

-- STATS maxD --

min ESS = 3.45277890271679

max BMK = 0.79985095208806

max MCSE = 14.1555373122257

all stationary: FALSE

burn: 1428

-- STATS 2D --

min ESS = 476.584635187811

max BMK = 0.126034727946859

max MCSE = 3.86917252161272

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.231707178859224

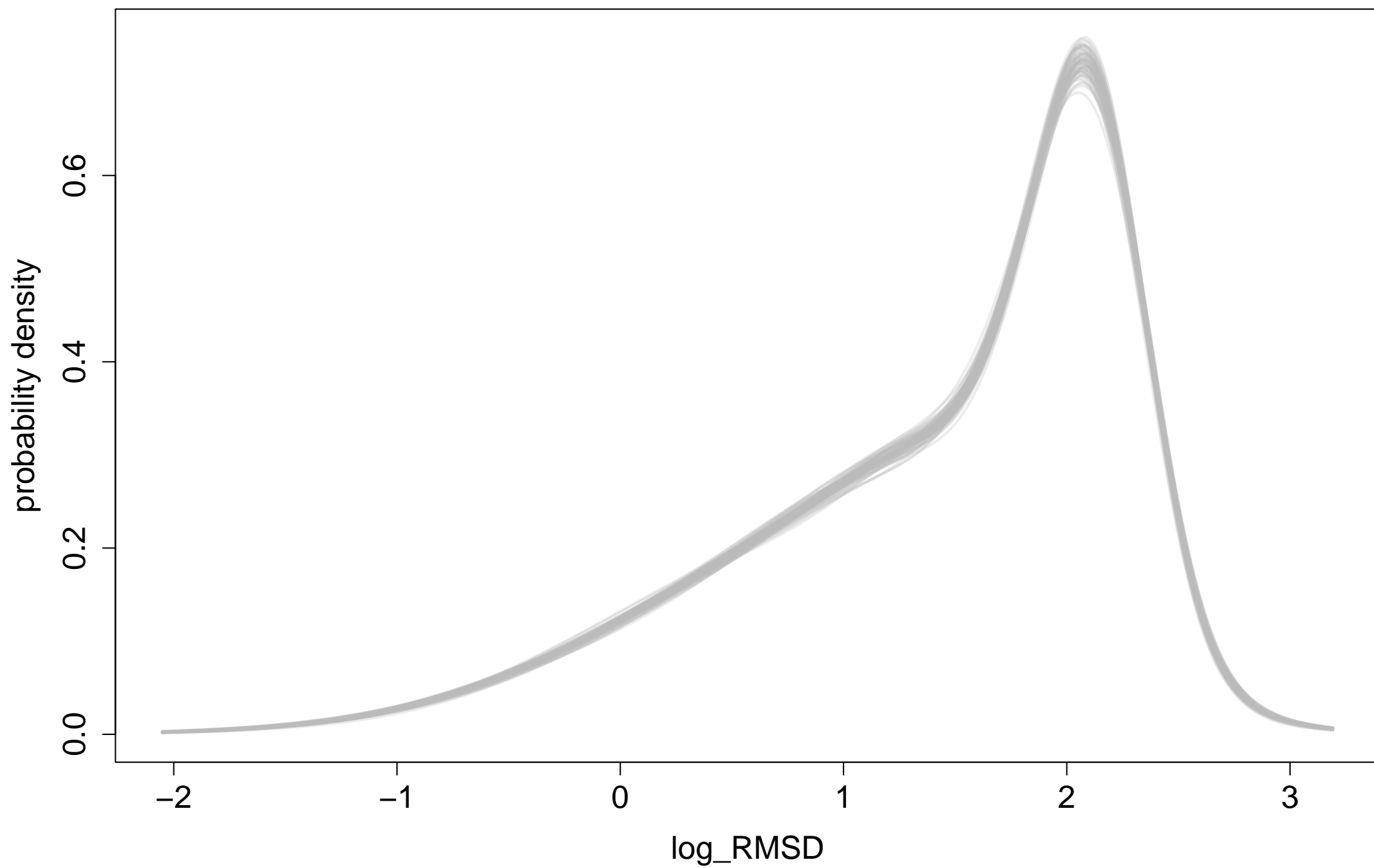
max MCSE = NaN

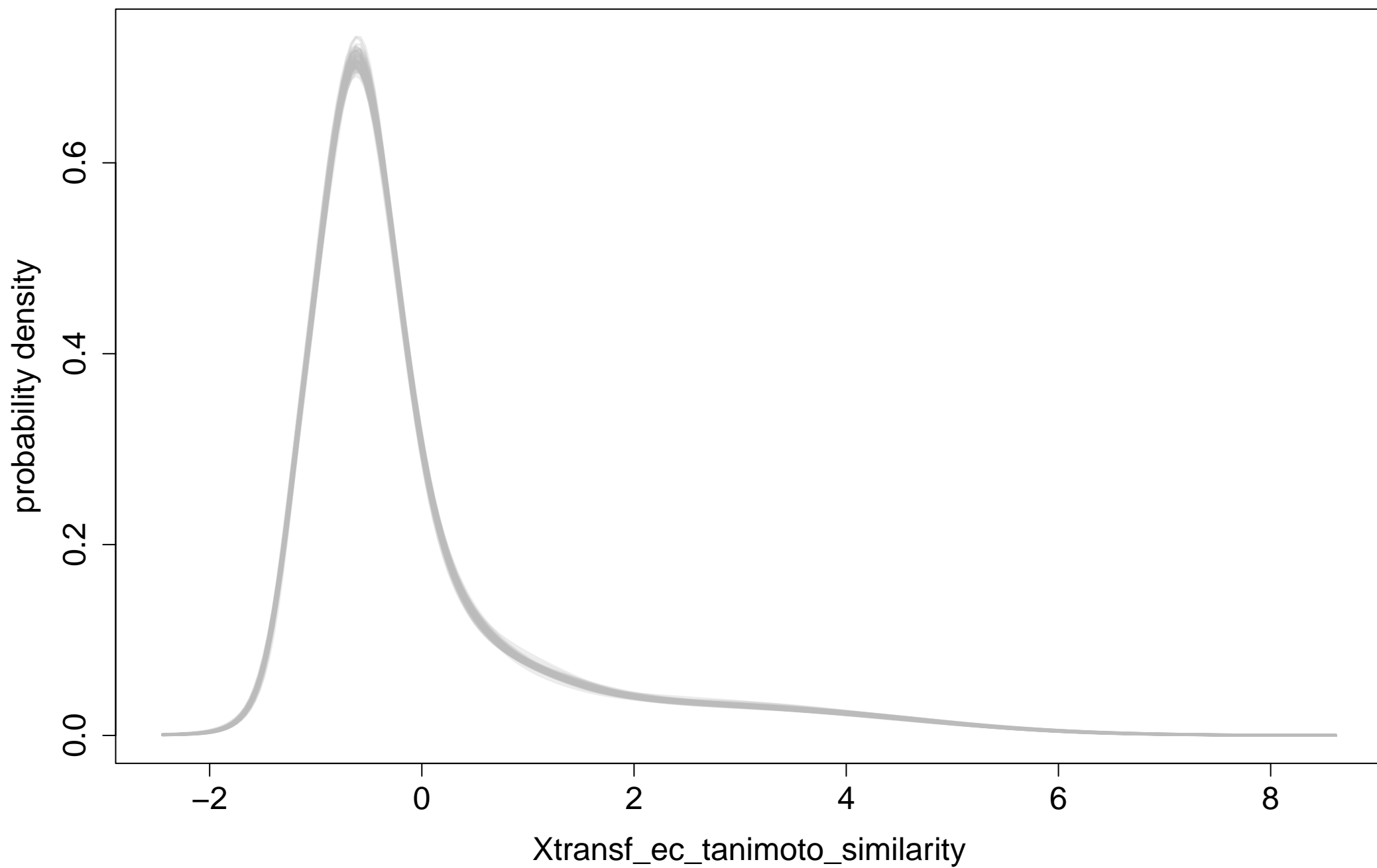
all stationary: FALSE

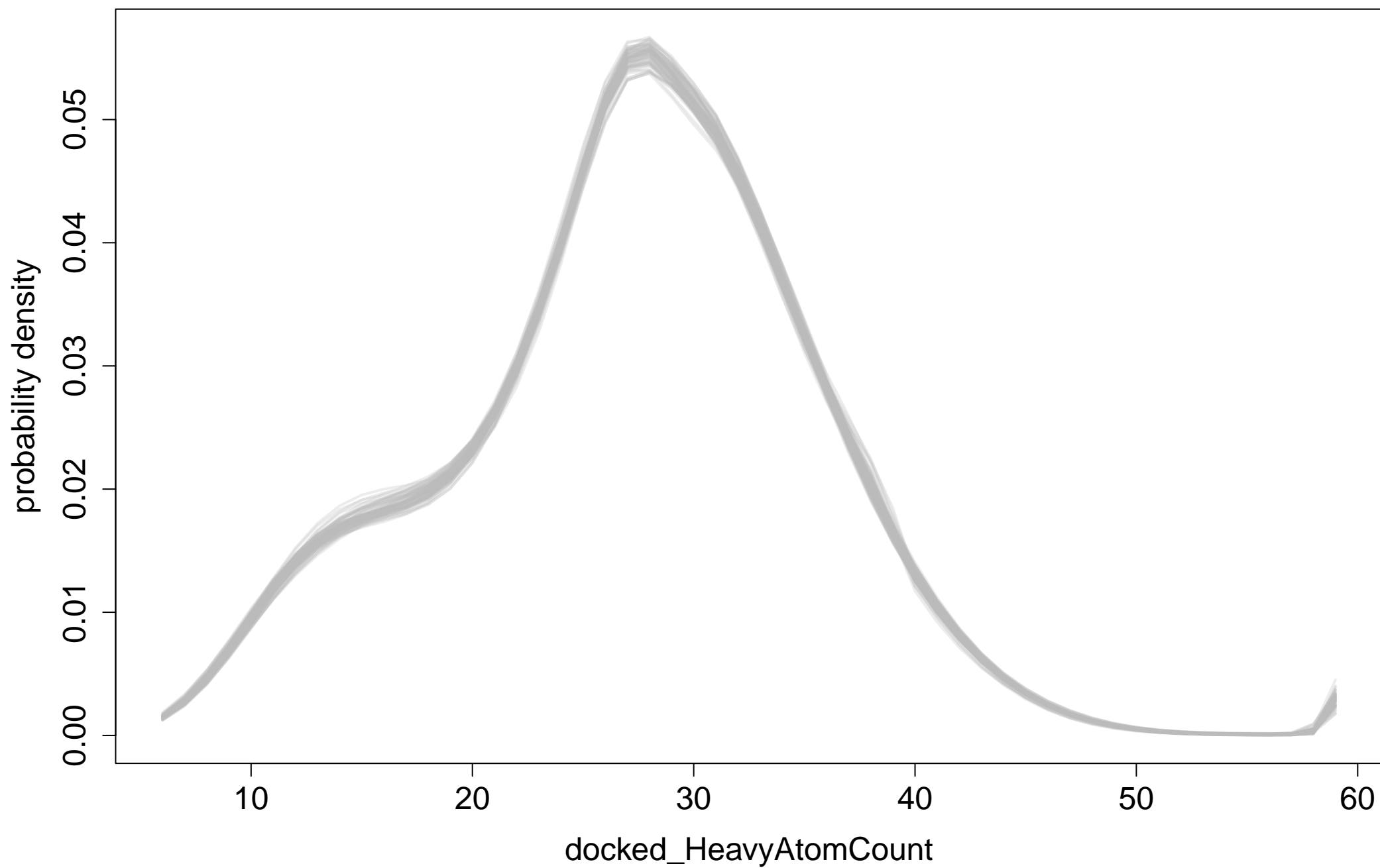
burn: 2040

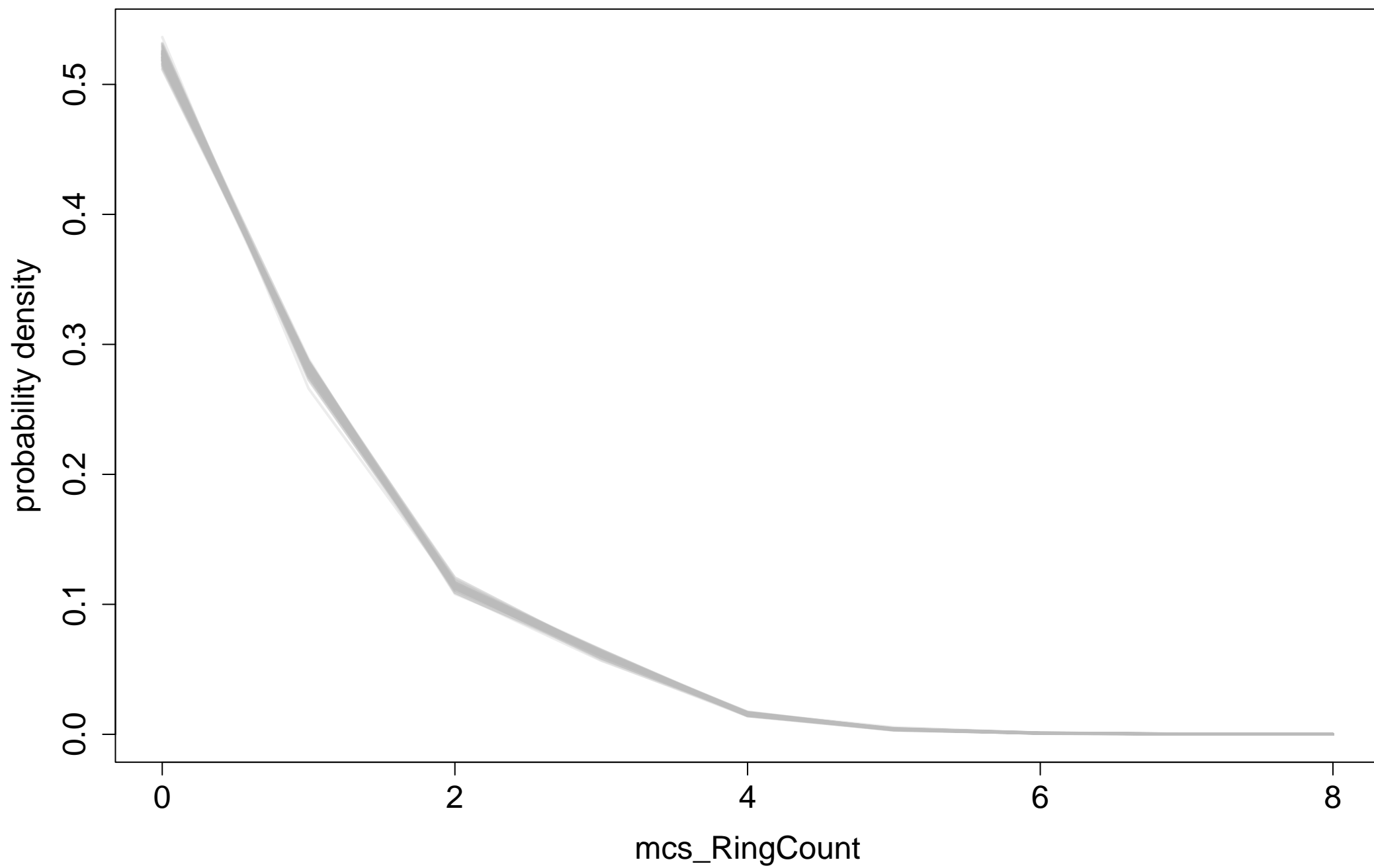
Occupied clusters: 70 of 91

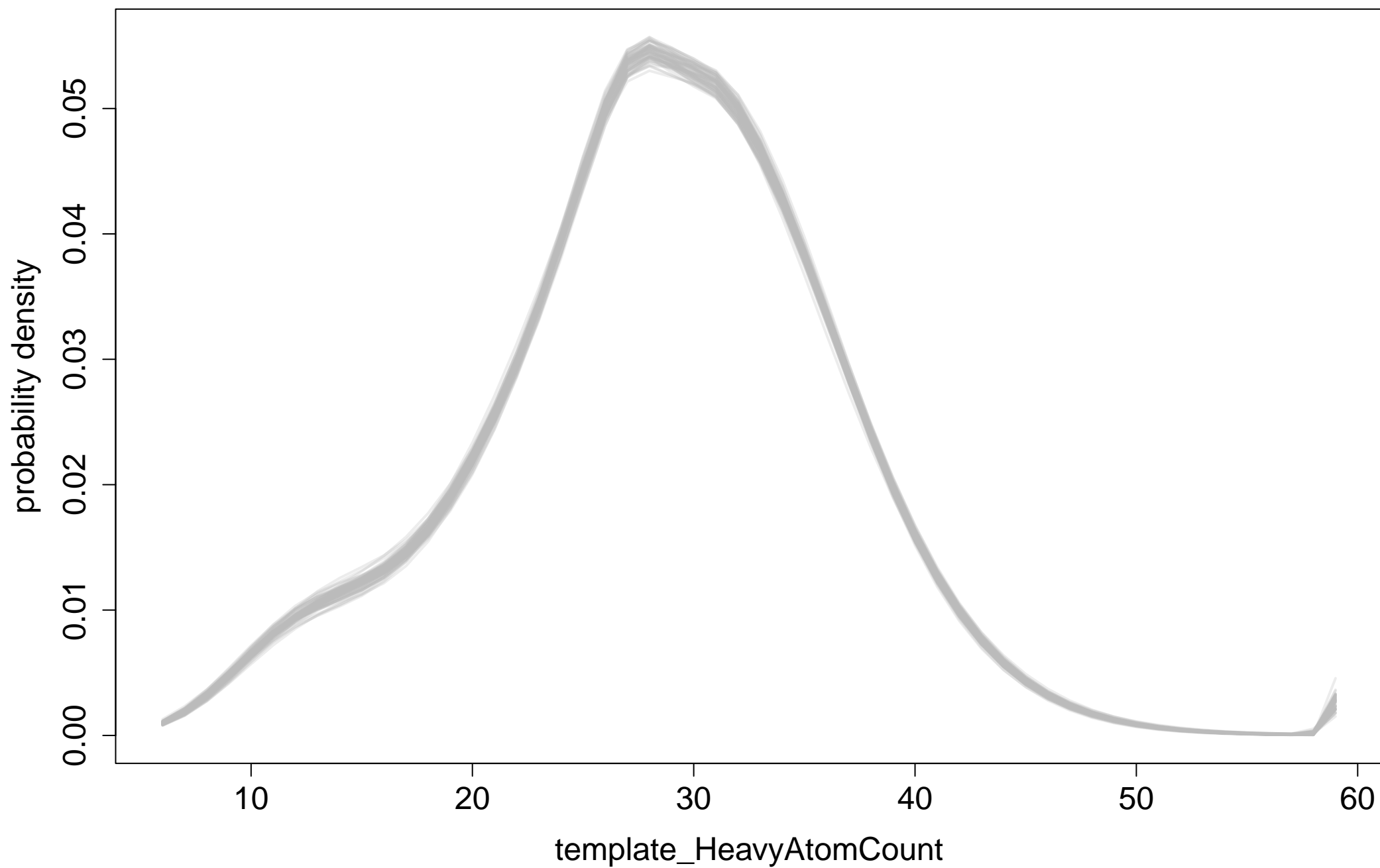
LL: -110000 +- 64.5

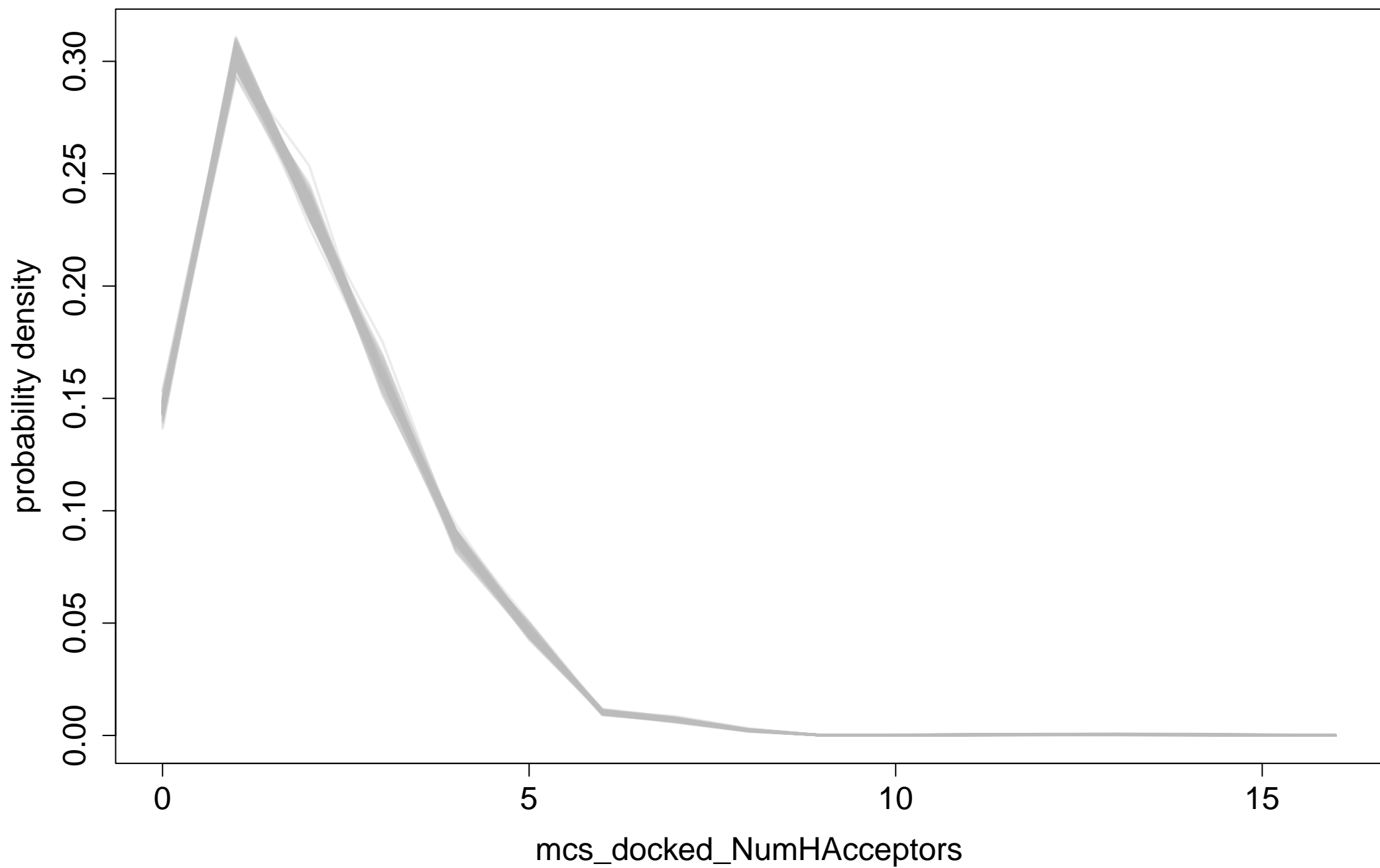


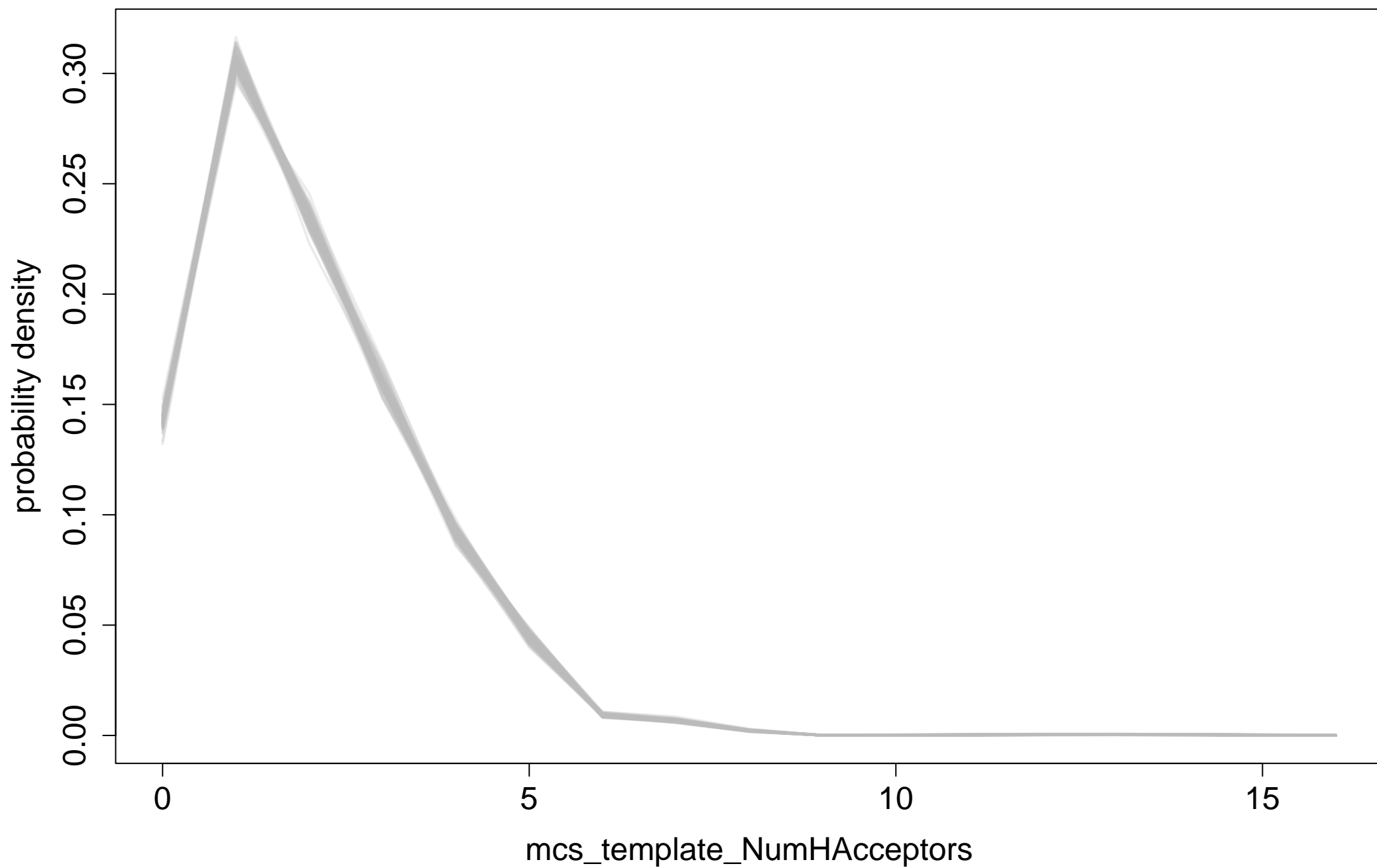


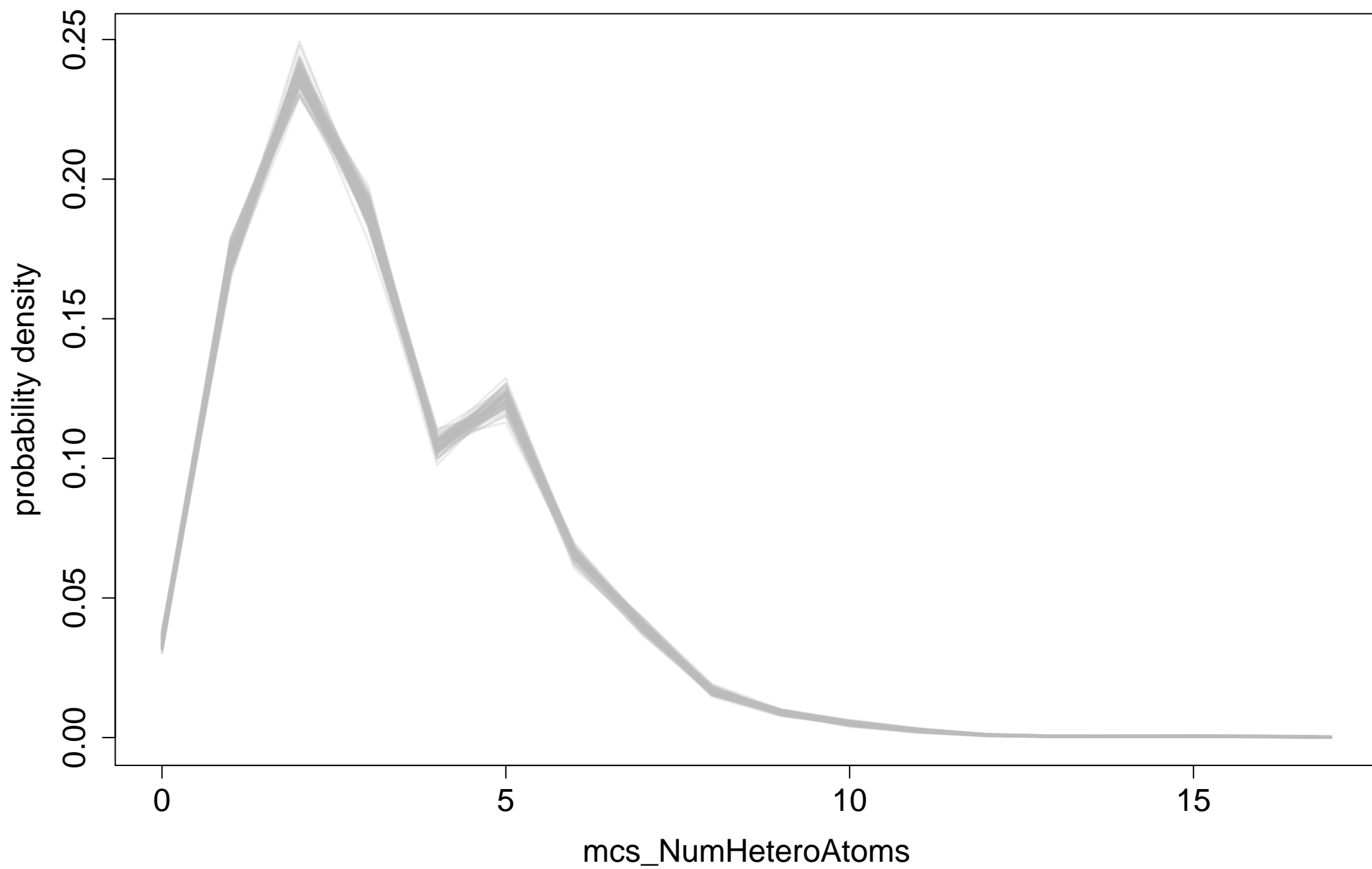


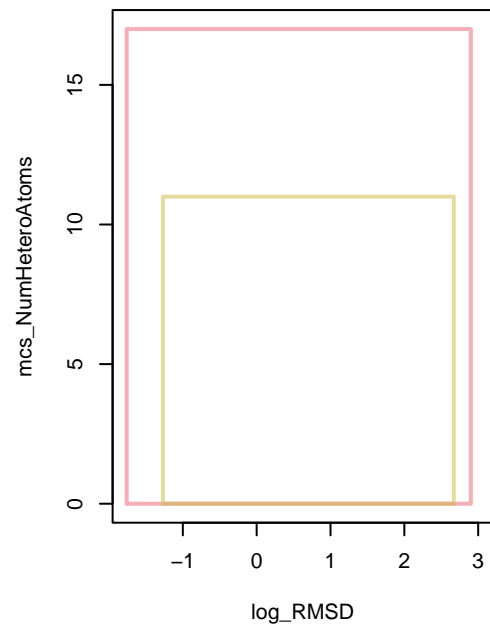
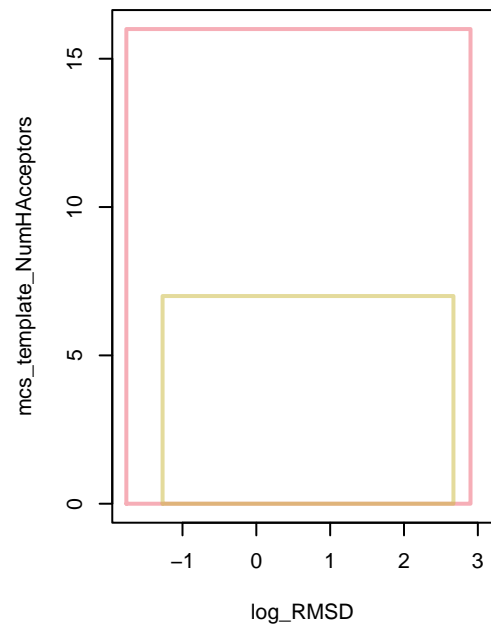
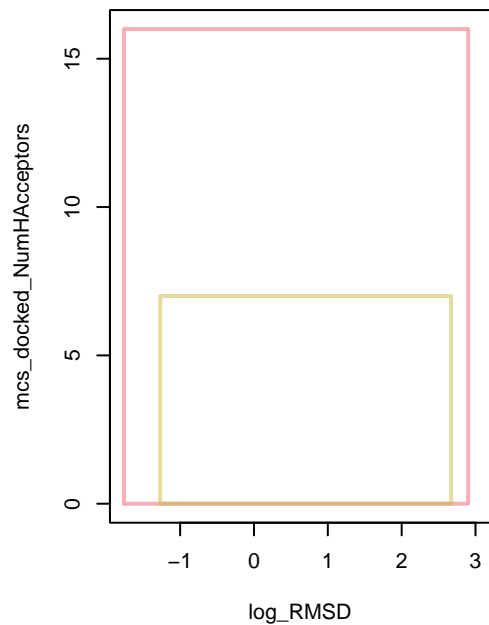
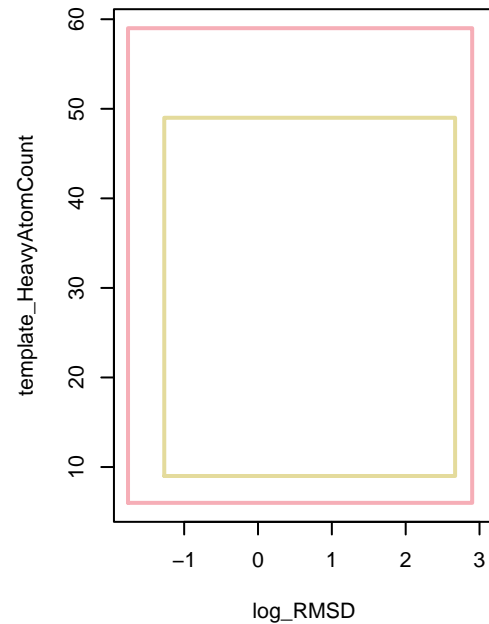
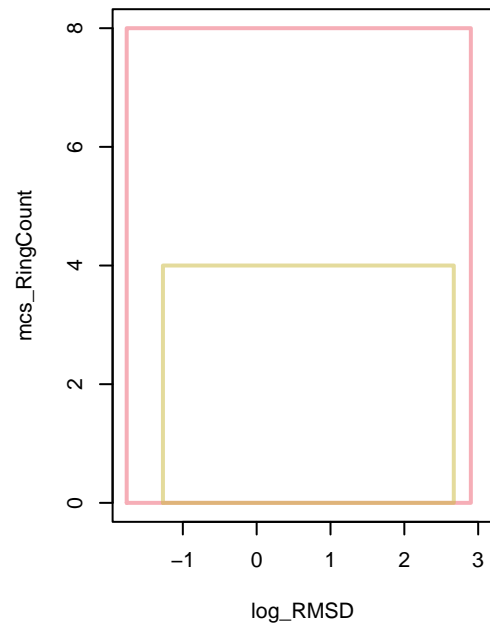
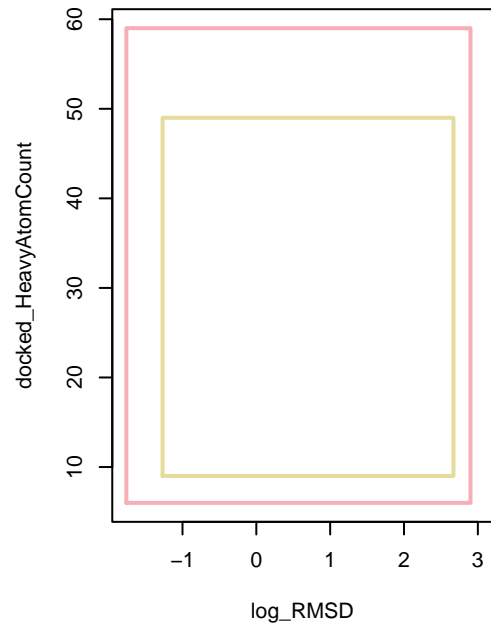
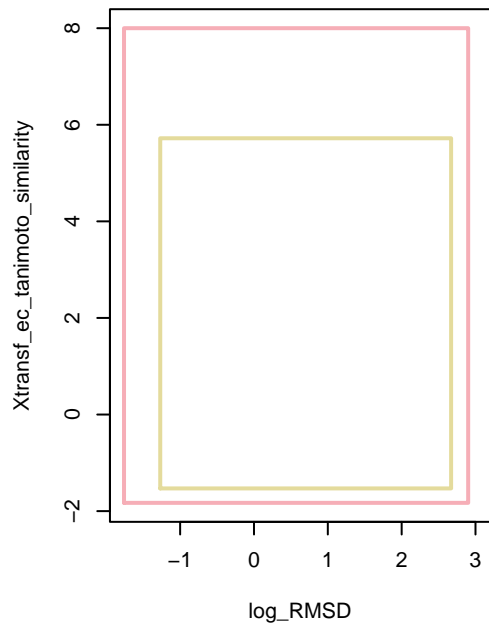




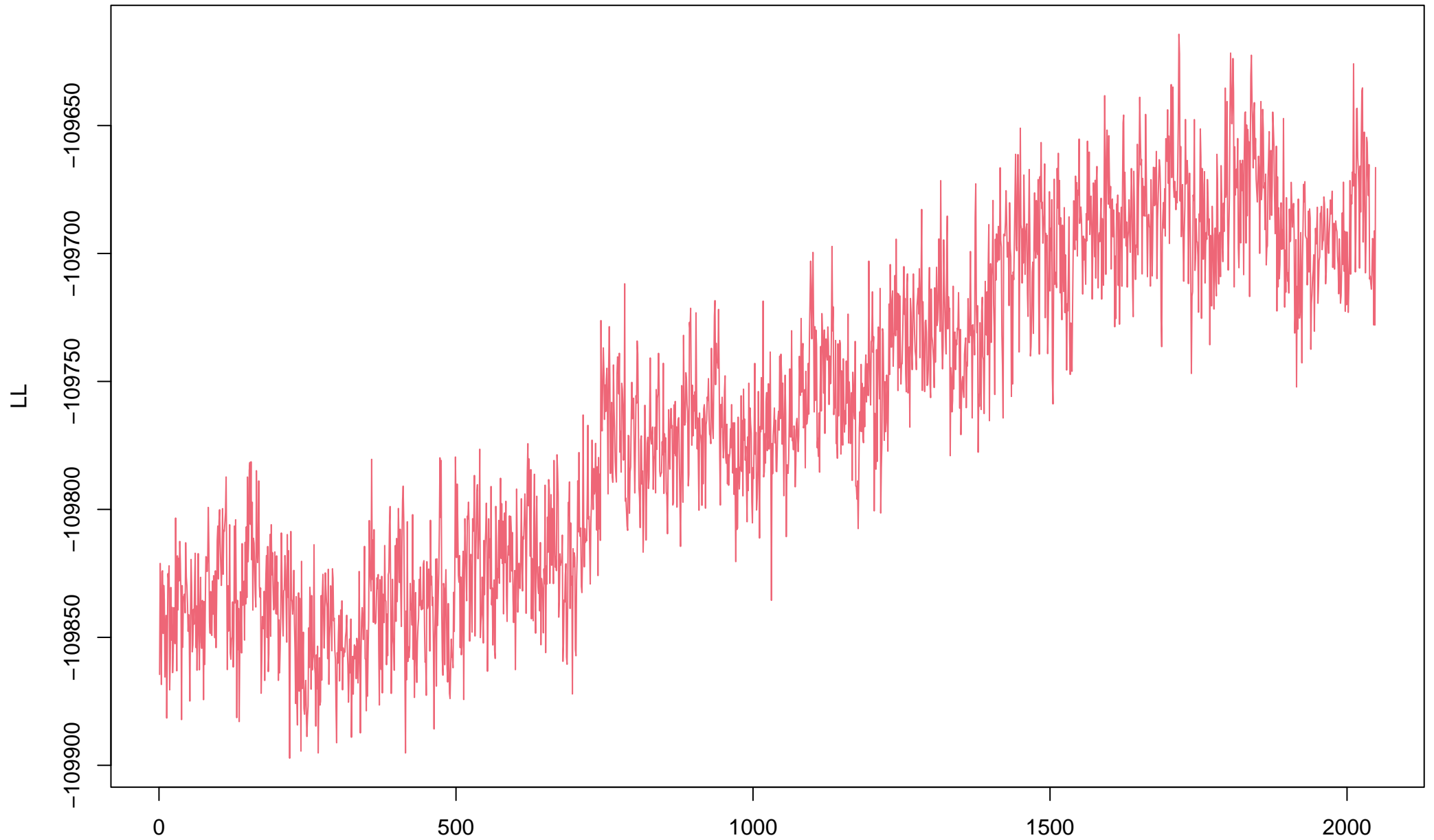




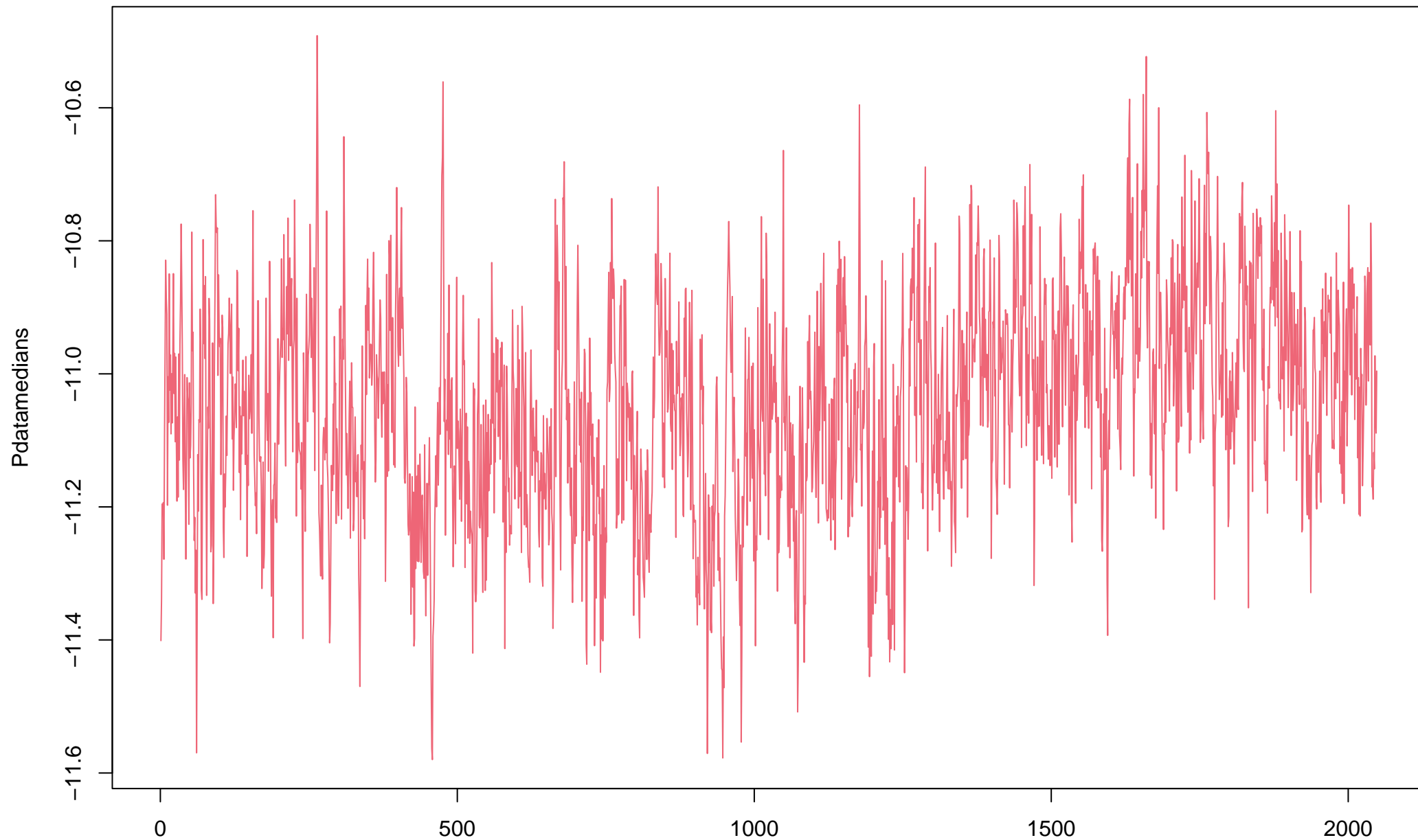




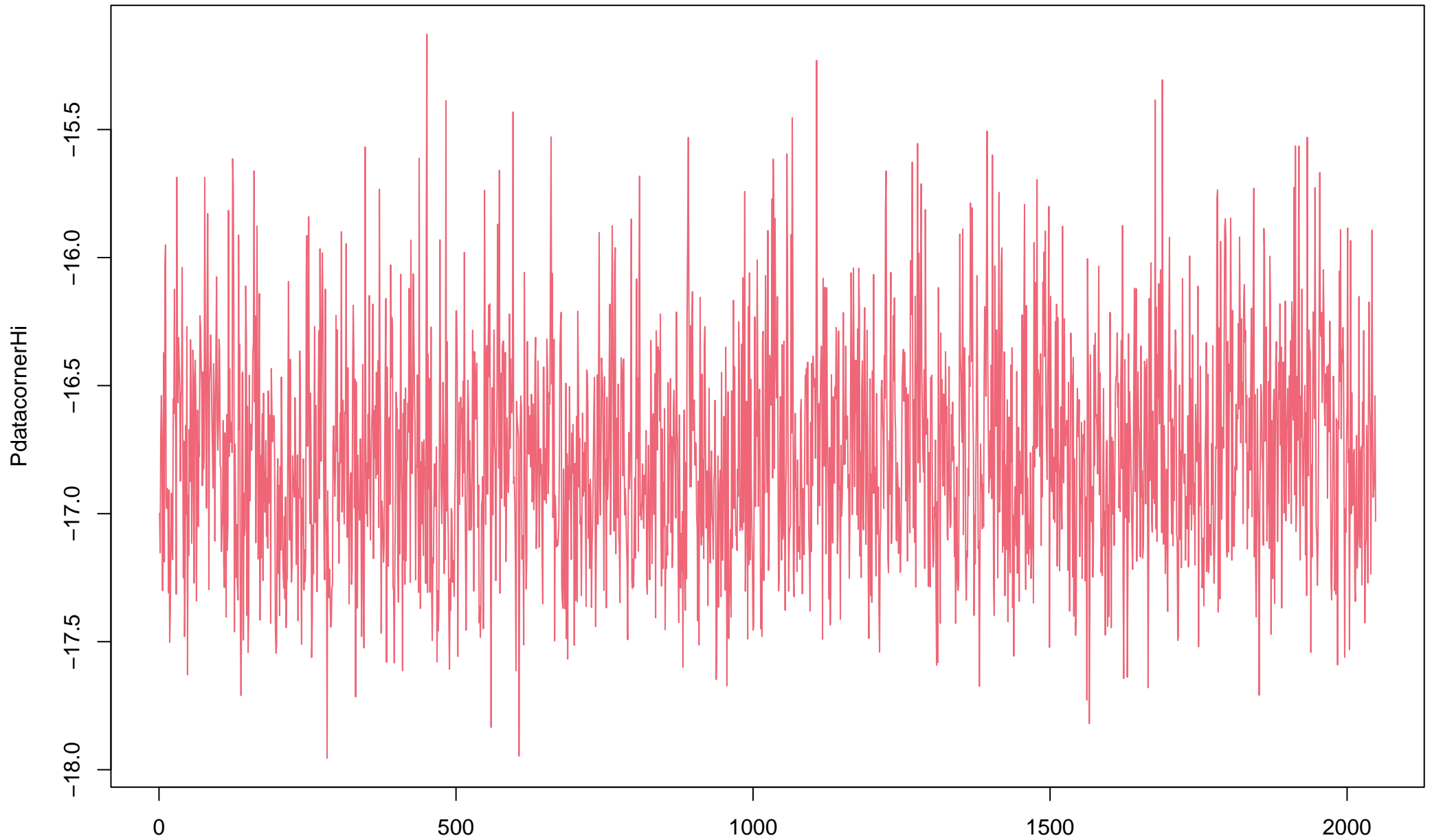
LL
ESS = 3.45 | BMK = 0.8 | MCSE(6.27) = 14.2 | stat: FALSE | burn: 0



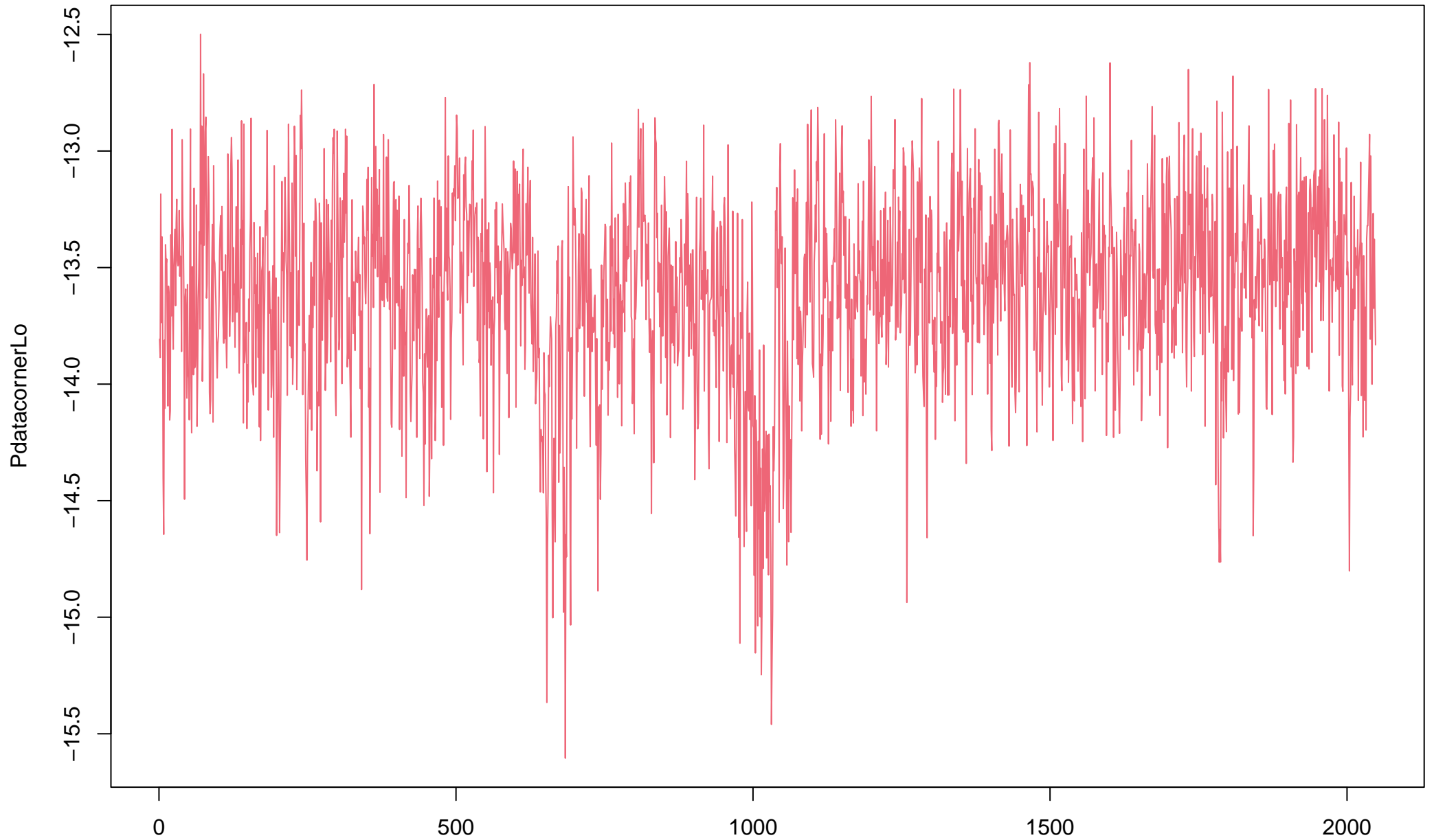
Pdatamedians
ESS = 173 | BMK = 0.198 | MCSE(6.27) = 7.4 | stat: FALSE | burn: 0



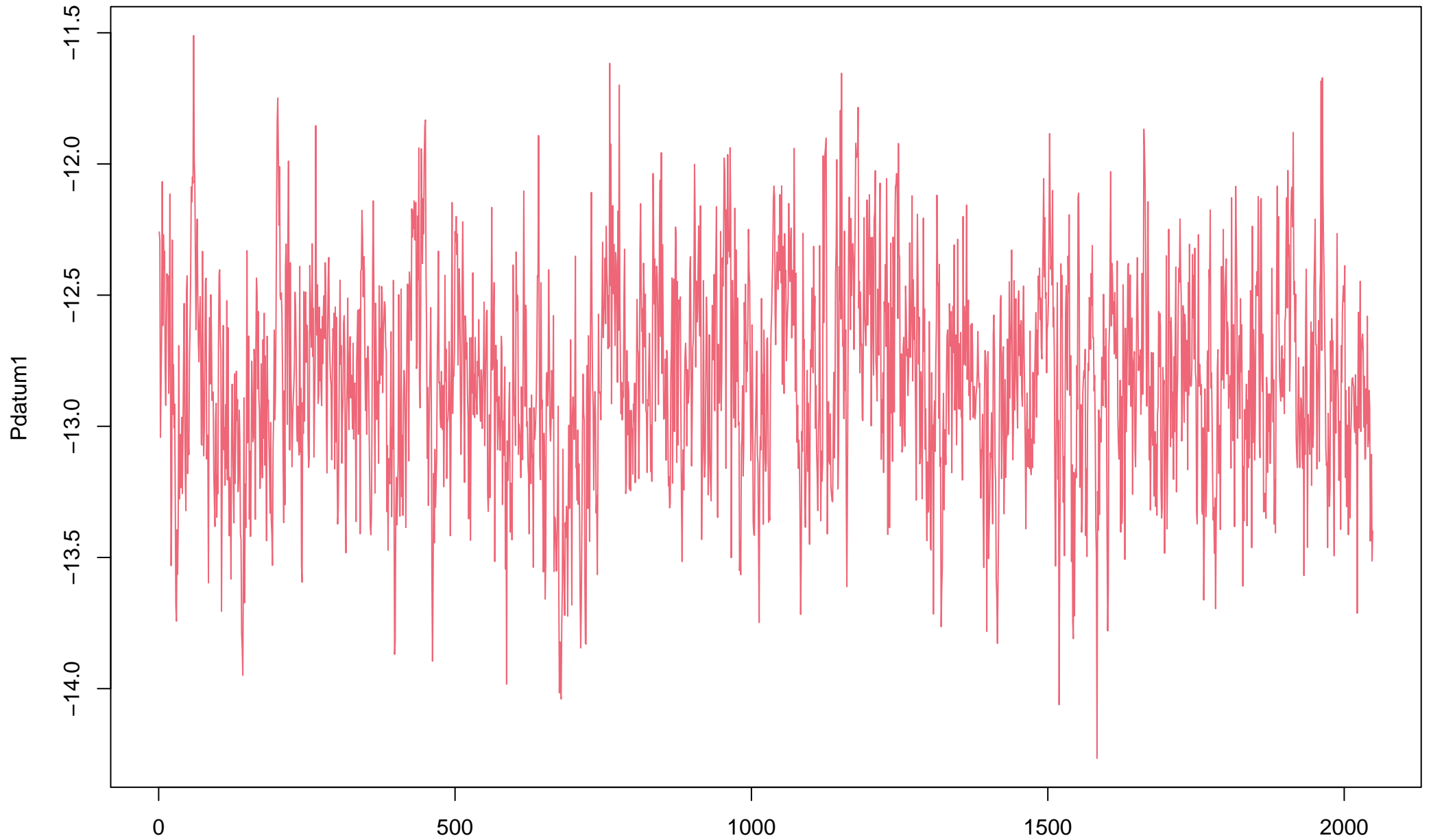
PdatacornerHi
ESS = 1220 | BMK = 0.0808 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0



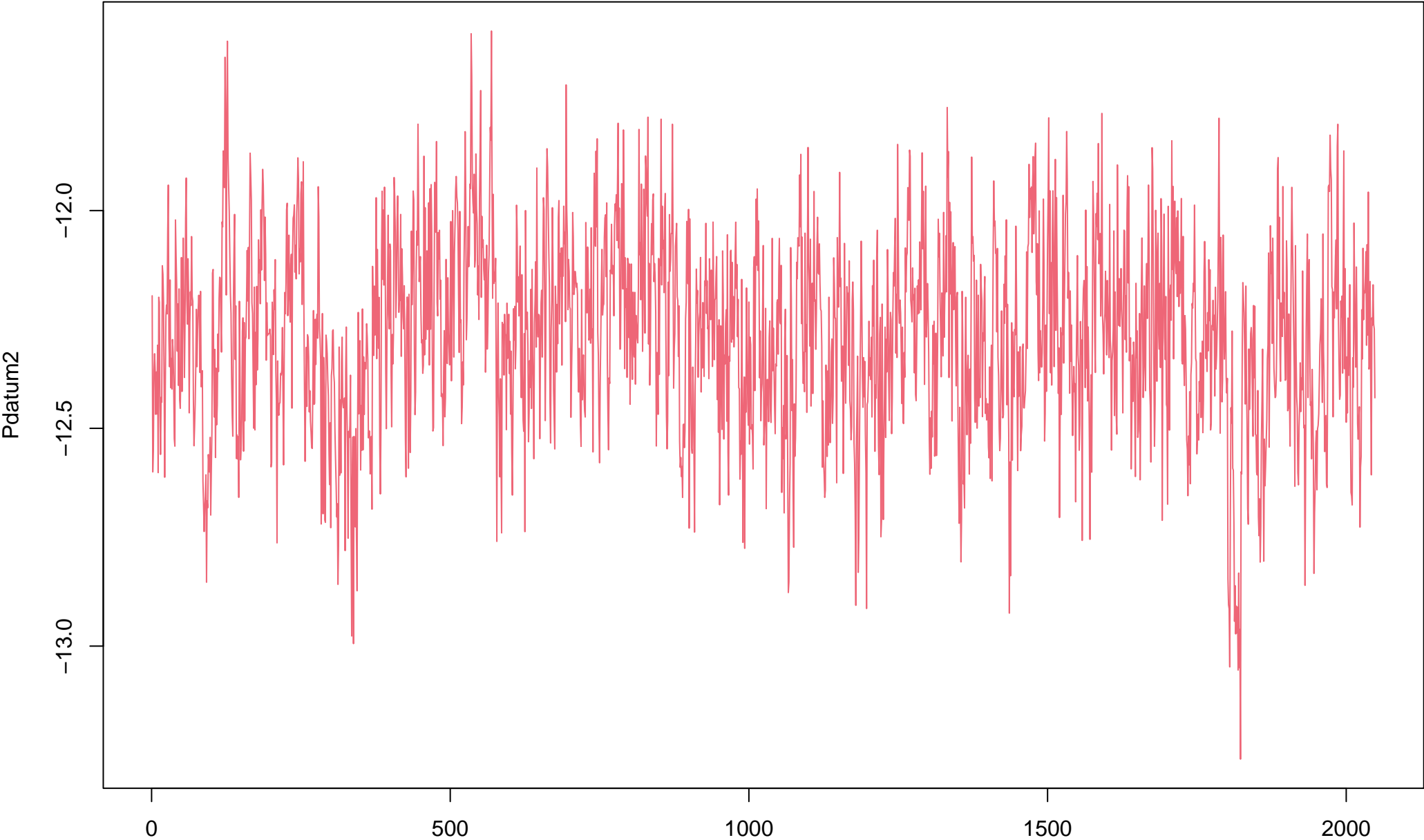
PdatacornerLo
ESS = 329 | BMK = 0.101 | MCSE(6.27) = 5.5 | stat: TRUE | burn: 0



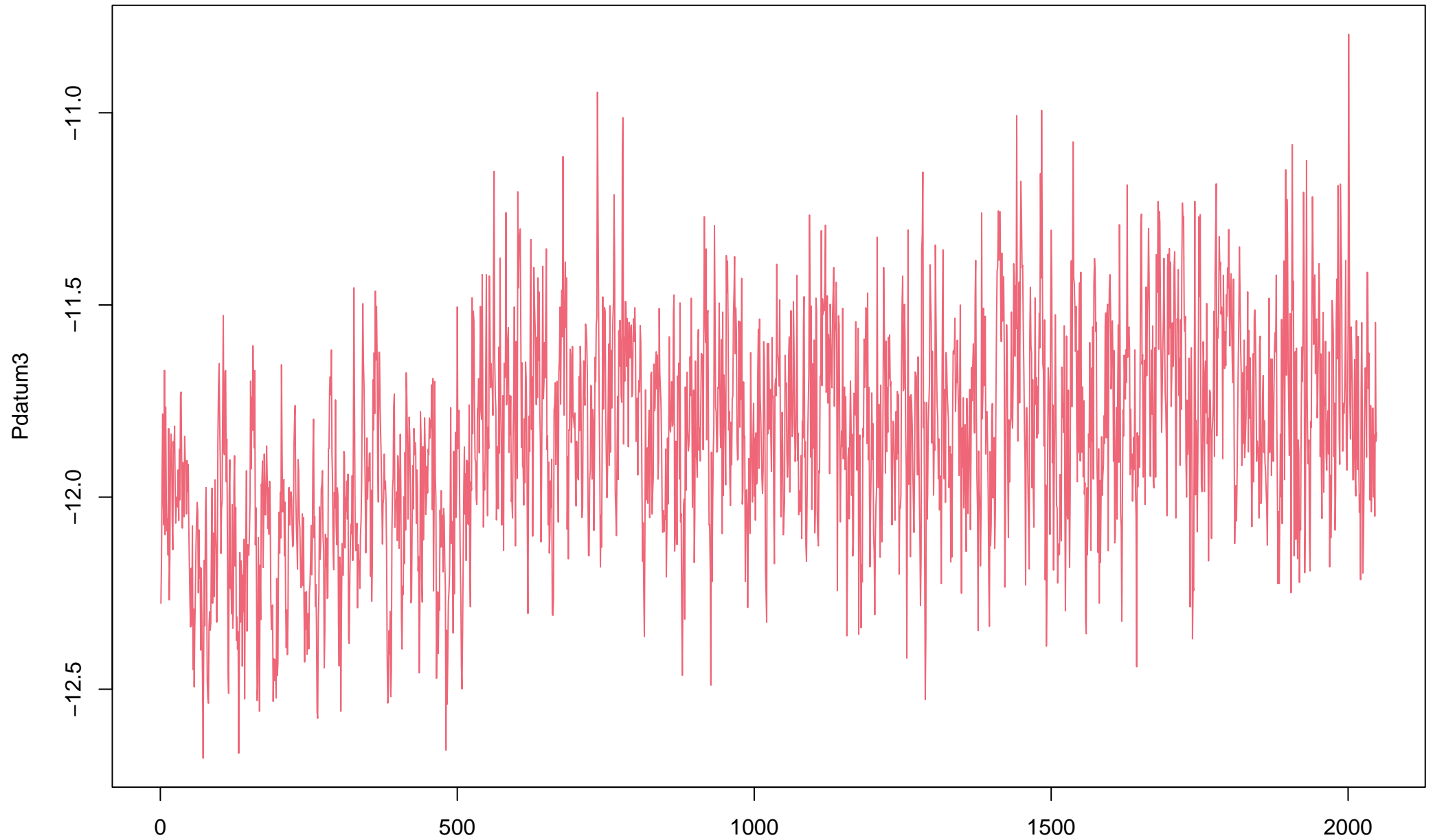
Pdatum1
ESS = 320 | BMK = 0.0582 | MCSE(6.27) = 5.8 | stat: TRUE | burn: 0



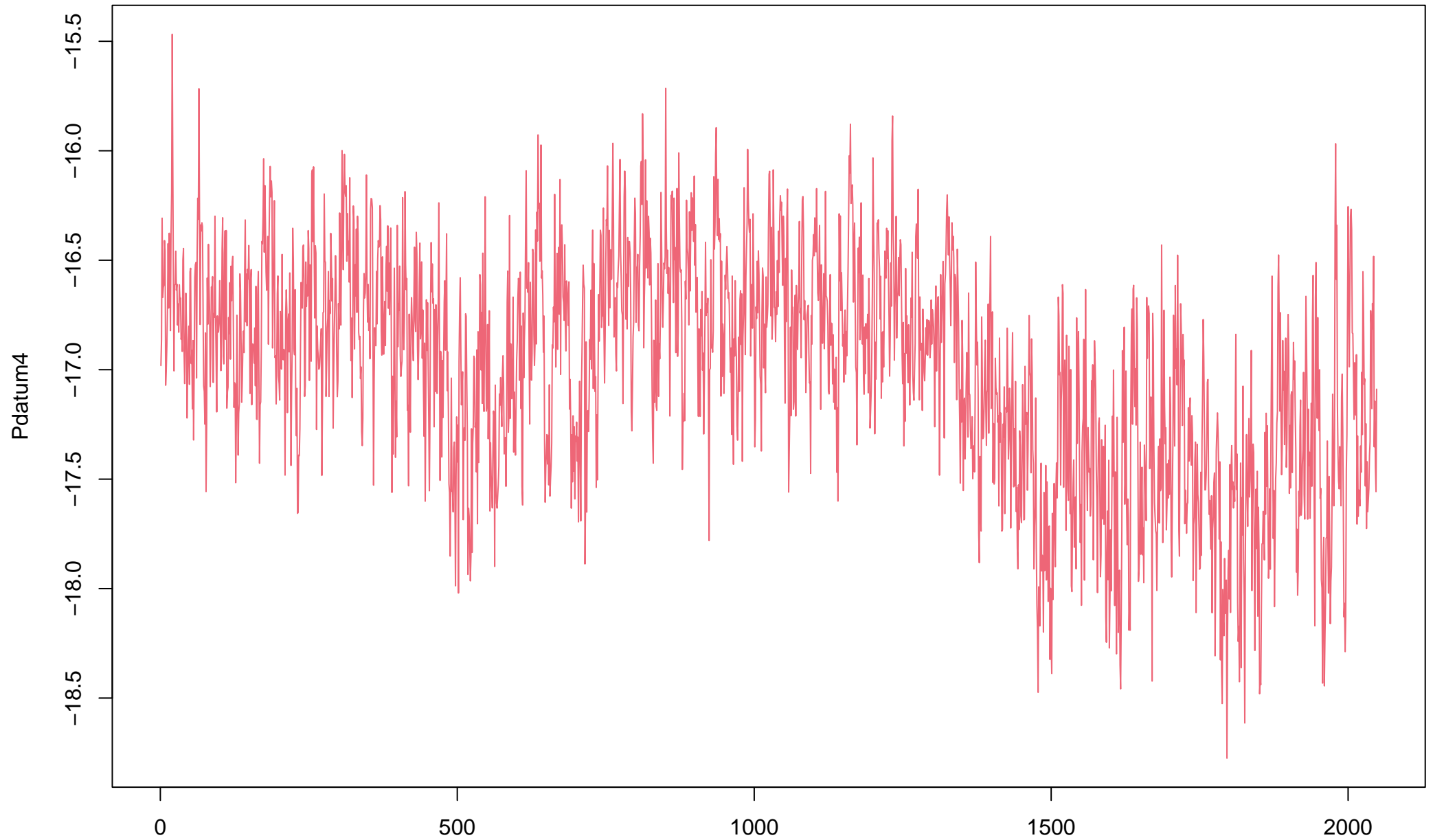
Pdatum2
ESS = 244 | BMK = 0.0975 | MCSE(6.27) = 6.31 | stat: TRUE | burn: 0



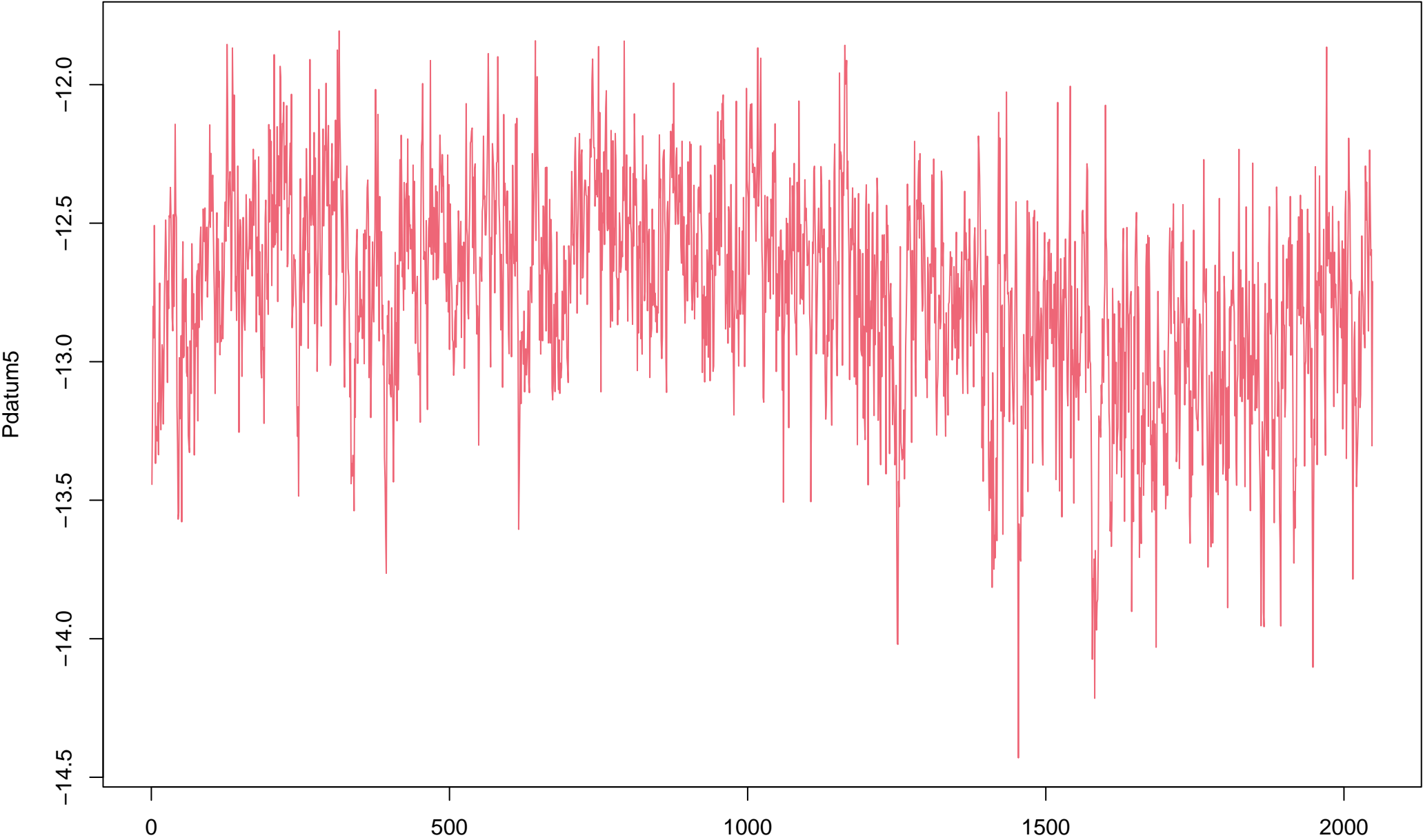
Pdatum3
ESS = 58.1 | BMK = 0.225 | MCSE(6.27) = 7.84 | stat: FALSE | burn: 0



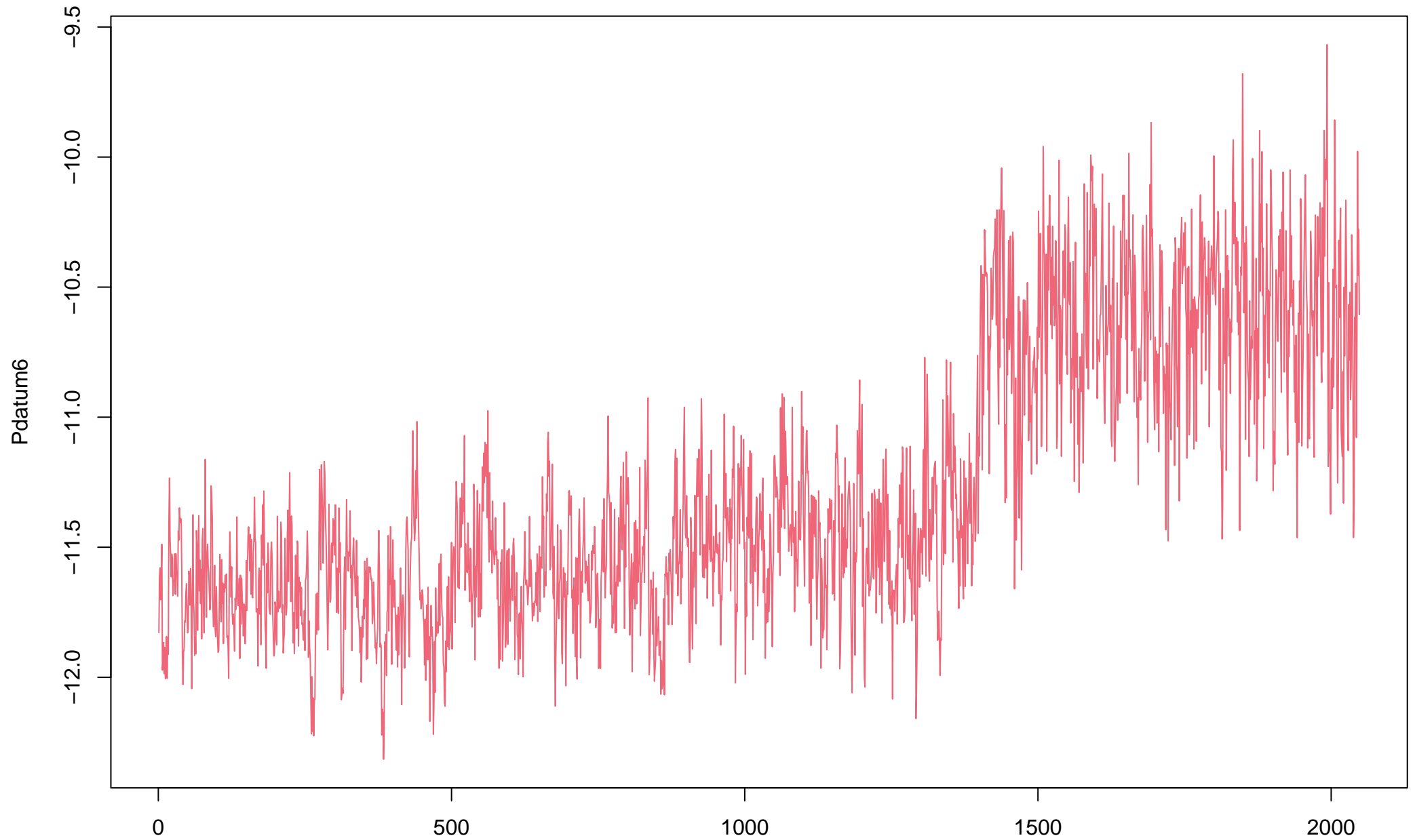
Pdatum4
ESS = 70.4 | BMK = 0.294 | MCSE(6.27) = 9.46 | stat: TRUE | burn: 0



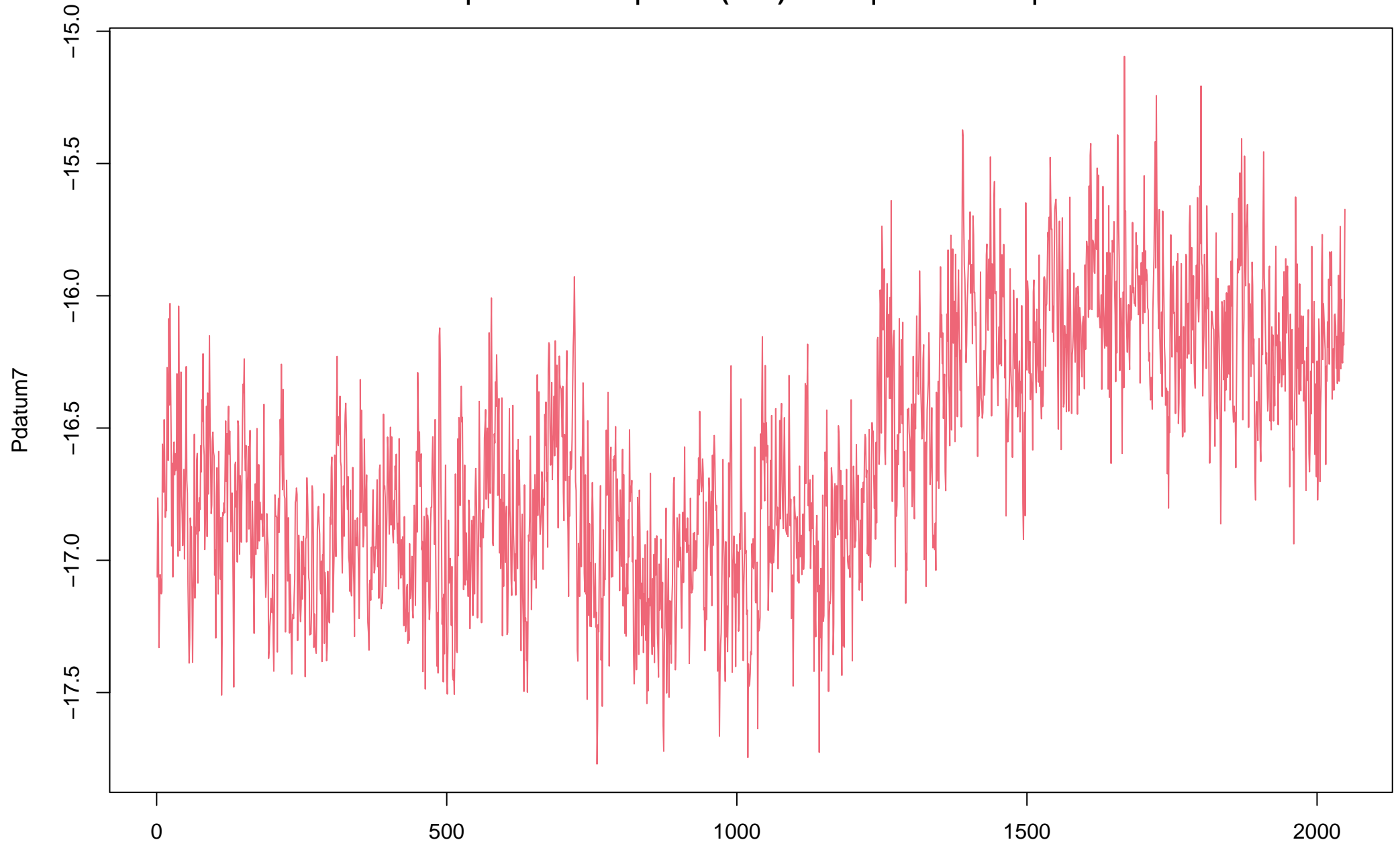
Pdatum5
ESS = 128 | BMK = 0.276 | MCSE(6.27) = 8.17 | stat: FALSE | burn: 0



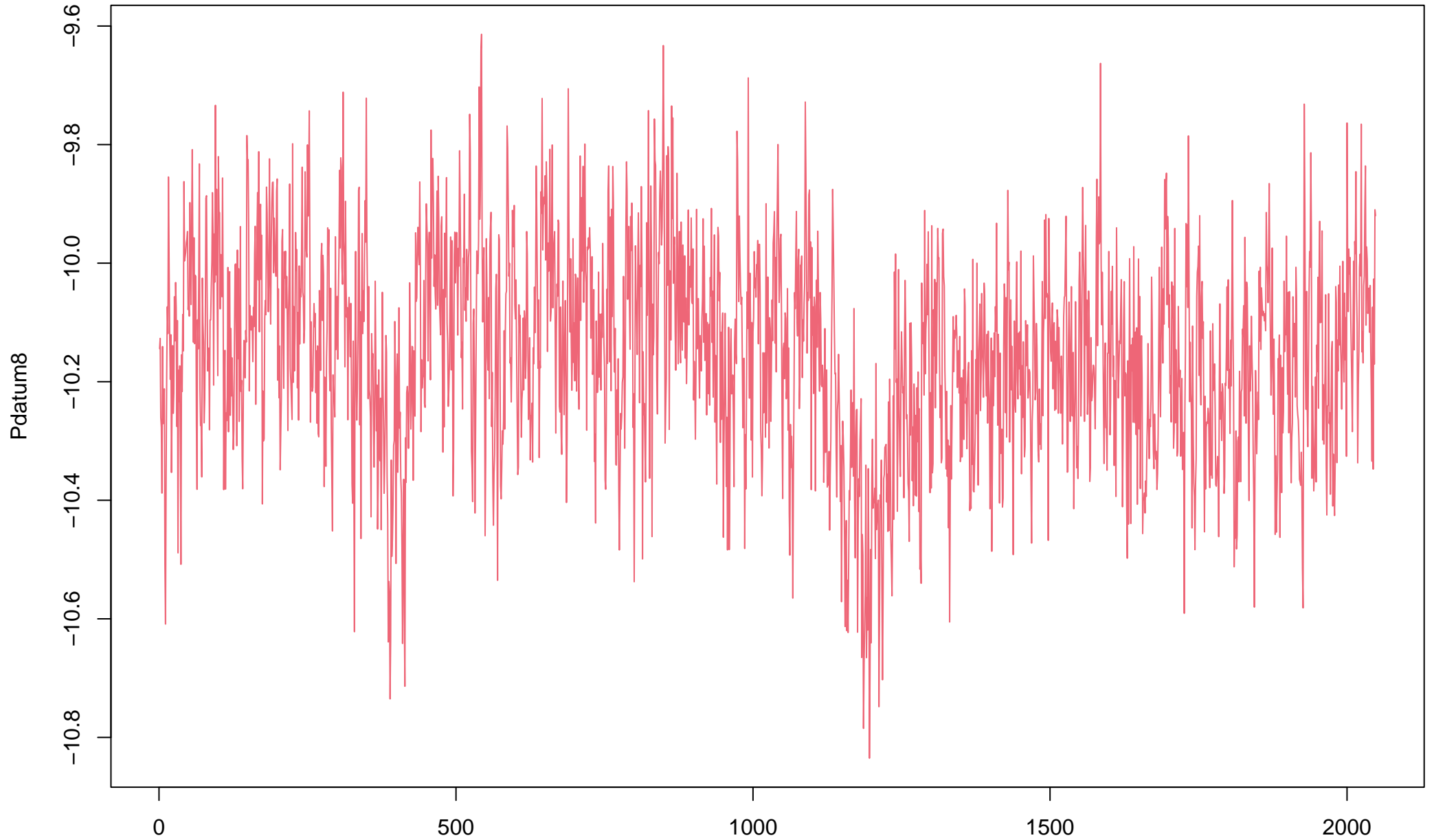
Pdatum6
ESS = 4.43 | BMK = 0.625 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 1428



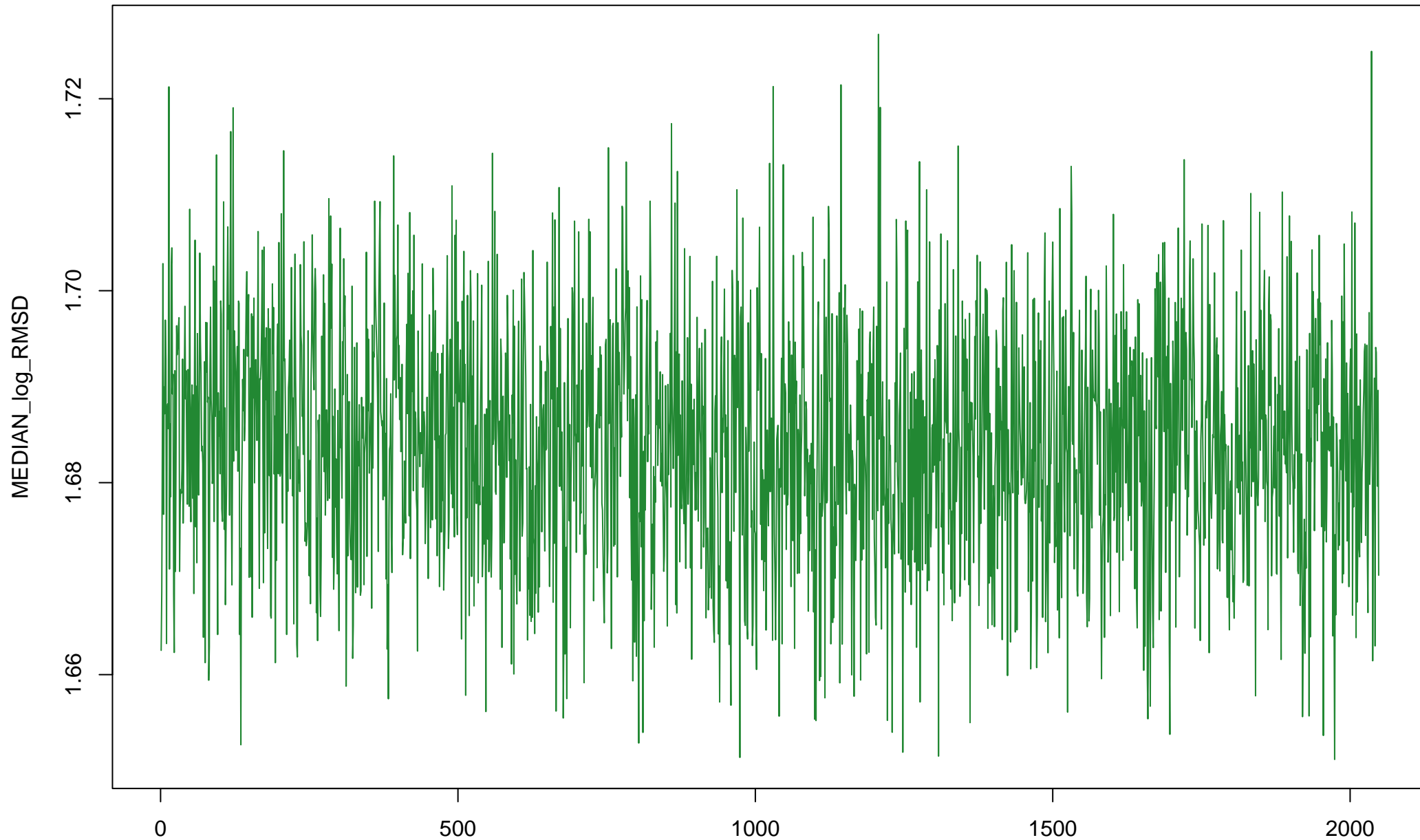
Pdatum7
ESS = 10.6 | BMK = 0.535 | MCSE(6.27) = 11.9 | stat: FALSE | burn: 1224



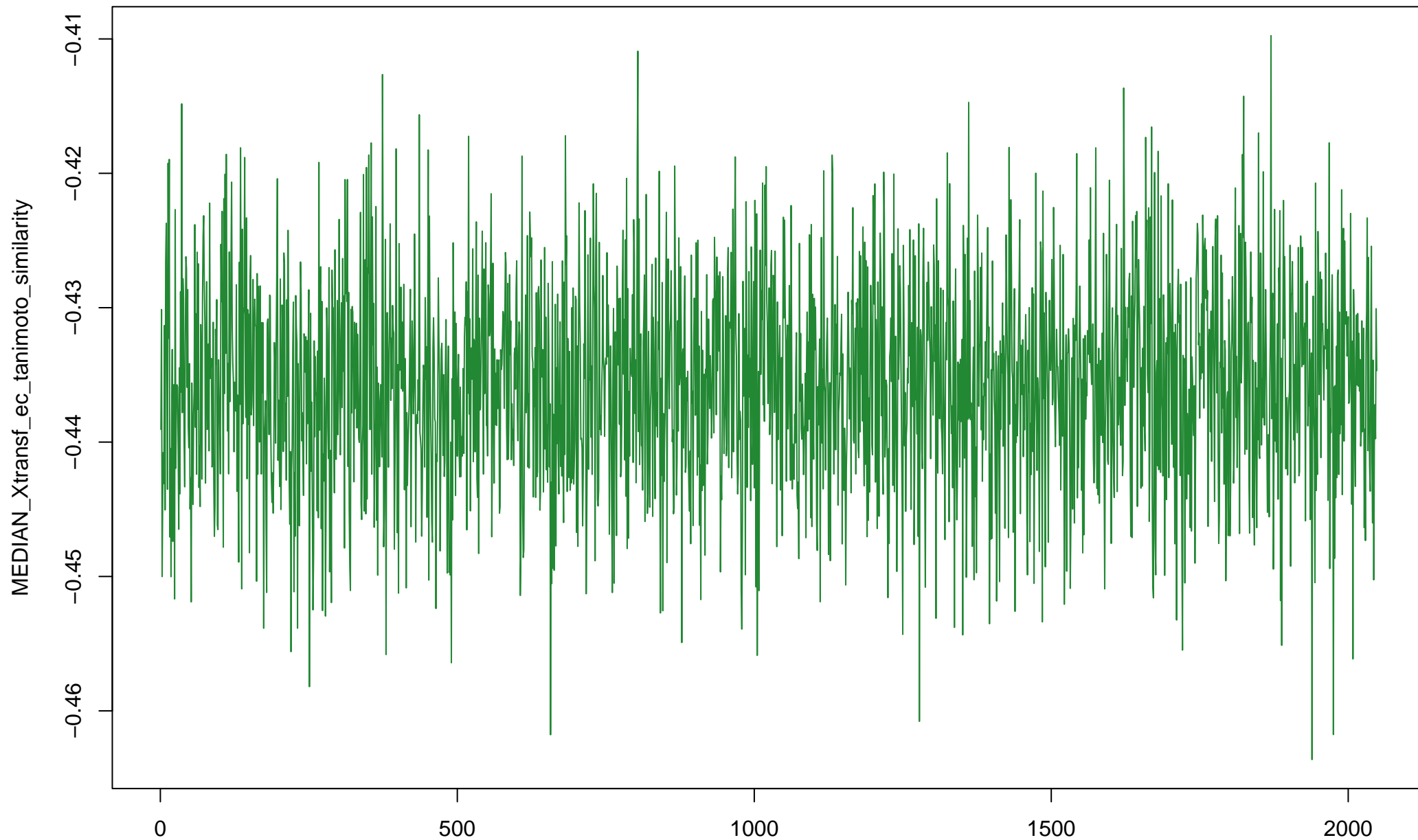
Pdatum8
ESS = 67.5 | BMK = 0.196 | MCSE(6.27) = 7.39 | stat: FALSE | burn: 0



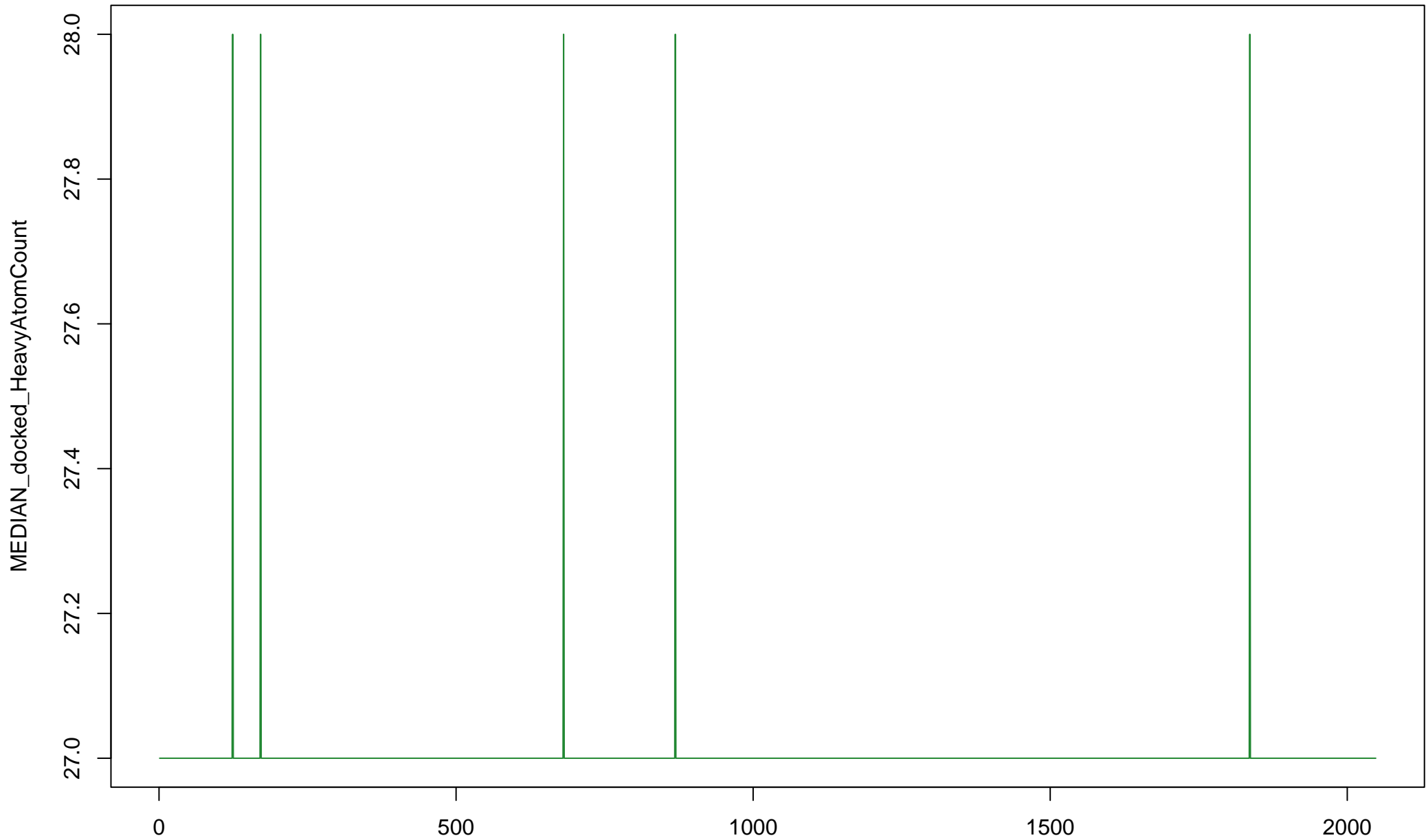
MEDIAN_log_RMSD
ESS = 1680 | BMK = 0.0572 | MCSE(6.27) = 2.48 | stat: FALSE | burn: 0



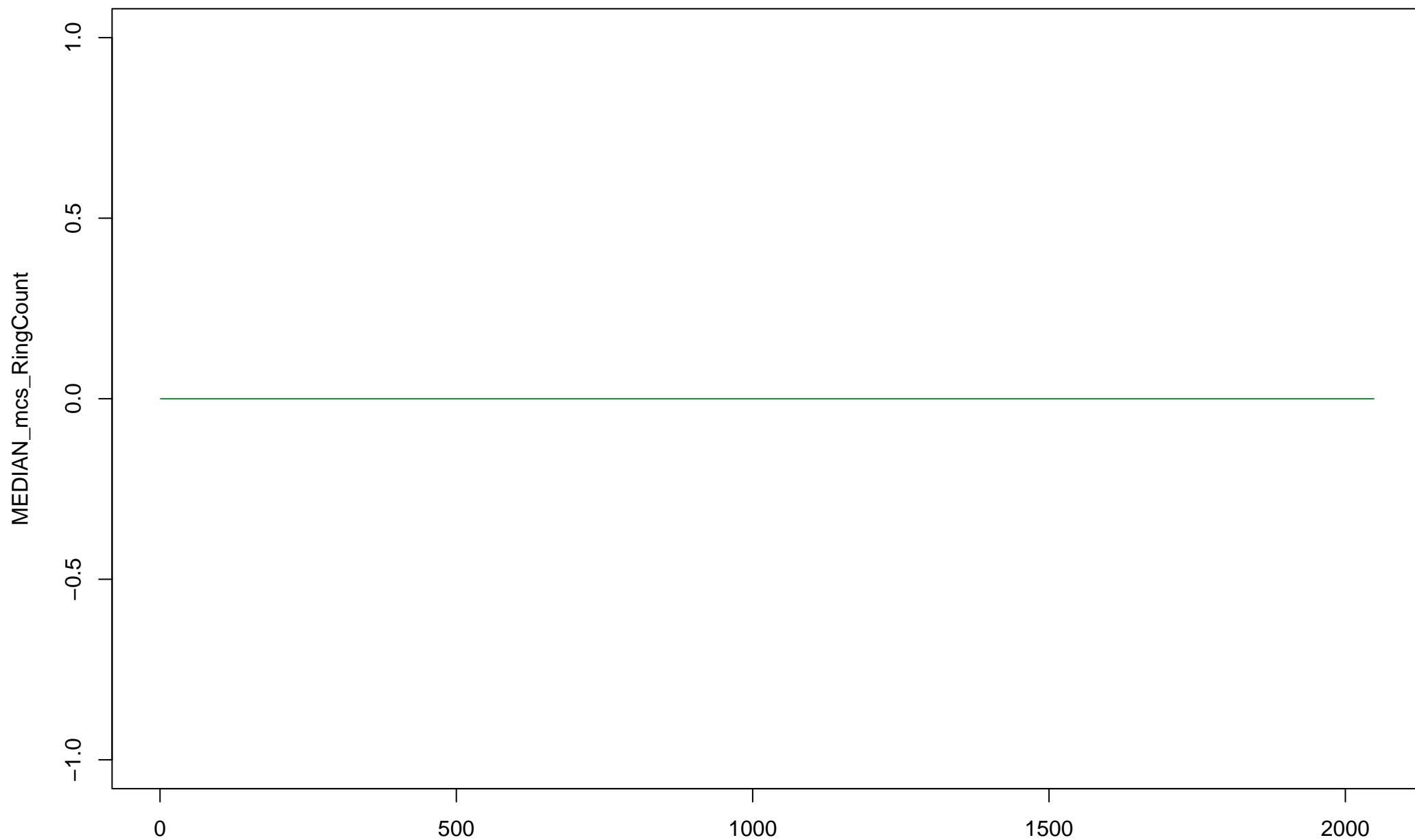
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1750 | BMK = 0.0435 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0



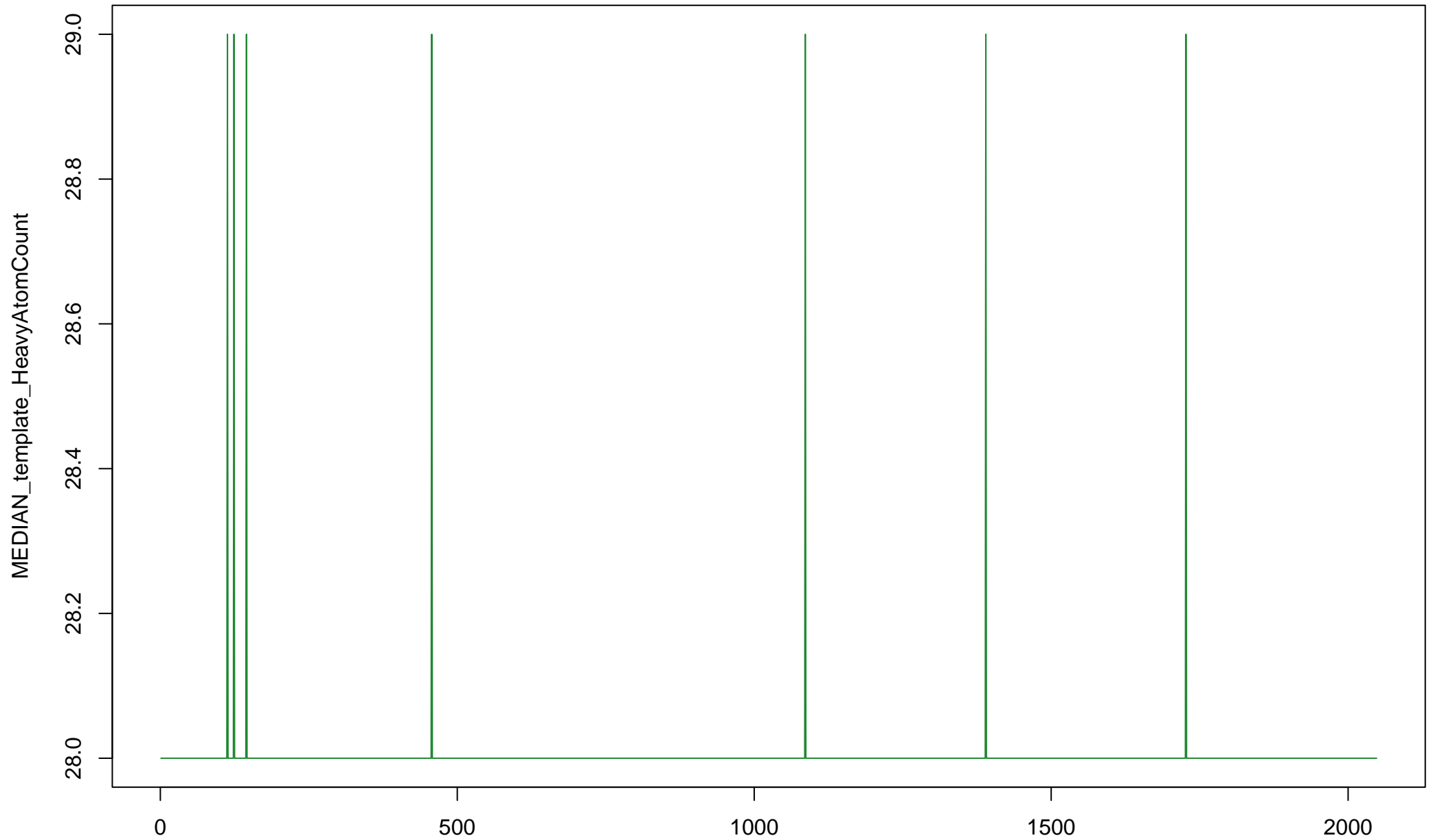
MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.232 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 2040



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



MEDIAN_template_HeavyAtomCount
ESS = 1130 | BMK = 0.051 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 2040



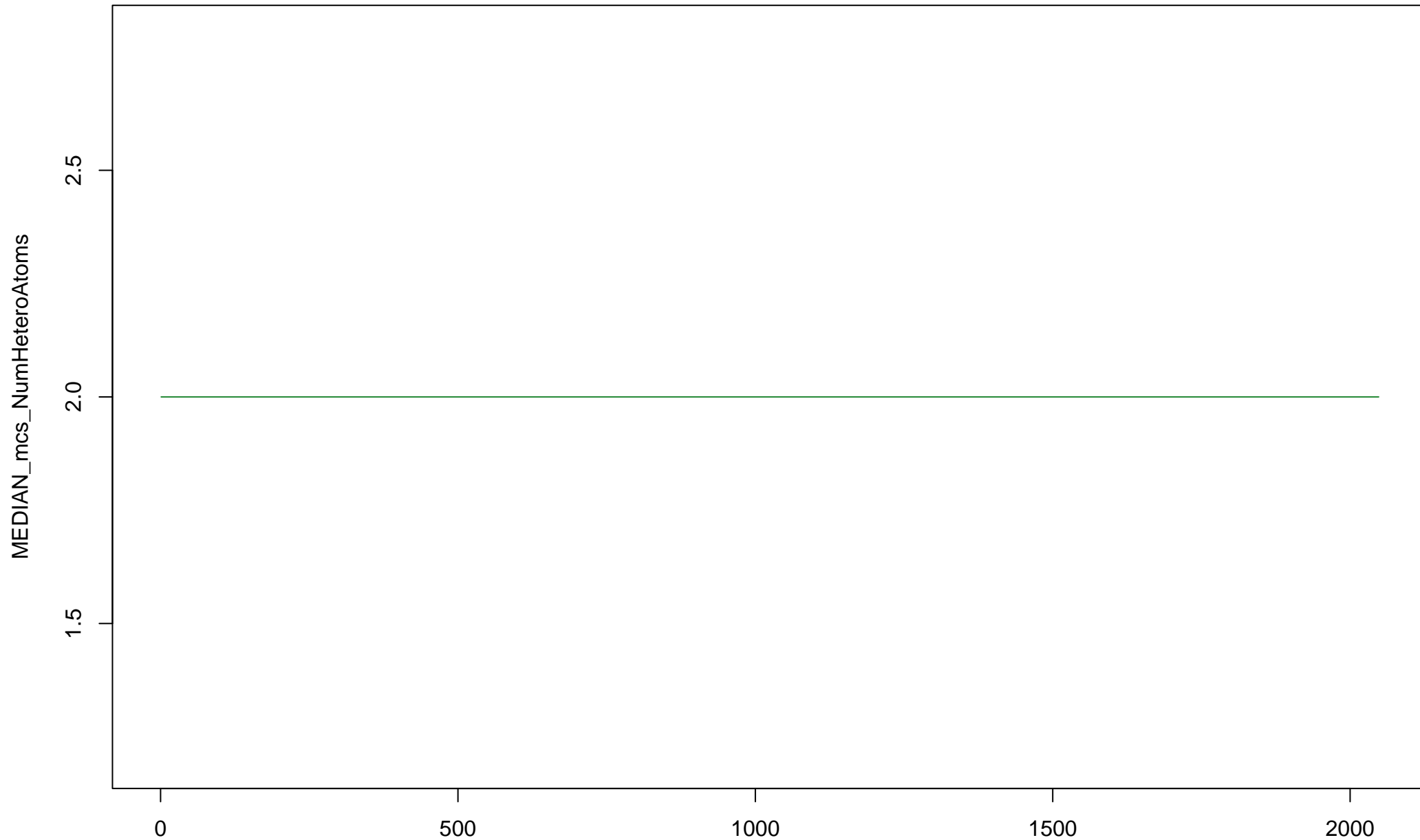
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



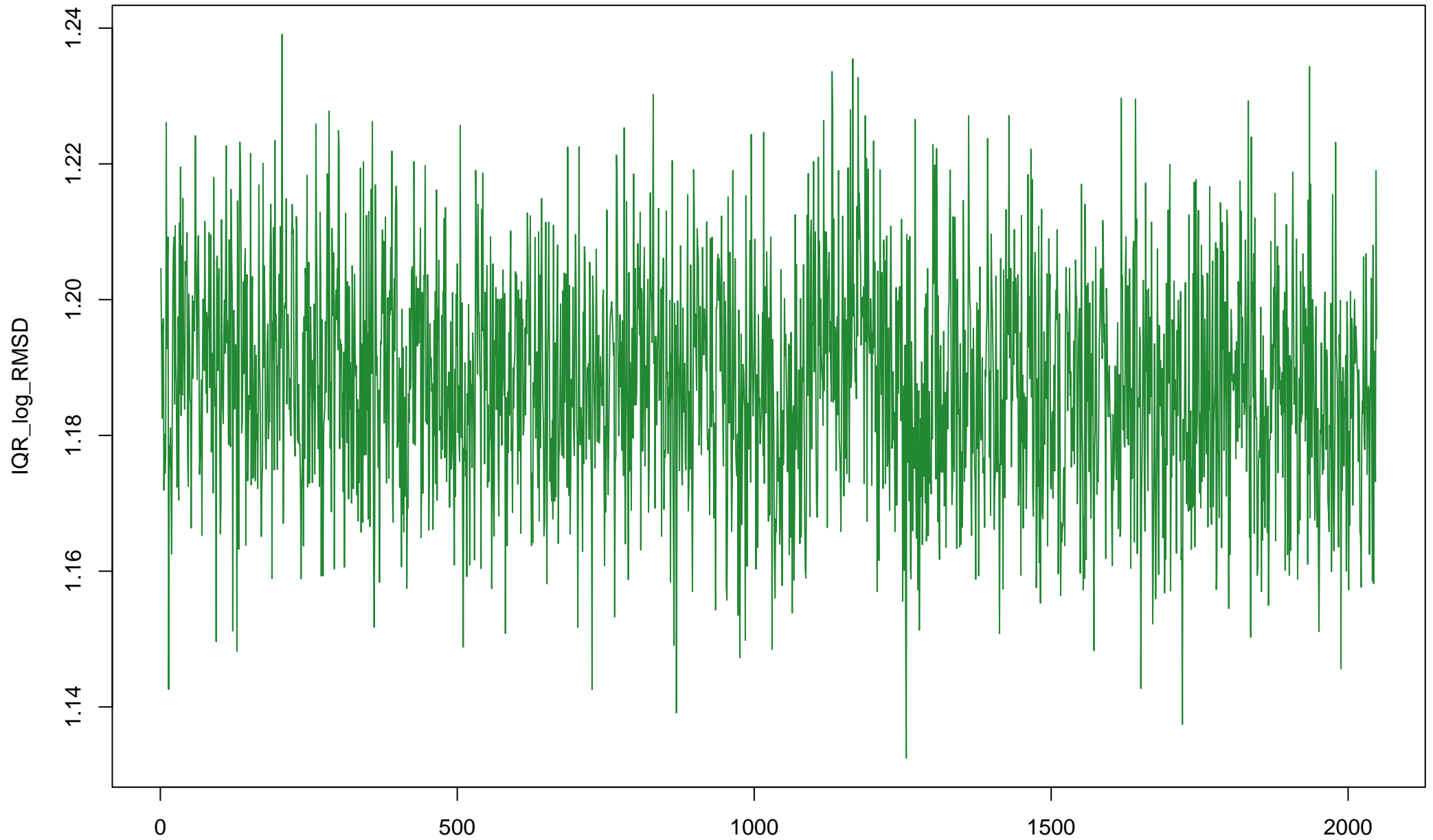
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



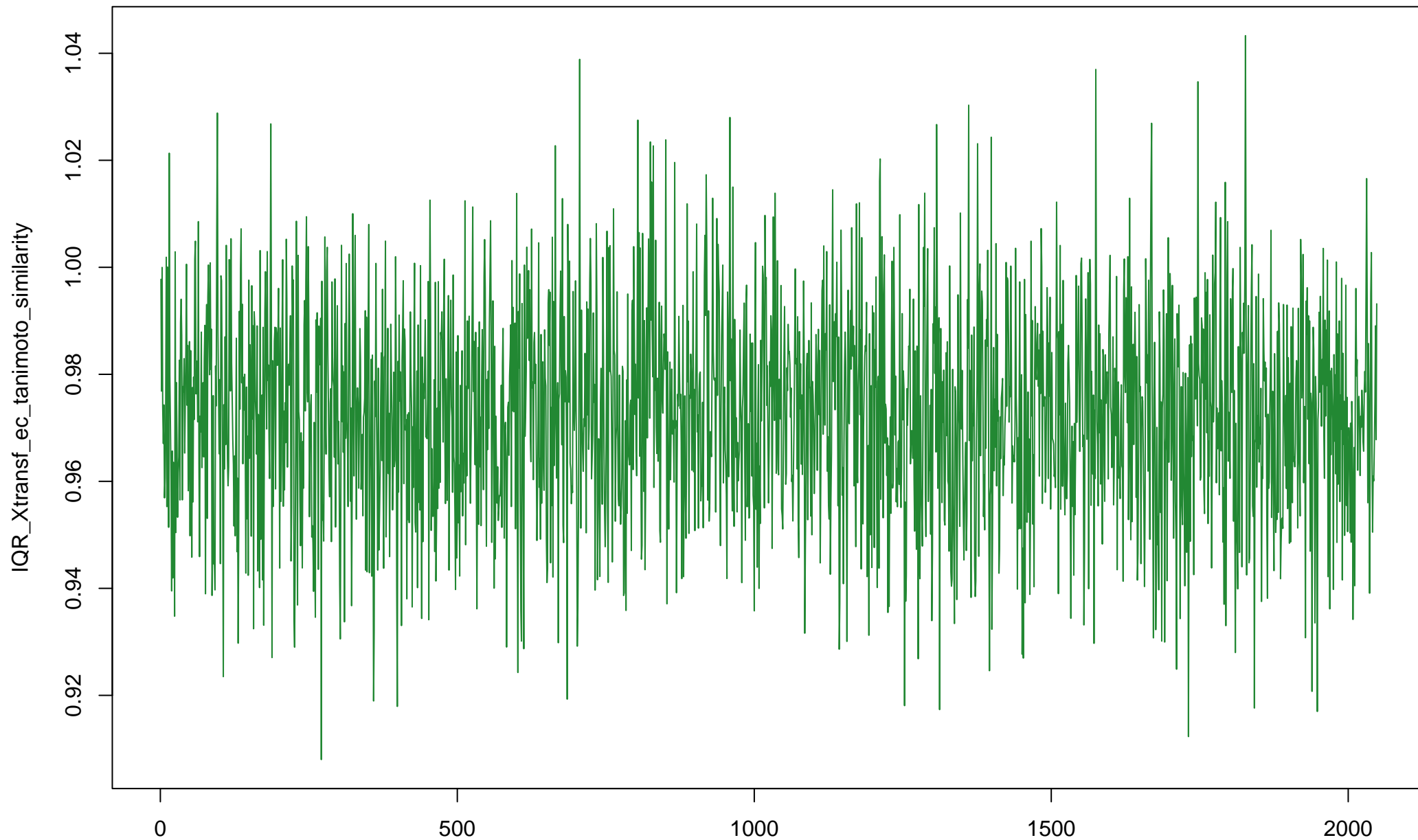
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



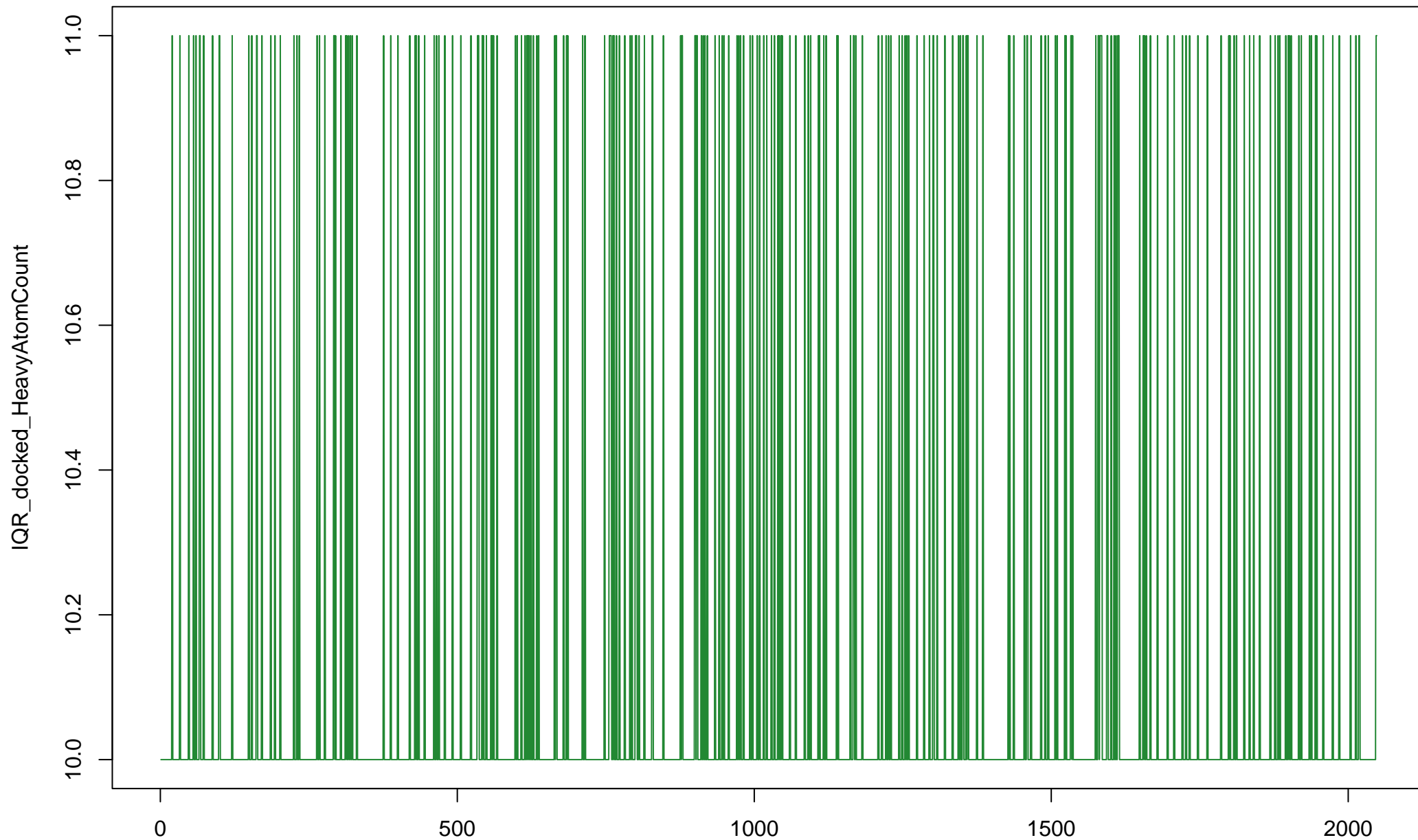
IQR_log_RMSD
ESS = 1170 | BMK = 0.0849 | MCSE(6.27) = 3.52 | stat: FALSE | burn: 0



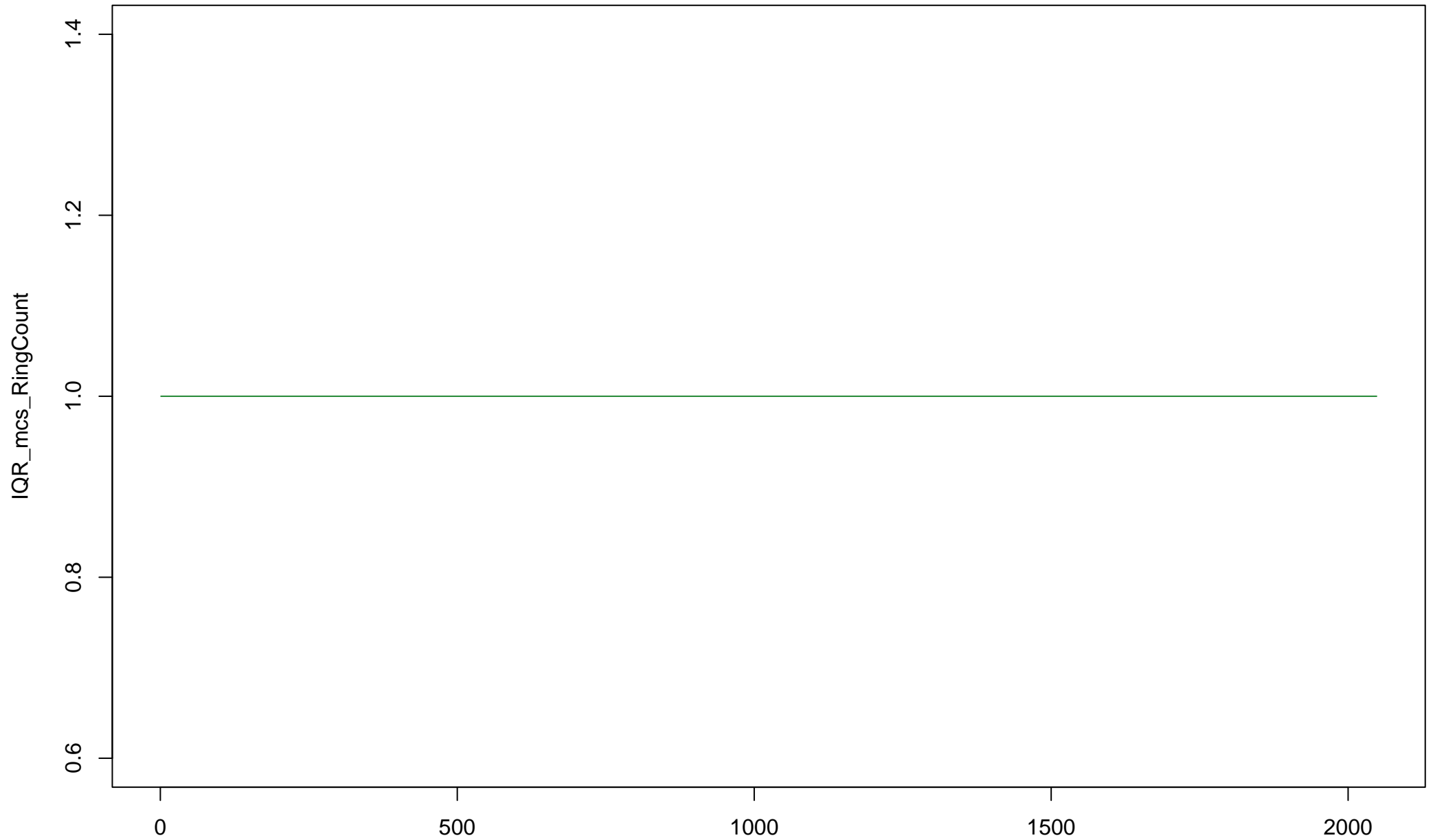
IQR_Xtransf_ec_tanimoto_similarity
ESS = 1740 | BMK = 0.0306 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0



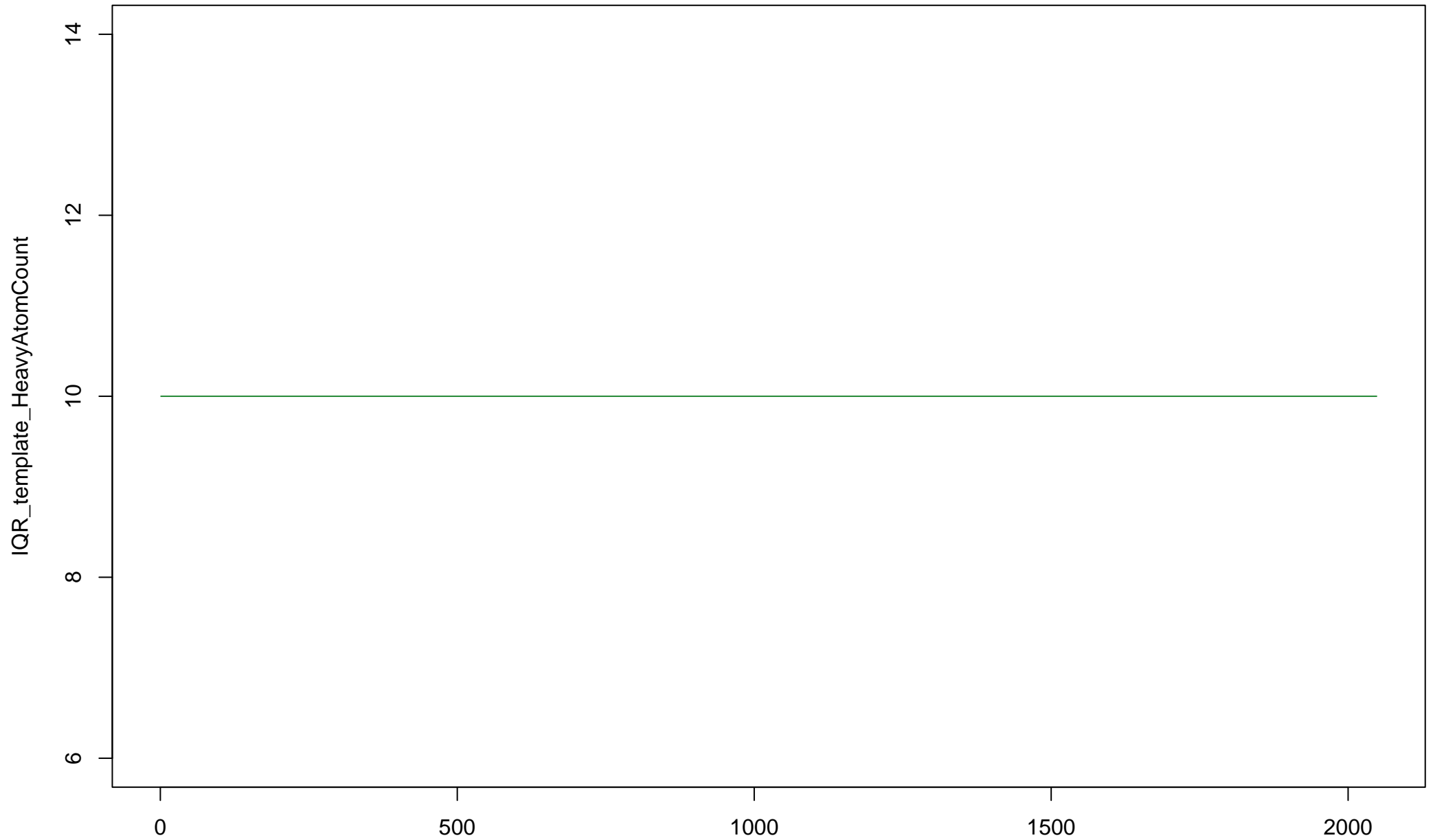
IQR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.15 | stat: FALSE | burn: 0



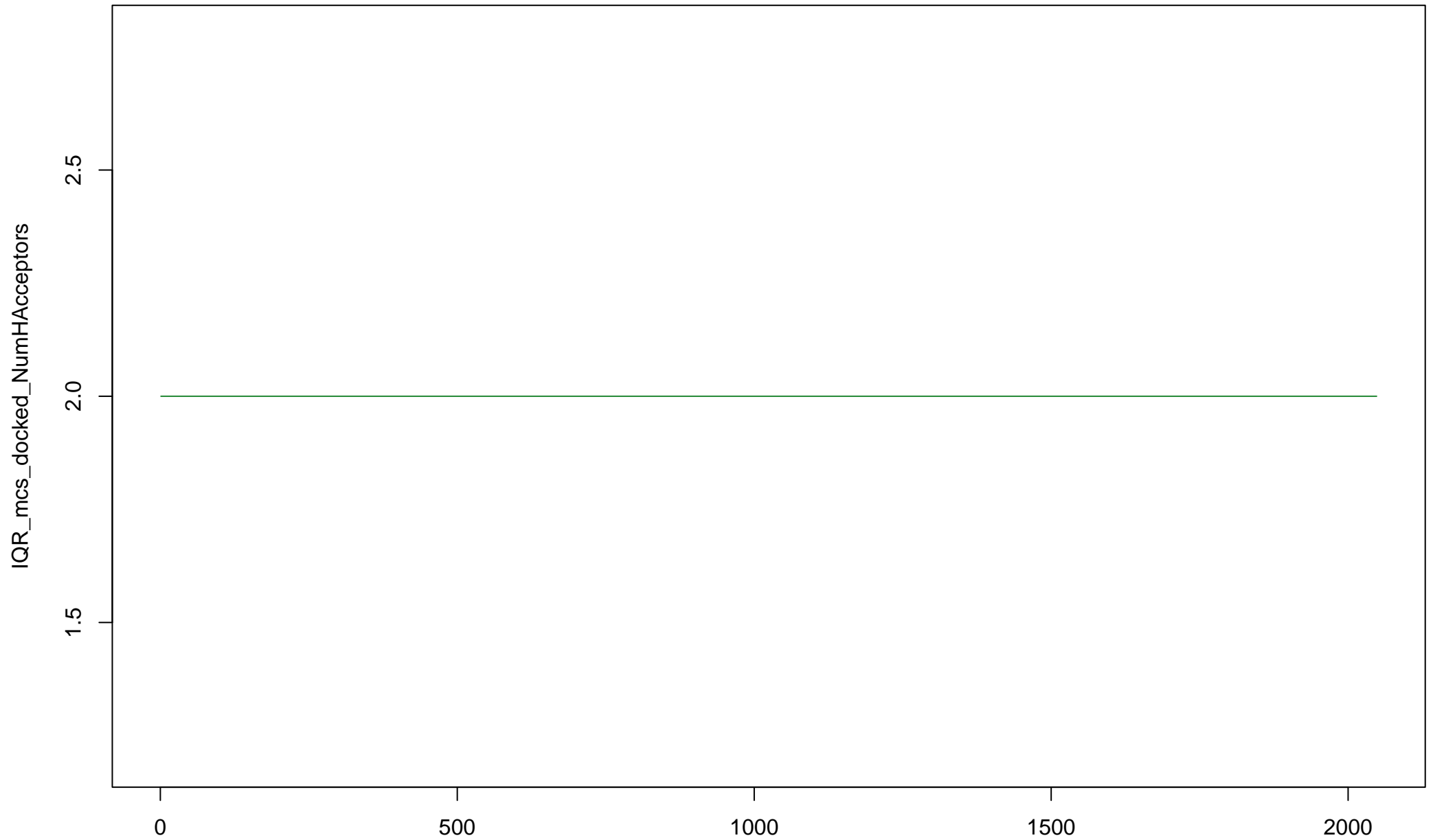
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



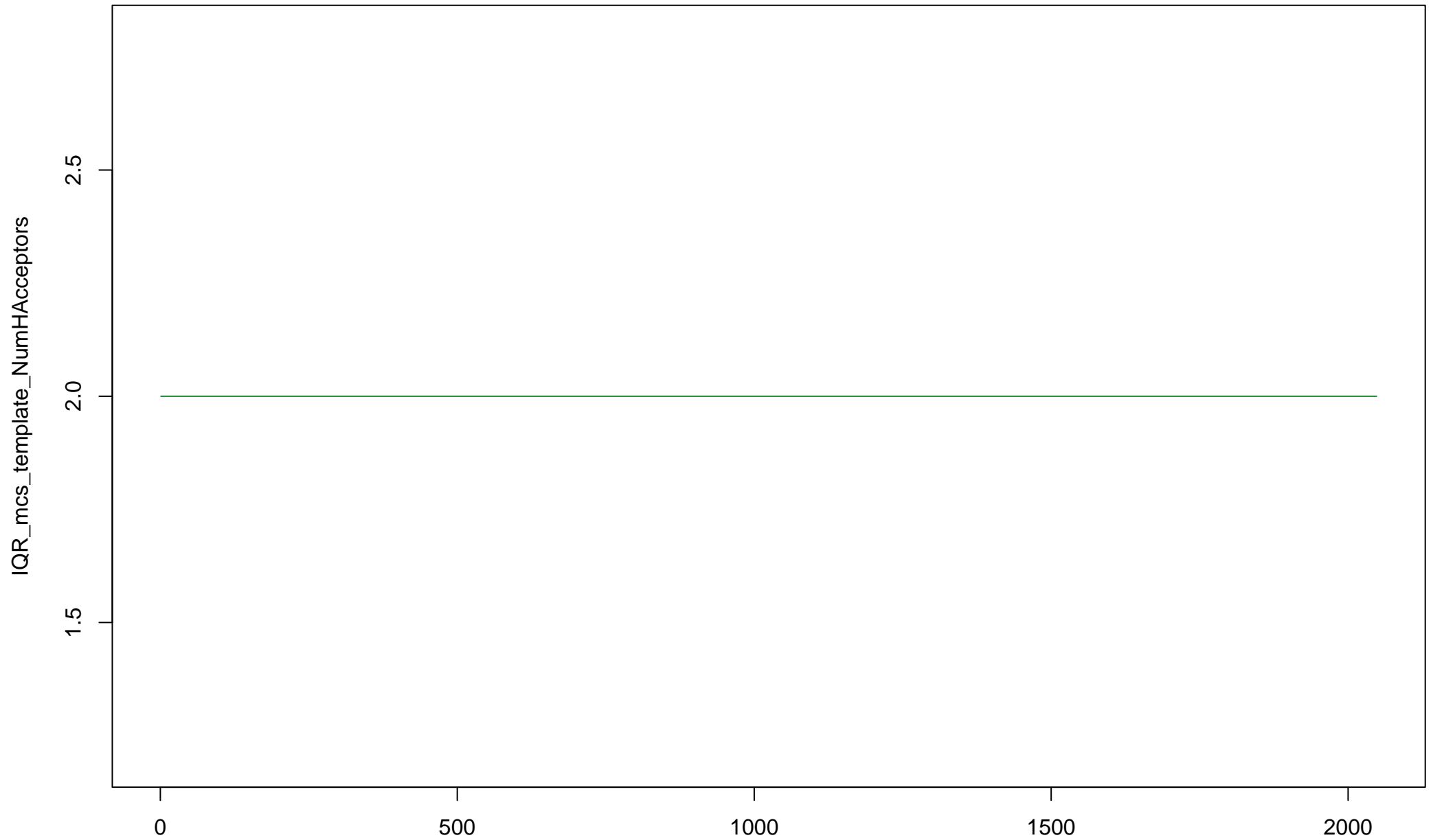
IQR_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



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



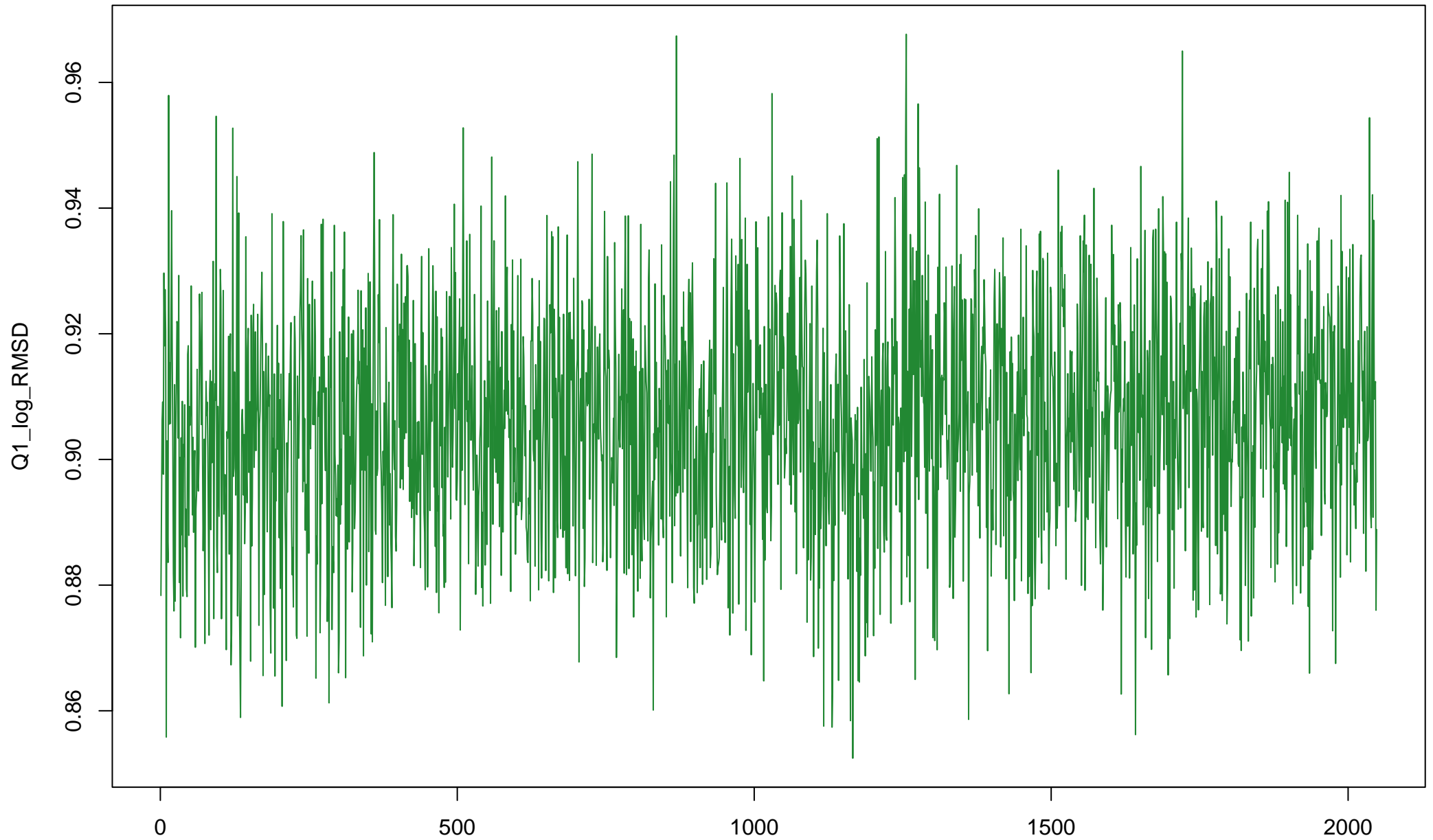
IQR_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



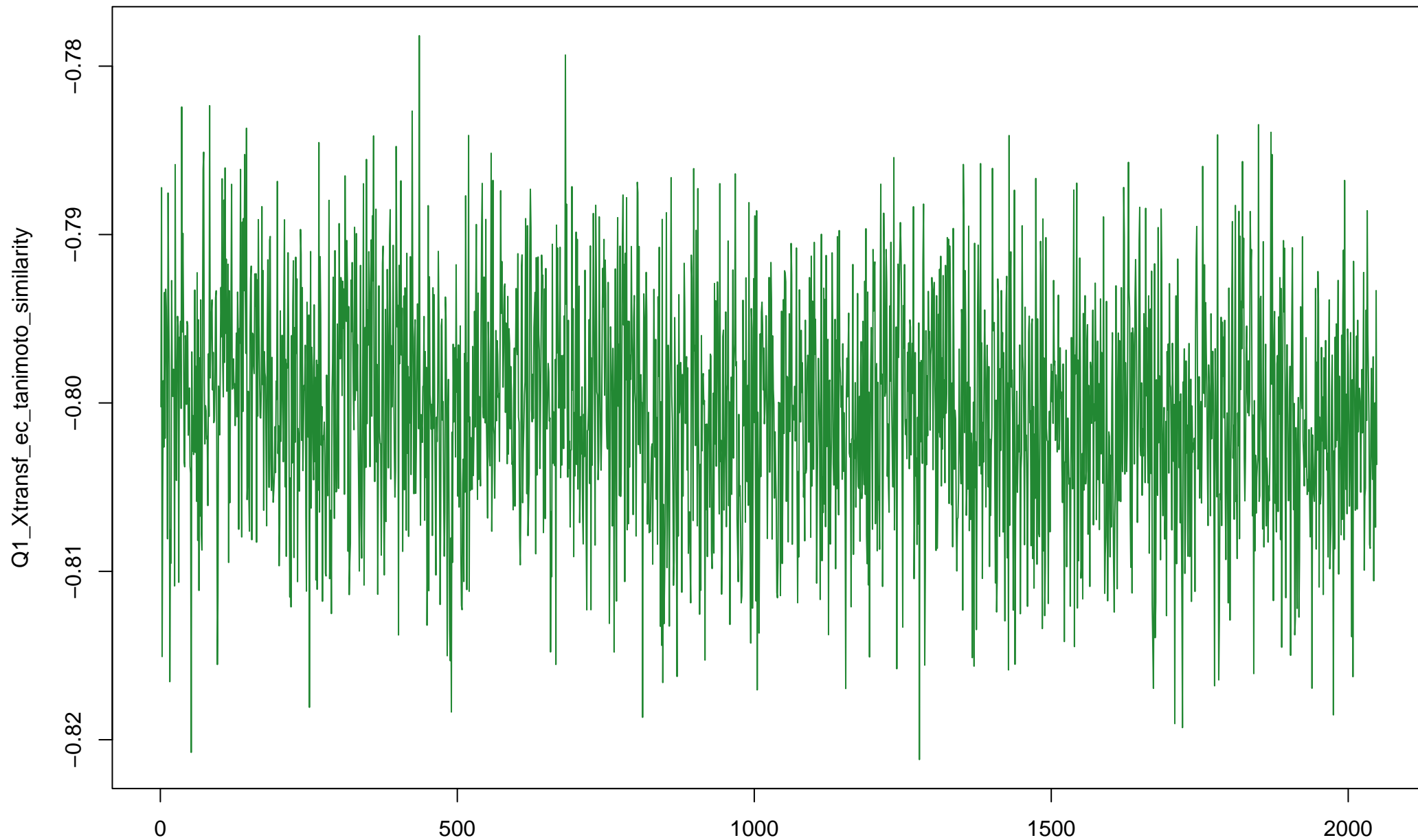
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



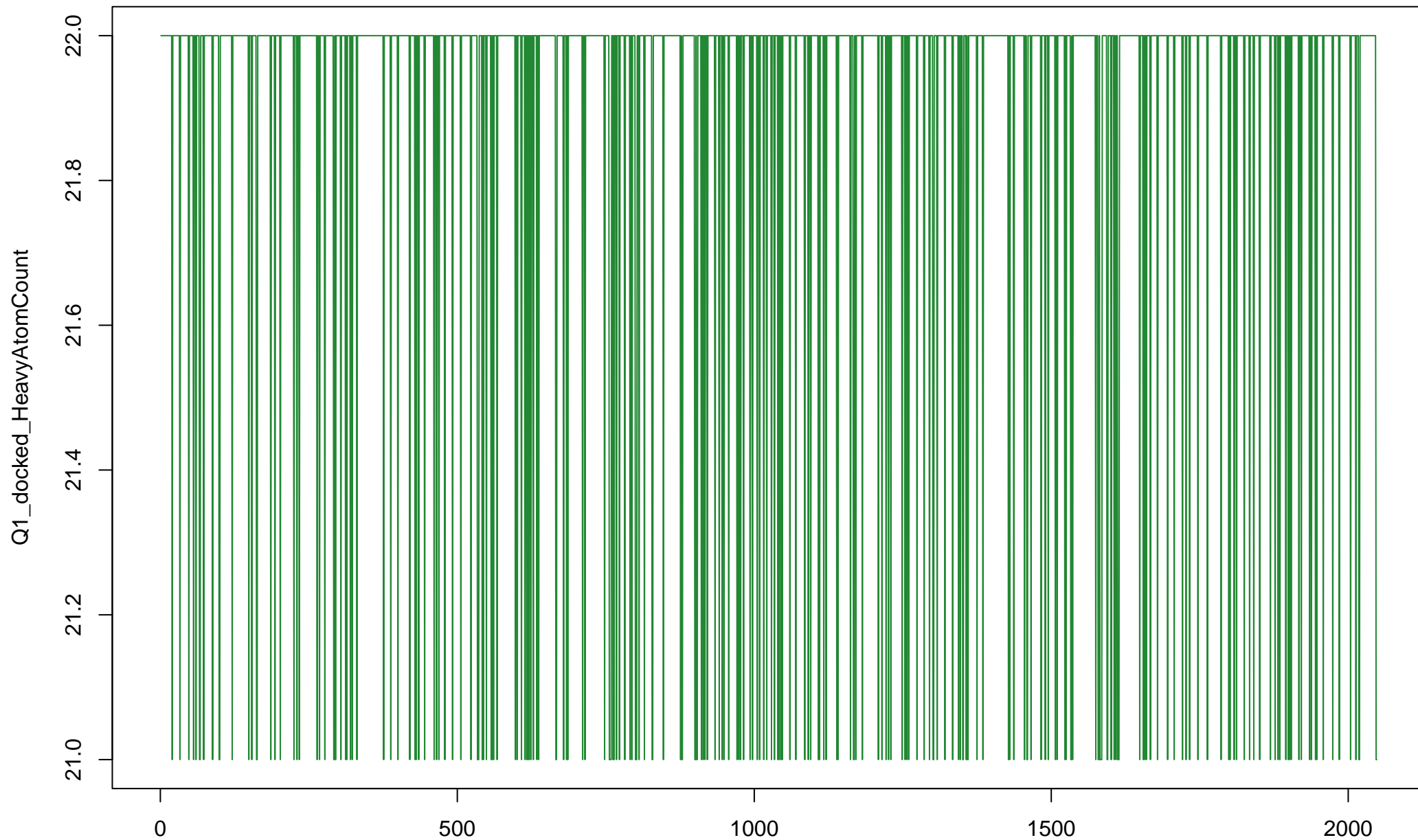
Q1_log_RMSD
ESS = 1780 | BMK = 0.0689 | MCSE(6.27) = 3 | stat: FALSE | burn: 0



Q1_Xtransf_ec_tanimoto_similarity
ESS = 1390 | BMK = 0.0692 | MCSE(6.27) = 3.23 | stat: FALSE | burn: 0



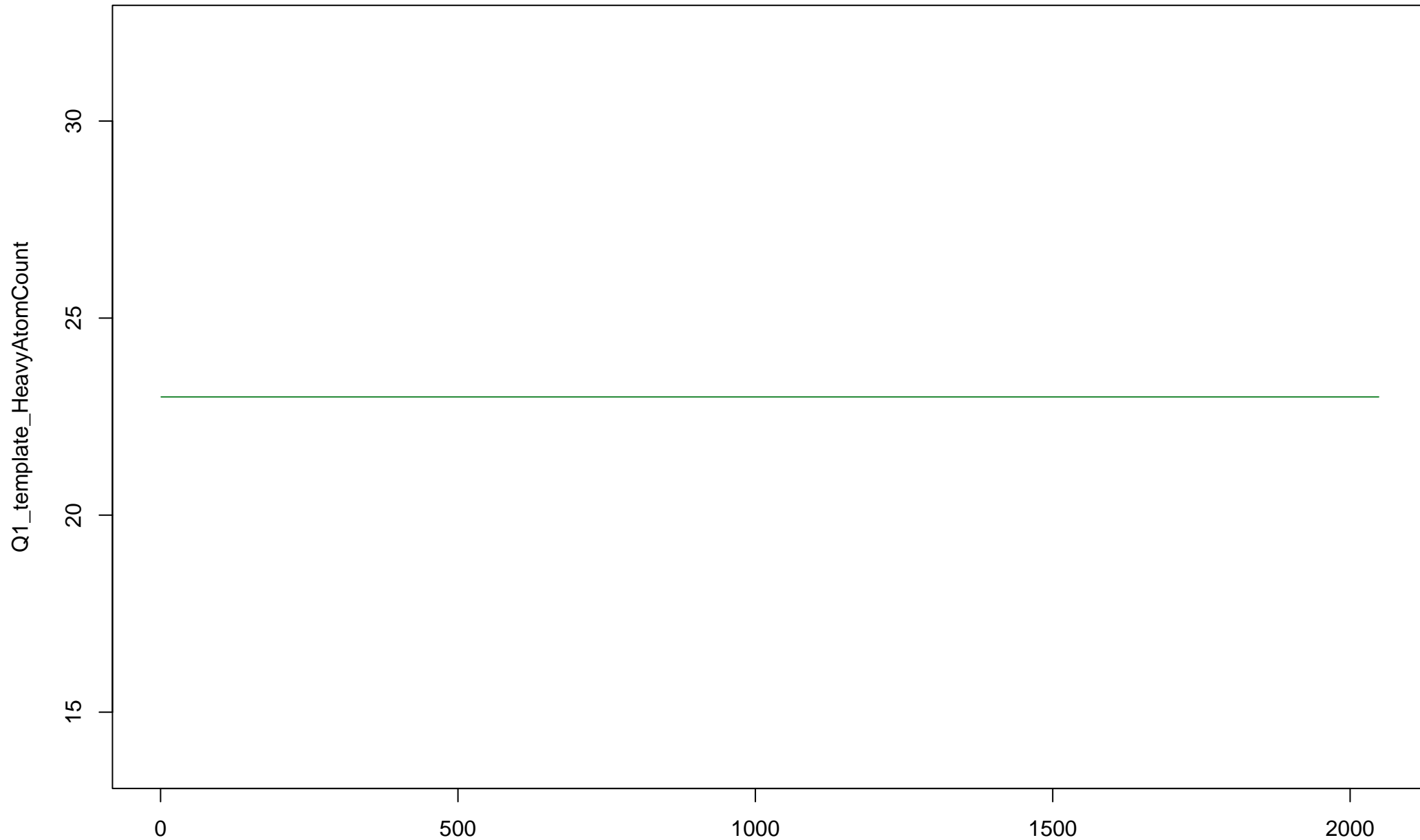
Q1_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.00289 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



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



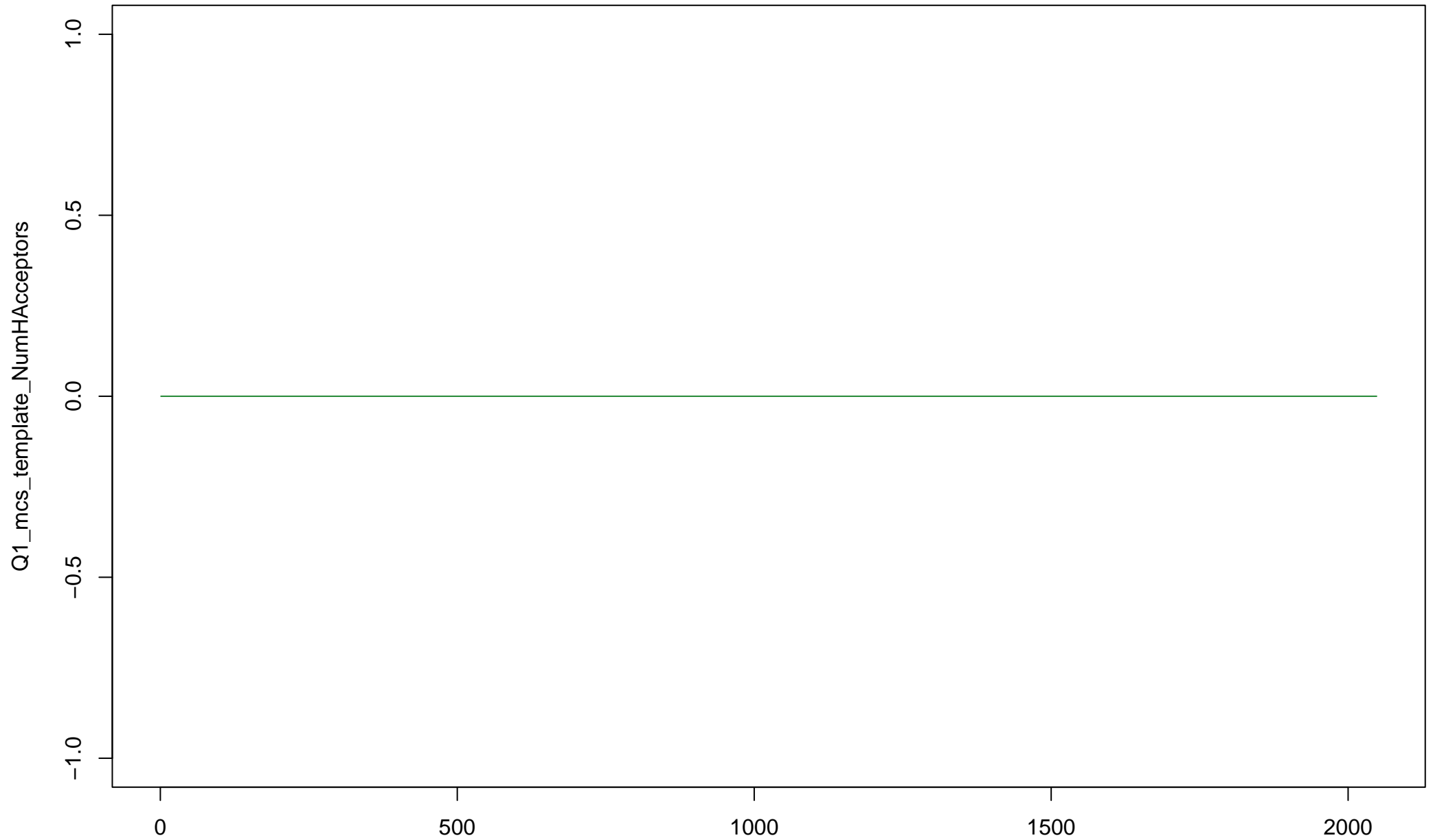
Q1_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



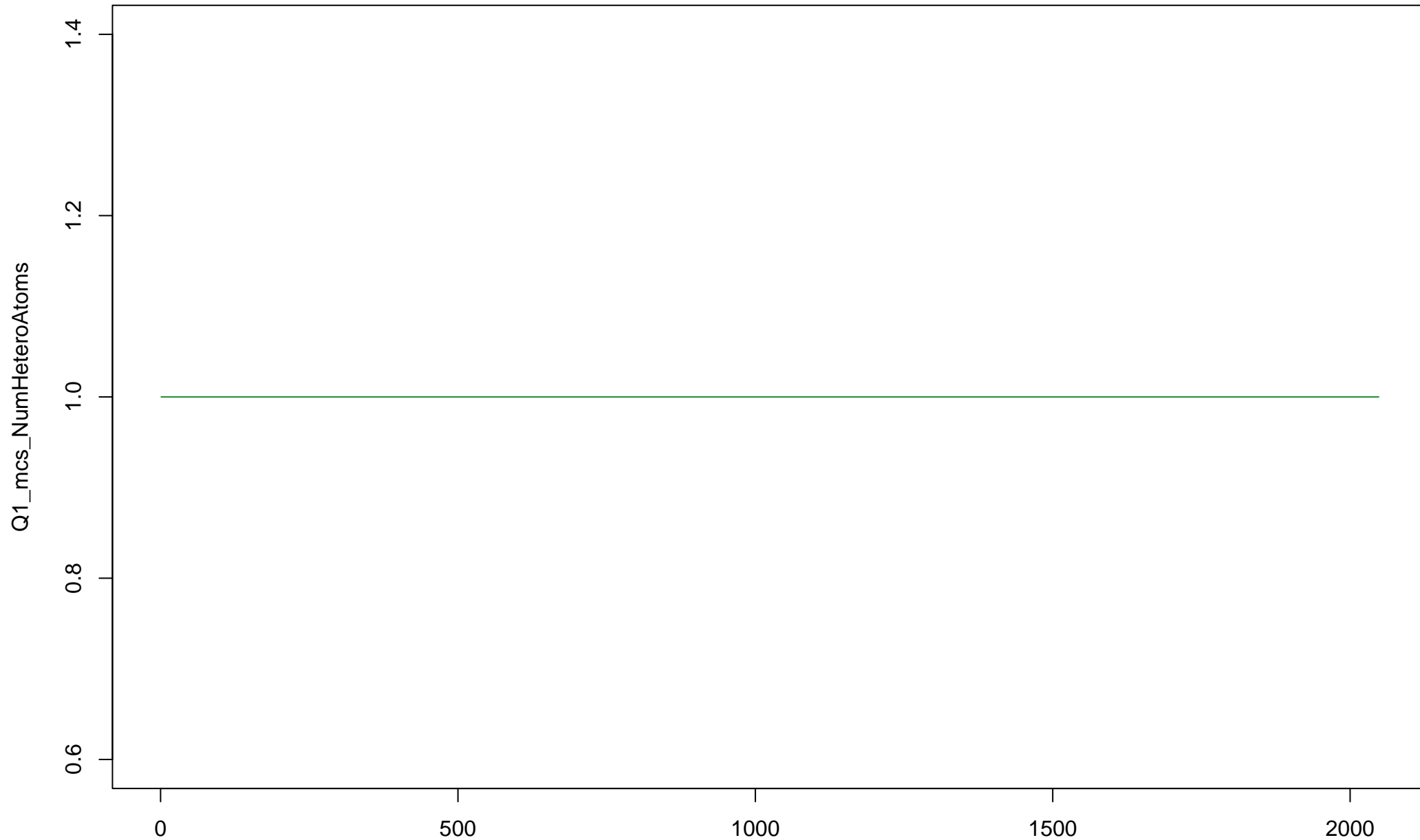
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



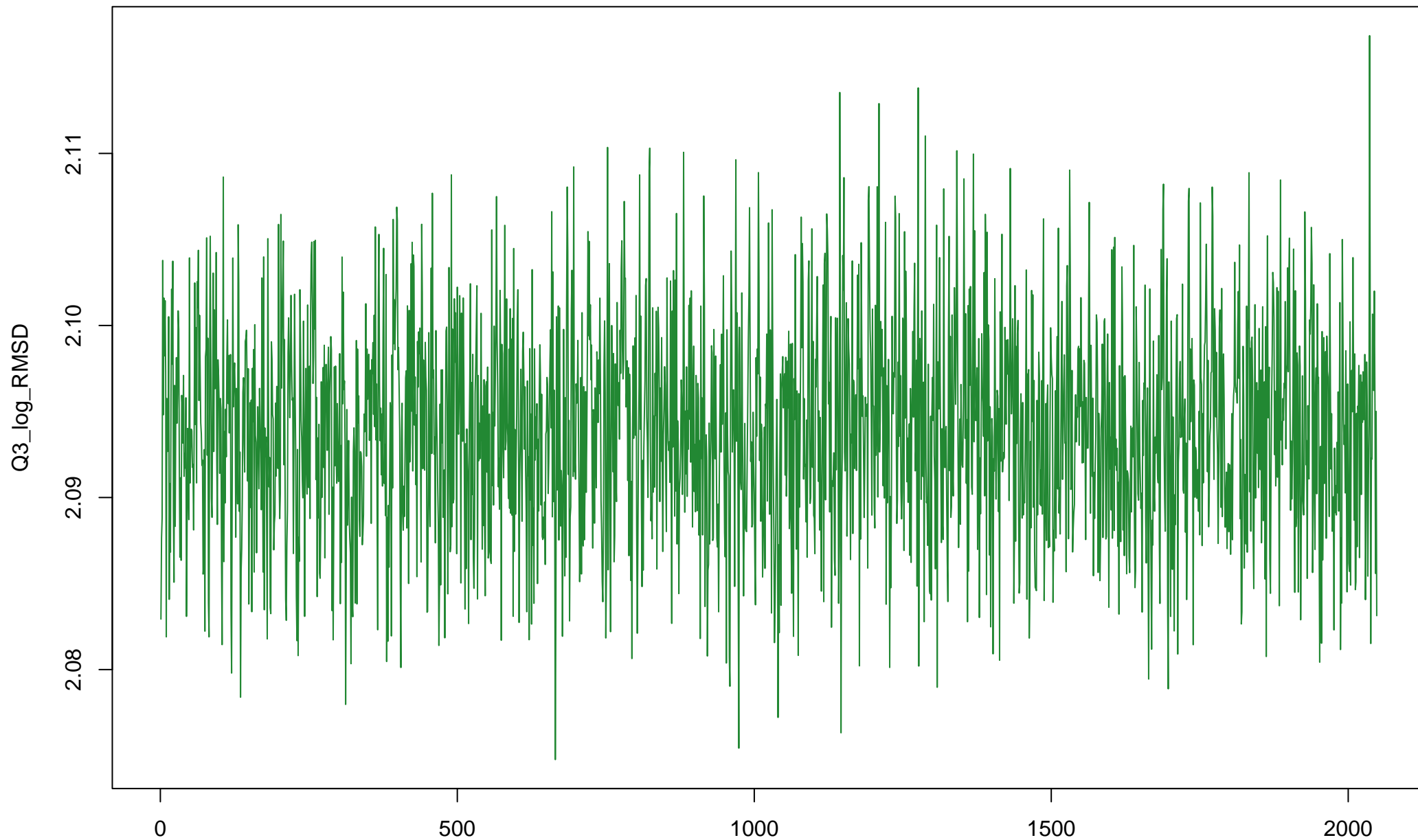
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



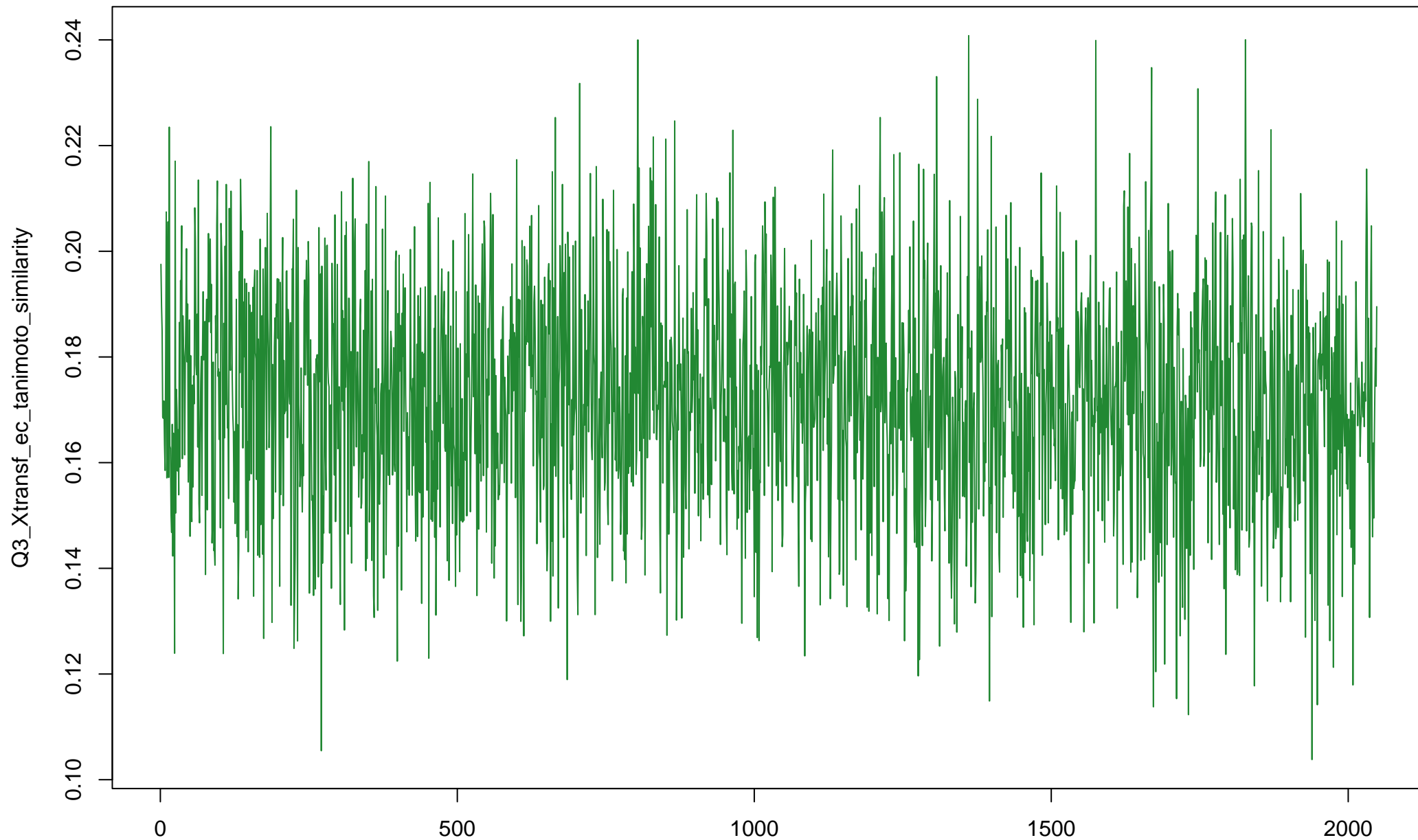
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



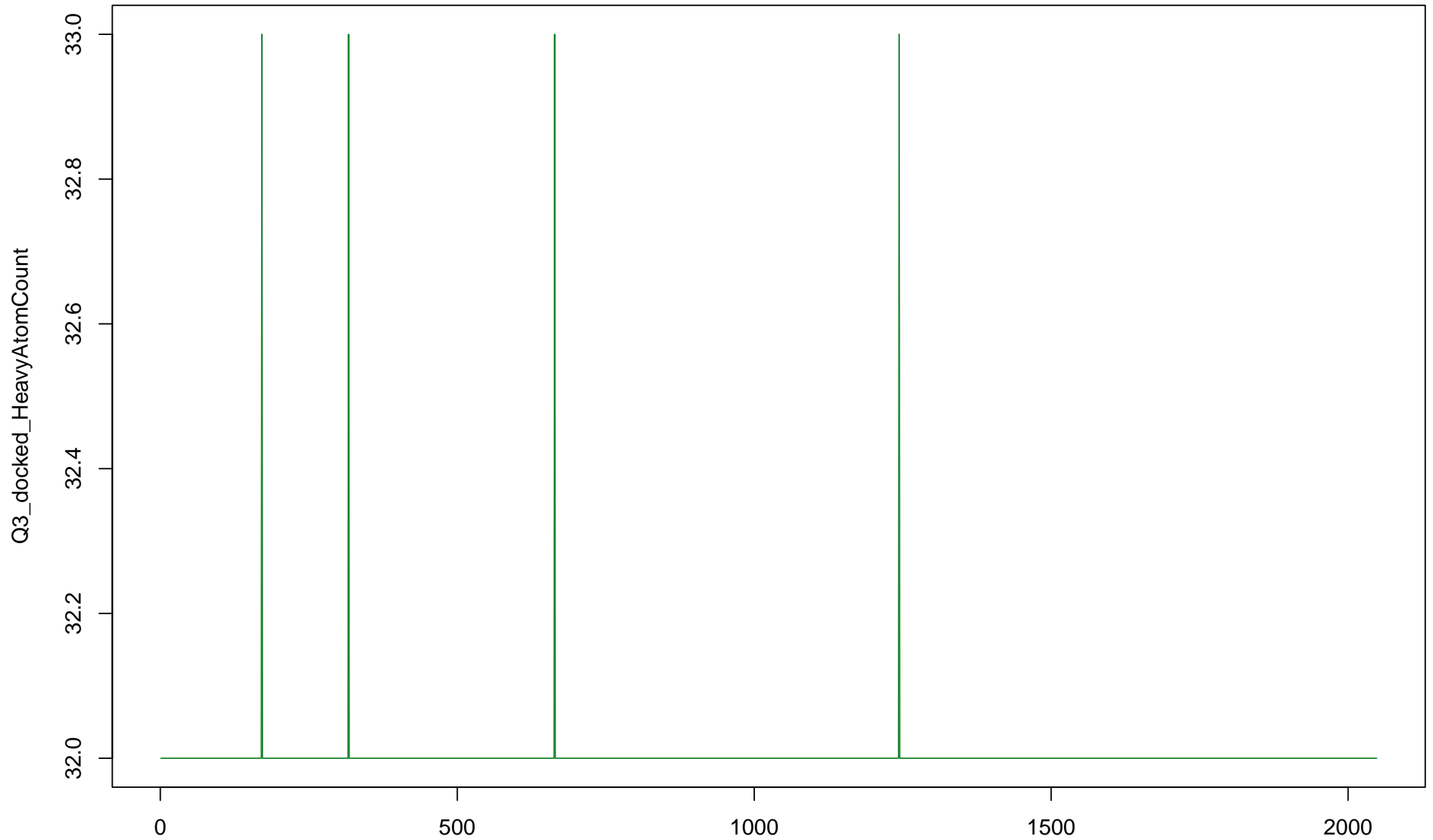
Q3_log_RMSD
ESS = 1590 | BMK = 0.0411 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 1850 | BMK = 0.0598 | MCSE(6.27) = 1.96 | stat: FALSE | burn: 0



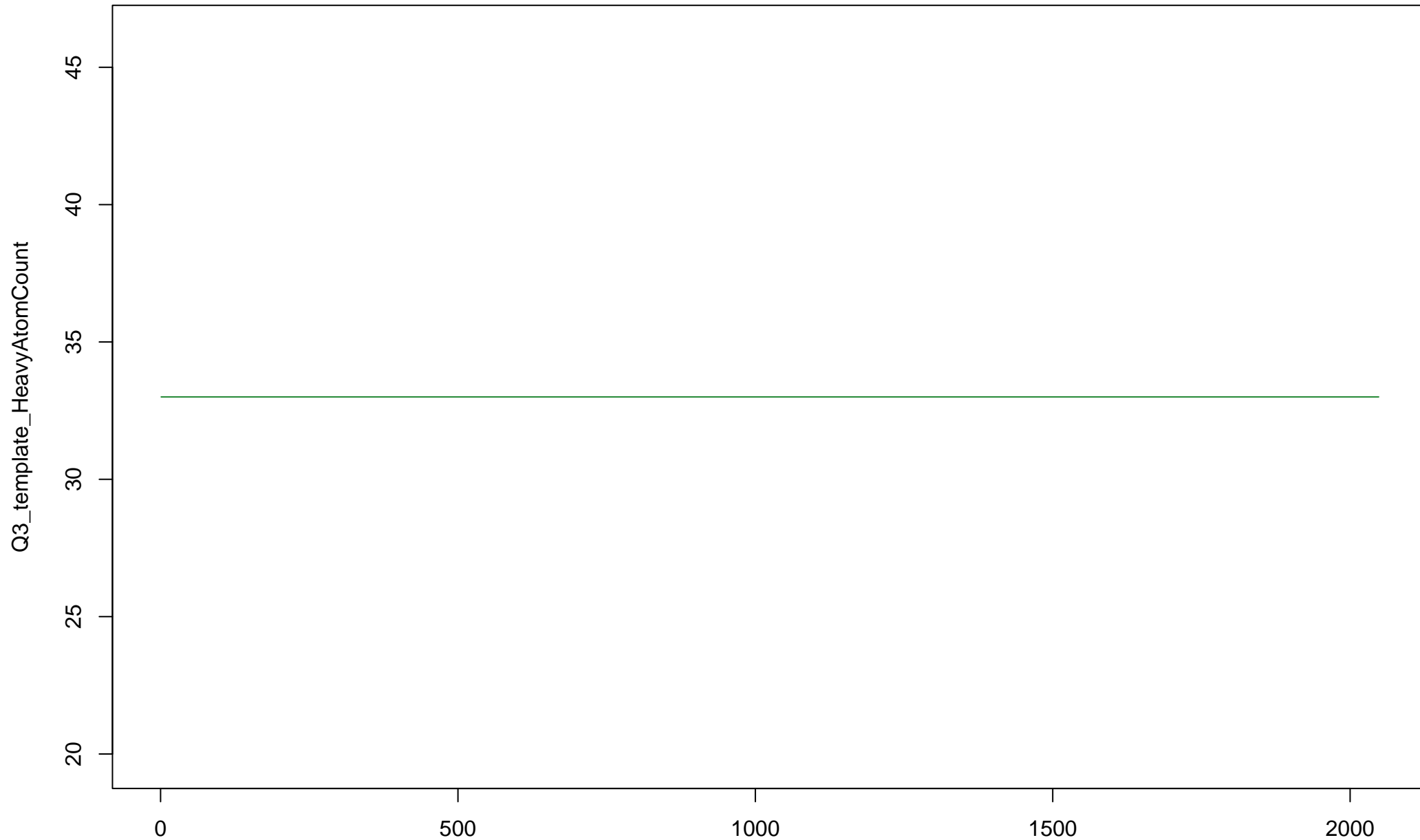
Q3_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1428



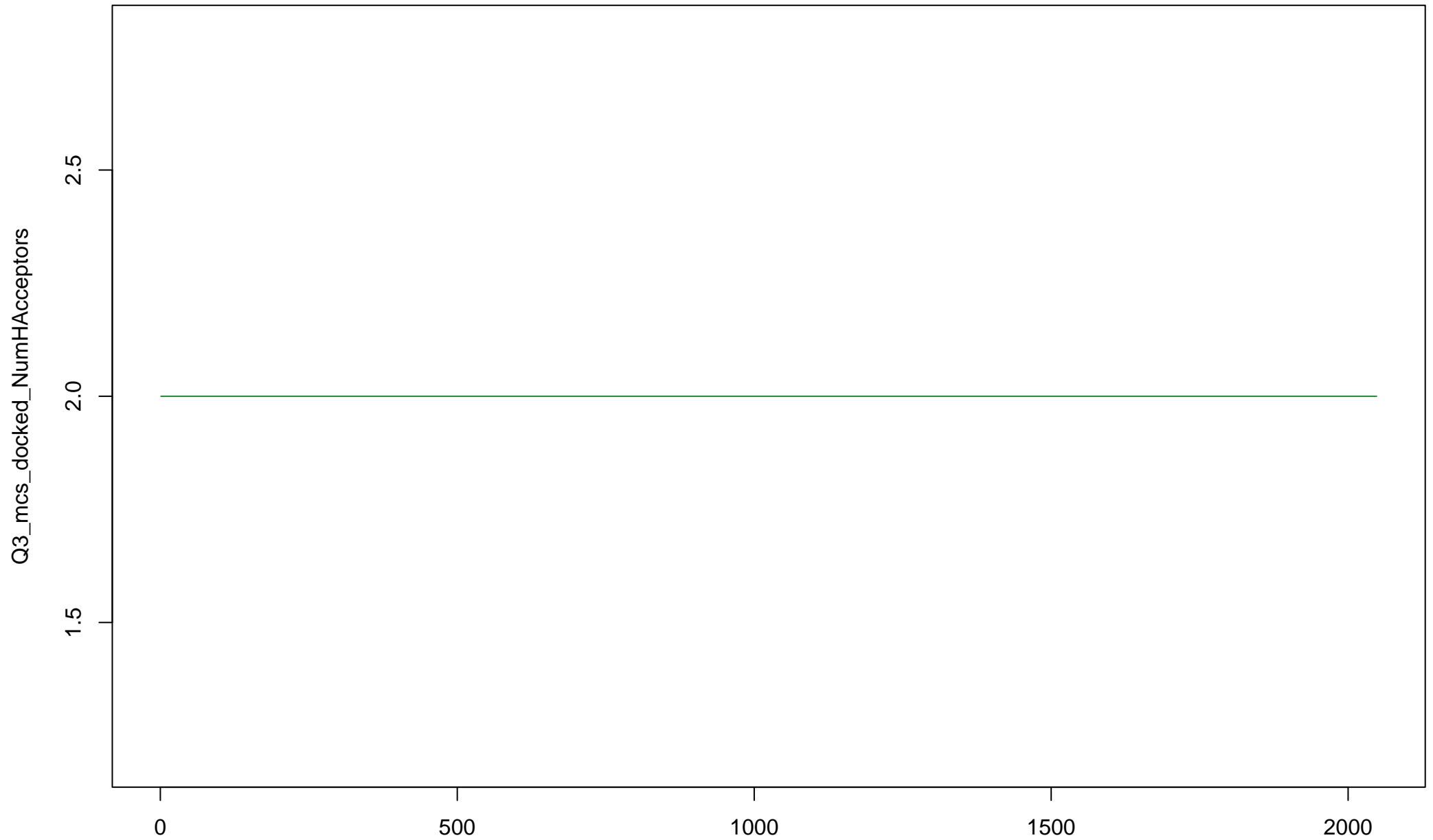
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



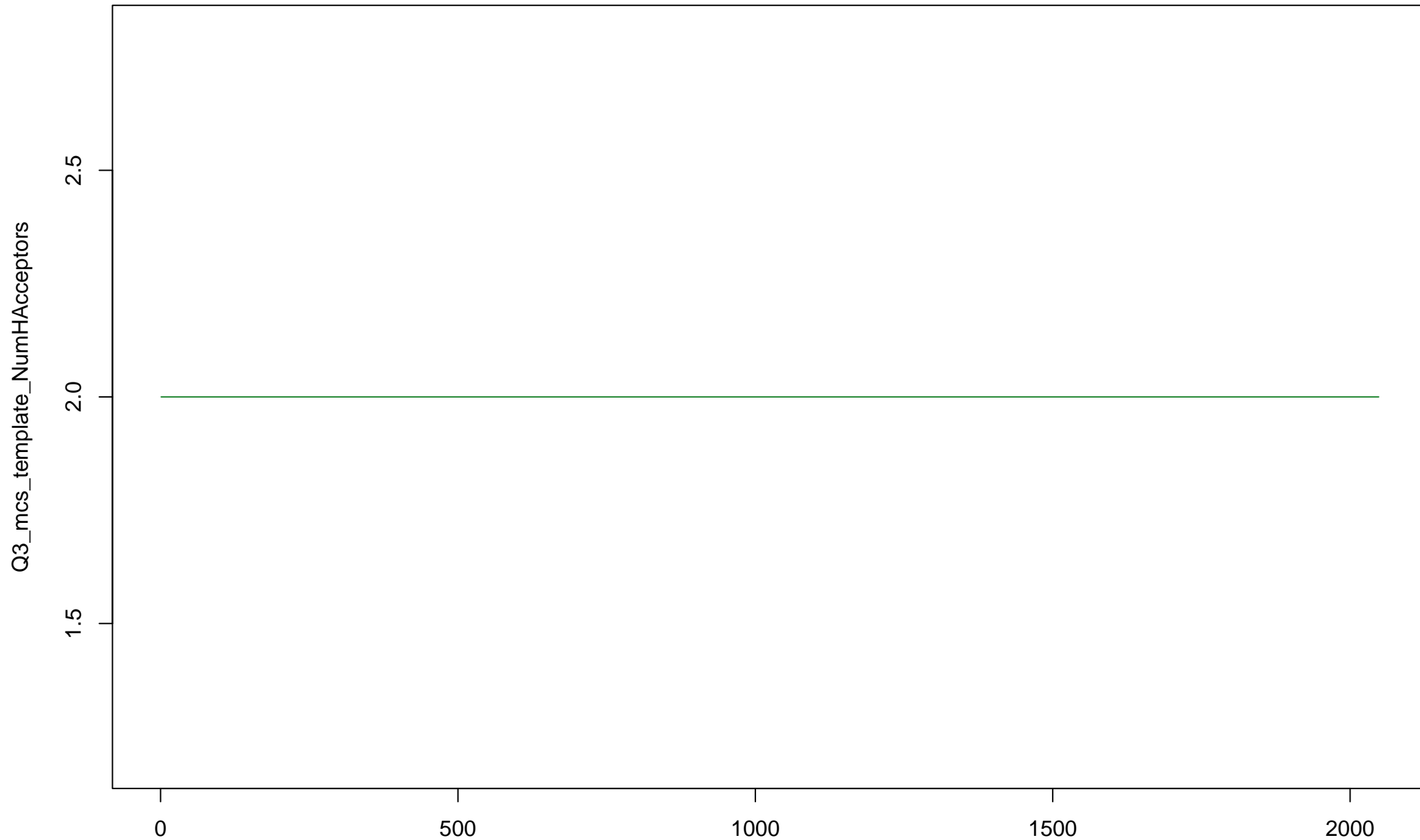
Q3_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



Q3_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



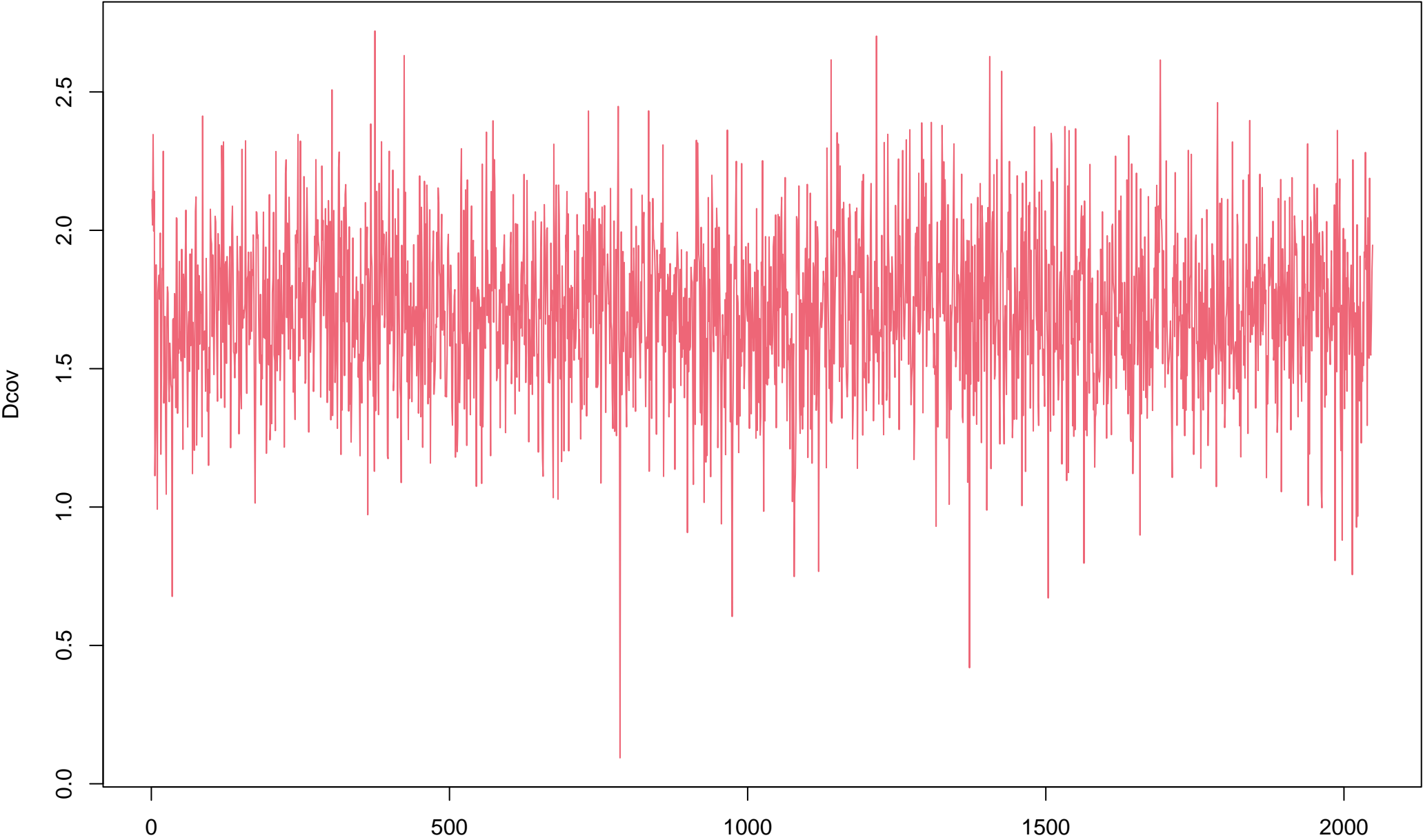
Q3_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



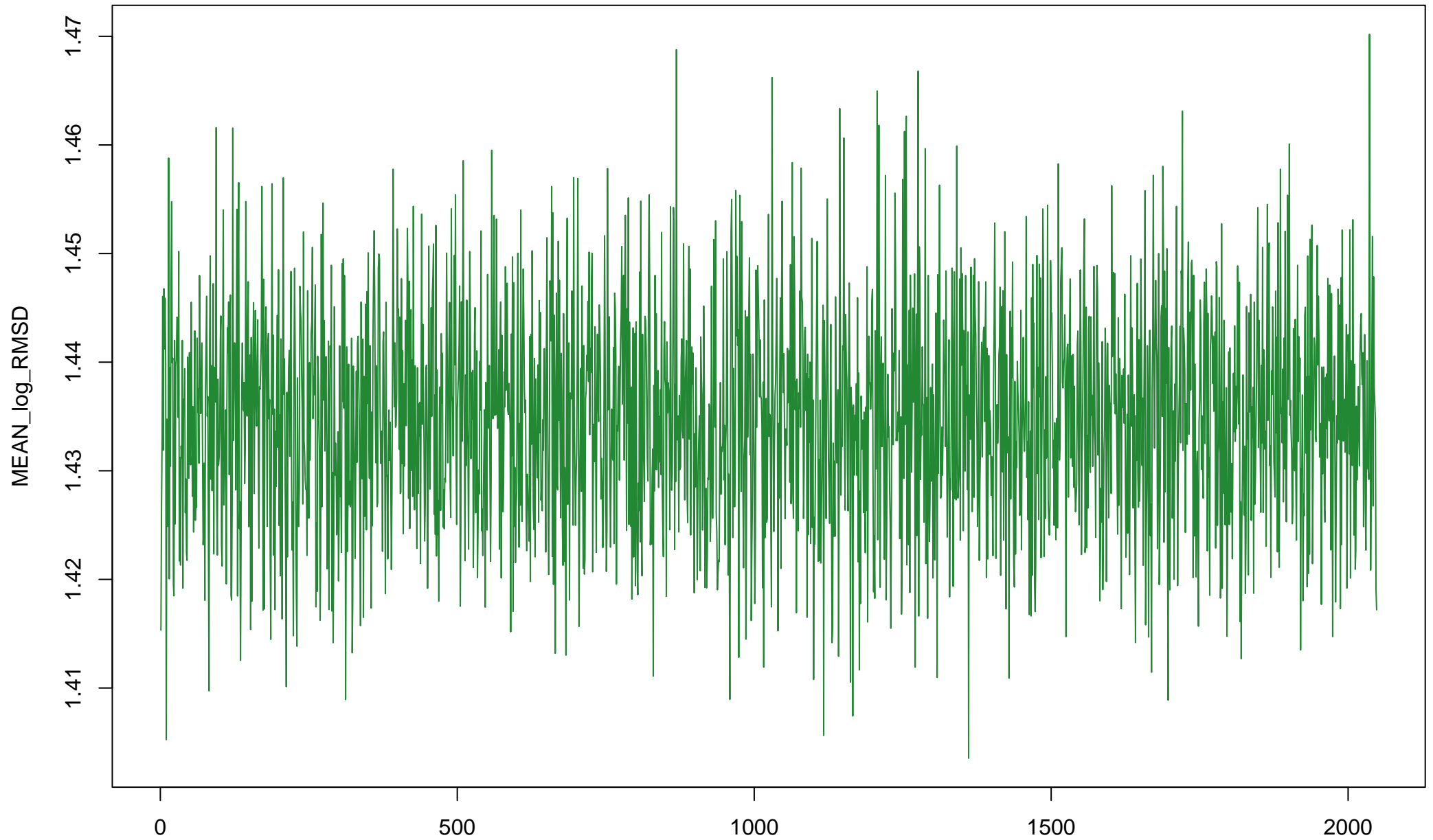
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



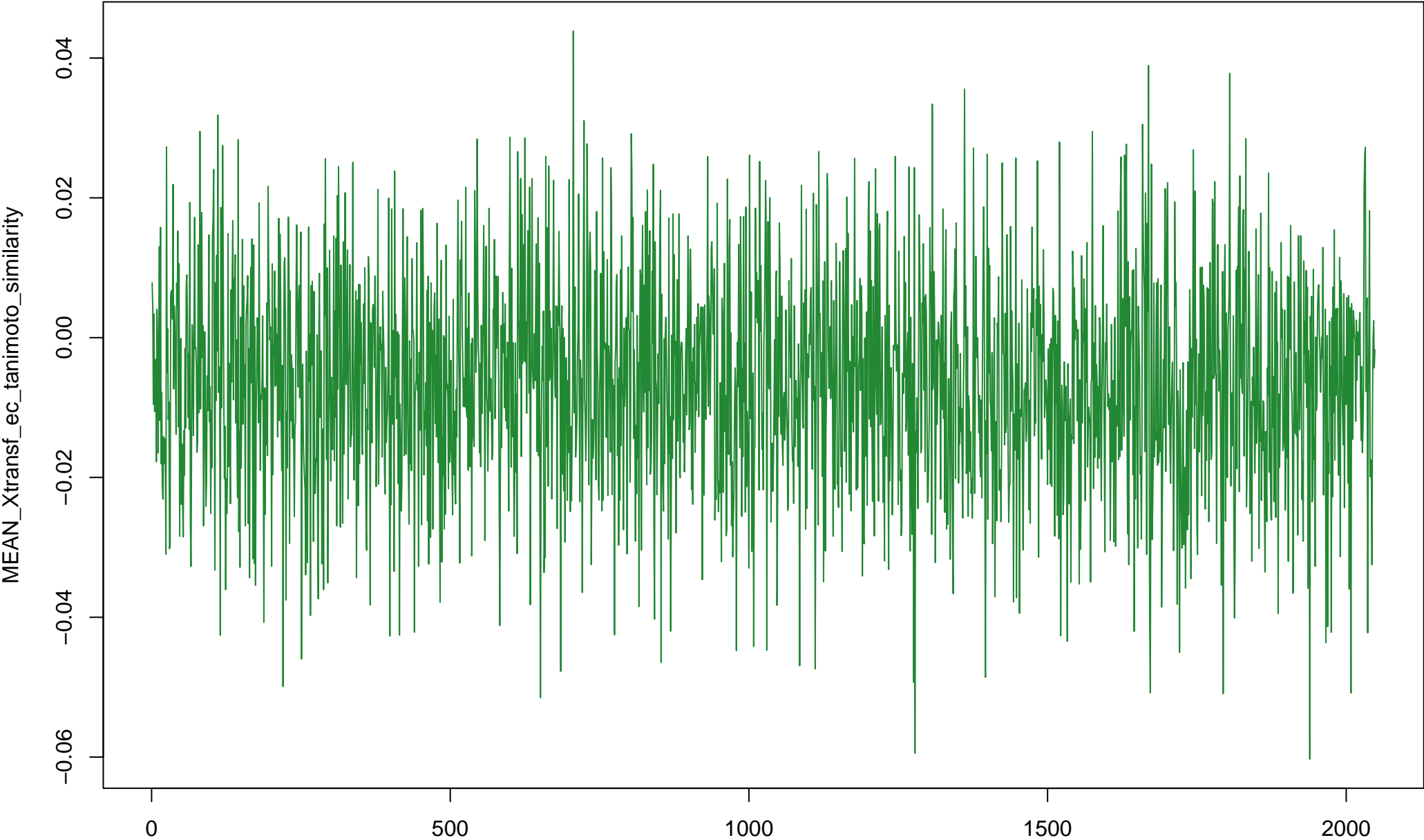
Dcov
ESS = 2050 | BMK = 0.0492 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0



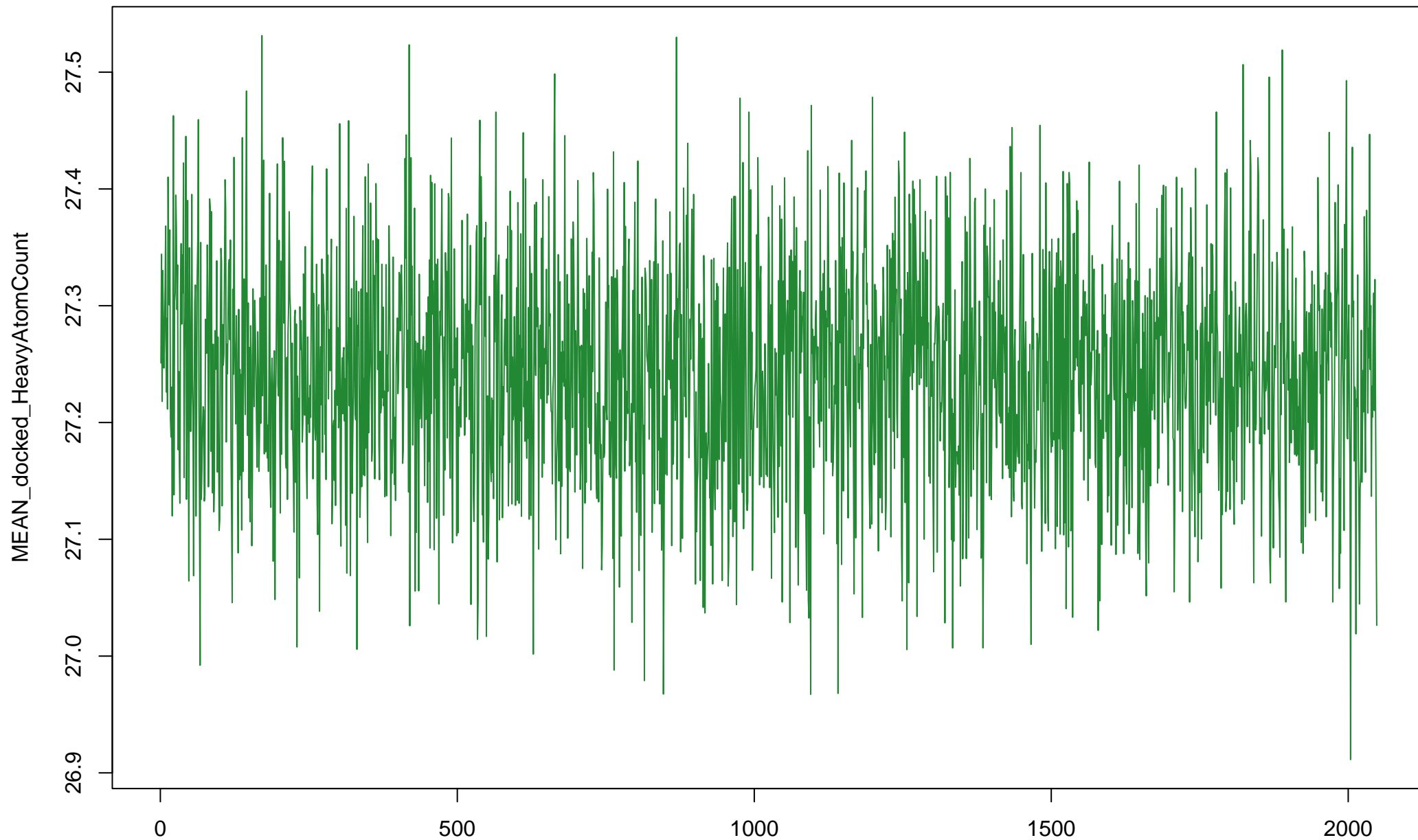
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0506 | MCSE(6.27) = 1.97 | stat: TRUE | burn: 0



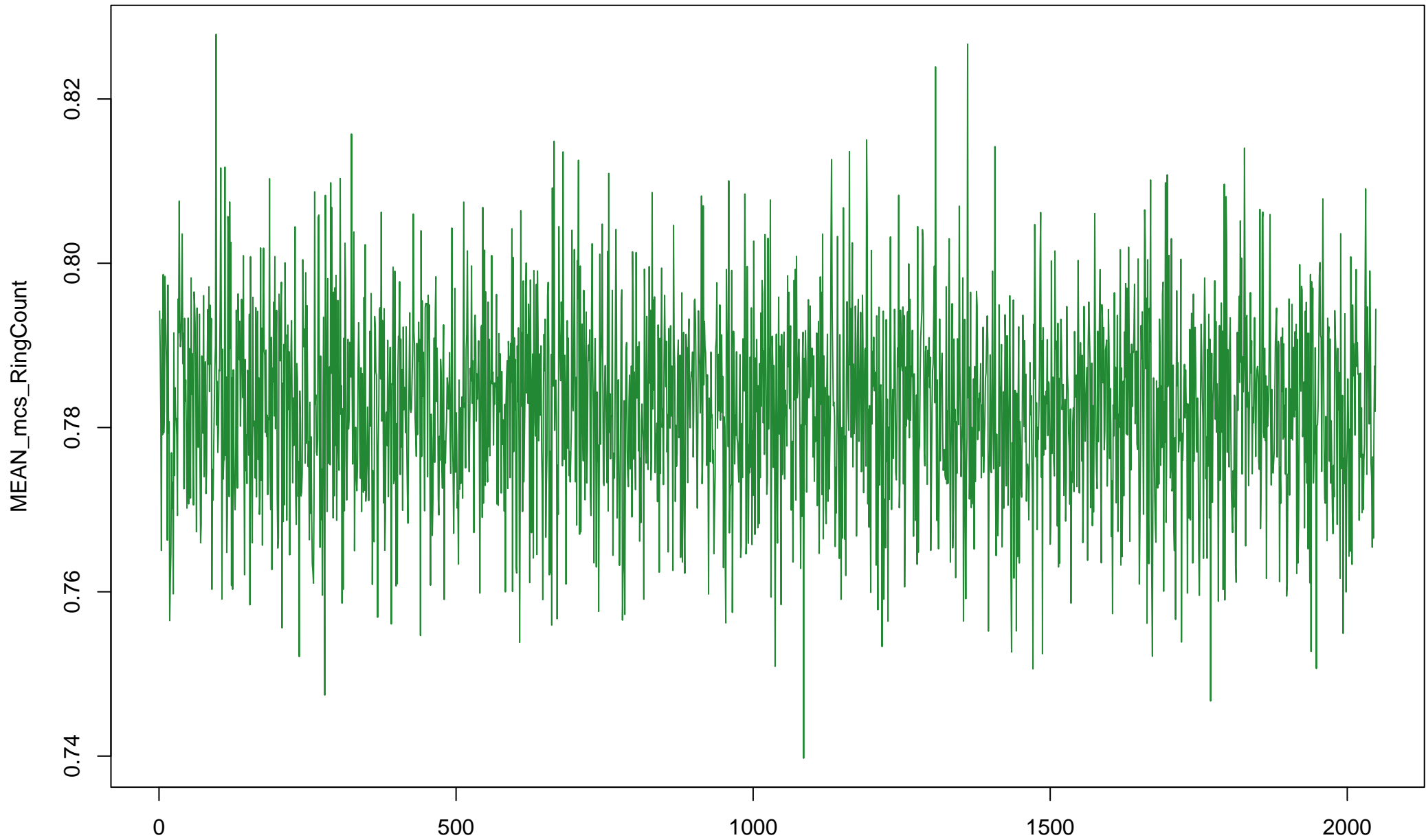
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0439 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0



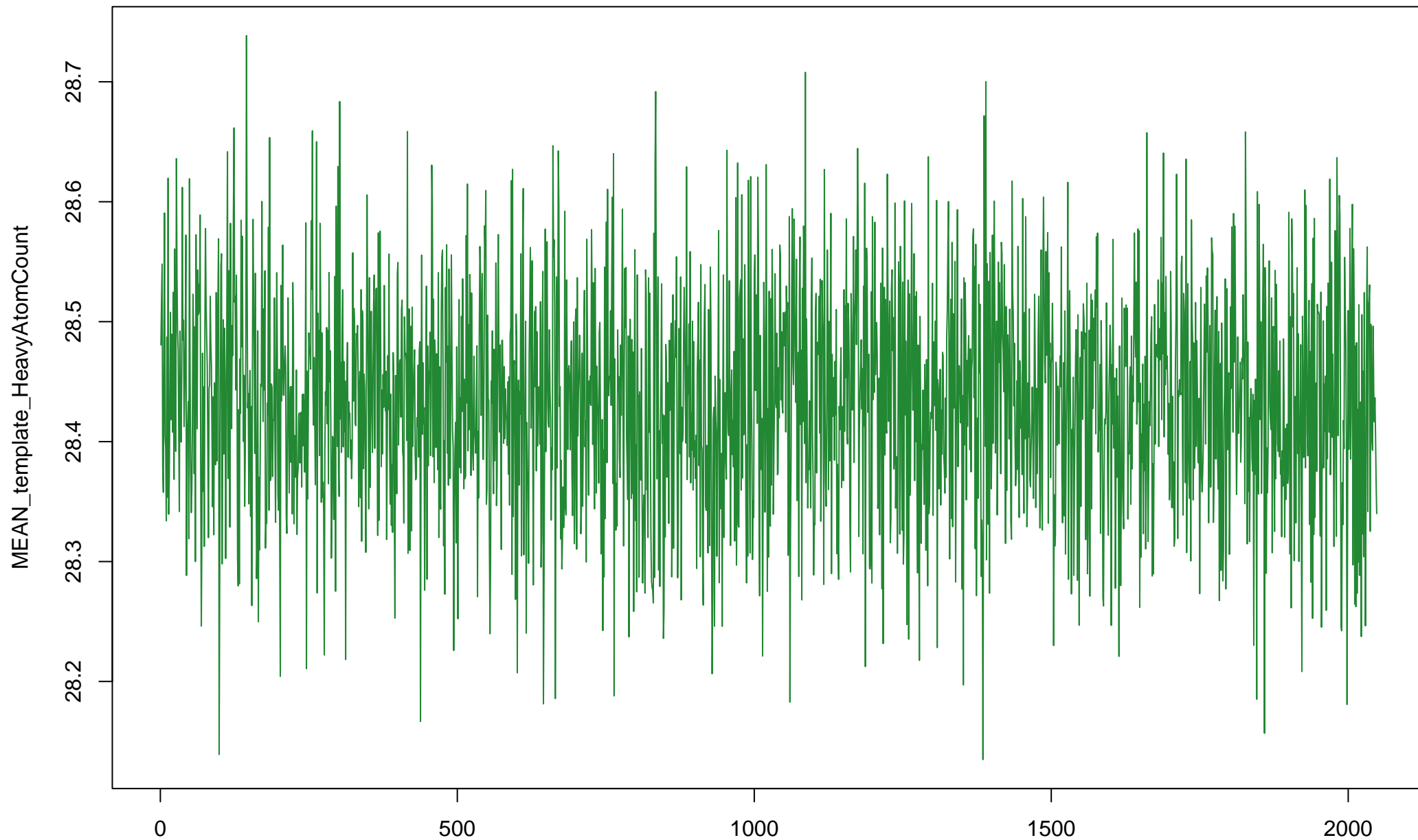
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0358 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



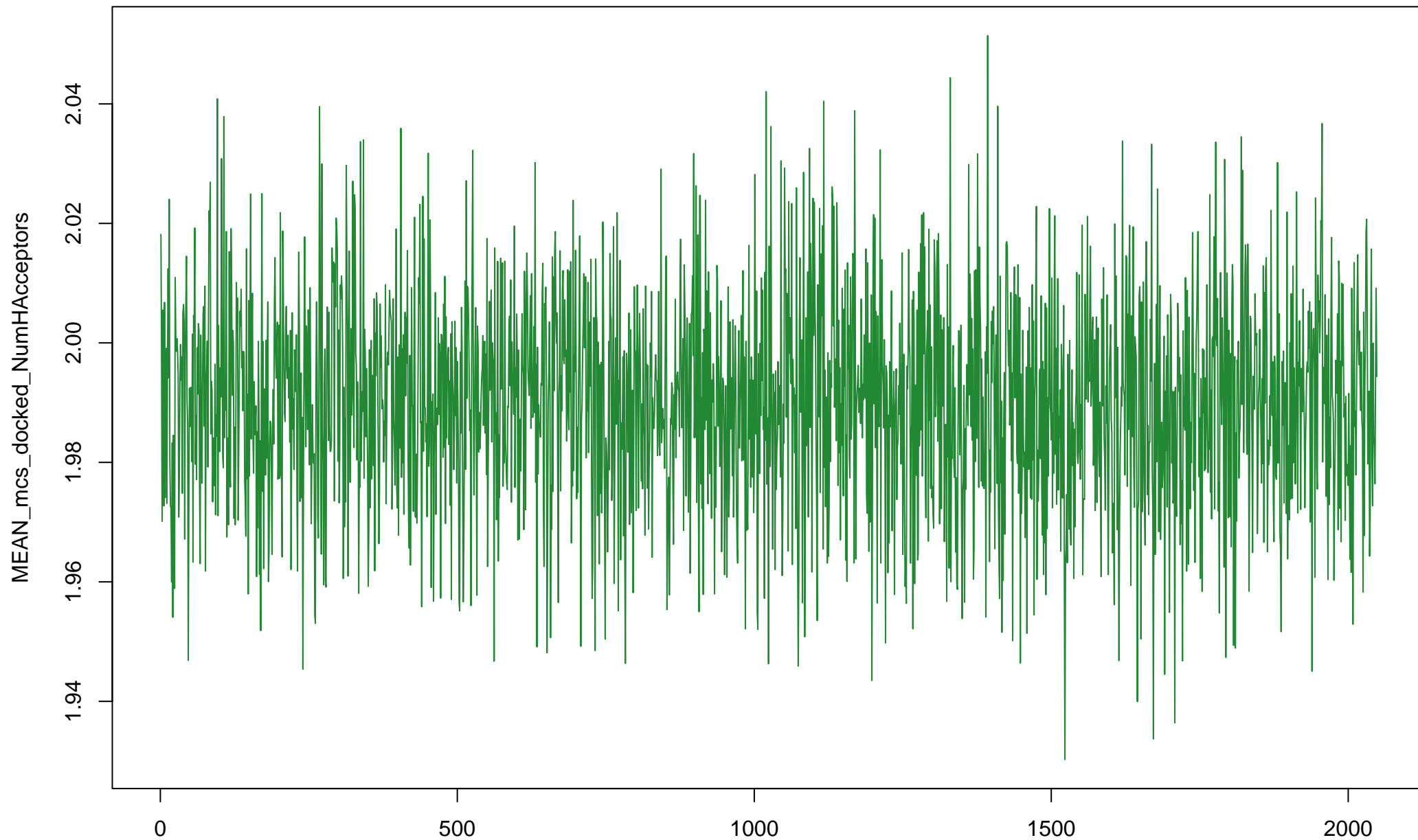
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0391 | MCSE(6.27) = 1.77 | stat: TRUE | burn: 0



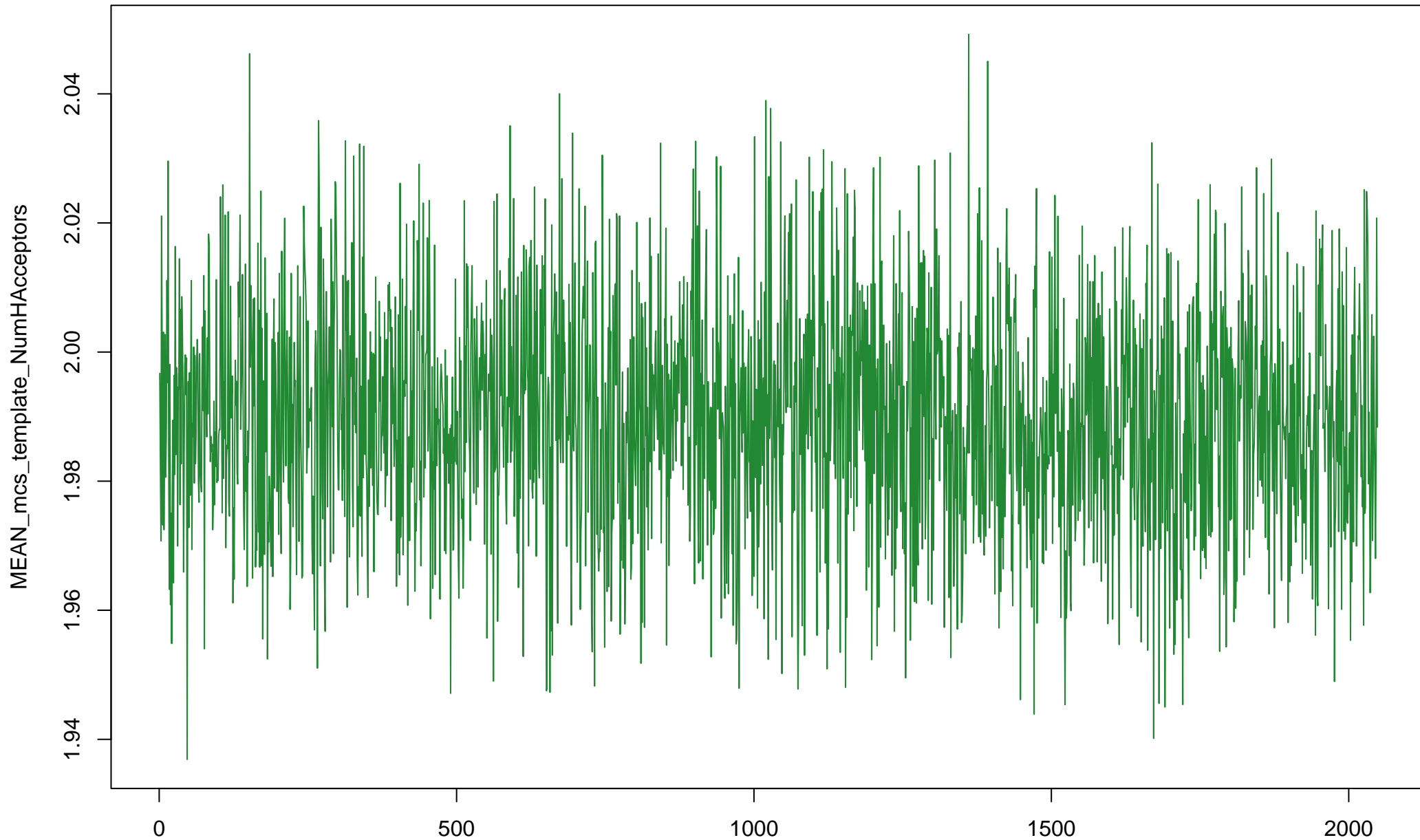
MEAN_template_HeavyAtomCount
ESS = 2020 | BMK = 0.0412 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0



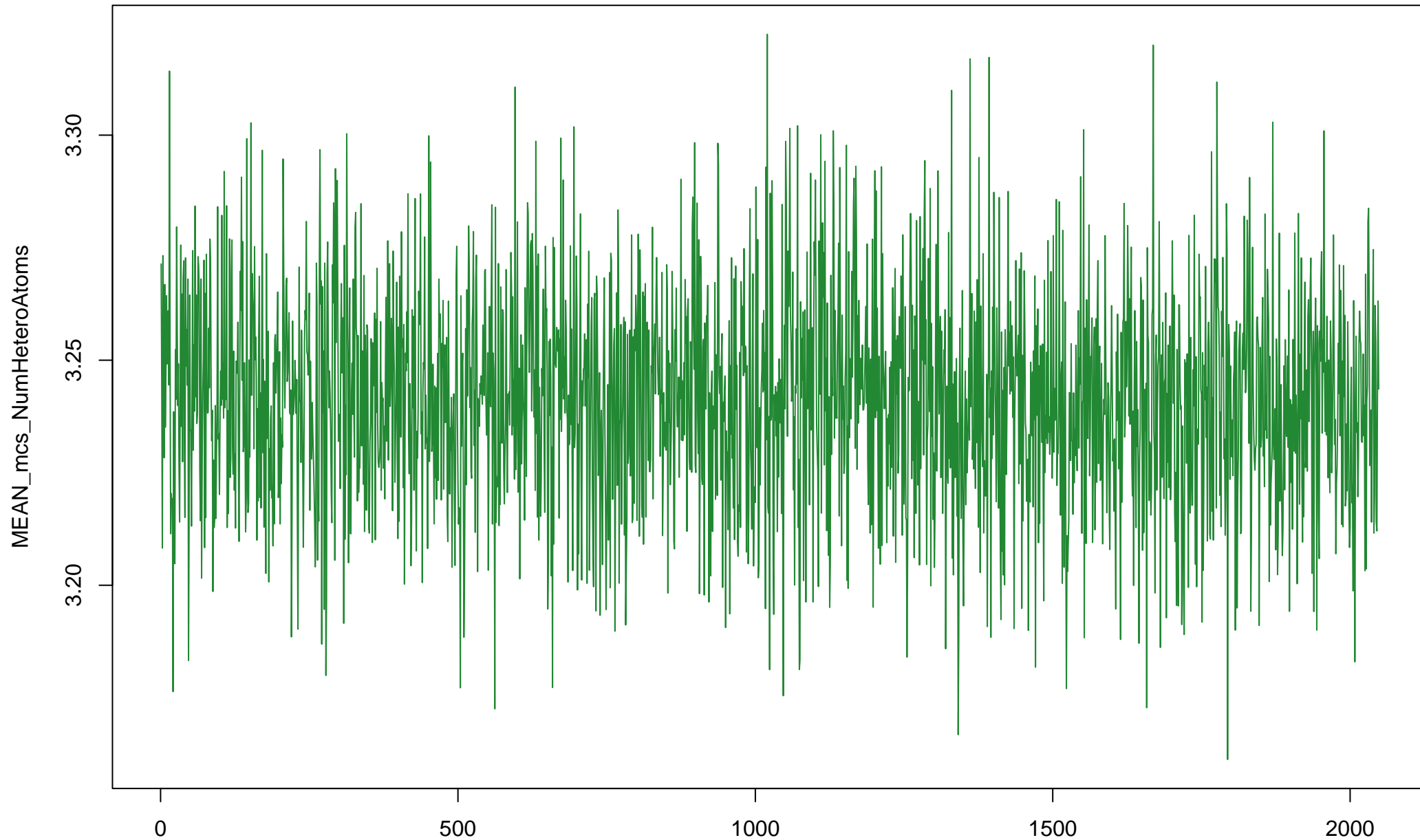
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0525 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0



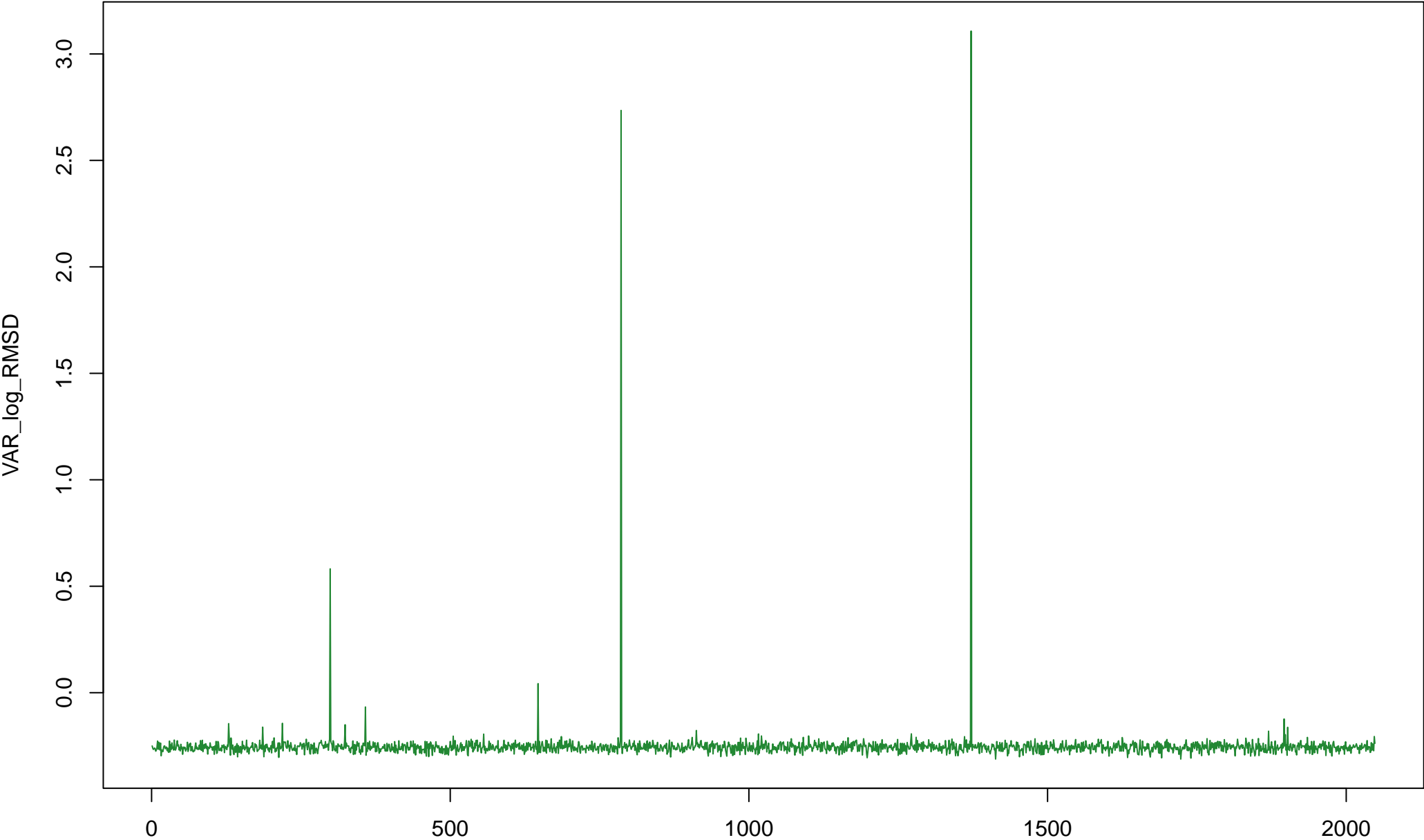
MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0387 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



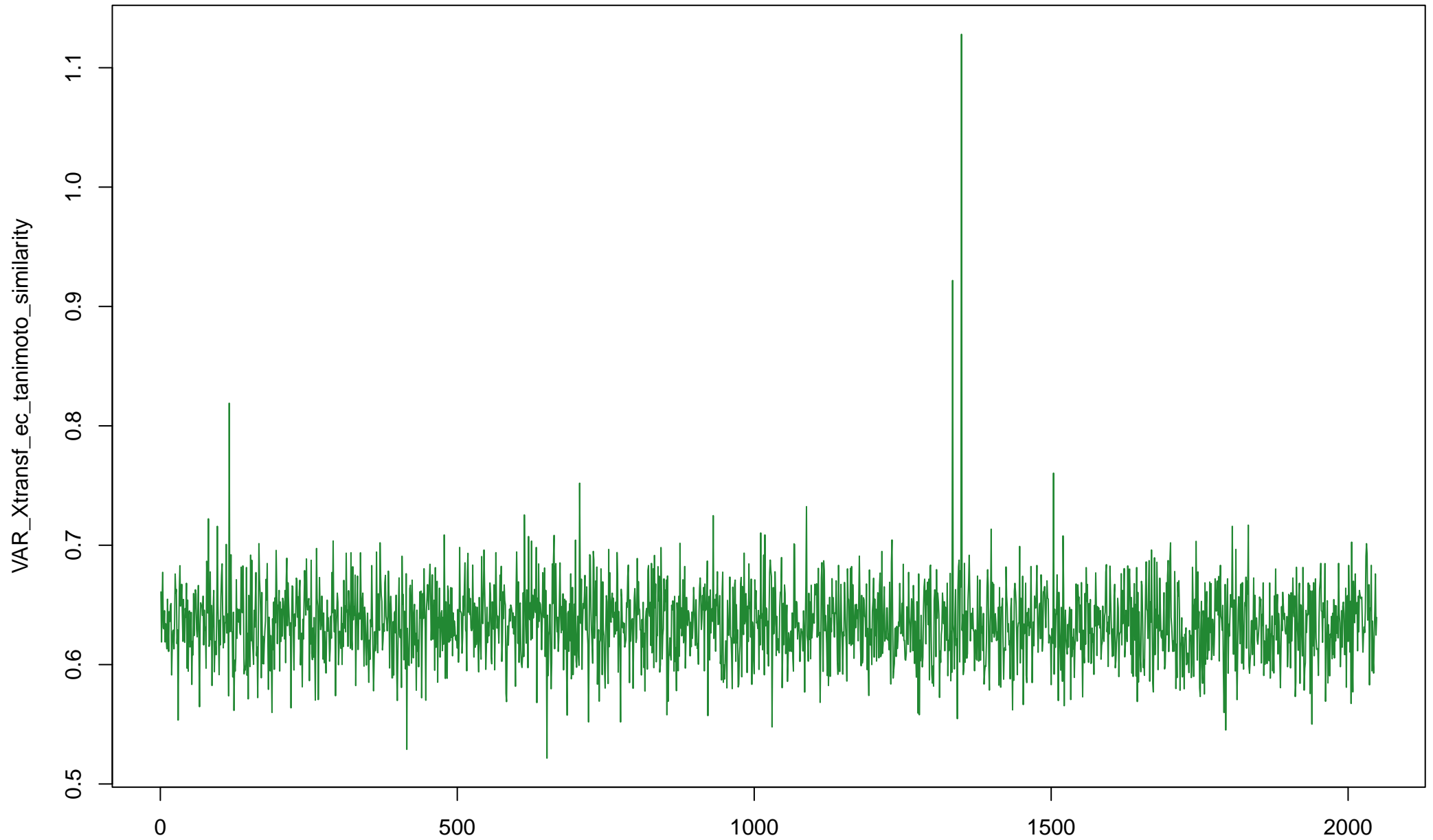
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0496 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0



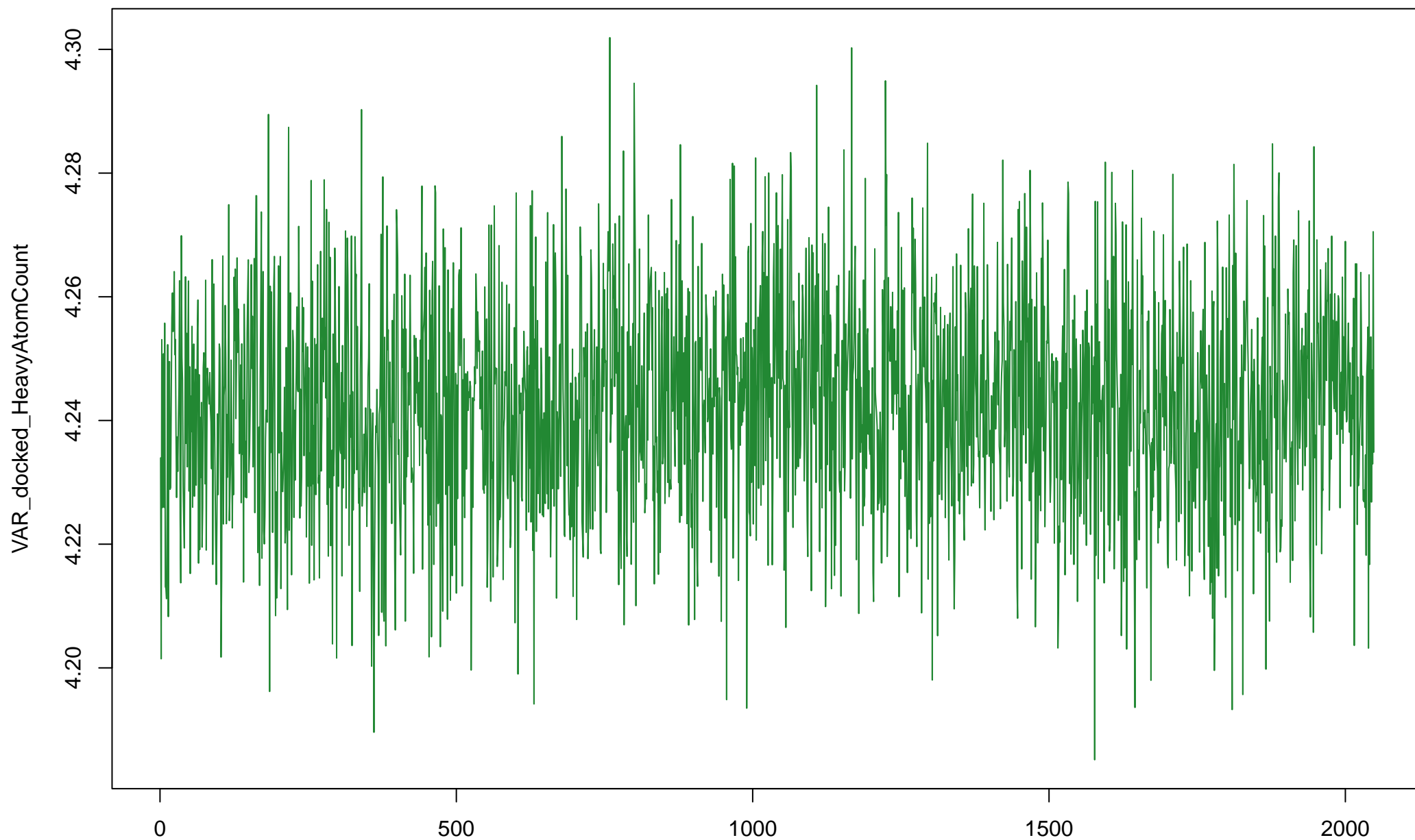
VAR_log_RMSD
ESS = 2050 | BMK = 0.0904 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



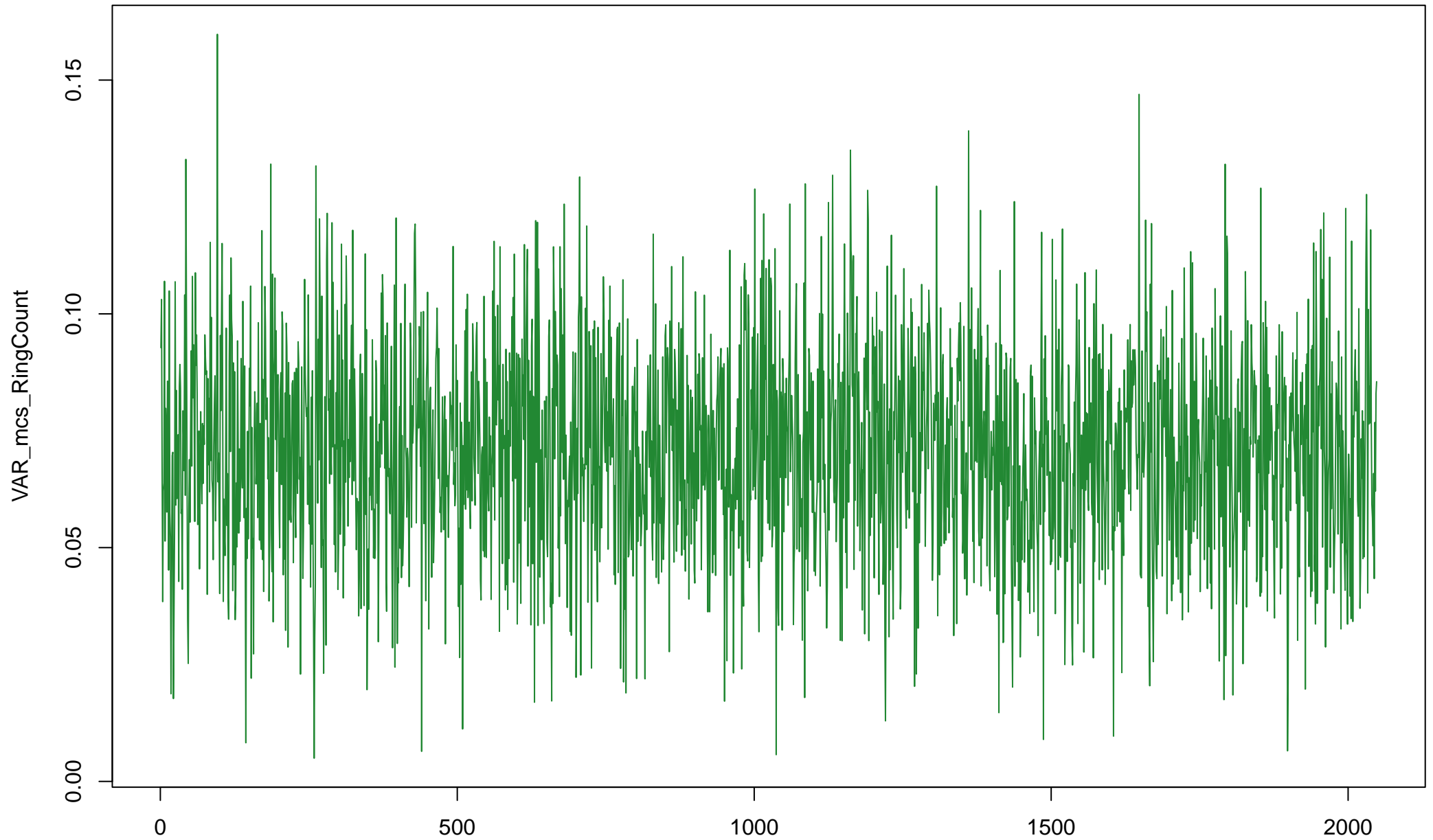
VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0684 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0



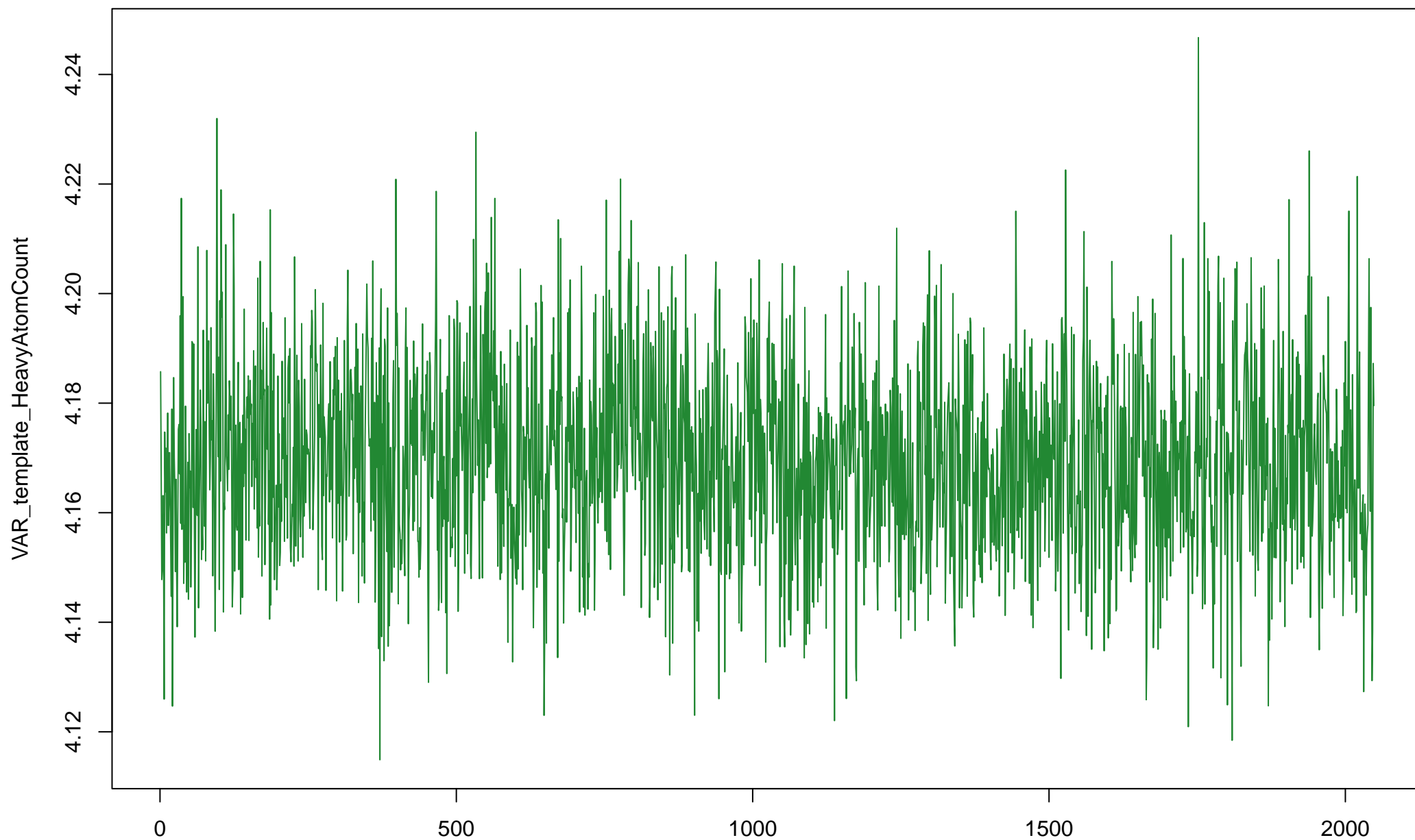
VAR_docked_HeavyAtomCount
ESS = 2020 | BMK = 0.0357 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0



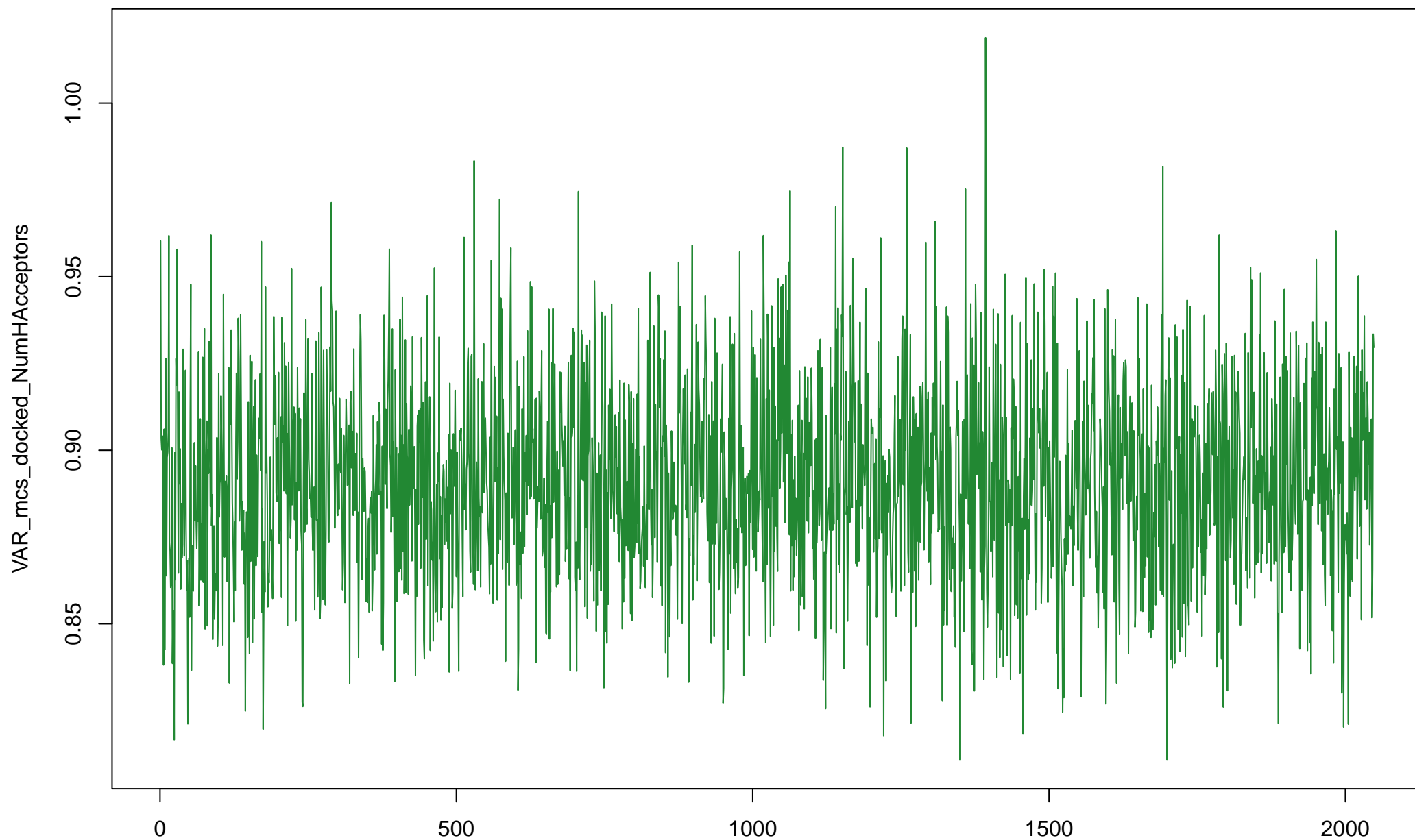
VAR_mcs_RingCount
ESS = 2050 | BMK = 0.0505 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



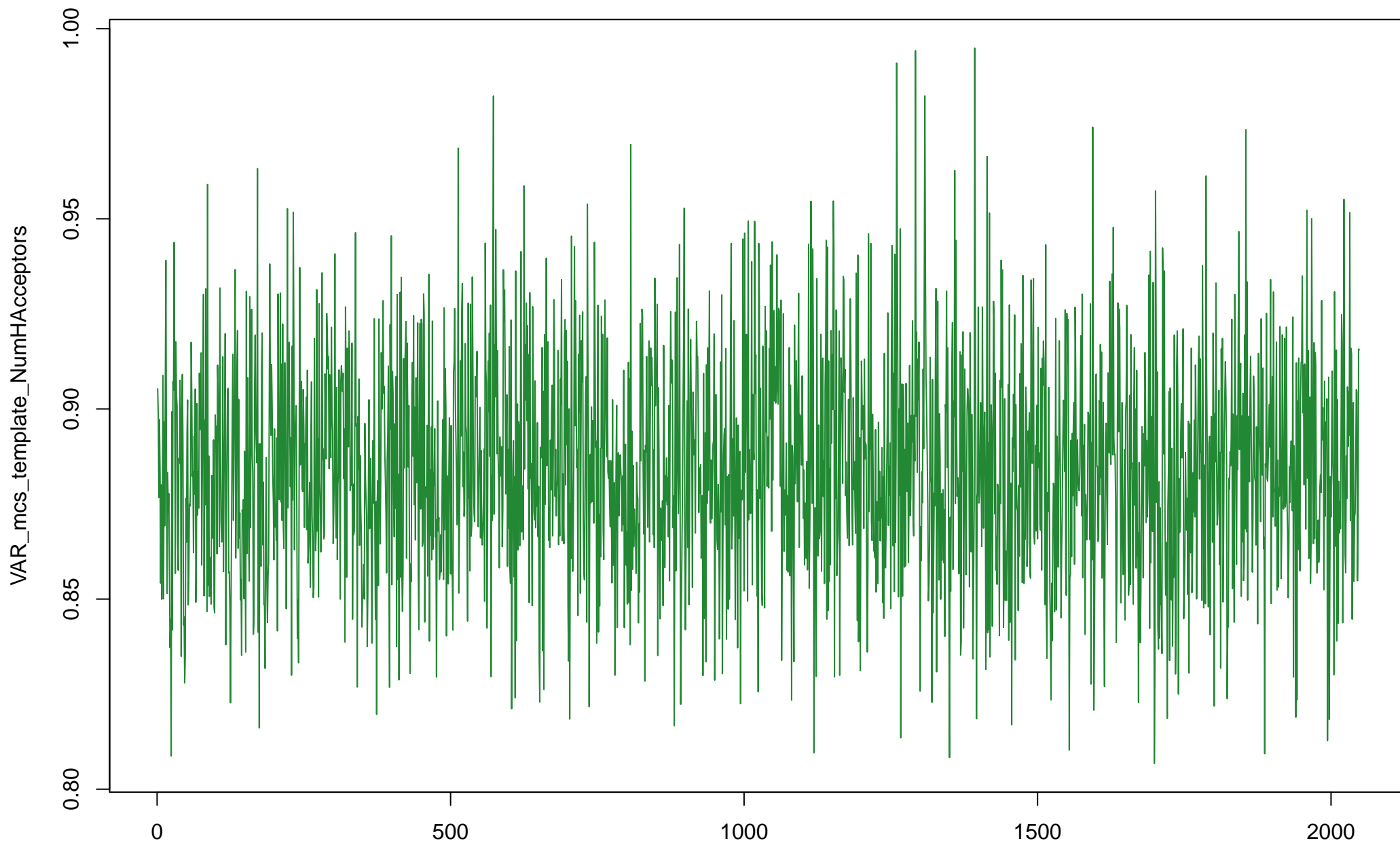
VAR_template_HeavyAtomCount
ESS = 1810 | BMK = 0.0615 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



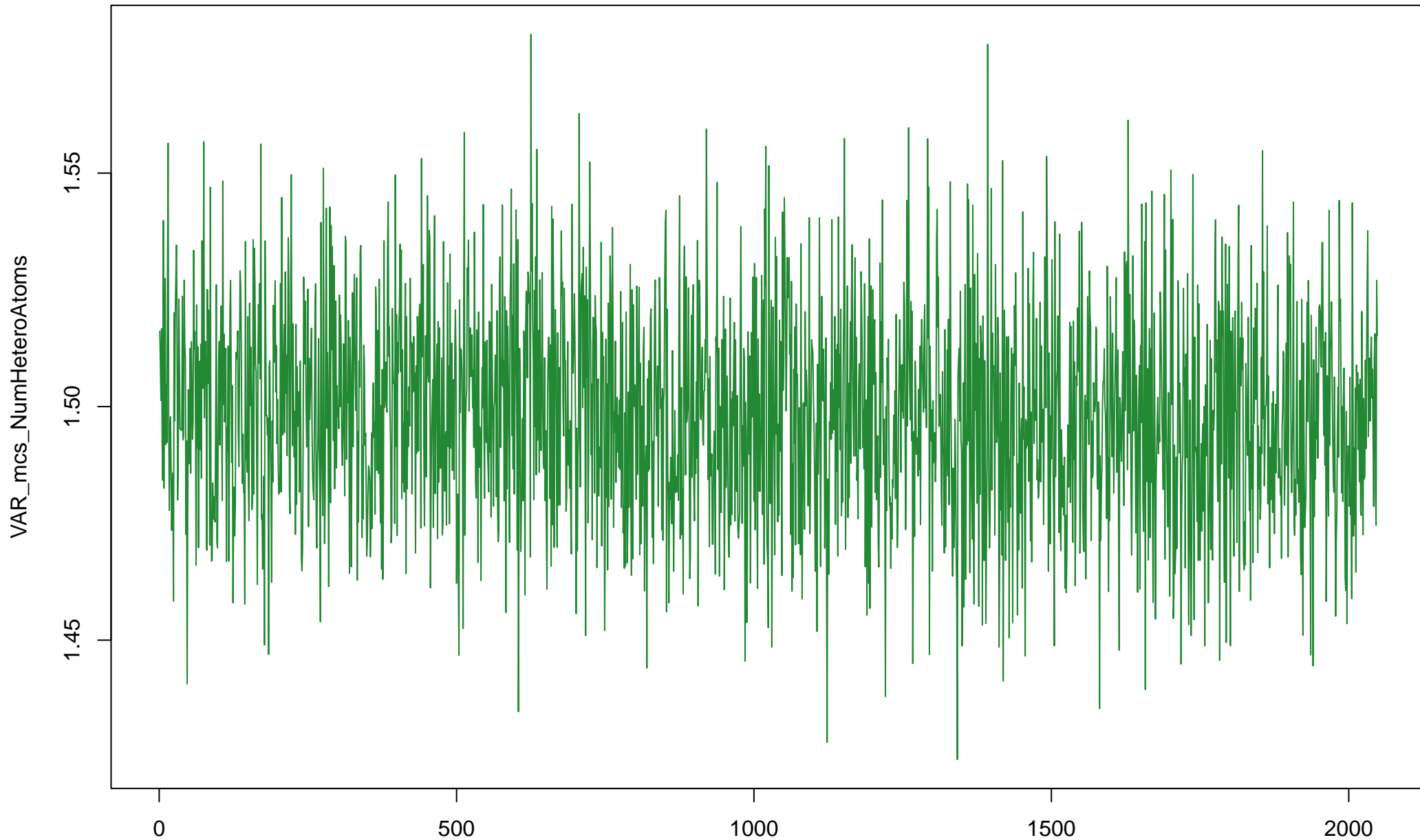
VAR_mcs_docked_NumHAcceptors
ESS = 1700 | BMK = 0.0496 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



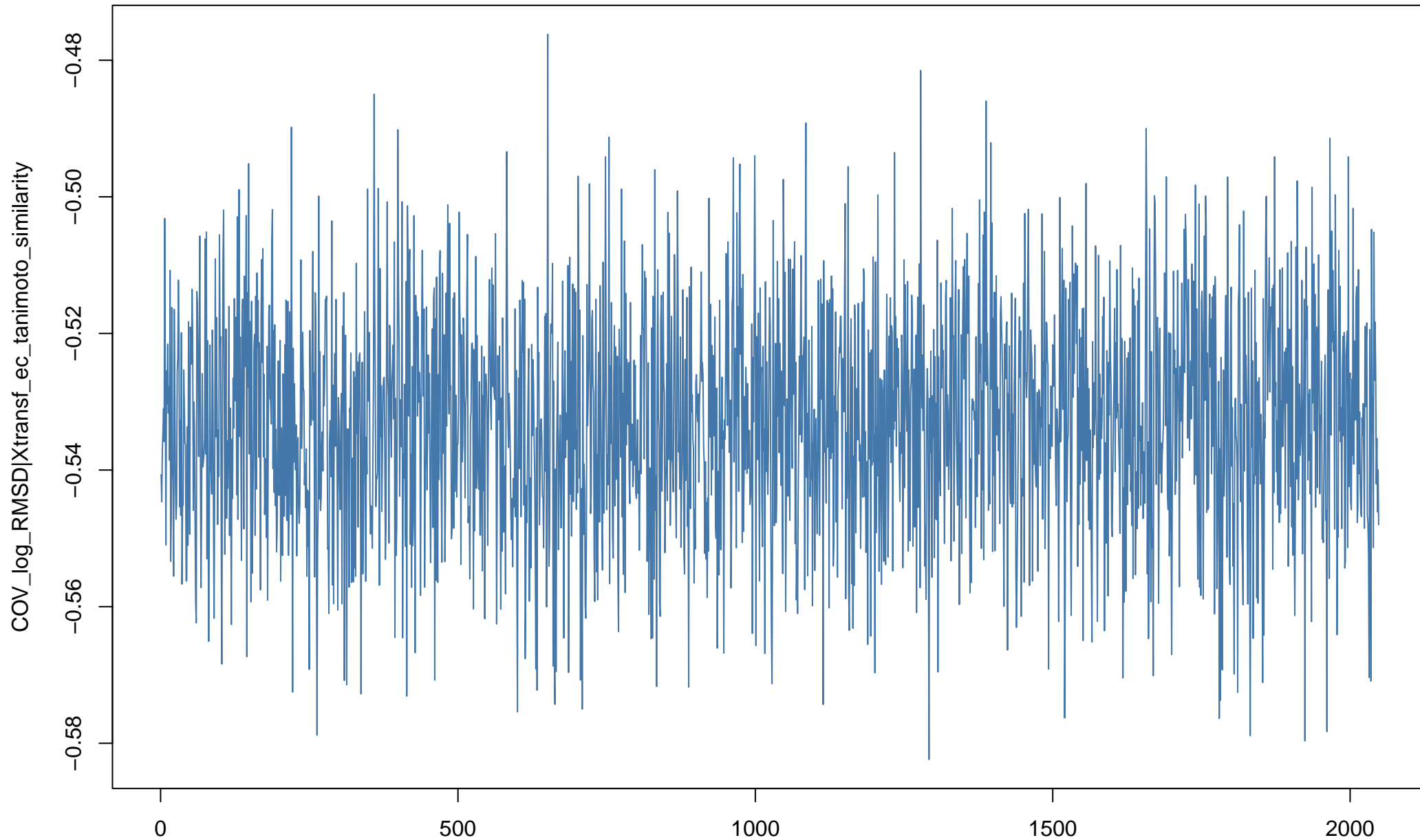
VAR_mcs_template_NumHAcceptors
ESS = 1820 | BMK = 0.0342 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



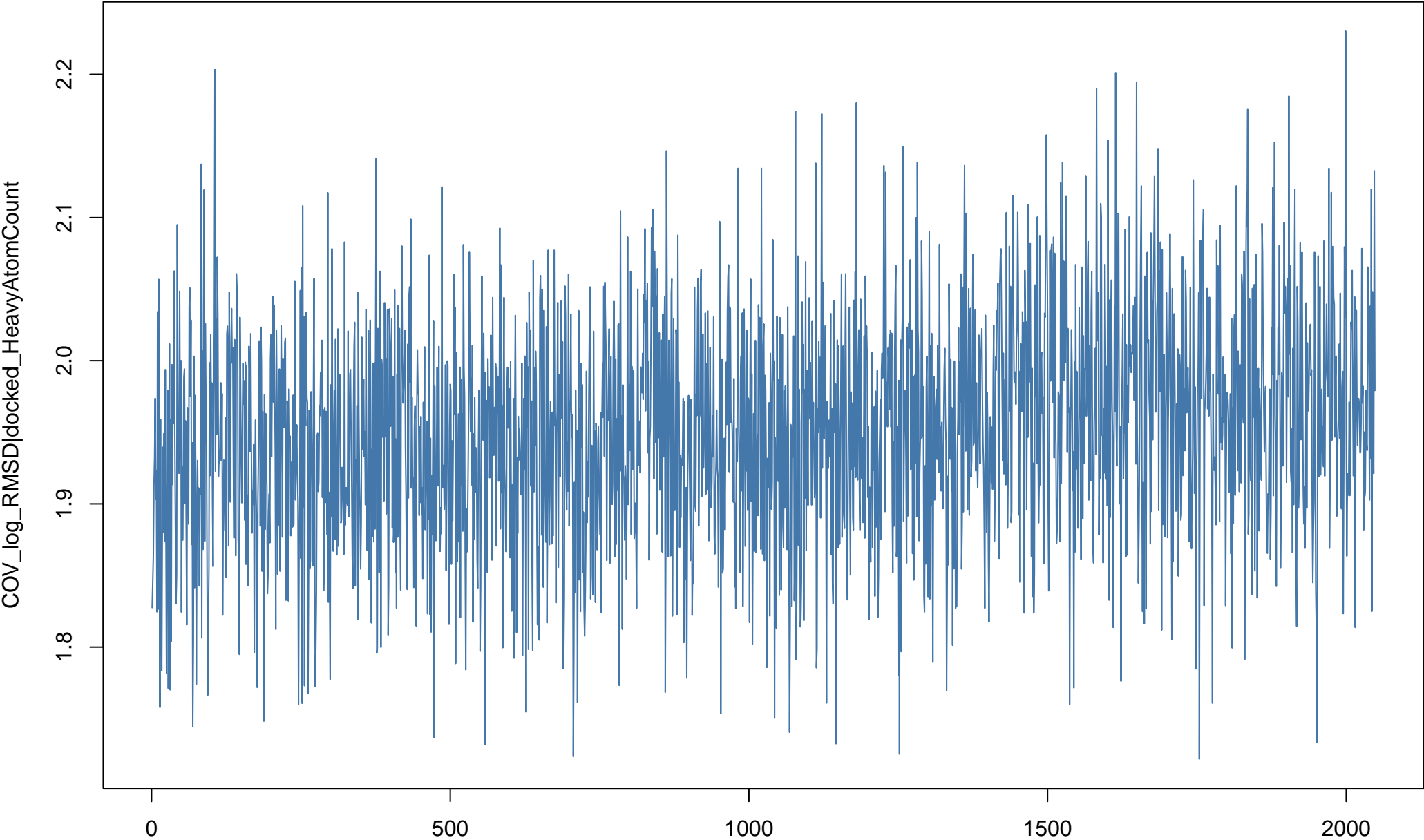
VAR_mcs_NumHeteroAtoms
ESS = 1540 | BMK = 0.0674 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0



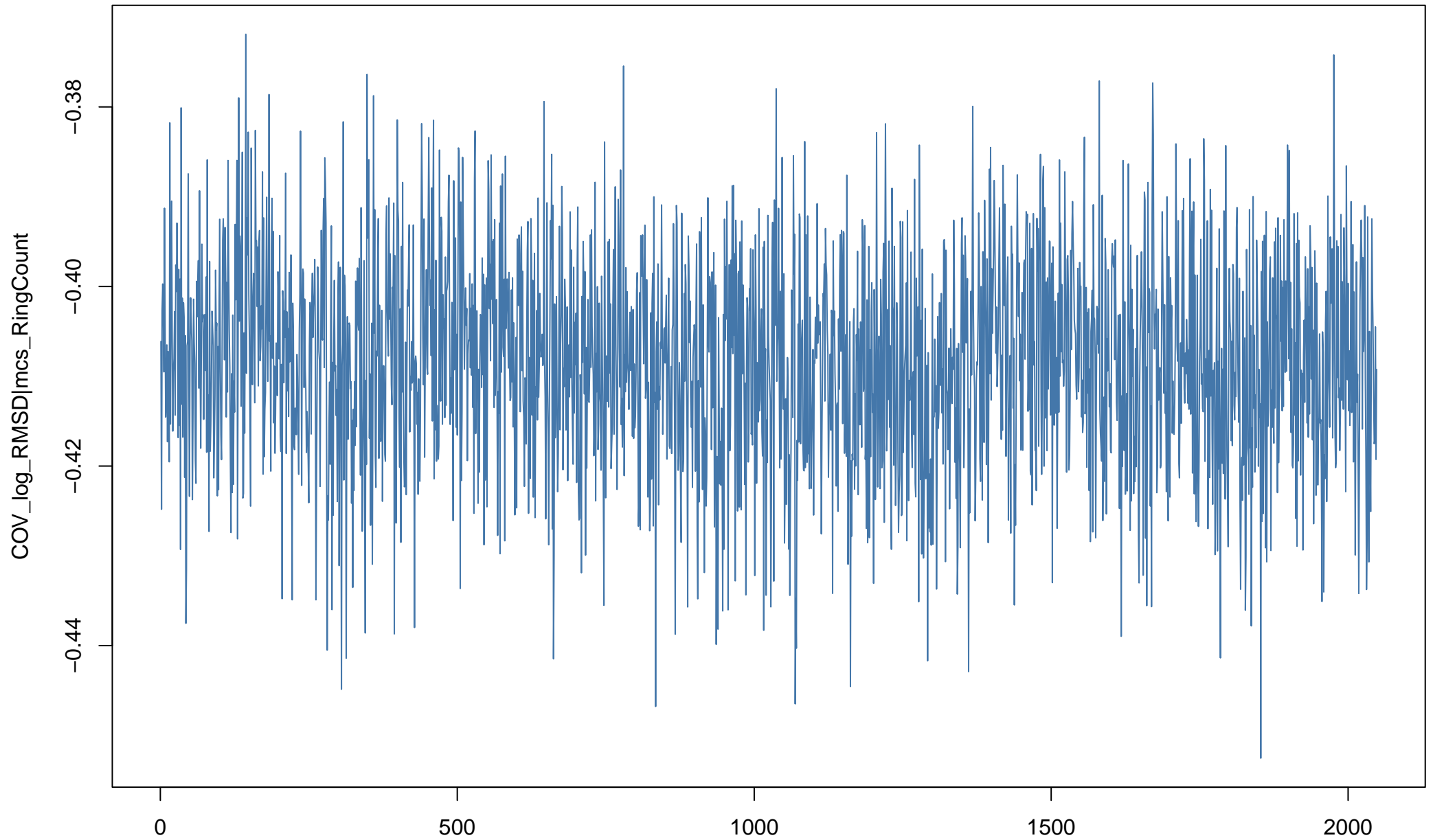
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0426 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0



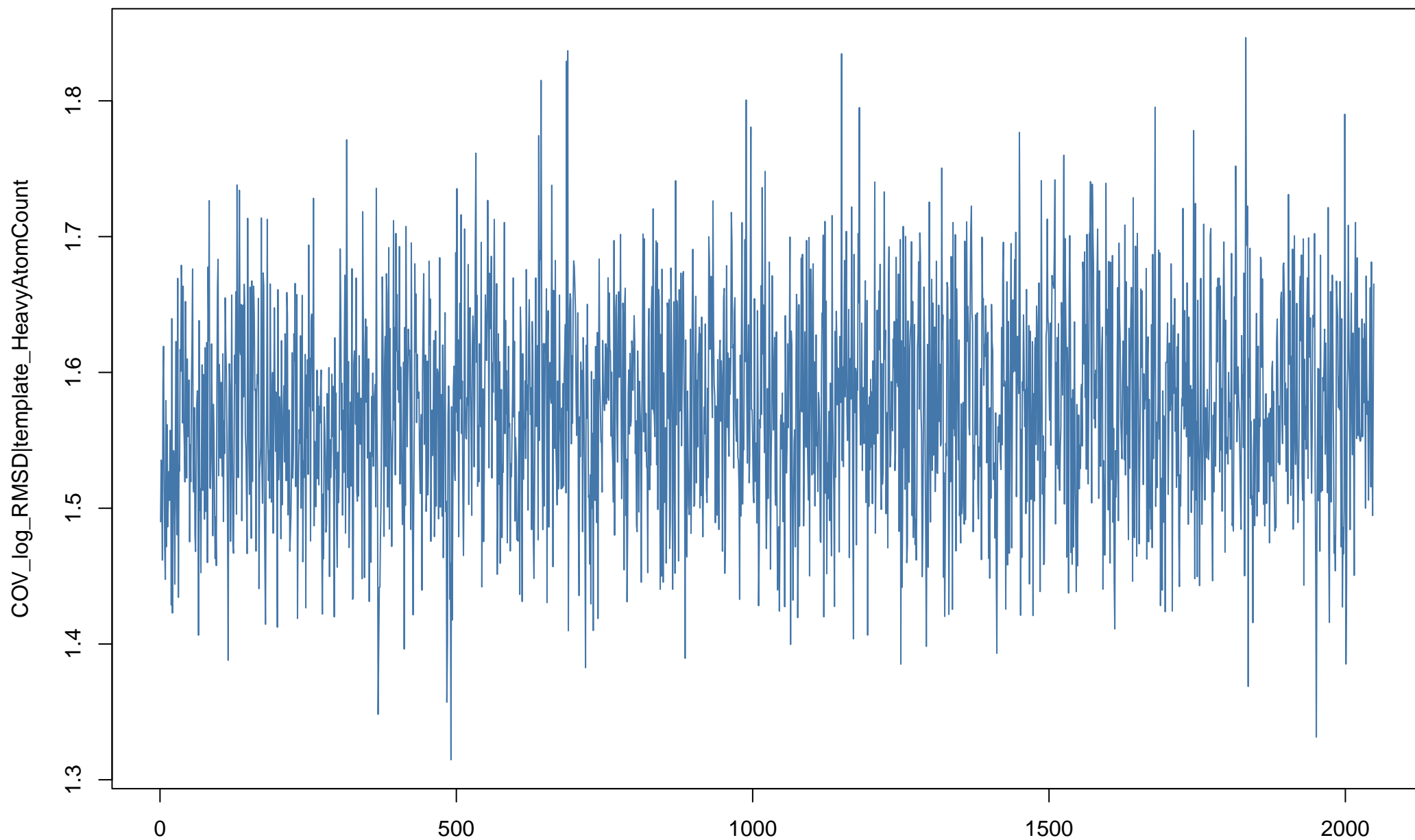
COV_log_RMSD|docked_HeavyAtomCount
ESS = 520 | BMK = 0.126 | MCSE(6.27) = 3.87 | stat: FALSE | burn: 0



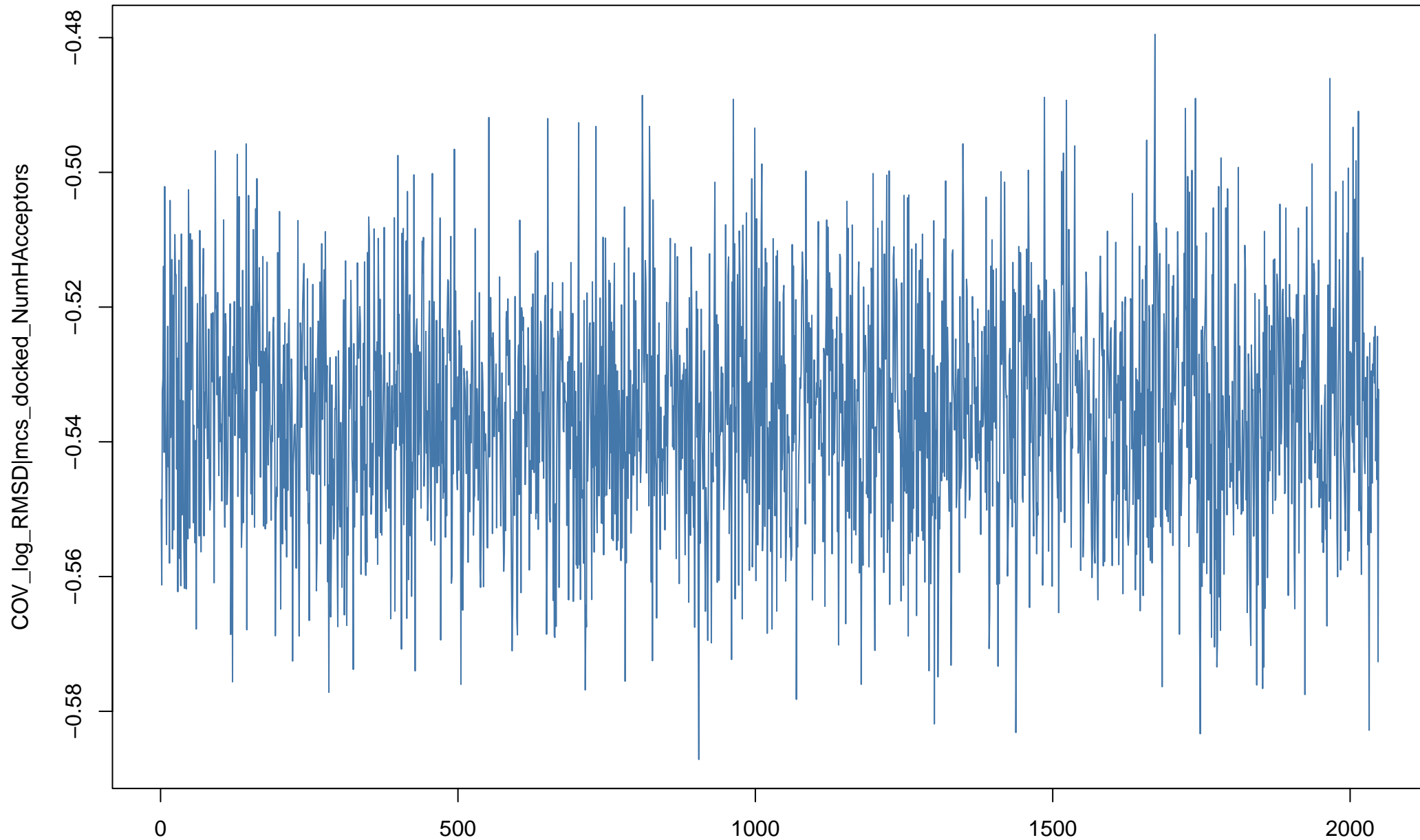
COV_log_RMSD|mcs_RingCount
ESS = 1860 | BMK = 0.0577 | MCSE(6.27) = 2.92 | stat: FALSE | burn: 0



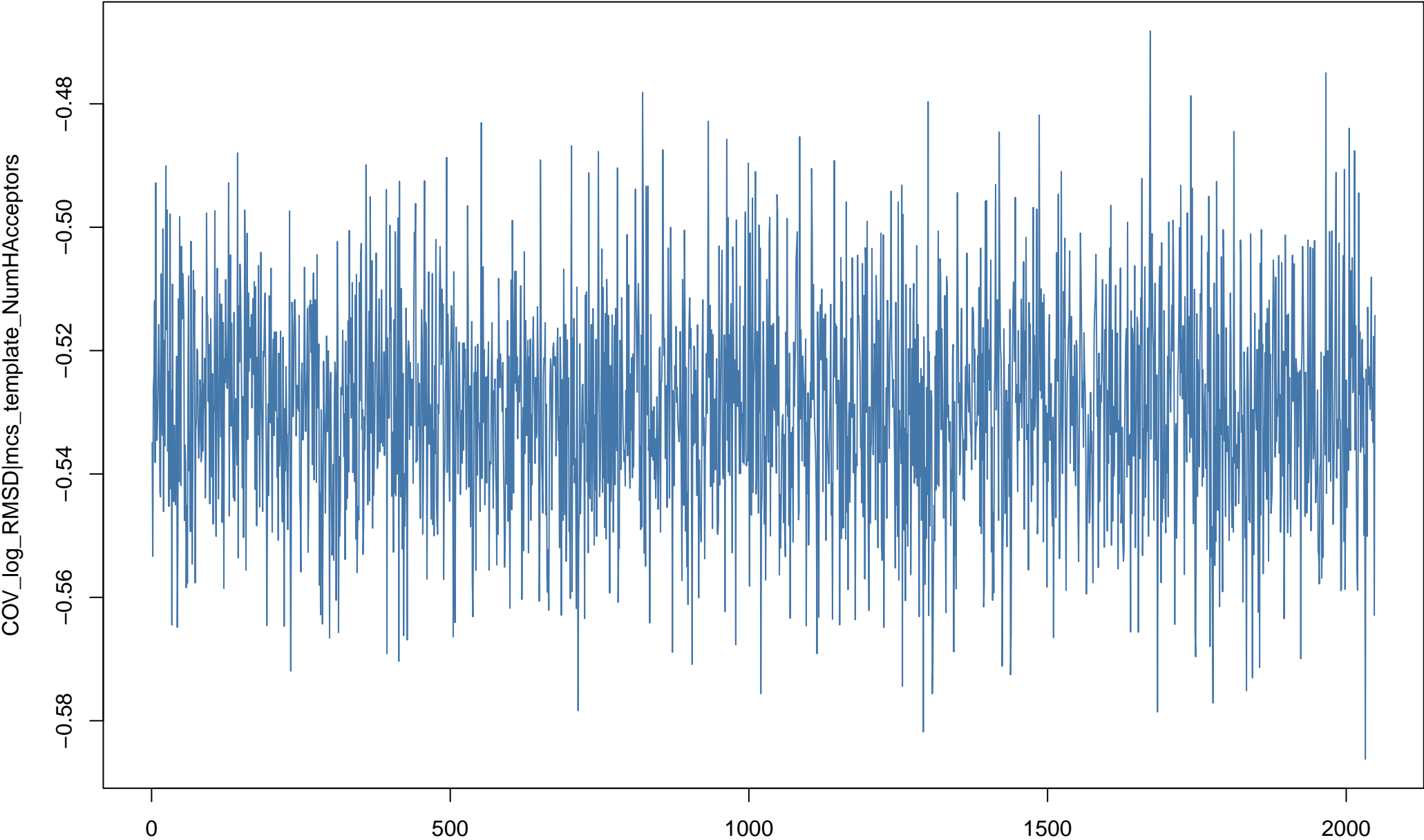
COV_log_RMSD|template_HeavyAtomCount
ESS = 1310 | BMK = 0.0489 | MCSE(6.27) = 2.69 | stat: FALSE | burn: 0



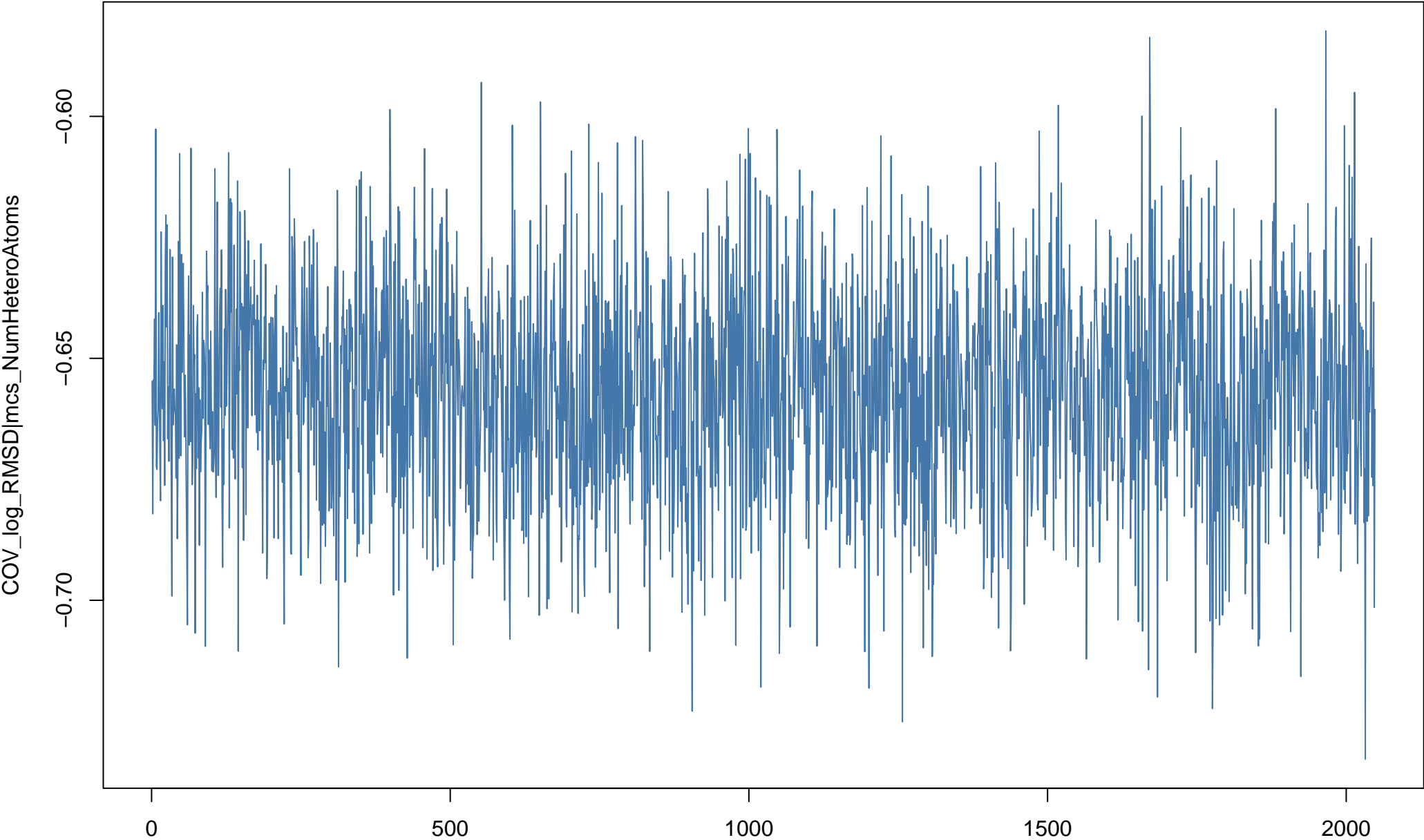
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 1770 | BMK = 0.0432 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0



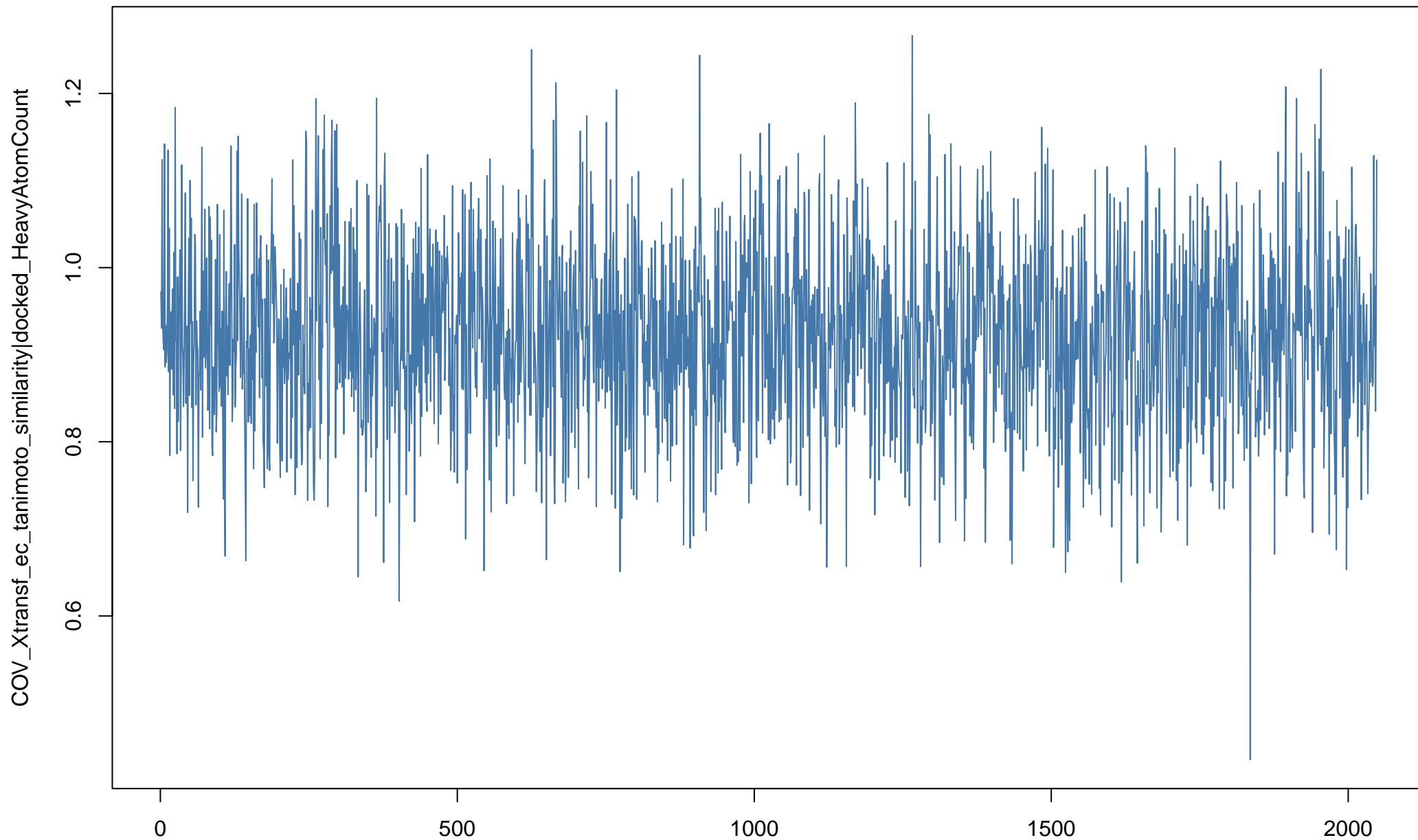
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.05 | MCSE(6.27) = 2.14 | stat: FALSE | burn: 0



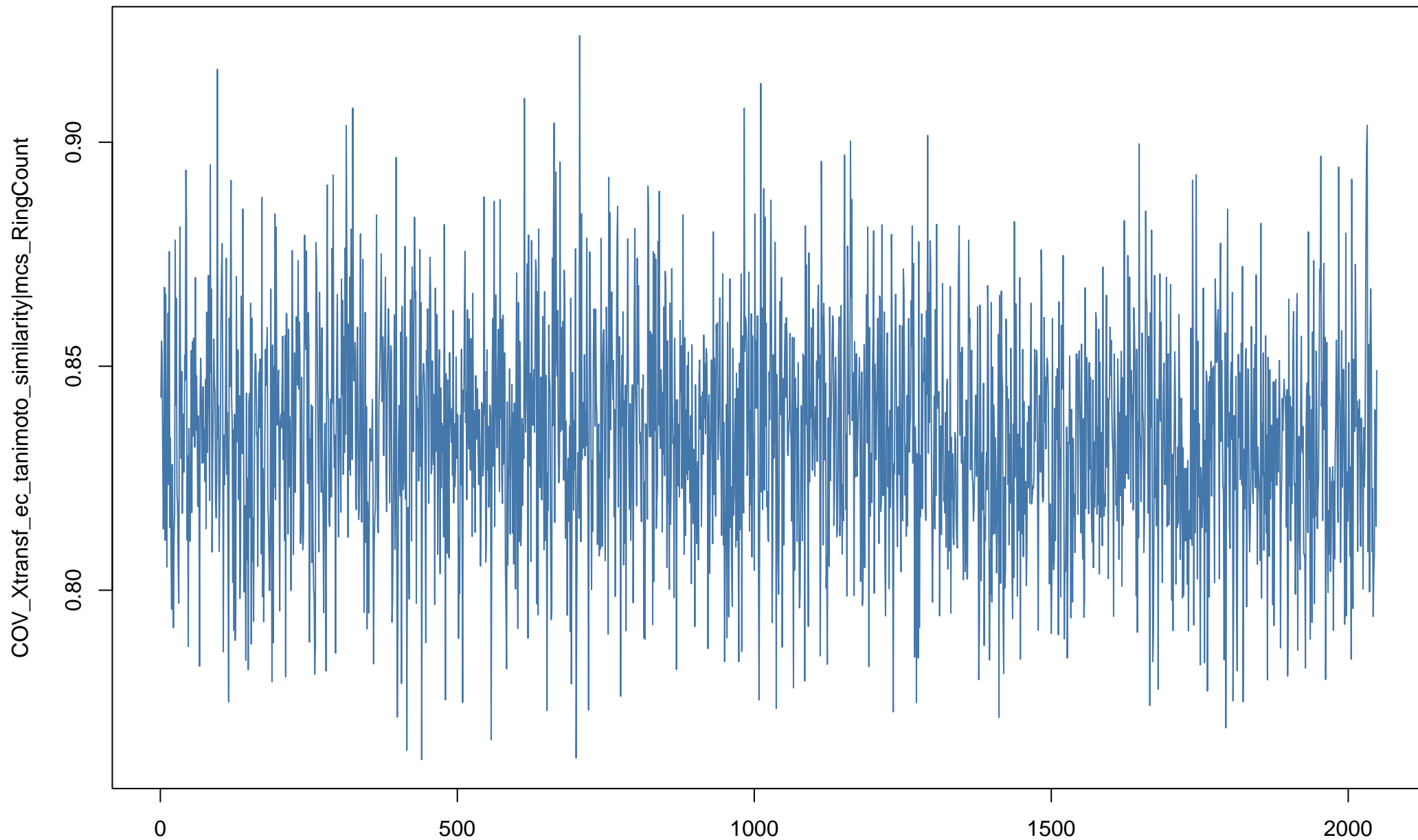
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.035 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0



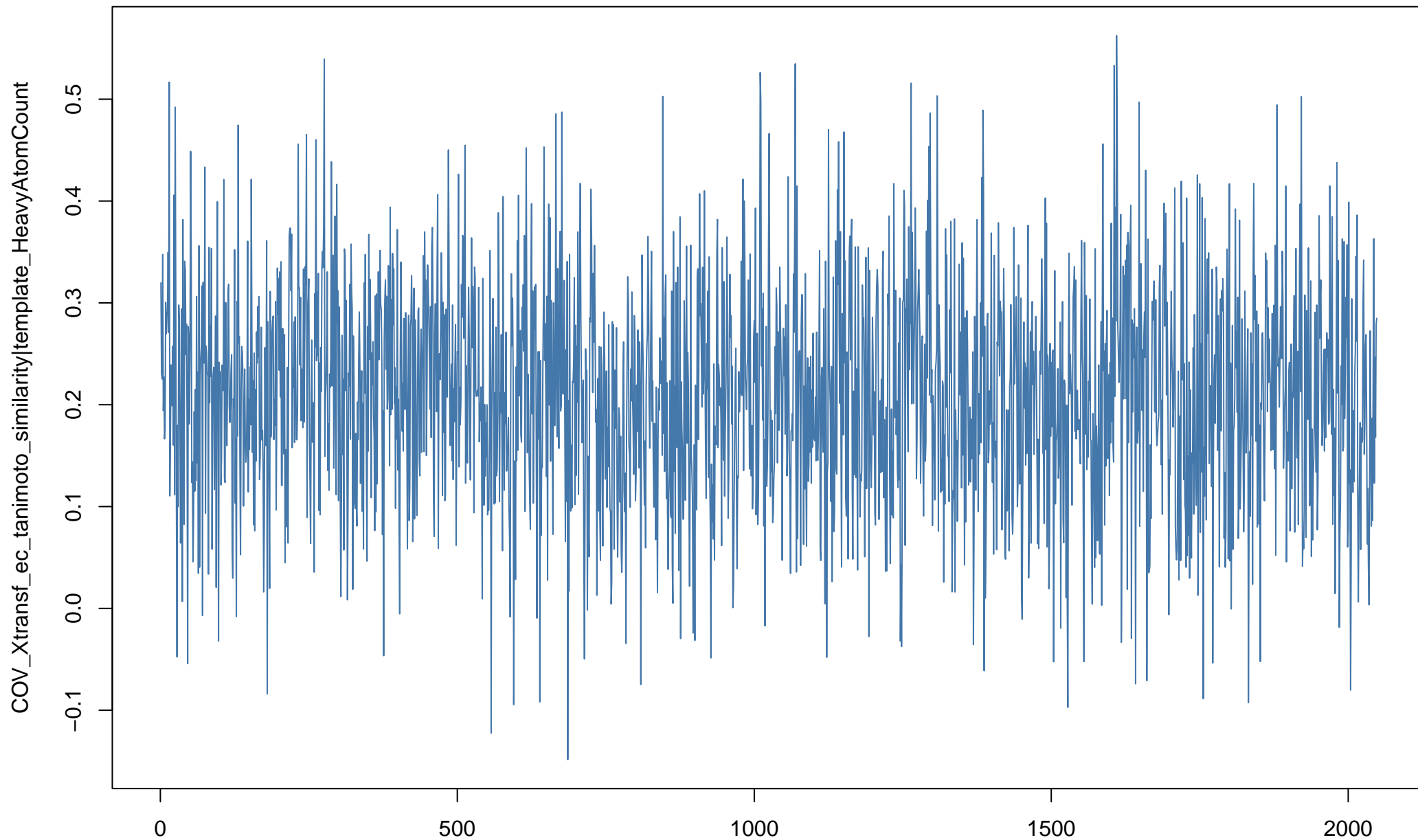
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1680 | BMK = 0.0391 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0



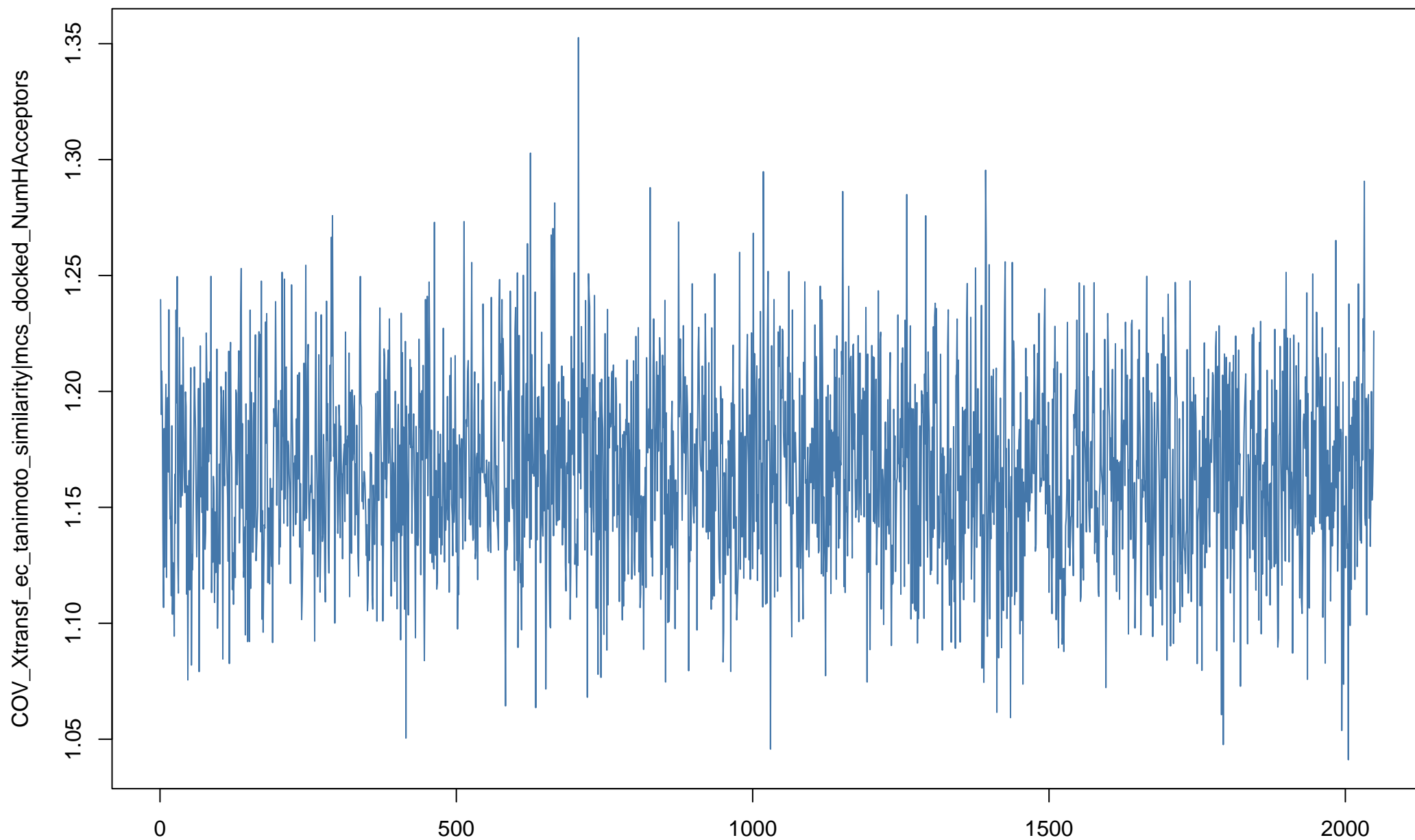
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1910 | BMK = 0.0716 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



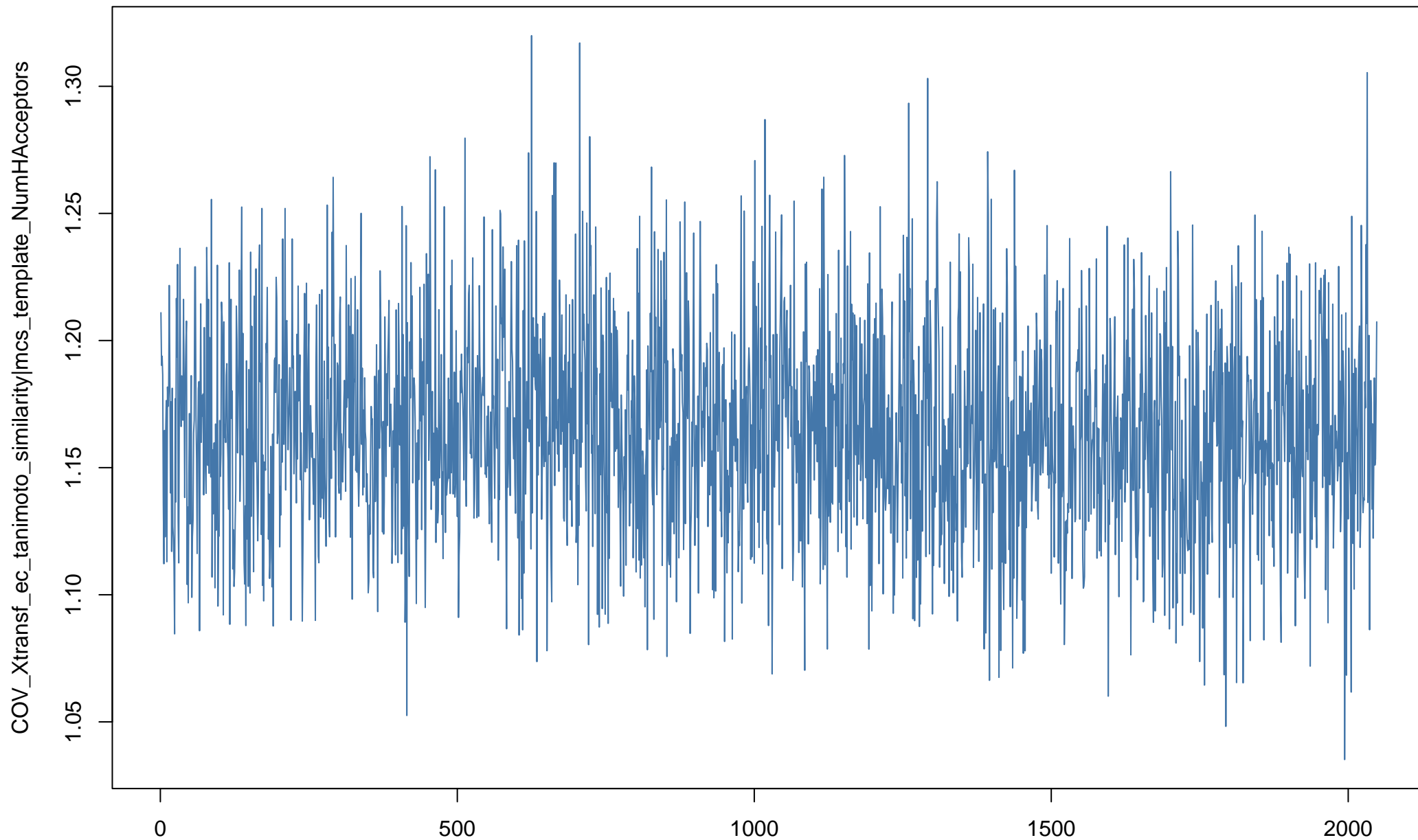
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1540 | BMK = 0.0513 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0



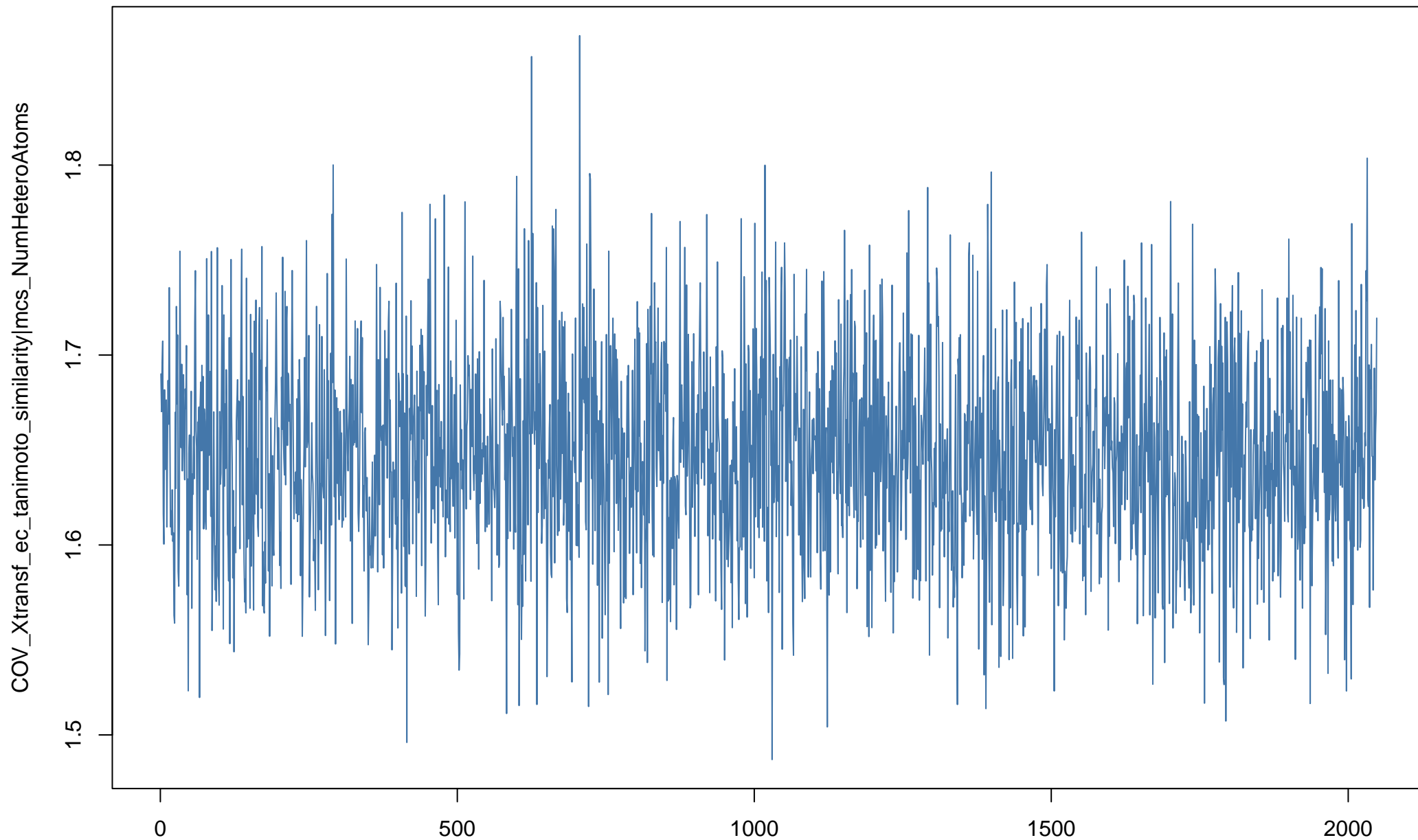
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 1780 | BMK = 0.0504 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0



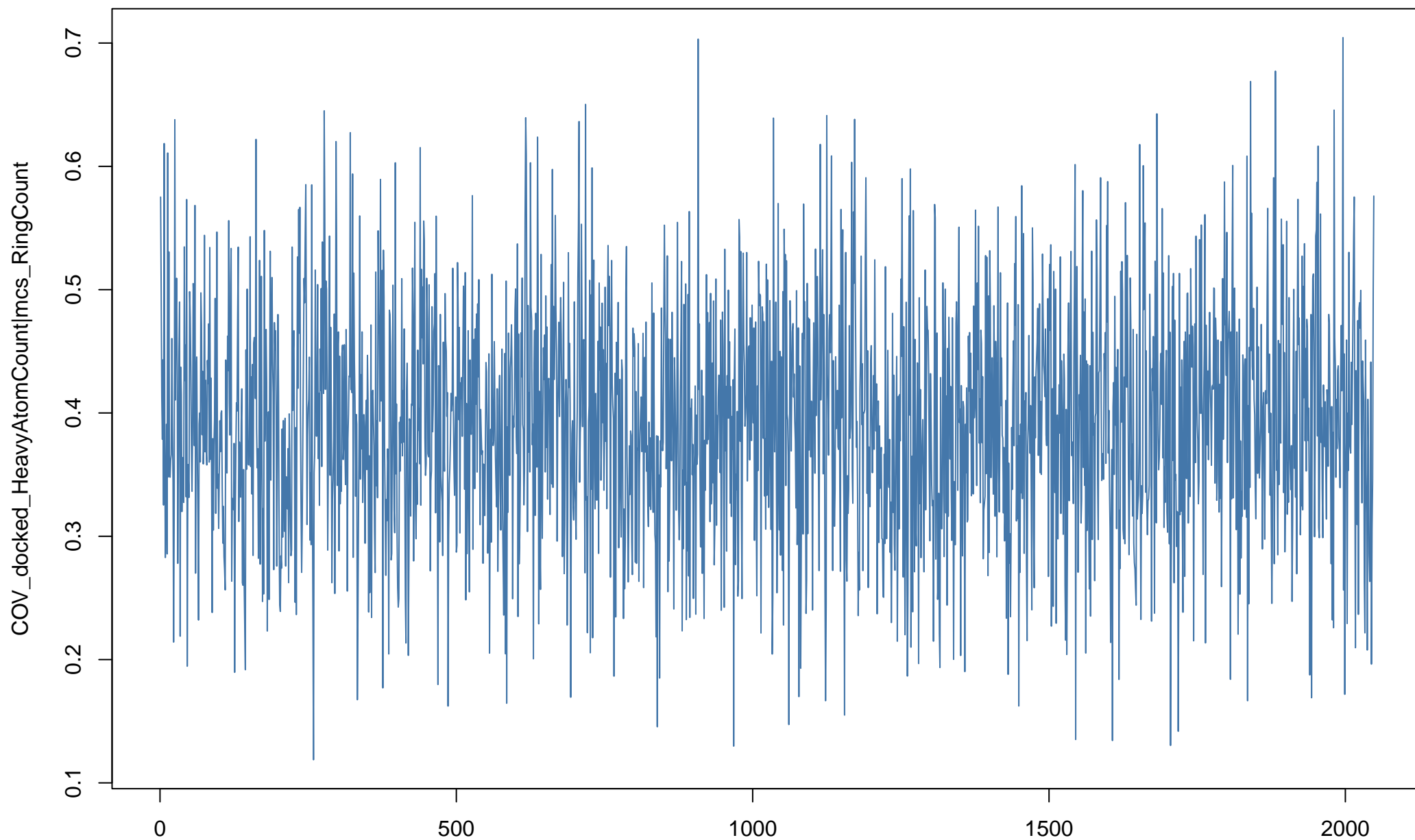
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 1820 | BMK = 0.0616 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0



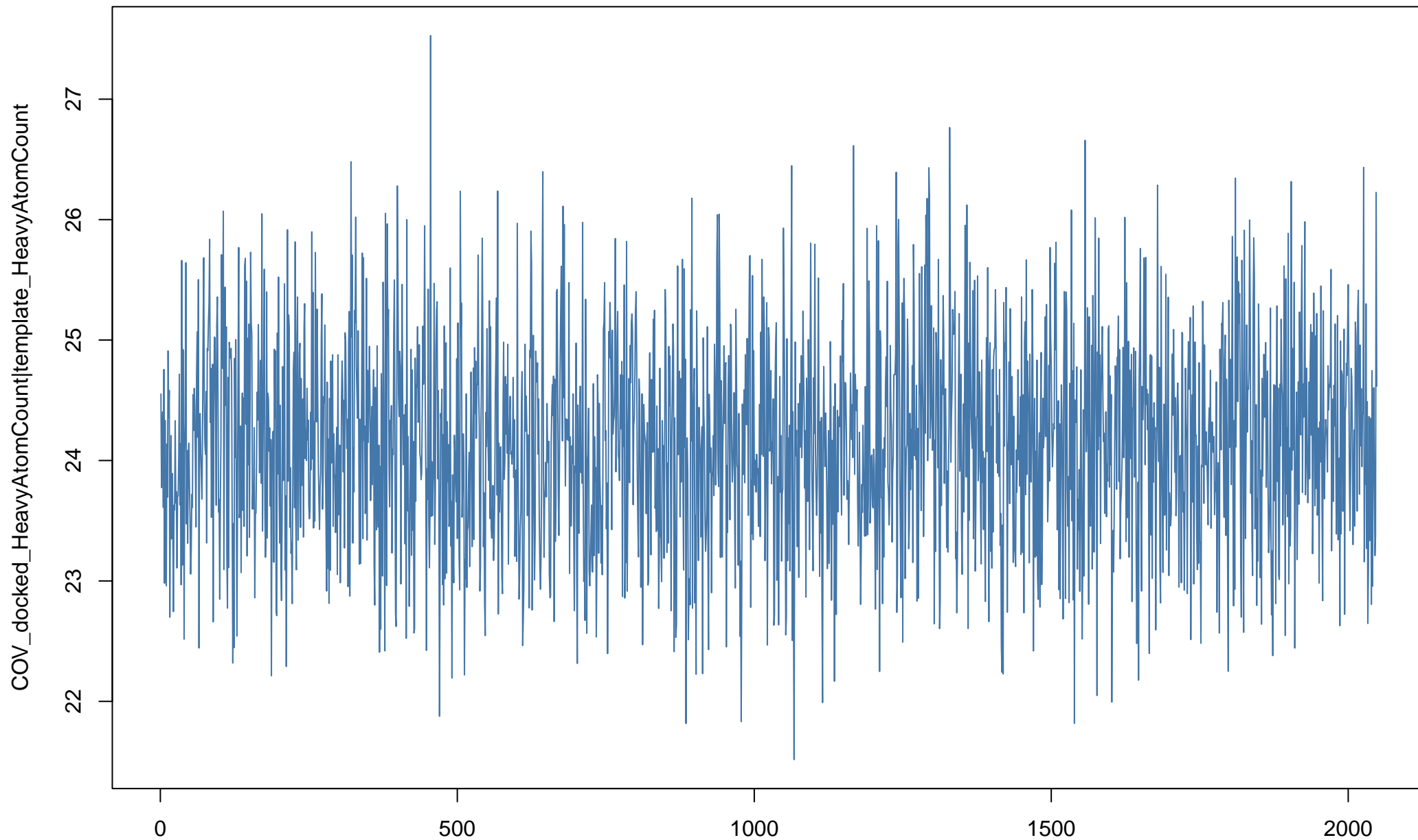
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1810 | BMK = 0.0425 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0



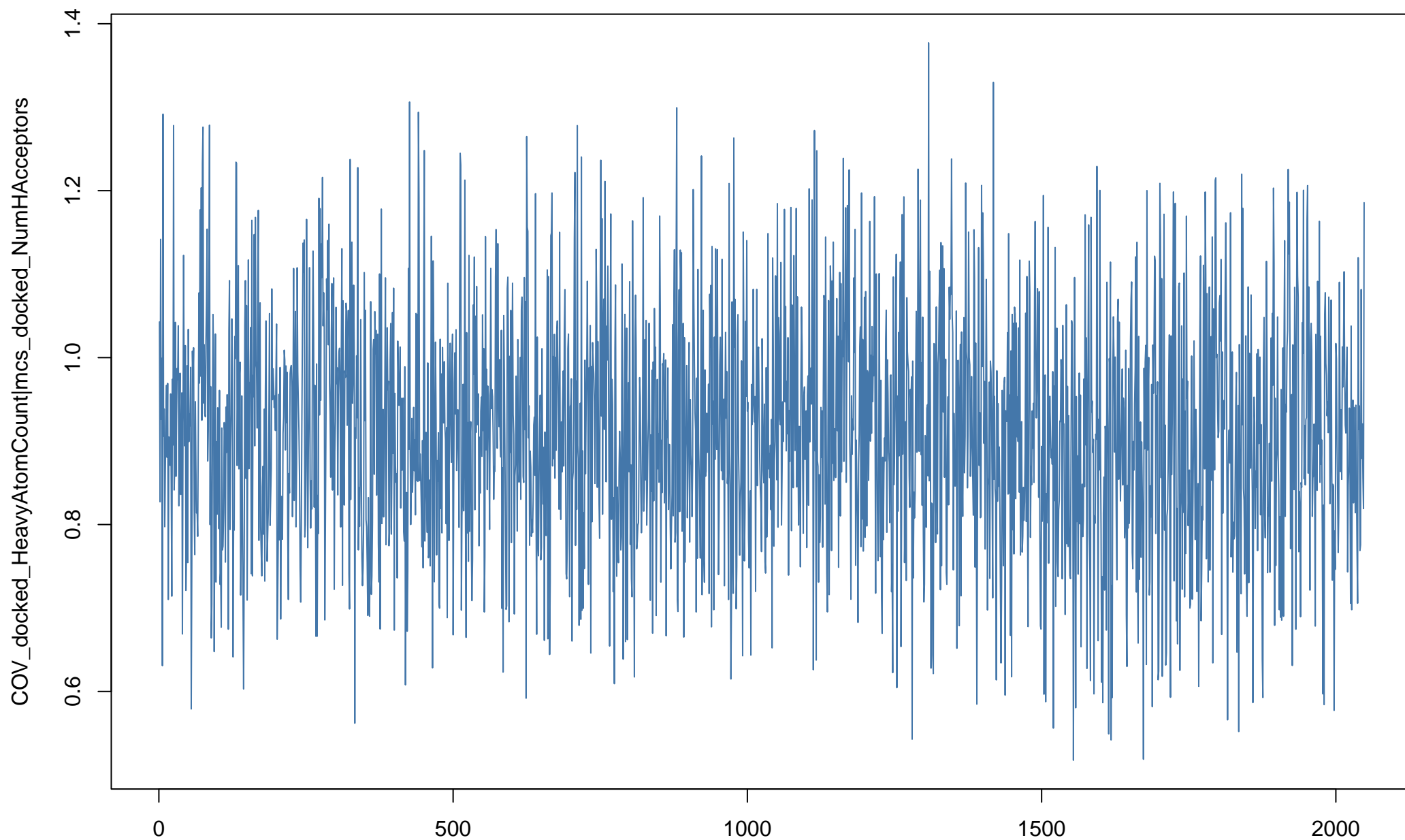
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1730 | BMK = 0.0429 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0



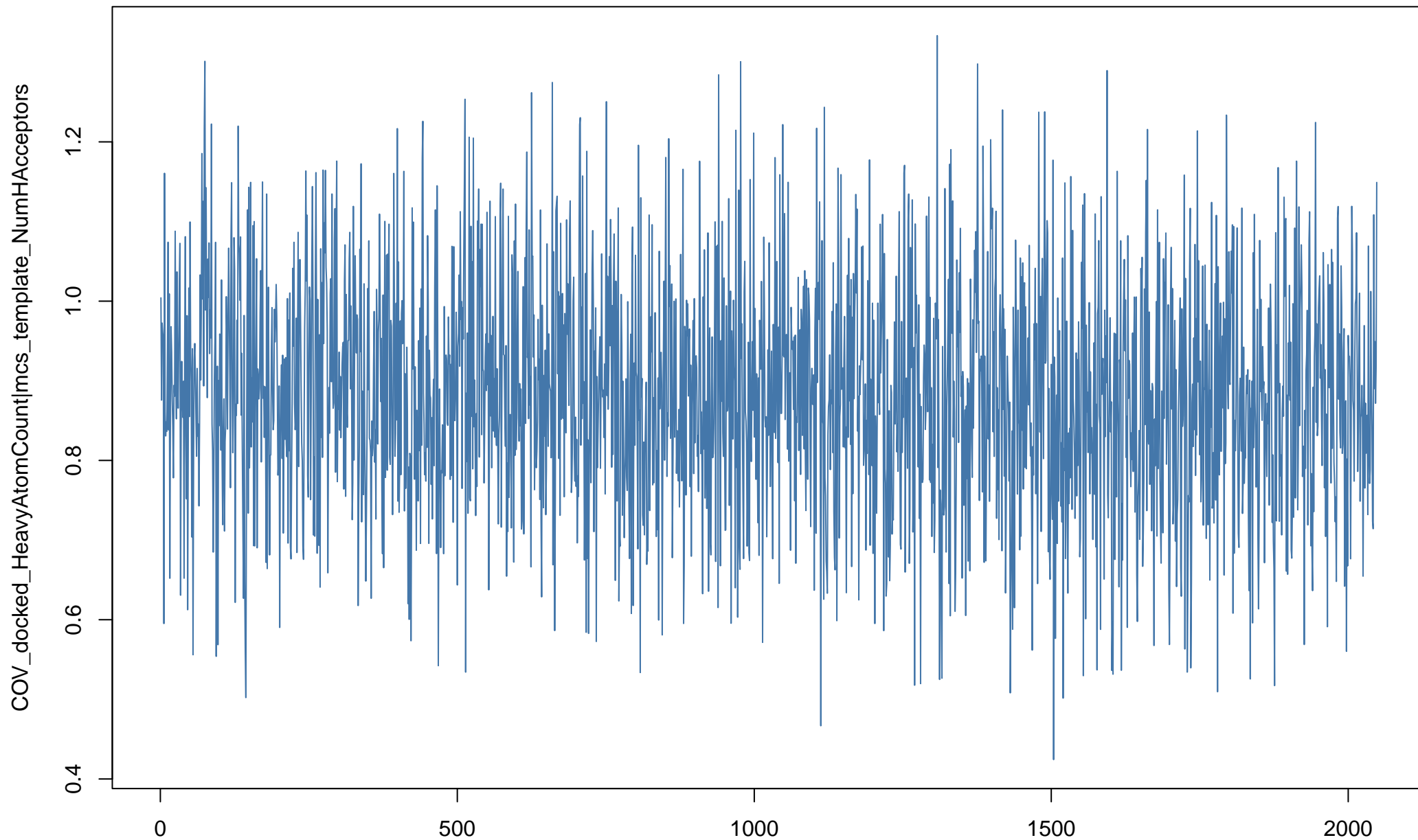
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1790 | BMK = 0.0435 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



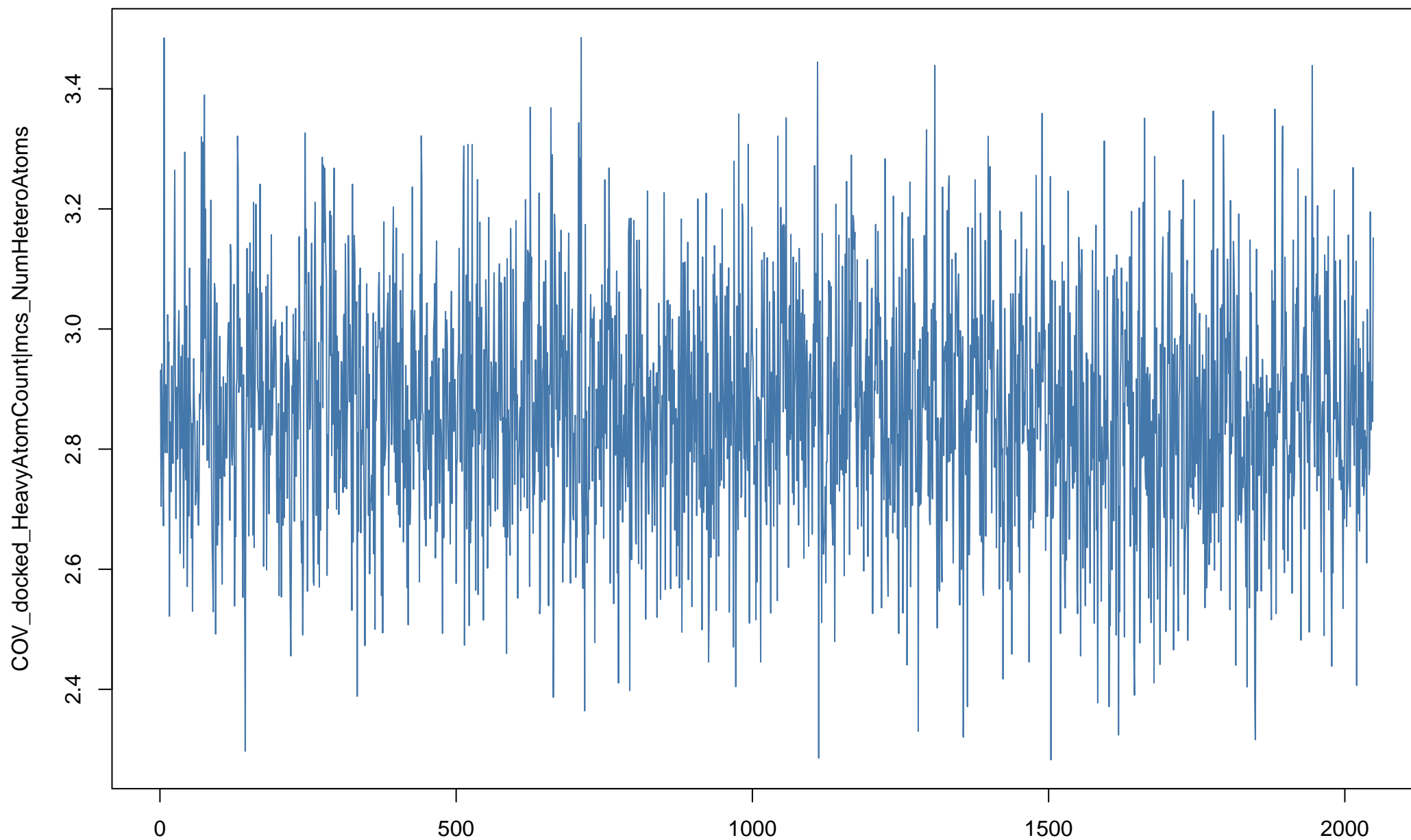
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0708 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0



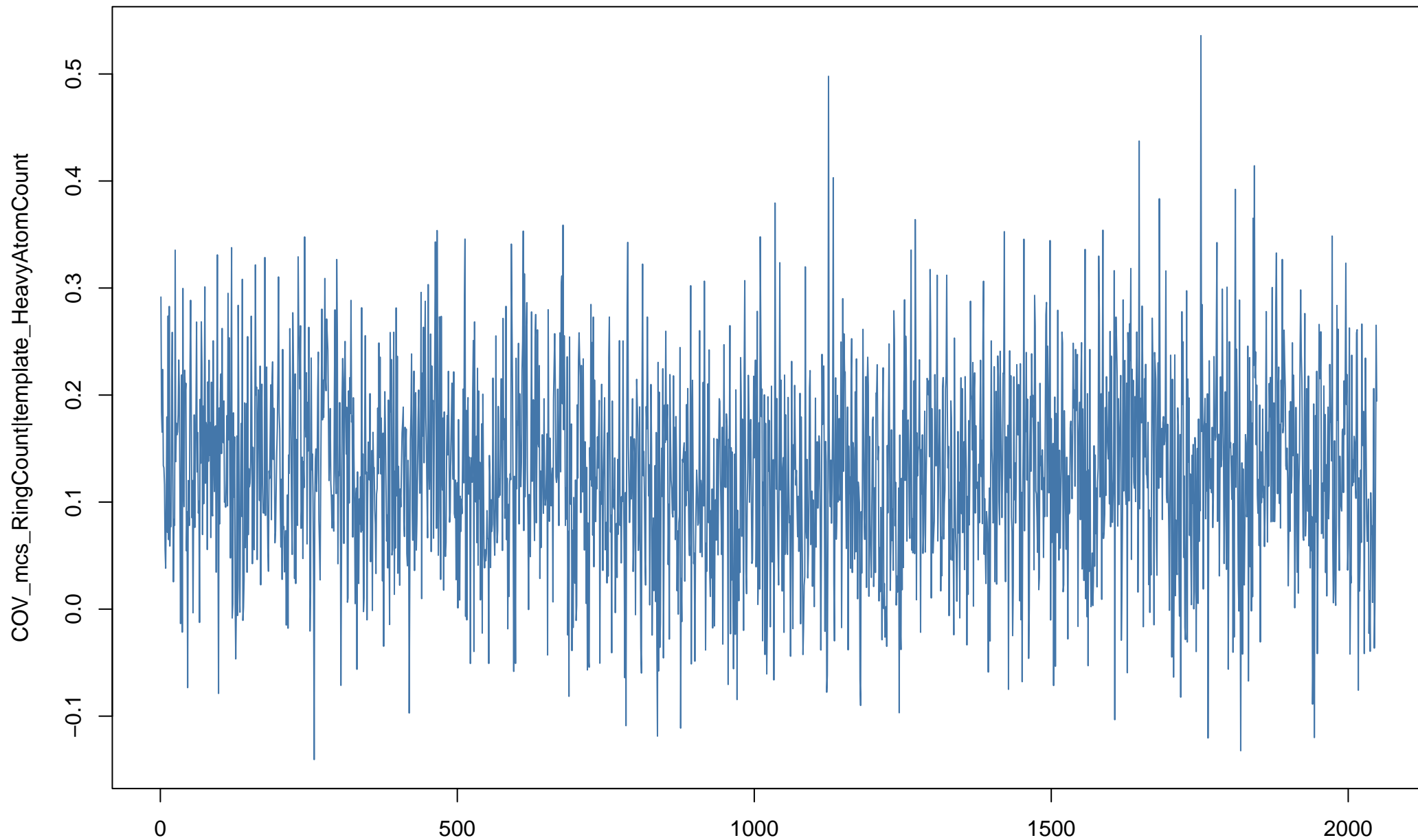
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0586 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0



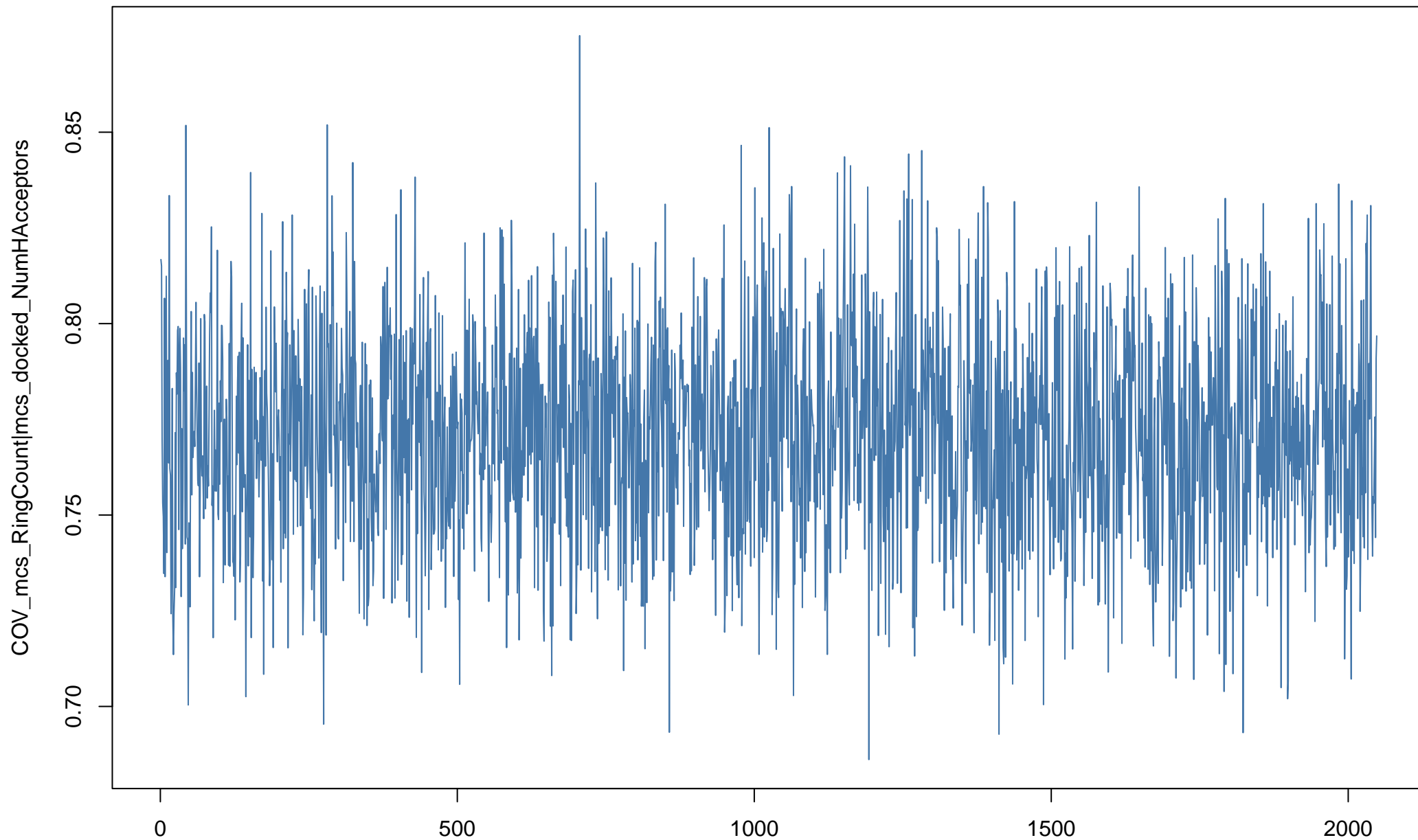
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0371 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0



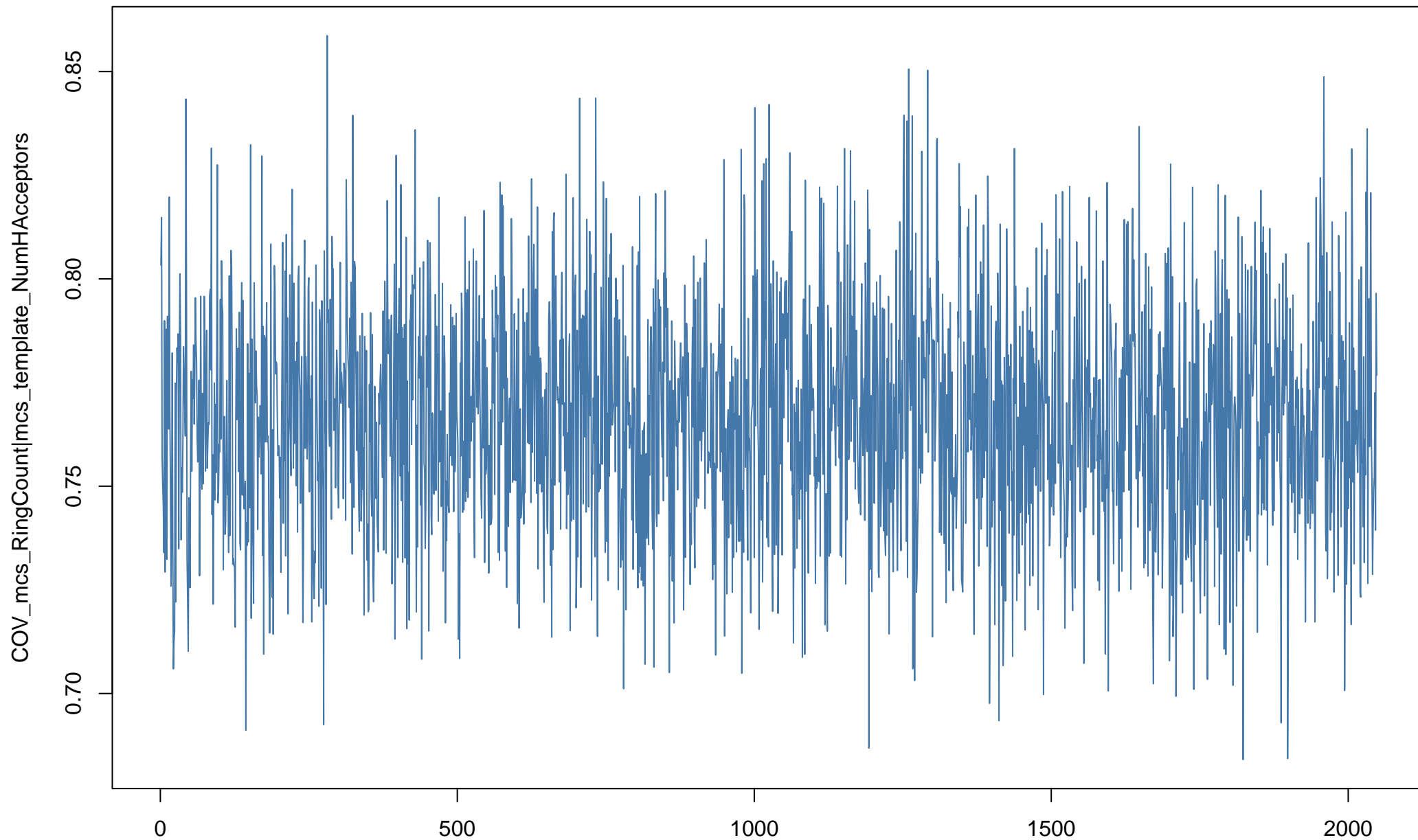
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1450 | BMK = 0.0597 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0



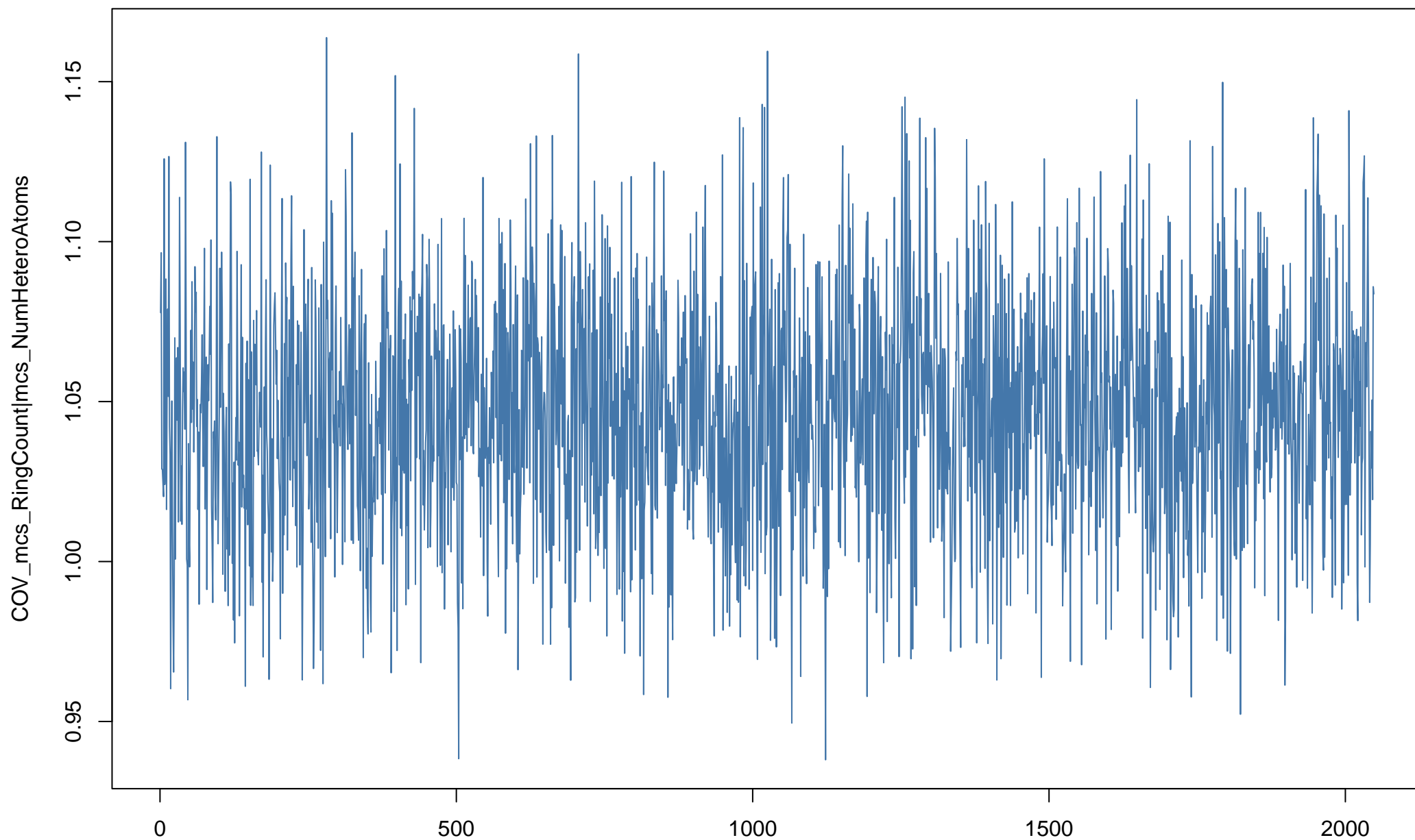
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.05 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



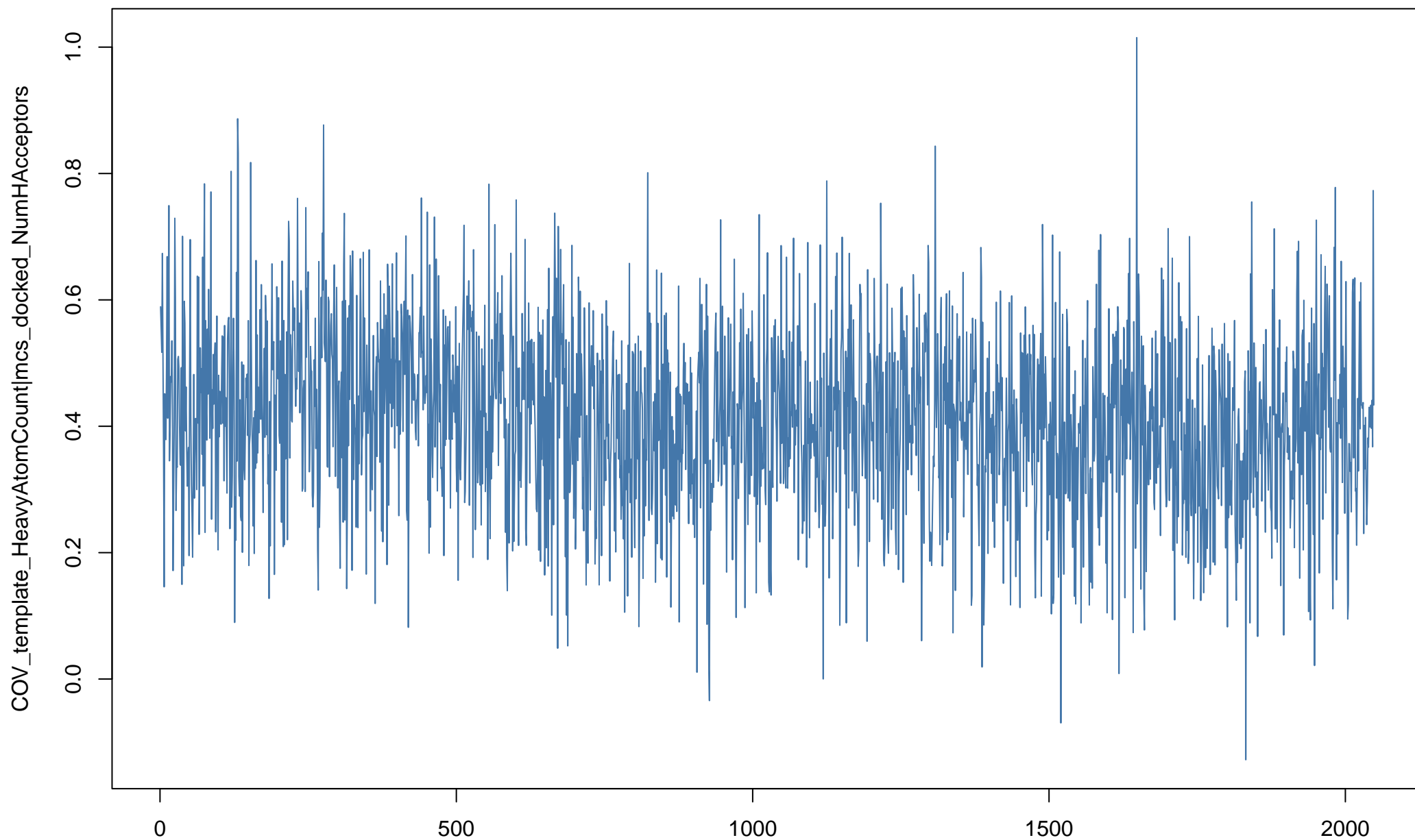
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 1550 | BMK = 0.0451 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



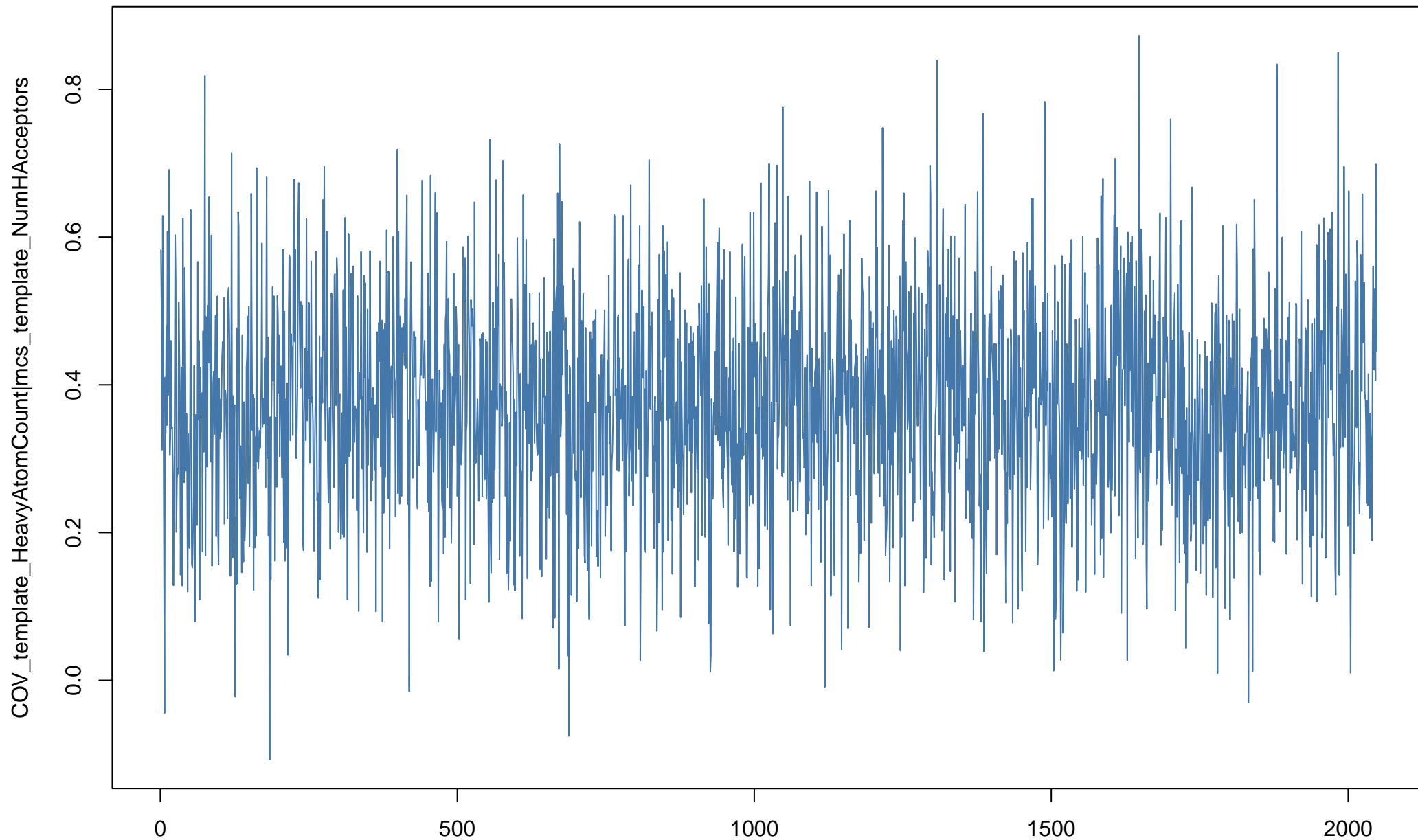
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0446 | MCSE(6.27) = 2.43 | stat: FALSE | burn: 0



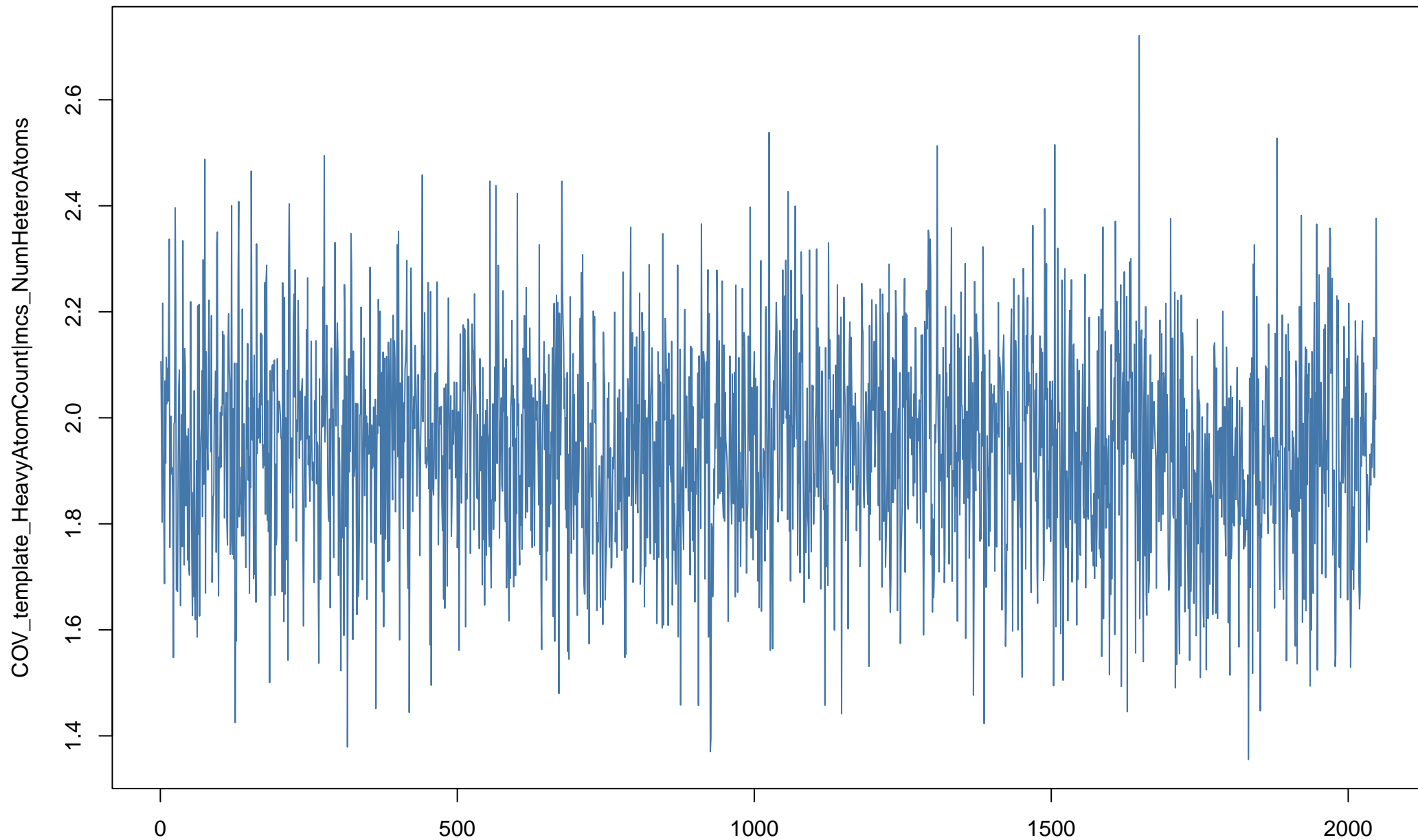
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 477 | BMK = 0.0991 | MCSE(6.27) = 3.66 | stat: FALSE | burn: 0



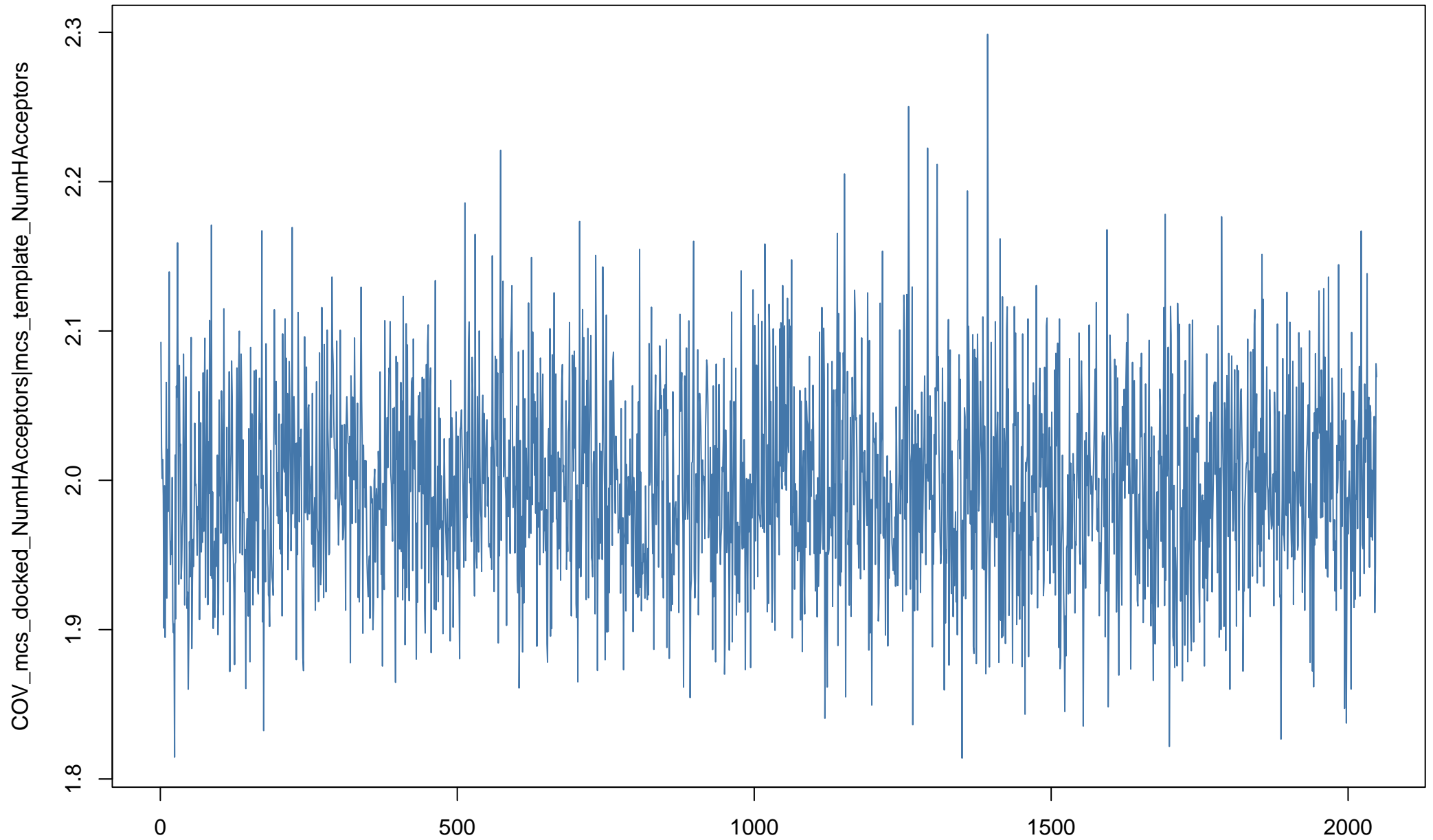
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0428 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



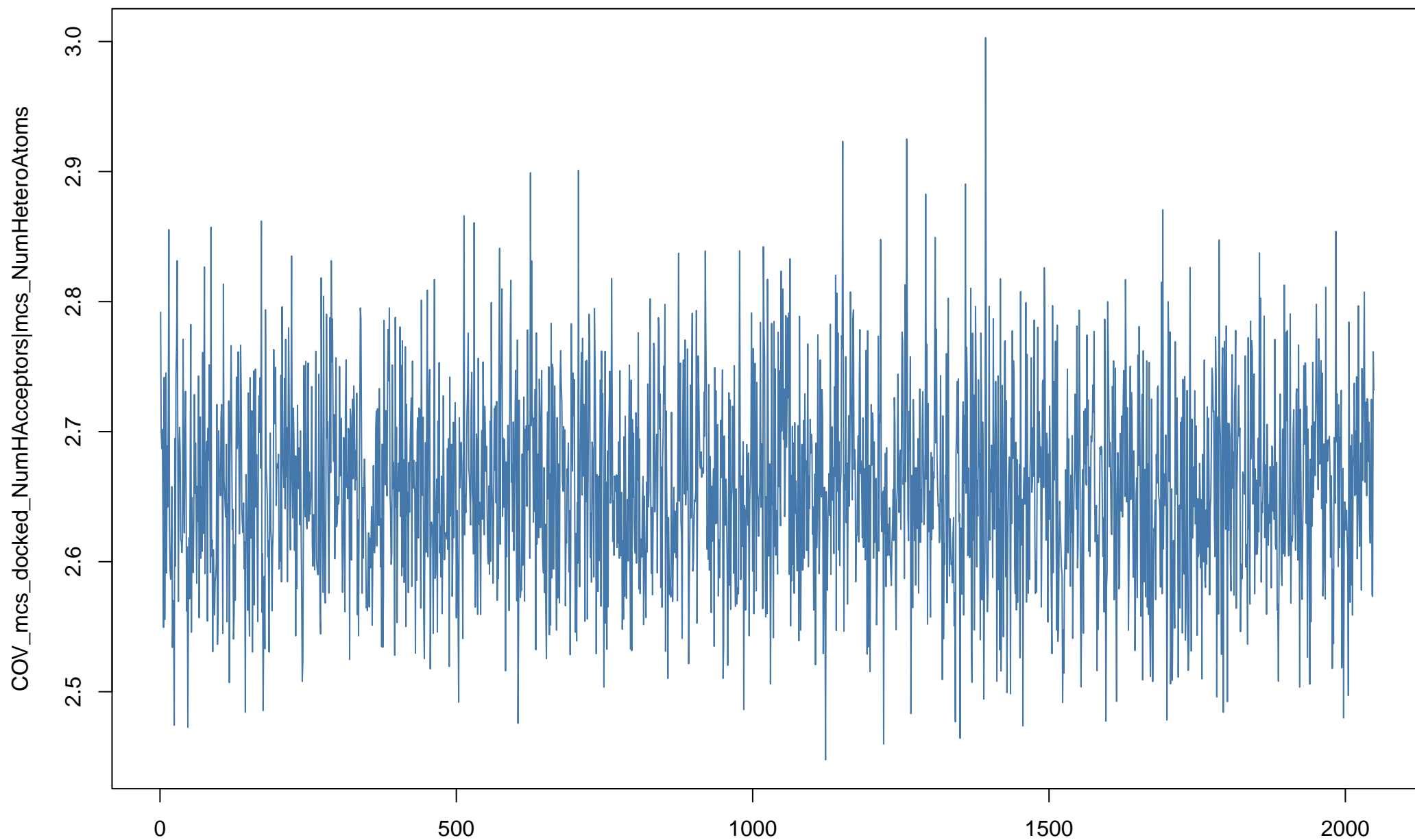
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1920 | BMK = 0.0466 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 1750 | BMK = 0.0552 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 1730 | BMK = 0.0561 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 1770 | BMK = 0.0454 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0

