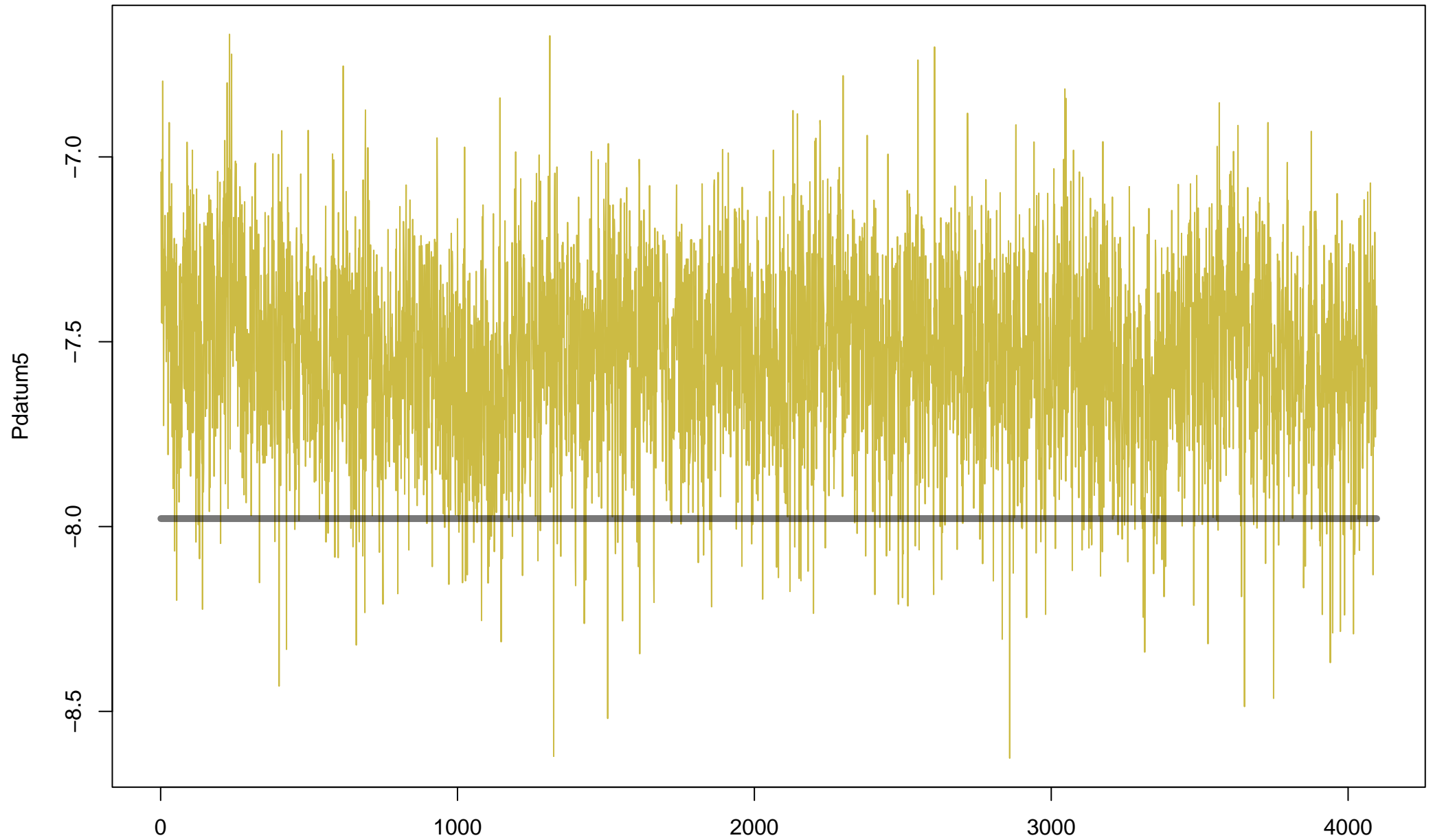


Pdatum4

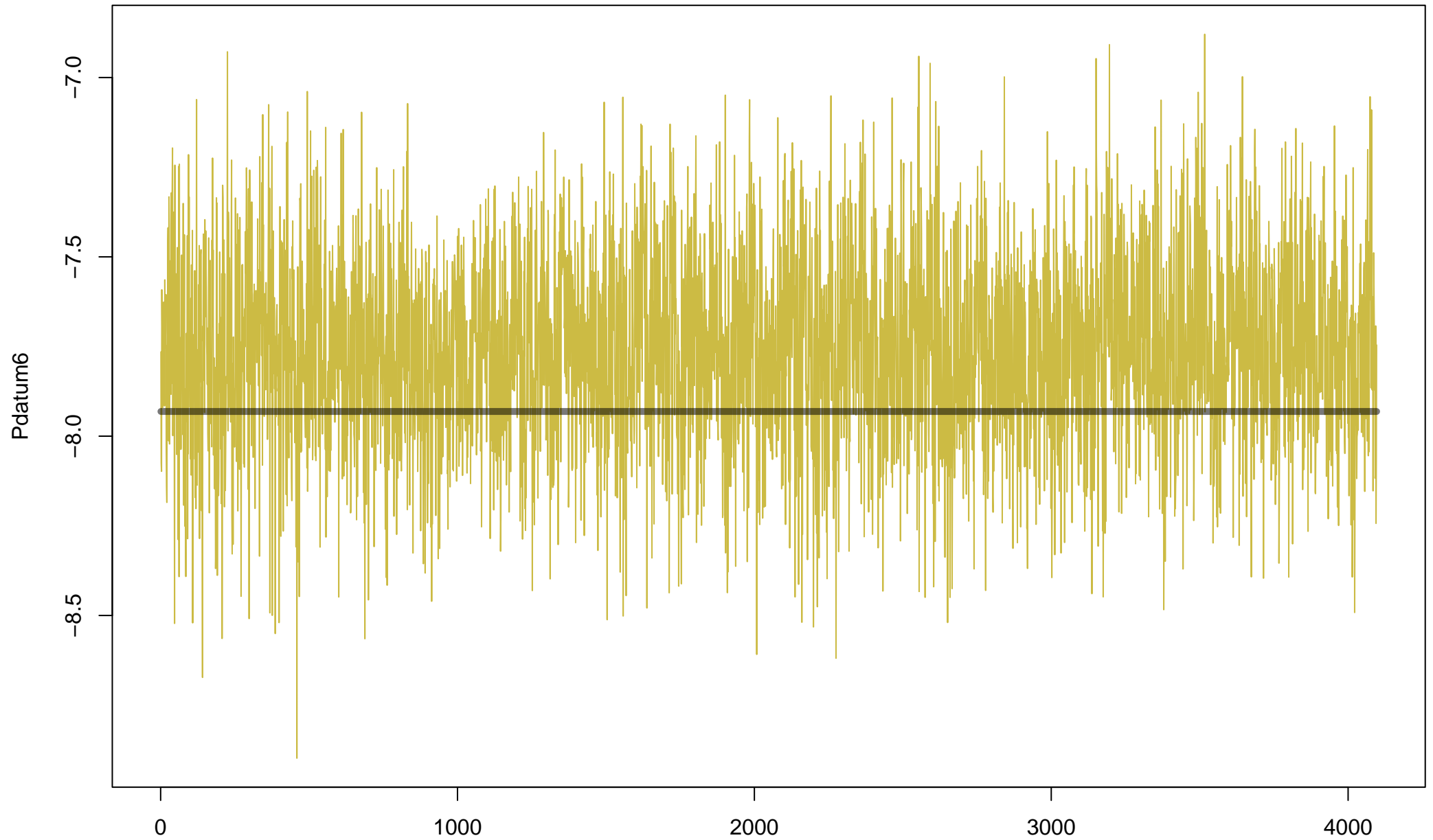
ESS = 1190 | BMK = 0.0476 | MCSE(6.27) = 3.54 | stat: FALSE | burn: 0 | rel.err: -0.0544



Pdatum5
ESS = 771 | BMK = 0.0405 | MCSE(6.27) = 3.14 | stat: FALSE | burn: 0 | rel.err: 1.49

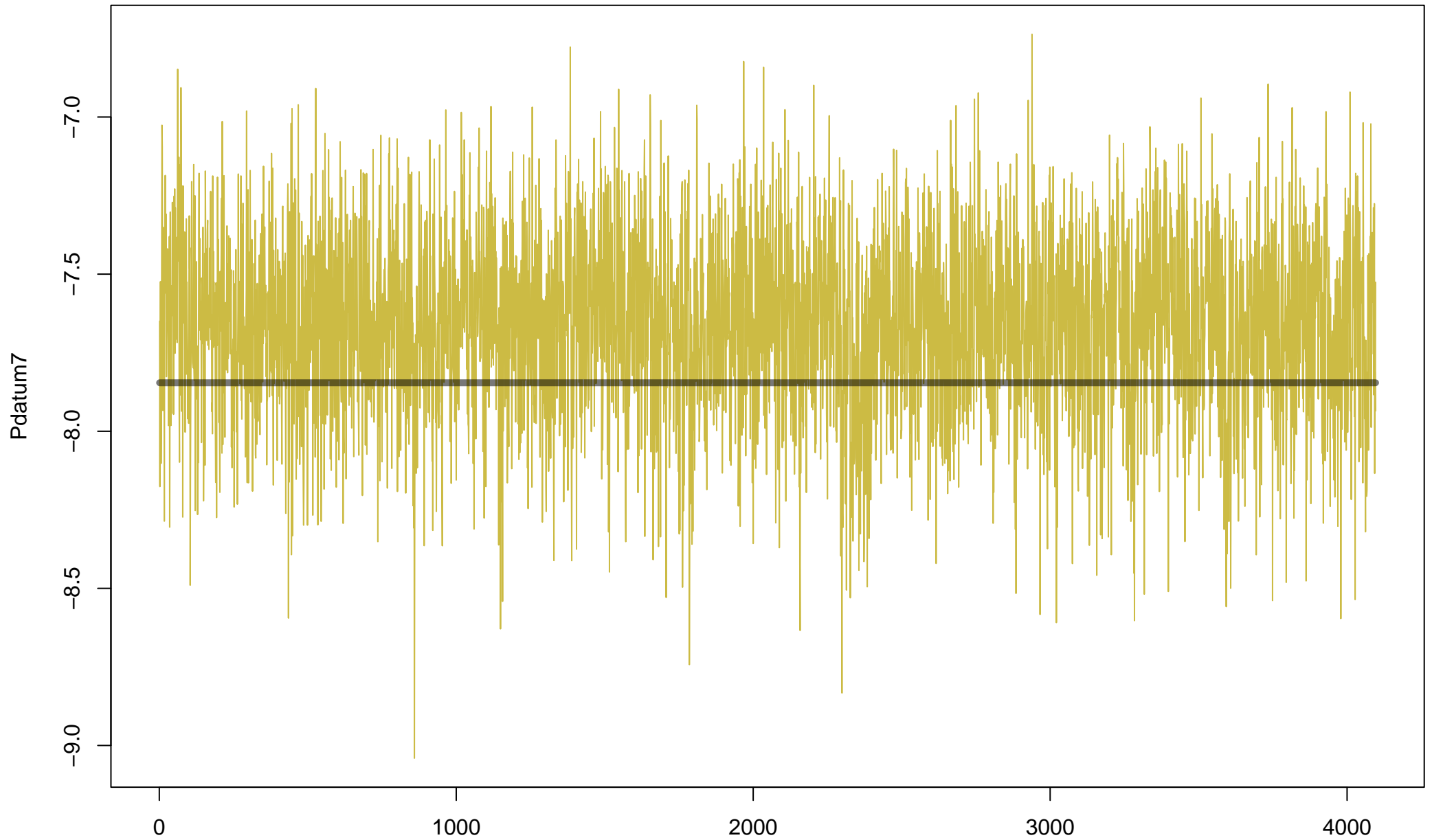


Pdatum6
ESS = 2290 | BMK = 0.034 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0 | rel.err: 0.692

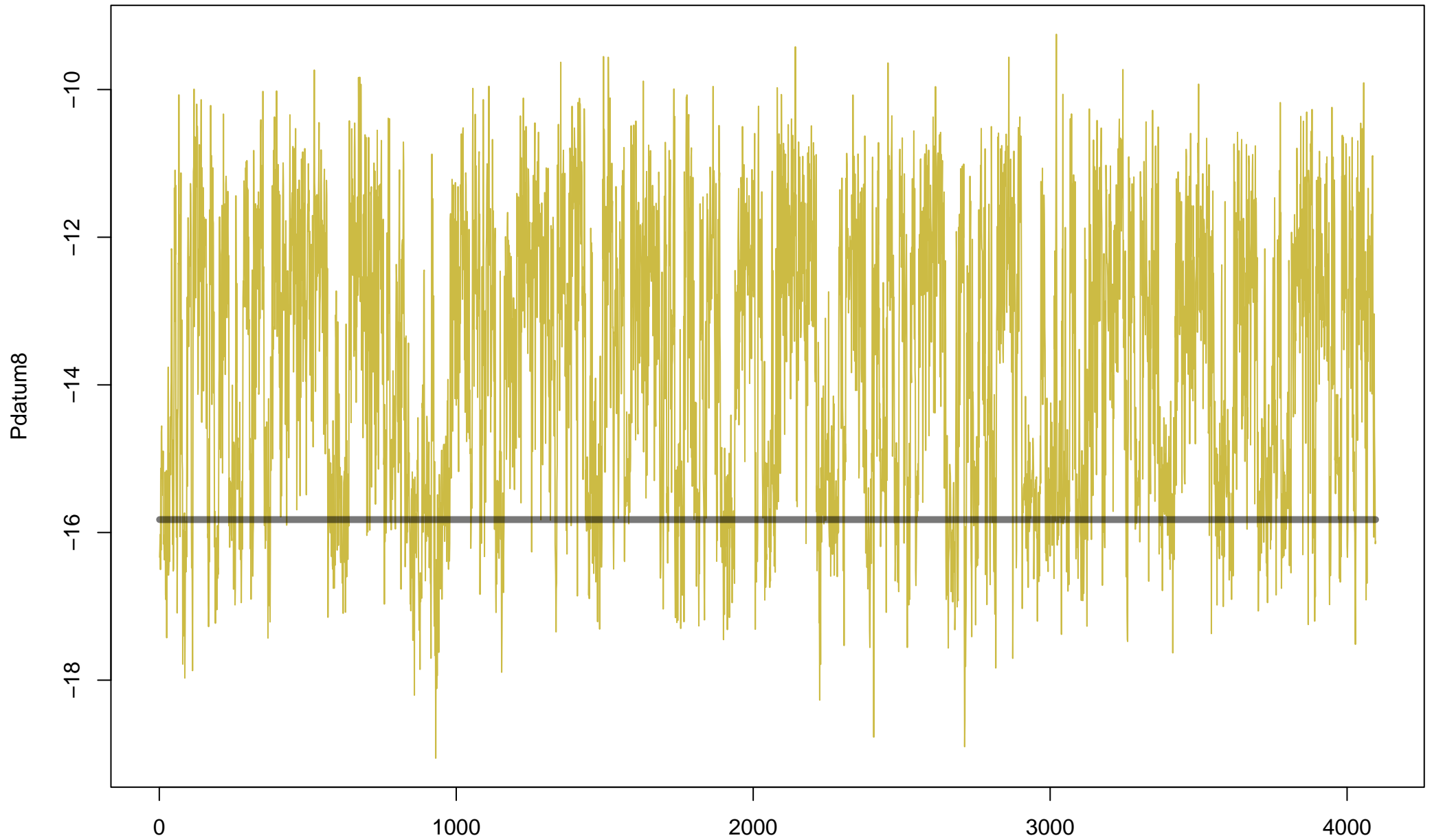


Pdatum7

ESS = 2900 | BMK = 0.0418 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | rel.err: 0.707

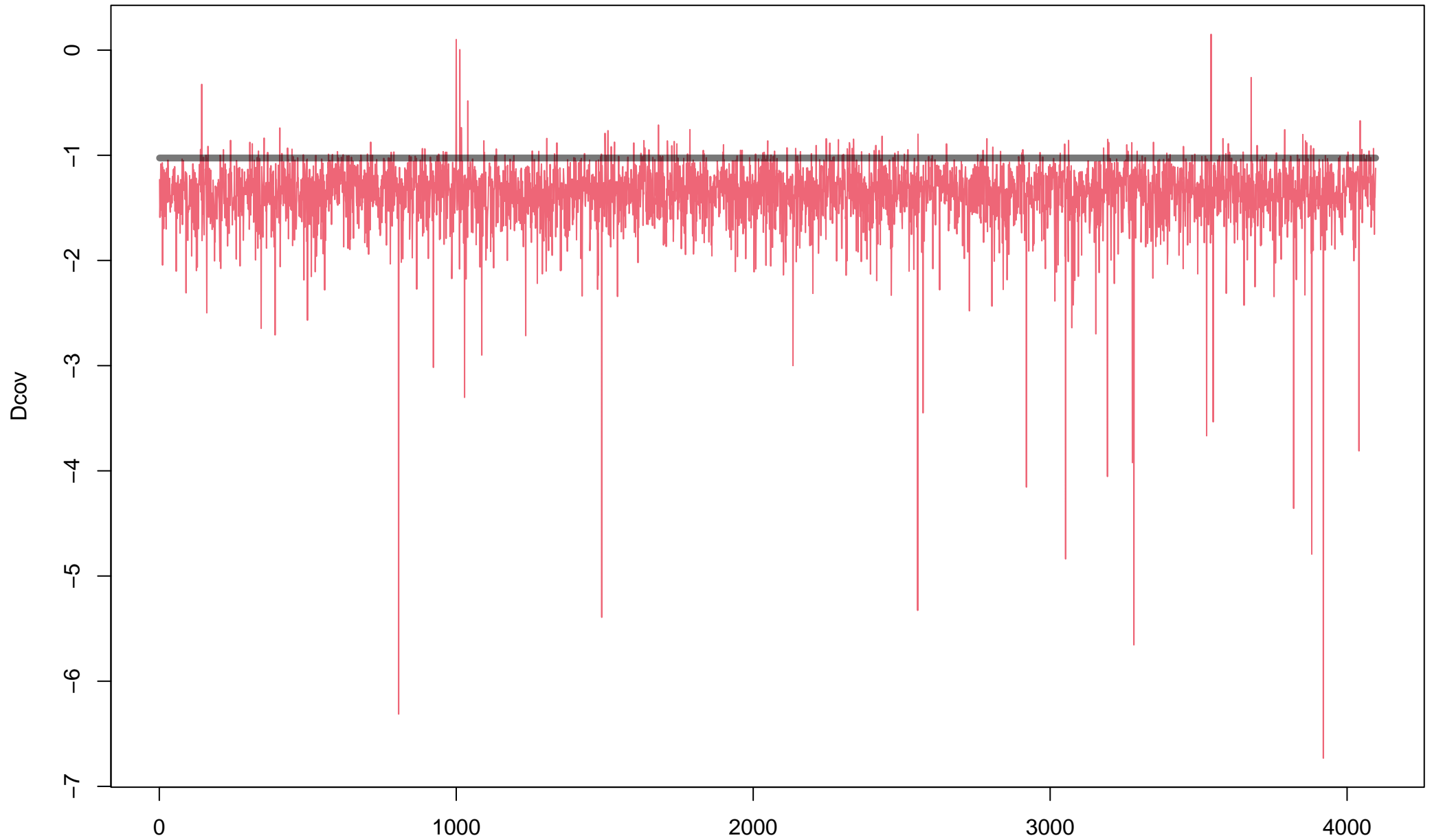


Pdatum8
ESS = 641 | BMK = 0.0722 | MCSE(6.27) = 3.54 | stat: TRUE | burn: 0 | rel.err: 0.579

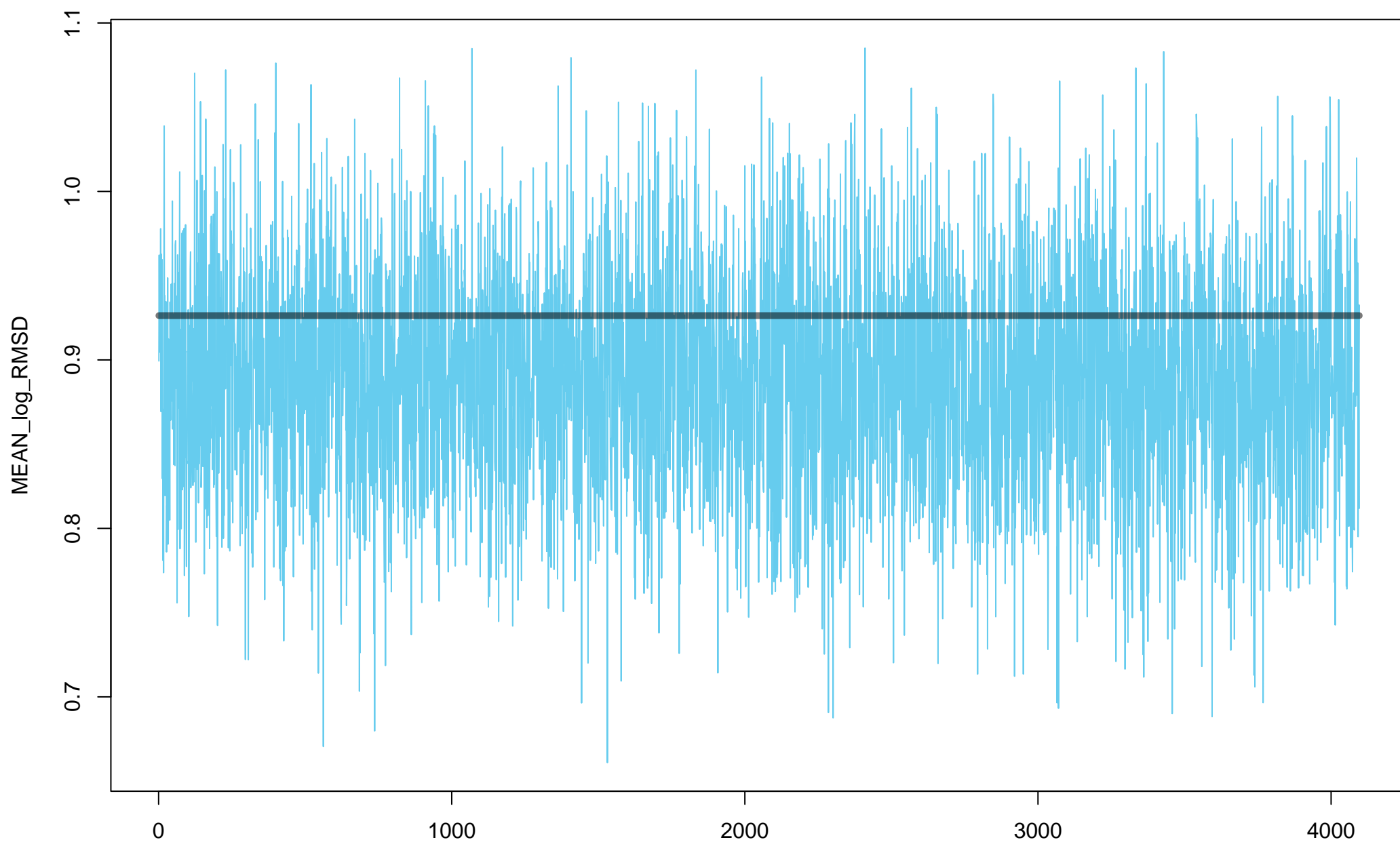


Dcov

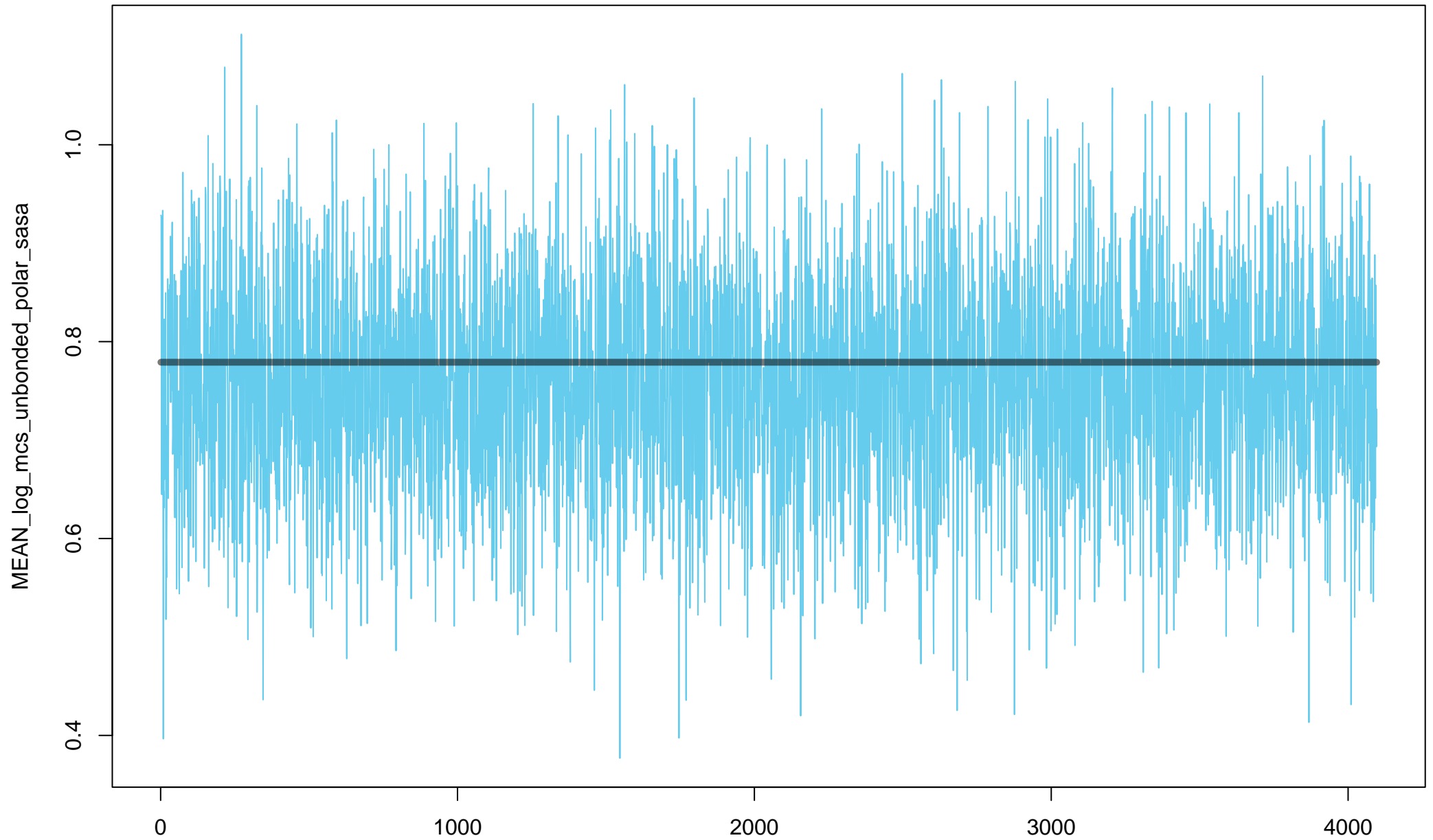
ESS = 3730 | BMK = 0.0673 | MCSE(6.27) = 1.66 | stat: TRUE | burn: 0 | rel.err: 1.31



MEAN_log_RMSD
ESS = 4100 | BMK = 0.0398 | MCSE(6.27) = 1.57 | stat: TRUE | burn: 0 | rel.err: -0.583

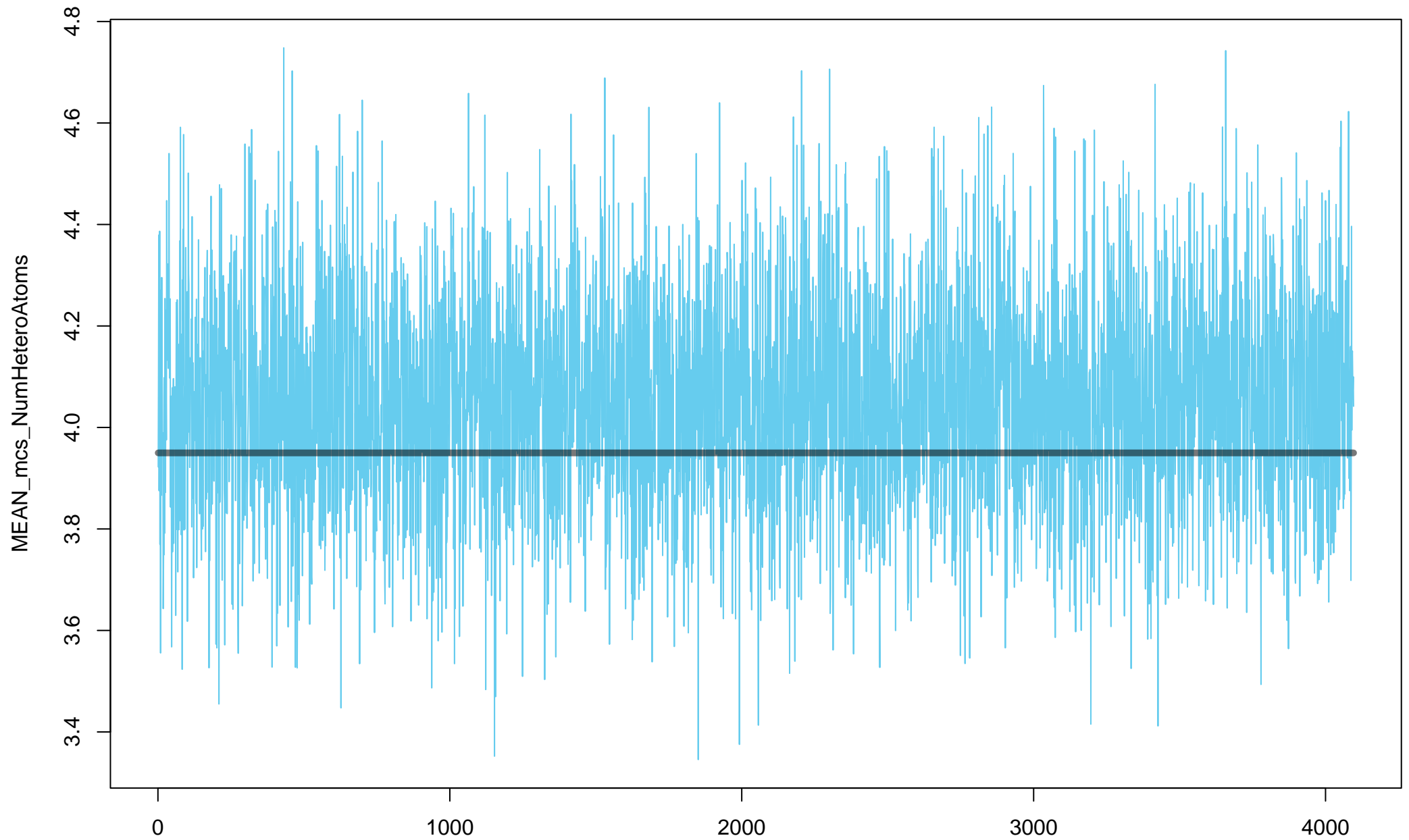


MEAN_log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.0338 | MCSE(6.27) = 1.34 | stat: TRUE | burn: 0 | rel.err: -0.2

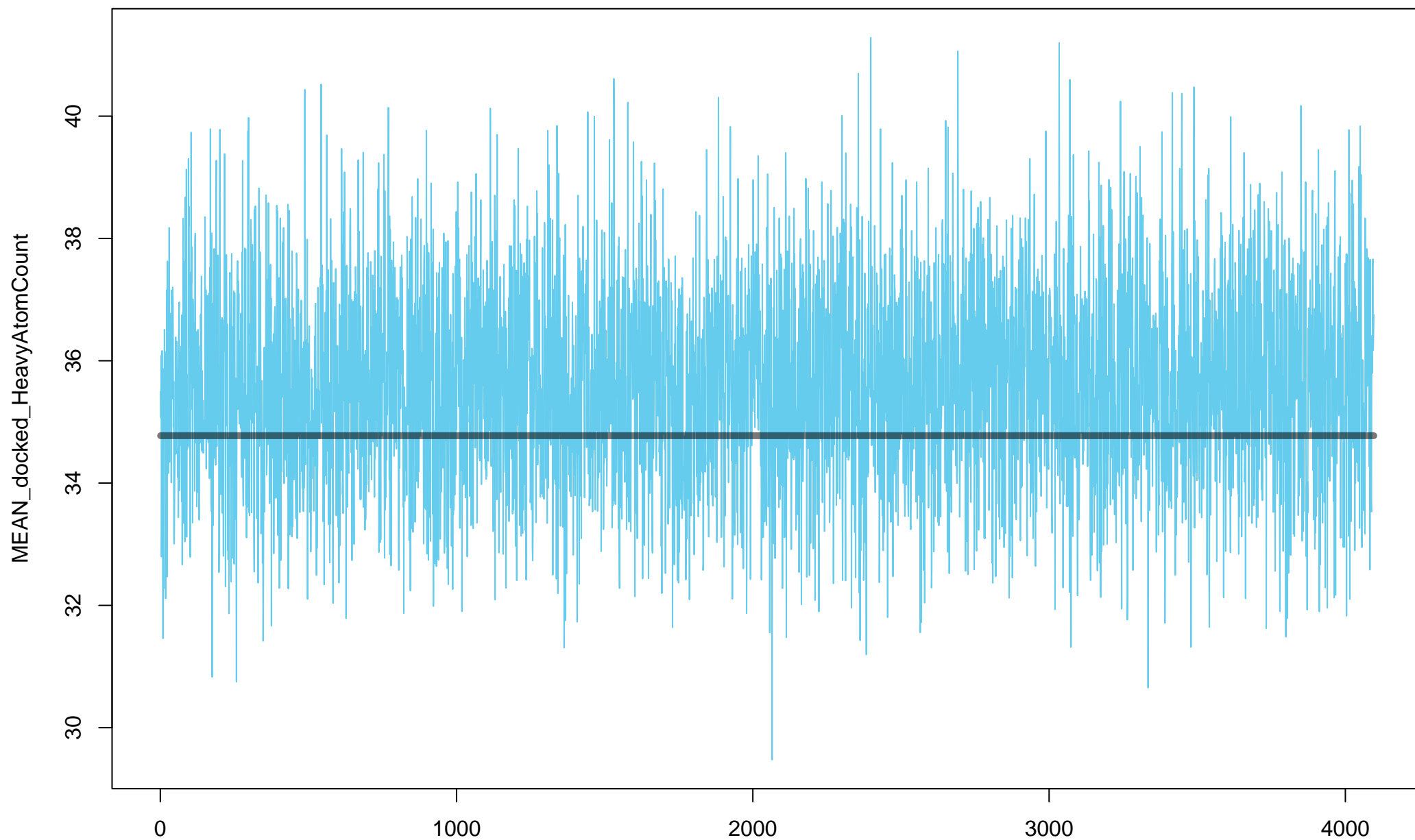


MEAN_mcs_NumHeteroAtoms

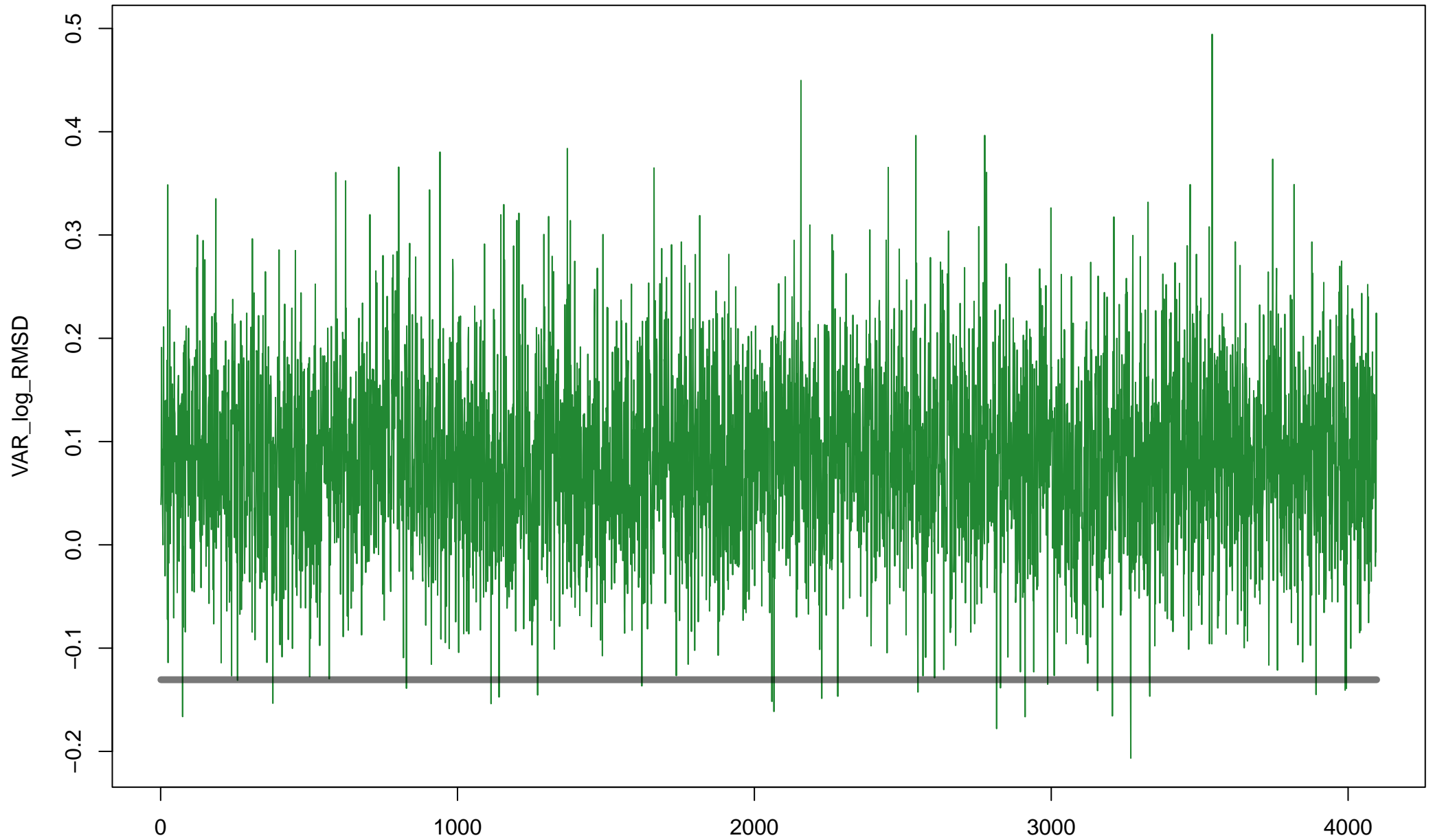
ESS = 4100 | BMK = 0.0348 | MCSE(6.27) = 1.58 | stat: TRUE | burn: 0 | rel.err: 0.497



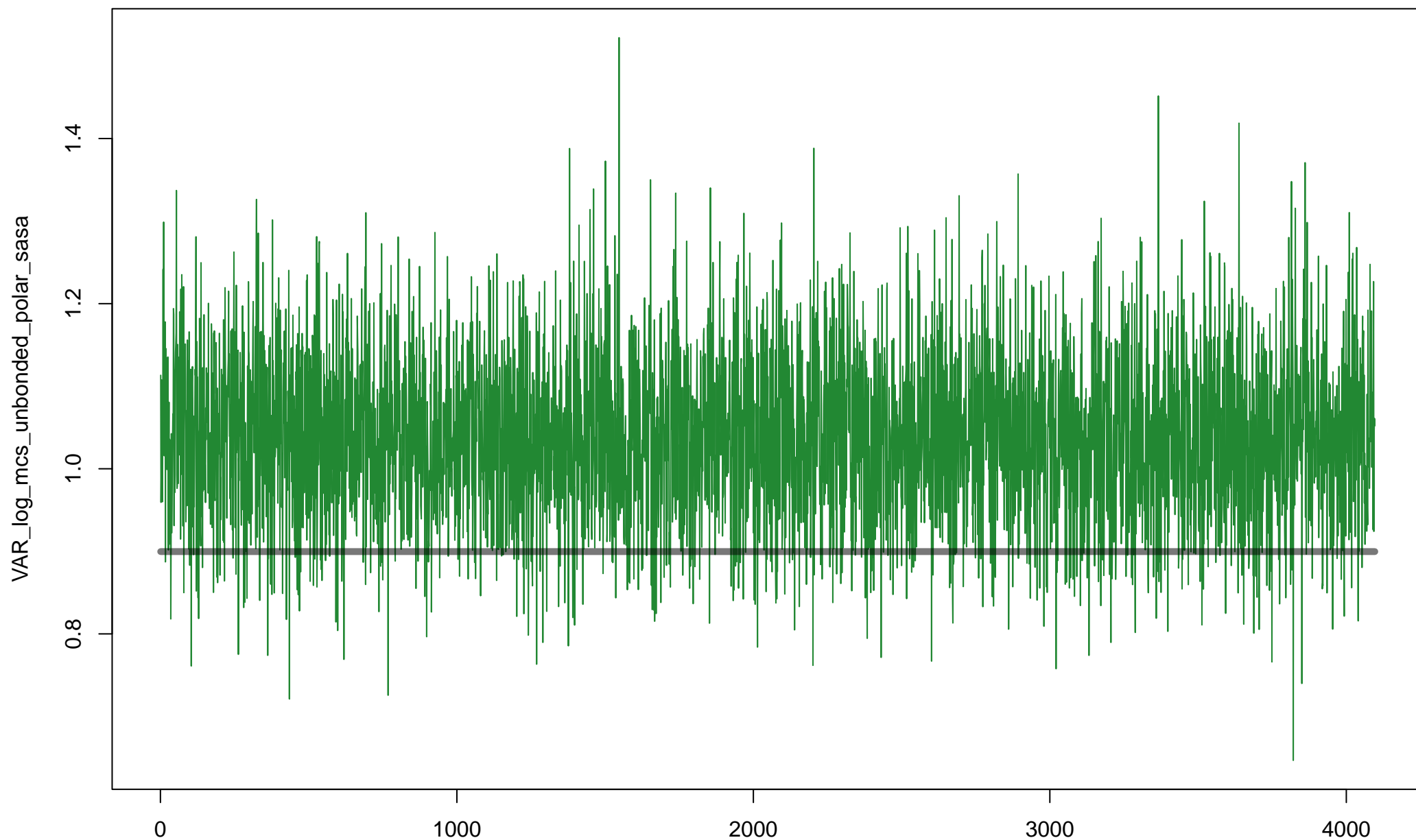
MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0432 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: 0.513



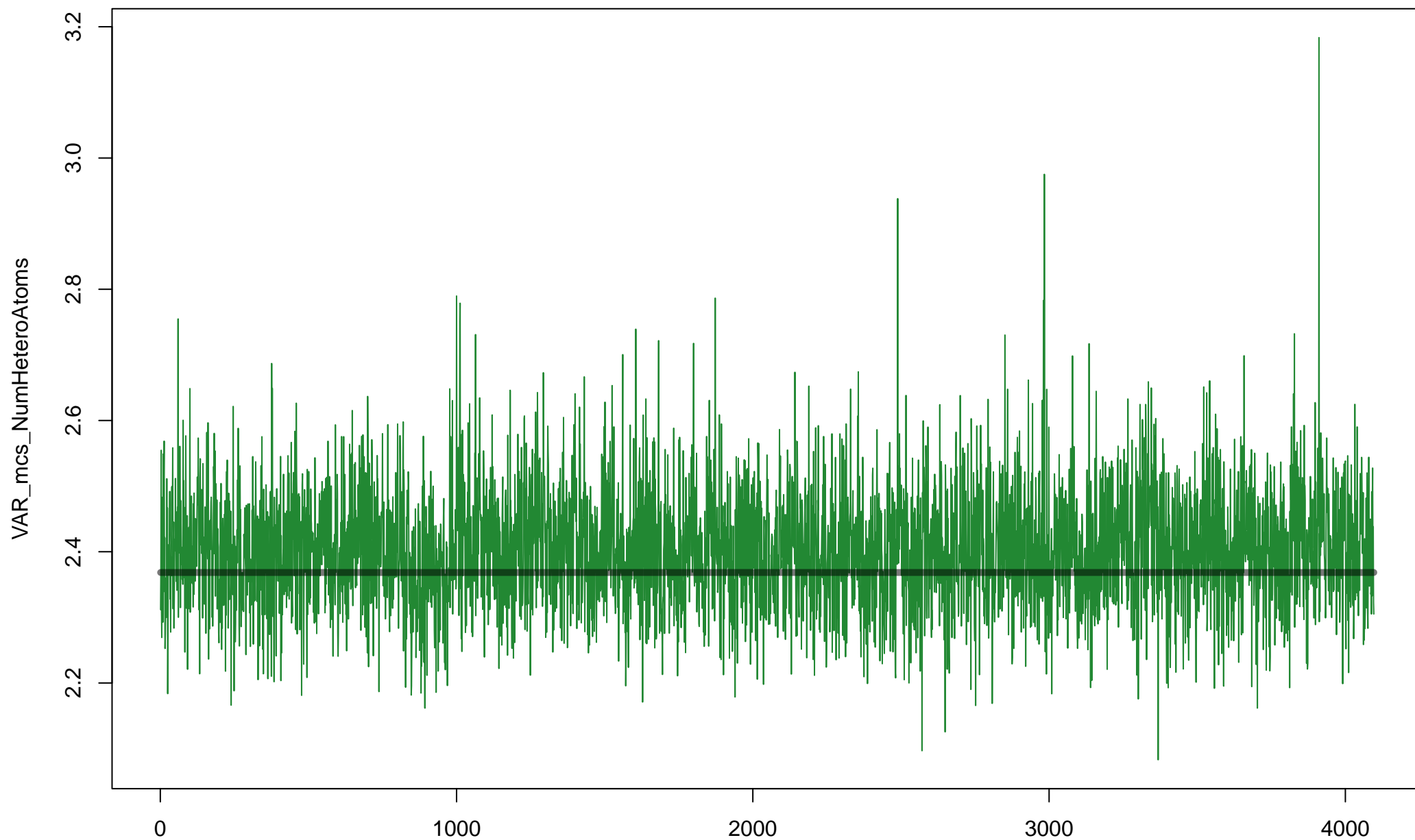
VAR_log_RMSD
ESS = 4100 | BMK = 0.0421 | MCSE(6.27) = 1.83 | stat: TRUE | burn: 0 | rel.err: 2.26



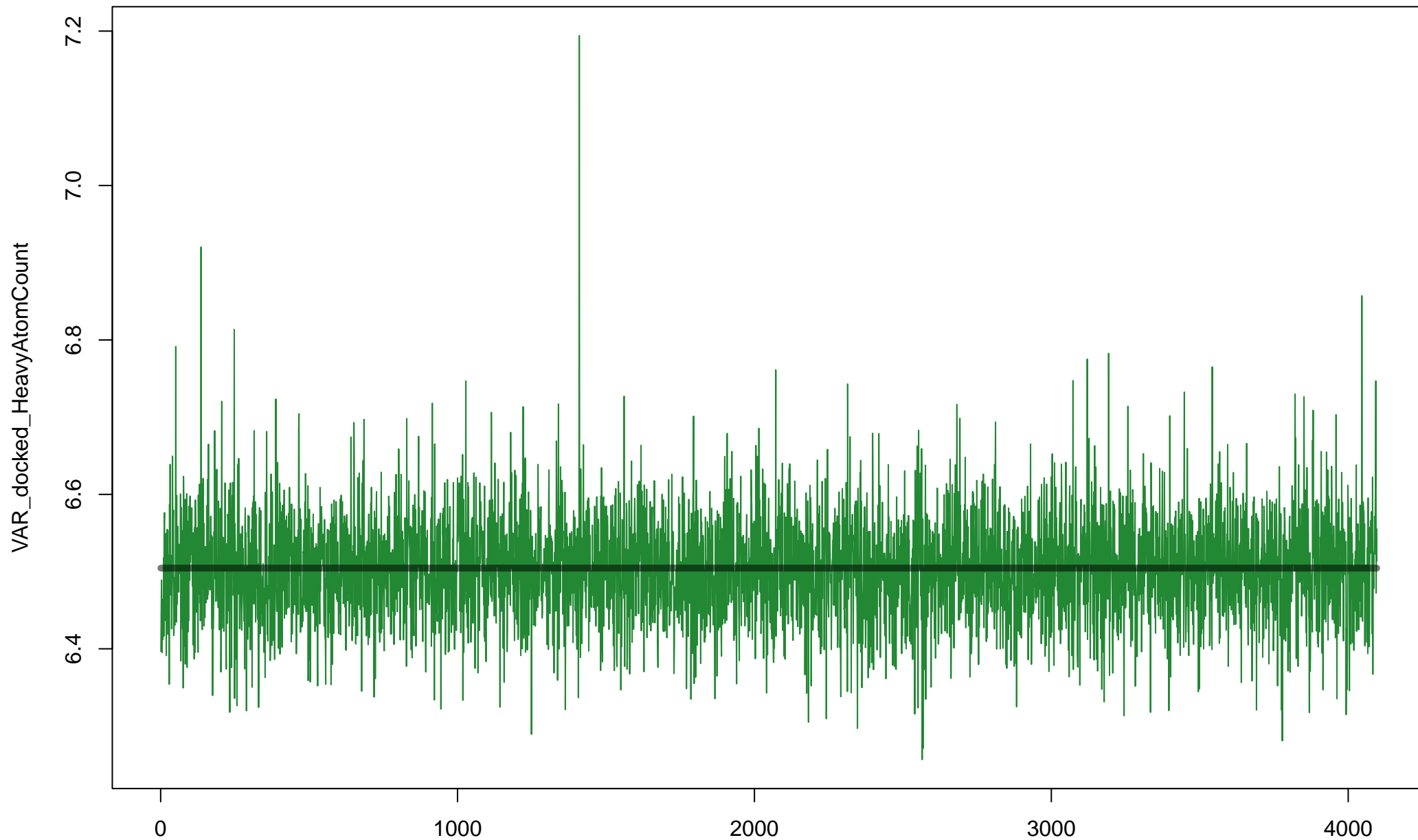
VAR_log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.0354 | MCSE(6.27) = 1.5 | stat: TRUE | burn: 0 | rel.err: 1.33



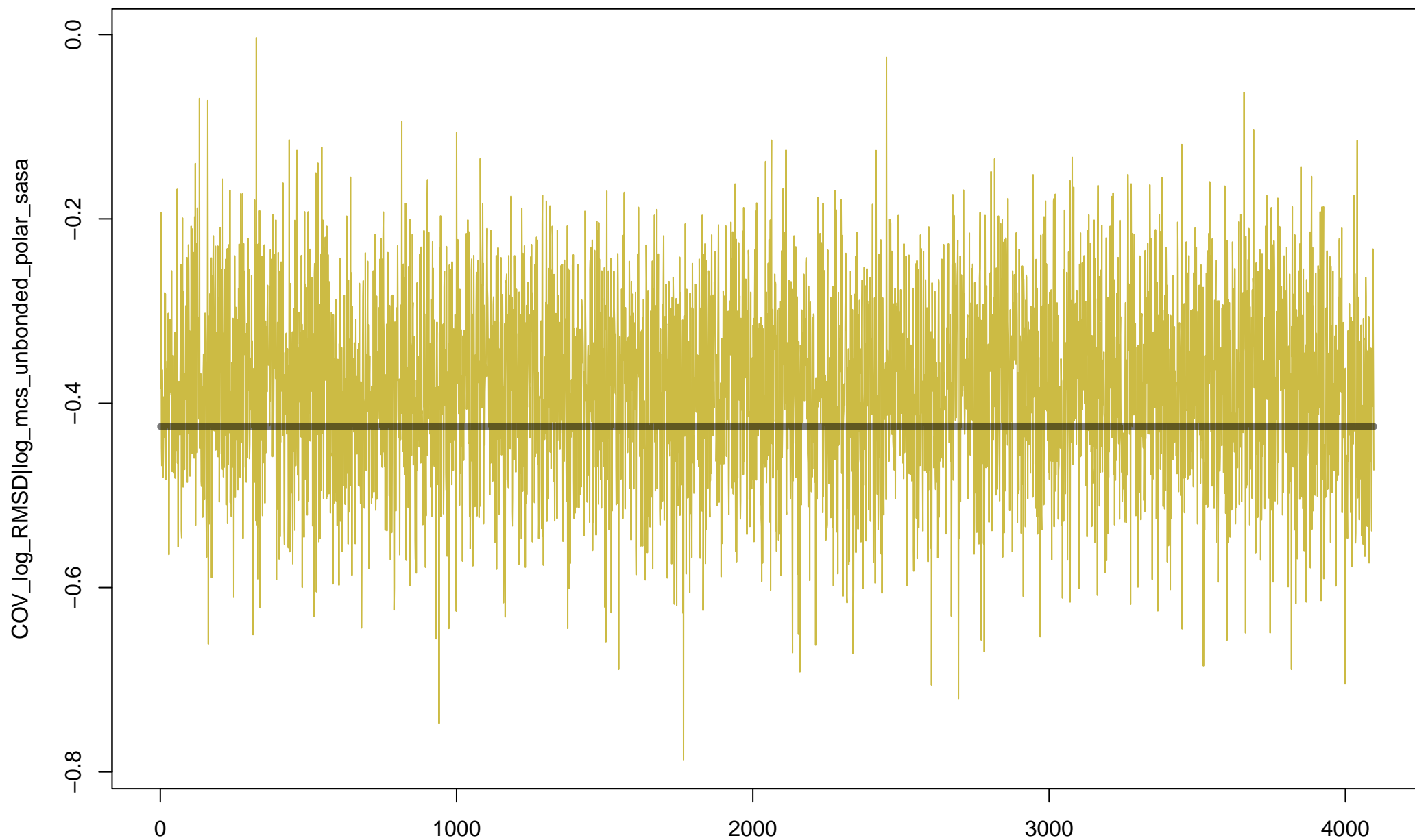
VAR_mcs_NumHeteroAtoms
ESS = 2380 | BMK = 0.0469 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.417



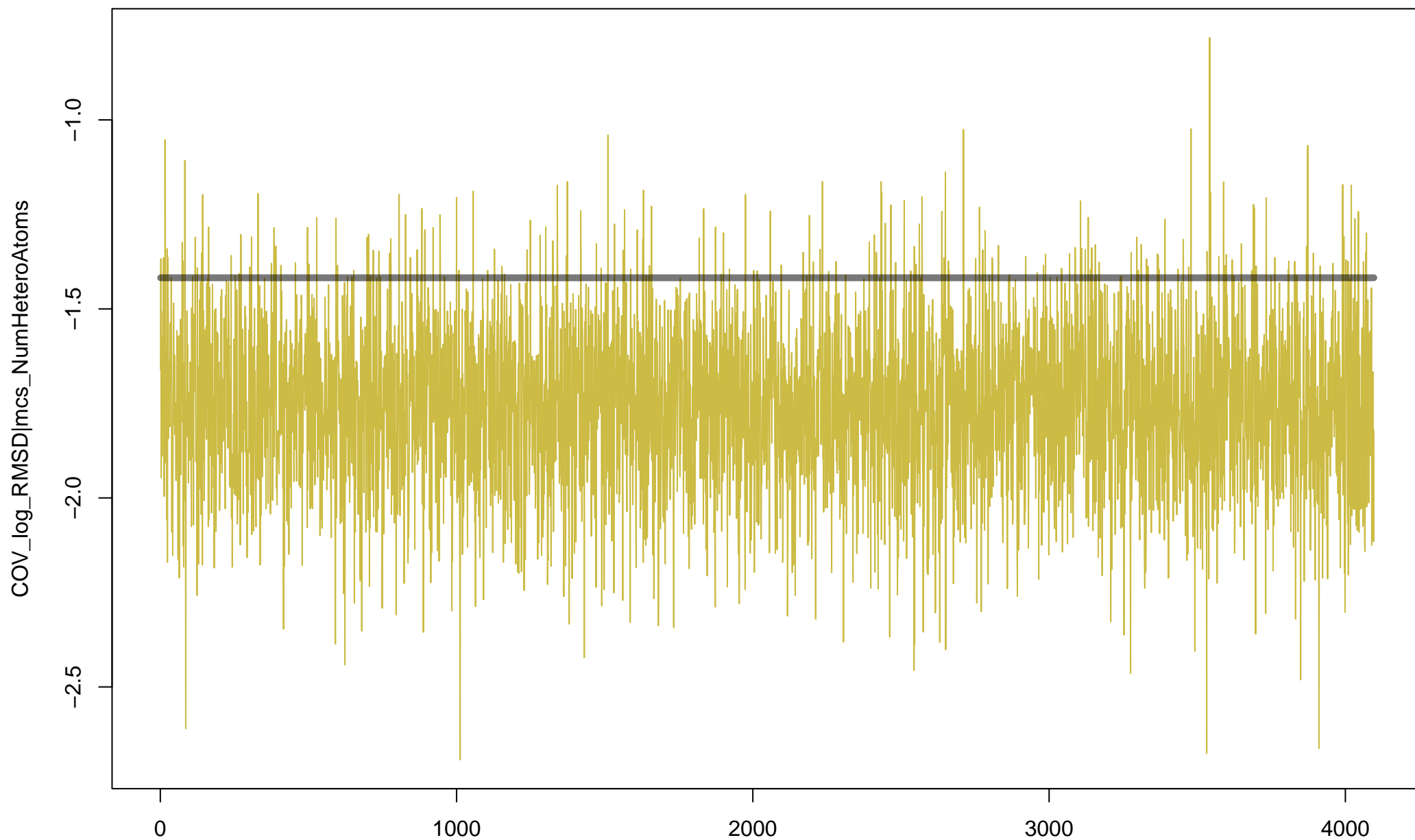
VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0497 | MCSE(6.27) = 1.59 | stat: TRUE | burn: 0 | rel.err: 0.0309



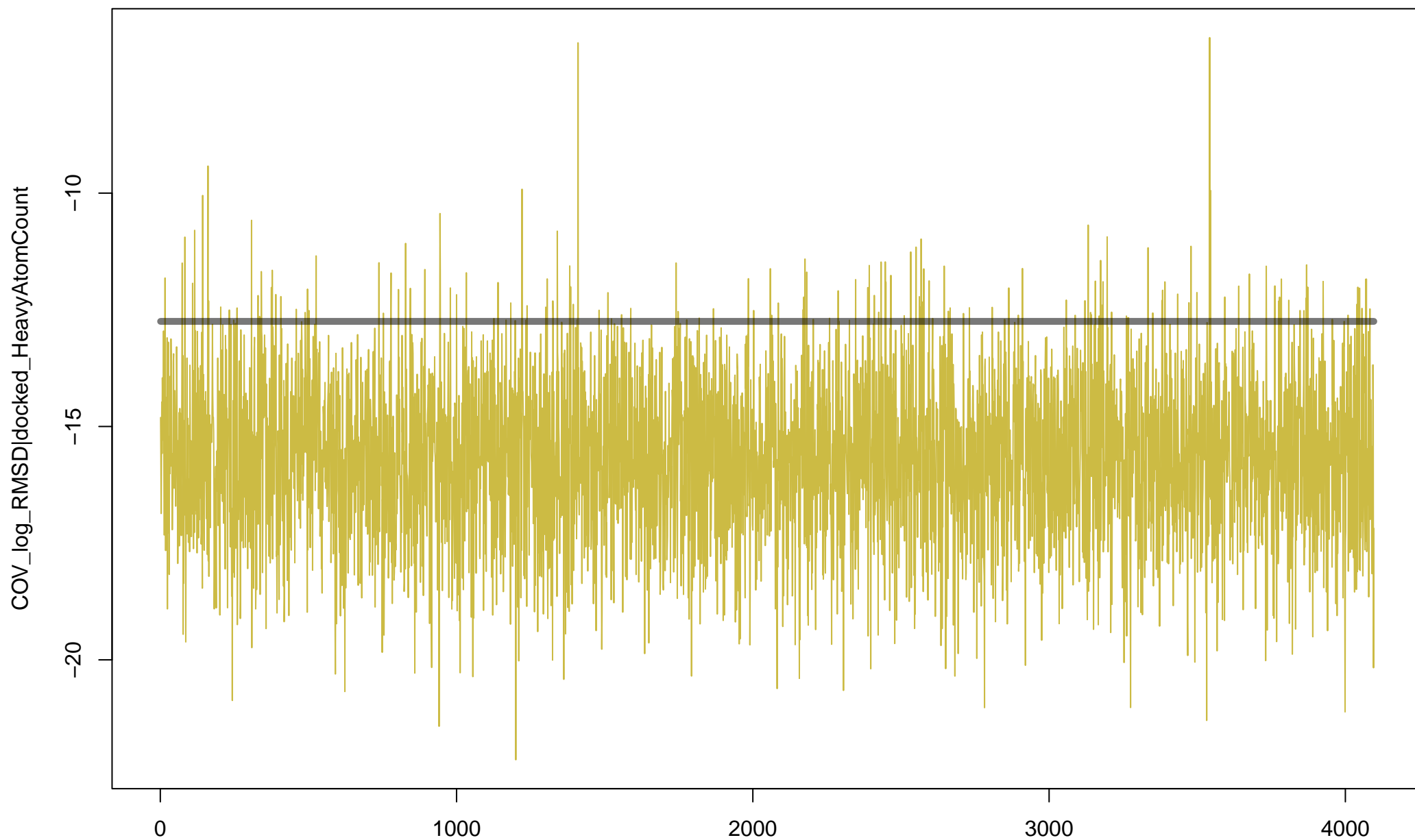
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3740 | BMK = 0.0329 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0 | rel.err: 0.453



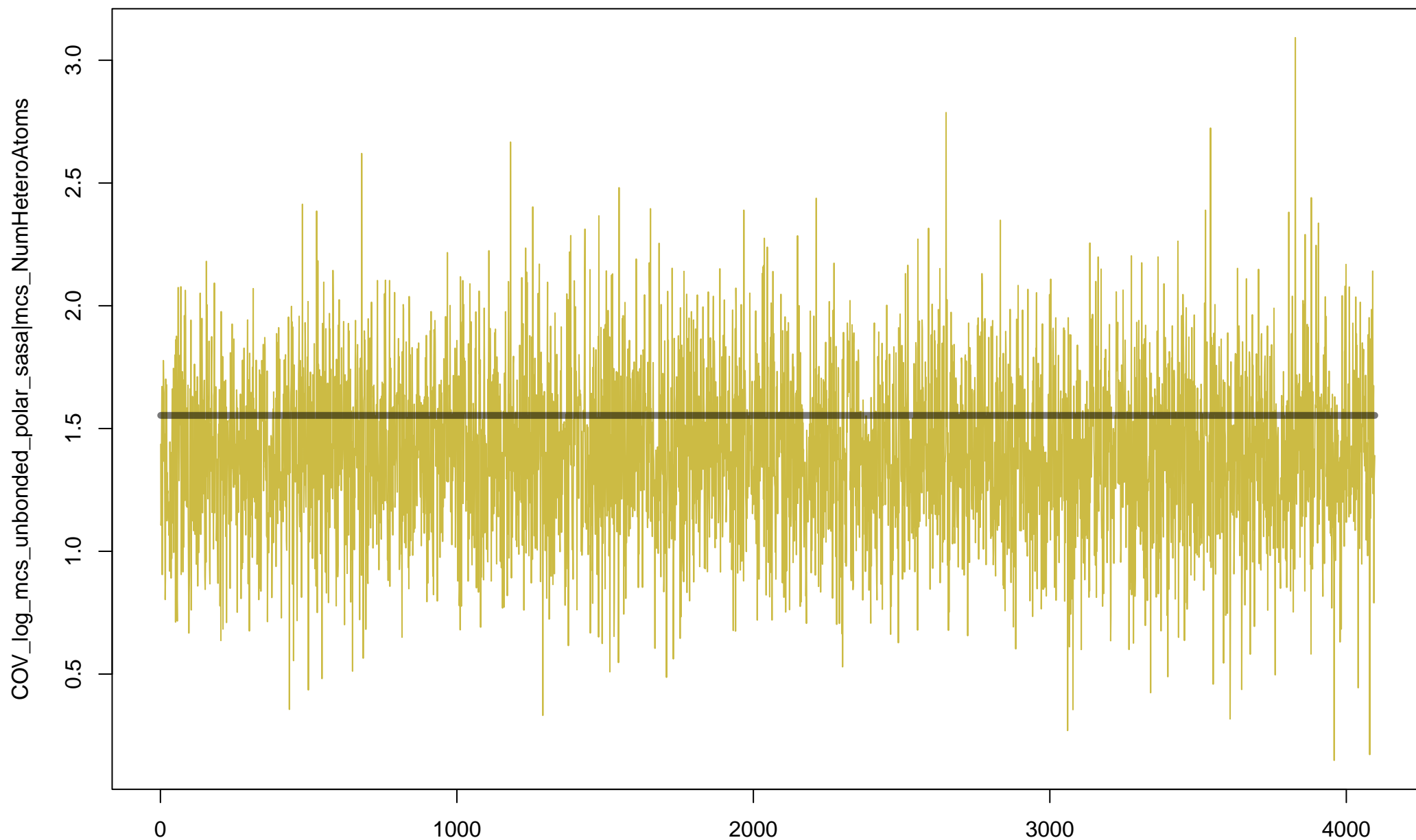
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0366 | MCSE(6.27) = 1.4 | stat: TRUE | burn: 0 | rel.err: -1.57



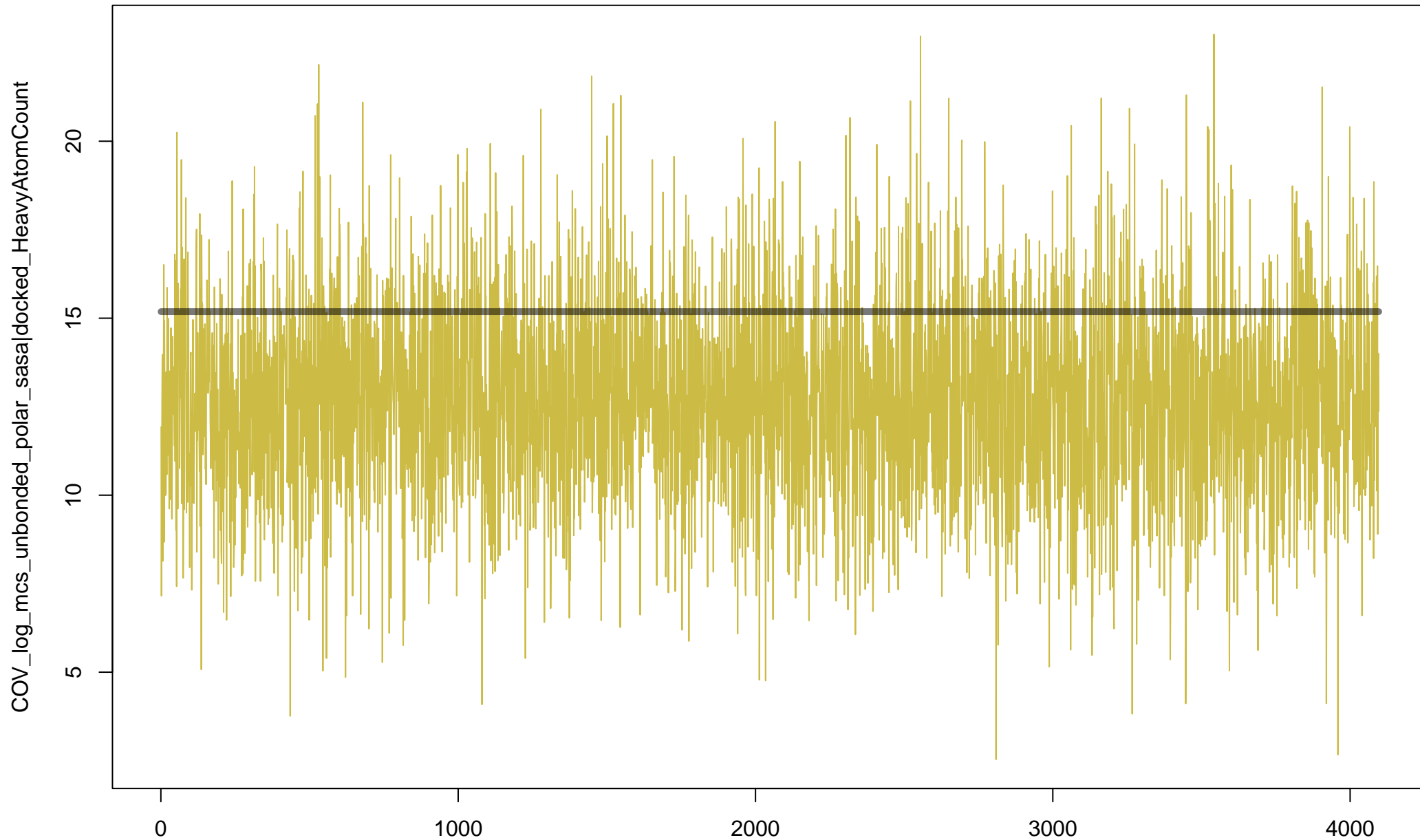
COV_log_RMSD|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0401 | MCSE(6.27) = 1.58 | stat: TRUE | burn: 0 | rel.err: -1.71



COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 3780 | BMK = 0.0403 | MCSE(6.27) = 1.65 | stat: TRUE | burn: 0 | rel.err: -0.467



COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0396 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: -0.944



COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0359 | MCSE(6.27) = 1.54 | stat: FALSE | burn: 0 | rel.err: 0.459

