

-- STATS maxD --

min ESS = 2.68359678111082

max BMK = 0.735309281845489

max MCSE = 14.2398877559166

all stationary: FALSE

burn: 2040

-- STATS 2D --

min ESS = 523.871673583216

max BMK = 0.114806279681349

max MCSE = 3.44010662849159

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.140775190889991

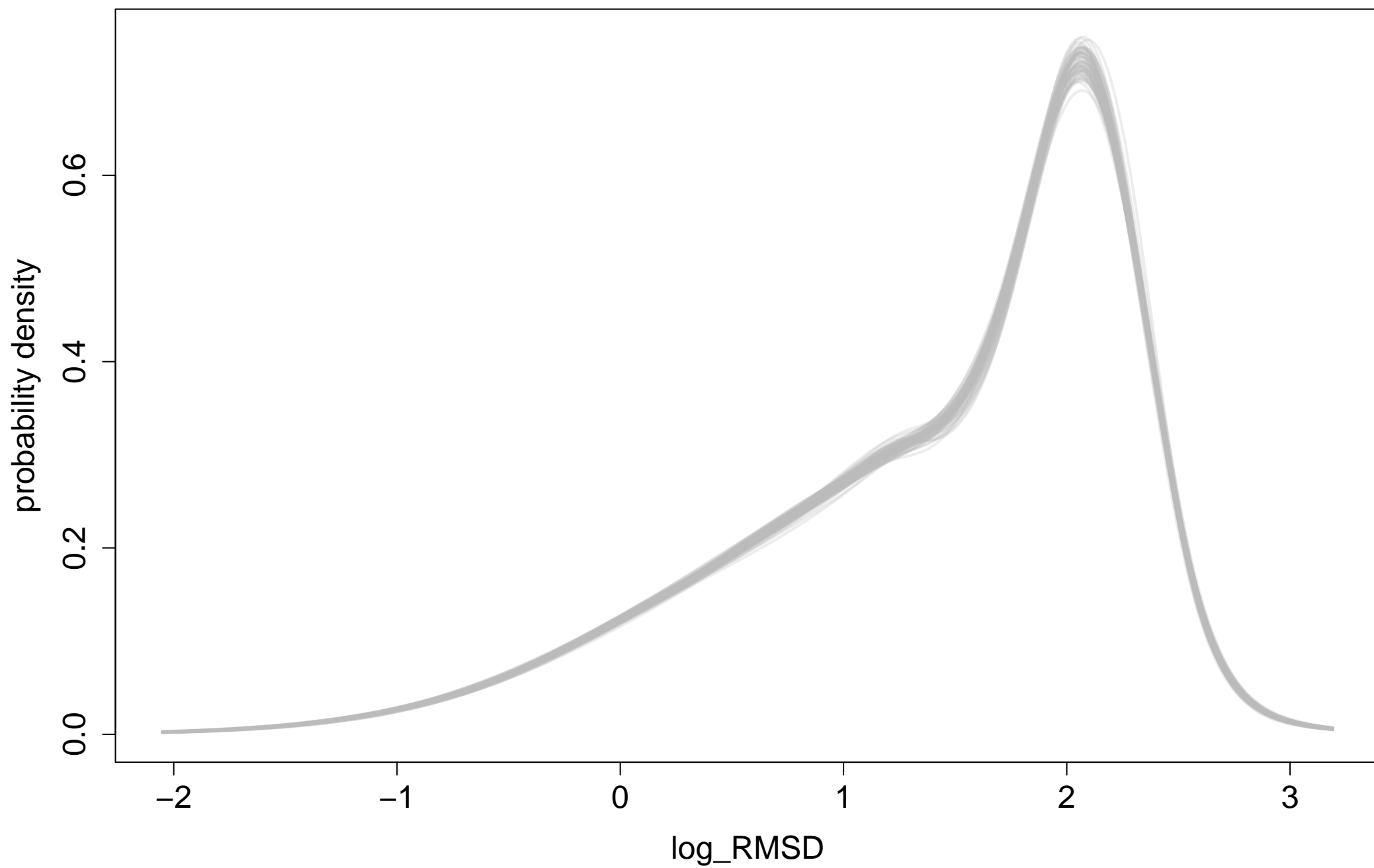
max MCSE = NaN

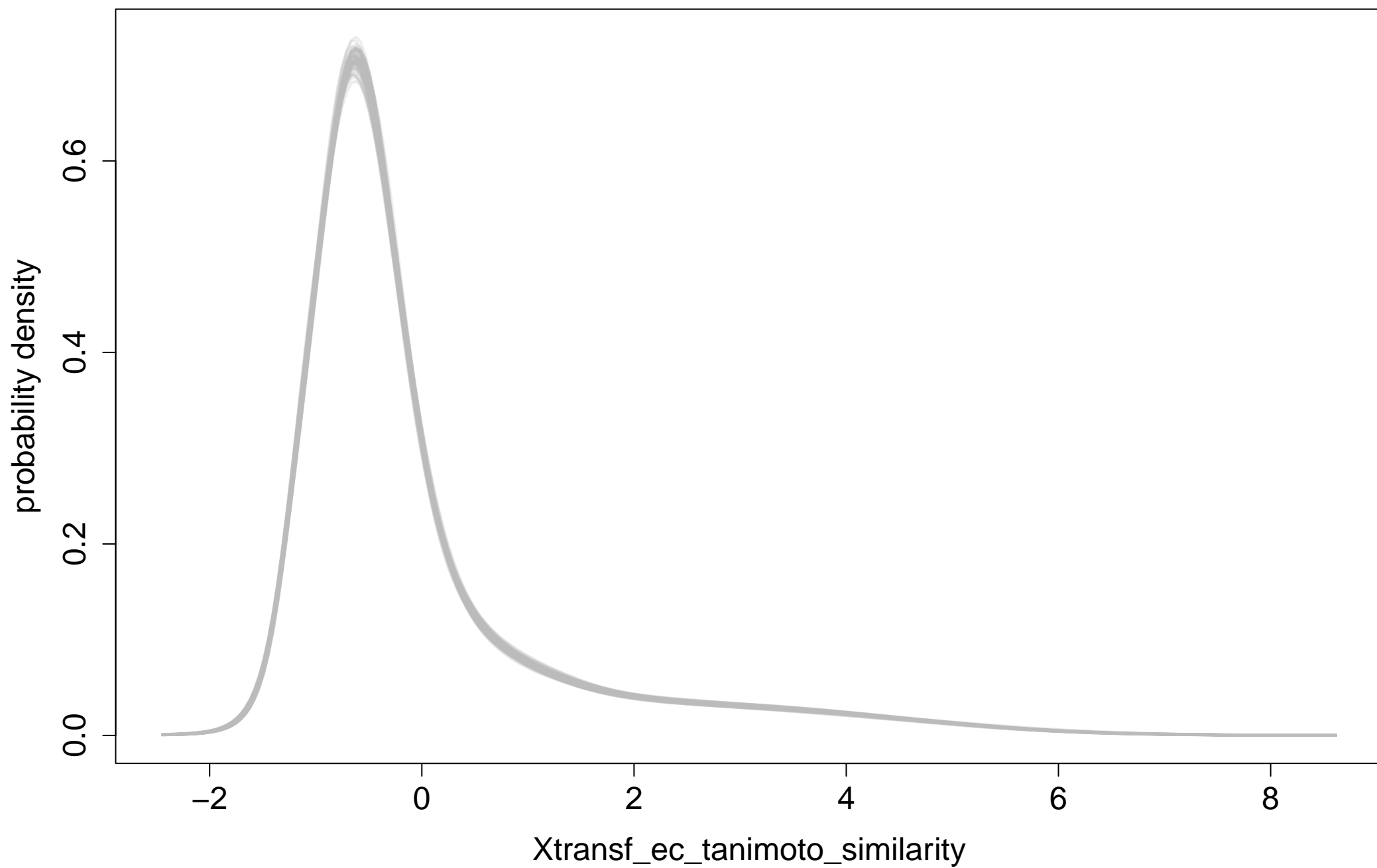
all stationary: FALSE

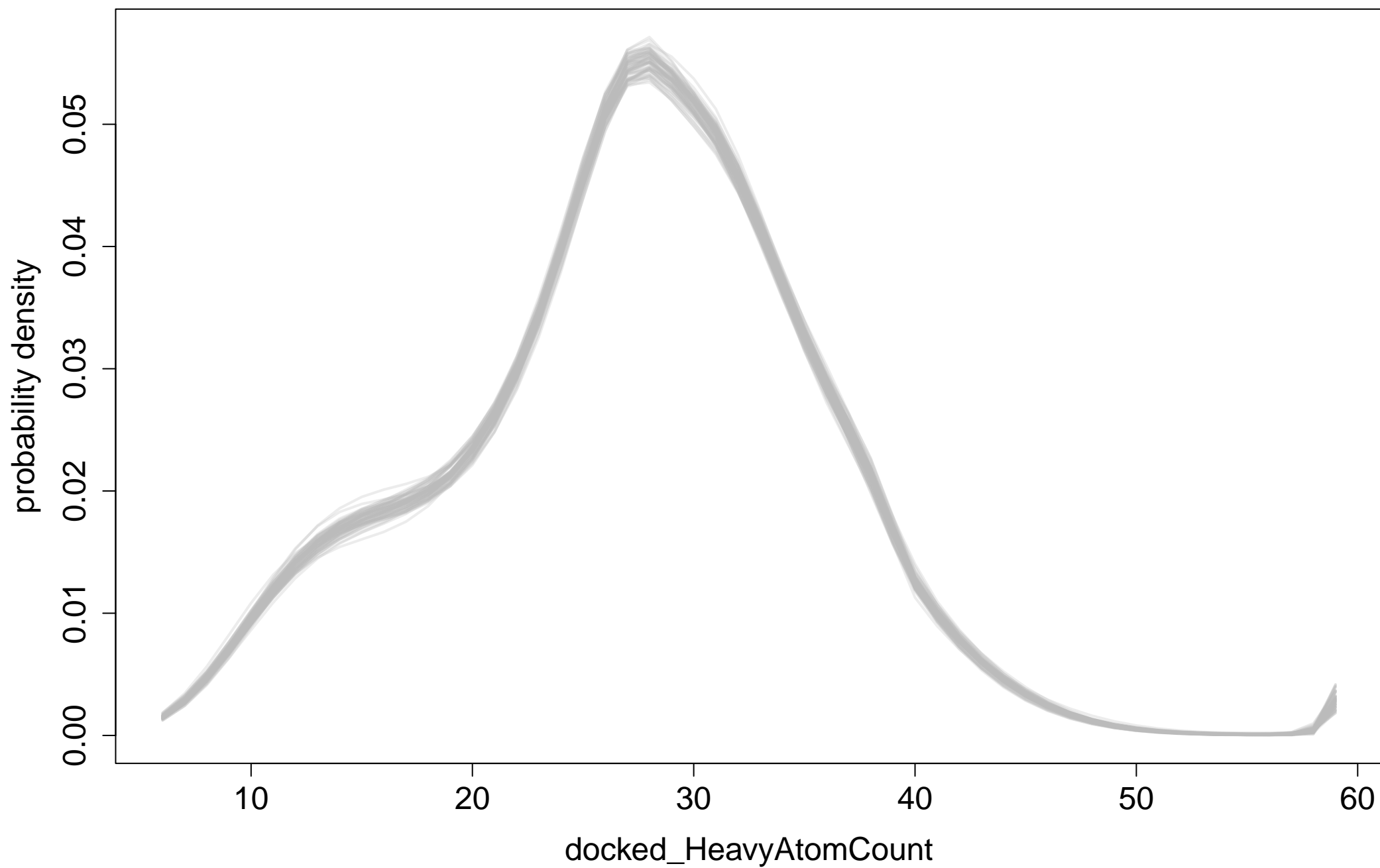
burn: 2040

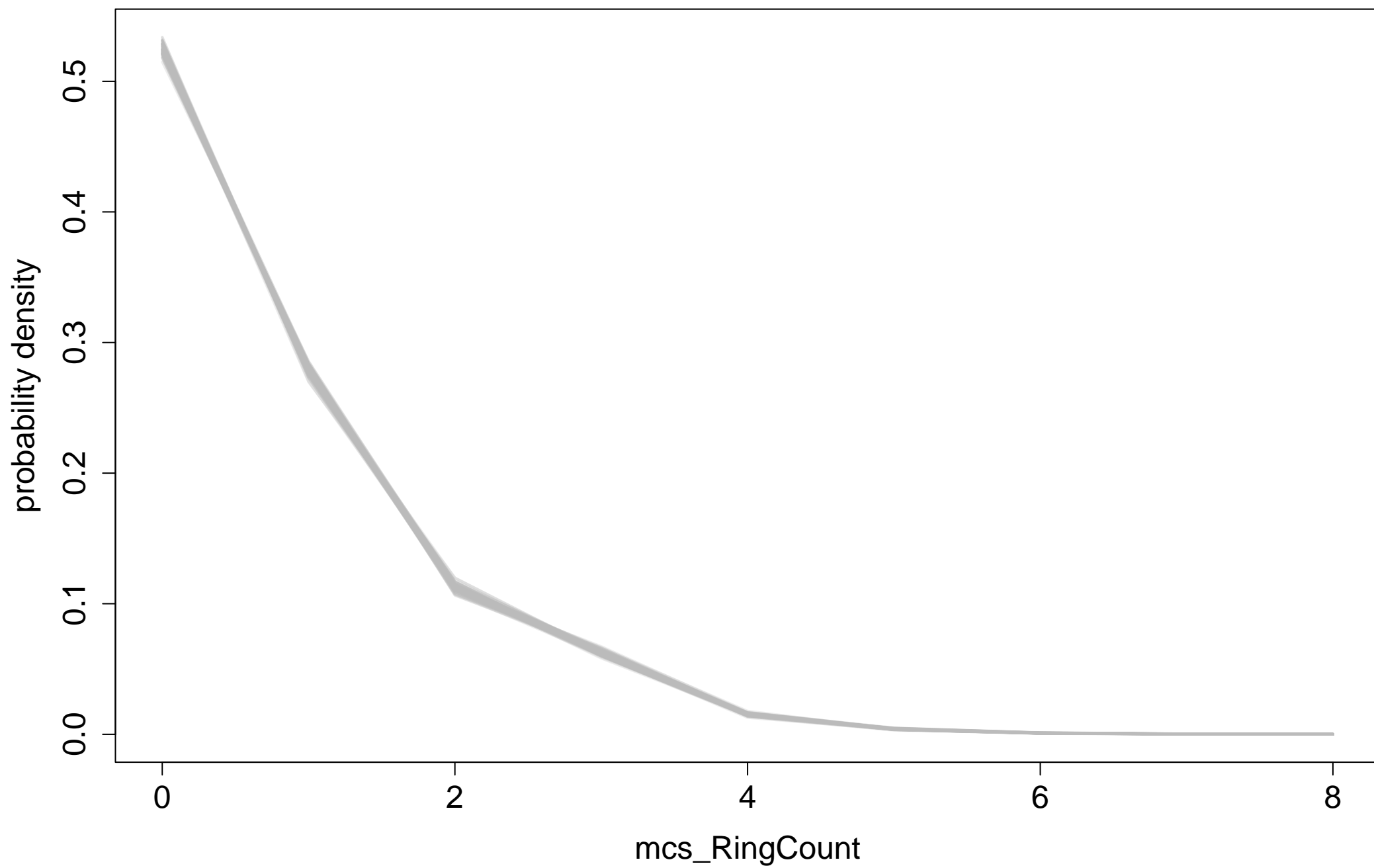
Occupied clusters: 72 of 91

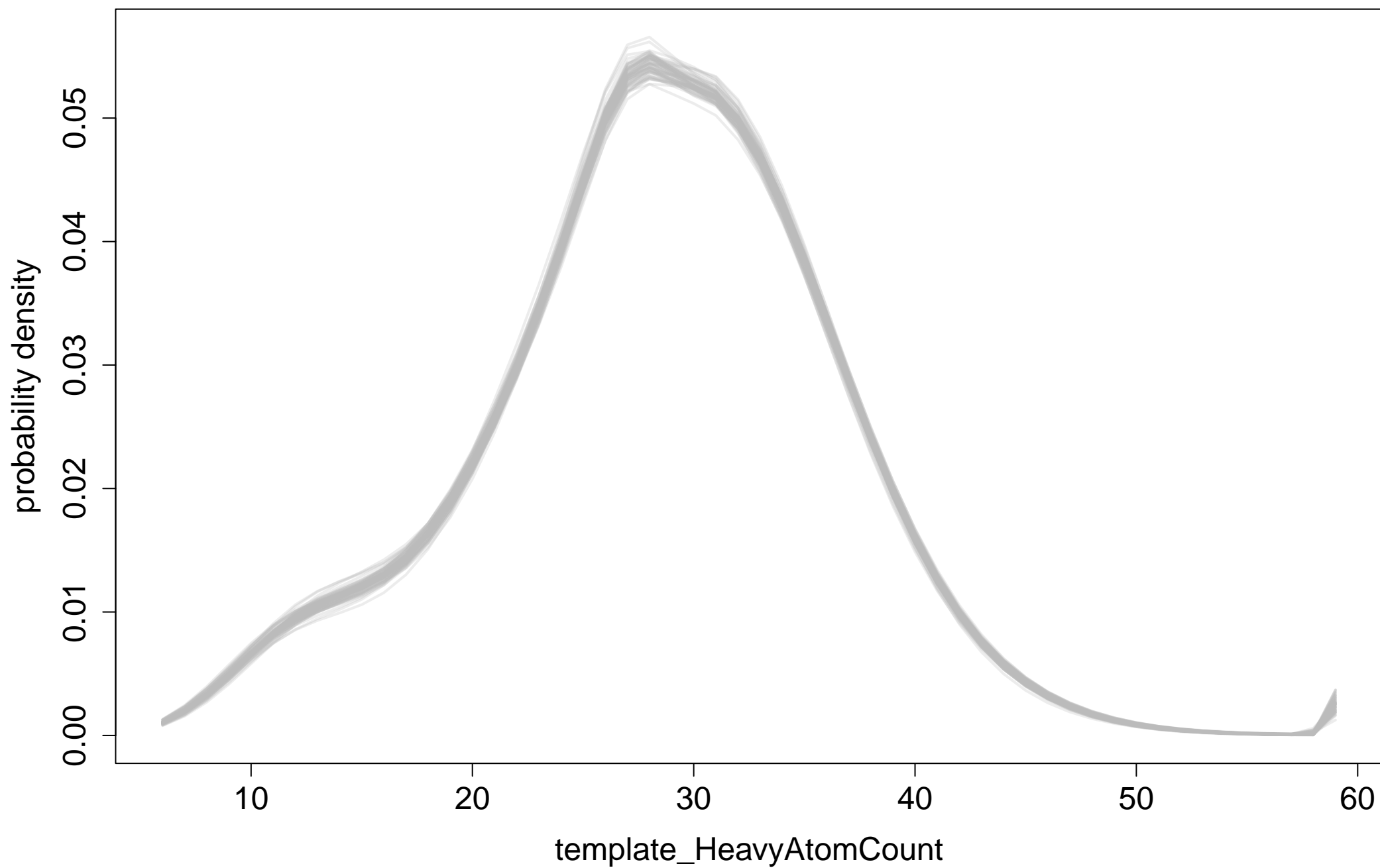
LL: -110000 +- 88.9

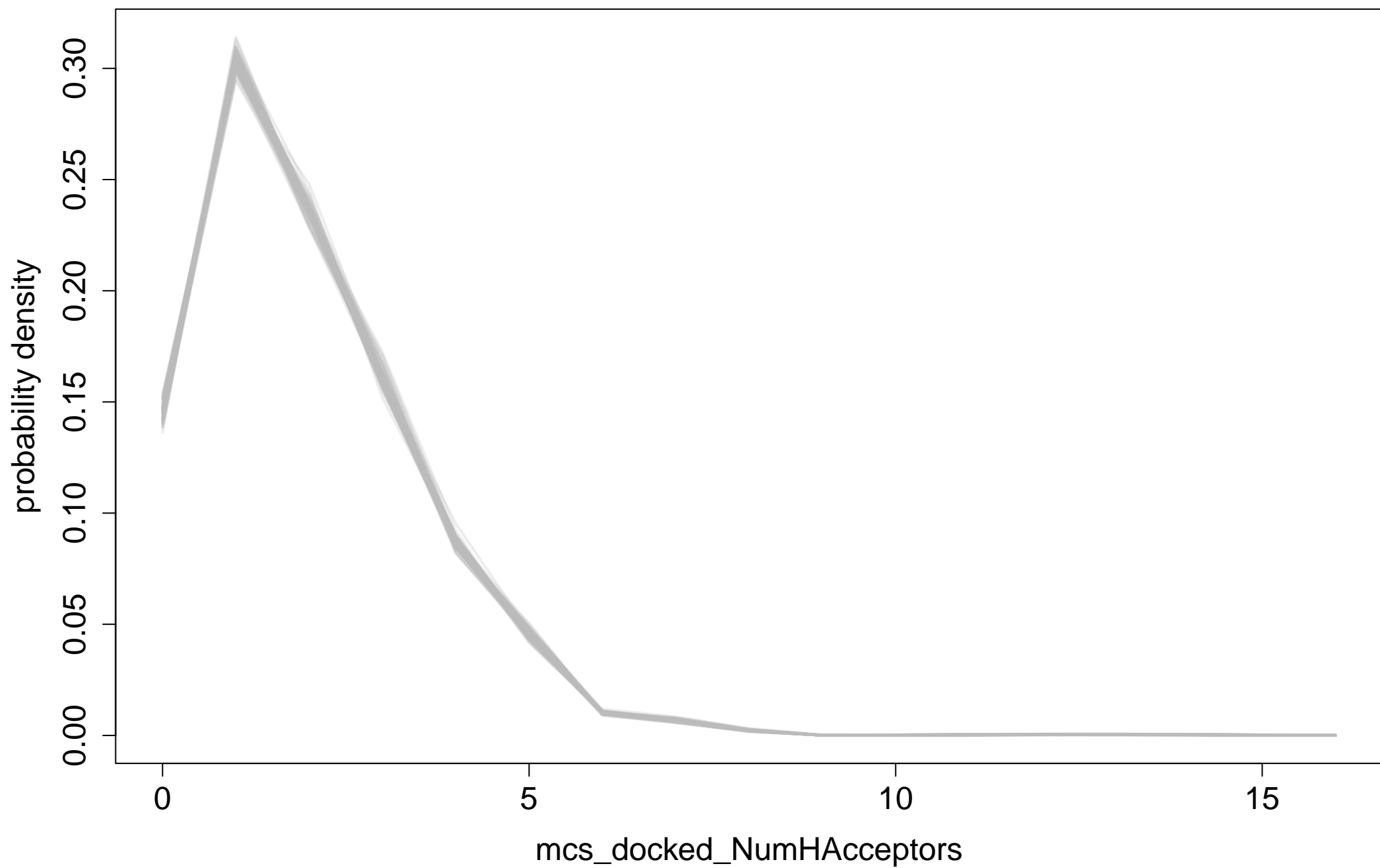


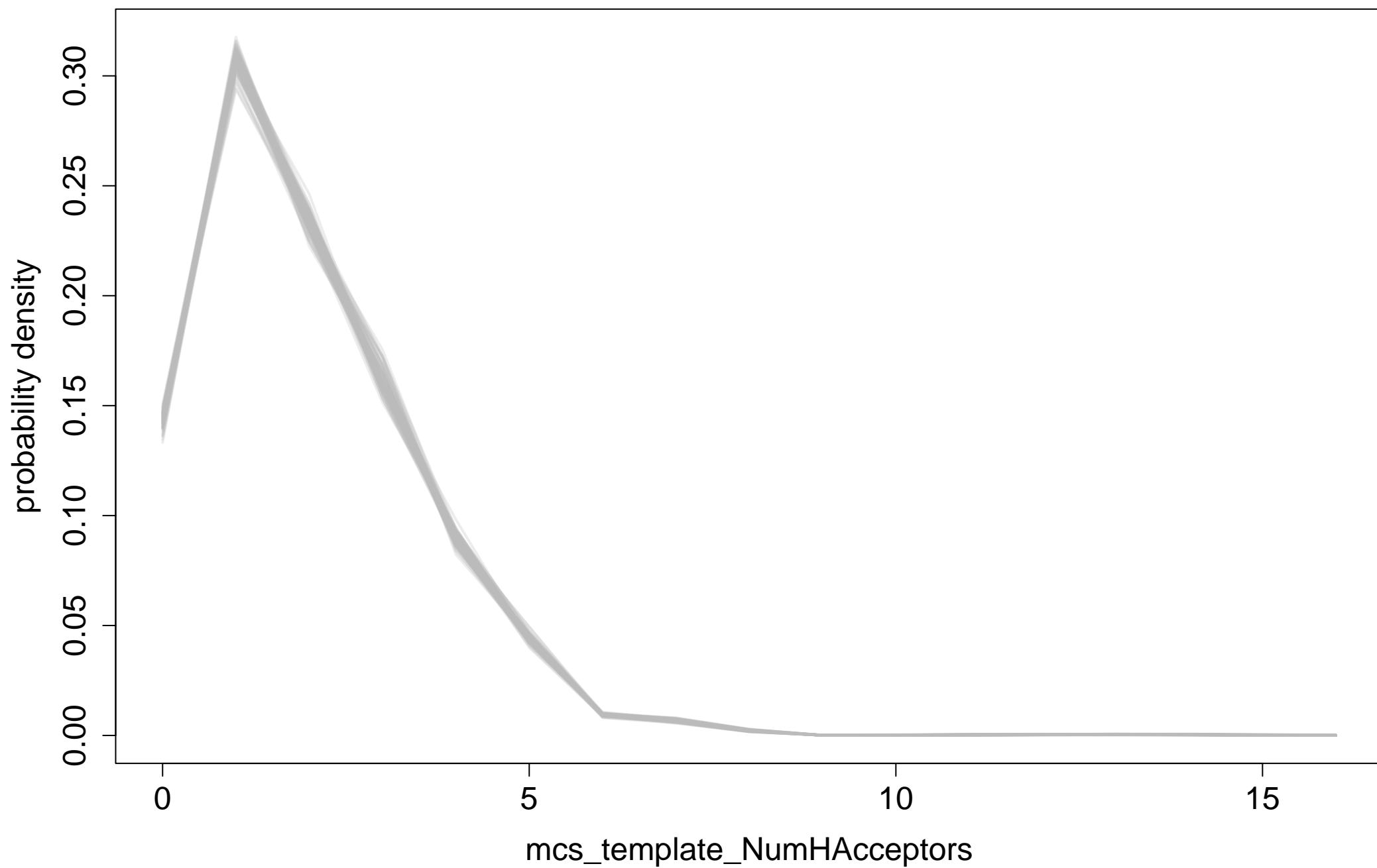


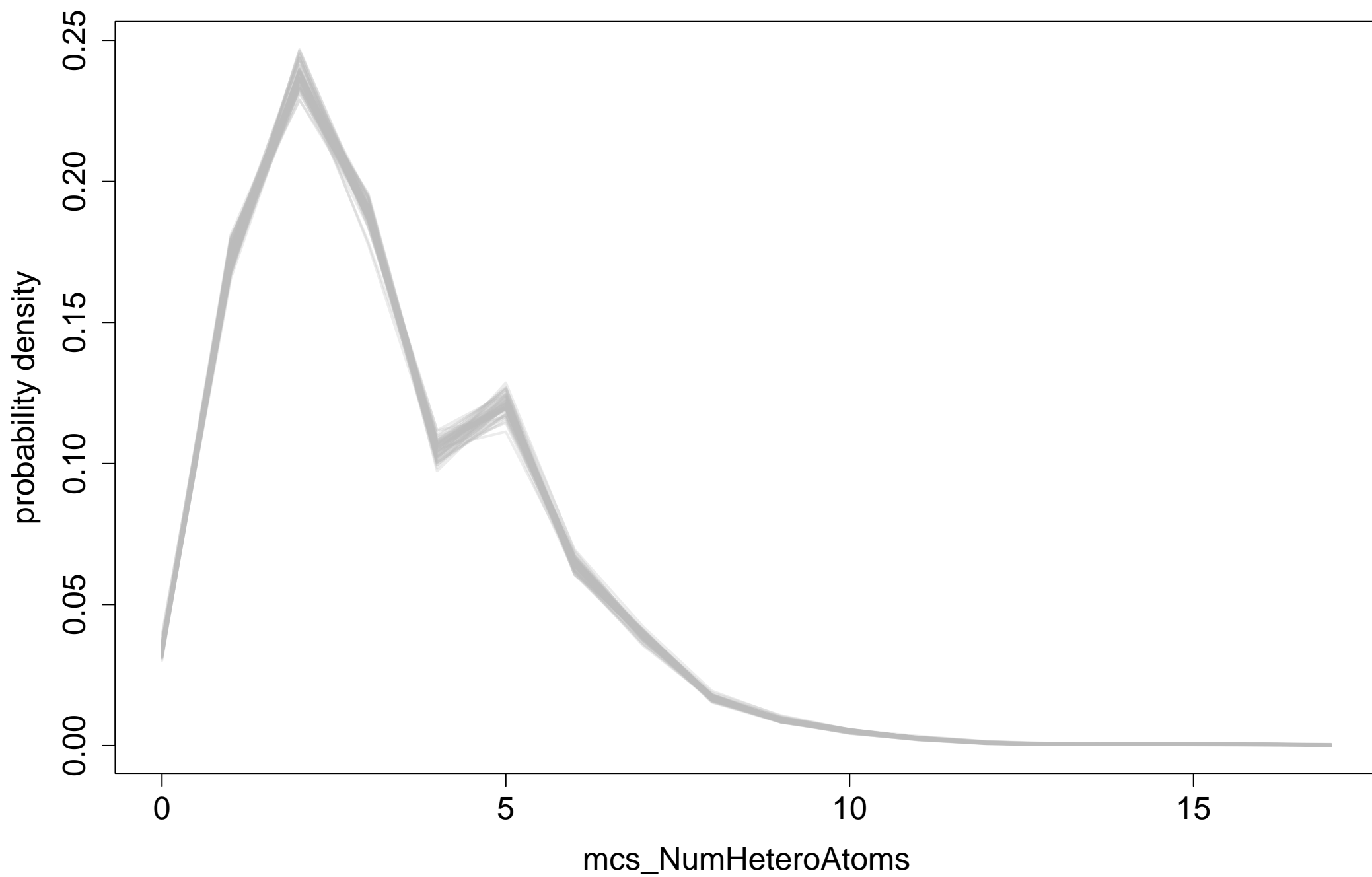


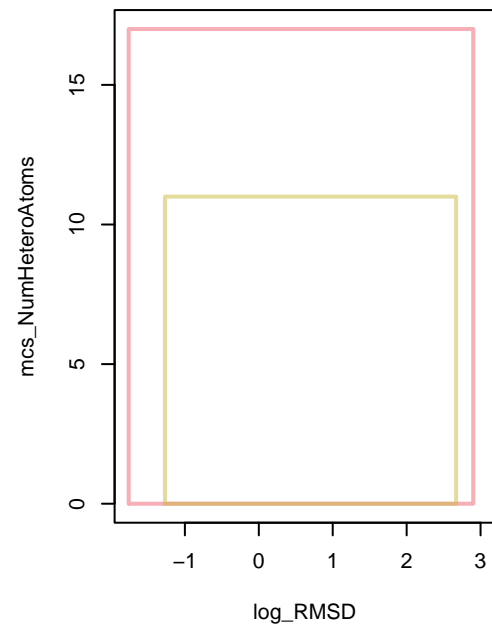
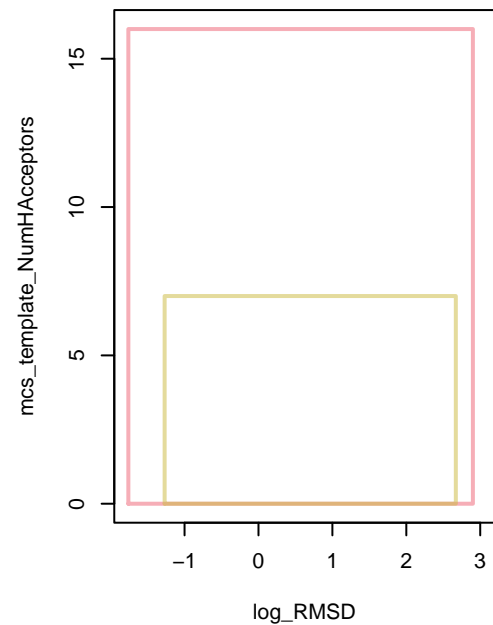
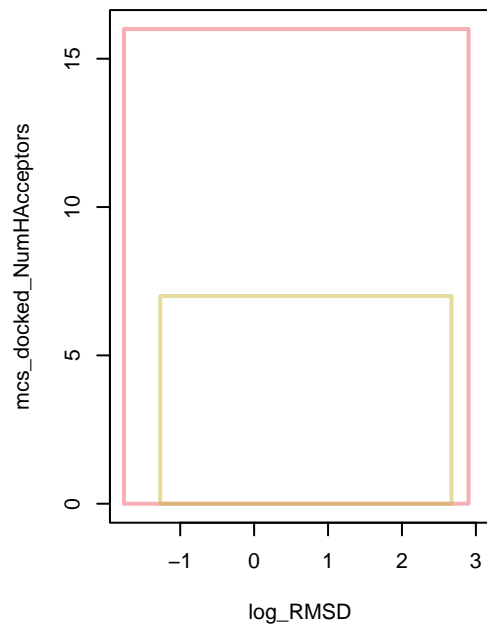
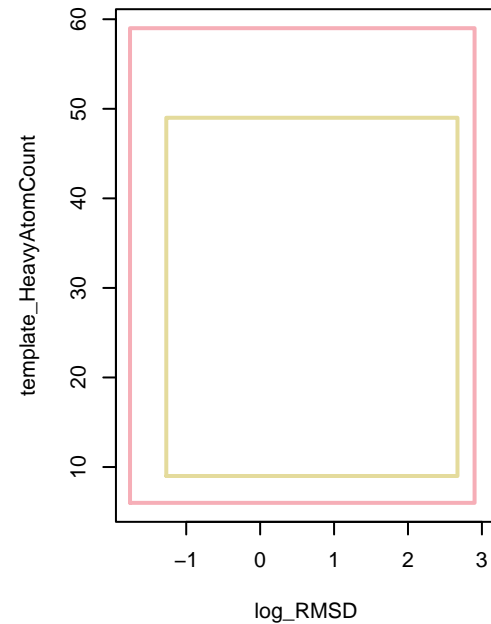
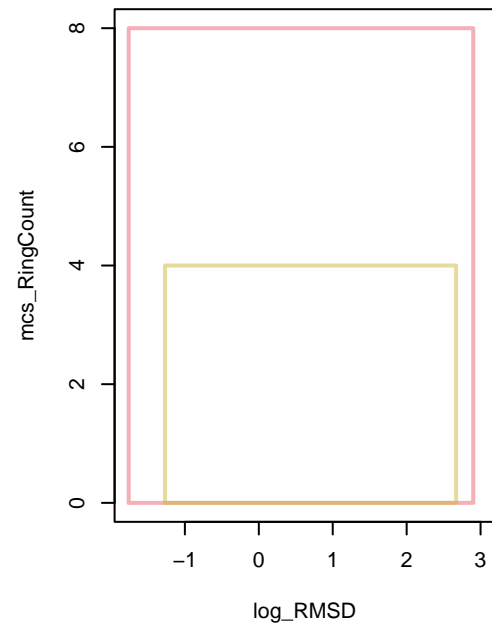
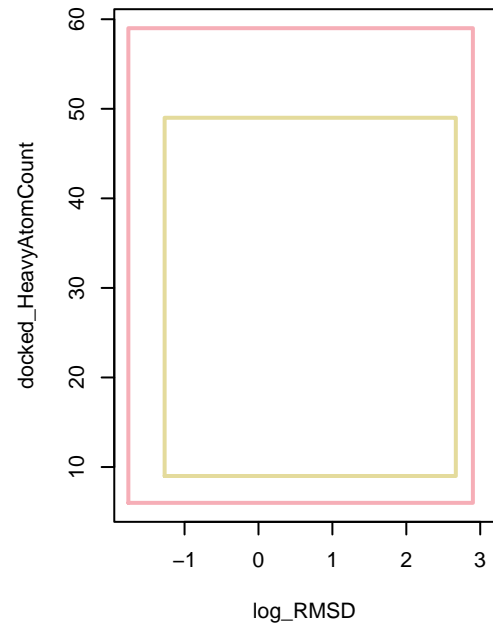
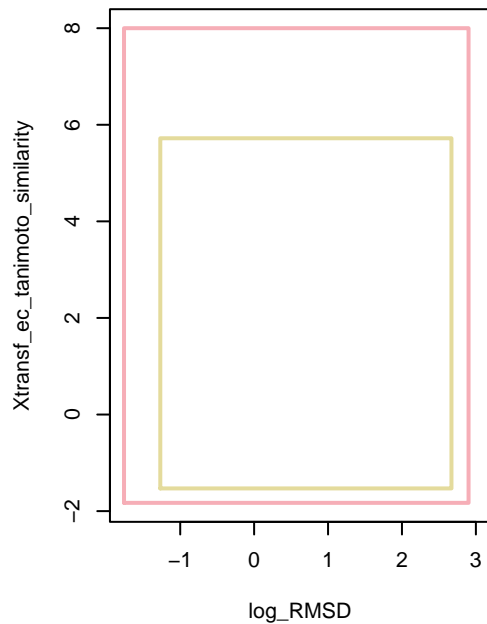




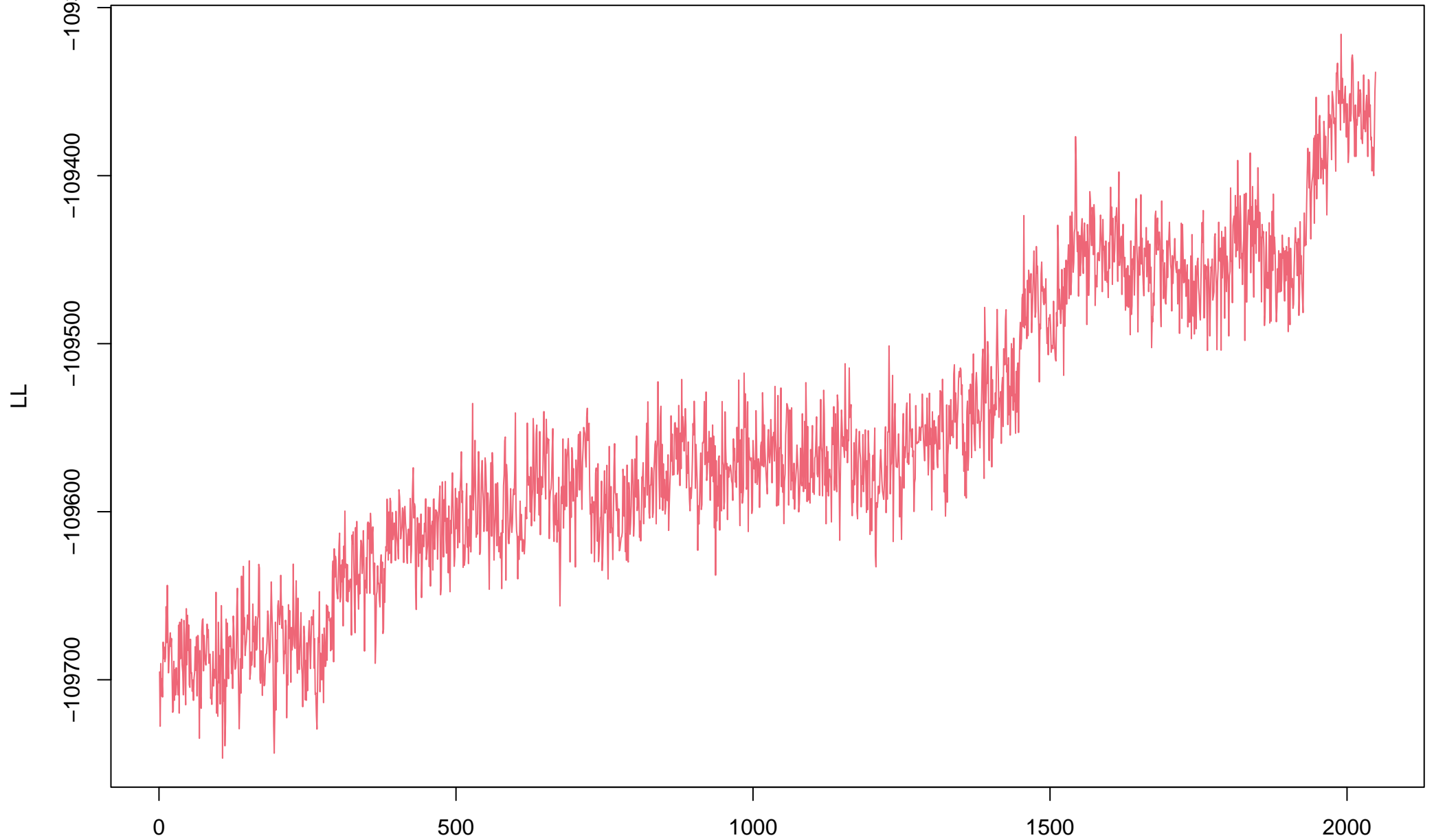




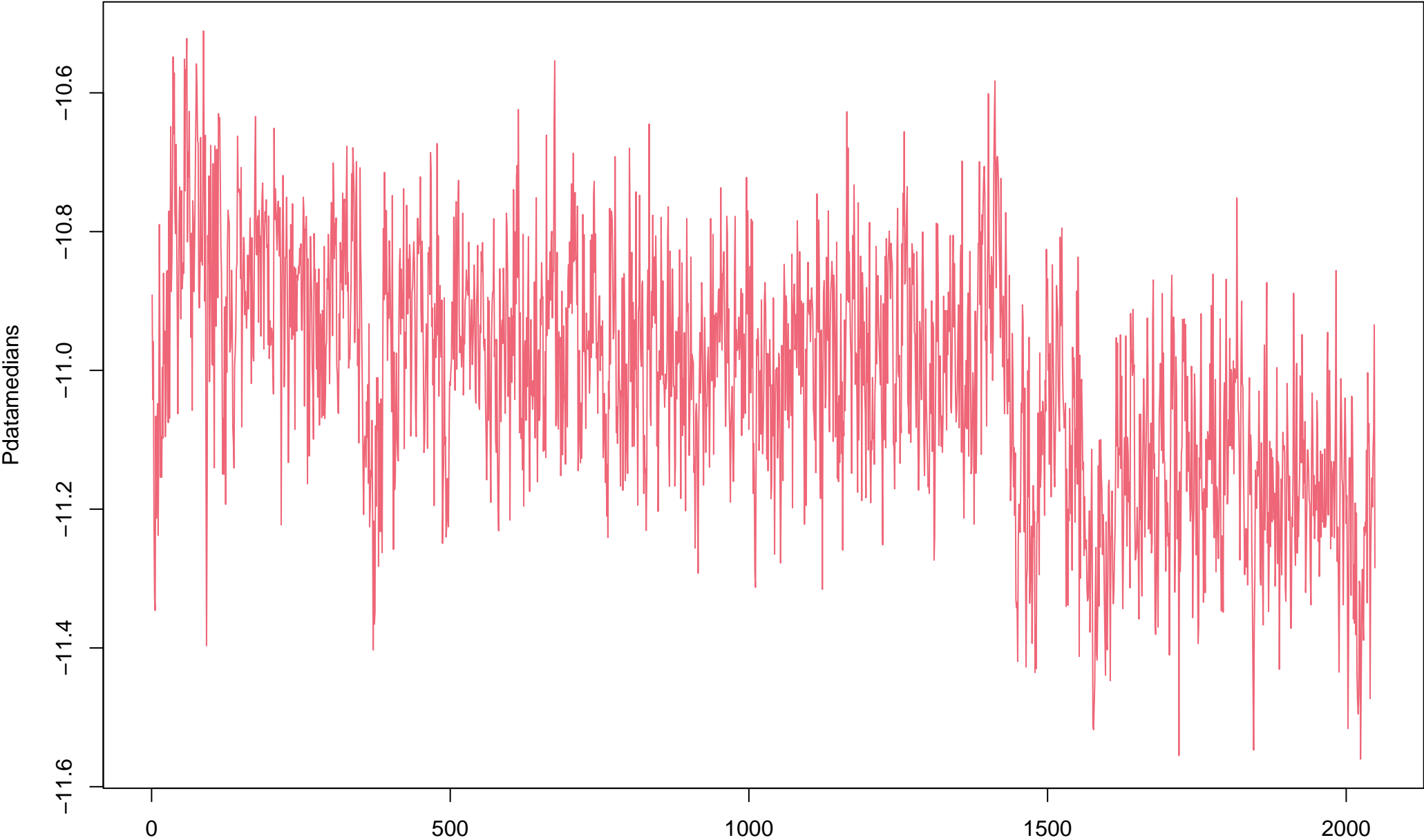




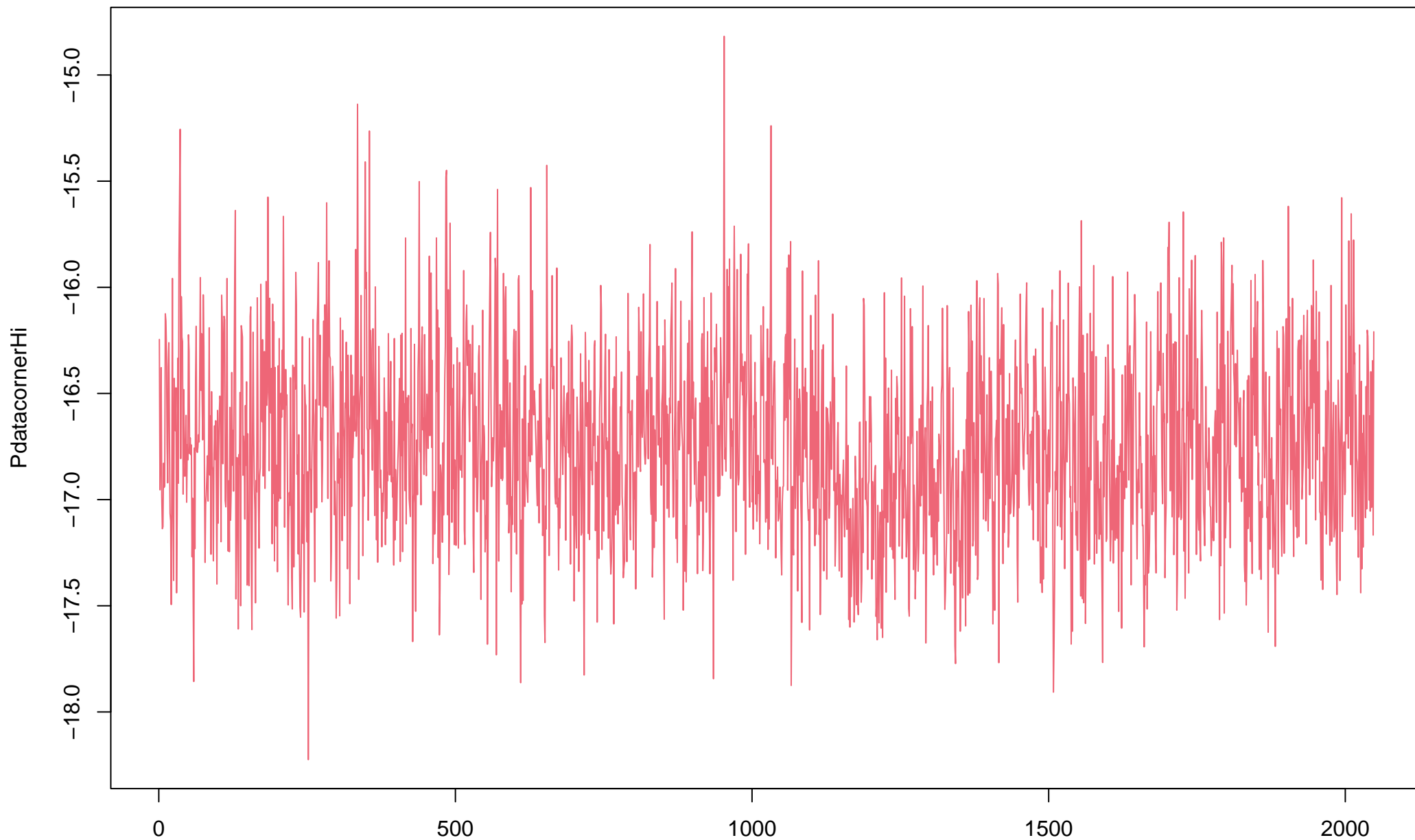
LL
ESS = 2.68 | BMK = 0.735 | MCSE(6.27) = 14.2 | stat: FALSE | burn: 2040



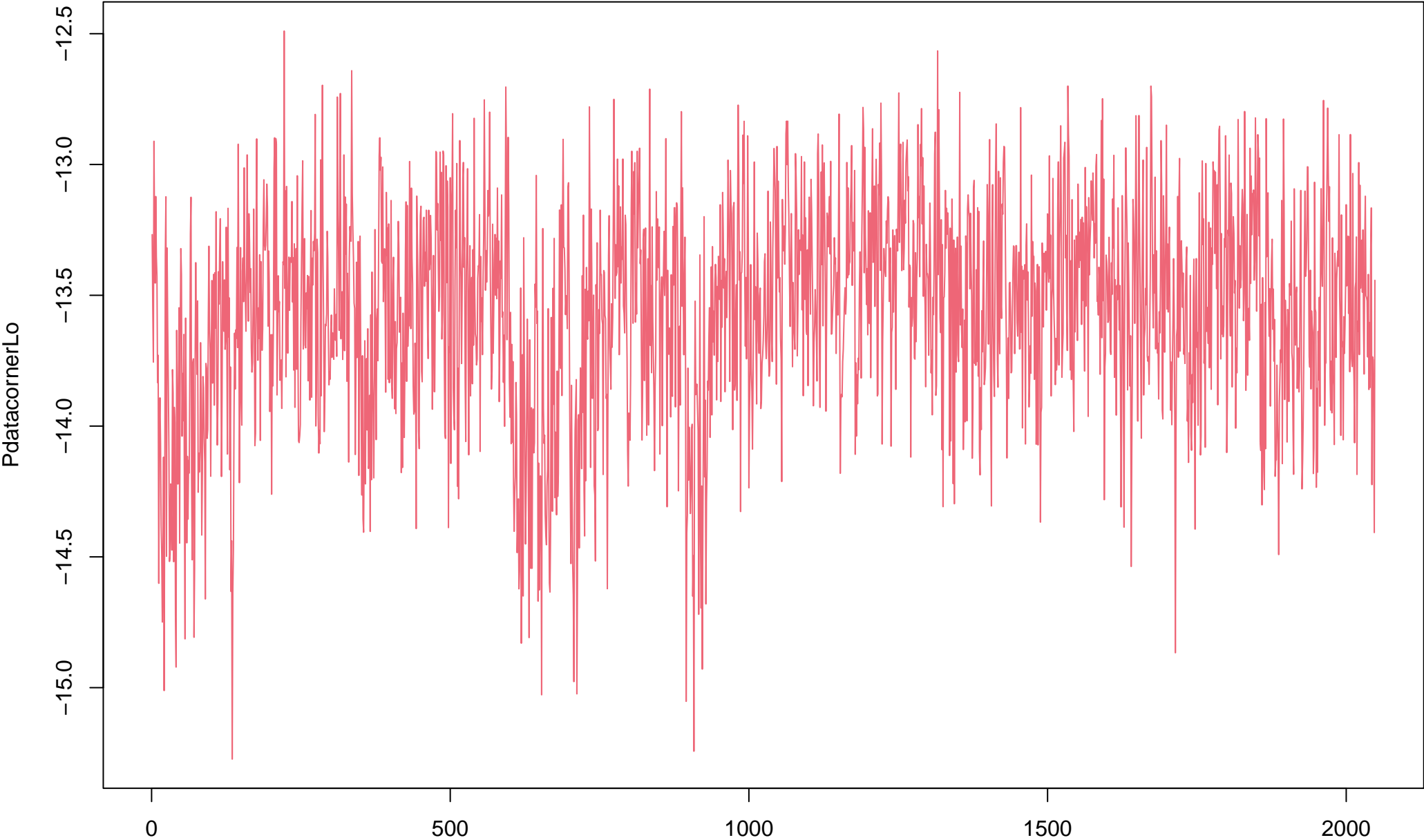
Pdatamedians
ESS = 37.8 | BMK = 0.317 | MCSE(6.27) = 9.62 | stat: FALSE | burn: 0



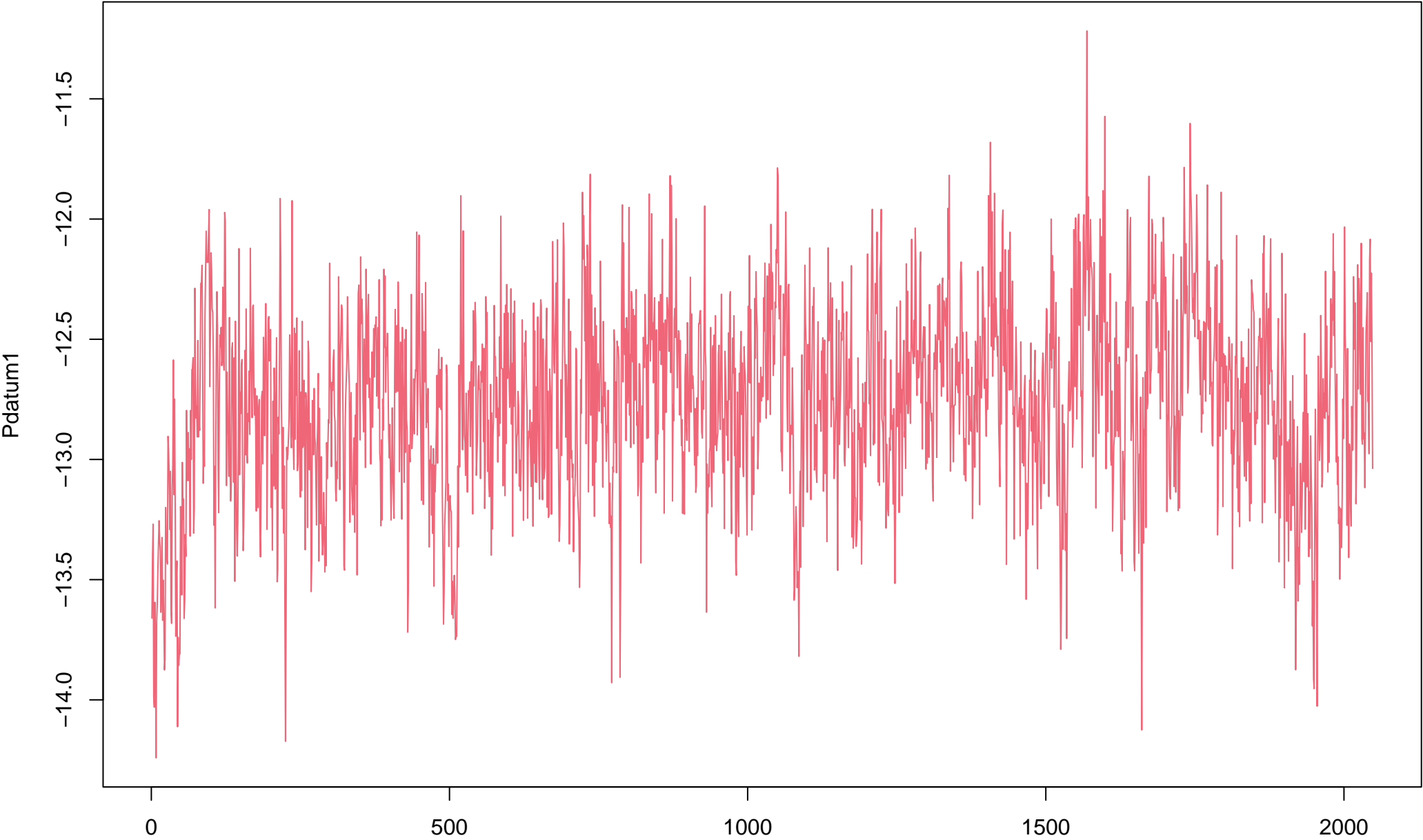
PdatacornerHi
ESS = 977 | BMK = 0.103 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0



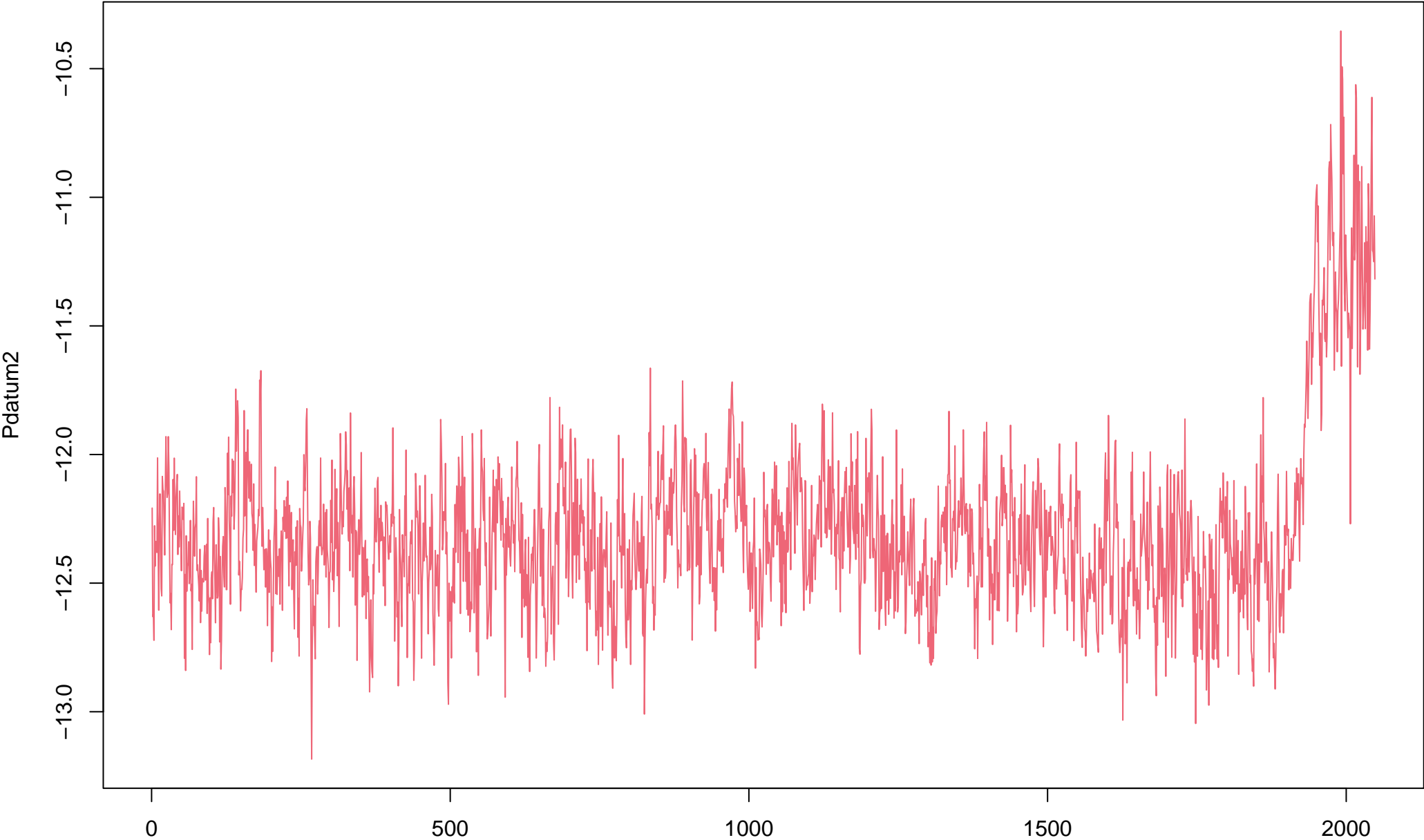
PdatacornerLo
ESS = 292 | BMK = 0.173 | MCSE(6.27) = 5.96 | stat: FALSE | burn: 0



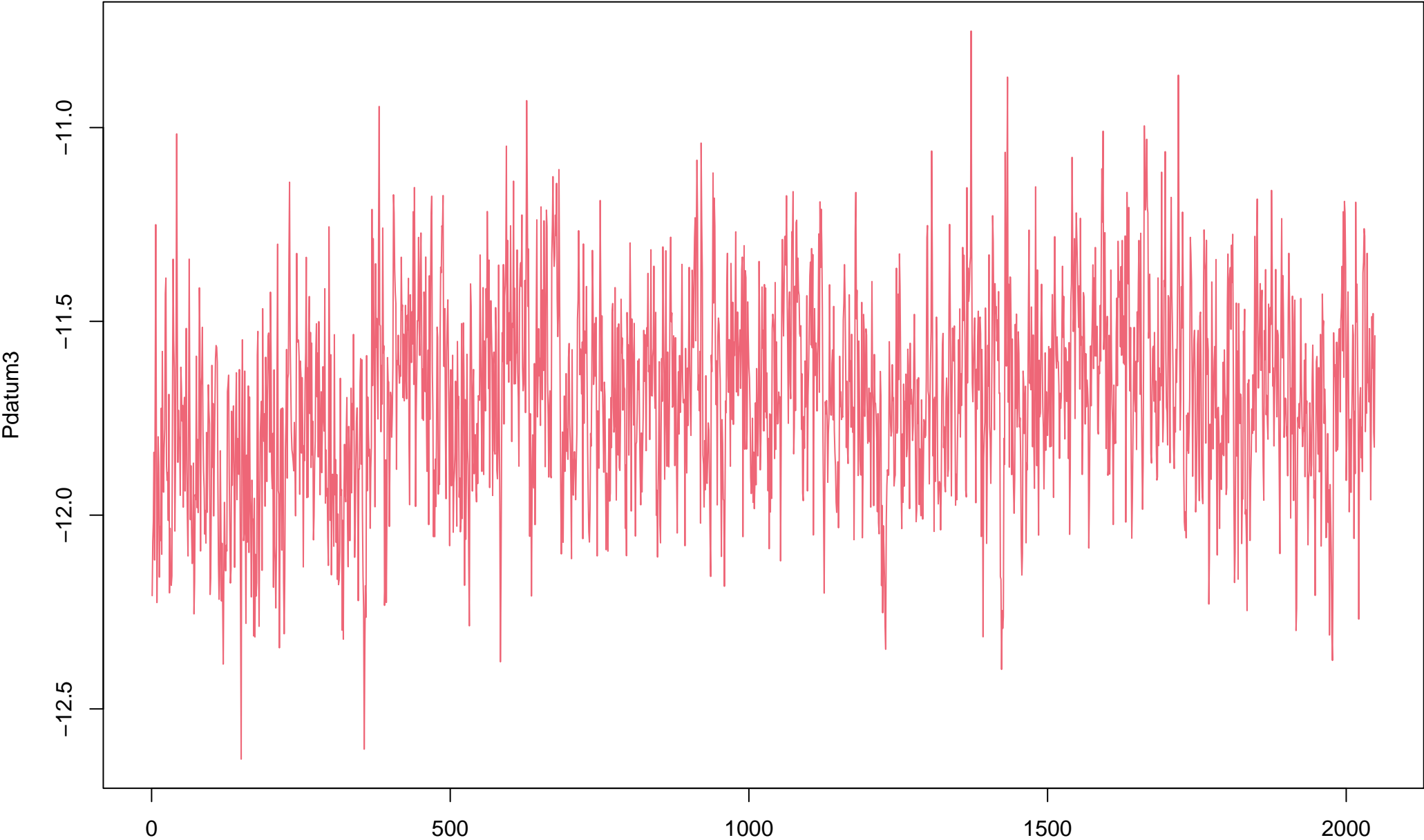
Pdatum1
ESS = 178 | BMK = 0.113 | MCSE(6.27) = 6.42 | stat: FALSE | burn: 0



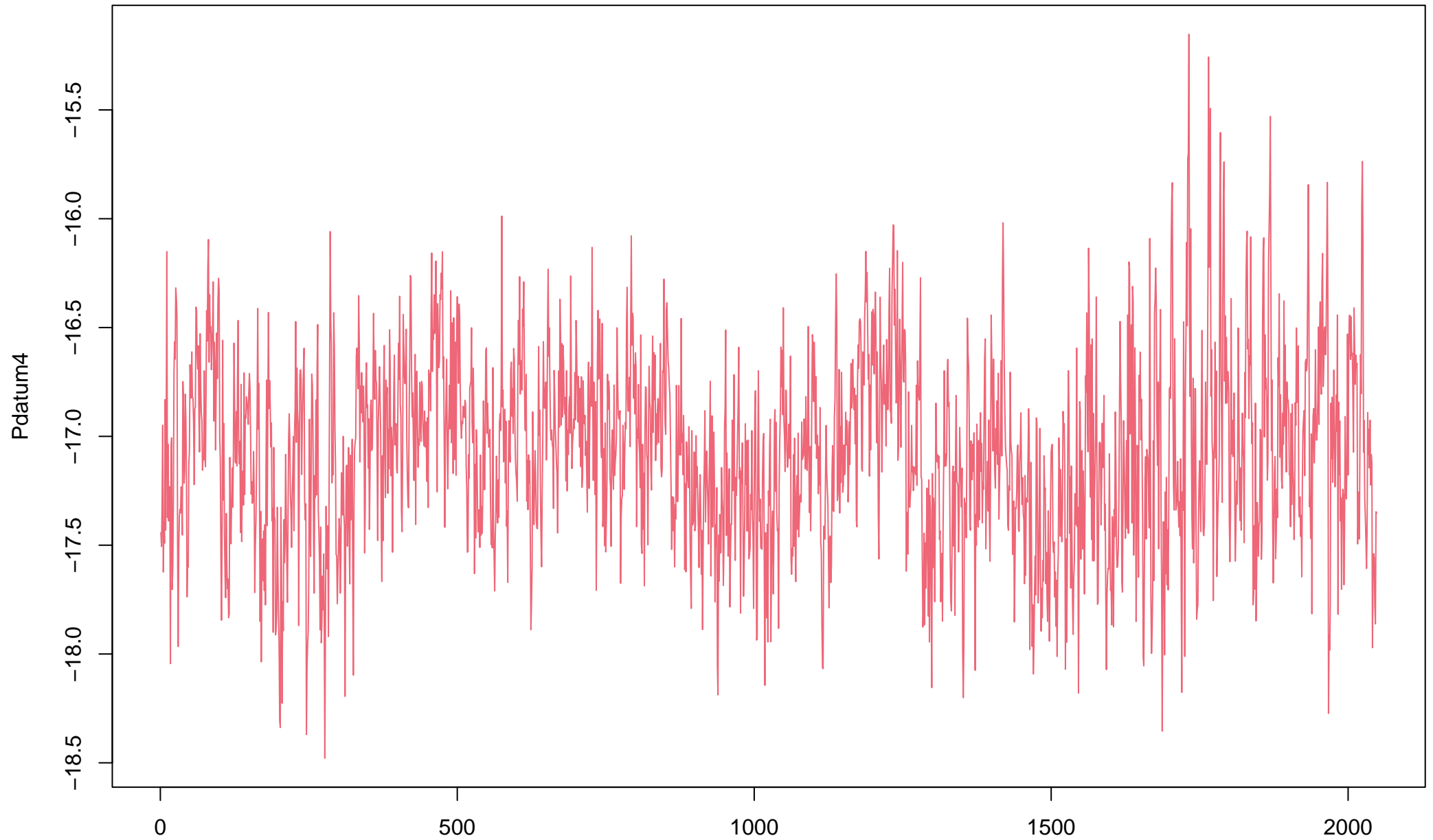
Pdatum2
ESS = 16 | BMK = 0.23 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 2040



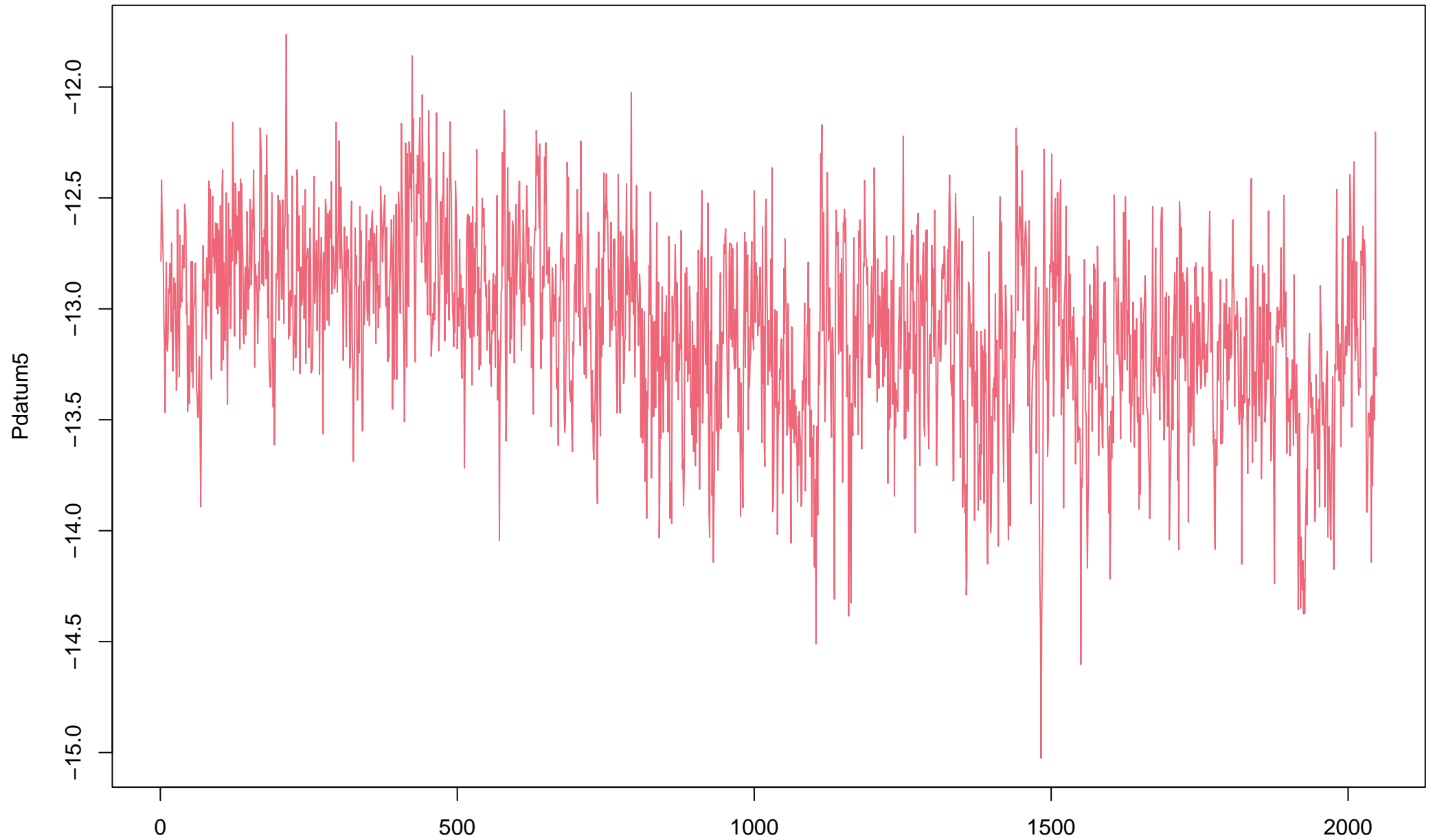
Pdatum3
ESS = 306 | BMK = 0.106 | MCSE(6.27) = 6.27 | stat: FALSE | burn: 0



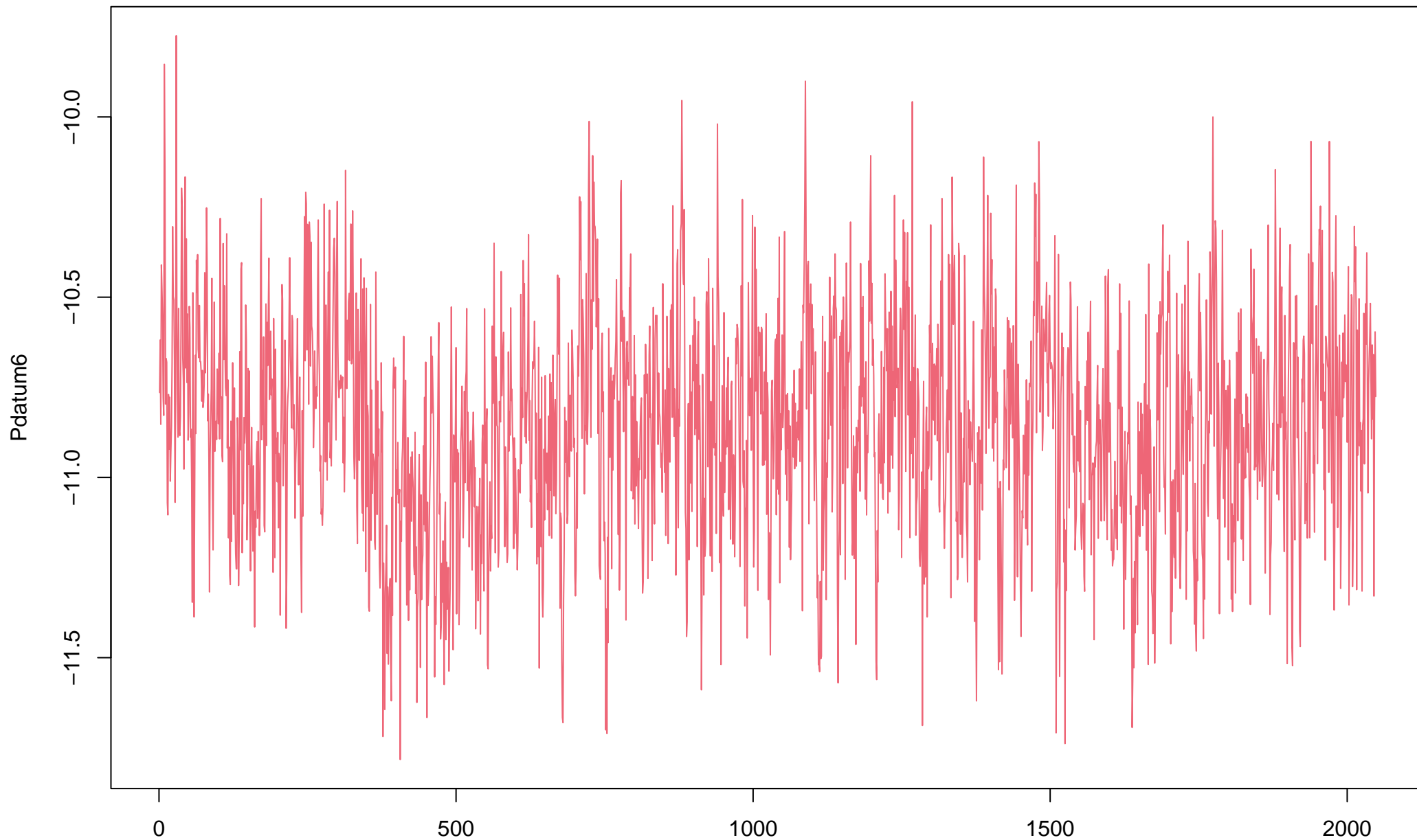
Pdatum4
ESS = 388 | BMK = 0.117 | MCSE(6.27) = 6.24 | stat: TRUE | burn: 0



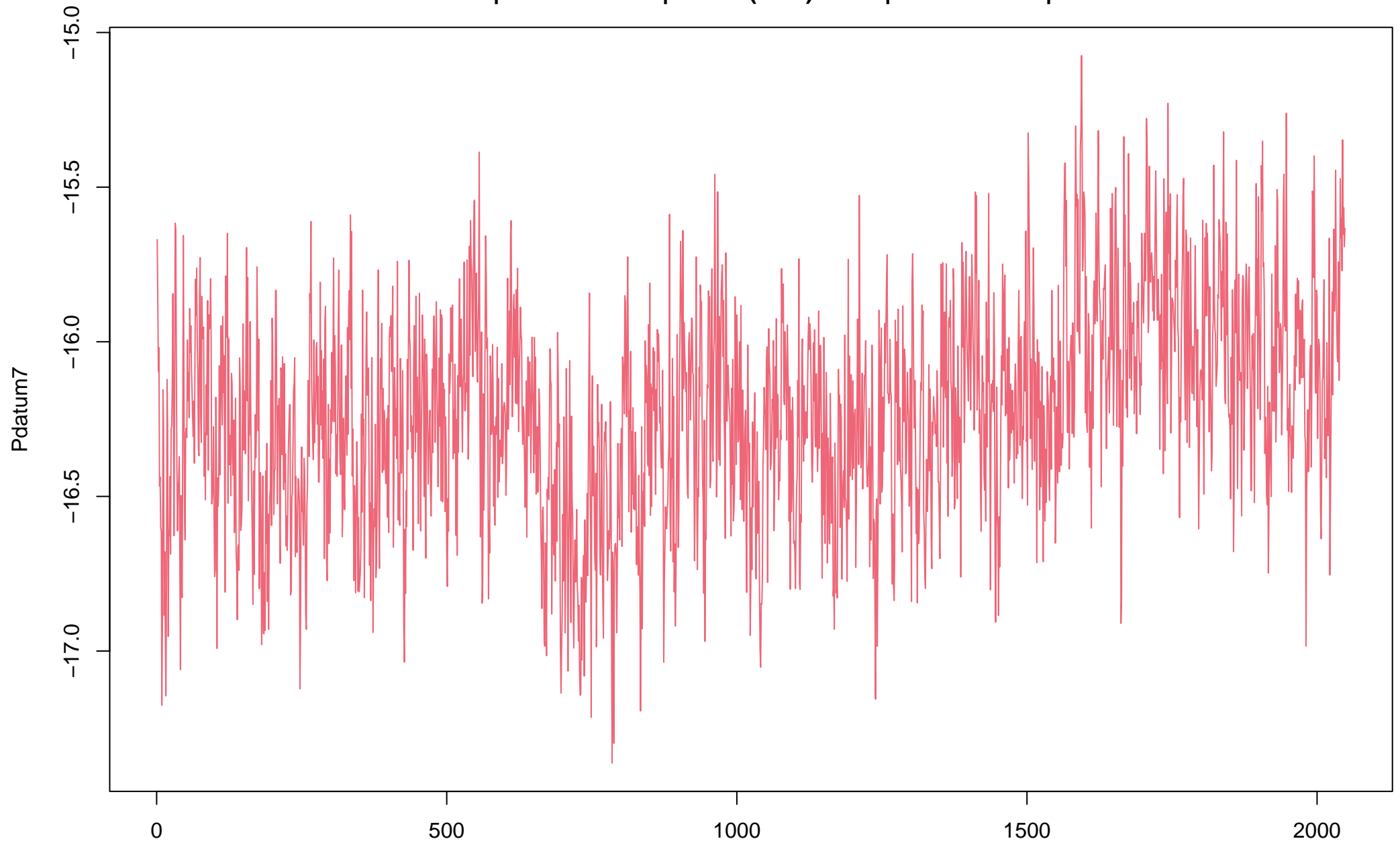
Pdatum5
ESS = 92.8 | BMK = 0.262 | MCSE(6.27) = 7.89 | stat: FALSE | burn: 0



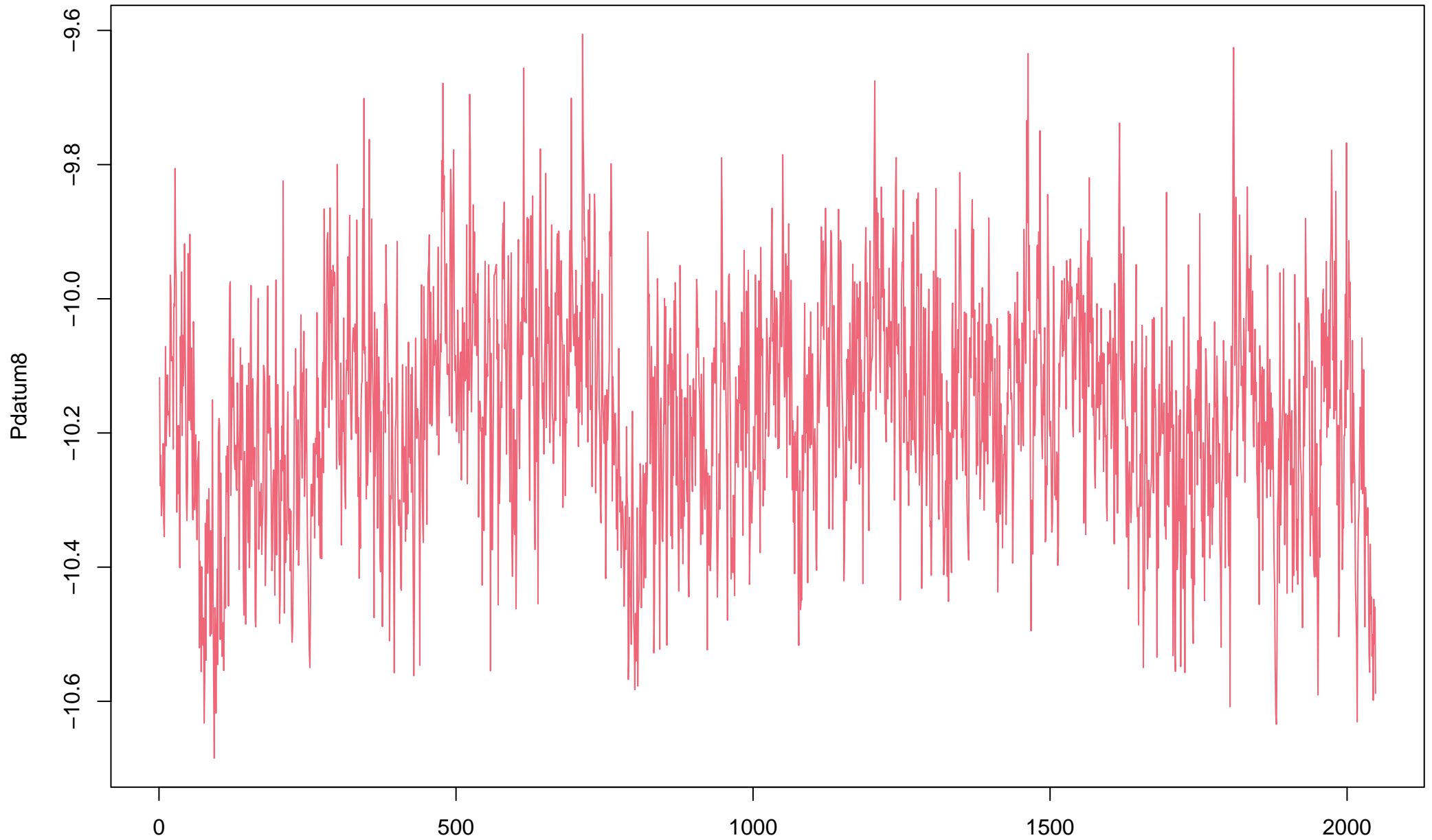
Pdatum6
ESS = 434 | BMK = 0.0483 | MCSE(6.27) = 5.1 | stat: TRUE | burn: 0



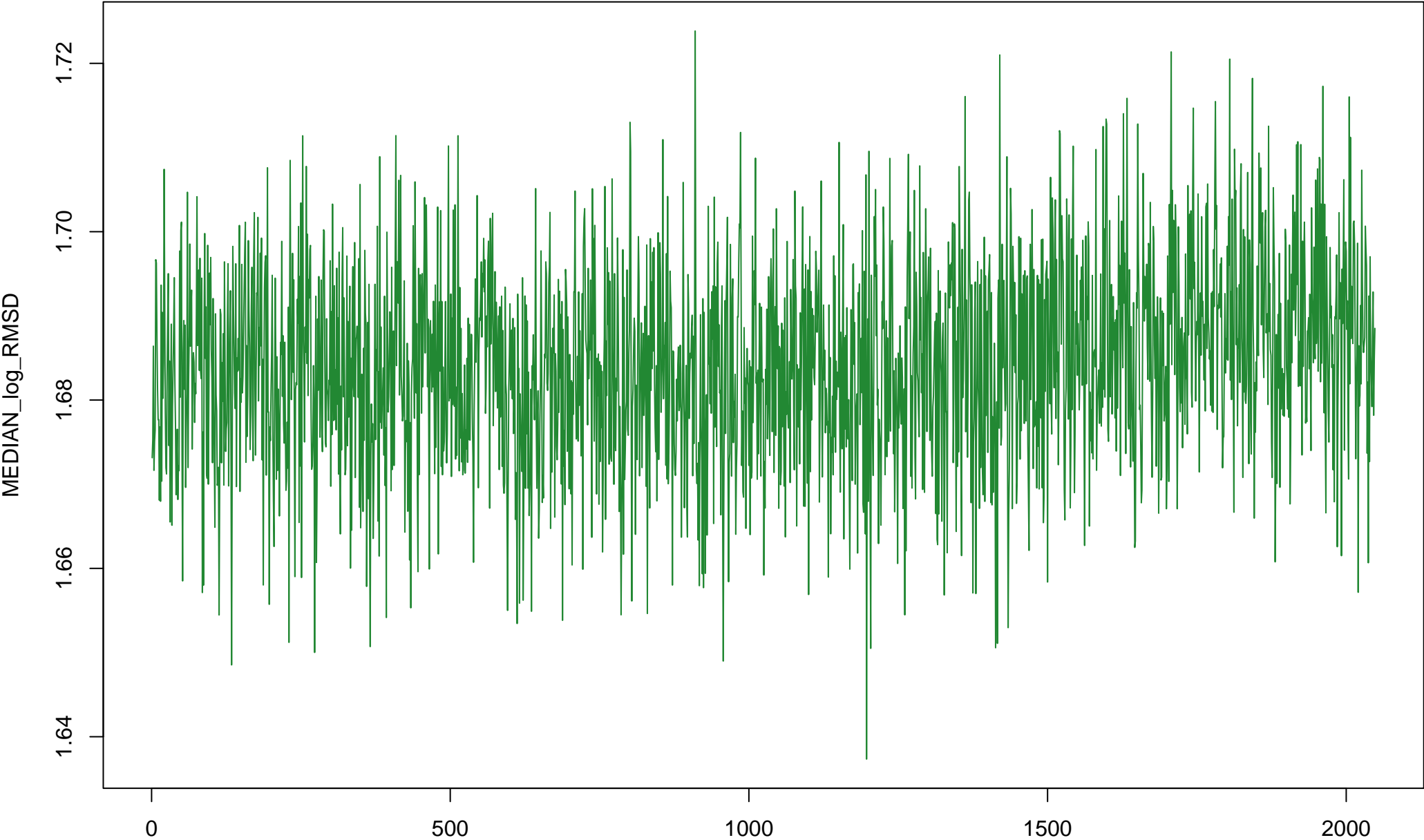
Pdatum7
ESS = 54.6 | BMK = 0.209 | MCSE(6.27) = 7.8 | stat: FALSE | burn: 0



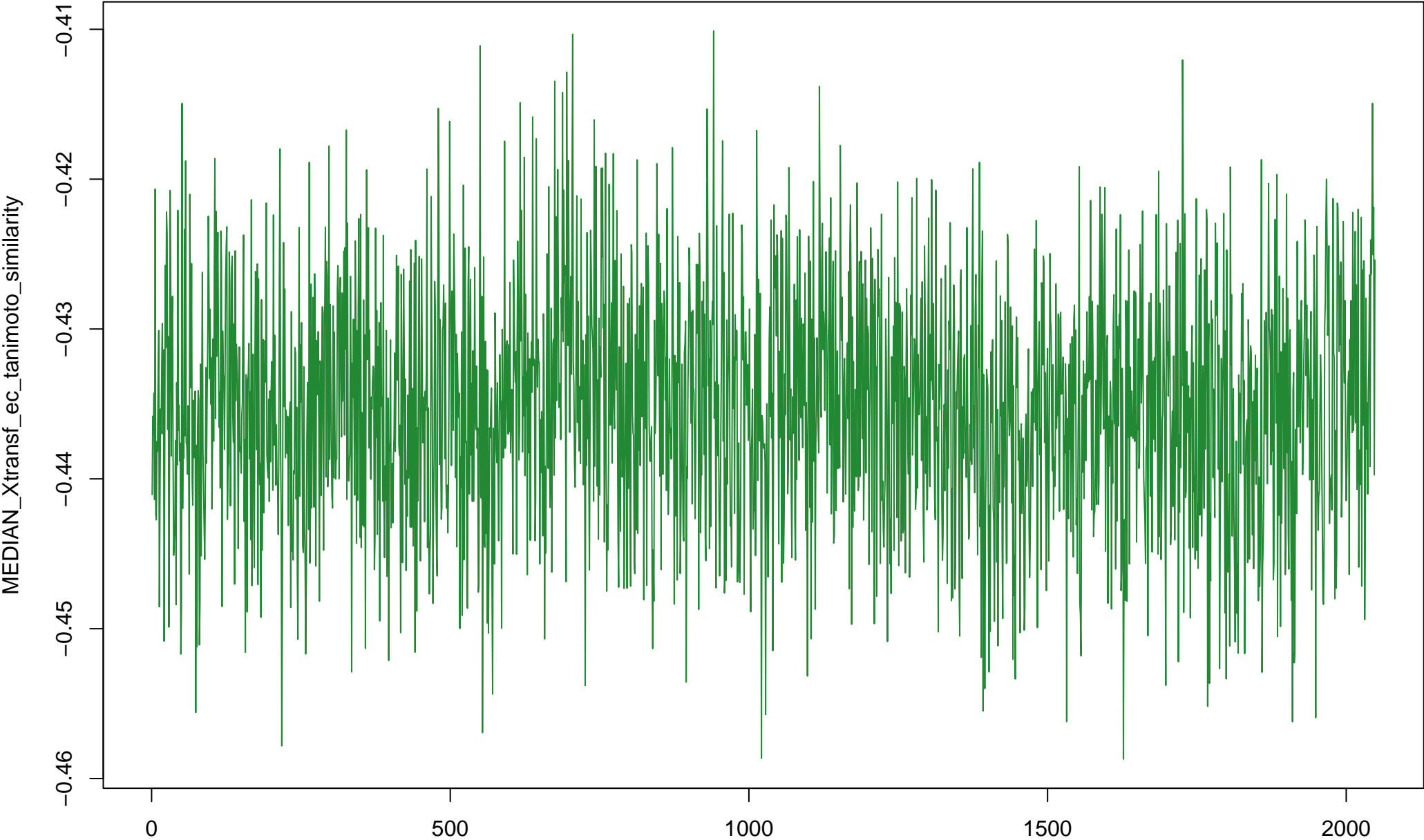
Pdatum8
ESS = 116 | BMK = 0.0572 | MCSE(6.27) = 7.08 | stat: FALSE | burn: 0



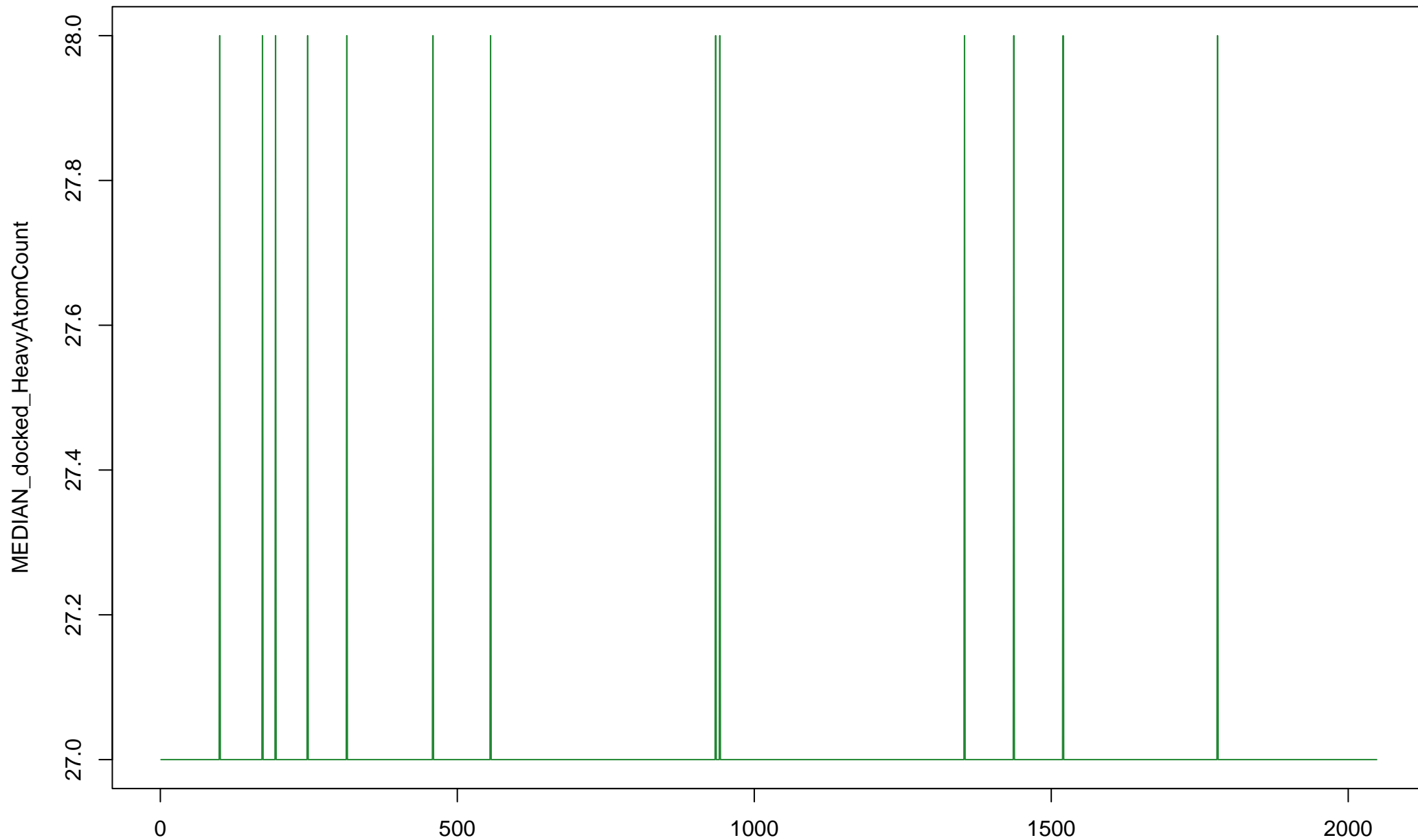
MEDIAN_log_RMSD
ESS = 638 | BMK = 0.114 | MCSE(6.27) = 4.06 | stat: FALSE | burn: 0



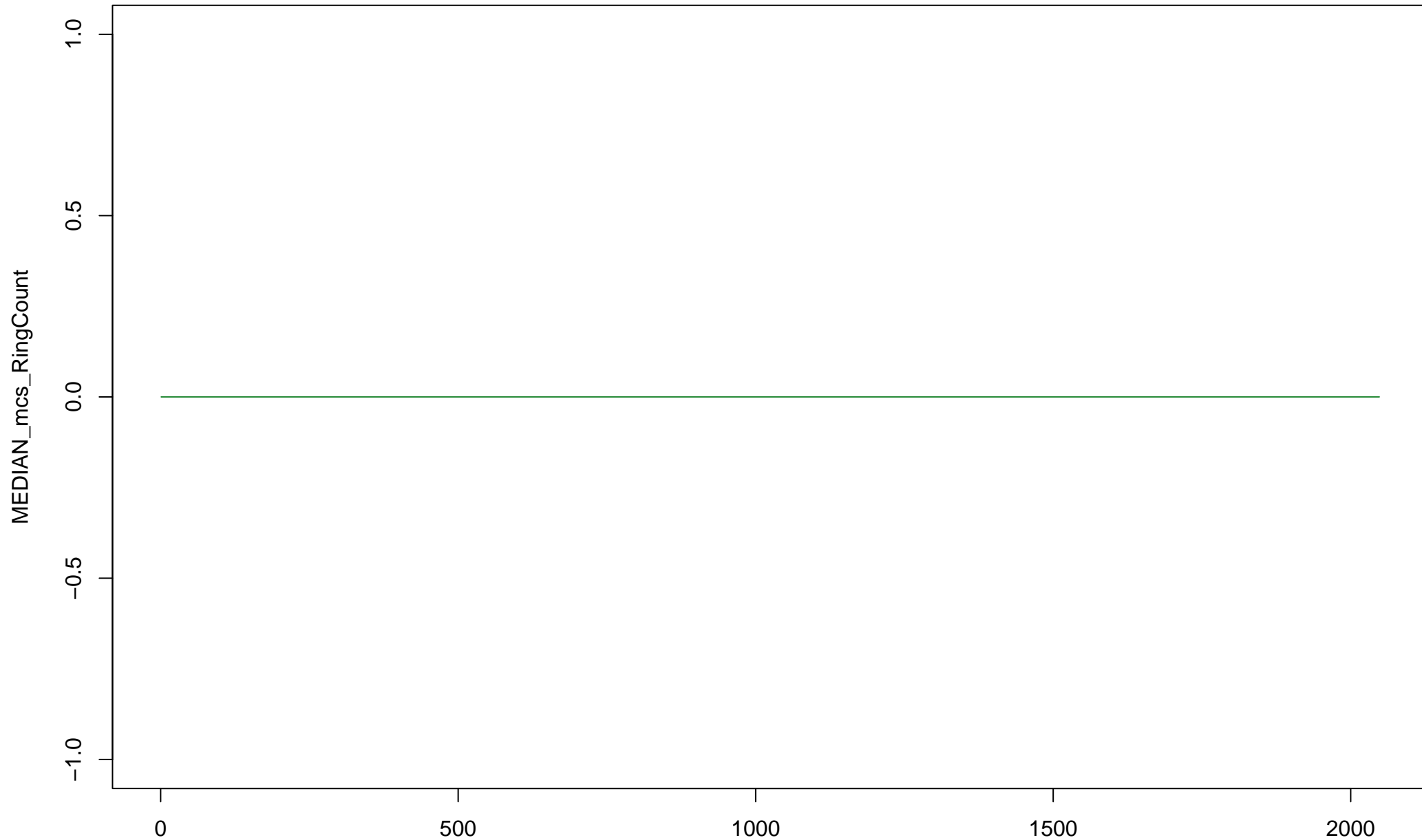
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1180 | BMK = 0.059 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0



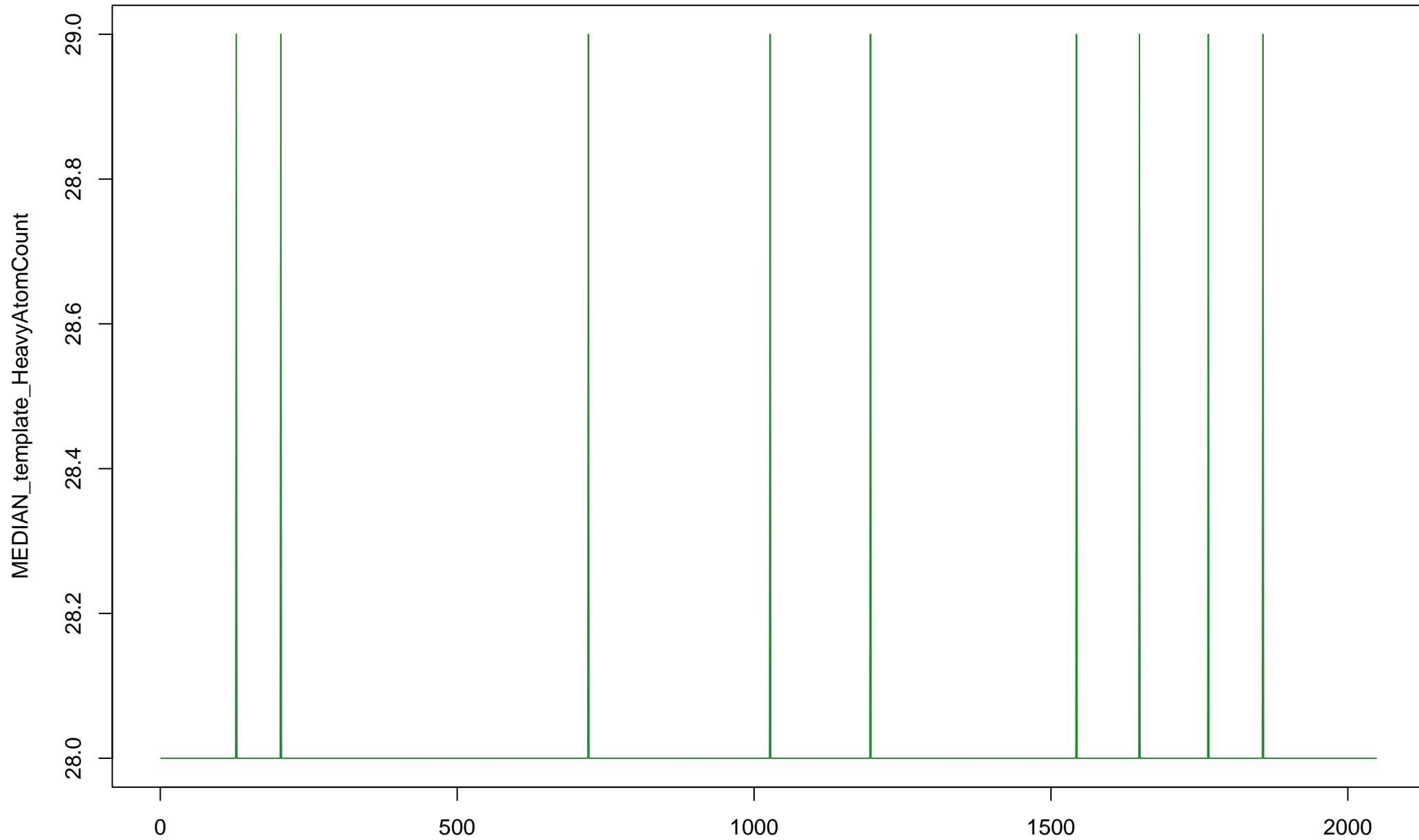
MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.141 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 2040



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



MEDIAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 1428



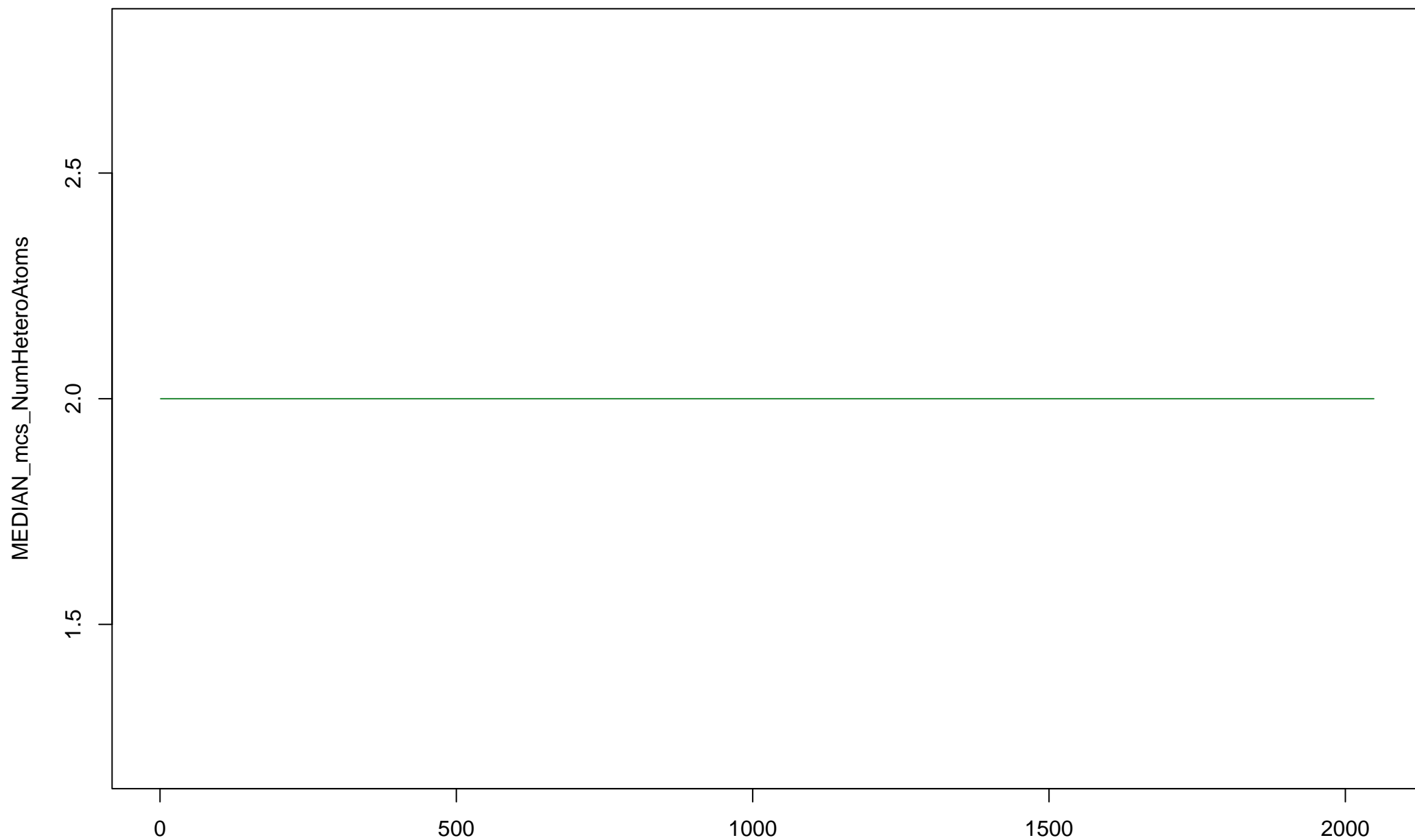
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



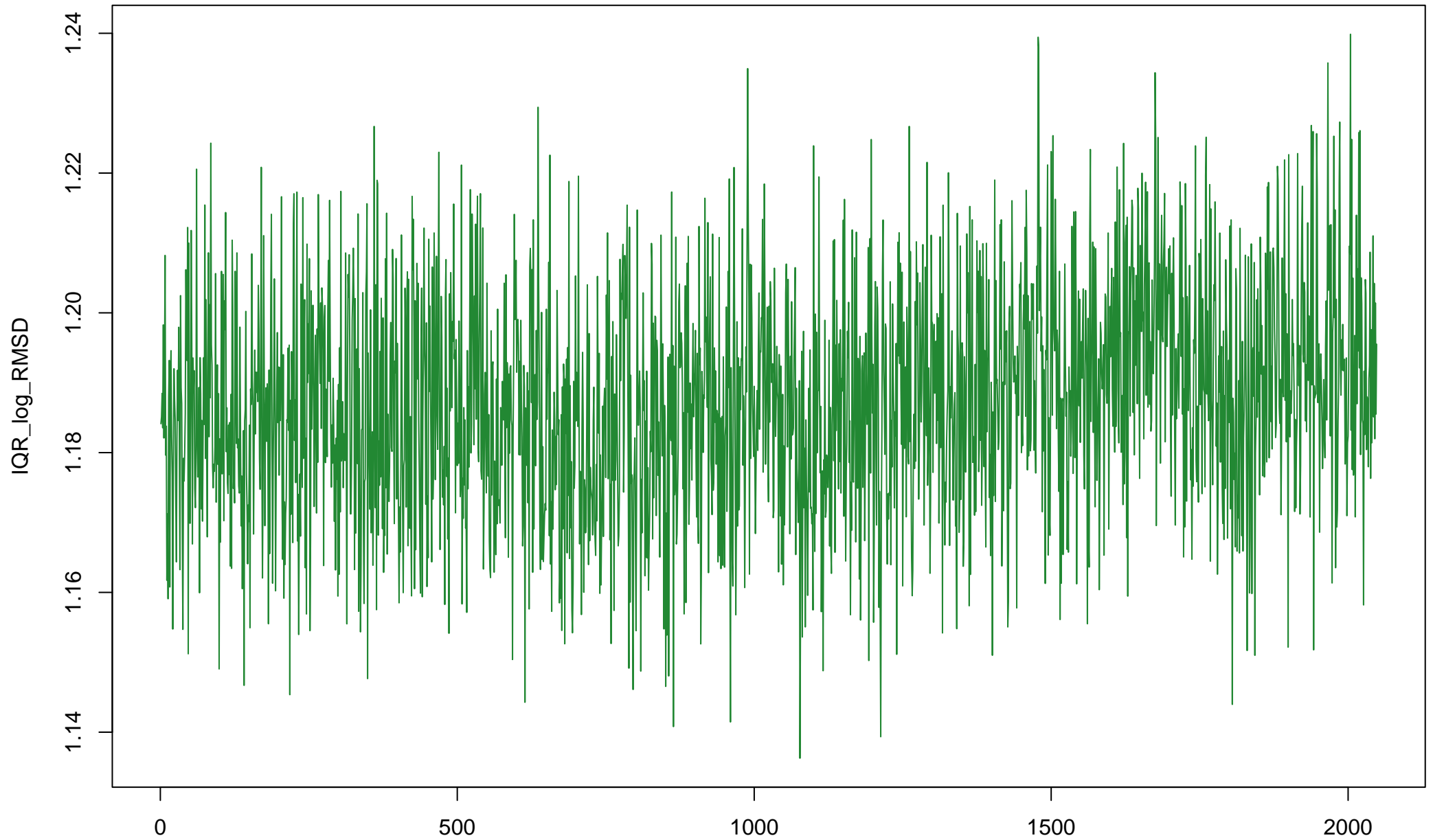
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



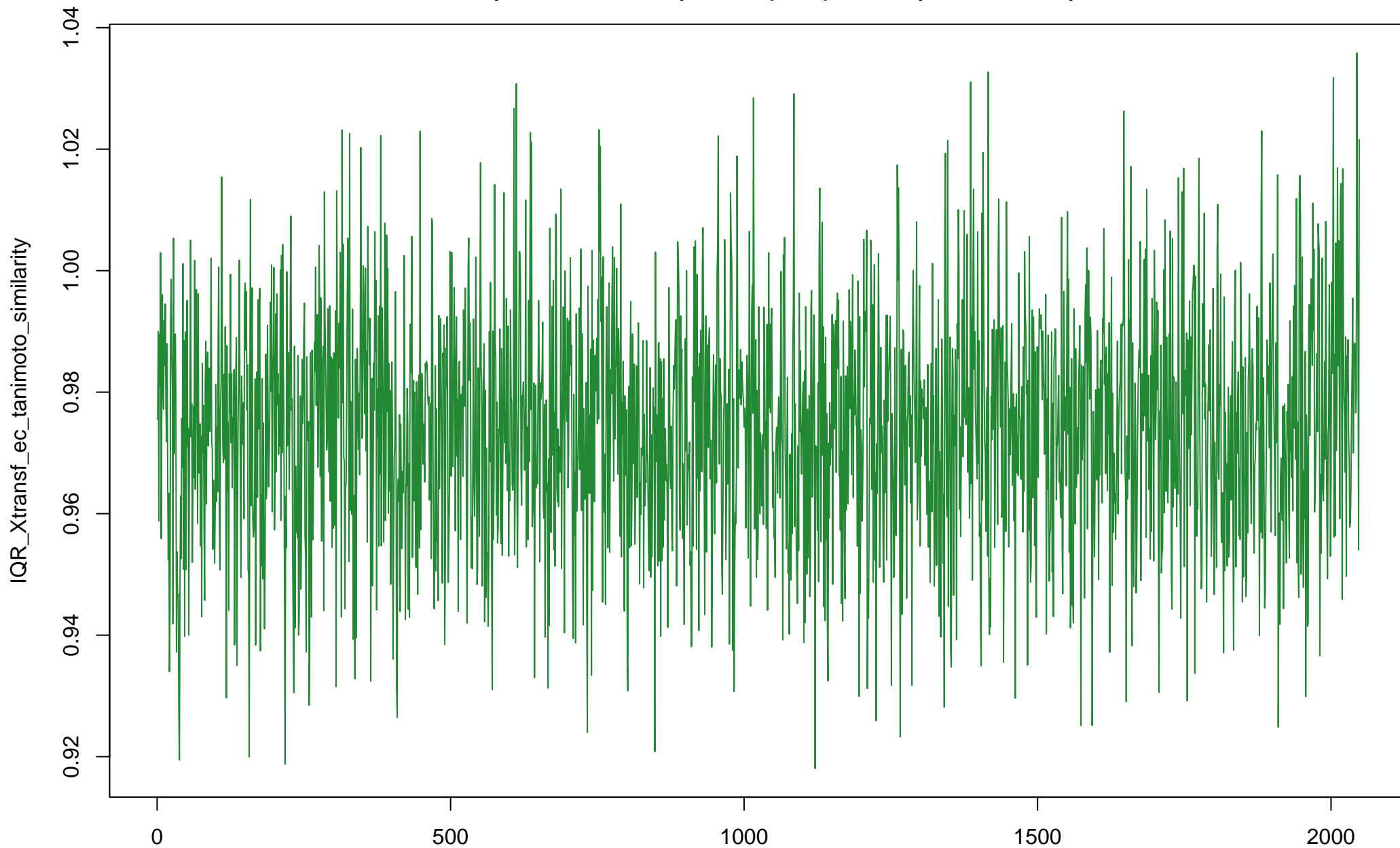
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



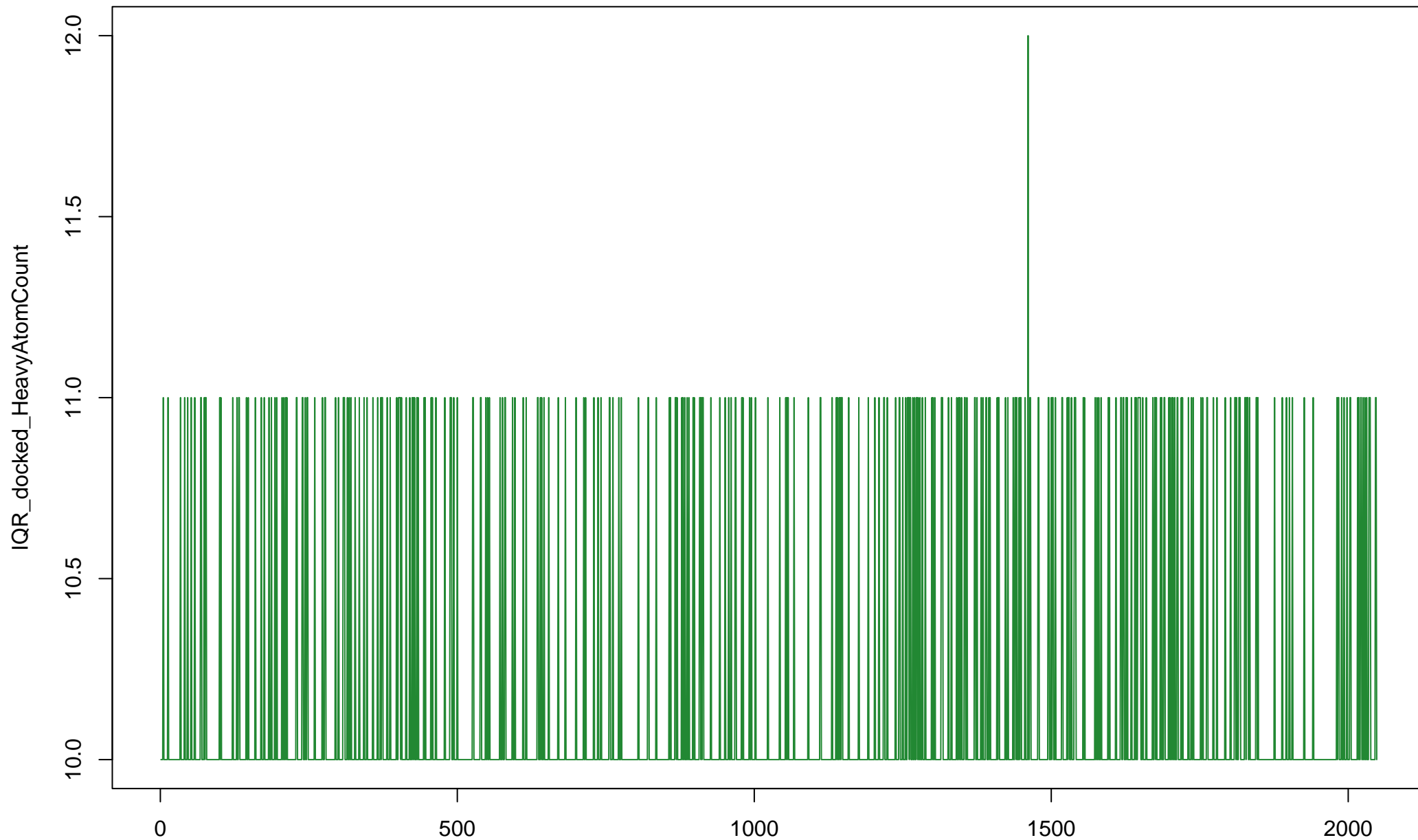
IQR_log_RMSD
ESS = 212 | BMK = 0.12 | MCSE(6.27) = 4.49 | stat: FALSE | burn: 0



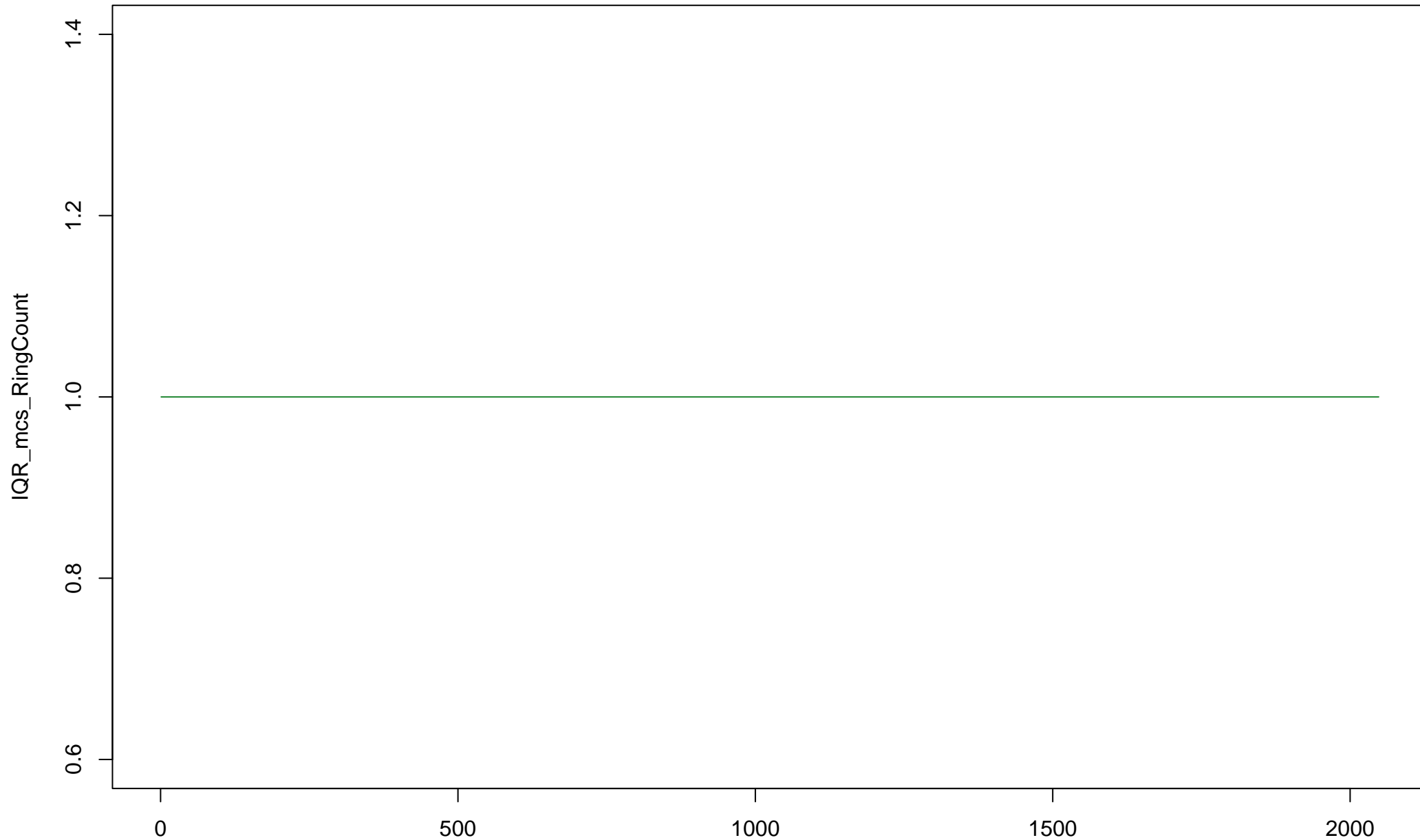
IQR_Xtransf_ec_tanimoto_similarity
ESS = 1650 | BMK = 0.0349 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0



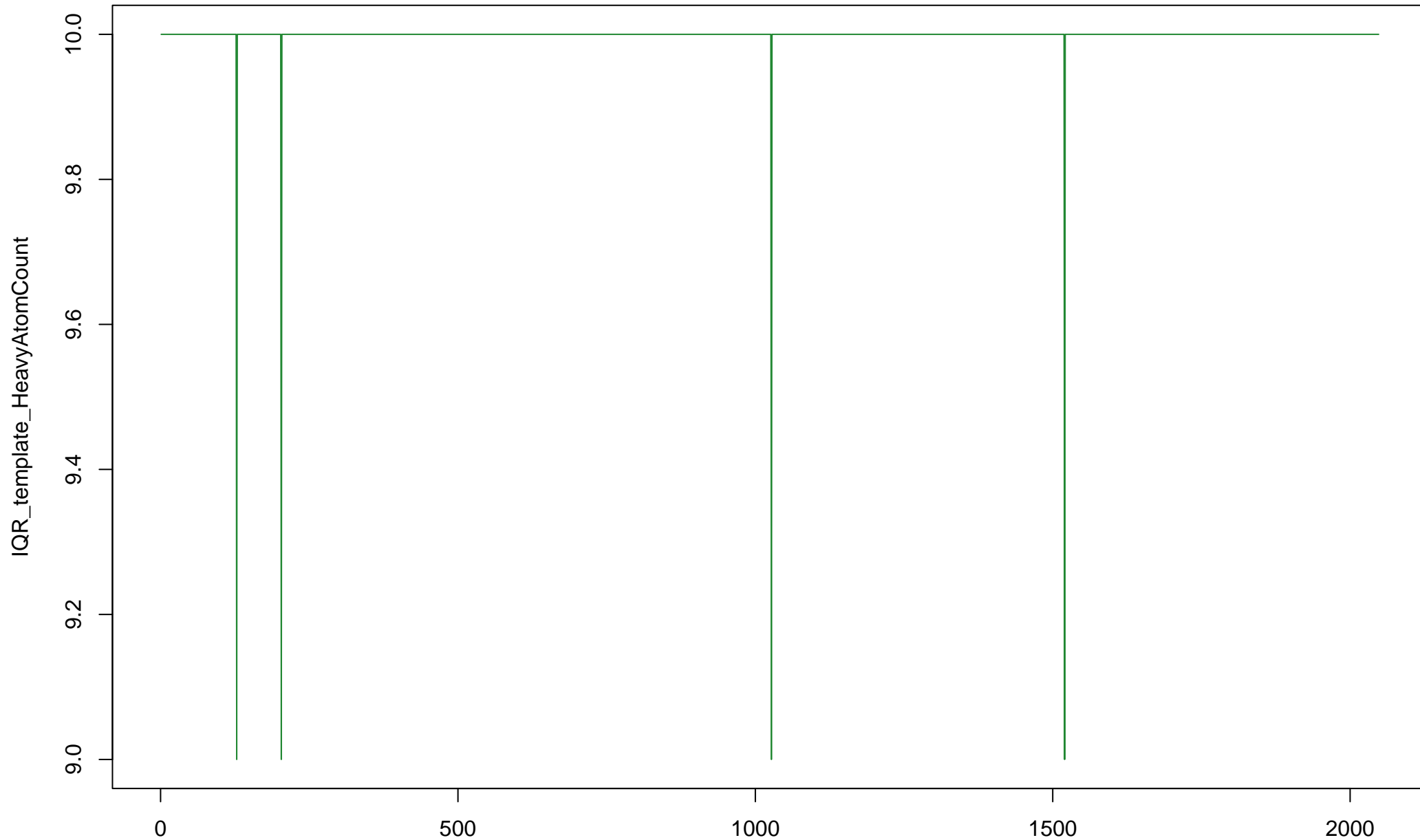
IQR_docked_HeavyAtomCount
ESS = 1870 | BMK = 0.0541 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0



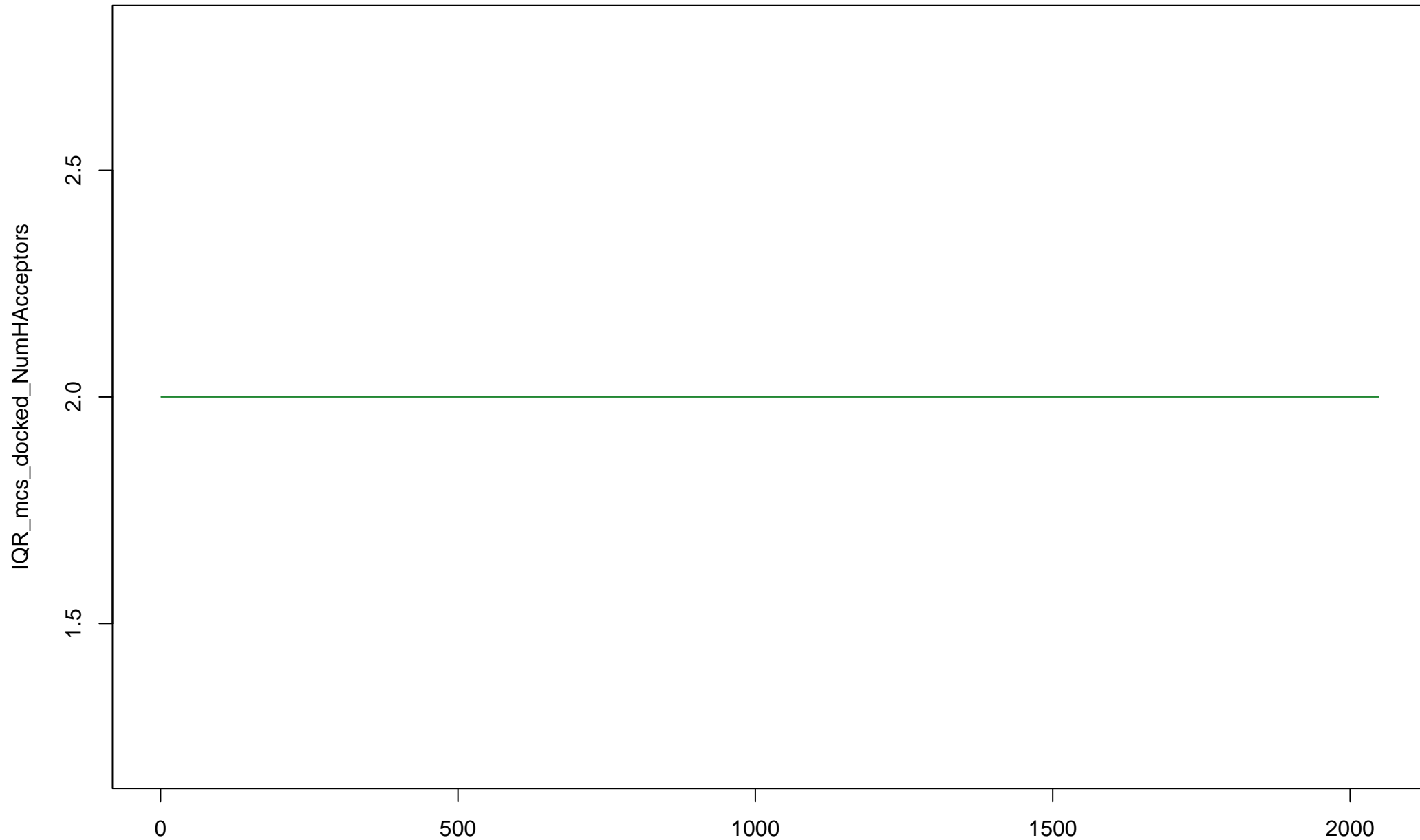
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



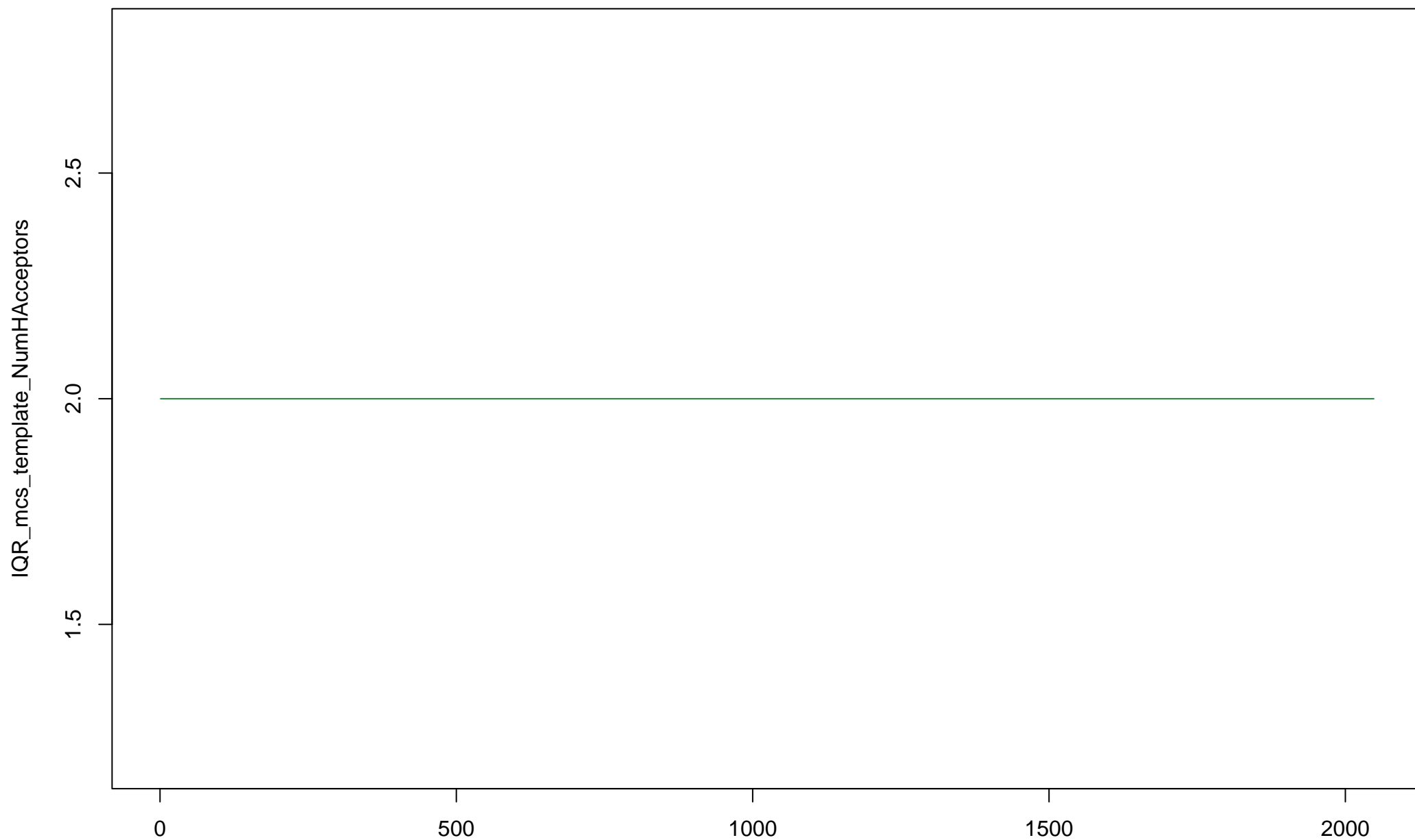
IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1632



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



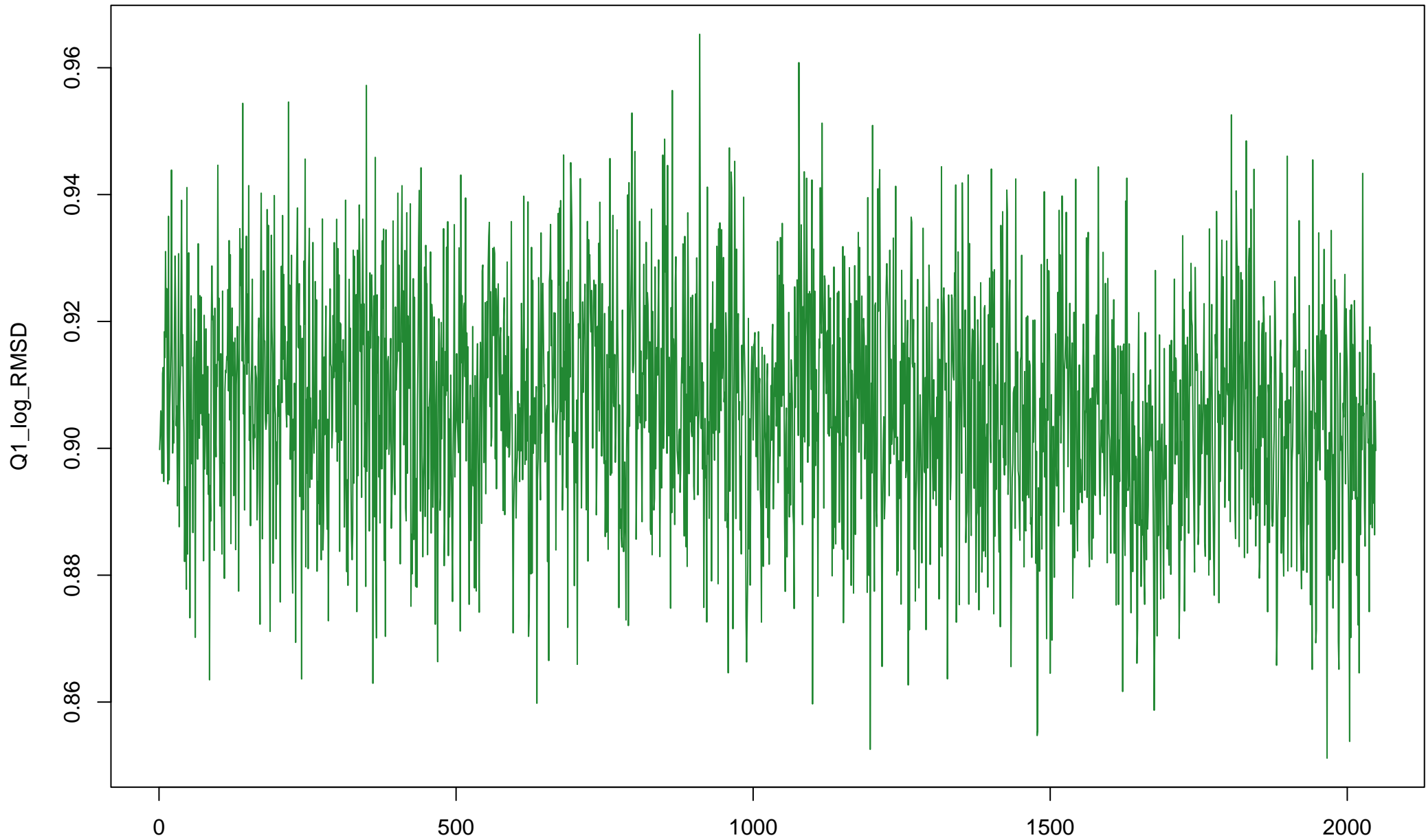
IQR_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



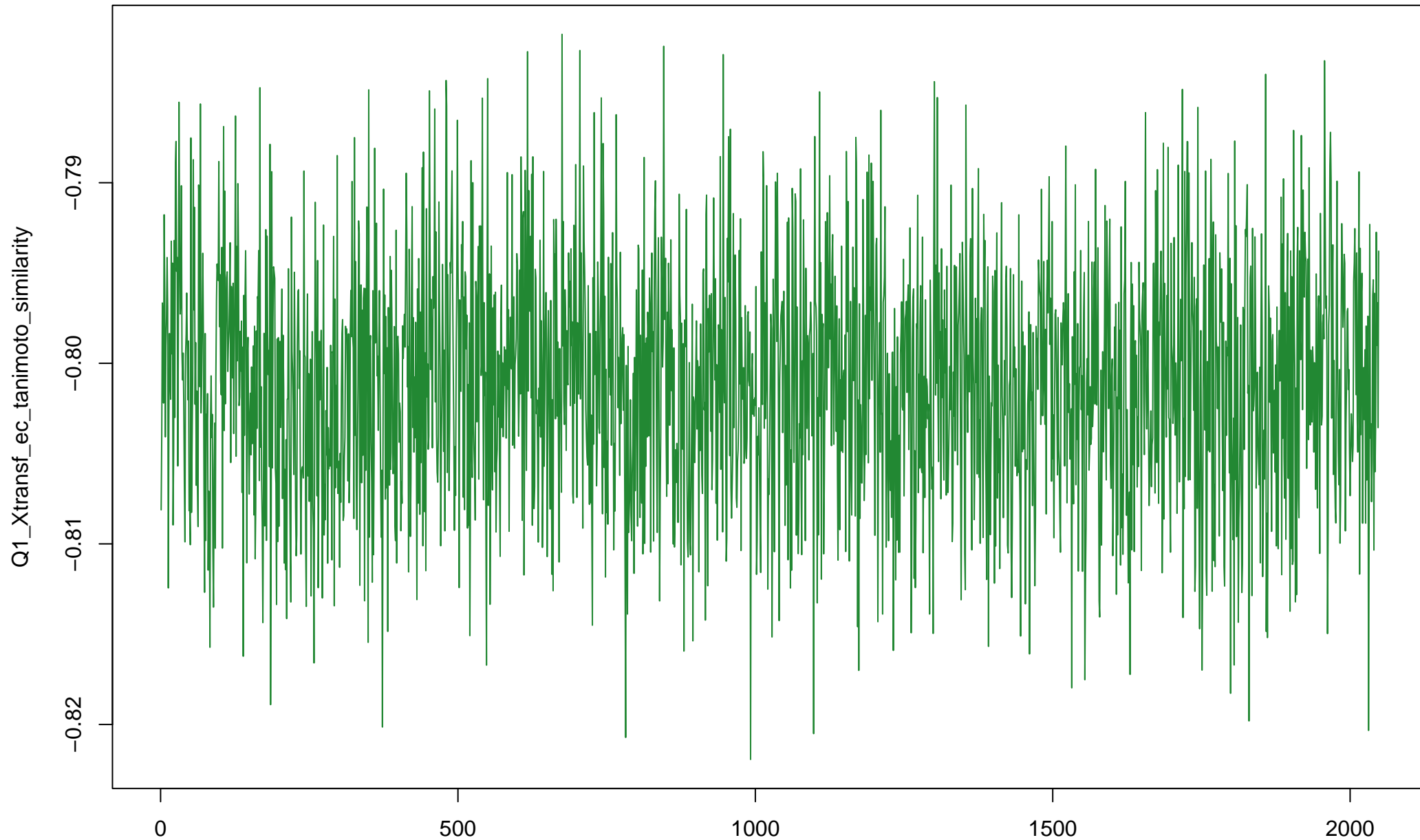
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



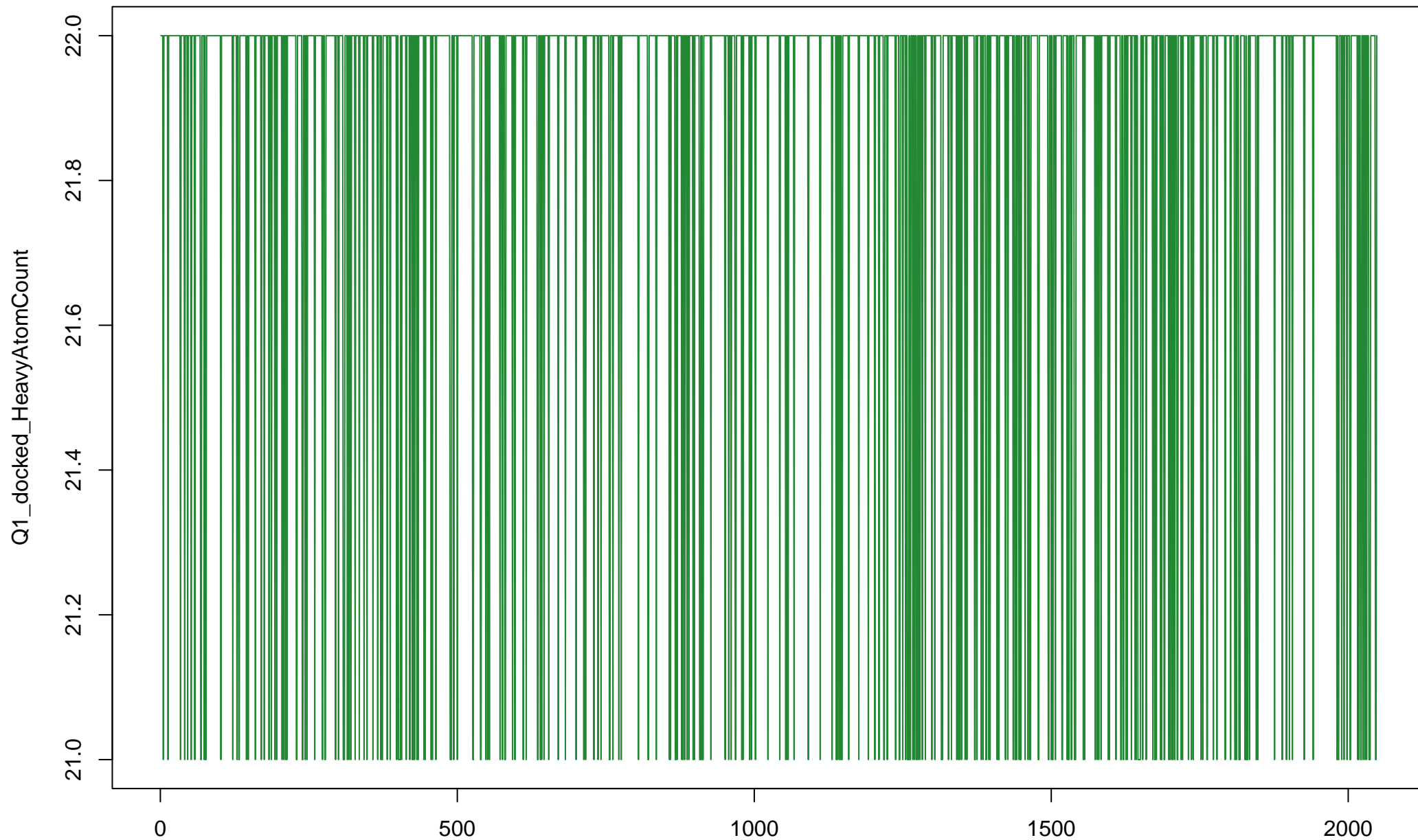
Q1_log_RMSD
ESS = 890 | BMK = 0.0898 | MCSE(6.27) = 3.61 | stat: FALSE | burn: 0



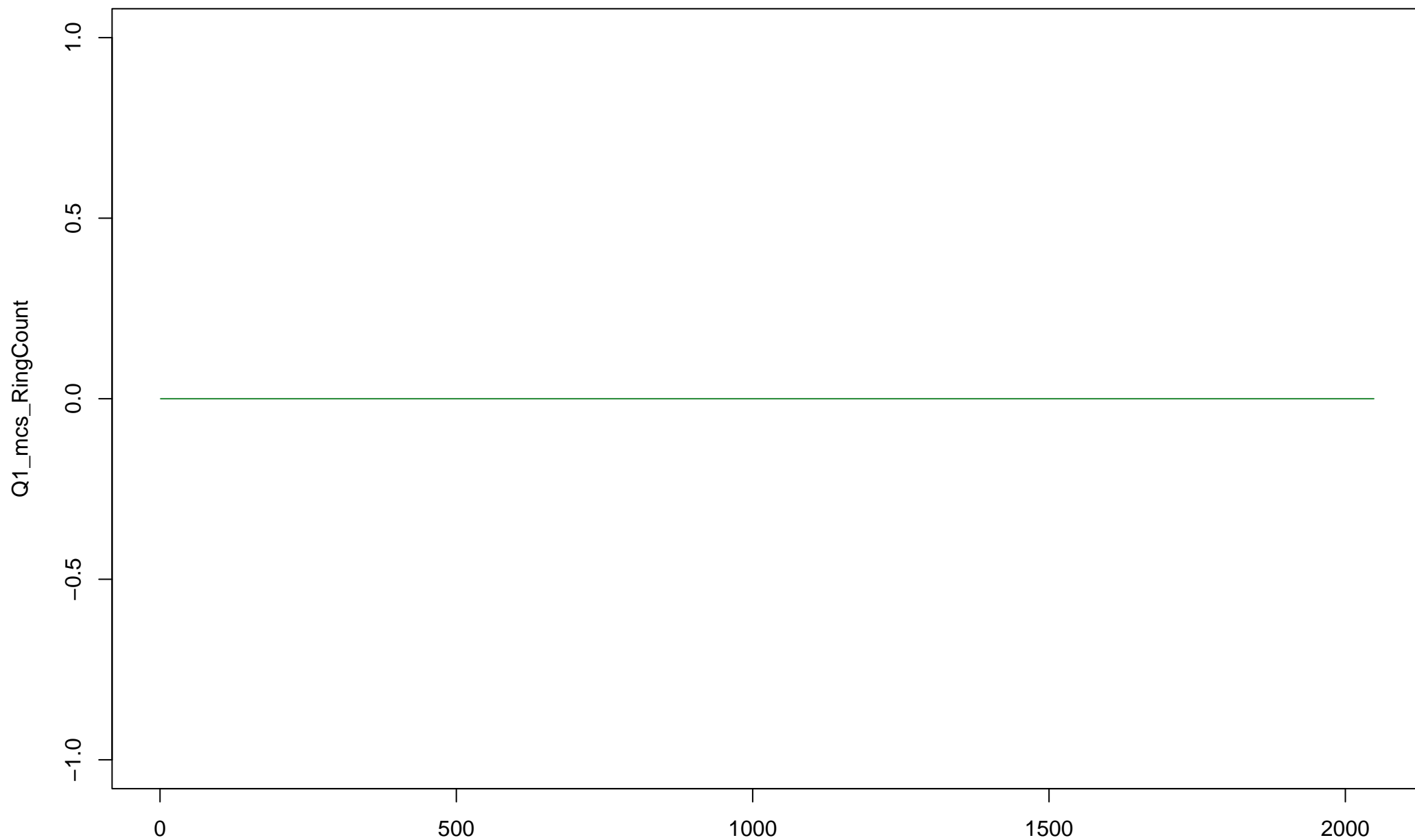
Q1_Xtransf_ec_tanimoto_similarity
ESS = 1830 | BMK = 0.0411 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0



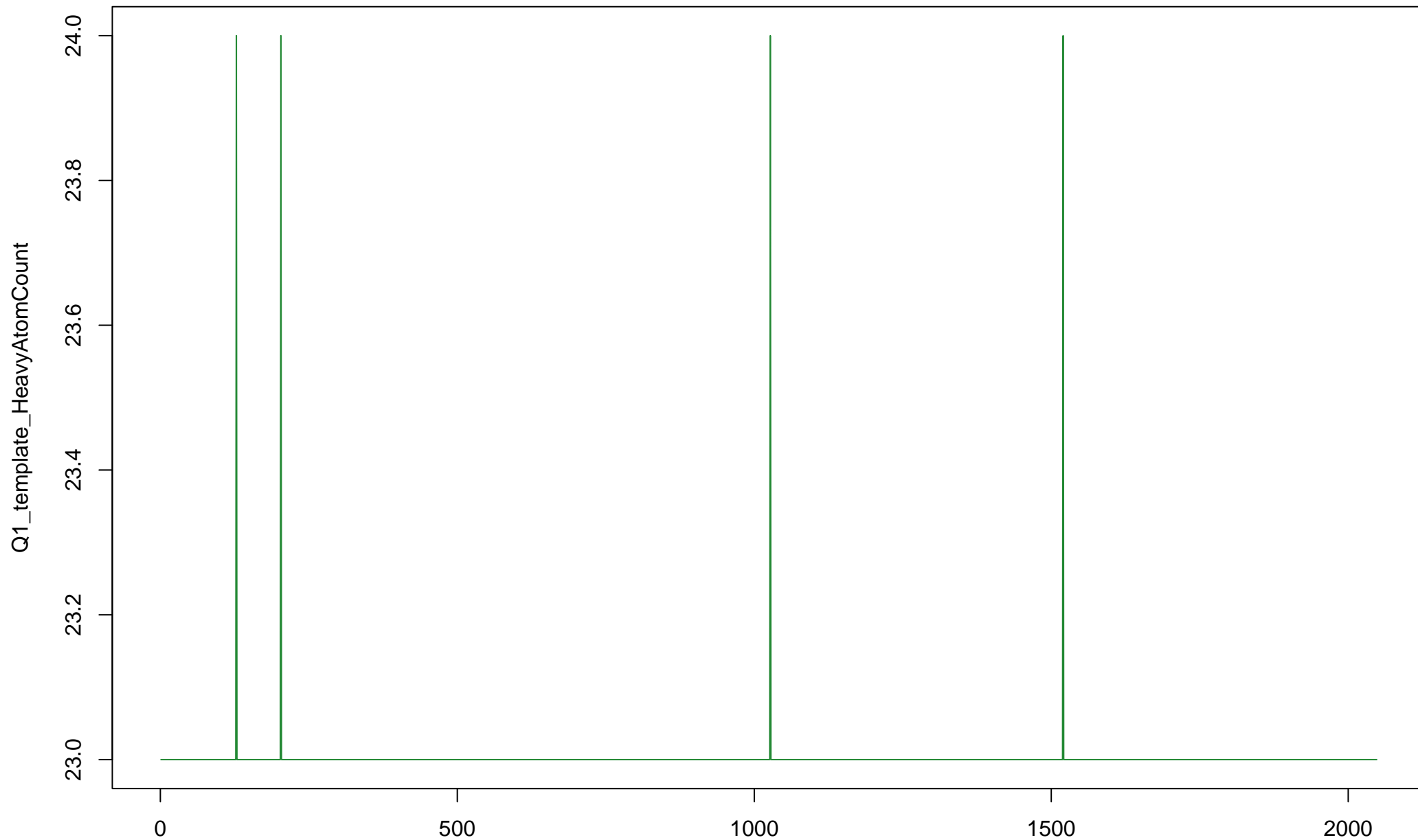
Q1_docked_HeavyAtomCount
ESS = 1870 | BMK = 0.0438 | MCSE(6.27) = 2.95 | stat: FALSE | burn: 0



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



Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1632



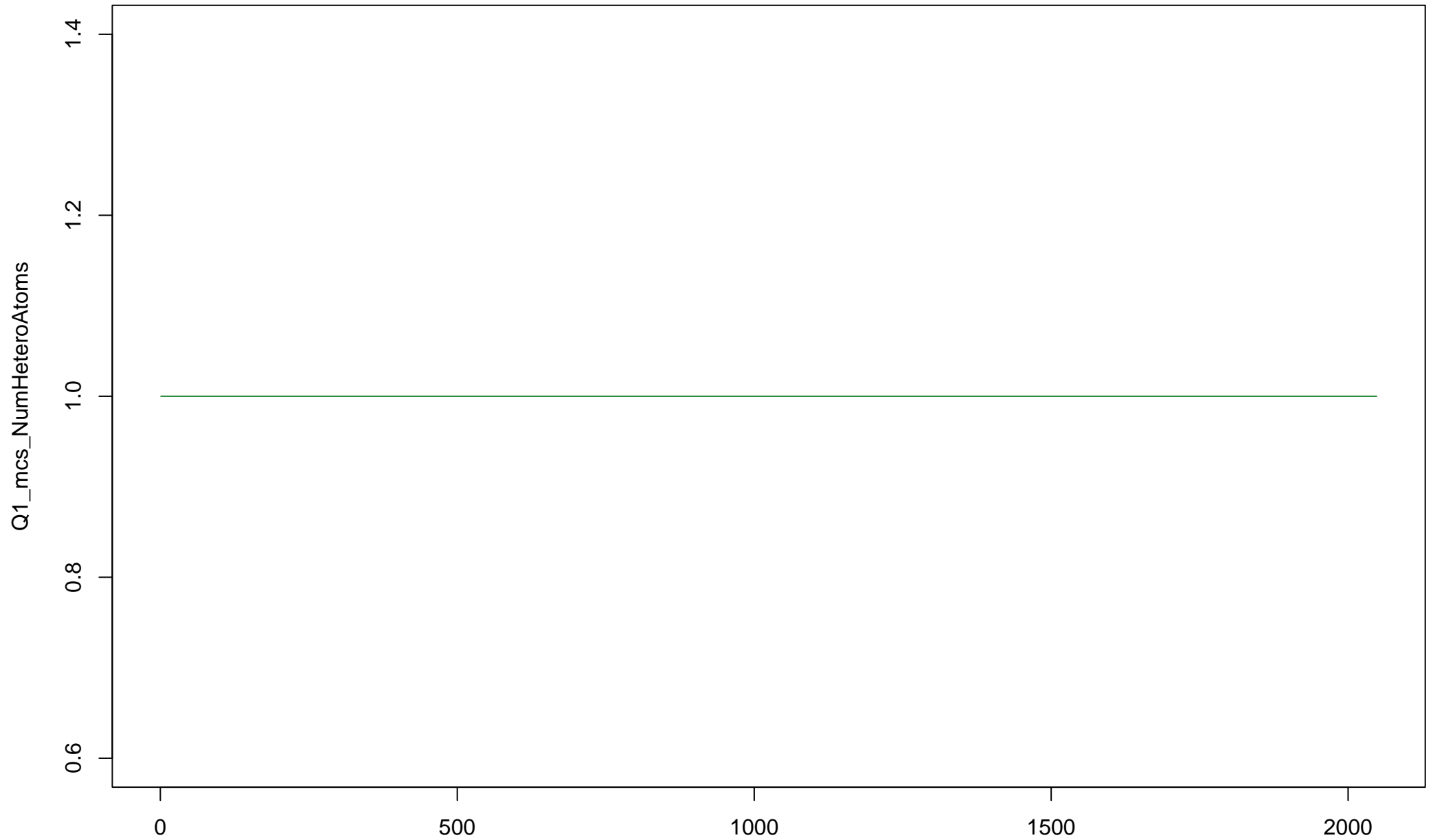
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



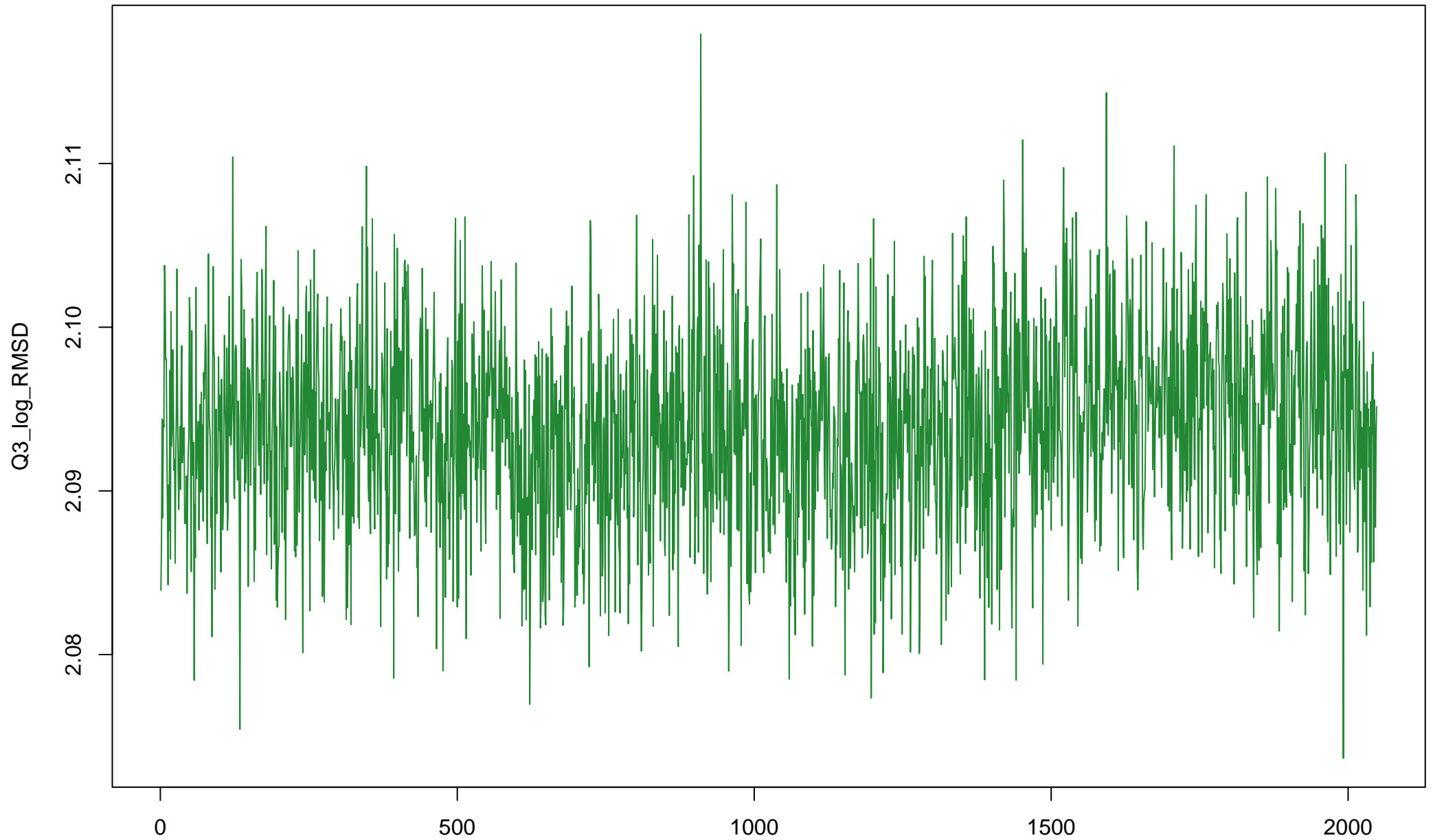
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



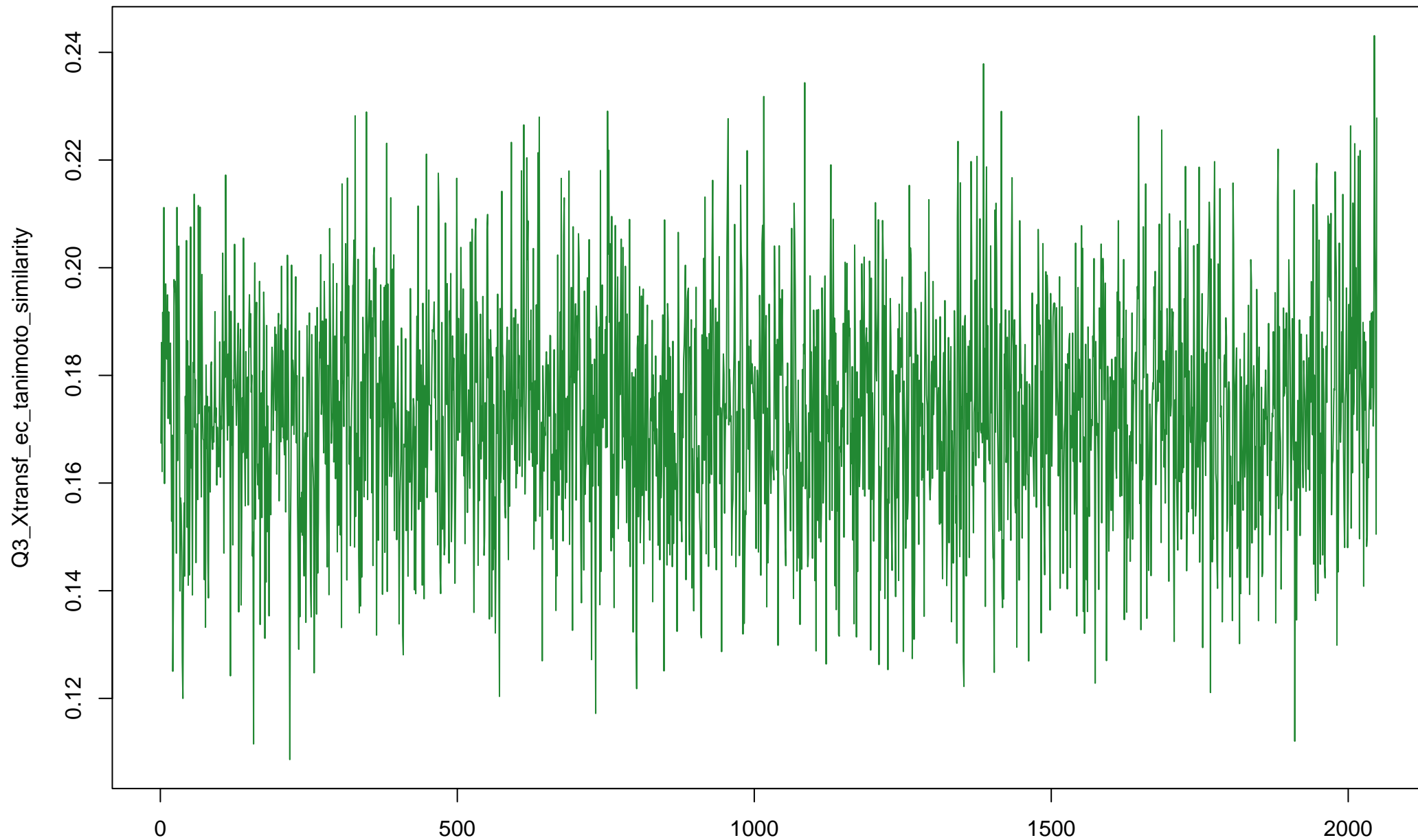
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



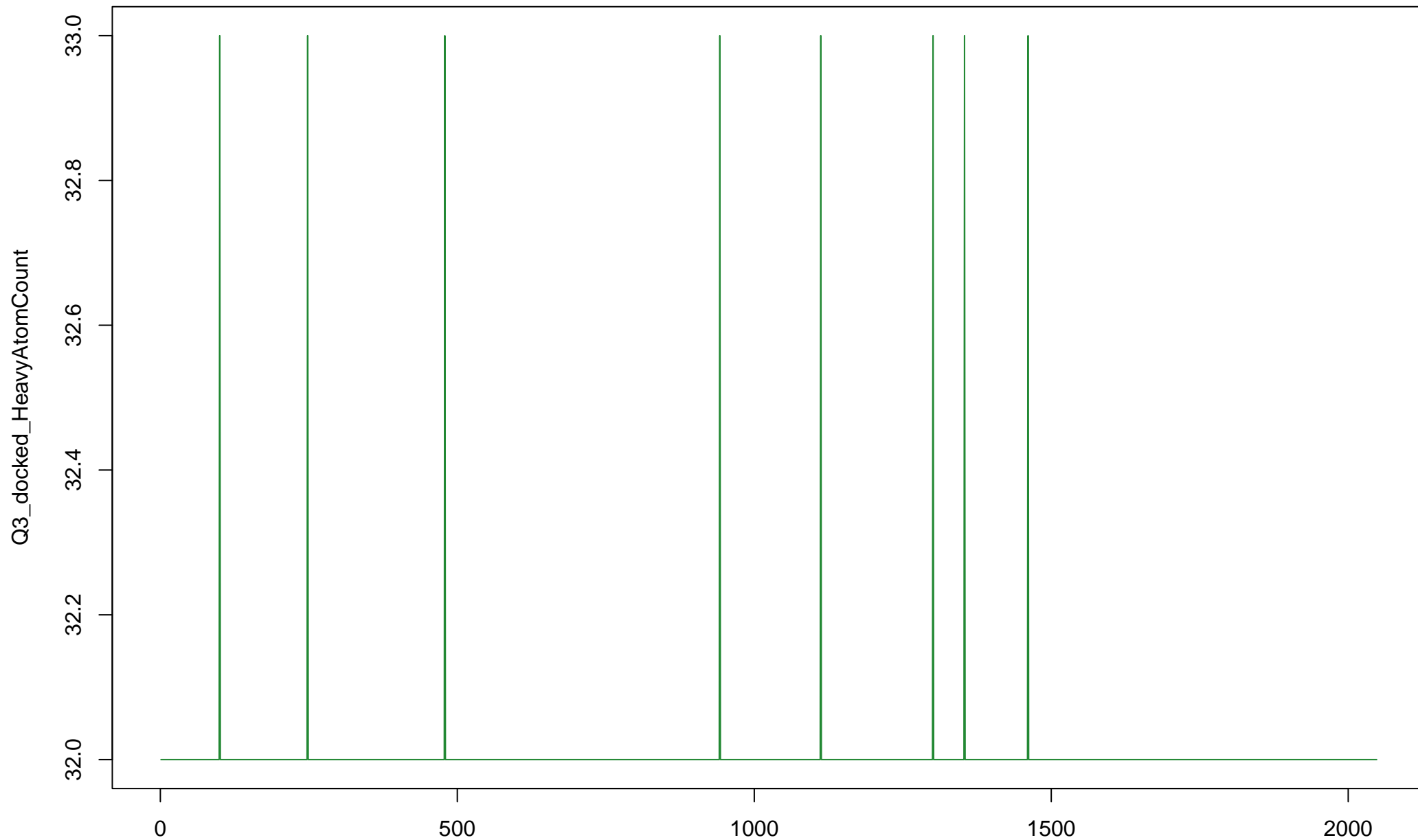
Q3_log_RMSD
ESS = 1000 | BMK = 0.0794 | MCSE(6.27) = 3.68 | stat: FALSE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 1850 | BMK = 0.0252 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0



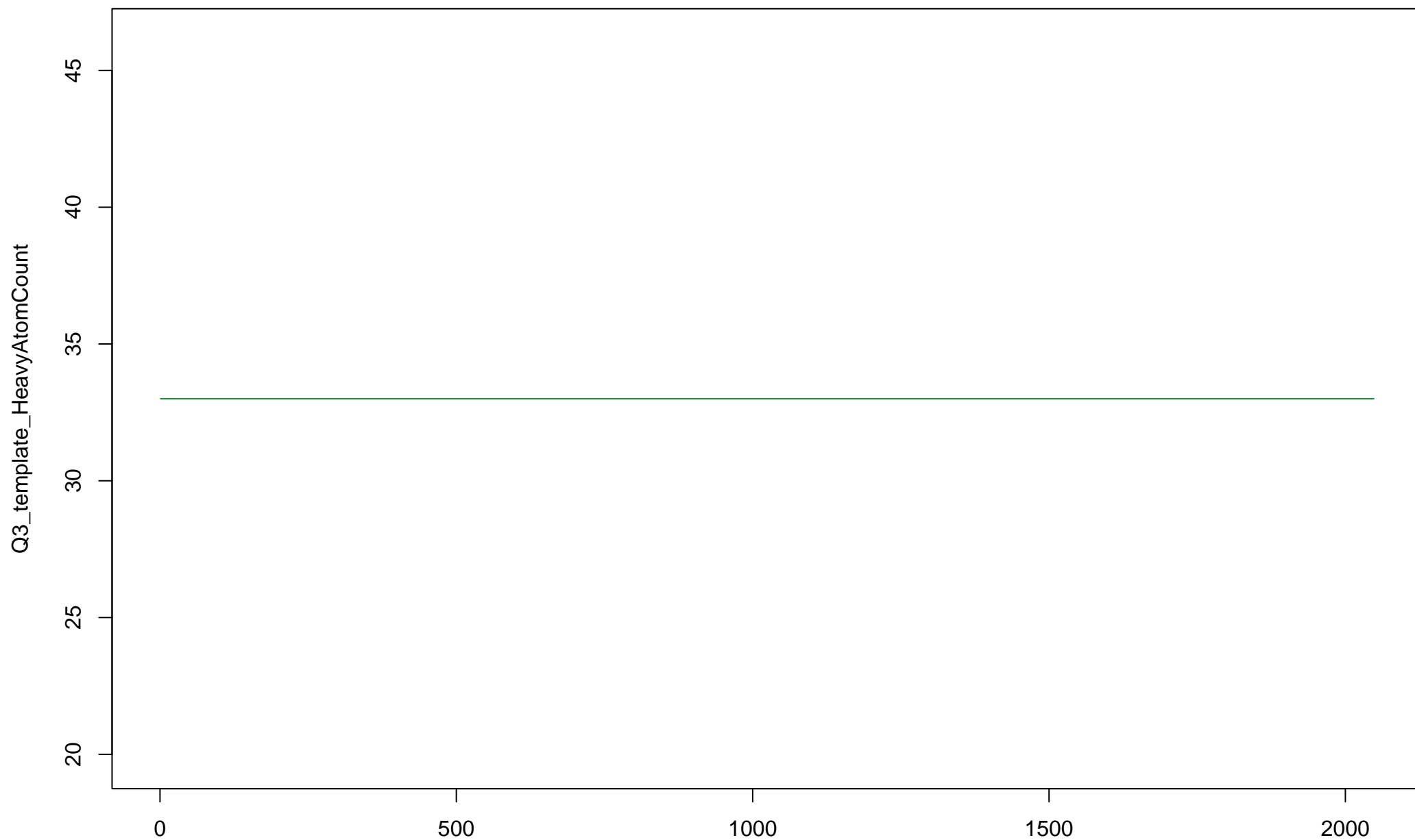
Q3_docked_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 1632



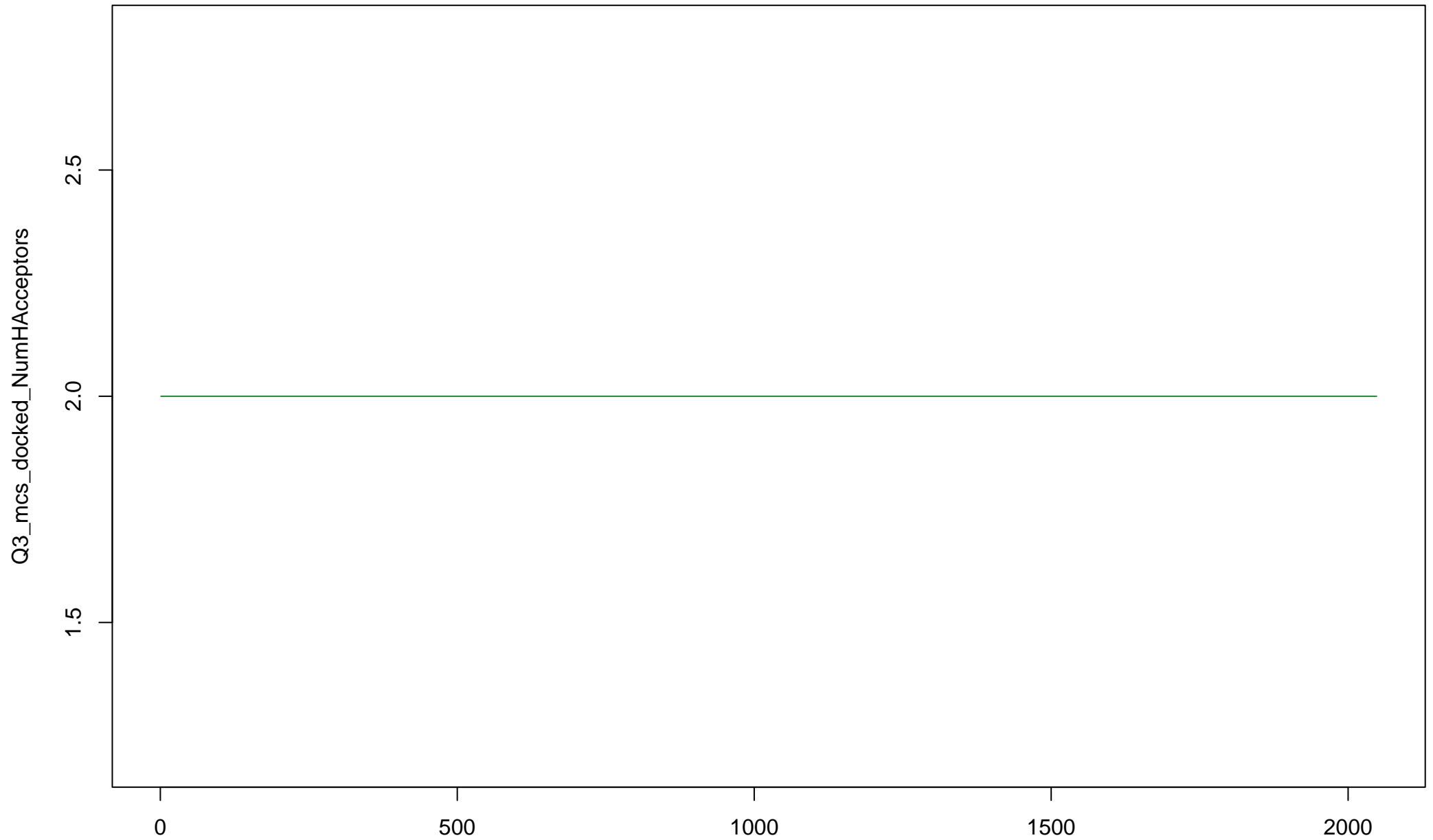
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



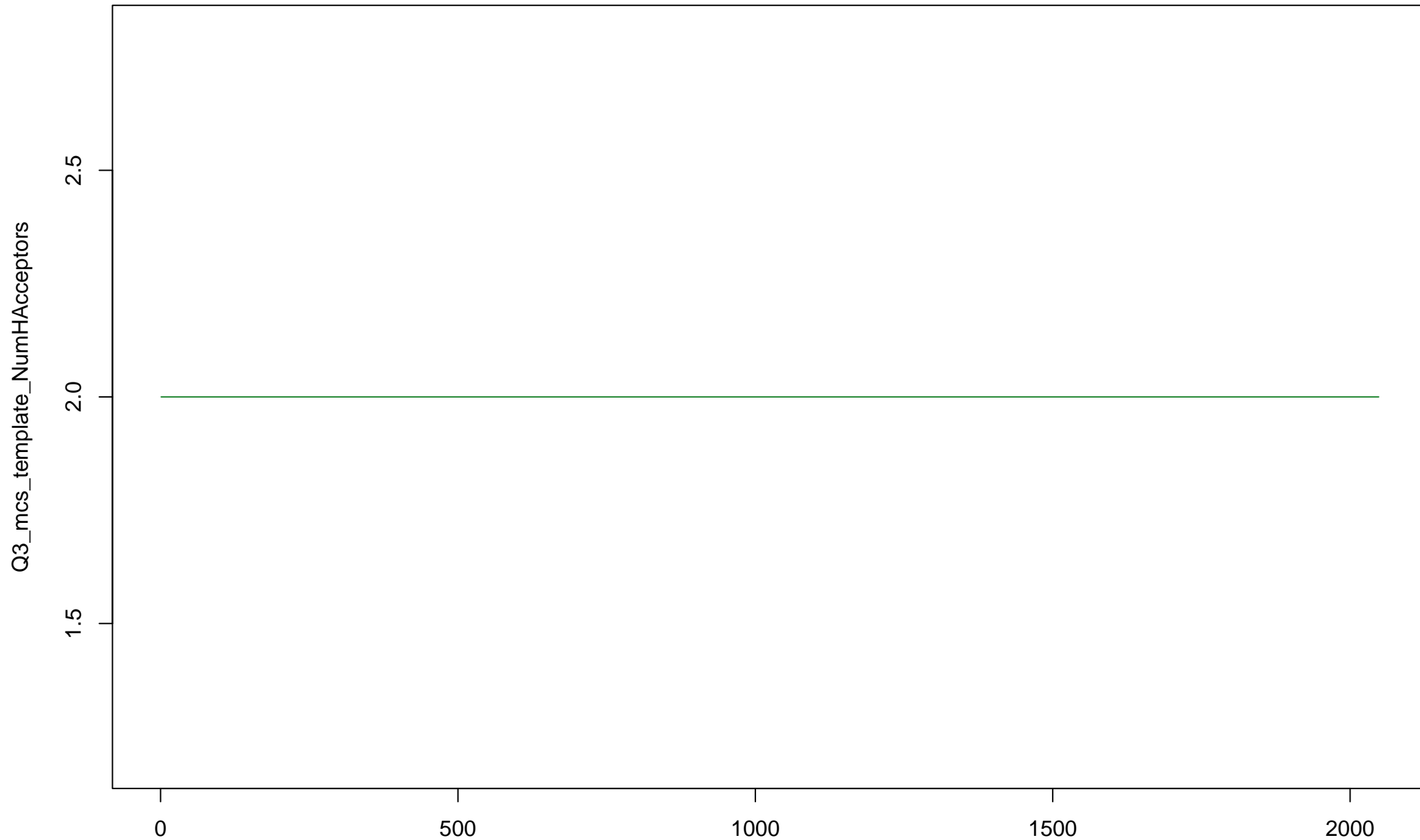
Q3_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



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



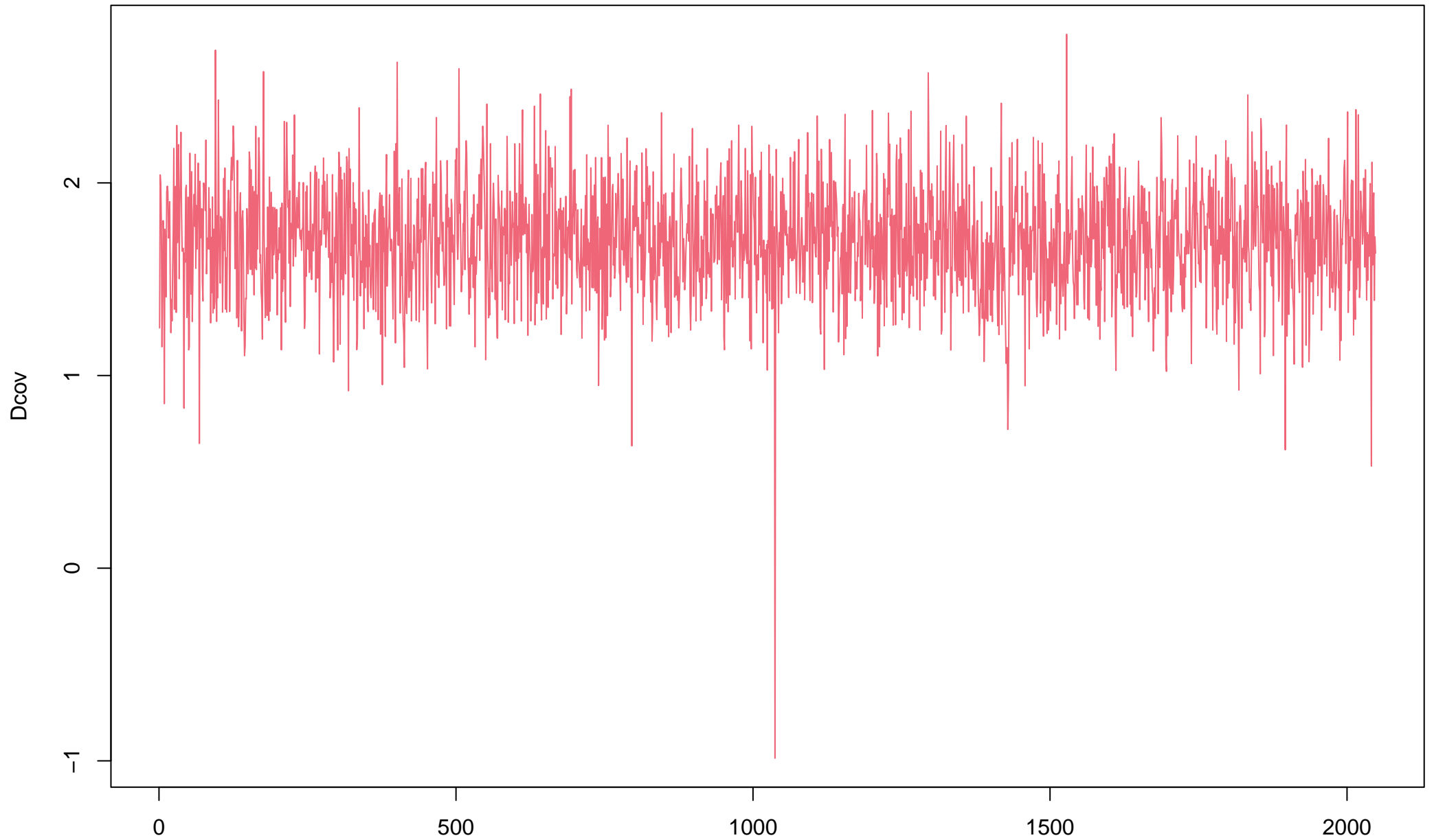
Q3_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



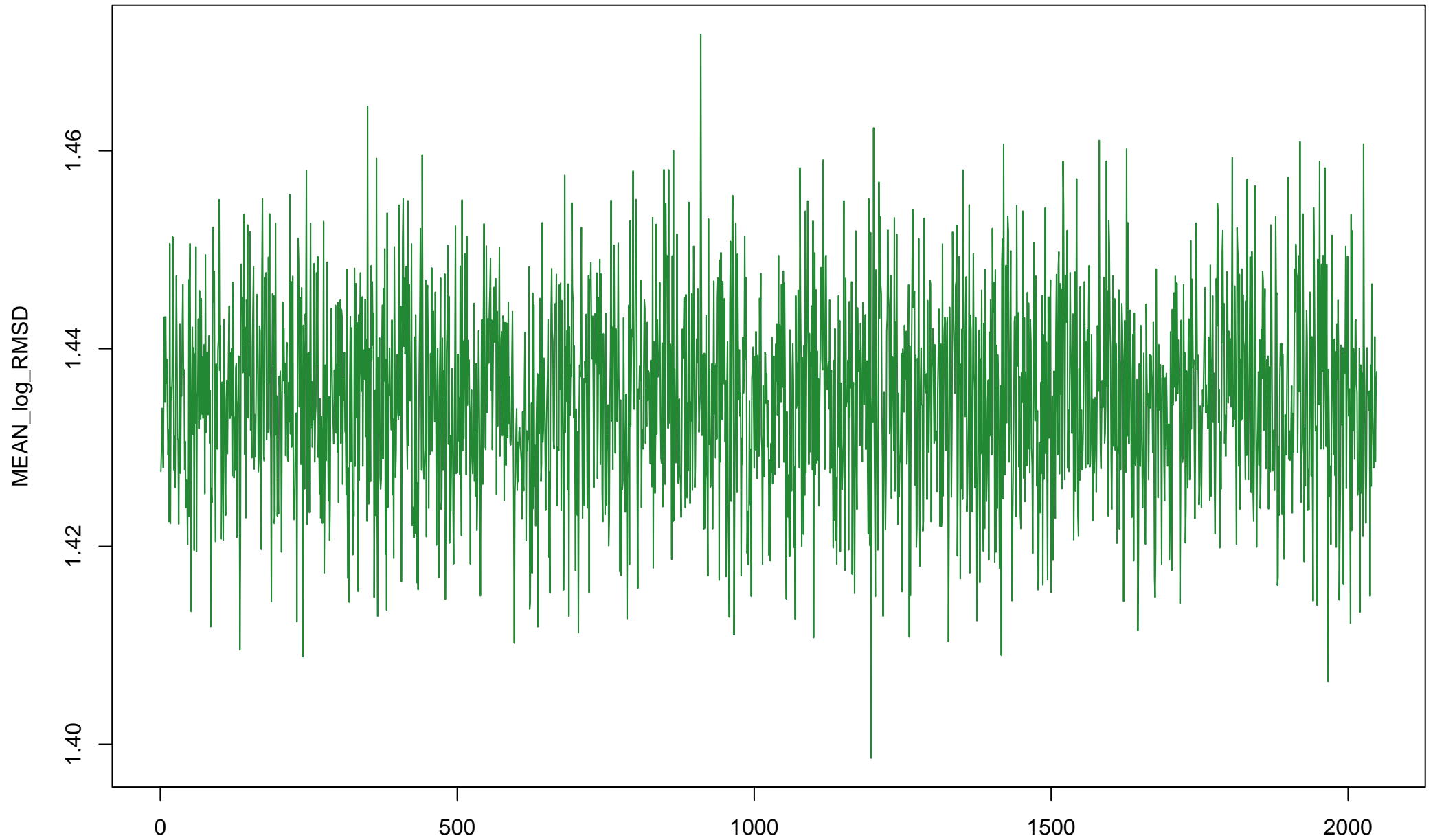
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



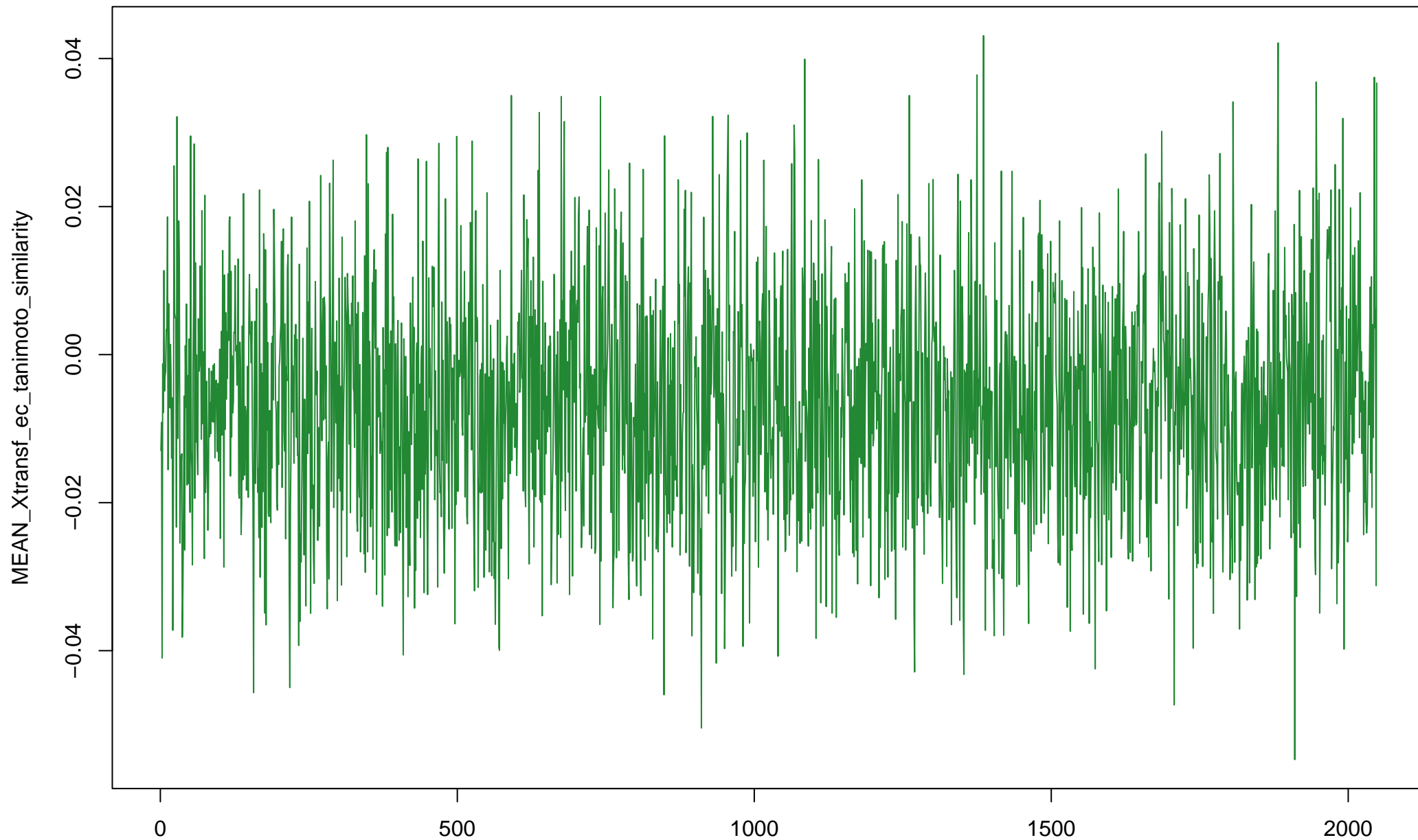
Dcov
ESS = 2050 | BMK = 0.0492 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0



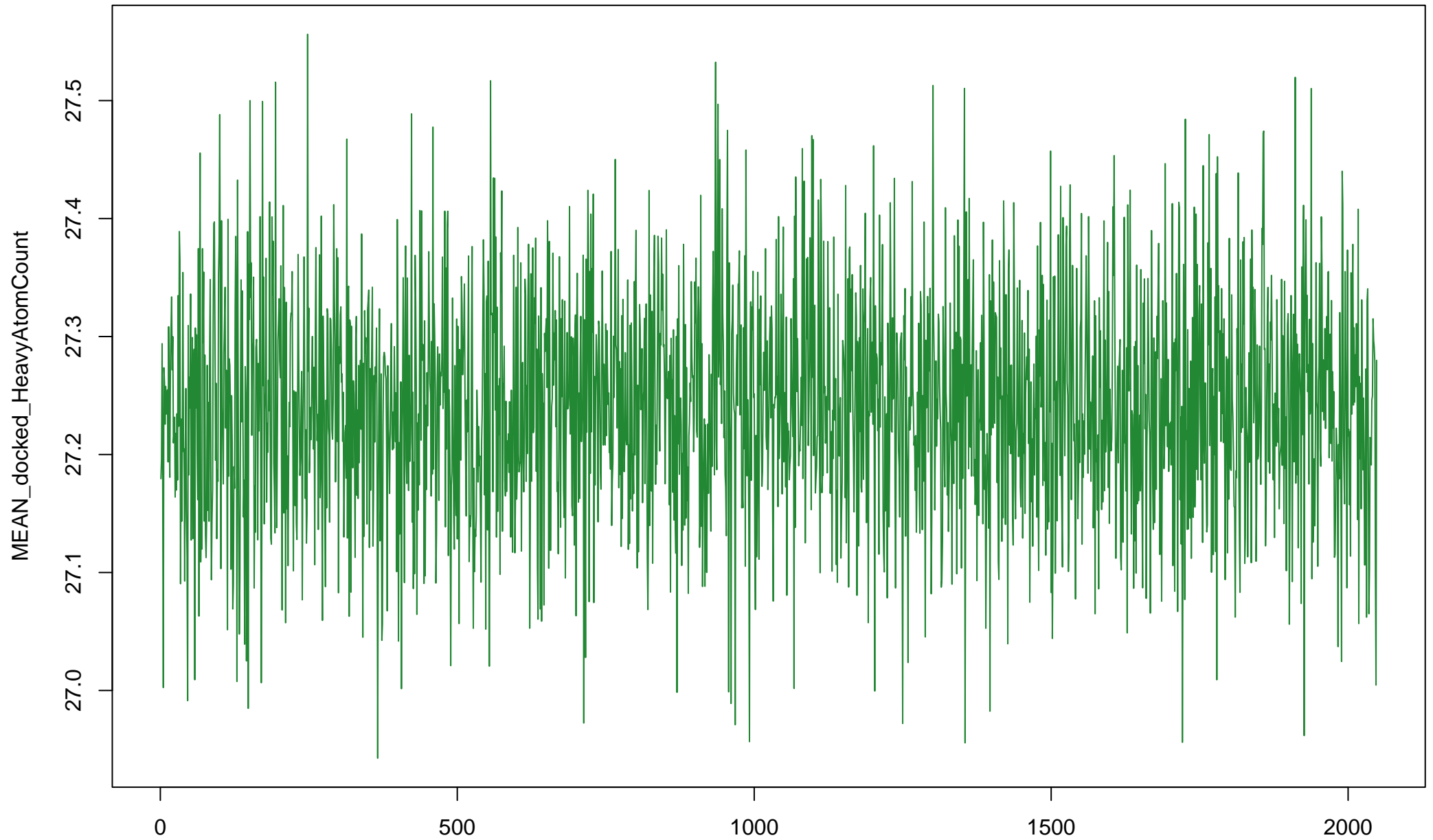
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0432 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0



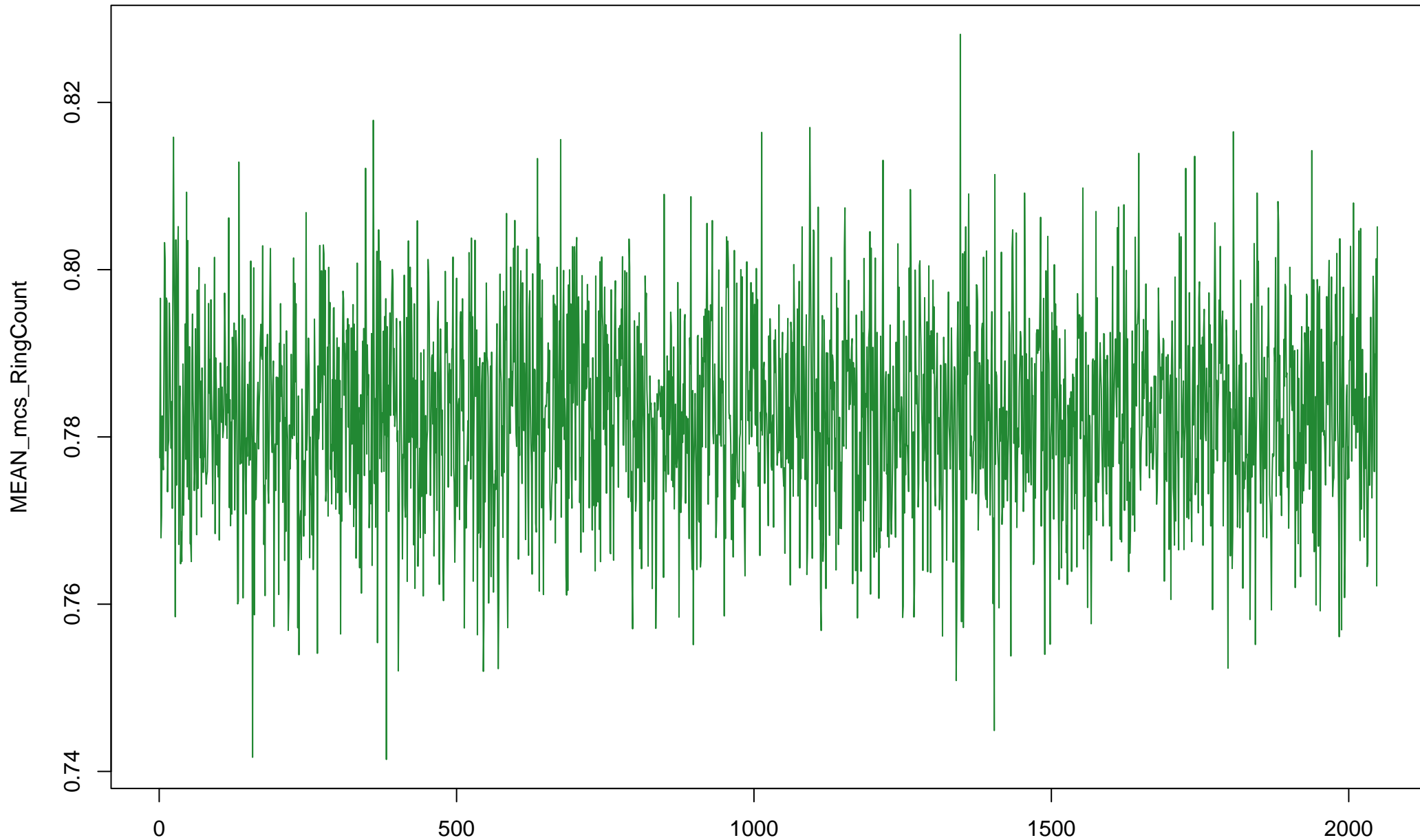
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0418 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0



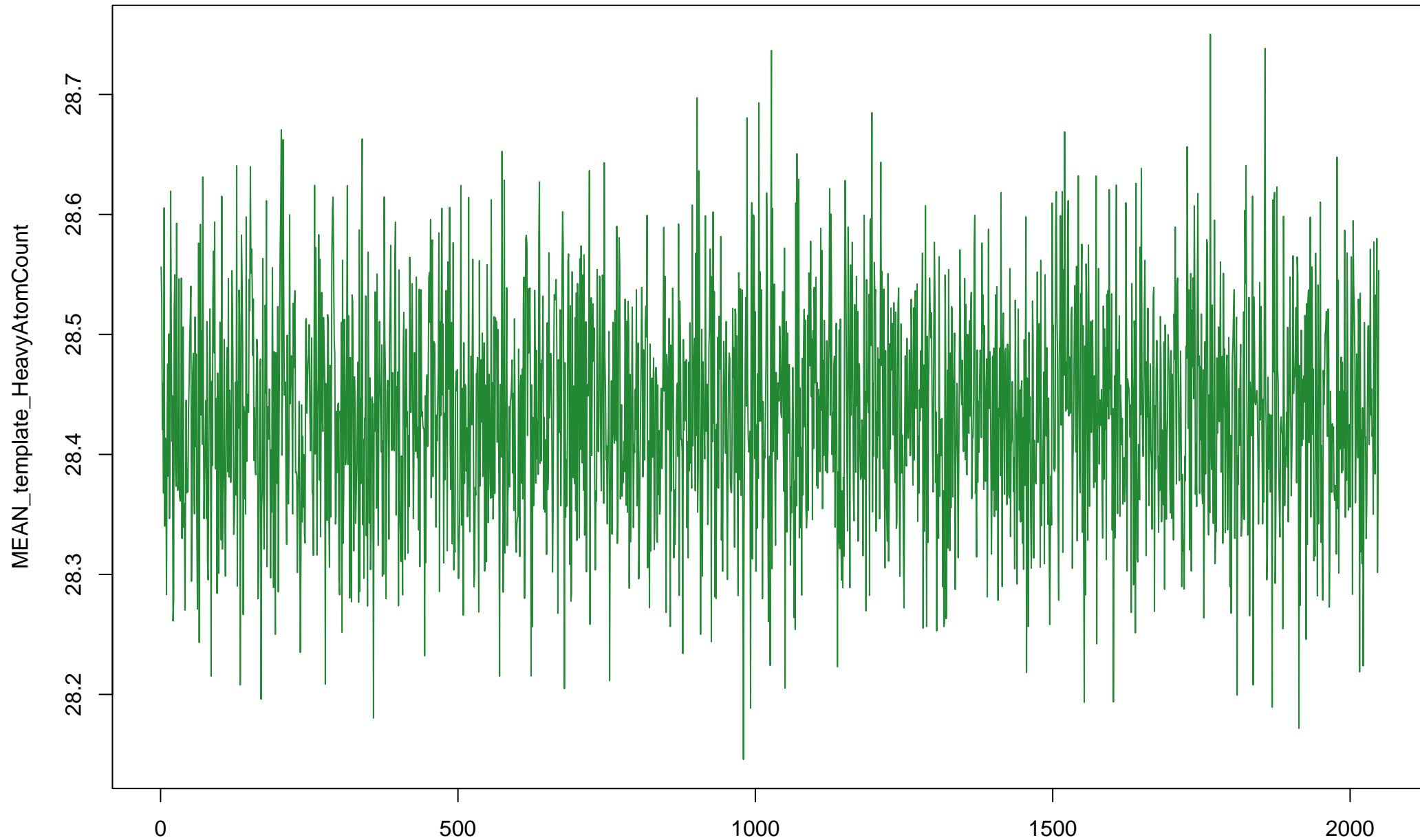
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.049 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0



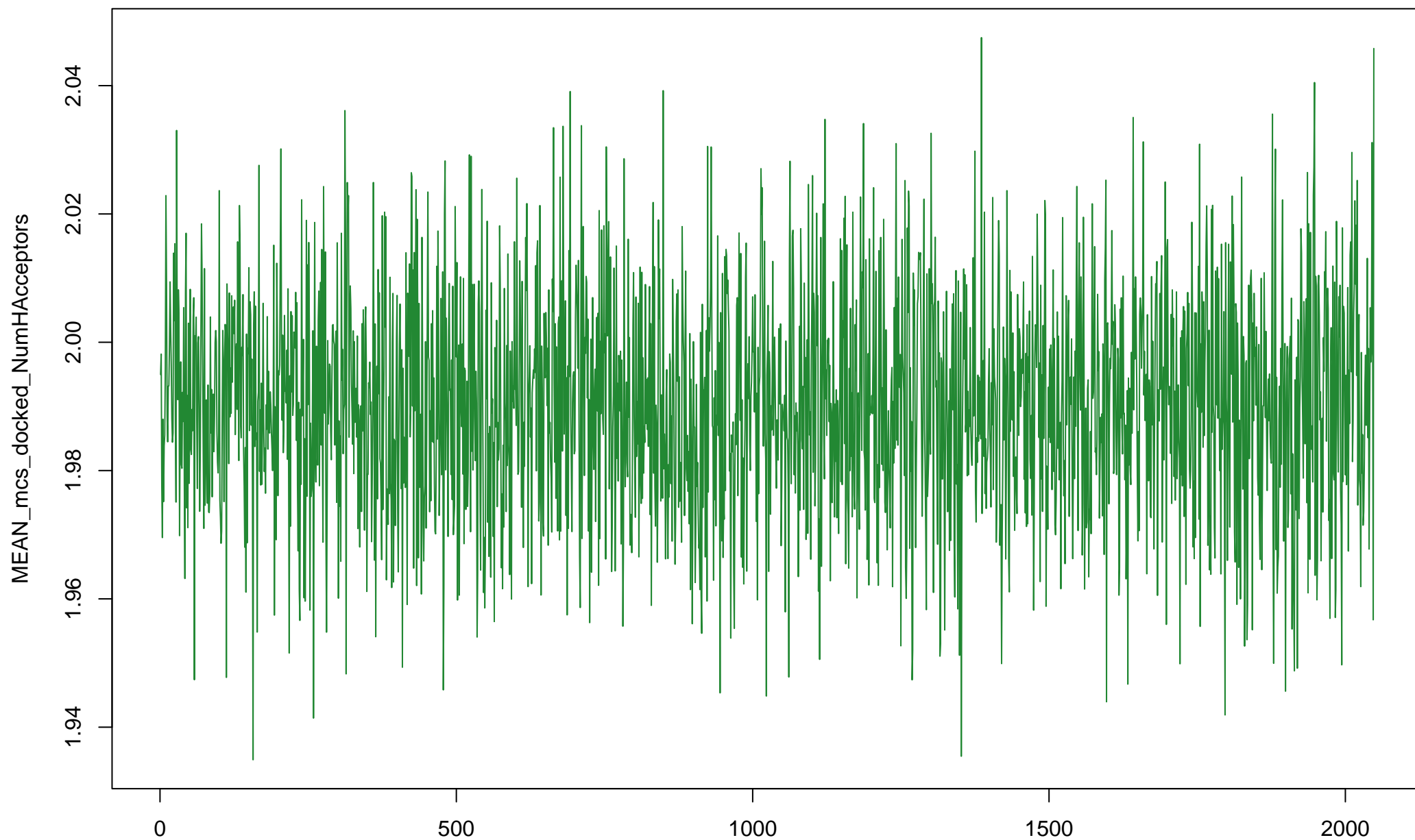
MEAN_mcs_RingCount
ESS = 1820 | BMK = 0.0475 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0



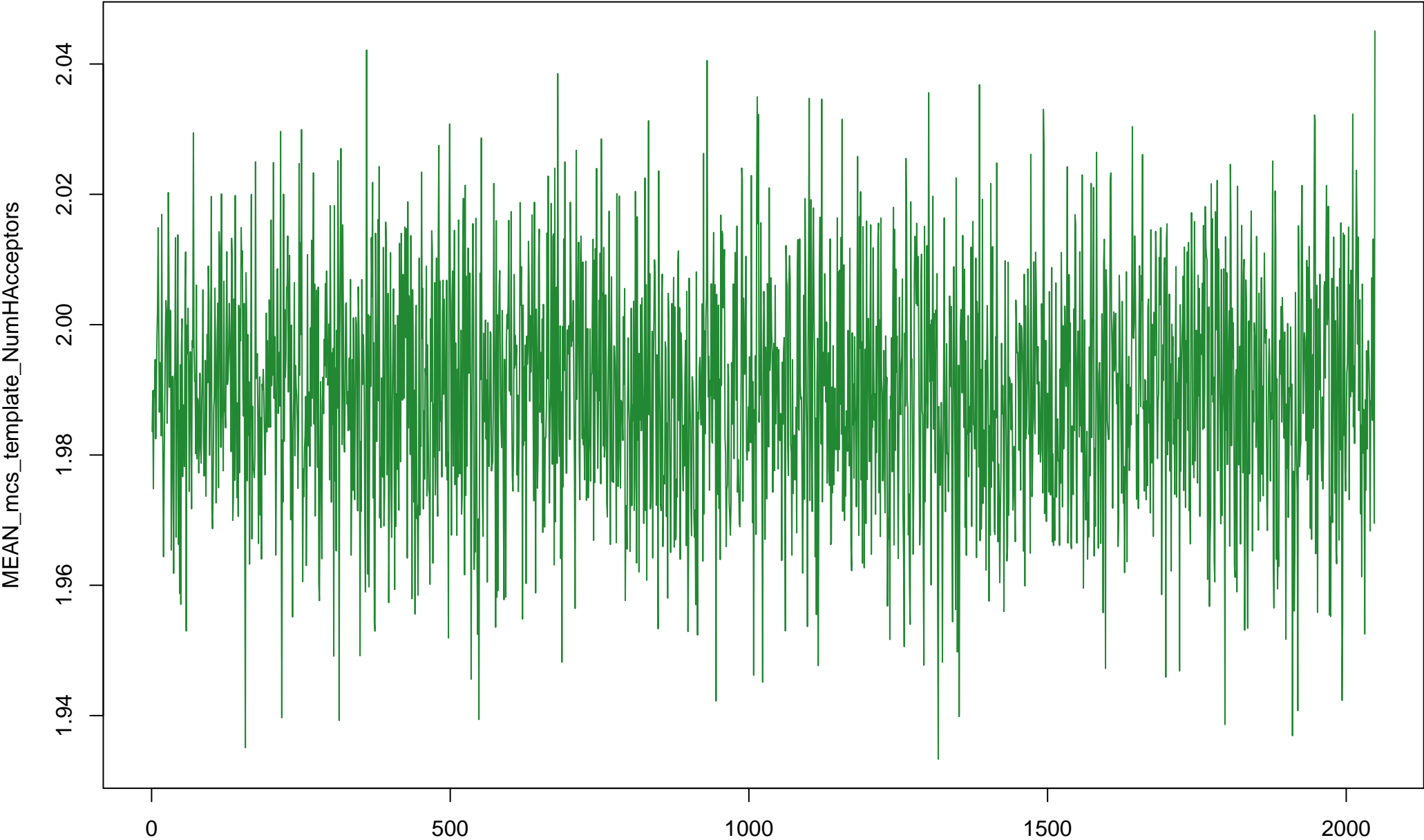
MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0369 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0



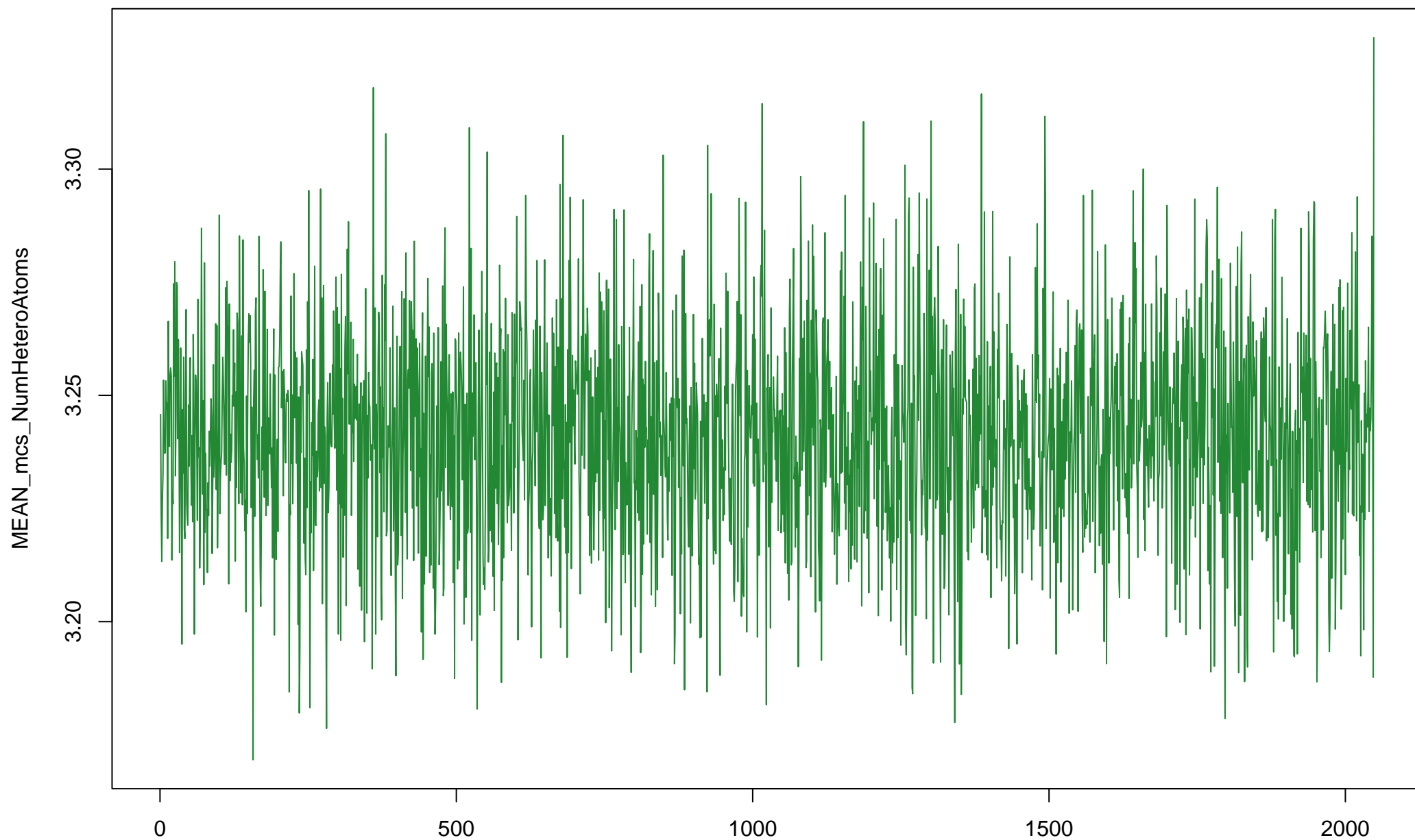
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0263 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0



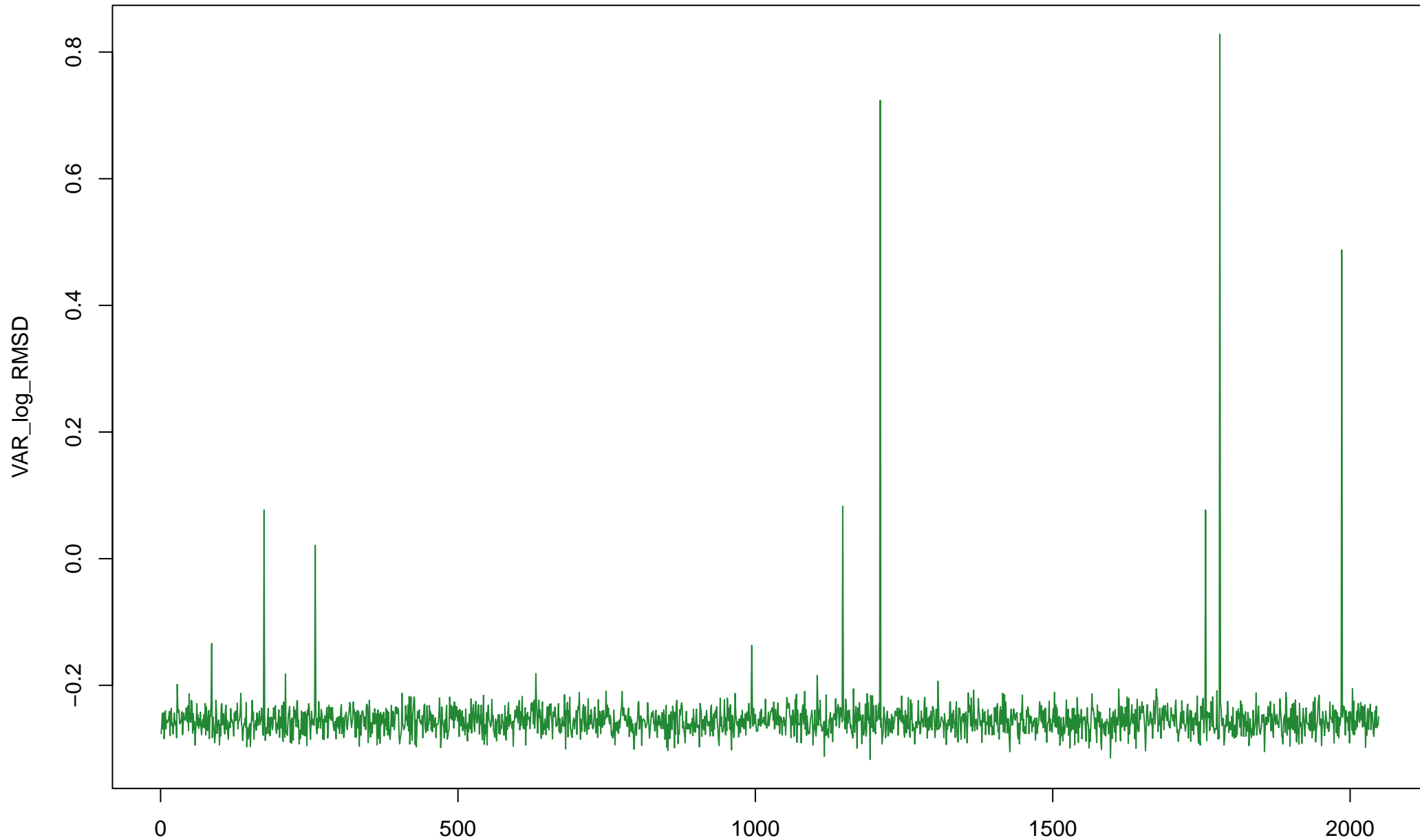
MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.028 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0



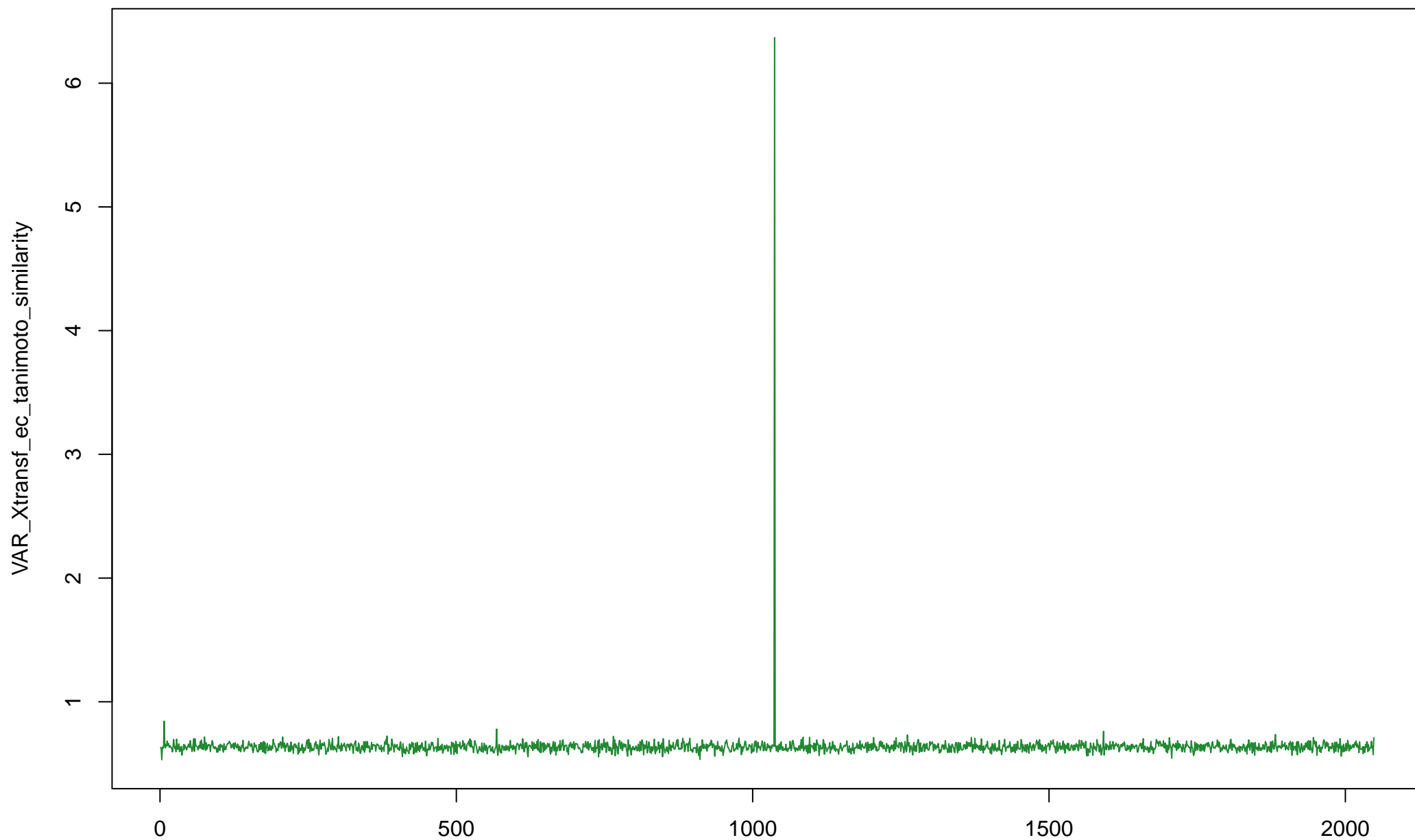
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0366 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0



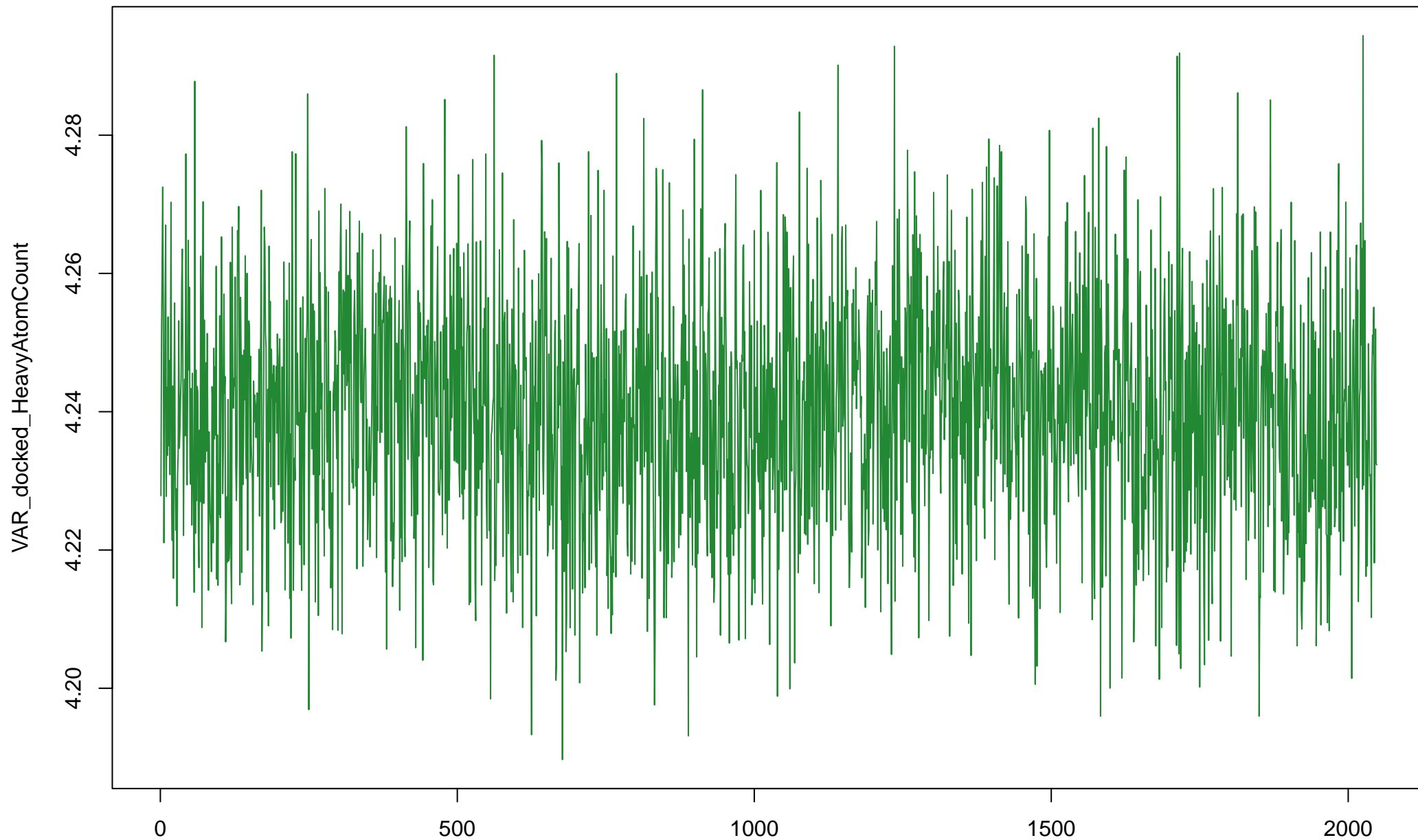
VAR_log_RMSD
ESS = 2050 | BMK = 0.0737 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0



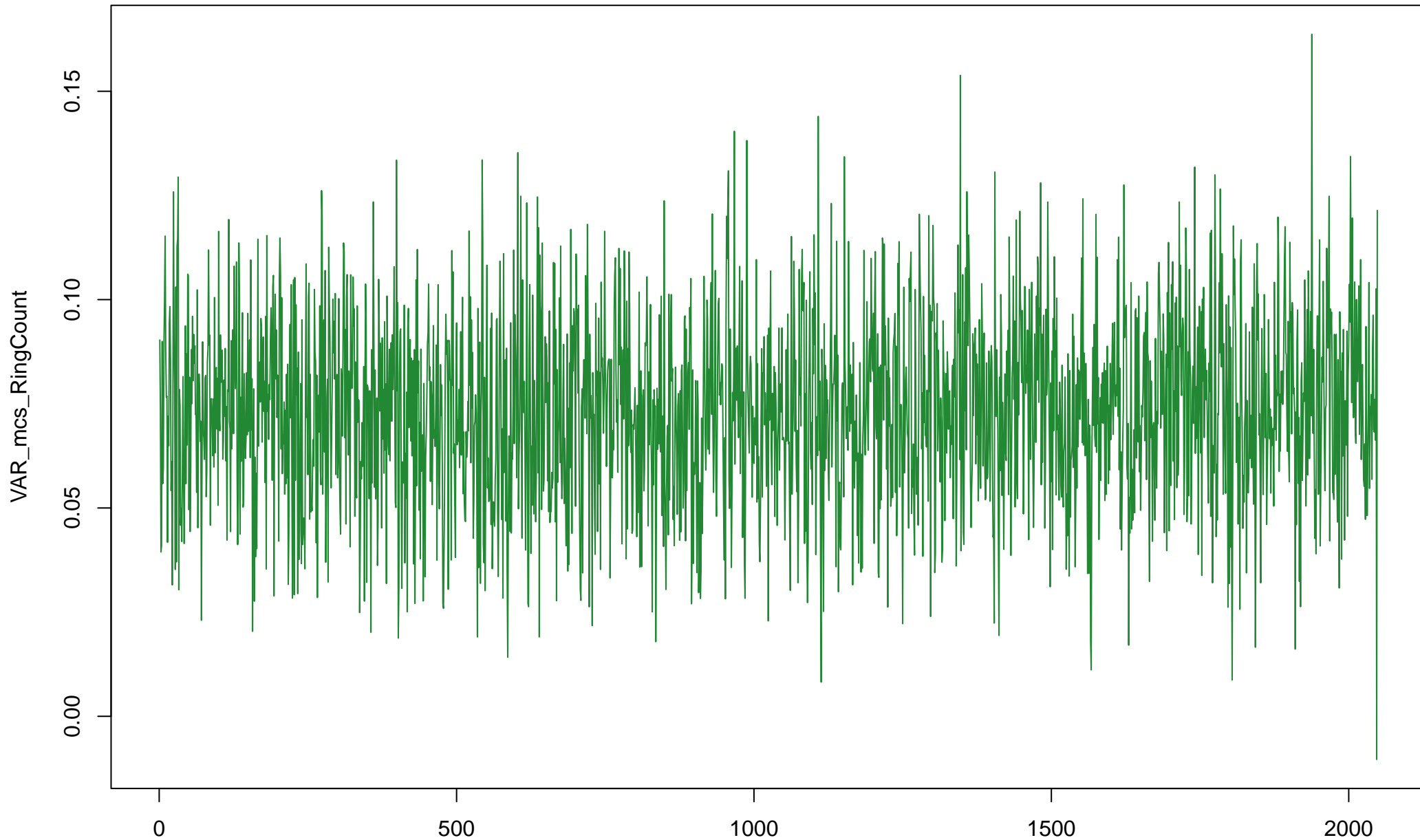
VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0994 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



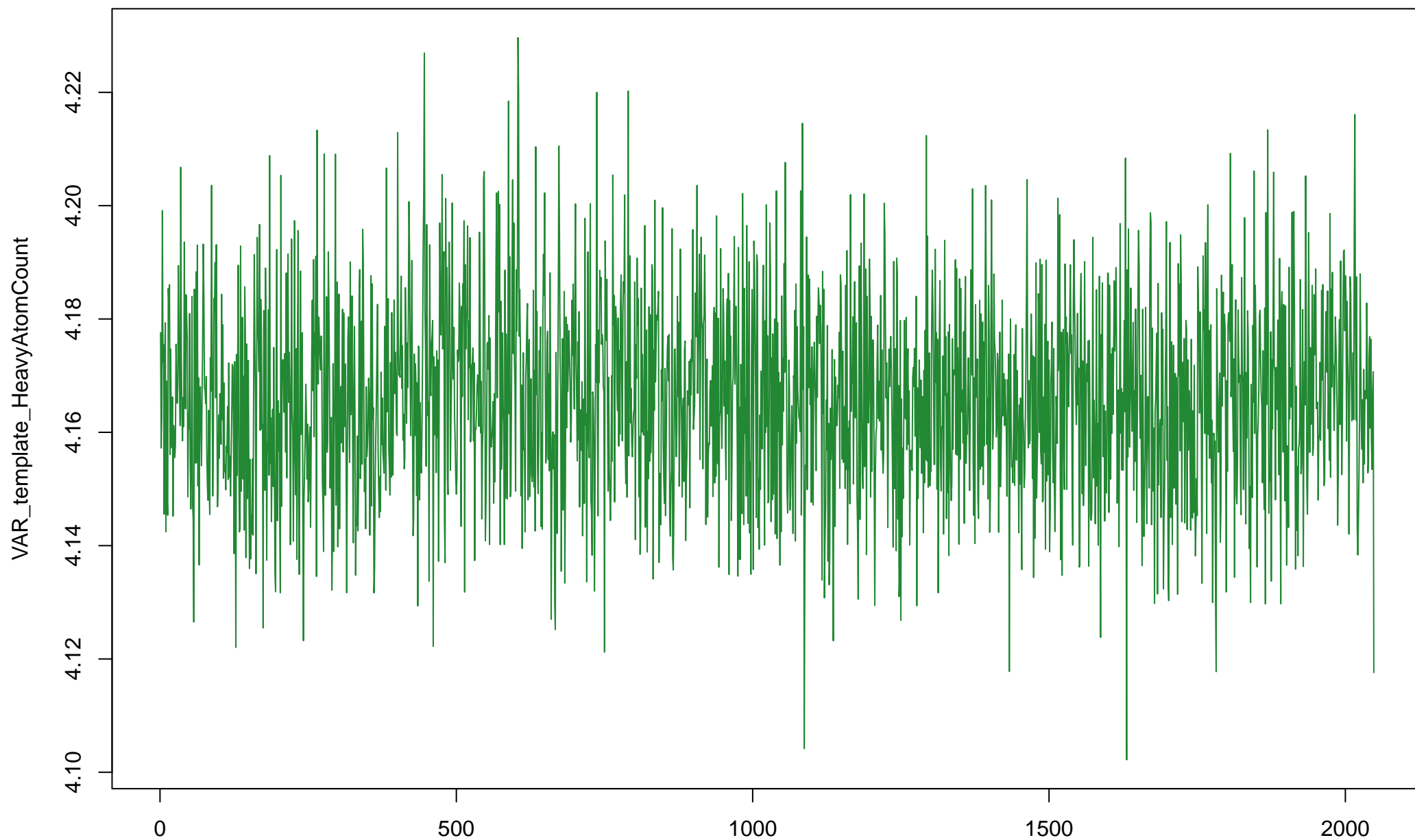
VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0384 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0



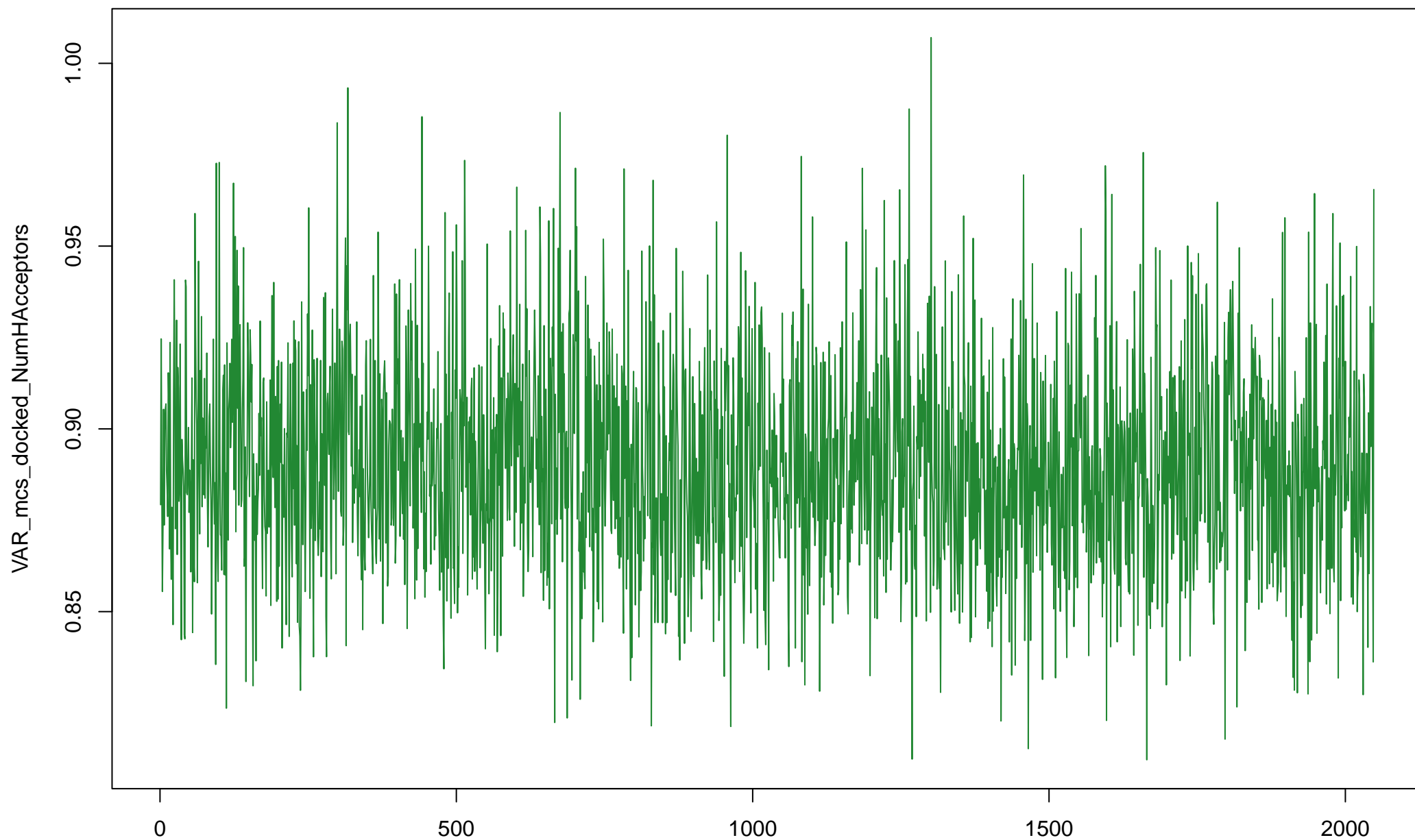
VAR_mcs_RingCount
ESS = 1610 | BMK = 0.0688 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



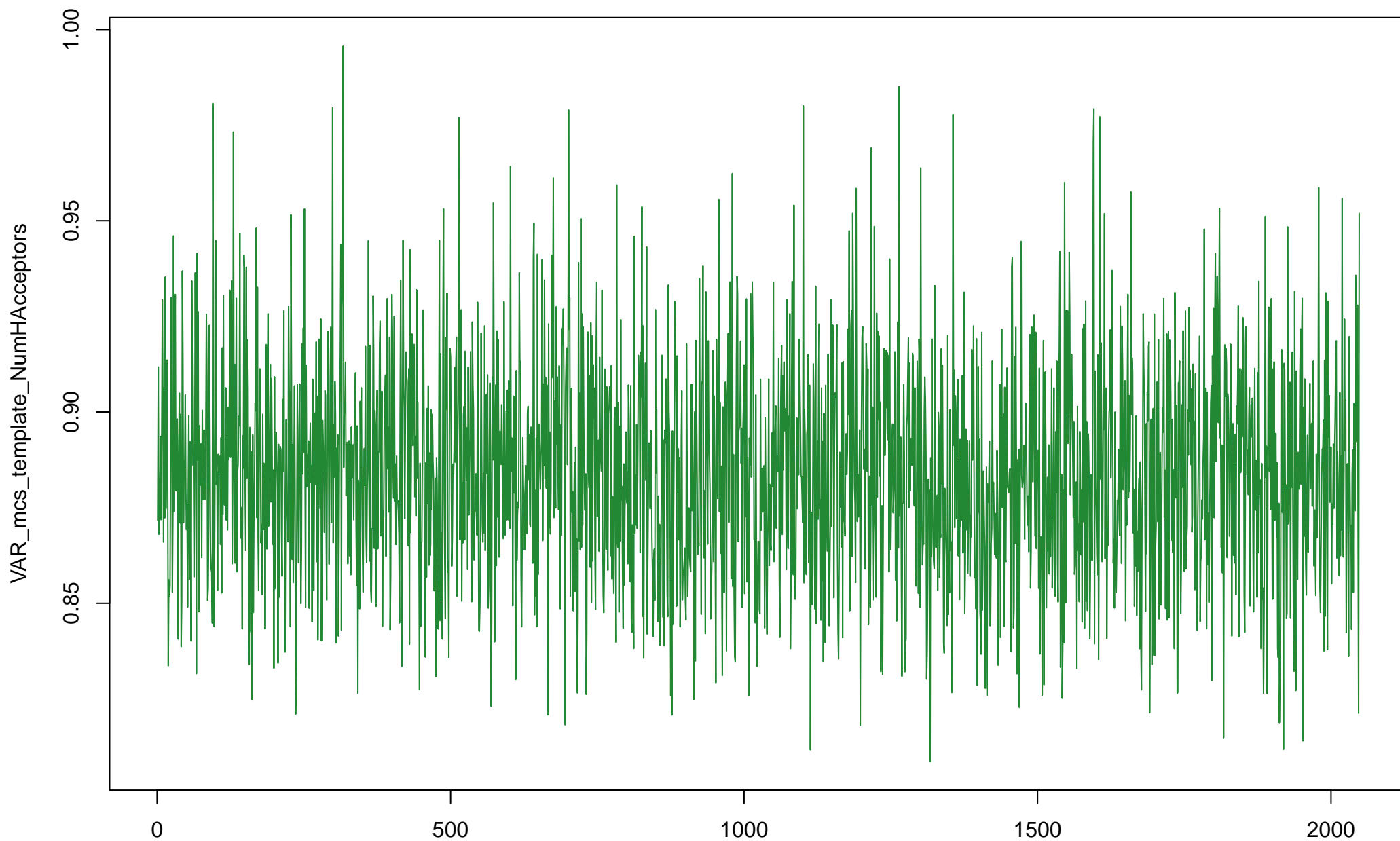
VAR_template_HeavyAtomCount
ESS = 1850 | BMK = 0.0541 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0



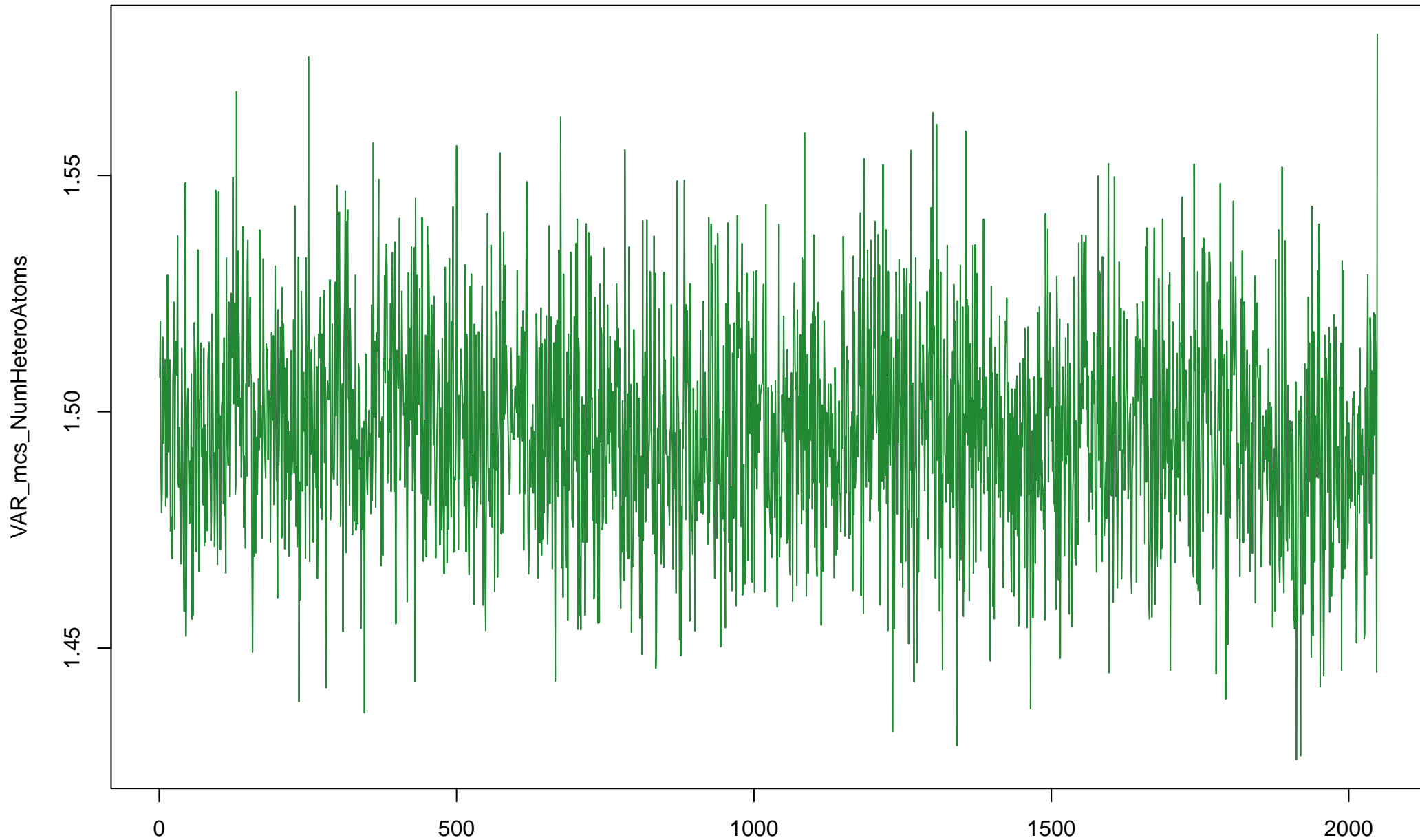
VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0466 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0



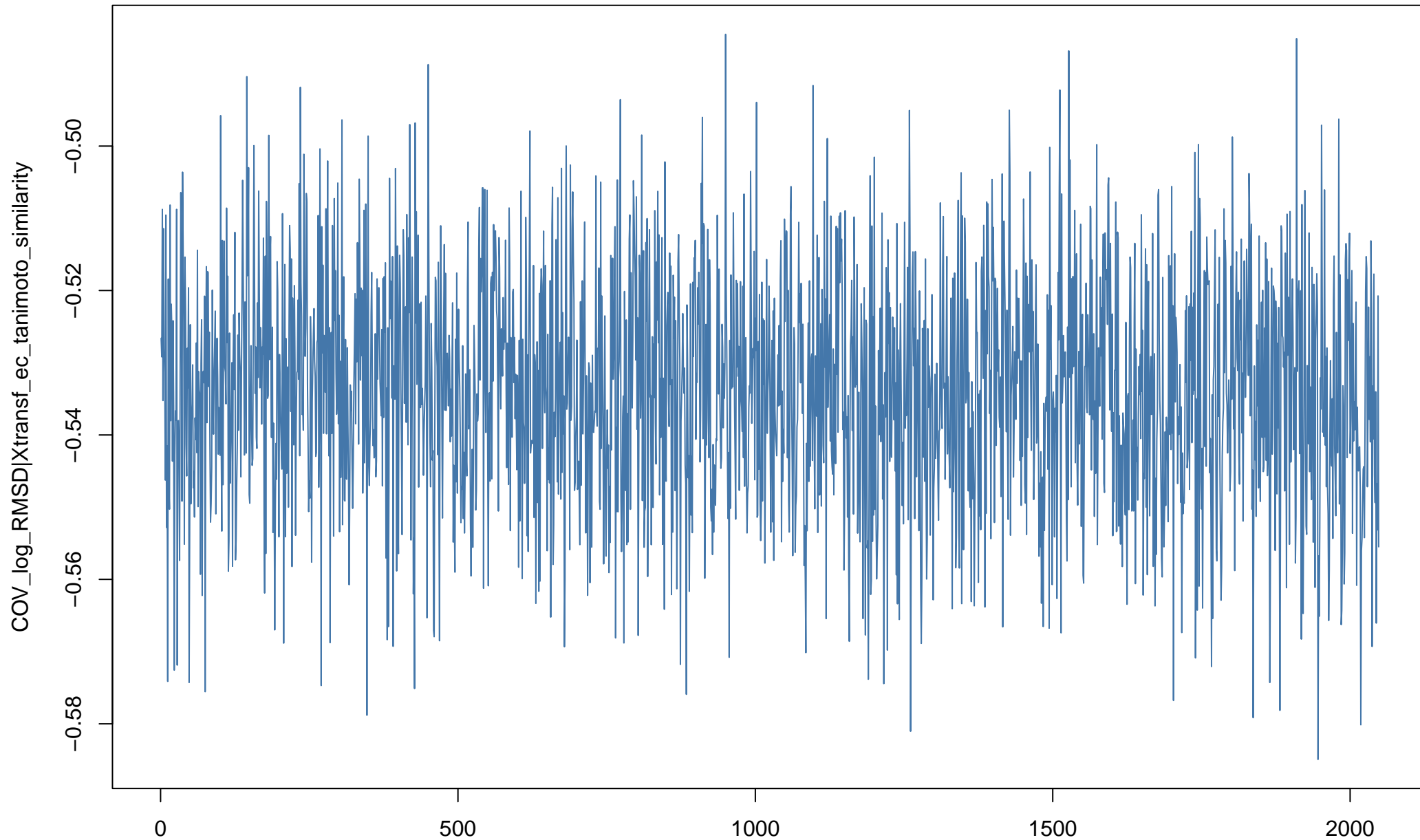
VAR_mcs_template_NumHAcceptors
ESS = 1140 | BMK = 0.0479 | MCSE(6.27) = 2.56 | stat: FALSE | burn: 0



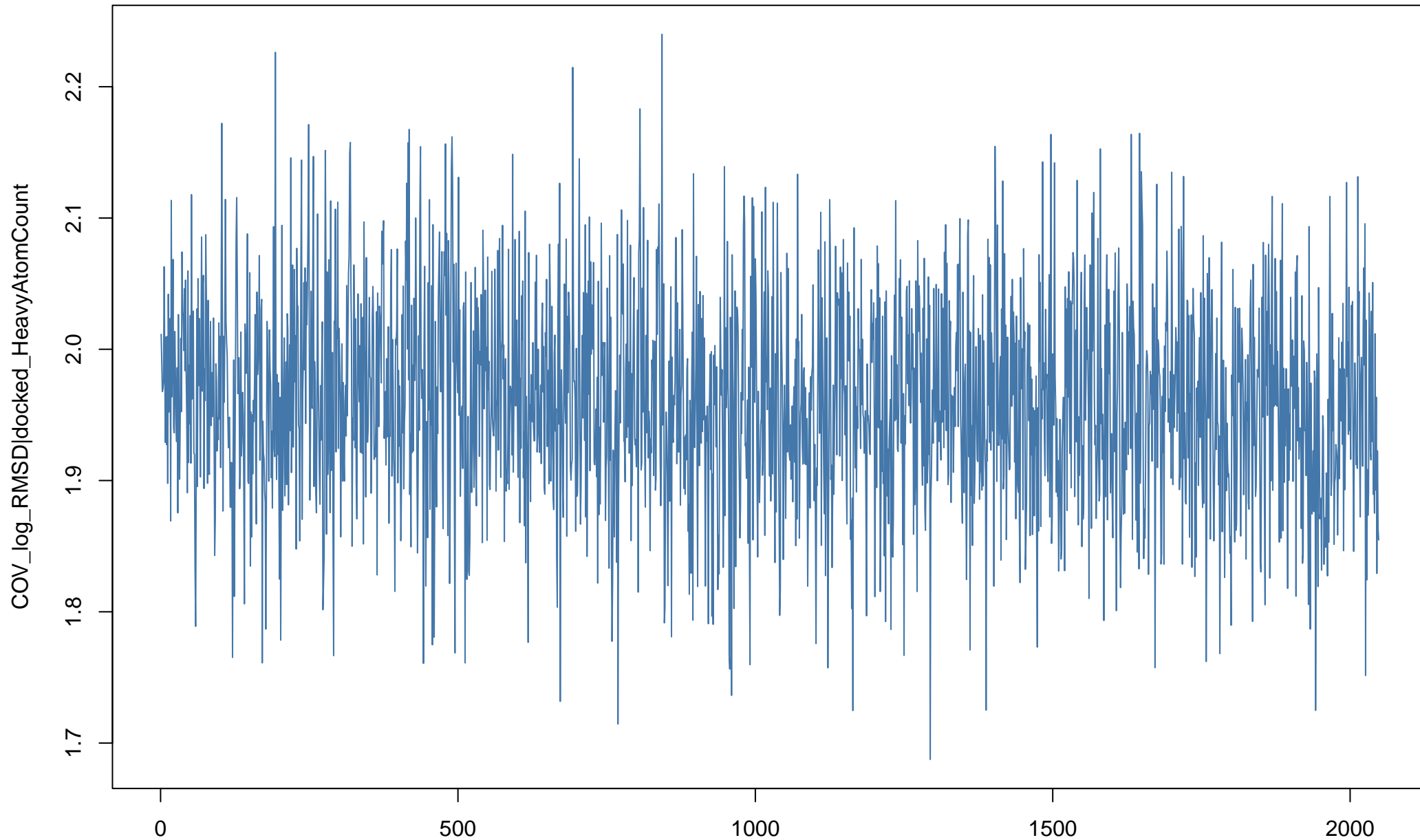
VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0528 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0



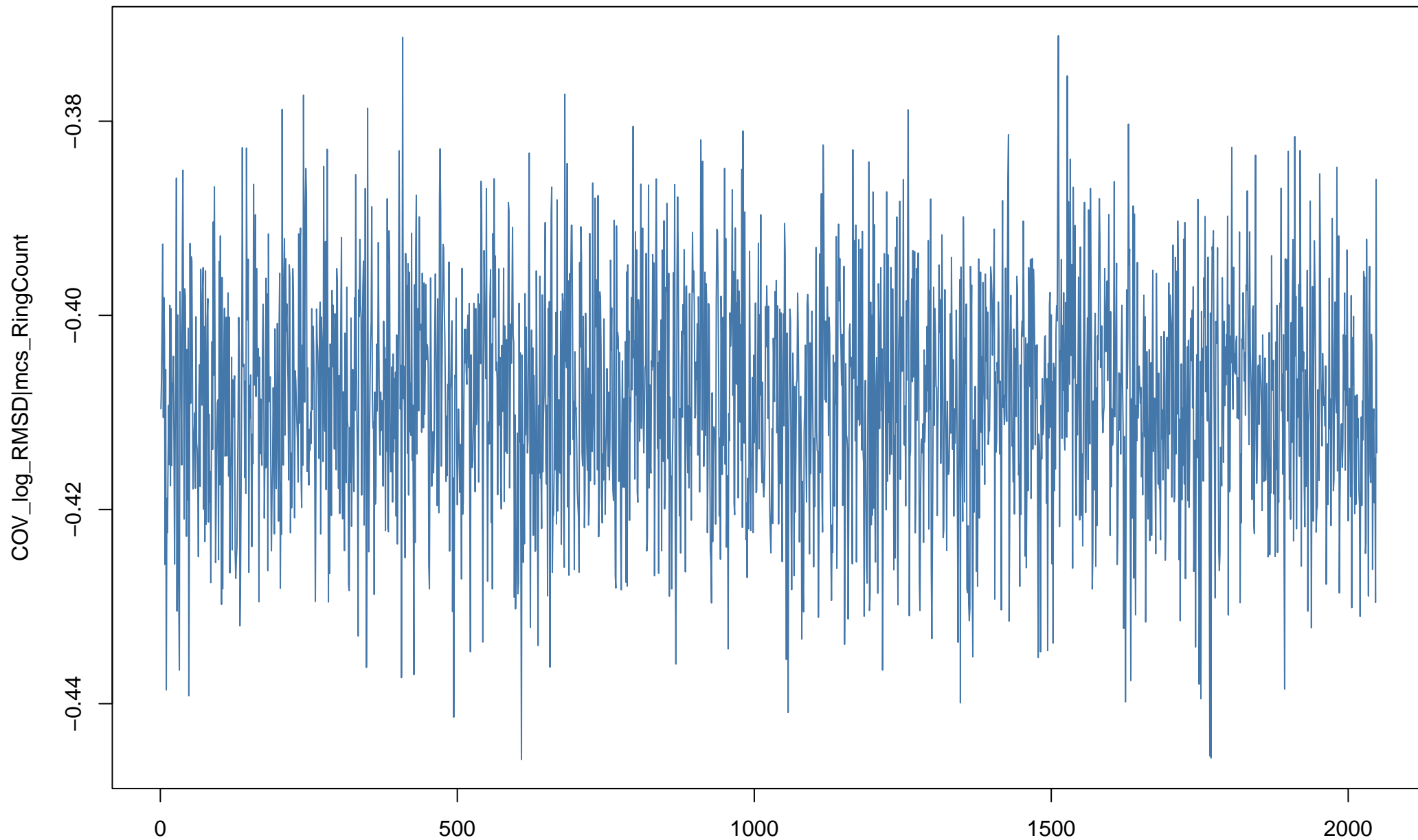
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1770 | BMK = 0.0526 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0



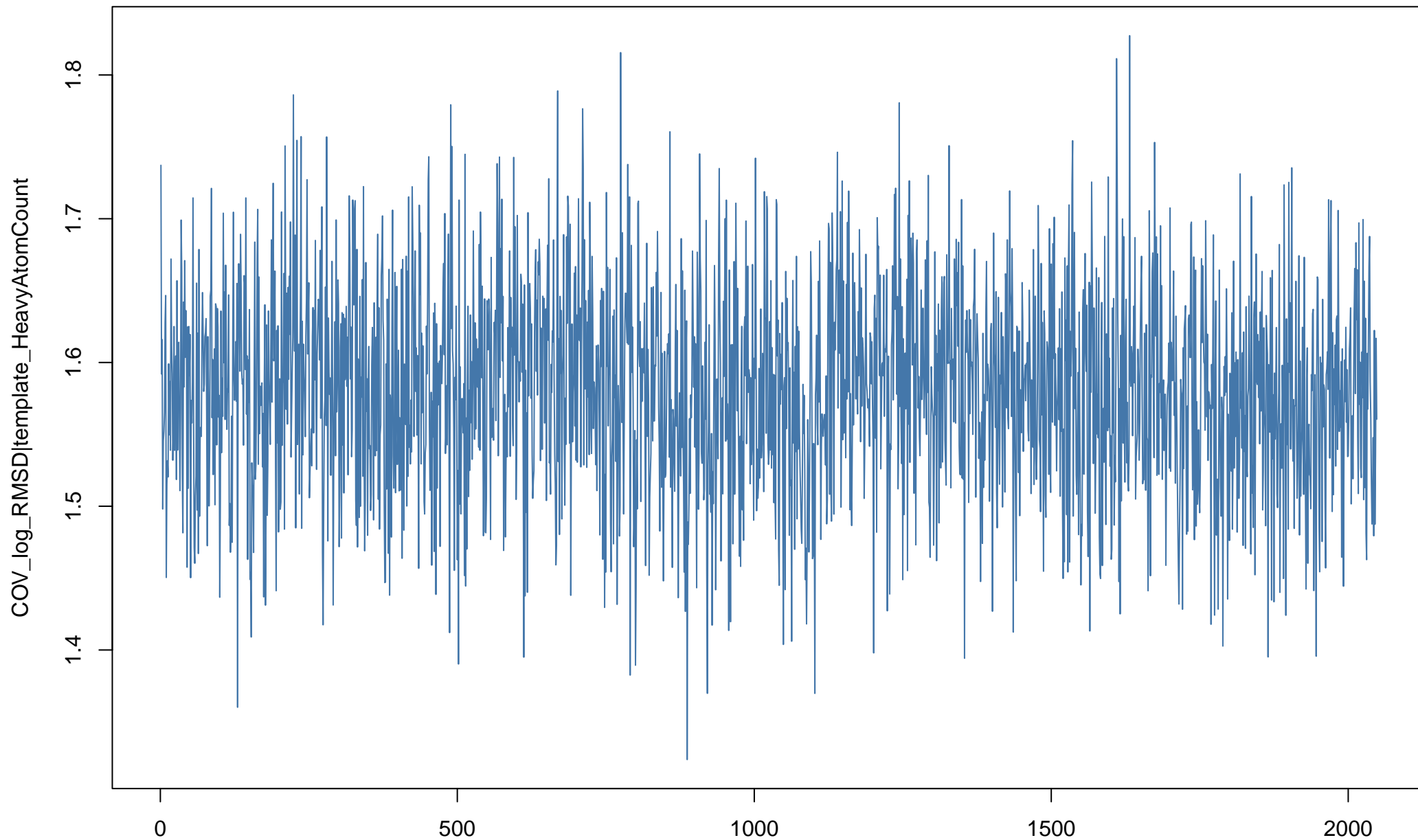
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1670 | BMK = 0.0737 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0



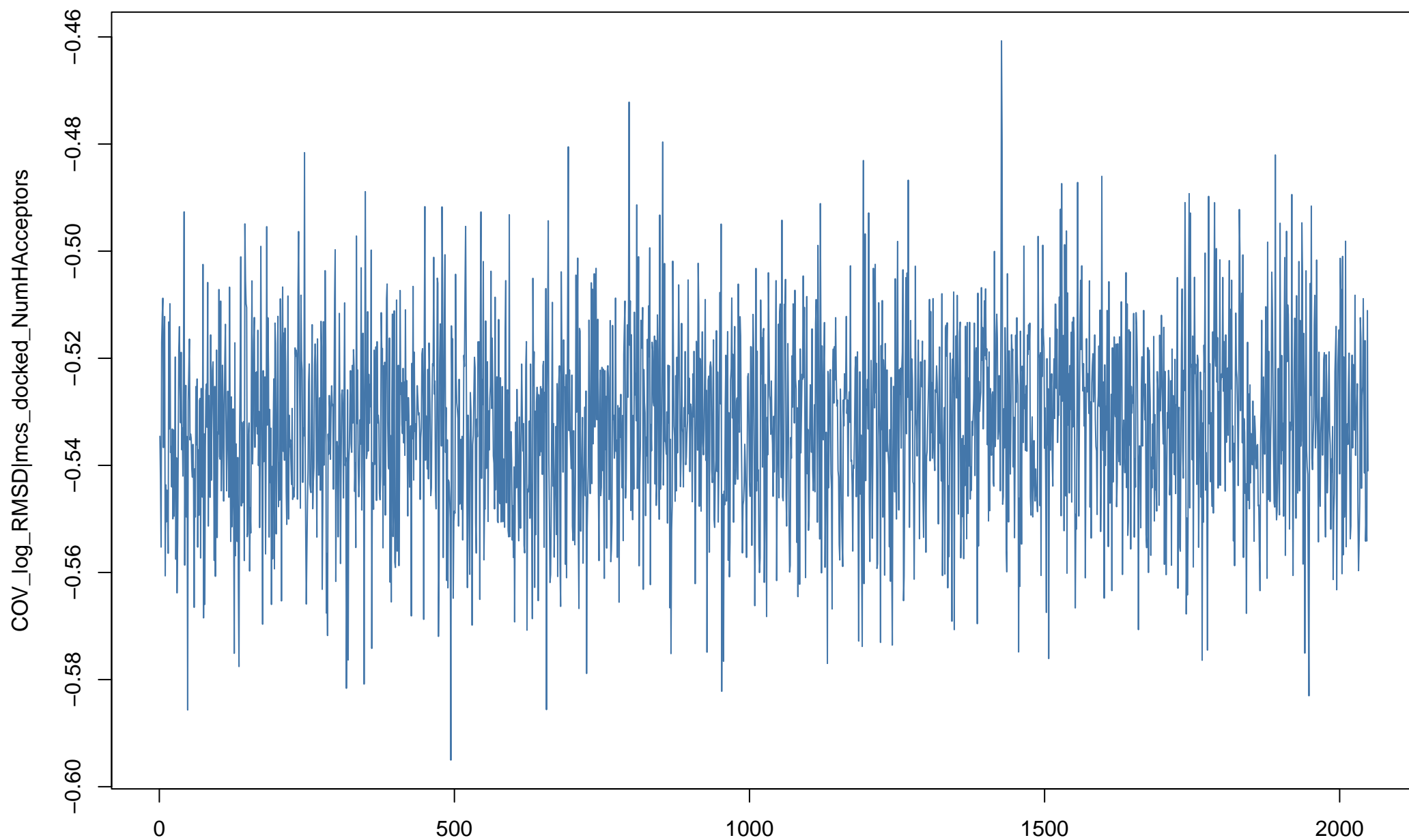
COV_log_RMSD|mcs_RingCount
ESS = 1770 | BMK = 0.0429 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0



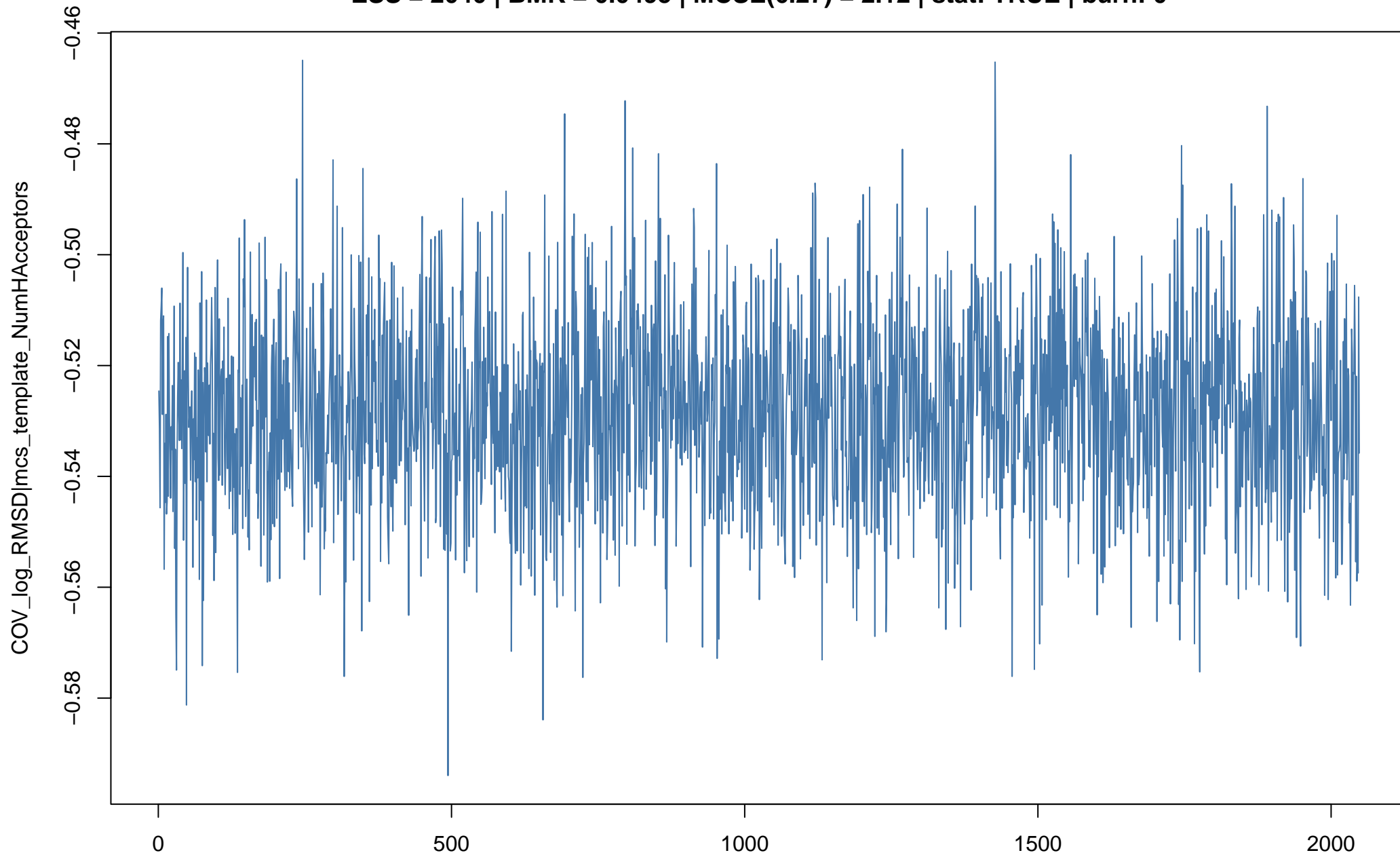
COV_log_RMSD|template_HeavyAtomCount
ESS = 1650 | BMK = 0.0524 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0



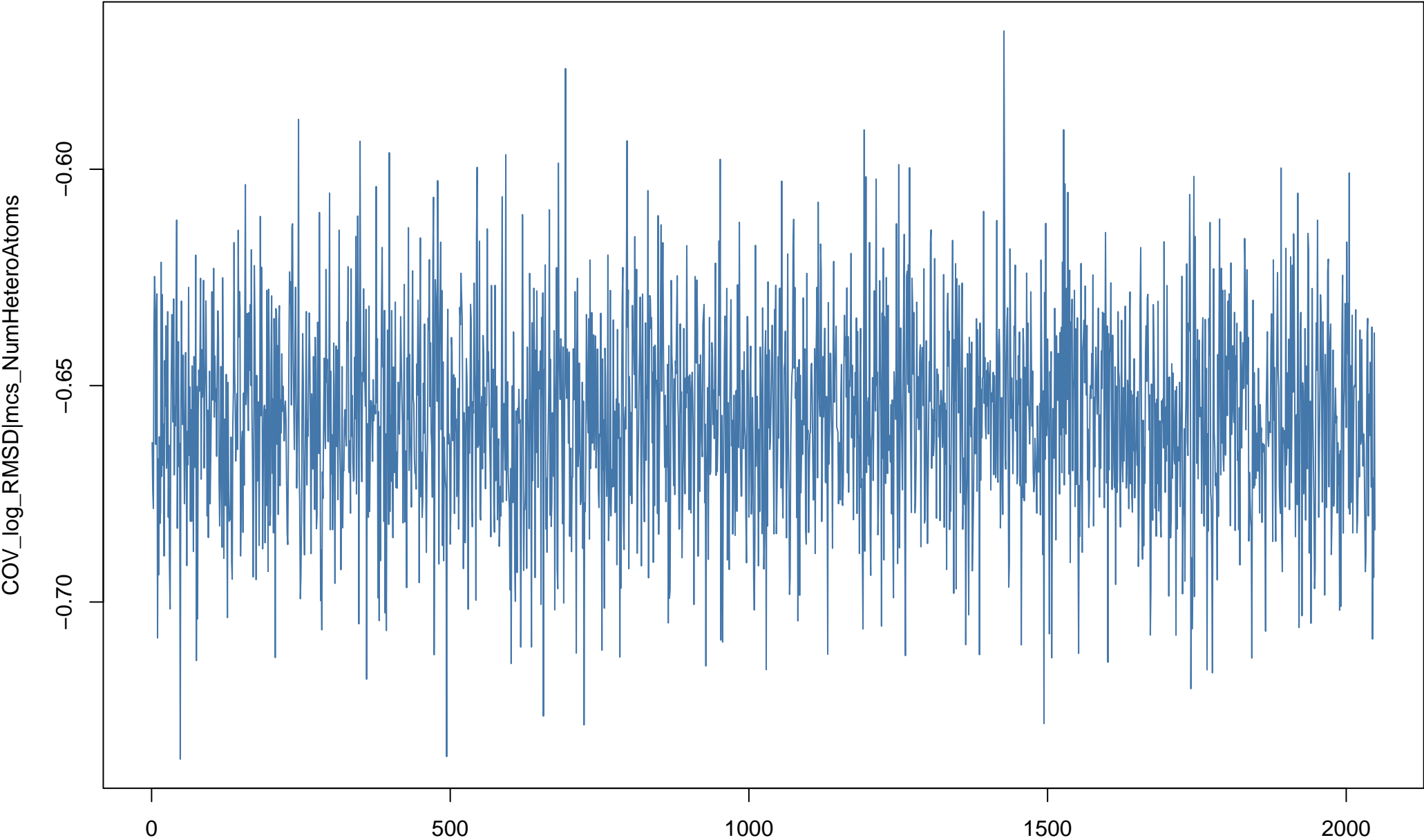
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 1960 | BMK = 0.0612 | MCSE(6.27) = 2.35 | stat: FALSE | burn: 0



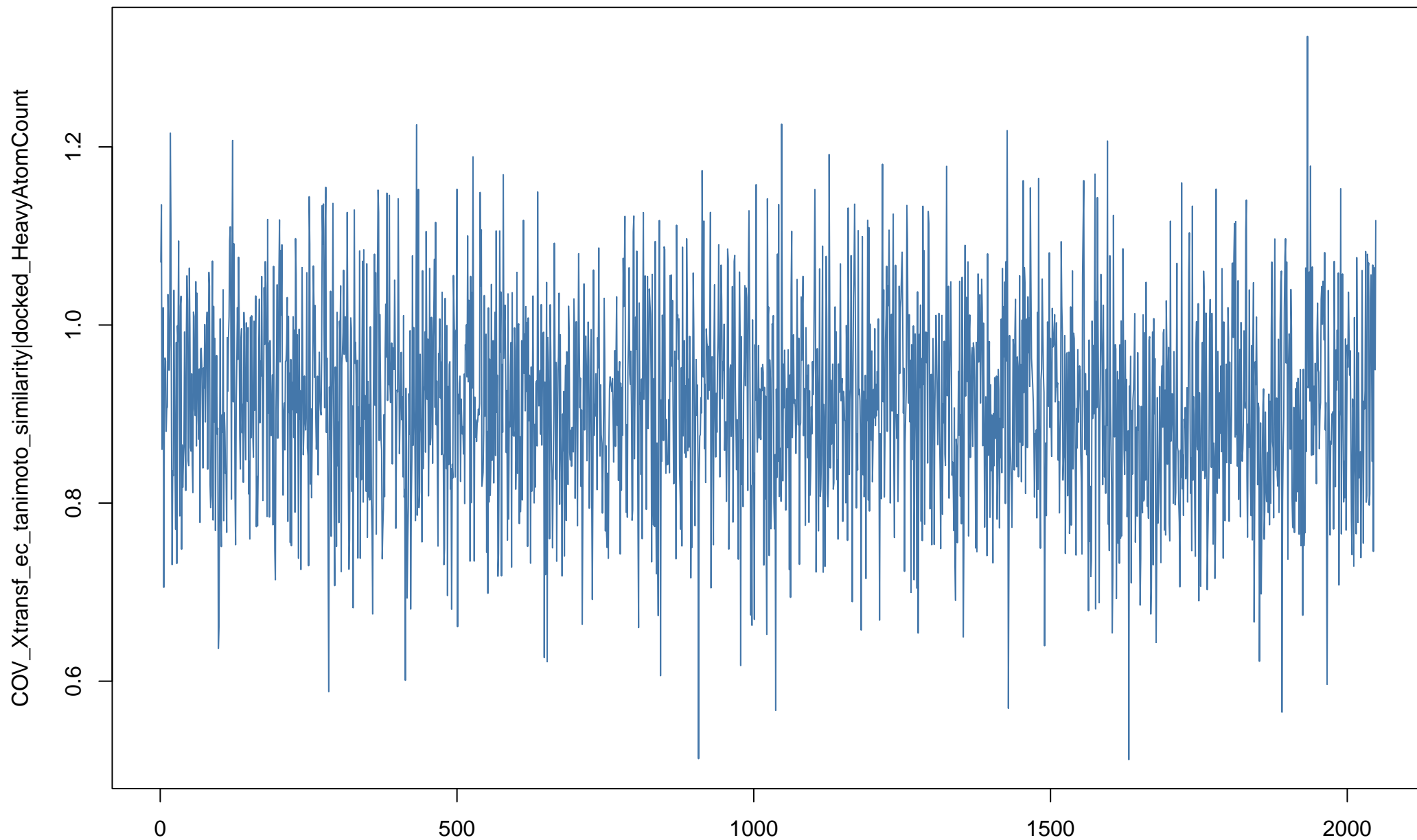
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2040 | BMK = 0.0495 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0



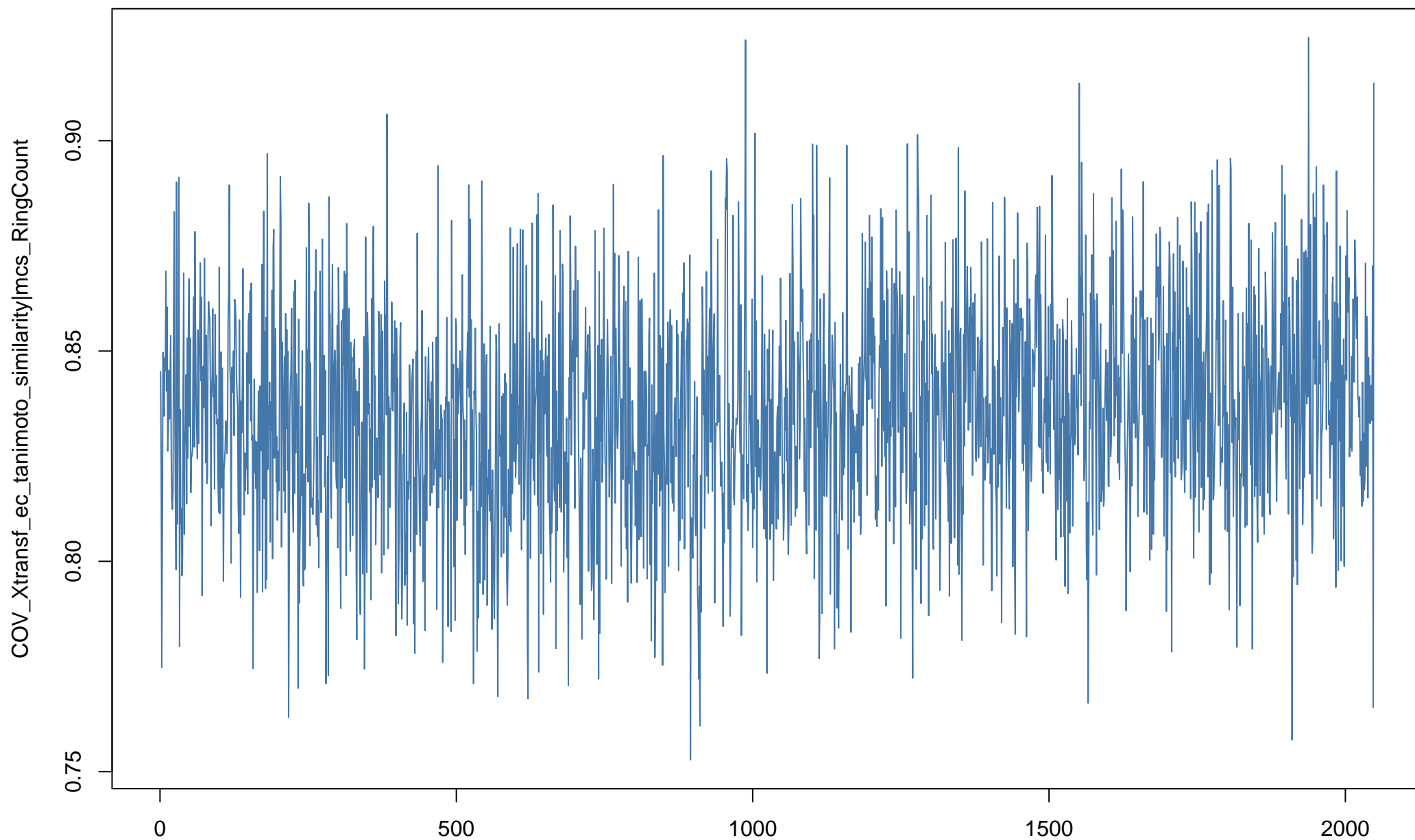
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.033 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0



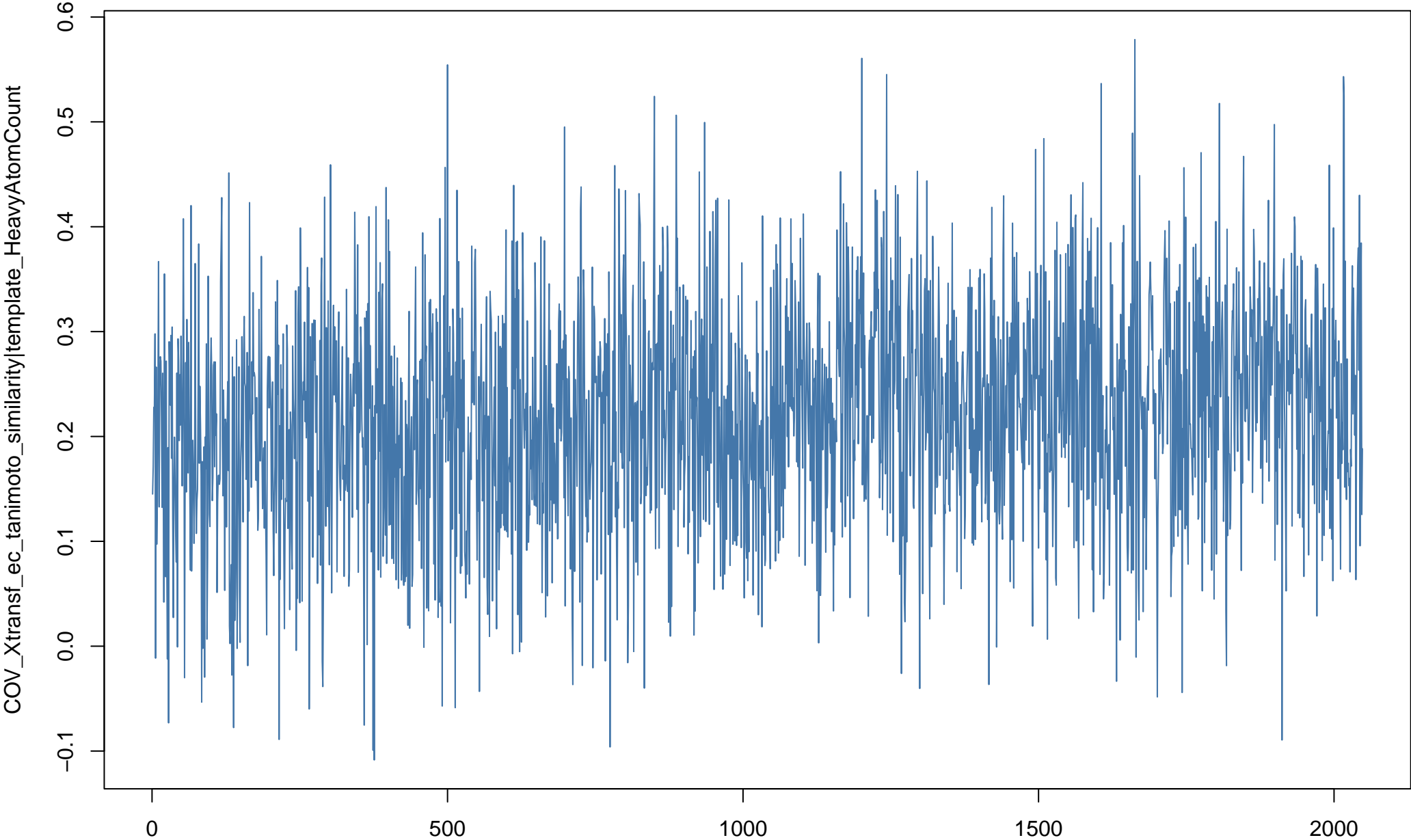
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1750 | BMK = 0.051 | MCSE(6.27) = 2.73 | stat: FALSE | burn: 0



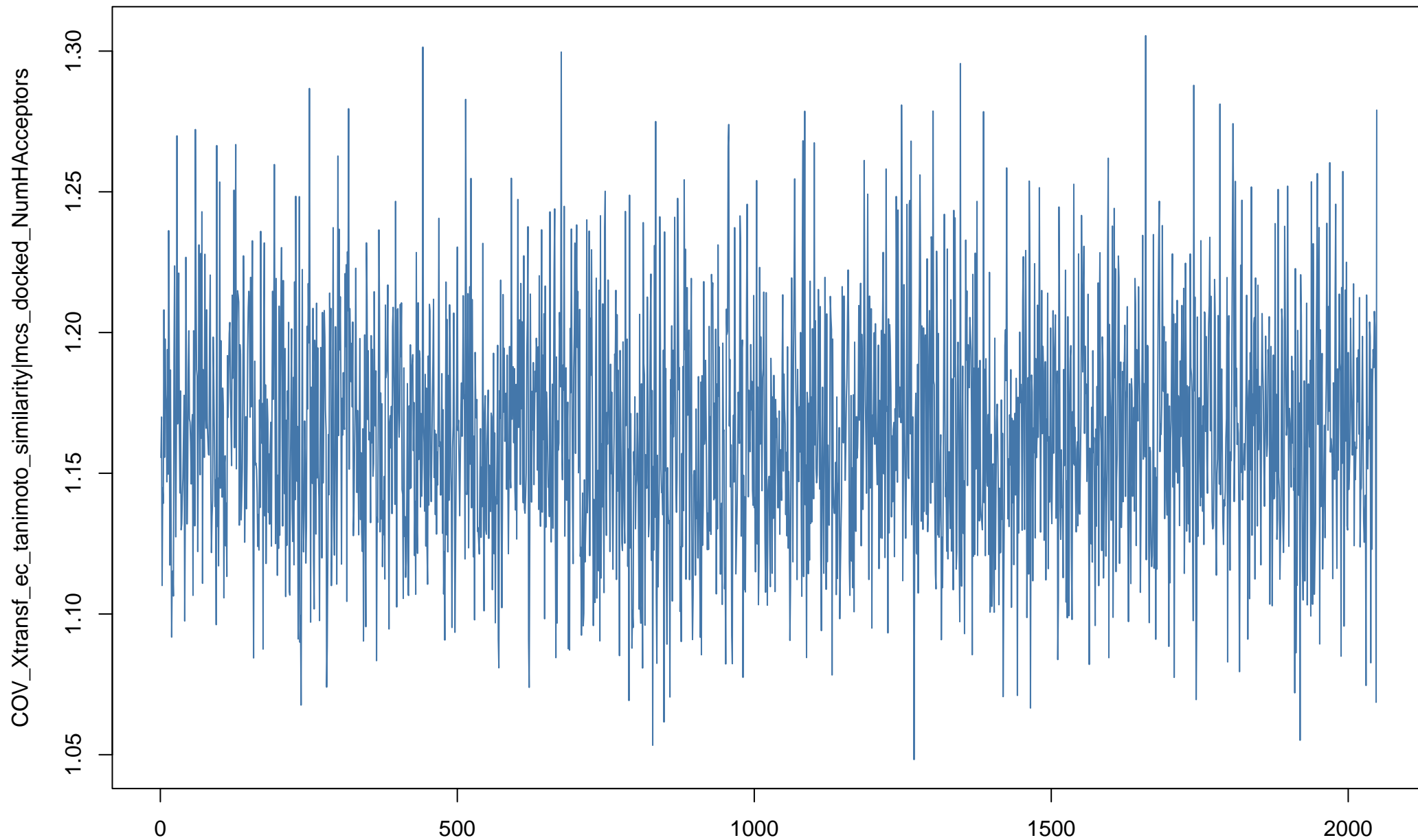
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1420 | BMK = 0.109 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0



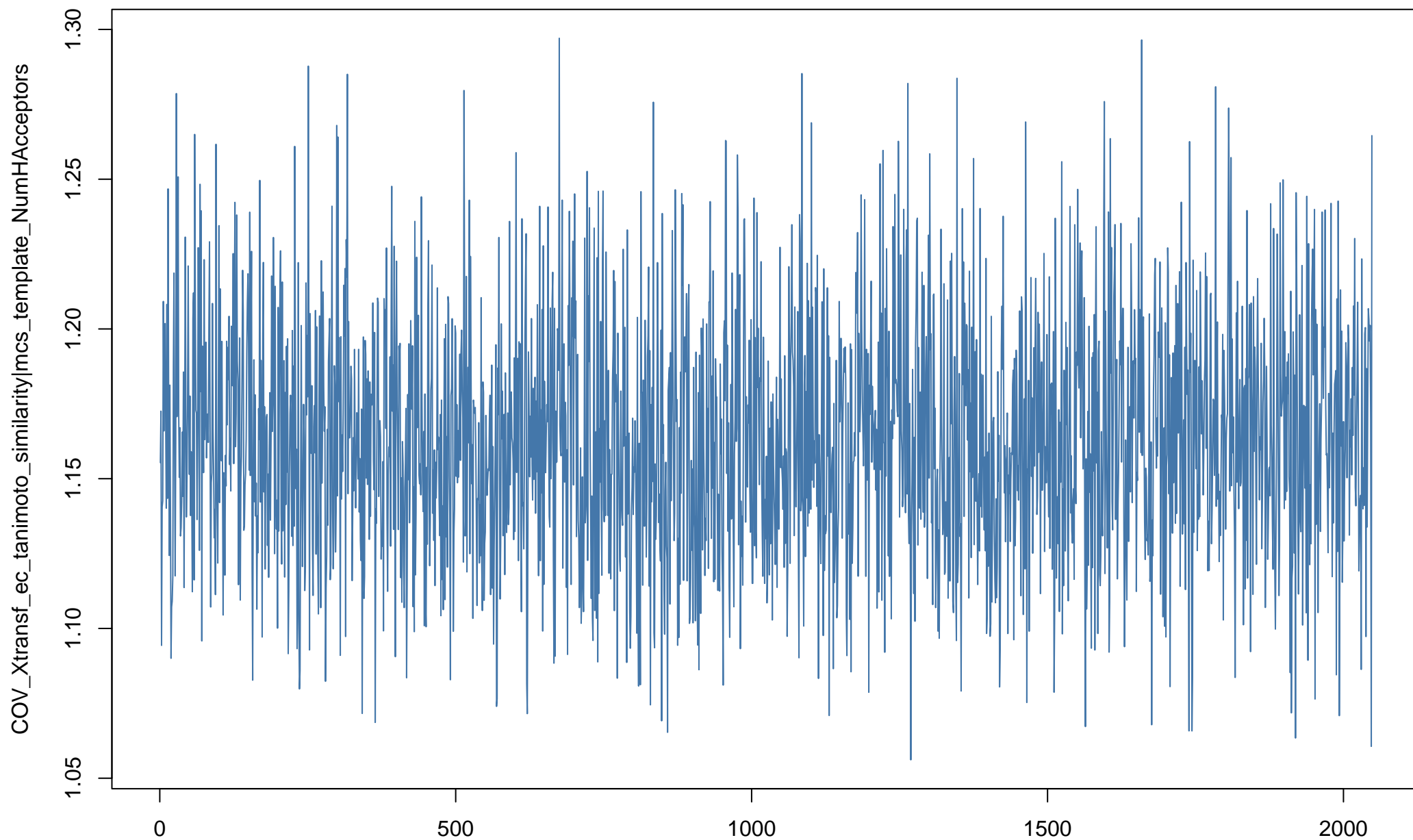
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 524 | BMK = 0.115 | MCSE(6.27) = 3.44 | stat: FALSE | burn: 0



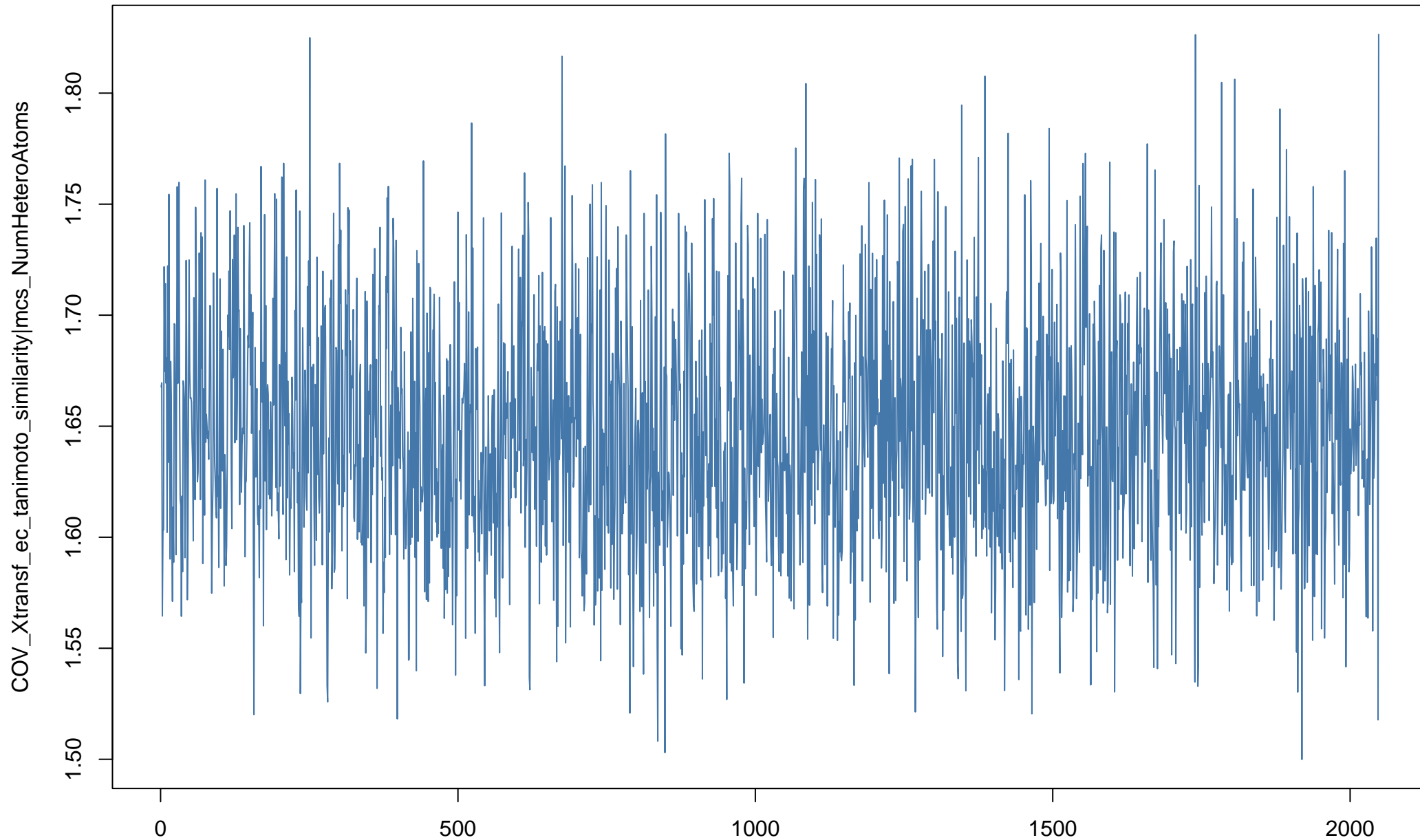
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0324 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0



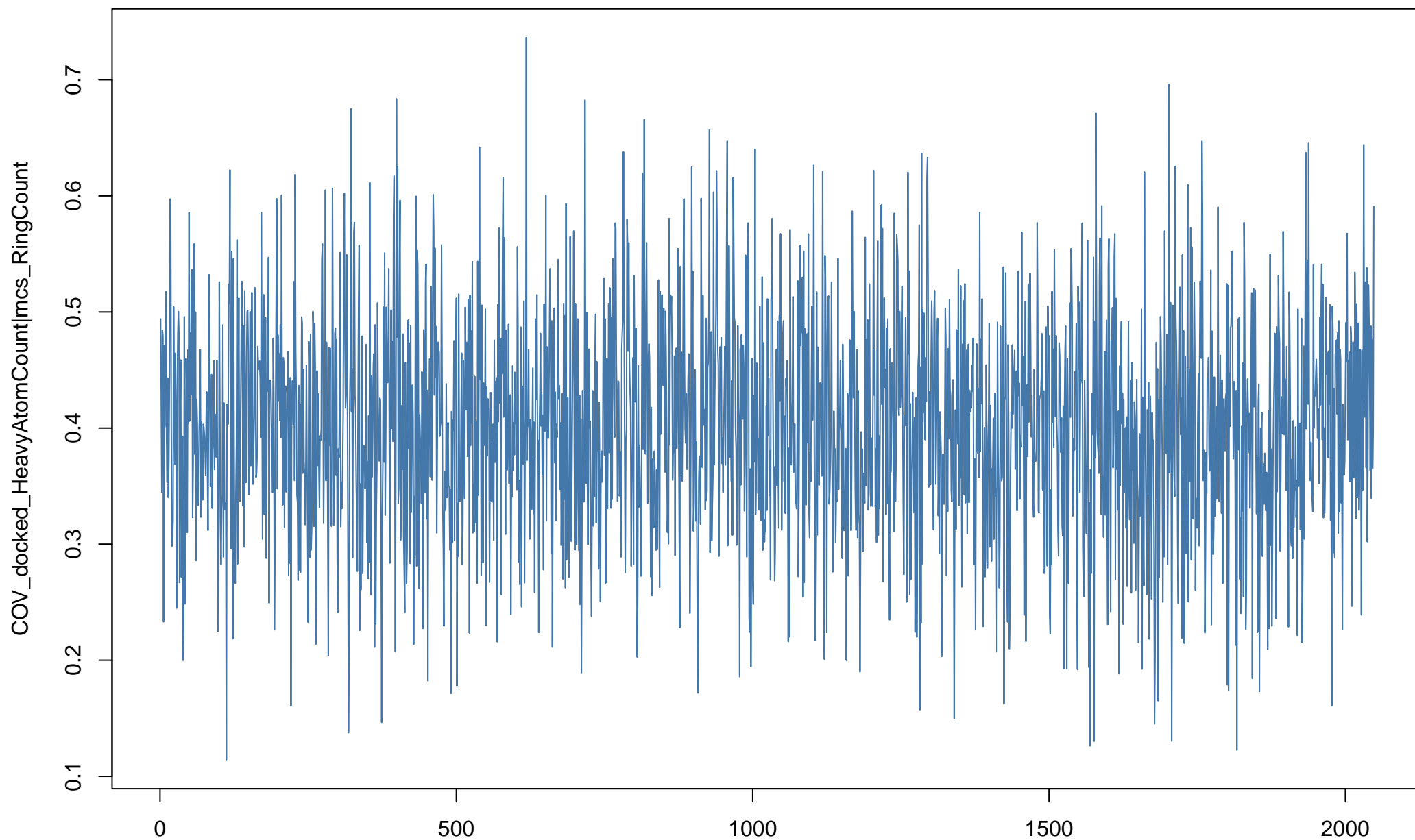
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0308 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0



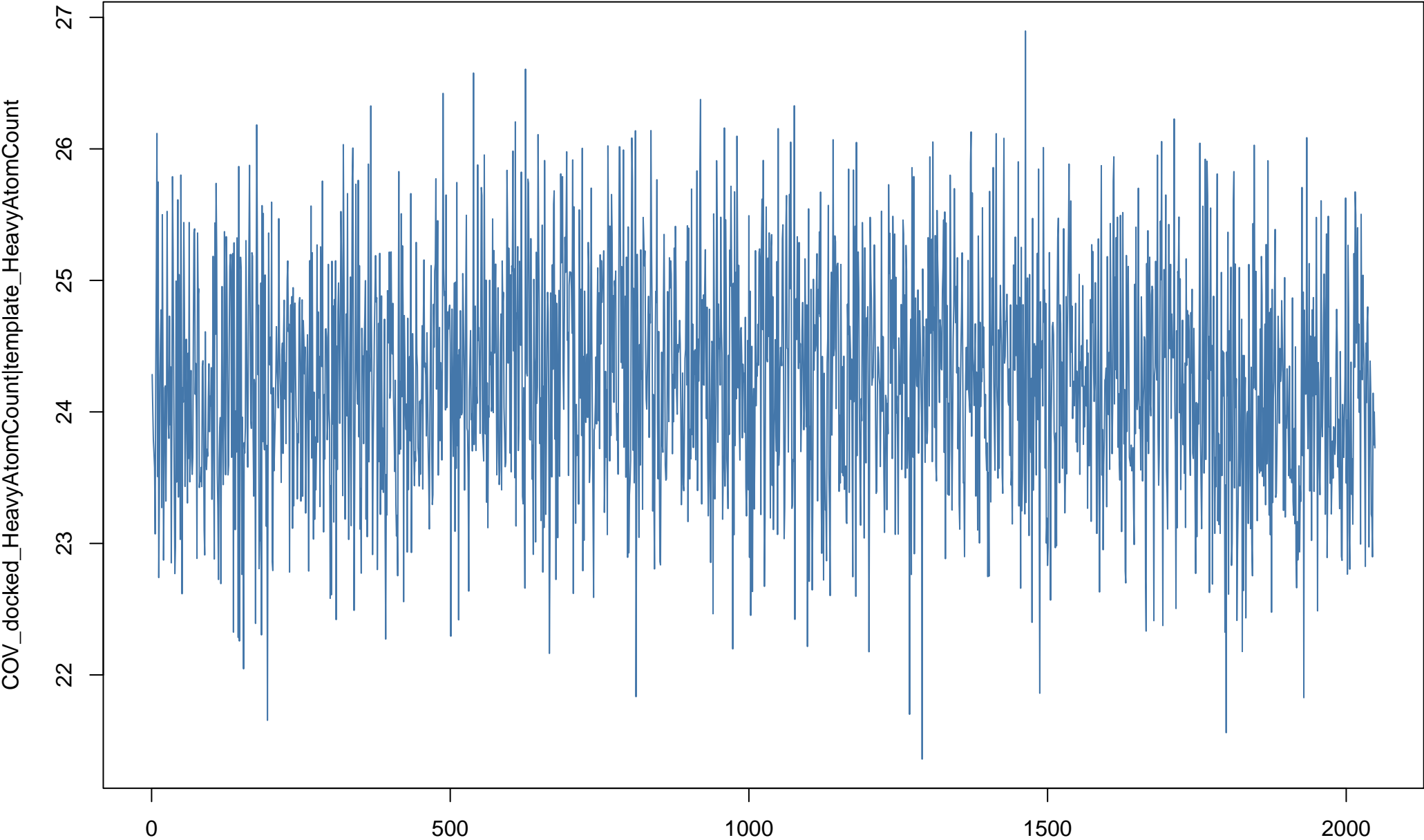
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0469 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0



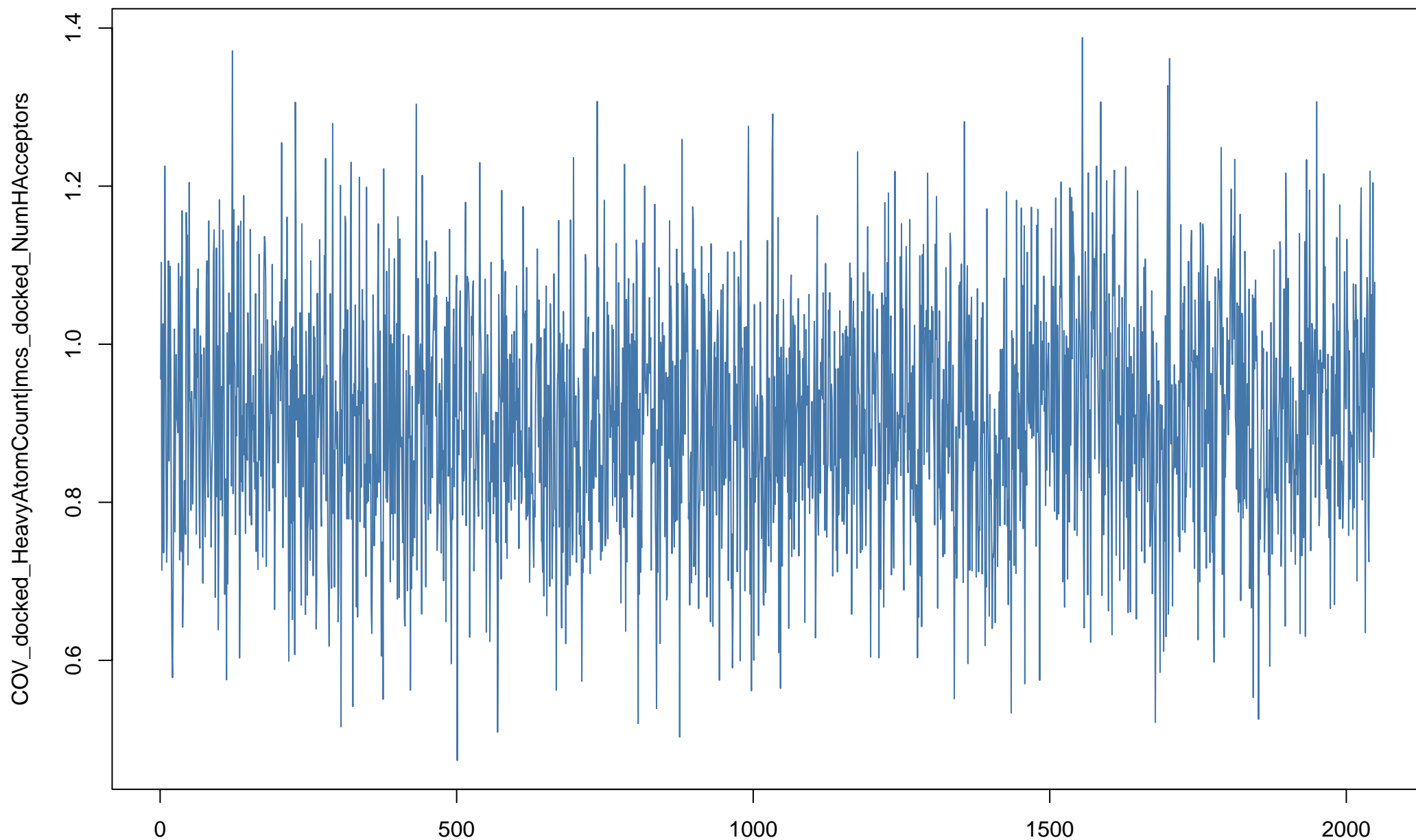
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1760 | BMK = 0.043 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



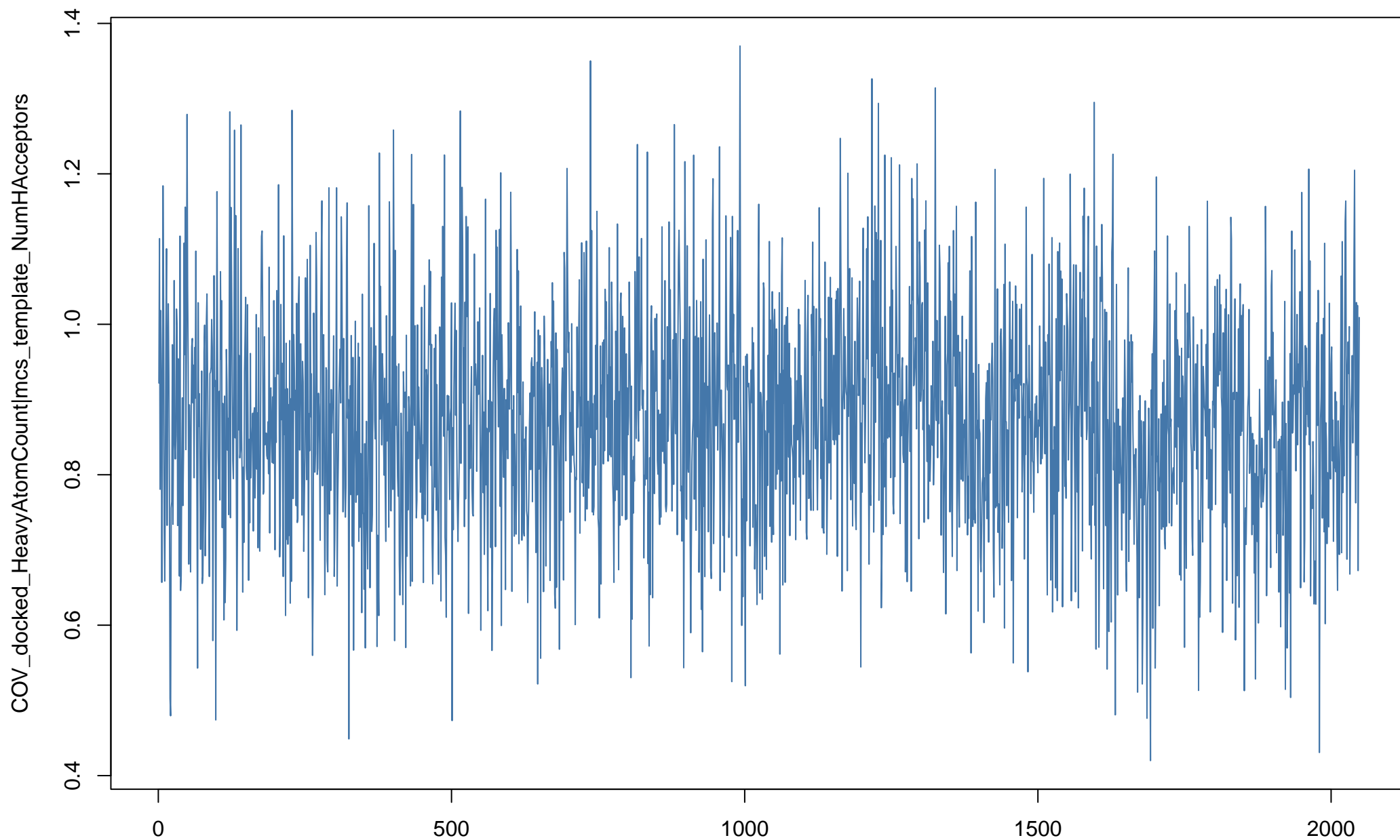
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1690 | BMK = 0.0422 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0



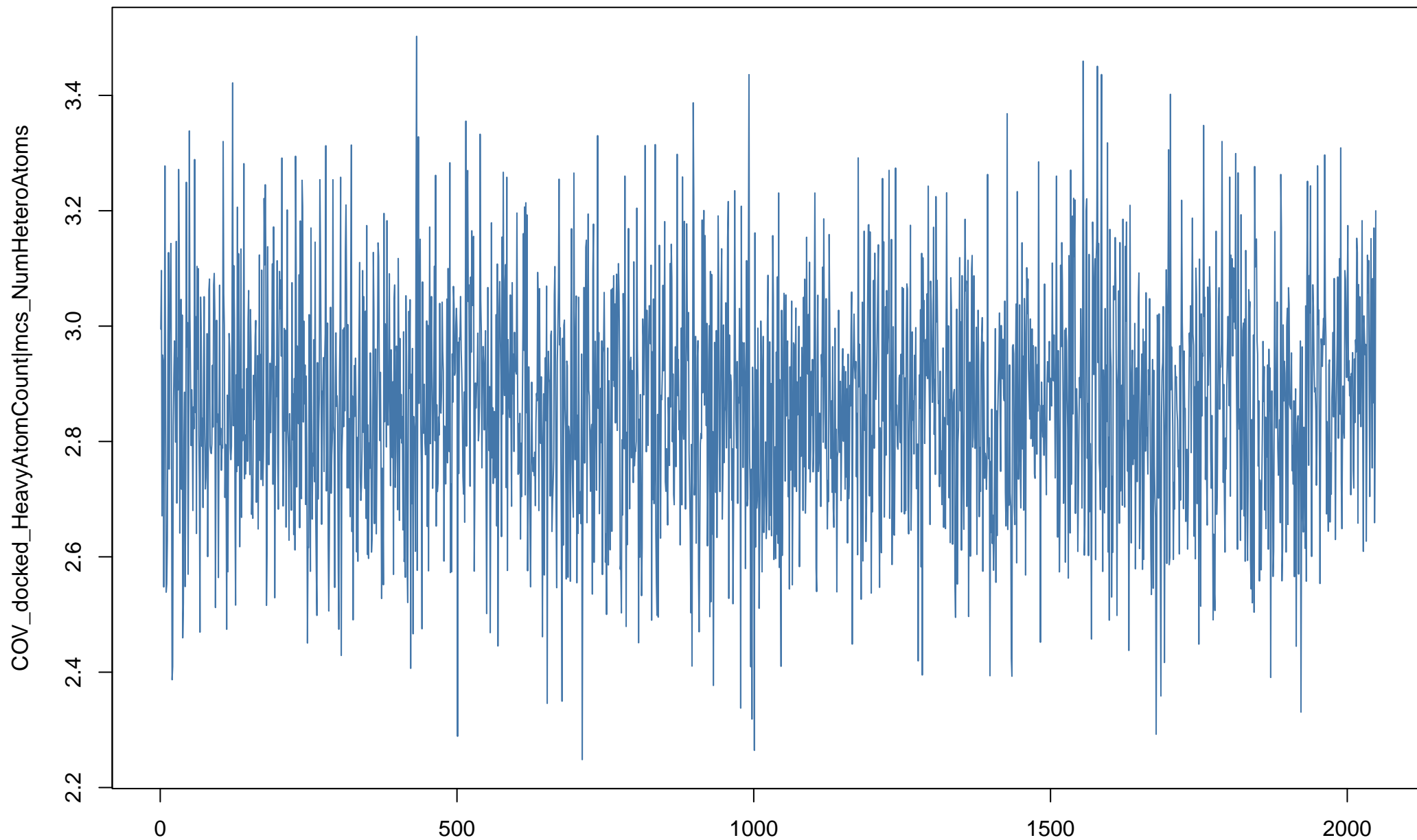
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1870 | BMK = 0.0459 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0



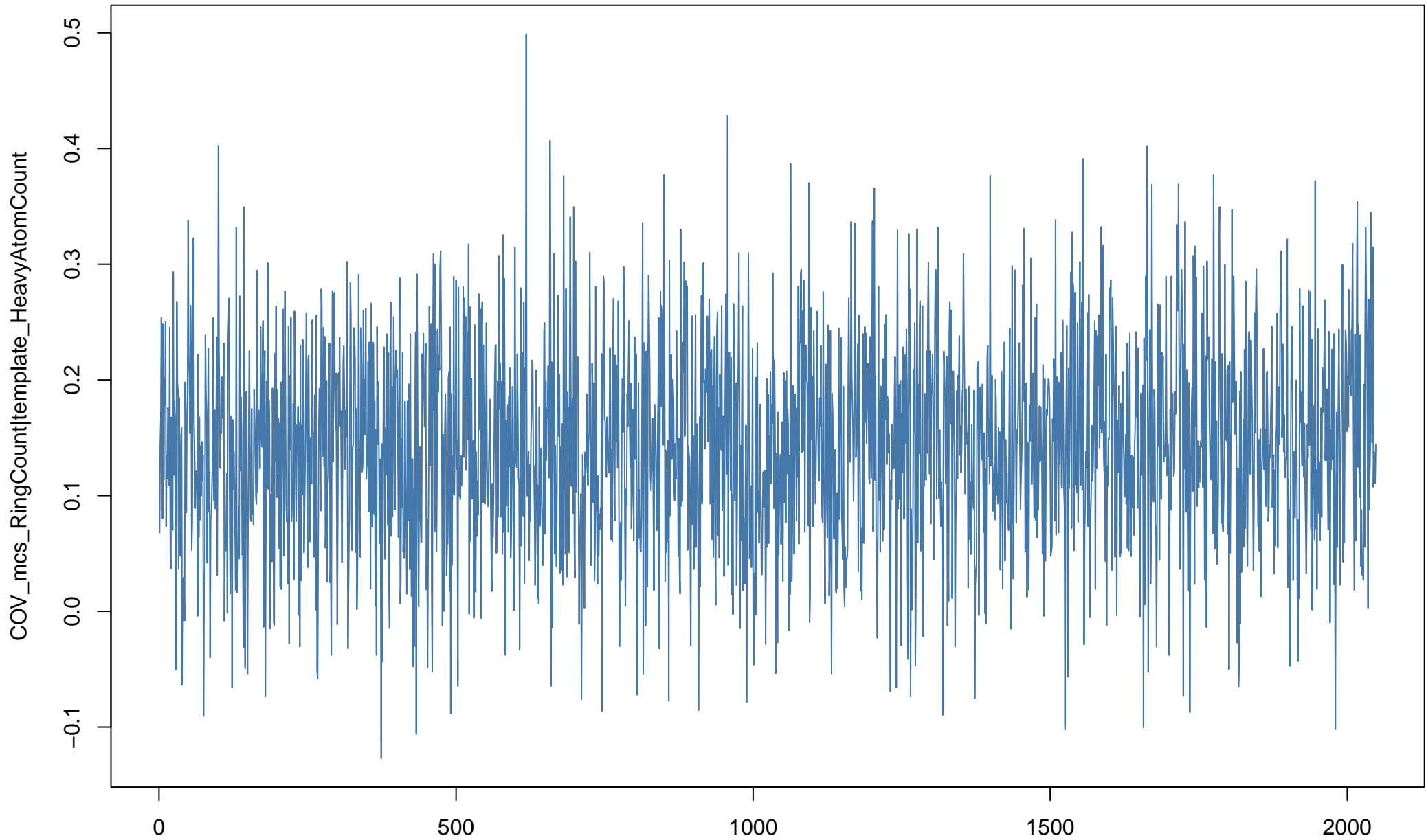
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1630 | BMK = 0.0321 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0



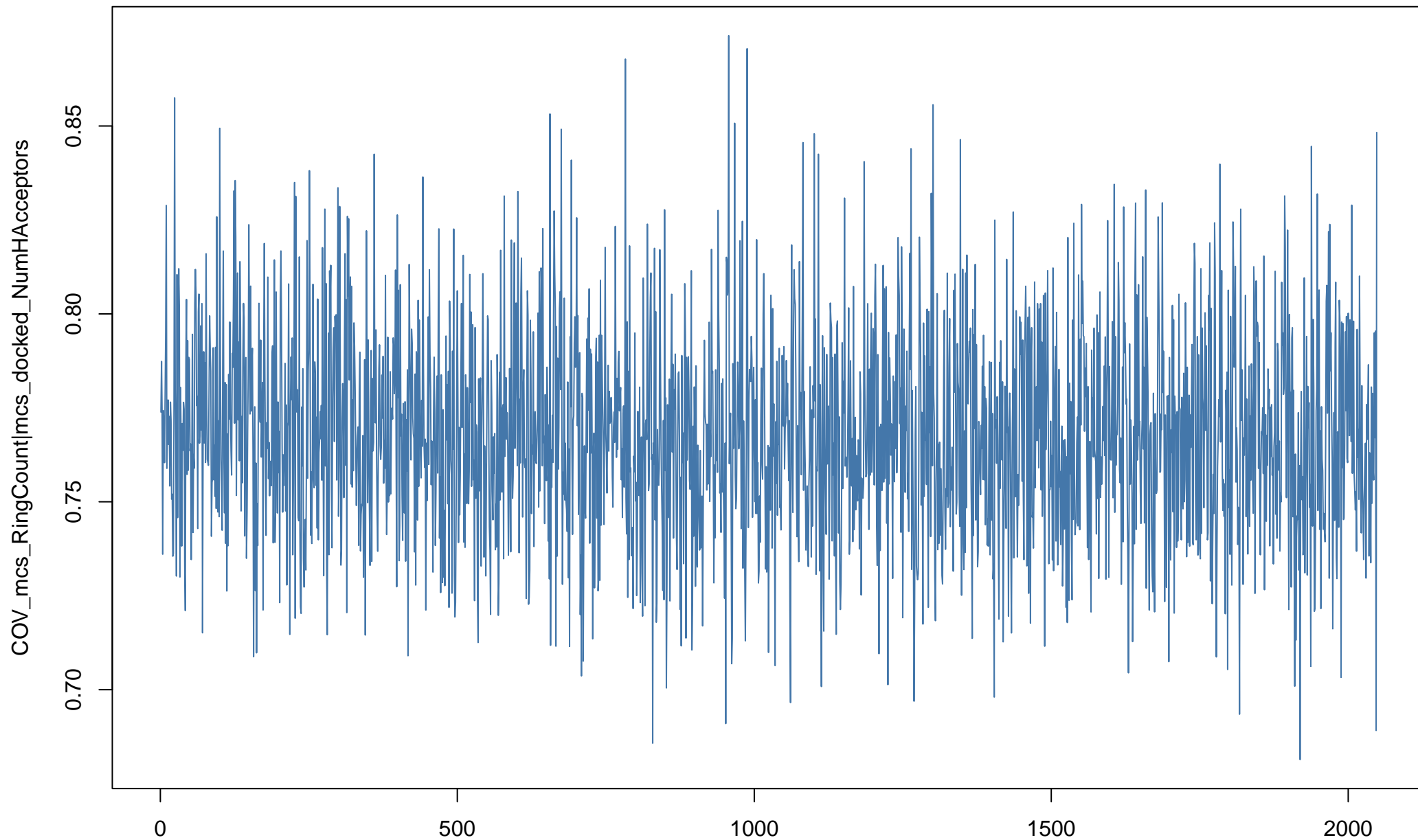
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1940 | BMK = 0.0479 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0



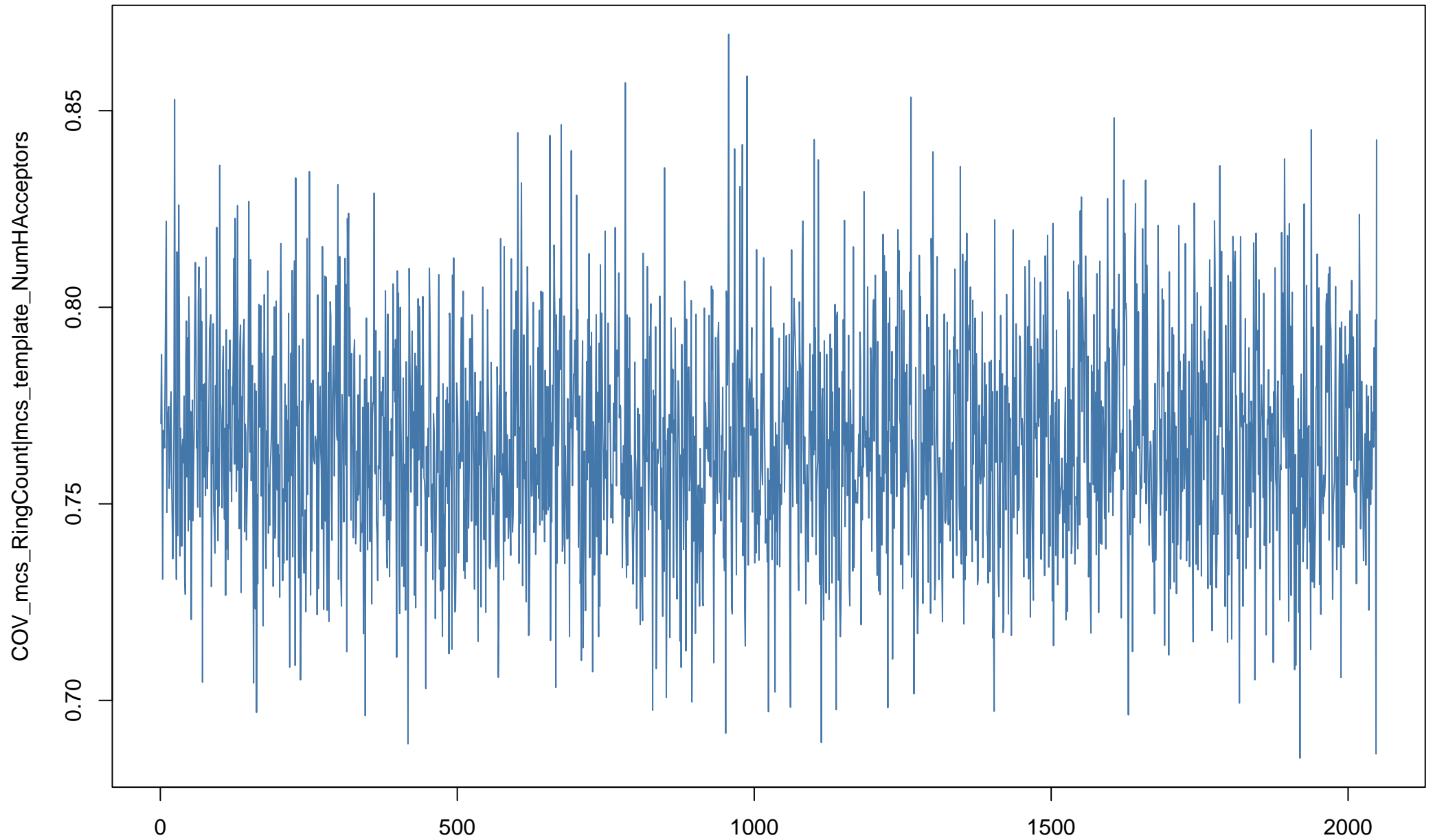
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1860 | BMK = 0.061 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0



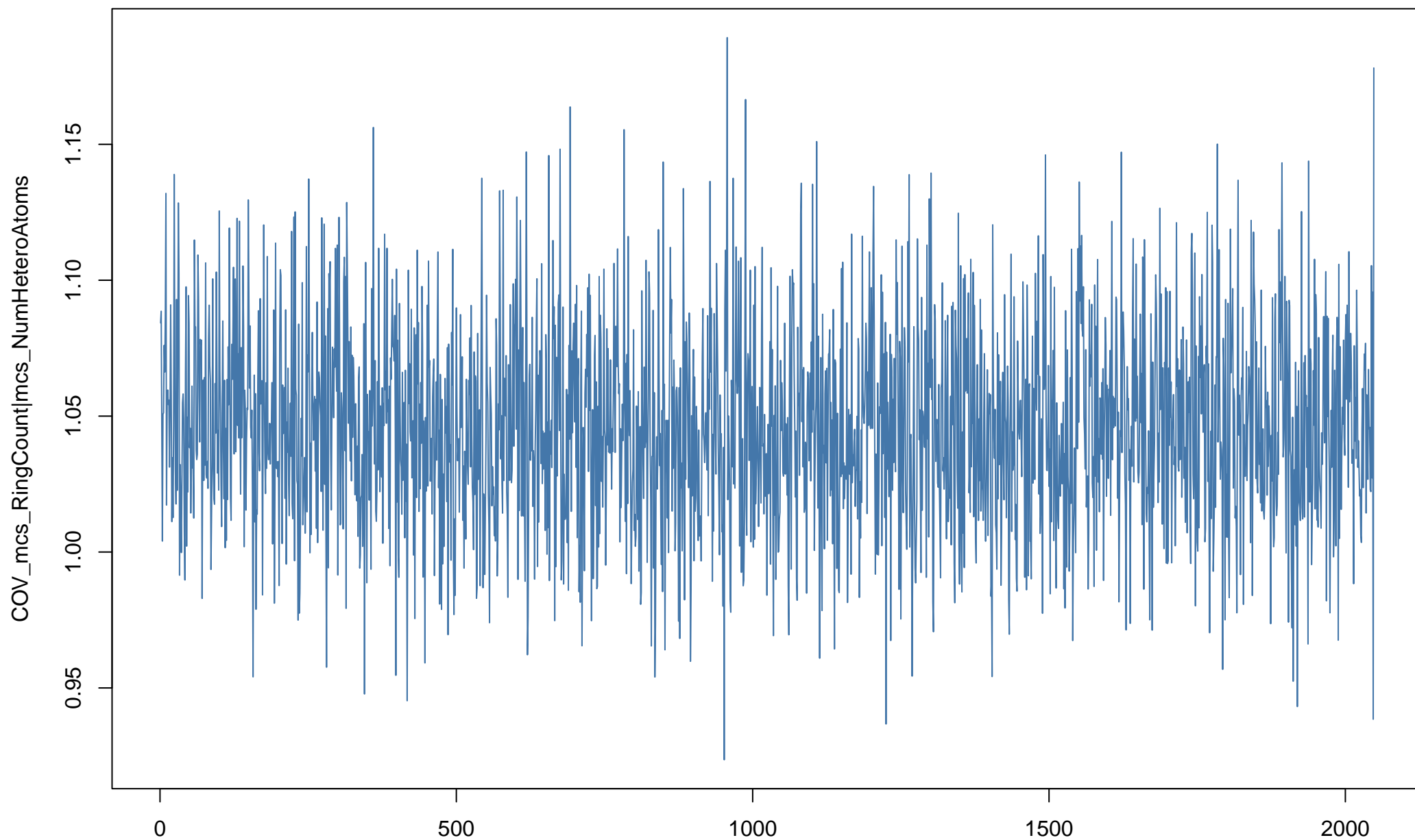
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 1900 | BMK = 0.0581 | MCSE(6.27) = 2.17 | stat: FALSE | burn: 0



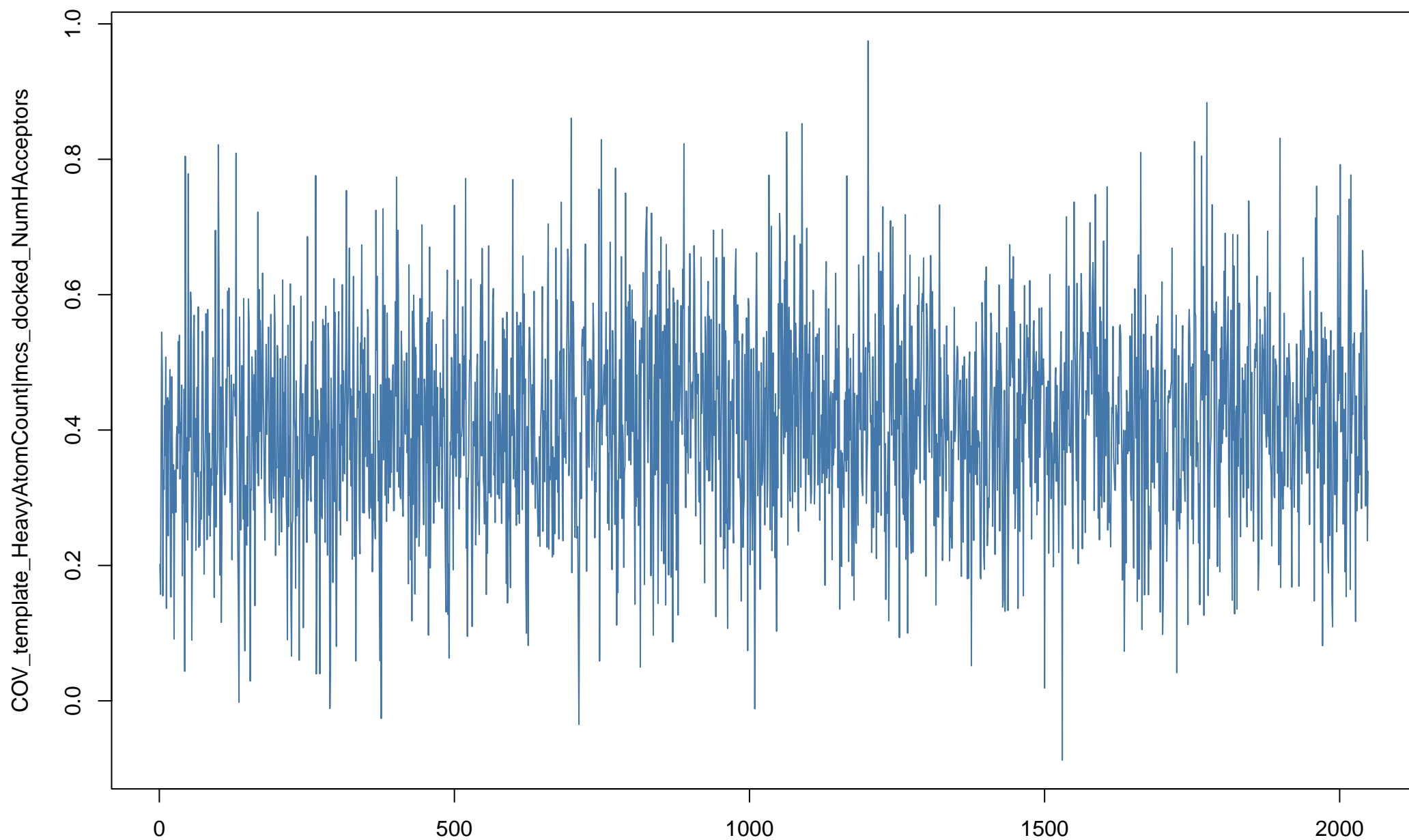
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0405 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0



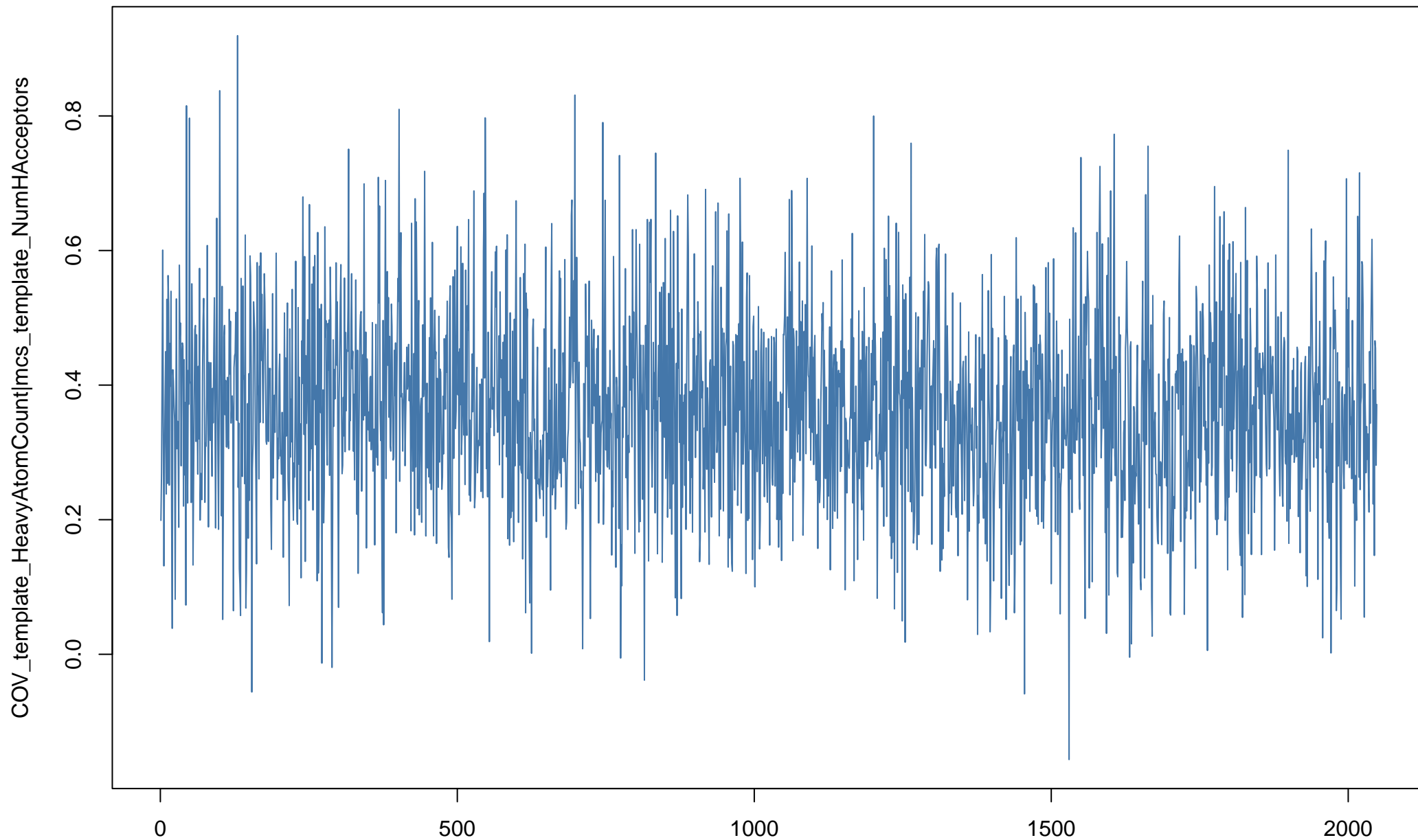
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 1920 | BMK = 0.0278 | MCSE(6.27) = 1.96 | stat: FALSE | burn: 0



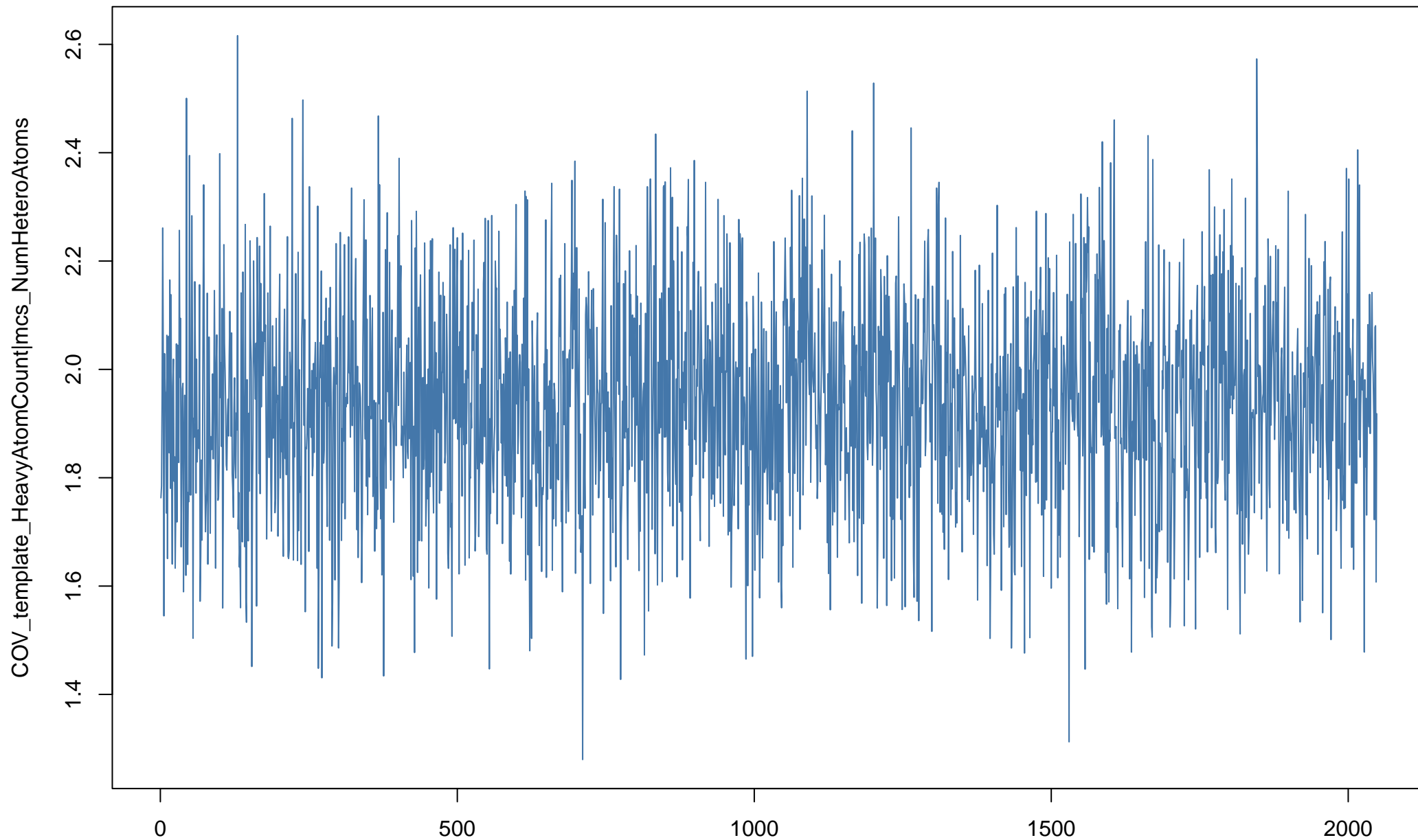
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1850 | BMK = 0.0707 | MCSE(6.27) = 2.56 | stat: FALSE | burn: 0



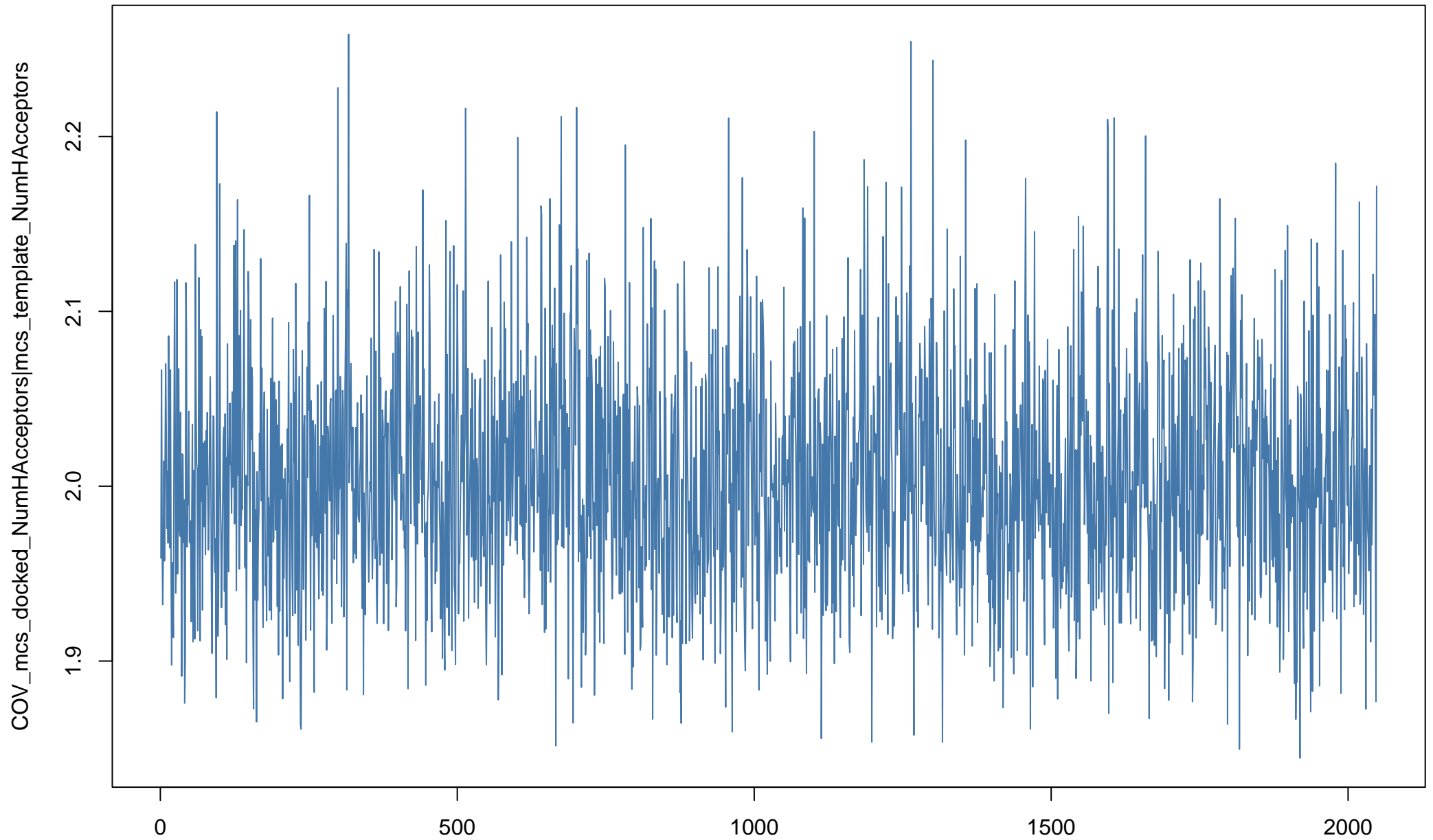
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.057 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0



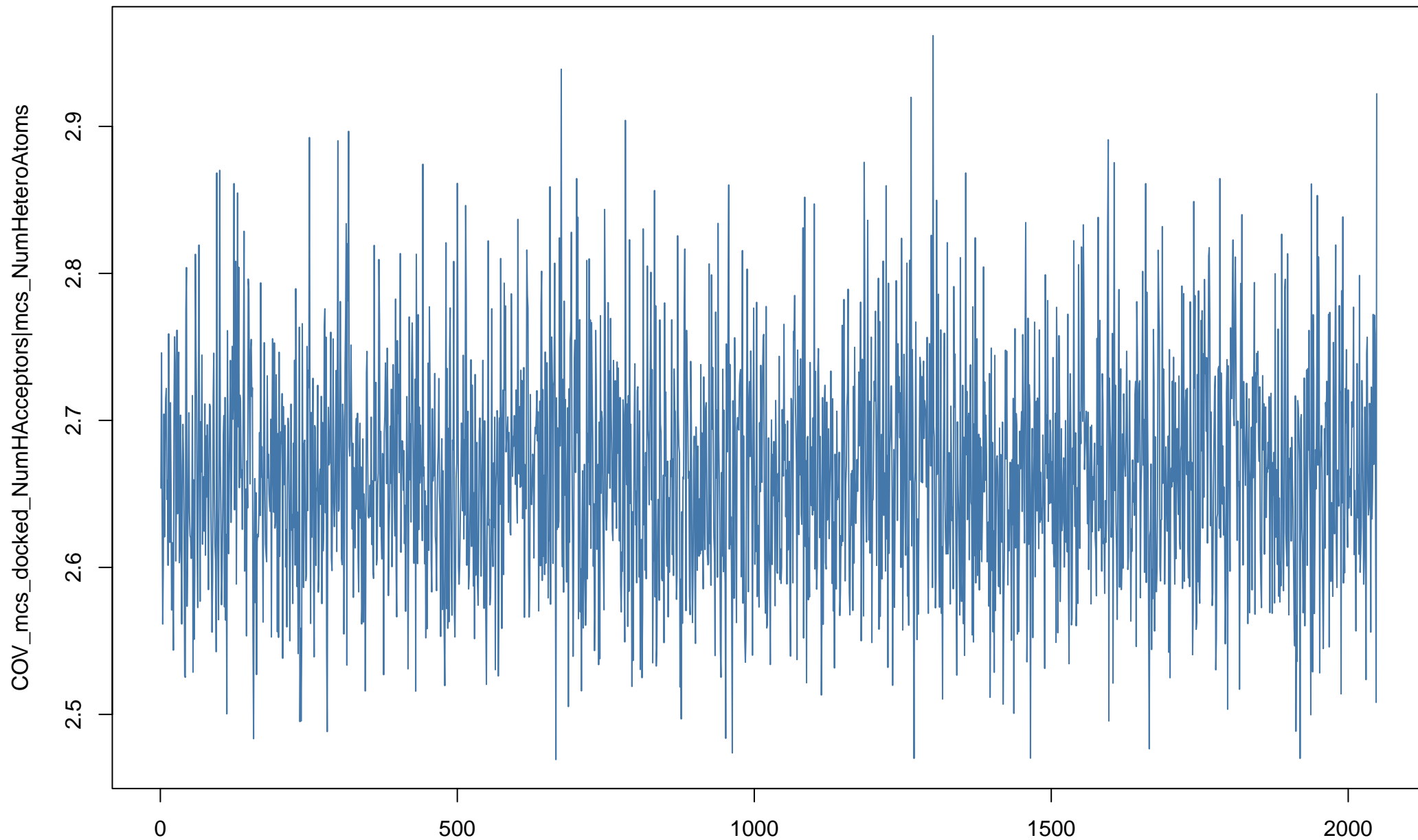
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0494 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0226 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0221 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0501 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0

