

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.933692059984056

max MCSE = 14.8623072900775

all stationary: FALSE

burn: 2040

-- STATS 2D --

min ESS = 112.093116858043

max BMK = 0.228949251472777

max MCSE = 5.49258632368607

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.410327466052744

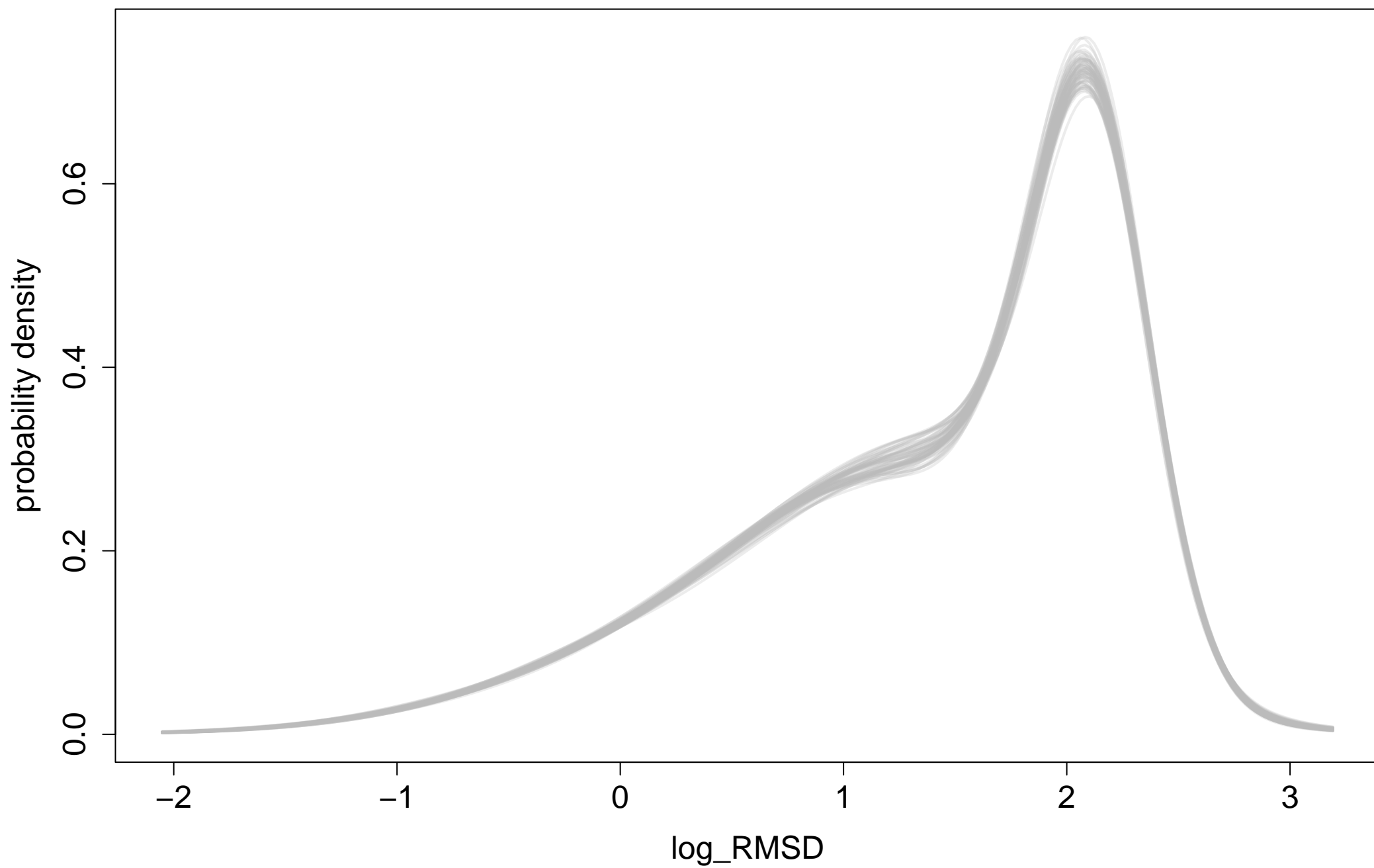
max MCSE = NaN

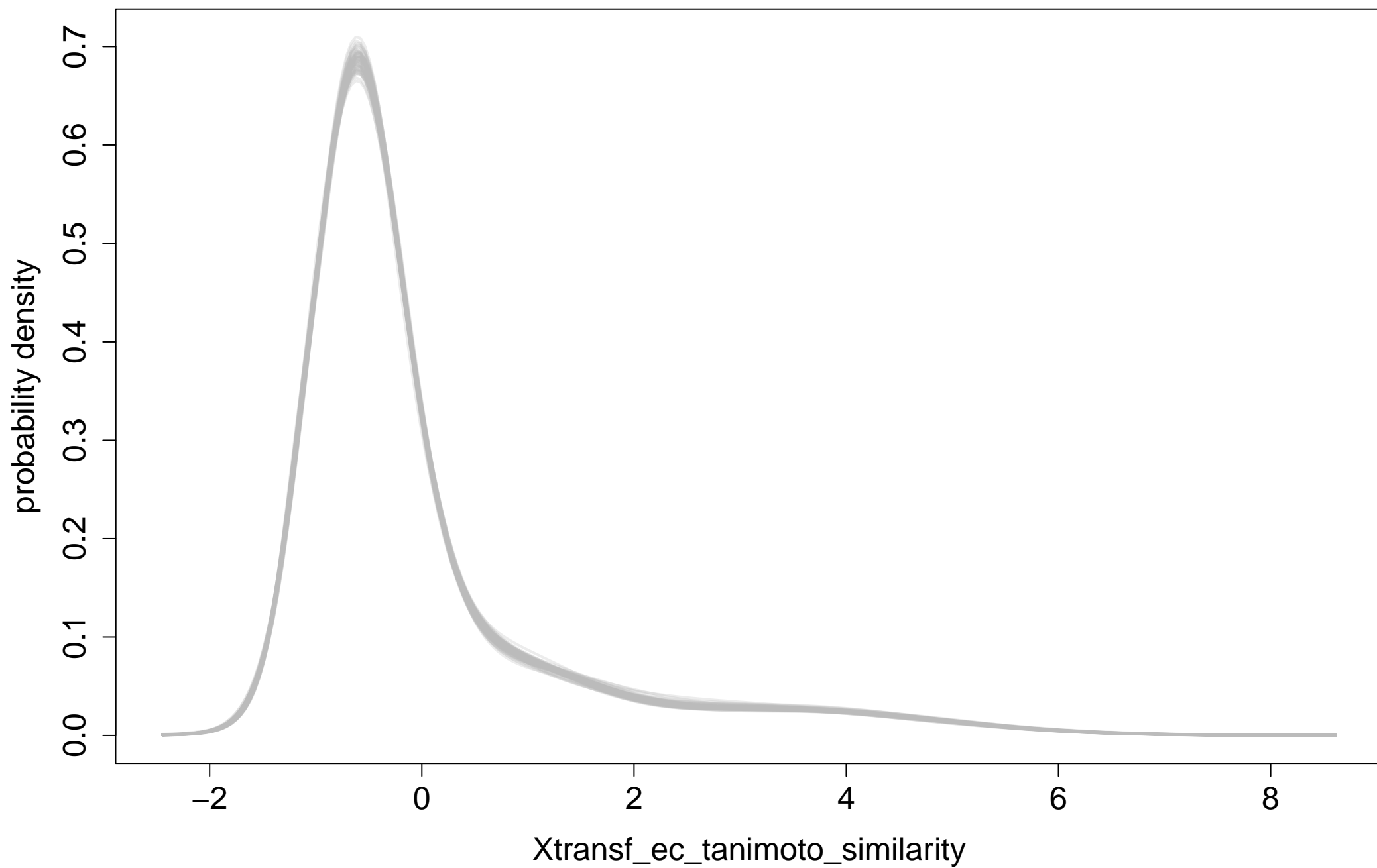
all stationary: FALSE

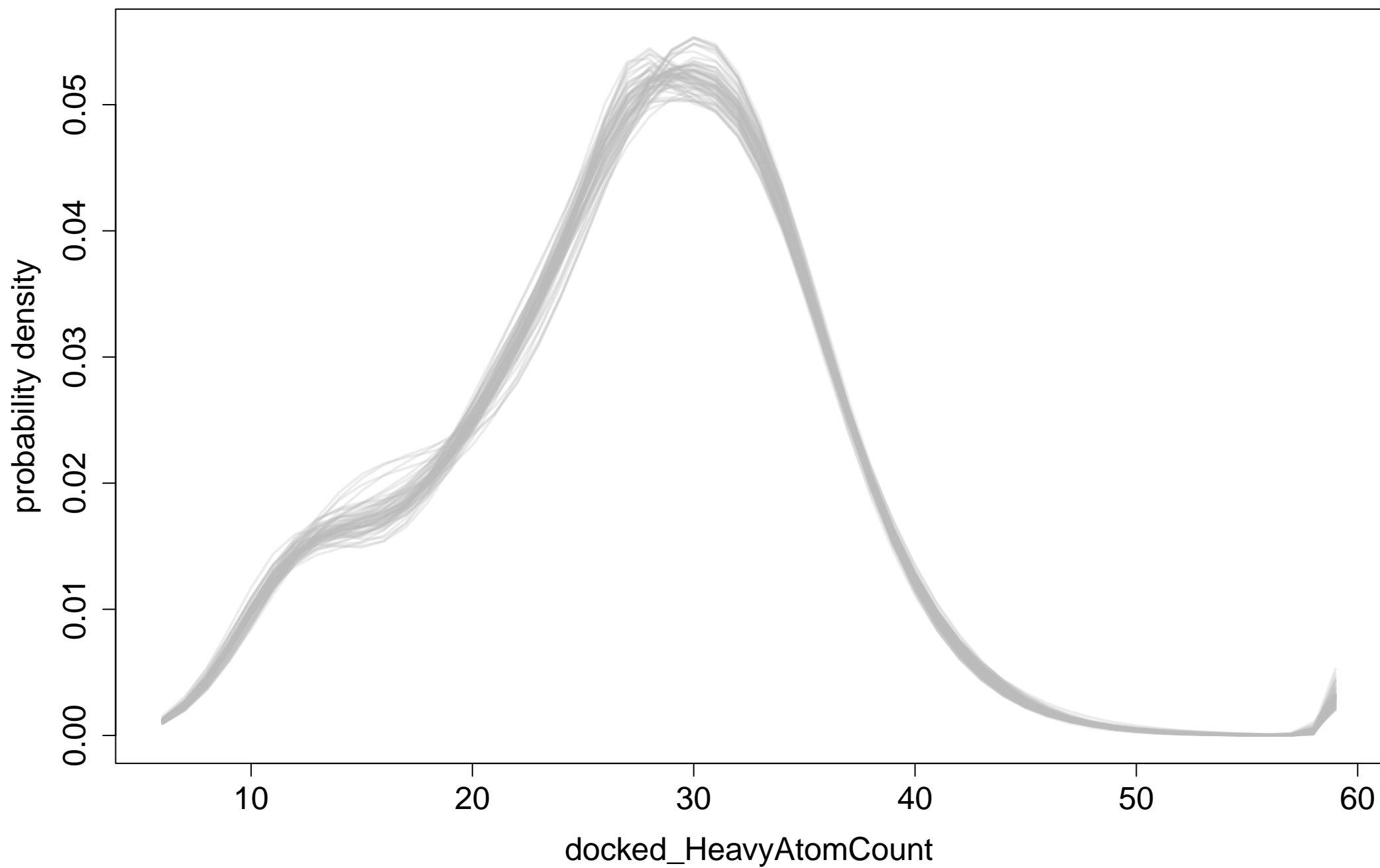
burn: 1428

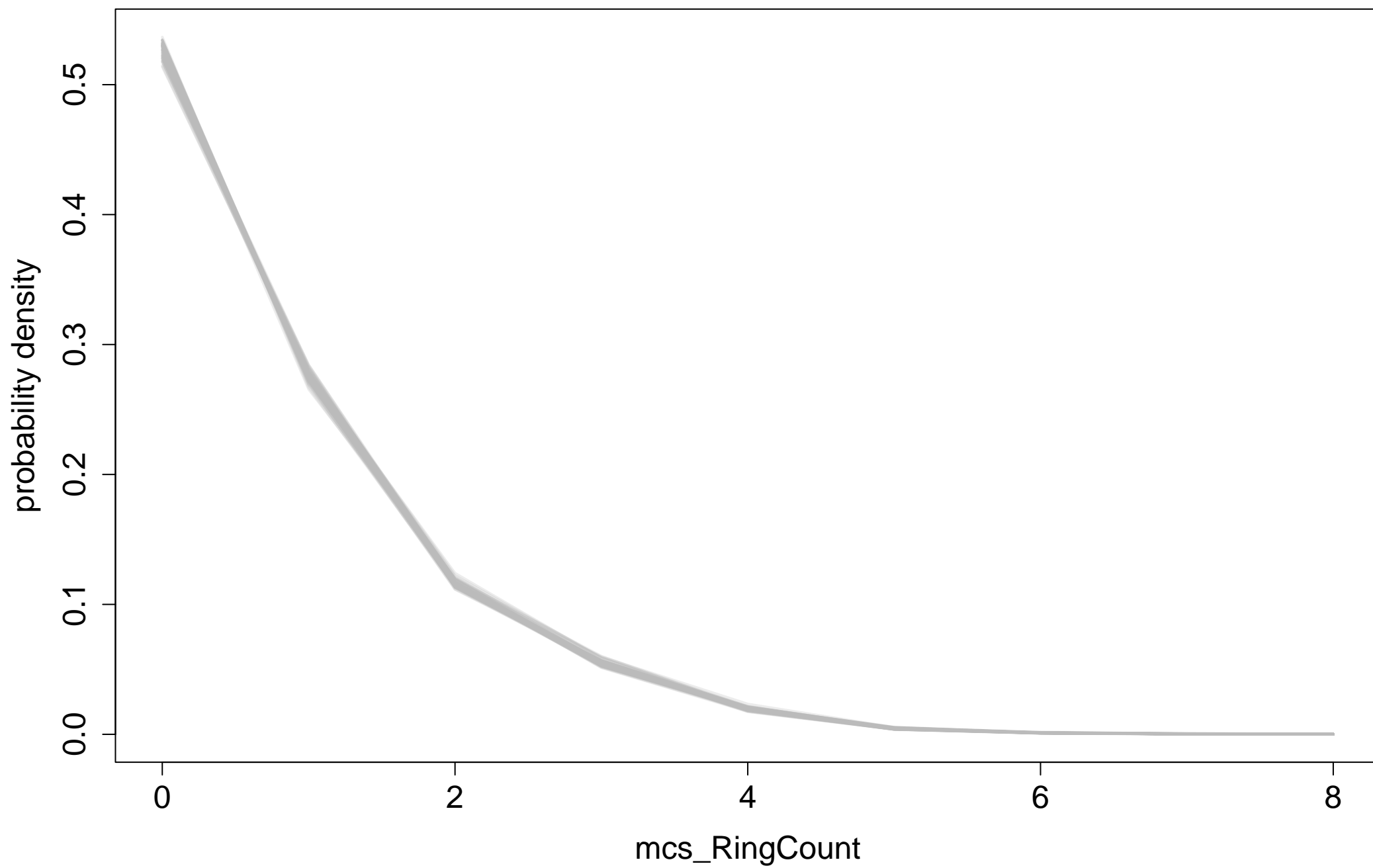
Occupied clusters: 39 of 91

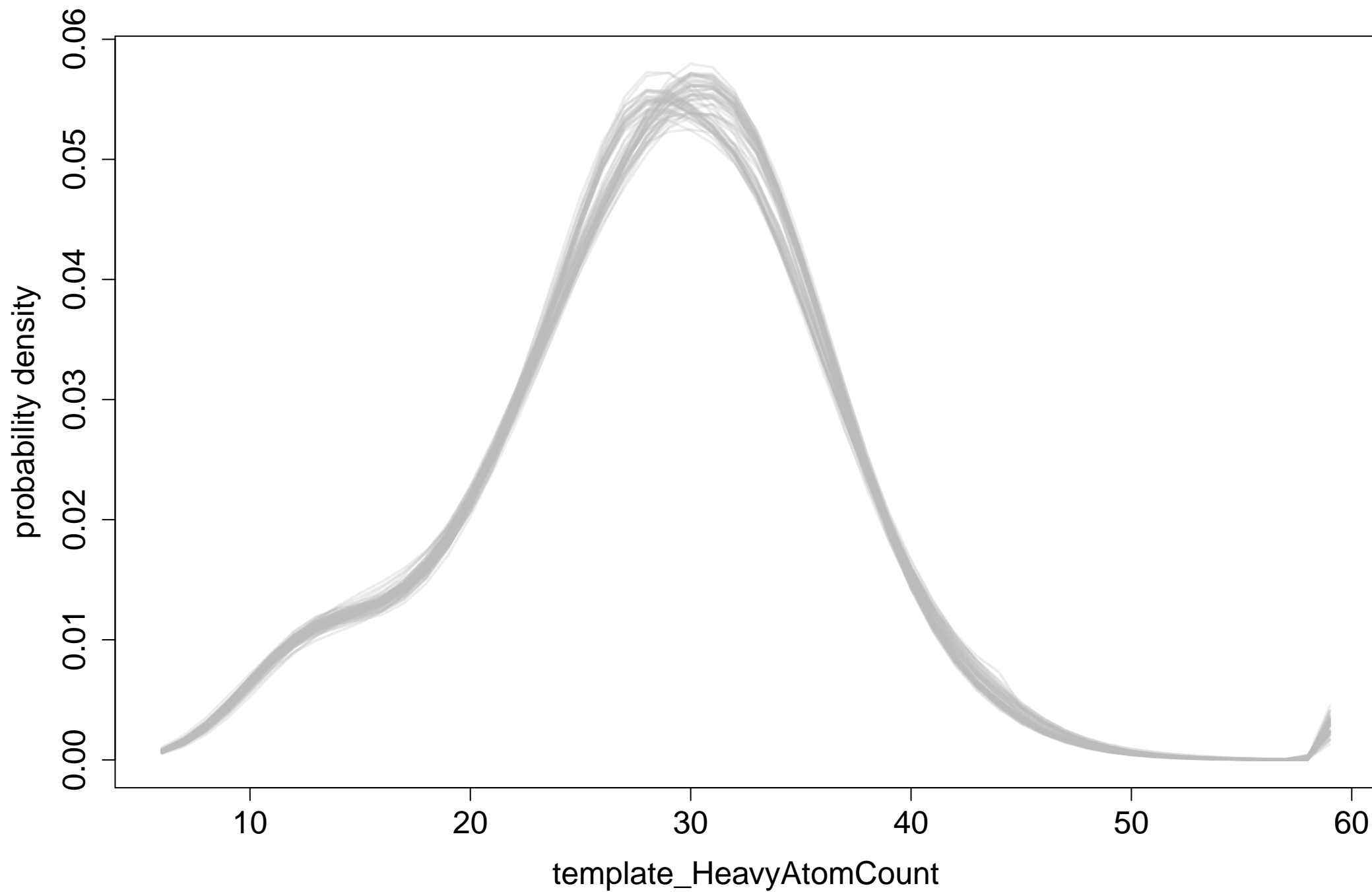
LL: -114000 +- 437

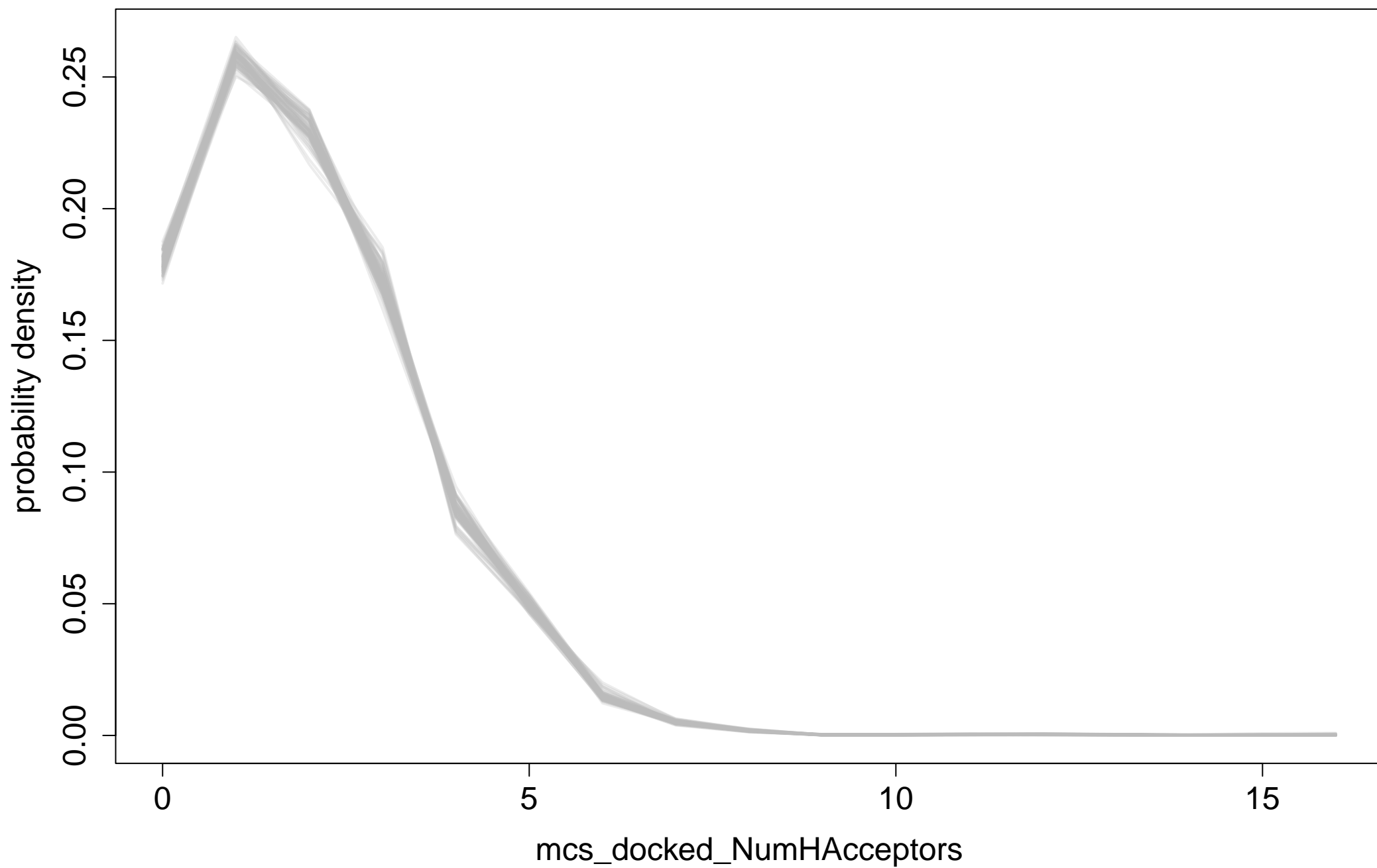


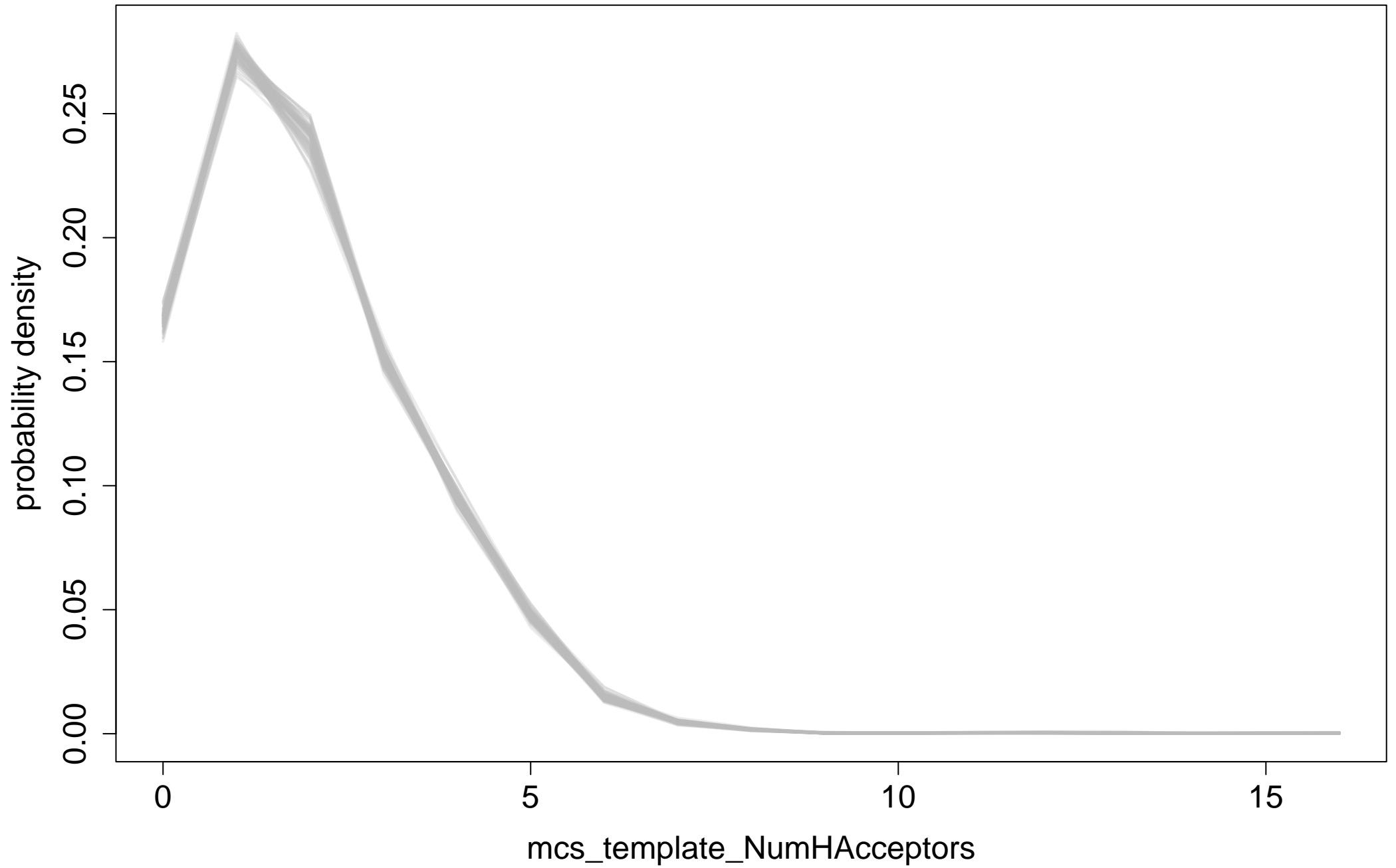


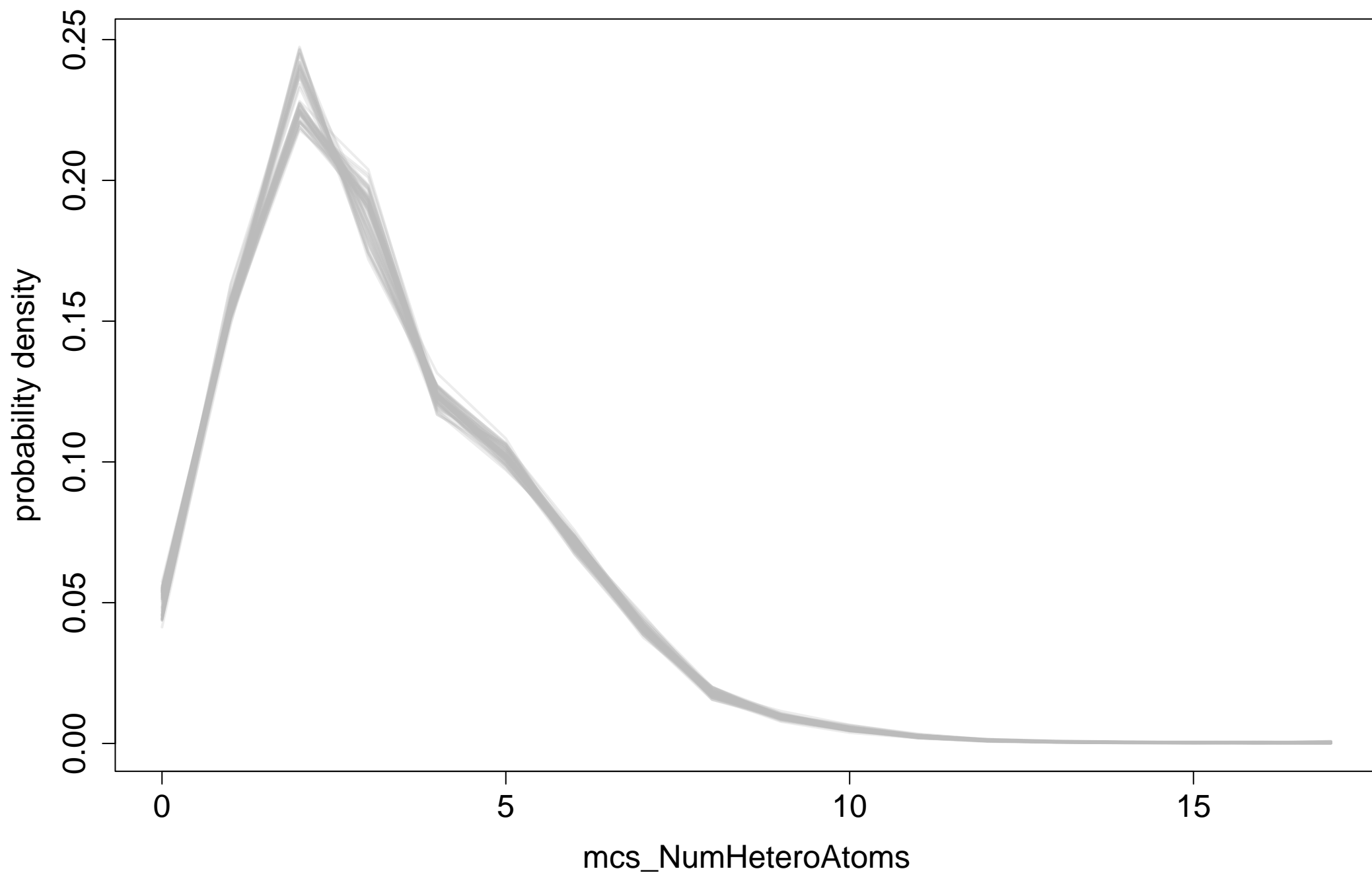


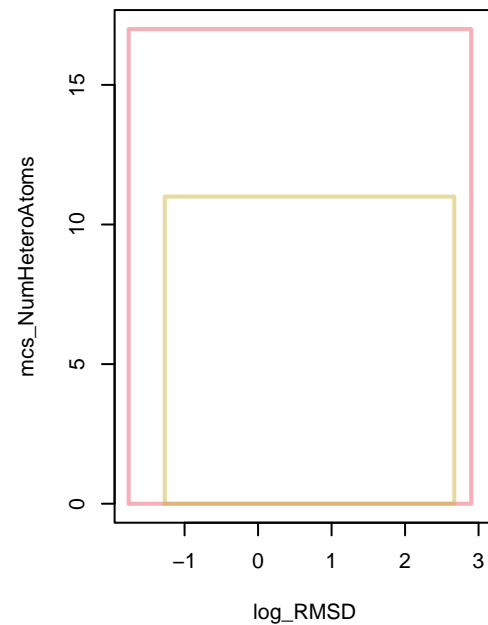
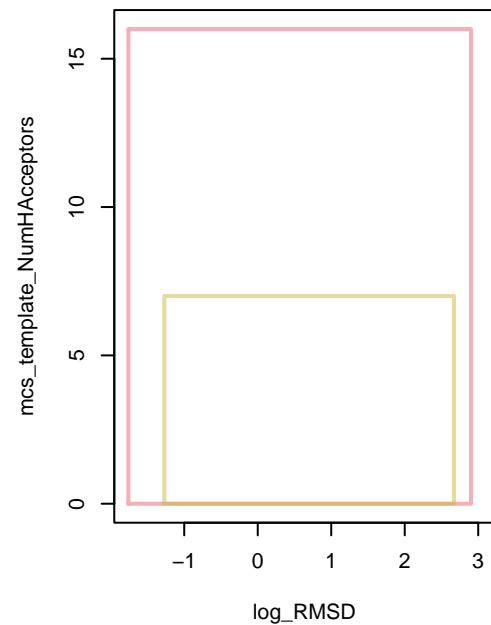
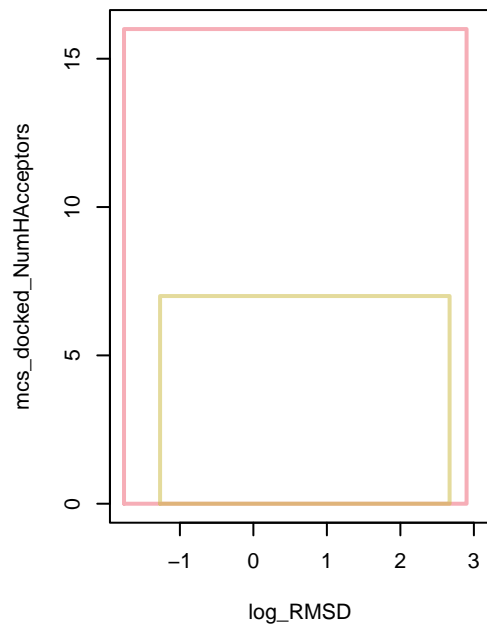
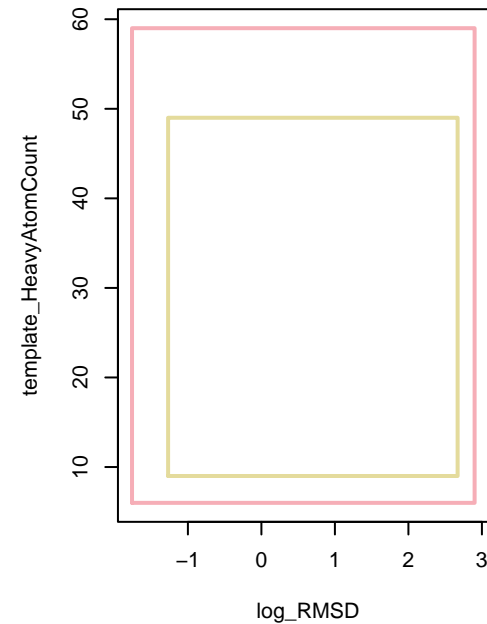
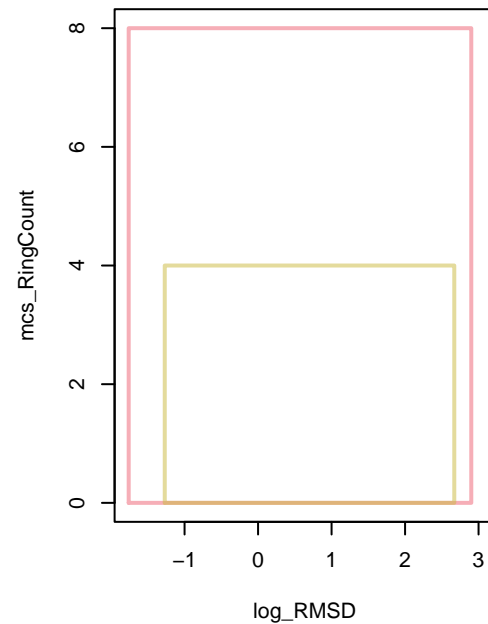
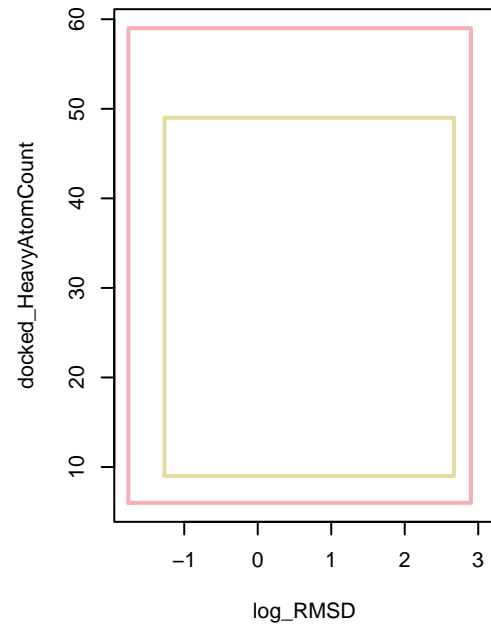
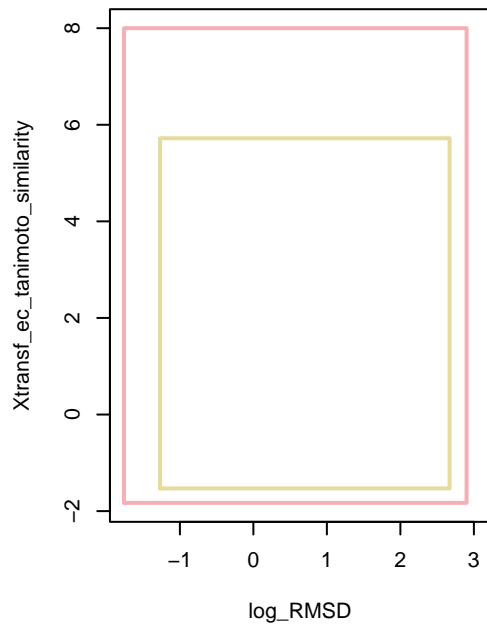




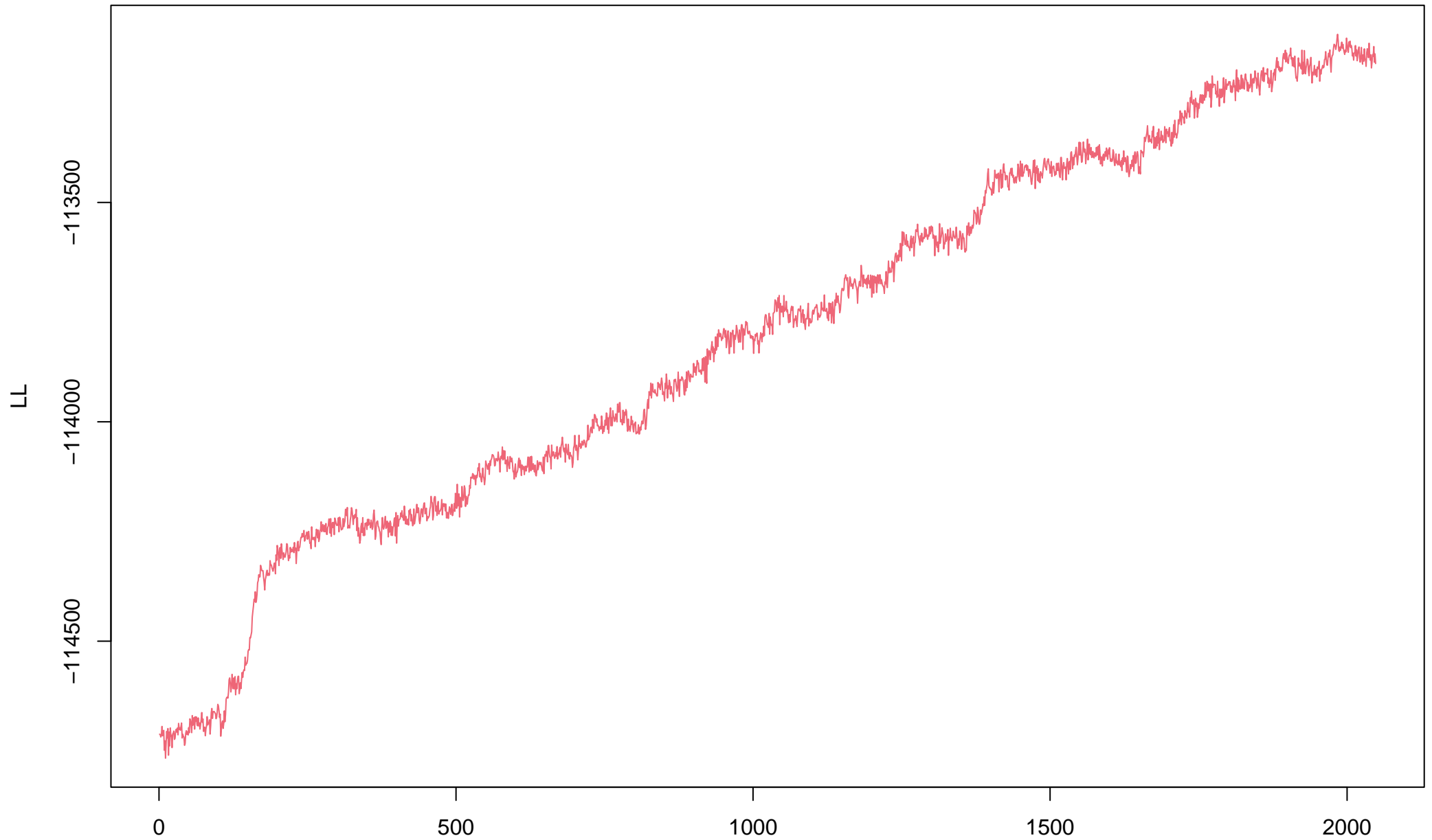




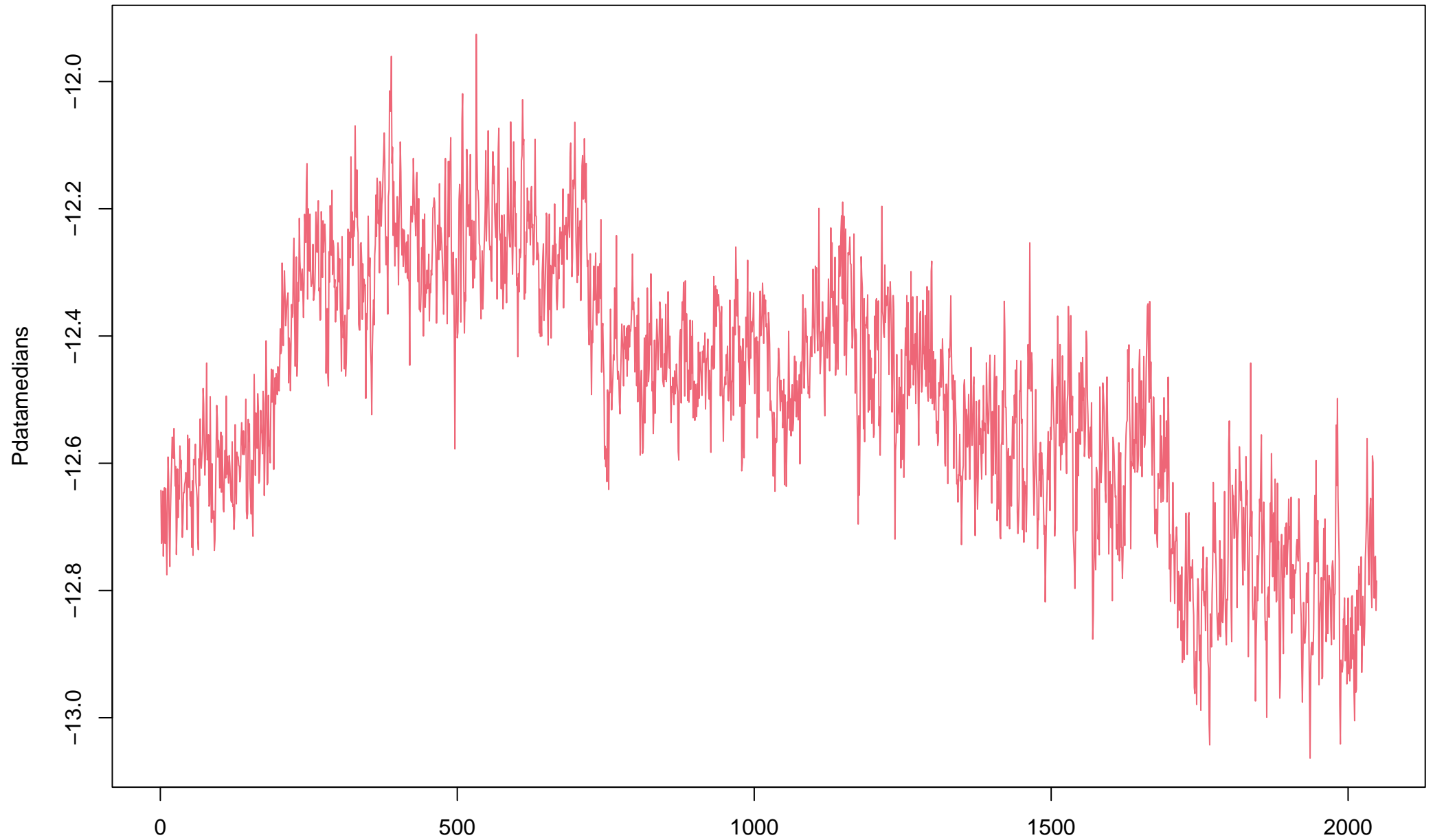




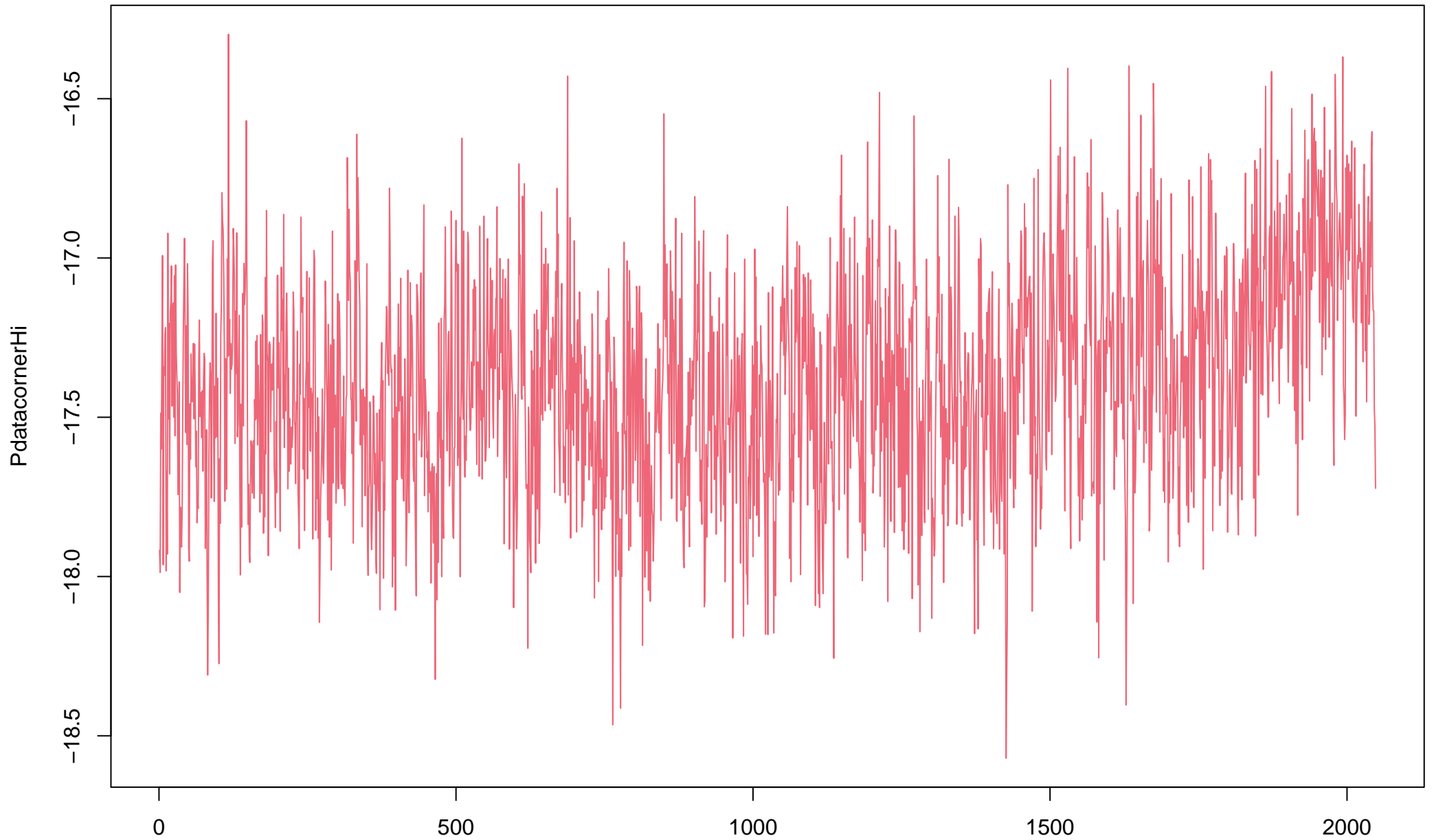
LL
ESS = 1.88 | BMK = 0.934 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 2040



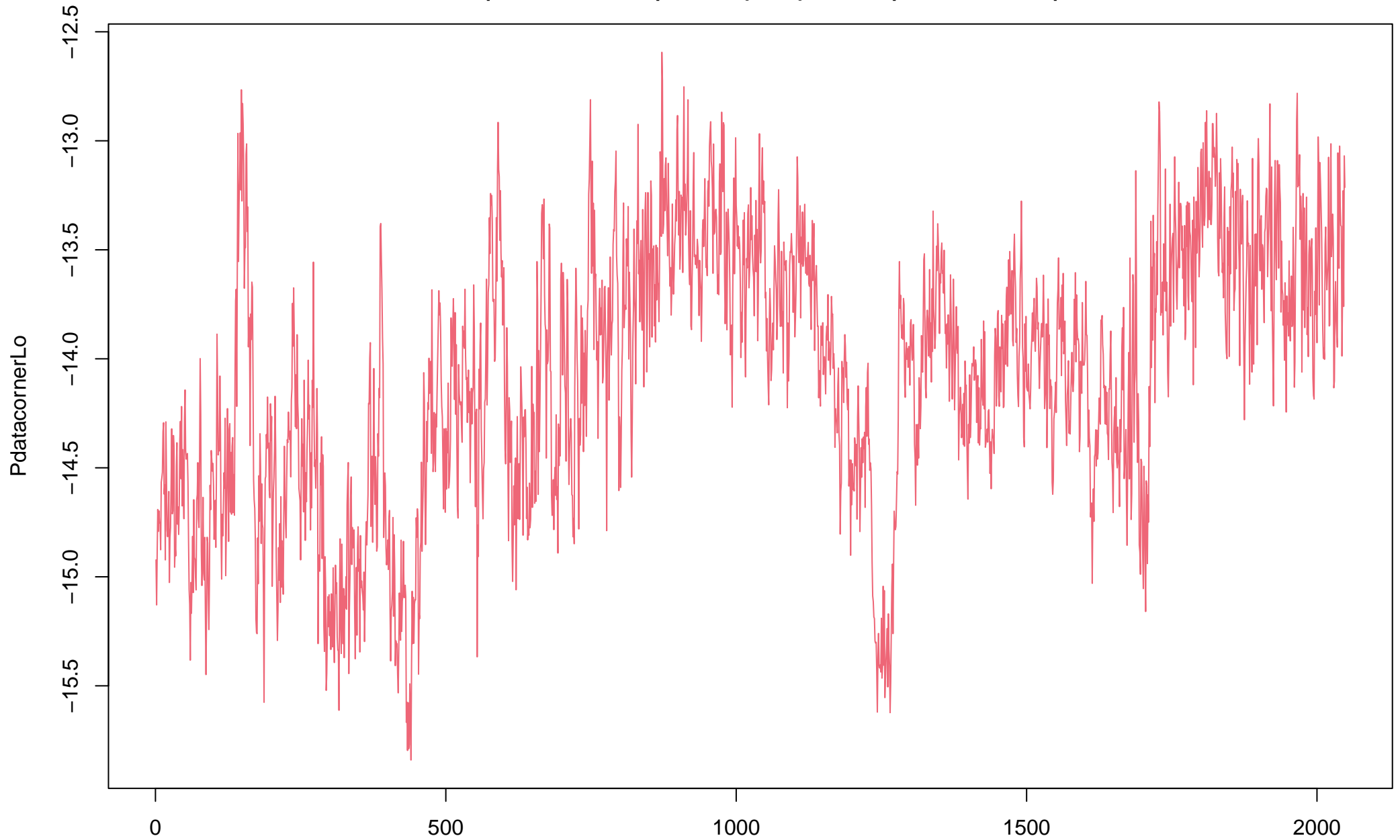
Pdatamedians
ESS = 4.81 | BMK = 0.473 | MCSE(6.27) = 13.5 | stat: TRUE | burn: 204



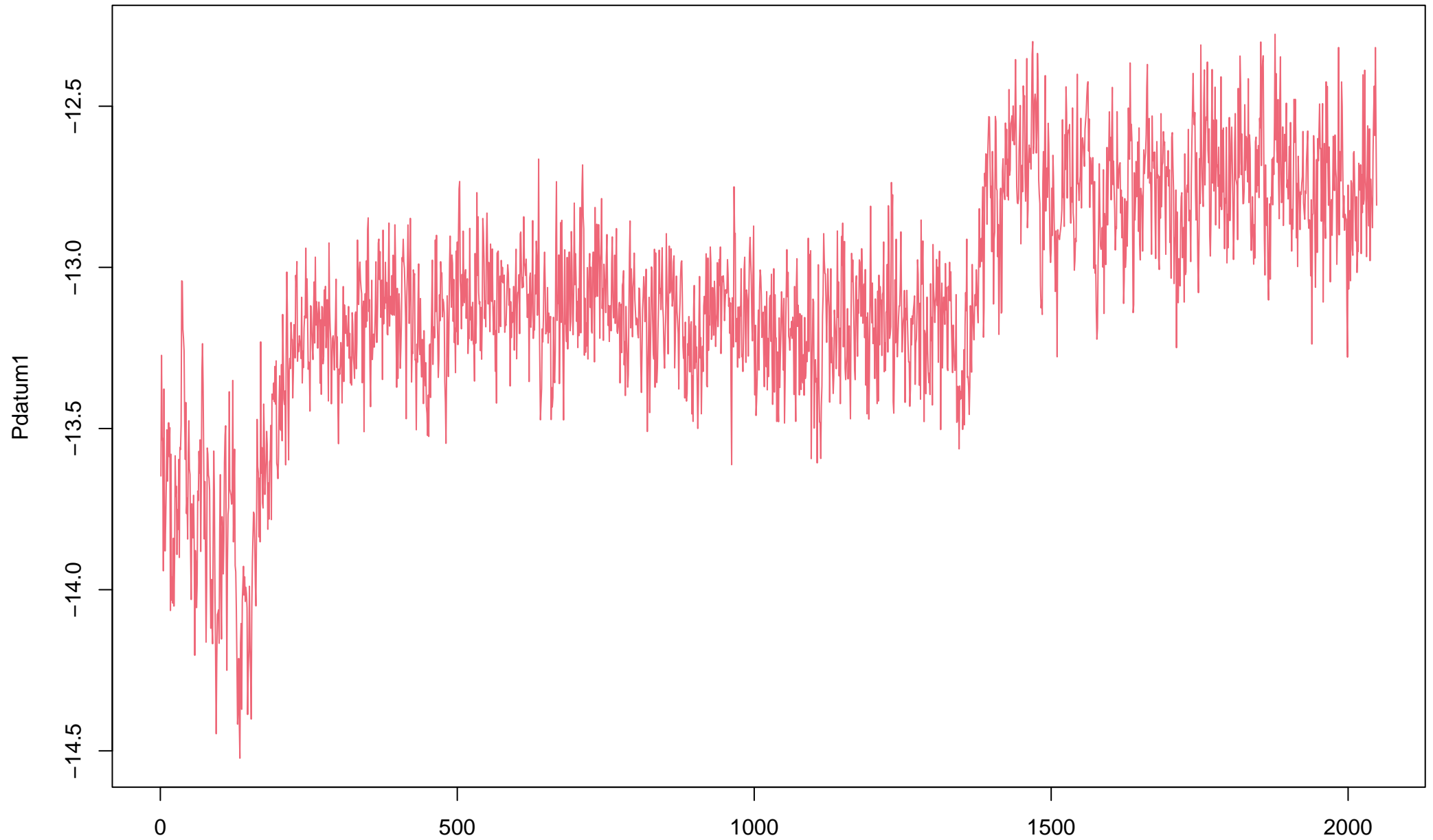
PdatacornerHi
ESS = 2.22e-16 | BMK = 0.189 | MCSE(6.27) = 6.72 | stat: FALSE | burn: 0



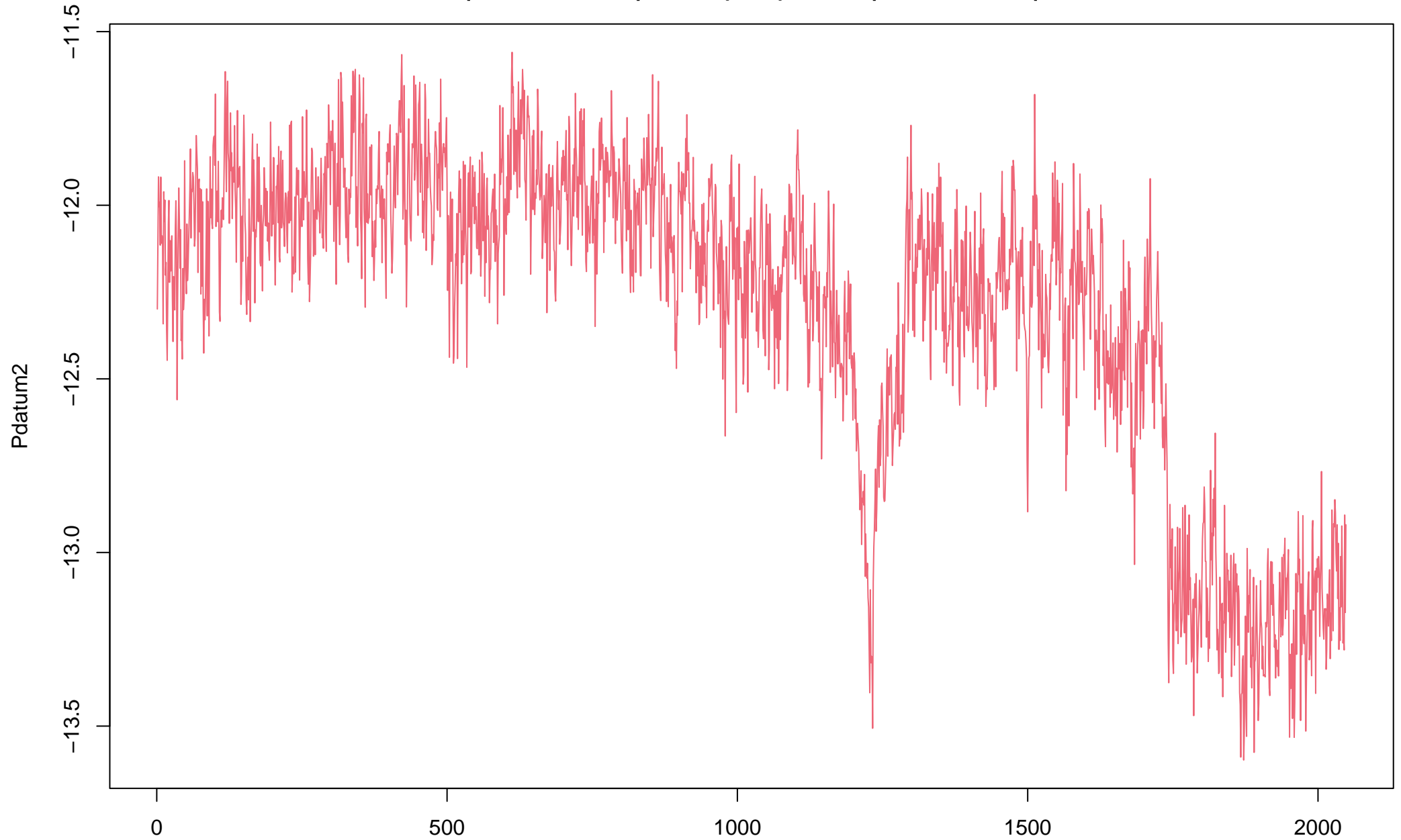
PdatacornerLo
ESS = 16.3 | BMK = 0.229 | MCSE(6.27) = 11.4 | stat: FALSE | burn: 0



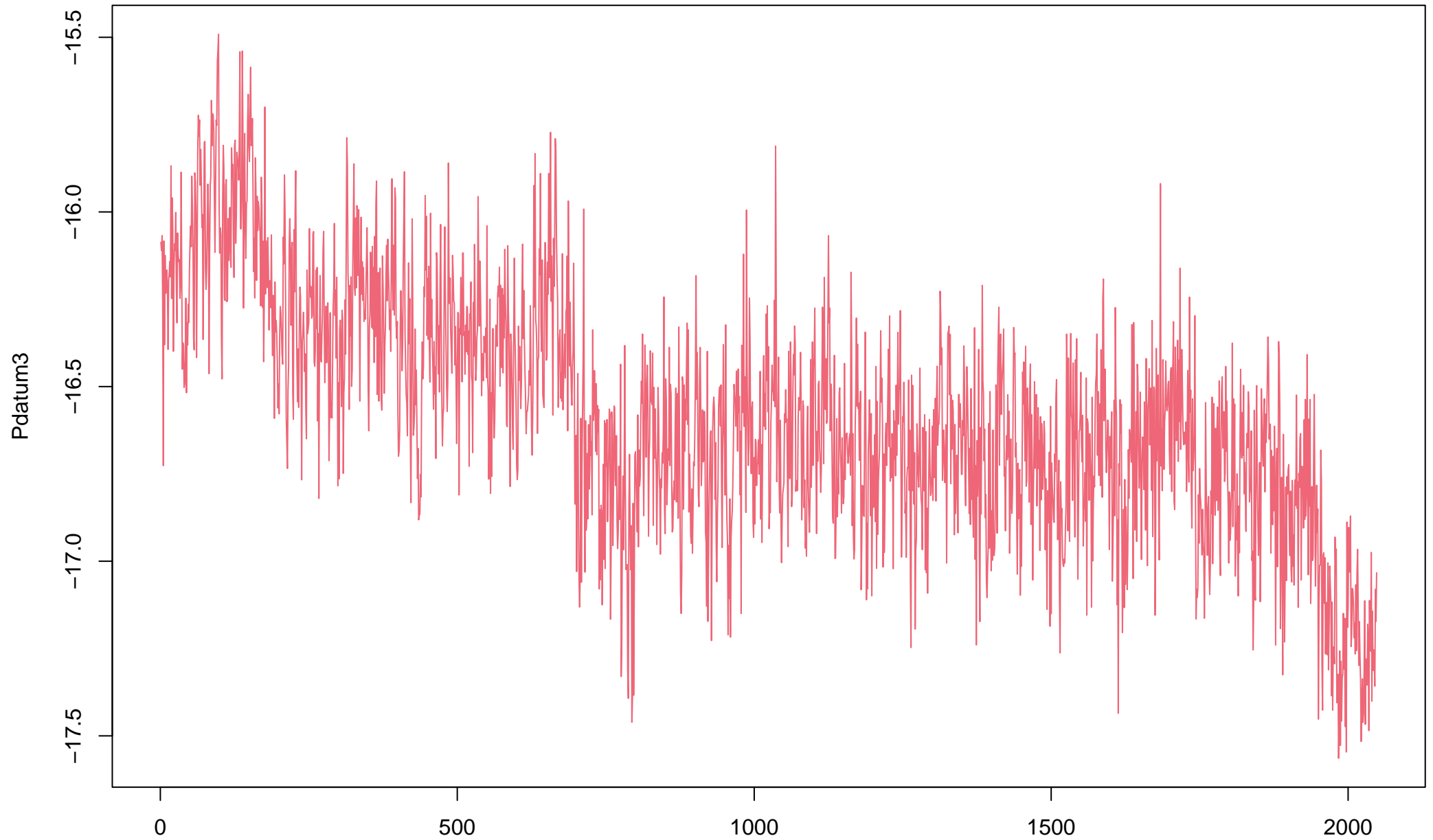
Pdatum1
ESS = 5.01 | BMK = 0.514 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 1428



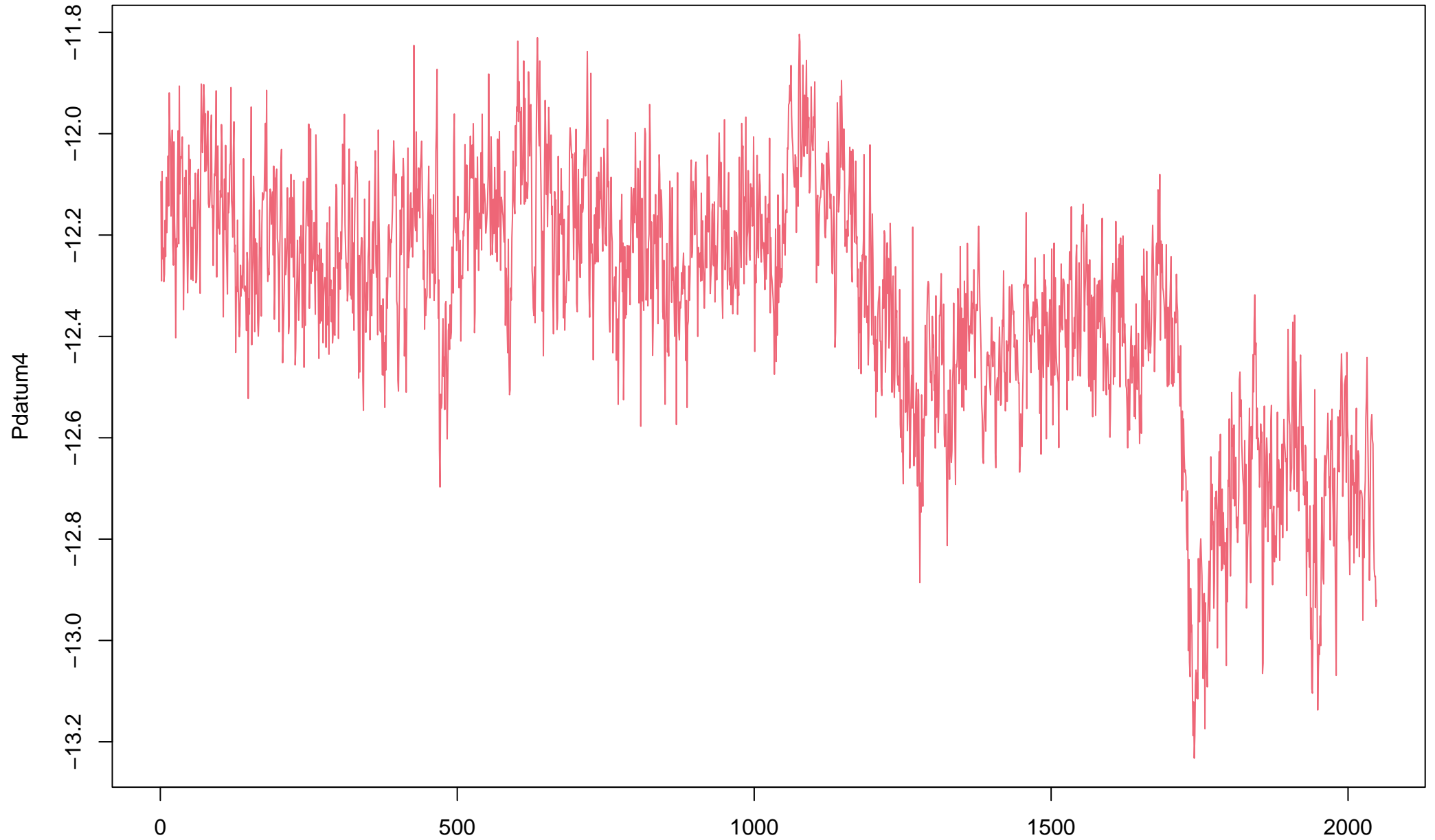
Pdatum2
ESS = 8.06 | BMK = 0.605 | MCSE(6.27) = 13.1 | stat: FALSE | burn: 2040



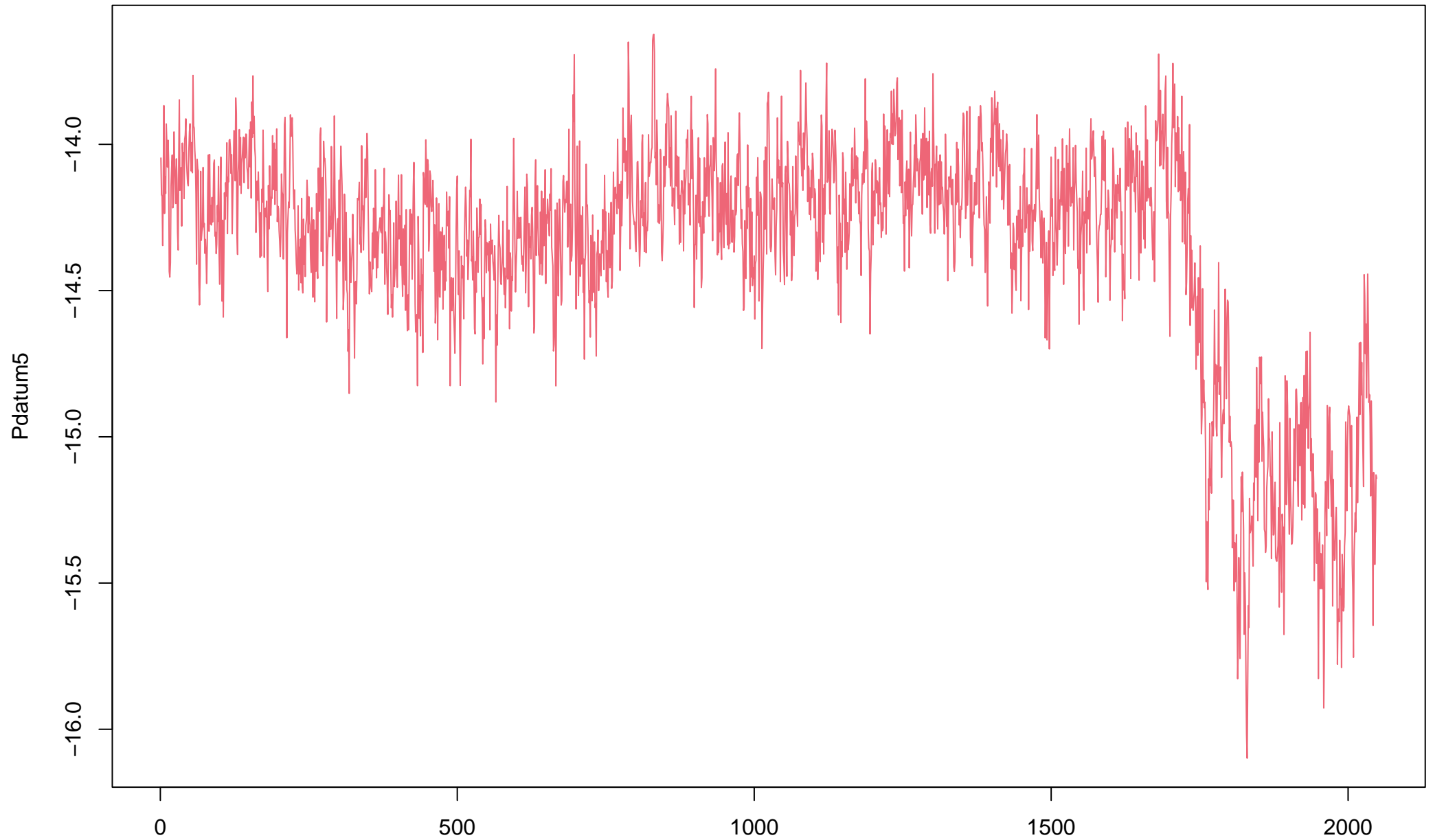
Pdatum3
ESS = 14.3 | BMK = 0.433 | MCSE(6.27) = 11.8 | stat: FALSE | burn: 0



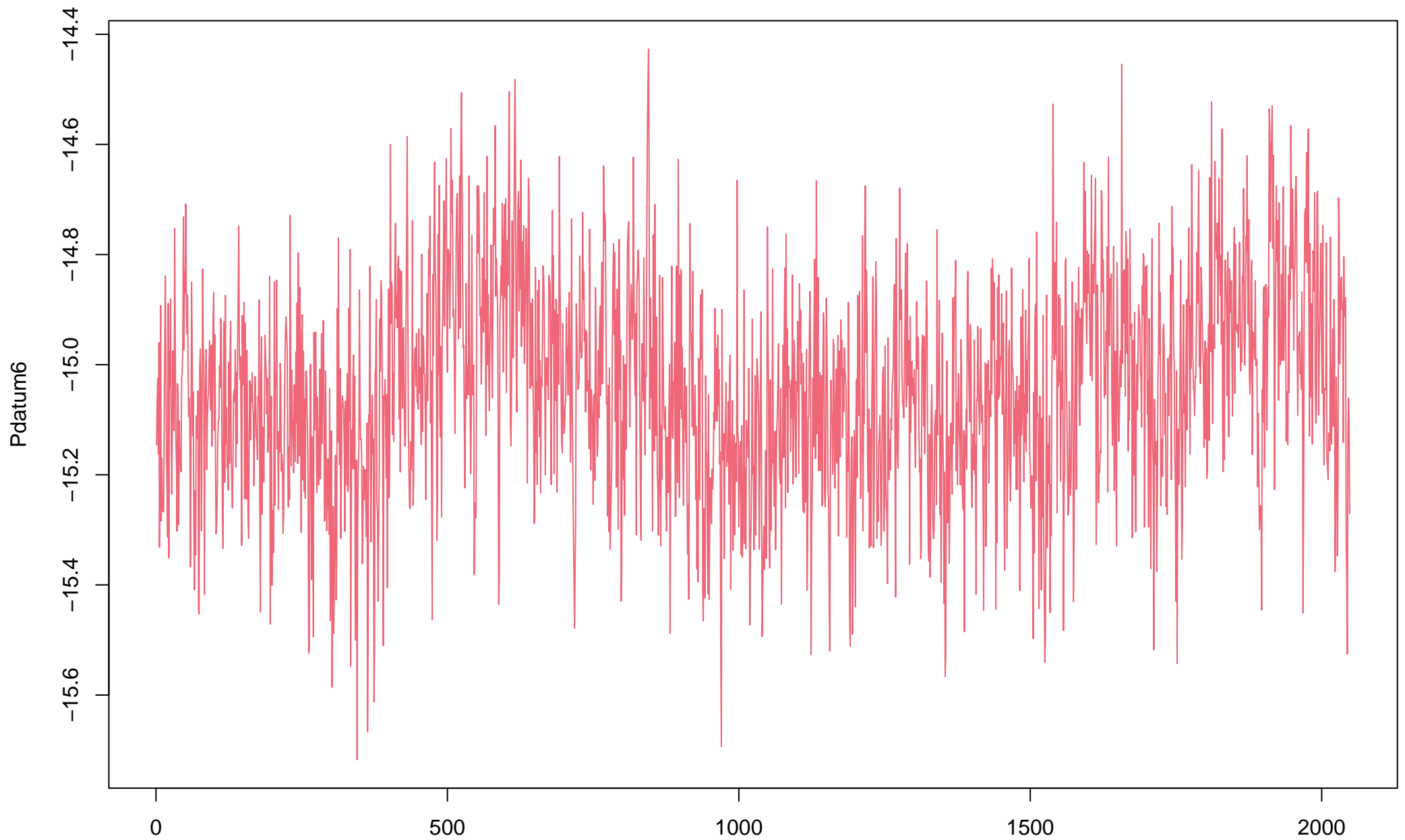
Pdatum4
ESS = 15.5 | BMK = 0.492 | MCSE(6.27) = 12.2 | stat: FALSE | burn: 1224



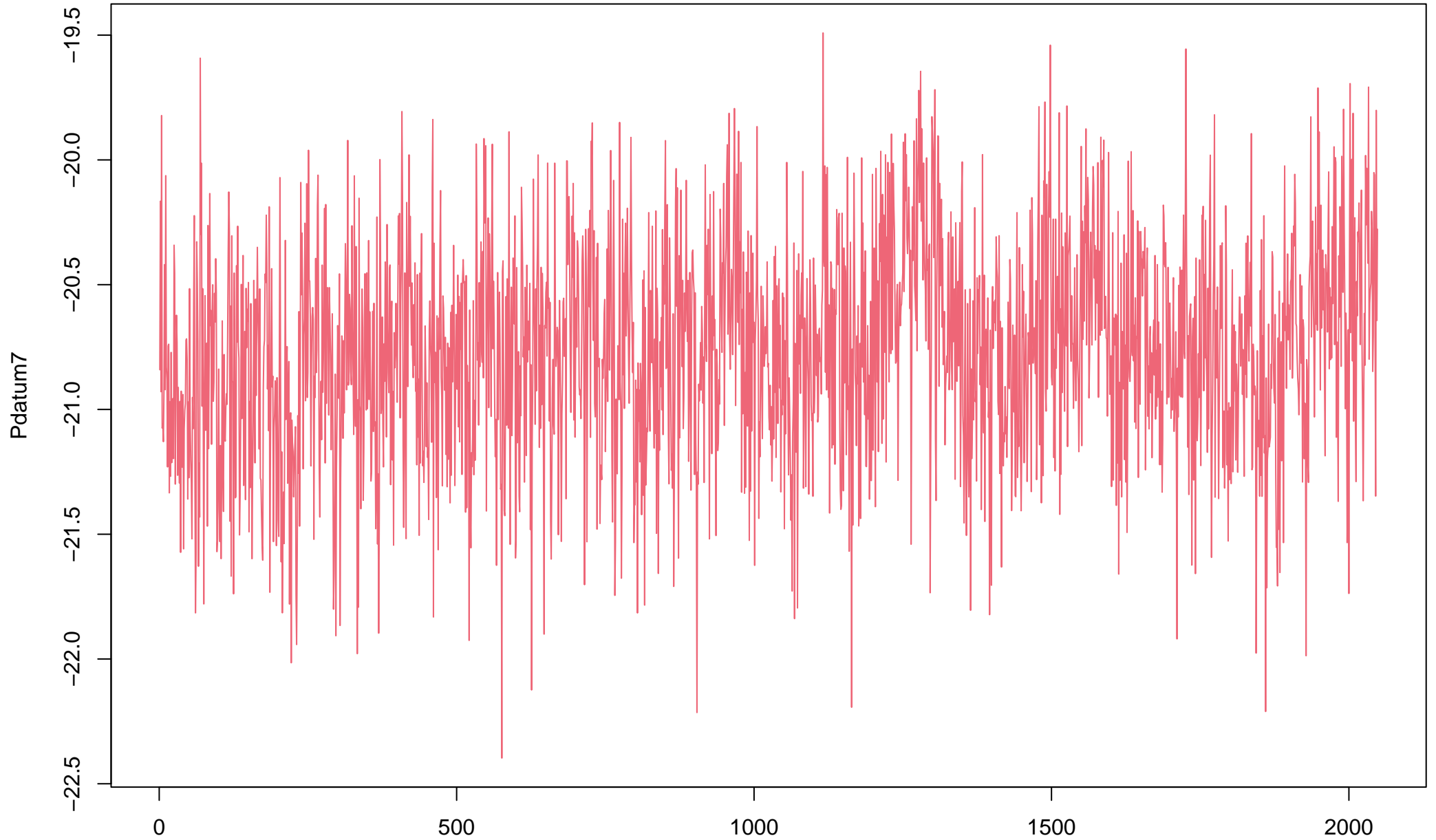
Pdatum5
ESS = 11.8 | BMK = 0.364 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 2040



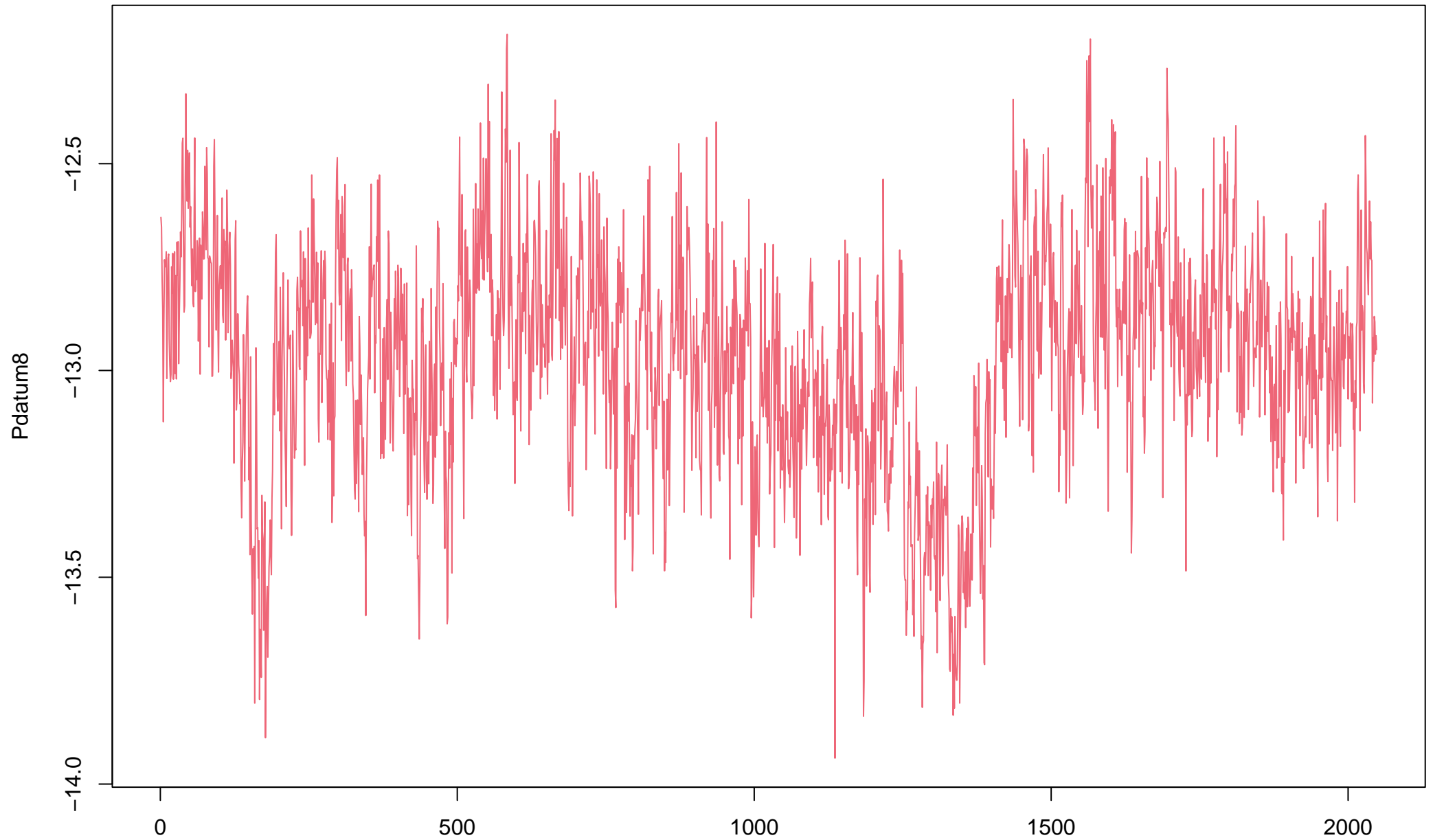
Pdatum6
ESS = 134 | BMK = 0.0412 | MCSE(6.27) = 7.15 | stat: FALSE | burn: 0



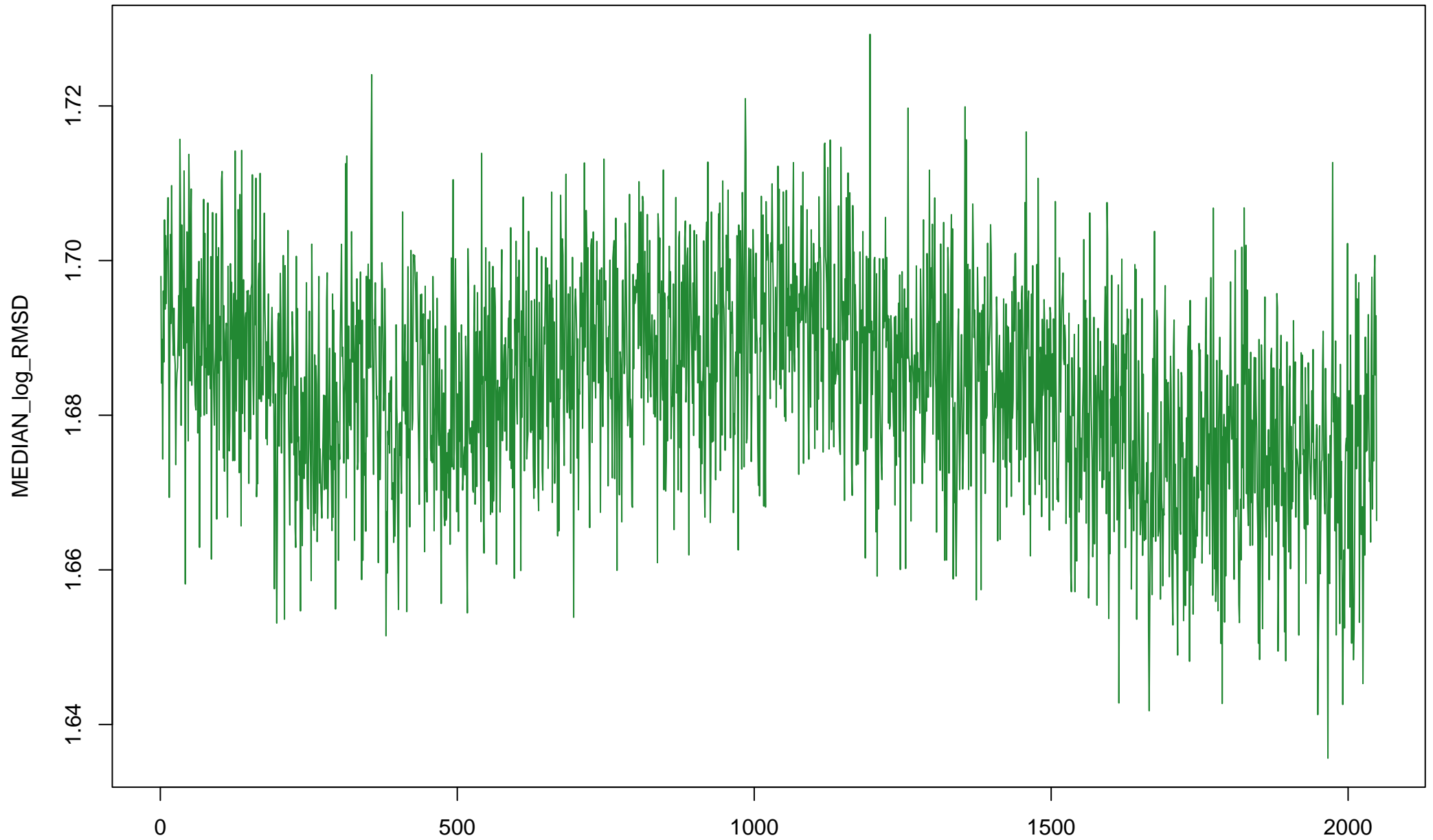
Pdatum7
ESS = 2.22e-16 | BMK = 0.103 | MCSE(6.27) = 5.28 | stat: TRUE | burn: 0



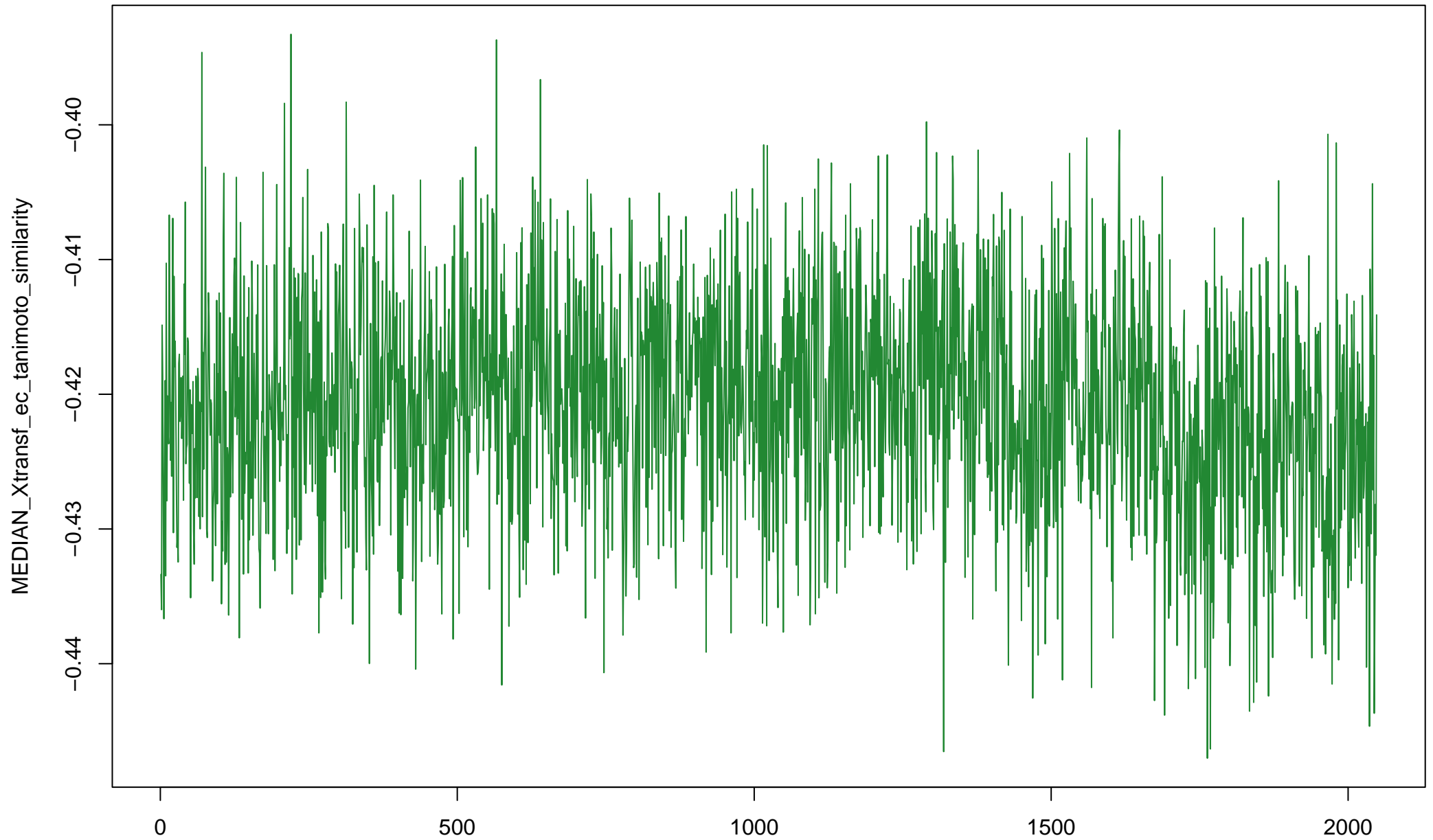
Pdatum8
ESS = 68.7 | BMK = 0.0876 | MCSE(6.27) = 9.37 | stat: TRUE | burn: 1428



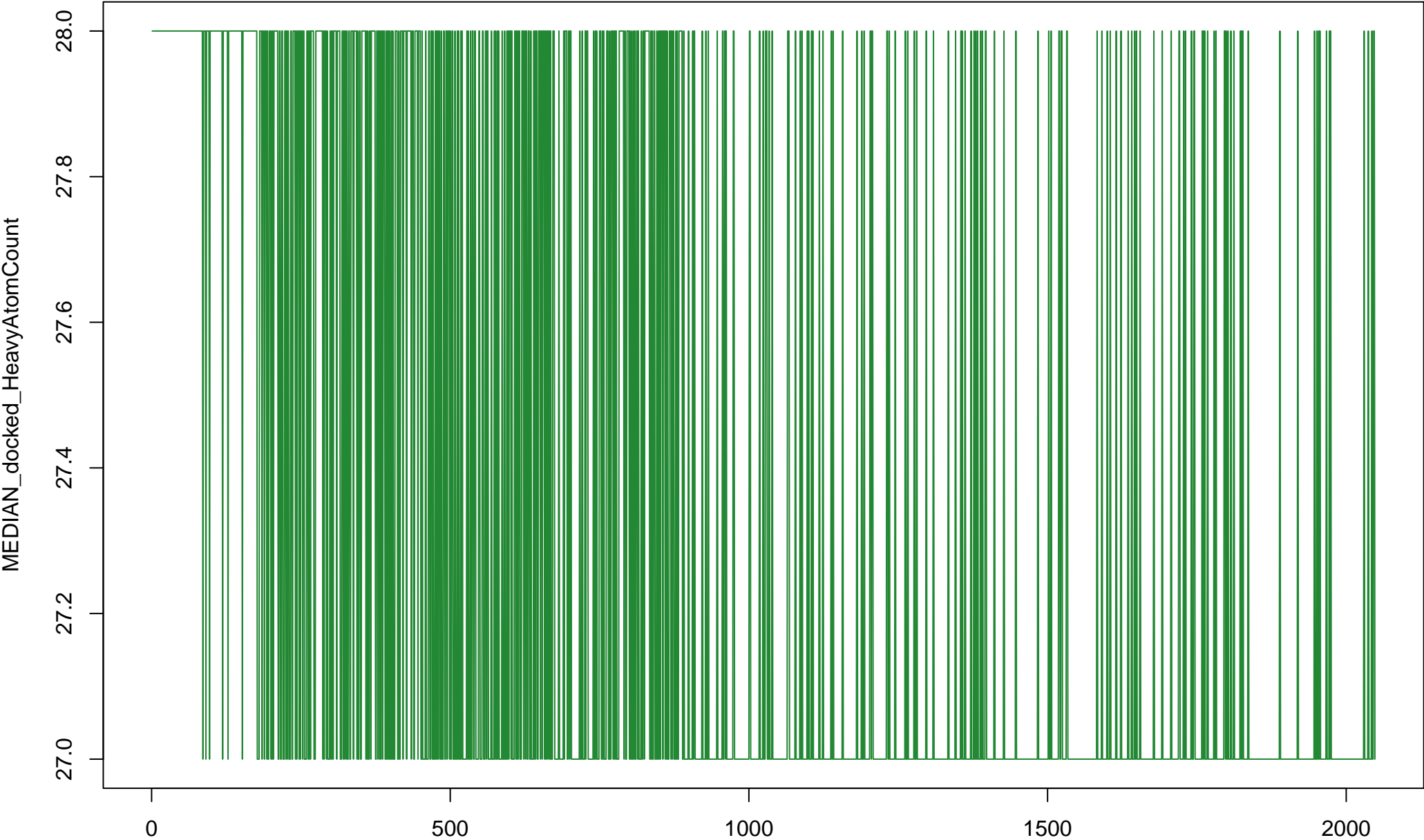
MEDIAN_log_RMSD
ESS = 55.9 | BMK = 0.144 | MCSE(6.27) = 7.29 | stat: FALSE | burn: 0



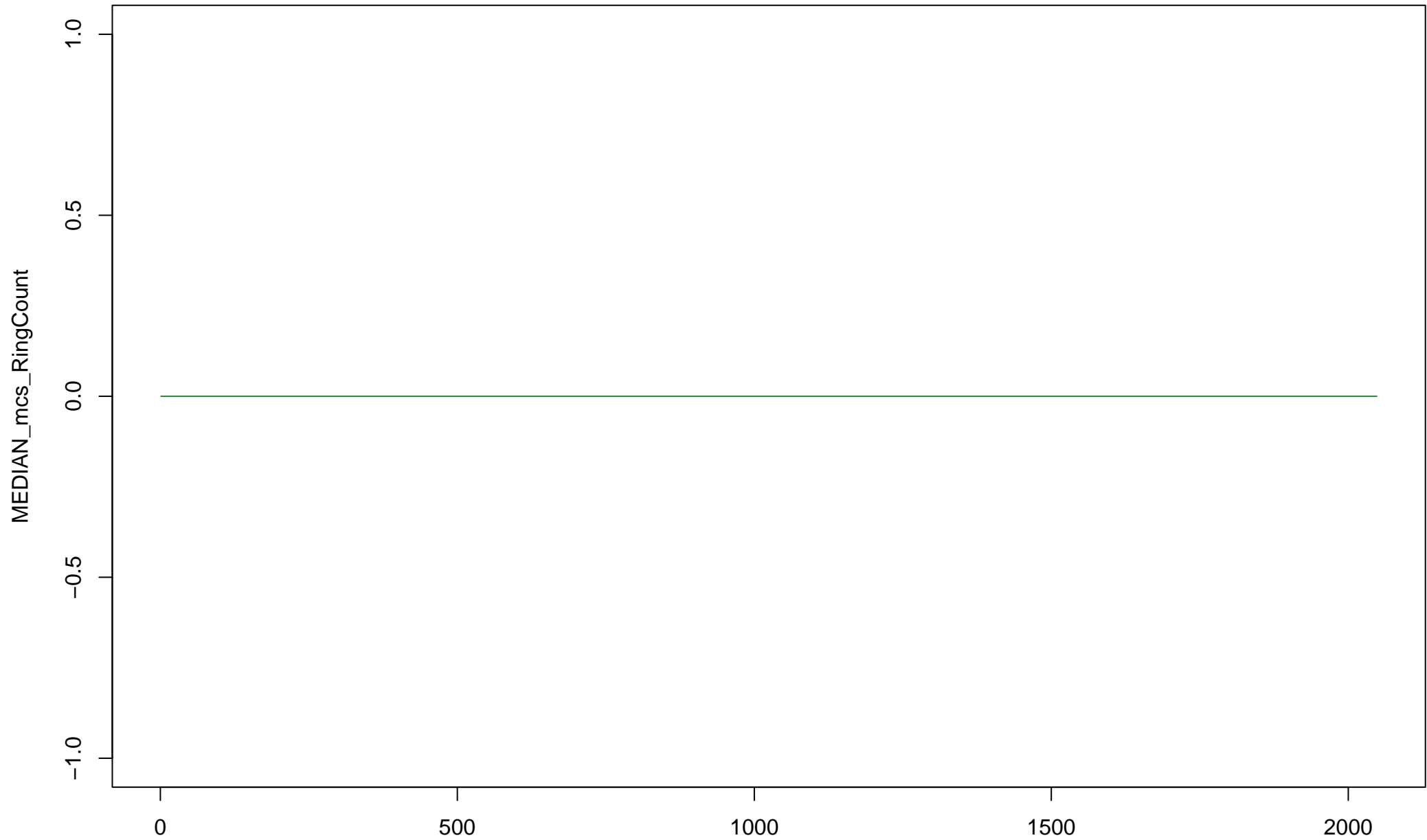
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 577 | BMK = 0.0856 | MCSE(6.27) = 4.08 | stat: TRUE | burn: 0



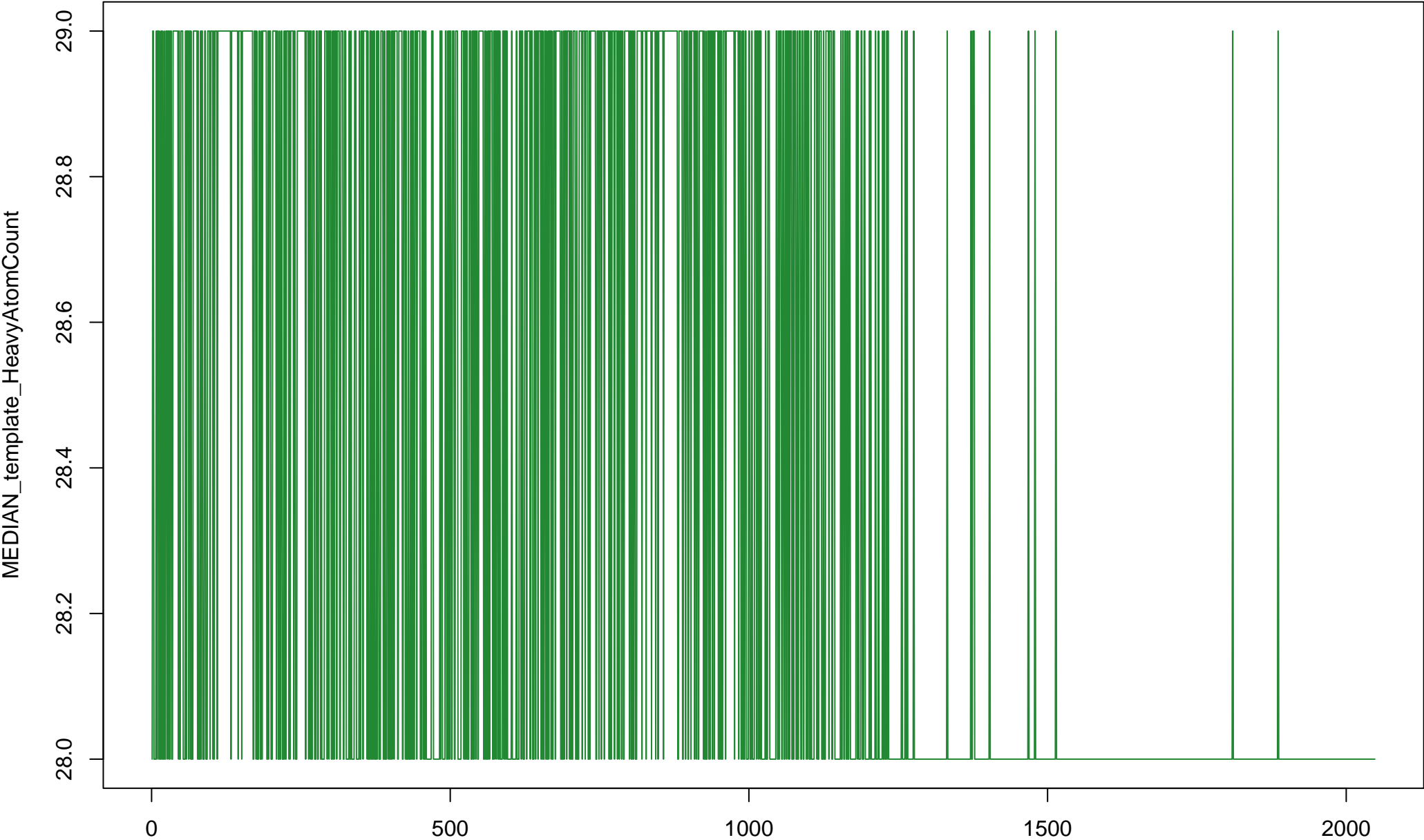
MEDIAN_docked_HeavyAtomCount
ESS = 15.1 | BMK = 0.284 | MCSE(6.27) = 9.04 | stat: FALSE | burn: 0



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



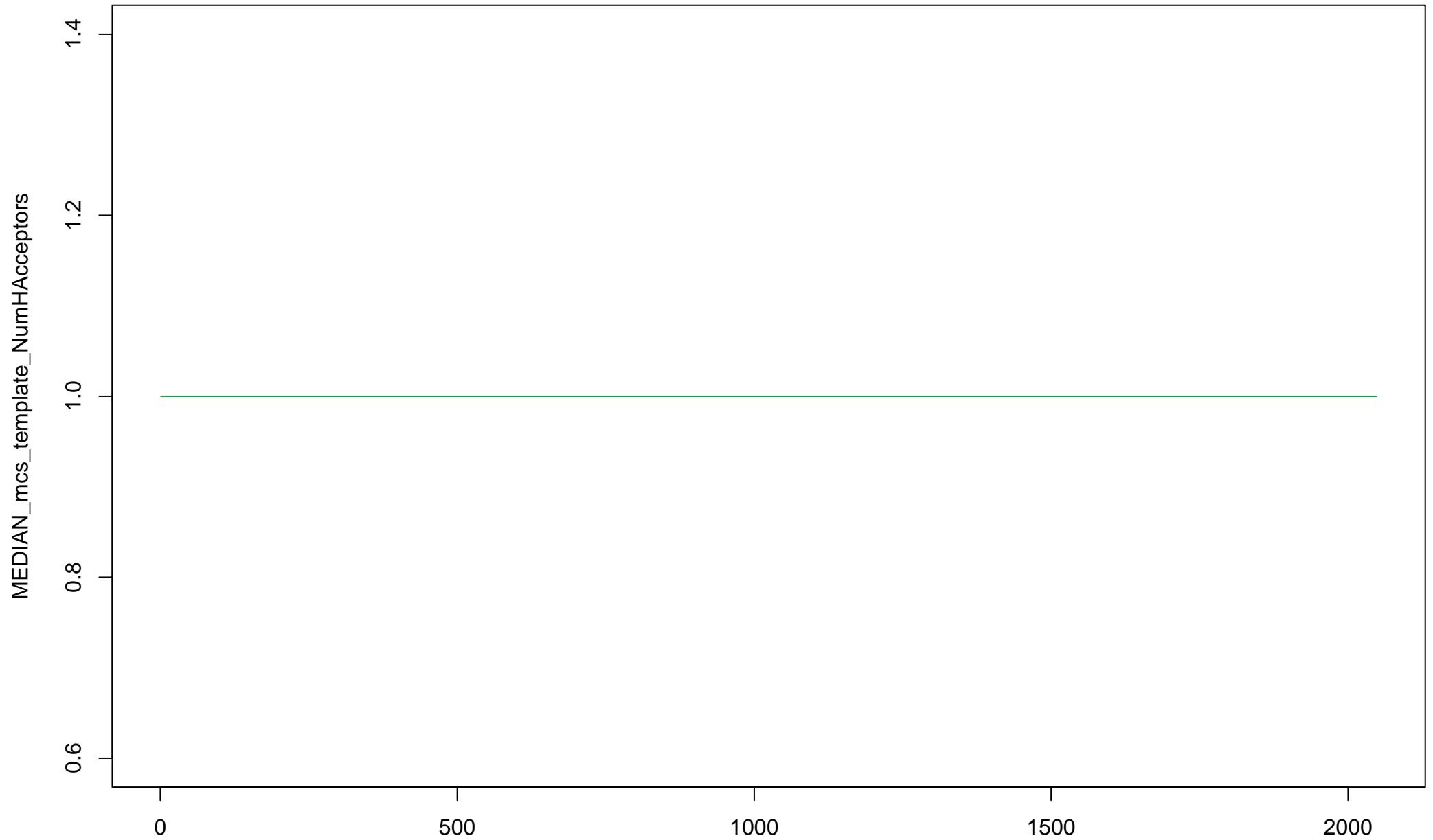
MEDIAN_template_HeavyAtomCount
ESS = 13.7 | BMK = 0.333 | MCSE(6.27) = 9.53 | stat: FALSE | burn: 0



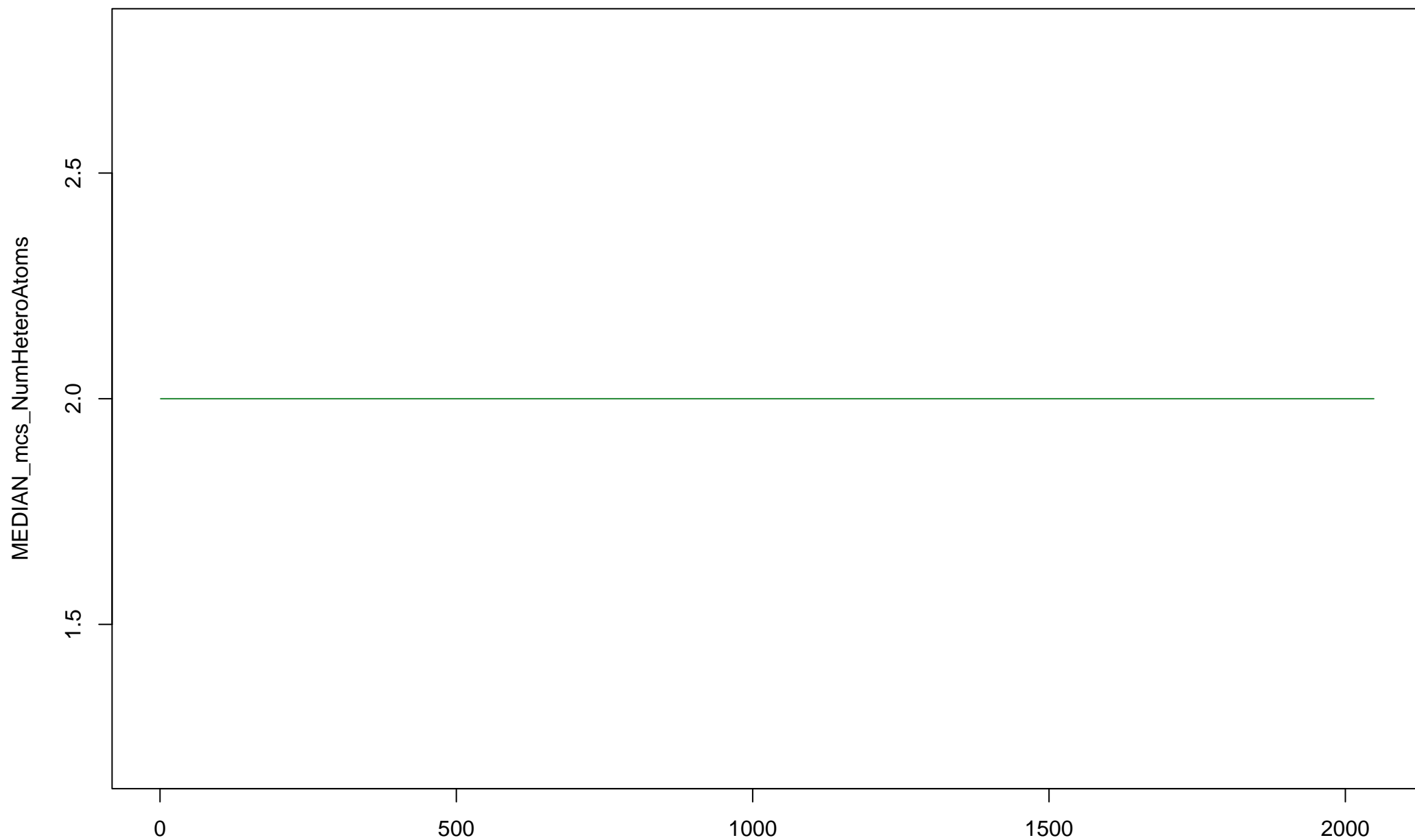
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



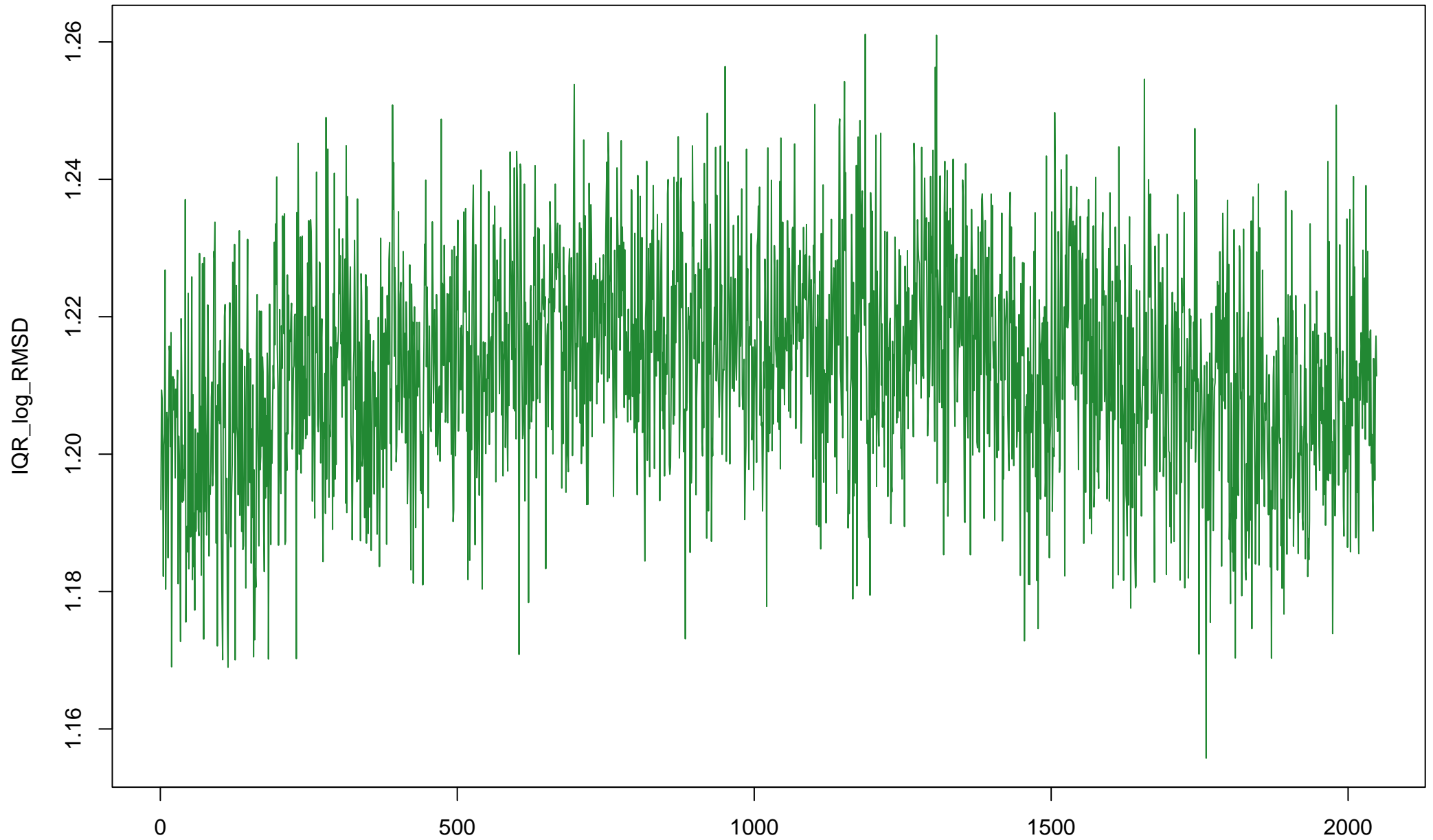
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



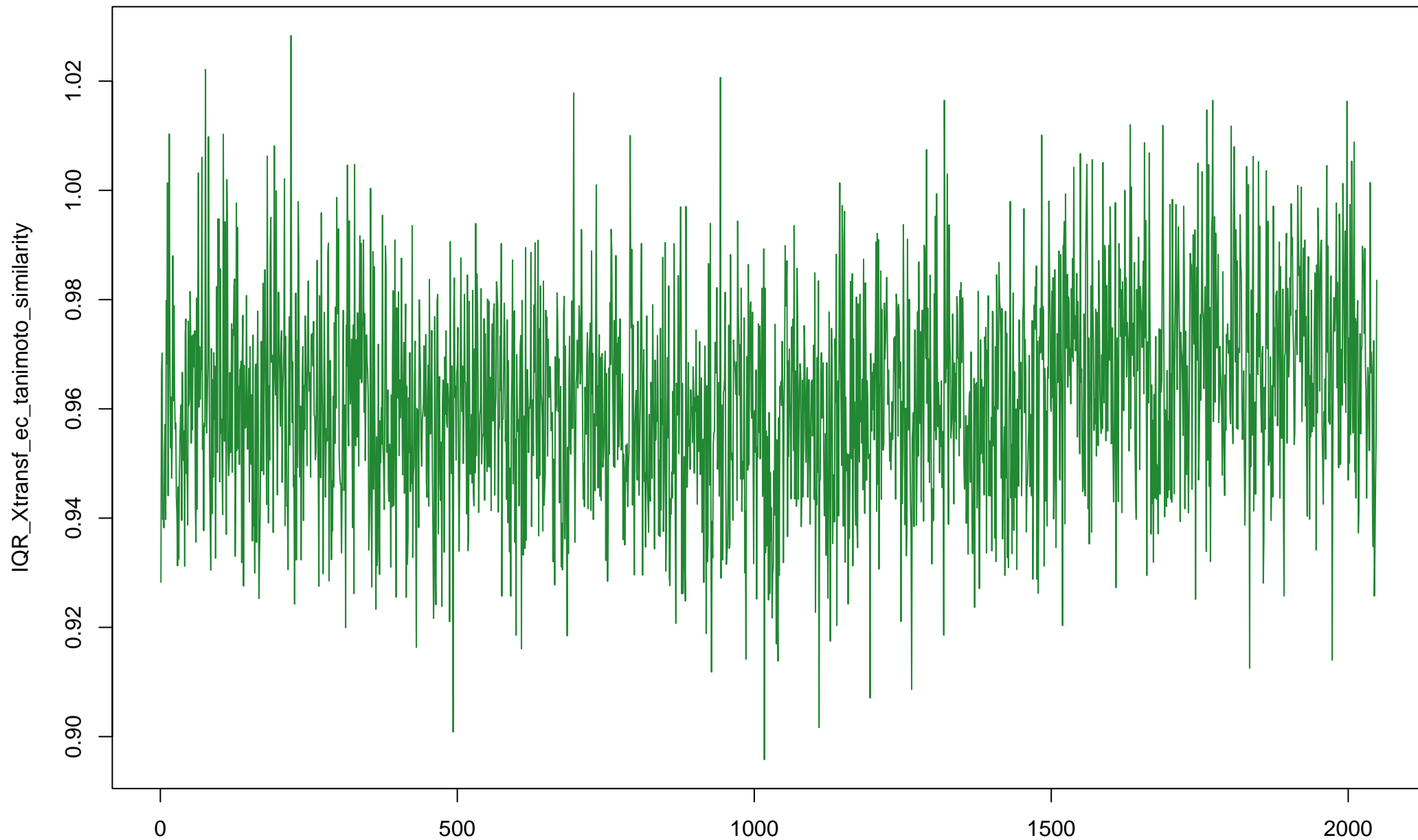
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



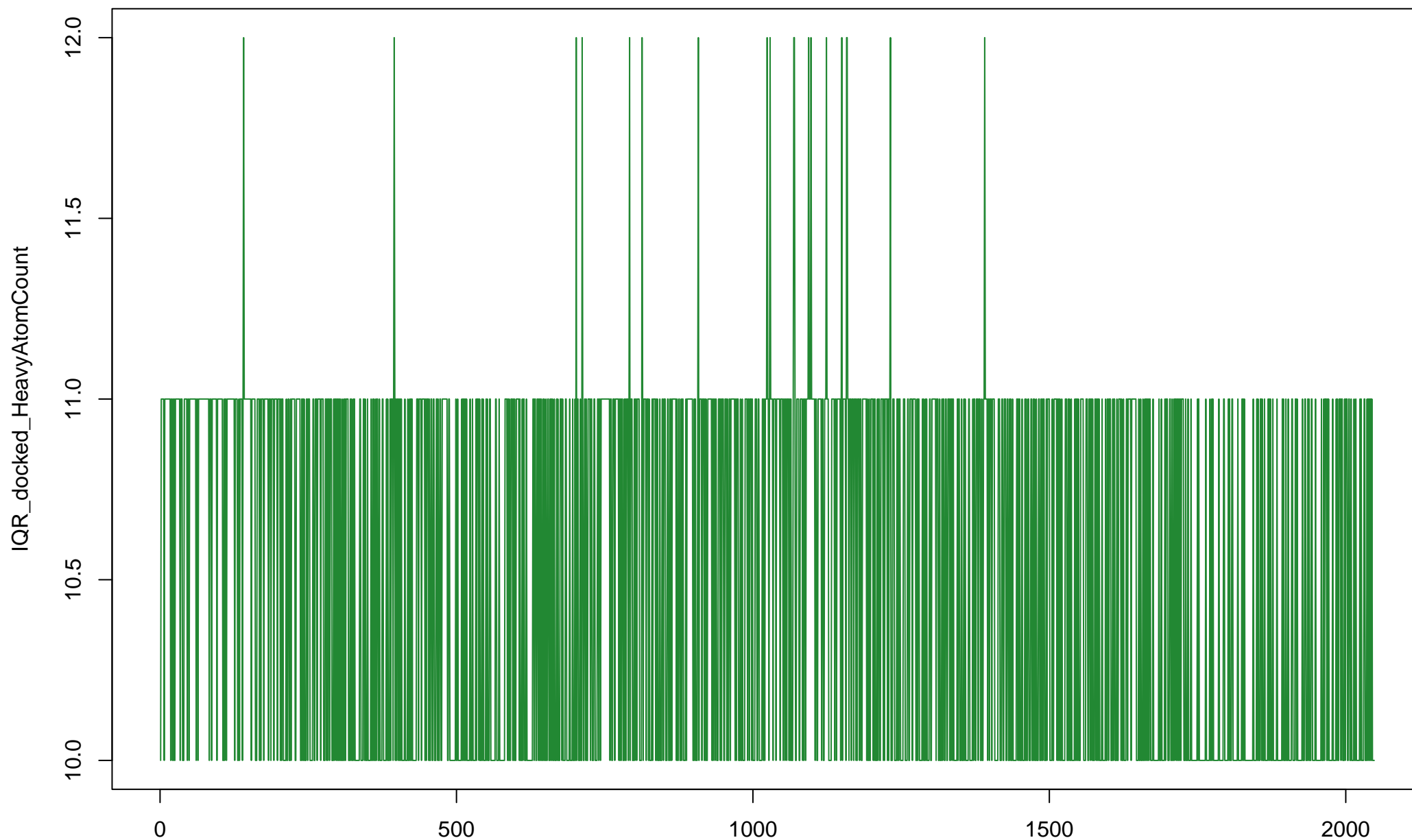
IQR_log_RMSD
ESS = 124 | BMK = 0.0398 | MCSE(6.27) = 5.82 | stat: FALSE | burn: 0



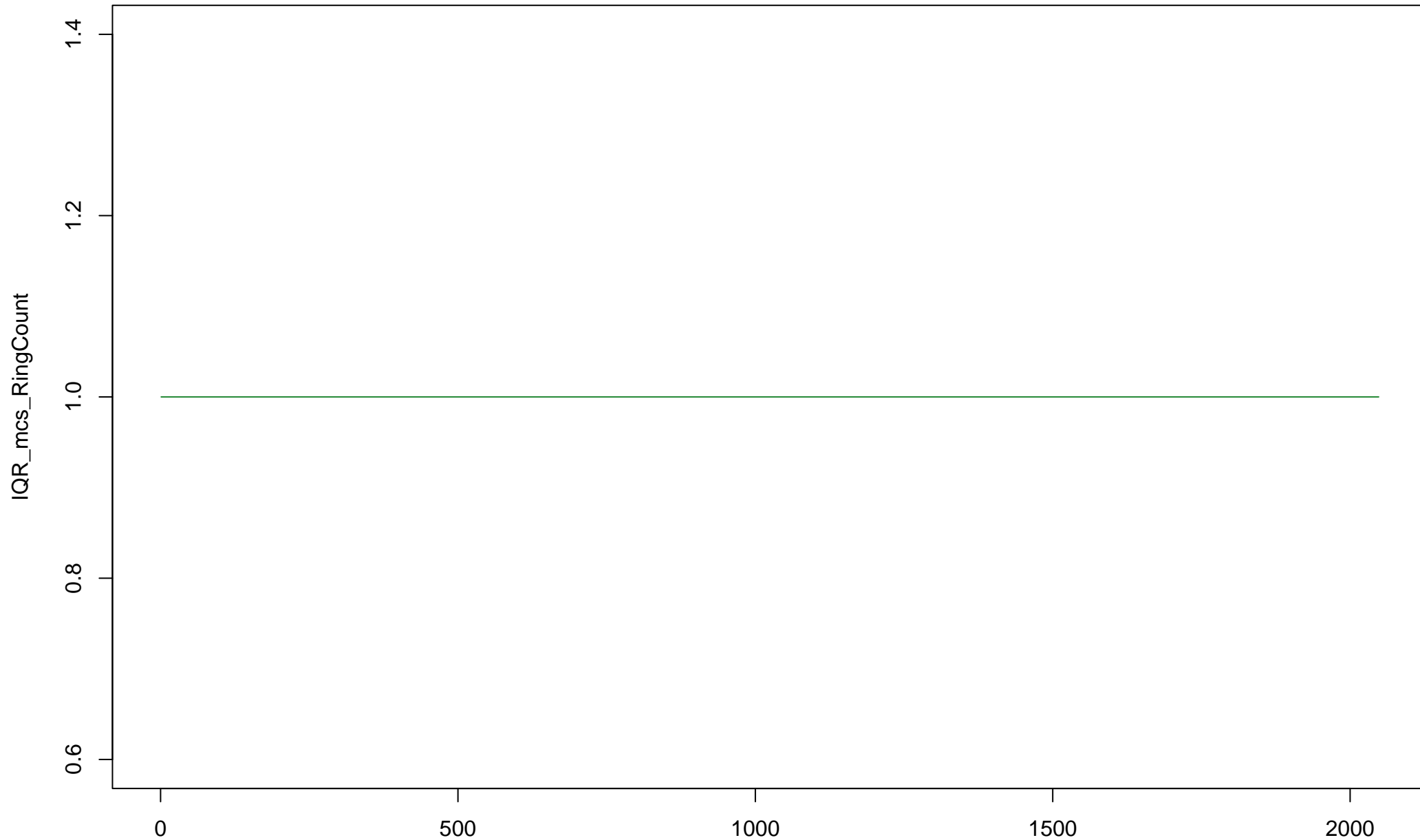
IQR_Xtransf_ec_tanimoto_similarity
ESS = 512 | BMK = 0.113 | MCSE(6.27) = 4.6 | stat: TRUE | burn: 0



IQR_docked_HeavyAtomCount
ESS = 140 | BMK = 0.0713 | MCSE(6.27) = 5.22 | stat: FALSE | burn: 0



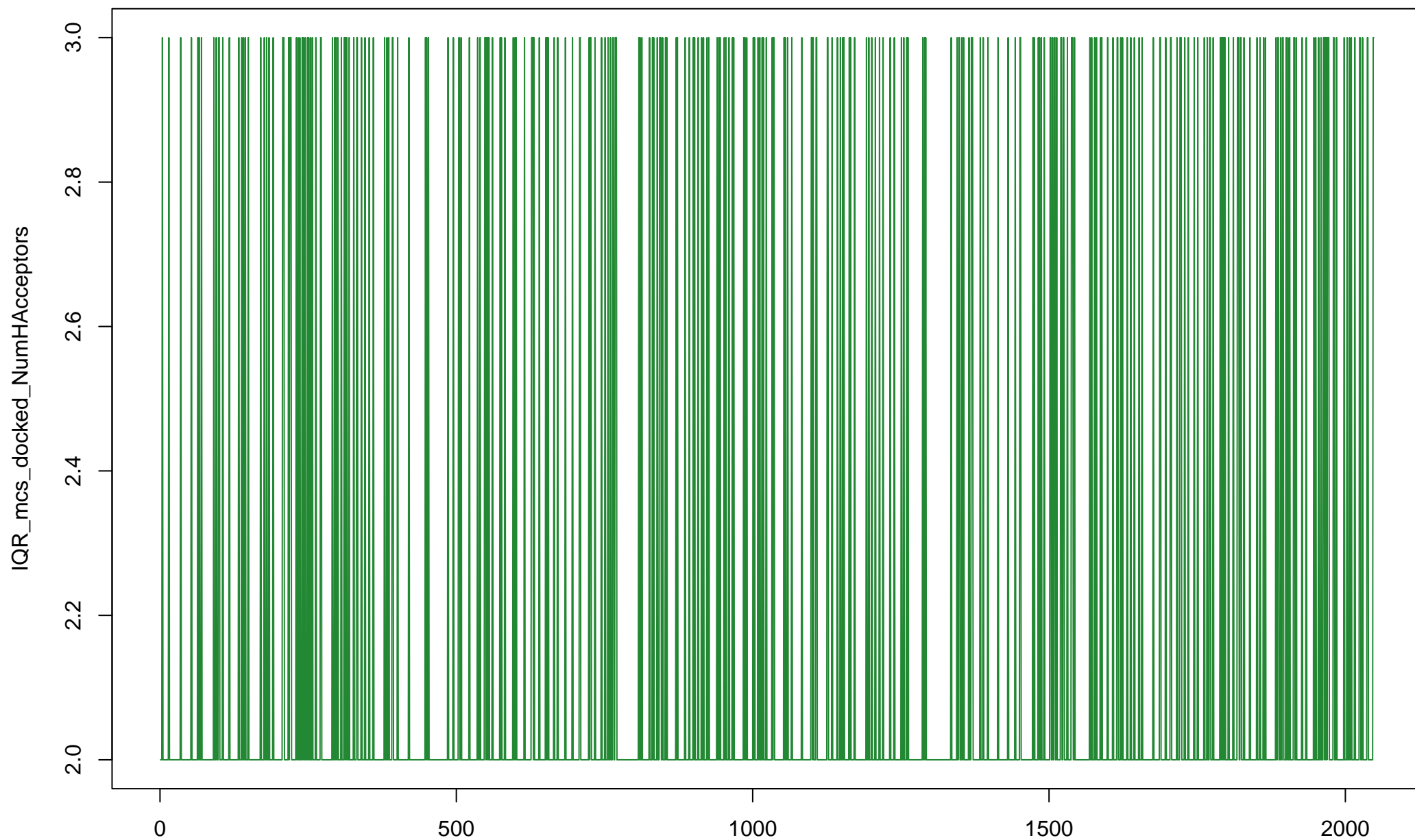
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



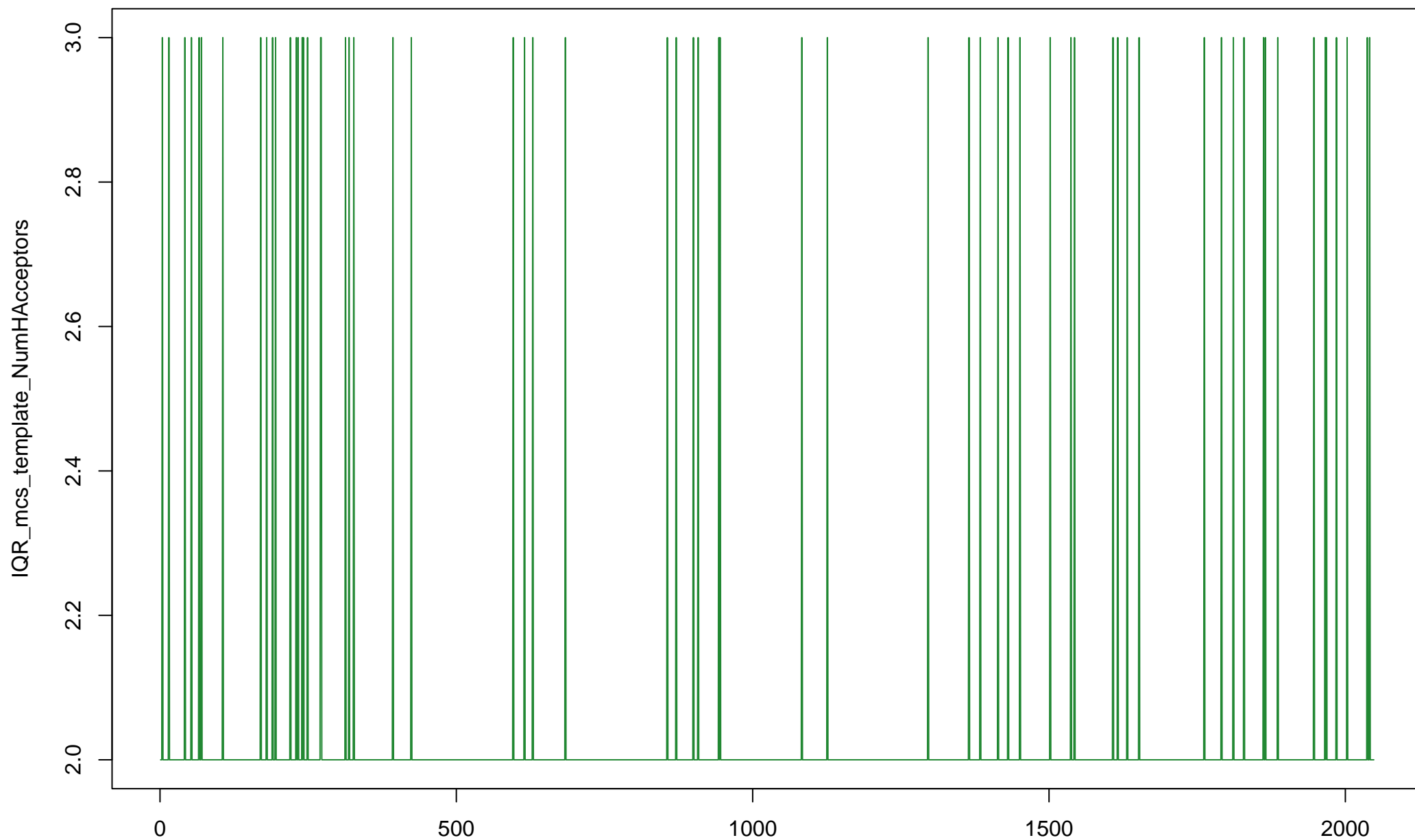
IQR_template_HeavyAtomCount
ESS = 1510 | BMK = 0.0394 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 1428



IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0131 | MCSE(6.27) = 2.23 | stat: FALSE | burn: 0



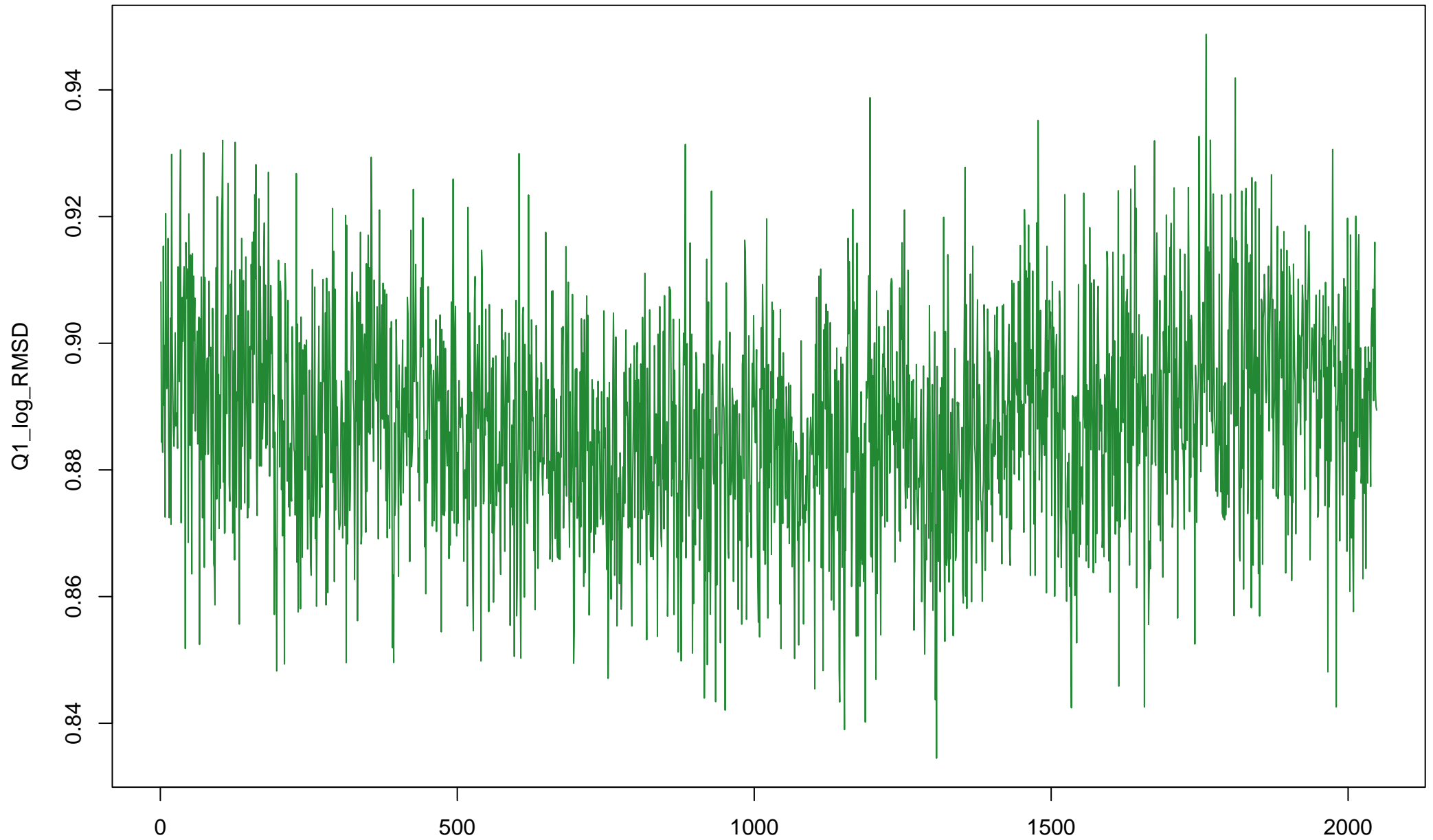
IQR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0282 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



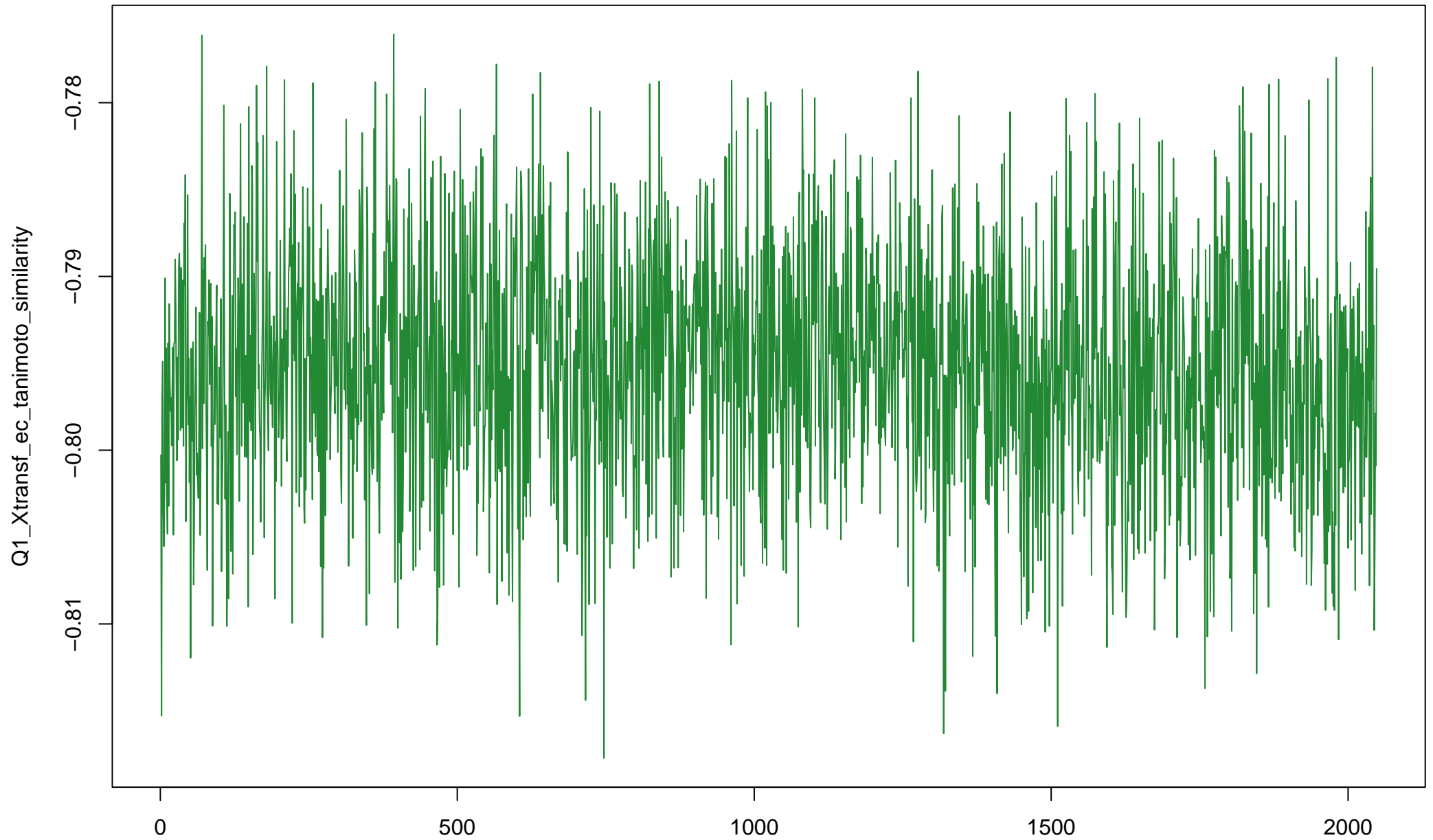
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



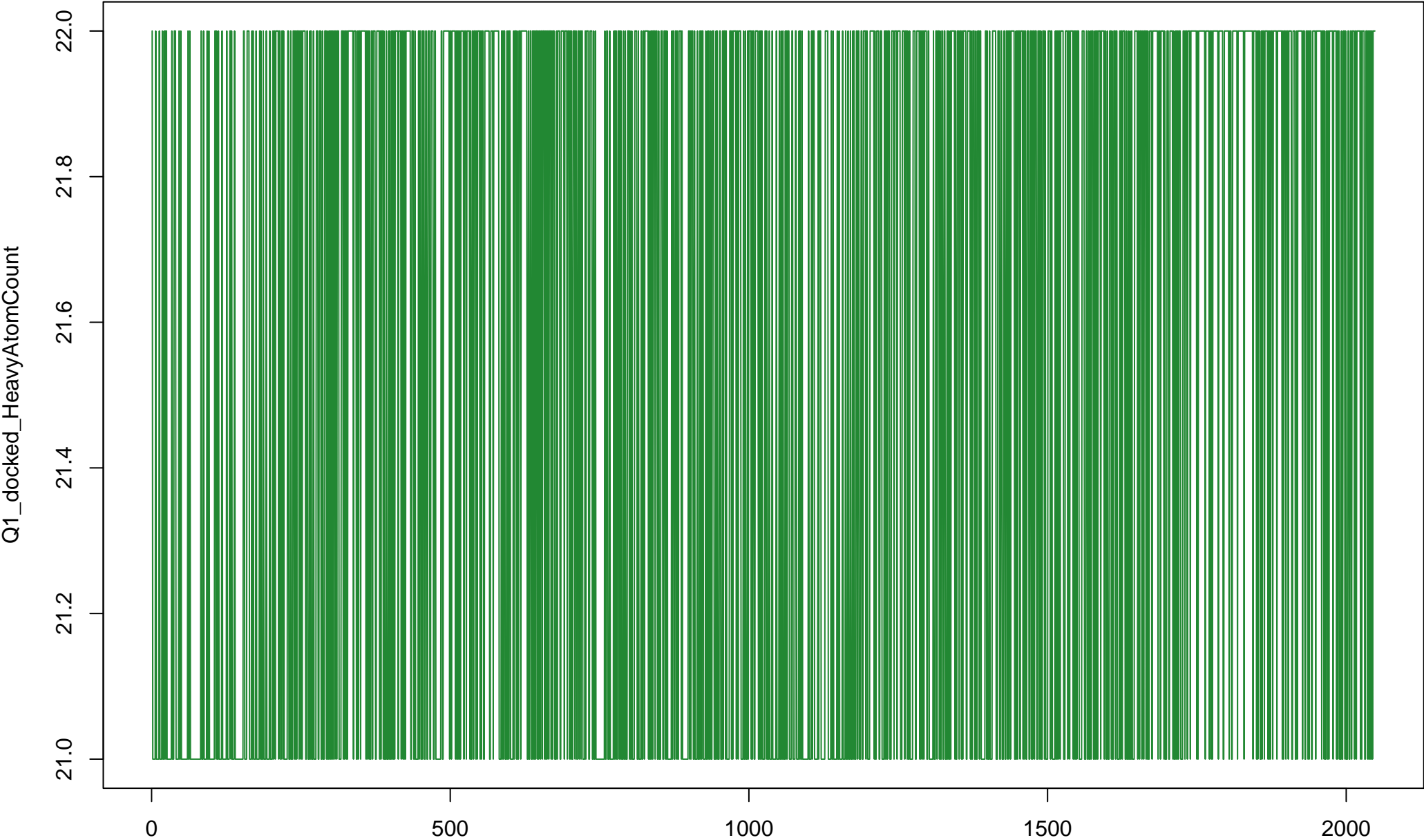
Q1_log_RMSD
ESS = 286 | BMK = 0.0554 | MCSE(6.27) = 4.84 | stat: FALSE | burn: 0



Q1_Xtransf_ec_tanimoto_similarity
ESS = 1160 | BMK = 0.0432 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0



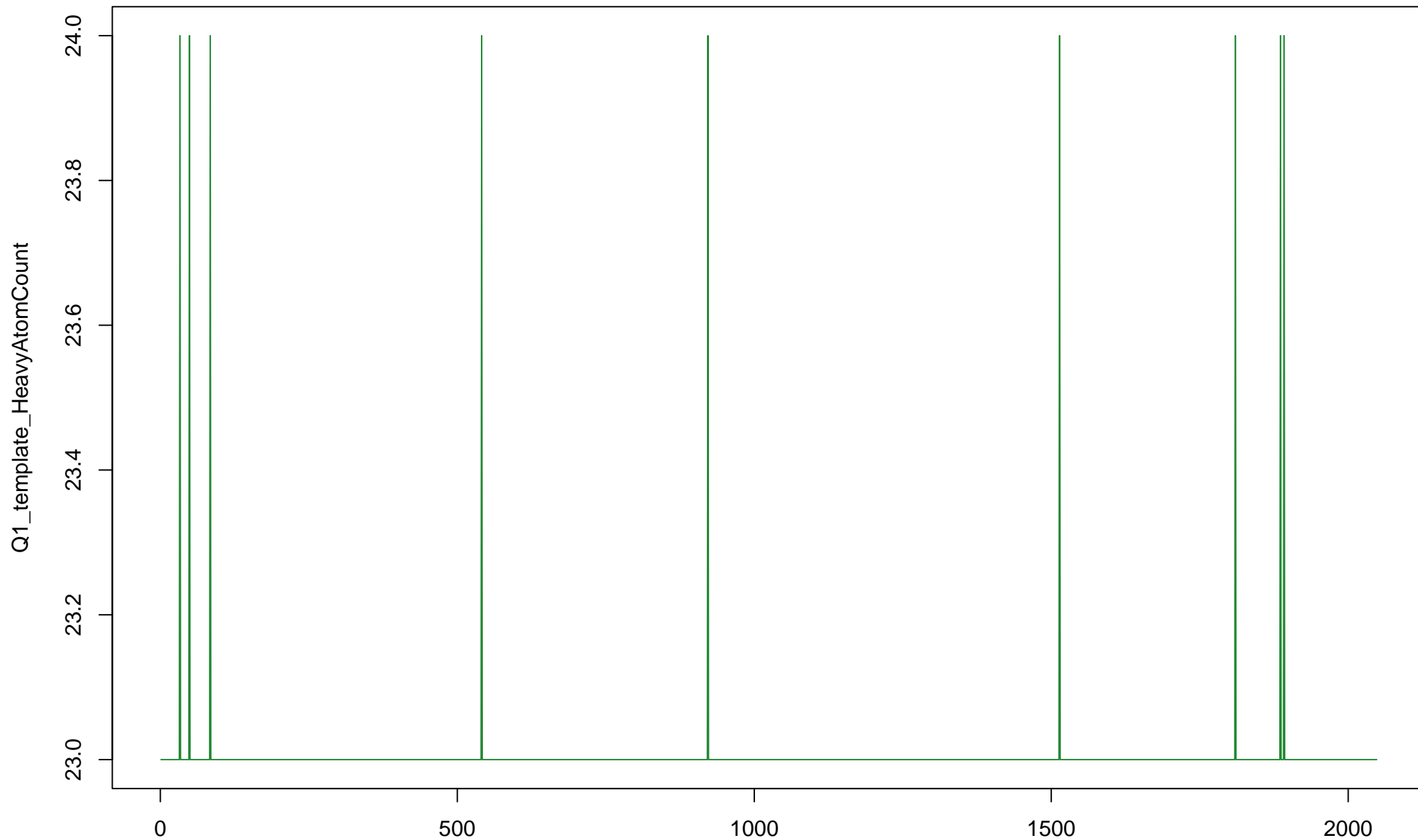
Q1_docked_HeavyAtomCount
ESS = 157 | BMK = 0.0562 | MCSE(6.27) = 5.1 | stat: FALSE | burn: 0



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



Q1_template_HeavyAtomCount
ESS = 1510 | BMK = 0.0394 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 1428



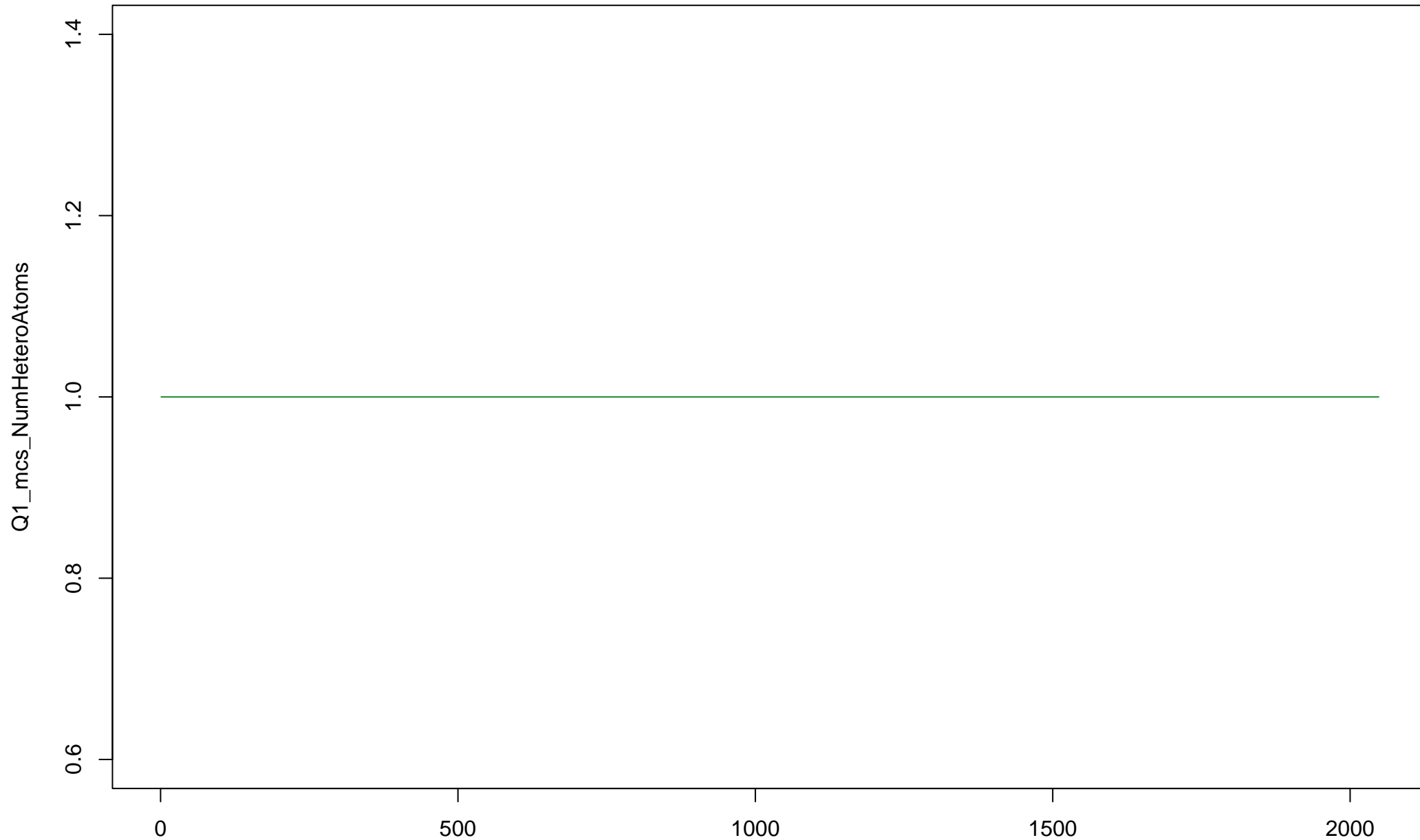
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



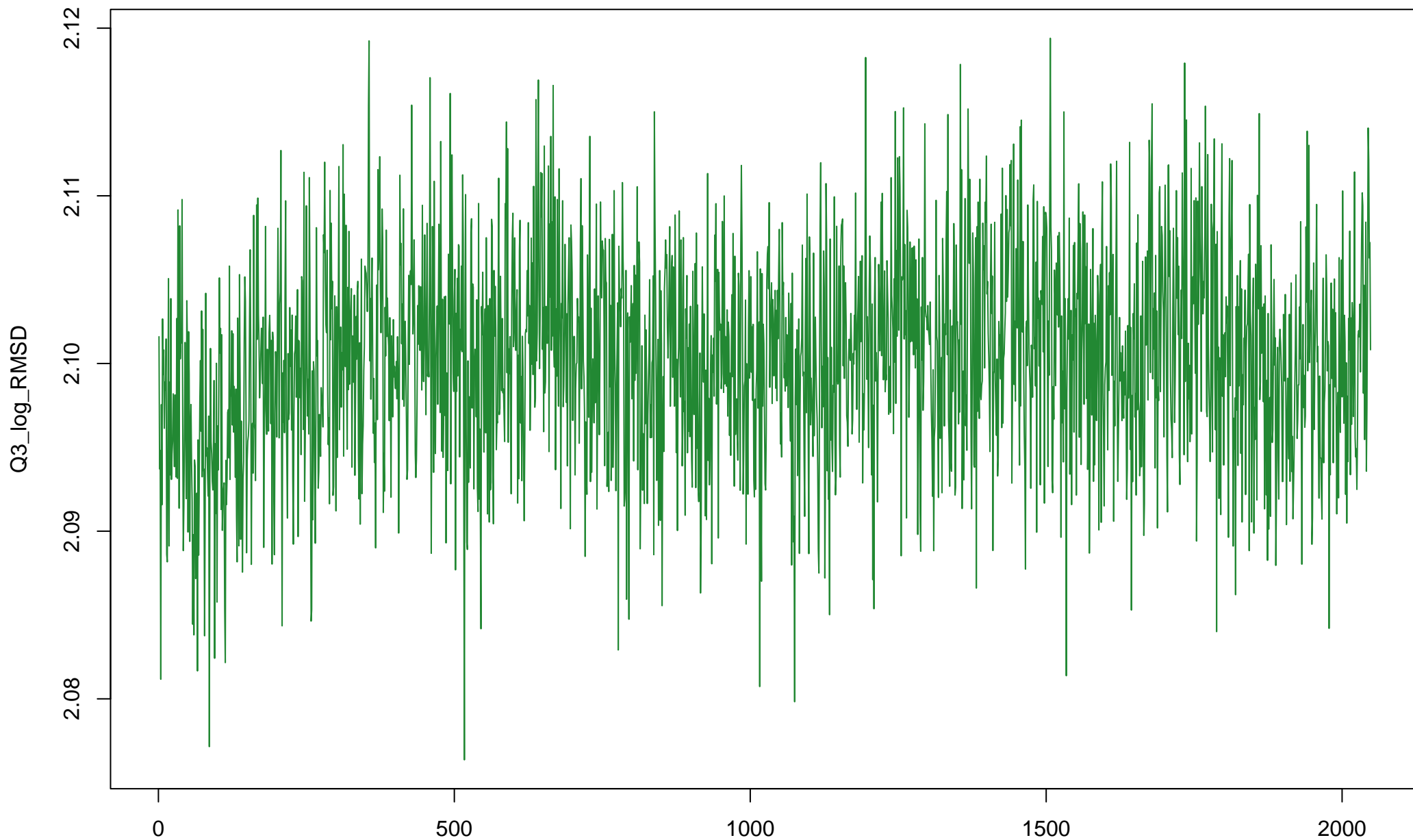
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



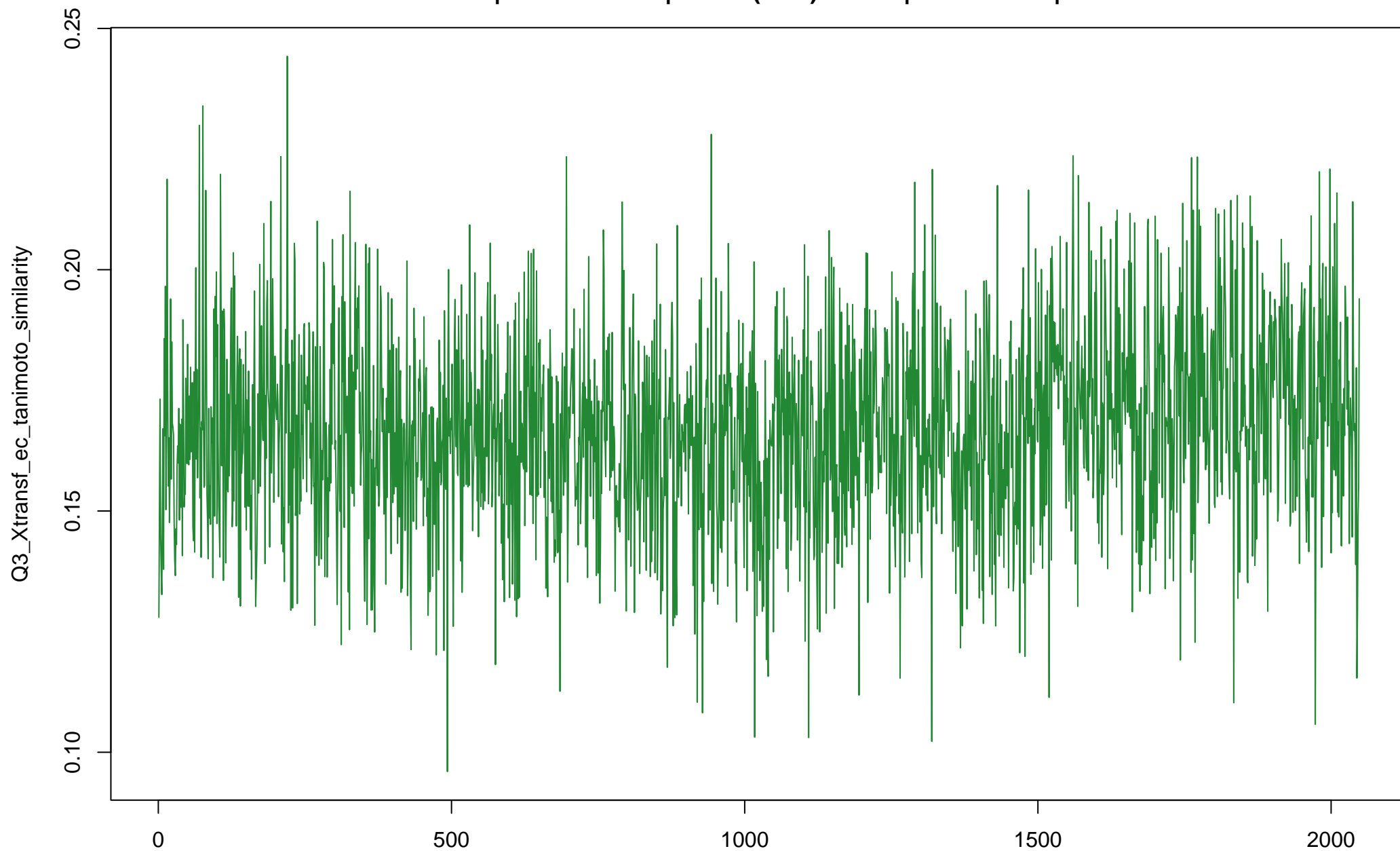
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



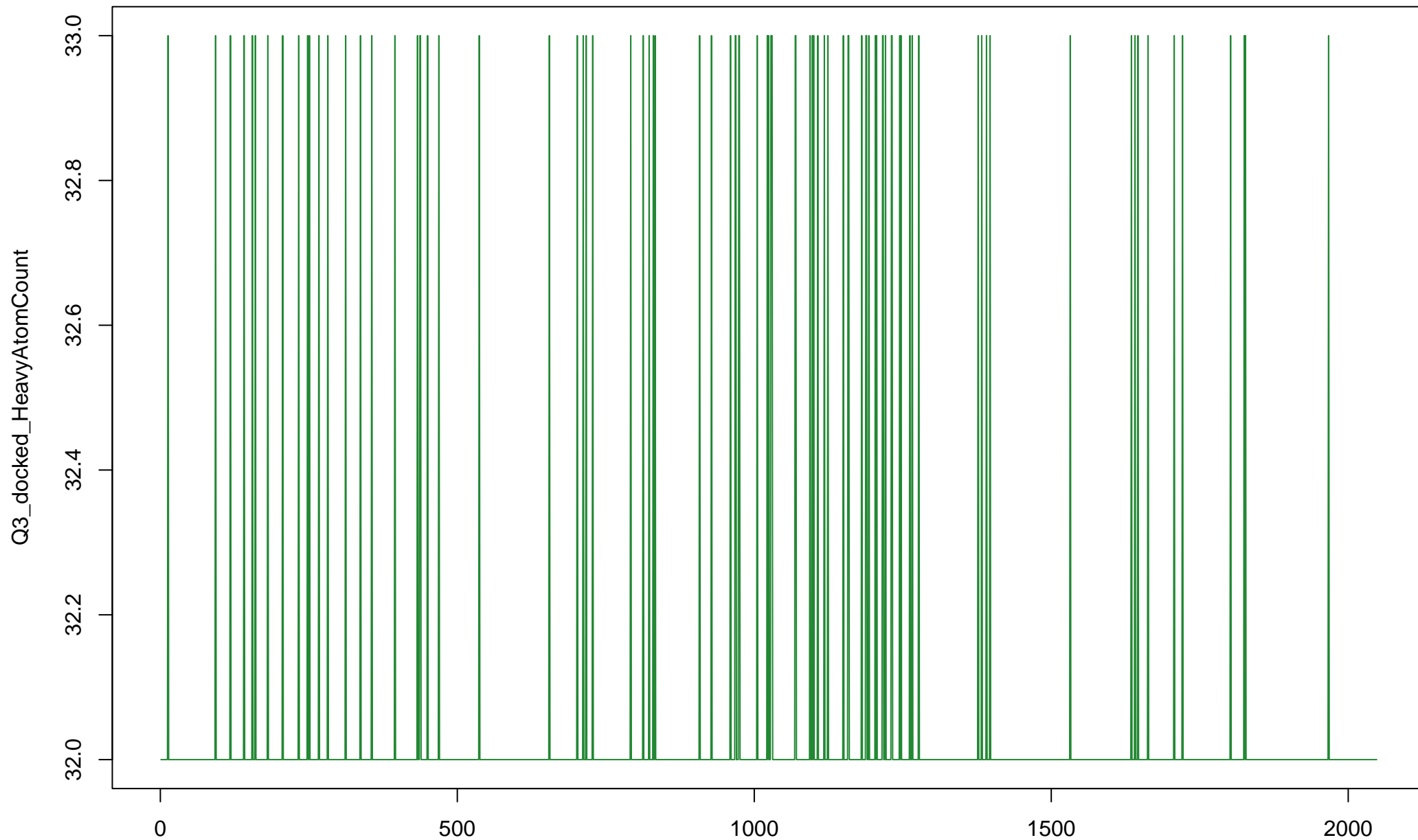
Q3_log_RMSD
ESS = 246 | BMK = 0.0764 | MCSE(6.27) = 4.96 | stat: FALSE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 784 | BMK = 0.102 | MCSE(6.27) = 3.81 | stat: TRUE | burn: 0



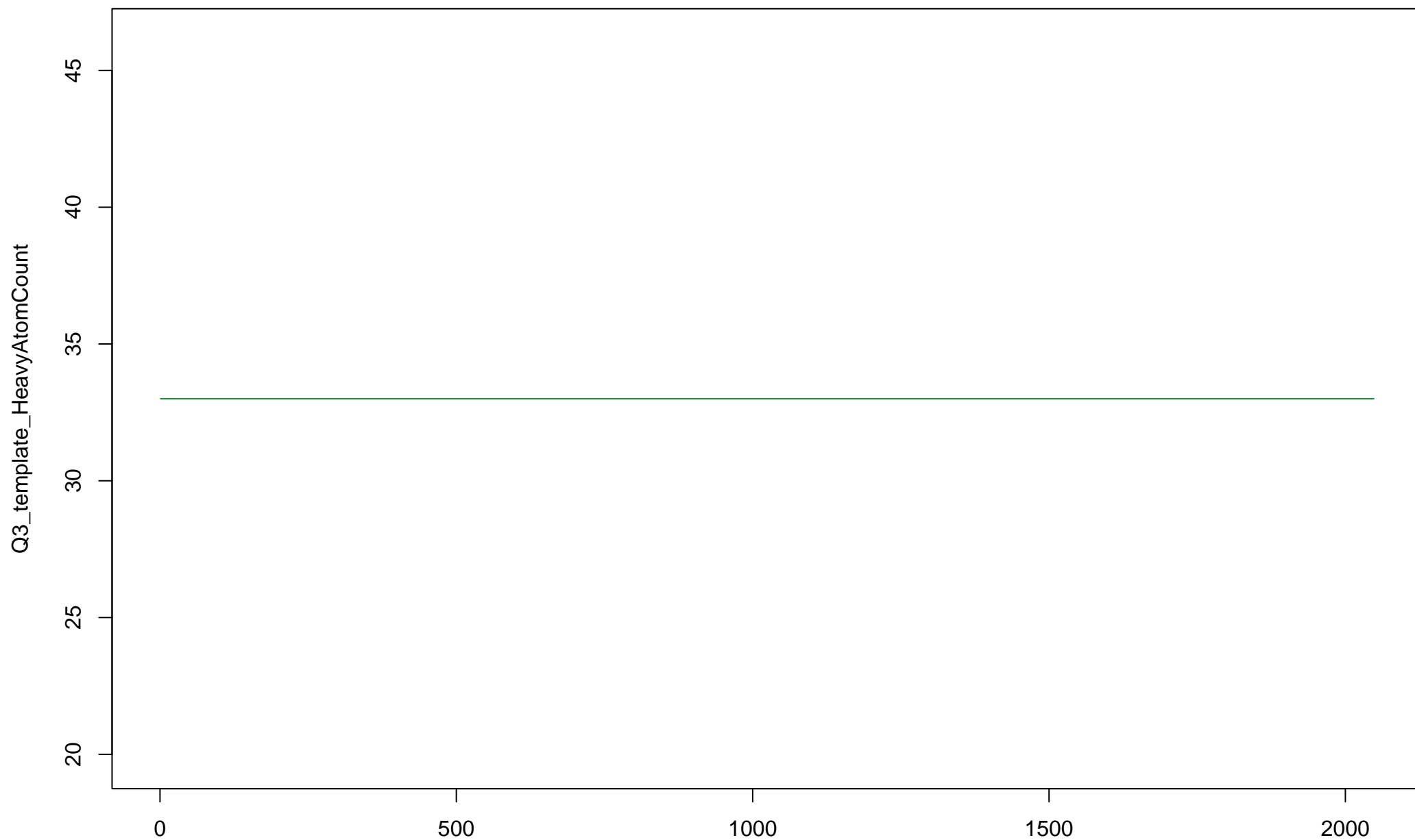
Q3_docked_HeavyAtomCount
ESS = 907 | BMK = 0.00805 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0



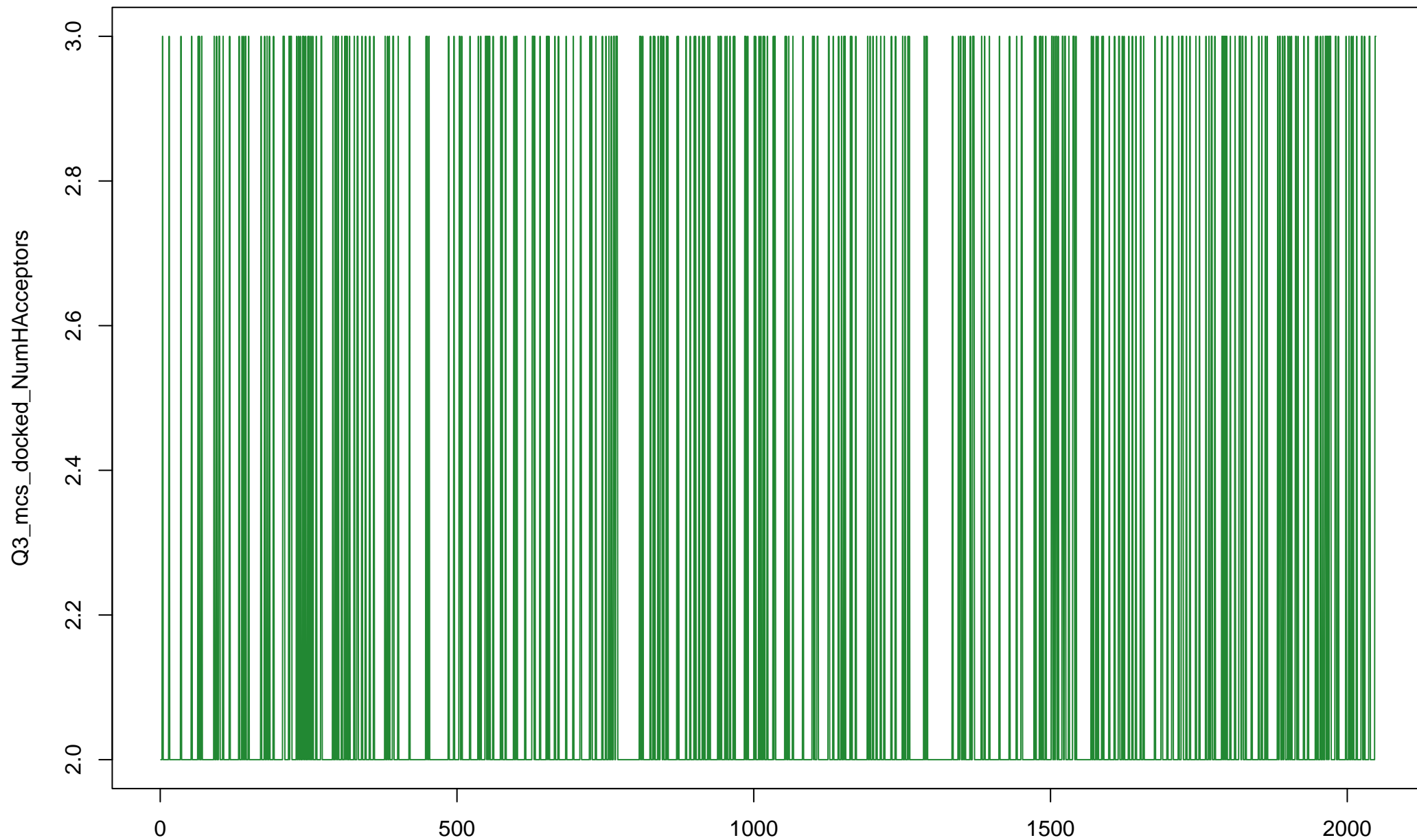
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



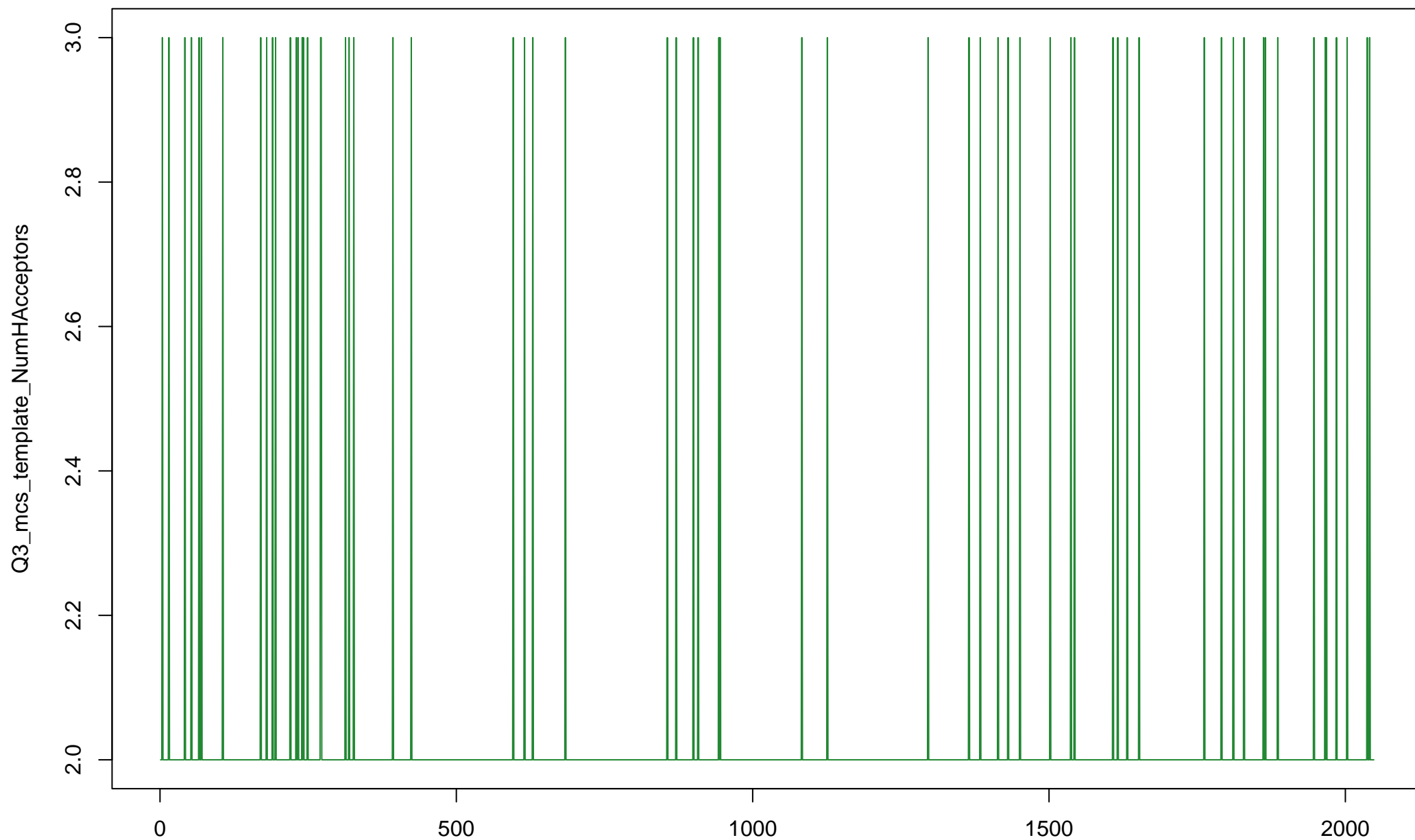
Q3_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0131 | MCSE(6.27) = 2.23 | stat: FALSE | burn: 0



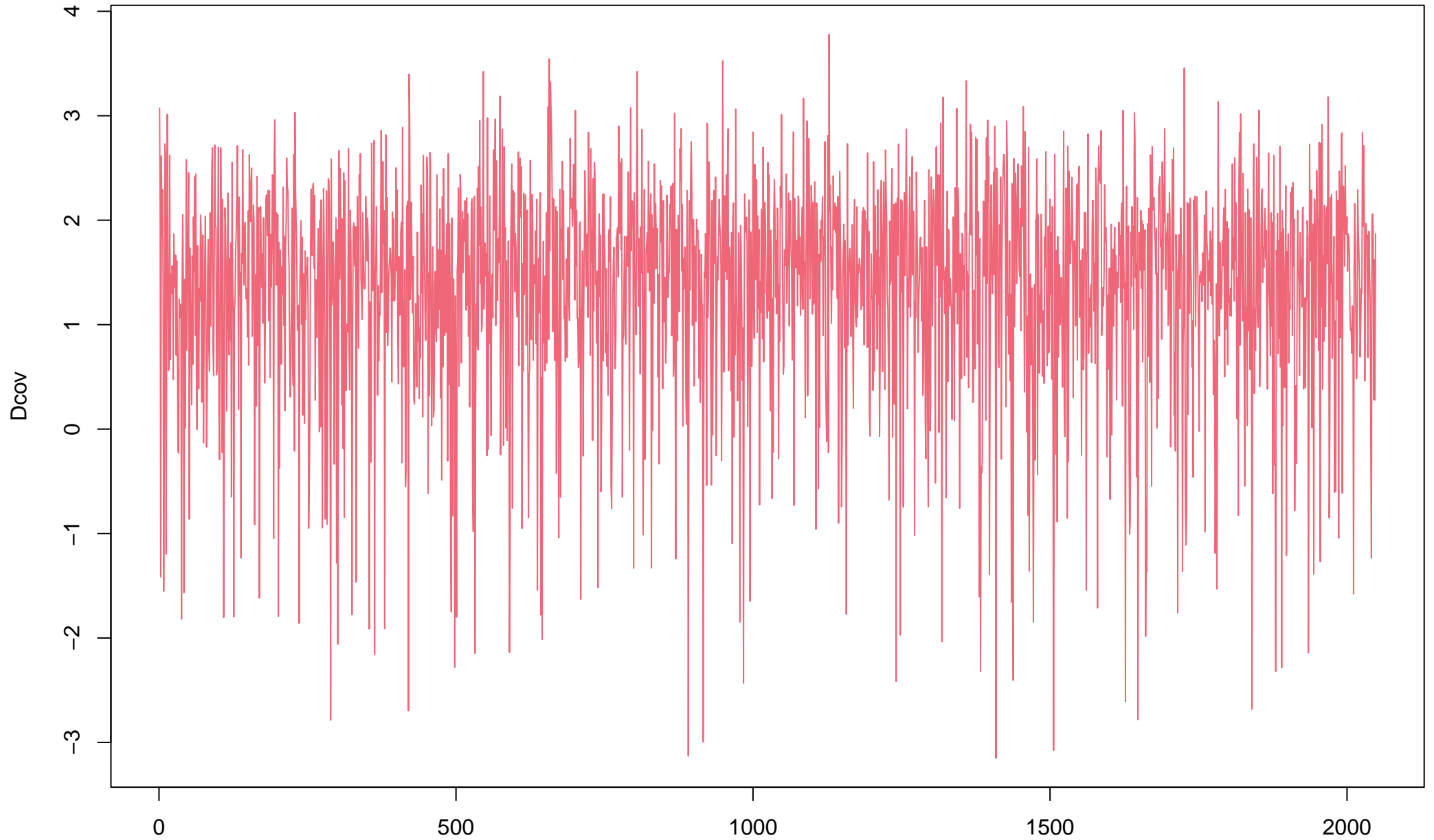
Q3_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0282 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



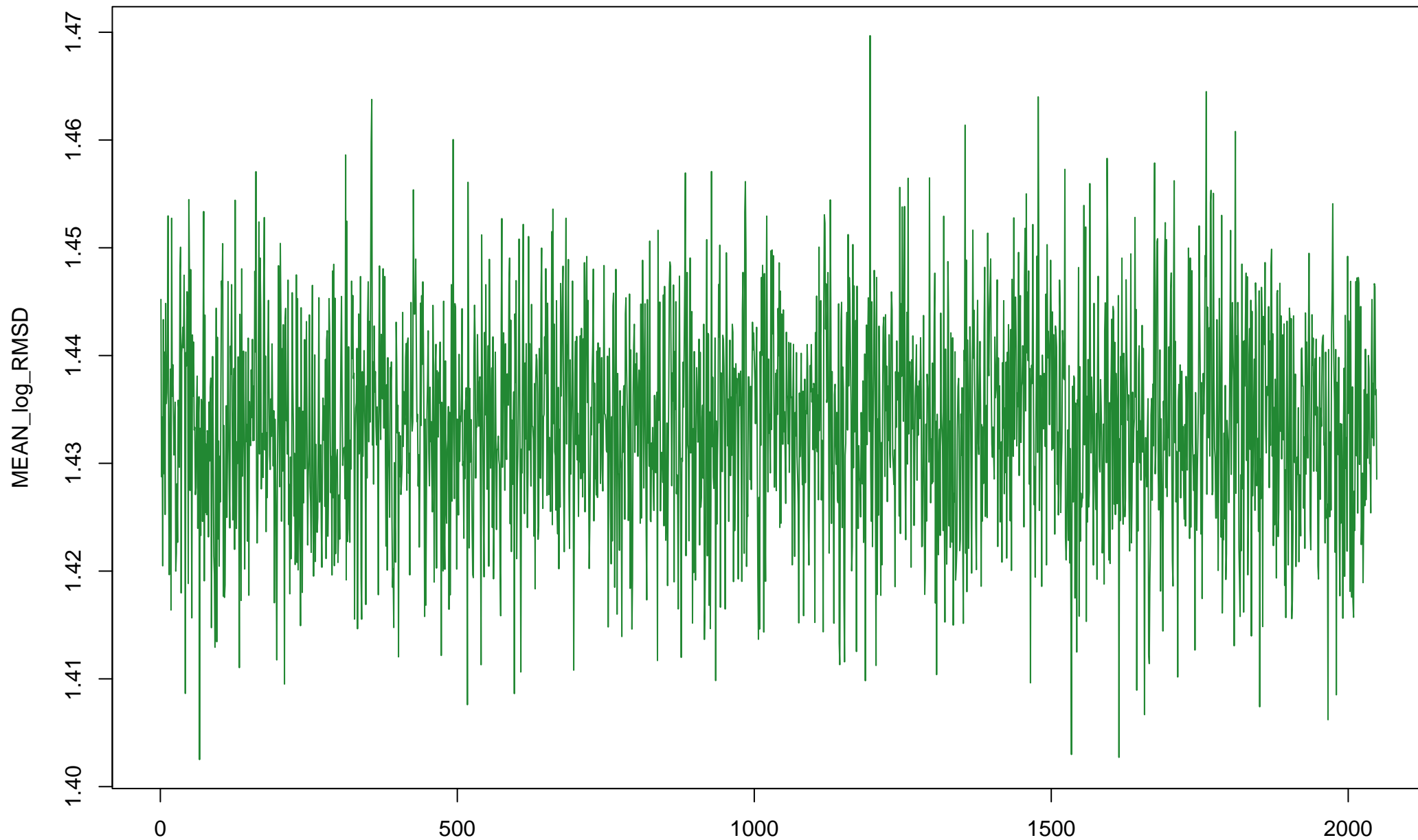
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



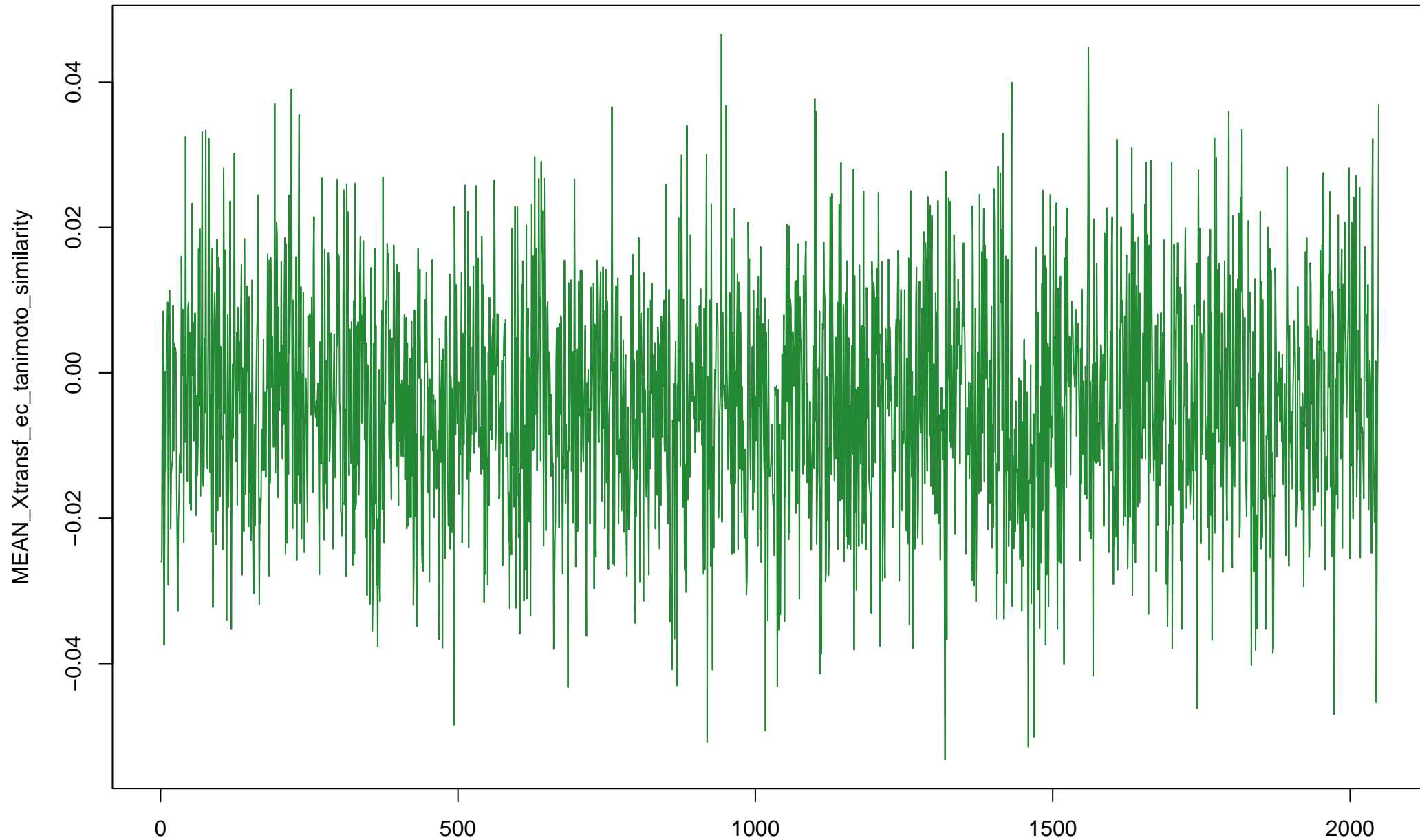
Dcov
ESS = 1950 | BMK = 0.0636 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0



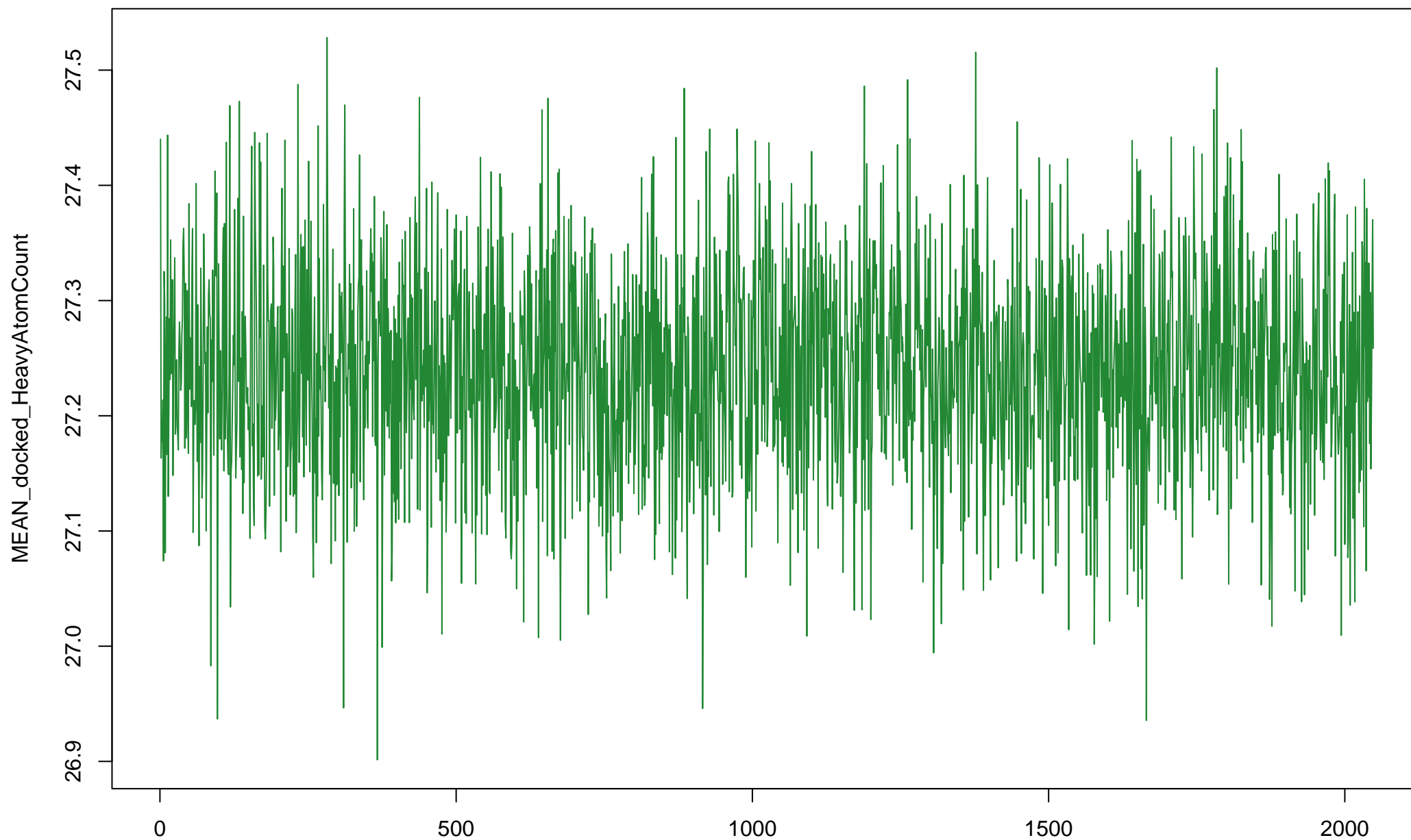
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0357 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0



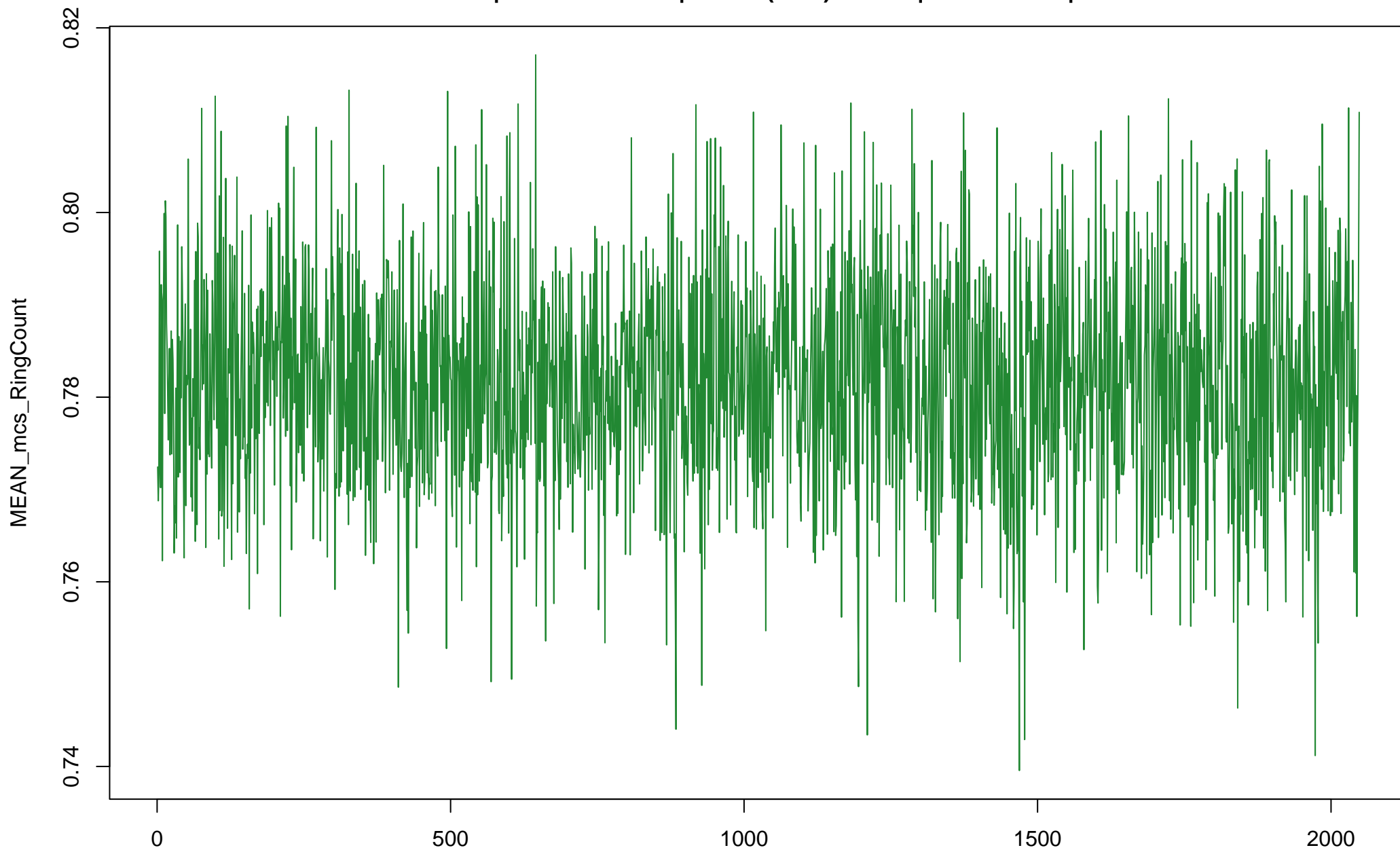
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0451 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0



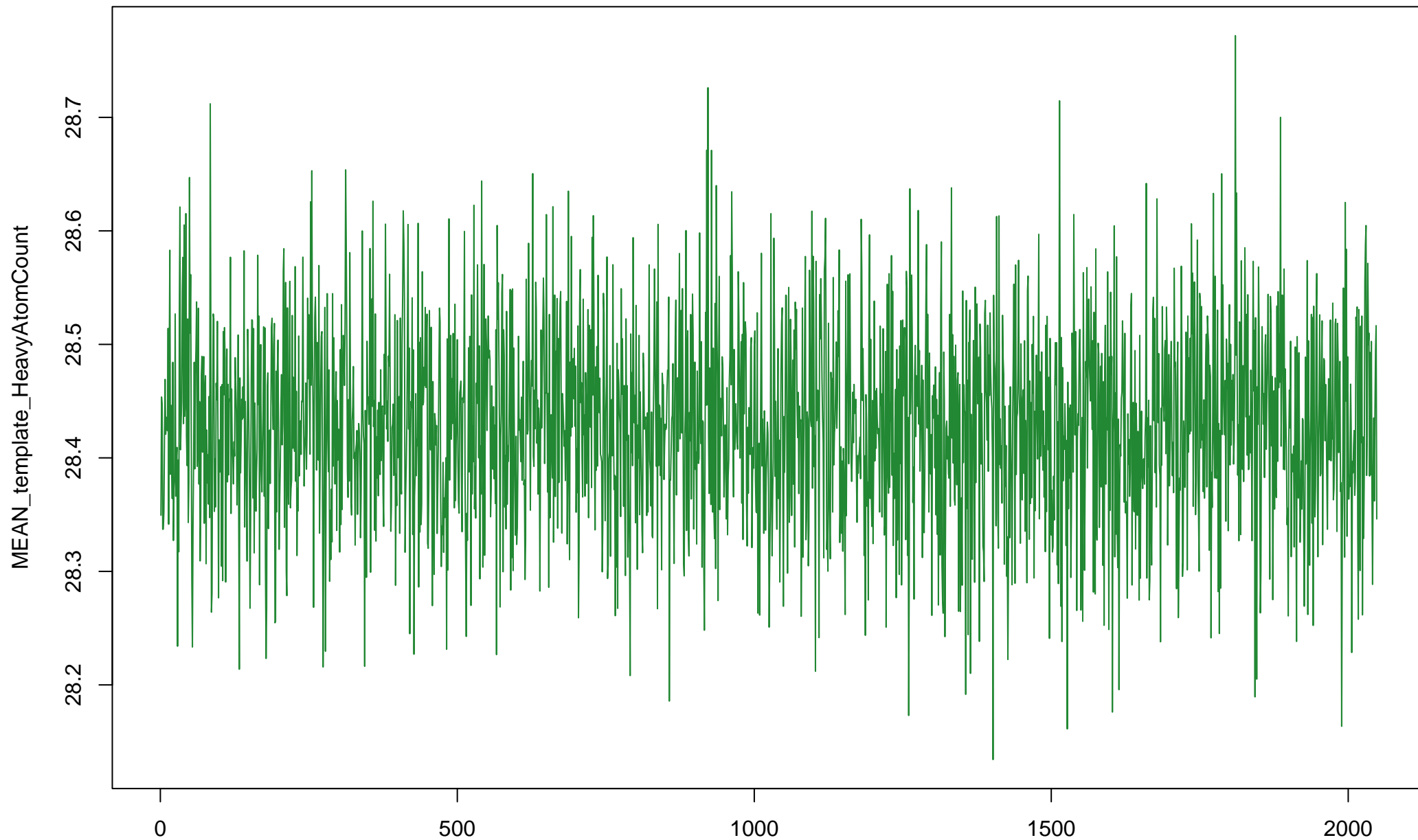
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0596 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0



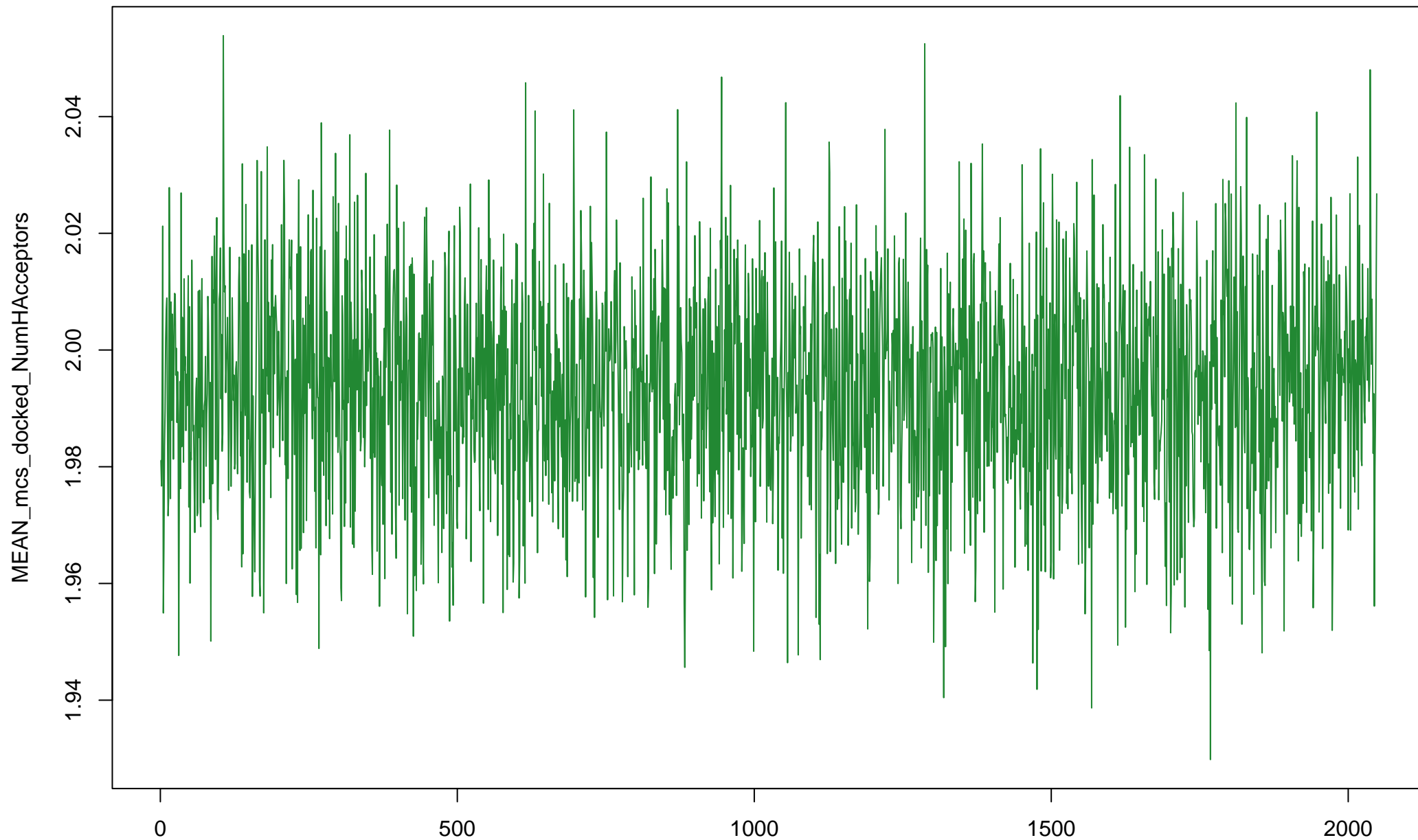
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0681 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0



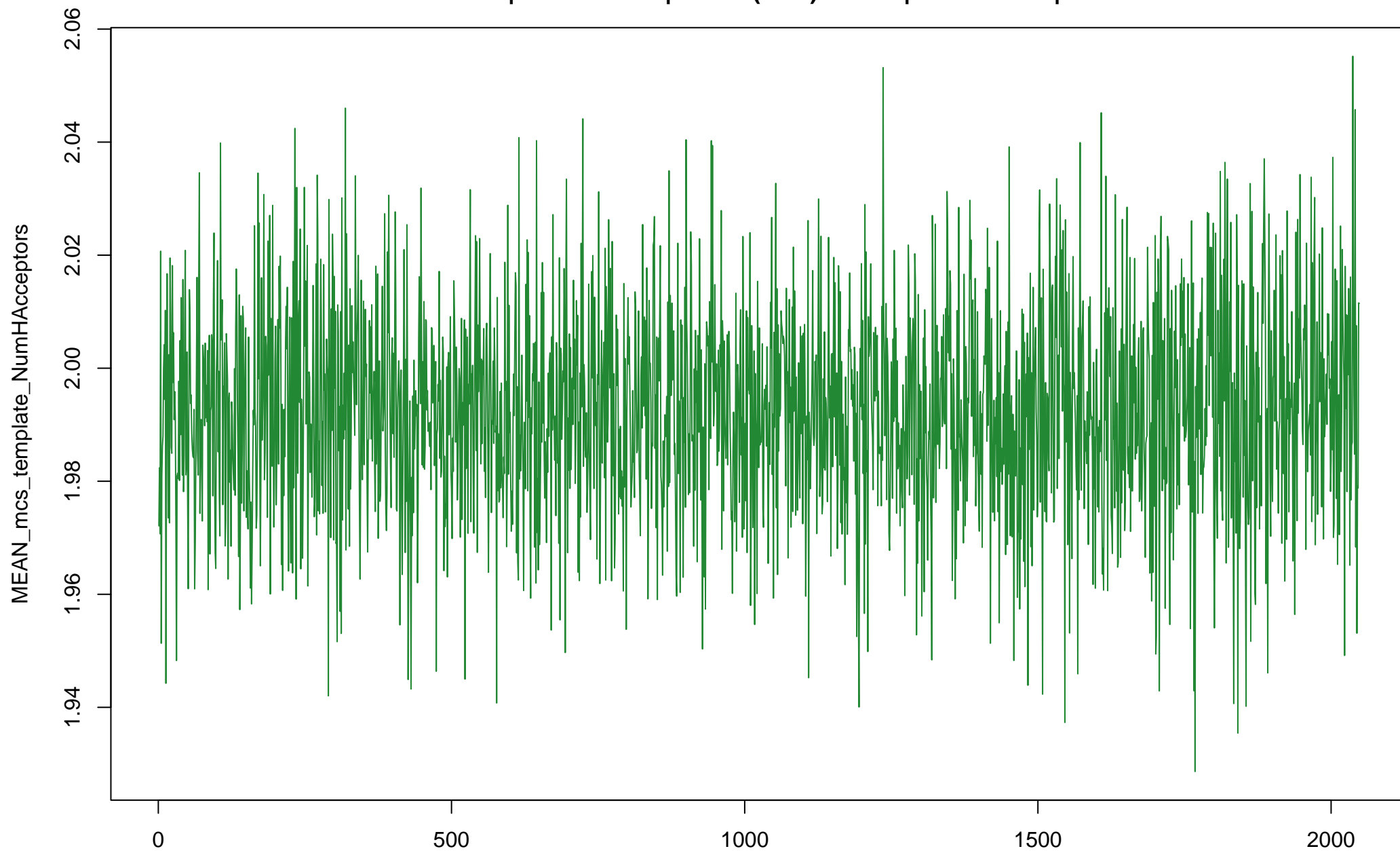
MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0568 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



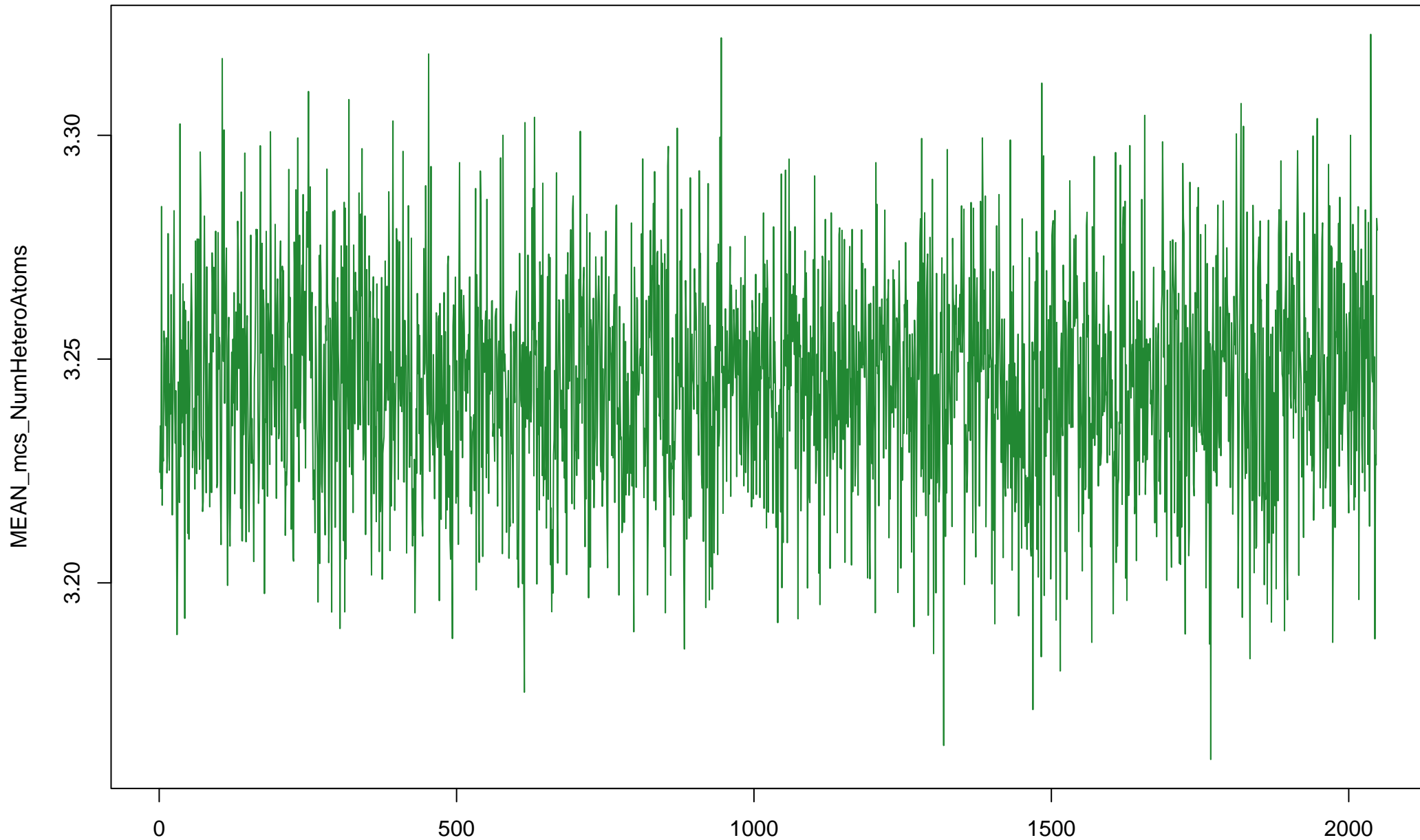
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 1.83 | stat: TRUE | burn: 0



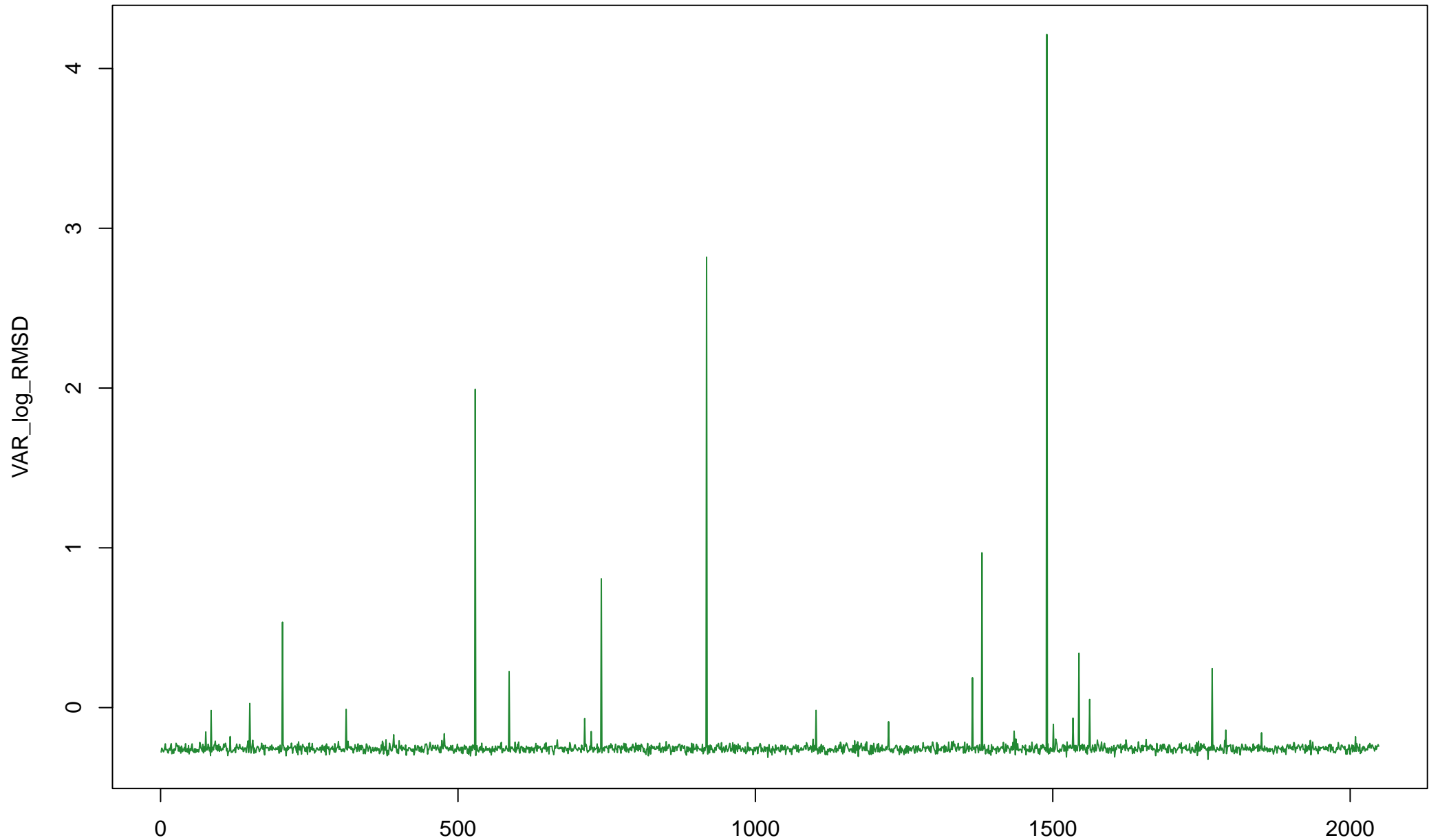
MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.05 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0



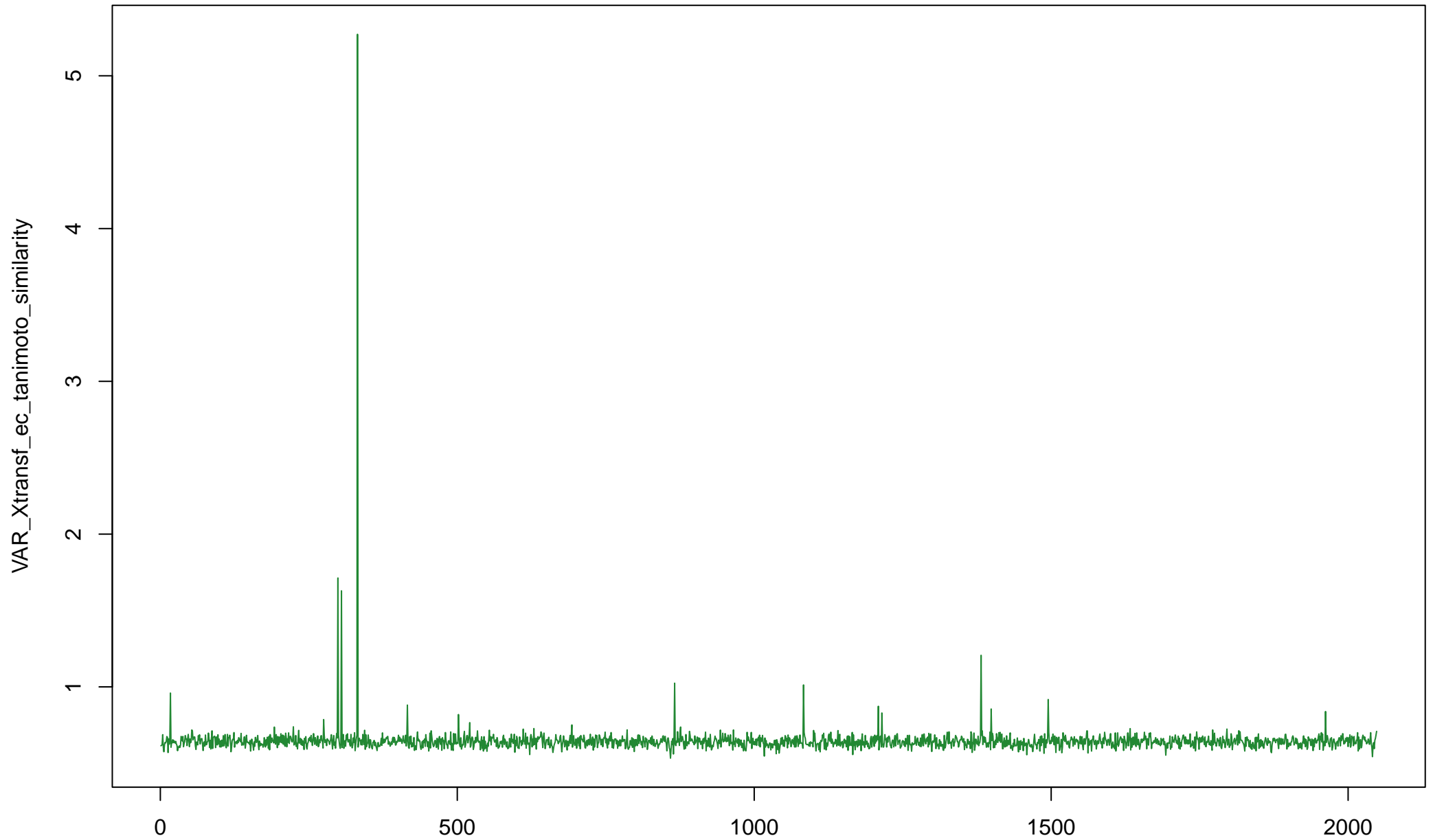
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0475 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0



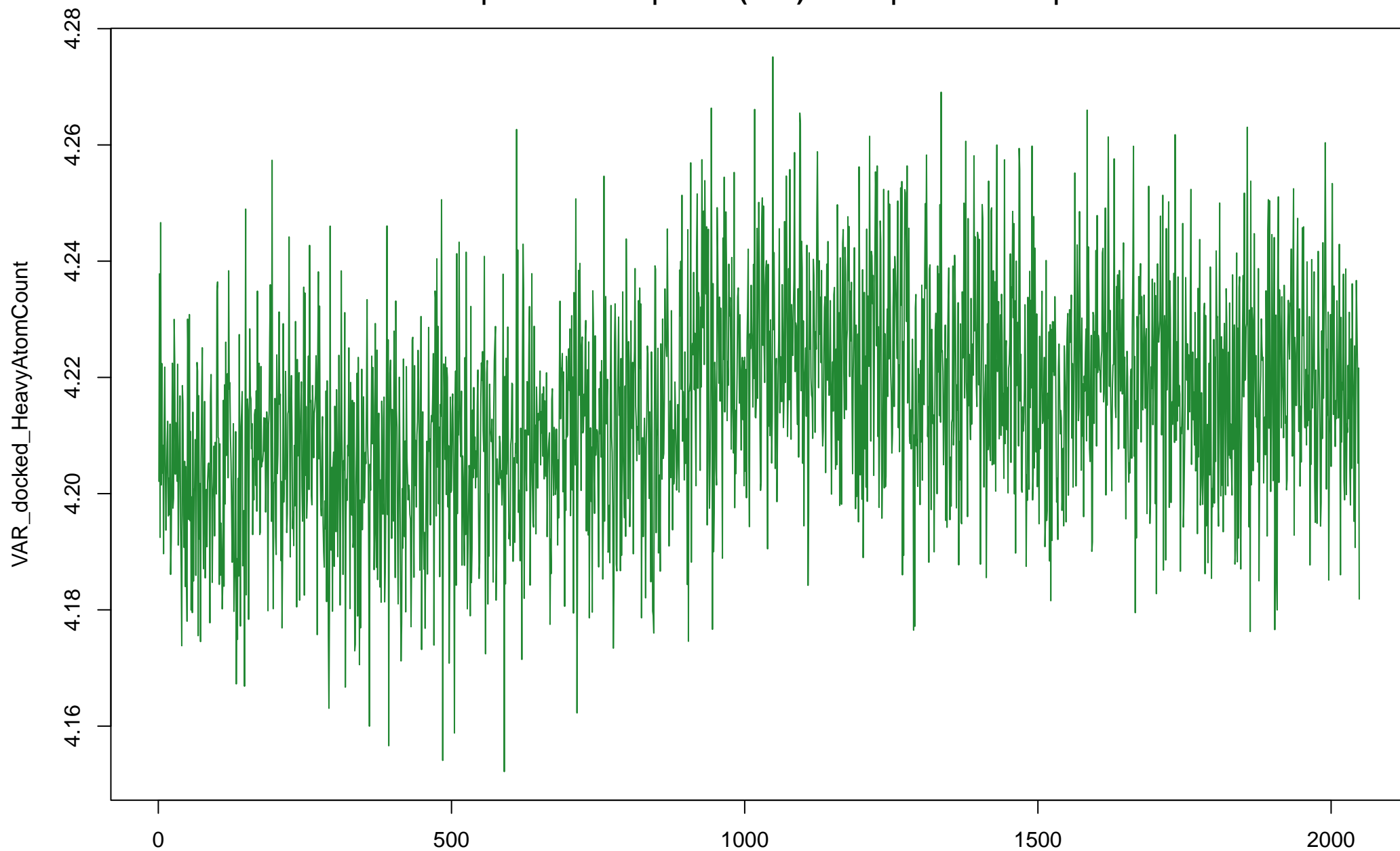
VAR_log_RMSD
ESS = 2050 | BMK = 0.202 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1428



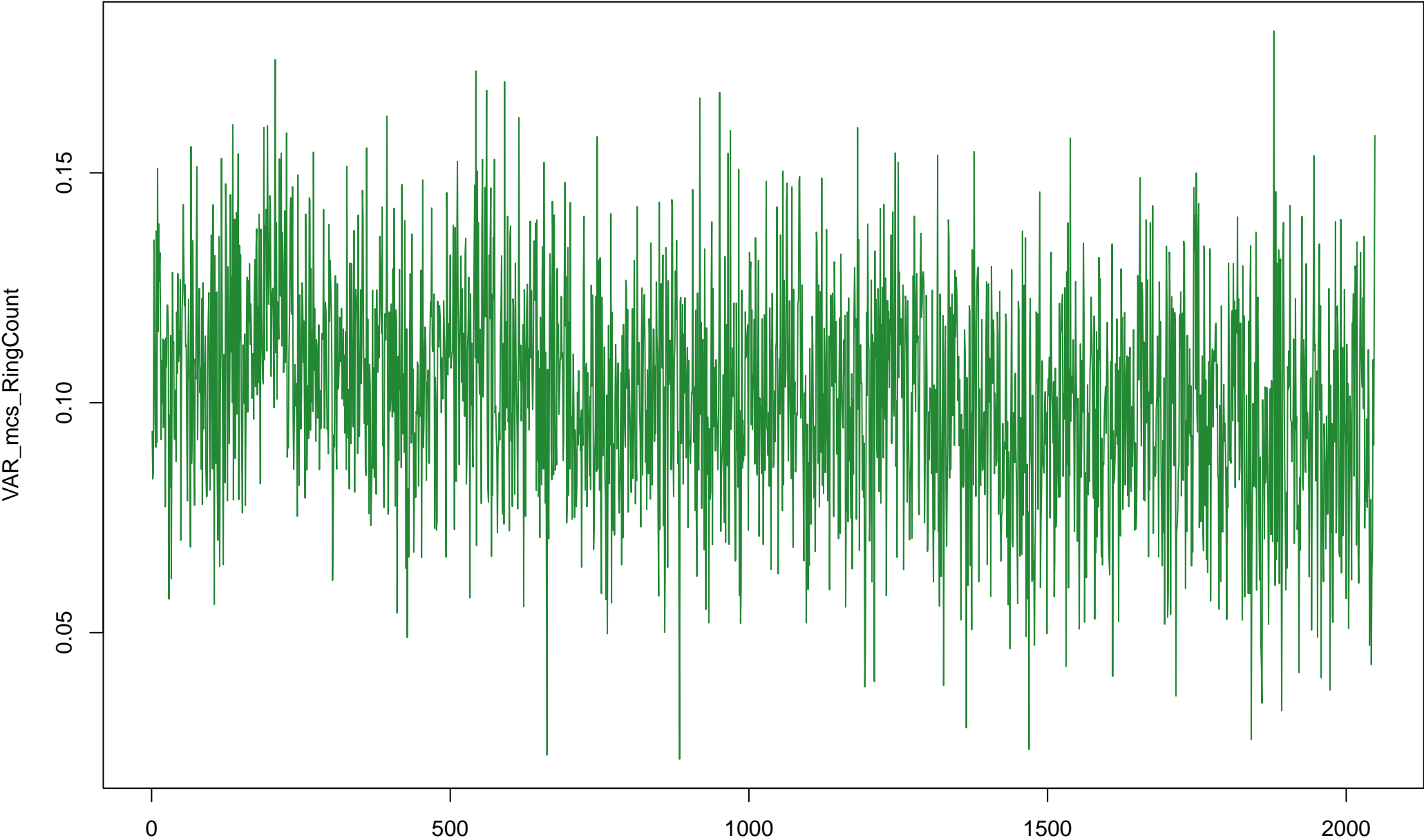
VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.116 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



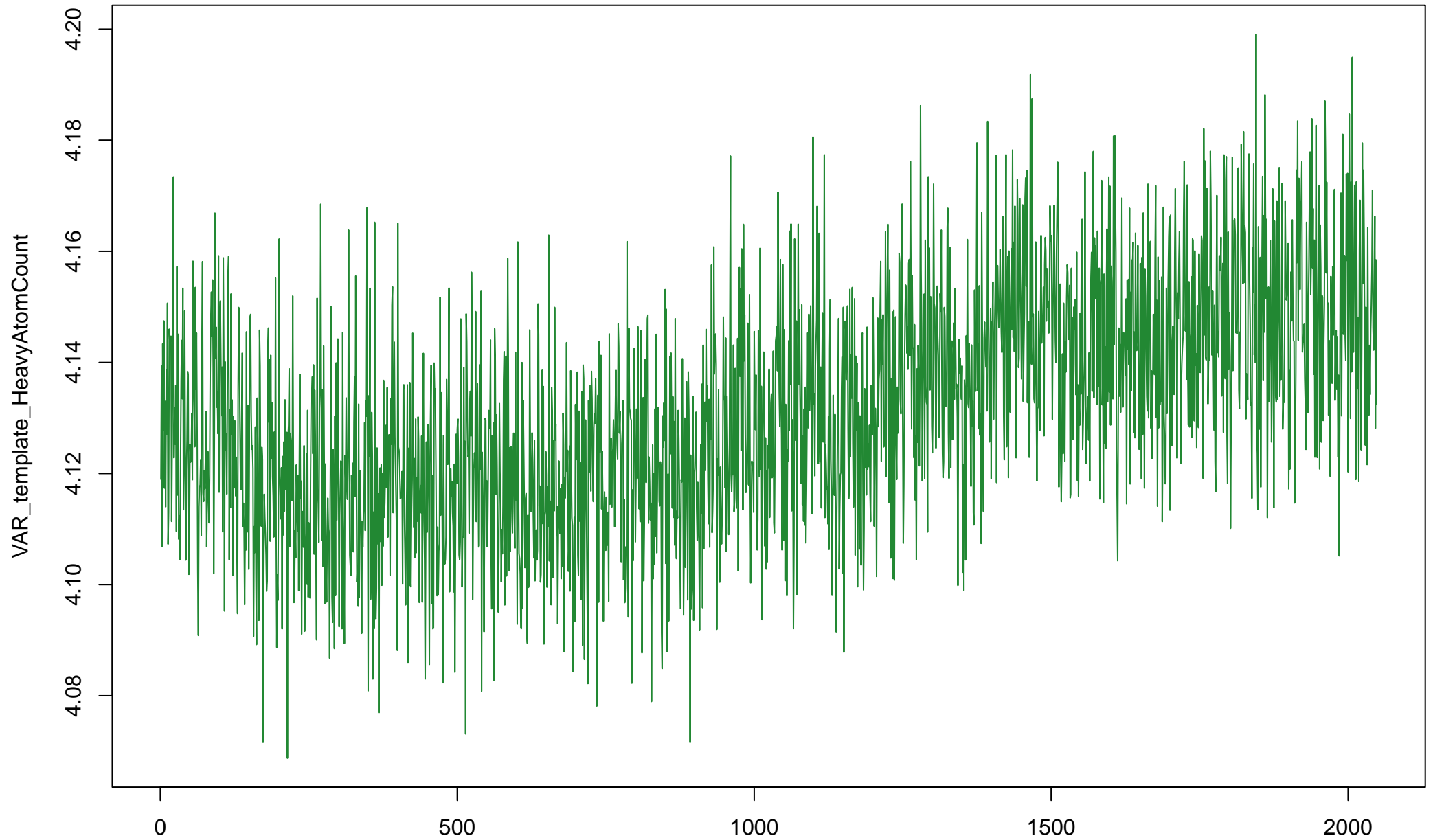
VAR_docked_HeavyAtomCount
ESS = 56 | BMK = 0.244 | MCSE(6.27) = 6.54 | stat: FALSE | burn: 0



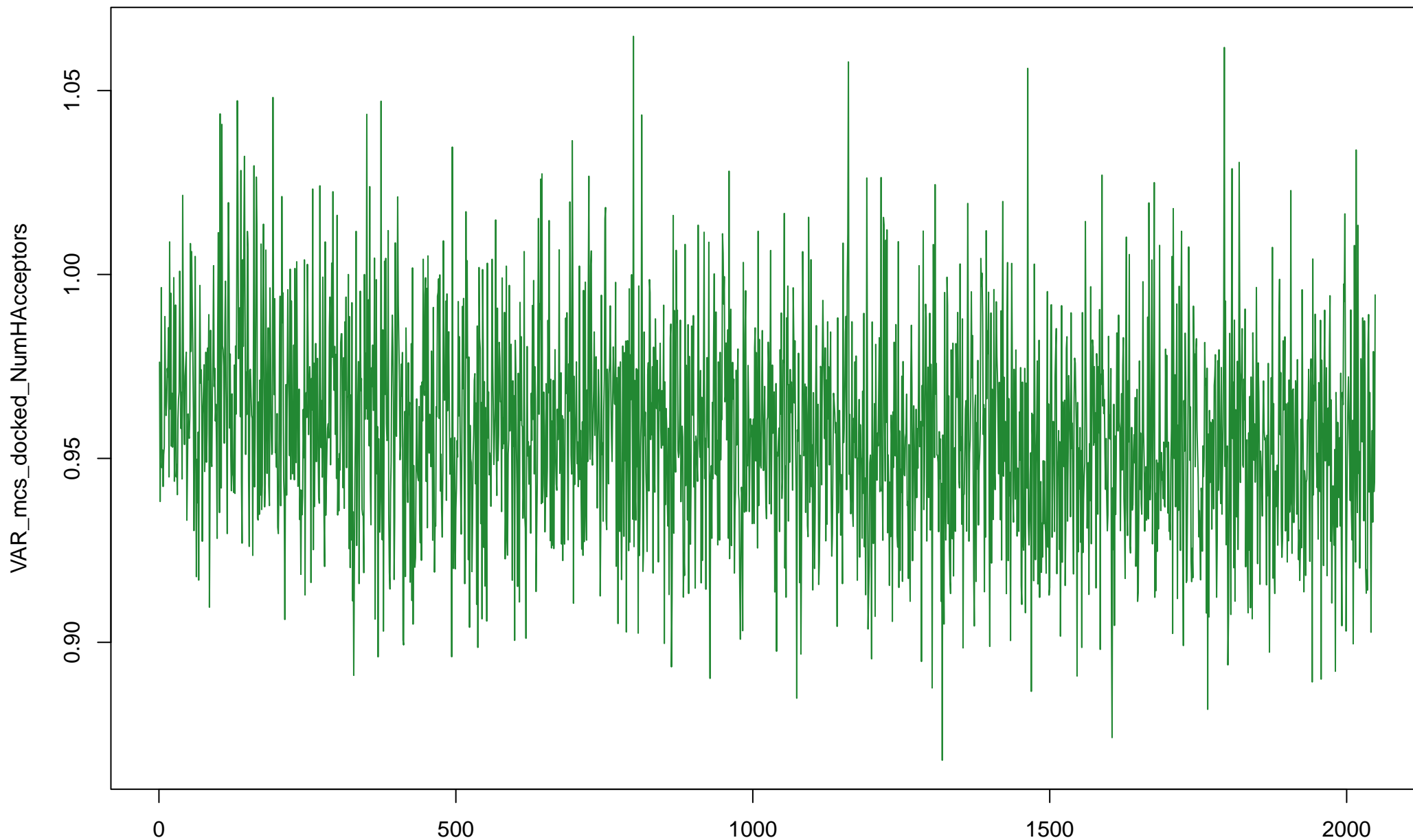
VAR_mcs_RingCount
ESS = 386 | BMK = 0.149 | MCSE(6.27) = 4.66 | stat: FALSE | burn: 0



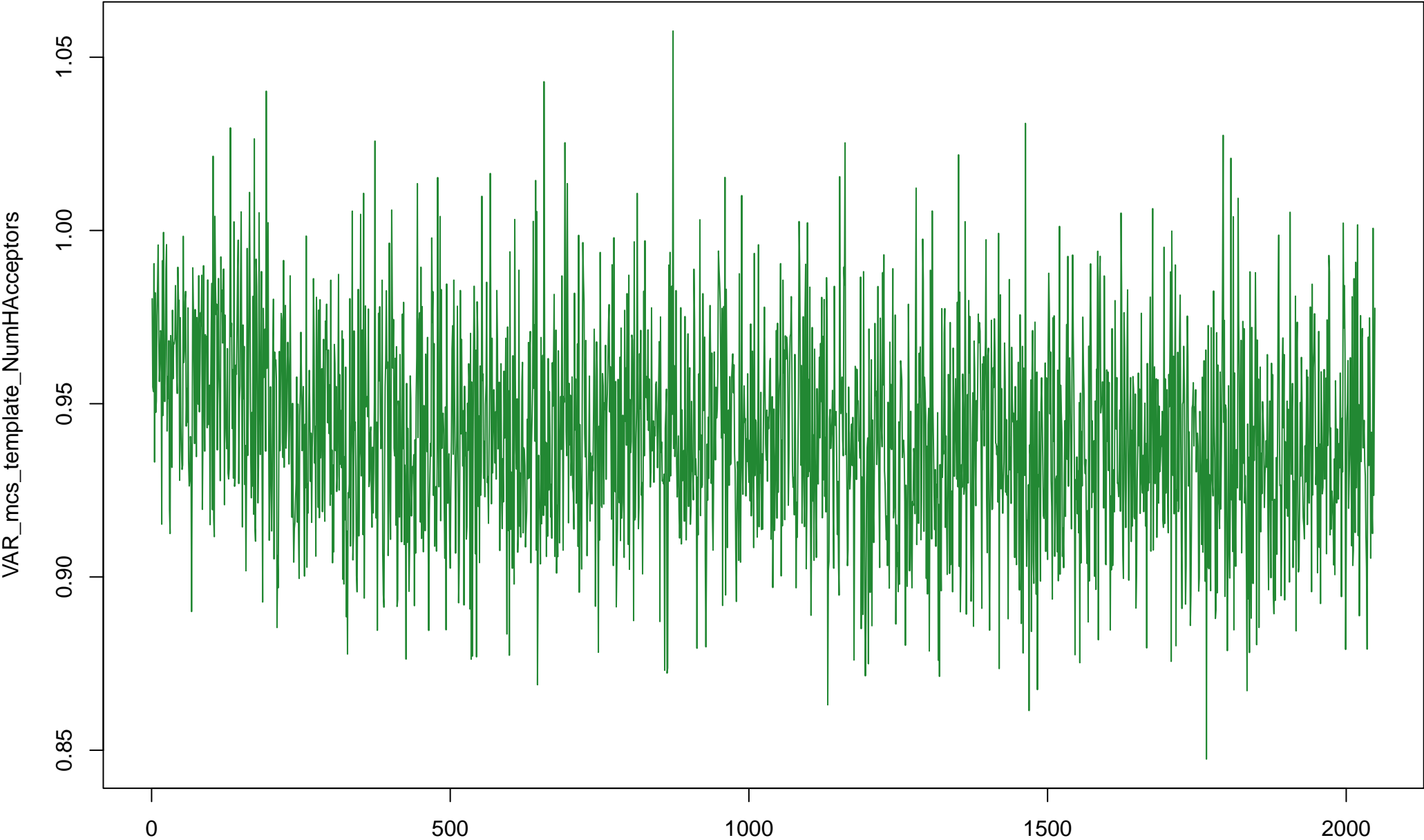
VAR_template_HeavyAtomCount
ESS = 12.1 | BMK = 0.41 | MCSE(6.27) = 9.13 | stat: FALSE | burn: 0



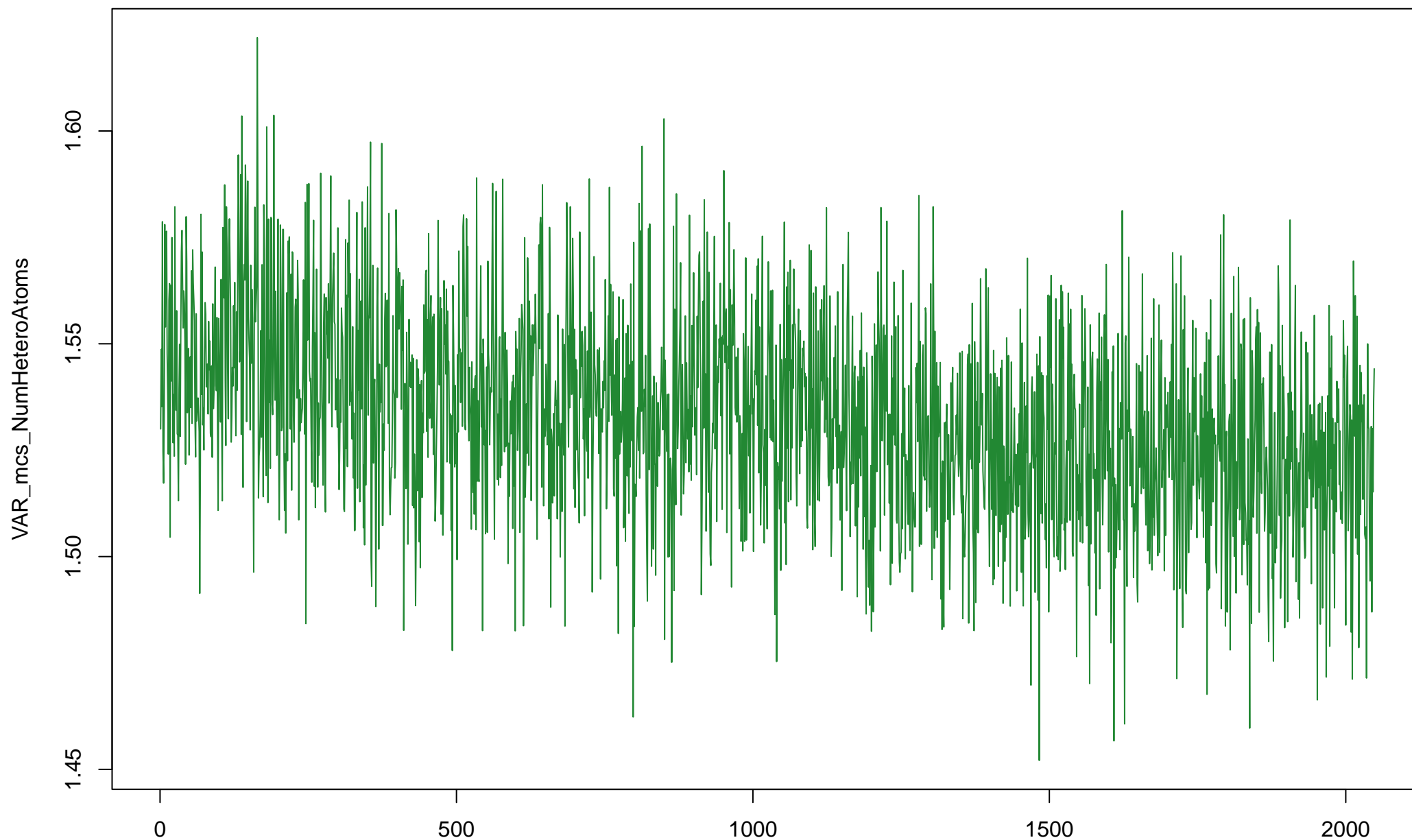
VAR_mcs_docked_NumHAcceptors
ESS = 1110 | BMK = 0.108 | MCSE(6.27) = 3.28 | stat: FALSE | burn: 0



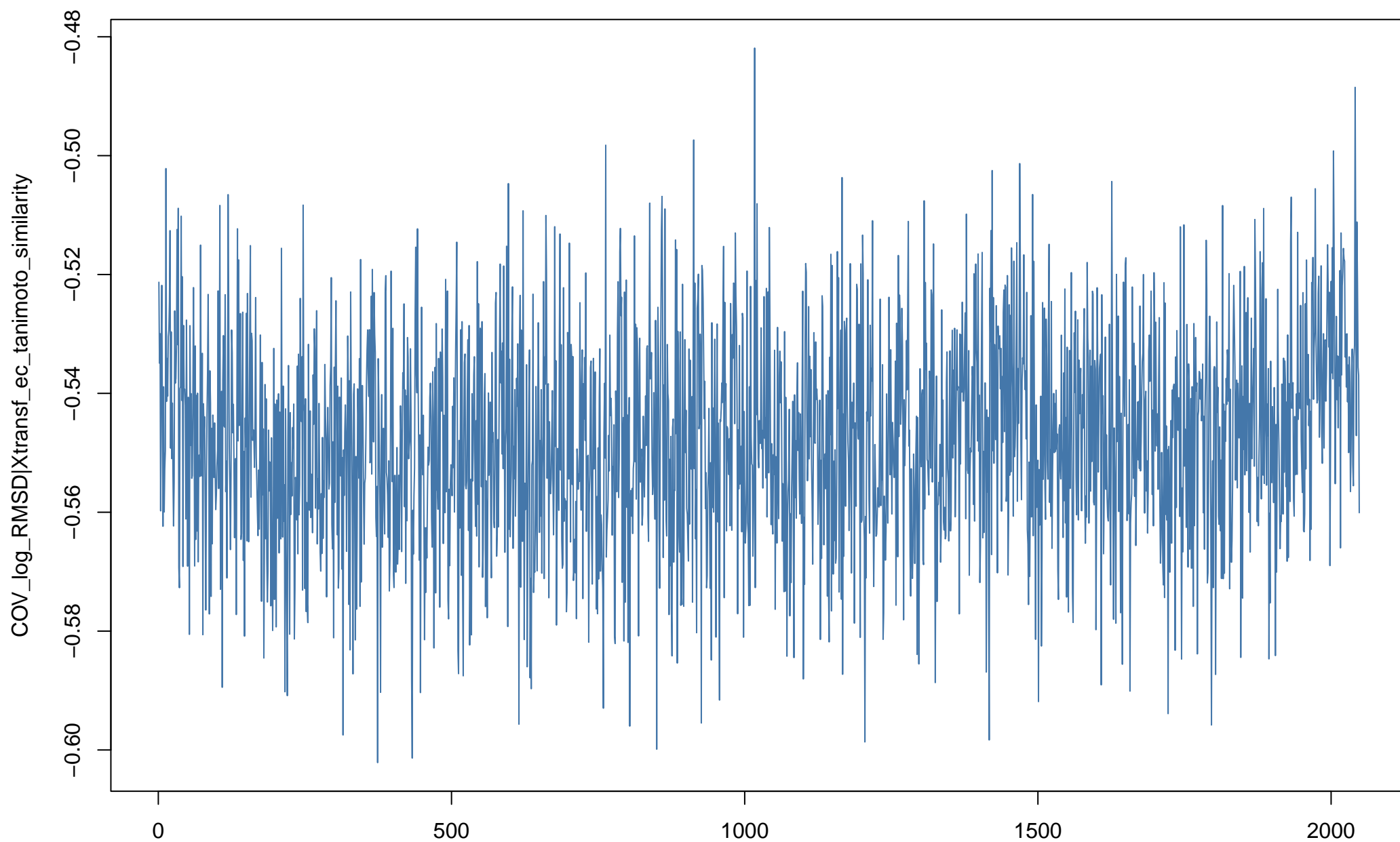
VAR_mcs_template_NumHAcceptors
ESS = 534 | BMK = 0.0976 | MCSE(6.27) = 3.8 | stat: FALSE | burn: 0



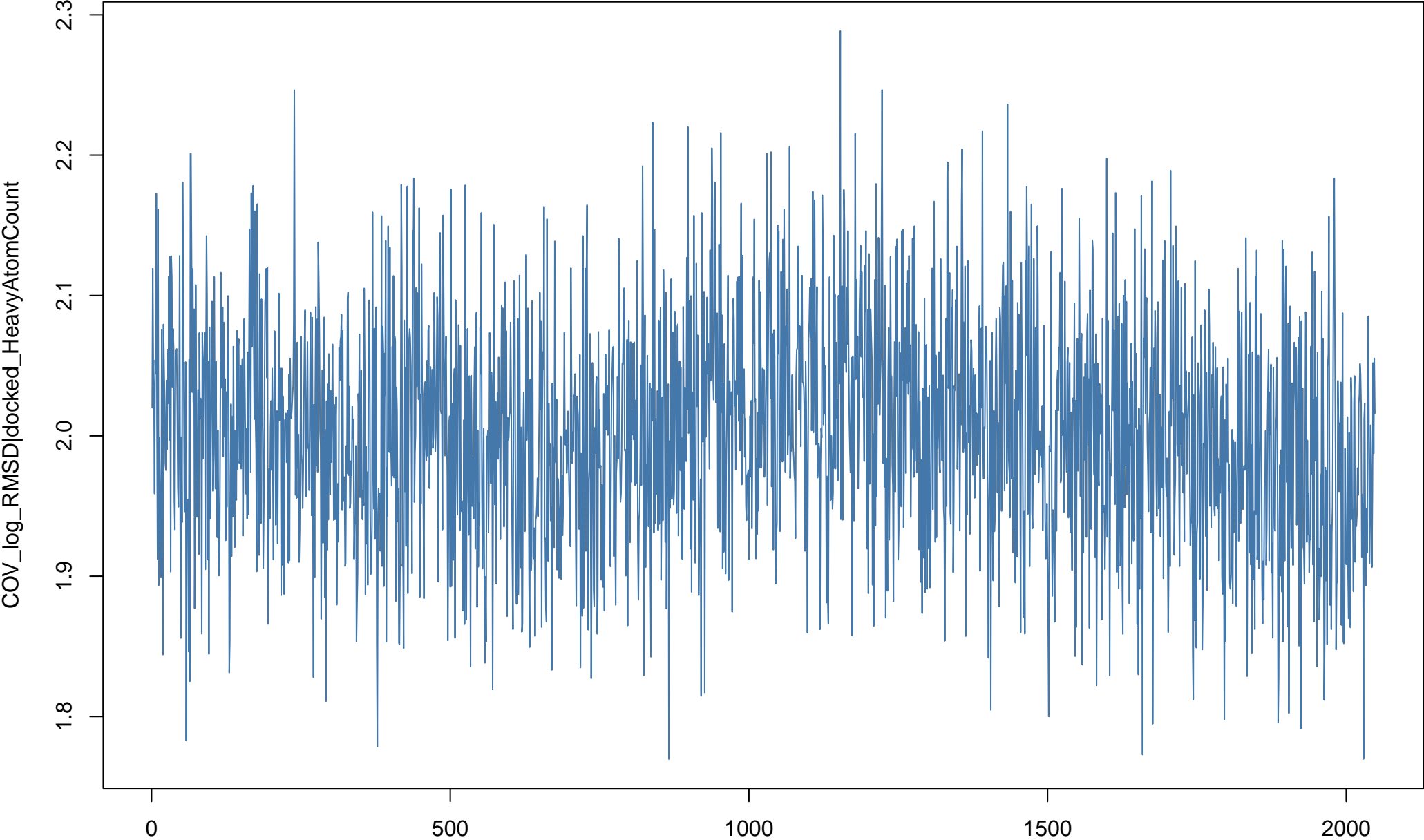
VAR_mcs_NumHeteroAtoms
ESS = 69.4 | BMK = 0.243 | MCSE(6.27) = 5.92 | stat: FALSE | burn: 0



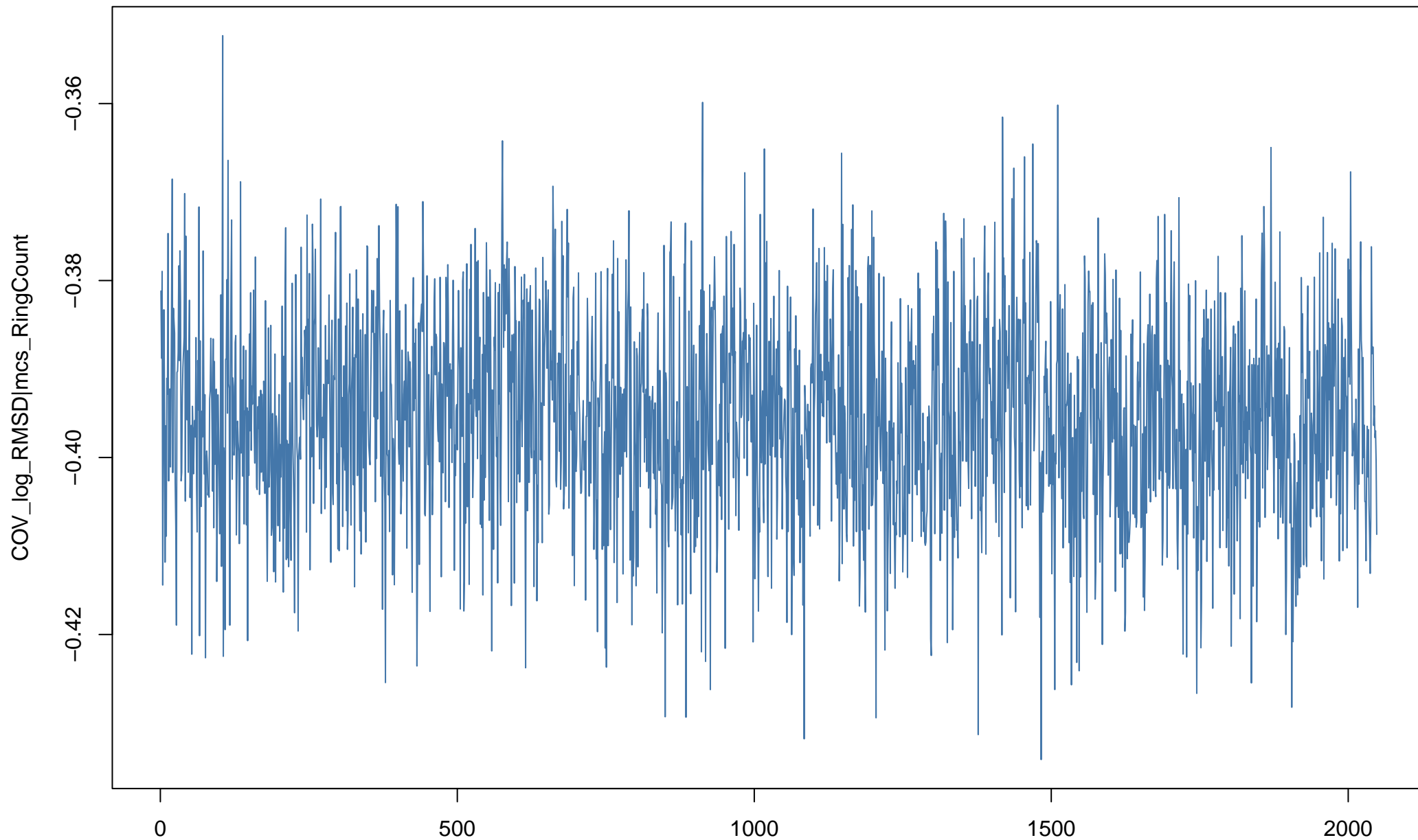
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 581 | BMK = 0.0736 | MCSE(6.27) = 3.68 | stat: TRUE | burn: 0



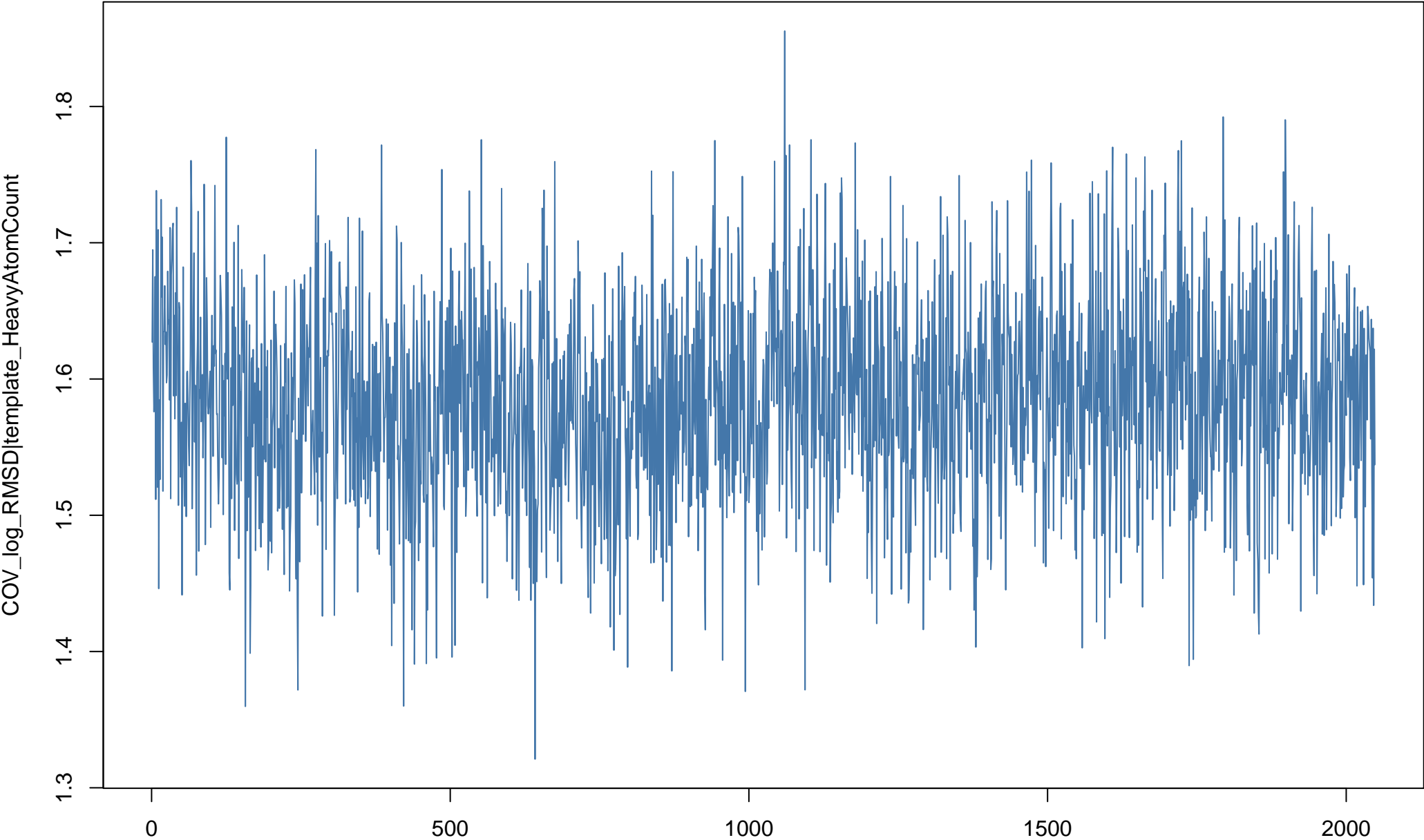
COV_log_RMSD|docked_HeavyAtomCount
ESS = 750 | BMK = 0.0372 | MCSE(6.27) = 3.81 | stat: TRUE | burn: 0



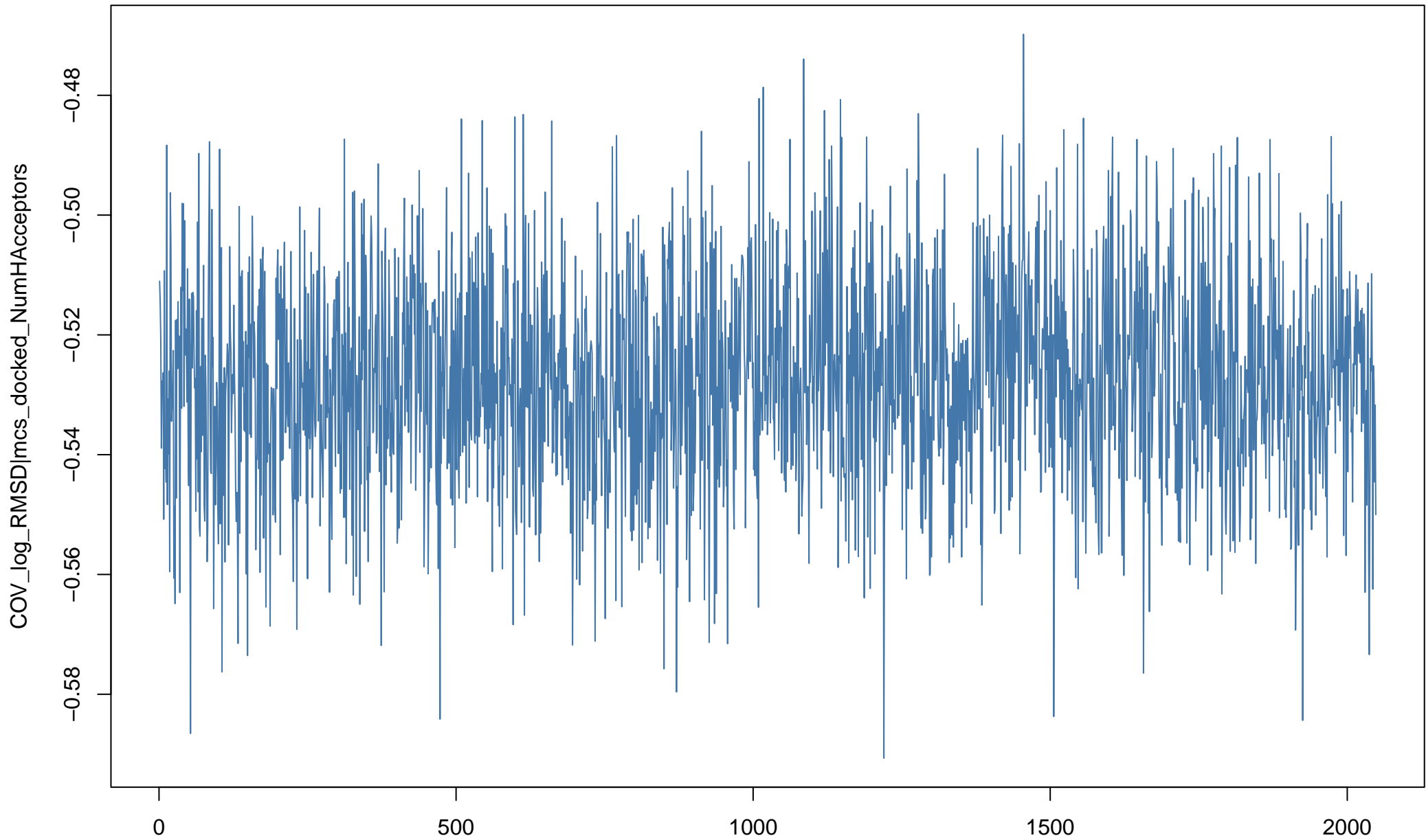
COV_log_RMSD|mcs_RingCount
ESS = 1550 | BMK = 0.06 | MCSE(6.27) = 3.4 | stat: TRUE | burn: 0



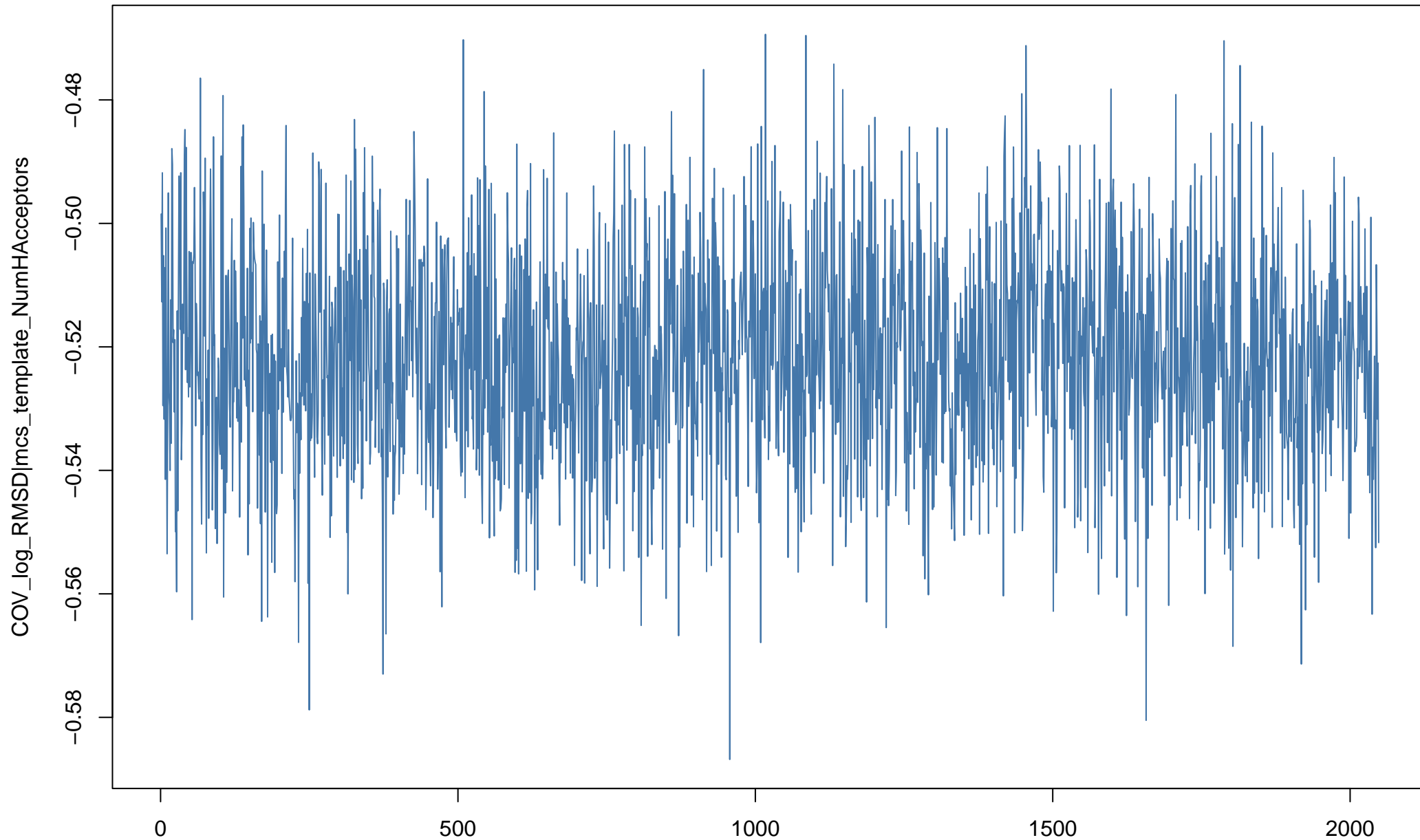
COV_log_RMSD|template_HeavyAtomCount
ESS = 697 | BMK = 0.0807 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0



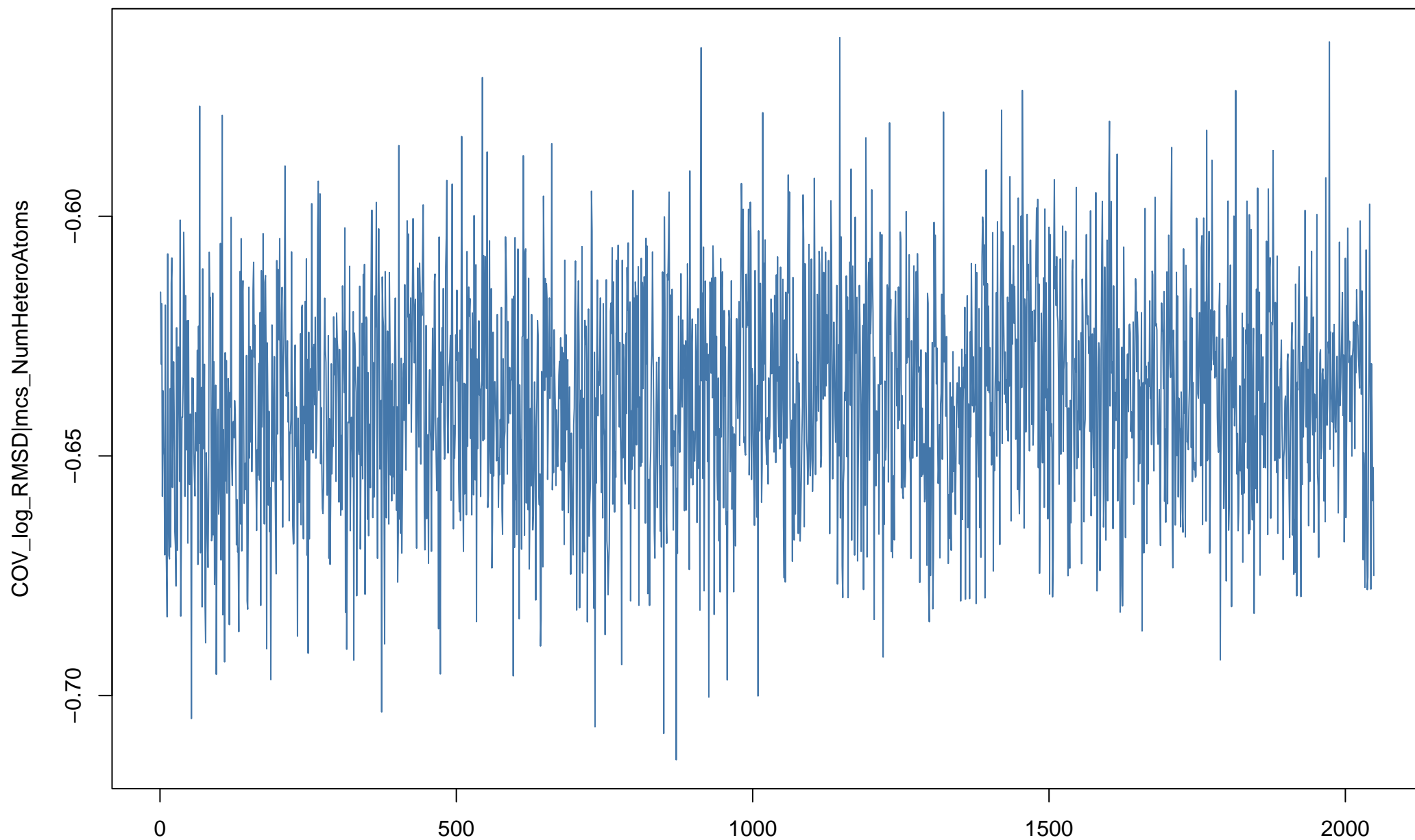
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 1800 | BMK = 0.0685 | MCSE(6.27) = 2.6 | stat: FALSE | burn: 0



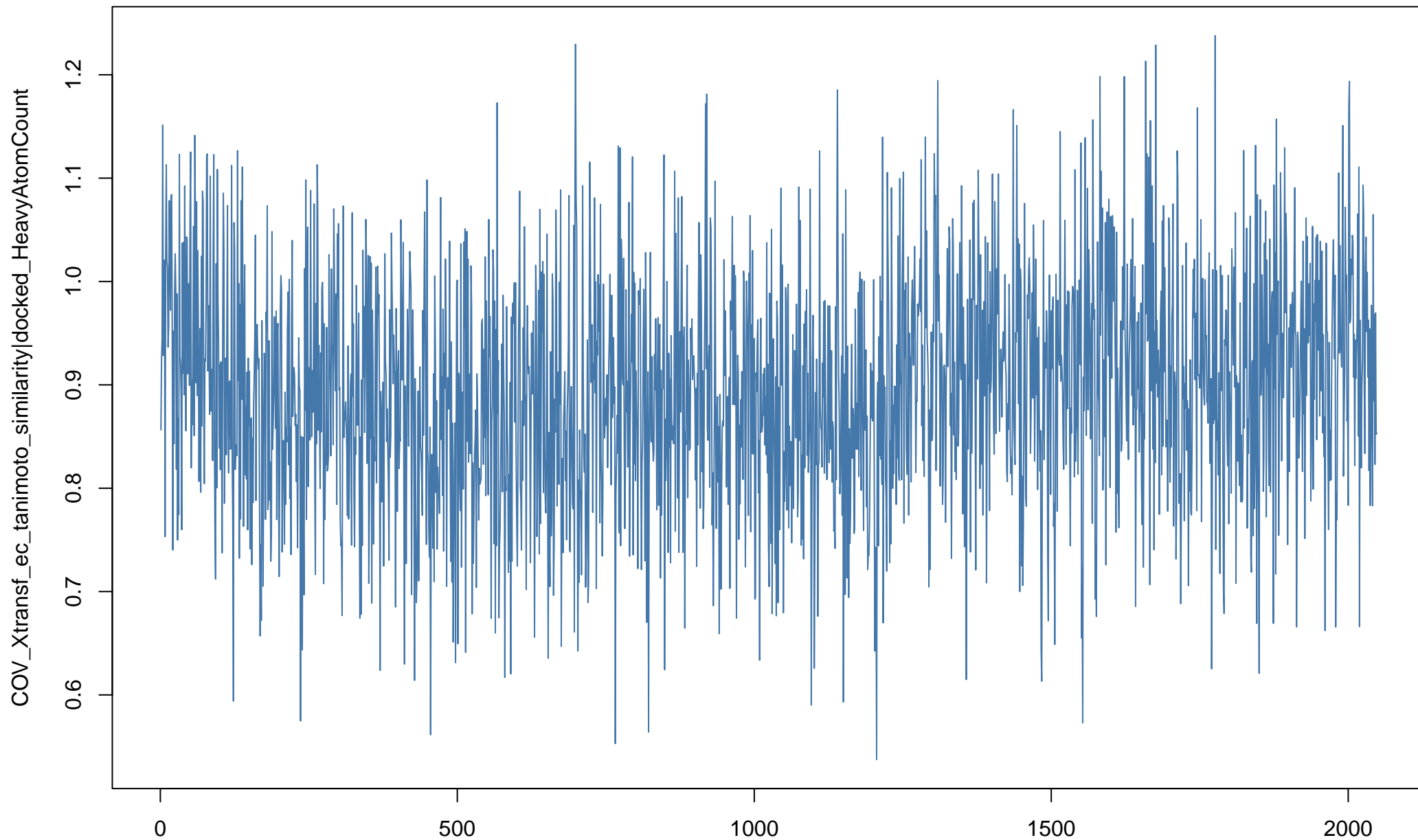
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 1630 | BMK = 0.0365 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0



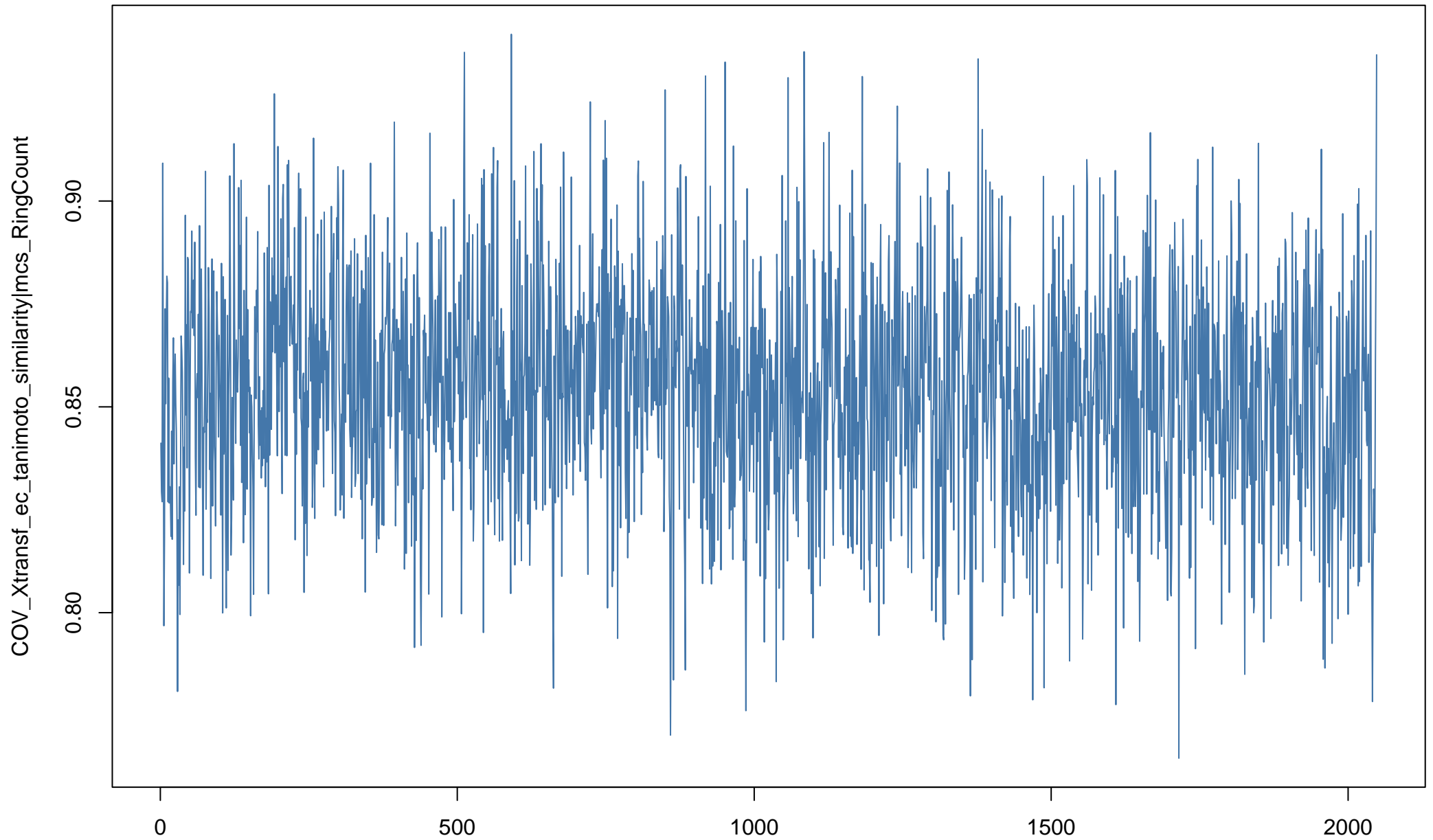
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1550 | BMK = 0.0951 | MCSE(6.27) = 3.05 | stat: FALSE | burn: 0



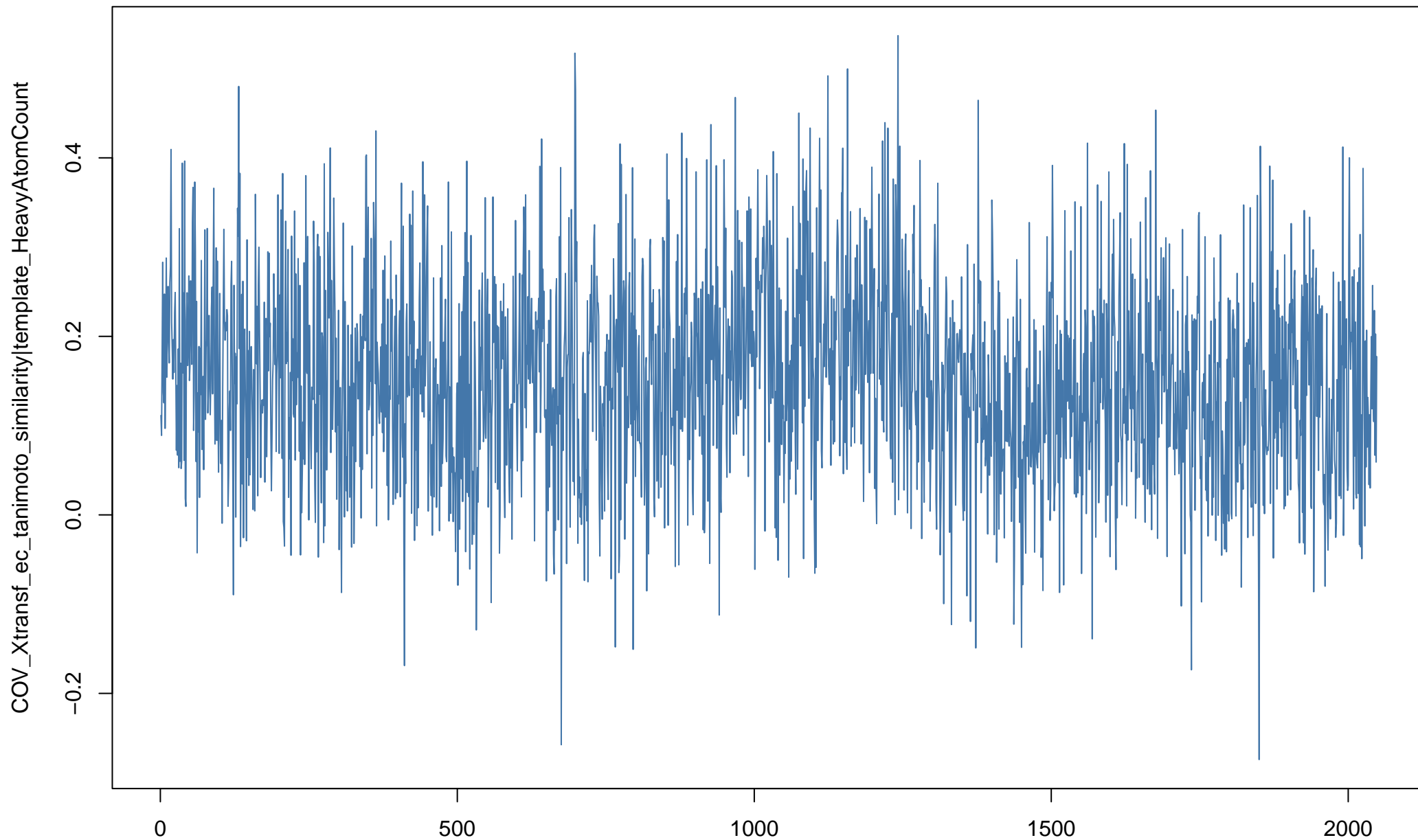
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 323 | BMK = 0.0779 | MCSE(6.27) = 3.92 | stat: TRUE | burn: 0



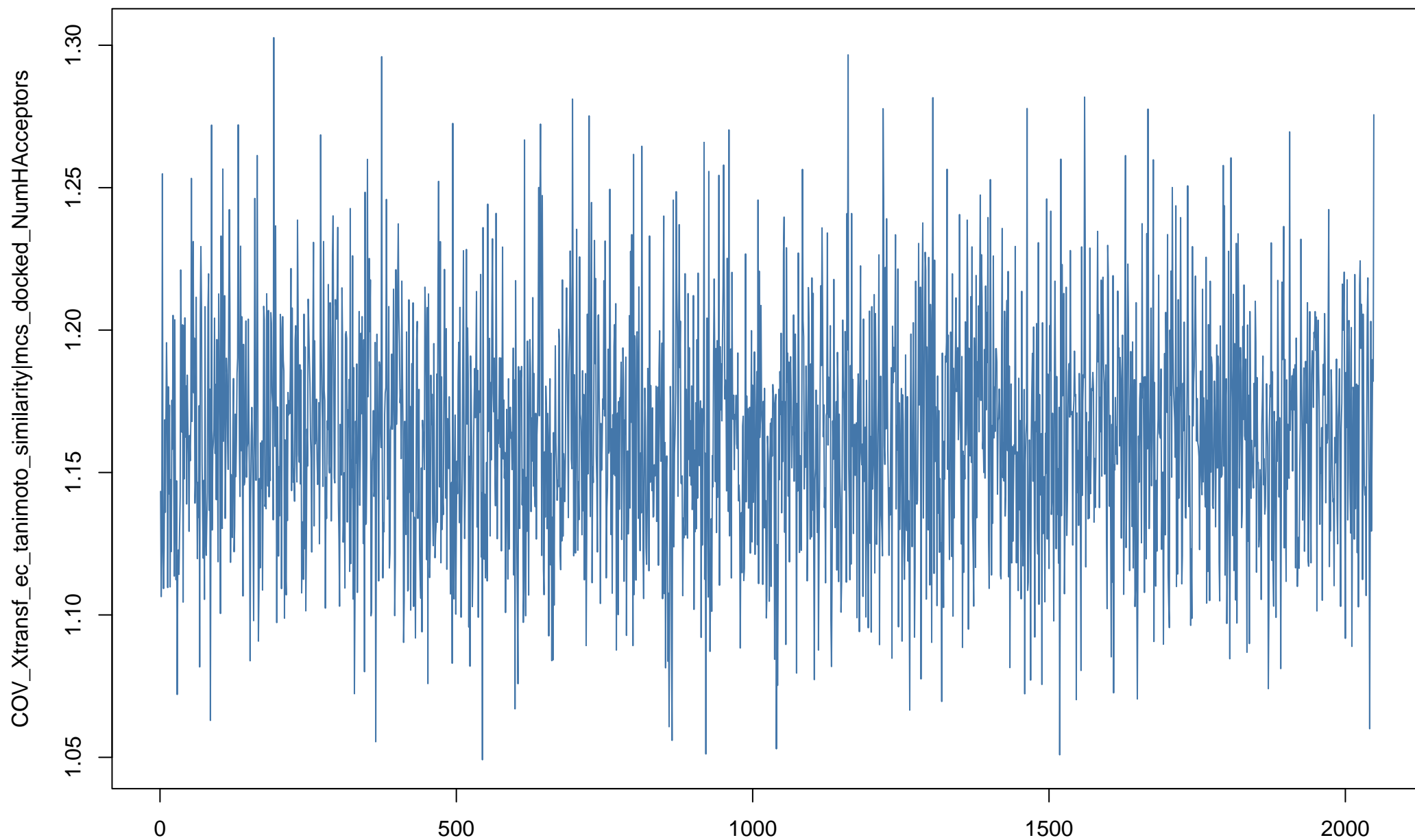
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 954 | BMK = 0.0703 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0



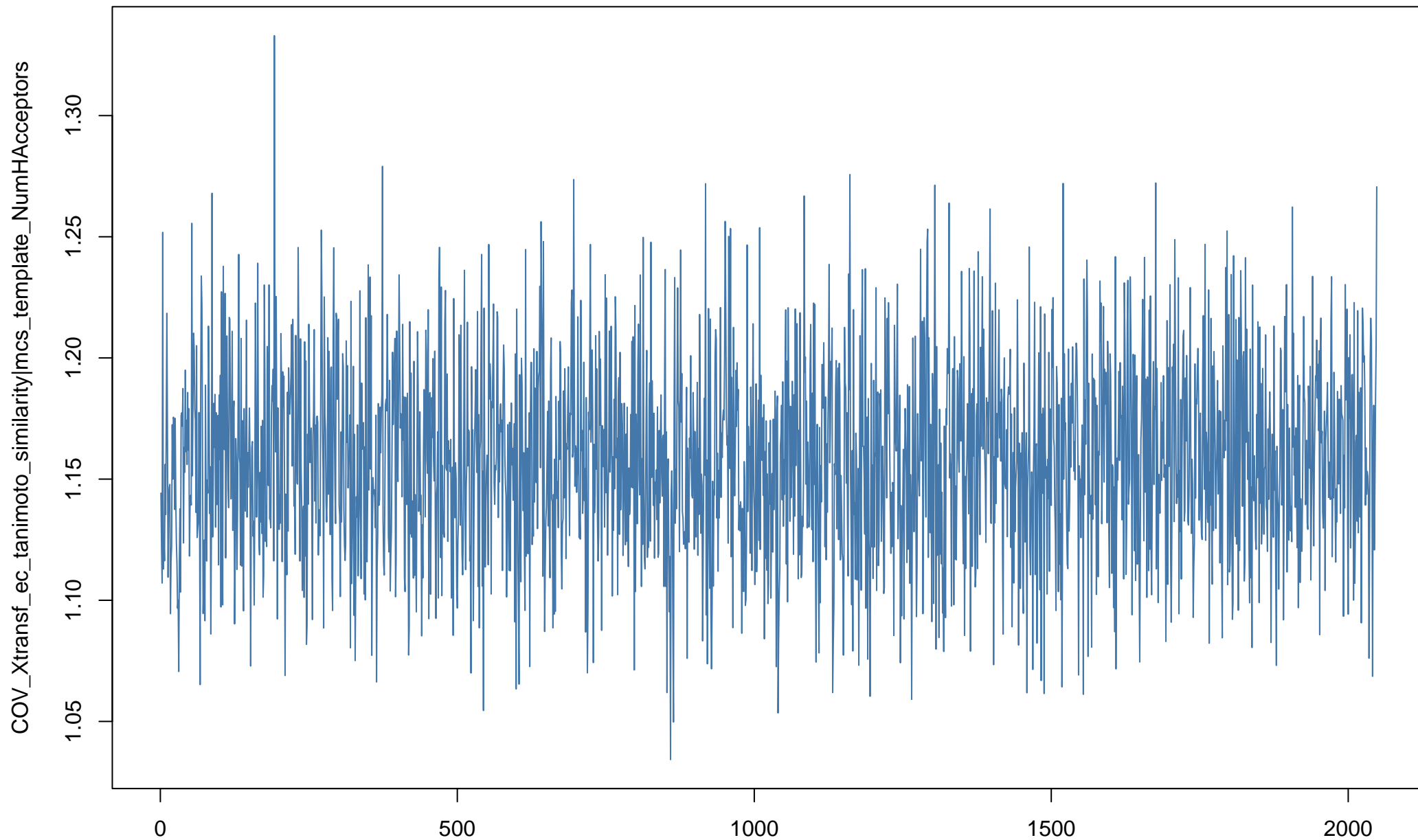
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 716 | BMK = 0.0546 | MCSE(6.27) = 3.99 | stat: FALSE | burn: 0



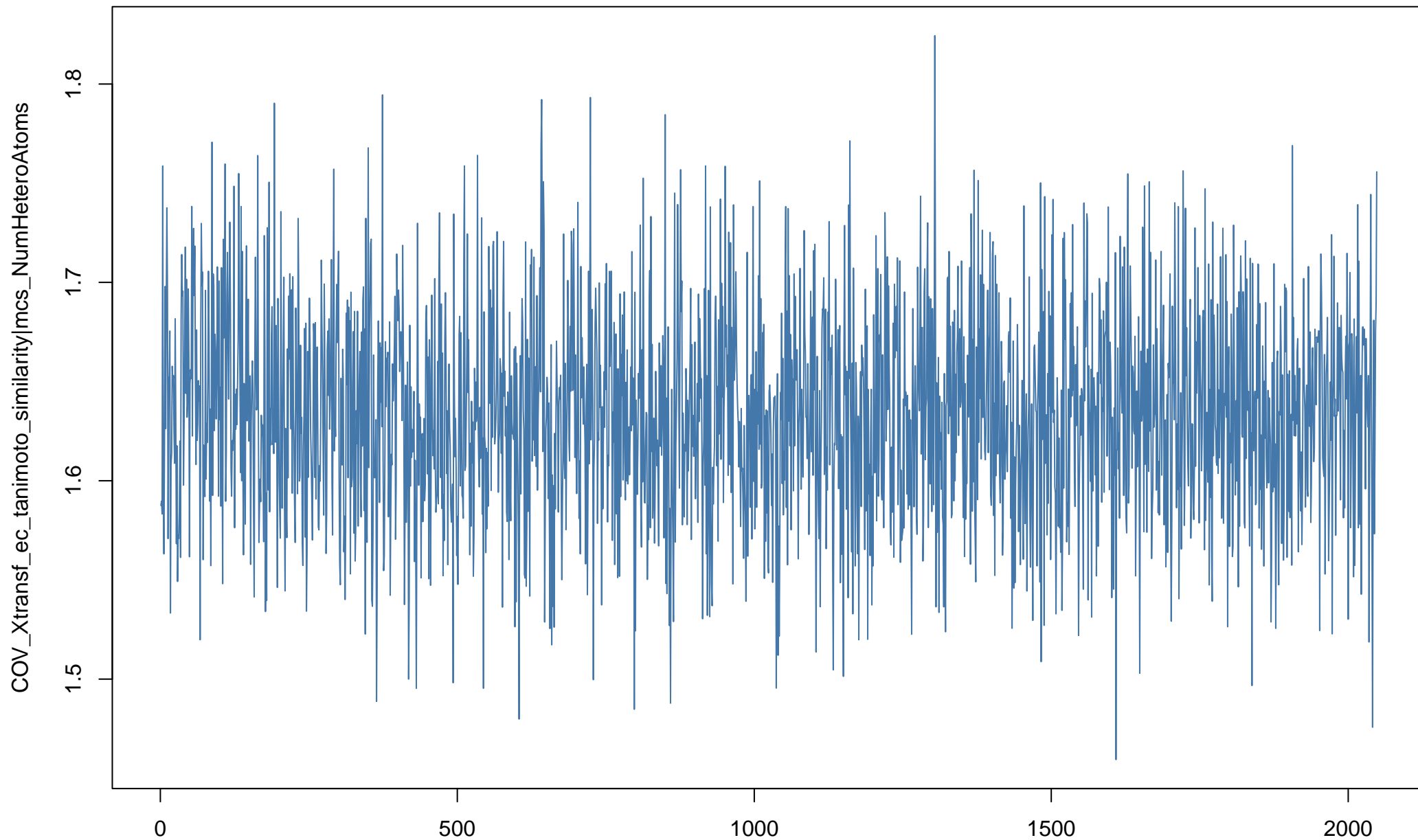
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0432 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0



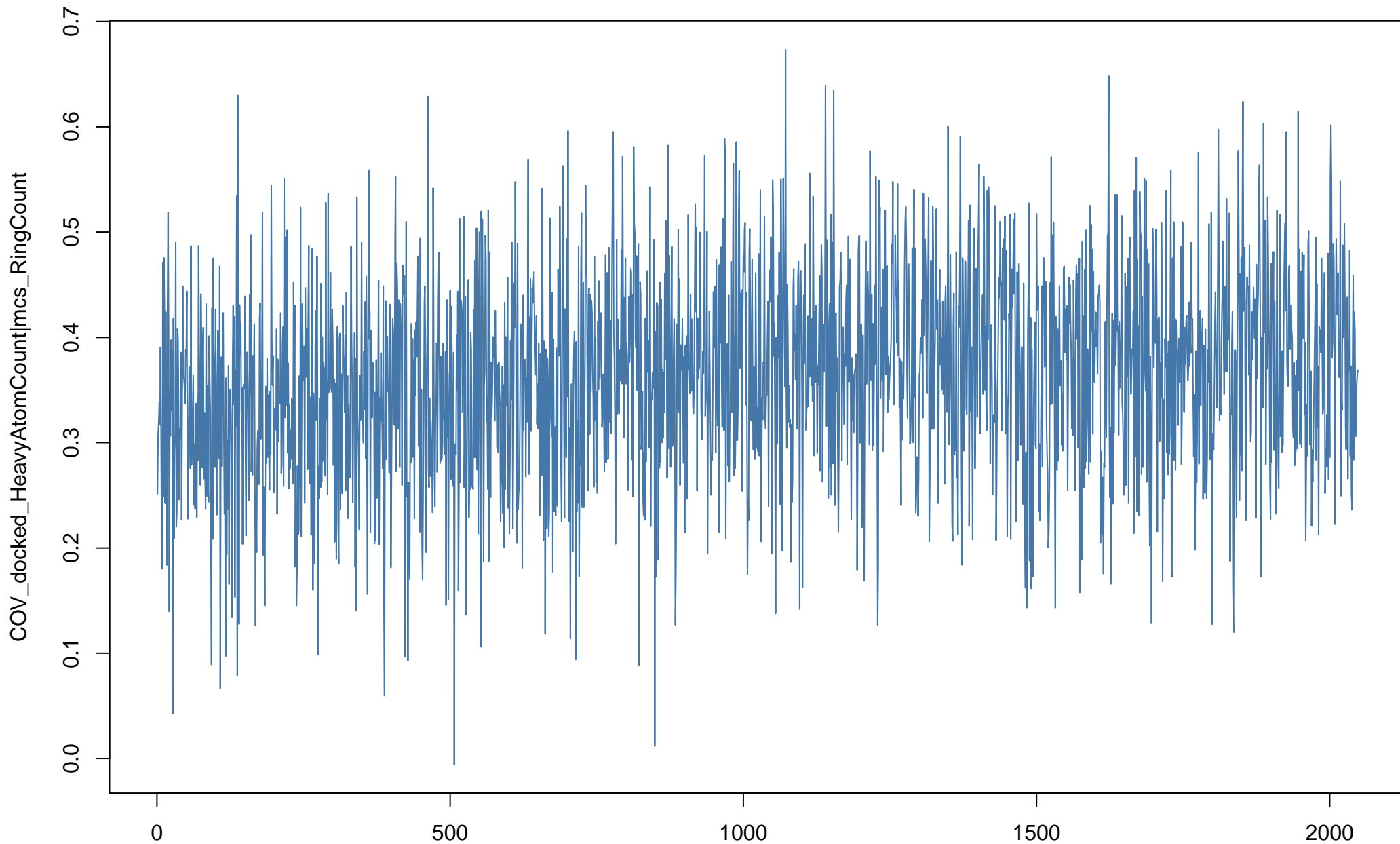
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0475 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



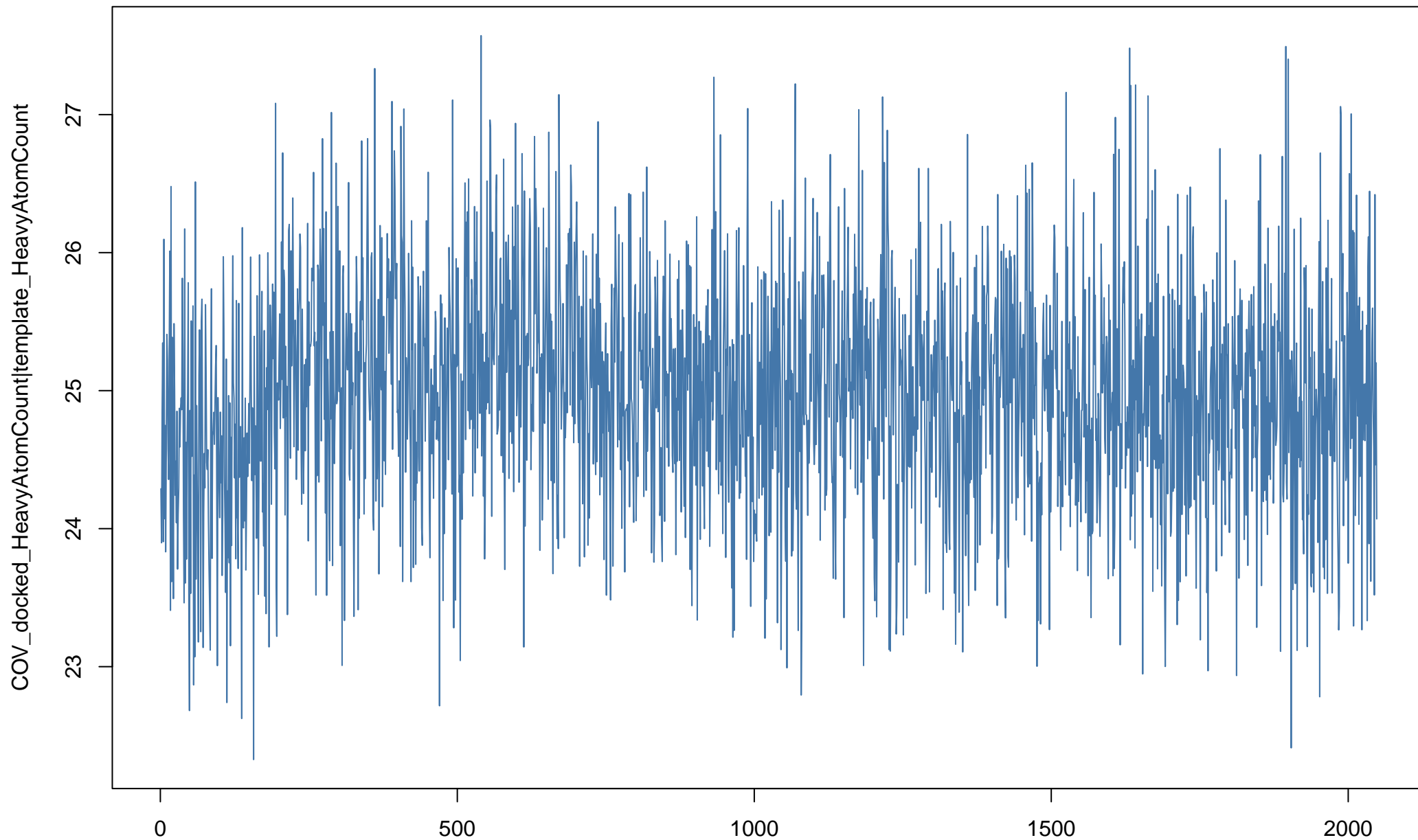
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0497 | MCSE(6.27) = 2.15 | stat: FALSE | burn: 0



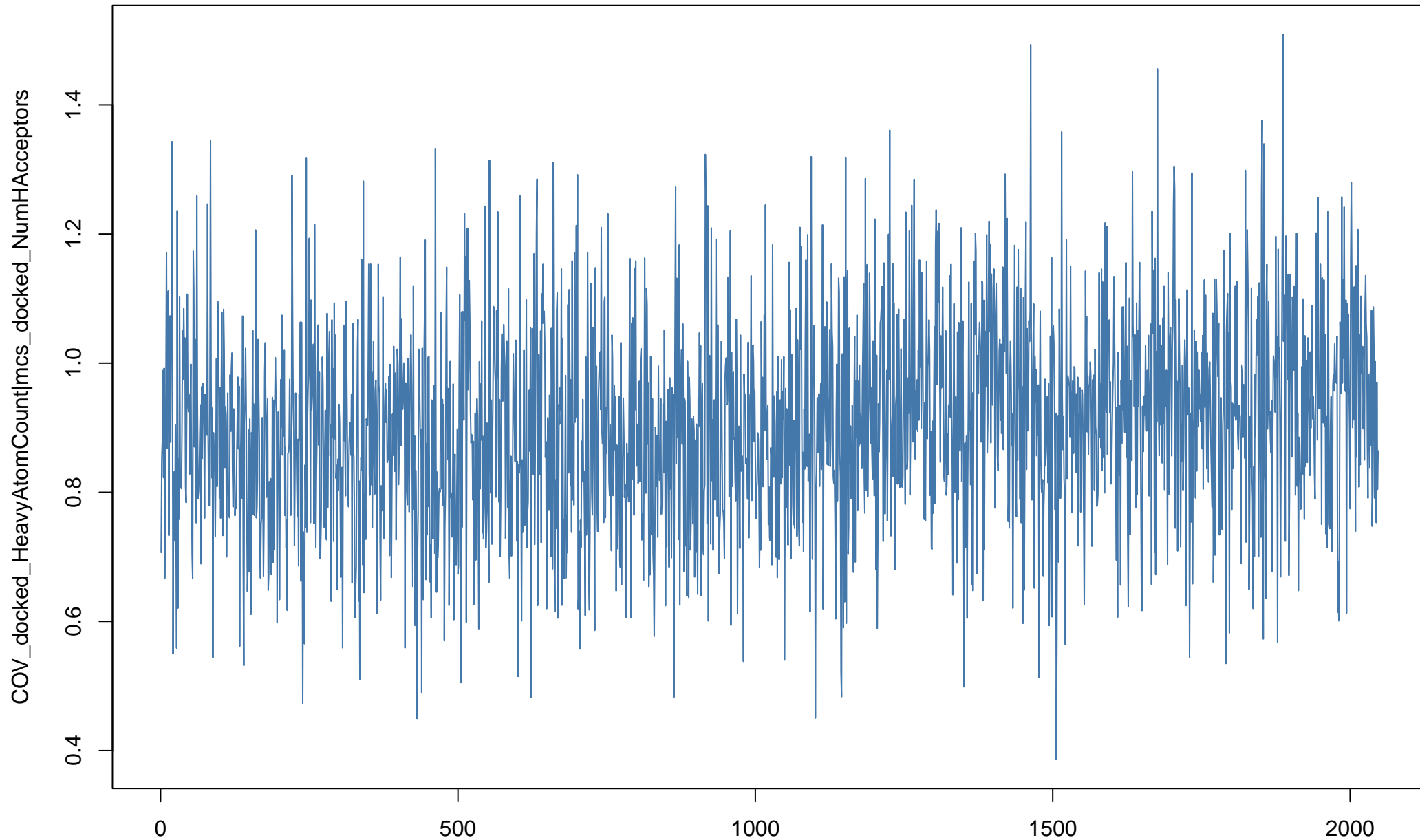
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1200 | BMK = 0.127 | MCSE(6.27) = 3.86 | stat: FALSE | burn: 0



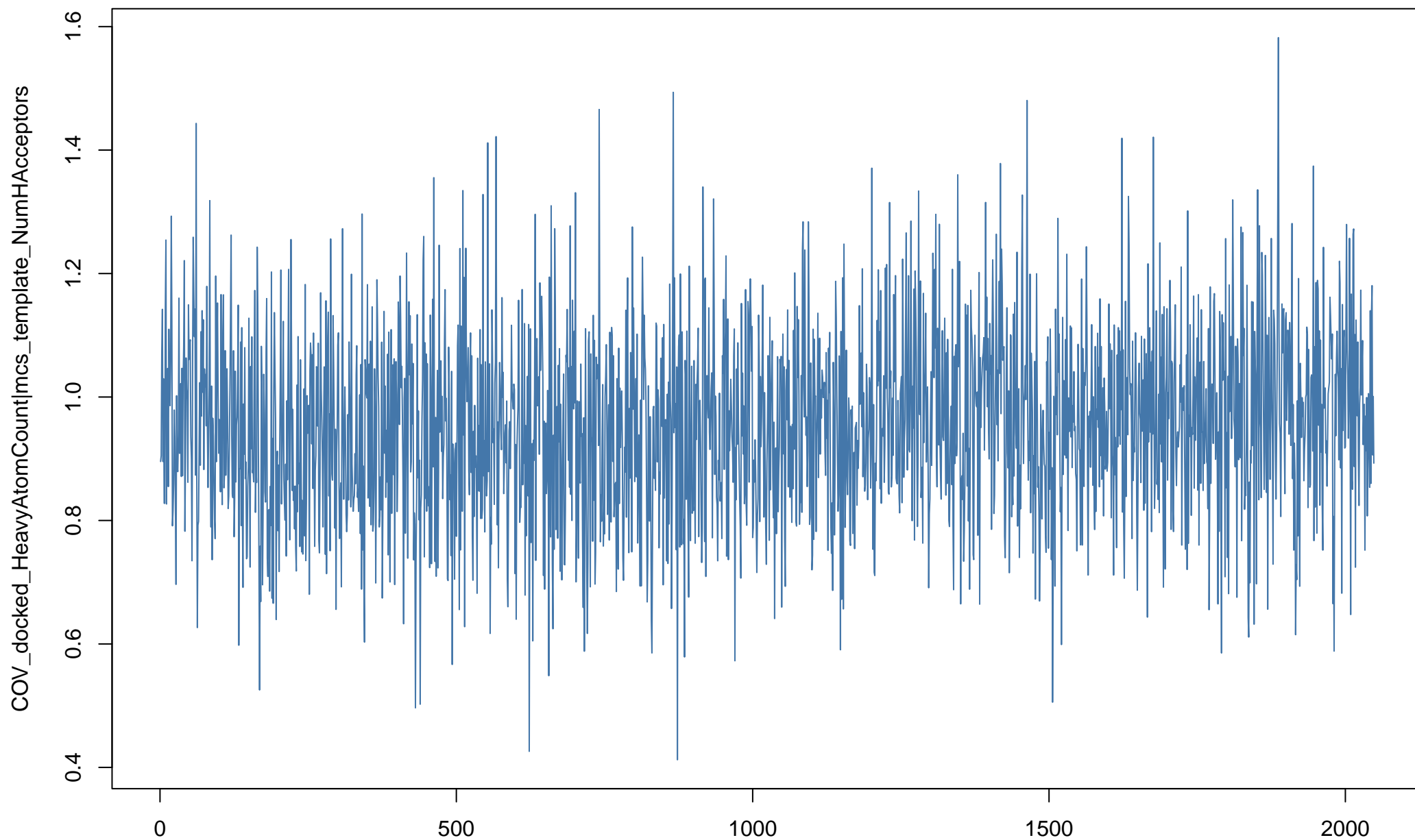
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 493 | BMK = 0.0439 | MCSE(6.27) = 3.61 | stat: FALSE | burn: 0



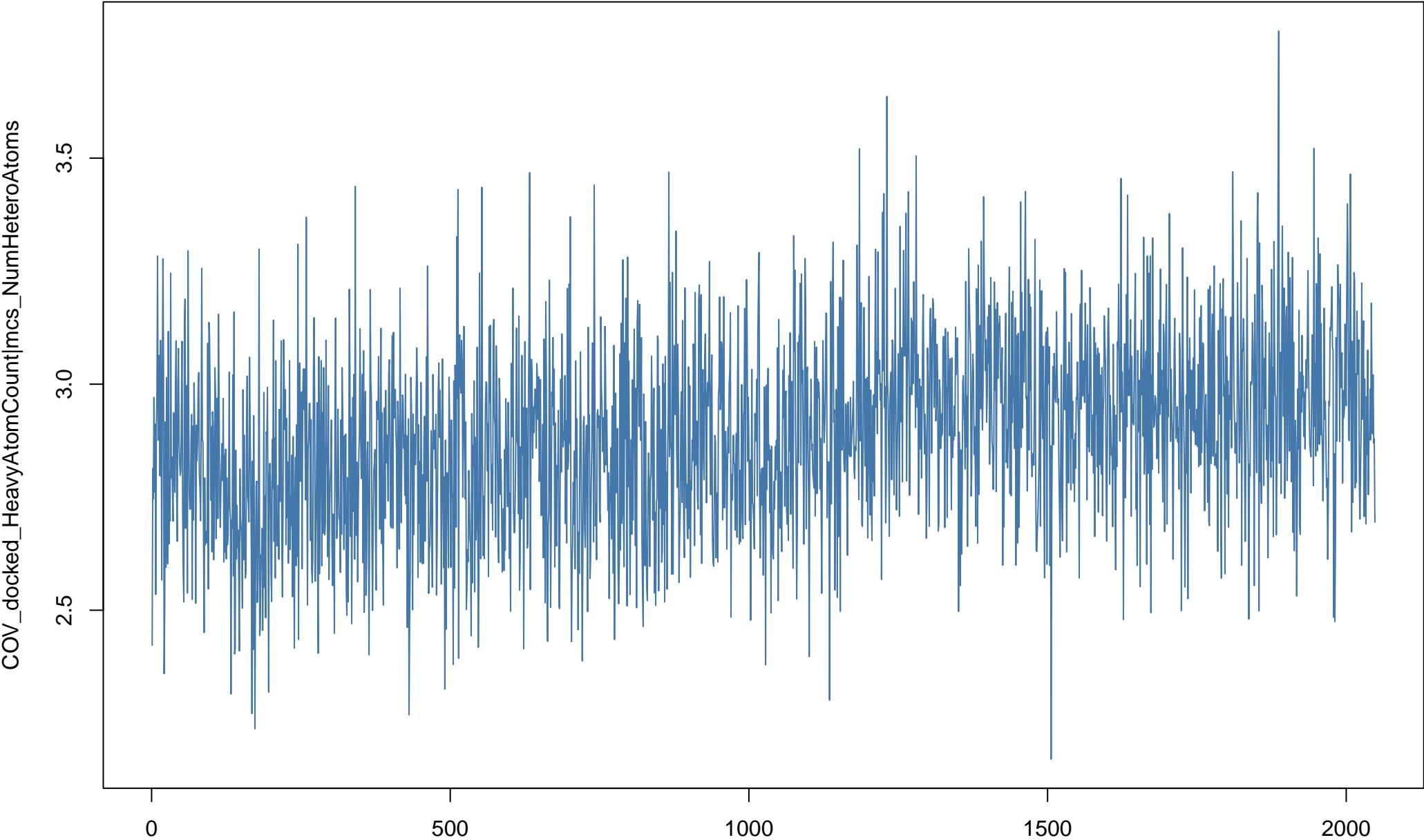
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 695 | BMK = 0.14 | MCSE(6.27) = 3.77 | stat: FALSE | burn: 0



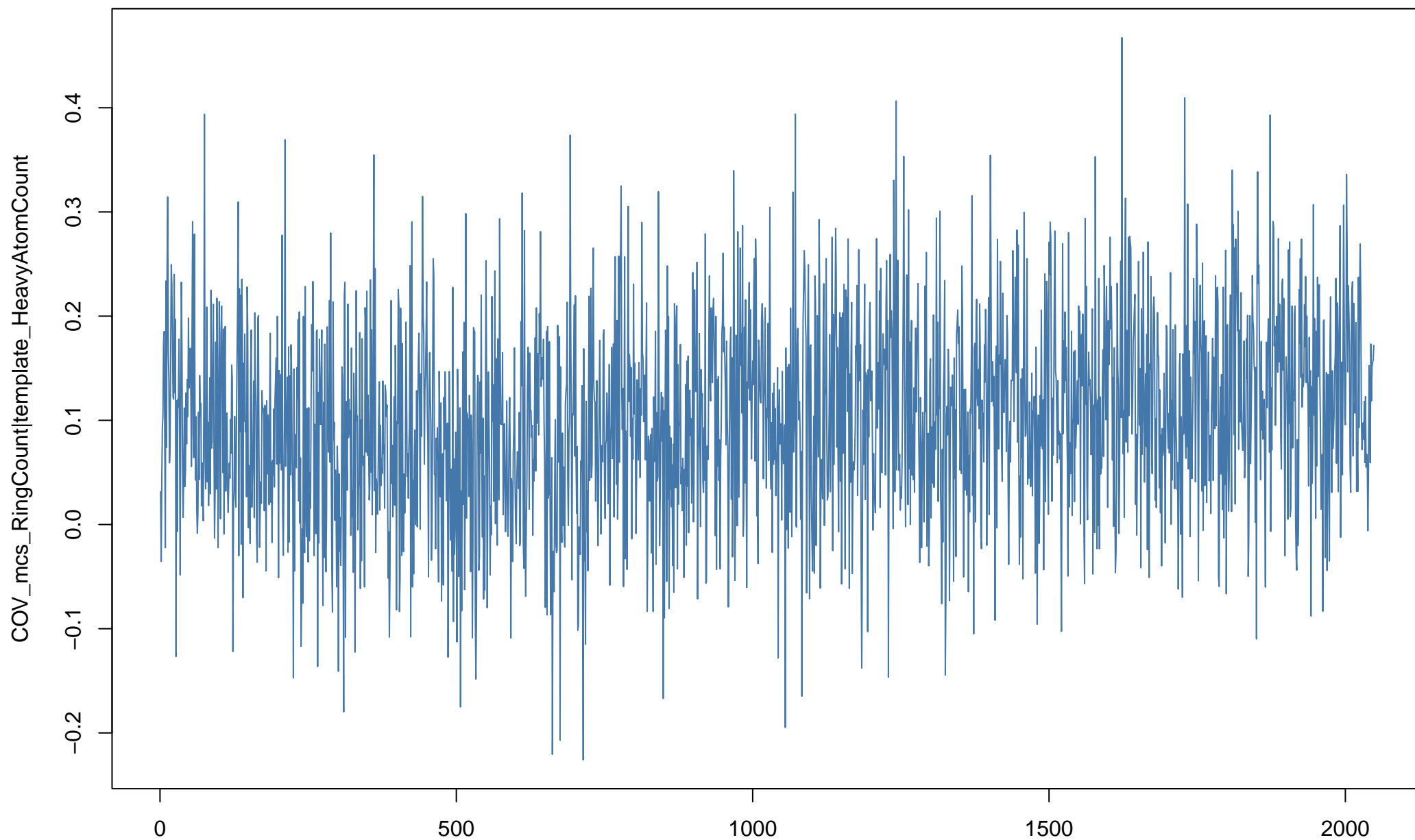
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1870 | BMK = 0.0954 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0



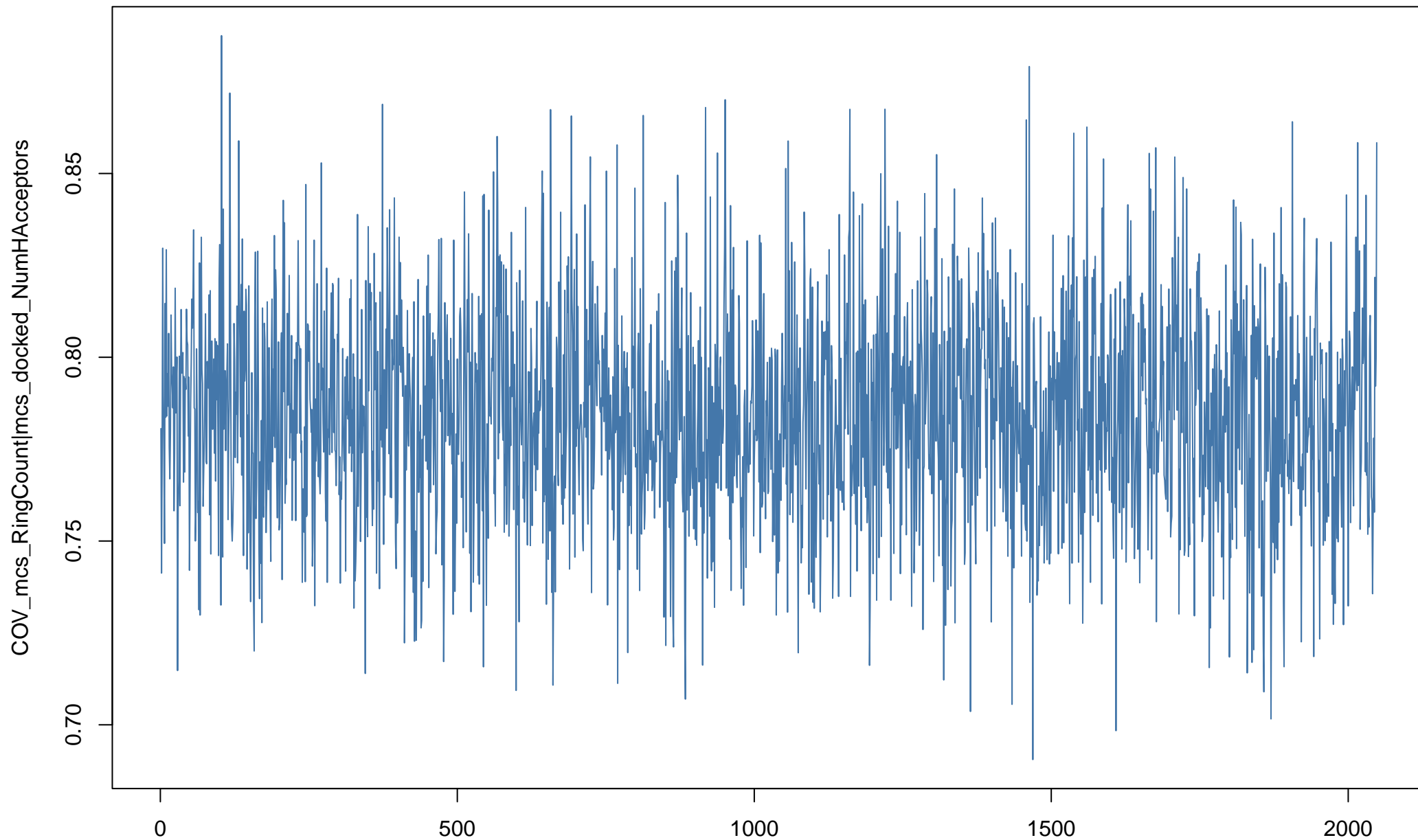
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 112 | BMK = 0.229 | MCSE(6.27) = 5.49 | stat: FALSE | burn: 0



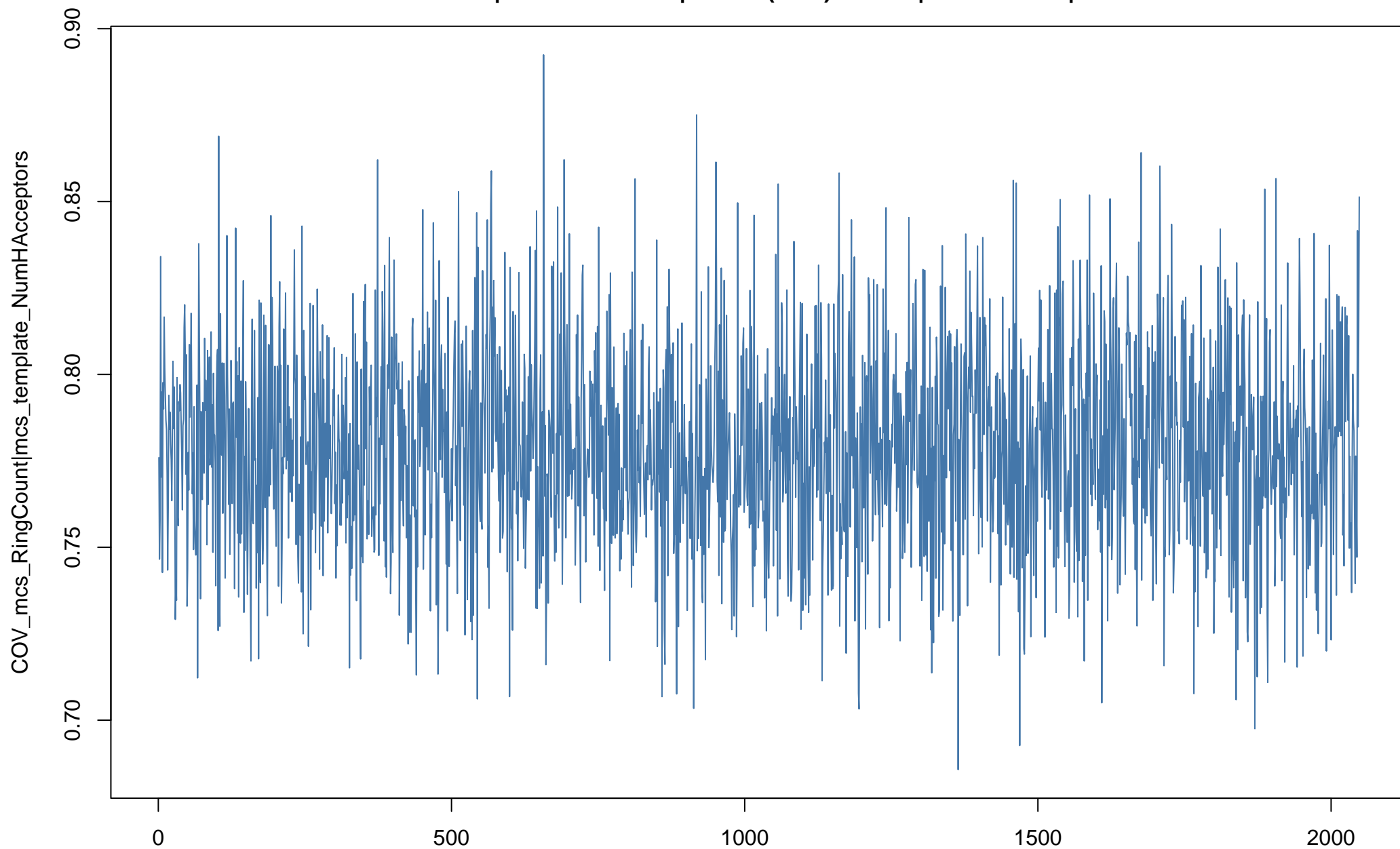
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 770 | BMK = 0.122 | MCSE(6.27) = 4.2 | stat: FALSE | burn: 0



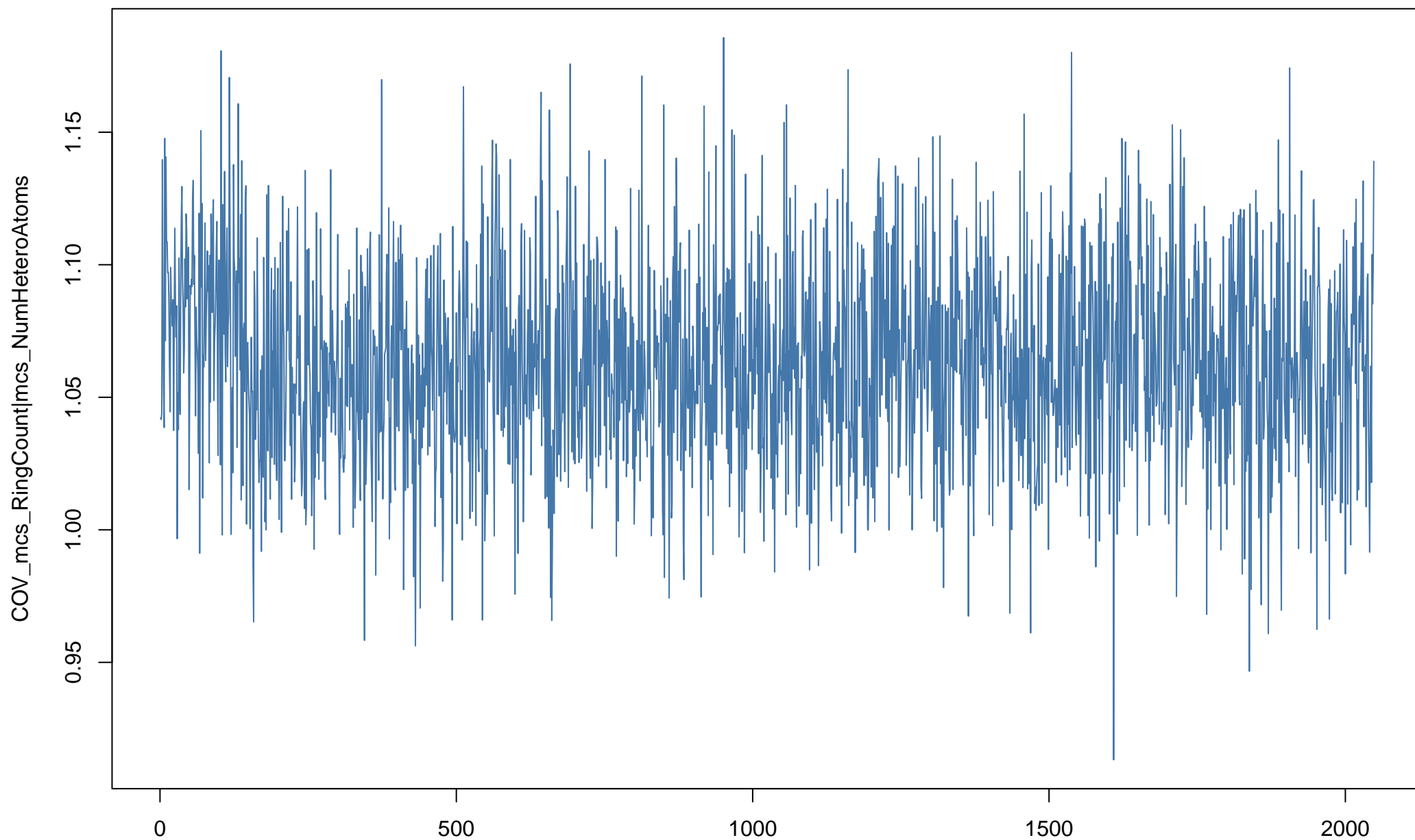
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0347 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0



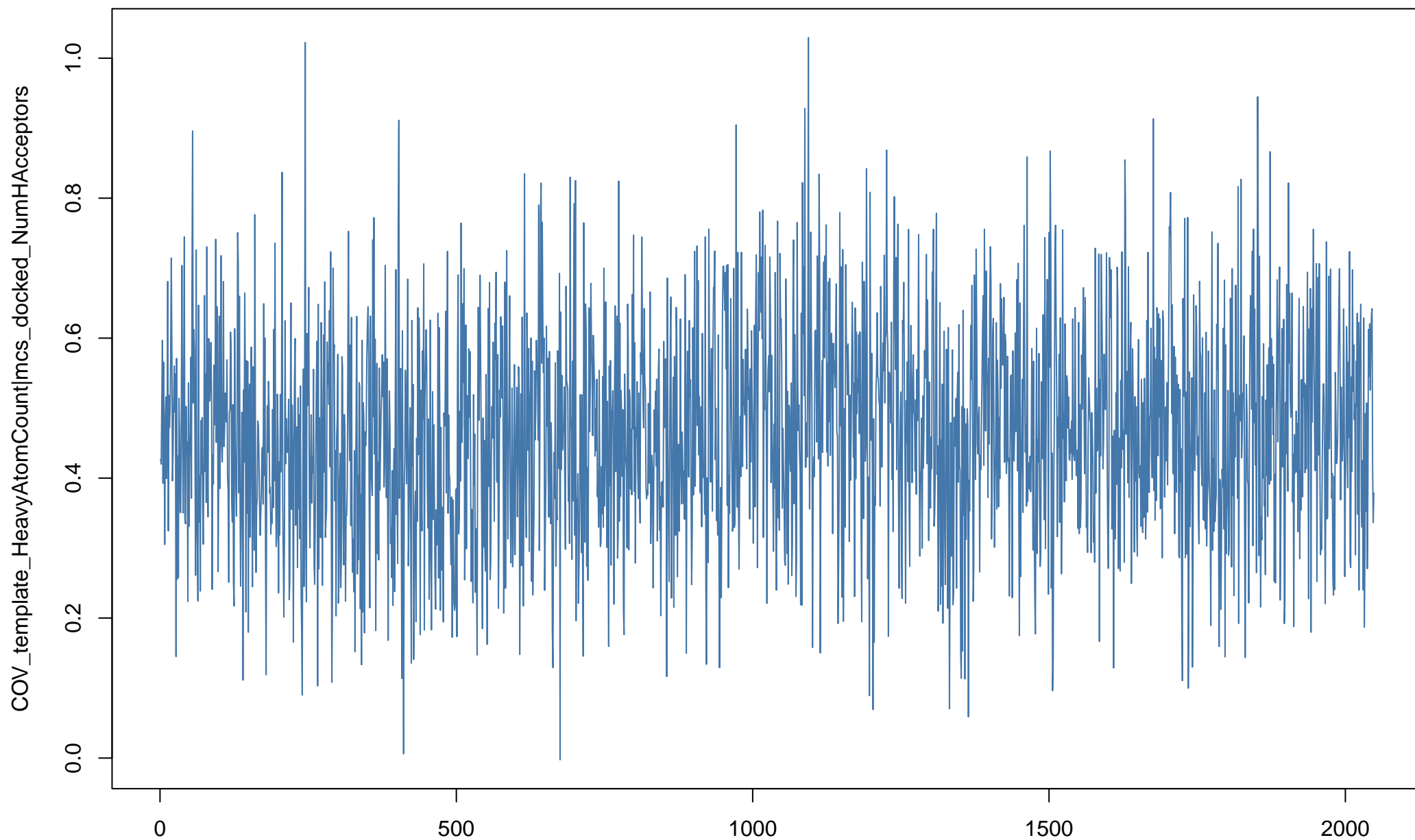
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0562 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



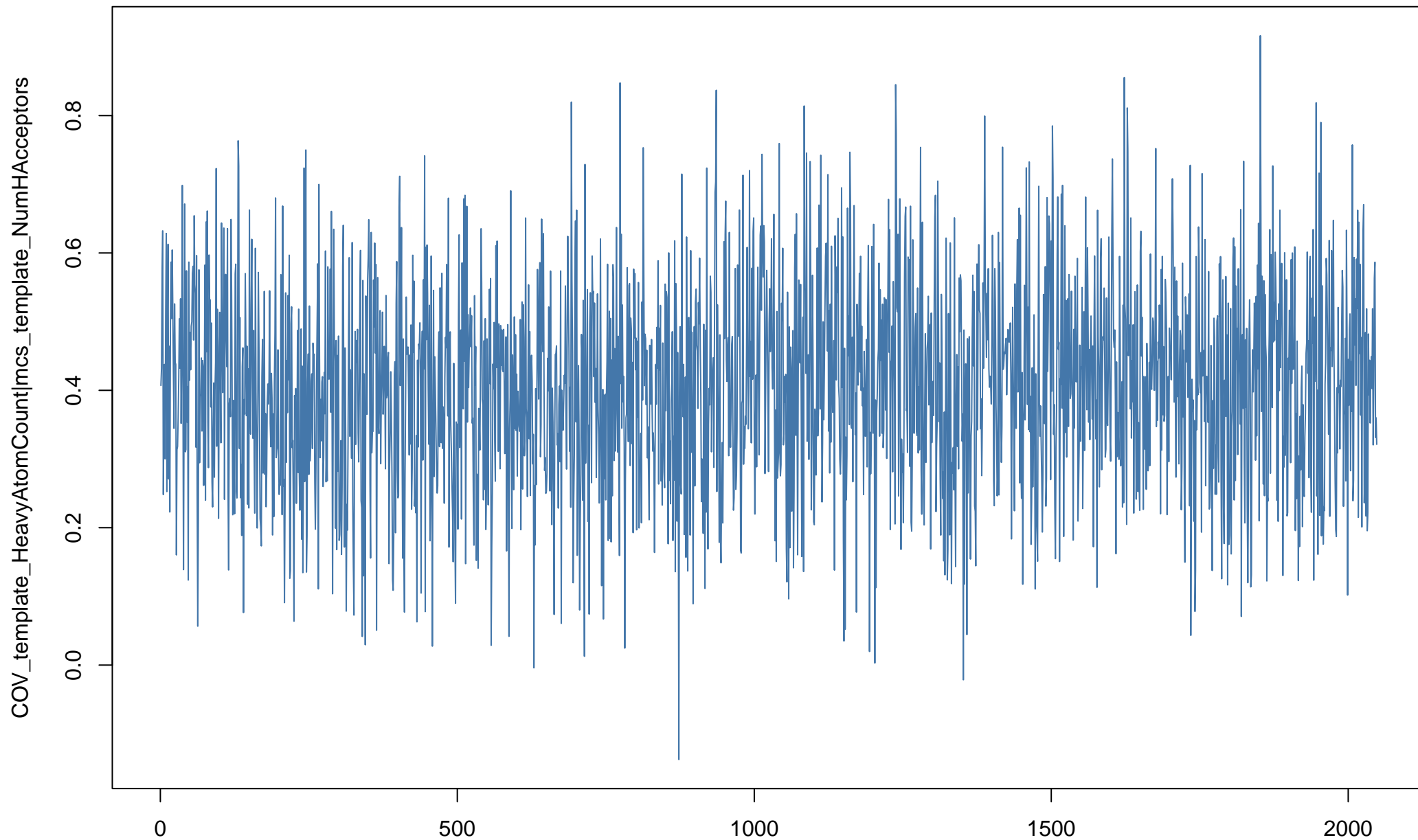
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 1470 | BMK = 0.0436 | MCSE(6.27) = 3.17 | stat: FALSE | burn: 0



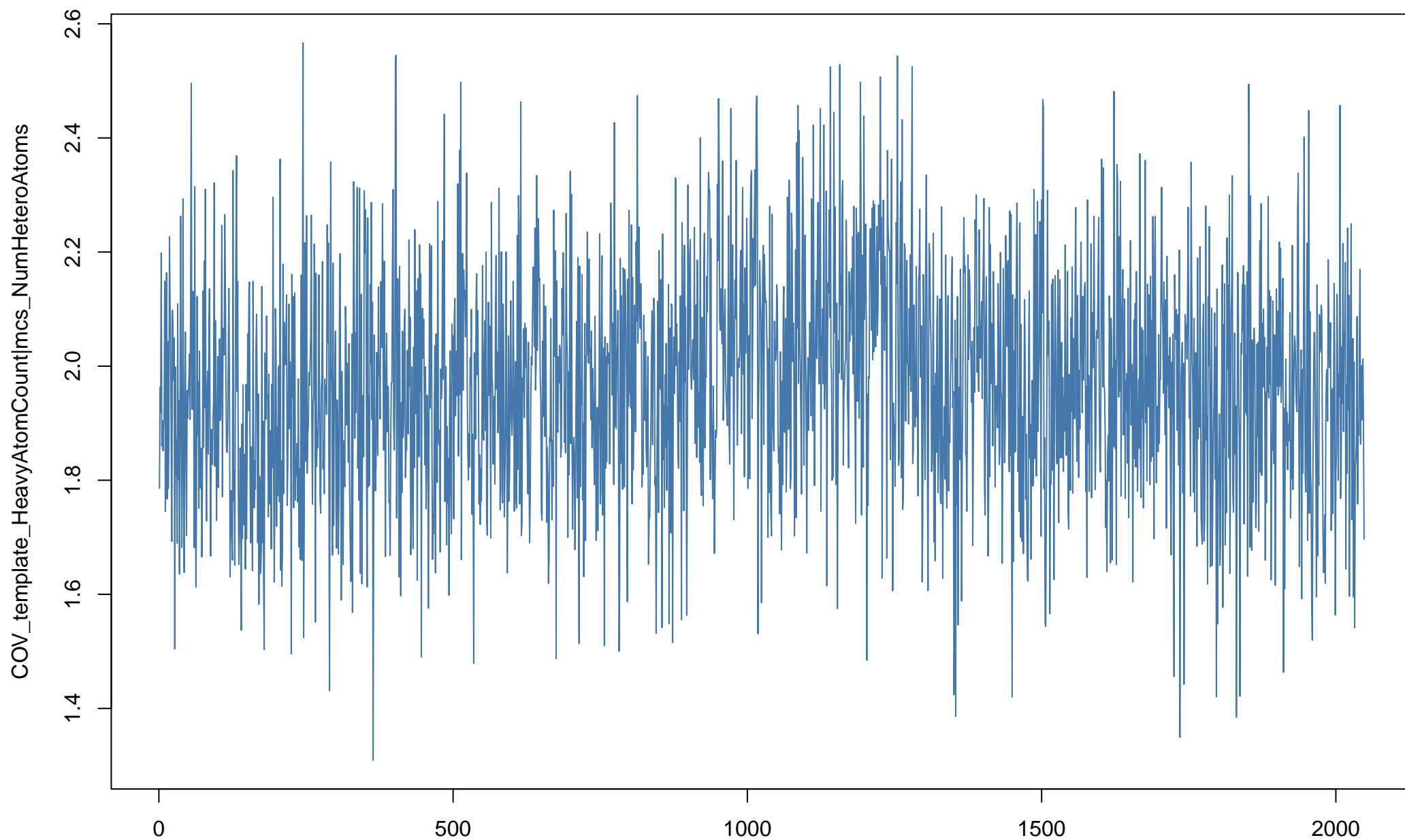
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1440 | BMK = 0.0697 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0



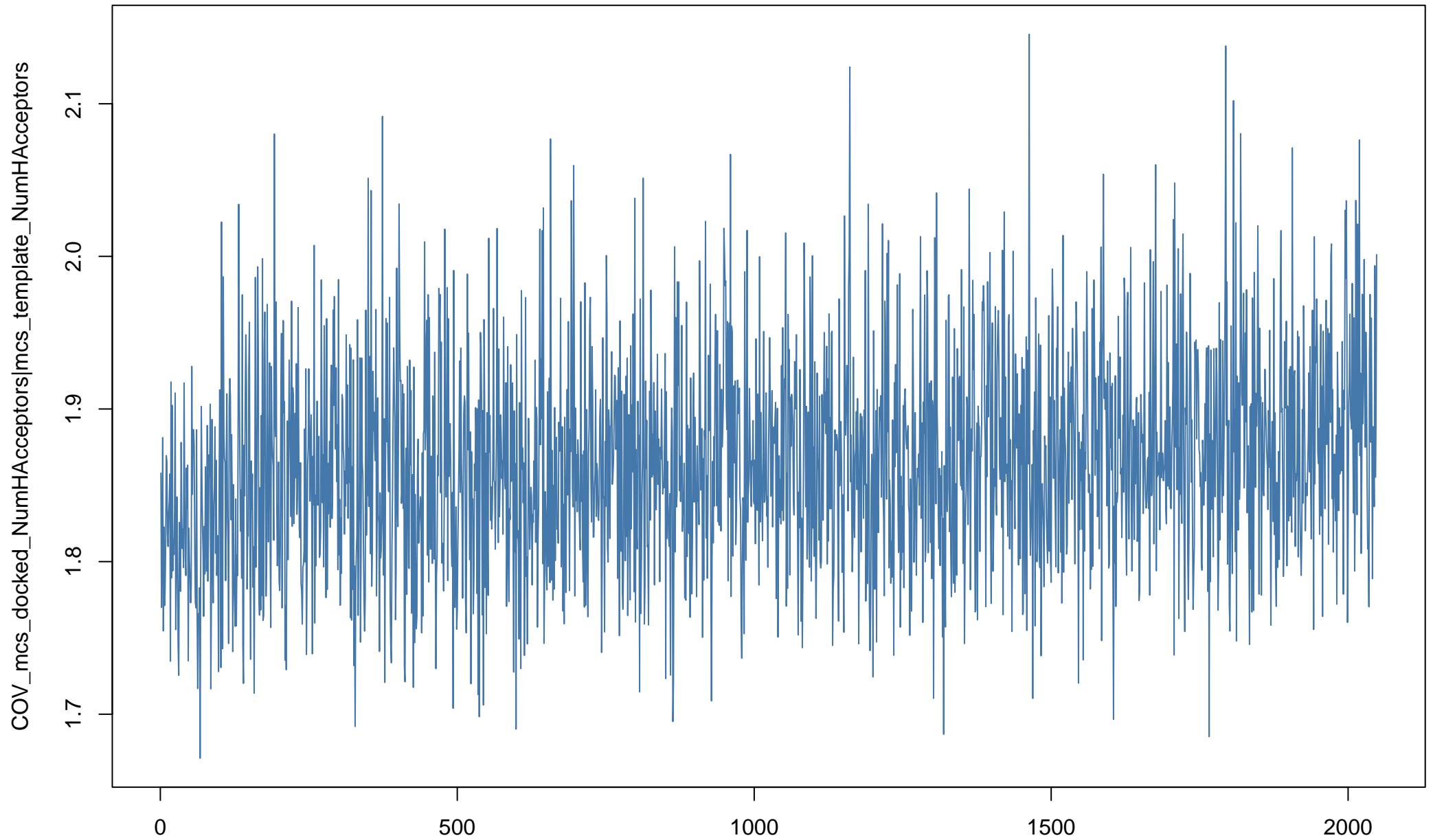
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1510 | BMK = 0.0649 | MCSE(6.27) = 3 | stat: TRUE | burn: 0



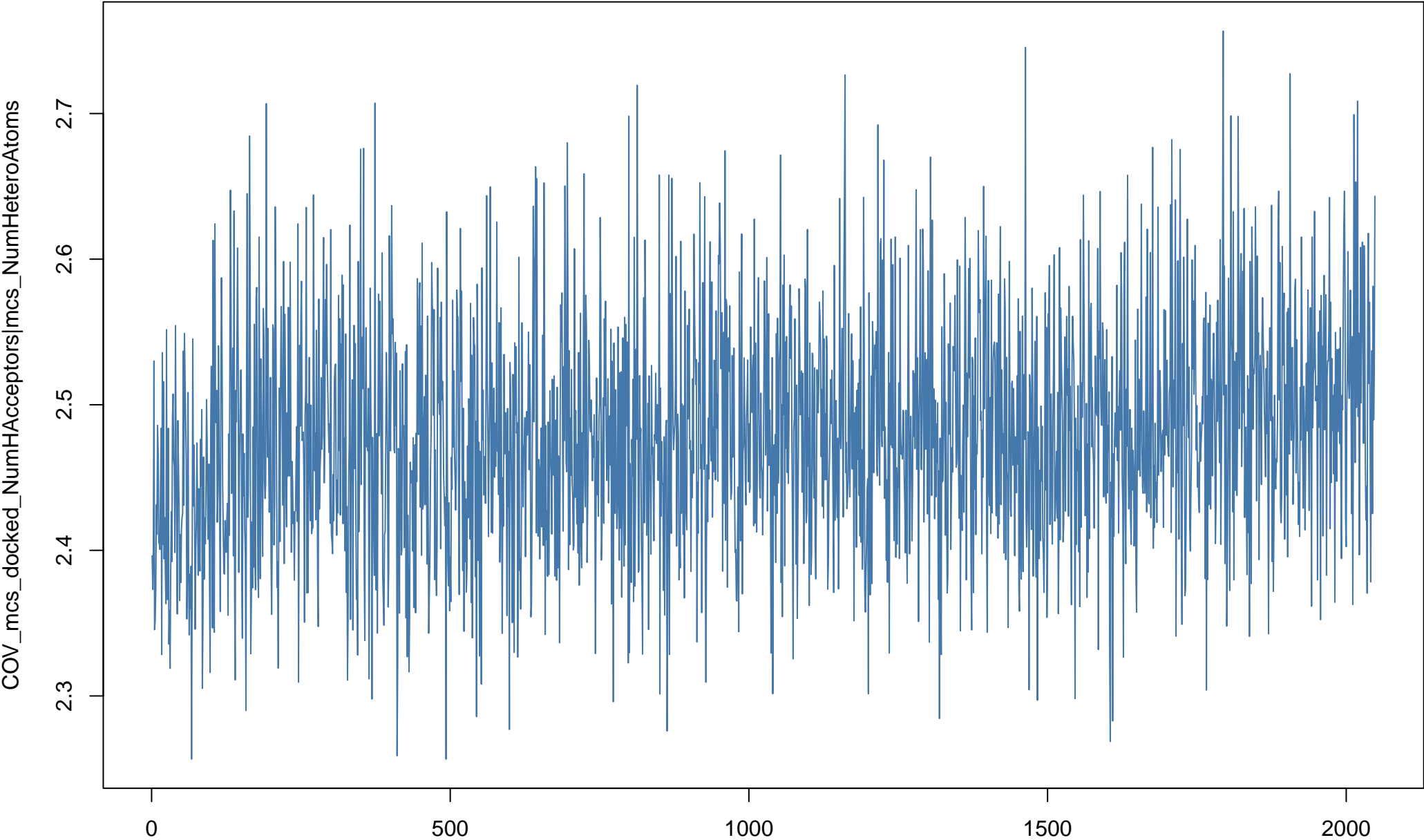
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 435 | BMK = 0.0618 | MCSE(6.27) = 4.14 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 876 | BMK = 0.117 | MCSE(6.27) = 3.72 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 849 | BMK = 0.112 | MCSE(6.27) = 3.72 | stat: FALSE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 526 | BMK = 0.117 | MCSE(6.27) = 4.05 | stat: FALSE | burn: 0

