

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.714913035607813

max MCSE = 12.370479805032

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 679.549364413631

max BMK = 0.118372604164297

max MCSE = 3.72599323609754

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.543537300194556

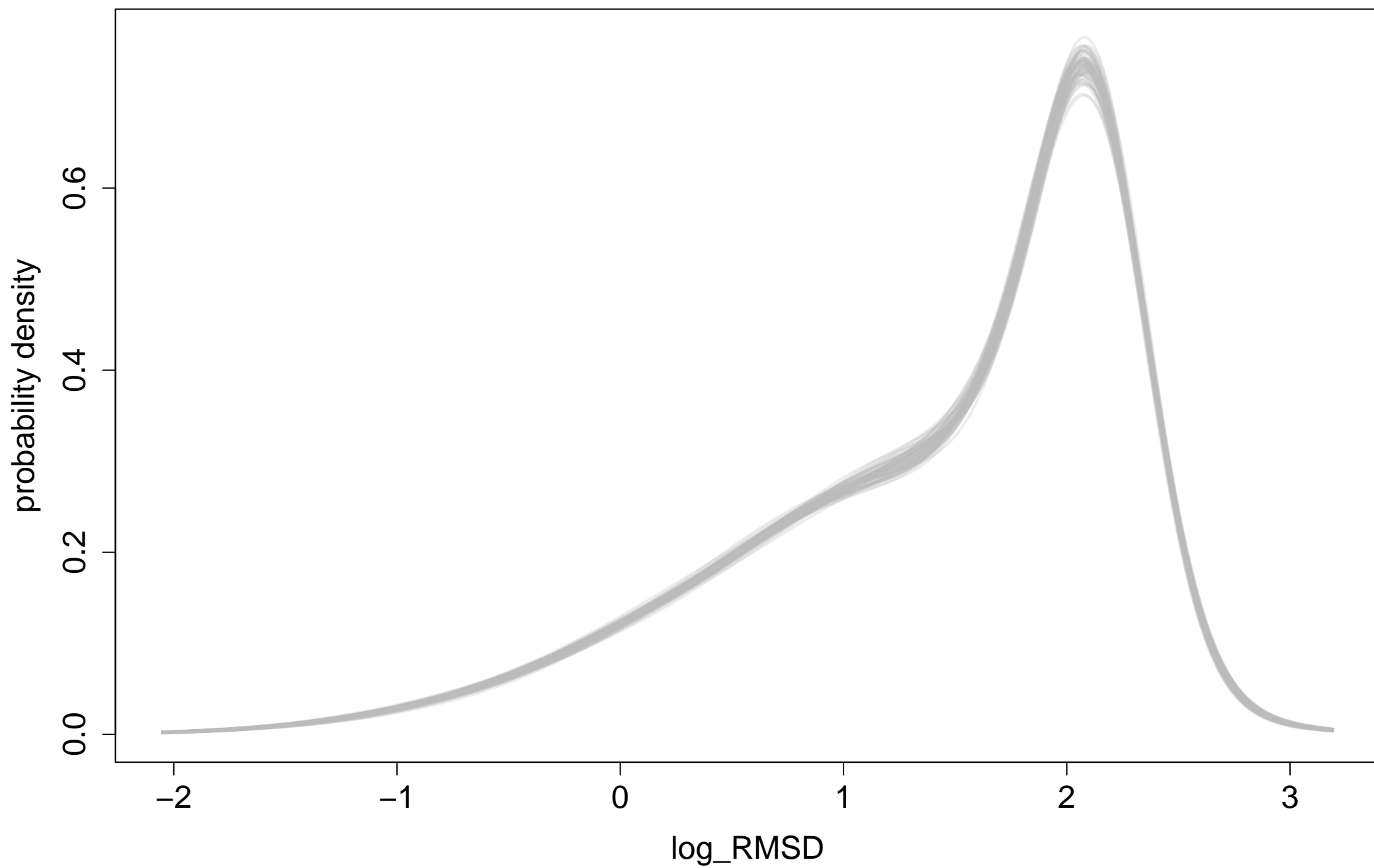
max MCSE = NaN

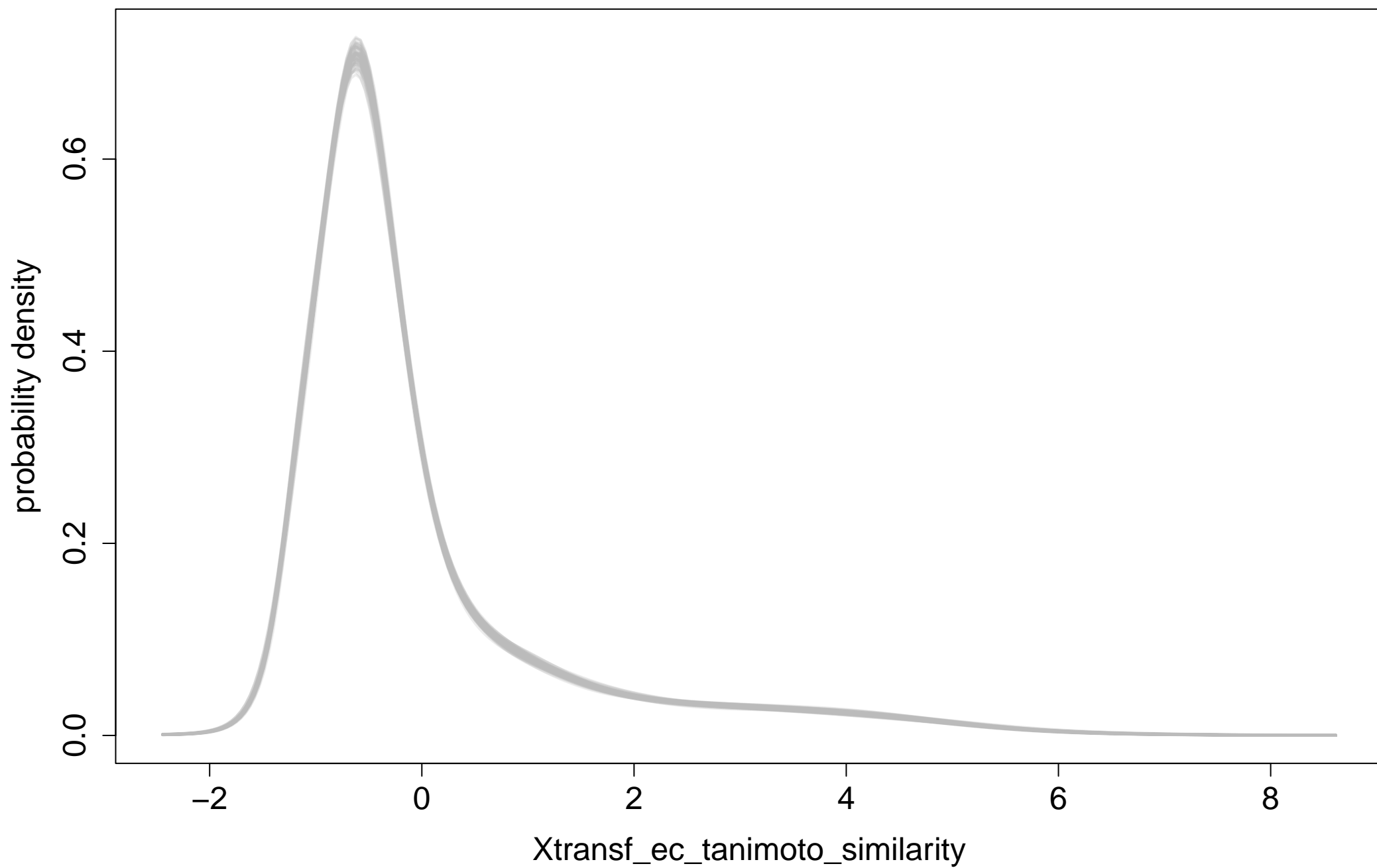
all stationary: FALSE

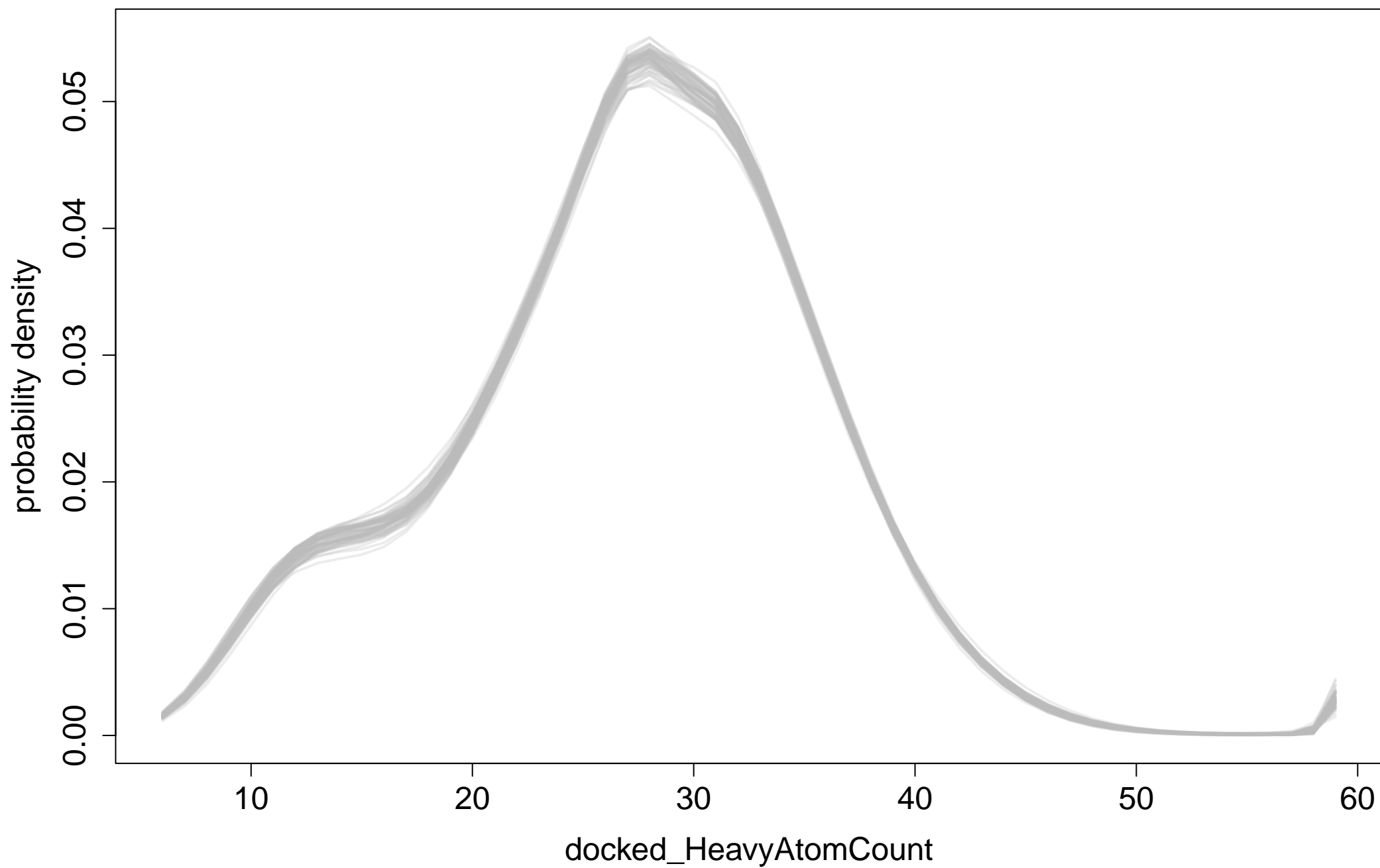
burn: 2040

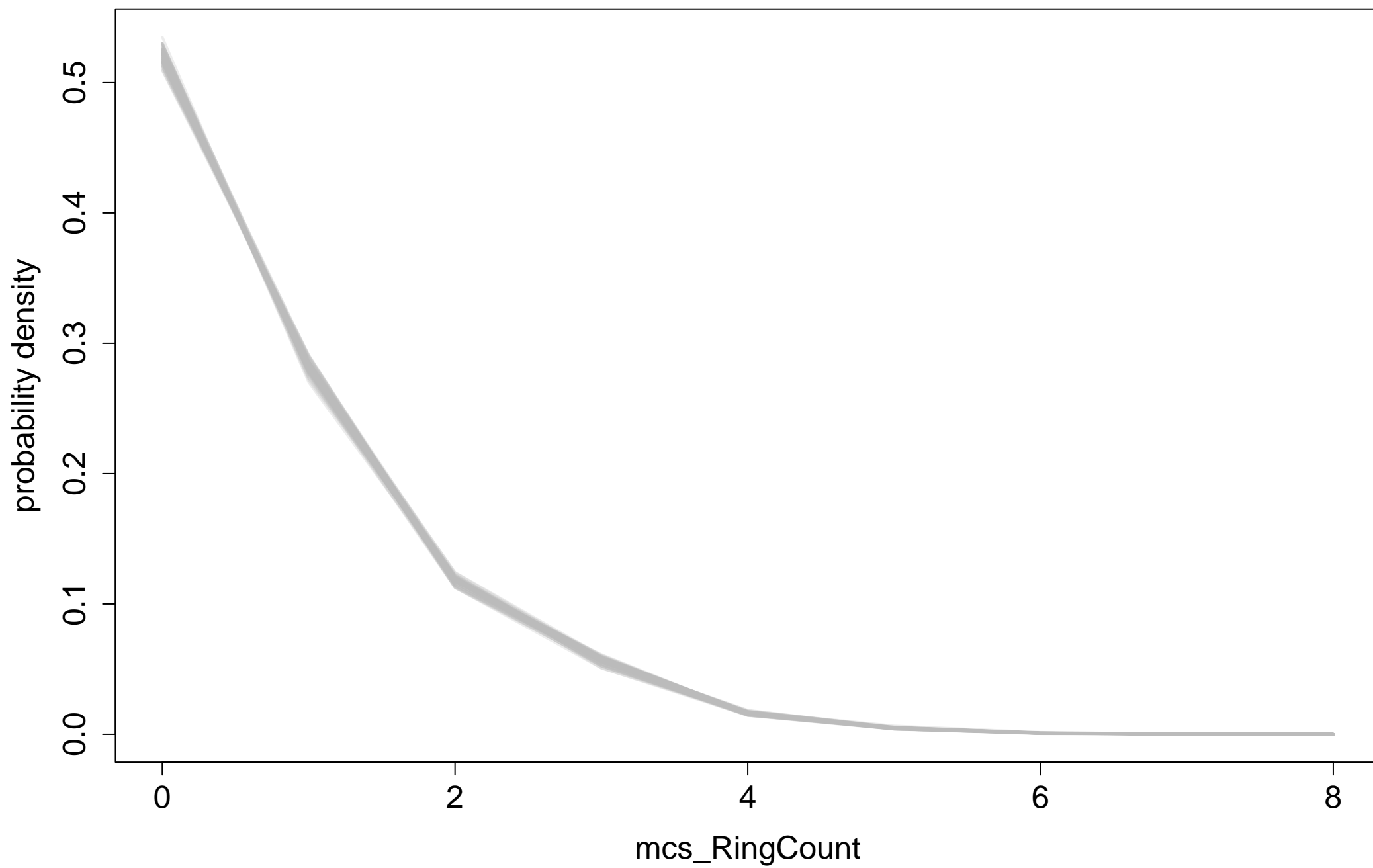
Occupied clusters: 61 of 64

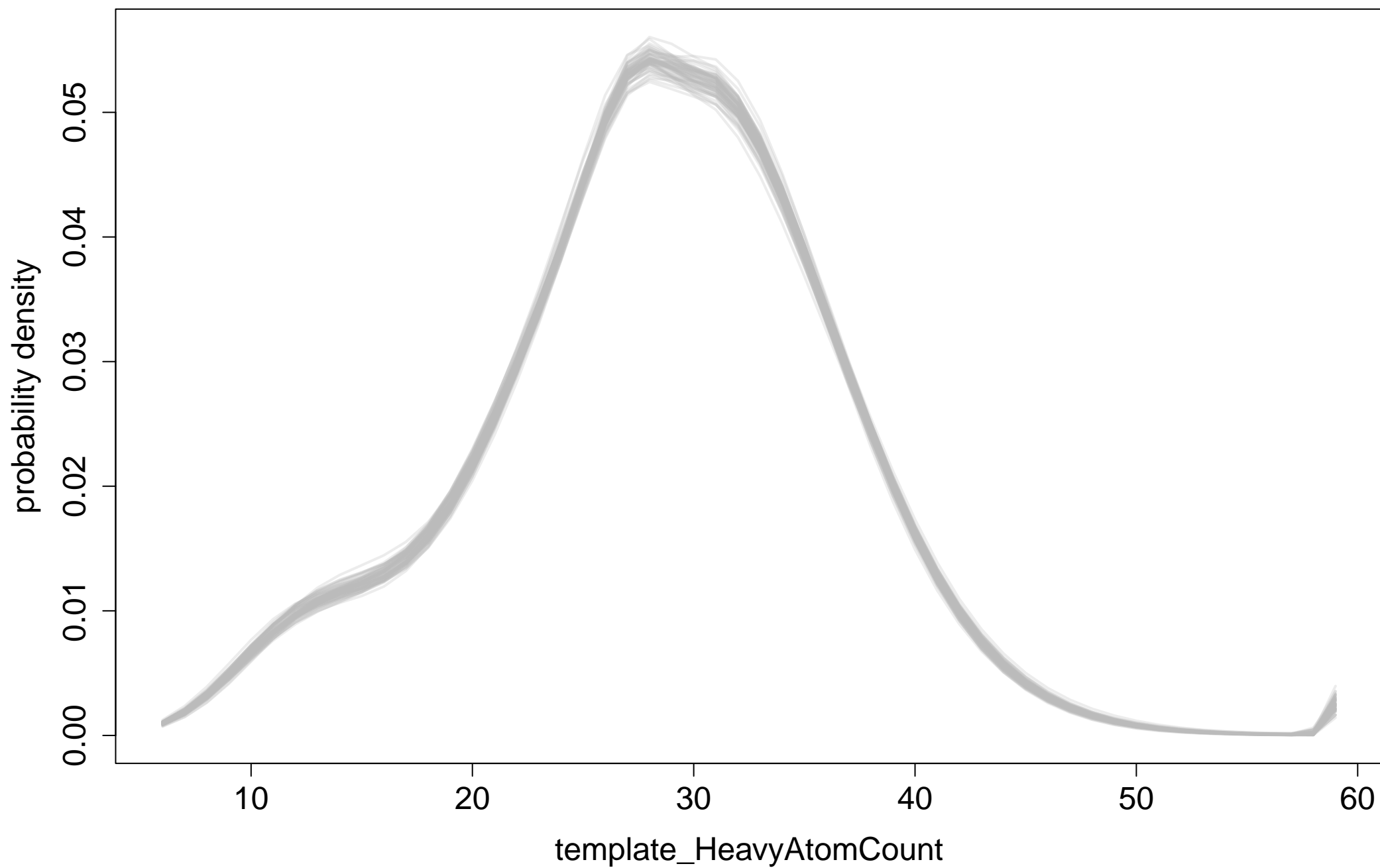
LL: -110000 +- 34.1

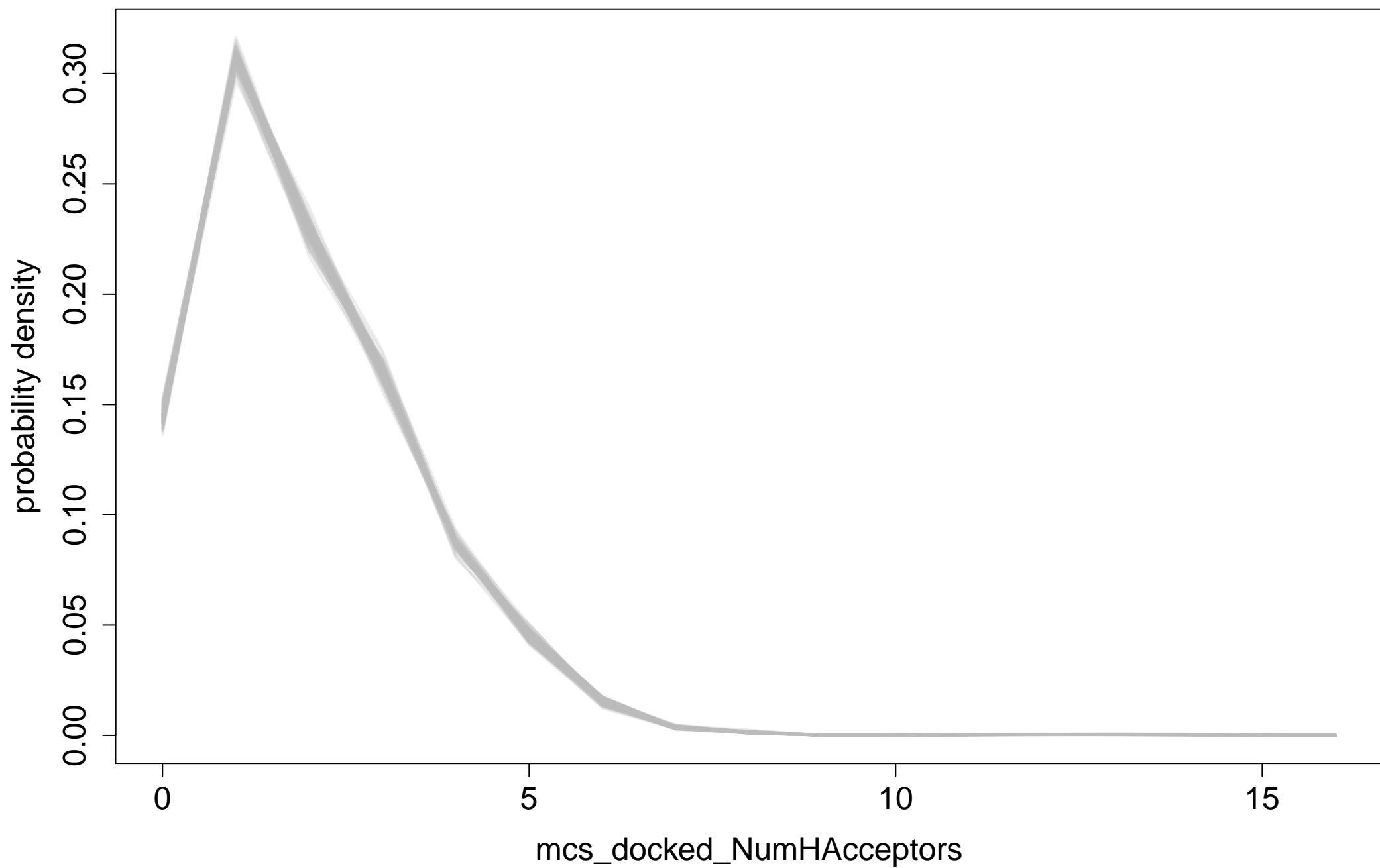


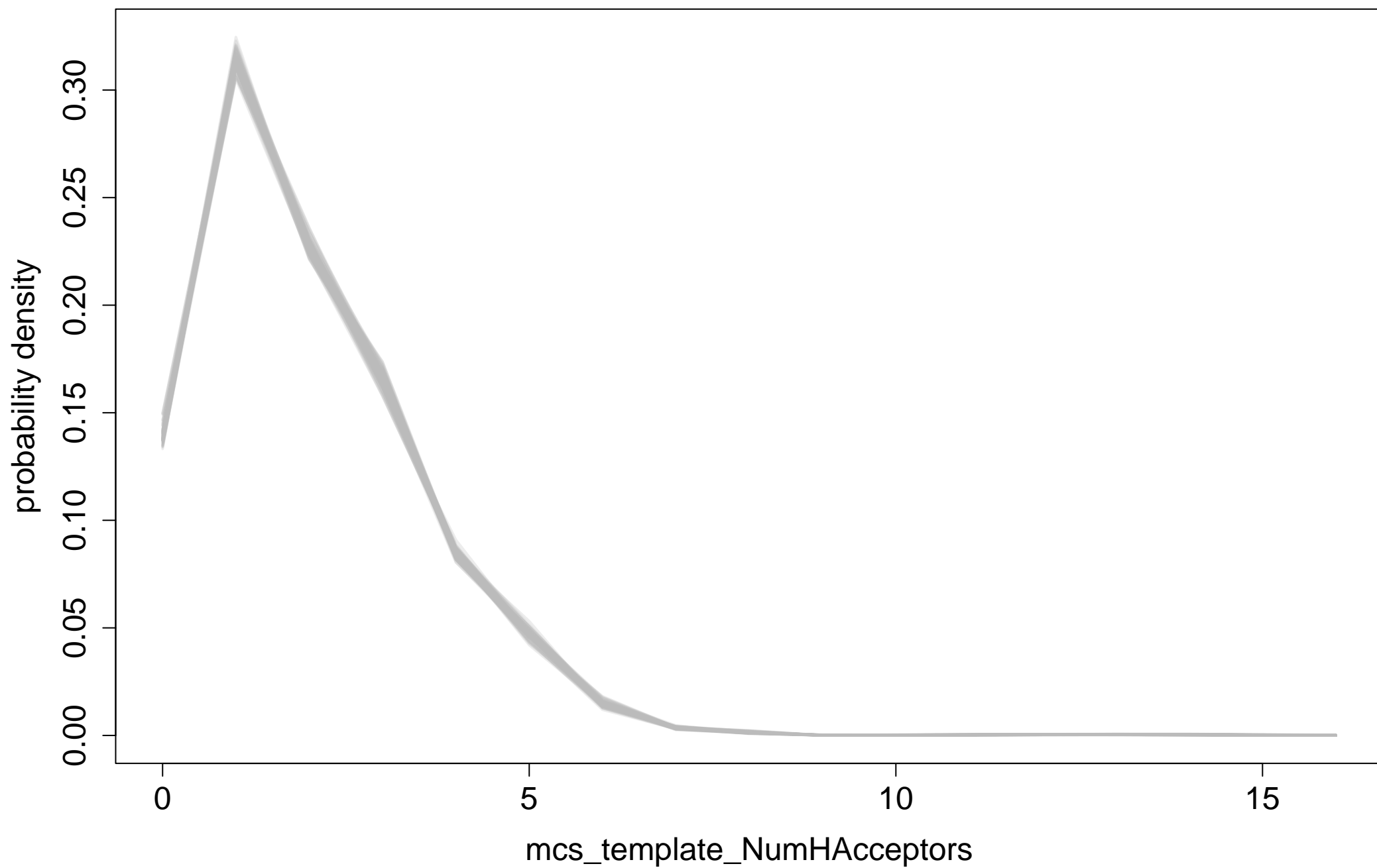


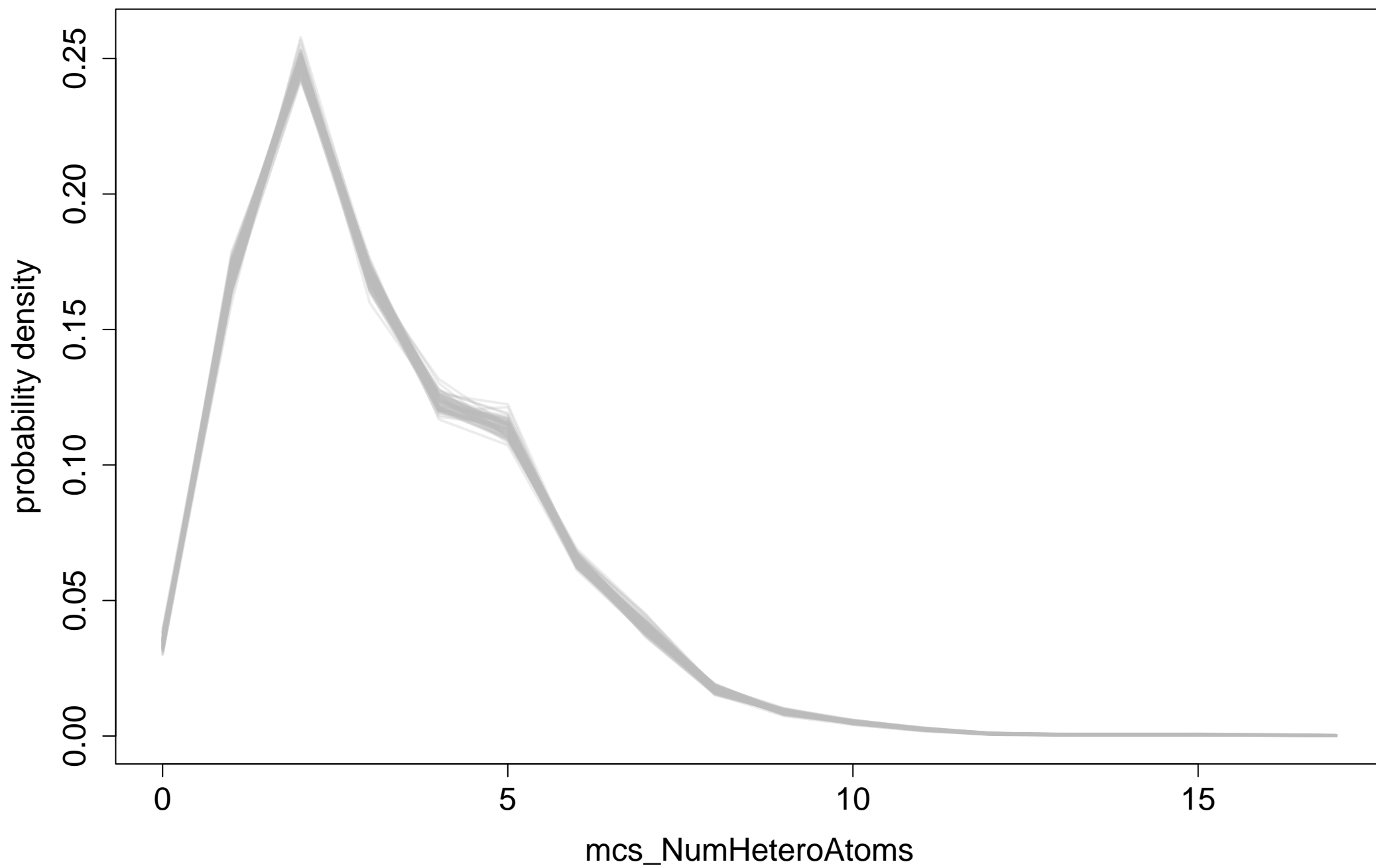


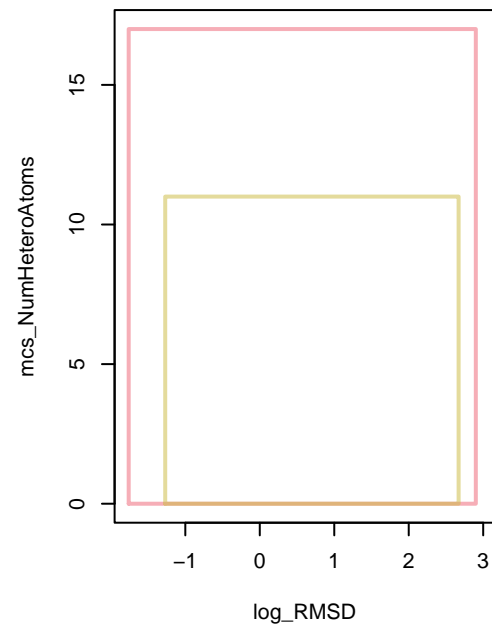
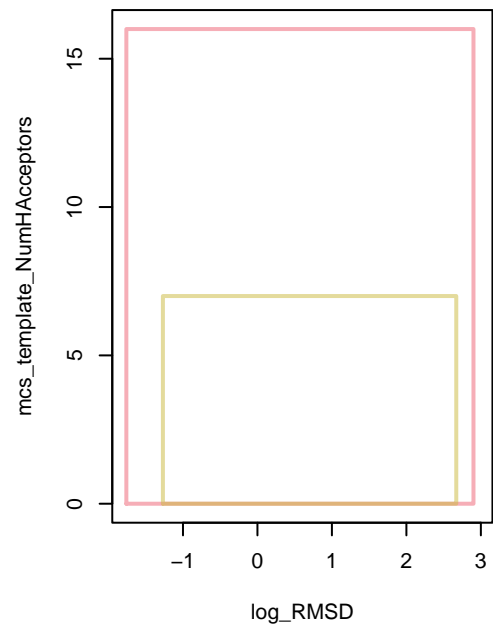
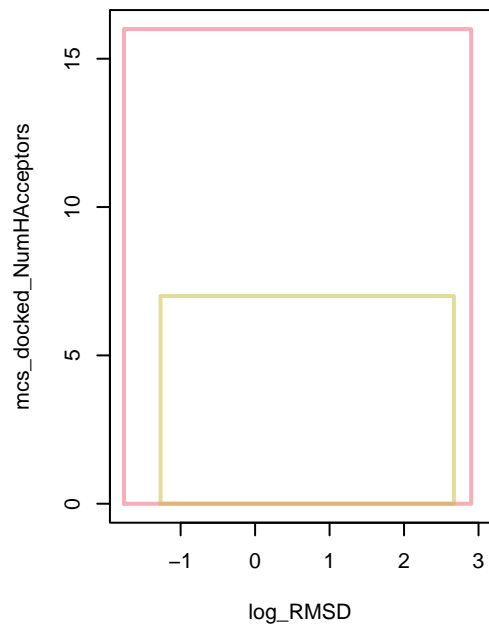
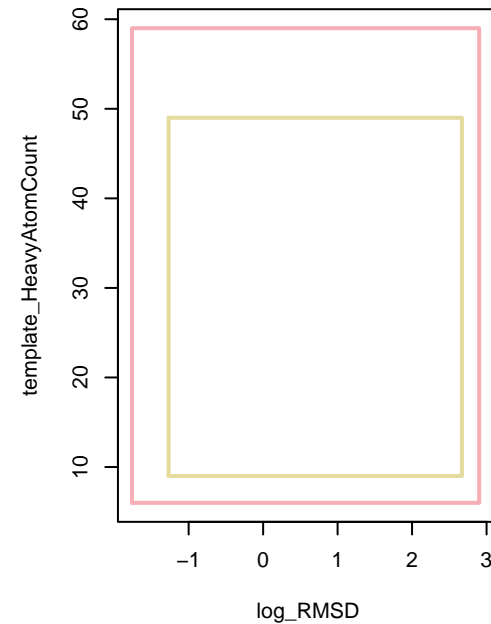
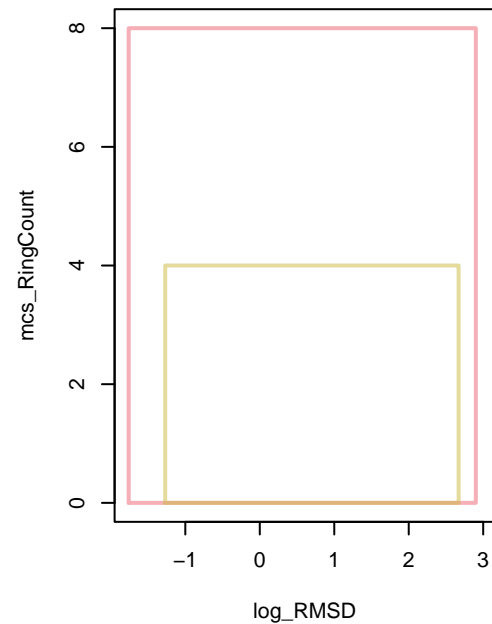
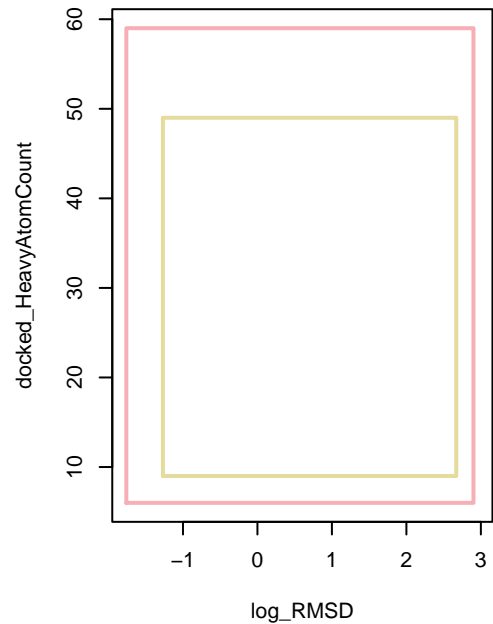
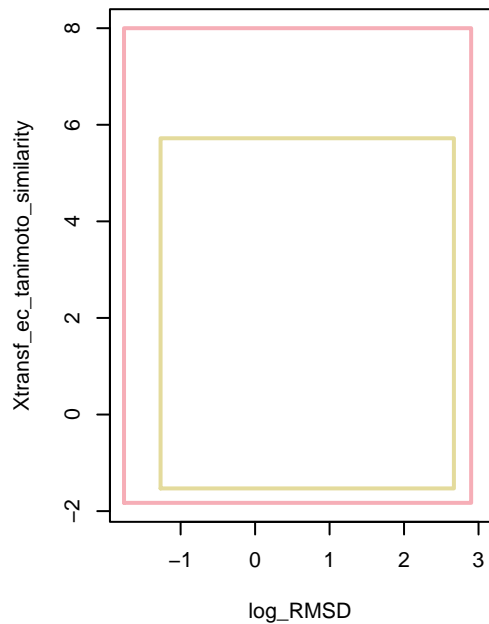




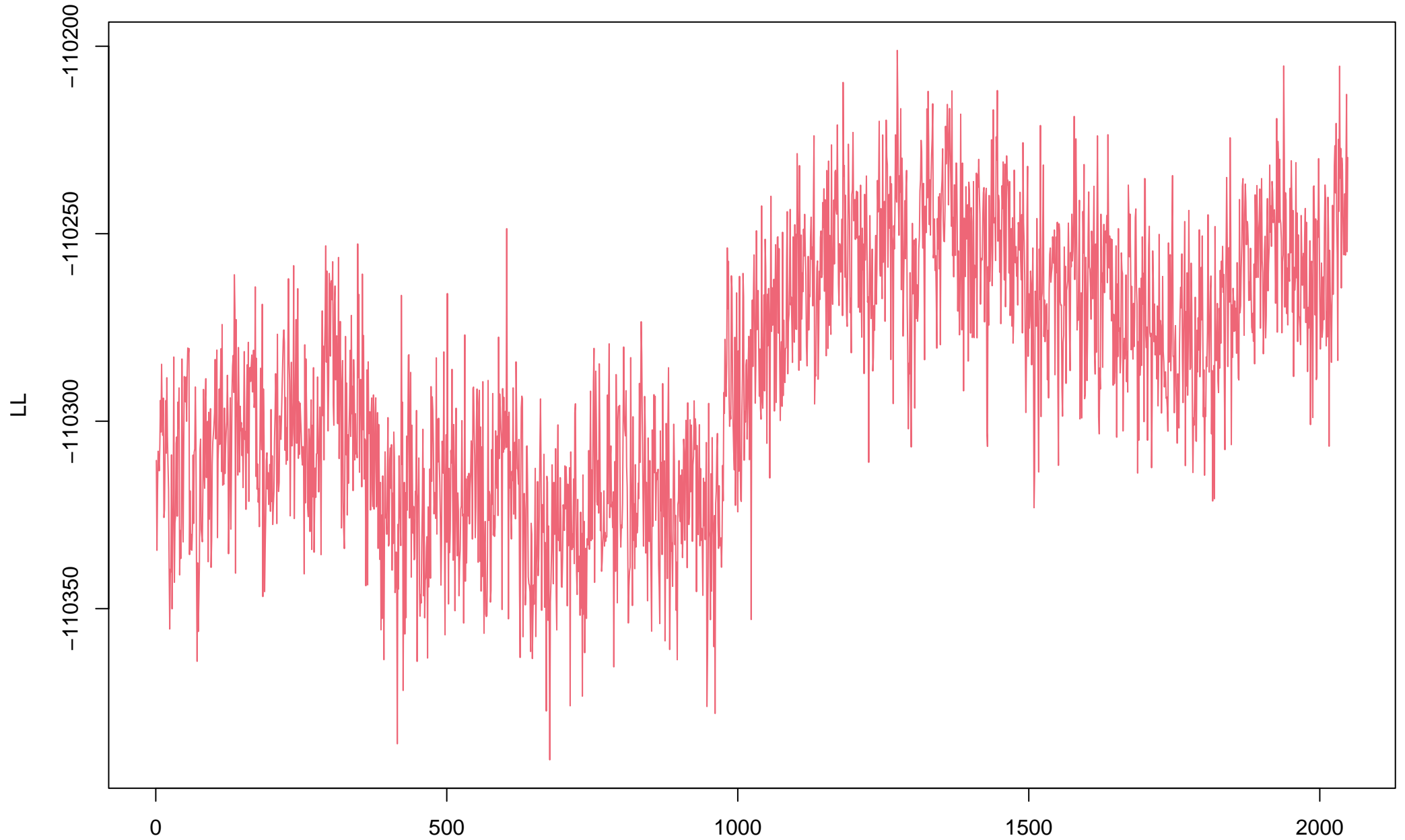




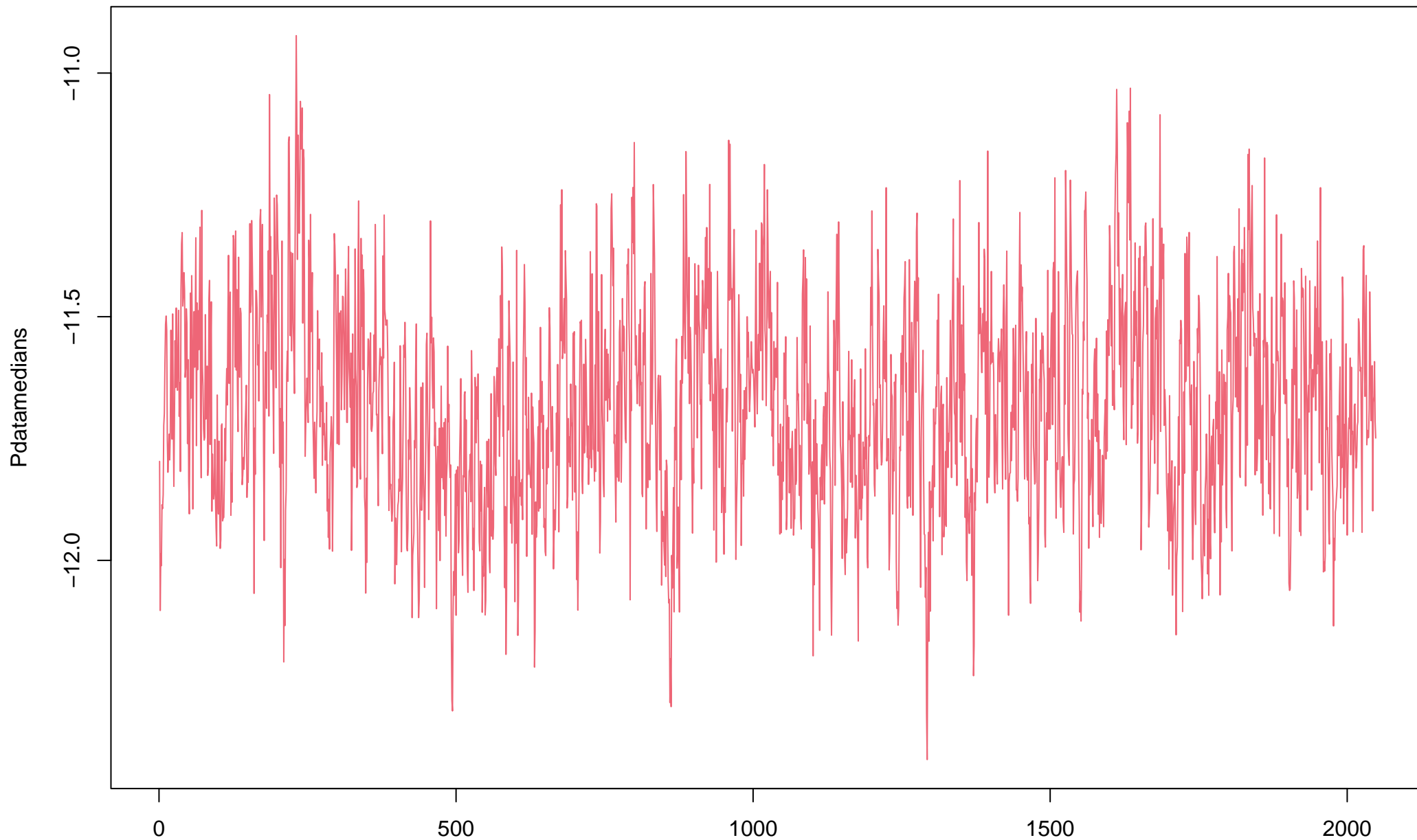




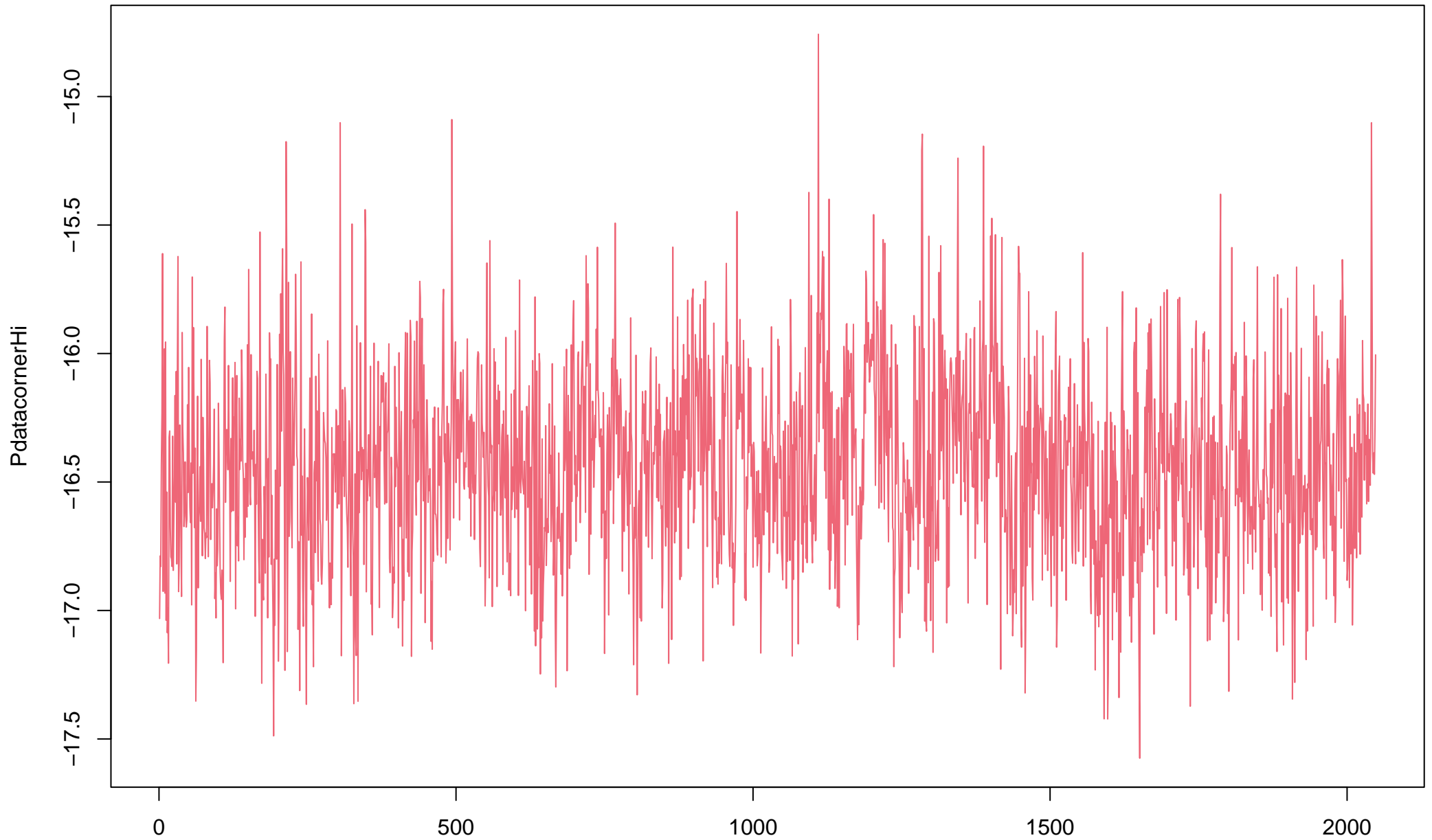
LL
ESS = 11.2 | BMK = 0.715 | MCSE(6.27) = 12.4 | stat: FALSE | burn: 1020



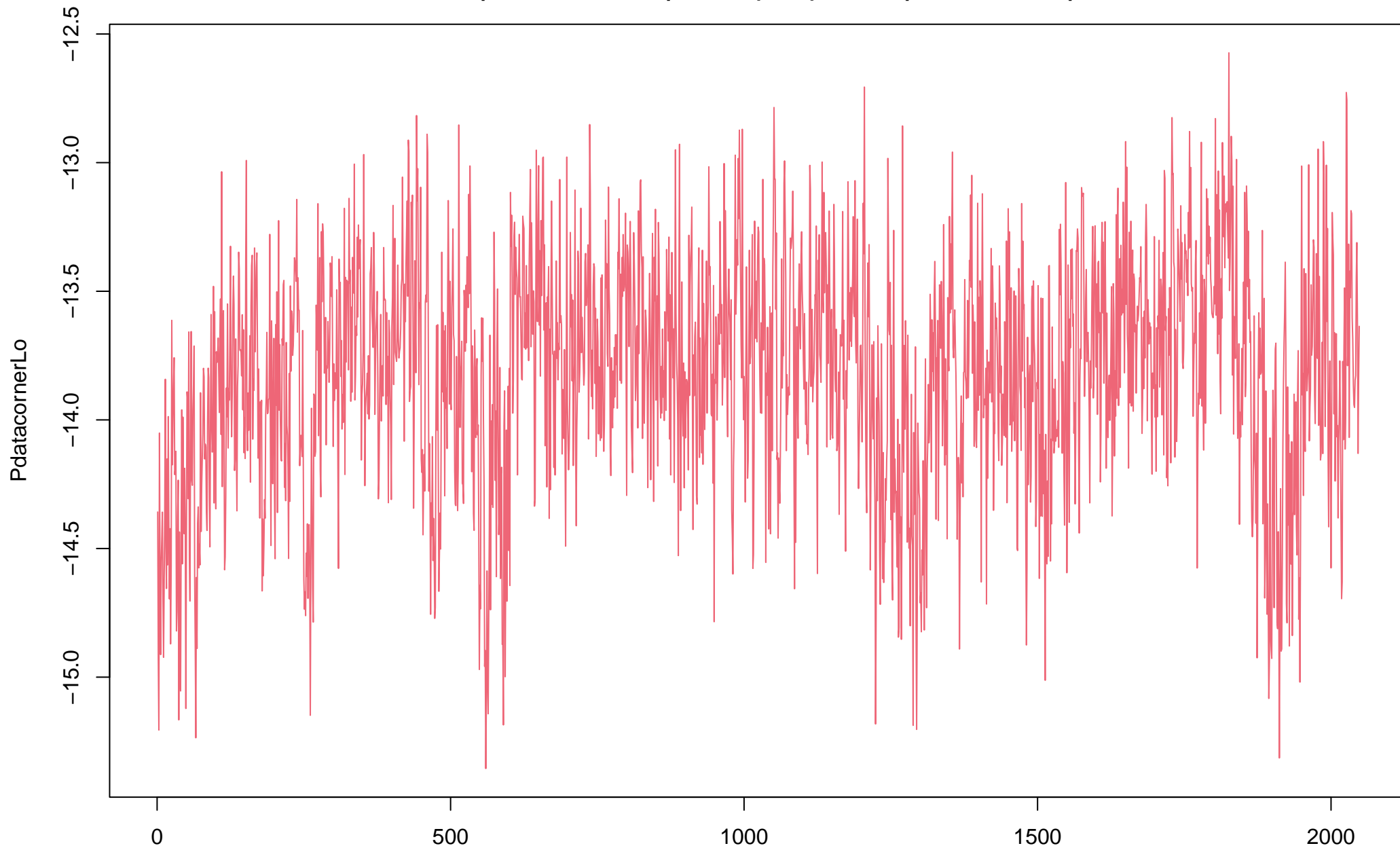
Pdatamedians
ESS = 191 | BMK = 0.0387 | MCSE(6.27) = 6.2 | stat: TRUE | burn: 0



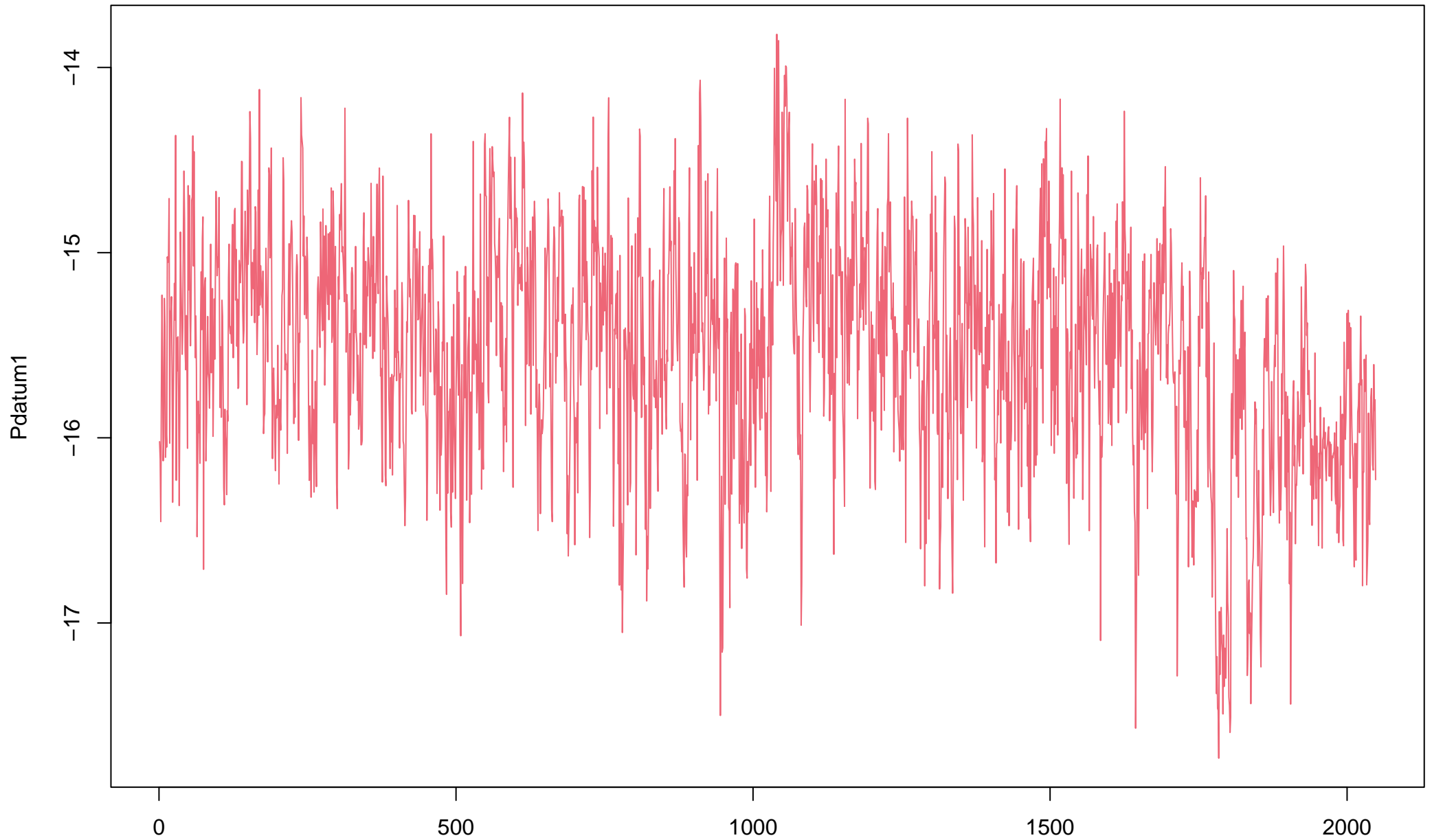
PdatacornerHi
ESS = 548 | BMK = 0.0609 | MCSE(6.27) = 3.46 | stat: FALSE | burn: 0



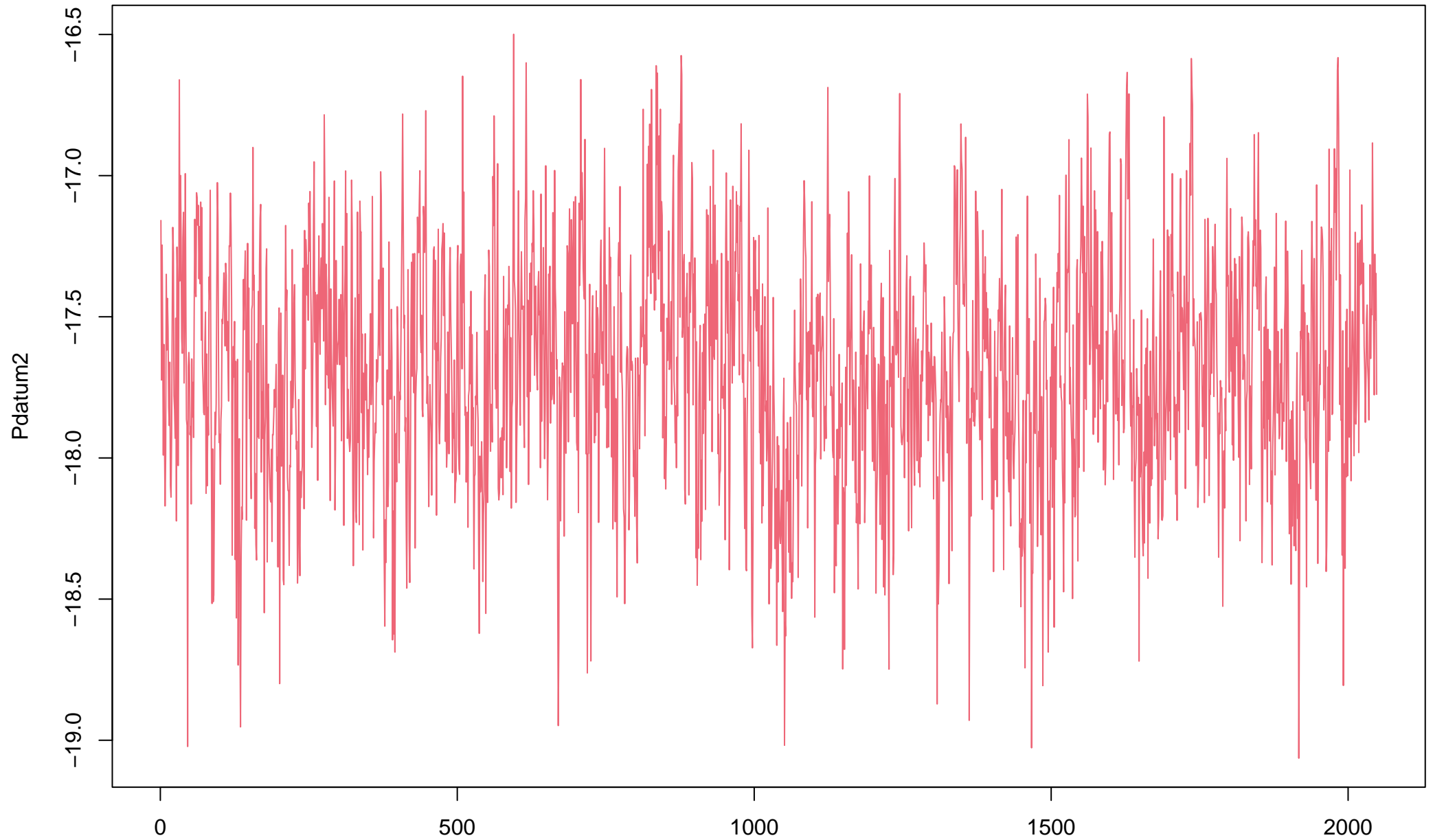
PdatacornerLo
ESS = 137 | BMK = 0.0538 | MCSE(6.27) = 6.97 | stat: FALSE | burn: 0



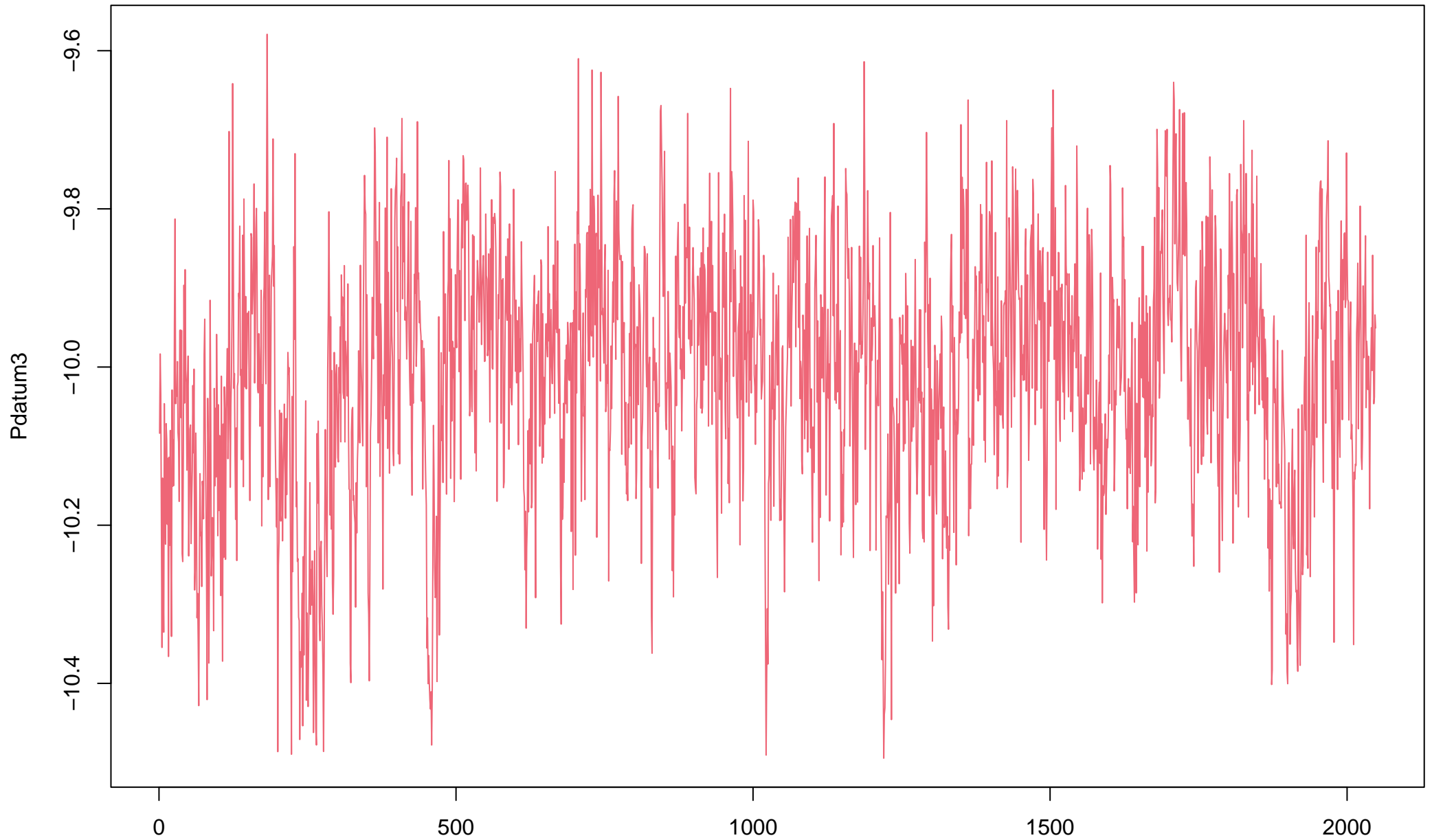
Pdatum1
ESS = 136 | BMK = 0.103 | MCSE(6.27) = 7.24 | stat: TRUE | burn: 0



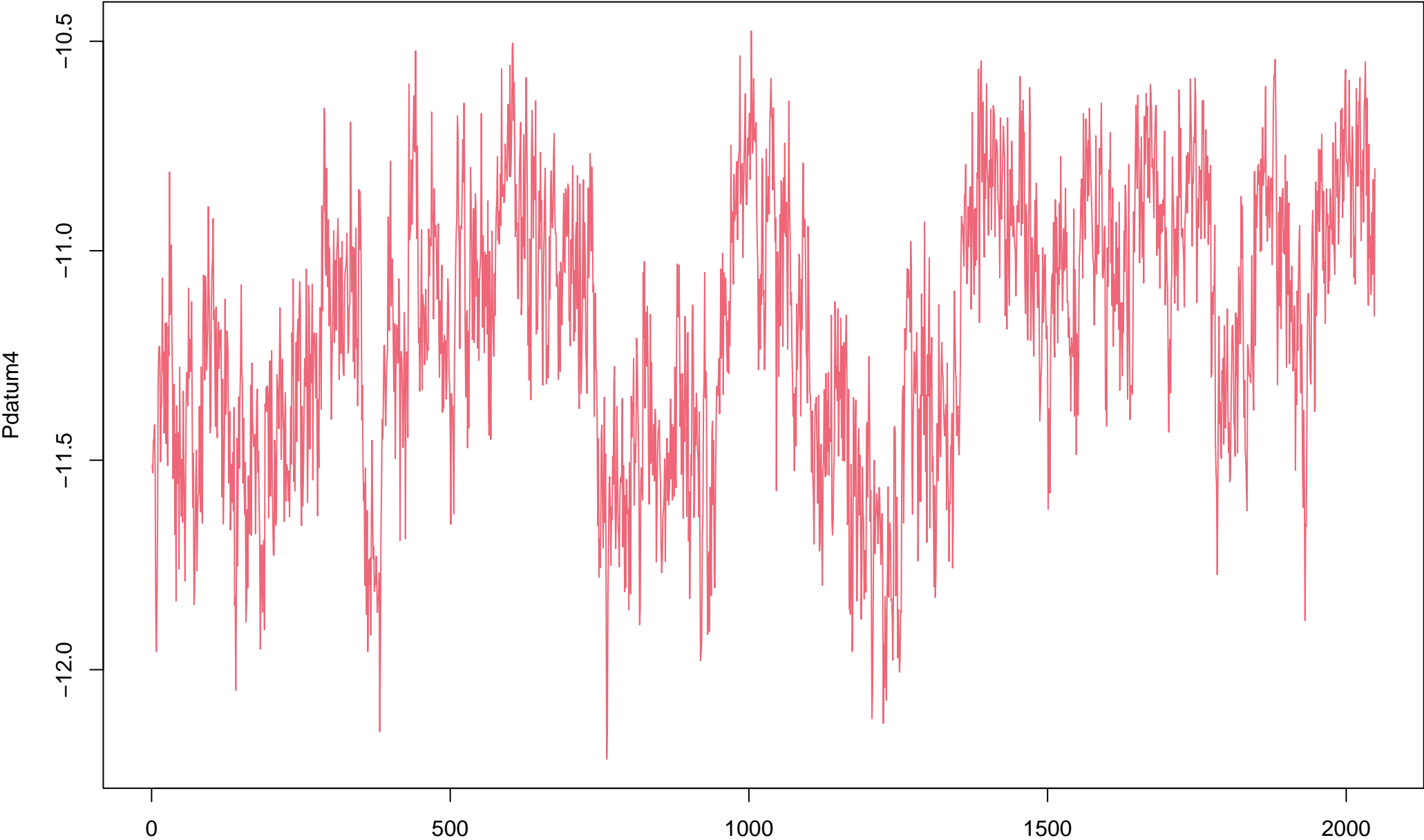
Pdatum2
ESS = 2.22e-16 | BMK = 0.0676 | MCSE(6.27) = 5 | stat: TRUE | burn: 0



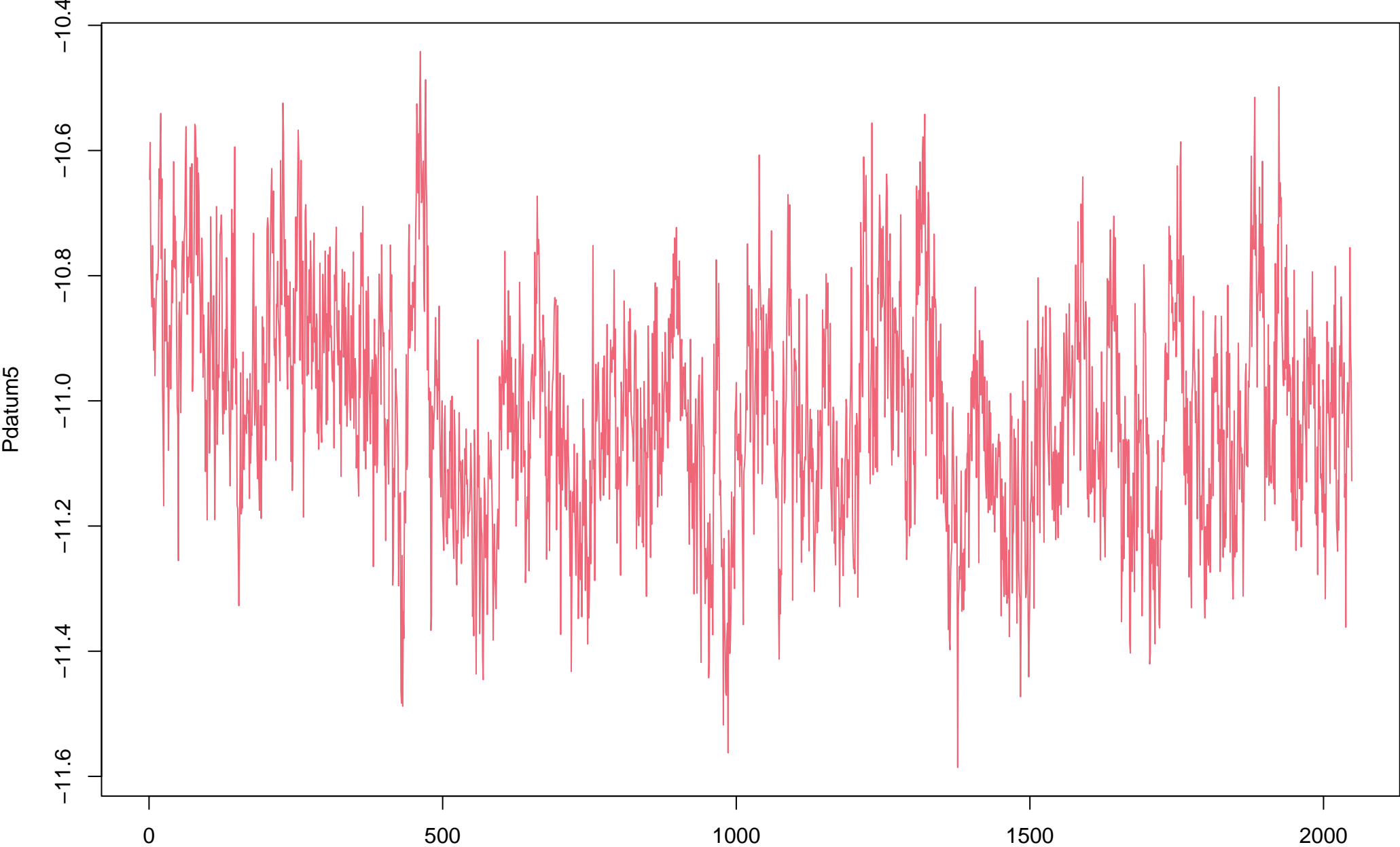
Pdatum3
ESS = 182 | BMK = 0.0688 | MCSE(6.27) = 7.34 | stat: FALSE | burn: 0



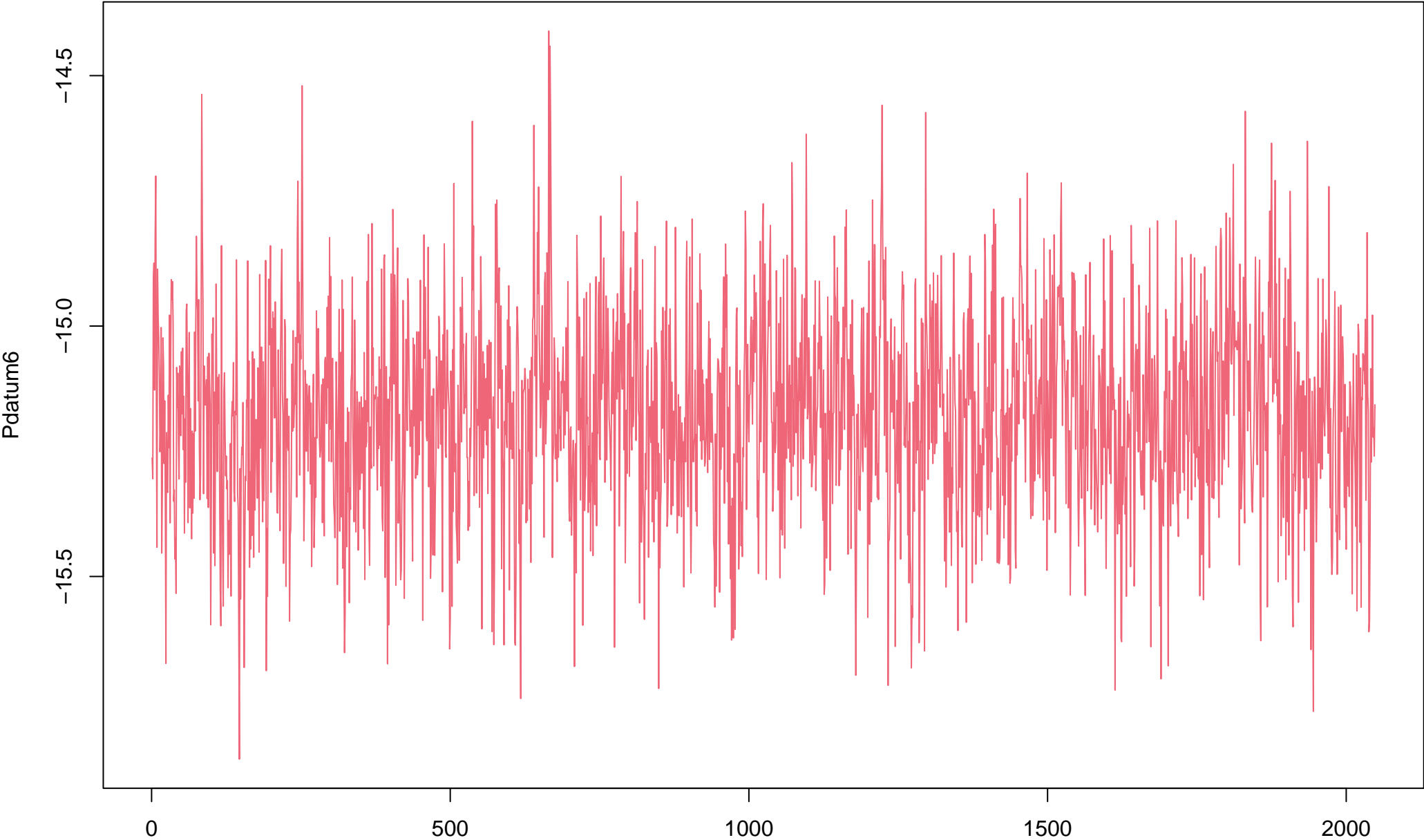
Pdatum4
ESS = 34.5 | BMK = 0.171 | MCSE(6.27) = 11.3 | stat: FALSE | burn: 0



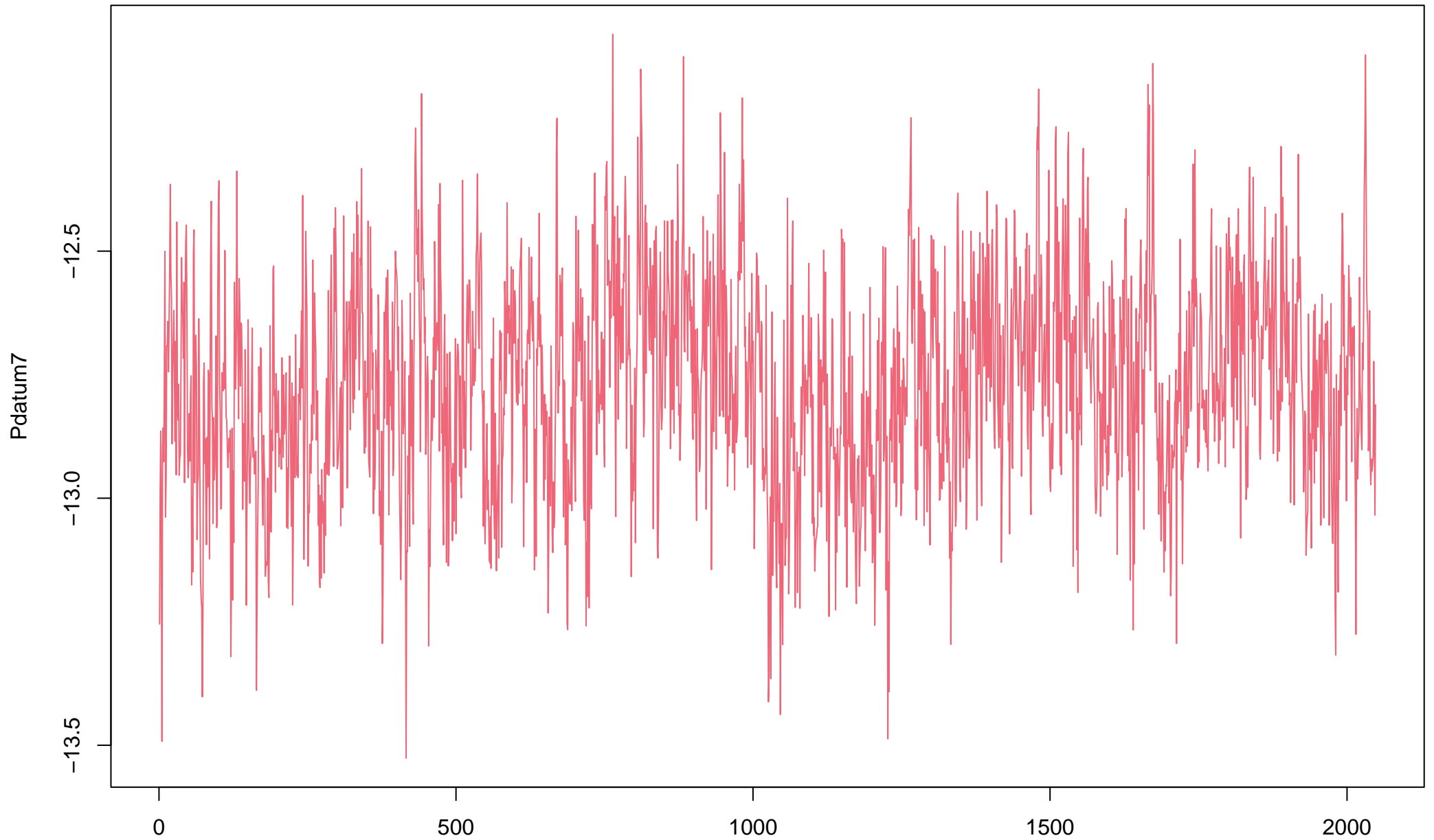
Pdatum5
ESS = 108 | BMK = 0.0792 | MCSE(6.27) = 8.9 | stat: FALSE | burn: 0



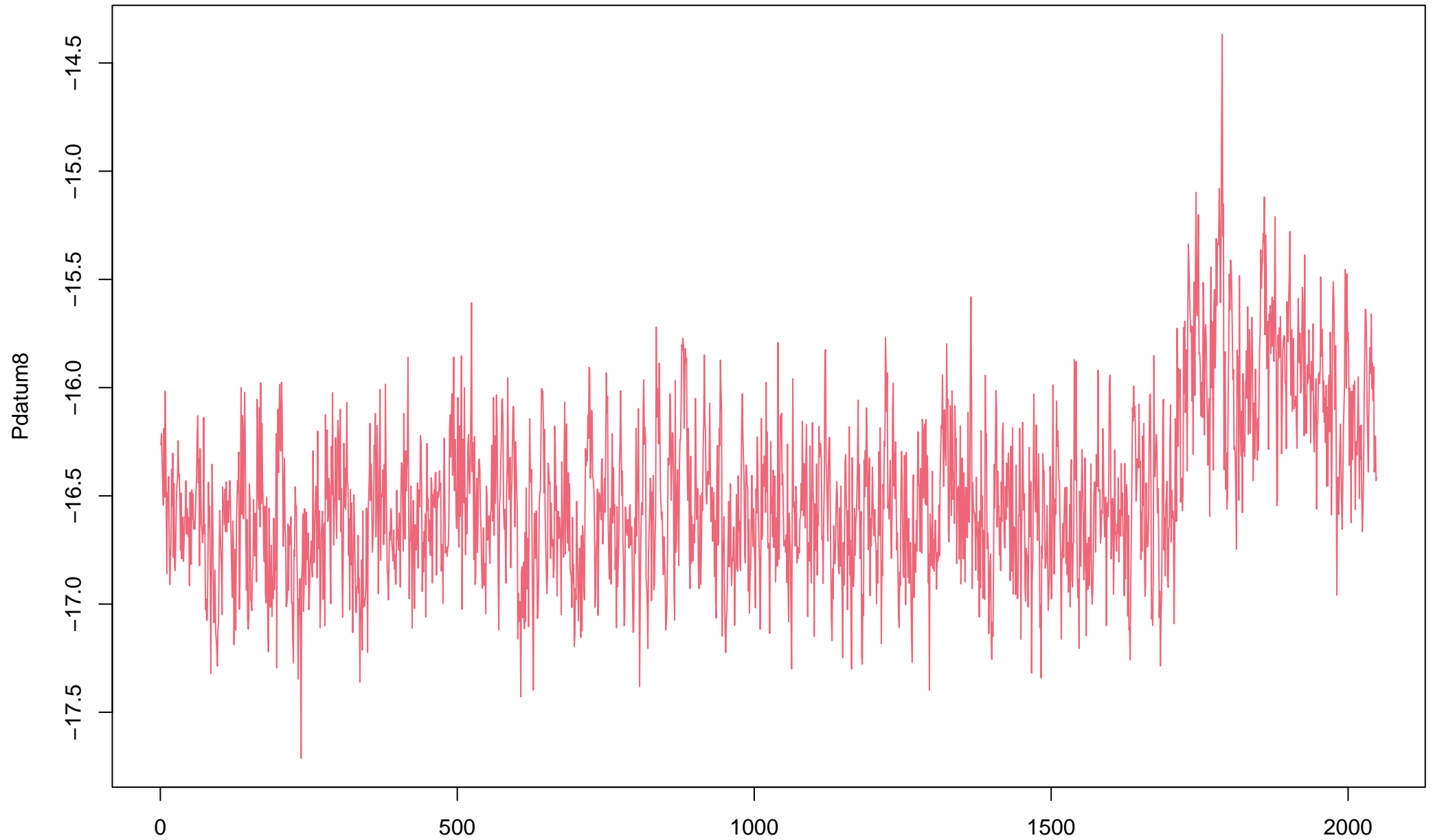
Pdatum6
ESS = 973 | BMK = 0.0449 | MCSE(6.27) = 3.88 | stat: TRUE | burn: 0



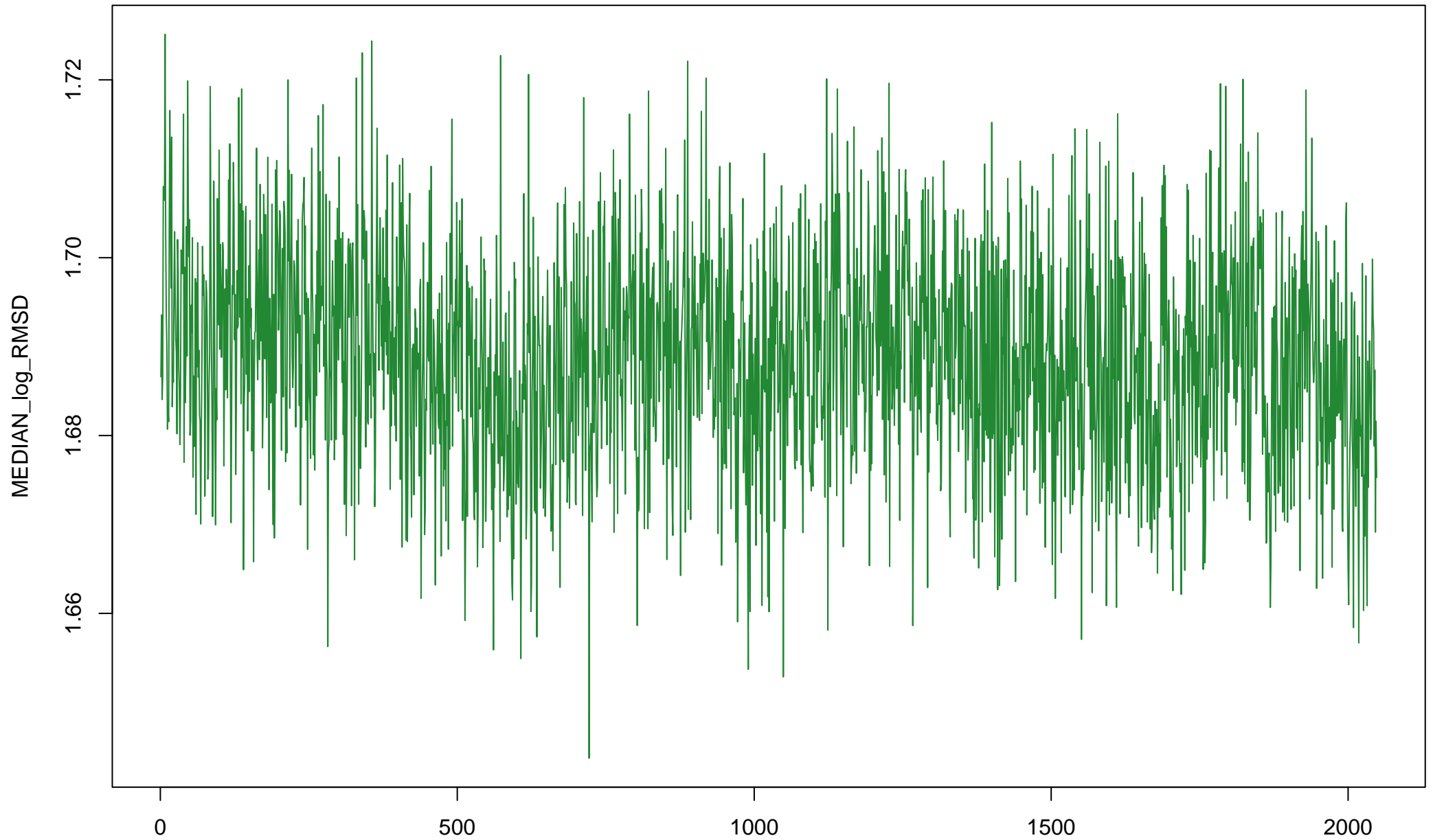
Pdatum7
ESS = 328 | BMK = 0.0285 | MCSE(6.27) = 6.07 | stat: FALSE | burn: 0



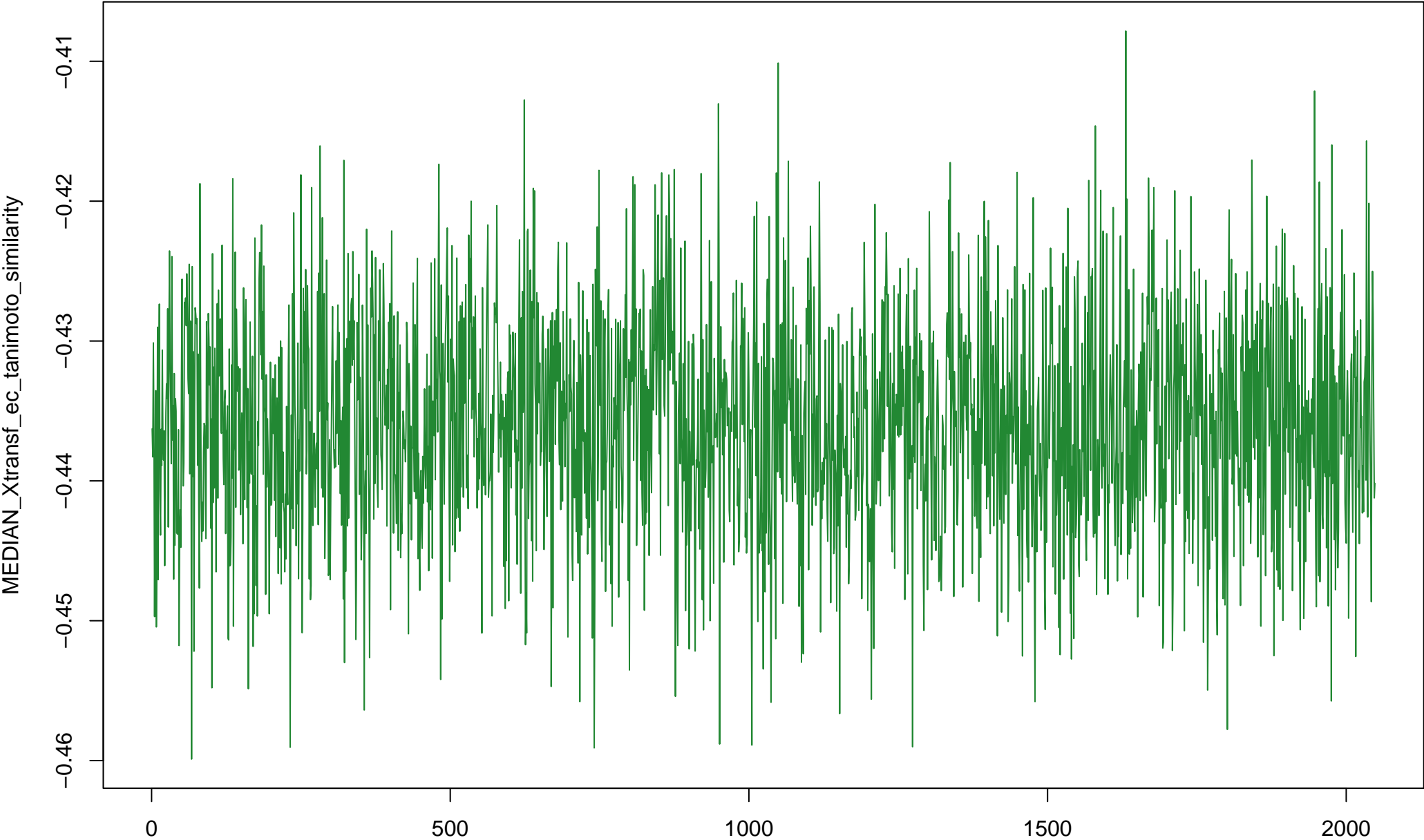
Pdatum8
ESS = 26.8 | BMK = 0.26 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 0



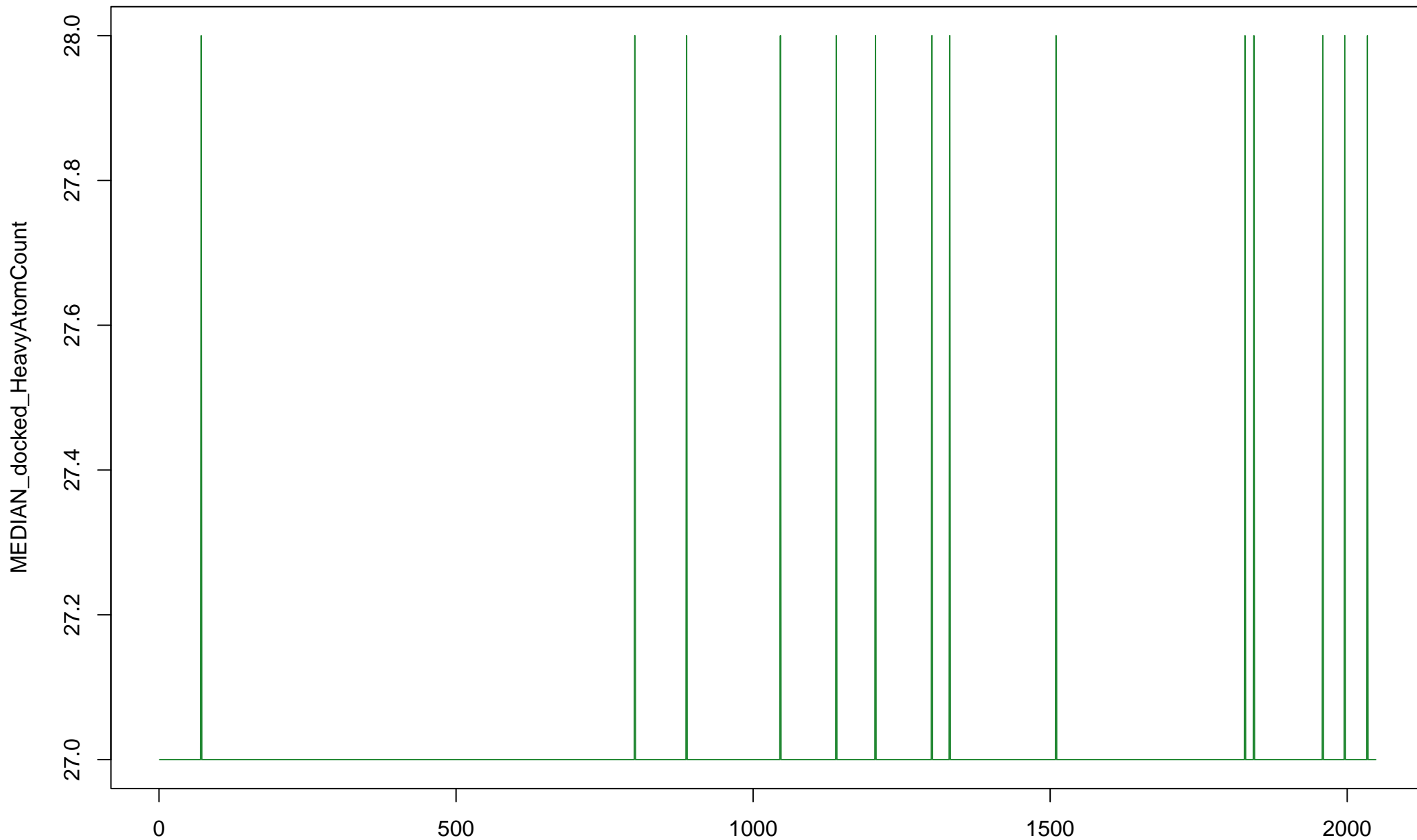
MEDIAN_log_RMSD
ESS = 746 | BMK = 0.0508 | MCSE(6.27) = 4.08 | stat: FALSE | burn: 0



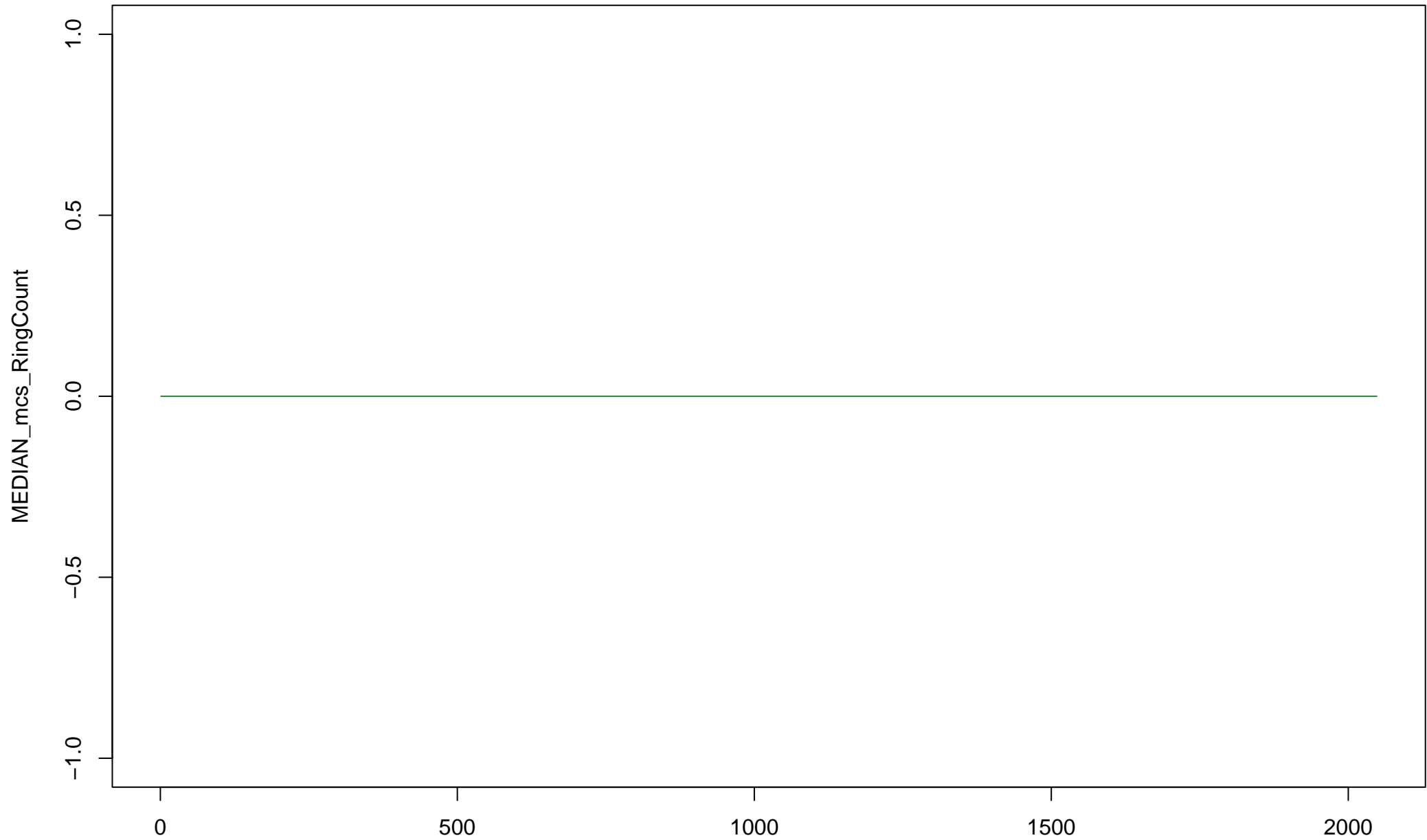
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1400 | BMK = 0.036 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0



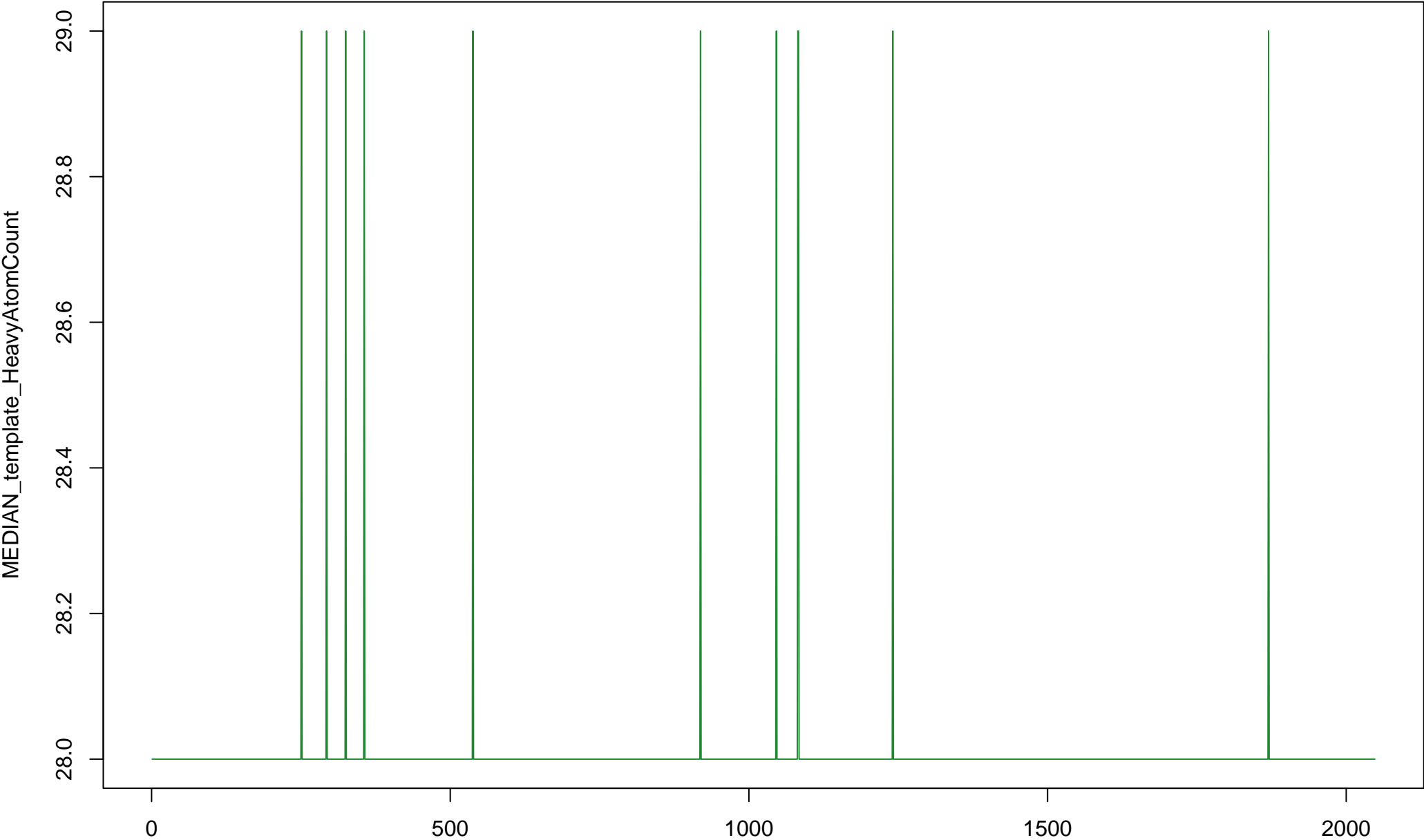
MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.218 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 612



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



MEDIAN_template_HeavyAtomCount
ESS = 1720 | BMK = 0.0324 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 2040



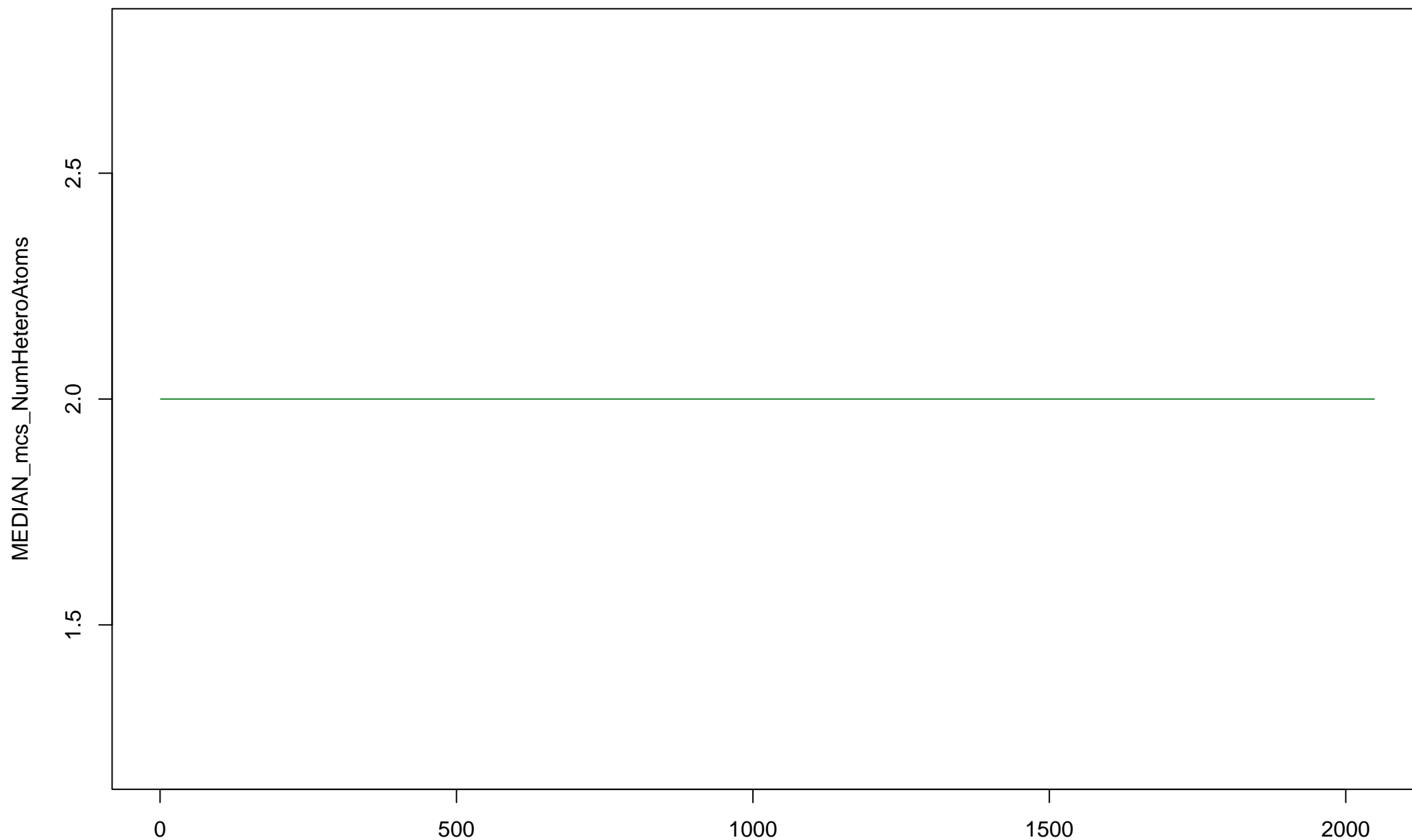
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



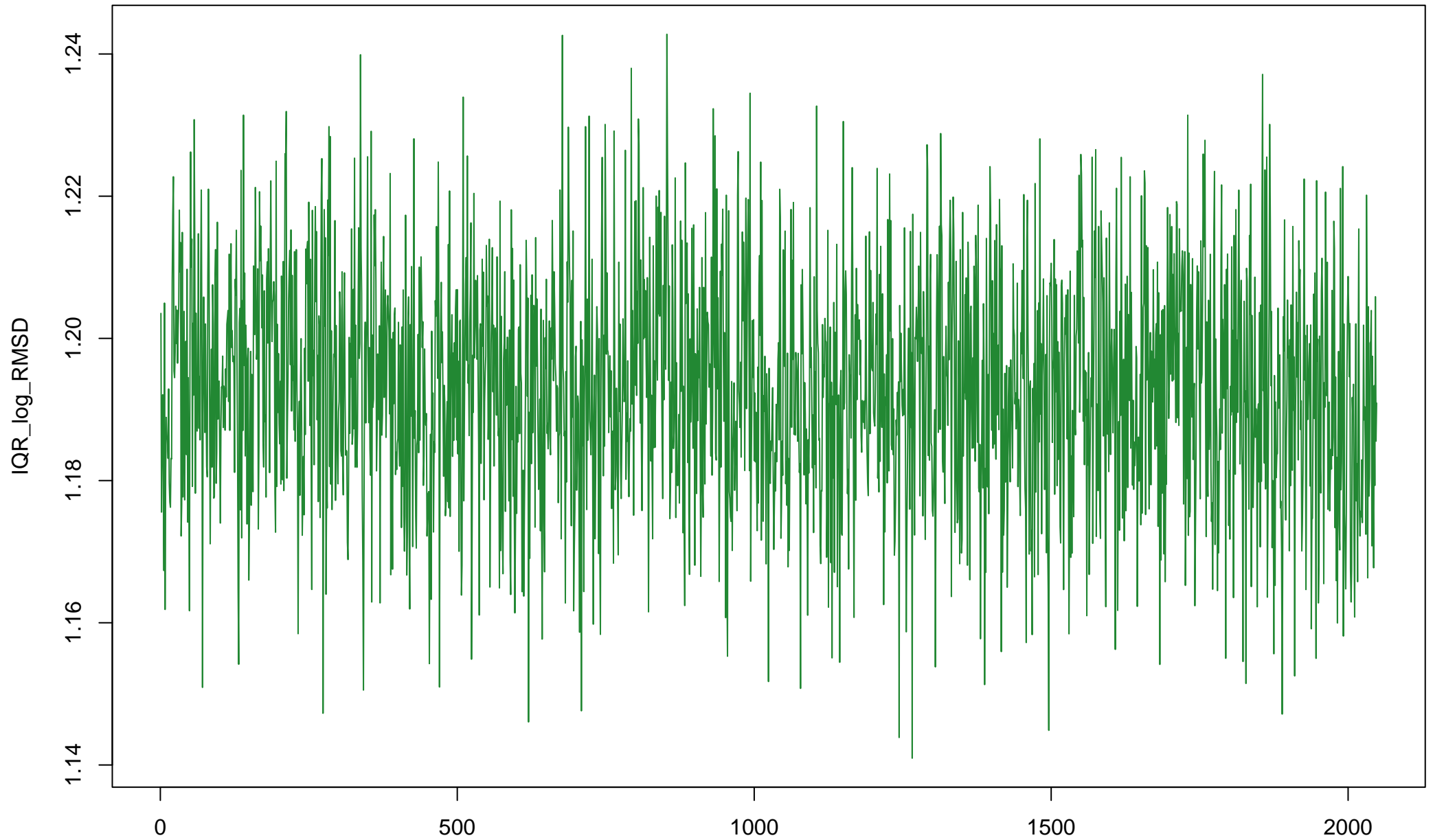
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



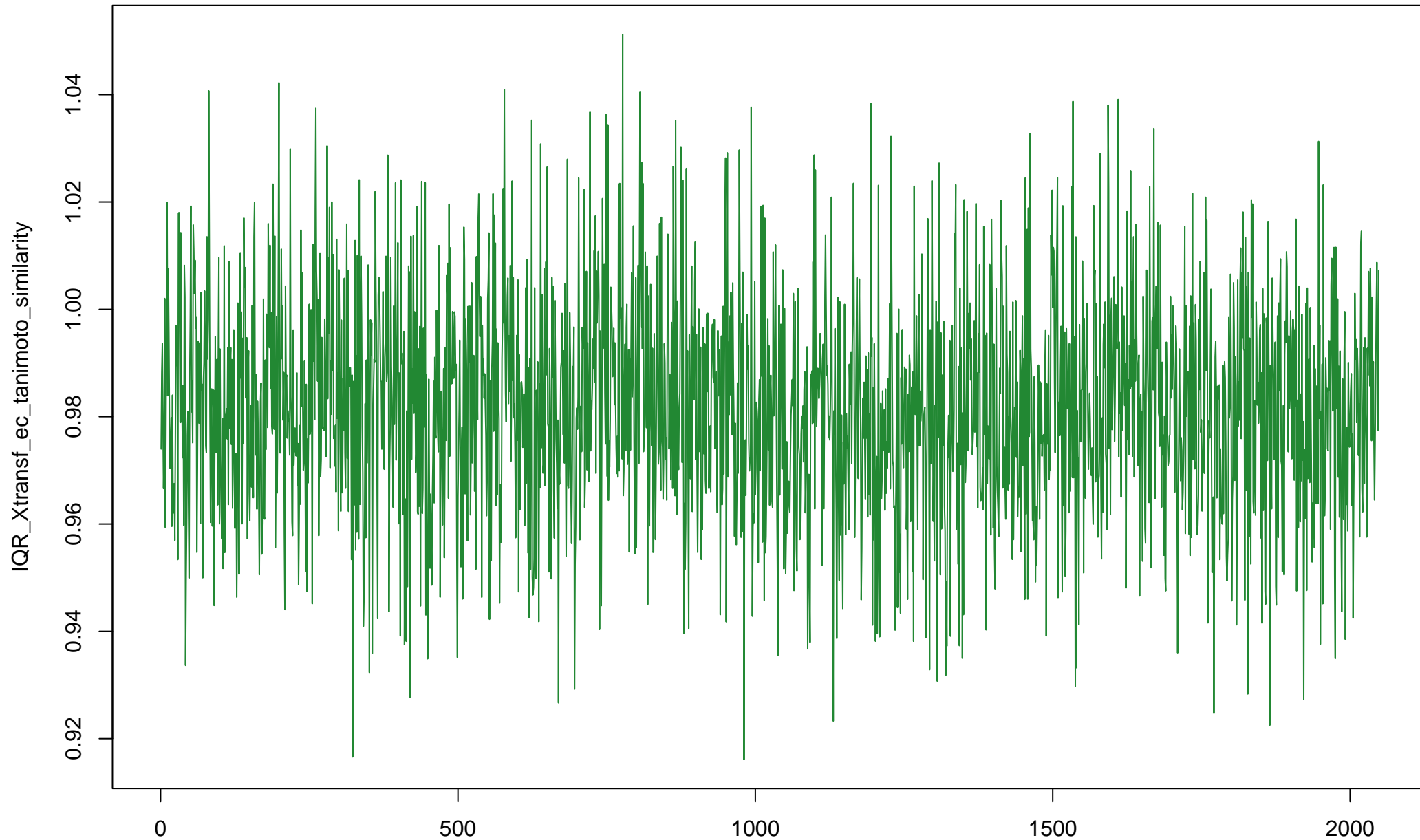
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



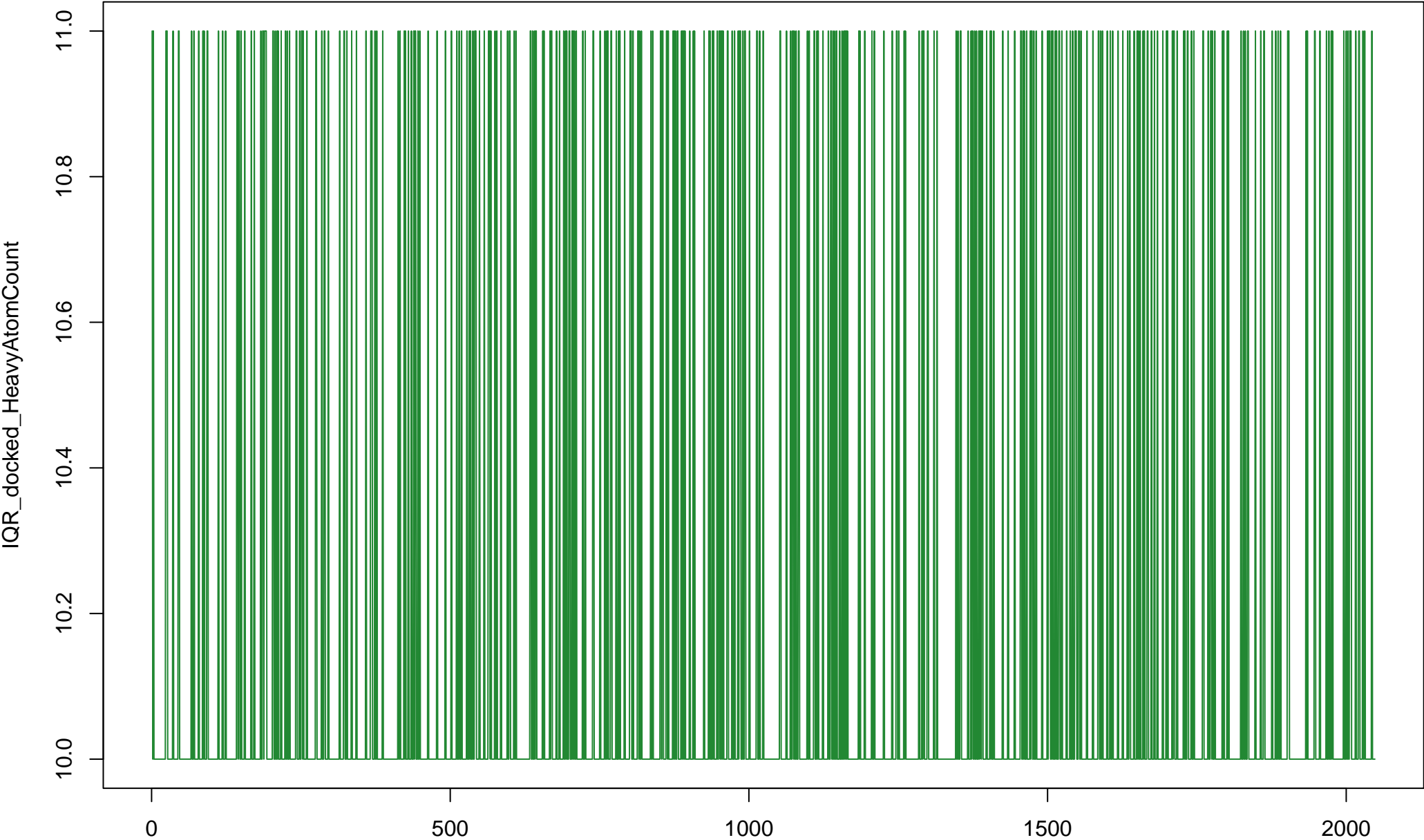
IQR_log_RMSD
ESS = 1530 | BMK = 0.0554 | MCSE(6.27) = 2.69 | stat: FALSE | burn: 0



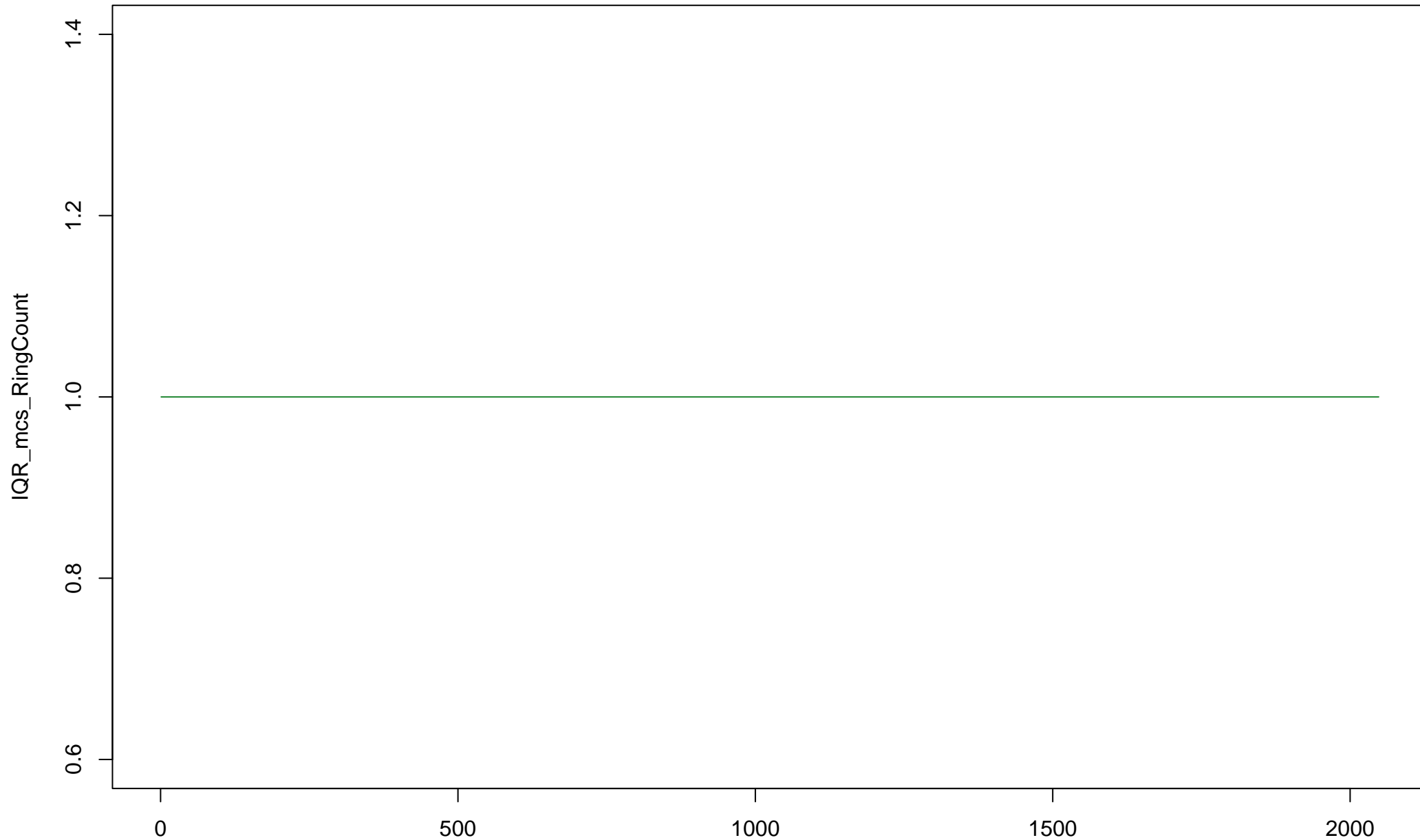
IQR_Xtransf_ec_tanimoto_similarity
ESS = 1510 | BMK = 0.0587 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0



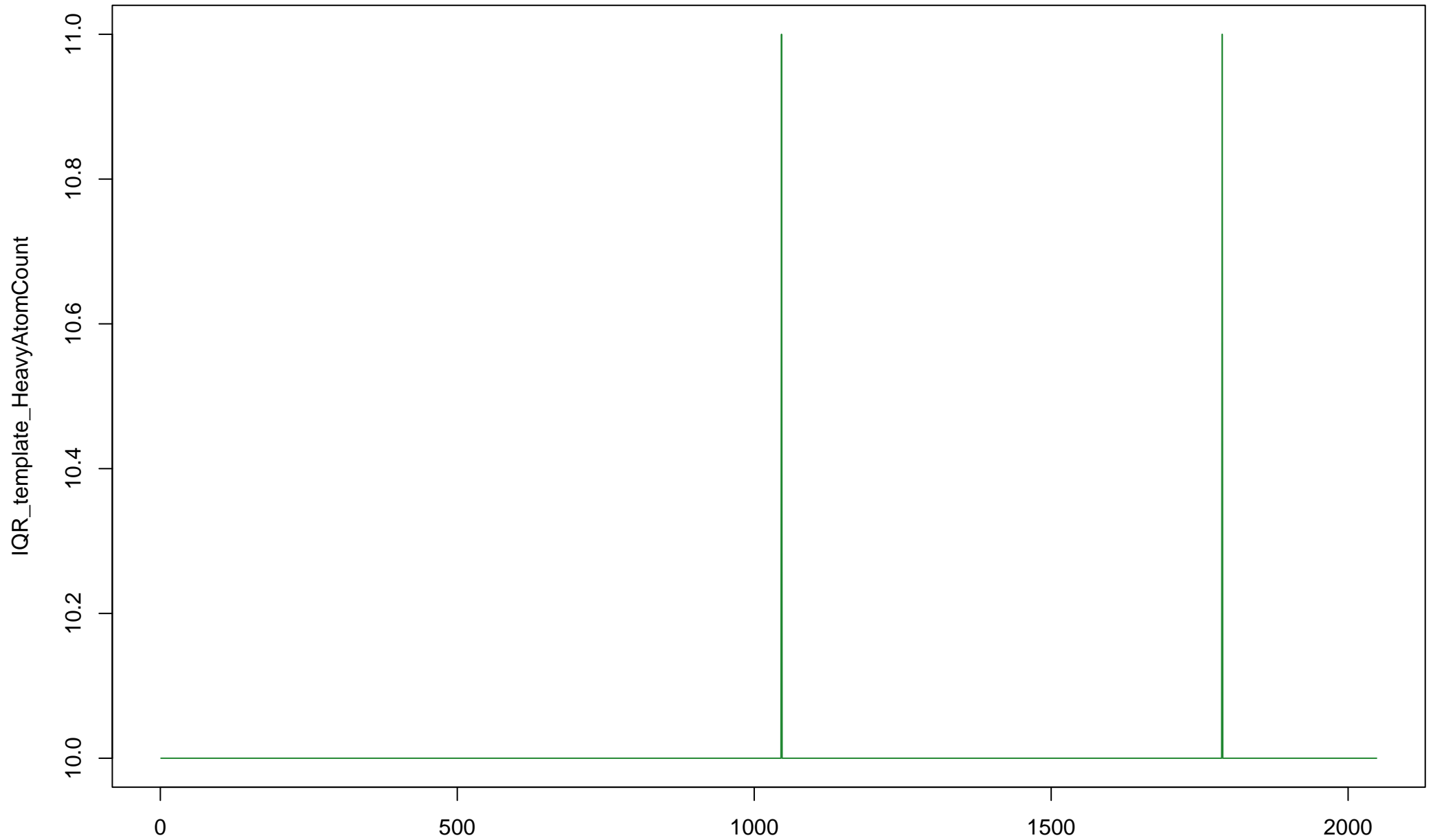
IQR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0103 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0



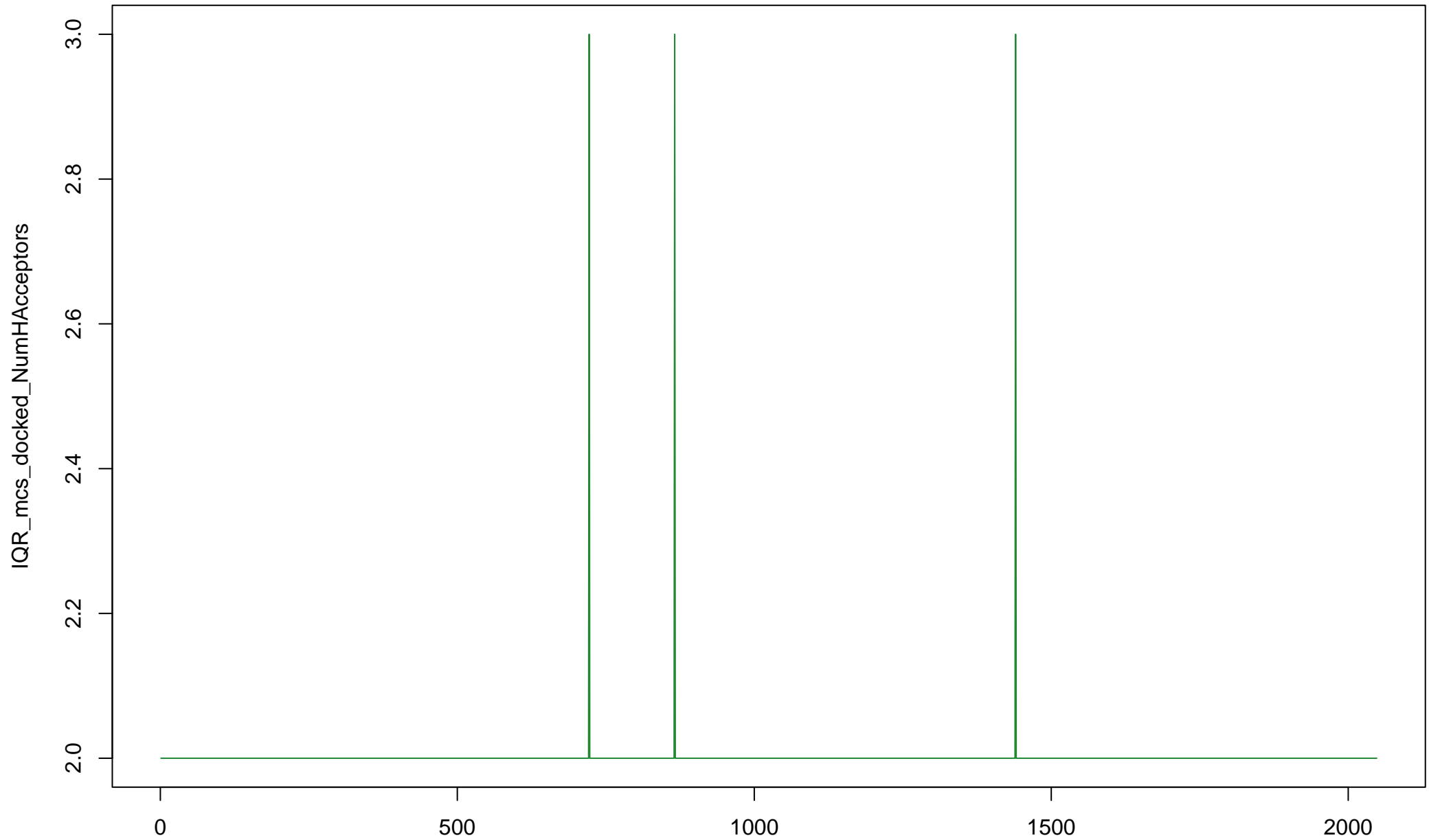
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



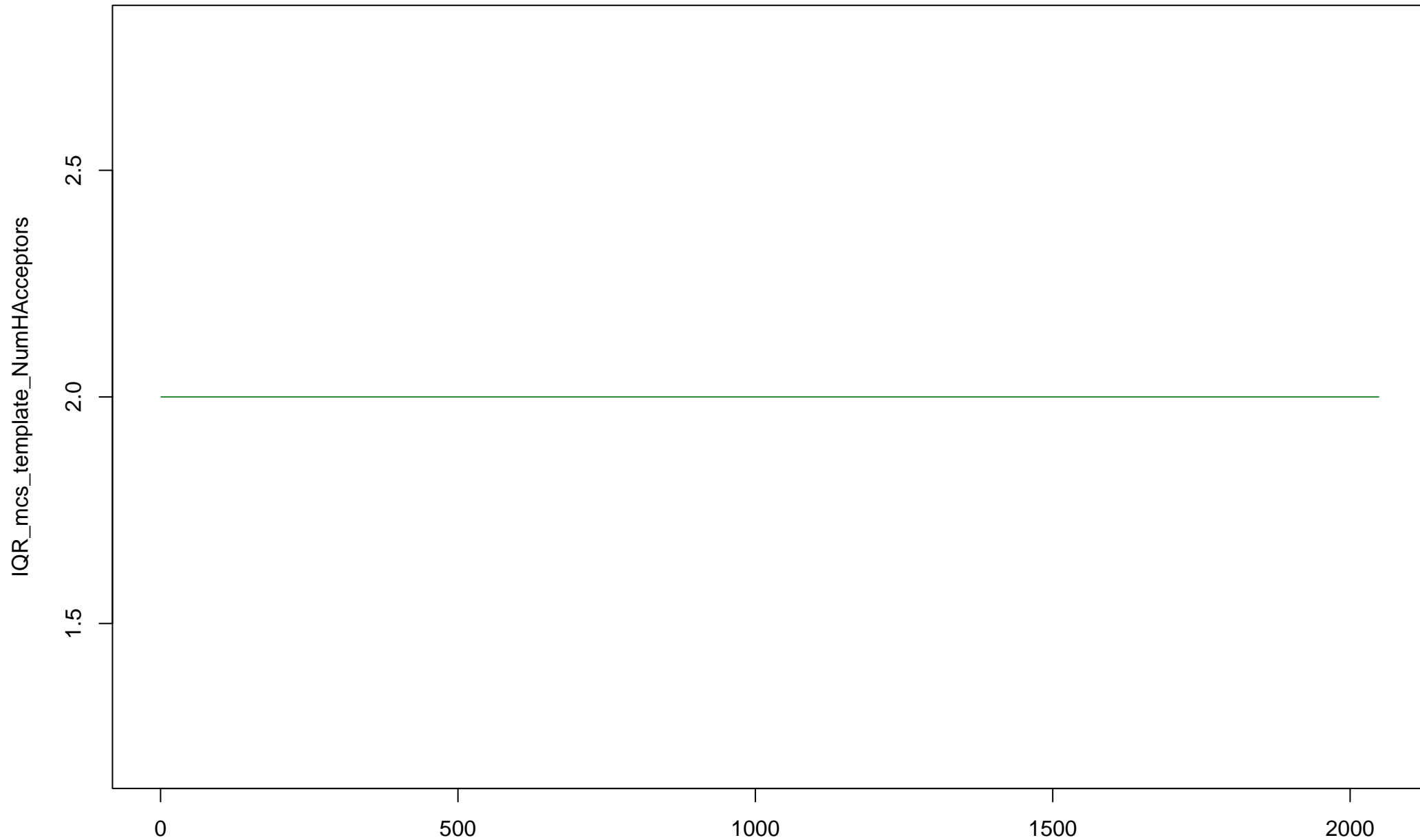
IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.544 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 2040



IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 1632



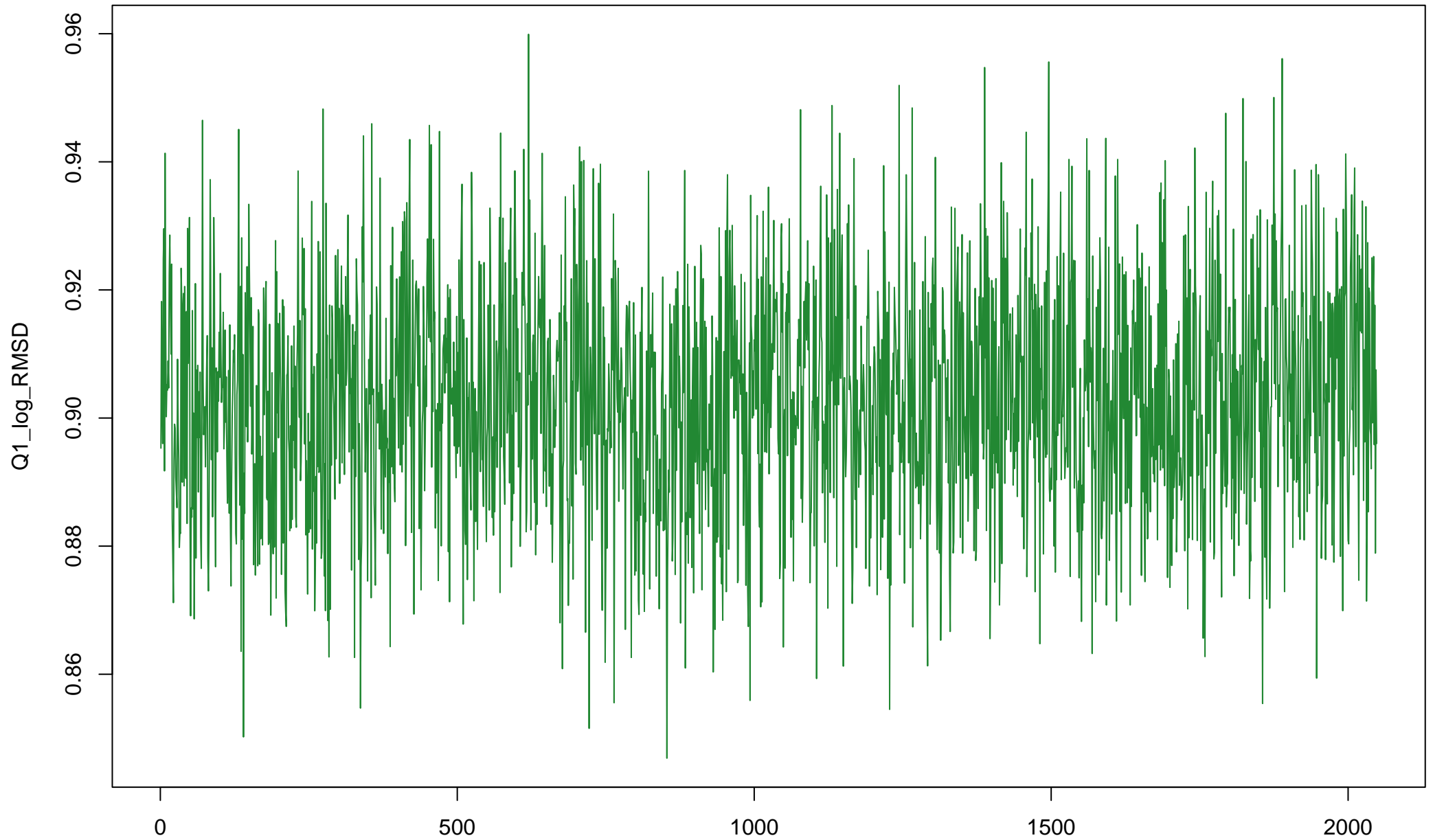
IQR_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



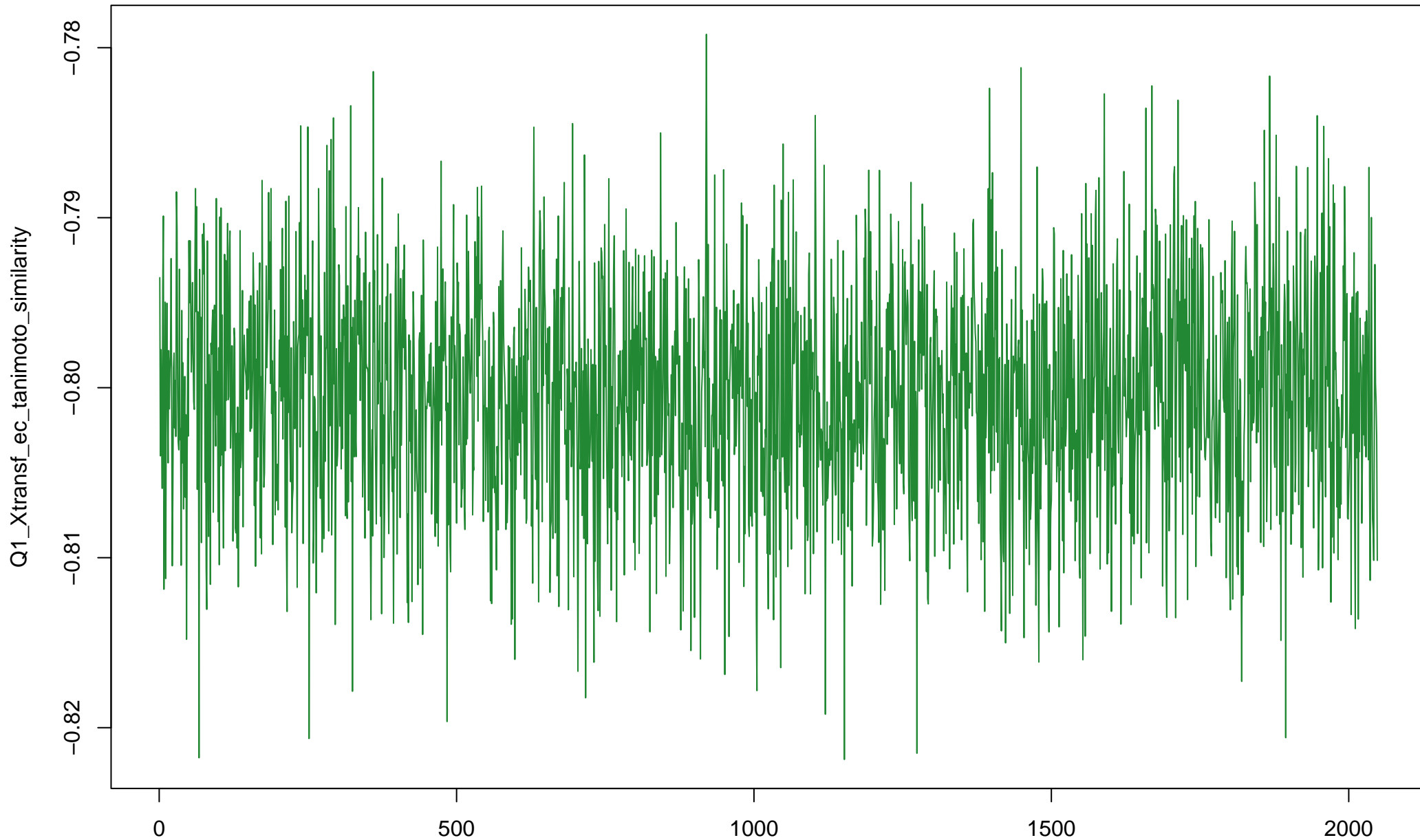
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



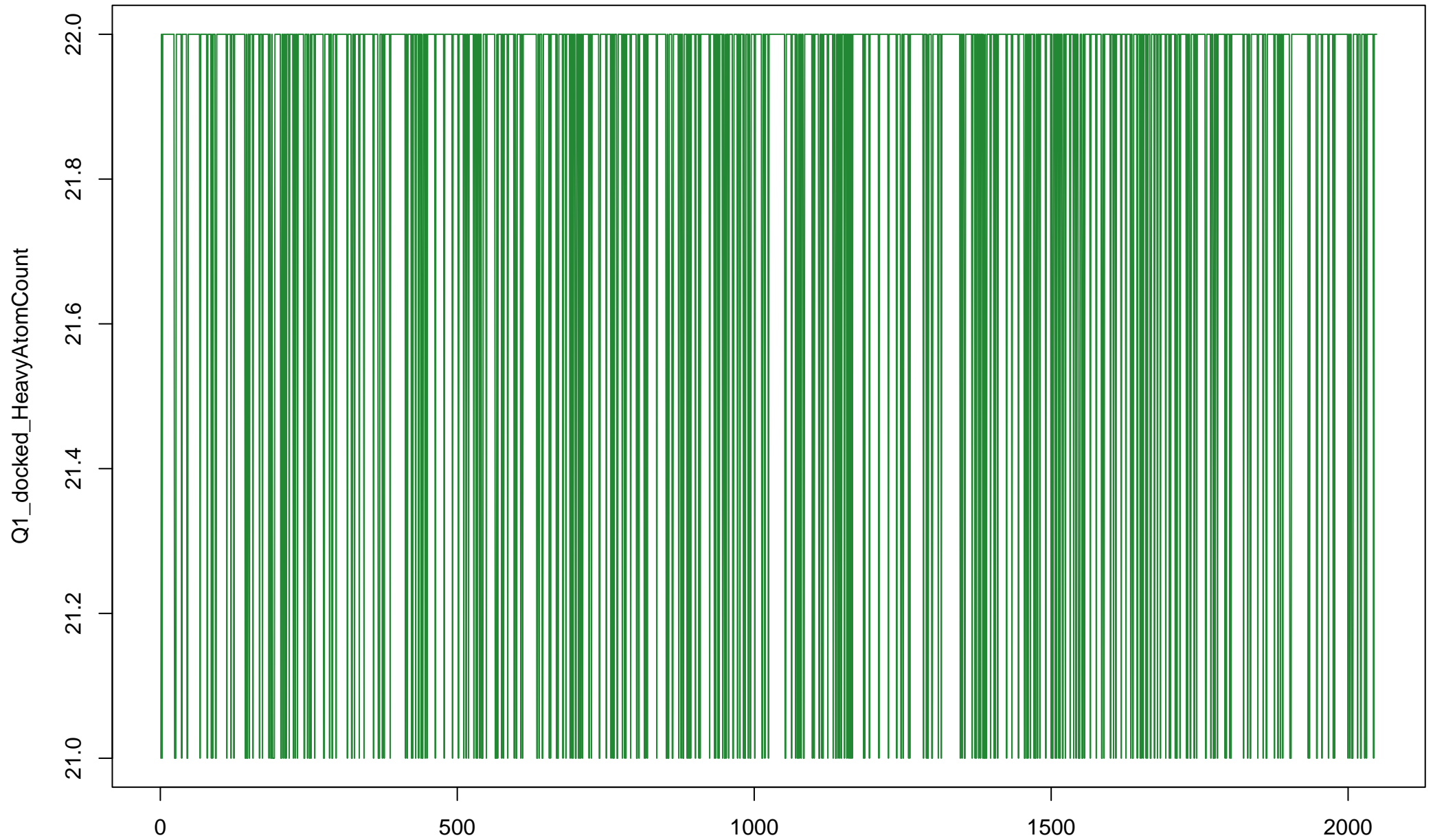
Q1_log_RMSD
ESS = 1560 | BMK = 0.051 | MCSE(6.27) = 2.69 | stat: FALSE | burn: 0



Q1_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0426 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0



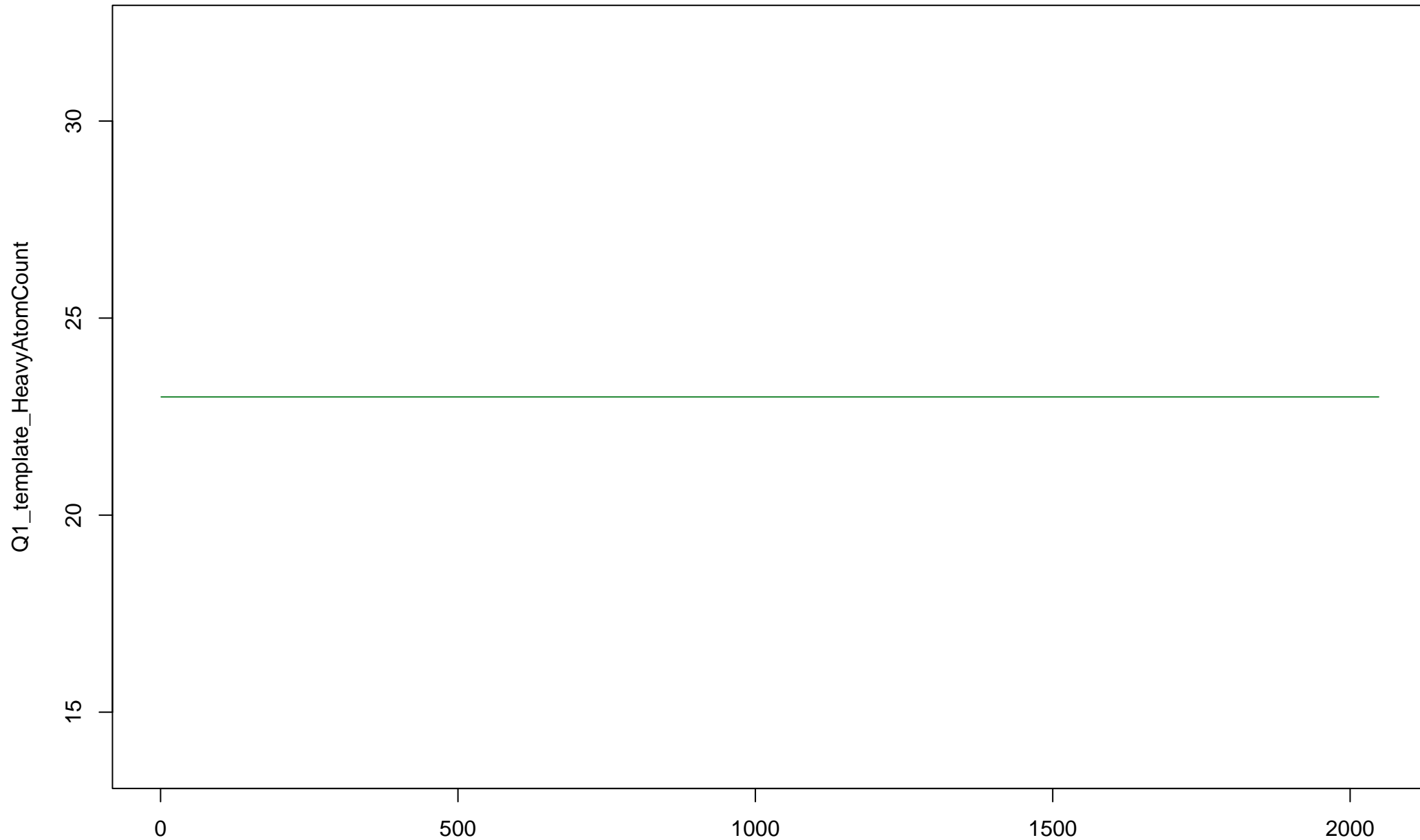
Q1_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.00784 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



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



Q1_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



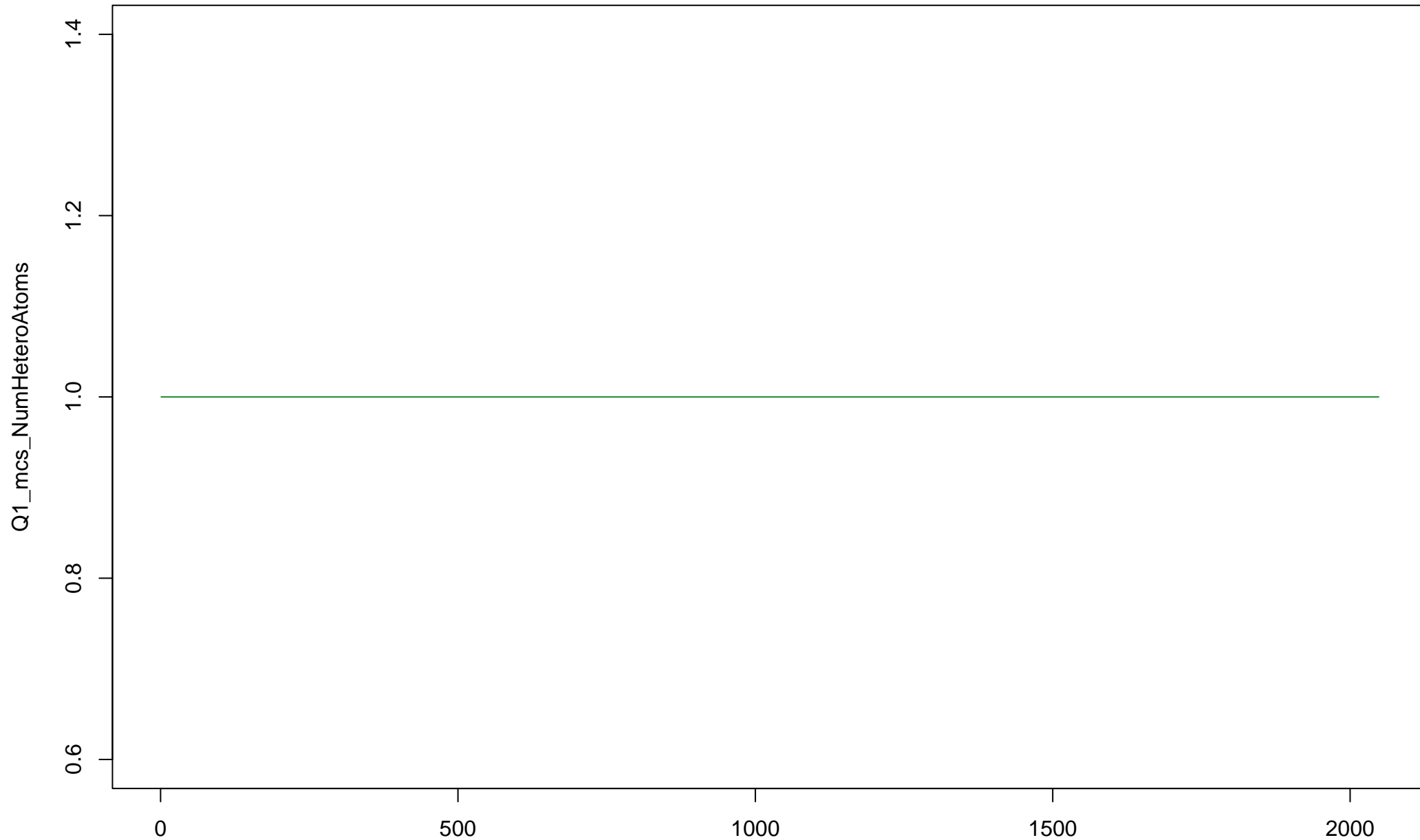
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



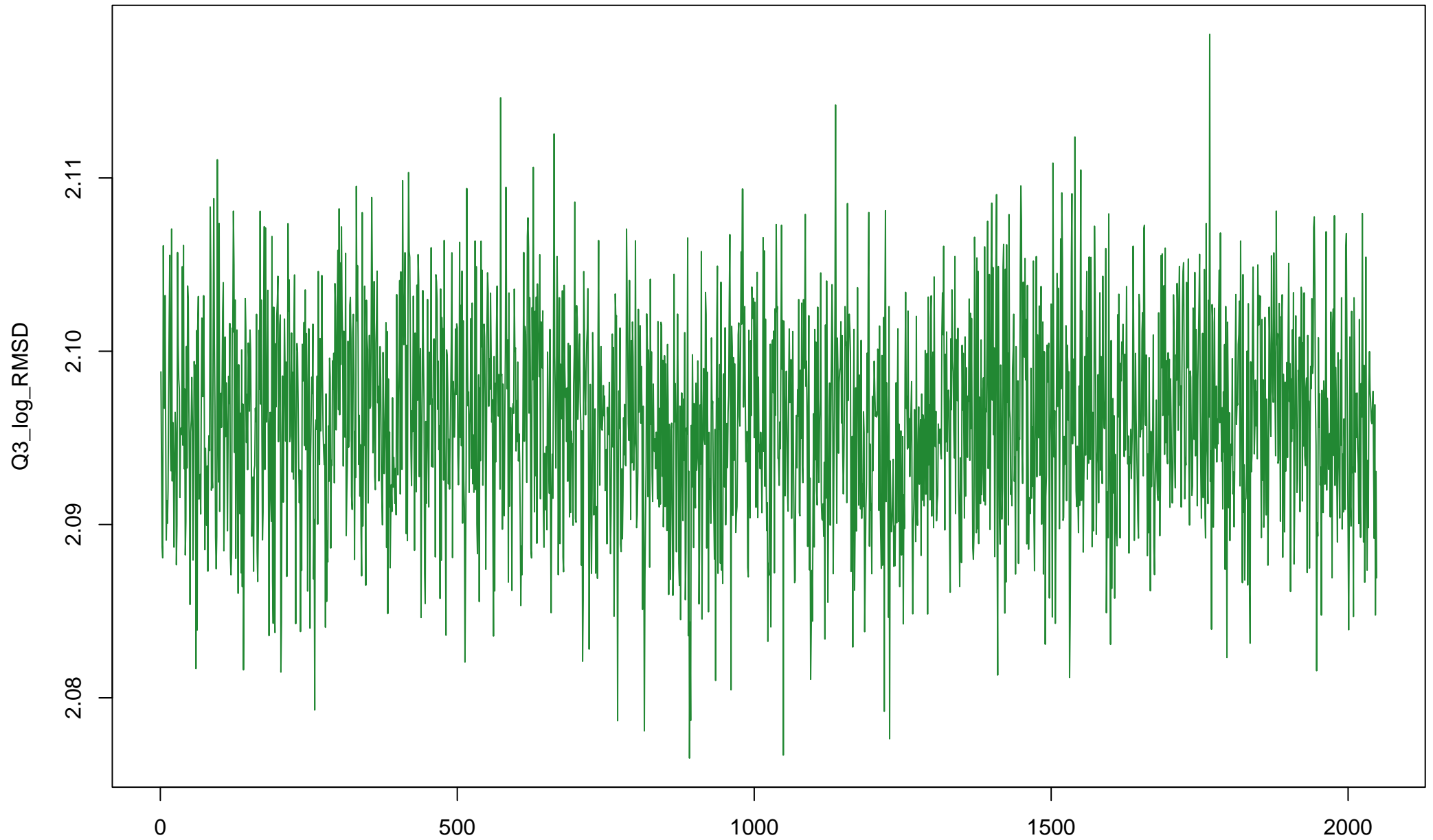
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



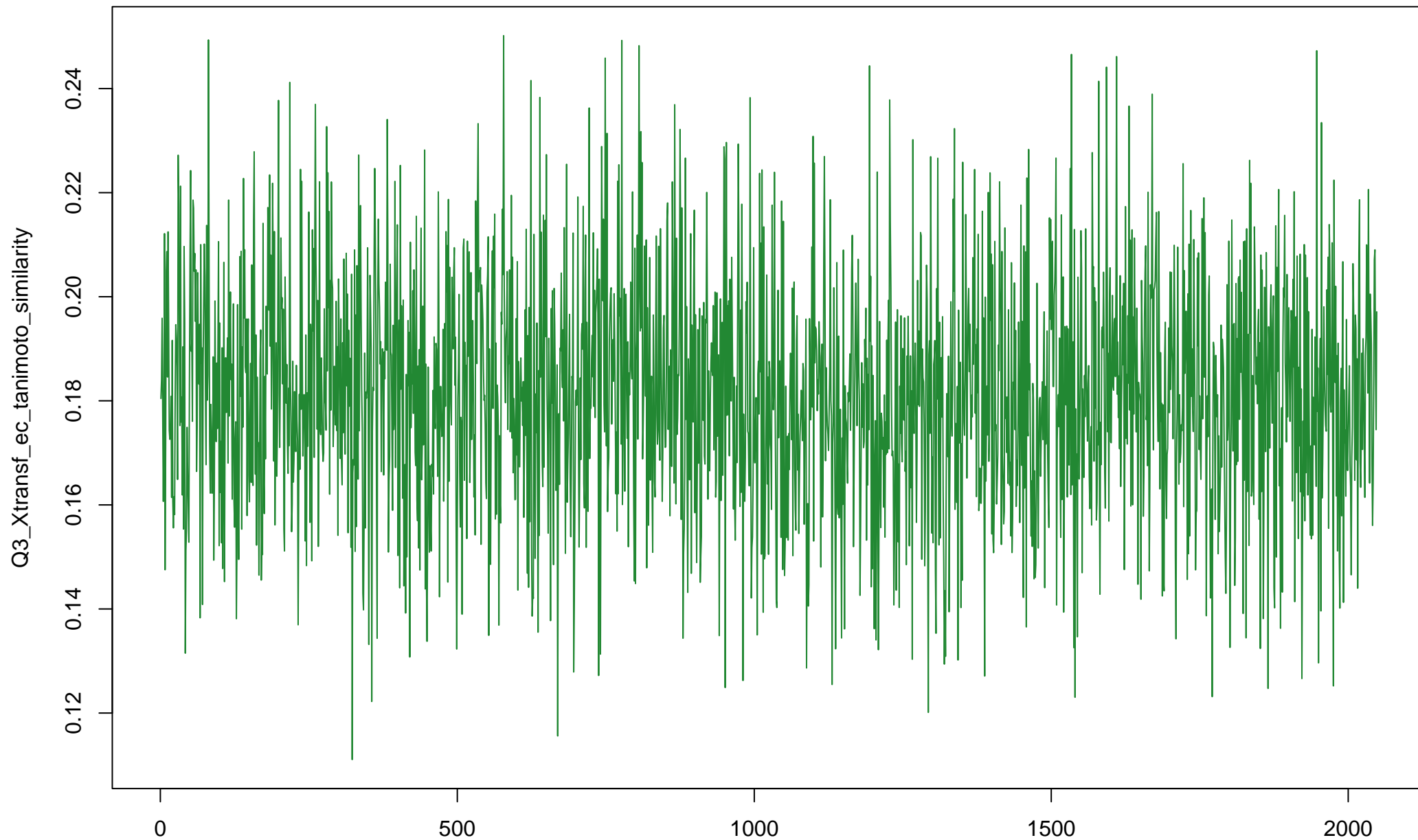
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



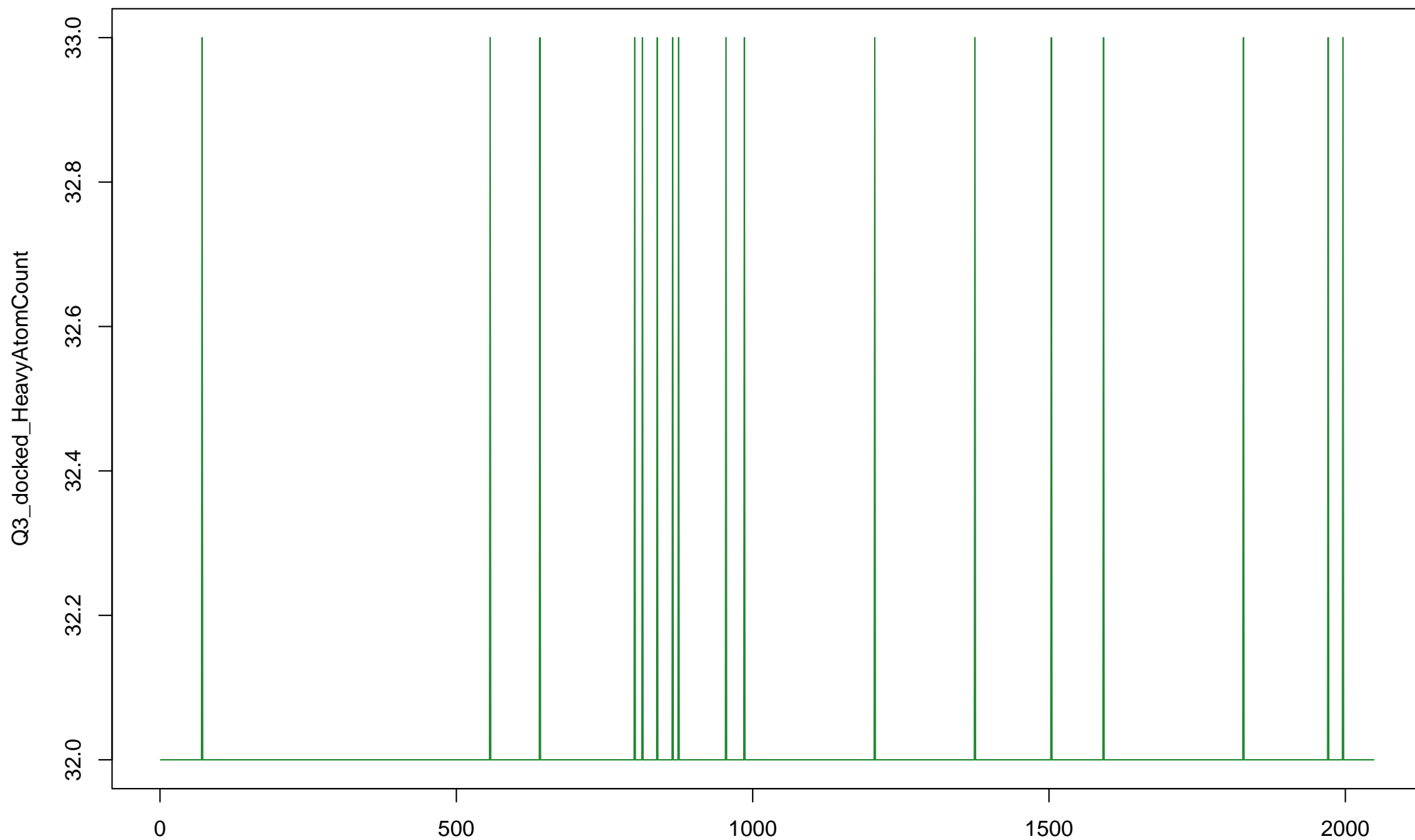
Q3_log_RMSD
ESS = 1670 | BMK = 0.0397 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 1630 | BMK = 0.0528 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0



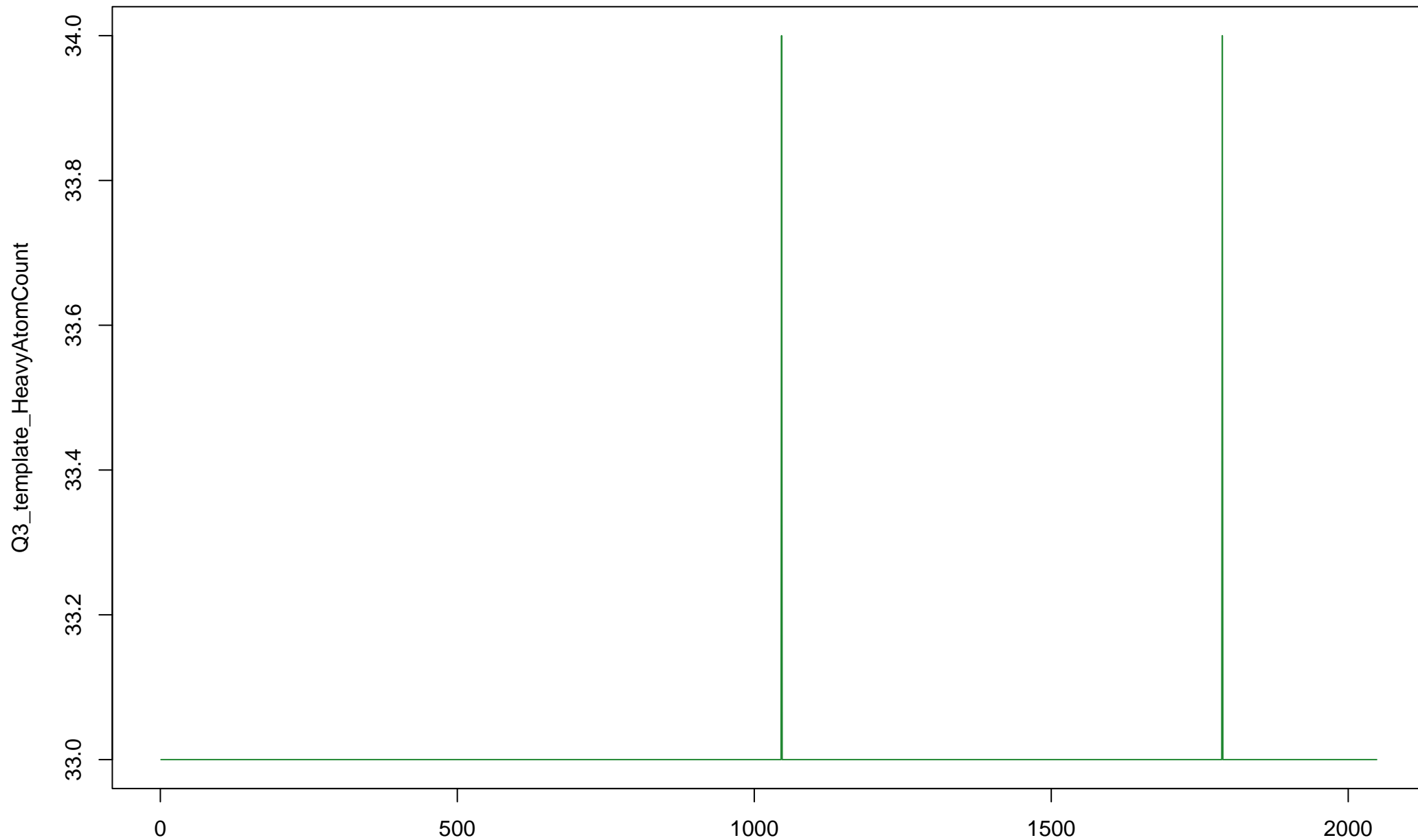
Q3_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.063 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 408



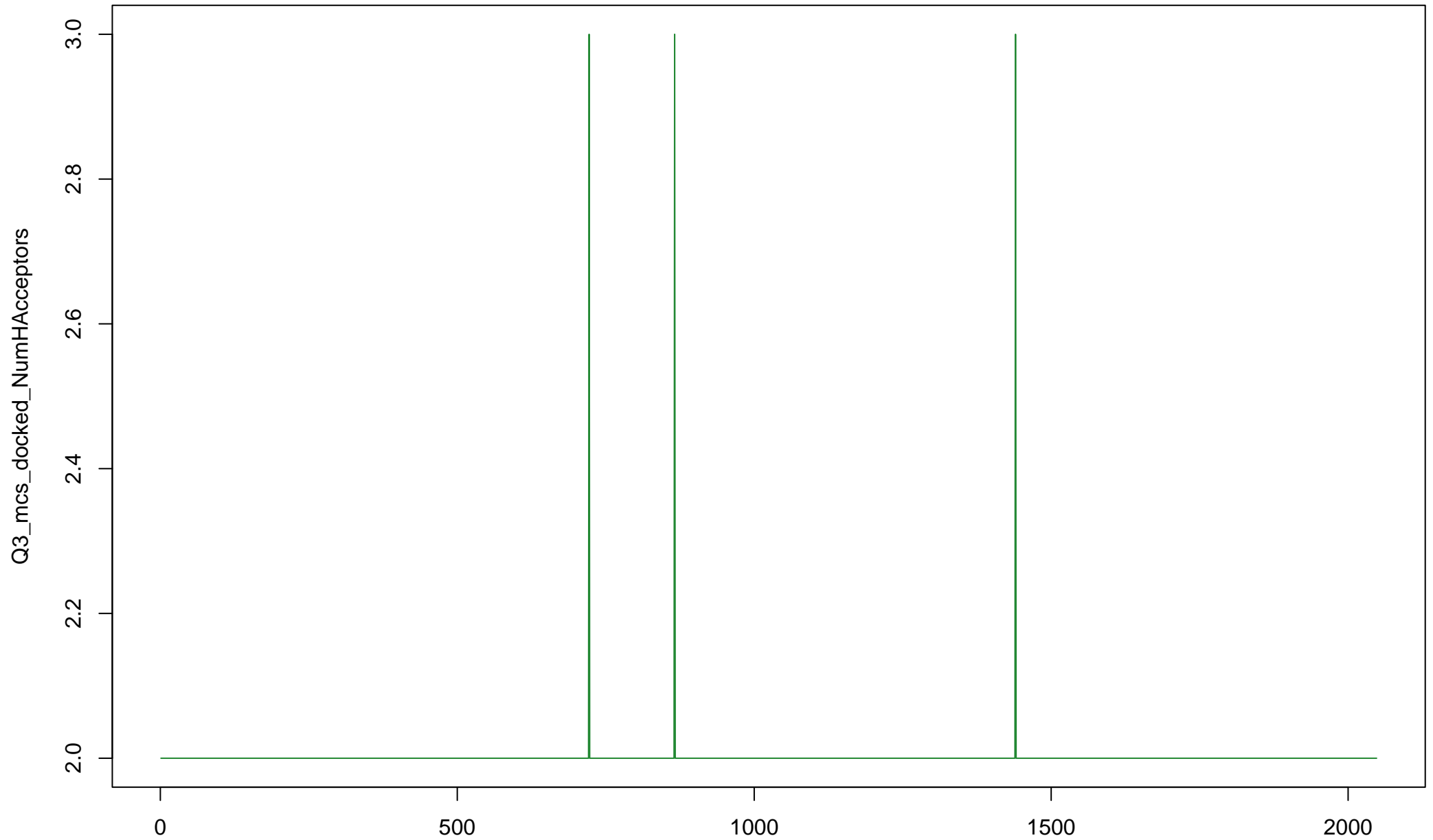
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



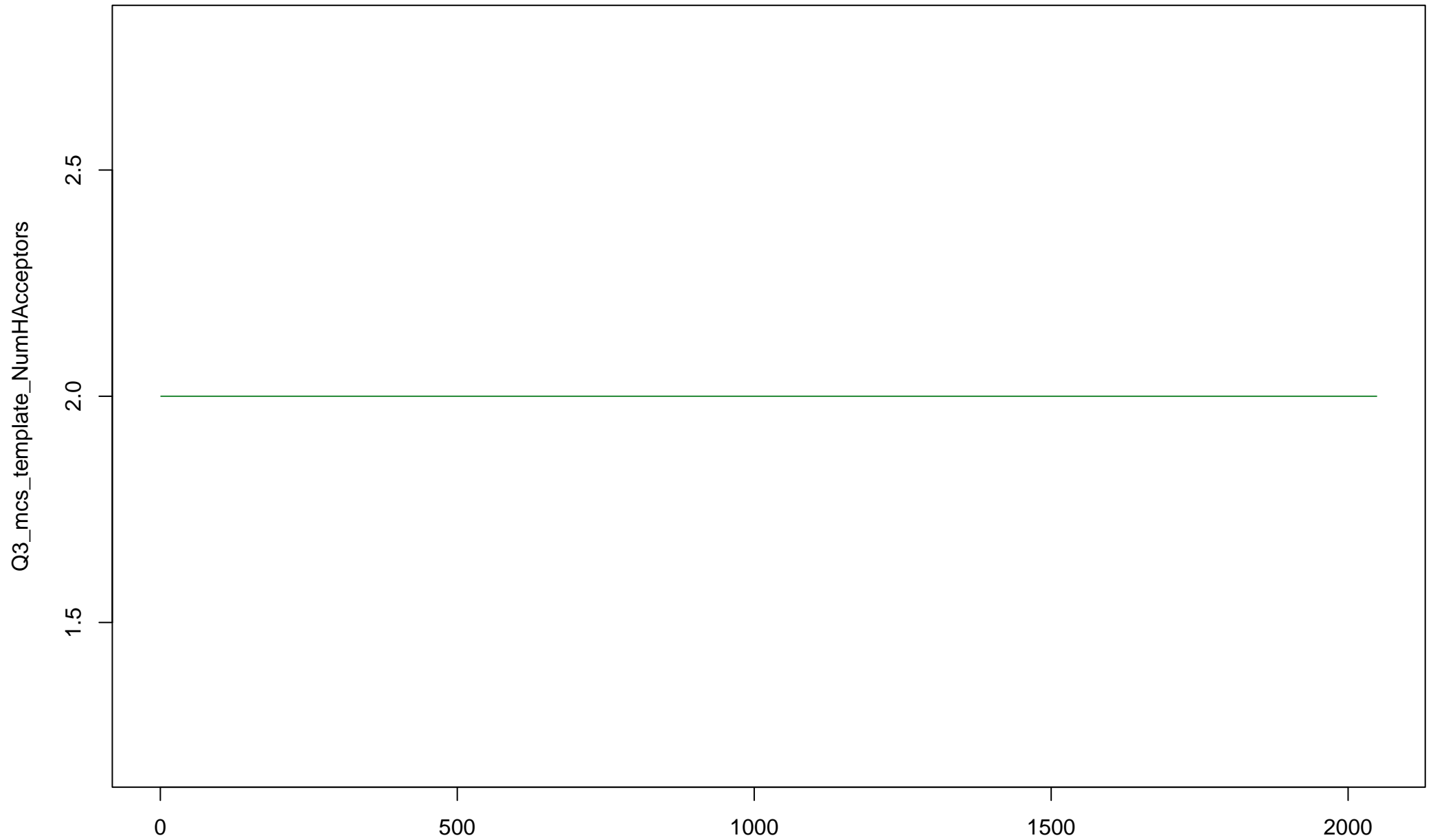
Q3_template_HeavyAtomCount
ESS = 2050 | BMK = 0.509 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 2040



Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 1632



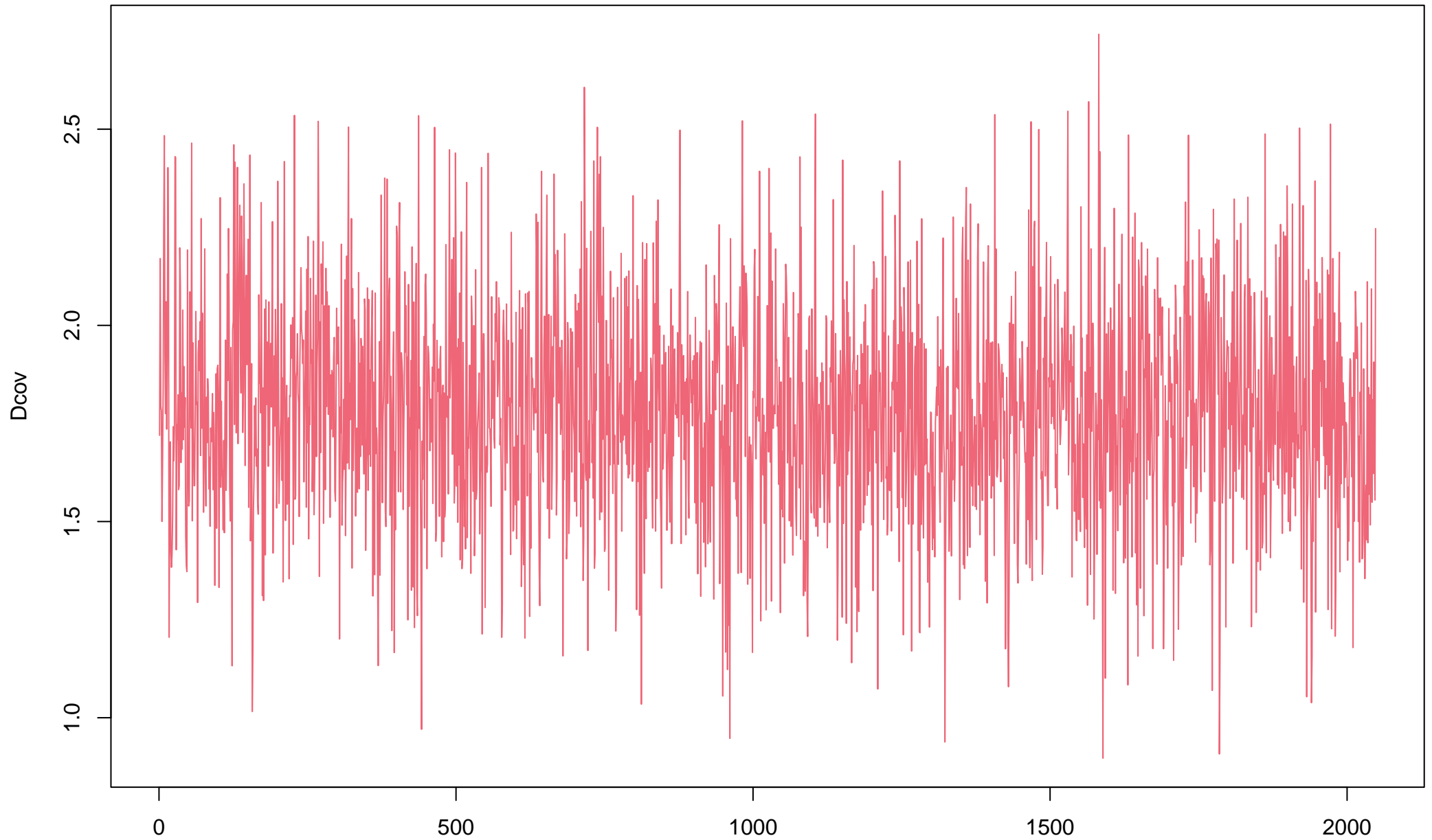
Q3_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



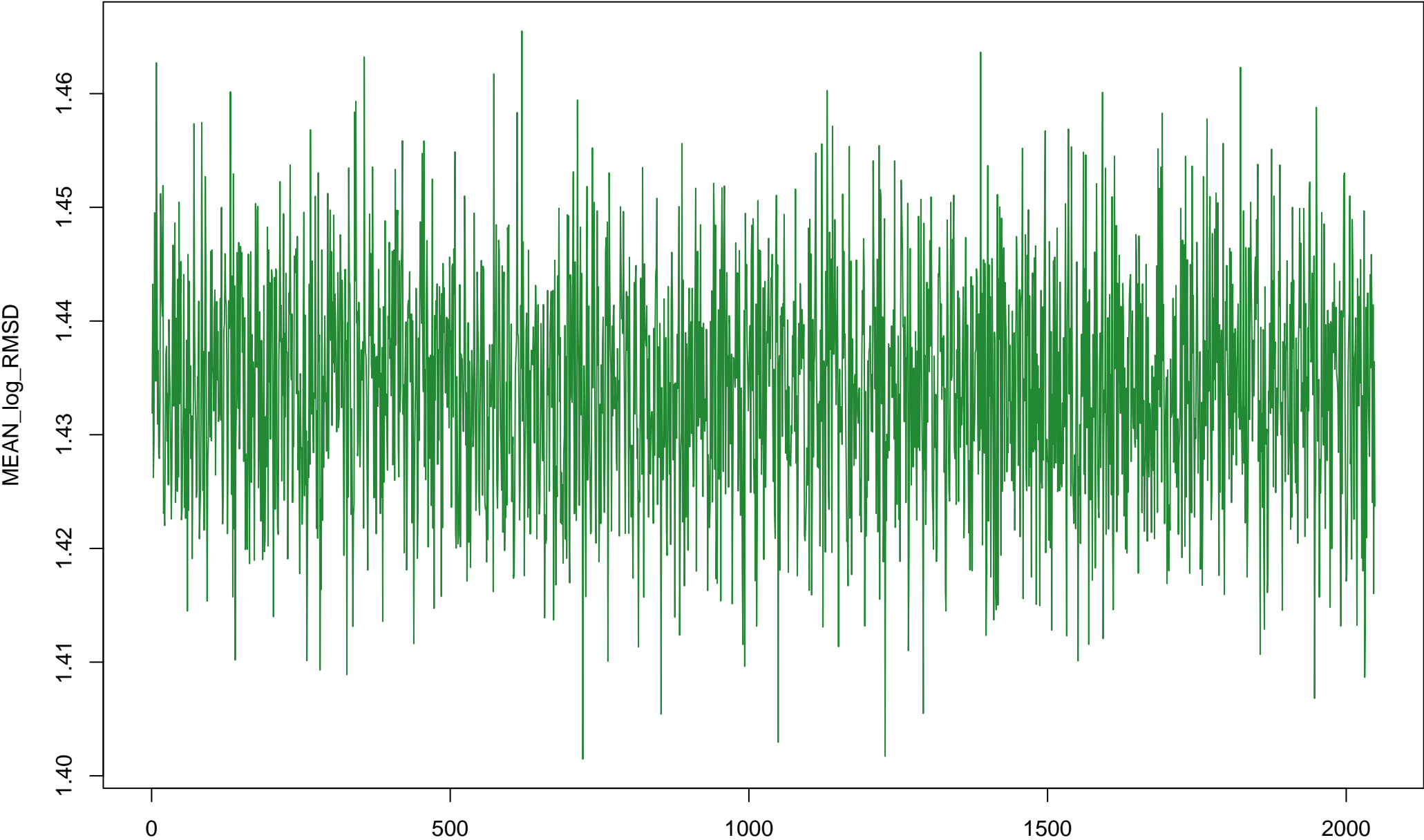
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



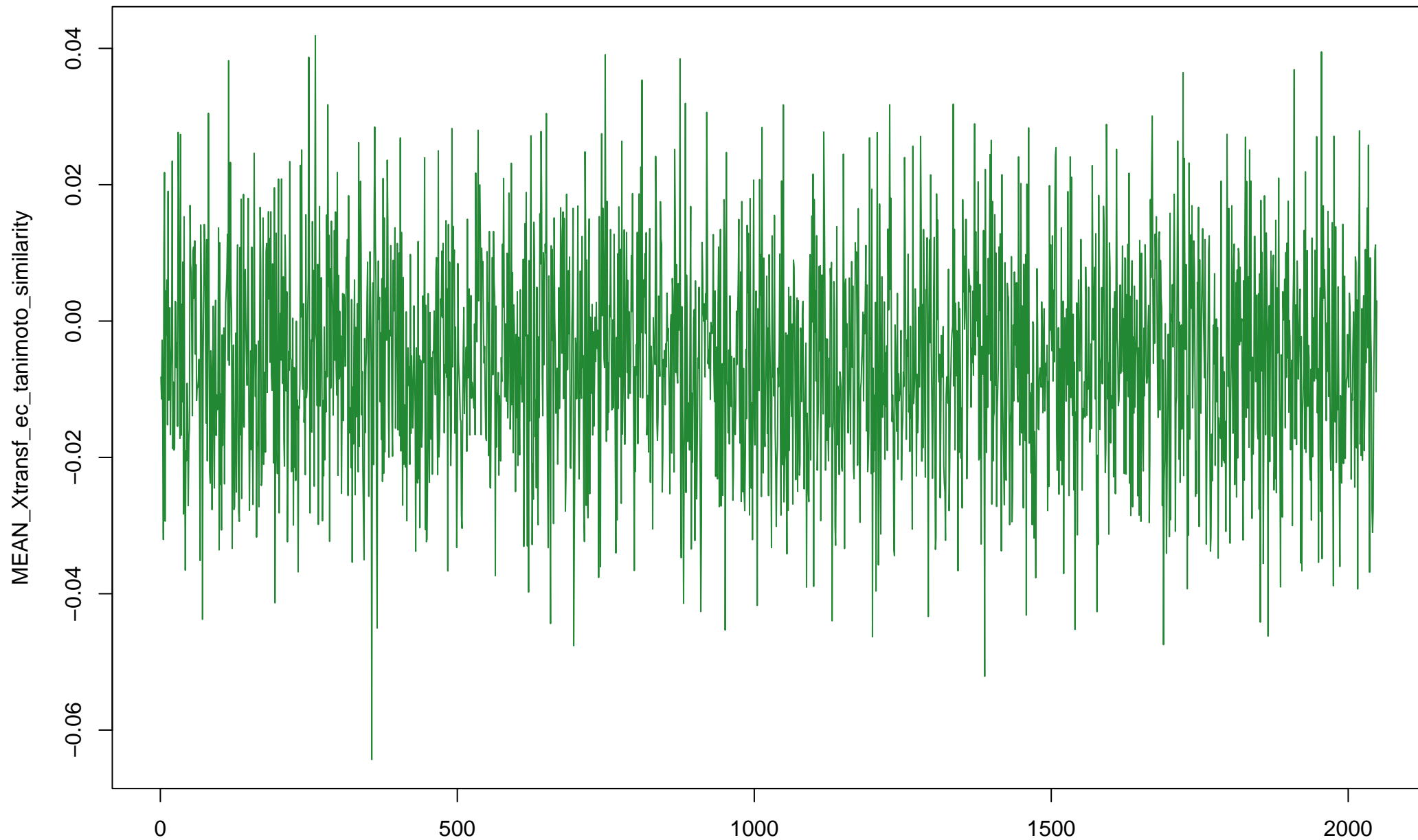
Dcov
ESS = 2050 | BMK = 0.0578 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0



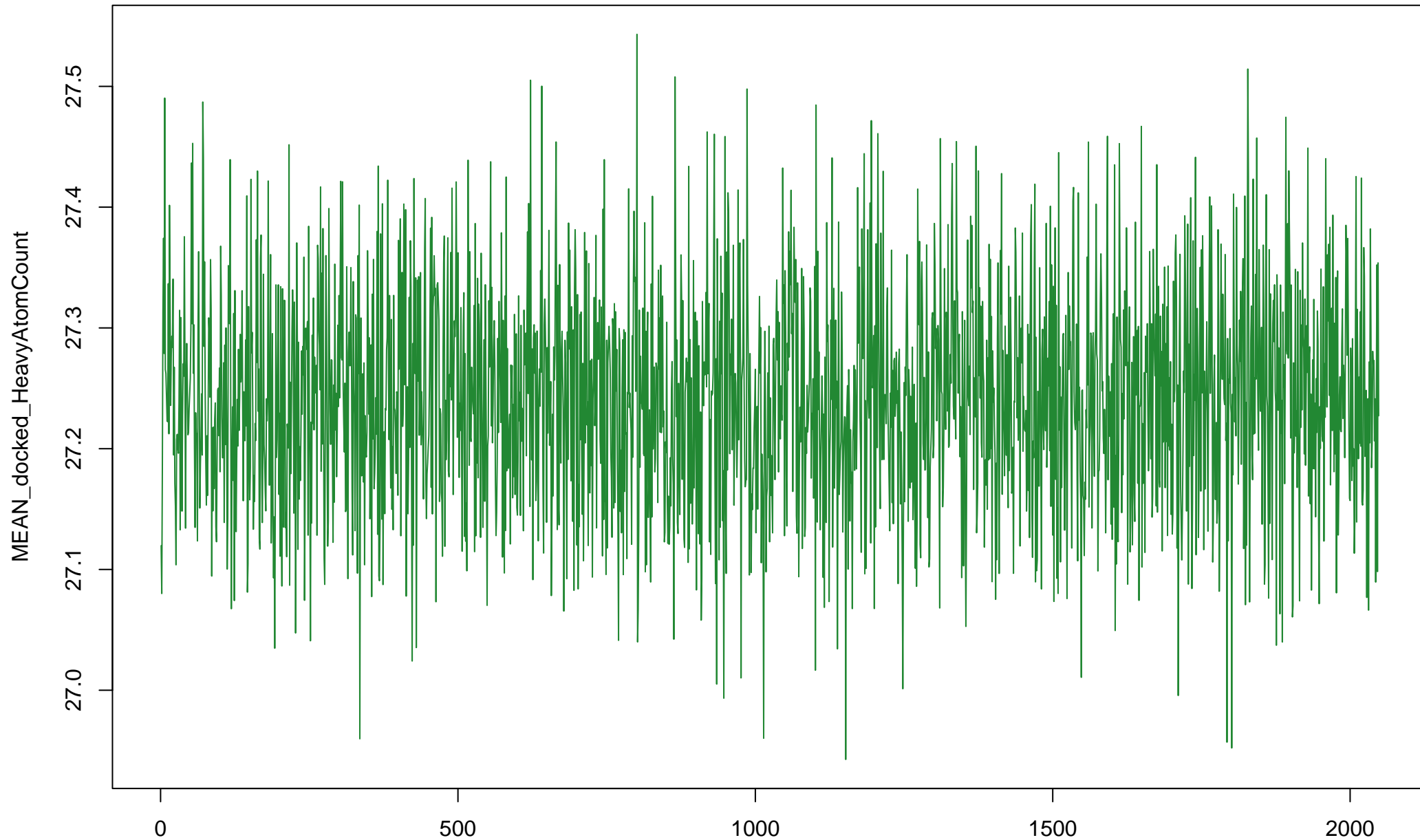
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0337 | MCSE(6.27) = 1.5 | stat: TRUE | burn: 0



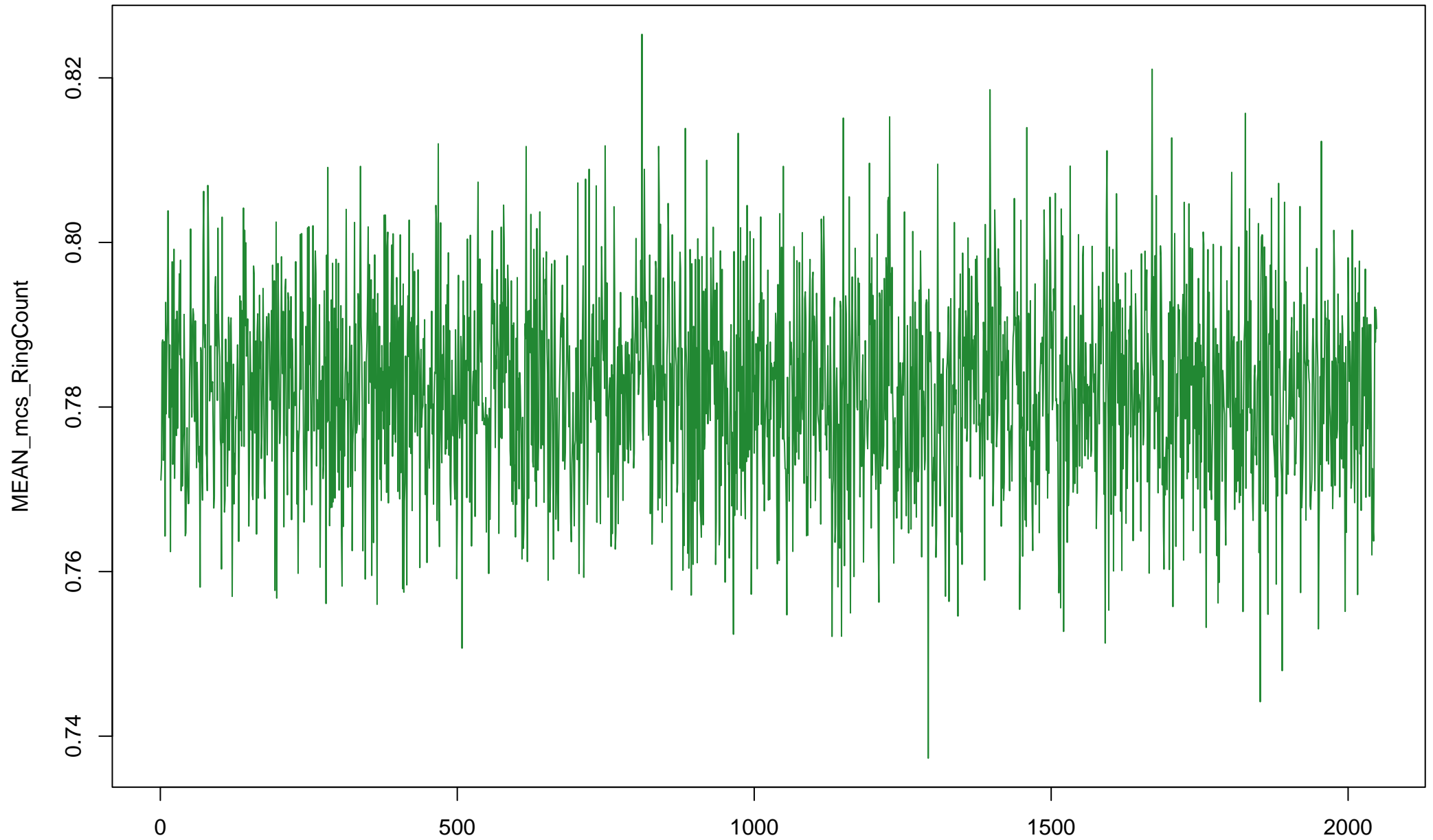
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0341 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0



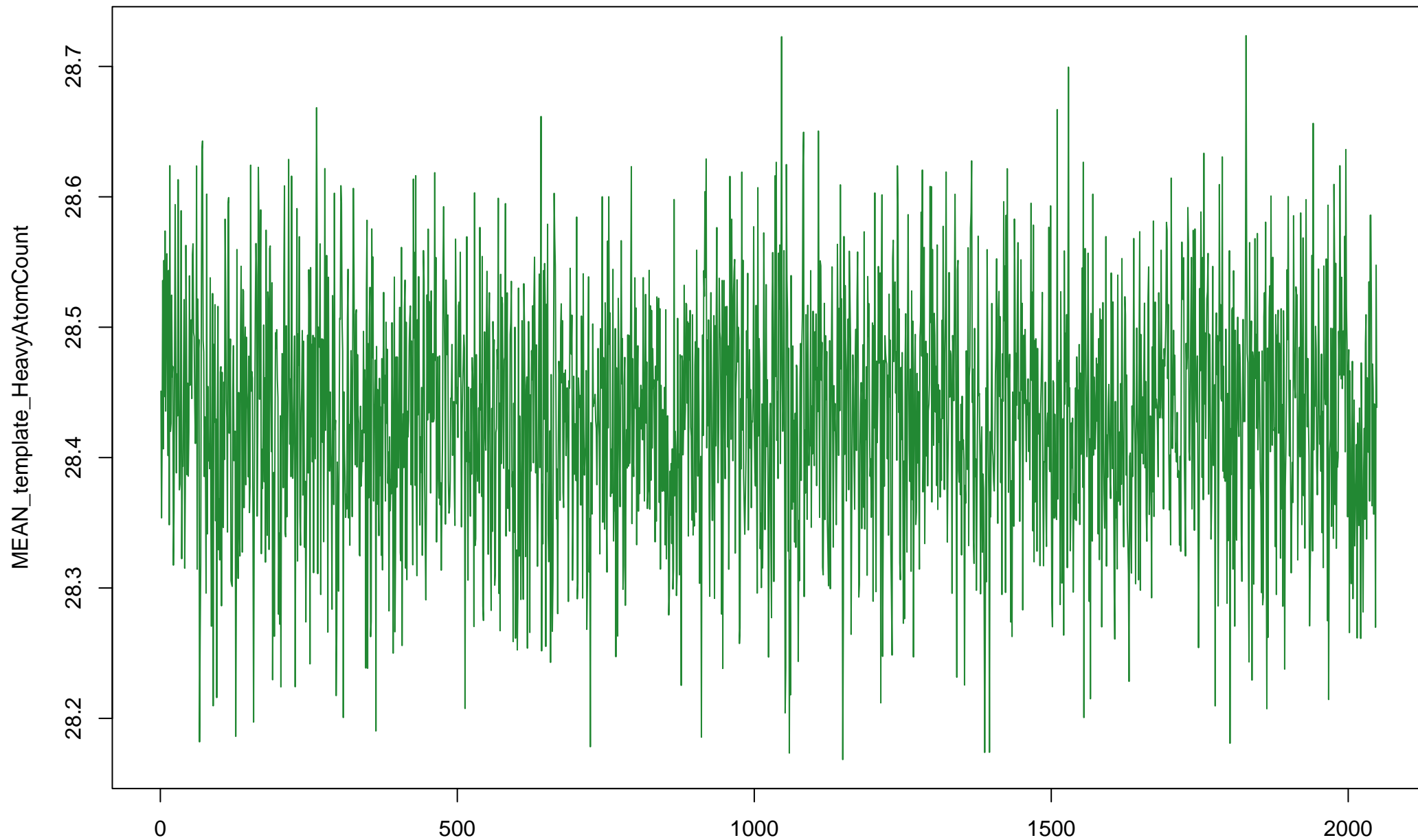
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0381 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0



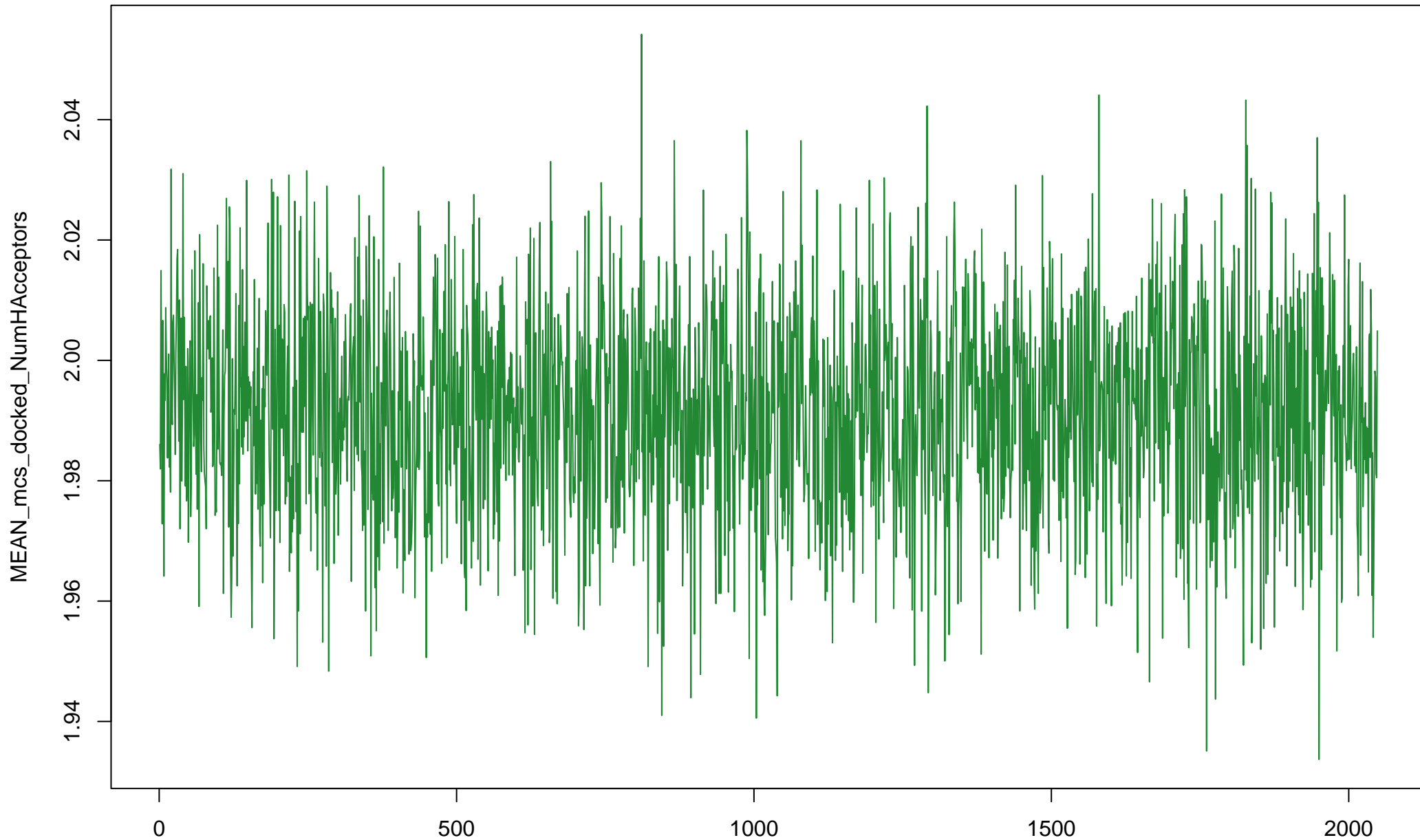
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0529 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0



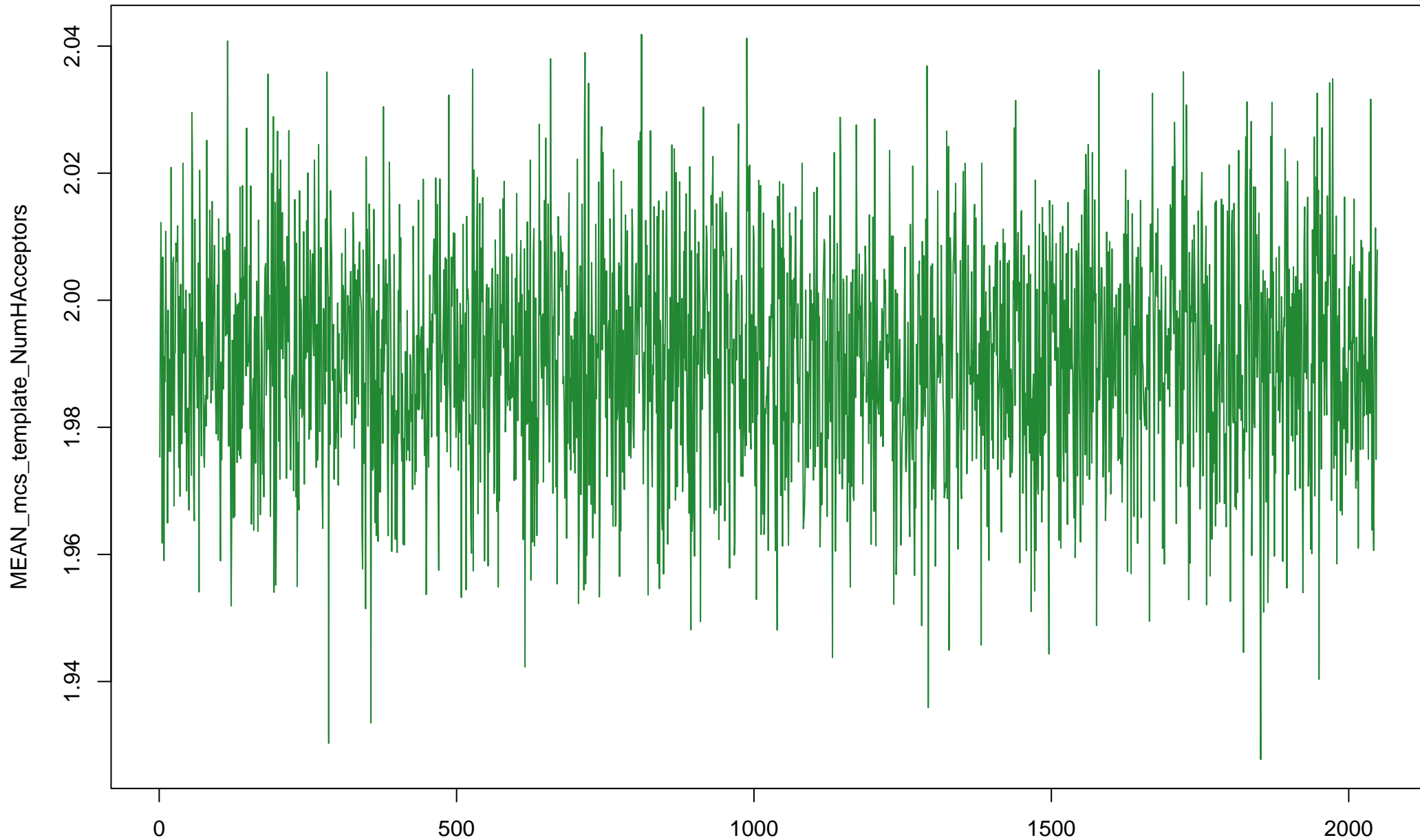
MEAN_template_HeavyAtomCount
ESS = 1920 | BMK = 0.0364 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



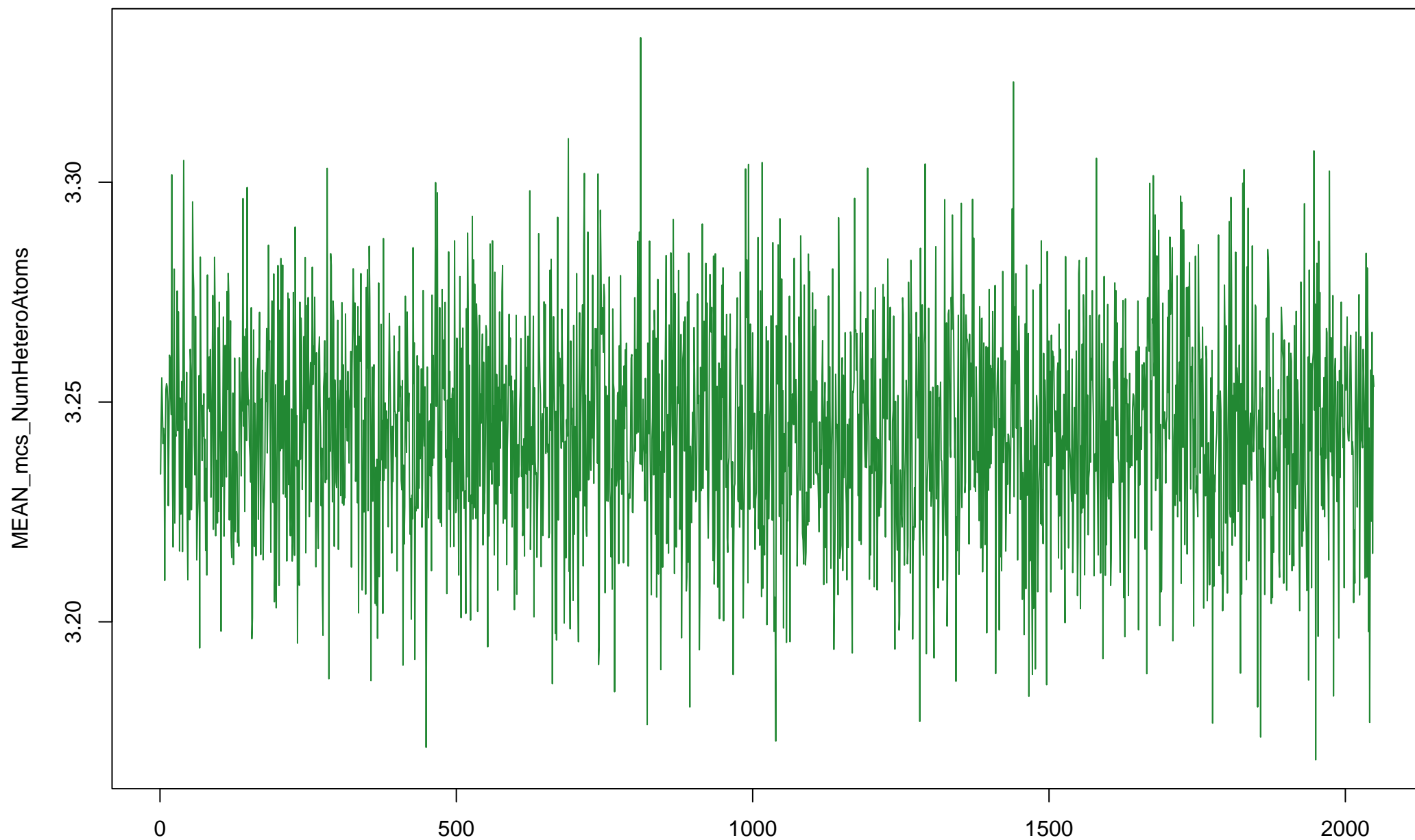
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0277 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



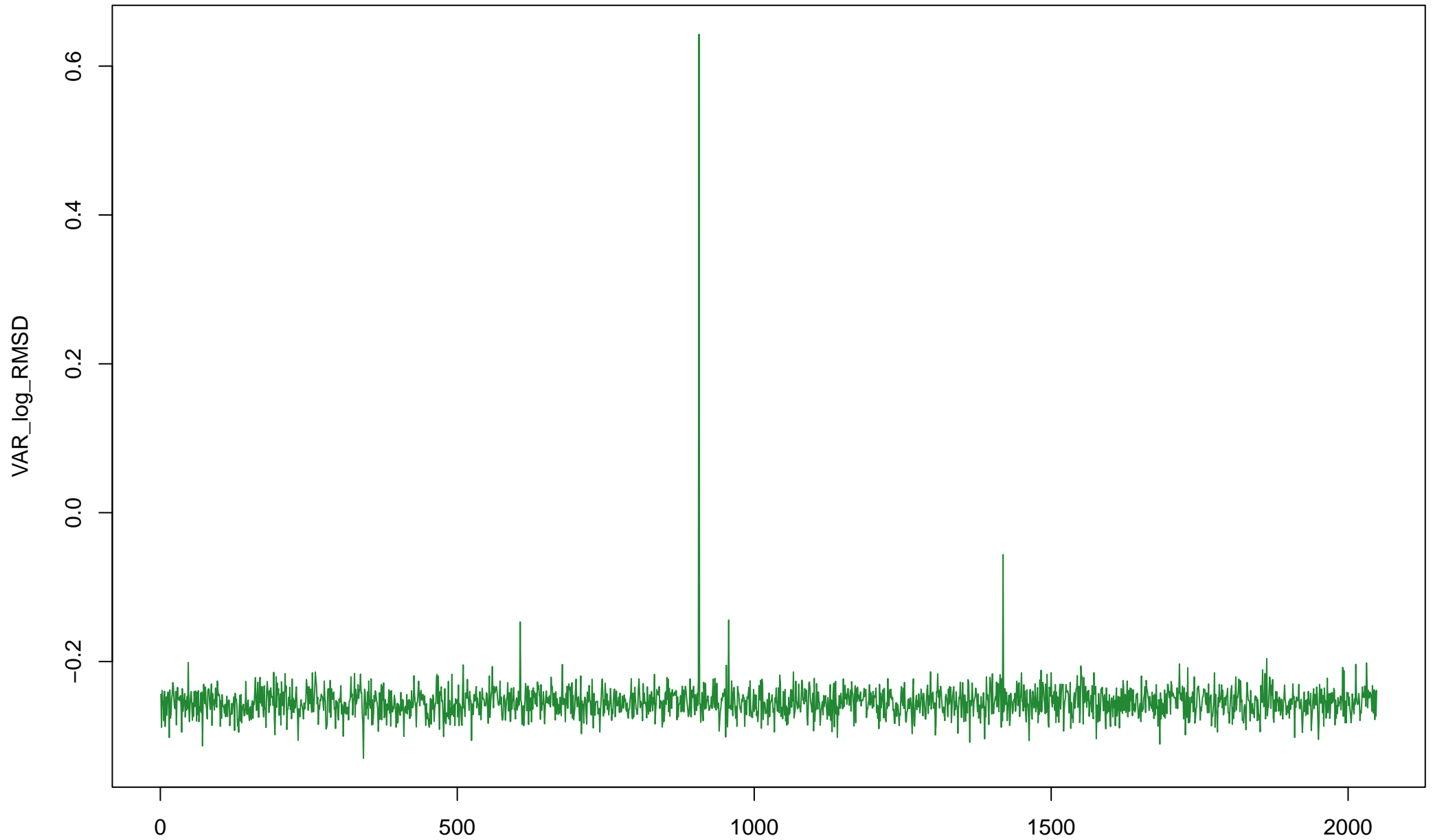
MEAN_mcs_template_NumHAcceptors
ESS = 1970 | BMK = 0.0339 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



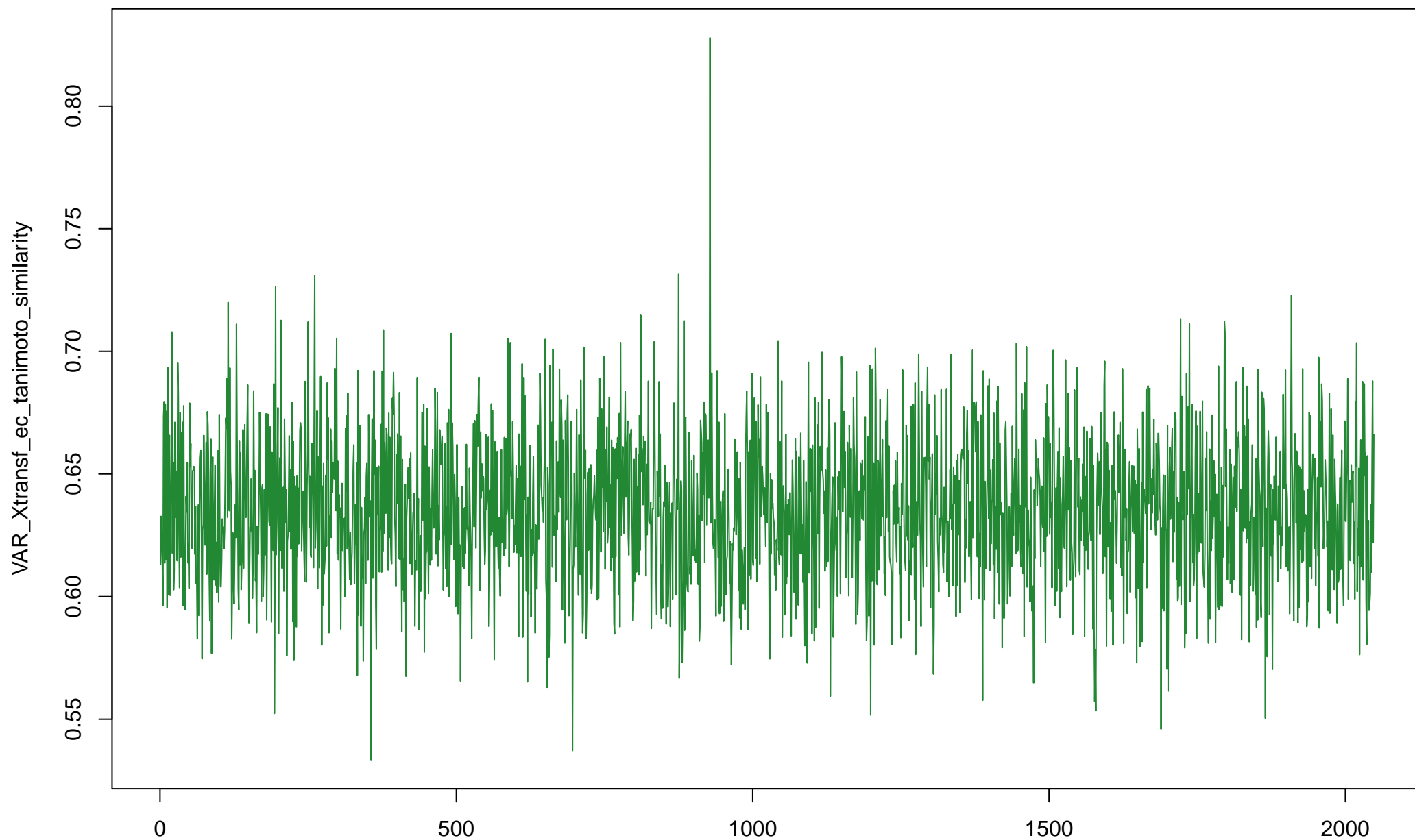
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0356 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



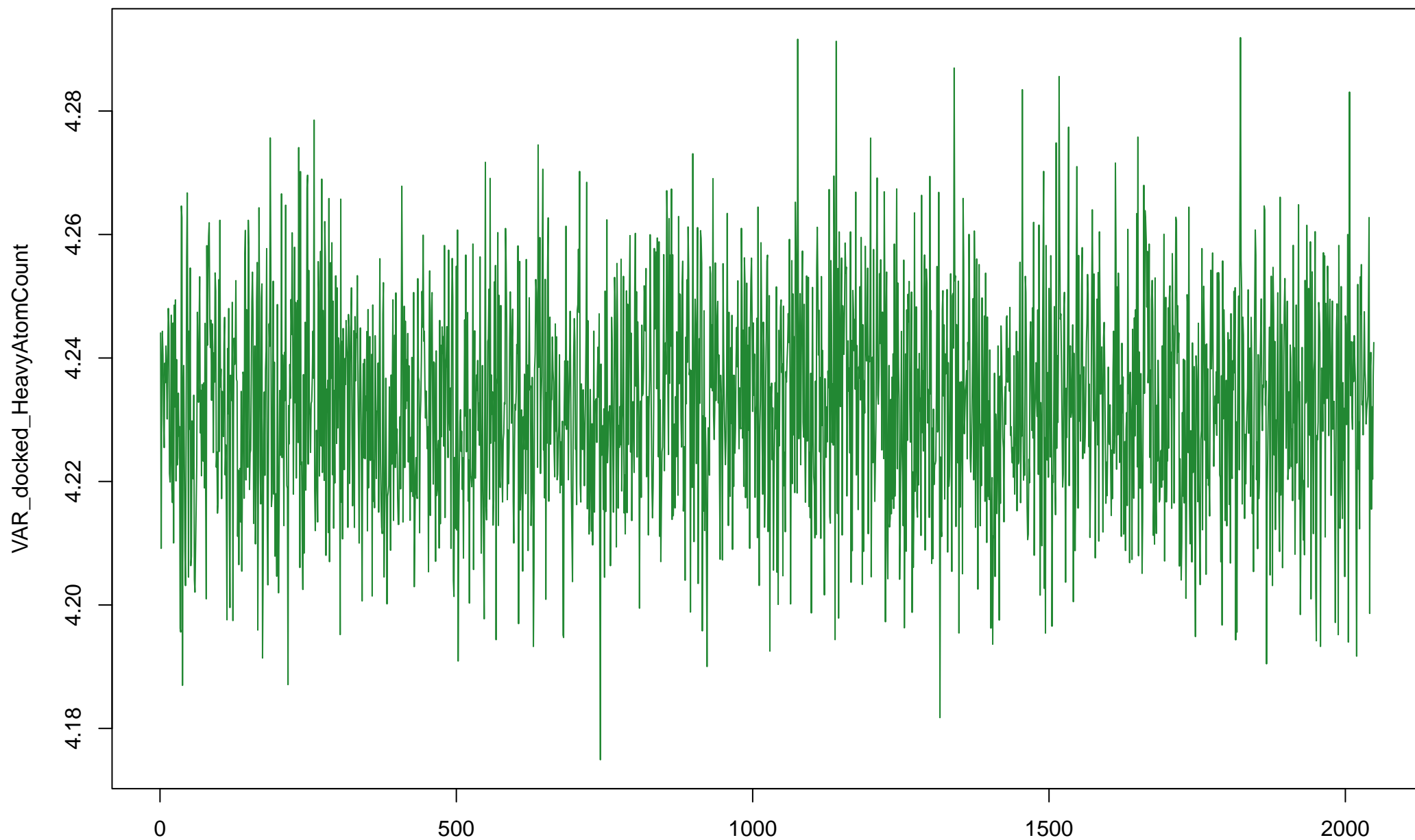
VAR_log_RMSD
ESS = 2050 | BMK = 0.0634 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0



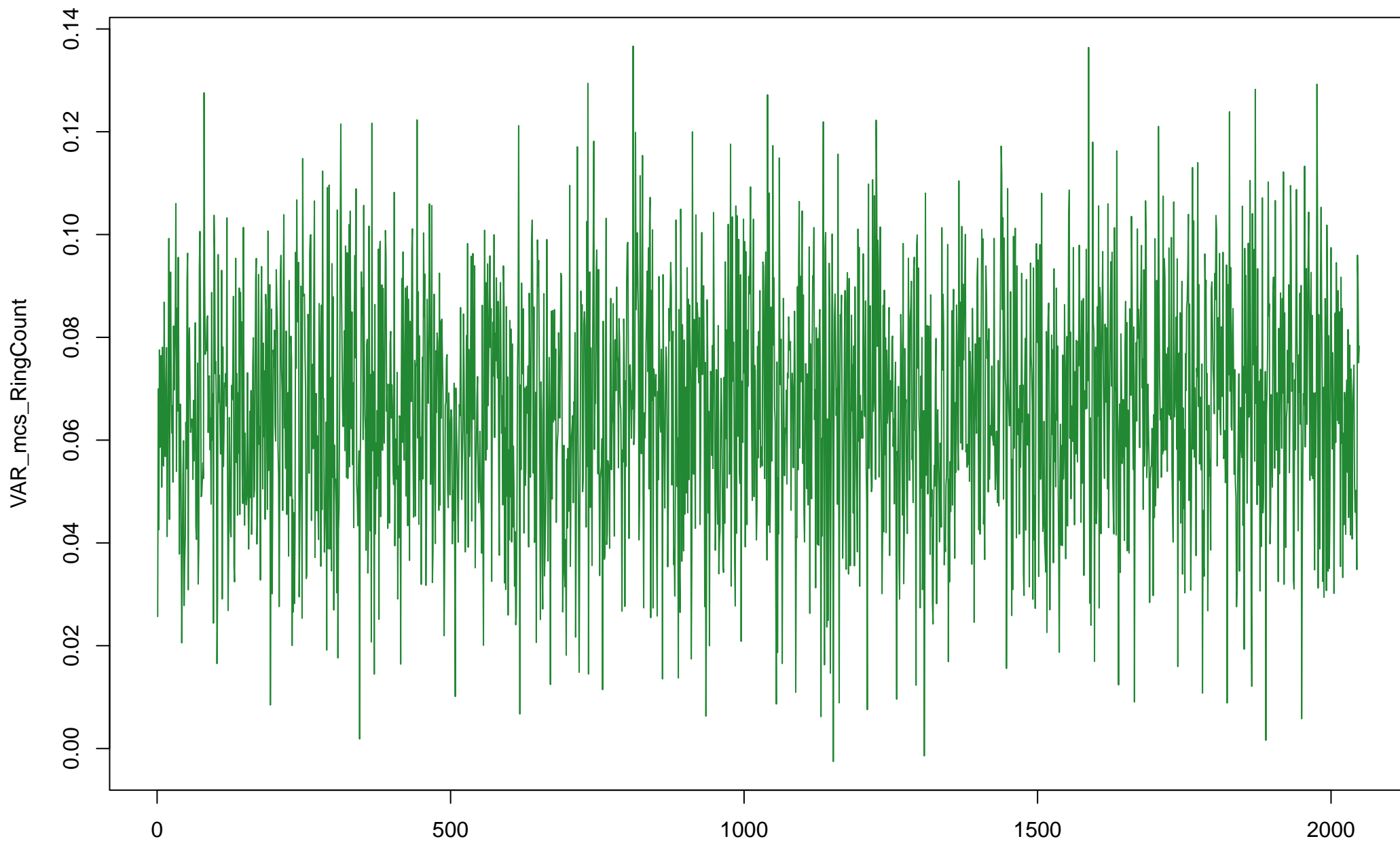
VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0526 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0



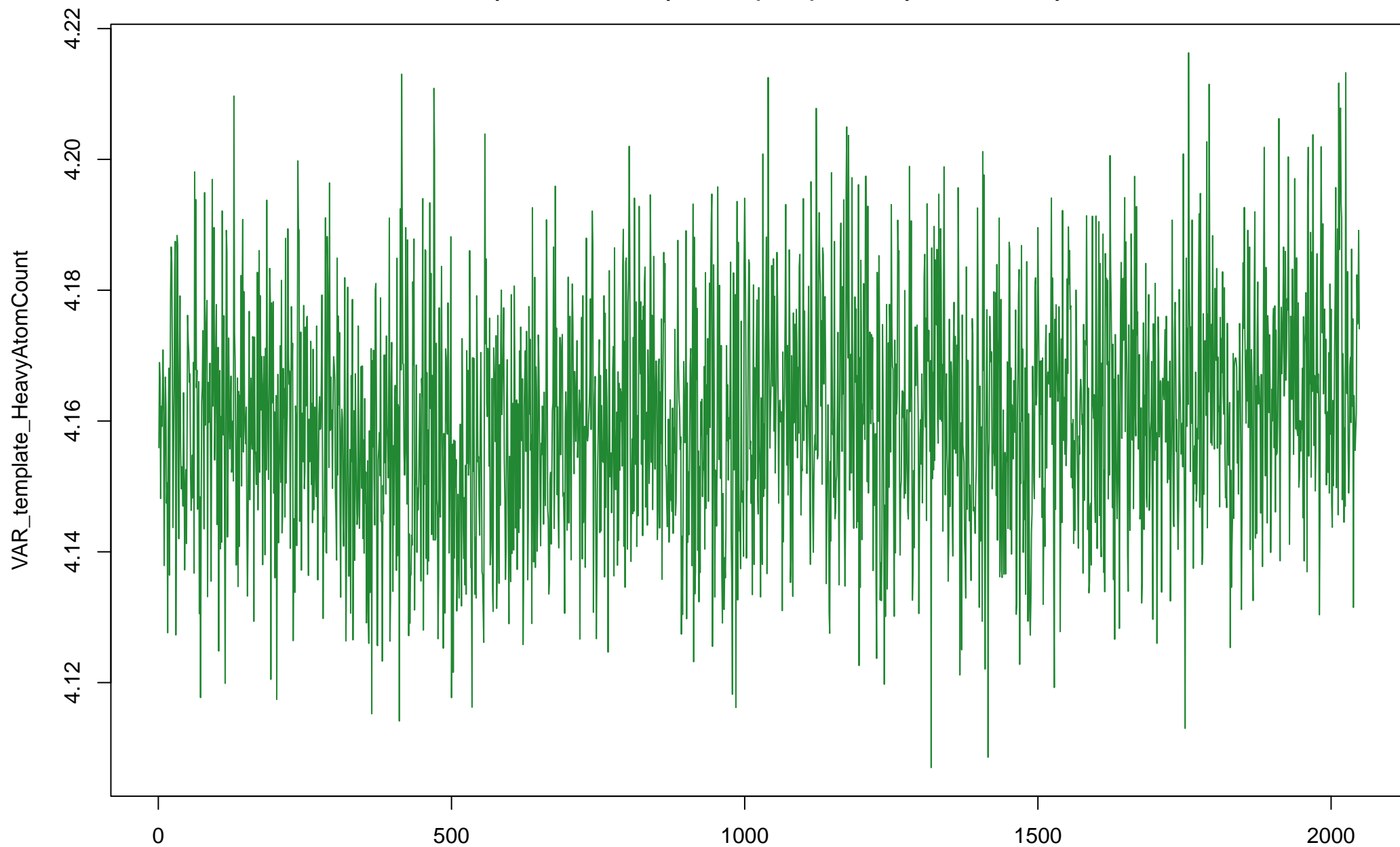
VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0525 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



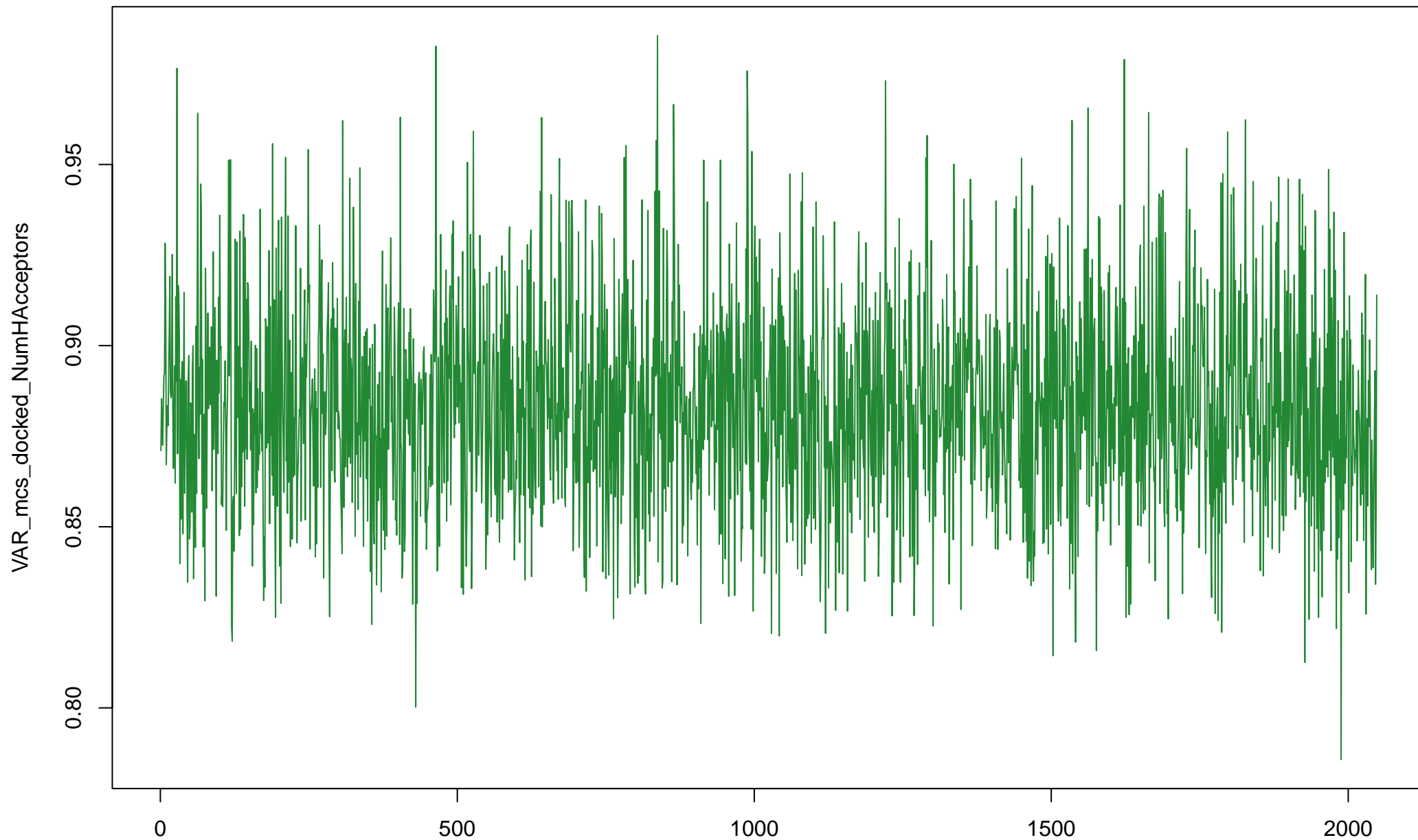
VAR_mcs_RingCount
ESS = 1890 | BMK = 0.0419 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



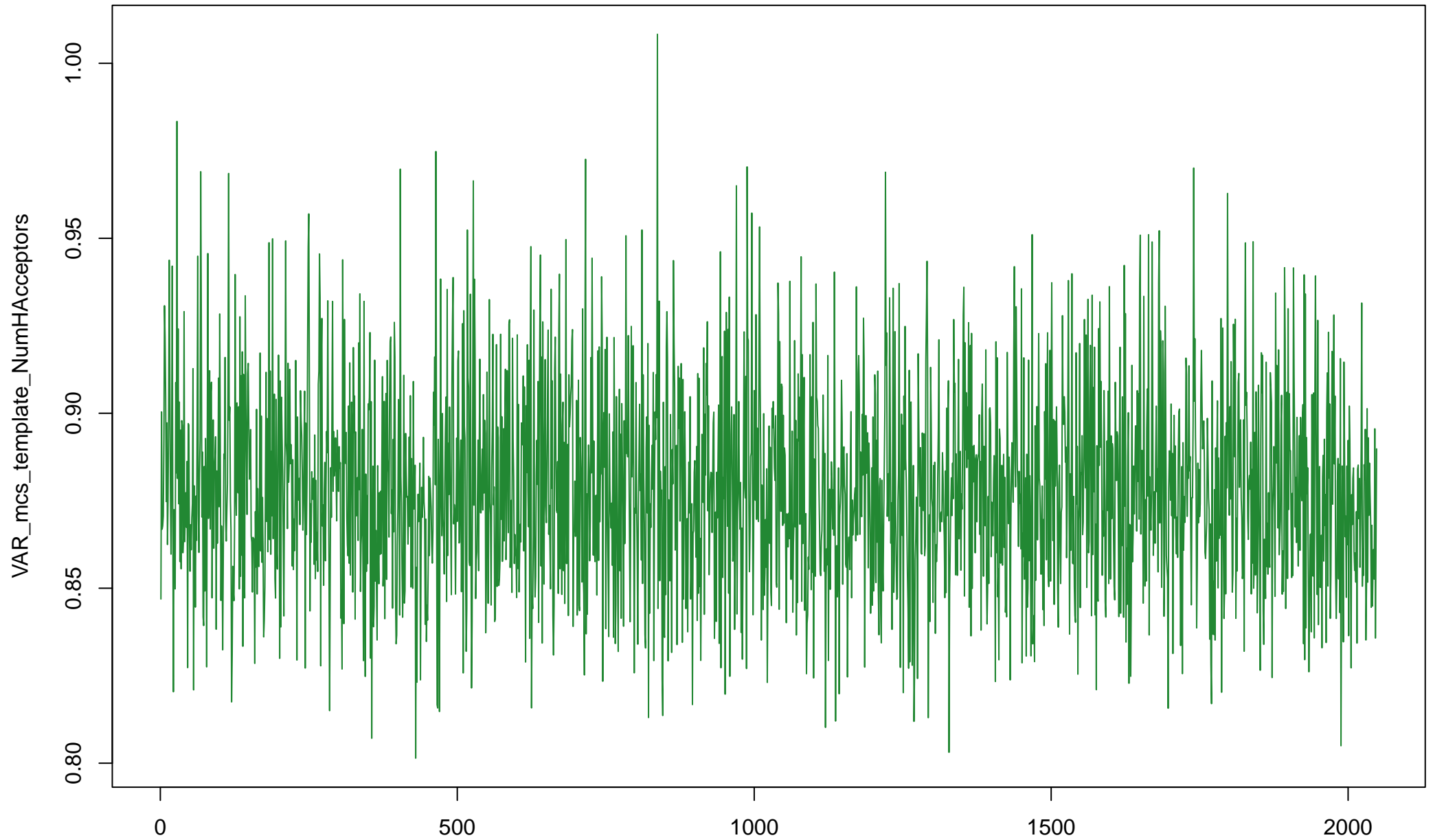
VAR_template_HeavyAtomCount
ESS = 452 | BMK = 0.105 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0



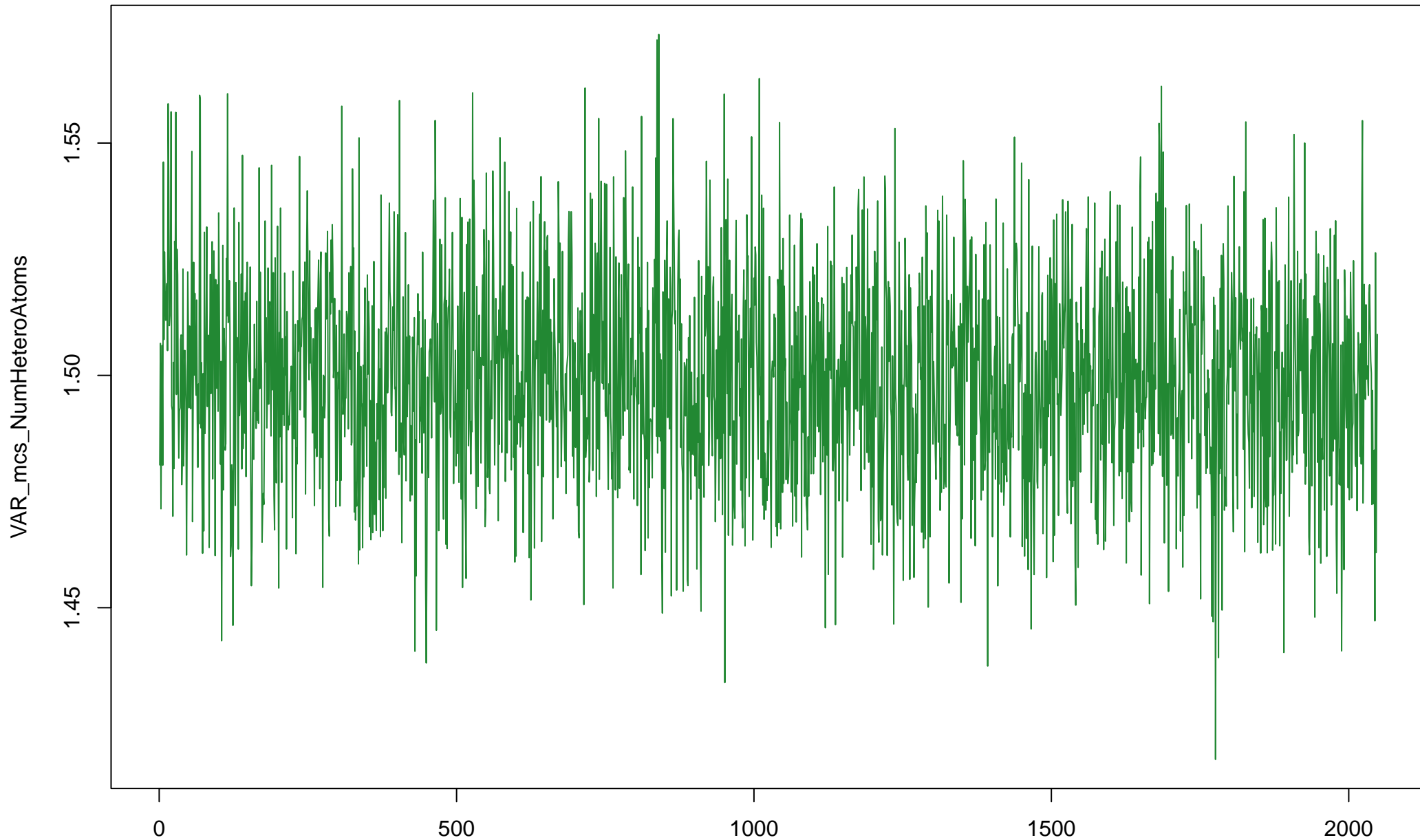
VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0428 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0



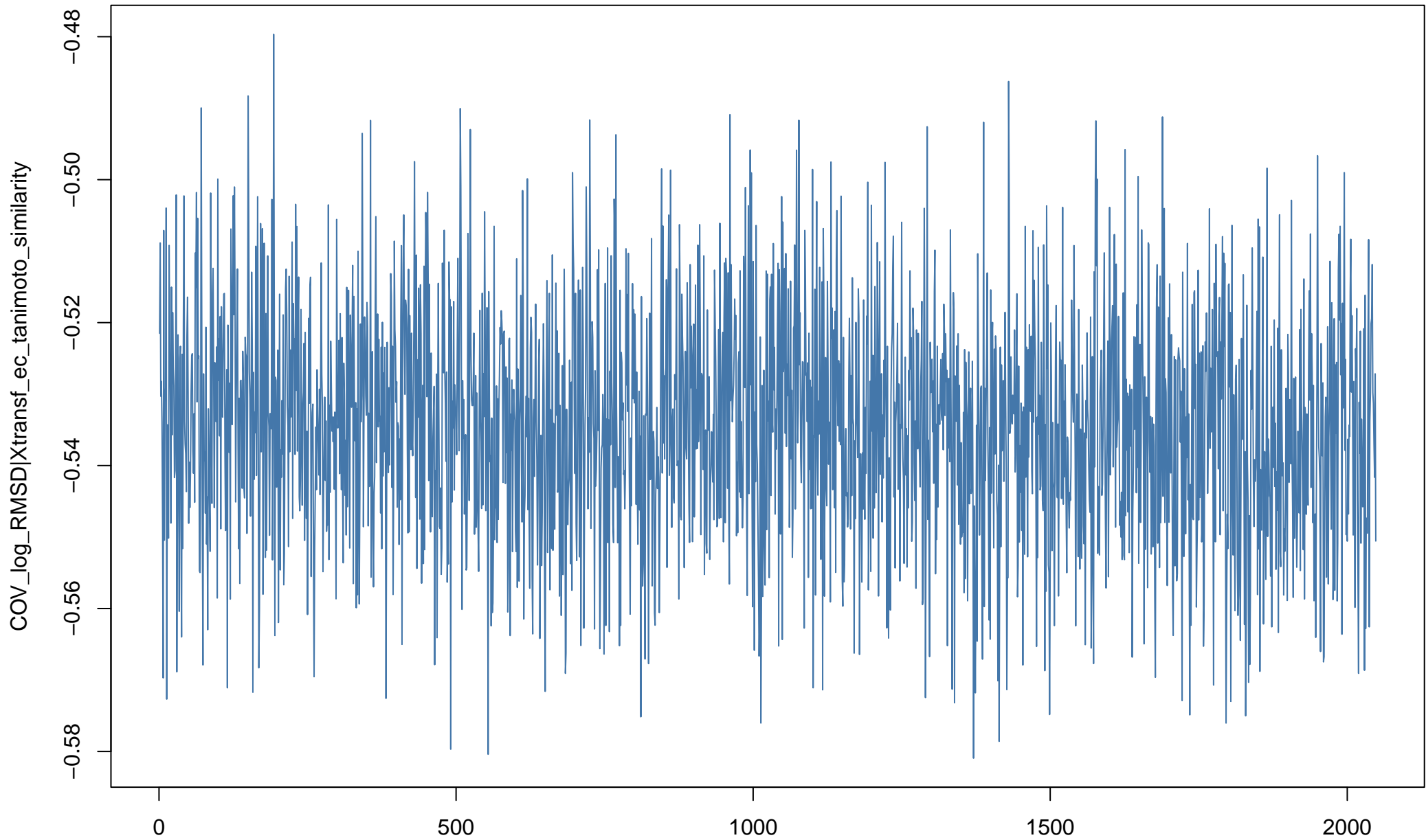
VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.053 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0



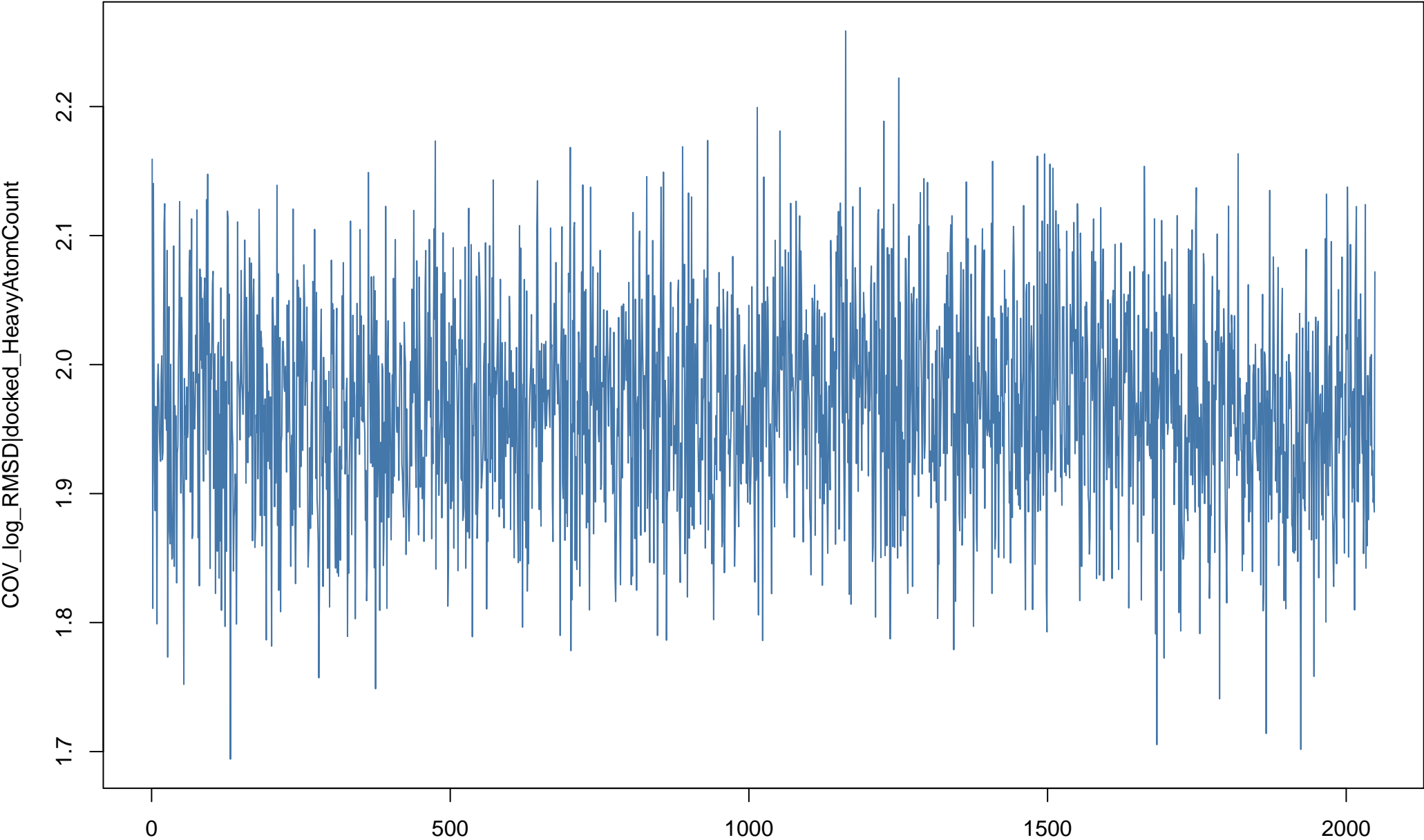
VAR_mcs_NumHeteroAtoms
ESS = 1810 | BMK = 0.0596 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



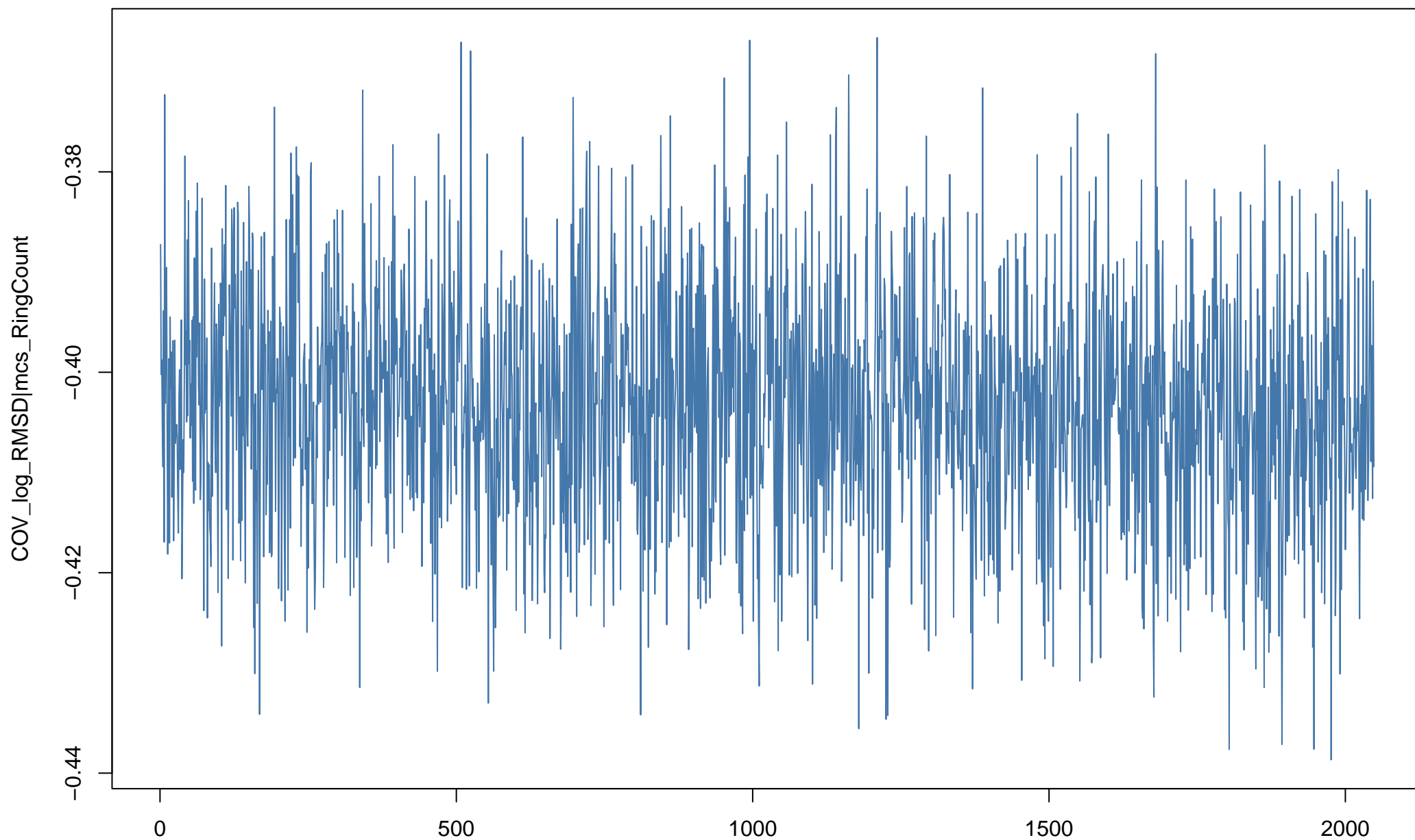
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1650 | BMK = 0.048 | MCSE(6.27) = 2.81 | stat: FALSE | burn: 0



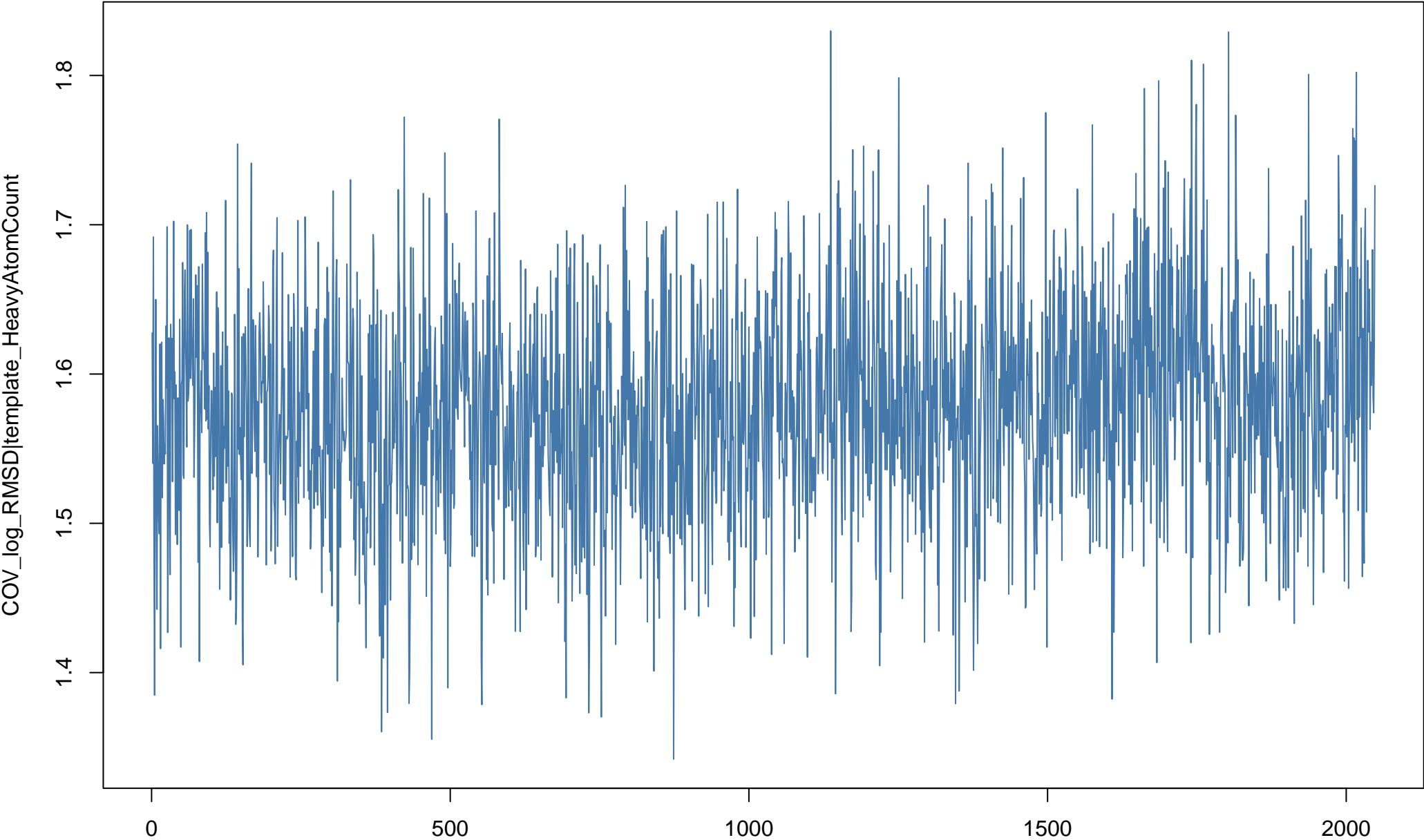
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1900 | BMK = 0.0481 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0



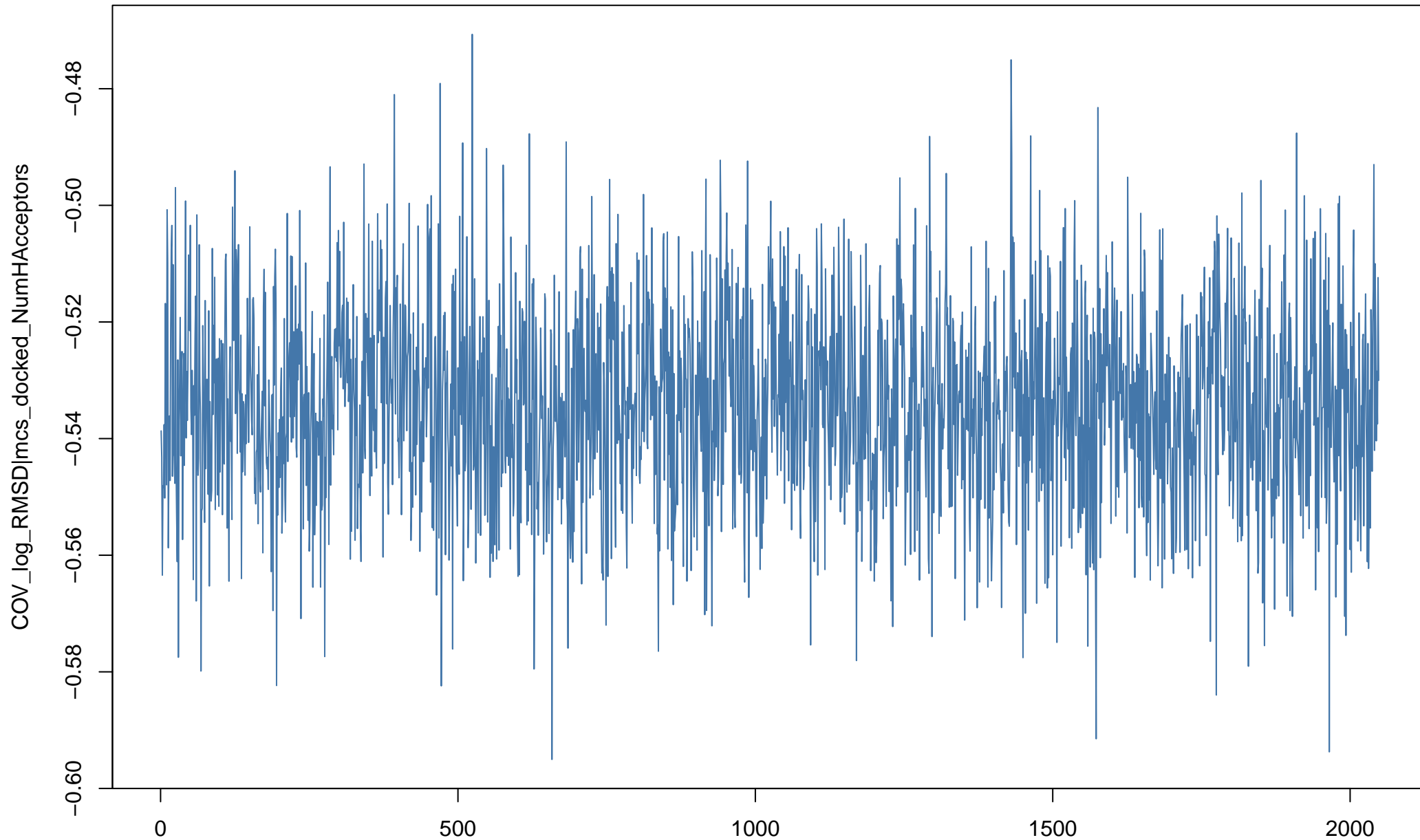
COV_log_RMSD|mcs_RingCount
ESS = 1770 | BMK = 0.0609 | MCSE(6.27) = 2.52 | stat: FALSE | burn: 0



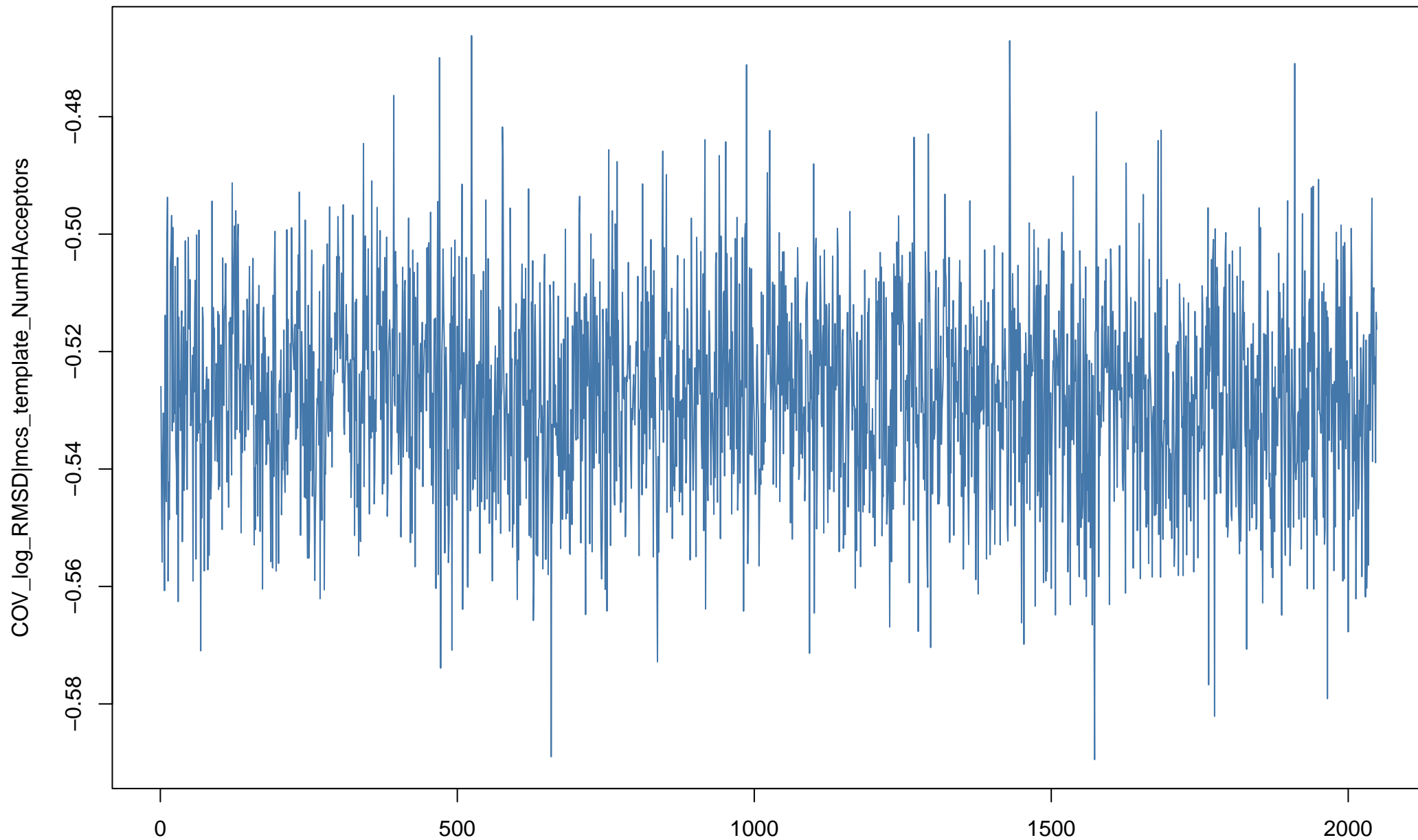
COV_log_RMSD|template_HeavyAtomCount
ESS = 680 | BMK = 0.118 | MCSE(6.27) = 3.73 | stat: FALSE | burn: 0



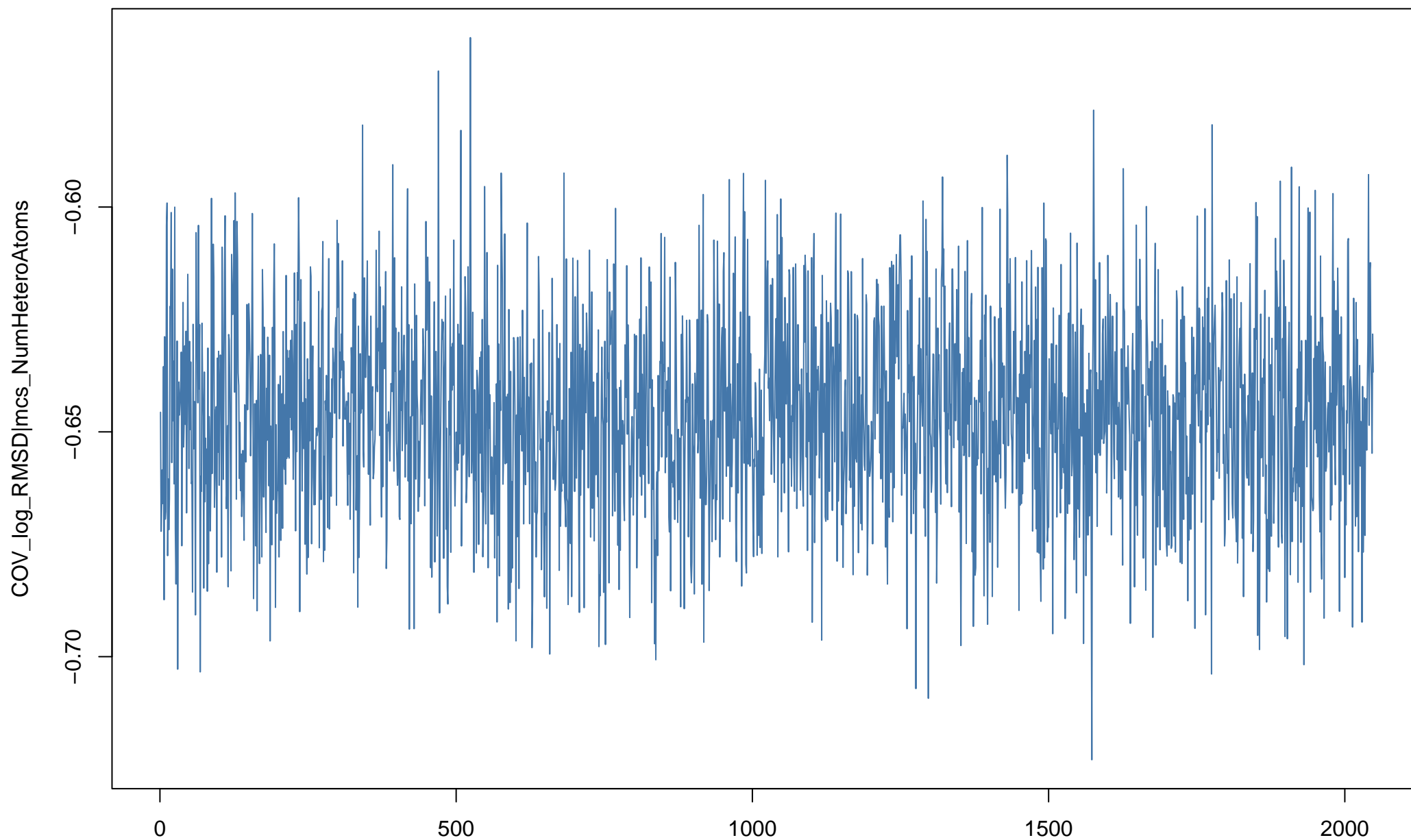
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 1900 | BMK = 0.0286 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0



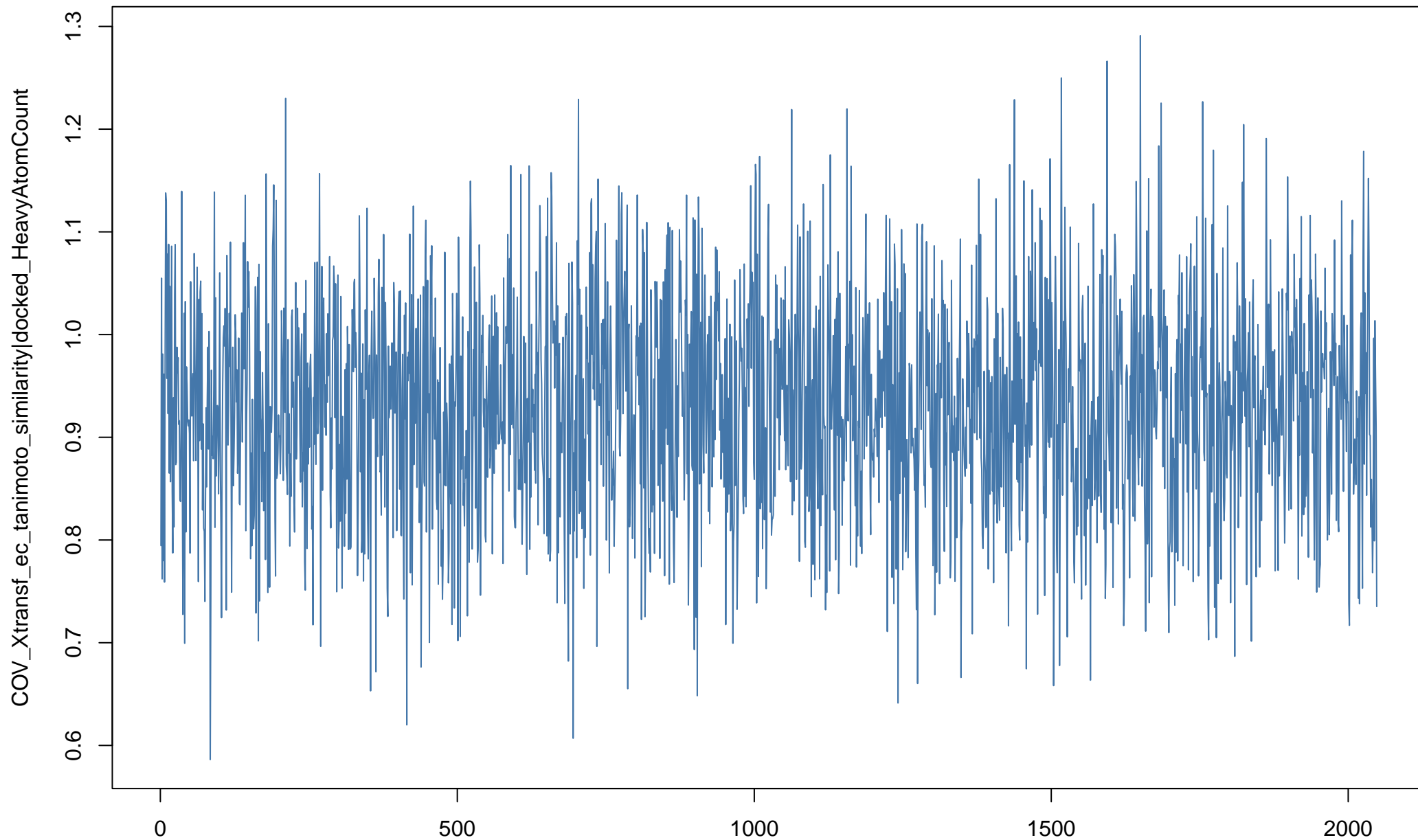
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0484 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0



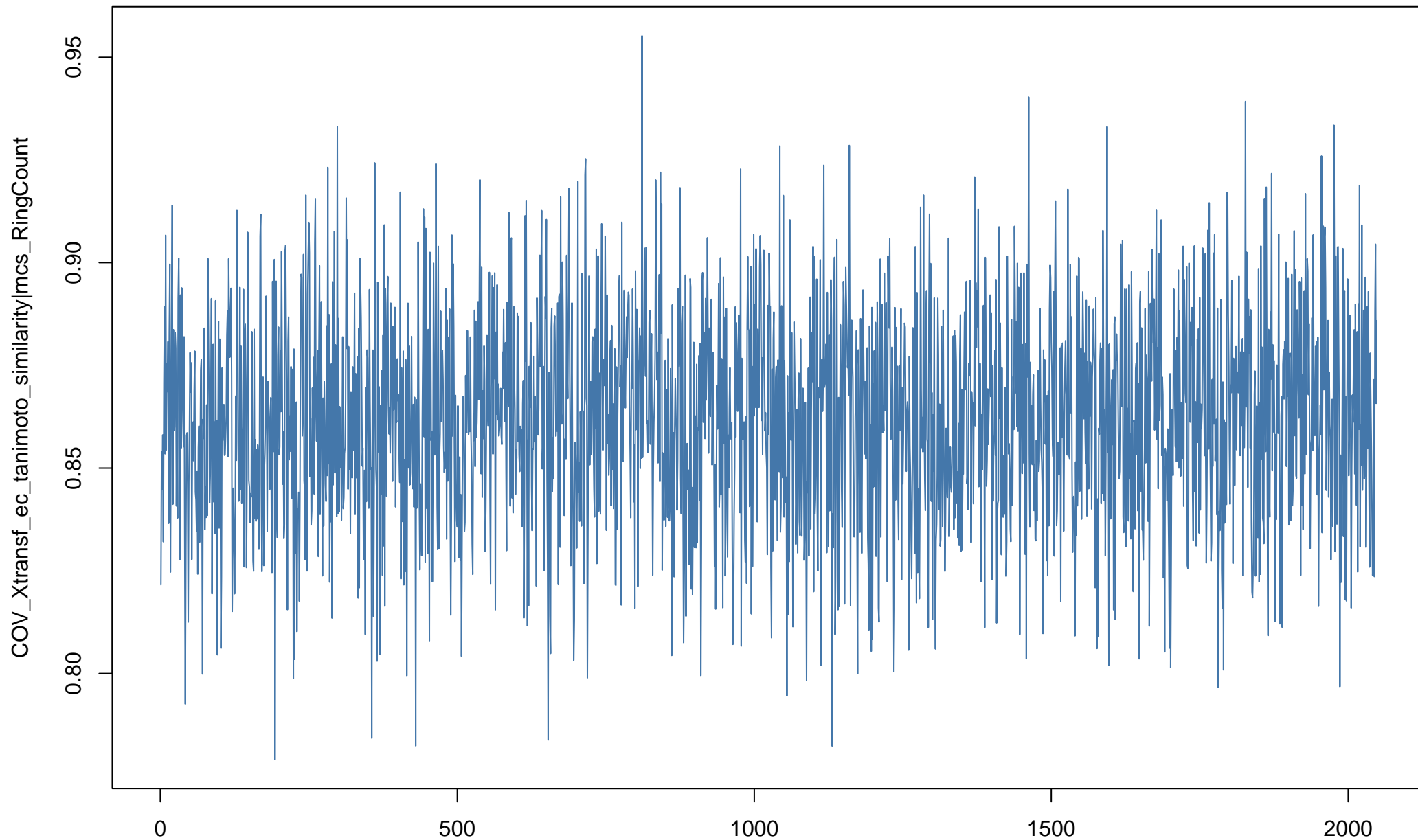
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1910 | BMK = 0.0482 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0



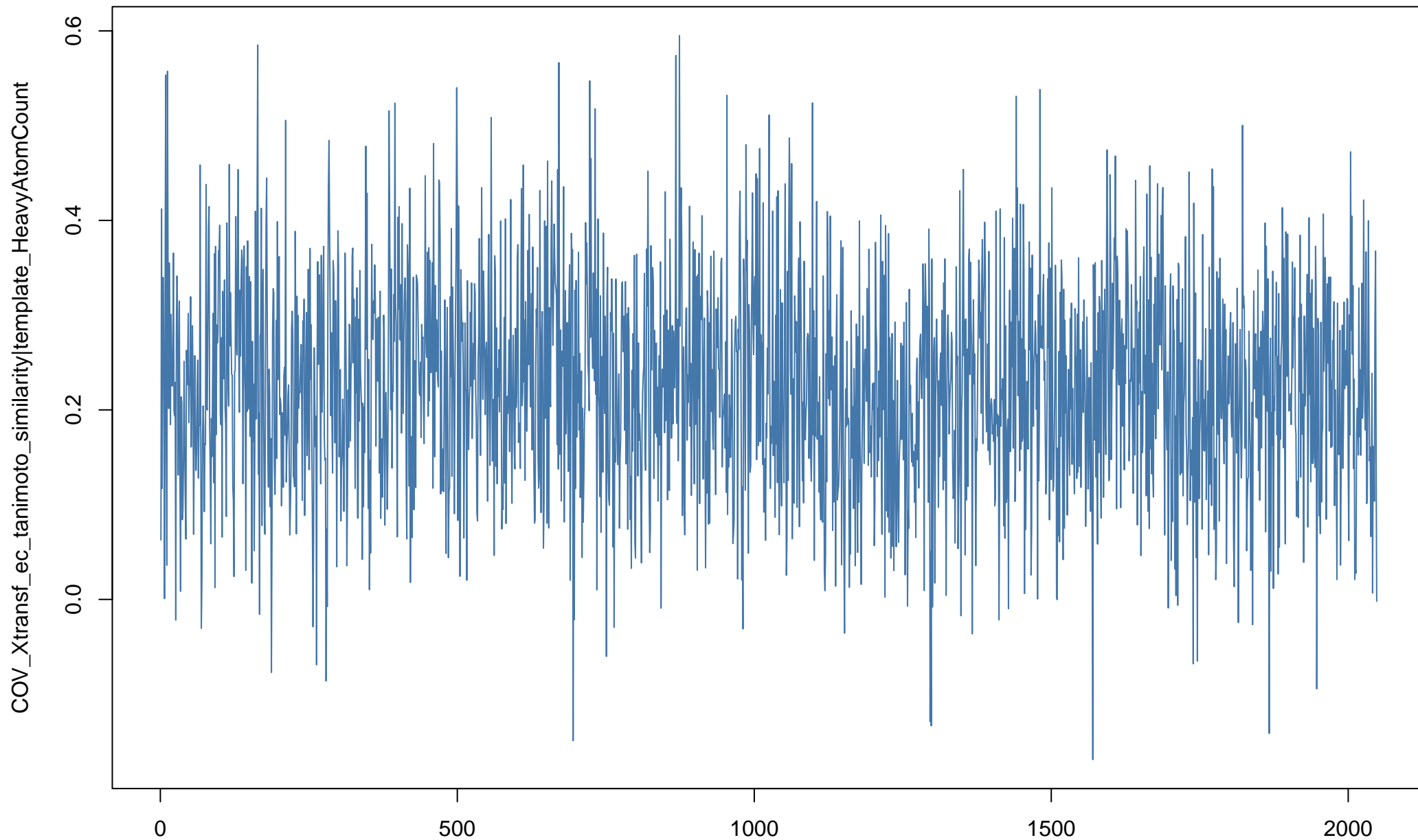
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1950 | BMK = 0.0519 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0



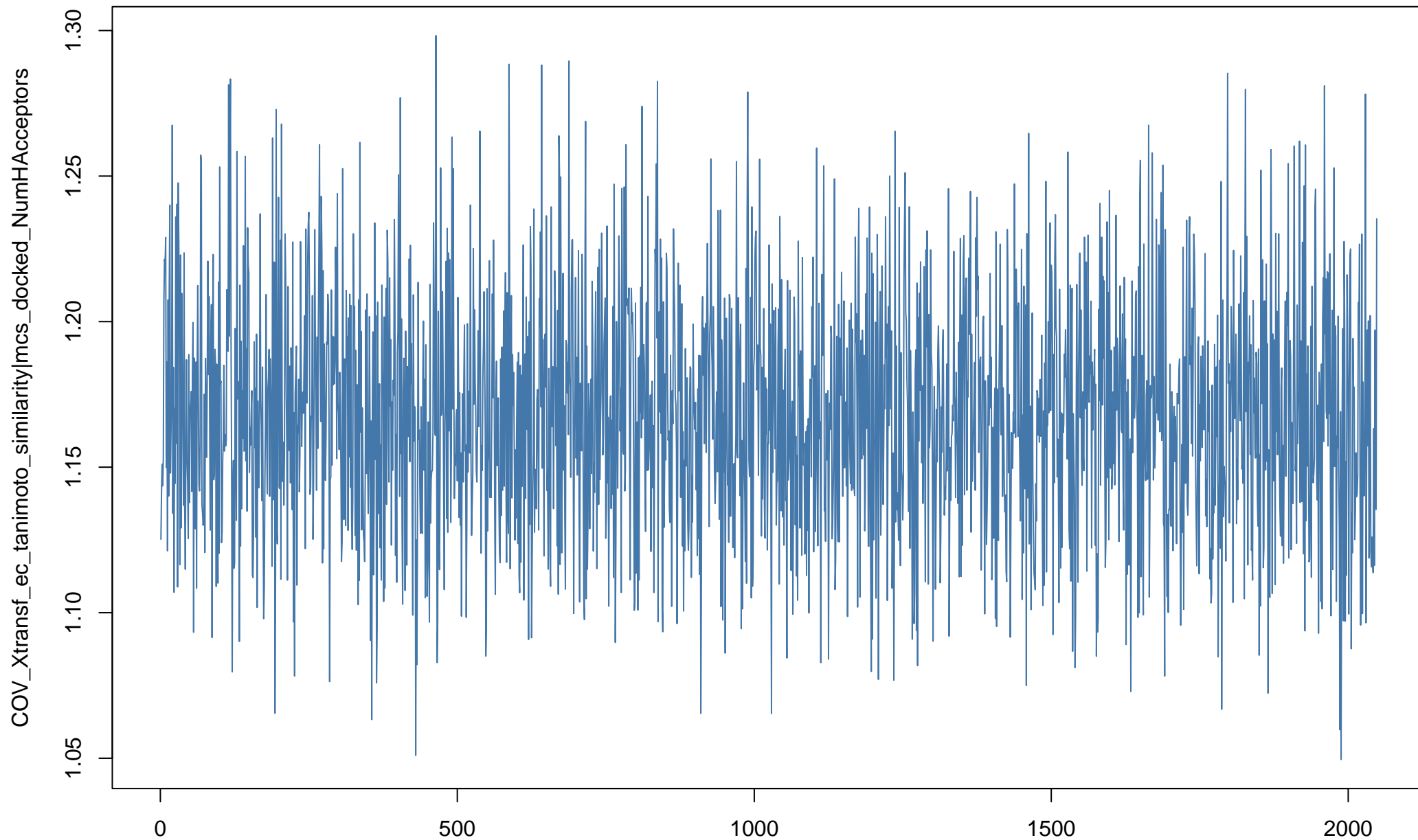
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 2050 | BMK = 0.0421 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0



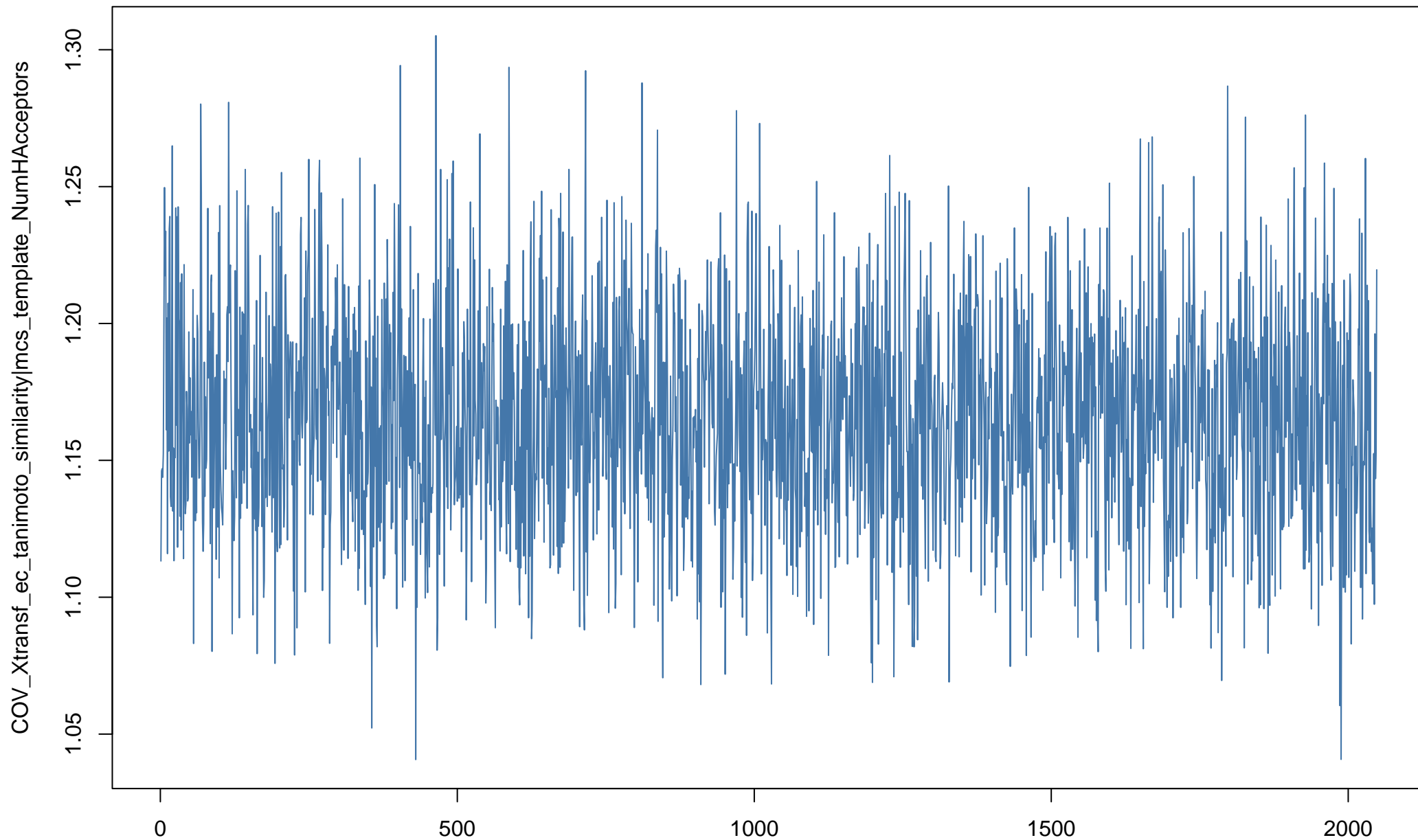
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1810 | BMK = 0.0675 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0



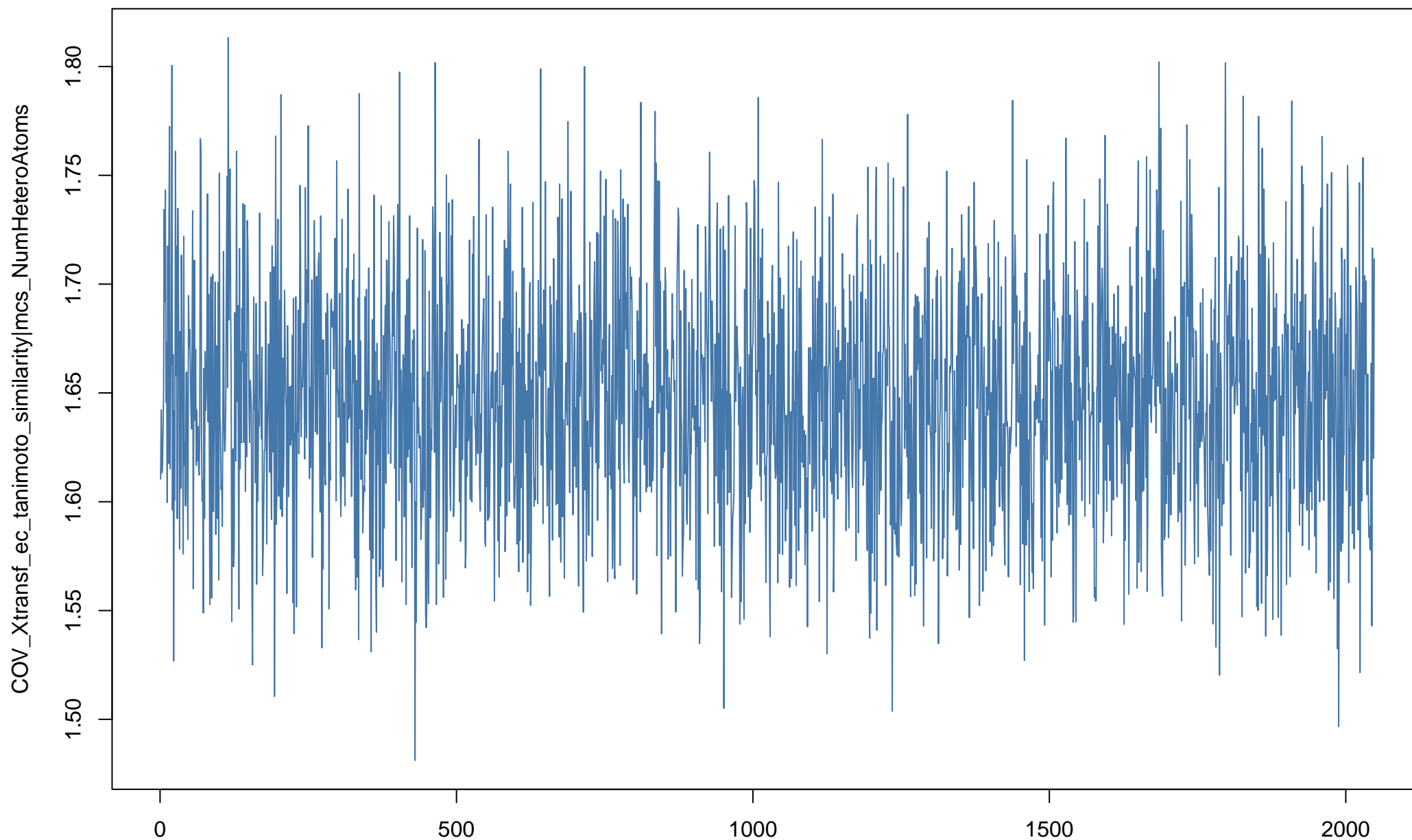
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0383 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0



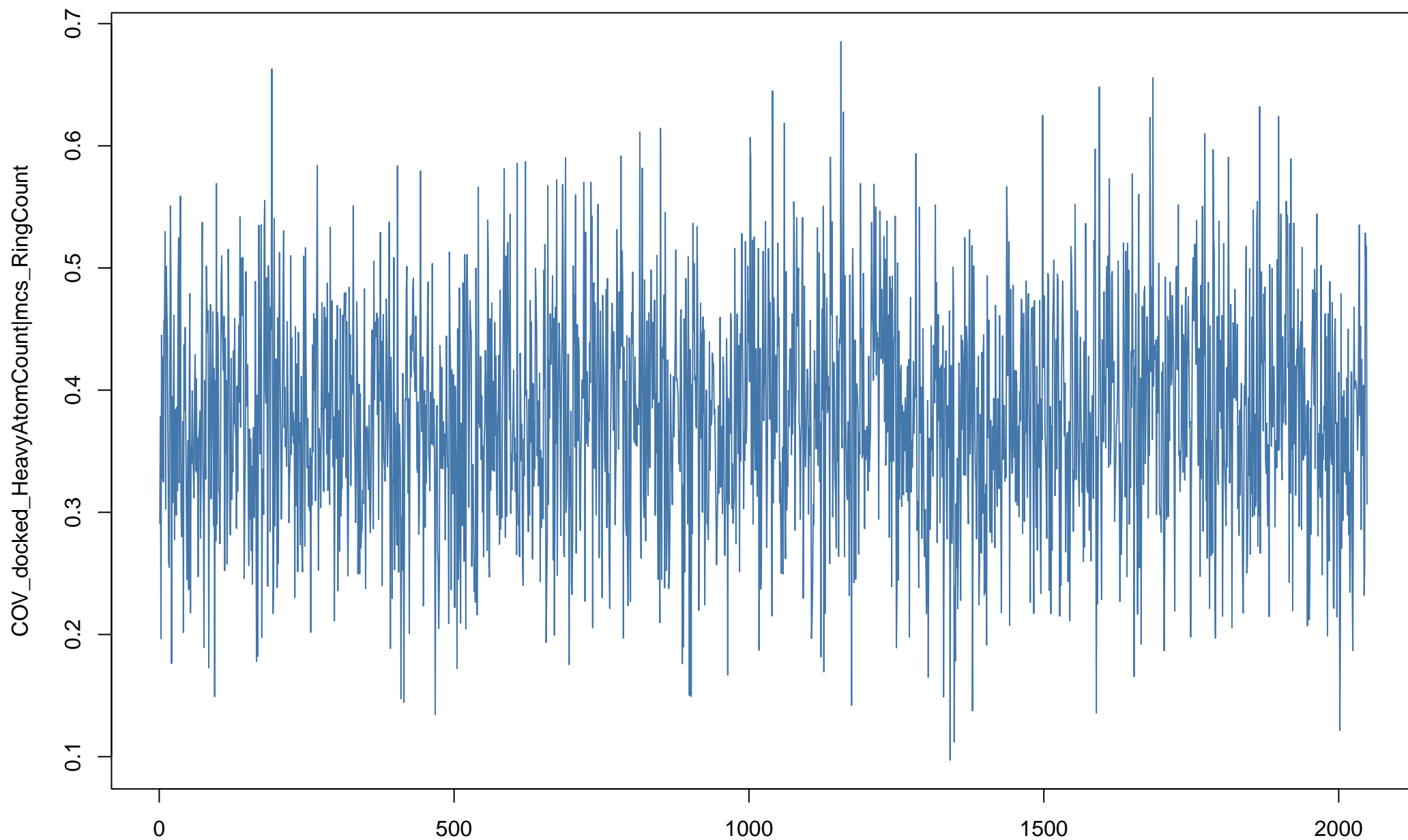
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0482 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



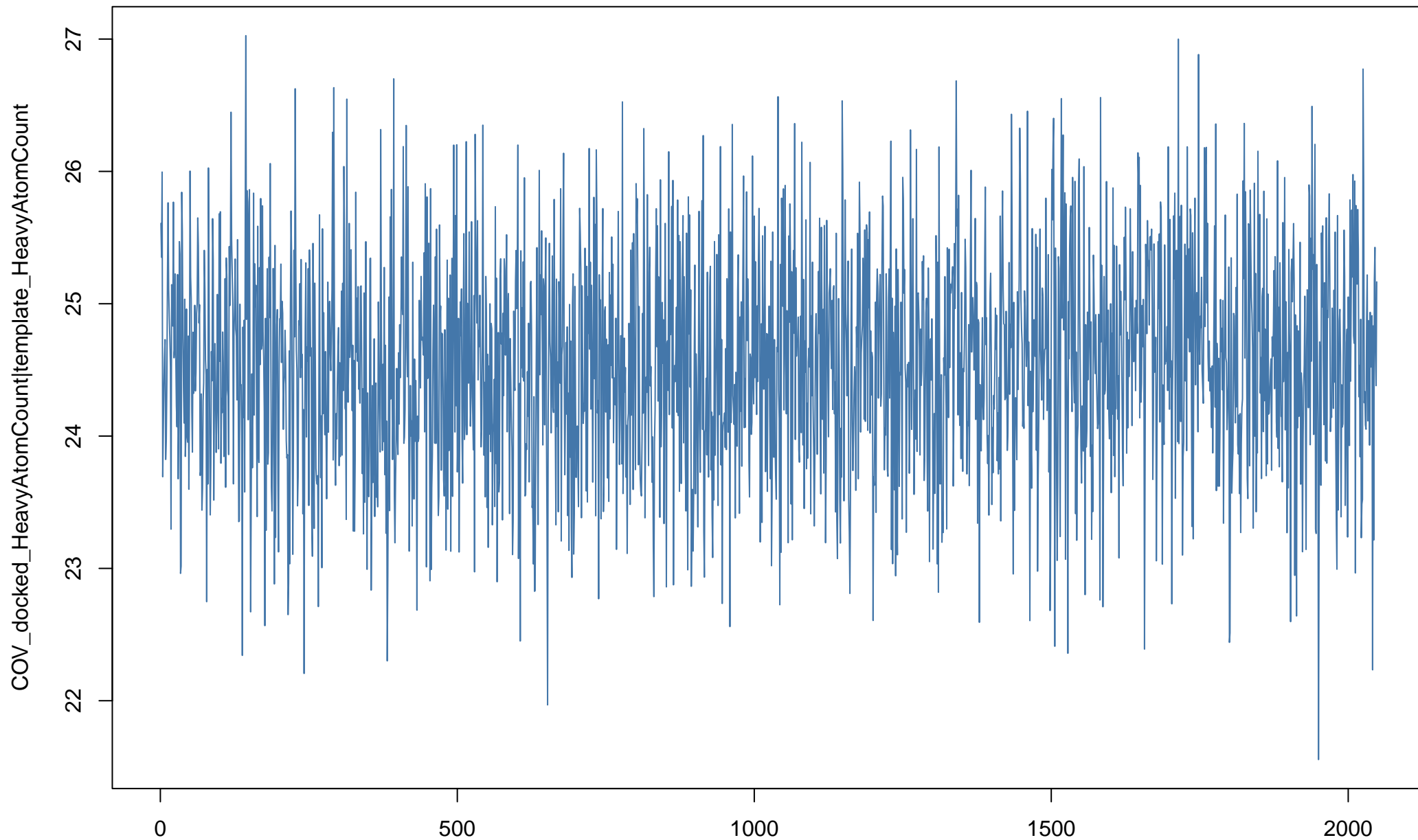
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0469 | MCSE(6.27) = 2 | stat: TRUE | burn: 0



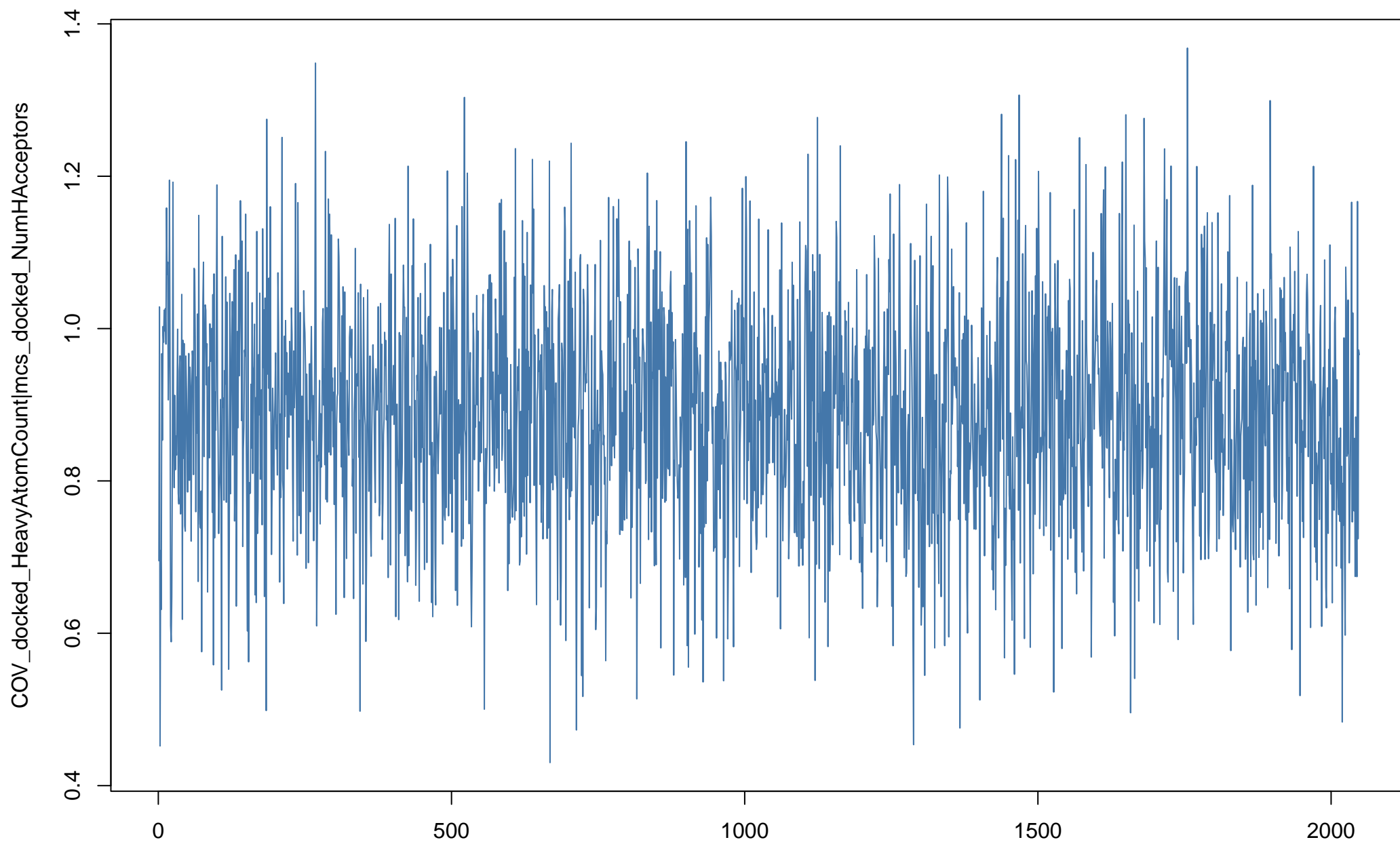
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1310 | BMK = 0.0447 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0



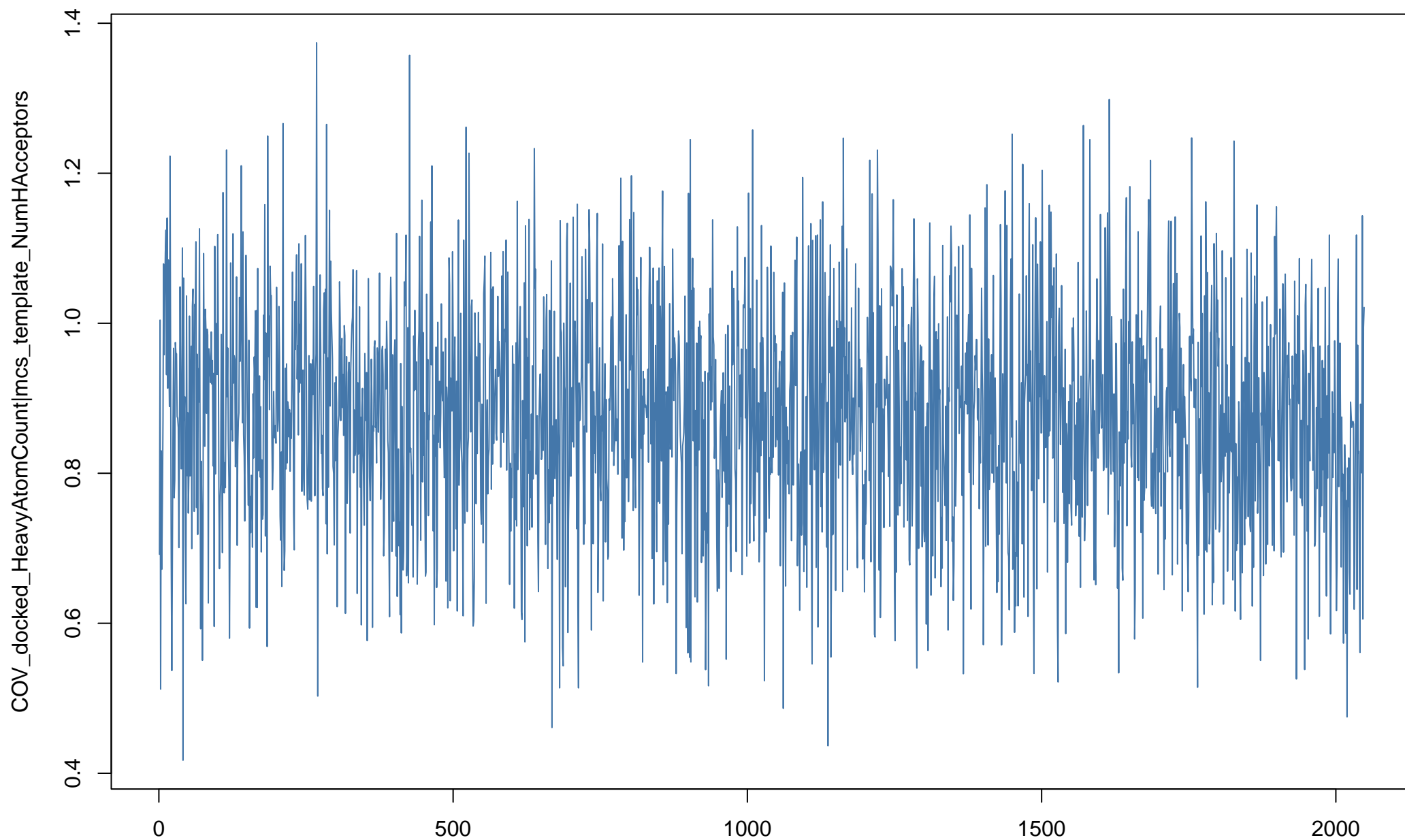
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1840 | BMK = 0.0618 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0



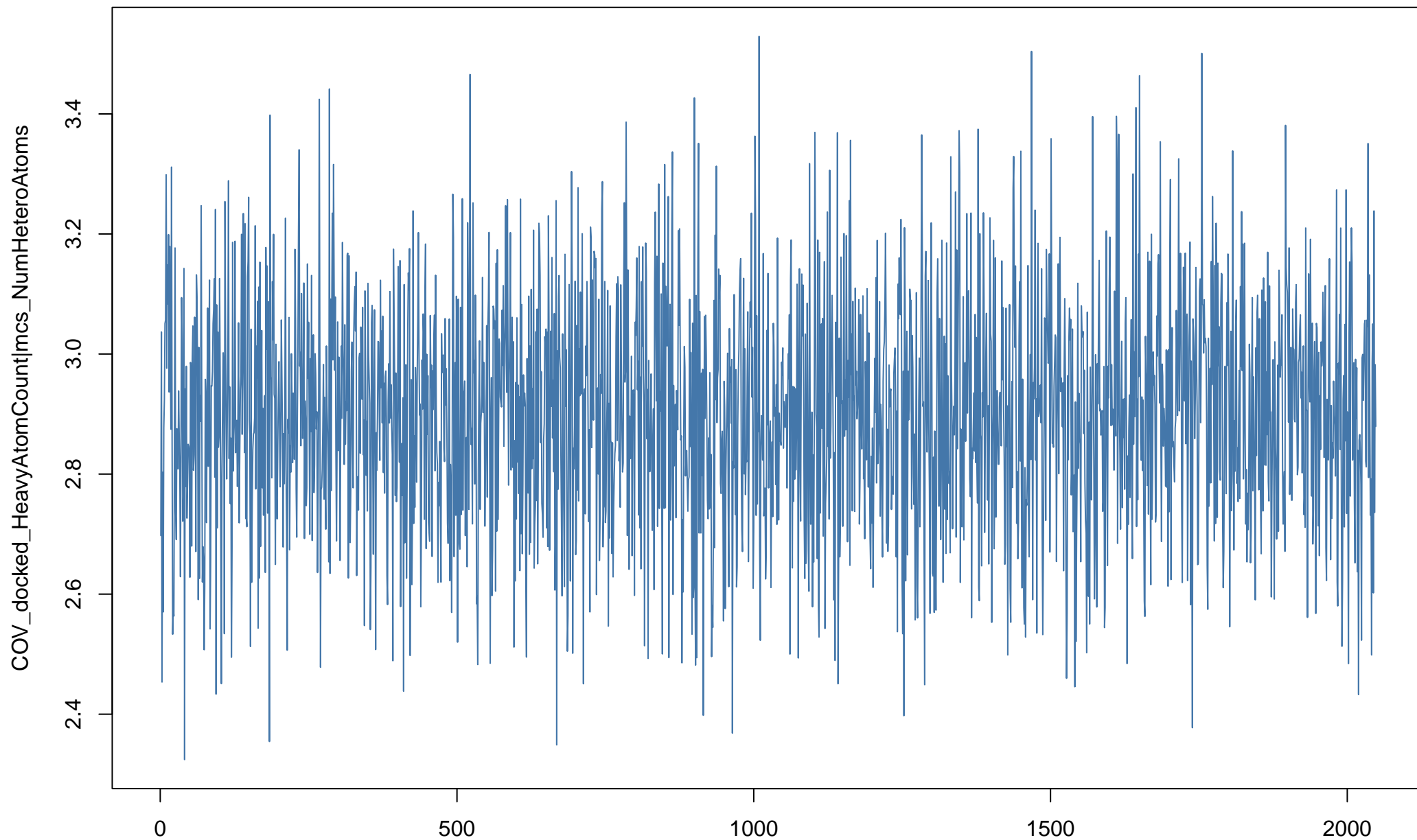
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1910 | BMK = 0.0401 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



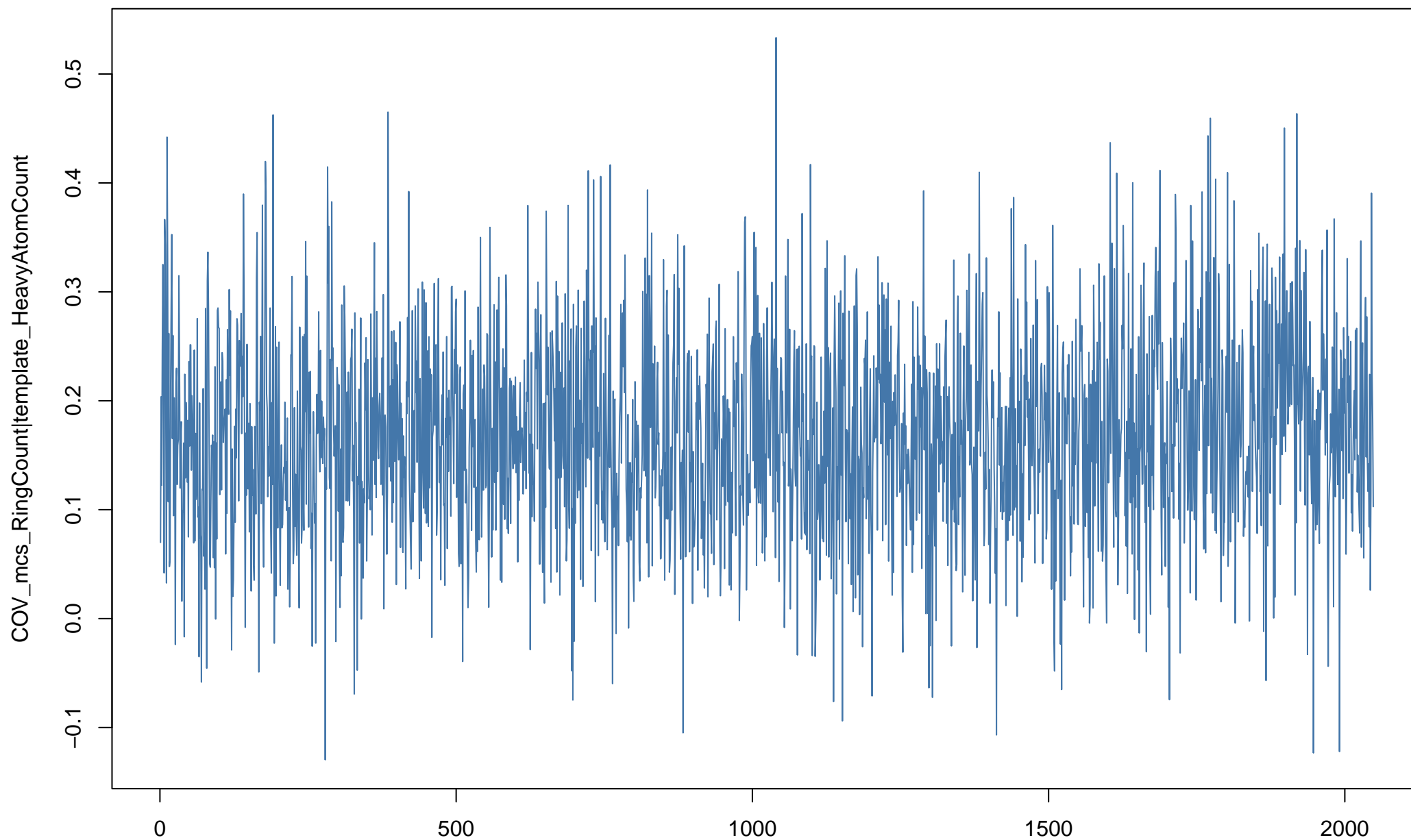
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2010 | BMK = 0.0428 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



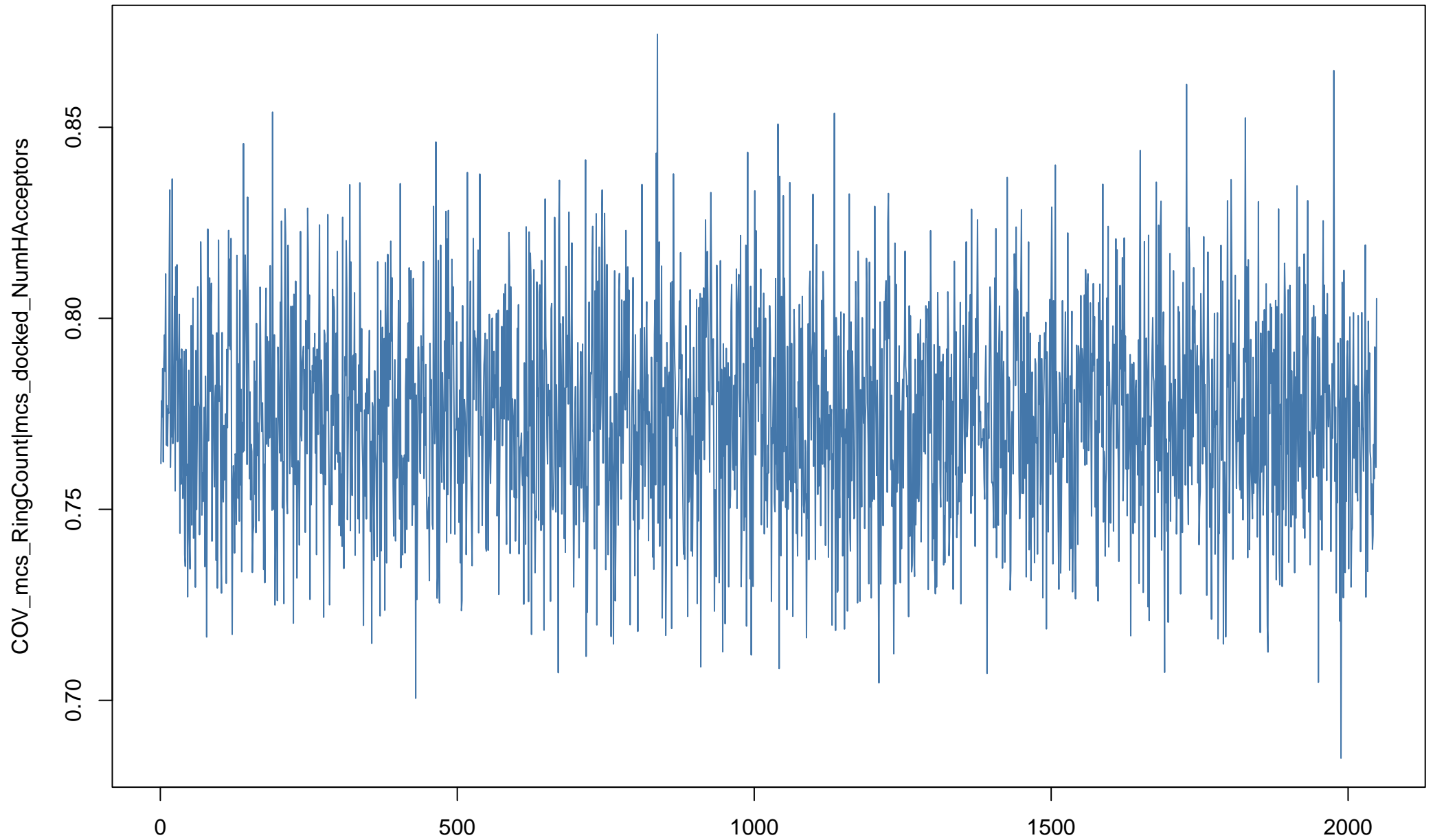
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0373 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0



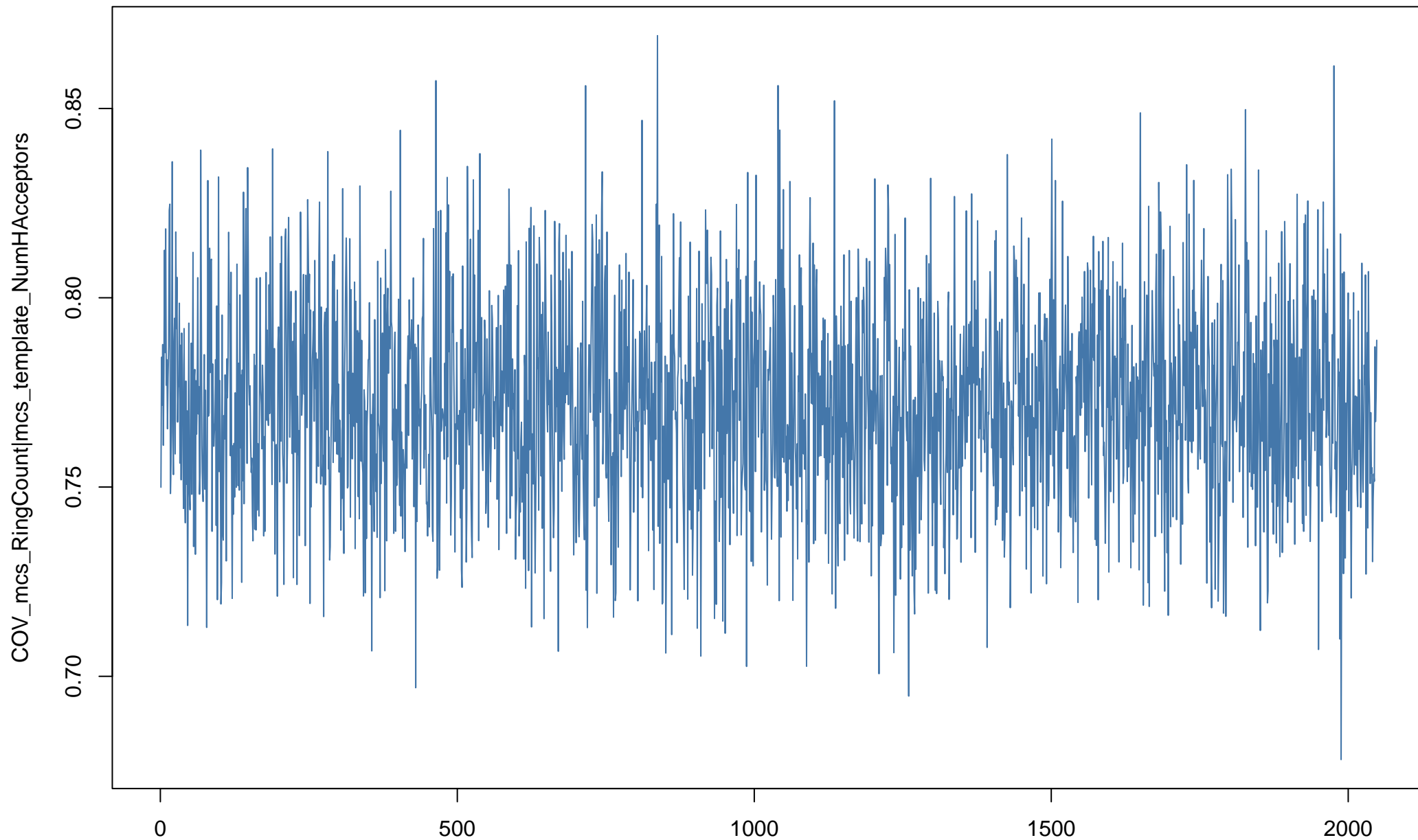
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1790 | BMK = 0.0556 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0



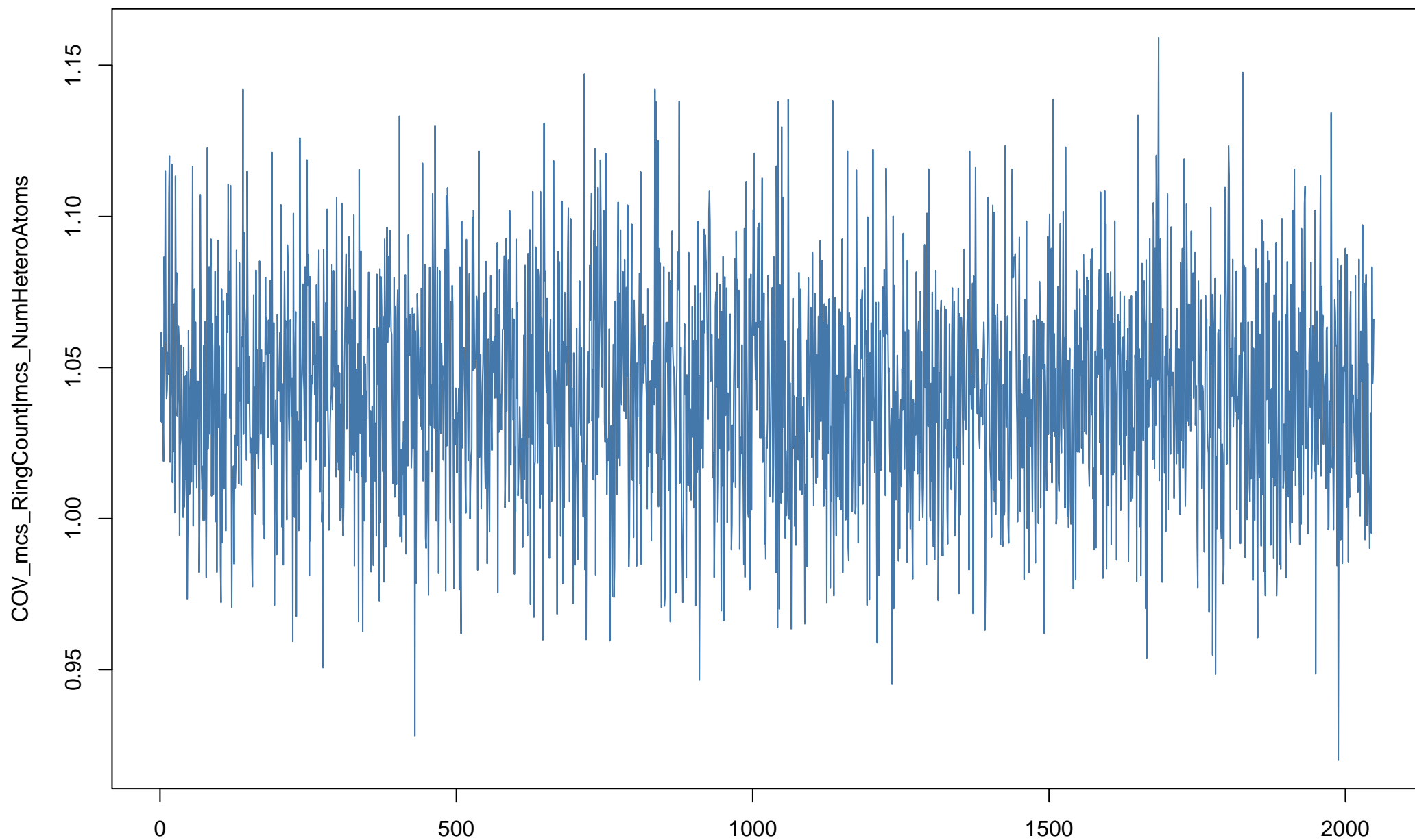
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2000 | BMK = 0.0378 | MCSE(6.27) = 1.7 | stat: TRUE | burn: 0



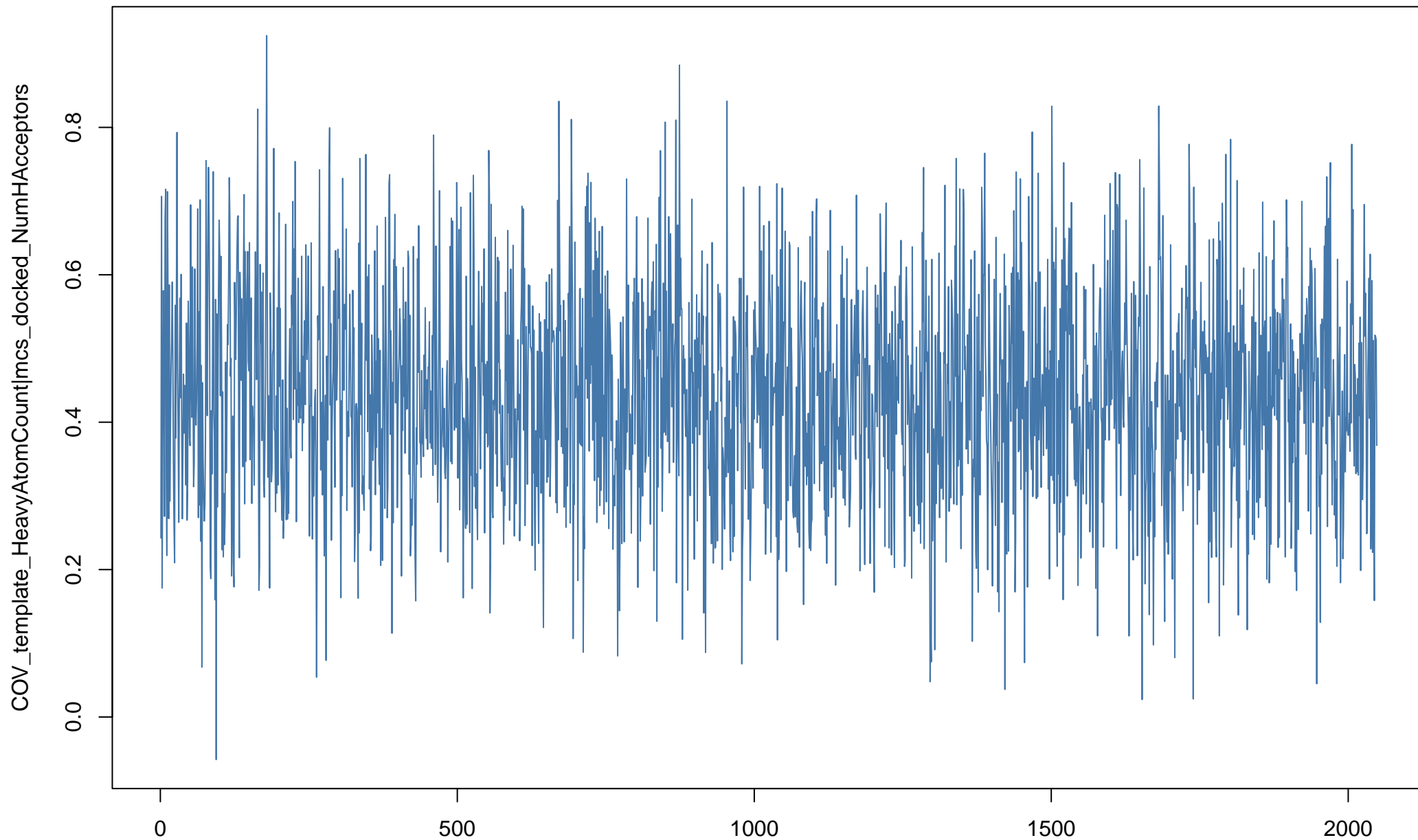
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 1920 | BMK = 0.0319 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0



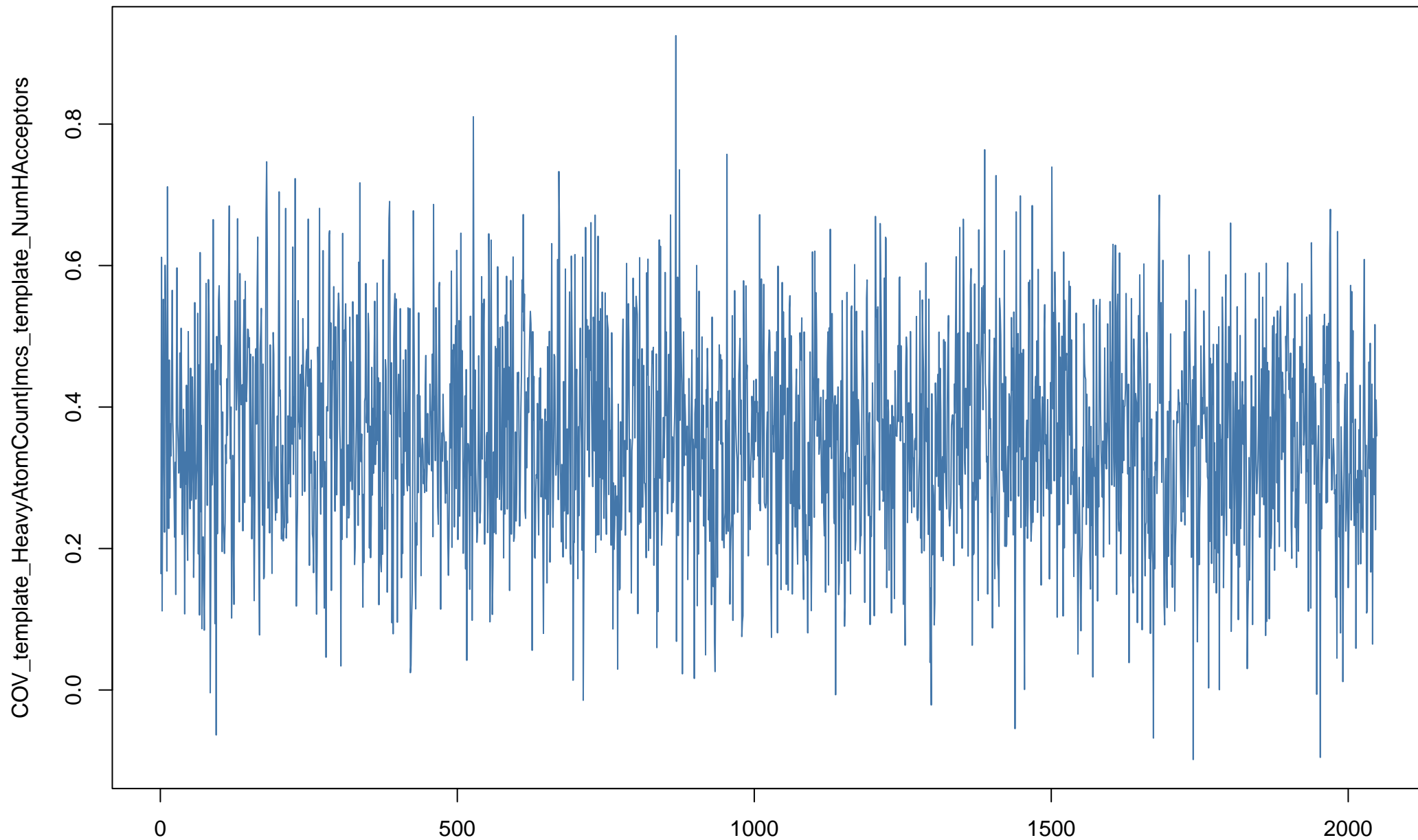
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 1870 | BMK = 0.0402 | MCSE(6.27) = 2.03 | stat: TRUE | burn: 0



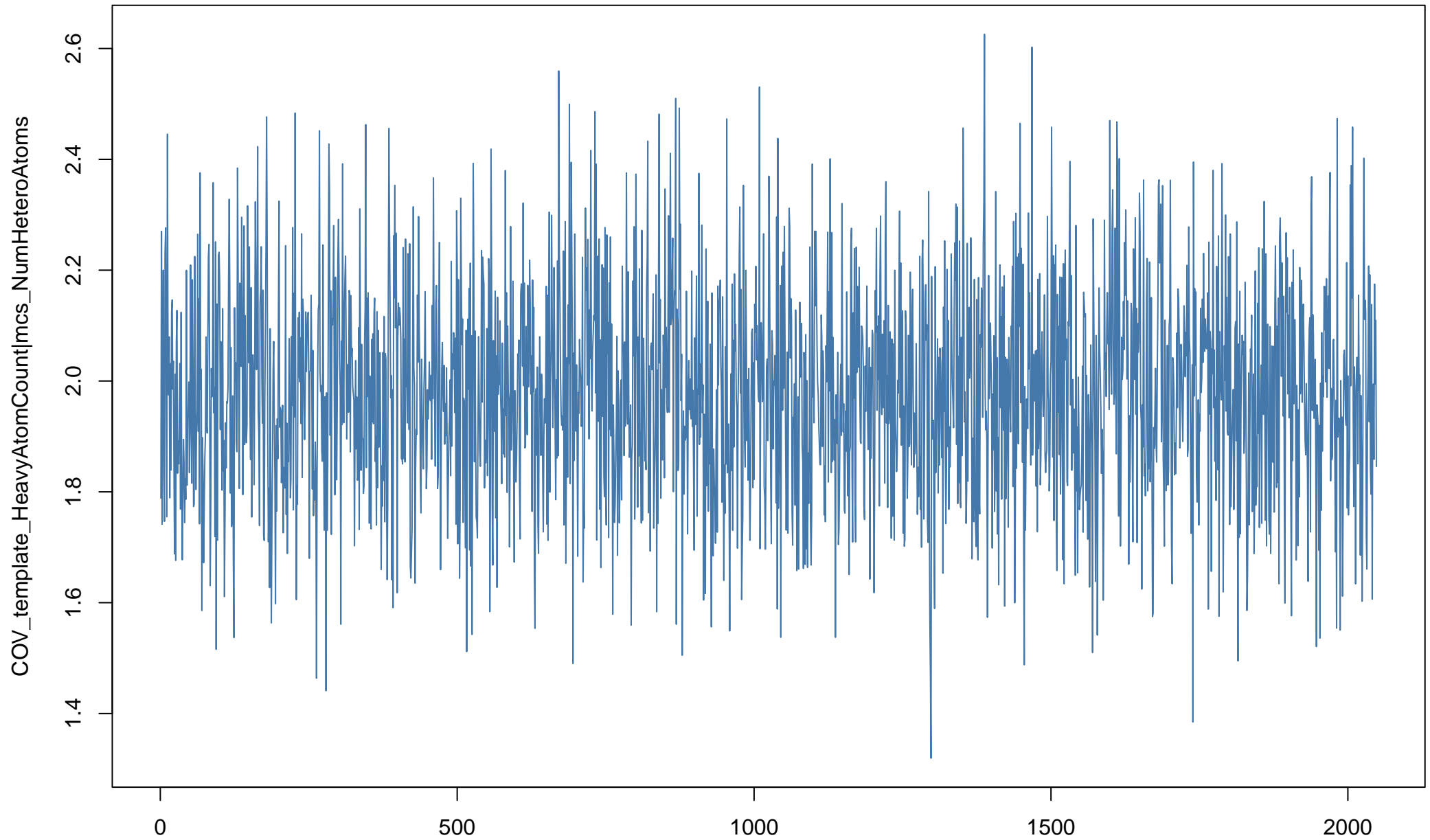
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1650 | BMK = 0.0412 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0



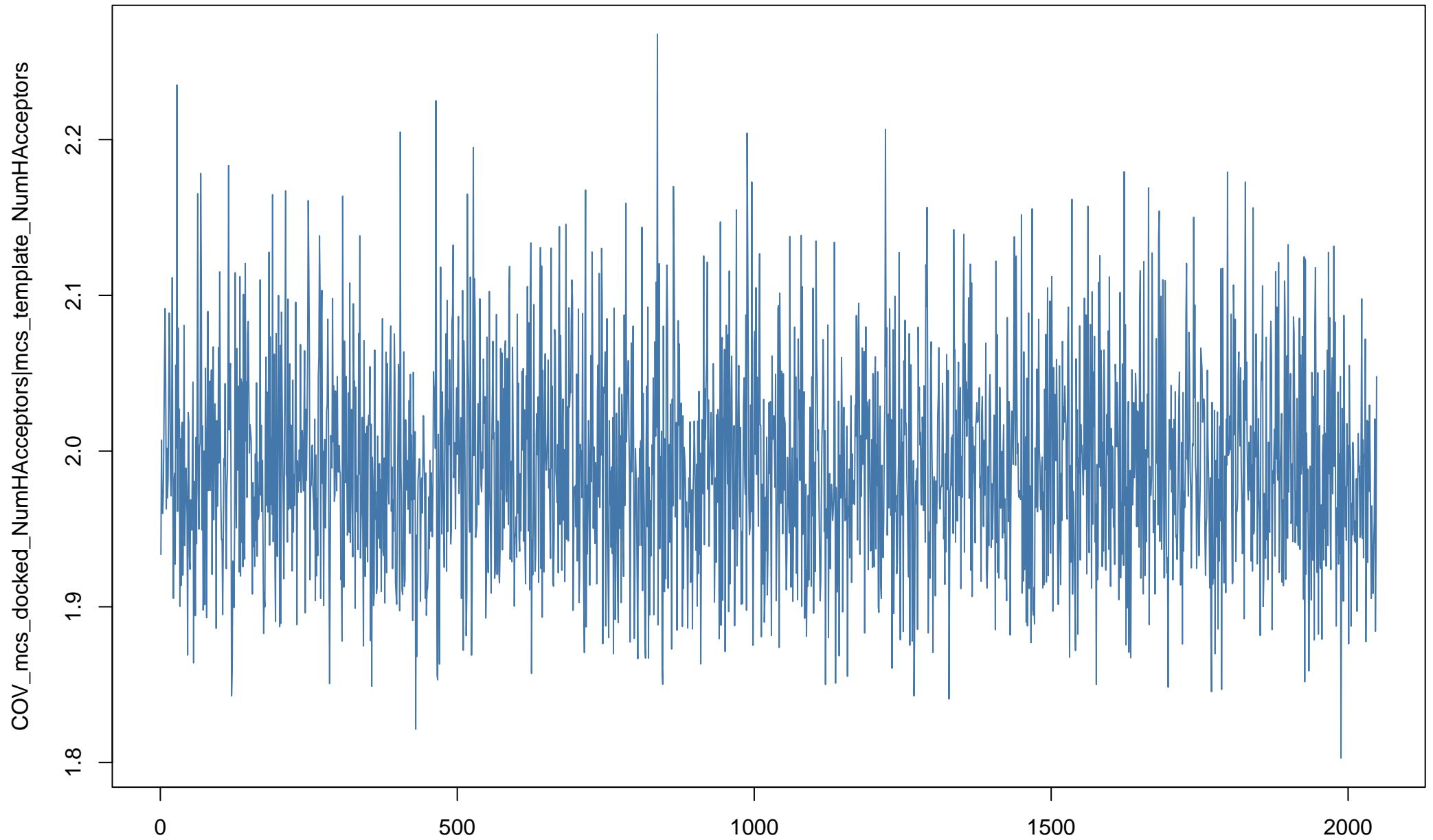
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1750 | BMK = 0.0476 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0



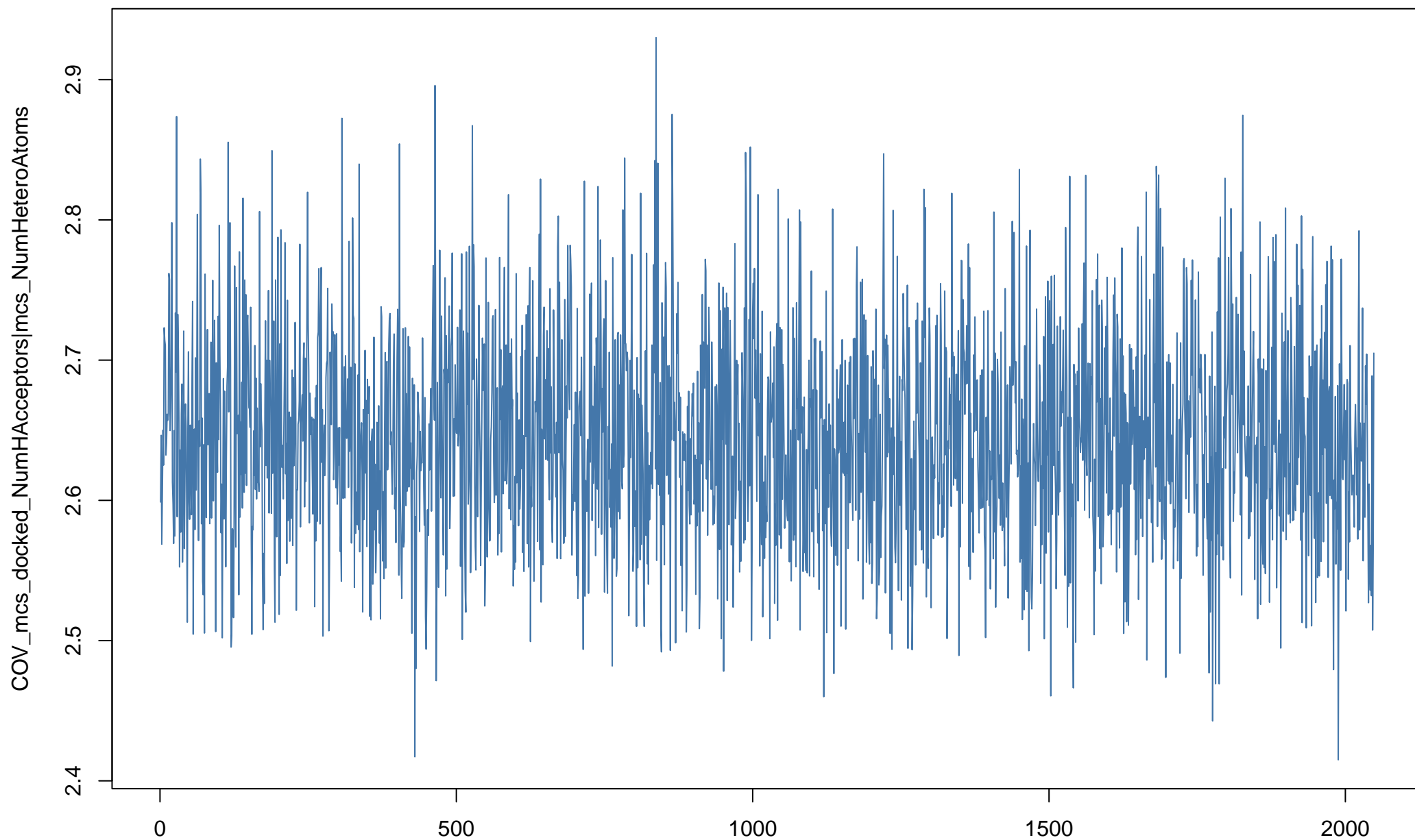
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1660 | BMK = 0.034 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0496 | MCSE(6.27) = 1.97 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0542 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0

