

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.425718397798298

max MCSE = 9.84132571672454

all stationary: FALSE

burn: 612

-- STATS 2D --

min ESS = 1069.89168534799

max BMK = 0.071590684677724

max MCSE = 3.30598713213212

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.263574718450252

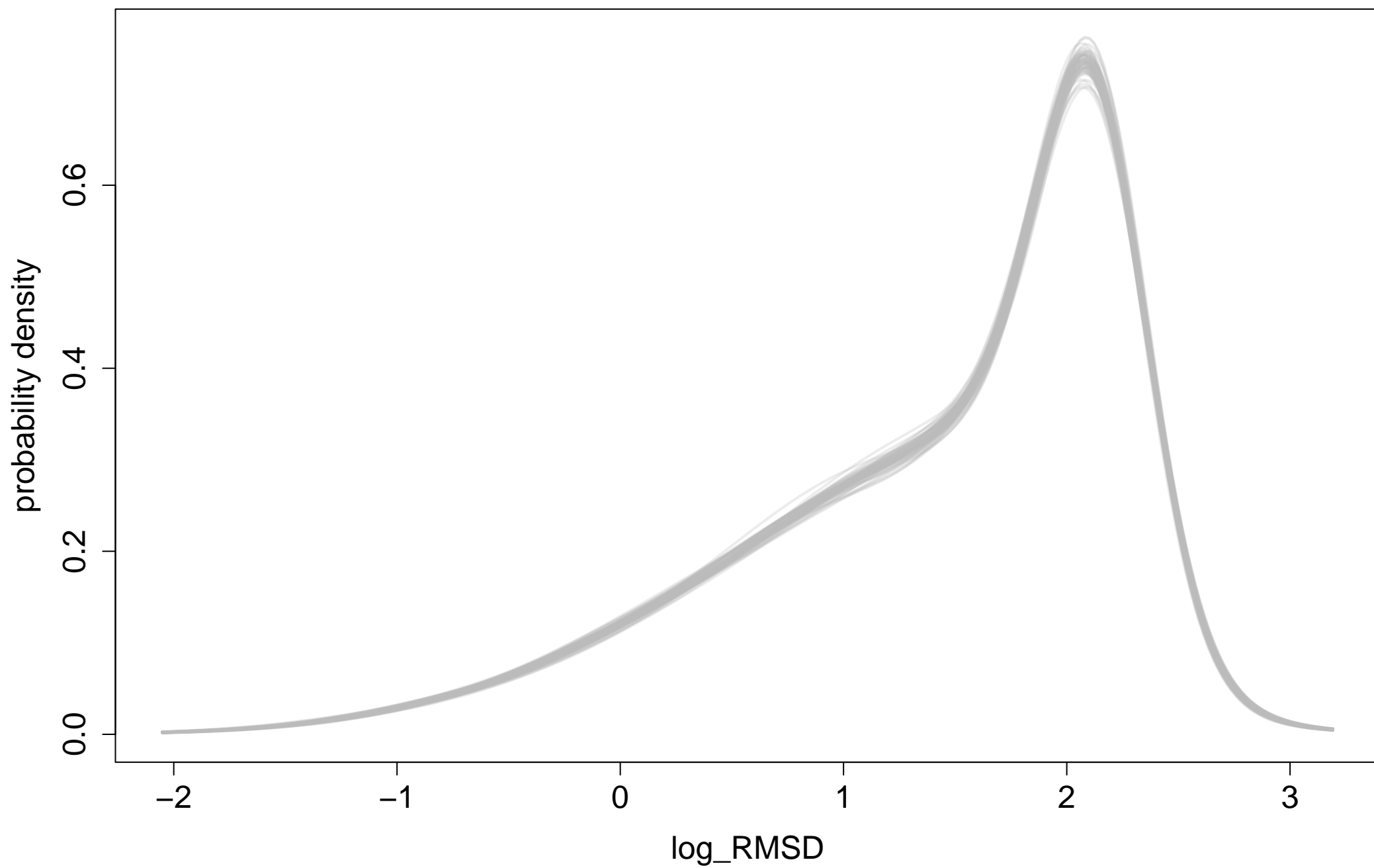
max MCSE = NaN

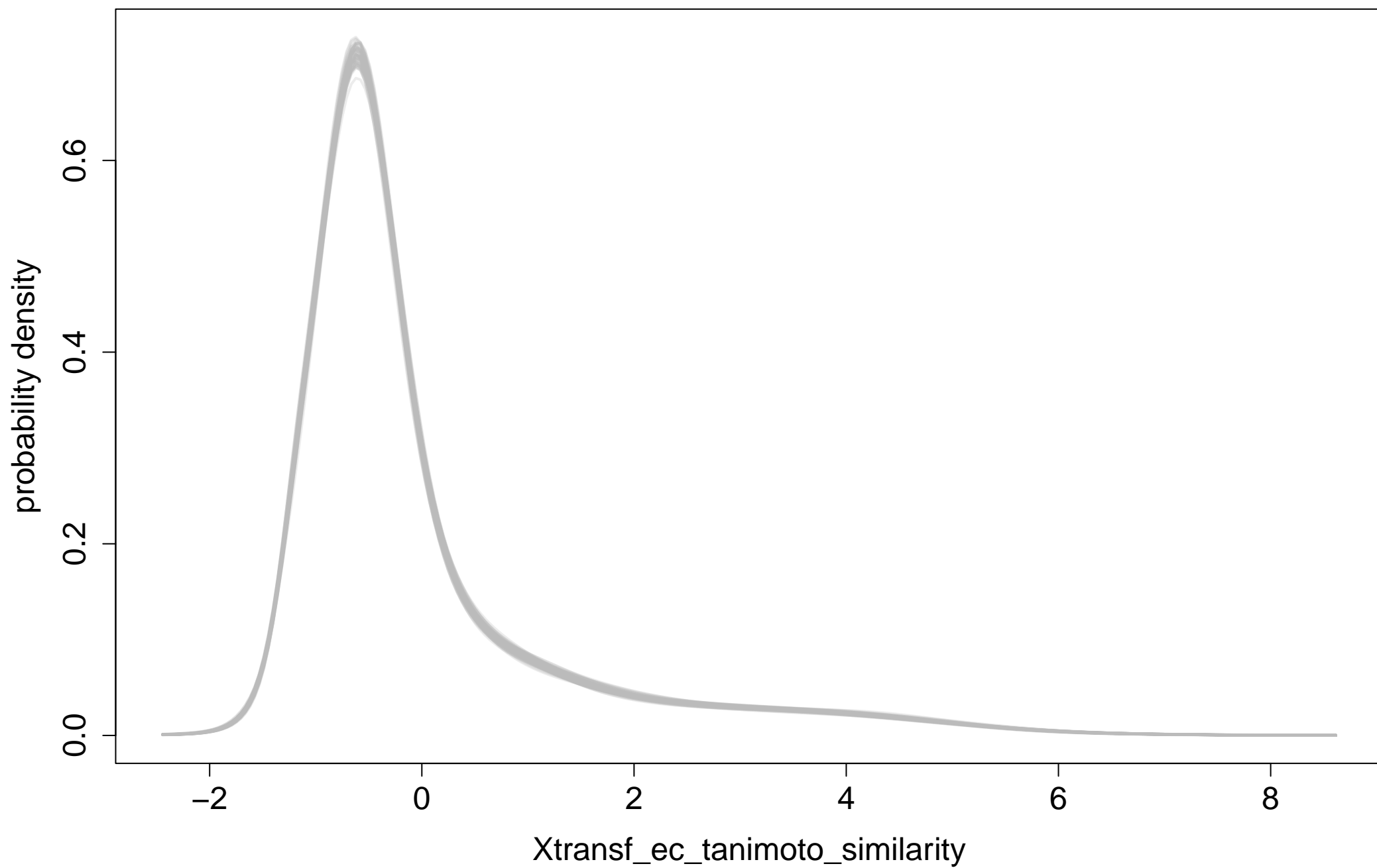
all stationary: FALSE

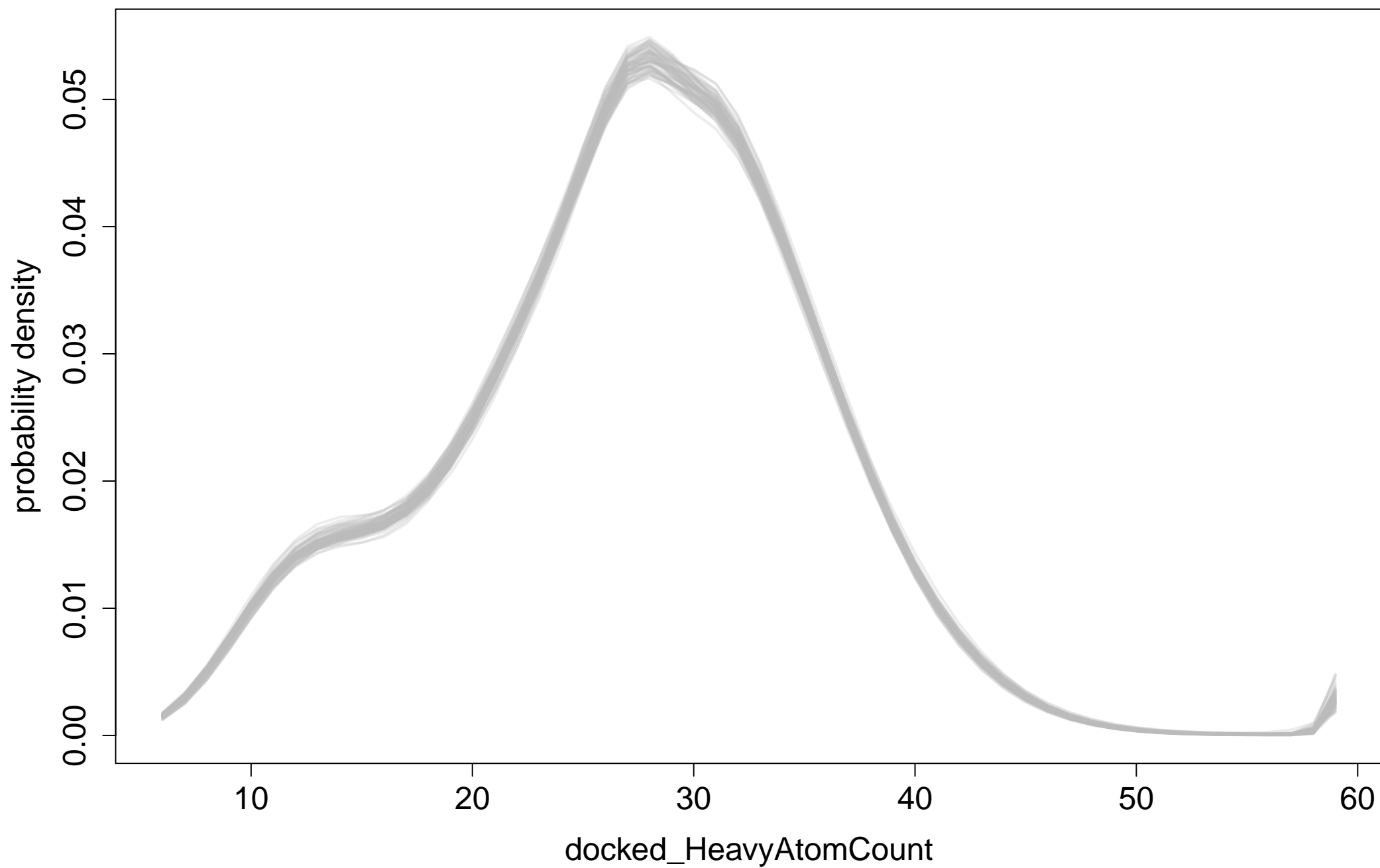
burn: 1632

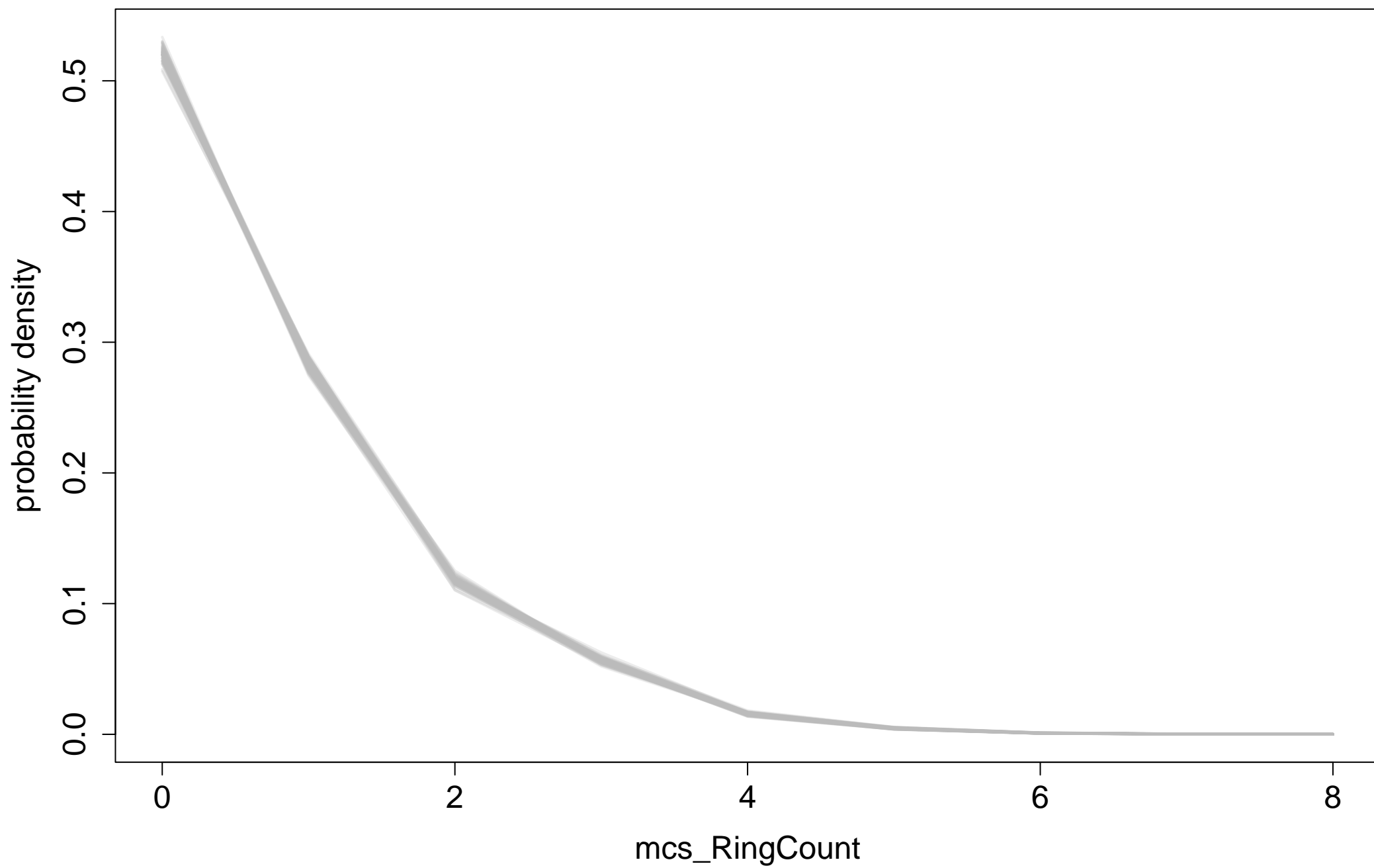
Occupied clusters: 61 of 64

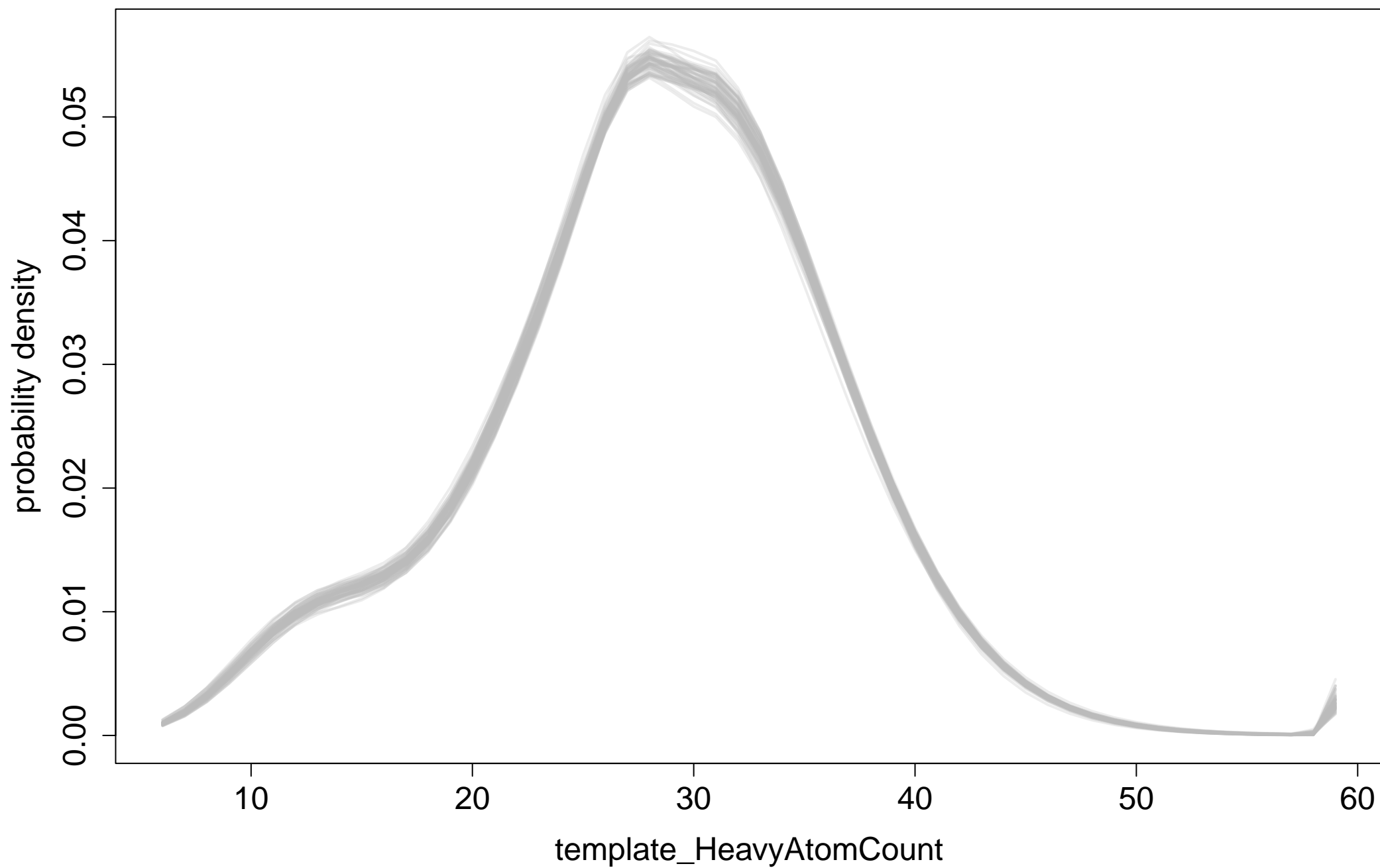
LL: -110000 +- 23.4

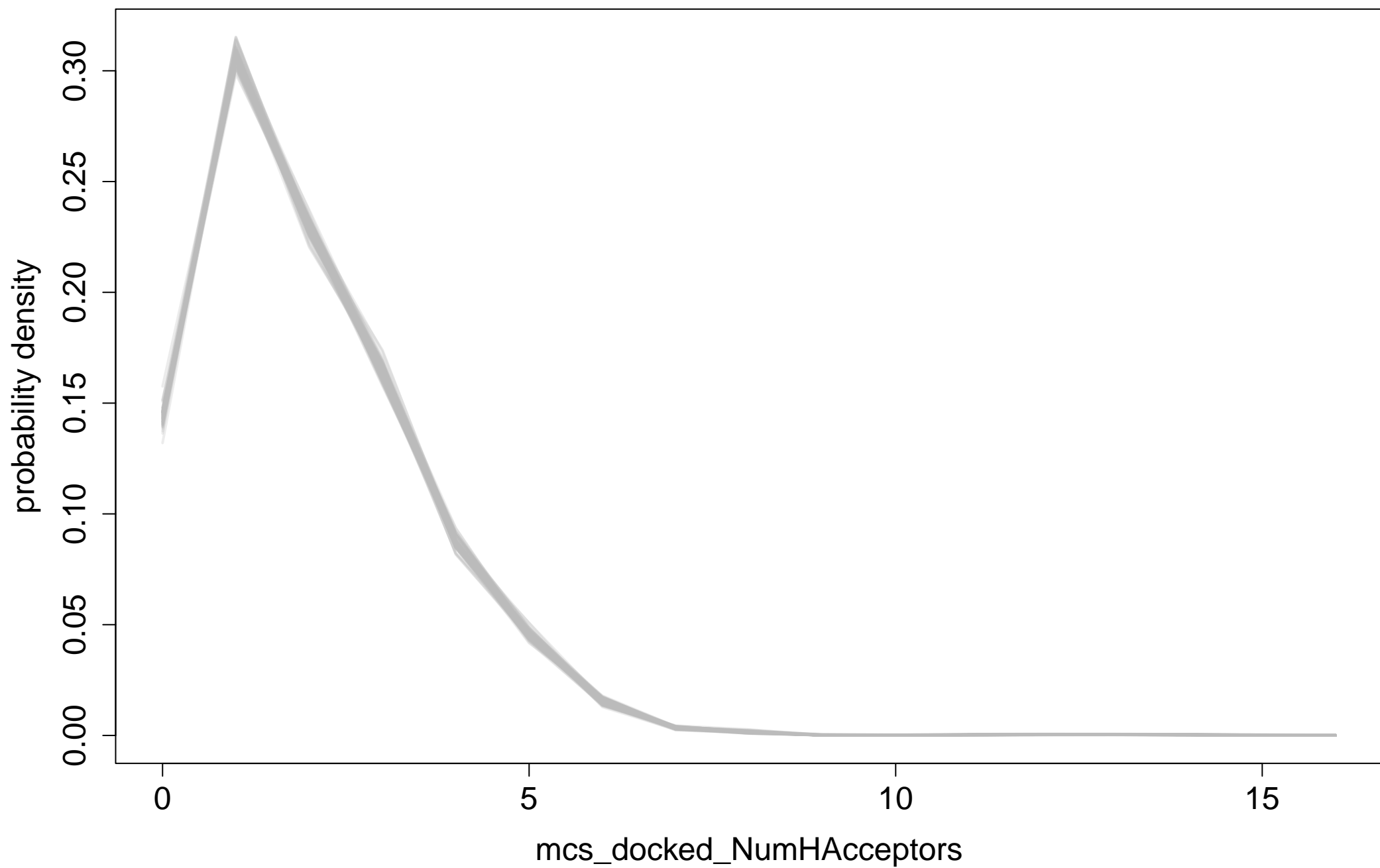


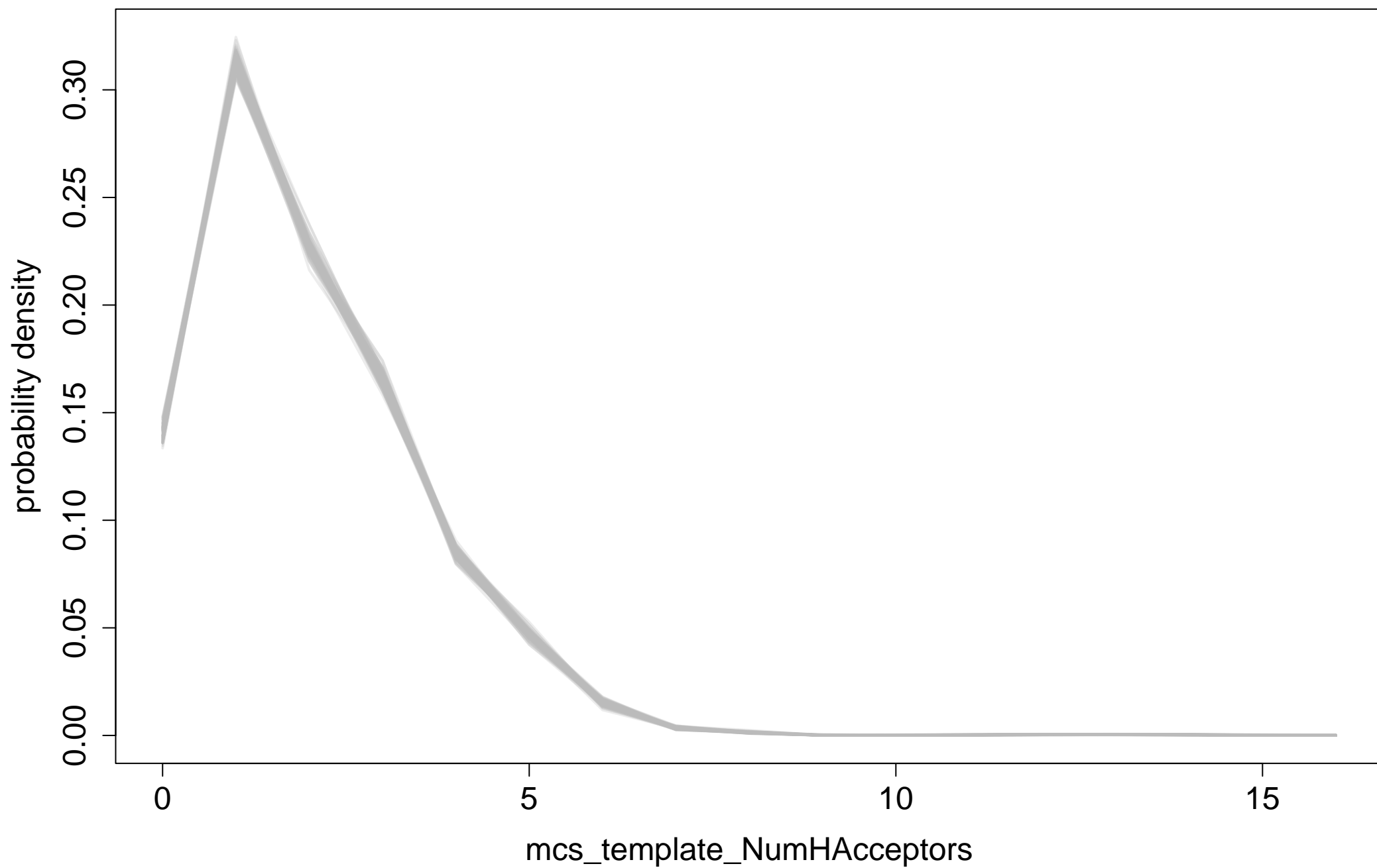


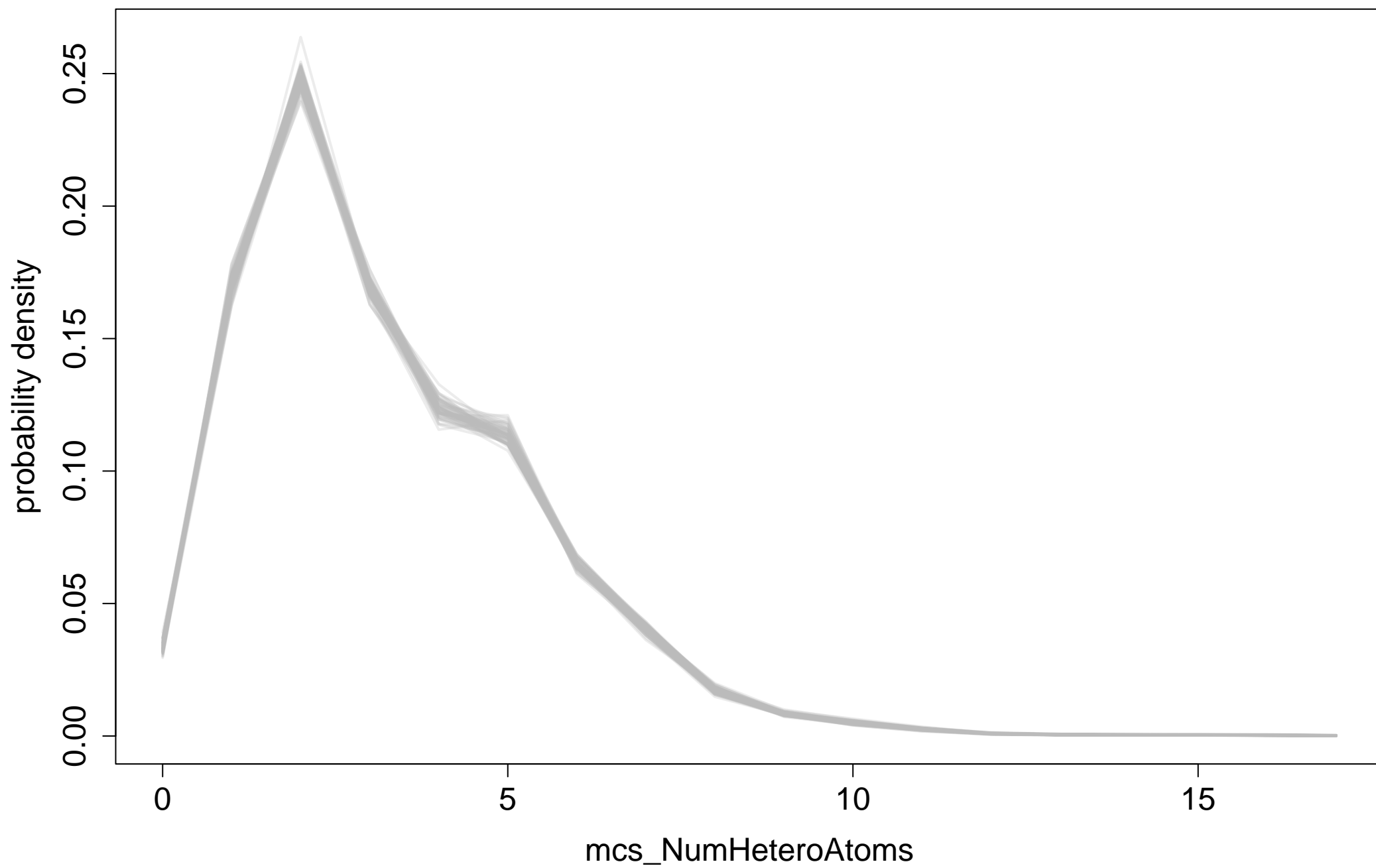


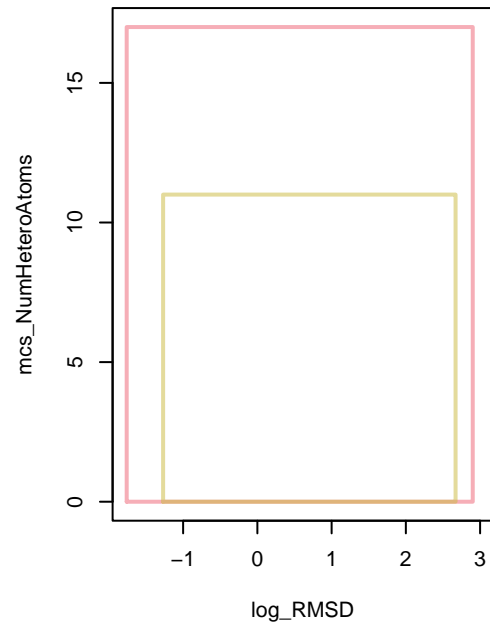
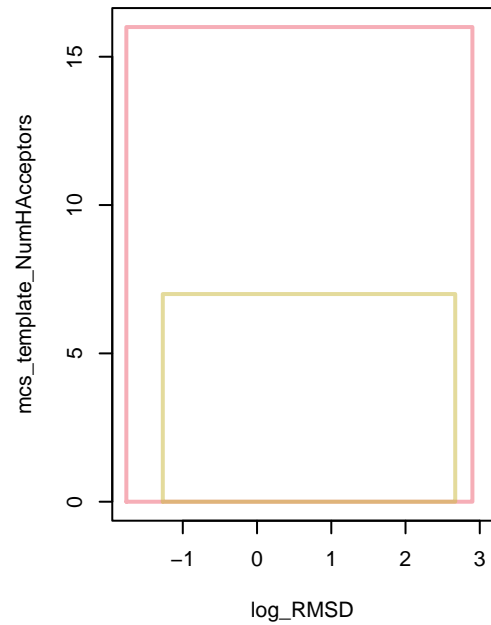
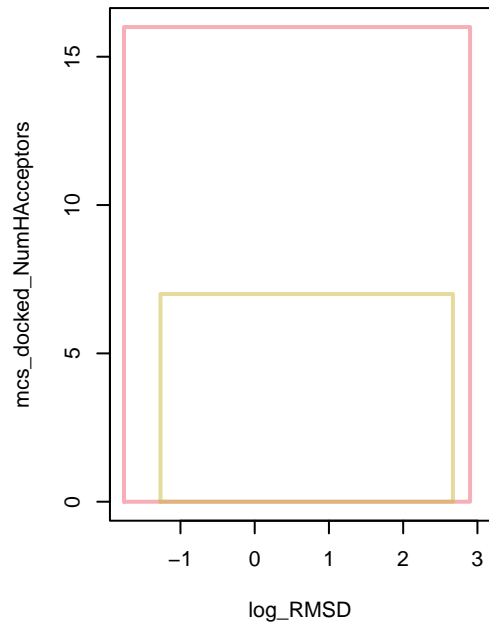
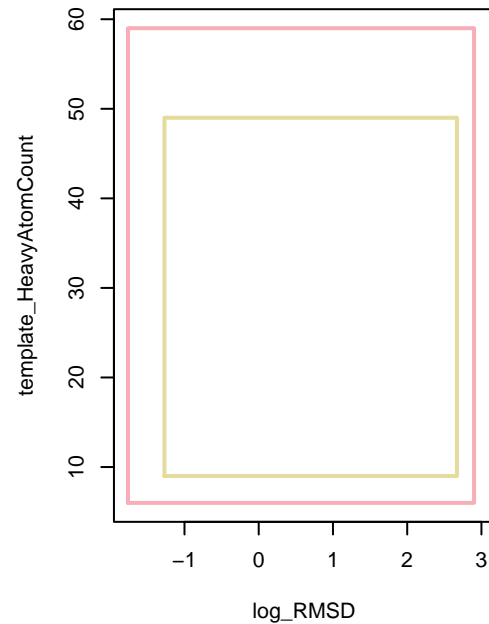
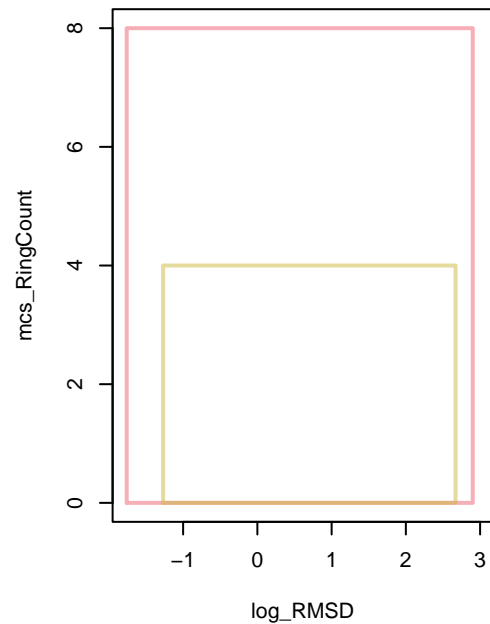
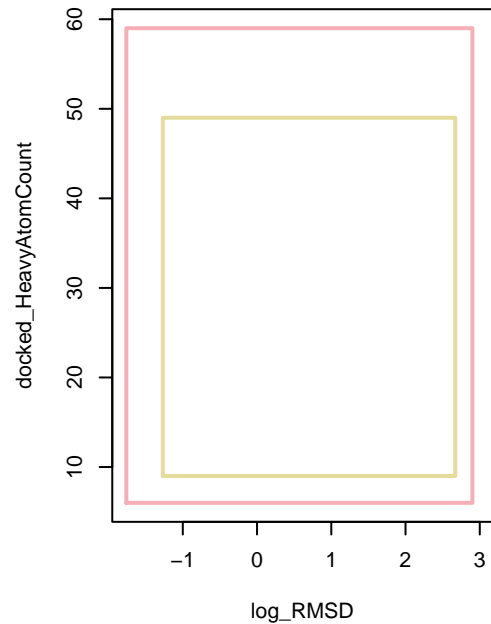
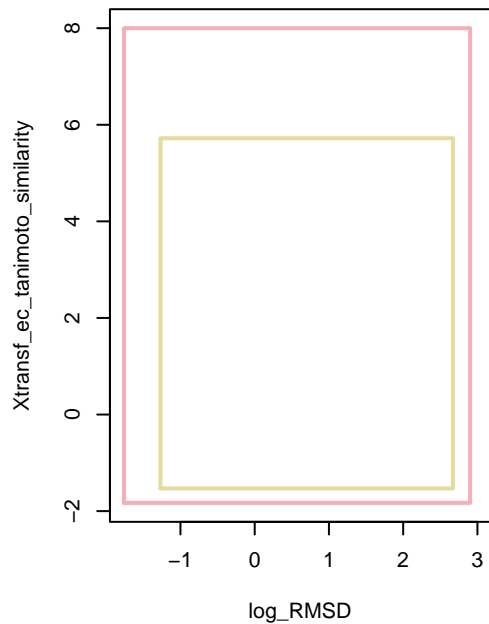




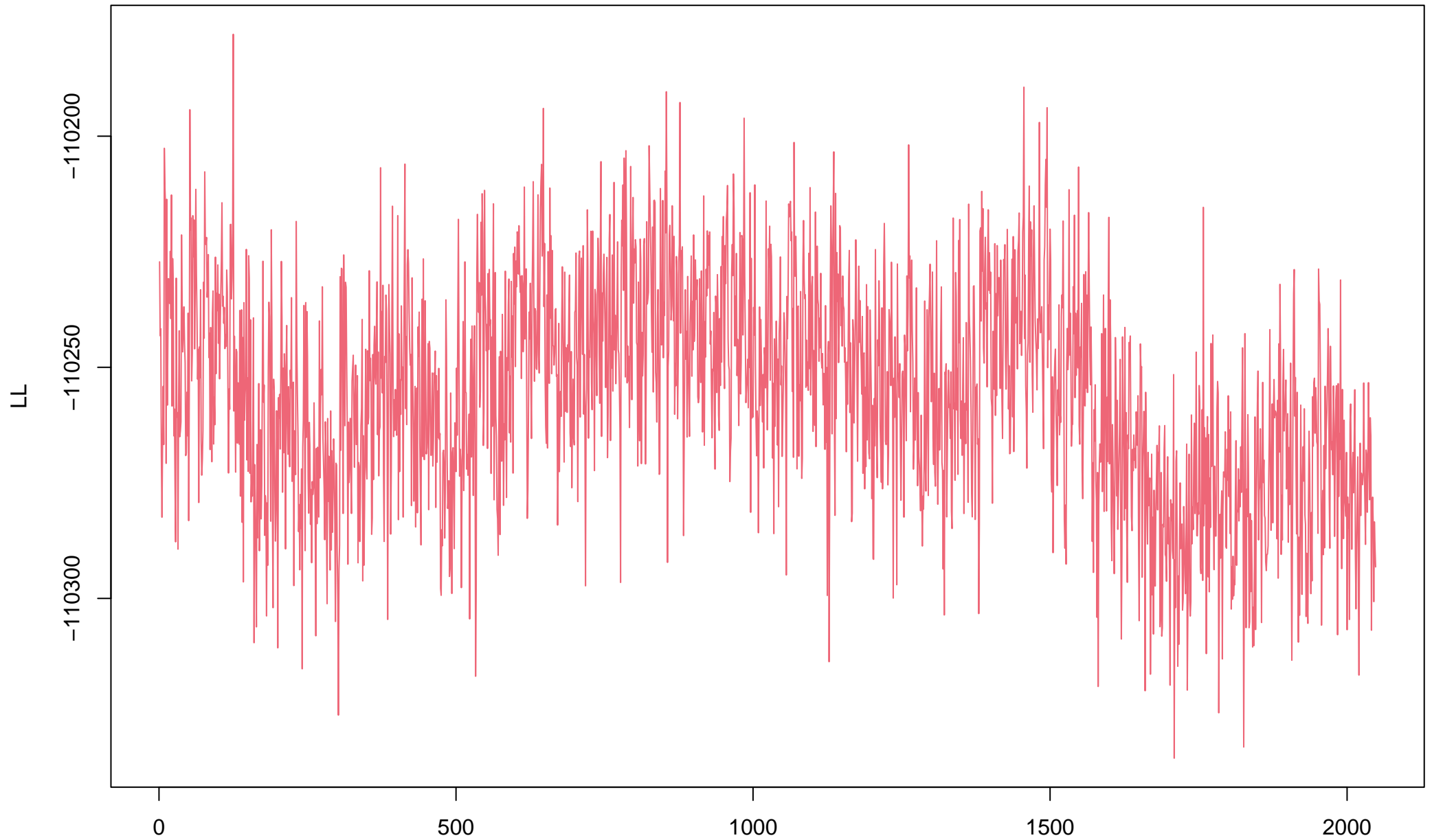




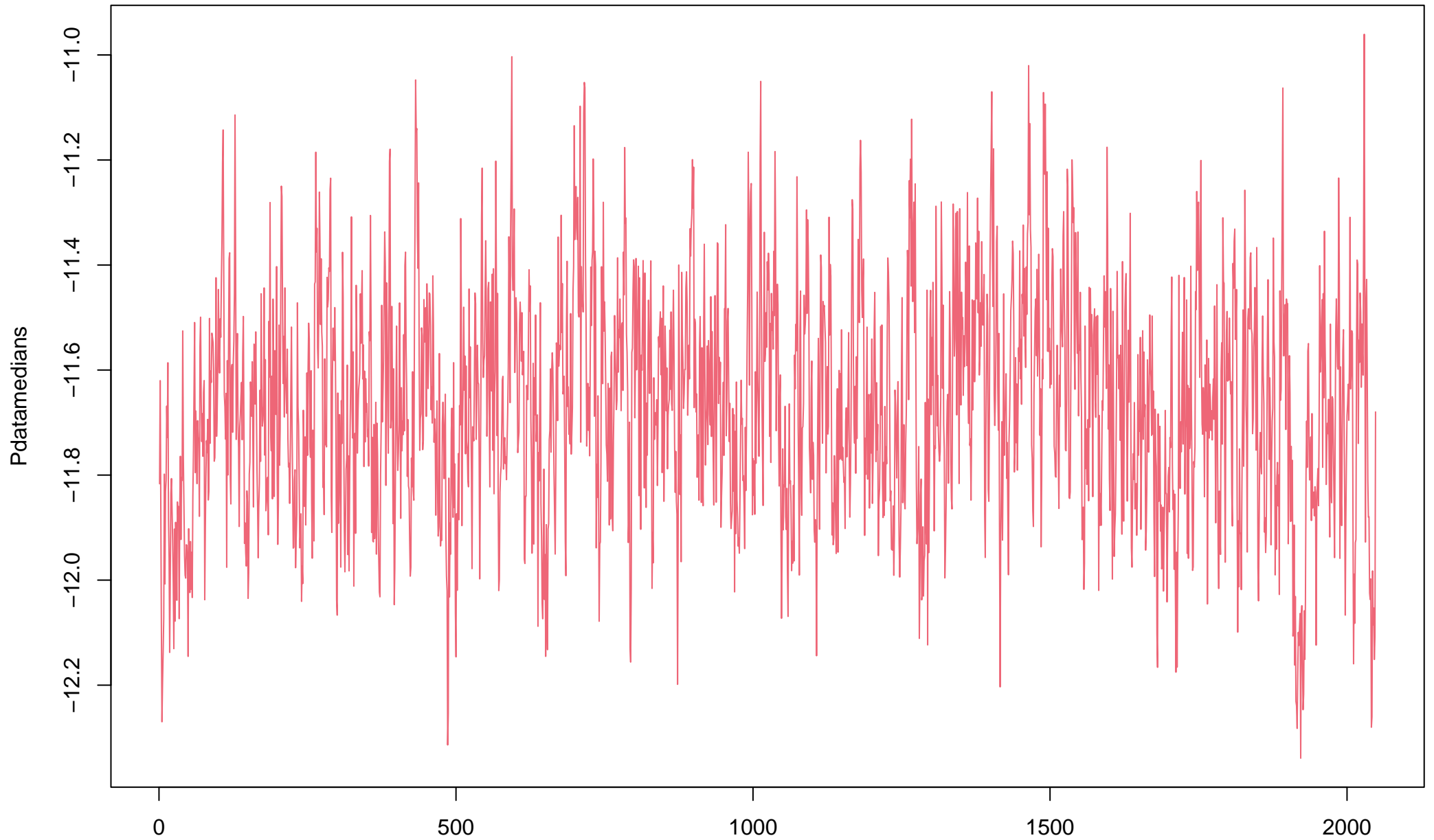




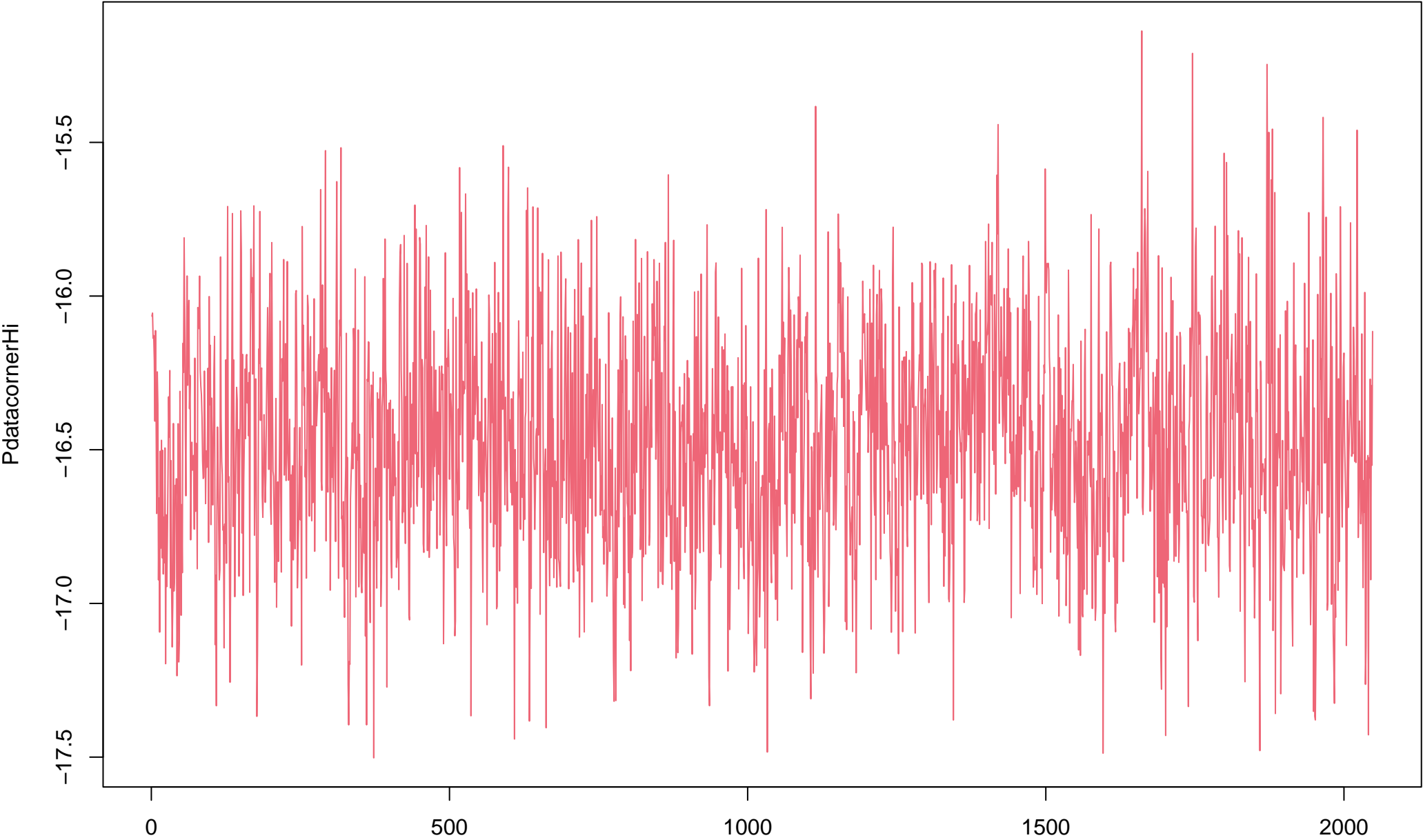
LL
ESS = 24.4 | BMK = 0.163 | MCSE(6.27) = 9.08 | stat: FALSE | burn: 0



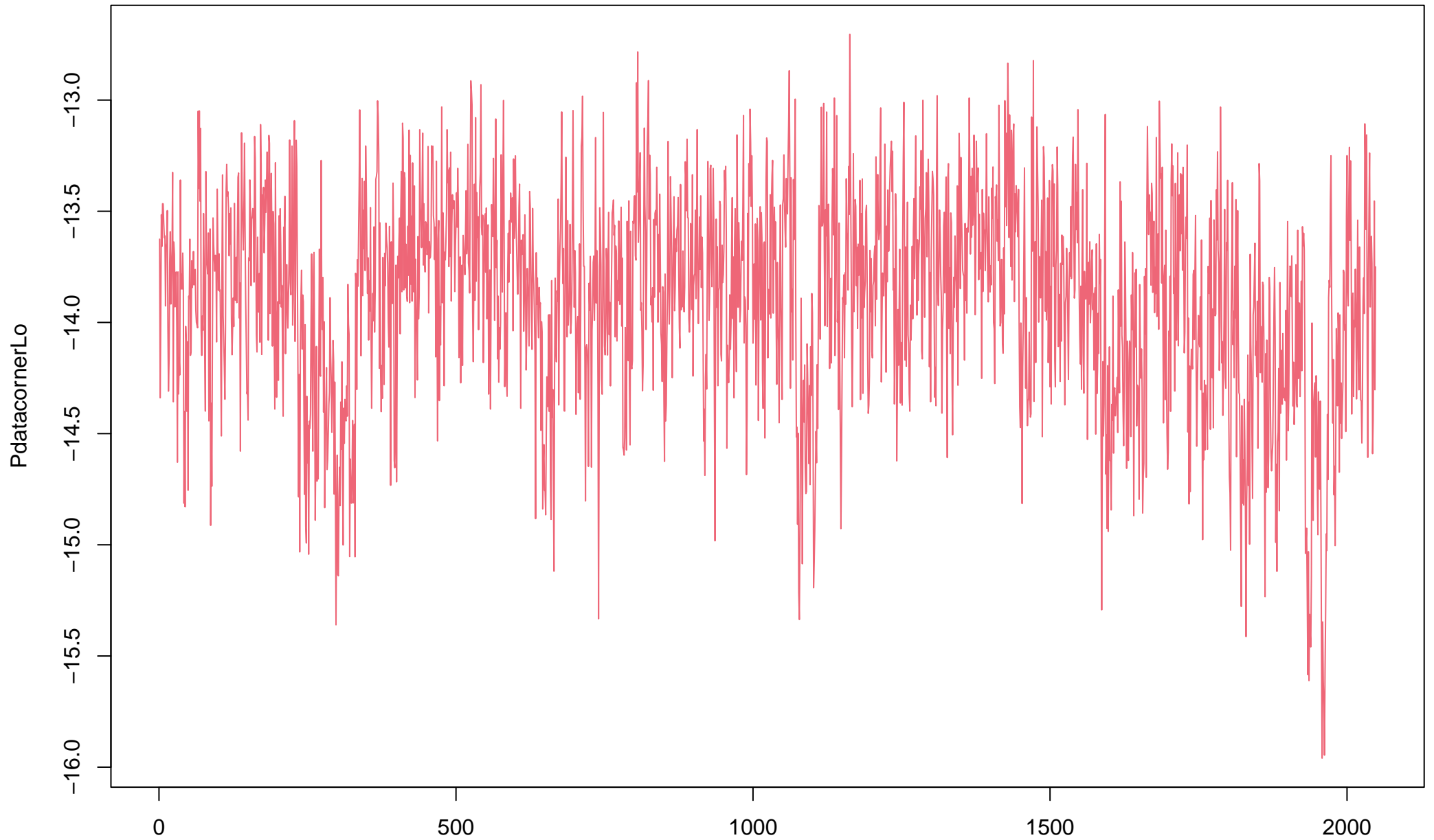
Pdatamedians
ESS = 332 | BMK = 0.0496 | MCSE(6.27) = 5.83 | stat: FALSE | burn: 0



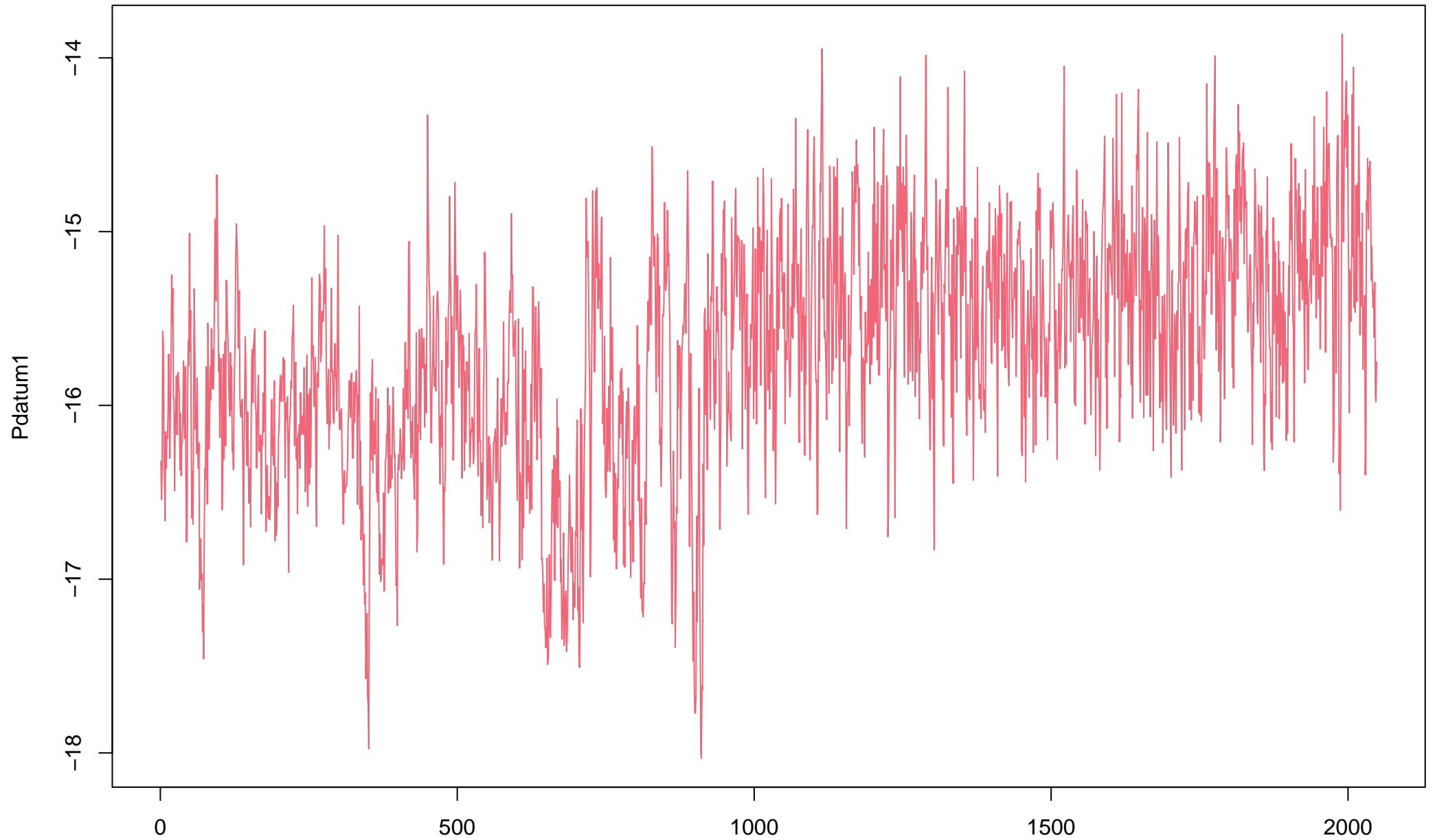
PdatacornerHi
ESS = 817 | BMK = 0.0743 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0



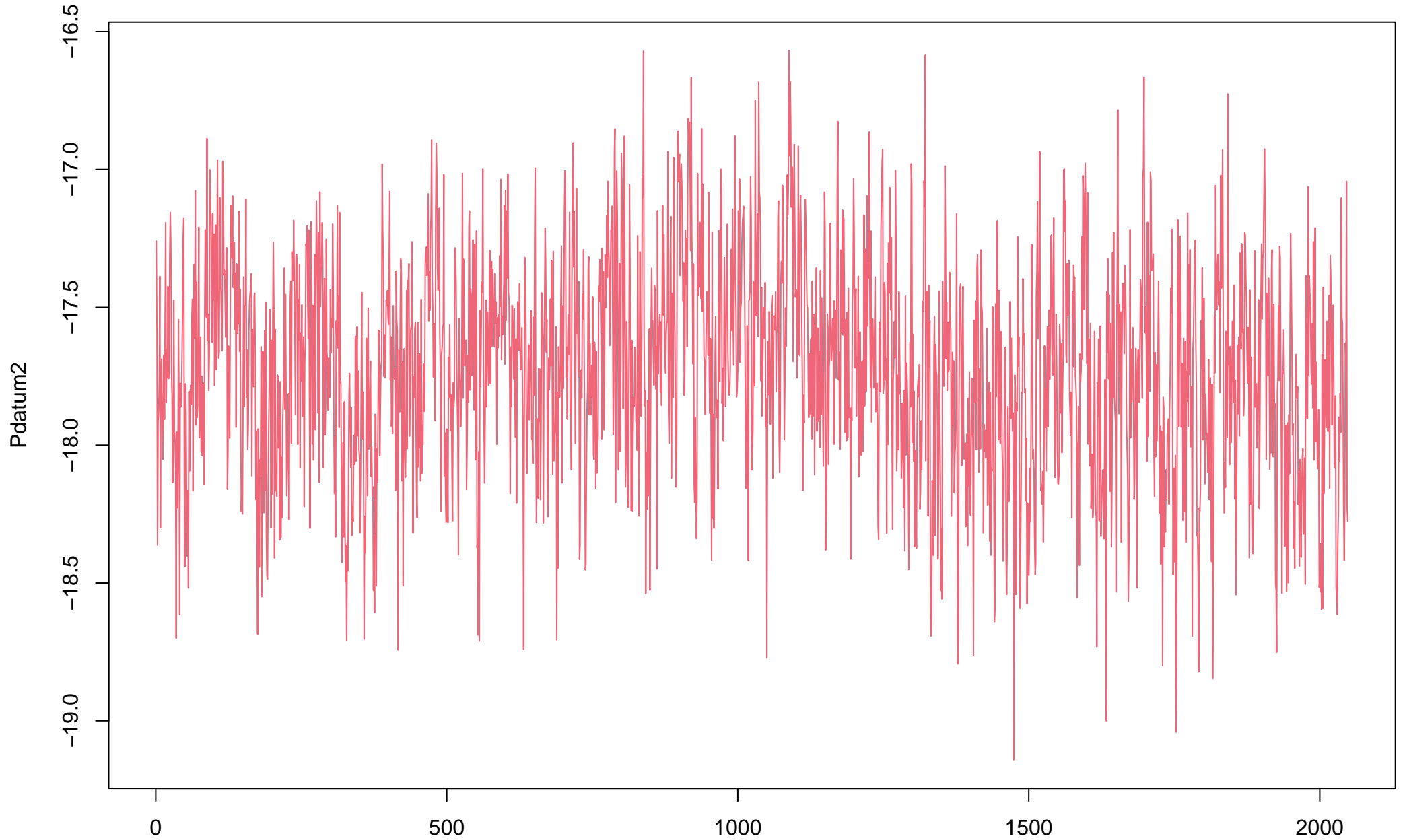
PdatacornerLo
ESS = 135 | BMK = 0.094 | MCSE(6.27) = 6.76 | stat: TRUE | burn: 0



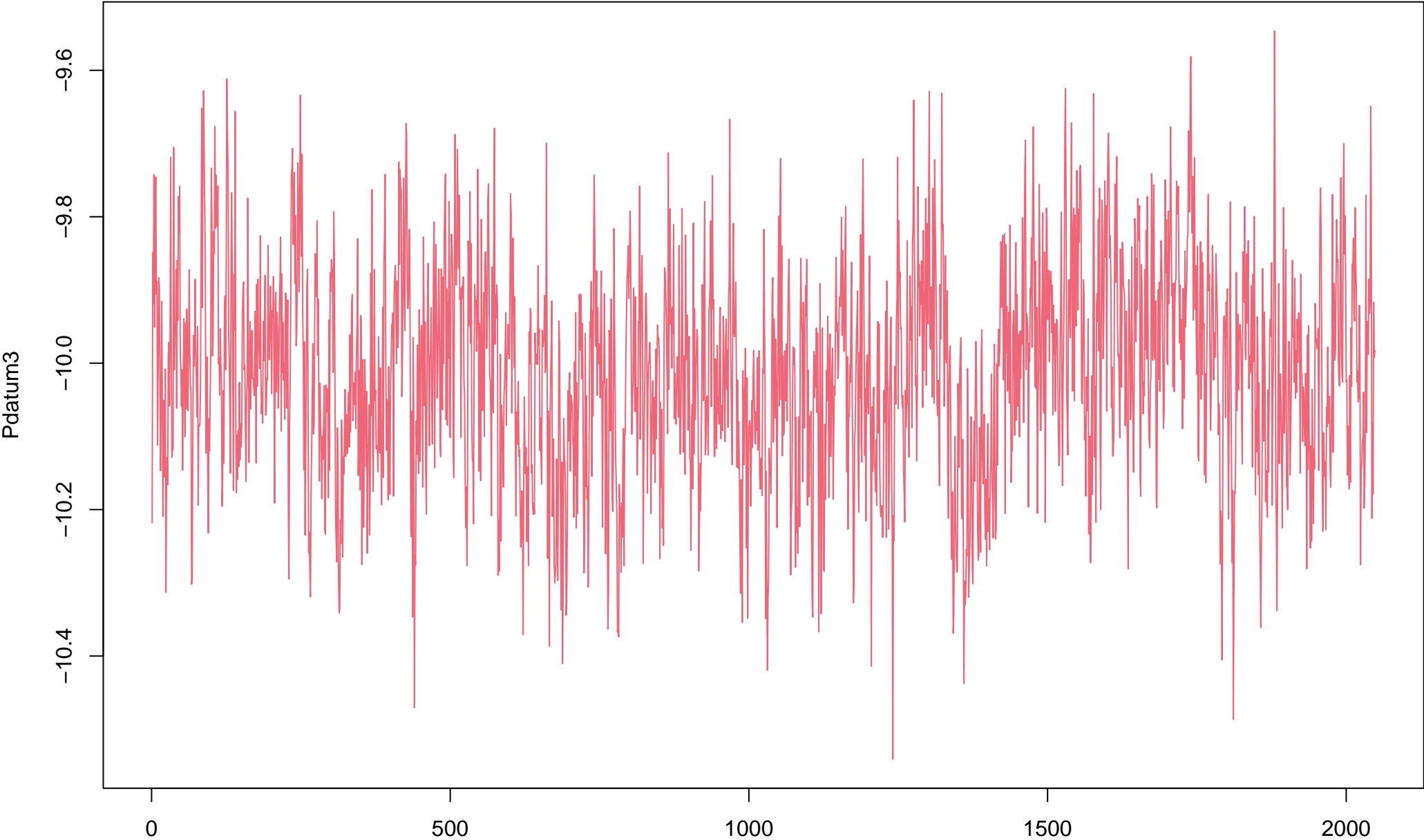
Pdatum1
ESS = 31.8 | BMK = 0.426 | MCSE(6.27) = 8.9 | stat: FALSE | burn: 0



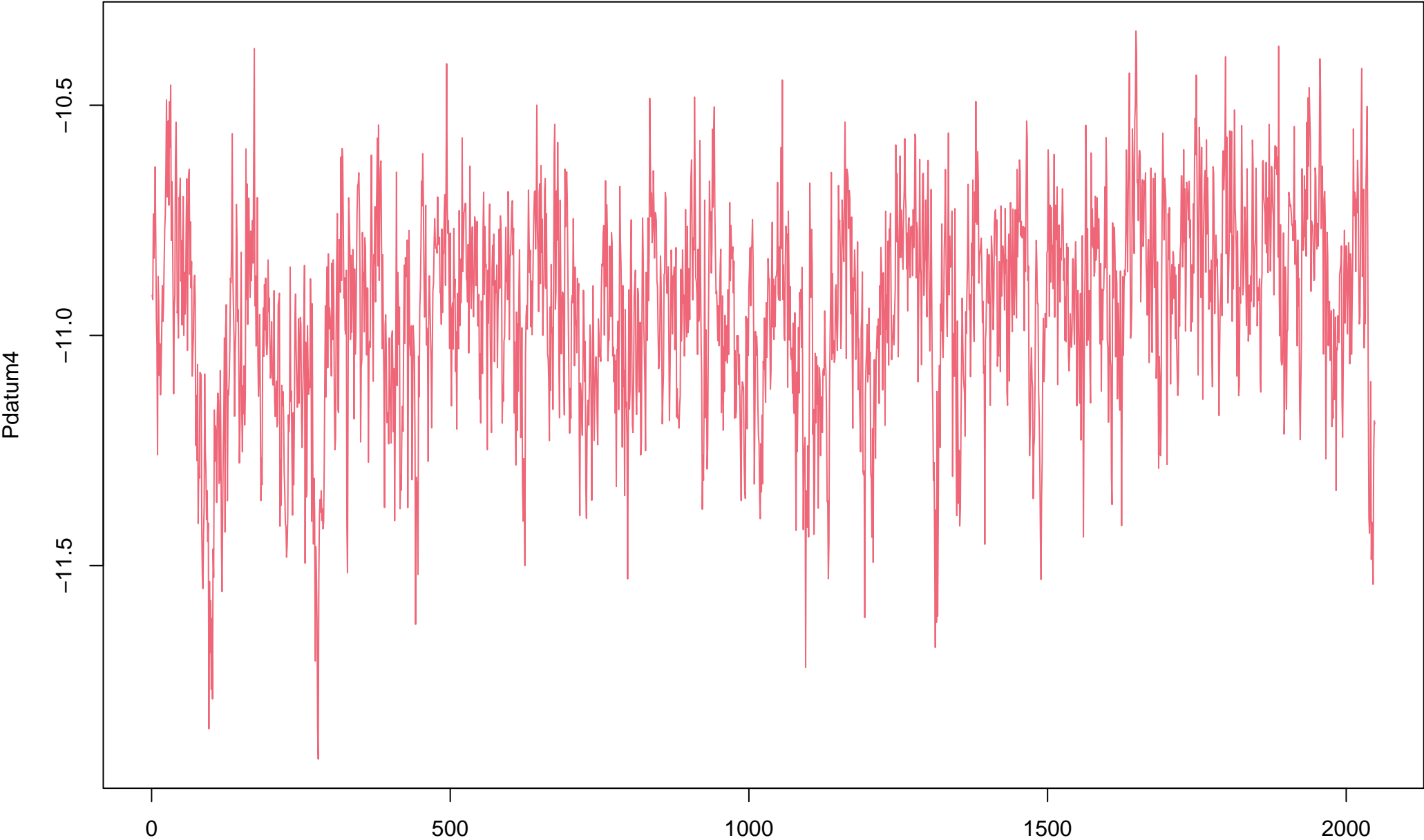
Pdatum2
ESS = 2.22e-16 | BMK = 0.0887 | MCSE(6.27) = 5.89 | stat: TRUE | burn: 0



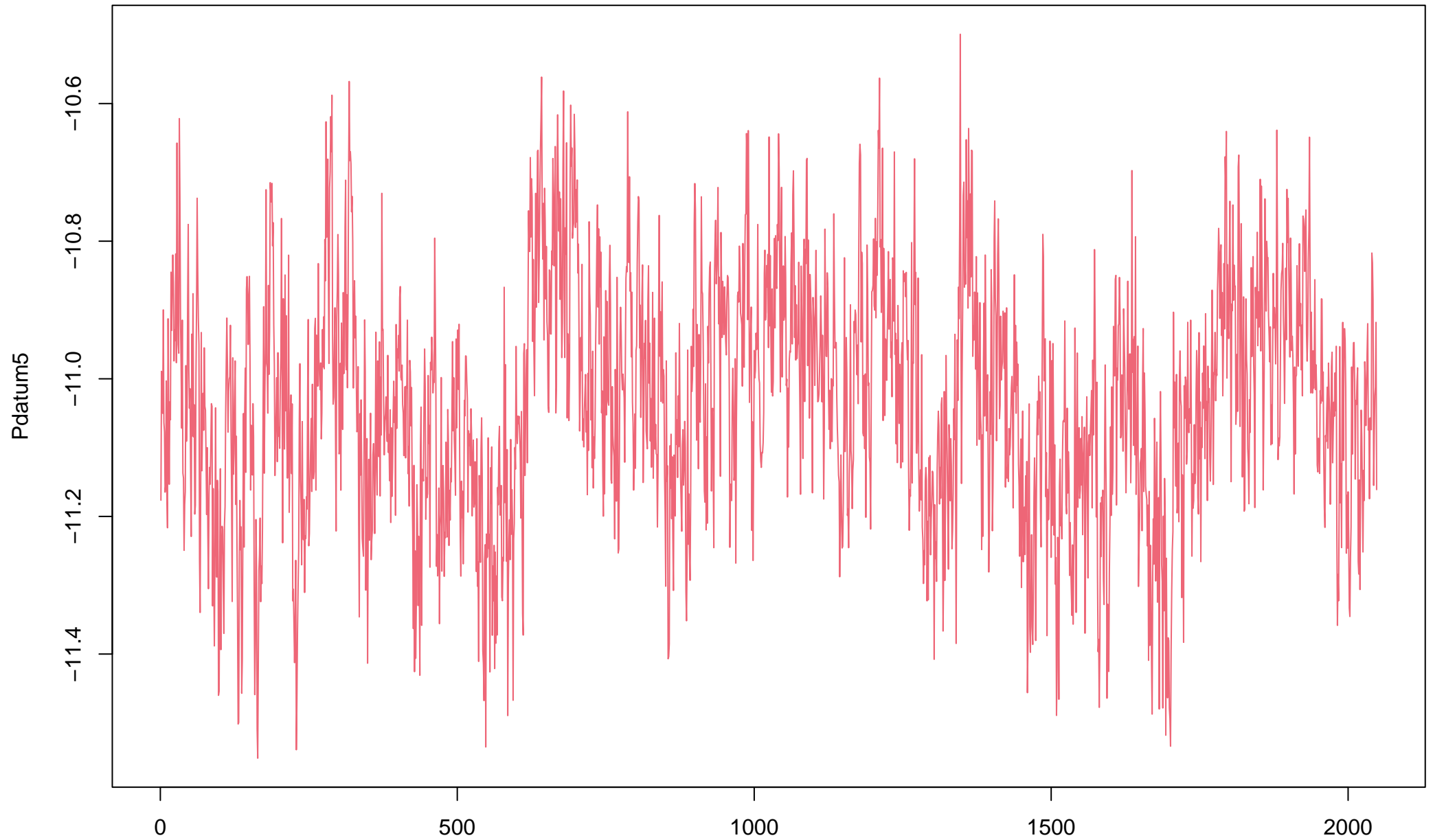
Pdatum3
ESS = 276 | BMK = 0.0629 | MCSE(6.27) = 5.92 | stat: TRUE | burn: 0



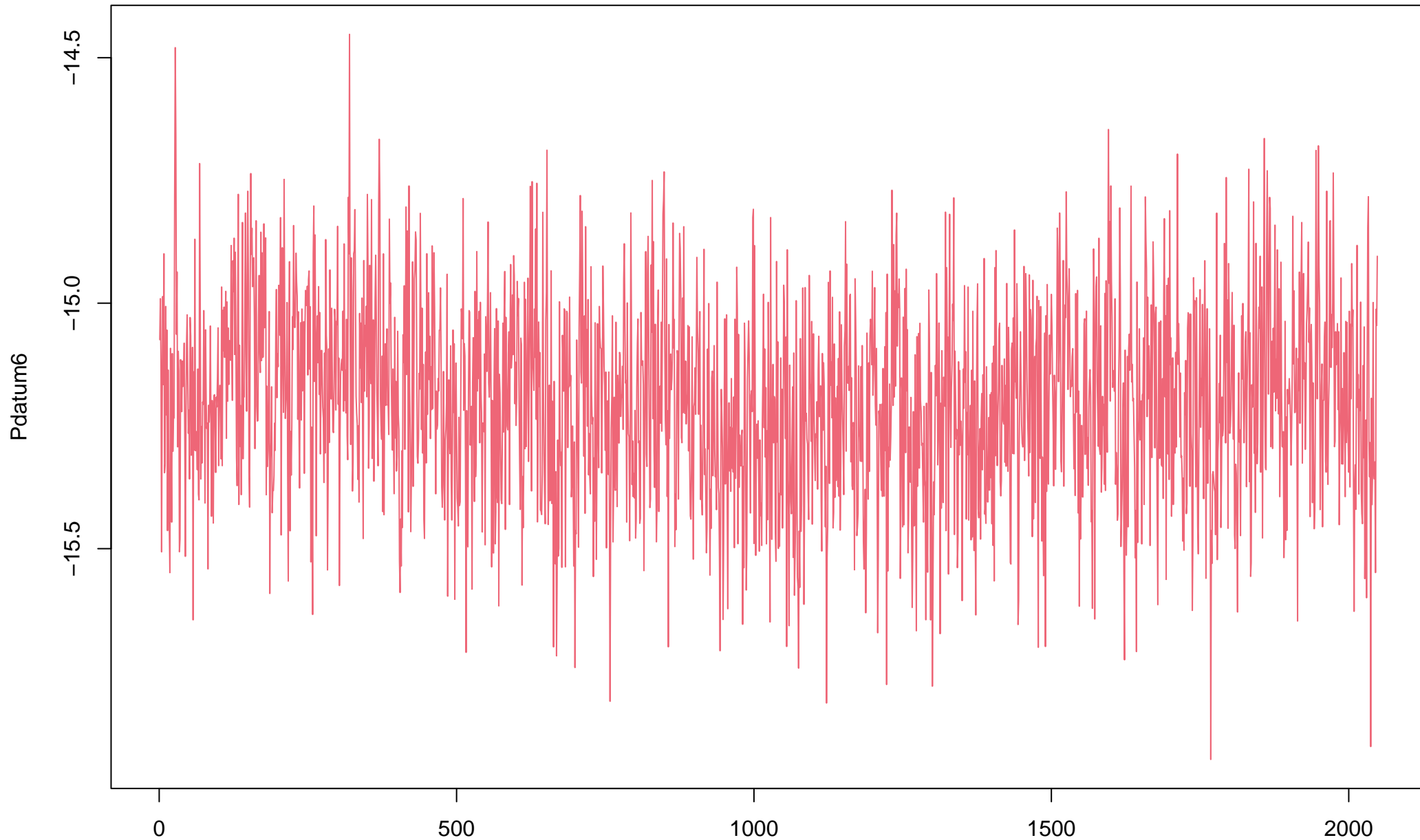
Pdatum4
ESS = 148 | BMK = 0.144 | MCSE(6.27) = 7.62 | stat: FALSE | burn: 0



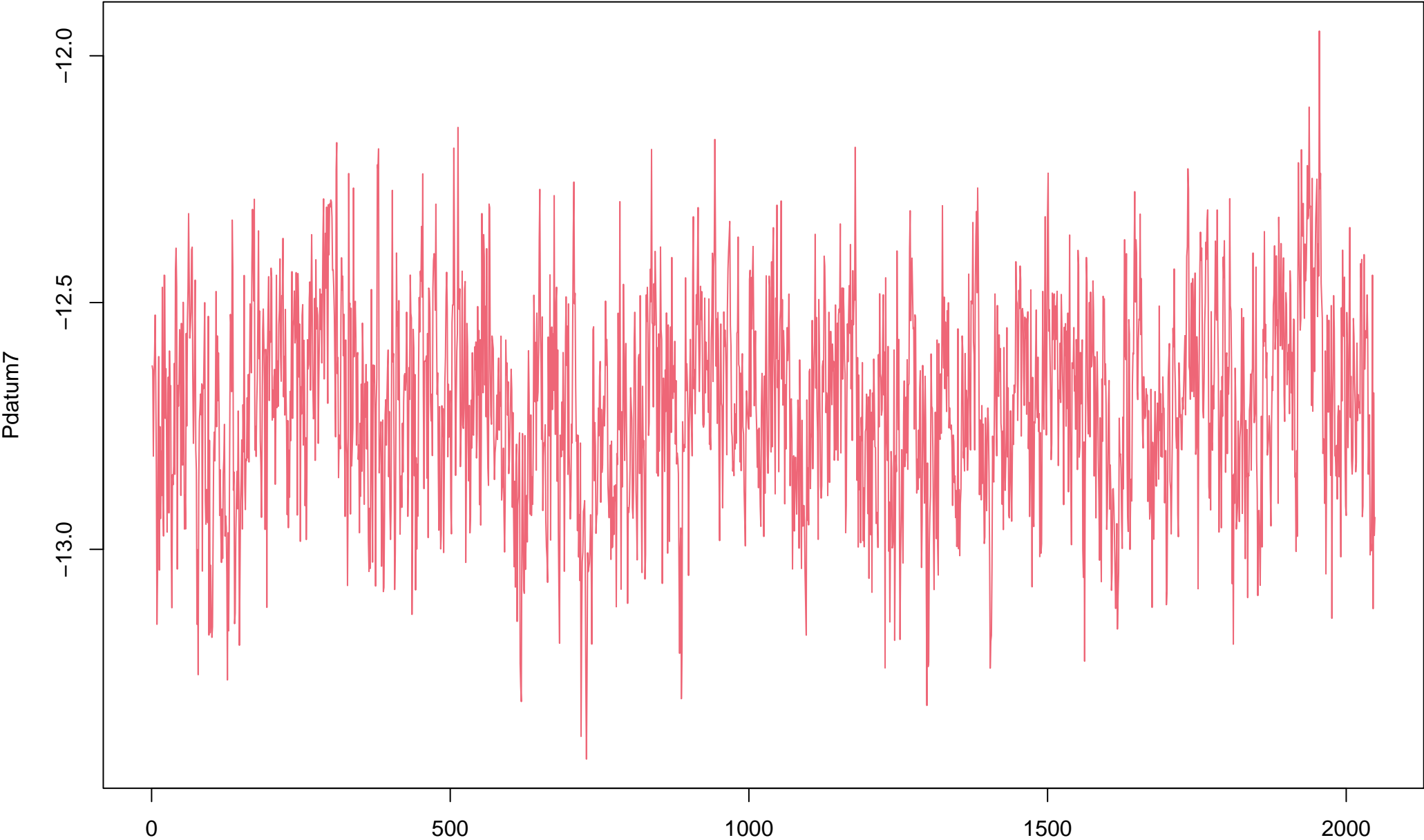
Pdatum5
ESS = 121 | BMK = 0.0602 | MCSE(6.27) = 8.98 | stat: TRUE | burn: 612



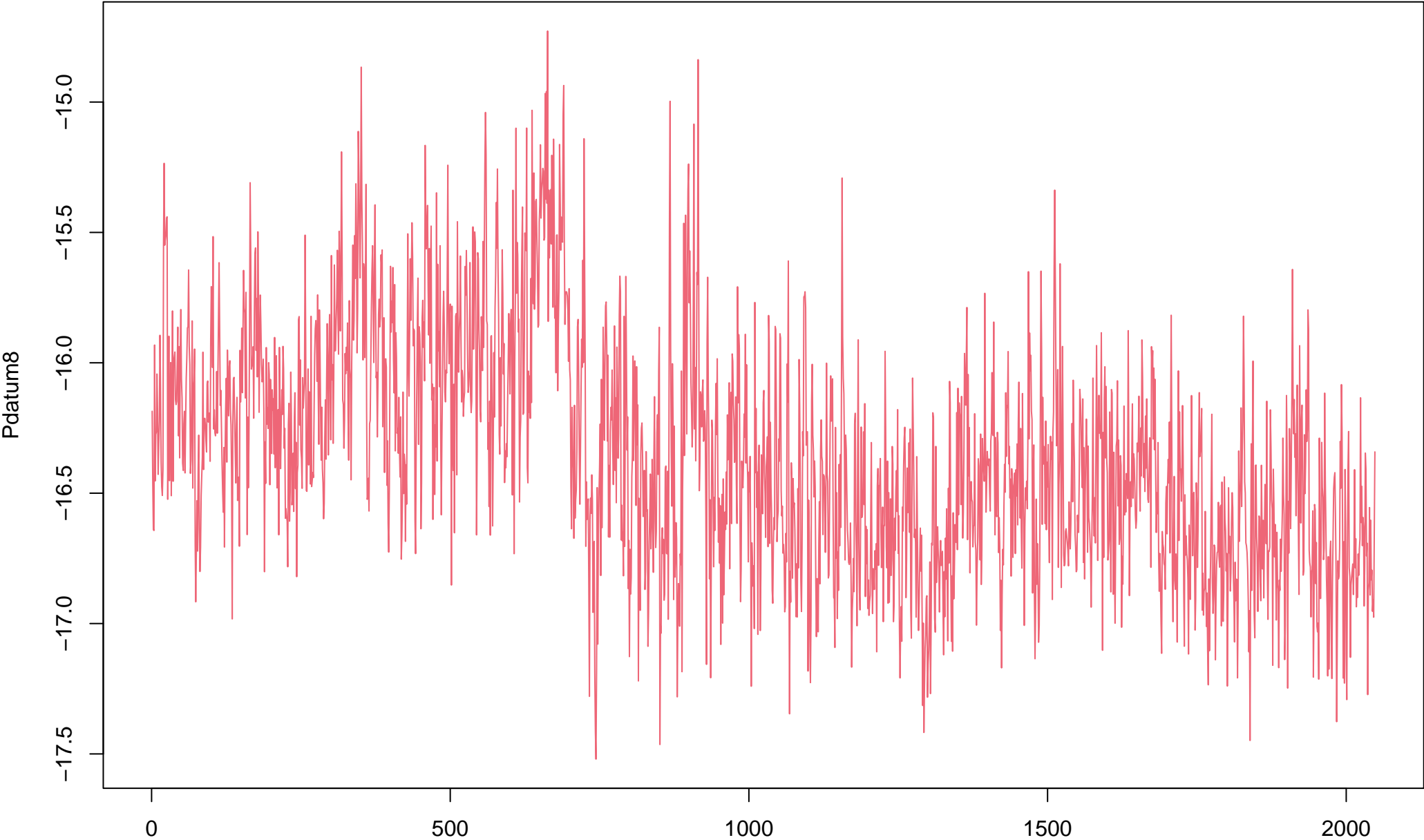
Pdatum6
ESS = 720 | BMK = 0.0632 | MCSE(6.27) = 4.39 | stat: FALSE | burn: 0



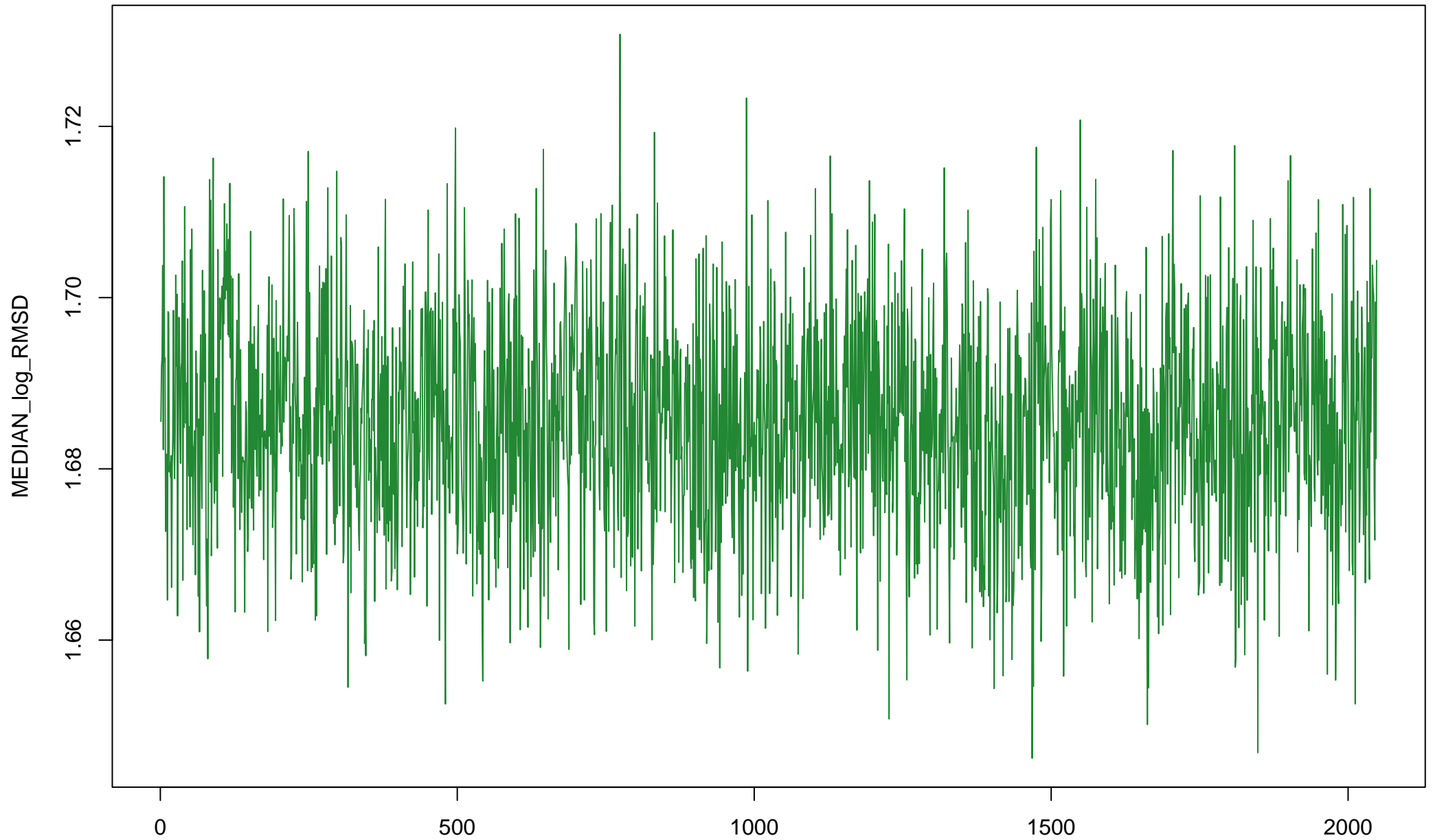
Pdatum7
ESS = 264 | BMK = 0.0432 | MCSE(6.27) = 6.21 | stat: TRUE | burn: 0



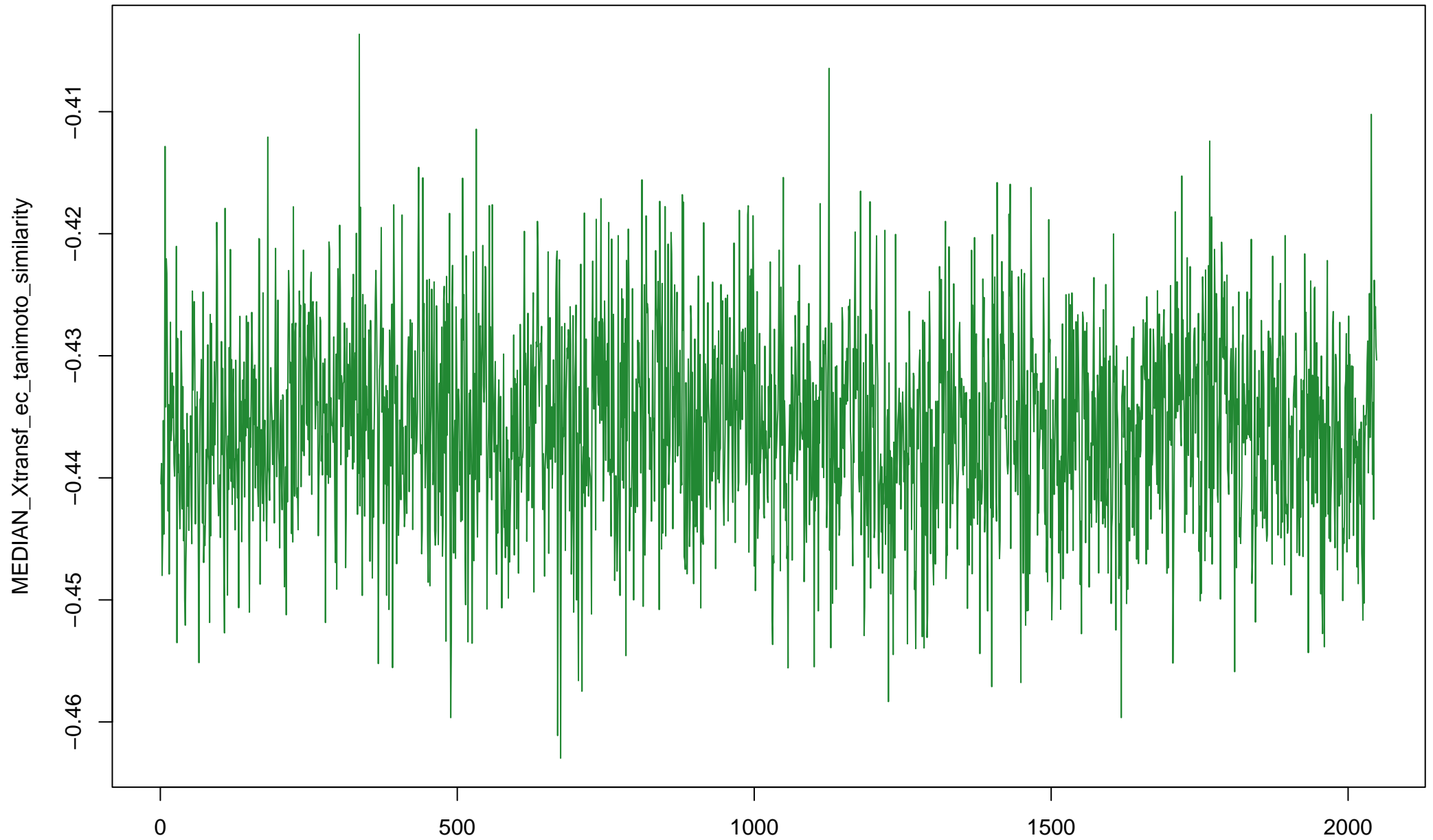
Pdatum8
ESS = 29.3 | BMK = 0.413 | MCSE(6.27) = 9.84 | stat: FALSE | burn: 0



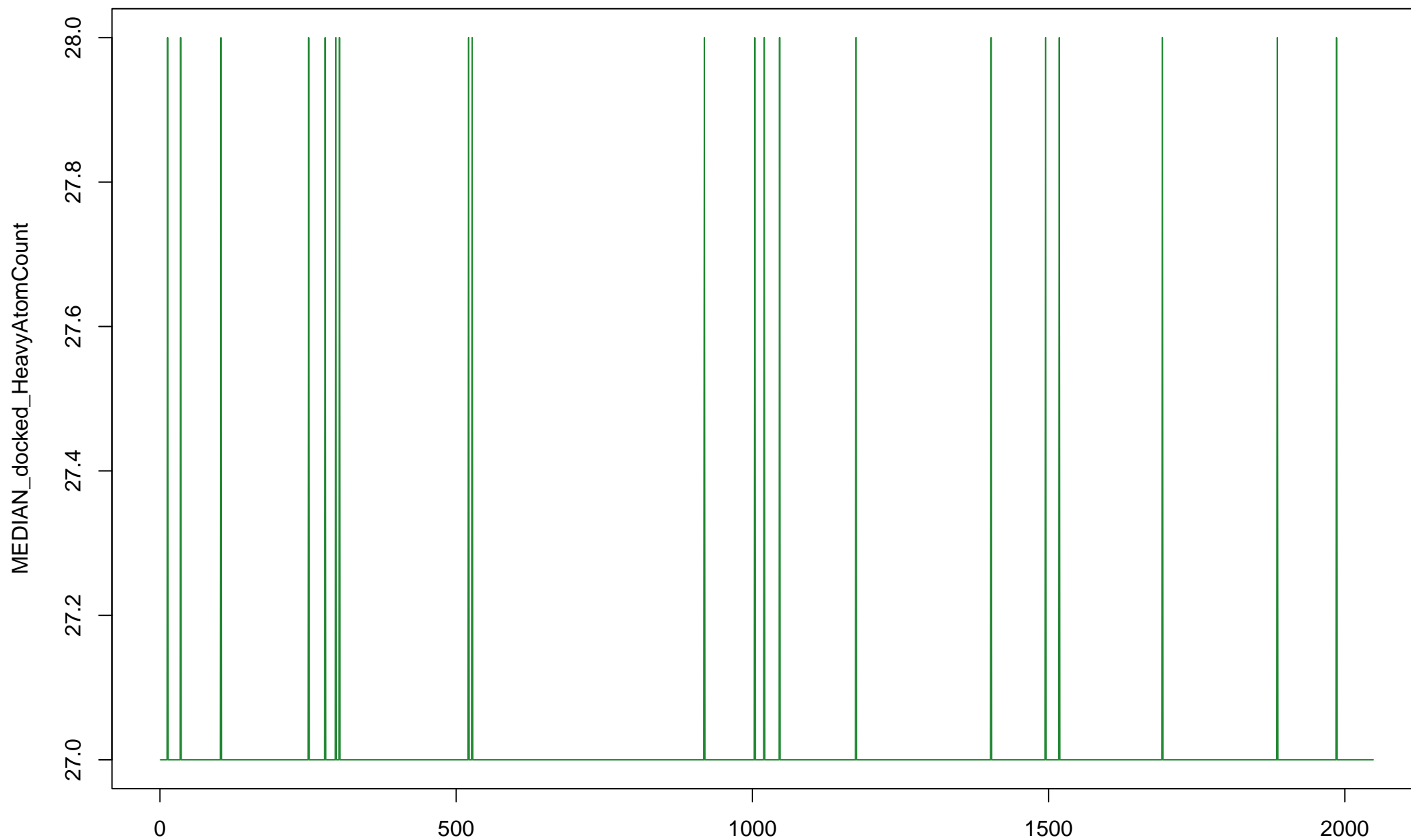
MEDIAN_log_RMSD
ESS = 1380 | BMK = 0.0451 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0



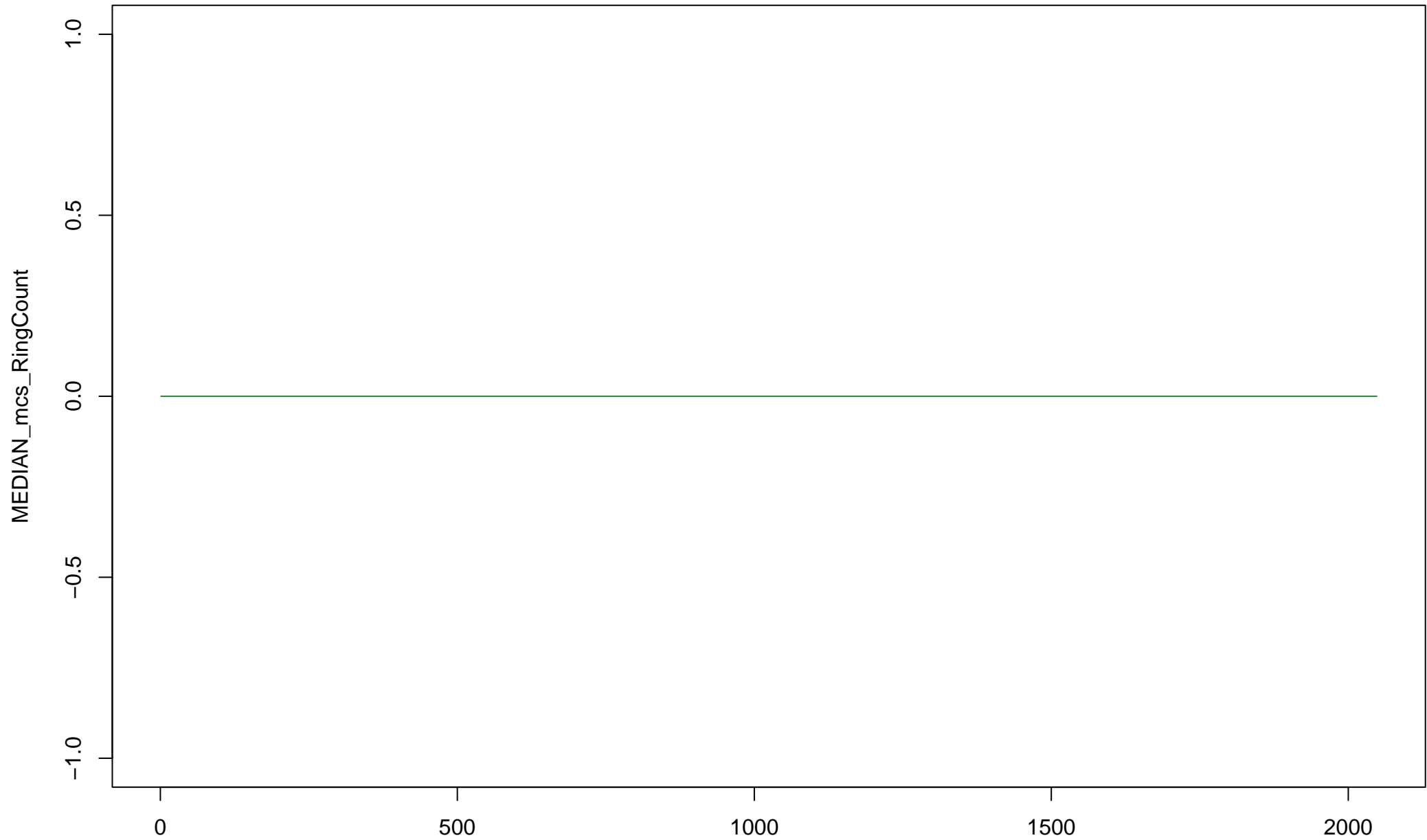
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1680 | BMK = 0.062 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0



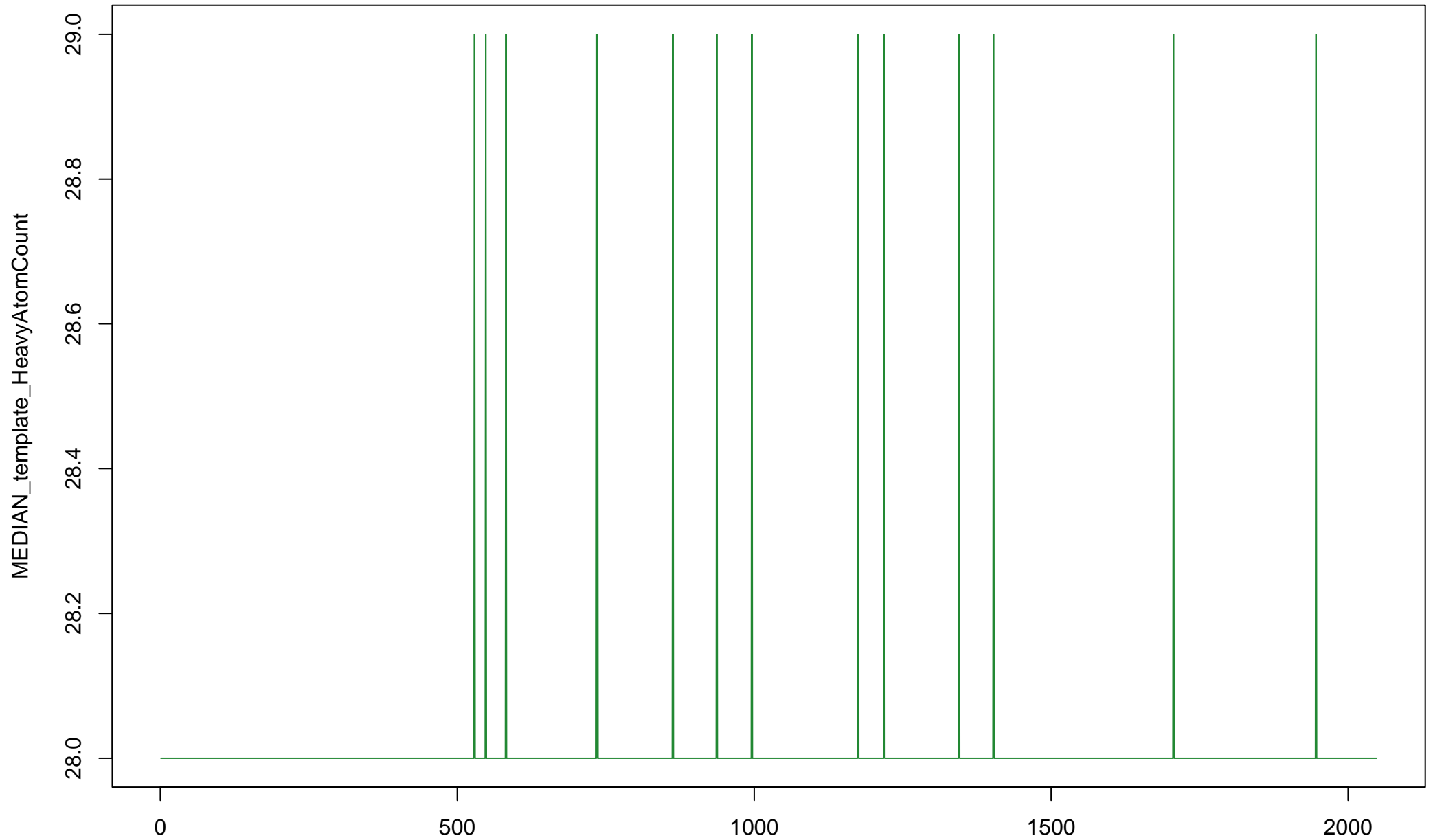
MEDIAN_docked_HeavyAtomCount
ESS = 1880 | BMK = 0.0716 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0



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



MEDIAN_template_HeavyAtomCount
ESS = 1820 | BMK = 0.0509 | MCSE(6.27) = 2.23 | stat: FALSE | burn: 1632



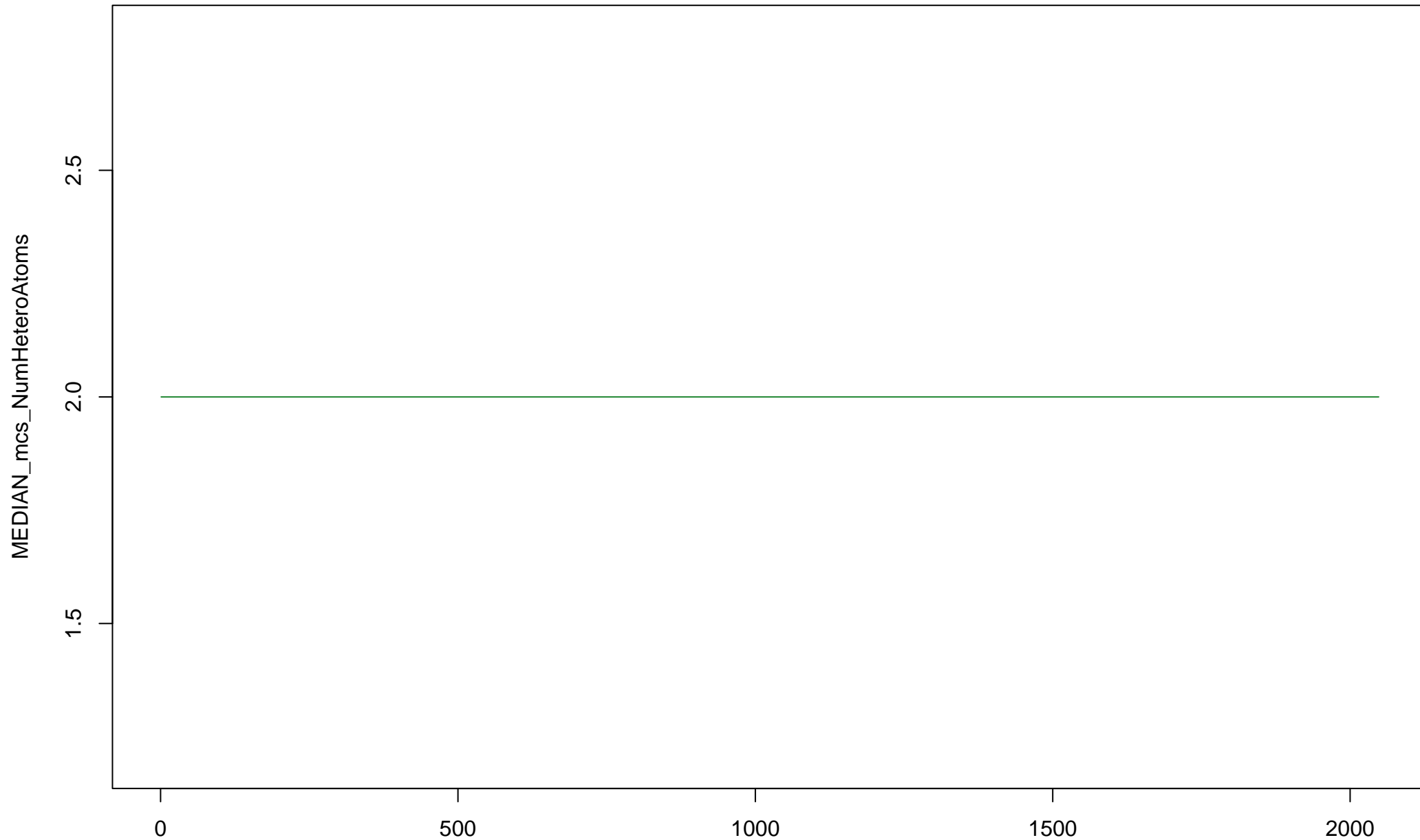
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



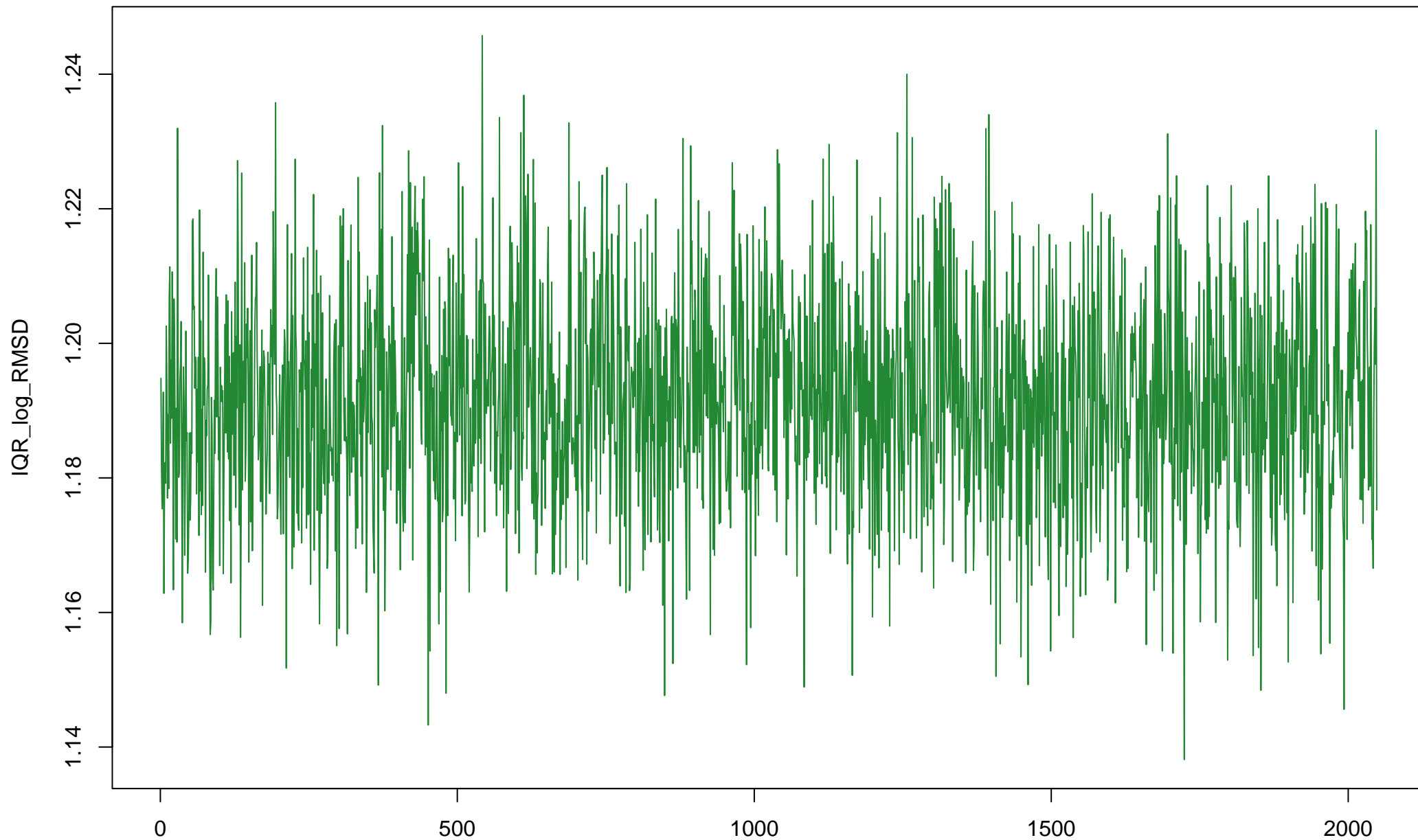
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



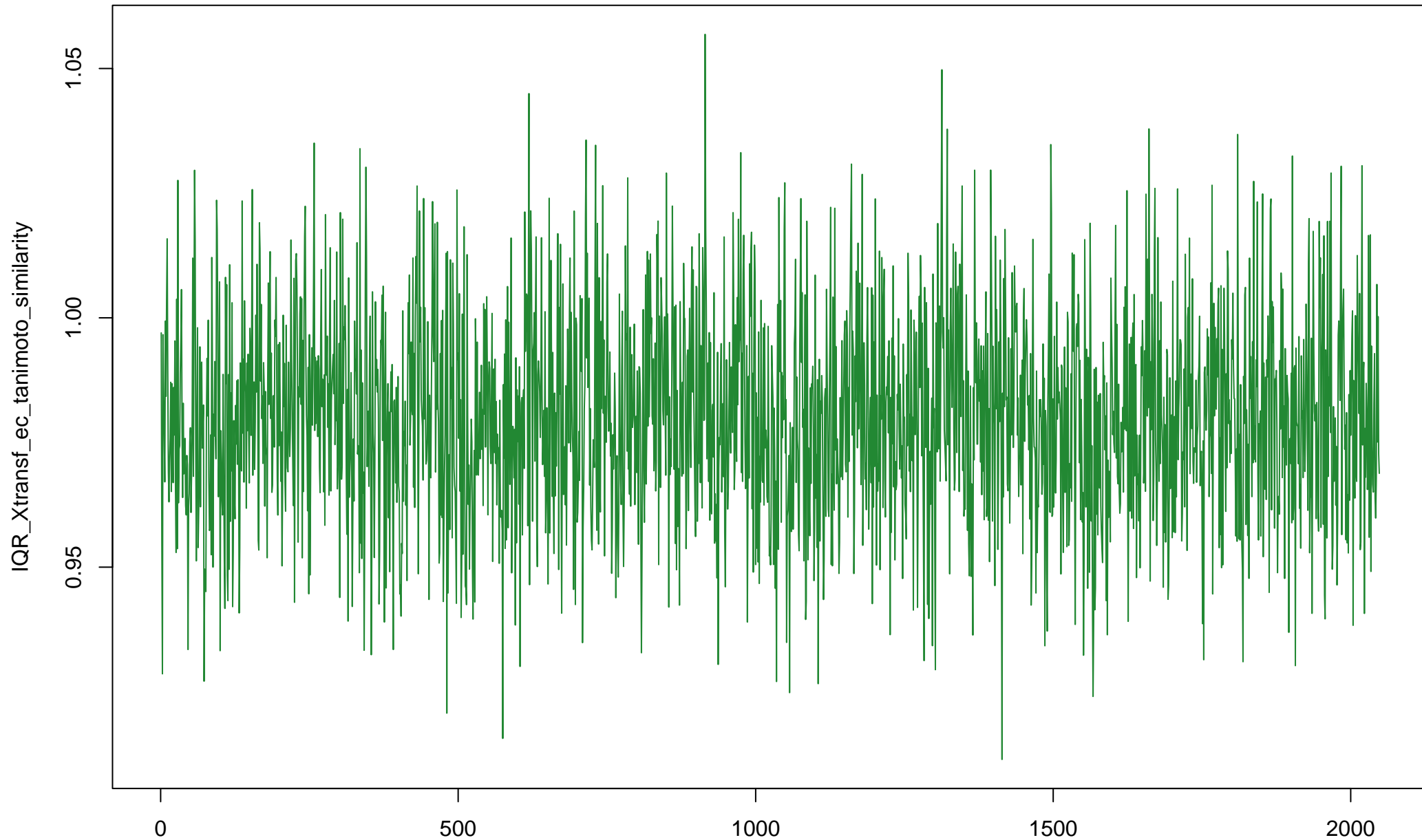
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



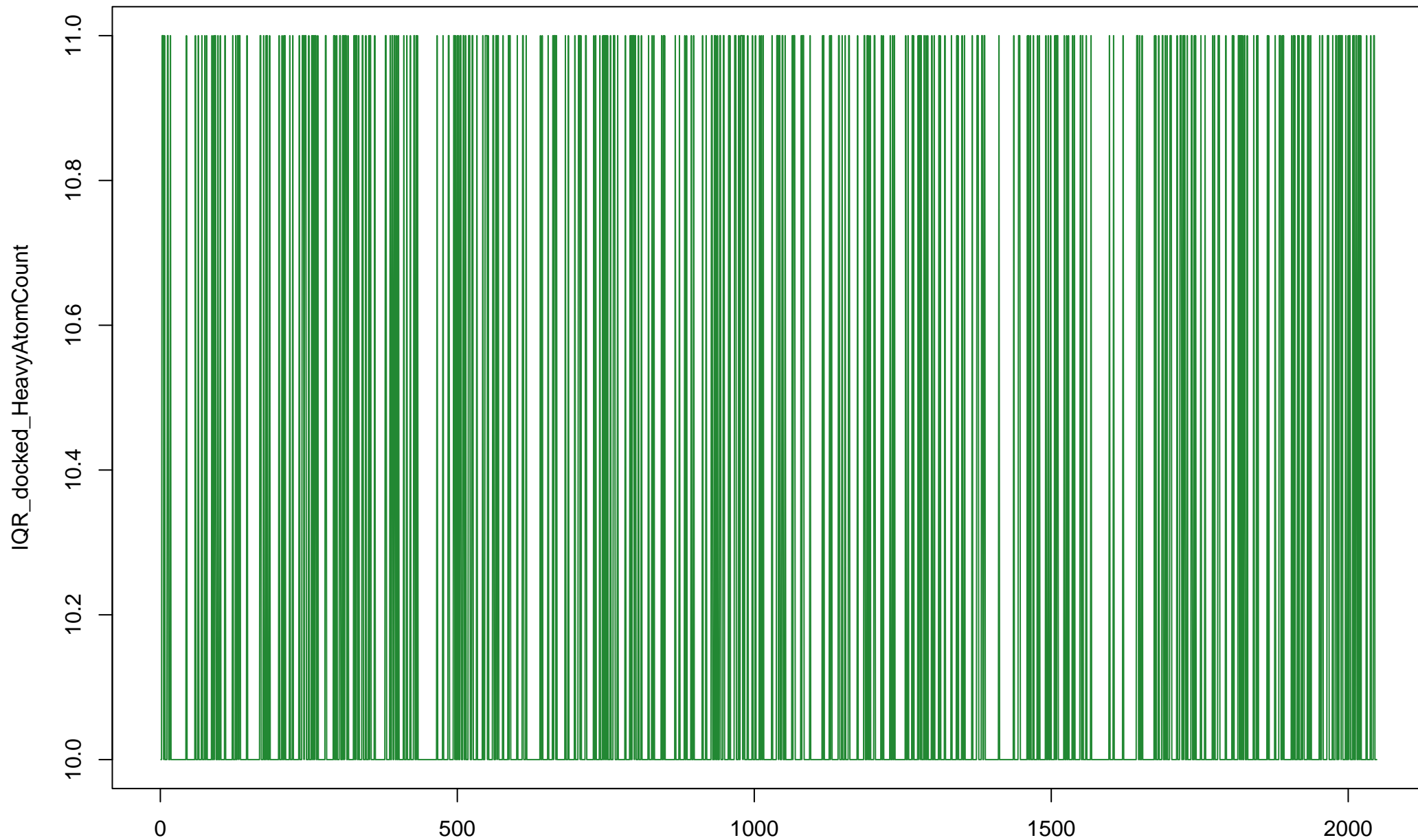
IQR_log_RMSD
ESS = 1670 | BMK = 0.0278 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0



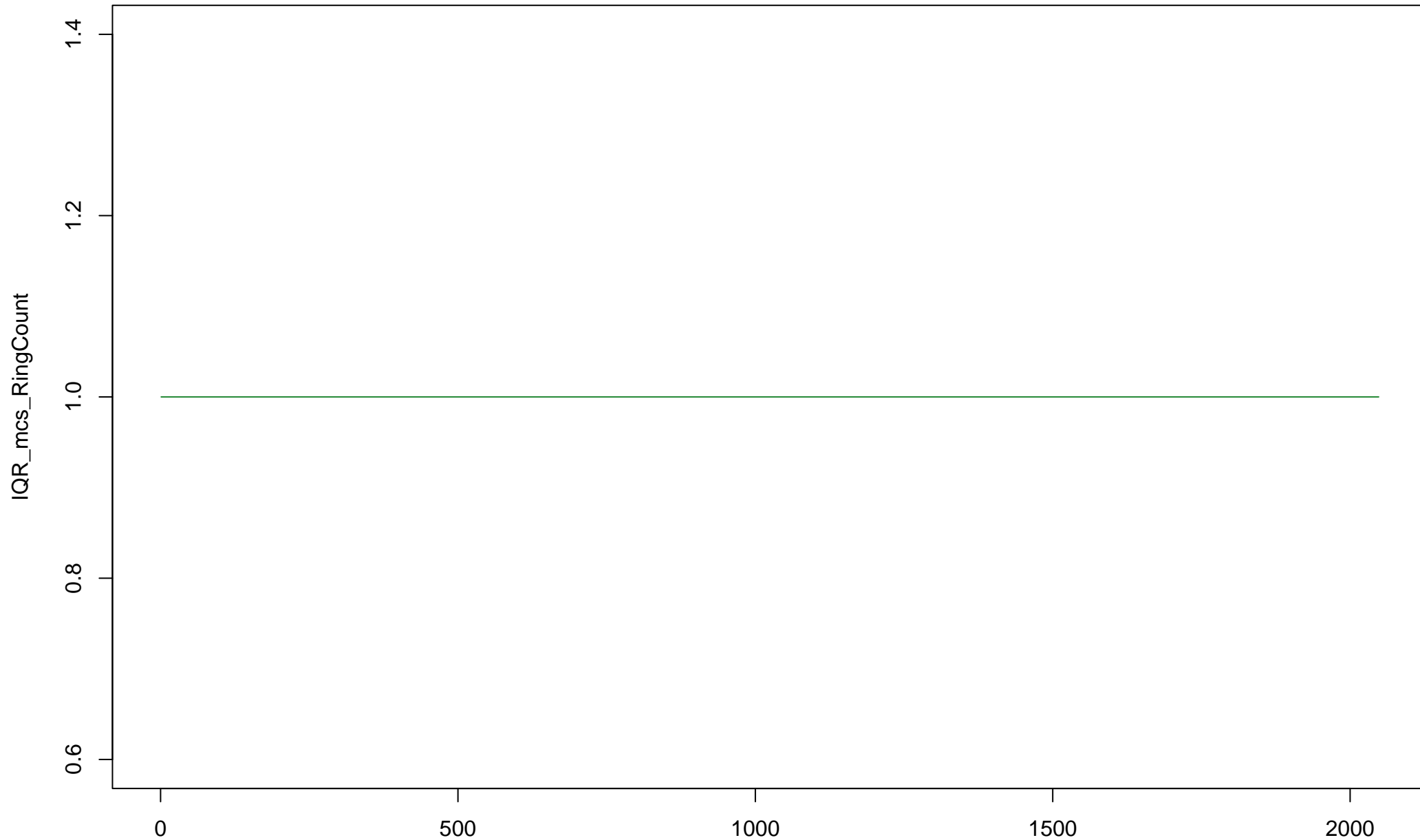
IQR_Xtransf_ec_tanimoto_similarity
ESS = 1800 | BMK = 0.0295 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0



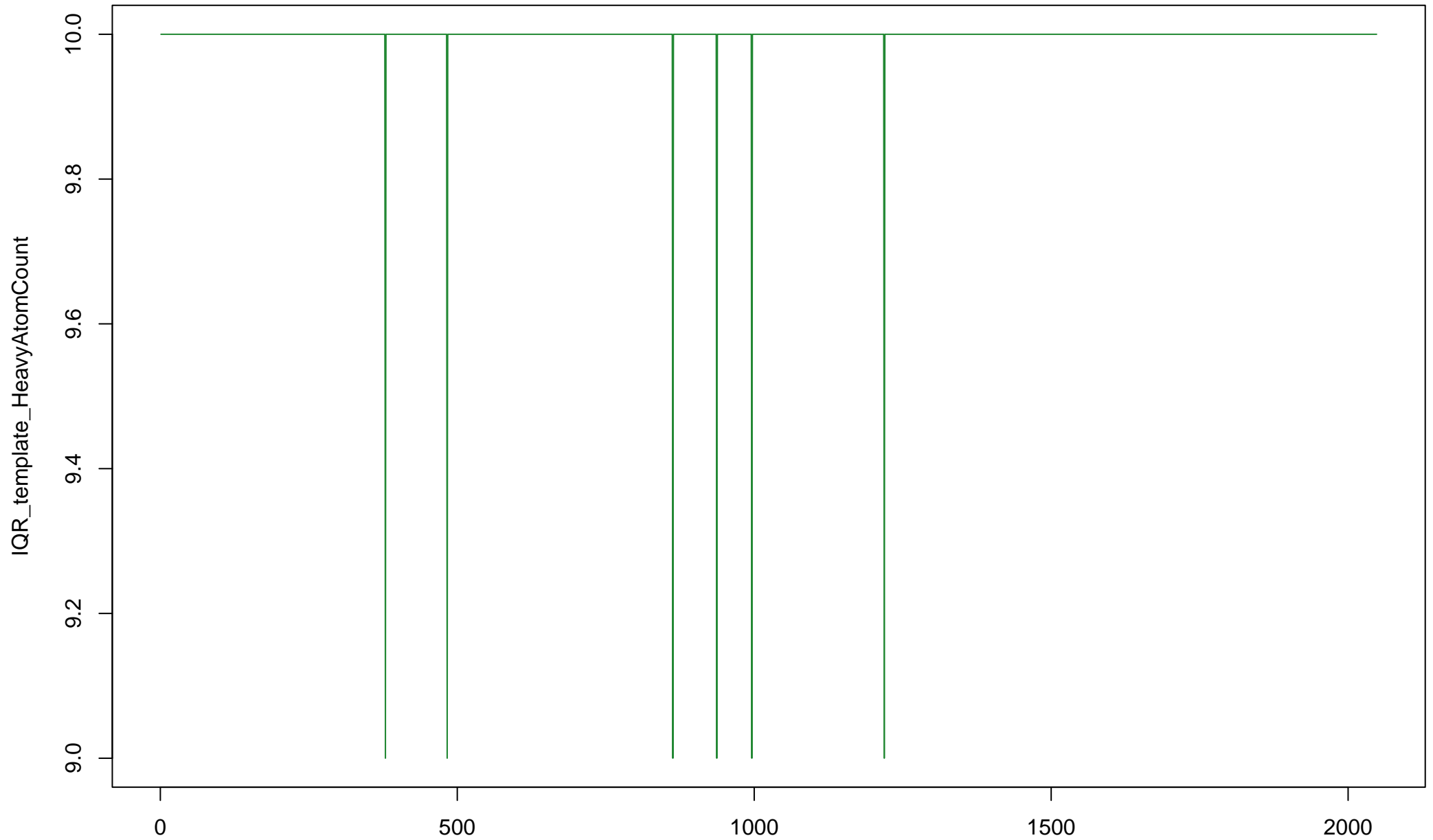
IQR_docked_HeavyAtomCount
ESS = 1800 | BMK = 0.0141 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0



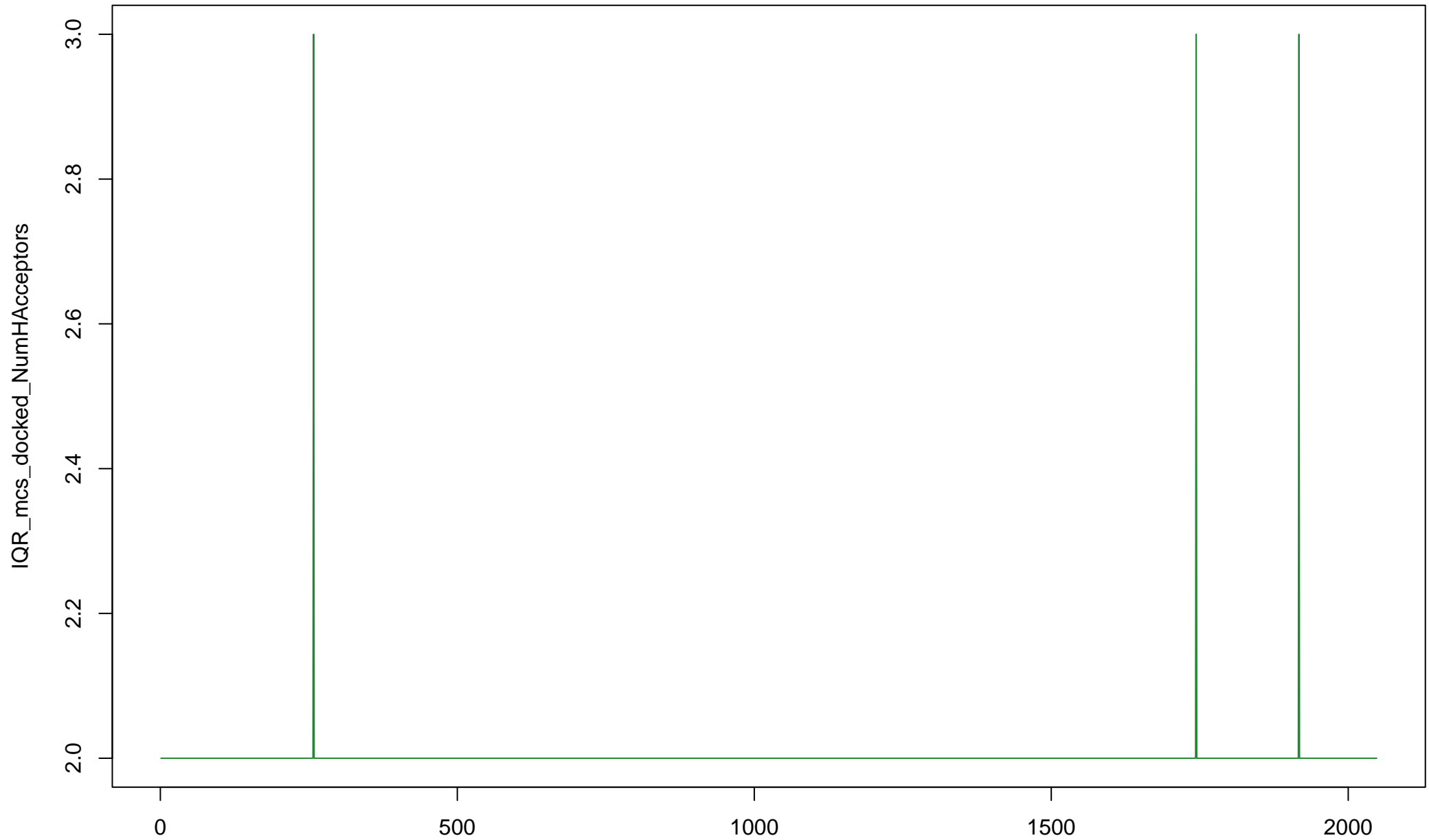
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



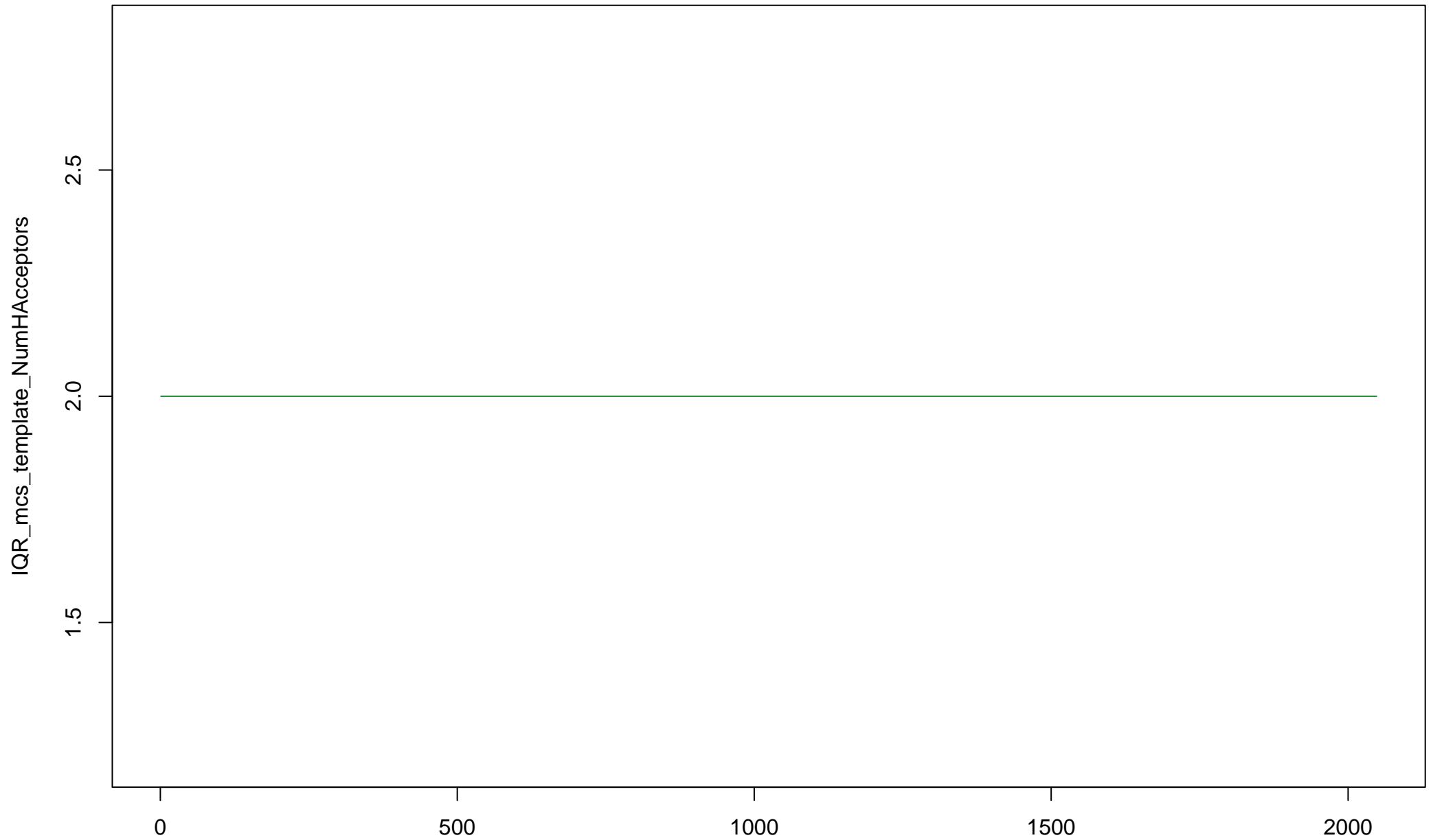
IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.264 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 1224



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



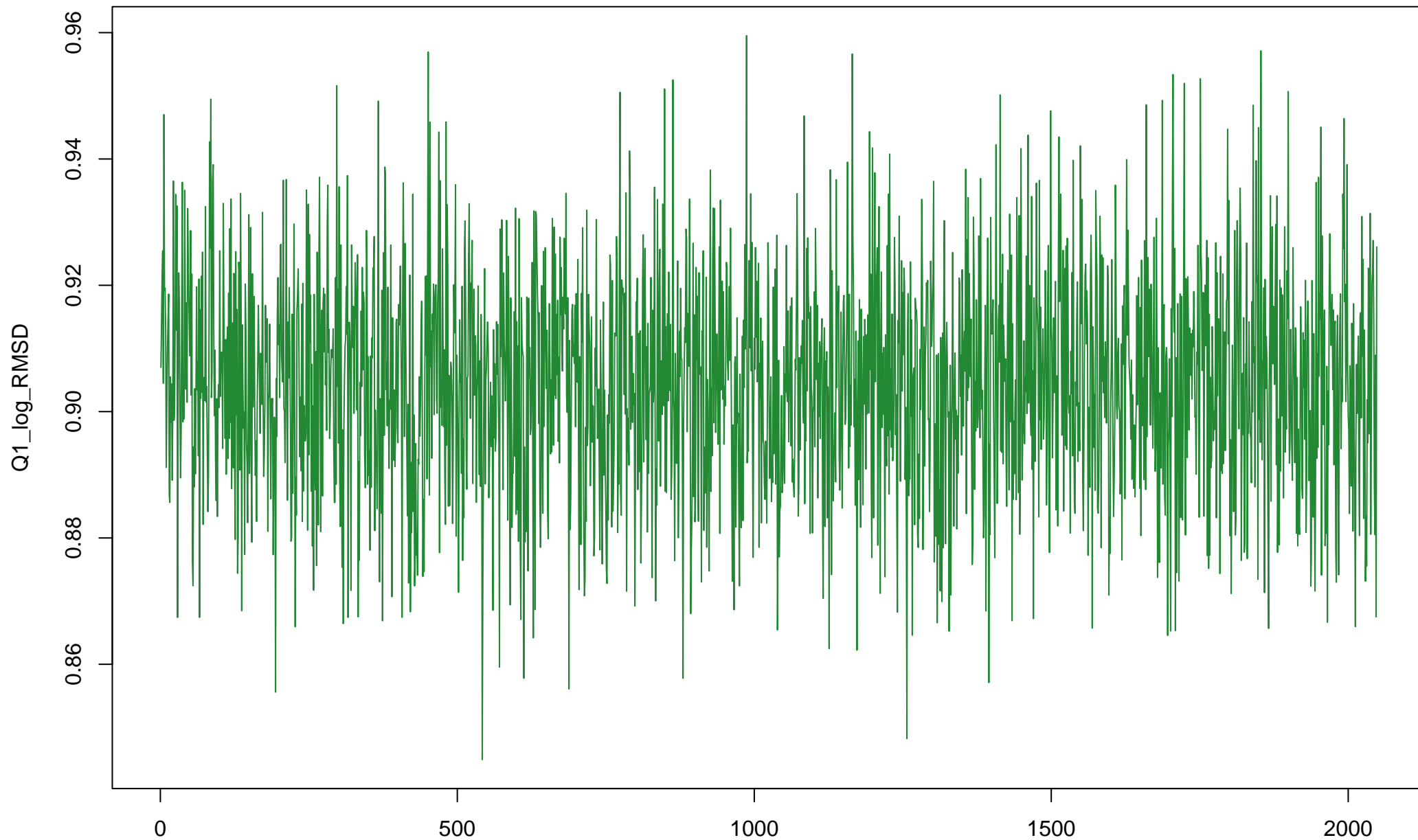
IQR_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



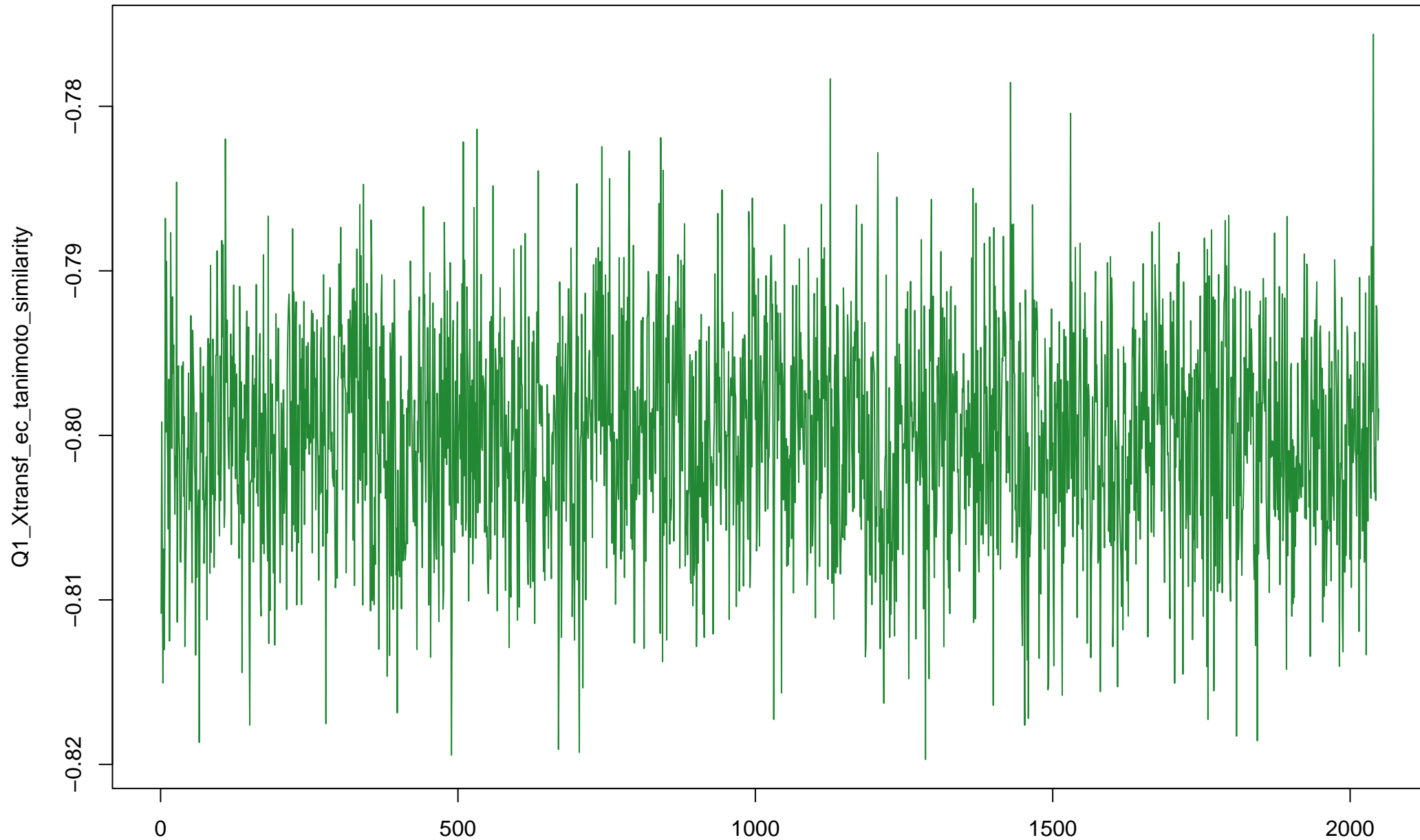
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



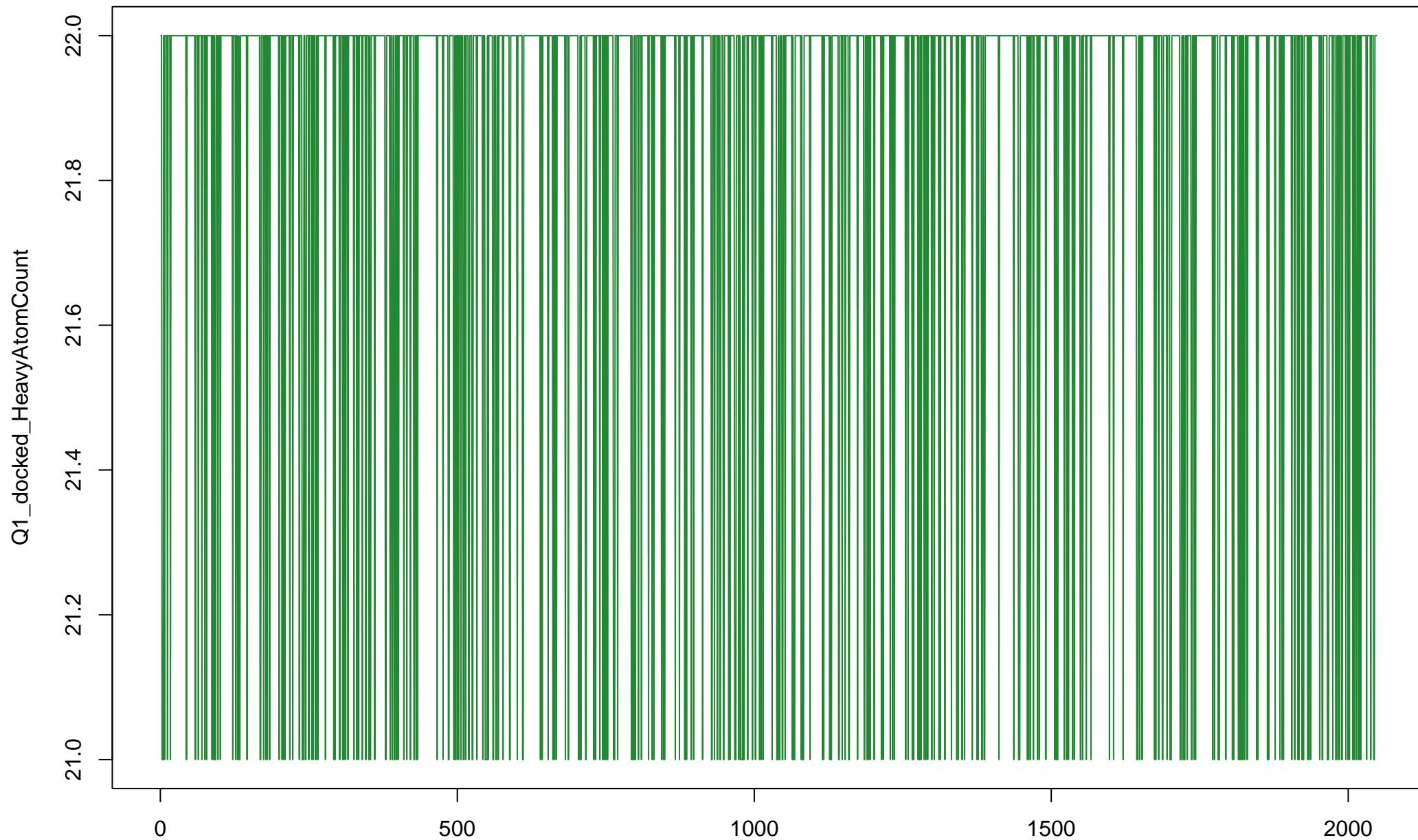
Q1_log_RMSD
ESS = 1880 | BMK = 0.0359 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0



Q1_Xtransf_ec_tanimoto_similarity
ESS = 1520 | BMK = 0.0536 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0



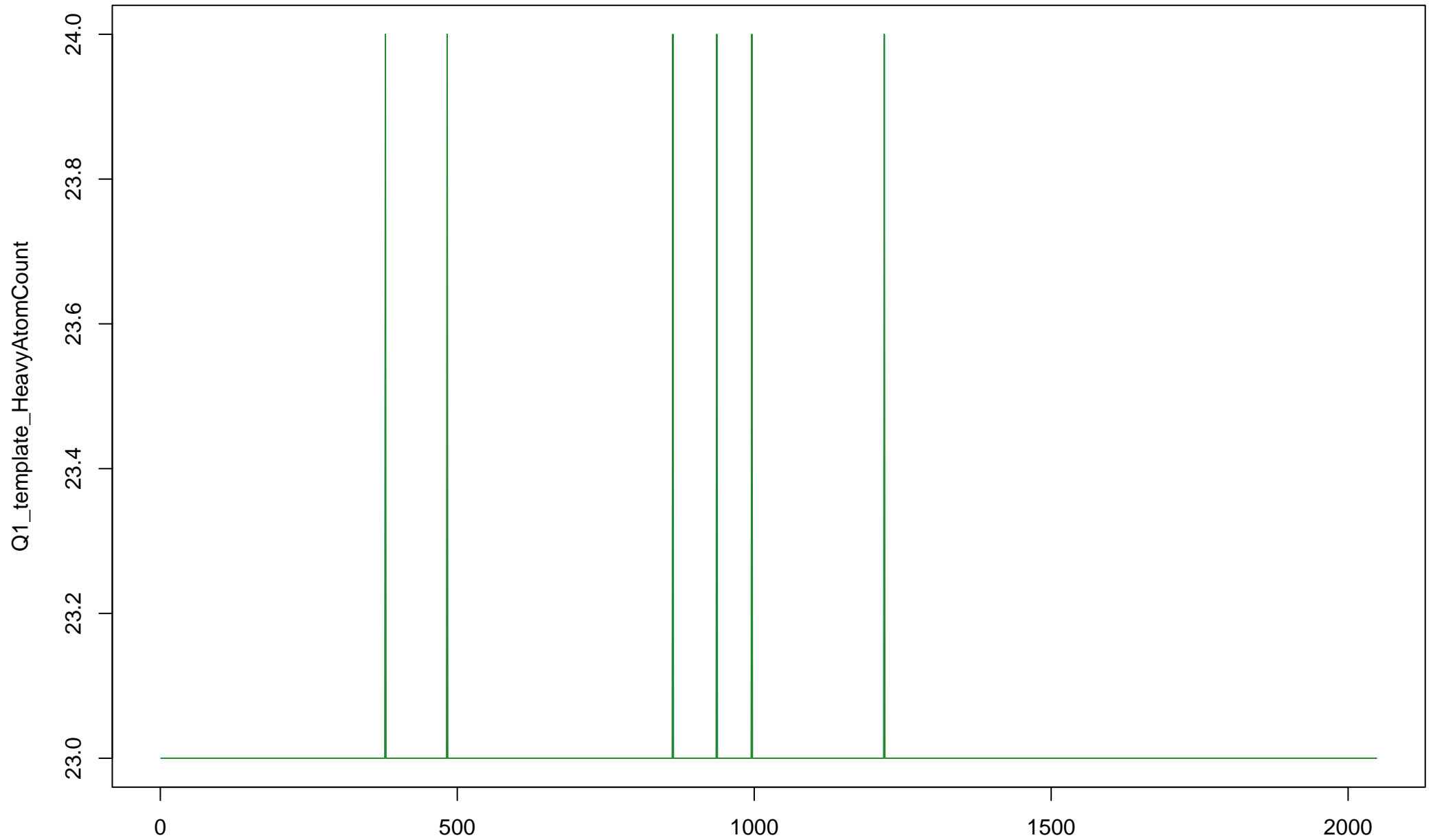
Q1_docked_HeavyAtomCount
ESS = 1850 | BMK = 0.00583 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0



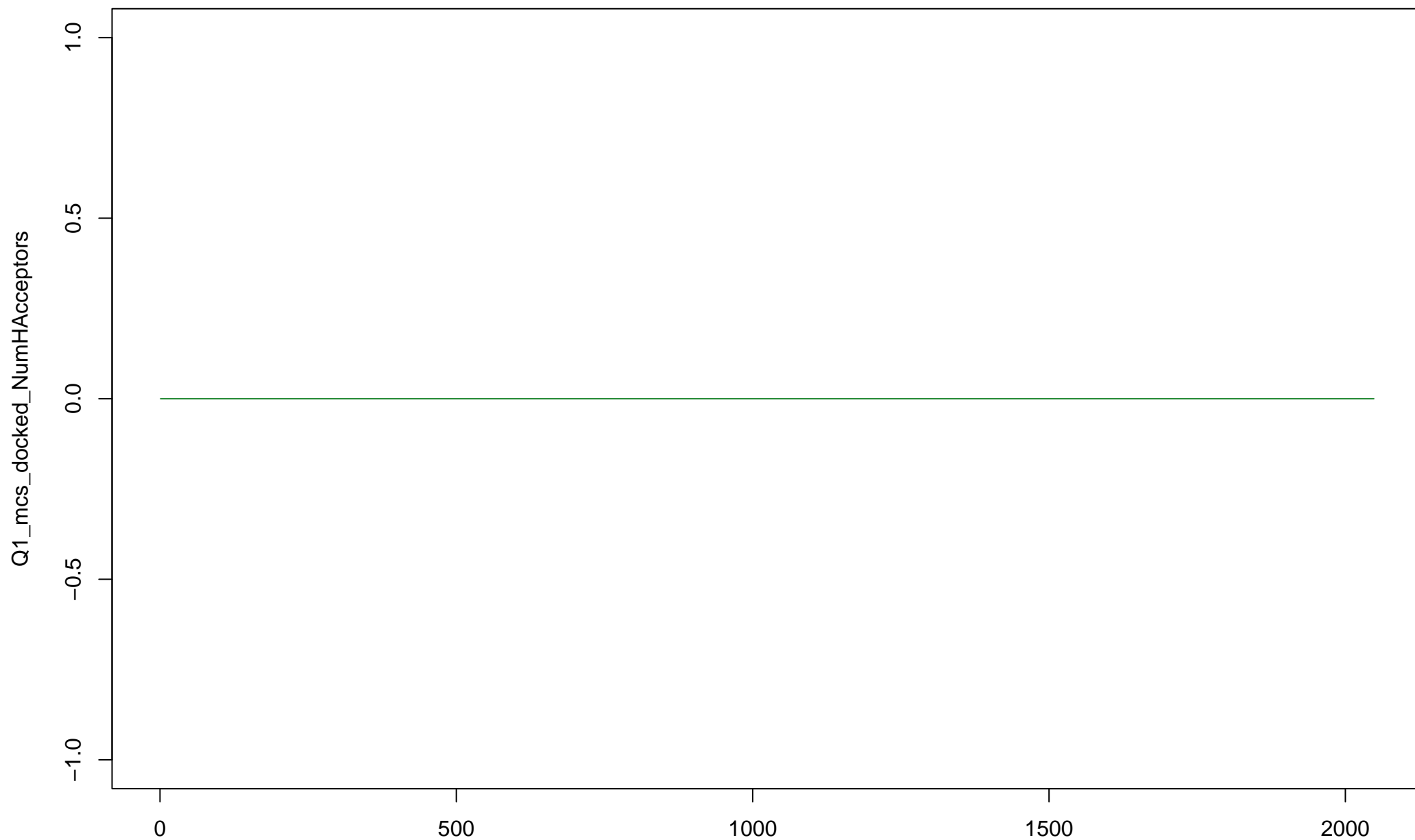
Q1_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



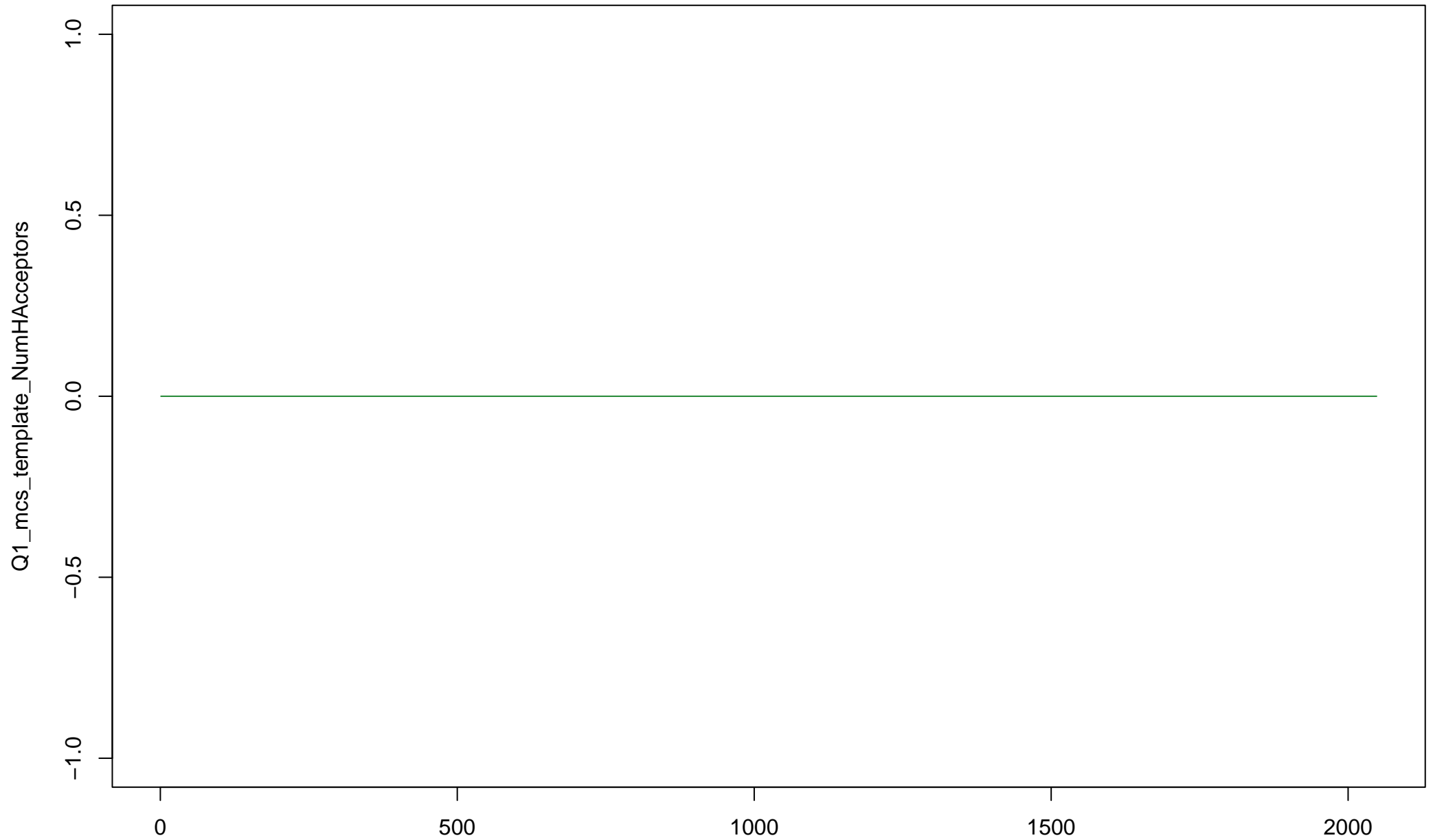
Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0.264 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 1224



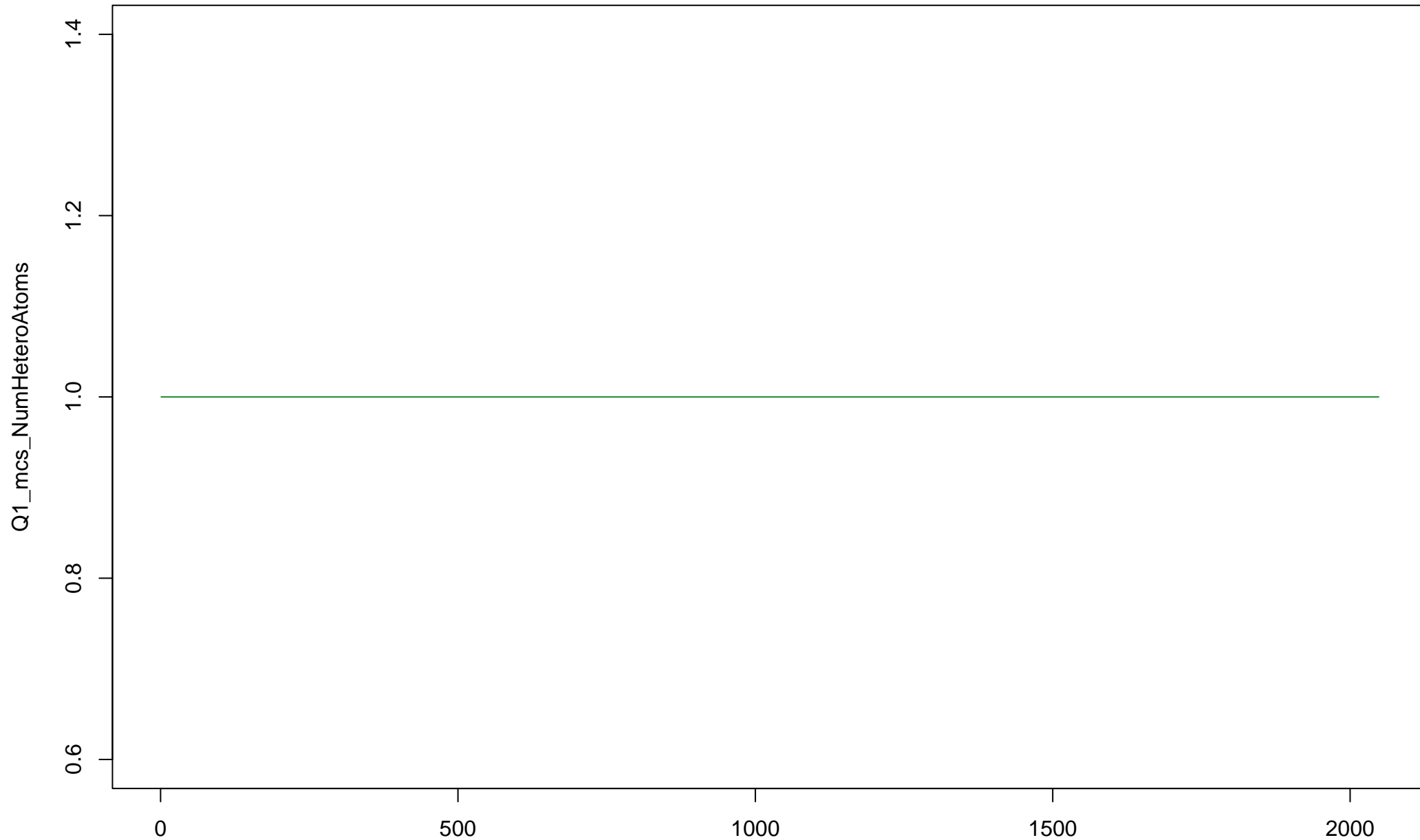
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



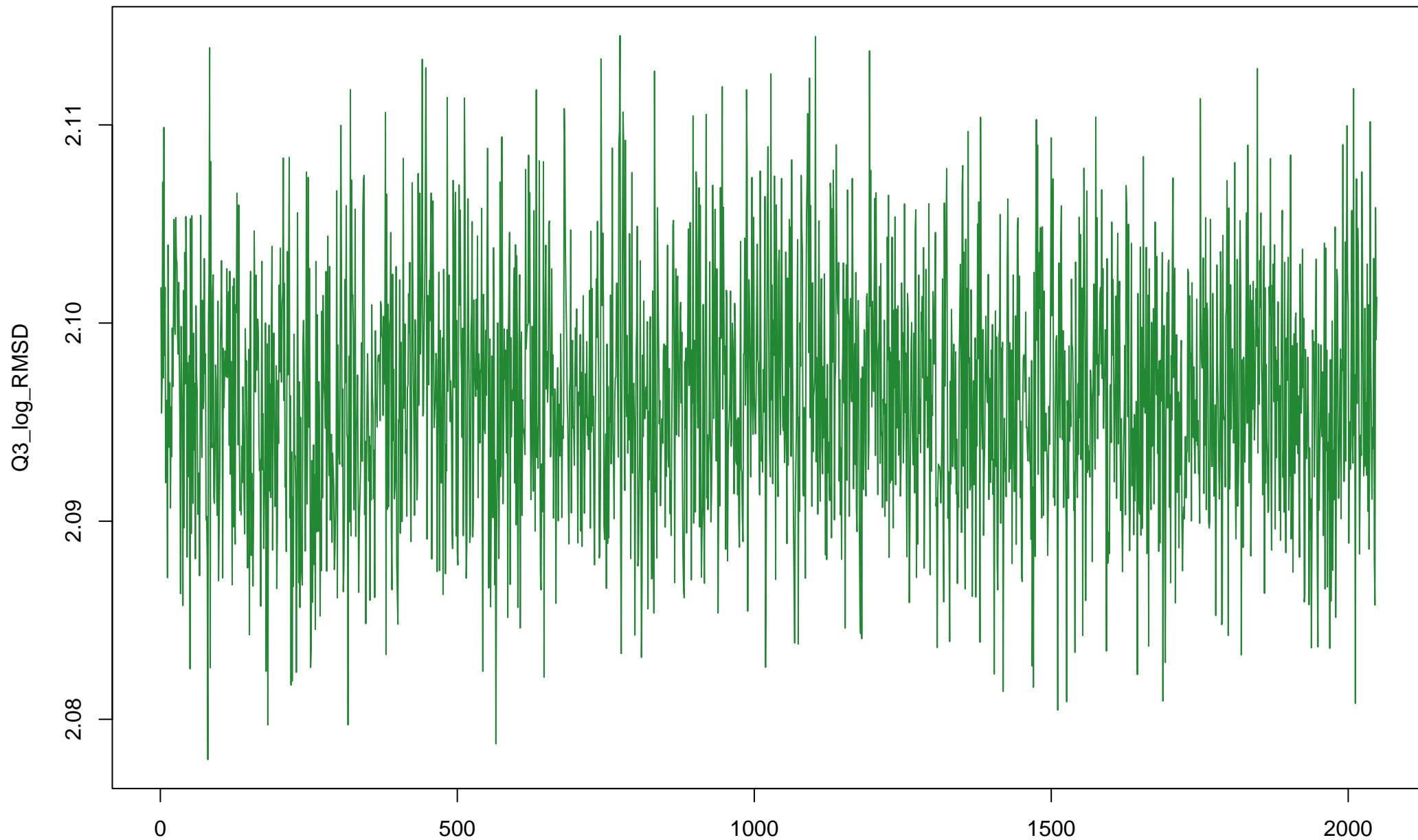
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



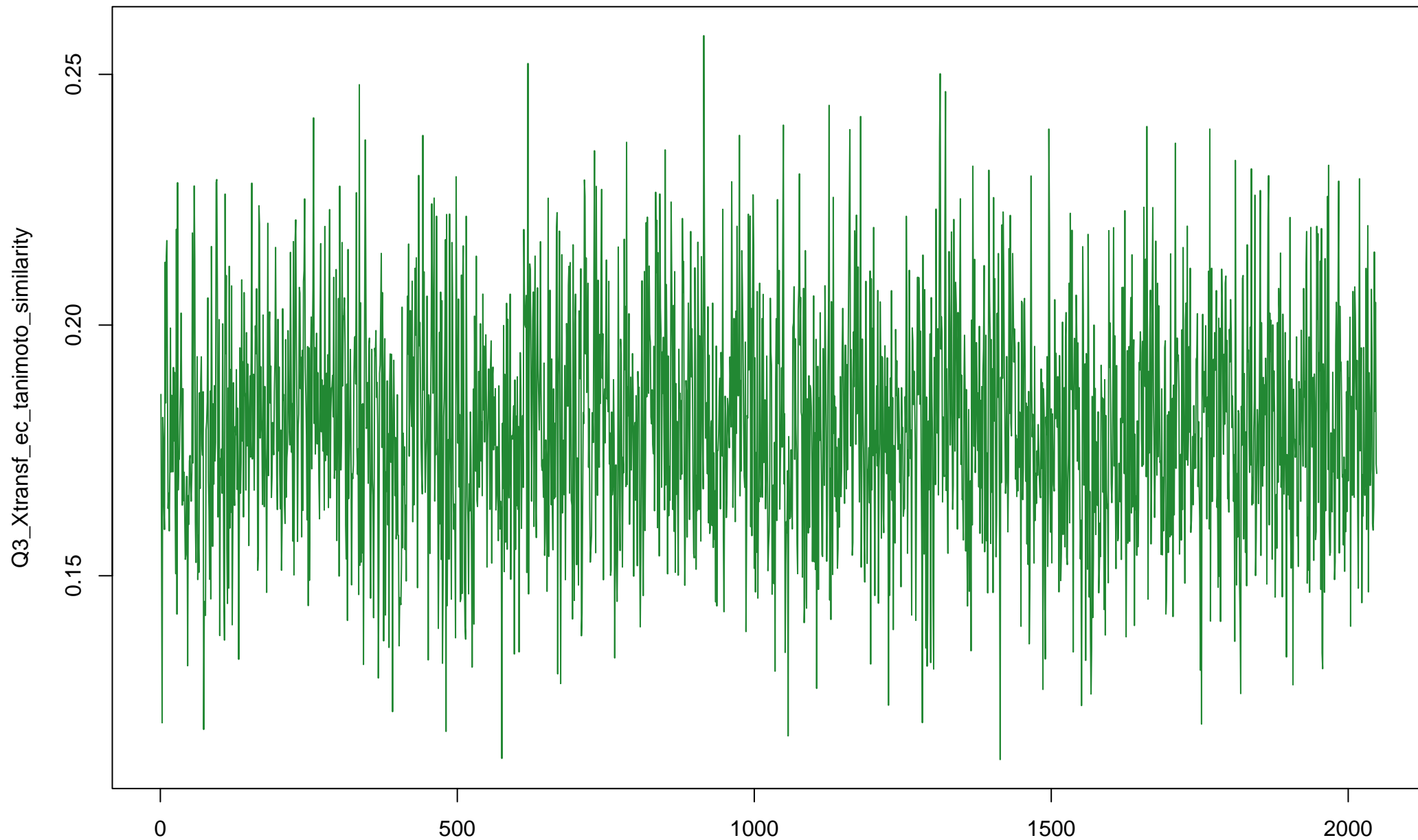
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



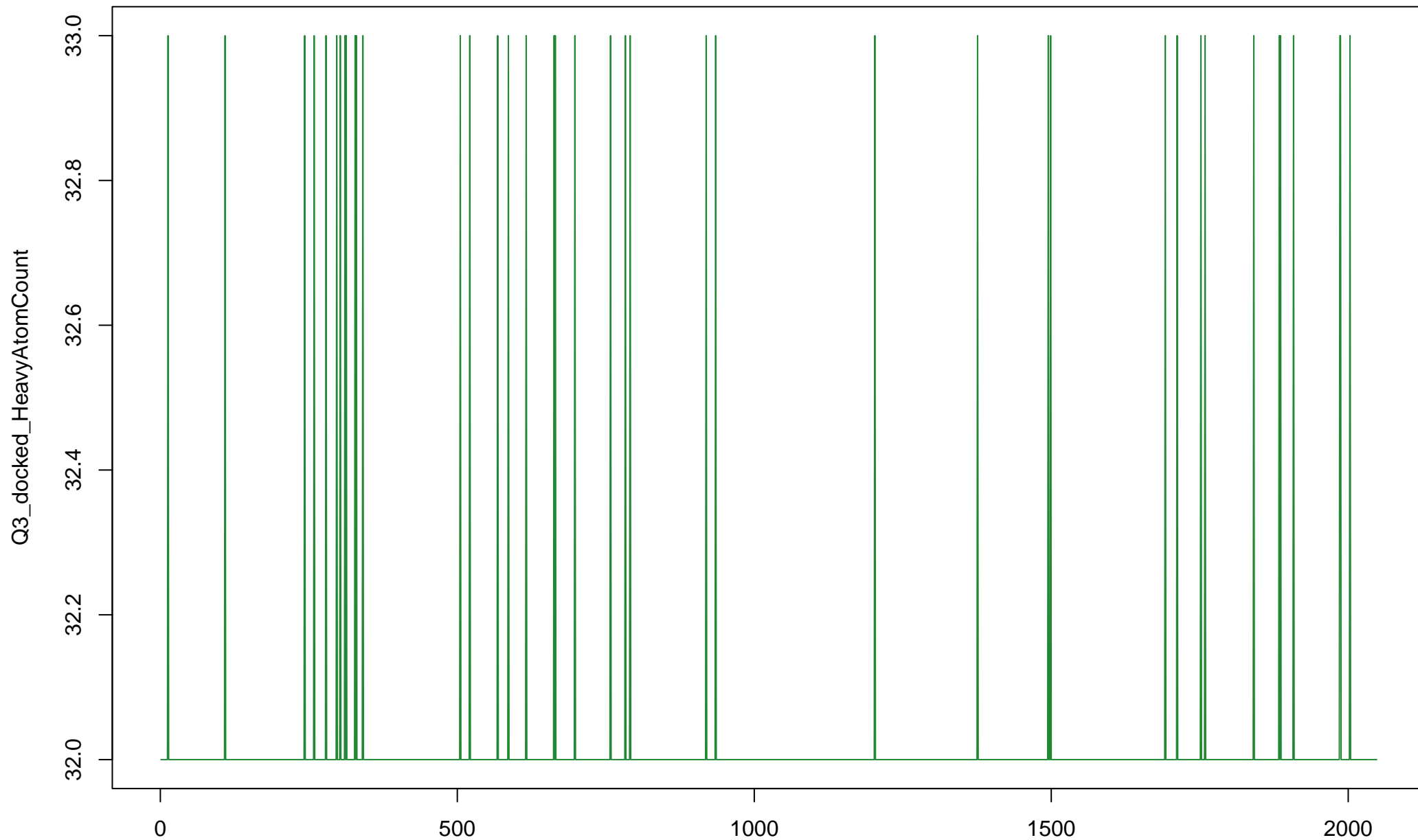
Q3_log_RMSD
ESS = 1740 | BMK = 0.0585 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 1720 | BMK = 0.0345 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0



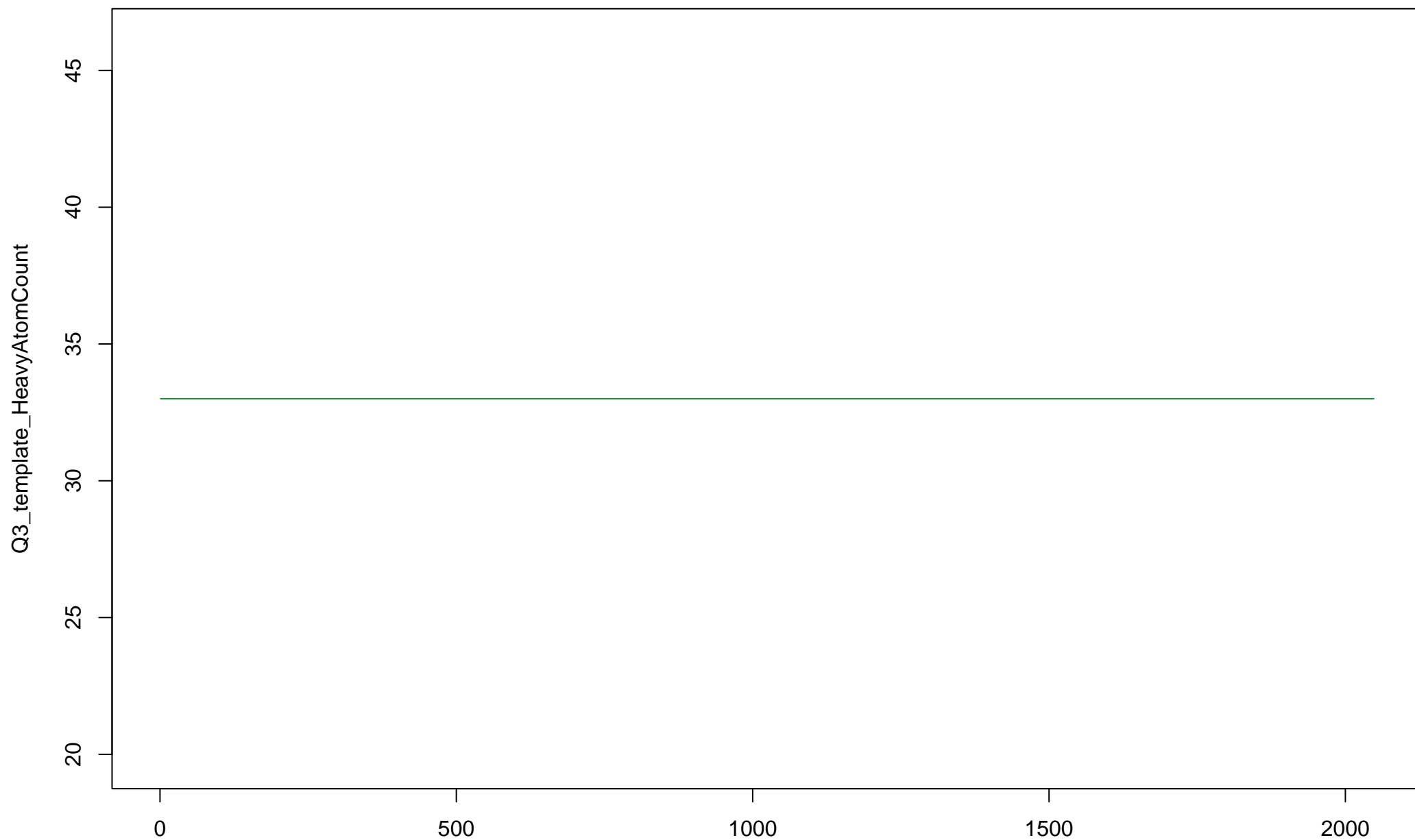
Q3_docked_HeavyAtomCount
ESS = 1250 | BMK = 0.0898 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0



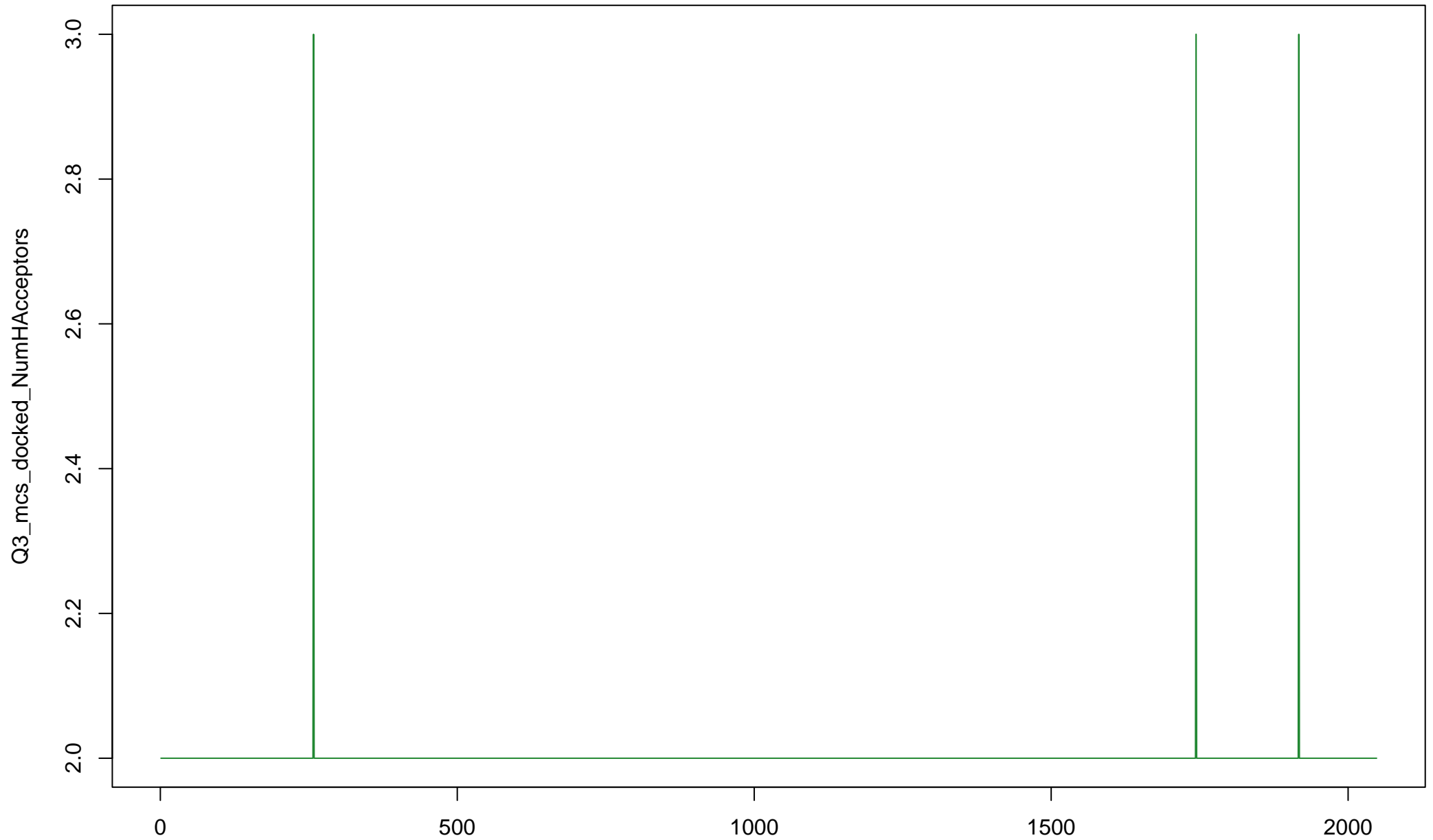
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



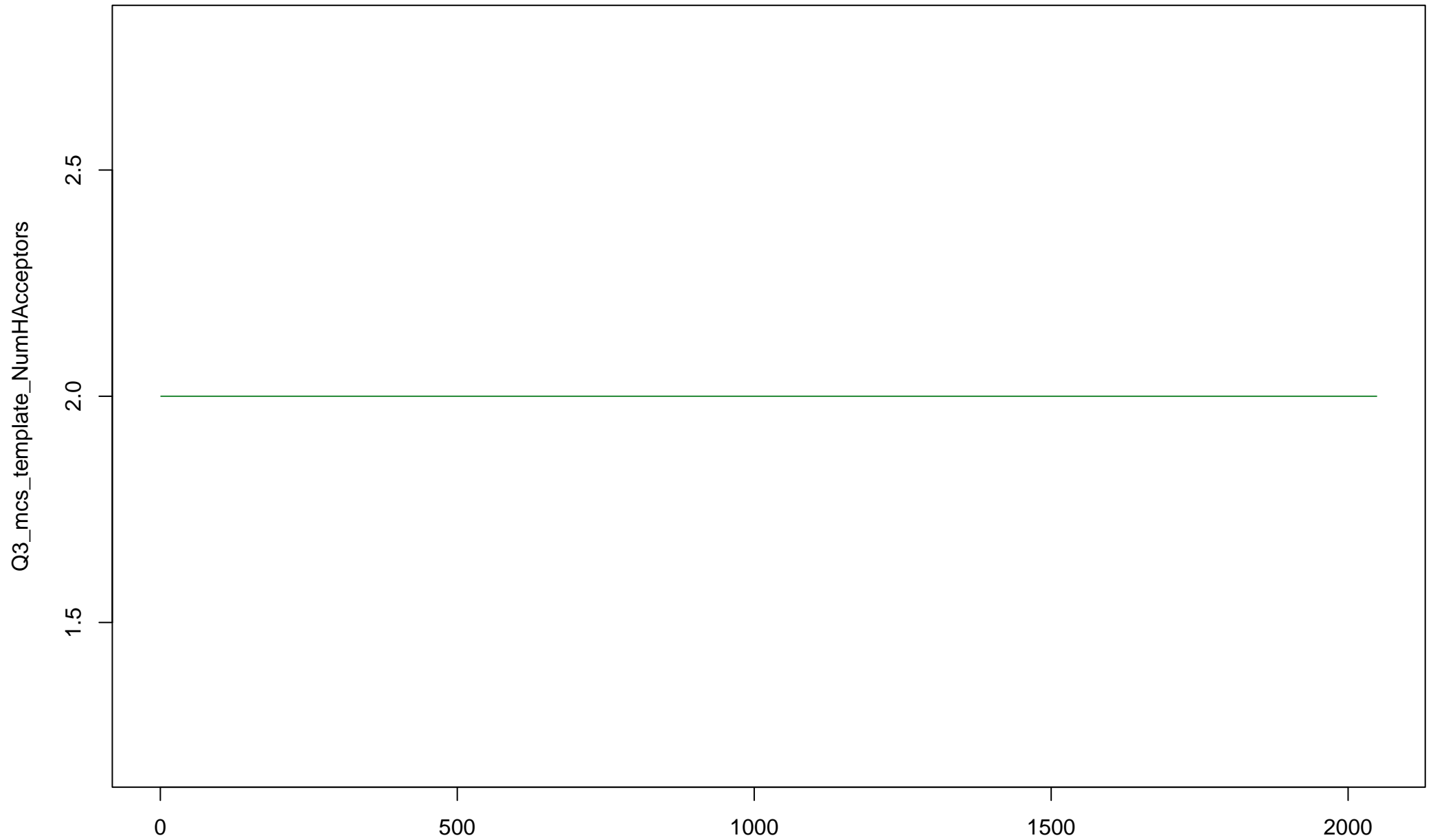
Q3_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



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



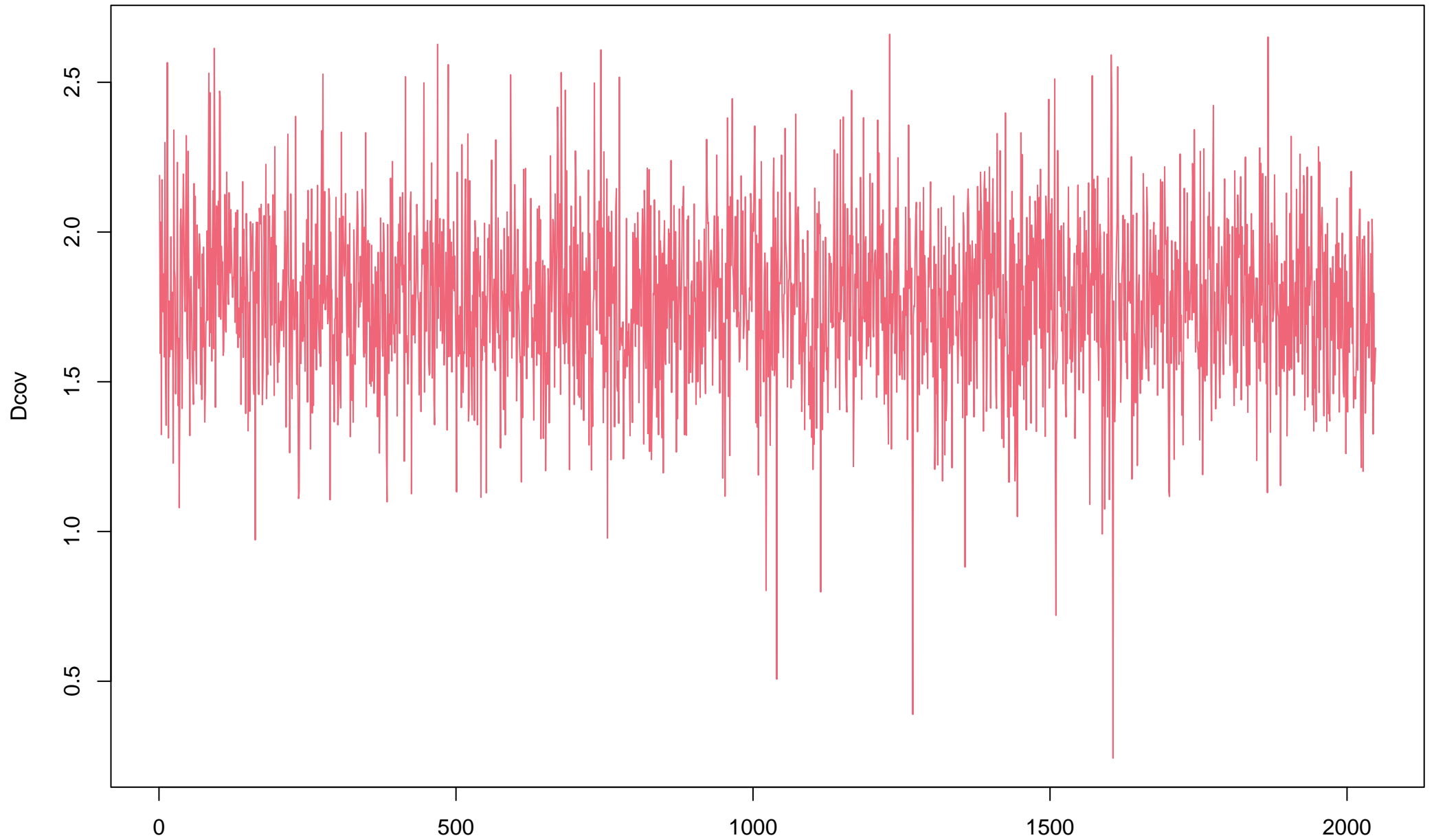
Q3_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



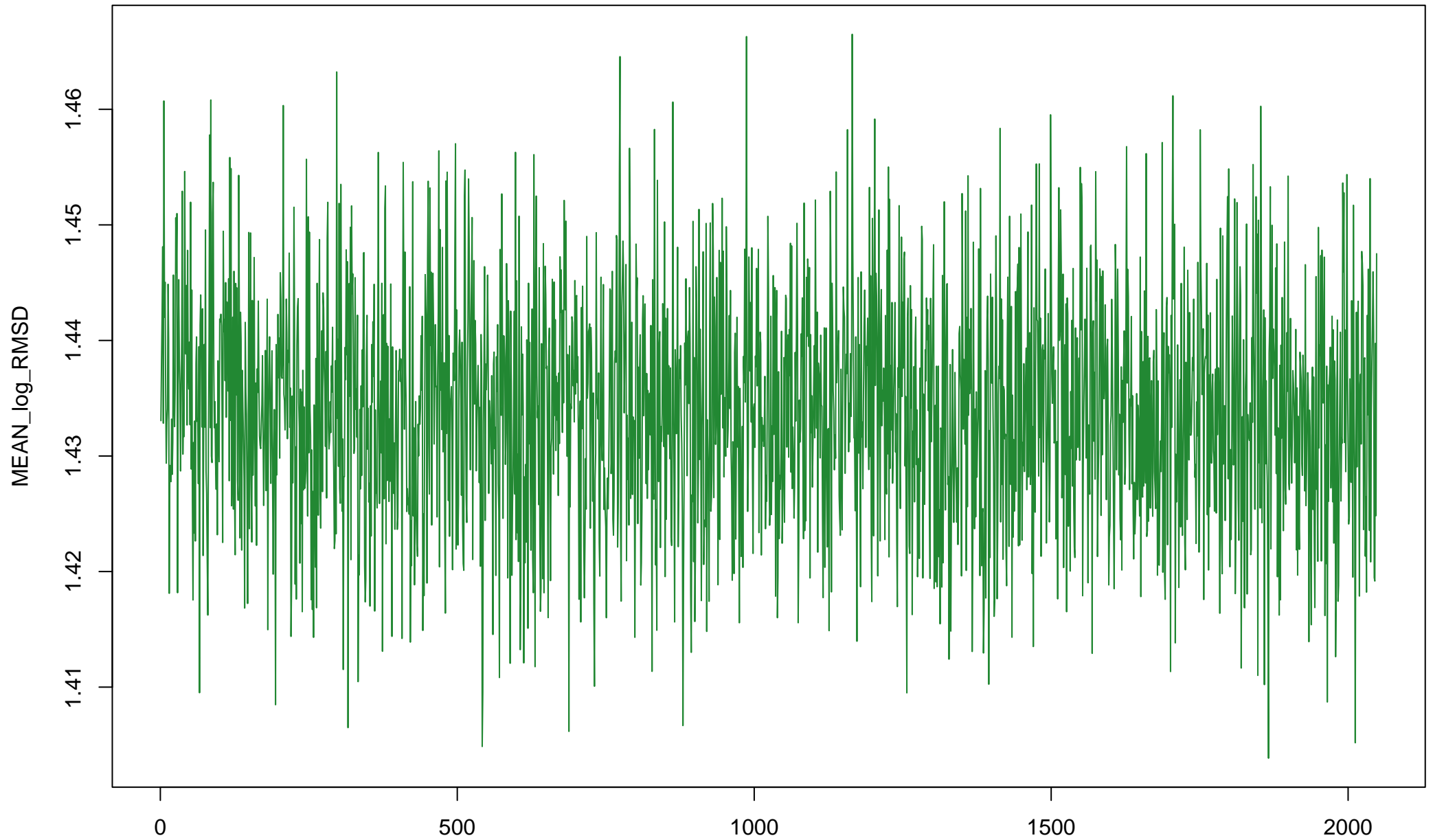
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



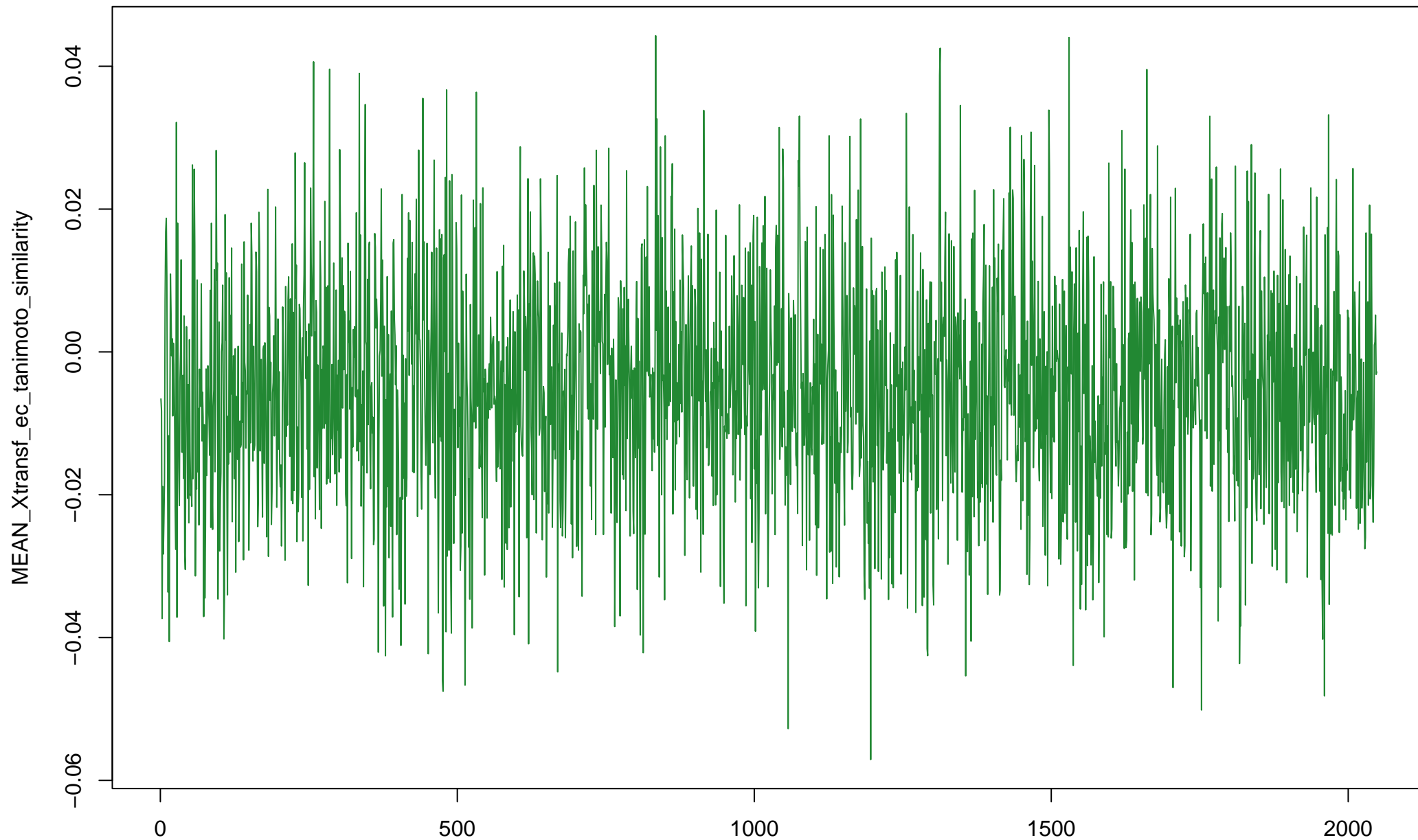
Dcov
ESS = 2050 | BMK = 0.0535 | MCSE(6.27) = 2.35 | stat: FALSE | burn: 0



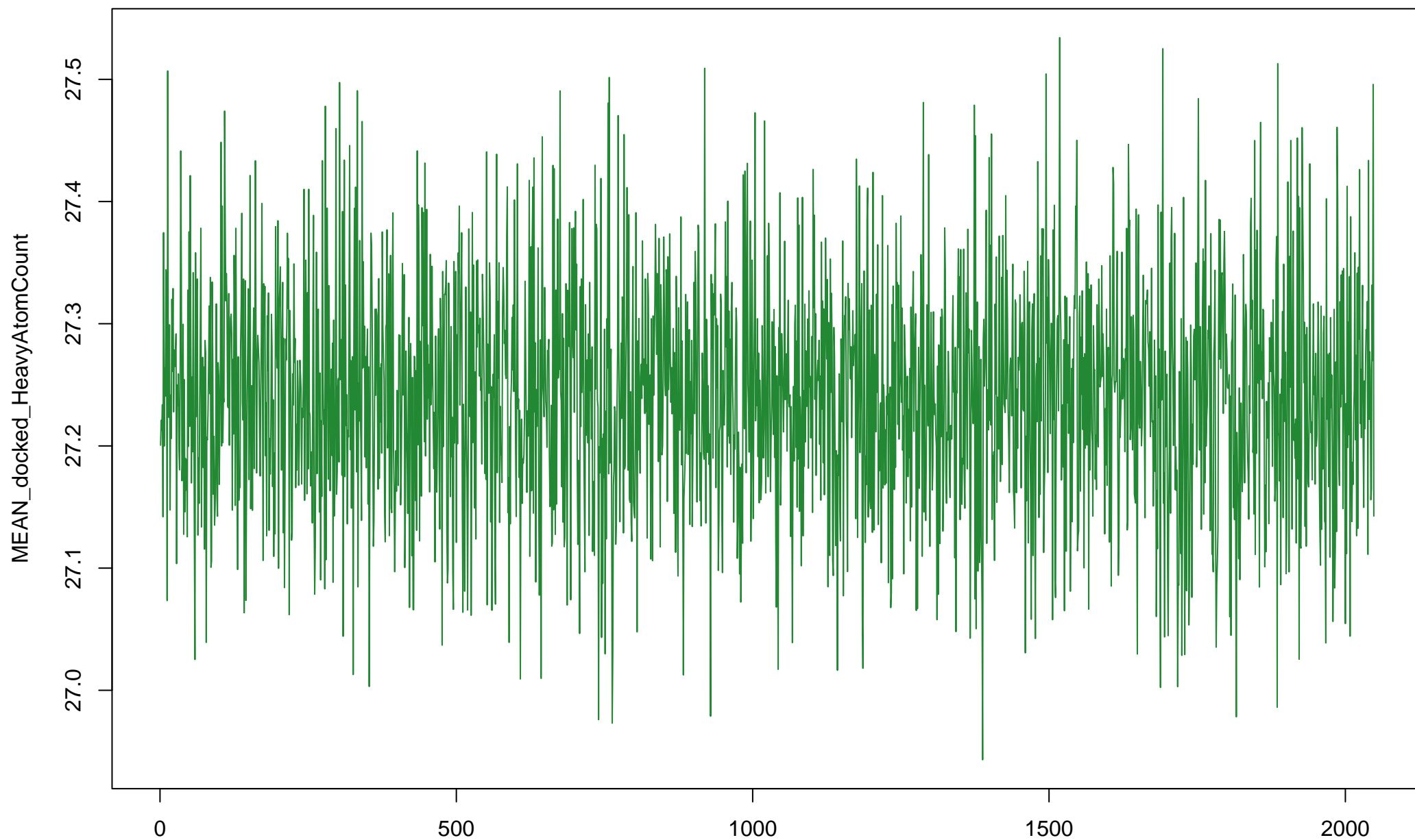
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0364 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0



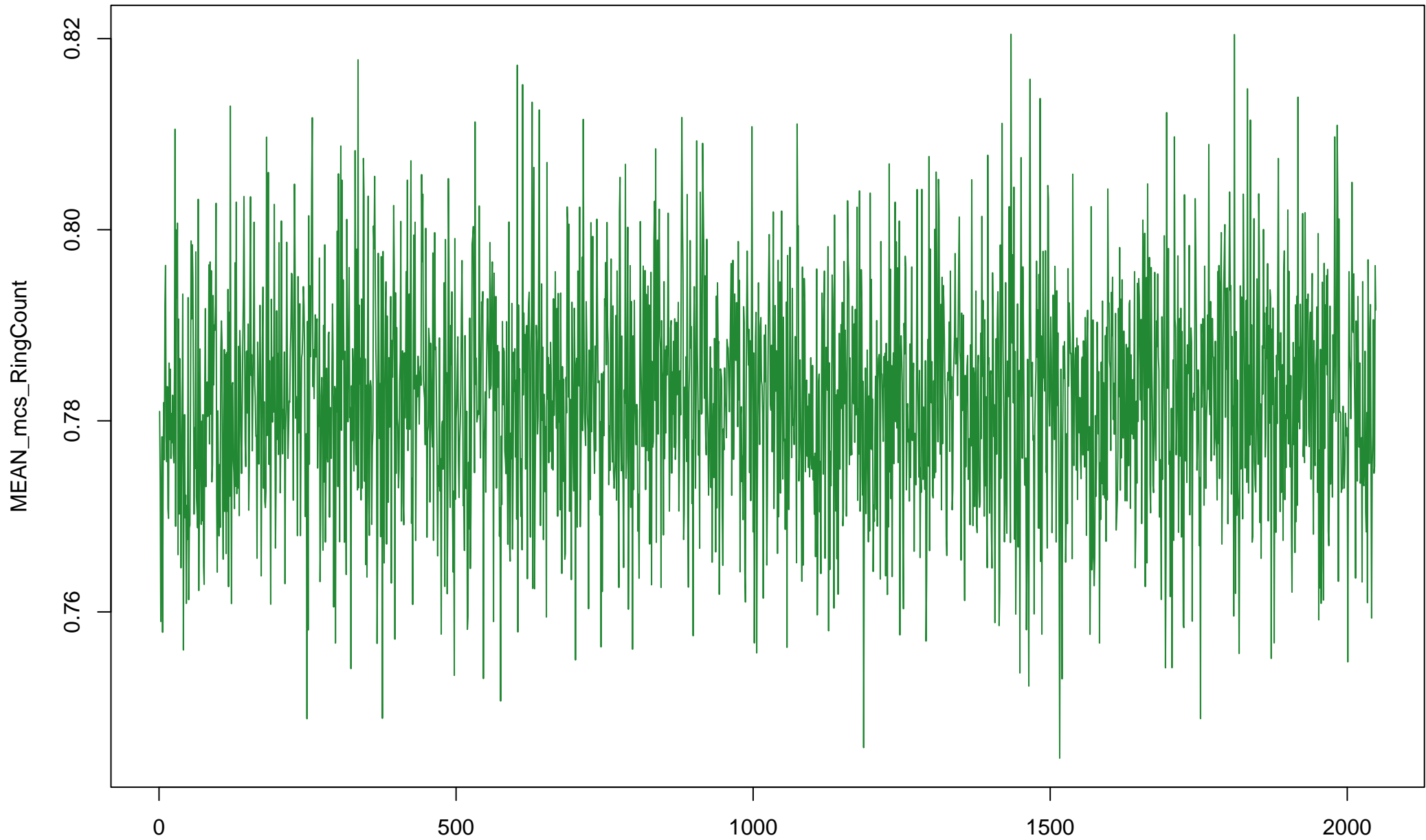
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0421 | MCSE(6.27) = 2.56 | stat: FALSE | burn: 0



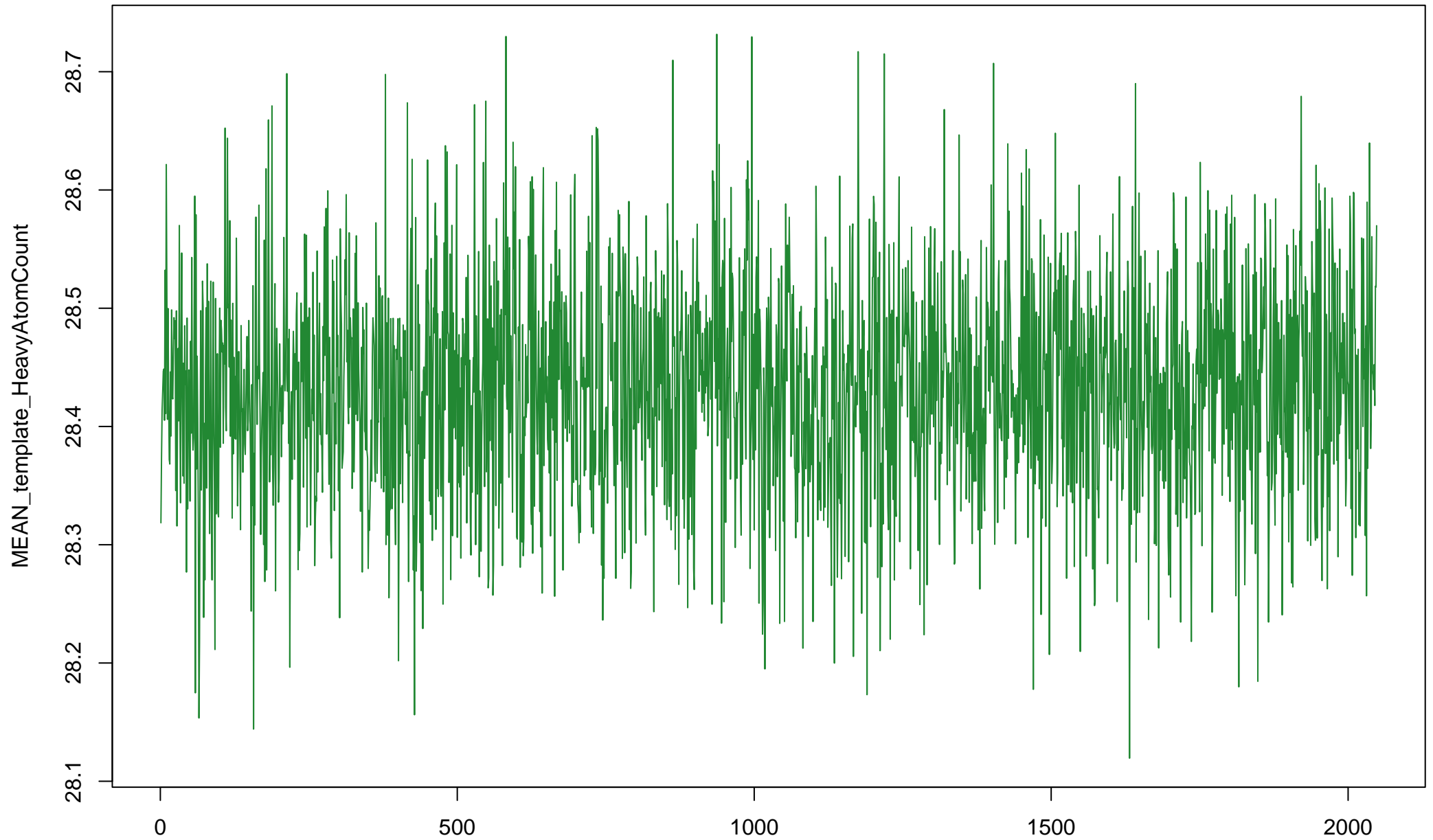
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0332 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0



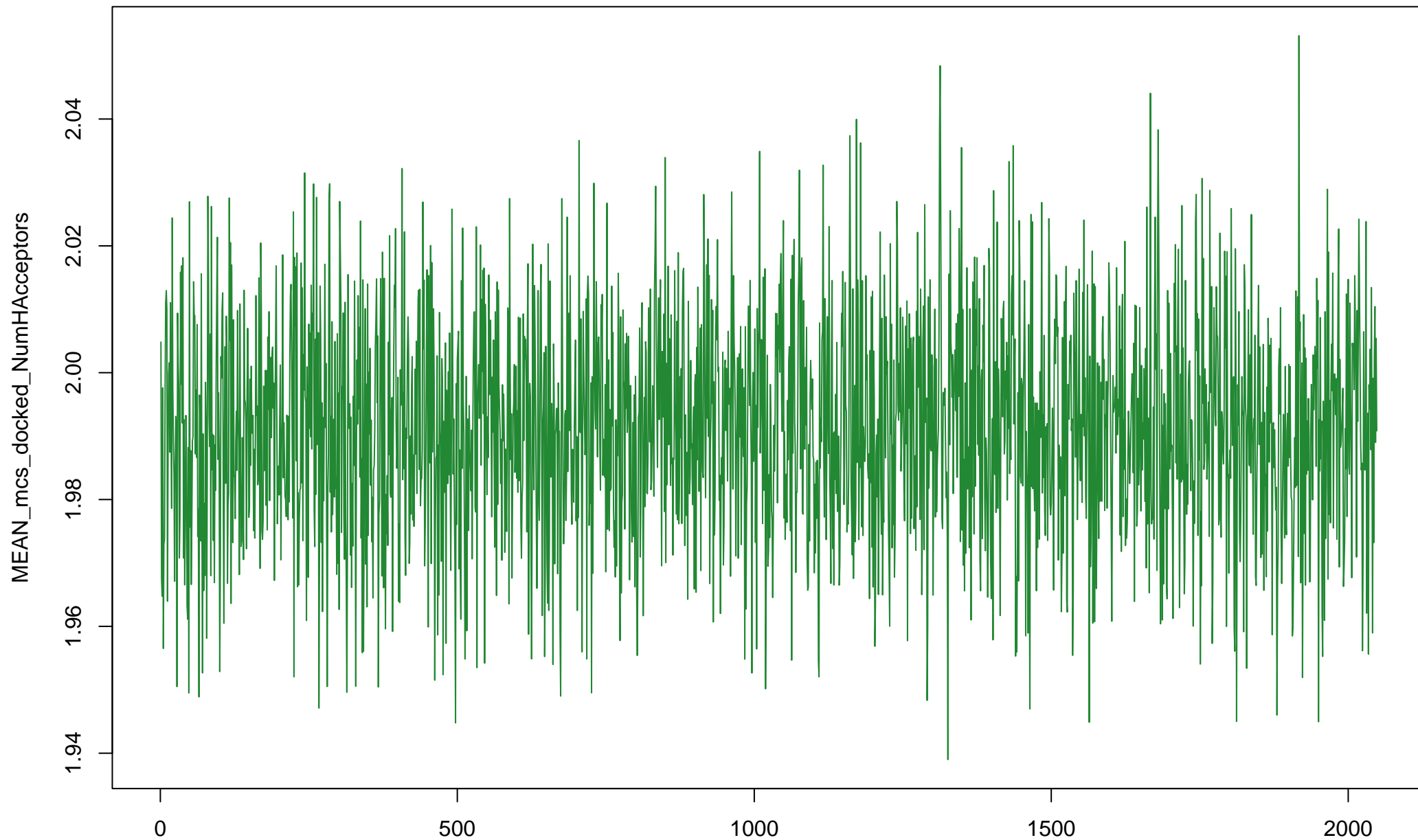
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0283 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



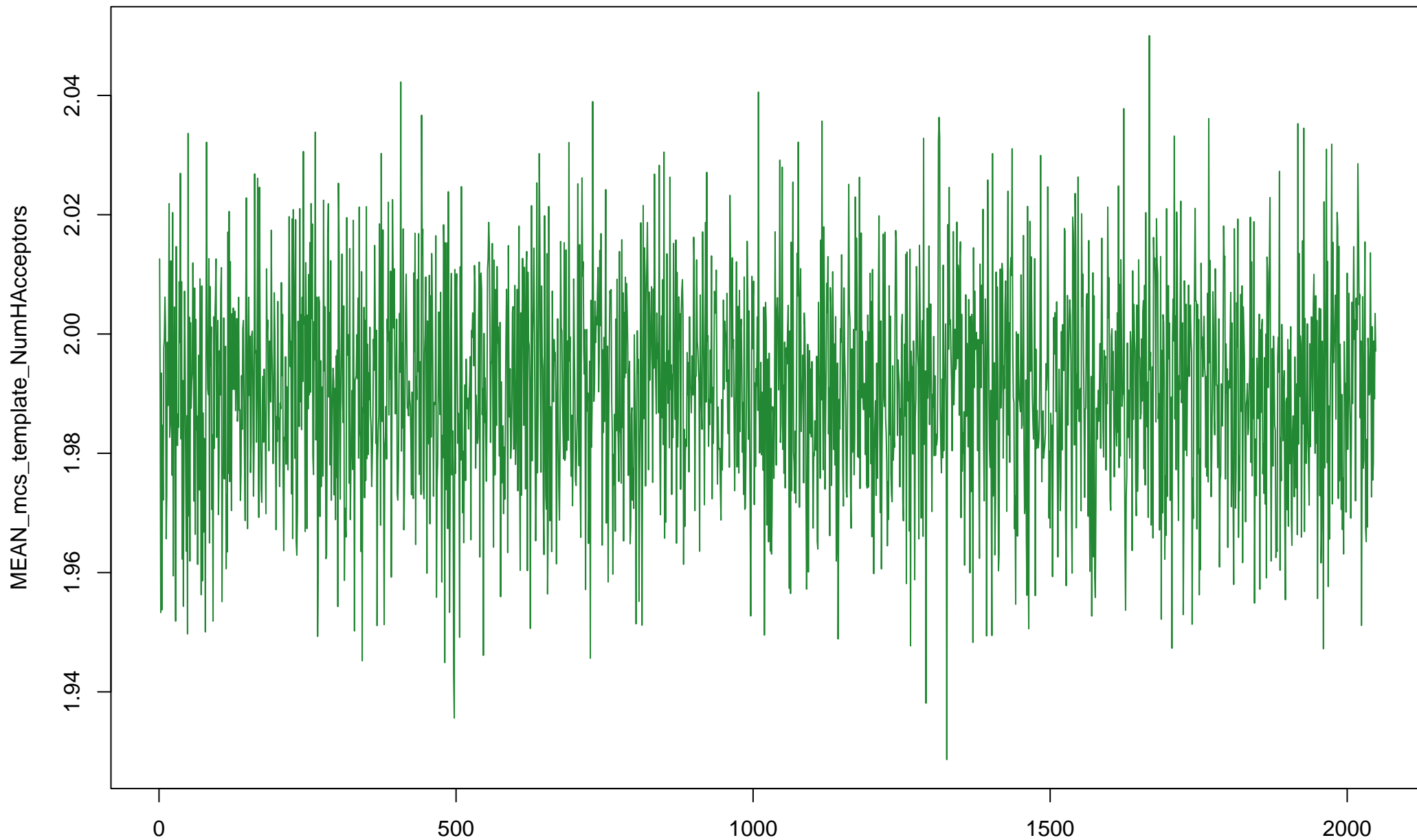
MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.047 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



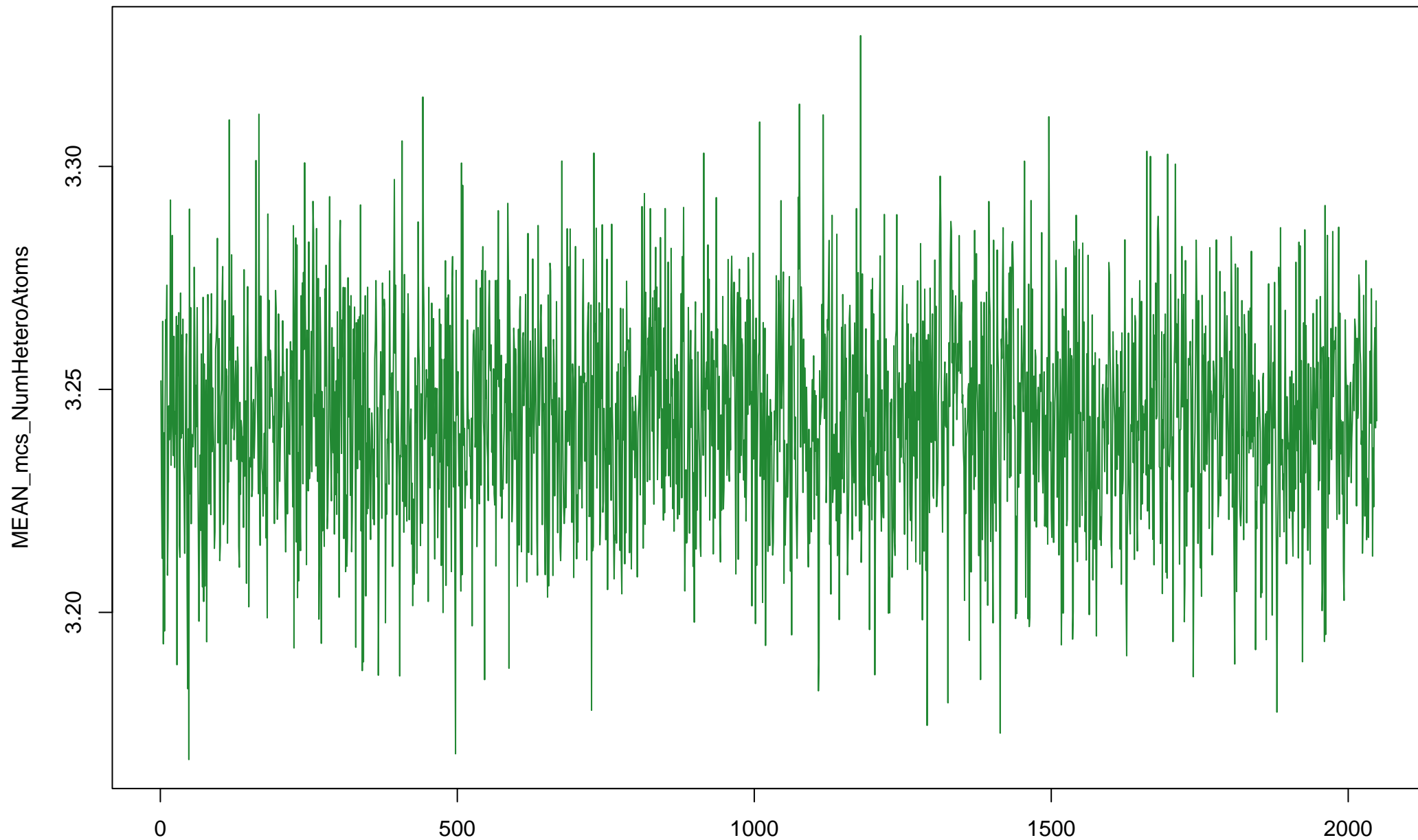
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0481 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0



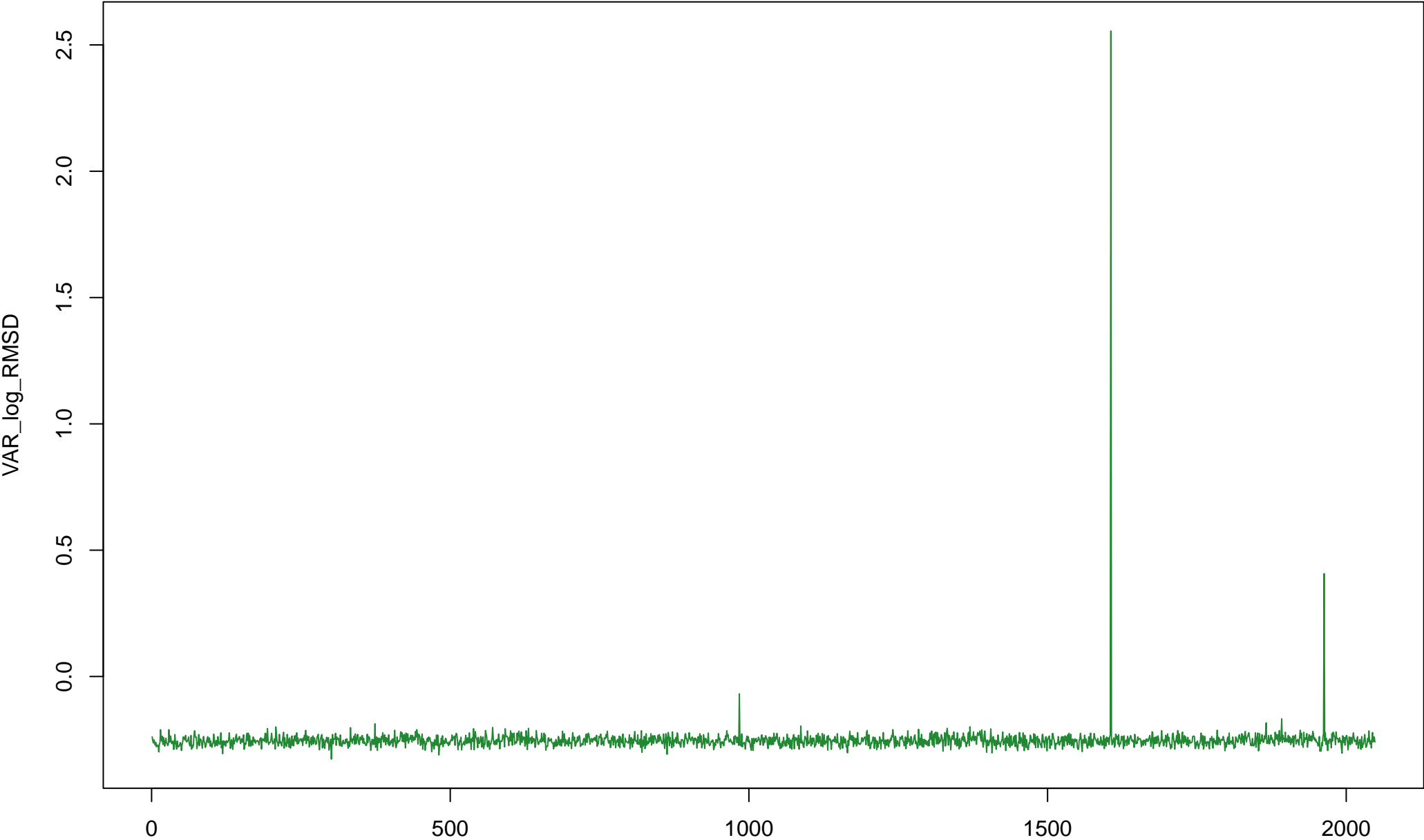
MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0382 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



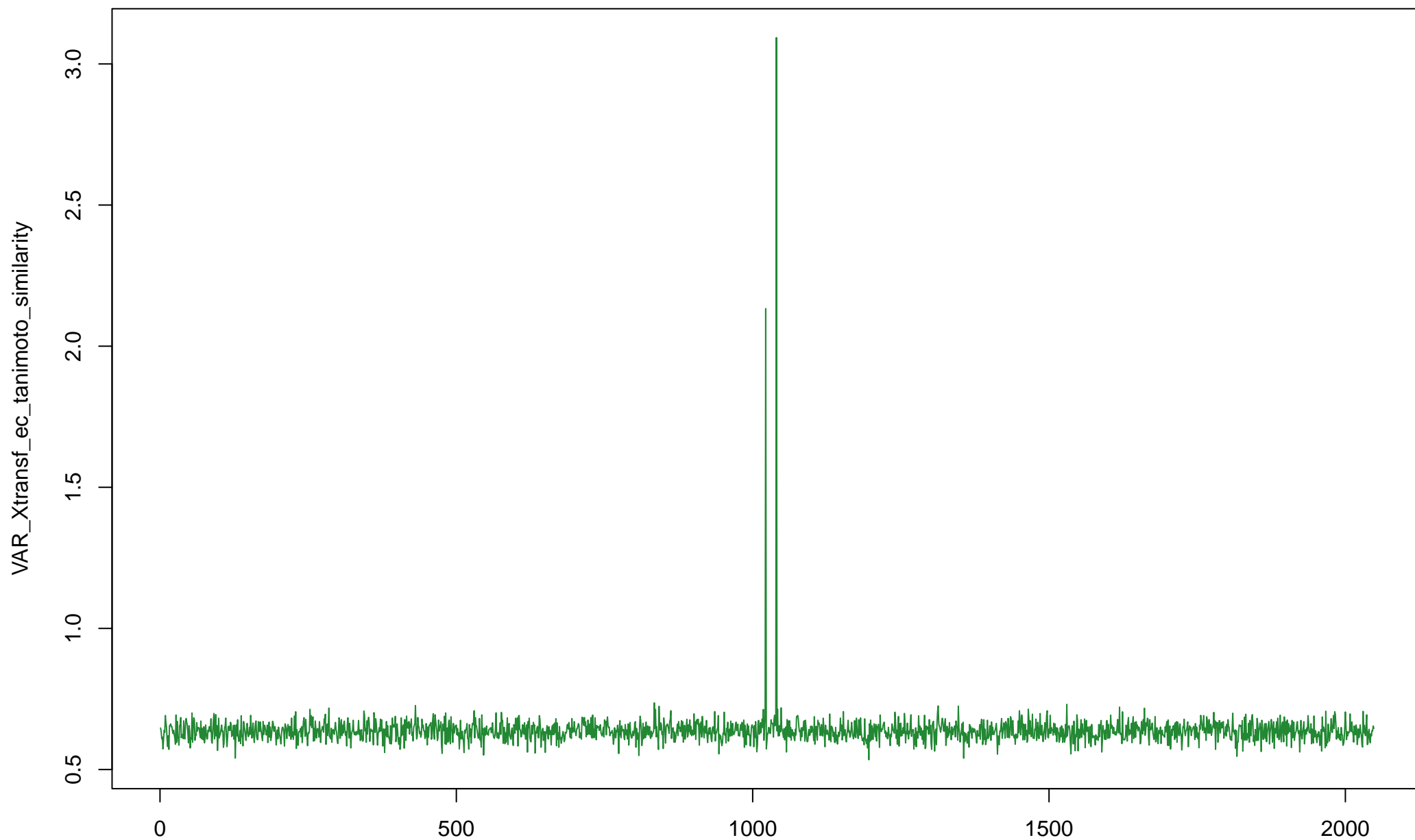
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0319 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



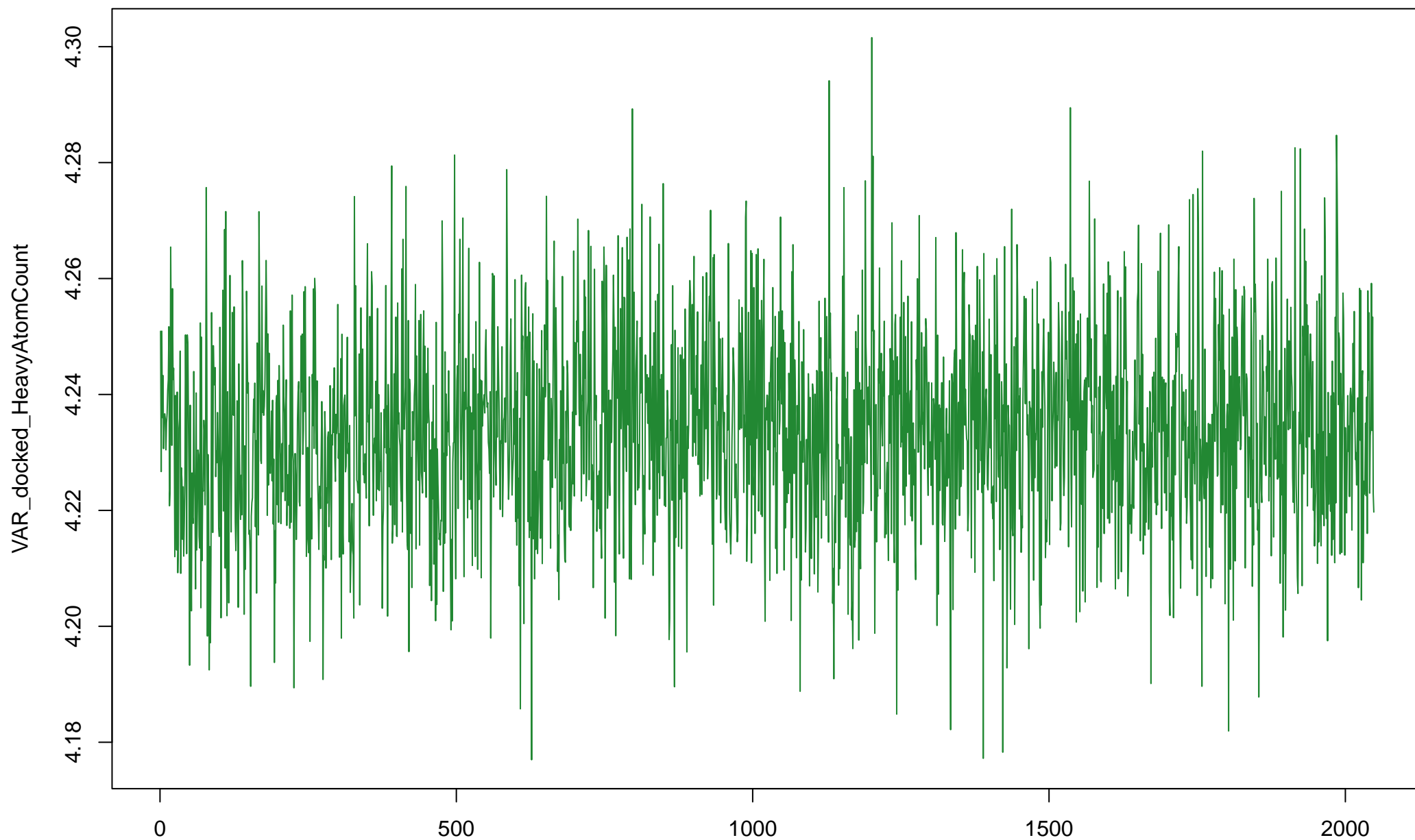
VAR_log_RMSD
ESS = 2050 | BMK = 0.089 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



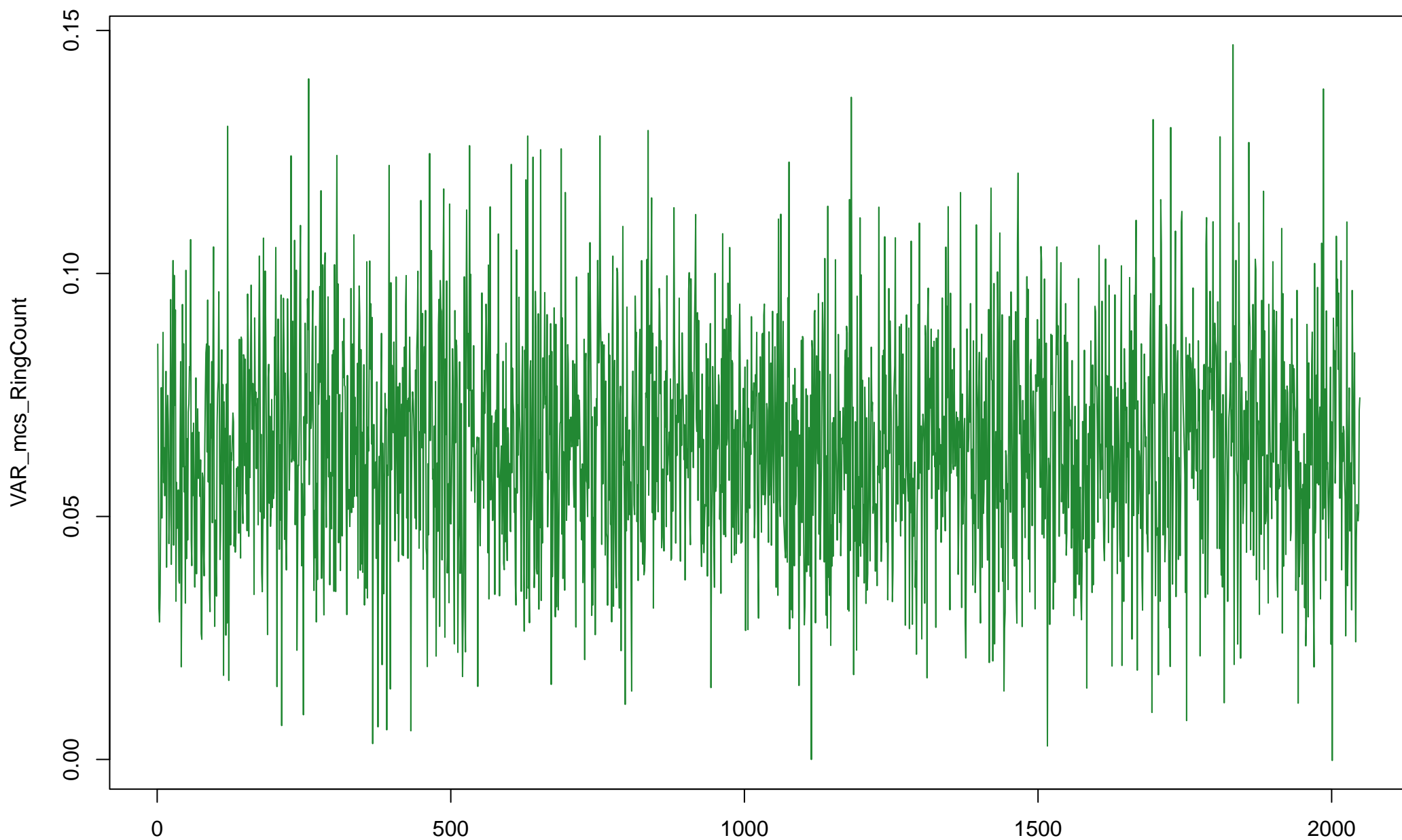
VAR_Xtransf_ec_tanimoto_similarity
ESS = 1080 | BMK = 0.0353 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0



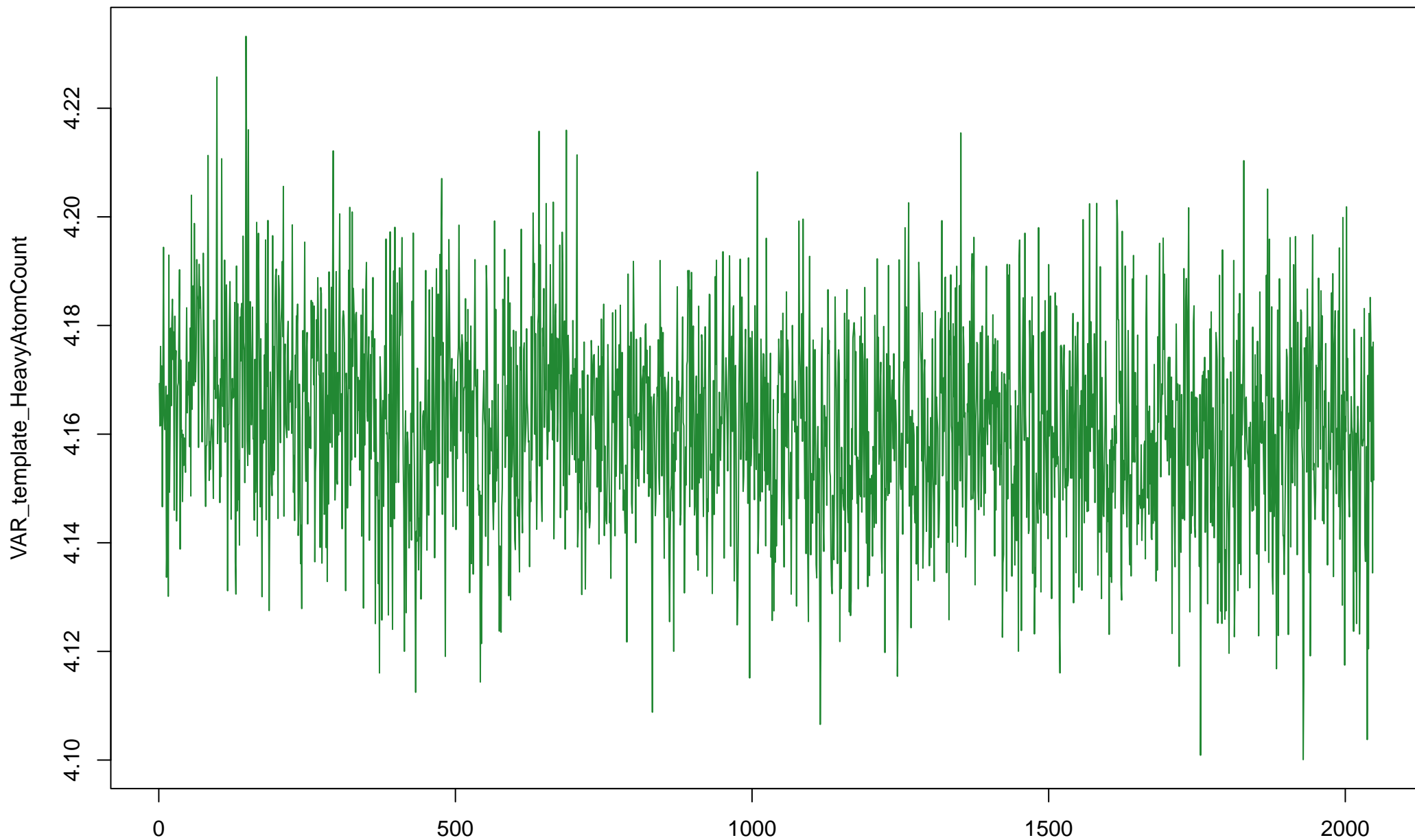
VAR_docked_HeavyAtomCount
ESS = 1670 | BMK = 0.0429 | MCSE(6.27) = 2.75 | stat: FALSE | burn: 0



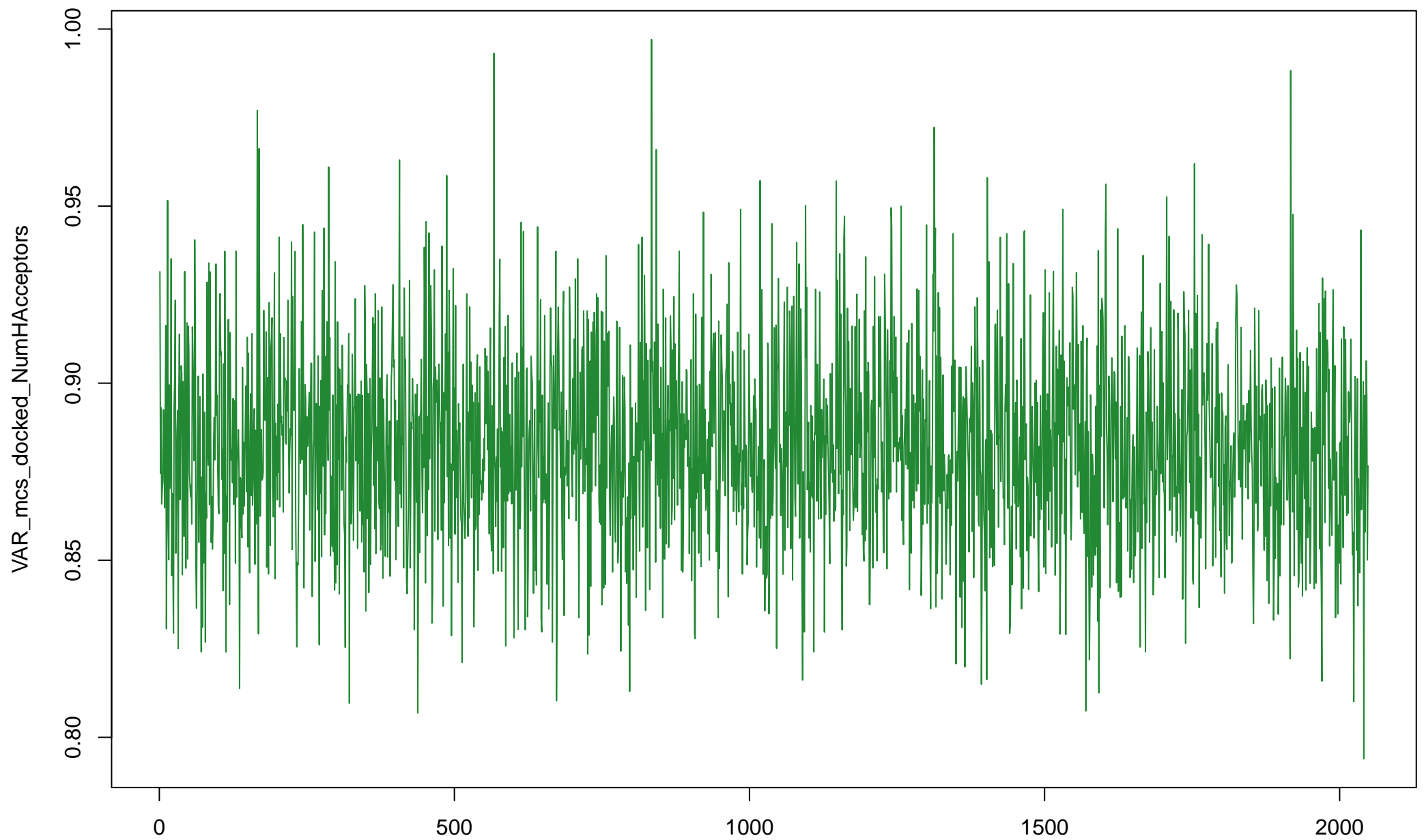
VAR_mcs_RingCount
ESS = 2050 | BMK = 0.0371 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0



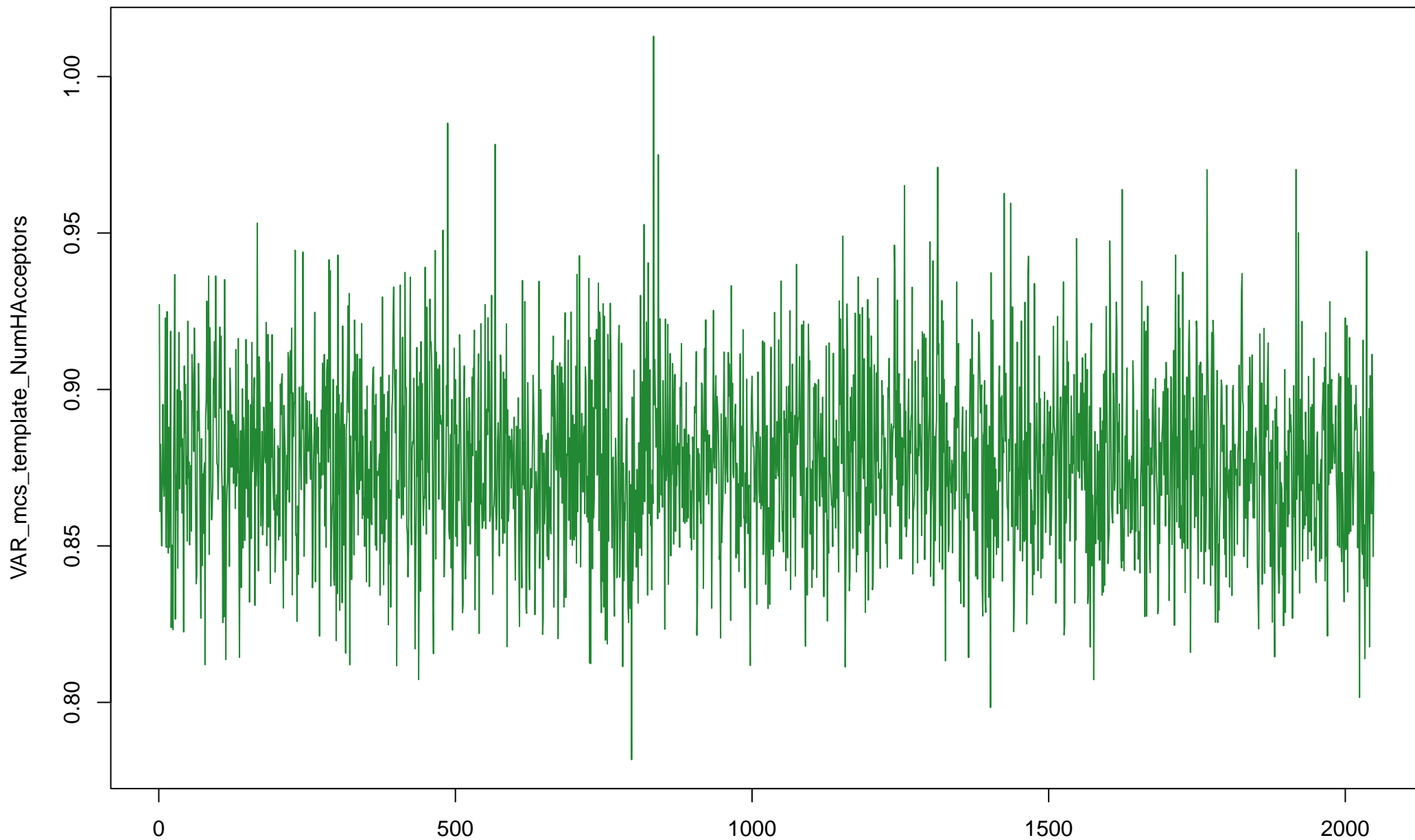
VAR_template_HeavyAtomCount
ESS = 1380 | BMK = 0.108 | MCSE(6.27) = 3.72 | stat: FALSE | burn: 0



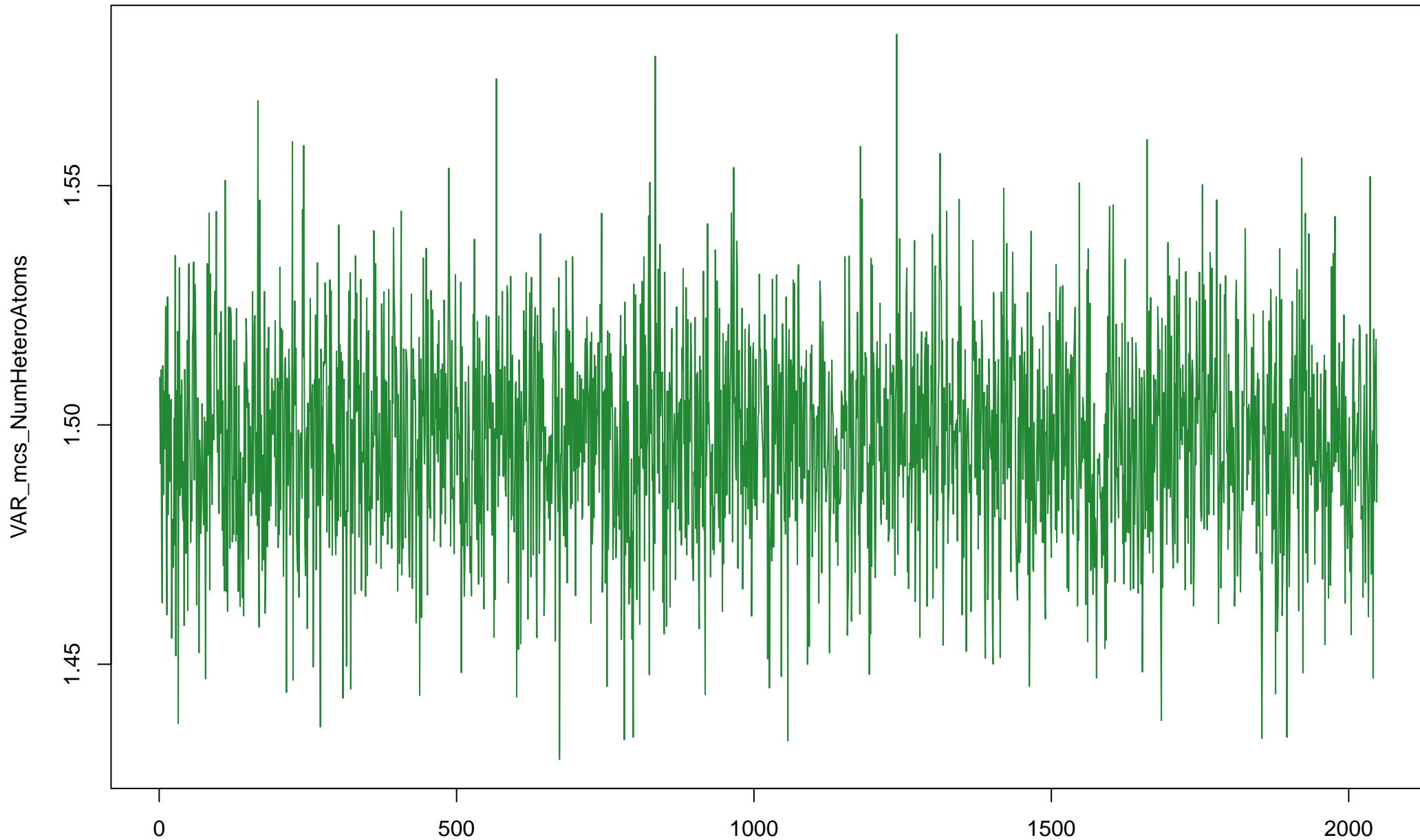
VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0352 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



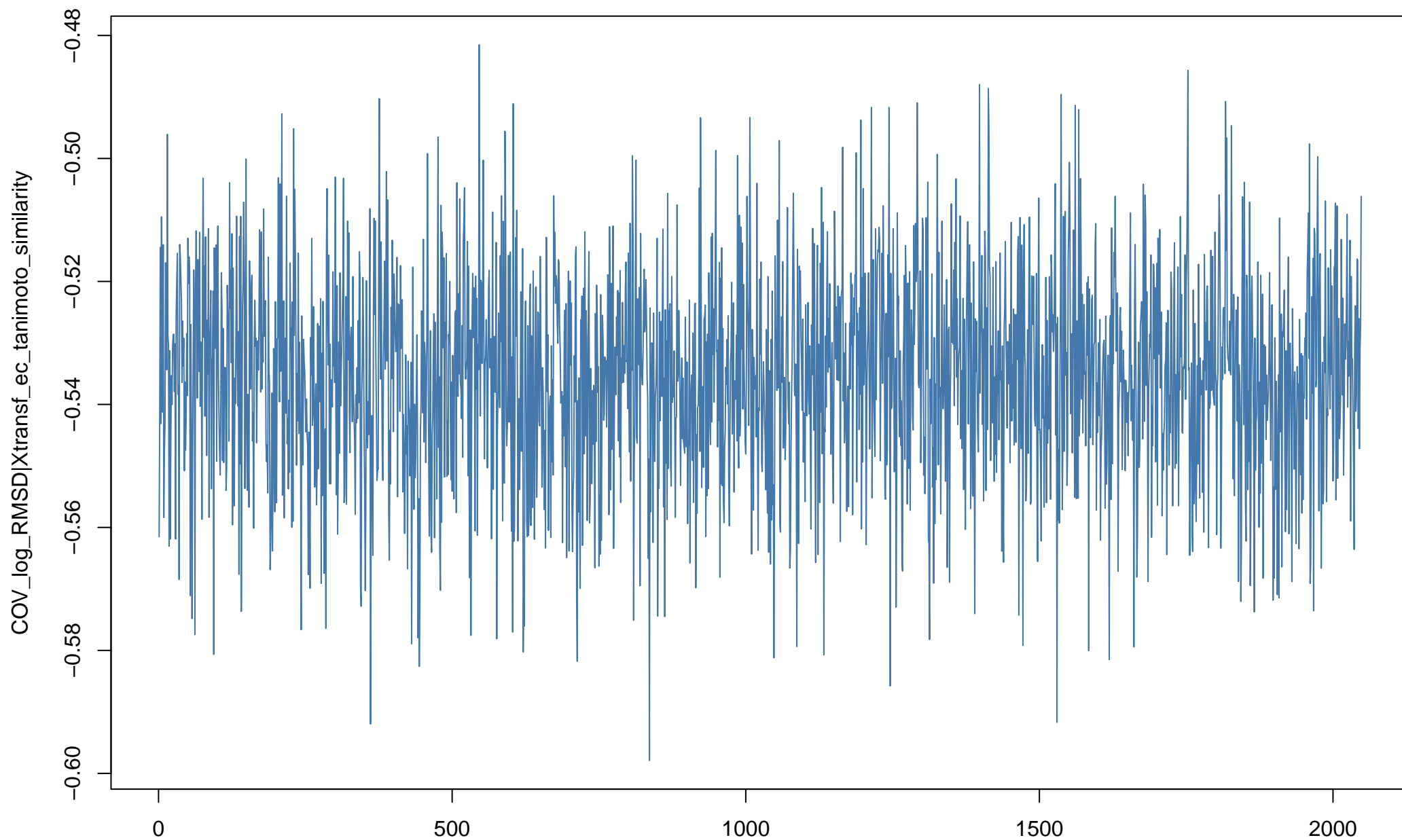
VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0555 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



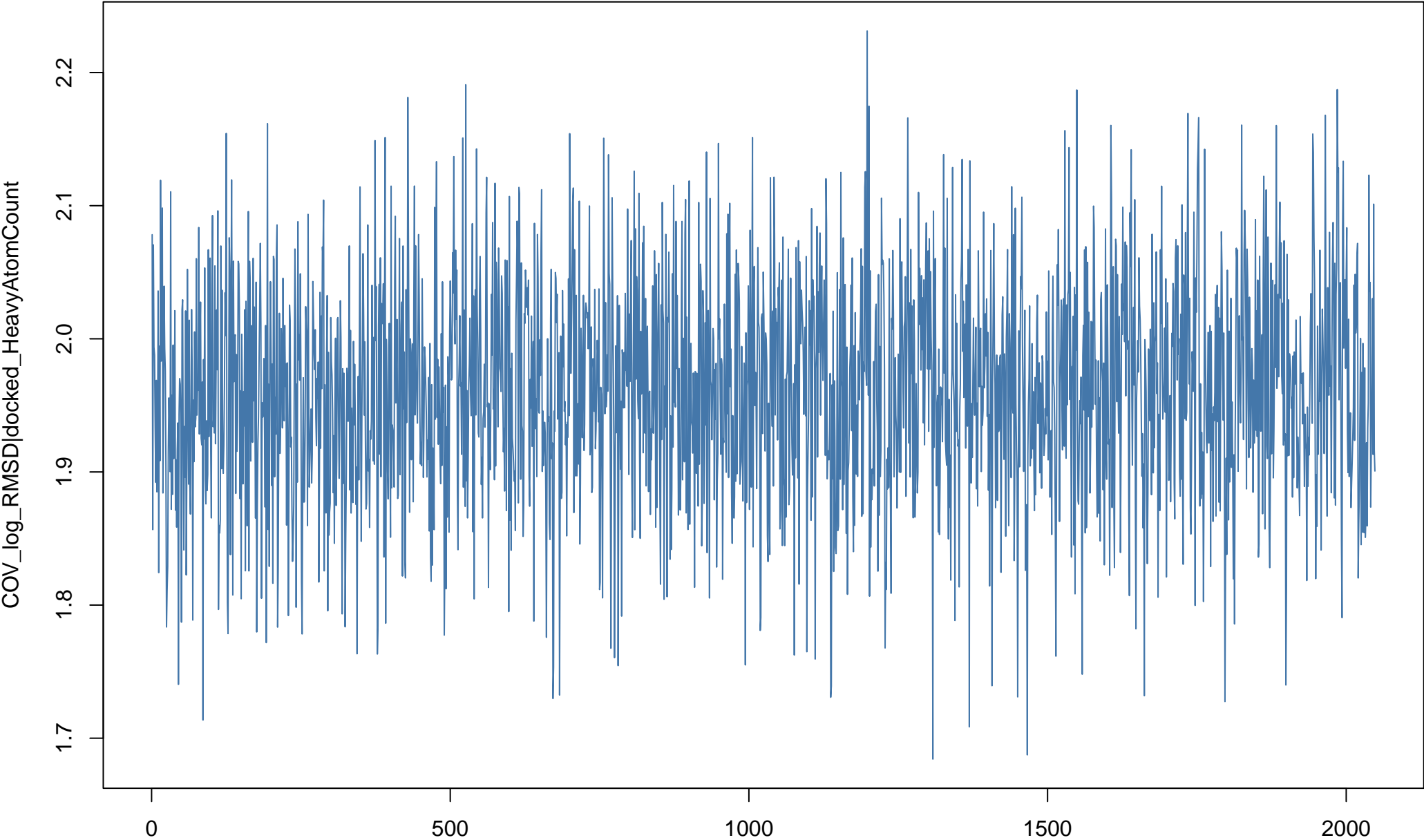
VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0368 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



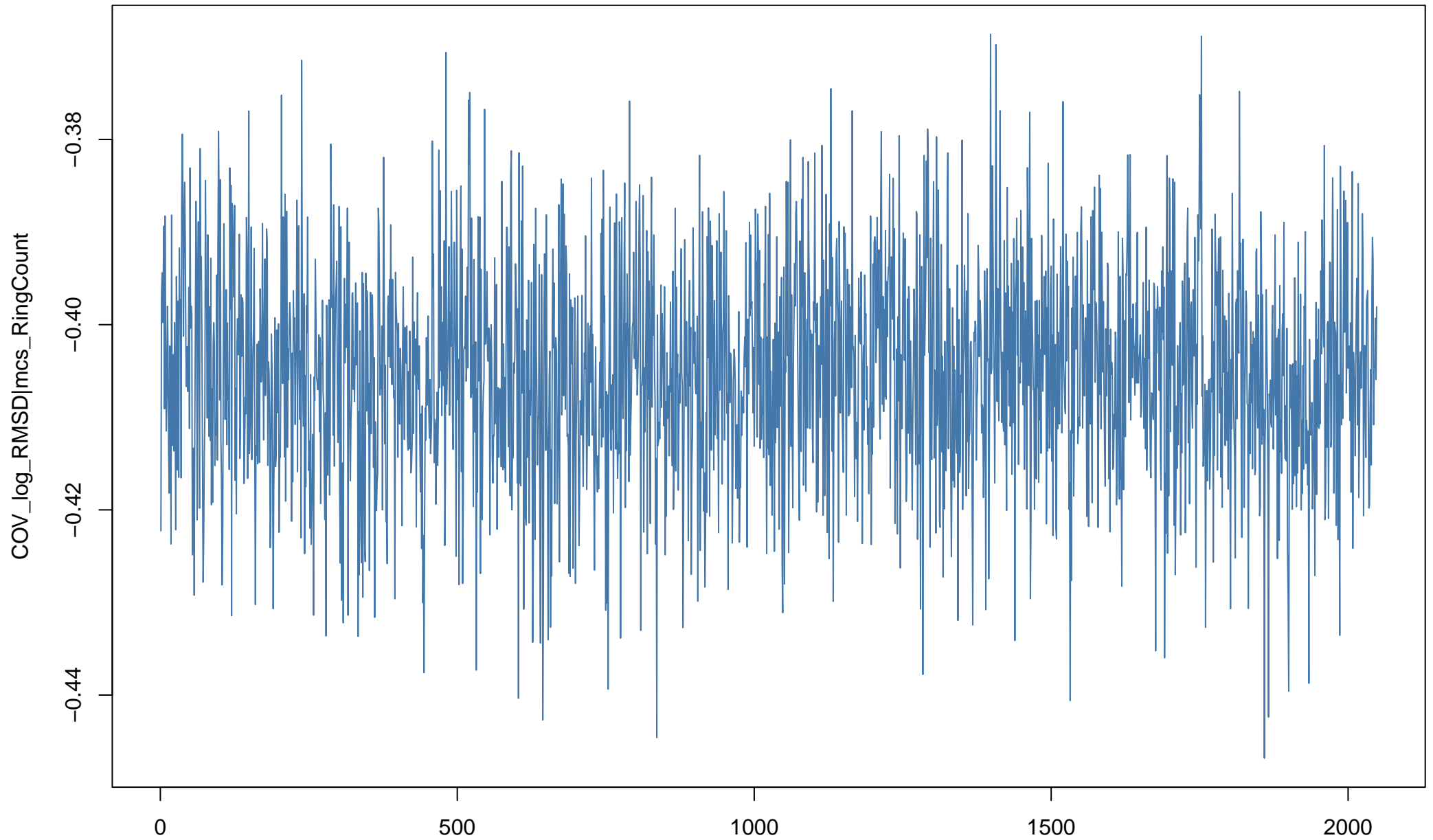
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1890 | BMK = 0.0409 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0



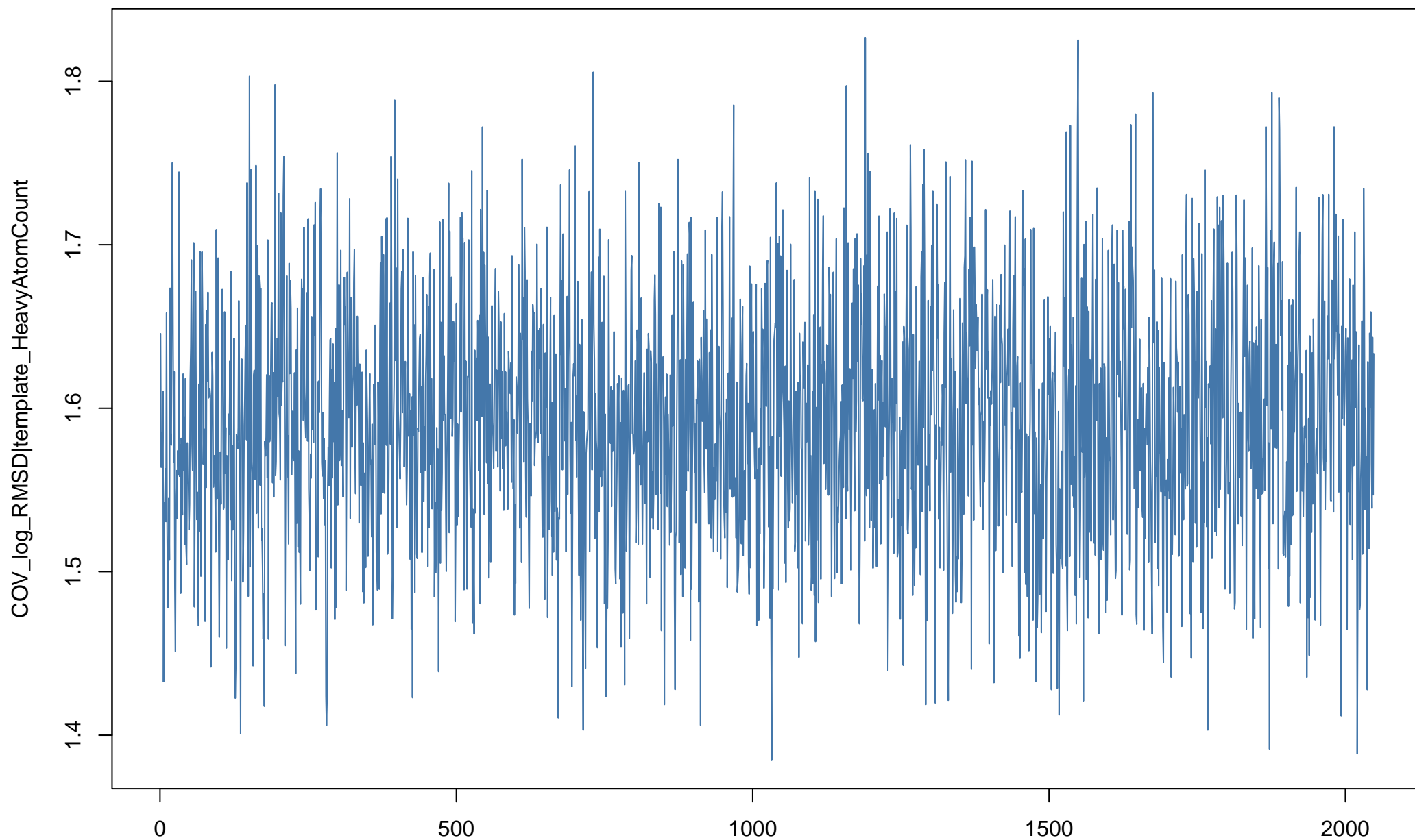
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1750 | BMK = 0.051 | MCSE(6.27) = 2.8 | stat: FALSE | burn: 0



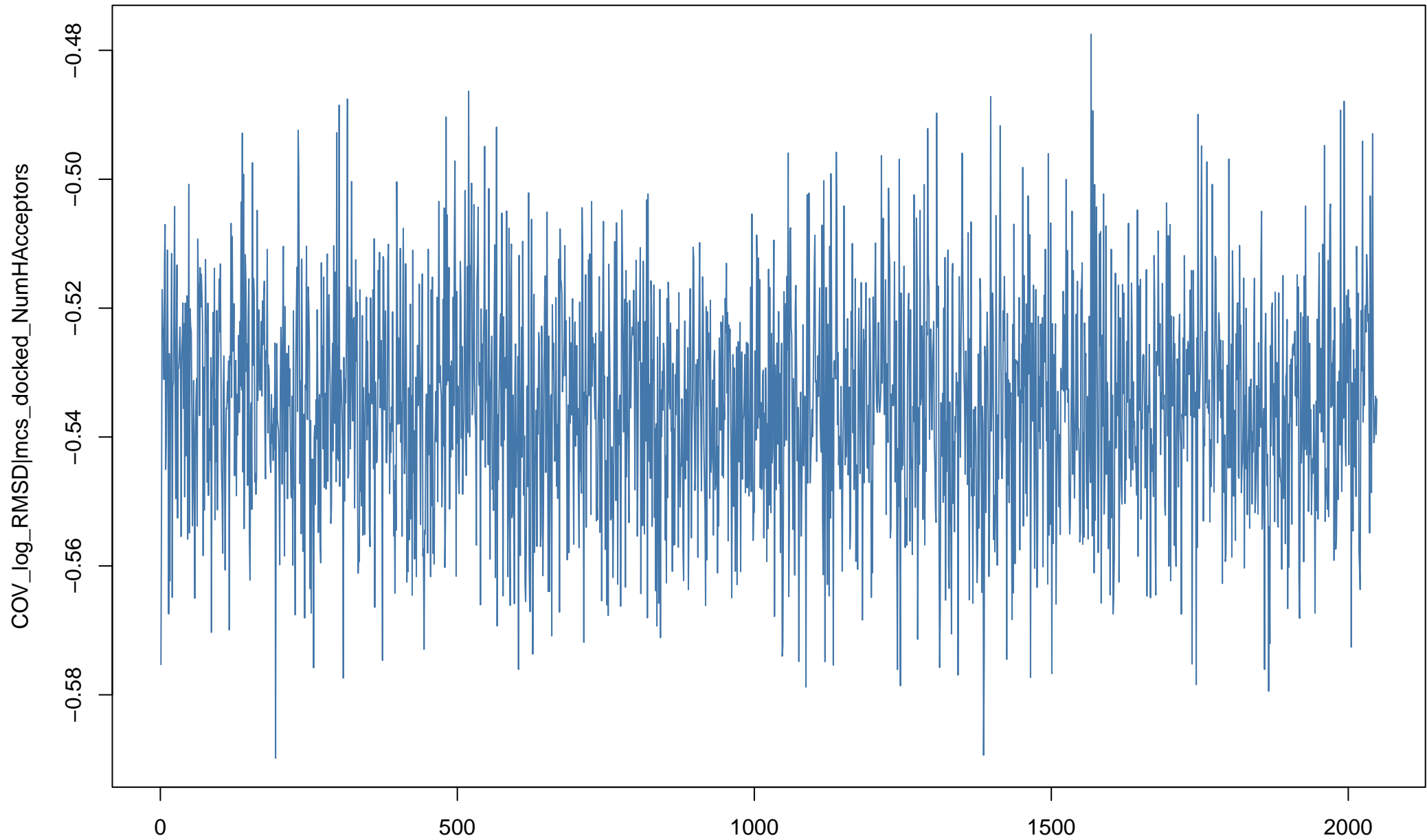
COV_log_RMSD|mcs_RingCount
ESS = 1690 | BMK = 0.0551 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0



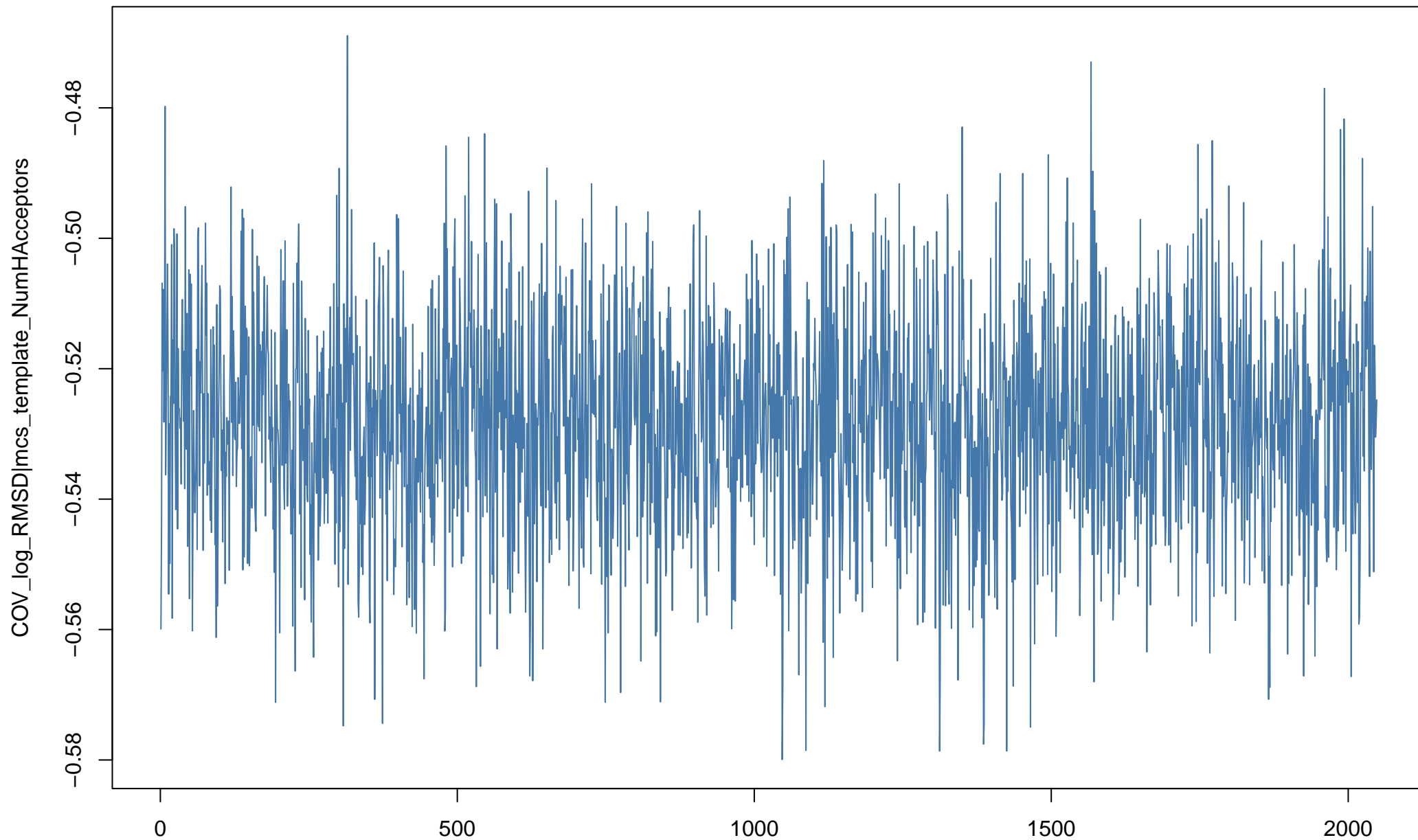
COV_log_RMSD|template_HeavyAtomCount
ESS = 1650 | BMK = 0.0474 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



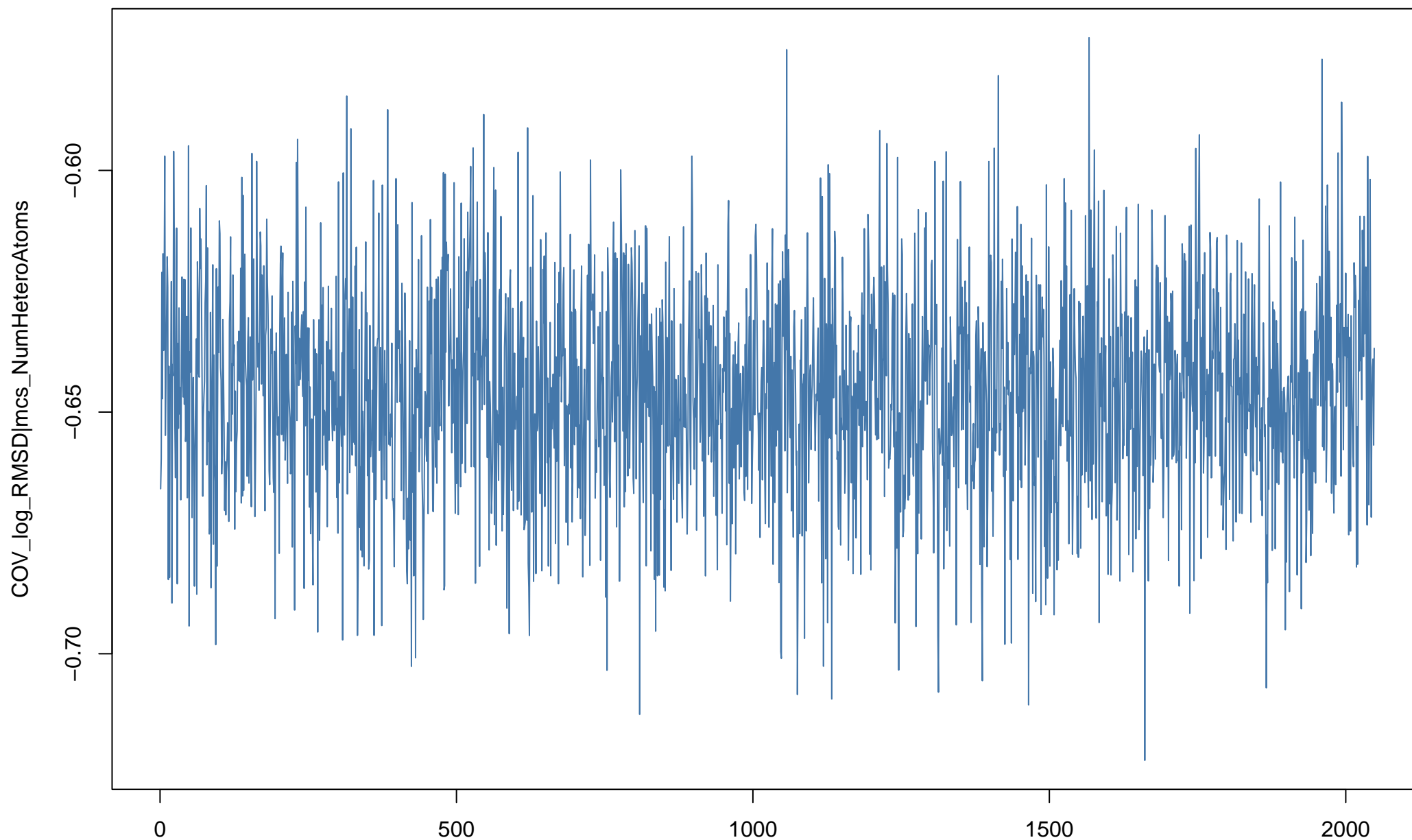
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0493 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0



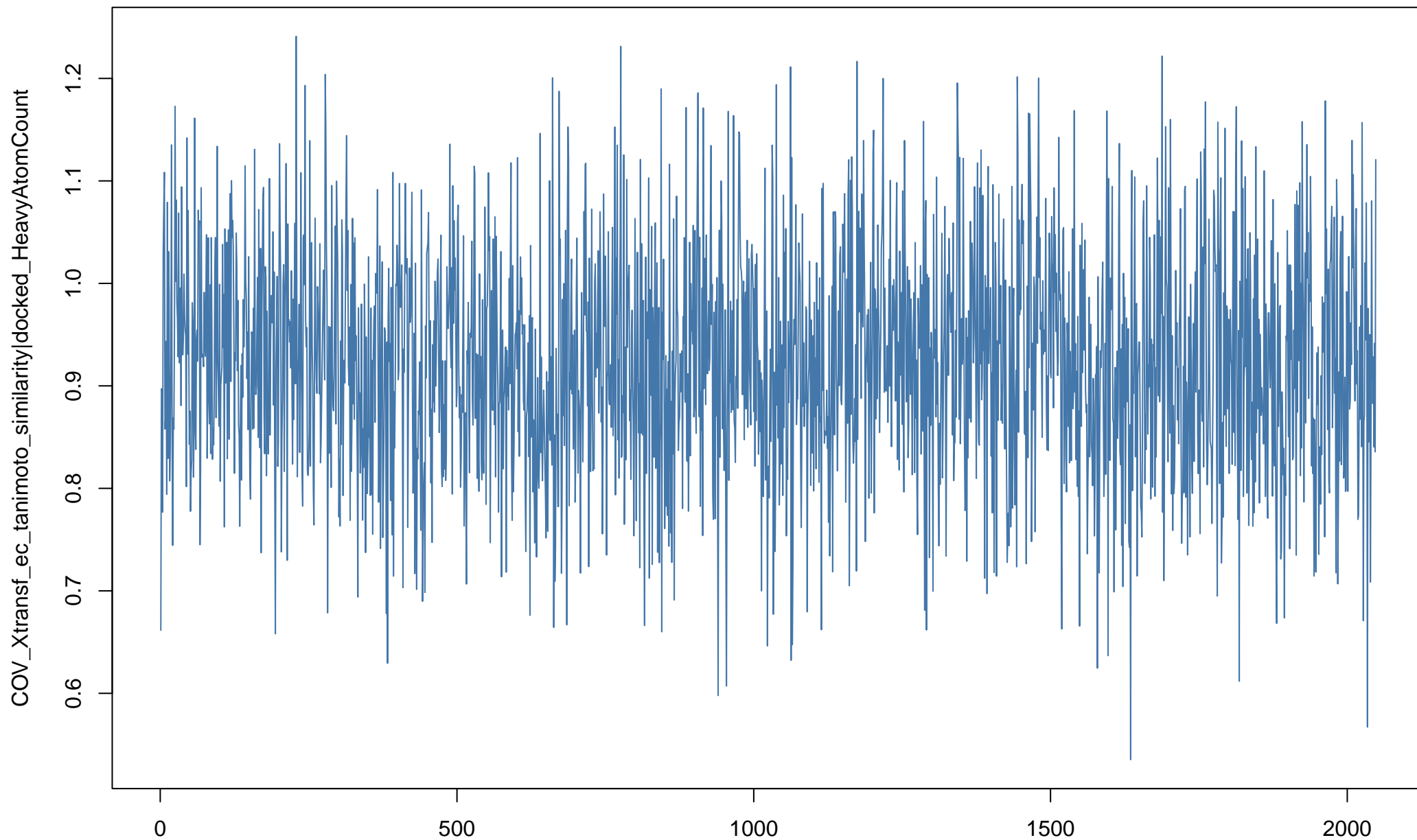
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0359 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0



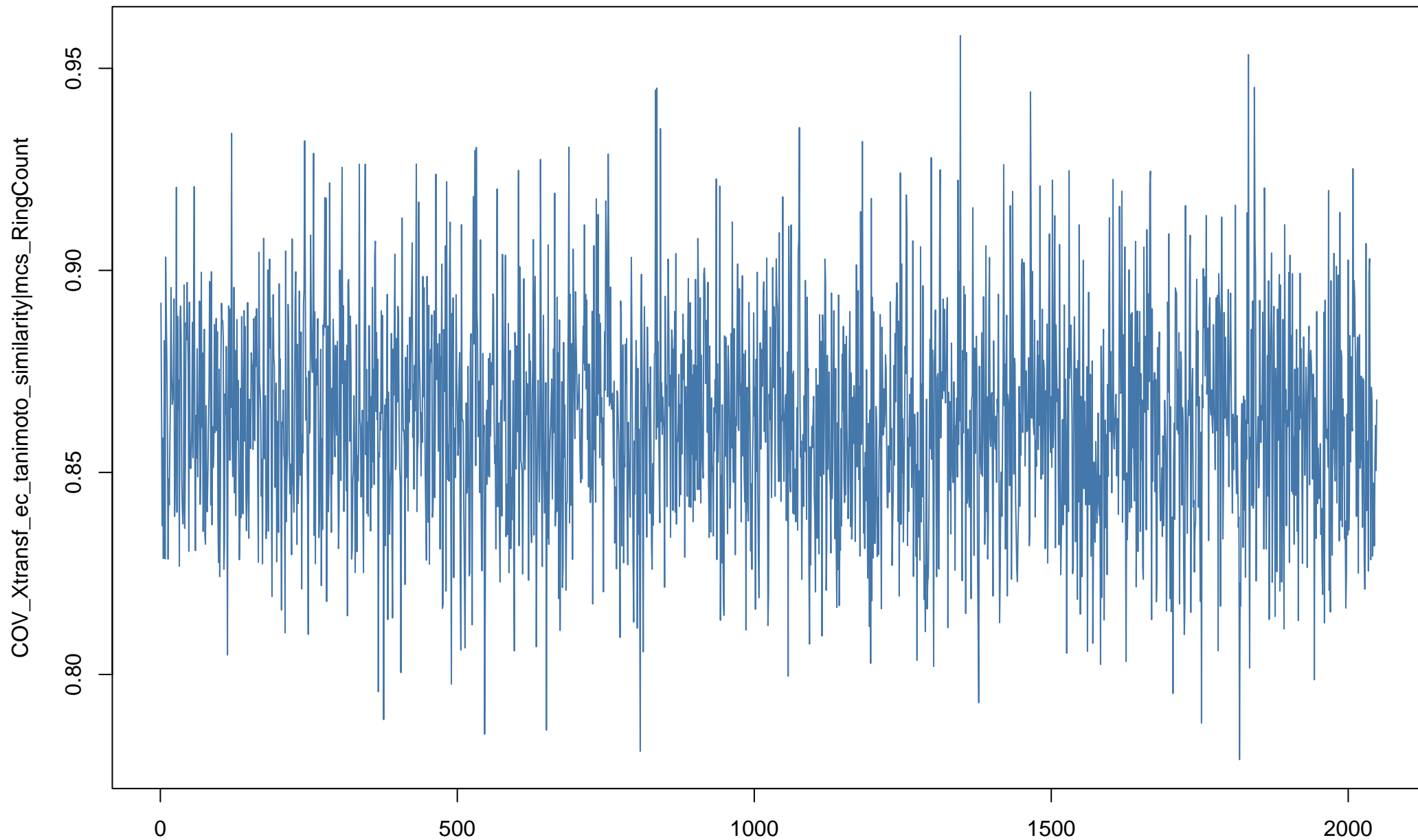
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0416 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0



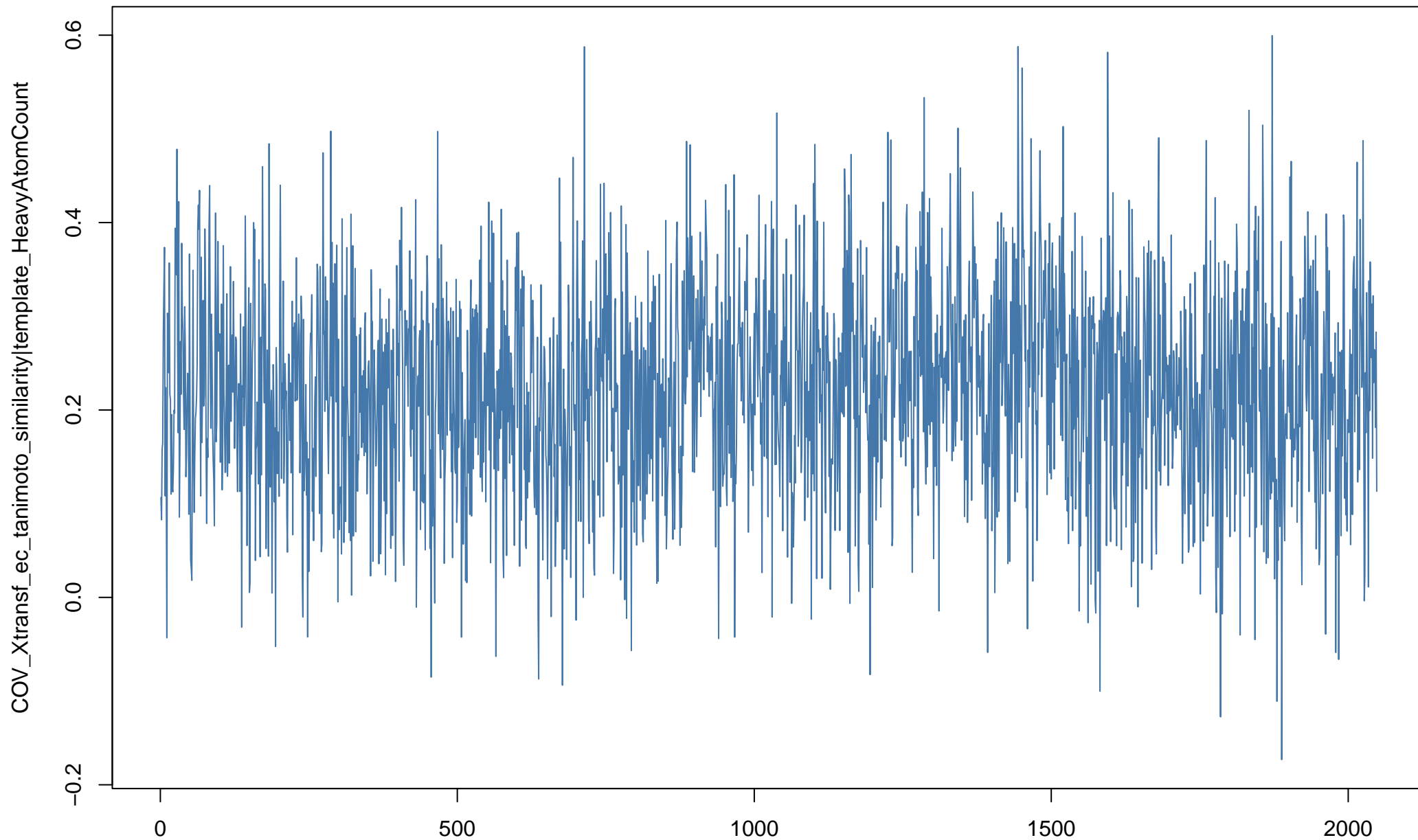
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1670 | BMK = 0.0384 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0



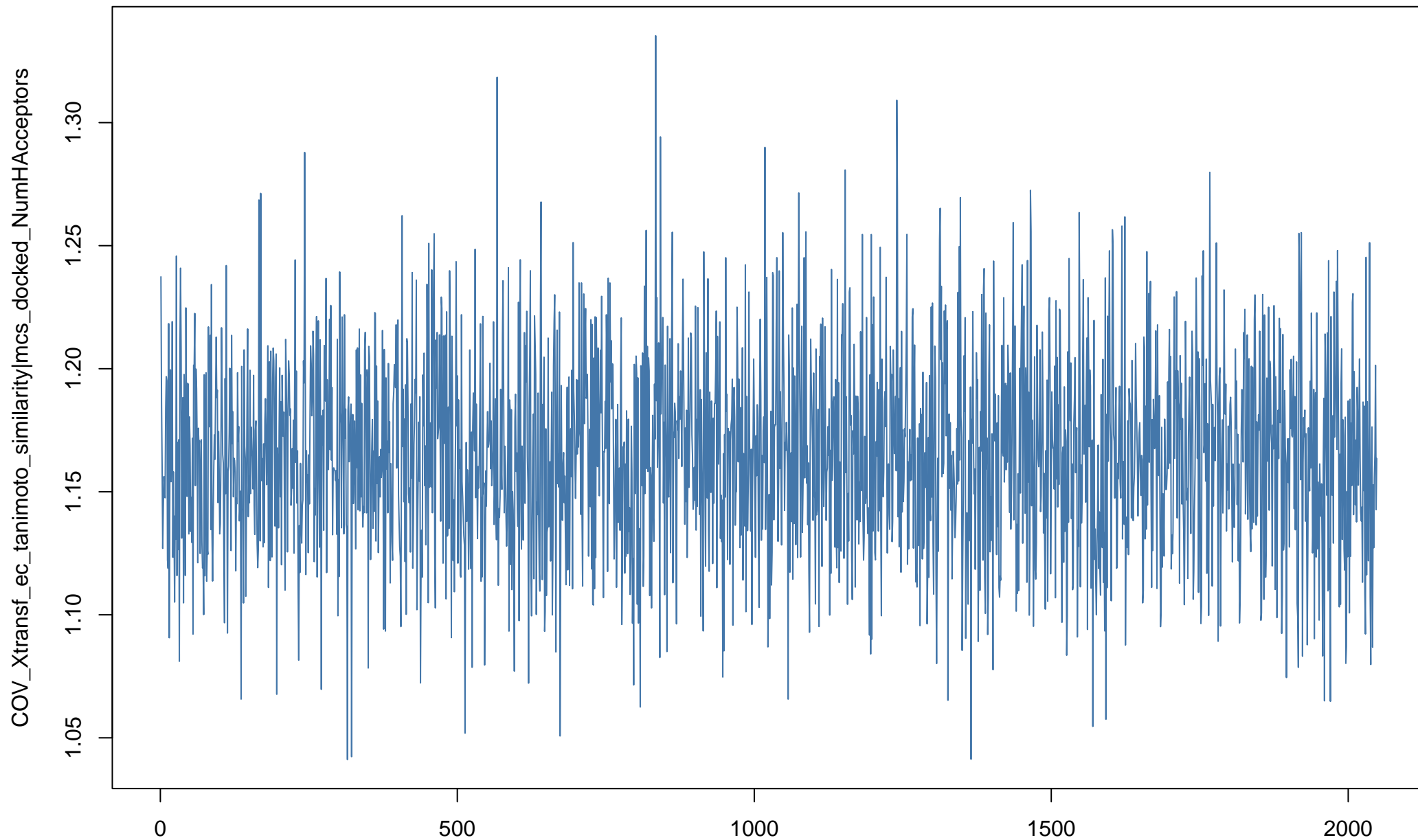
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 2050 | BMK = 0.0643 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



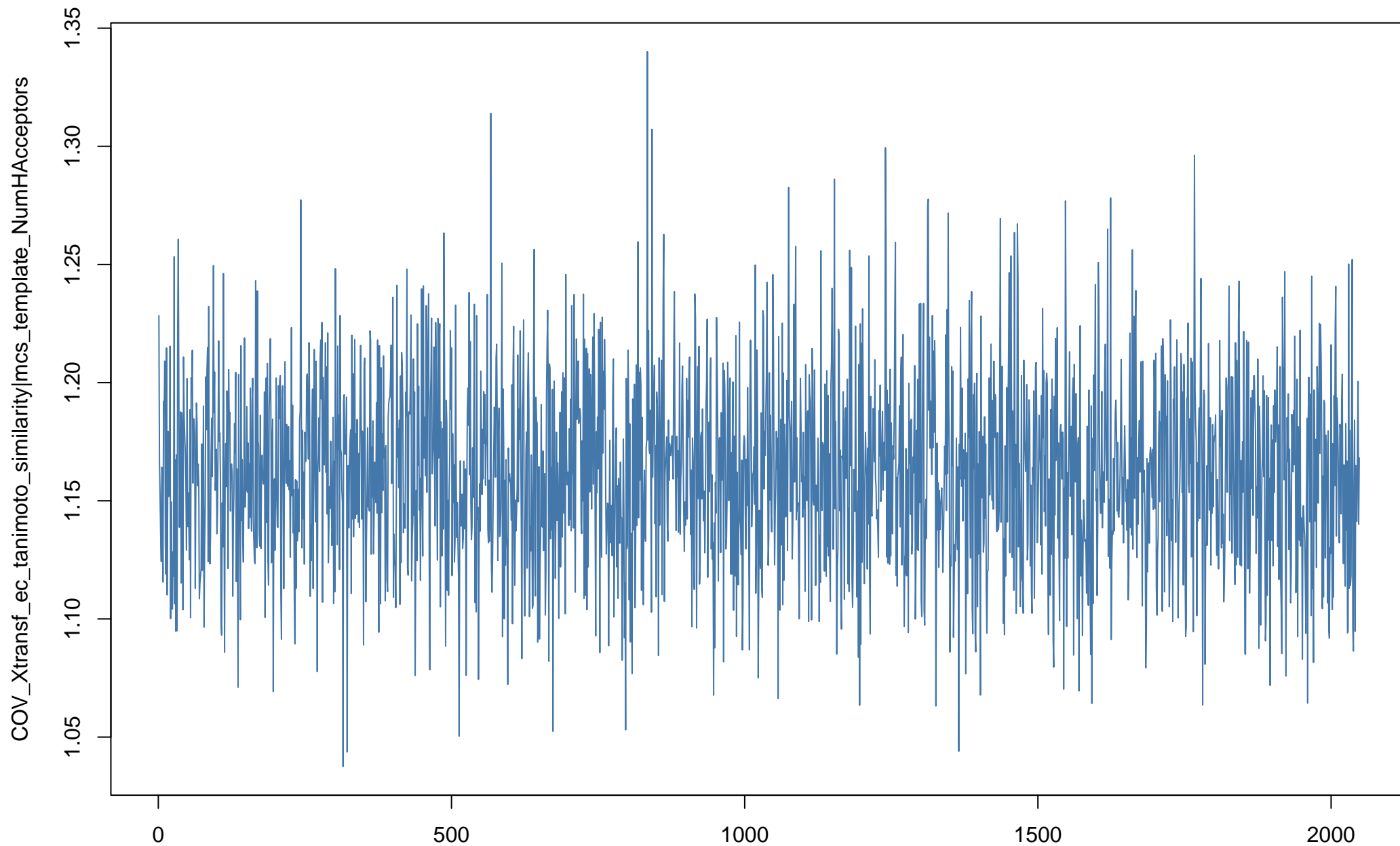
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1070 | BMK = 0.0647 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0



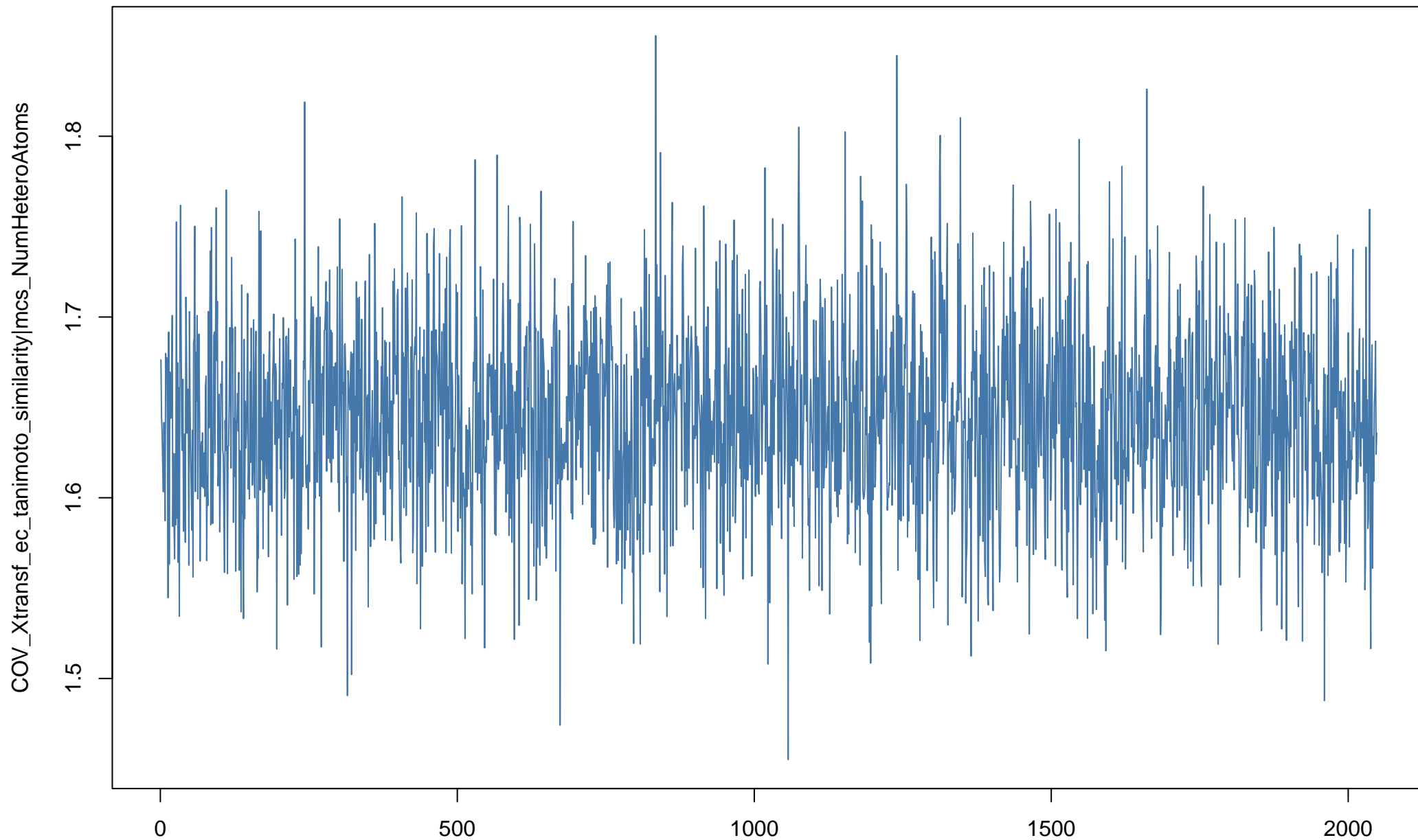
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0512 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0



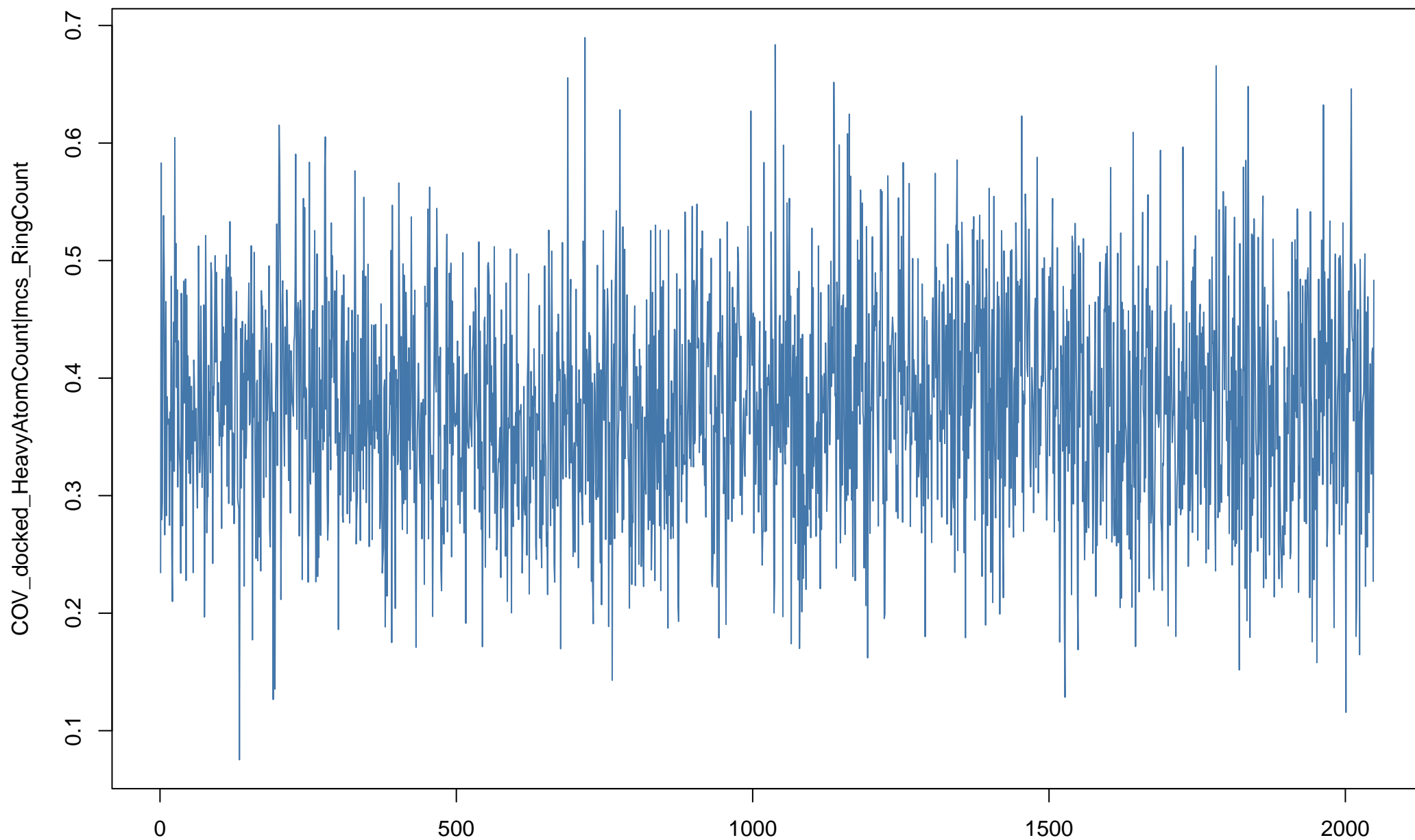
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0562 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0



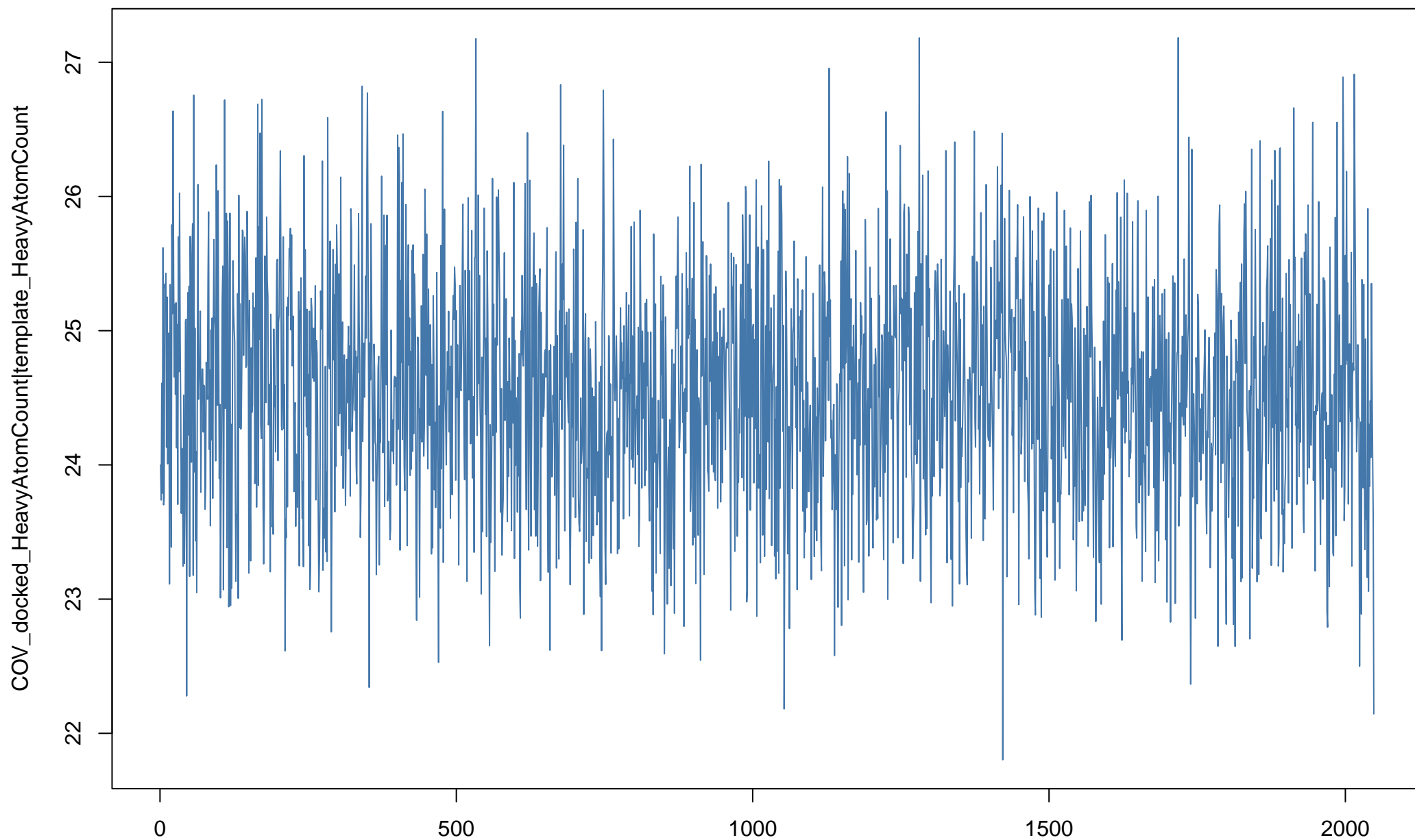
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0477 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0



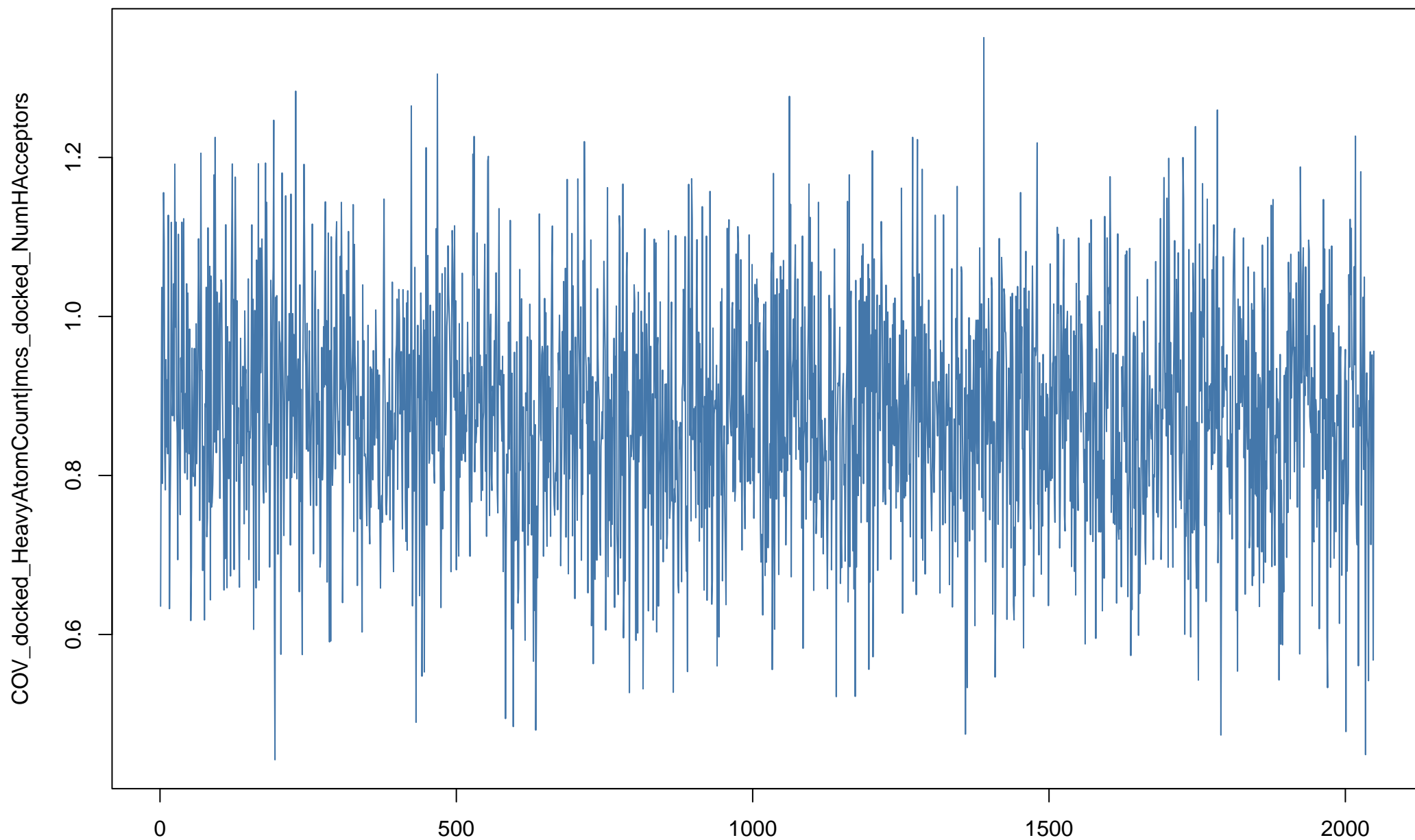
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1700 | BMK = 0.0716 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0



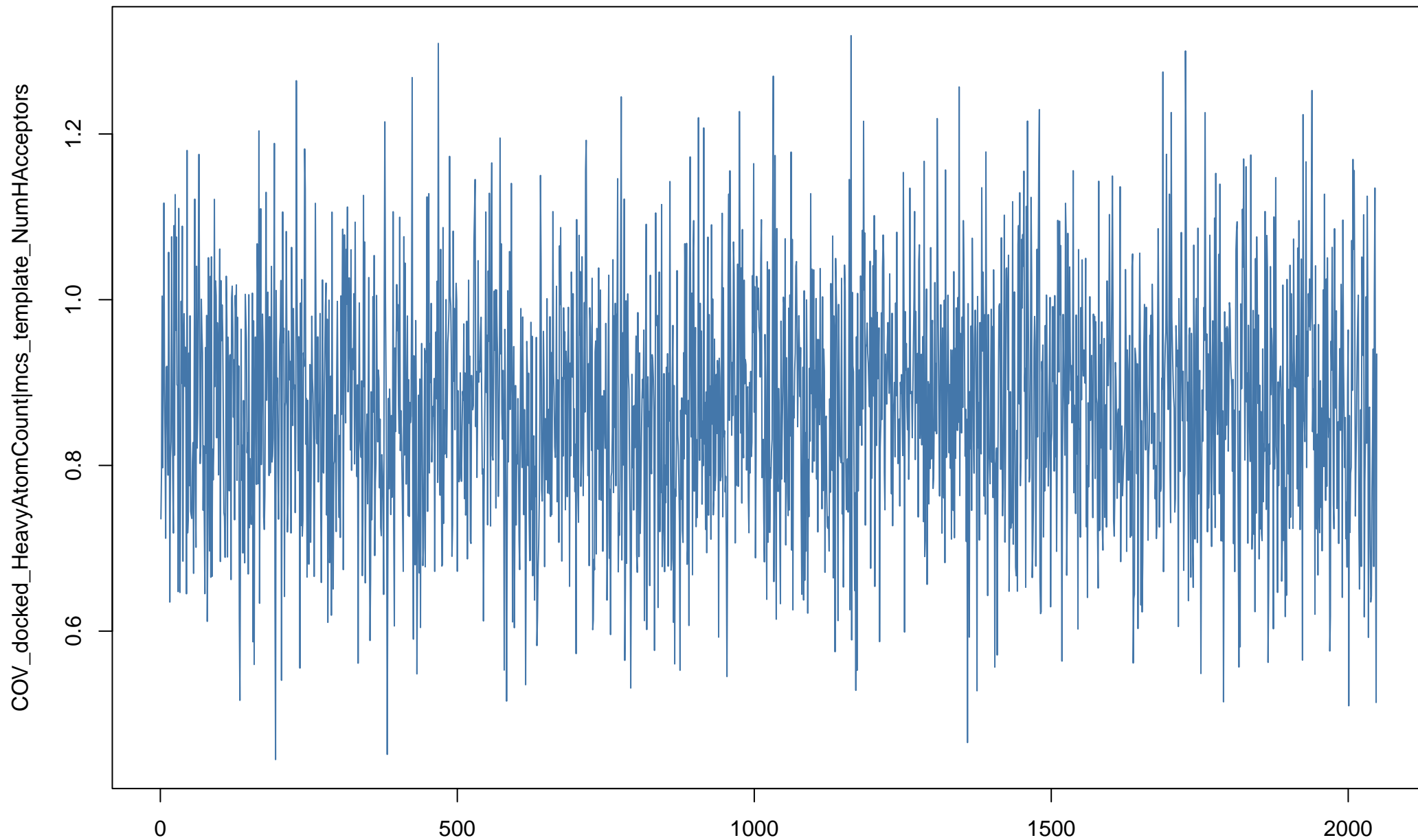
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1770 | BMK = 0.0332 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



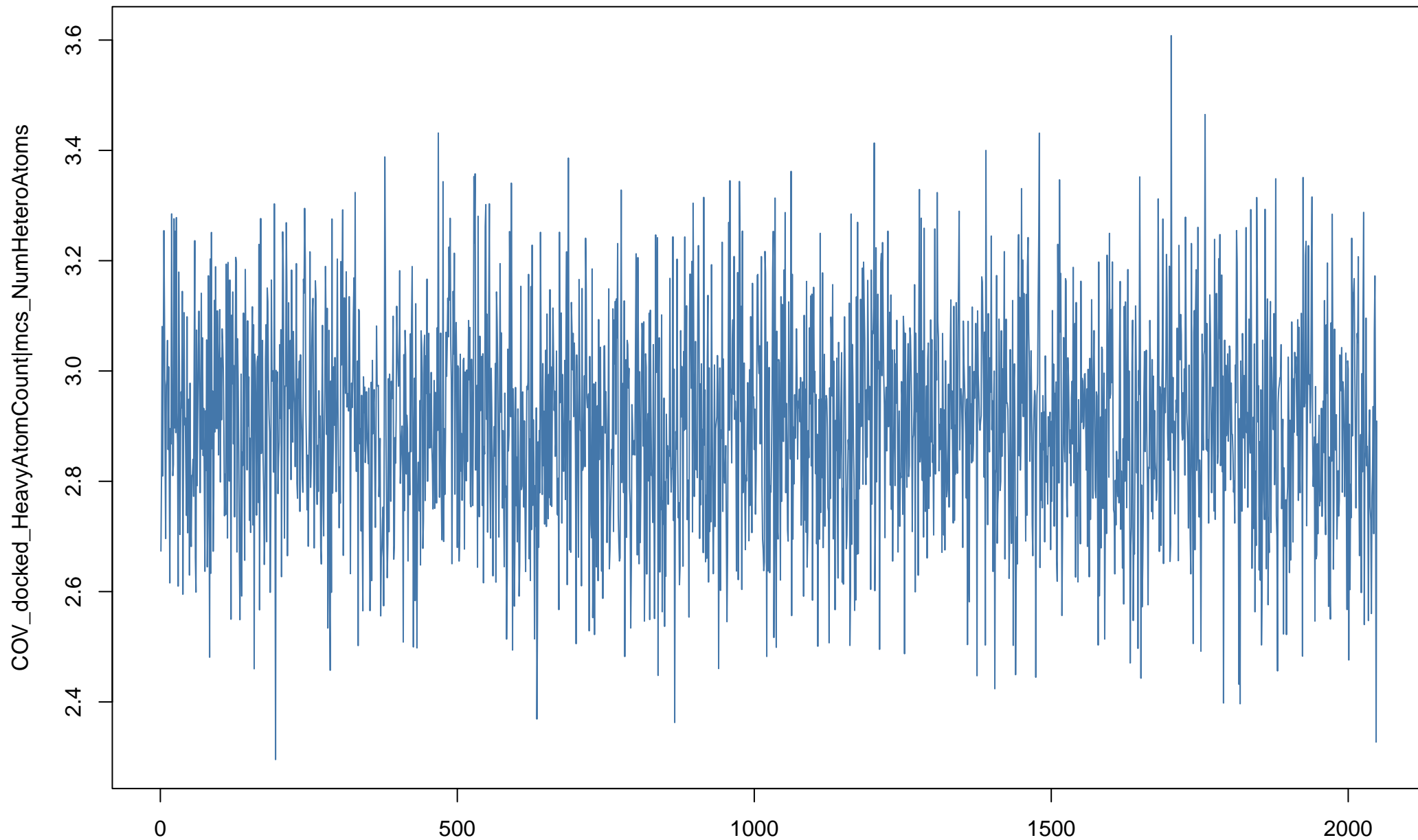
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0254 | MCSE(6.27) = 2.46 | stat: FALSE | burn: 0



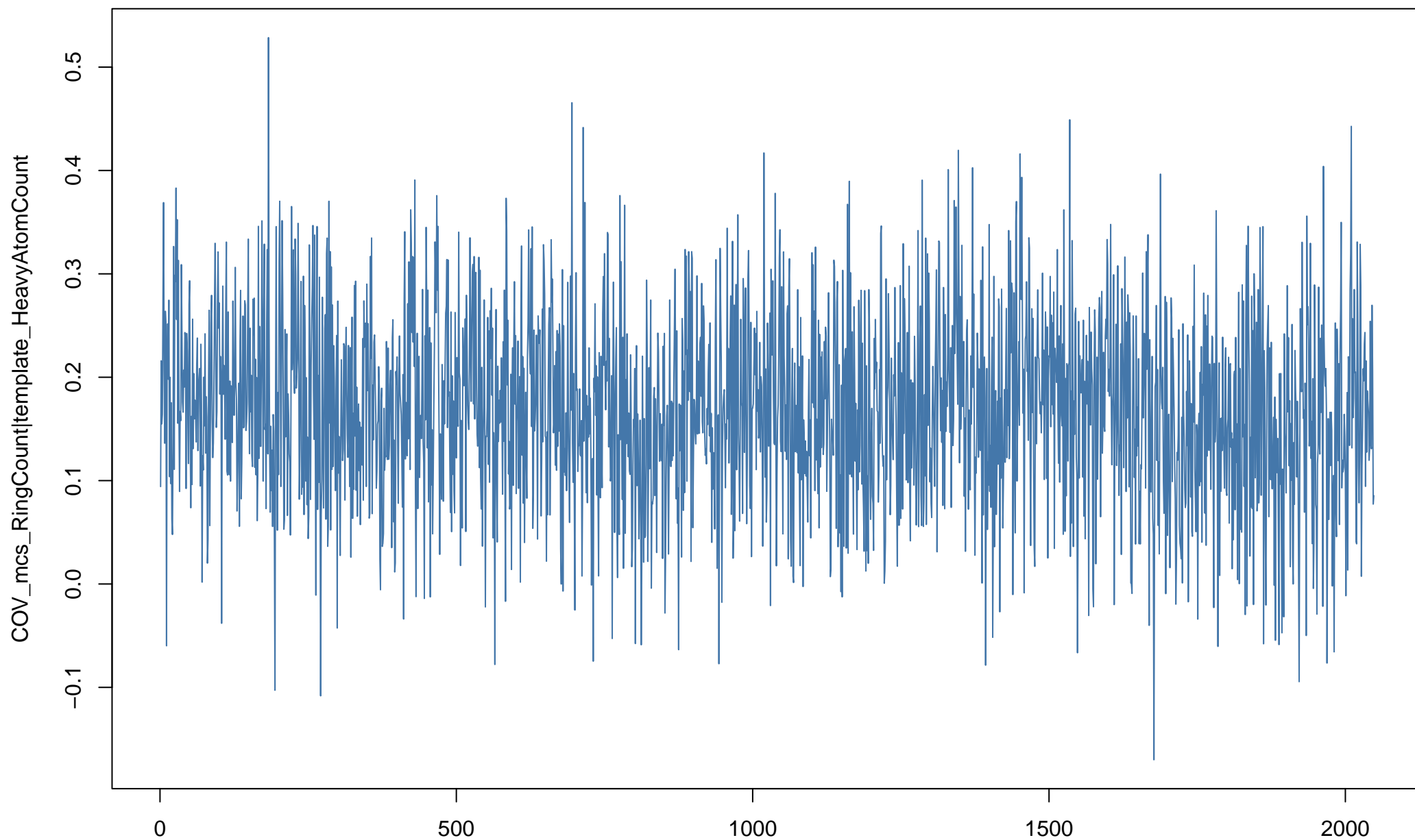
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0347 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0



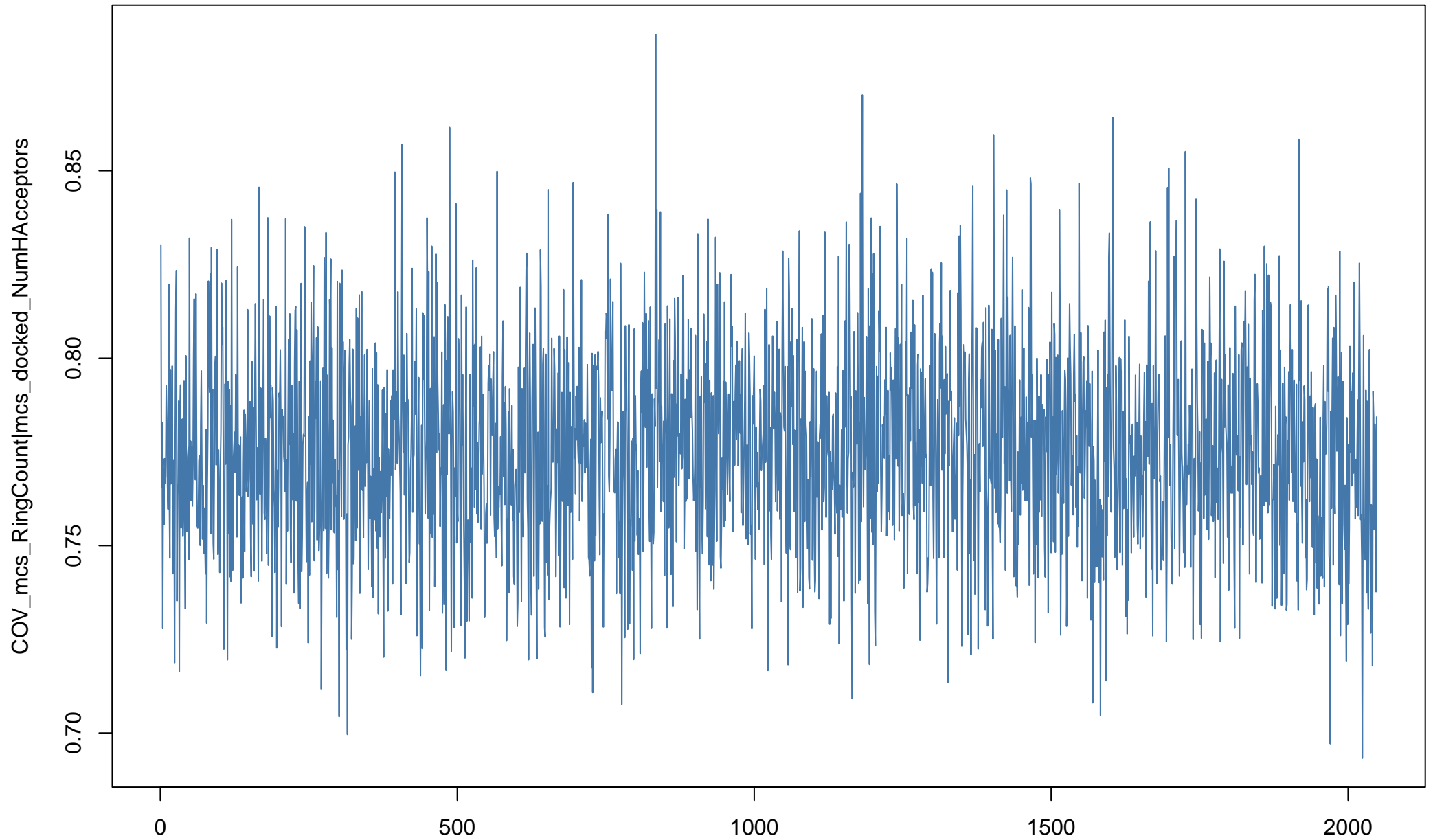
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0373 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0



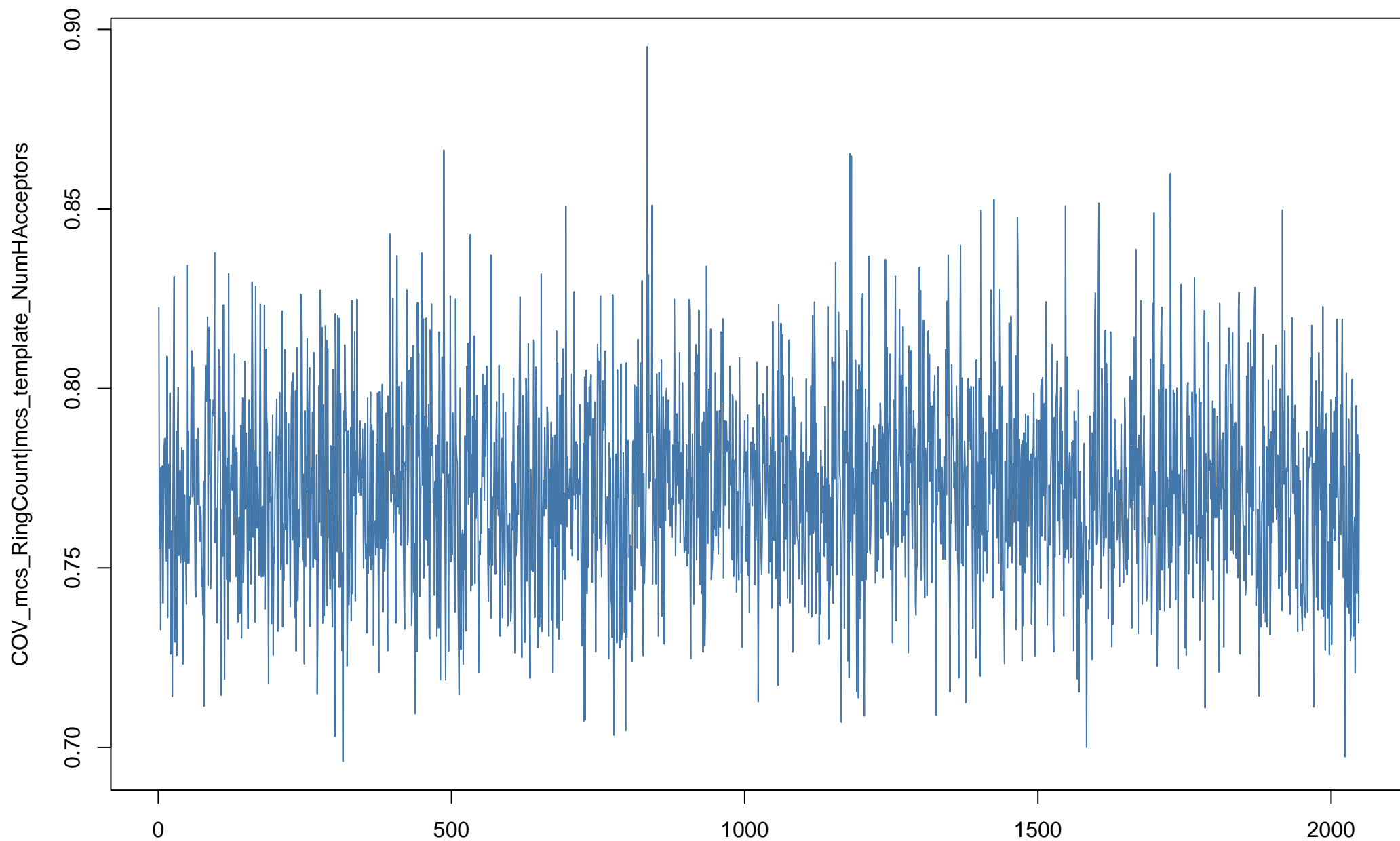
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1440 | BMK = 0.0608 | MCSE(6.27) = 3.31 | stat: FALSE | burn: 0



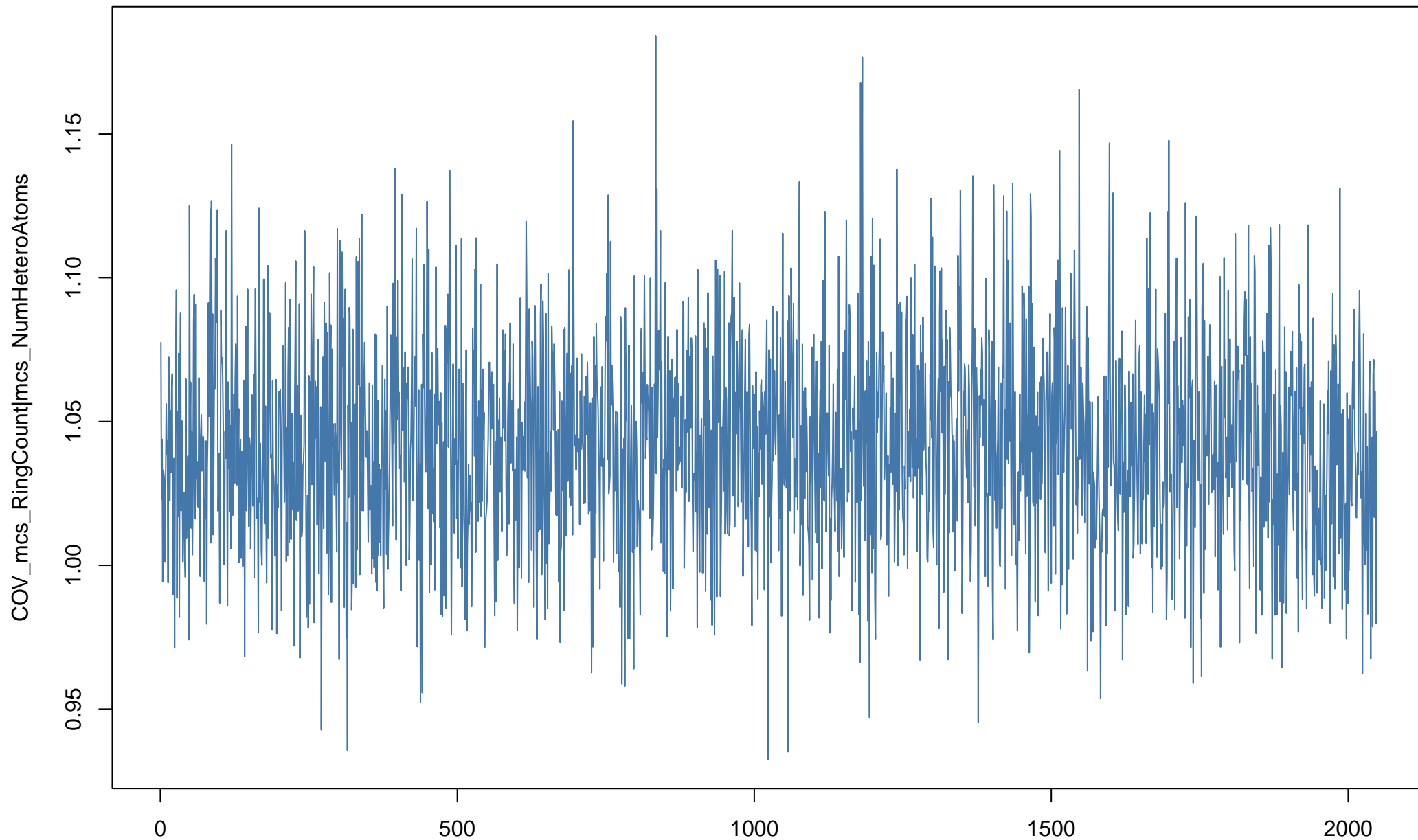
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0365 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0



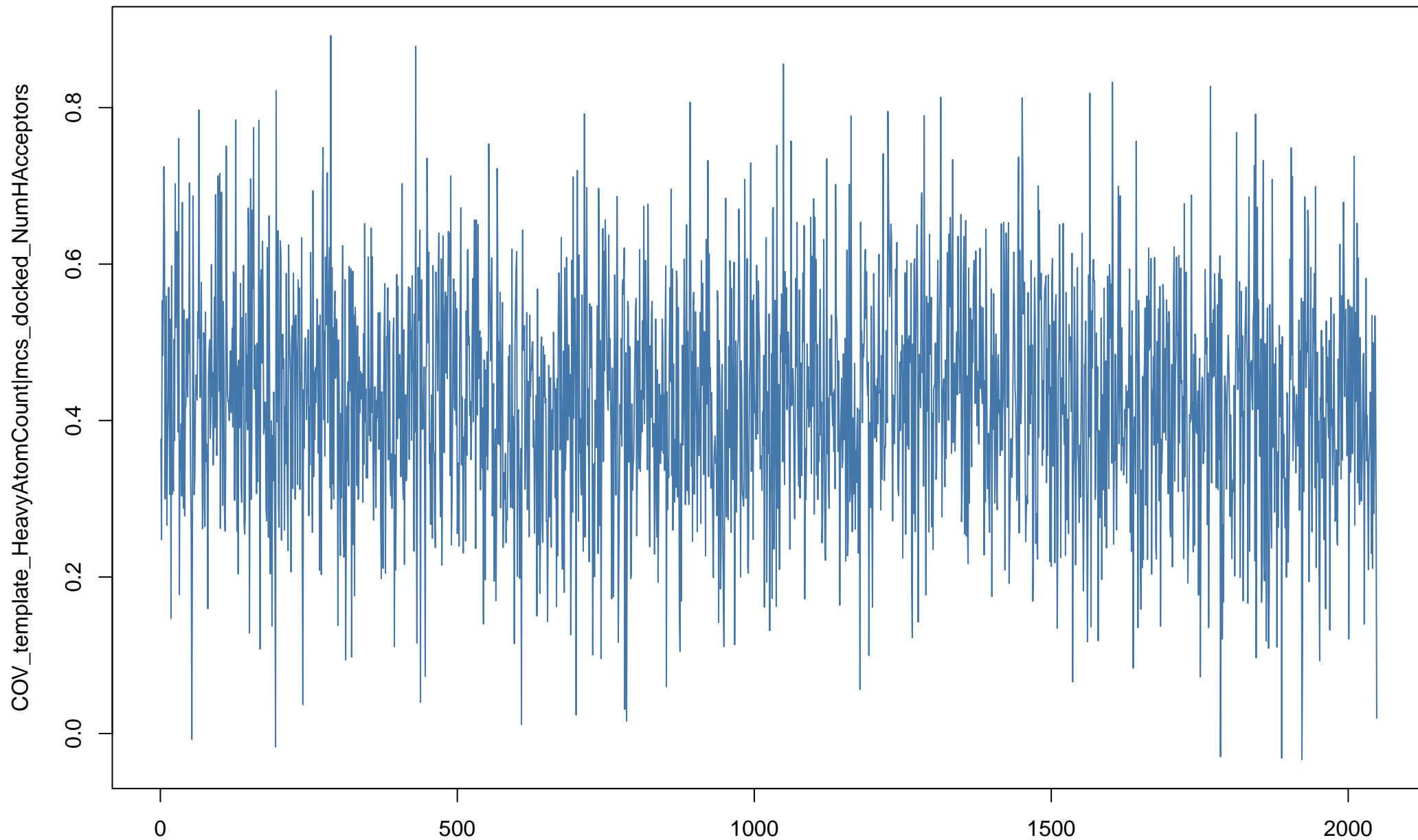
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.036 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



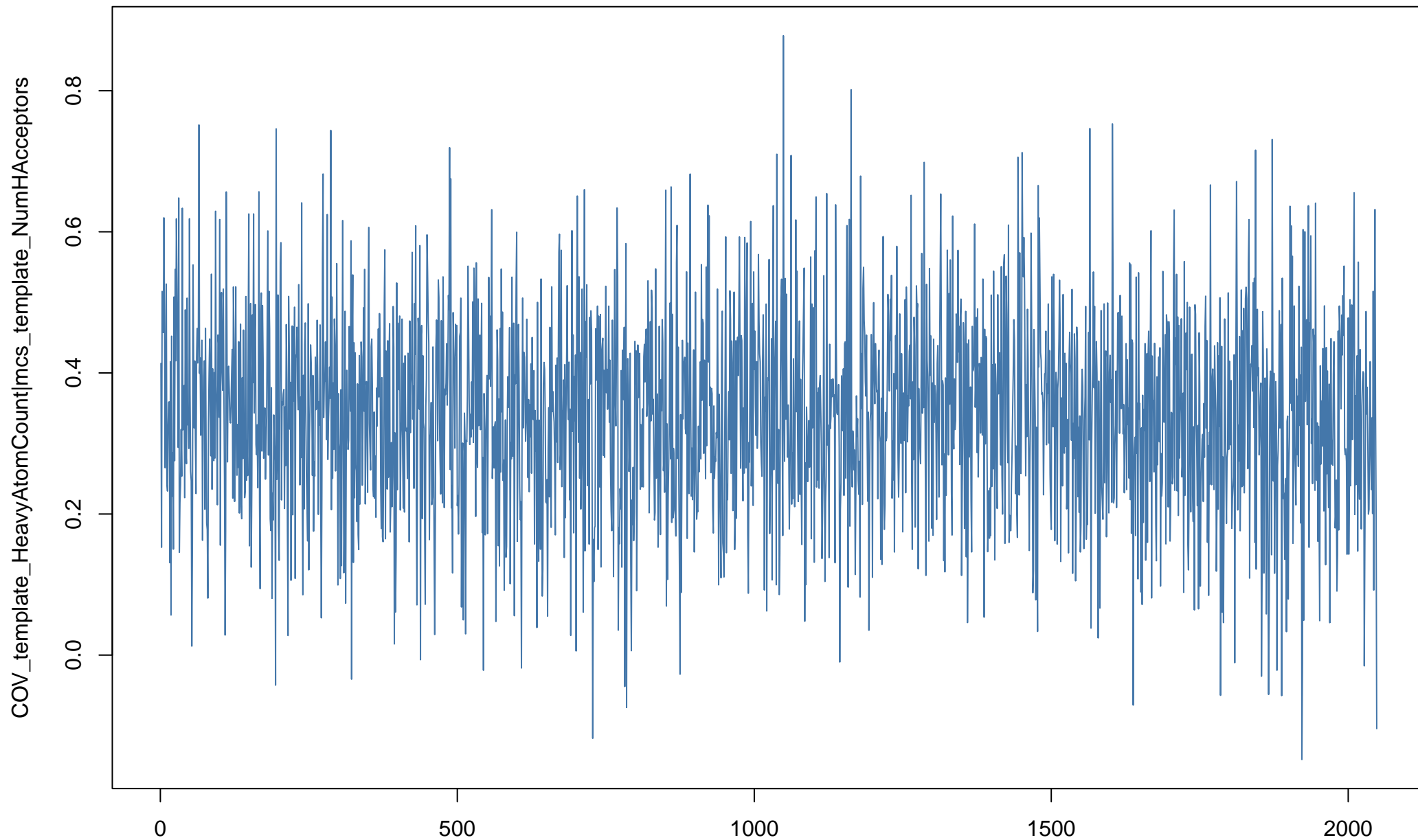
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0309 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0



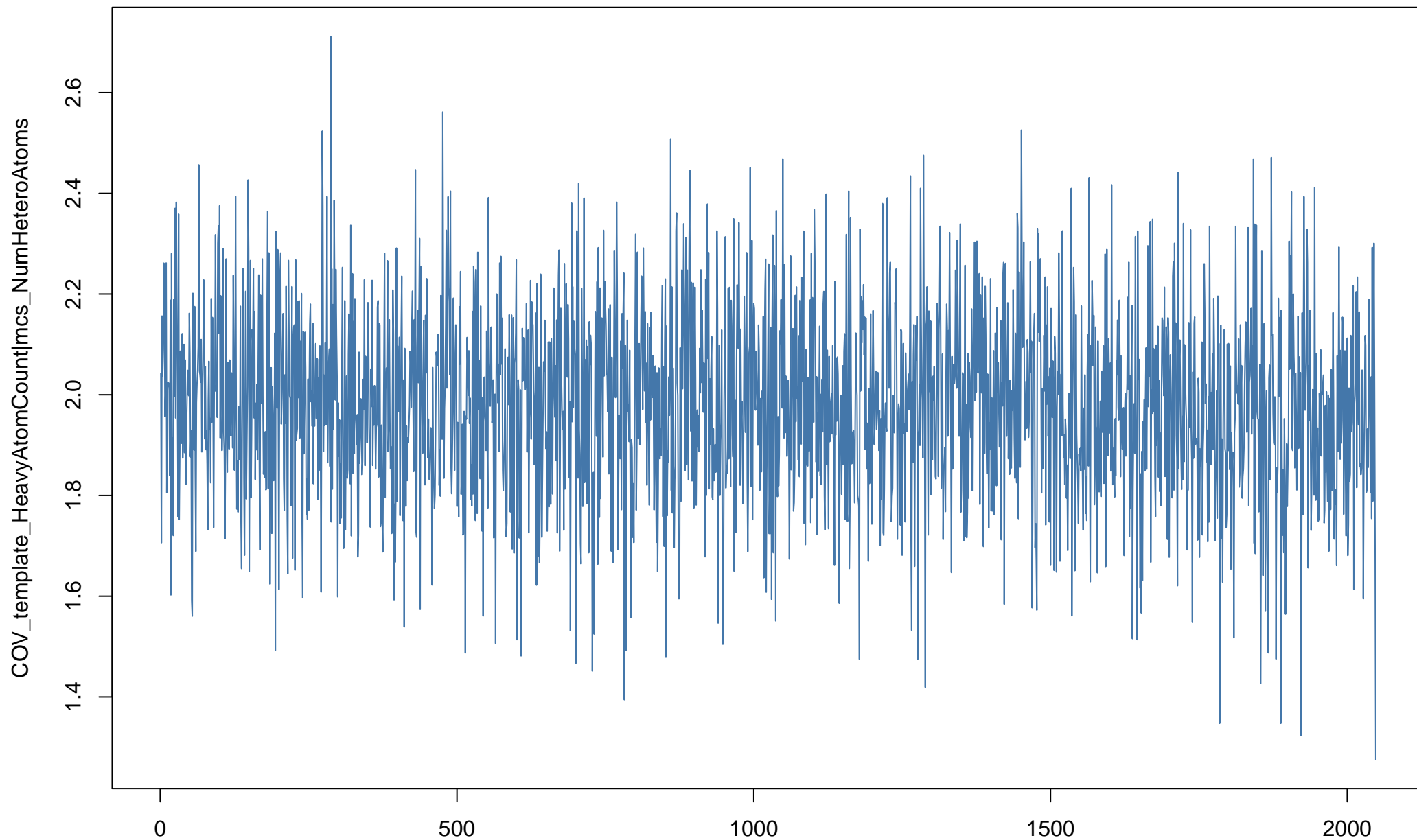
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1810 | BMK = 0.0332 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0



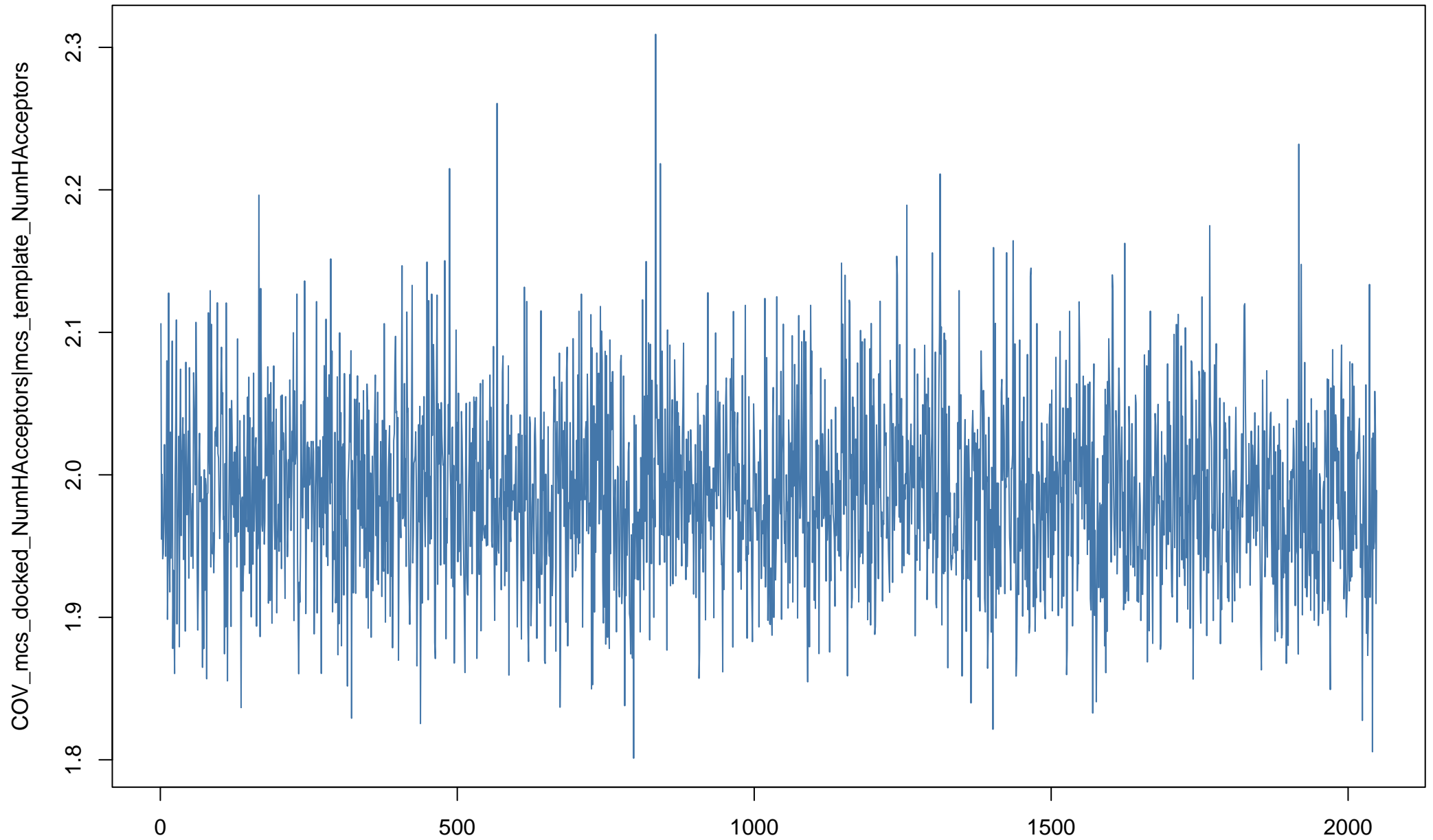
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0302 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0



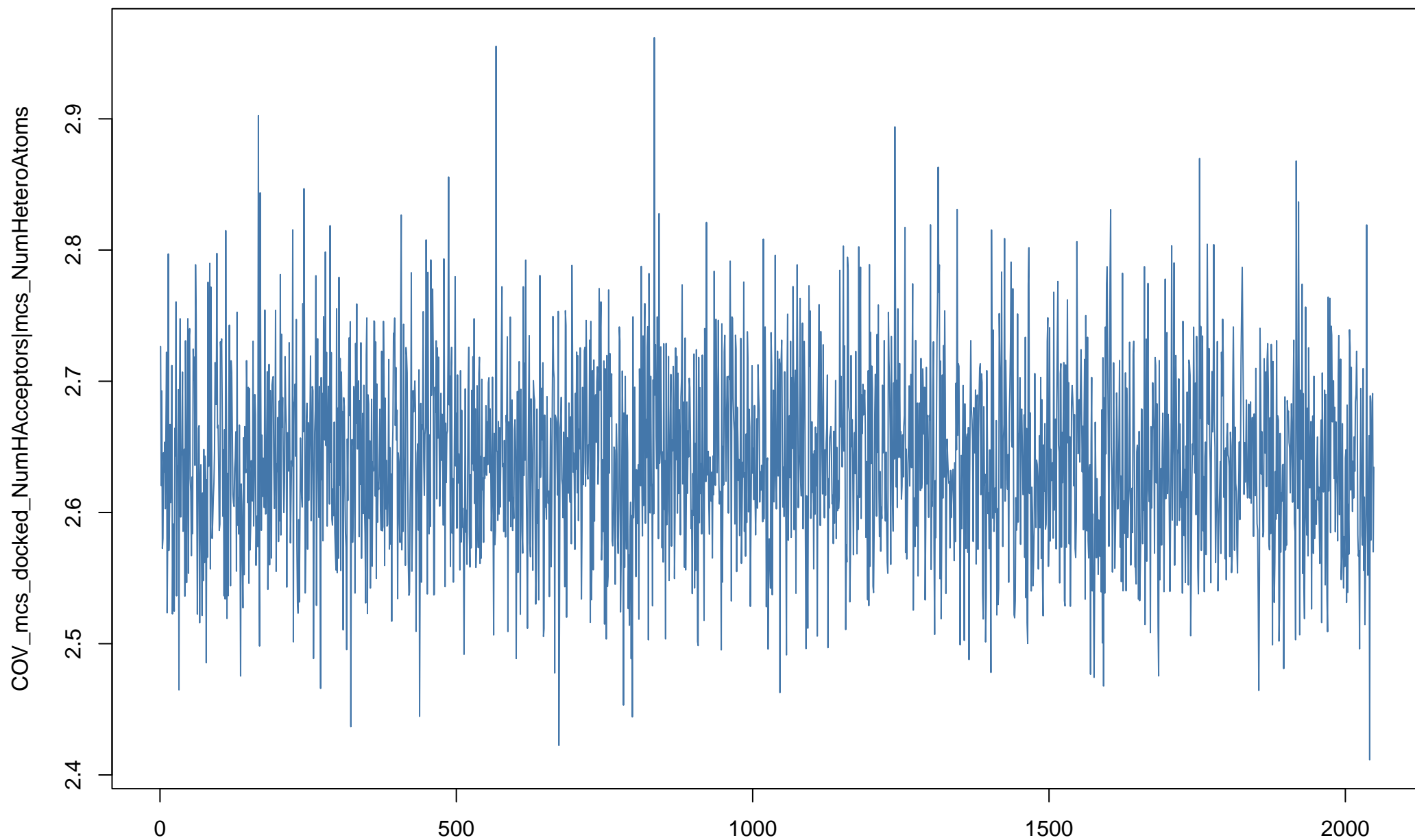
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1920 | BMK = 0.0537 | MCSE(6.27) = 2.08 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0542 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.042 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0585 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0

