

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.840980541800549

max MCSE = 14.8147315272357

all stationary: FALSE

burn: 2040

-- STATS 2D --

min ESS = 86.5364771651372

max BMK = 0.190268514173168

max MCSE = 5.11444627349547

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.799911400221765

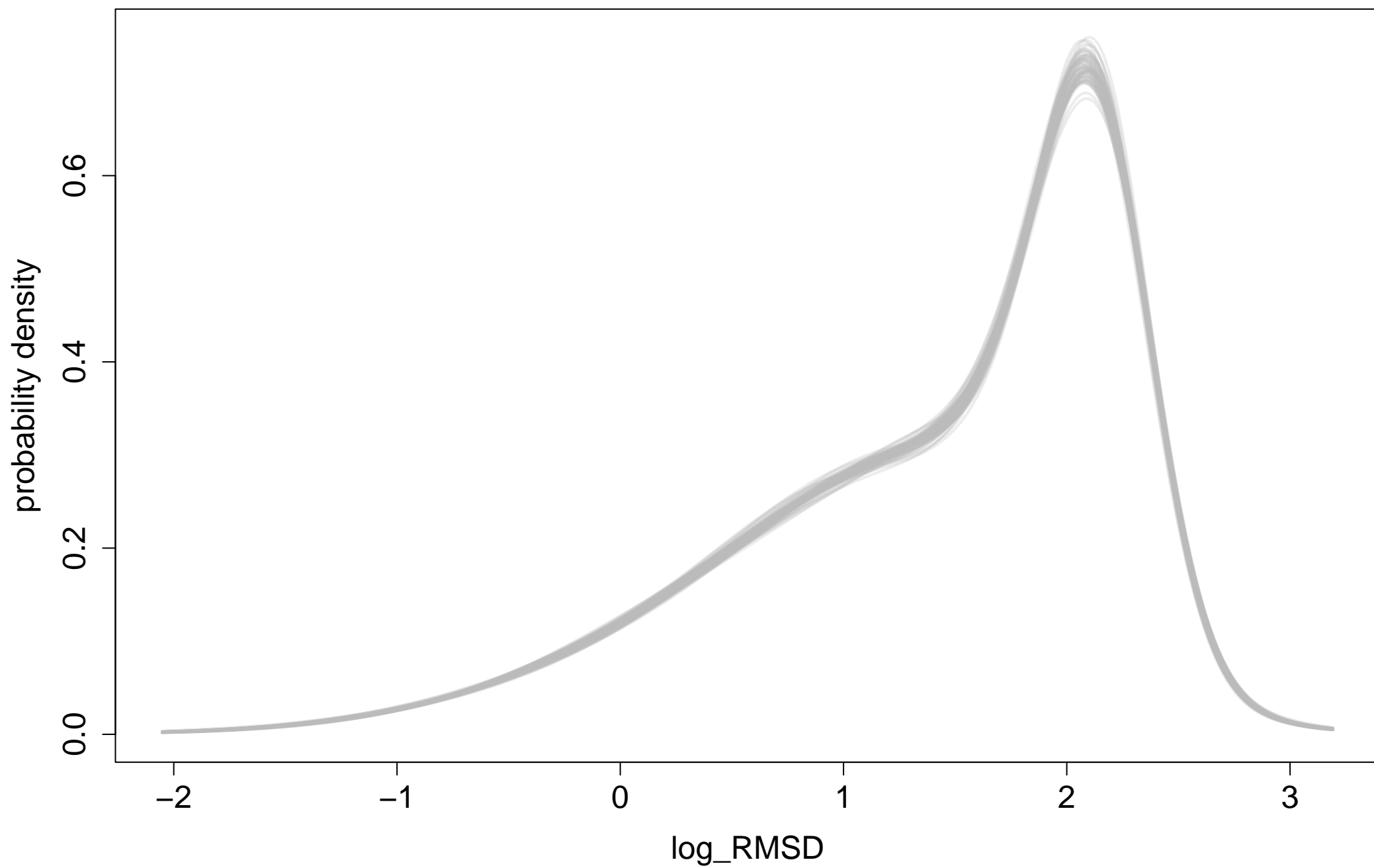
max MCSE = NaN

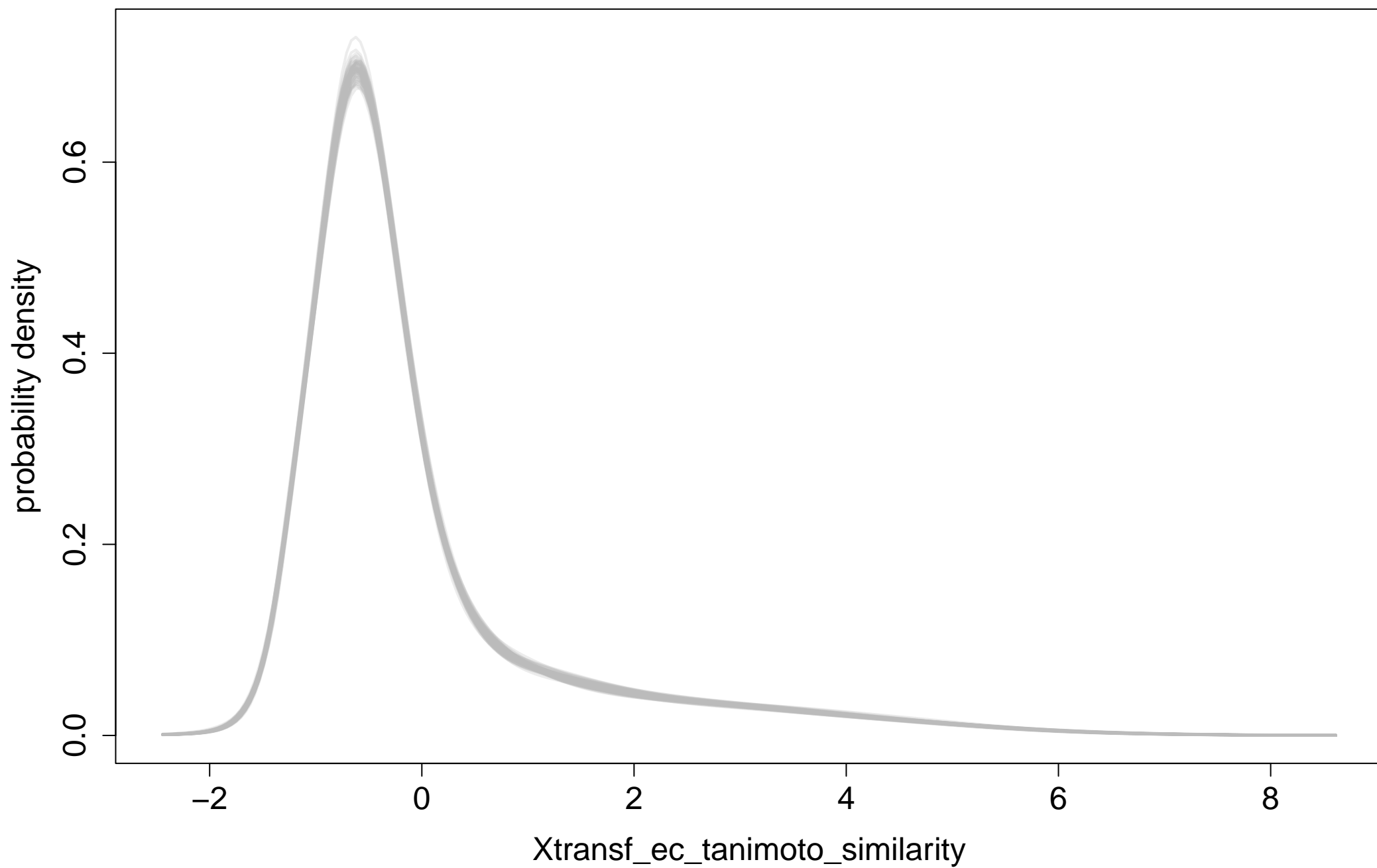
all stationary: FALSE

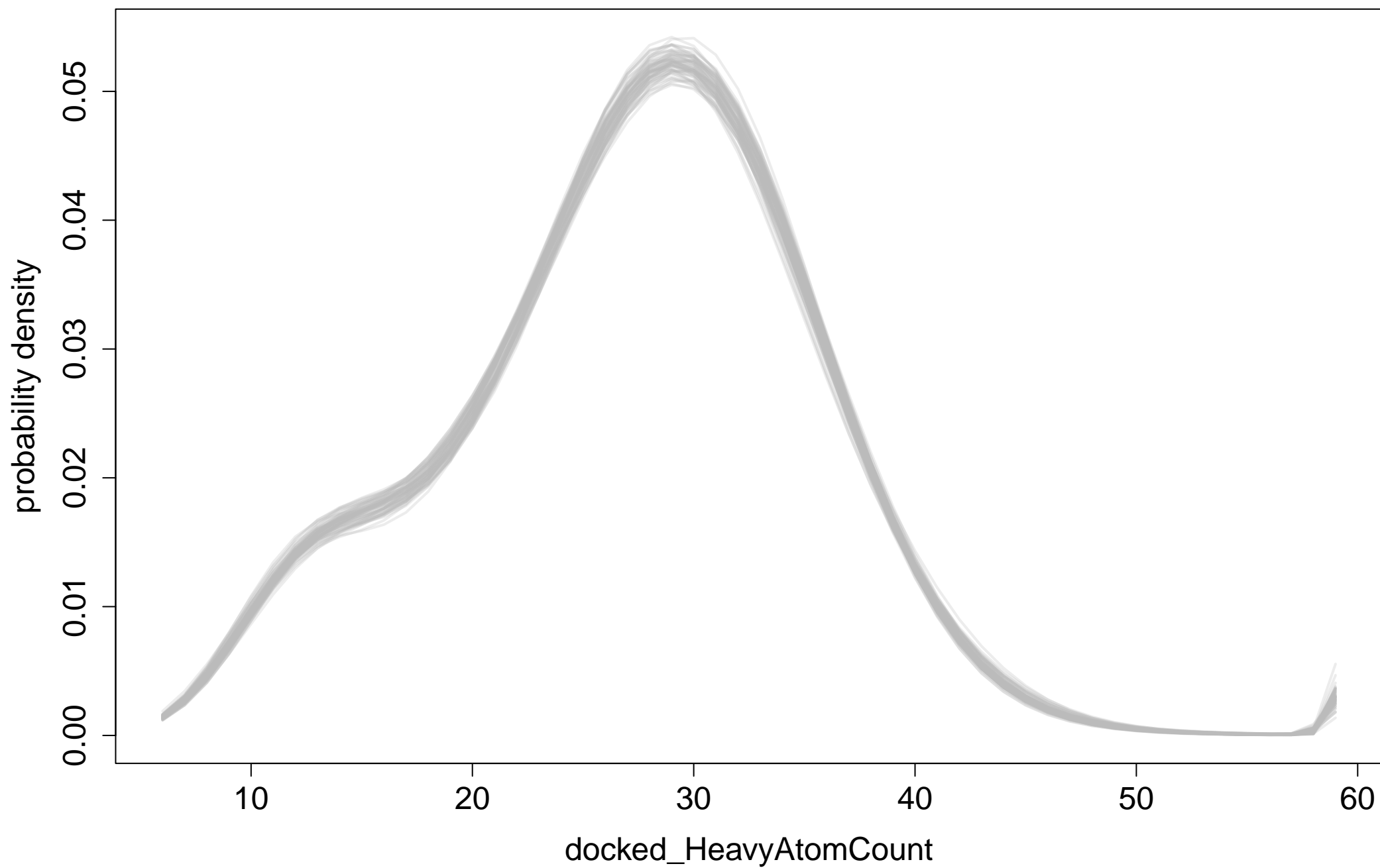
burn: 2040

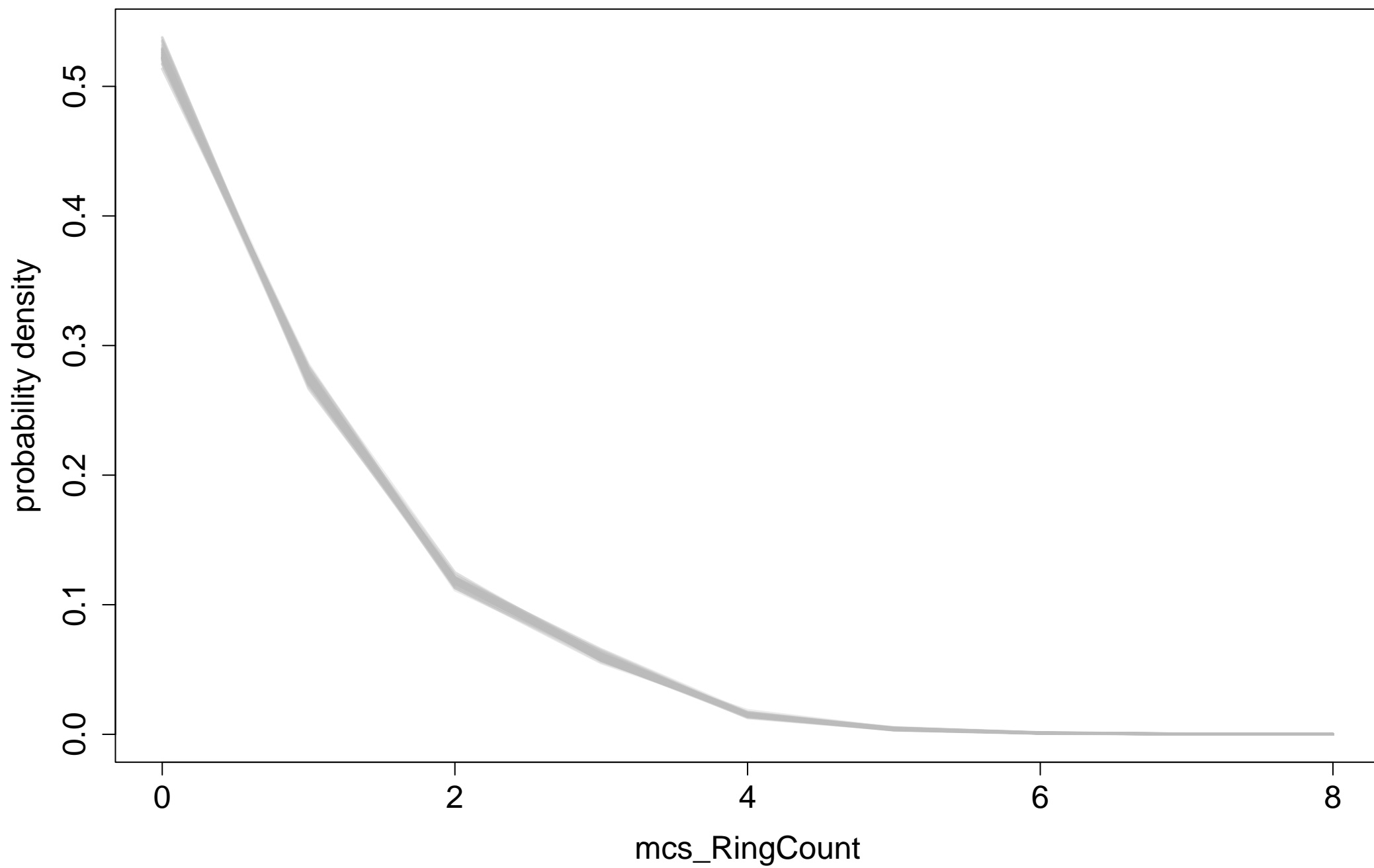
Occupied clusters: 45 of 91

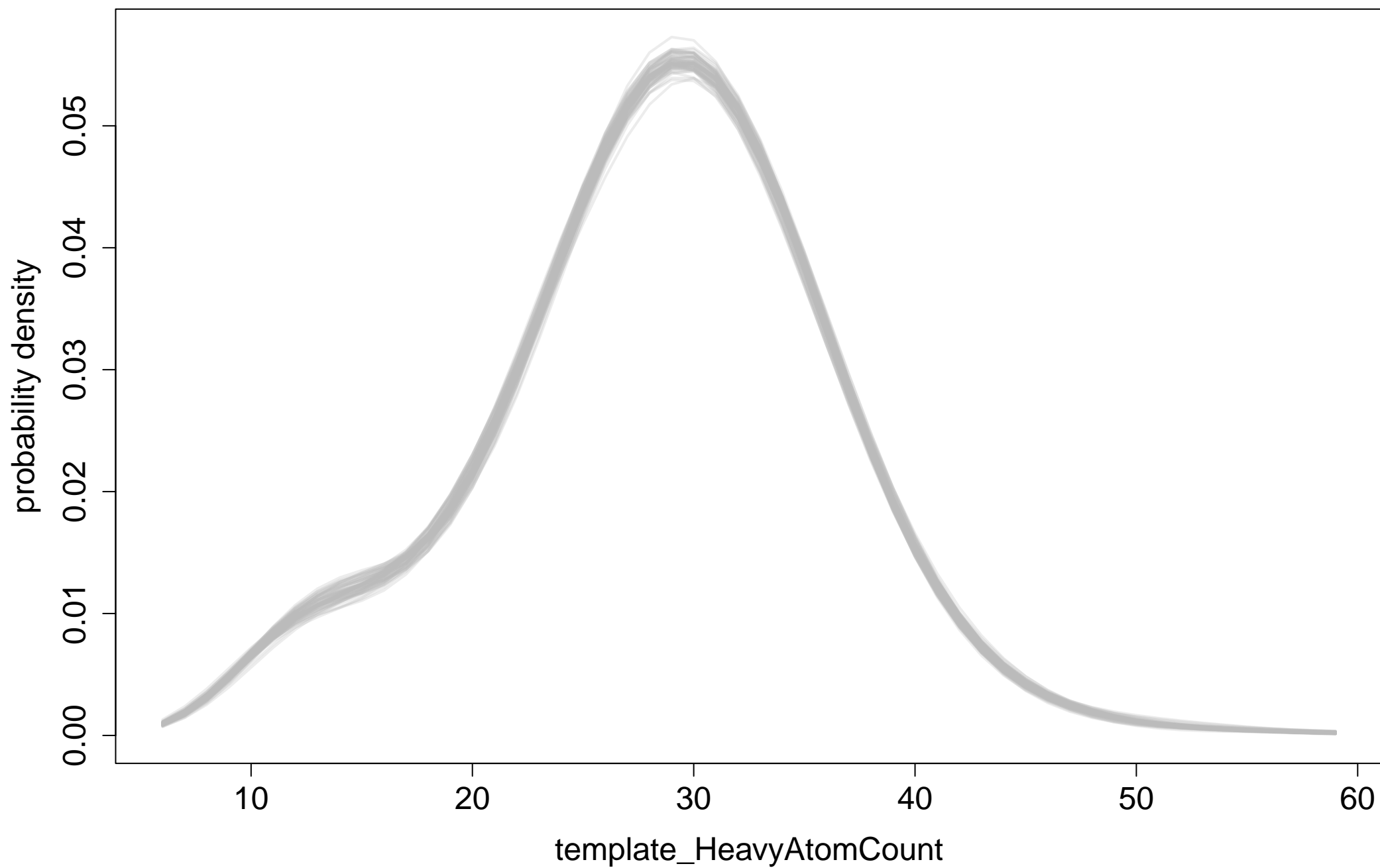
LL: -112000 +- 412

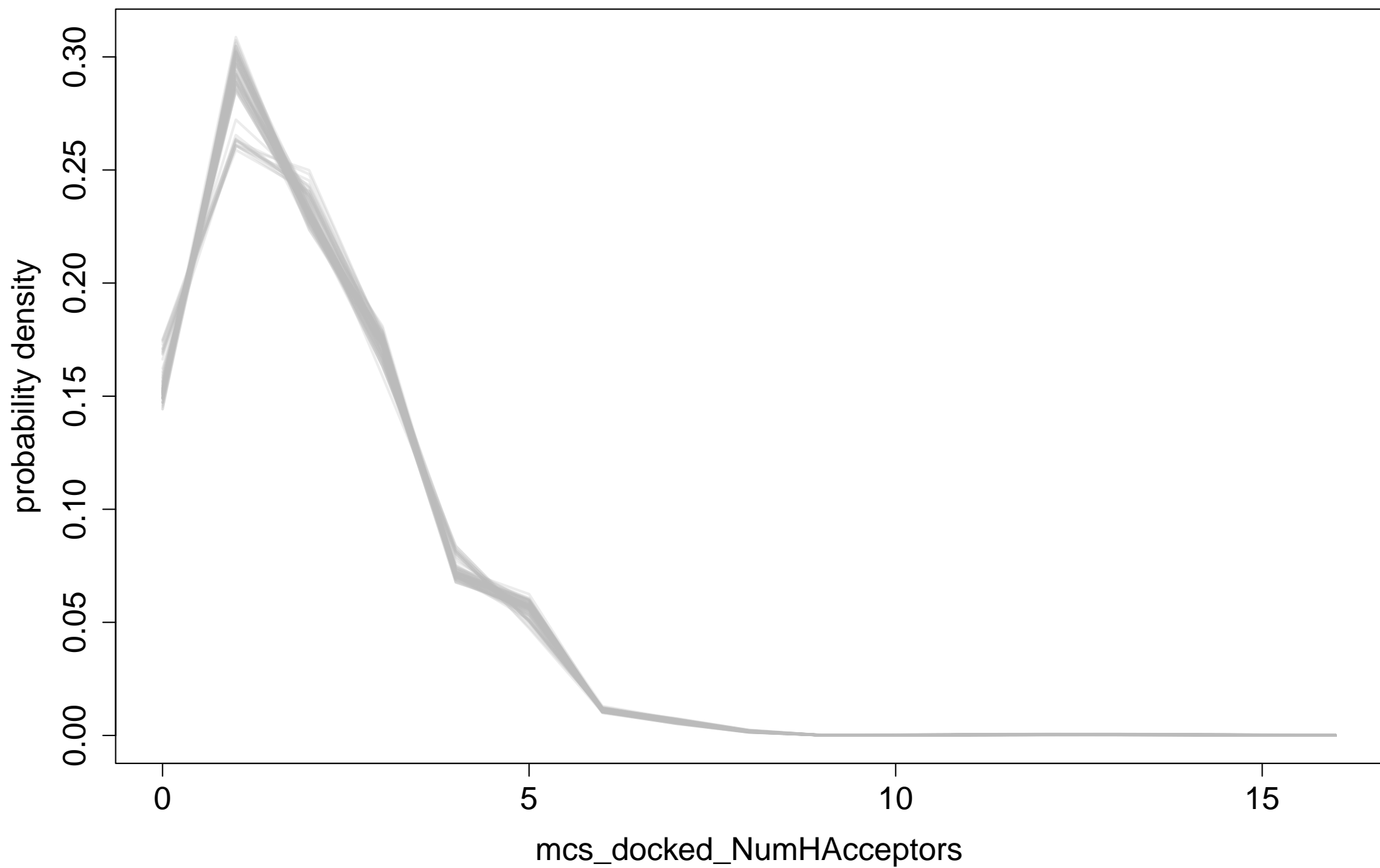


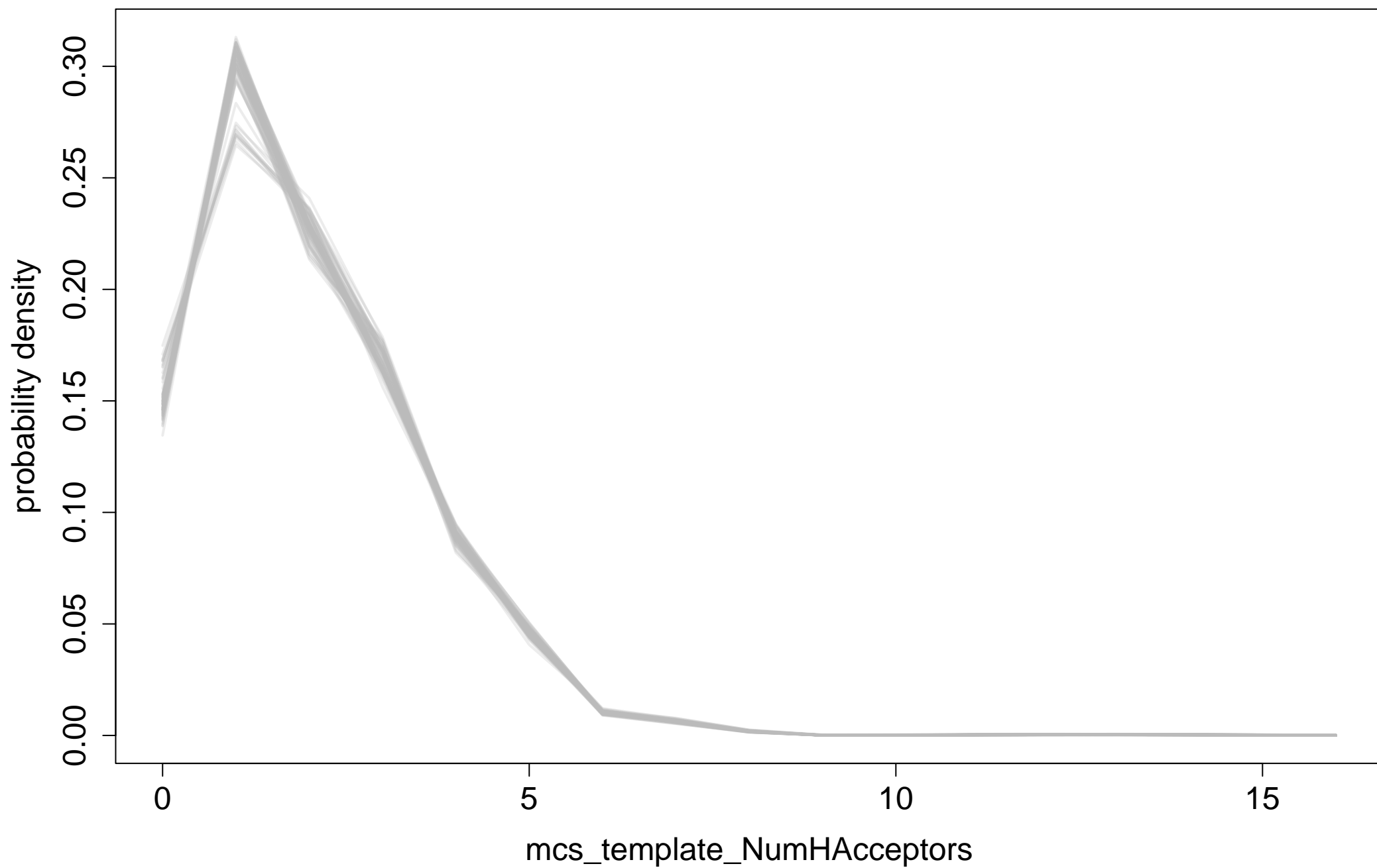


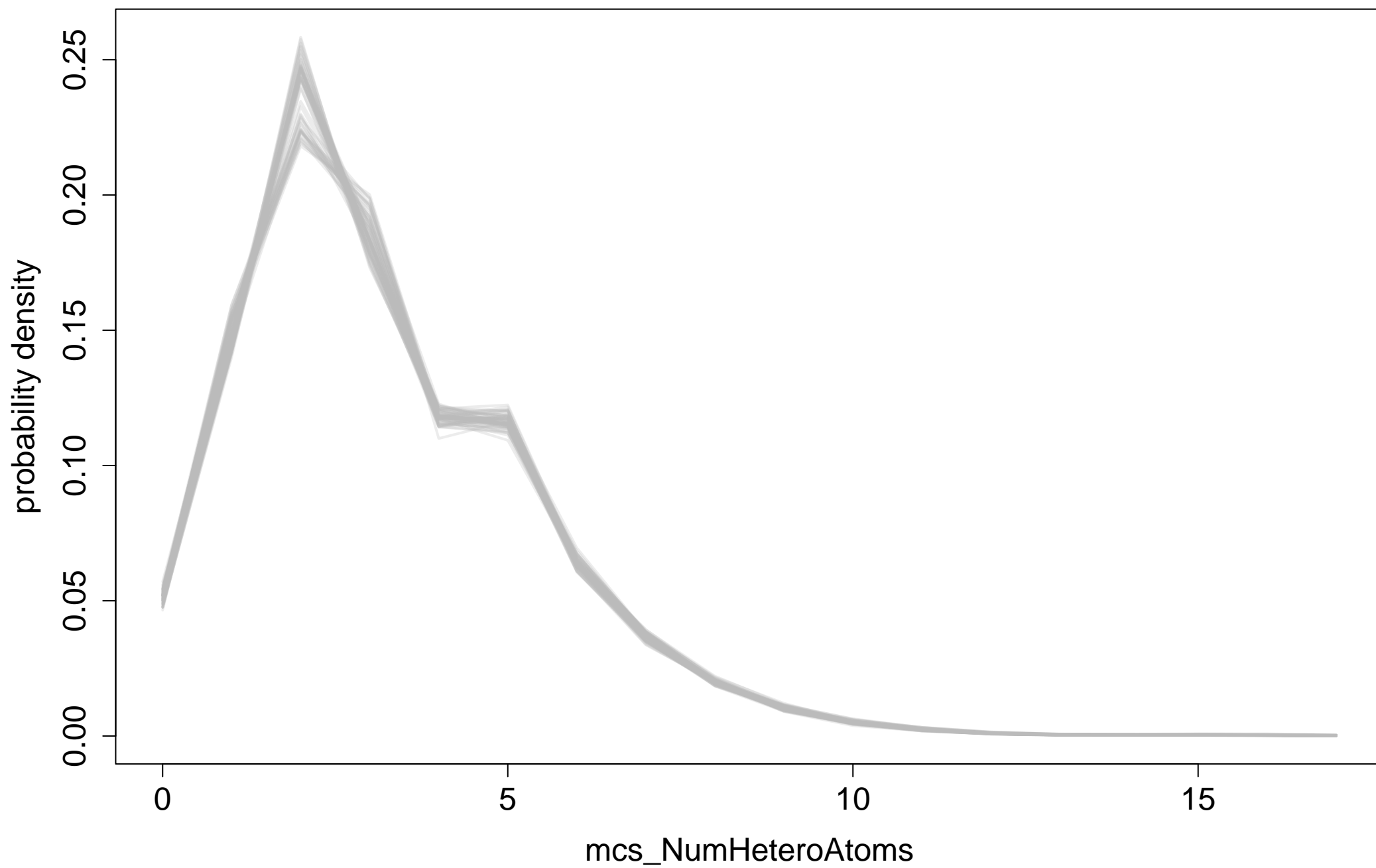


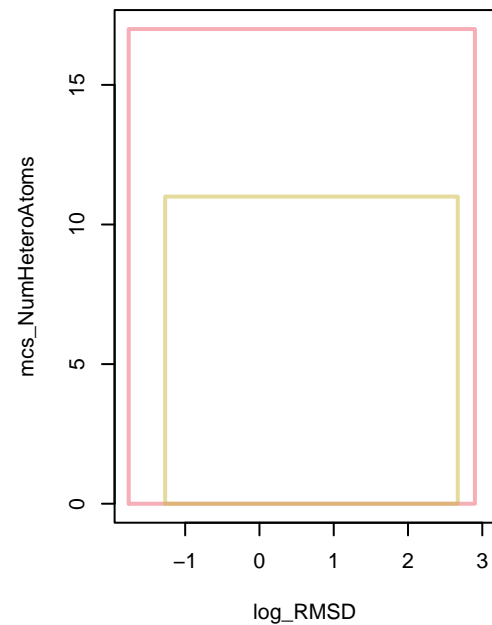
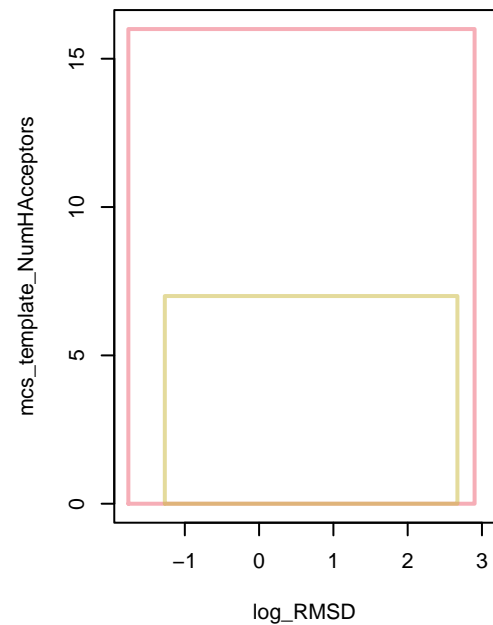
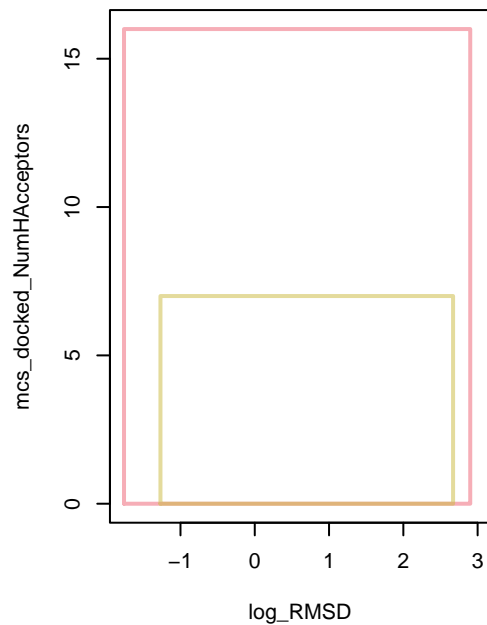
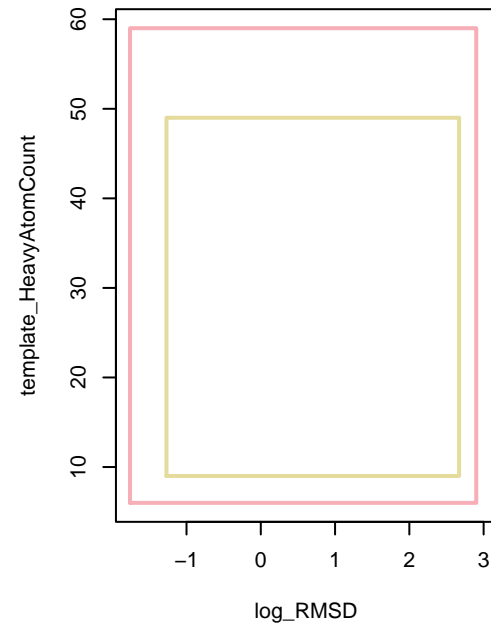
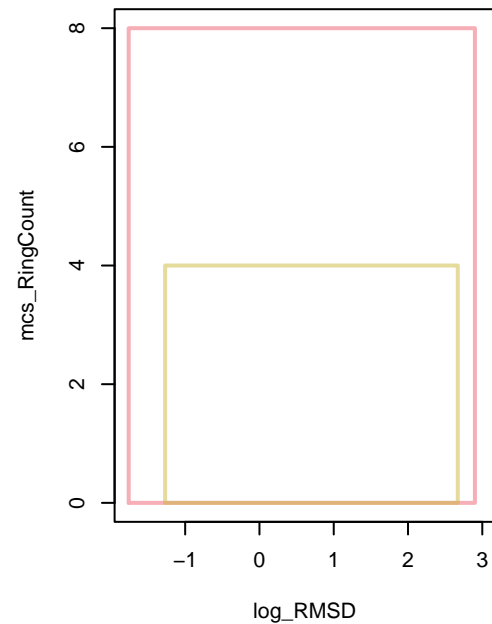
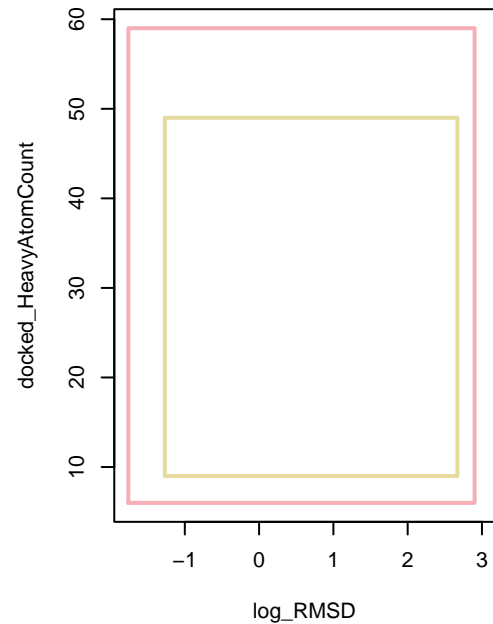
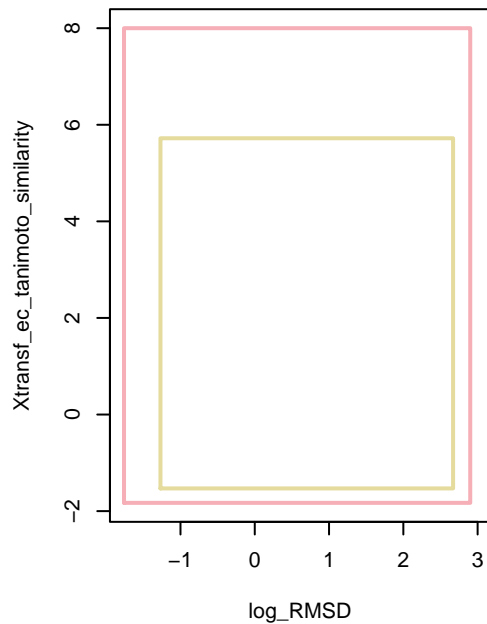




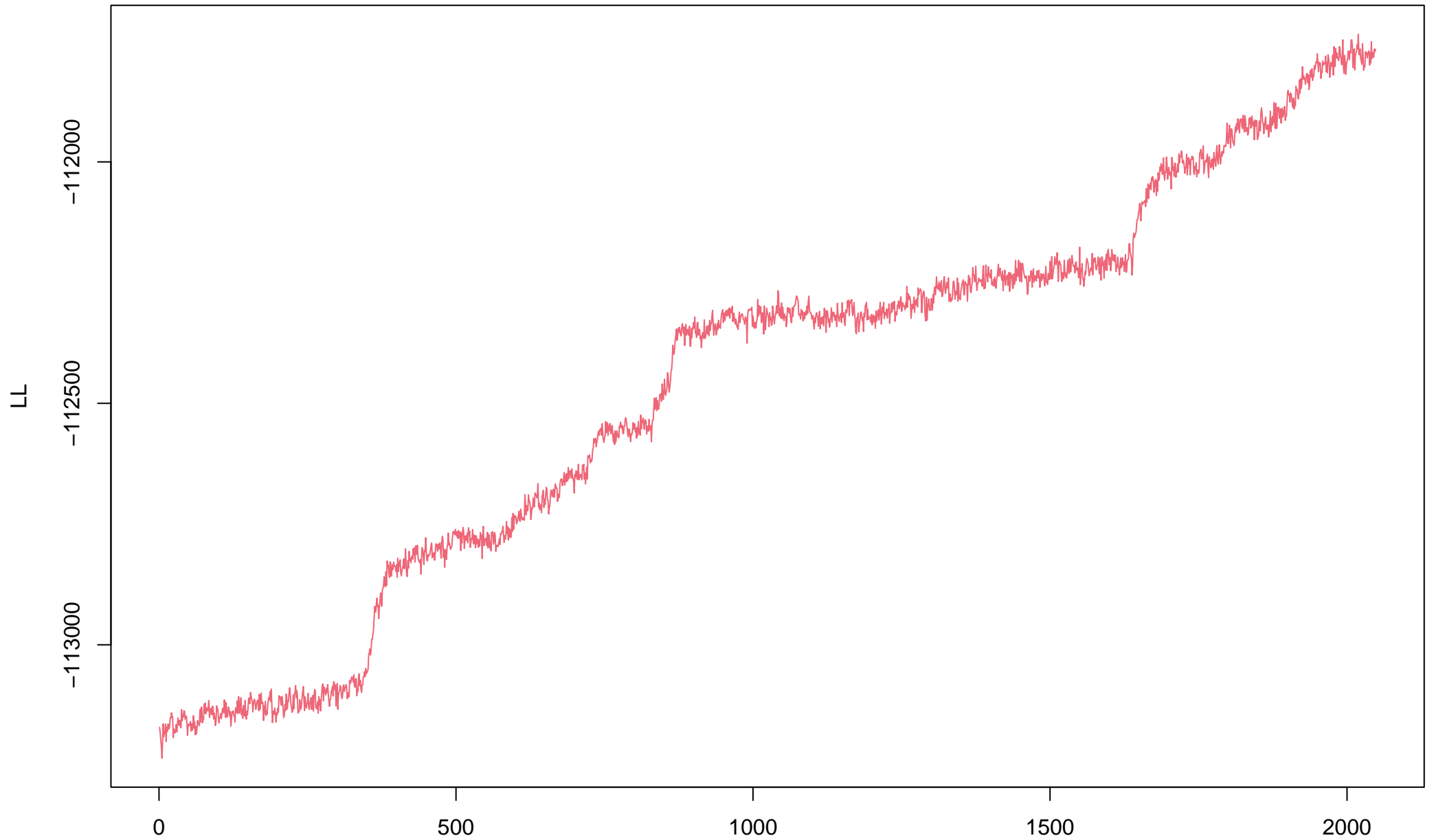




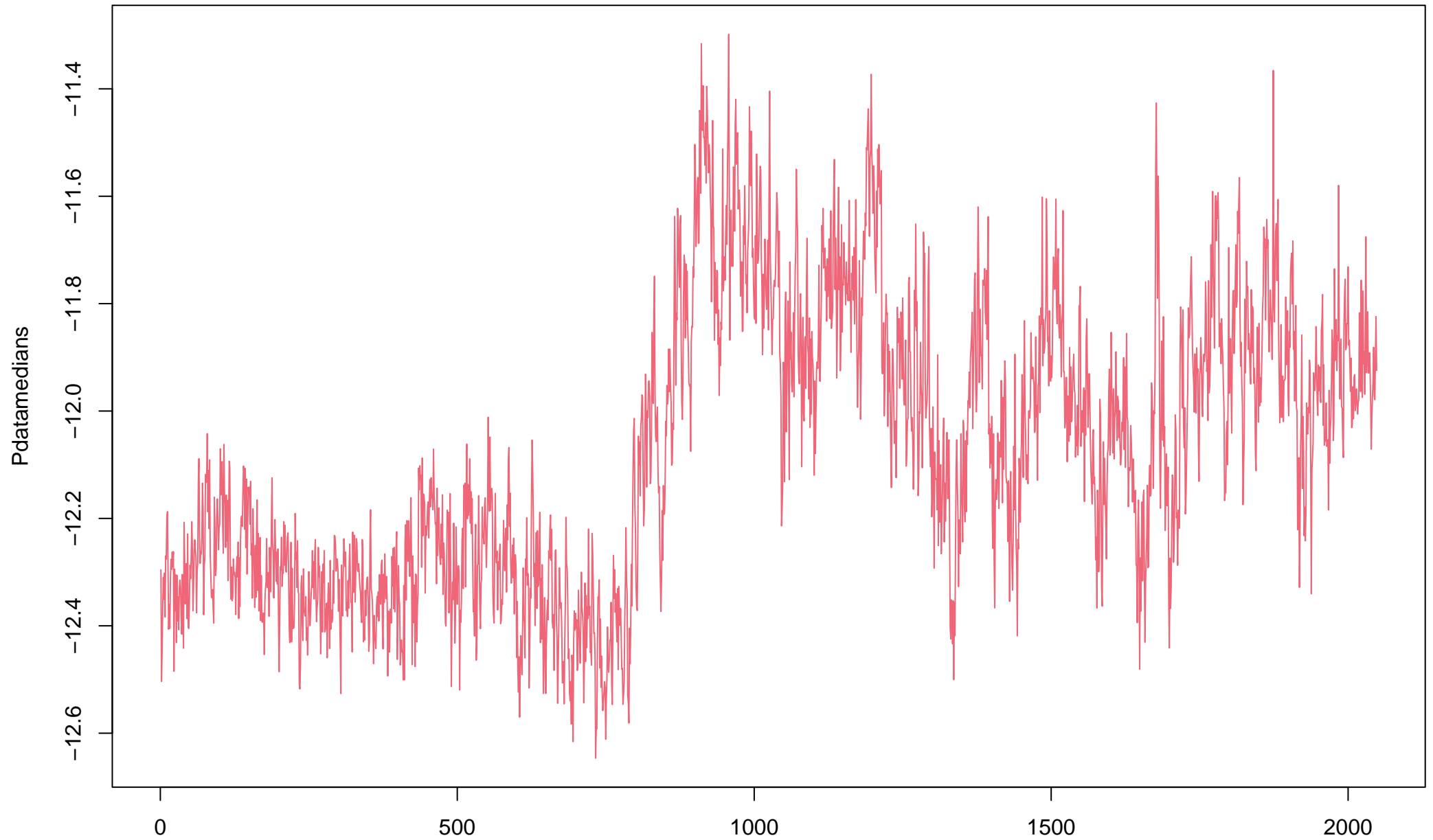




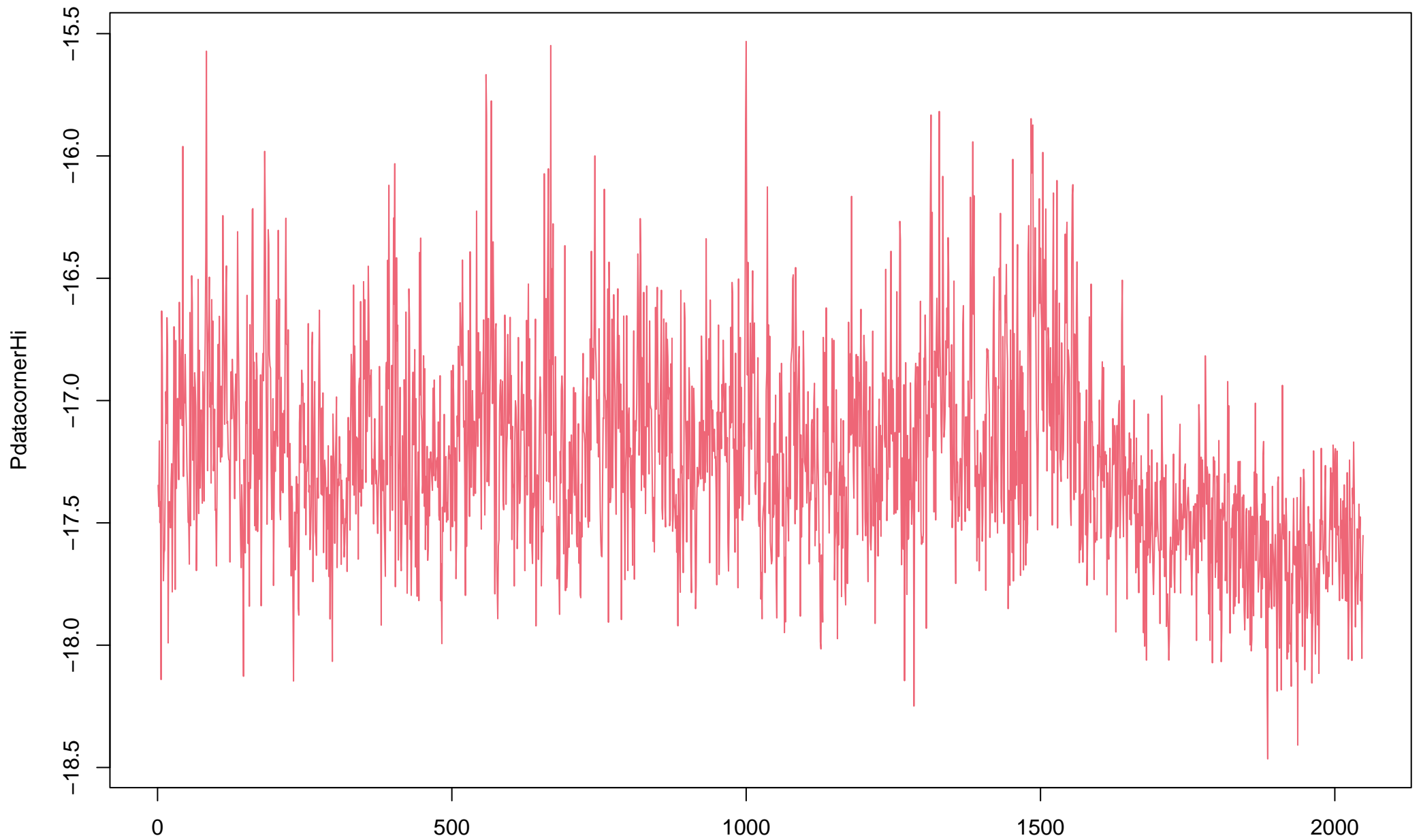
LL
ESS = 1.65 | BMK = 0.841 | MCSE(6.27) = 14.8 | stat: FALSE | burn: 2040



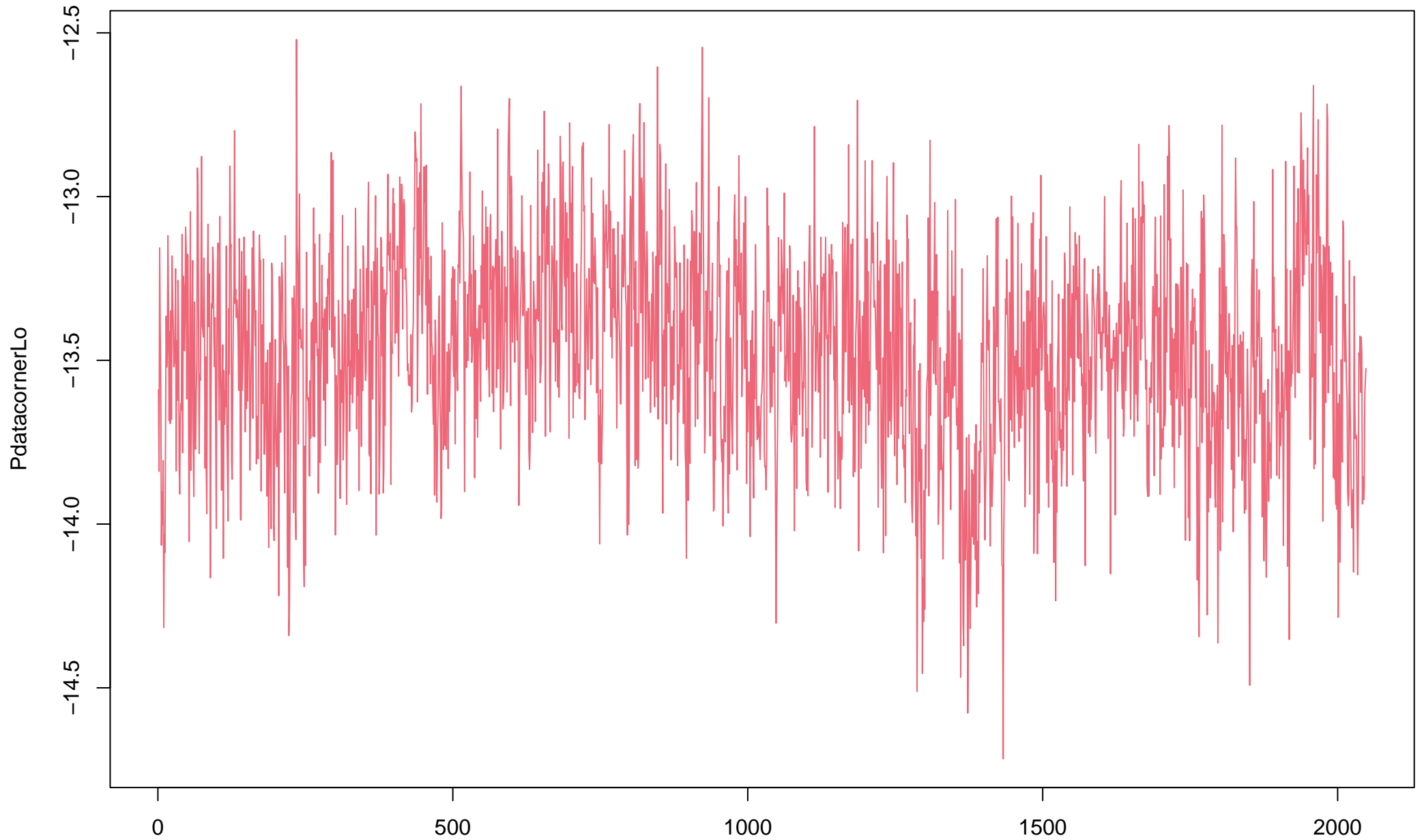
Pdatamedians
ESS = 15.9 | BMK = 0.519 | MCSE(6.27) = 13.1 | stat: FALSE | burn: 816



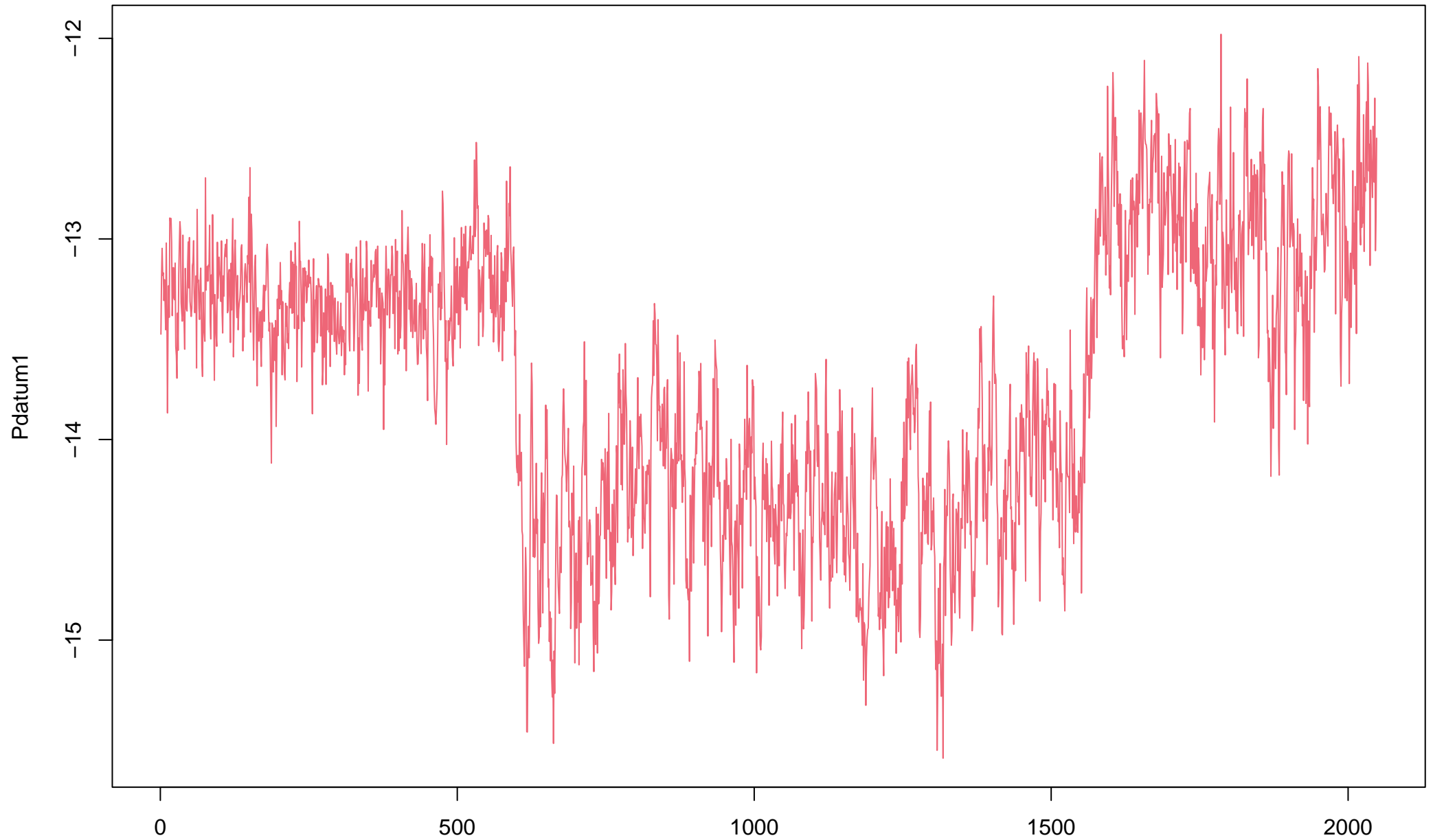
PdatacornerHi
ESS = 199 | BMK = 0.175 | MCSE(6.27) = 6.72 | stat: TRUE | burn: 0



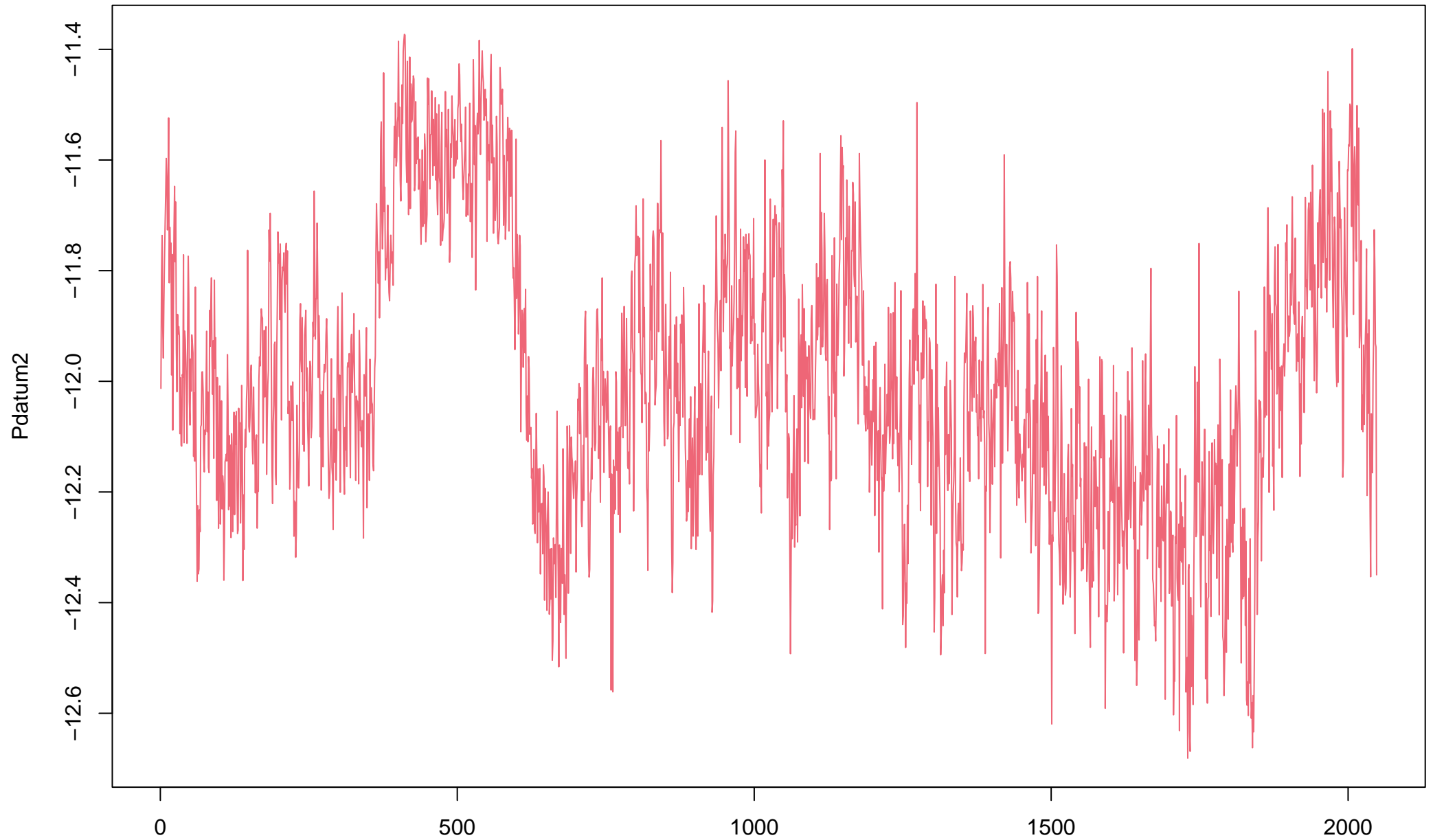
PdatacornerLo
ESS = 348 | BMK = 0.138 | MCSE(6.27) = 6.02 | stat: TRUE | burn: 0



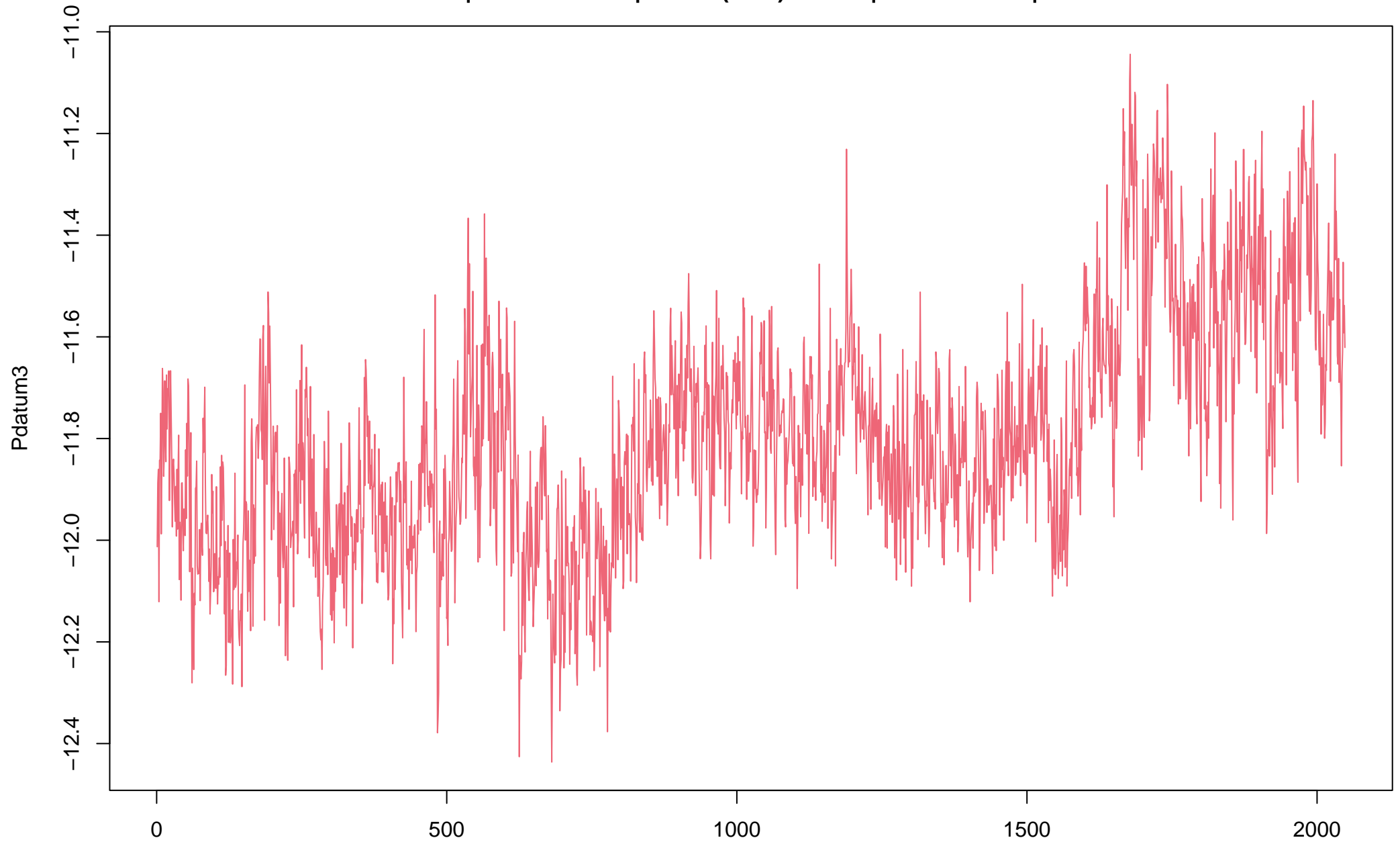
Pdatum1
ESS = 10.2 | BMK = 0.312 | MCSE(6.27) = 12.3 | stat: TRUE | burn: 1632



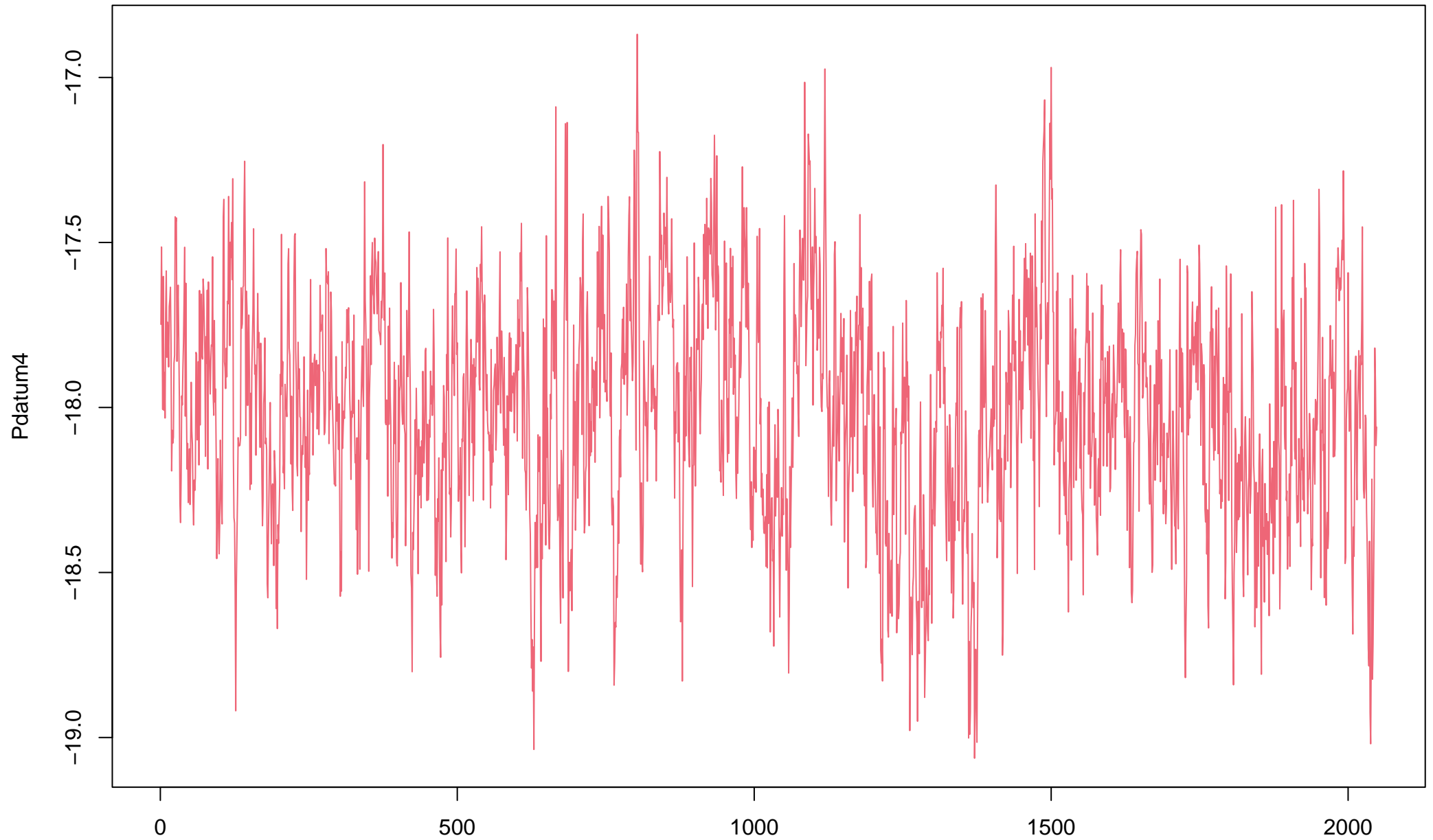
Pdatum2
ESS = 10.5 | BMK = 0.213 | MCSE(6.27) = 12.3 | stat: TRUE | burn: 2040



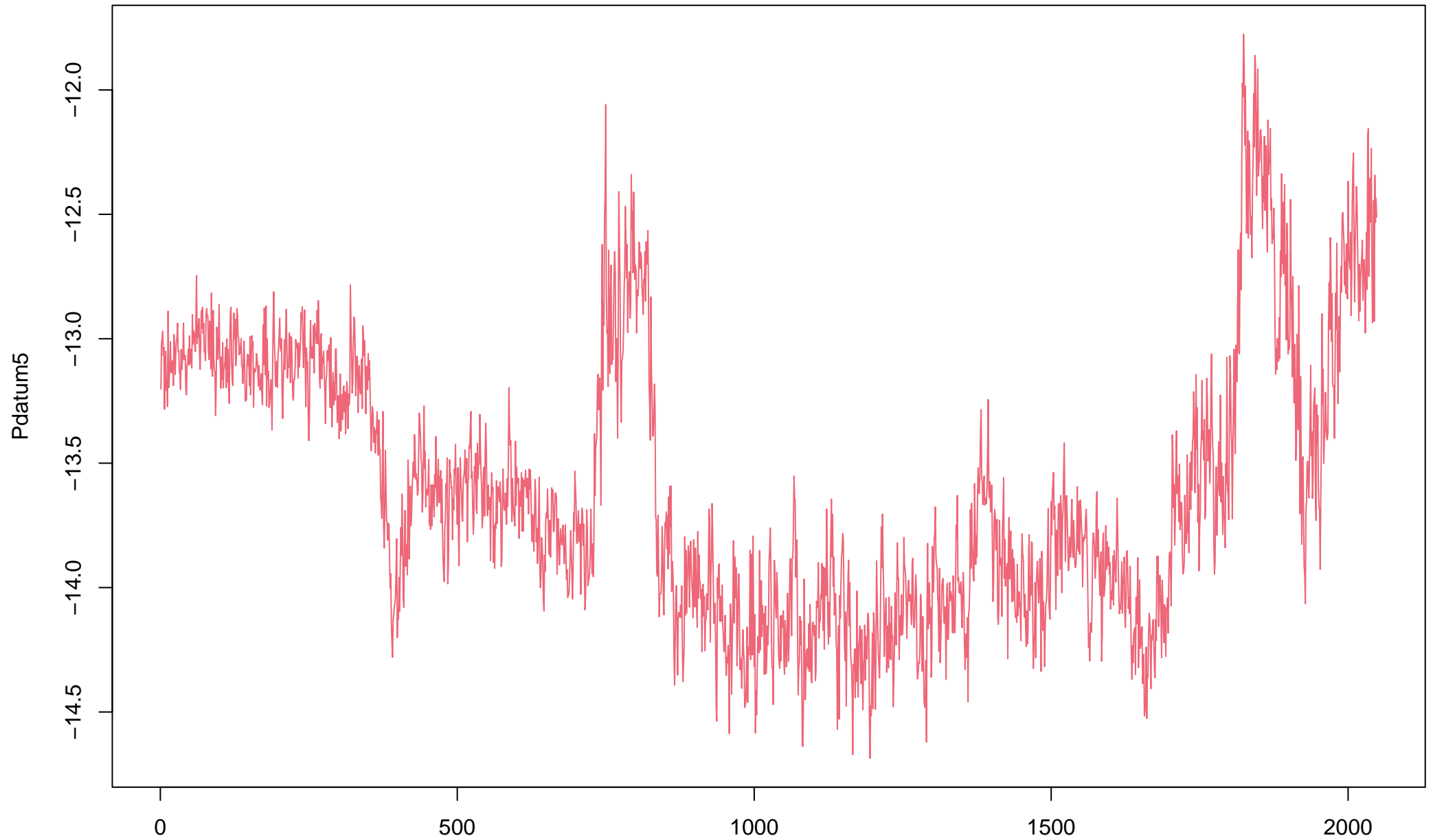
Pdatum3
ESS = 18.6 | BMK = 0.405 | MCSE(6.27) = 11.7 | stat: FALSE | burn: 1632



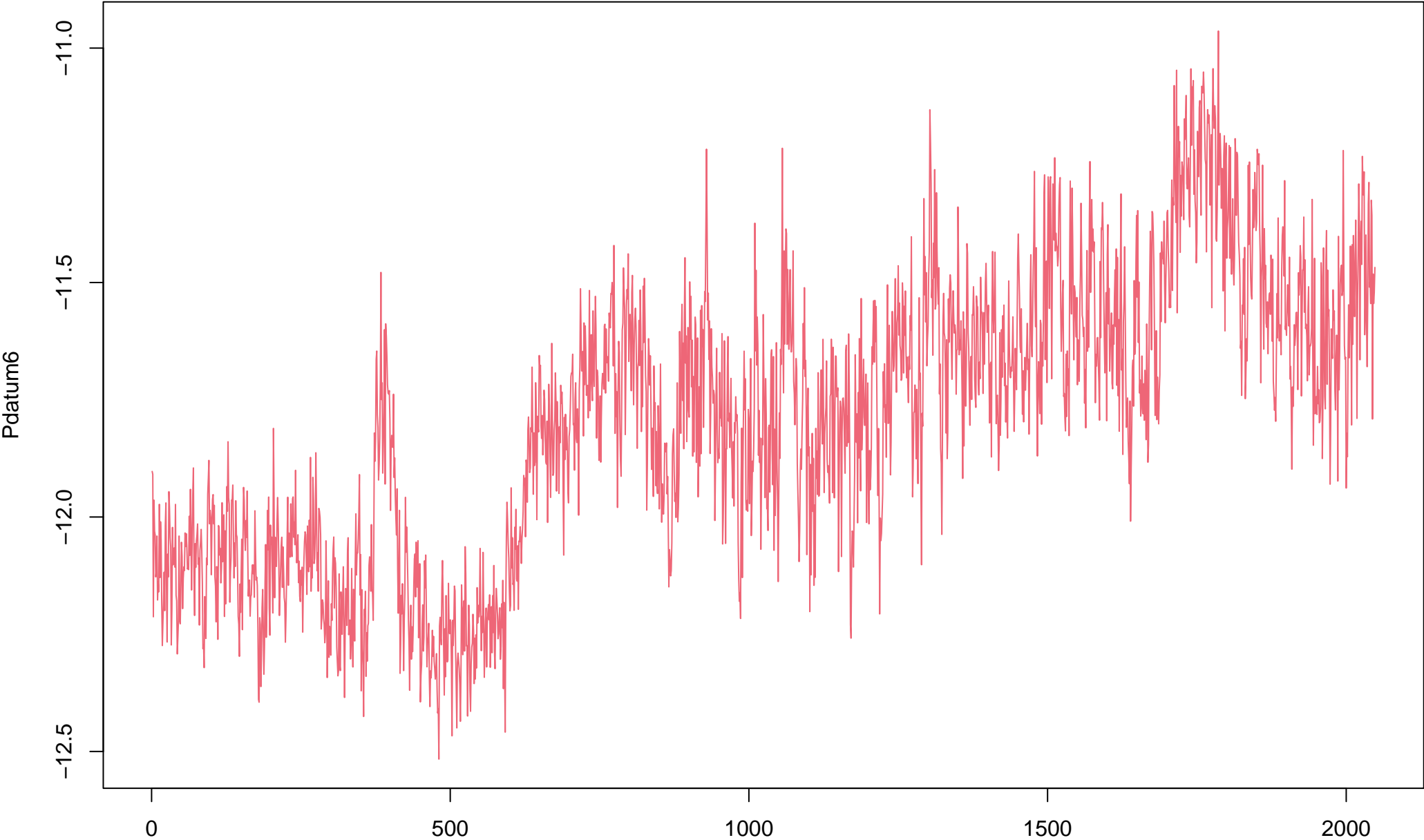
Pdatum4
ESS = 2.22e-16 | BMK = 0.122 | MCSE(6.27) = 6.91 | stat: TRUE | burn: 0



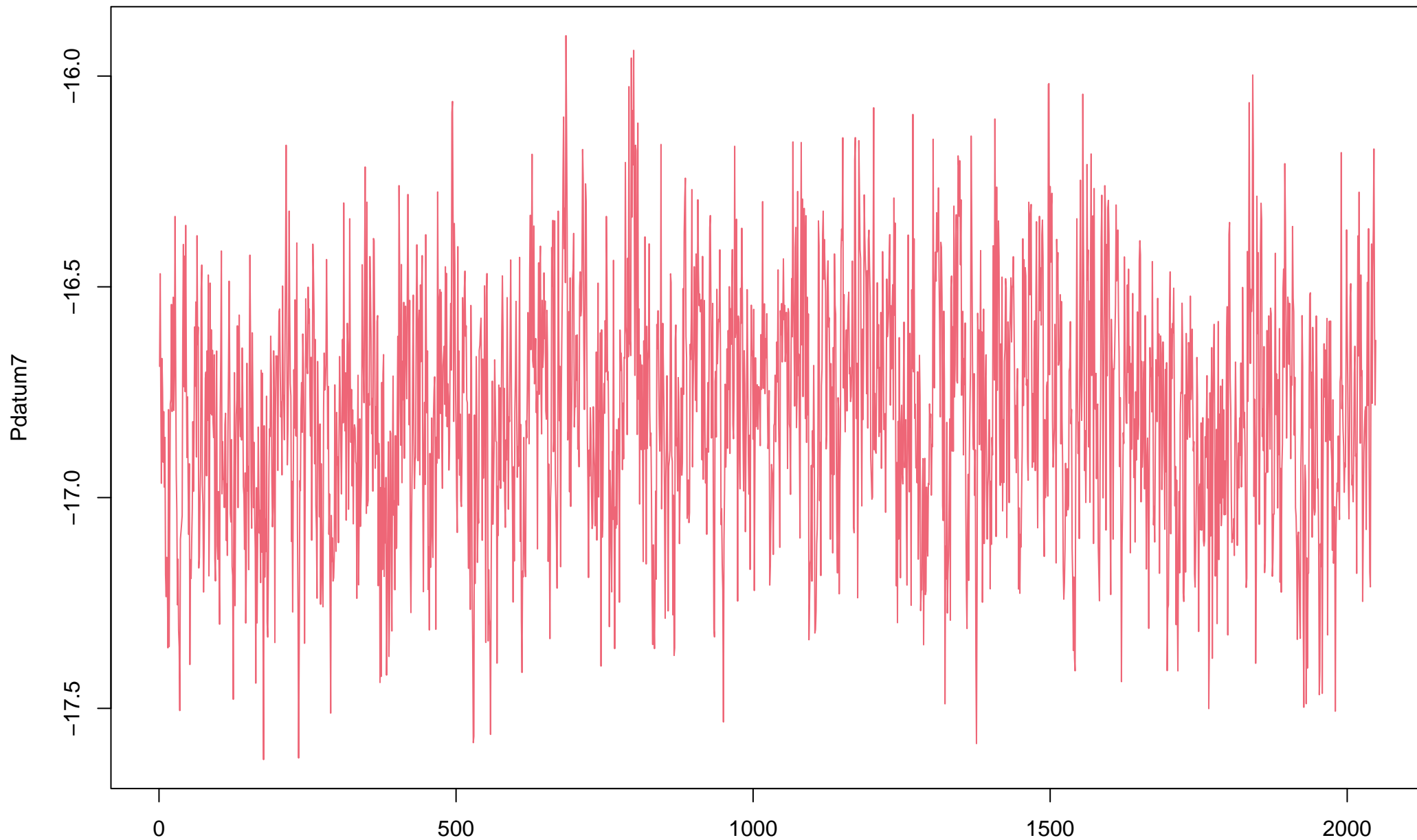
Pdatum5
ESS = 17.7 | BMK = 0.329 | MCSE(6.27) = 12.7 | stat: FALSE | burn: 612



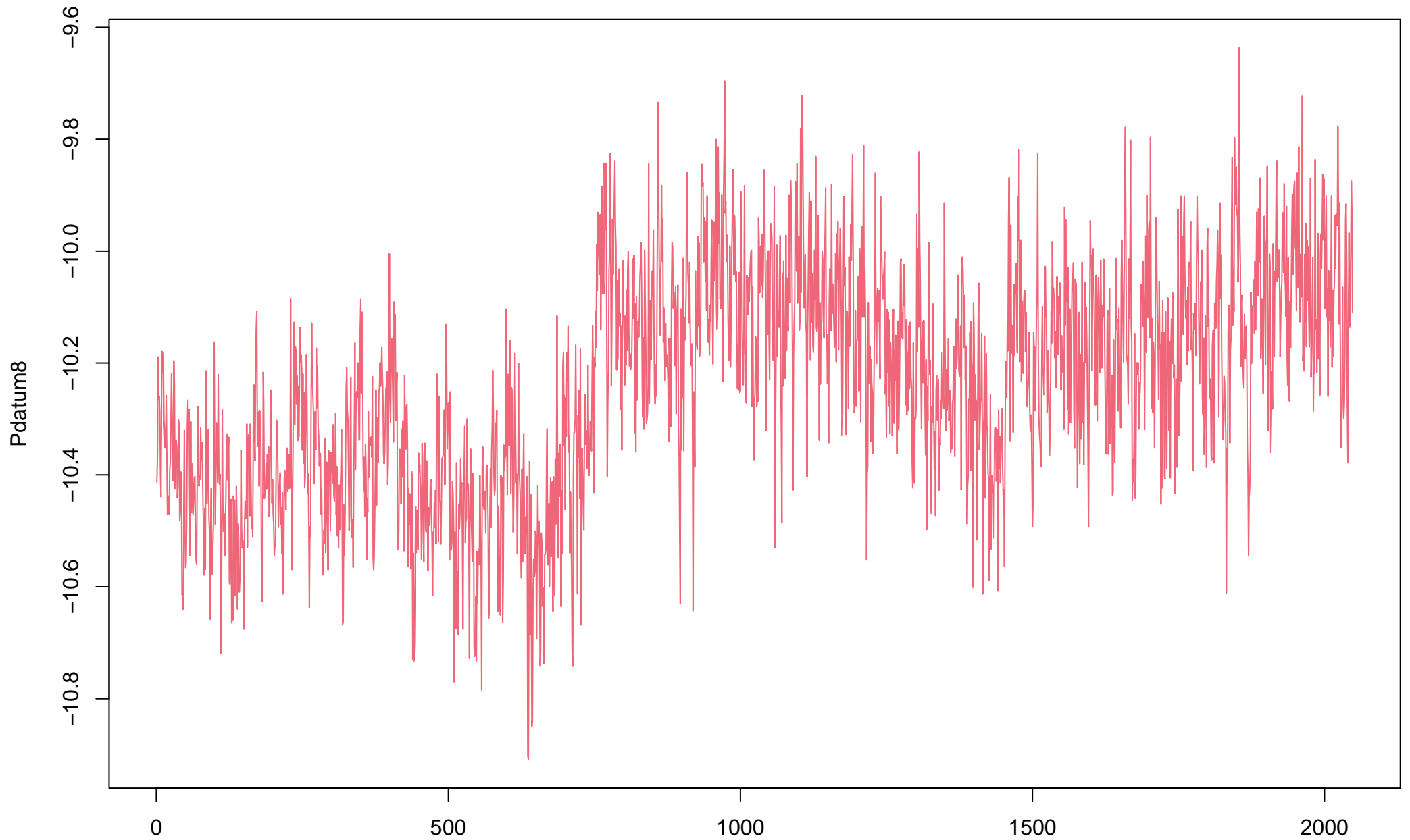
Pdatum6
ESS = 9.3 | BMK = 0.552 | MCSE(6.27) = 13 | stat: FALSE | burn: 612



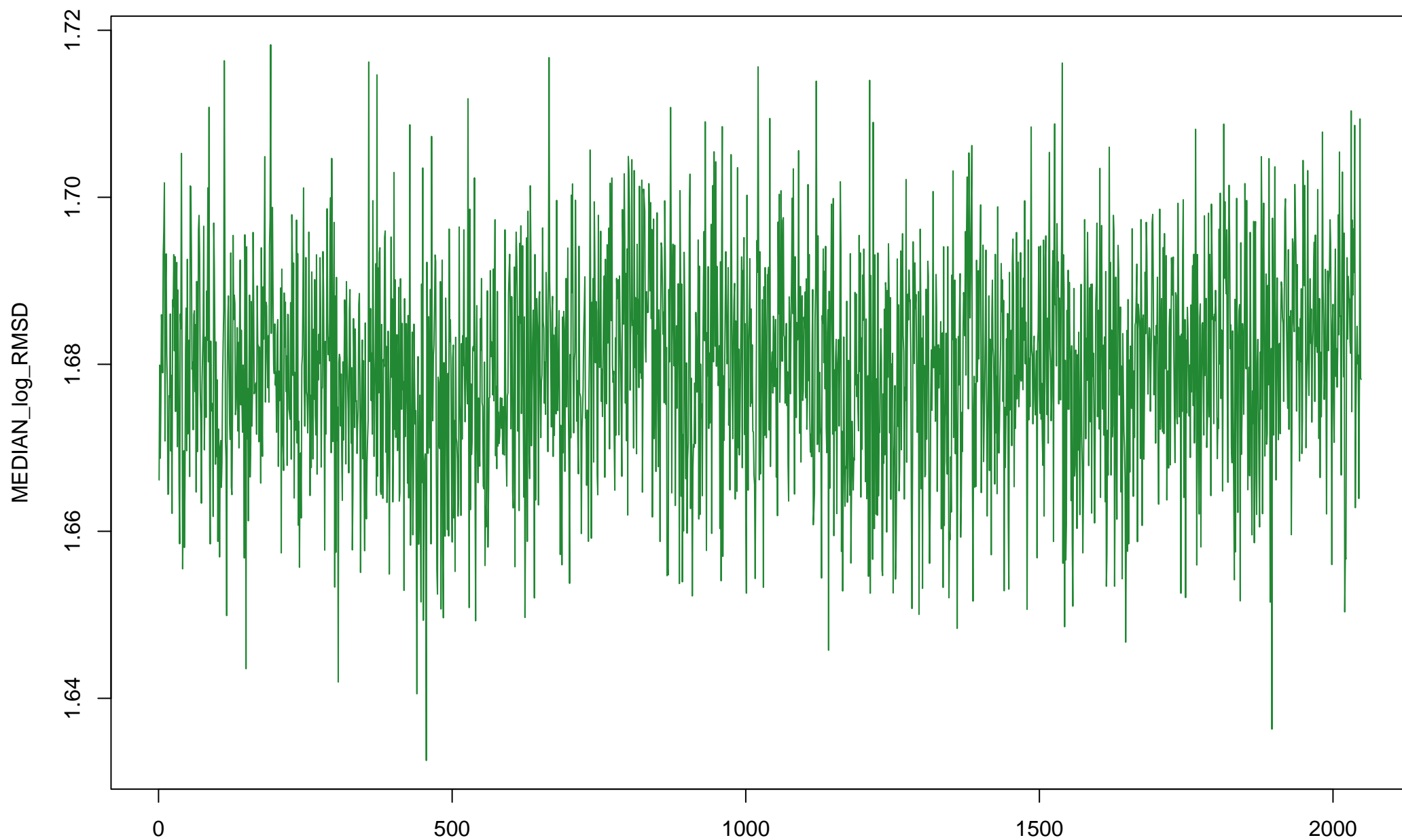
Pdatum7
ESS = 426 | BMK = 0.0624 | MCSE(6.27) = 5.01 | stat: FALSE | burn: 0



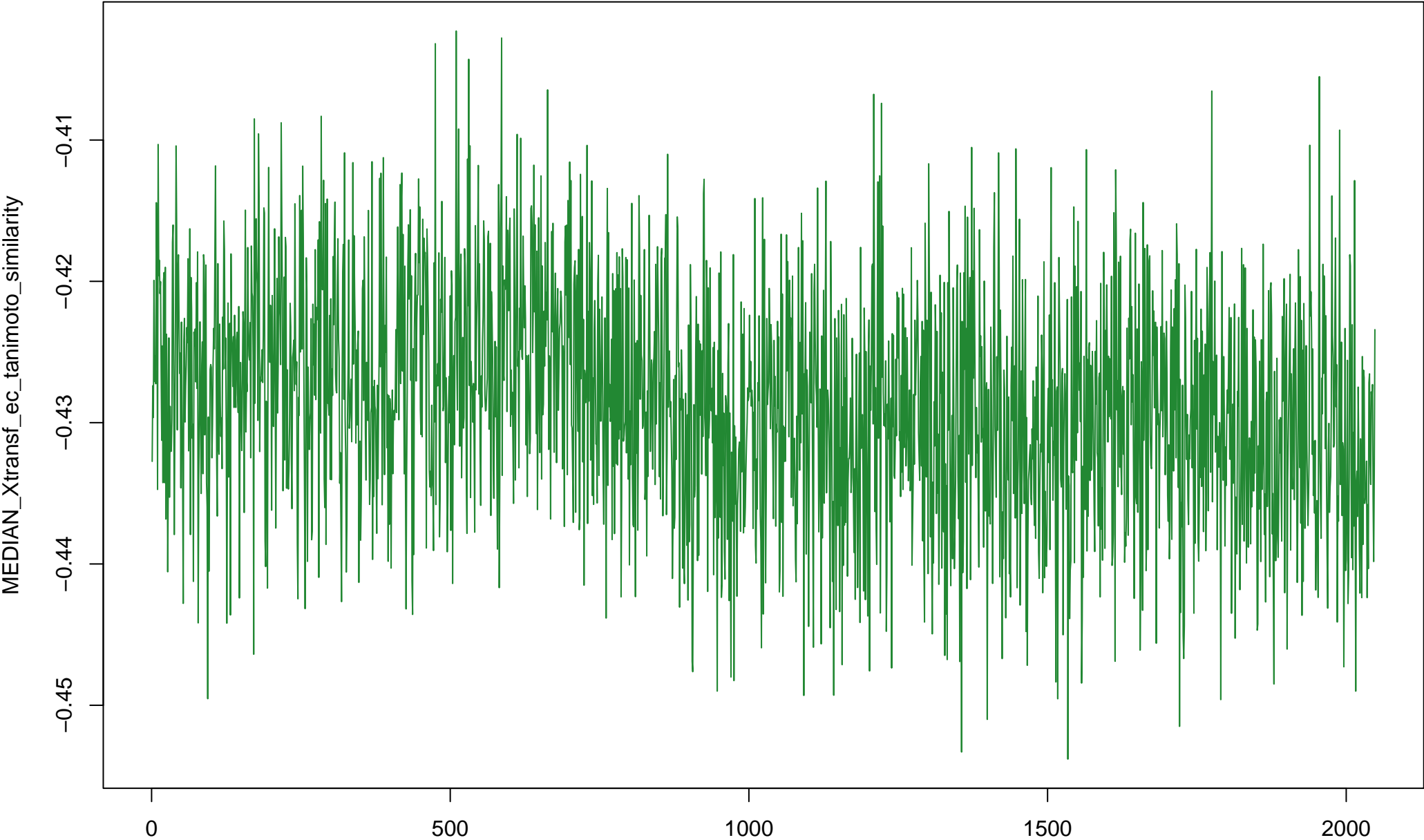
Pdatum8
ESS = 18.3 | BMK = 0.366 | MCSE(6.27) = 10.9 | stat: FALSE | burn: 0



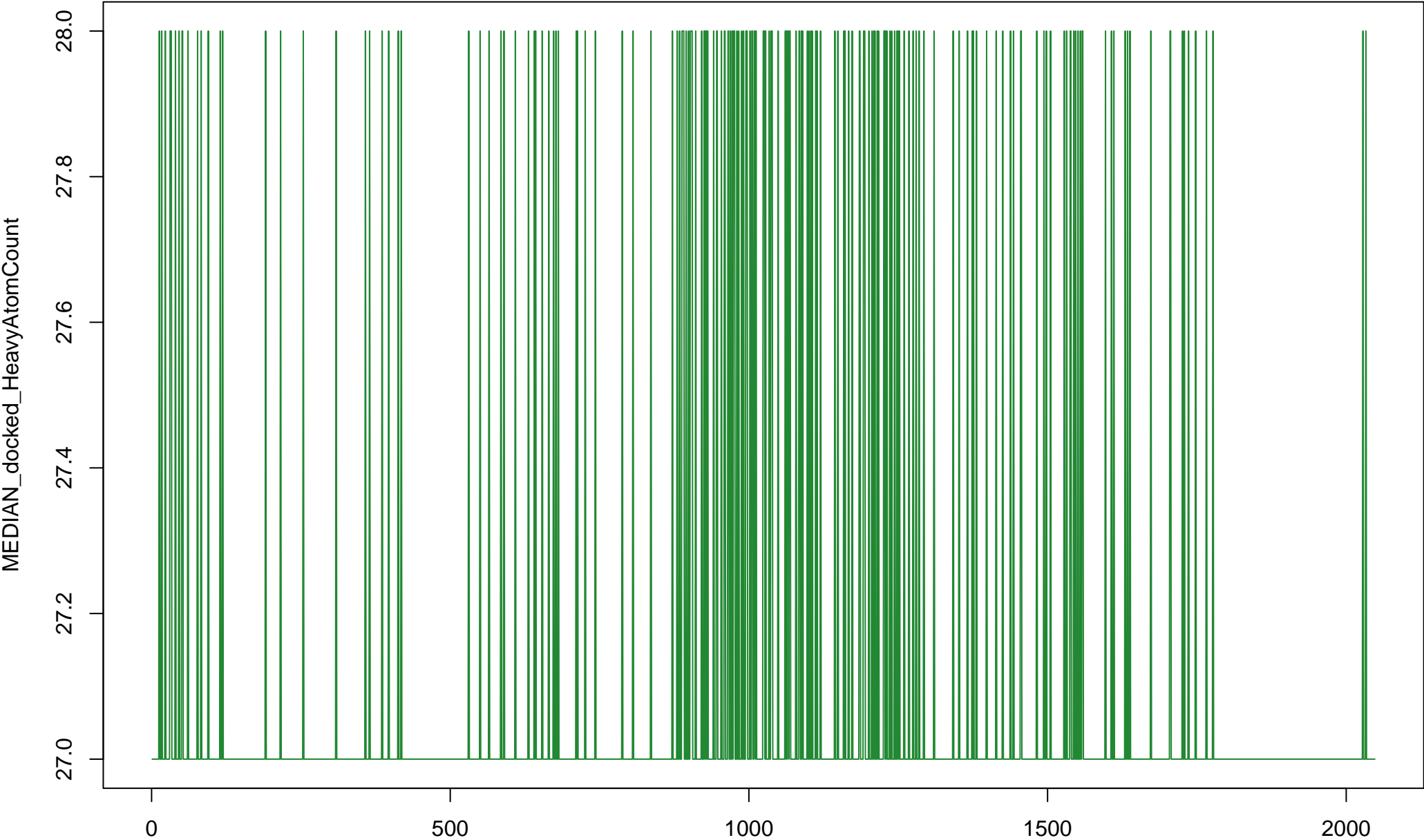
MEDIAN_log_RMSD
ESS = 804 | BMK = 0.048 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0



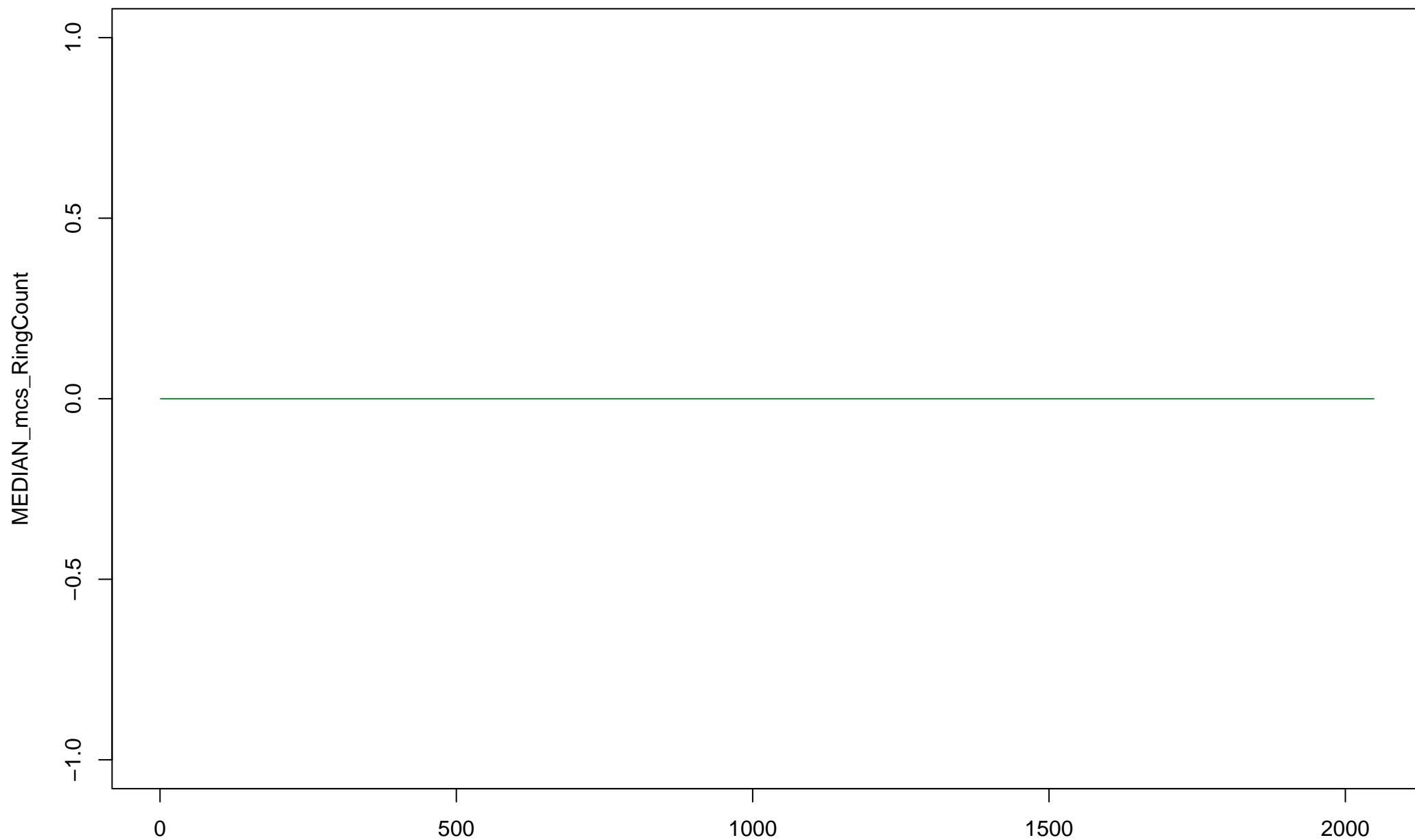
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 182 | BMK = 0.161 | MCSE(6.27) = 4.87 | stat: FALSE | burn: 0



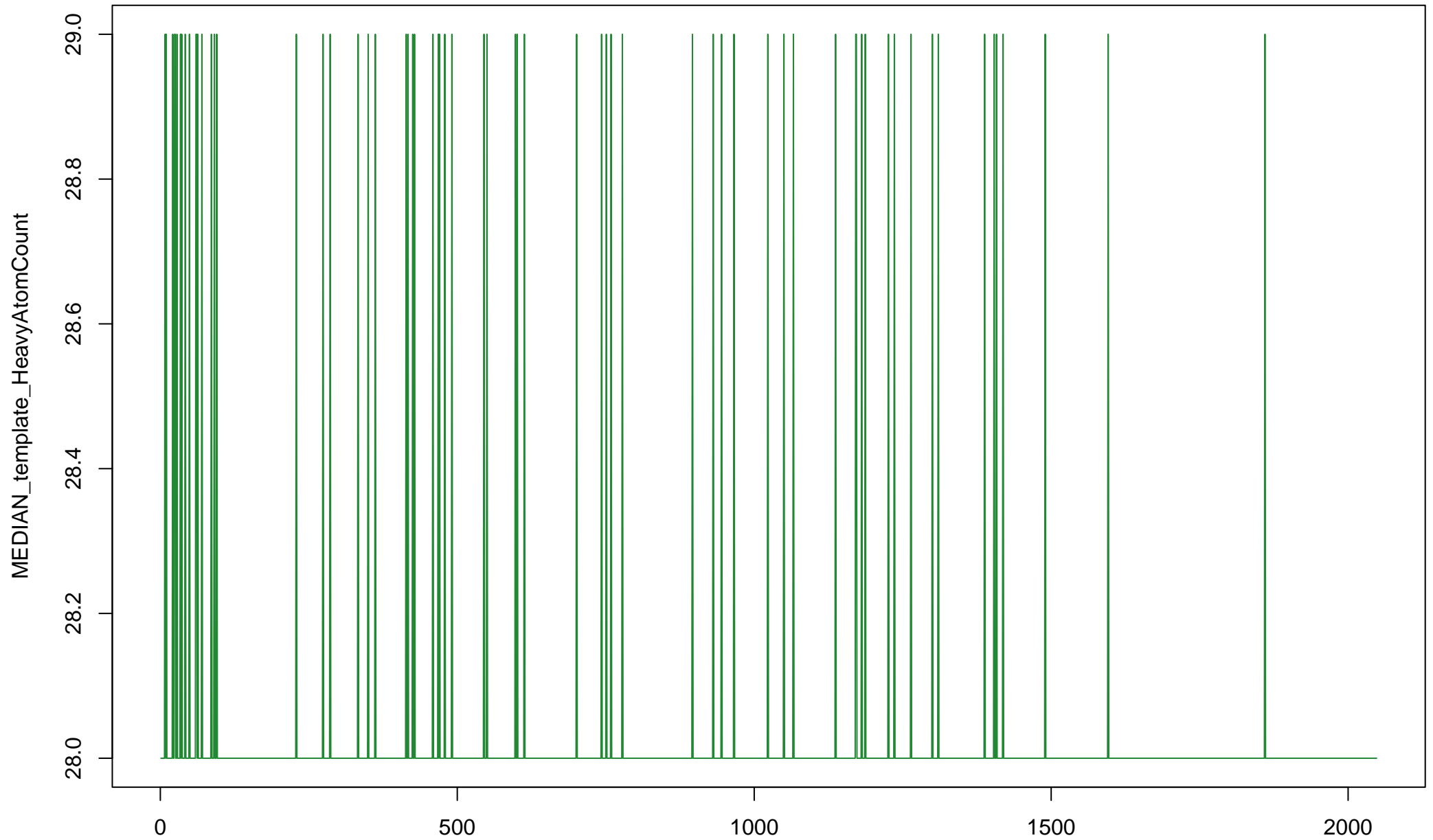
MEDIAN_docked_HeavyAtomCount
ESS = 139 | BMK = 0.0199 | MCSE(6.27) = 4.64 | stat: TRUE | burn: 0



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



MEDIAN_template_HeavyAtomCount
ESS = 672 | BMK = 0.156 | MCSE(6.27) = 3.43 | stat: FALSE | burn: 2040



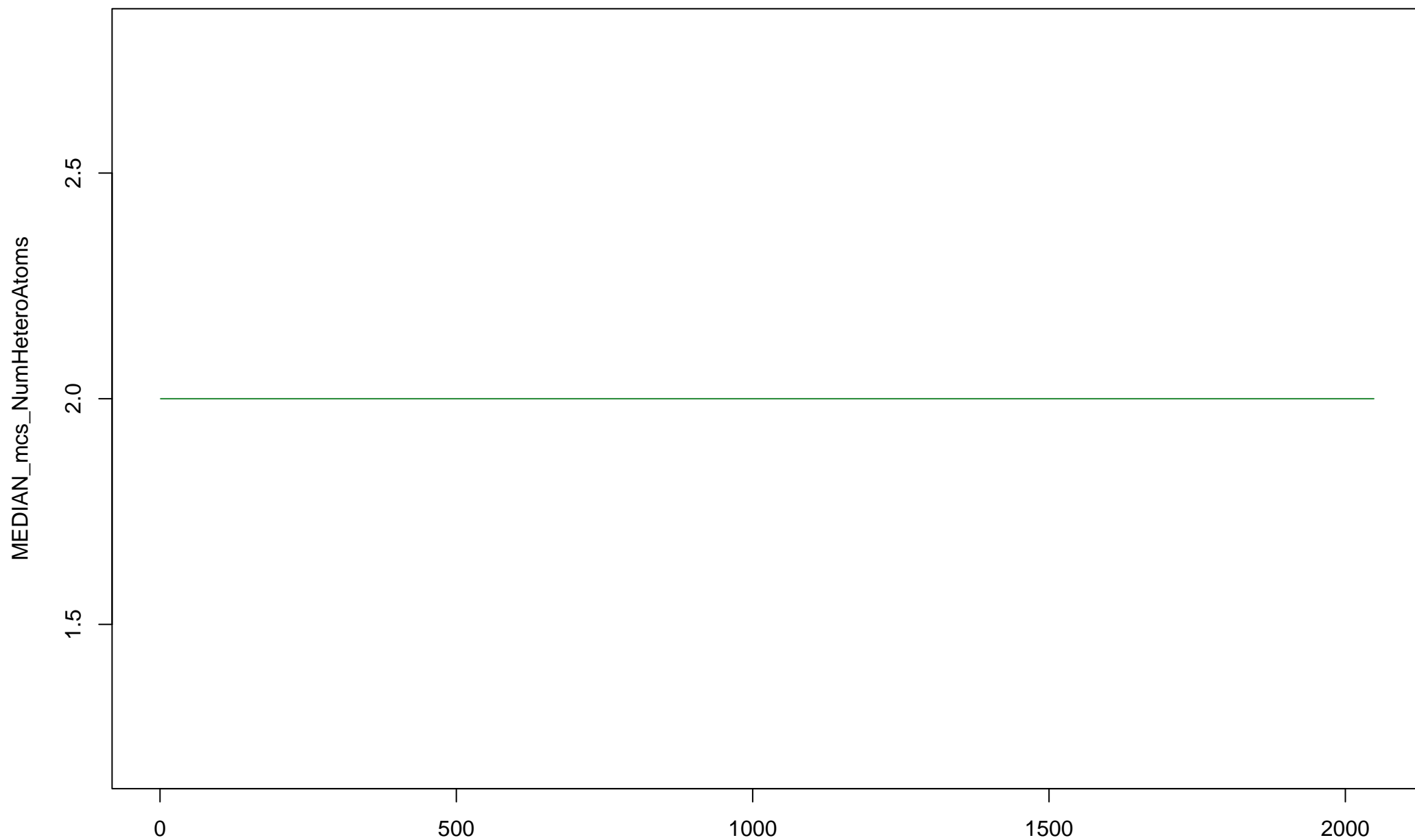
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



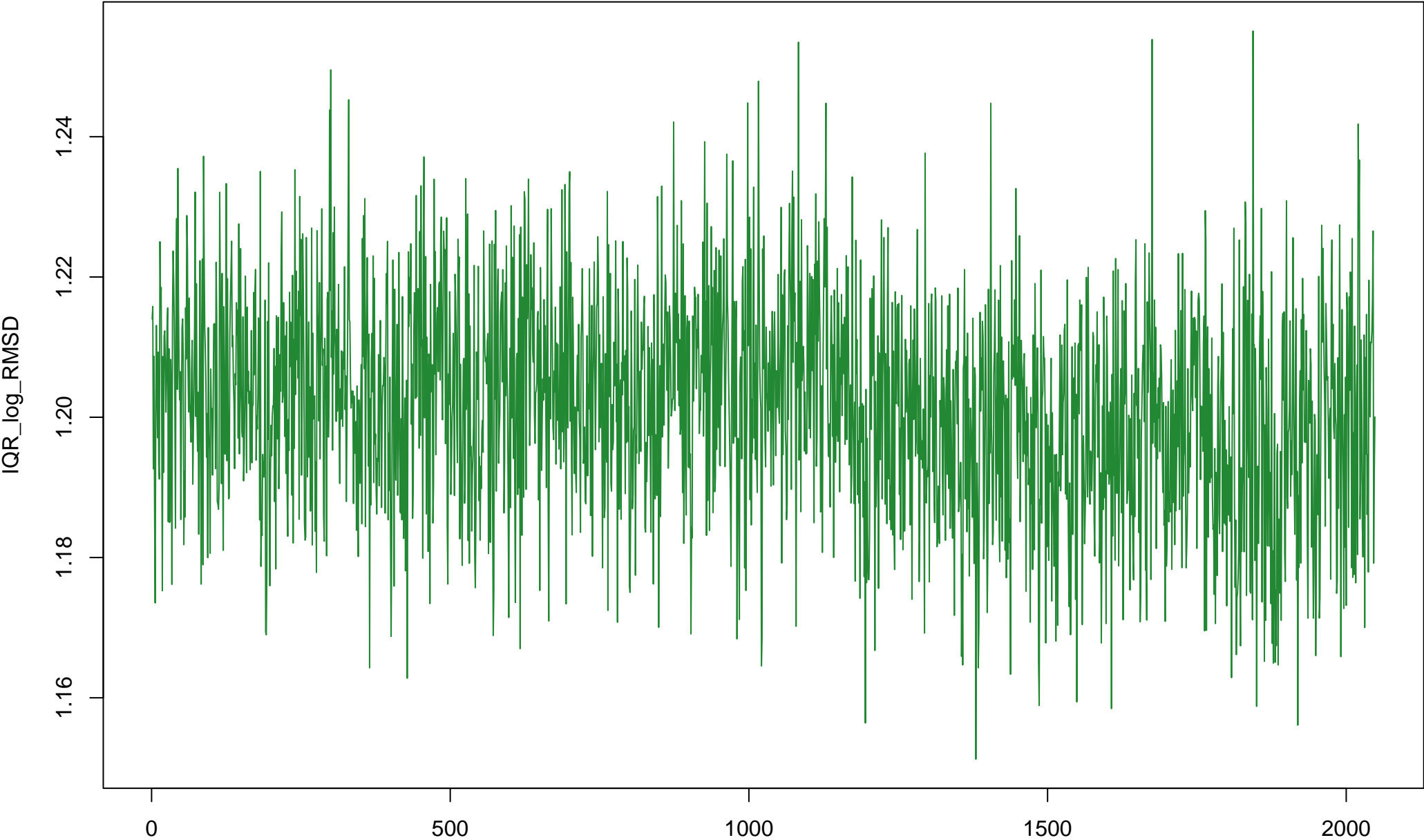
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



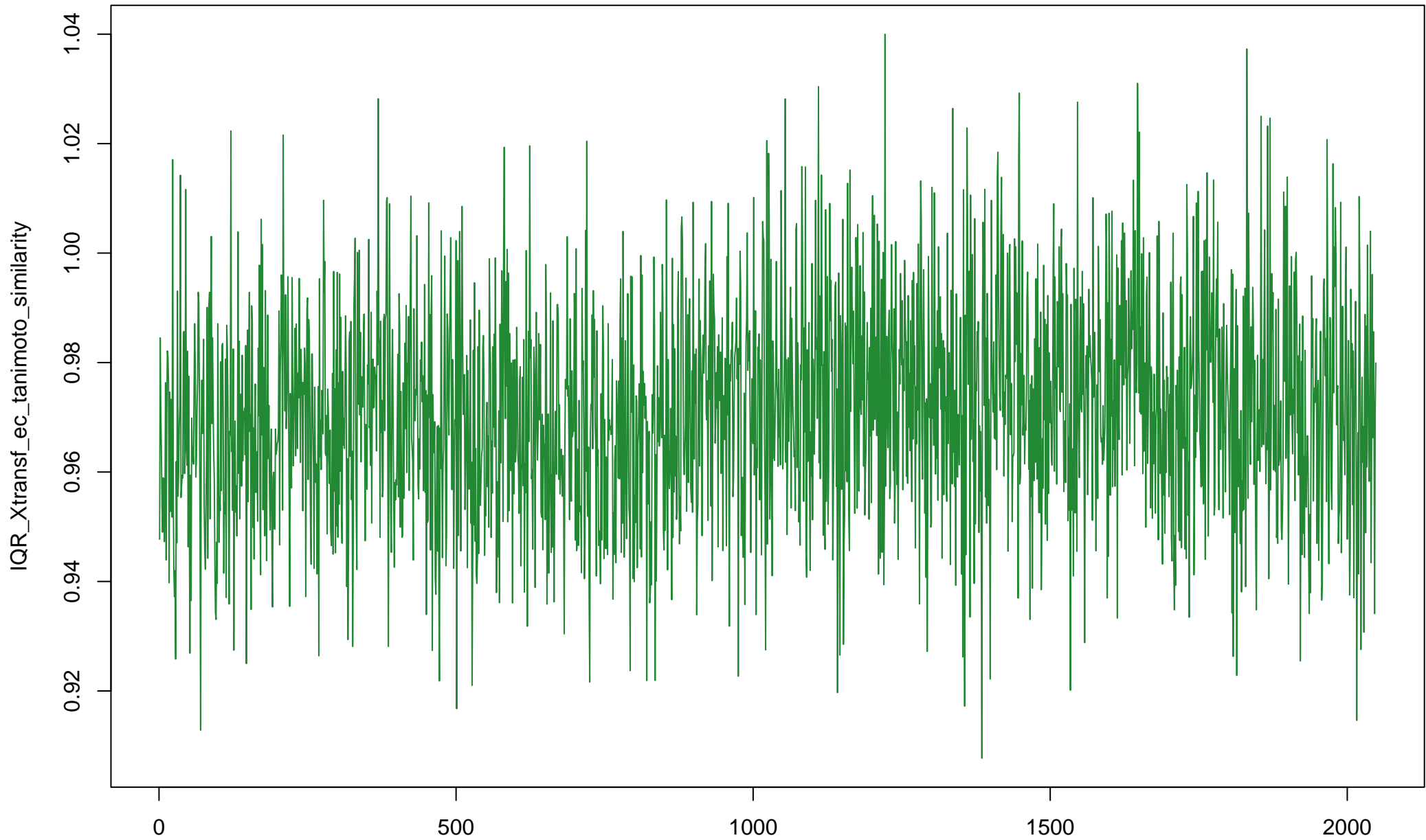
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



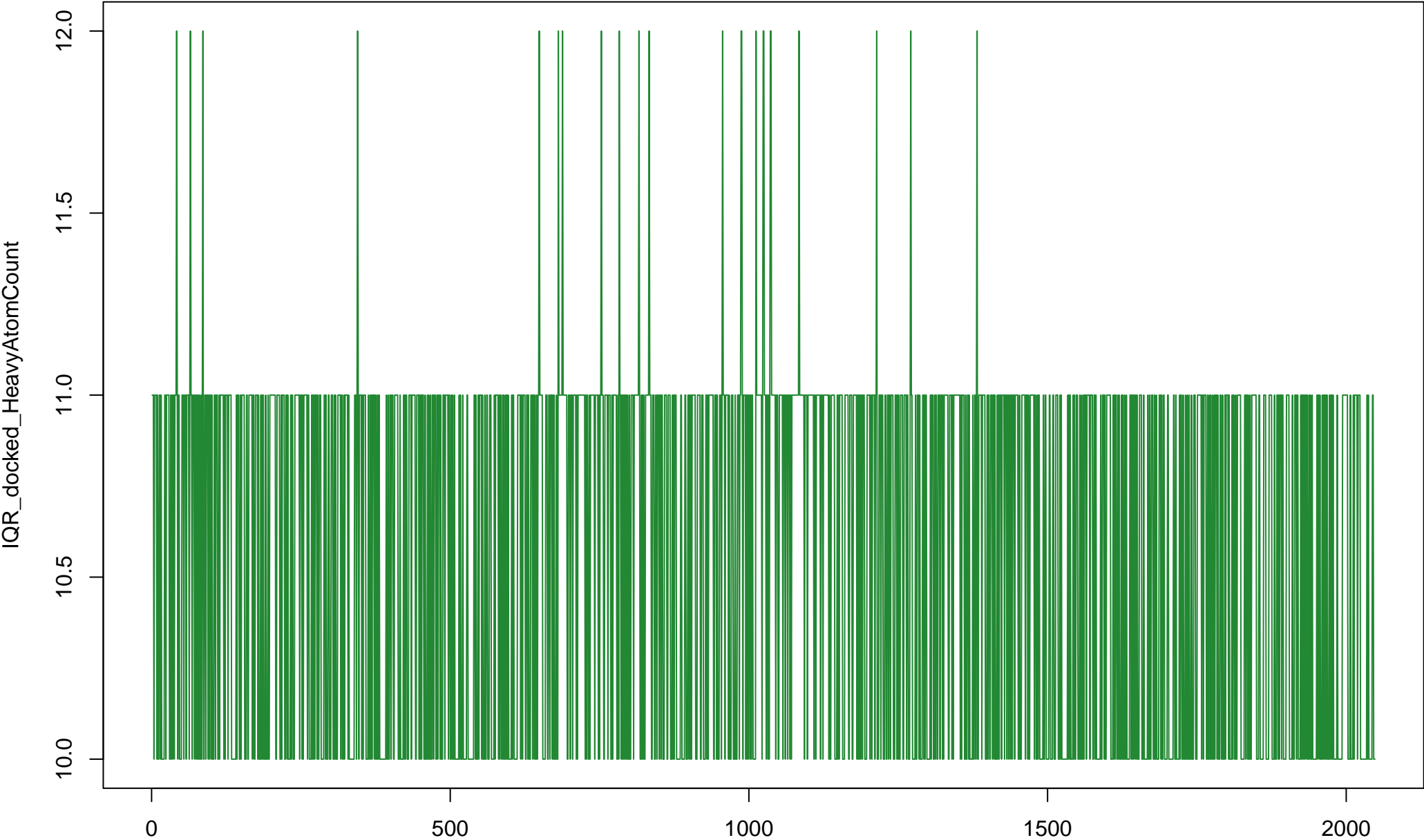
IQR_log_RMSD
ESS = 385 | BMK = 0.143 | MCSE(6.27) = 4.56 | stat: FALSE | burn: 0



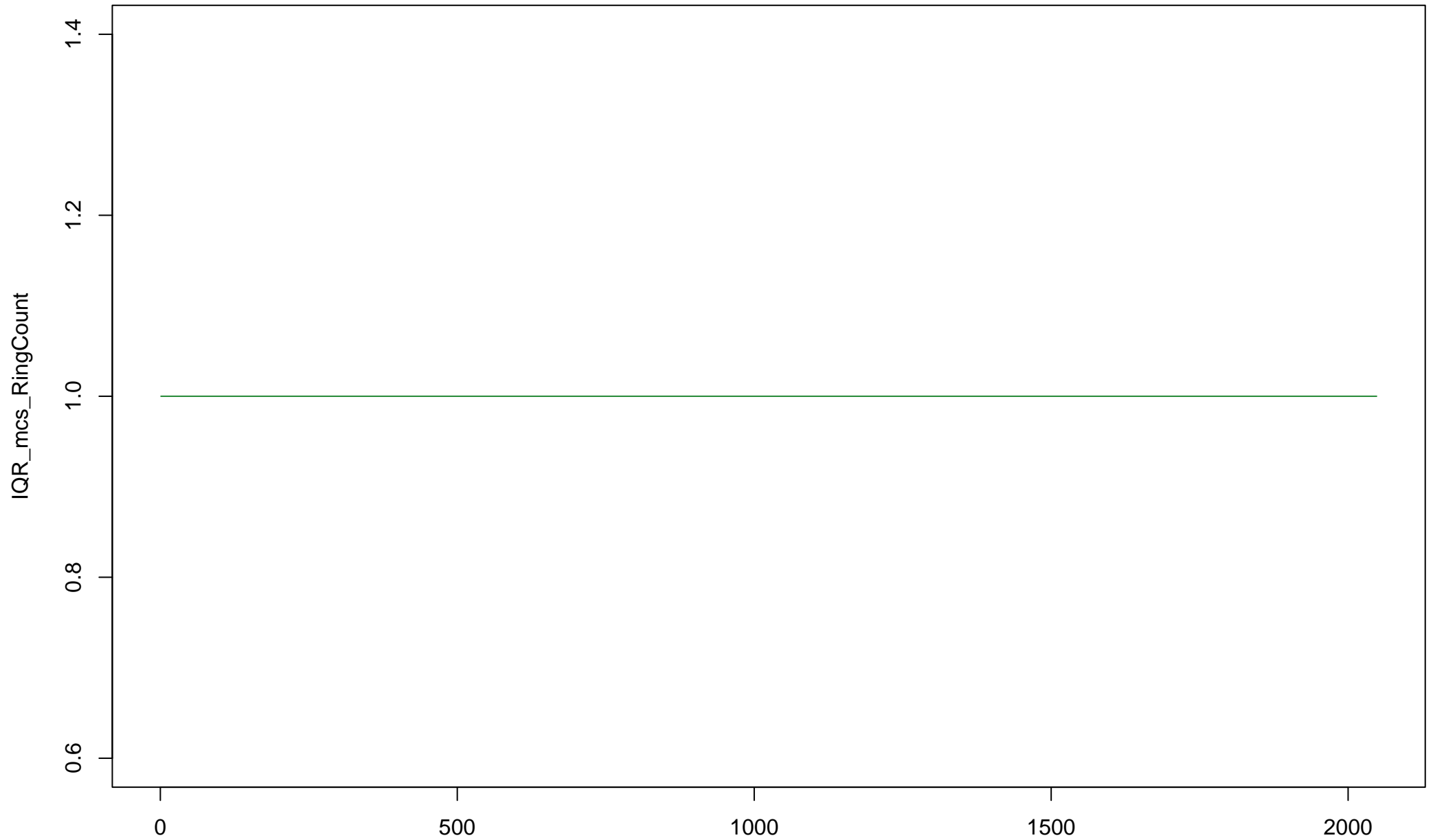
IQR_Xtransf_ec_tanimoto_similarity
ESS = 1180 | BMK = 0.111 | MCSE(6.27) = 3.33 | stat: FALSE | burn: 0



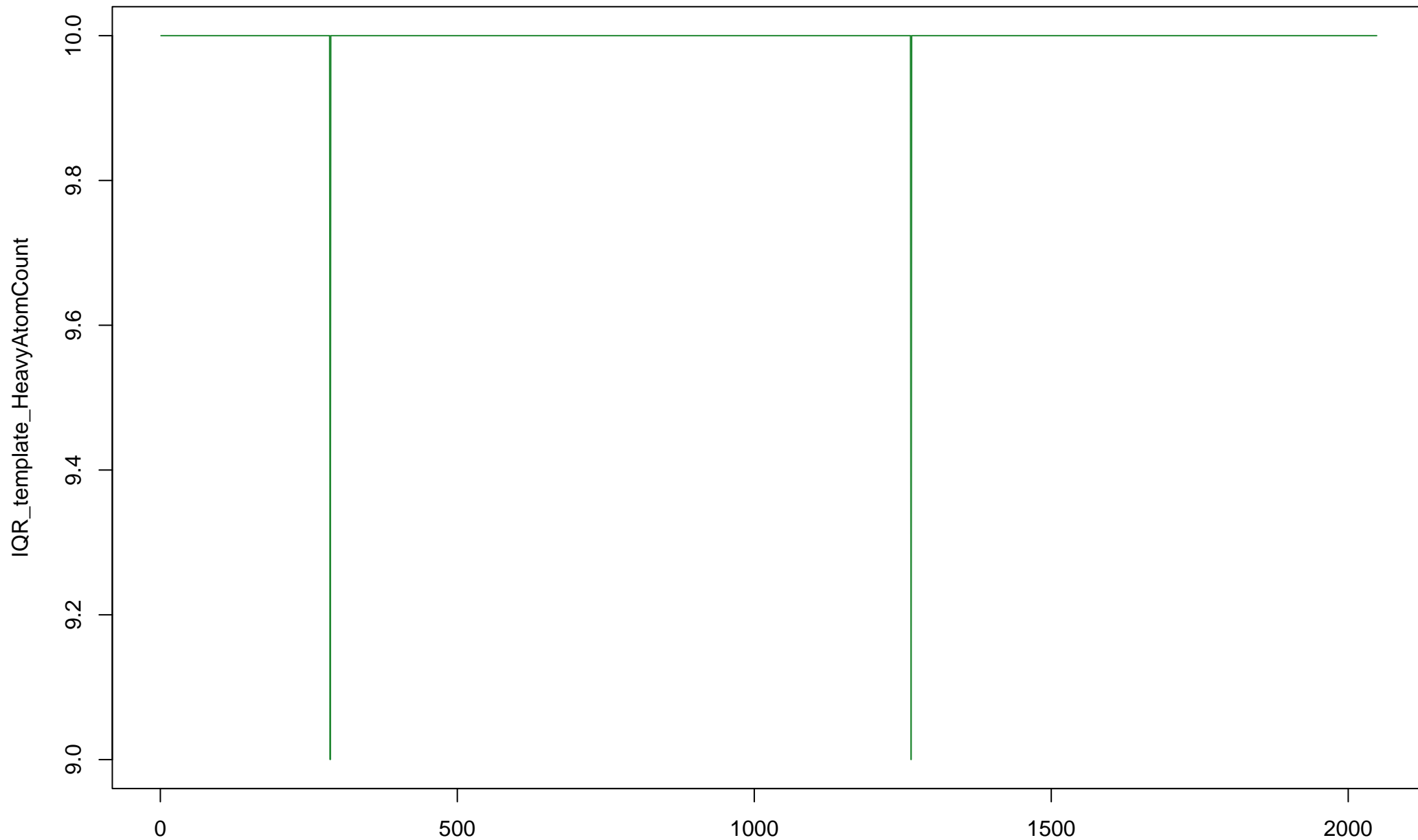
IQR_docked_HeavyAtomCount
ESS = 490 | BMK = 0.0322 | MCSE(6.27) = 4.18 | stat: TRUE | burn: 0



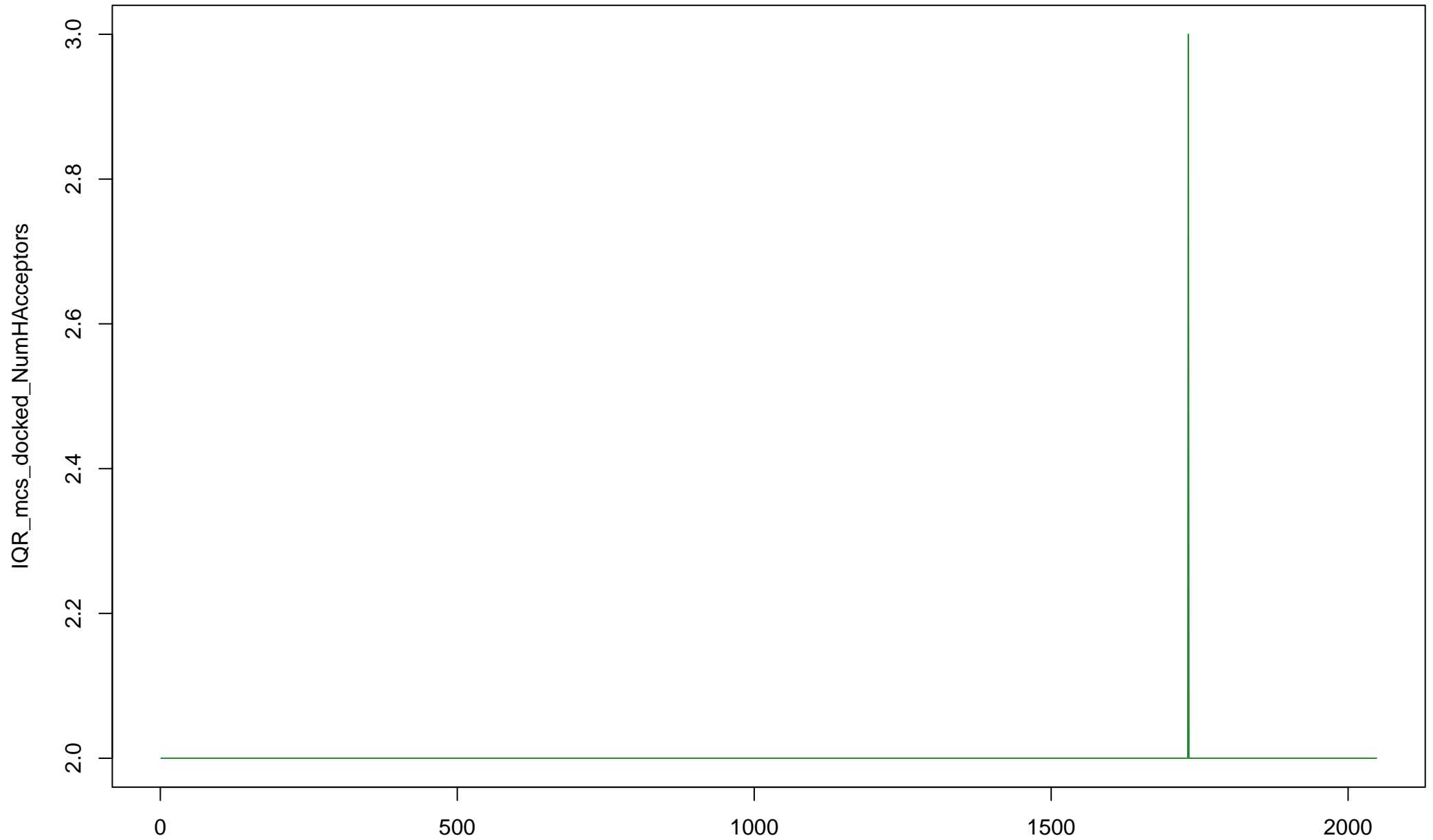
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



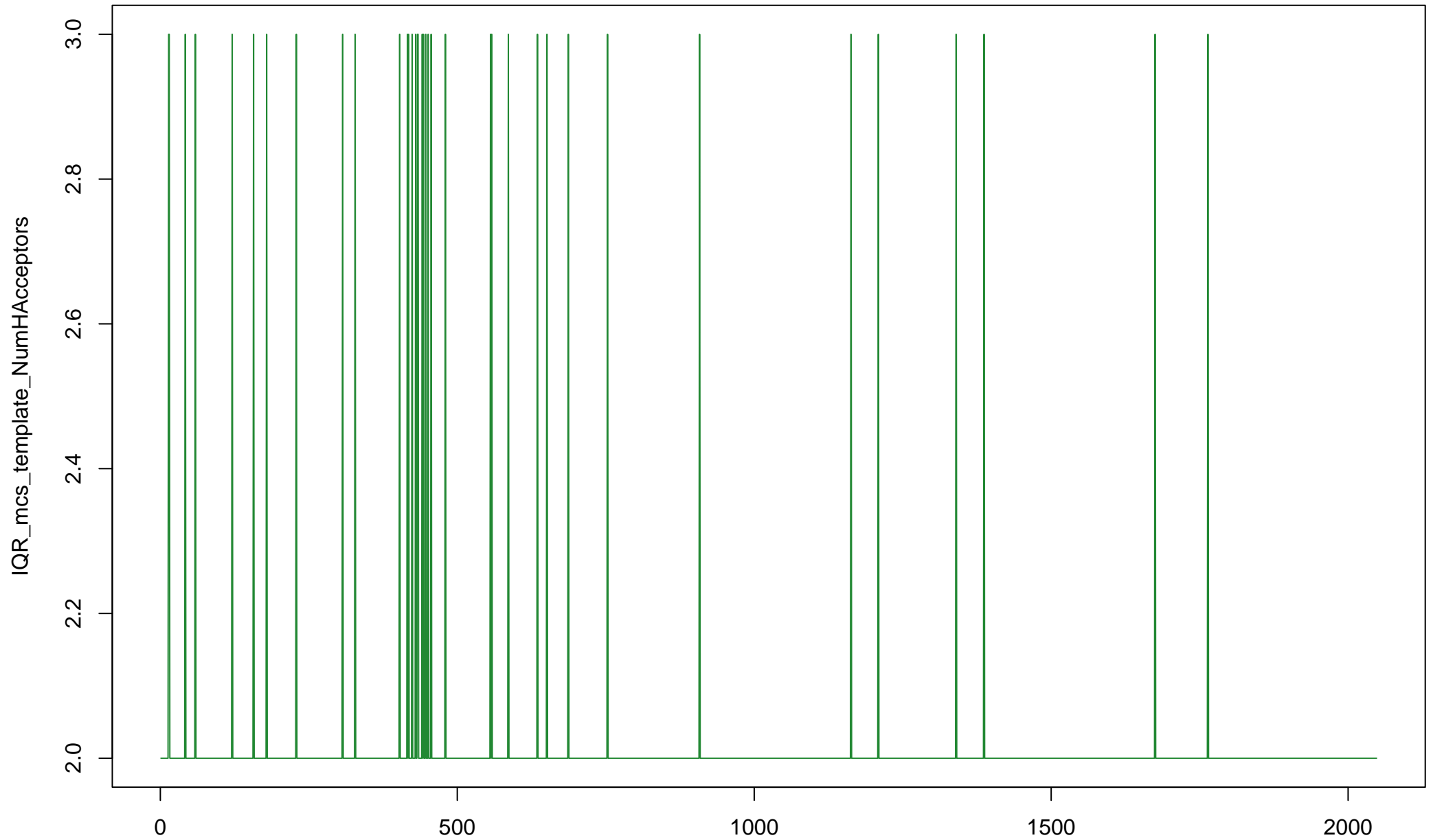
IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1428



IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.644 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 2040



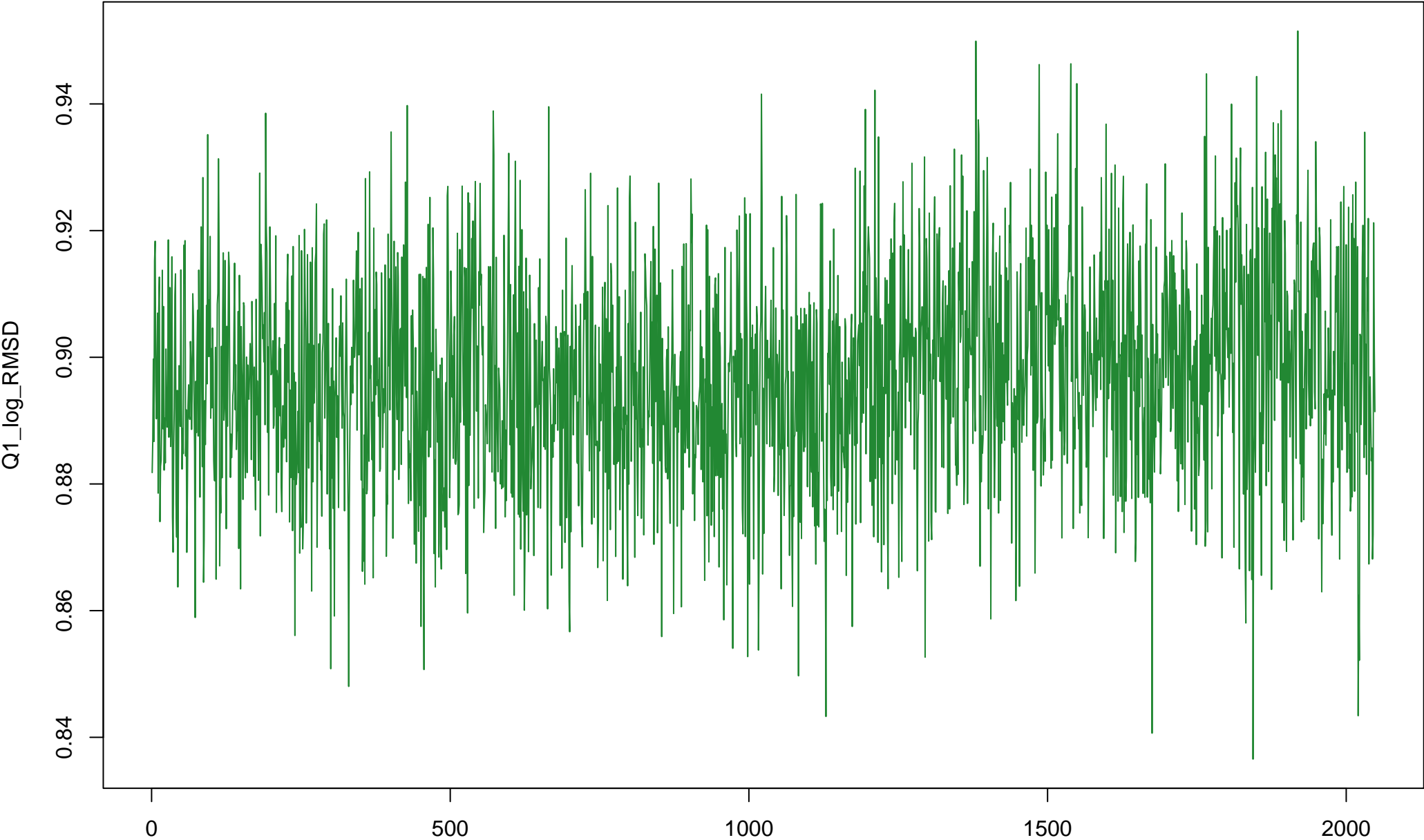
IQR_mcs_template_NumHAcceptors
ESS = 427 | BMK = 0.268 | MCSE(6.27) = 3.66 | stat: TRUE | burn: 2040



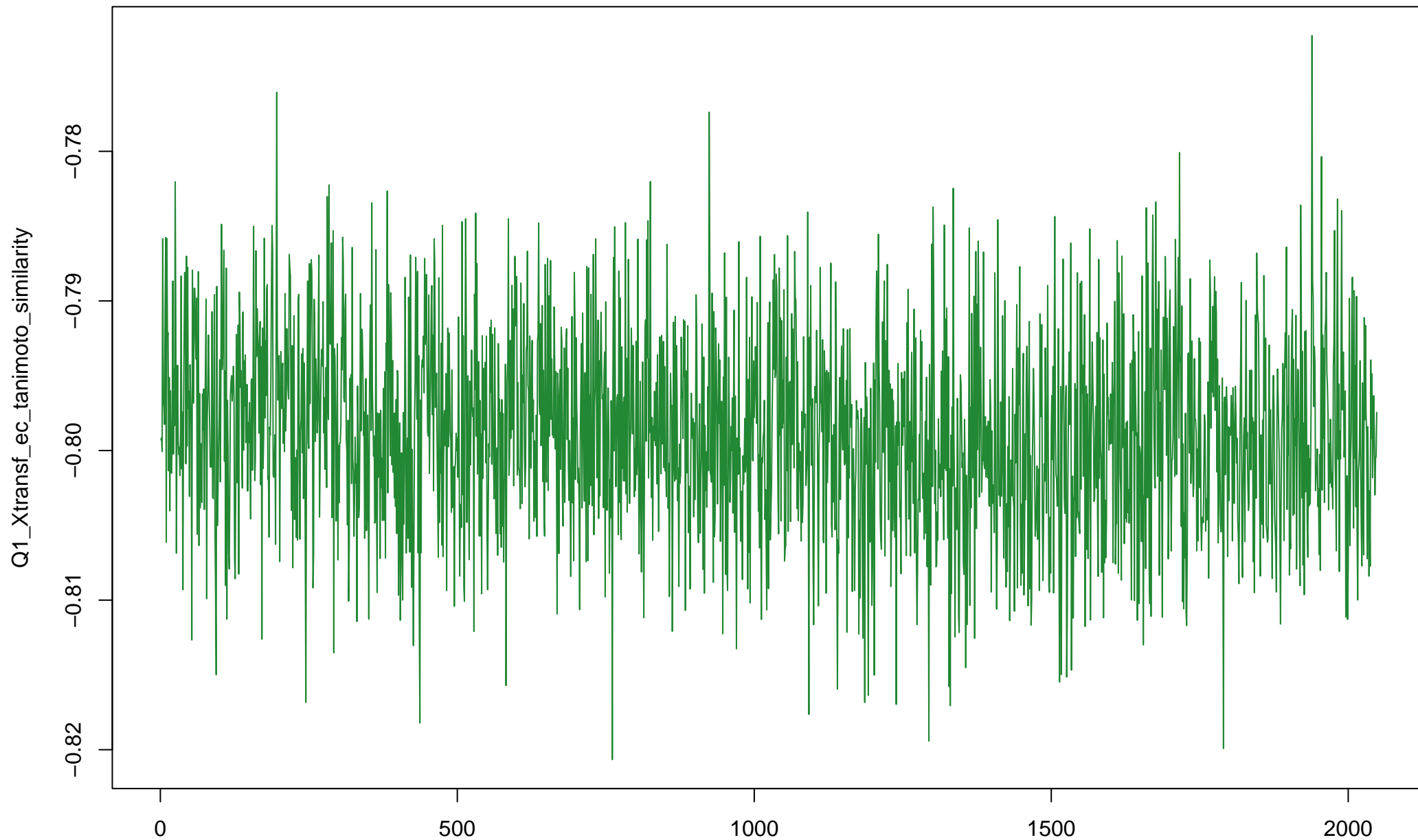
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



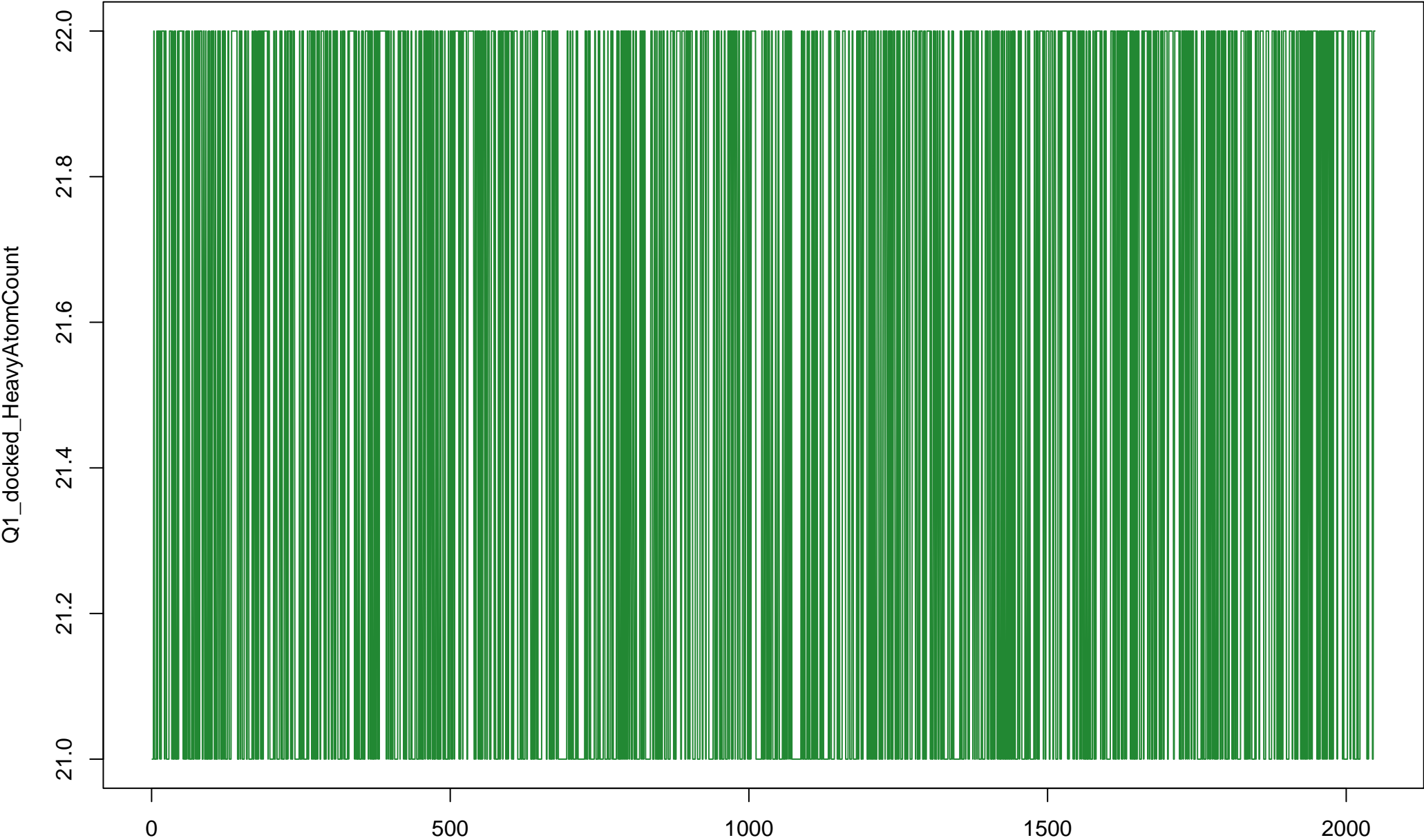
Q1_log_RMSD
ESS = 1440 | BMK = 0.107 | MCSE(6.27) = 3.4 | stat: FALSE | burn: 0



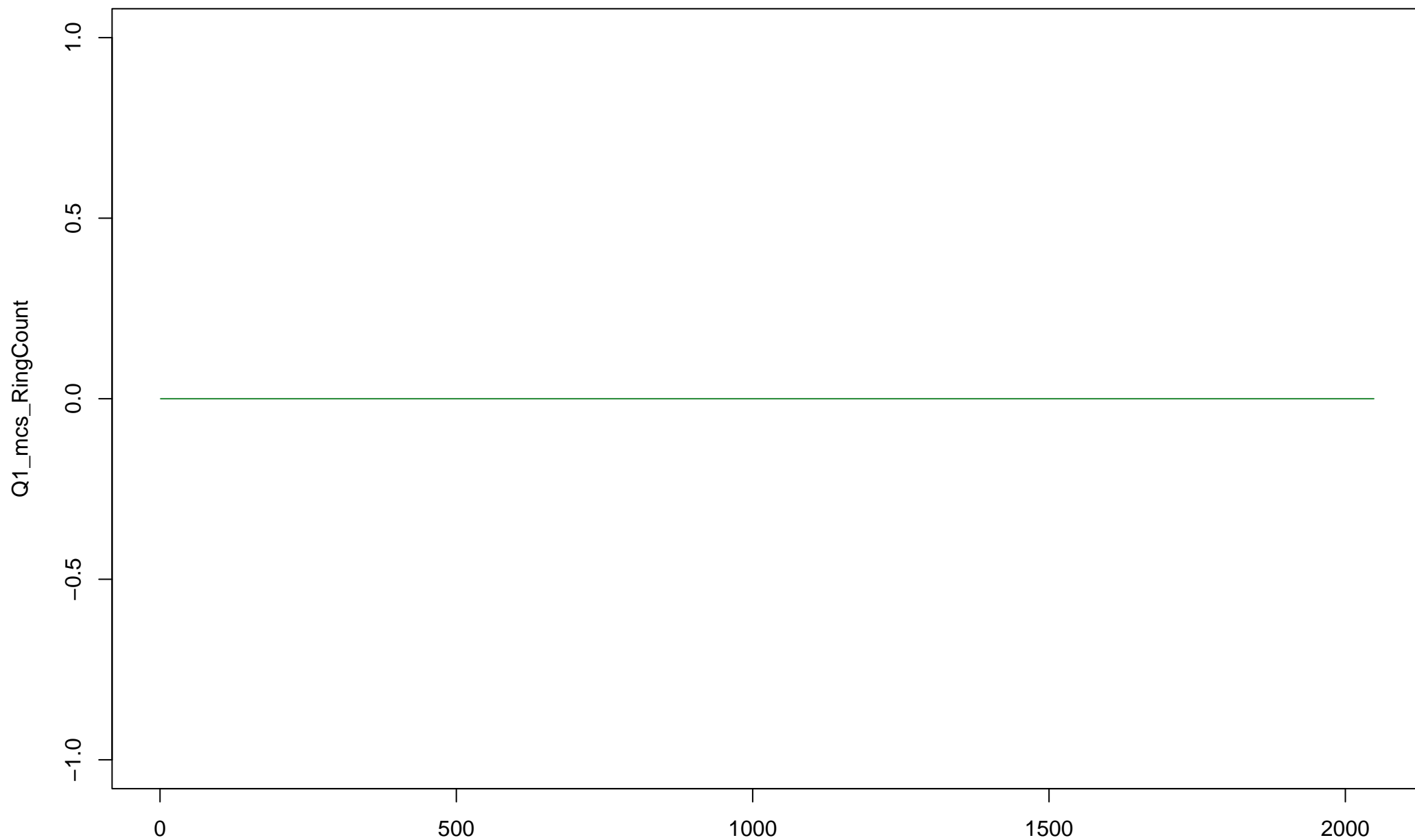
Q1_Xtransf_ec_tanimoto_similarity
ESS = 1400 | BMK = 0.0921 | MCSE(6.27) = 3.38 | stat: FALSE | burn: 0



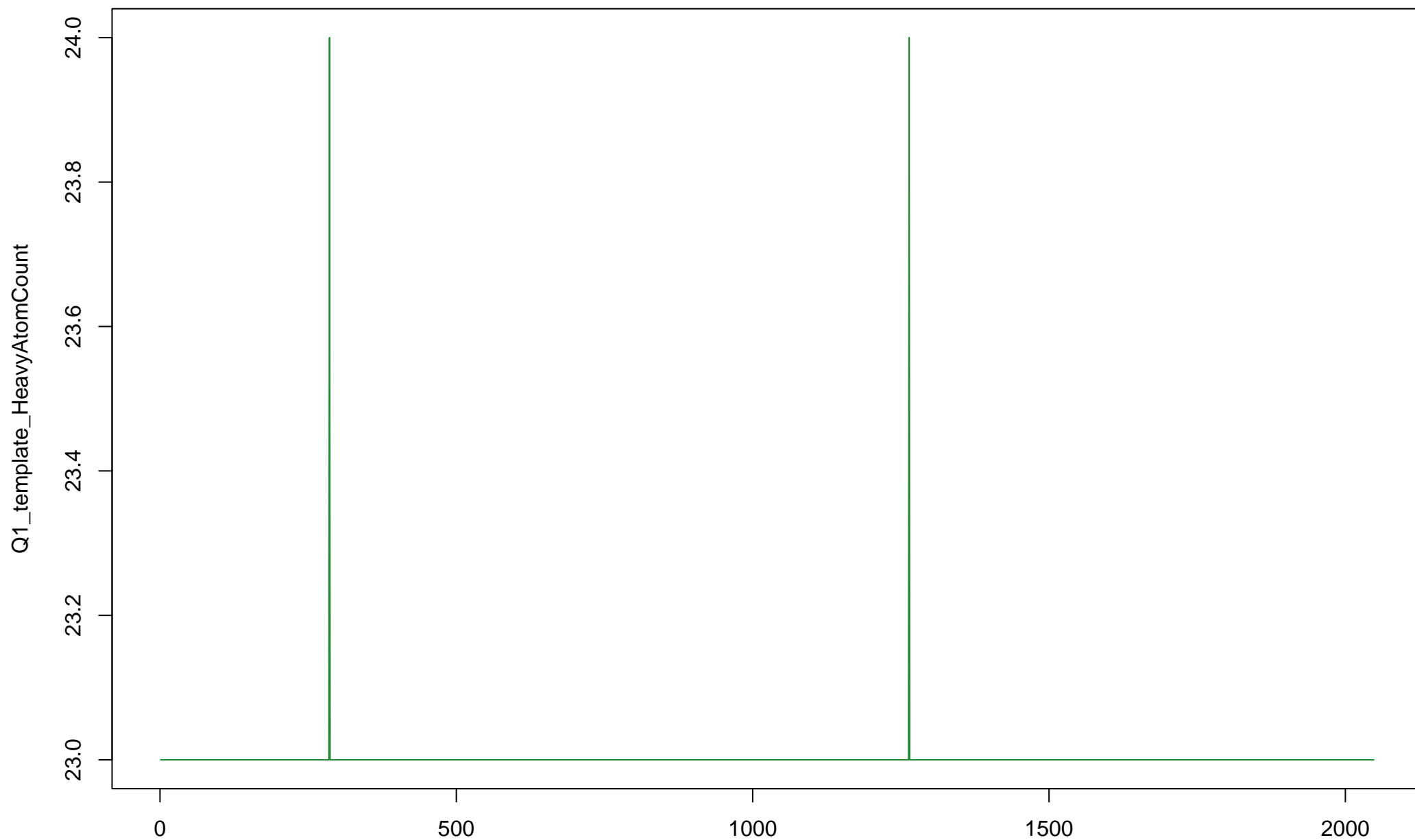
Q1_docked_HeavyAtomCount
ESS = 917 | BMK = 0.0137 | MCSE(6.27) = 3.51 | stat: TRUE | burn: 0



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



Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1428



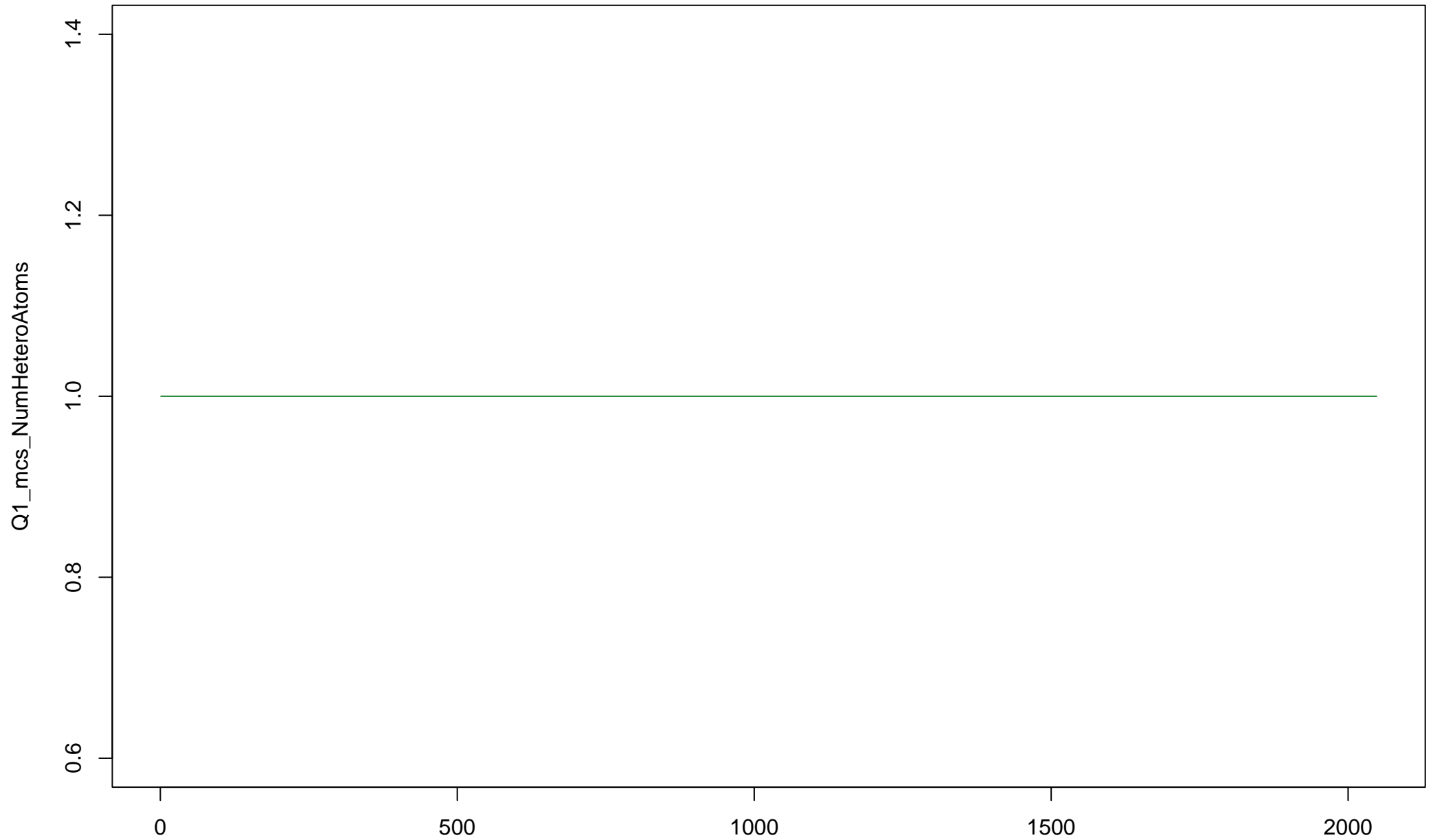
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



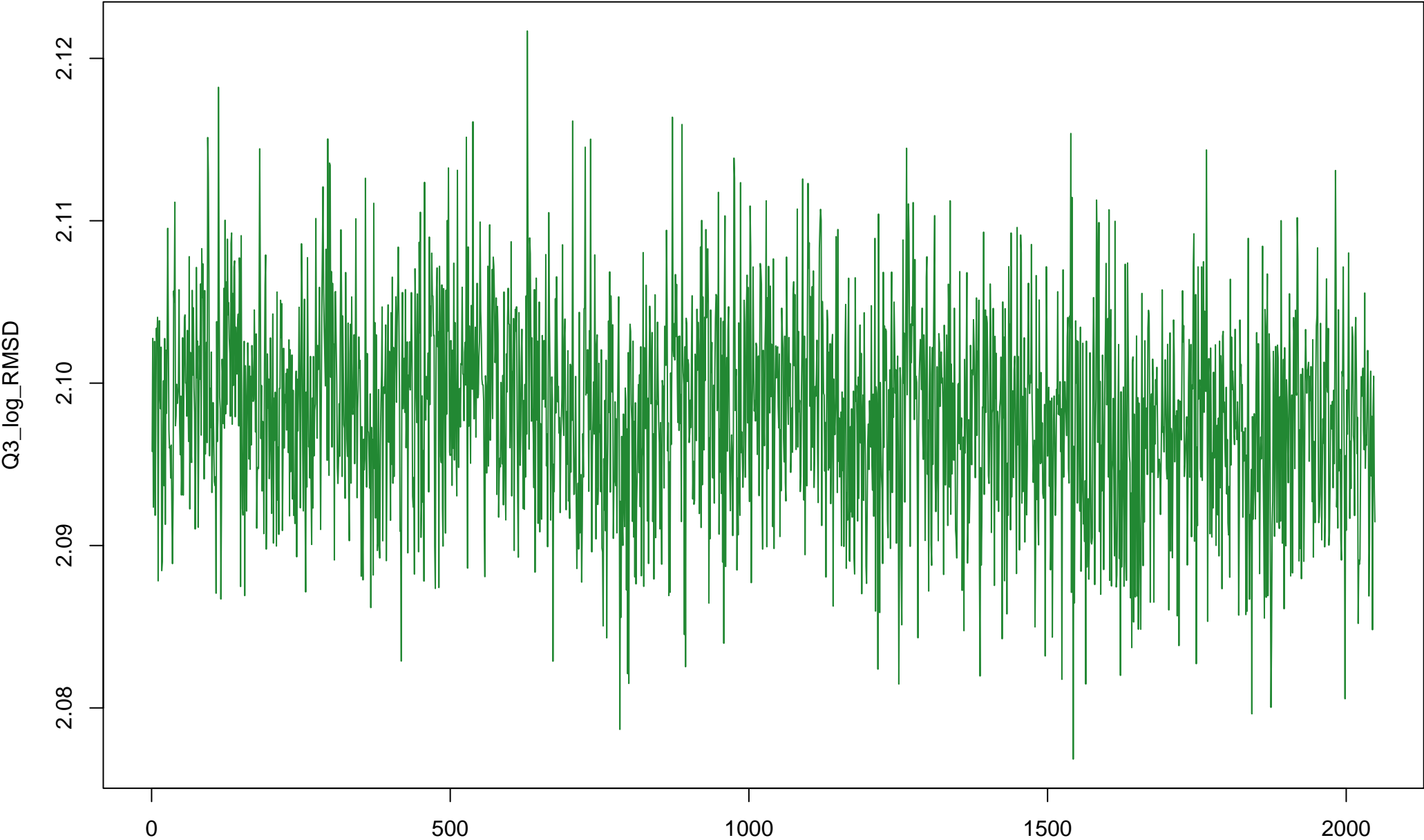
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



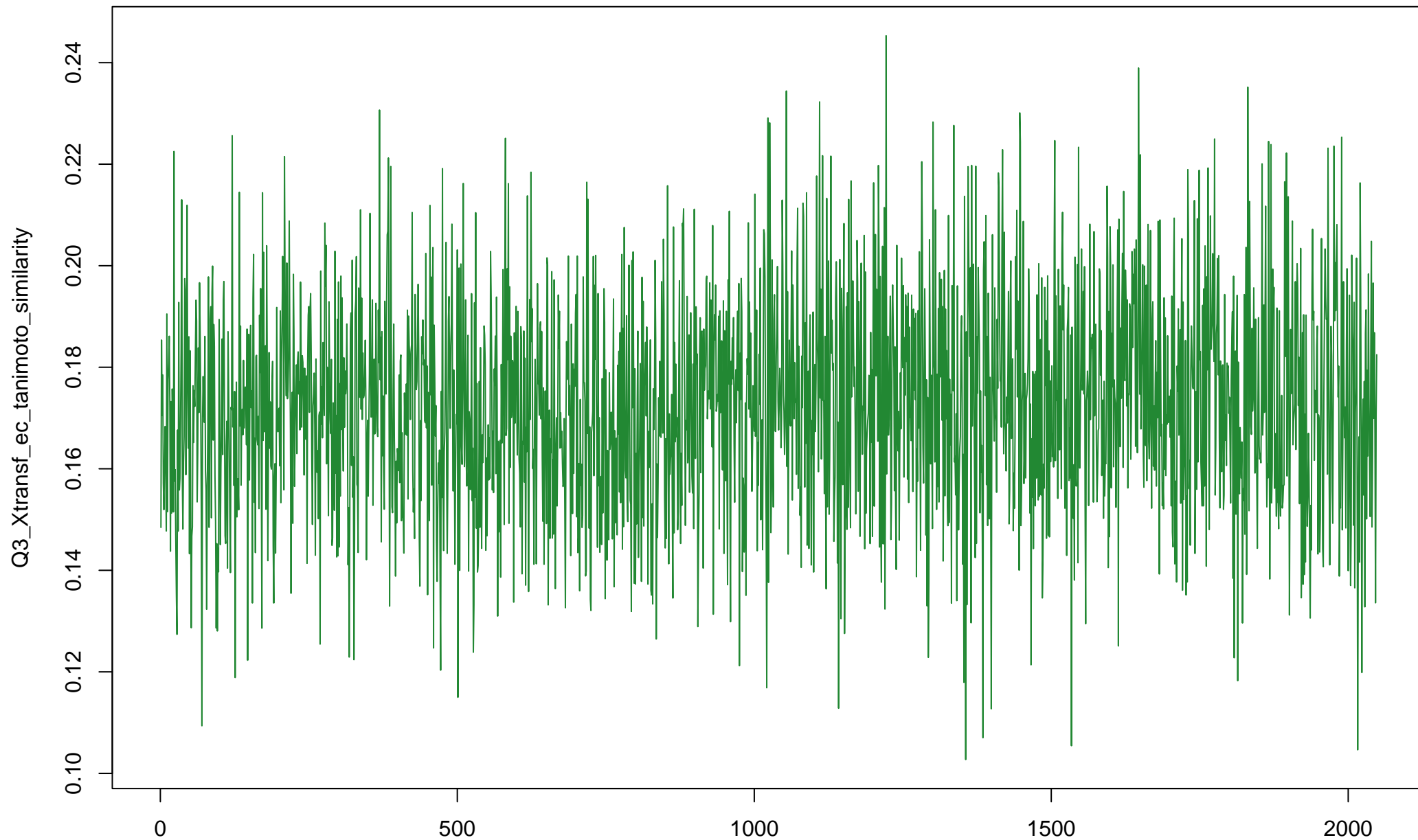
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



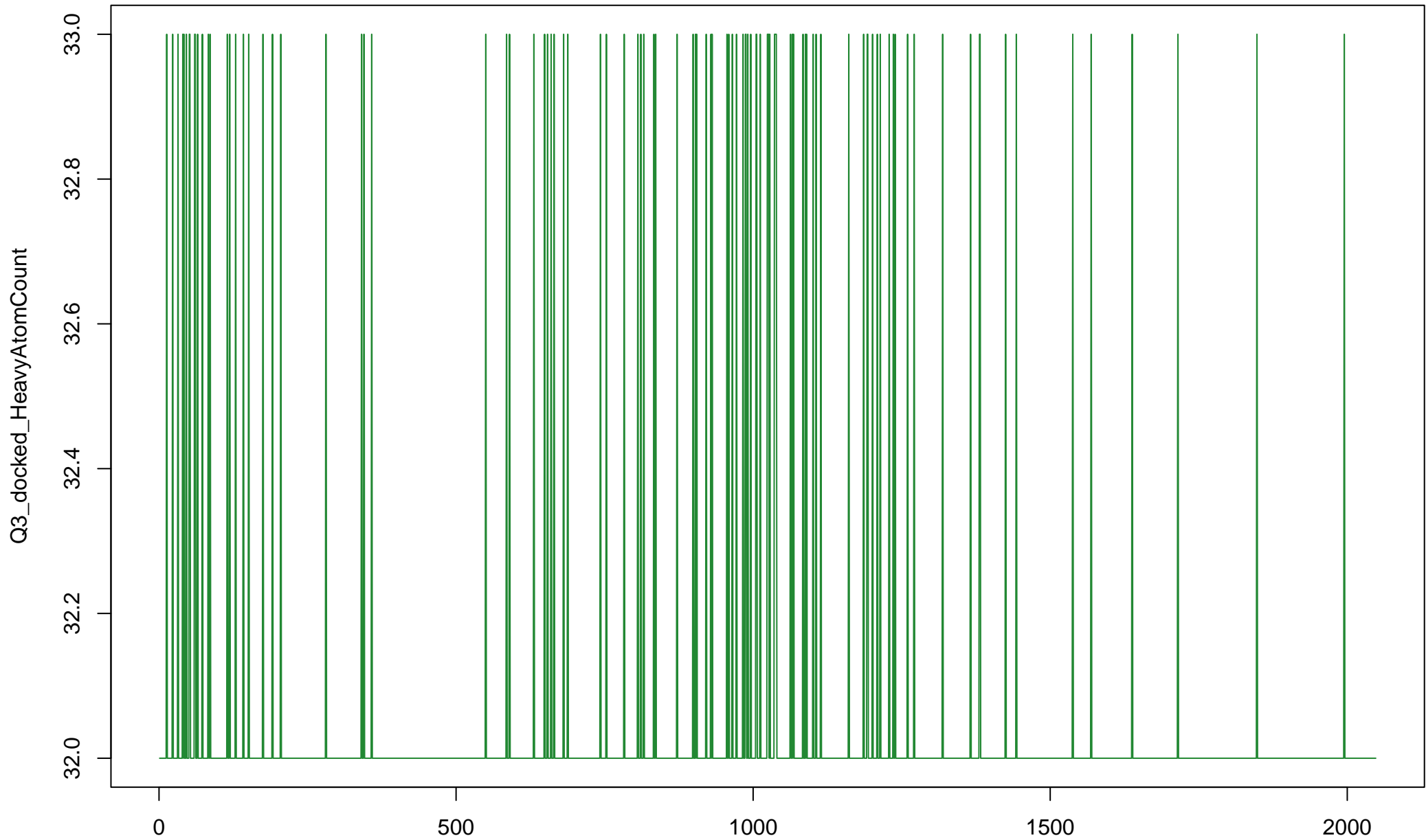
Q3_log_RMSD
ESS = 618 | BMK = 0.102 | MCSE(6.27) = 4.11 | stat: FALSE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0973 | MCSE(6.27) = 2.62 | stat: FALSE | burn: 0



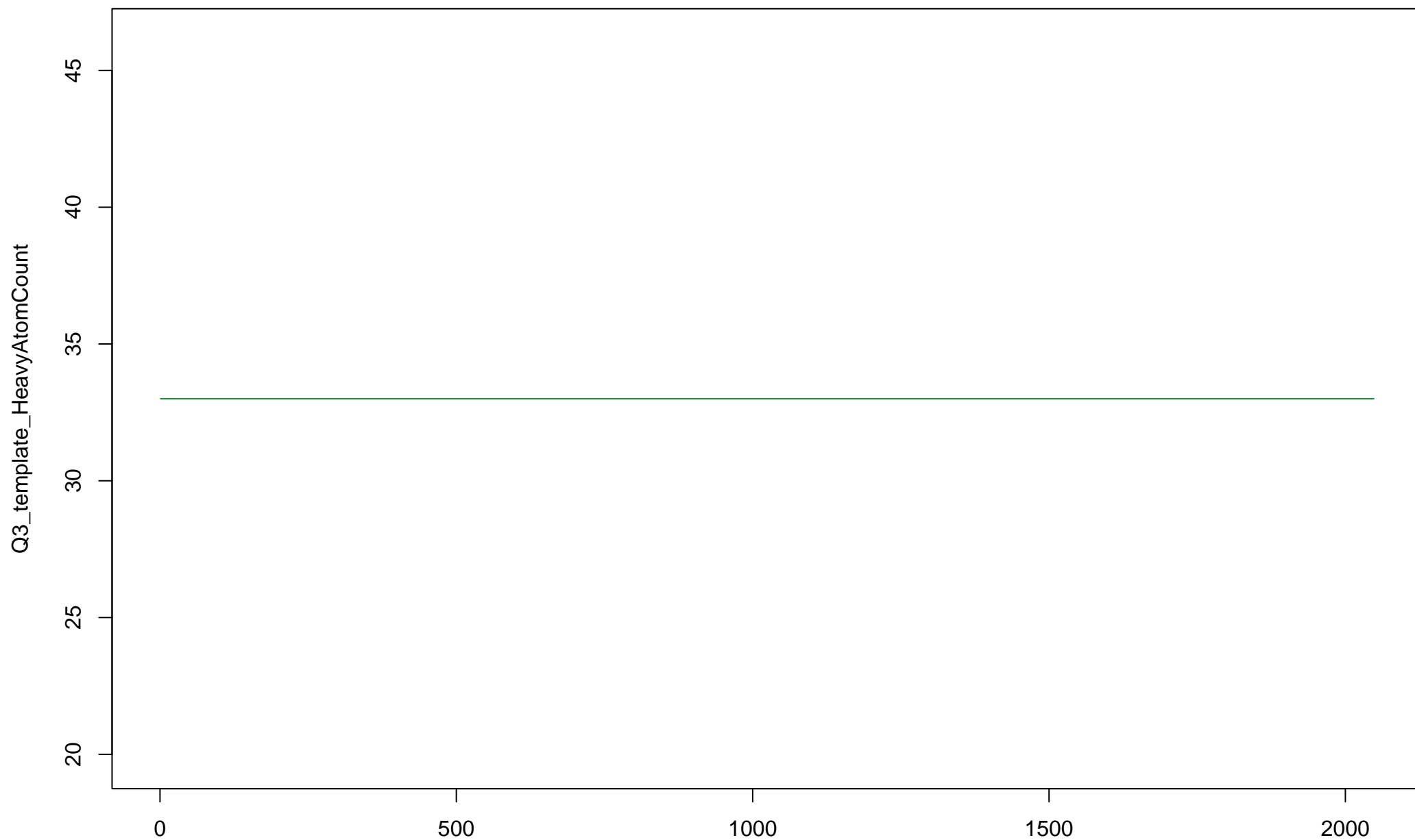
Q3_docked_HeavyAtomCount
ESS = 256 | BMK = 0.0828 | MCSE(6.27) = 3.74 | stat: FALSE | burn: 0



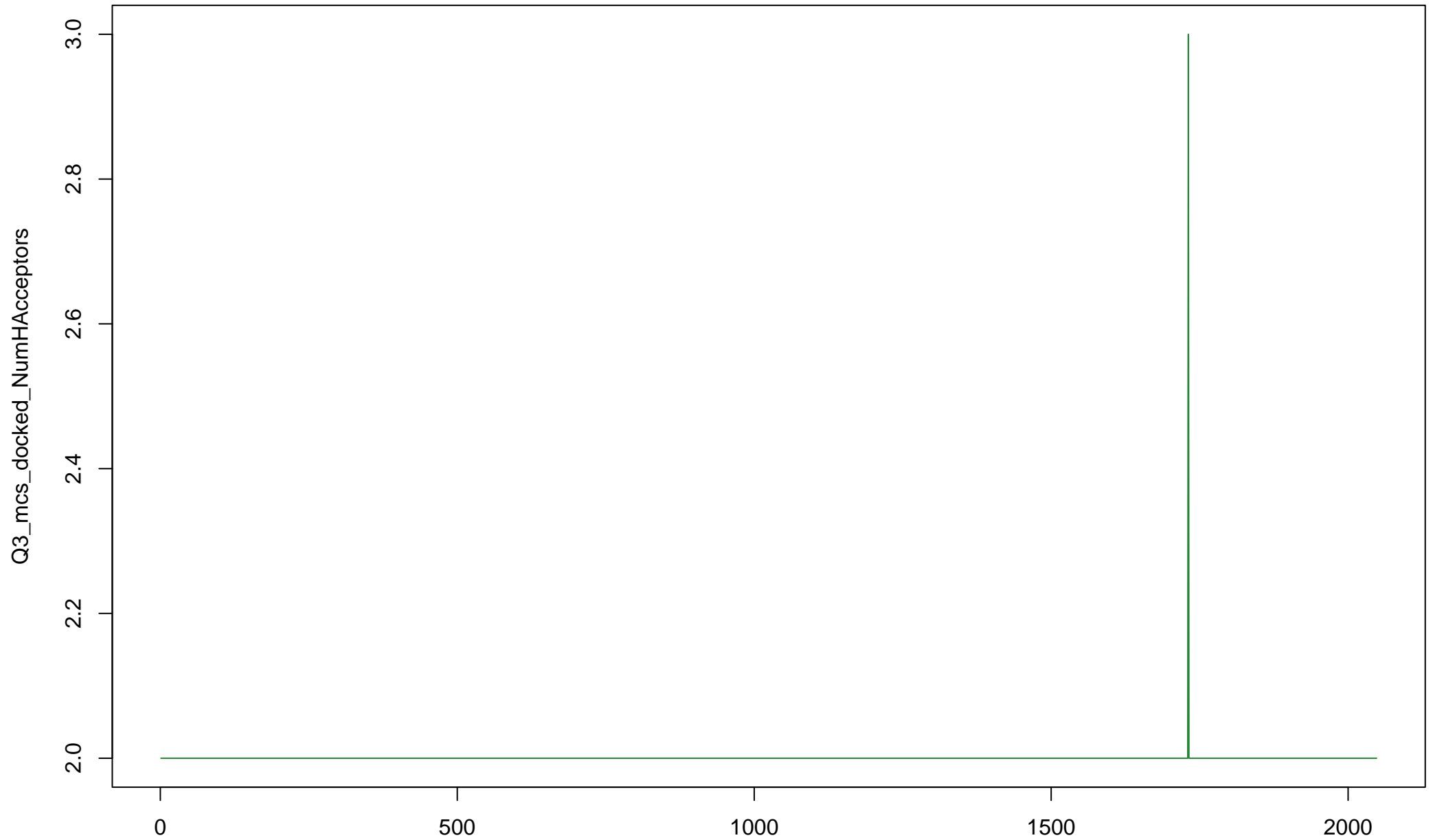
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



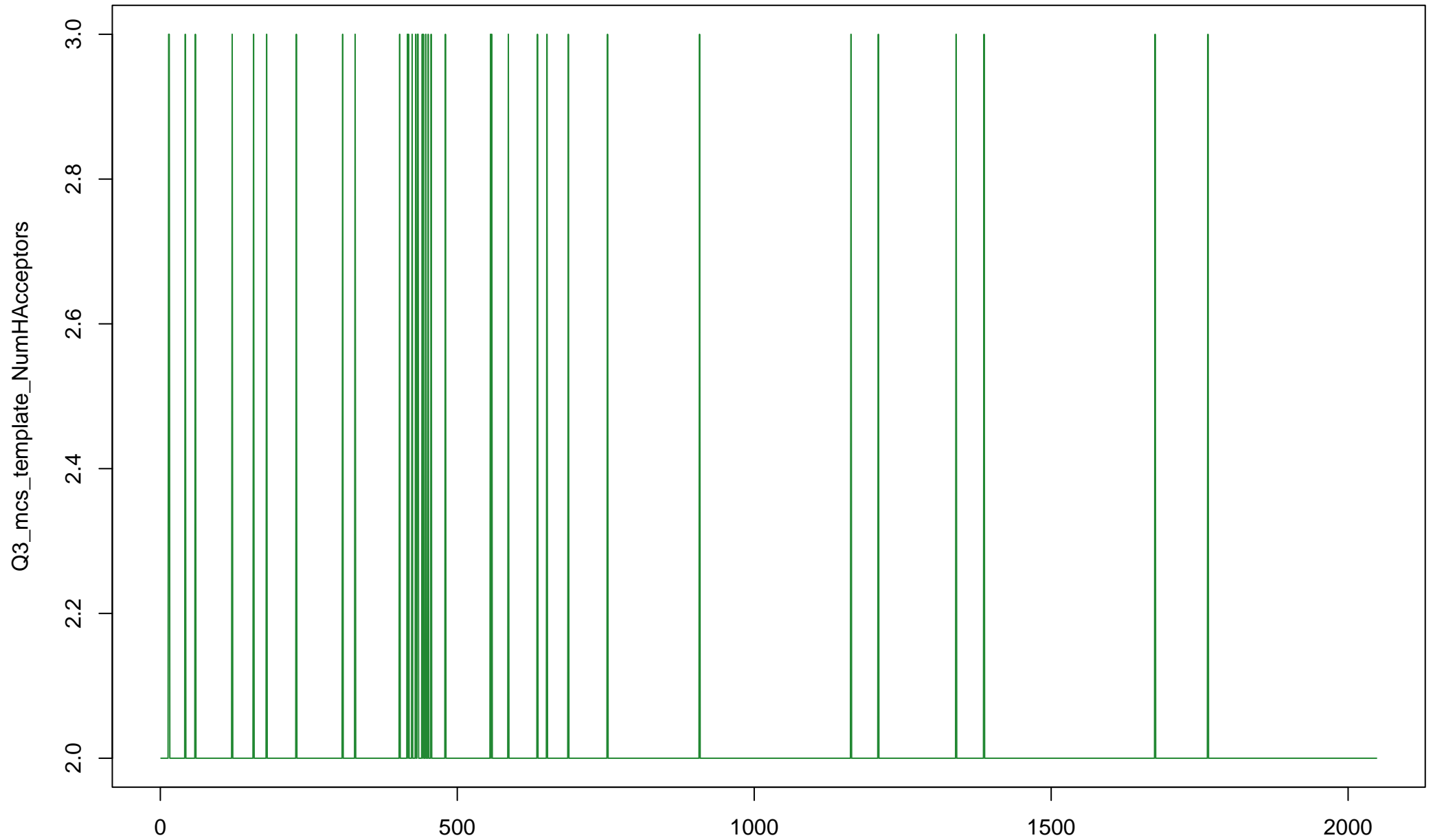
Q3_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.644 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 2040



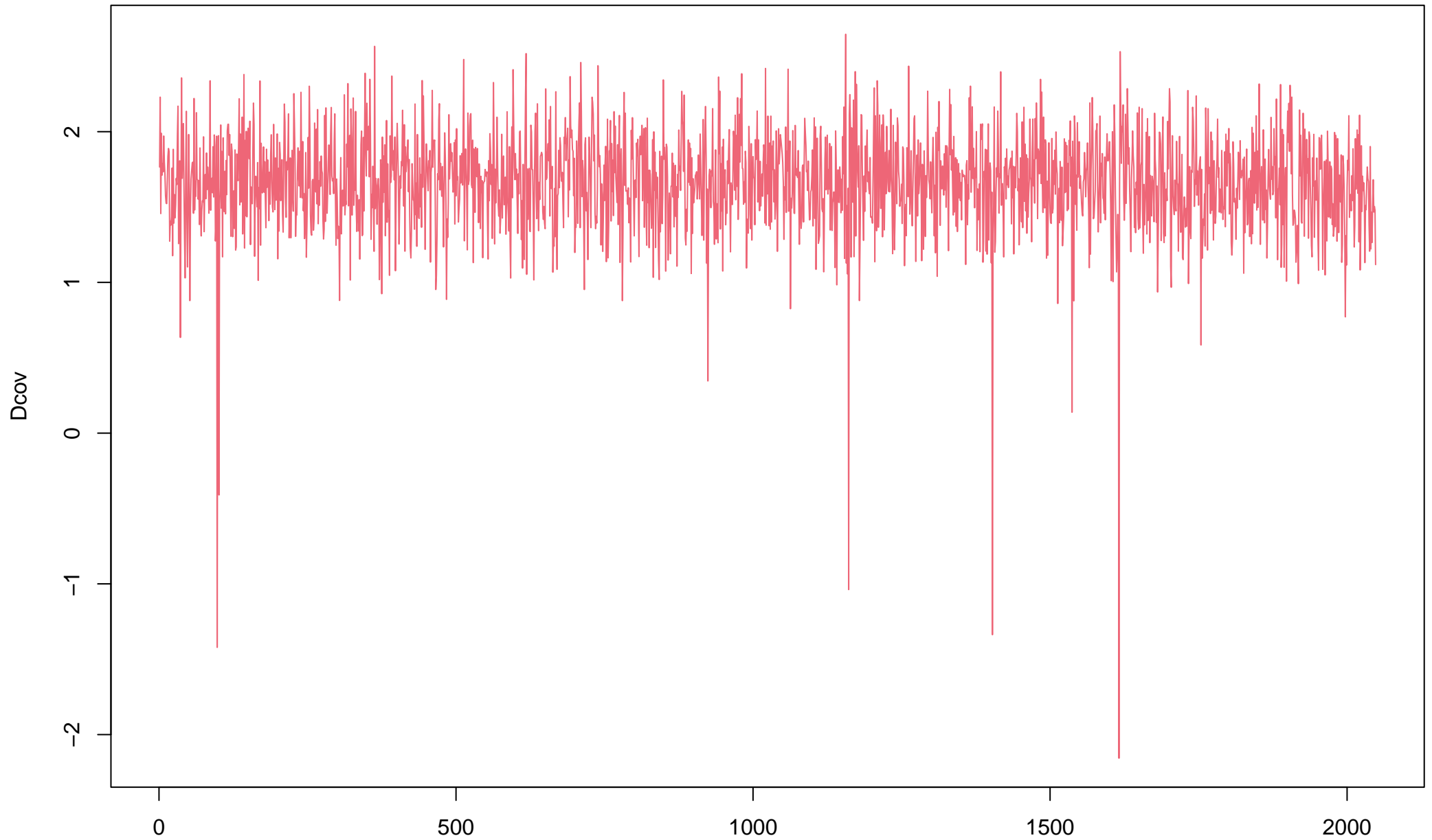
Q3_mcs_template_NumHAcceptors
ESS = 427 | BMK = 0.268 | MCSE(6.27) = 3.66 | stat: TRUE | burn: 2040



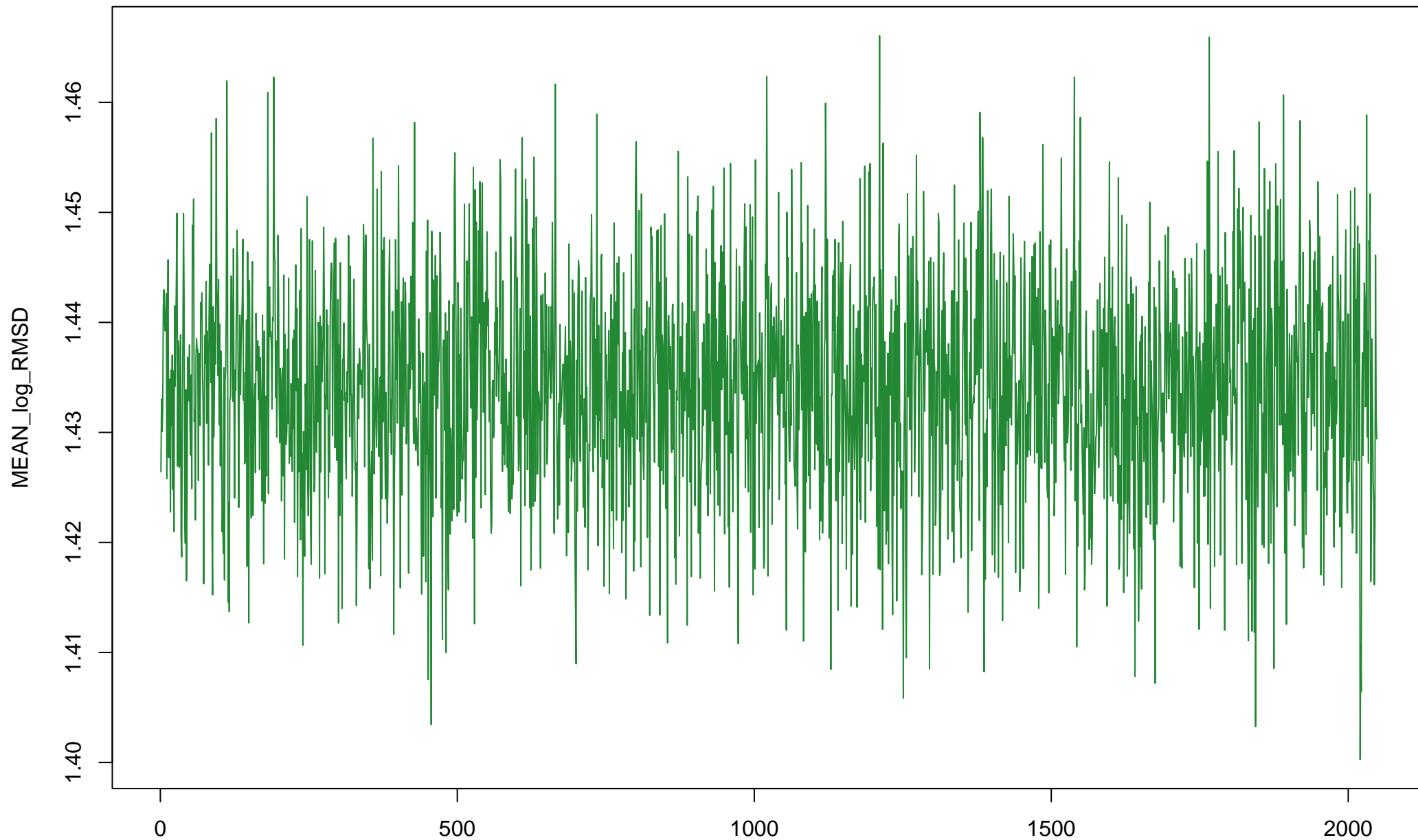
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



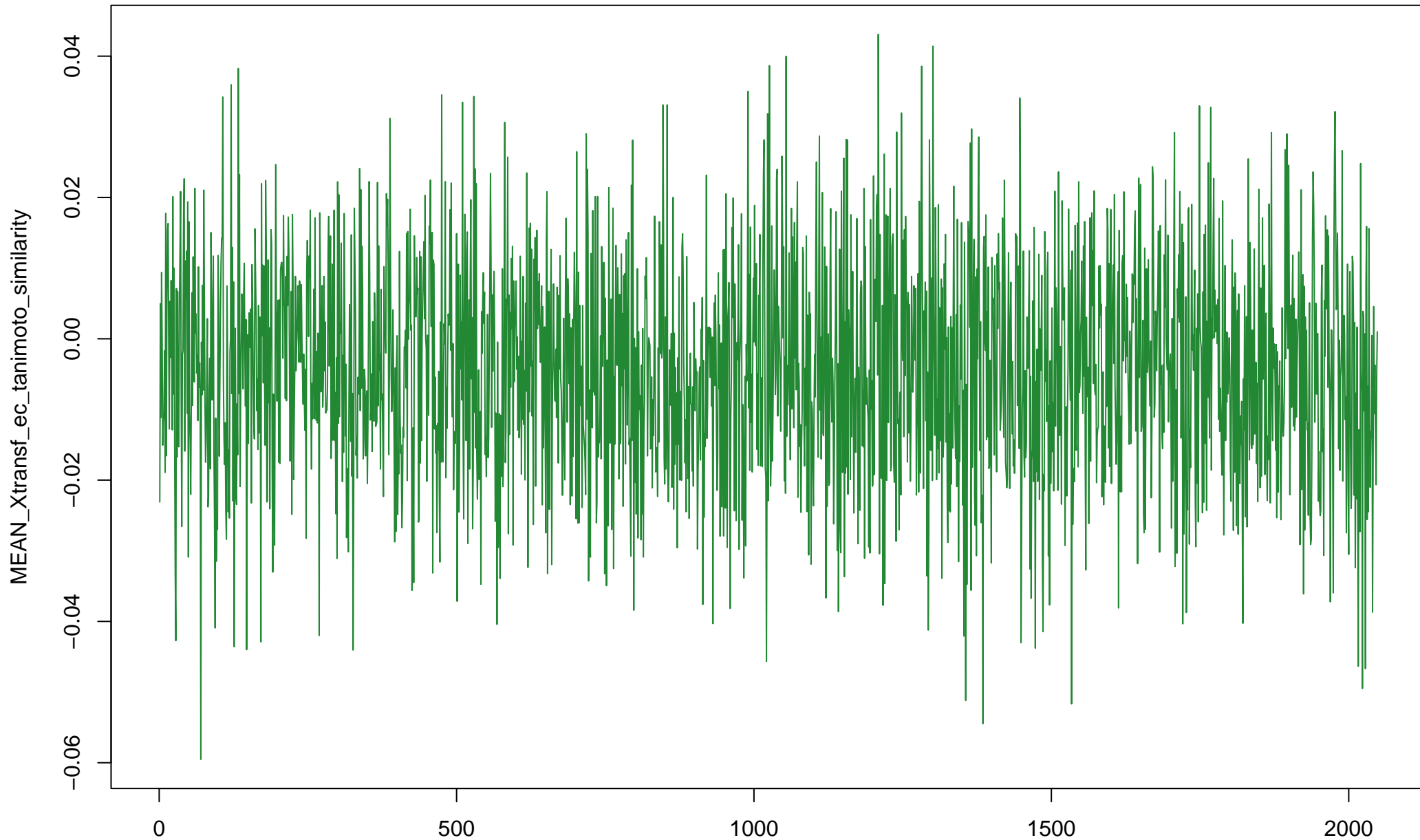
Dcov
ESS = 2050 | BMK = 0.0407 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0



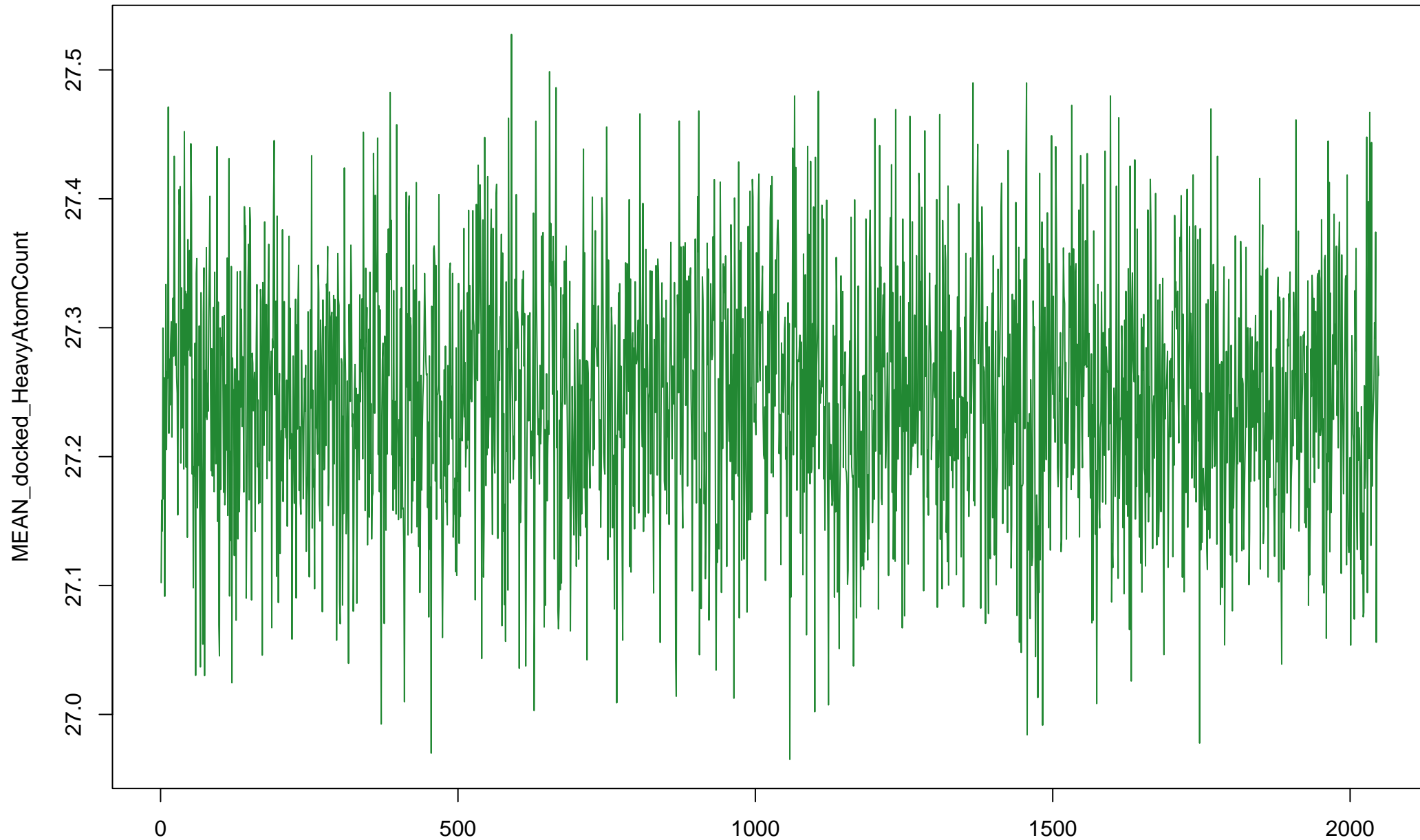
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0405 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



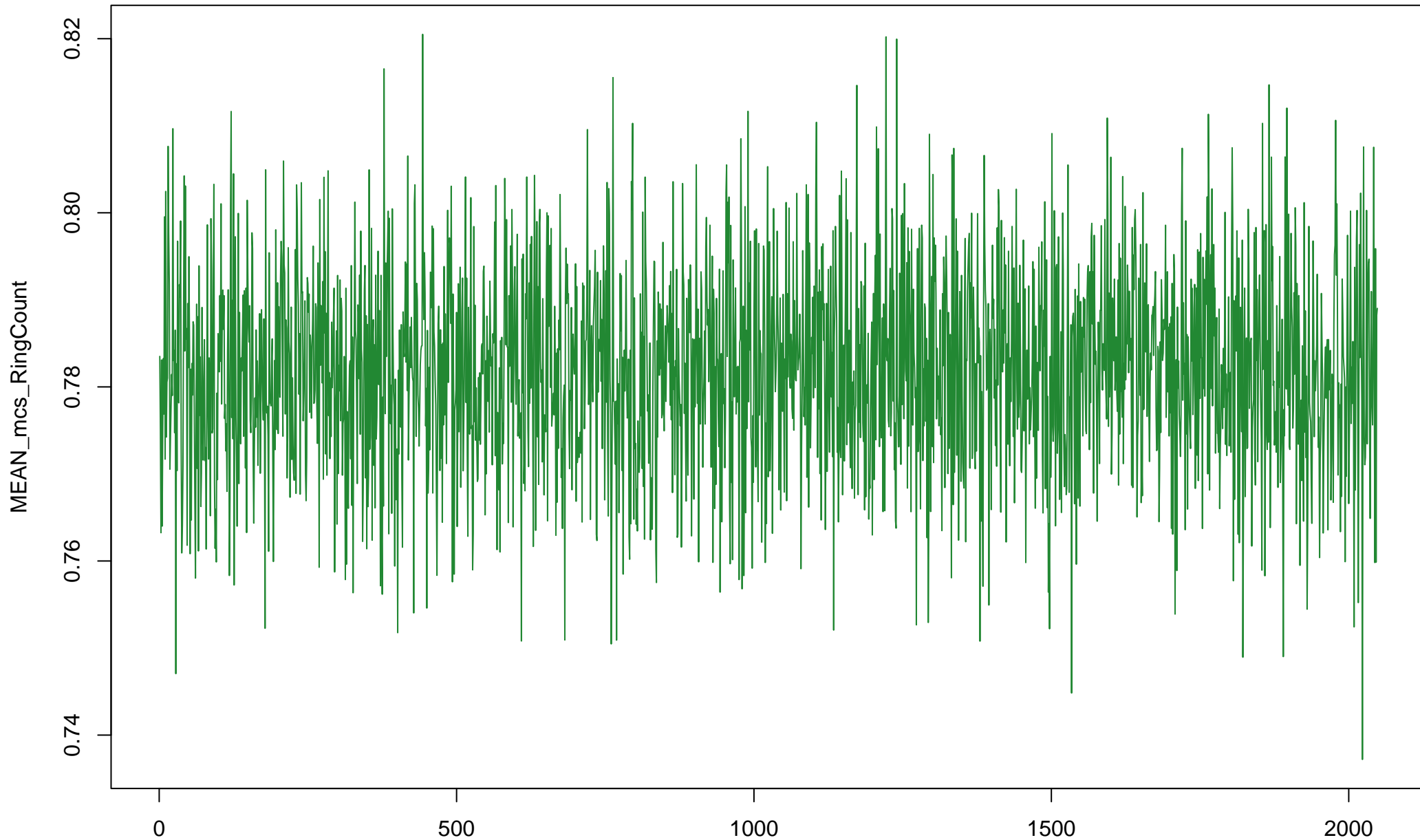
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 1830 | BMK = 0.0476 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0



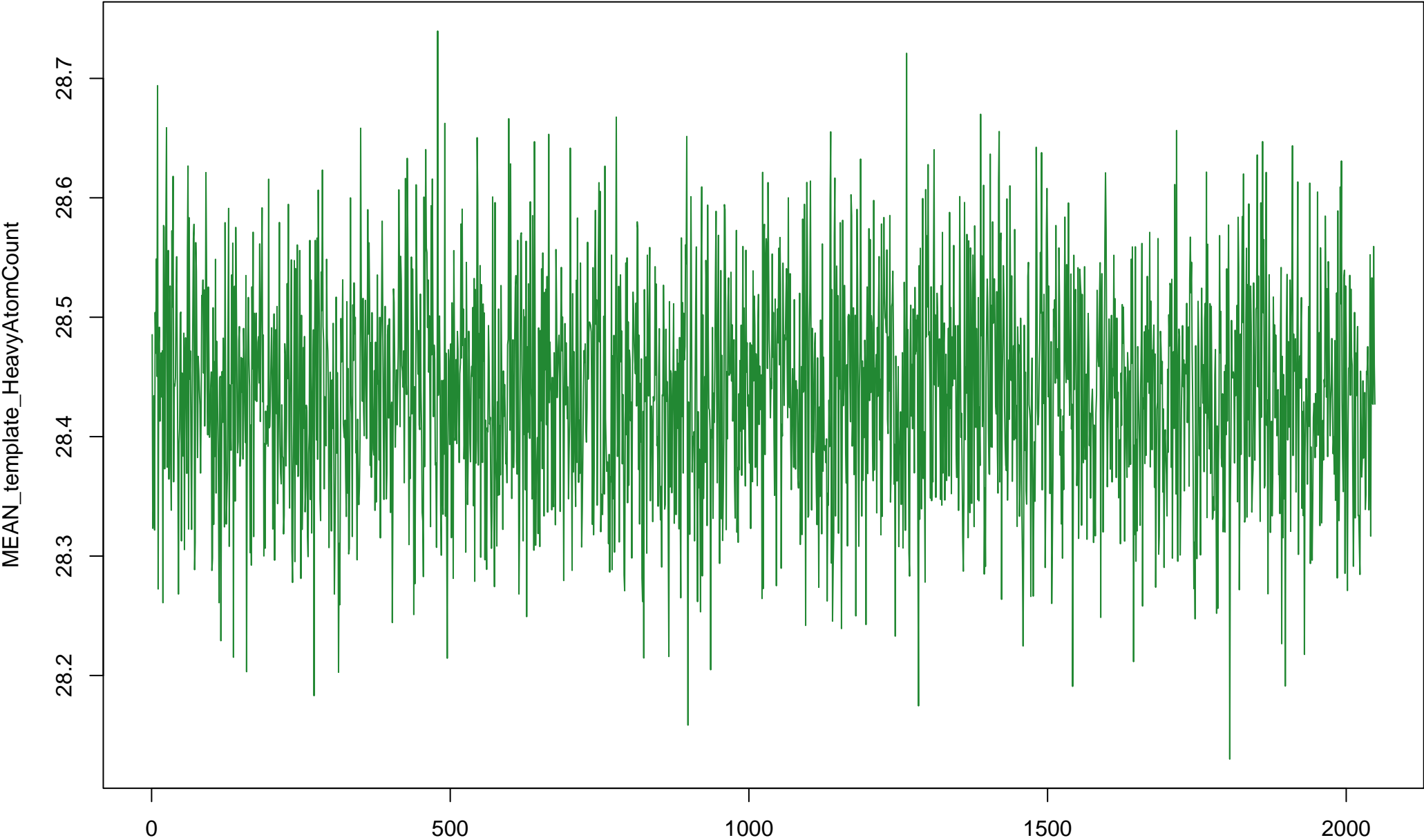
MEAN_docked_HeavyAtomCount
ESS = 1780 | BMK = 0.0519 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0



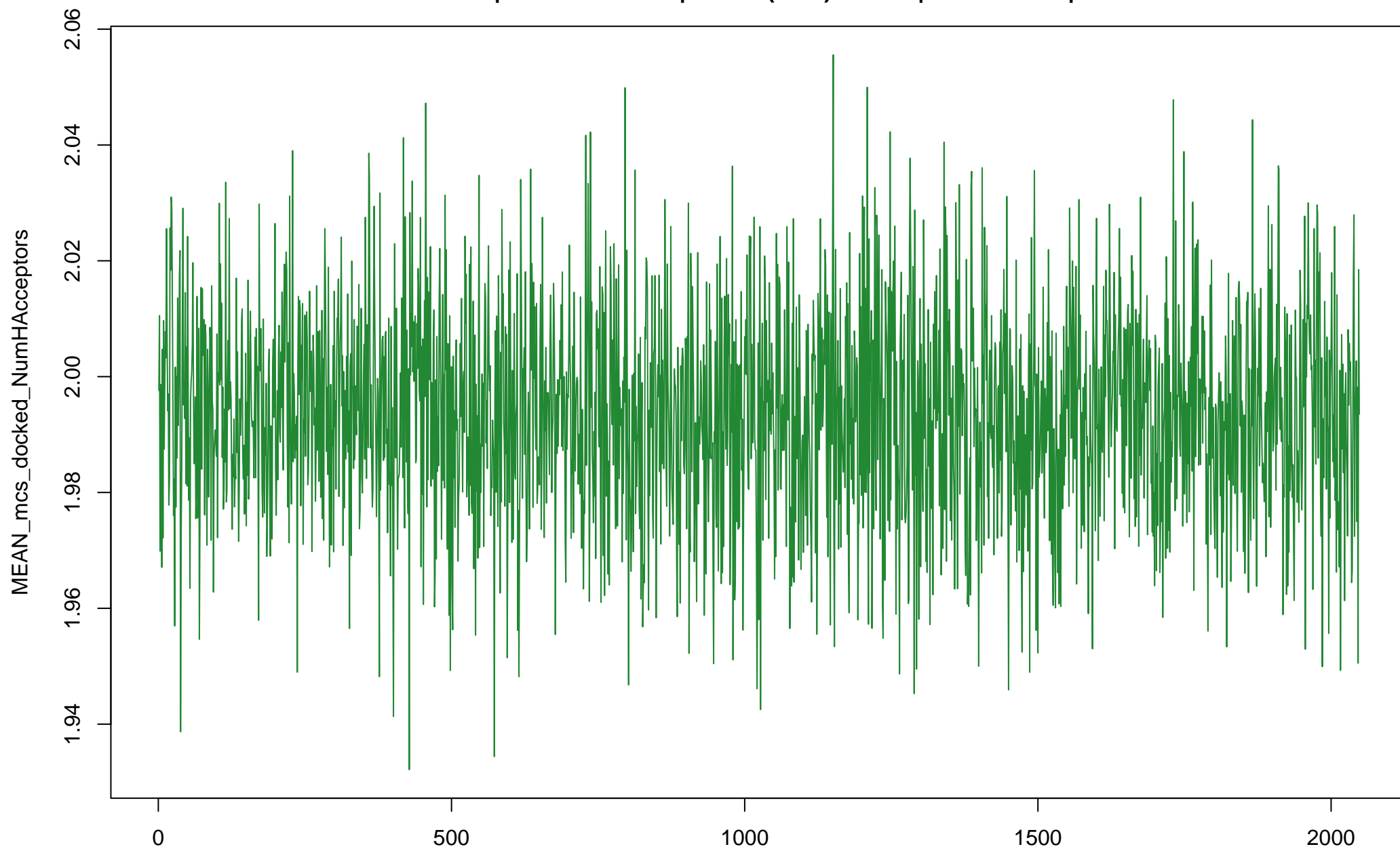
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0549 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0



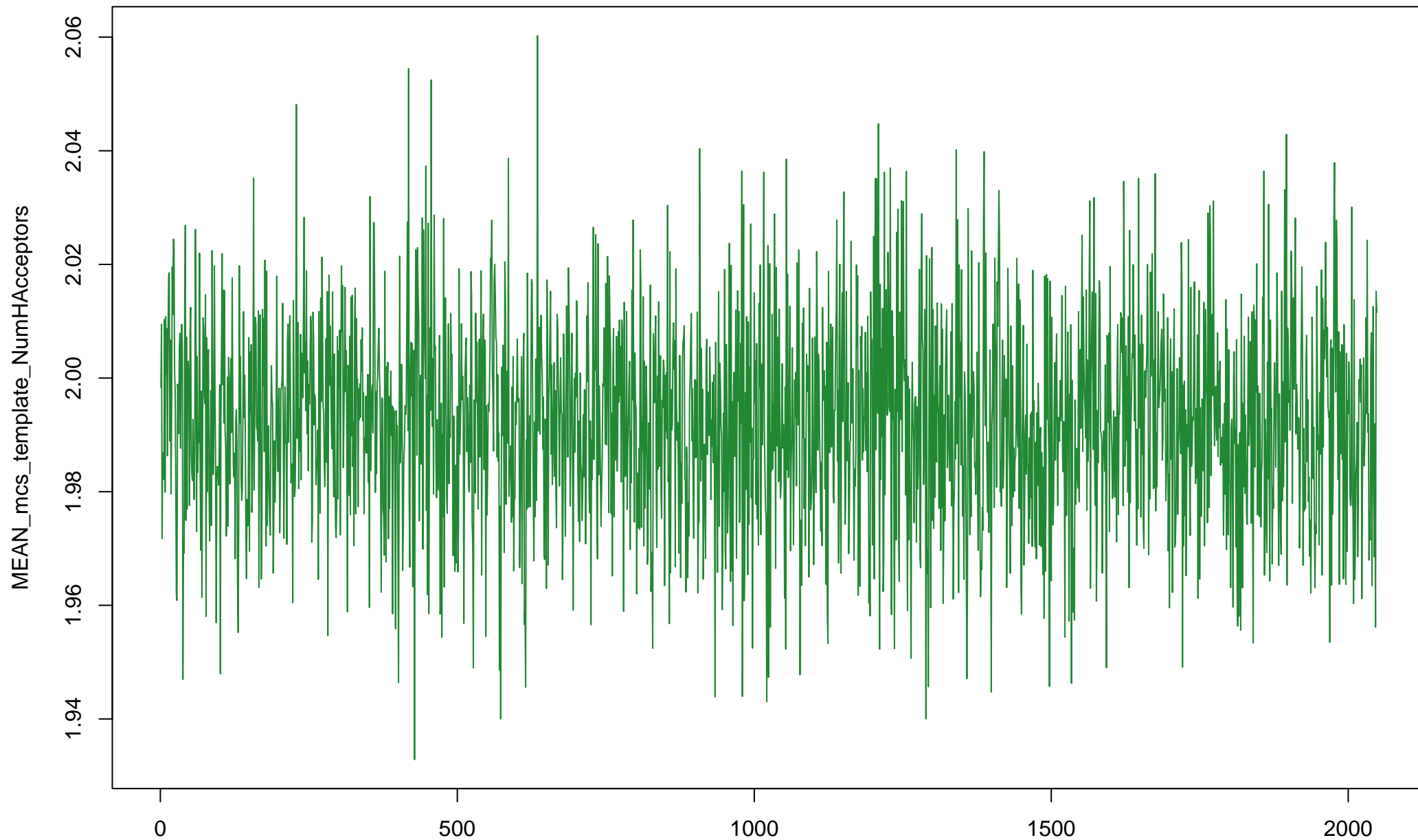
MEAN_template_HeavyAtomCount
ESS = 1890 | BMK = 0.0288 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0



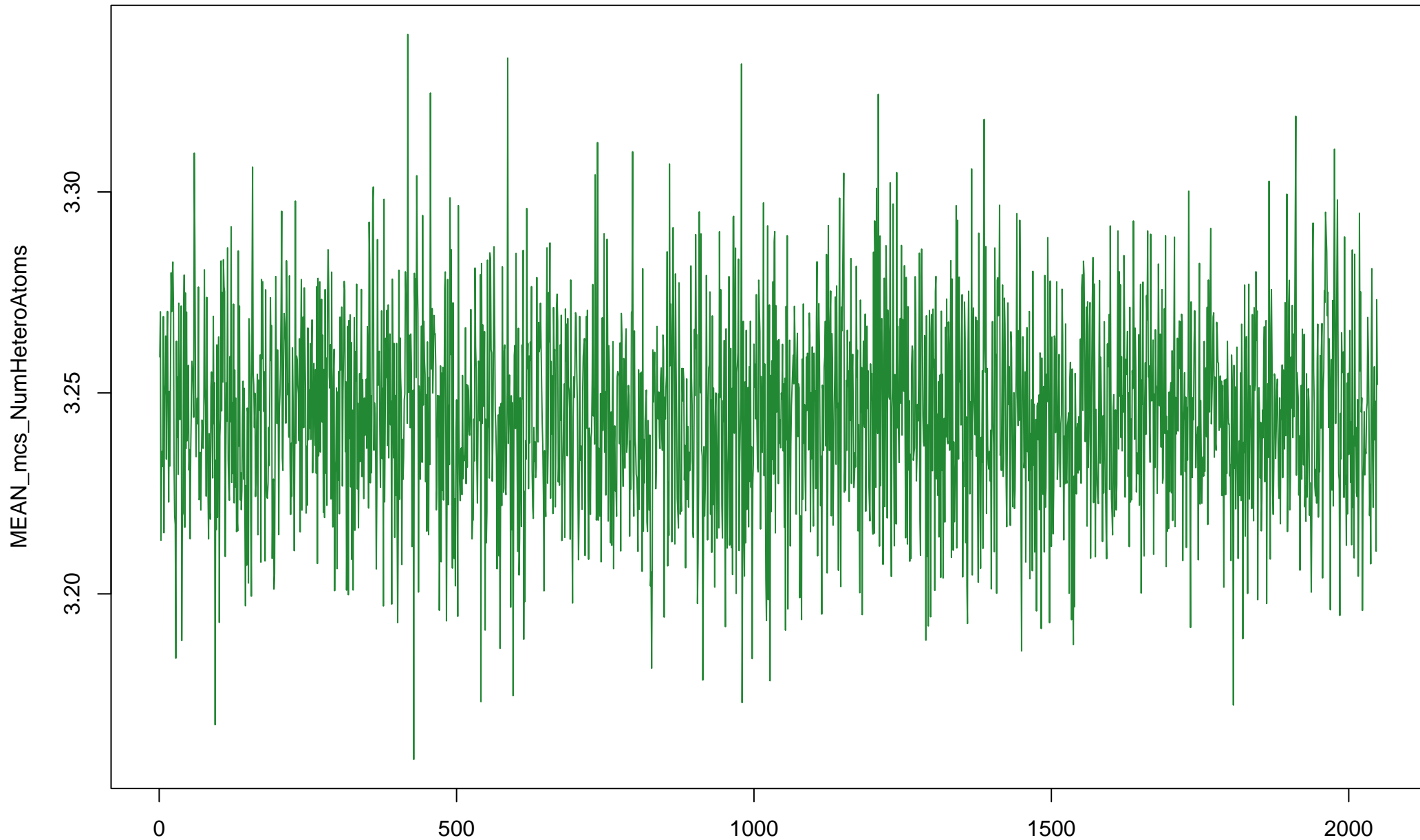
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0419 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



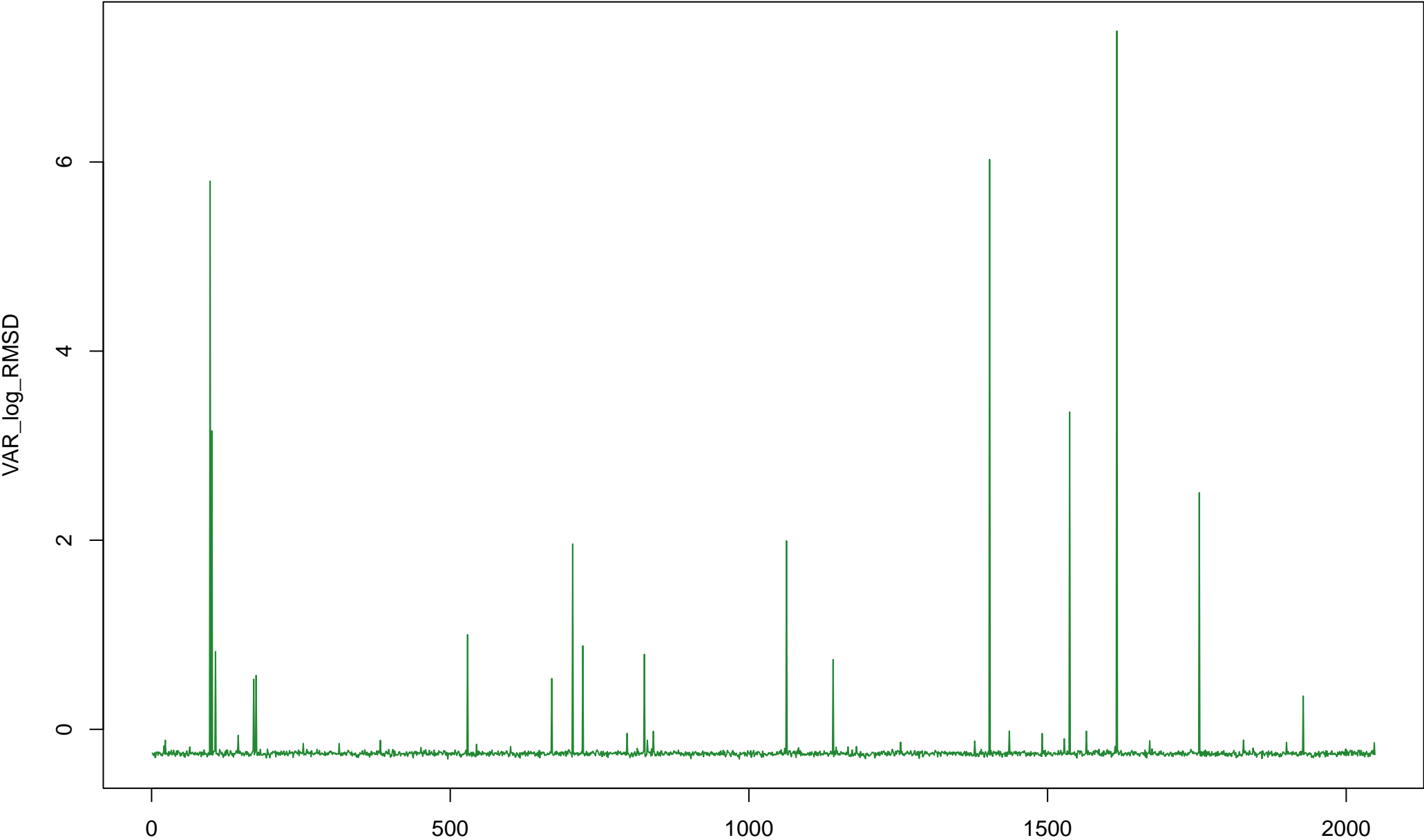
MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0584 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



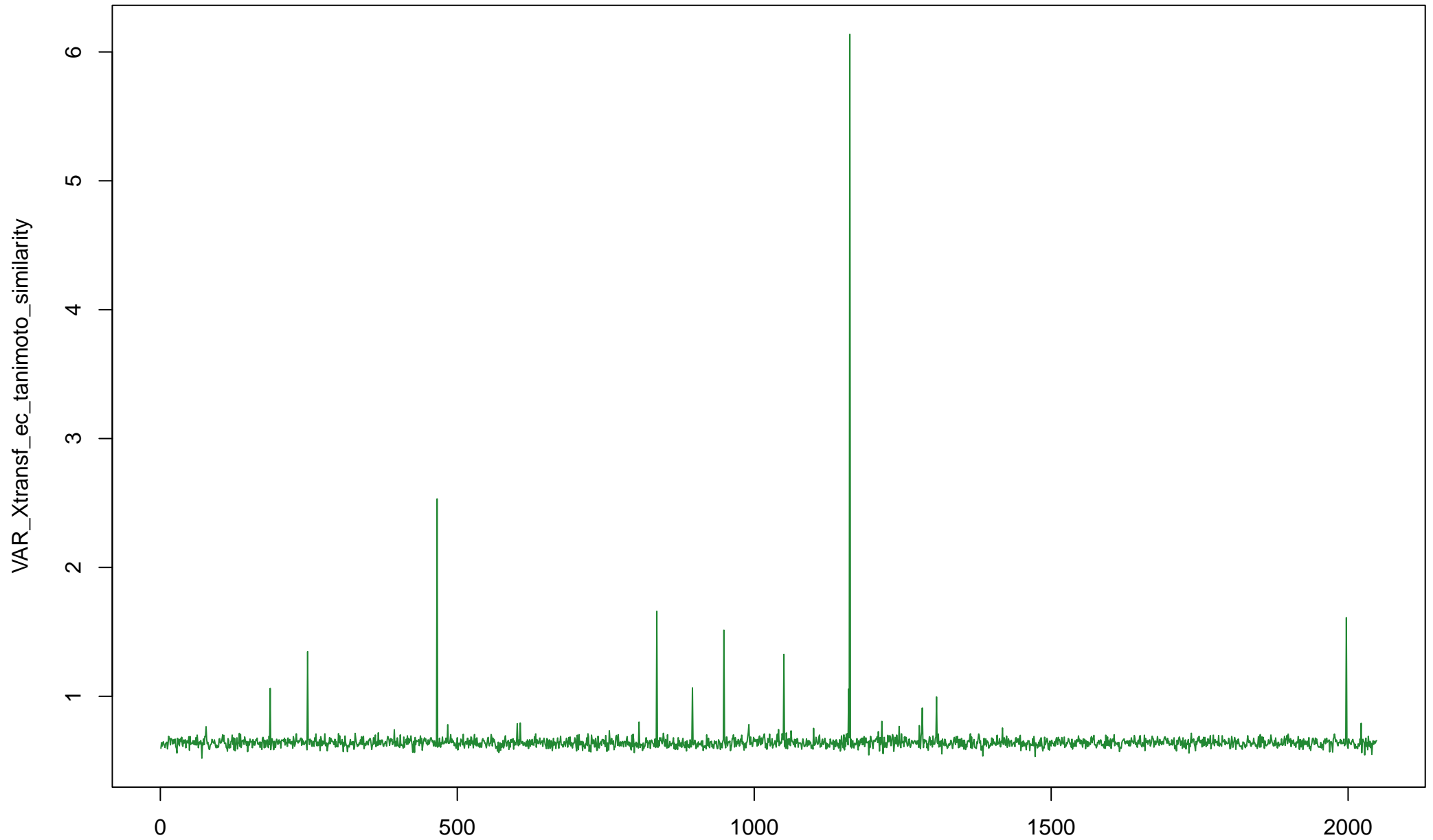
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0426 | MCSE(6.27) = 1.97 | stat: TRUE | burn: 0



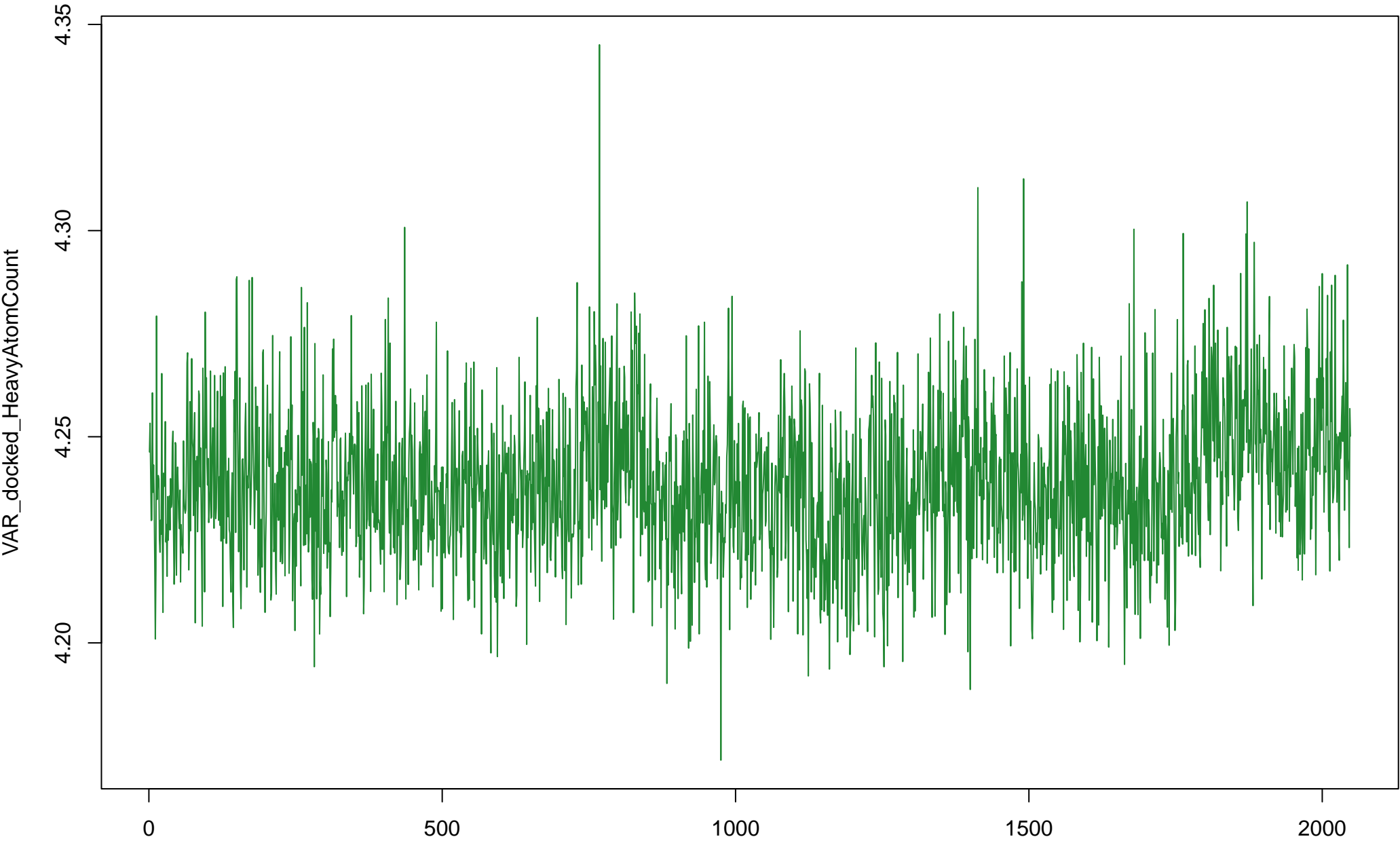
VAR_log_RMSD
ESS = 2050 | BMK = 0.8 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1632



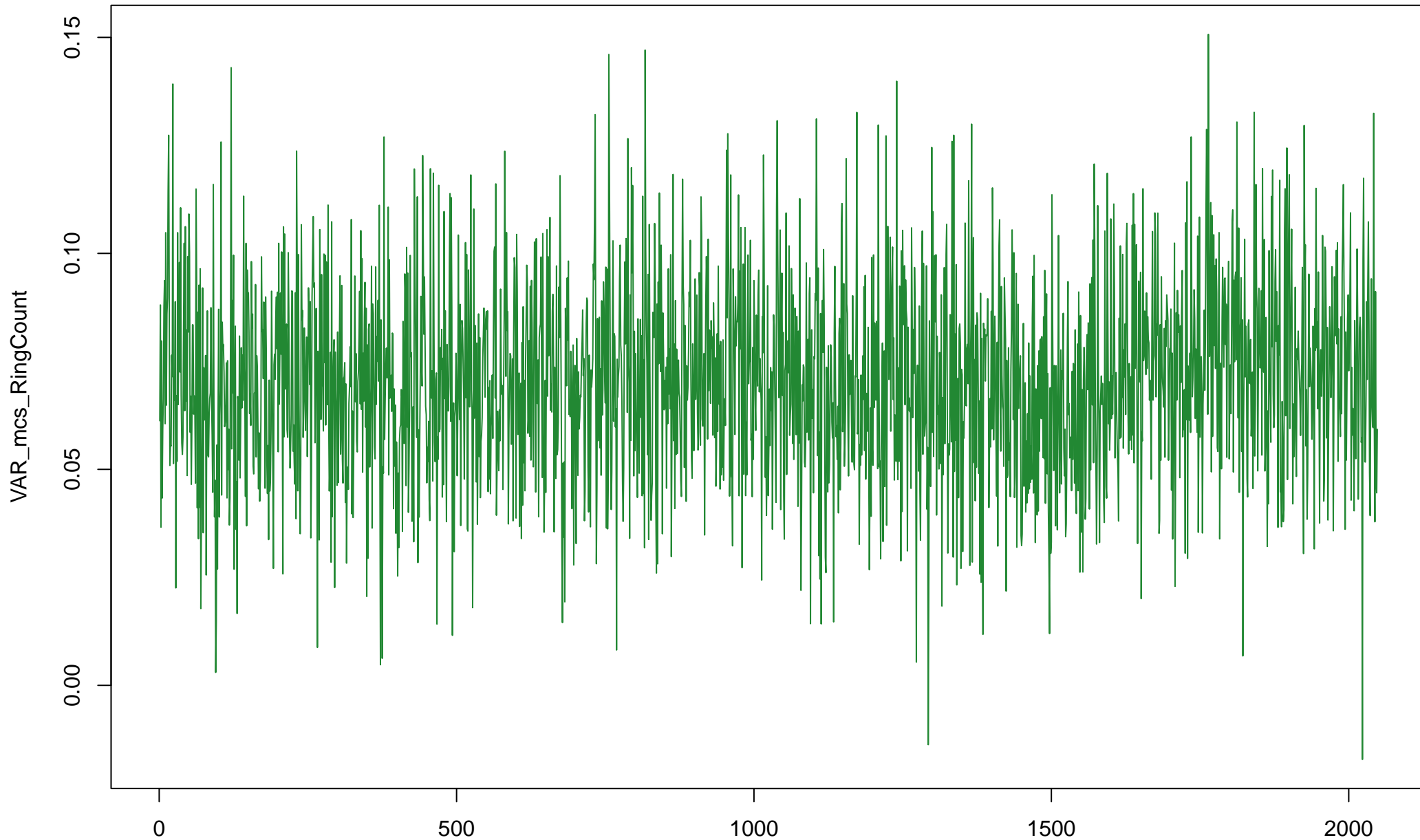
VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.141 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



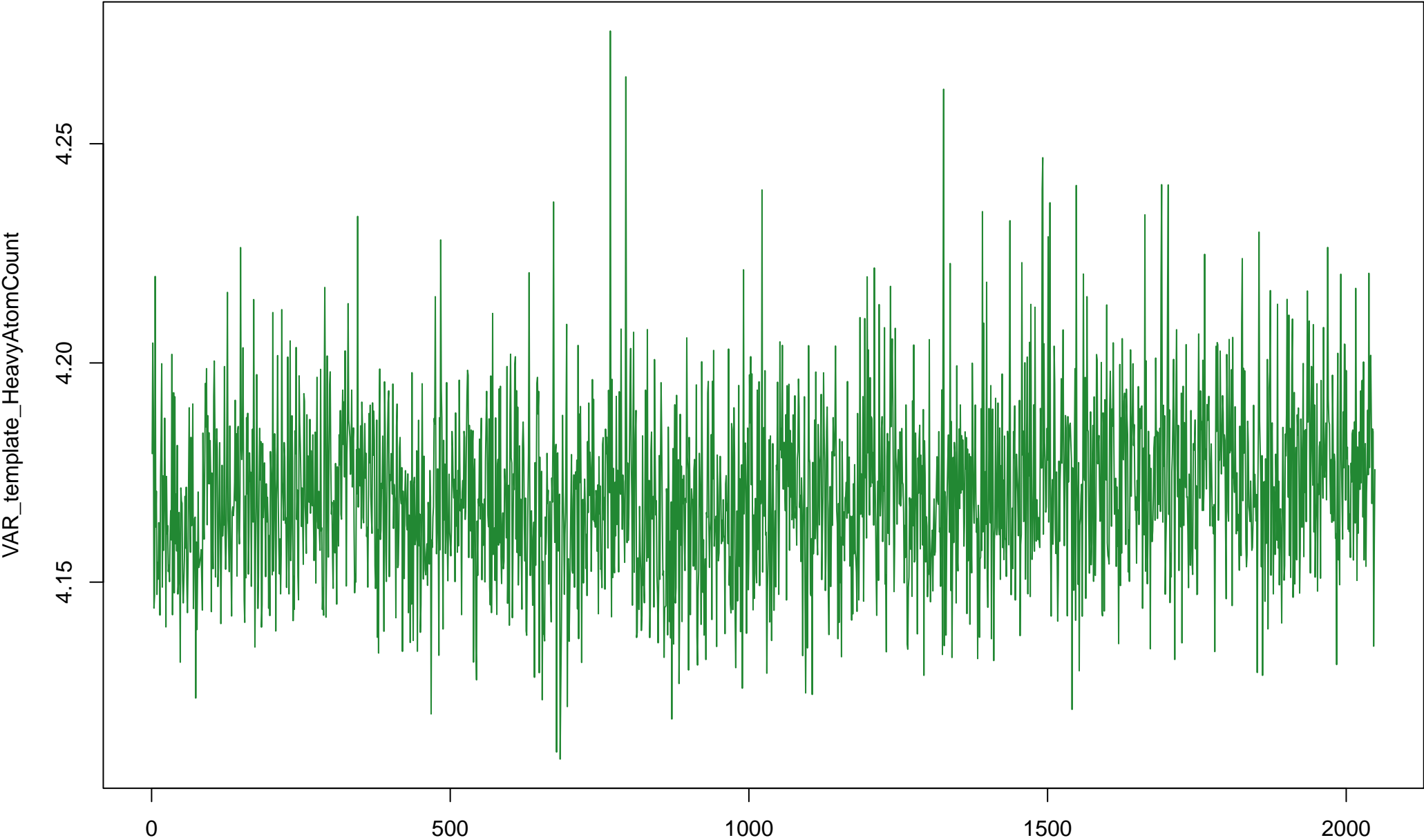
VAR_docked_HeavyAtomCount
ESS = 174 | BMK = 0.0827 | MCSE(6.27) = 4.75 | stat: TRUE | burn: 0



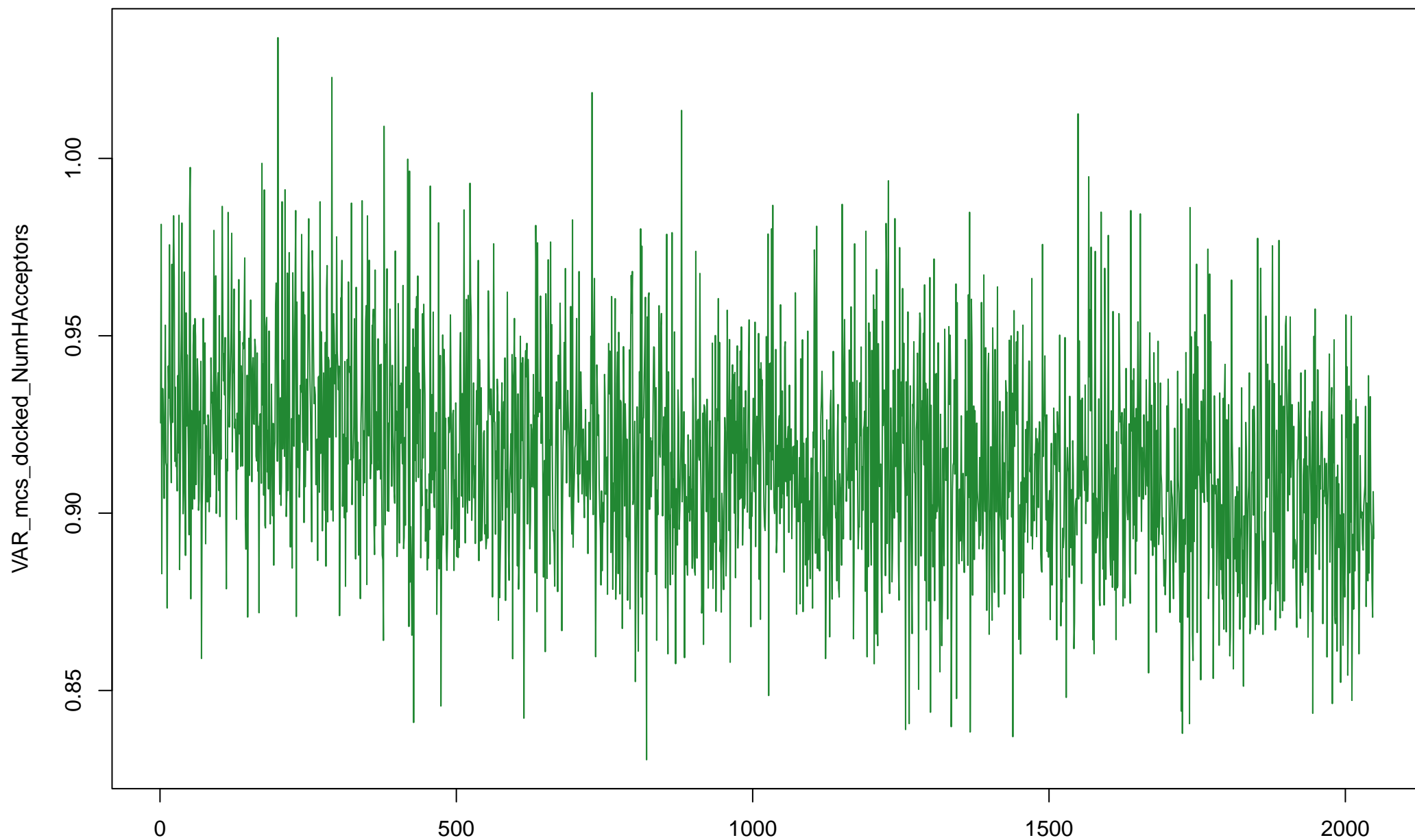
VAR_mcs_RingCount
ESS = 1780 | BMK = 0.0422 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0



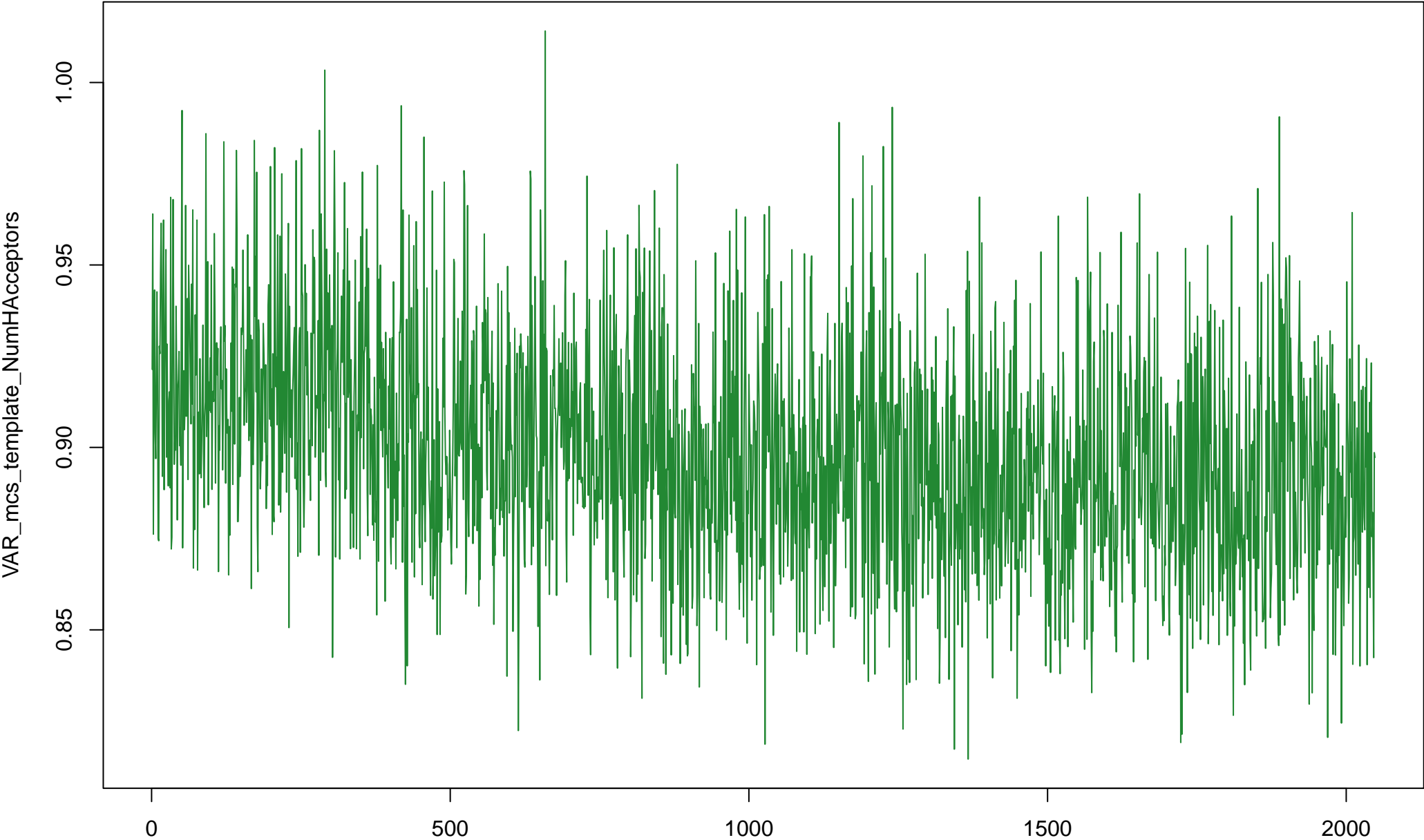
VAR_template_HeavyAtomCount
ESS = 804 | BMK = 0.112 | MCSE(6.27) = 3.95 | stat: FALSE | burn: 0



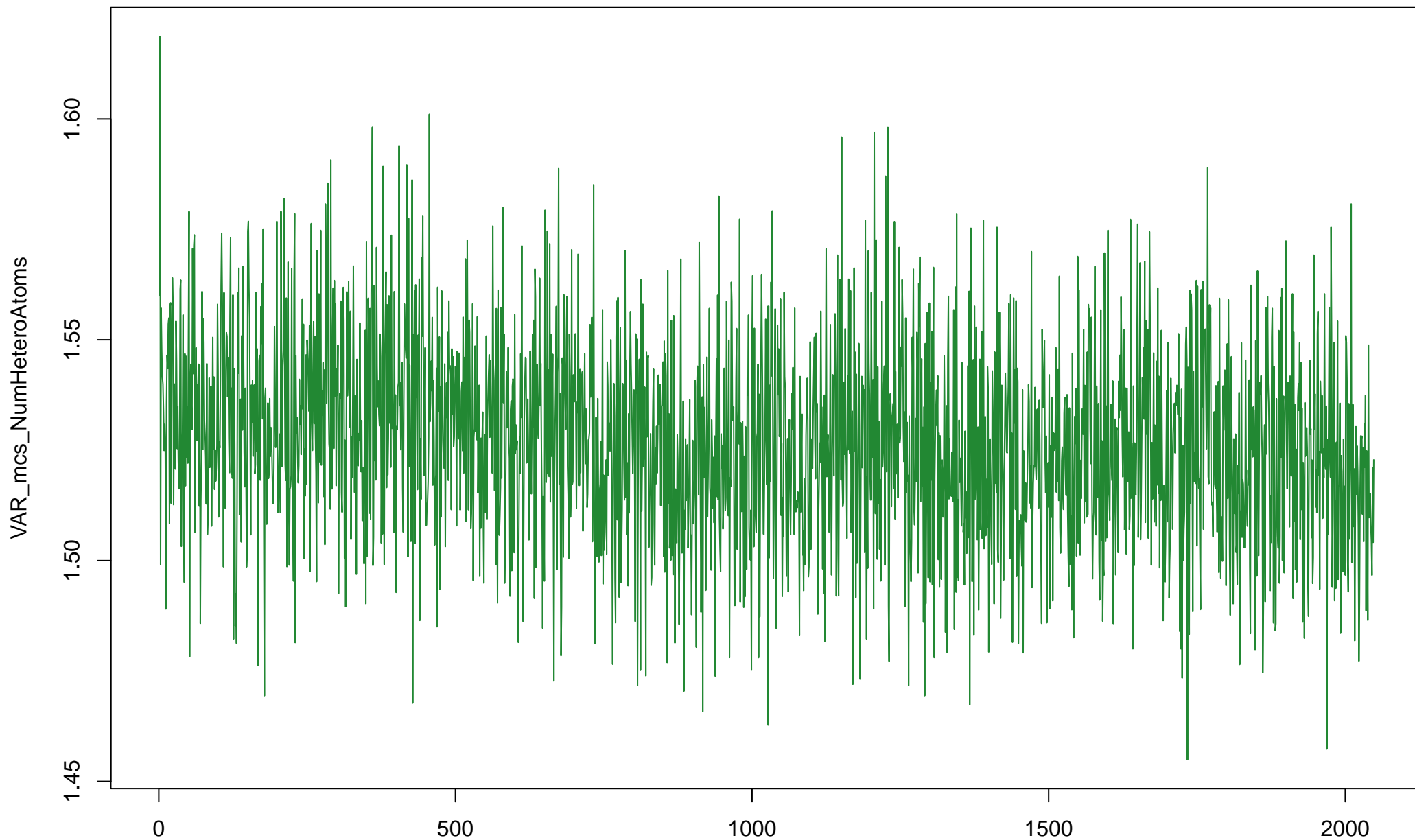
VAR_mcs_docked_NumHAcceptors
ESS = 178 | BMK = 0.151 | MCSE(6.27) = 4.58 | stat: FALSE | burn: 0



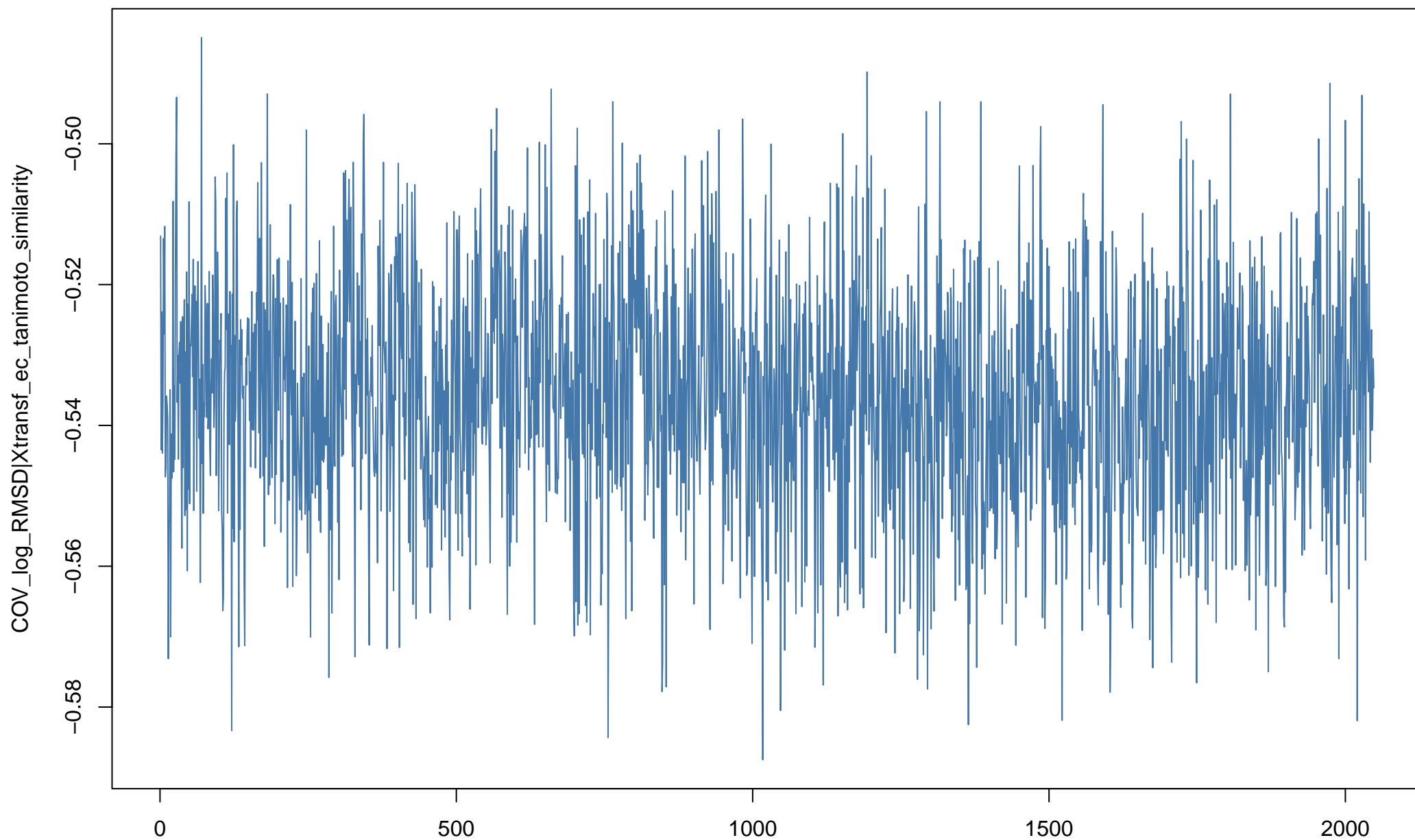
VAR_mcs_template_NumHAcceptors
ESS = 118 | BMK = 0.173 | MCSE(6.27) = 5.37 | stat: FALSE | burn: 0



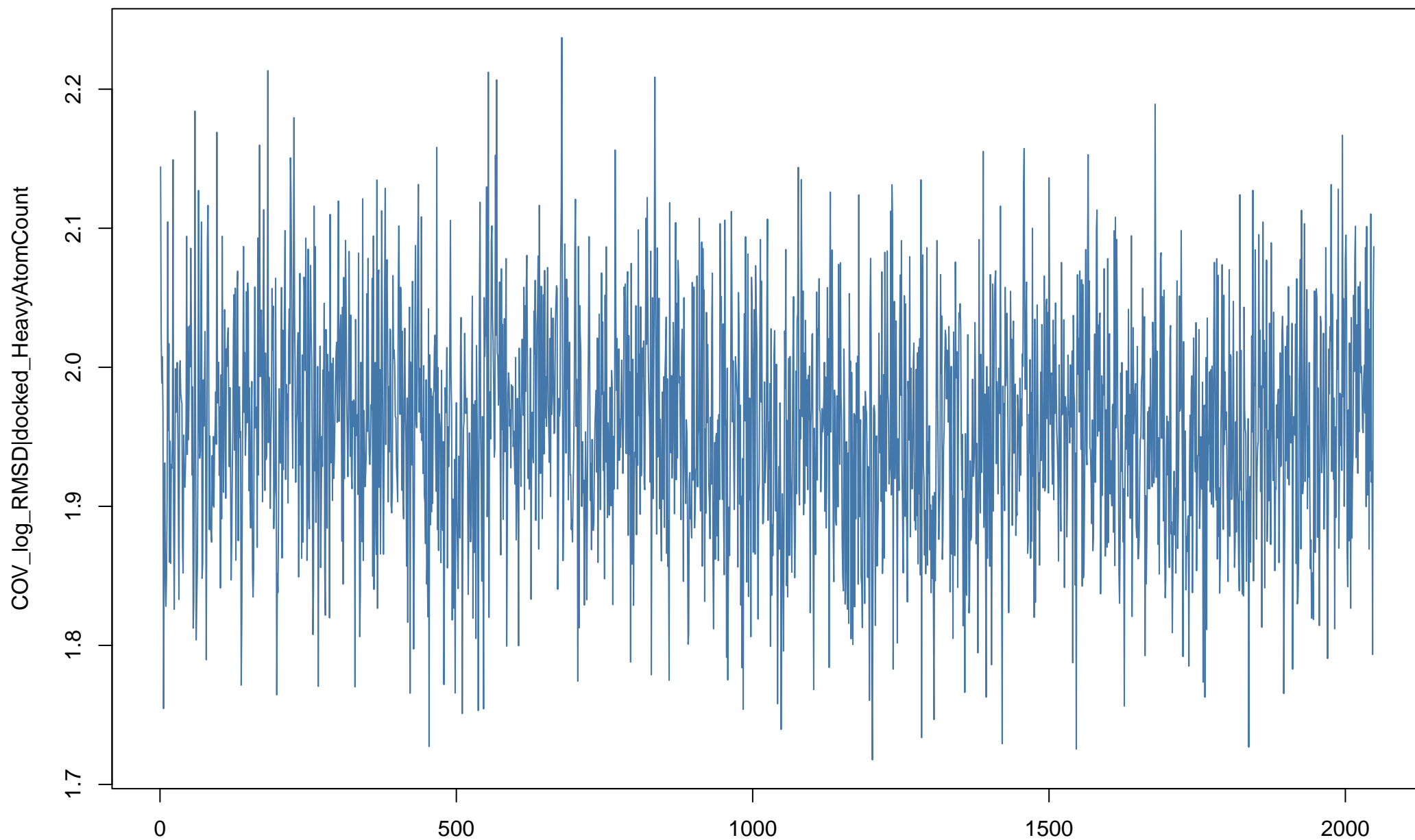
VAR_mcs_NumHeteroAtoms
ESS = 570 | BMK = 0.101 | MCSE(6.27) = 3.84 | stat: FALSE | burn: 0



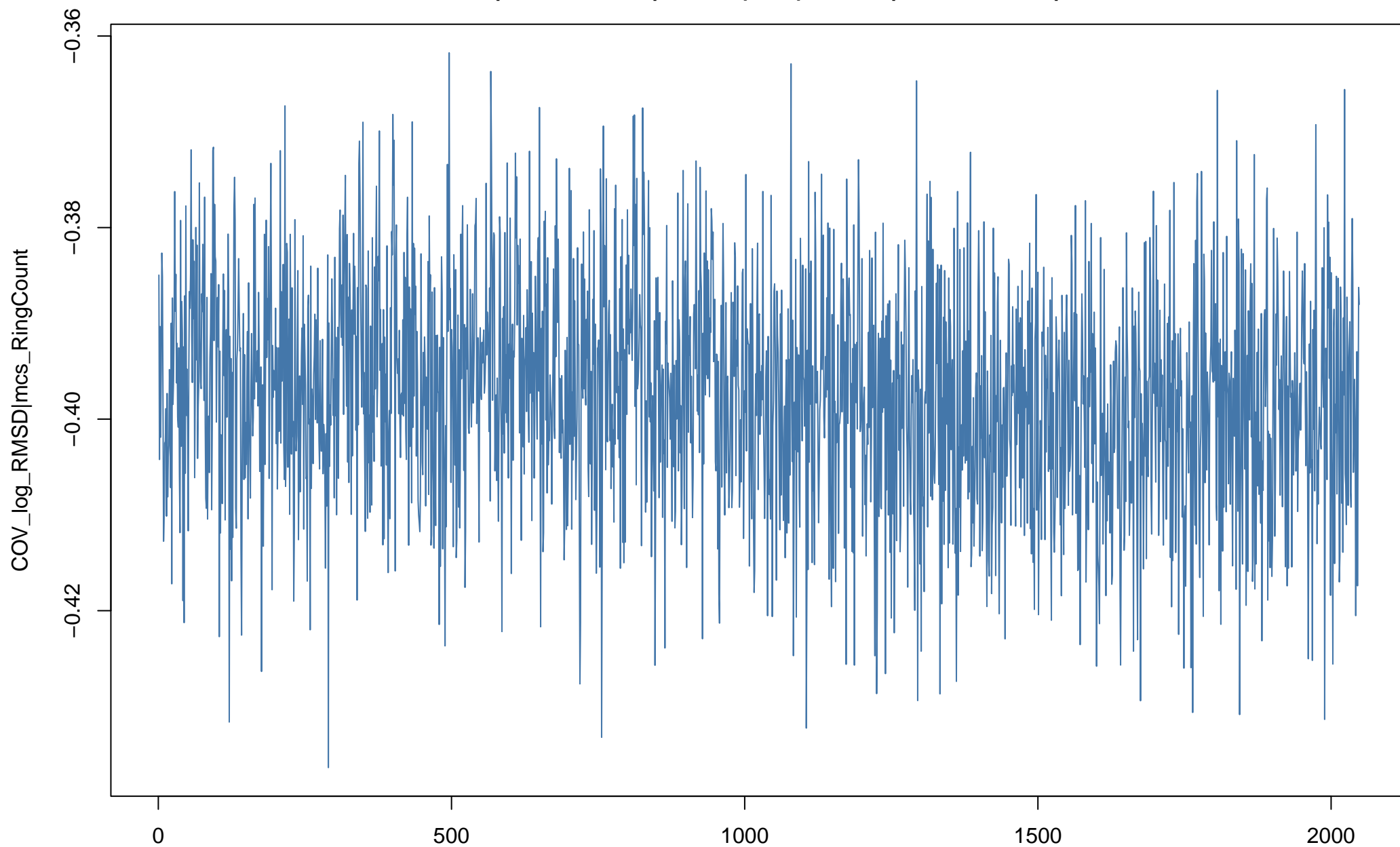
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1670 | BMK = 0.0841 | MCSE(6.27) = 3.12 | stat: FALSE | burn: 0



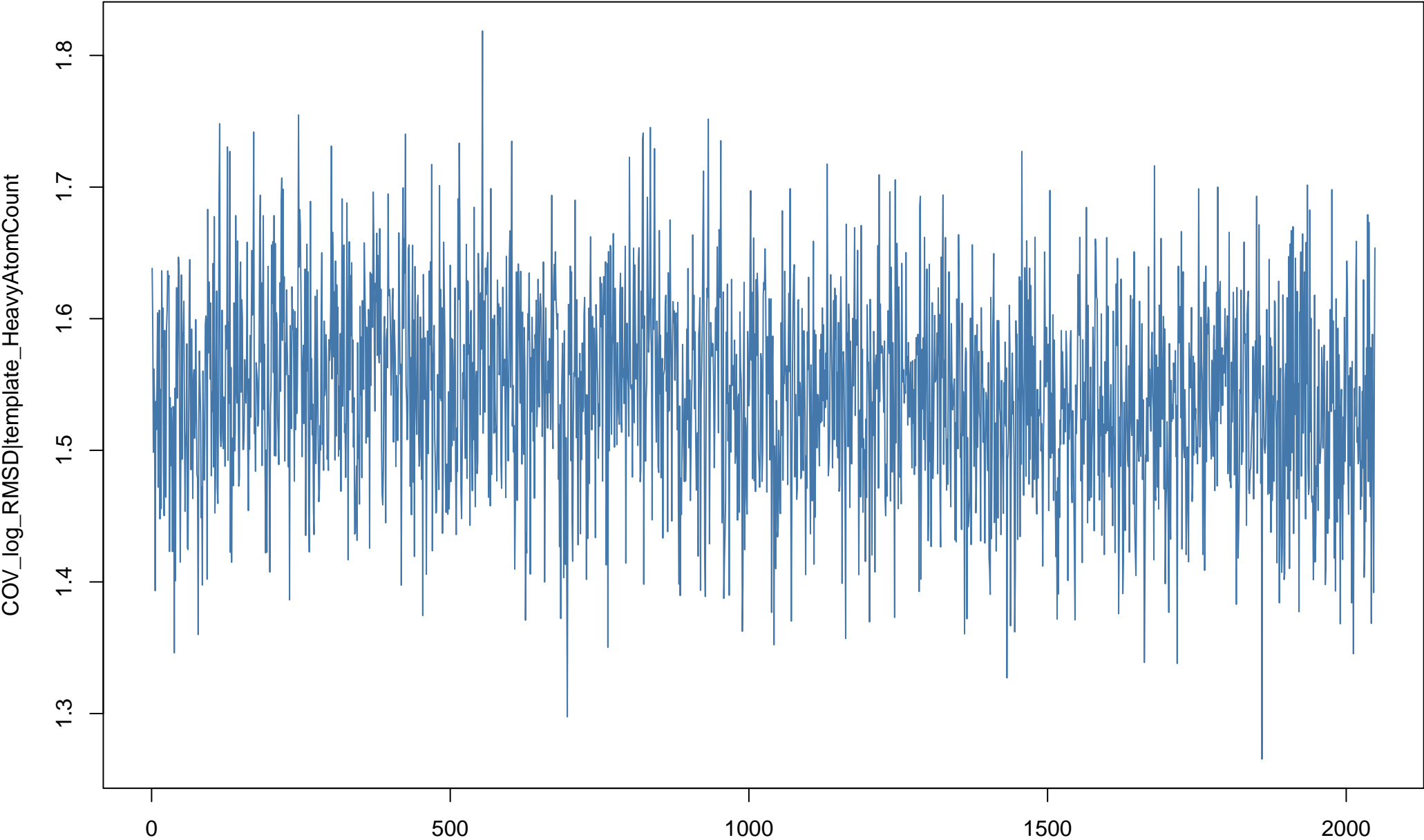
COV_log_RMSD|docked_HeavyAtomCount
ESS = 950 | BMK = 0.065 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0



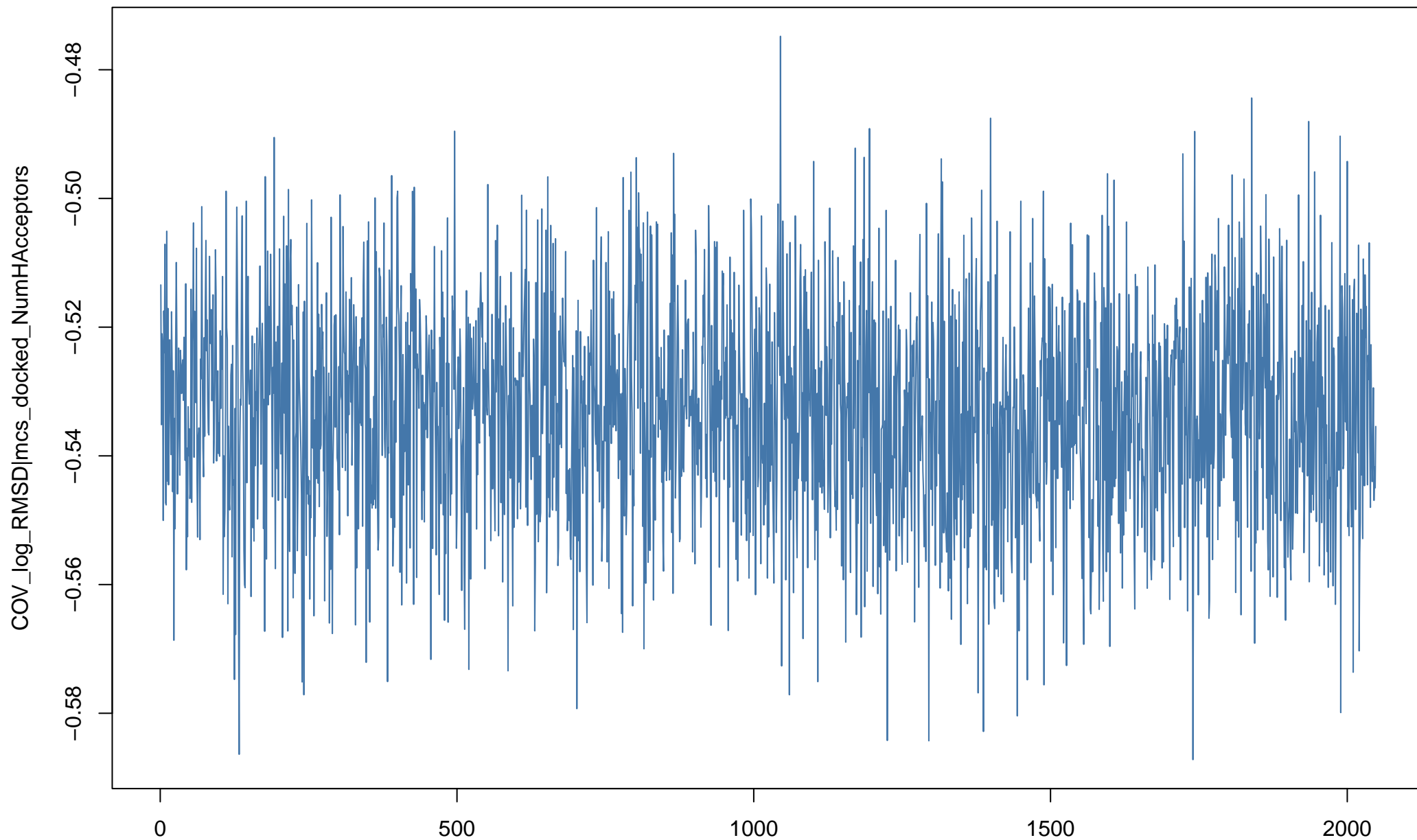
COV_log_RMSD|mcs_RingCount
ESS = 552 | BMK = 0.13 | MCSE(6.27) = 3.57 | stat: FALSE | burn: 0



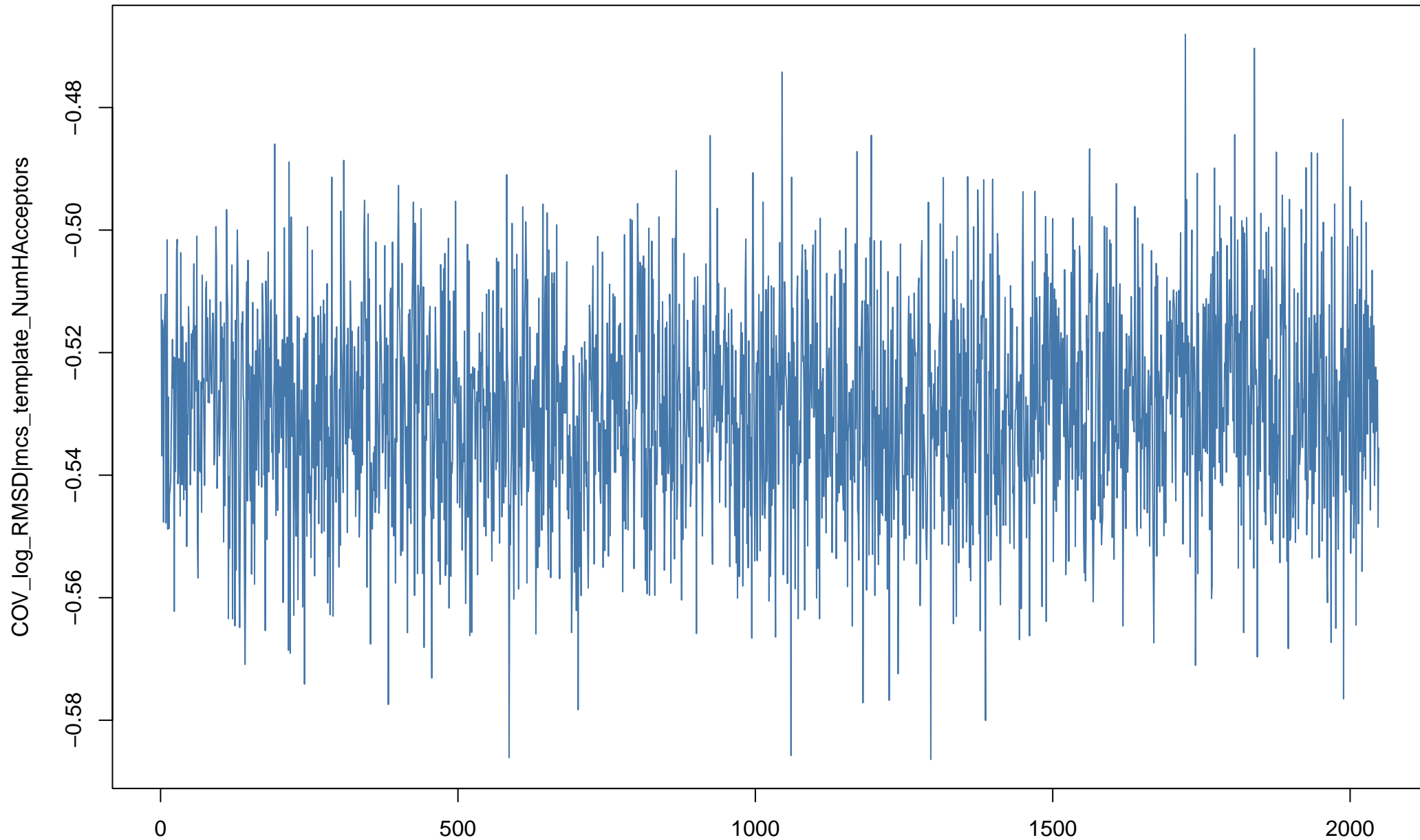
COV_log_RMSD|template_HeavyAtomCount
ESS = 958 | BMK = 0.115 | MCSE(6.27) = 3.74 | stat: FALSE | burn: 0



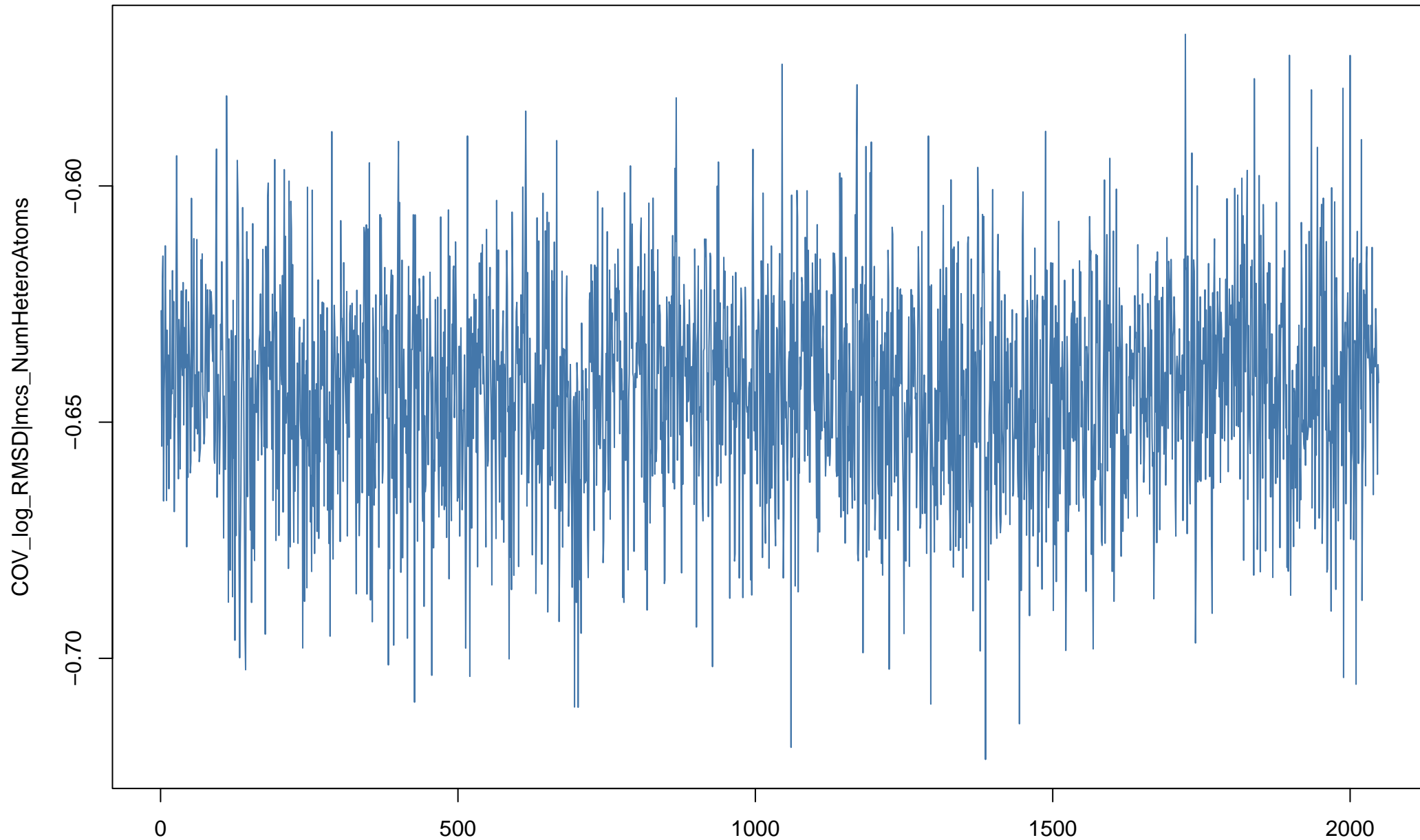
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0699 | MCSE(6.27) = 2.45 | stat: FALSE | burn: 0



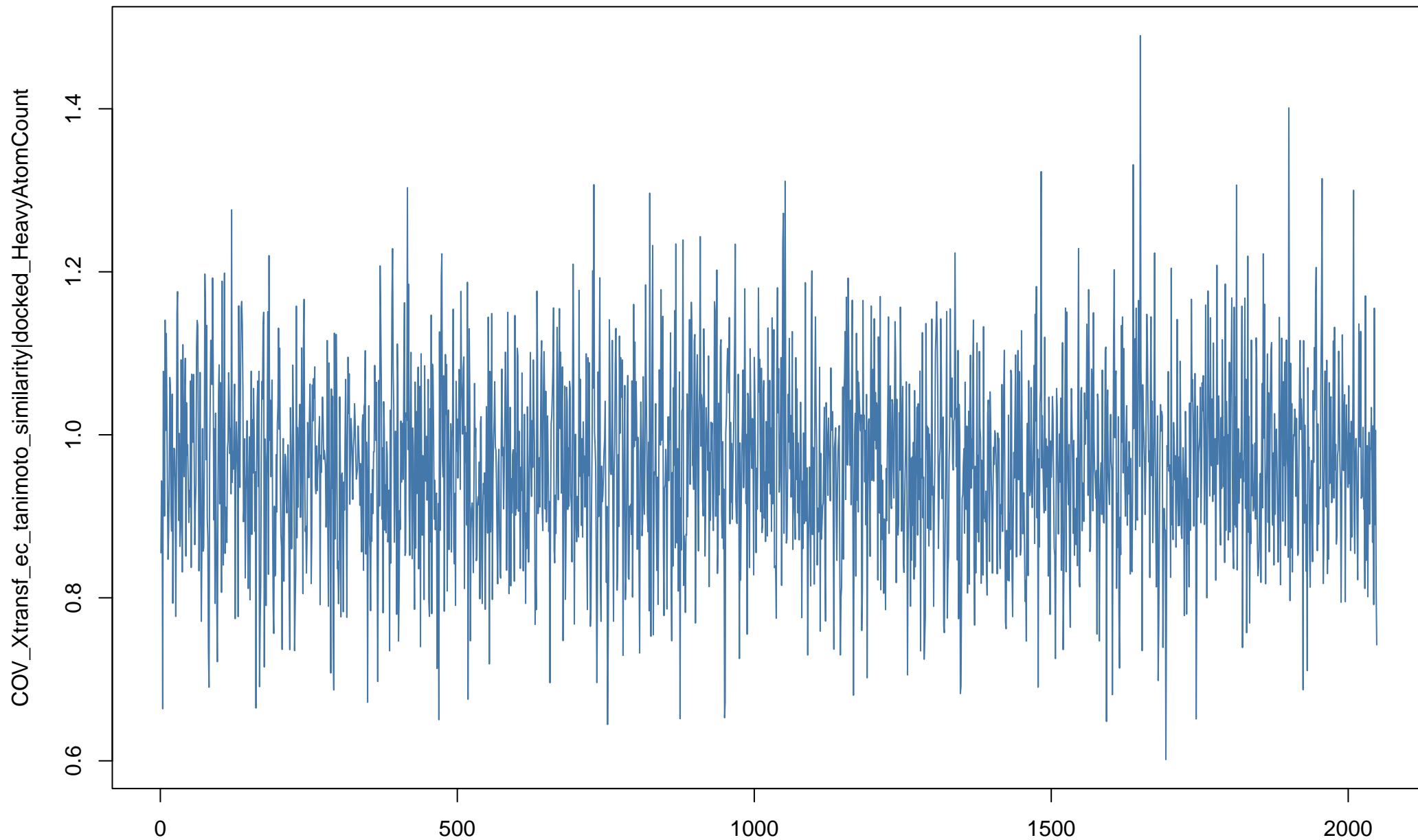
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0565 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0



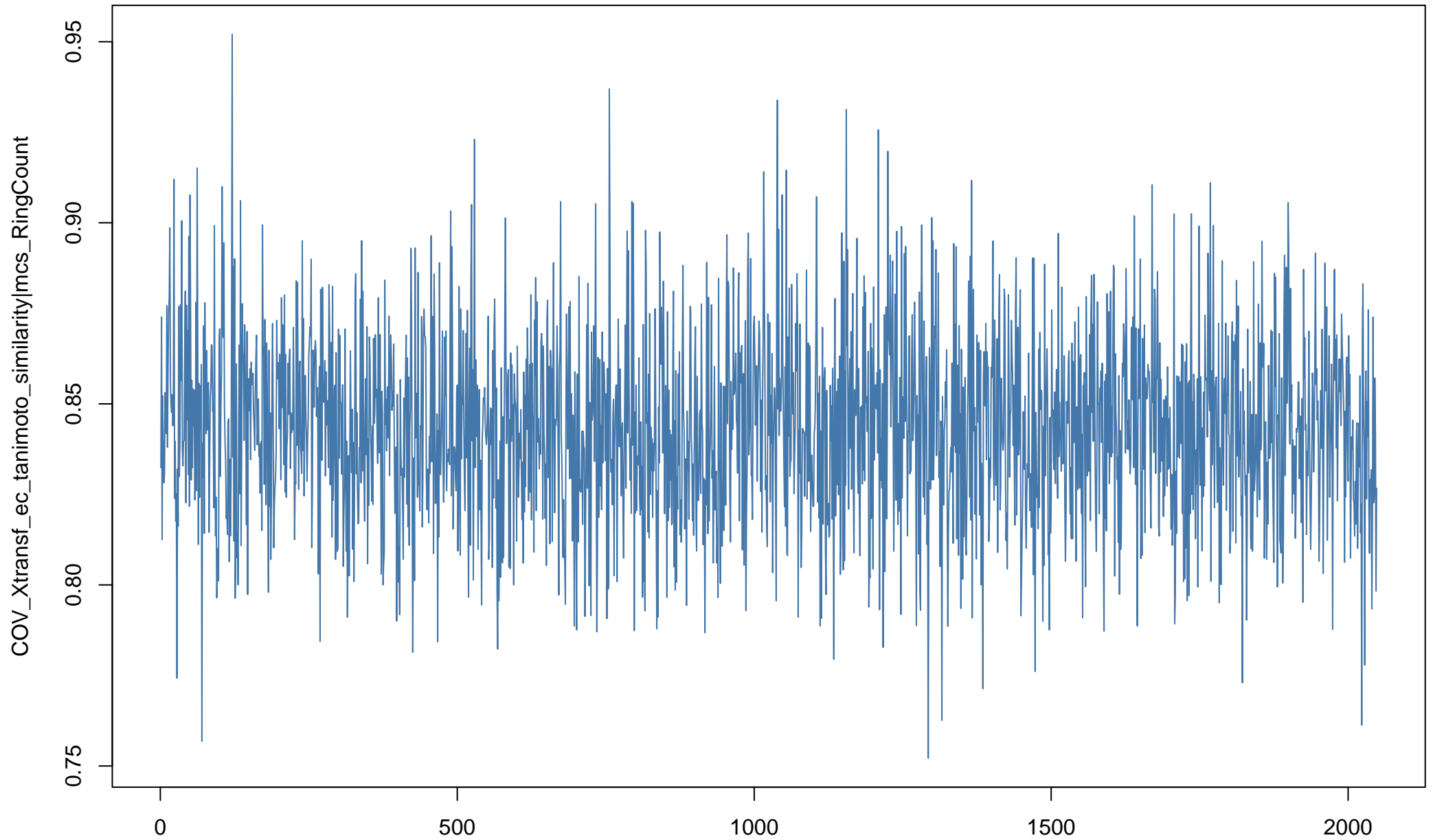
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0608 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0



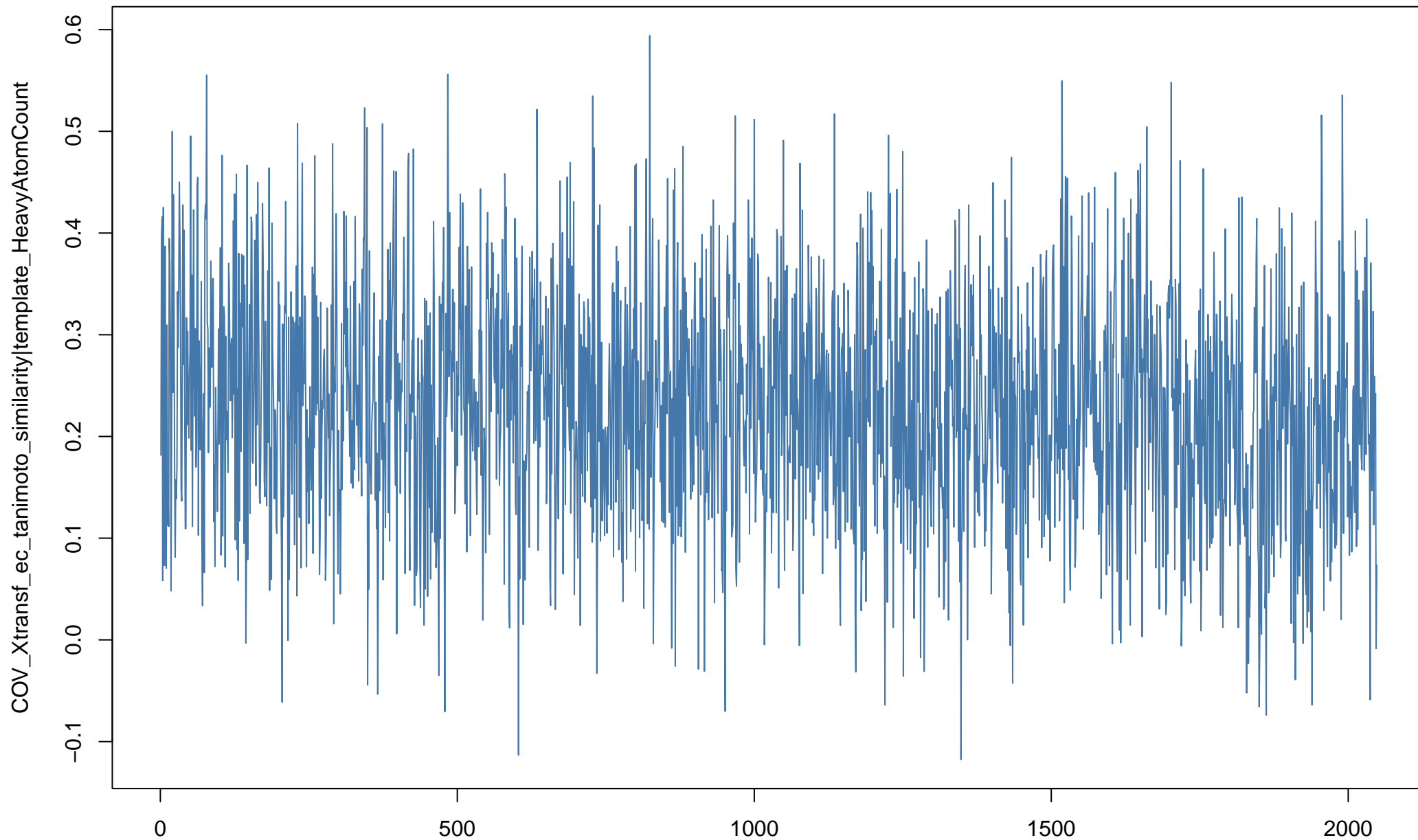
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0489 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0



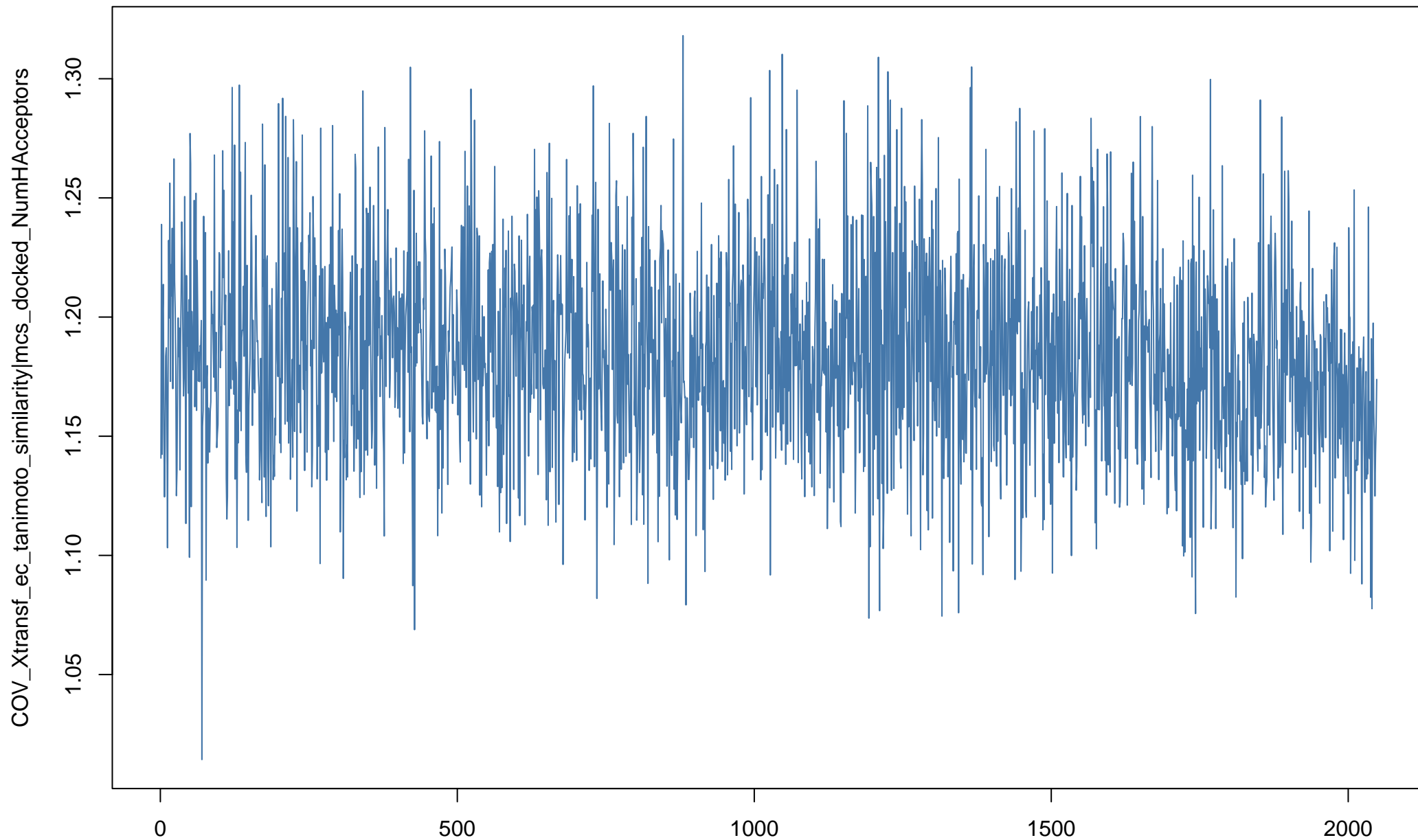
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1780 | BMK = 0.0367 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0



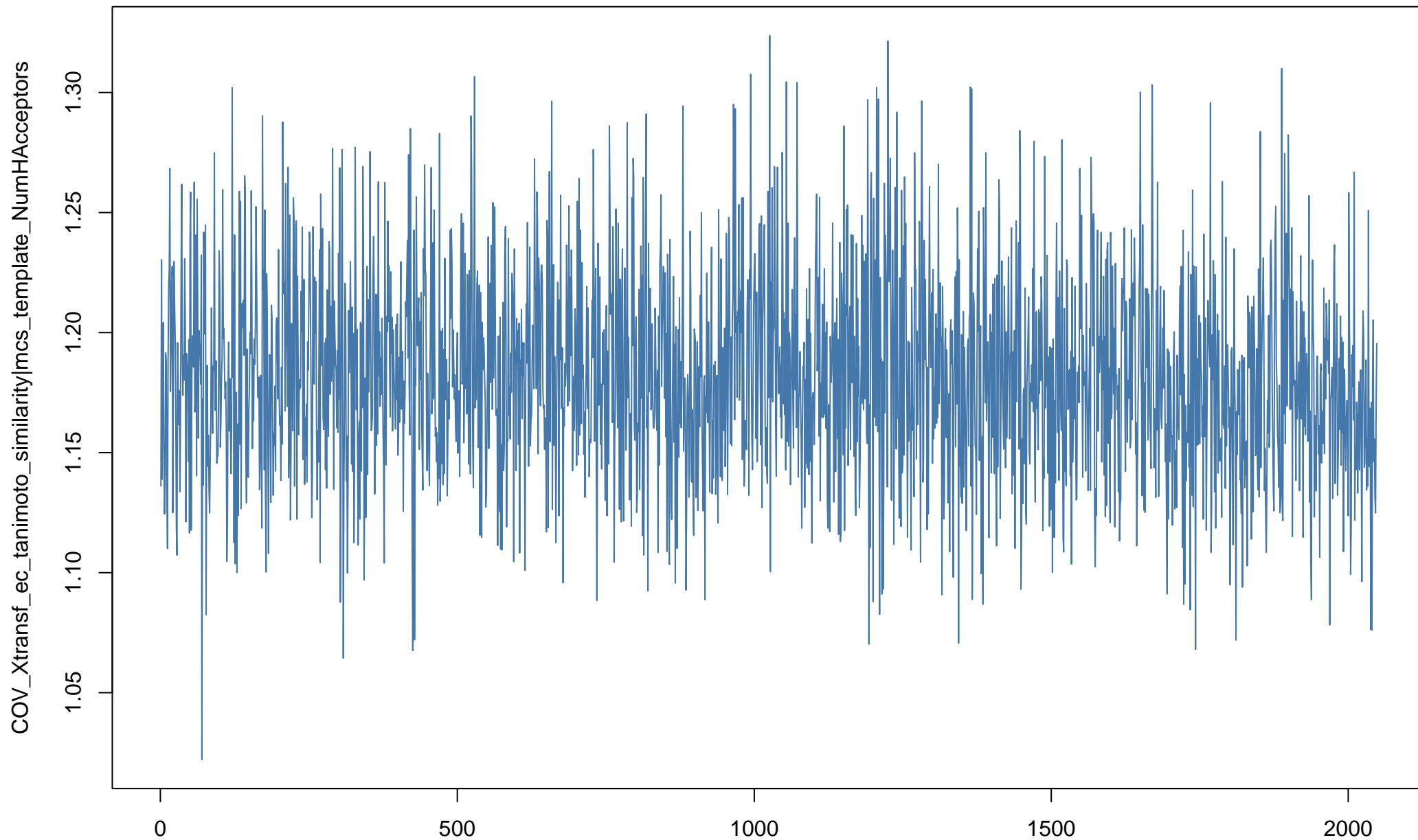
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1760 | BMK = 0.0691 | MCSE(6.27) = 2.96 | stat: FALSE | burn: 0



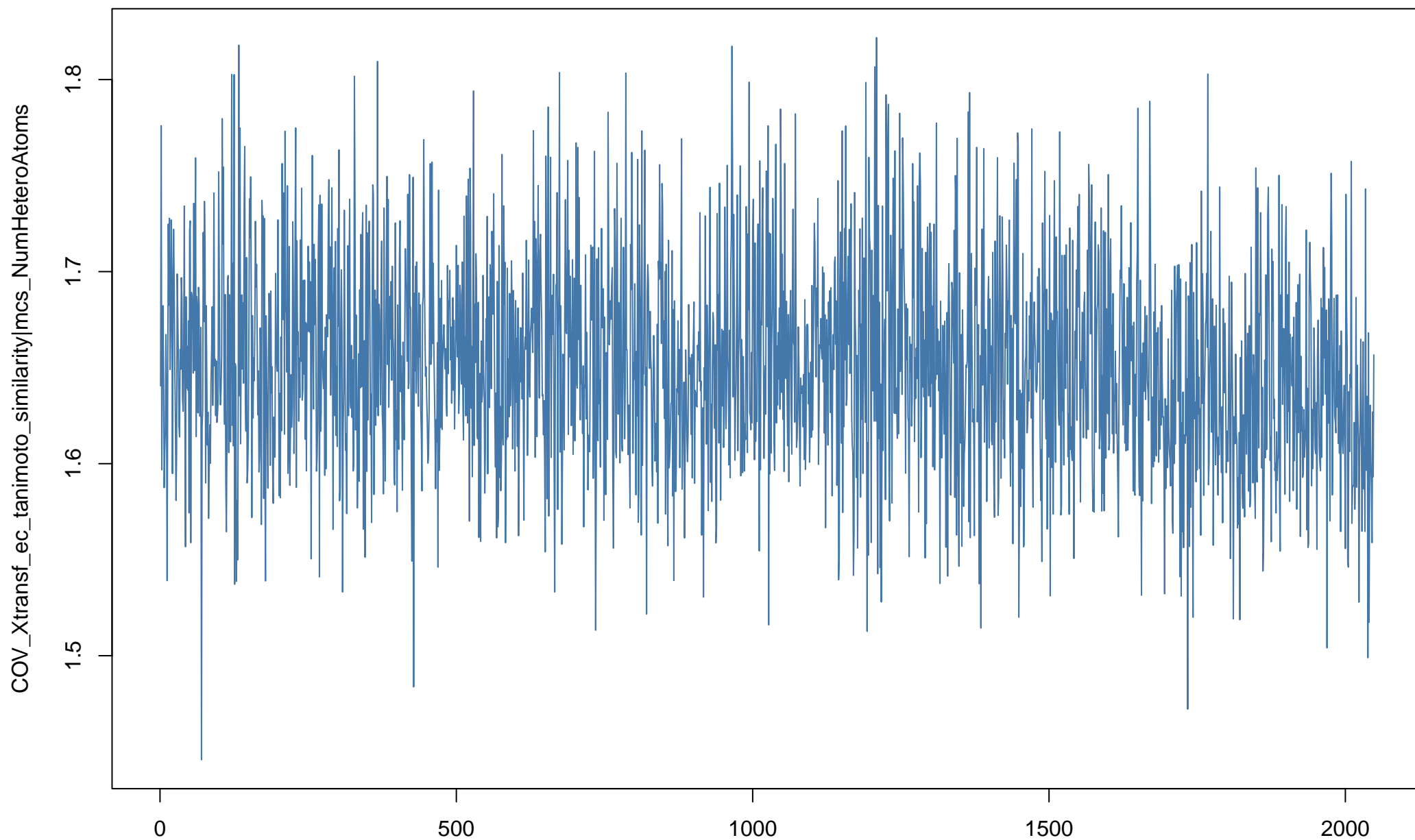
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 1060 | BMK = 0.0685 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0



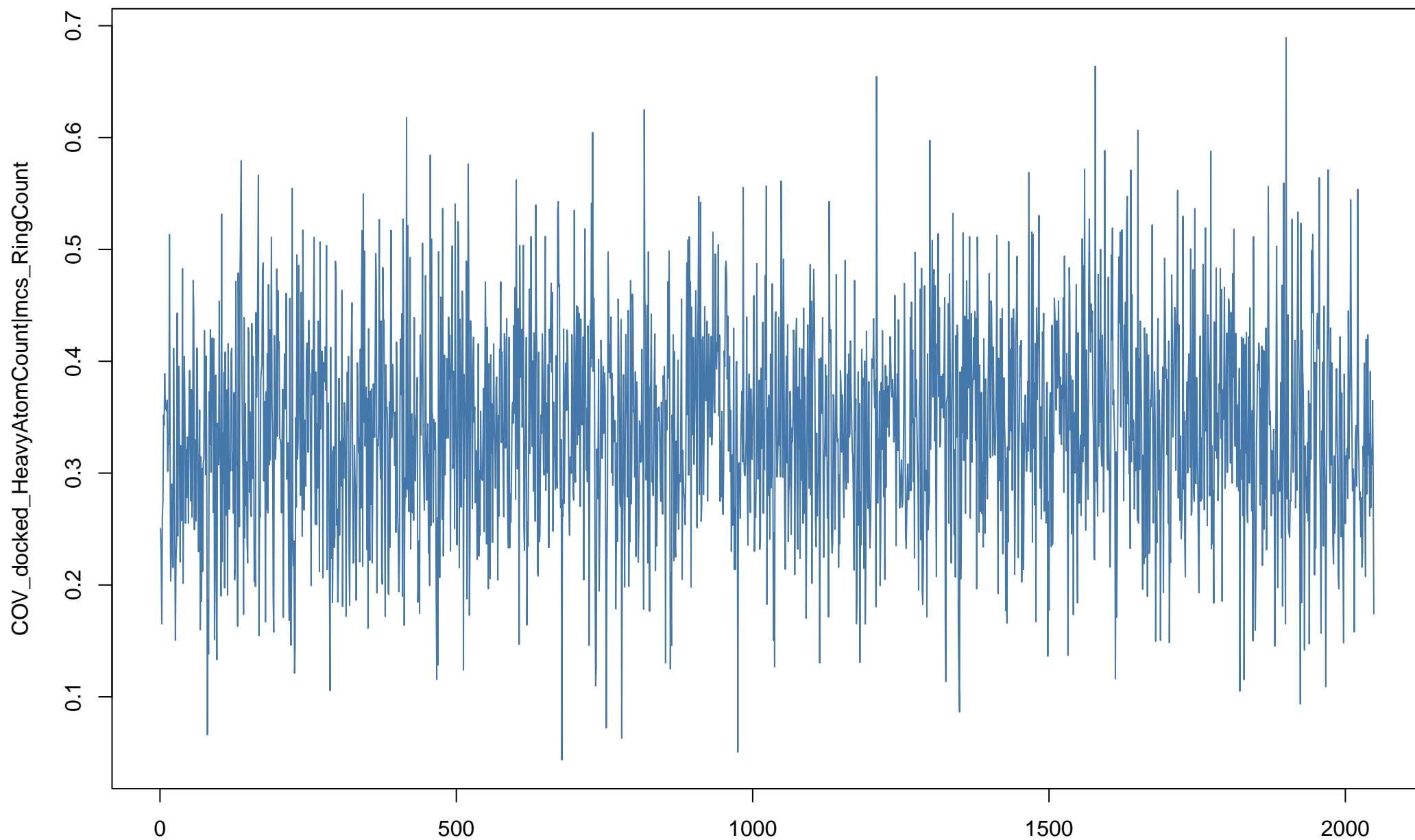
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0591 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0



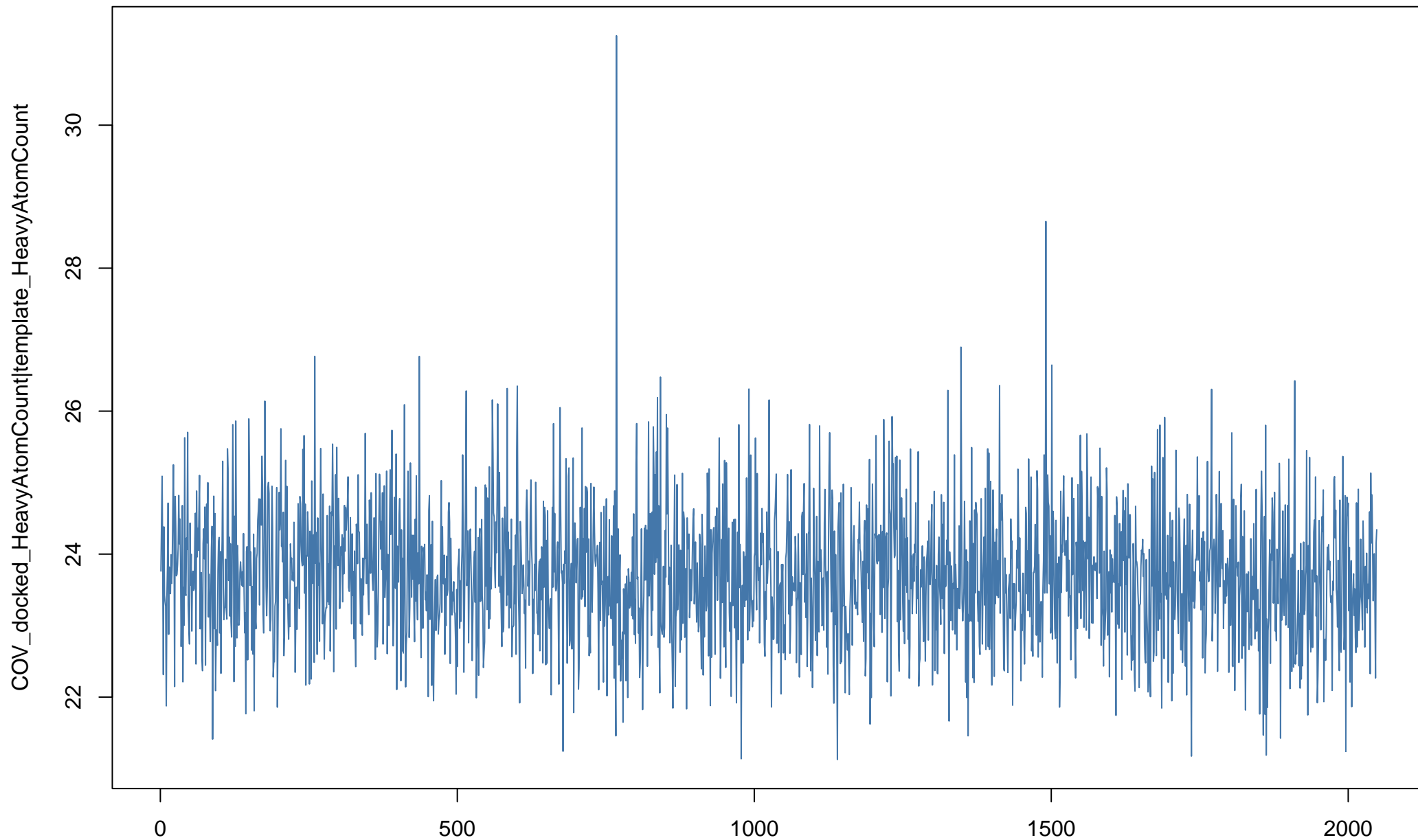
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 932 | BMK = 0.0763 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0



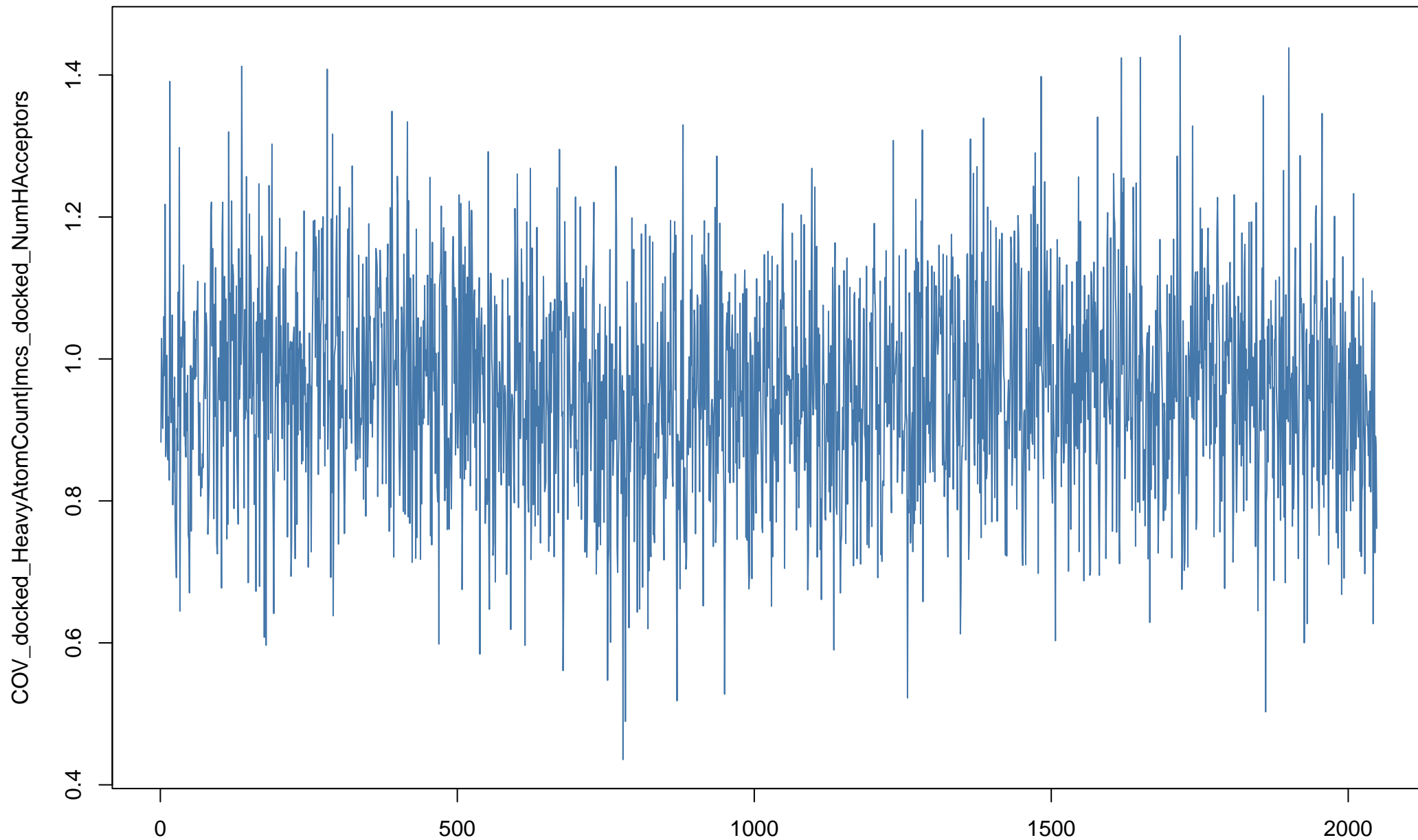
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1790 | BMK = 0.0462 | MCSE(6.27) = 2.47 | stat: FALSE | burn: 0



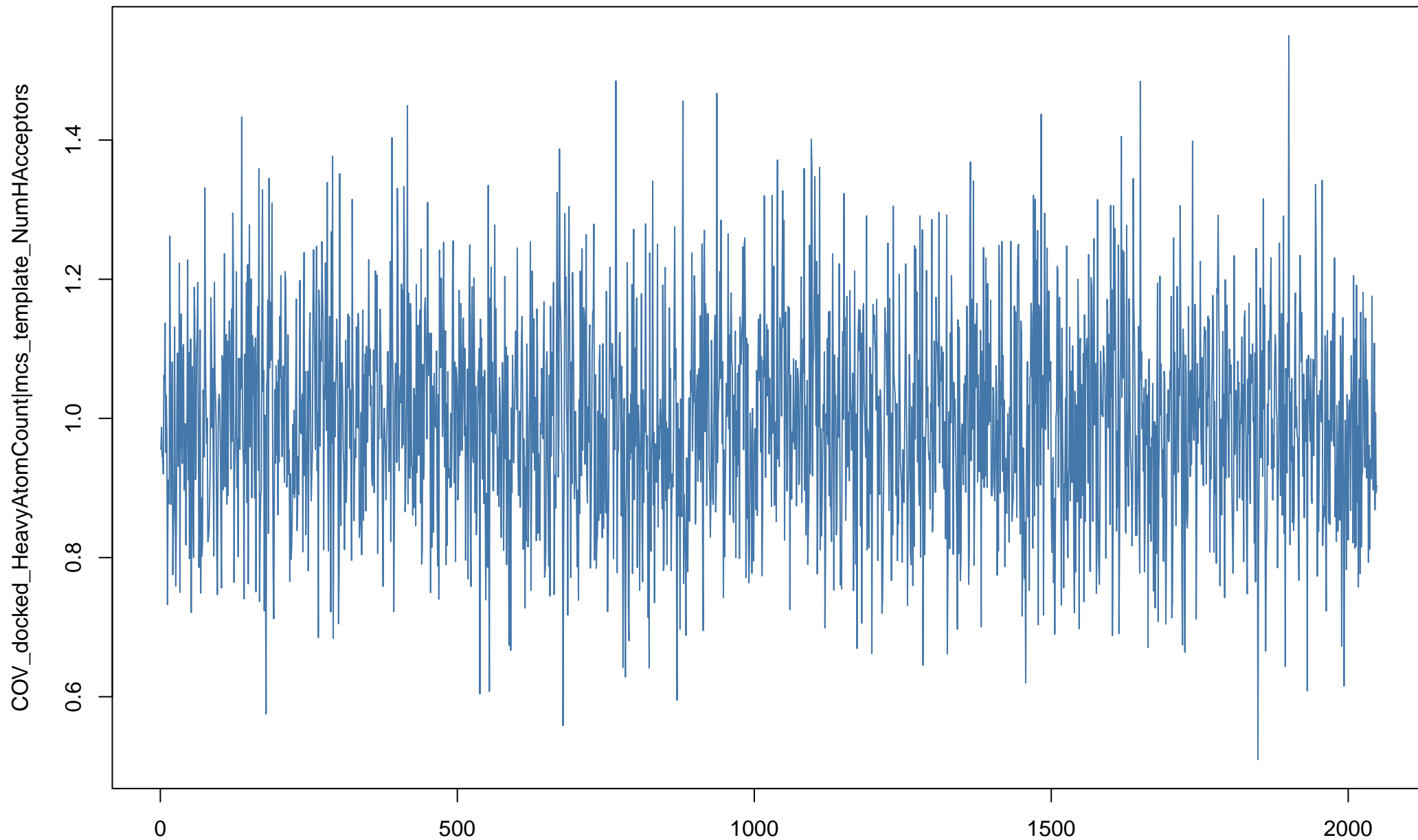
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1920 | BMK = 0.054 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0



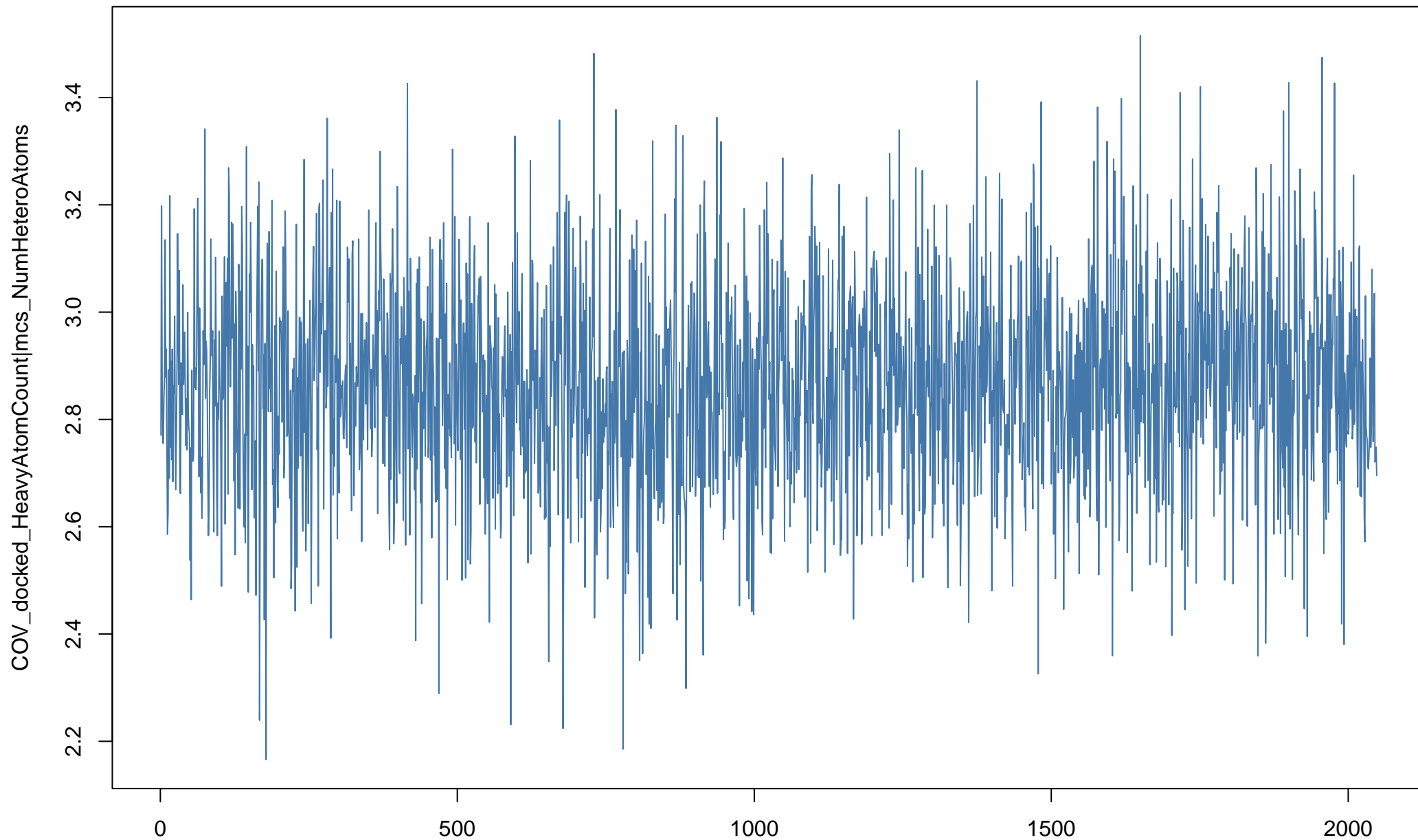
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1790 | BMK = 0.0345 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0



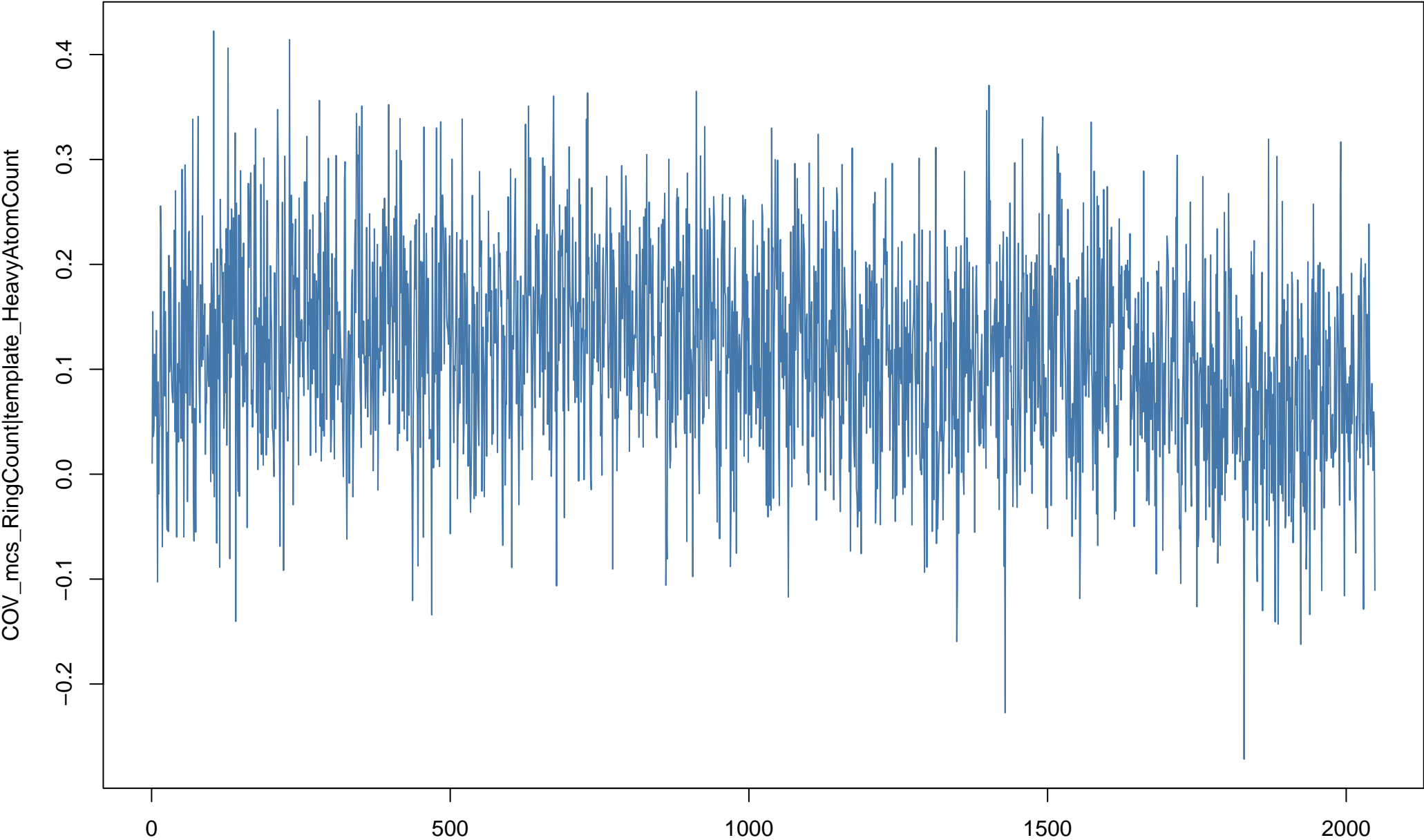
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1850 | BMK = 0.0411 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0



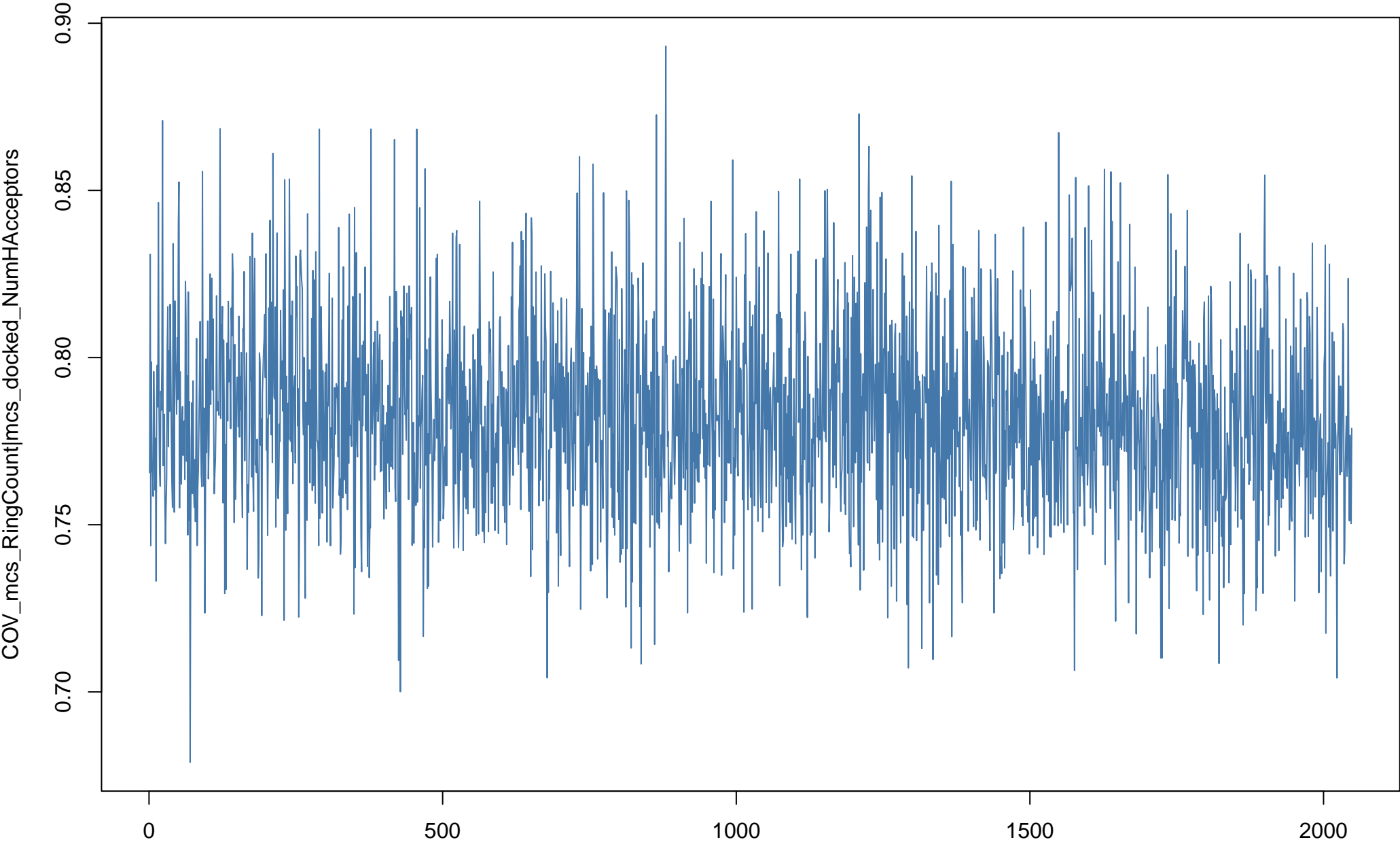
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0629 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0



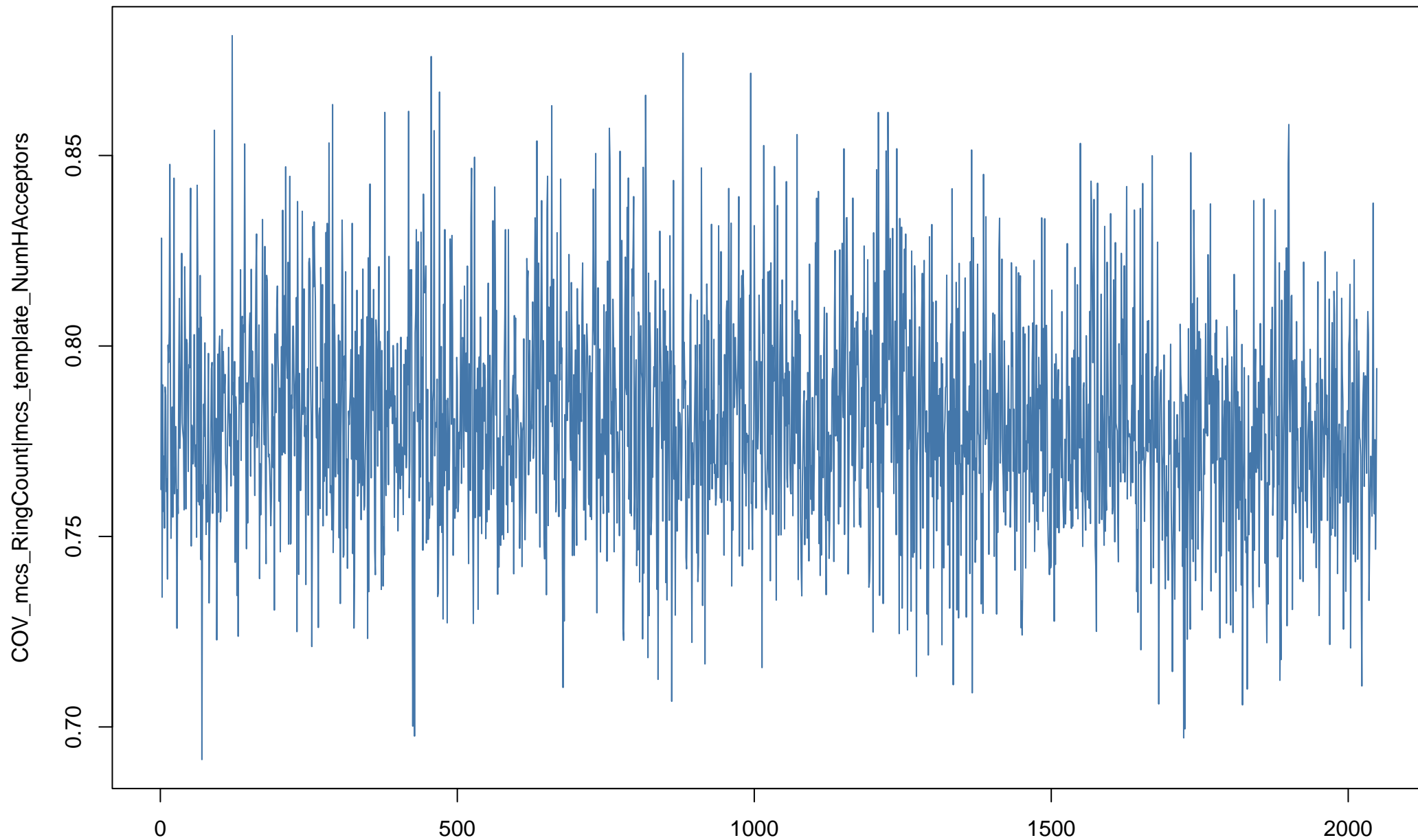
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 181 | BMK = 0.149 | MCSE(6.27) = 4.46 | stat: FALSE | burn: 0



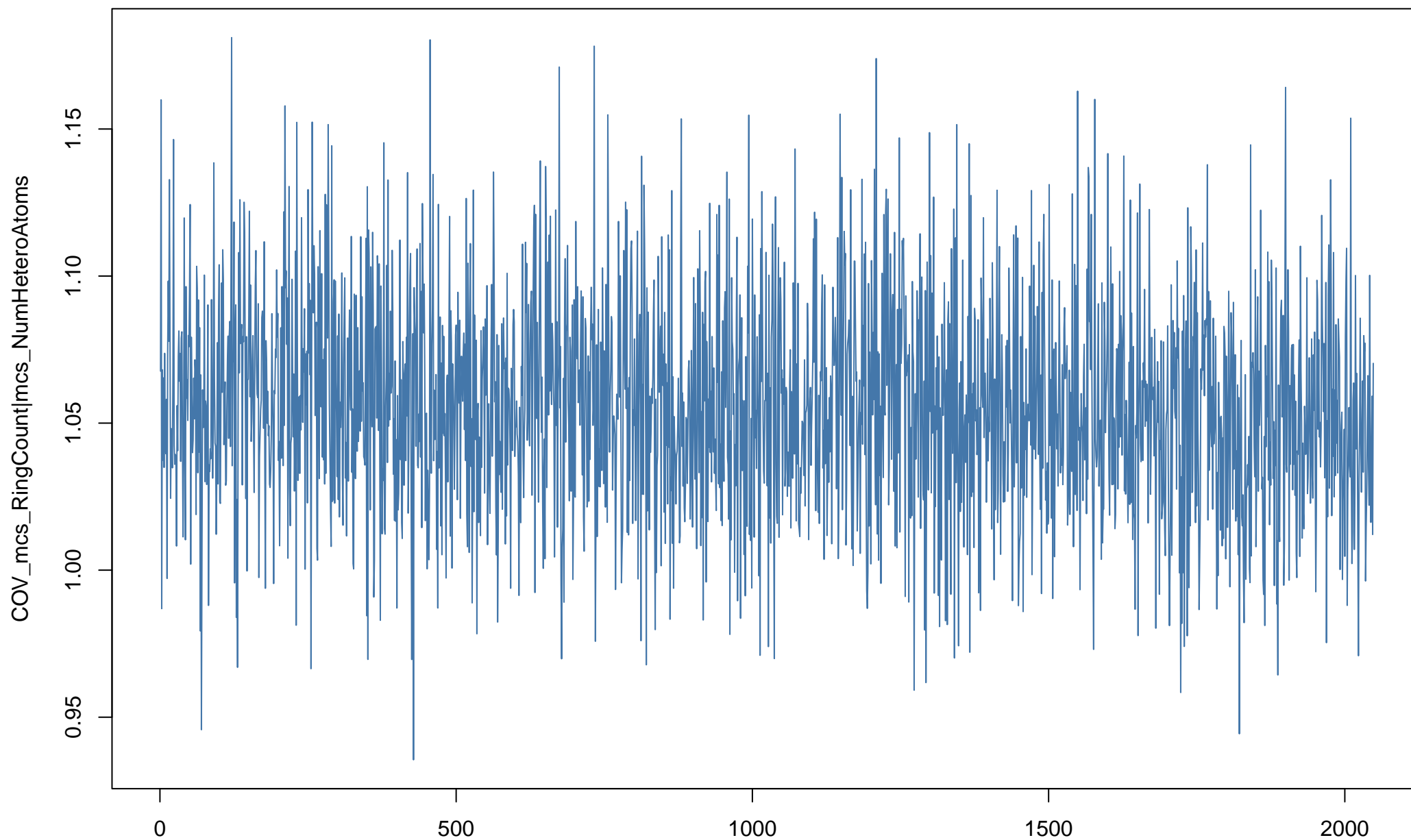
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.055 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0



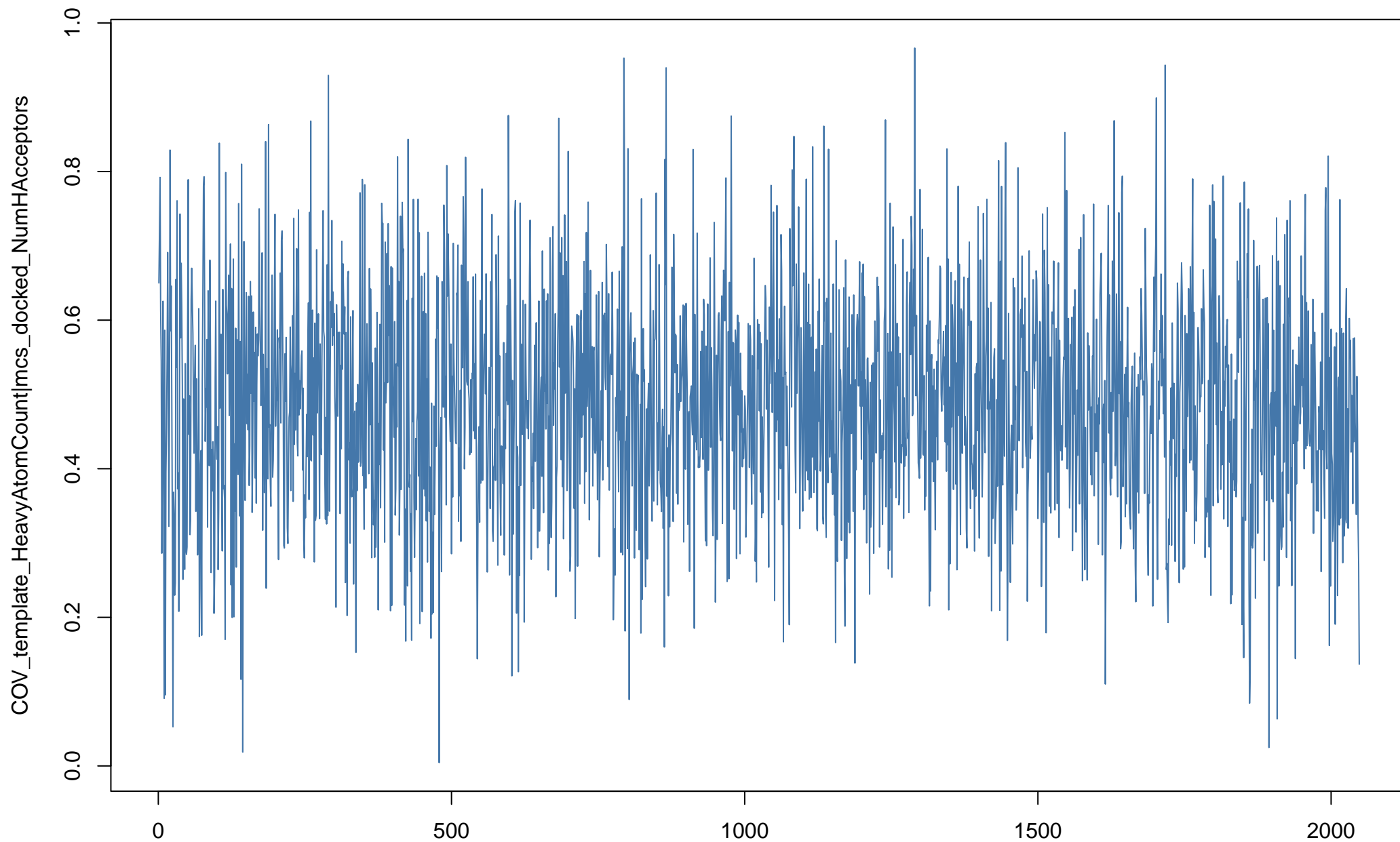
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0701 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



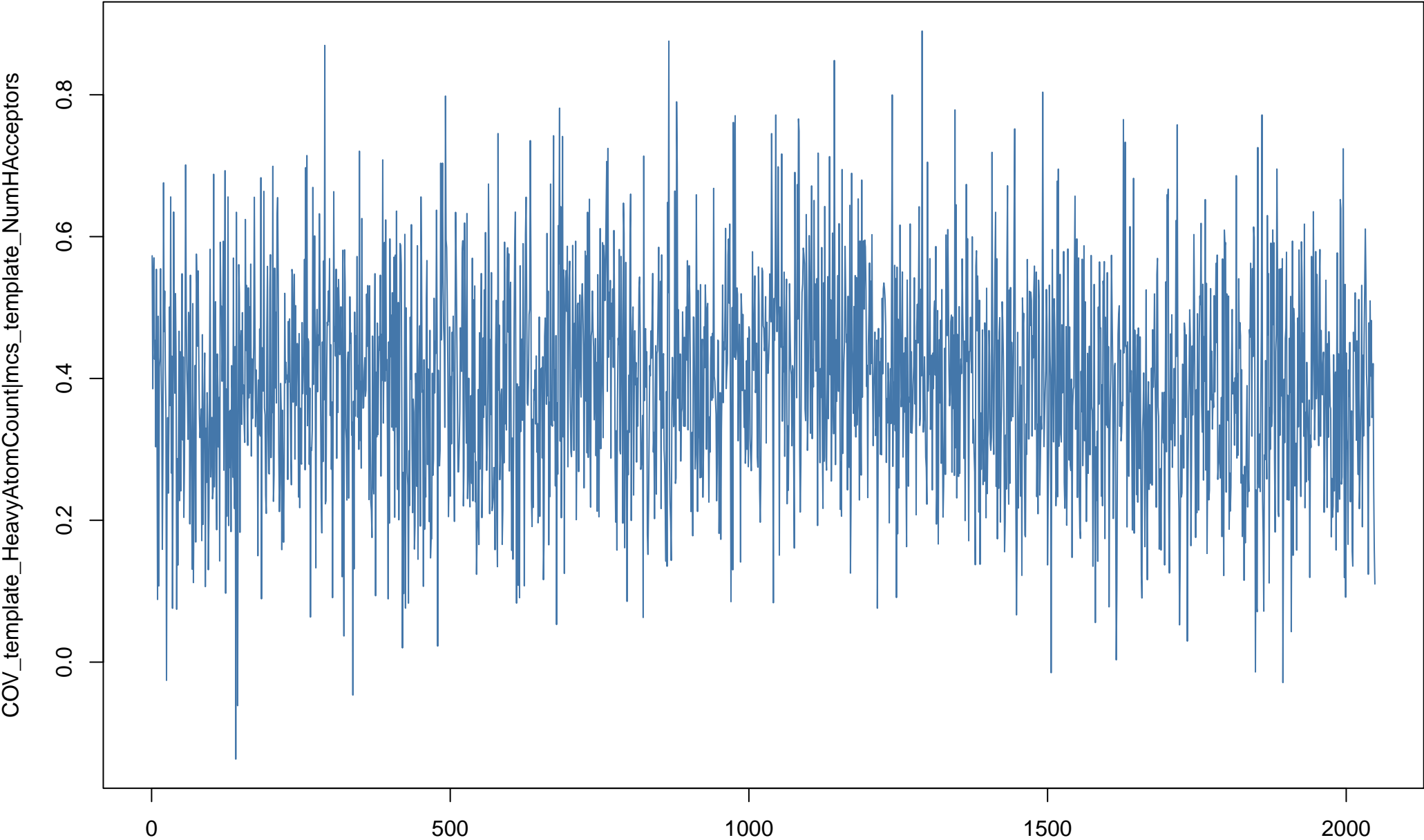
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0525 | MCSE(6.27) = 2.59 | stat: FALSE | burn: 0



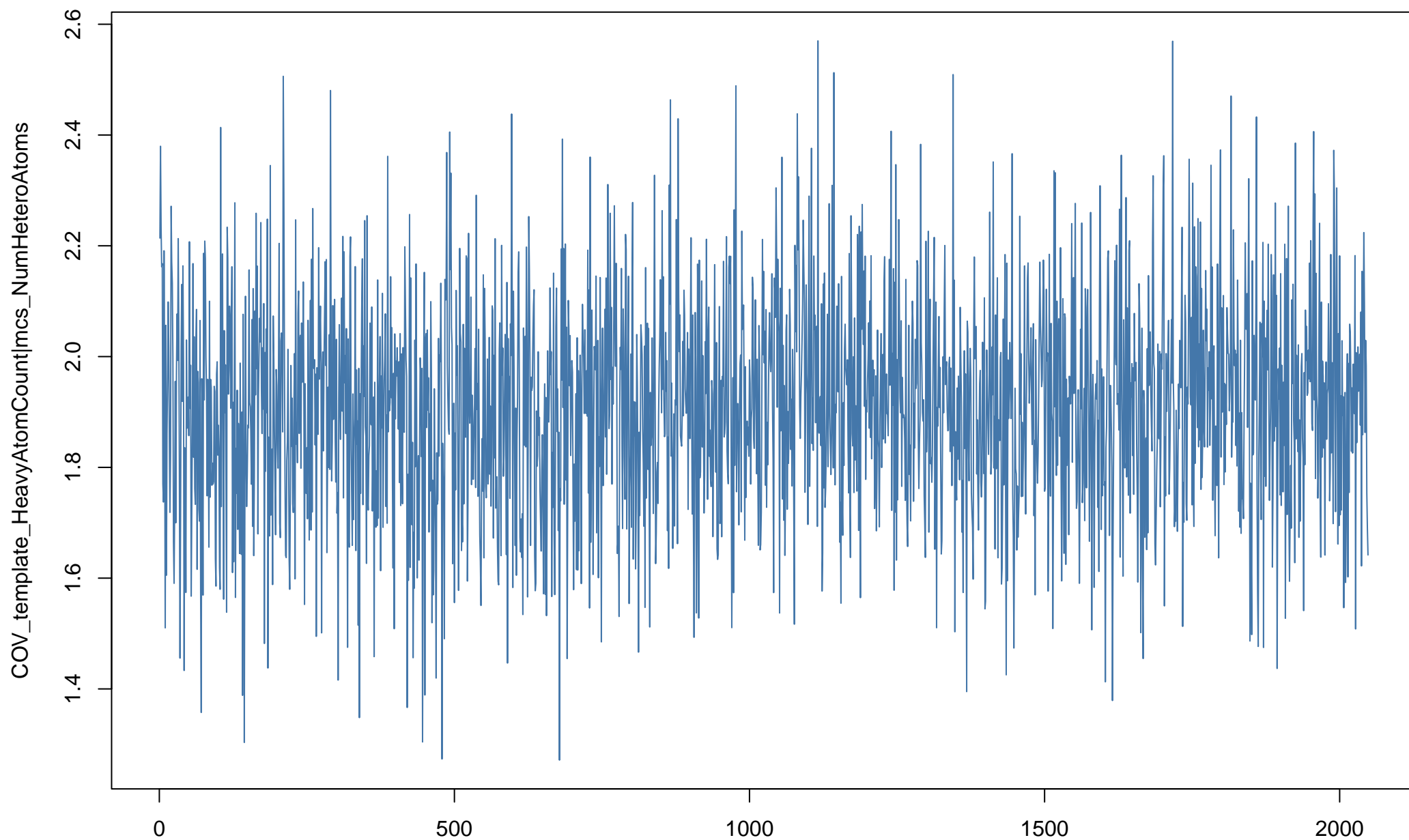
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1860 | BMK = 0.0335 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0



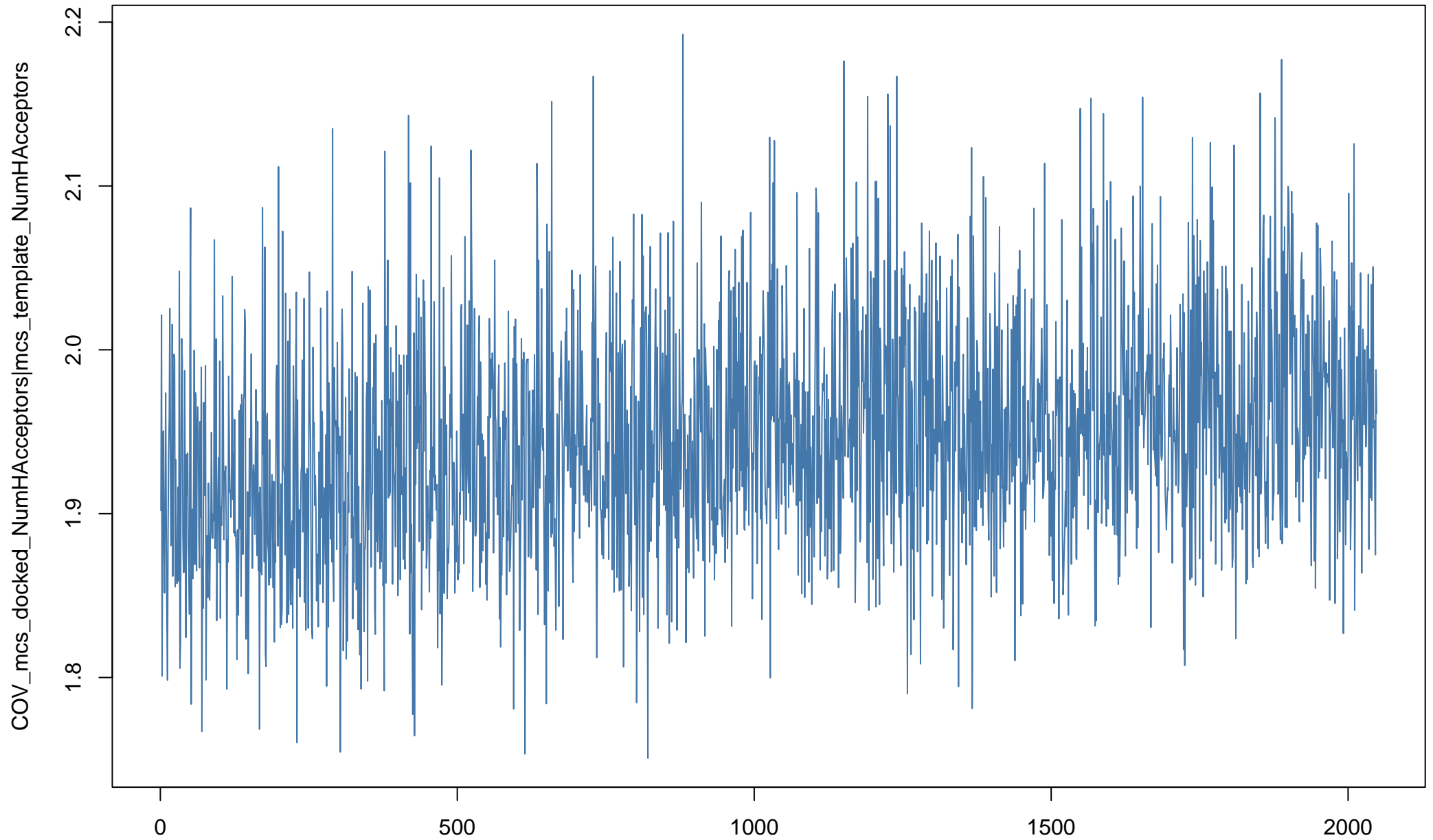
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1660 | BMK = 0.031 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0



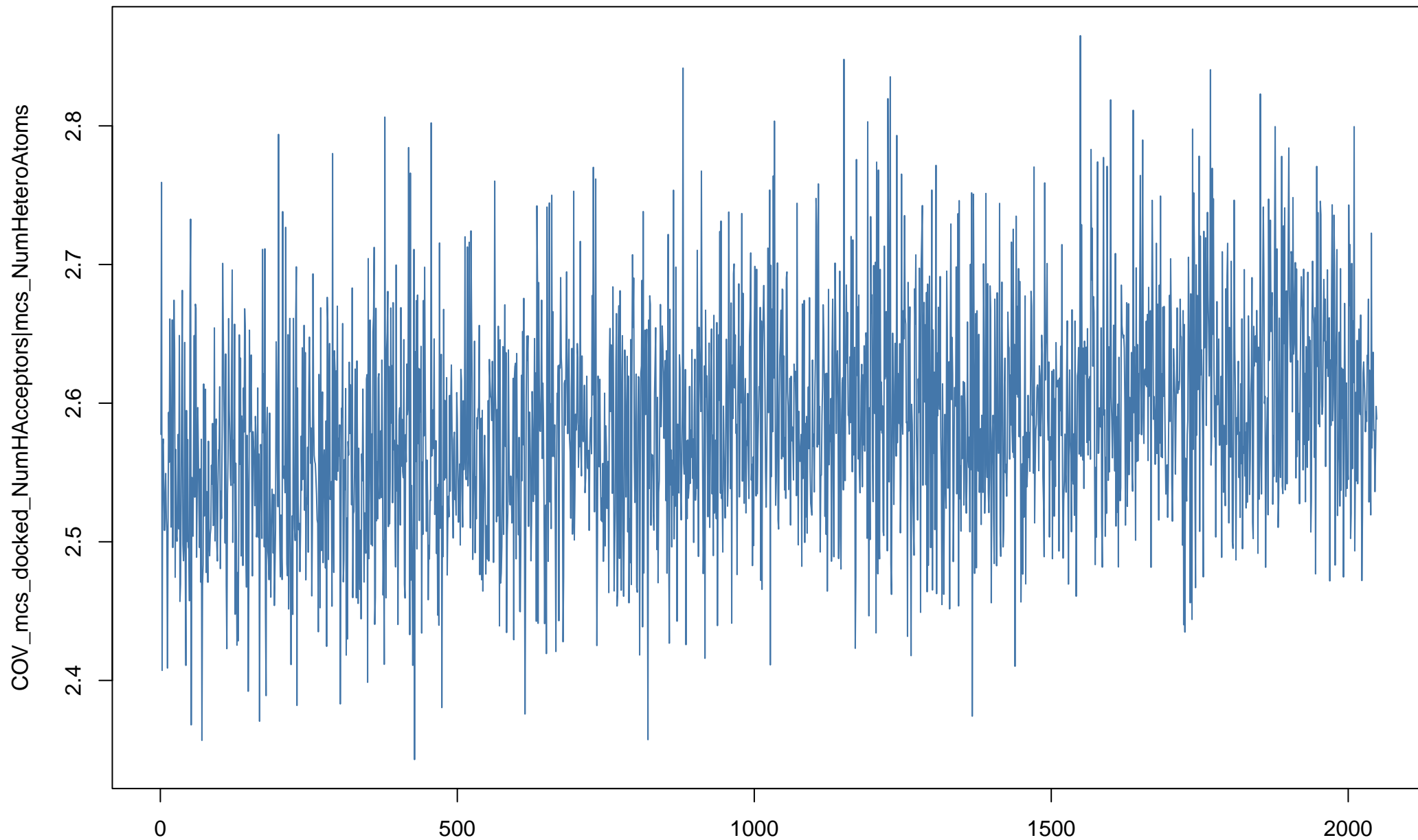
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1870 | BMK = 0.0728 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 122 | BMK = 0.172 | MCSE(6.27) = 4.6 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 102 | BMK = 0.18 | MCSE(6.27) = 4.79 | stat: FALSE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 86.5 | BMK = 0.19 | MCSE(6.27) = 5.11 | stat: FALSE | burn: 0

