

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.78981063755515

max MCSE = 14.533385529391

all stationary: FALSE

burn: 1020

-- STATS 2D --

min ESS = 193.77898632991

max BMK = 0.167307380107956

max MCSE = 4.56275144569721

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.809212070807686

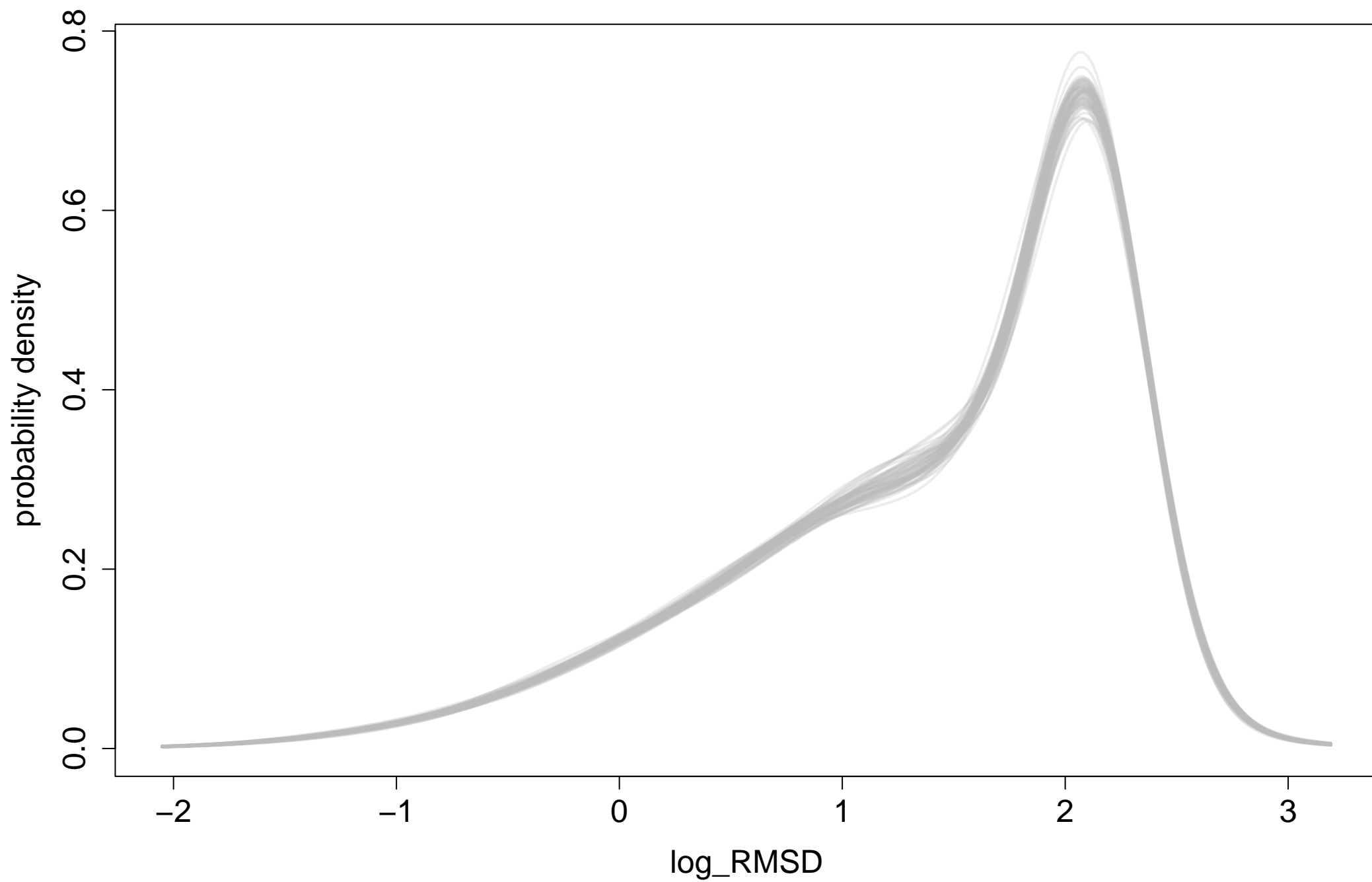
max MCSE = NaN

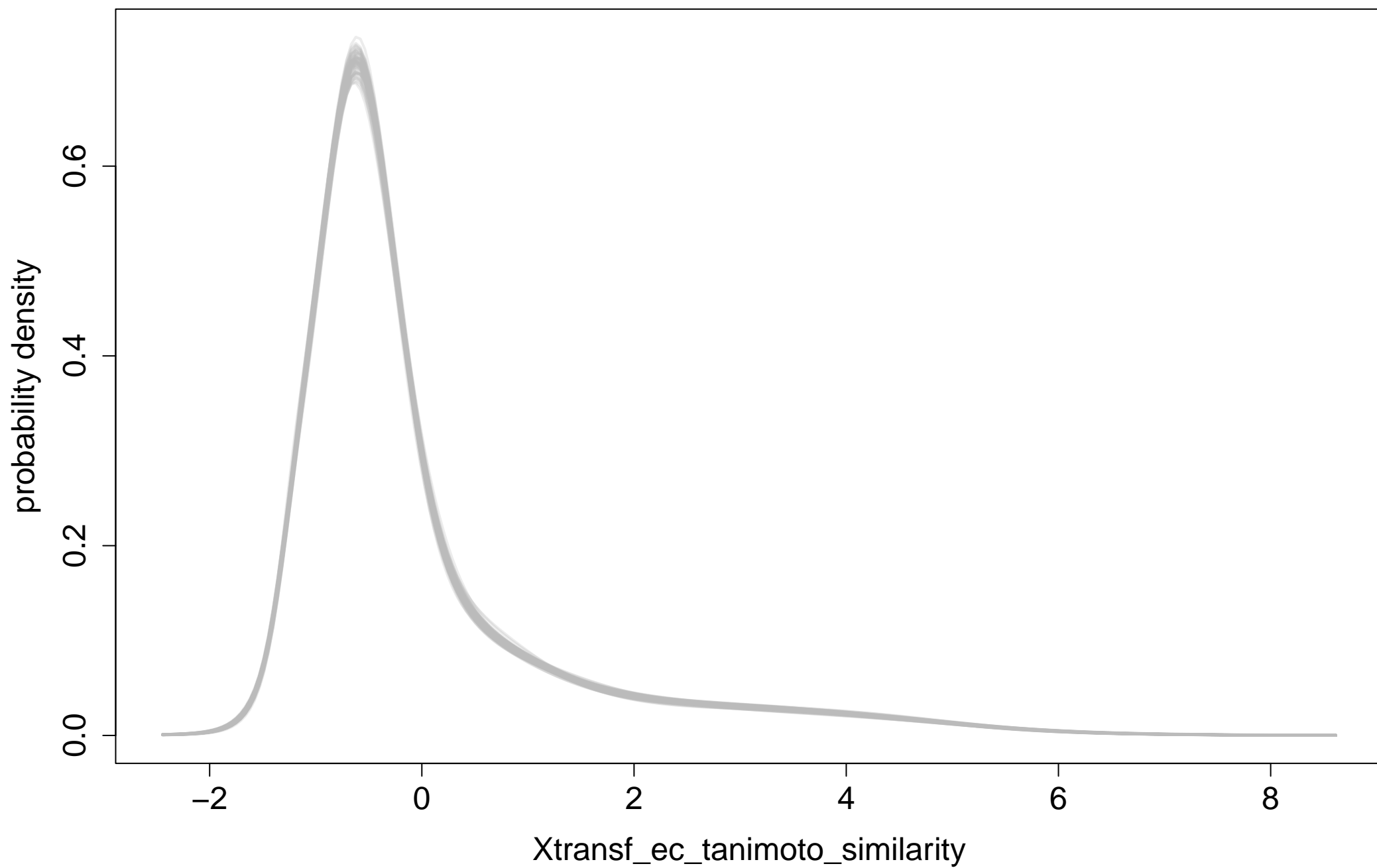
all stationary: FALSE

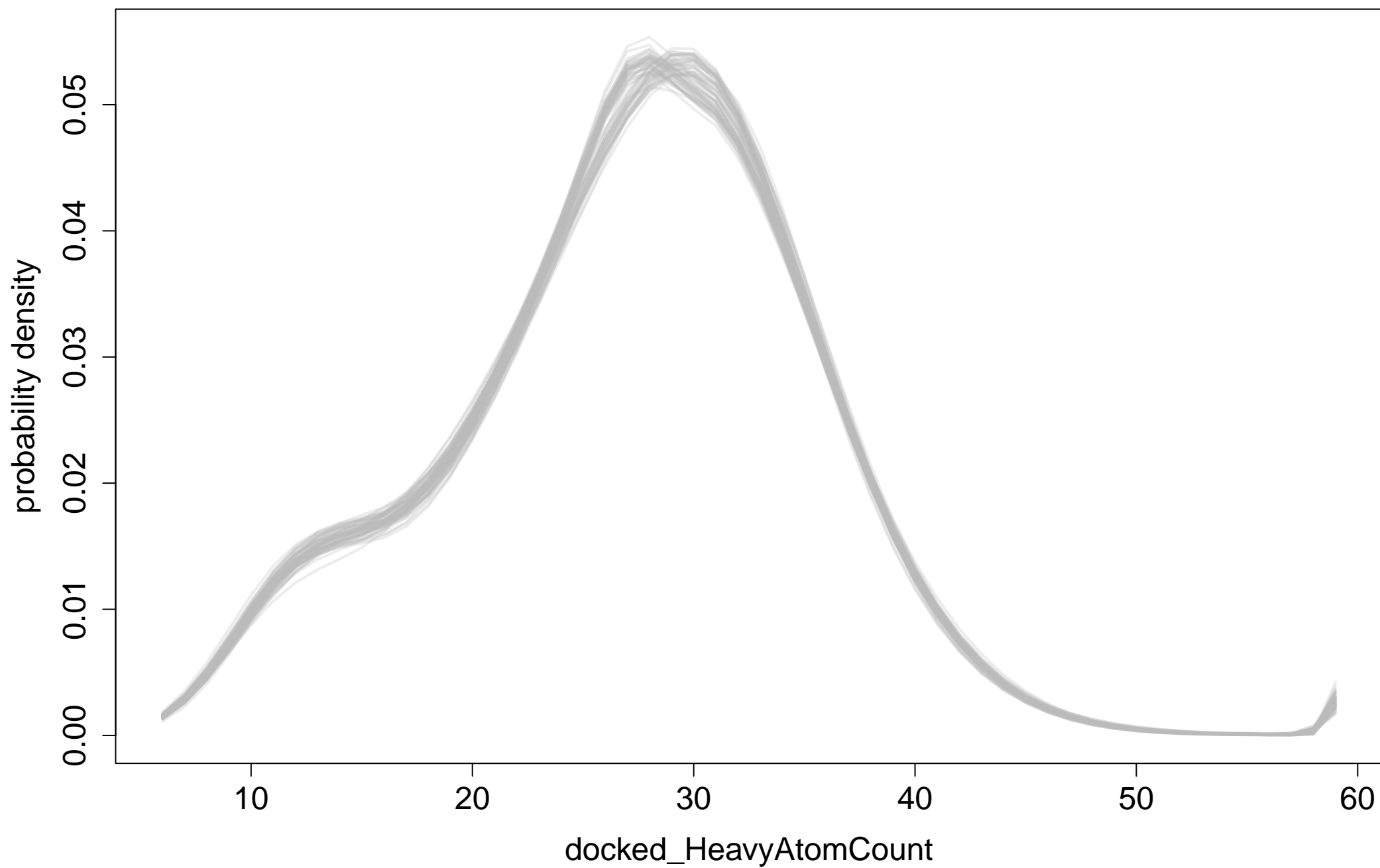
burn: 2040

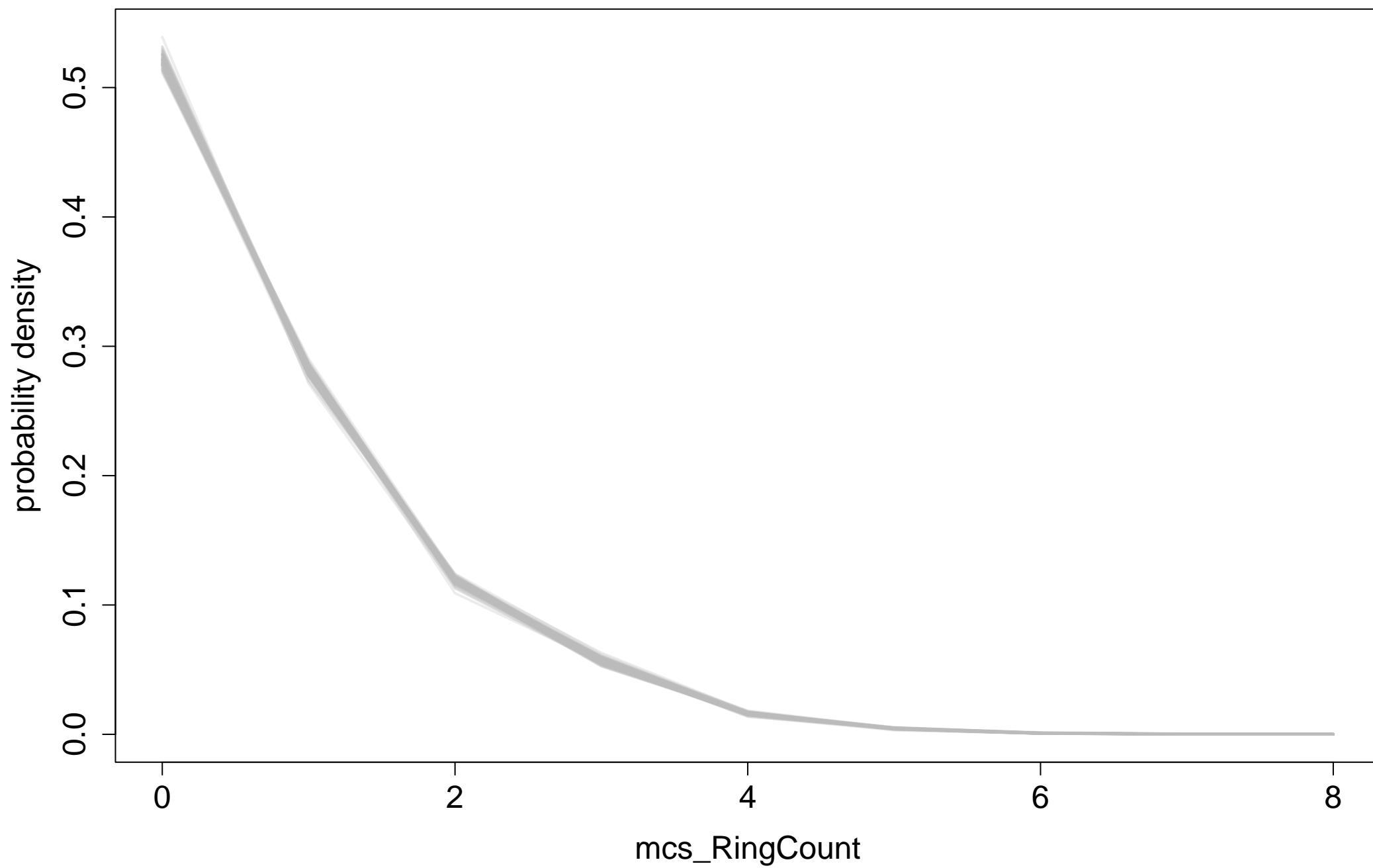
Occupied clusters: 60 of 64

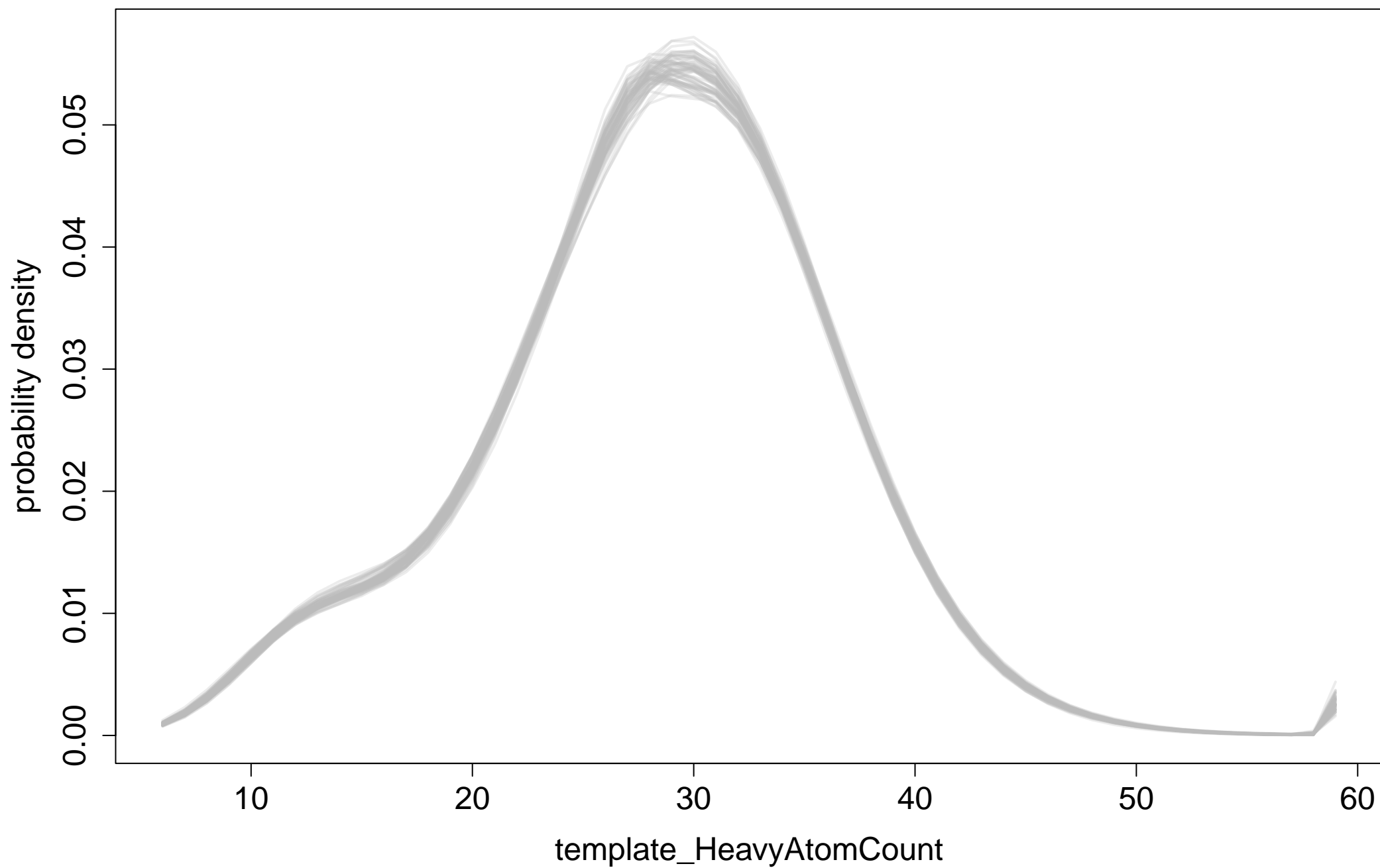
LL: -110000 +- 78.6

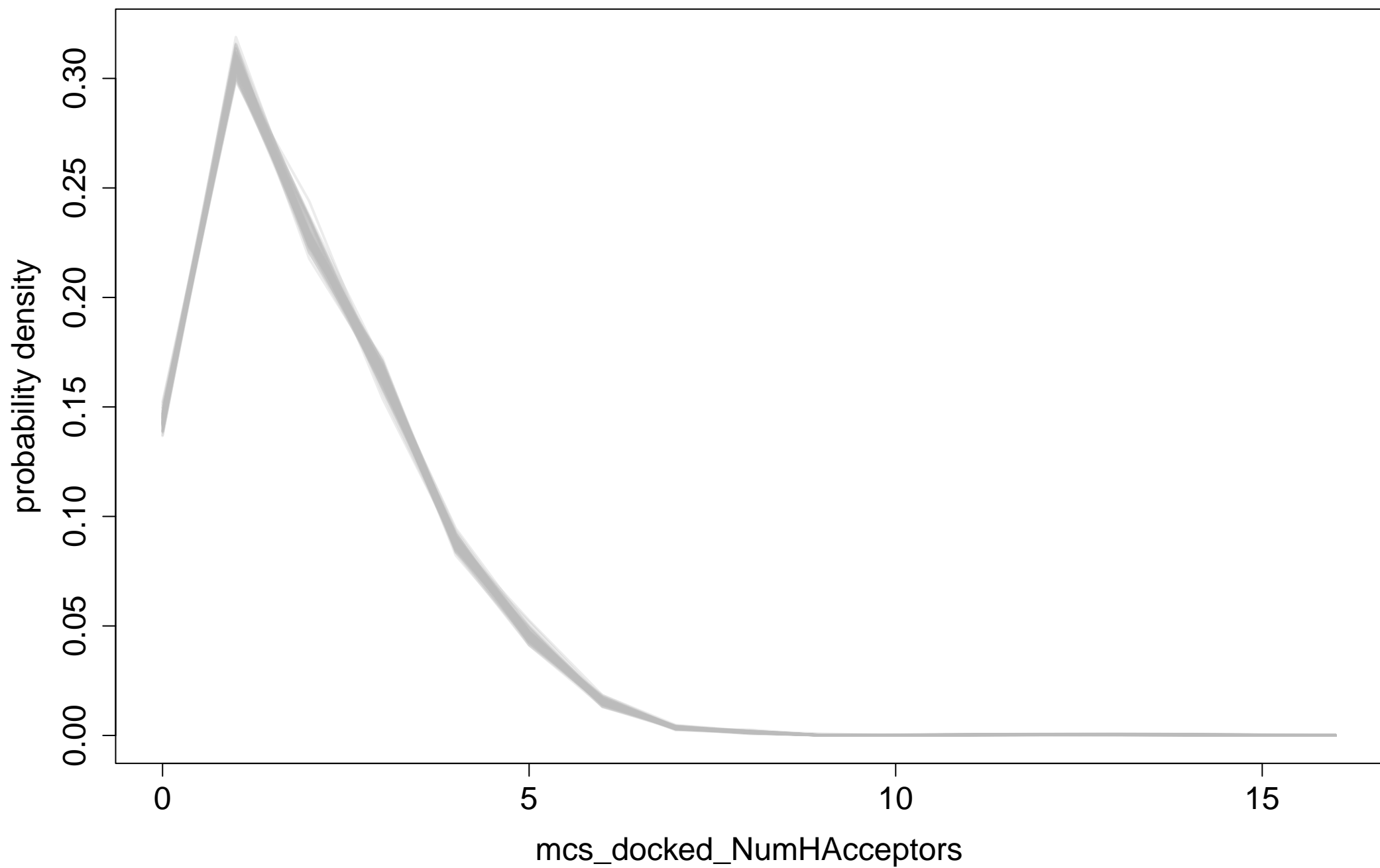


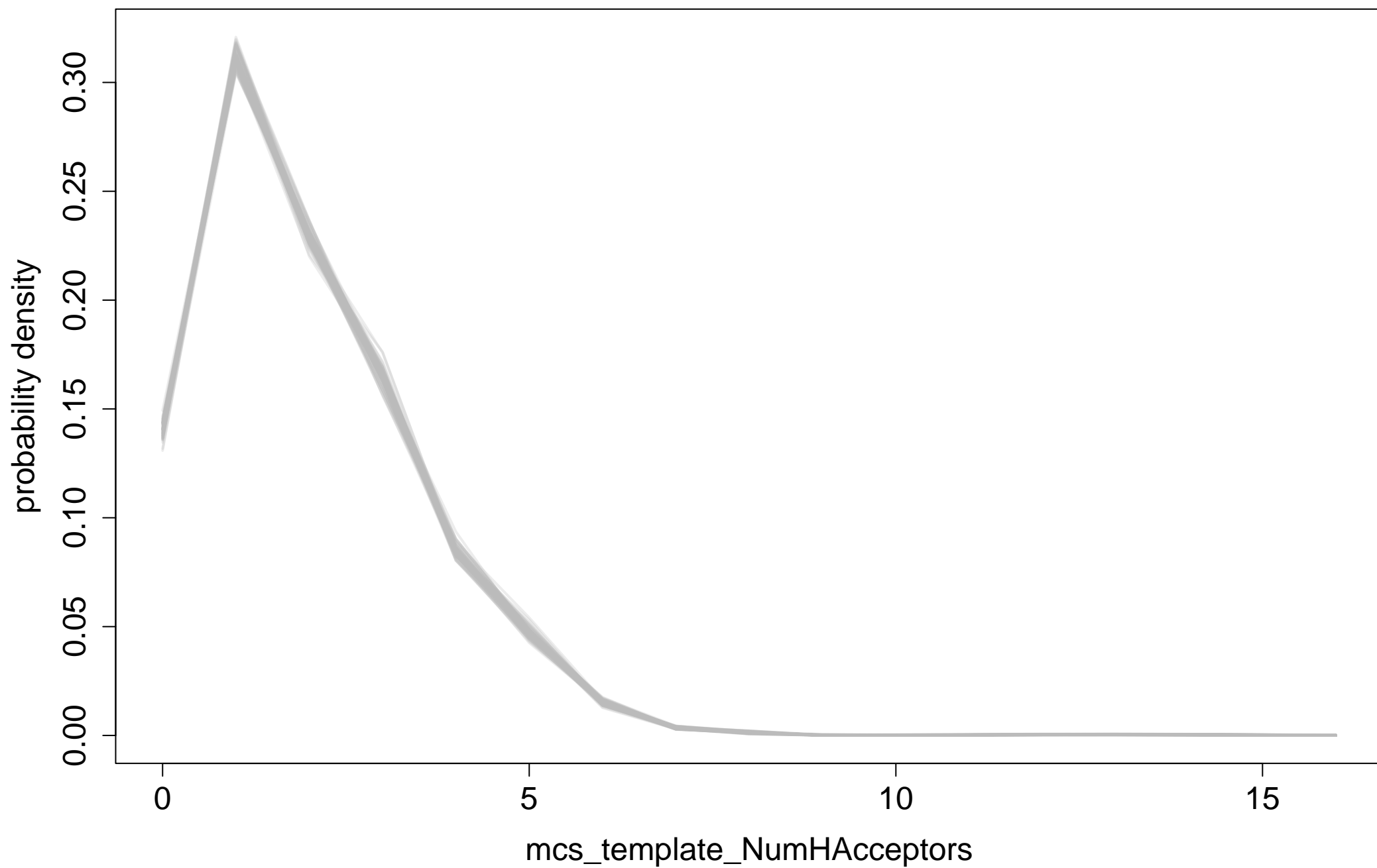


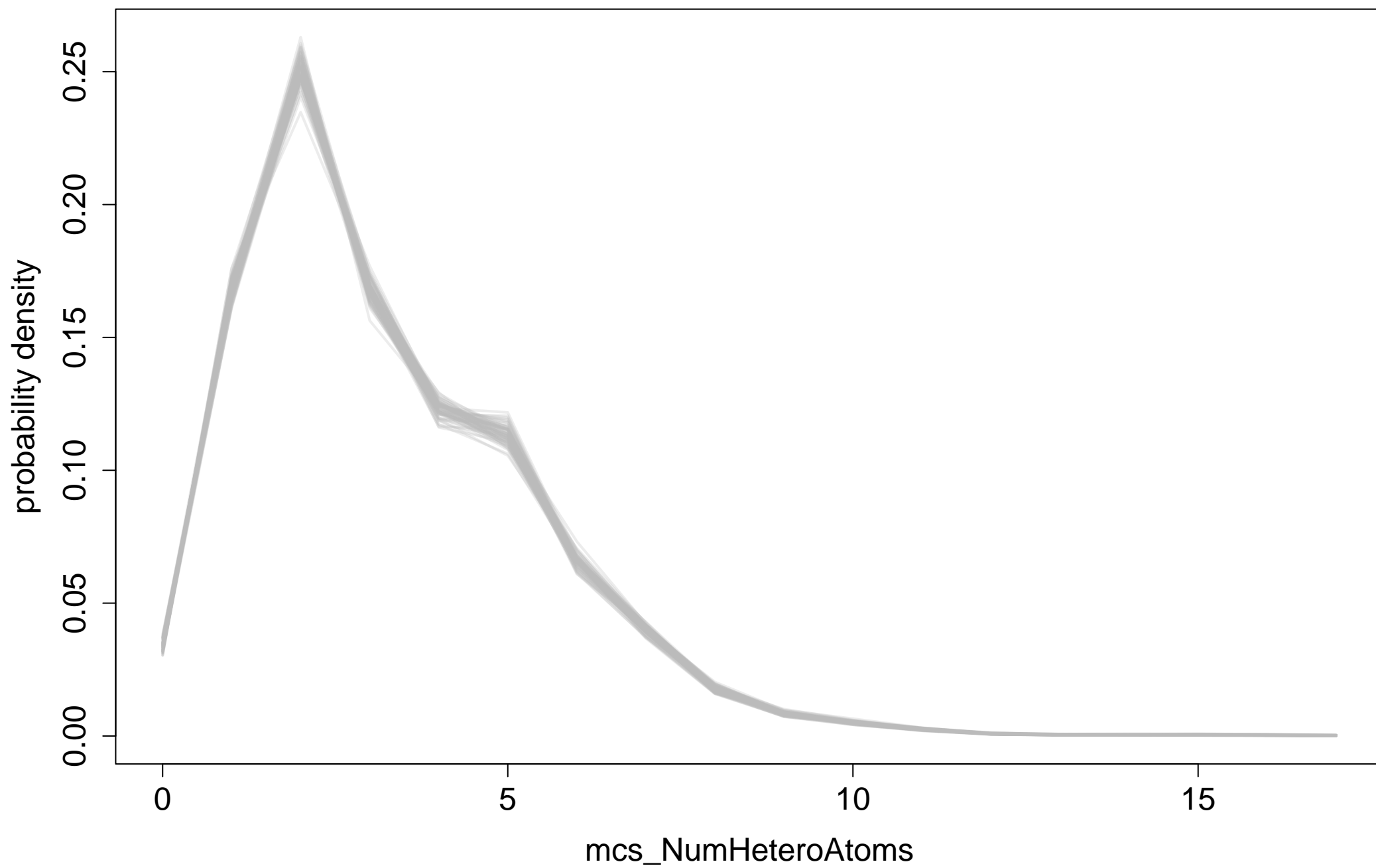


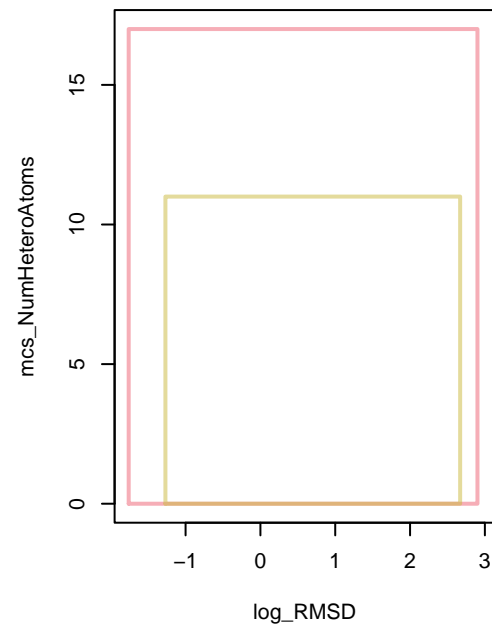
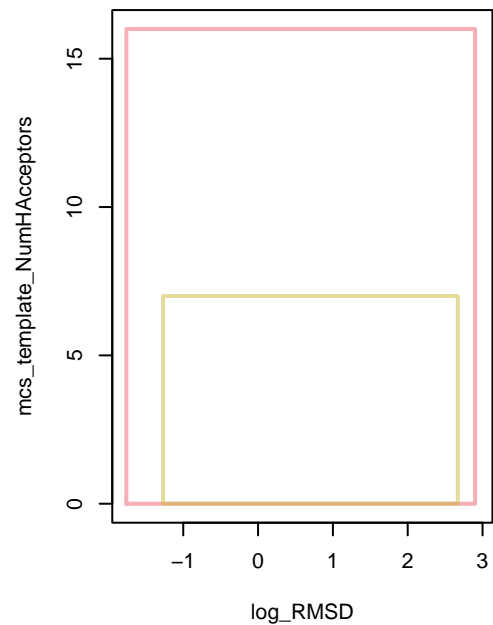
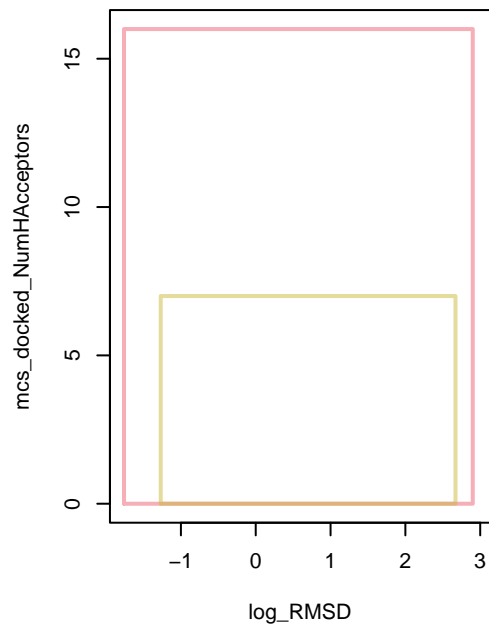
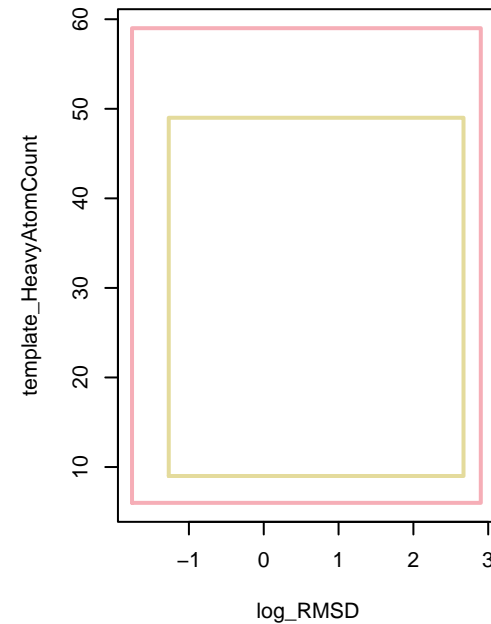
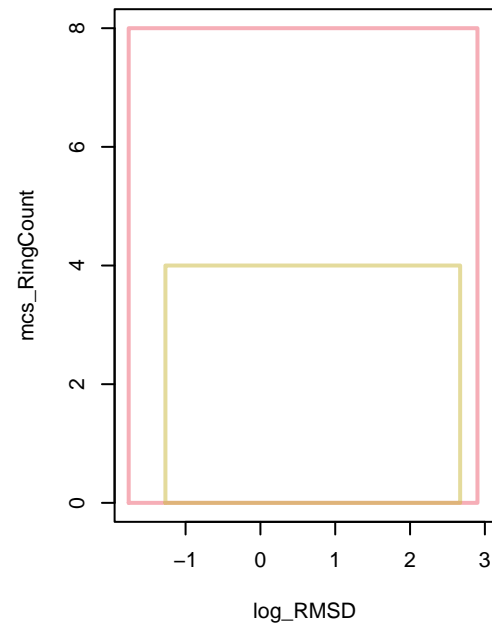
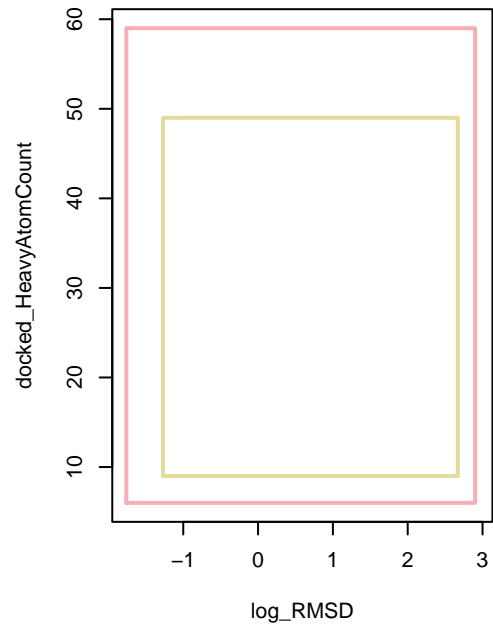
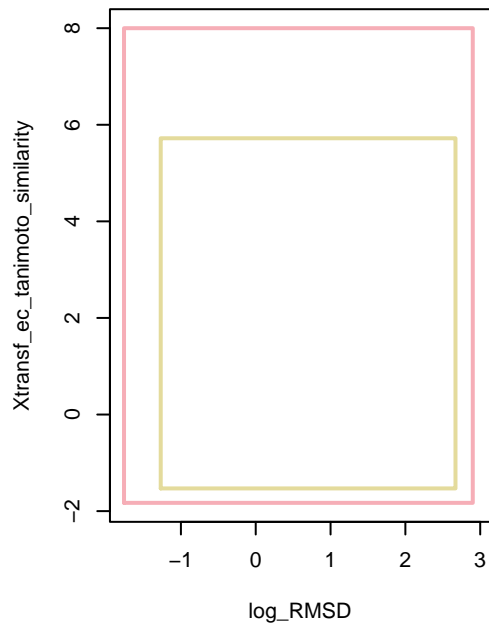




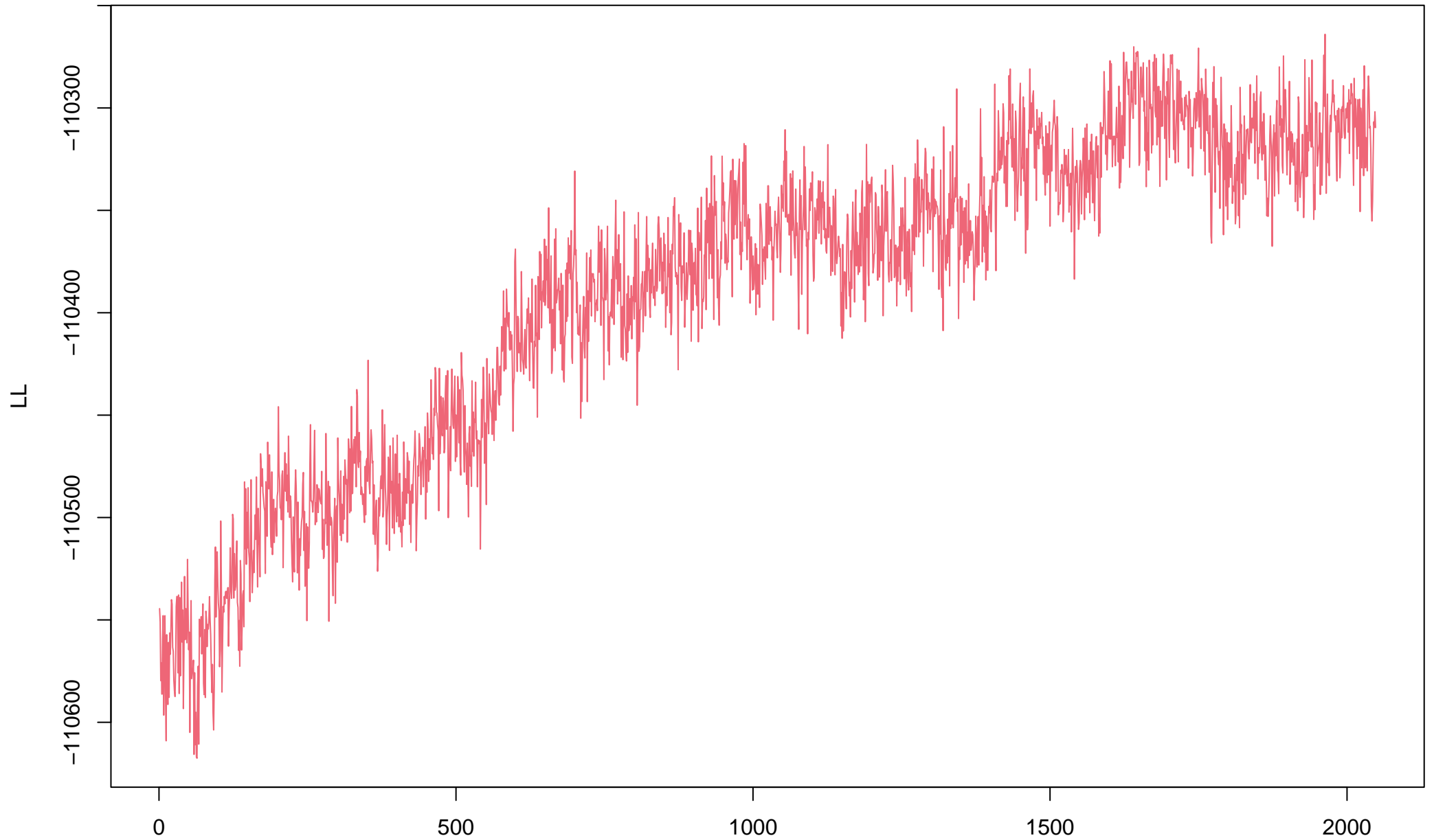




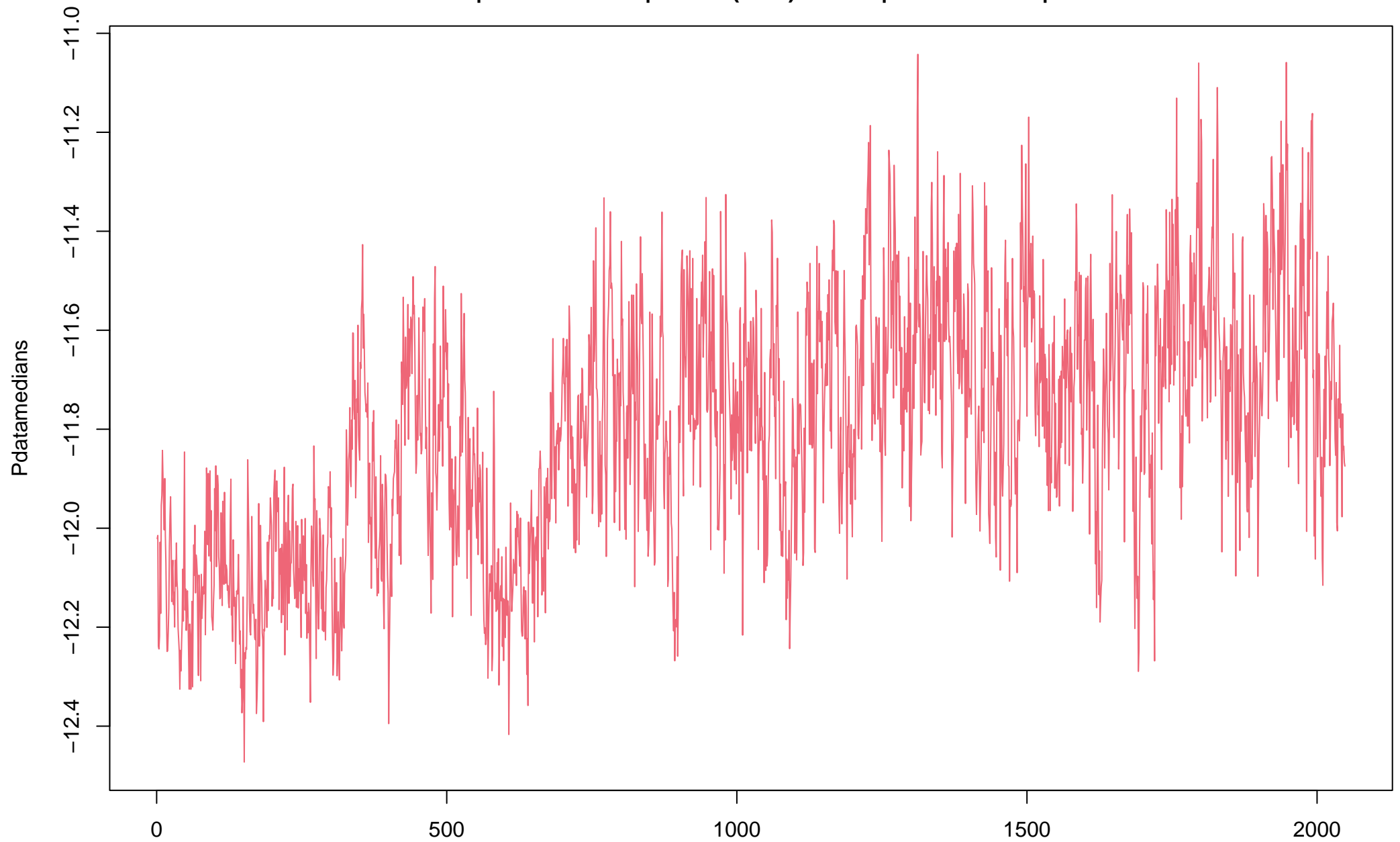




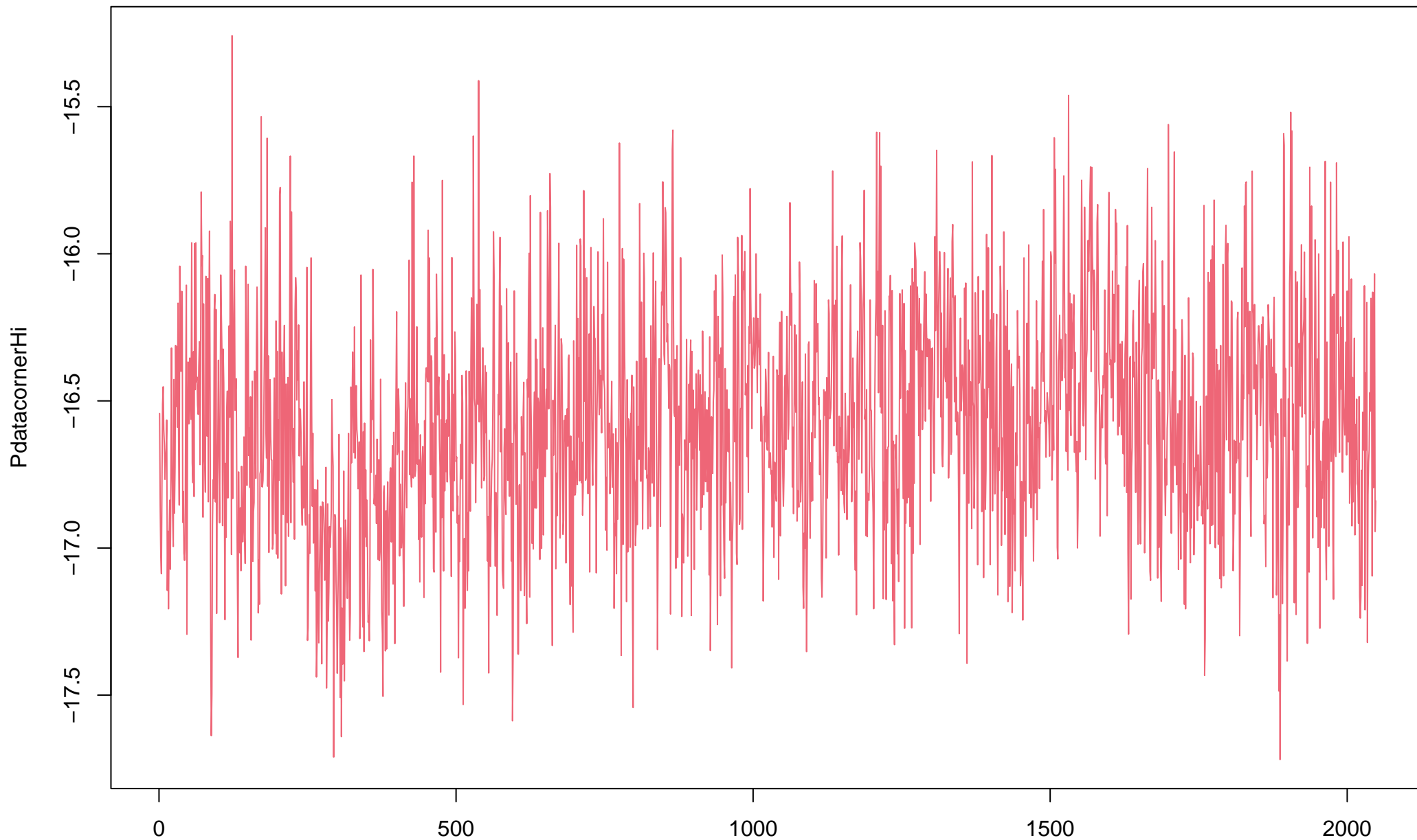
LL
ESS = 2.81 | BMK = 0.745 | MCSE(6.27) = 14.5 | stat: FALSE | burn: 612



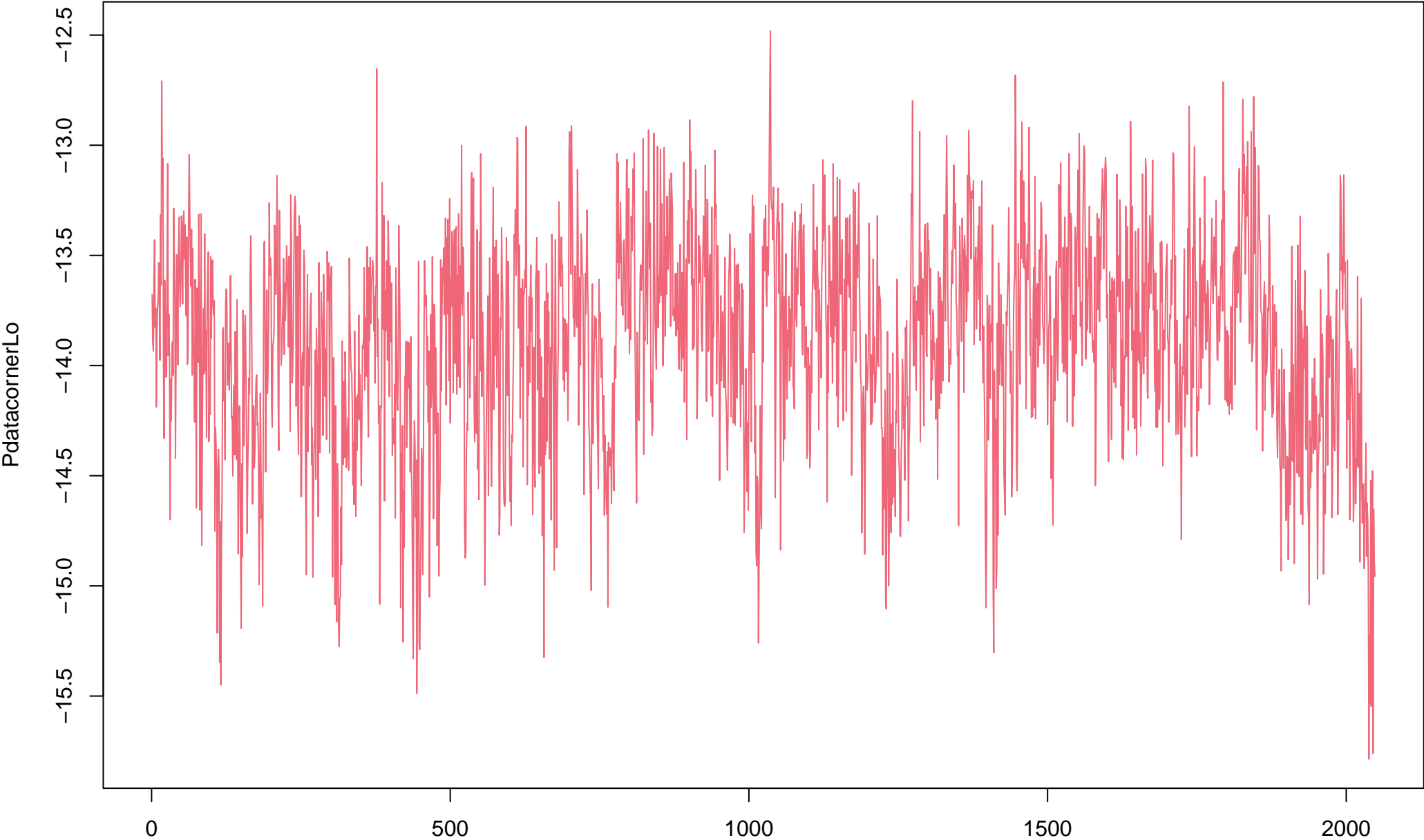
Pdatamedians
ESS = 44 | BMK = 0.387 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 0



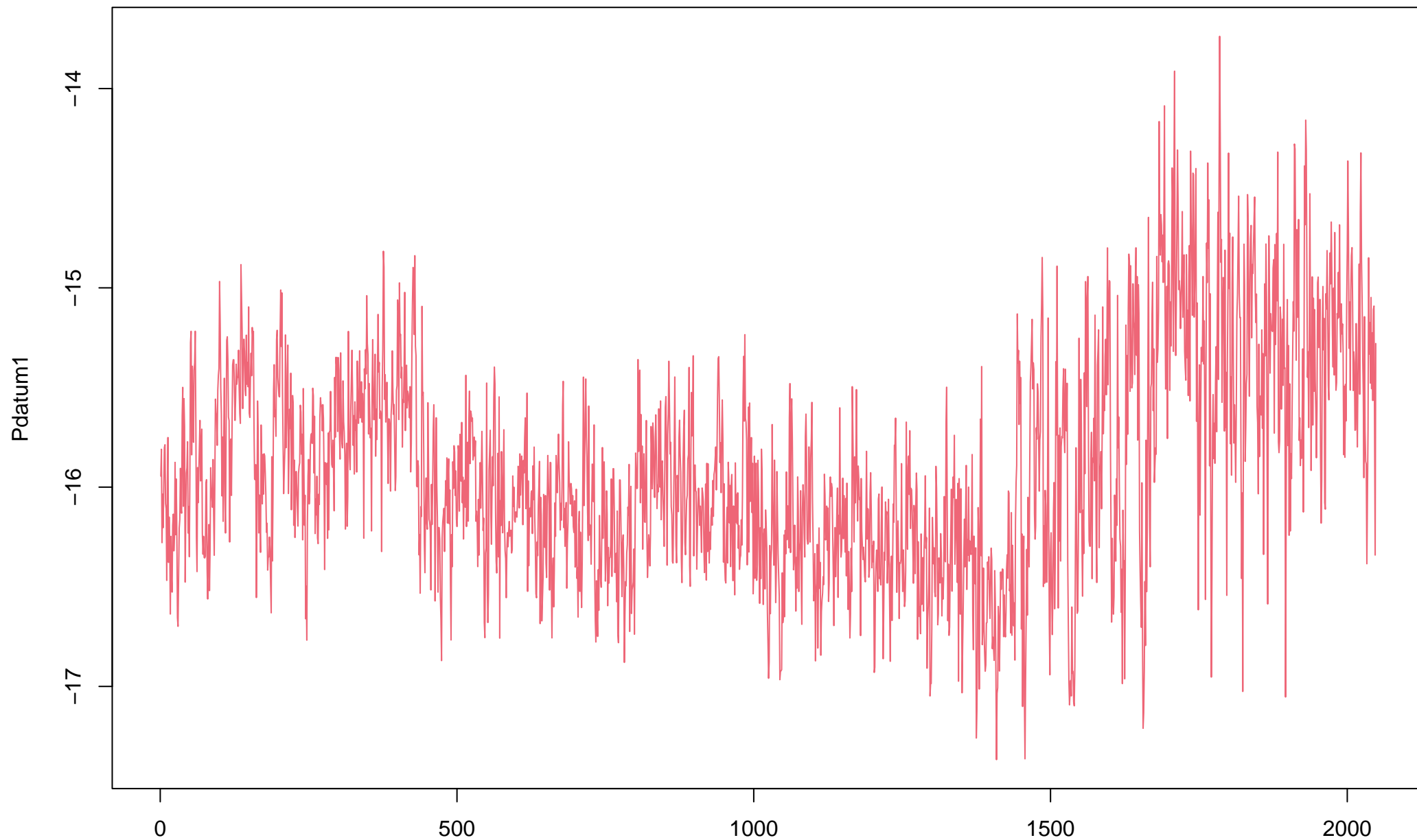
PdatacornerHi
ESS = 407 | BMK = 0.125 | MCSE(6.27) = 4.95 | stat: TRUE | burn: 0



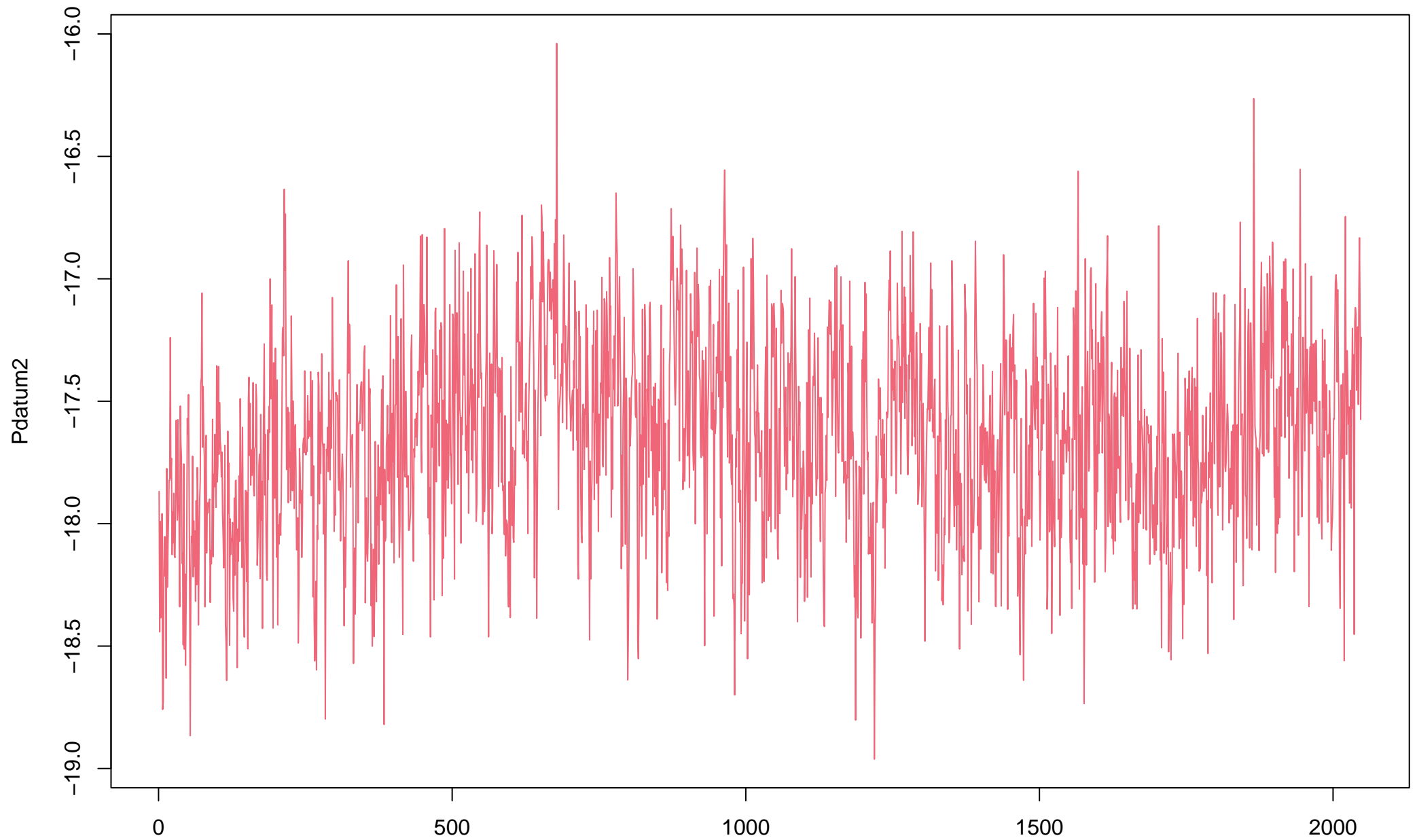
PdatacornerLo
ESS = 176 | BMK = 0.0818 | MCSE(6.27) = 6.57 | stat: TRUE | burn: 0



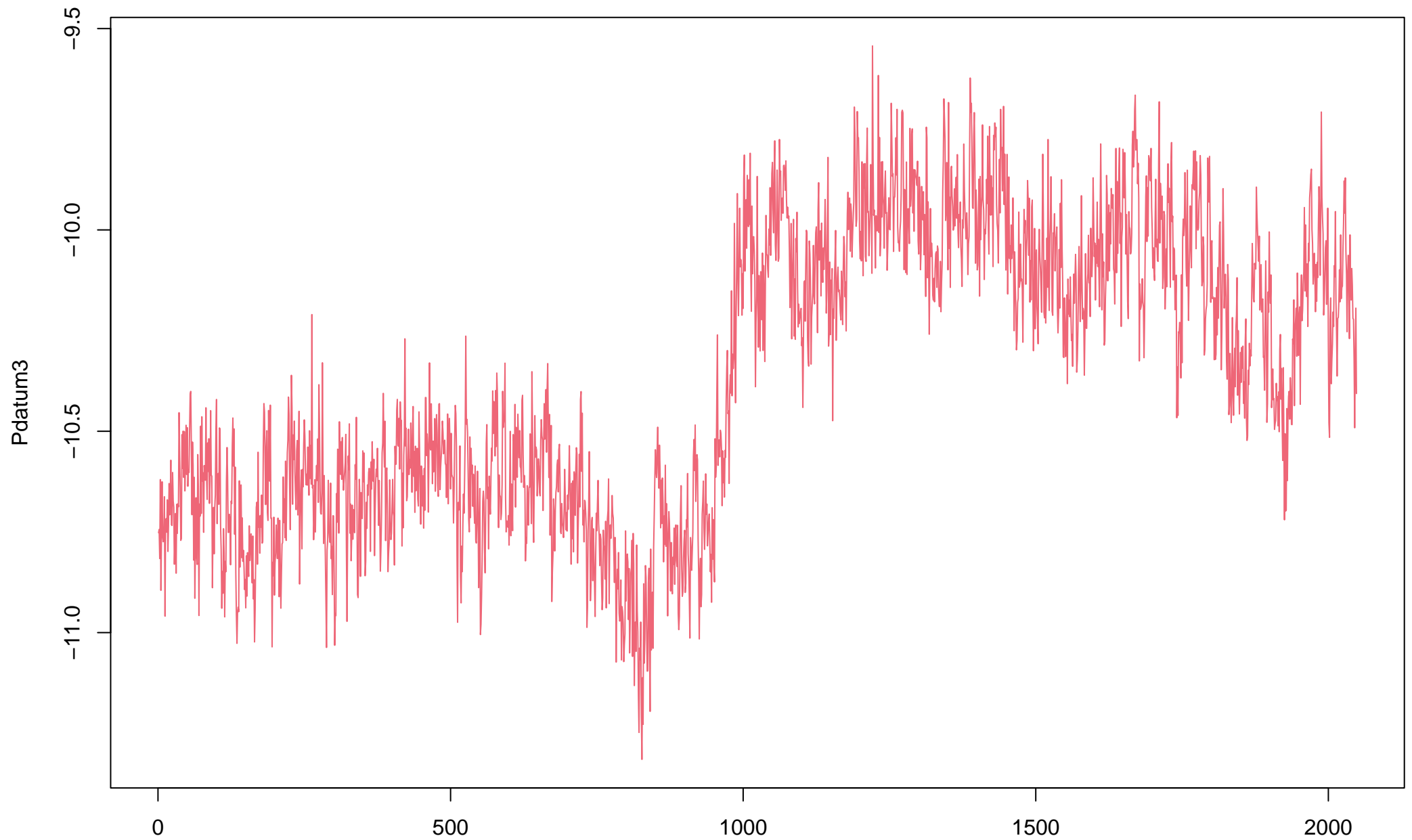
Pdatum1
ESS = 24 | BMK = 0.304 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 0



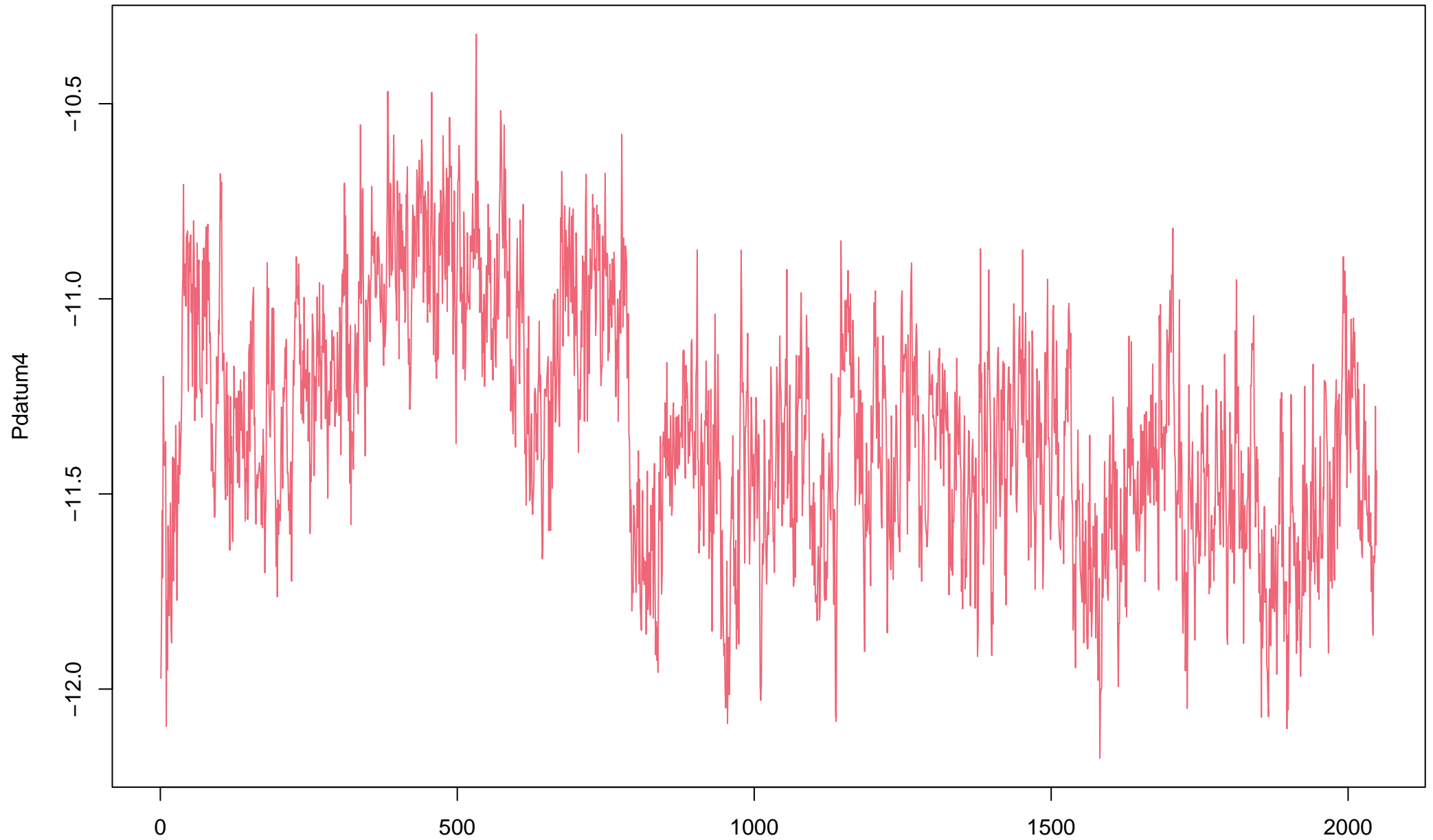
Pdatum2
ESS = 2.22e-16 | BMK = 0.072 | MCSE(6.27) = 6.11 | stat: FALSE | burn: 0



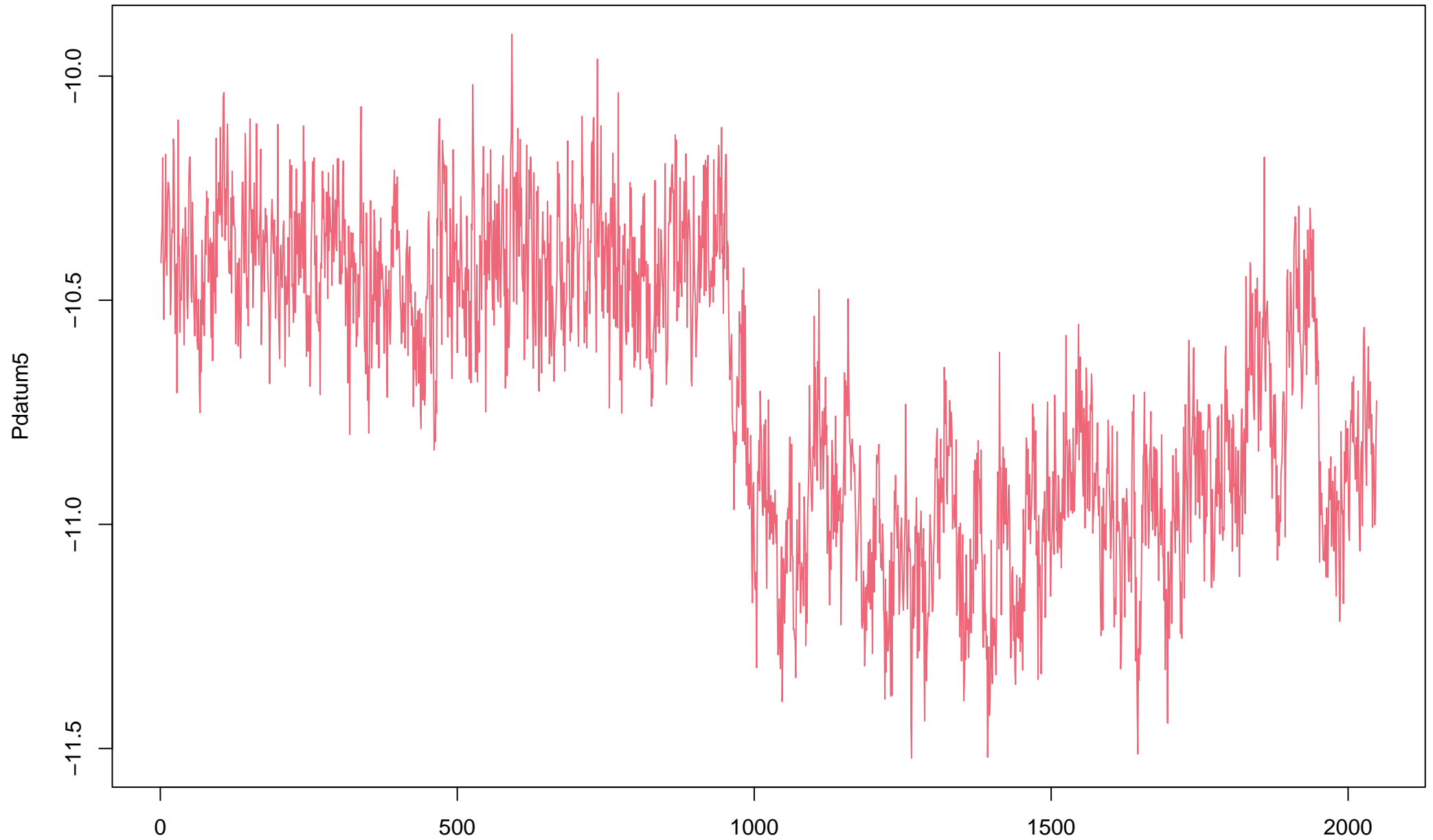
Pdatum3
ESS = 4.94 | BMK = 0.79 | MCSE(6.27) = 13.7 | stat: FALSE | burn: 1020



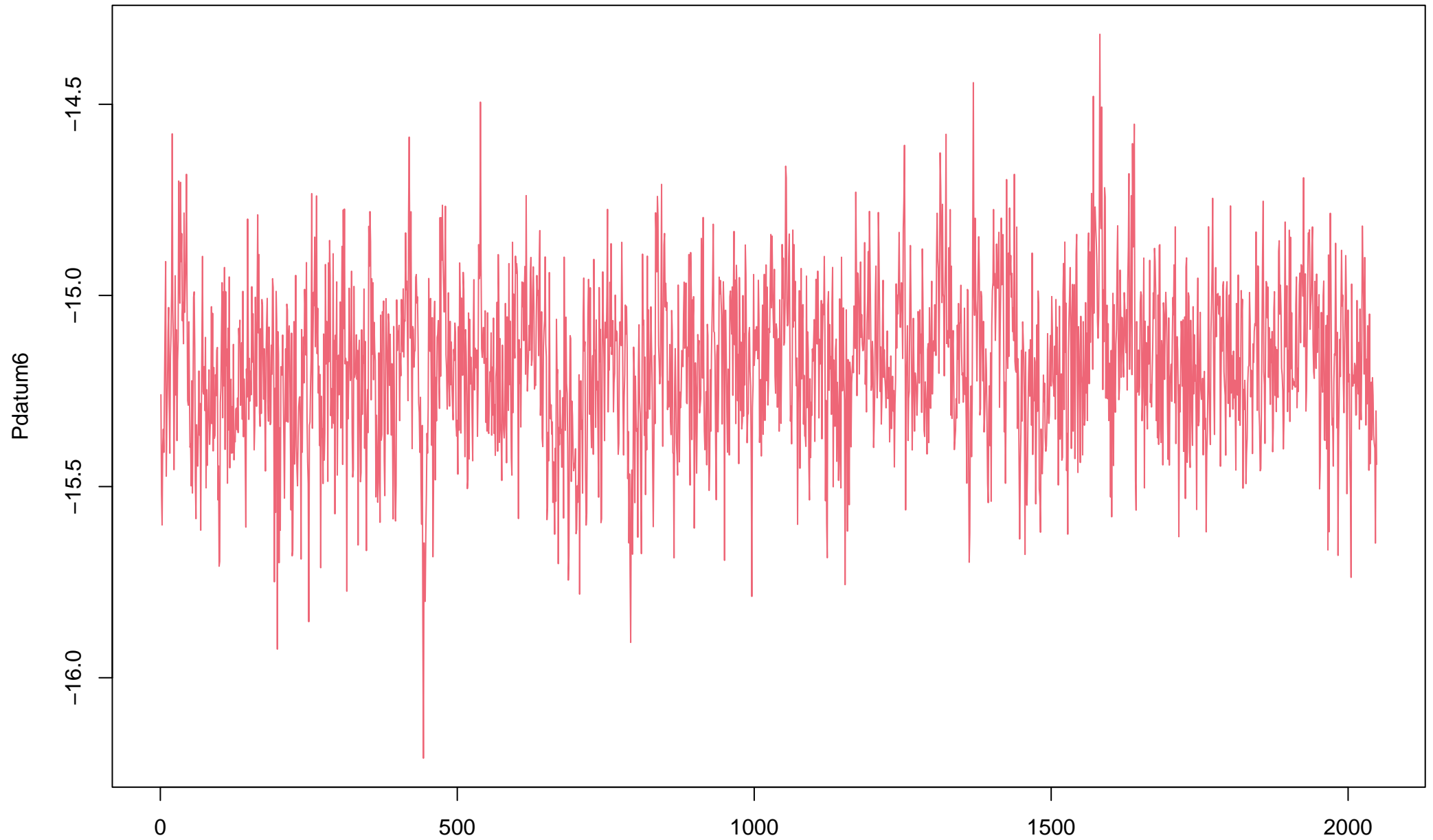
Pdatum4
ESS = 29.2 | BMK = 0.372 | MCSE(6.27) = 11.4 | stat: FALSE | burn: 0



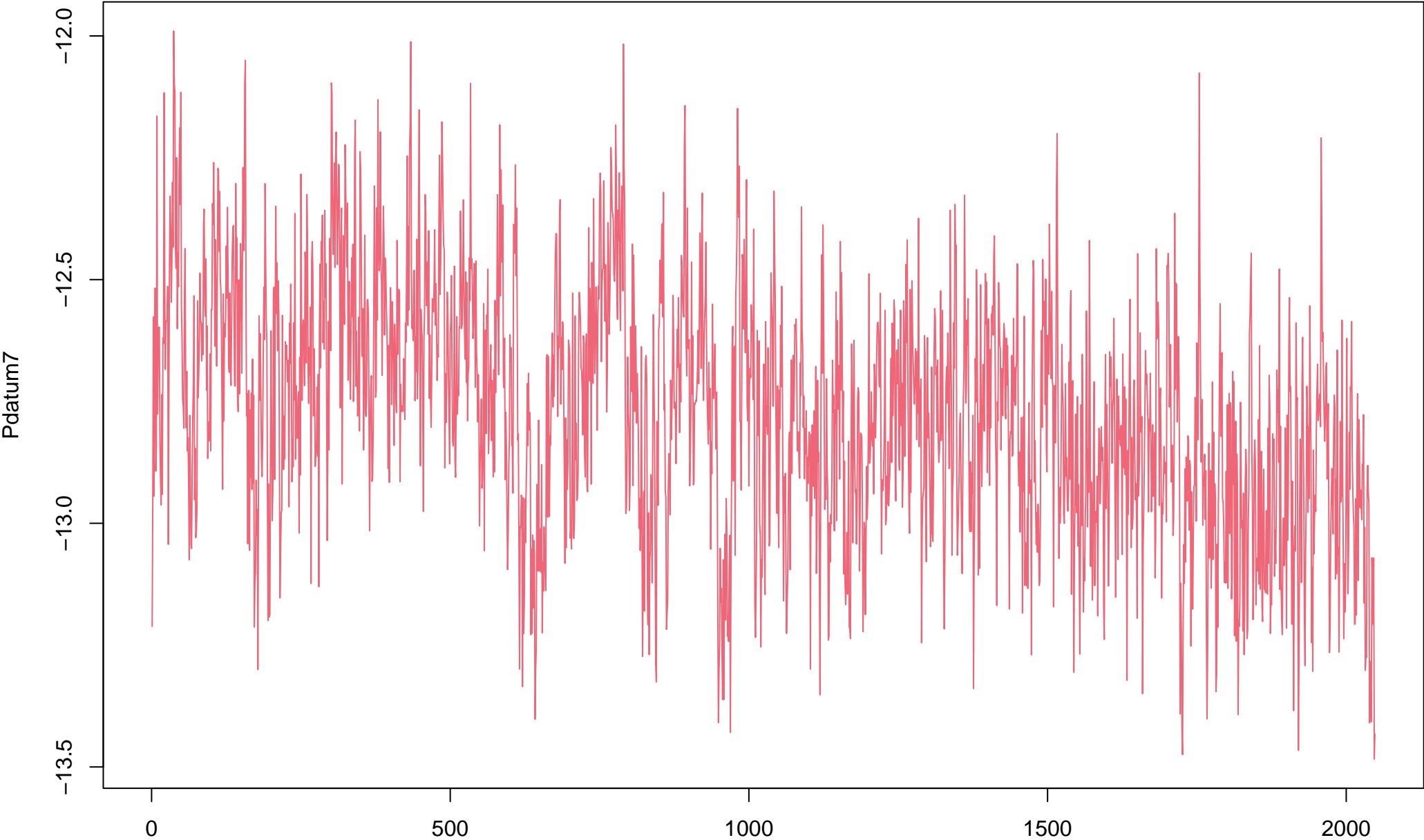
Pdatum5
ESS = 7.25 | BMK = 0.698 | MCSE(6.27) = 13.1 | stat: FALSE | burn: 1020



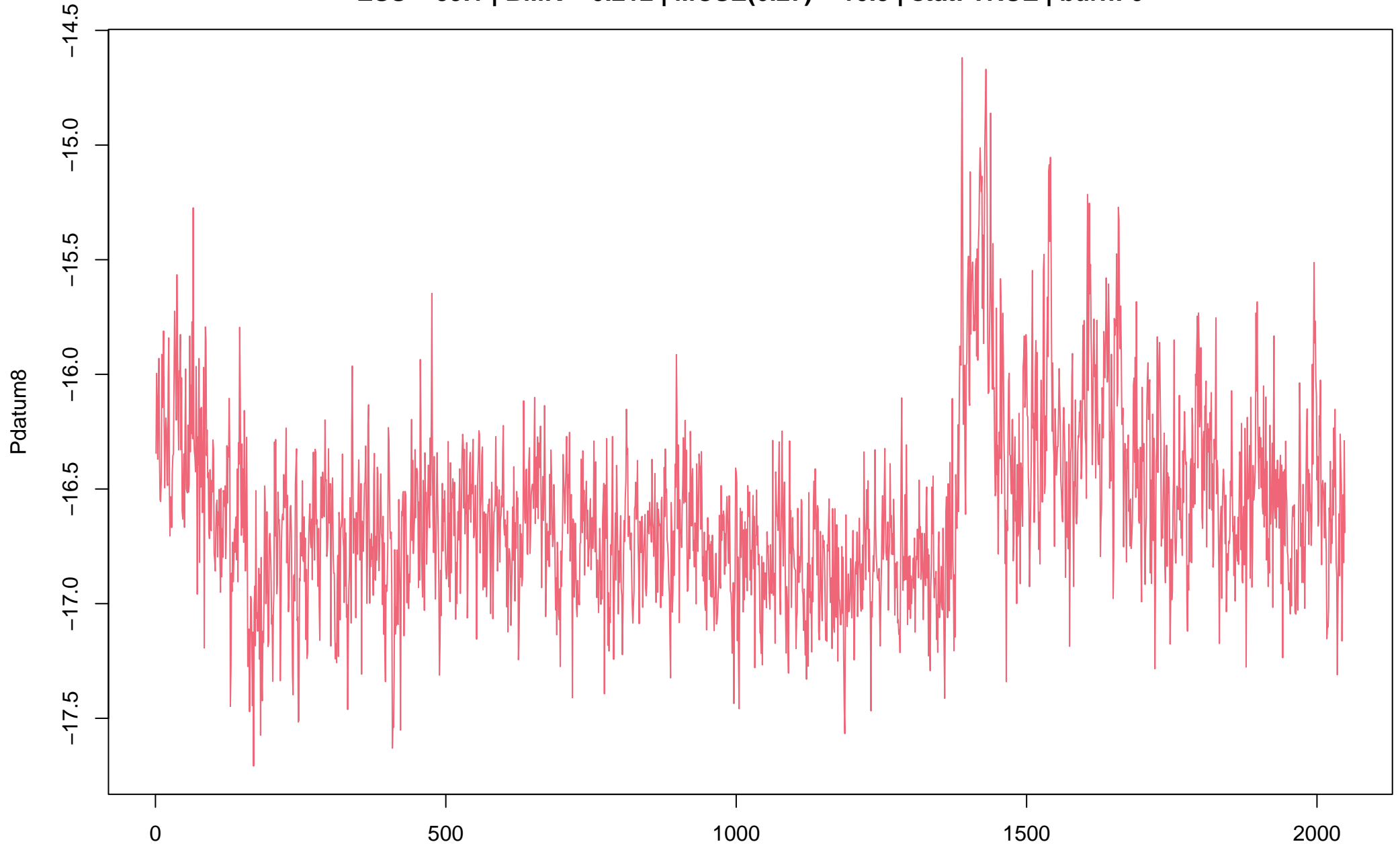
Pdatum6
ESS = 362 | BMK = 0.112 | MCSE(6.27) = 5.1 | stat: FALSE | burn: 0



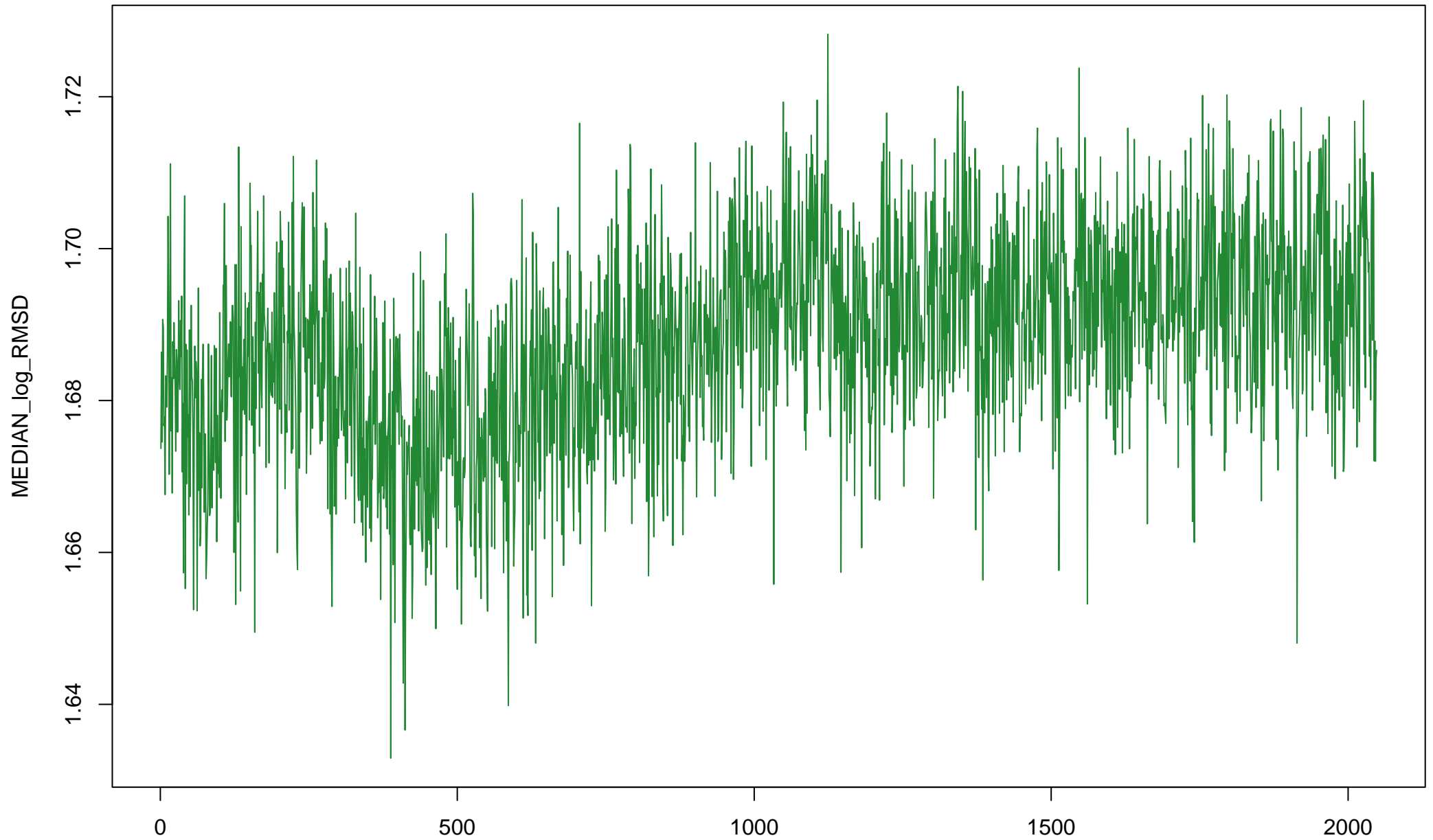
Pdatum7
ESS = 112 | BMK = 0.289 | MCSE(6.27) = 7.88 | stat: FALSE | burn: 0



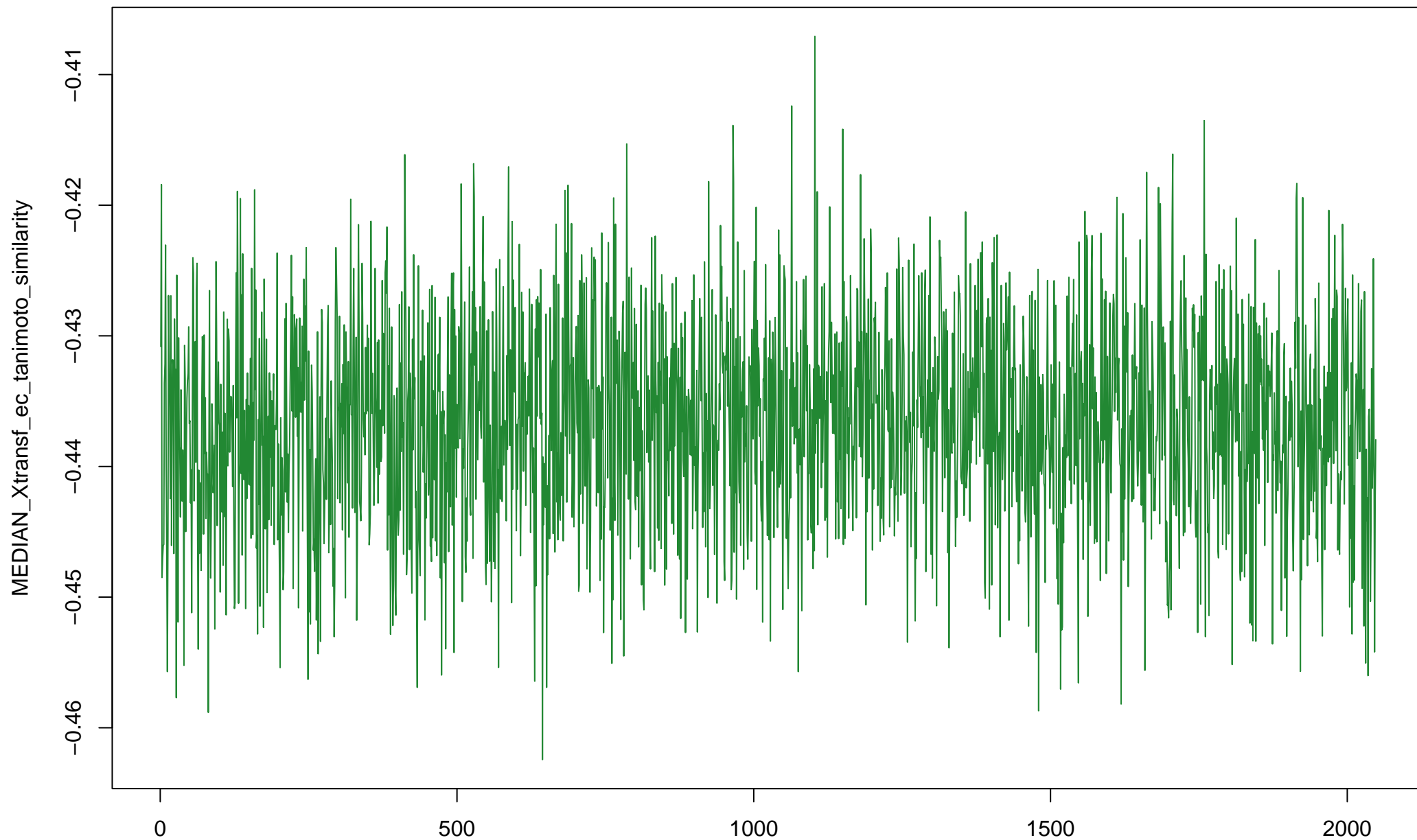
Pdatum8
ESS = 39.1 | BMK = 0.212 | MCSE(6.27) = 10.3 | stat: TRUE | burn: 0



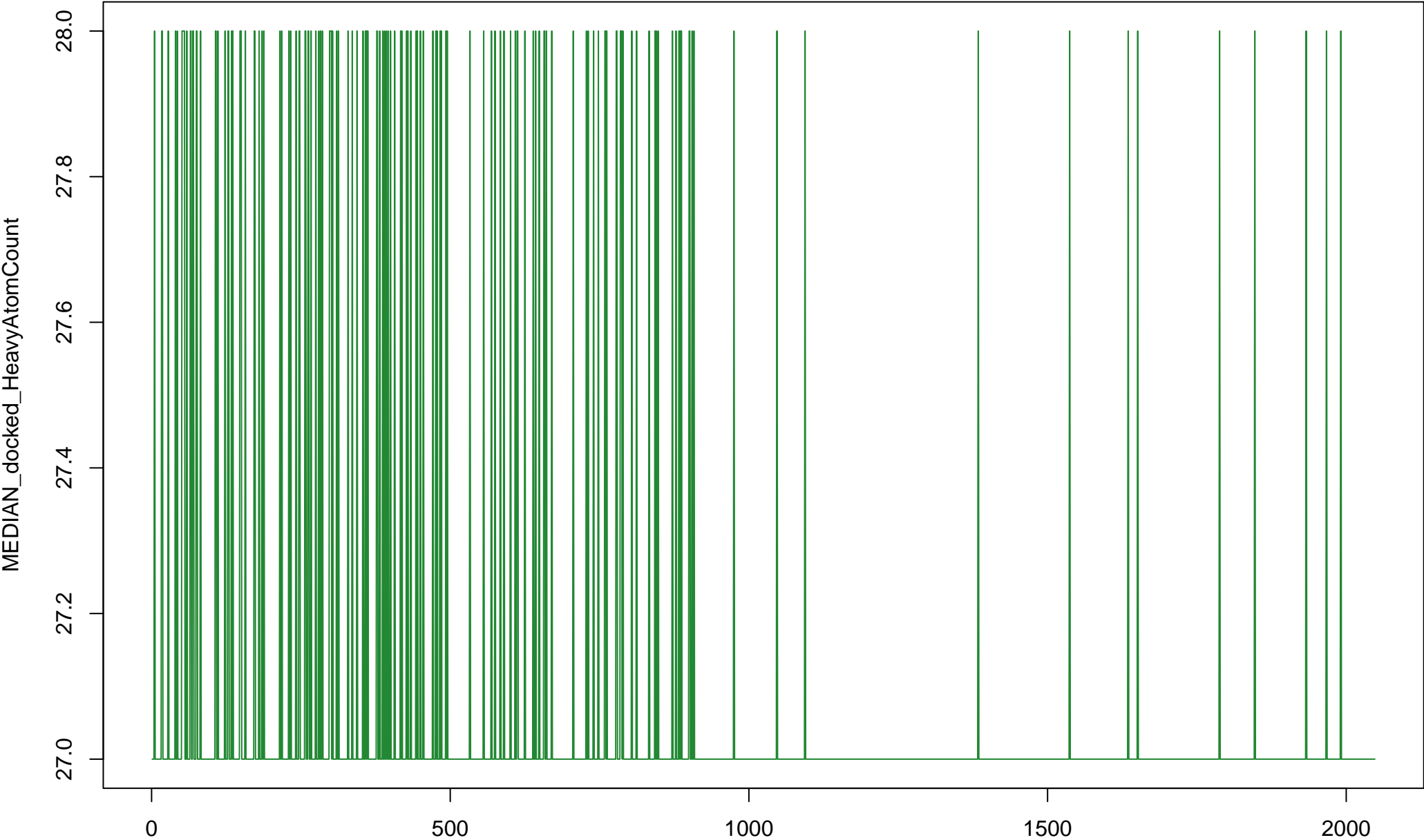
MEDIAN_log_RMSD
ESS = 31.1 | BMK = 0.324 | MCSE(6.27) = 8.08 | stat: FALSE | burn: 0



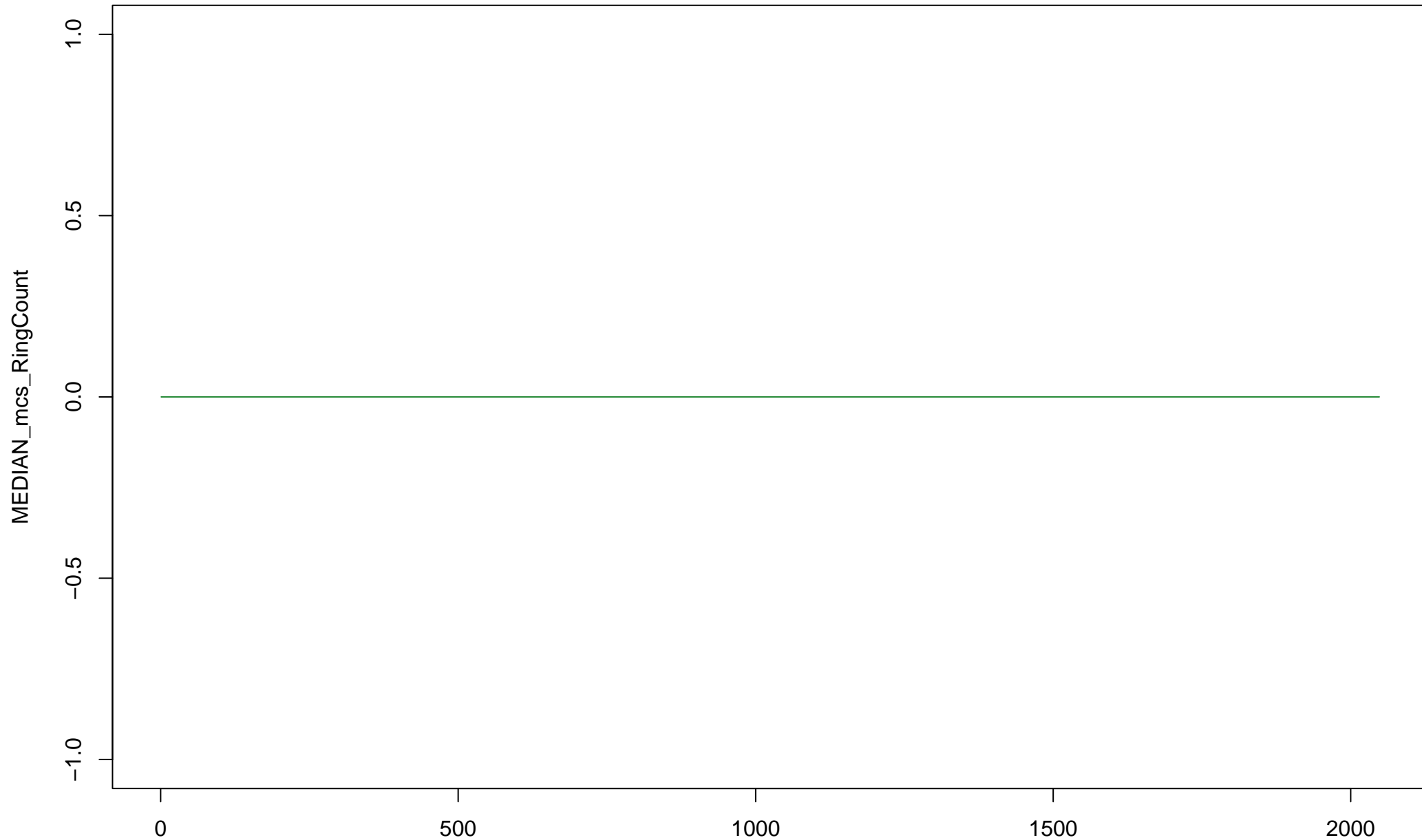
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1830 | BMK = 0.0562 | MCSE(6.27) = 2.24 | stat: FALSE | burn: 0



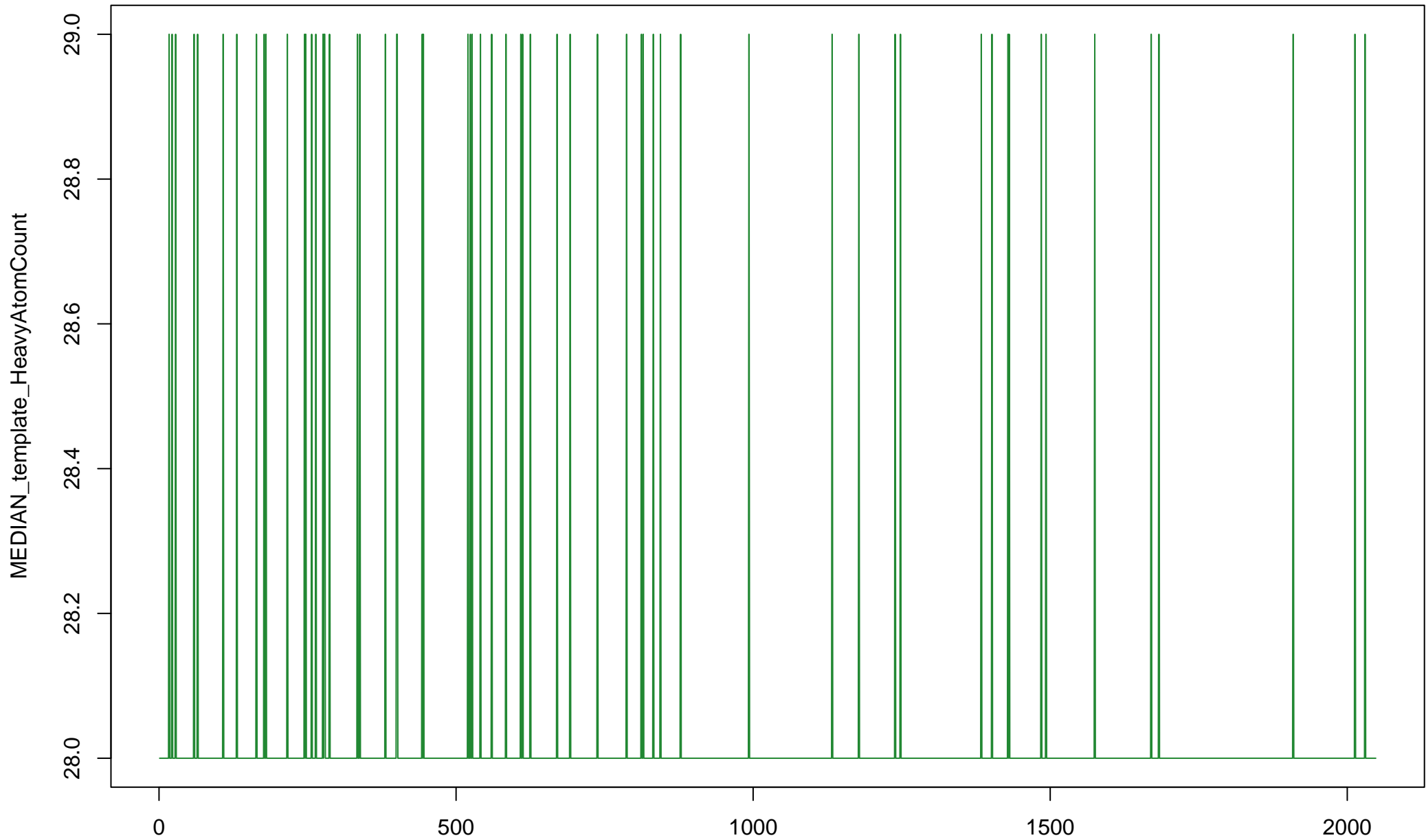
MEDIAN_docked_HeavyAtomCount
ESS = 206 | BMK = 0.379 | MCSE(6.27) = 4.68 | stat: FALSE | burn: 0



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



MEDIAN_template_HeavyAtomCount
ESS = 1700 | BMK = 0.177 | MCSE(6.27) = 2.44 | stat: FALSE | burn: 0



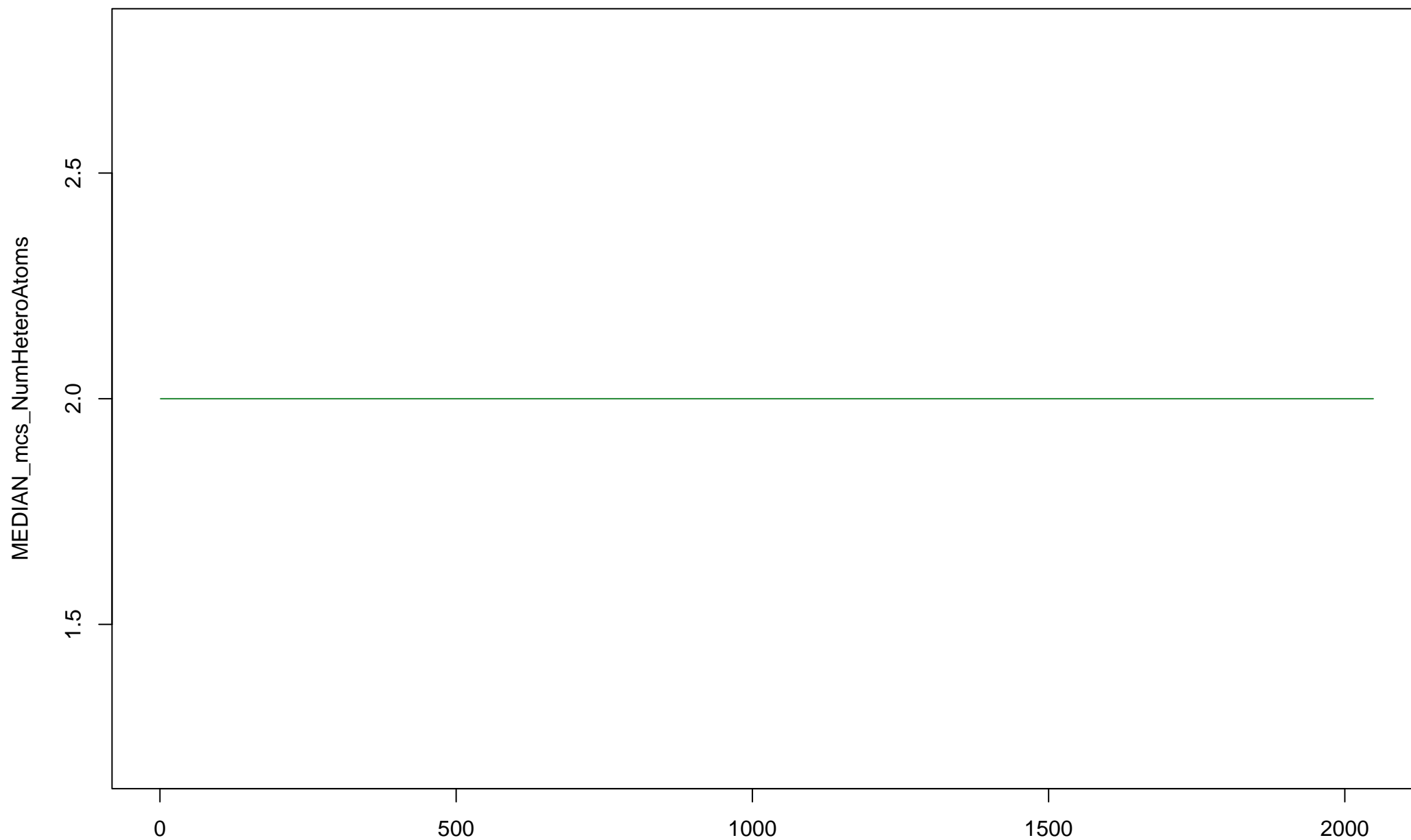
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



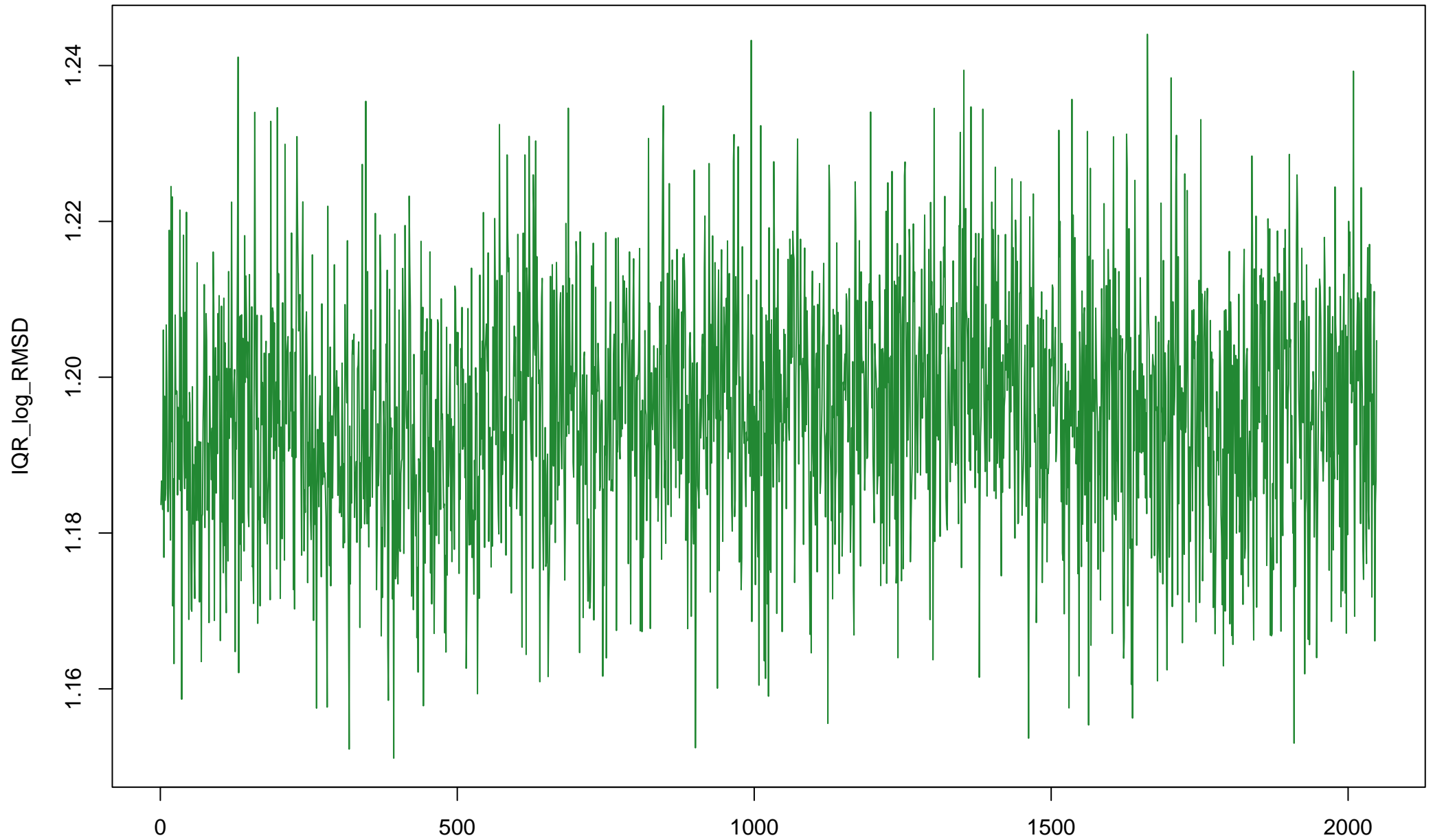
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



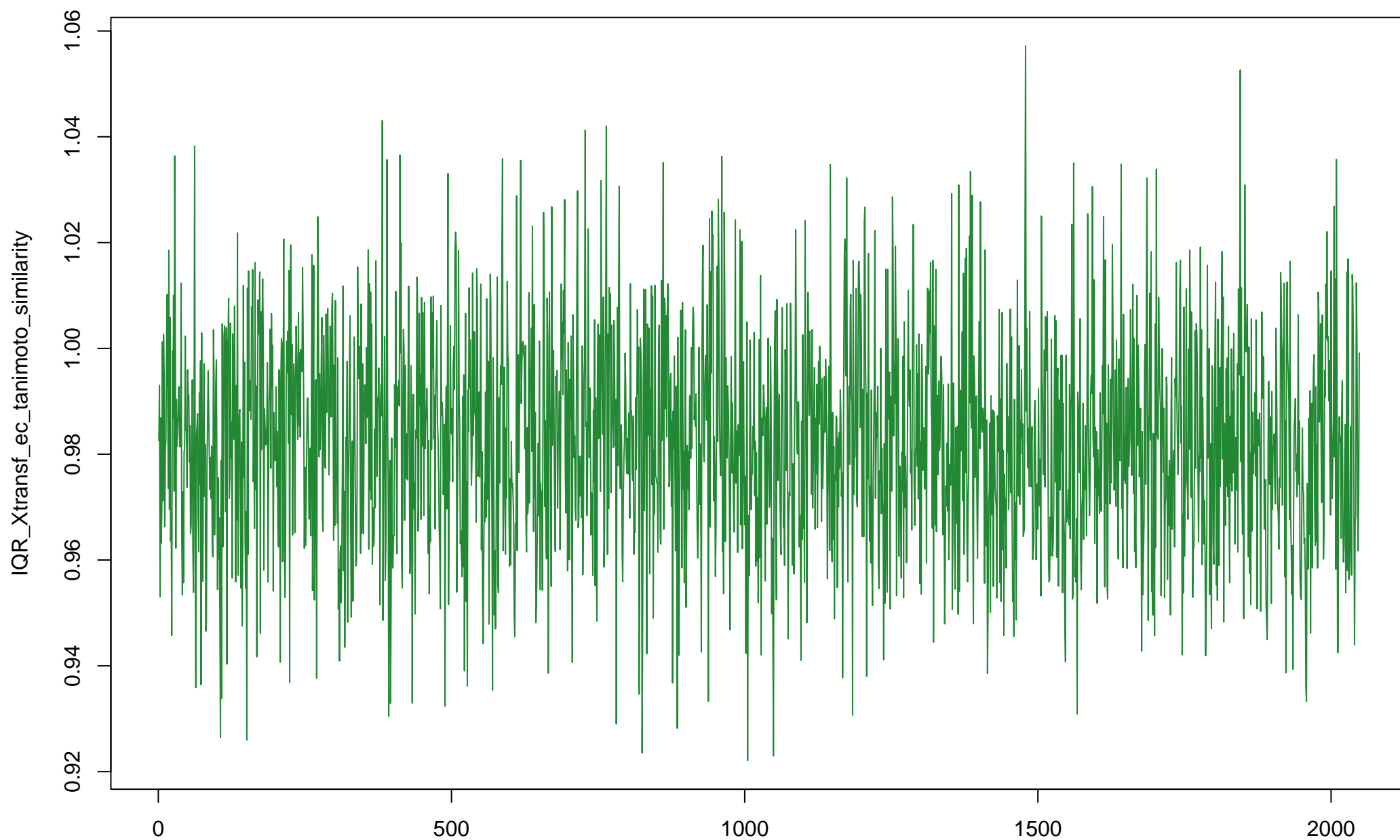
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



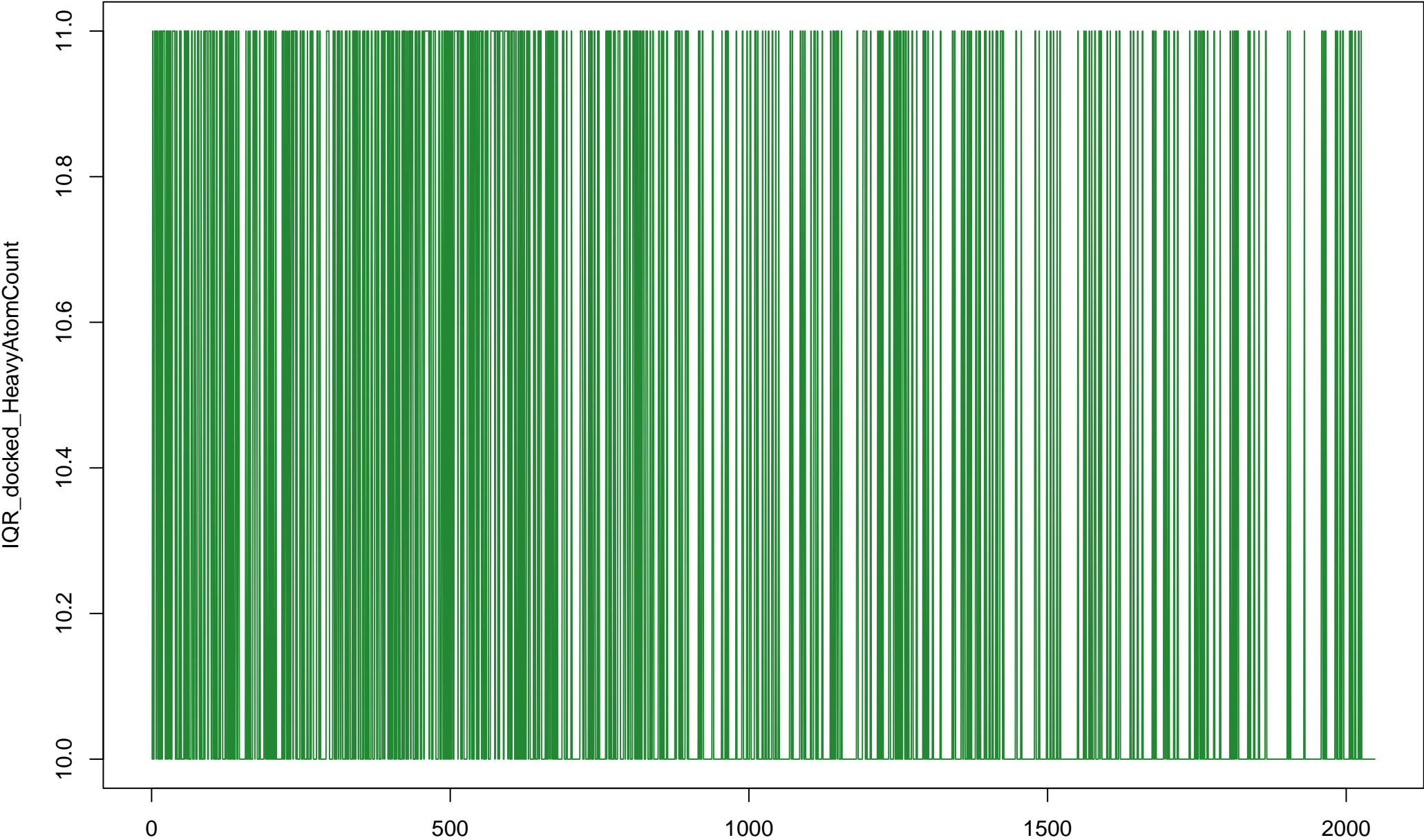
IQR_log_RMSD
ESS = 1080 | BMK = 0.076 | MCSE(6.27) = 3.26 | stat: FALSE | burn: 0



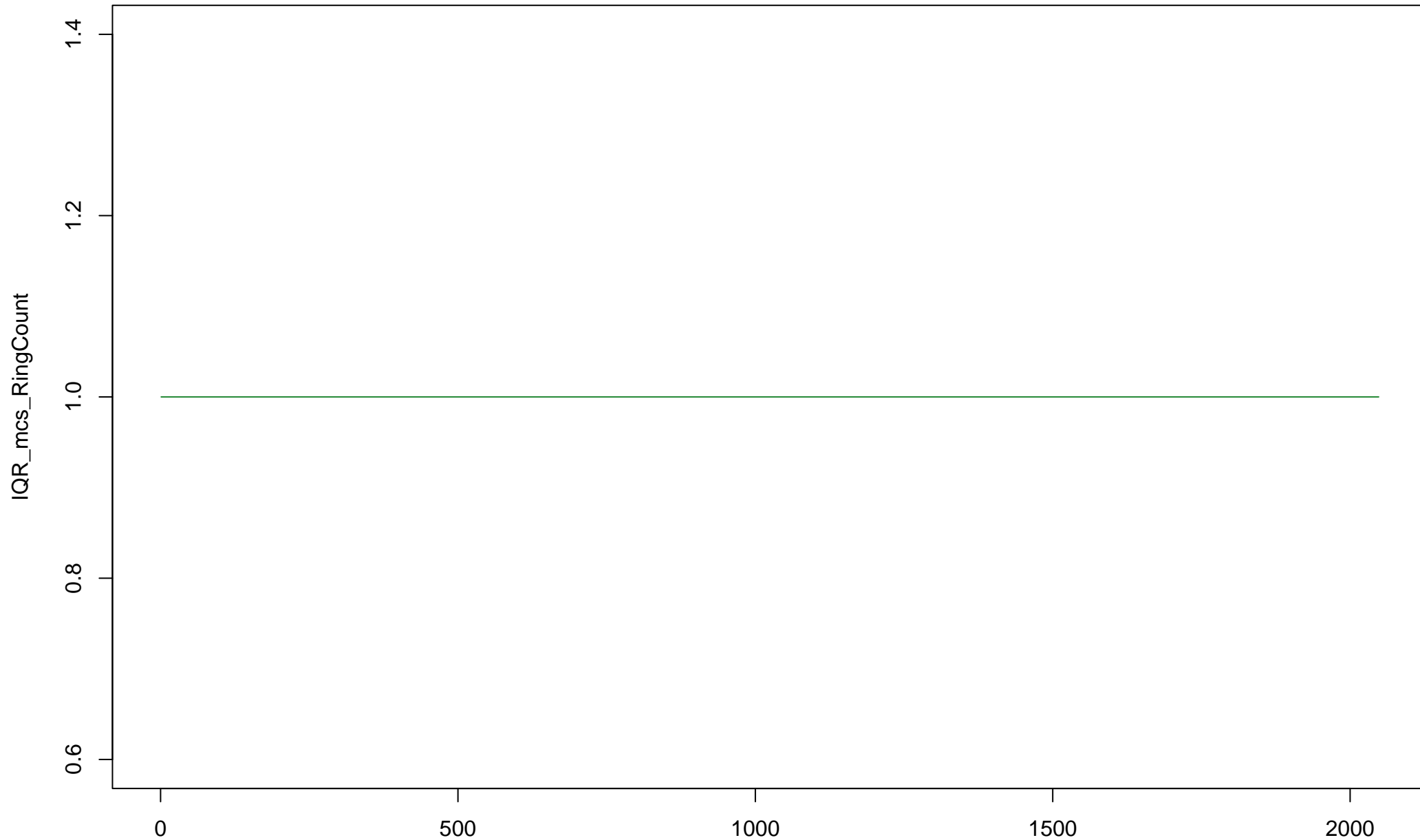
IQR_Xtransf_ec_tanimoto_similarity
ESS = 1620 | BMK = 0.0673 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



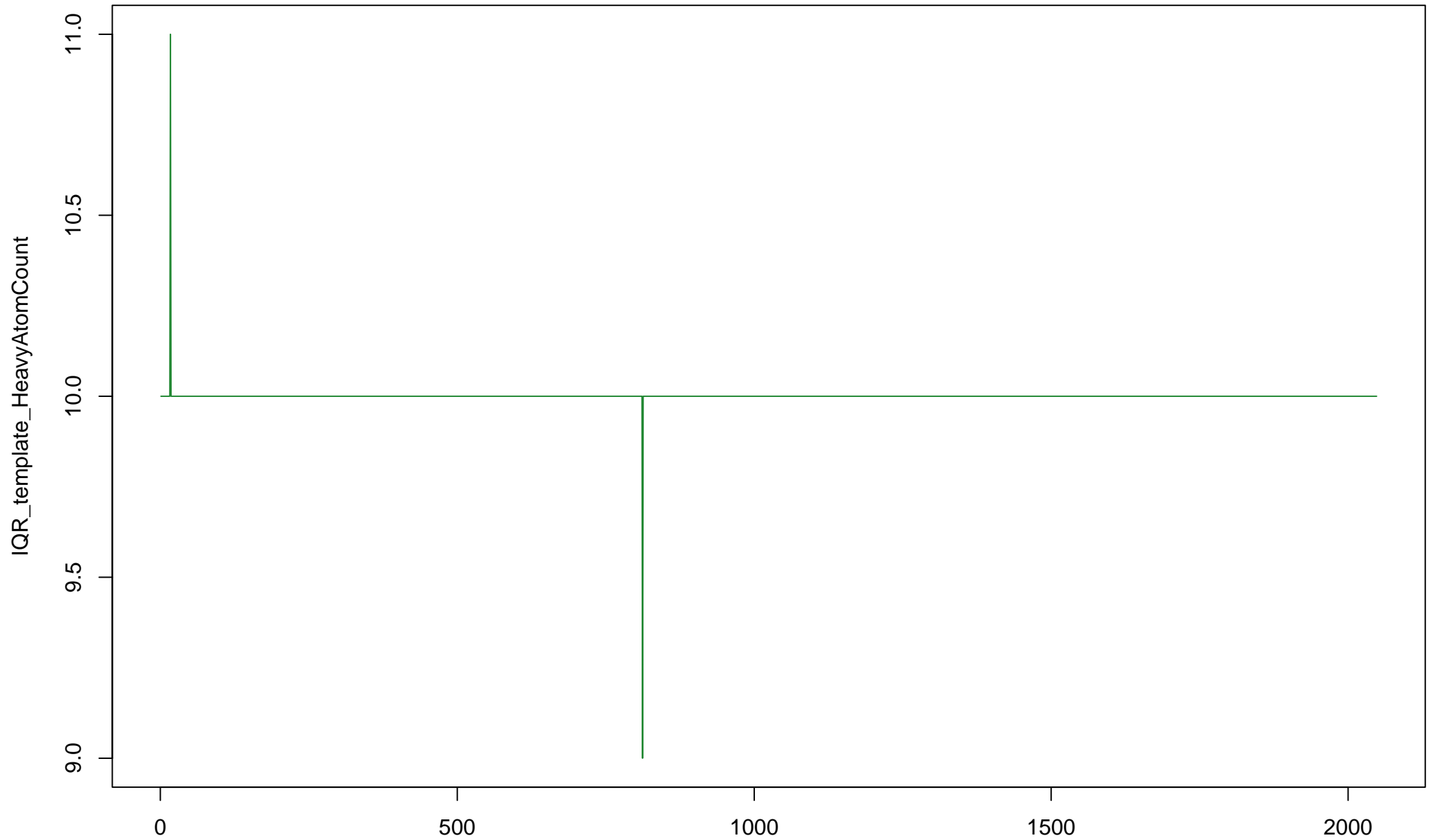
IQR_docked_HeavyAtomCount
ESS = 232 | BMK = 0.156 | MCSE(6.27) = 5.03 | stat: FALSE | burn: 0



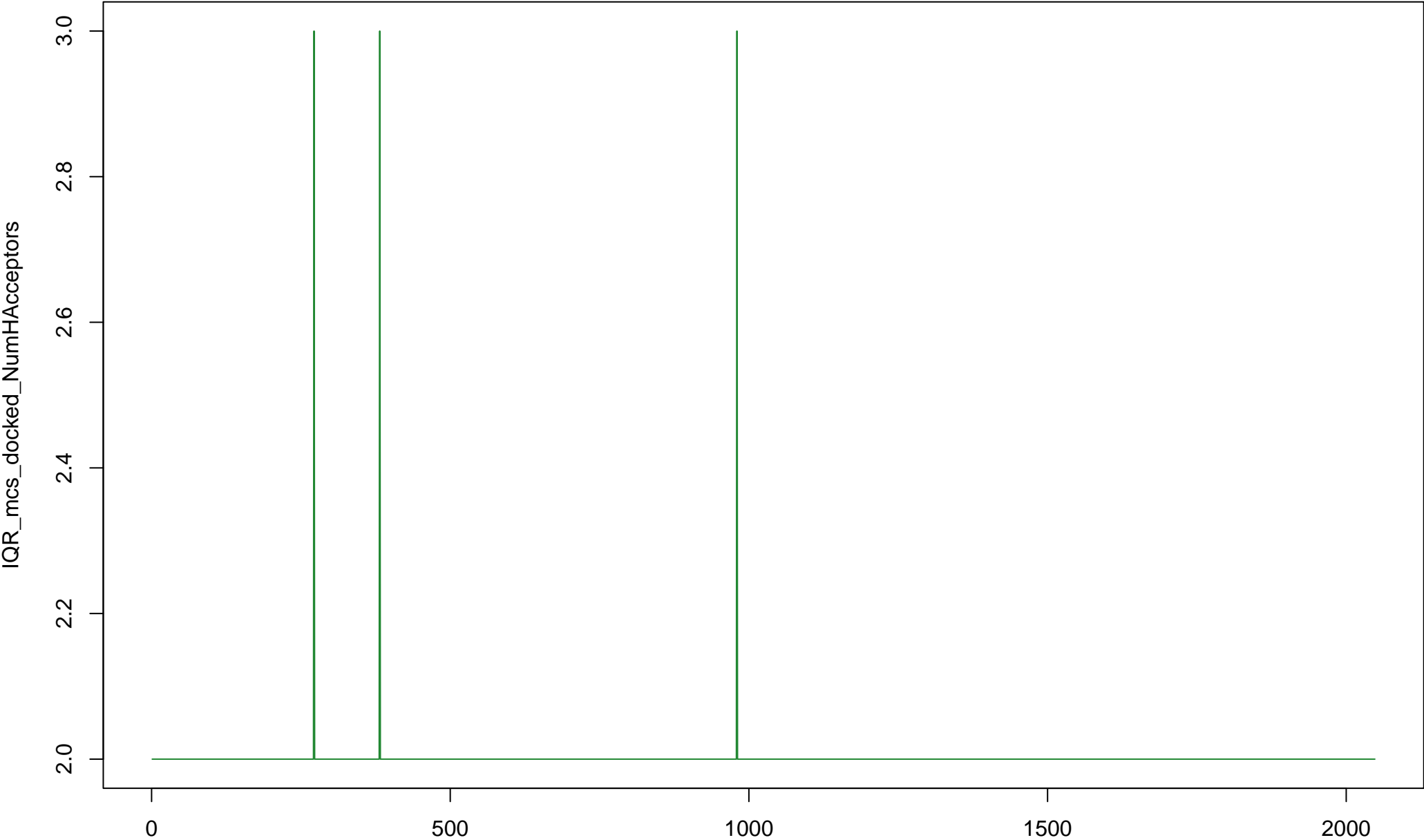
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



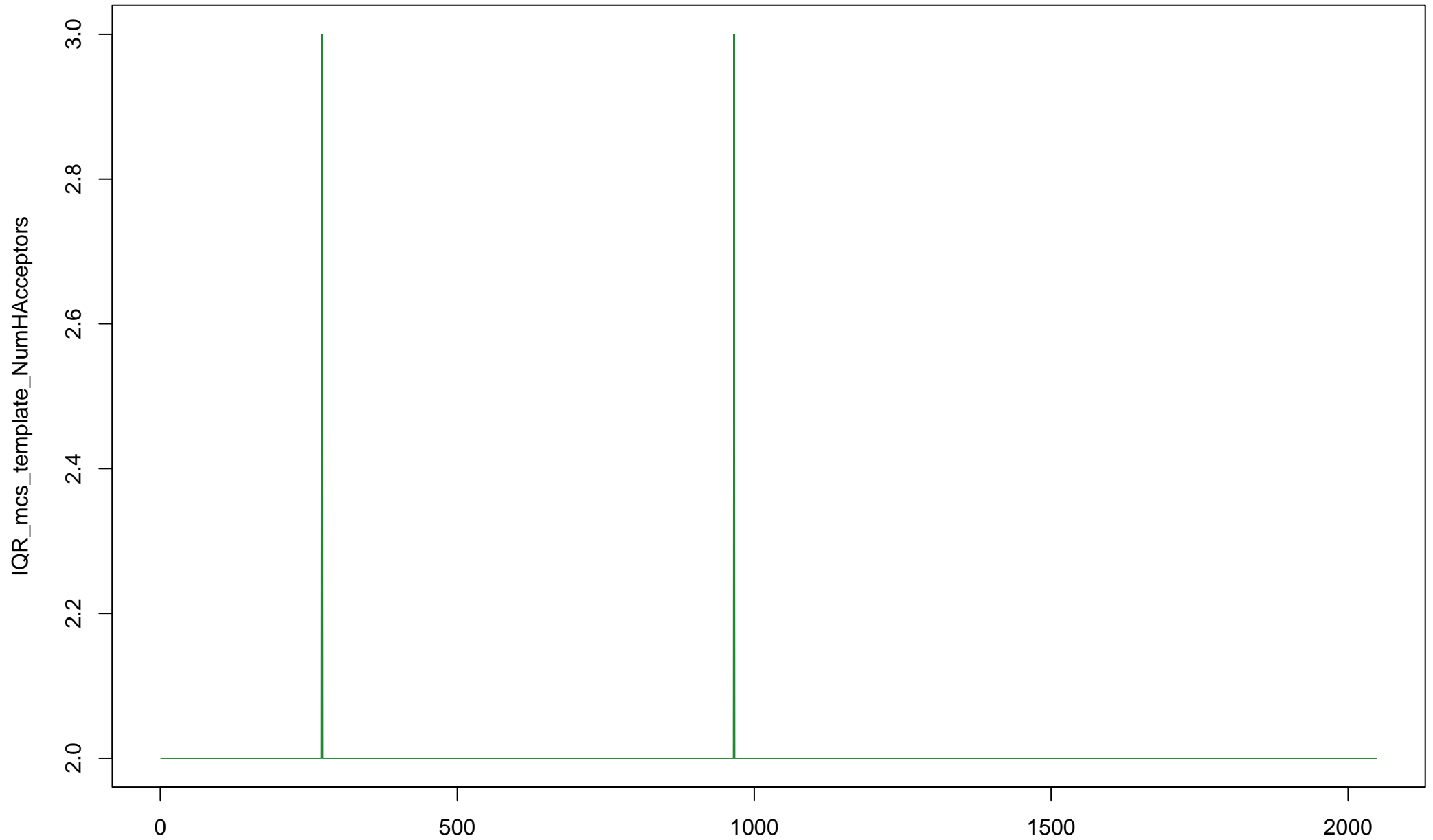
IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.758 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 816



IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.617 | MCSE(6.27) = 2.17 | stat: FALSE | burn: 1020



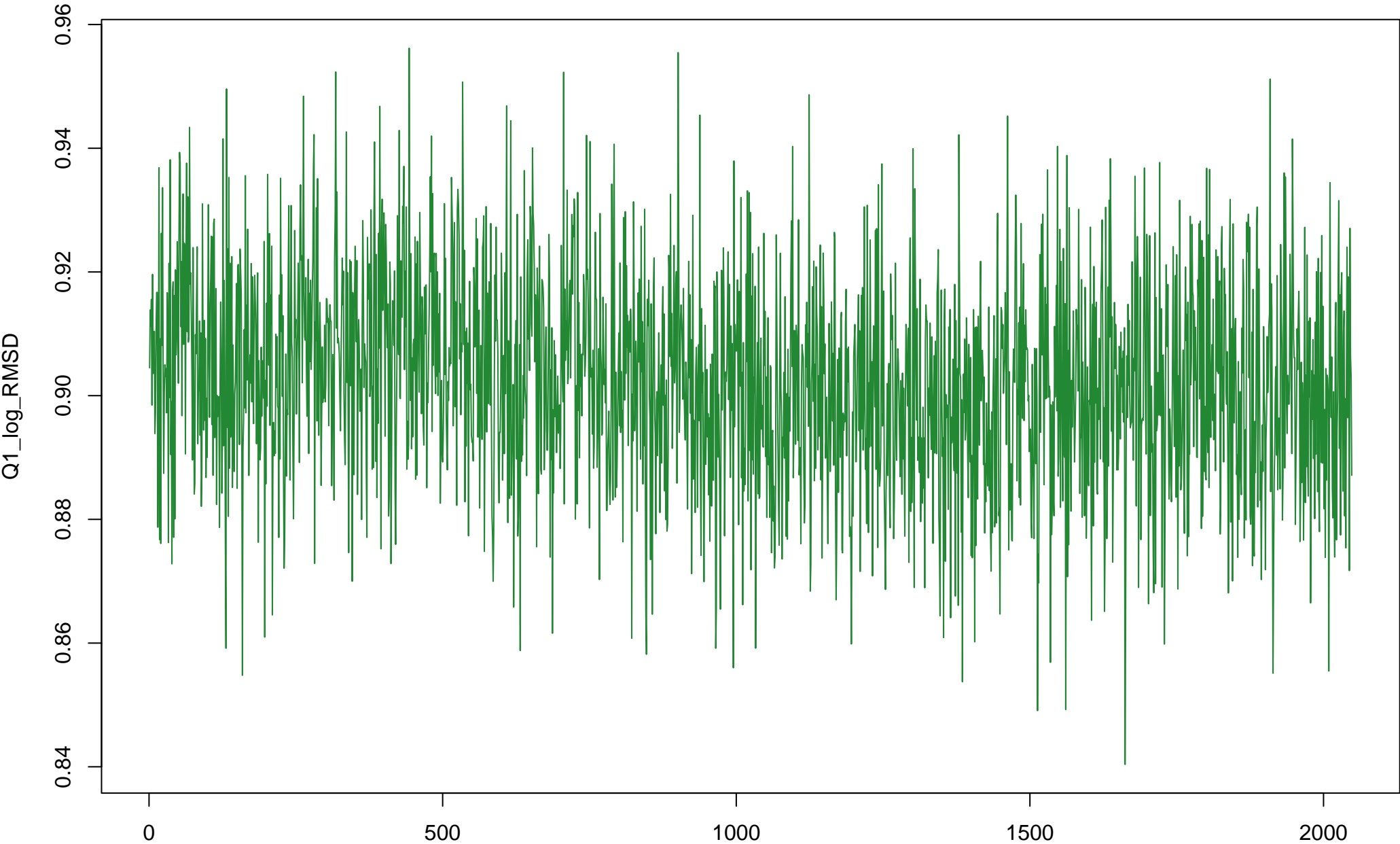
IQR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.628 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 1020



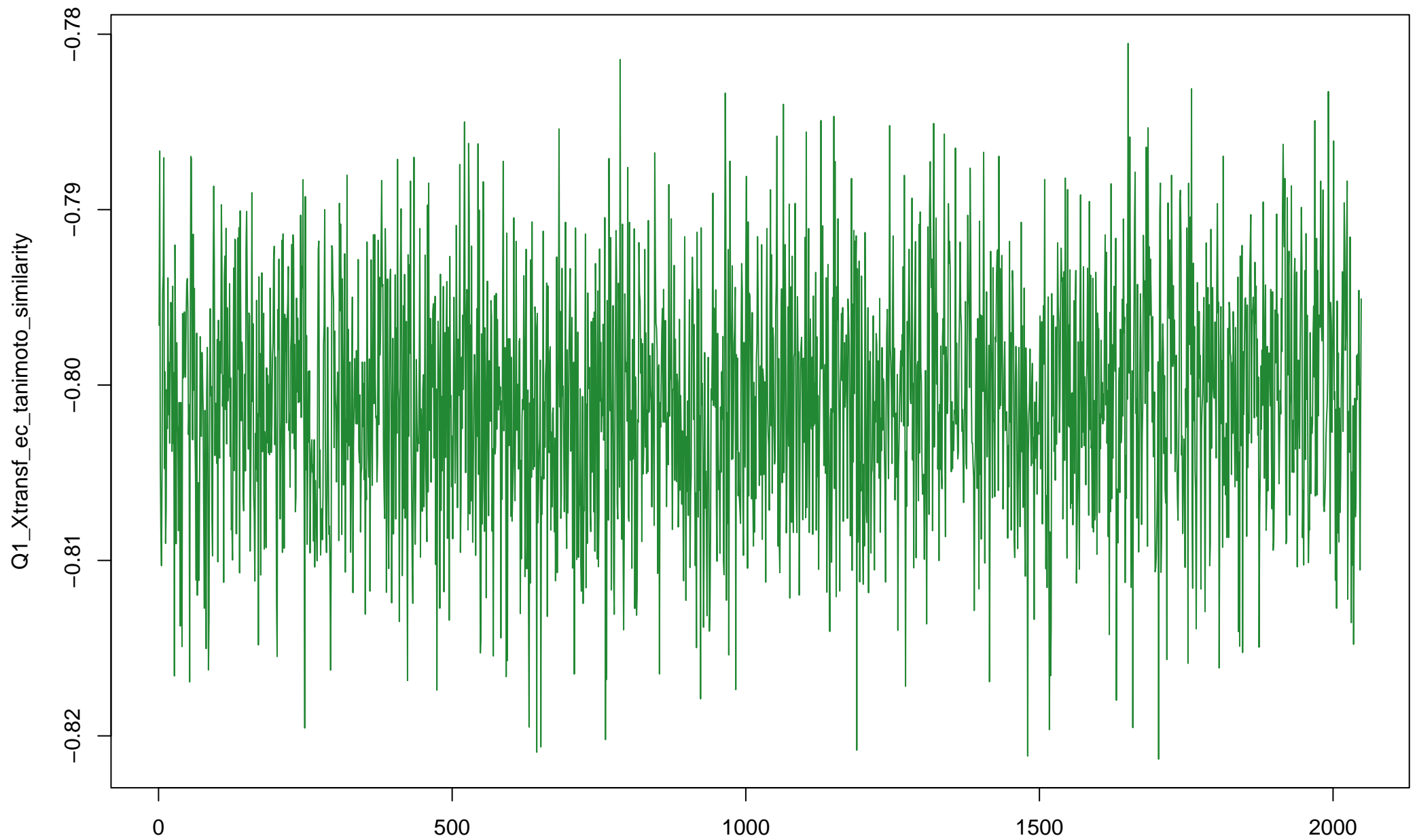
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



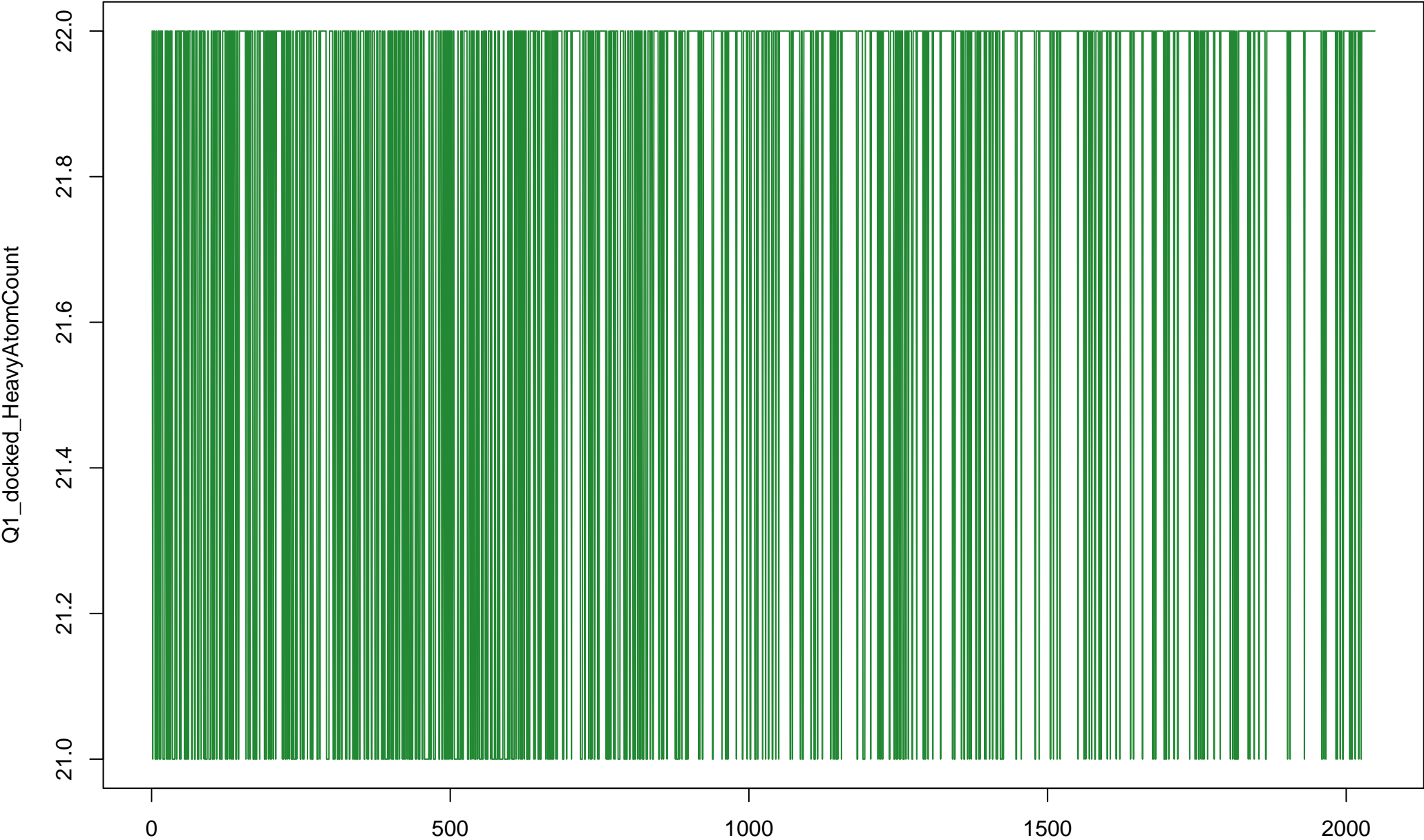
Q1_log_RMSD
ESS = 598 | BMK = 0.133 | MCSE(6.27) = 3.88 | stat: FALSE | burn: 0



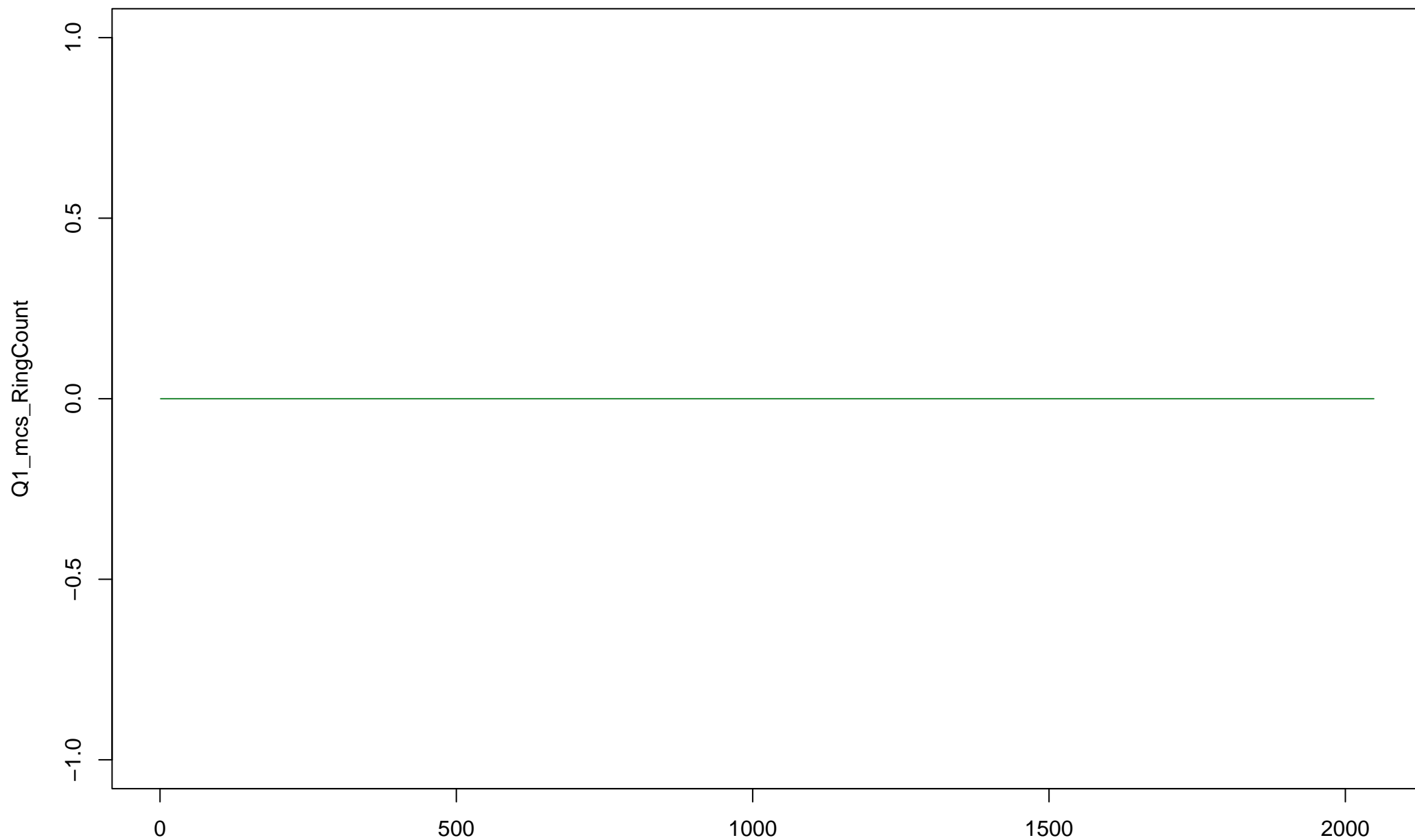
Q1_Xtransf_ec_tanimoto_similarity
ESS = 1860 | BMK = 0.059 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0



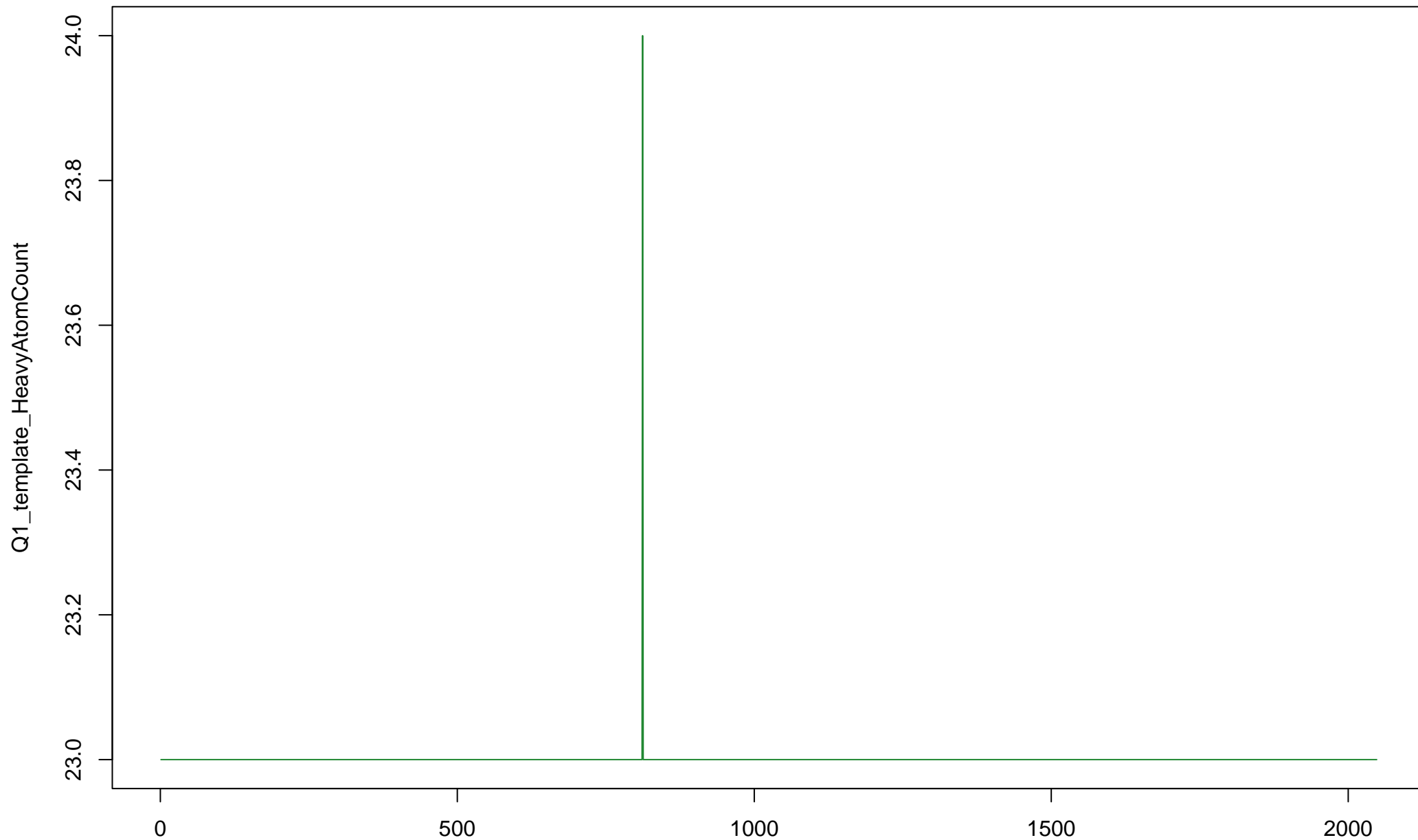
Q1_docked_HeavyAtomCount
ESS = 140 | BMK = 0.161 | MCSE(6.27) = 5.01 | stat: FALSE | burn: 0



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: 816



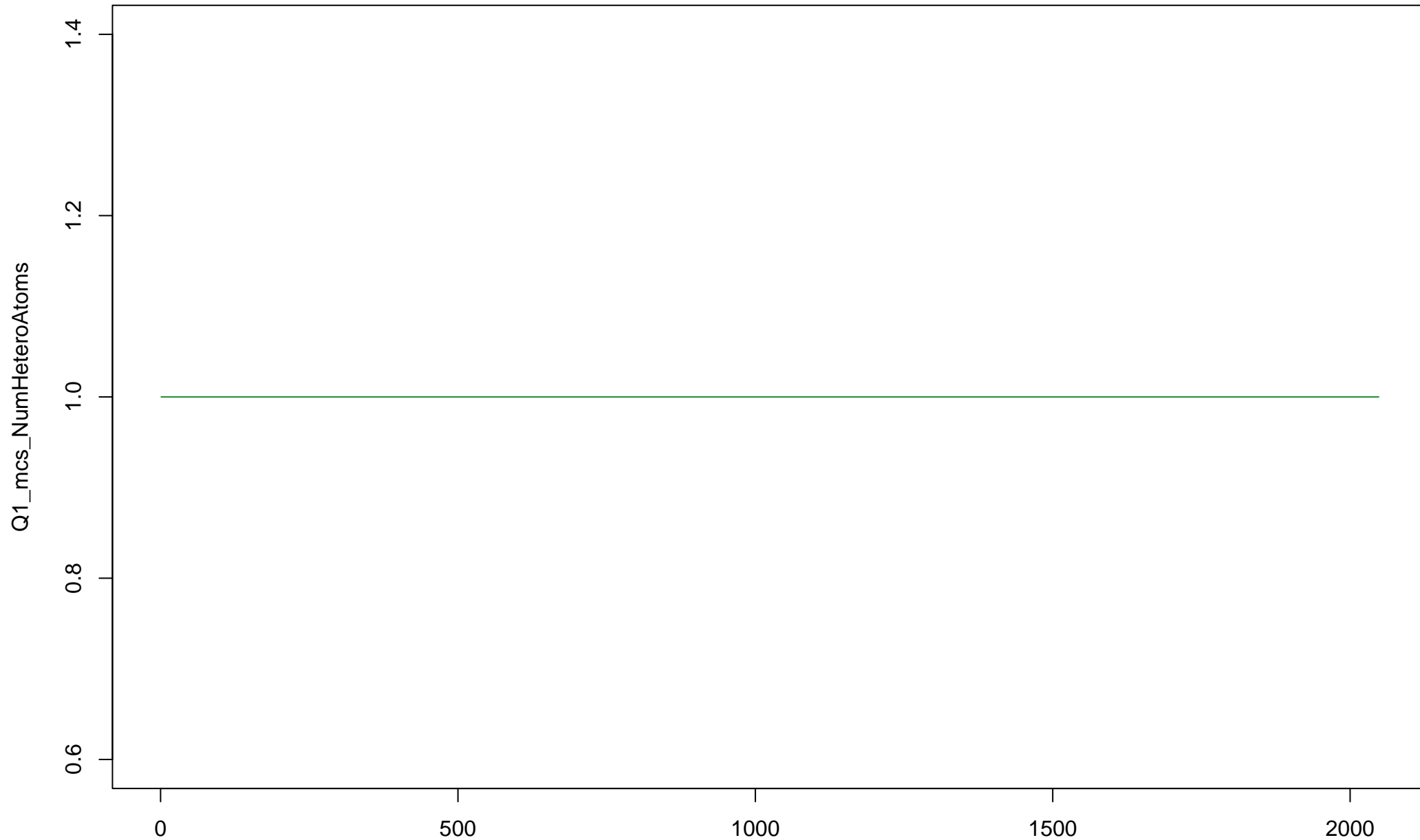
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



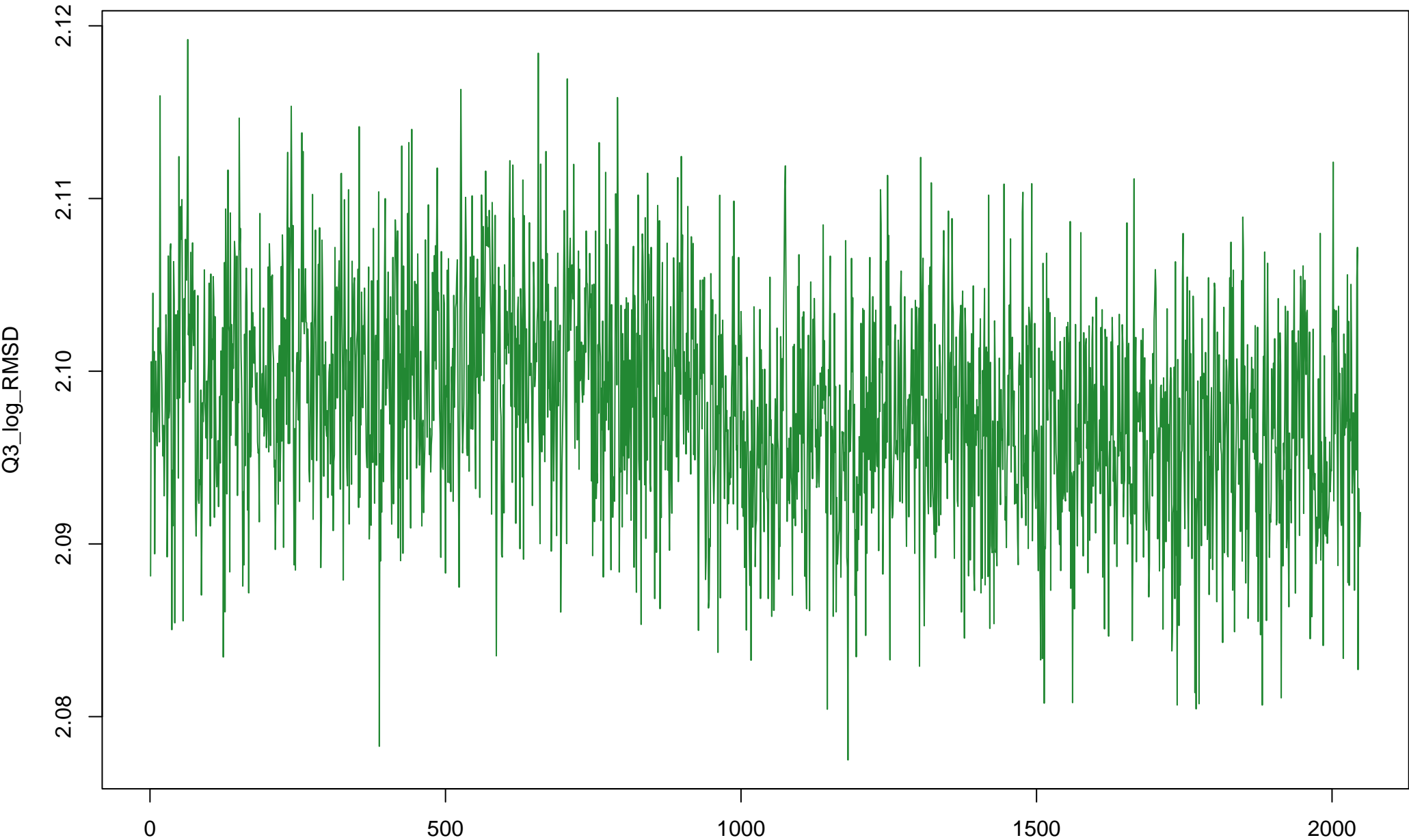
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



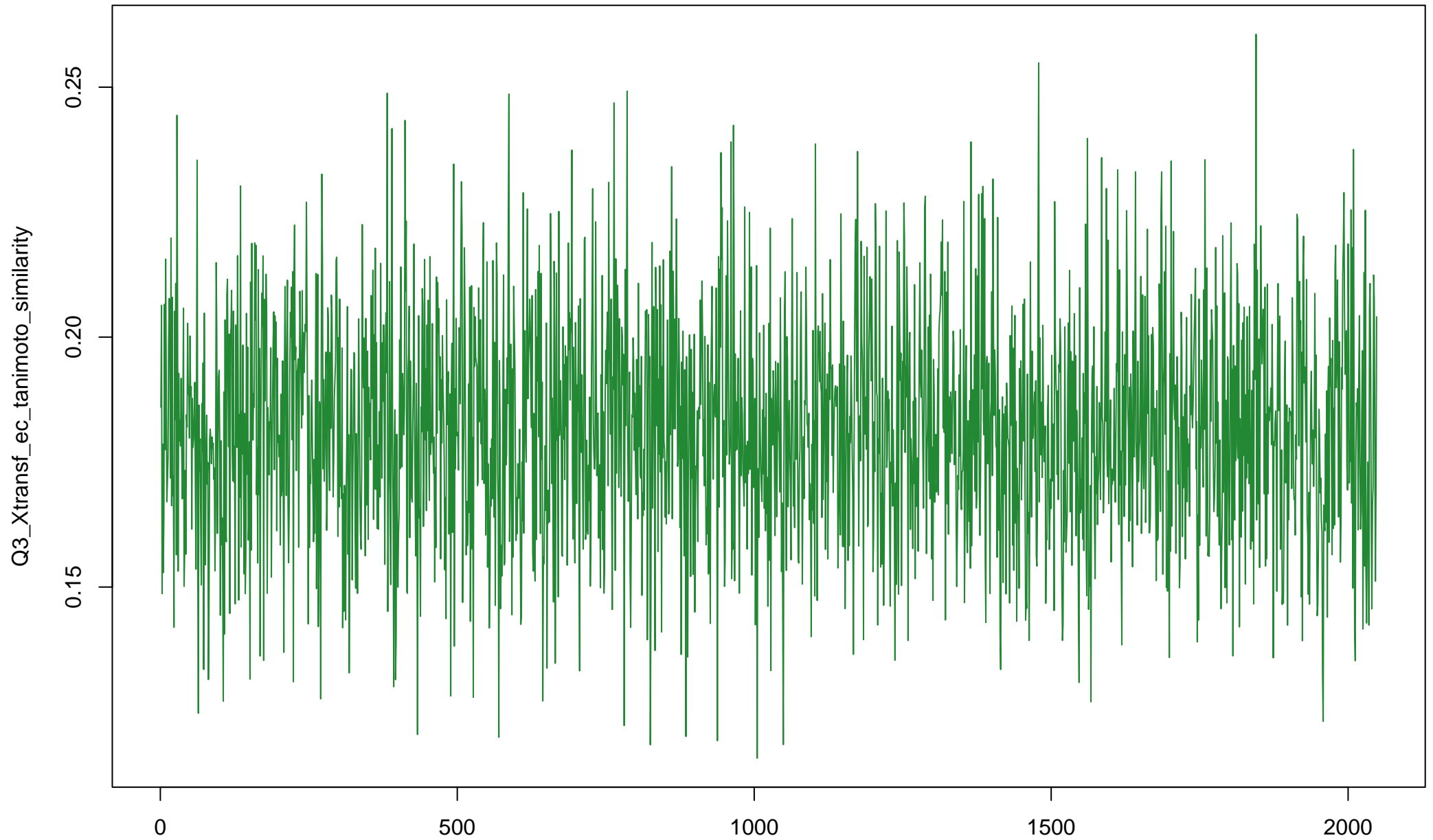
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



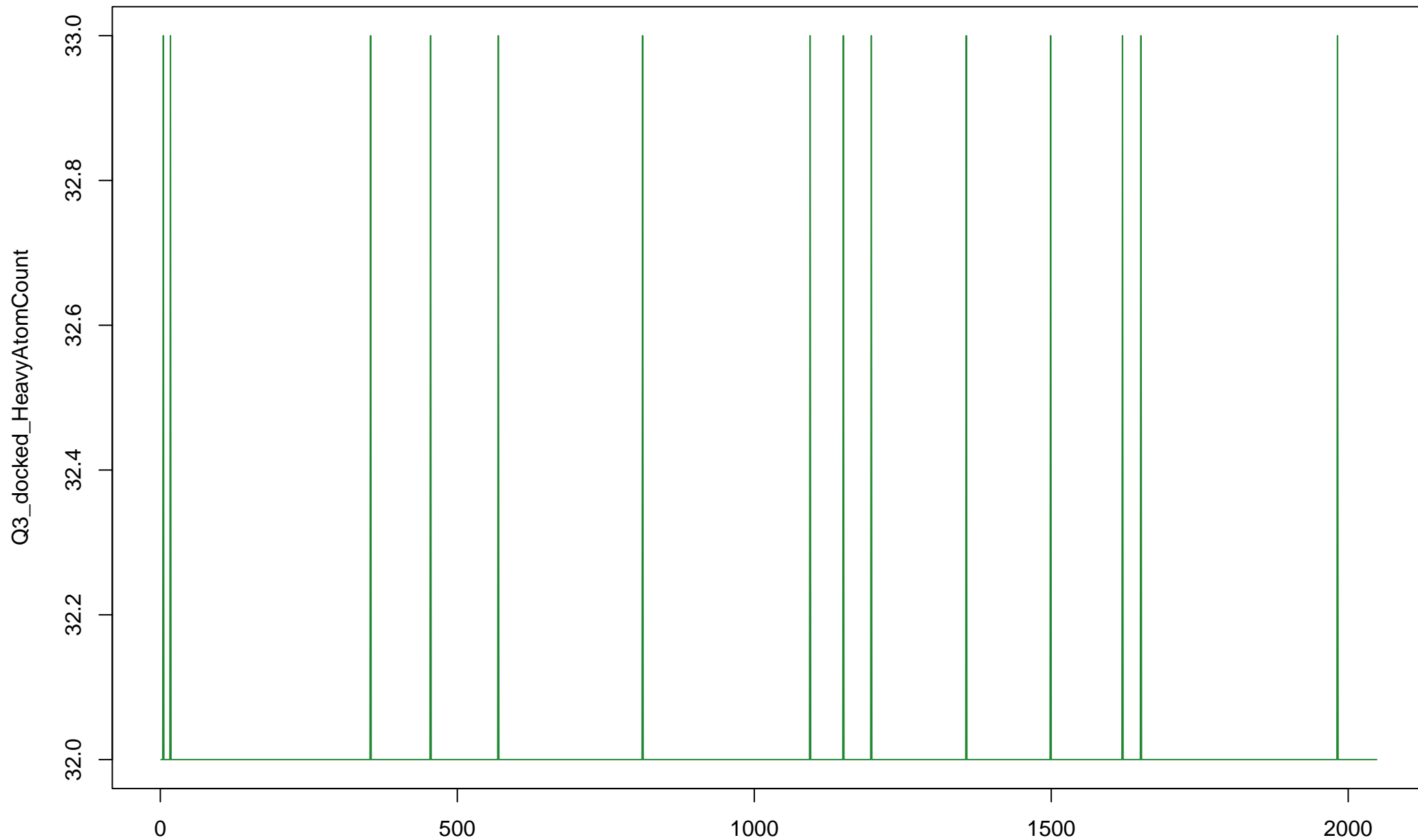
Q3_log_RMSD
ESS = 284 | BMK = 0.204 | MCSE(6.27) = 5.13 | stat: FALSE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 1740 | BMK = 0.0656 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0



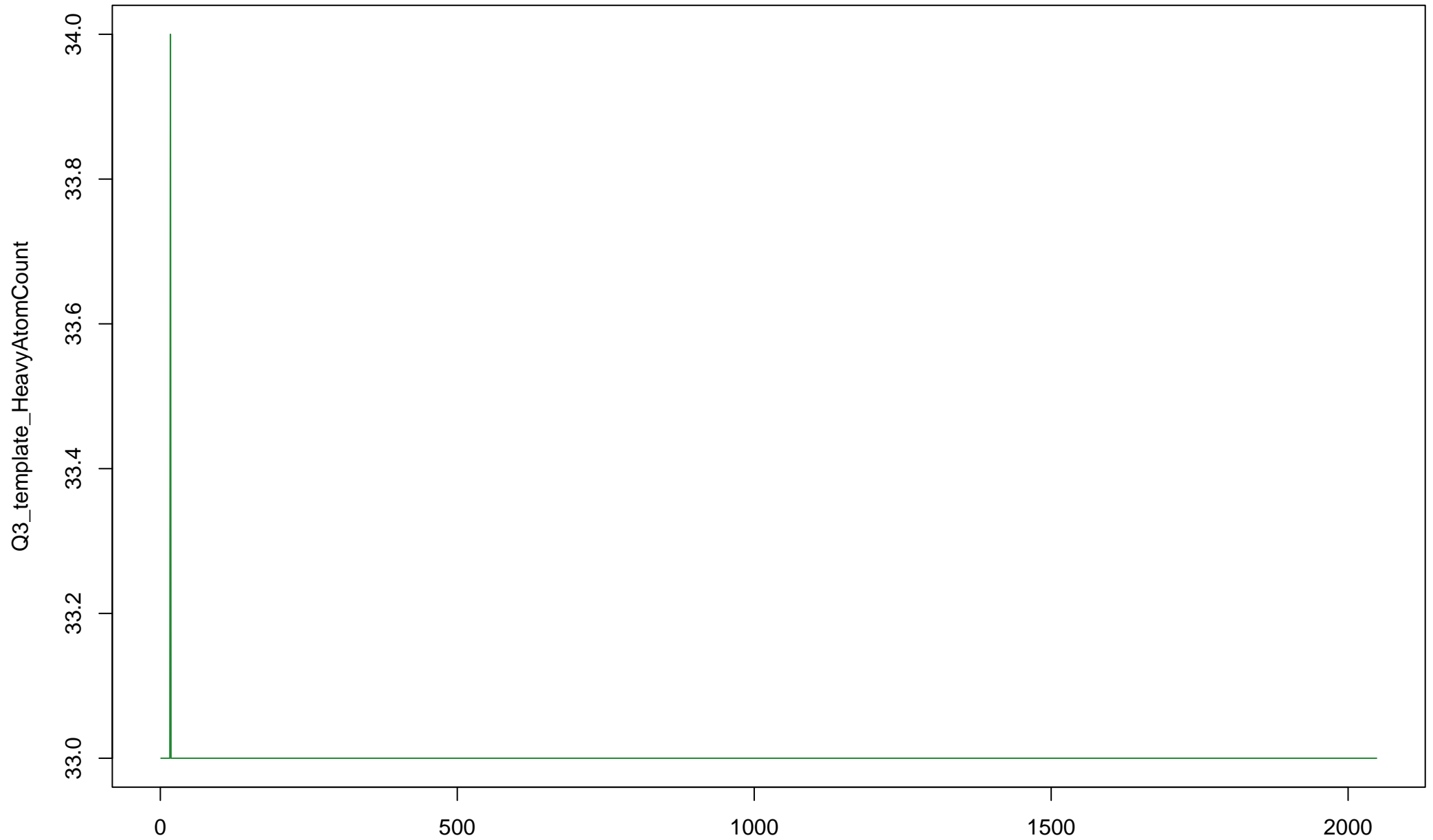
Q3_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0509 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 816



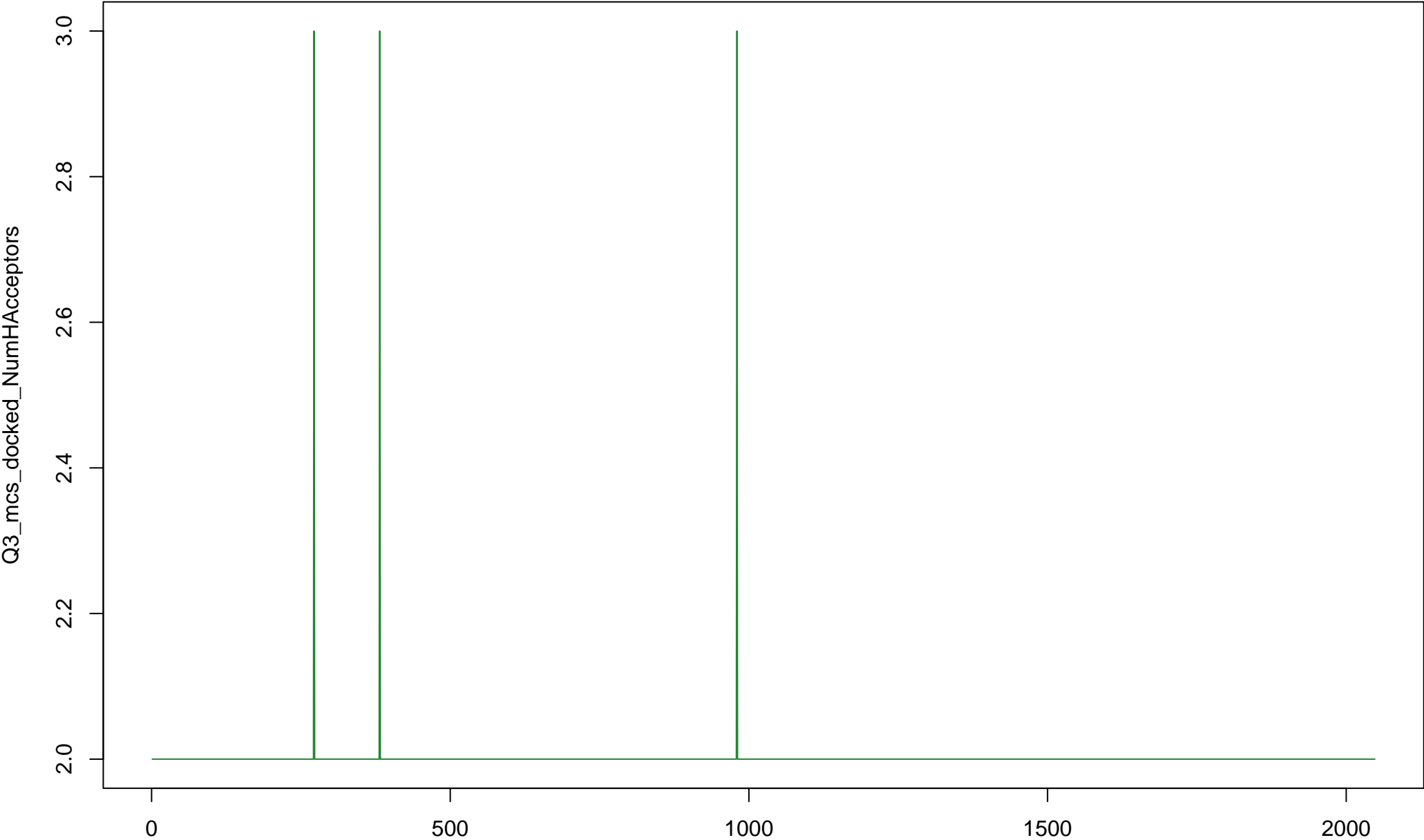
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



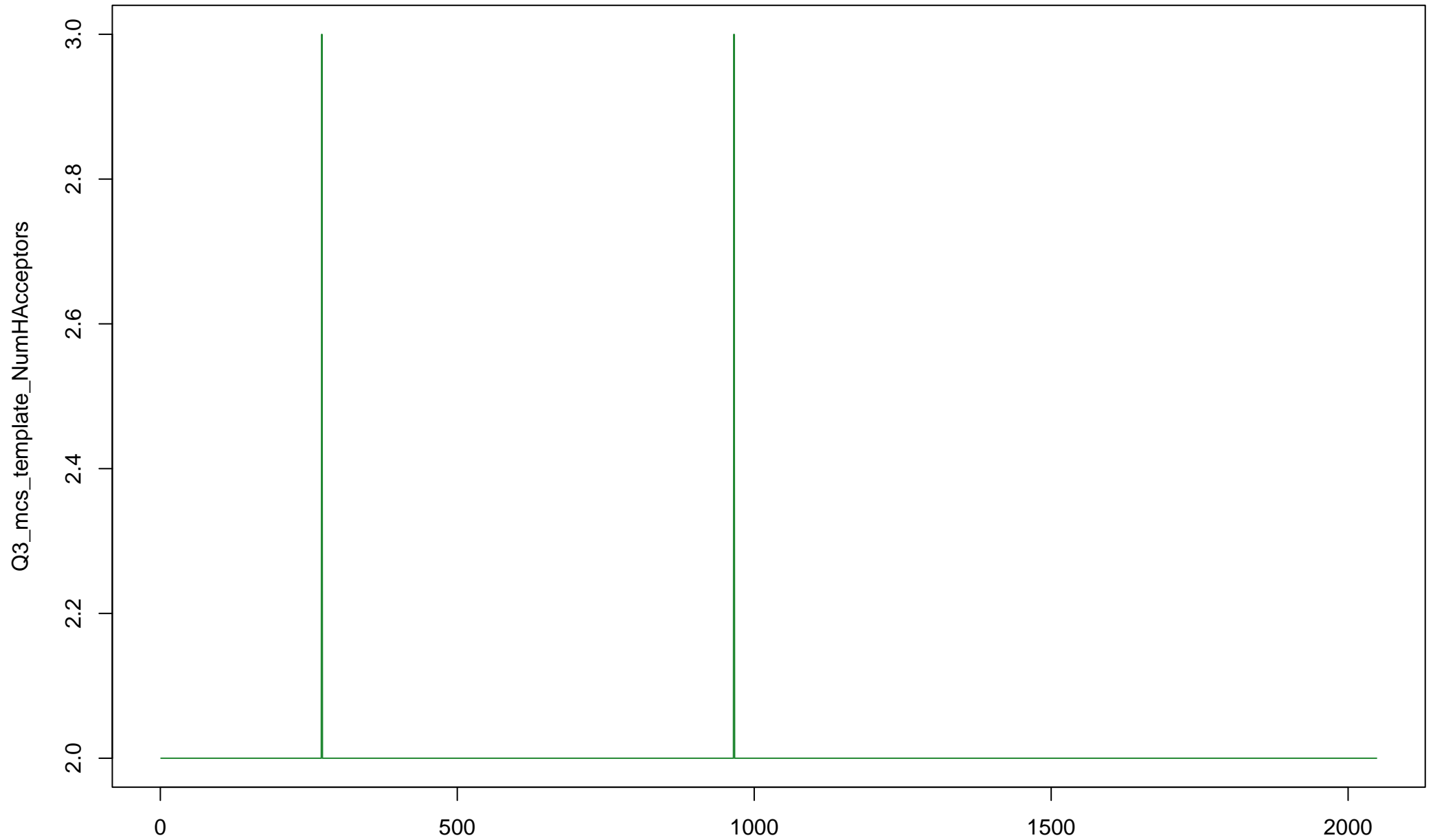
Q3_template_HeavyAtomCount
ESS = 2050 | BMK = 0.517 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 204



Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.617 | MCSE(6.27) = 2.17 | stat: FALSE | burn: 1020



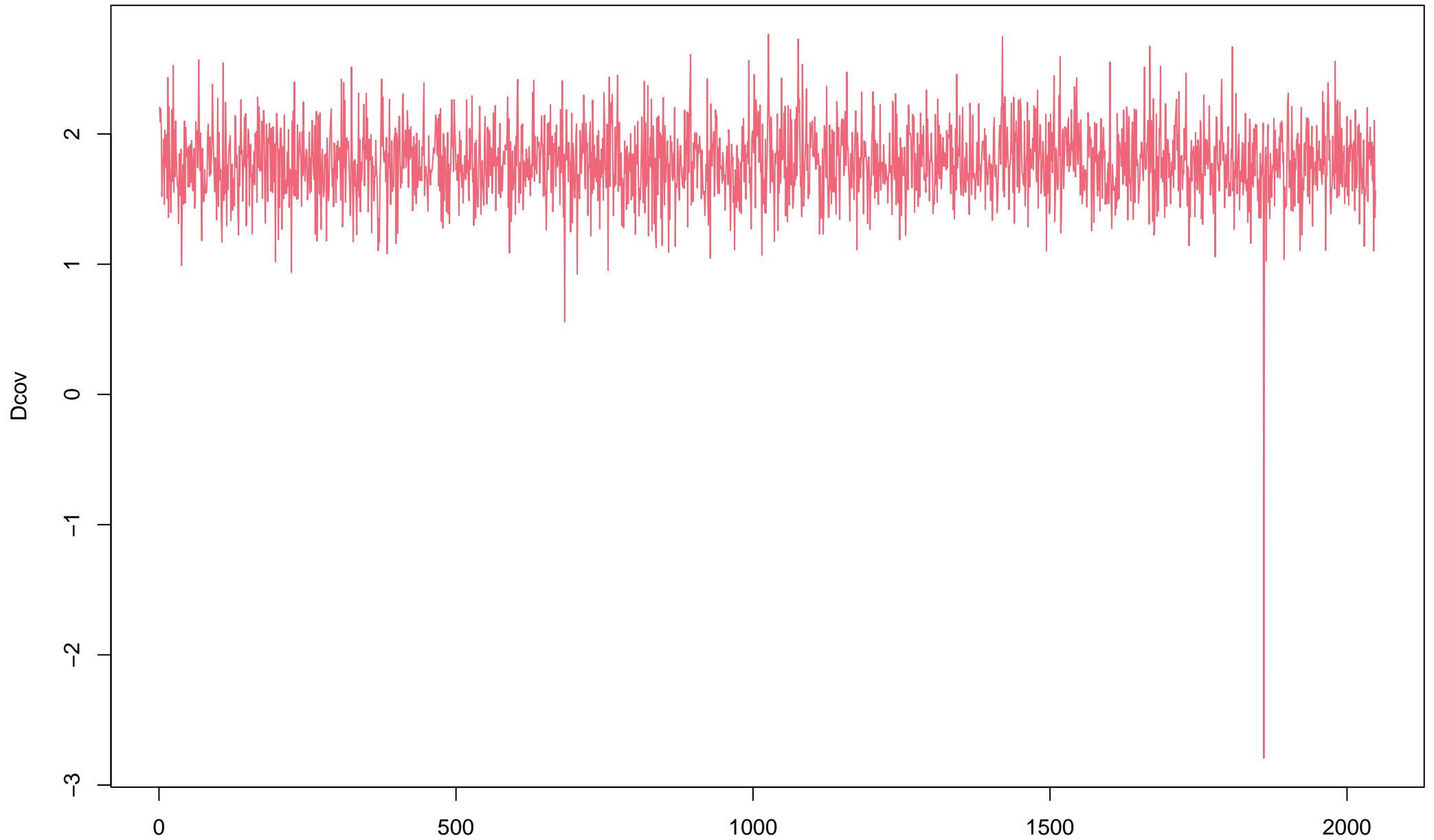
Q3_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.628 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 1020



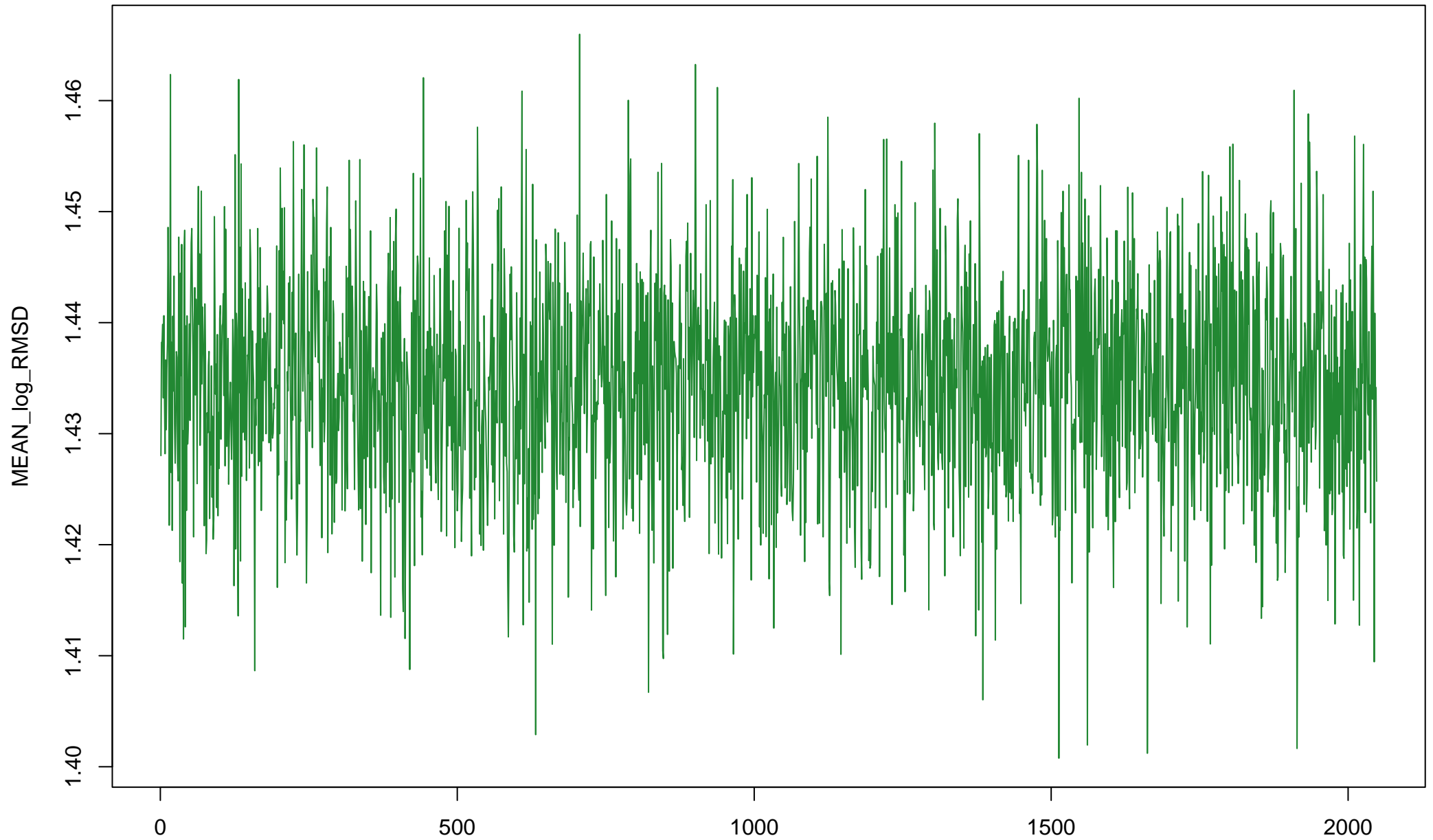
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



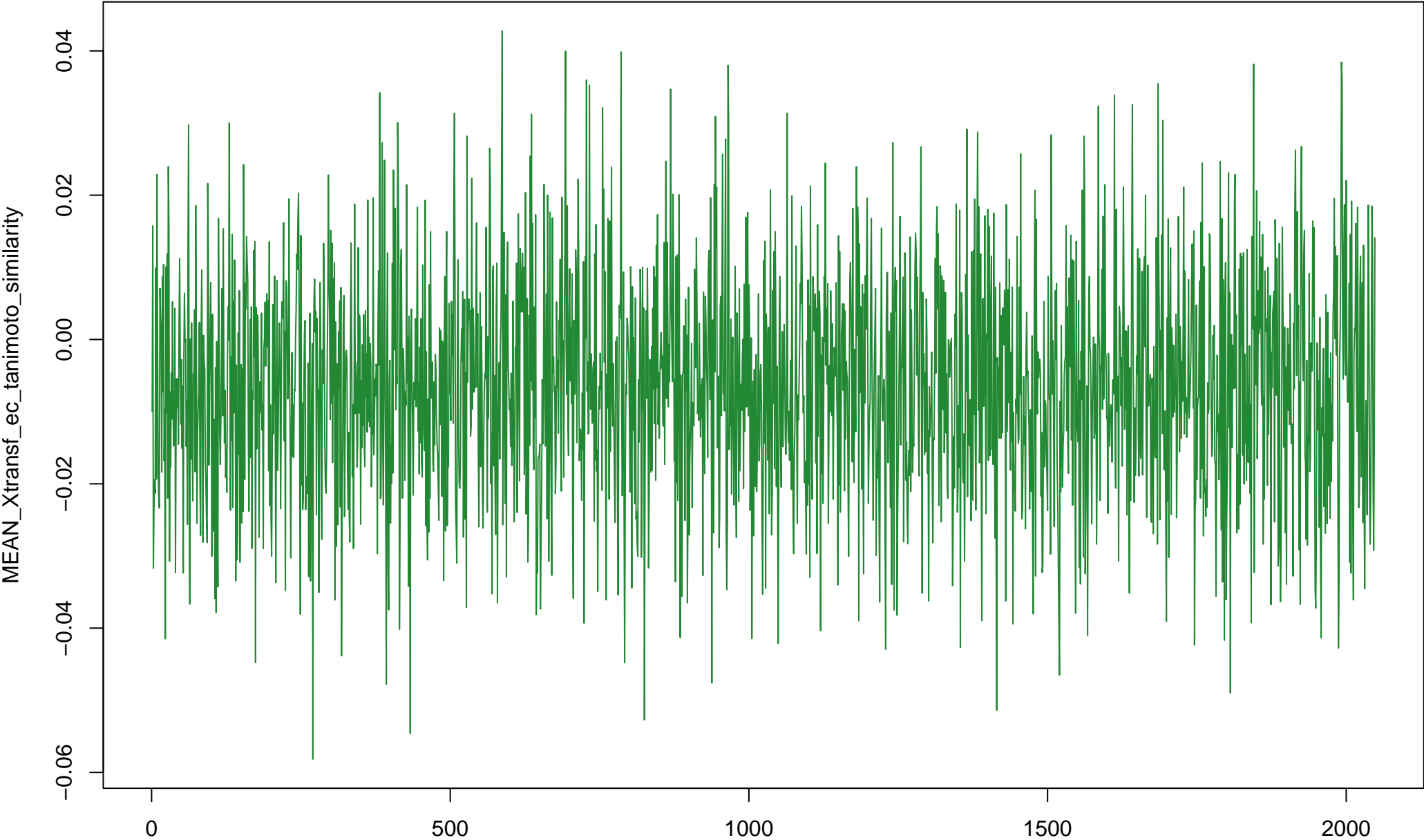
Dcov
ESS = 2050 | BMK = 0.0704 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0



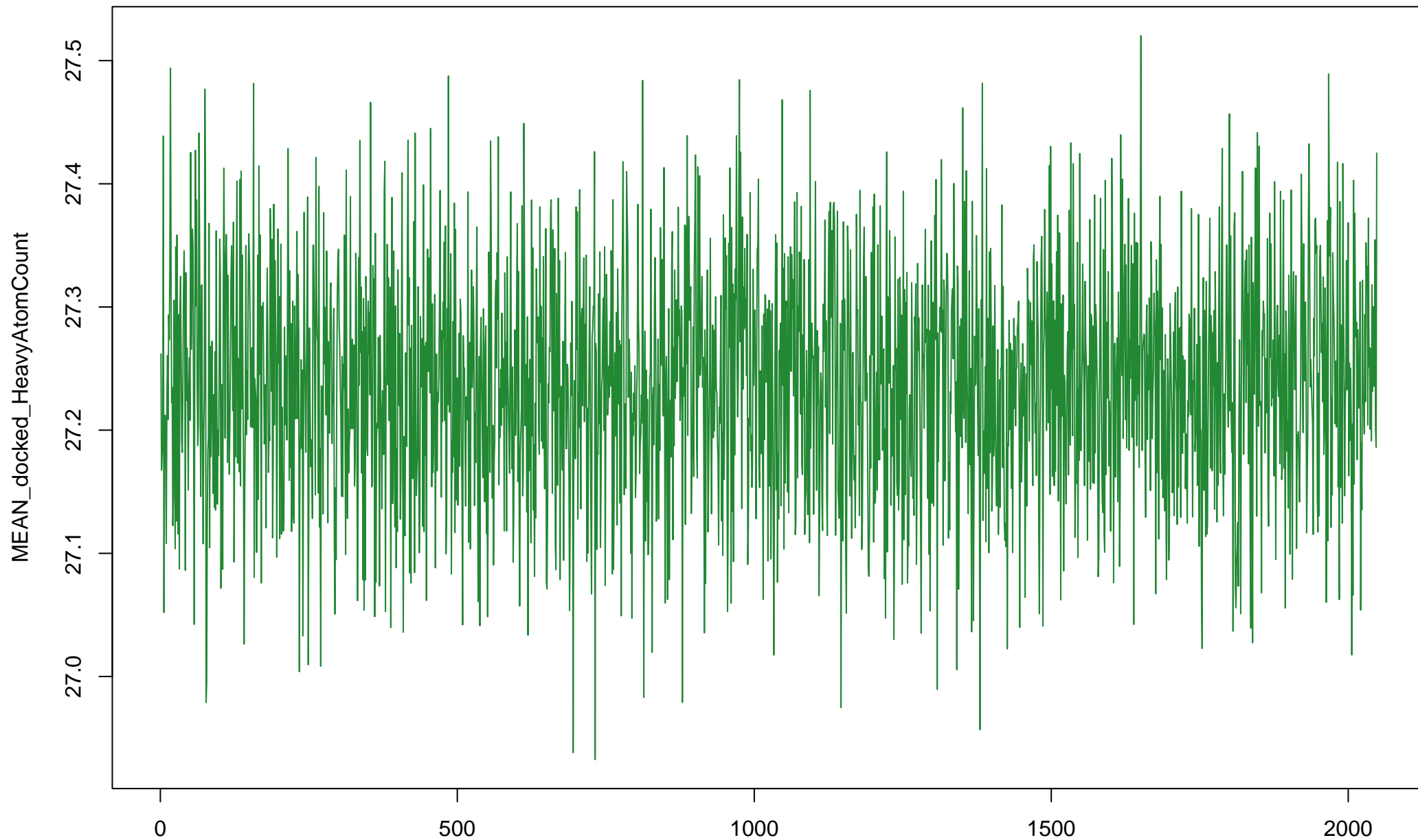
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0398 | MCSE(6.27) = 1.81 | stat: TRUE | burn: 0



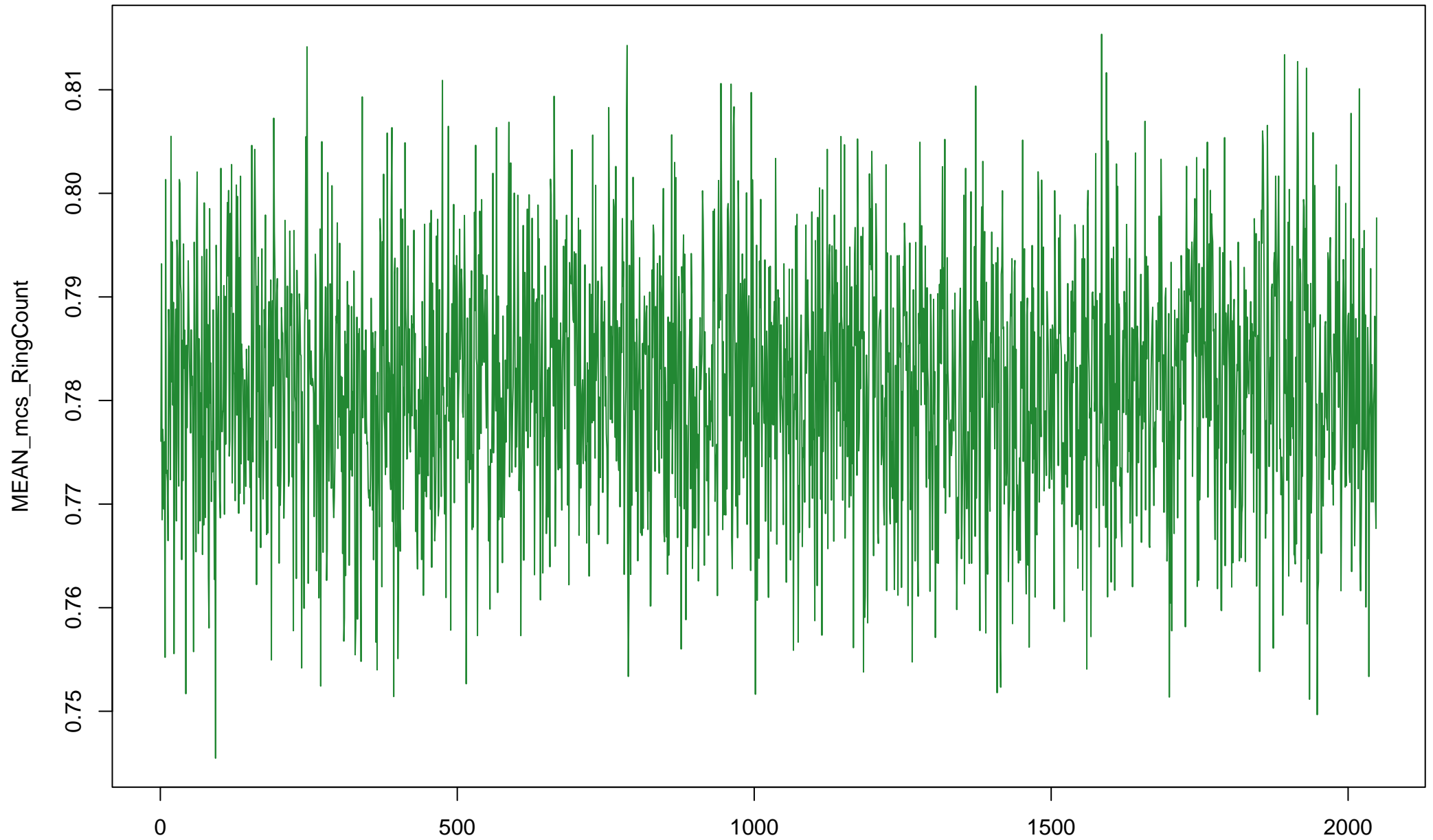
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.035 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0



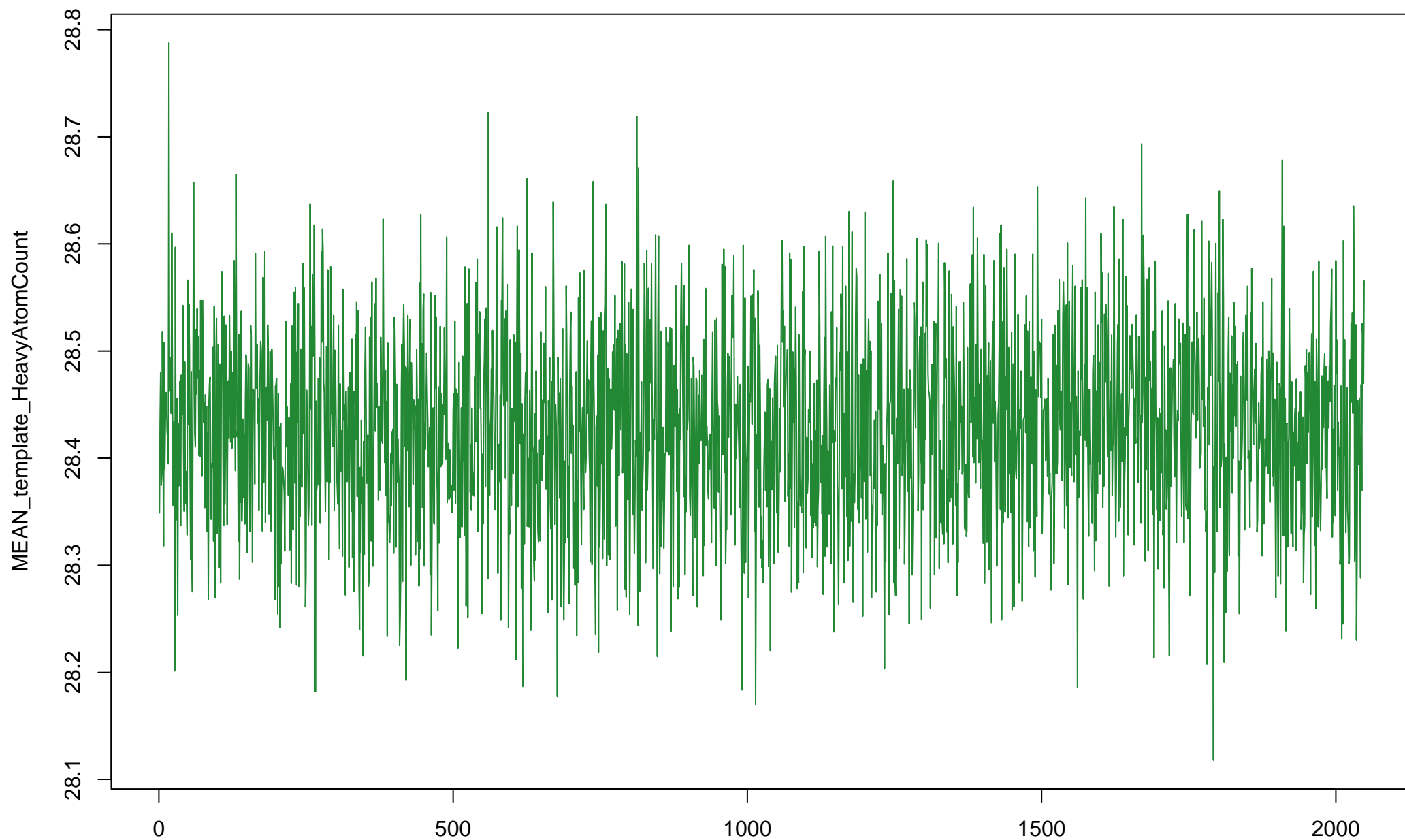
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0395 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0



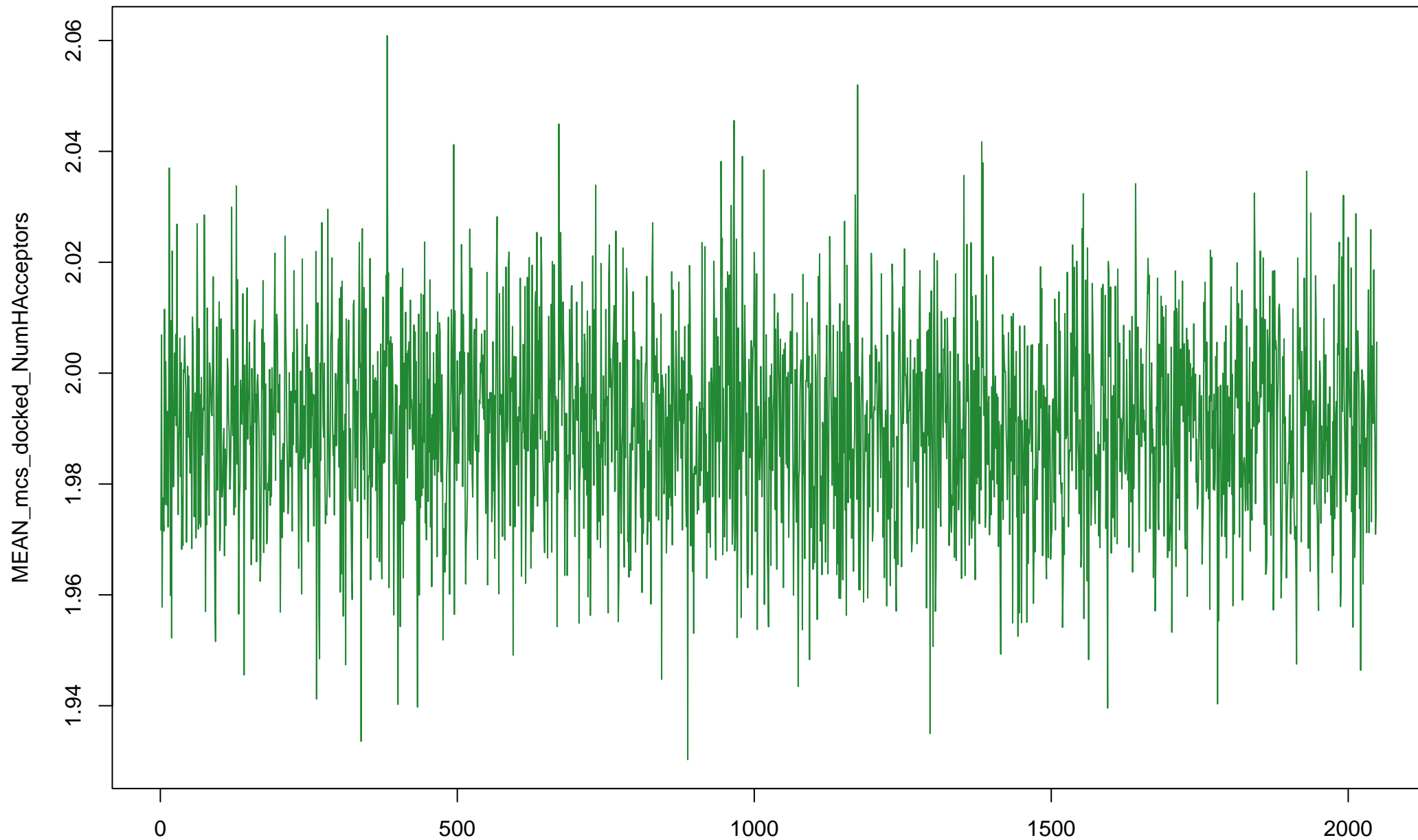
MEAN_mcs_RingCount
ESS = 1900 | BMK = 0.035 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0



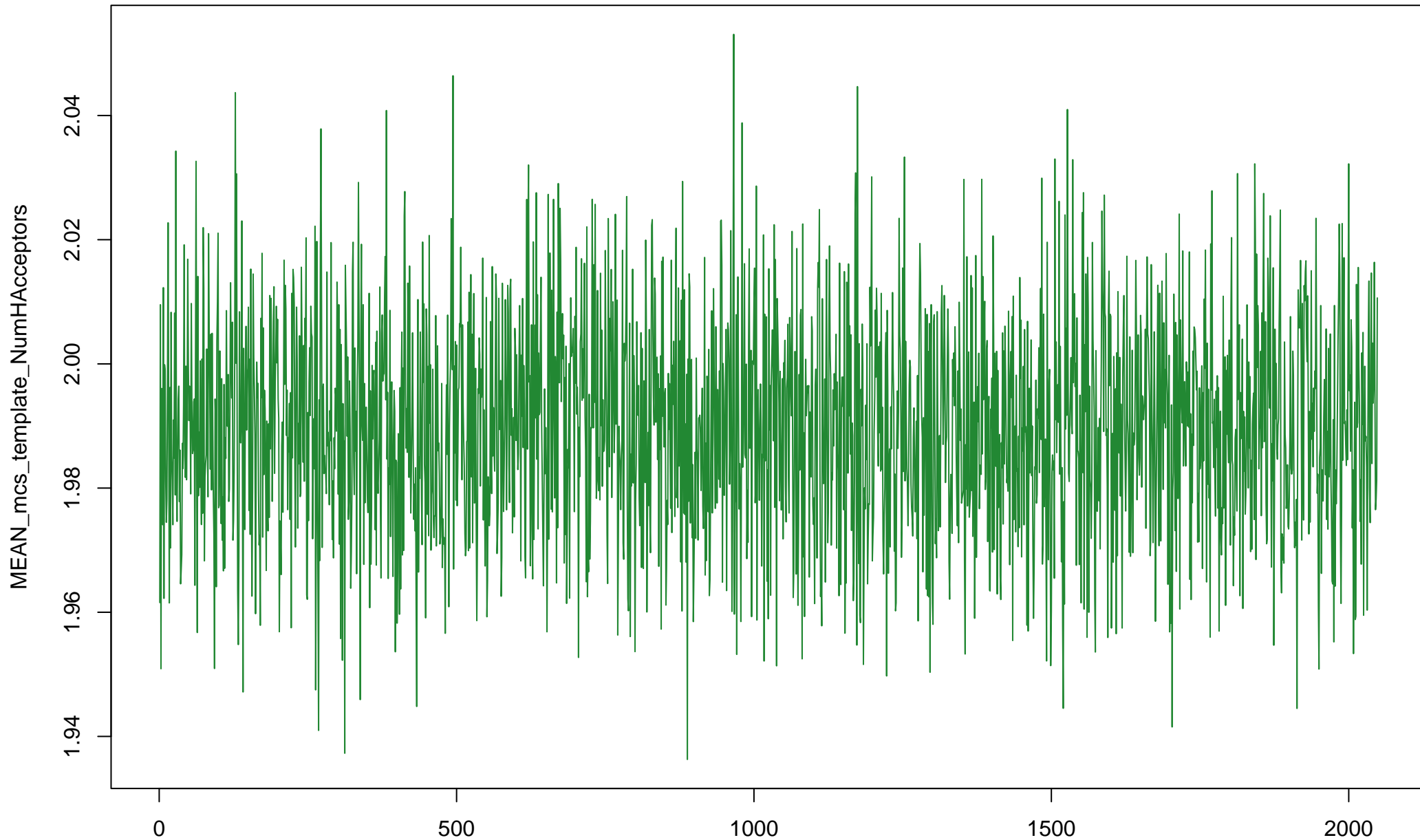
MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0477 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0



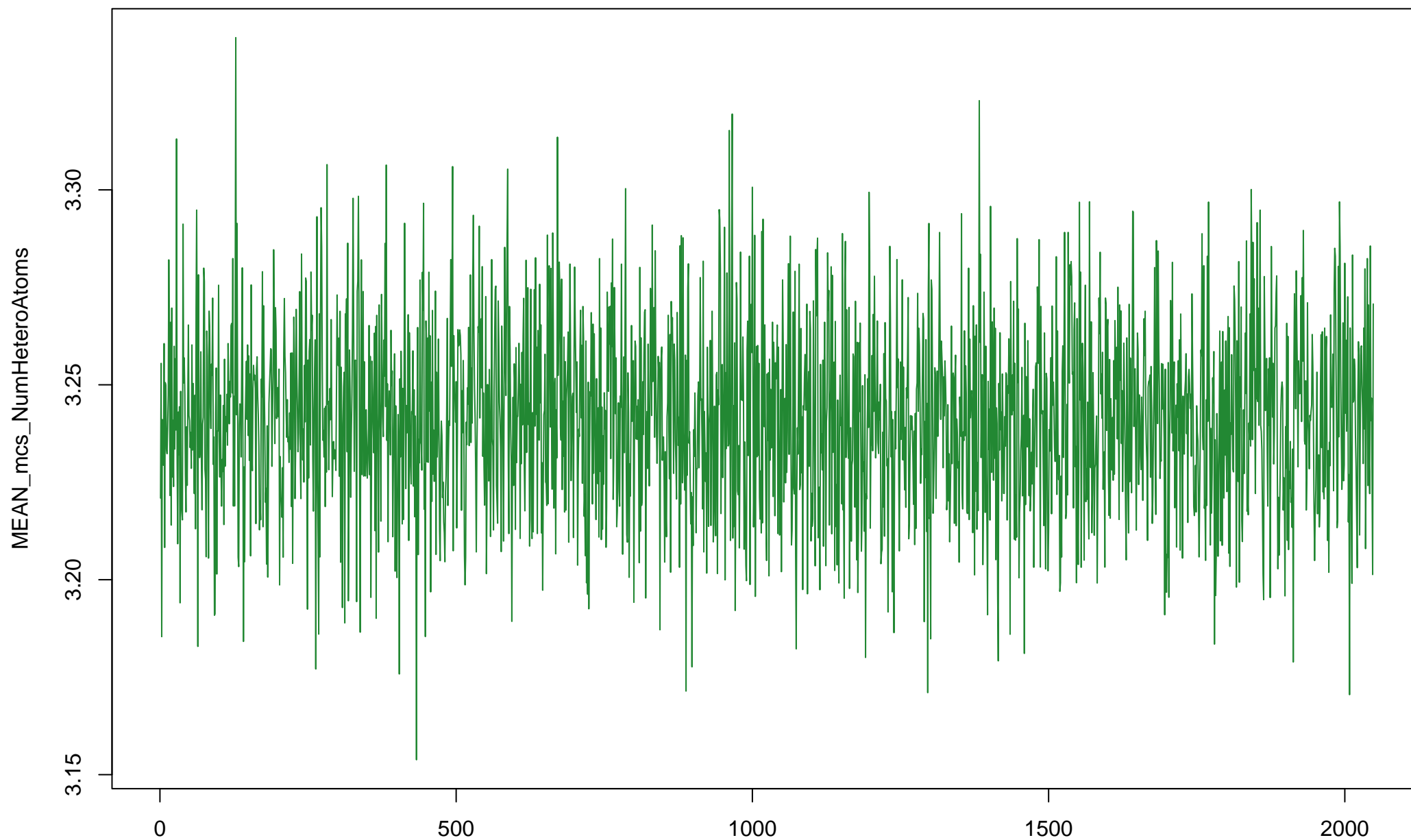
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0354 | MCSE(6.27) = 1.87 | stat: TRUE | burn: 0



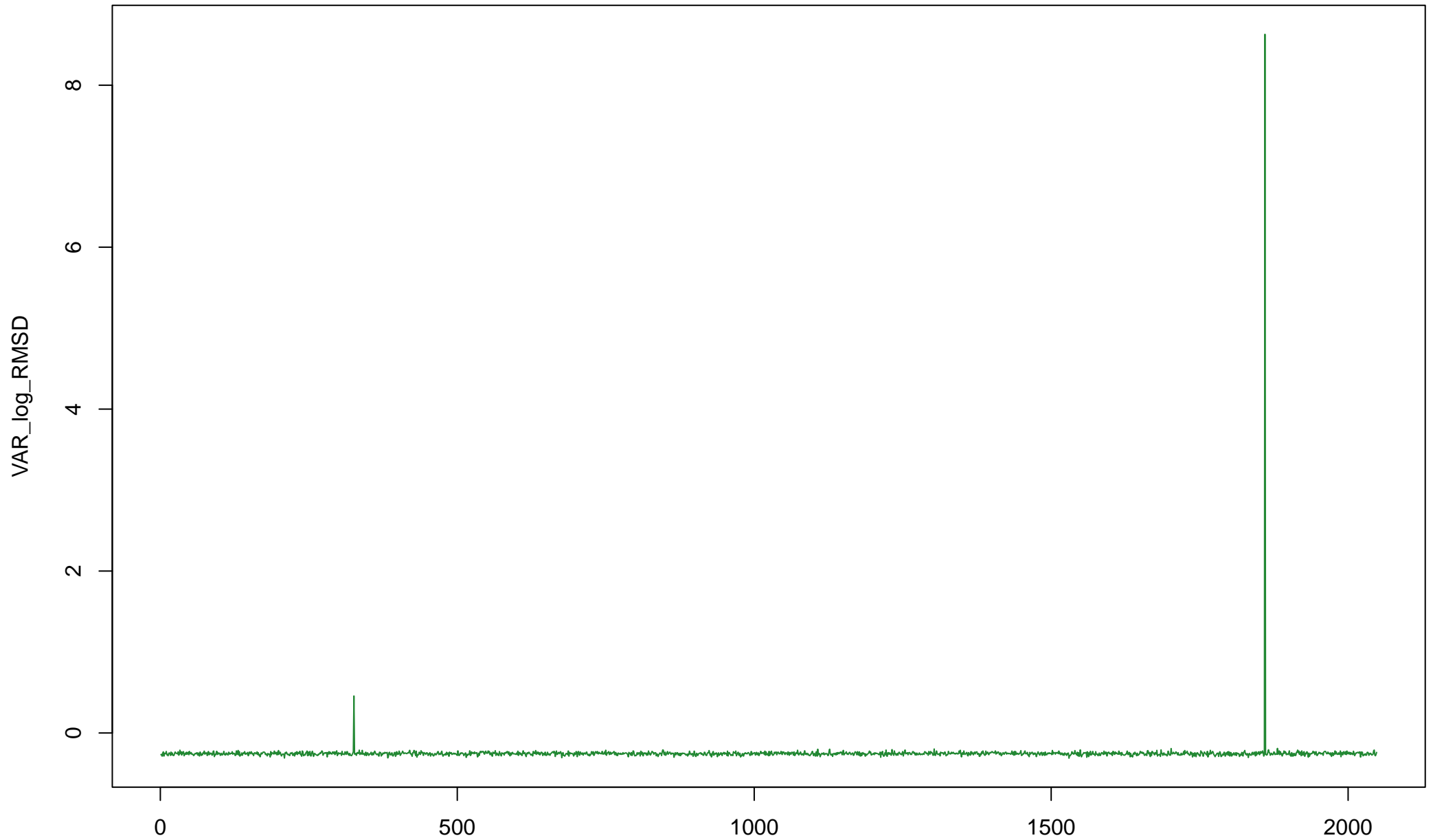
MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0327 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0



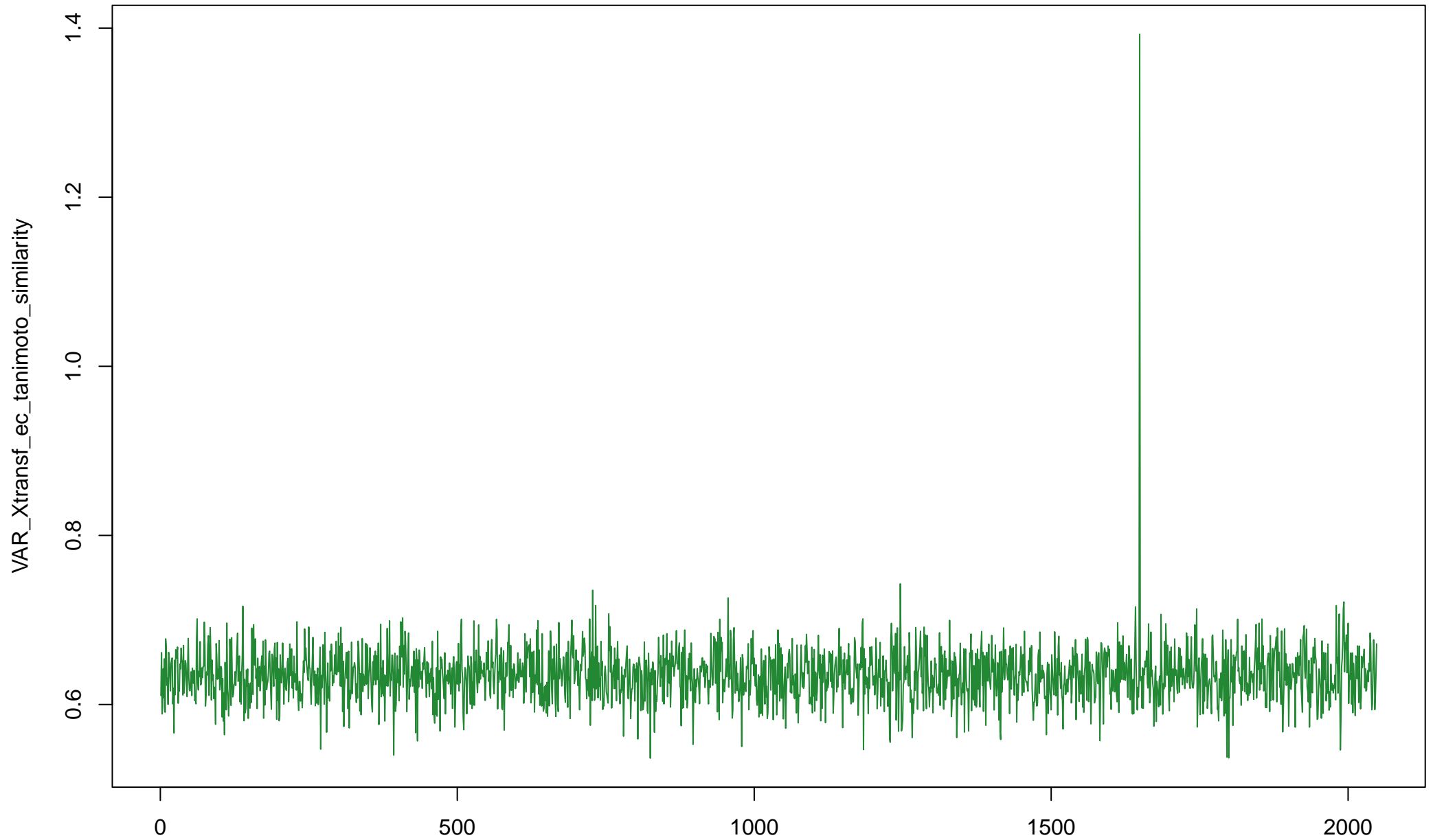
MEAN_mcs_NumHeteroAtoms
ESS = 1740 | BMK = 0.0491 | MCSE(6.27) = 1.72 | stat: TRUE | burn: 0



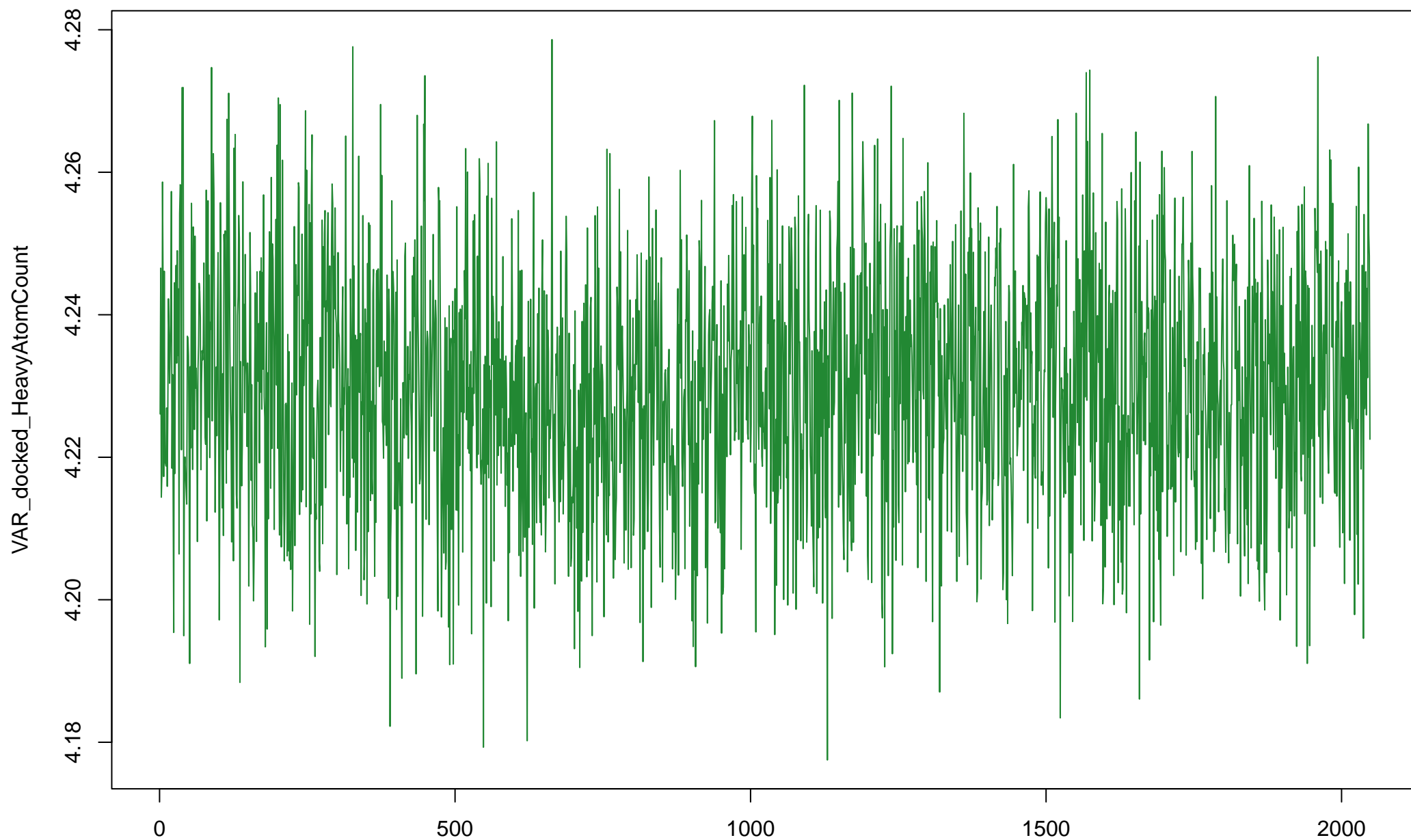
VAR_log_RMSD
ESS = 2050 | BMK = 0.809 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 2040



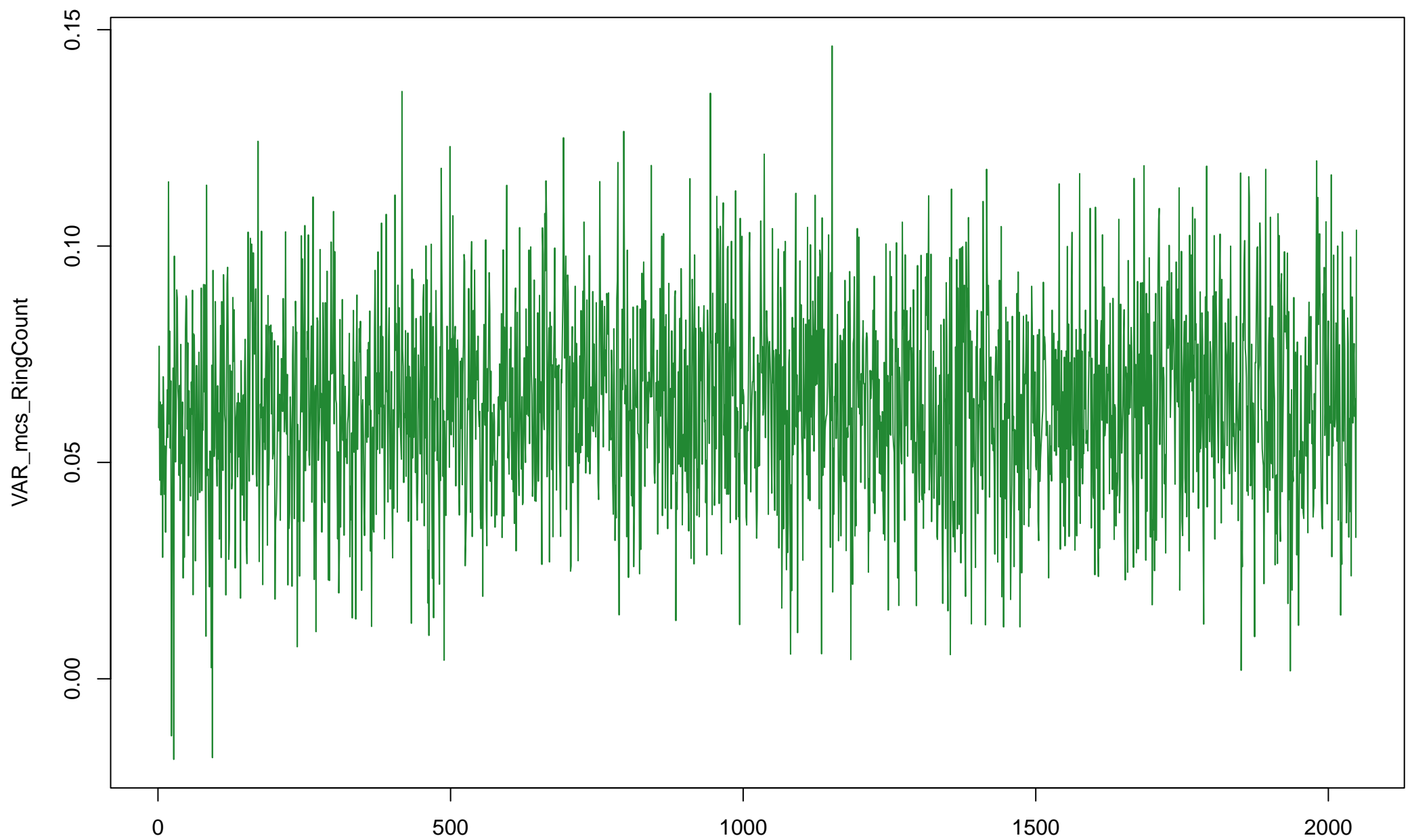
VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0414 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0



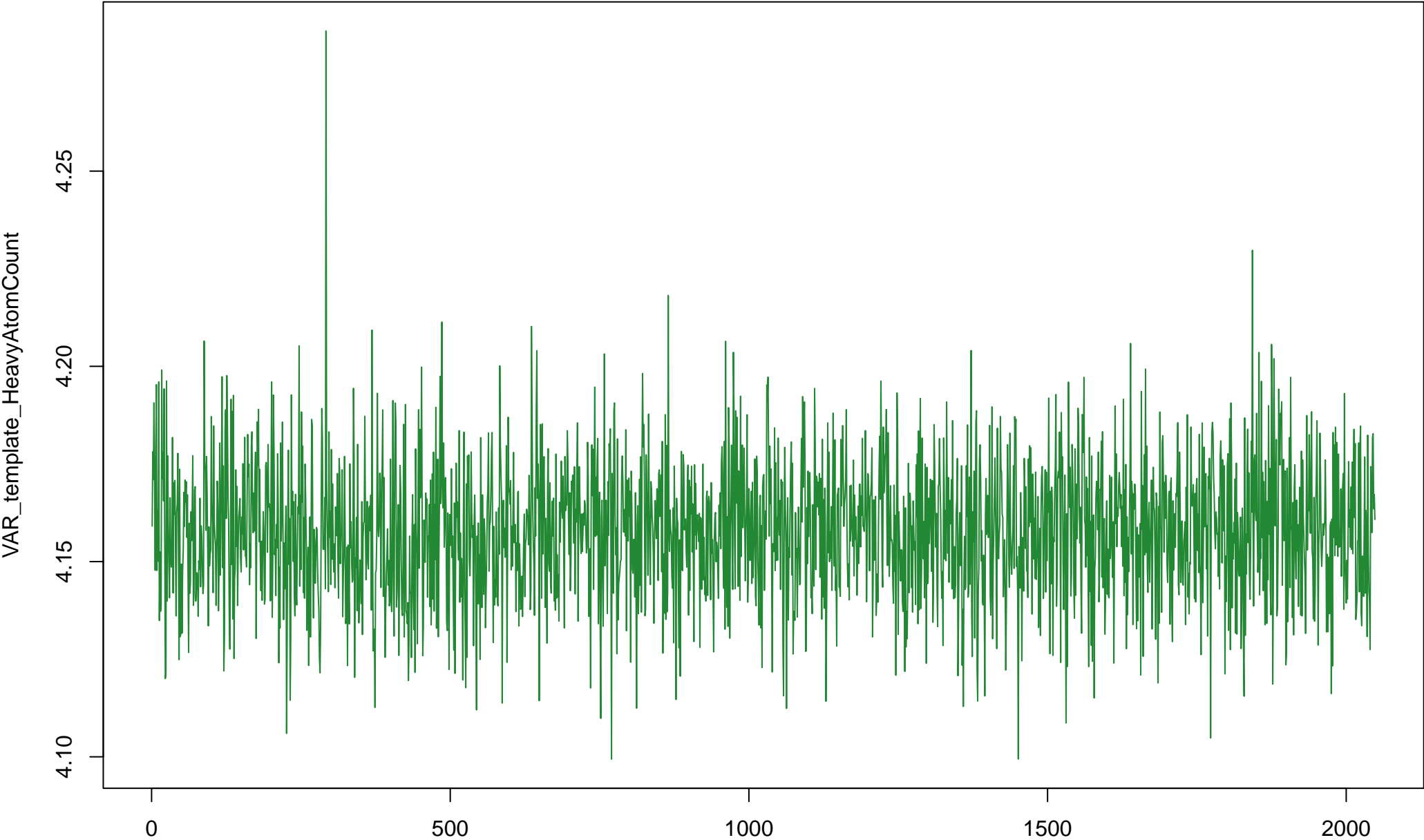
VAR_docked_HeavyAtomCount
ESS = 1650 | BMK = 0.0585 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0



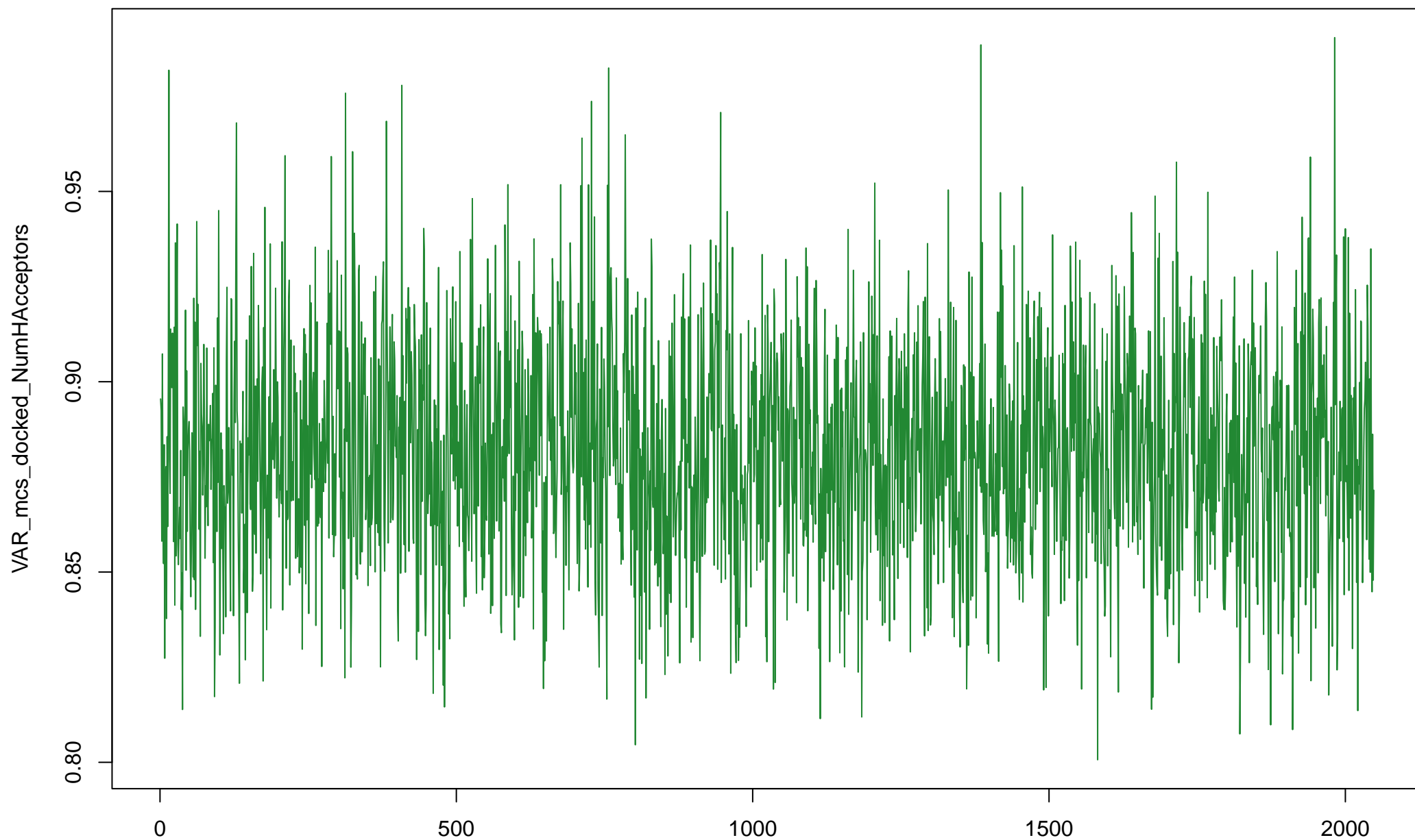
VAR_mcs_RingCount
ESS = 2050 | BMK = 0.0601 | MCSE(6.27) = 2.34 | stat: FALSE | burn: 0



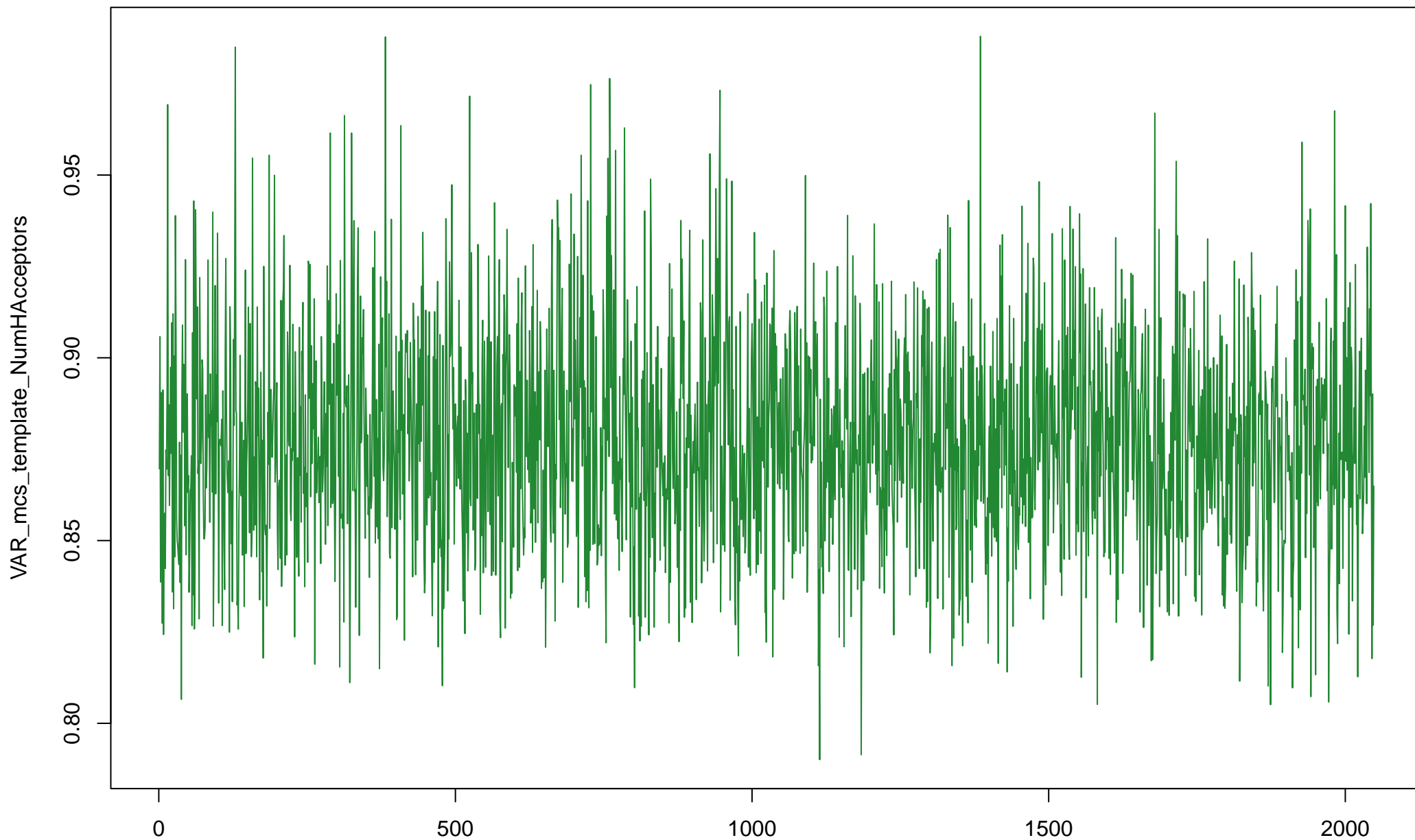
VAR_template_HeavyAtomCount
ESS = 1890 | BMK = 0.0541 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0



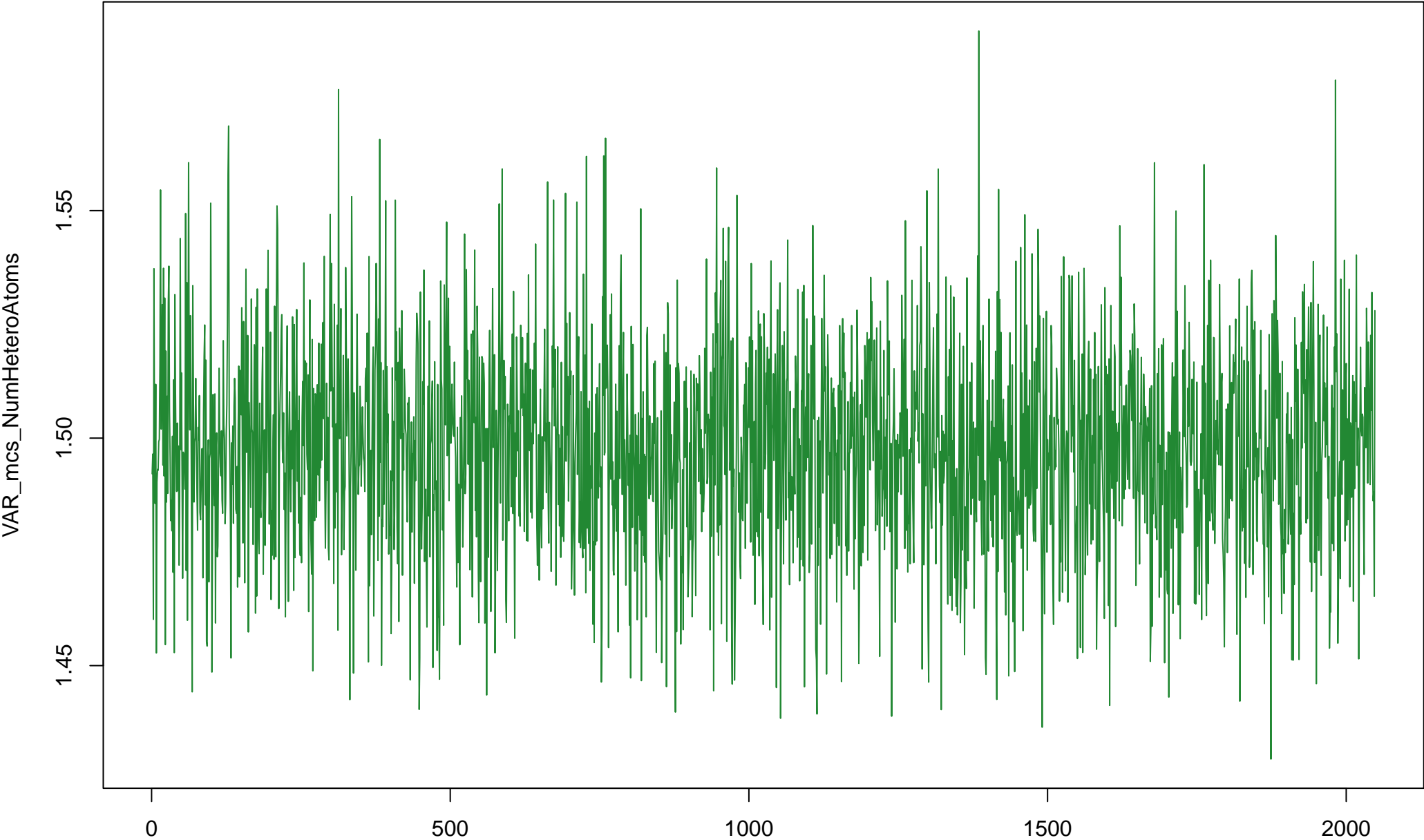
VAR_mcs_docked_NumHAcceptors
ESS = 1740 | BMK = 0.0588 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0



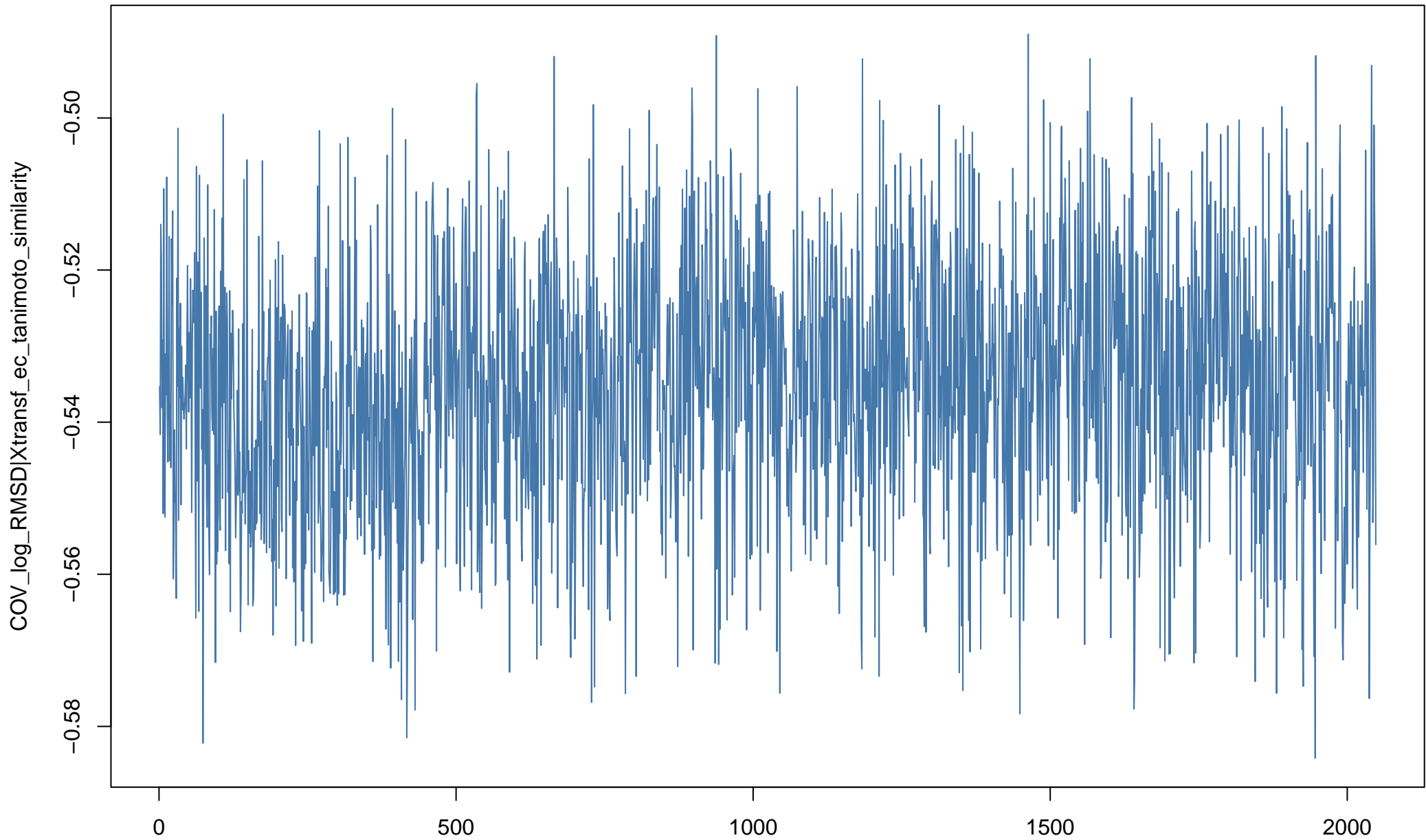
VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0749 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0



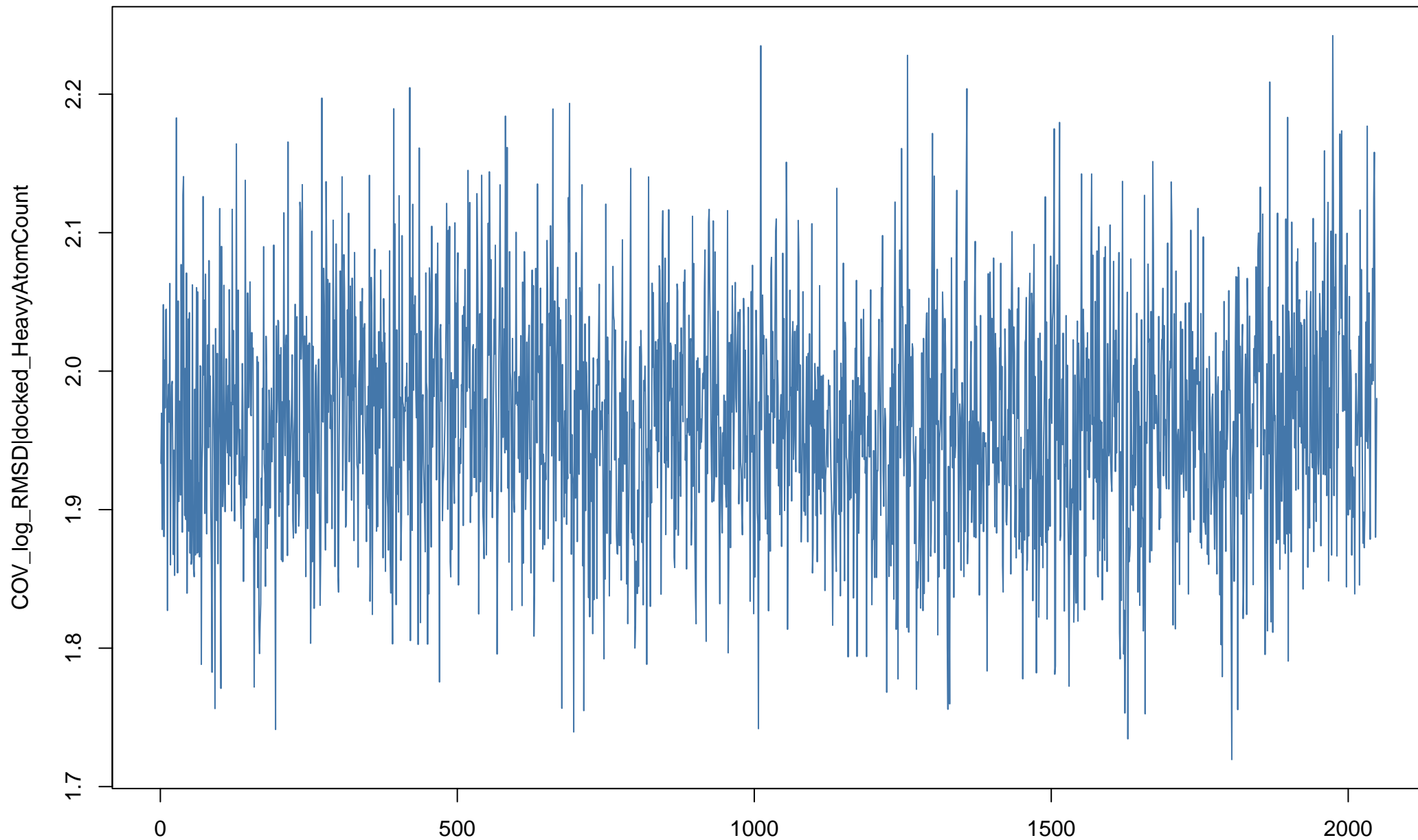
VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.051 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0



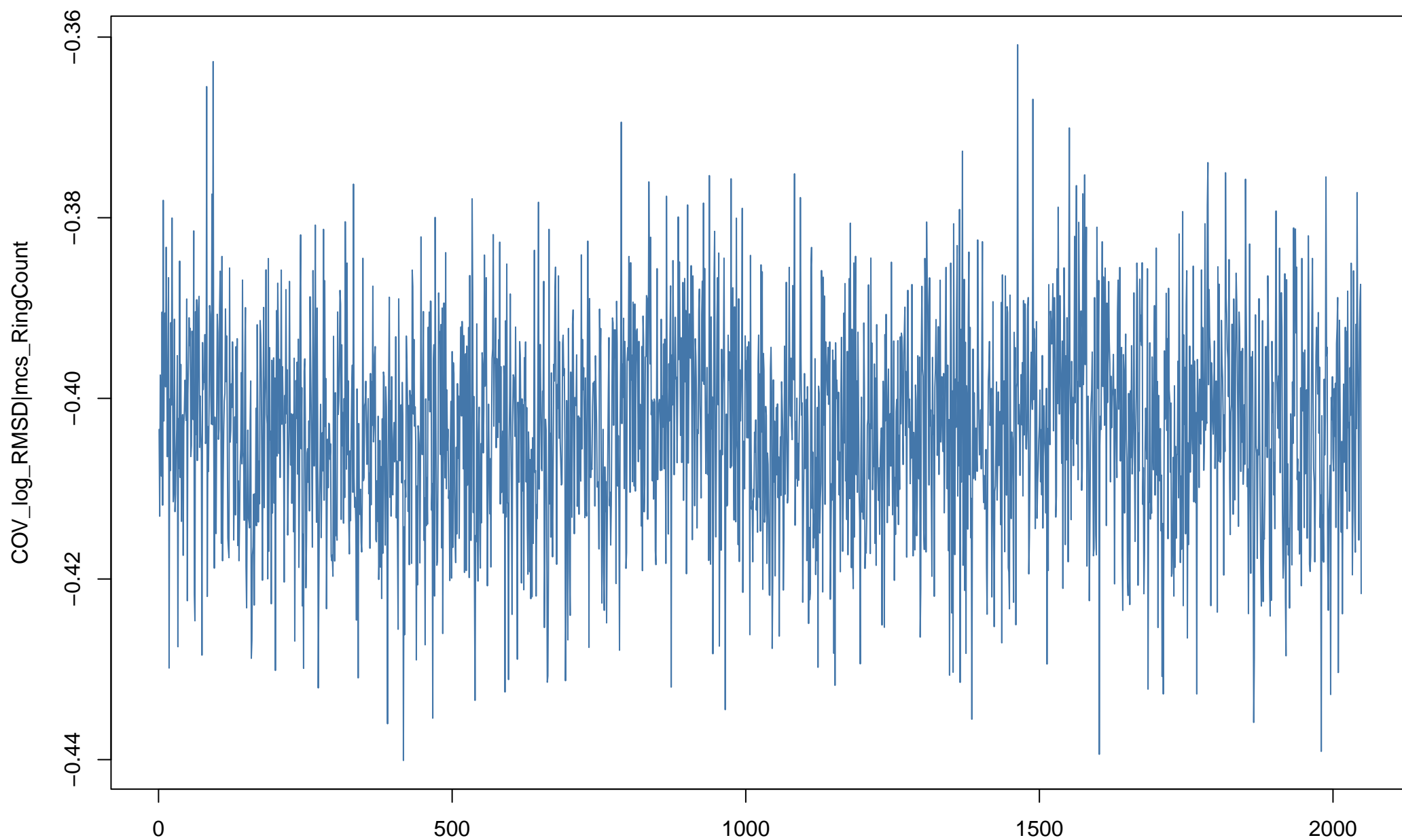
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 560 | BMK = 0.0789 | MCSE(6.27) = 3.79 | stat: FALSE | burn: 0



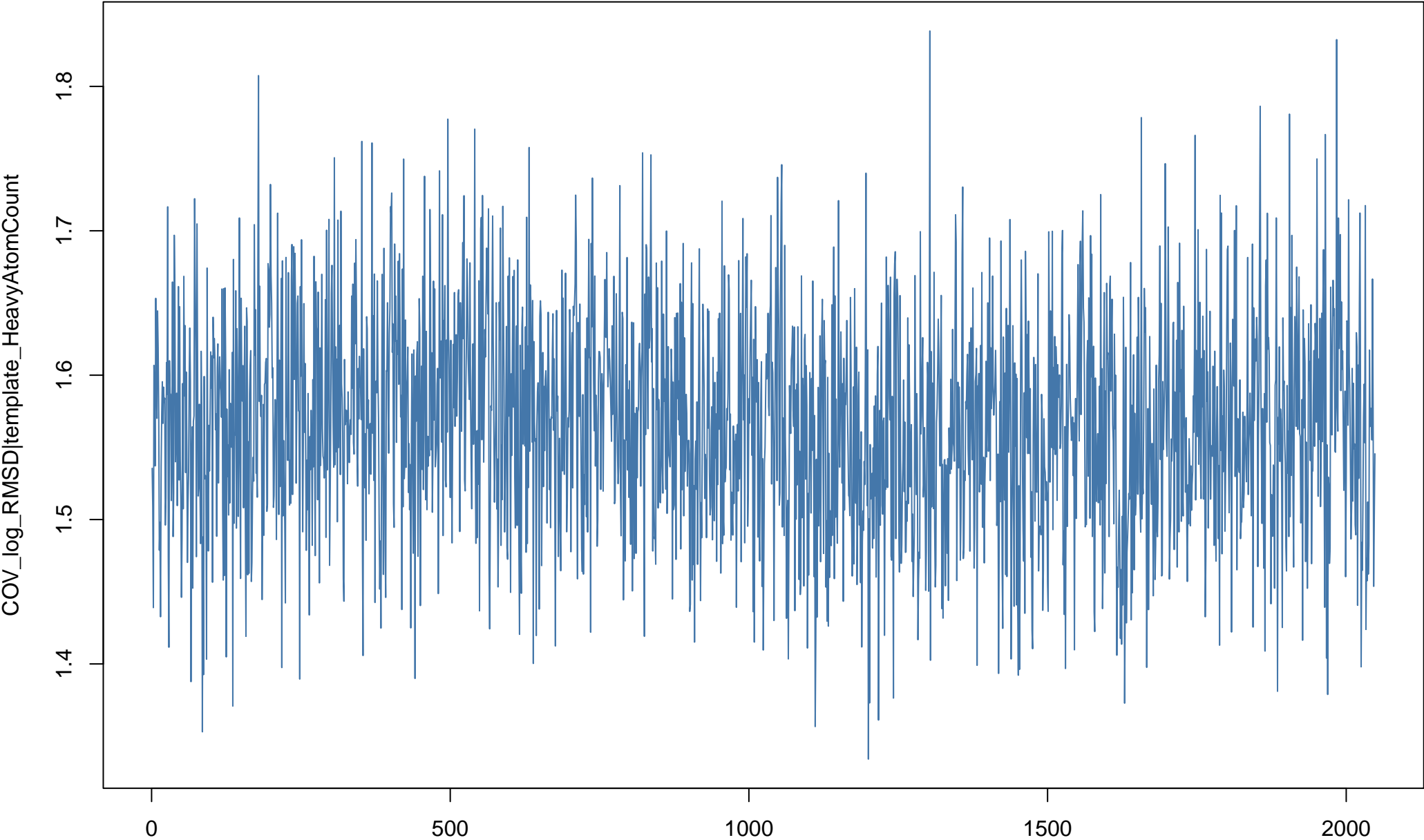
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1610 | BMK = 0.0423 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0



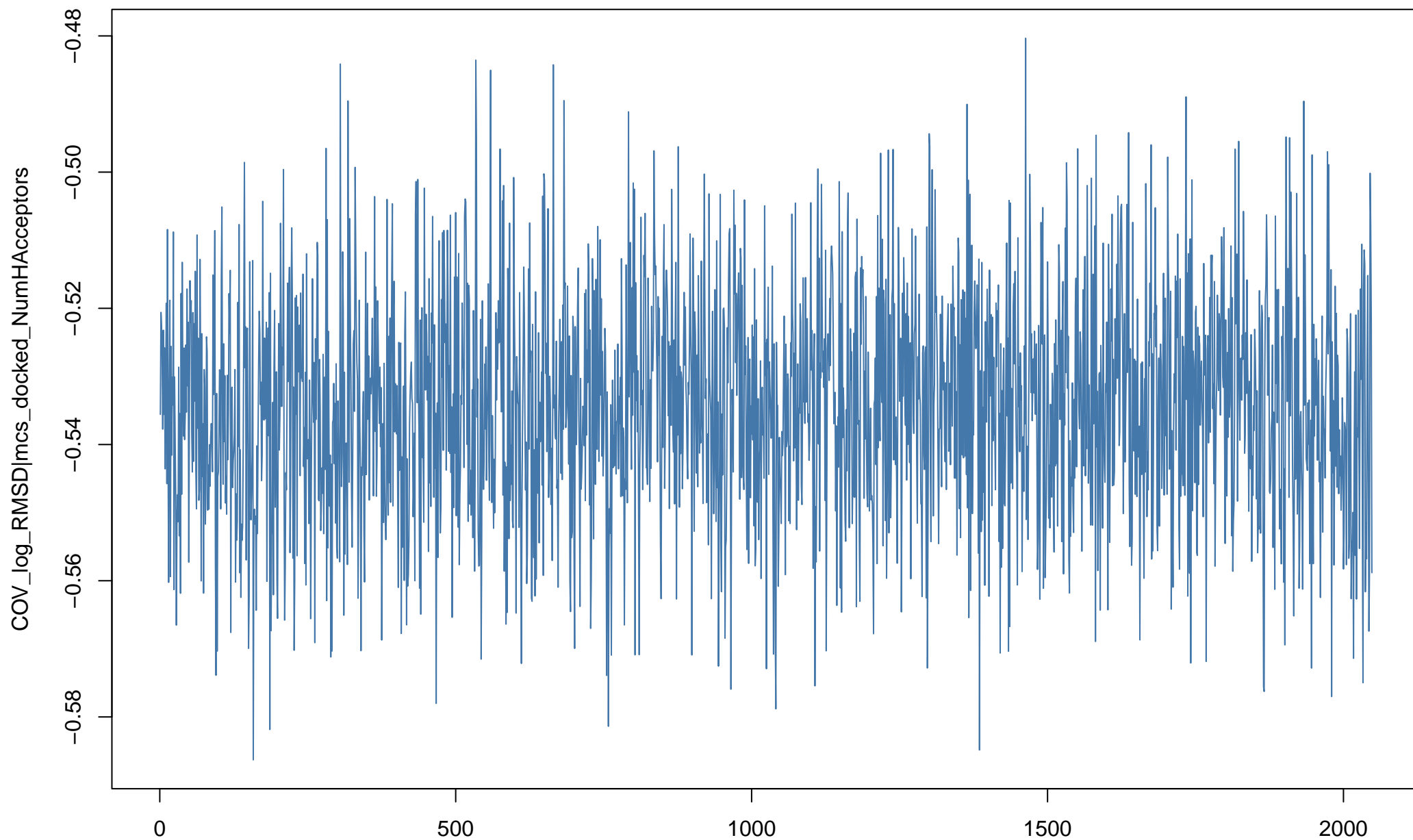
COV_log_RMSD|mcs_RingCount
ESS = 1290 | BMK = 0.0331 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0



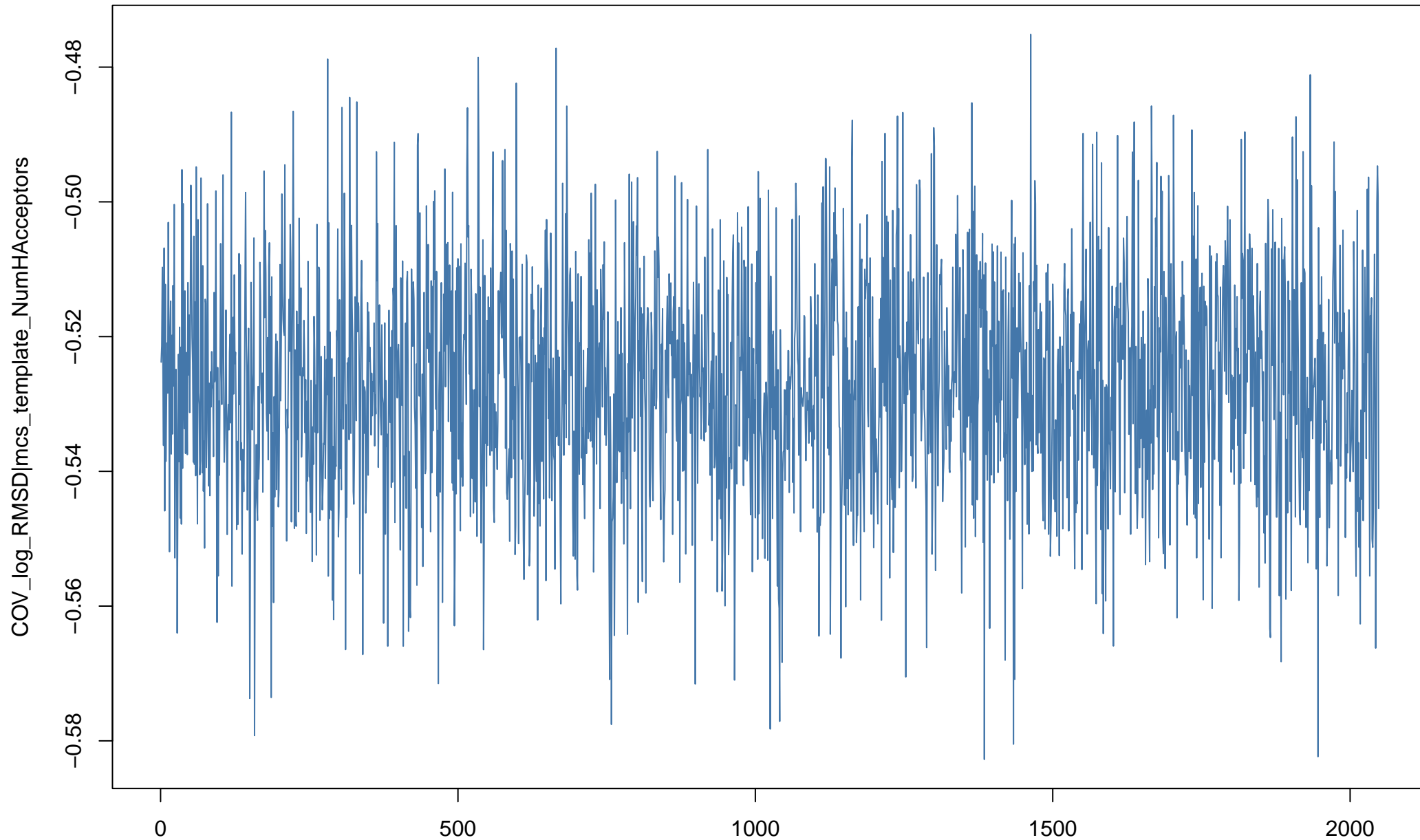
COV_log_RMSD|template_HeavyAtomCount
ESS = 1240 | BMK = 0.085 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0



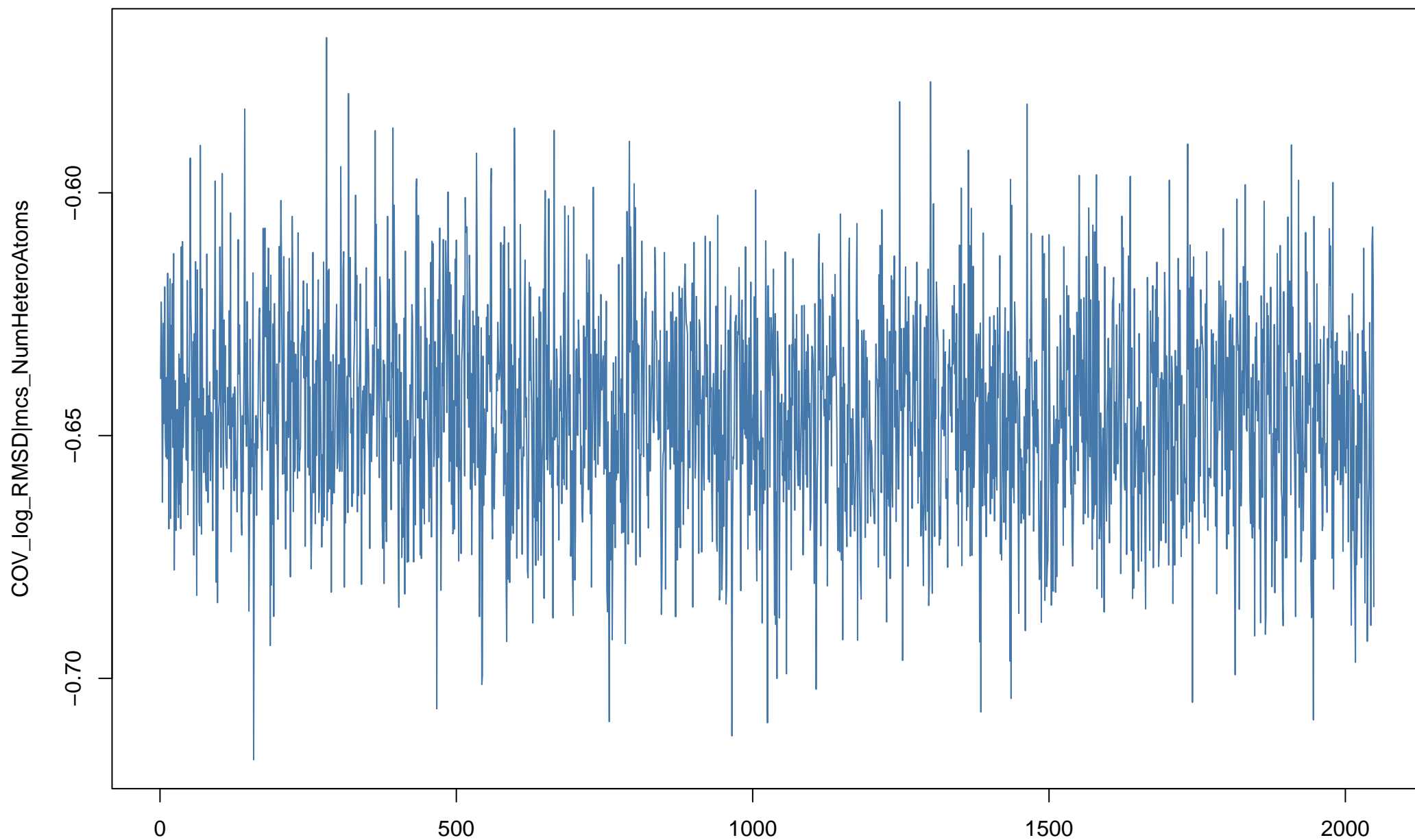
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 1650 | BMK = 0.0485 | MCSE(6.27) = 2.46 | stat: FALSE | burn: 0



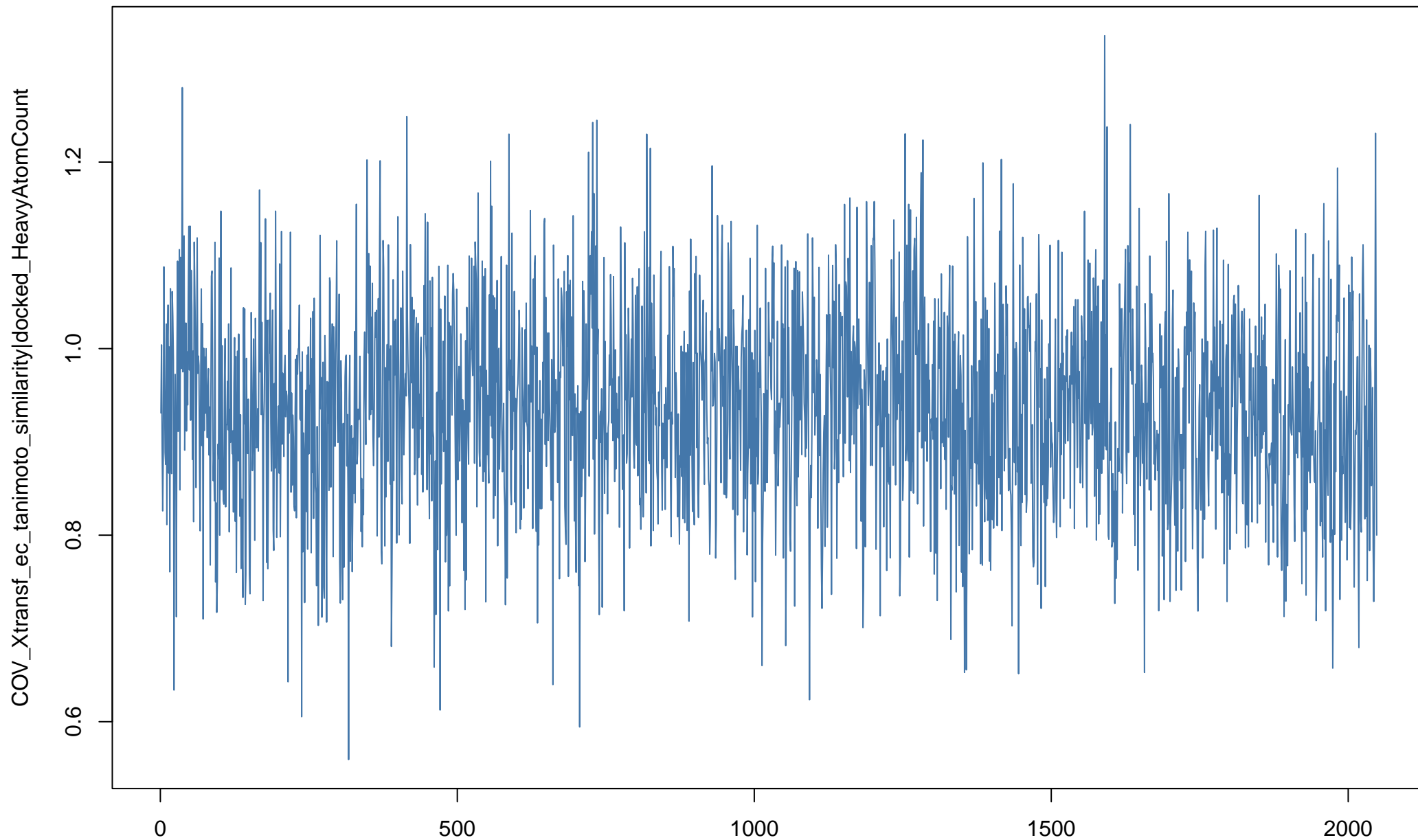
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 1680 | BMK = 0.0365 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0



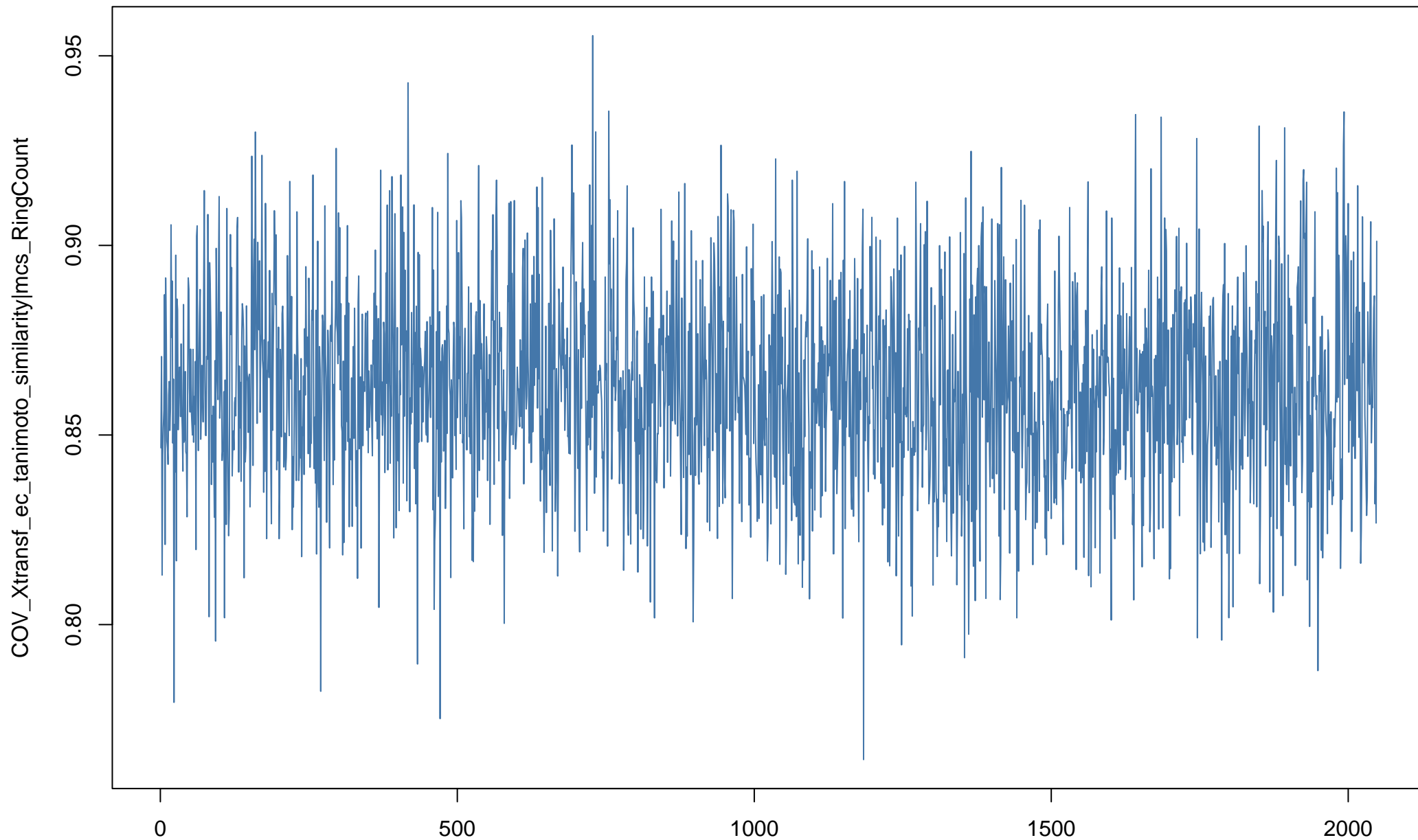
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1720 | BMK = 0.0585 | MCSE(6.27) = 2.07 | stat: FALSE | burn: 0



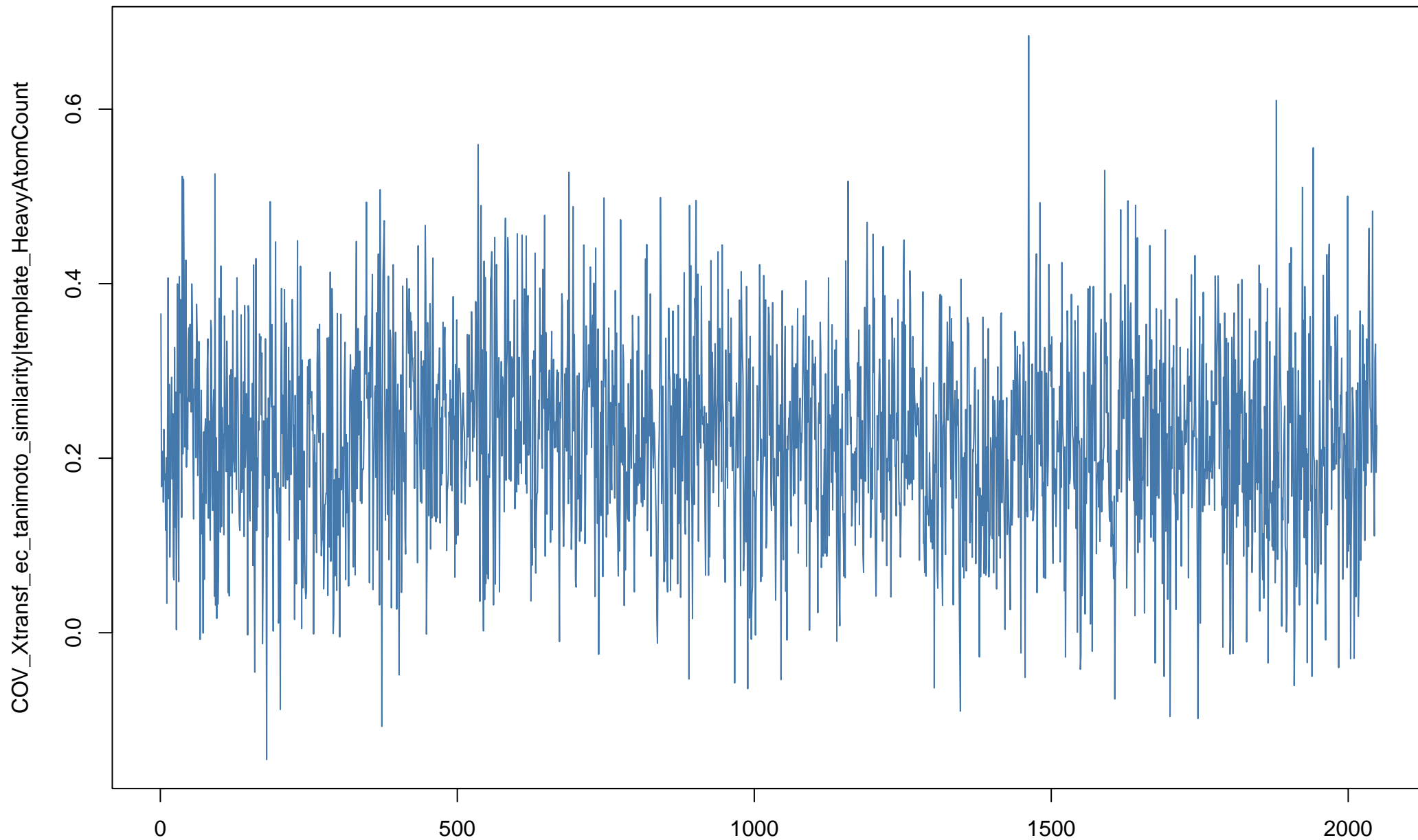
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1510 | BMK = 0.0473 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0



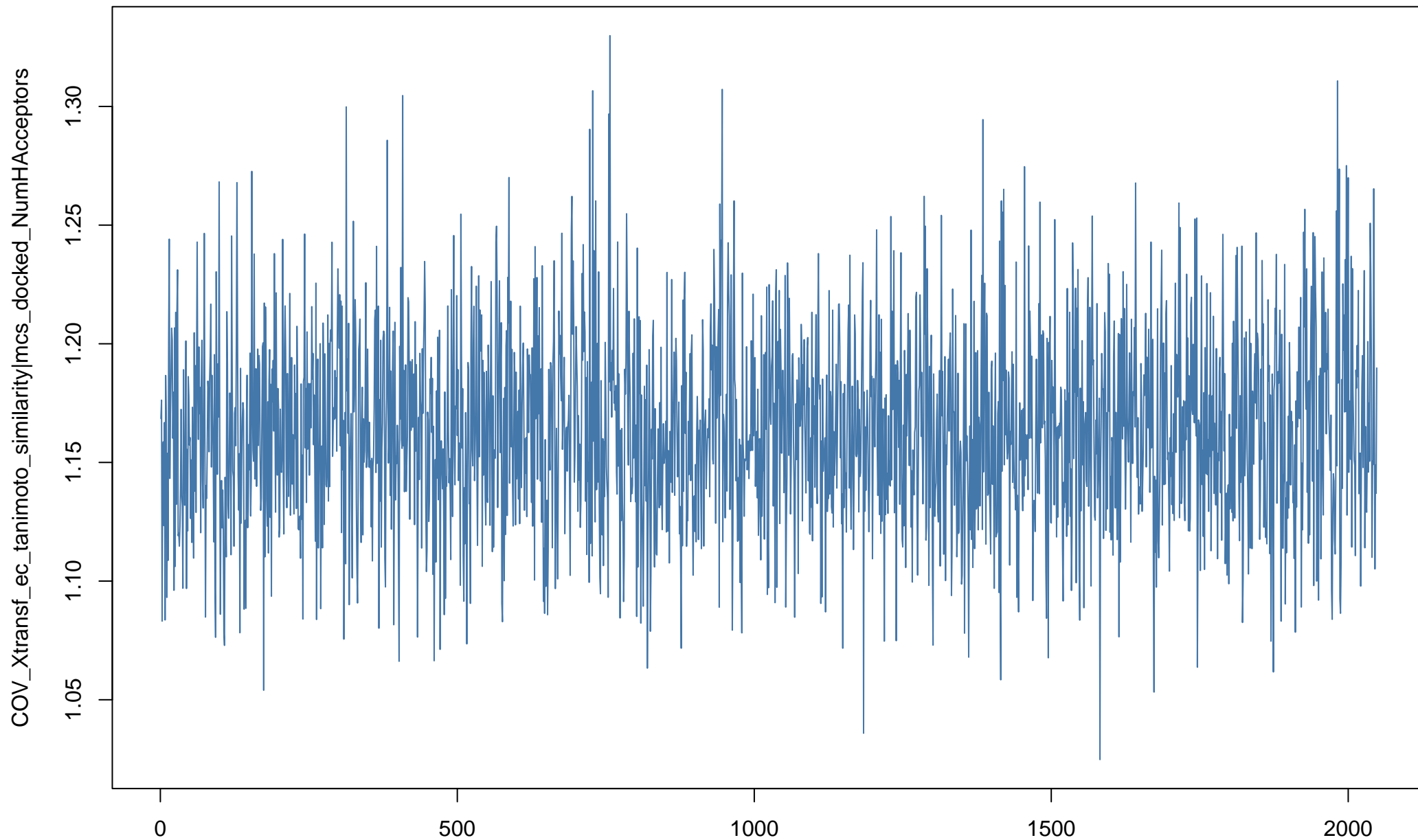
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1810 | BMK = 0.0765 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0



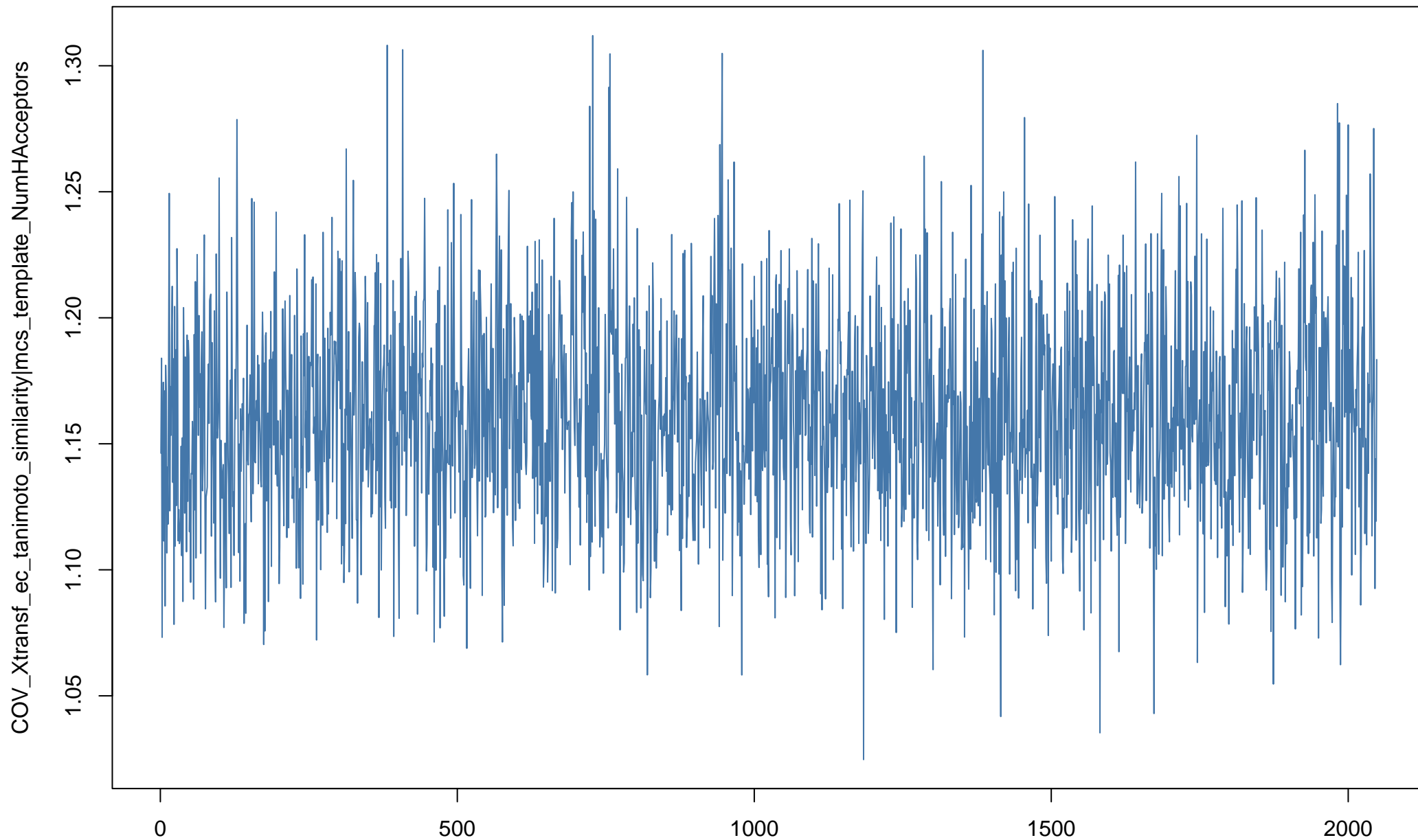
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1590 | BMK = 0.0711 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0



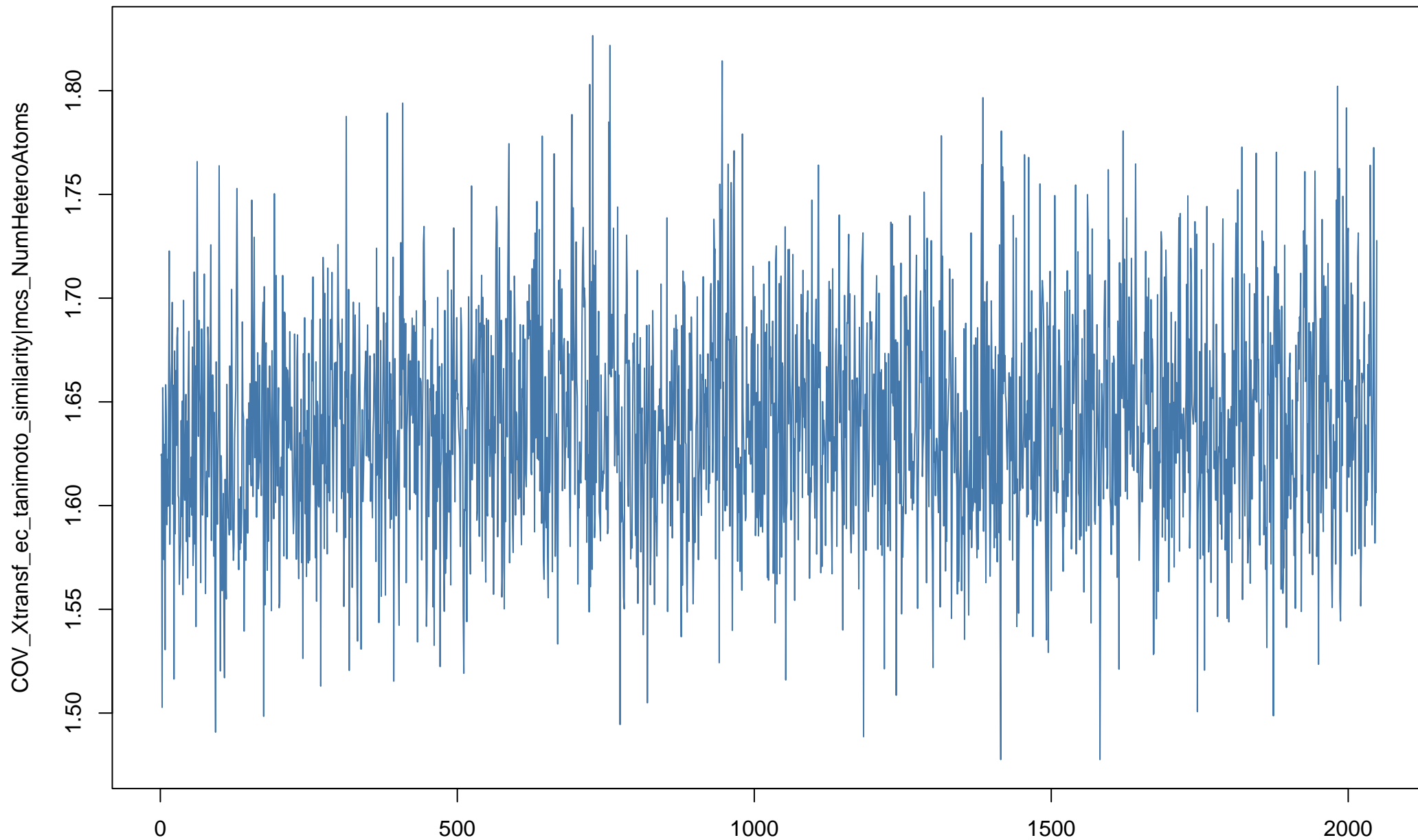
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 1700 | BMK = 0.0439 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0



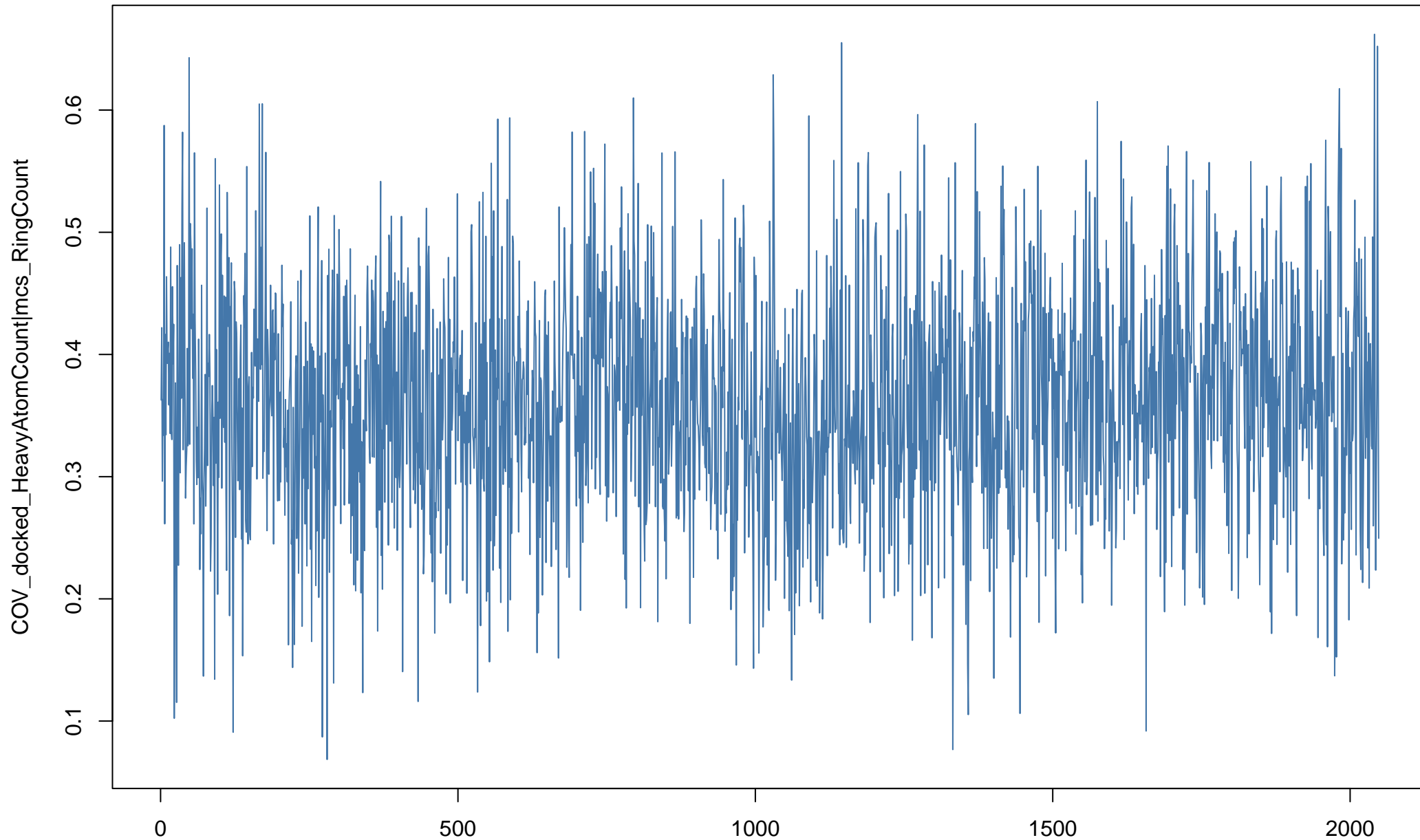
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 1810 | BMK = 0.046 | MCSE(6.27) = 2.13 | stat: FALSE | burn: 0



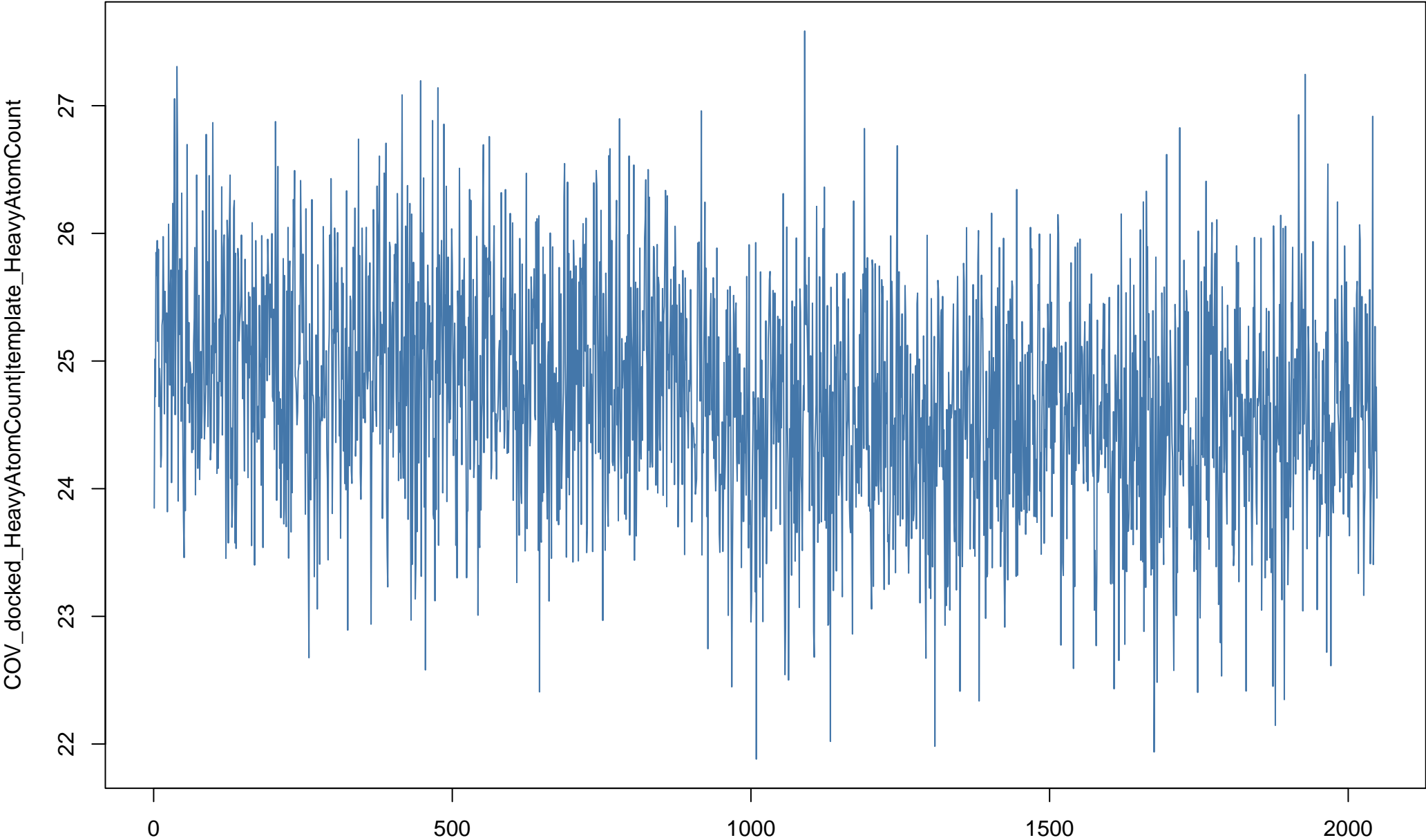
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1700 | BMK = 0.0567 | MCSE(6.27) = 2.79 | stat: FALSE | burn: 0



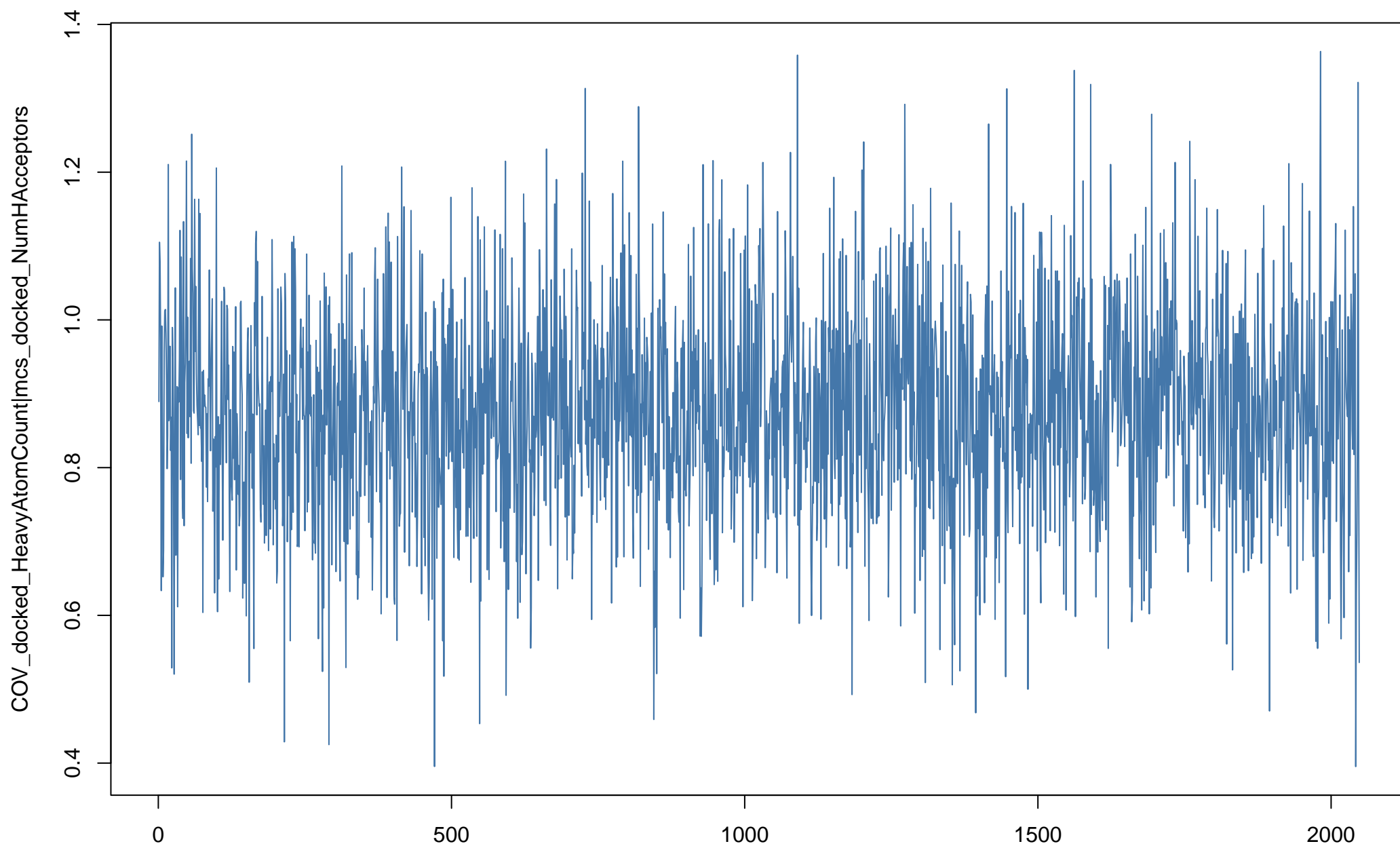
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1680 | BMK = 0.0438 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0



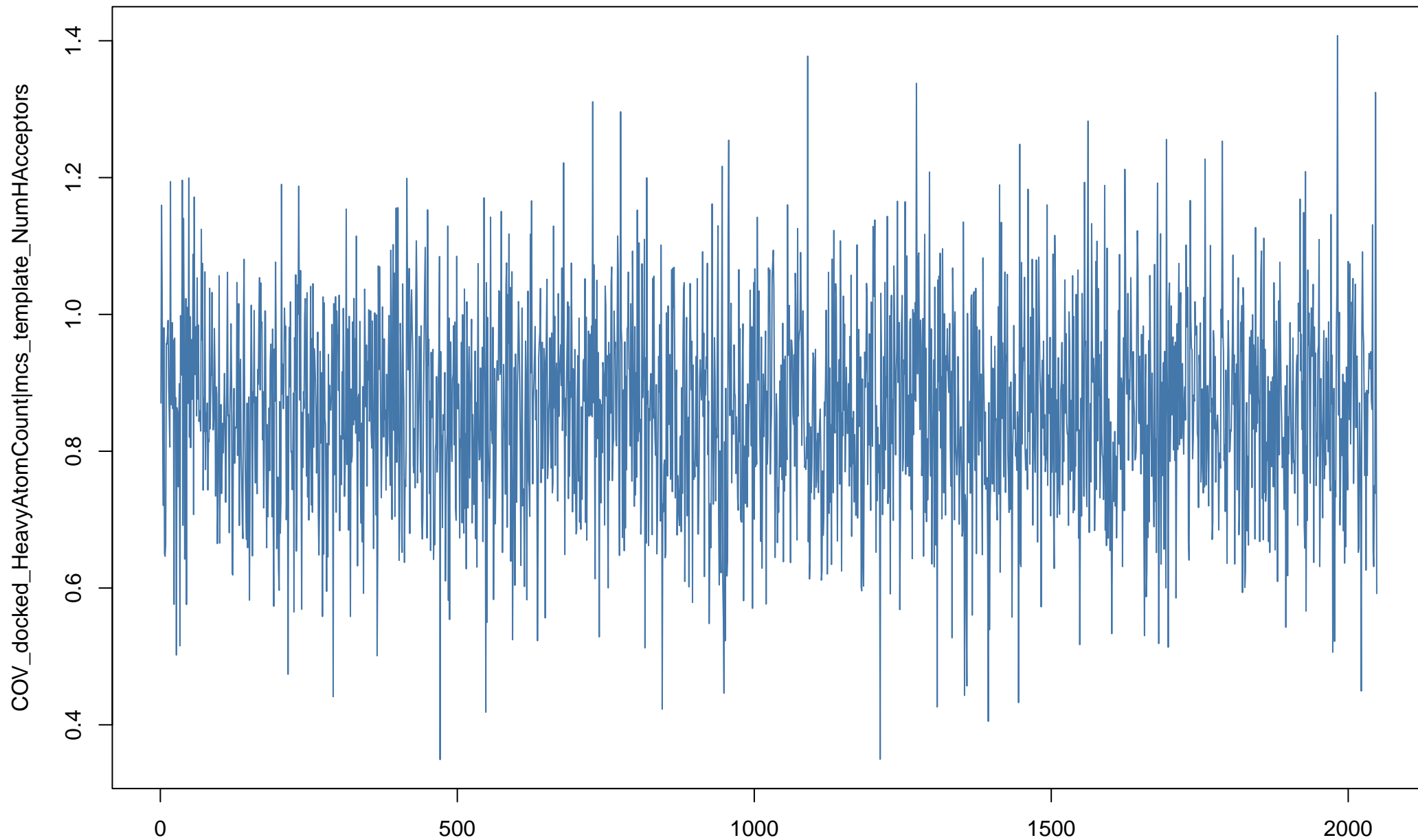
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 194 | BMK = 0.167 | MCSE(6.27) = 4.56 | stat: FALSE | burn: 0



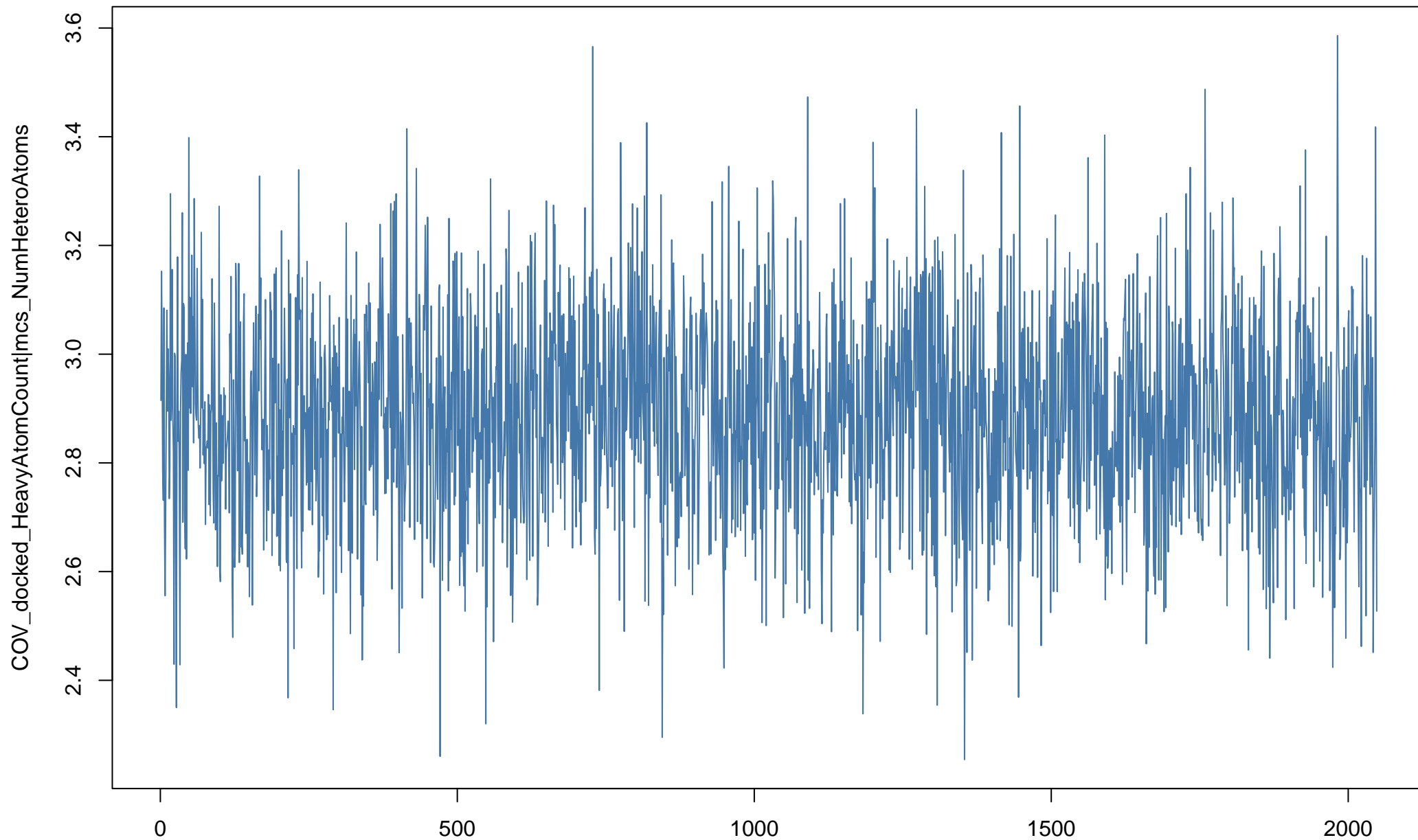
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0512 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0



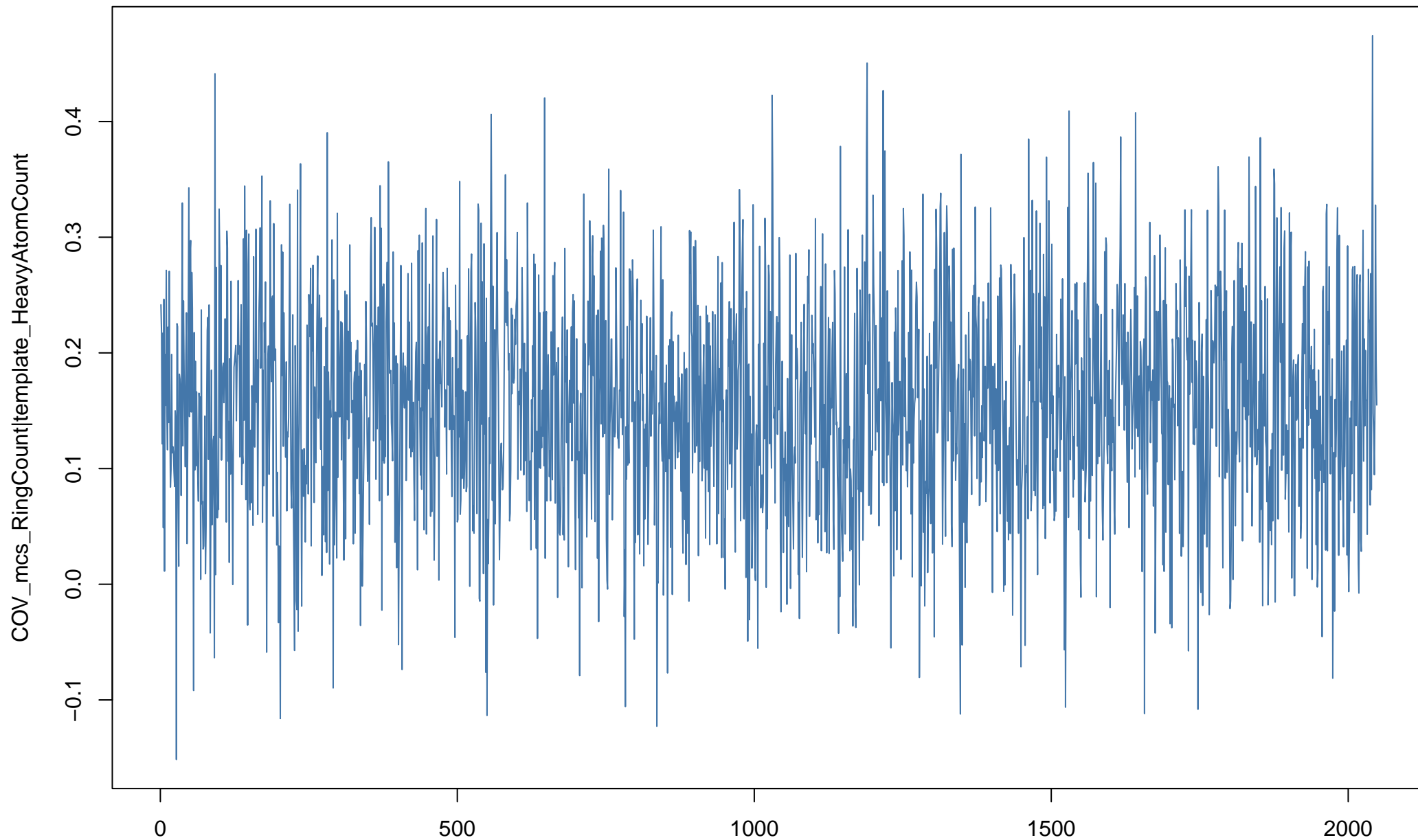
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0447 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0



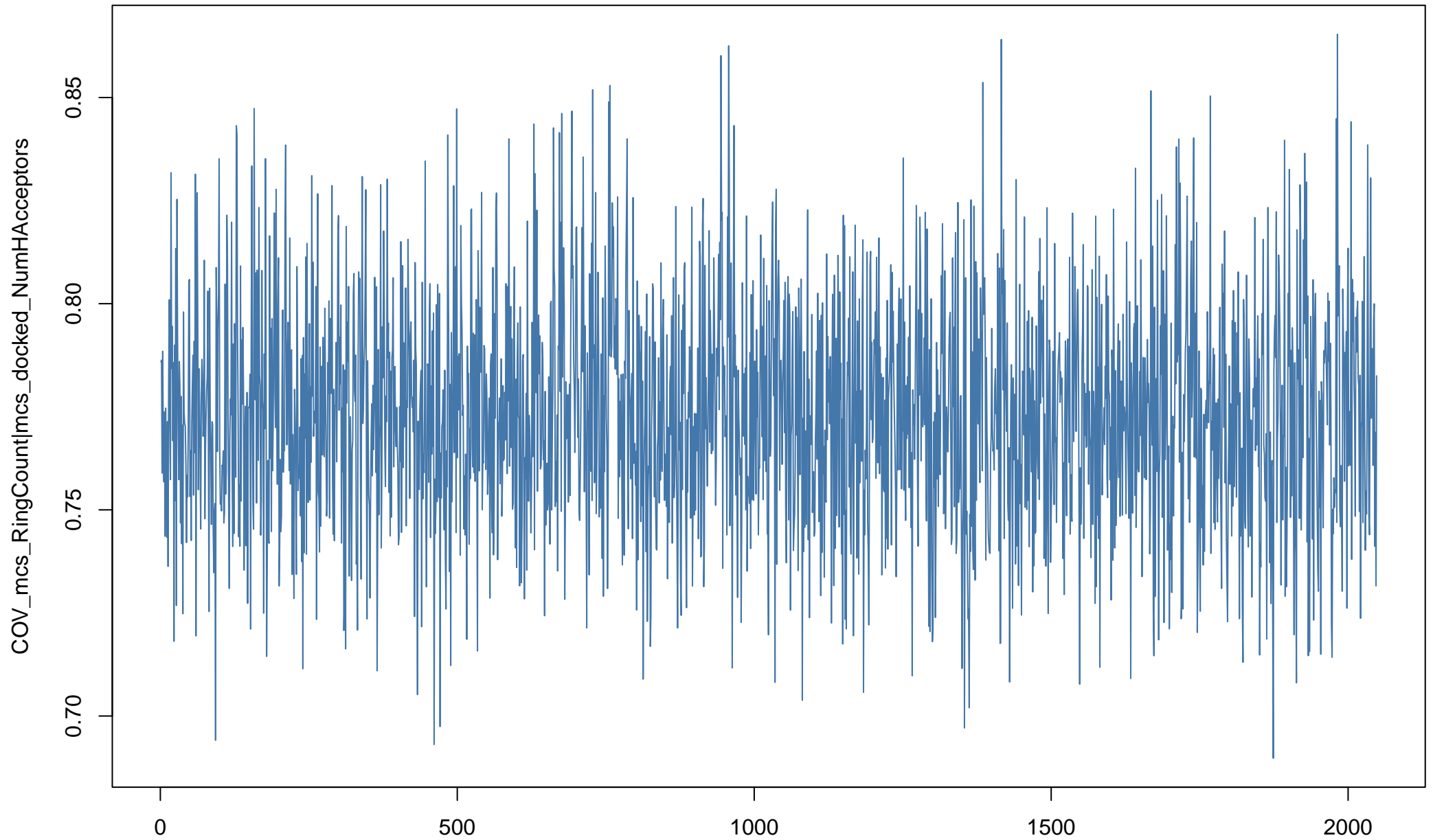
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0443 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



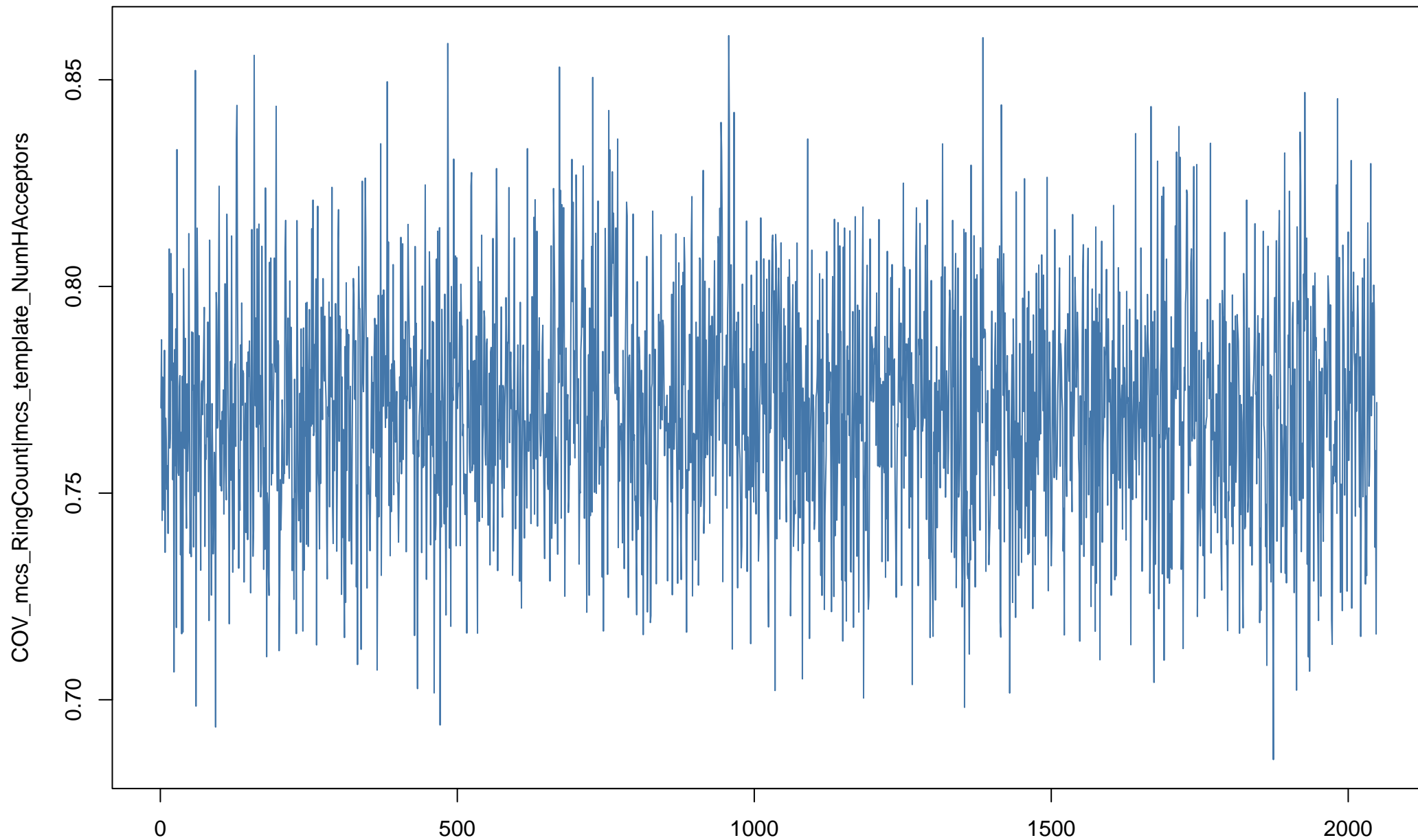
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1780 | BMK = 0.0388 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



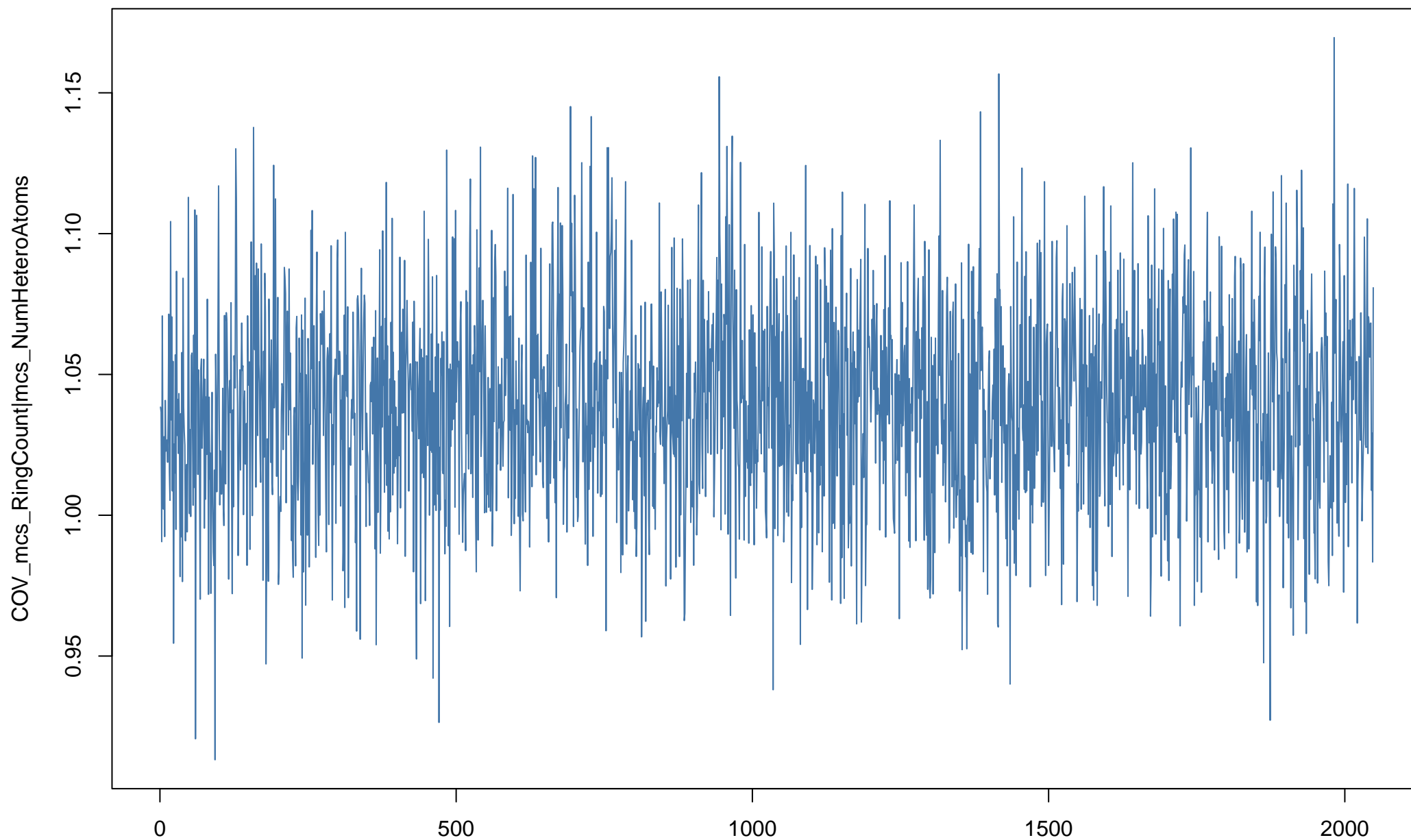
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 1770 | BMK = 0.0553 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



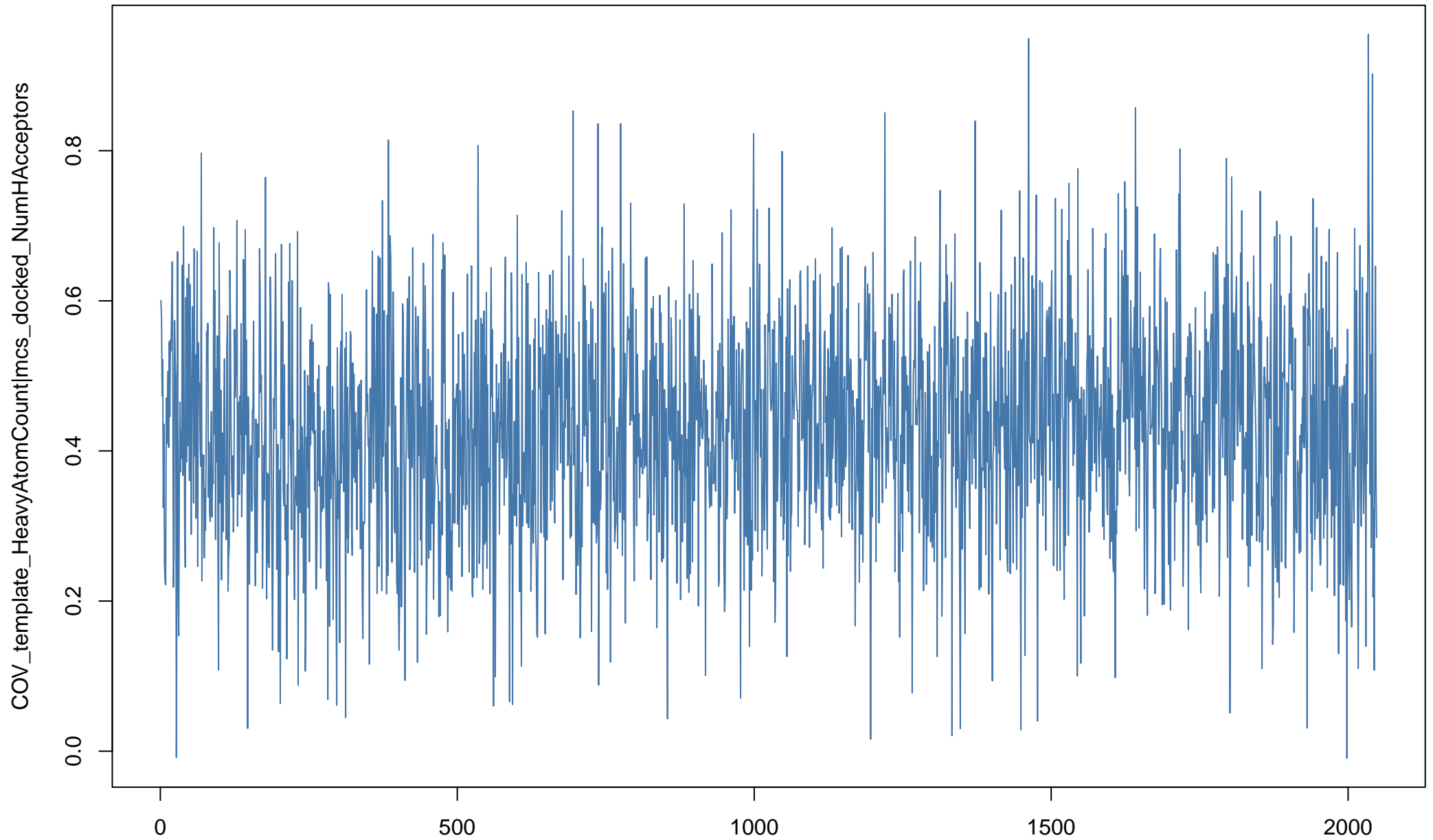
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0503 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0



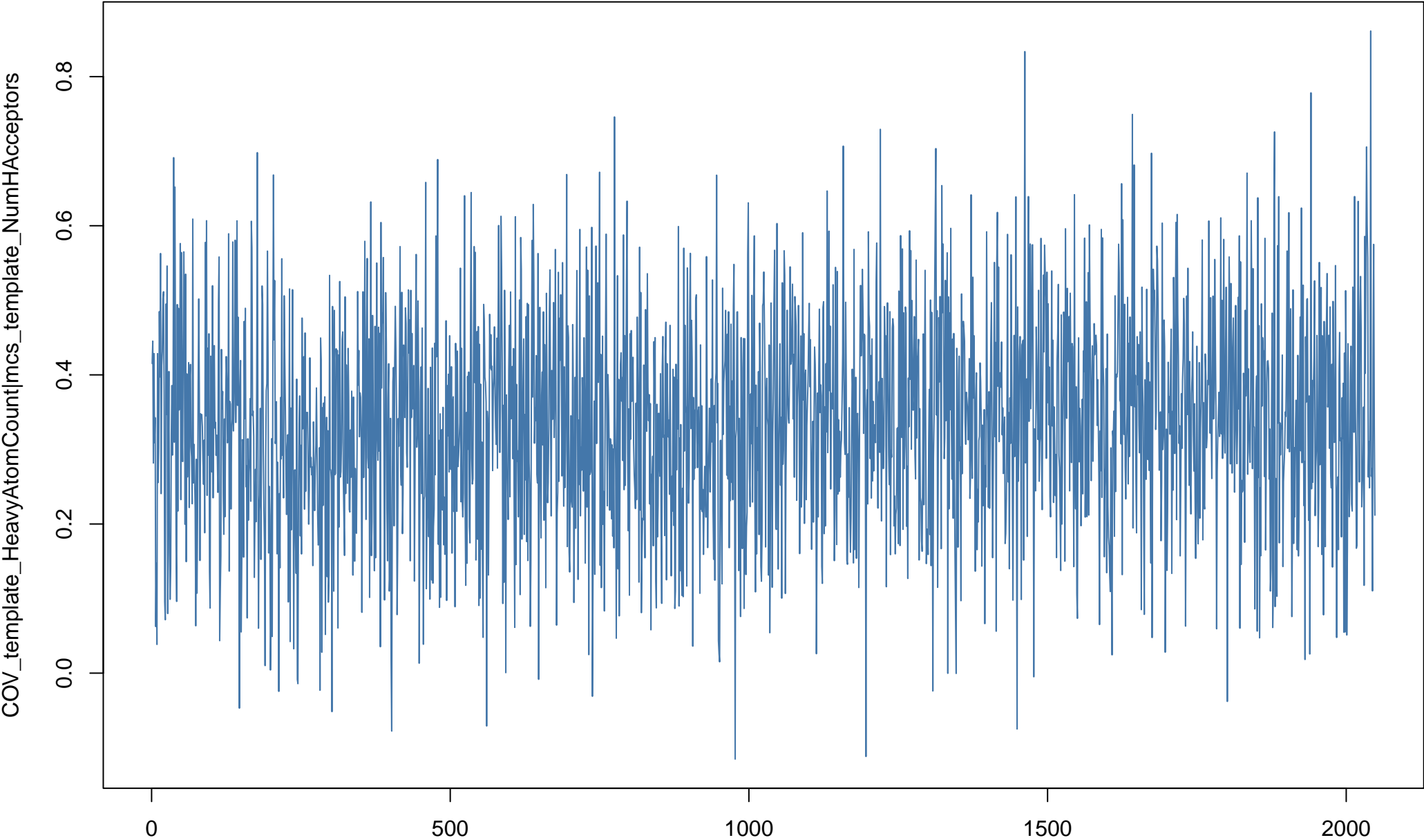
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 1800 | BMK = 0.0531 | MCSE(6.27) = 2.38 | stat: FALSE | burn: 0



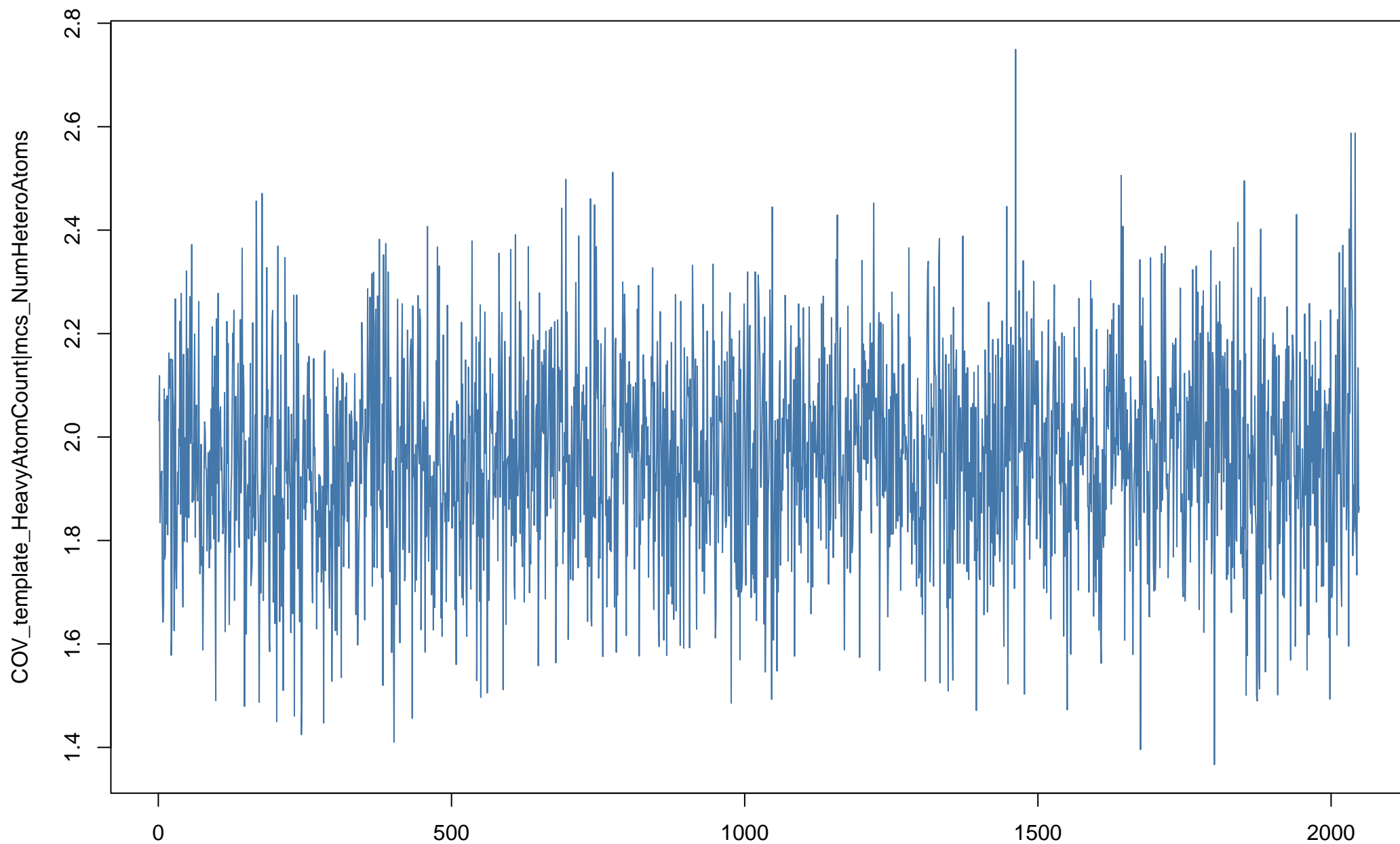
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0725 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0



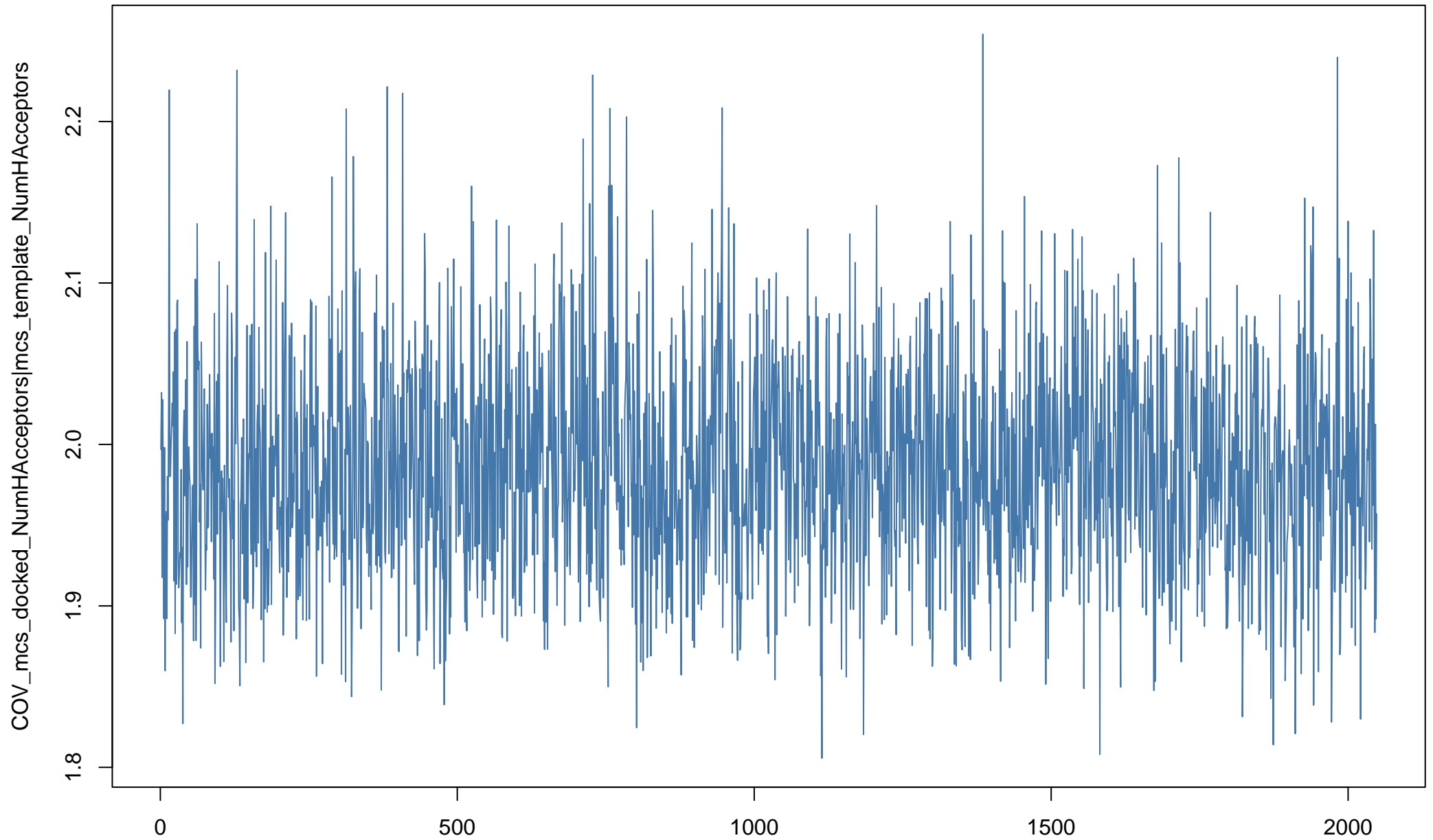
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.082 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0



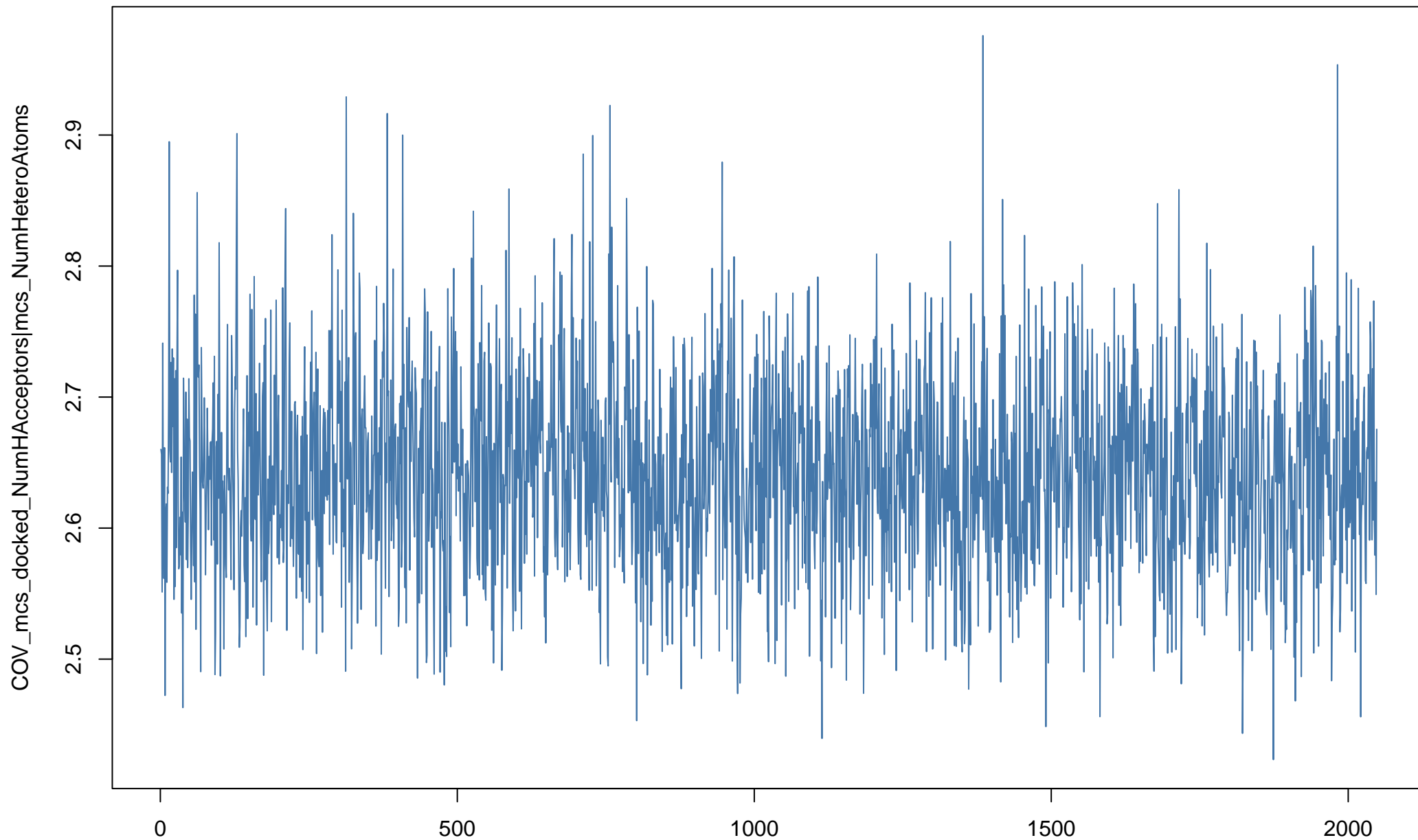
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0593 | MCSE(6.27) = 2.42 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 1820 | BMK = 0.069 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 1740 | BMK = 0.0642 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.066 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0

