

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.302034658228532

max MCSE = 9.88821348042167

all stationary: FALSE

burn: 0

-- STATS 2D --

min ESS = 1444.13509047222

max BMK = 0.0694714285255469

max MCSE = 2.77799971263735

all stationary: TRUE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.145333519404941

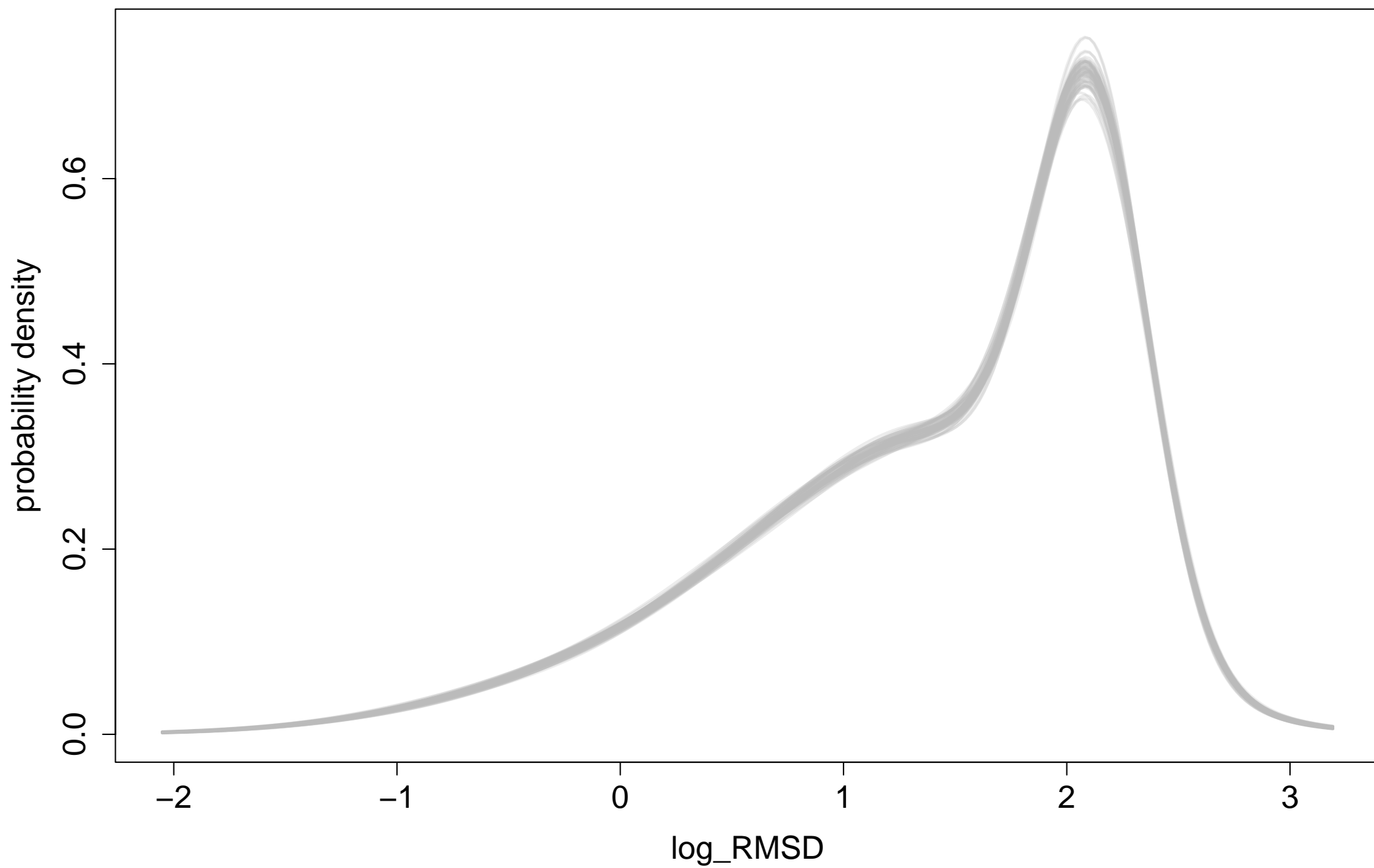
max MCSE = NaN

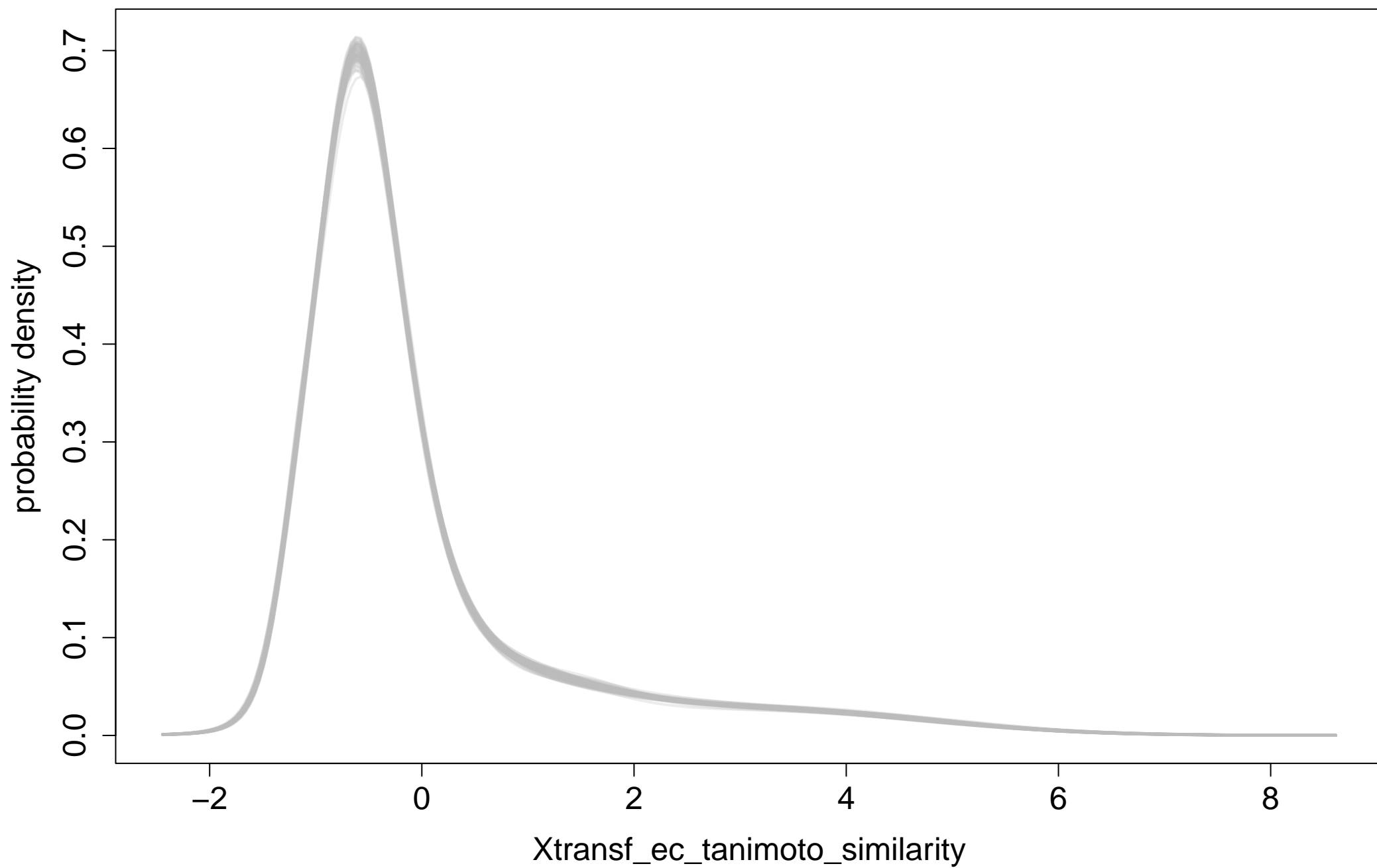
all stationary: FALSE

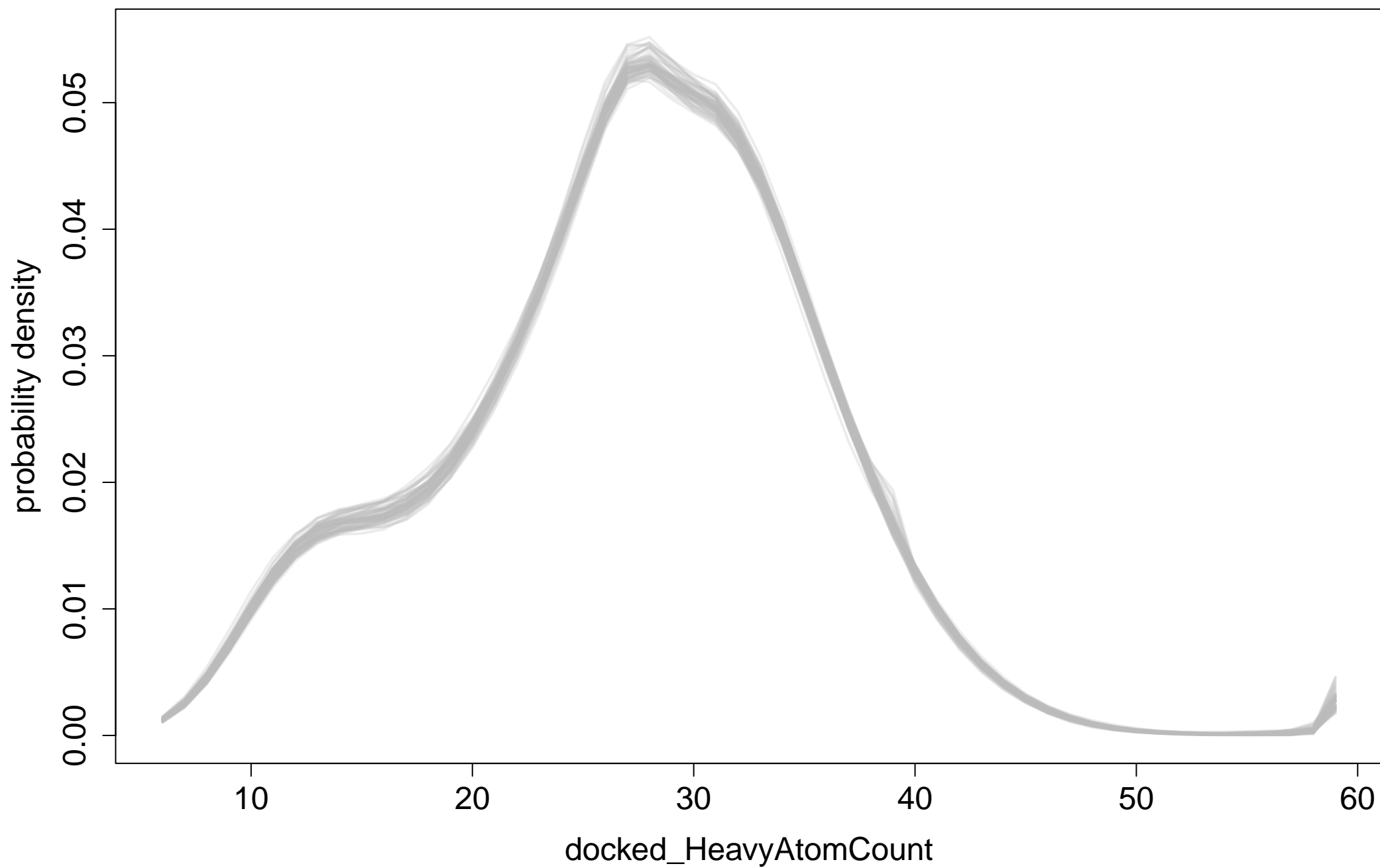
burn: 612

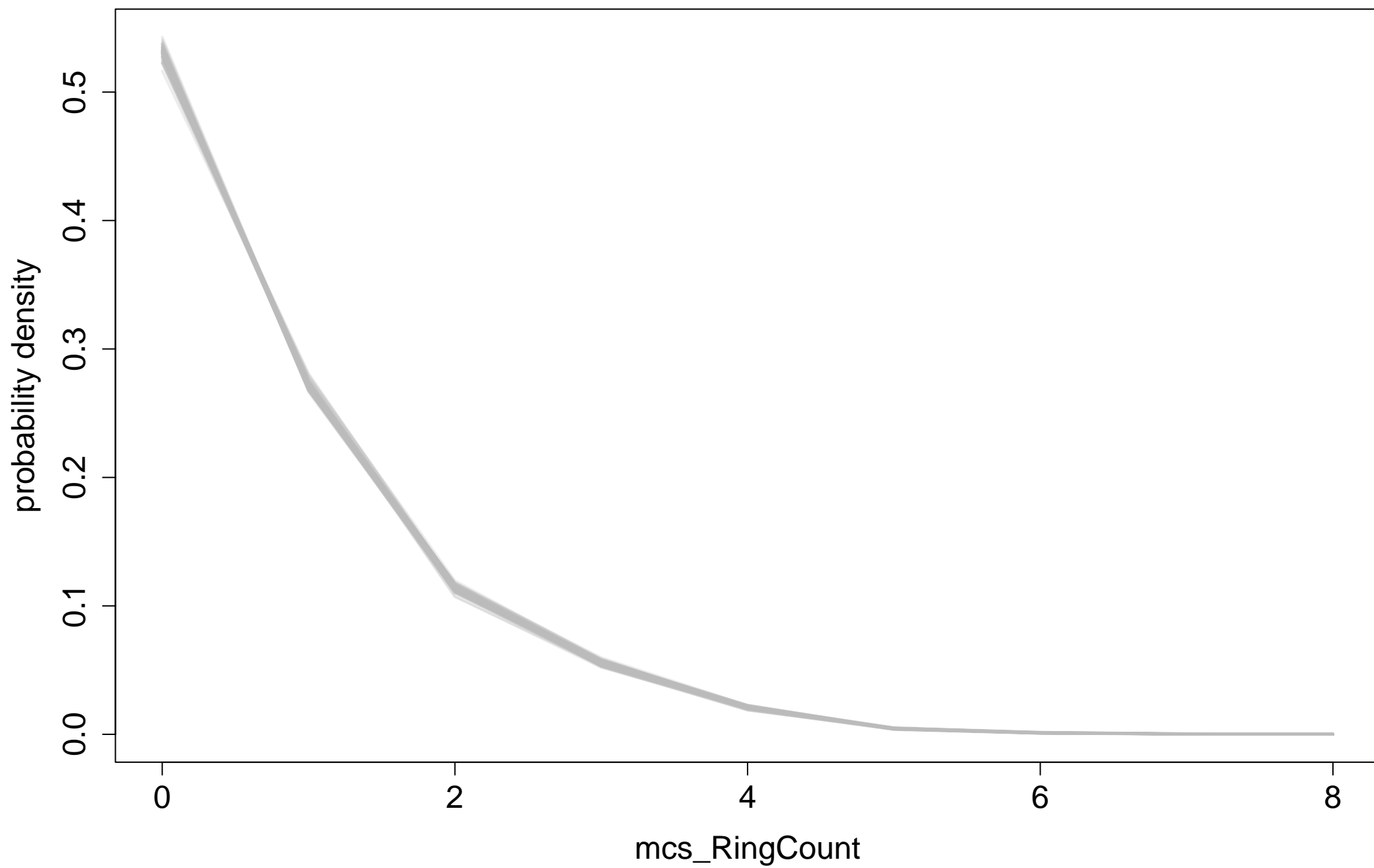
Occupied clusters: 50 of 91

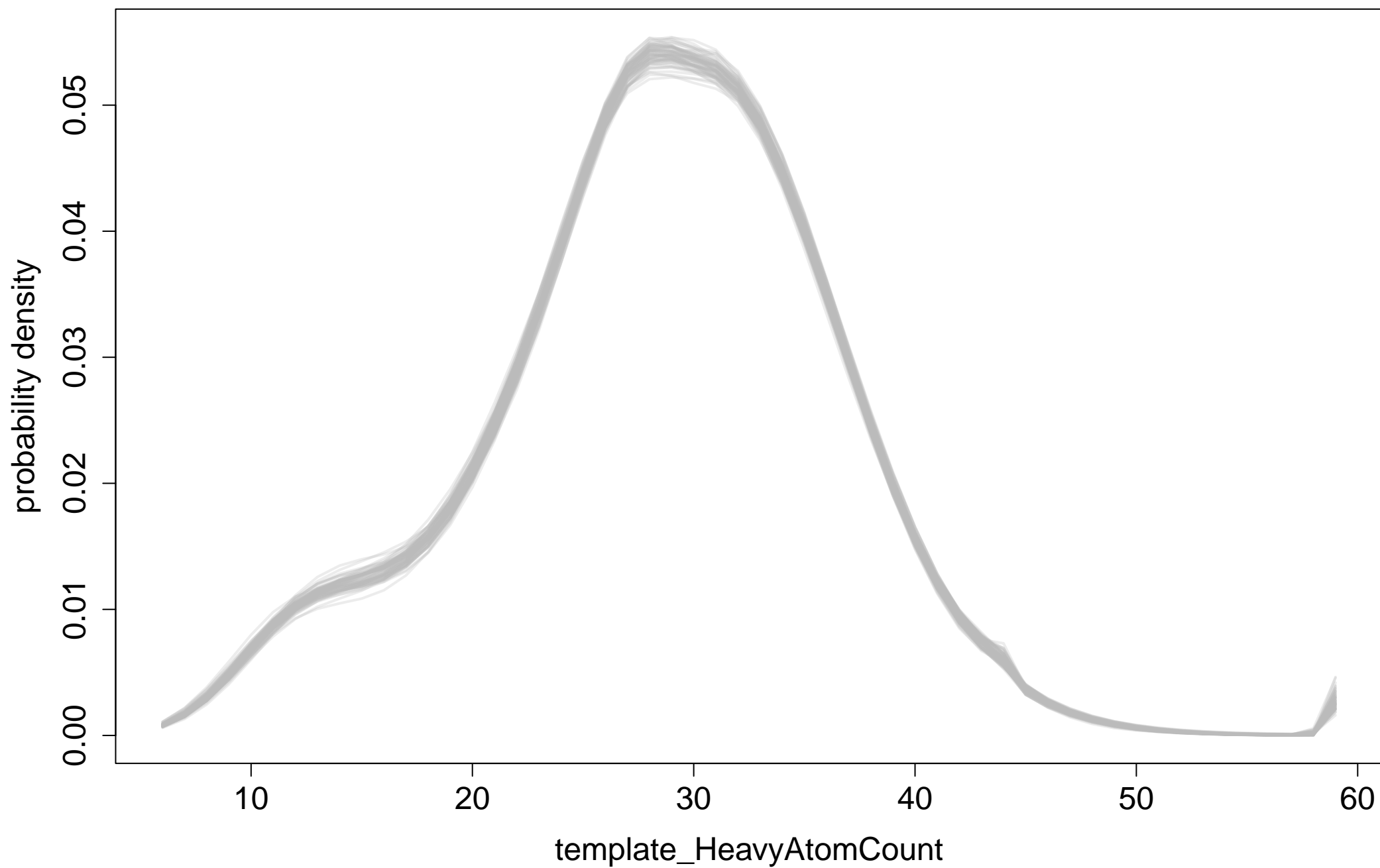
LL: -112000 +- 25.4

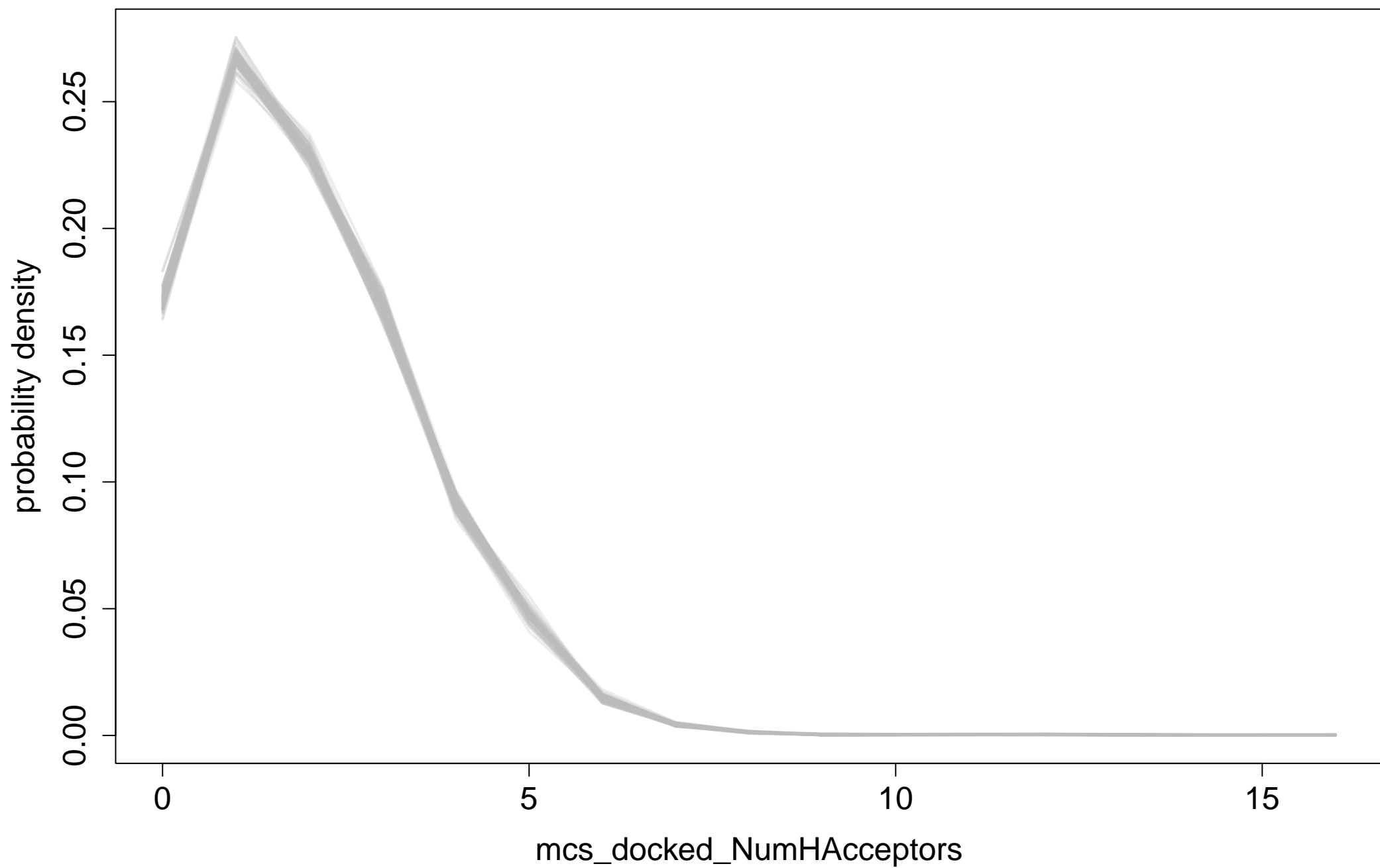


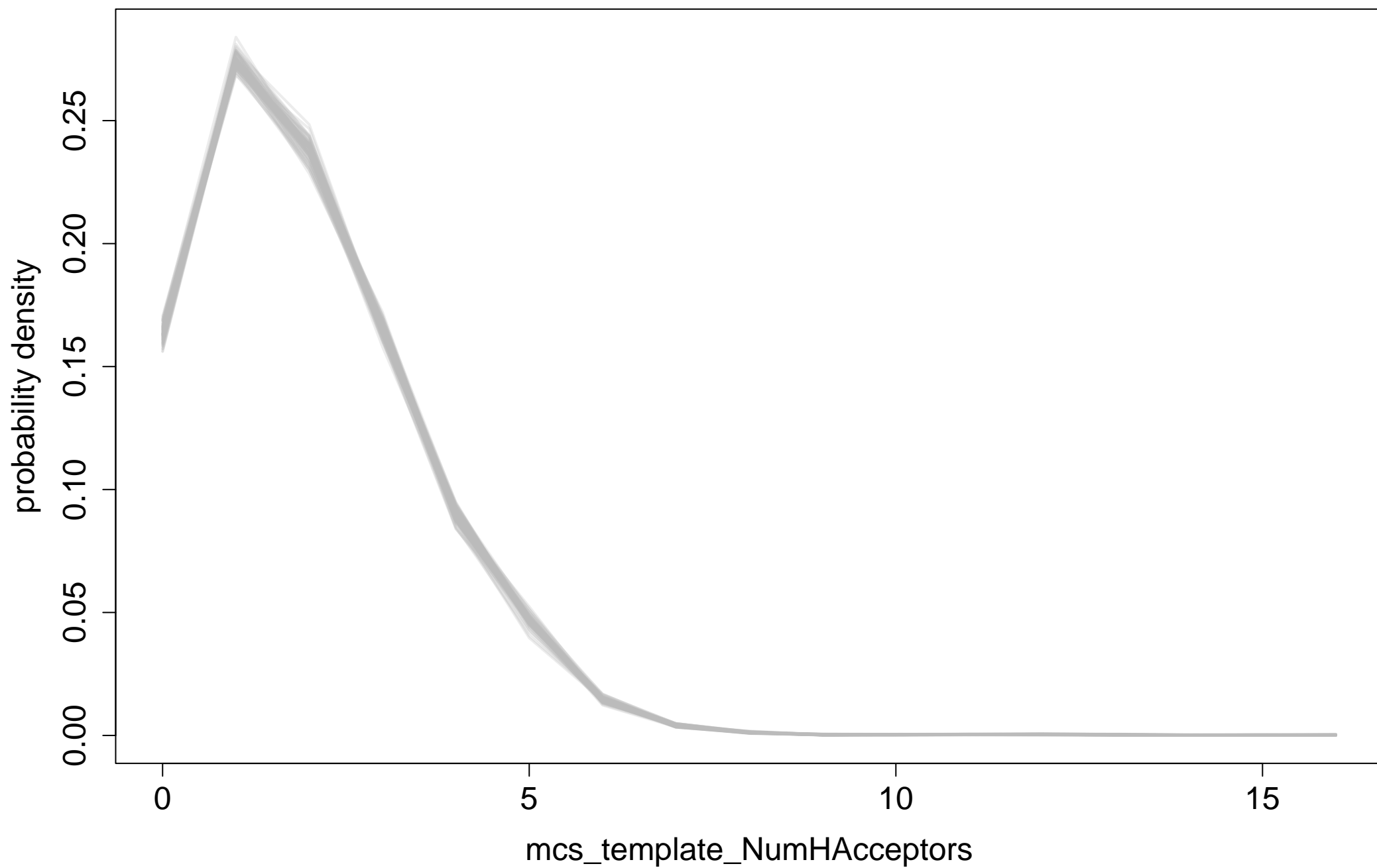


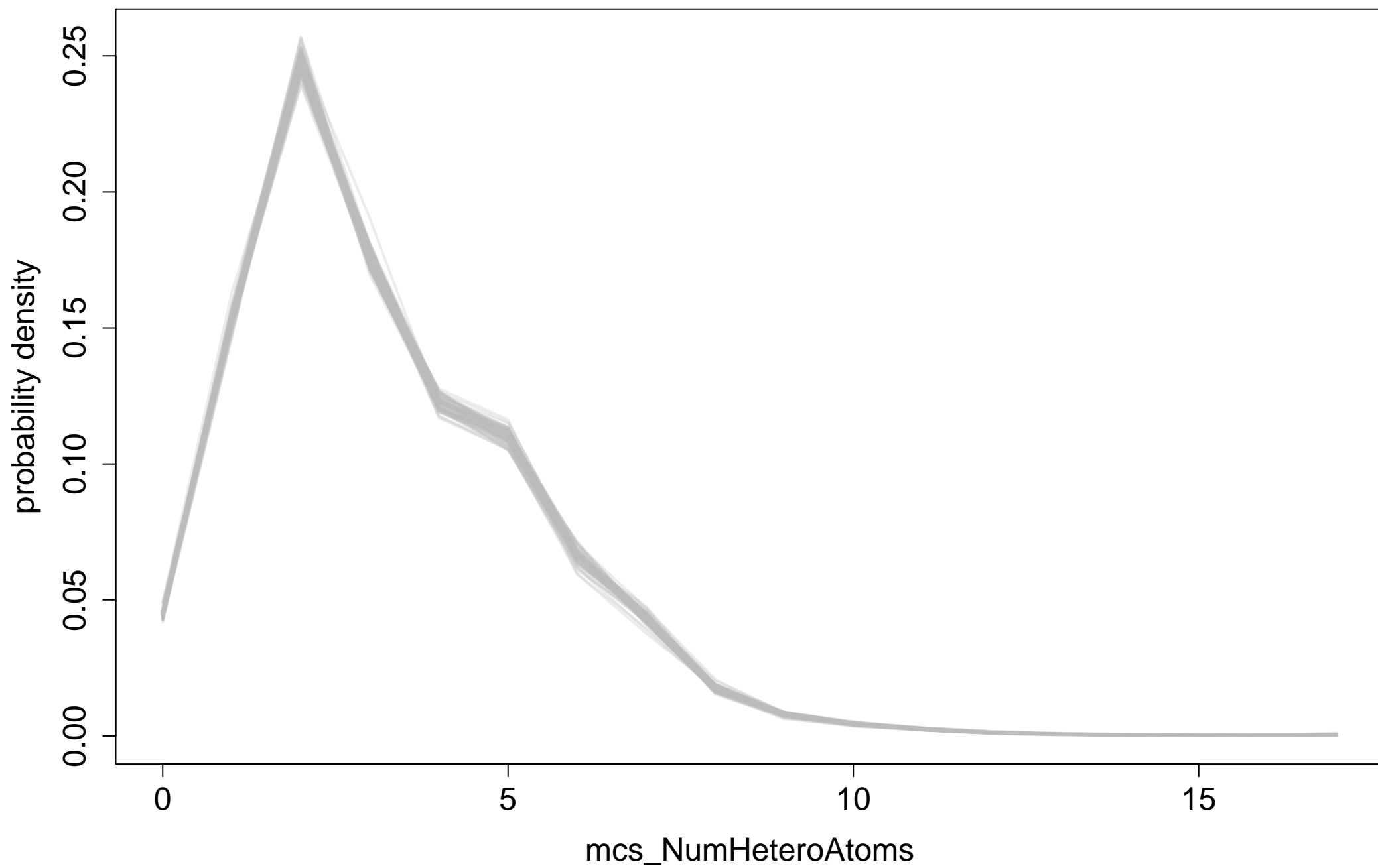


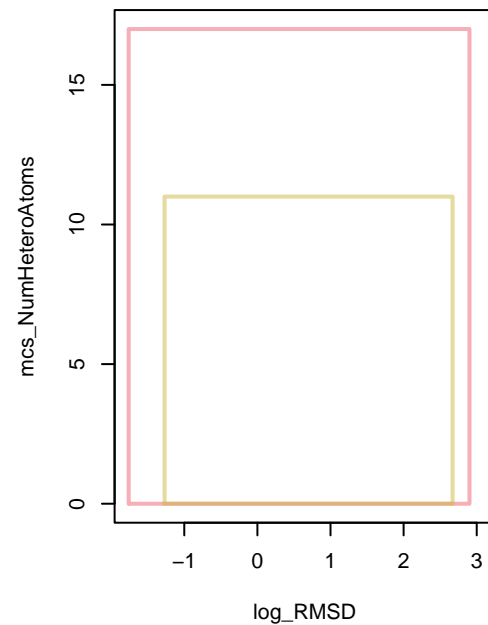
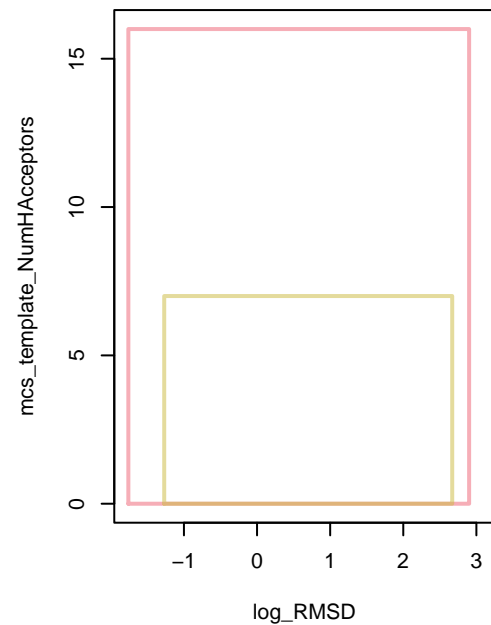
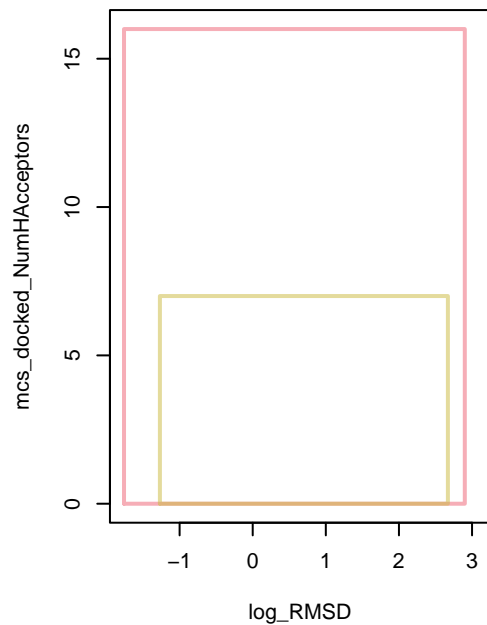
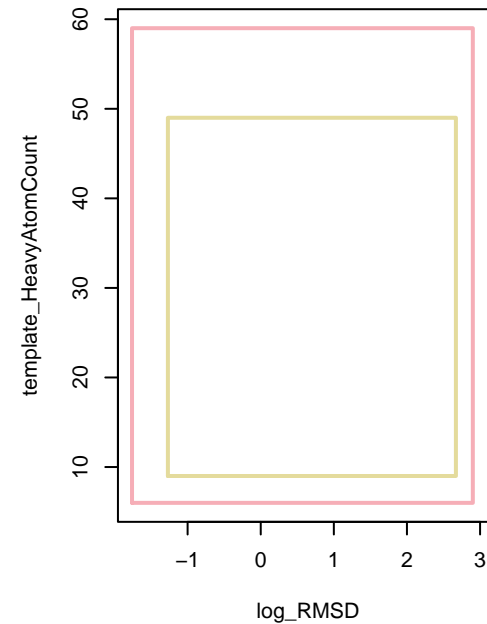
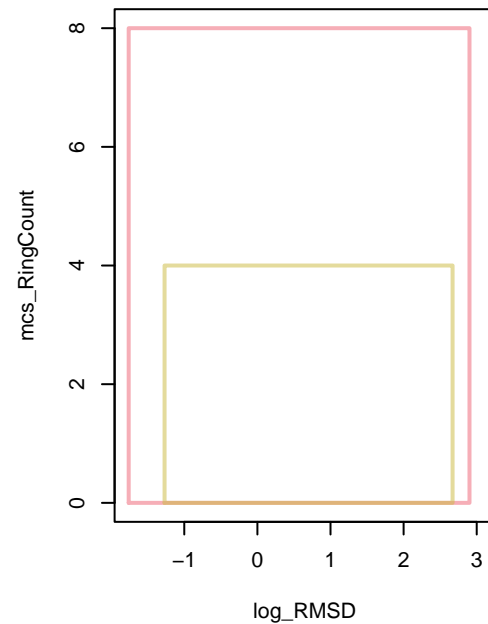
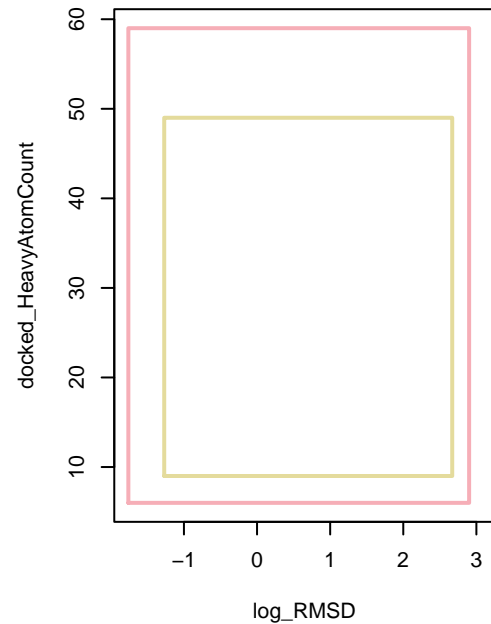
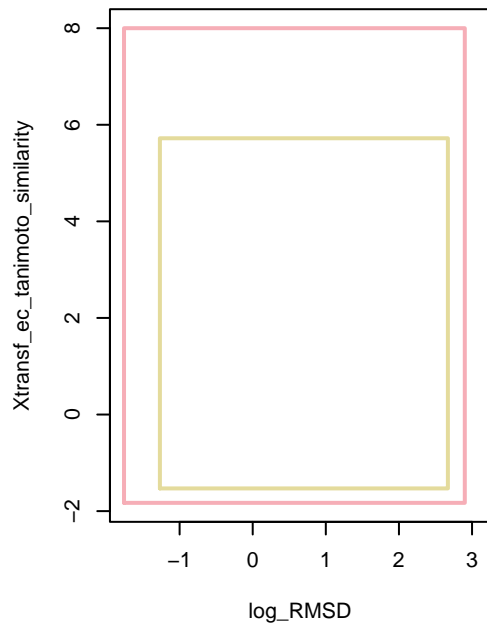




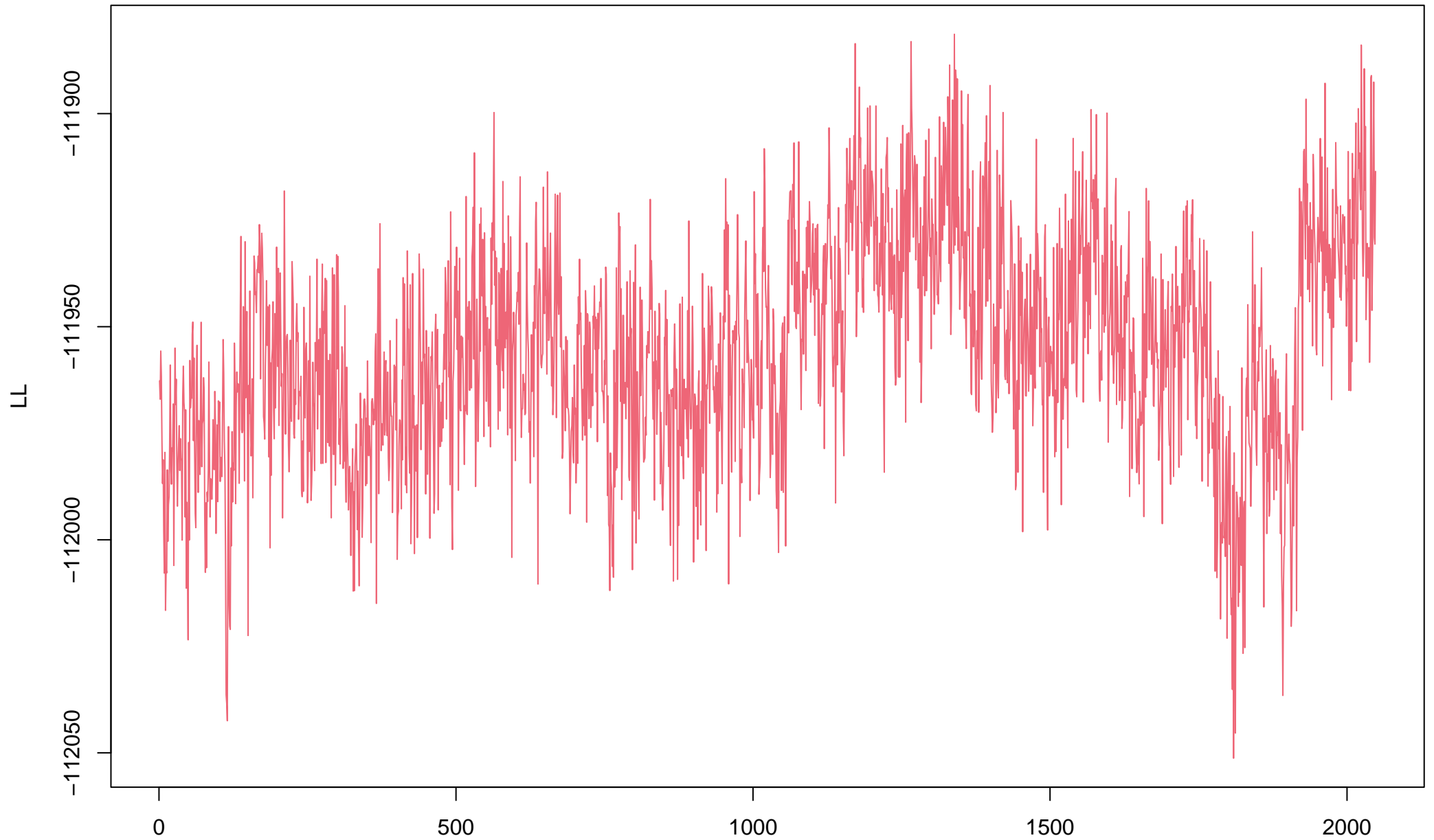




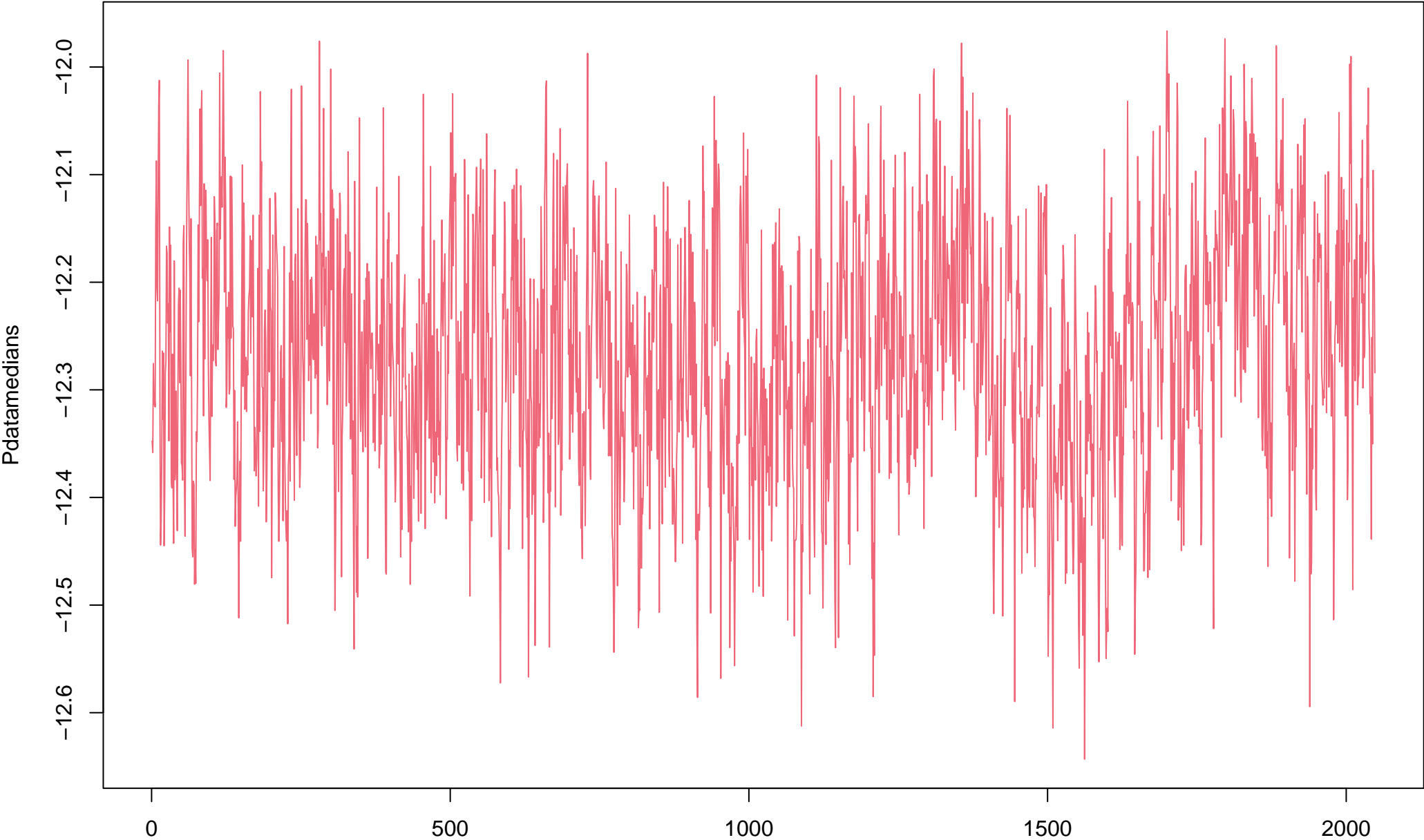




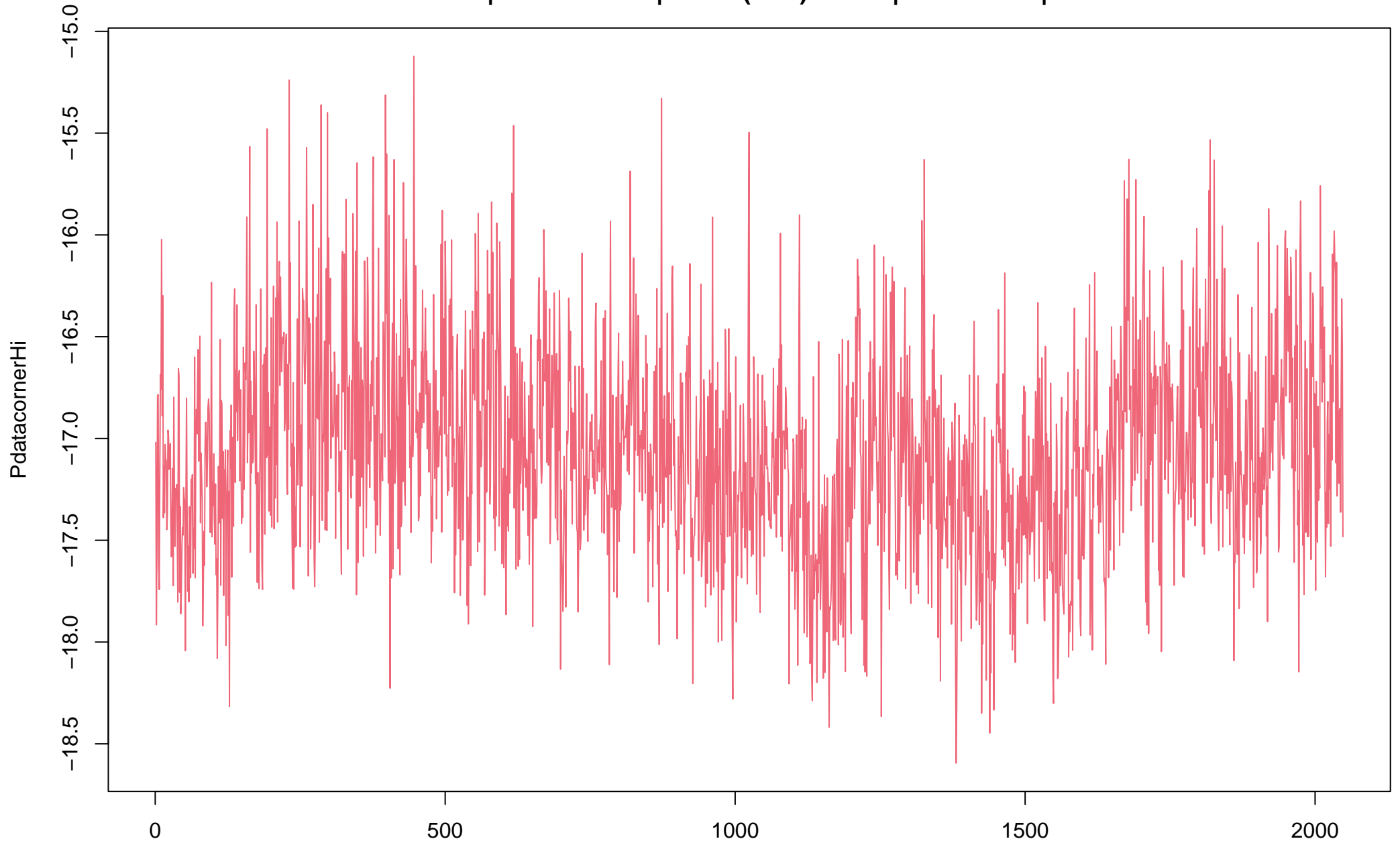
LL
ESS = 42.6 | BMK = 0.302 | MCSE(6.27) = 9.89 | stat: FALSE | burn: 0



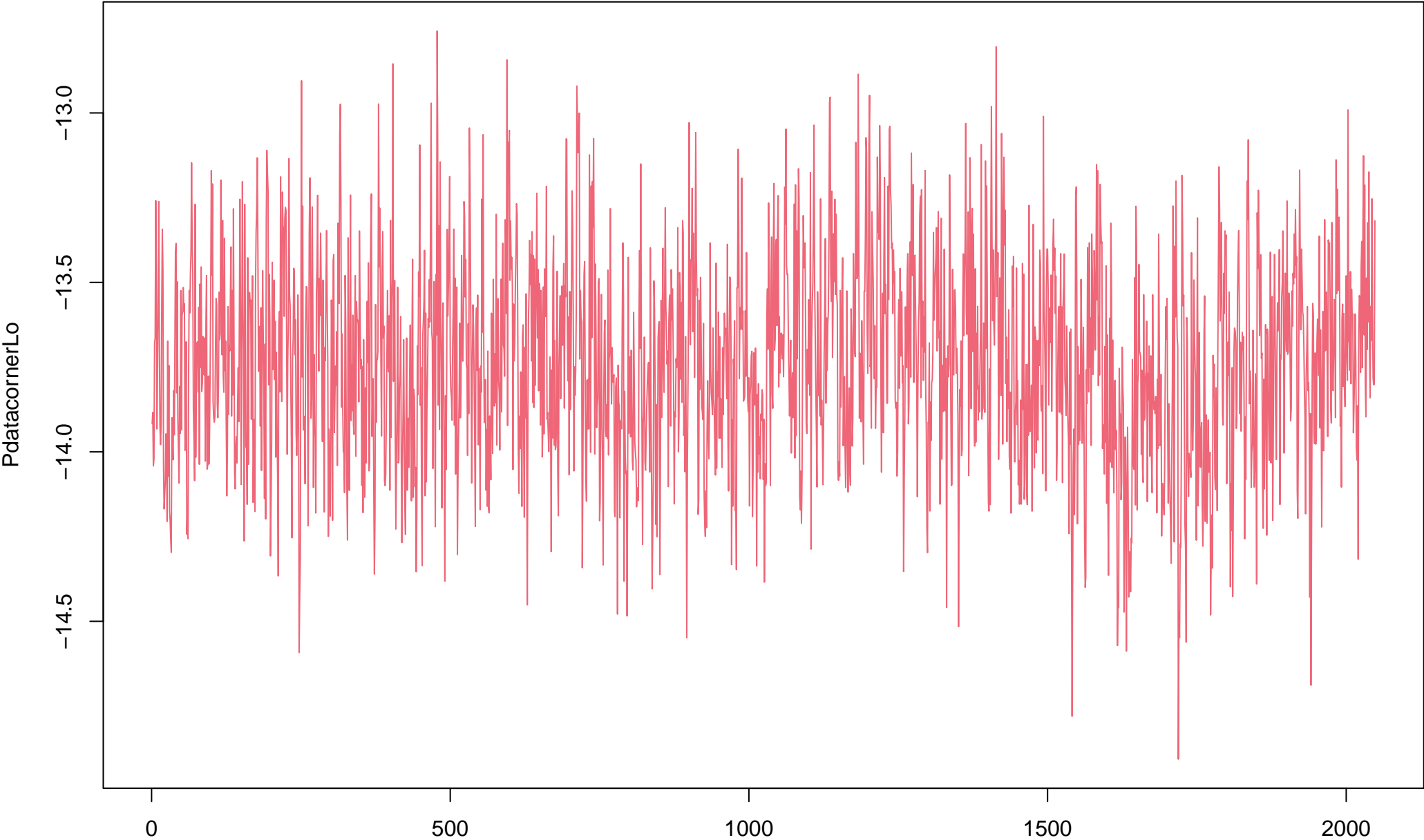
Pdatamedians
ESS = 396 | BMK = 0.0709 | MCSE(6.27) = 5.79 | stat: TRUE | burn: 0



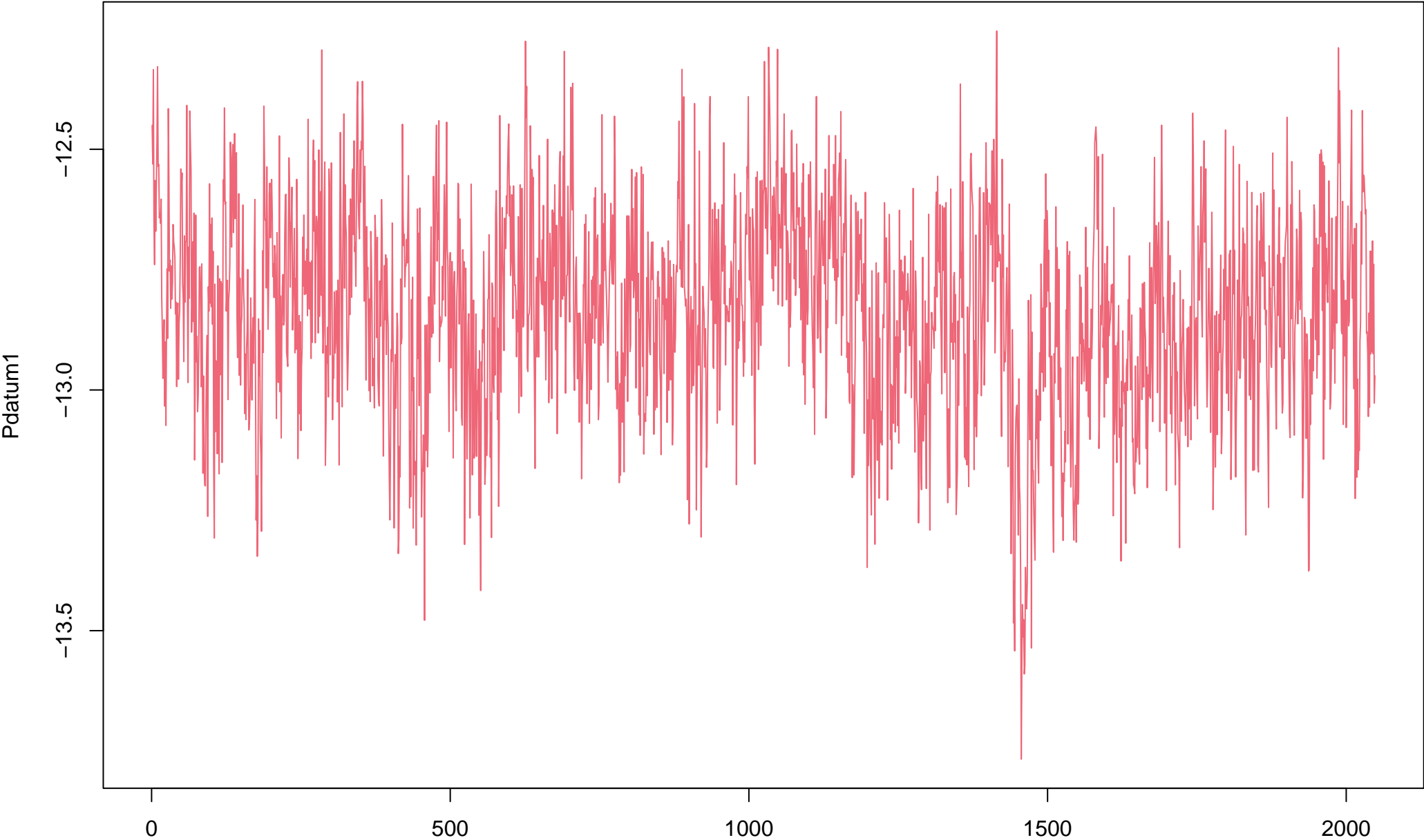
PdatacornerHi
ESS = 150 | BMK = 0.116 | MCSE(6.27) = 5.52 | stat: TRUE | burn: 0



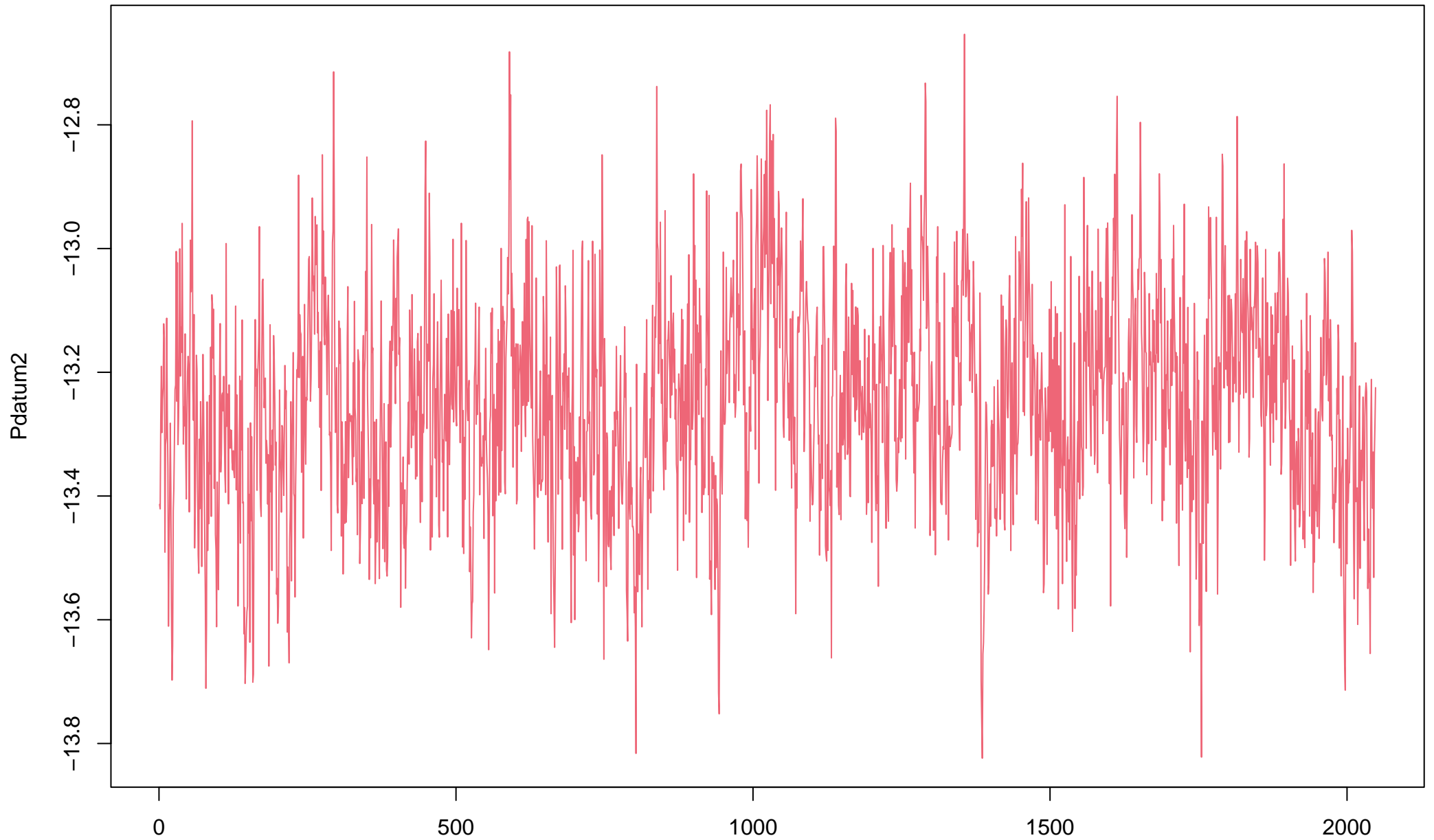
PdatacornerLo
ESS = 559 | BMK = 0.0541 | MCSE(6.27) = 4.49 | stat: TRUE | burn: 0



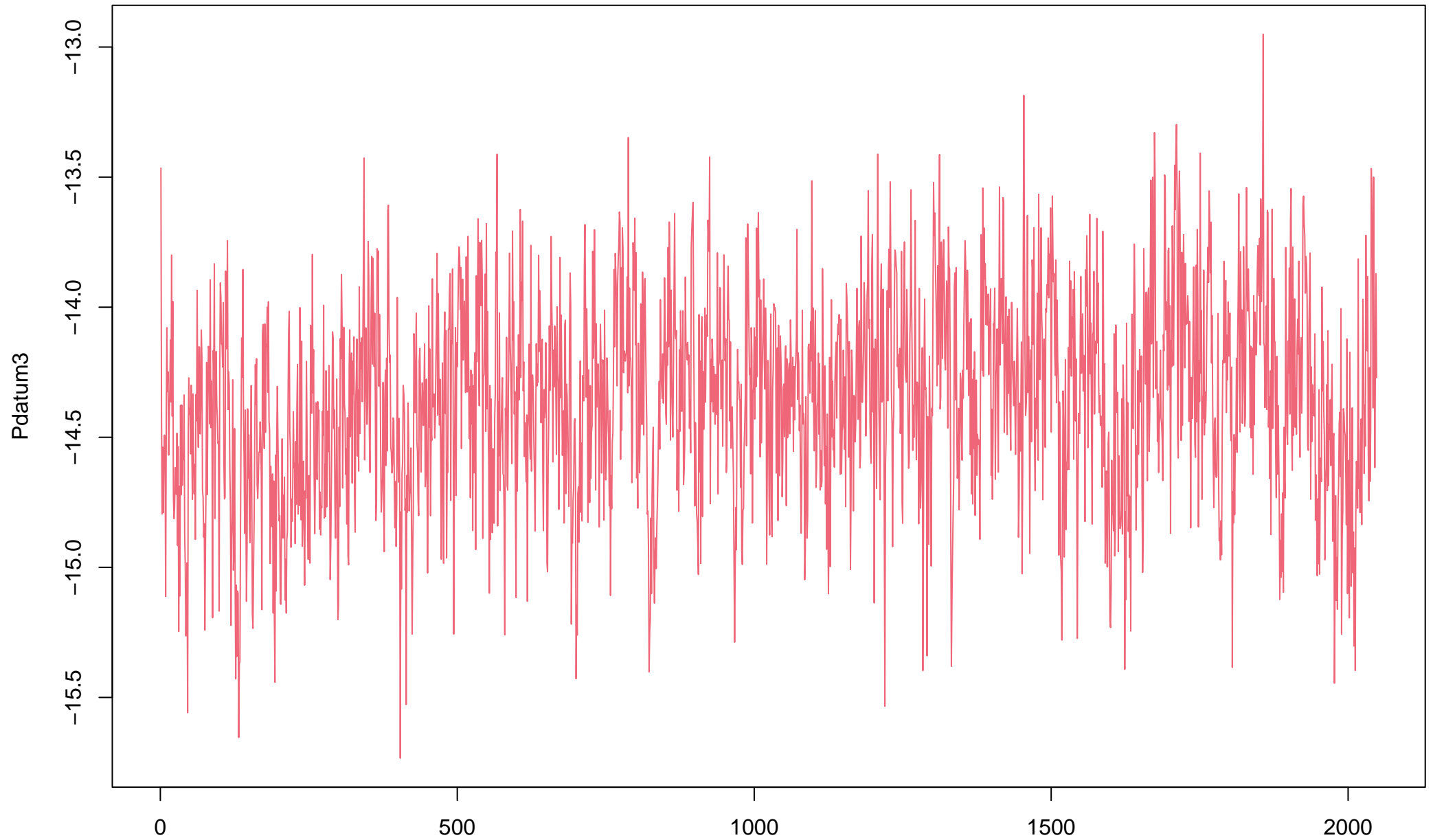
Pdatum1
ESS = 224 | BMK = 0.0996 | MCSE(6.27) = 6.75 | stat: TRUE | burn: 0



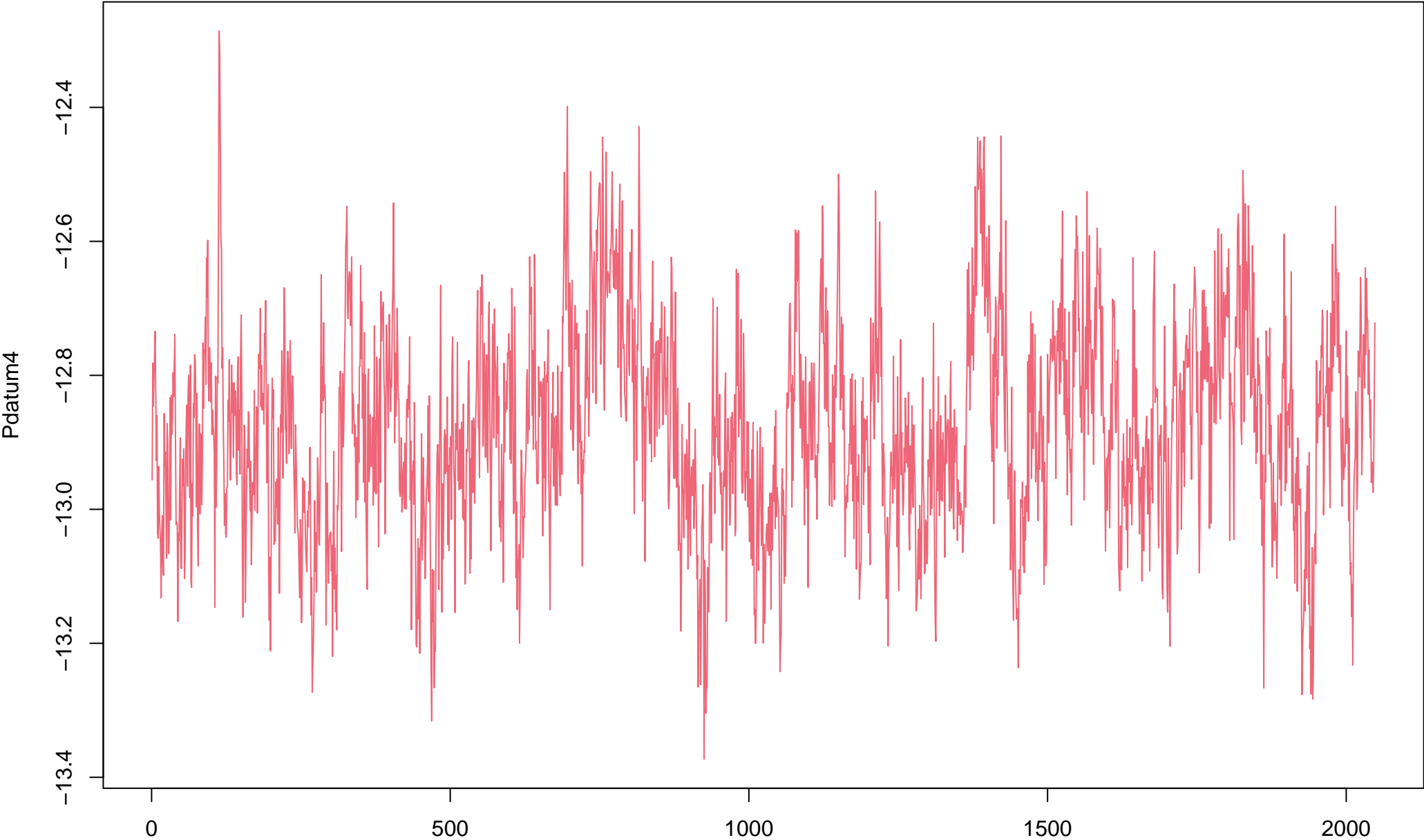
Pdatum2
ESS = 220 | BMK = 0.0944 | MCSE(6.27) = 6.19 | stat: FALSE | burn: 0



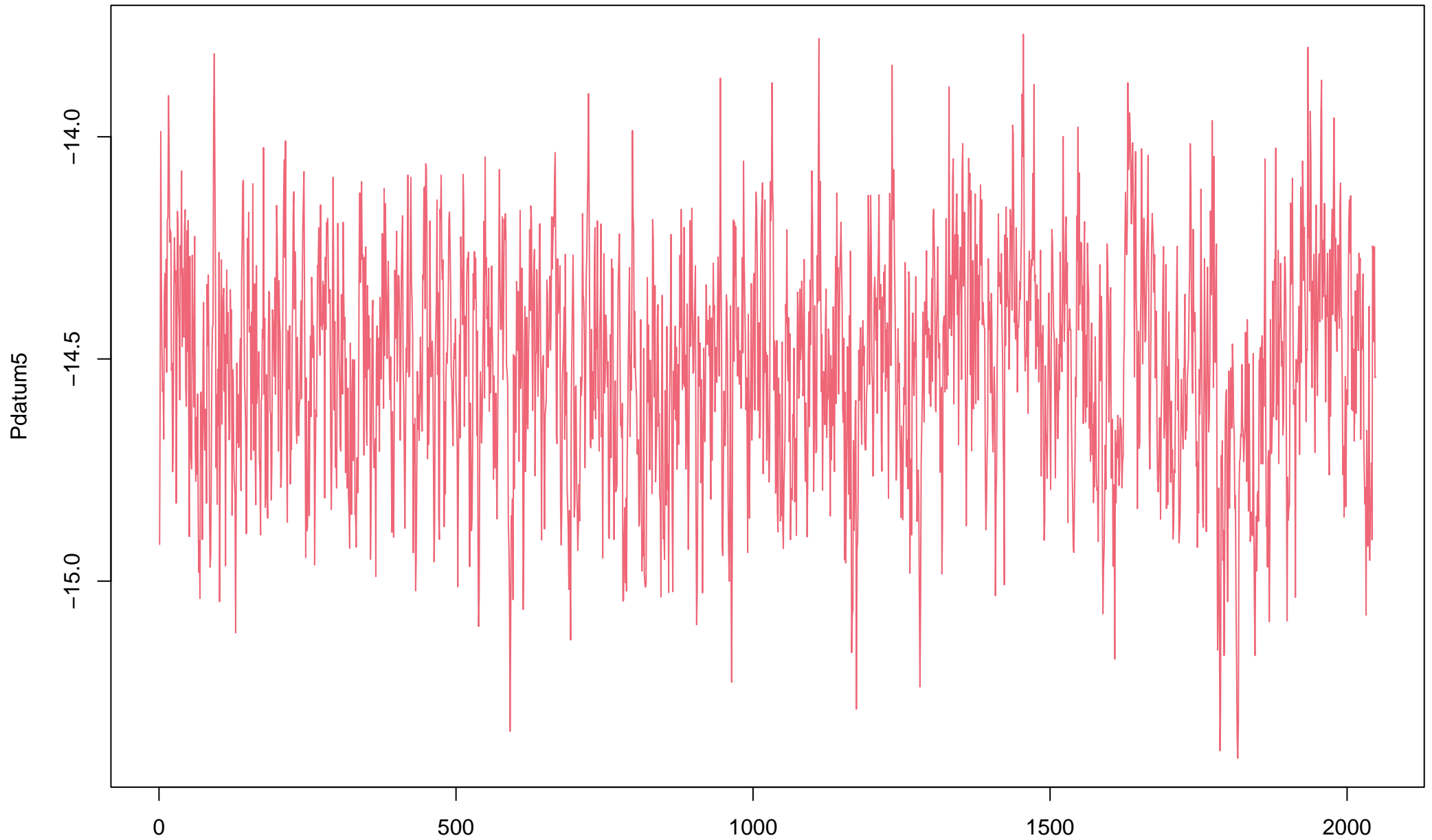
Pdatum3
ESS = 319 | BMK = 0.122 | MCSE(6.27) = 6 | stat: FALSE | burn: 0



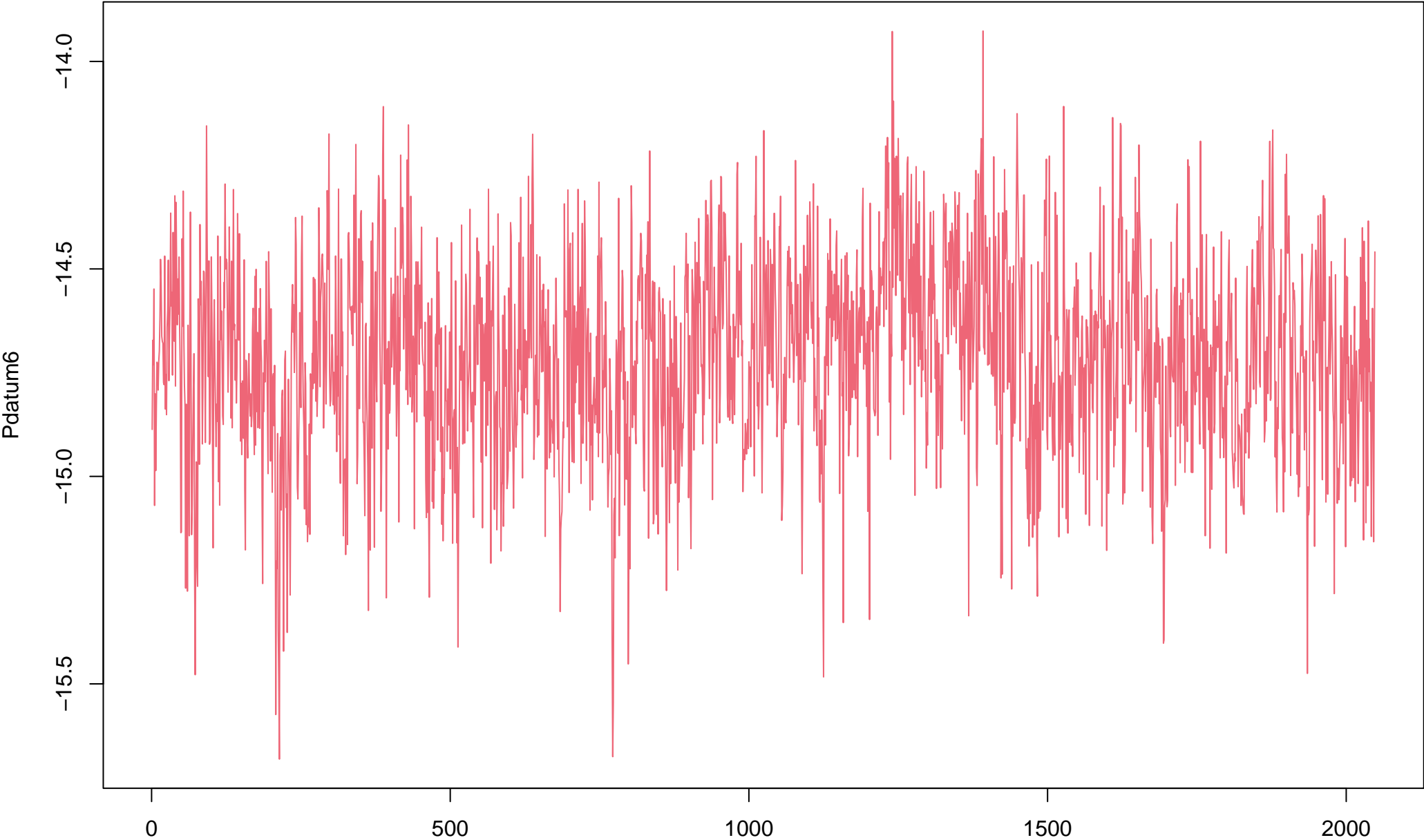
Pdatum4
ESS = 127 | BMK = 0.0564 | MCSE(6.27) = 8.37 | stat: TRUE | burn: 0



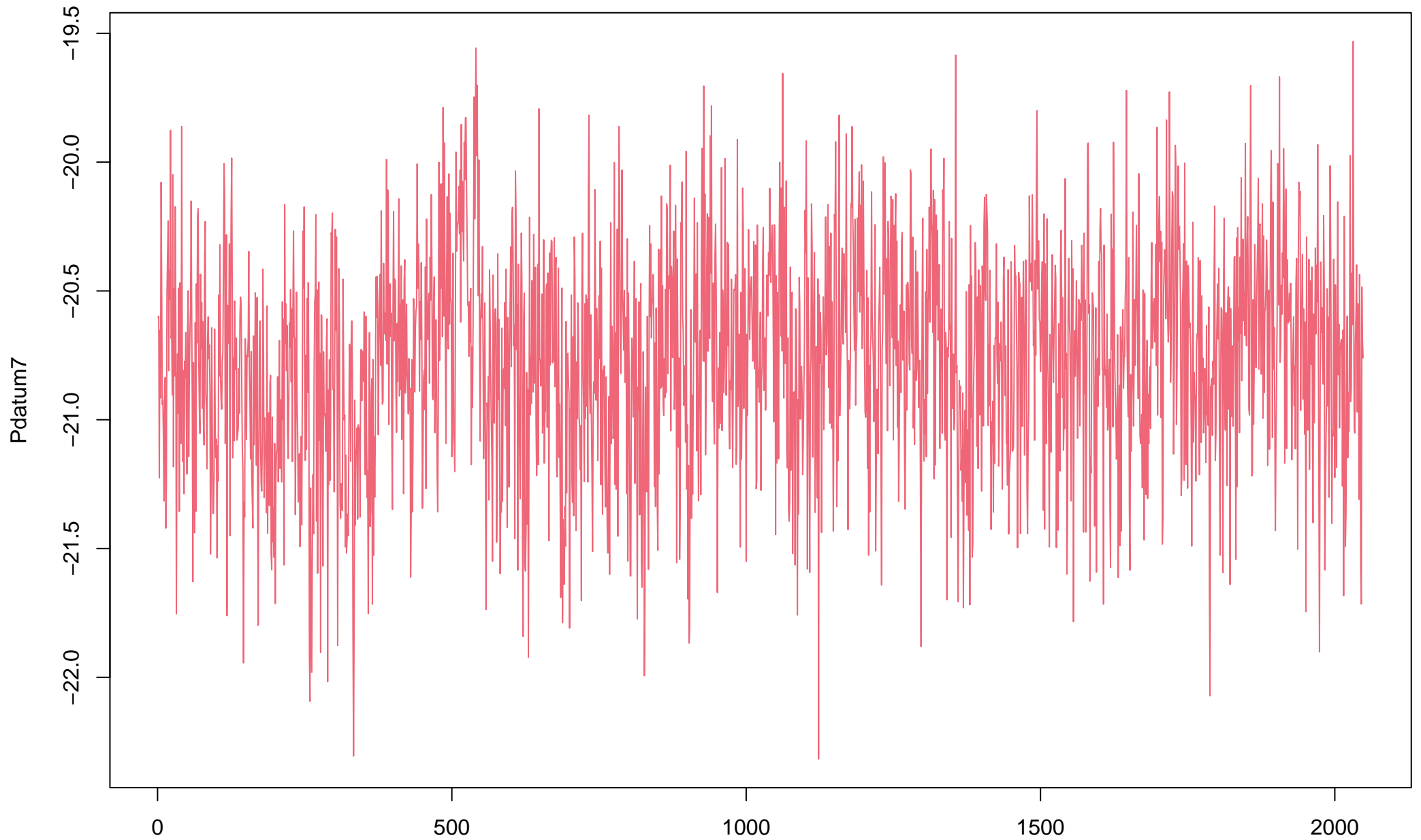
Pdatum5
ESS = 423 | BMK = 0.059 | MCSE(6.27) = 5.68 | stat: TRUE | burn: 0



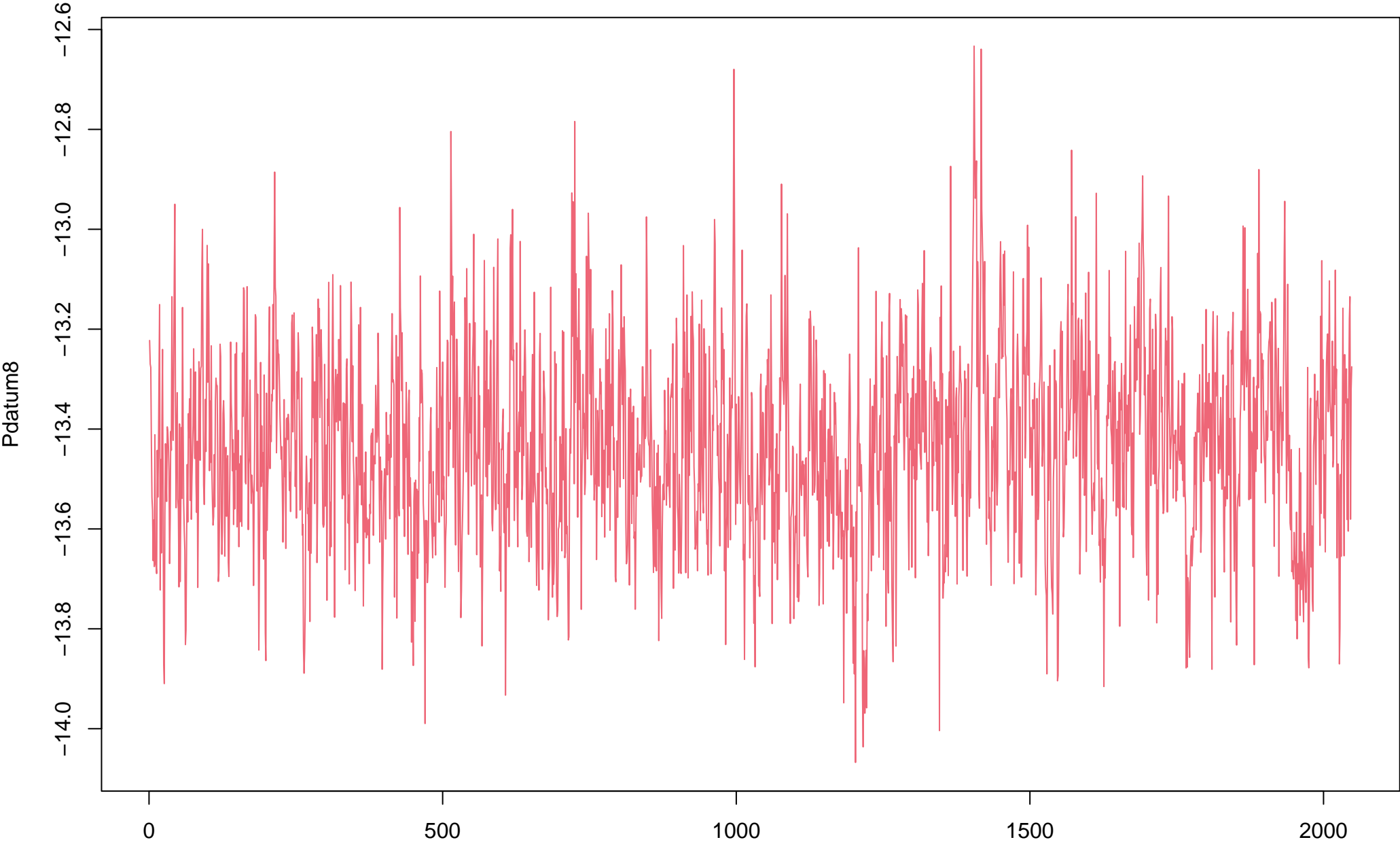
Pdatum6
ESS = 324 | BMK = 0.0864 | MCSE(6.27) = 5.49 | stat: TRUE | burn: 0



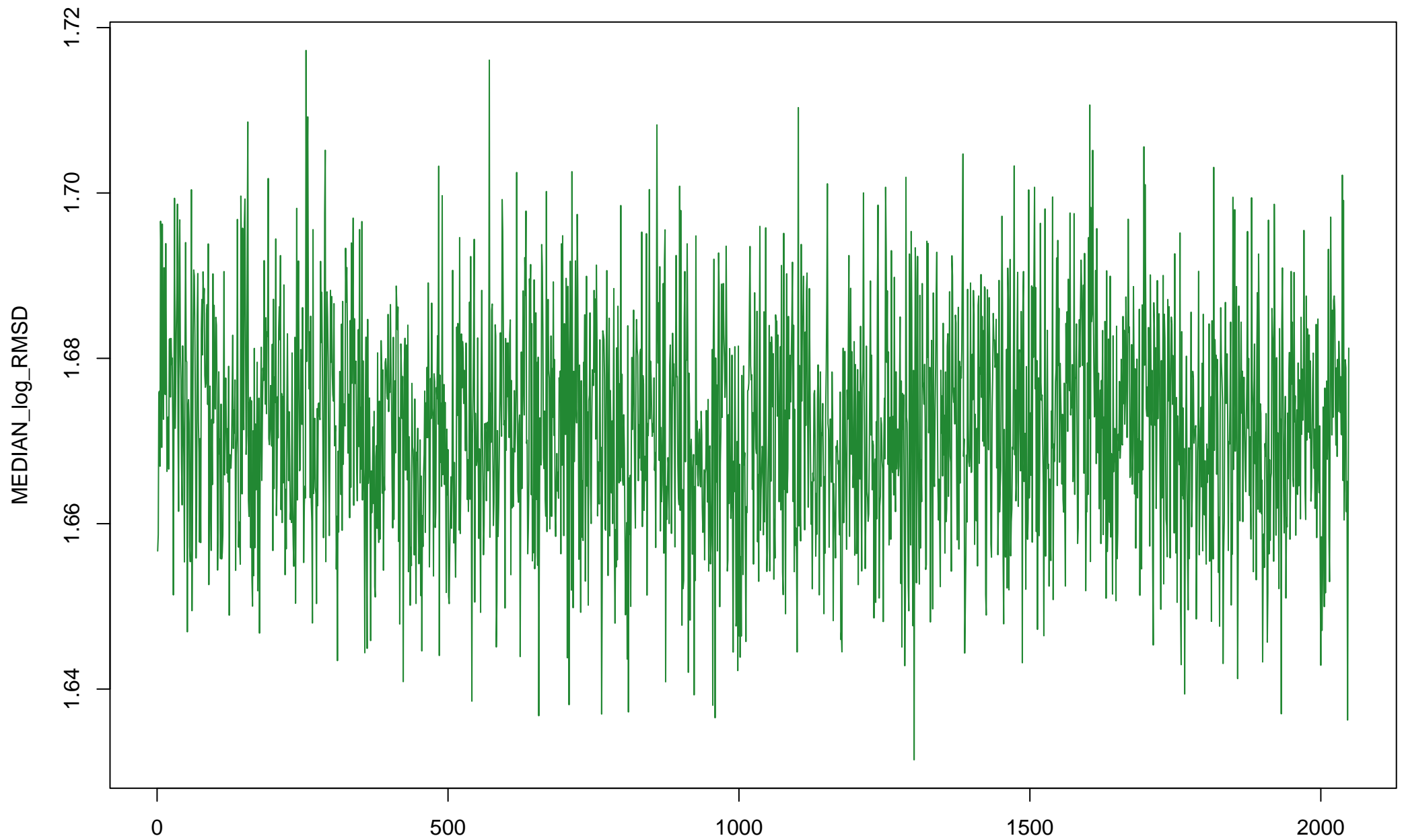
Pdatum7
ESS = 2.22e-16 | BMK = 0.0873 | MCSE(6.27) = 4.94 | stat: TRUE | burn: 0



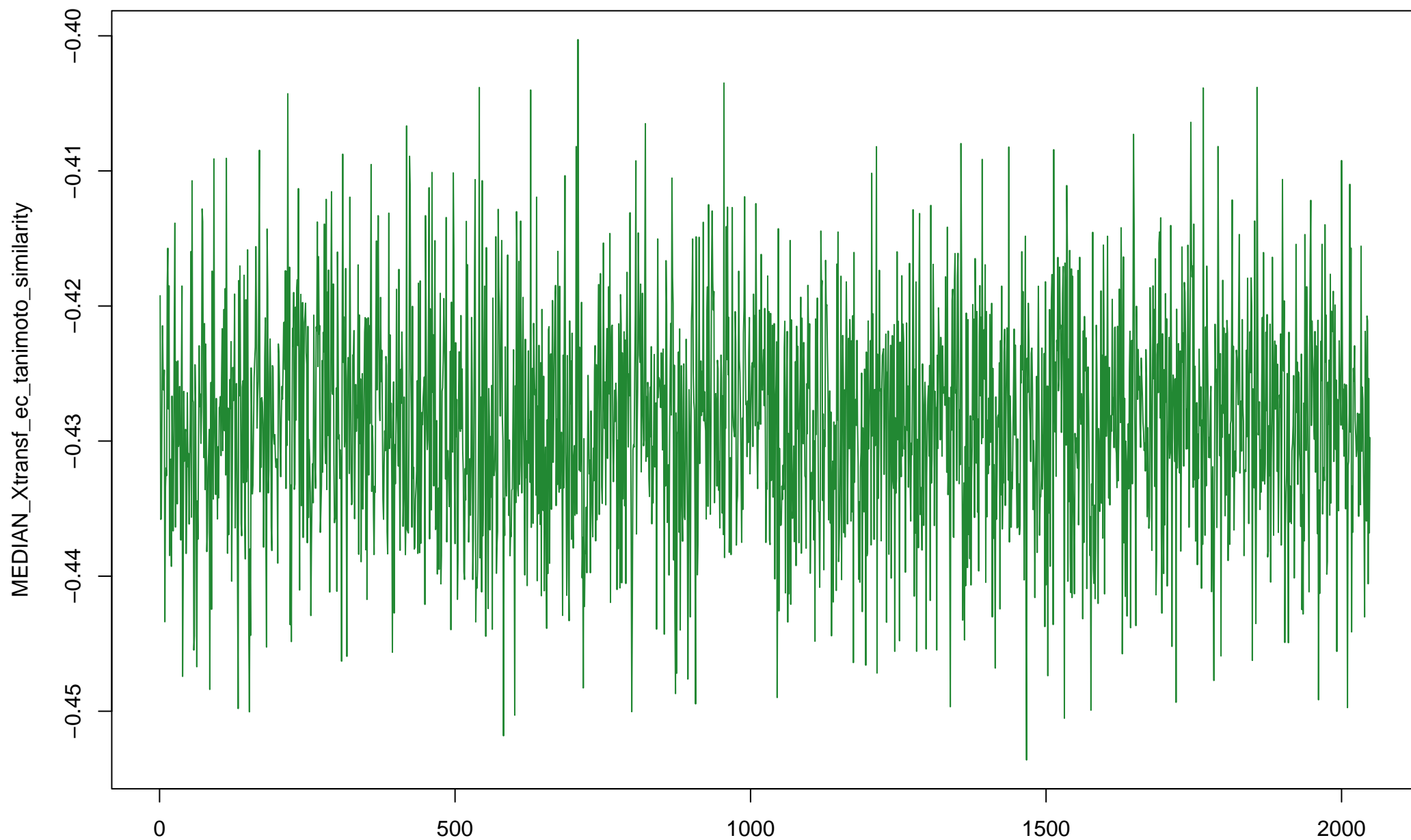
Pdatum8
ESS = 447 | BMK = 0.0807 | MCSE(6.27) = 5.01 | stat: TRUE | burn: 0



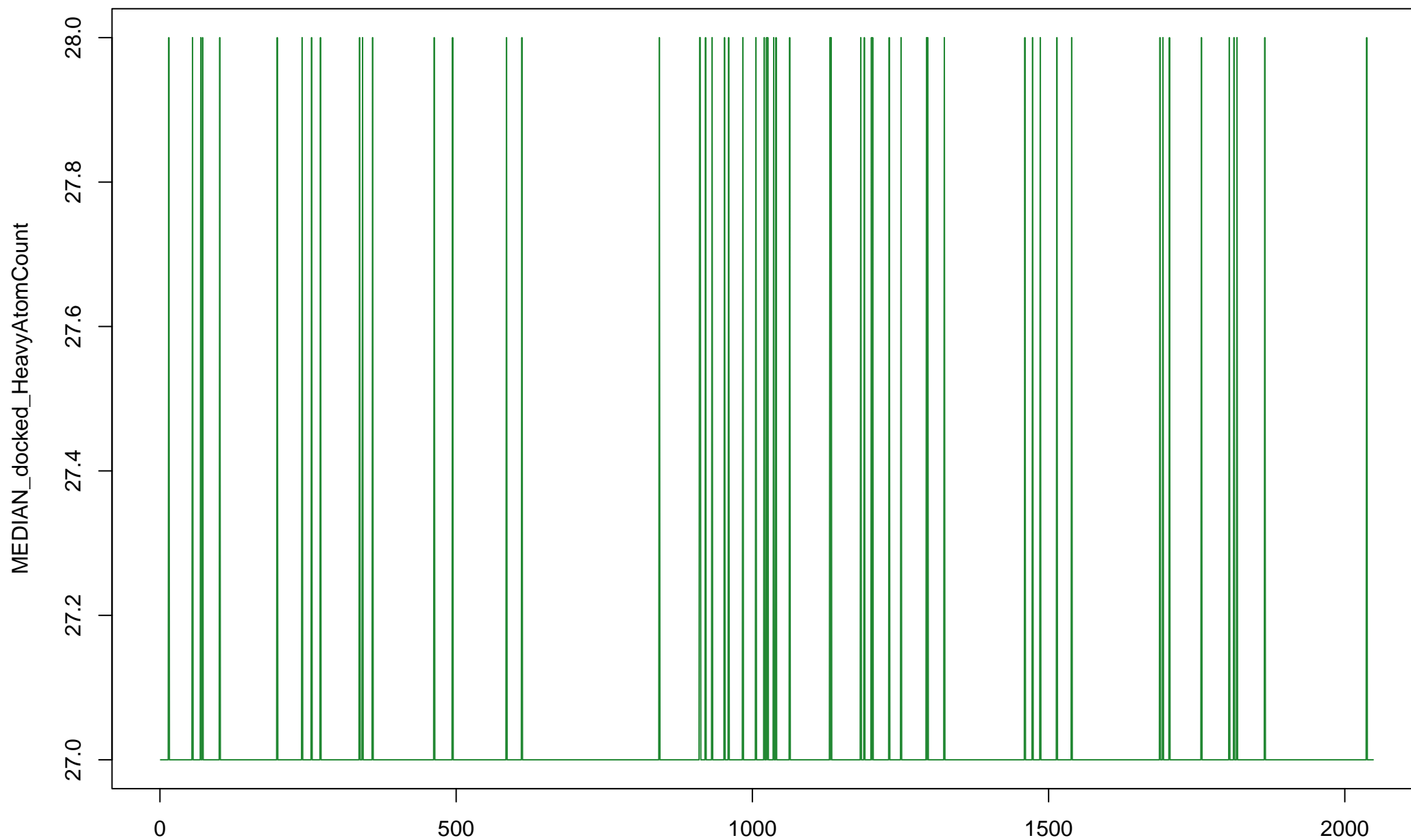
MEDIAN_log_RMSD
ESS = 1380 | BMK = 0.0349 | MCSE(6.27) = 3.05 | stat: FALSE | burn: 0



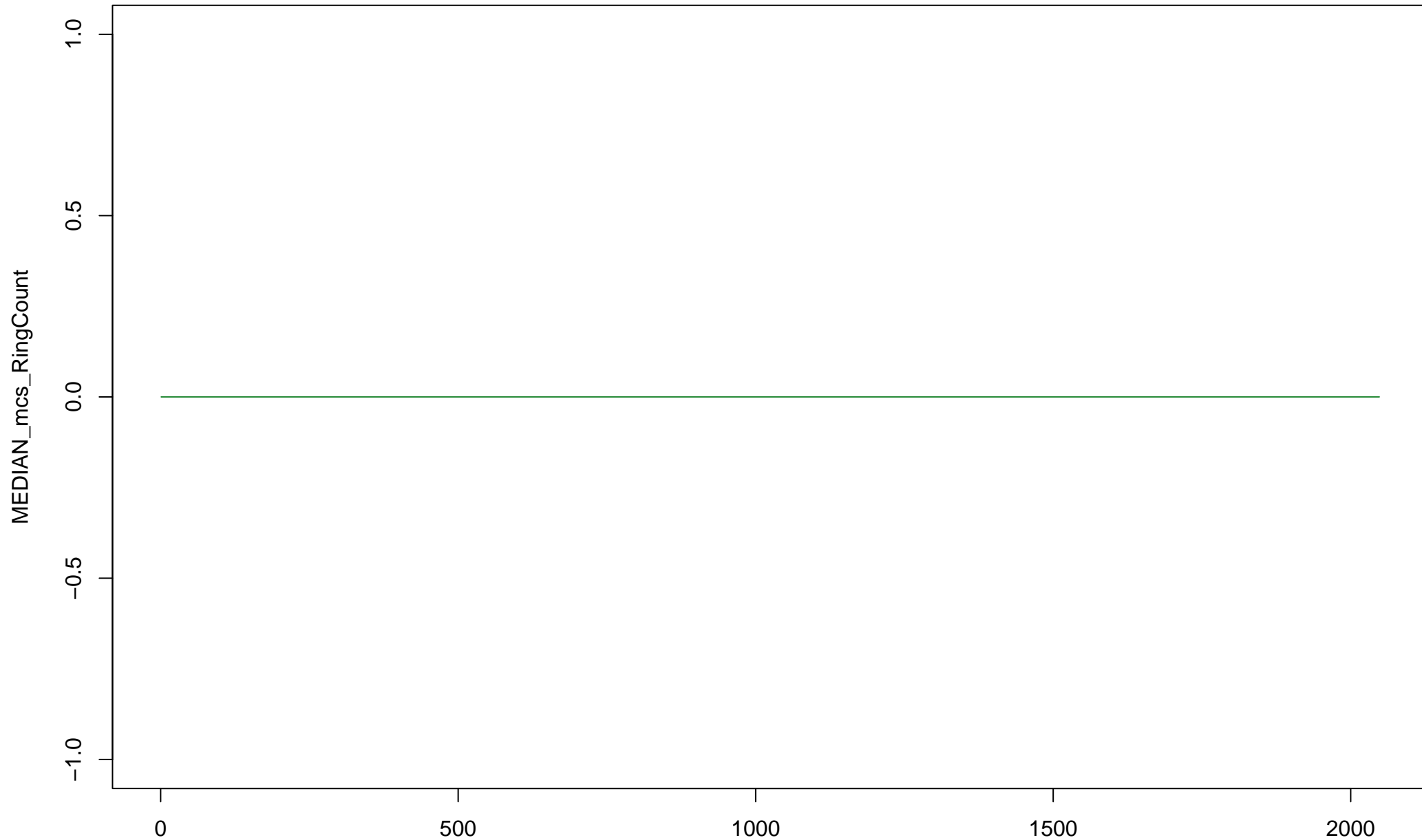
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0454 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



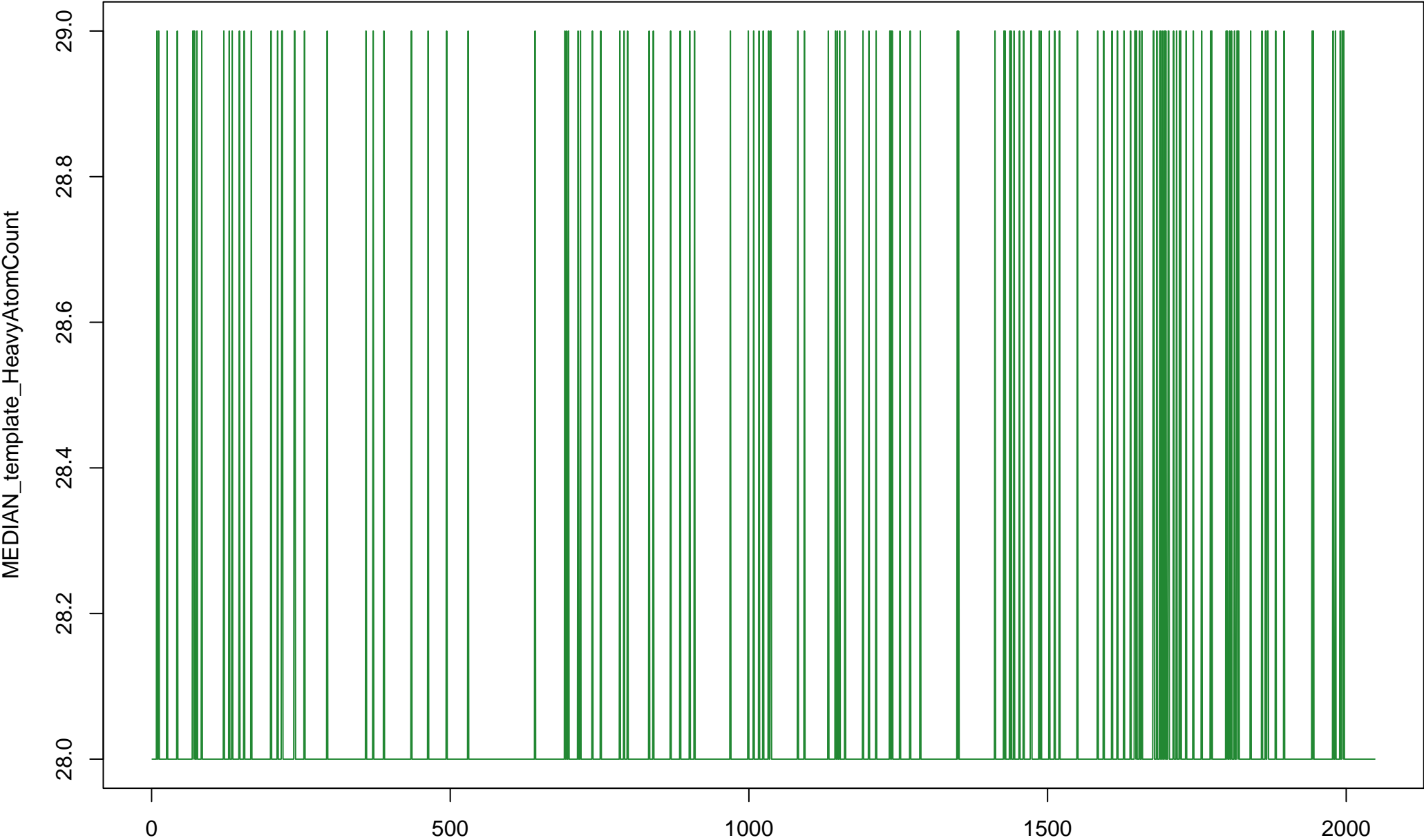
MEDIAN_docked_HeavyAtomCount
ESS = 1910 | BMK = 0.0127 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0



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



MEDIAN_template_HeavyAtomCount
ESS = 1720 | BMK = 0.0965 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0



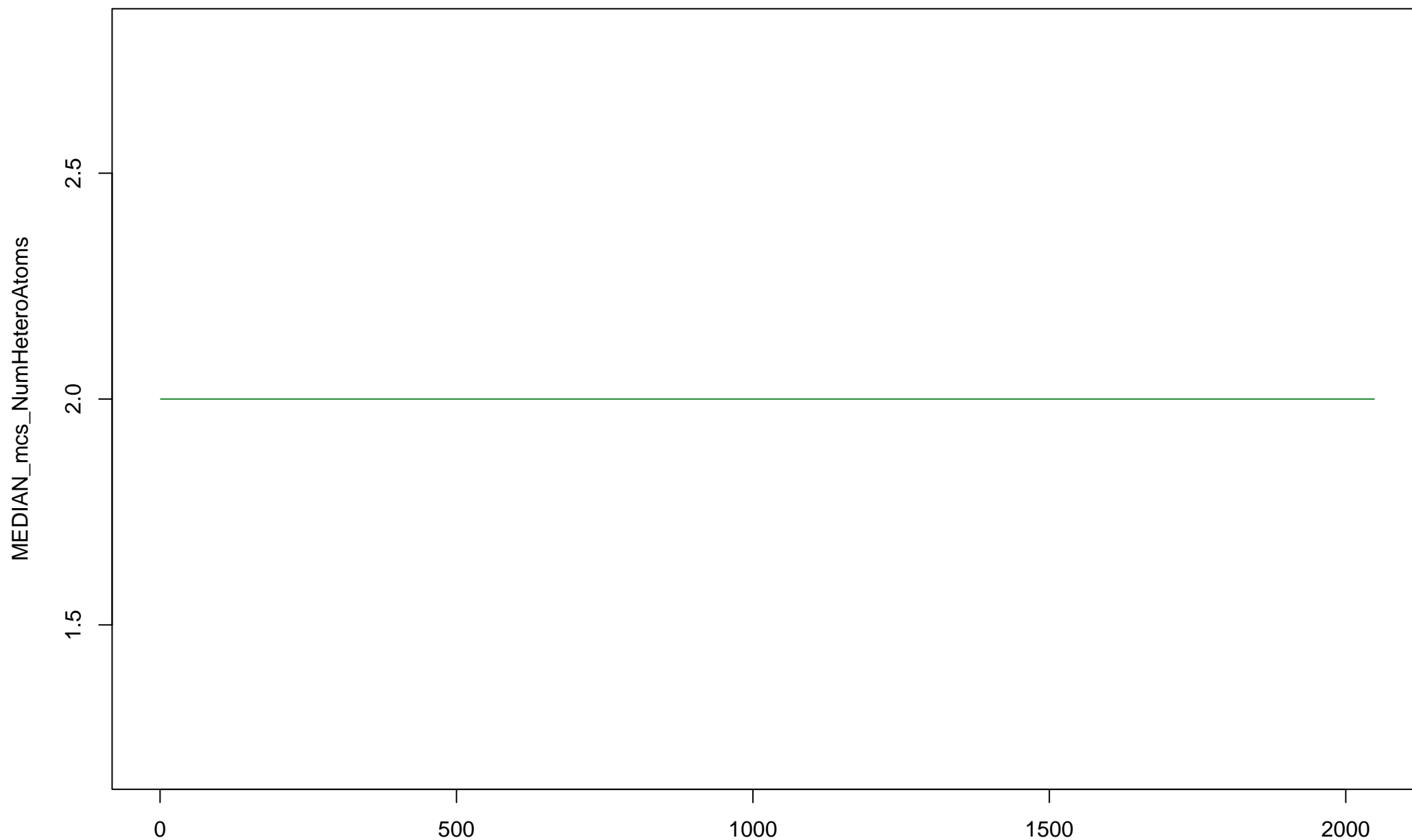
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



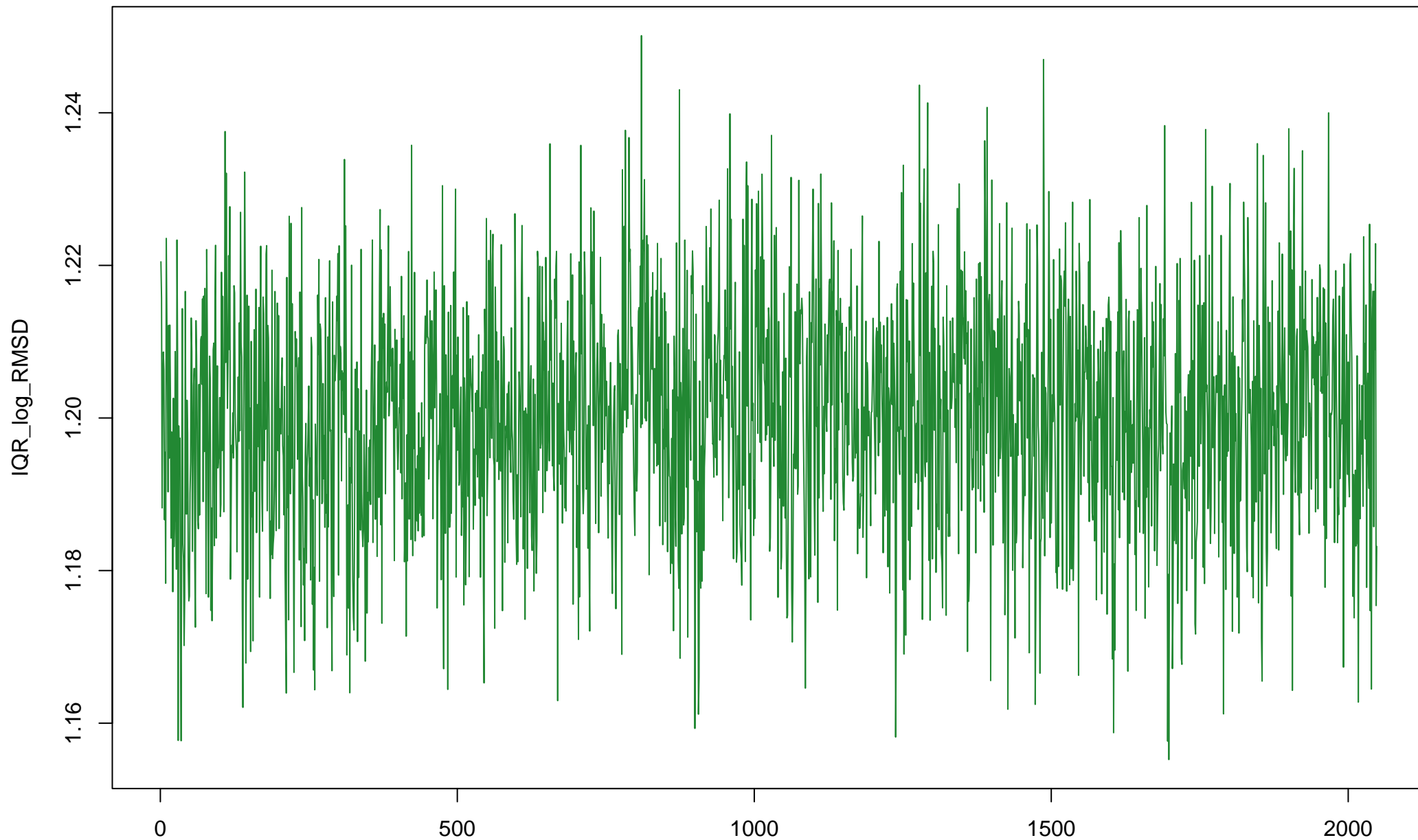
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



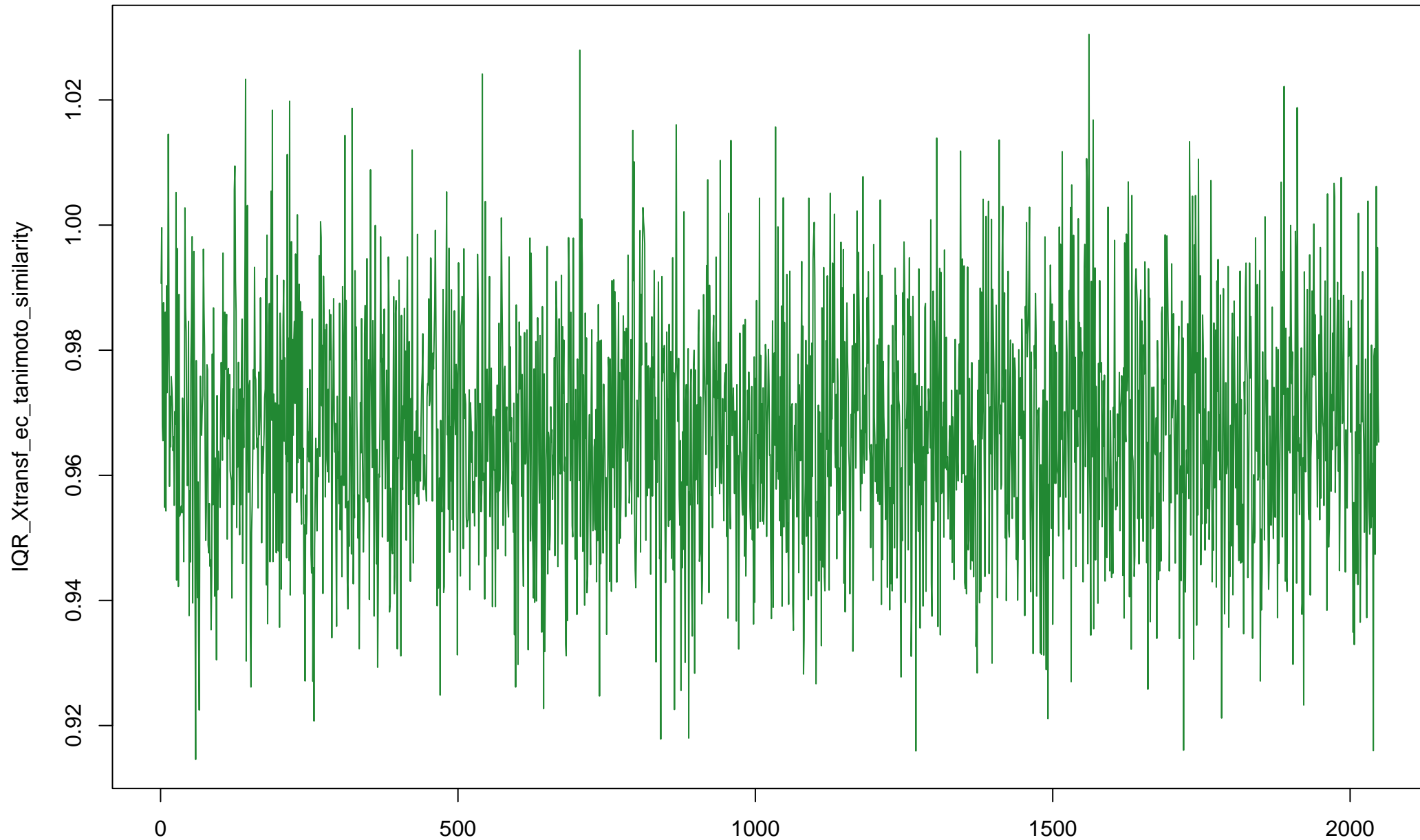
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



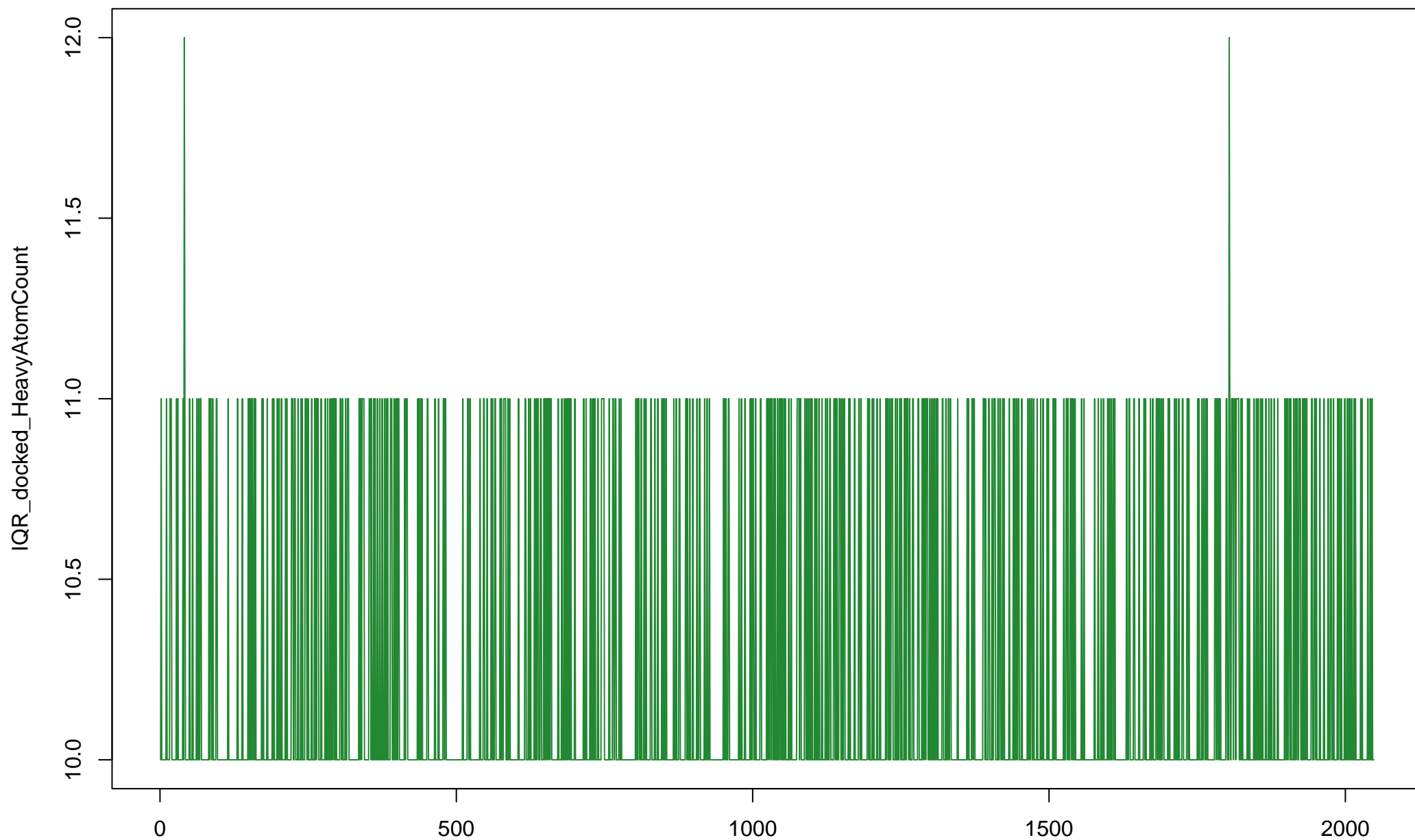
IQR_log_RMSD
ESS = 1020 | BMK = 0.0324 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0



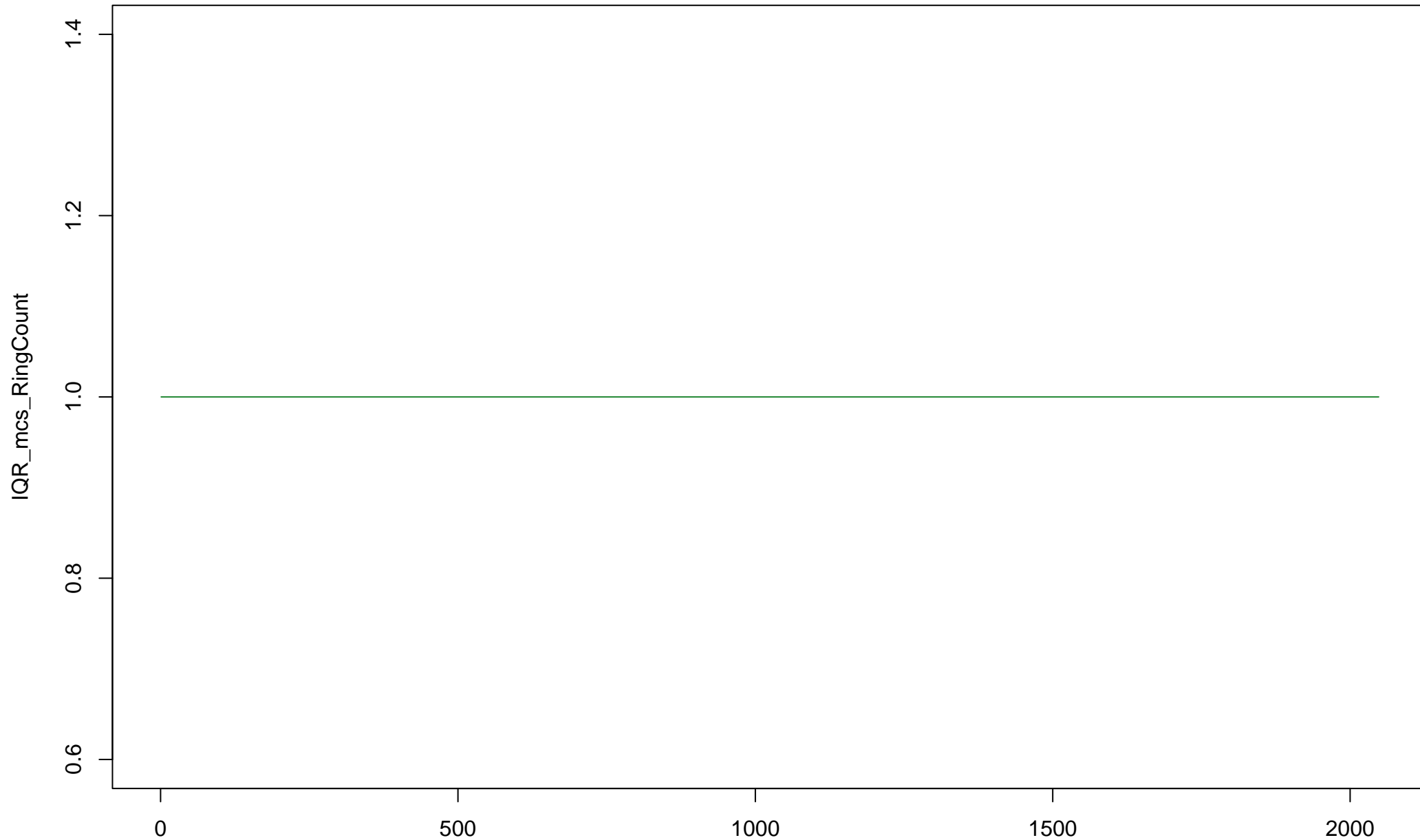
IQR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0479 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0



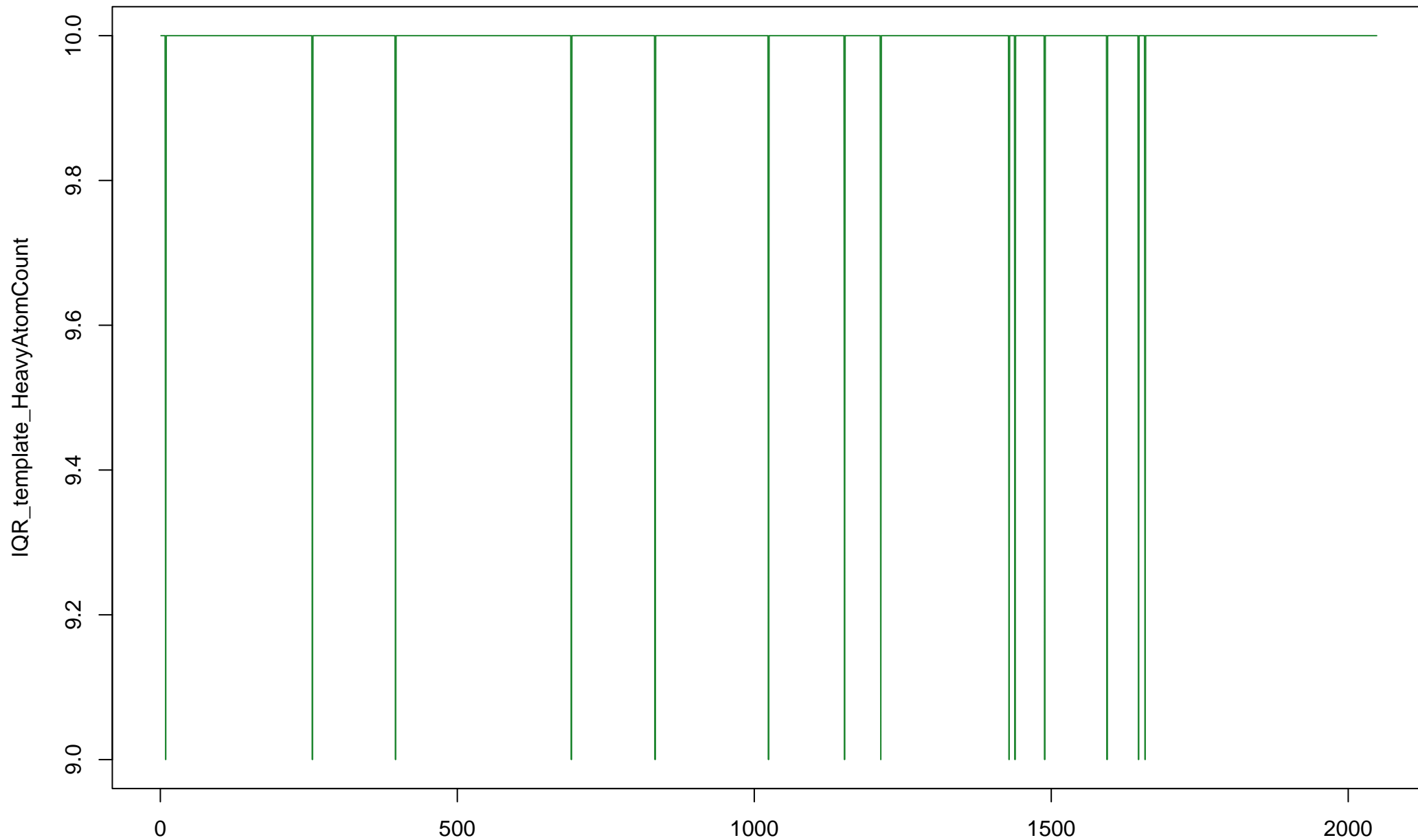
IQR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0434 | MCSE(6.27) = 2.48 | stat: FALSE | burn: 0



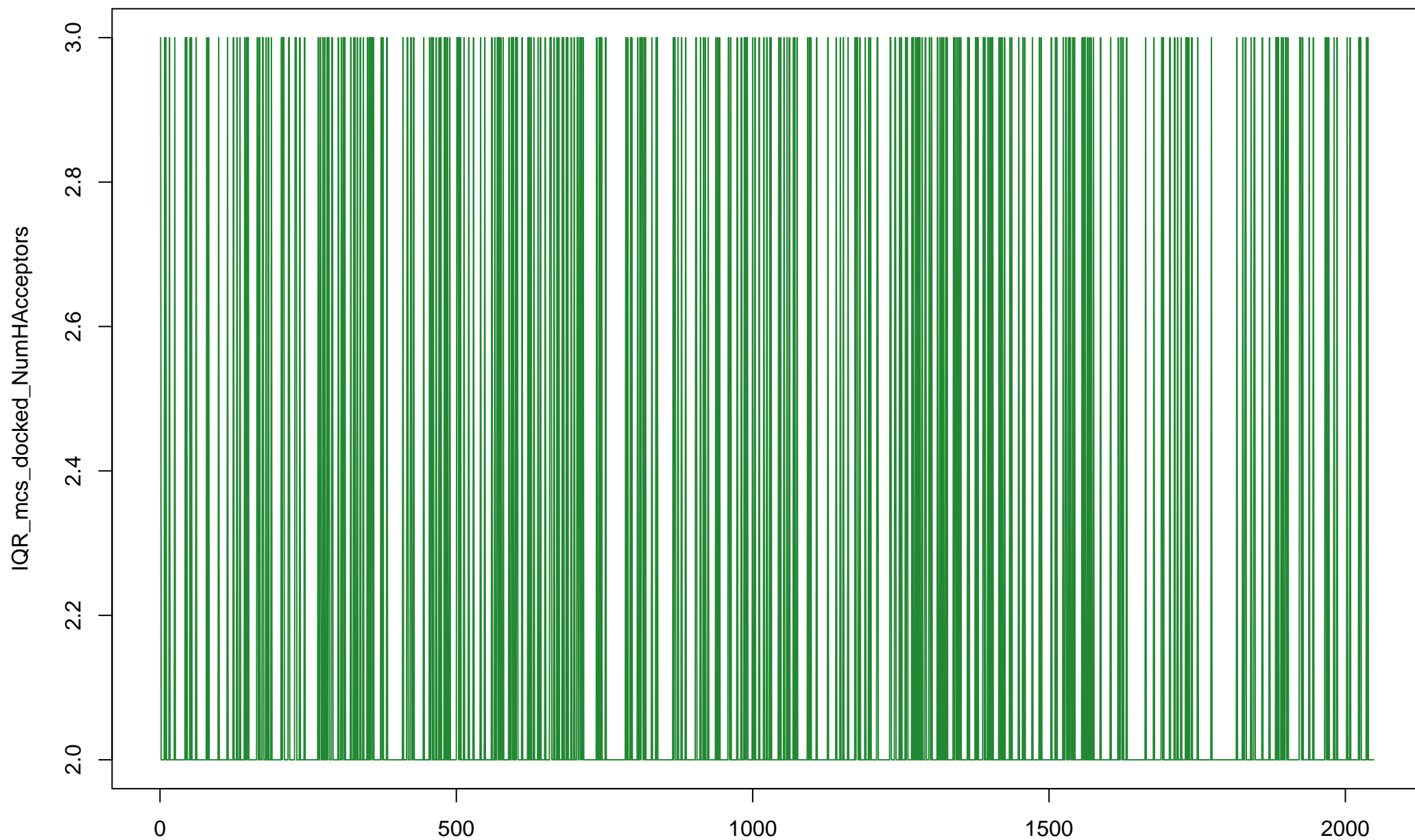
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



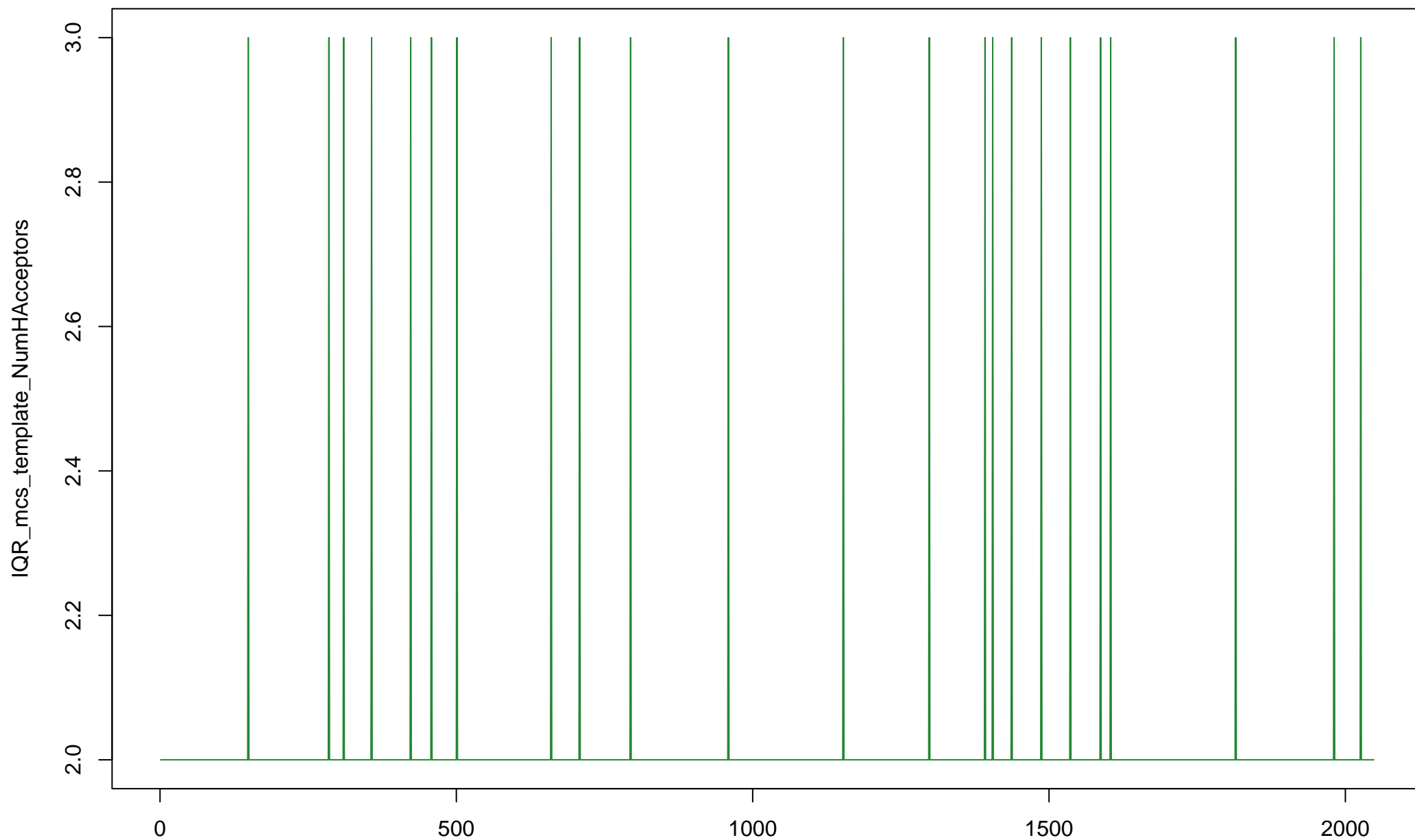
IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0509 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 612



IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0259 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



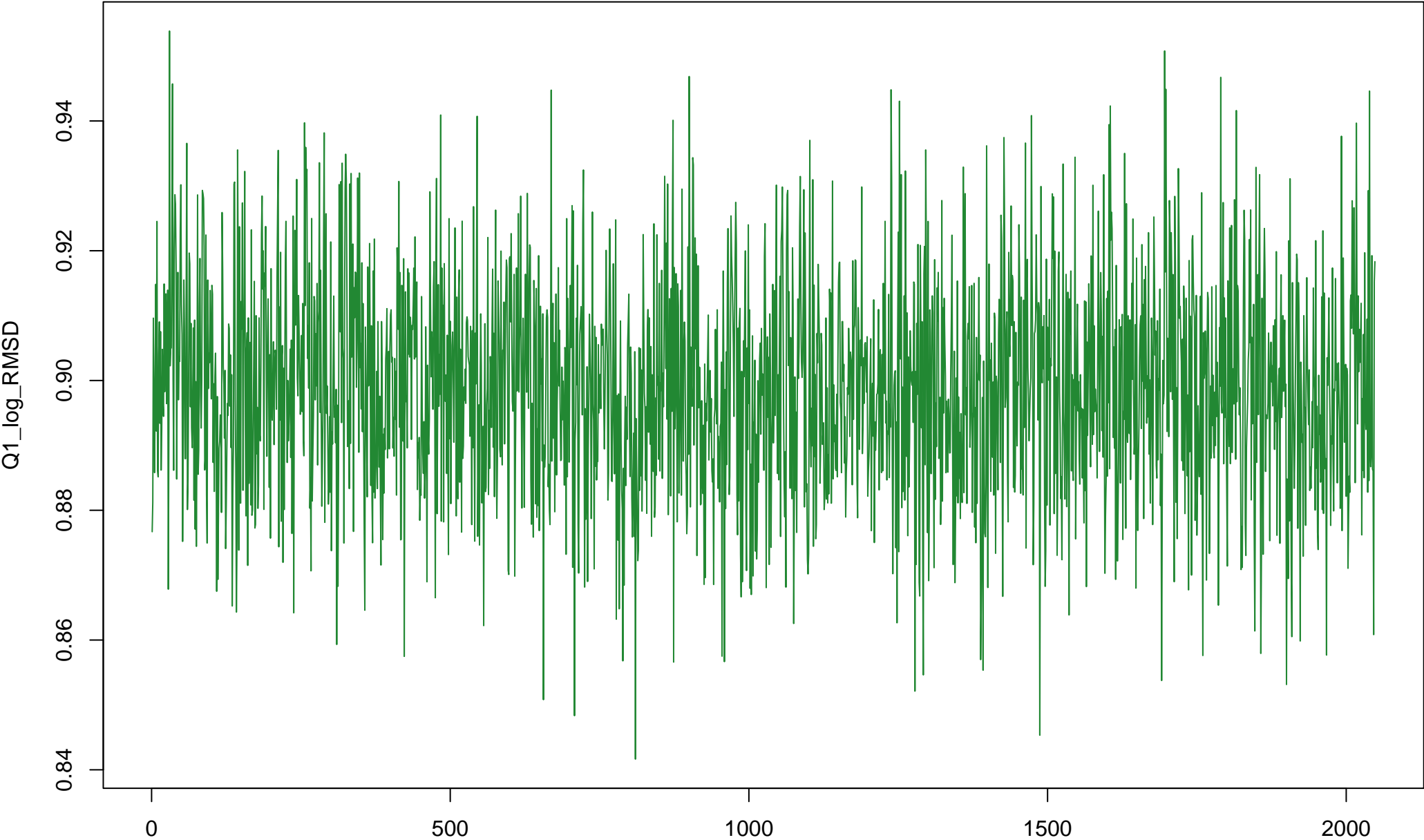
IQR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0154 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0



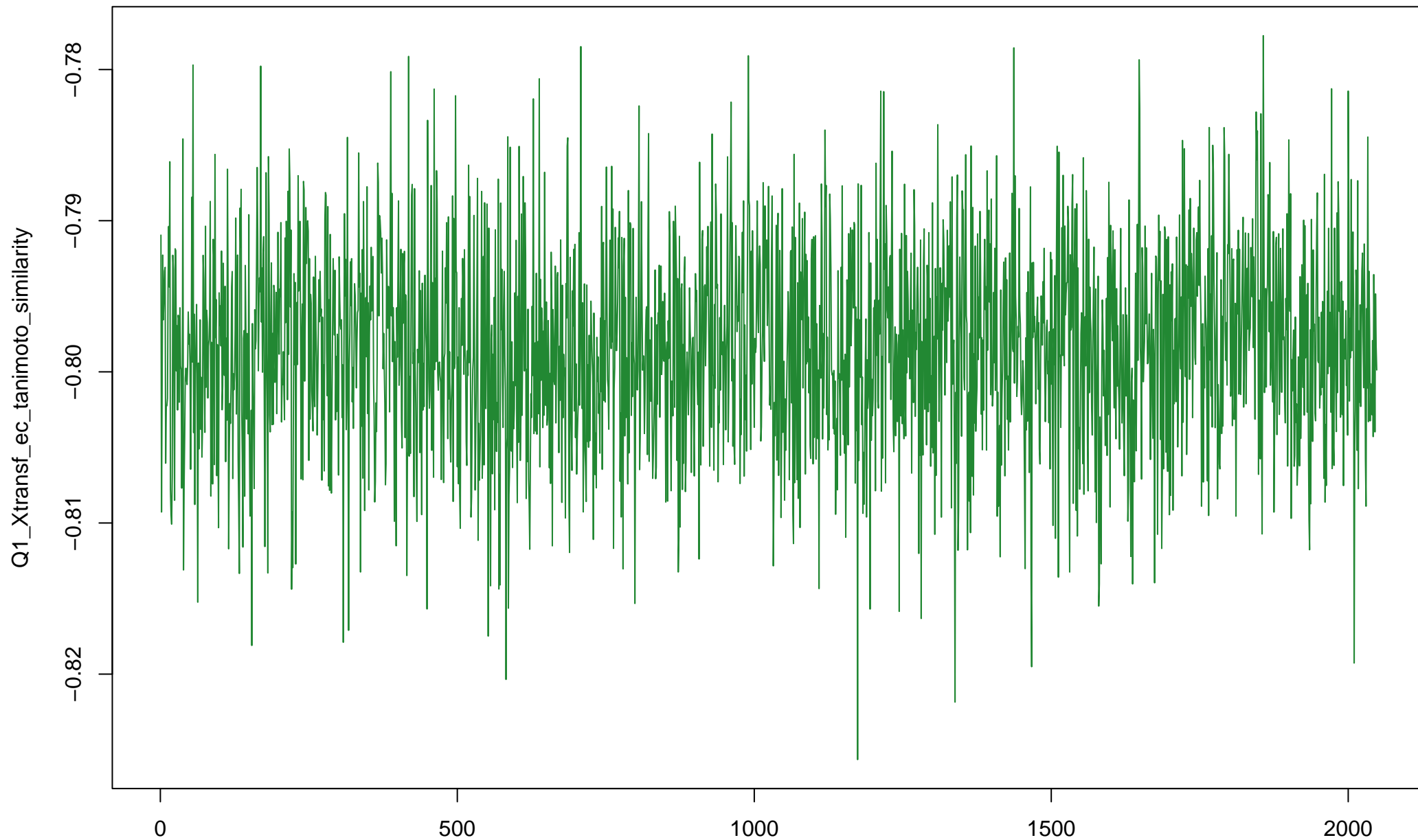
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



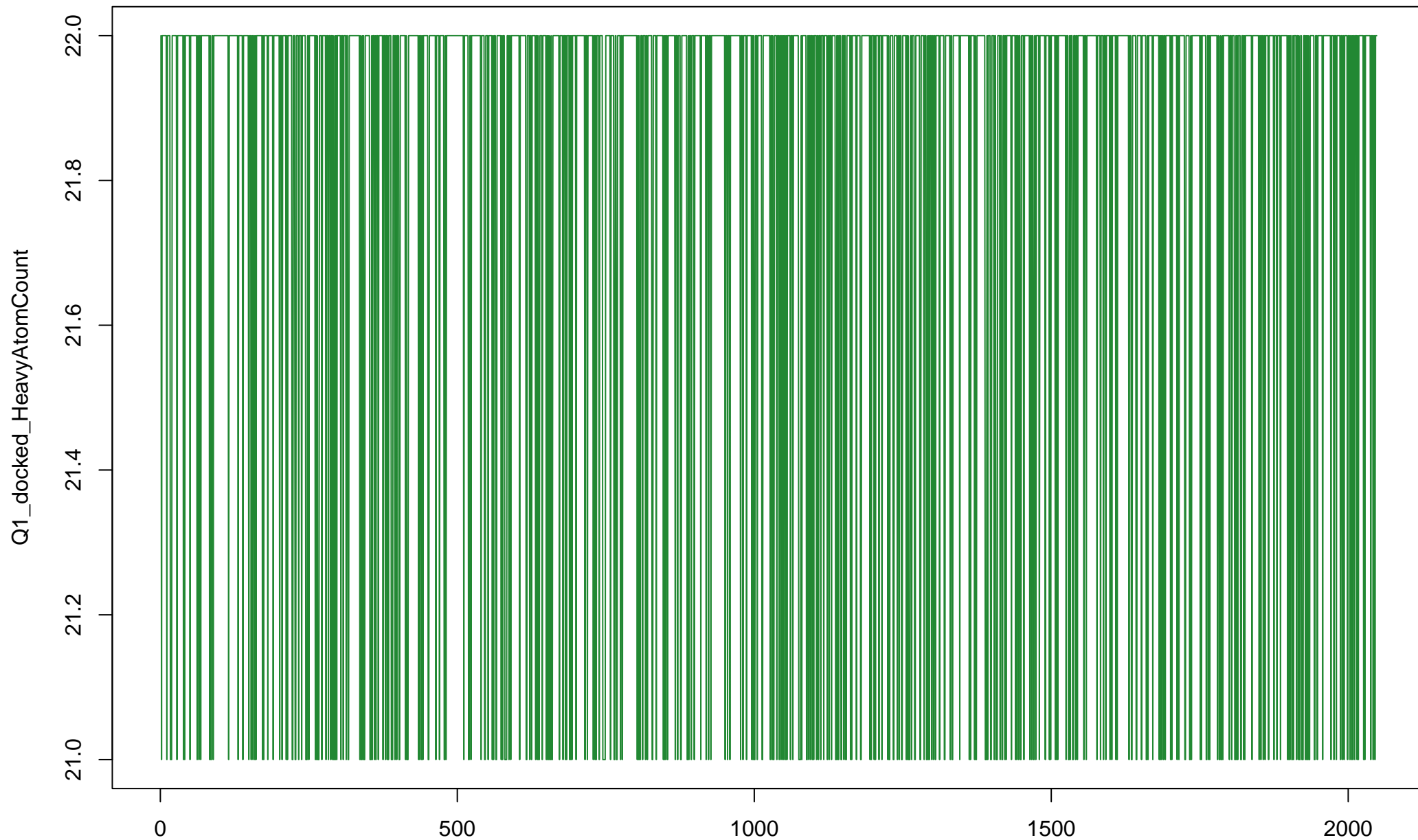
Q1_log_RMSD
ESS = 1840 | BMK = 0.0276 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0



Q1_Xtransf_ec_tanimoto_similarity
ESS = 1600 | BMK = 0.0371 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0



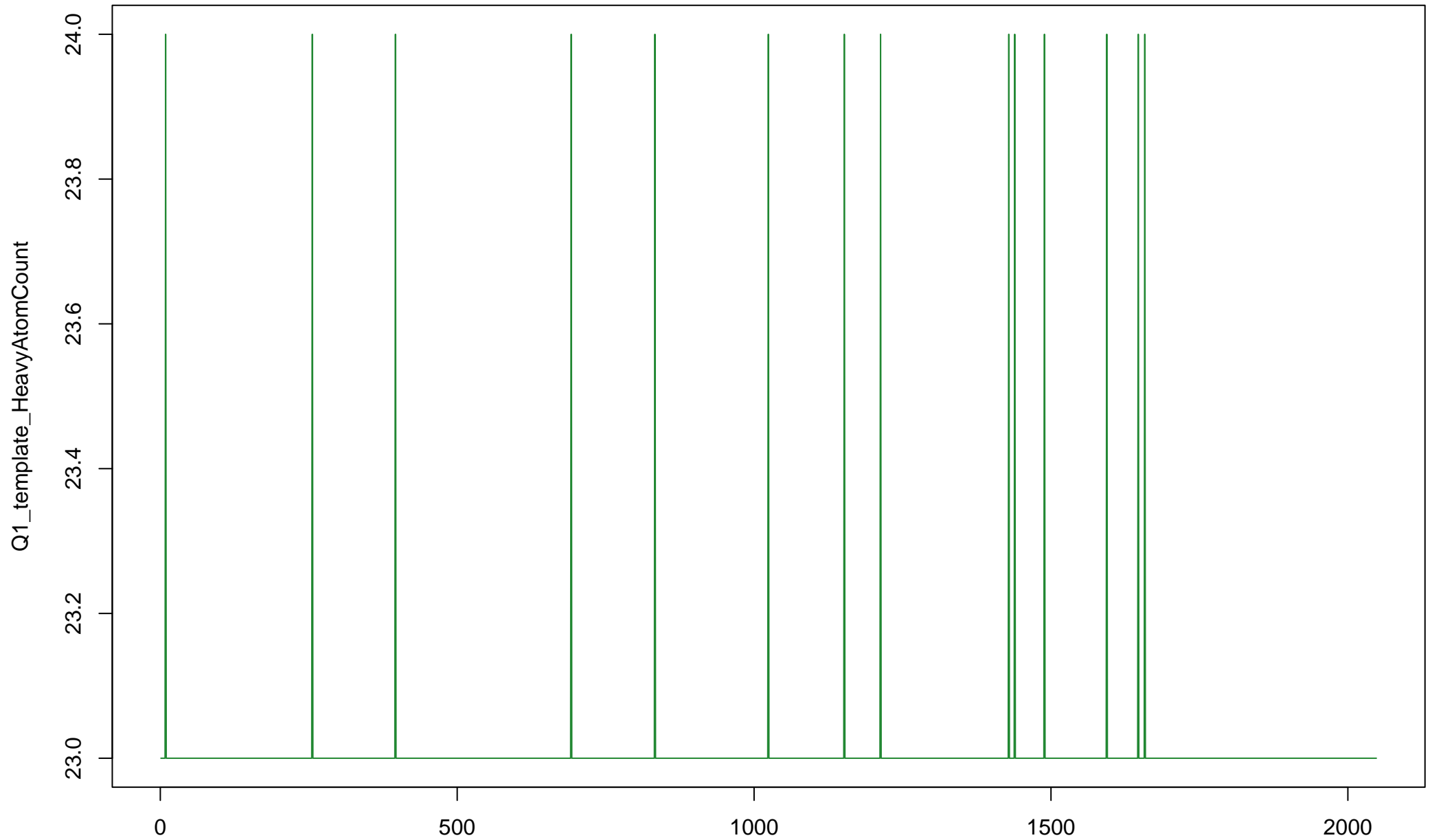
Q1_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0284 | MCSE(6.27) = 2.45 | stat: FALSE | burn: 0



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



Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0509 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 612



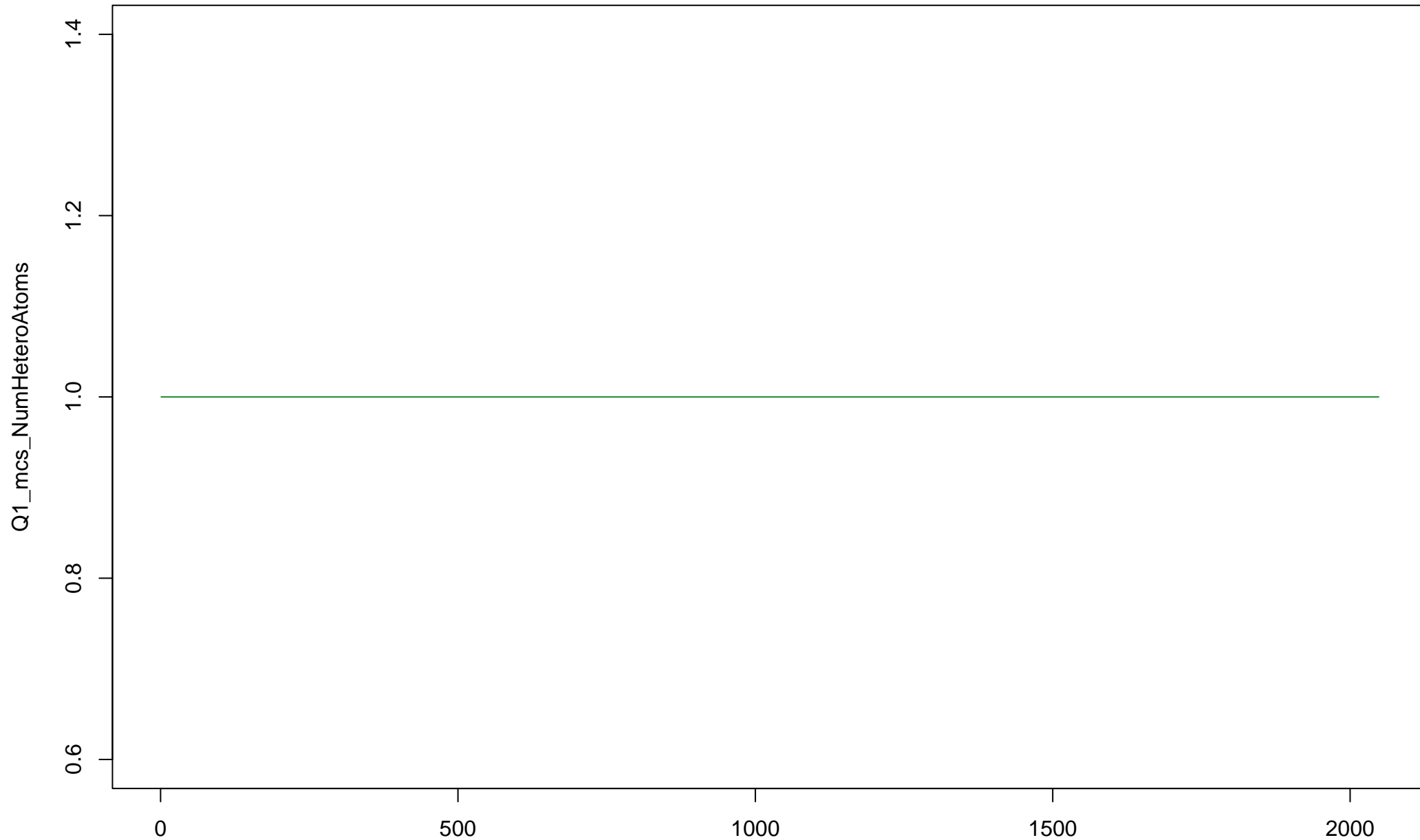
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



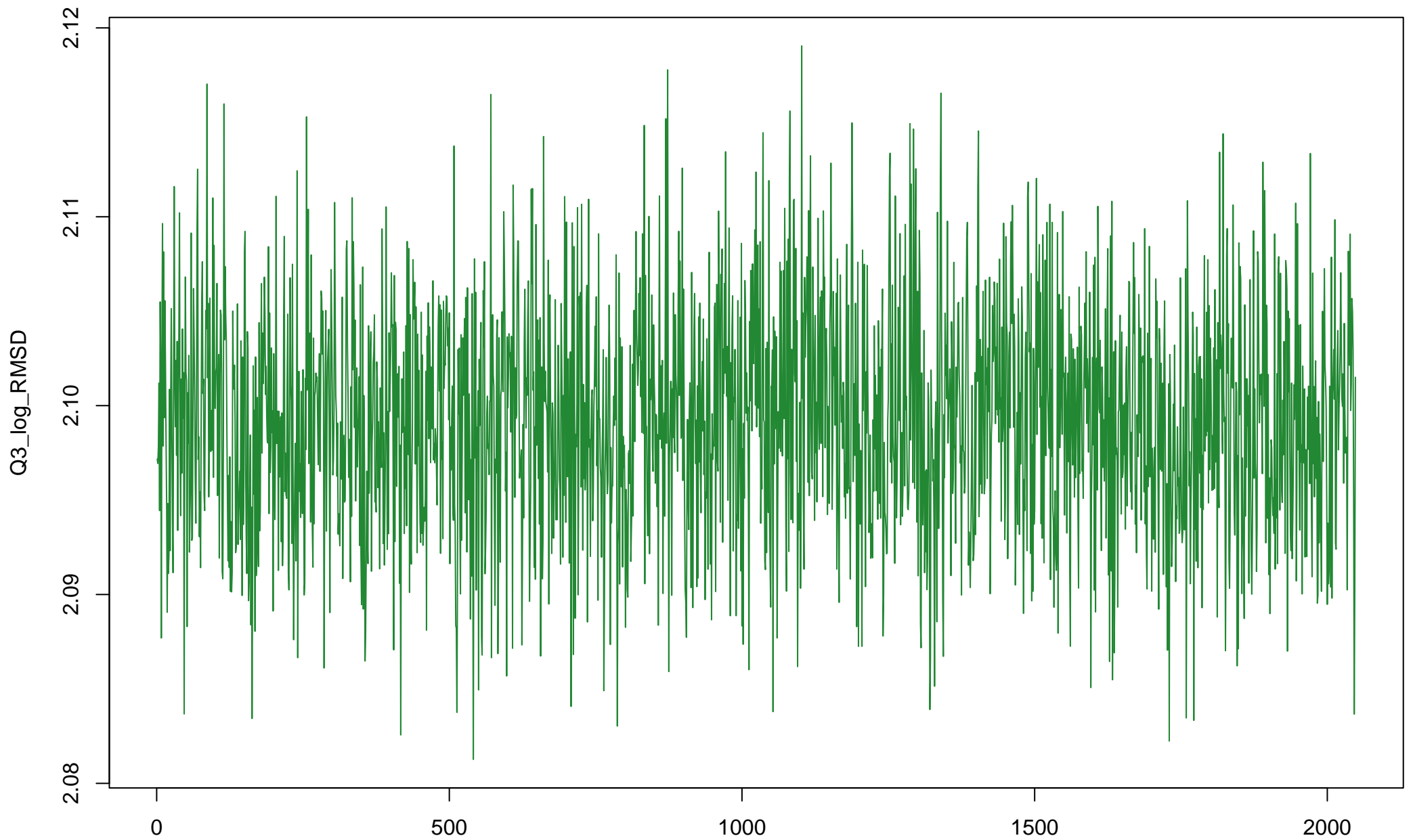
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



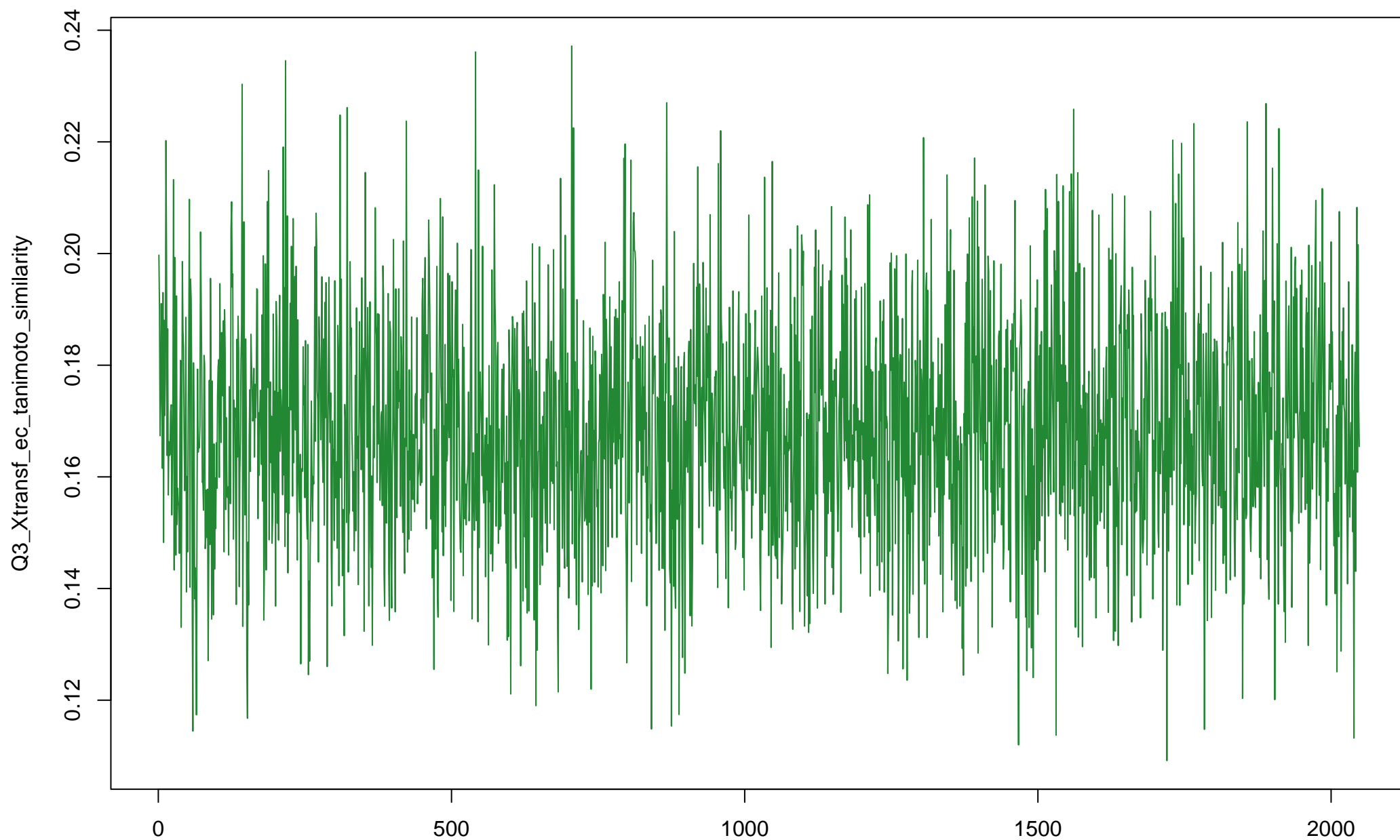
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



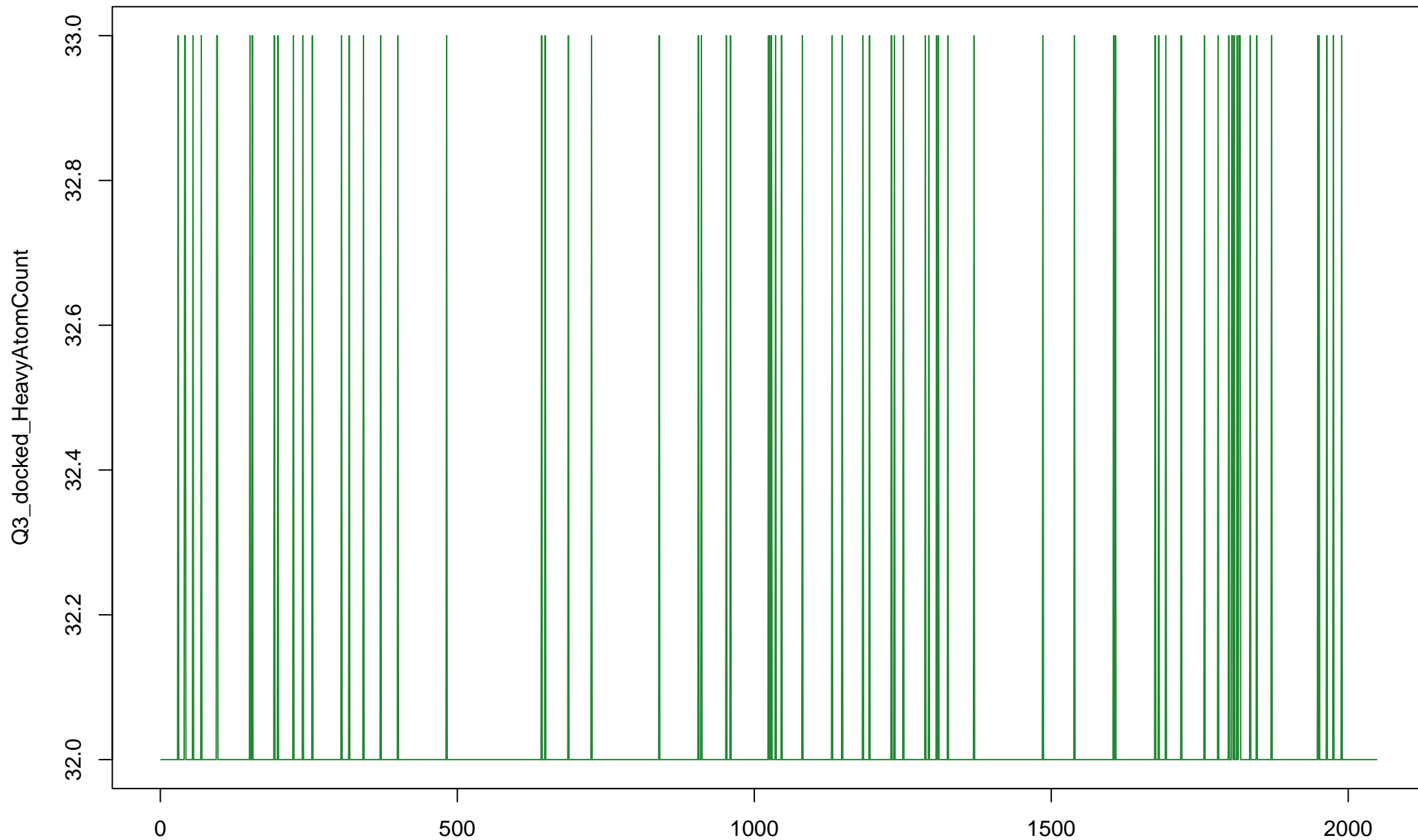
Q3_log_RMSD
ESS = 1730 | BMK = 0.0435 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0458 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



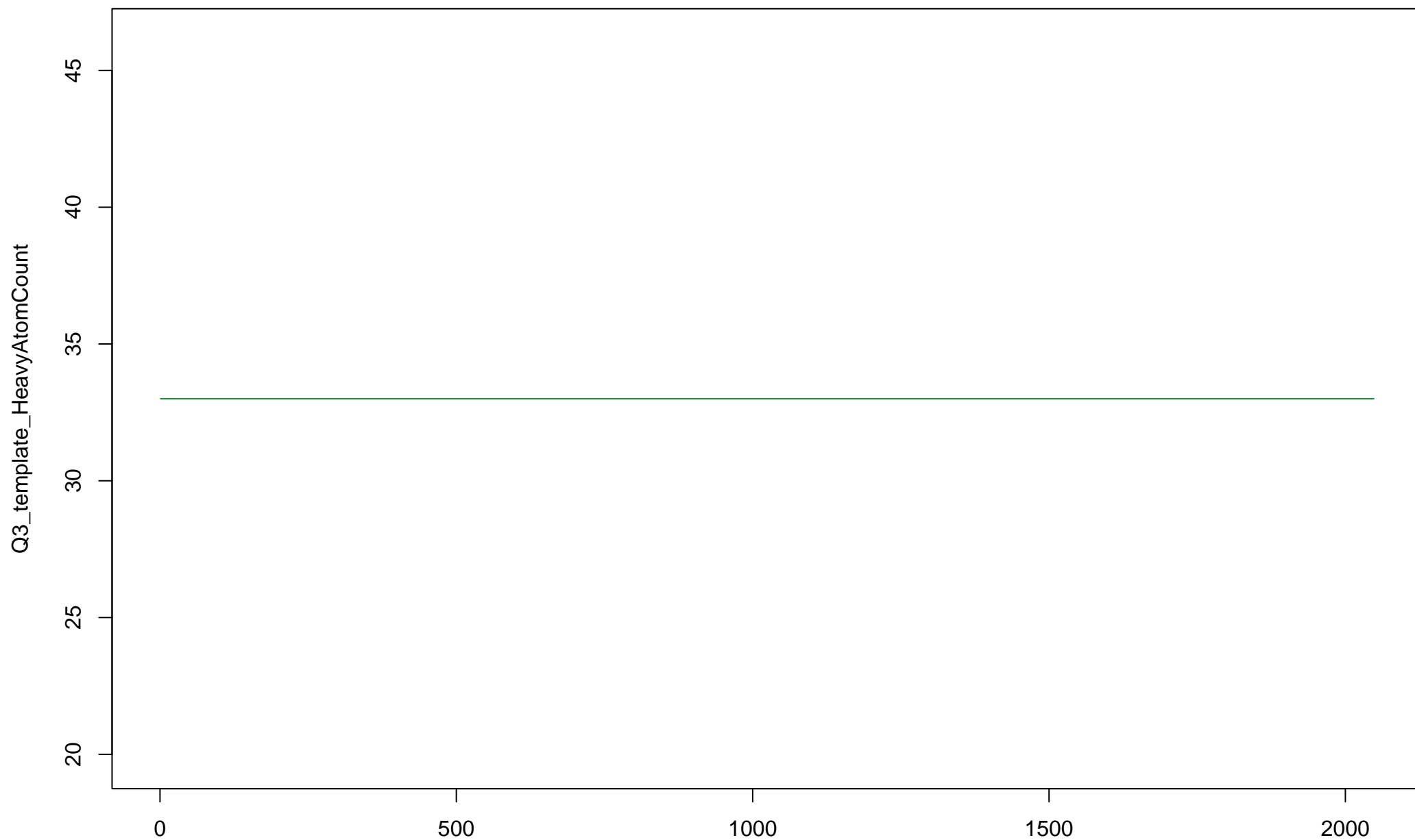
Q3_docked_HeavyAtomCount
ESS = 1920 | BMK = 0.0676 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



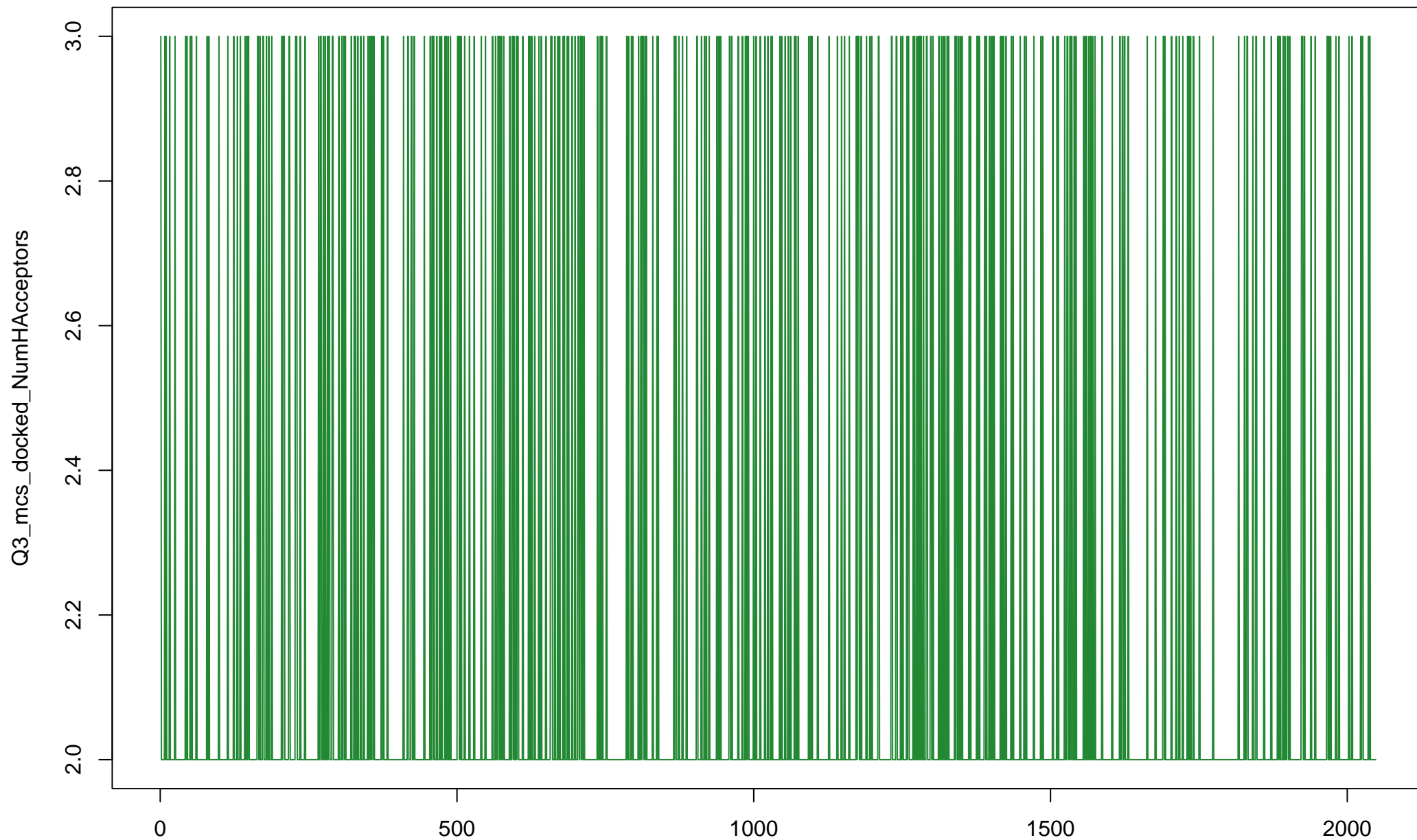
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



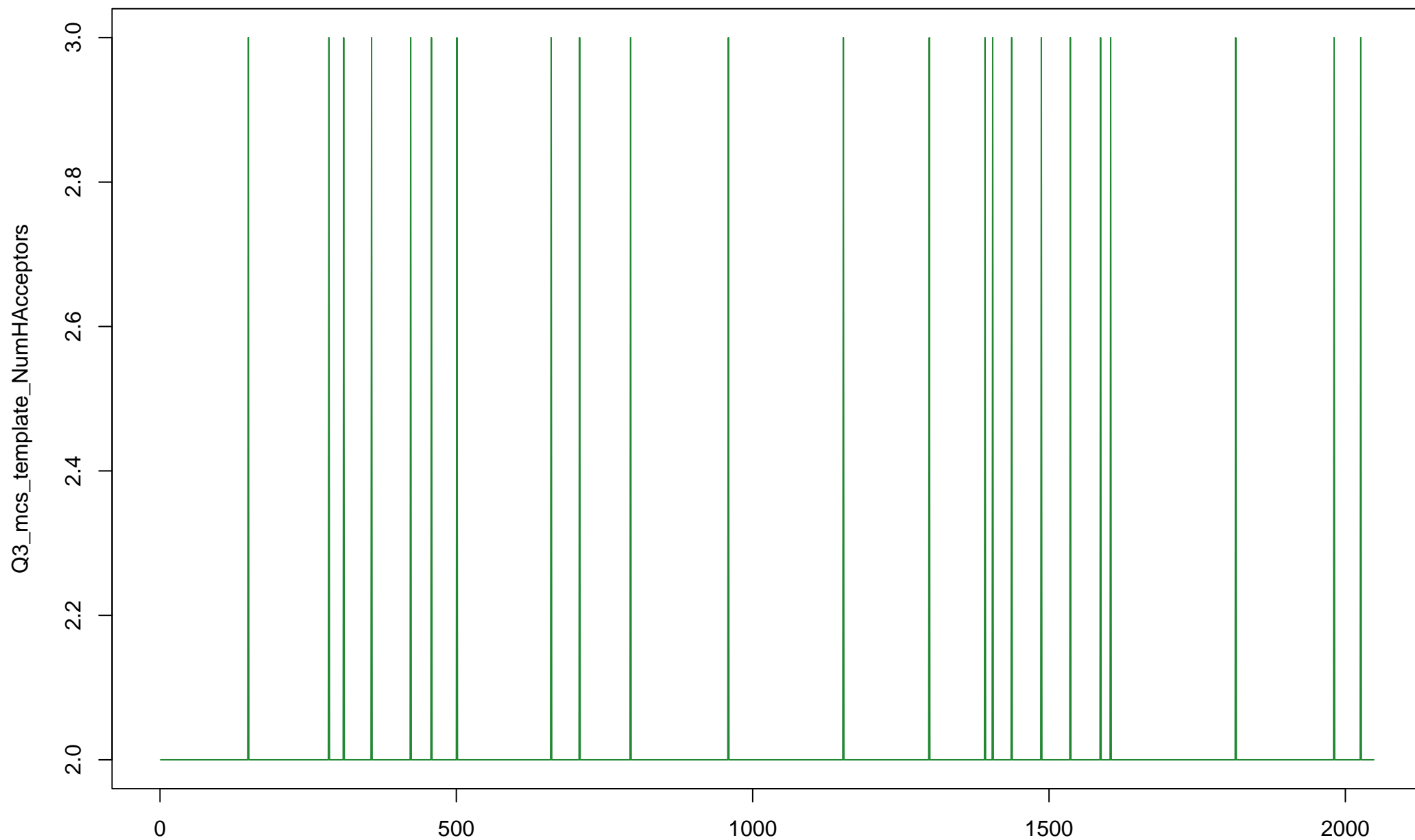
Q3_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0259 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



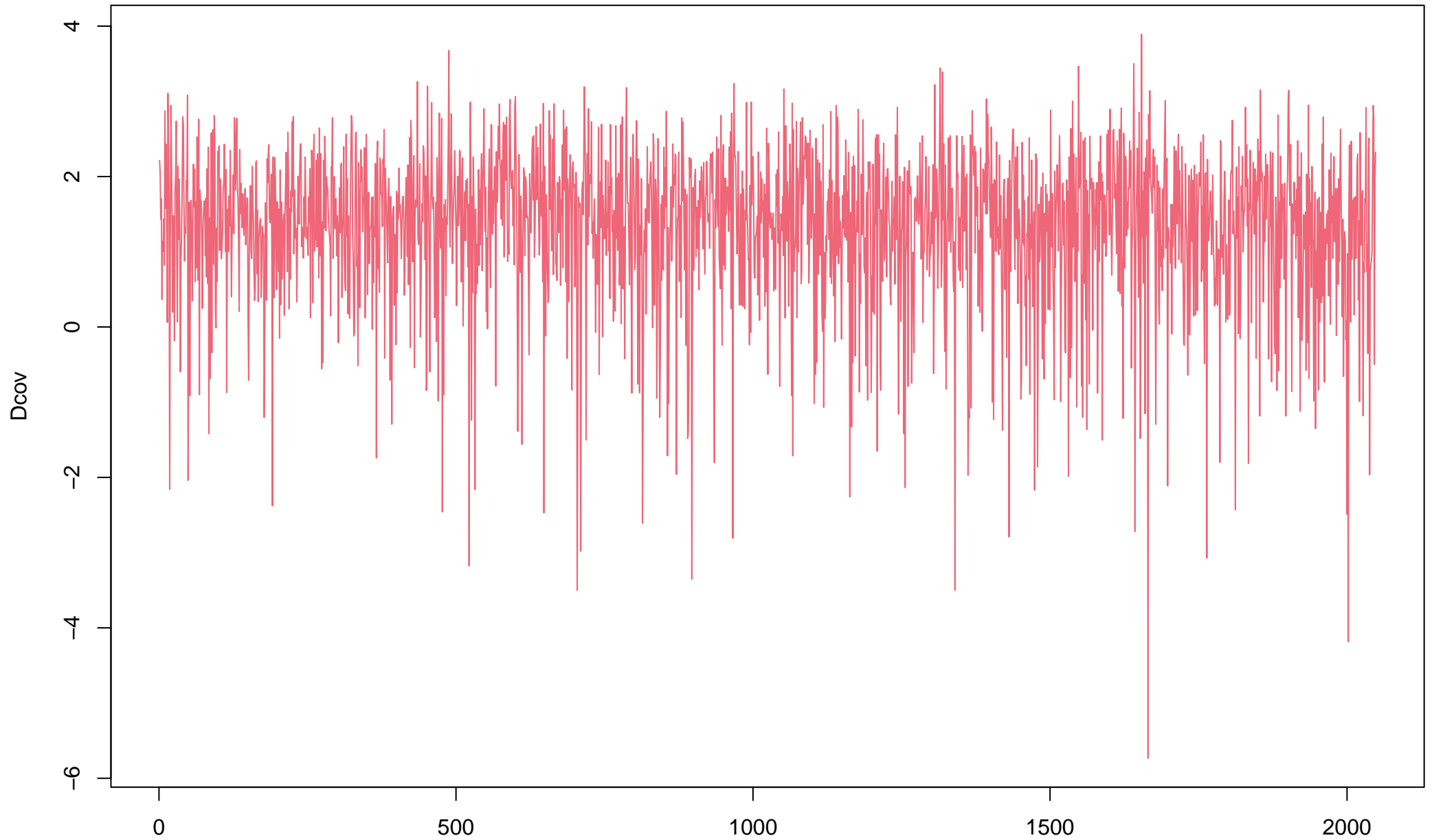
Q3_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0154 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0



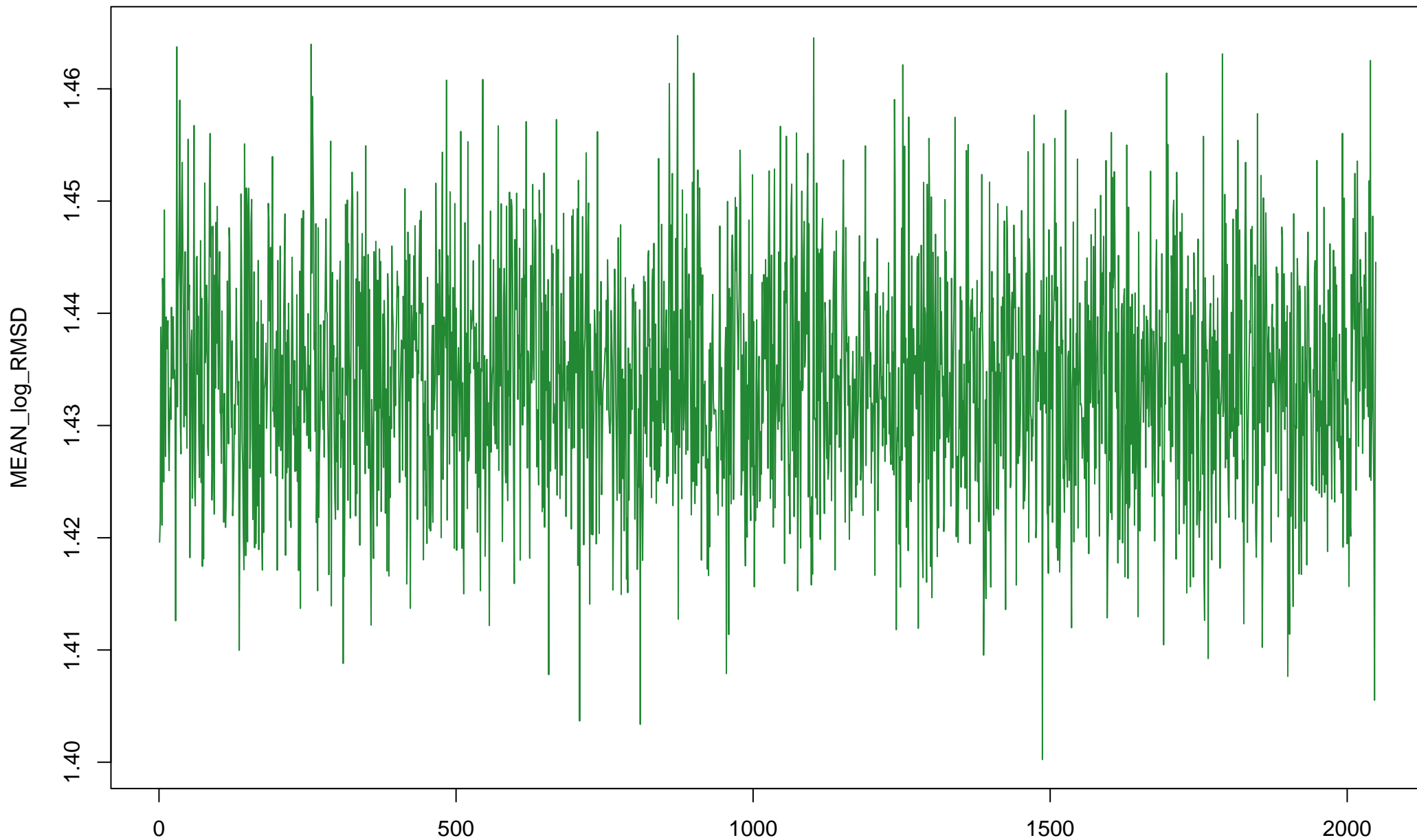
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



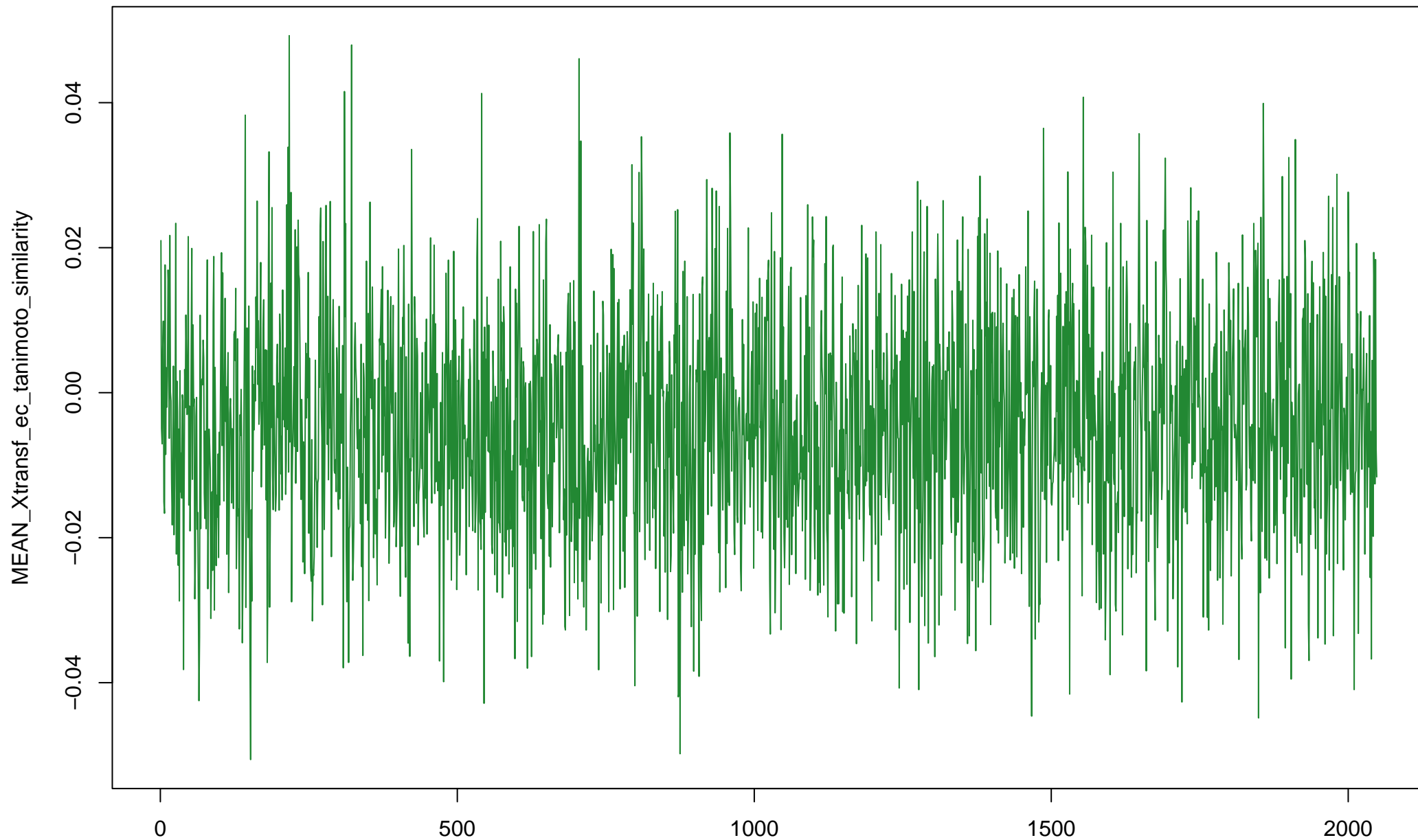
Dcov
ESS = 2050 | BMK = 0.1 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0



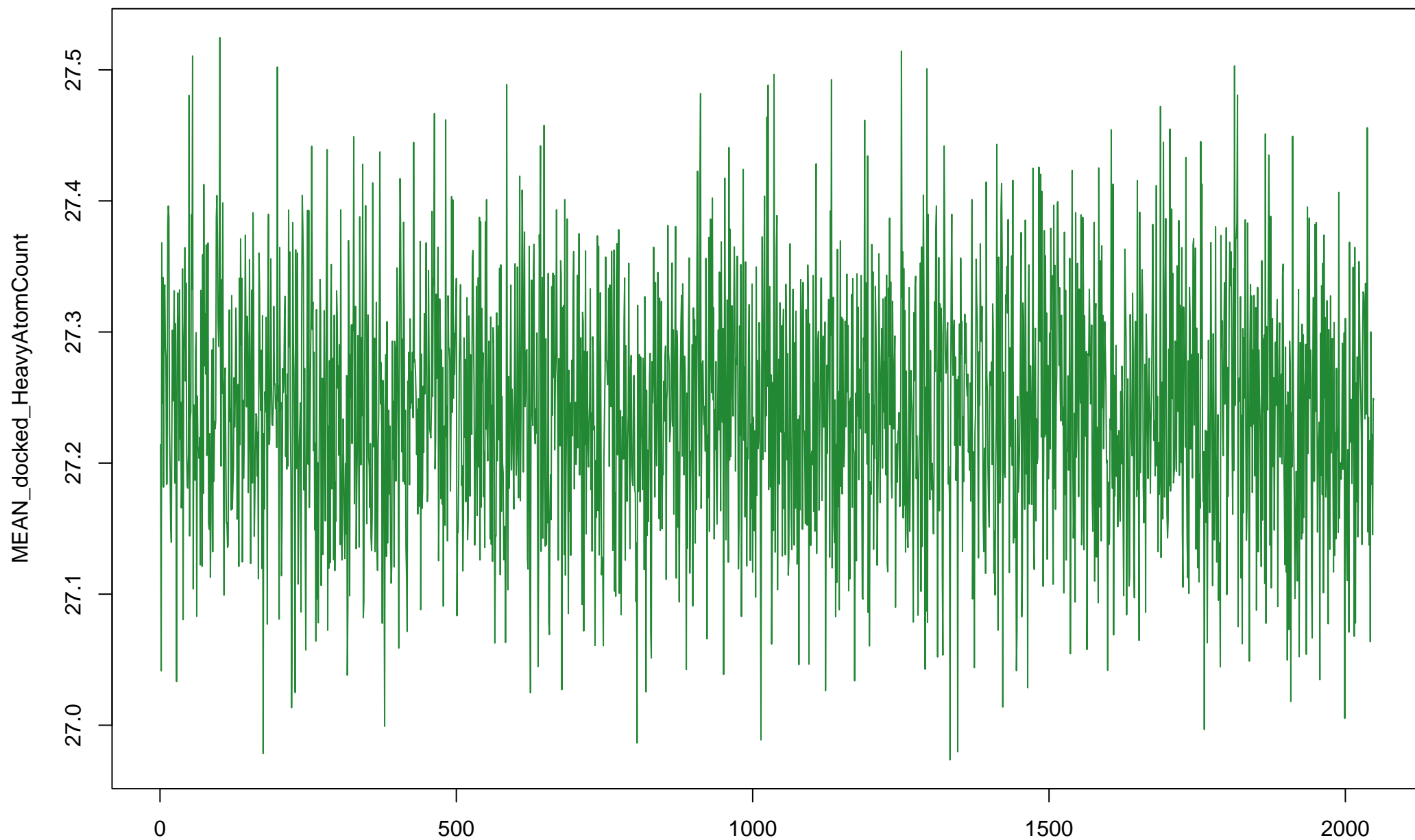
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0293 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0



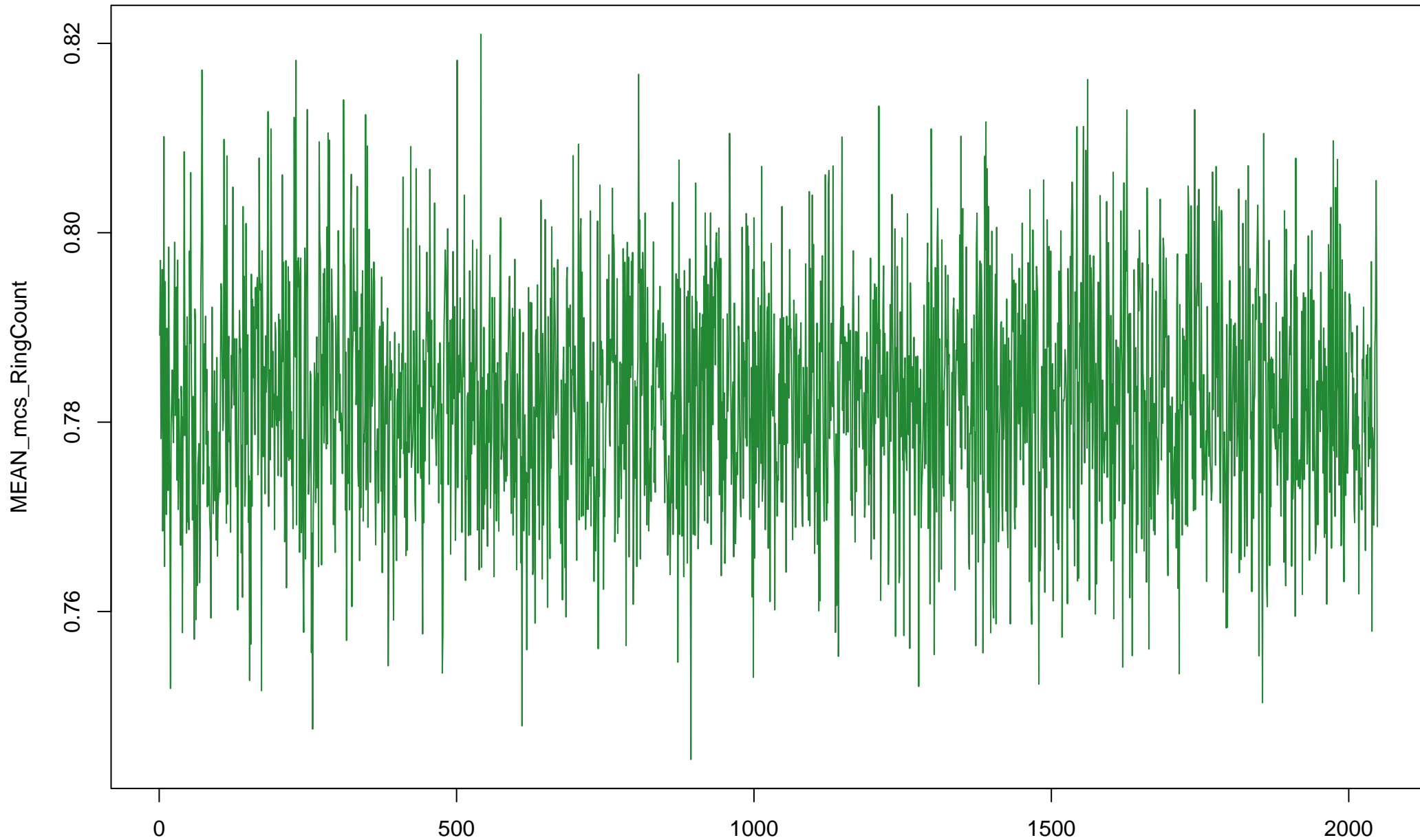
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0442 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0



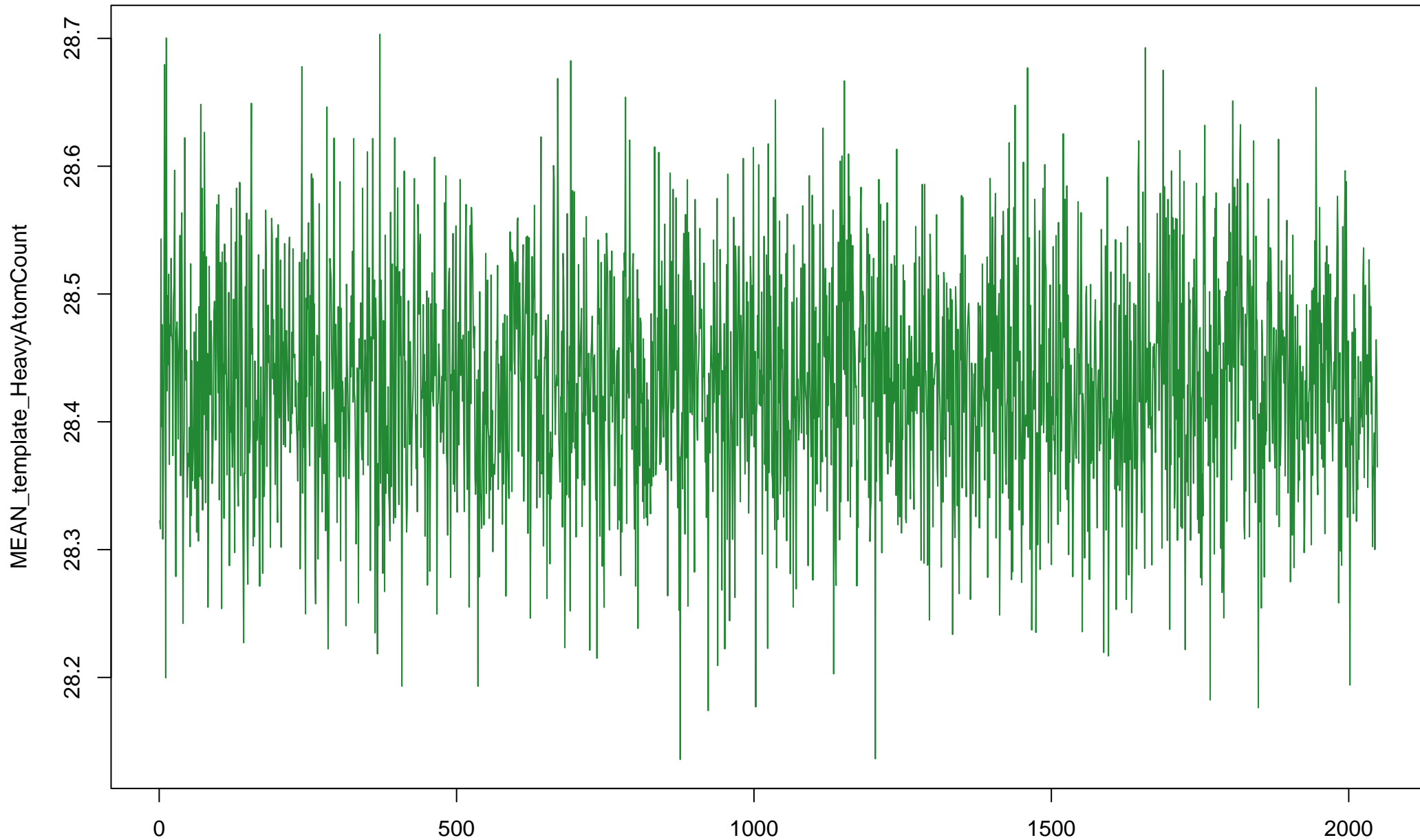
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0354 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



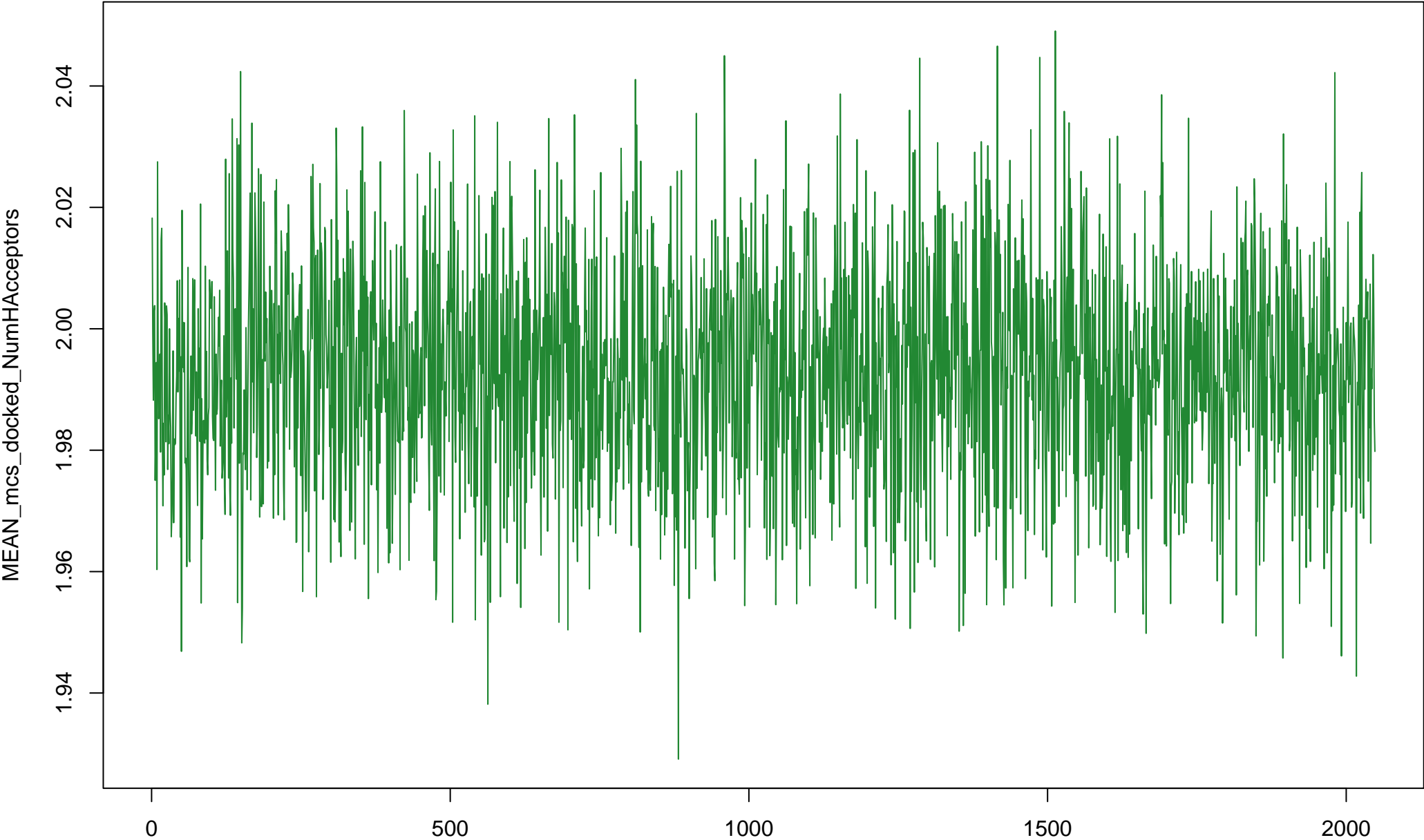
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0529 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



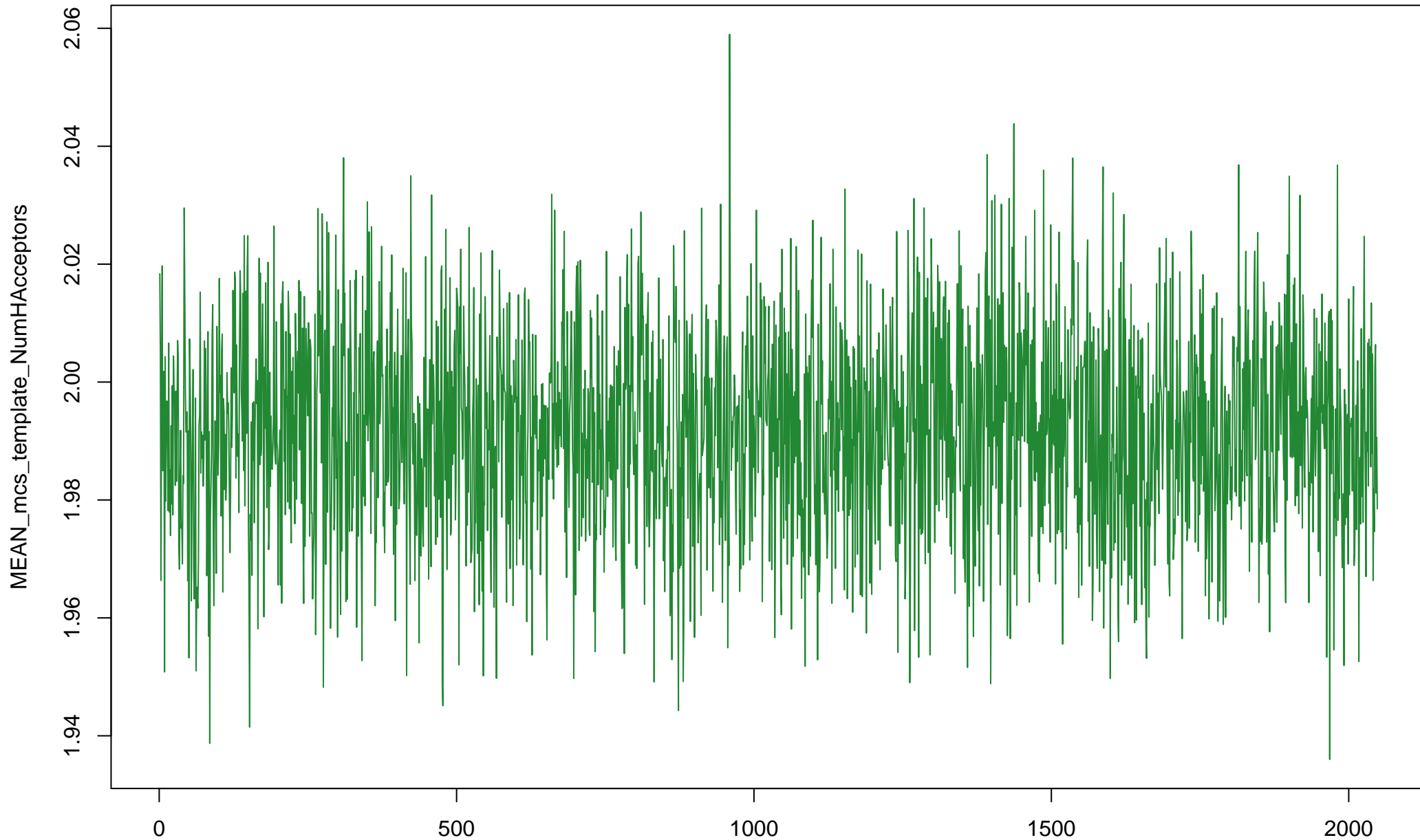
MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0309 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



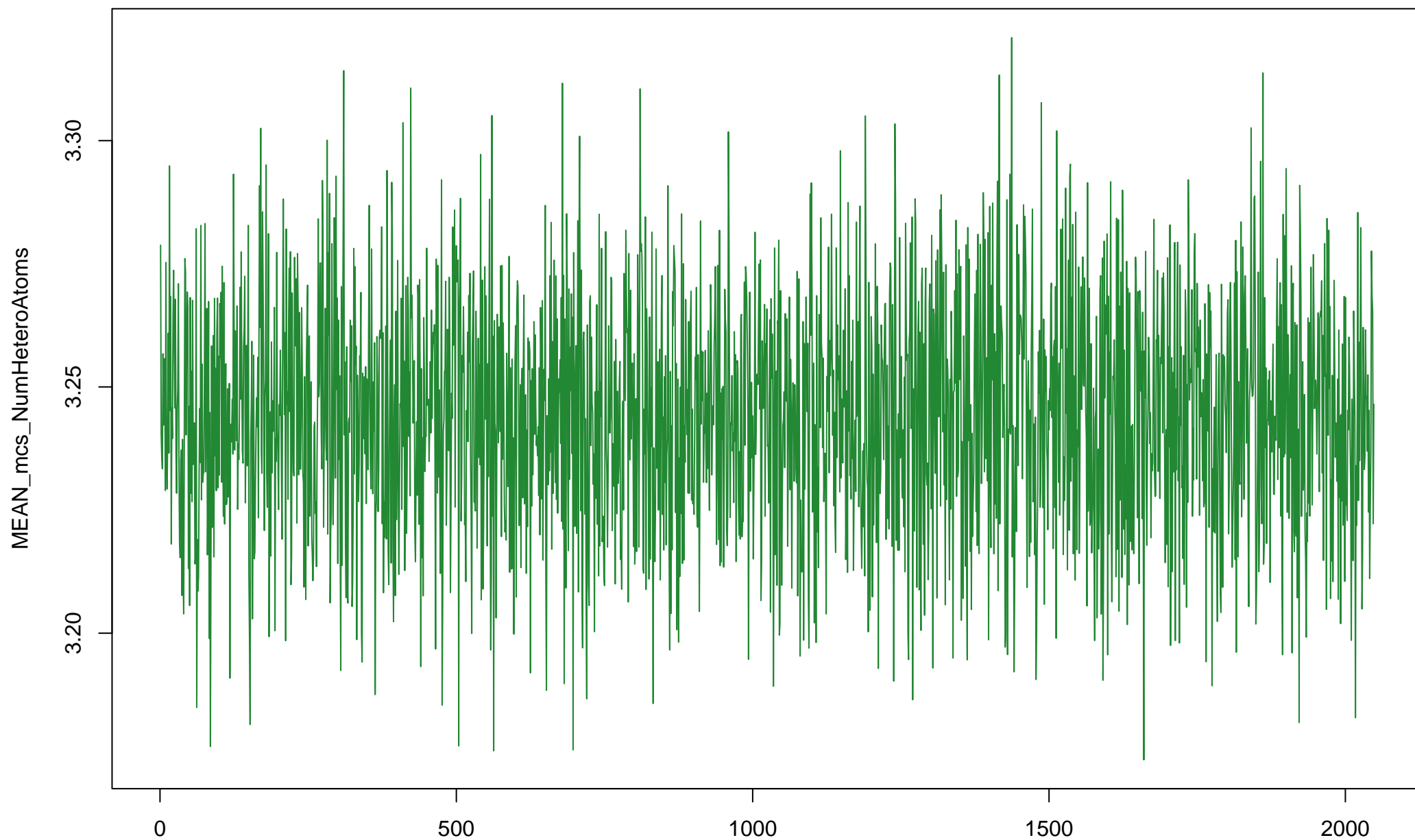
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.043 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0



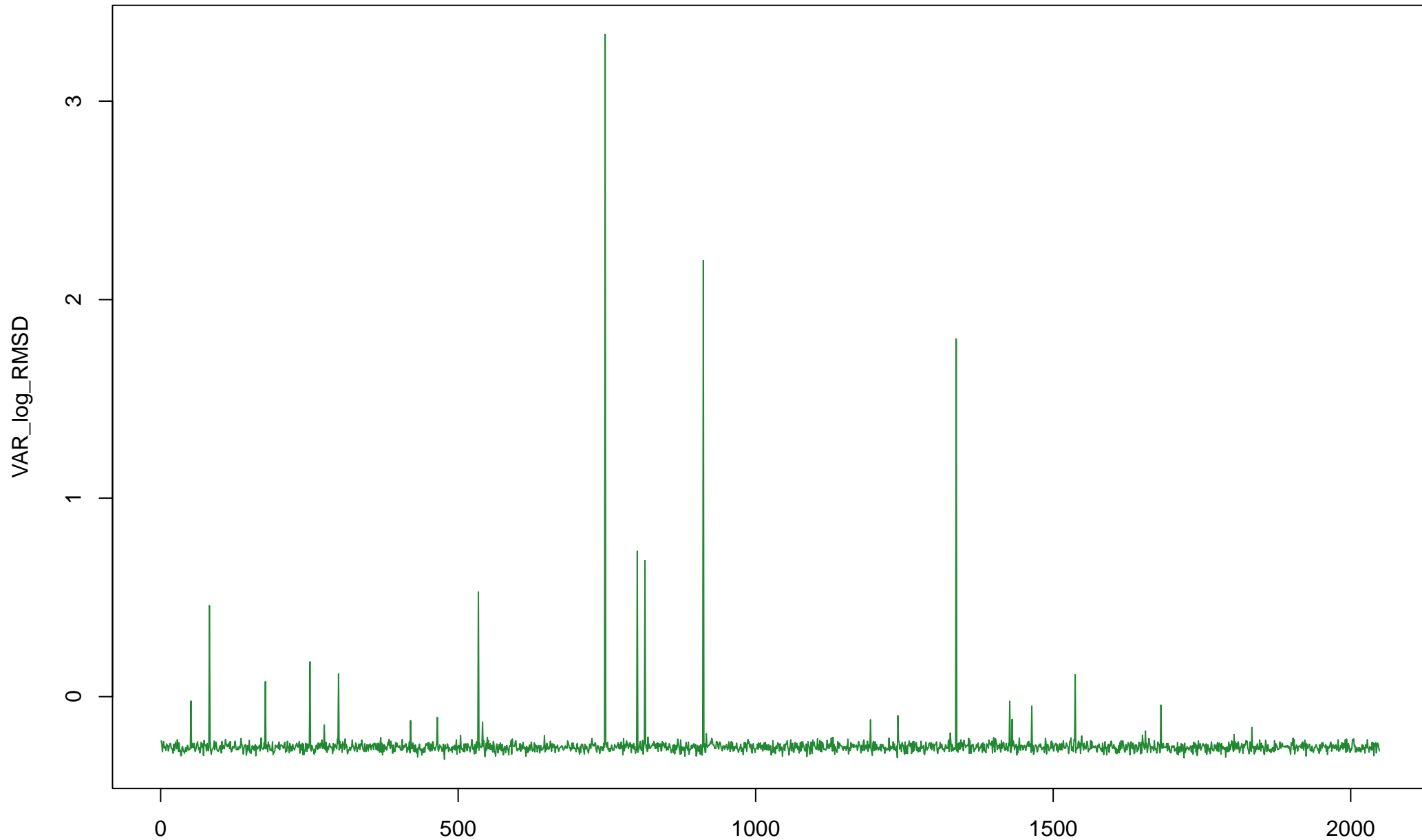
MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0463 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



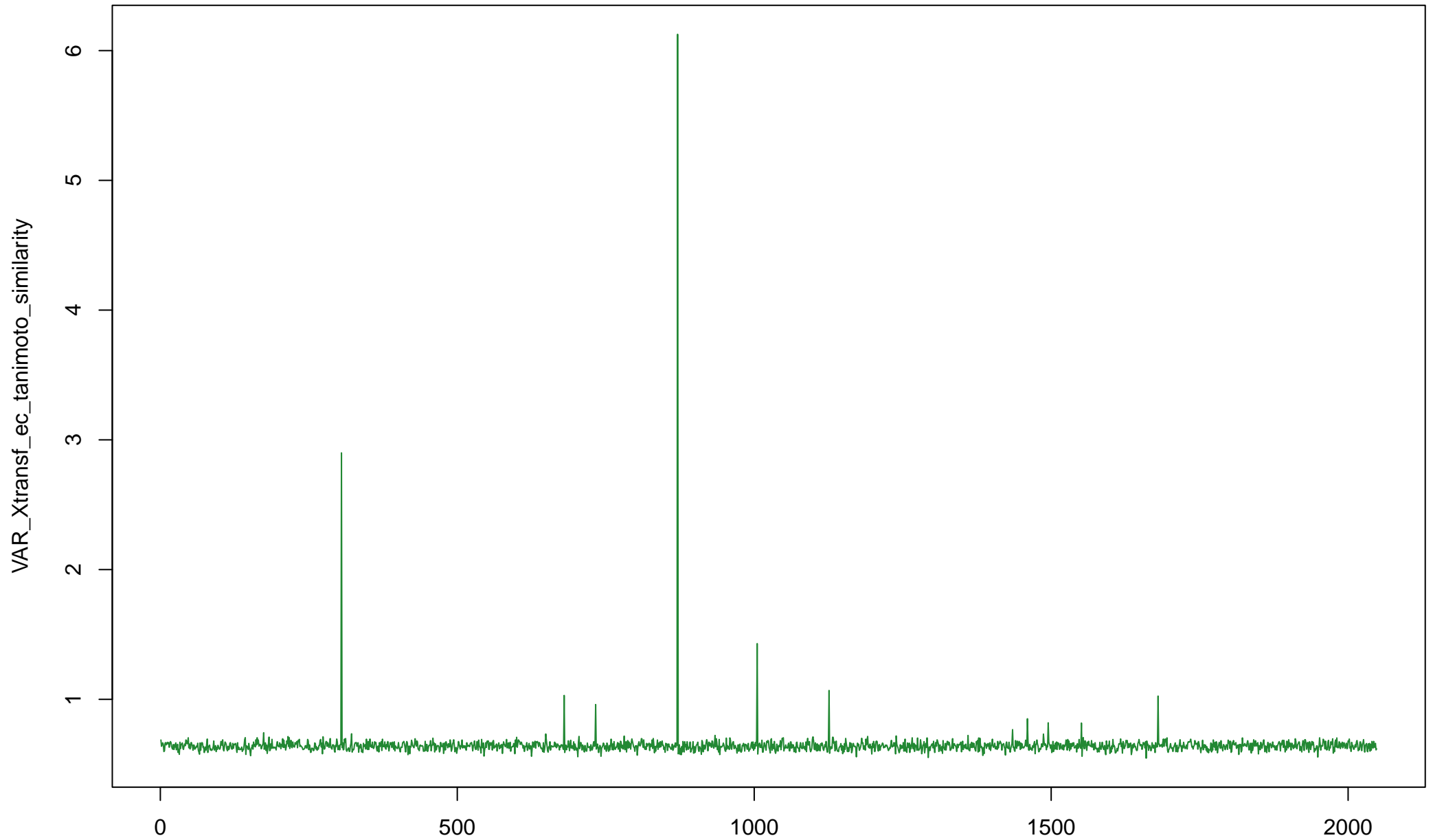
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0423 | MCSE(6.27) = 1.88 | stat: TRUE | burn: 0



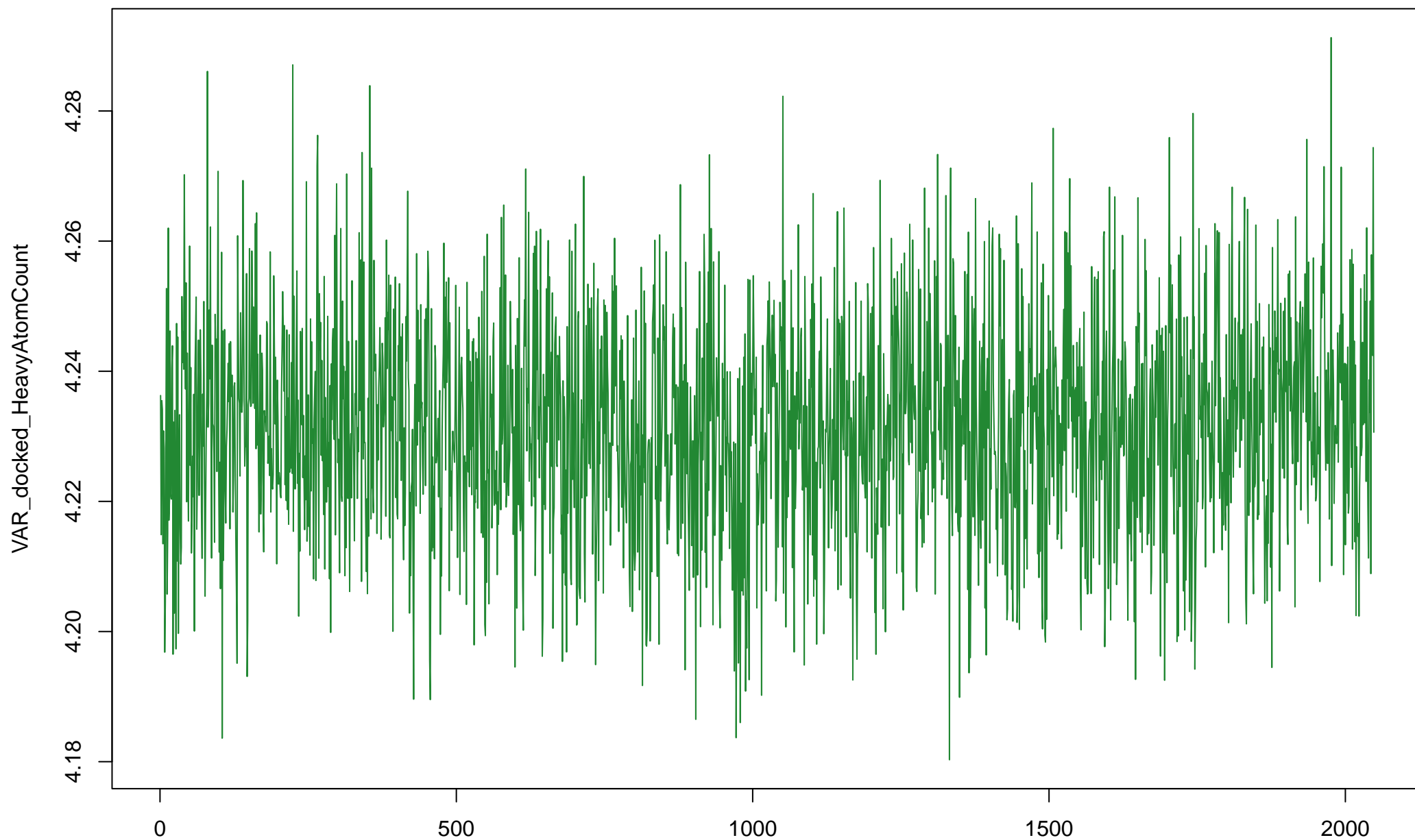
VAR_log_RMSD
ESS = 2050 | BMK = 0.13 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



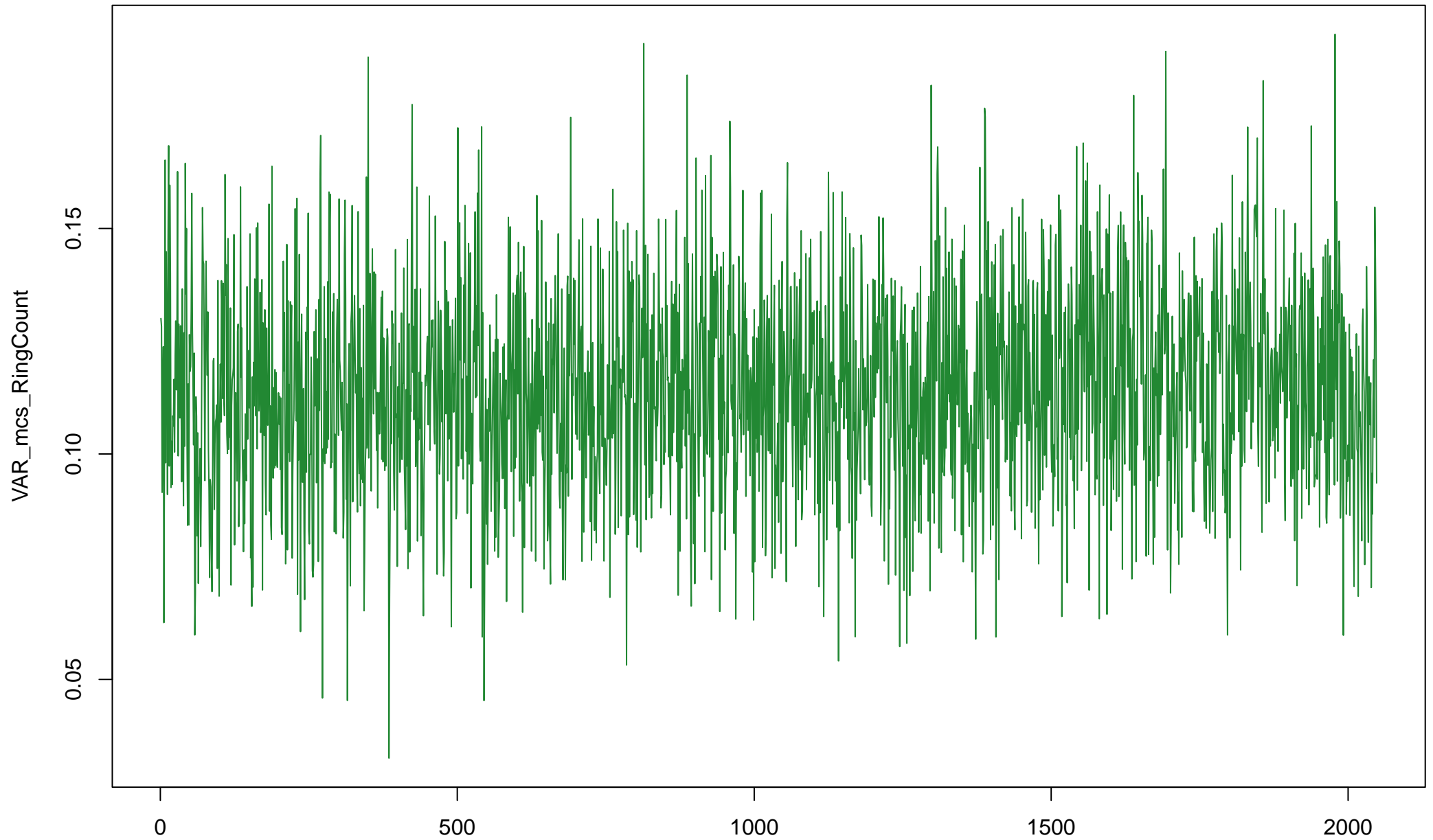
VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.145 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



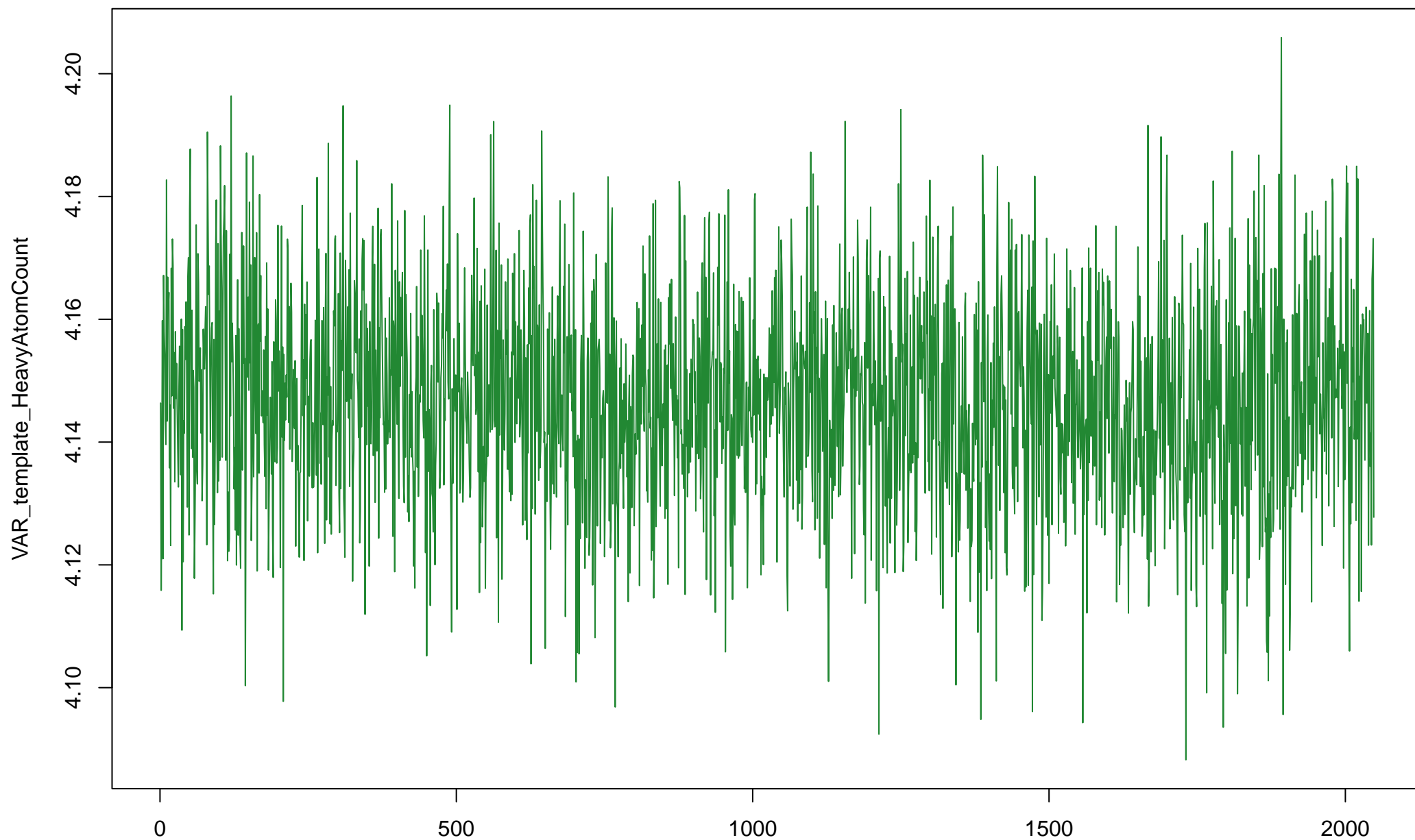
VAR_docked_HeavyAtomCount
ESS = 1370 | BMK = 0.0491 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0



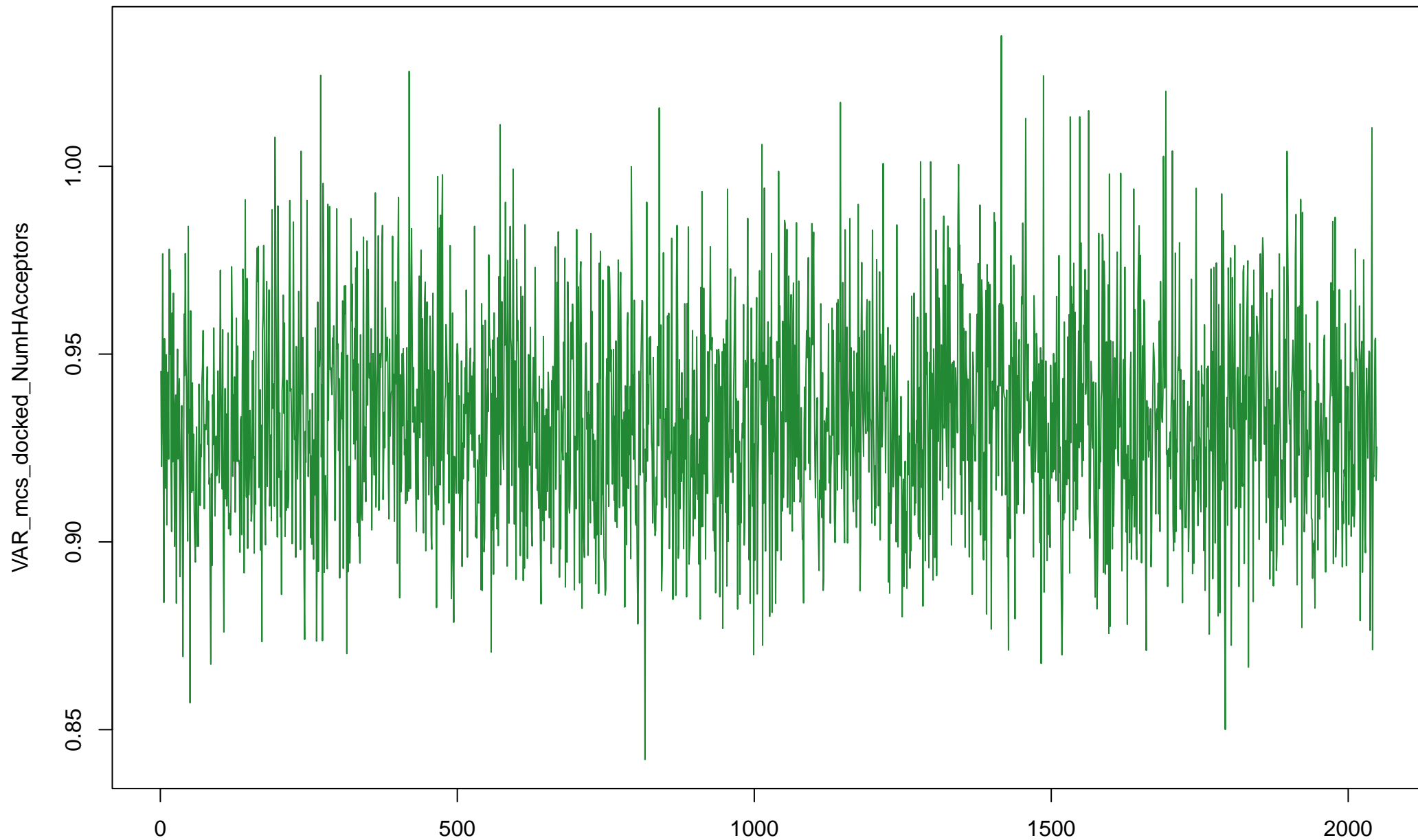
VAR_mcs_RingCount
ESS = 1570 | BMK = 0.0623 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0



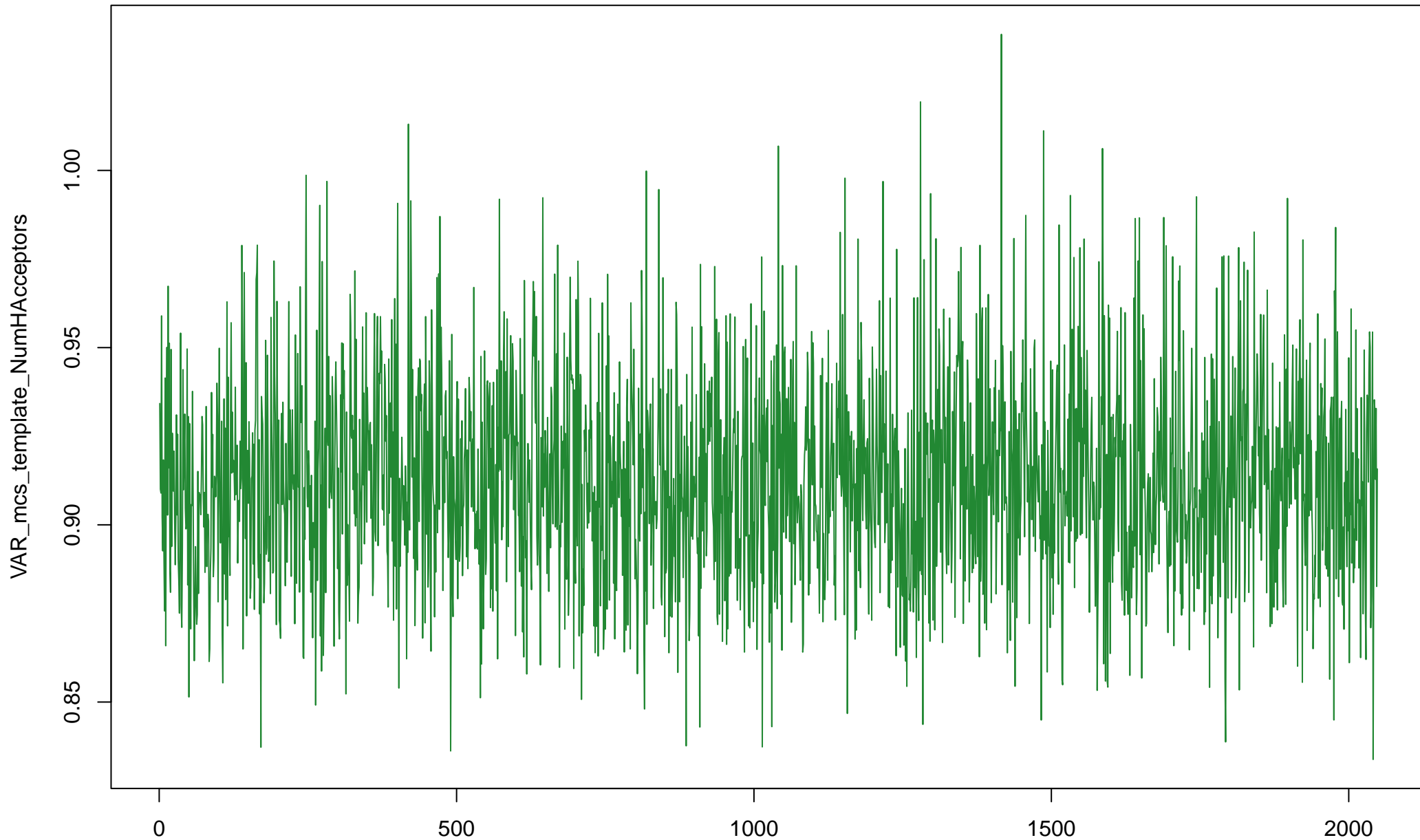
VAR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0502 | MCSE(6.27) = 2.47 | stat: FALSE | burn: 0



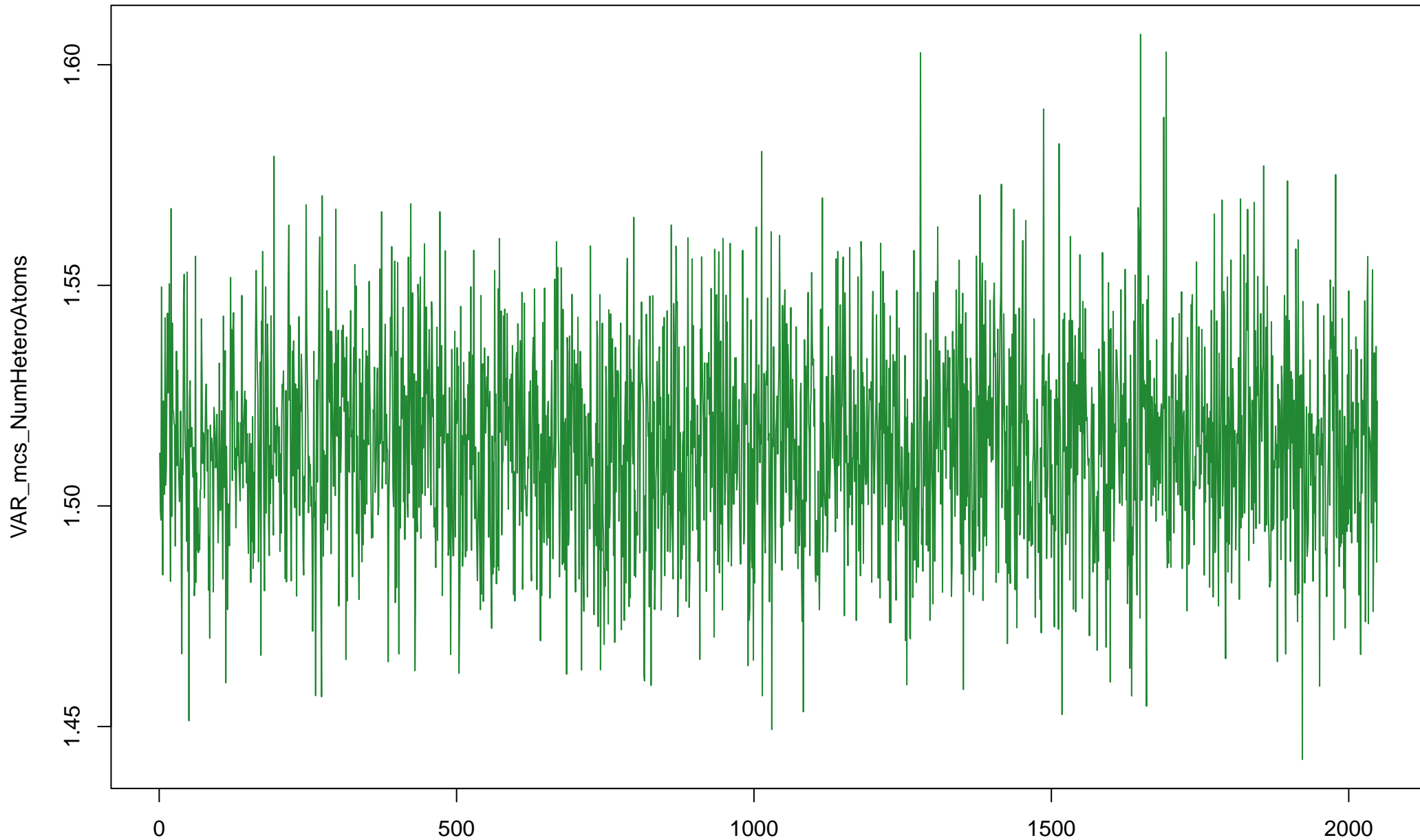
VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0289 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0



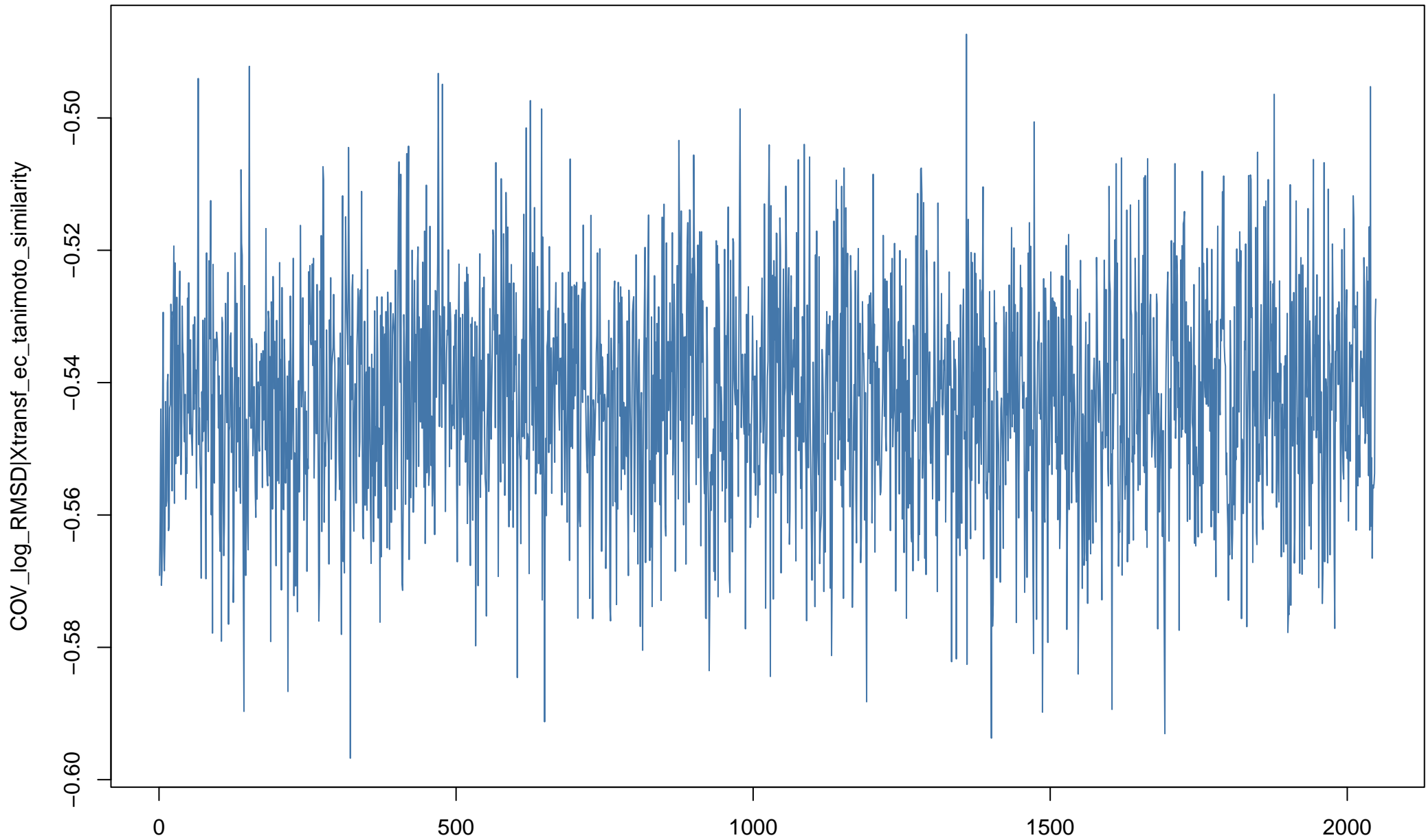
VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0468 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0



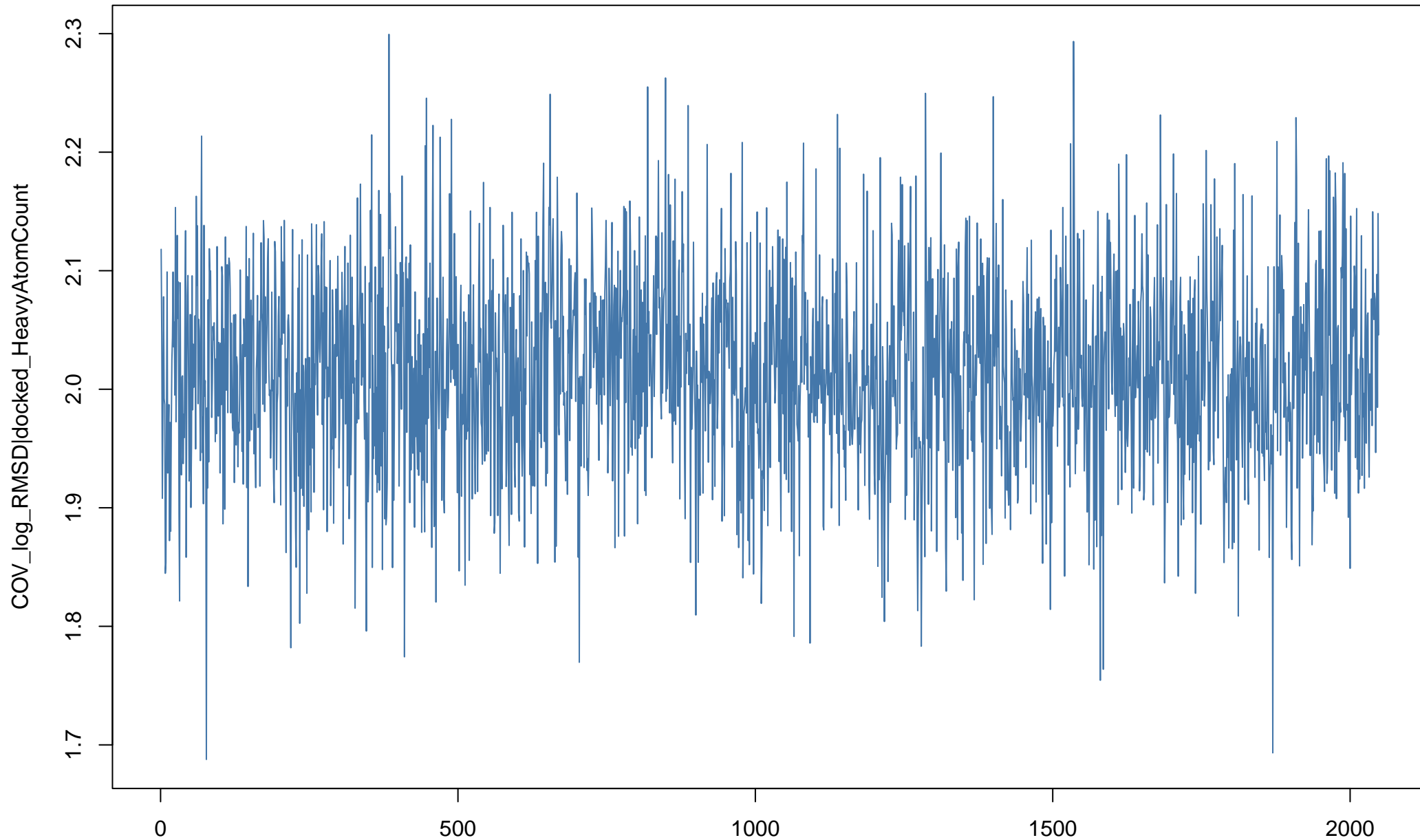
VAR_mcs_NumHeteroAtoms
ESS = 2030 | BMK = 0.0484 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0



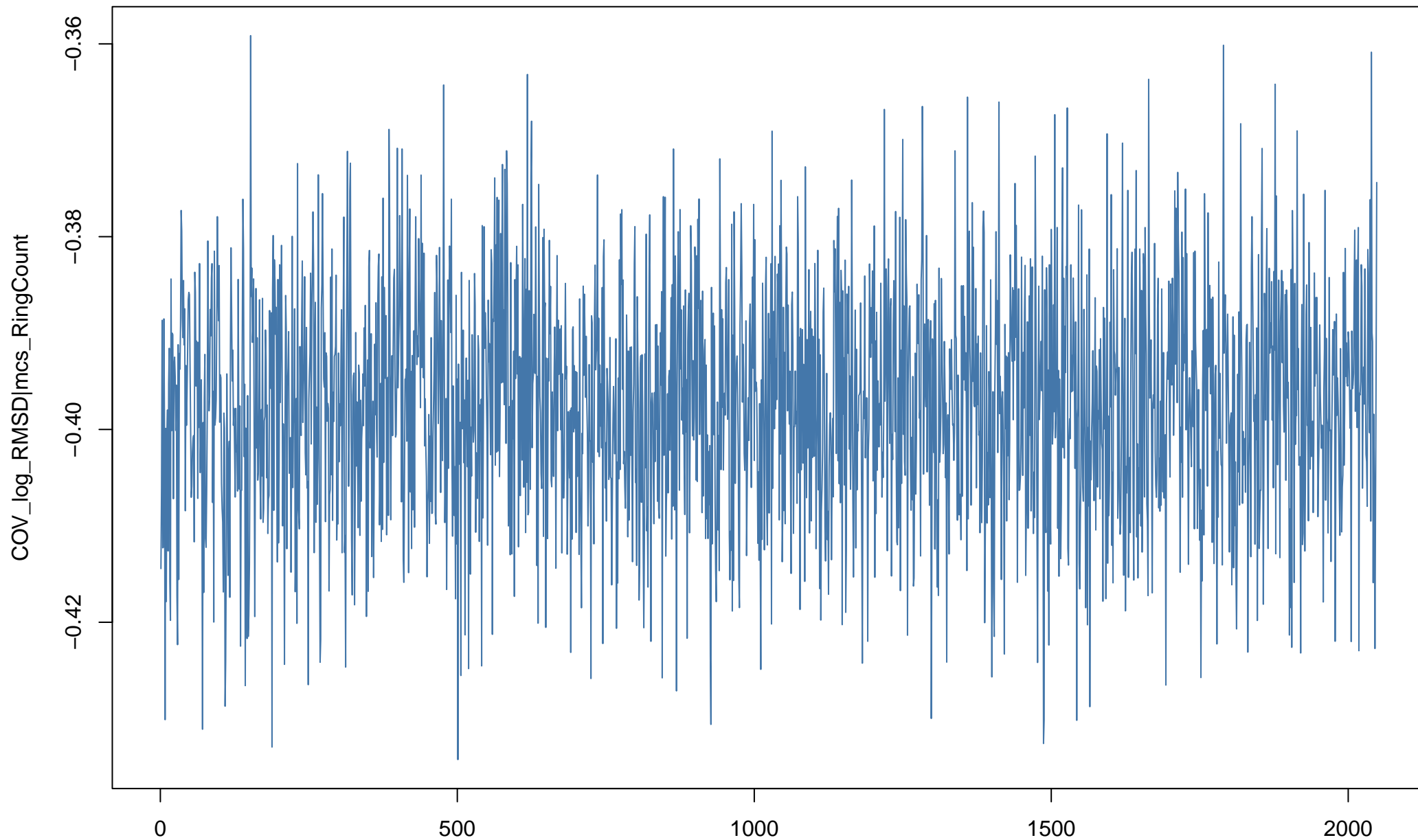
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1850 | BMK = 0.0531 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0



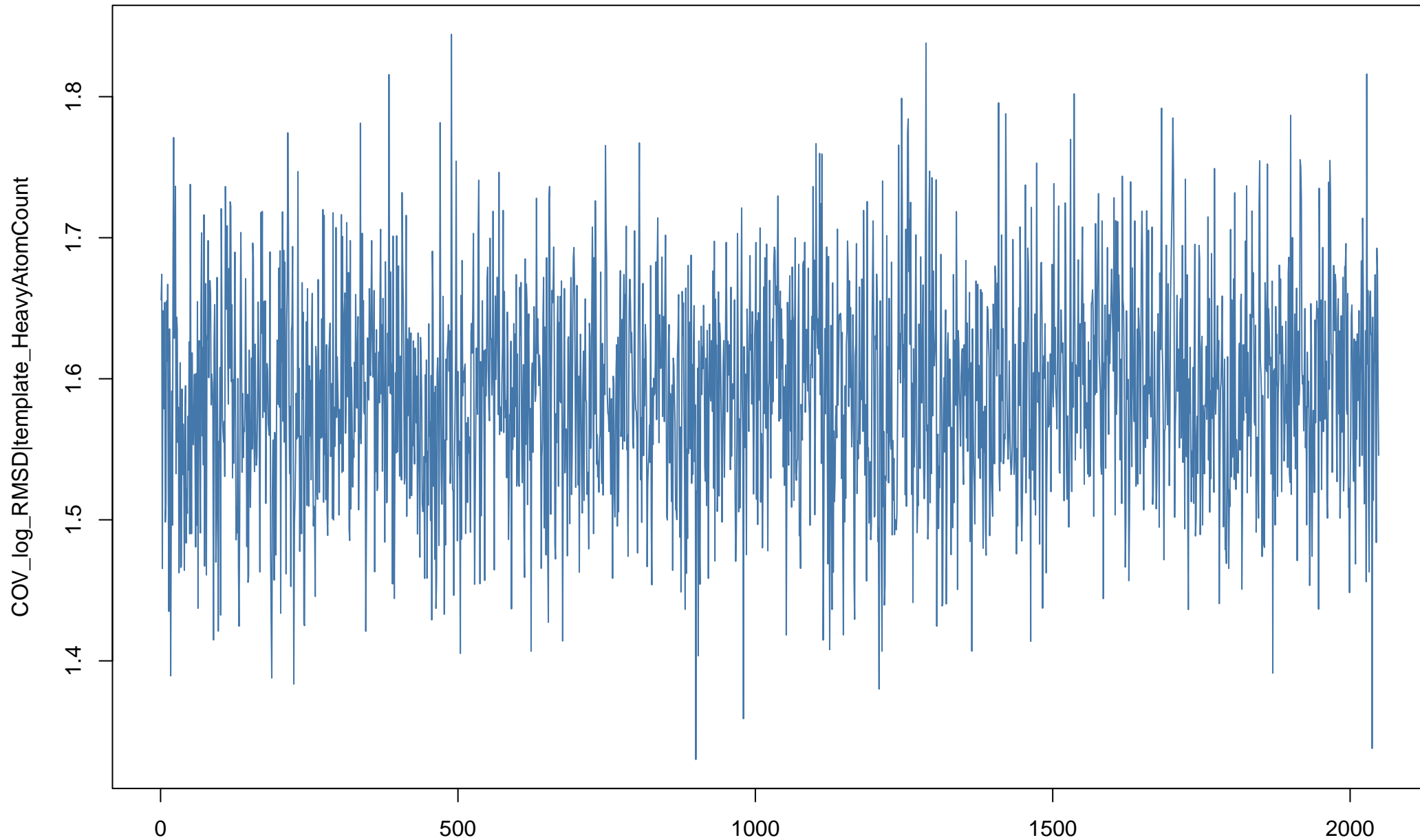
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1440 | BMK = 0.0567 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0



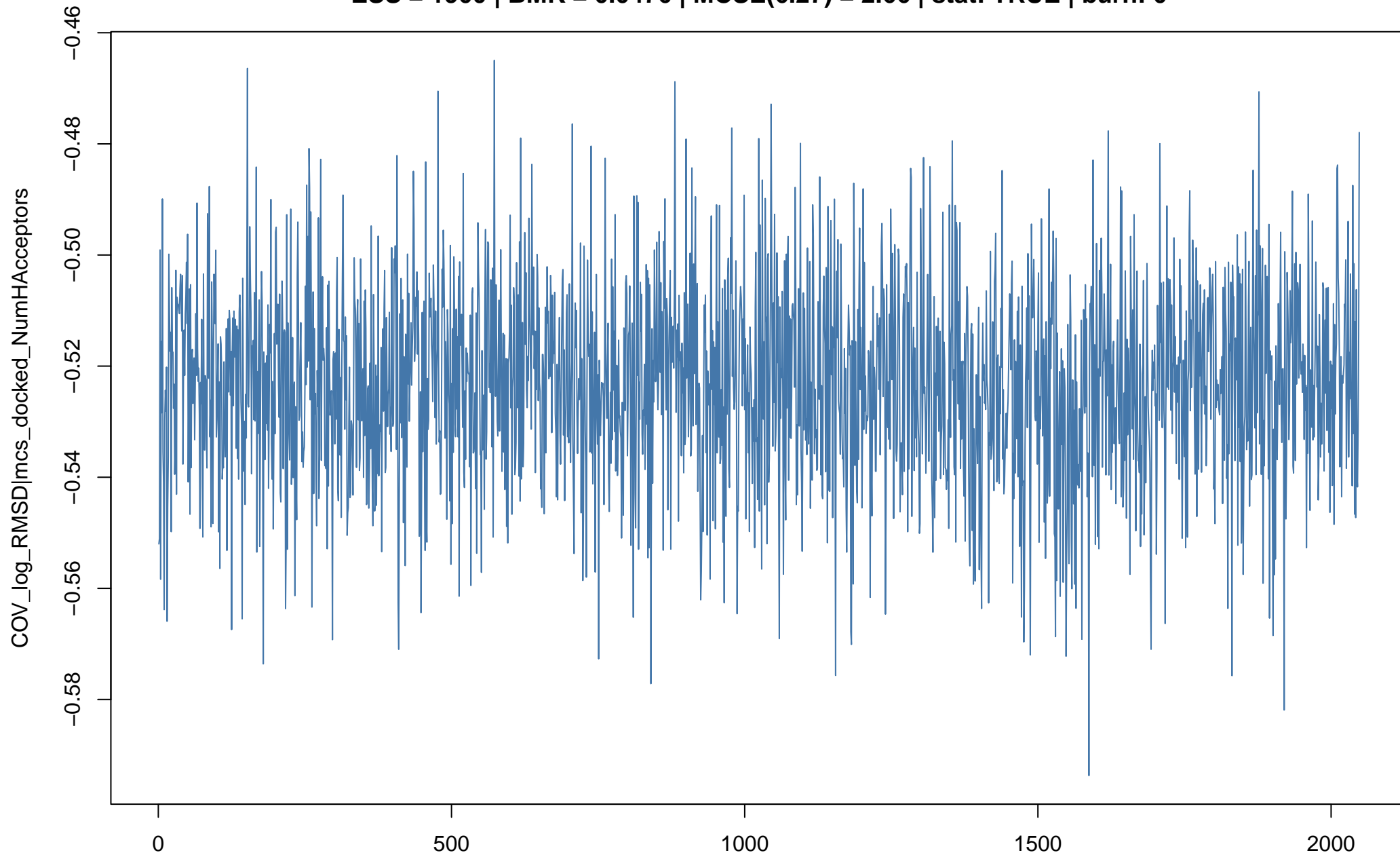
COV_log_RMSD|mcs_RingCount
ESS = 1840 | BMK = 0.0336 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0



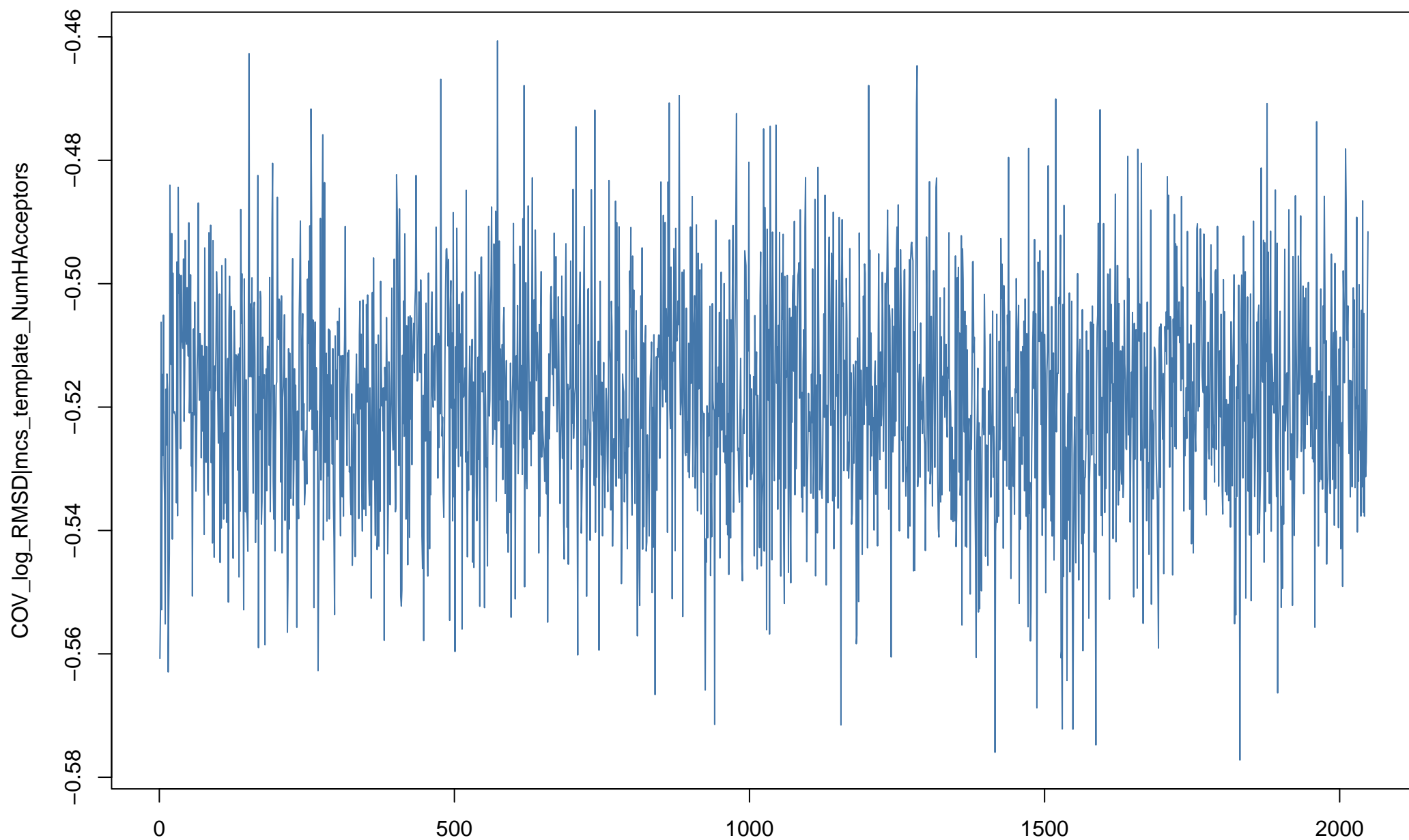
COV_log_RMSD|template_HeavyAtomCount
ESS = 1640 | BMK = 0.0664 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0



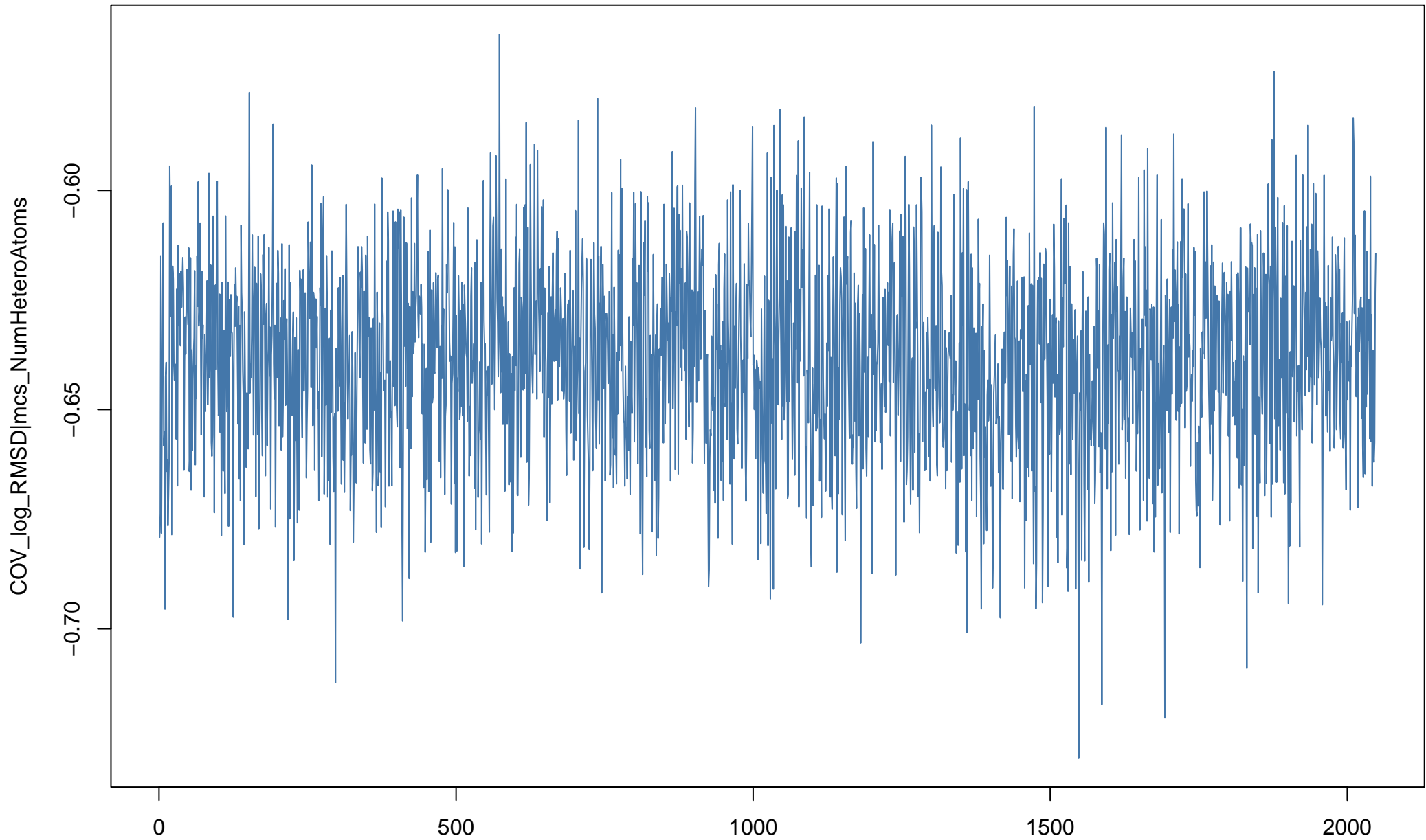
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 1900 | BMK = 0.0476 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0



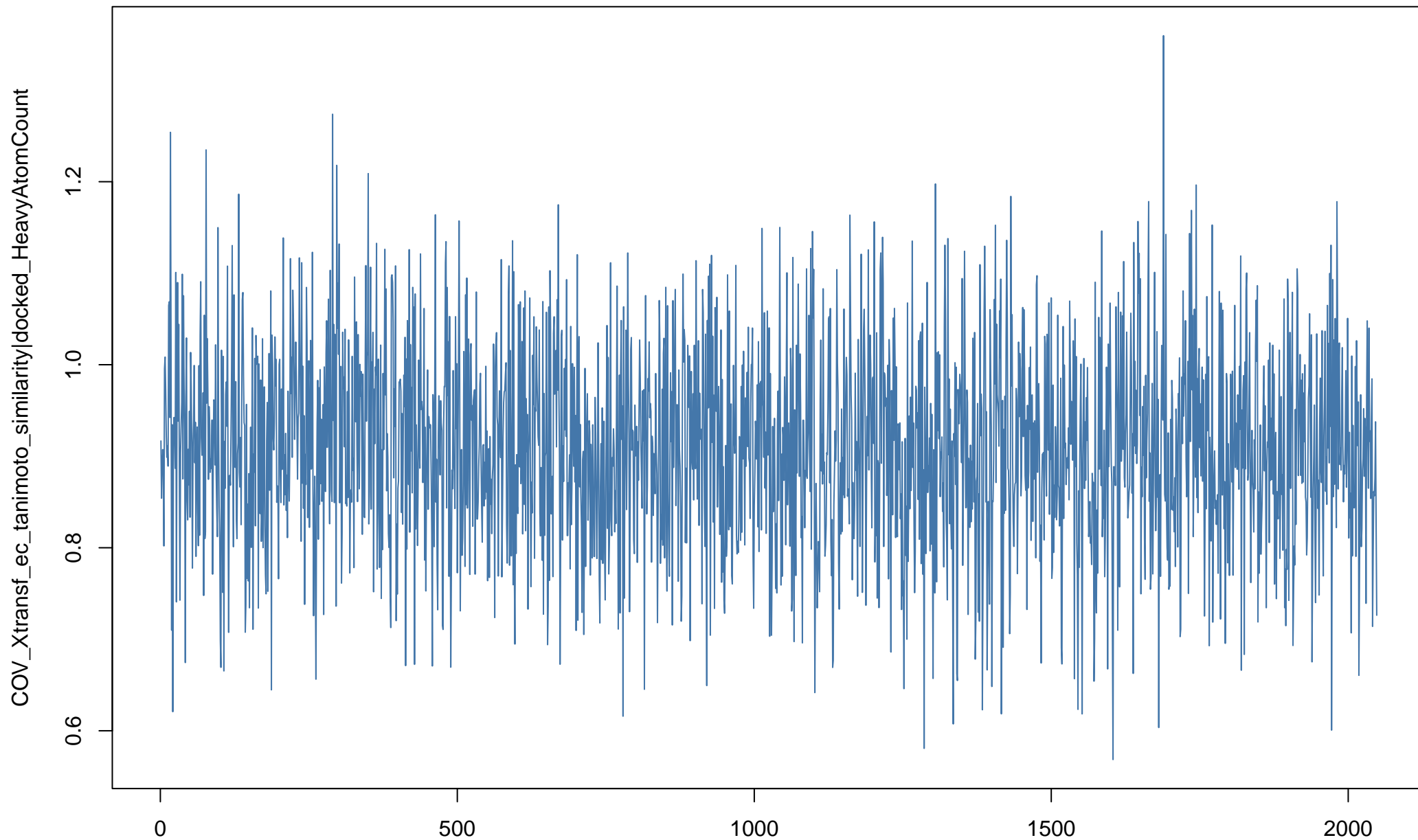
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 1860 | BMK = 0.0501 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0



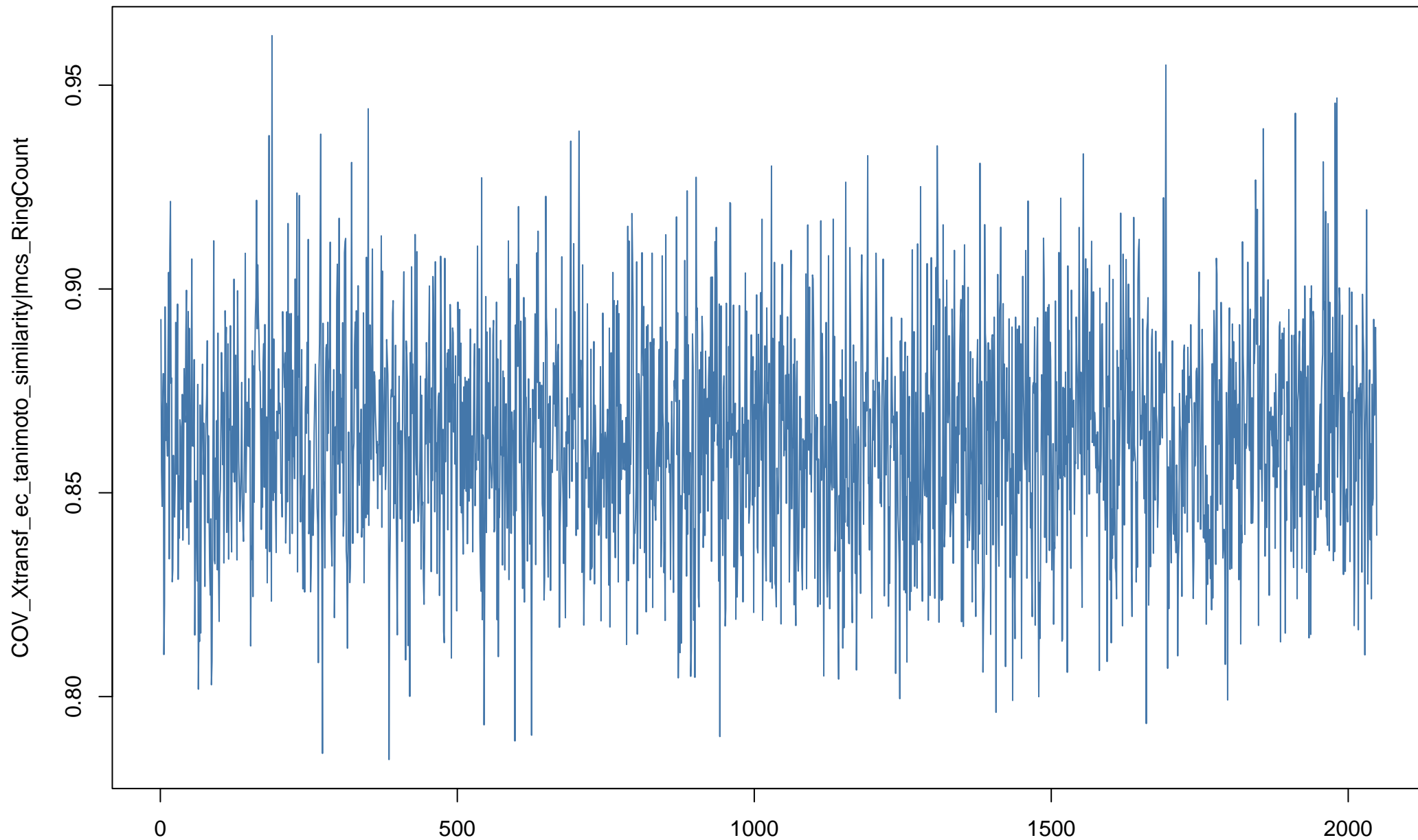
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1790 | BMK = 0.0563 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0



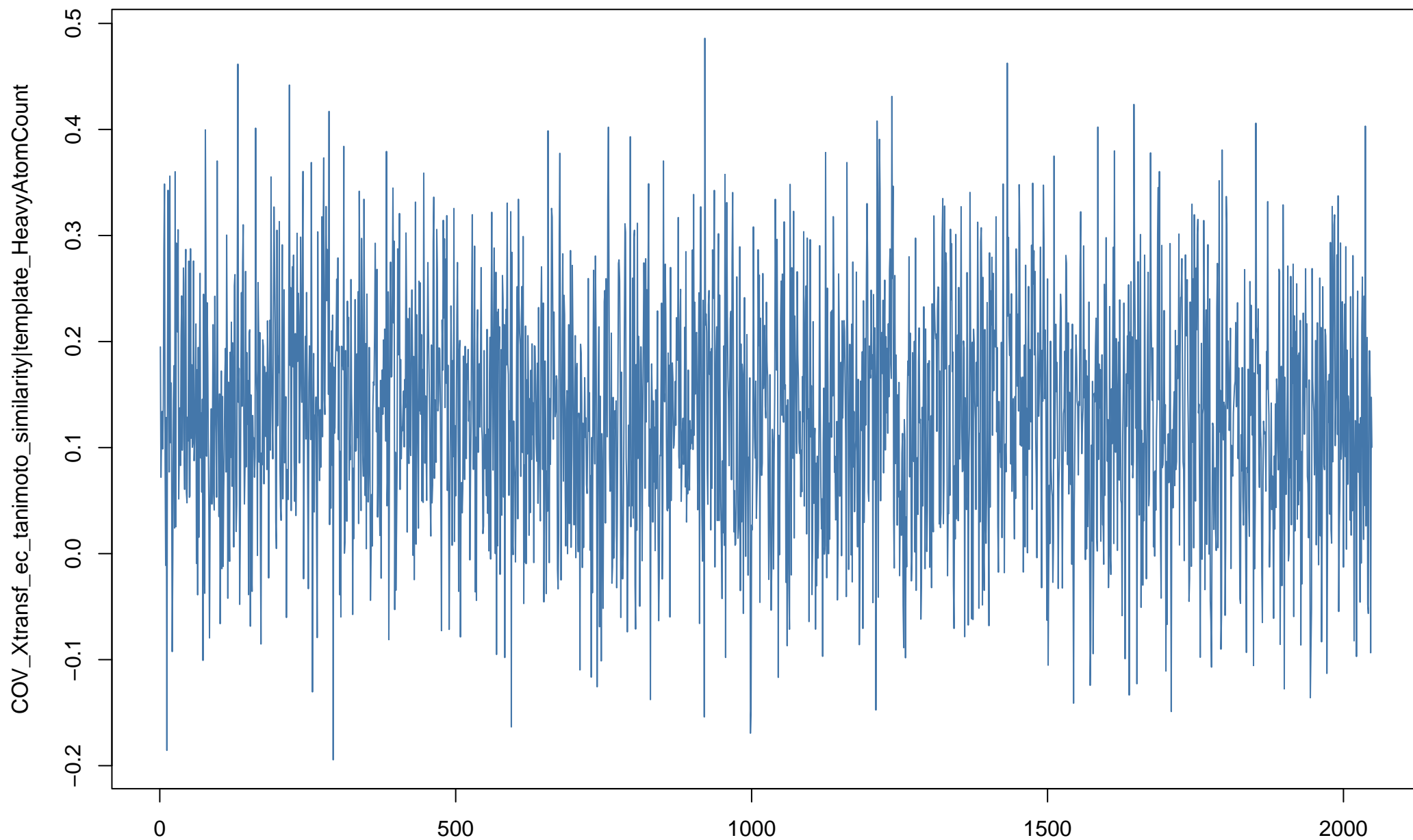
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0692 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0



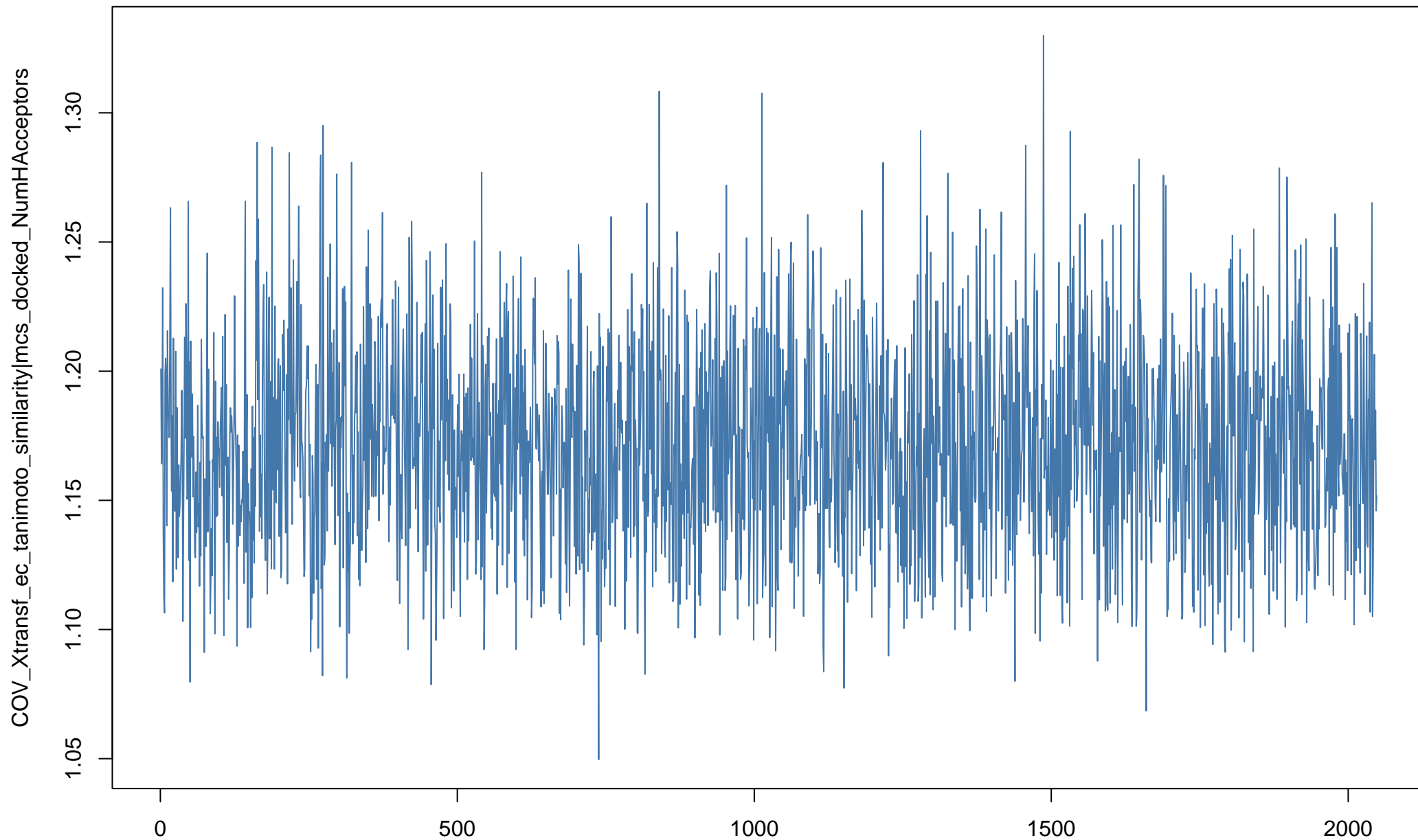
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1840 | BMK = 0.0372 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0



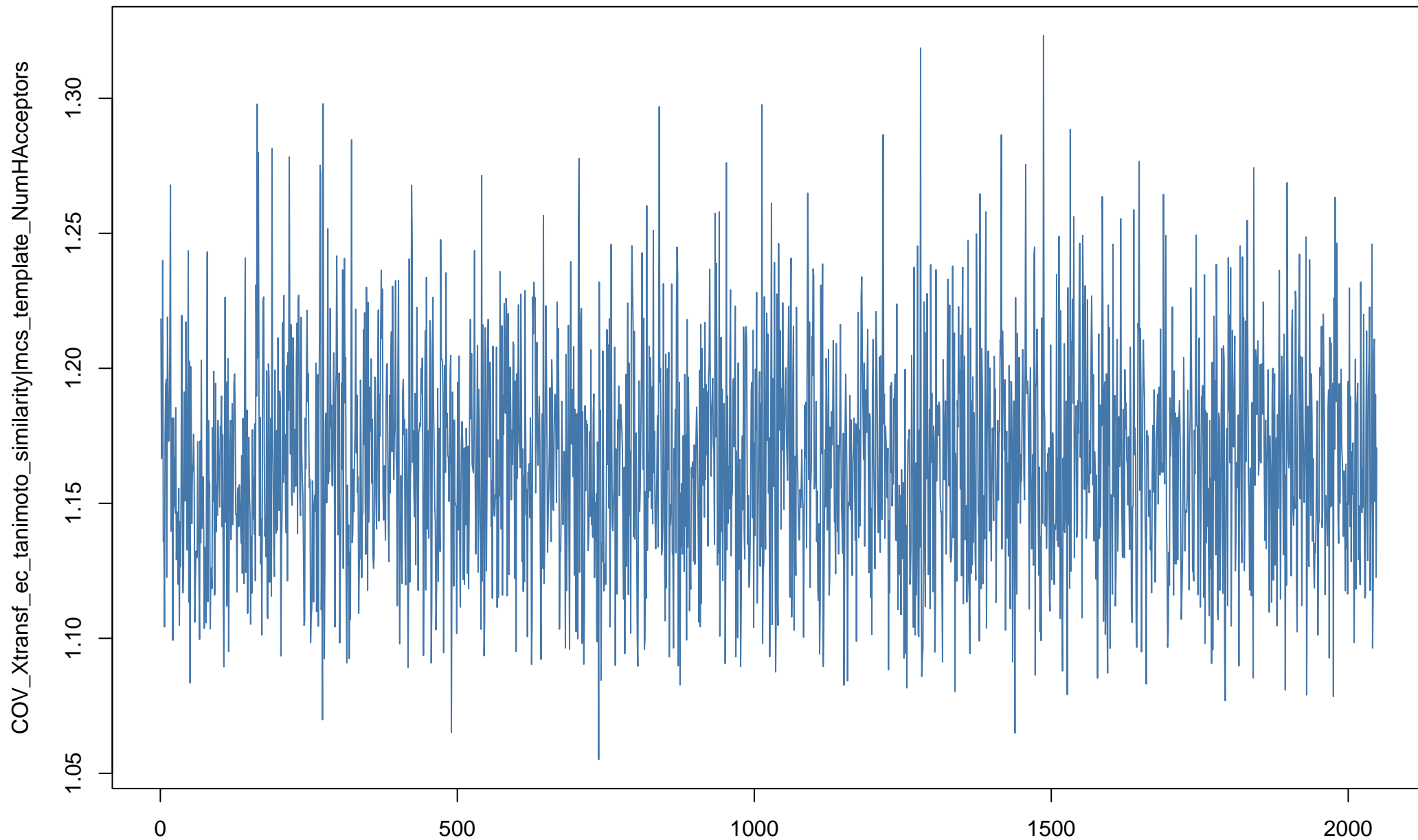
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1870 | BMK = 0.049 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



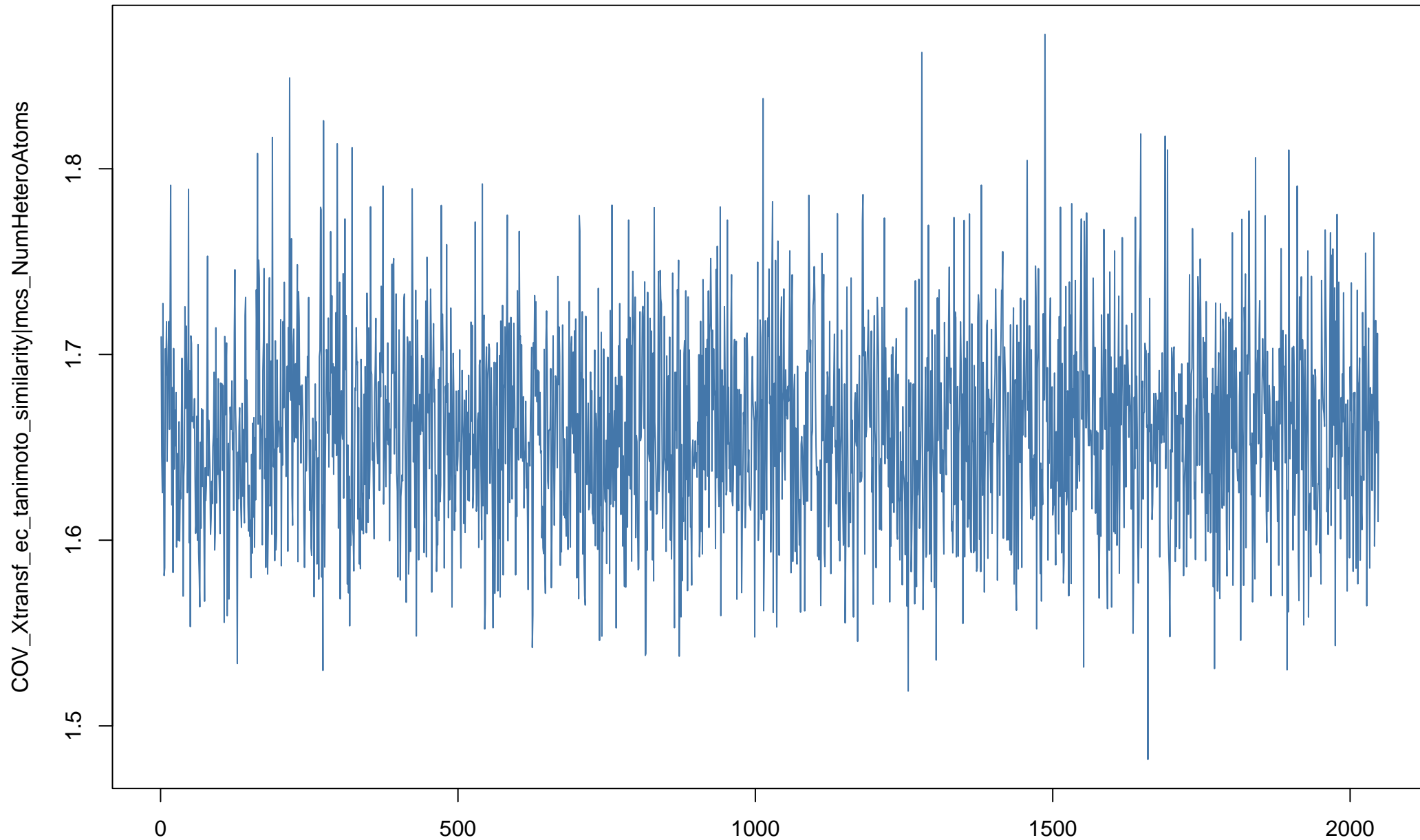
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 1920 | BMK = 0.0323 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



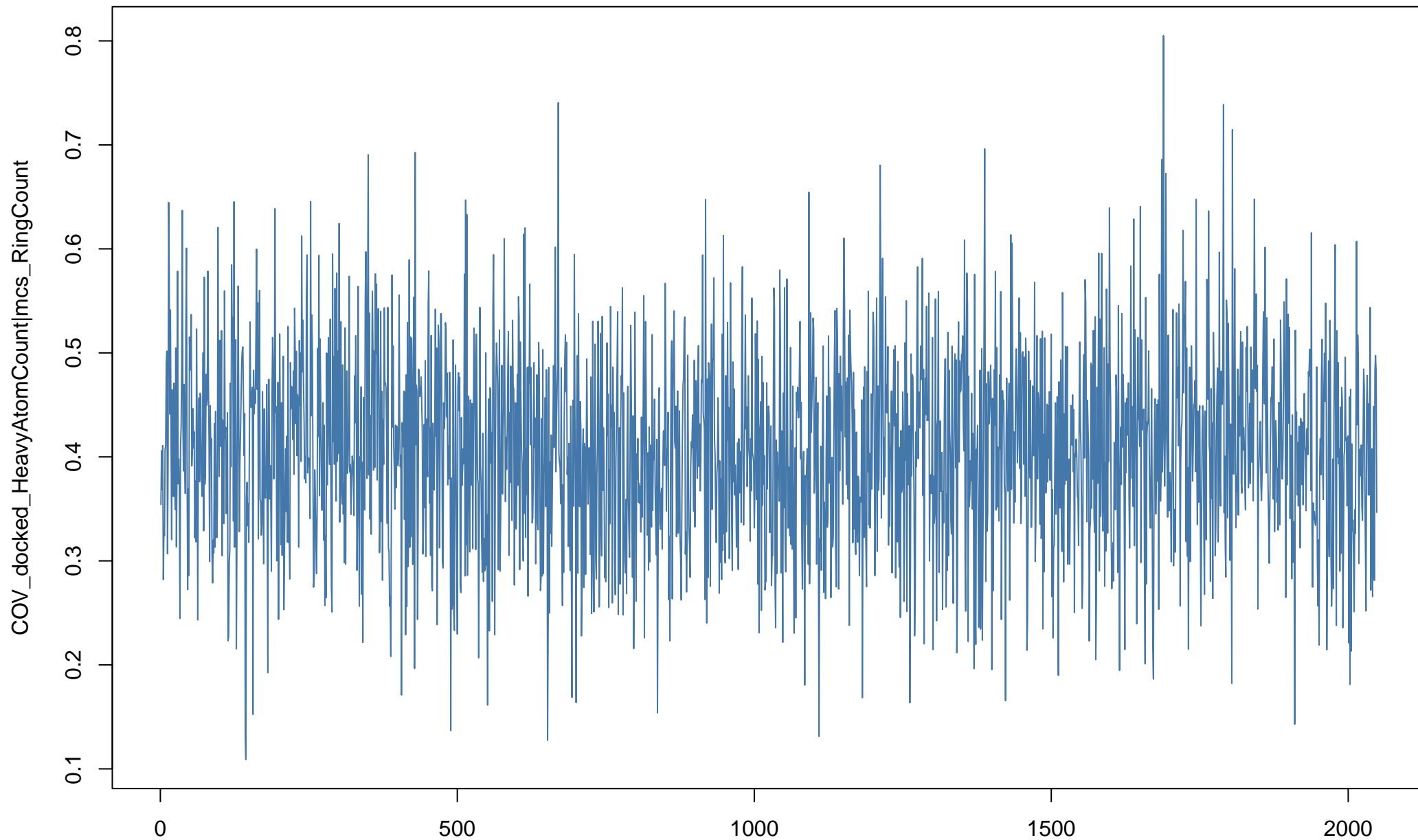
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 1920 | BMK = 0.0369 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0



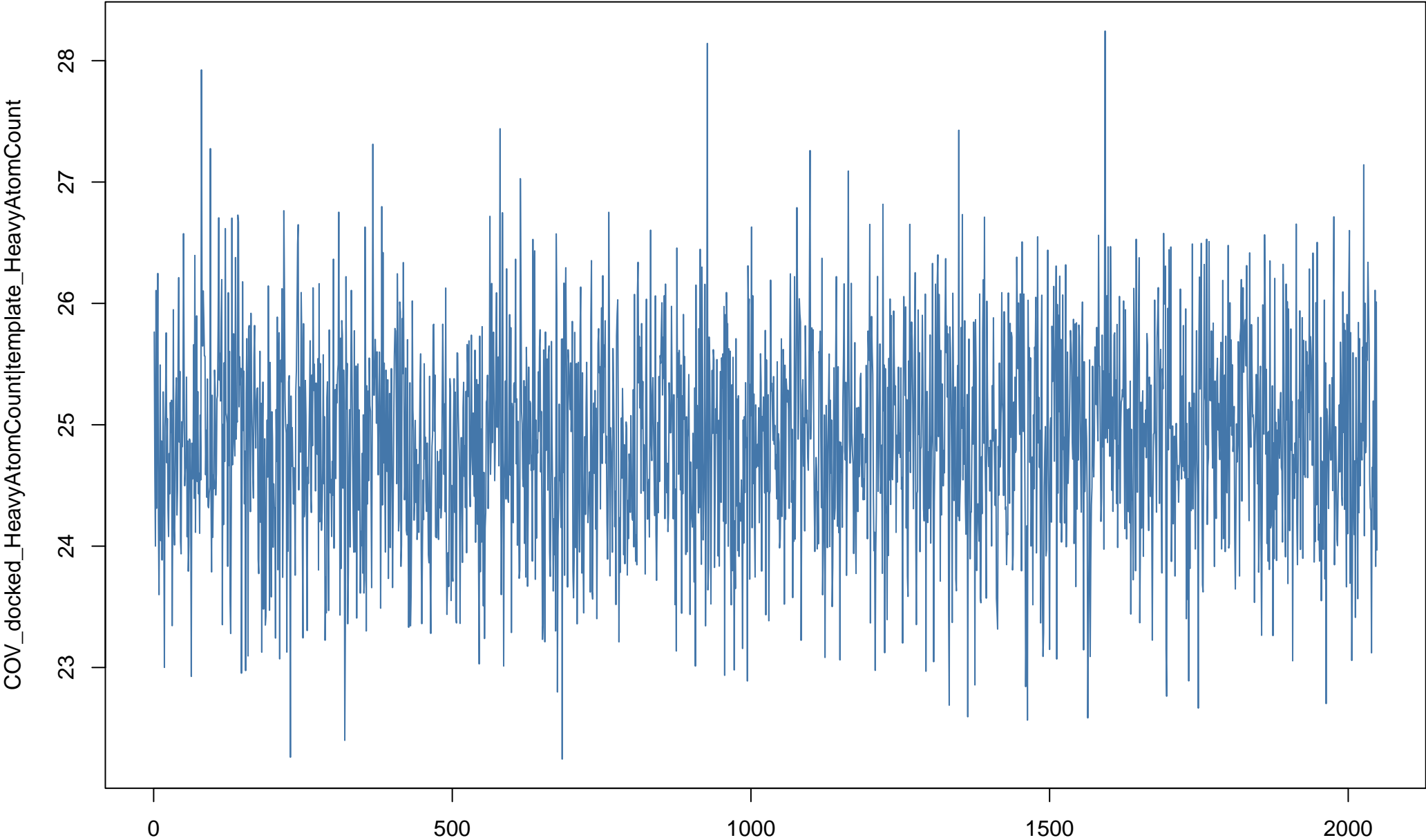
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0444 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



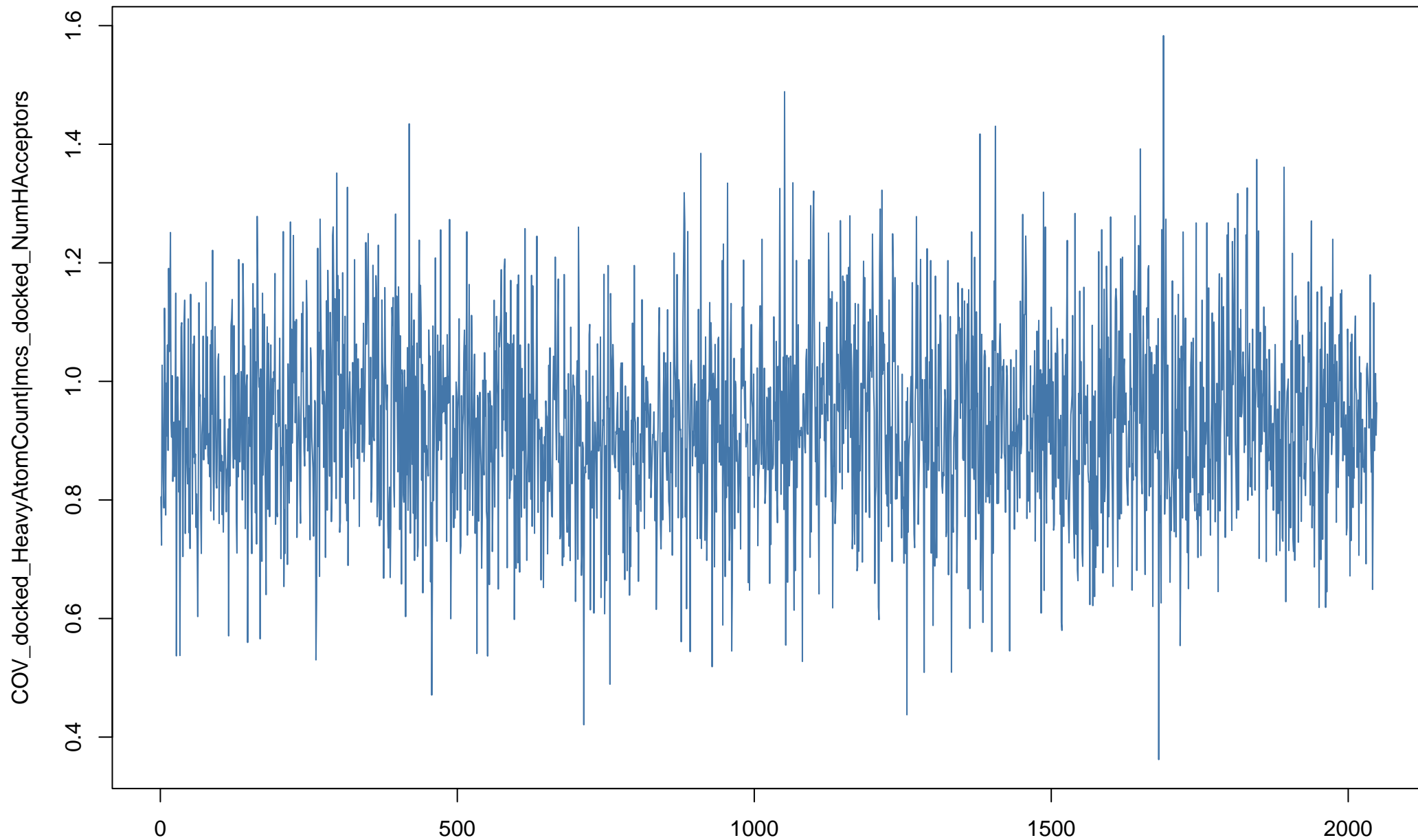
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1920 | BMK = 0.047 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0



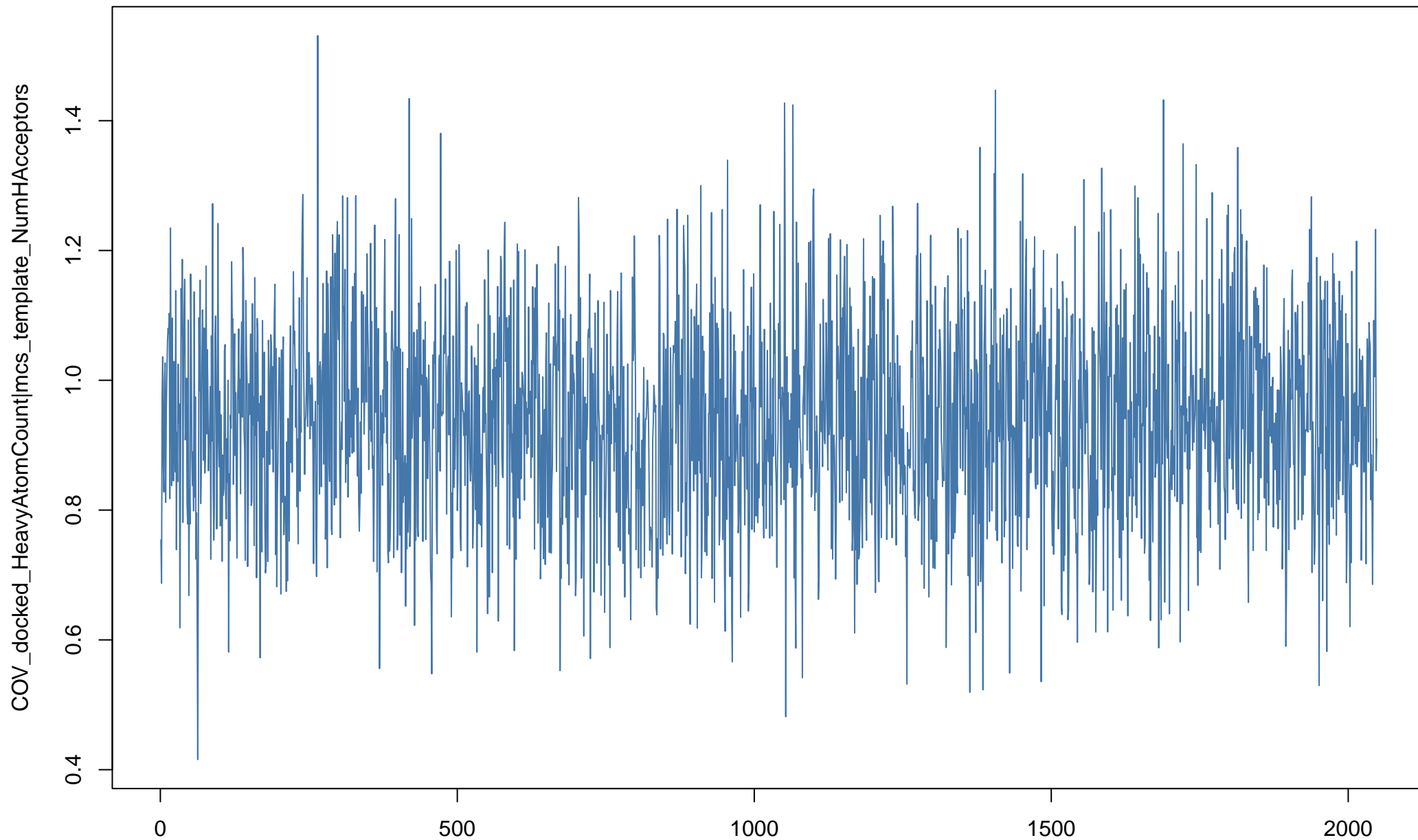
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1640 | BMK = 0.0695 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0



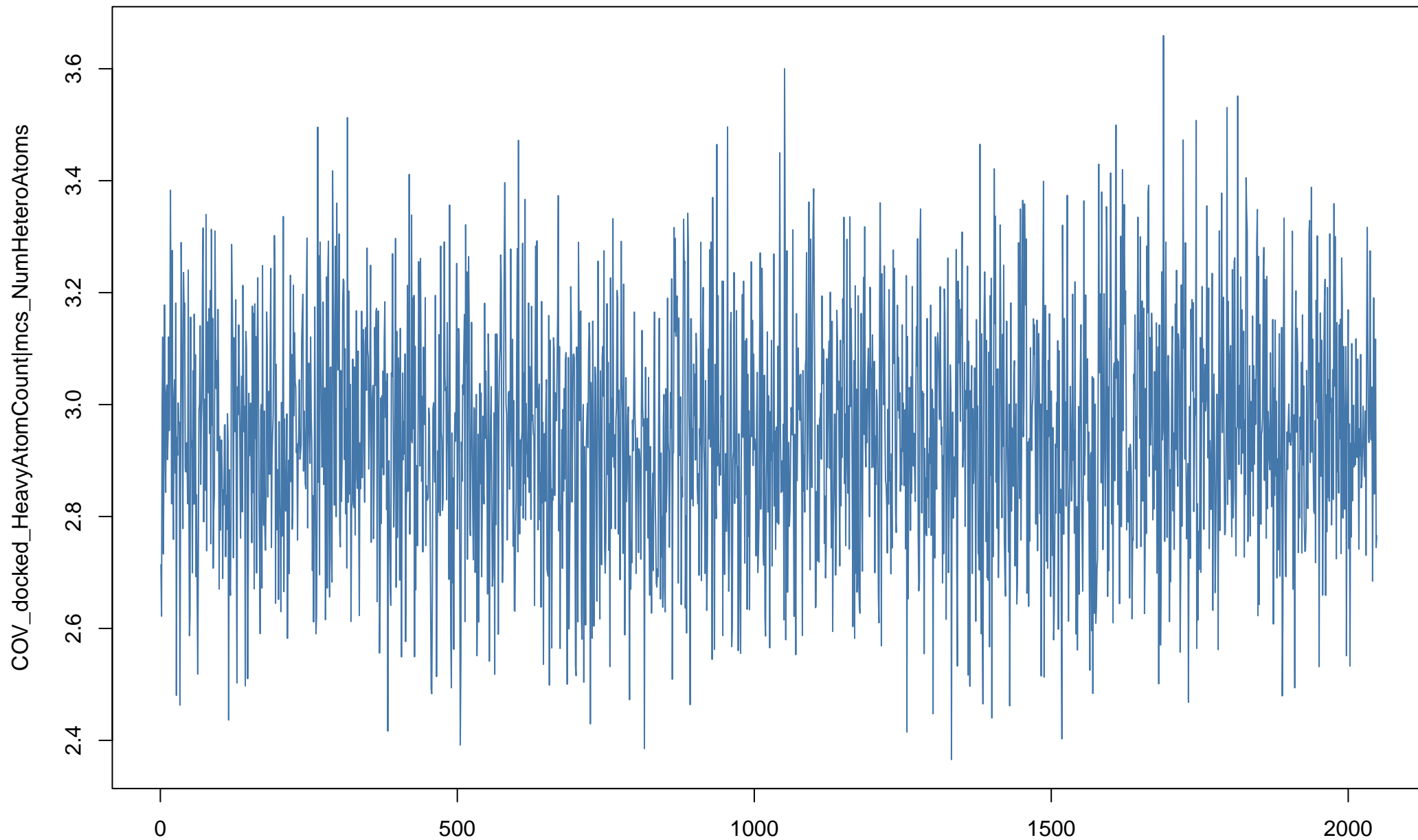
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0476 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0



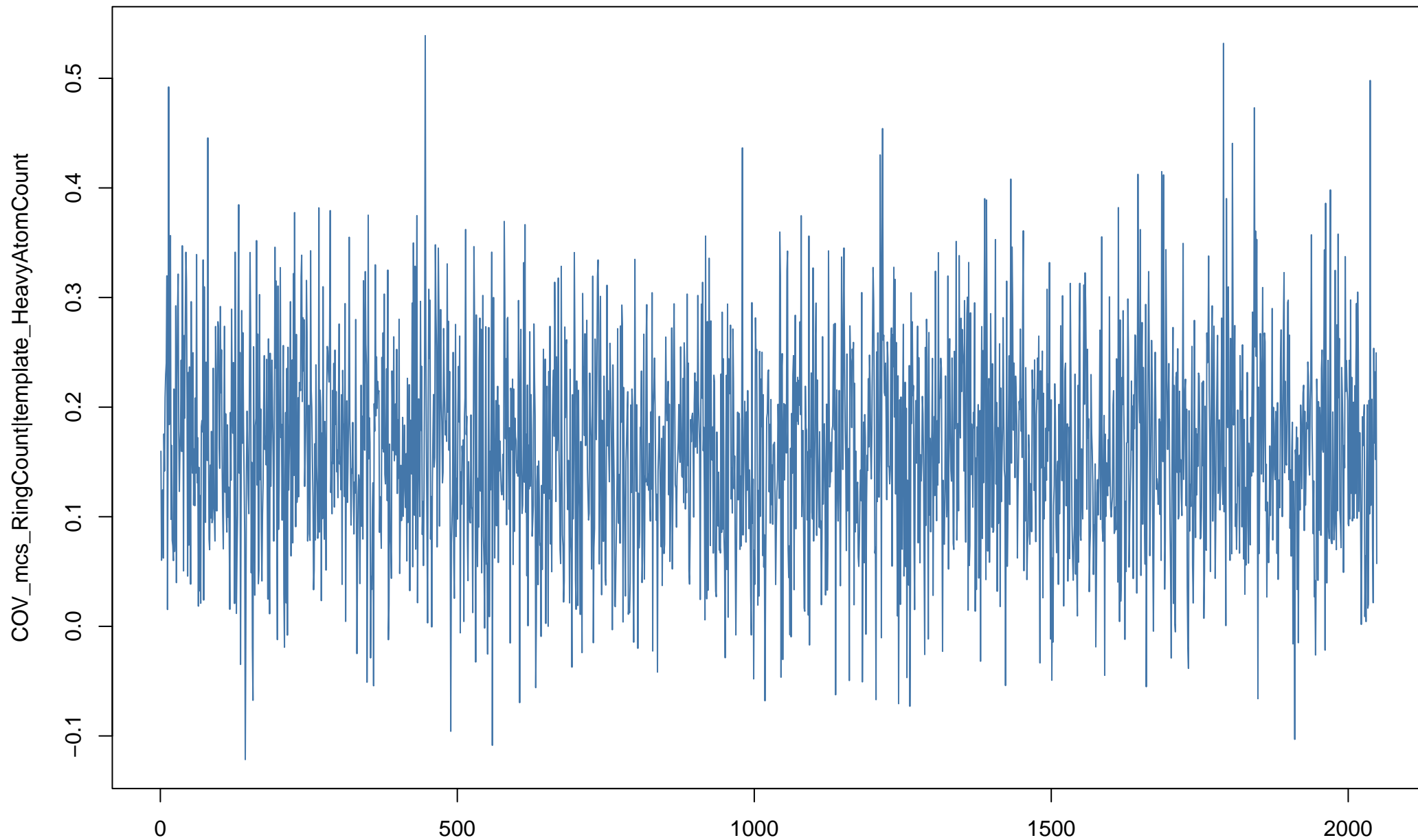
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1880 | BMK = 0.0482 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



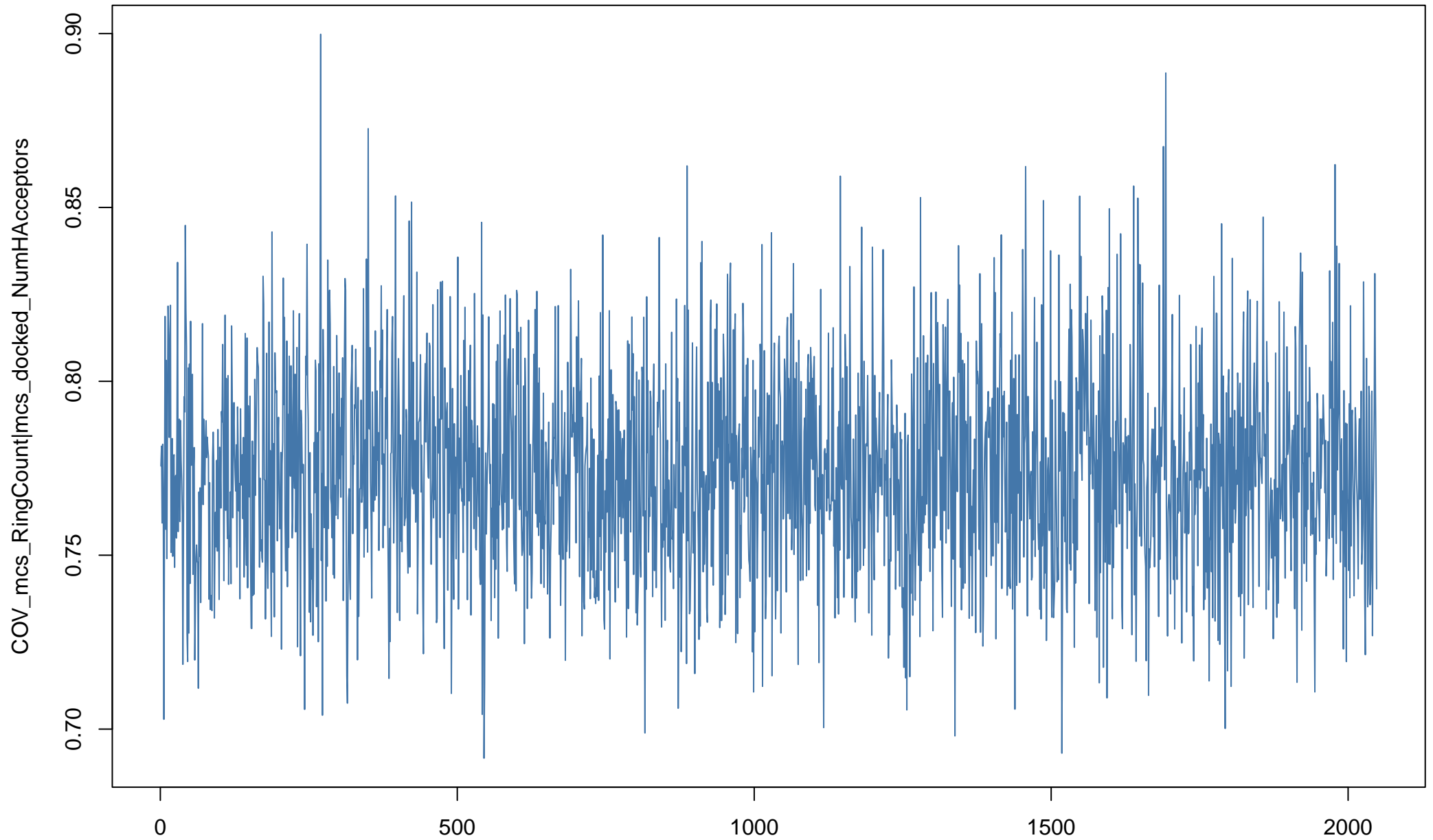
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1910 | BMK = 0.0493 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0



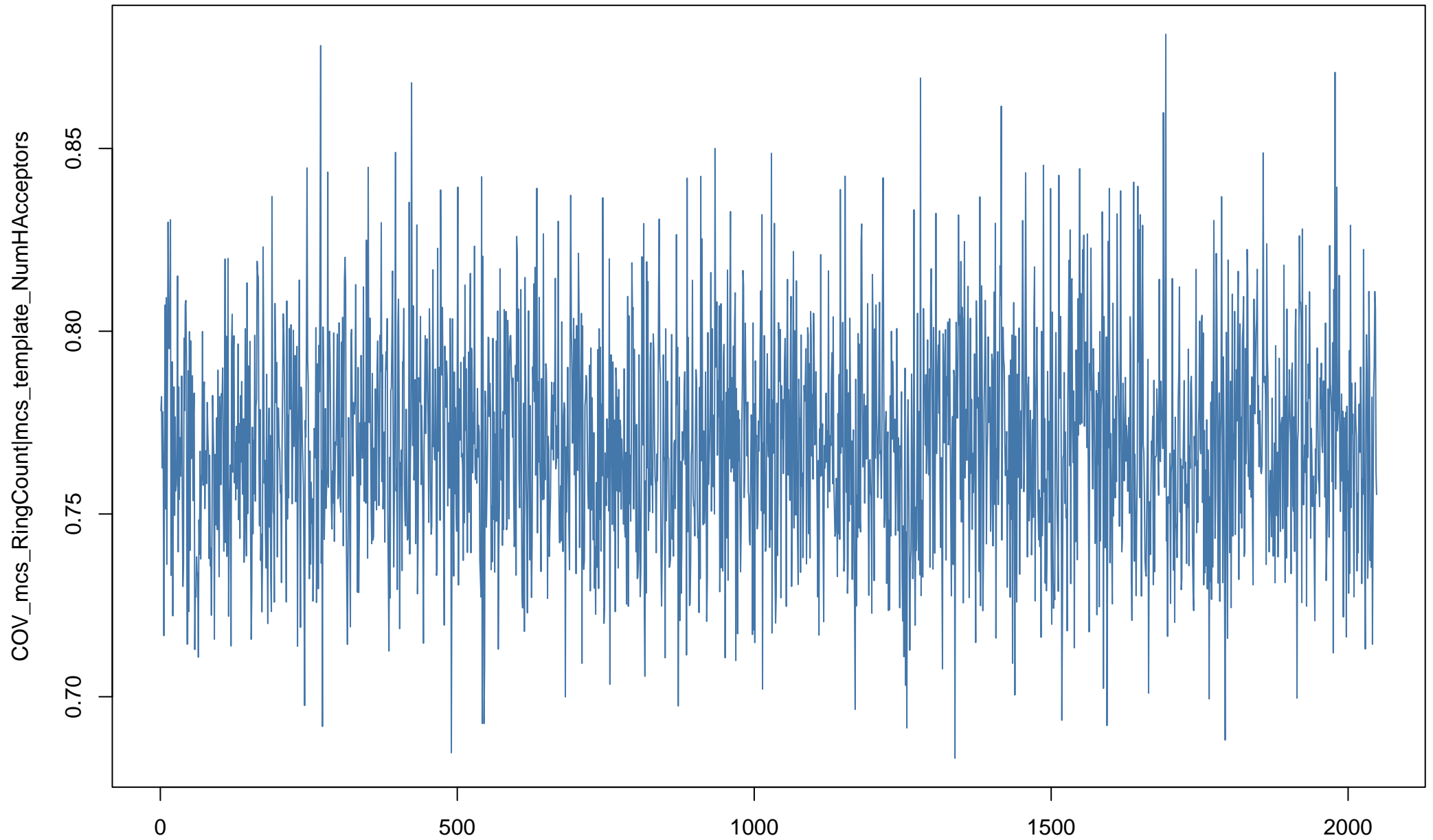
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1780 | BMK = 0.0435 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



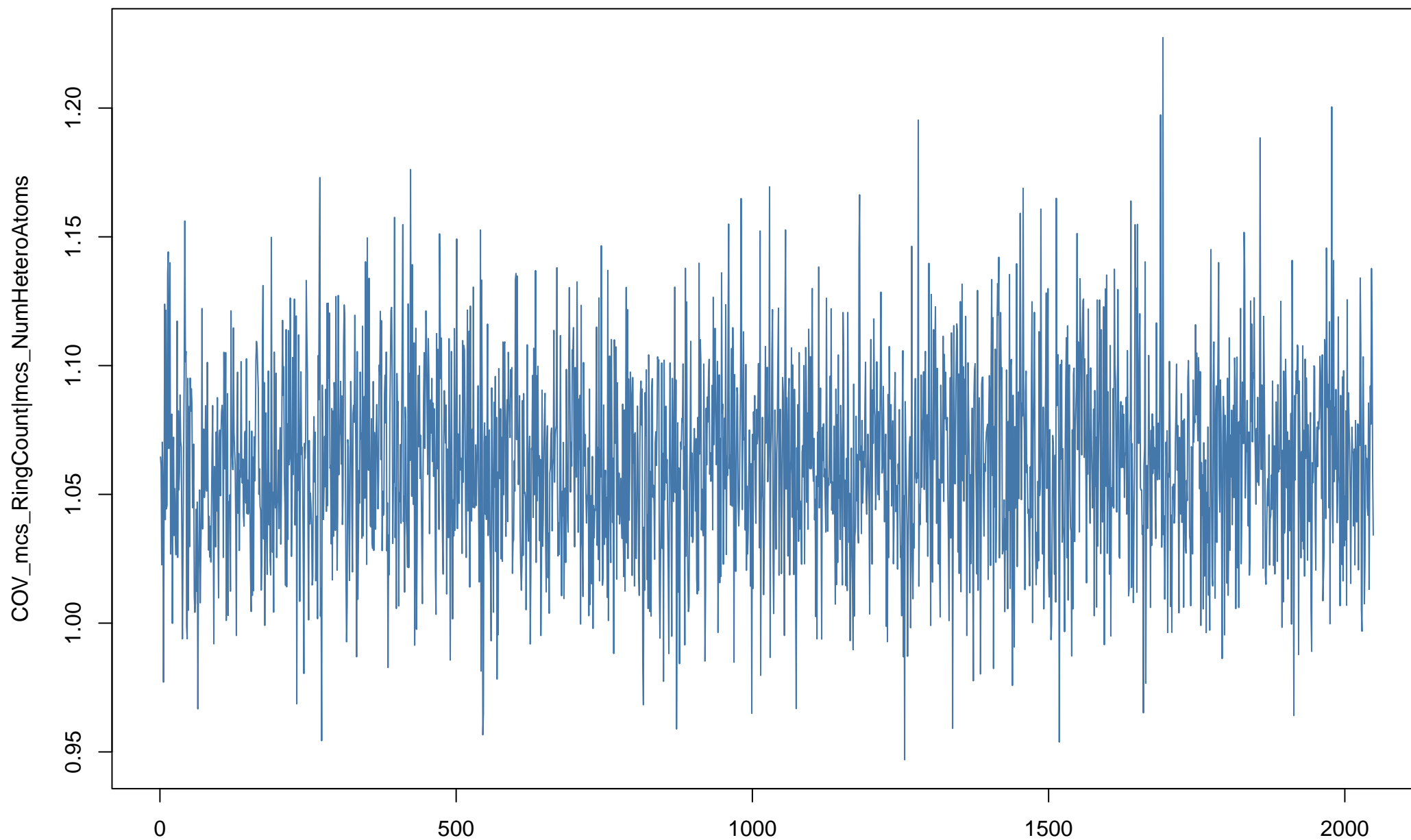
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2040 | BMK = 0.035 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0



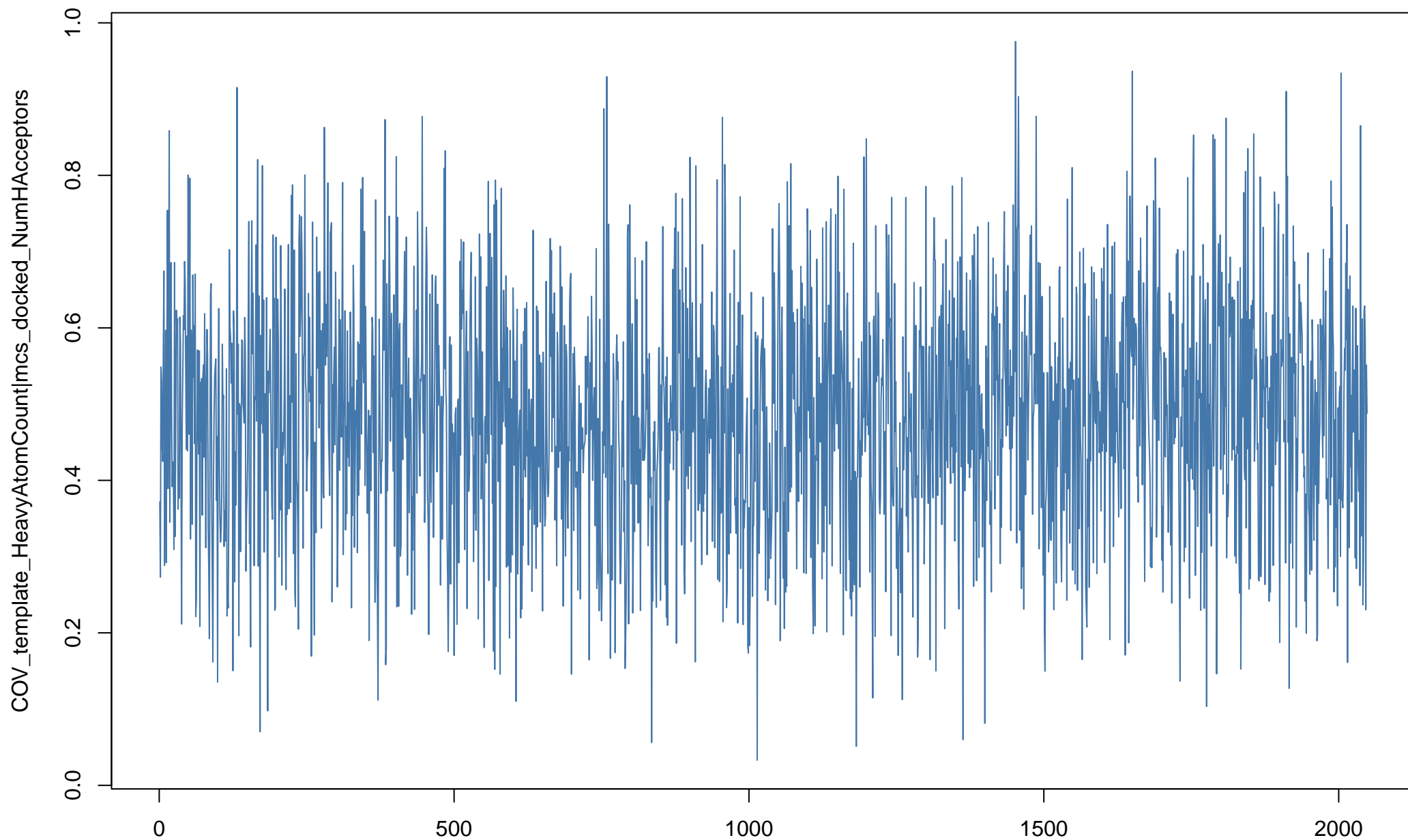
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0337 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0



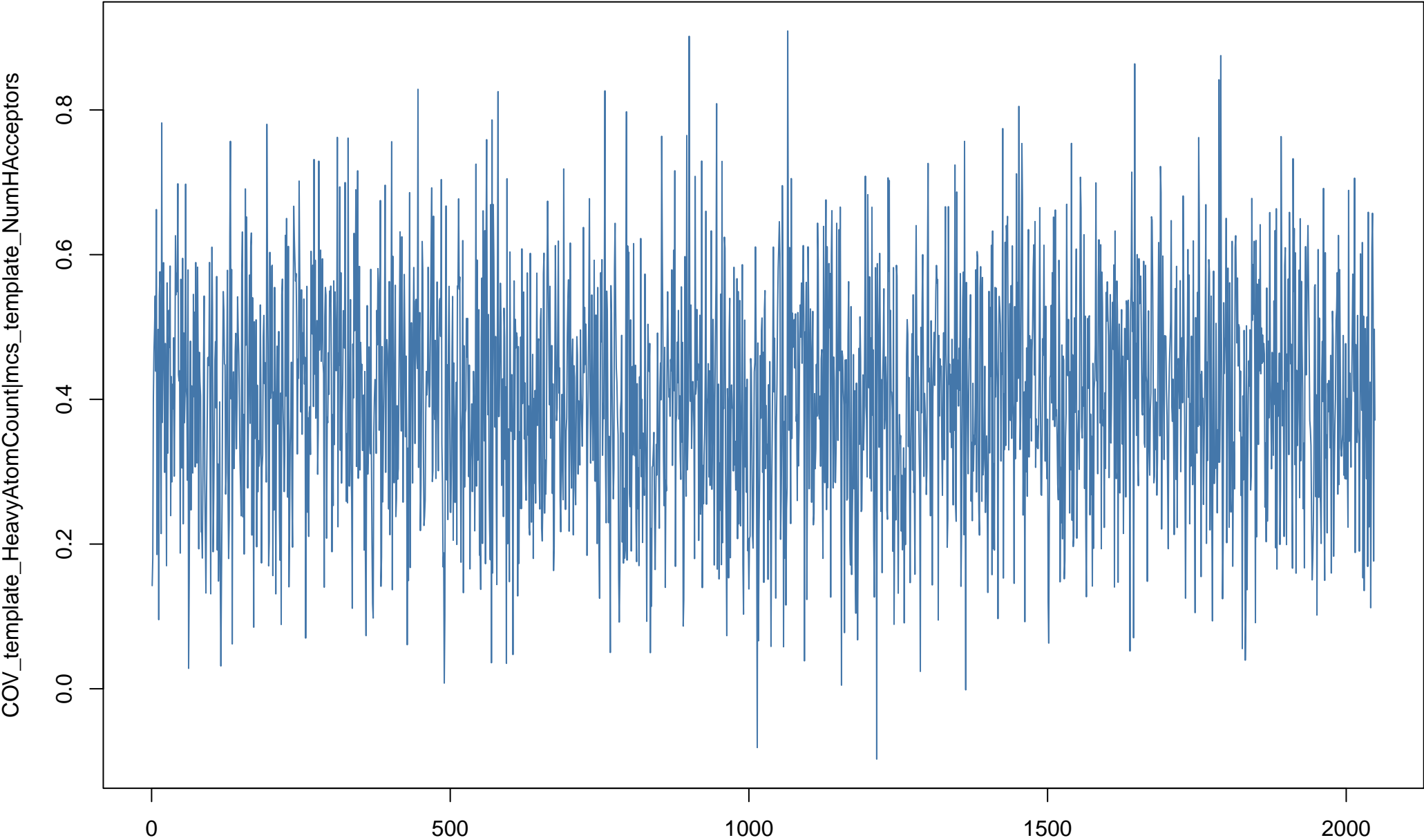
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0491 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0



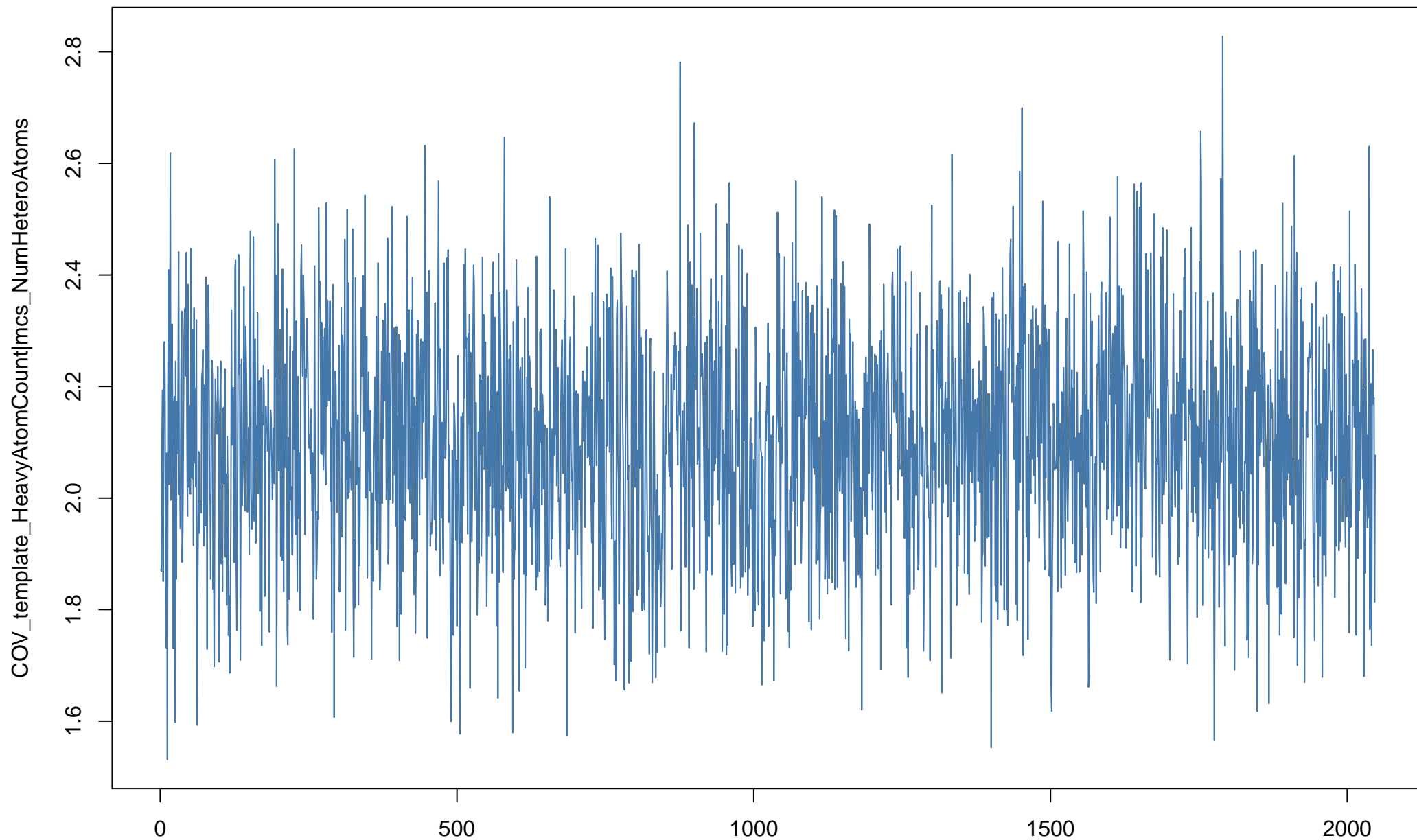
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1870 | BMK = 0.0358 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0



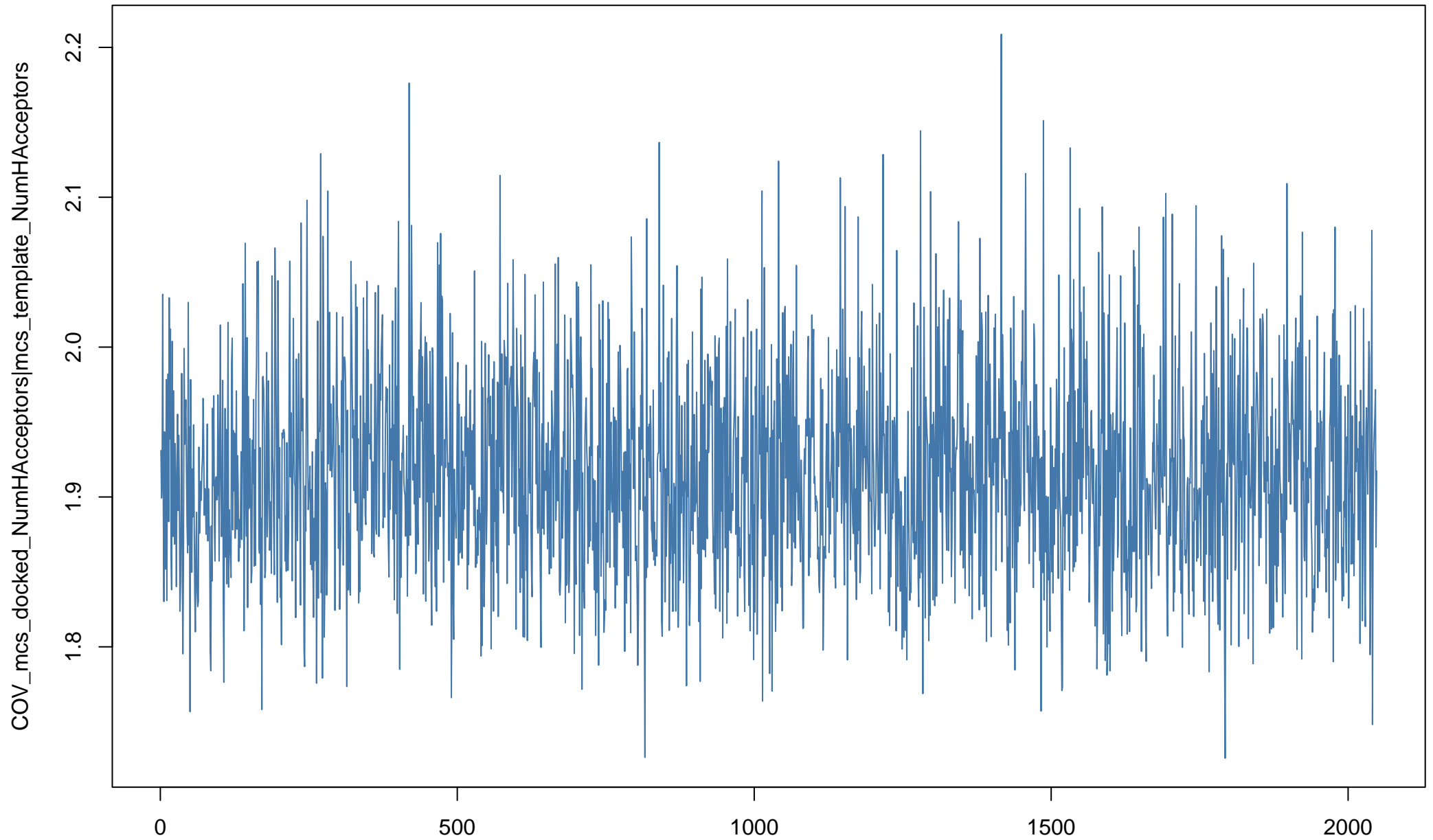
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1870 | BMK = 0.0465 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0



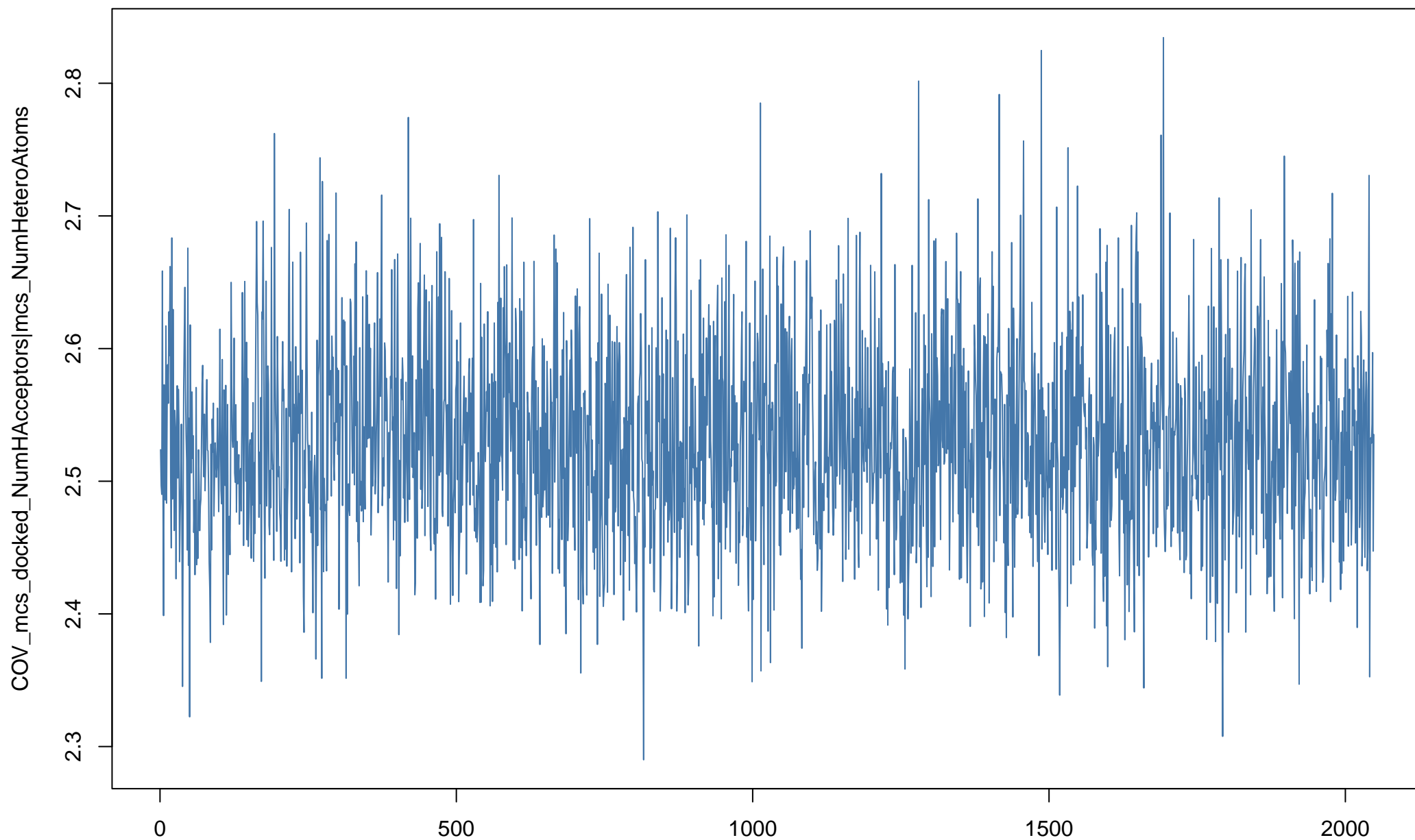
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1910 | BMK = 0.0434 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0474 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0334 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0457 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0

