

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.208740697688651

max MCSE = 10.0019176718116

all stationary: FALSE

burn: 0

-- STATS 2D --

min ESS = 1172.49399888686

max BMK = 0.0607795479945052

max MCSE = 3.03861014387686

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.517210613073053

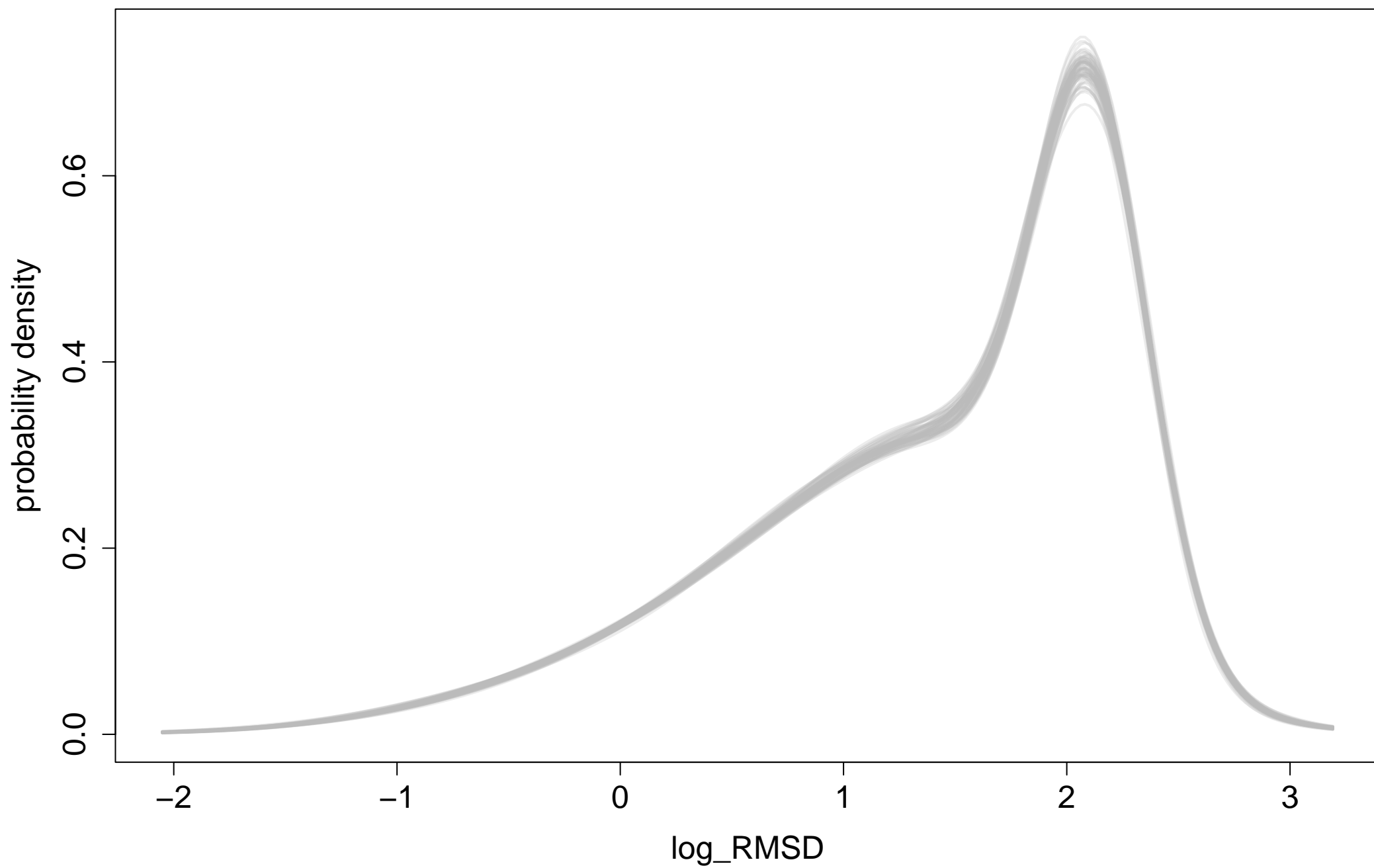
max MCSE = NaN

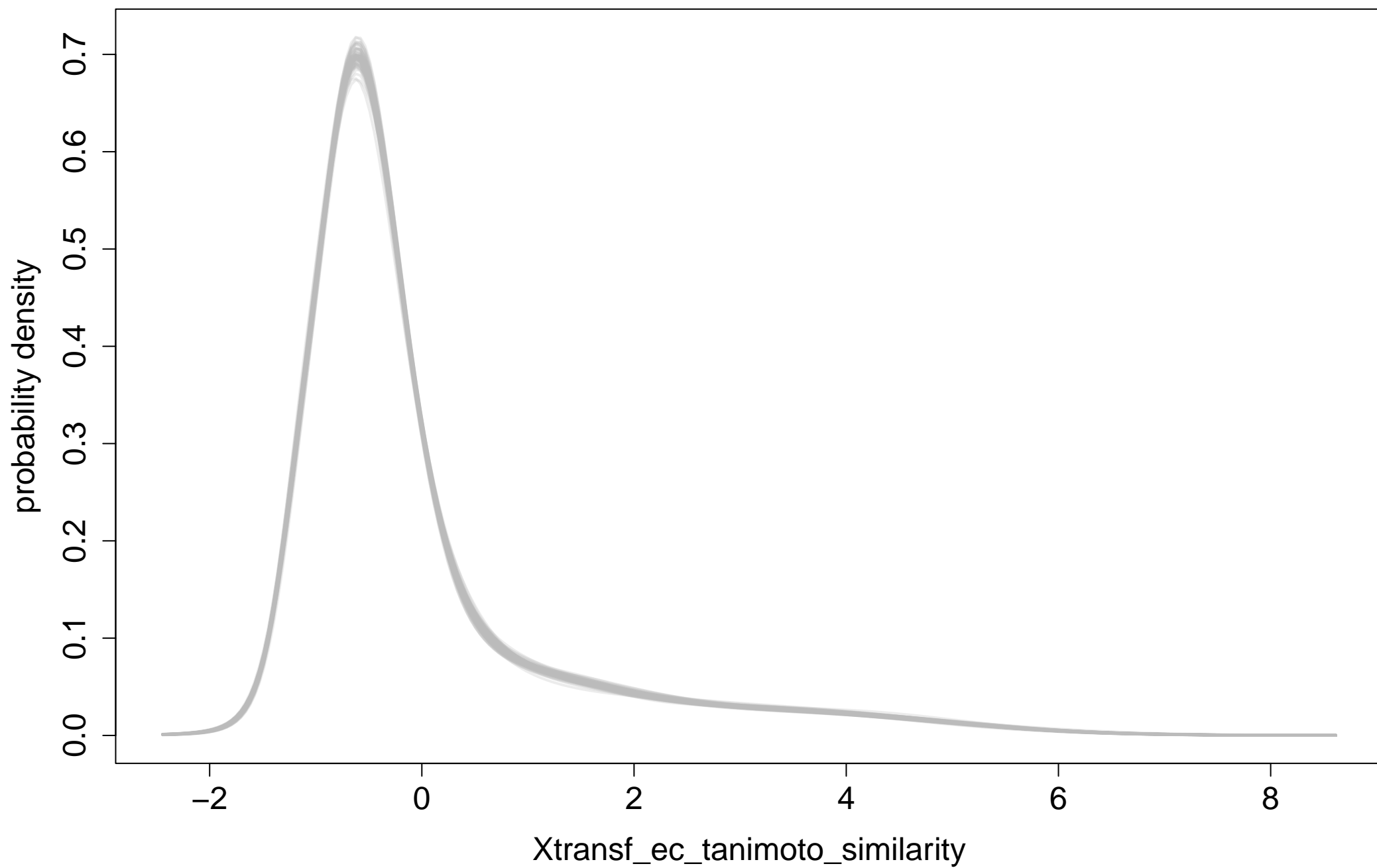
all stationary: FALSE

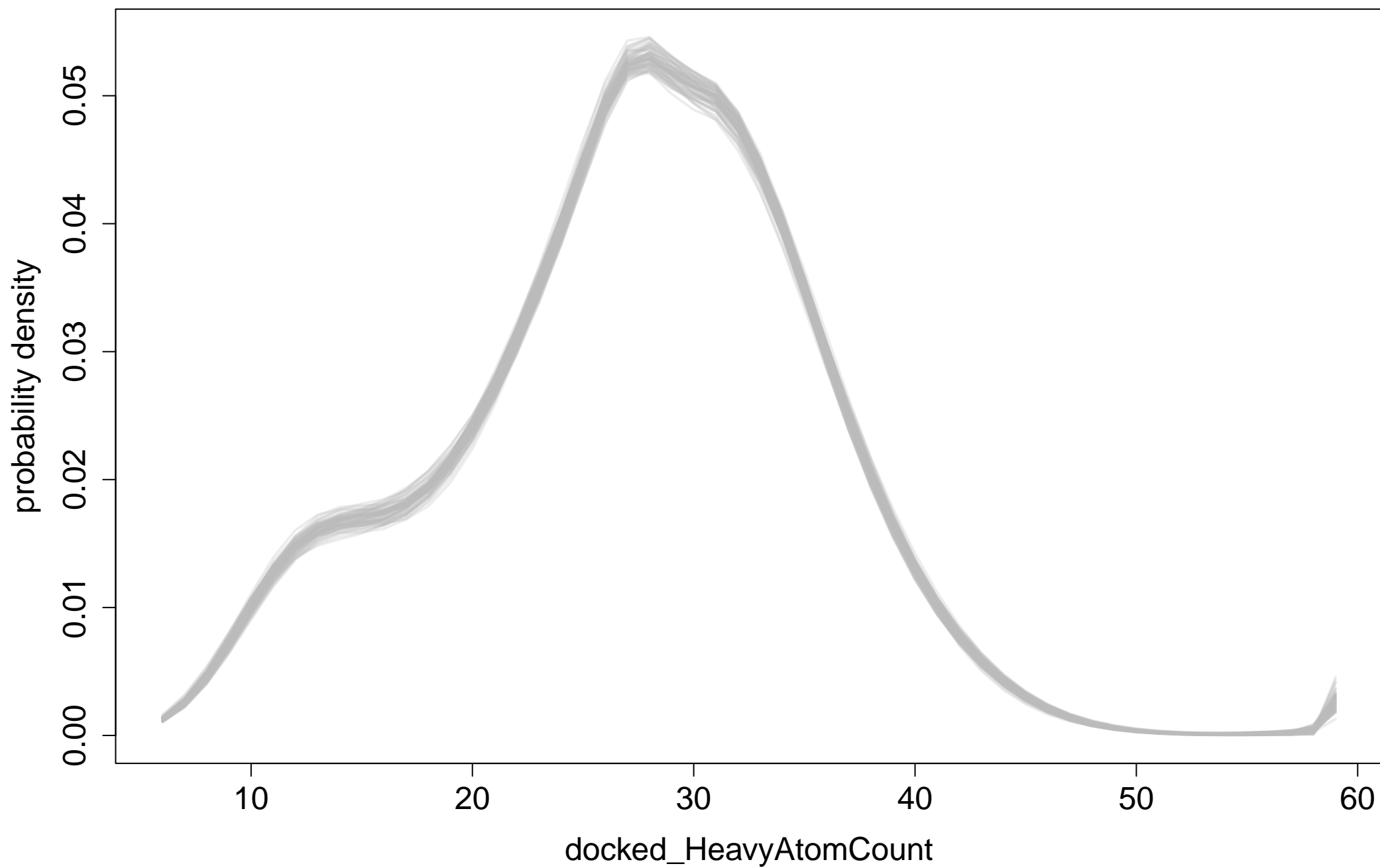
burn: 1632

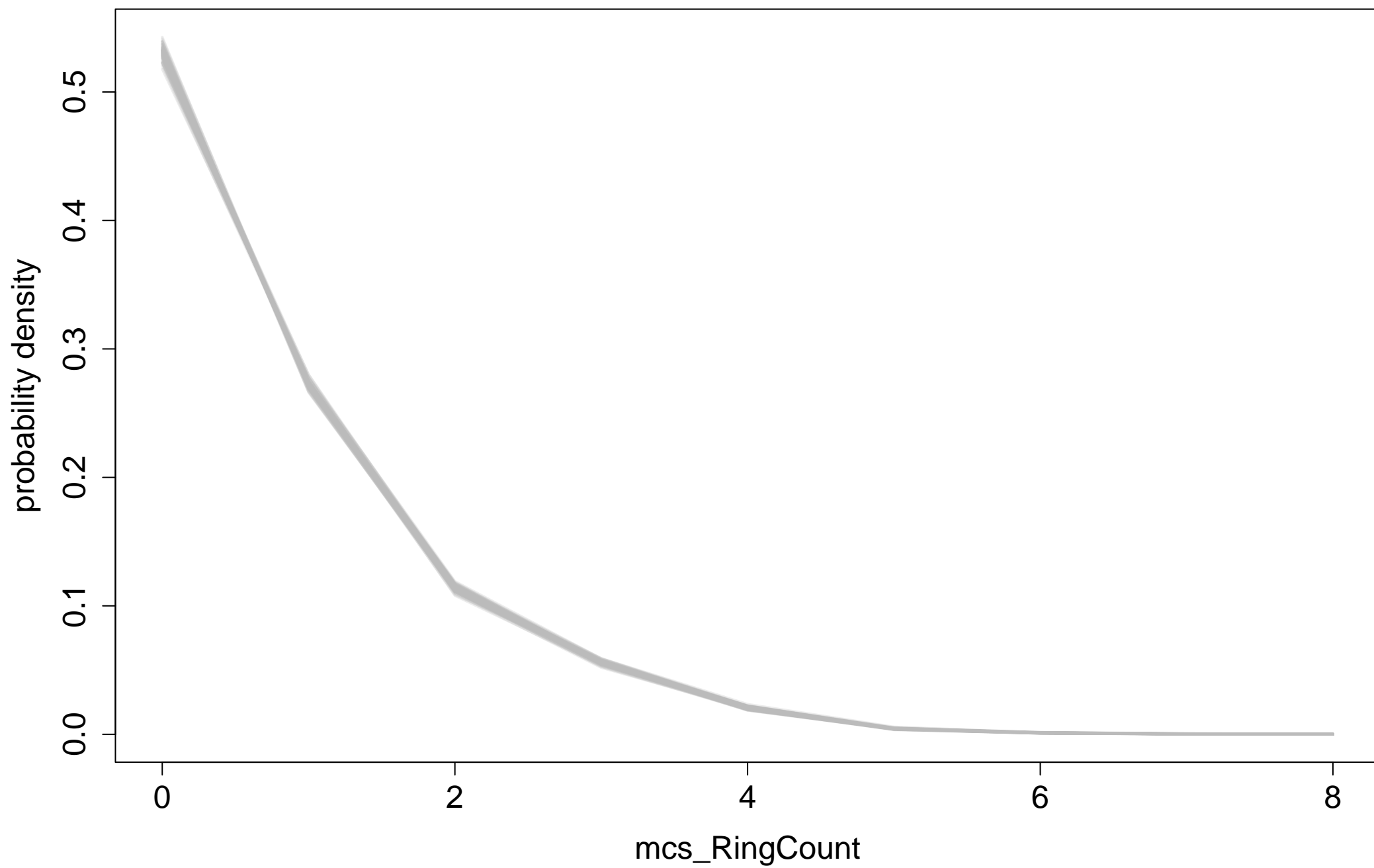
Occupied clusters: 48 of 91

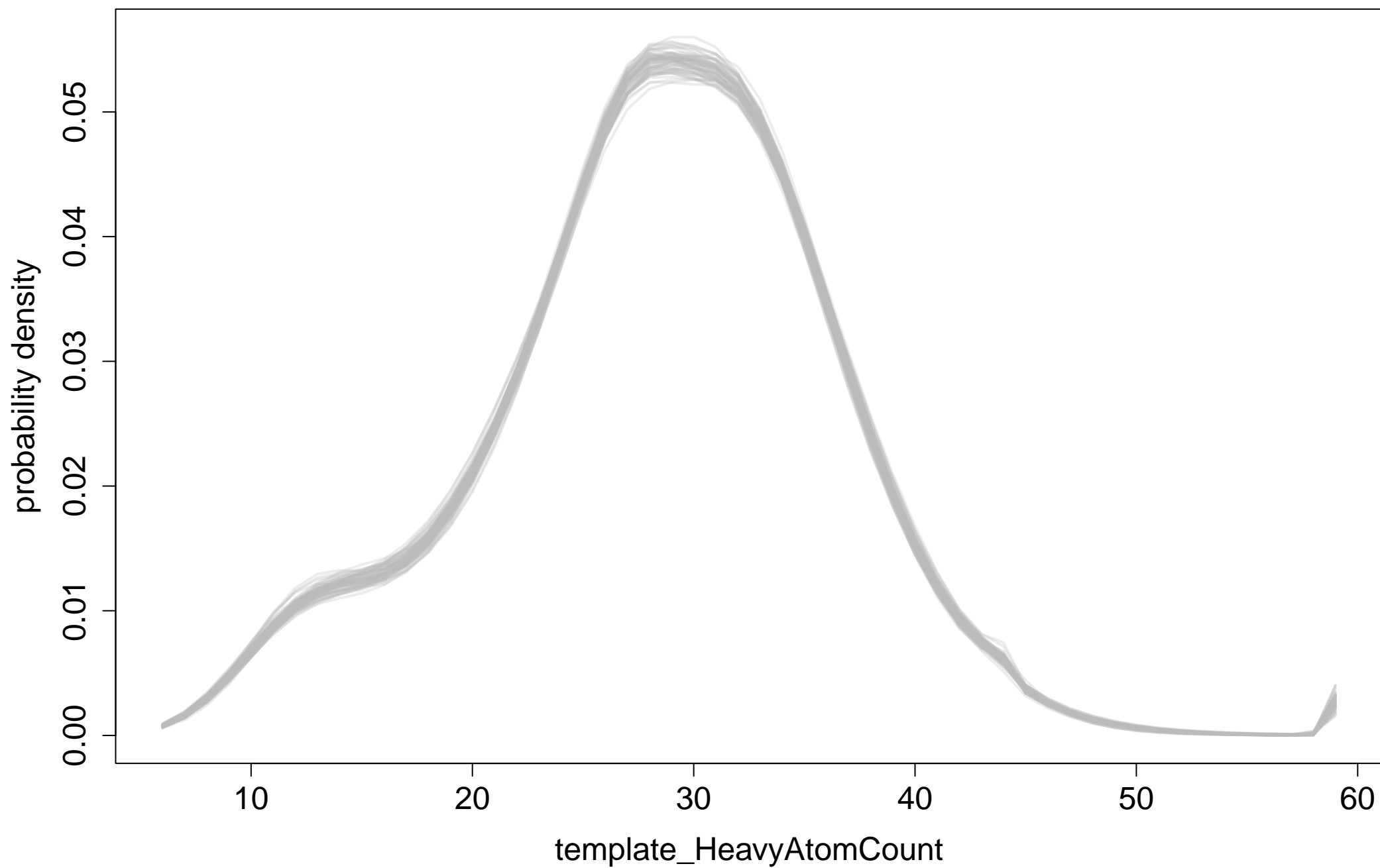
LL: -112000 +- 24.3

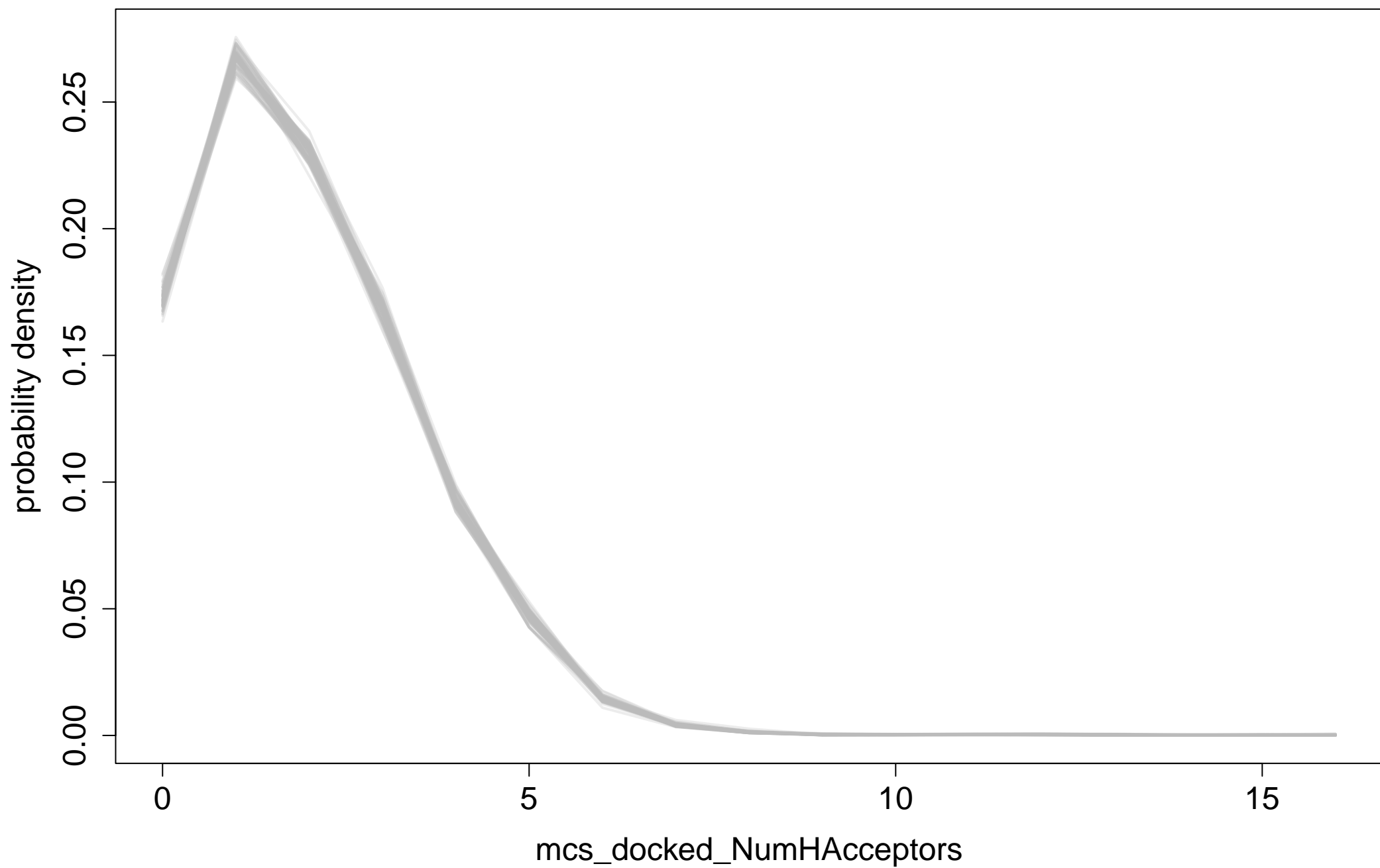


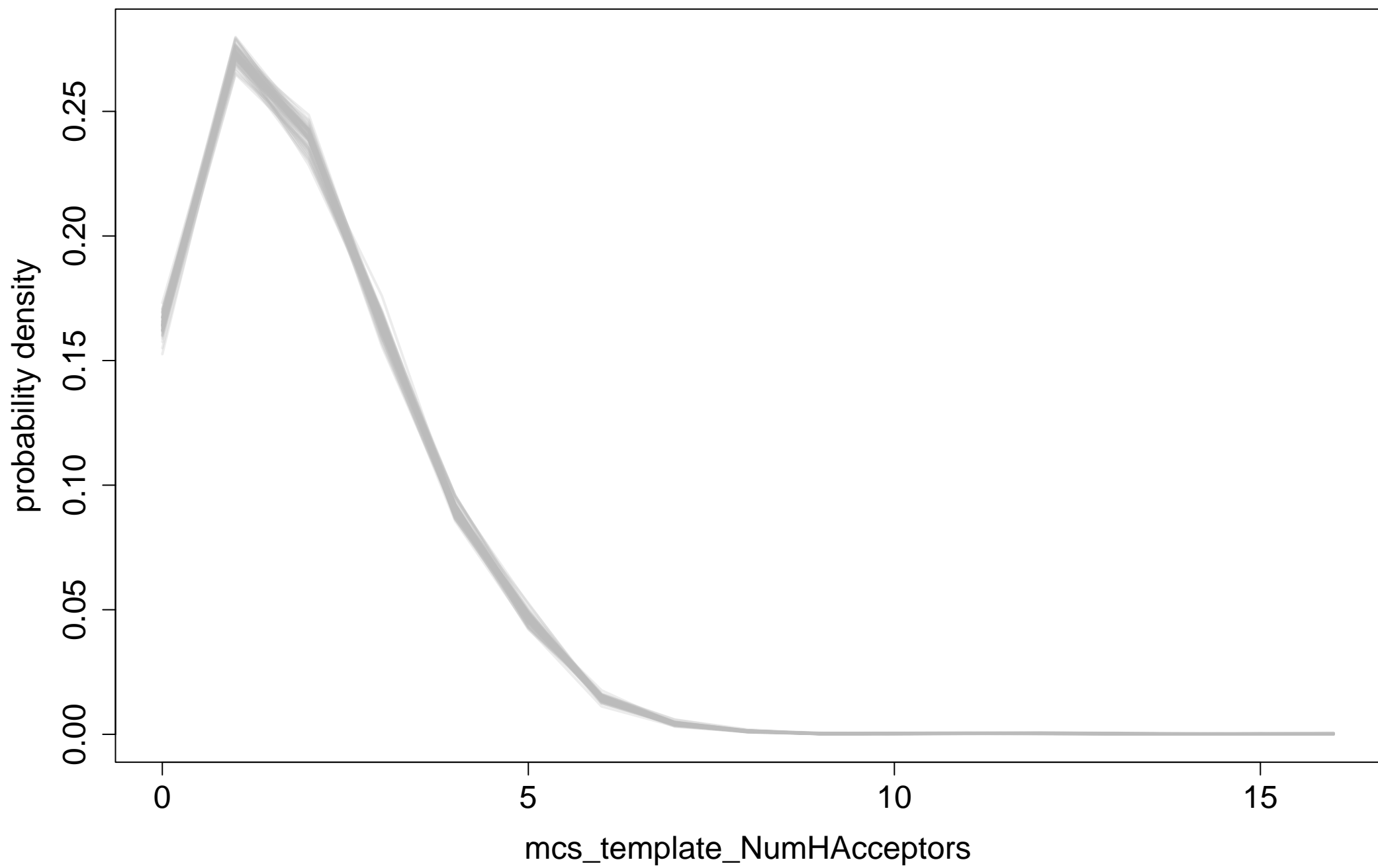


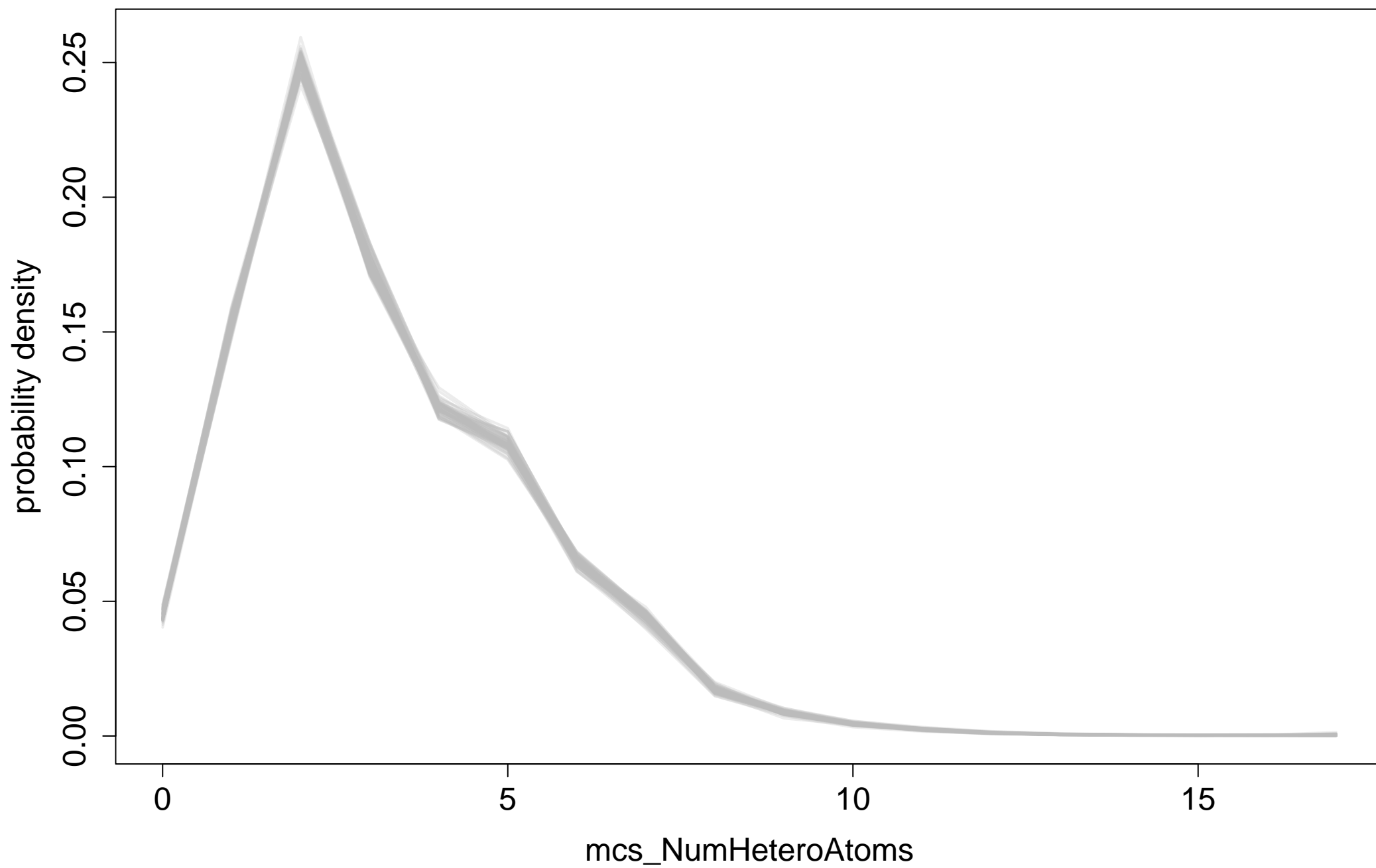


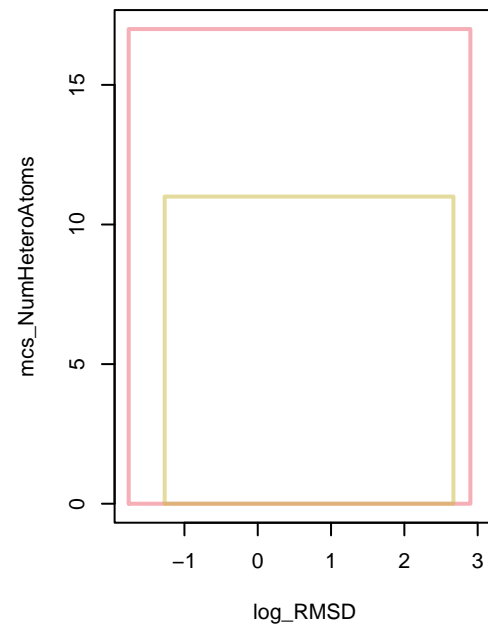
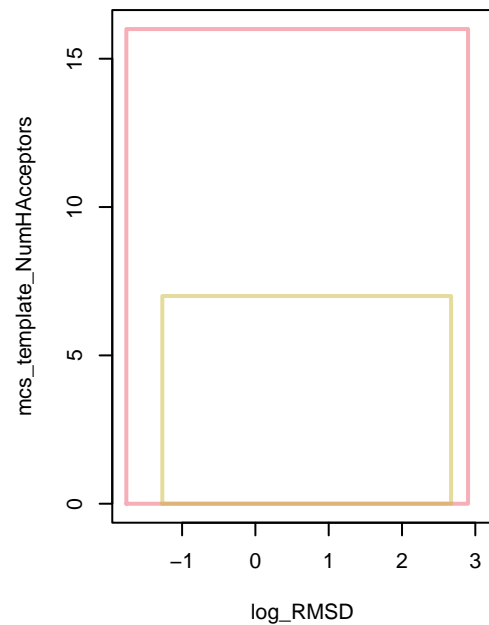
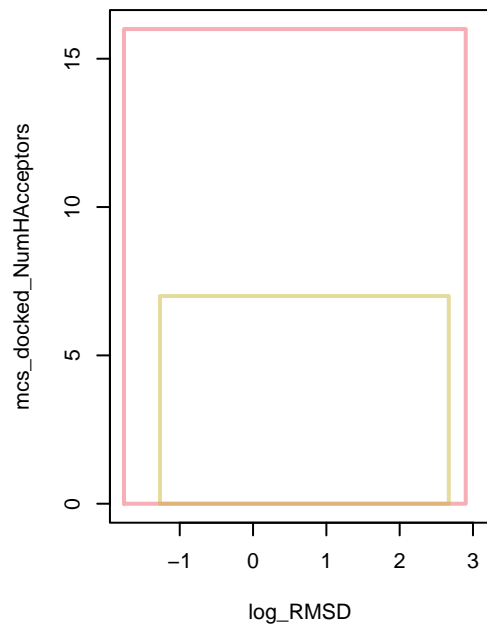
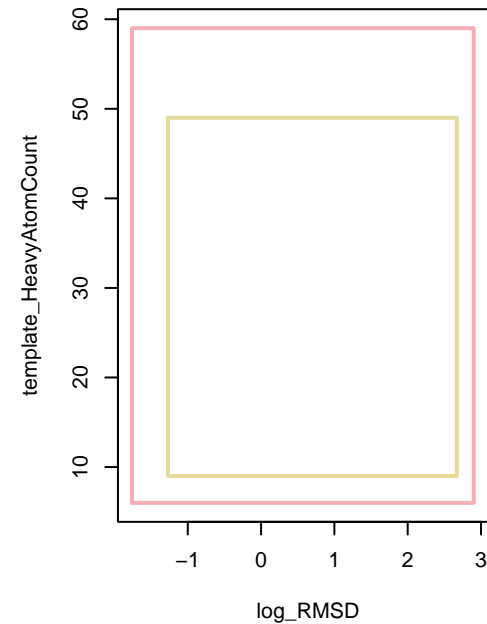
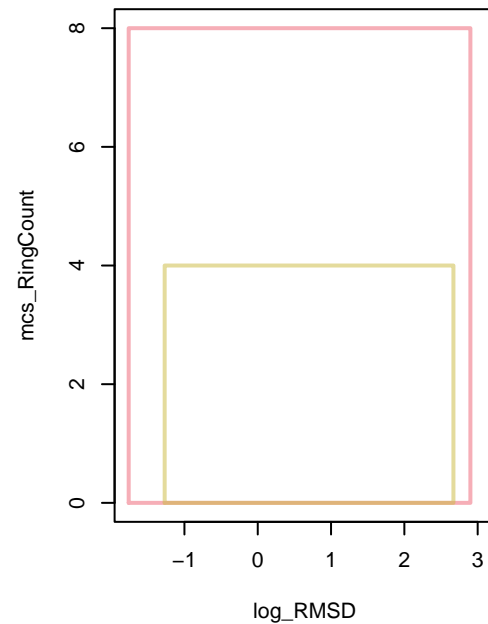
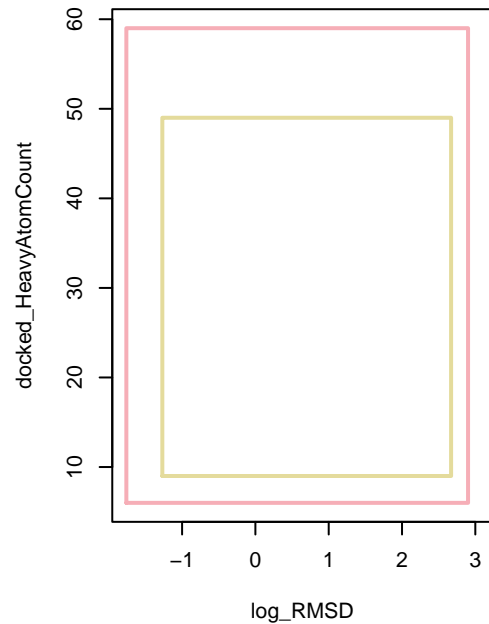
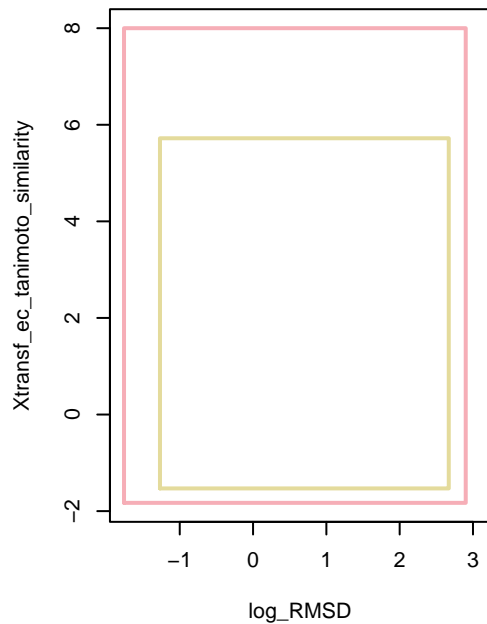




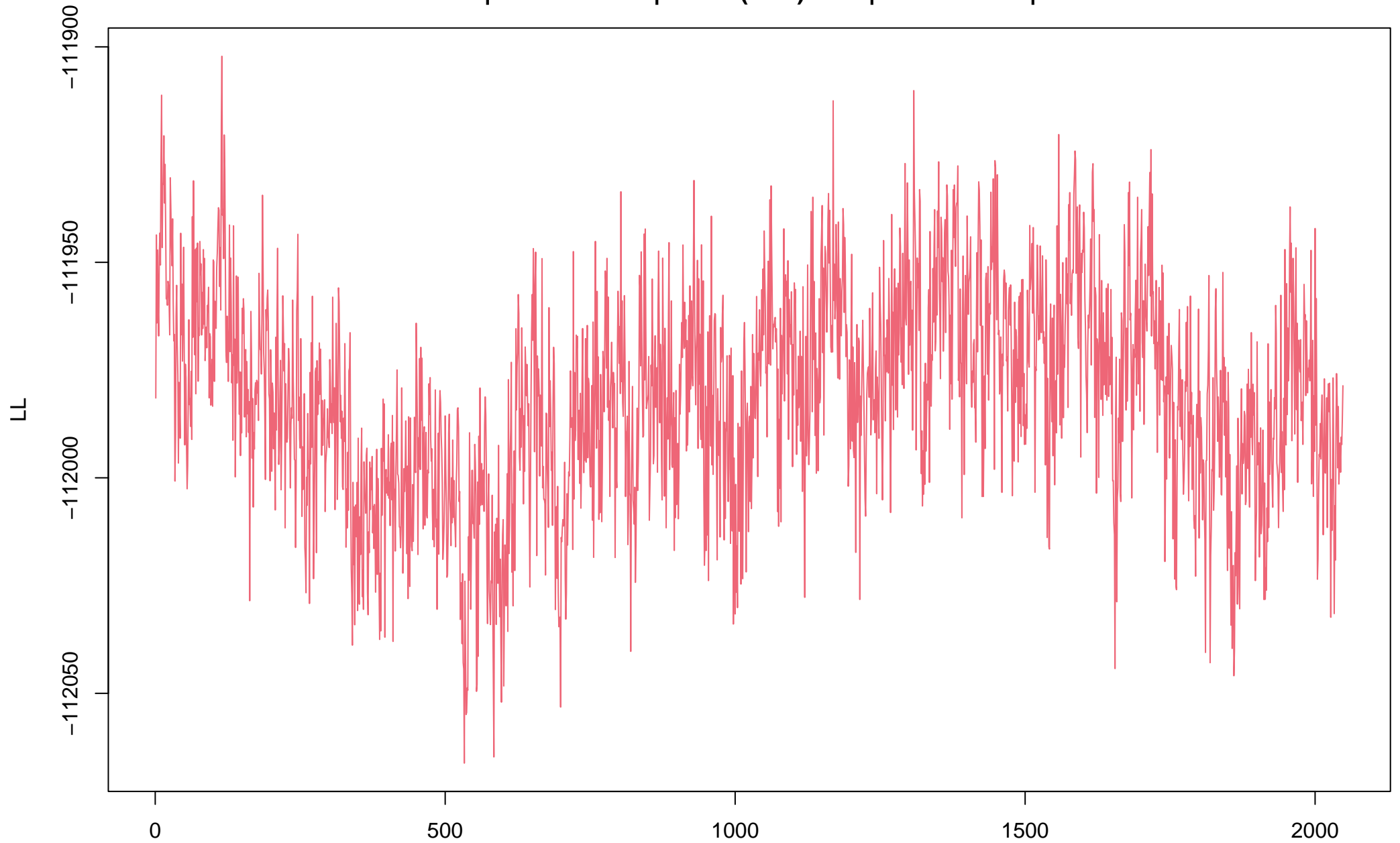




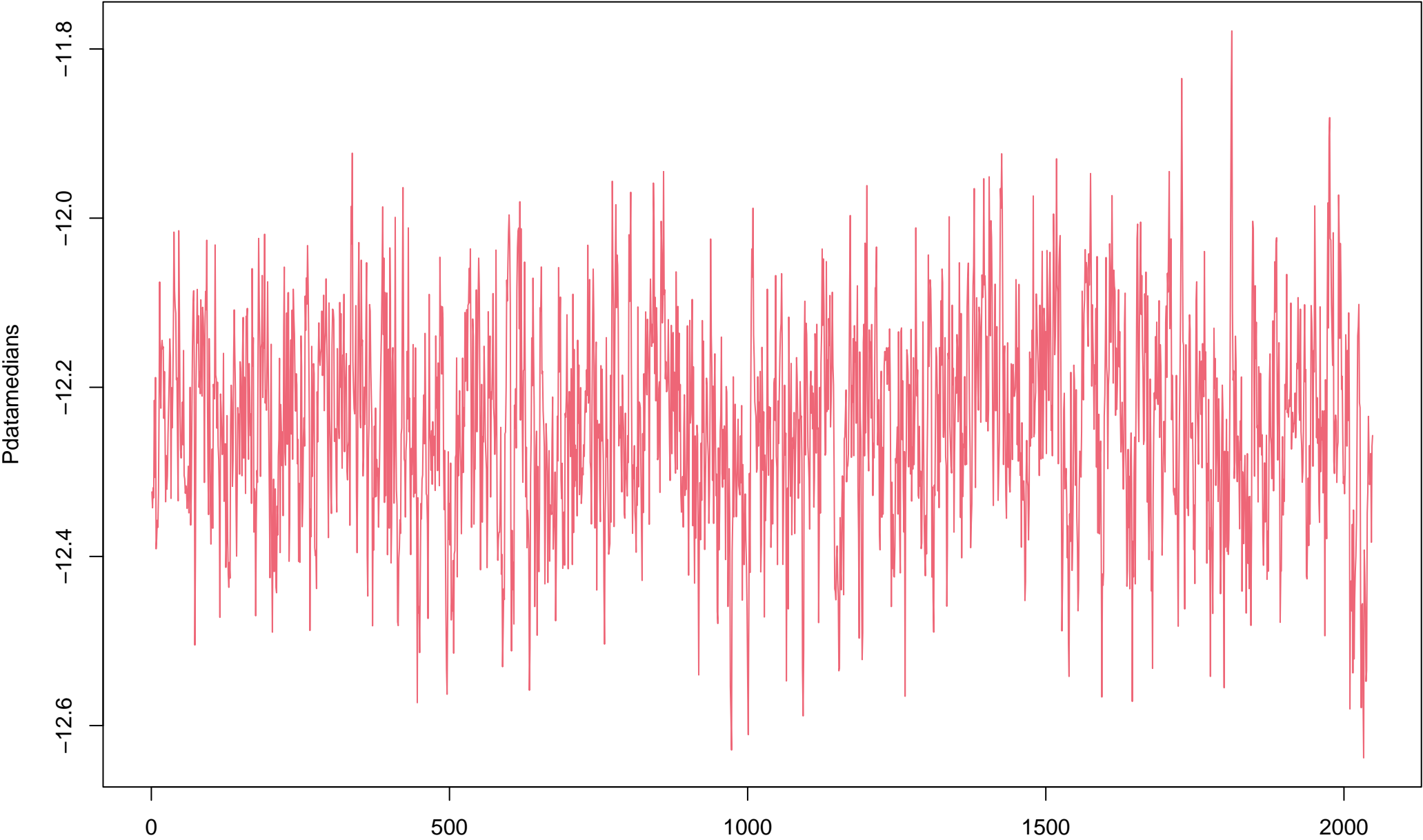




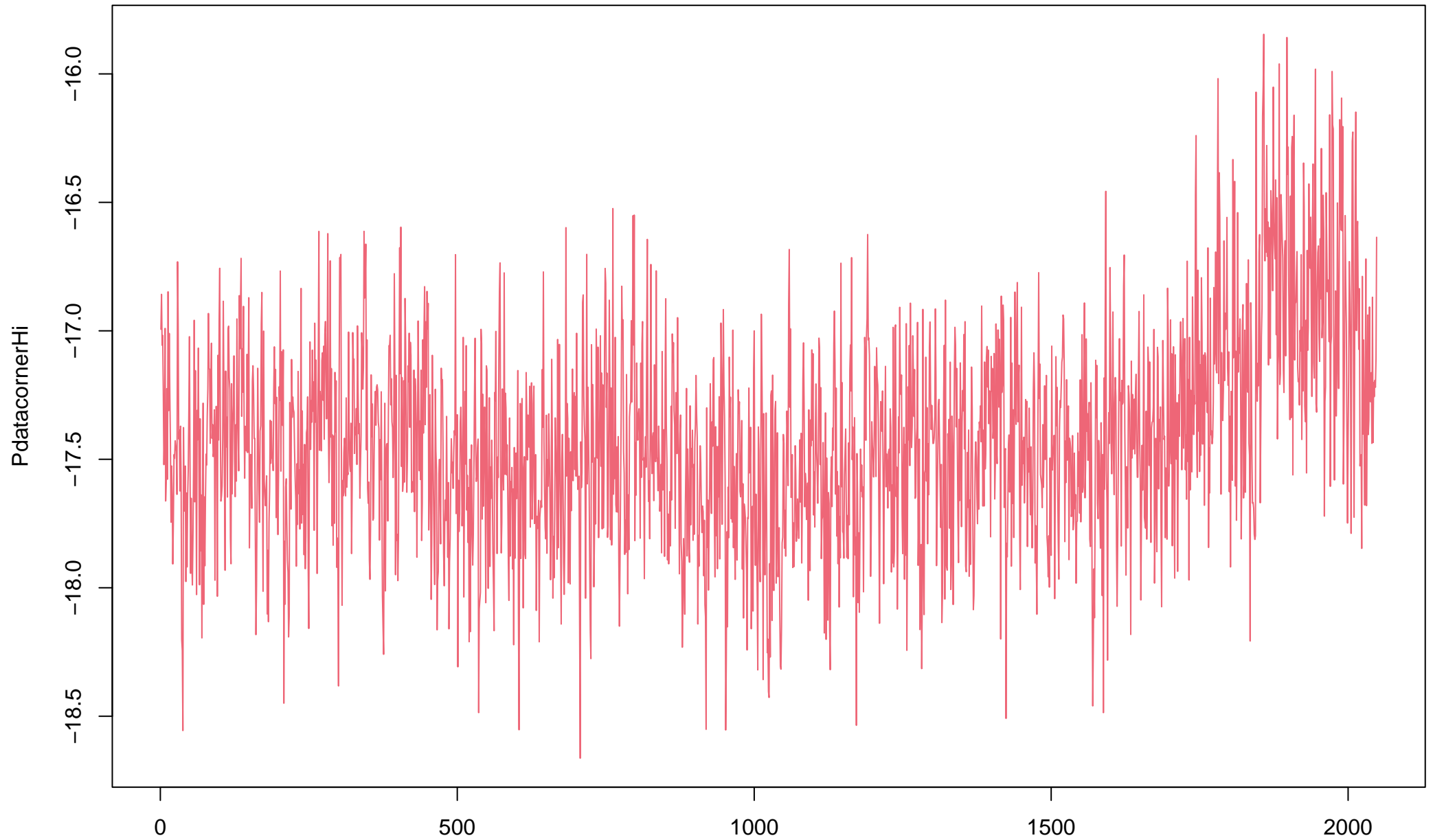
LL
ESS = 47 | BMK = 0.209 | MCSE(6.27) = 10 | stat: FALSE | burn: 0



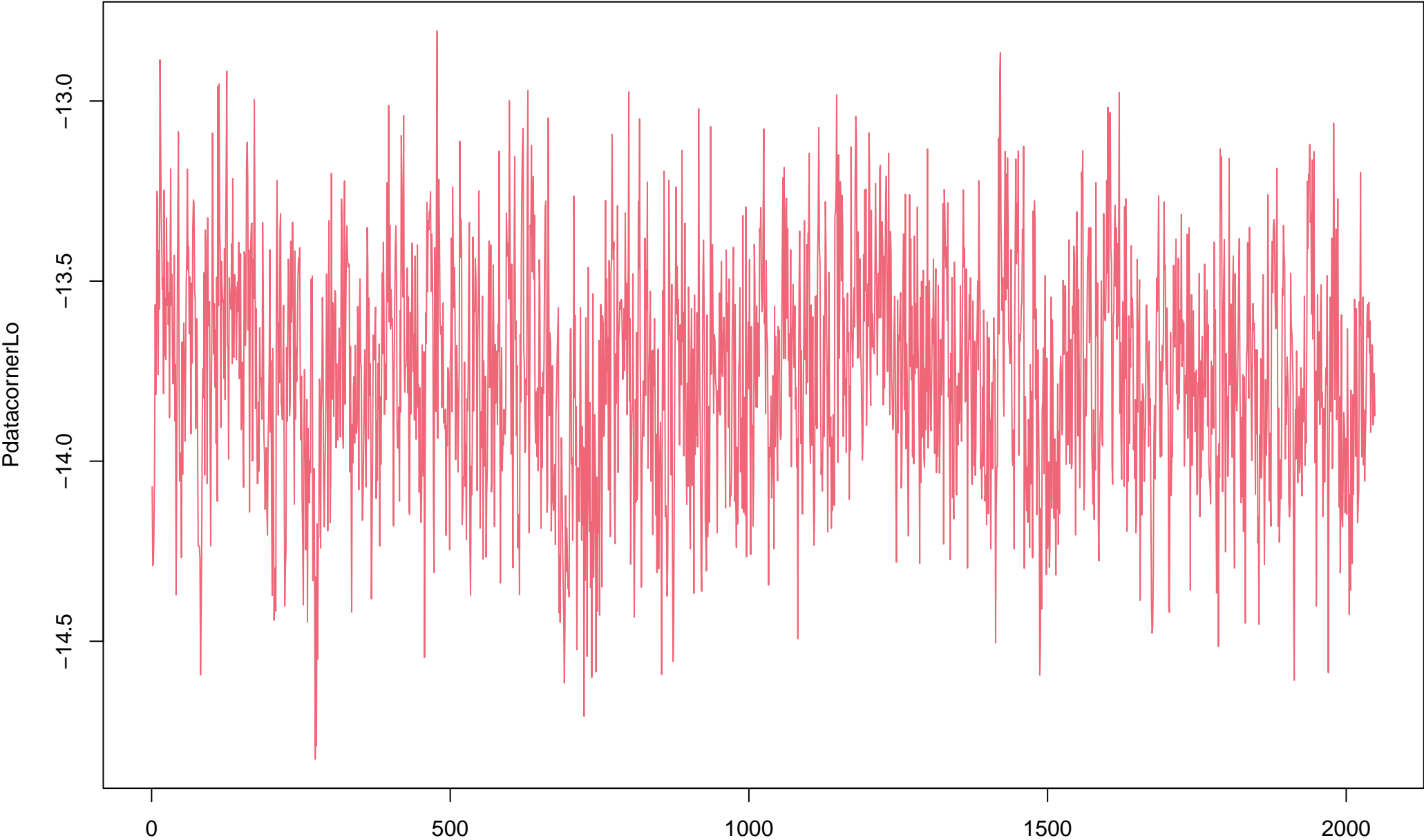
Pdatamedians
ESS = 406 | BMK = 0.0626 | MCSE(6.27) = 4.16 | stat: TRUE | burn: 0



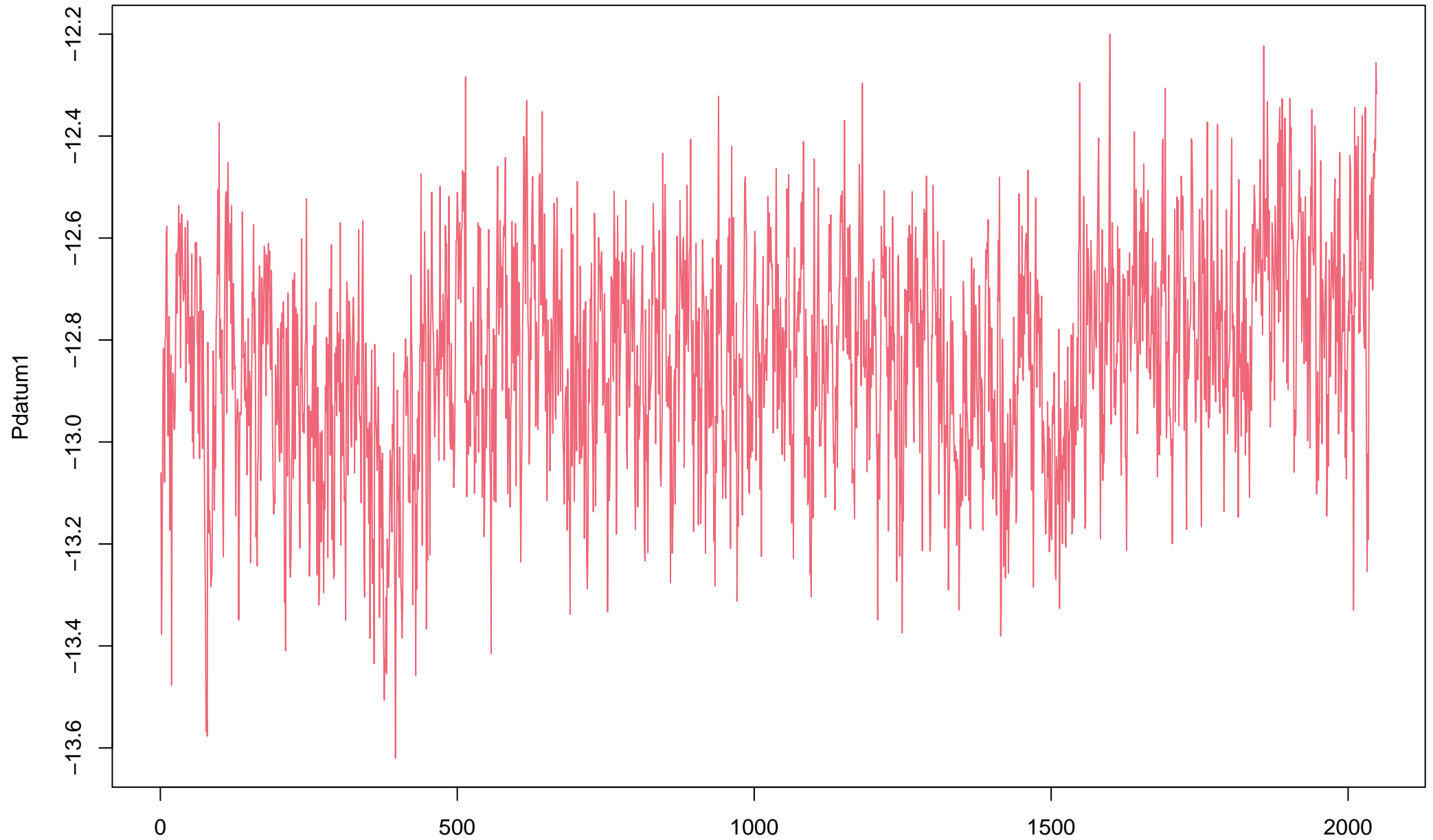
PdatacornerHi
ESS = 2.22e-16 | BMK = 0.182 | MCSE(6.27) = 8.49 | stat: FALSE | burn: 0



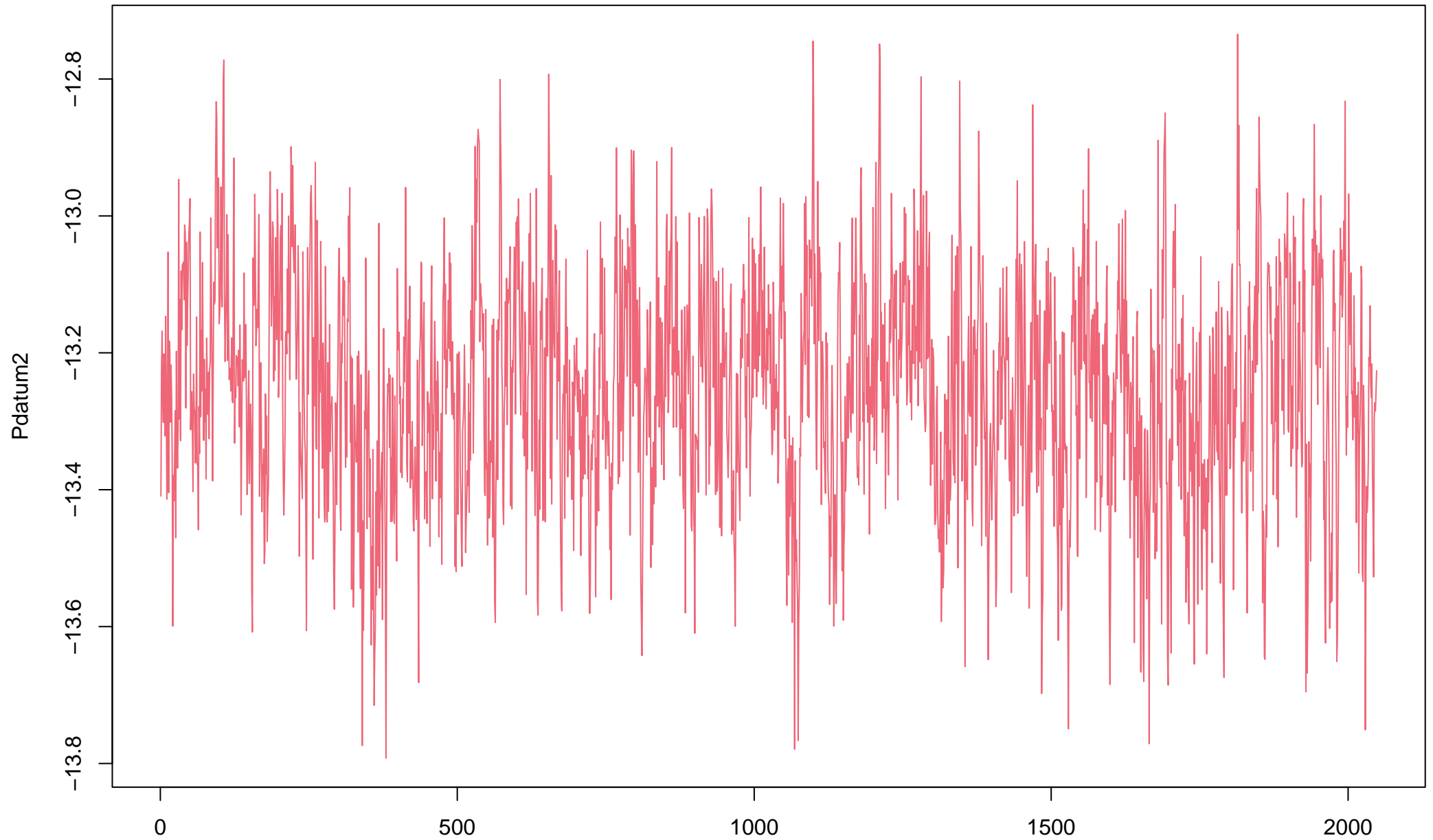
PdatacornerLo
ESS = 409 | BMK = 0.0711 | MCSE(6.27) = 4.82 | stat: TRUE | burn: 0



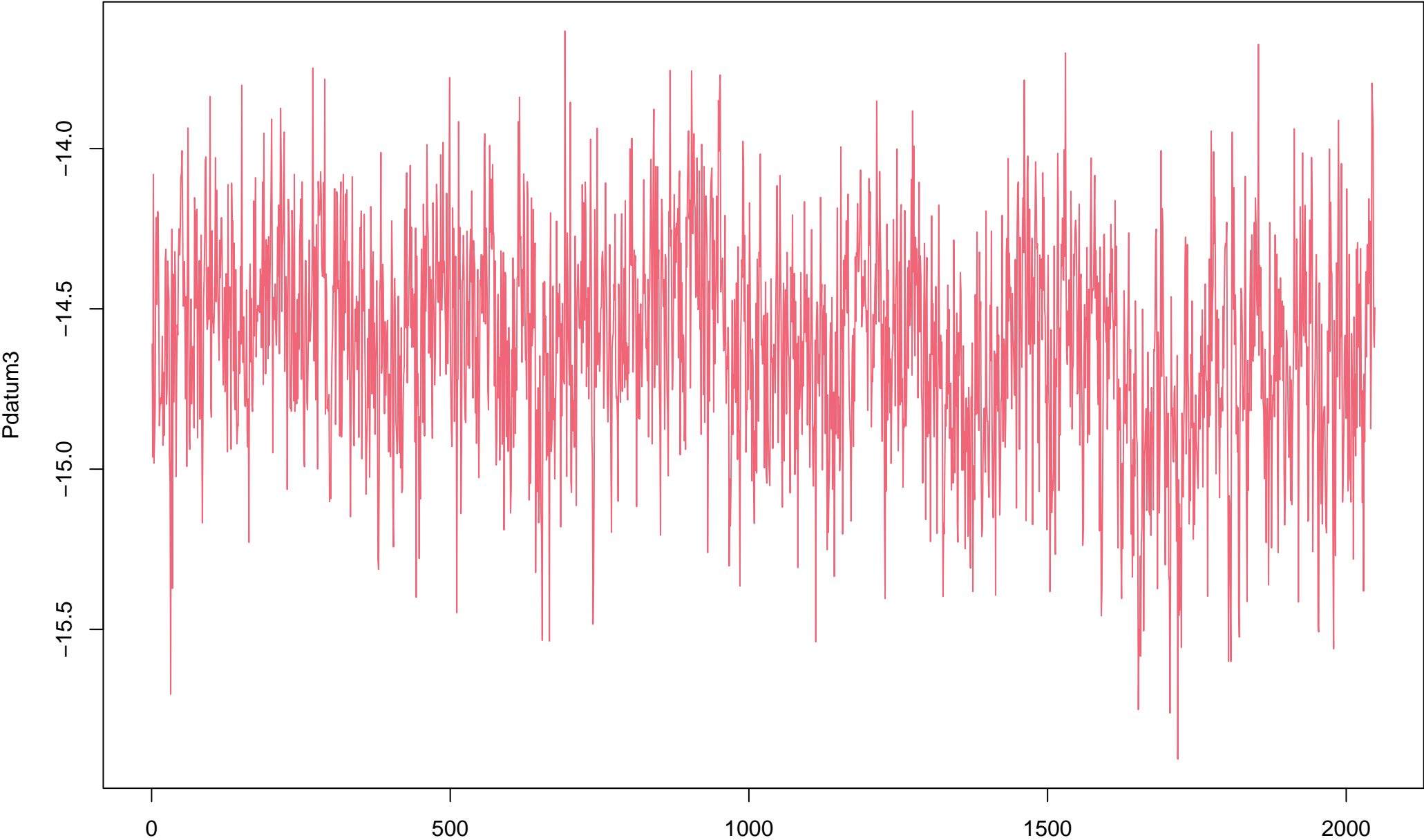
Pdatum1
ESS = 118 | BMK = 0.127 | MCSE(6.27) = 6.78 | stat: TRUE | burn: 0



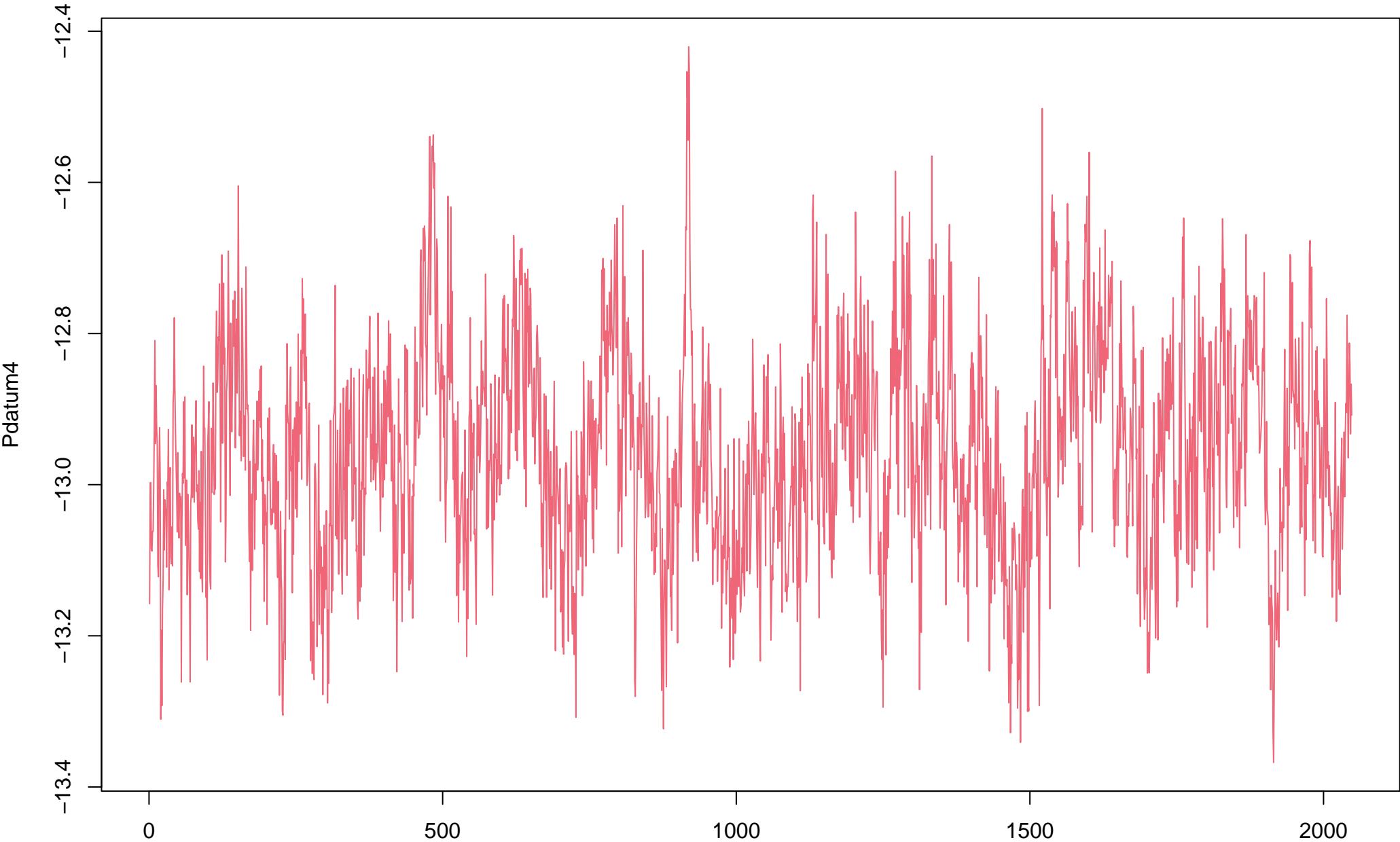
Pdatum2
ESS = 400 | BMK = 0.069 | MCSE(6.27) = 5.5 | stat: FALSE | burn: 0



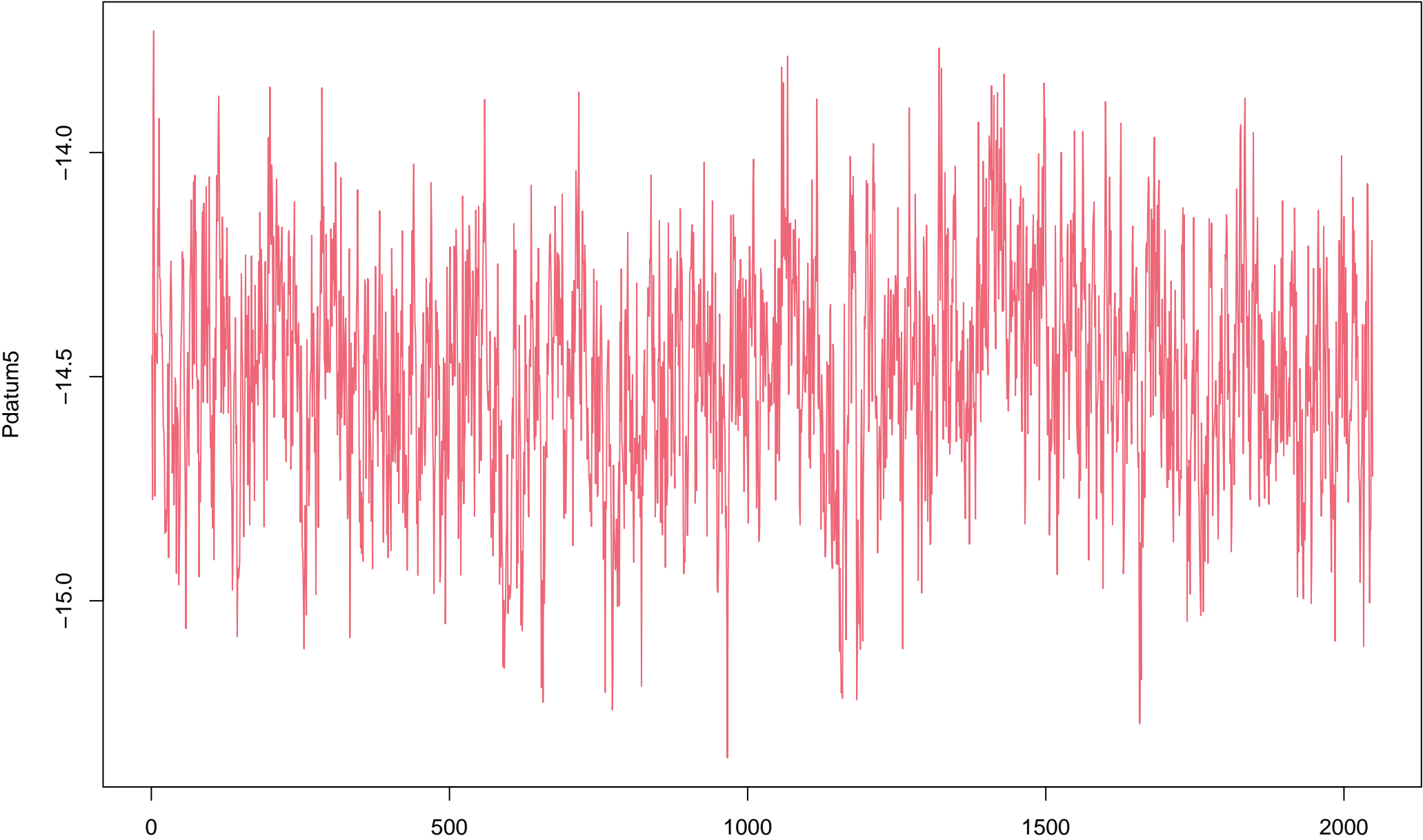
Pdatum3
ESS = 295 | BMK = 0.152 | MCSE(6.27) = 5.72 | stat: FALSE | burn: 0



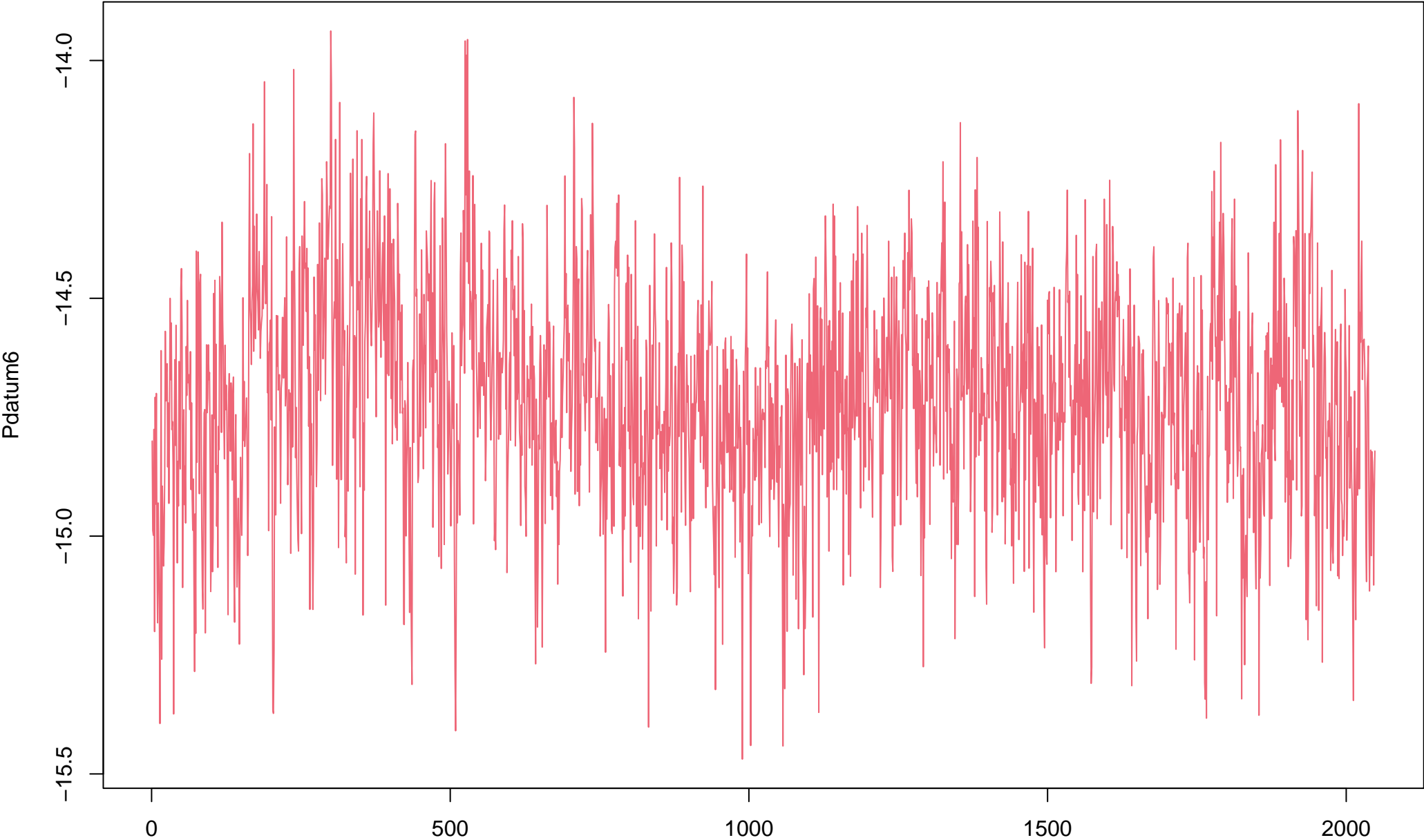
Pdatum4
ESS = 121 | BMK = 0.0694 | MCSE(6.27) = 8.28 | stat: TRUE | burn: 0



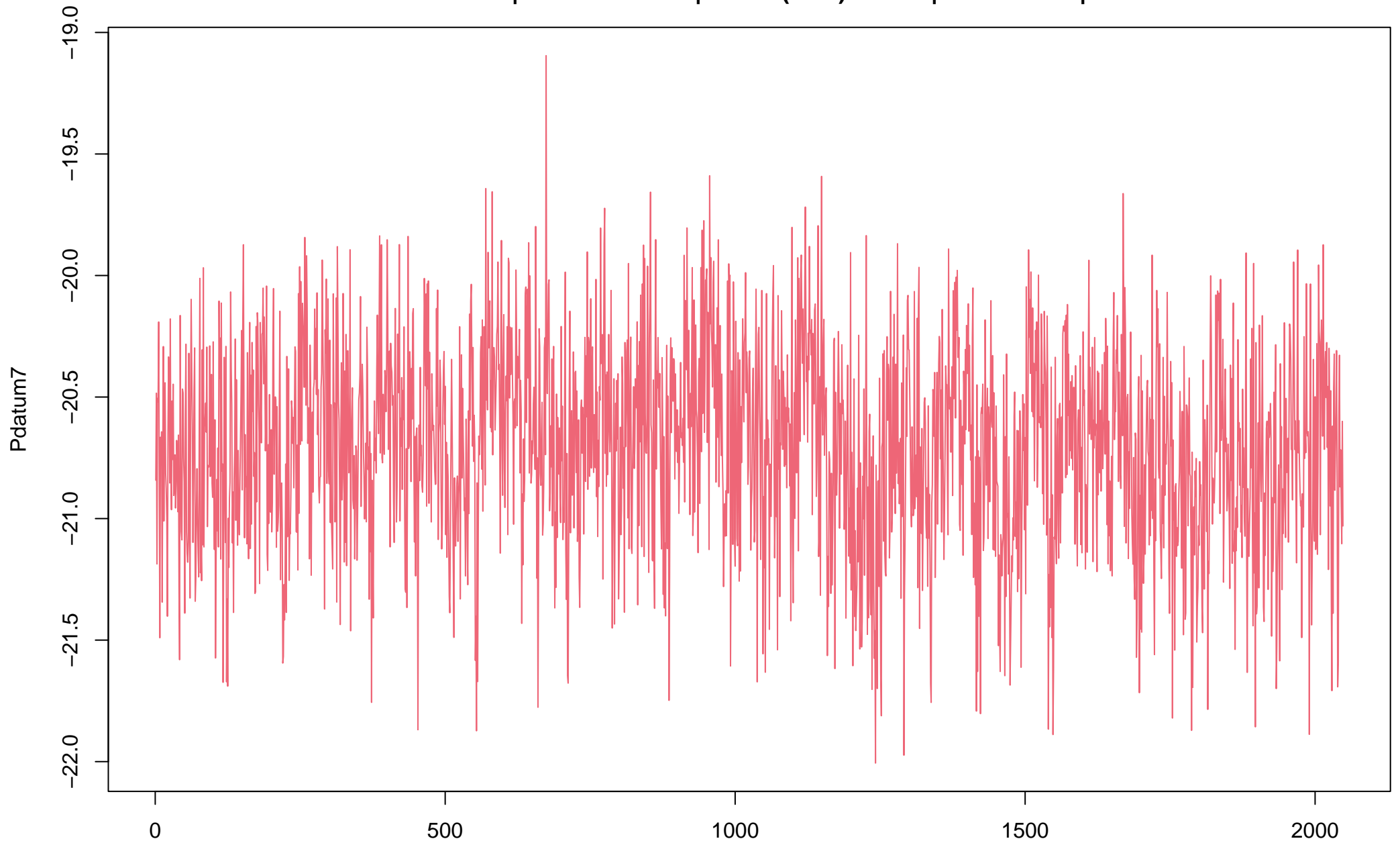
Pdatum5
ESS = 358 | BMK = 0.0914 | MCSE(6.27) = 6.31 | stat: TRUE | burn: 0



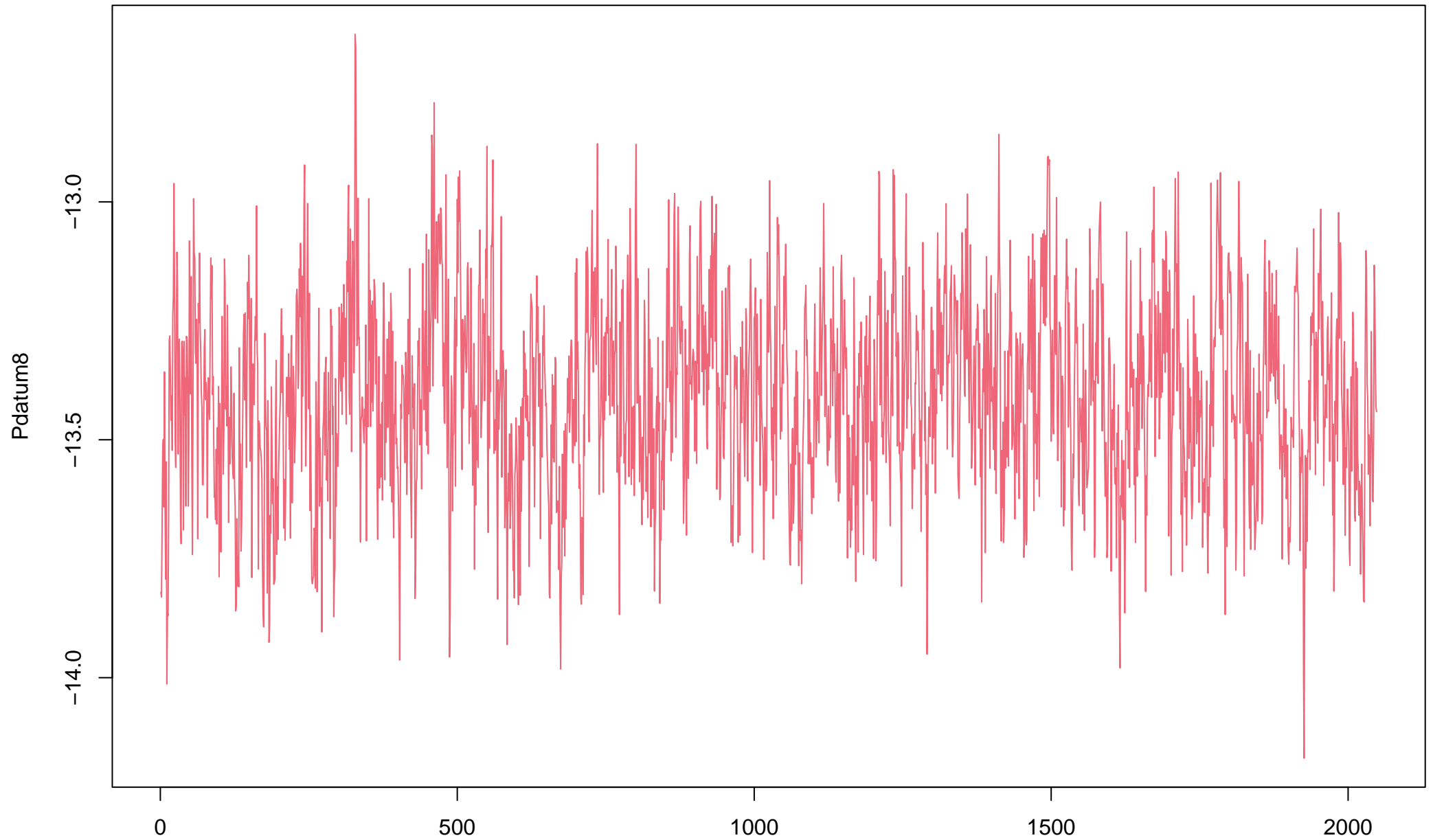
Pdatum6
ESS = 343 | BMK = 0.0711 | MCSE(6.27) = 5.29 | stat: TRUE | burn: 0



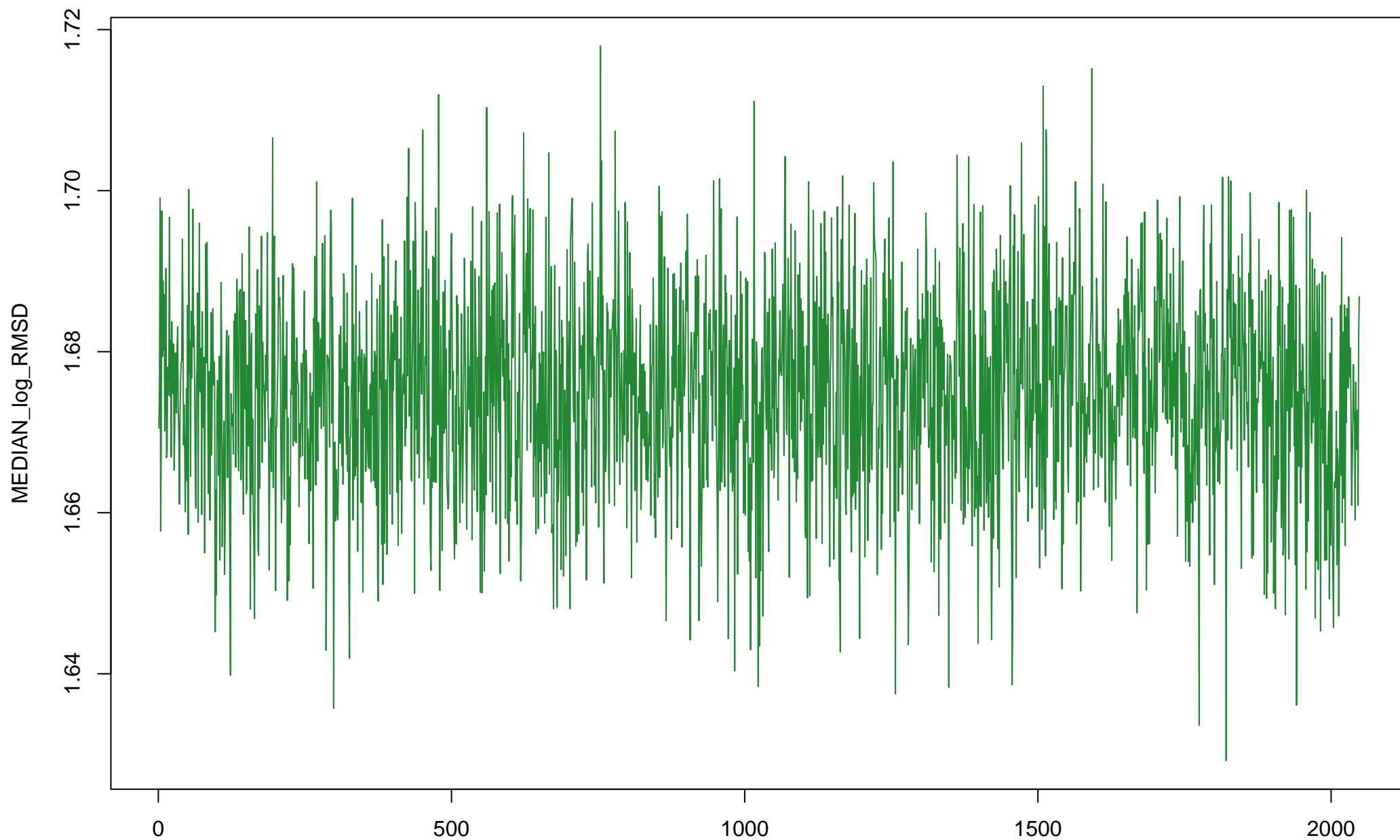
Pdatum7
ESS = 2.22e-16 | BMK = 0.0874 | MCSE(6.27) = 4.73 | stat: TRUE | burn: 0



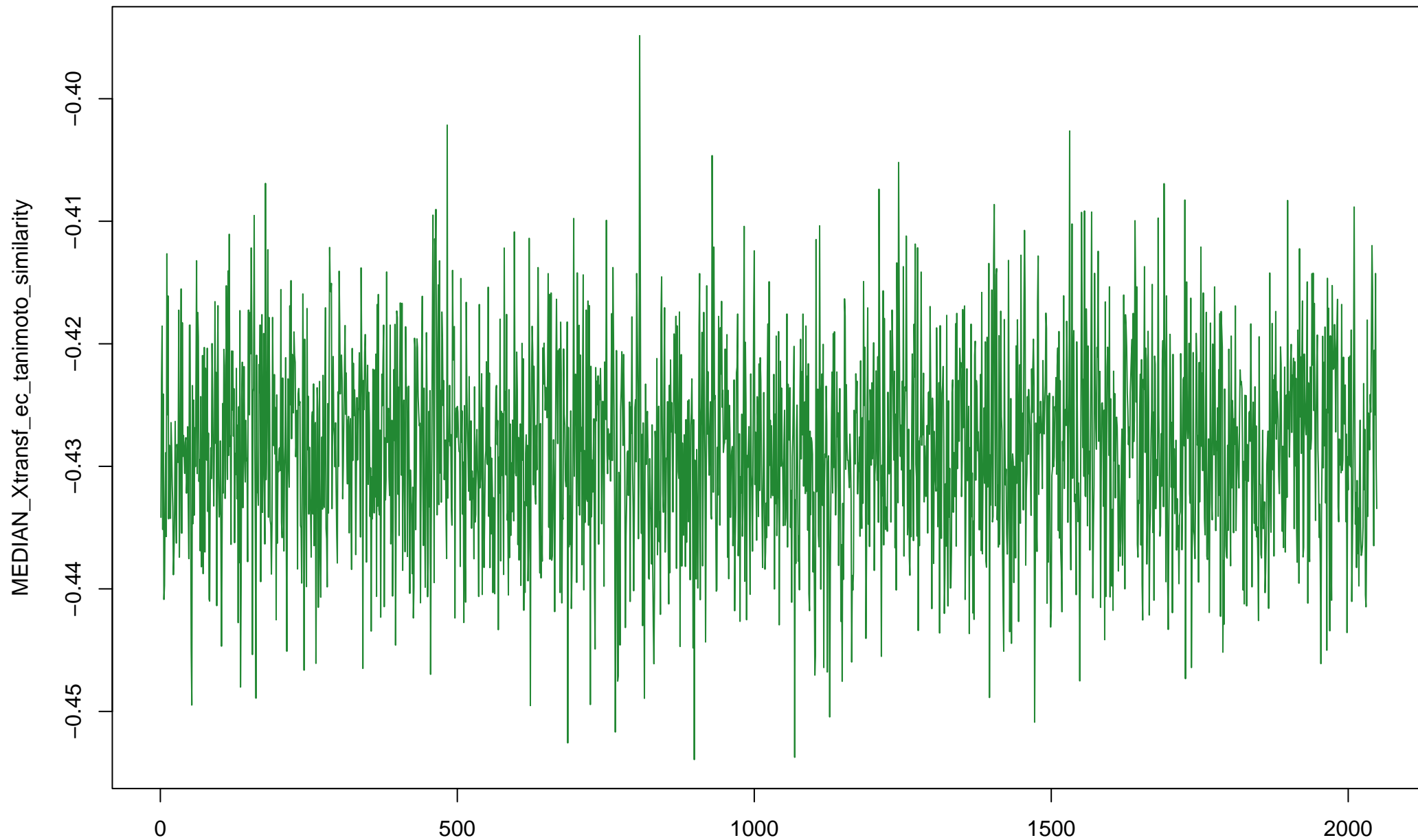
Pdatum8
ESS = 403 | BMK = 0.0614 | MCSE(6.27) = 5.25 | stat: FALSE | burn: 0



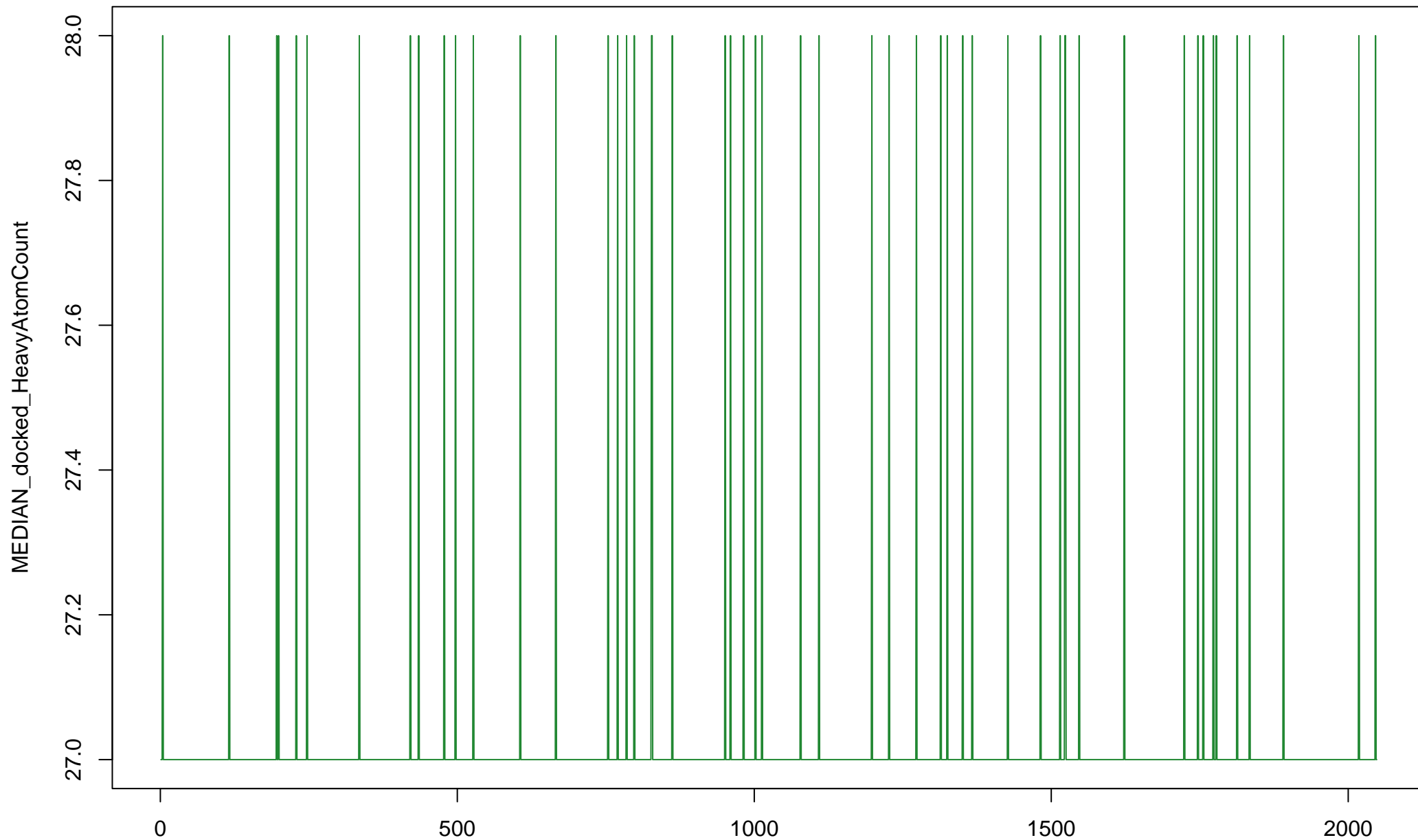
MEDIAN_log_RMSD
ESS = 1620 | BMK = 0.0383 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0



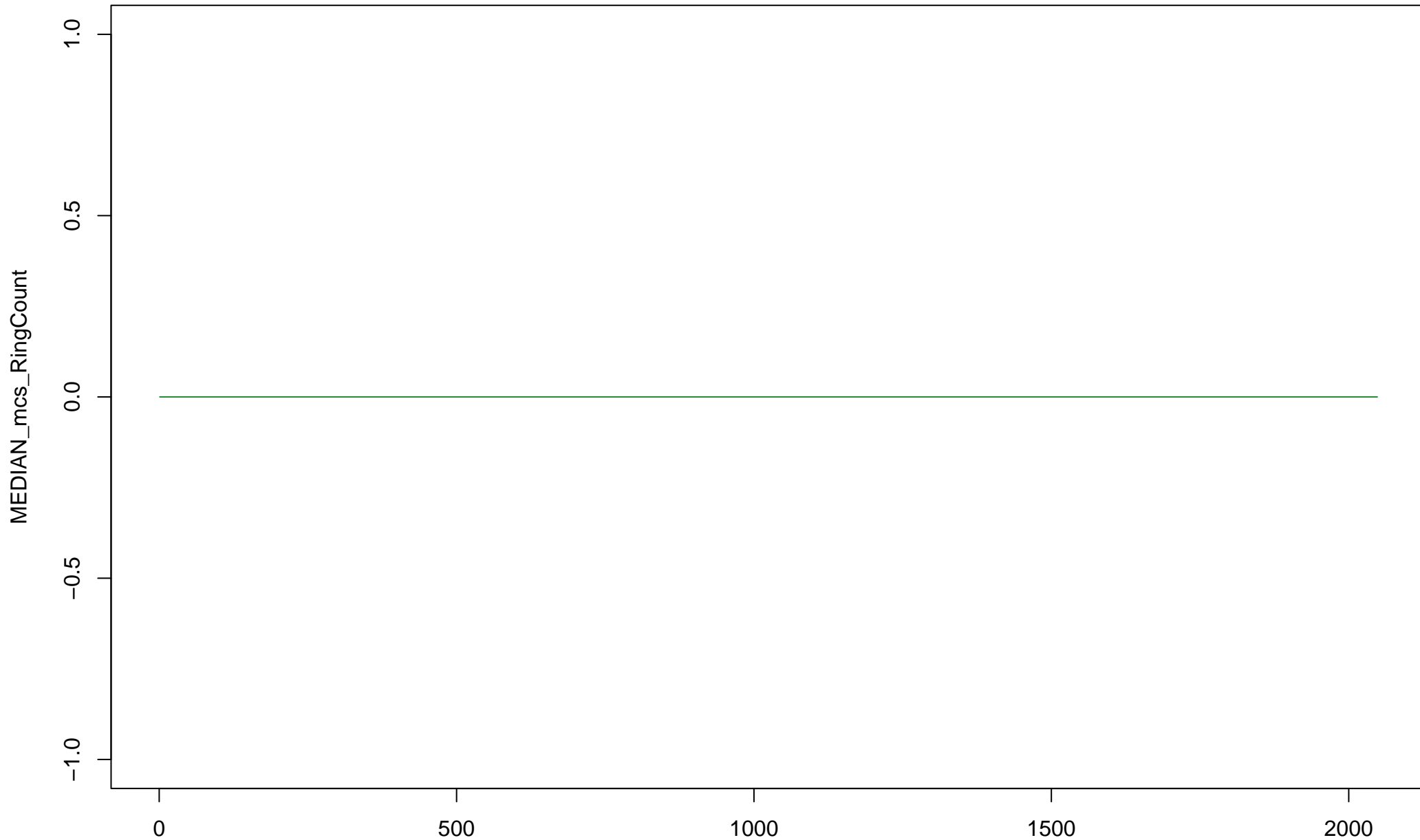
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1870 | BMK = 0.0327 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0



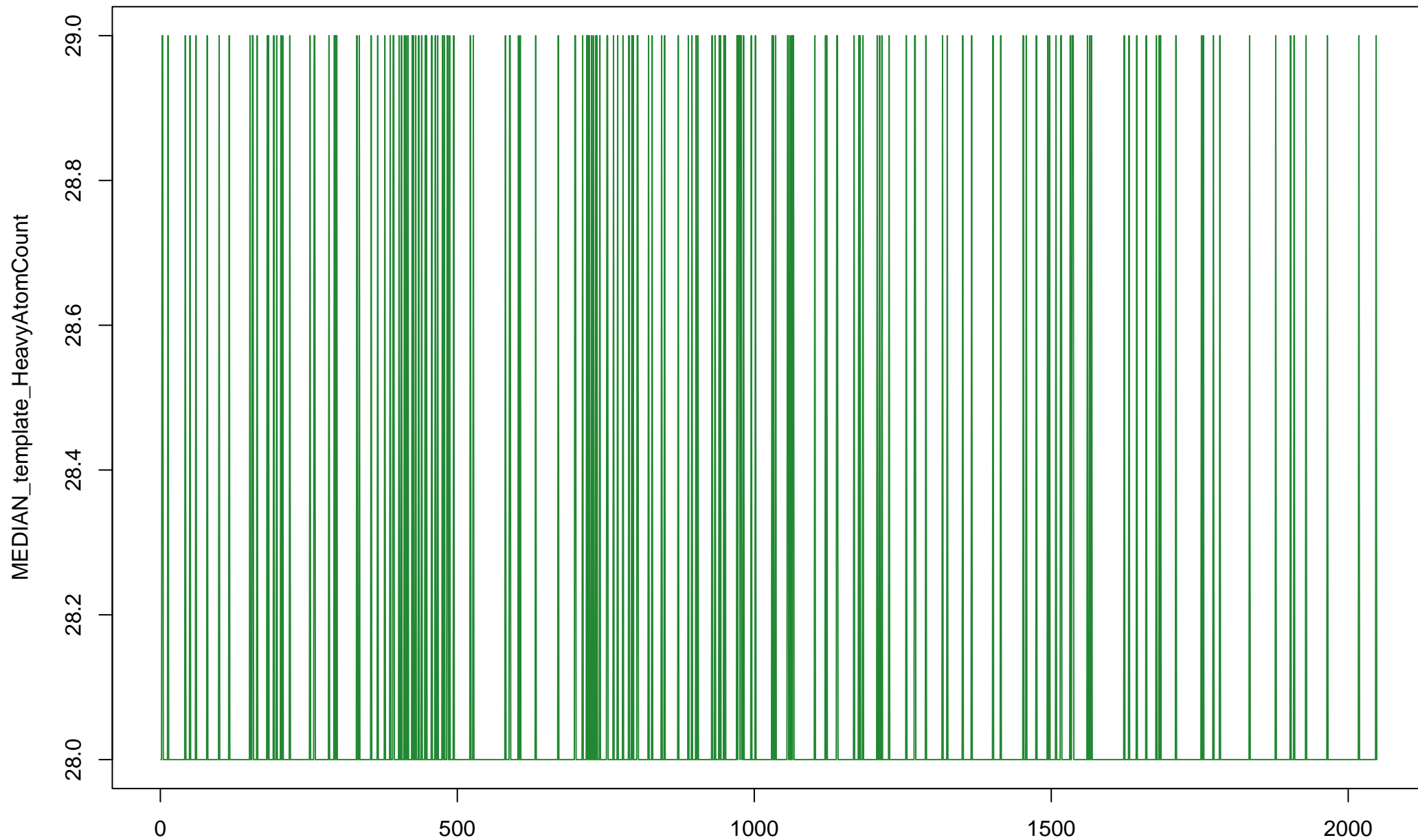
MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0



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



MEDIAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0875 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0



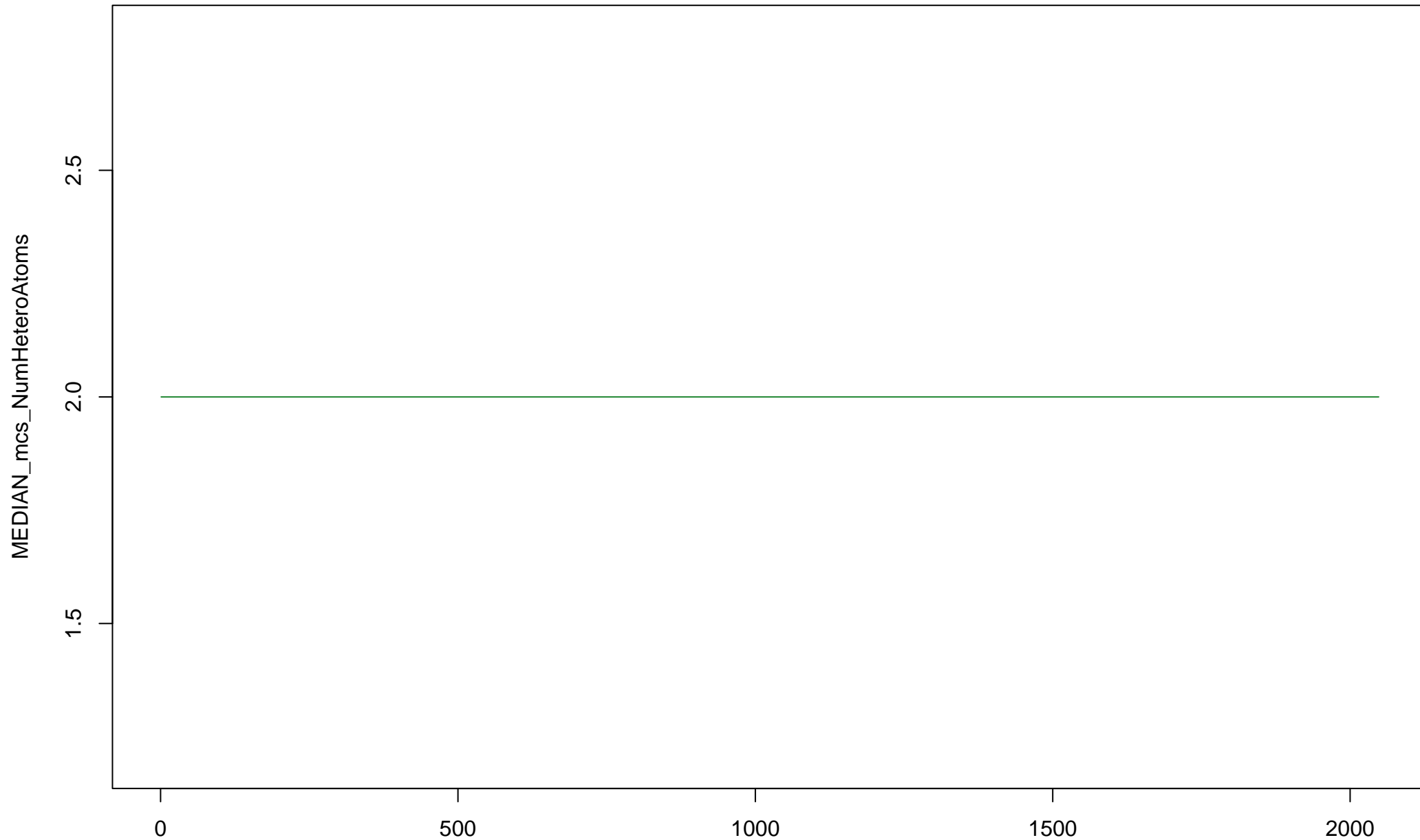
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



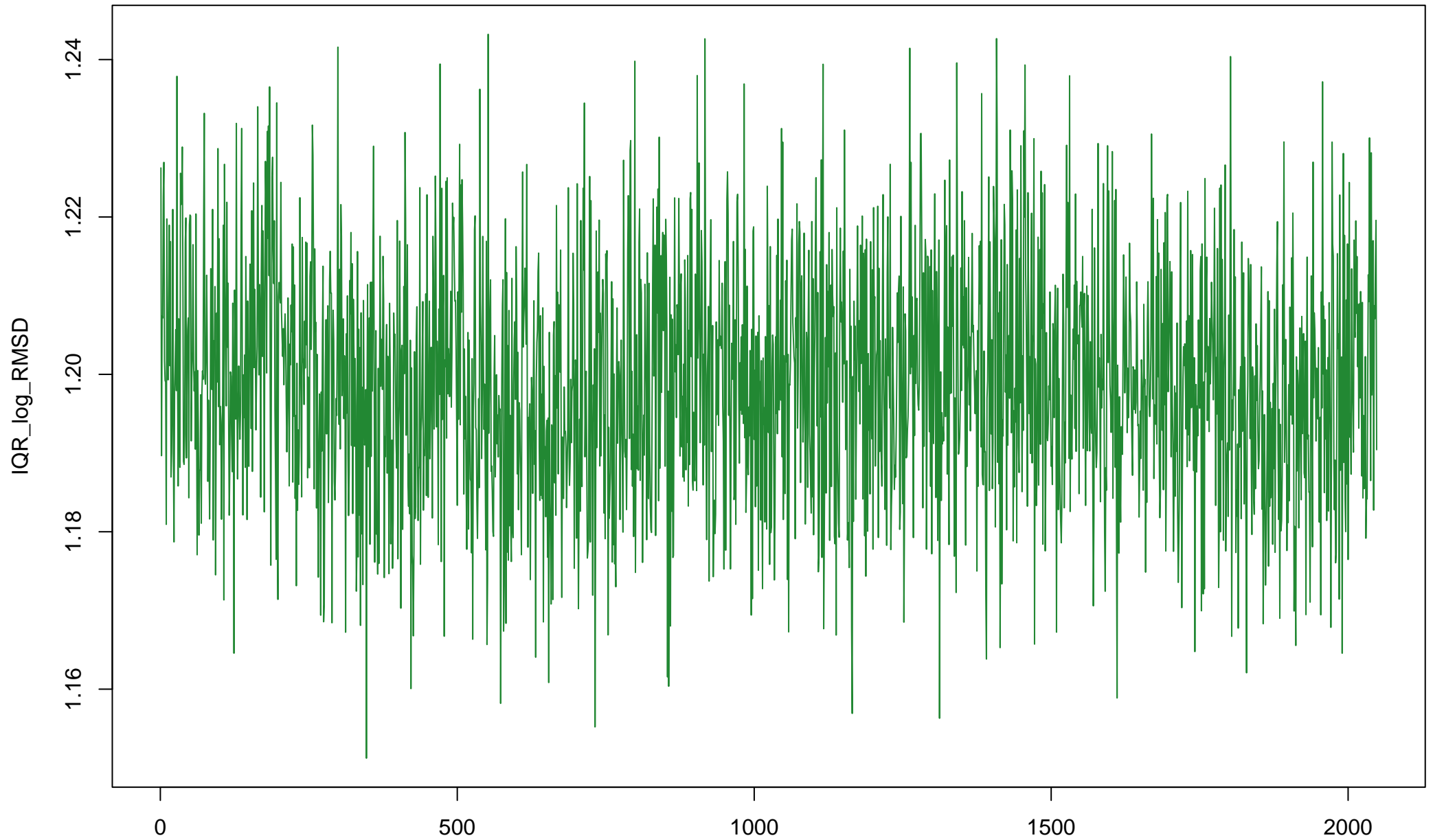
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



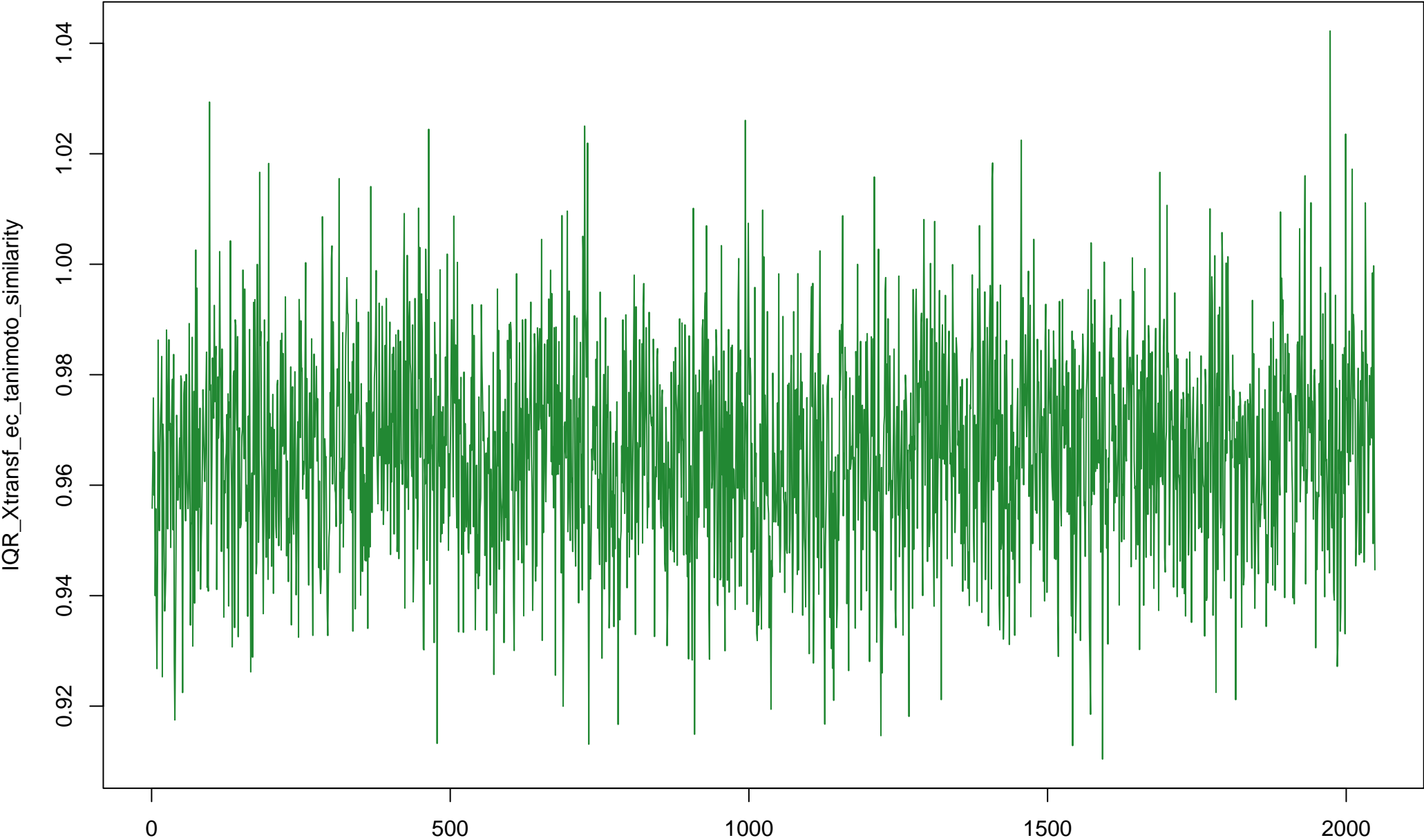
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



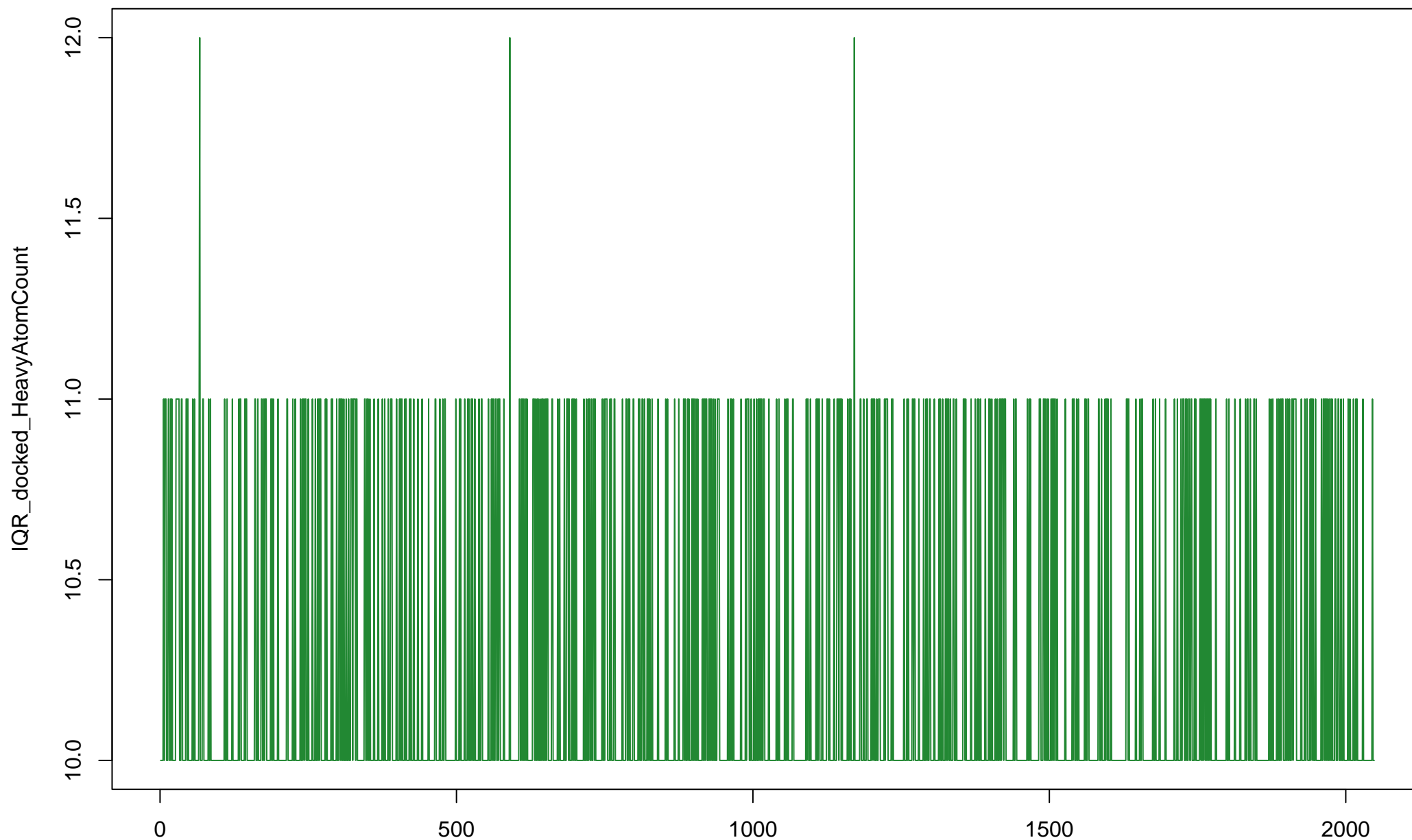
IQR_log_RMSD
ESS = 1440 | BMK = 0.0245 | MCSE(6.27) = 3.44 | stat: FALSE | burn: 0



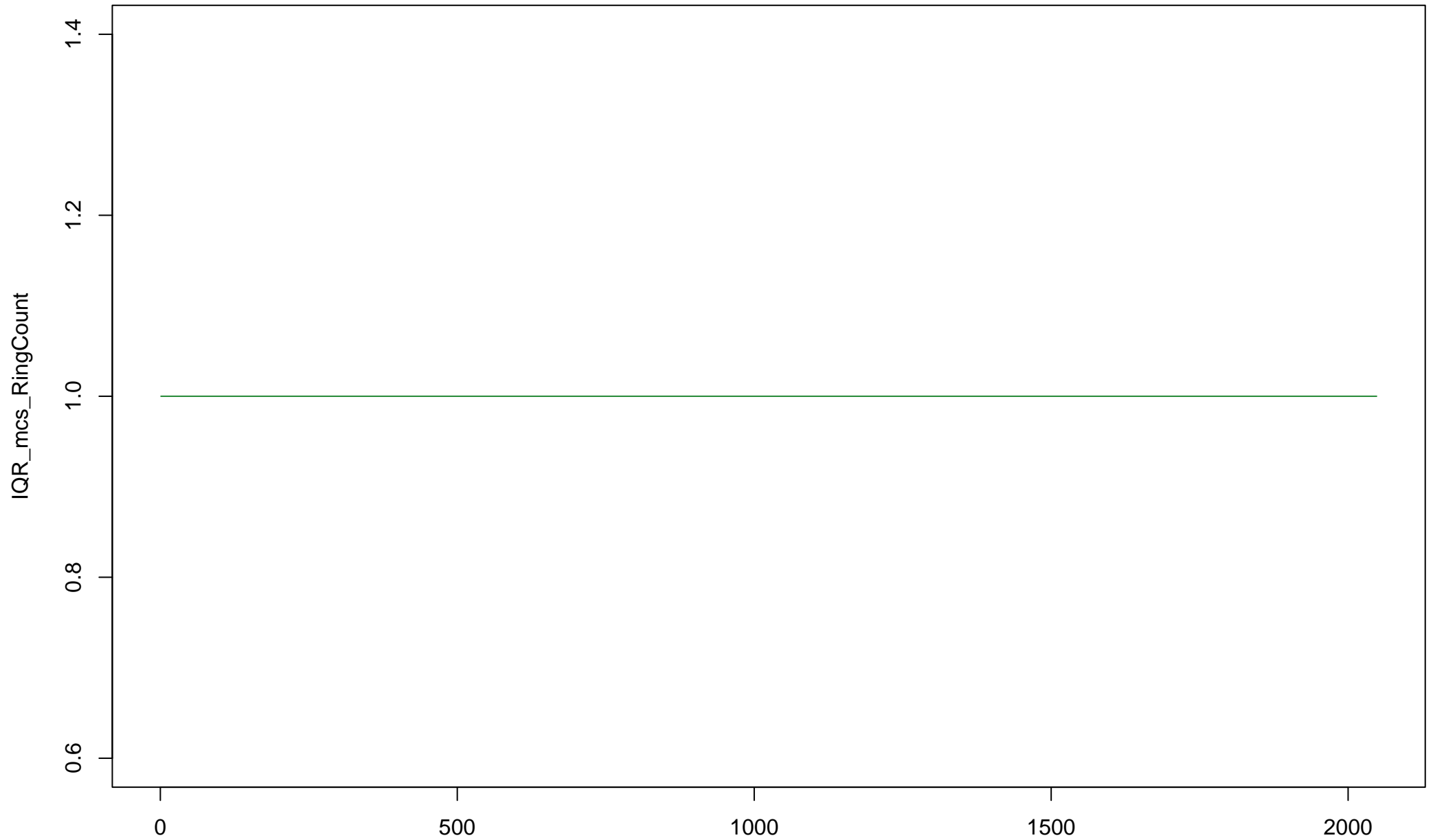
IQR_Xtransf_ec_tanimoto_similarity
ESS = 1720 | BMK = 0.035 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0



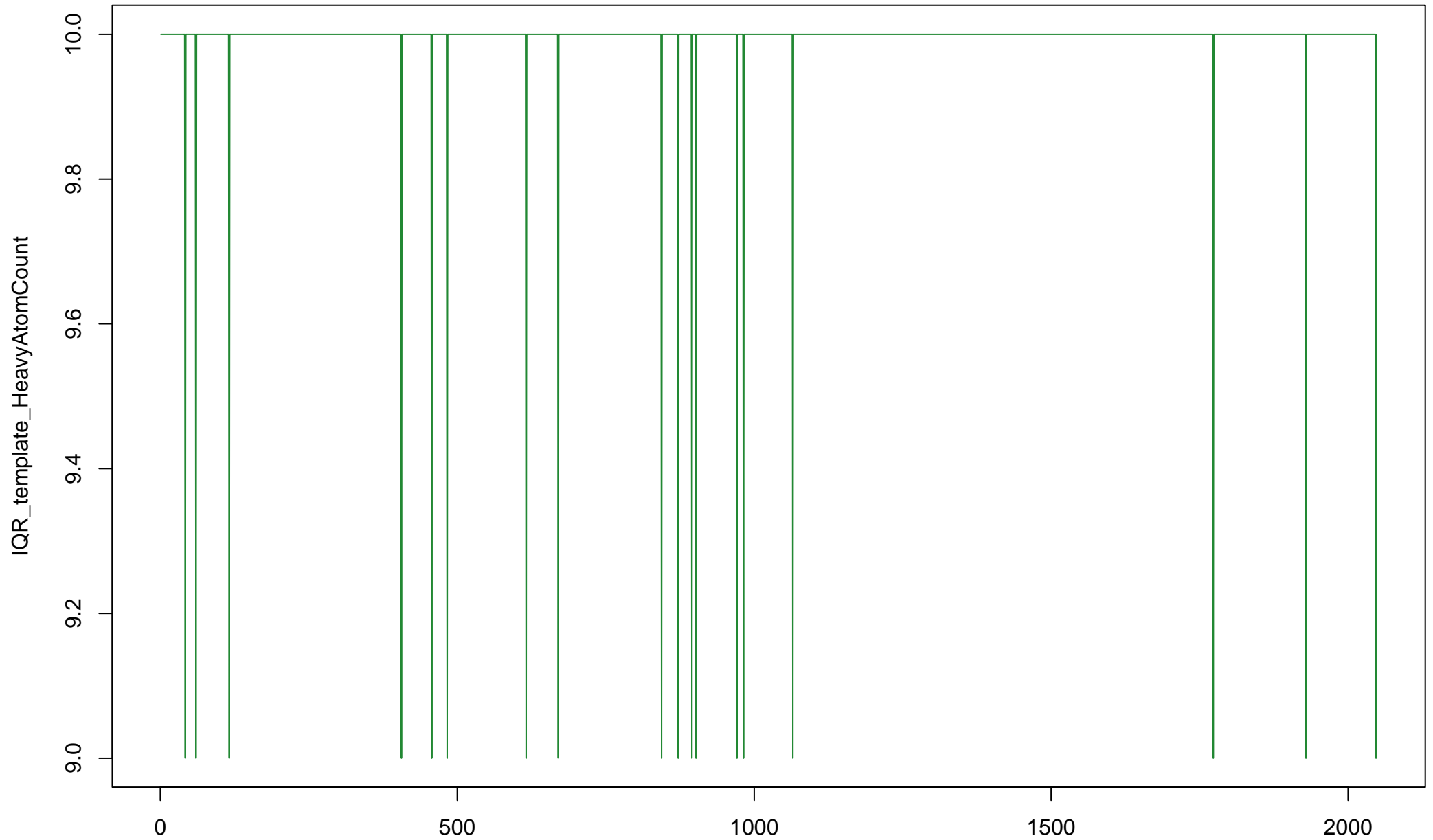
IQR_docked_HeavyAtomCount
ESS = 1740 | BMK = 0.0198 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0



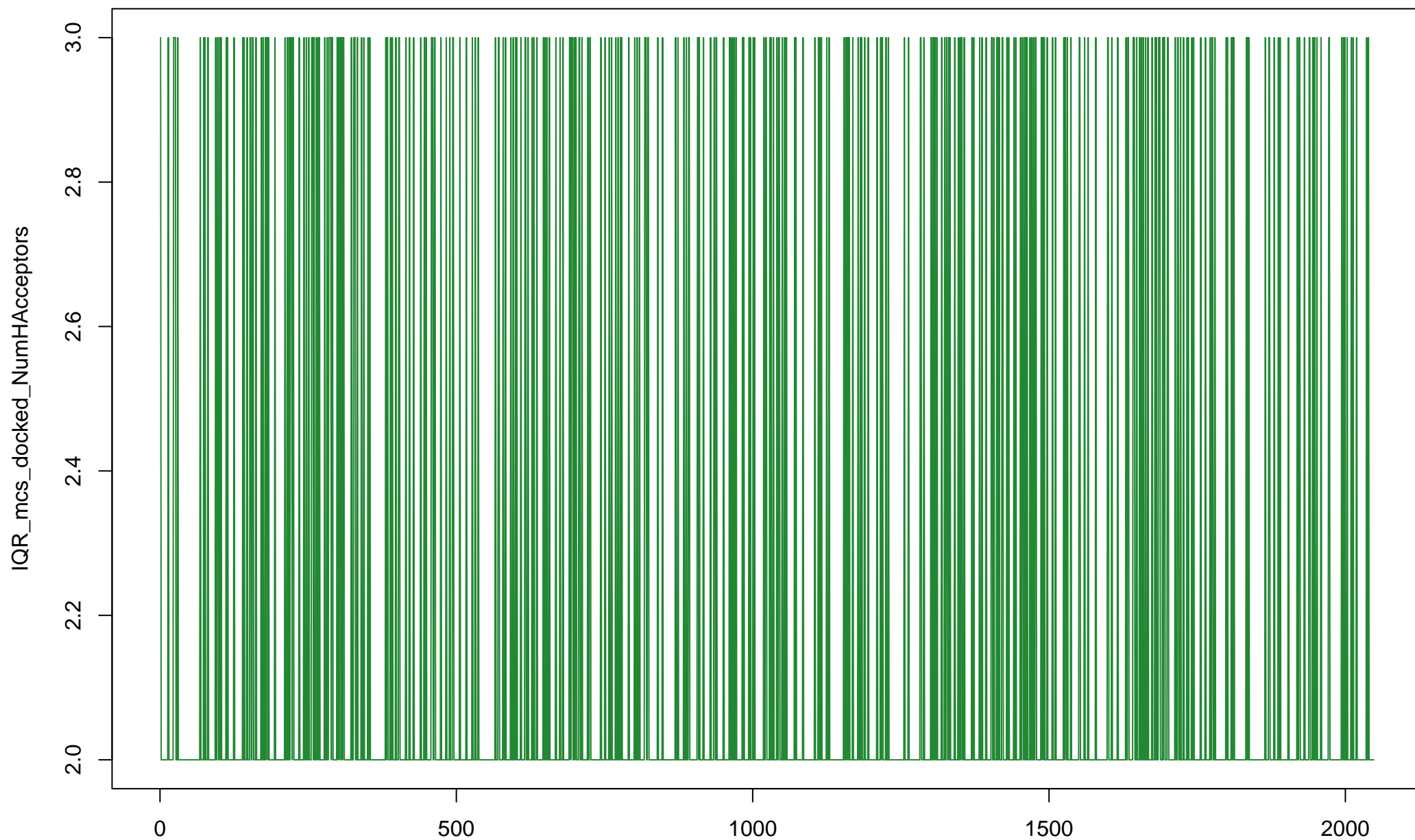
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



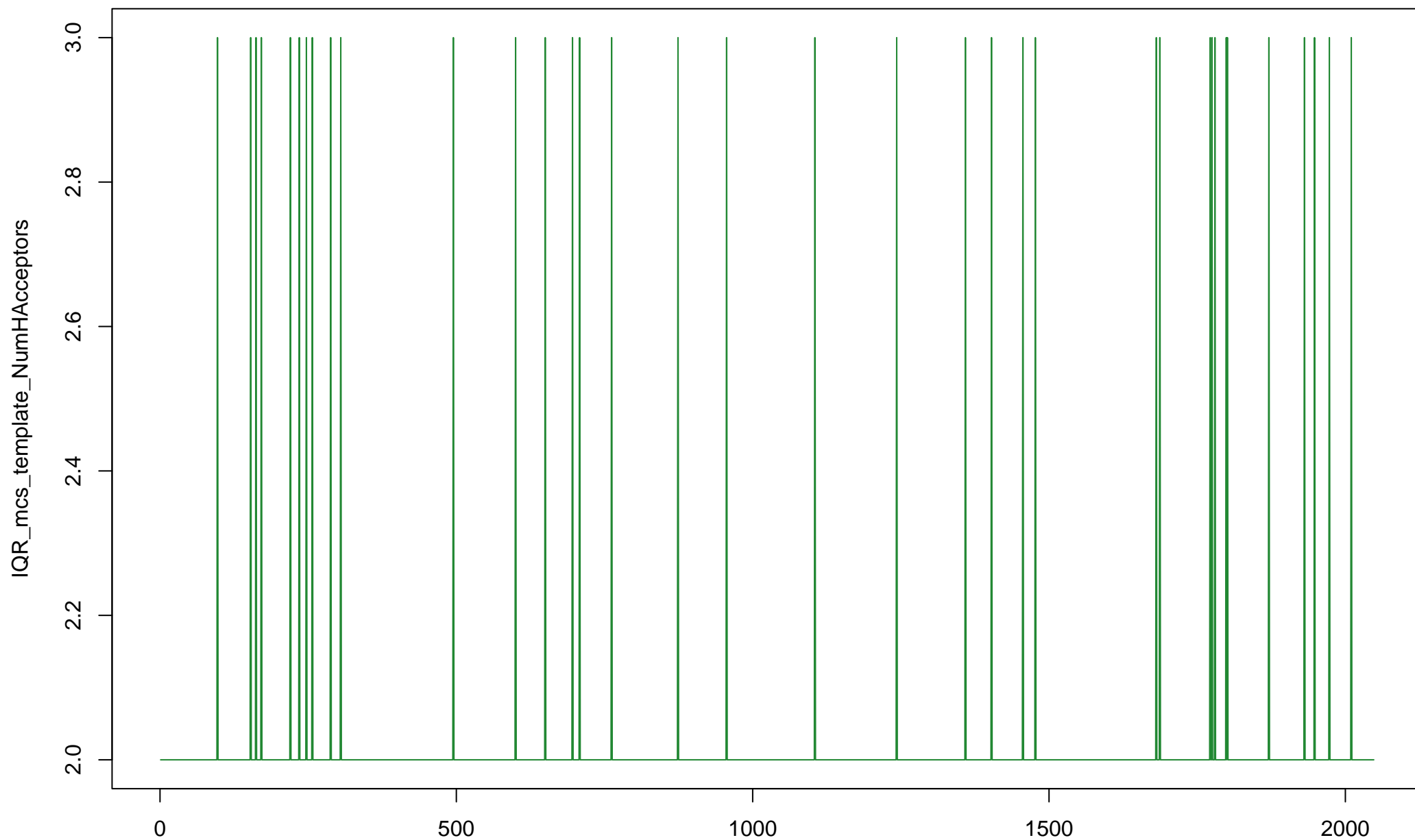
IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.211 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 1632



IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0117 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



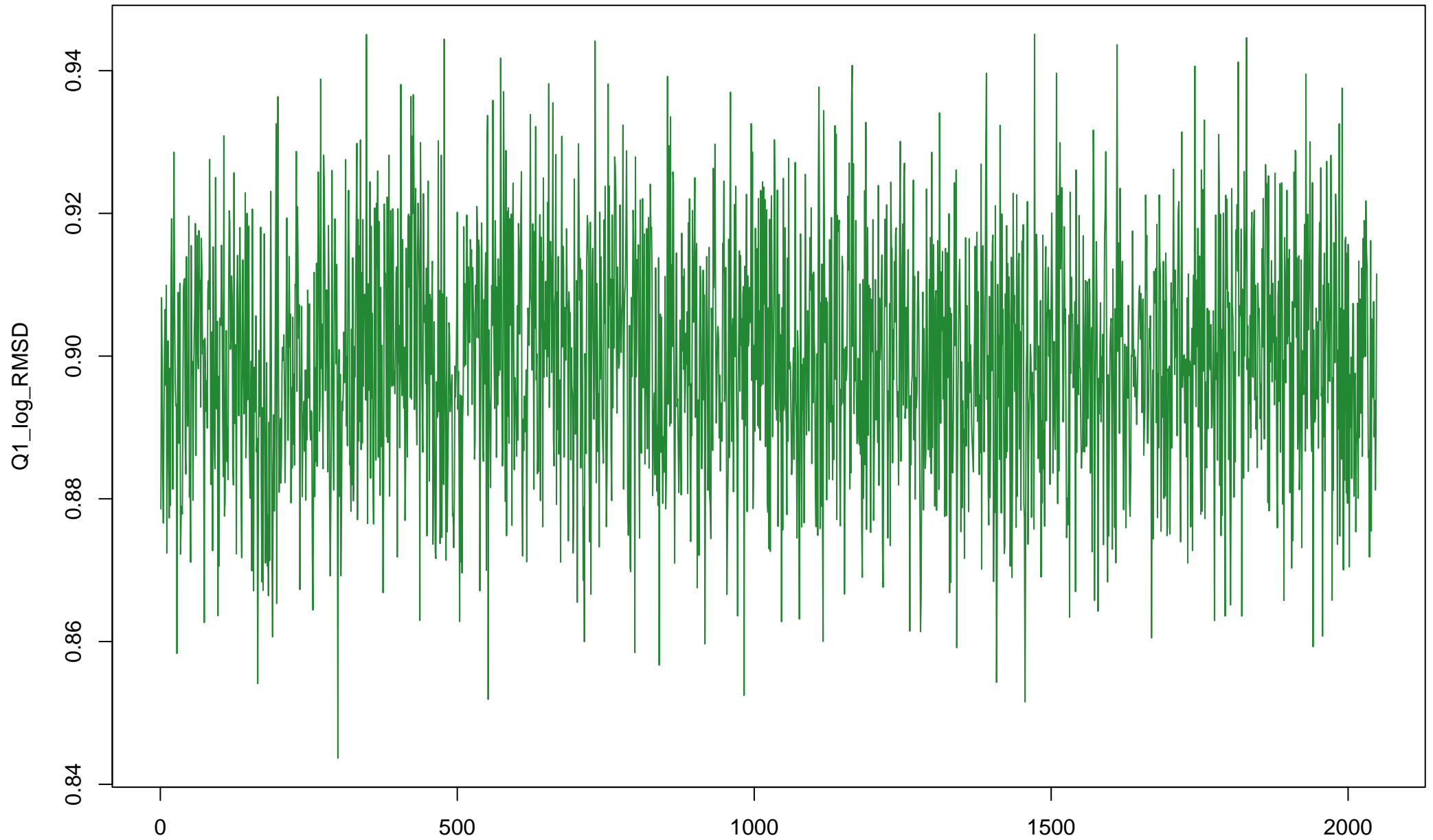
IQR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



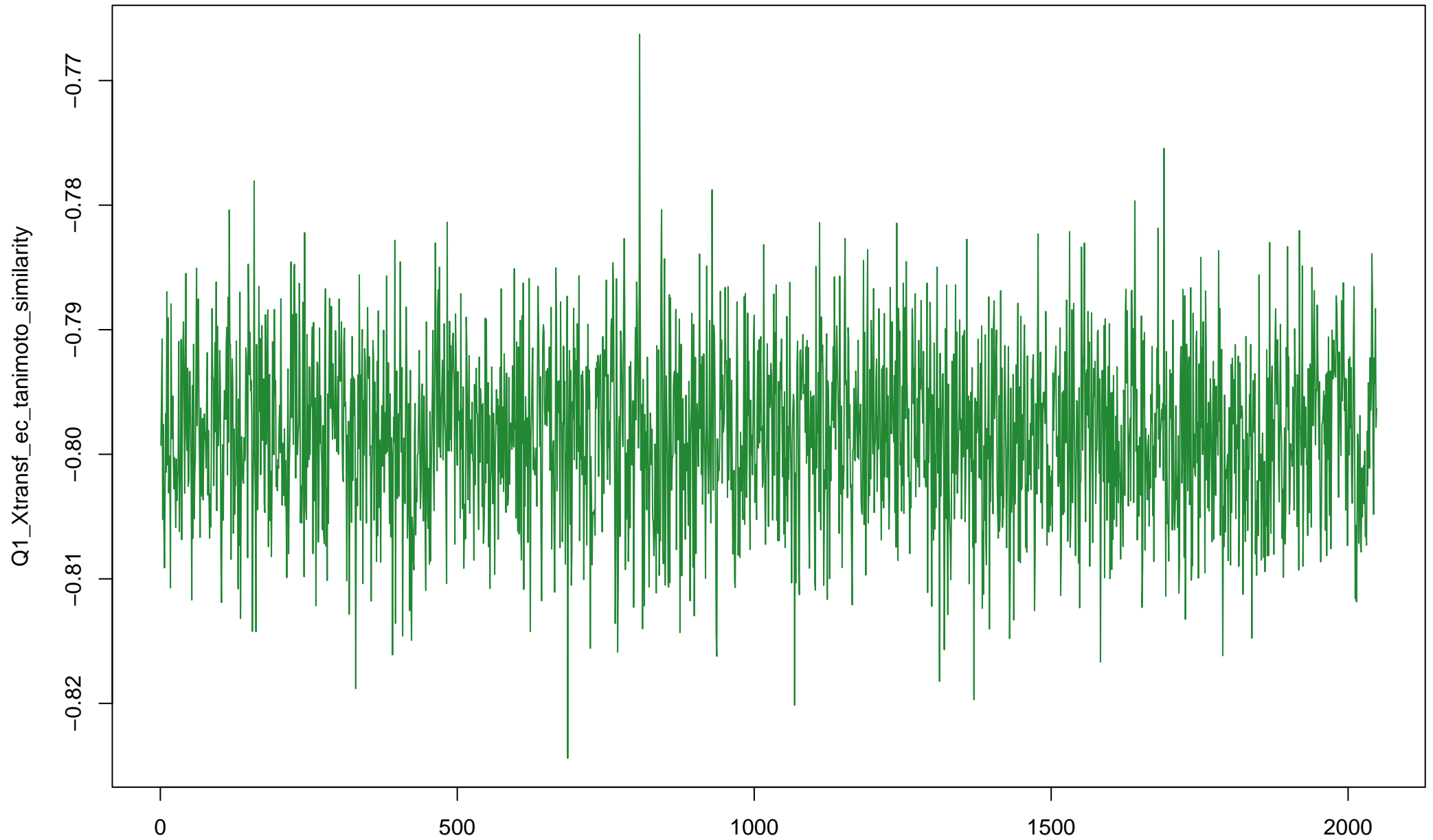
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



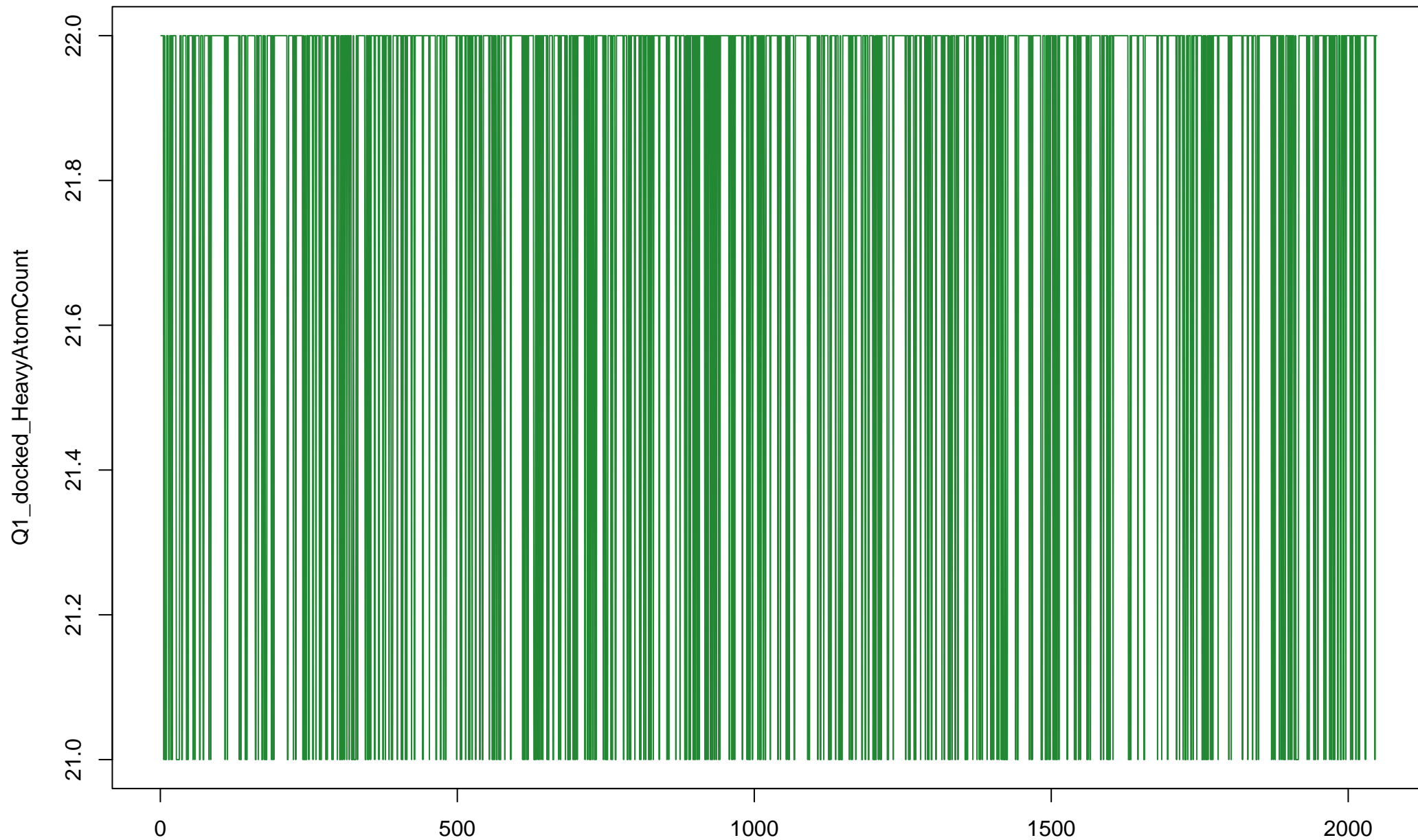
Q1_log_RMSD
ESS = 2050 | BMK = 0.0281 | MCSE(6.27) = 2.89 | stat: FALSE | burn: 0



Q1_Xtransf_ec_tanimoto_similarity
ESS = 1580 | BMK = 0.0434 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



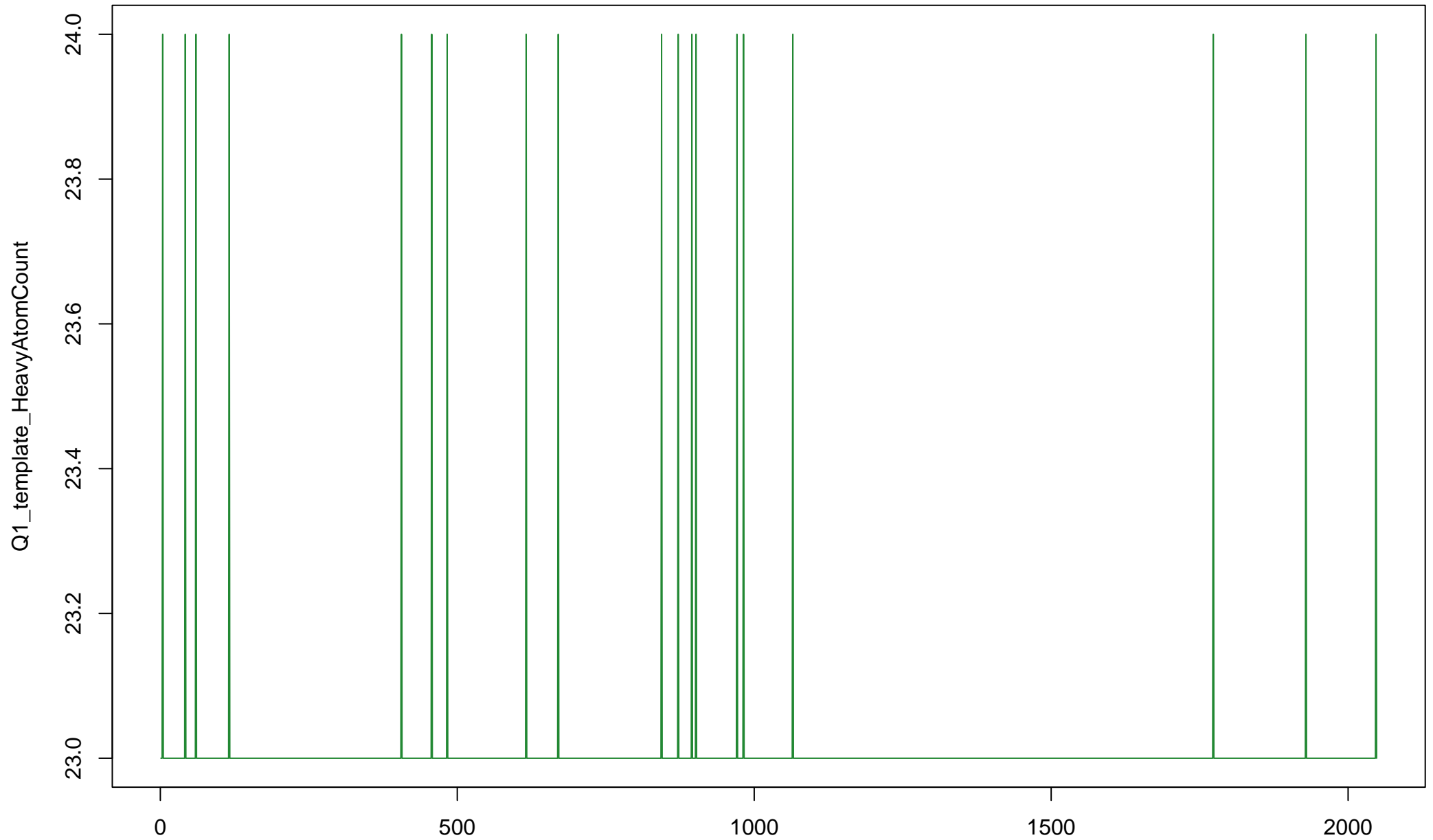
Q1_docked_HeavyAtomCount
ESS = 1610 | BMK = 0.0173 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0



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



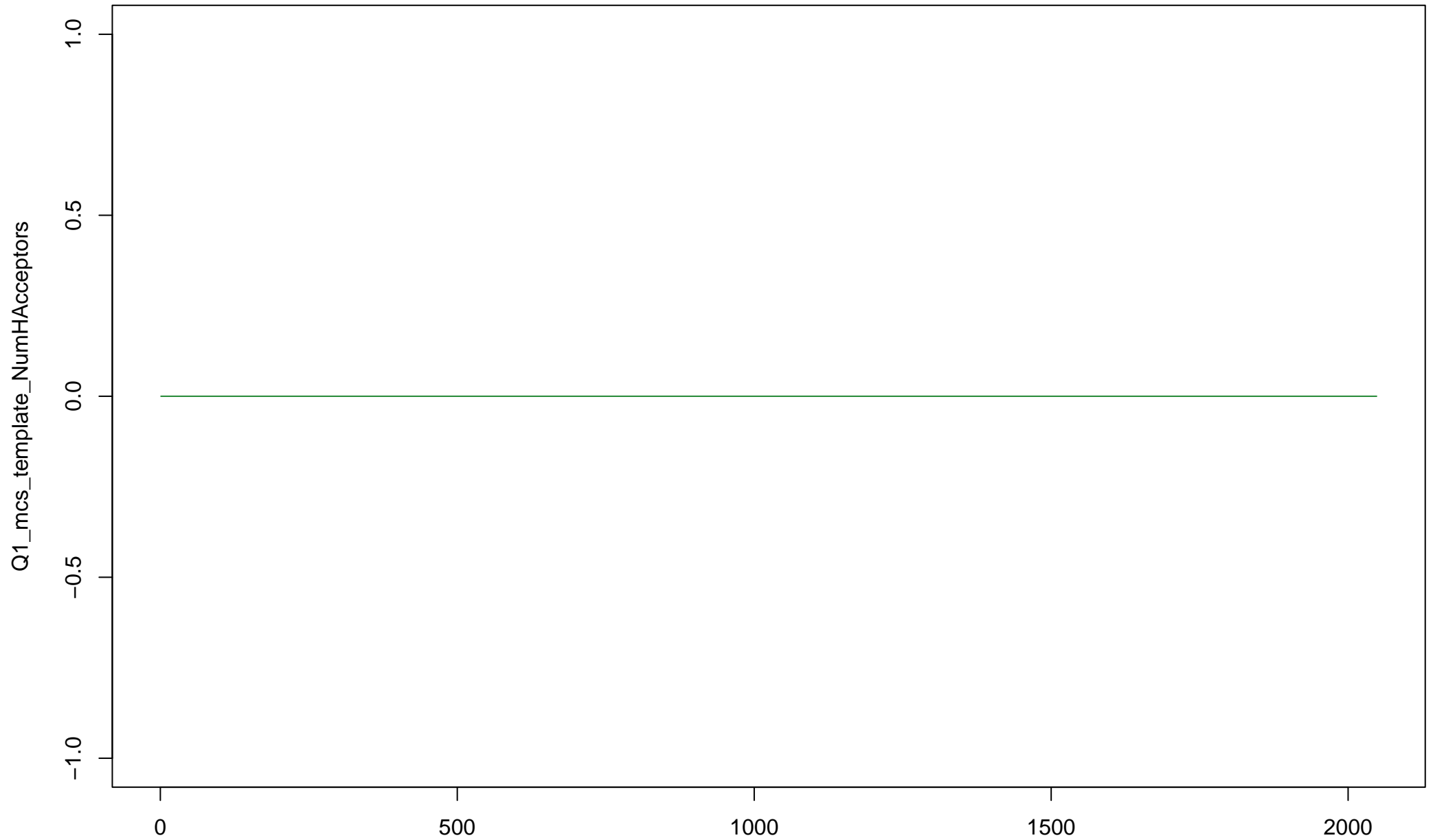
Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0.221 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 1632



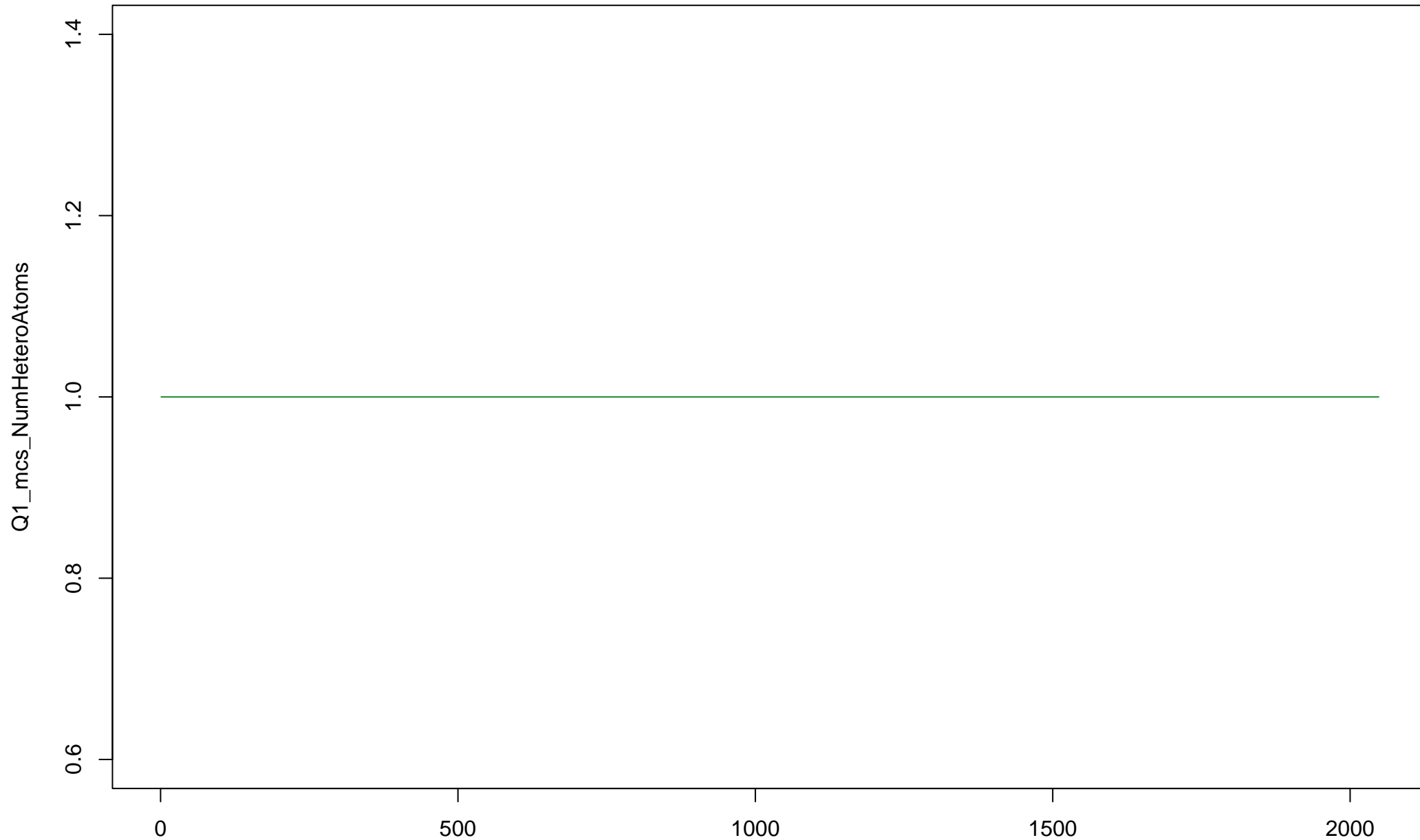
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



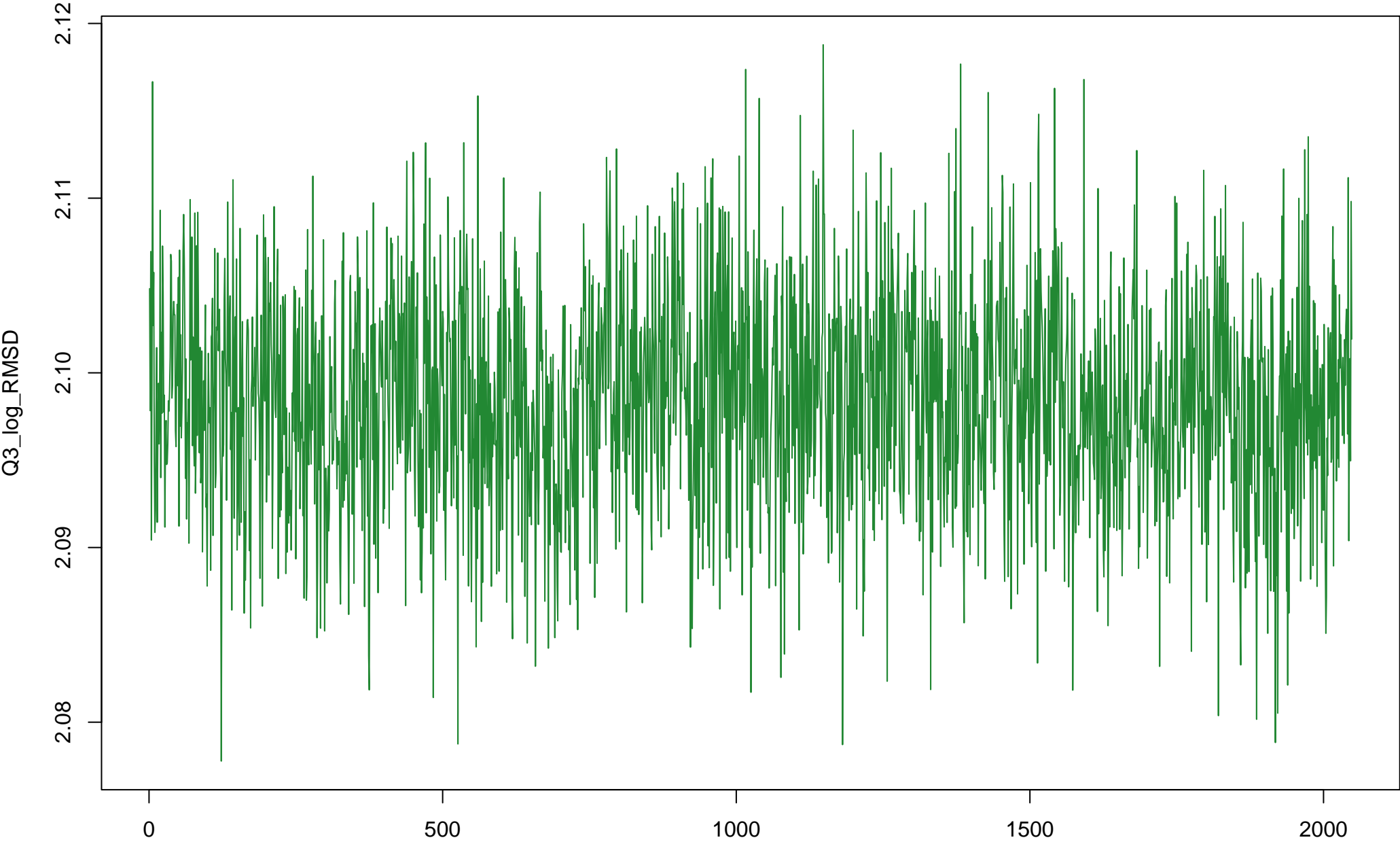
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



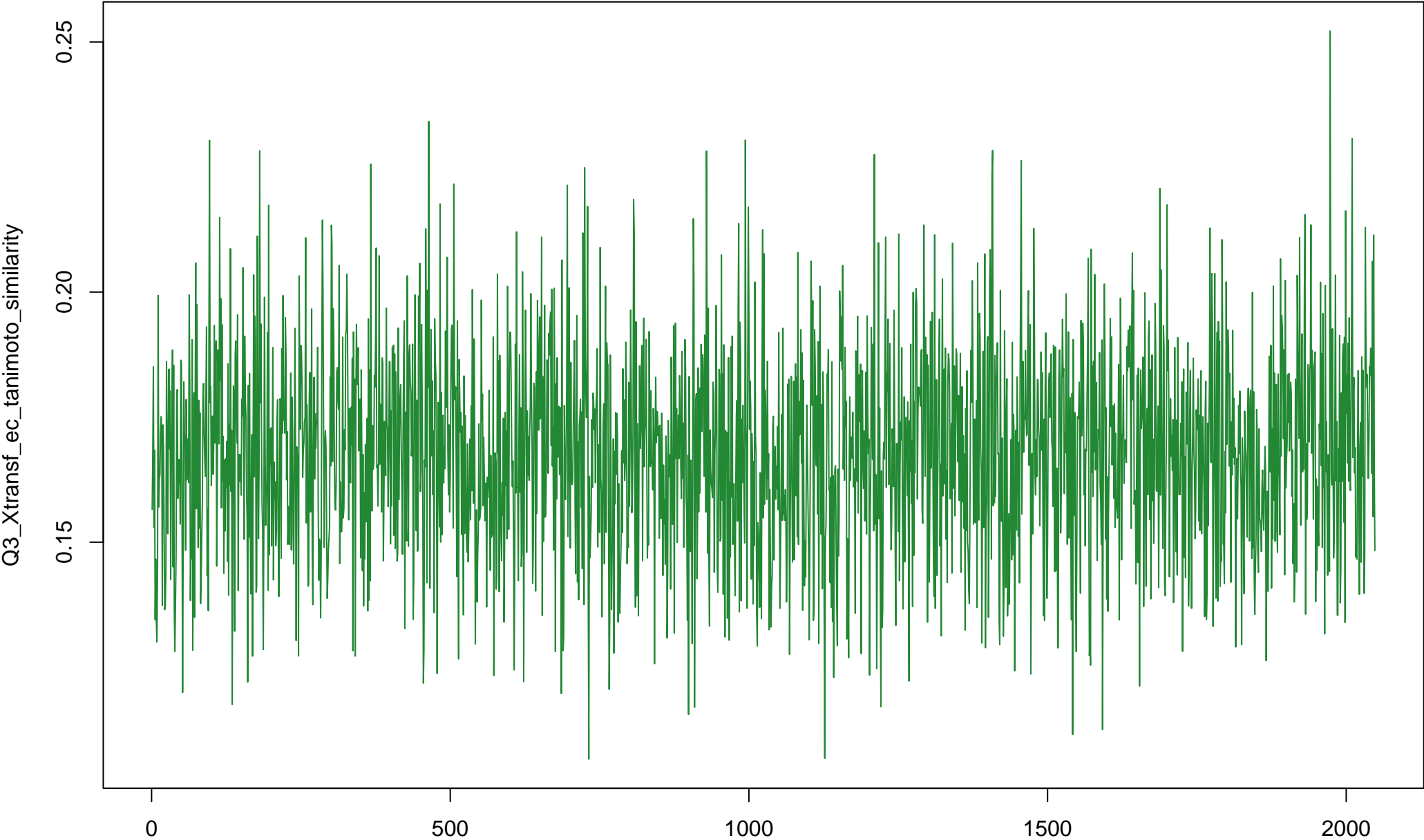
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



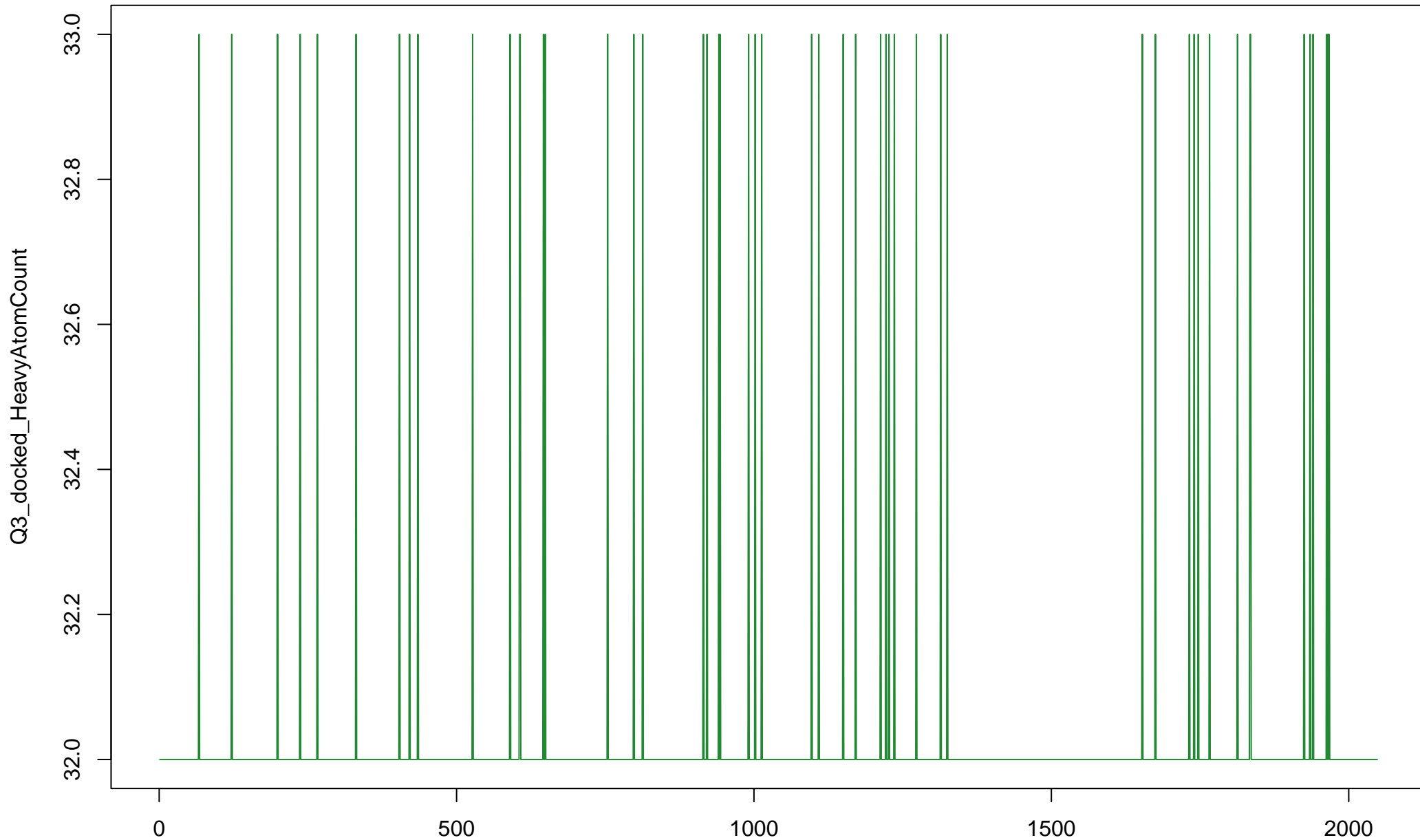
Q3_log_RMSD
ESS = 858 | BMK = 0.0509 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 1850 | BMK = 0.0337 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0



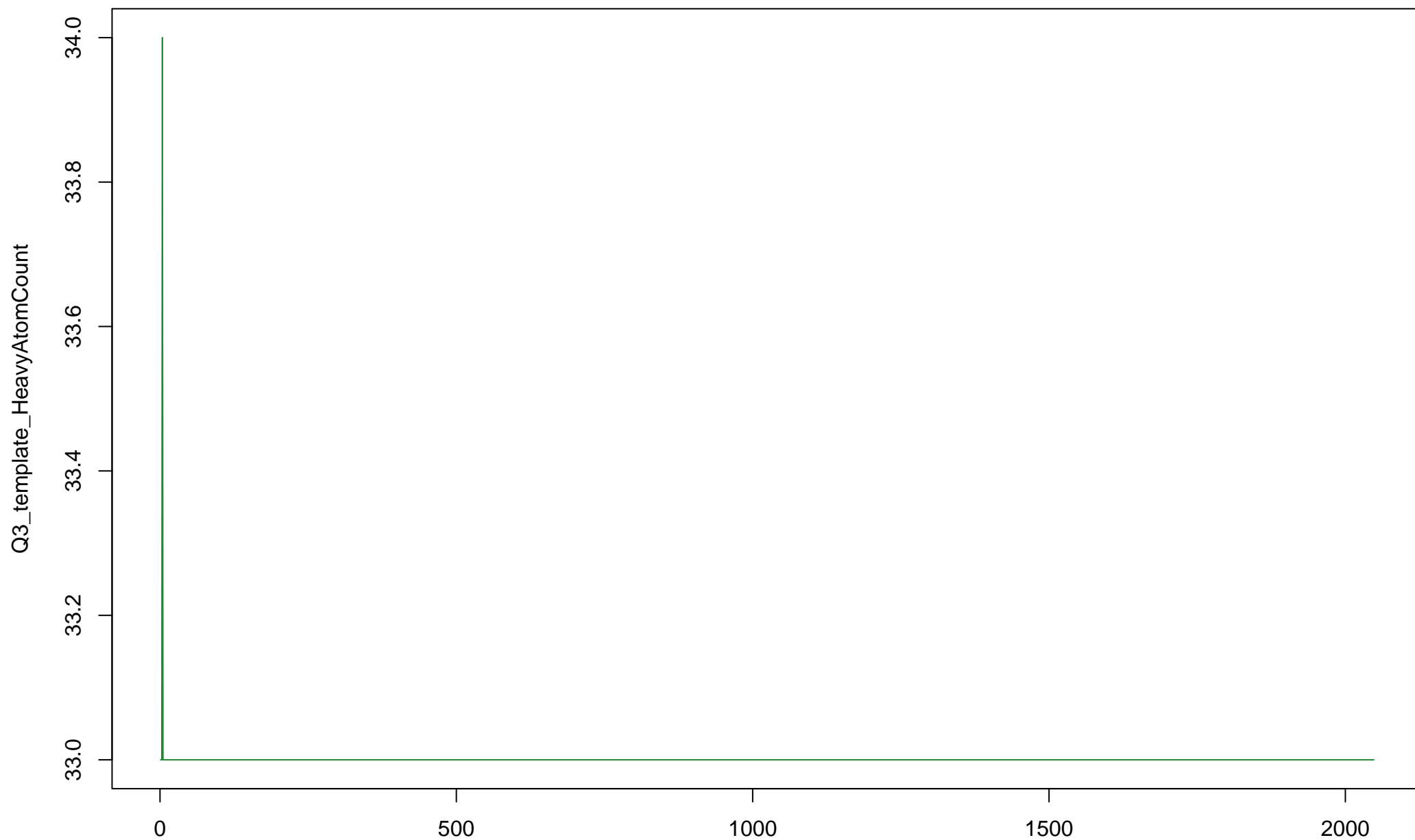
Q3_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.00693 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0



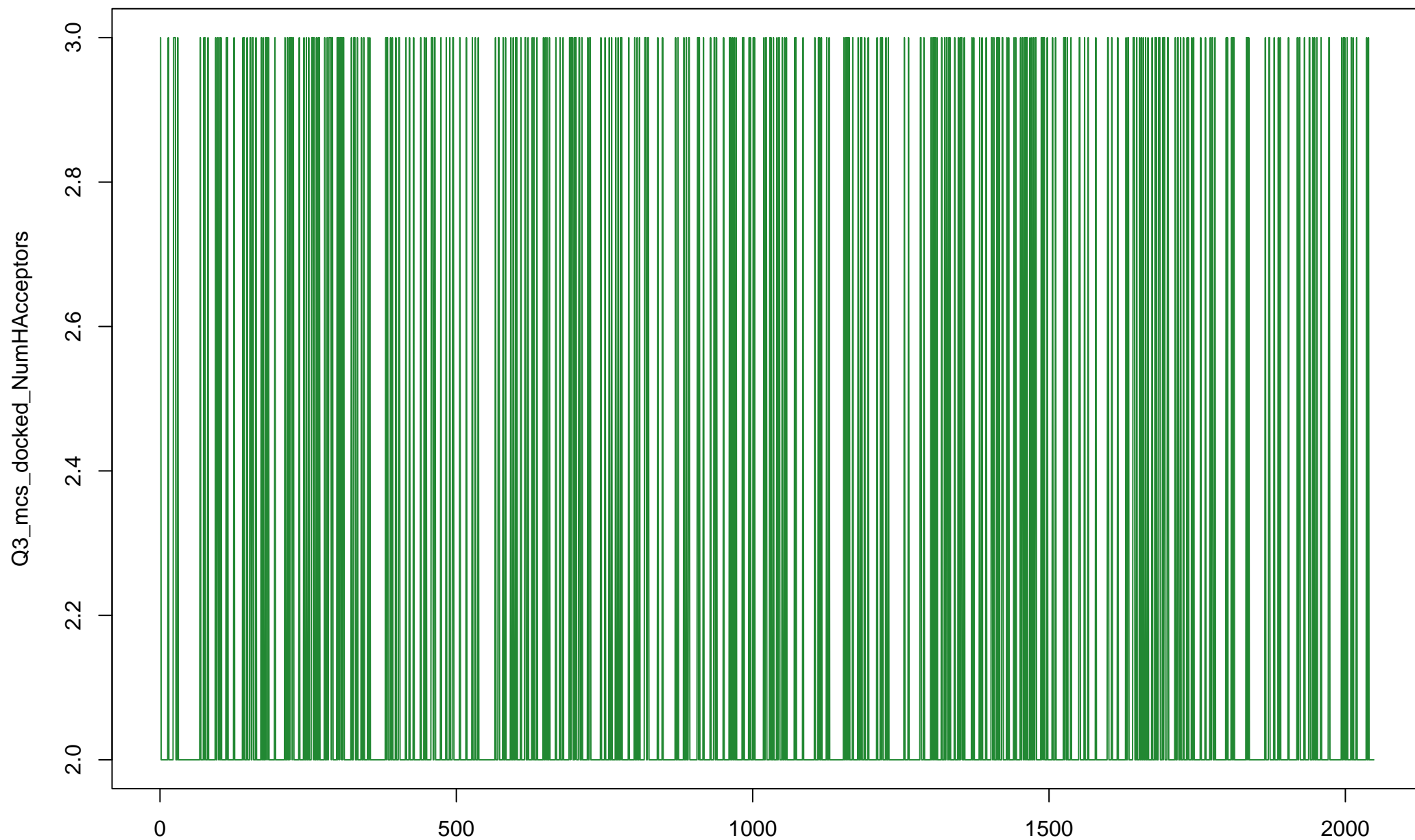
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



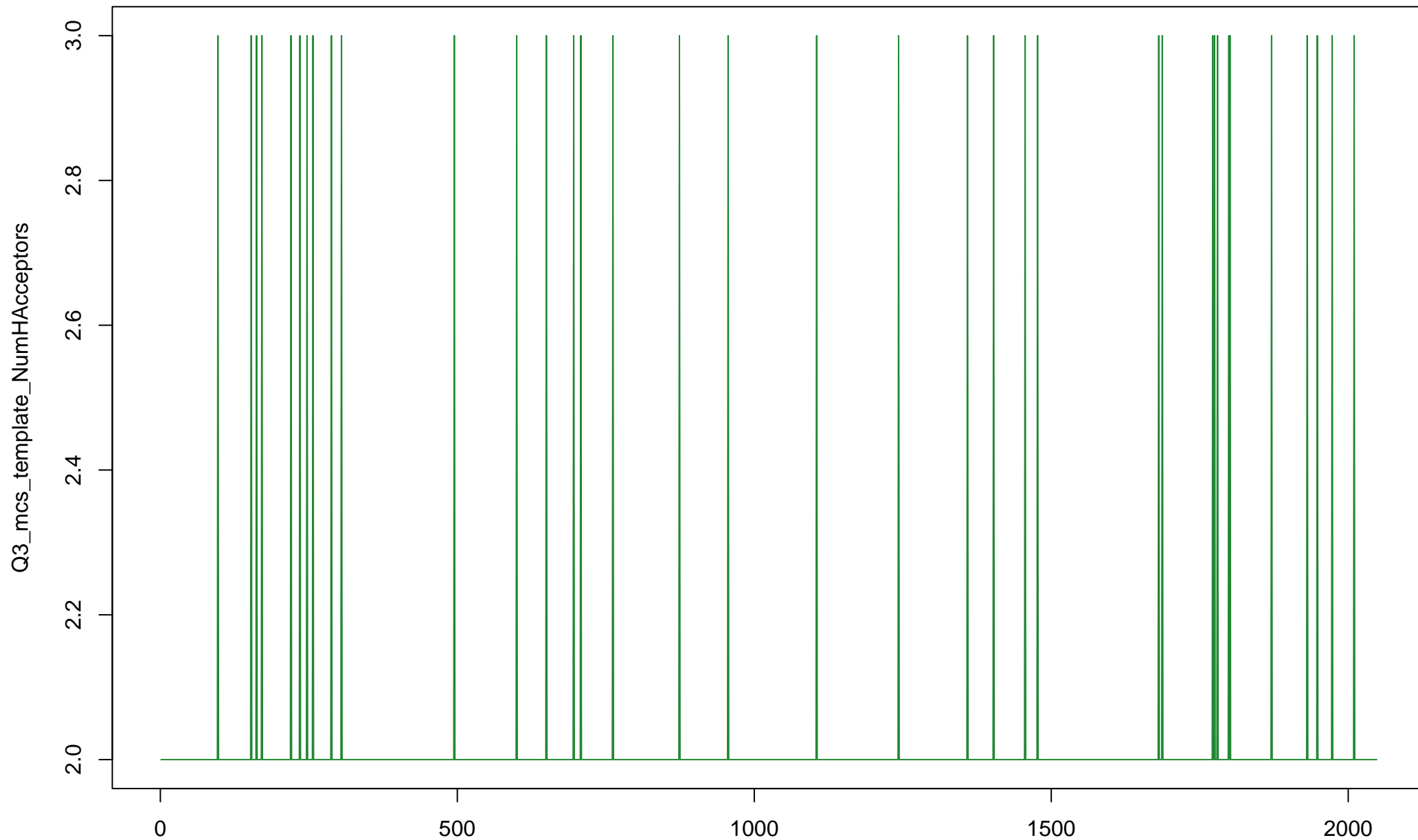
Q3_template_HeavyAtomCount
ESS = 2050 | BMK = 0.517 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 204



Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0117 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



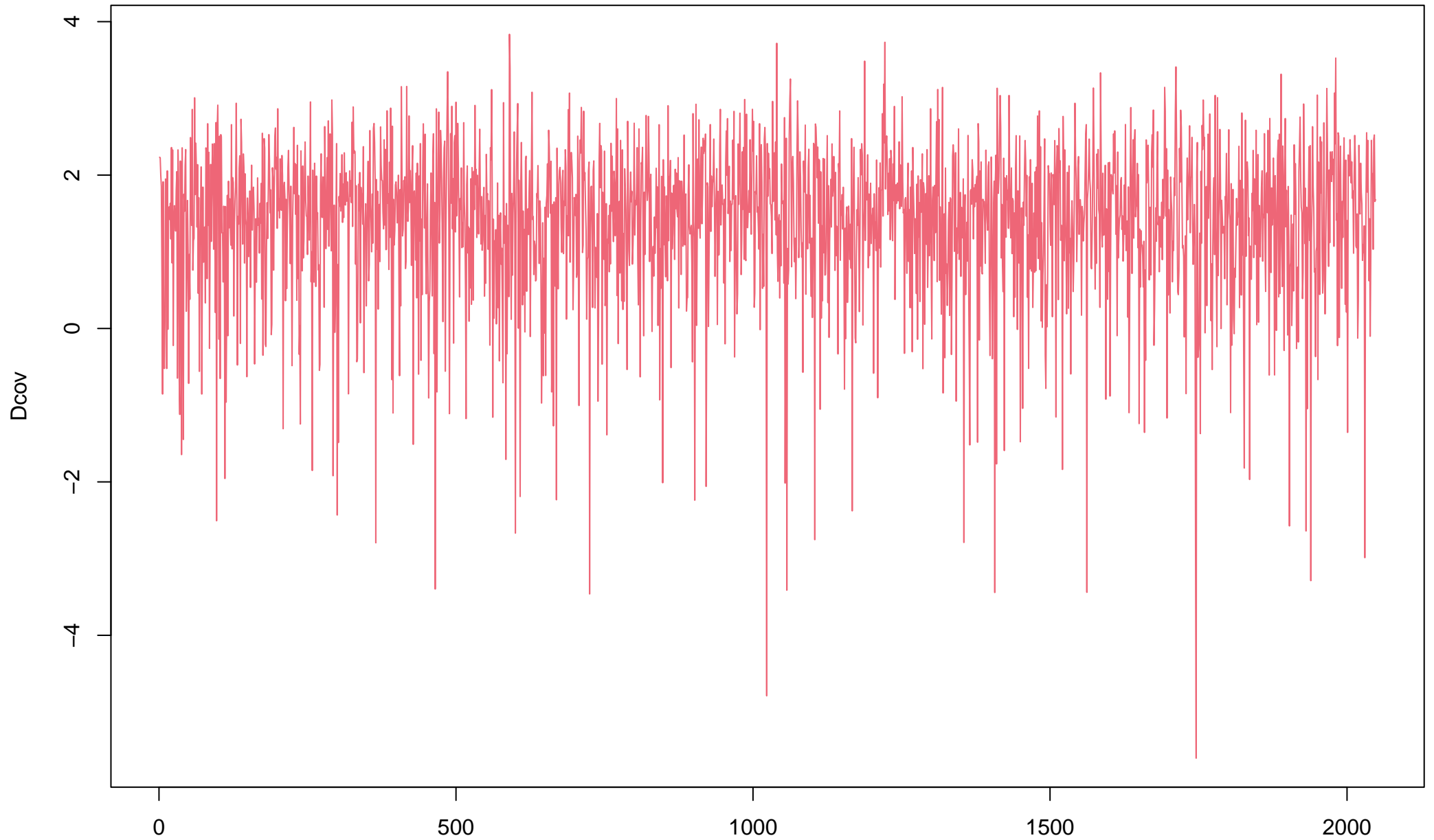
Q3_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



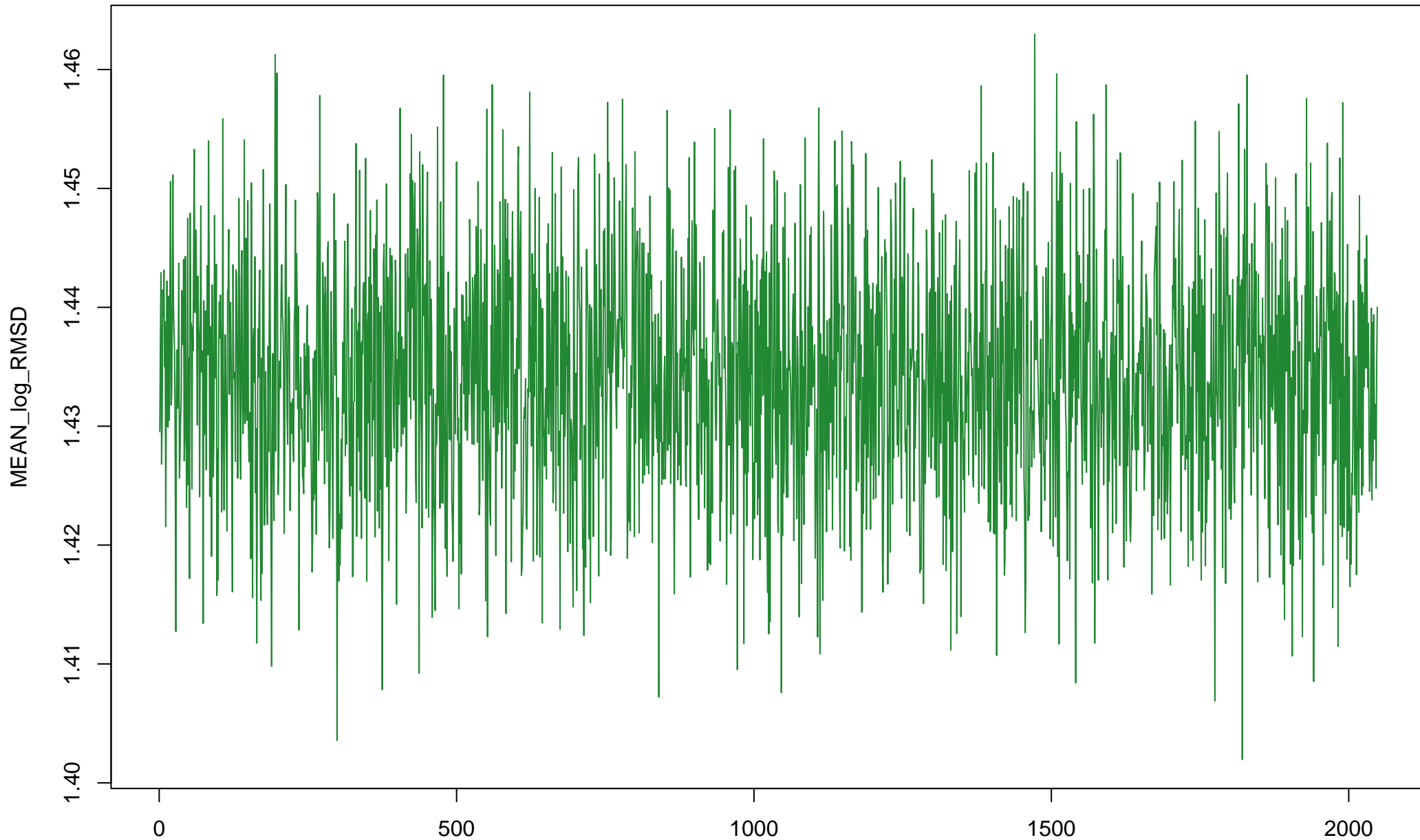
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



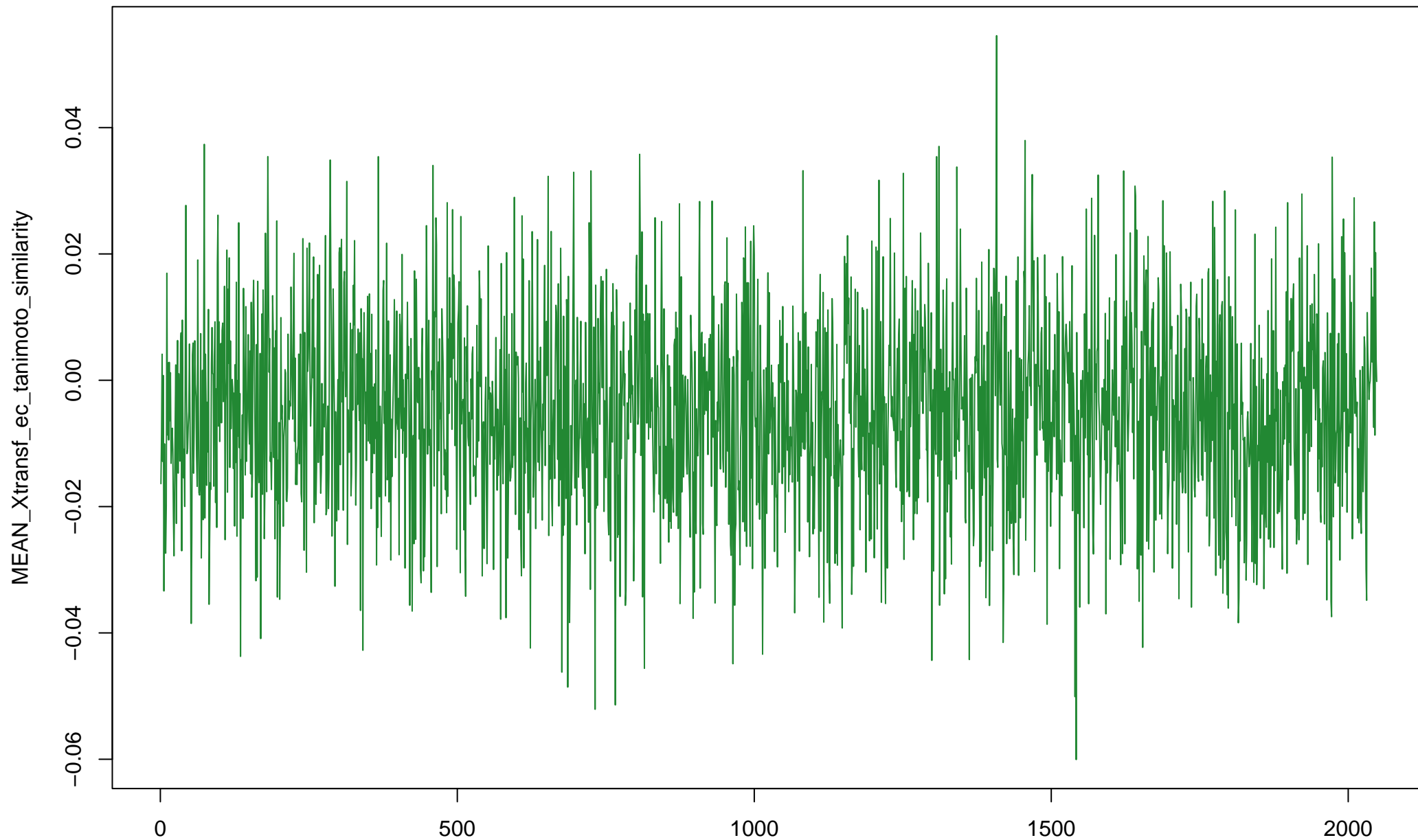
Dcov
ESS = 2050 | BMK = 0.0854 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



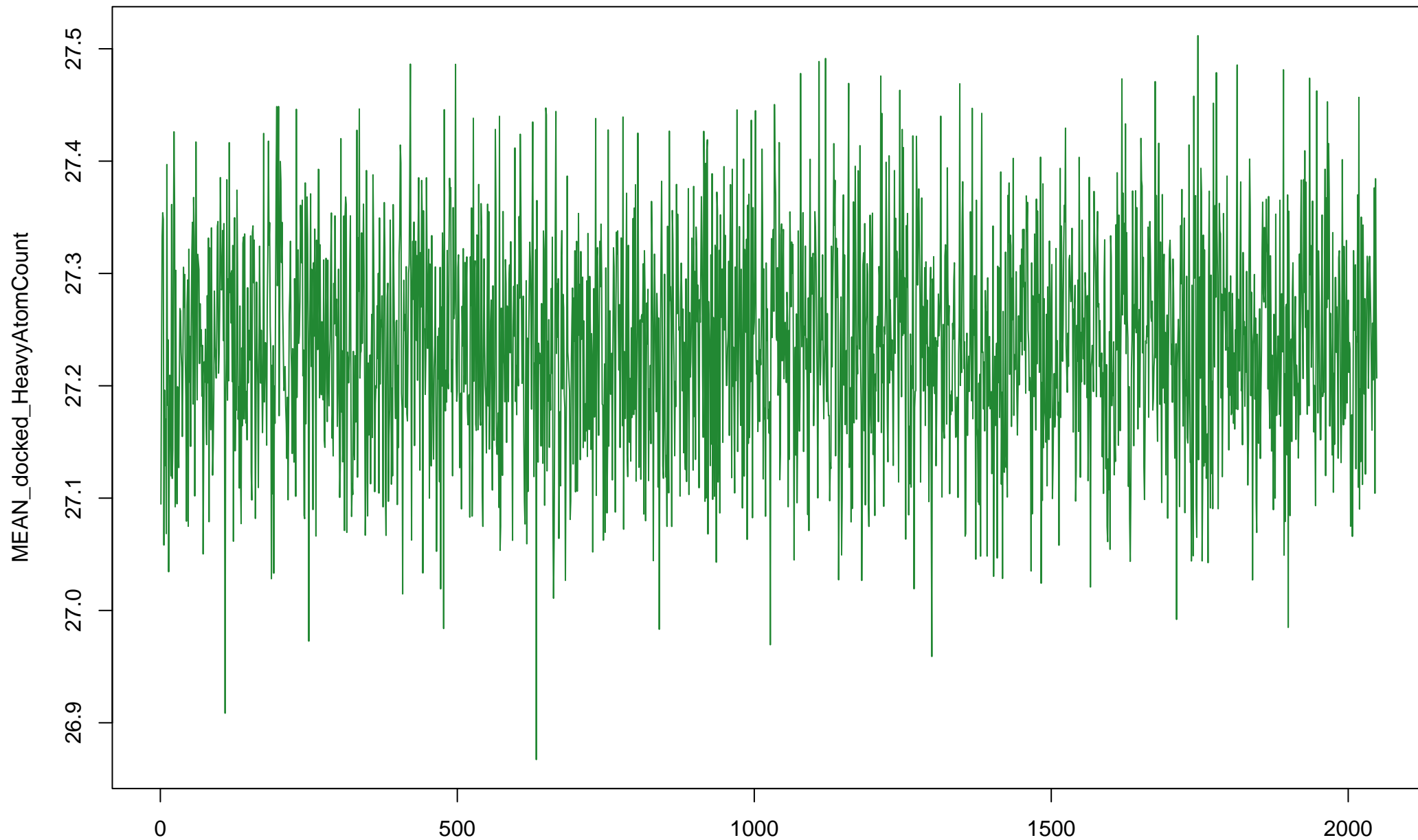
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0276 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0



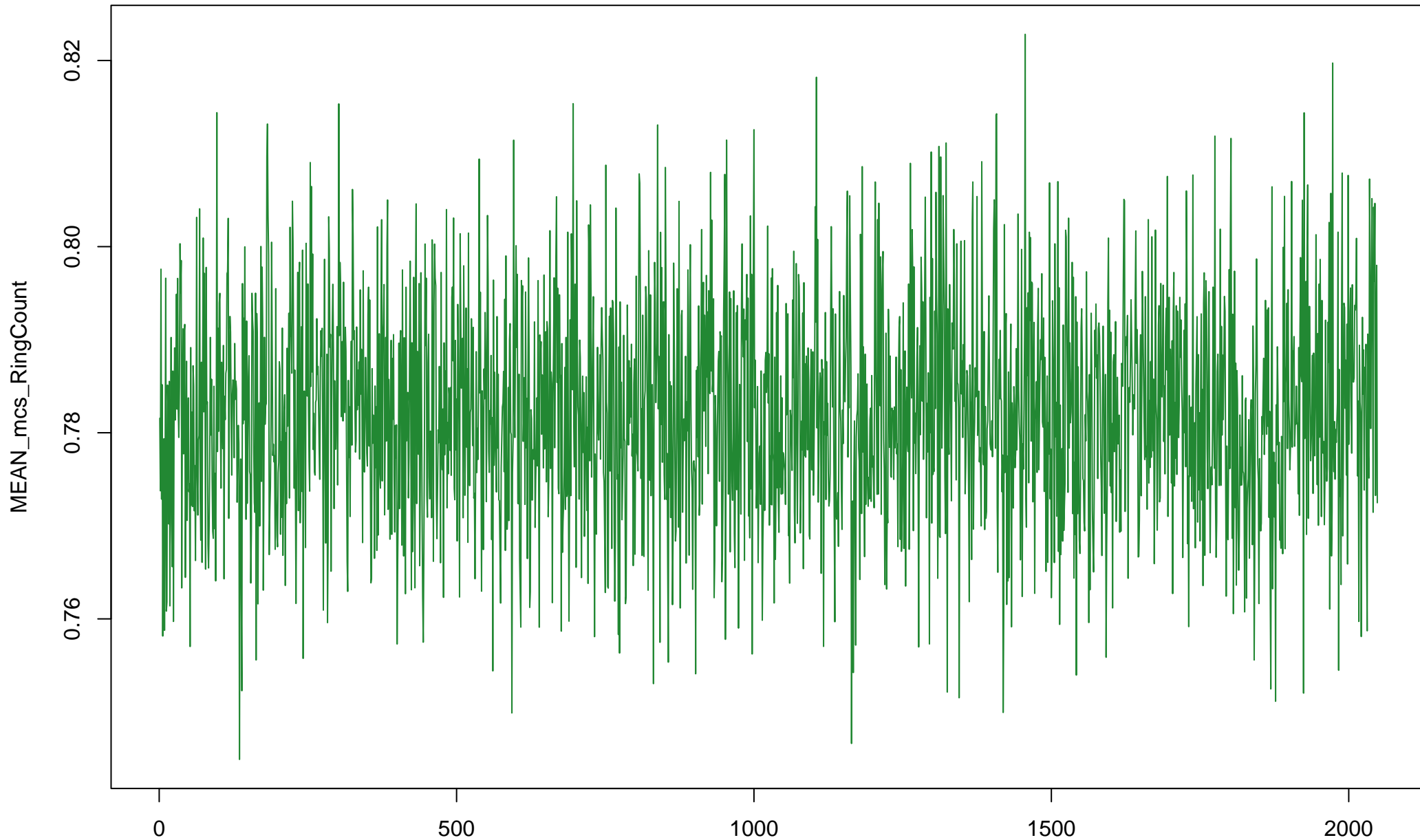
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0



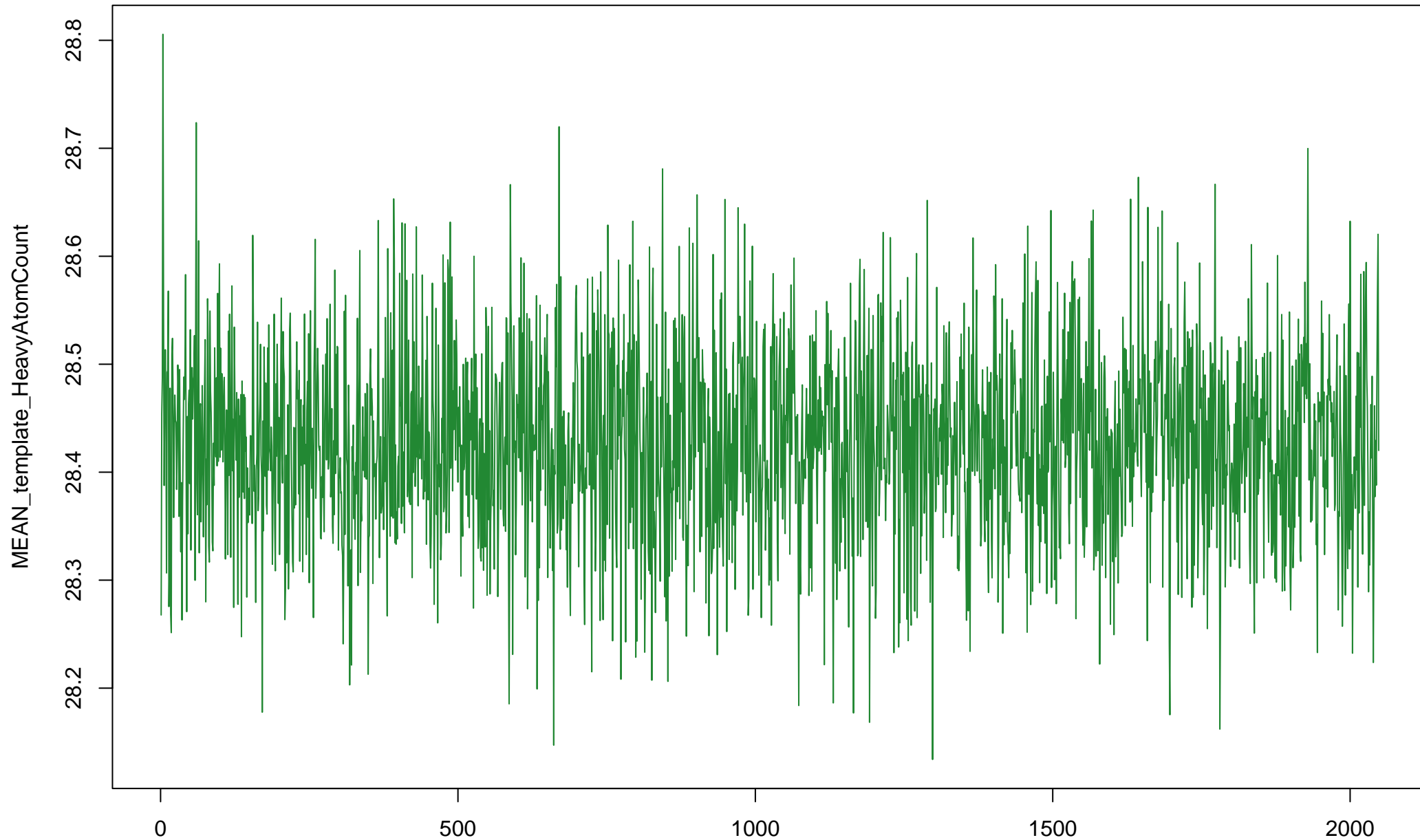
MEAN_docked_HeavyAtomCount
ESS = 1920 | BMK = 0.0527 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0



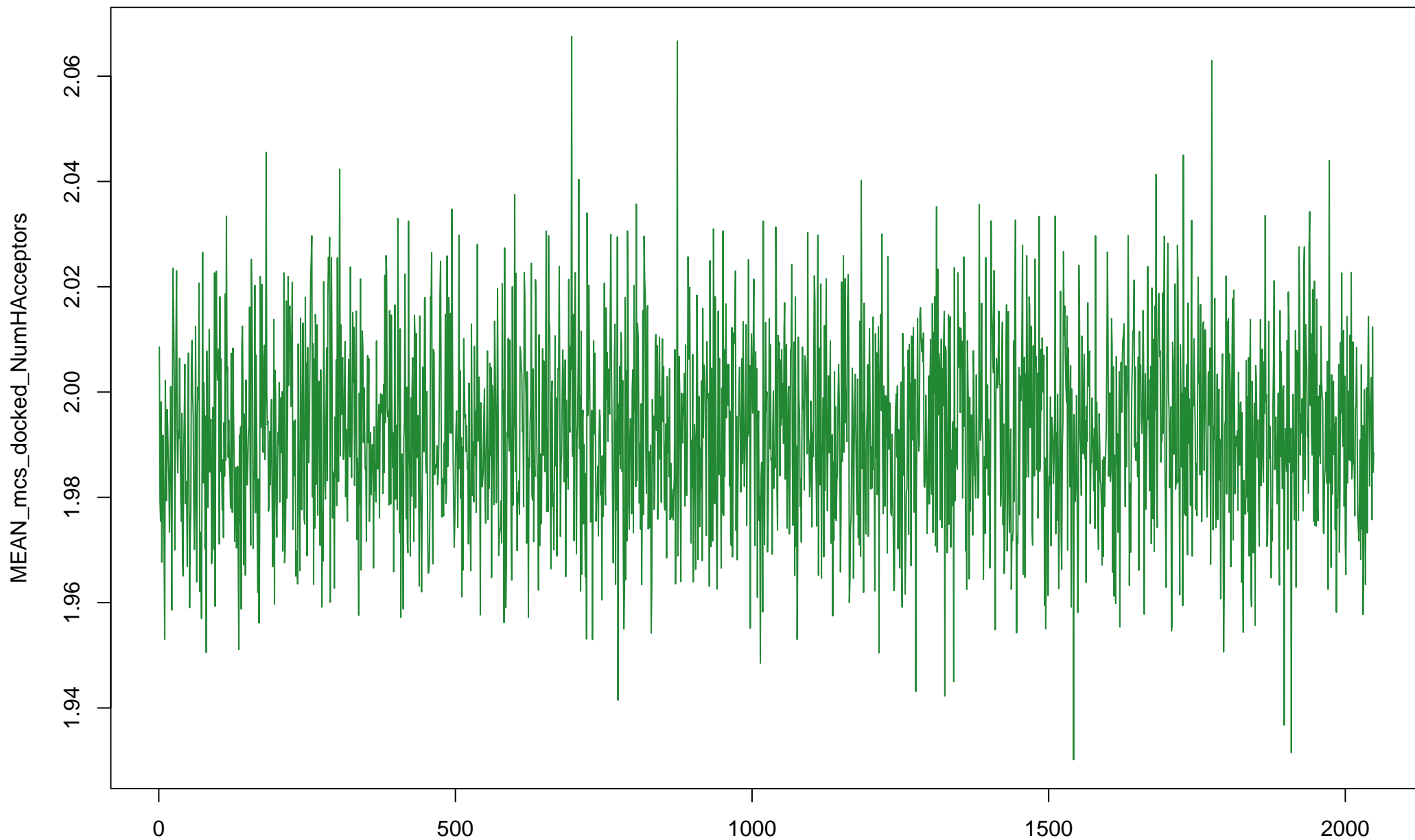
MEAN_mcs_RingCount
ESS = 1900 | BMK = 0.0473 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0



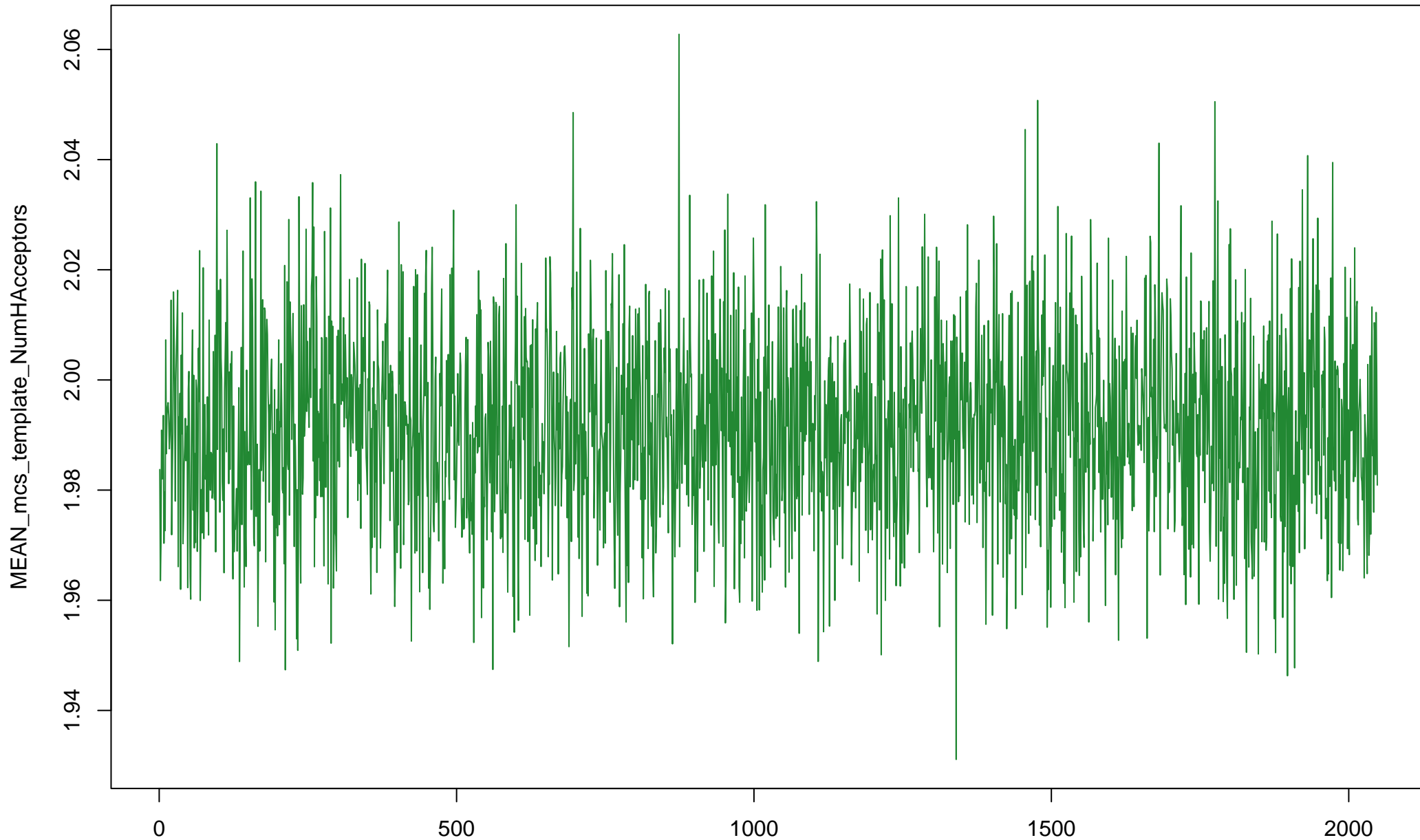
MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0471 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0



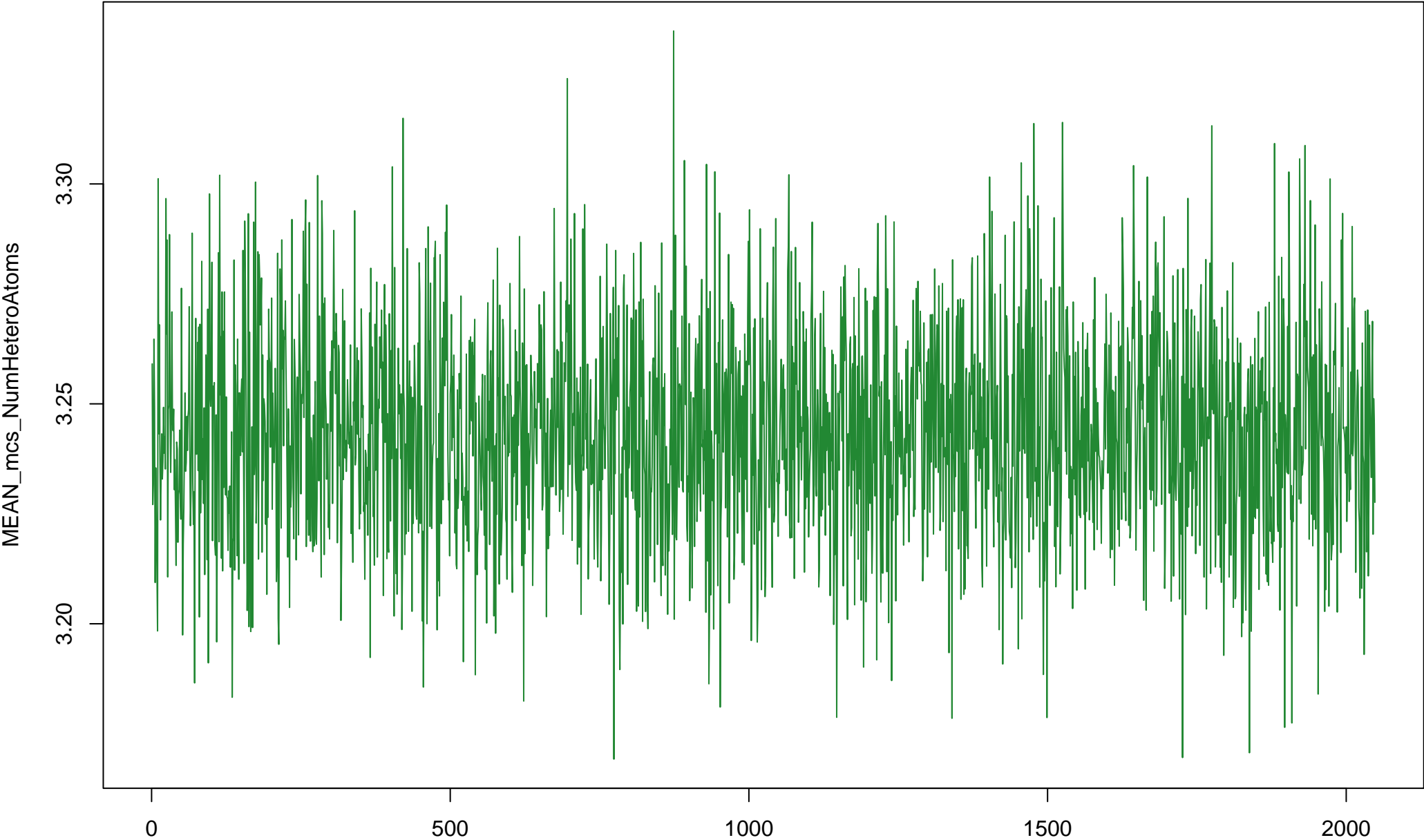
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.048 | MCSE(6.27) = 2.12 | stat: FALSE | burn: 0



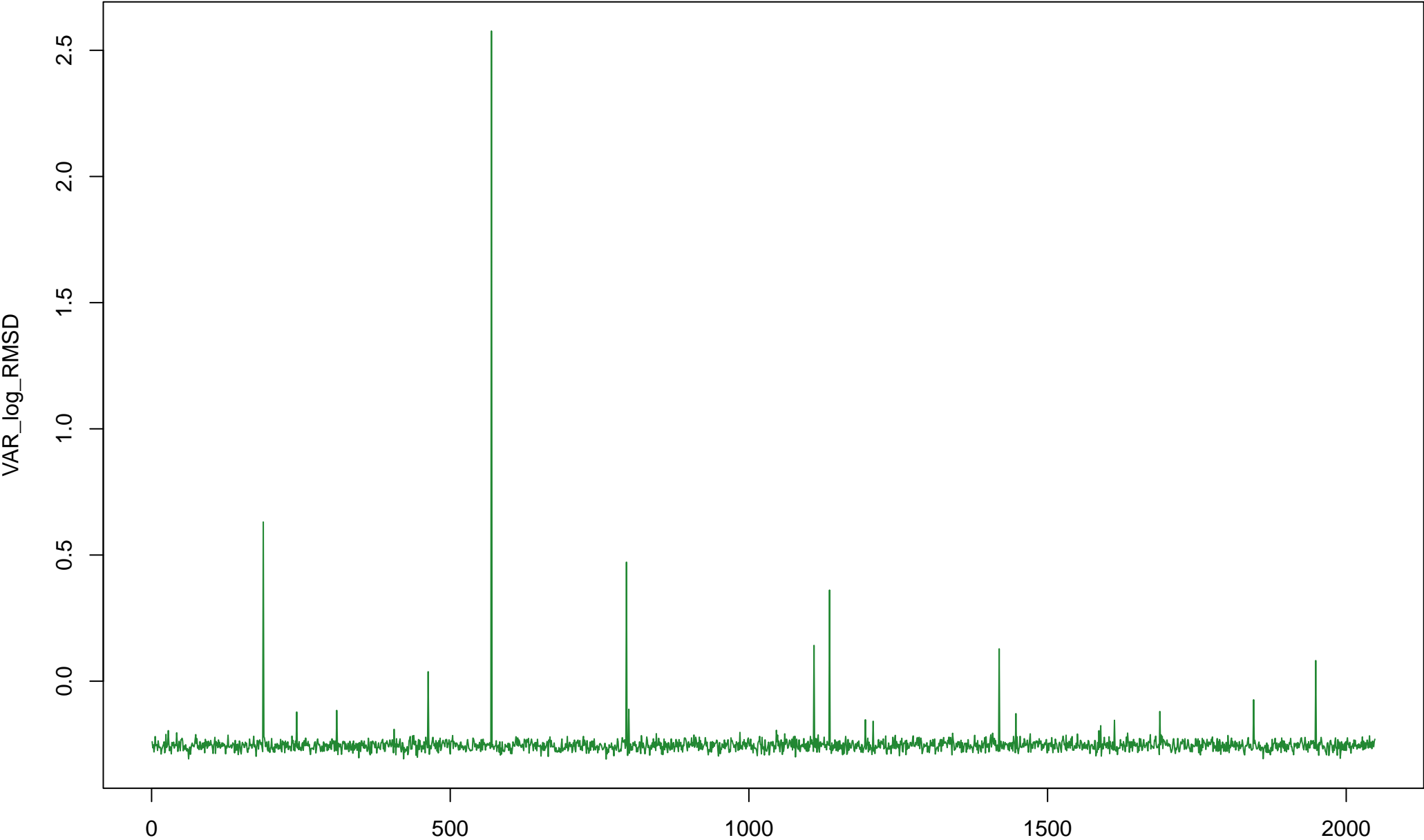
MEAN_mcs_template_NumHAcceptors
ESS = 1900 | BMK = 0.0299 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0



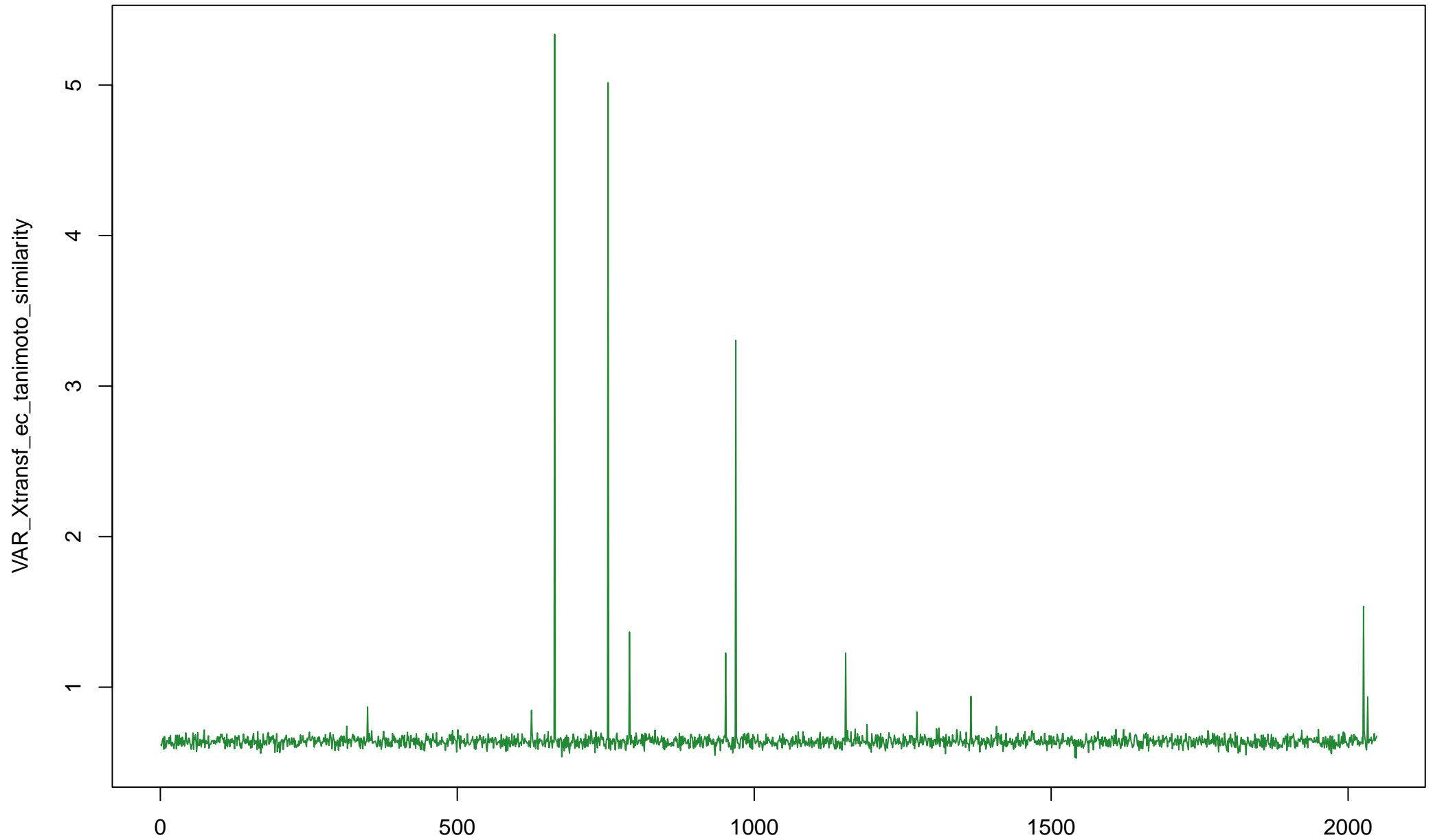
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.047 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0



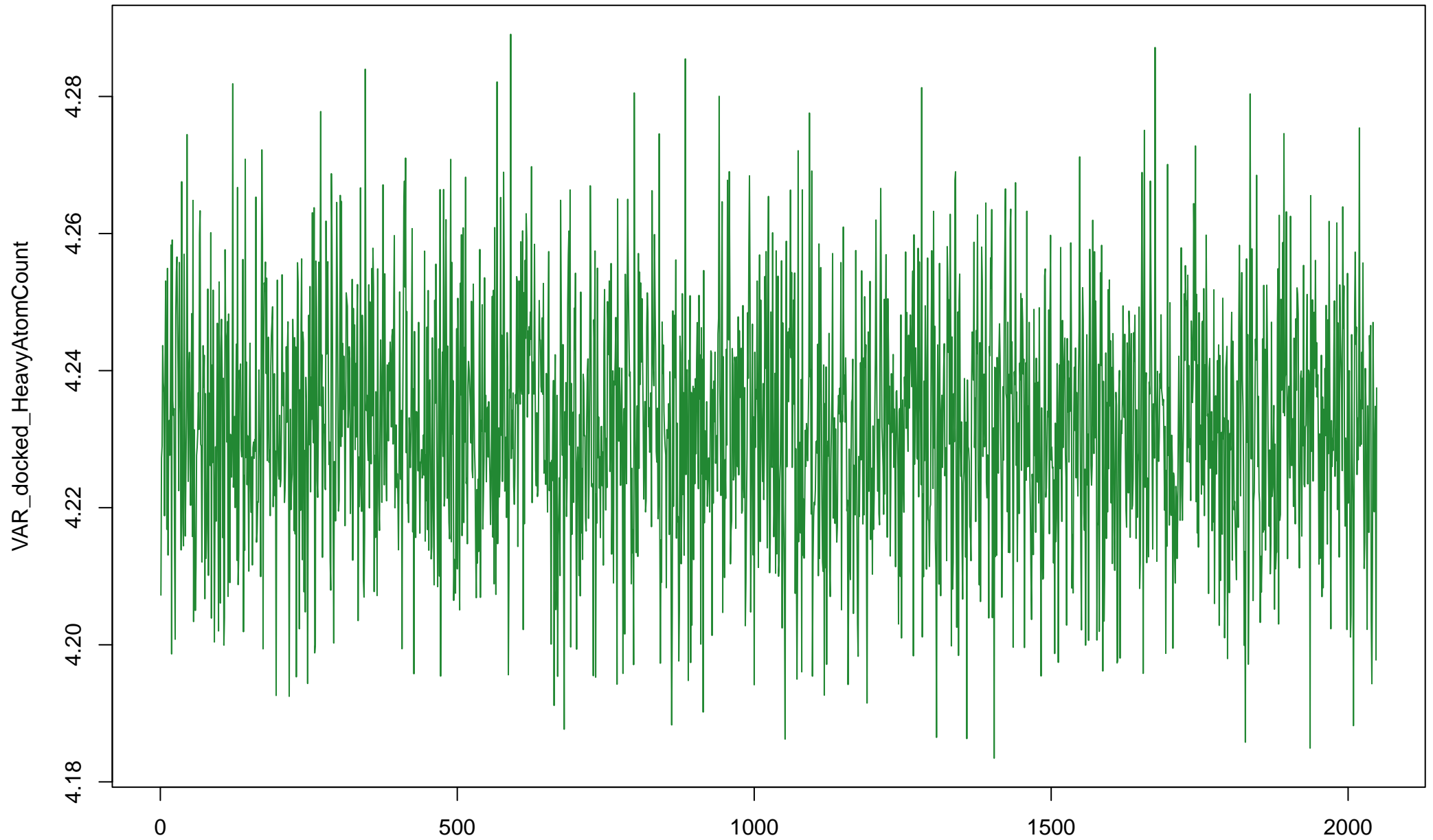
VAR_log_RMSD
ESS = 2050 | BMK = 0.105 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



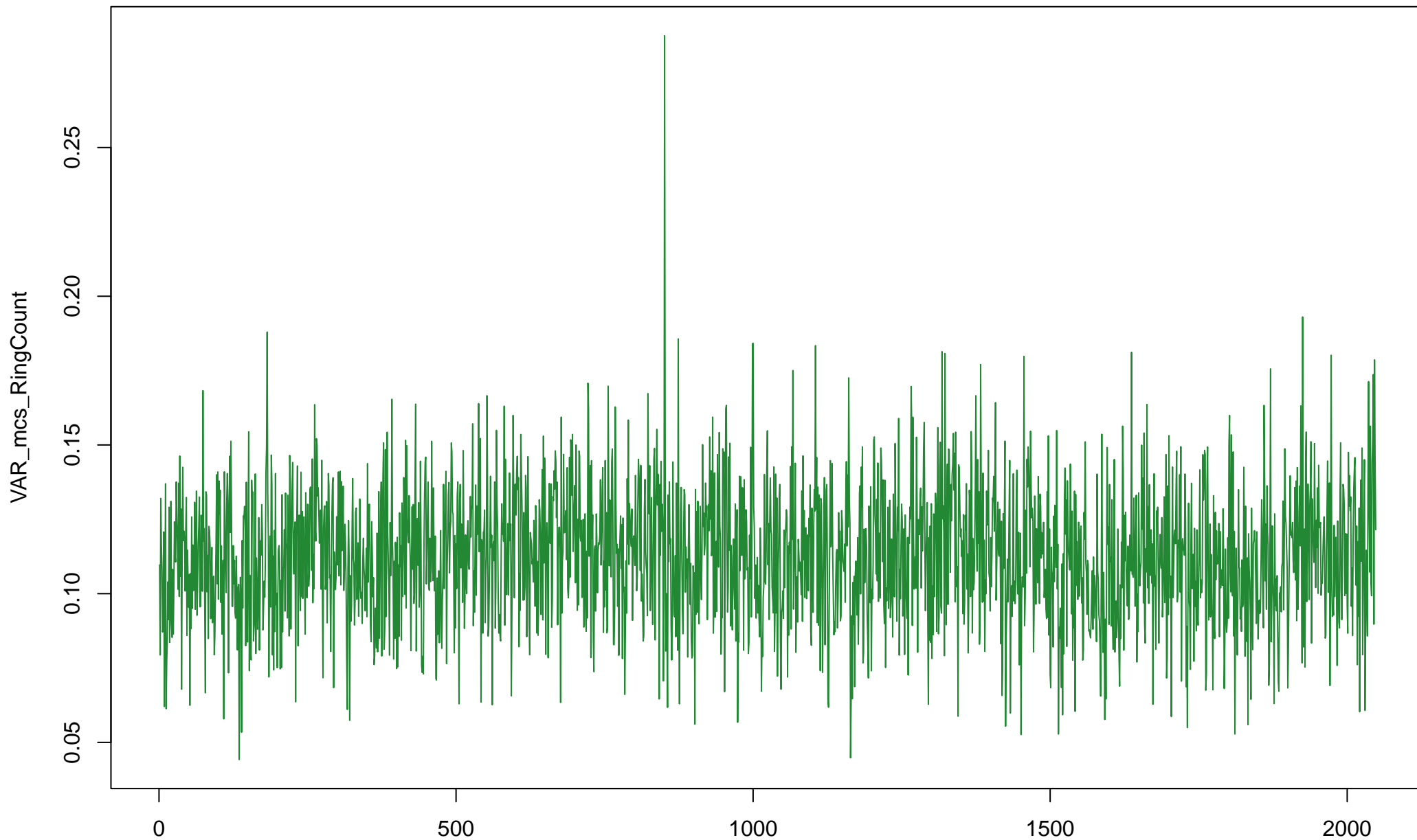
VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.137 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0



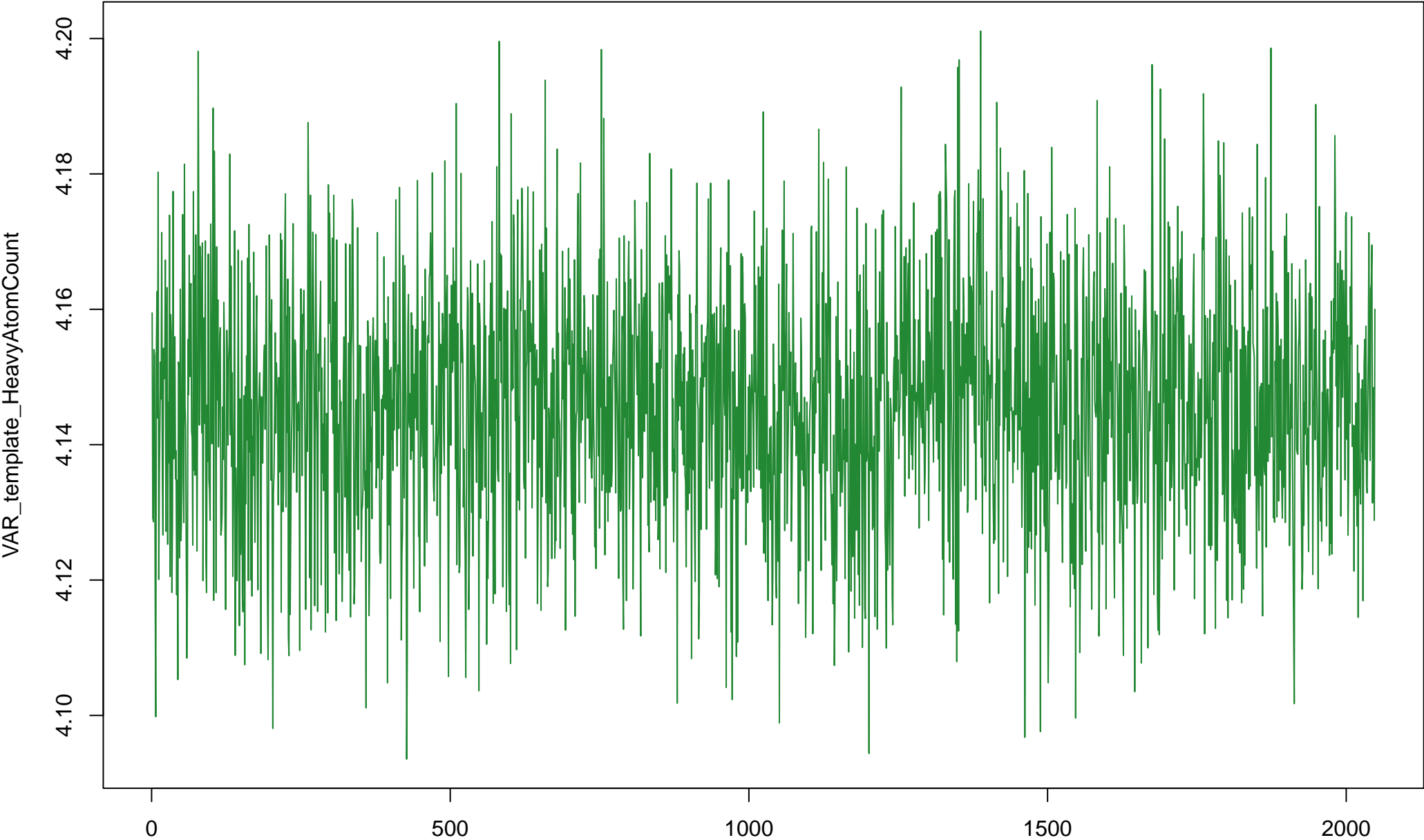
VAR_docked_HeavyAtomCount
ESS = 1950 | BMK = 0.042 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0



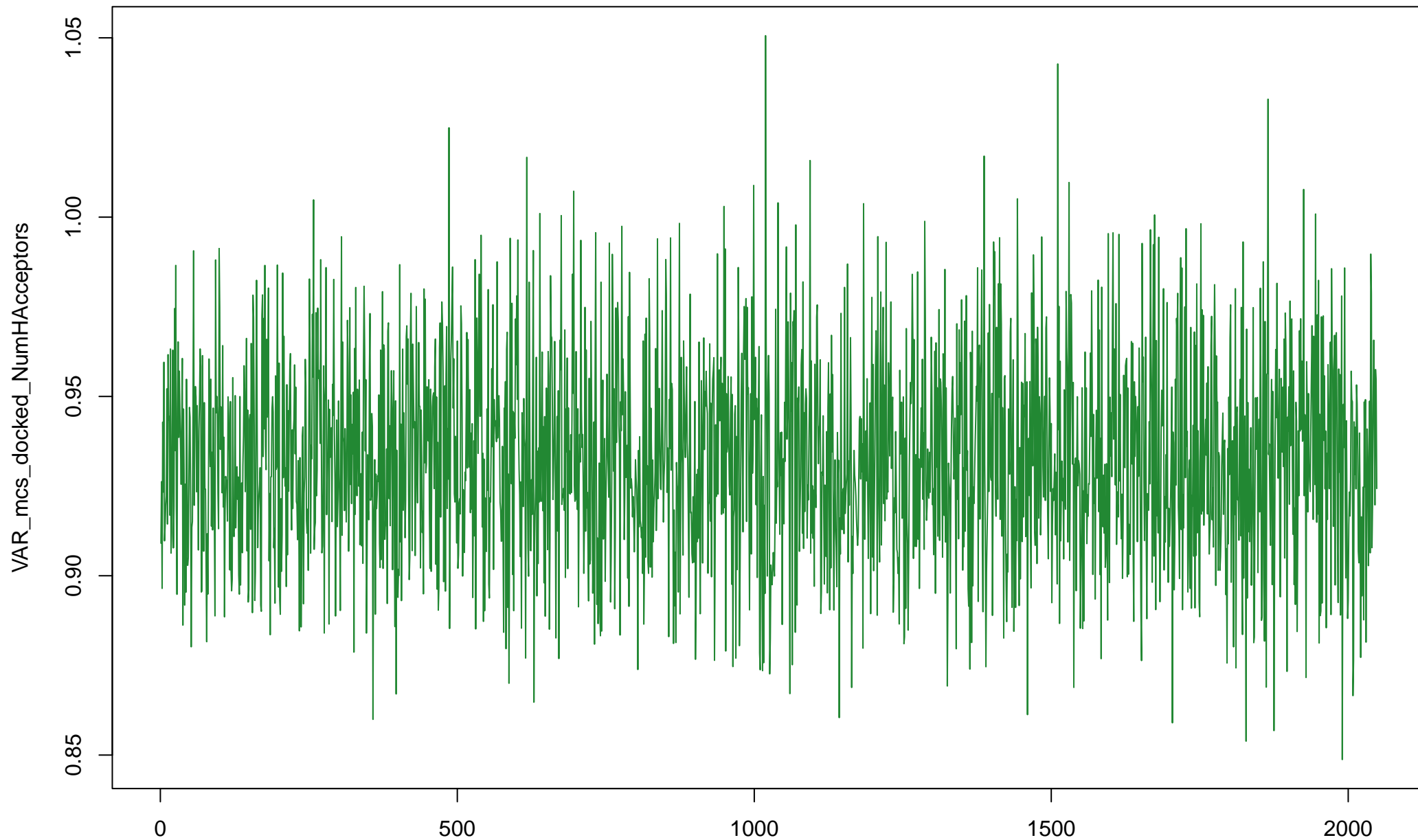
VAR_mcs_RingCount
ESS = 1190 | BMK = 0.0564 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0



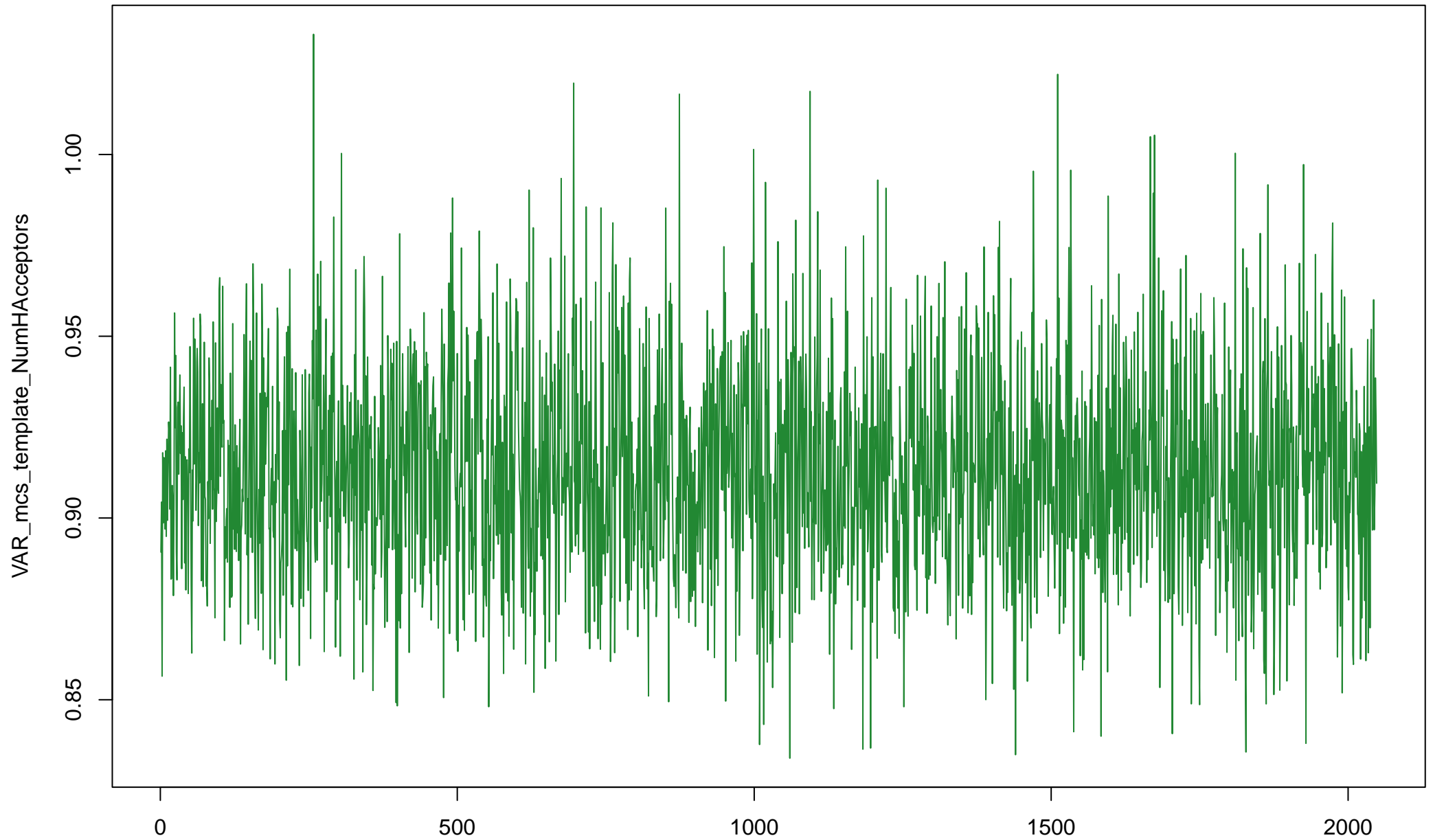
VAR_template_HeavyAtomCount
ESS = 1680 | BMK = 0.0457 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0



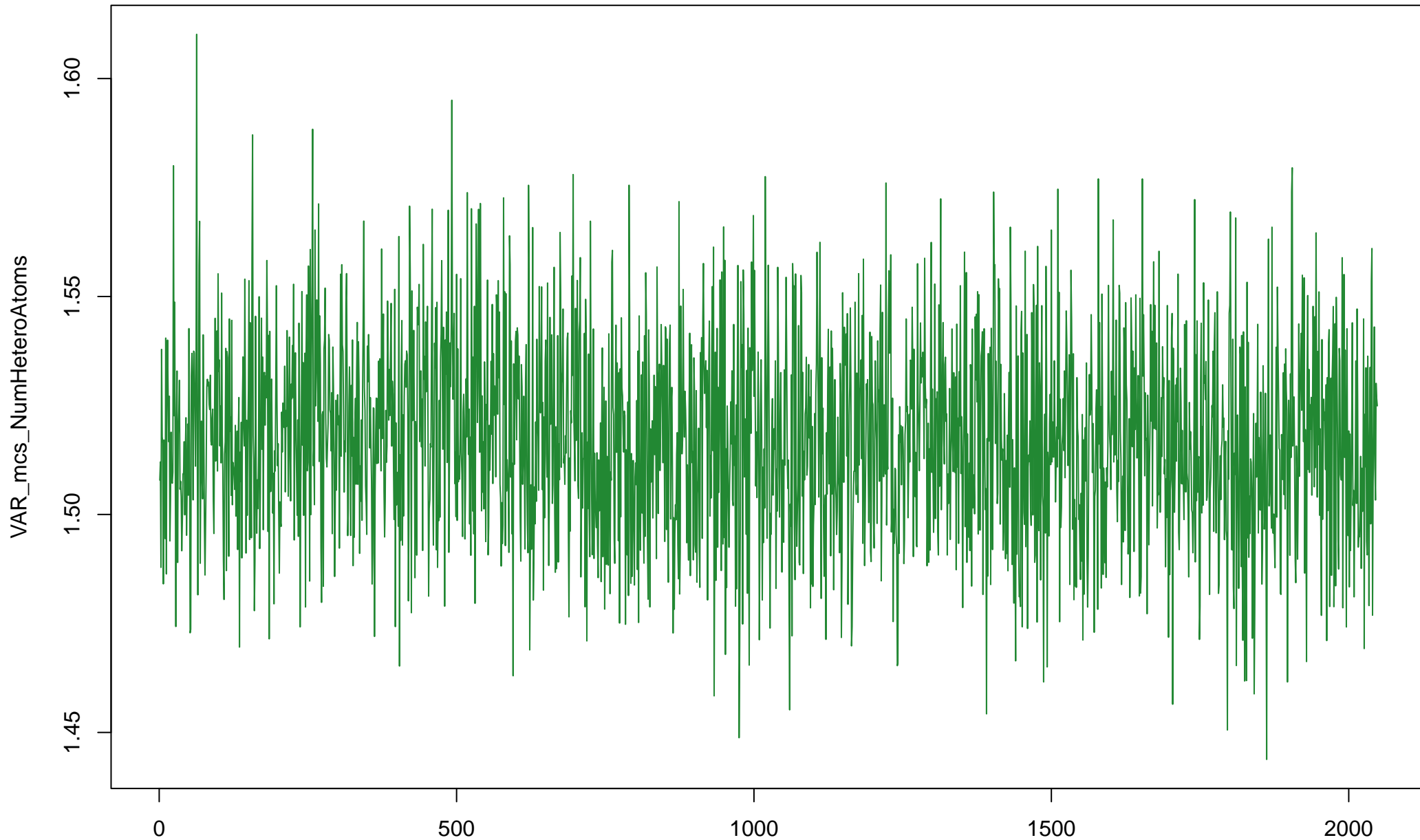
VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0435 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0



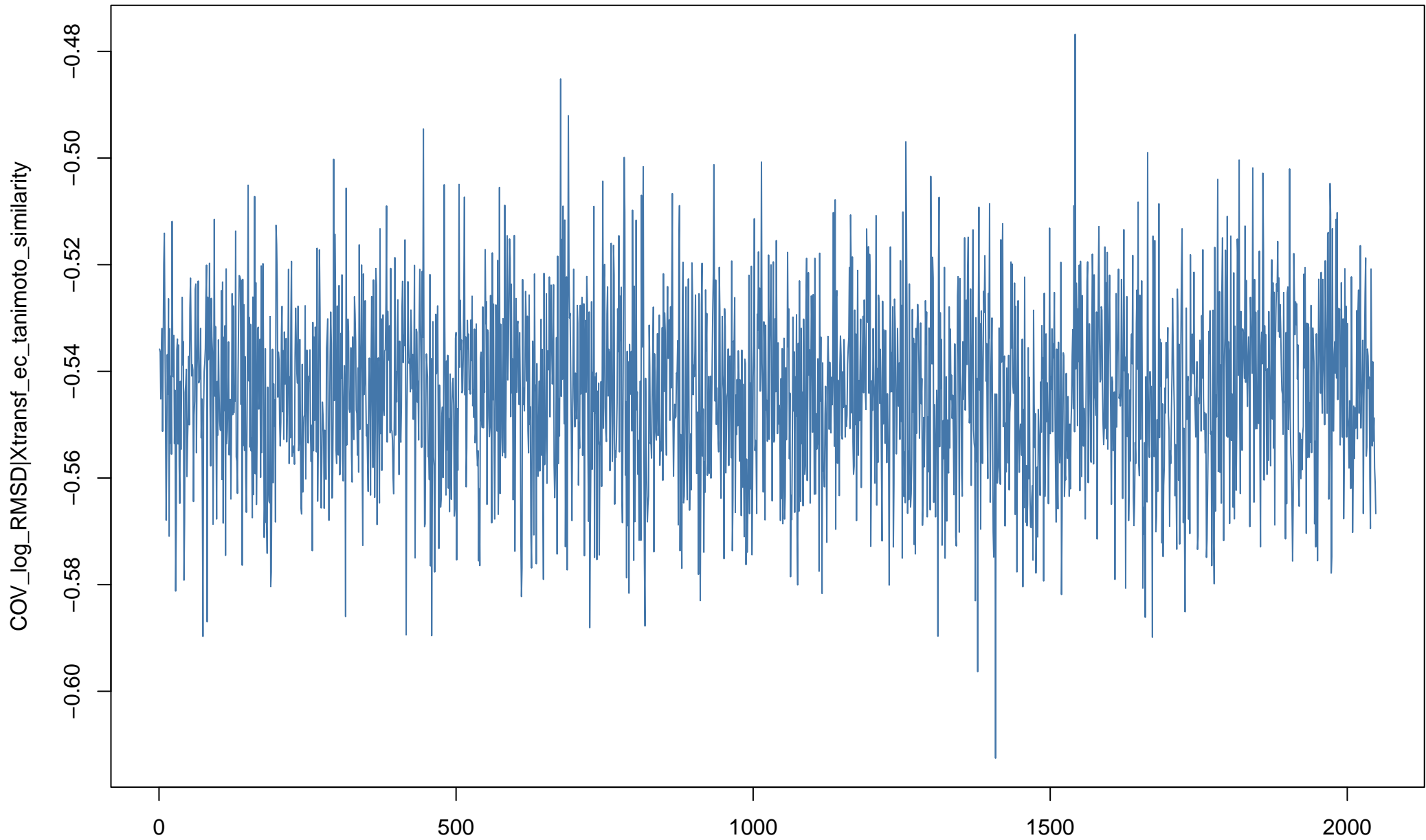
VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0348 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0



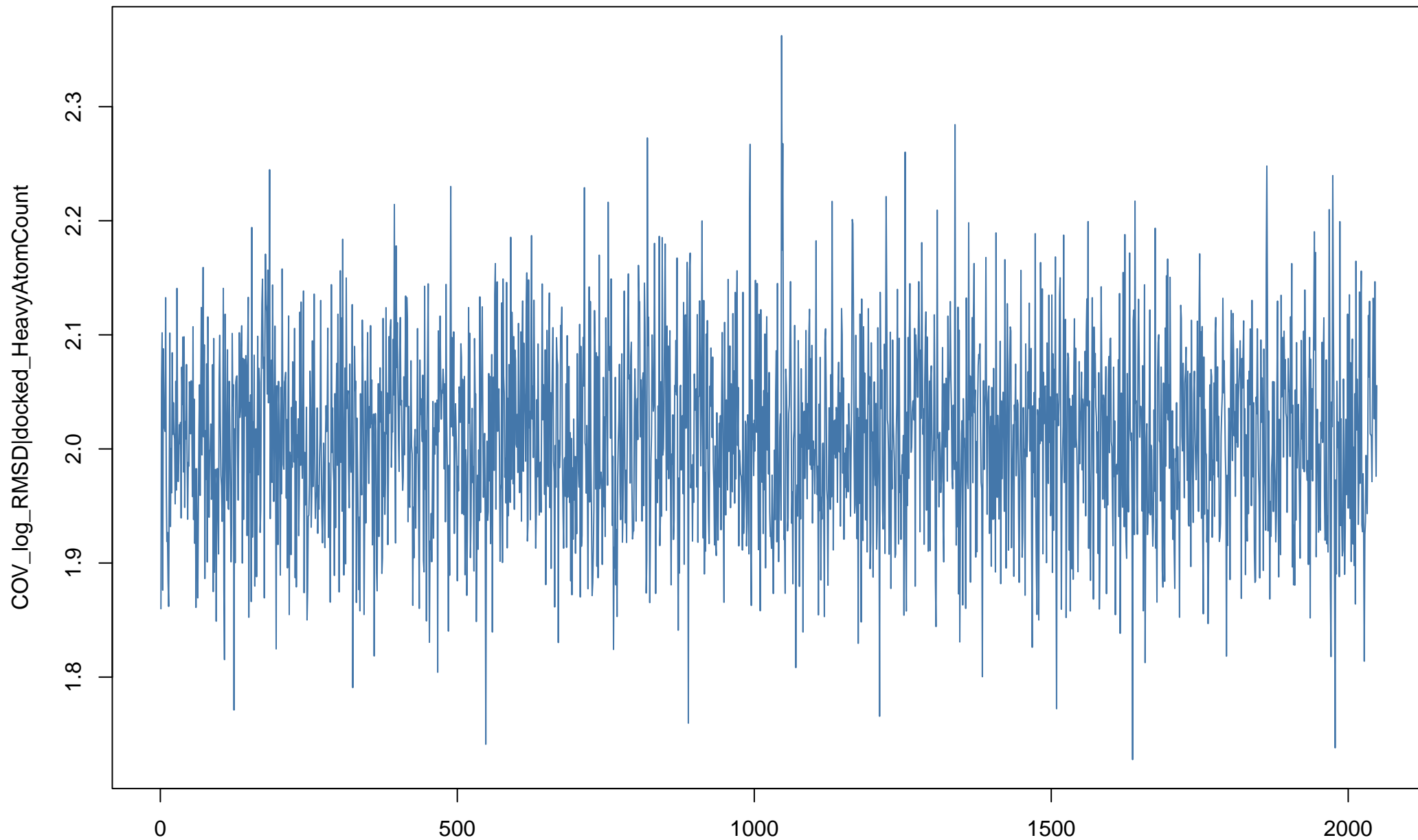
VAR_mcs_NumHeteroAtoms
ESS = 1790 | BMK = 0.0639 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0



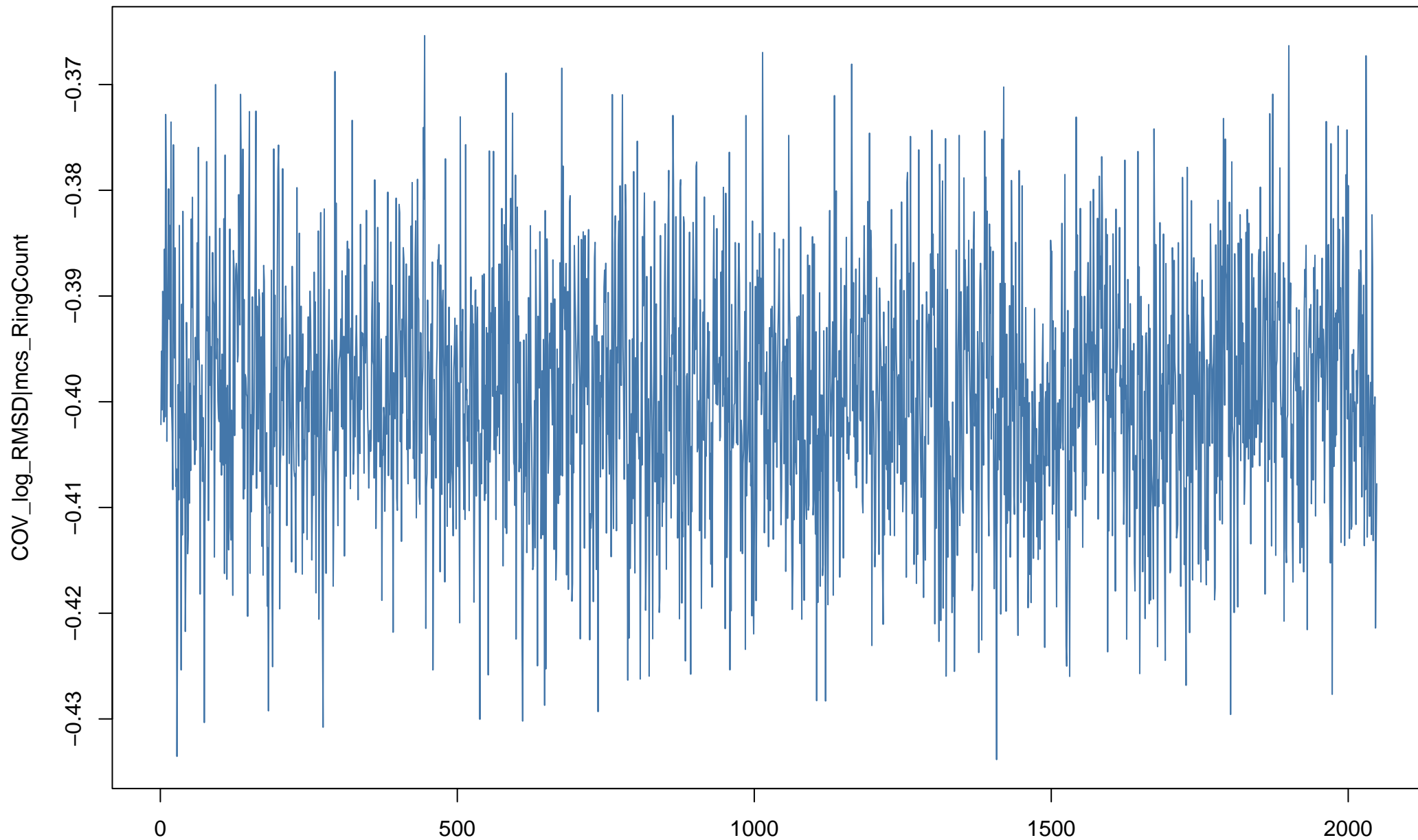
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1170 | BMK = 0.0454 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0



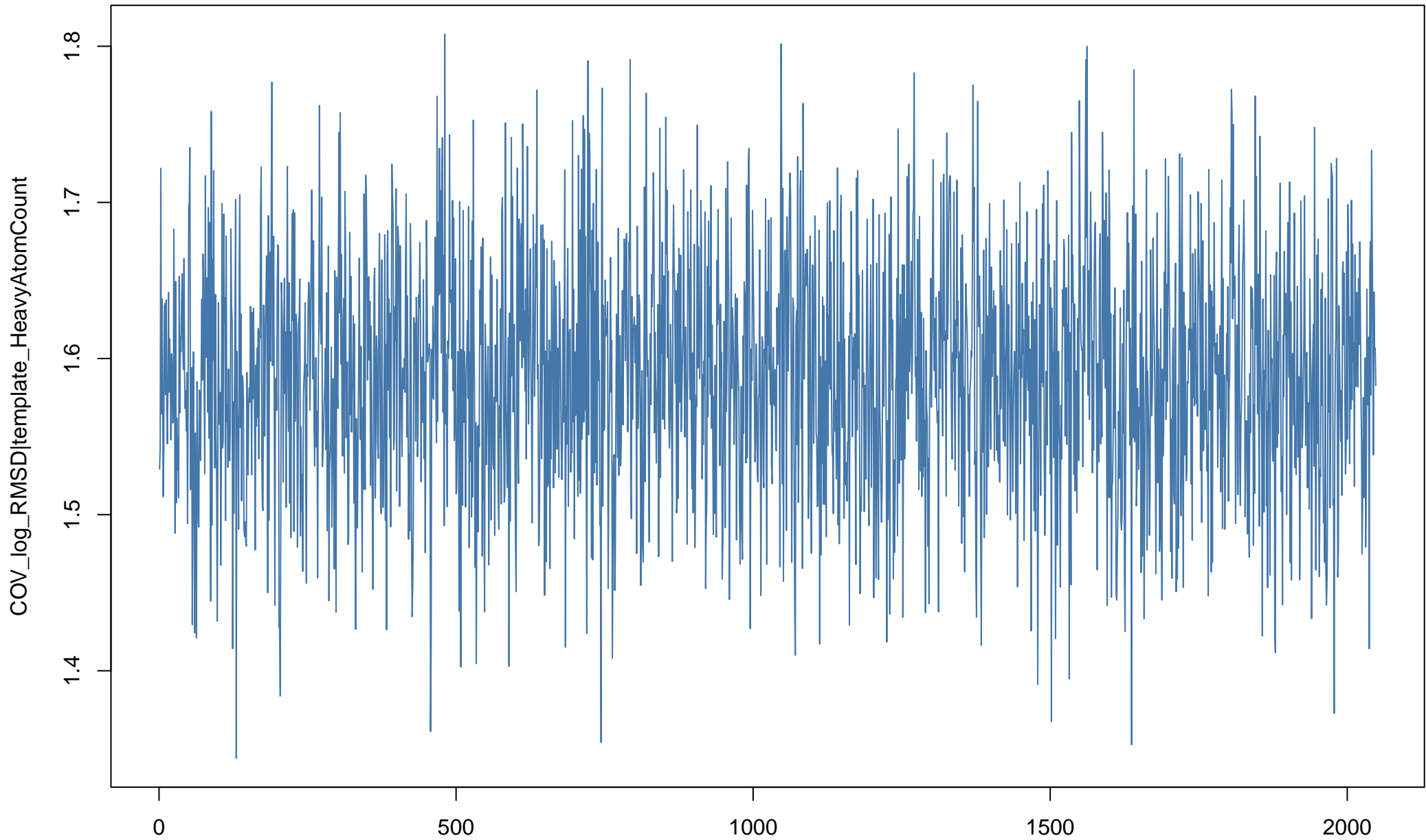
COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0358 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0



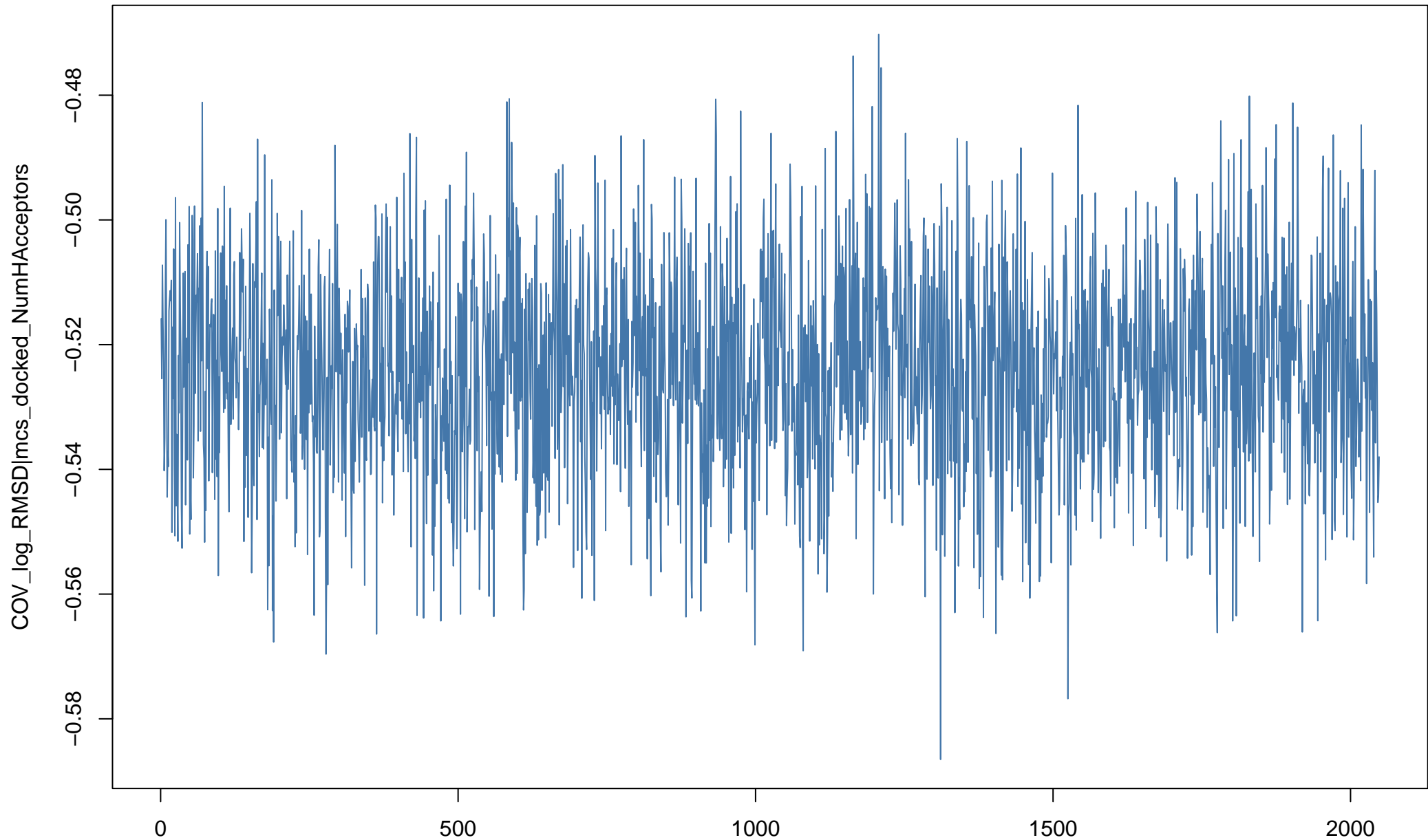
COV_log_RMSD|mcs_RingCount
ESS = 1730 | BMK = 0.0416 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0



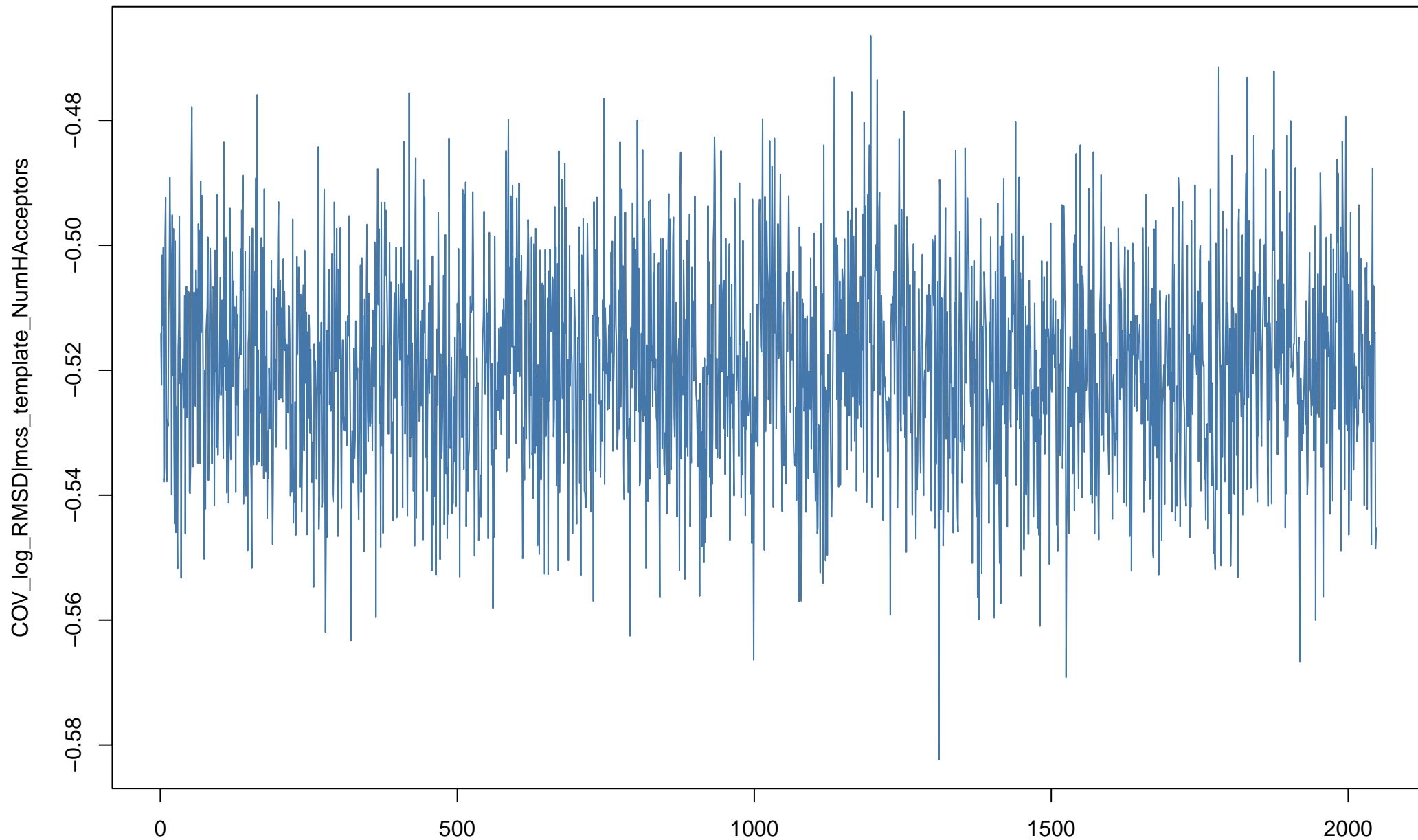
COV_log_RMSD|template_HeavyAtomCount
ESS = 1610 | BMK = 0.0269 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0



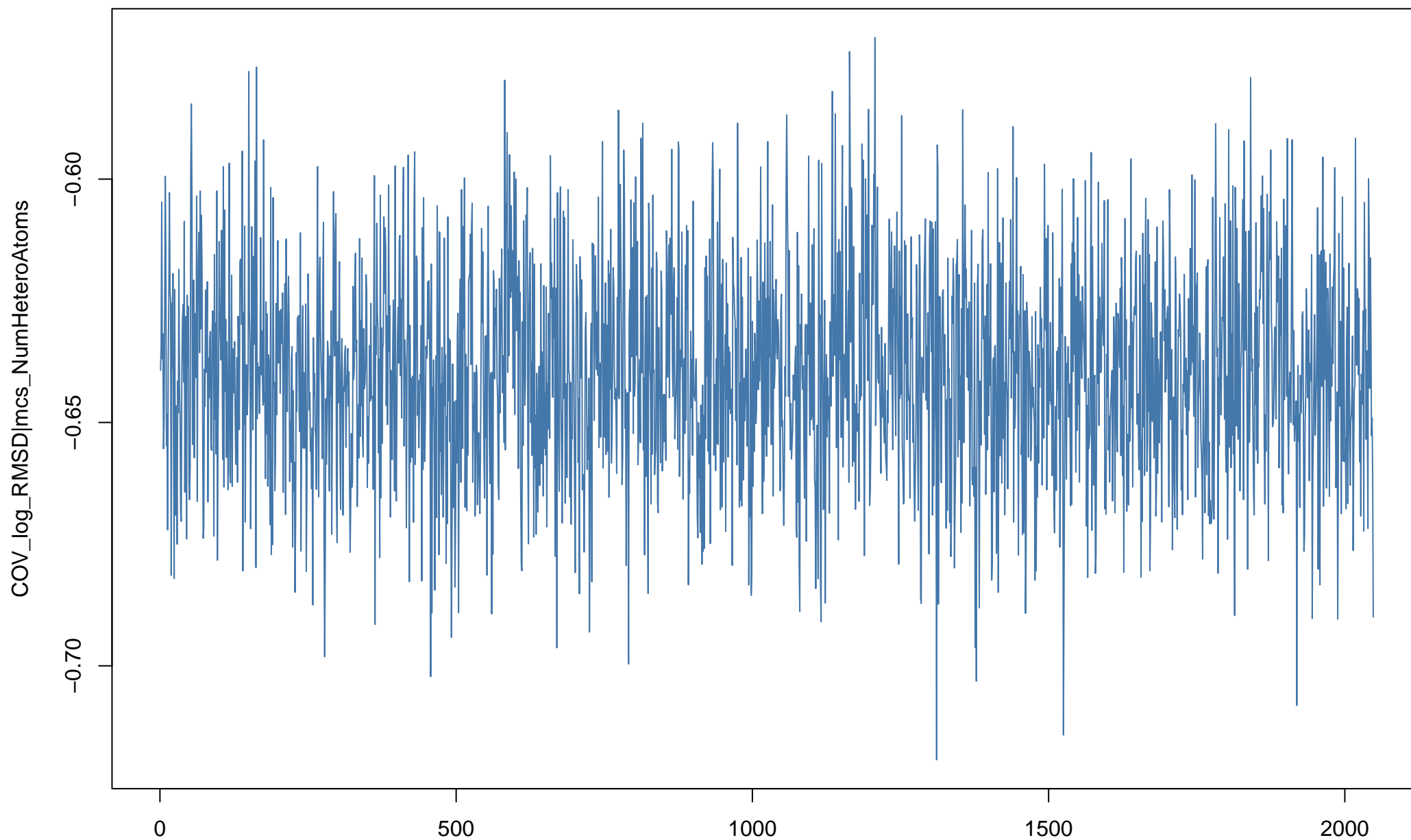
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0437 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0



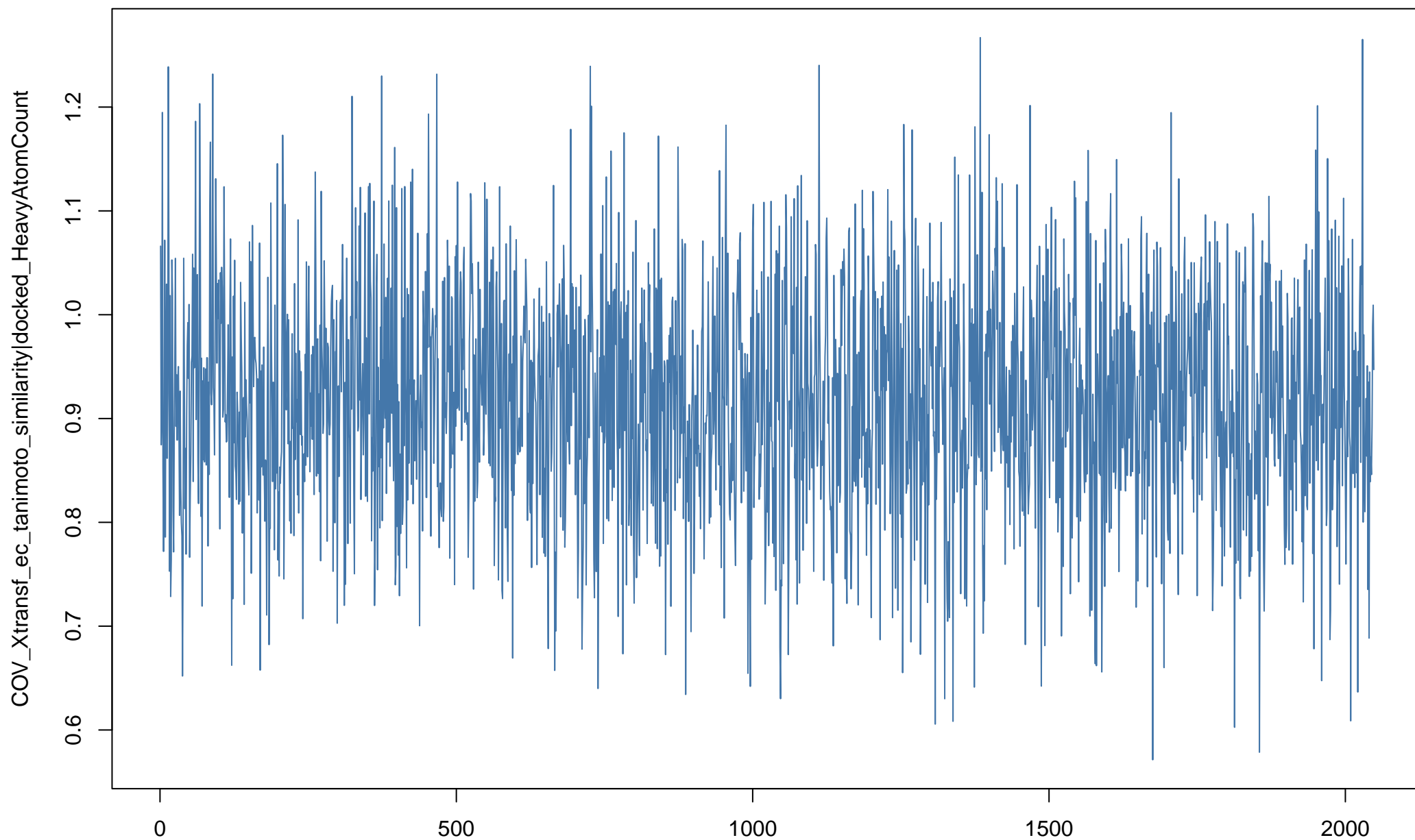
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 1810 | BMK = 0.0493 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0



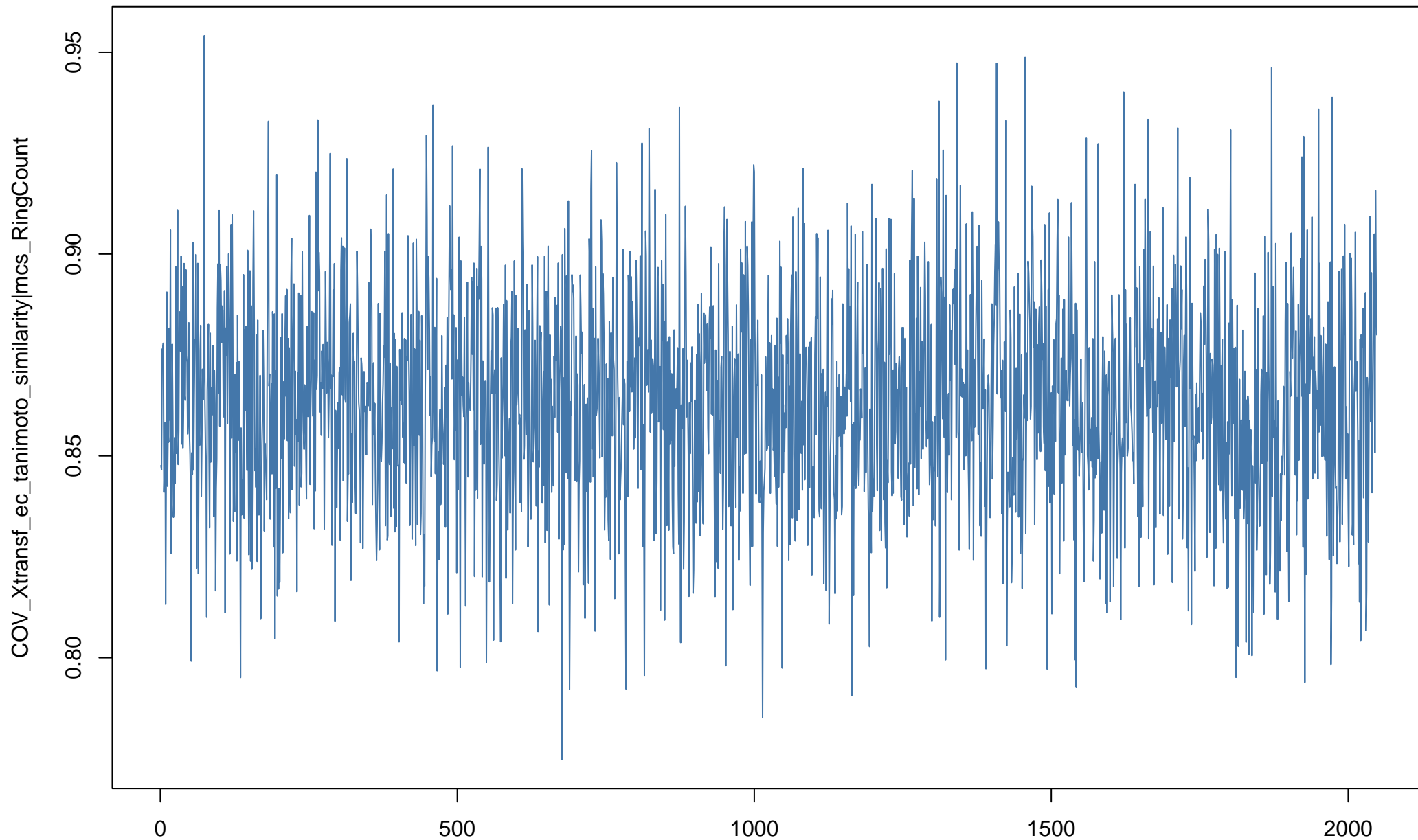
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1720 | BMK = 0.0351 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0



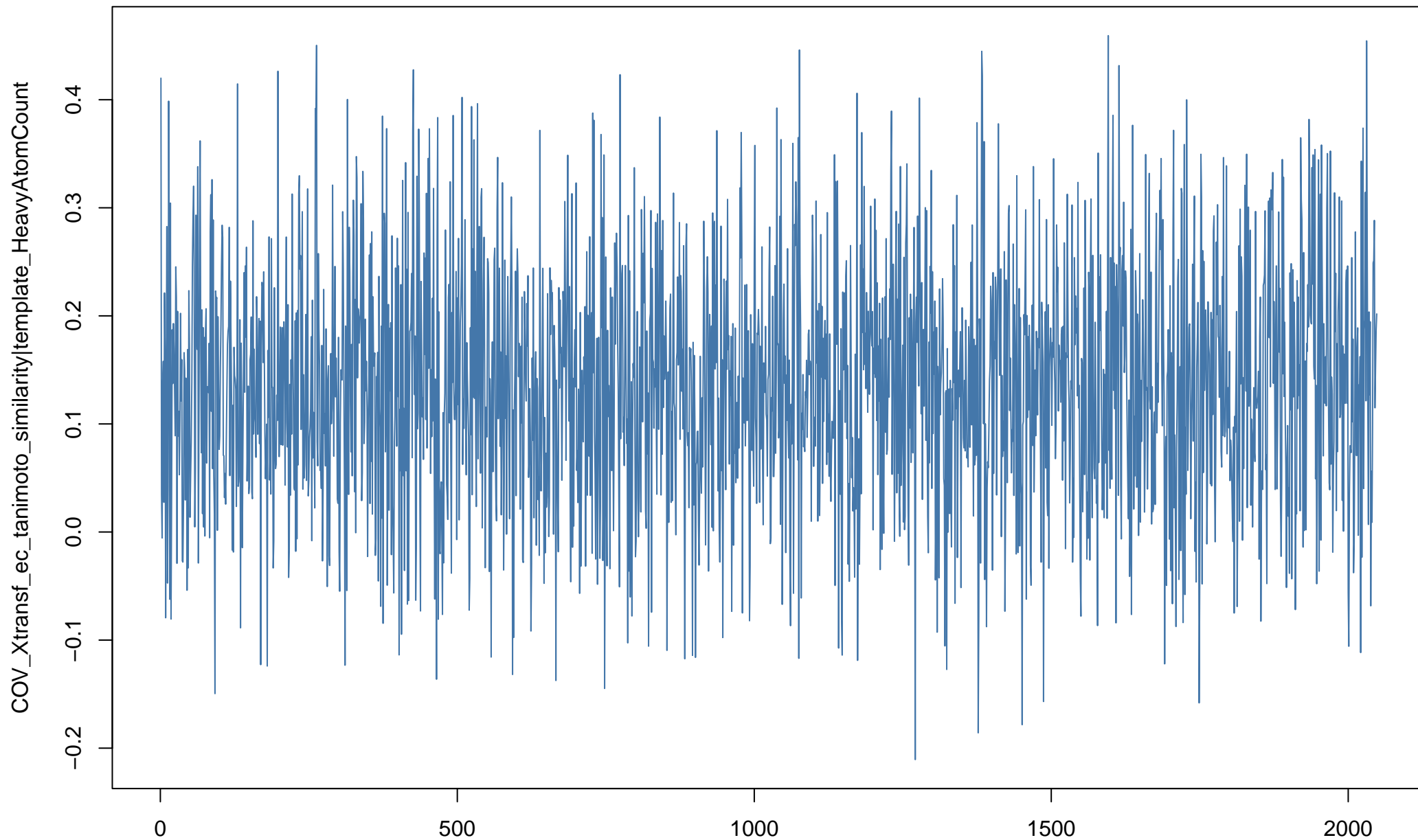
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1770 | BMK = 0.0538 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0



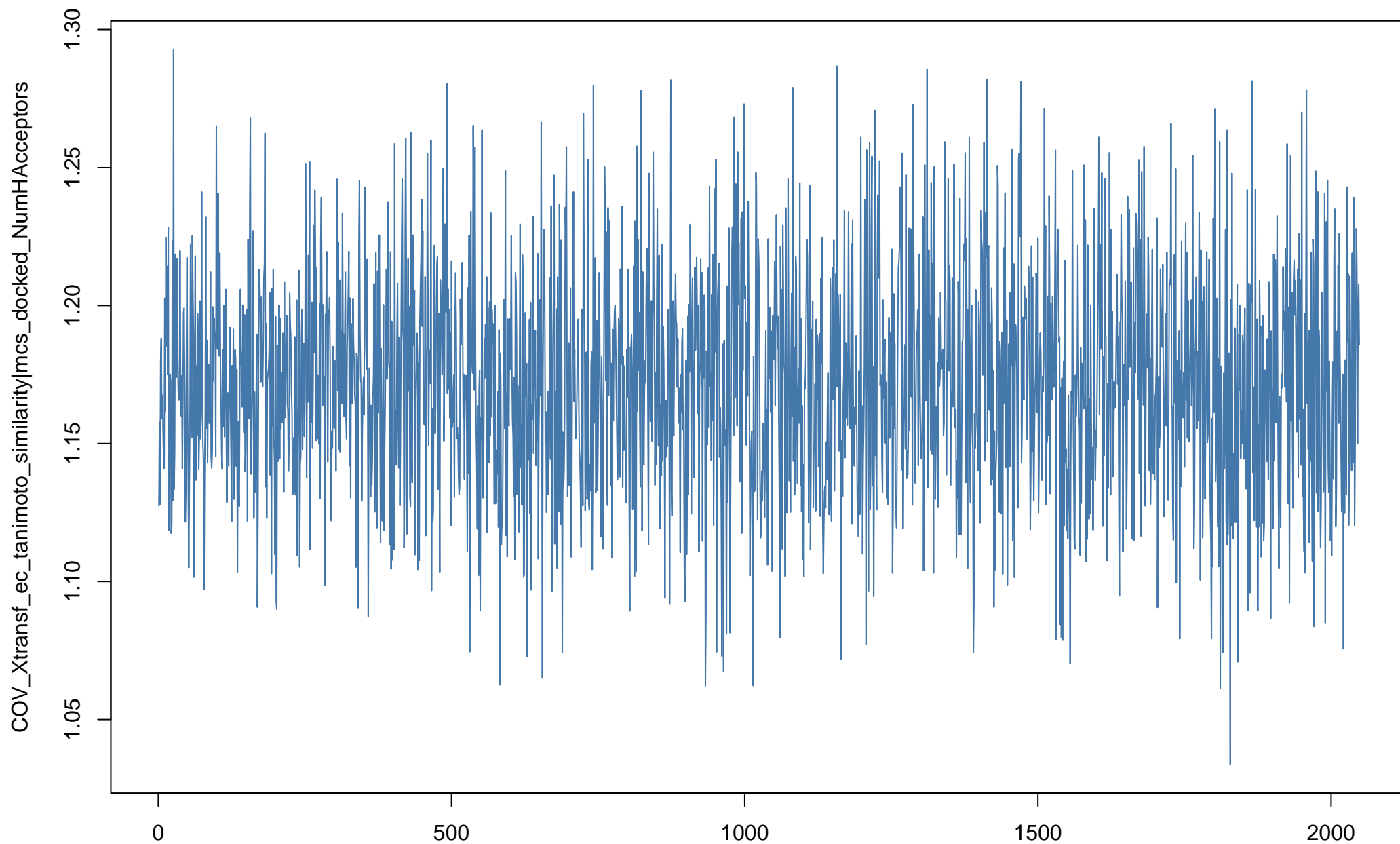
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1810 | BMK = 0.0409 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0



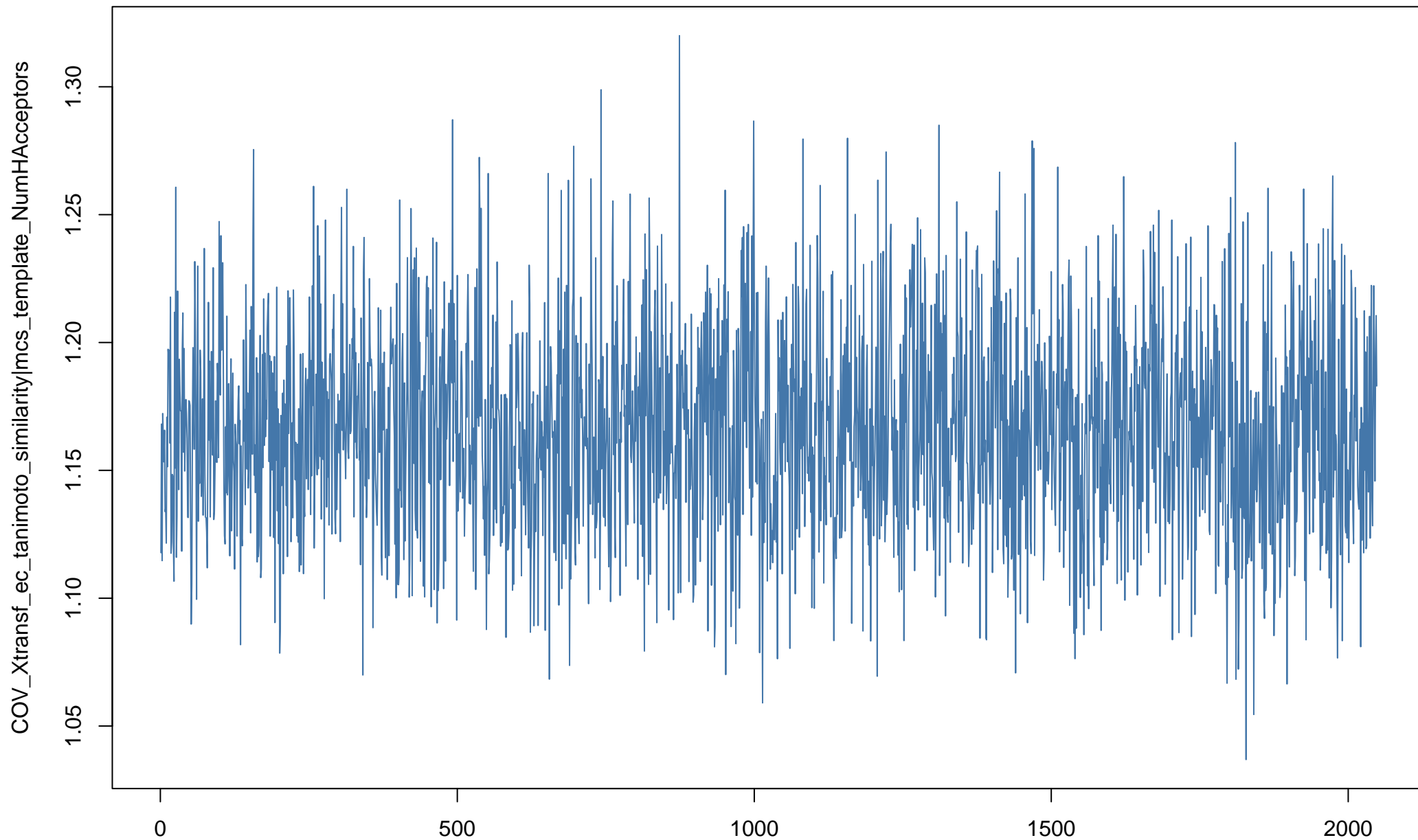
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 2050 | BMK = 0.0386 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



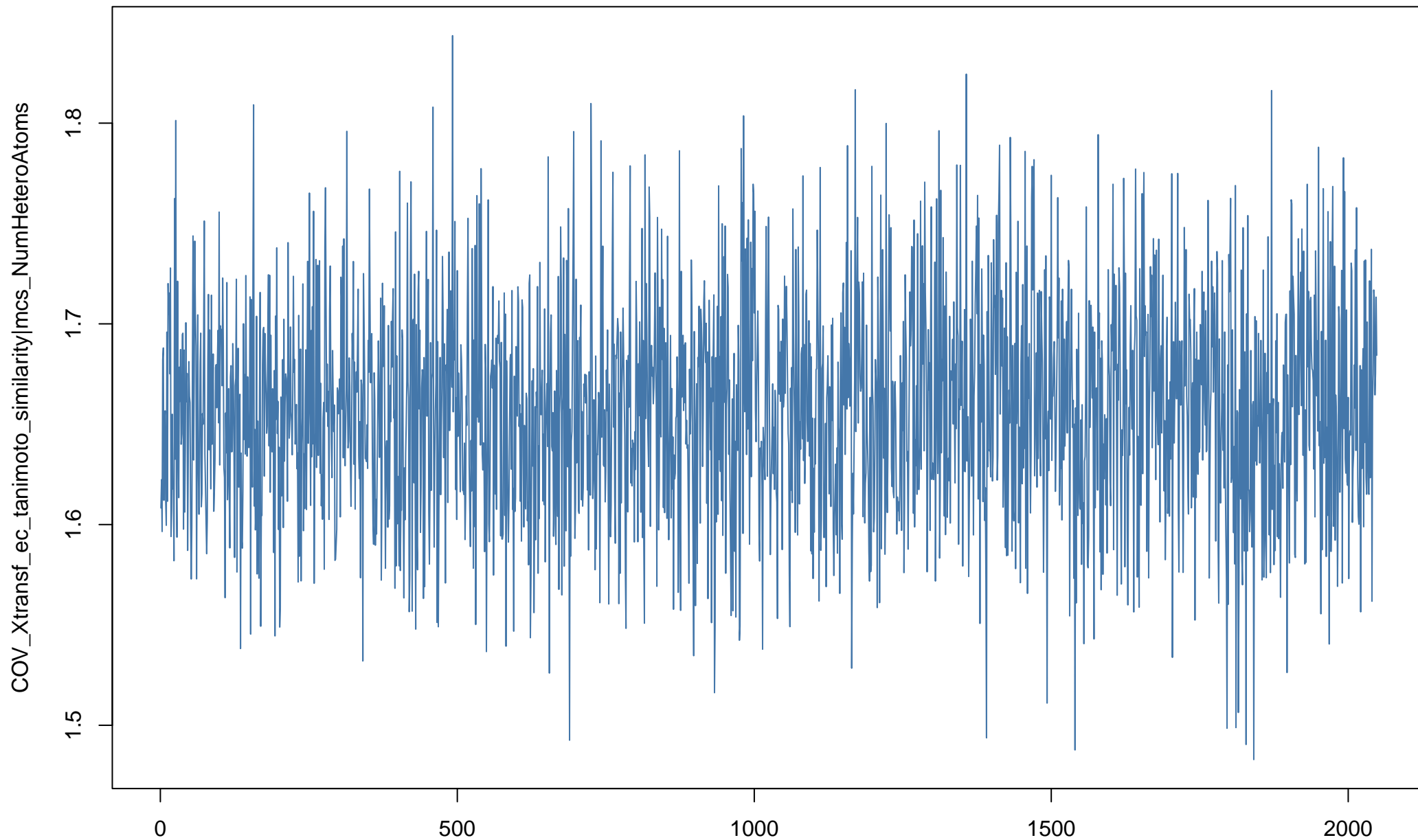
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0449 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0



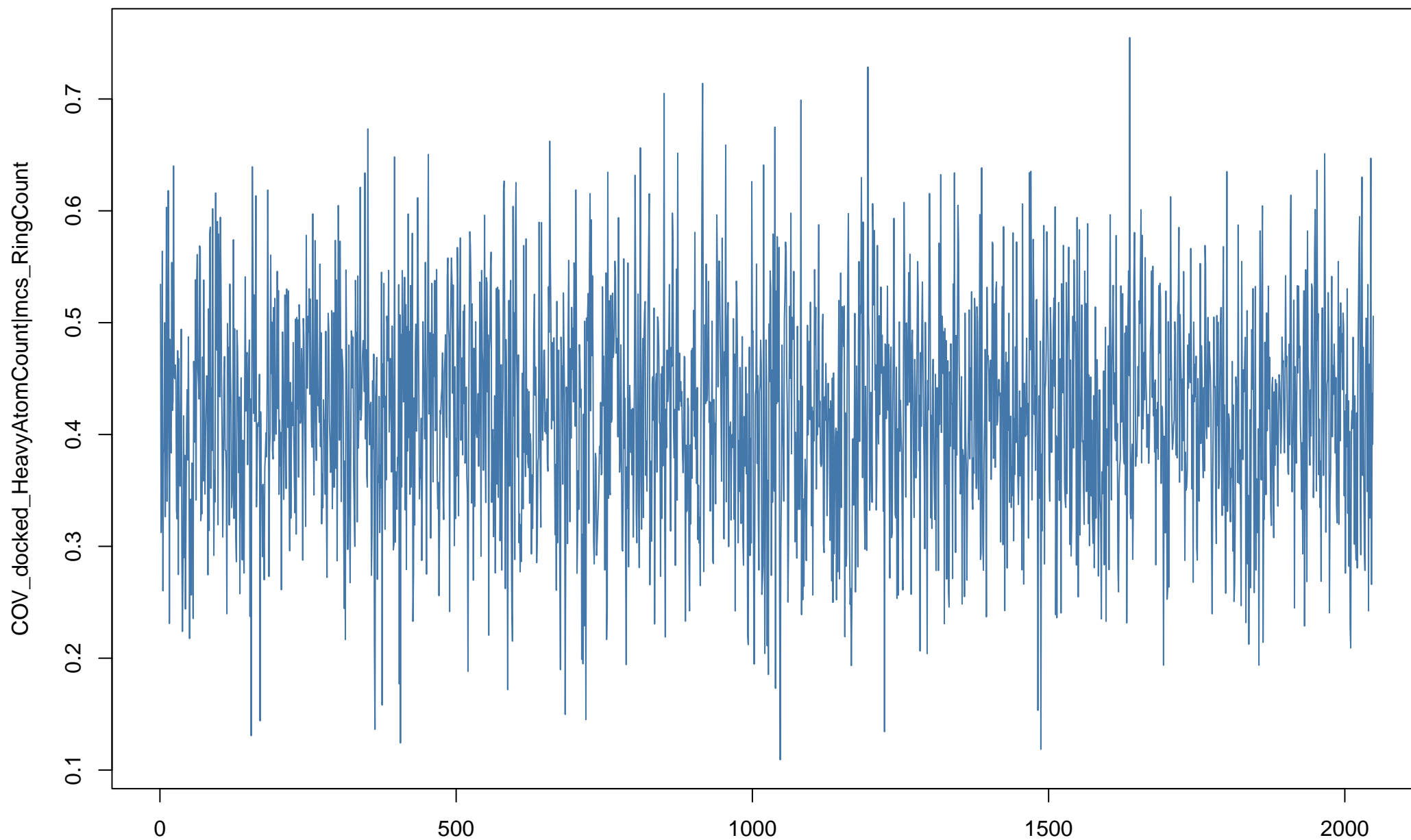
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0482 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0



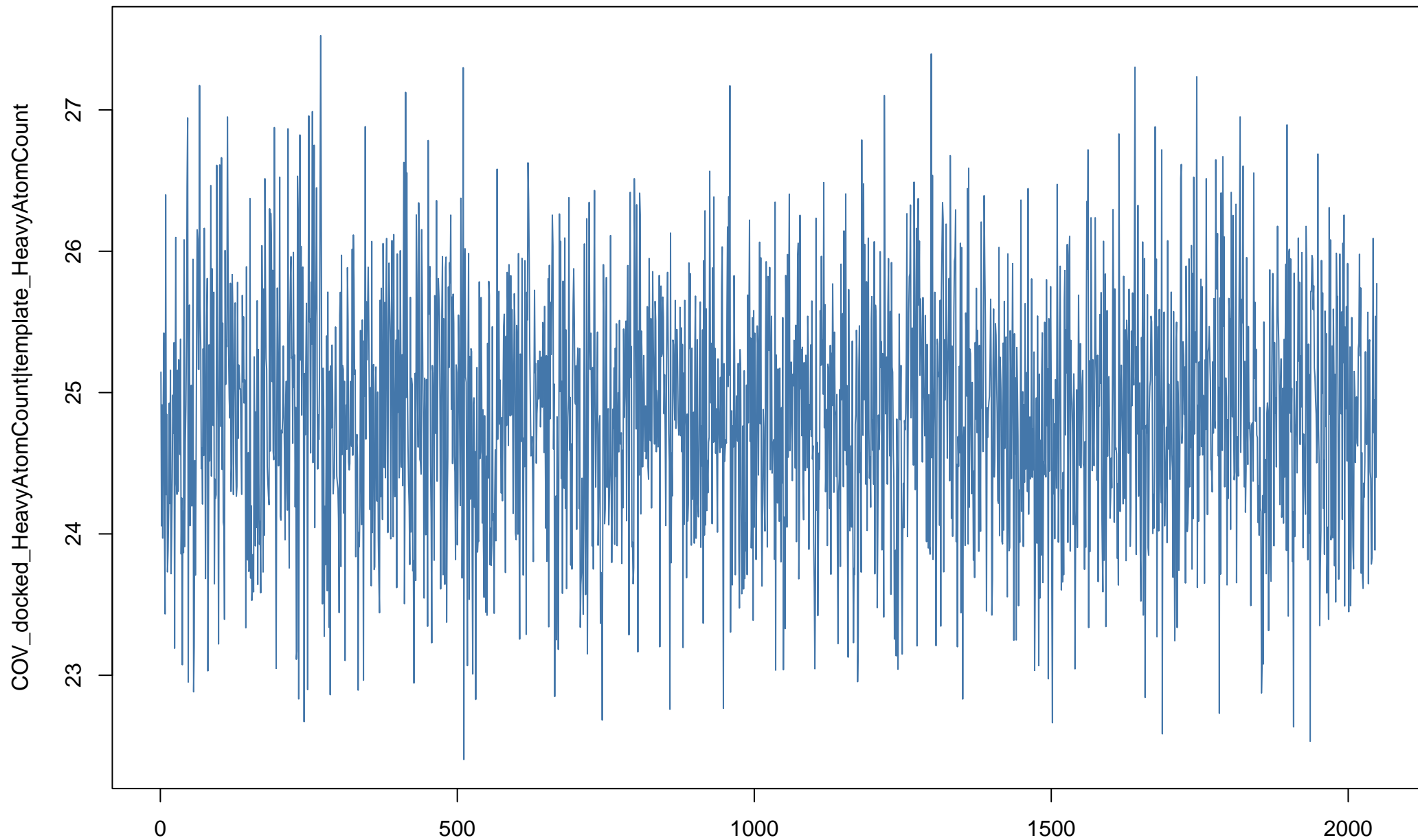
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1800 | BMK = 0.0608 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0



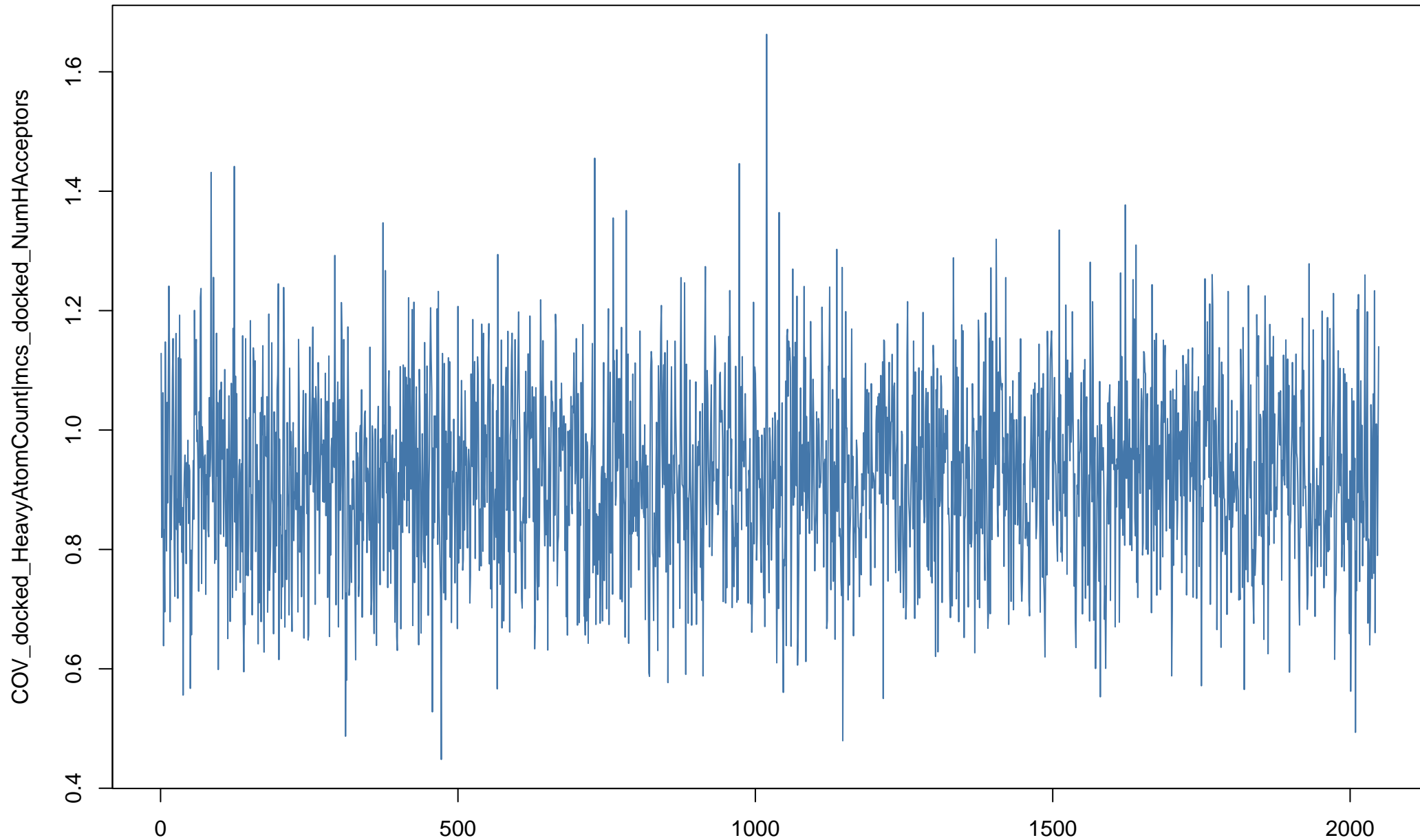
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1750 | BMK = 0.0401 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0



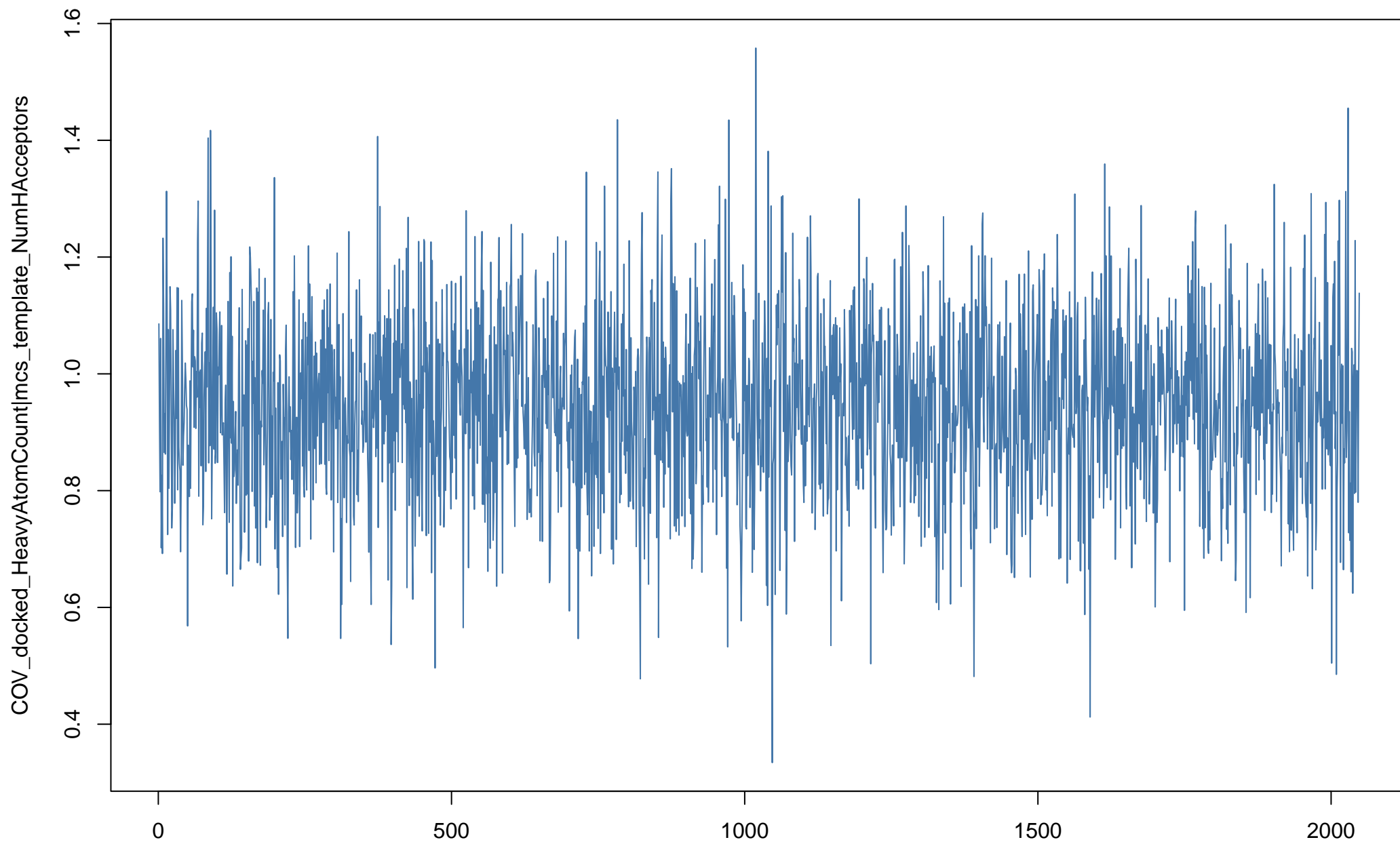
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1700 | BMK = 0.0238 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0



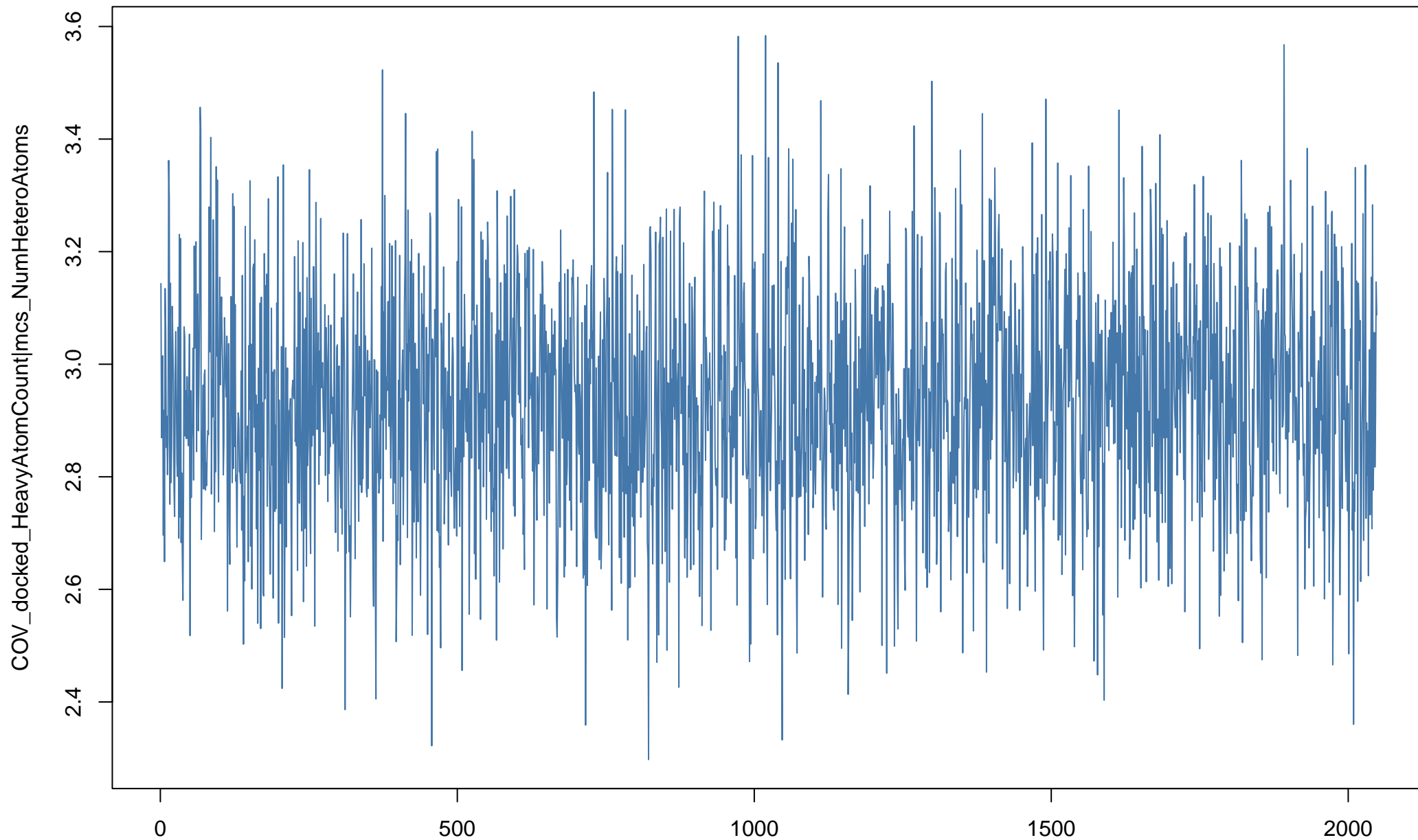
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0542 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0



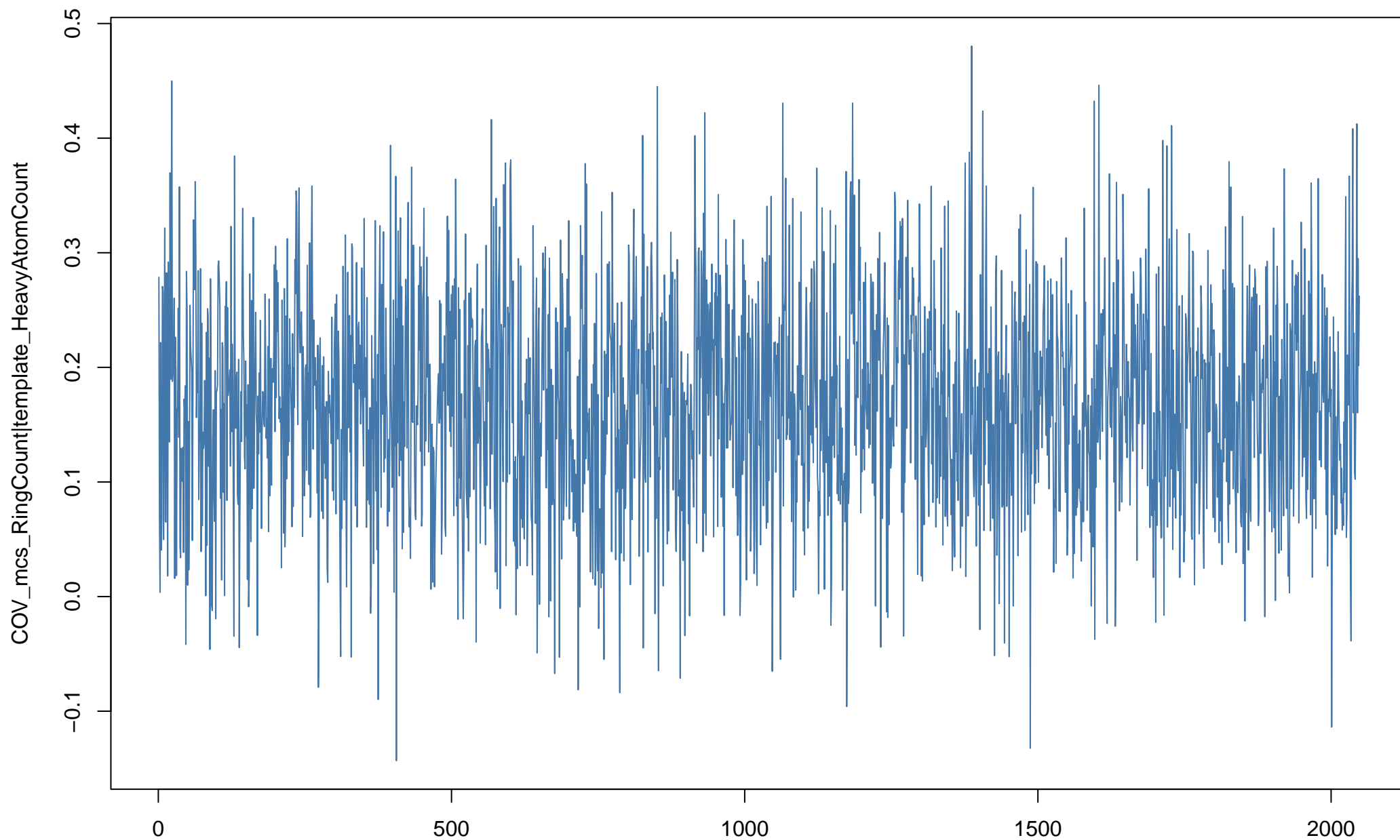
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0402 | MCSE(6.27) = 1.83 | stat: TRUE | burn: 0



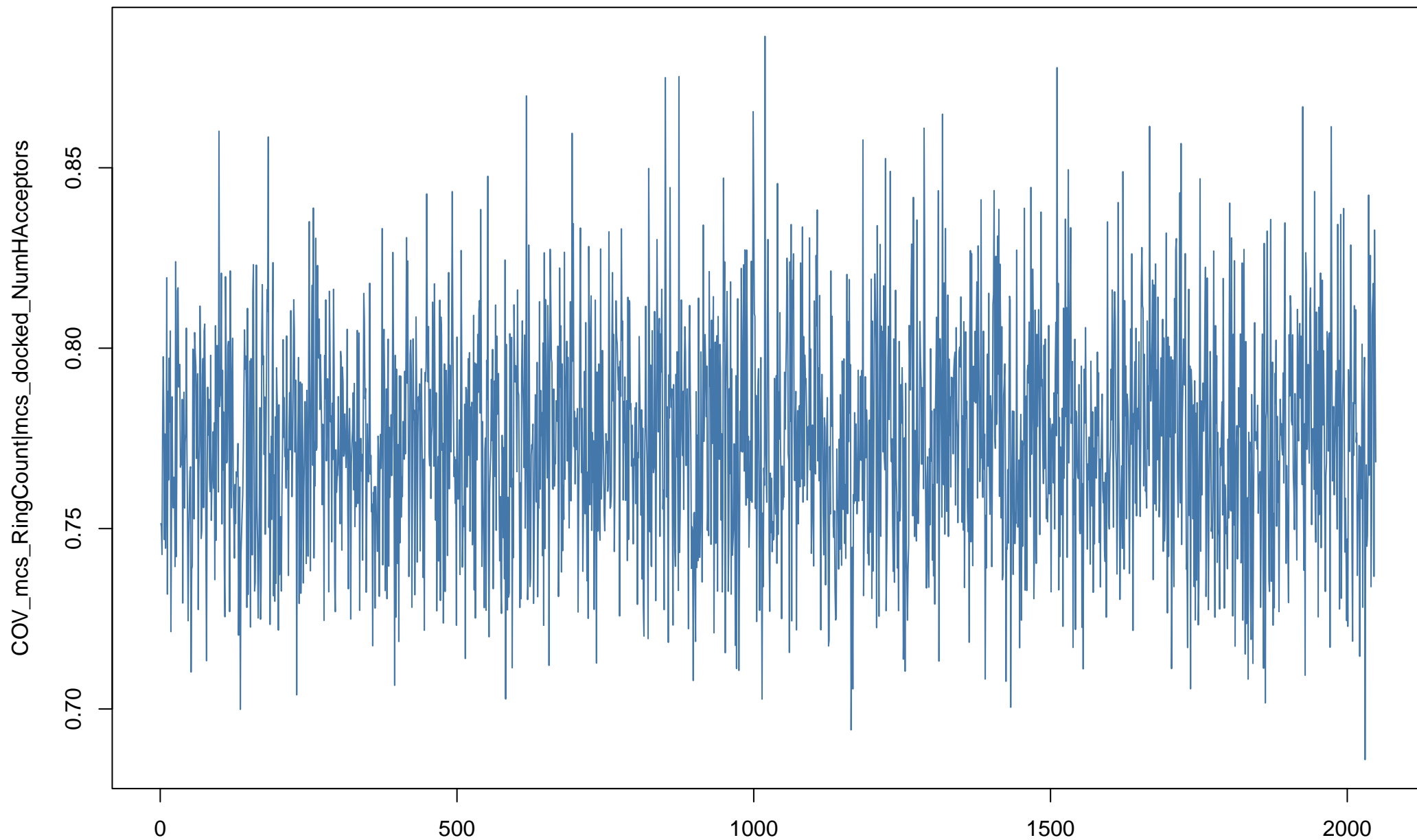
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0386 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0



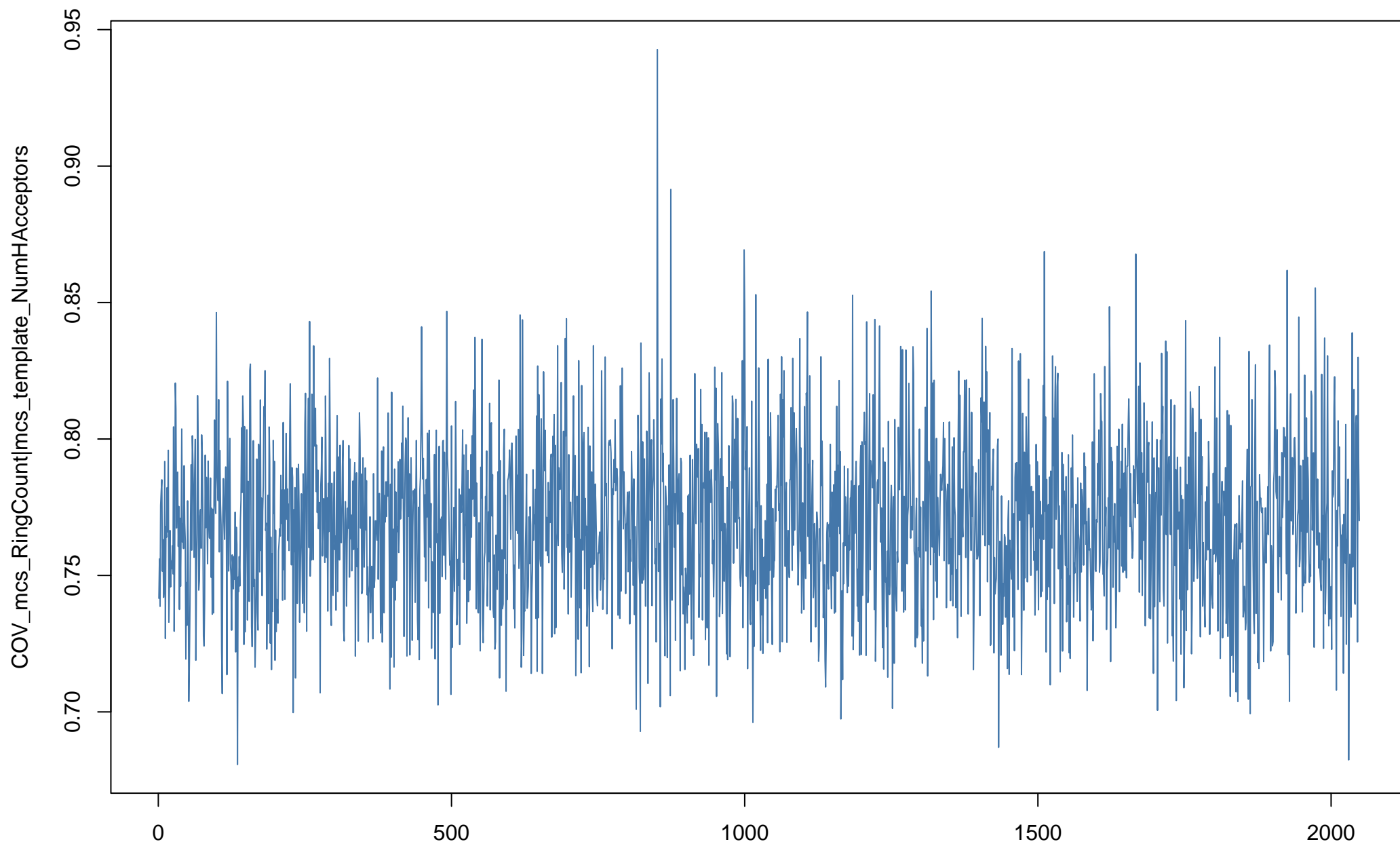
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1860 | BMK = 0.0528 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0



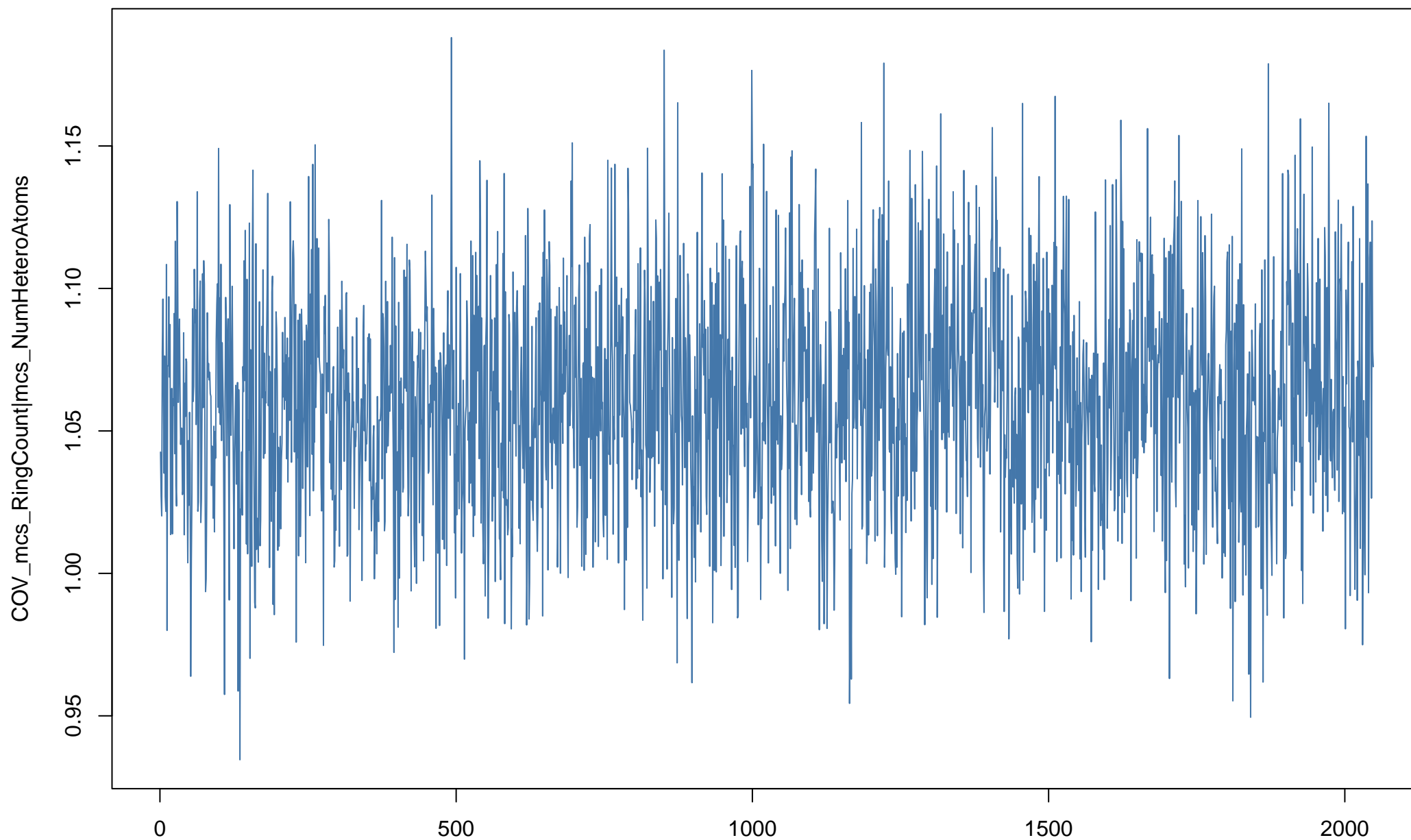
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 1910 | BMK = 0.0571 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



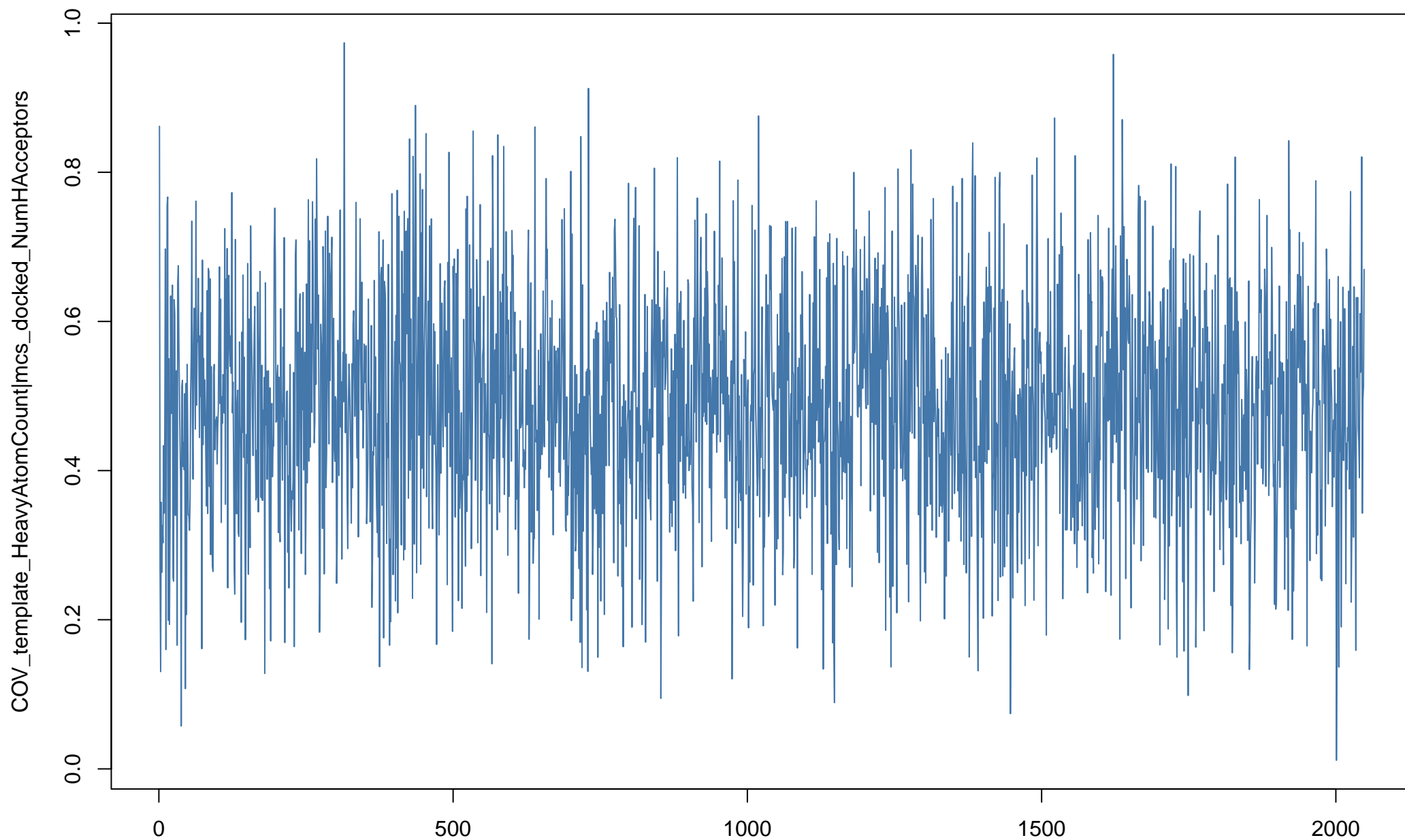
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 1870 | BMK = 0.0536 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



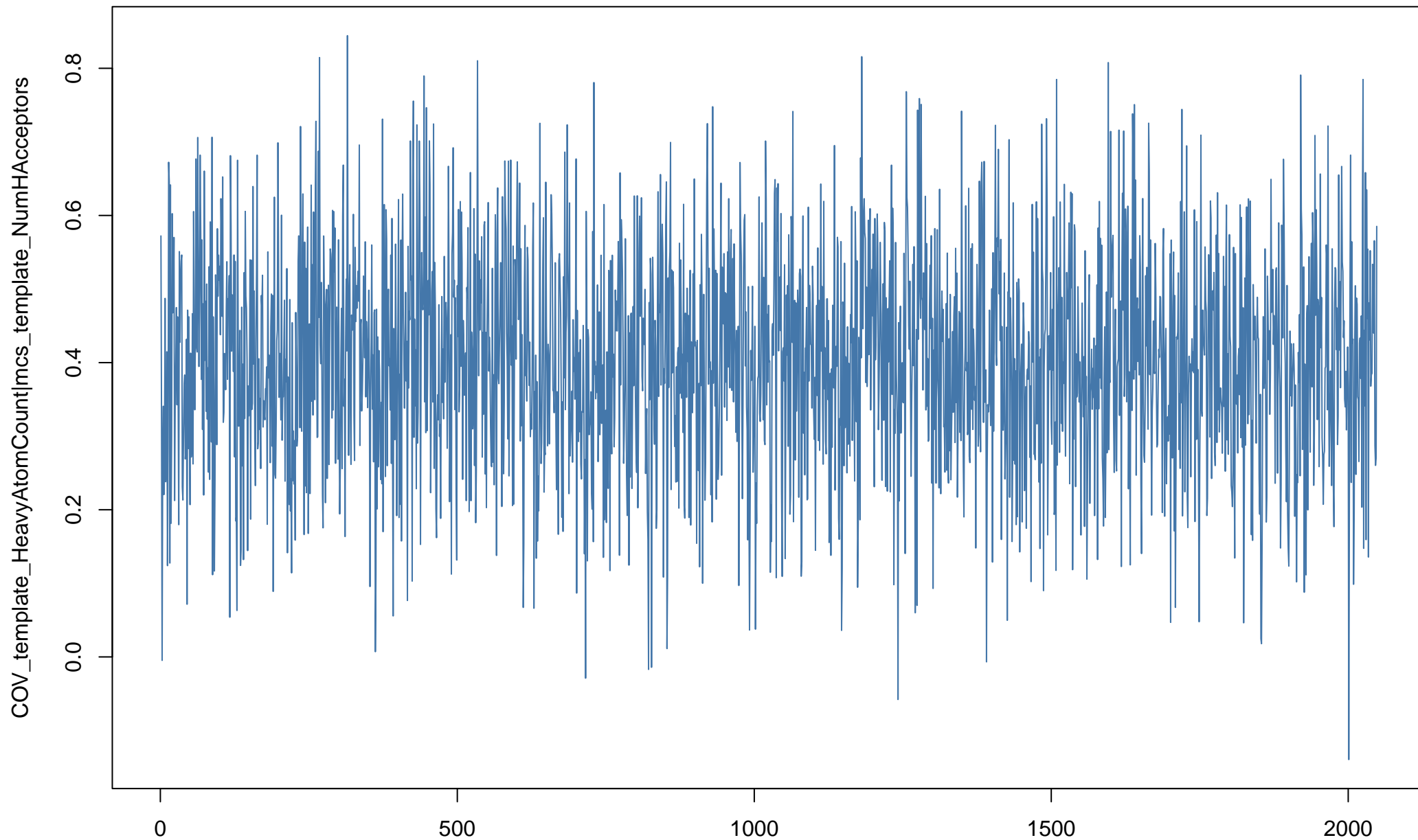
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 1250 | BMK = 0.0574 | MCSE(6.27) = 2.72 | stat: FALSE | burn: 0



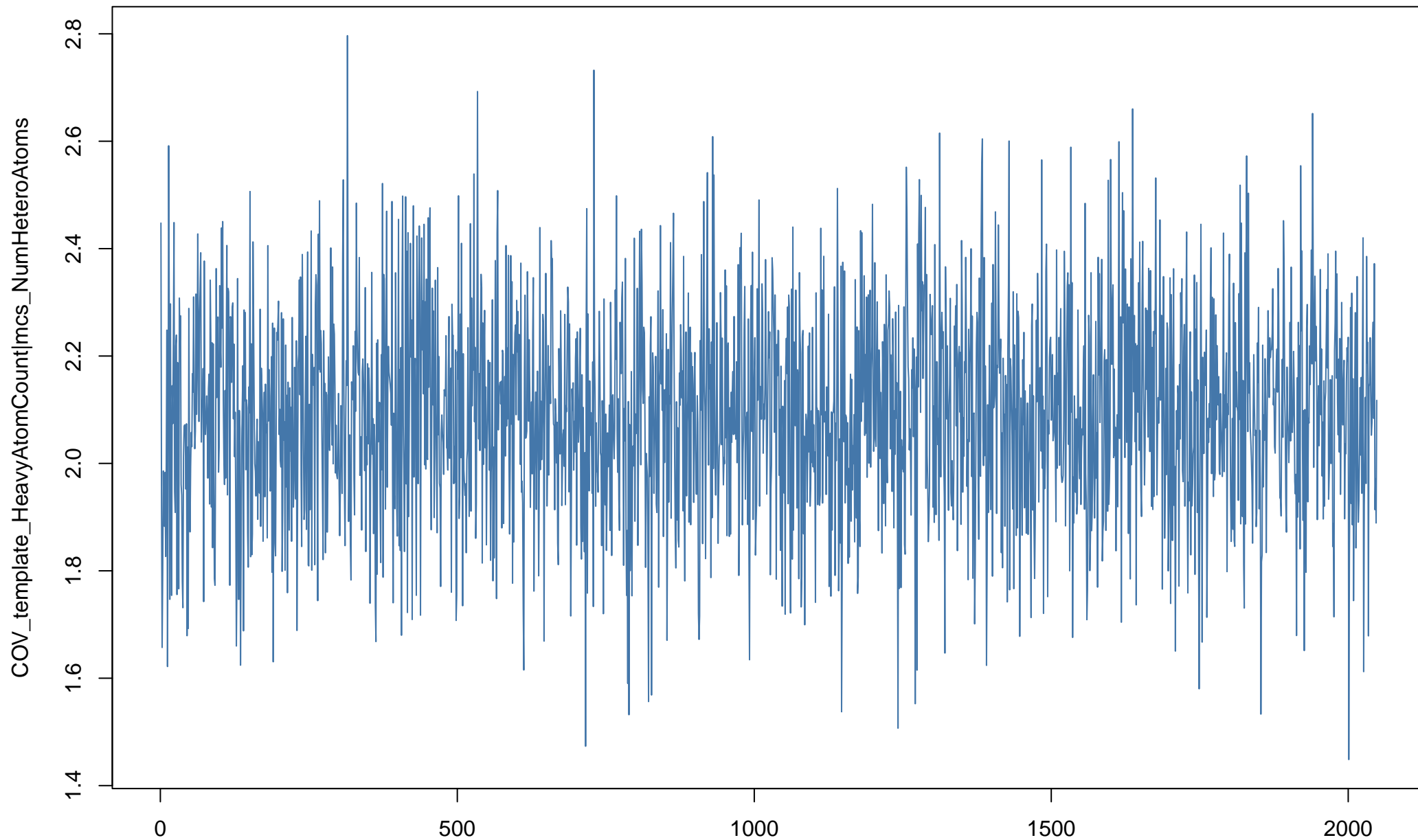
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0335 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



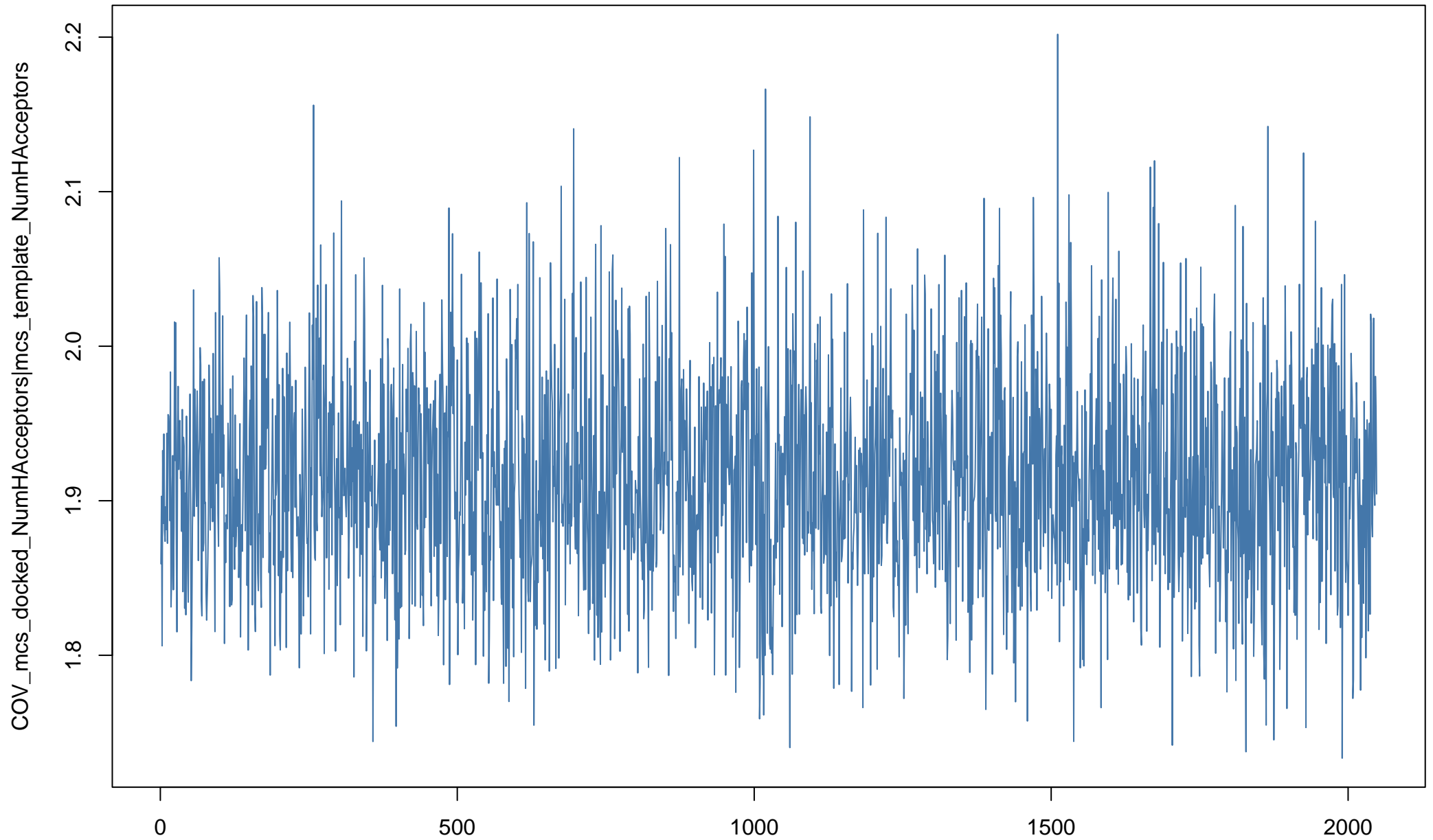
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0352 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0



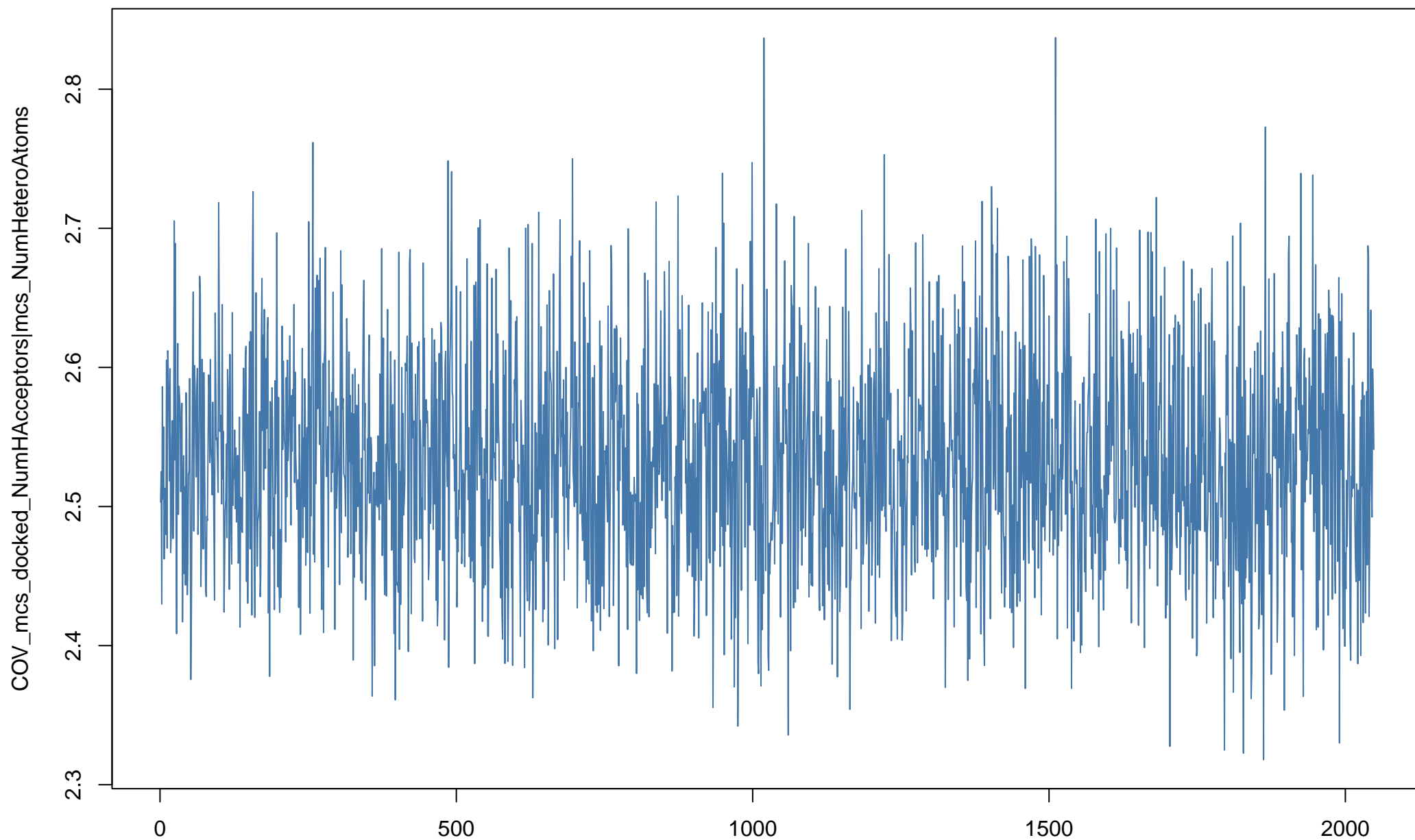
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0377 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0449 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0342 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0

