

-- STATS maxD --

min ESS = 6.62698397555167

max BMK = 0.55797827113591

max MCSE = 12.352433381488

all stationary: FALSE

burn: 1224

-- STATS 2D --

min ESS = 1272.89202777971

max BMK = 0.0694123389669299

max MCSE = 3.05380308273306

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.523854130455817

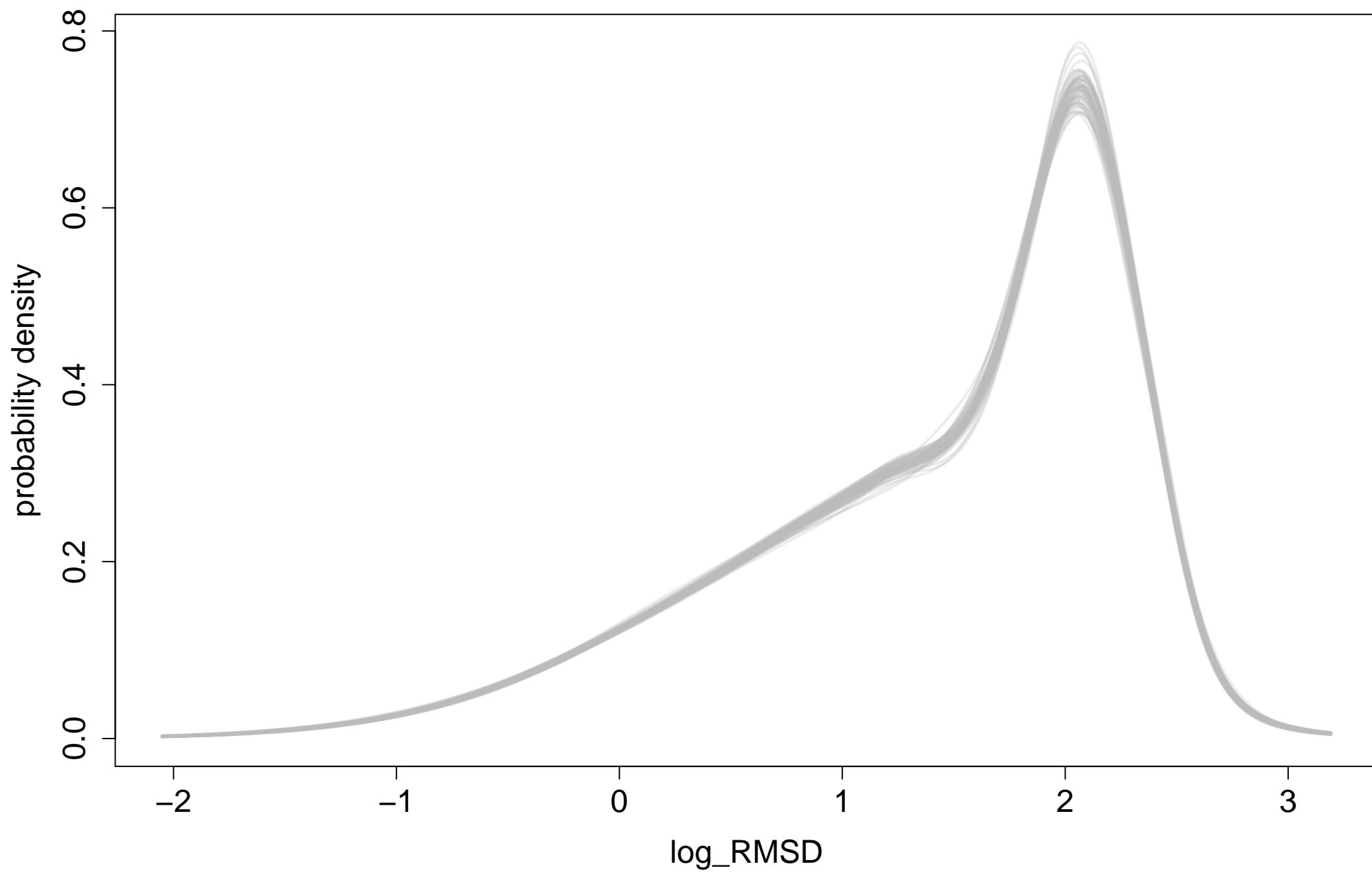
max MCSE = NaN

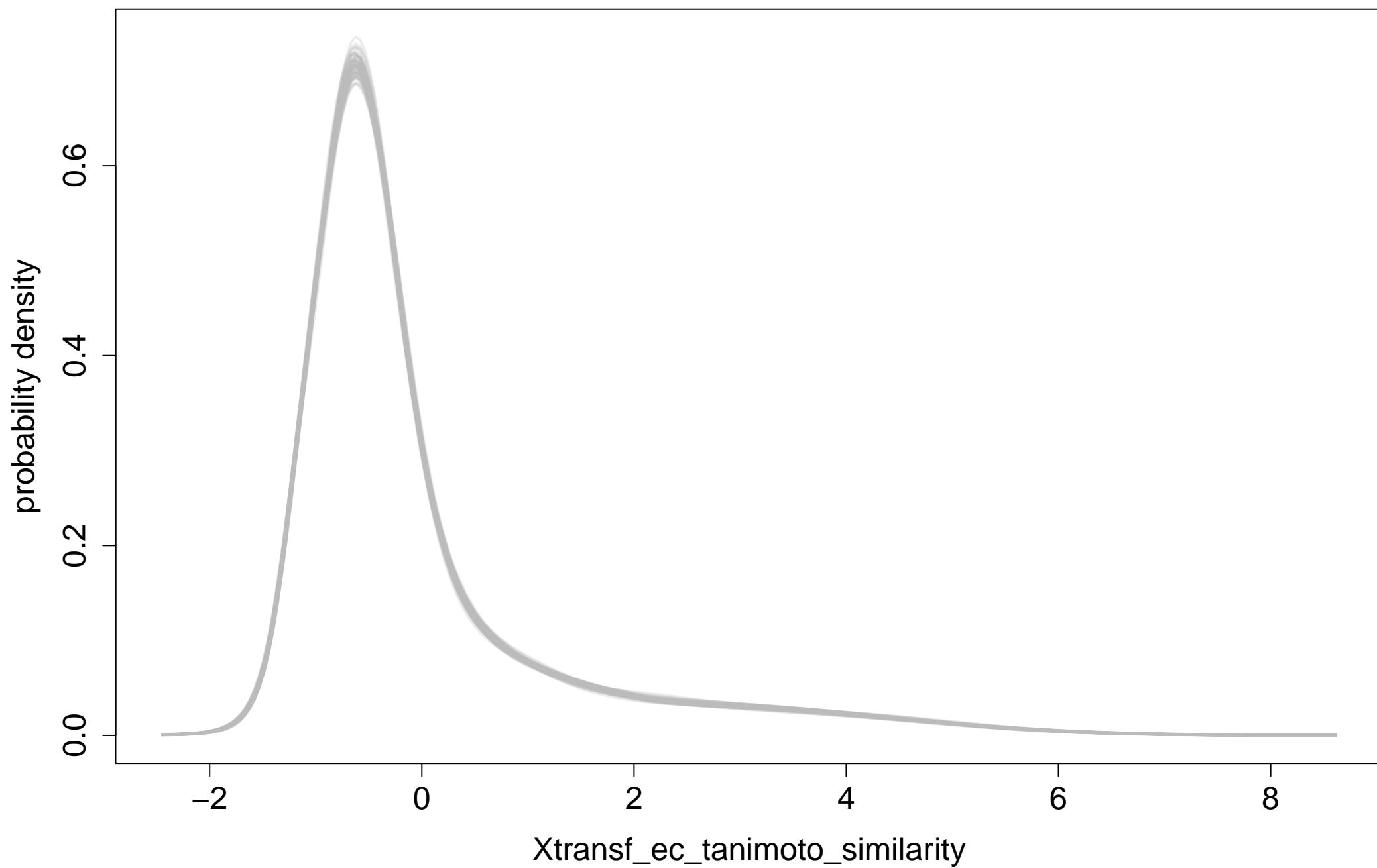
all stationary: FALSE

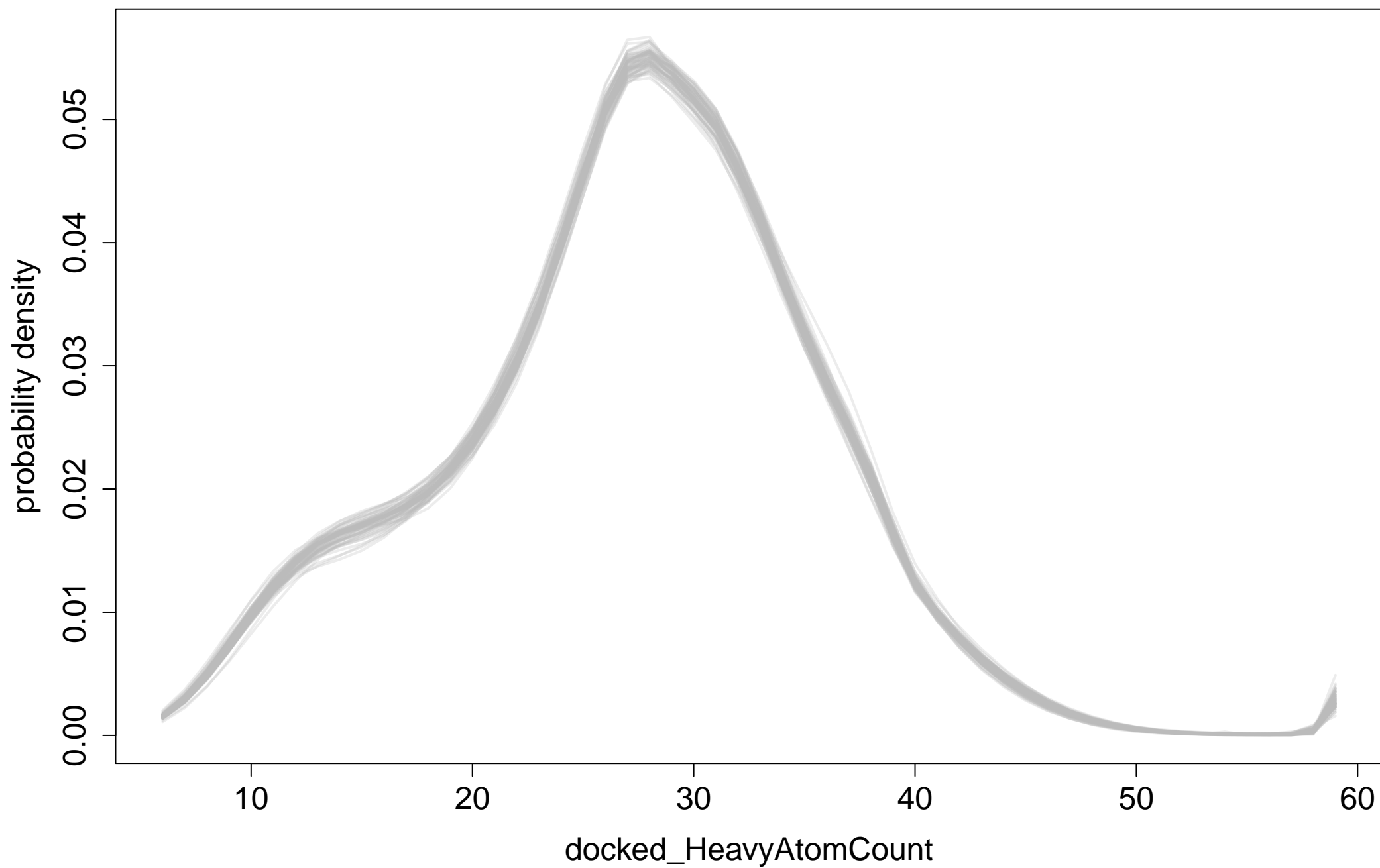
burn: 2040

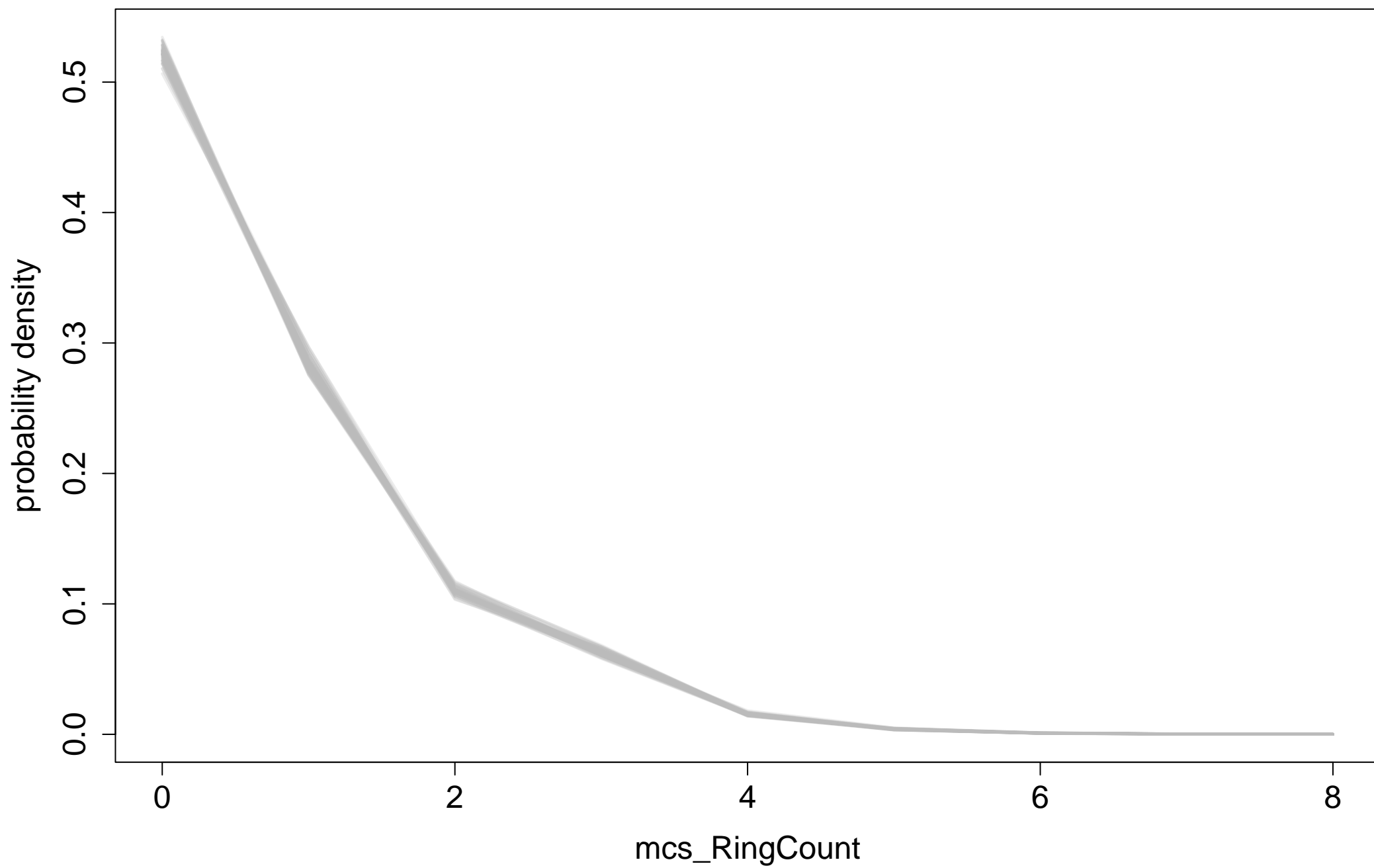
Occupied clusters: 74 of 91

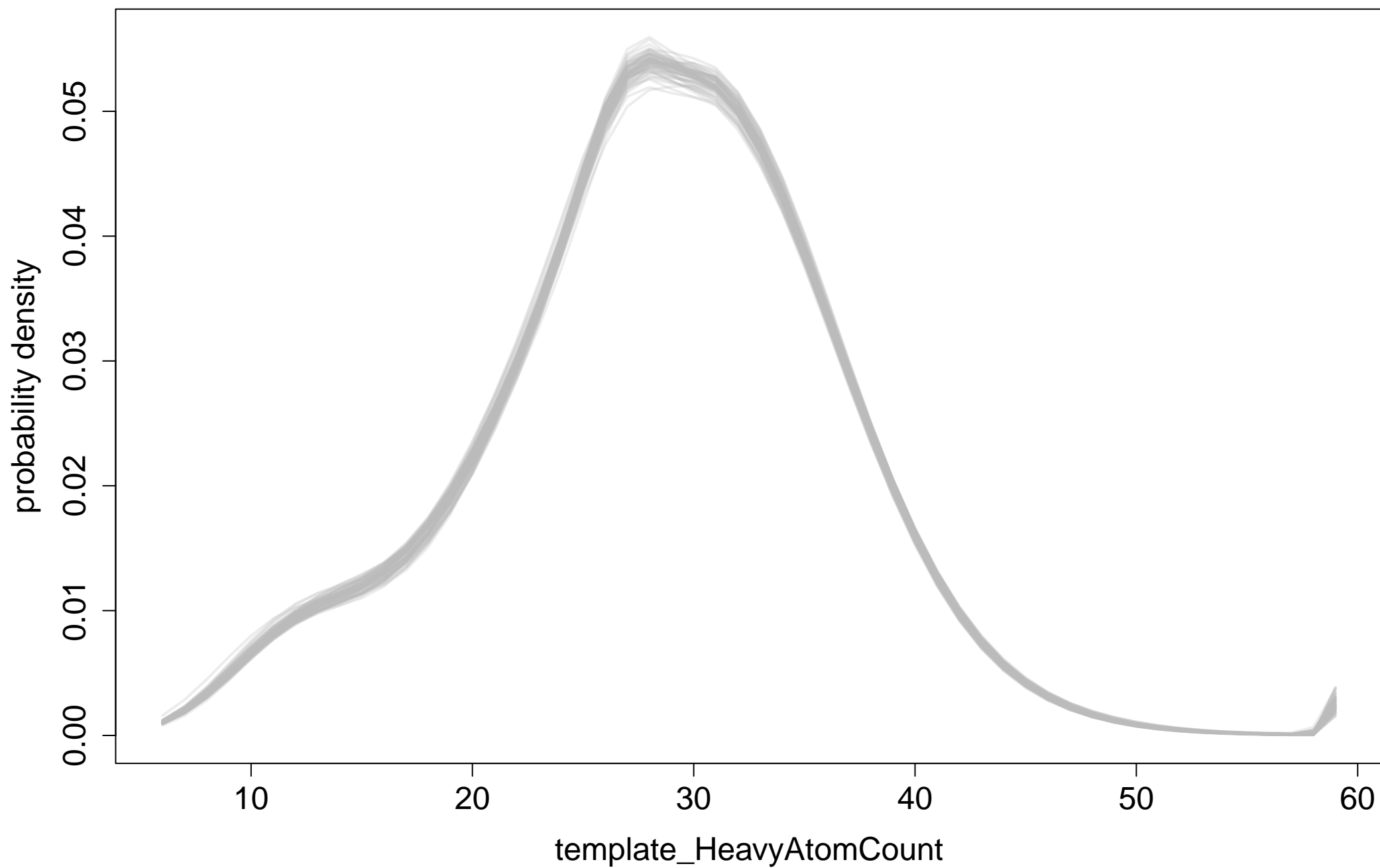
LL: -109000 +- 38.8

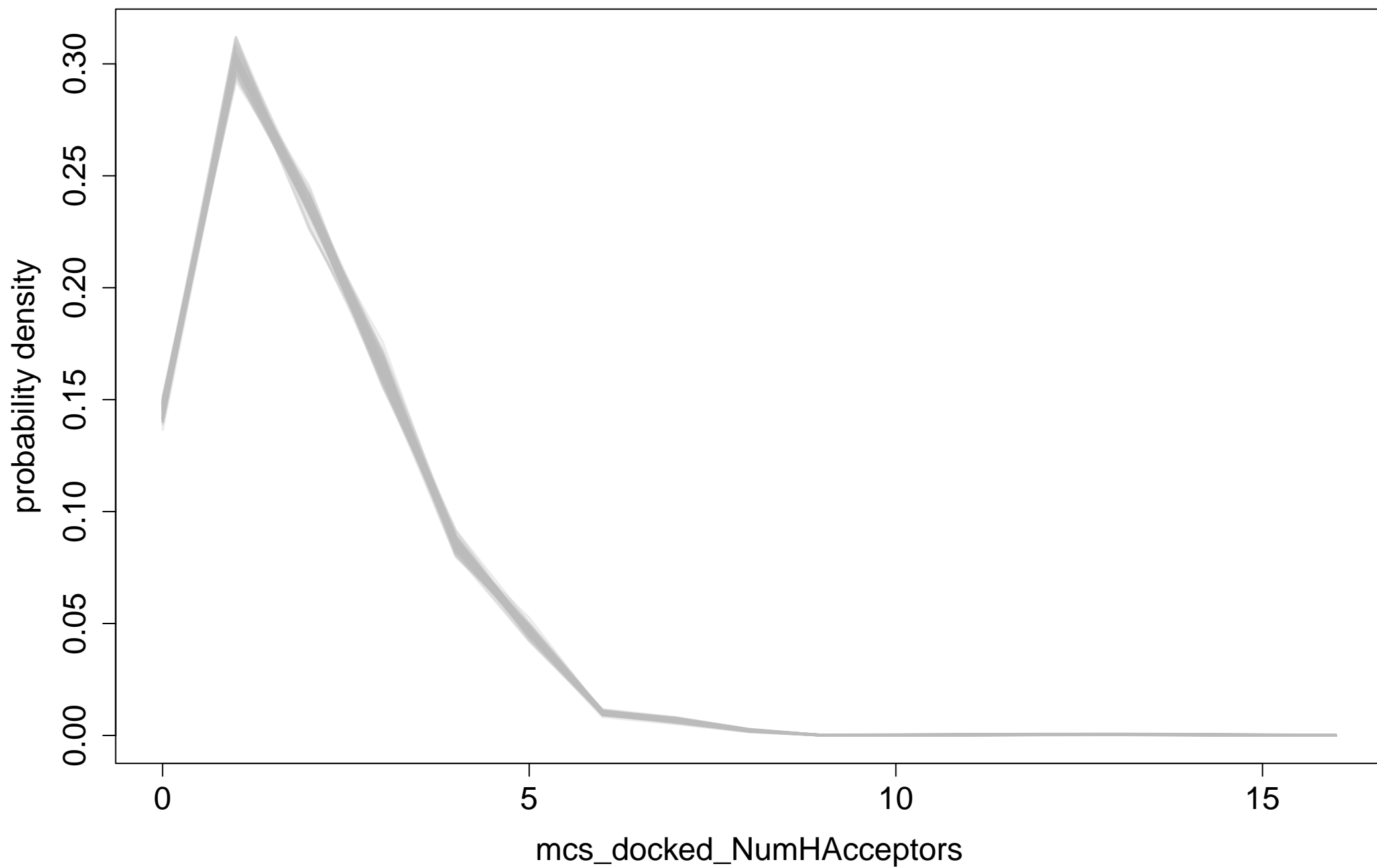


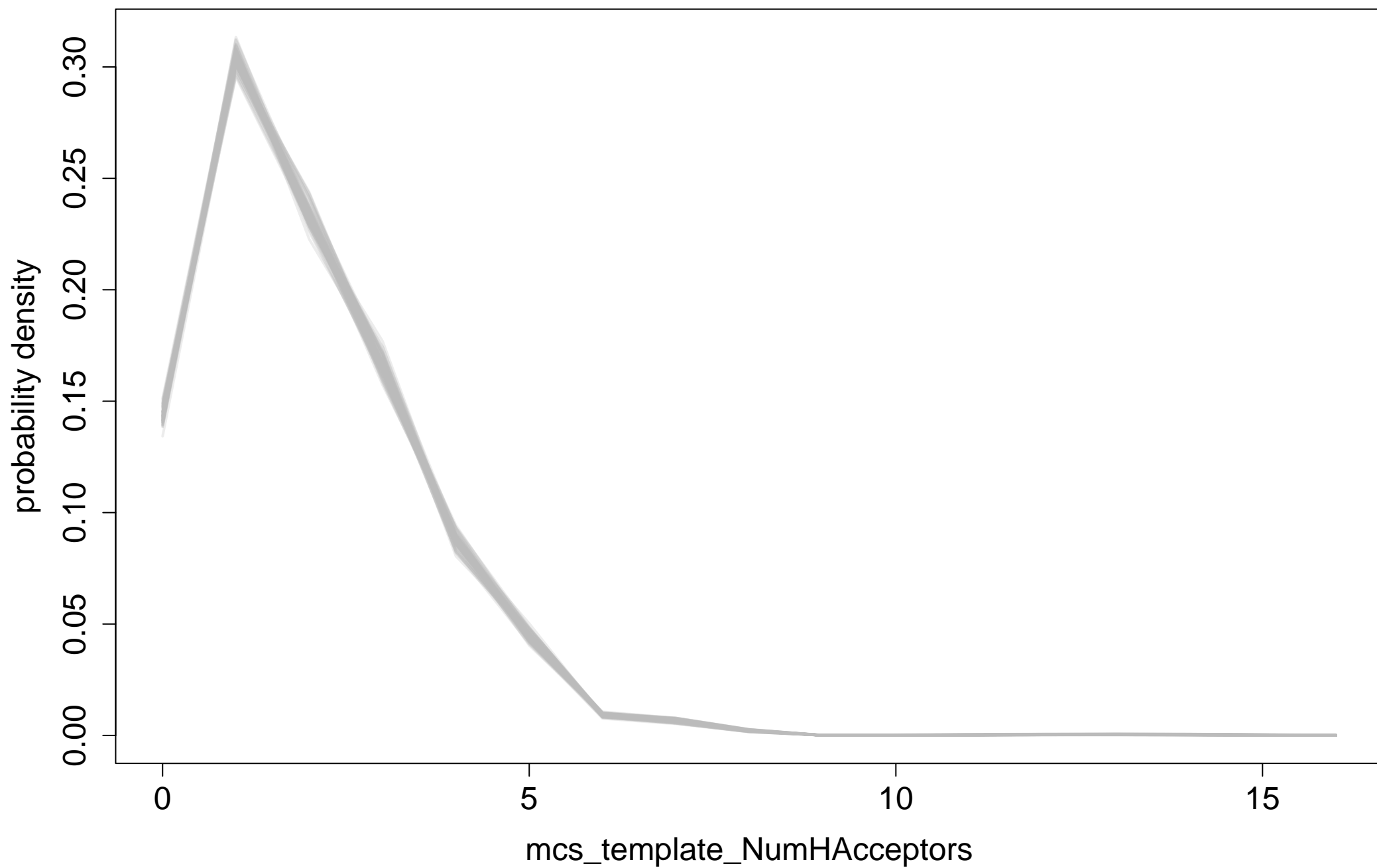


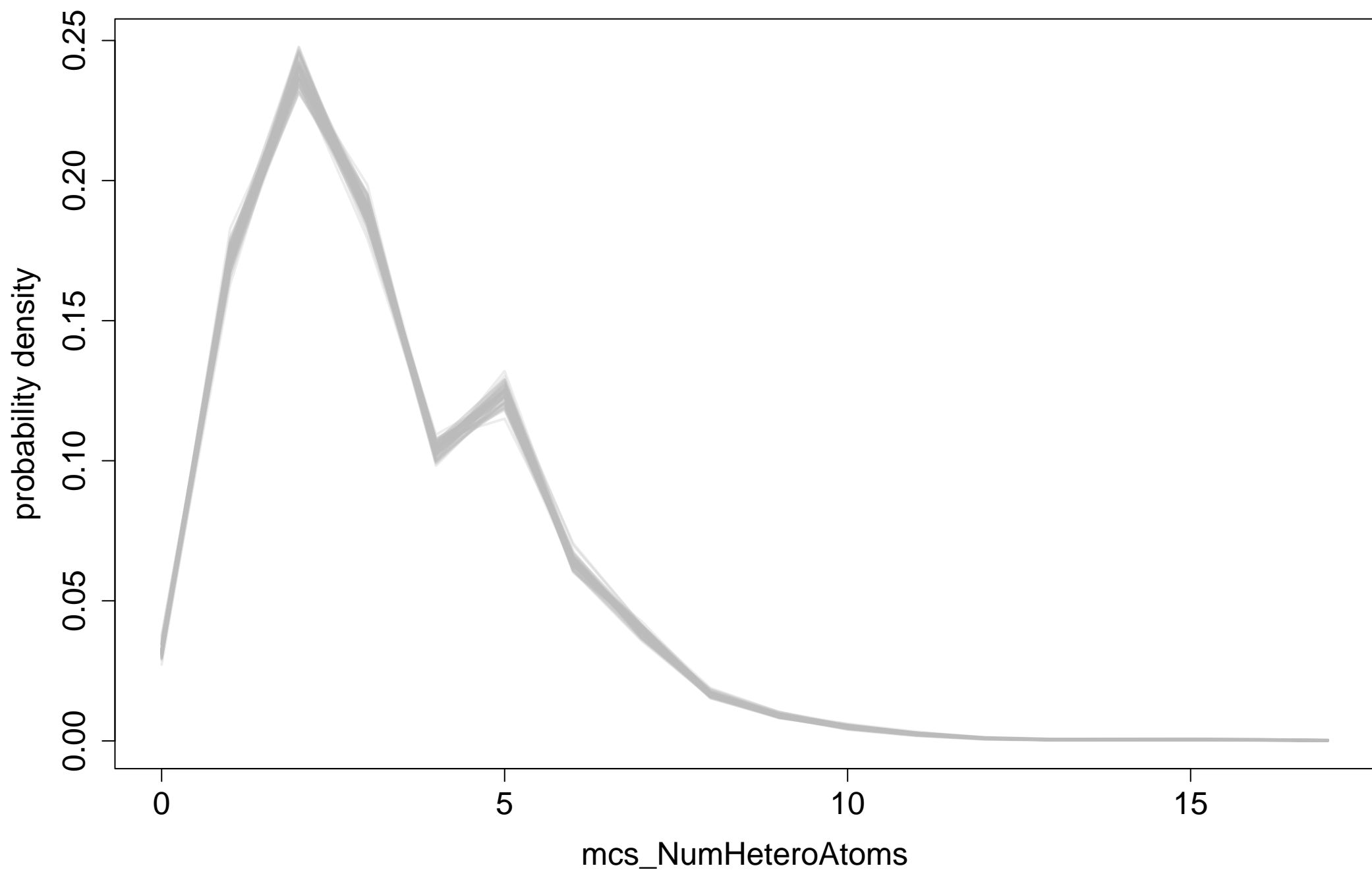


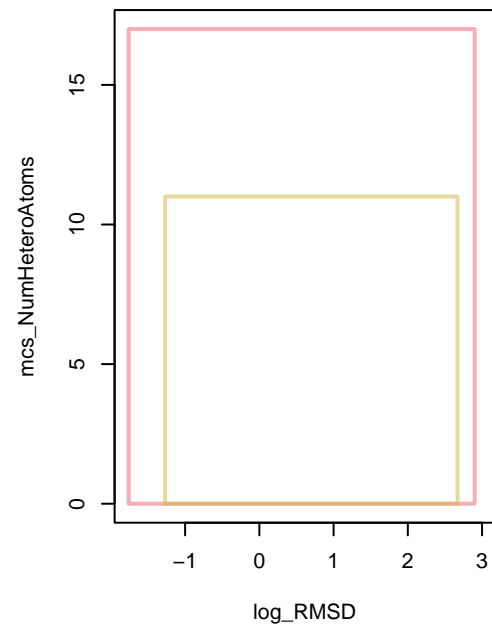
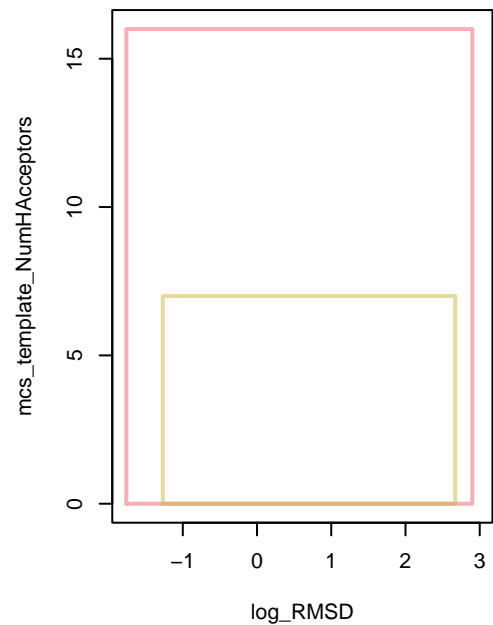
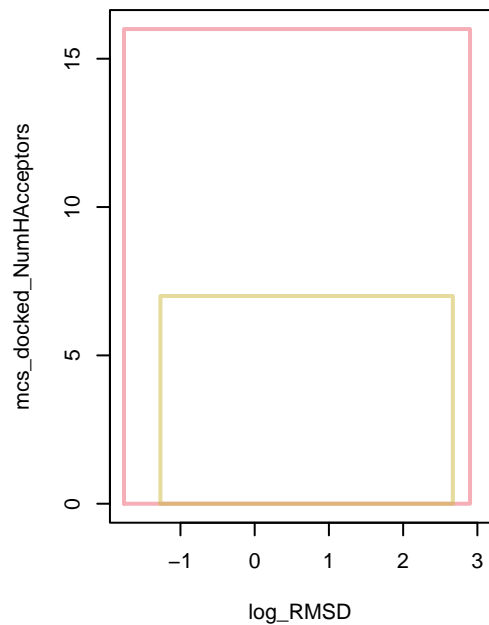
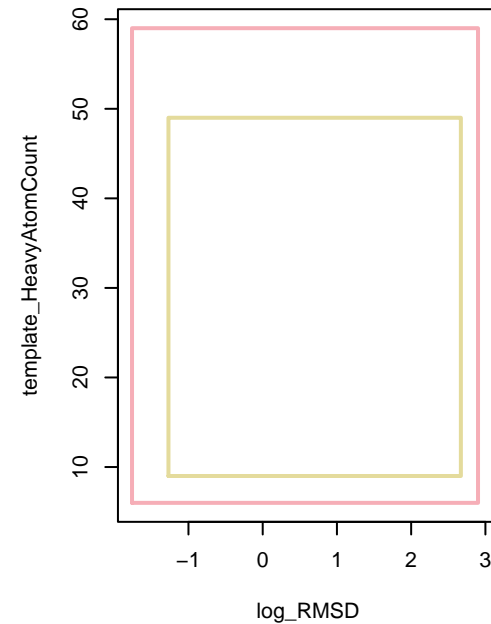
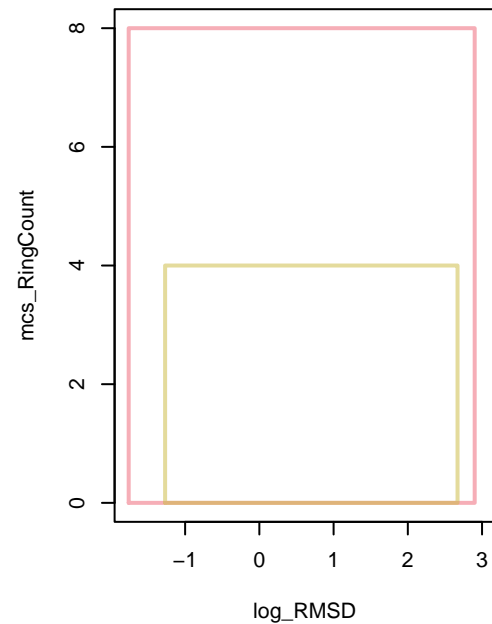
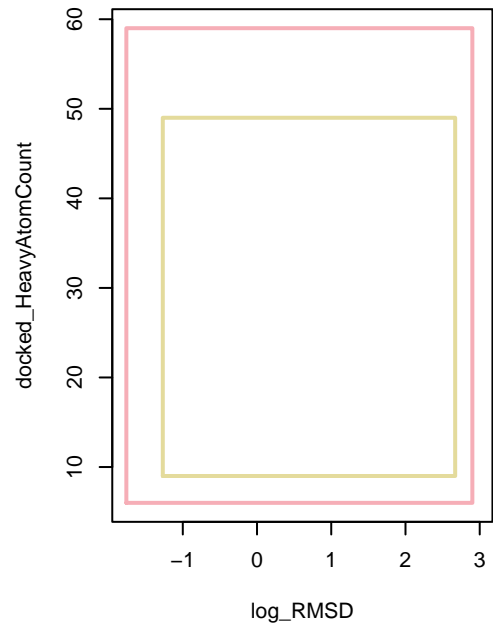
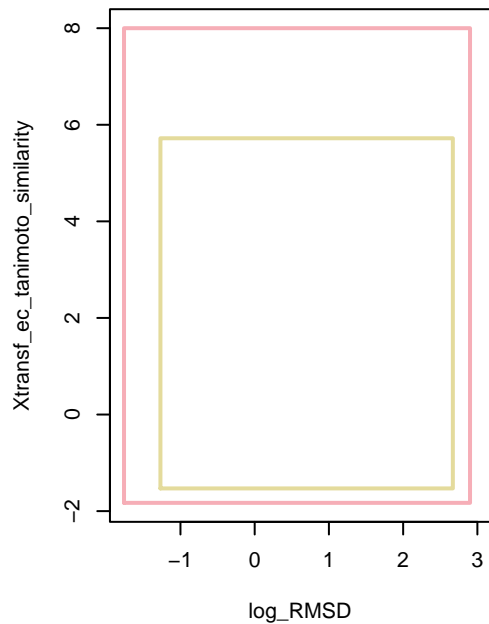




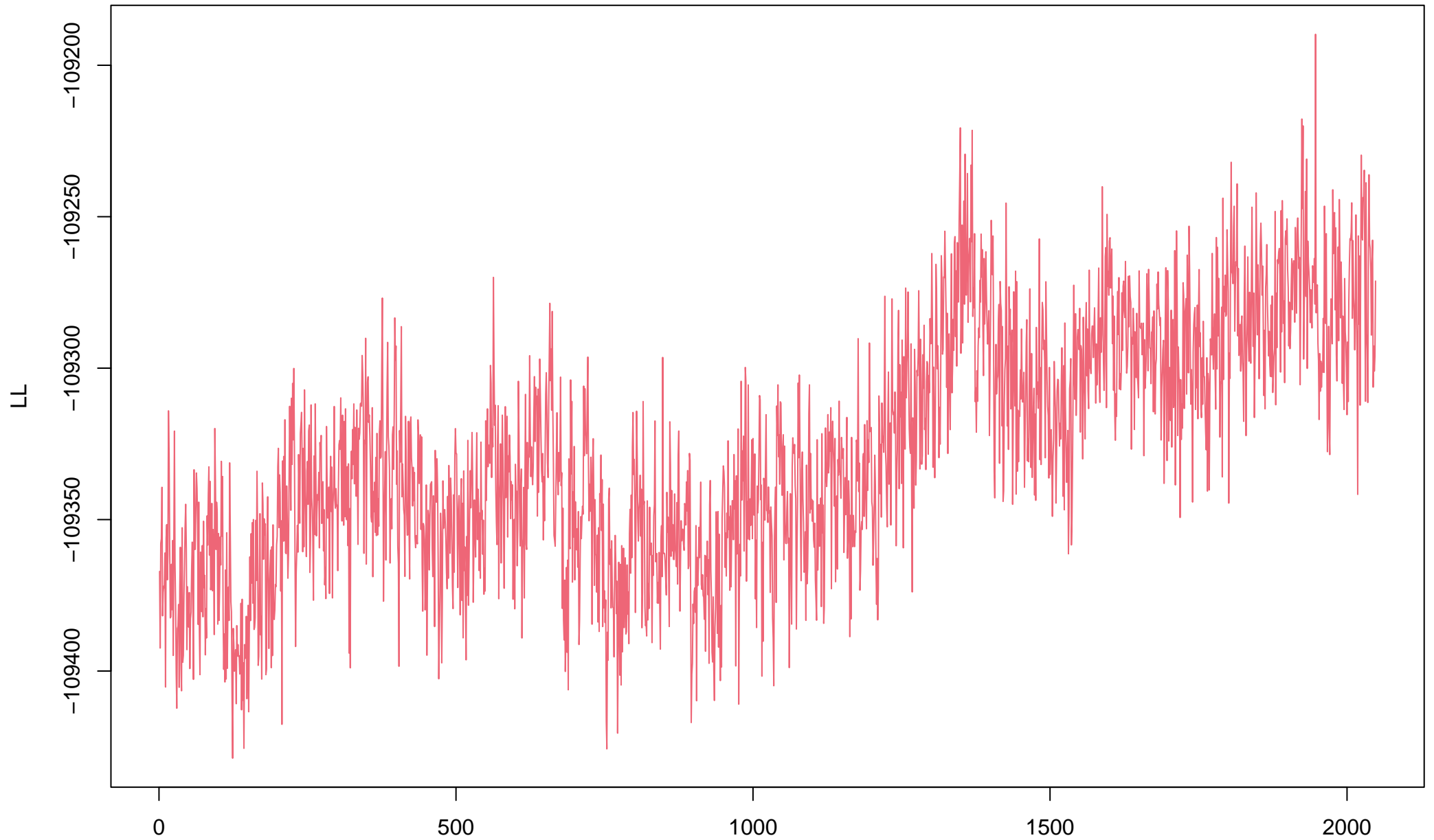




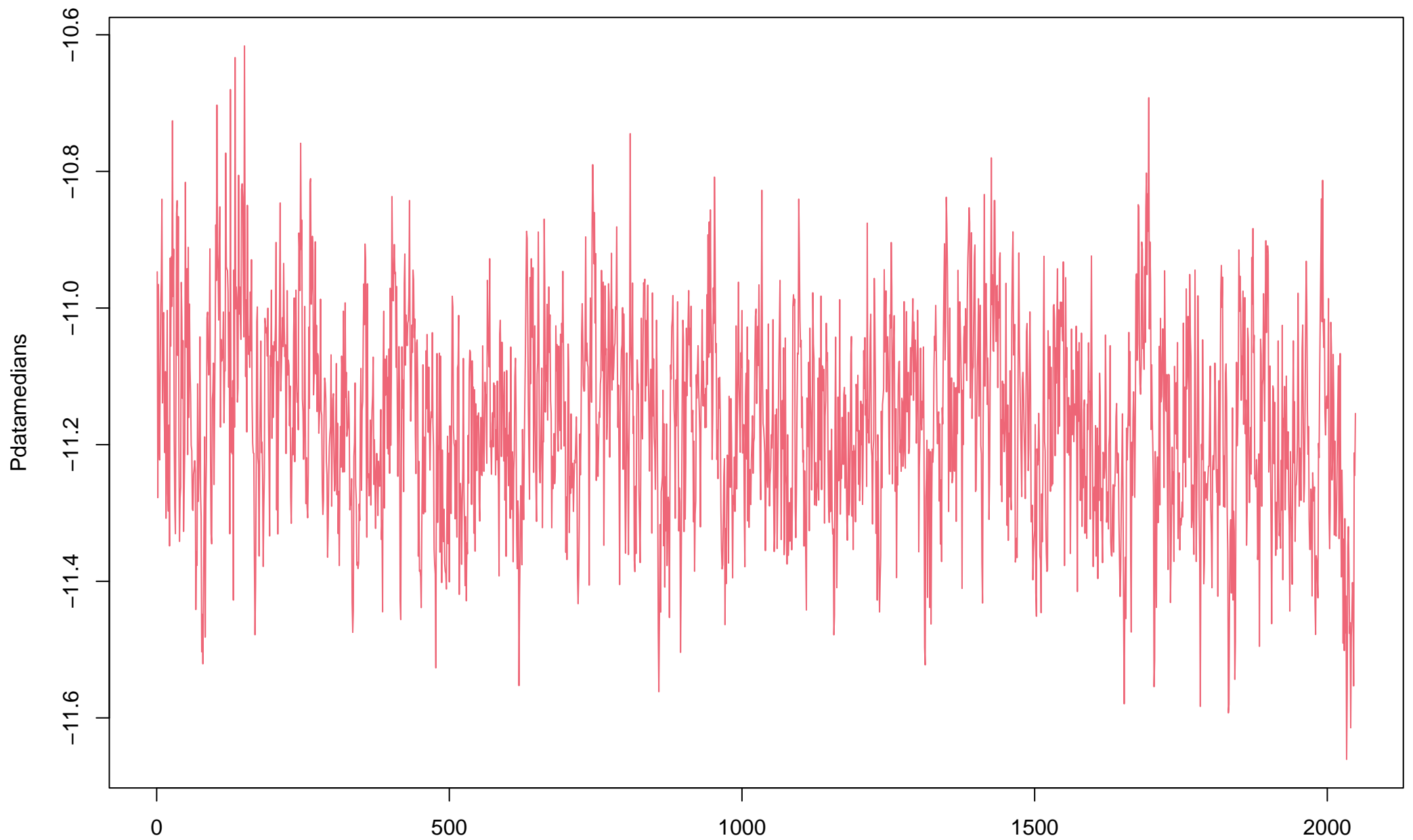




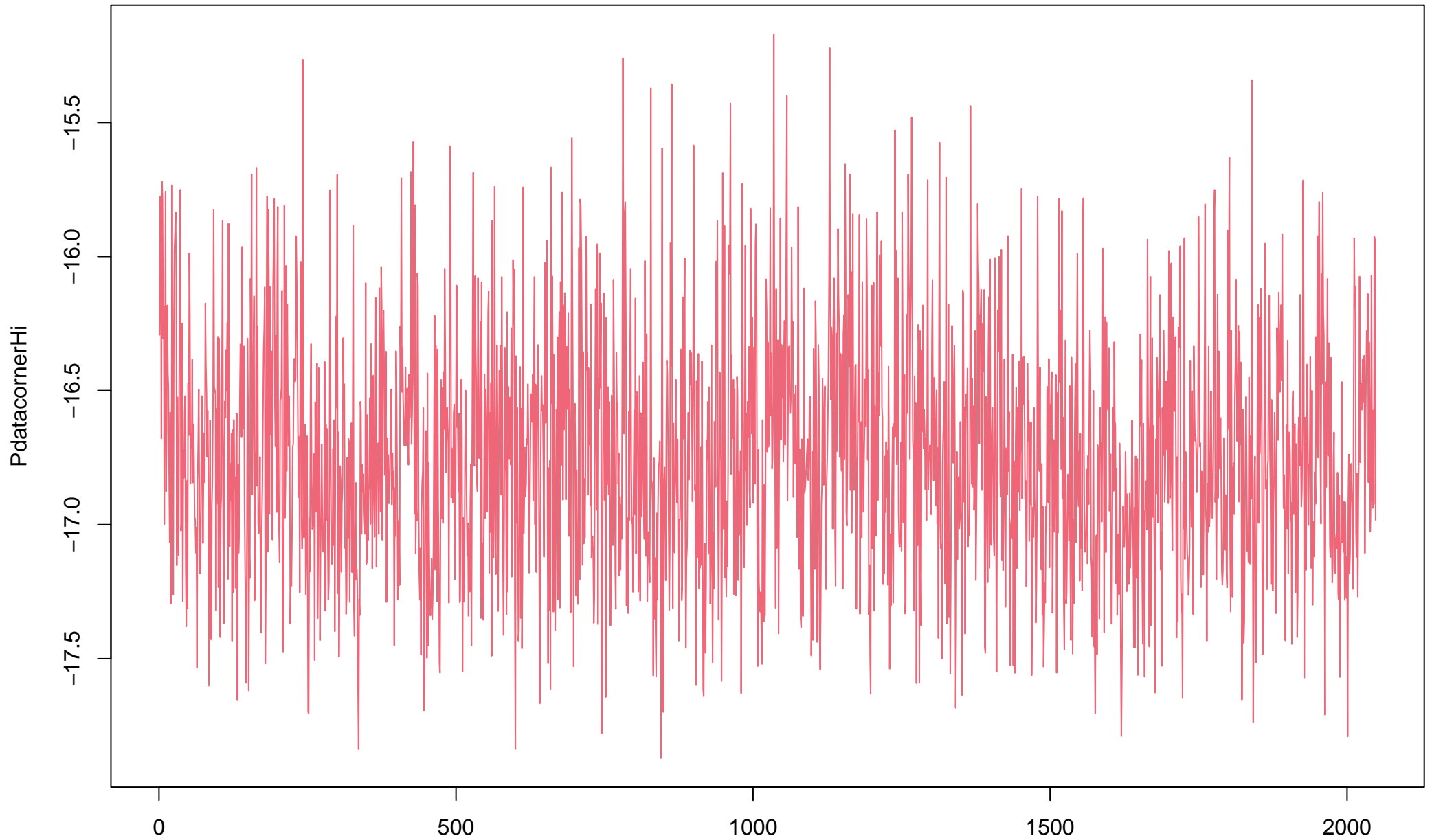
LL
ESS = 6.63 | BMK = 0.558 | MCSE(6.27) = 12.4 | stat: FALSE | burn: 1224



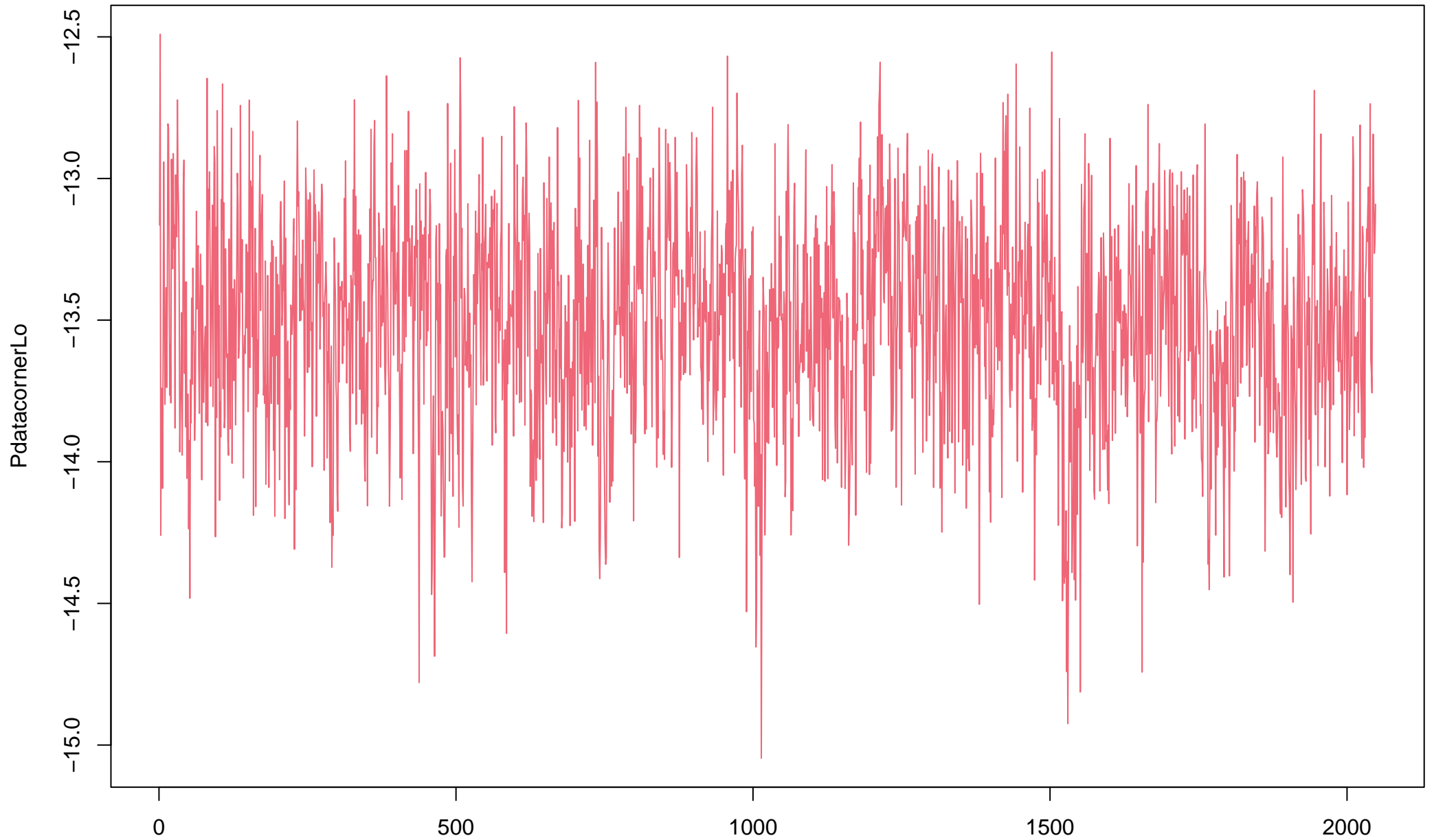
Pdatamedians
ESS = 260 | BMK = 0.0794 | MCSE(6.27) = 5.94 | stat: FALSE | burn: 0



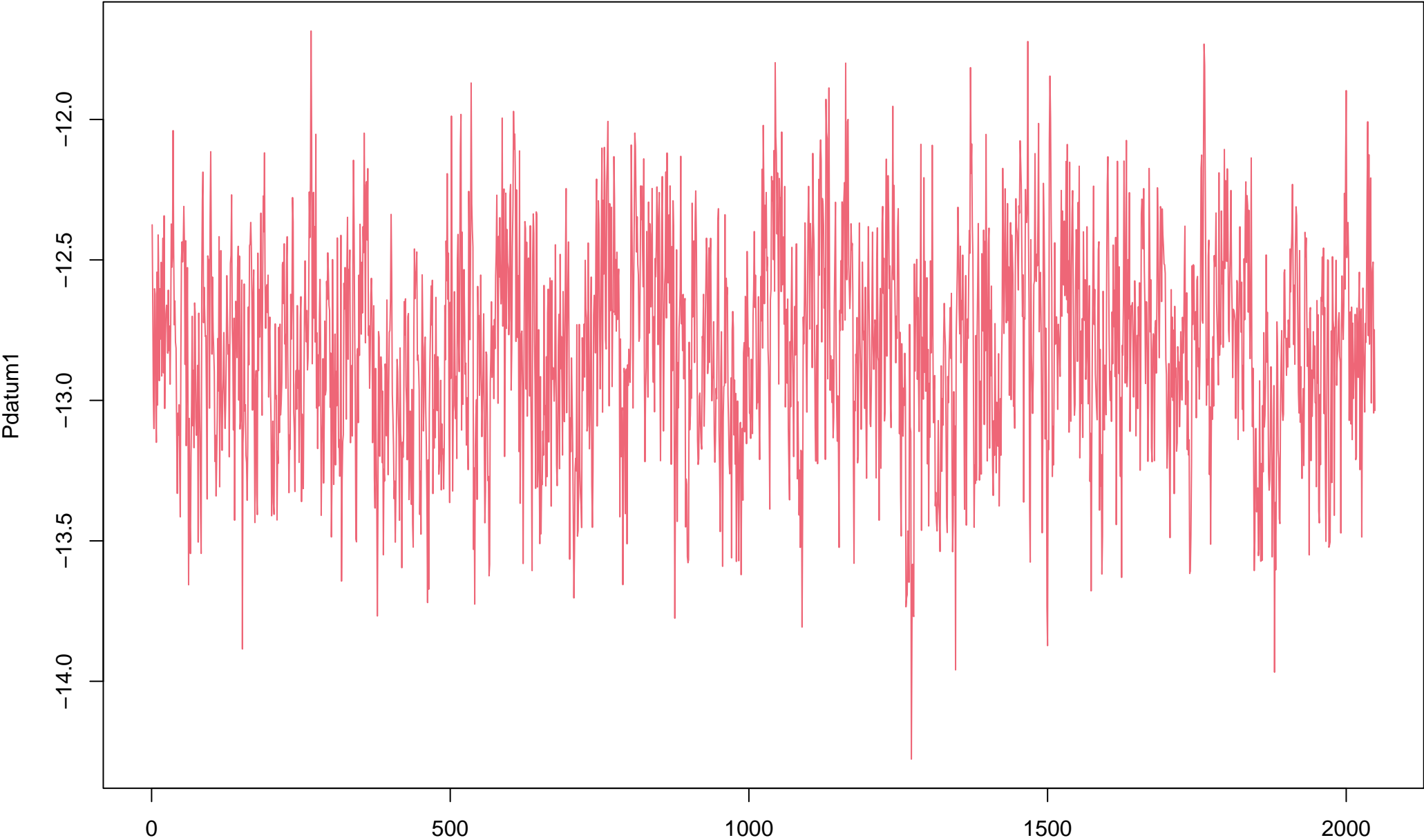
PdatacornerHi
ESS = 1200 | BMK = 0.0554 | MCSE(6.27) = 3.79 | stat: TRUE | burn: 0



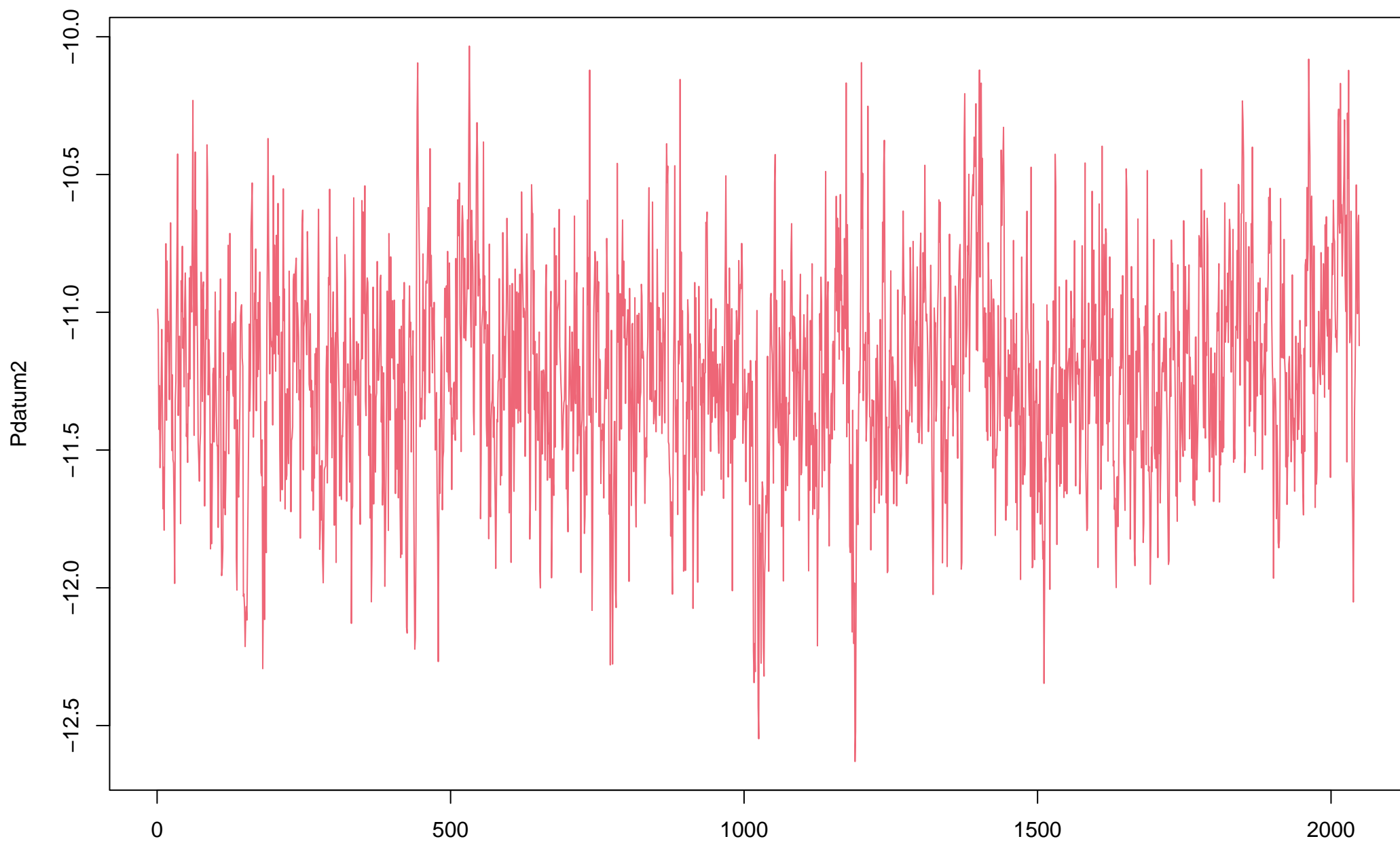
PdatacornerLo
ESS = 502 | BMK = 0.044 | MCSE(6.27) = 4.12 | stat: TRUE | burn: 0



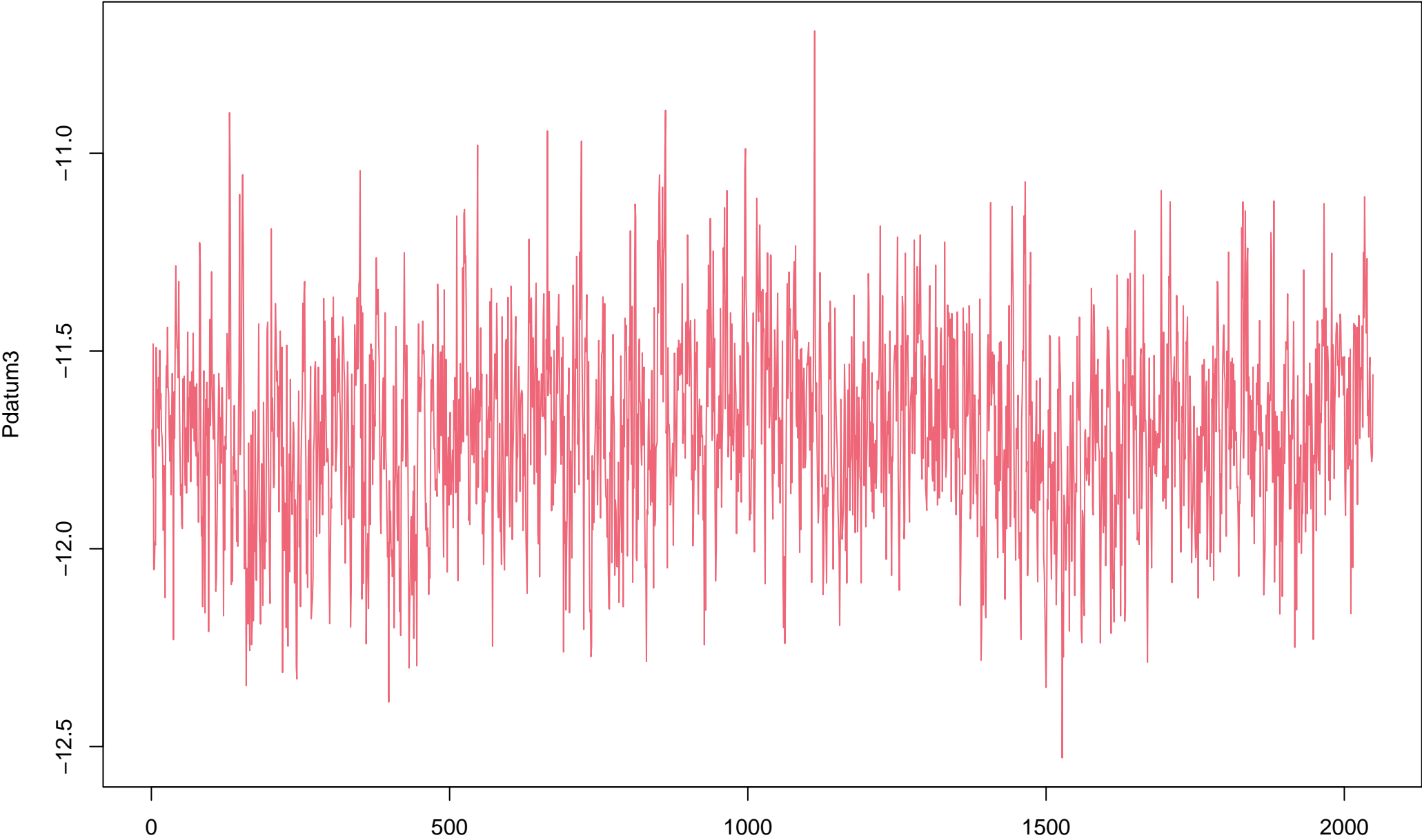
Pdatum1
ESS = 383 | BMK = 0.0792 | MCSE(6.27) = 5.66 | stat: TRUE | burn: 0



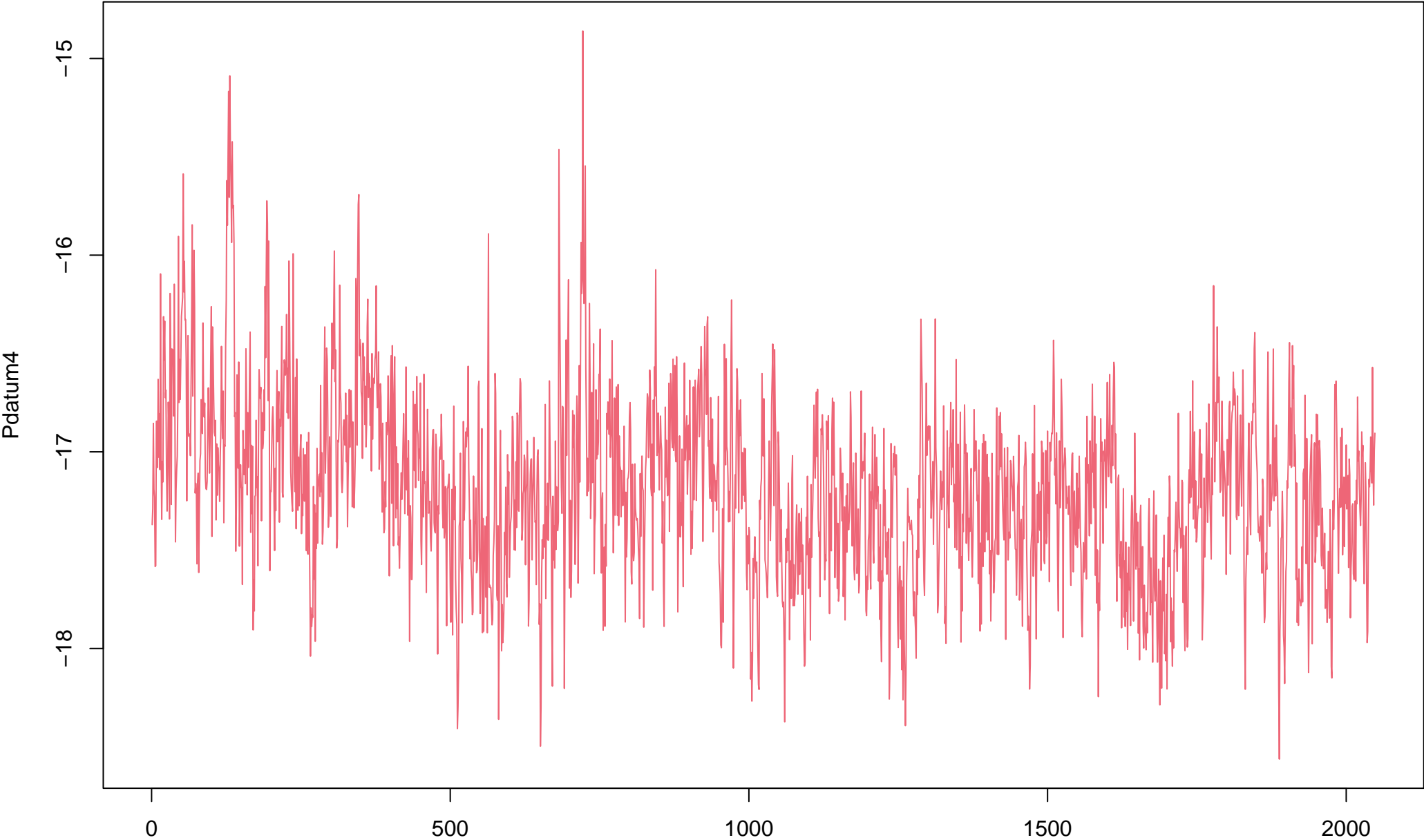
Pdatum2
ESS = 503 | BMK = 0.069 | MCSE(6.27) = 4.75 | stat: TRUE | burn: 0



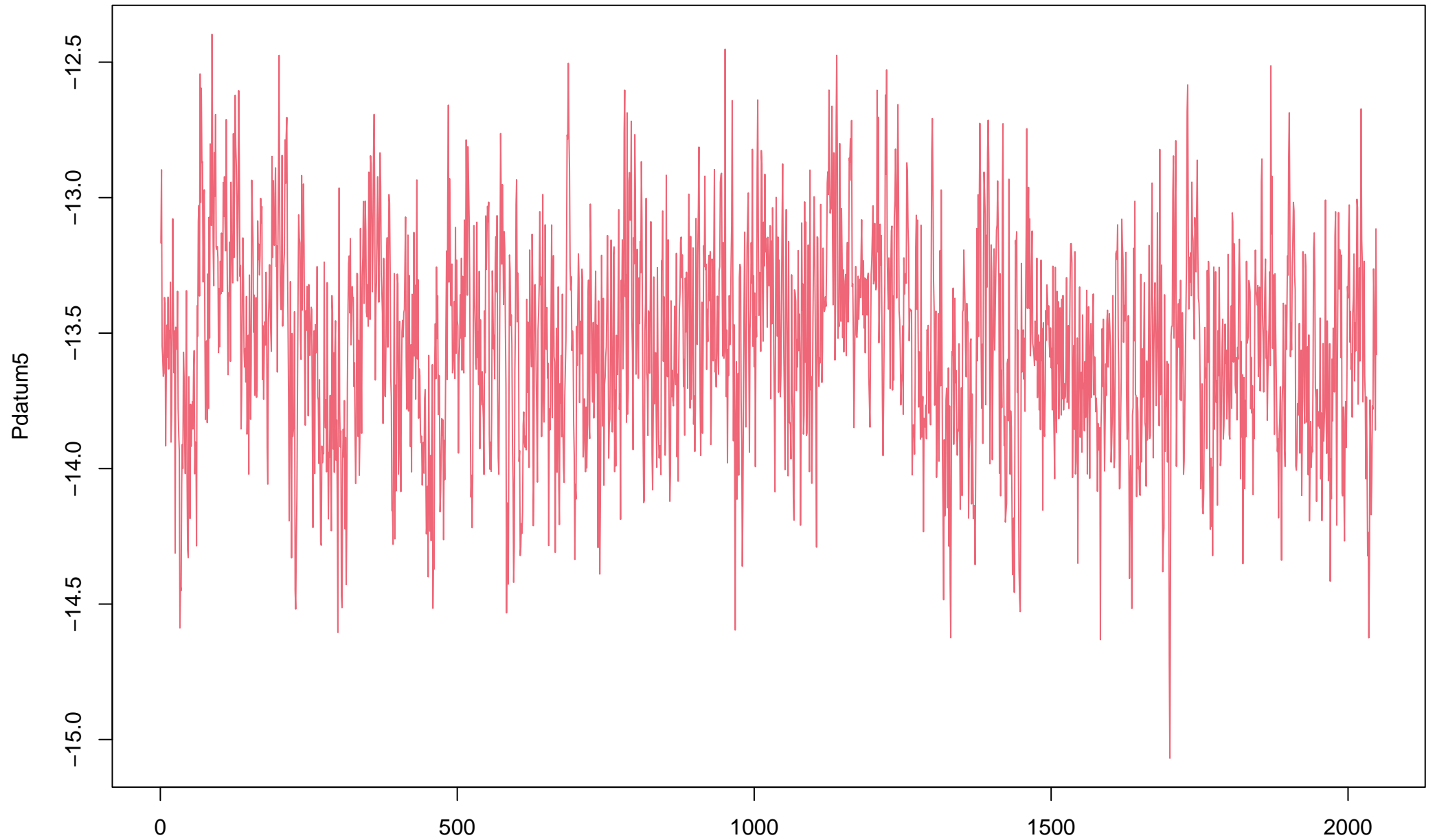
Pdatum3
ESS = 554 | BMK = 0.0782 | MCSE(6.27) = 4.48 | stat: TRUE | burn: 0



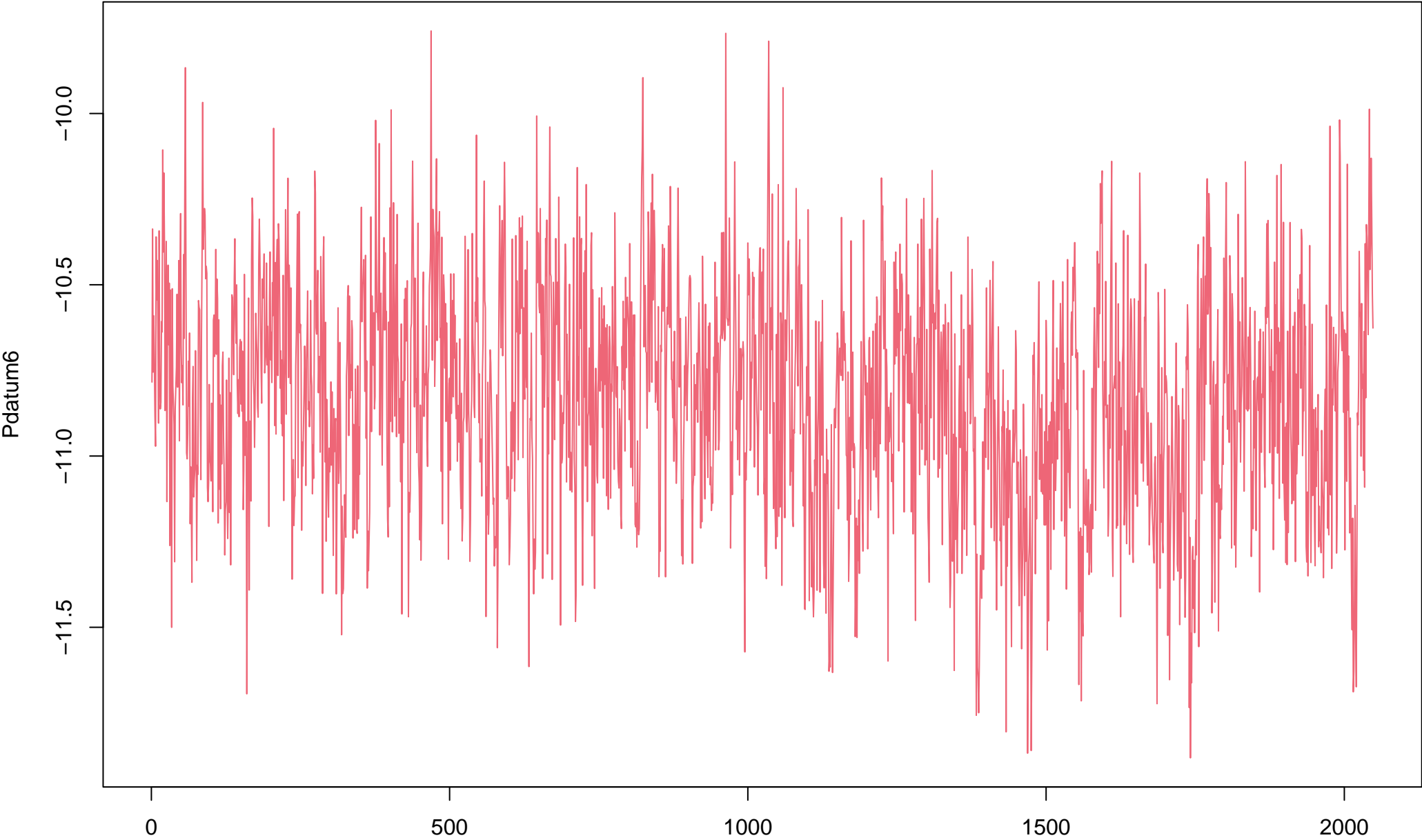
Pdatum4
ESS = 155 | BMK = 0.252 | MCSE(6.27) = 7.42 | stat: FALSE | burn: 0



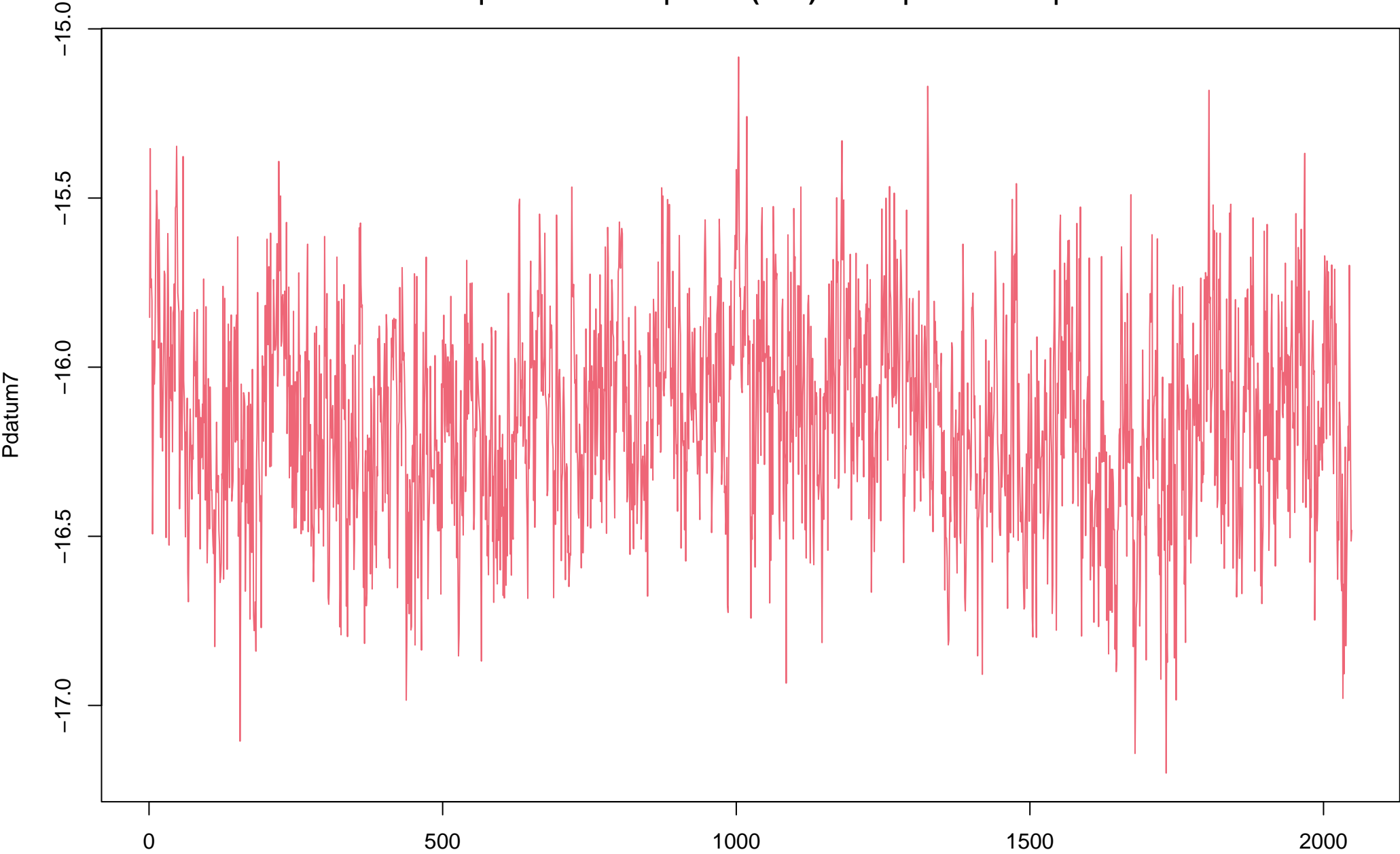
Pdatum5
ESS = 206 | BMK = 0.0534 | MCSE(6.27) = 6.18 | stat: FALSE | burn: 0



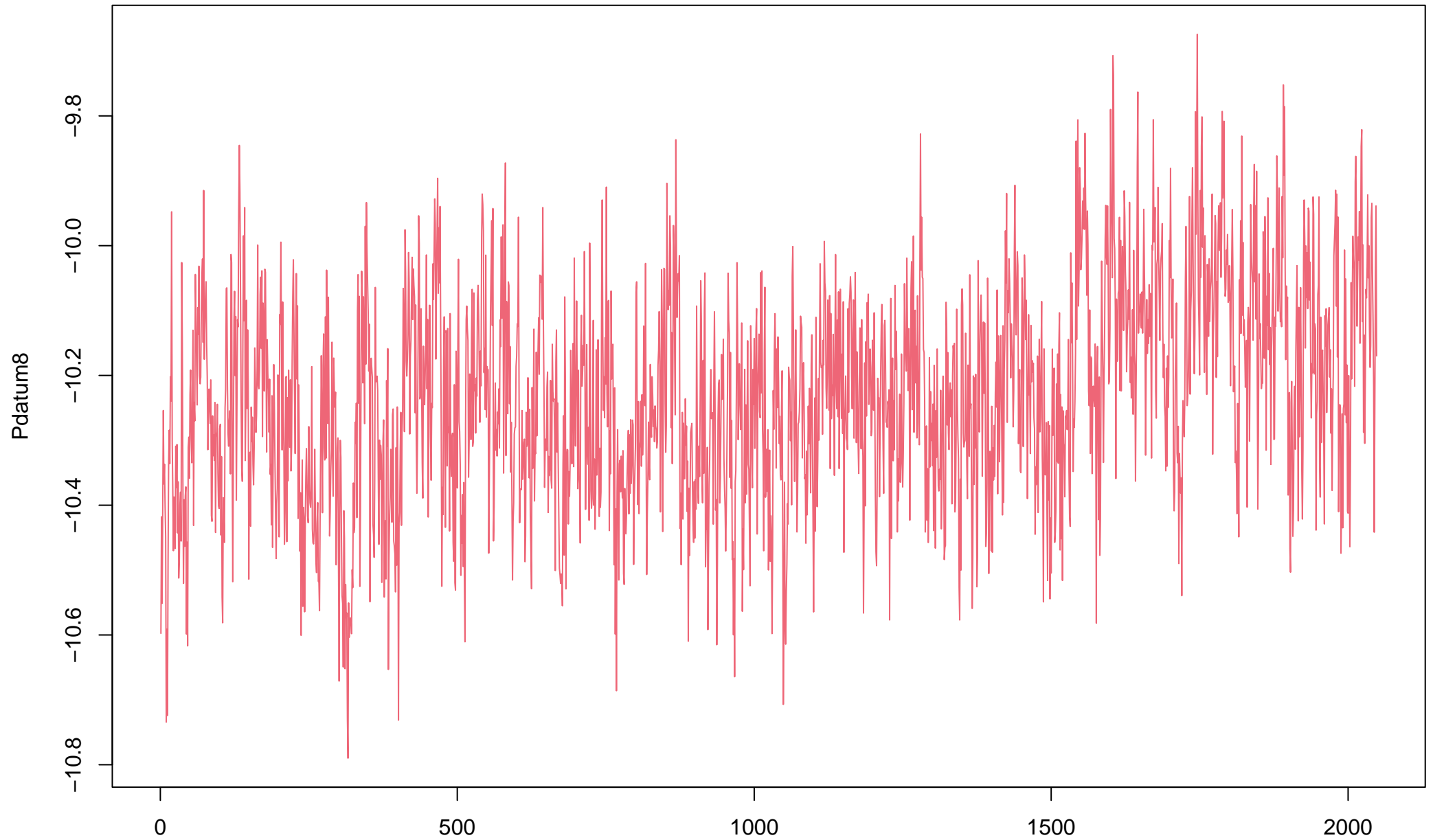
Pdatum6
ESS = 209 | BMK = 0.156 | MCSE(6.27) = 5.31 | stat: FALSE | burn: 0



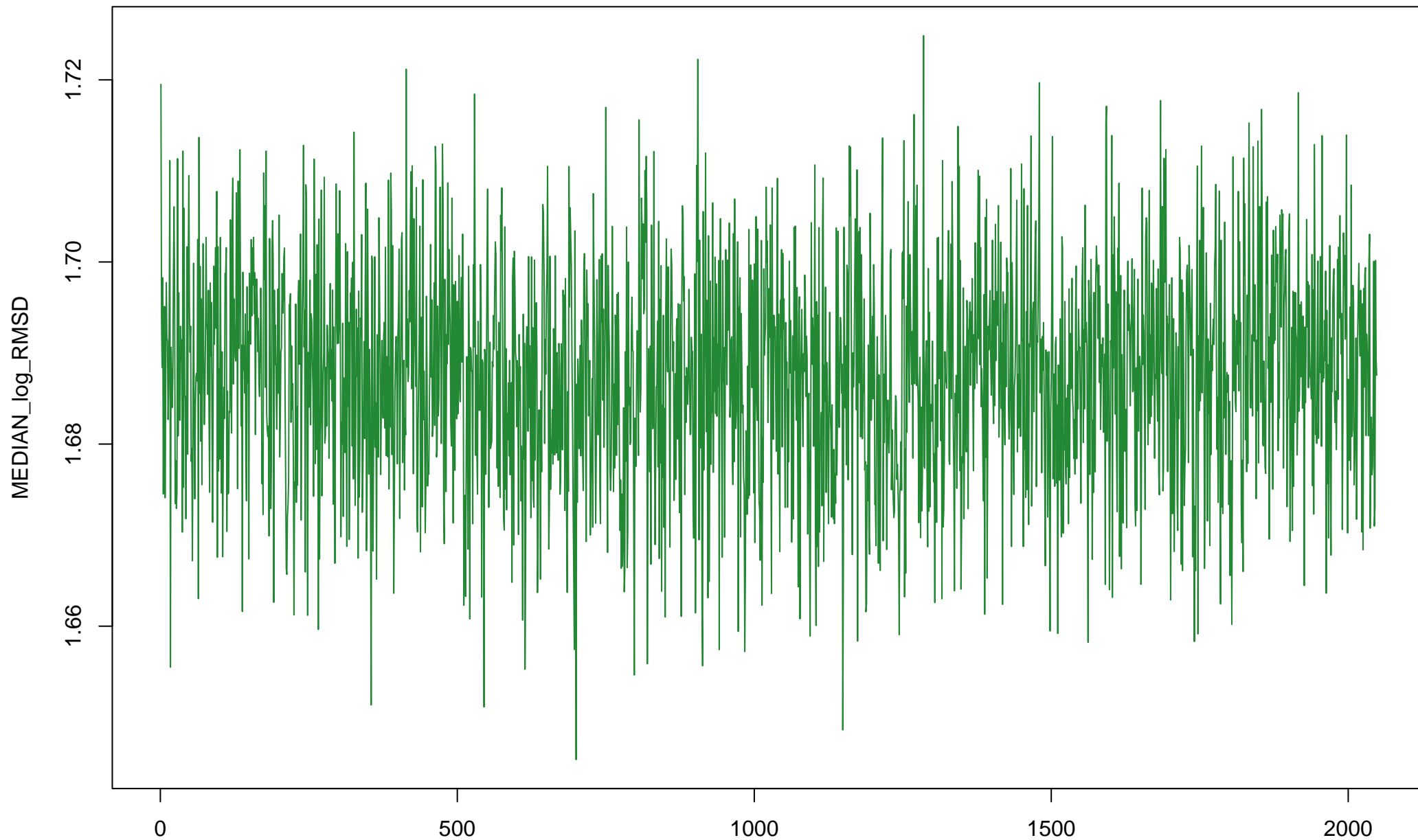
Pdatum7
ESS = 297 | BMK = 0.0529 | MCSE(6.27) = 5.93 | stat: TRUE | burn: 0



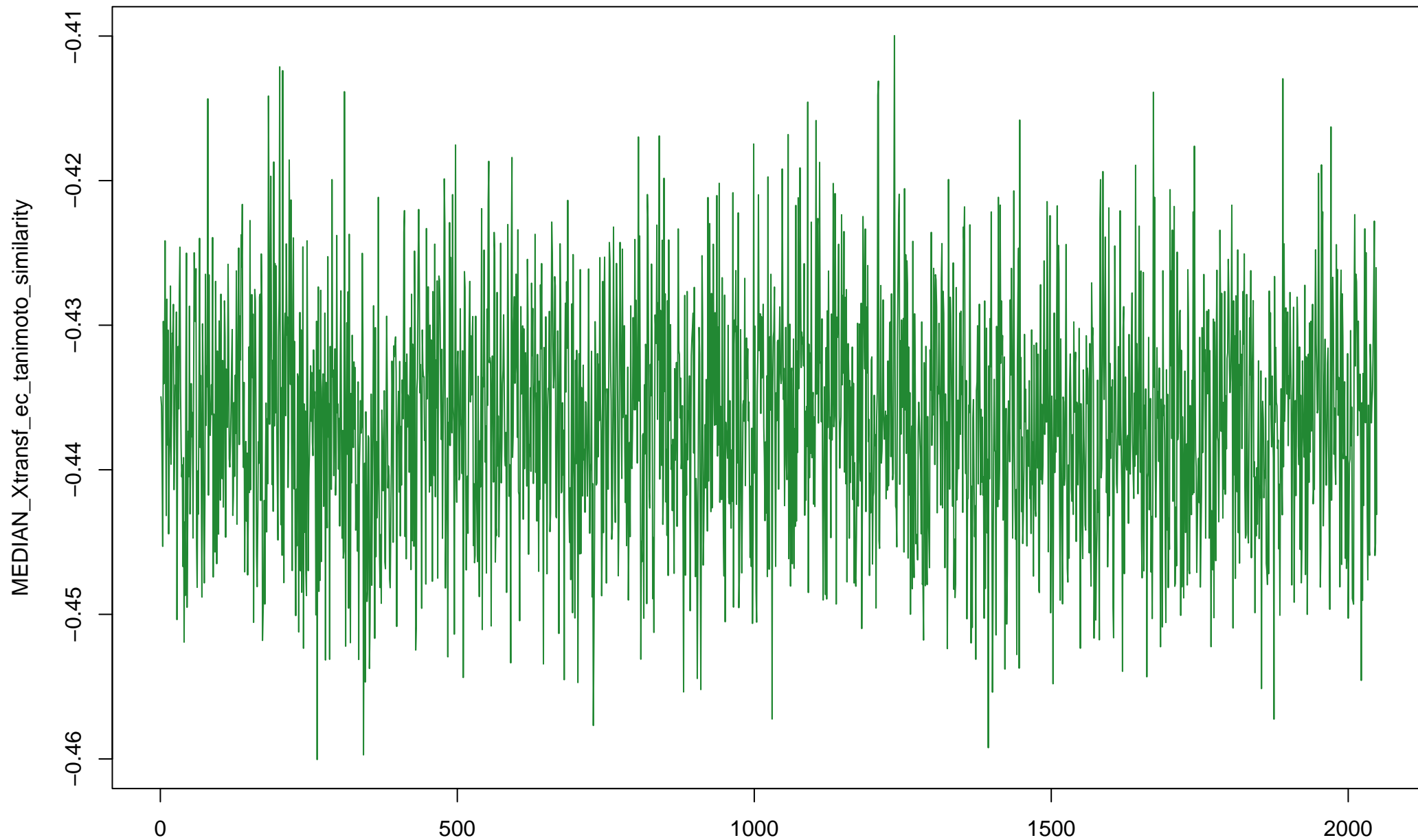
Pdatum8
ESS = 117 | BMK = 0.202 | MCSE(6.27) = 7.6 | stat: FALSE | burn: 0



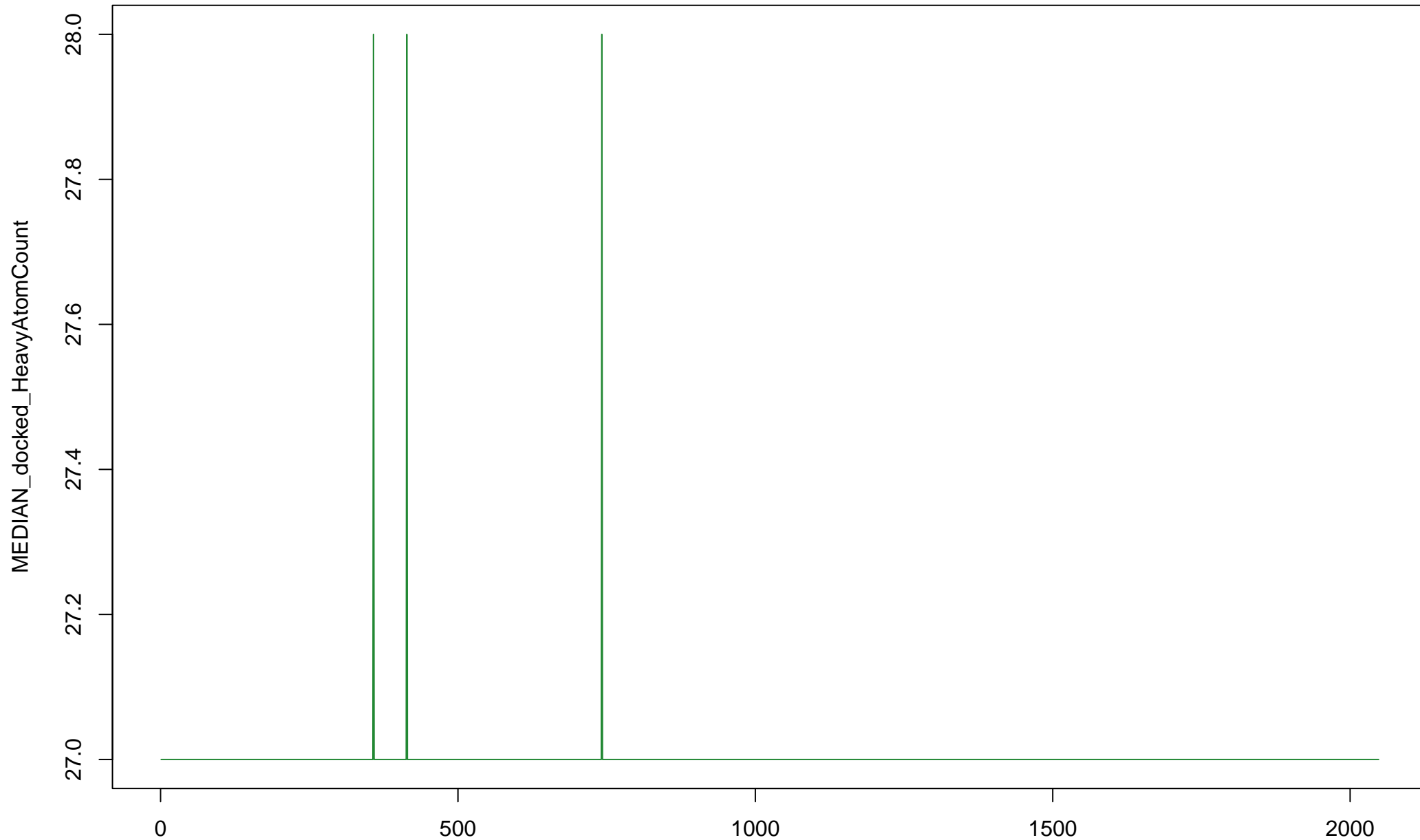
MEDIAN_log_RMSD
ESS = 1900 | BMK = 0.0349 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0



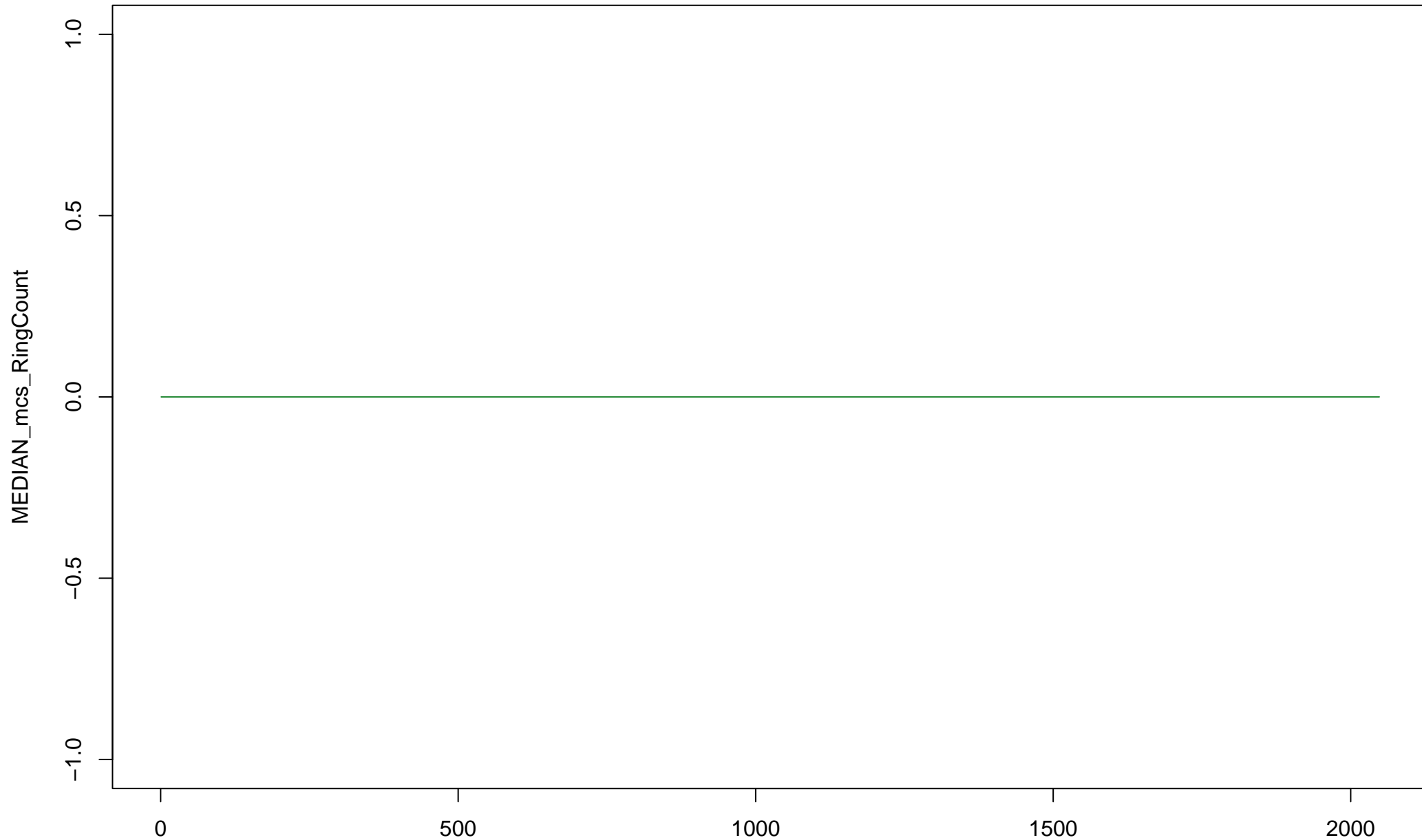
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1820 | BMK = 0.0237 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0



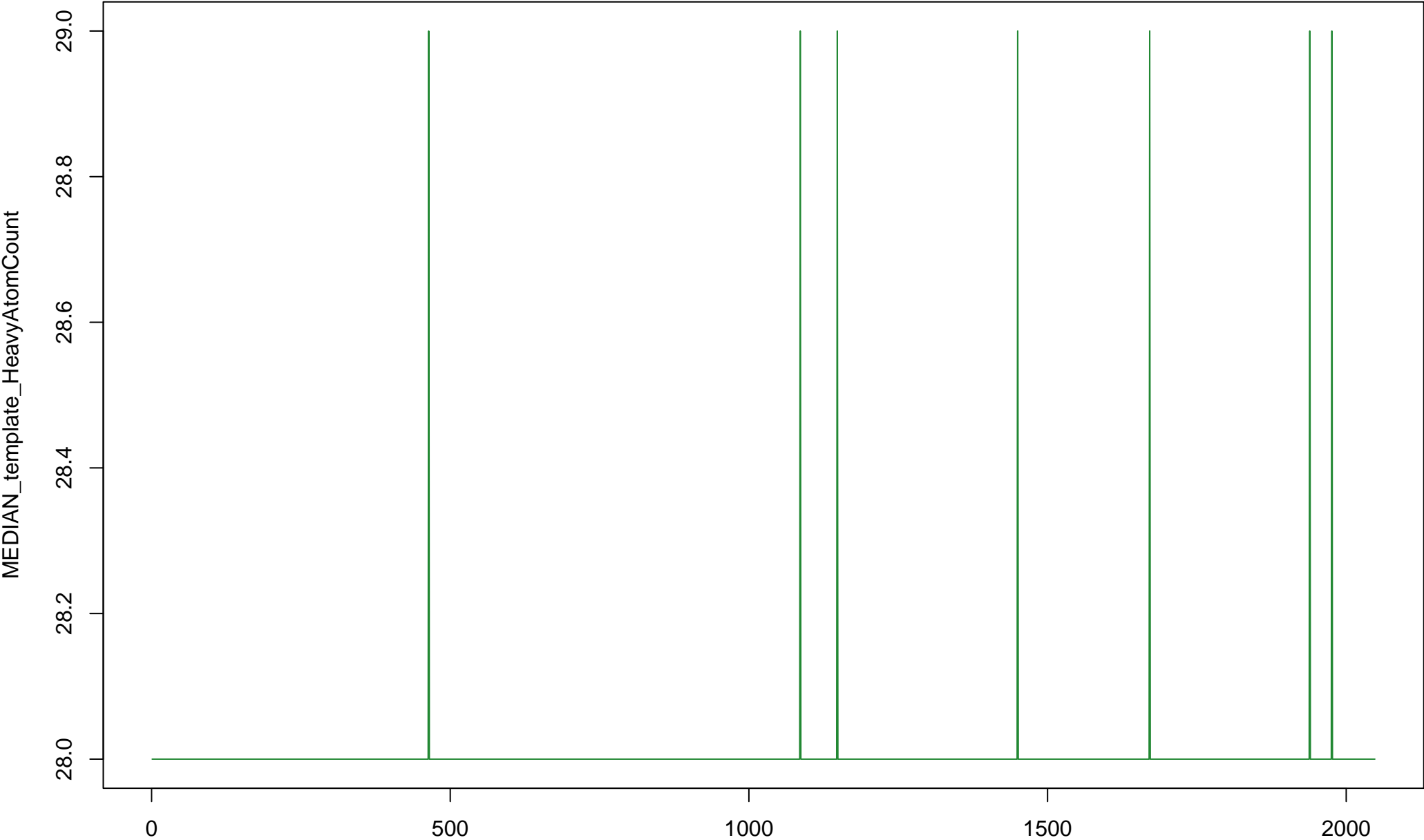
MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.507 | MCSE(6.27) = 2.17 | stat: FALSE | burn: 816



MEDIAN_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



MEDIAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.288 | MCSE(6.27) = 2.39 | stat: FALSE | burn: 1428



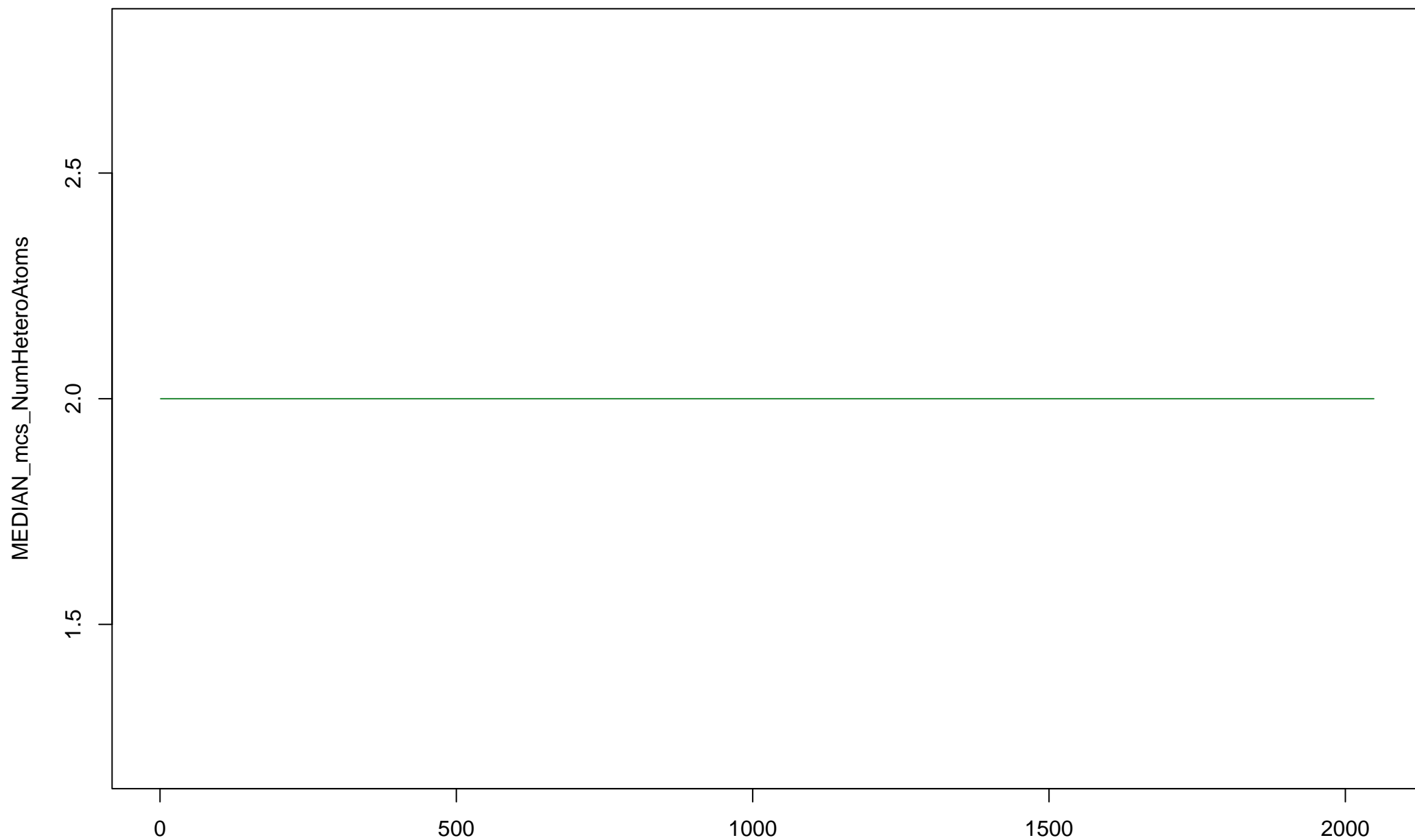
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



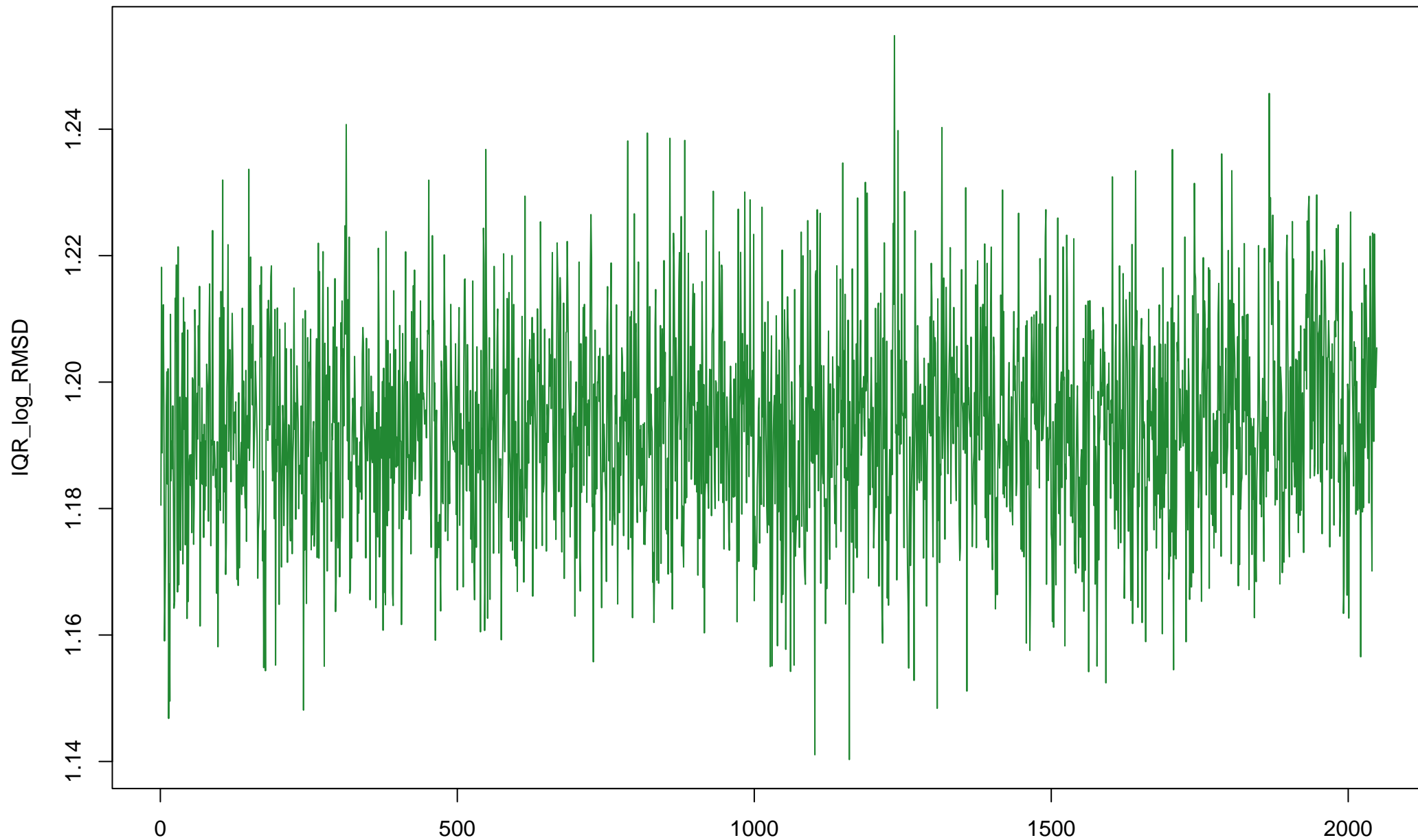
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



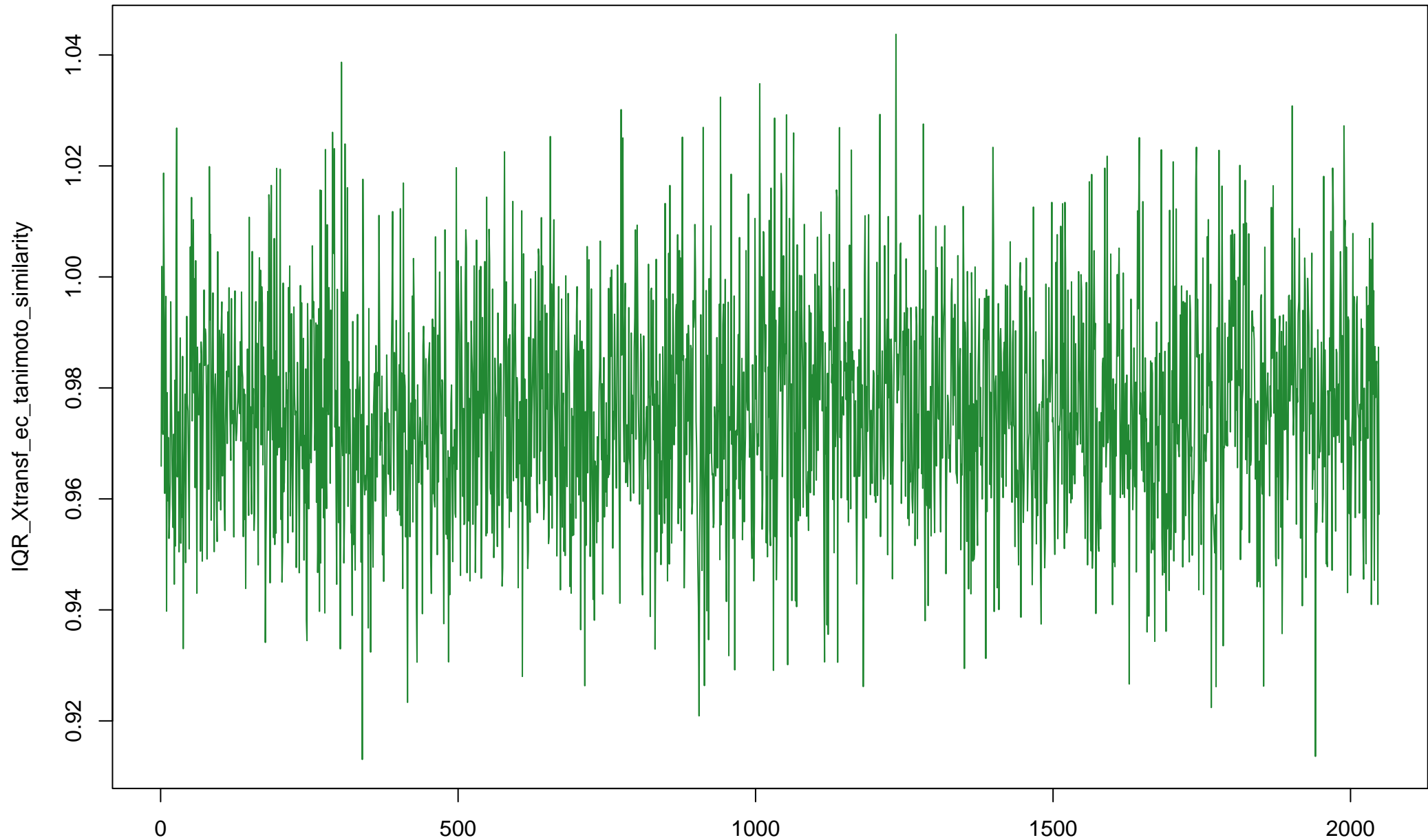
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



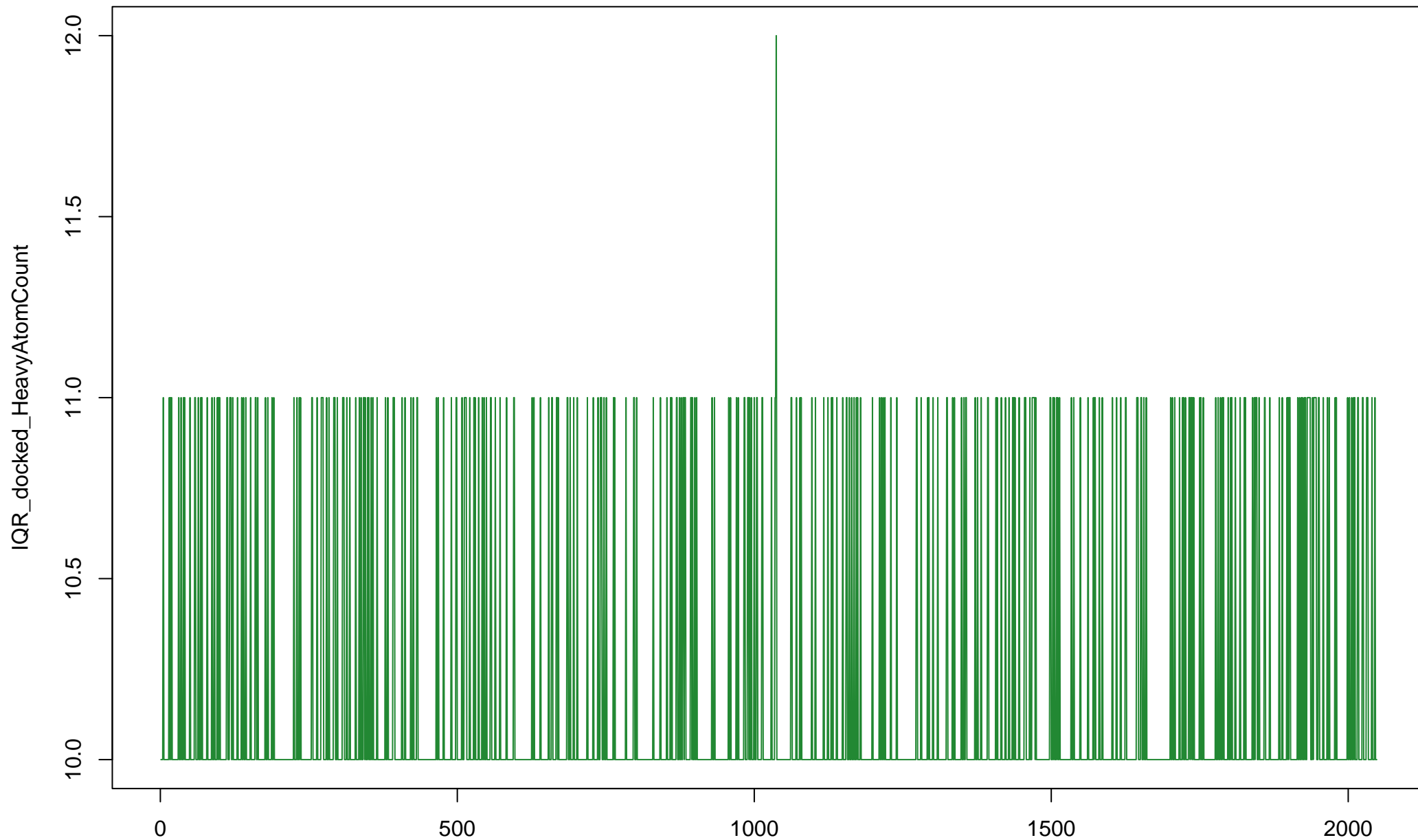
IQR_log_RMSD
ESS = 1460 | BMK = 0.0562 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



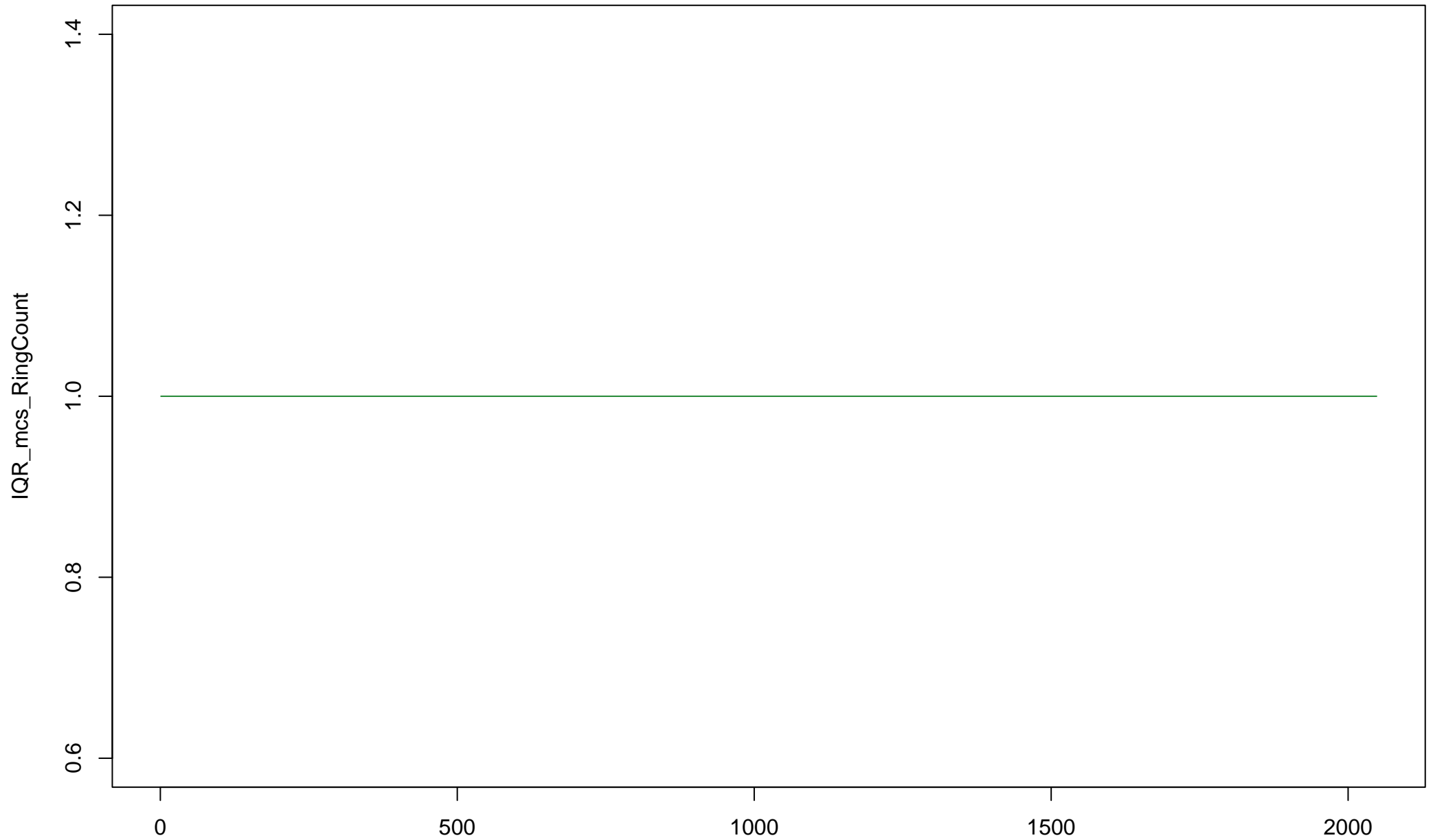
IQR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0427 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0



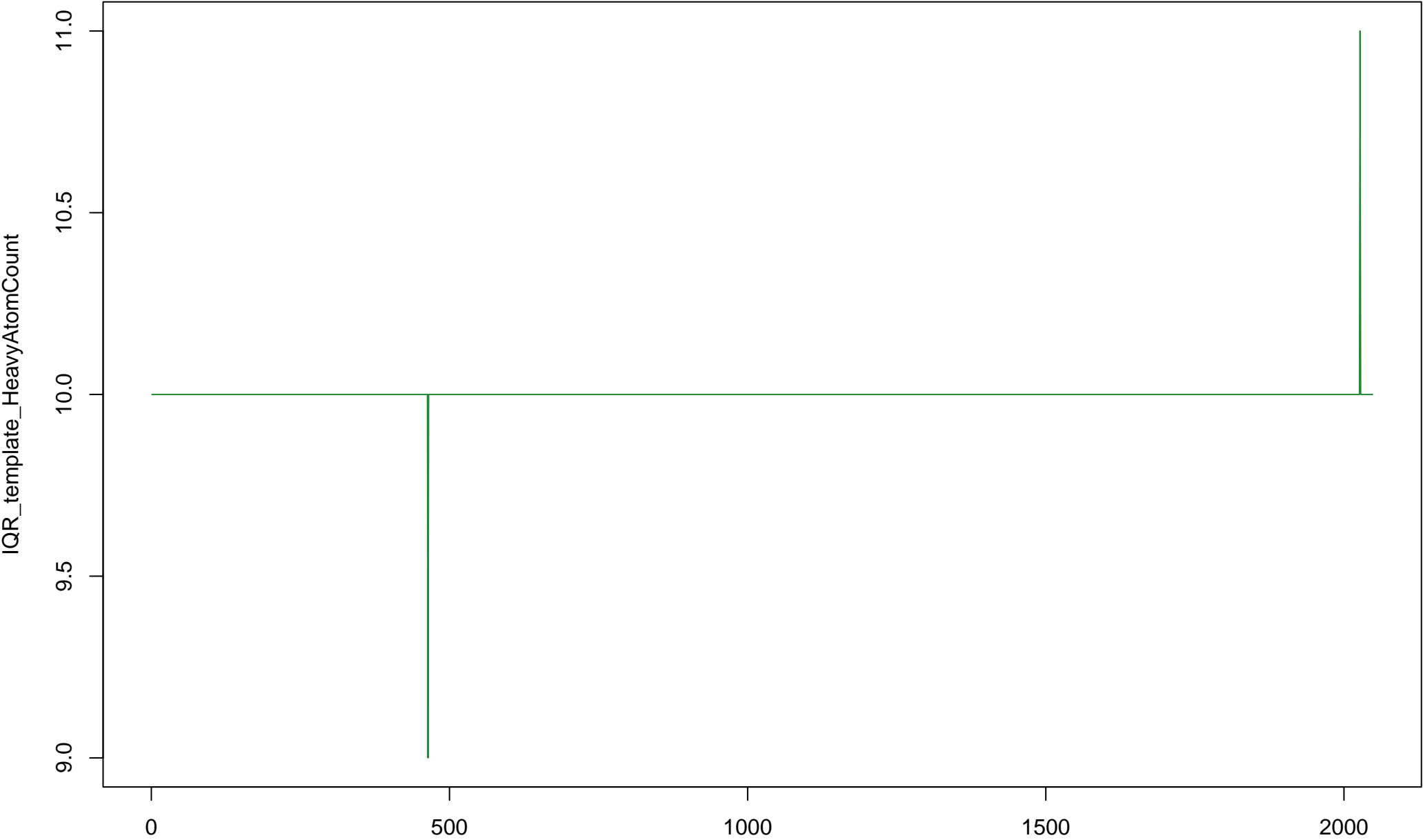
IQR_docked_HeavyAtomCount
ESS = 1820 | BMK = 0.0222 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0



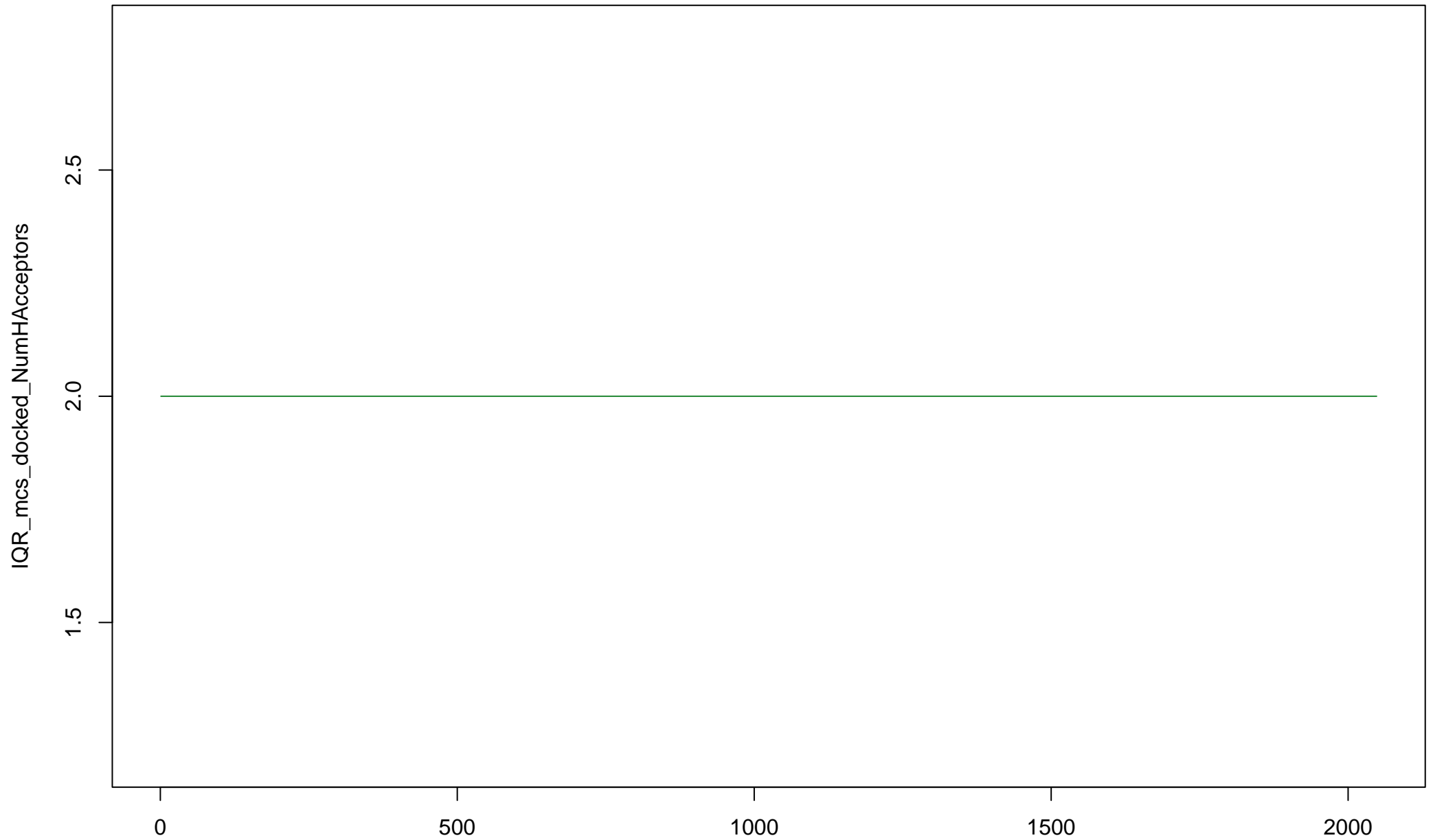
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



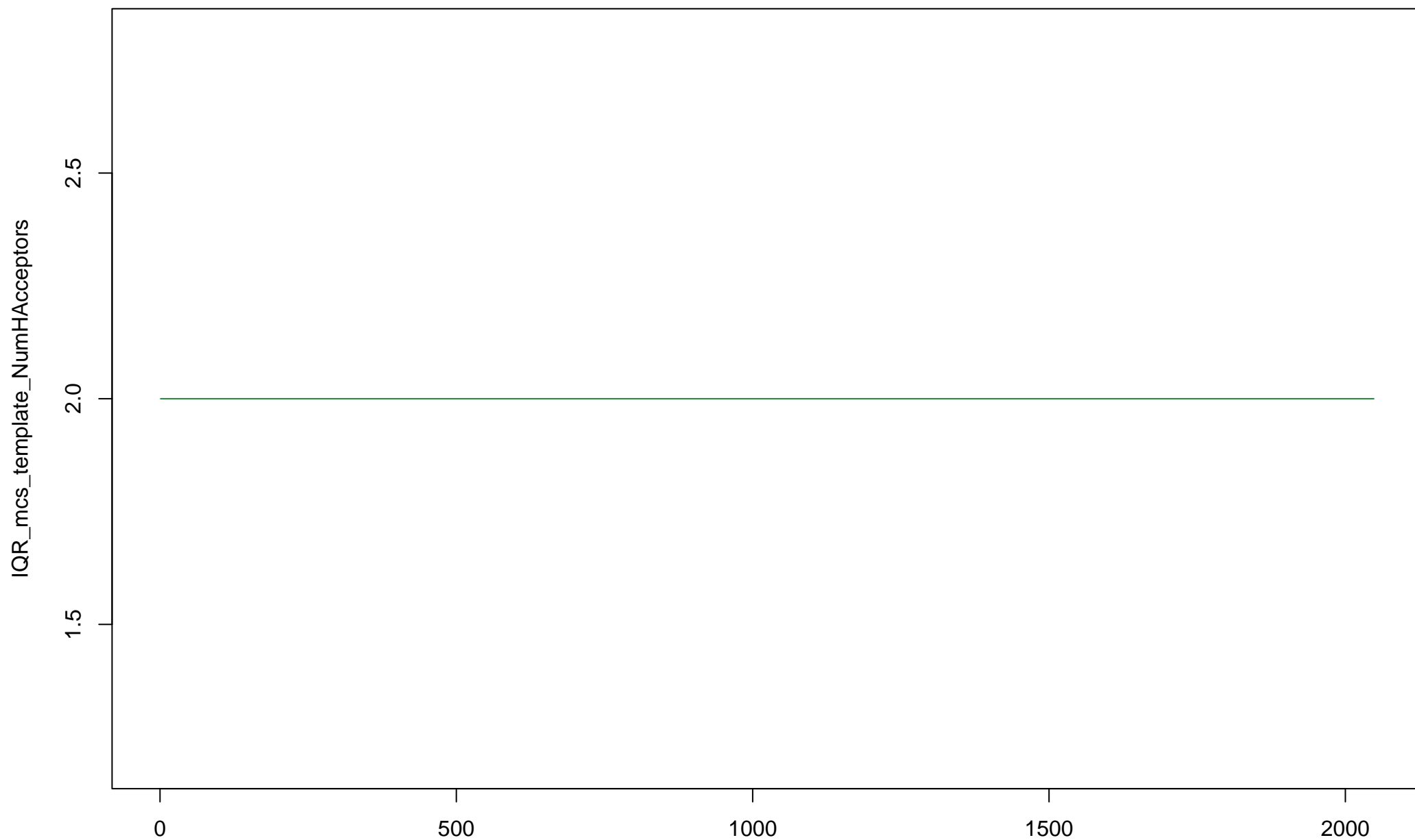
IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0233 | MCSE(6.27) = 1.57 | stat: TRUE | burn: 2040



IQR_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



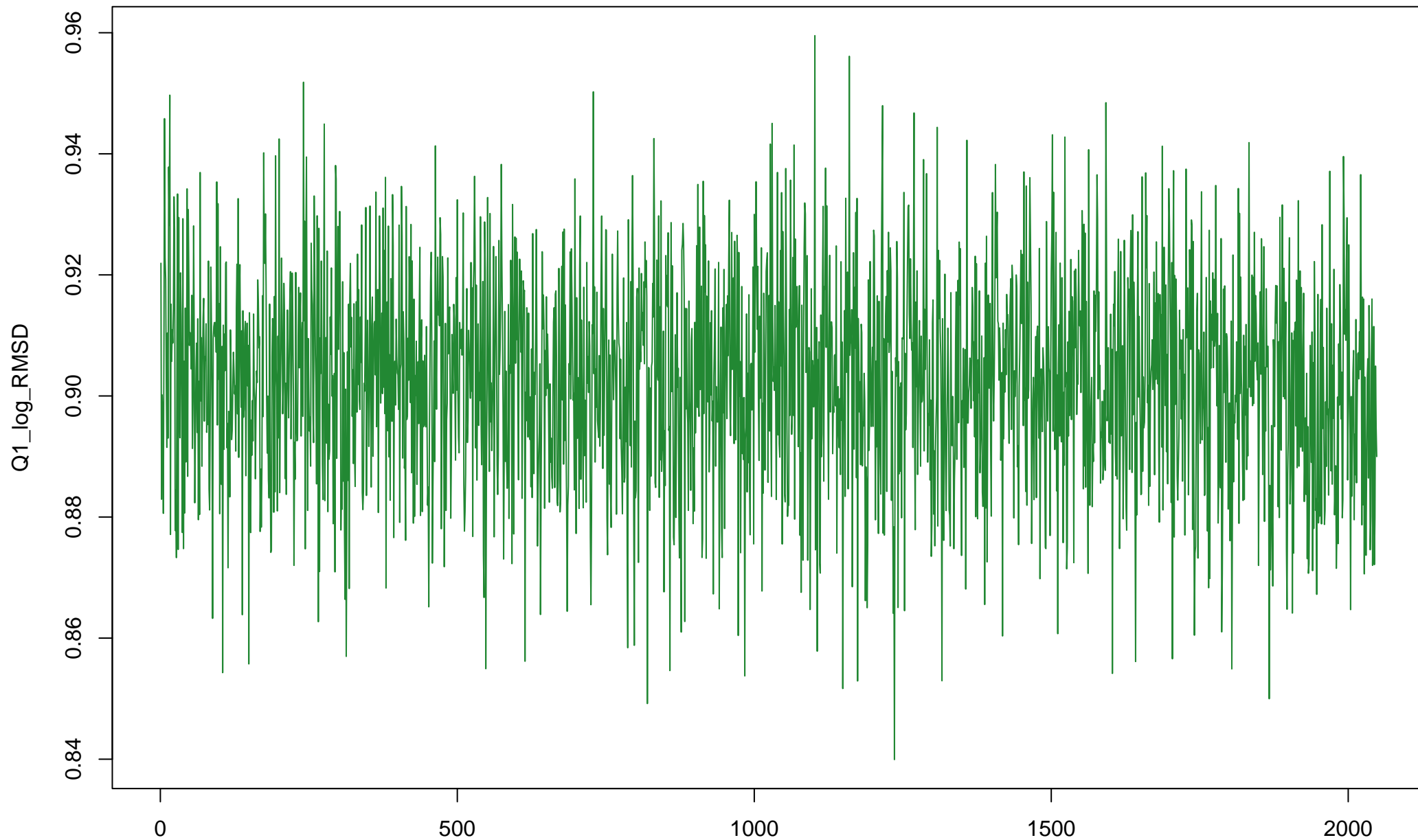
IQR_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



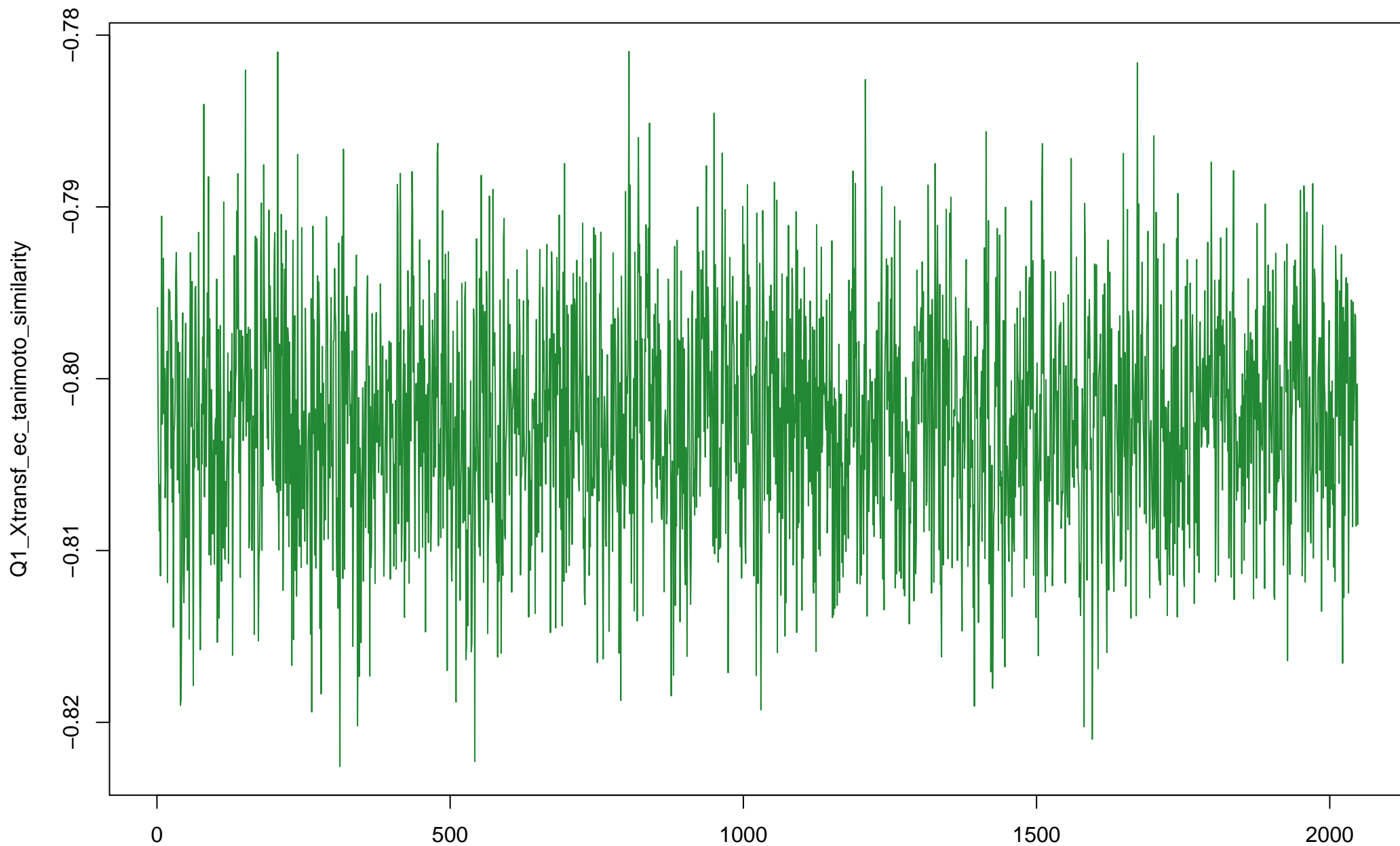
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



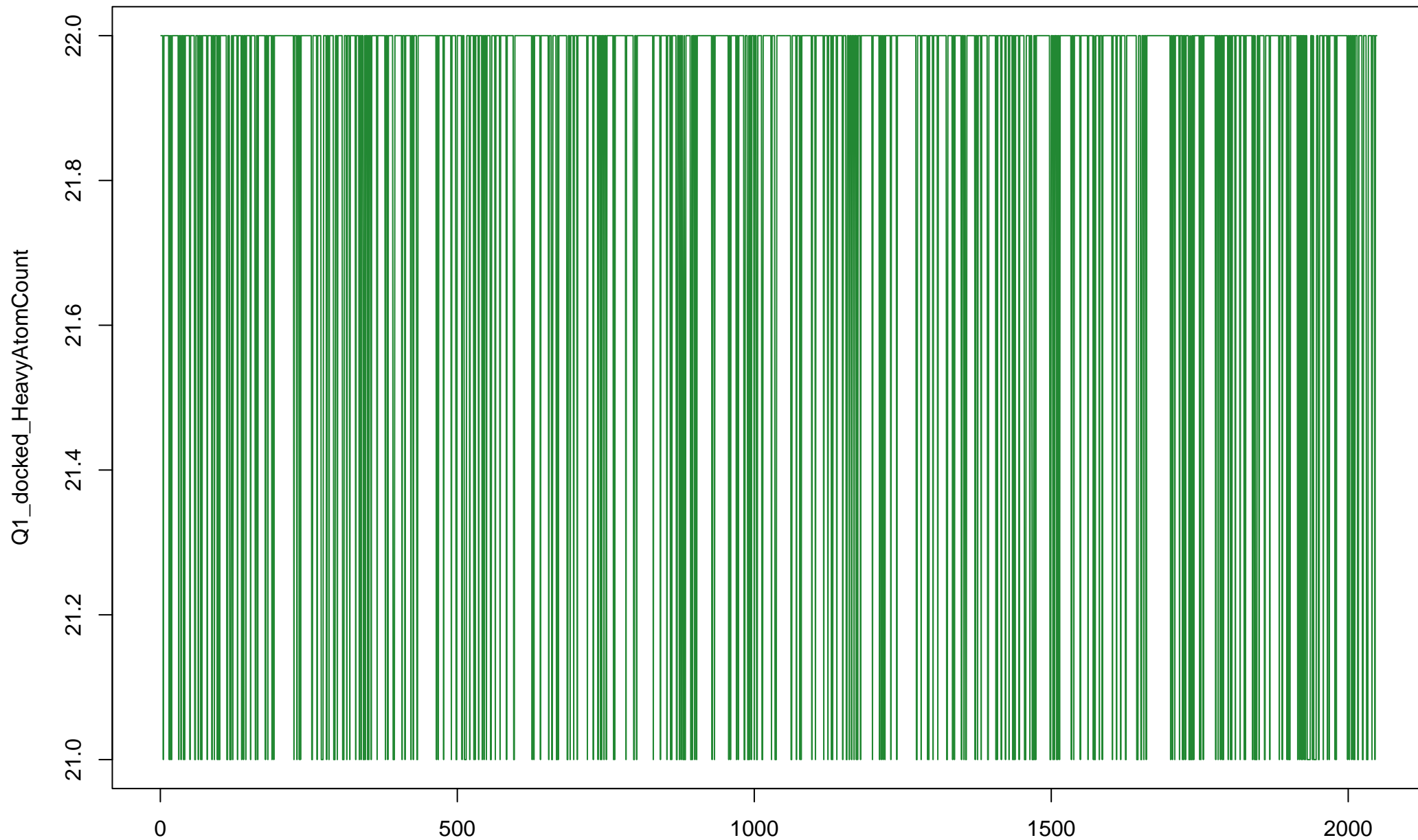
Q1_log_RMSD
ESS = 2050 | BMK = 0.0429 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



Q1_Xtransf_ec_tanimoto_similarity
ESS = 1890 | BMK = 0.0508 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



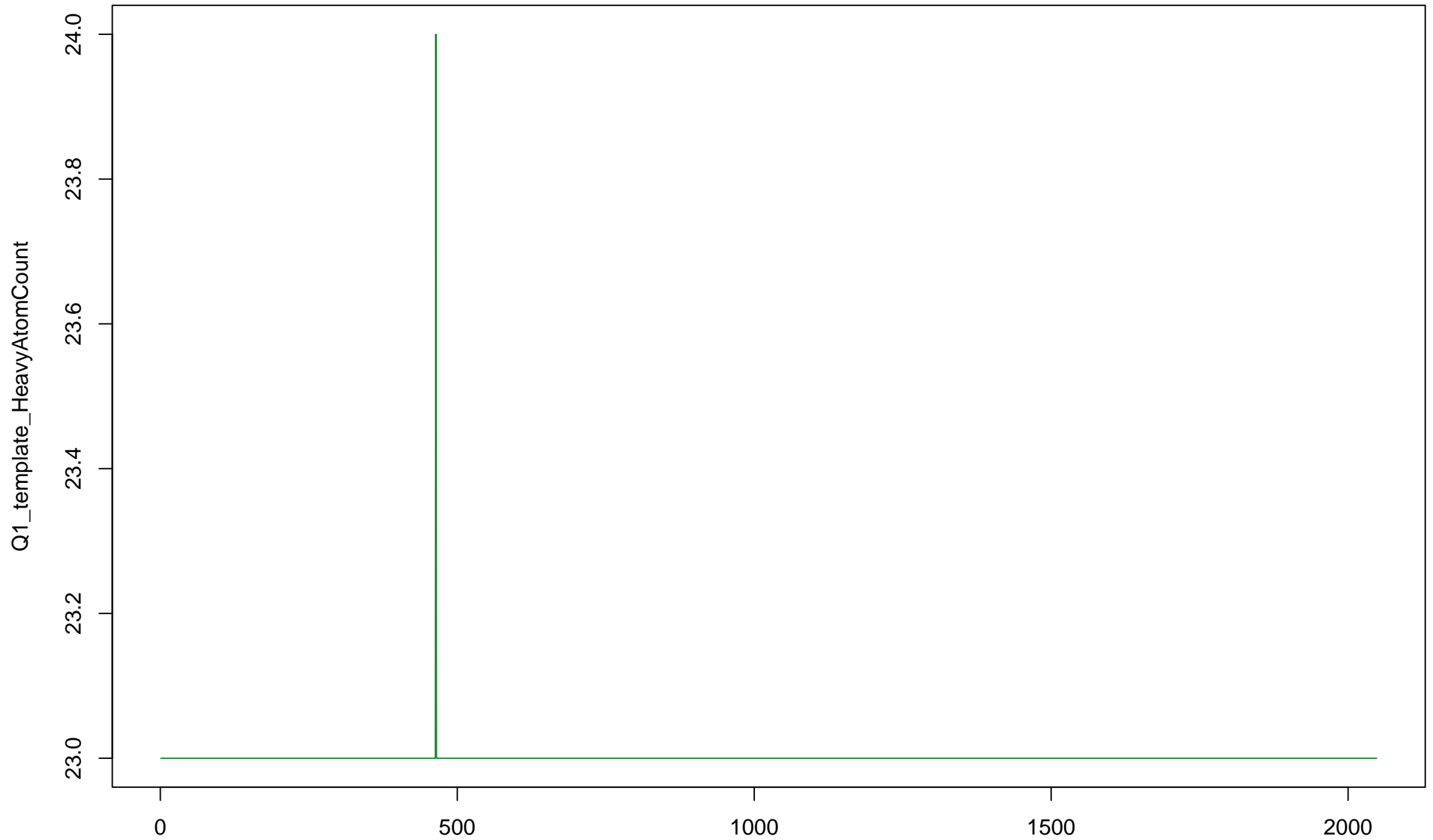
Q1_docked_HeavyAtomCount
ESS = 1860 | BMK = 0.0125 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0



Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0.524 | MCSE(6.27) = 2.22 | stat: FALSE | burn: 612



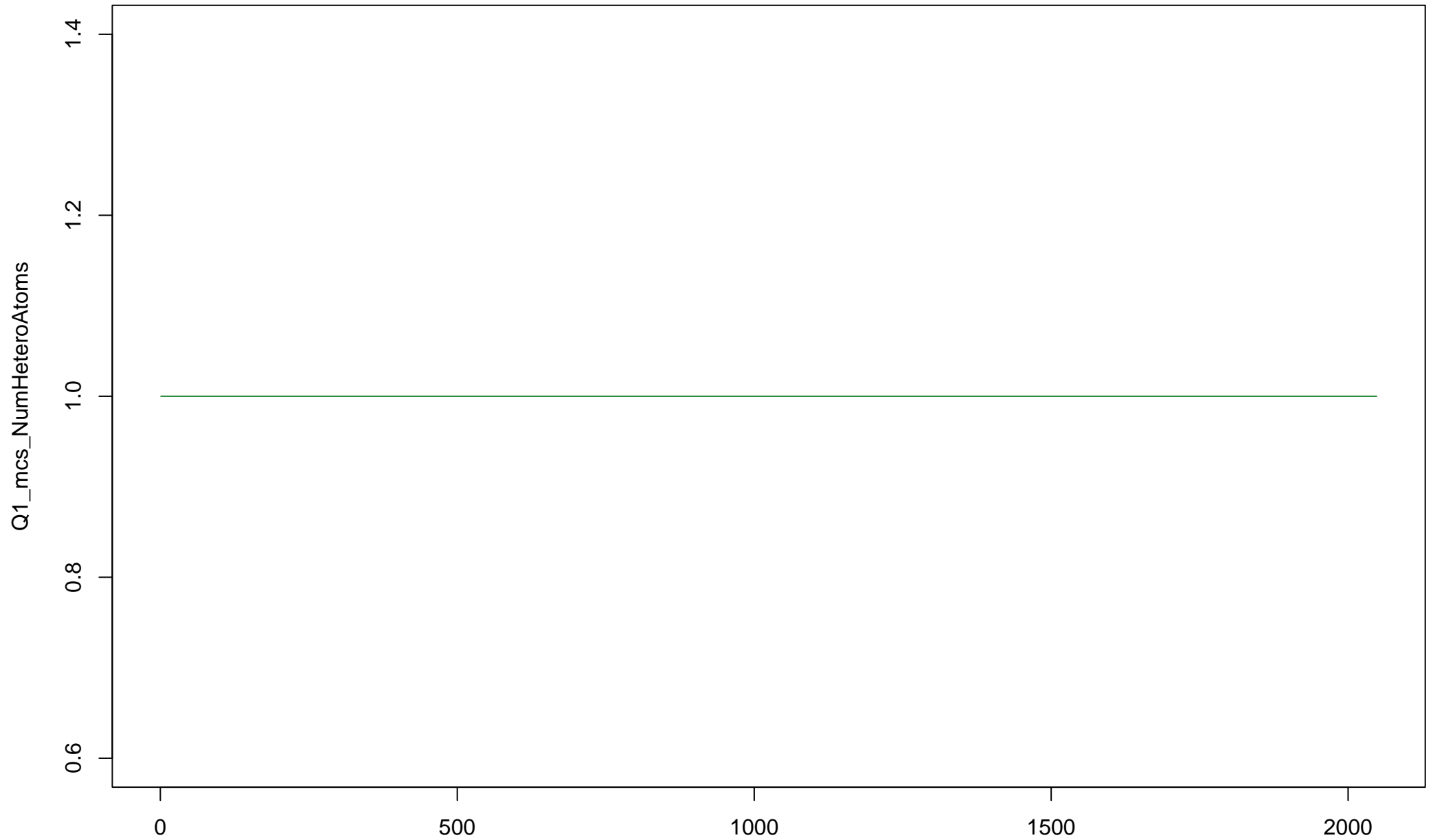
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



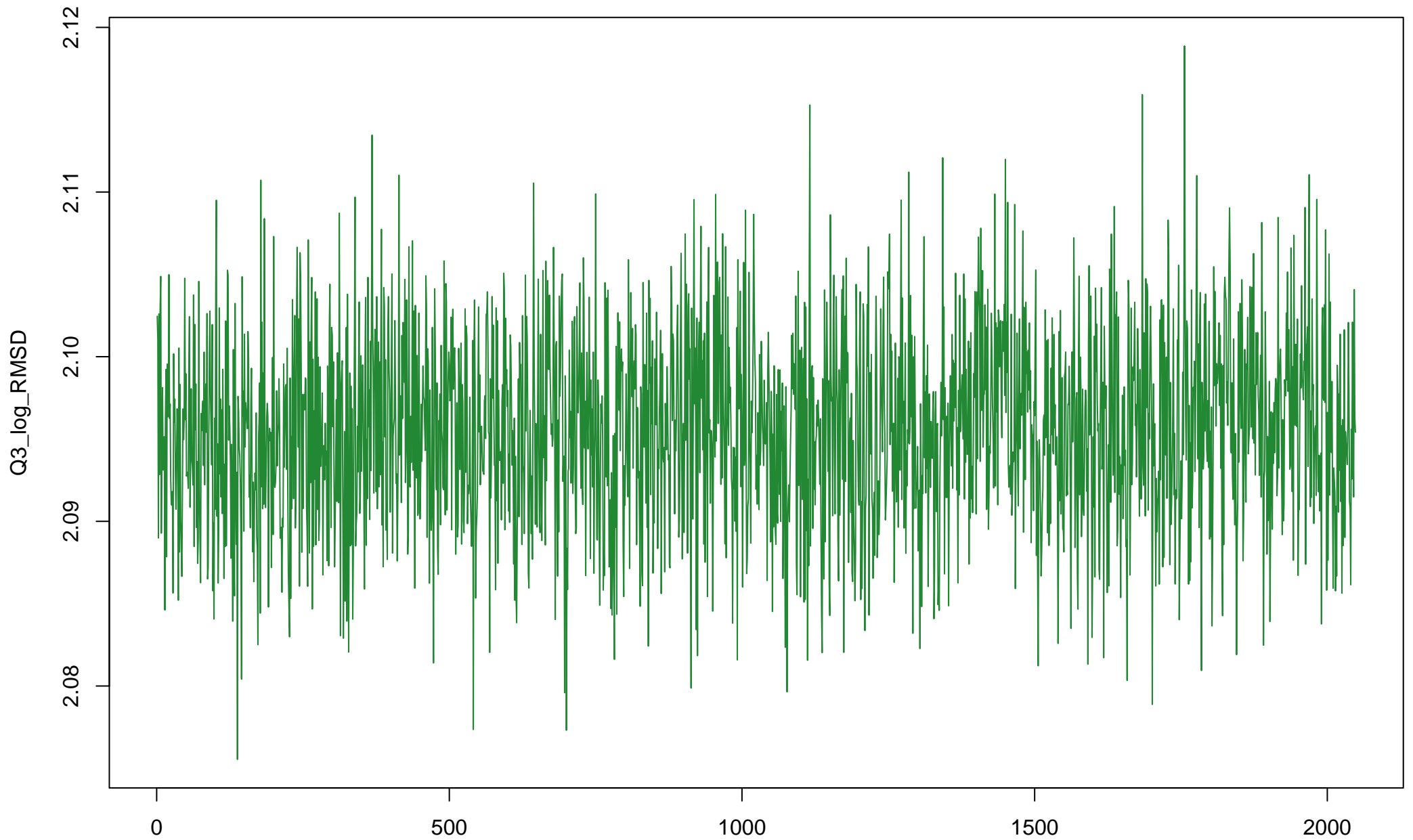
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



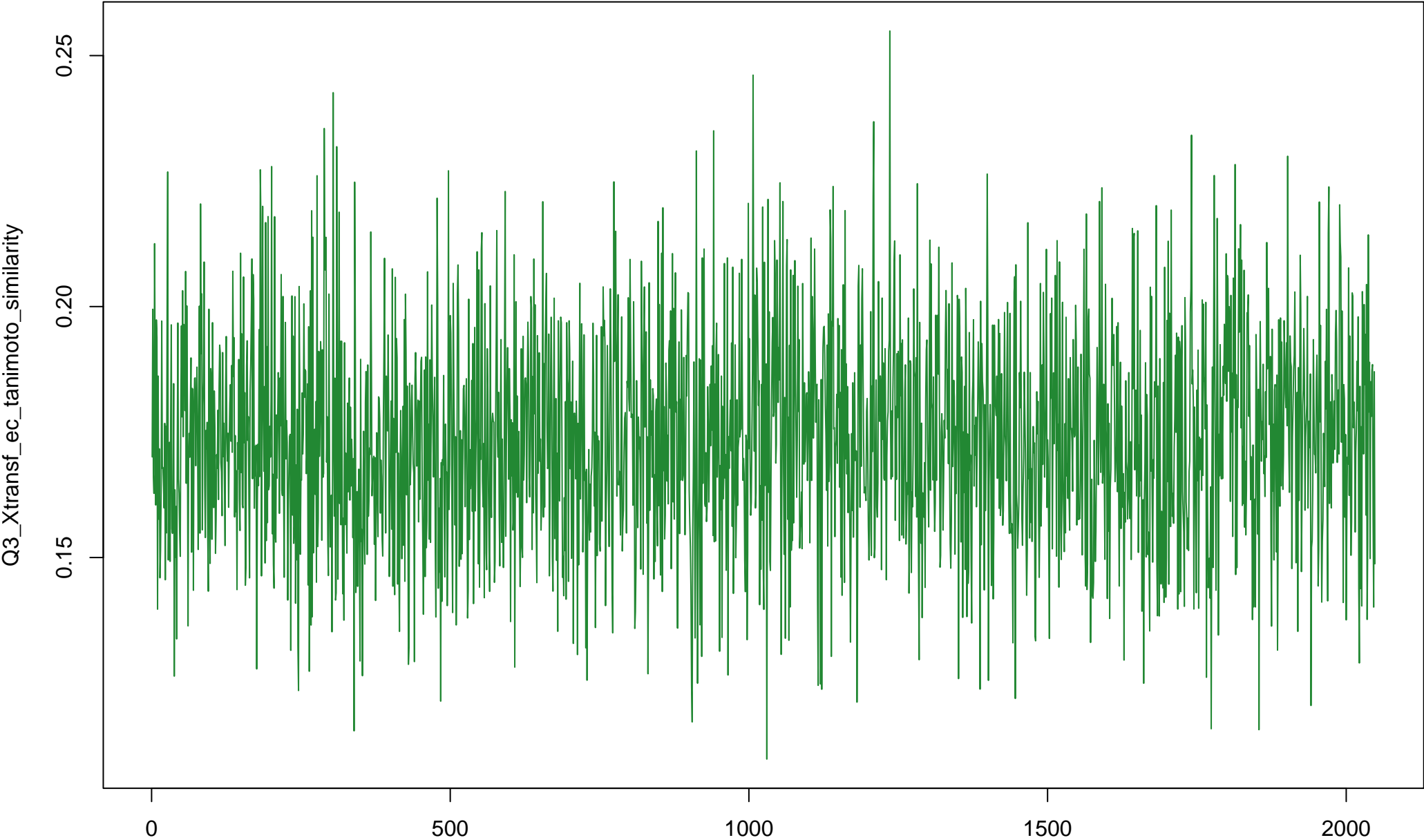
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



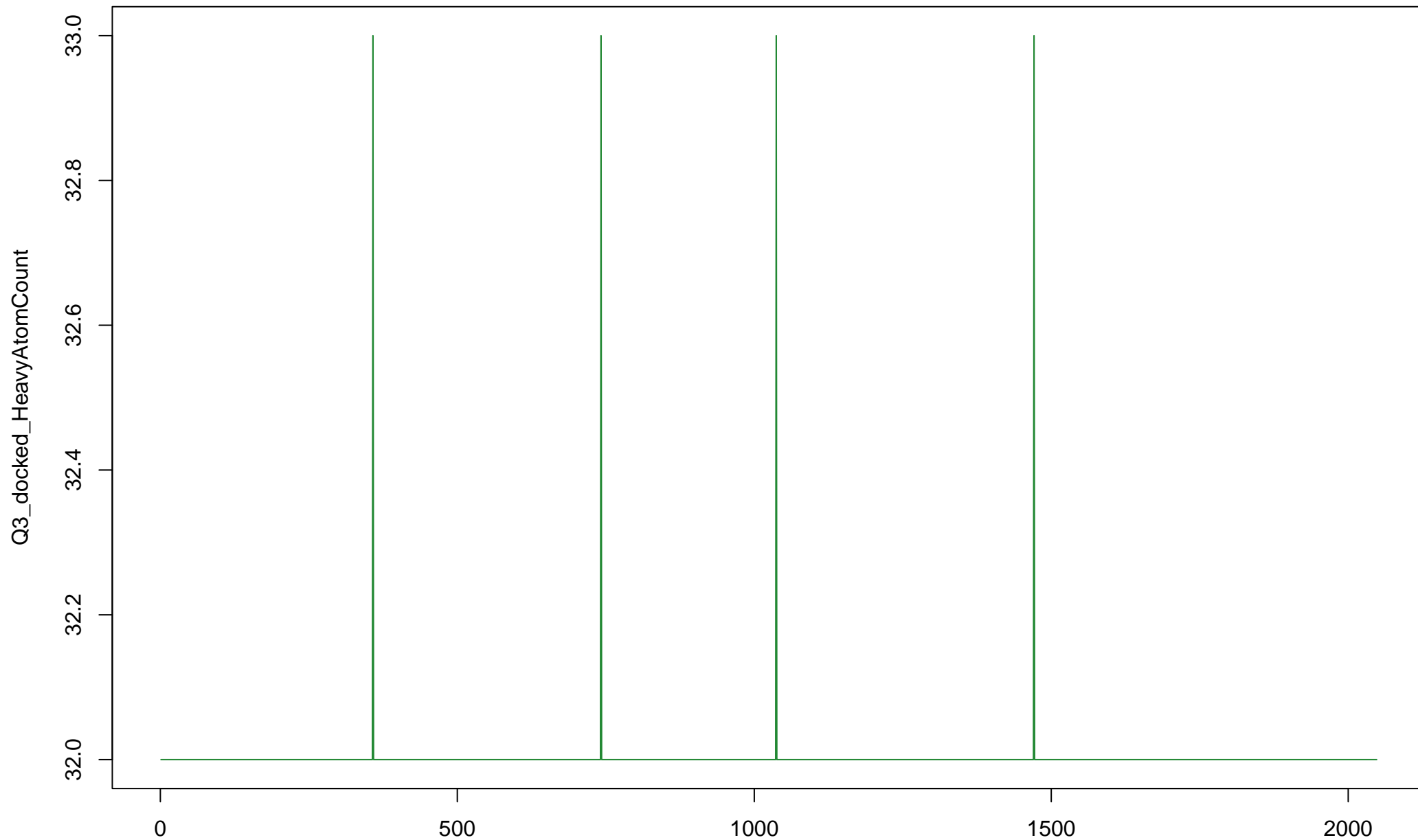
Q3_log_RMSD
ESS = 1520 | BMK = 0.0479 | MCSE(6.27) = 2.9 | stat: FALSE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0468 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0



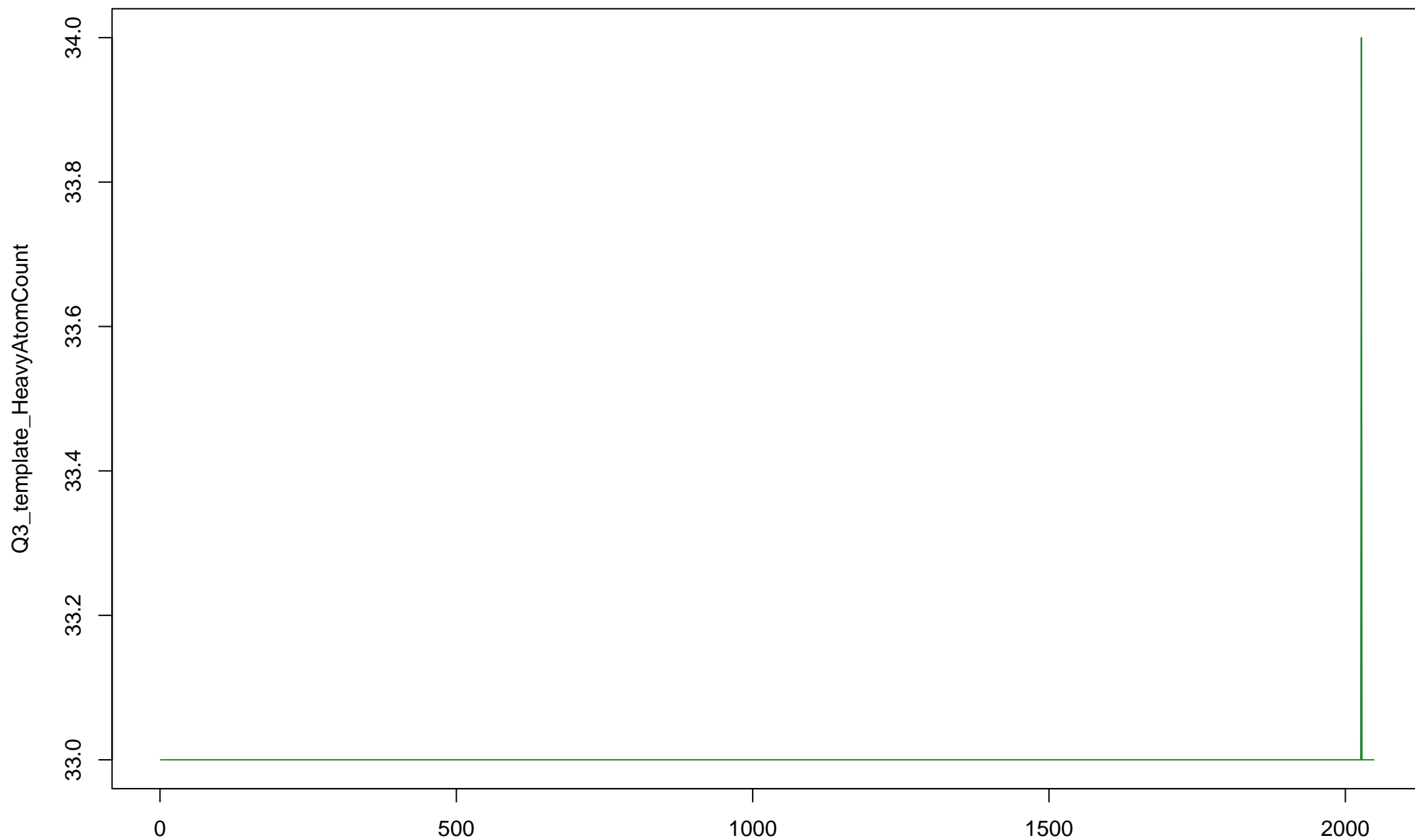
Q3_docked_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1632



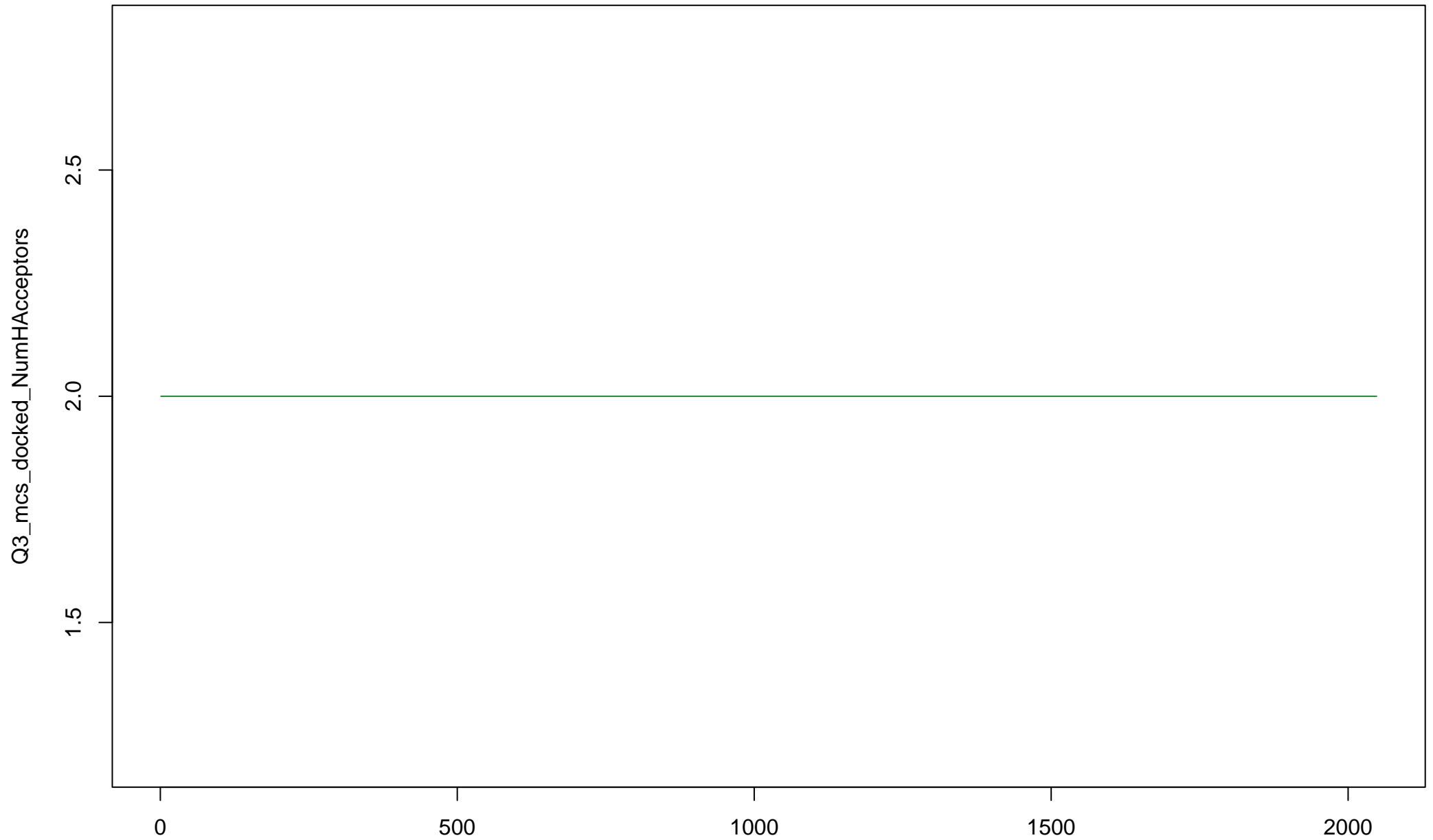
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



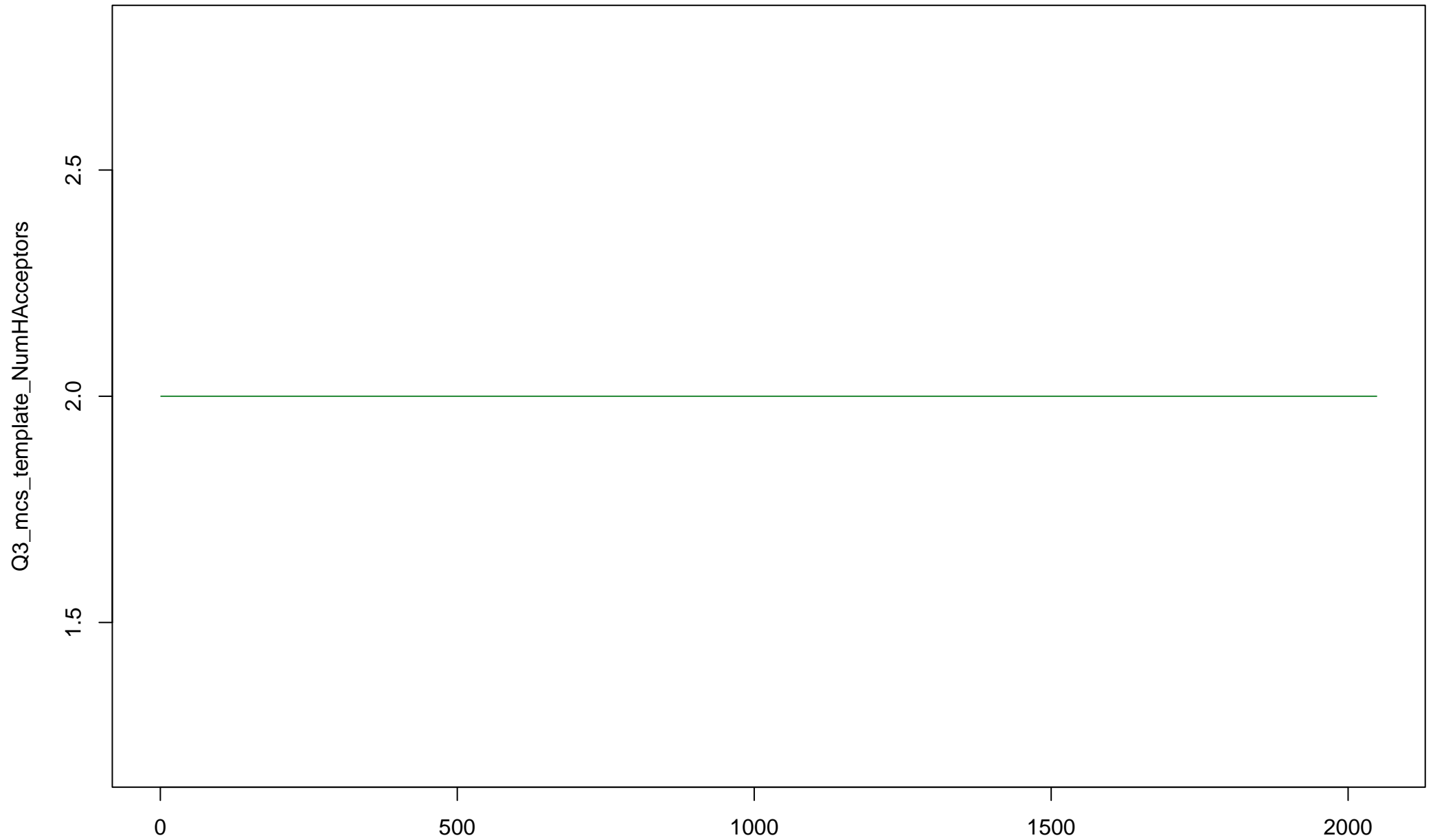
Q3_template_HeavyAtomCount
ESS = 2050 | BMK = 0.517 | MCSE(6.27) = 0 | stat: TRUE | burn: 2040



Q3_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



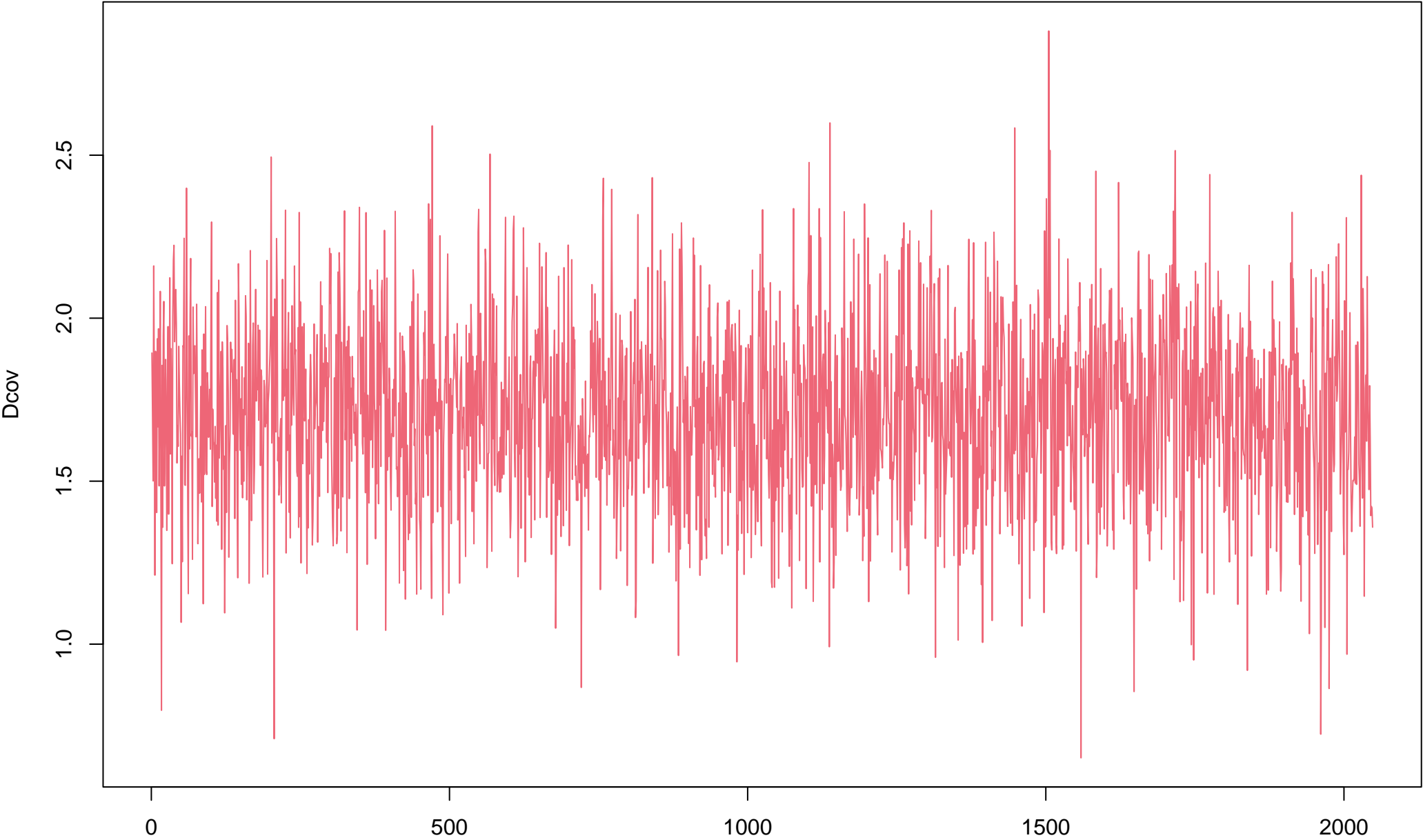
Q3_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



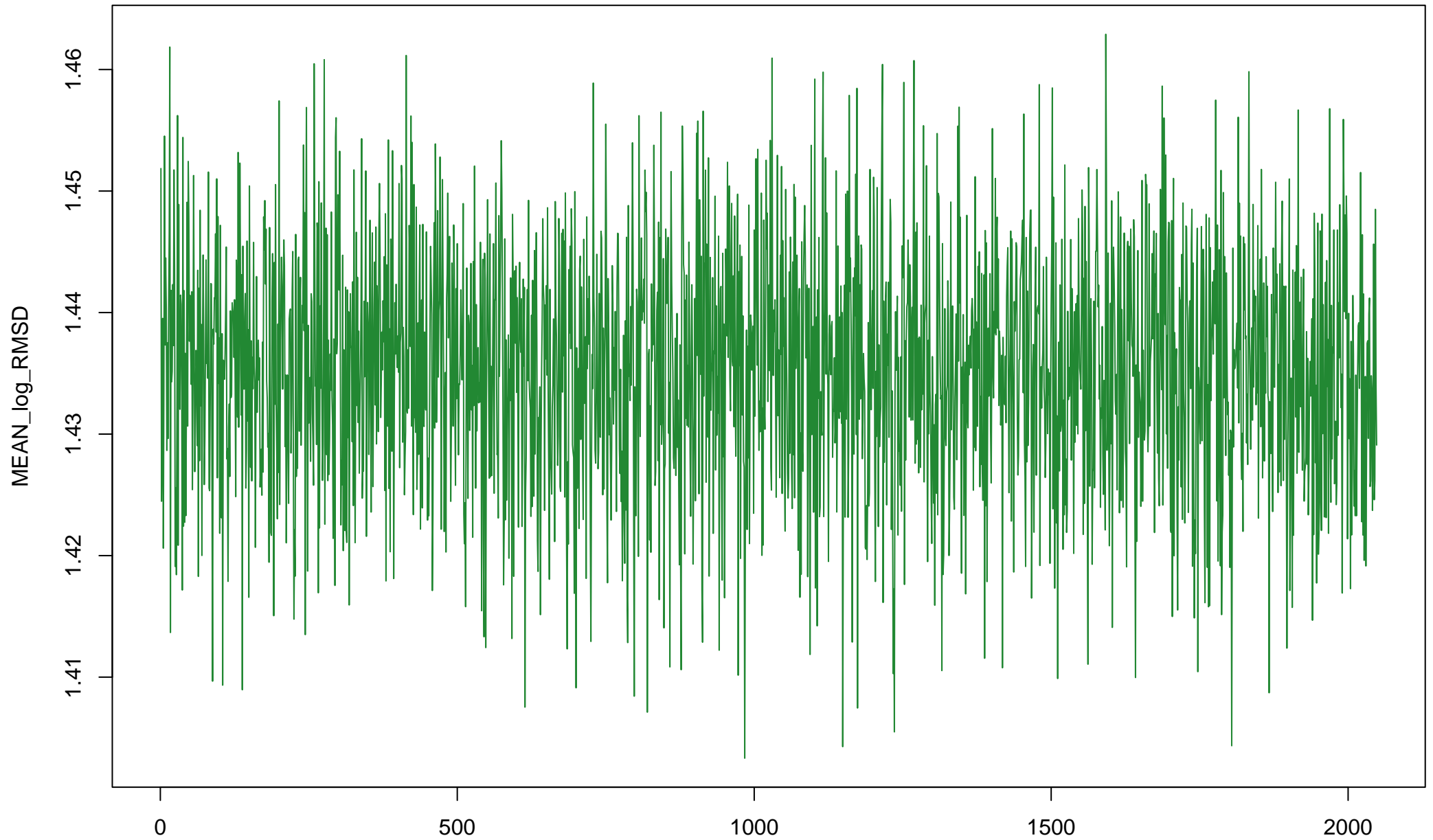
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



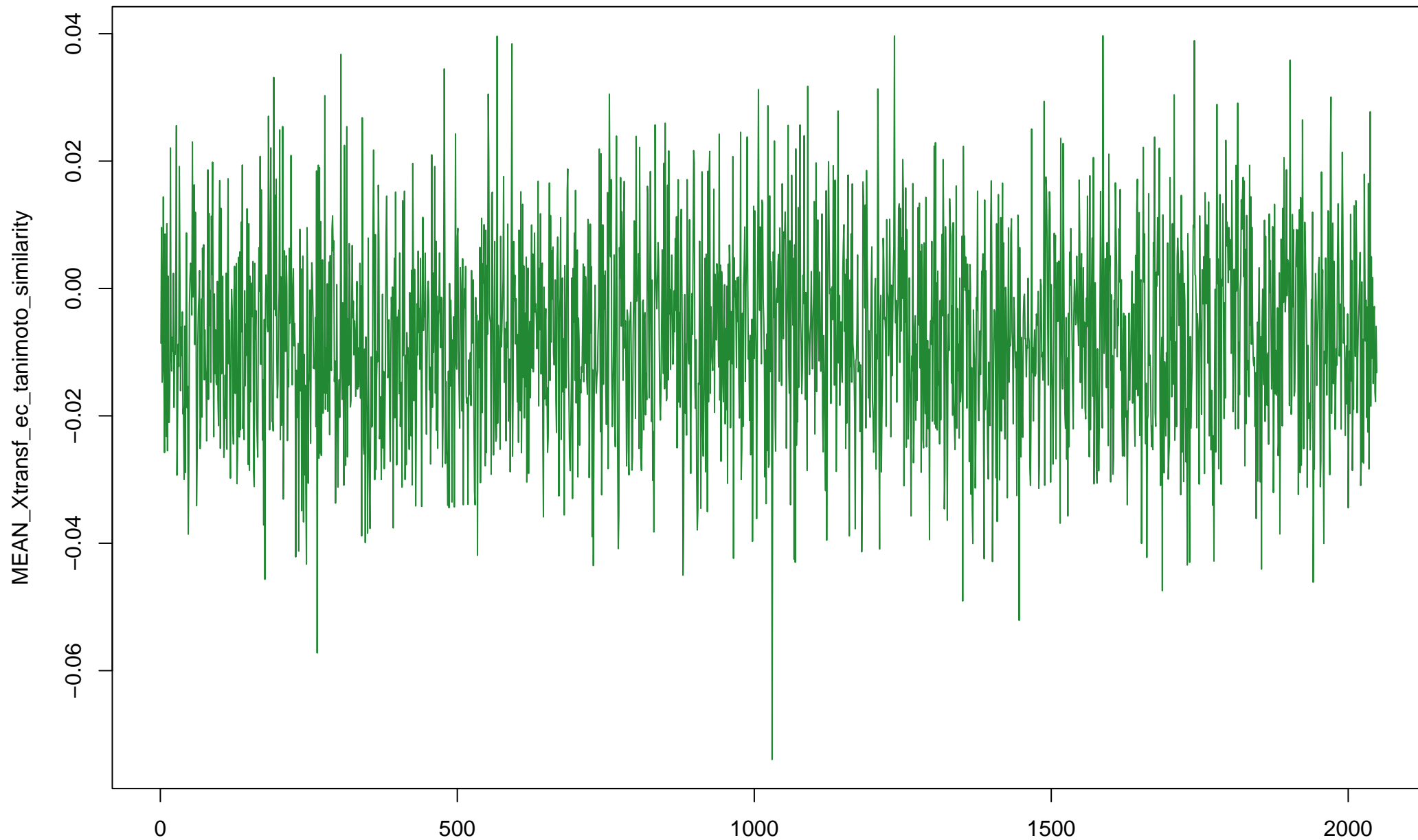
Dcov
ESS = 2020 | BMK = 0.0384 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0



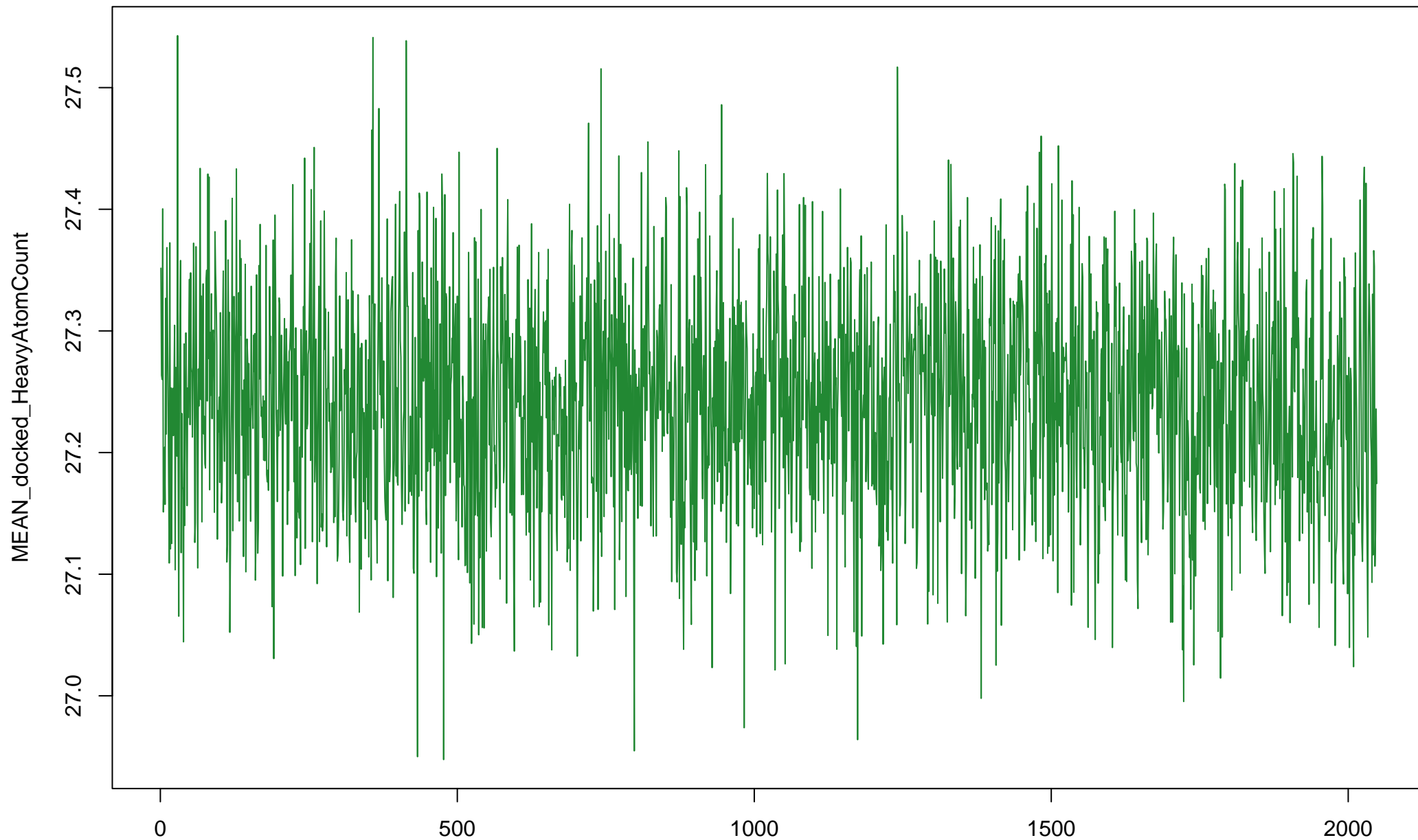
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0343 | MCSE(6.27) = 1.84 | stat: TRUE | burn: 0



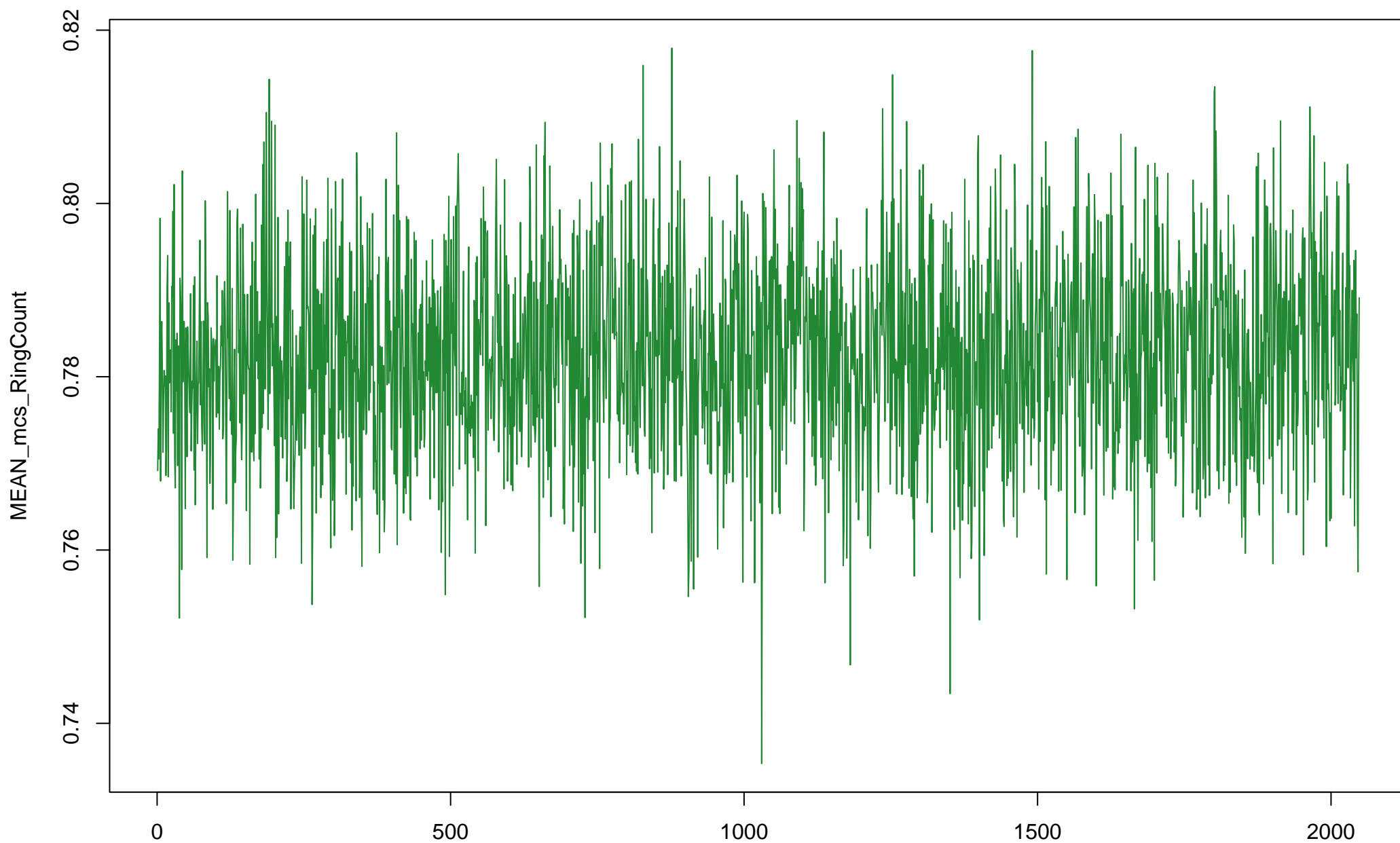
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0



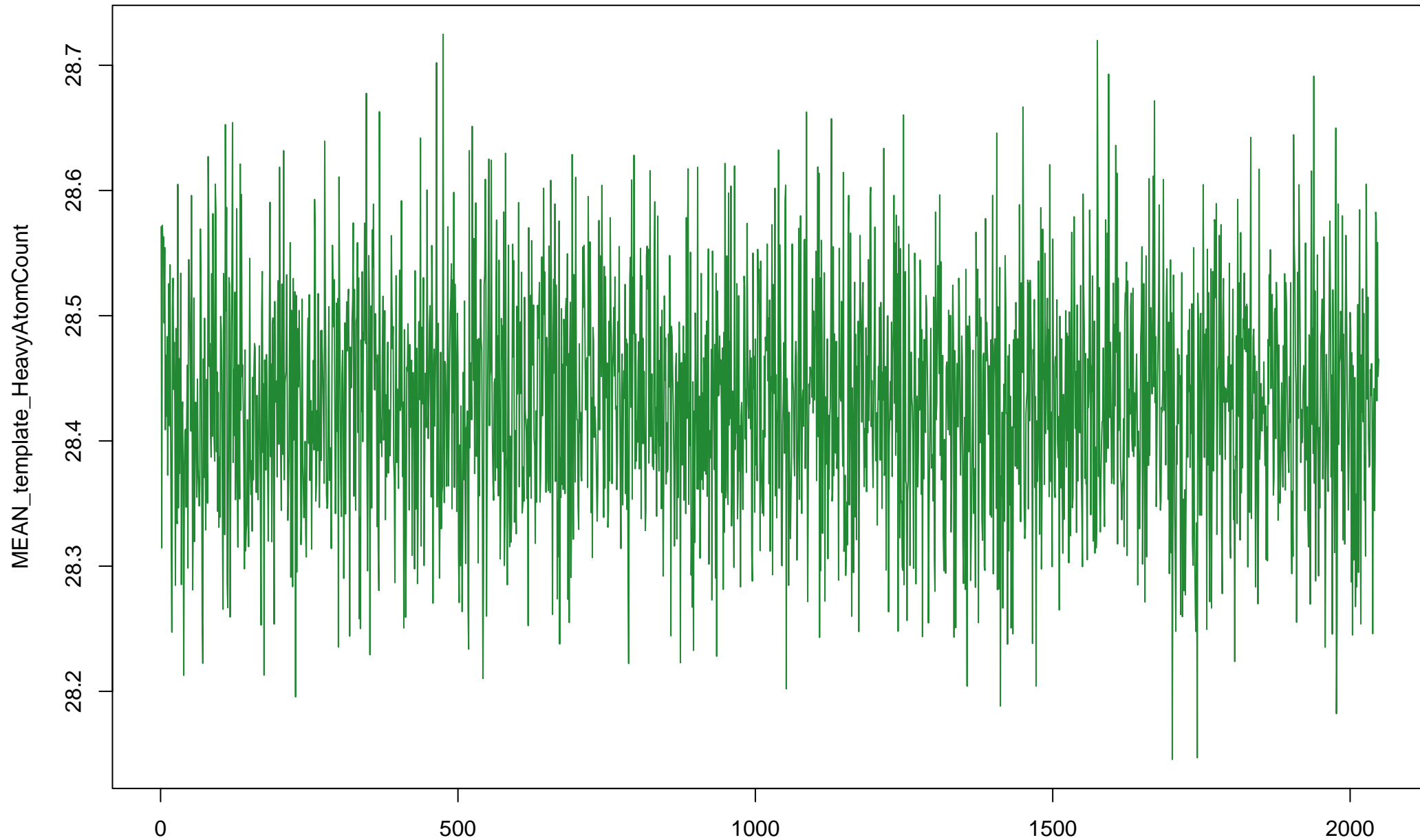
MEAN_docked_HeavyAtomCount
ESS = 1810 | BMK = 0.0447 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



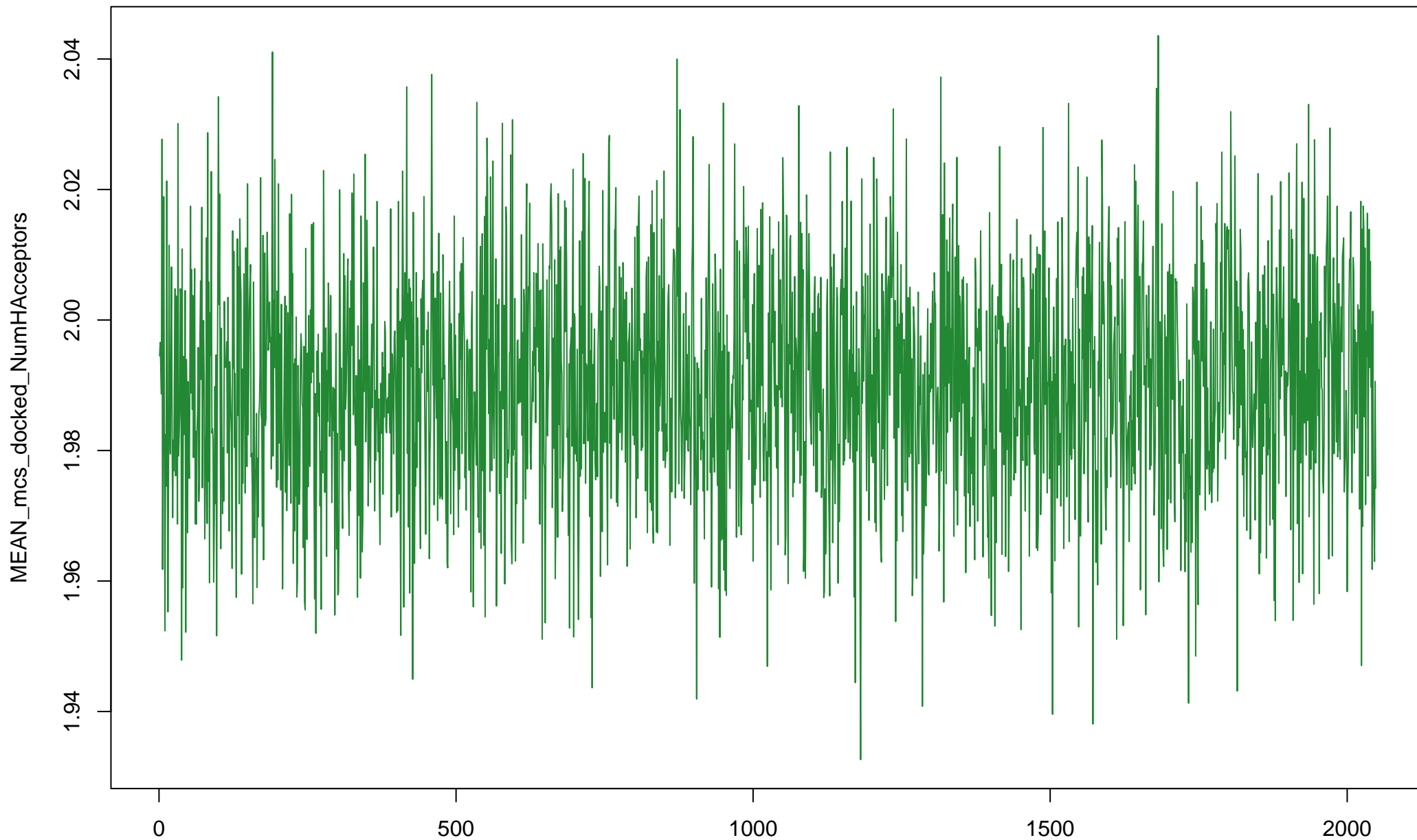
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0571 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0



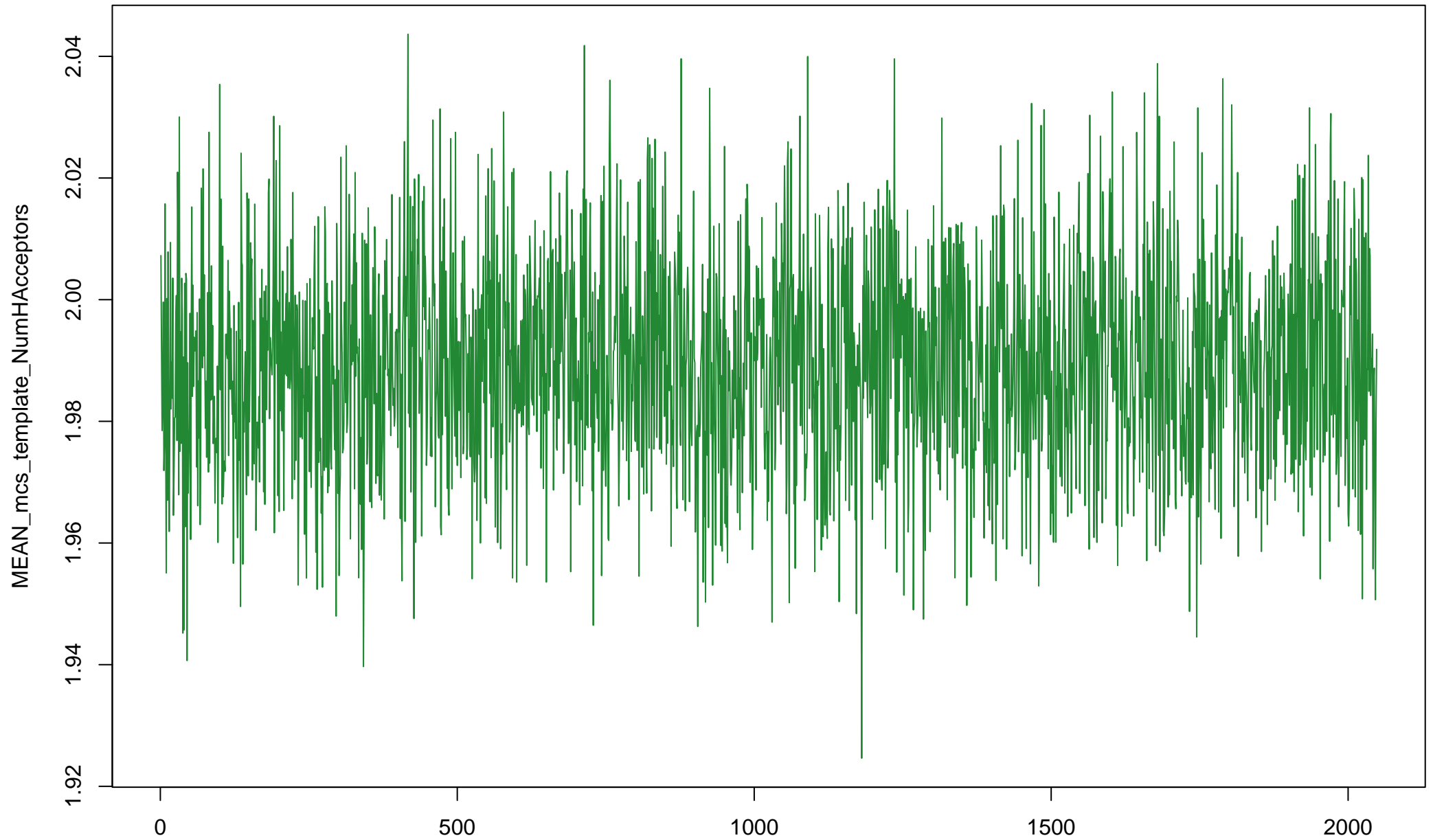
MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0451 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0



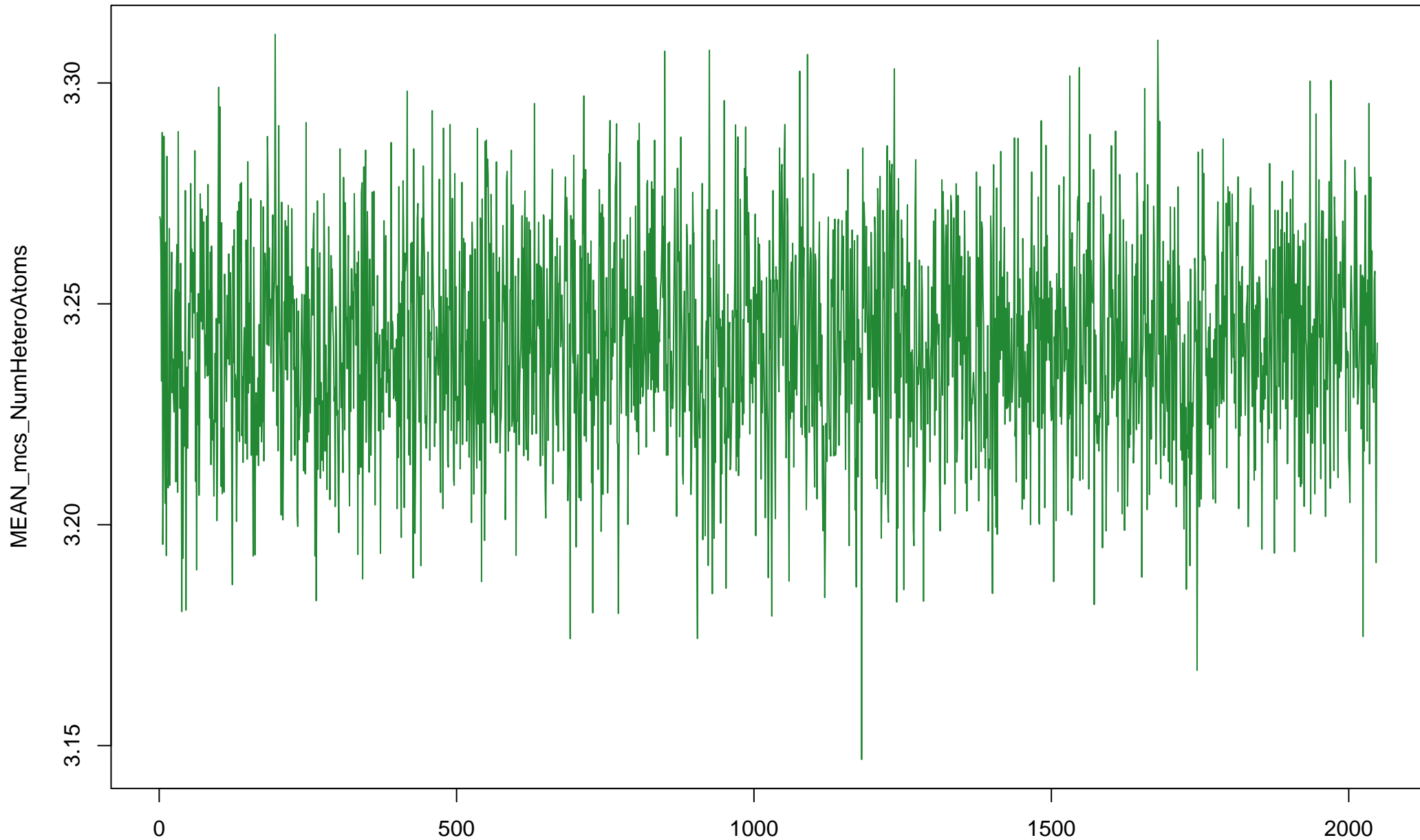
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0434 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



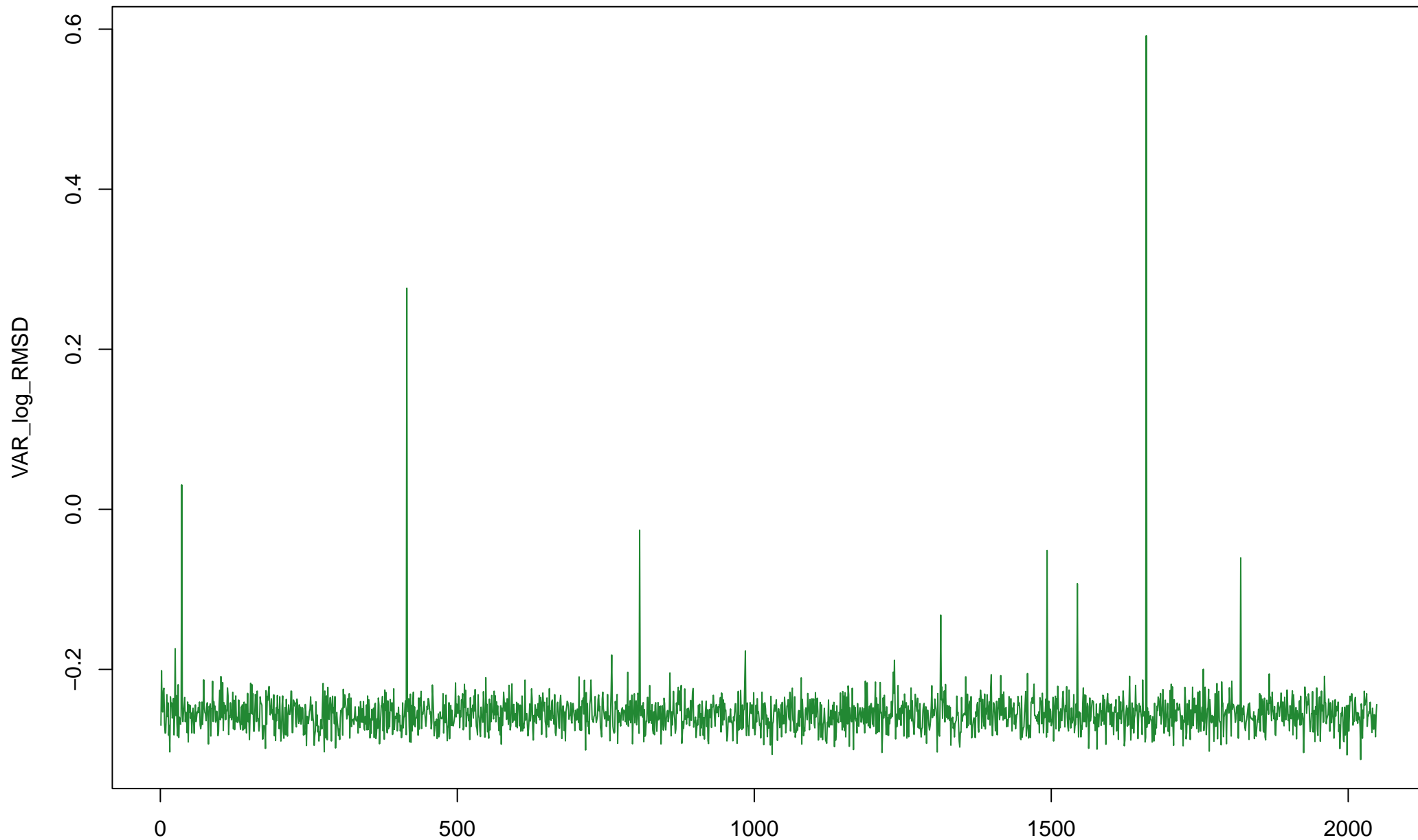
MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0402 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0



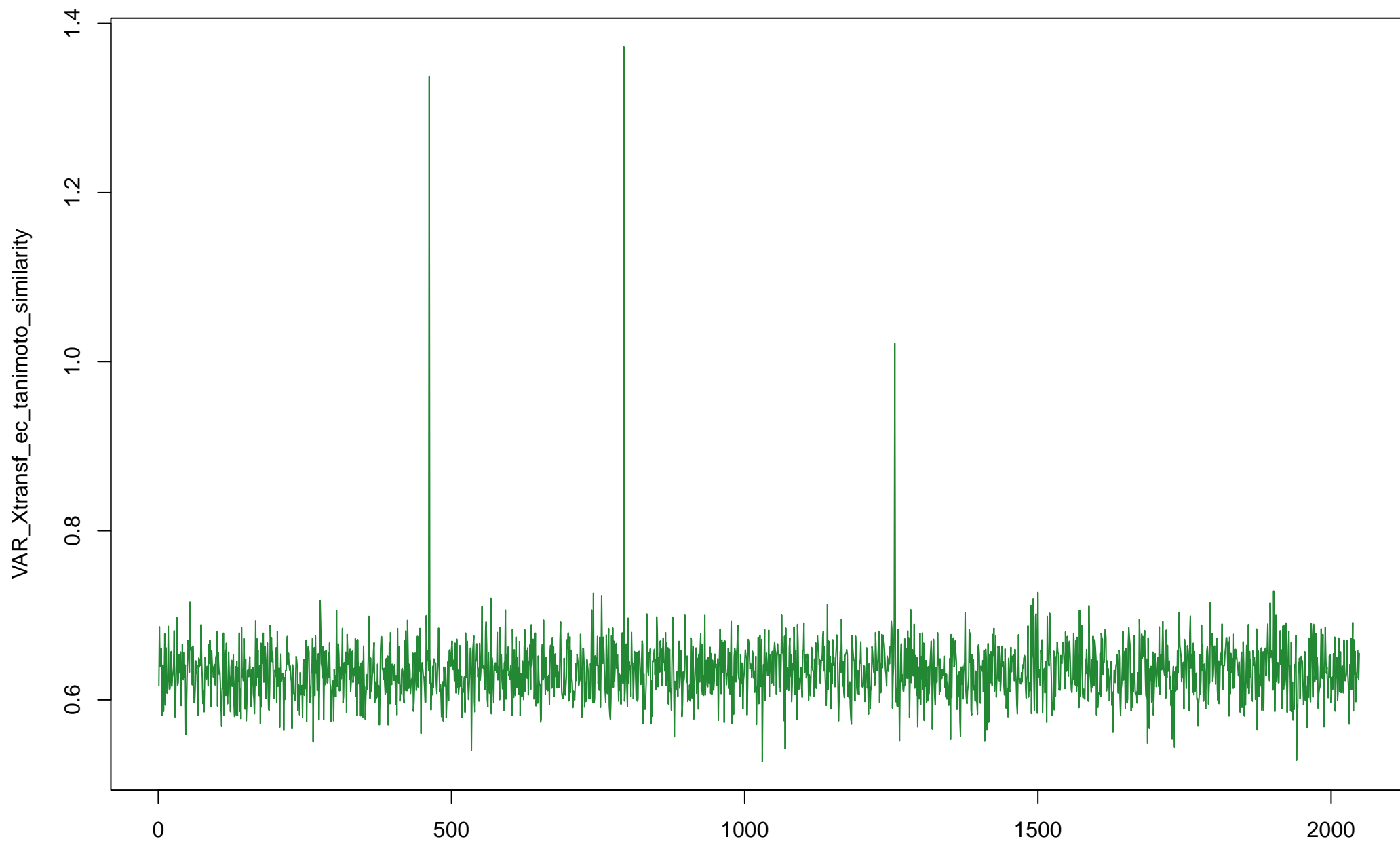
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0405 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0



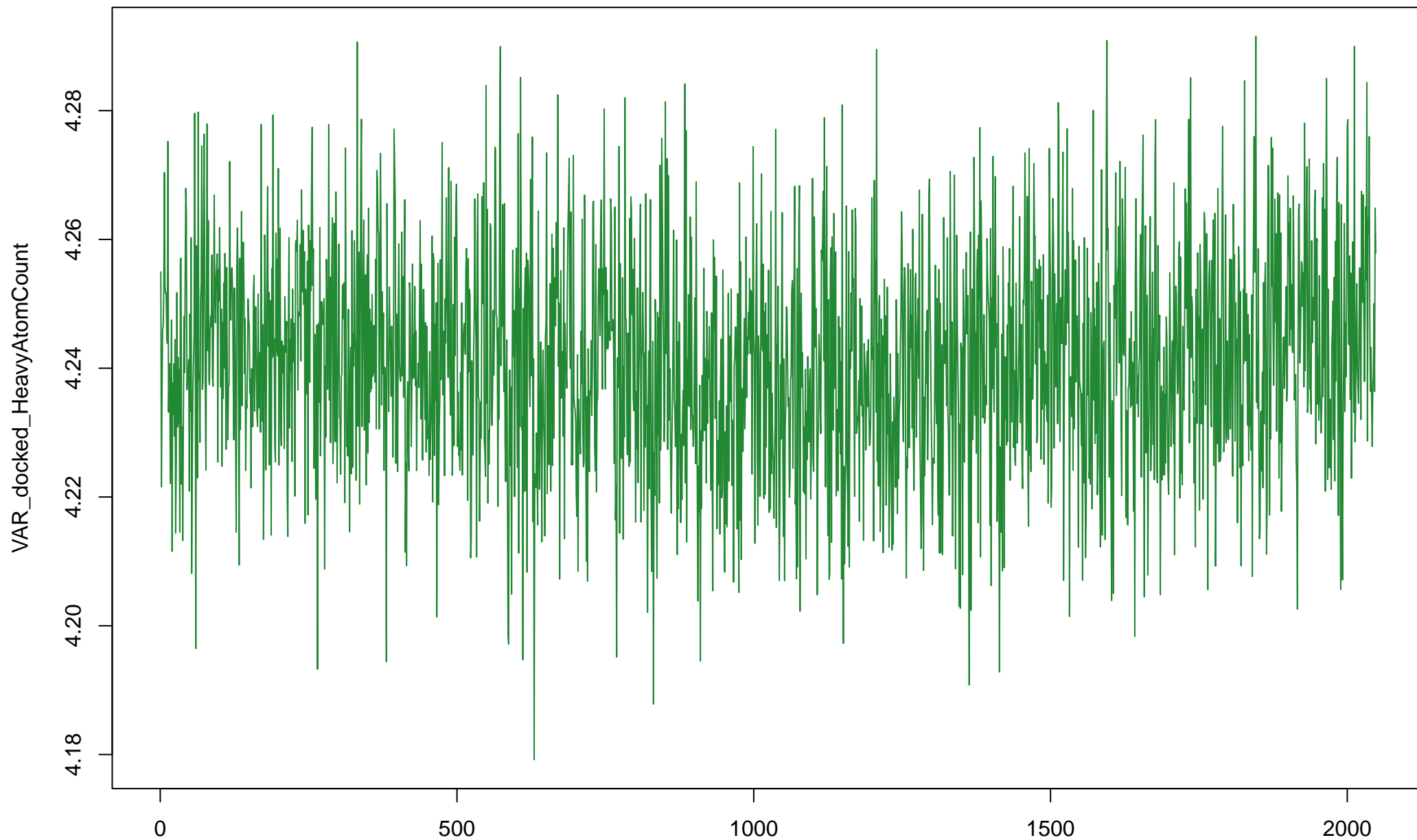
VAR_log_RMSD
ESS = 2050 | BMK = 0.0773 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0



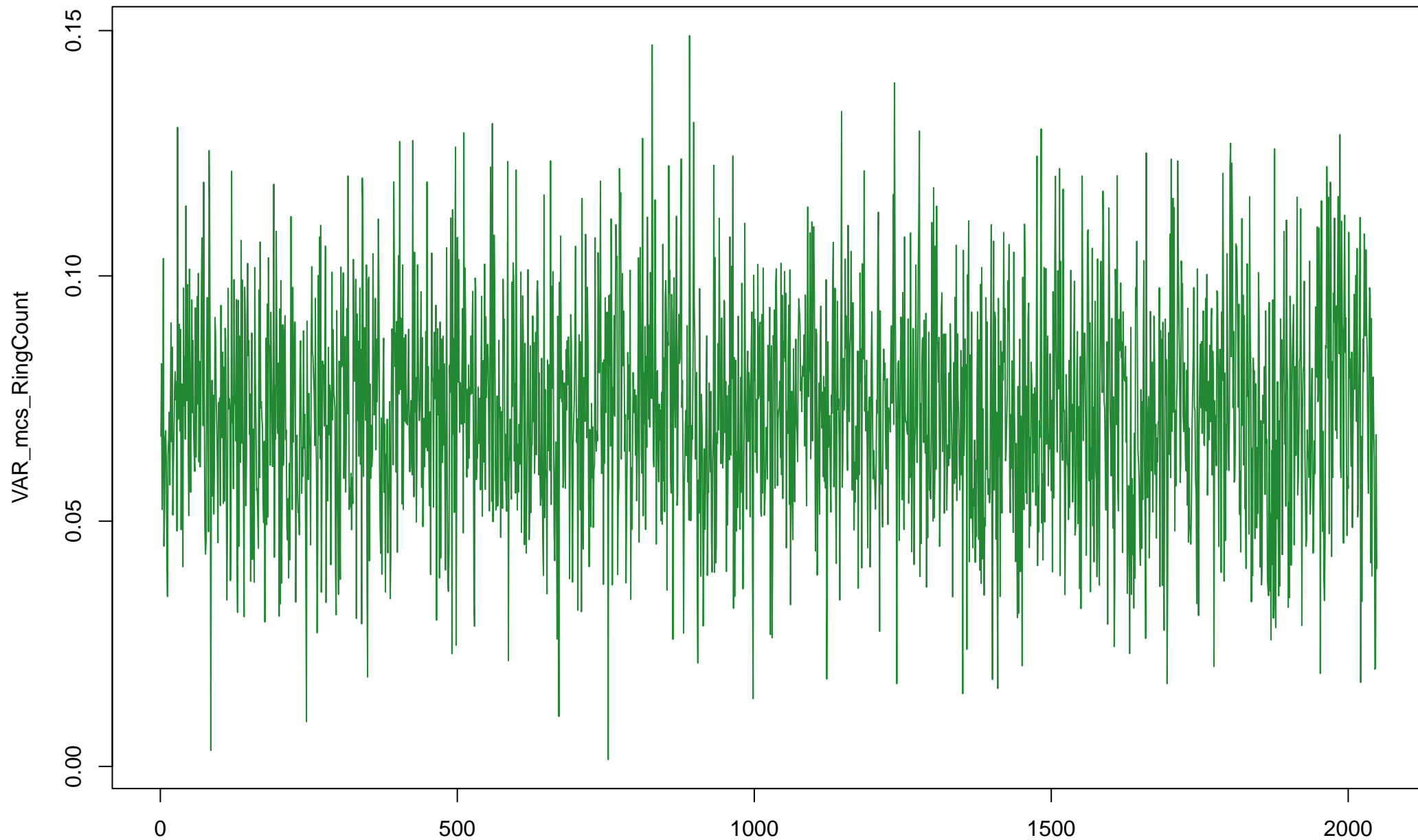
VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0635 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



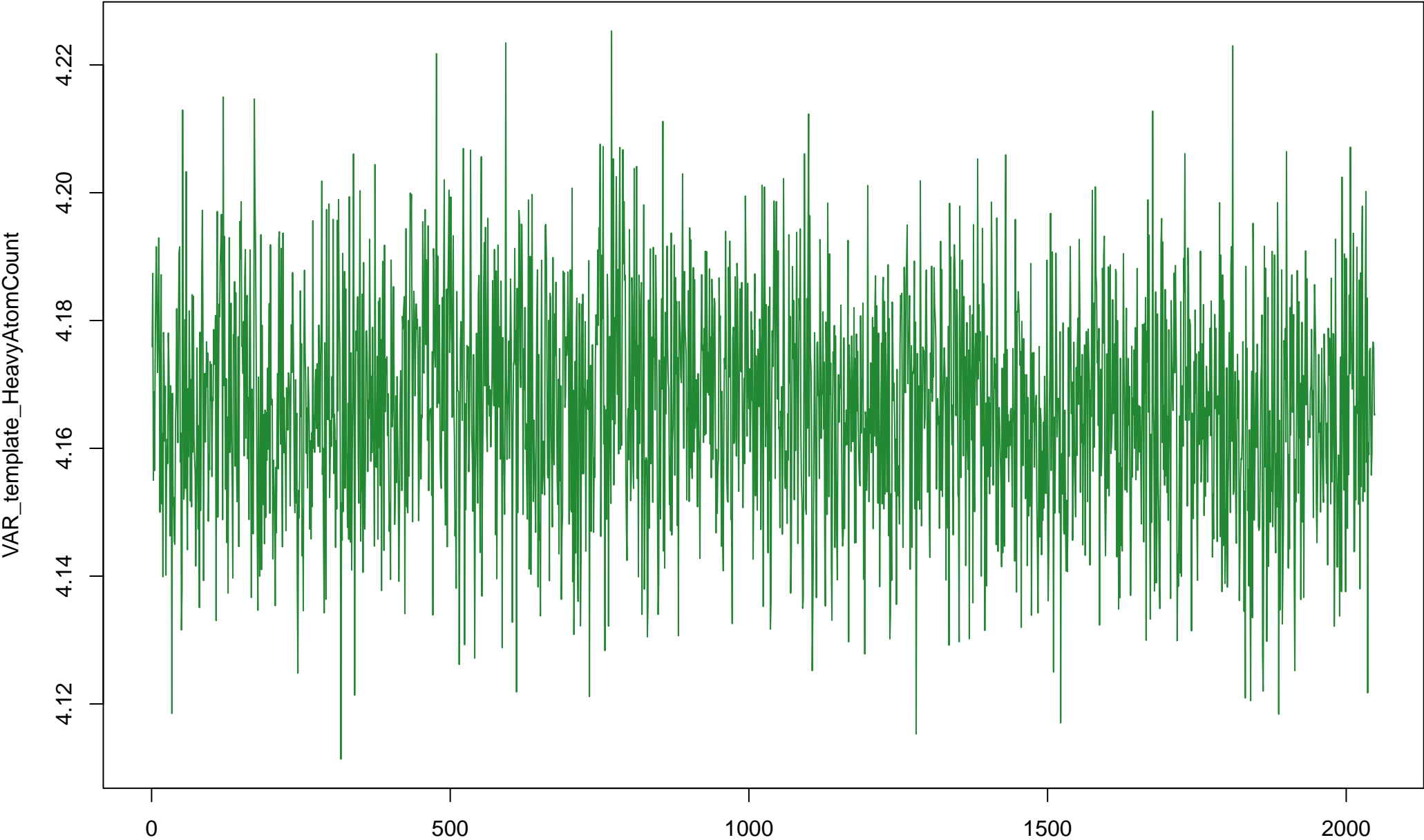
VAR_docked_HeavyAtomCount
ESS = 1160 | BMK = 0.05 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0



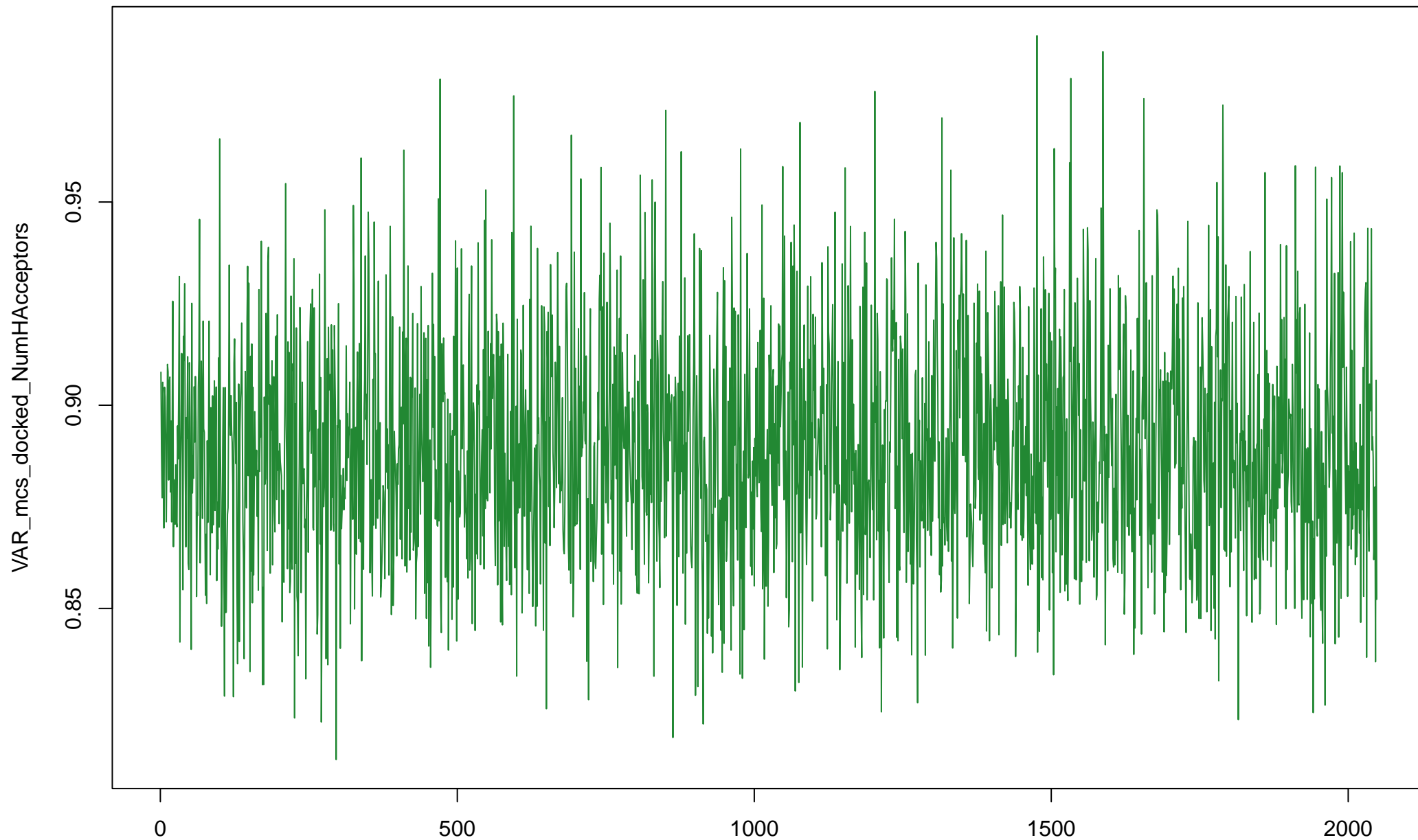
VAR_mcs_RingCount
ESS = 2050 | BMK = 0.0494 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0



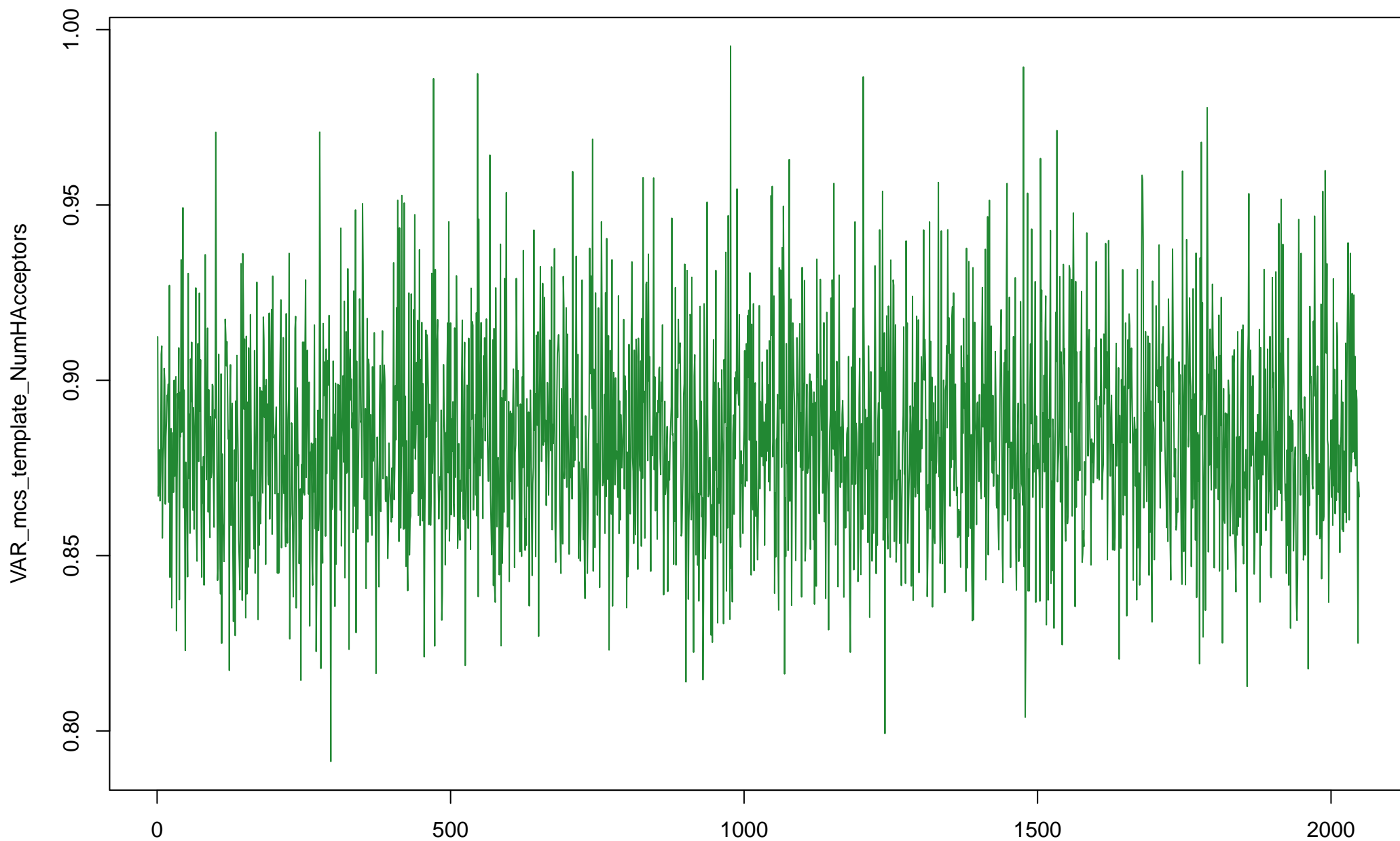
VAR_template_HeavyAtomCount
ESS = 1800 | BMK = 0.0615 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0



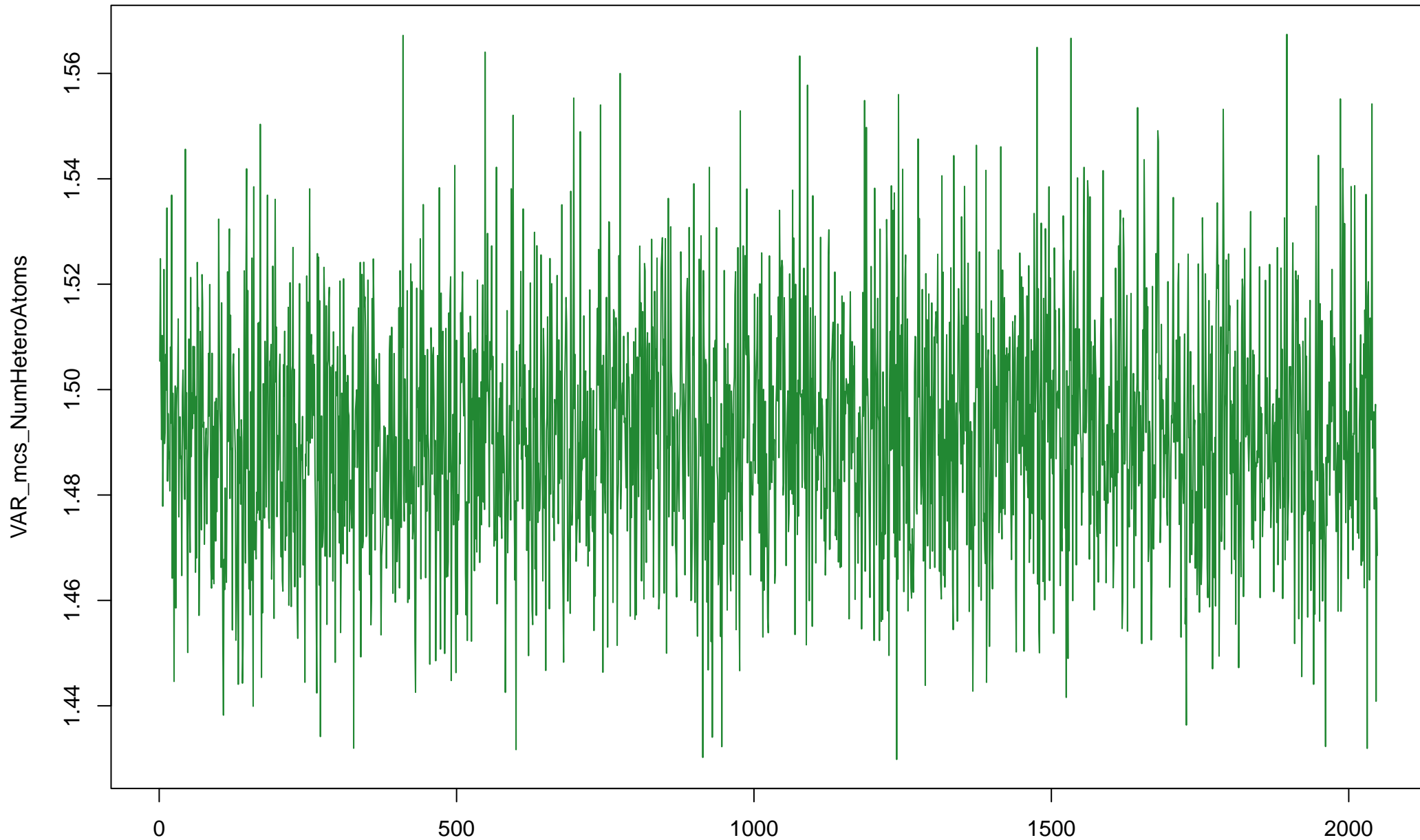
VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0419 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



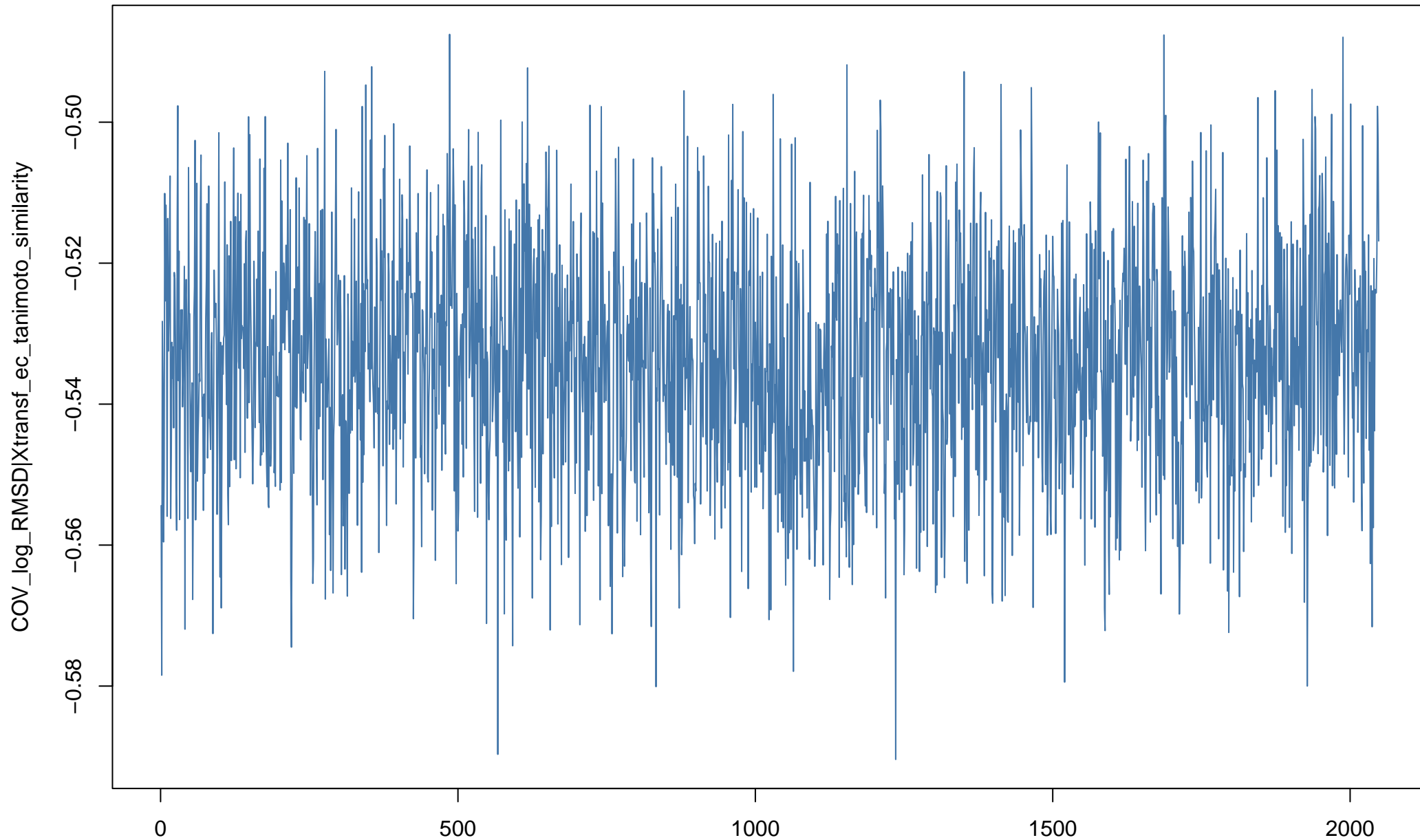
VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0409 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



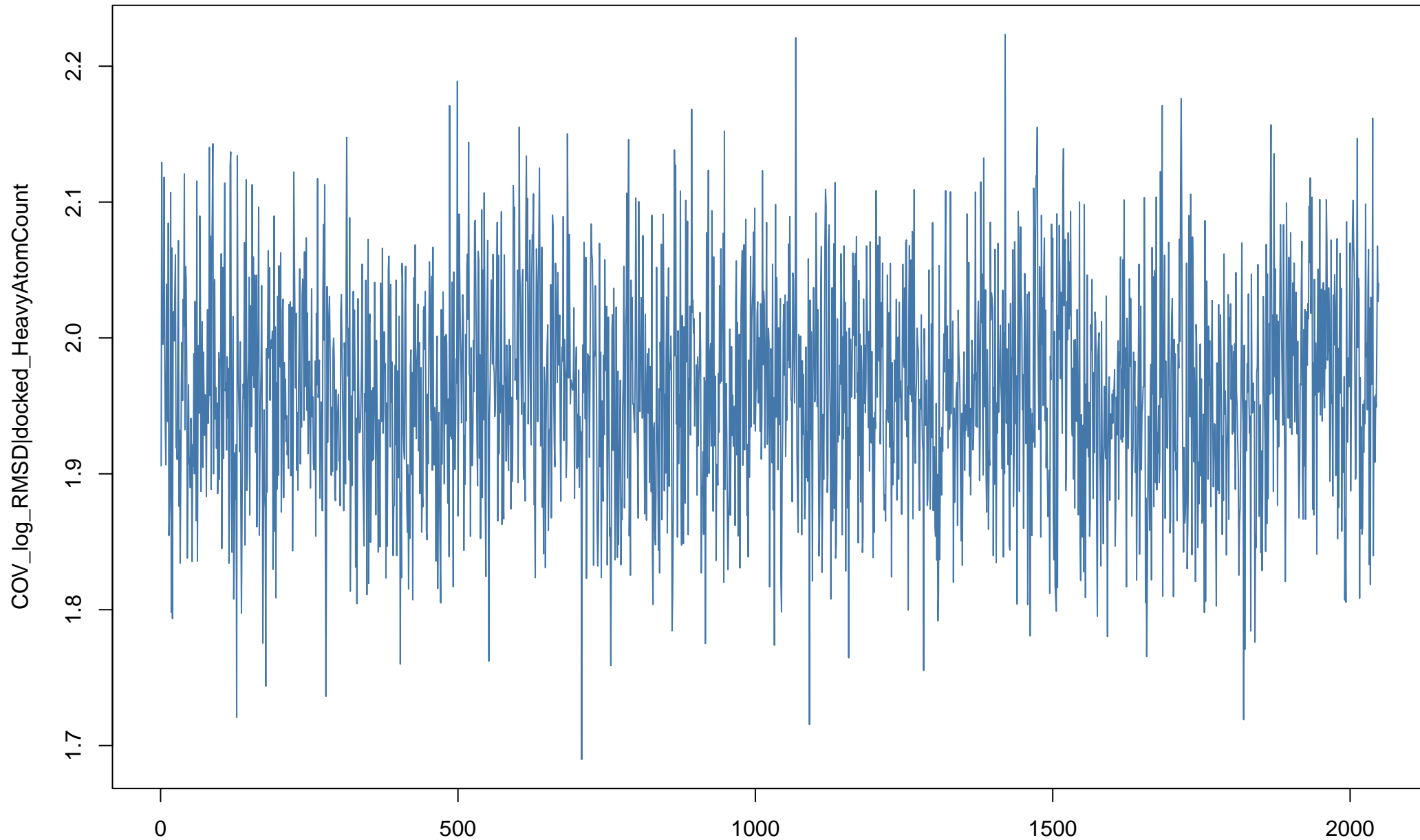
VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0493 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0



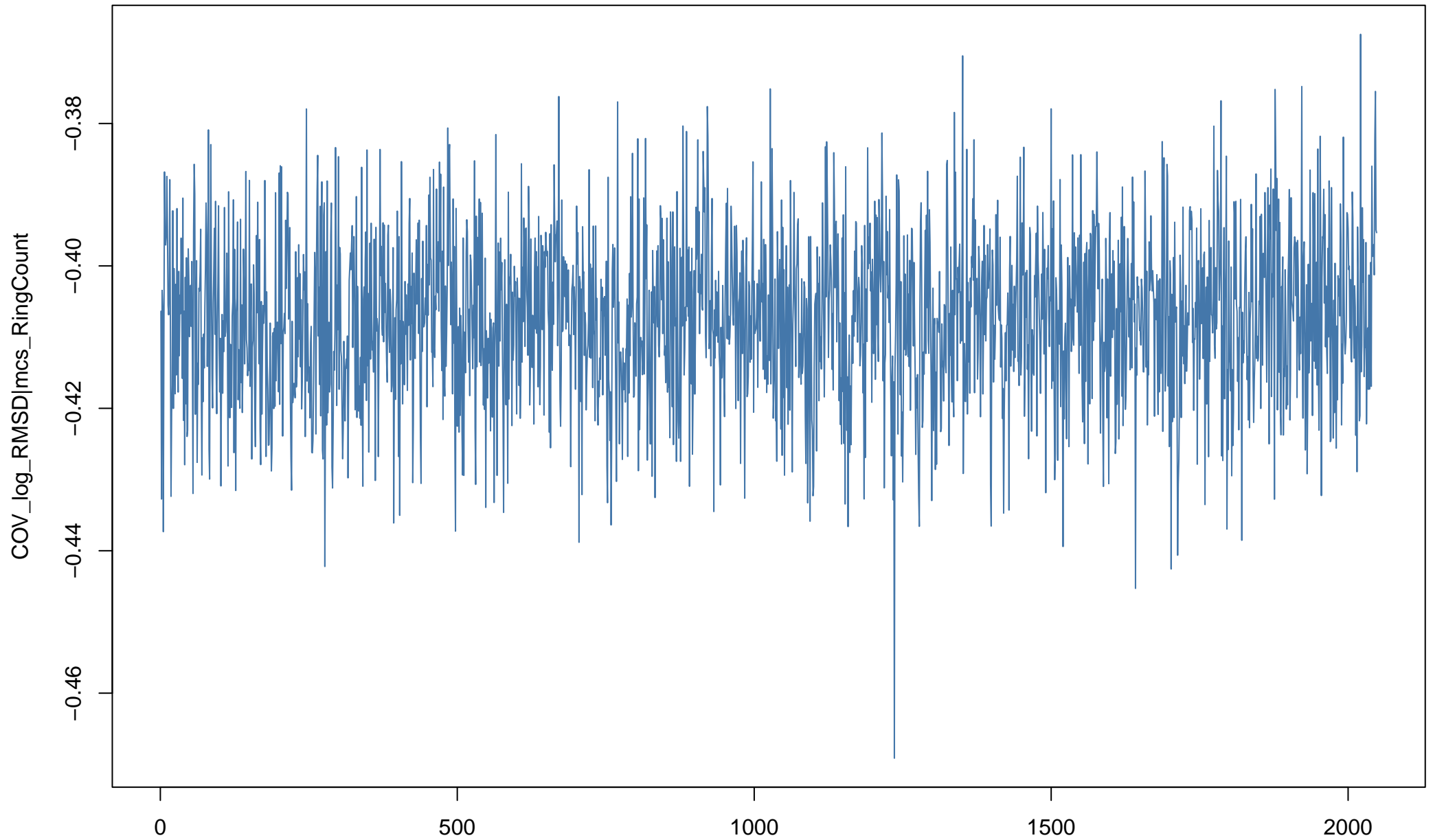
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1760 | BMK = 0.0492 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0



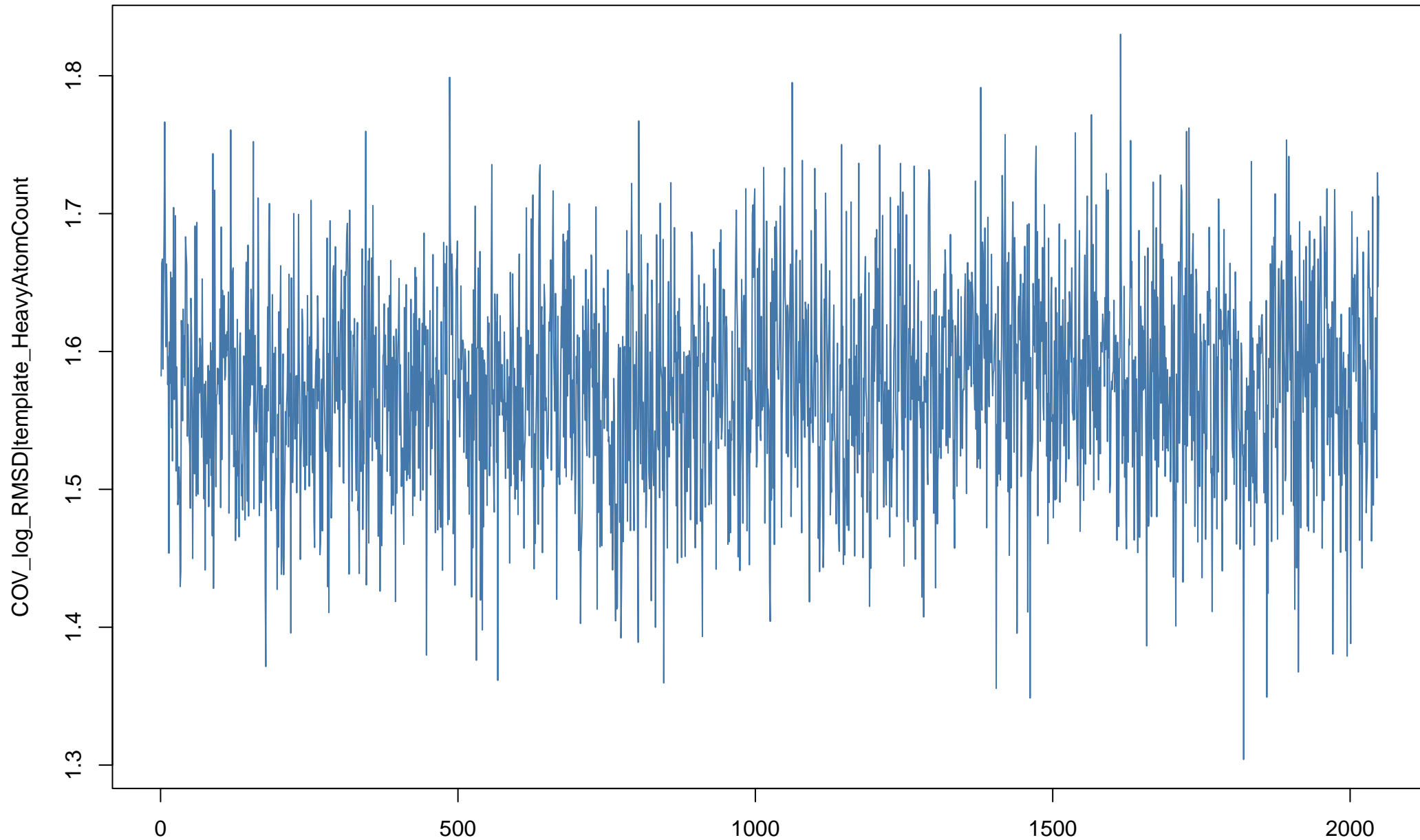
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1360 | BMK = 0.0387 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0



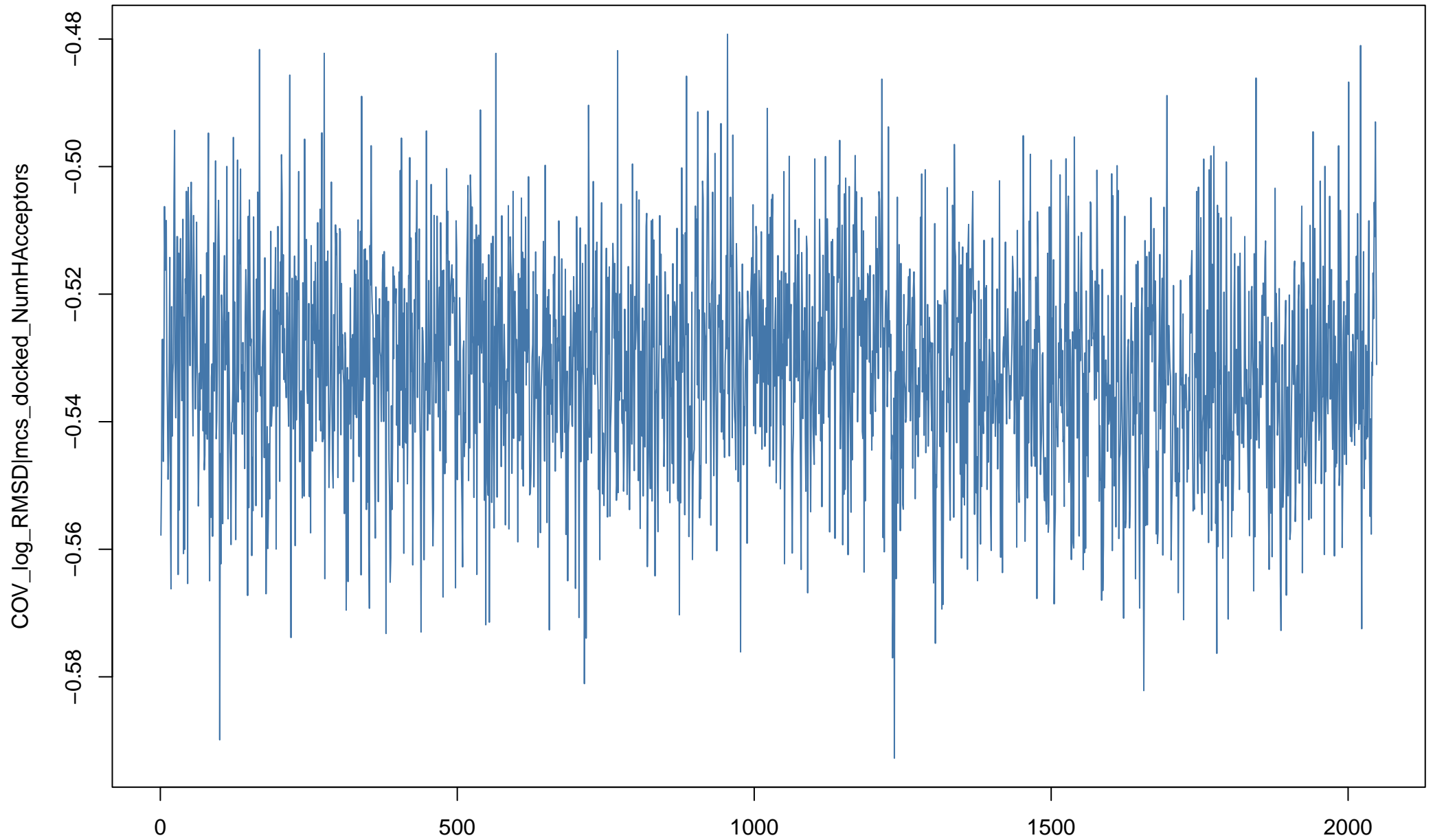
COV_log_RMSD|mcs_RingCount
ESS = 1270 | BMK = 0.047 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0



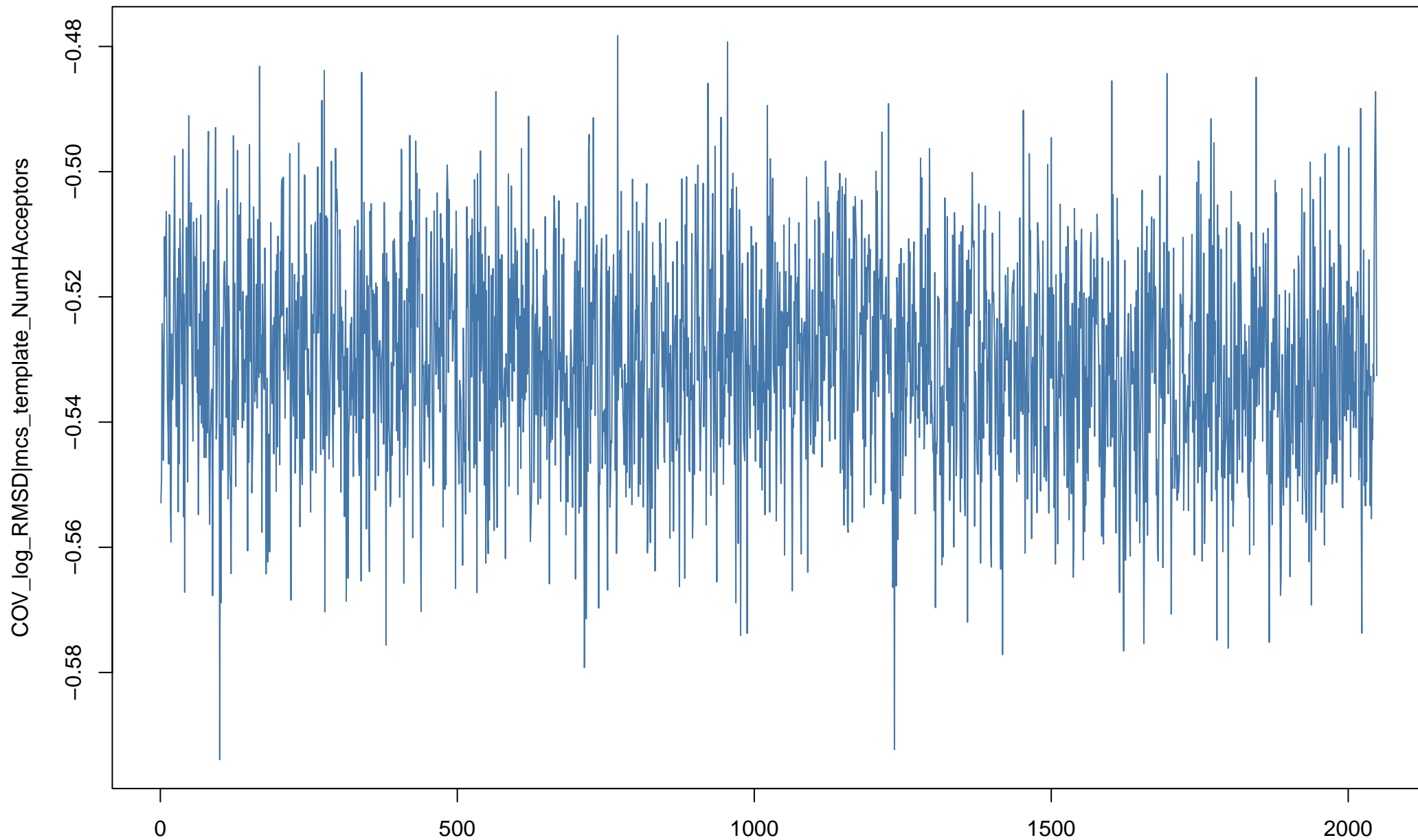
COV_log_RMSD|template_HeavyAtomCount
ESS = 1570 | BMK = 0.0694 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0



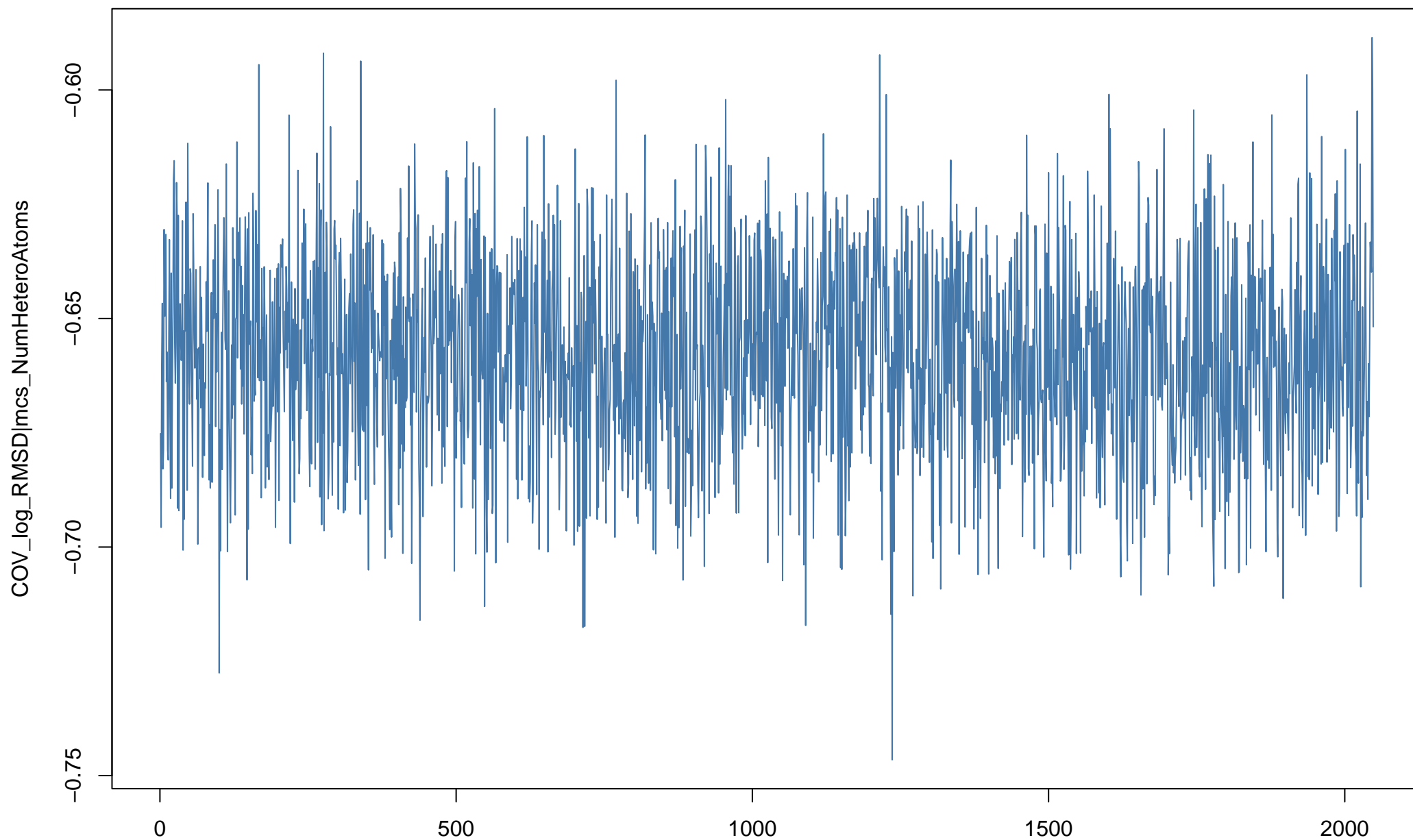
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 1800 | BMK = 0.051 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0



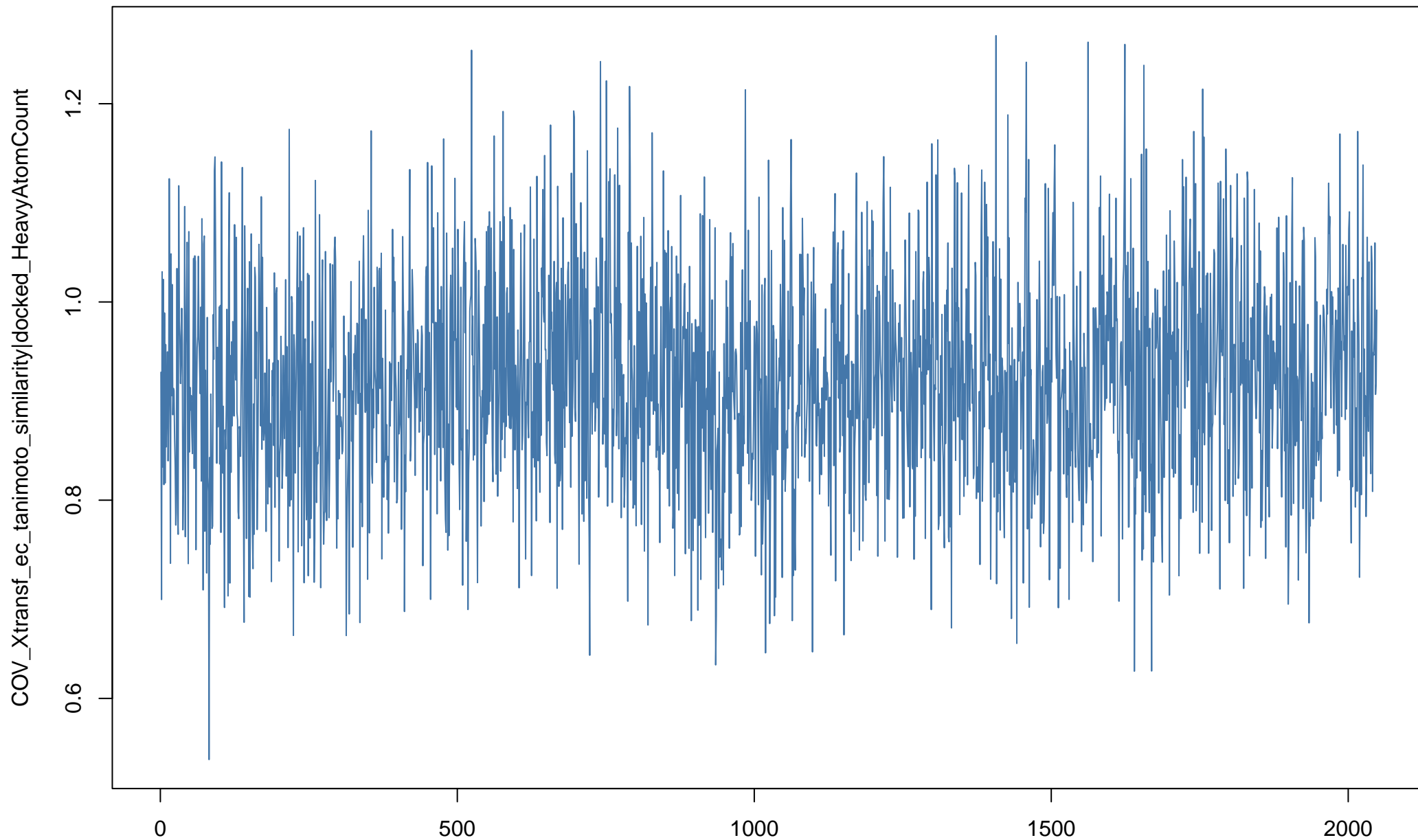
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 1760 | BMK = 0.0551 | MCSE(6.27) = 2.58 | stat: FALSE | burn: 0



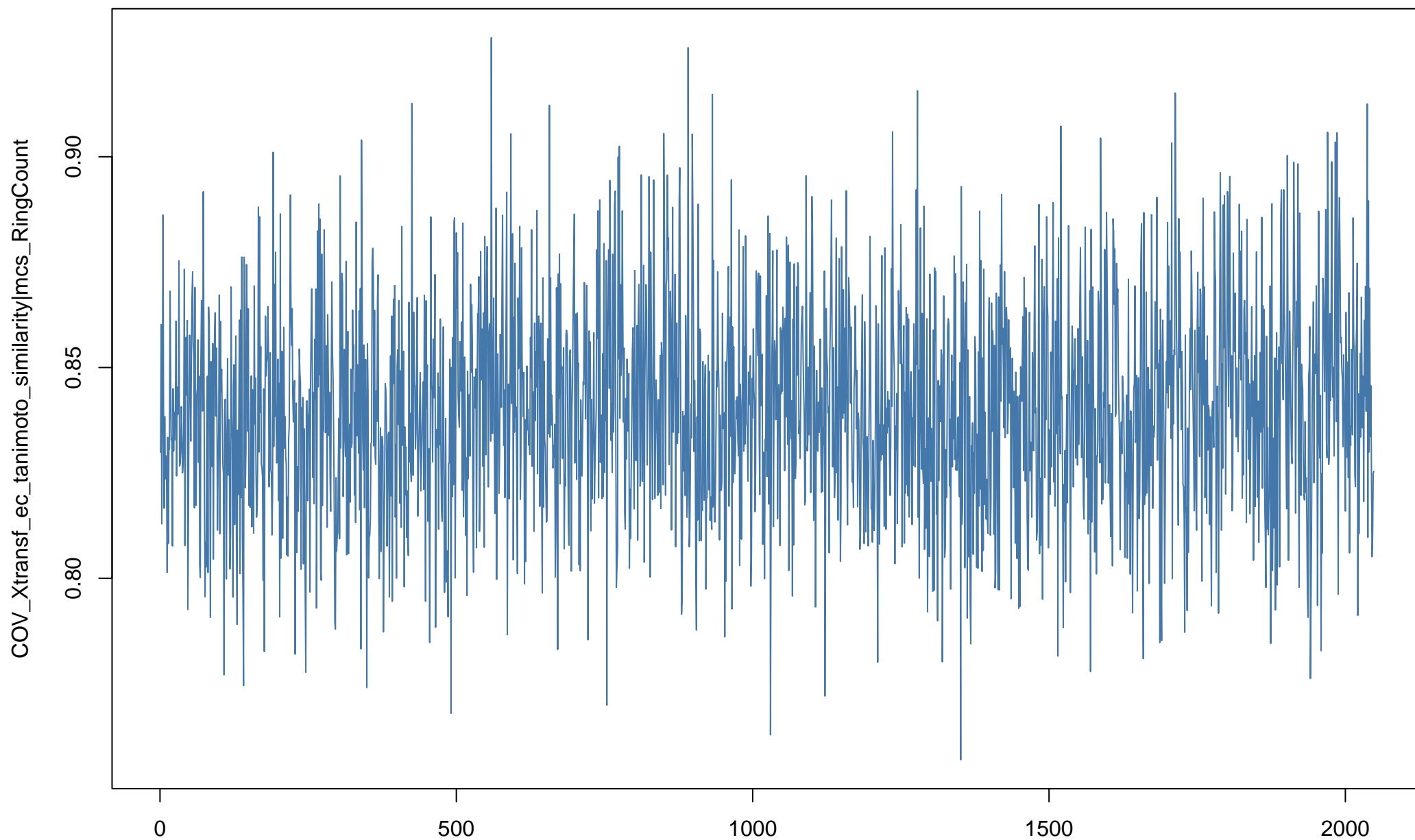
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0479 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



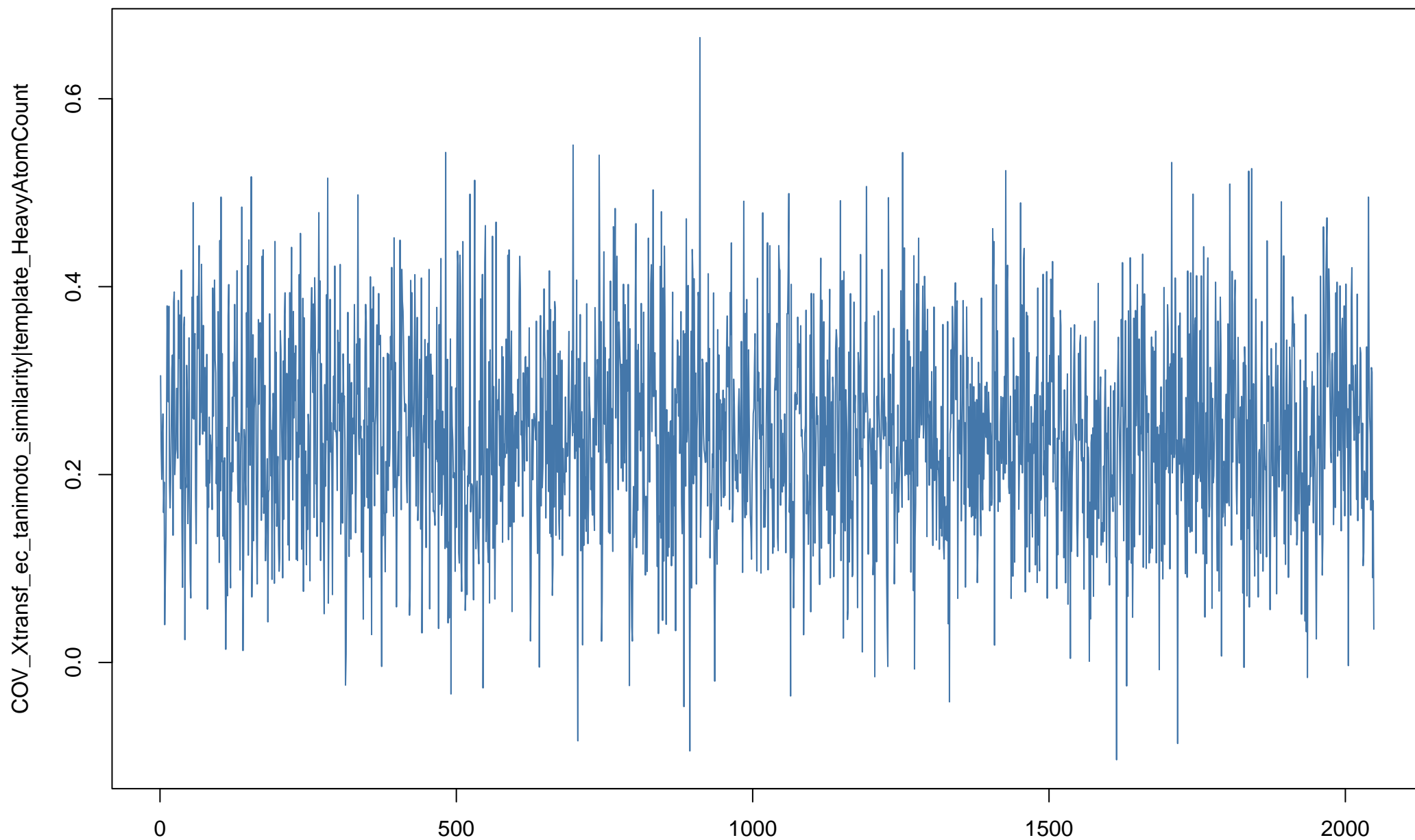
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0451 | MCSE(6.27) = 2.69 | stat: FALSE | burn: 0



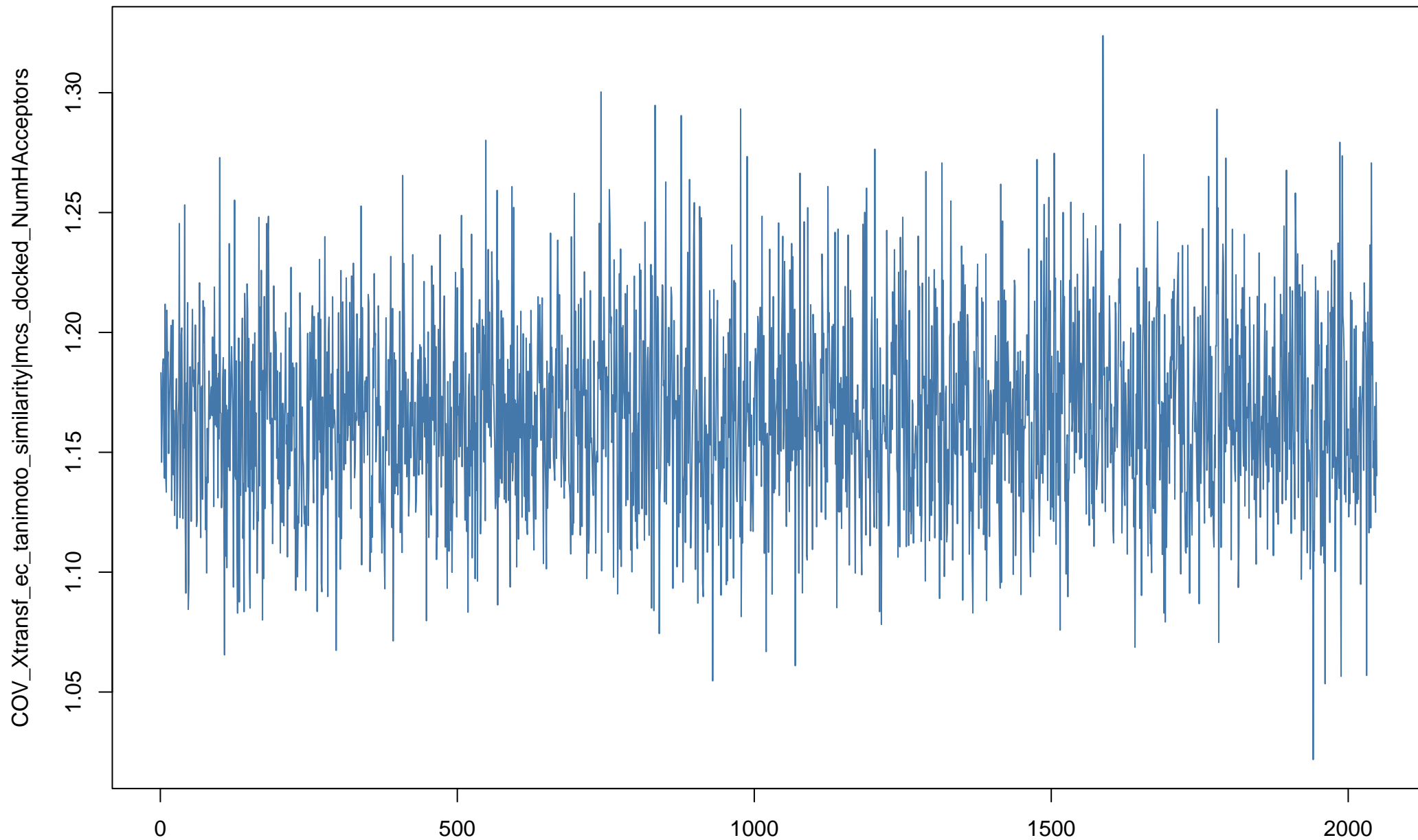
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1320 | BMK = 0.0351 | MCSE(6.27) = 3.05 | stat: FALSE | burn: 0



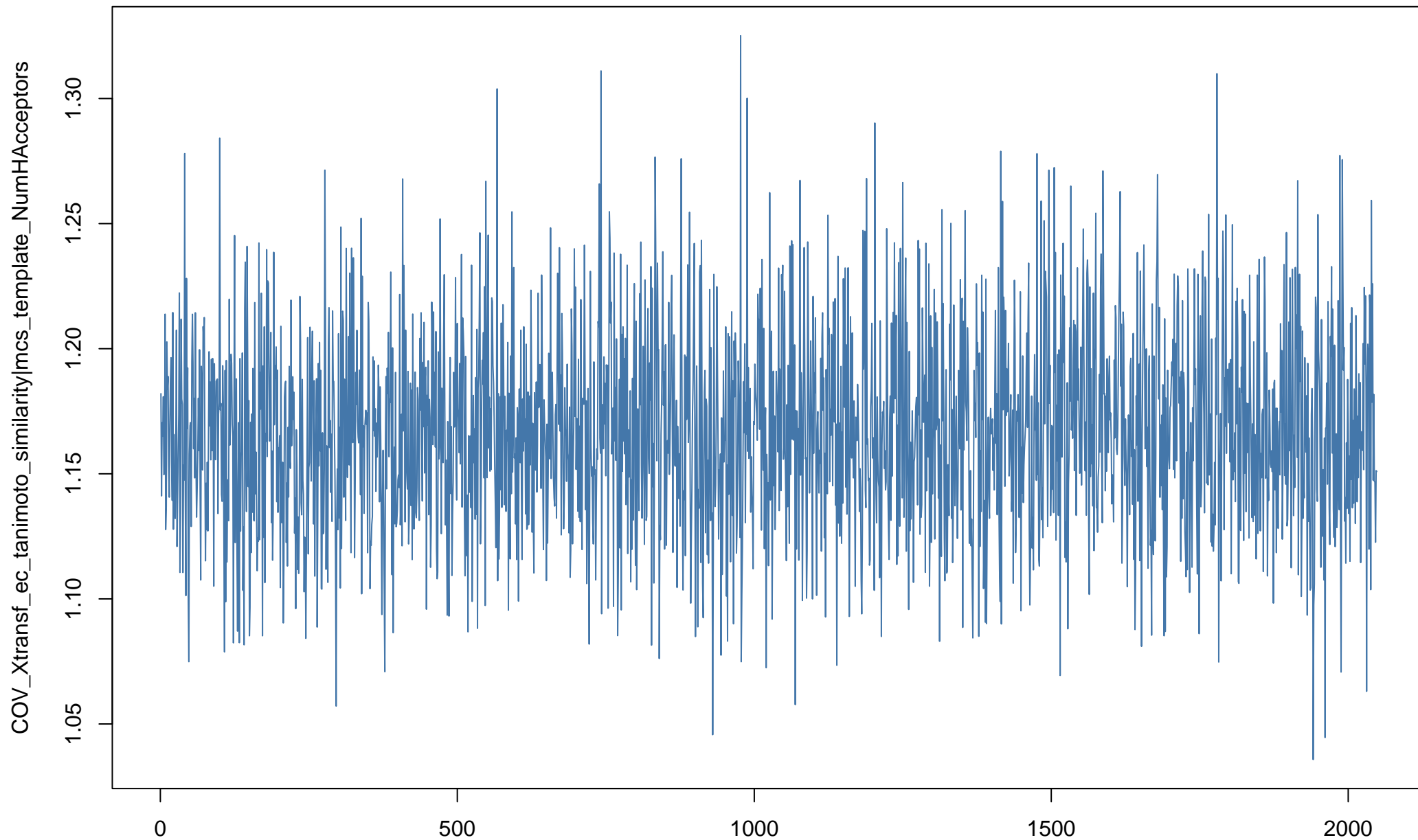
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1840 | BMK = 0.0414 | MCSE(6.27) = 2 | stat: TRUE | burn: 0



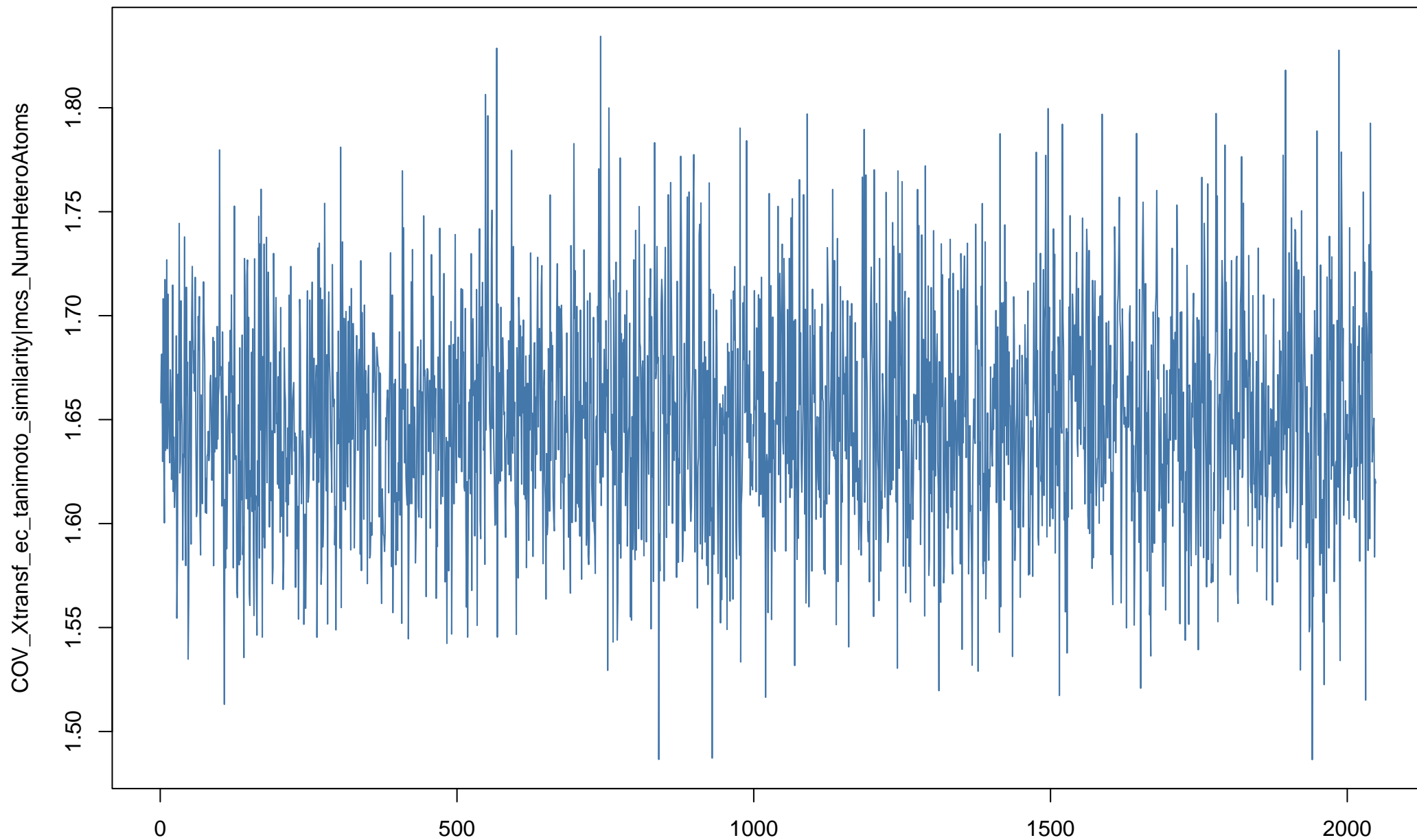
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0555 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



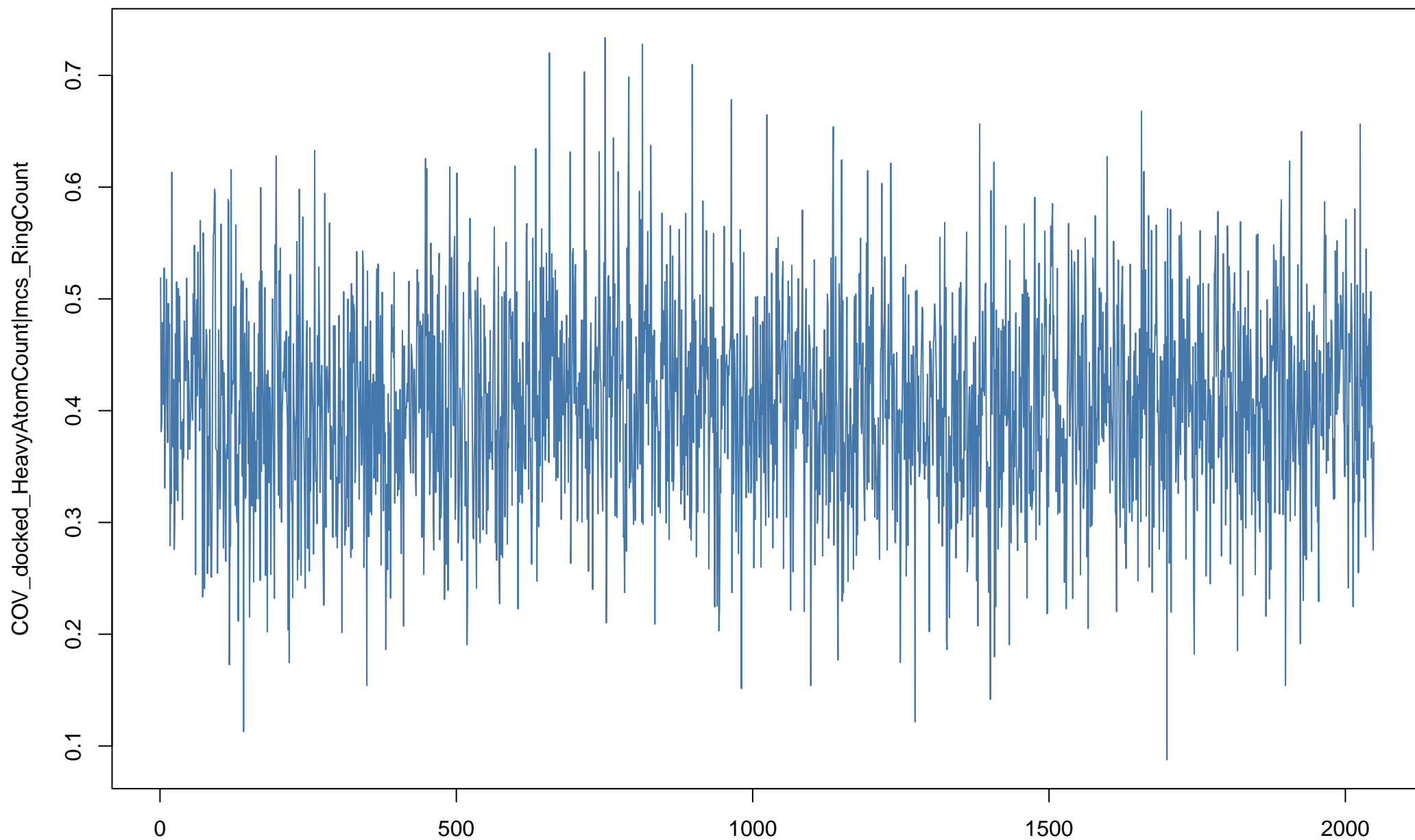
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.057 | MCSE(6.27) = 2.36 | stat: FALSE | burn: 0



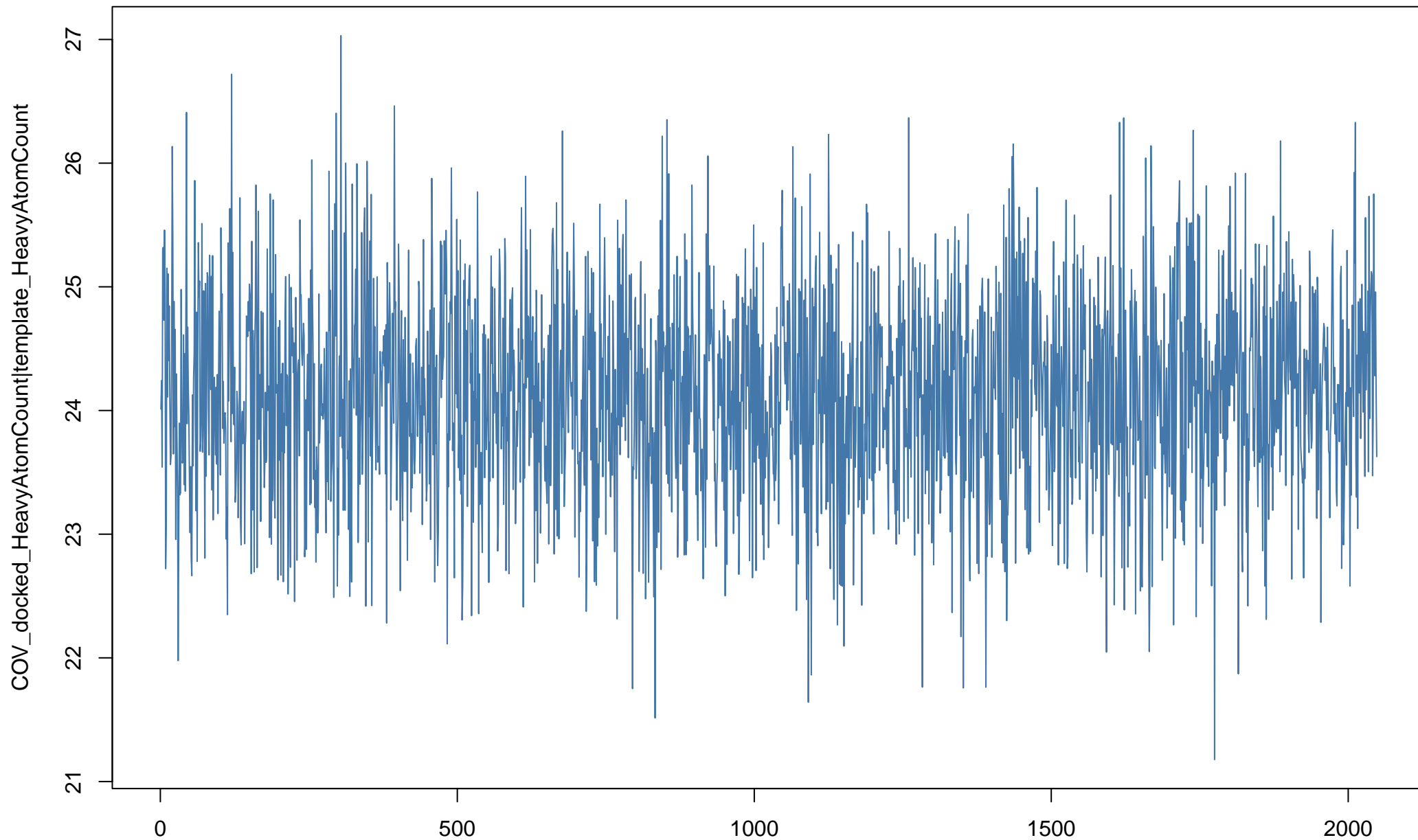
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0483 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0



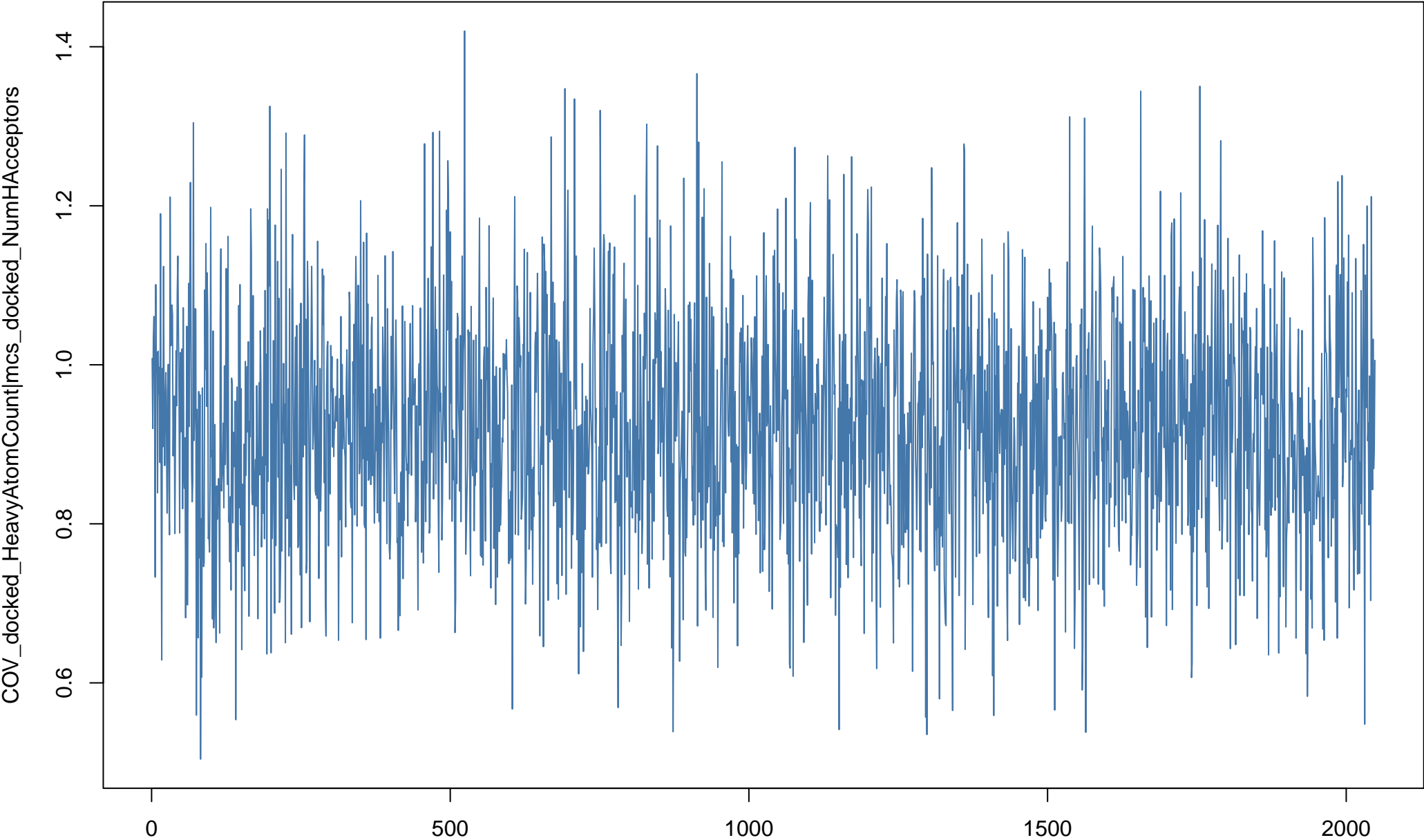
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1880 | BMK = 0.0489 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0



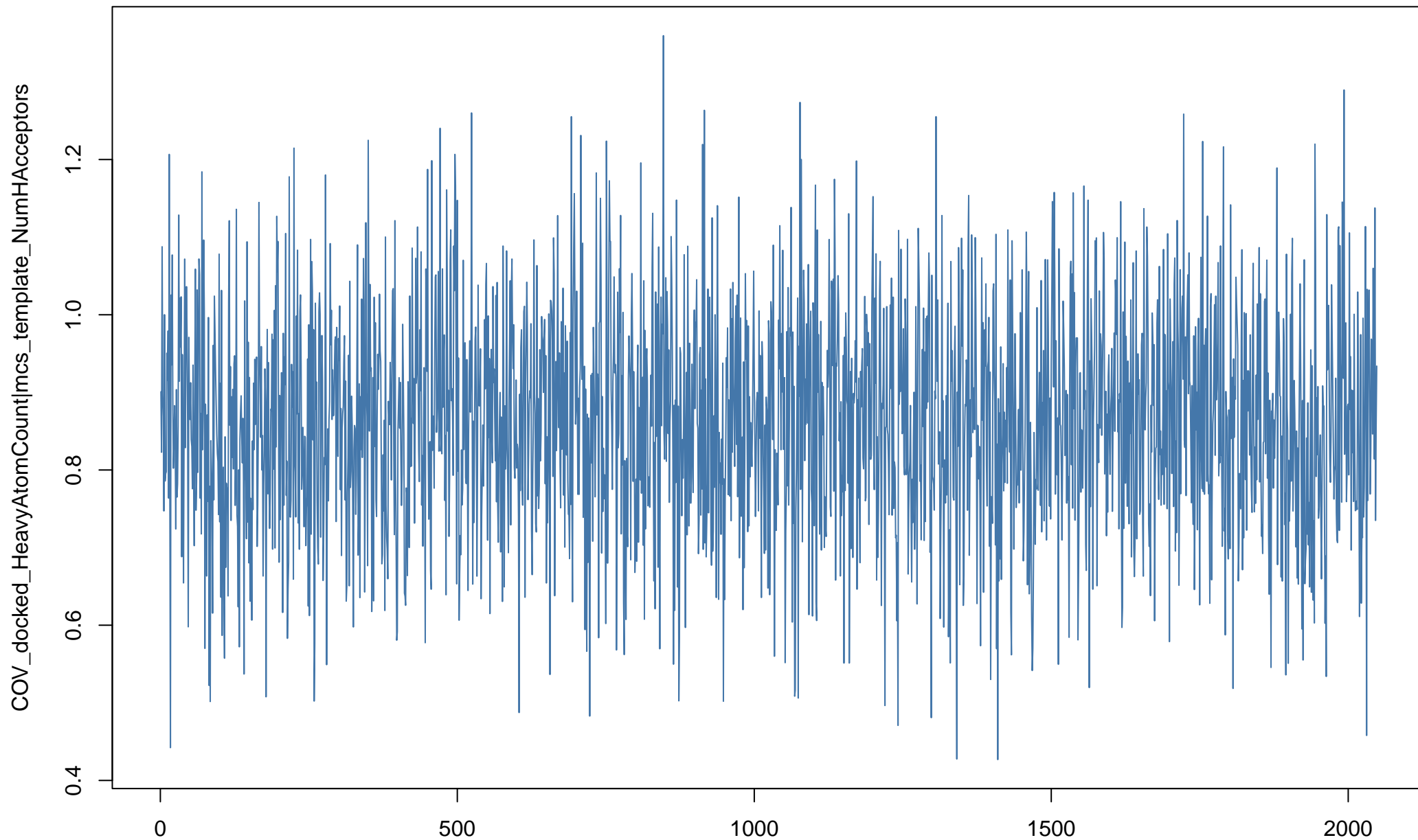
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 2050 | BMK = 0.0396 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0



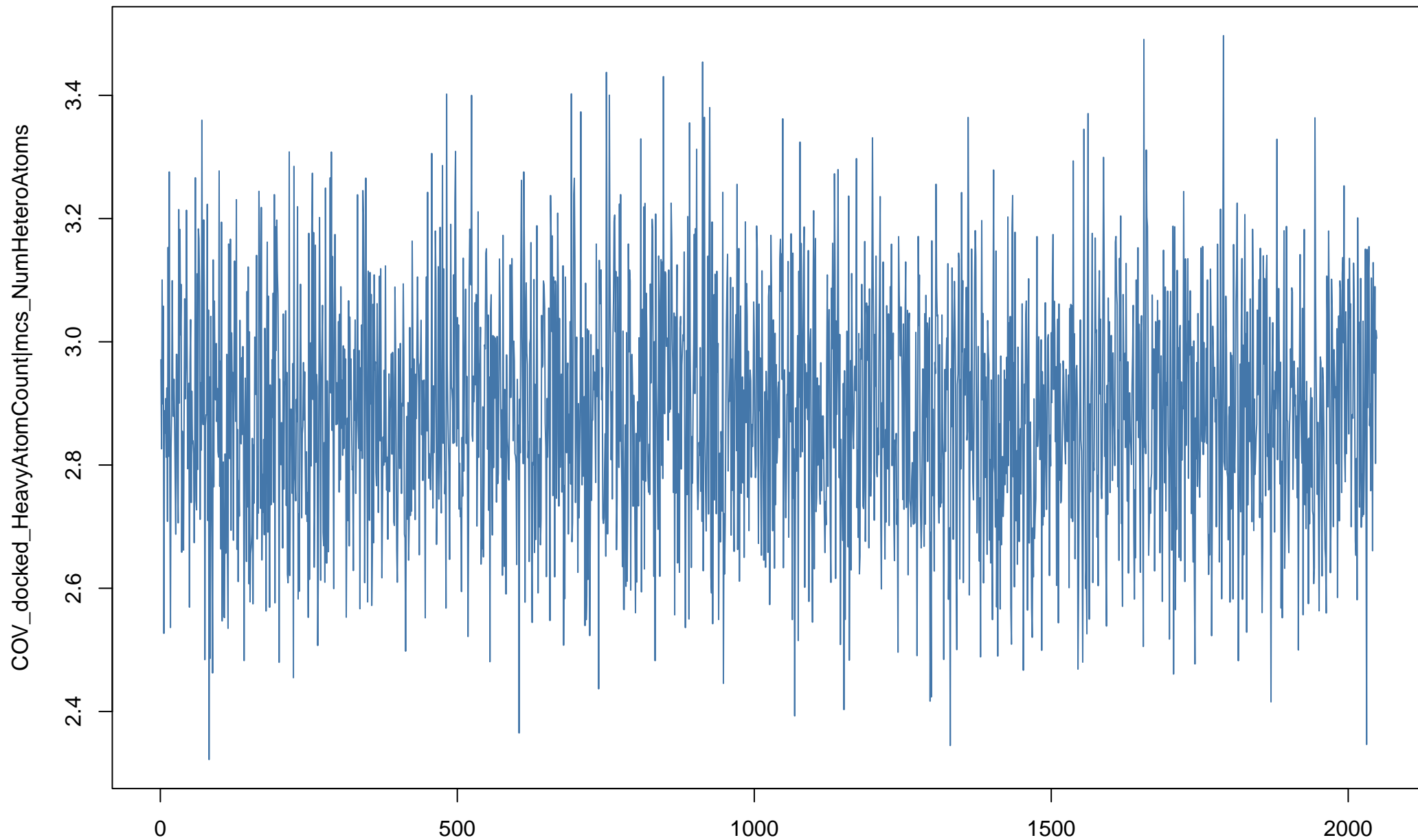
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1890 | BMK = 0.0351 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0



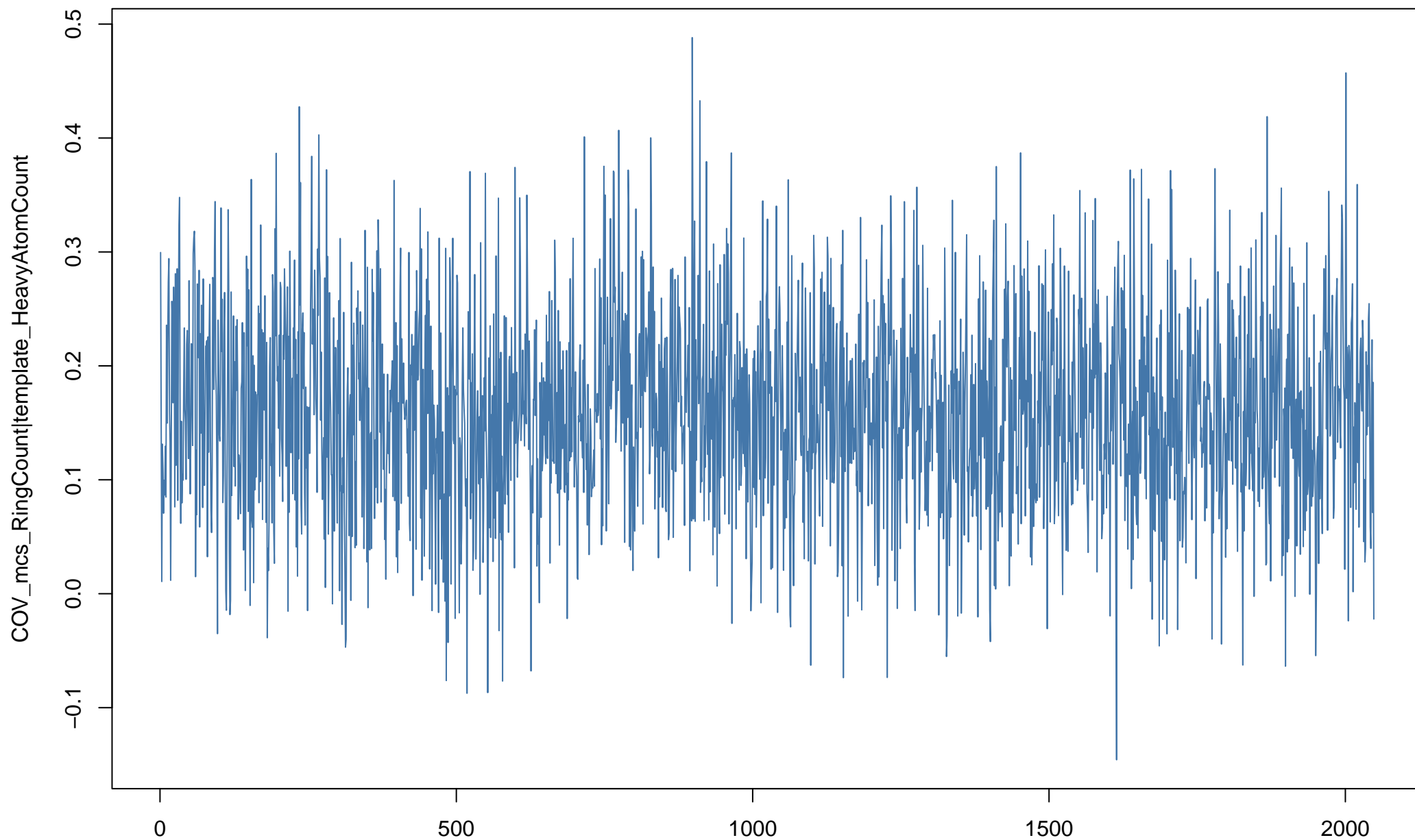
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1890 | BMK = 0.0377 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



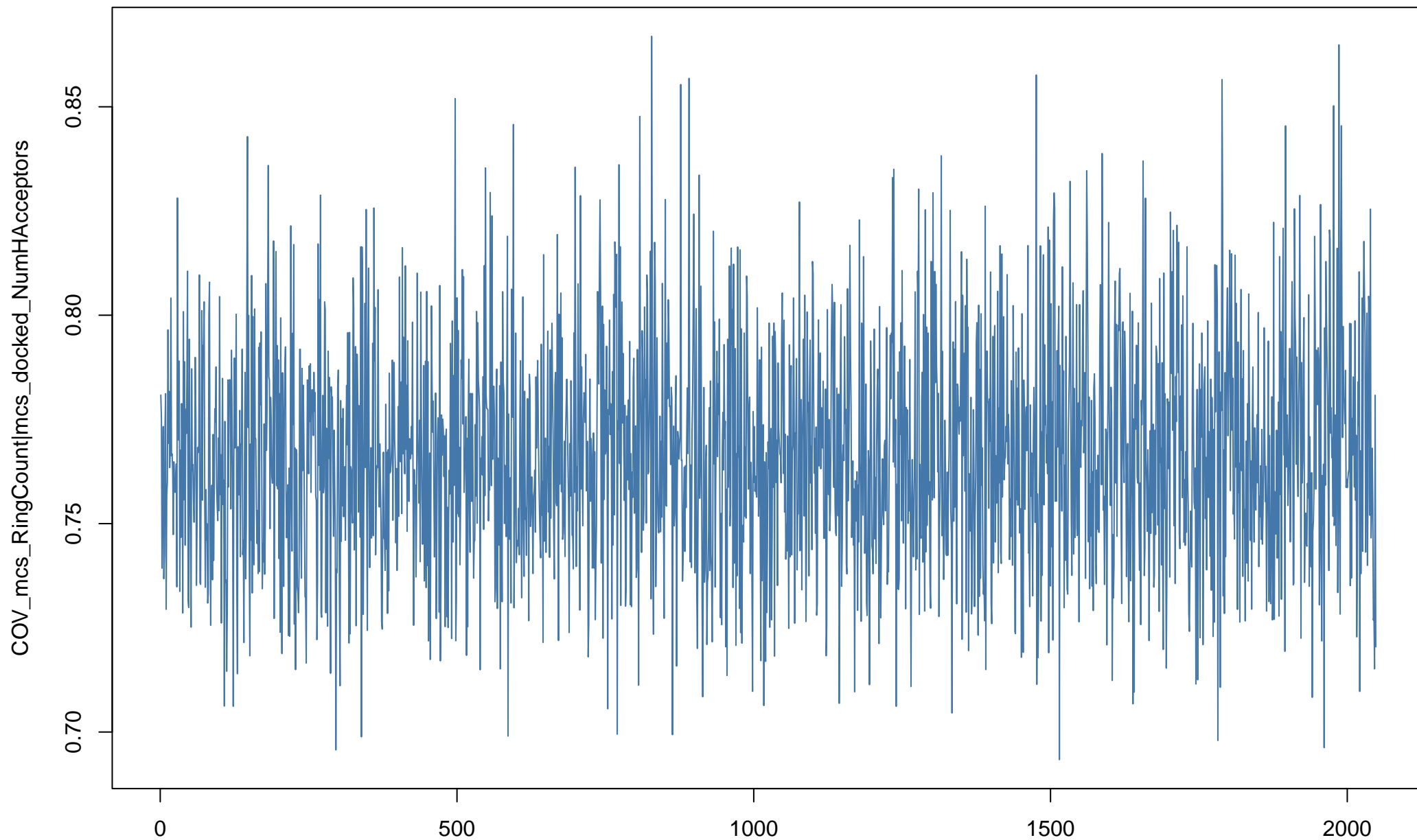
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0507 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0



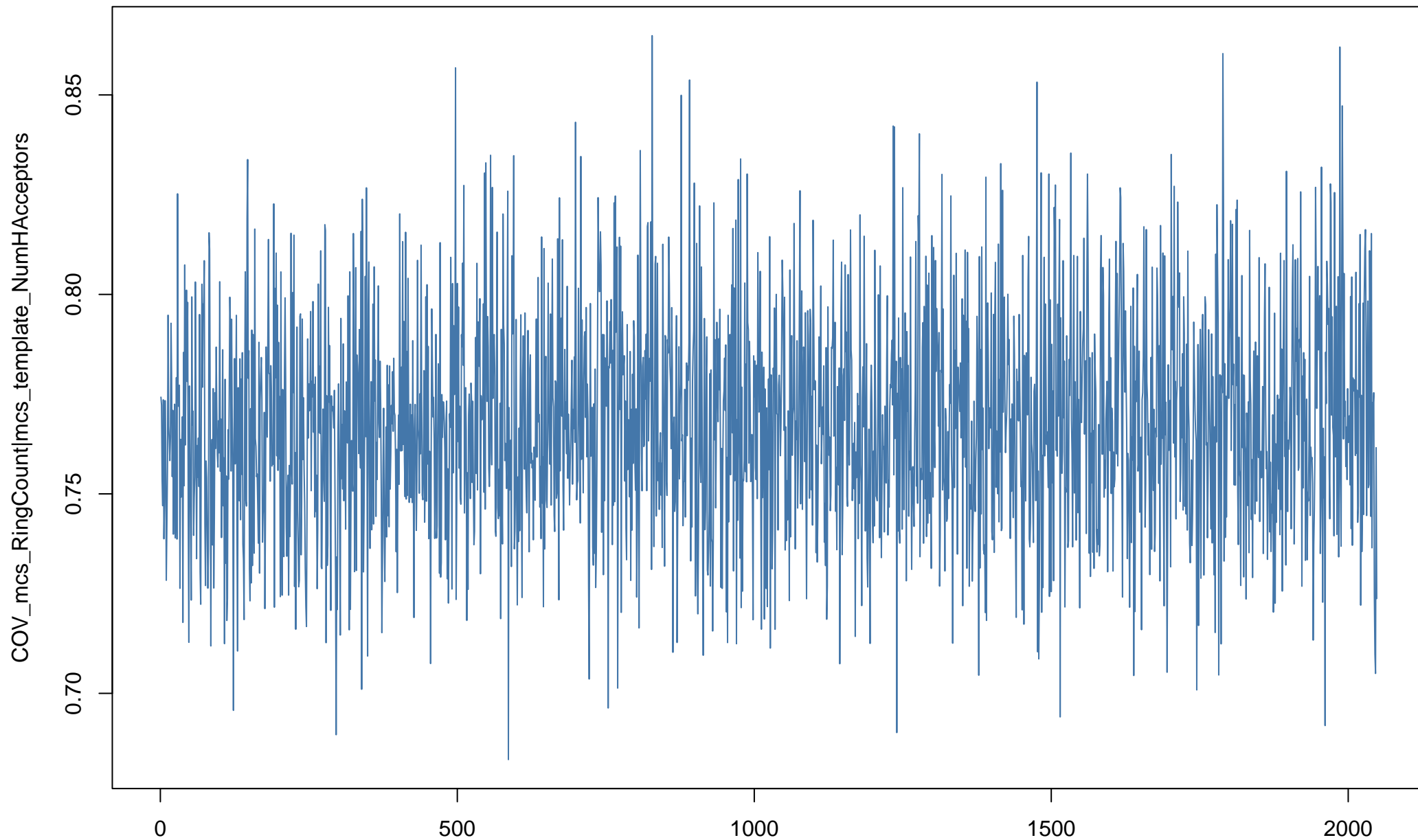
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1600 | BMK = 0.0402 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0



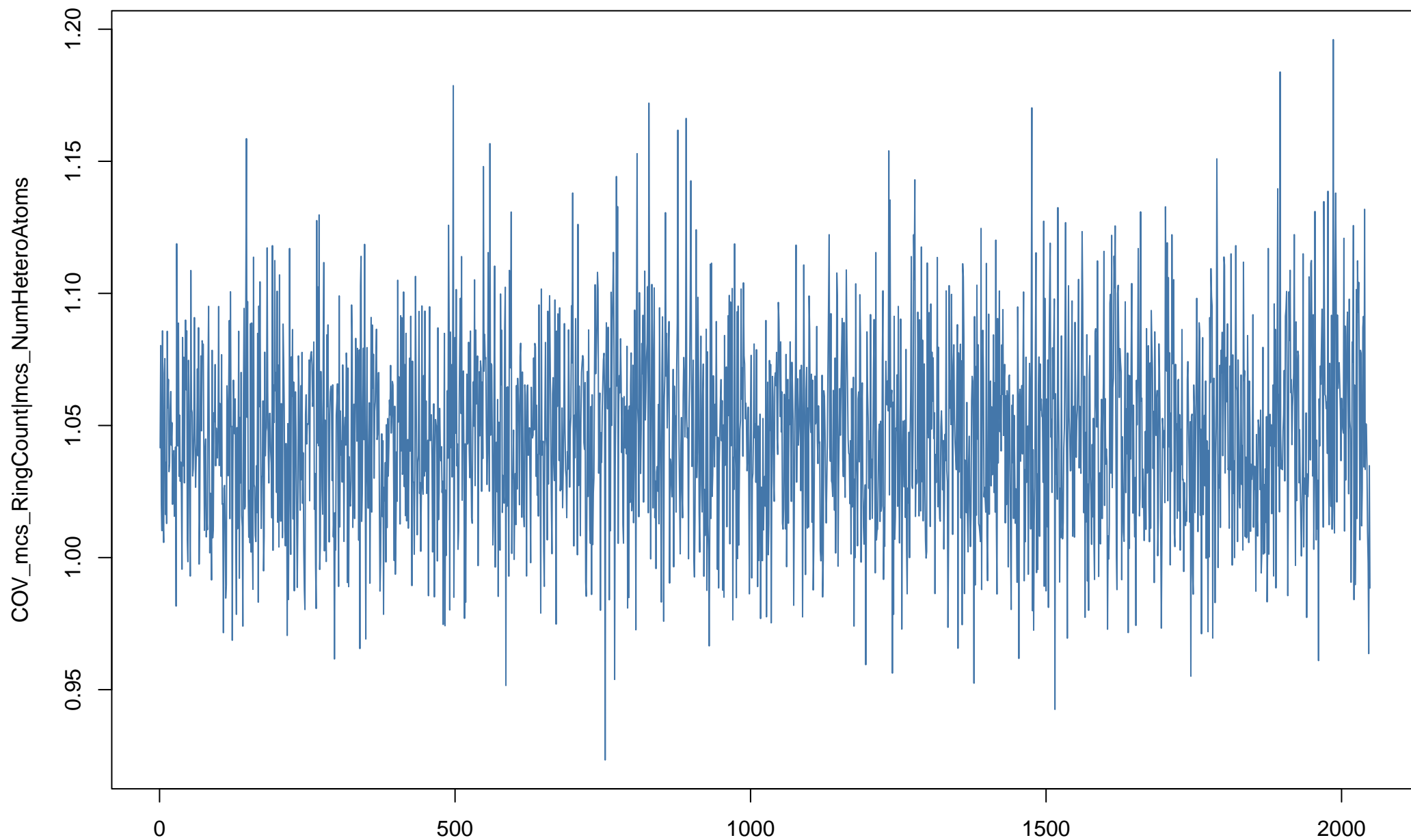
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0442 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0



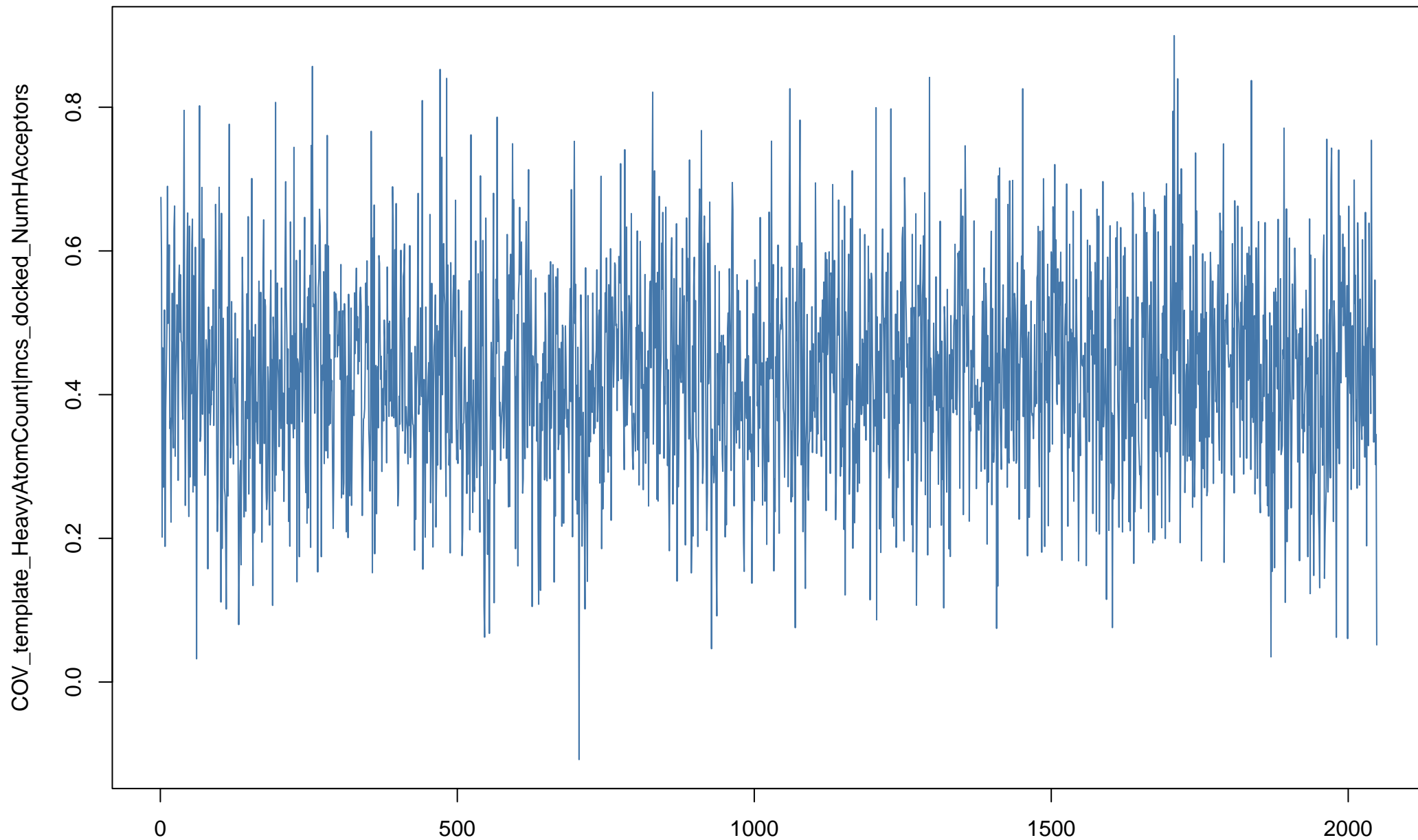
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2010 | BMK = 0.0423 | MCSE(6.27) = 2.5 | stat: FALSE | burn: 0



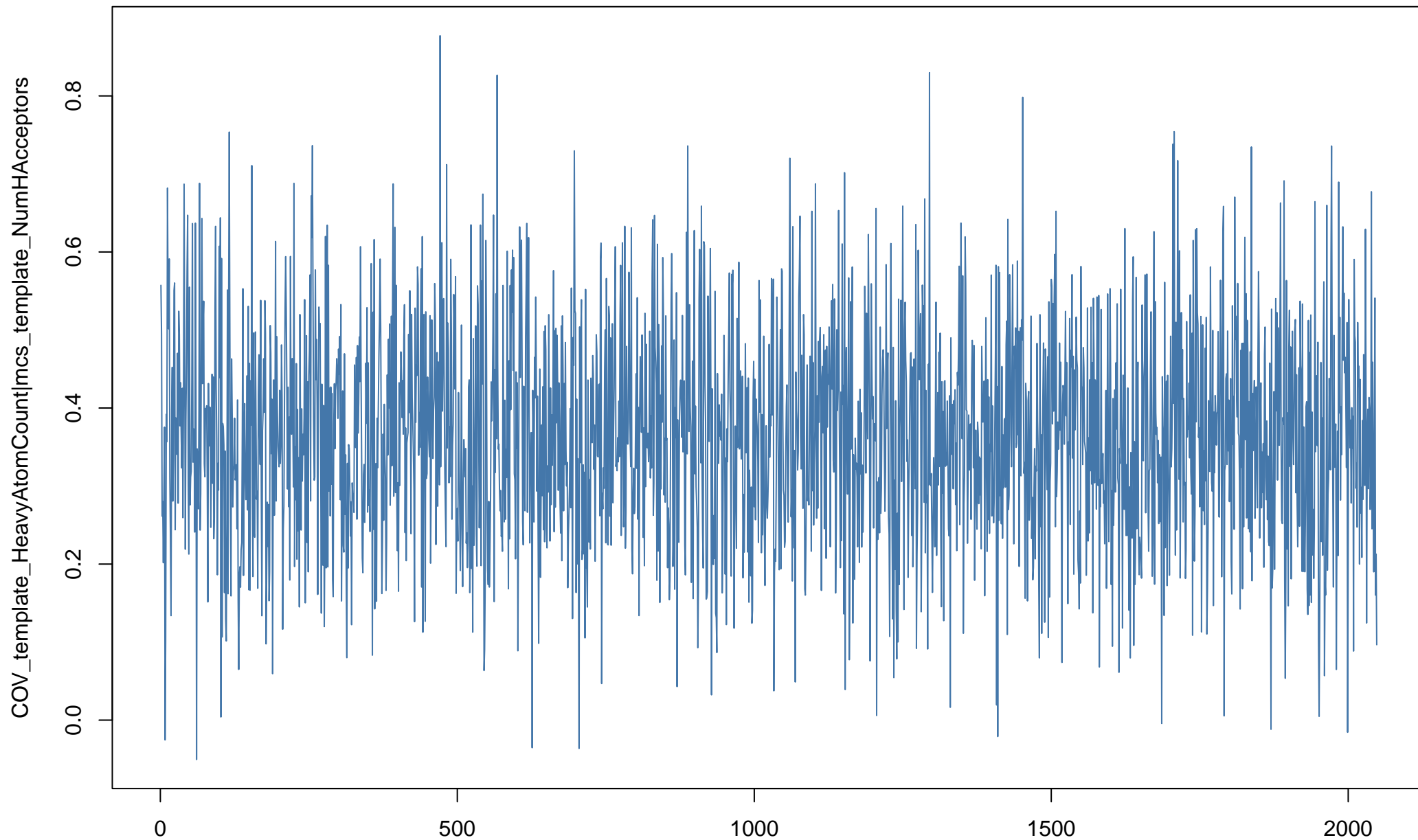
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0549 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0



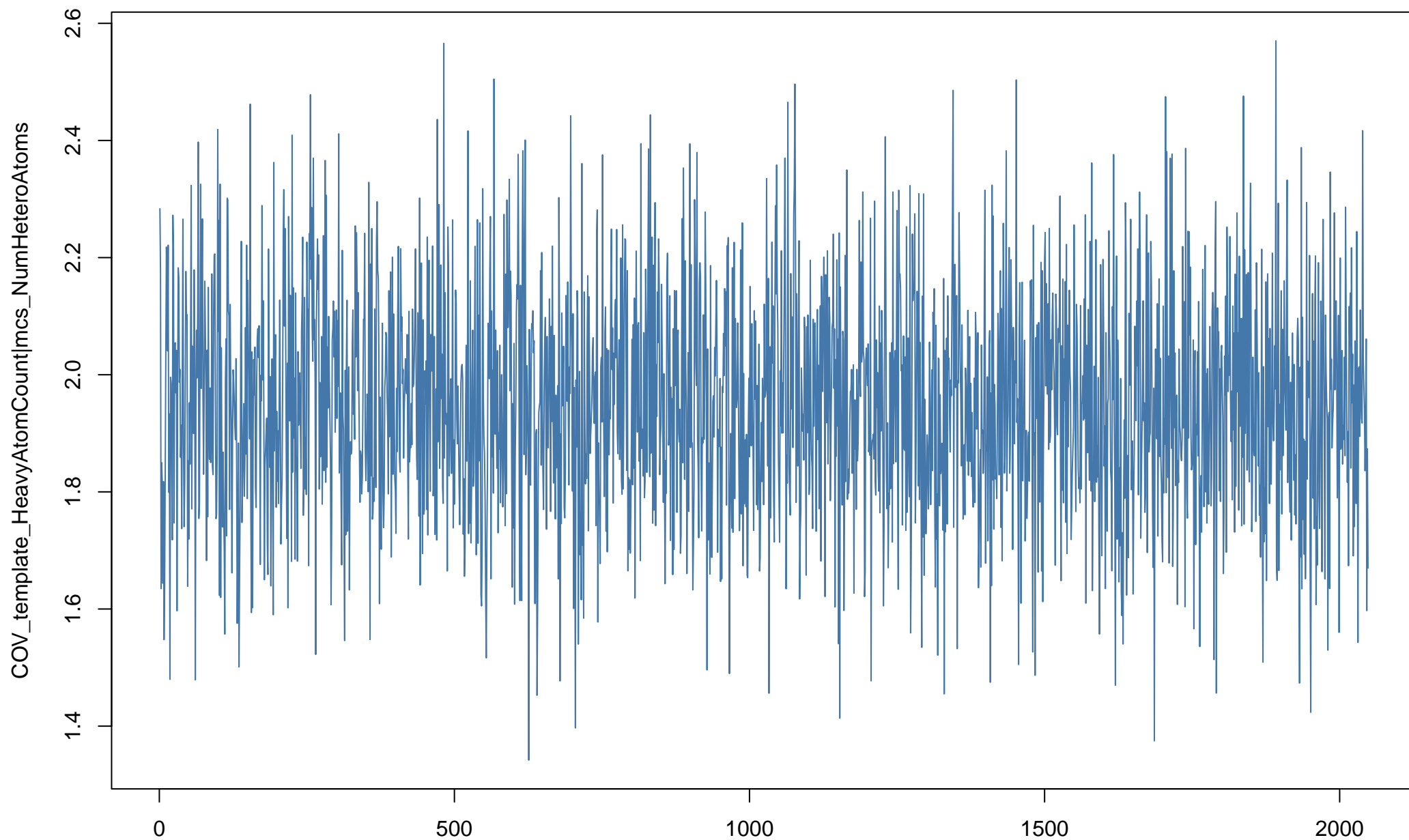
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0414 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0



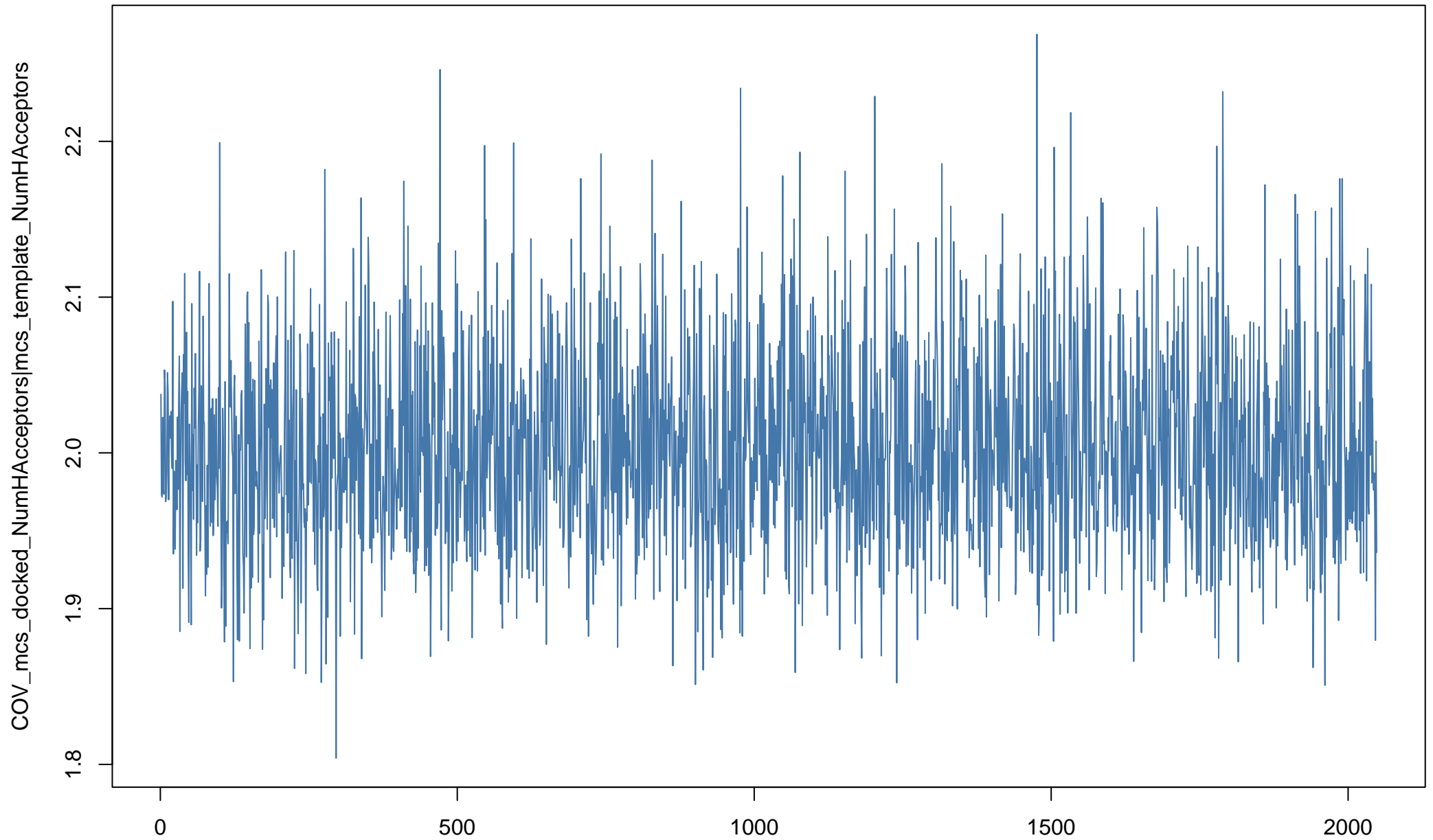
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0402 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0



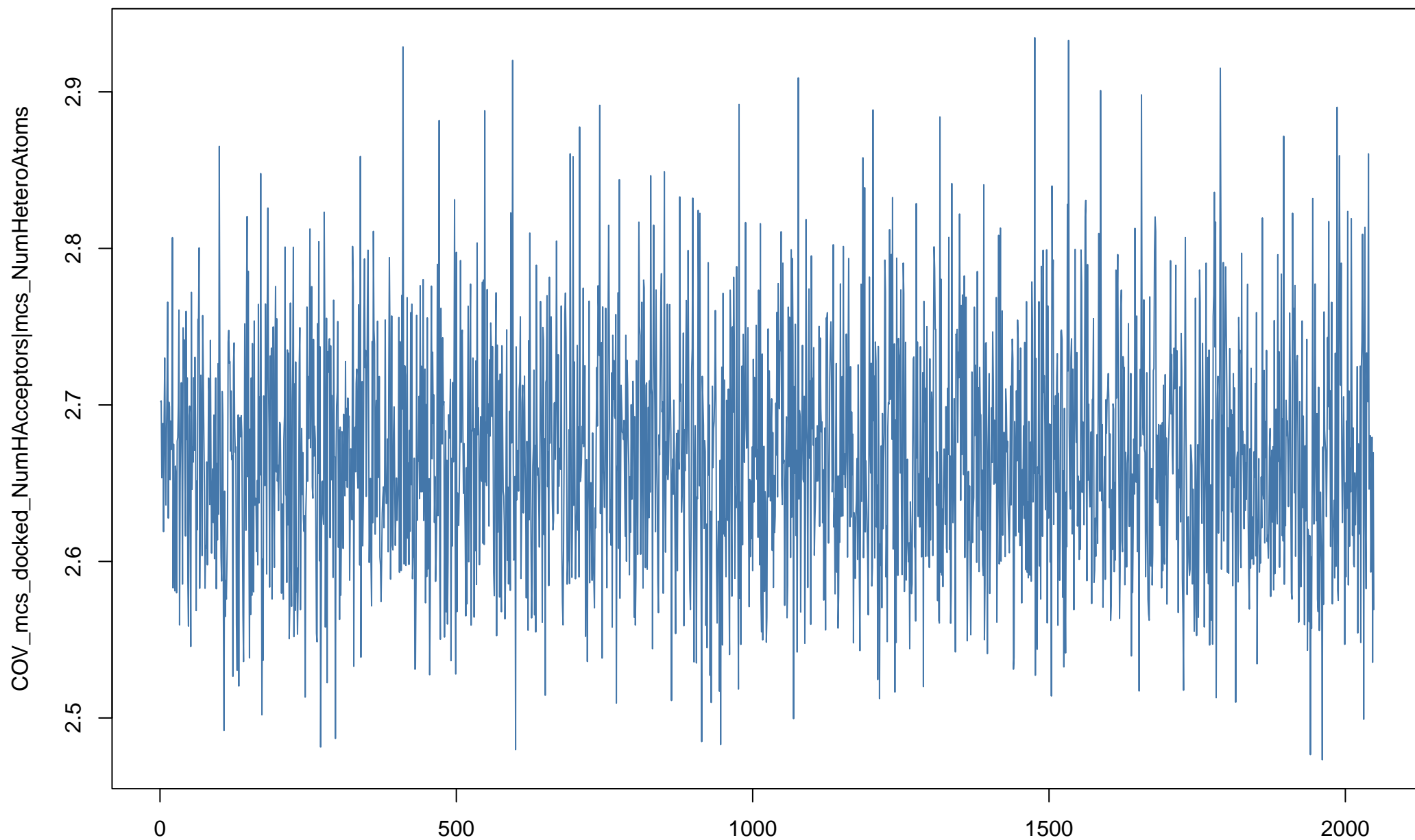
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0279 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.047 | MCSE(6.27) = 2.29 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0441 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0421 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0

