

-- STATS maxD --

min ESS = 2.22044604925031e-16

max BMK = 0.891944997973009

max MCSE = 14.775615208424

all stationary: FALSE

burn: 2040

-- STATS 2D --

min ESS = 216.999720393668

max BMK = 0.17185980280573

max MCSE = 4.82626639684503

all stationary: FALSE

burn: 0

-- STATS 1D --

min ESS = 2.22044604925031e-16

max BMK = 0.26357471844246

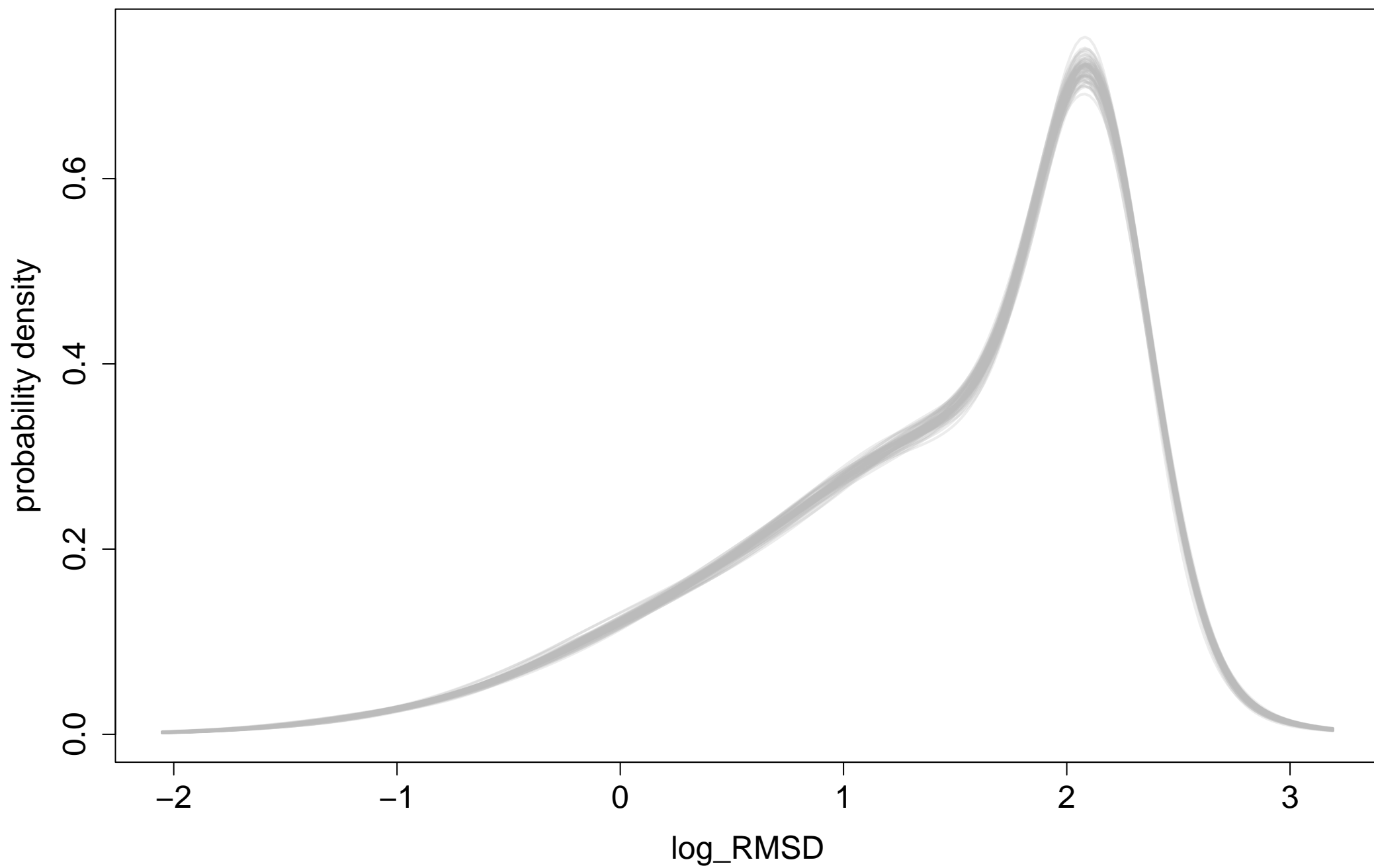
max MCSE = NaN

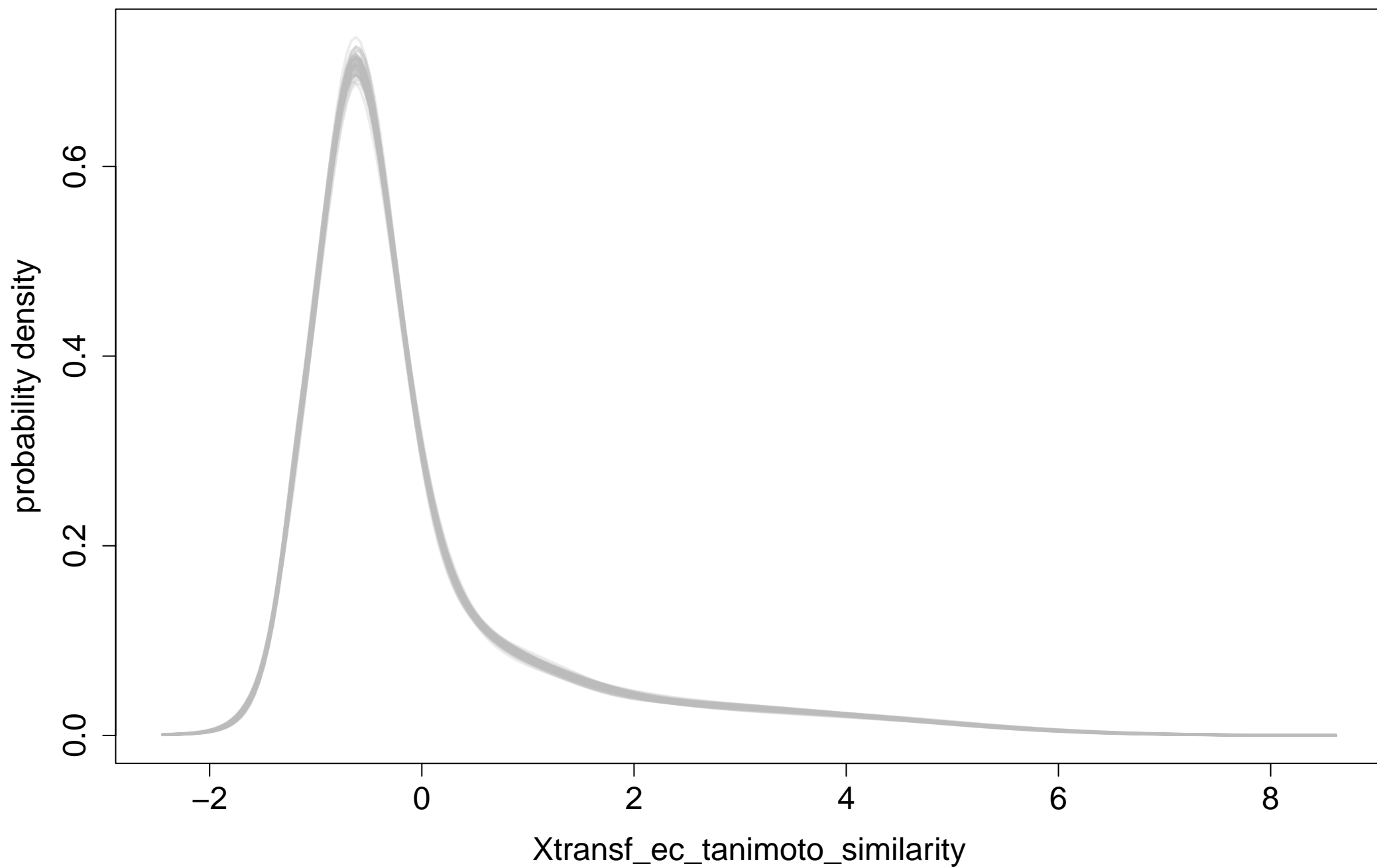
all stationary: FALSE

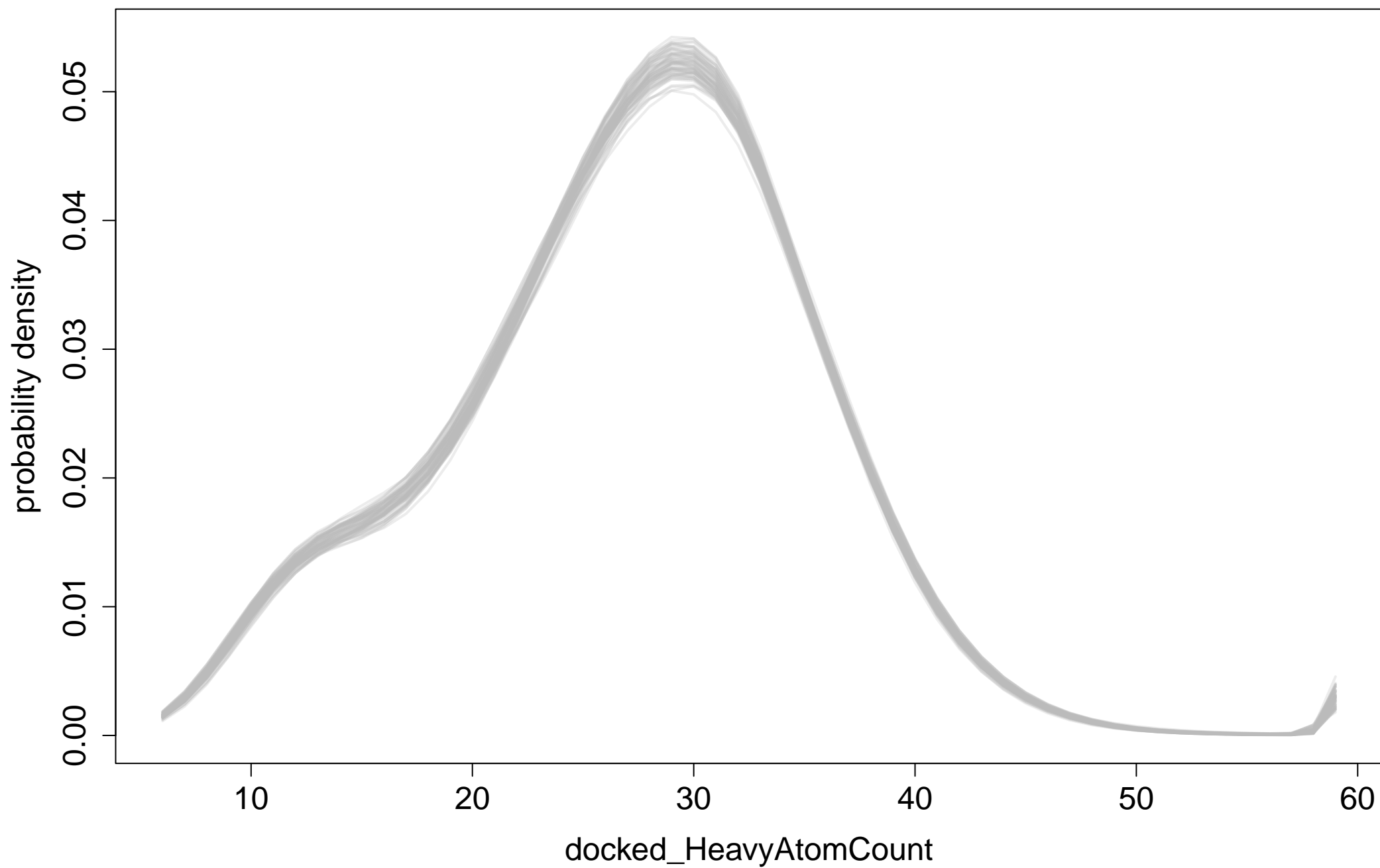
burn: 2040

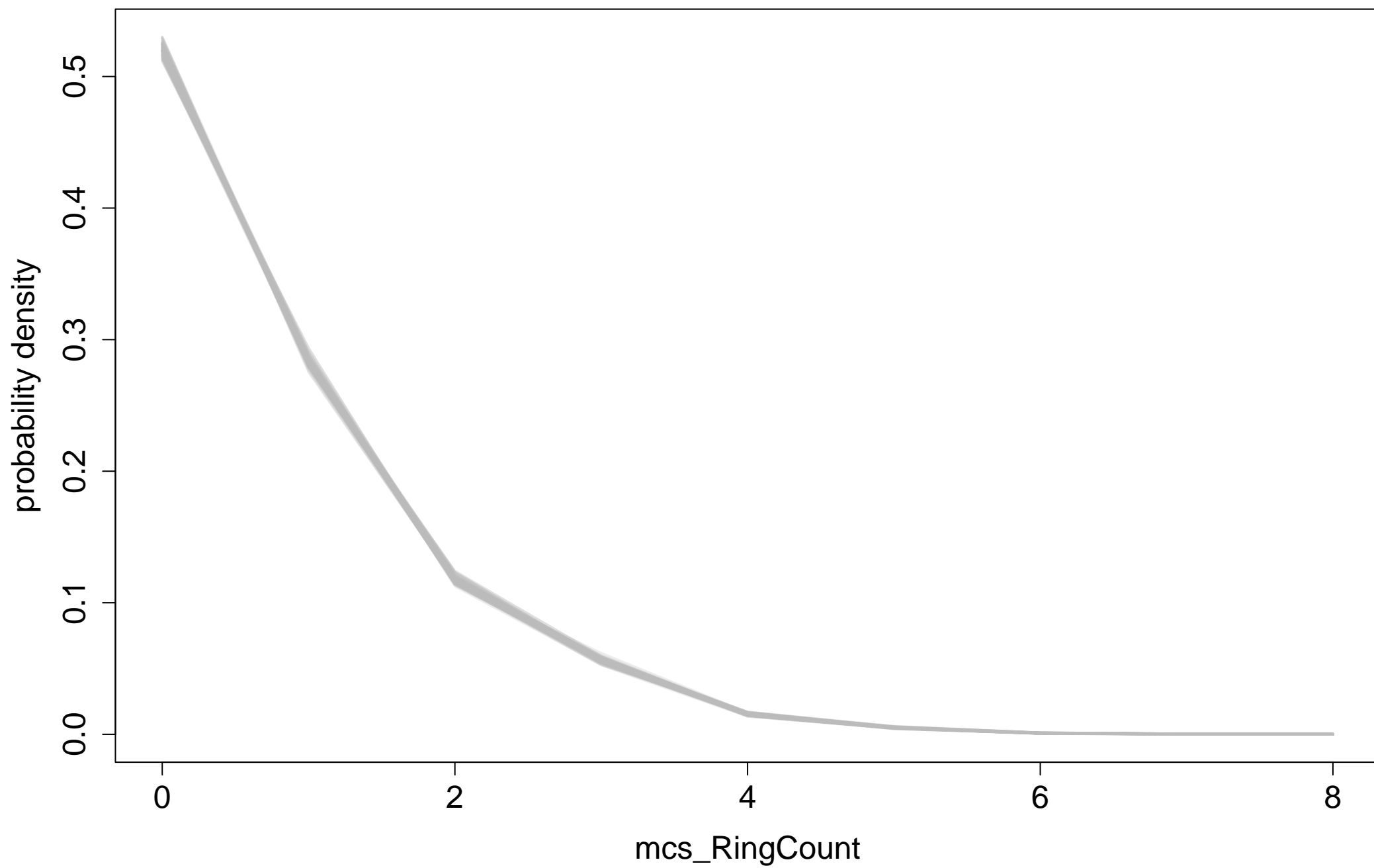
Occupied clusters: 57 of 64

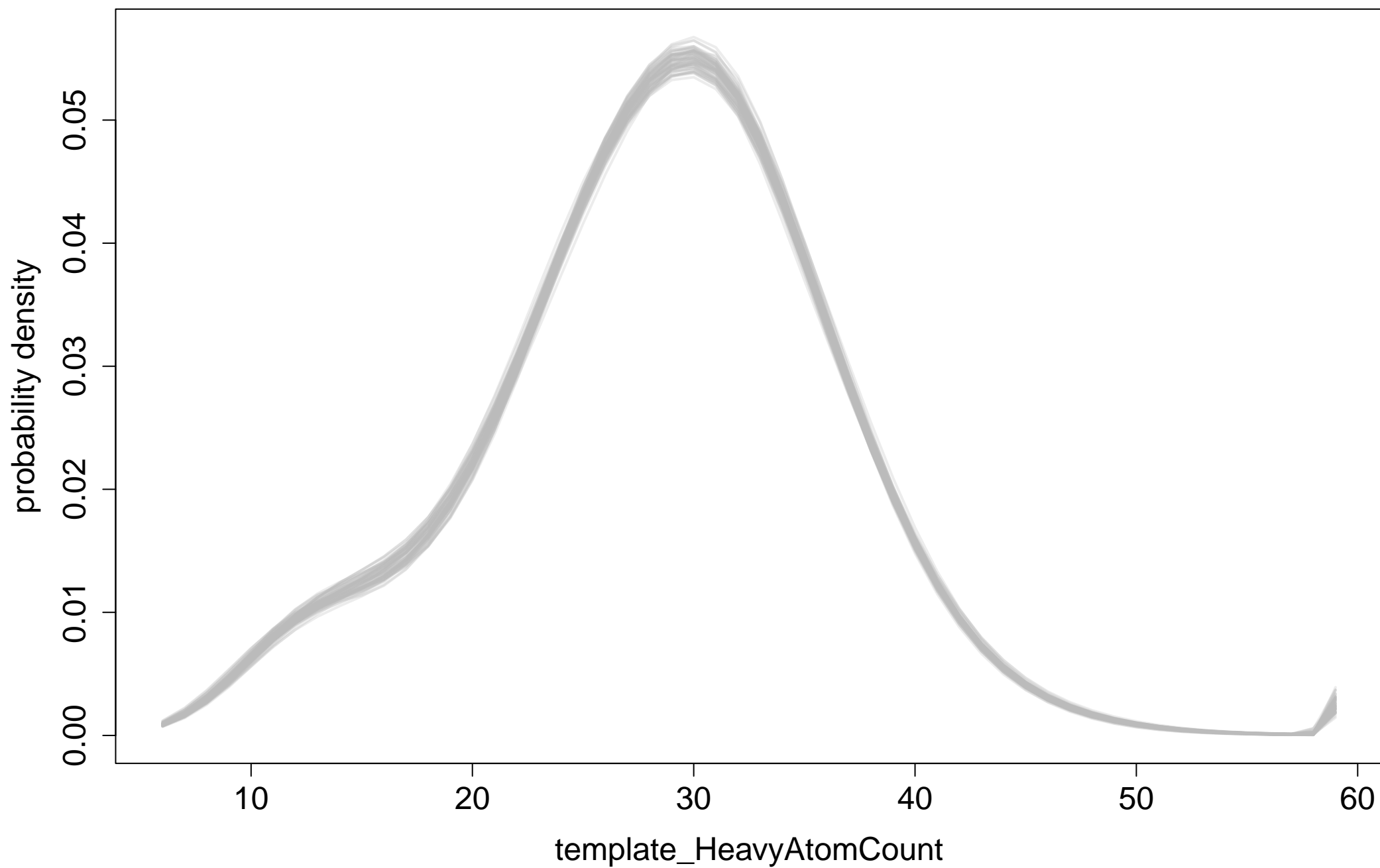
LL: -111000 +- 154

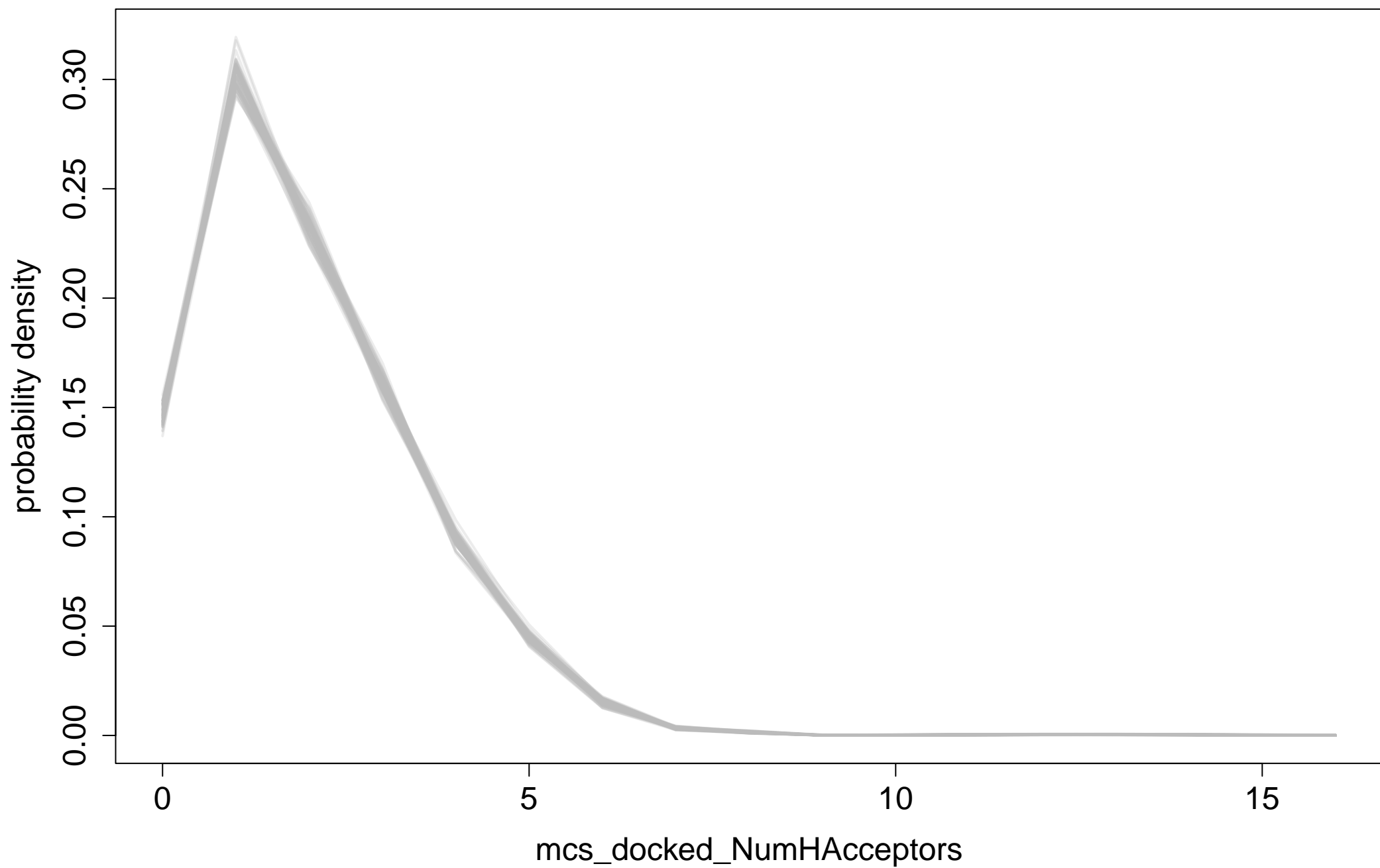


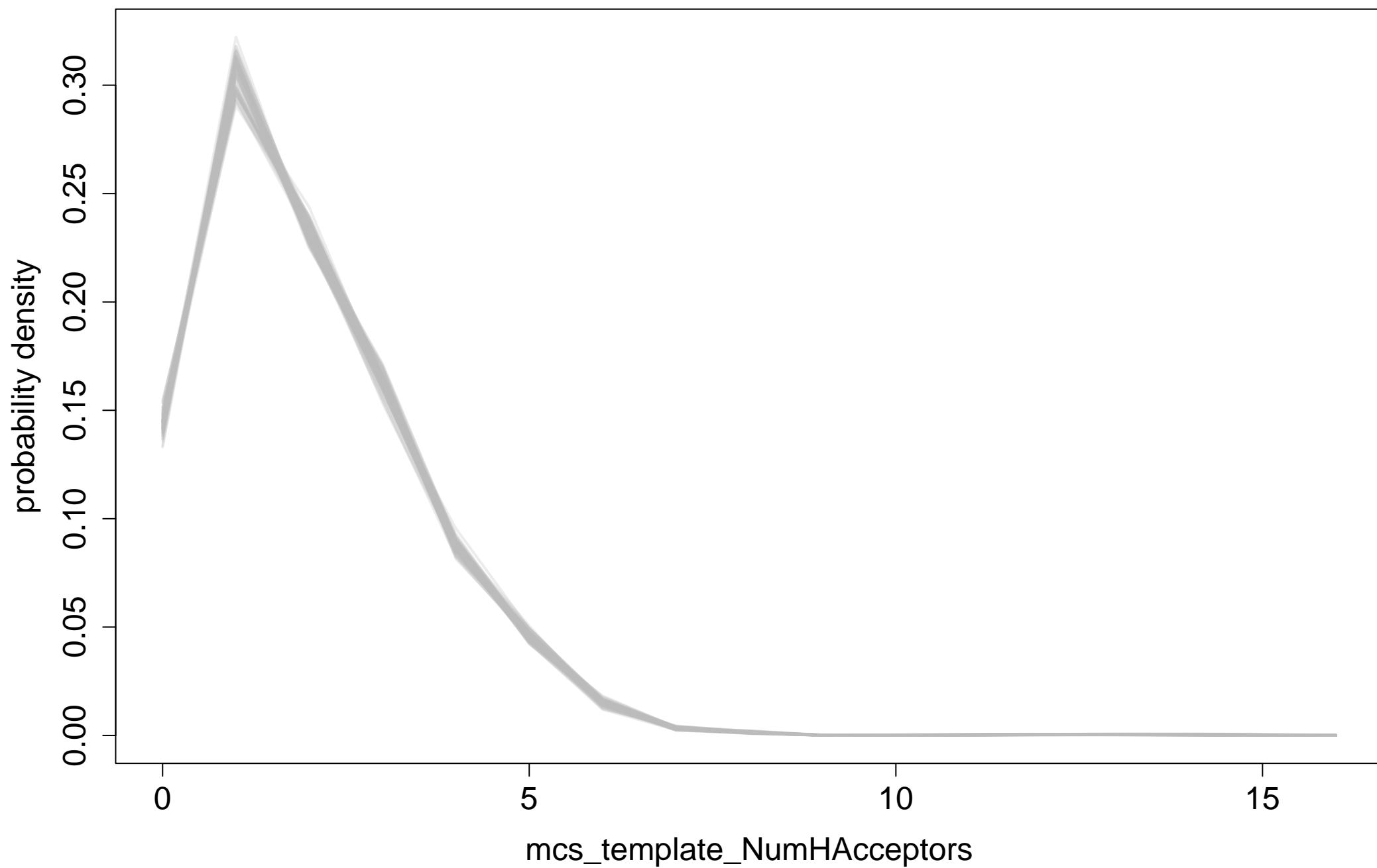


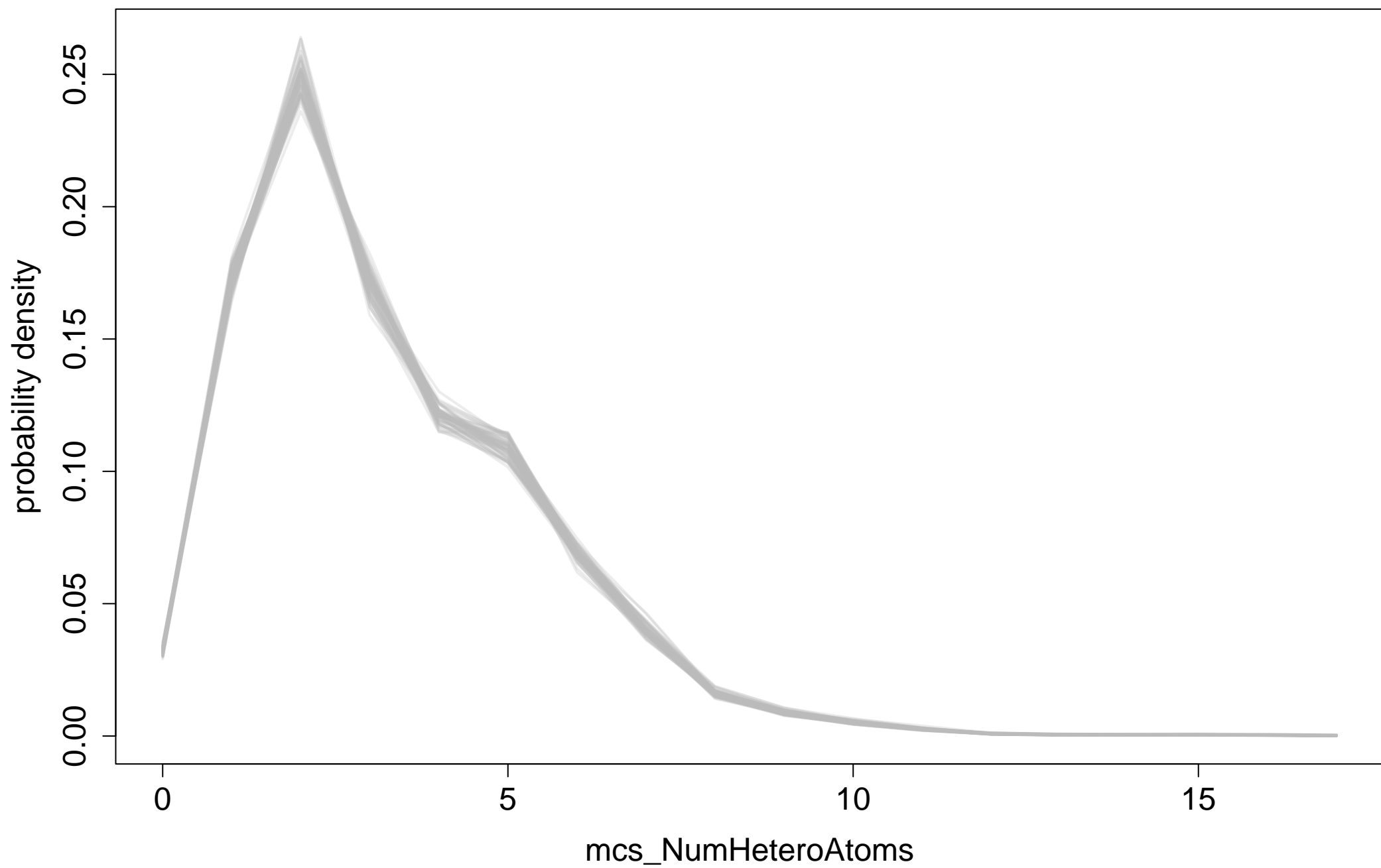


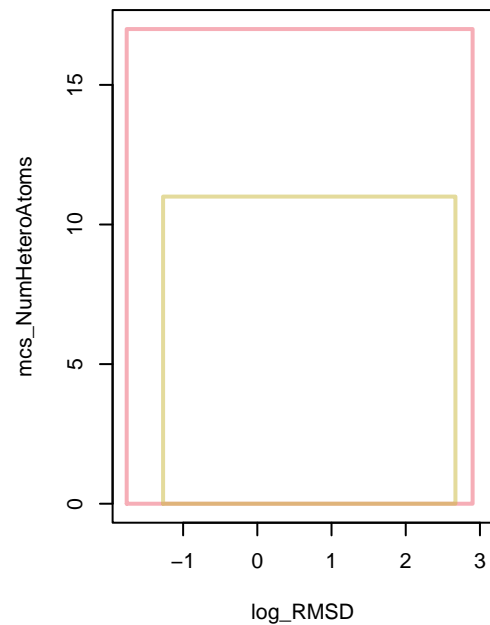
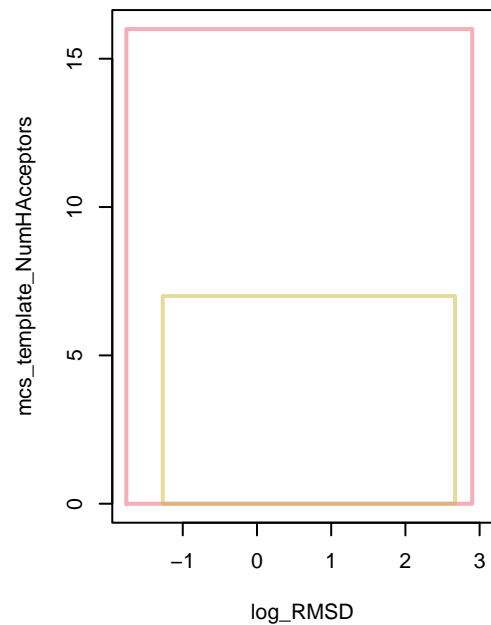
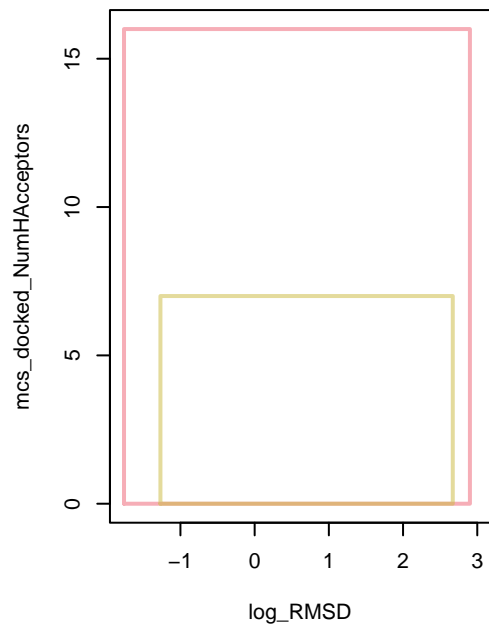
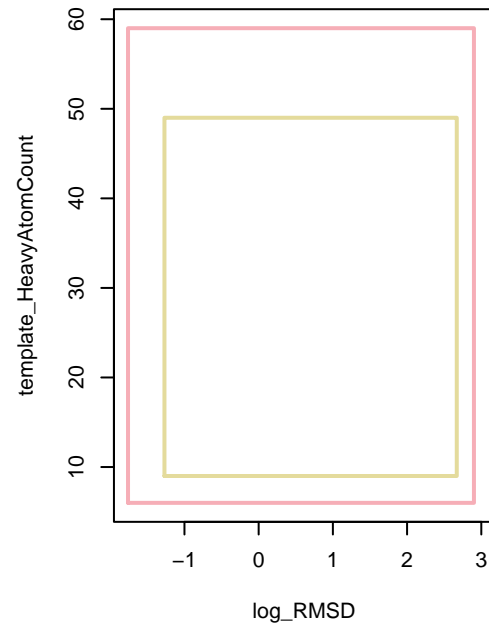
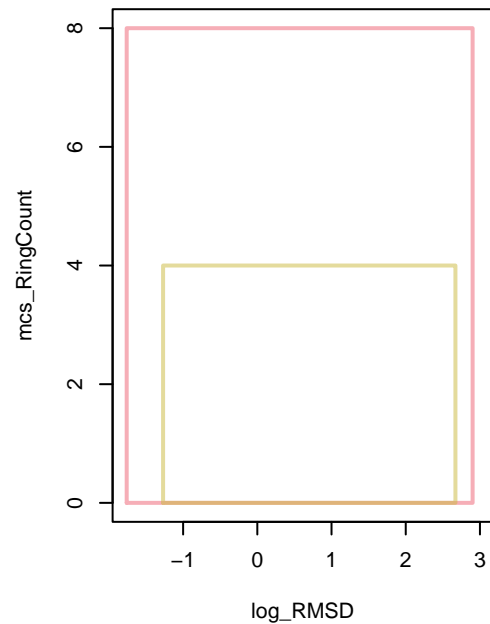
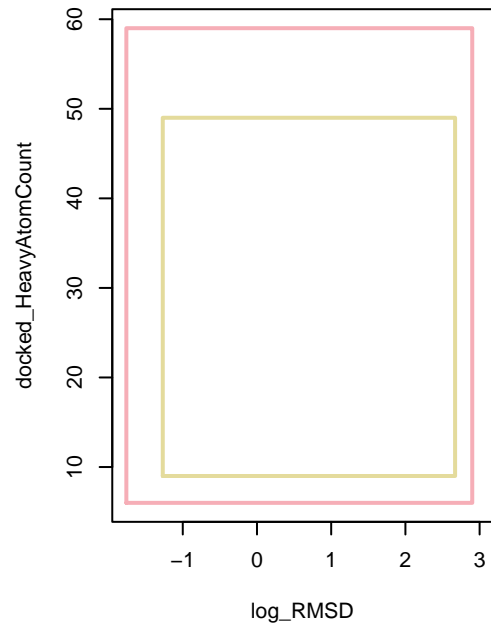
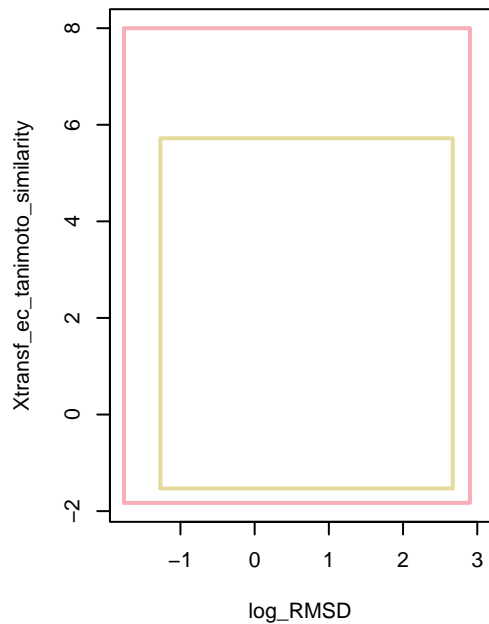




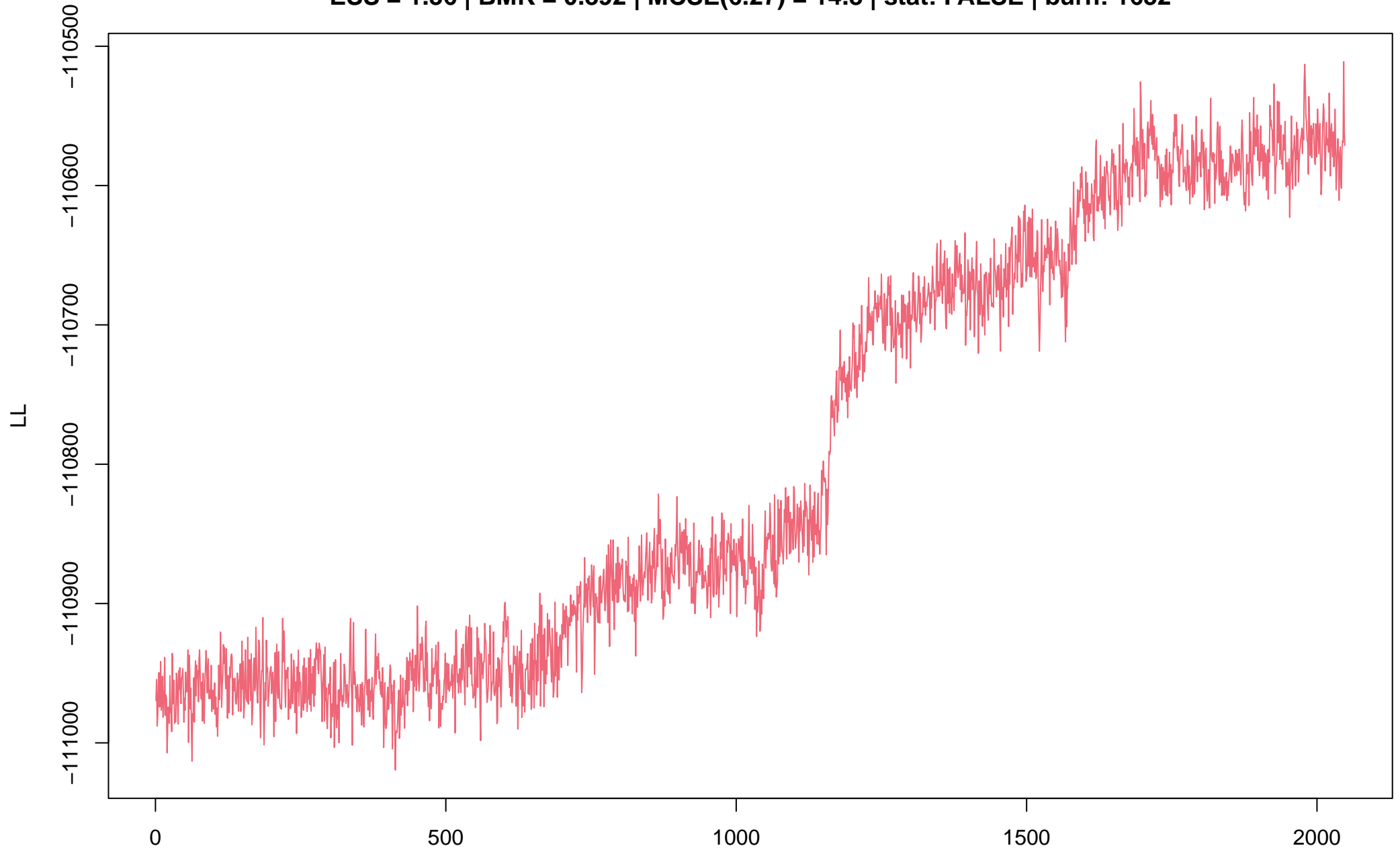




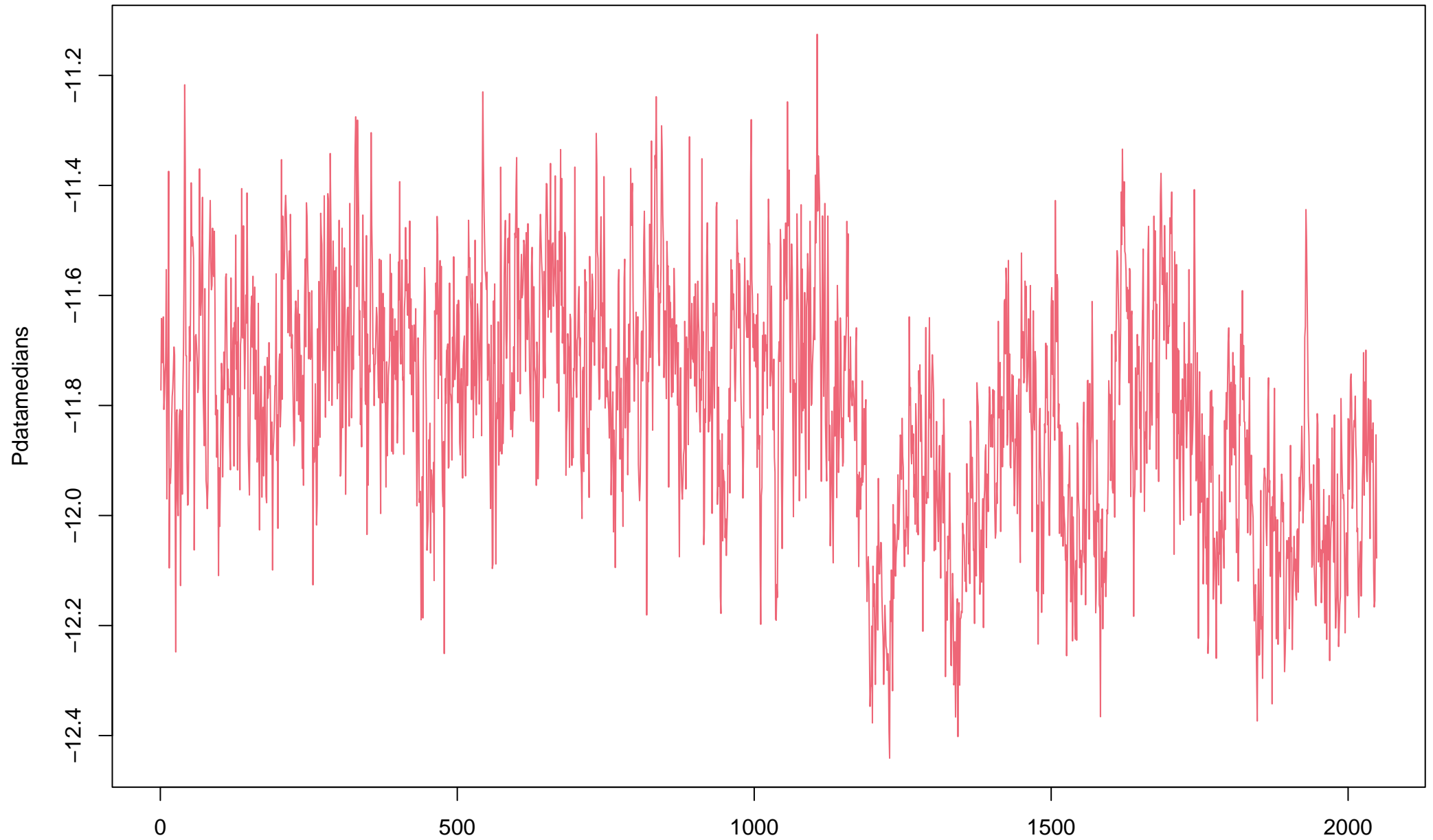




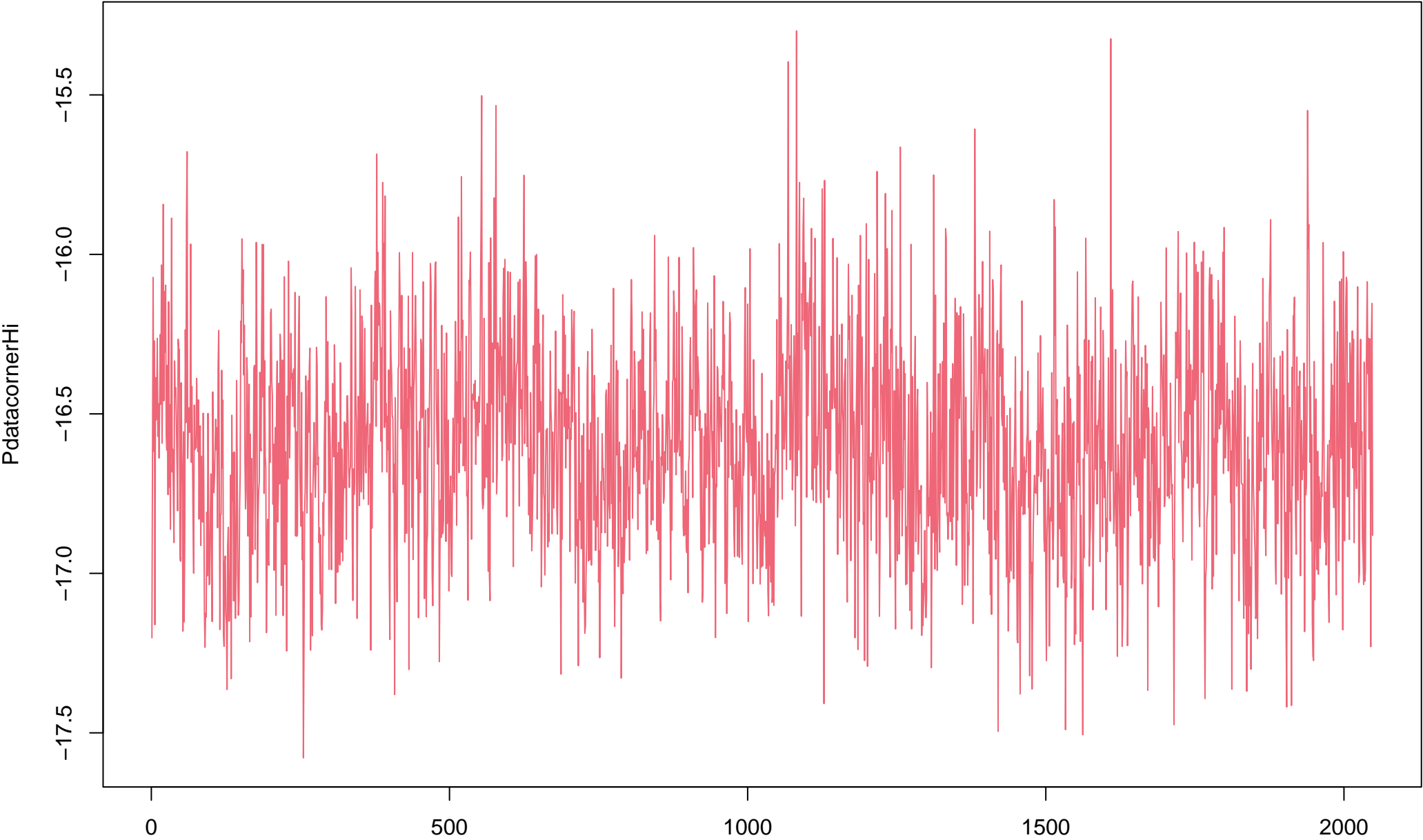
LL
ESS = 1.36 | BMK = 0.892 | MCSE(6.27) = 14.8 | stat: FALSE | burn: 1632



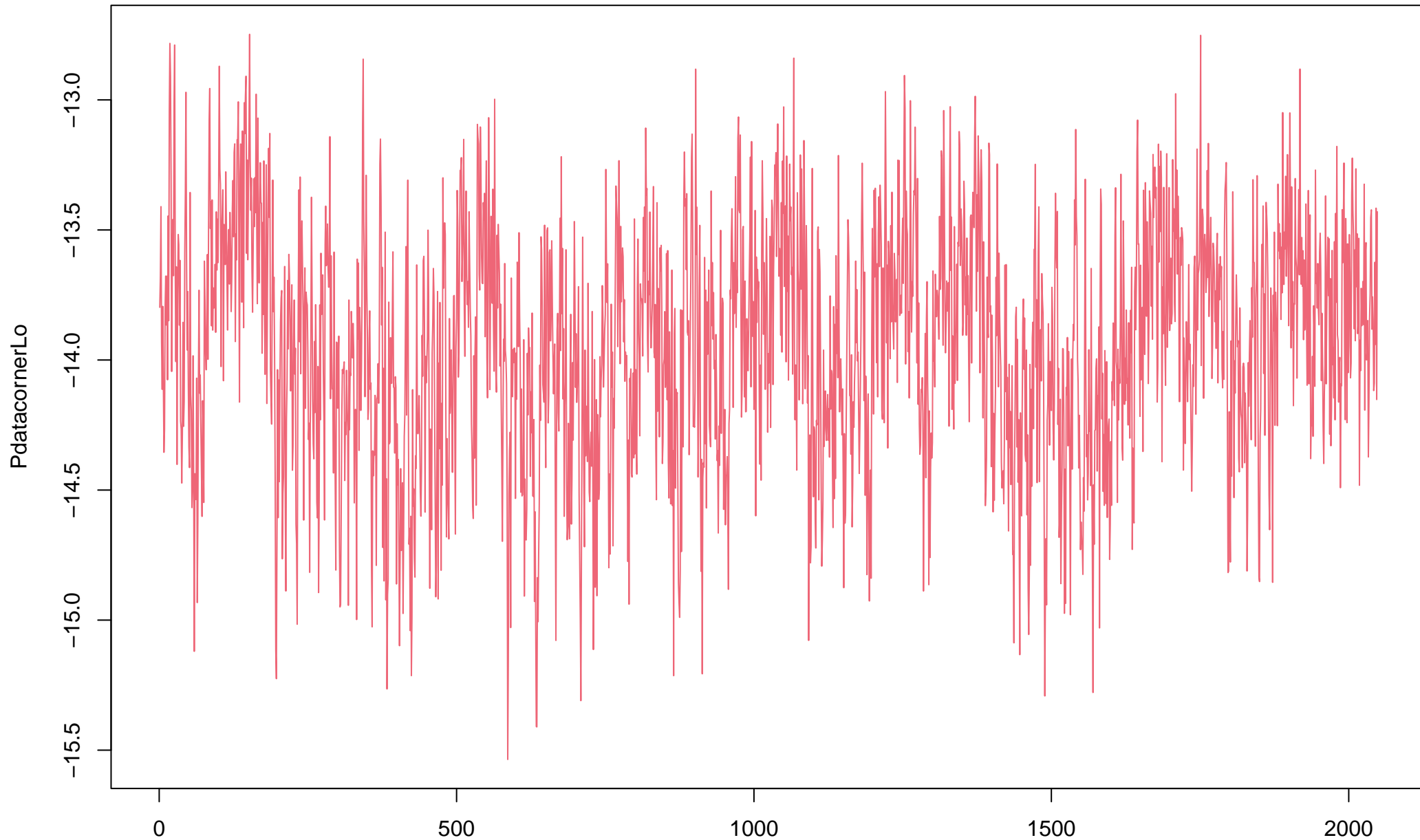
Pdatamedians
ESS = 69.1 | BMK = 0.348 | MCSE(6.27) = 9.58 | stat: FALSE | burn: 0



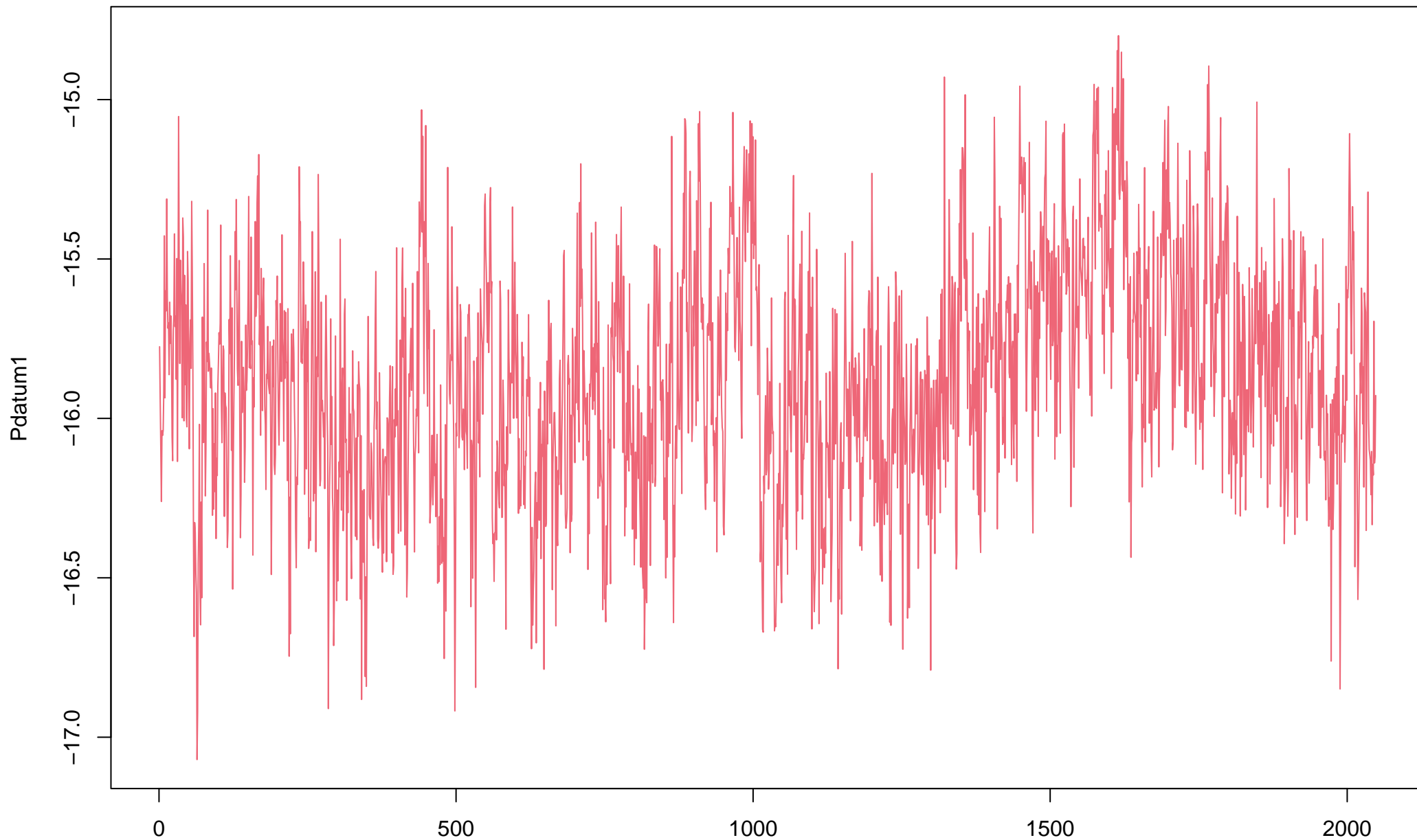
PdatacornerHi
ESS = 264 | BMK = 0.0665 | MCSE(6.27) = 4.75 | stat: TRUE | burn: 0



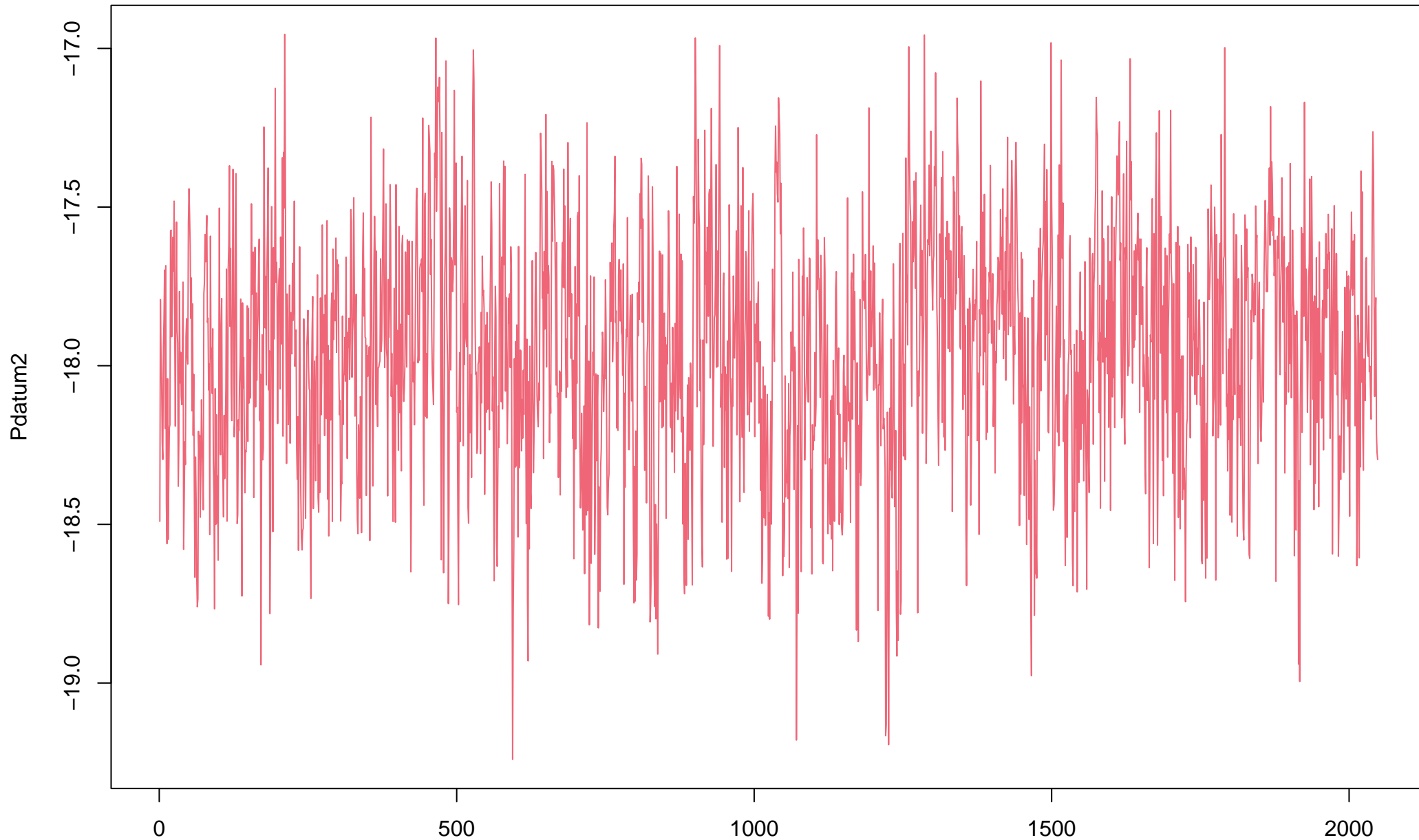
PdatacornerLo
ESS = 118 | BMK = 0.0776 | MCSE(6.27) = 7.26 | stat: FALSE | burn: 0



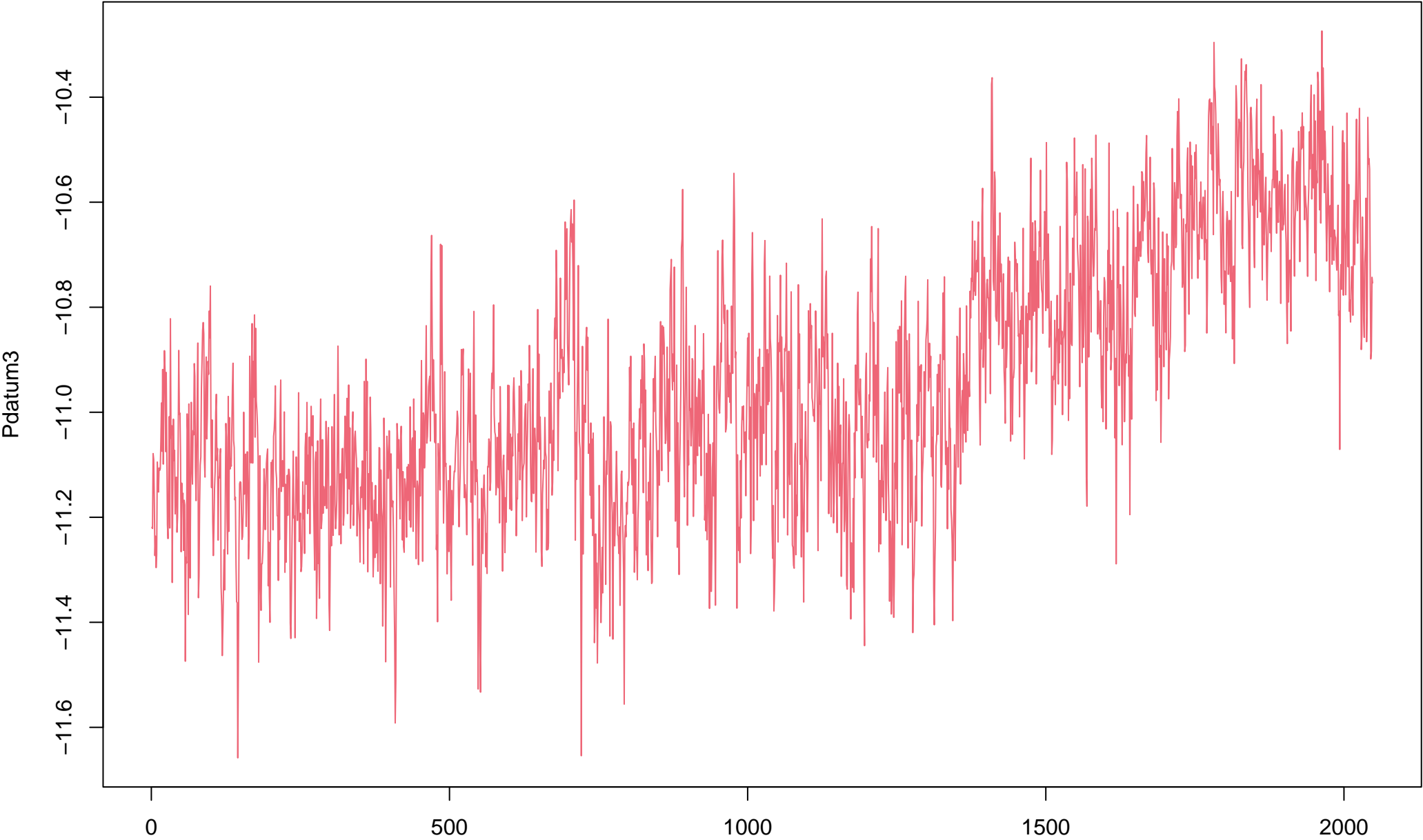
Pdatum1
ESS = 113 | BMK = 0.138 | MCSE(6.27) = 8.13 | stat: TRUE | burn: 0



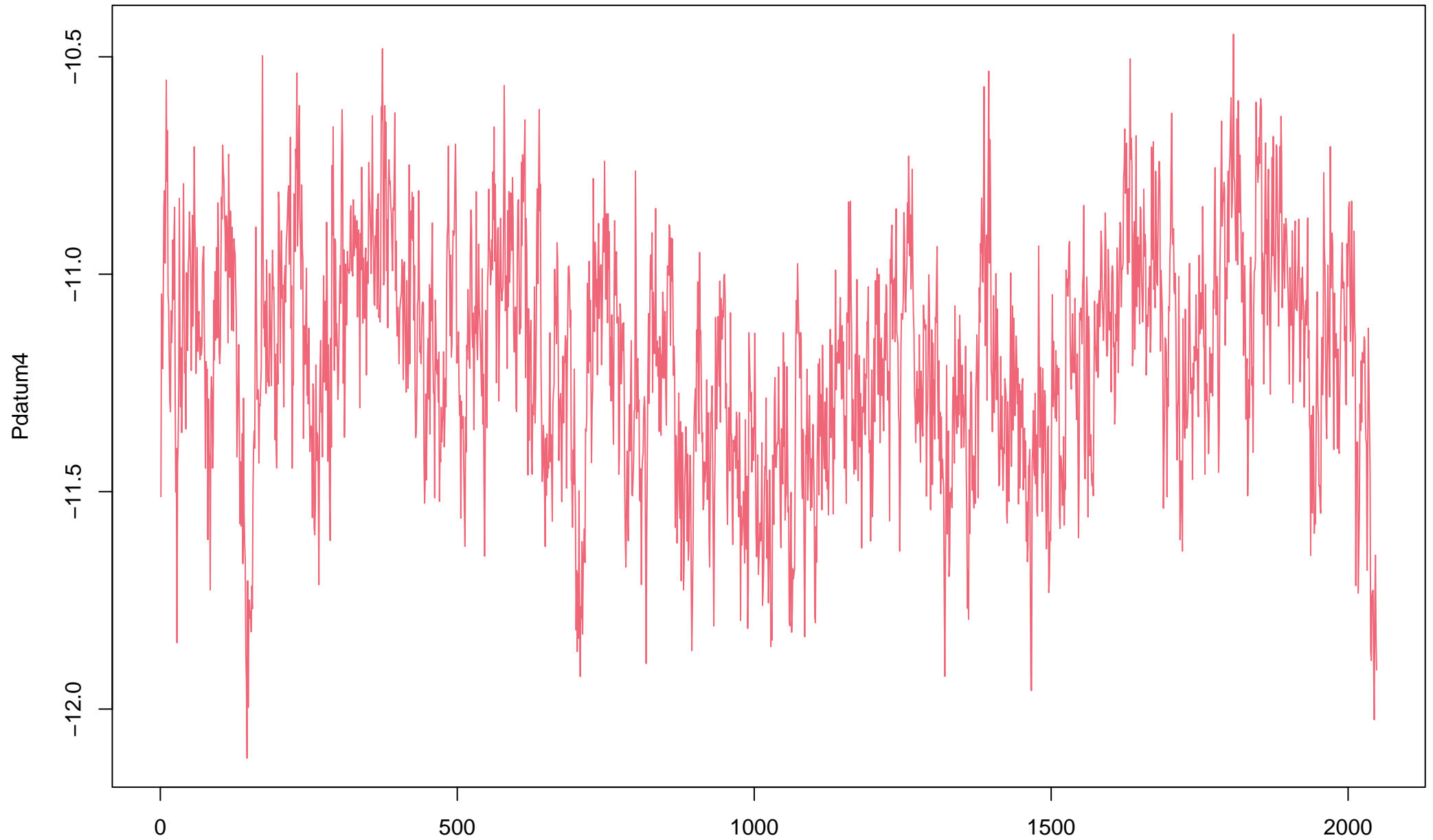
Pdatum2
ESS = 2.22e-16 | BMK = 0.0586 | MCSE(6.27) = 5.35 | stat: TRUE | burn: 0



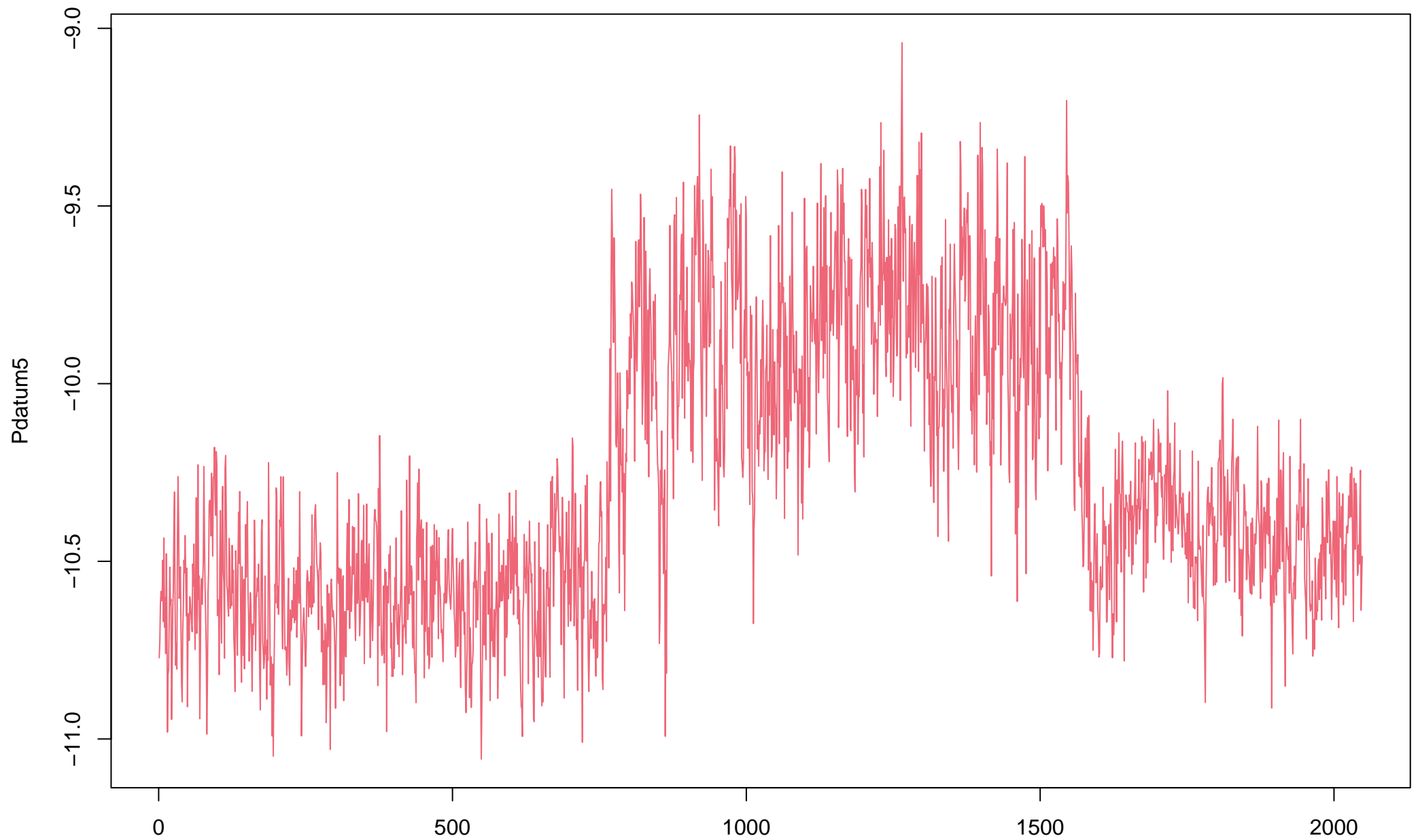
Pdatum3
ESS = 11.3 | BMK = 0.492 | MCSE(6.27) = 12.4 | stat: FALSE | burn: 0



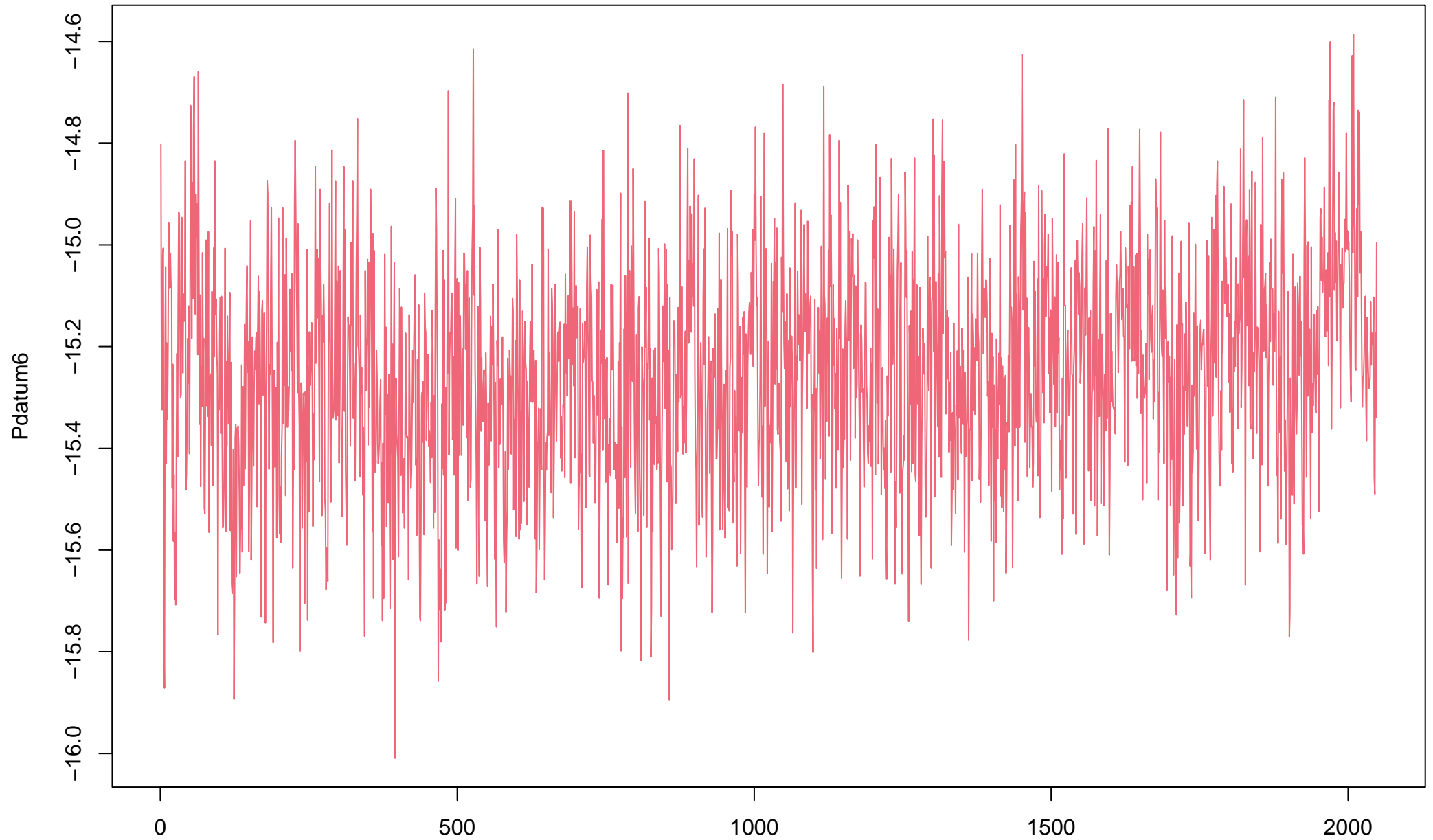
Pdatum4
ESS = 95.2 | BMK = 0.059 | MCSE(6.27) = 8.99 | stat: TRUE | burn: 0



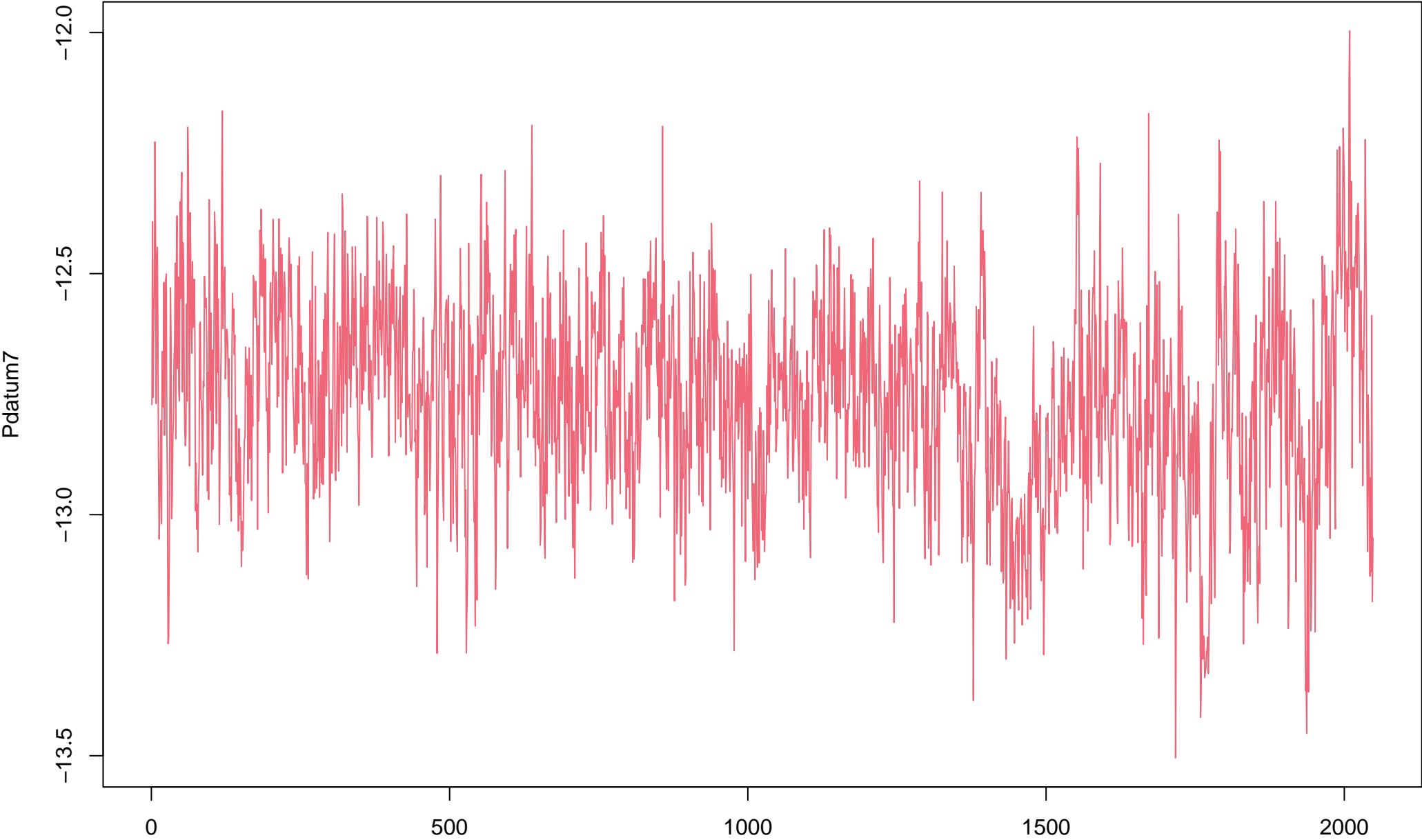
Pdatum5
ESS = 7.35 | BMK = 0.321 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 1632



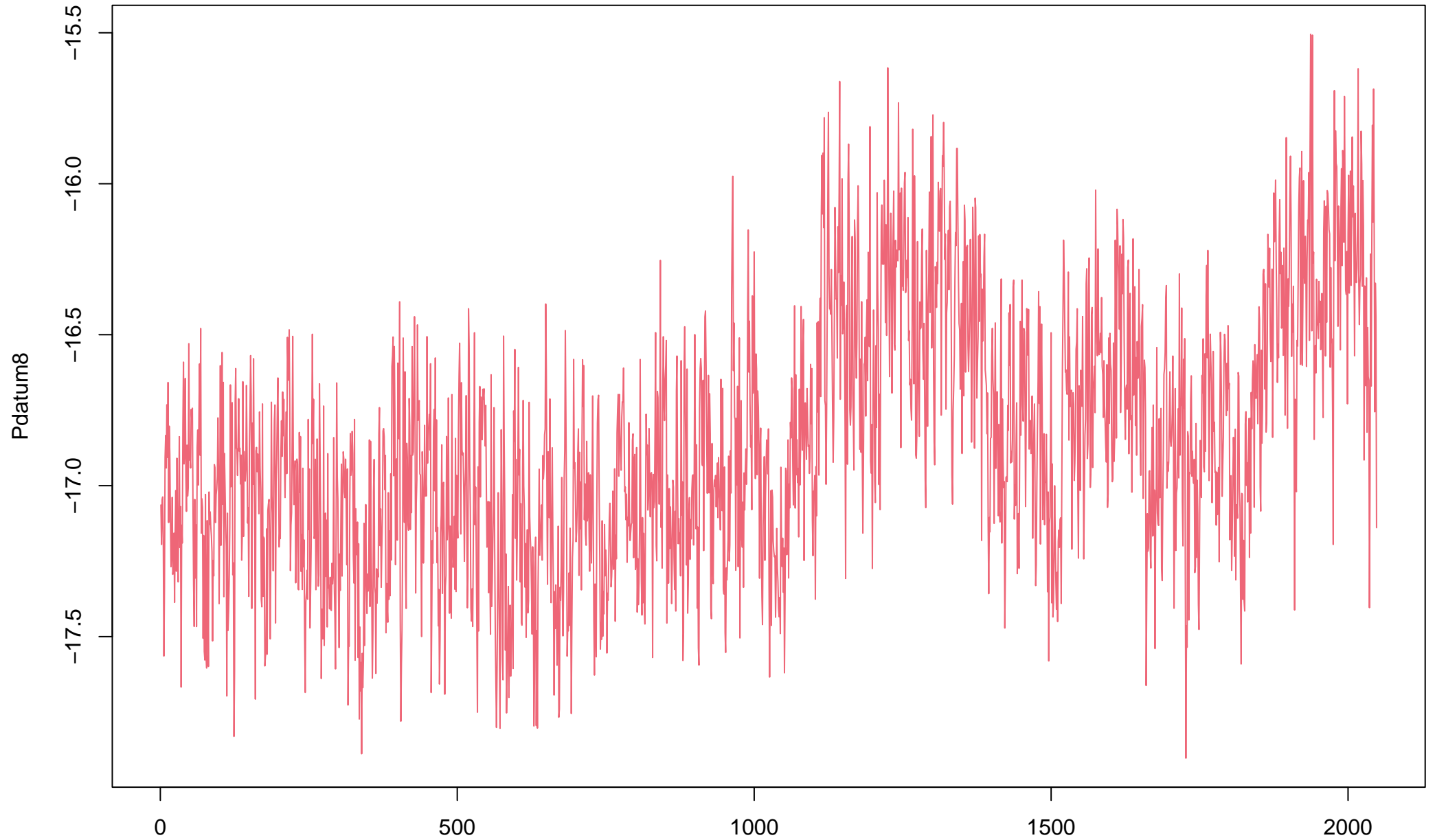
Pdatum6
ESS = 307 | BMK = 0.126 | MCSE(6.27) = 5.02 | stat: TRUE | burn: 0



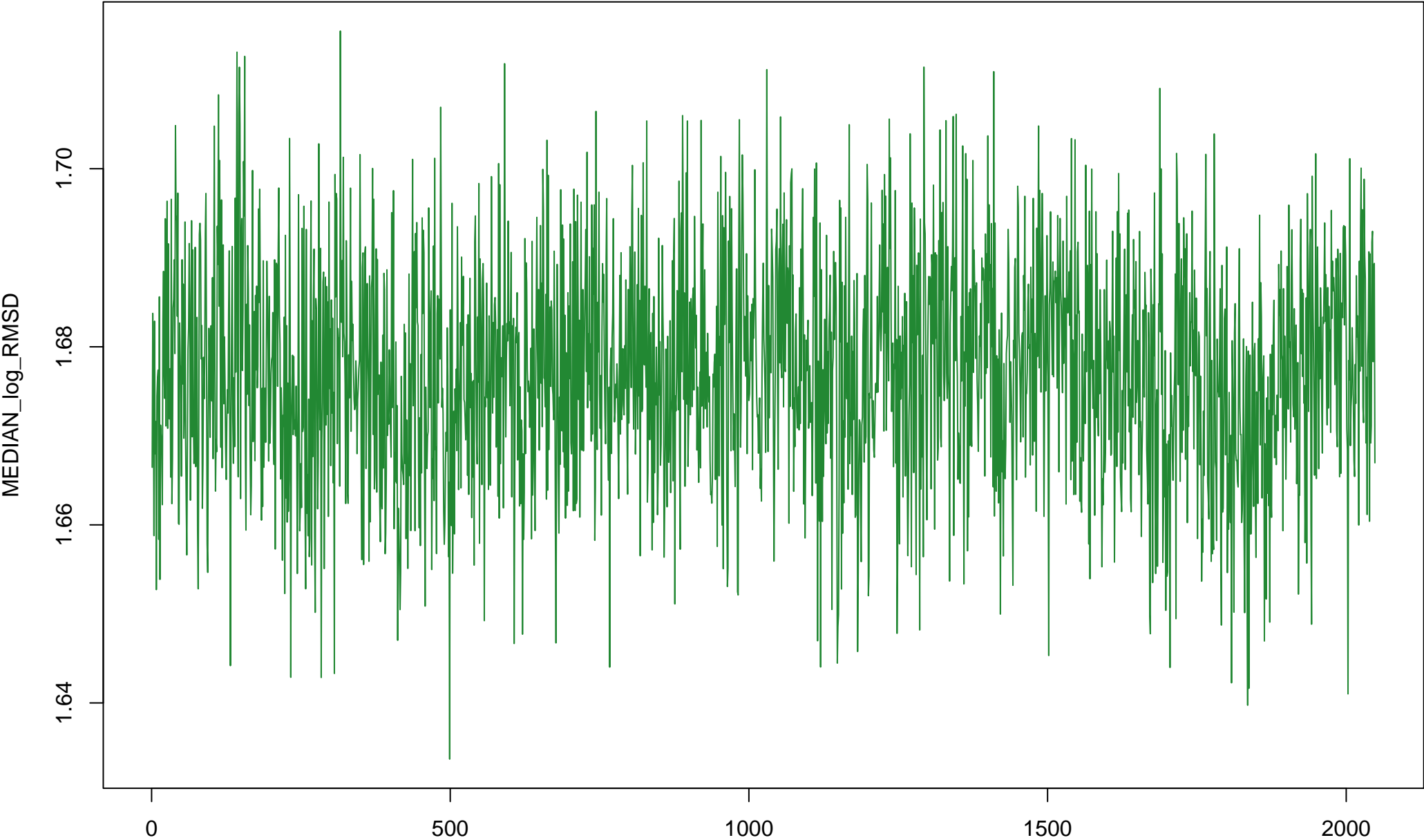
Pdatum7
ESS = 180 | BMK = 0.139 | MCSE(6.27) = 6.75 | stat: FALSE | burn: 0



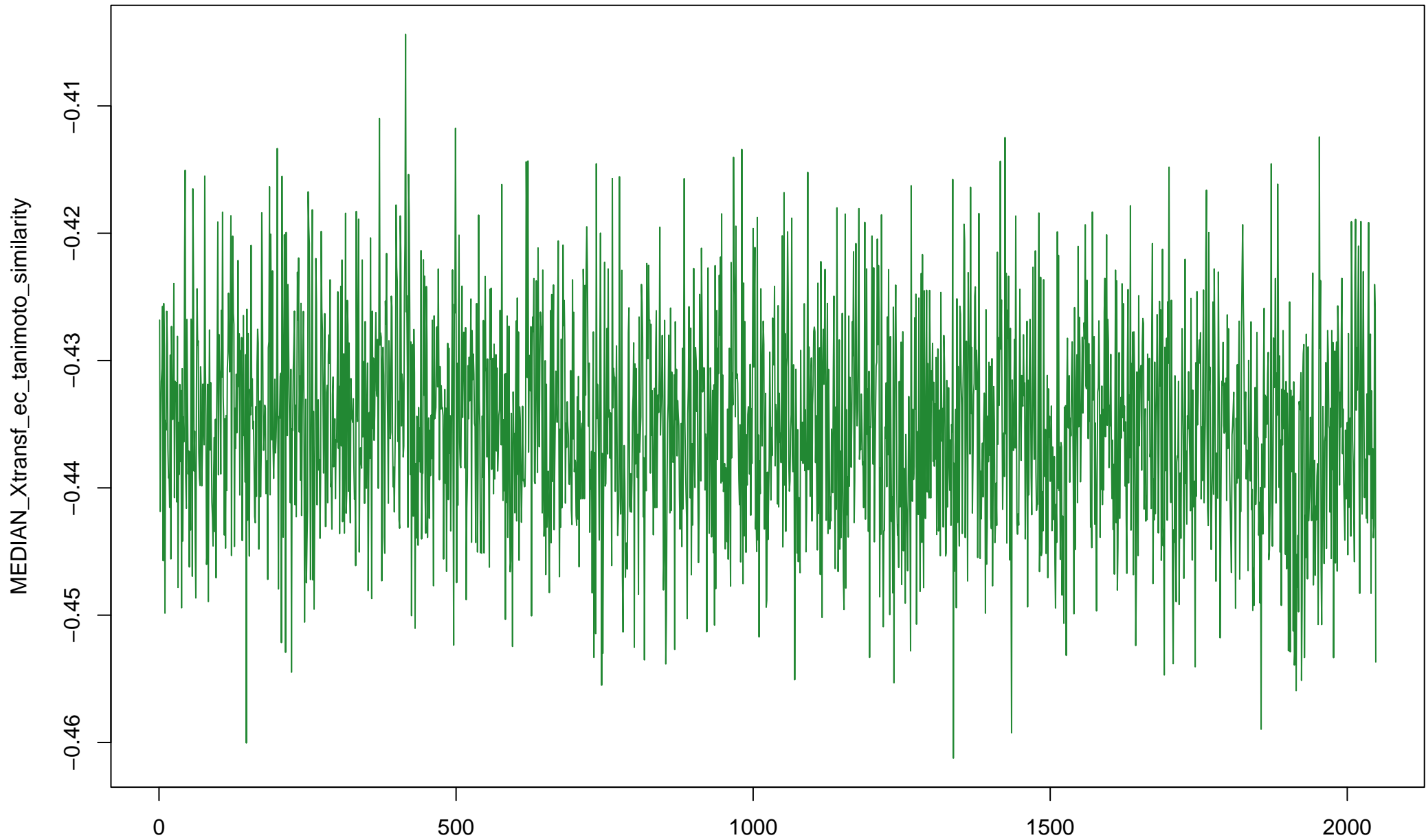
Pdatum8
ESS = 14.9 | BMK = 0.439 | MCSE(6.27) = 10.8 | stat: FALSE | burn: 2040



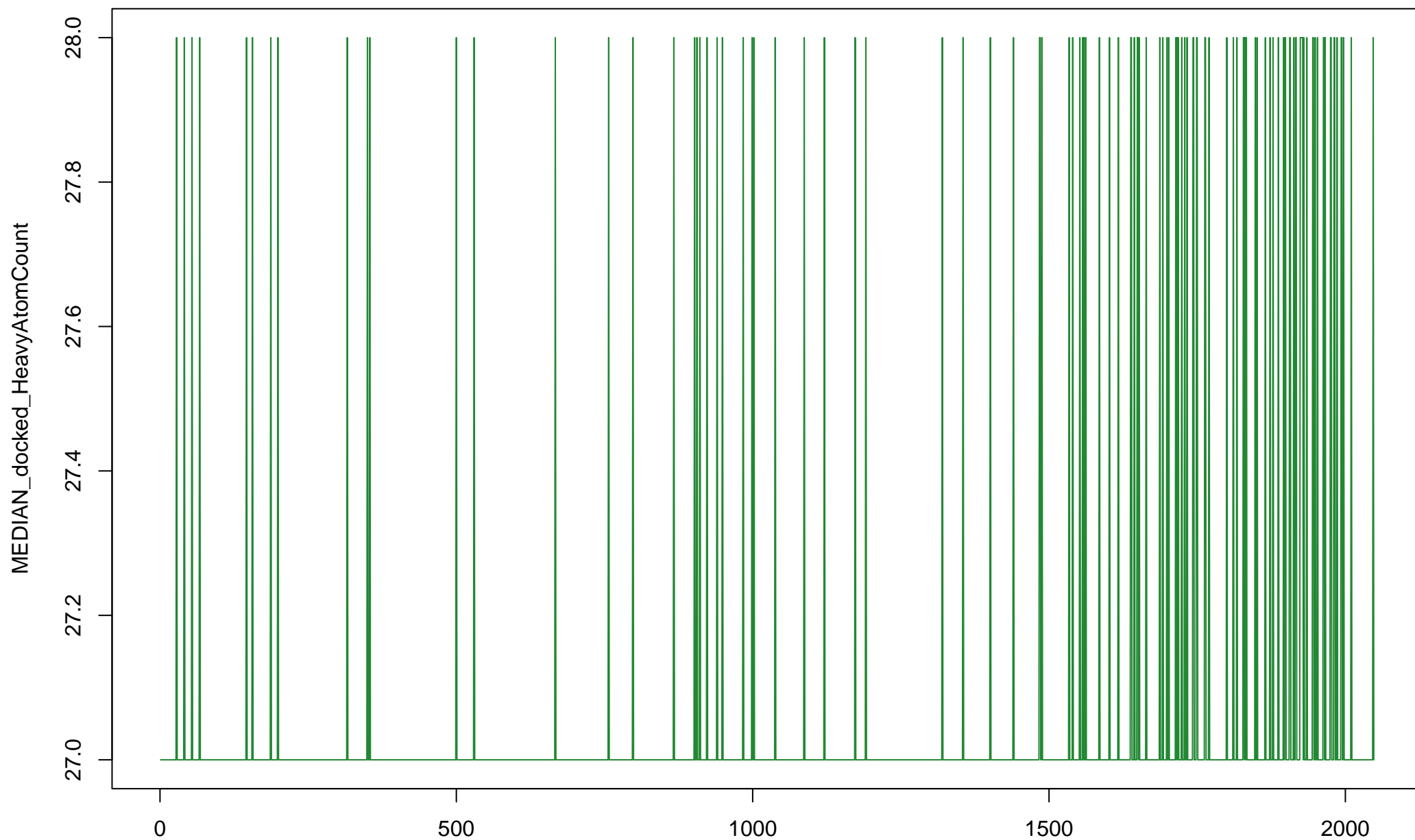
MEDIAN_log_RMSD
ESS = 848 | BMK = 0.0557 | MCSE(6.27) = 4.04 | stat: TRUE | burn: 0



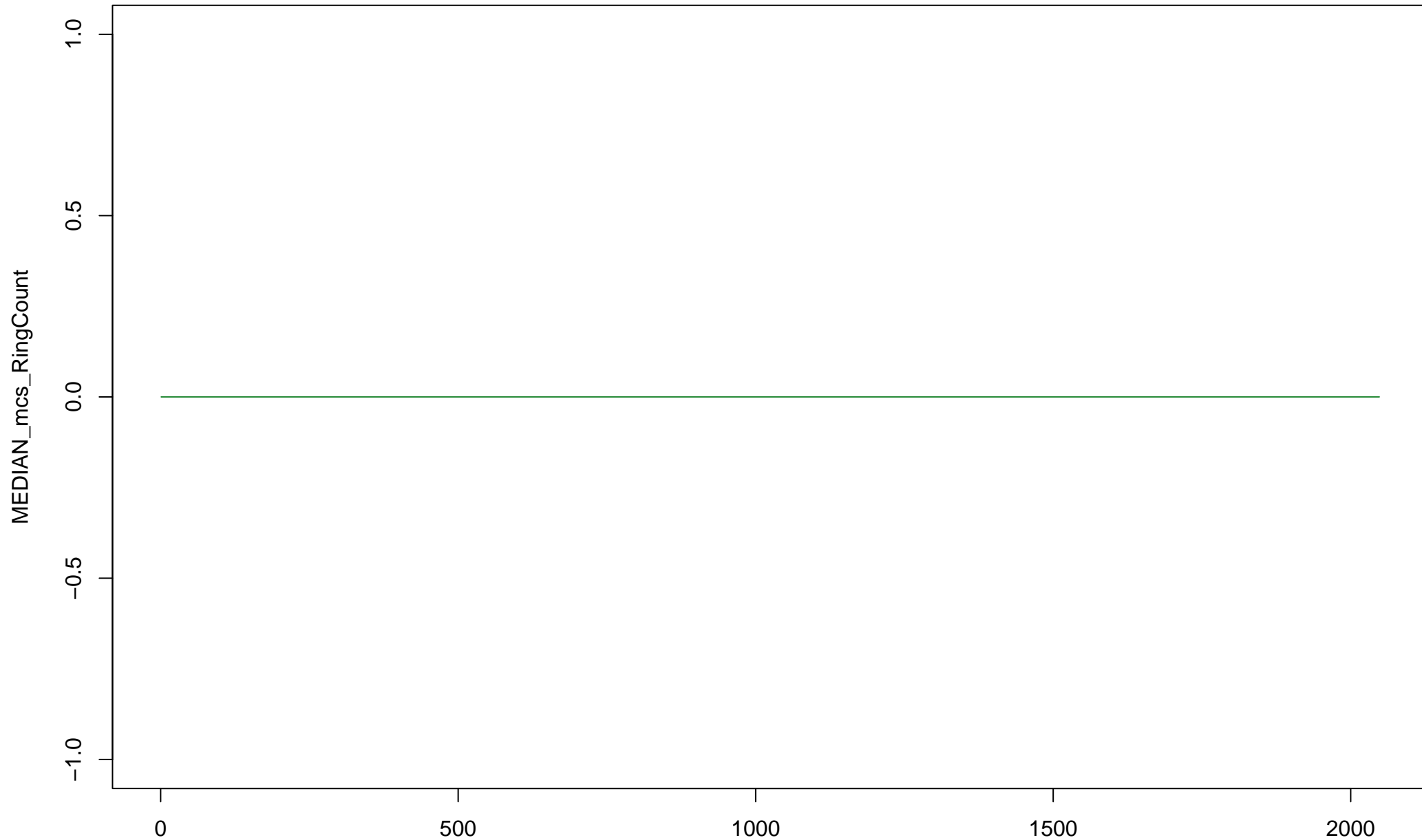
MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1850 | BMK = 0.063 | MCSE(6.27) = 3.04 | stat: FALSE | burn: 0



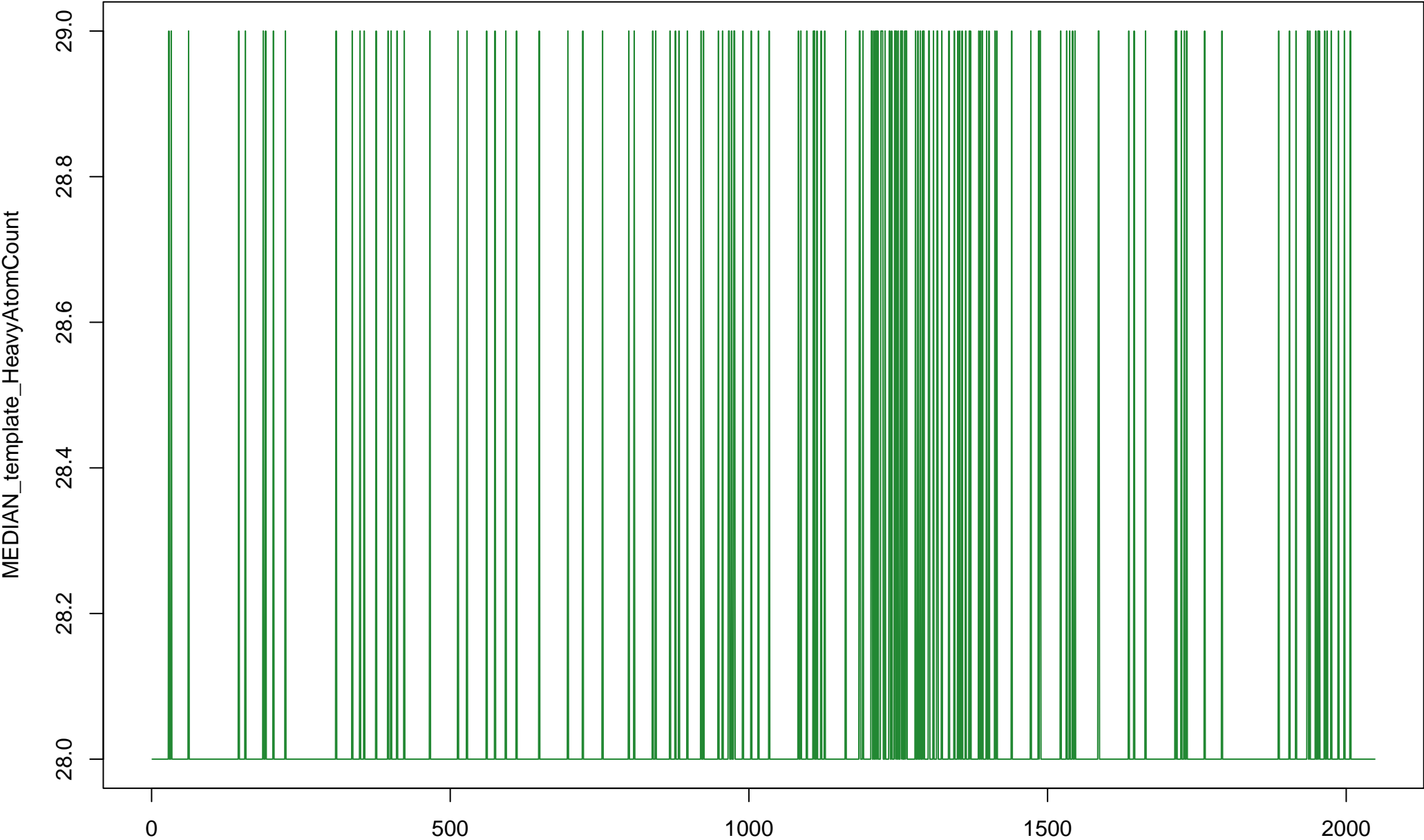
MEDIAN_docked_HeavyAtomCount
ESS = 215 | BMK = 0.21 | MCSE(6.27) = 4.53 | stat: FALSE | burn: 0



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



MEDIAN_template_HeavyAtomCount
ESS = 409 | BMK = 0.125 | MCSE(6.27) = 4.01 | stat: FALSE | burn: 0



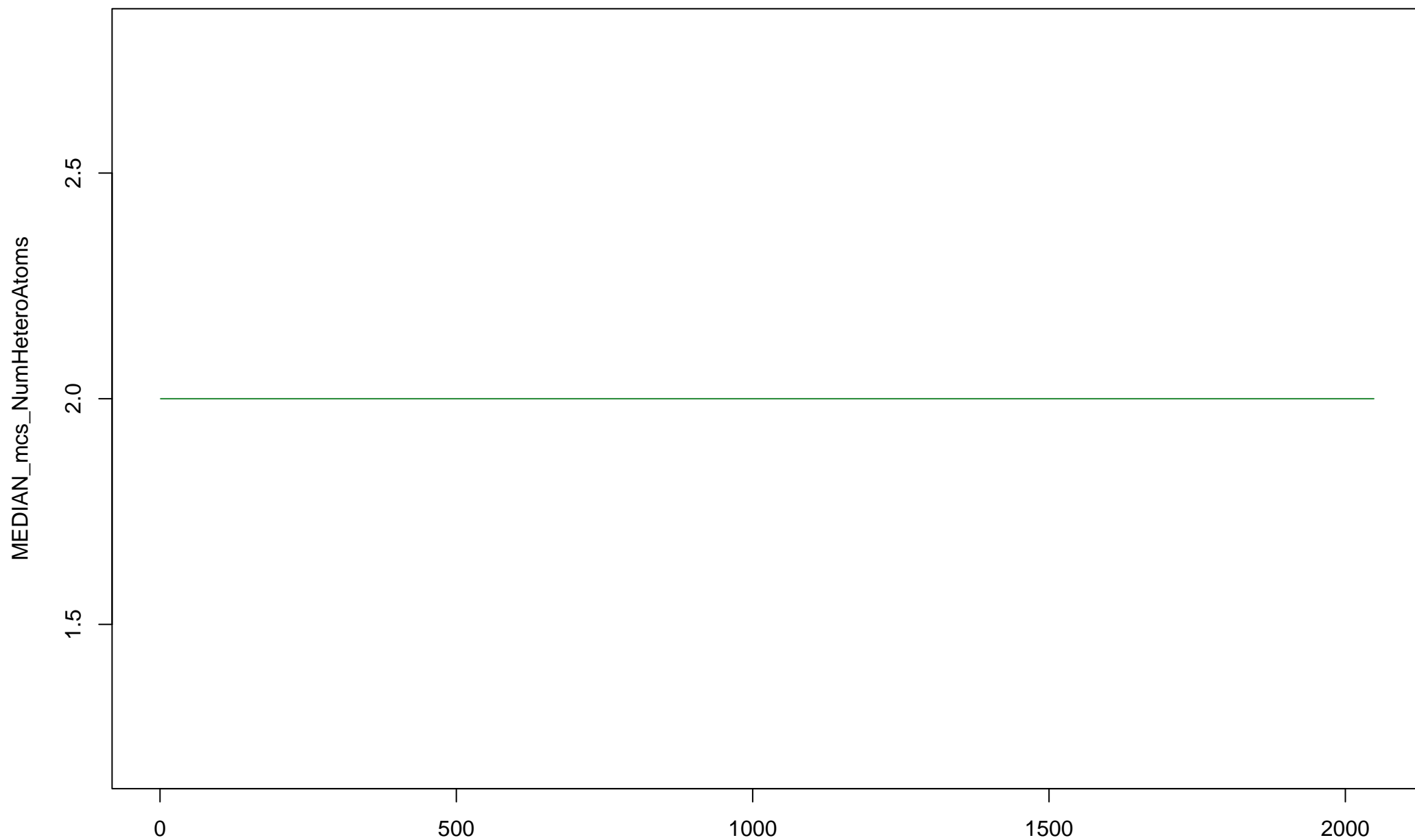
MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



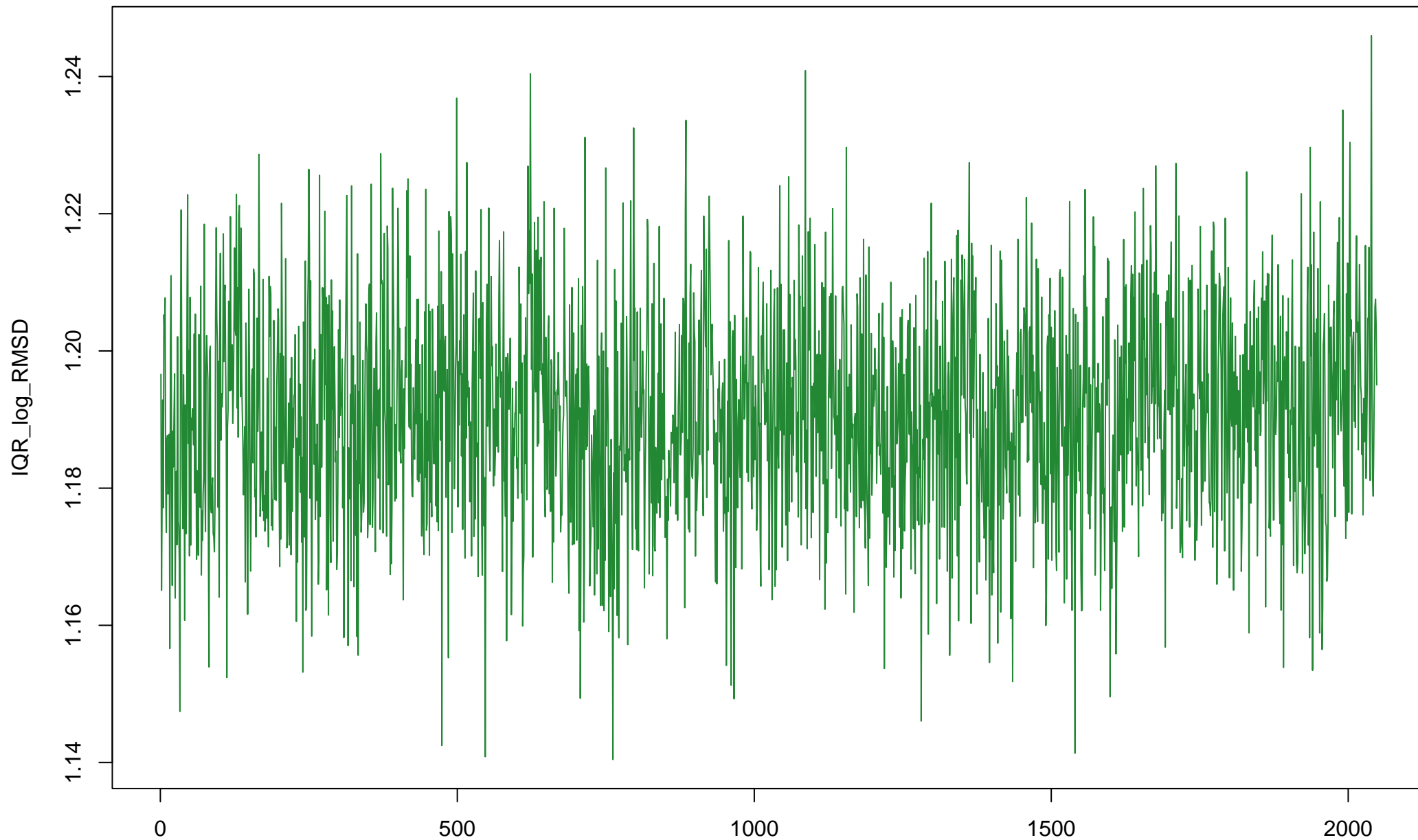
MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



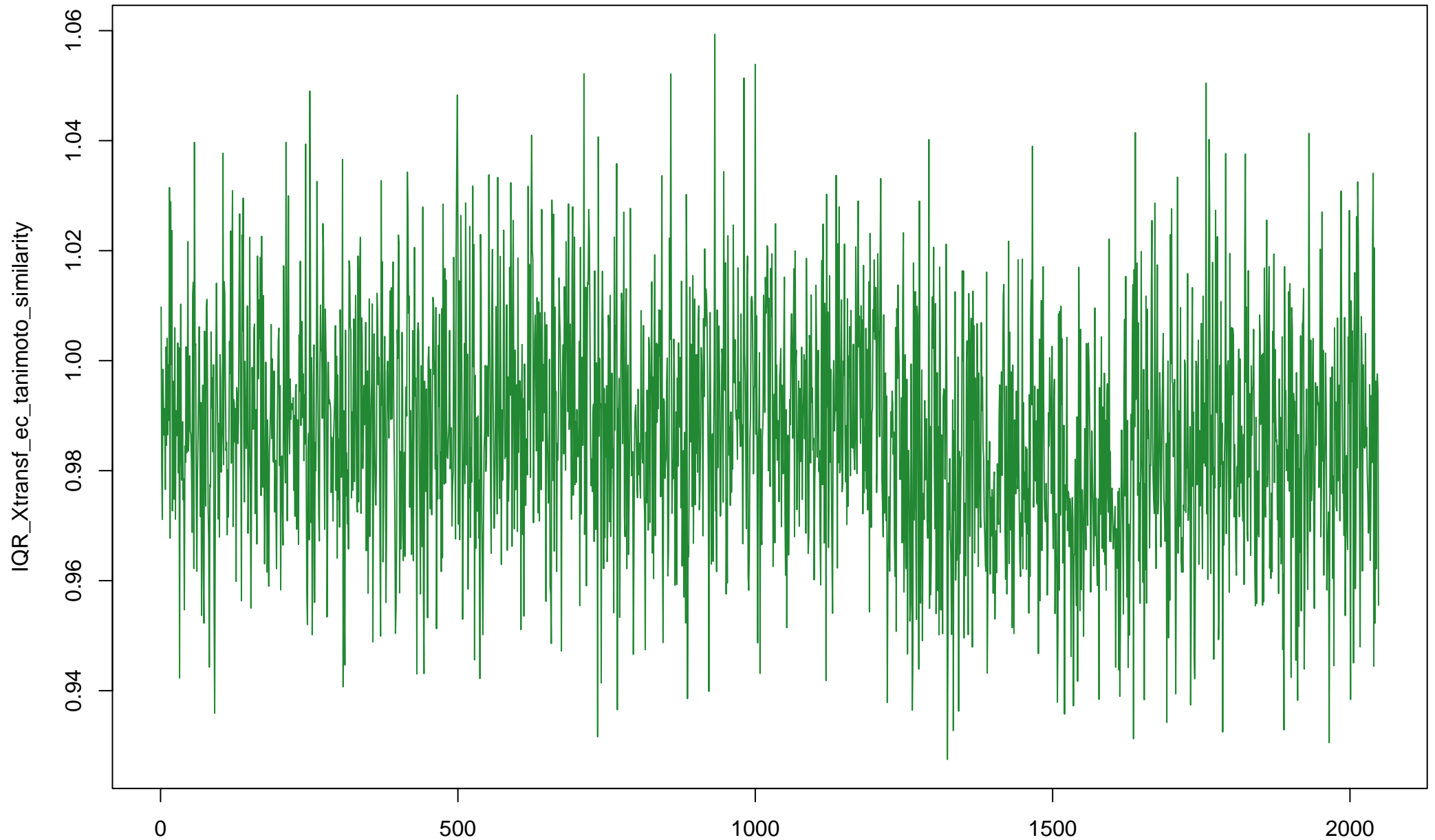
MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



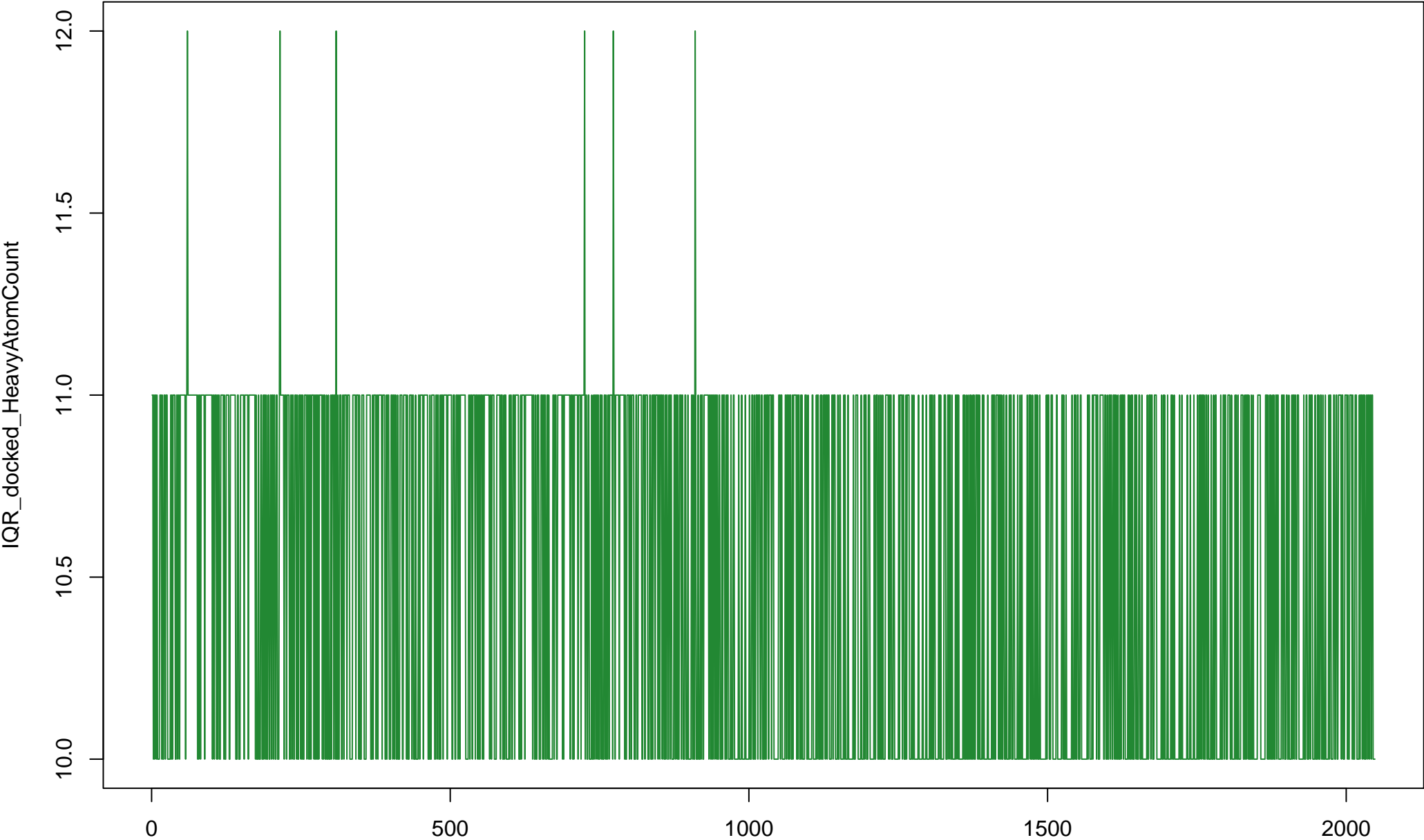
IQR_log_RMSD
ESS = 697 | BMK = 0.048 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0



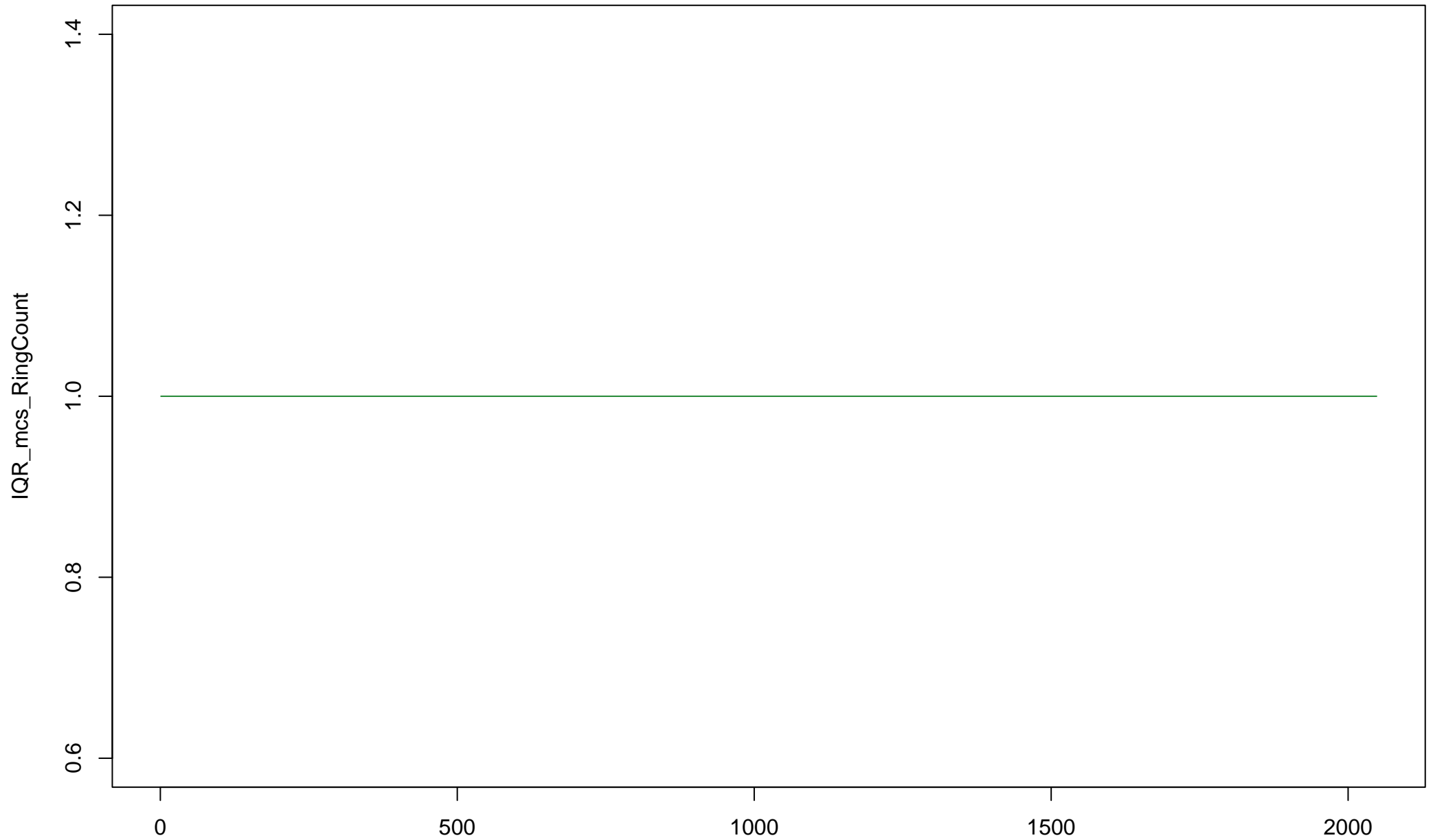
IQR_Xtransf_ec_tanimoto_similarity
ESS = 701 | BMK = 0.12 | MCSE(6.27) = 3.91 | stat: FALSE | burn: 0



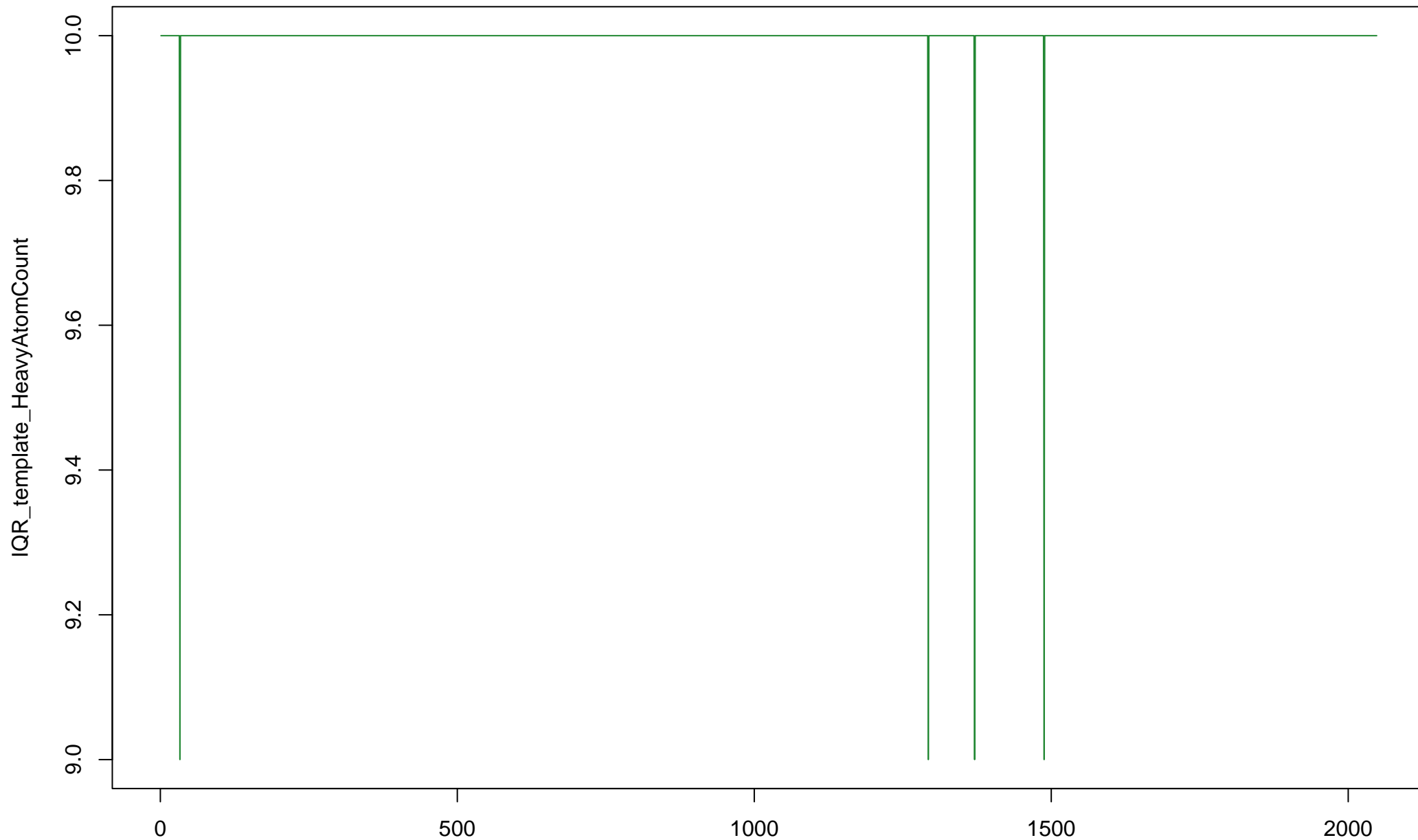
IQR_docked_HeavyAtomCount
ESS = 225 | BMK = 0.151 | MCSE(6.27) = 4.87 | stat: FALSE | burn: 0



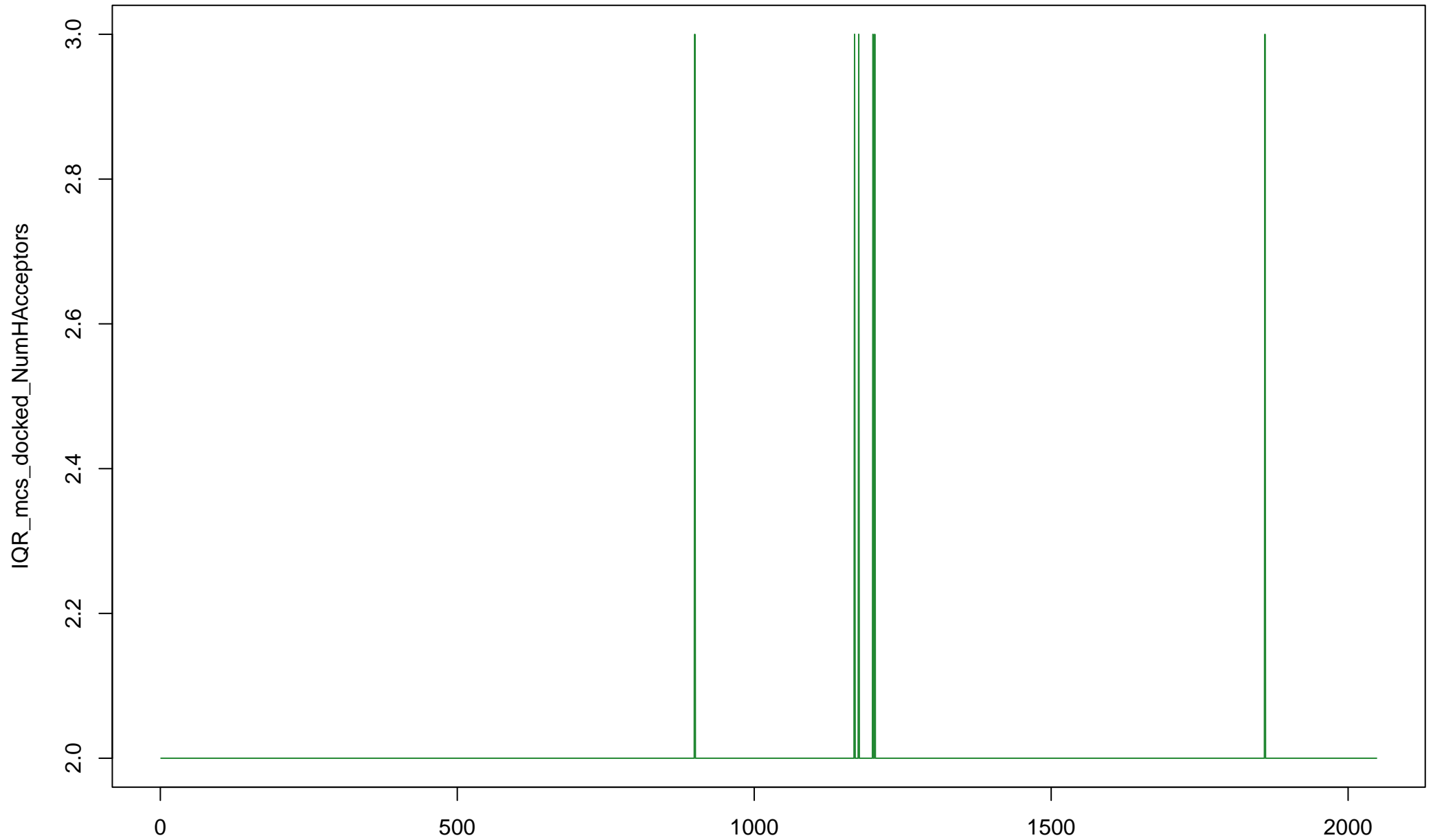
IQR_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



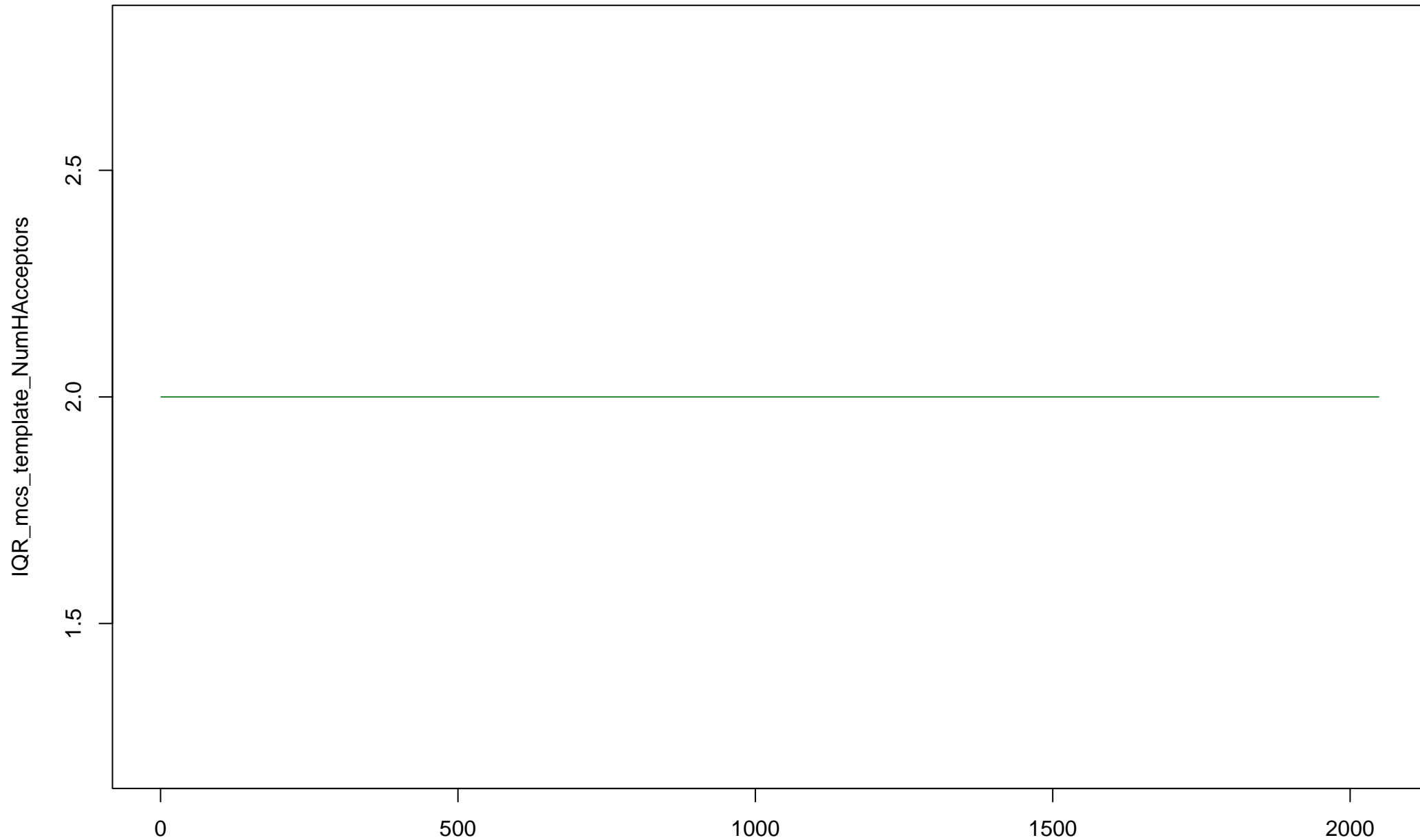
IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1632



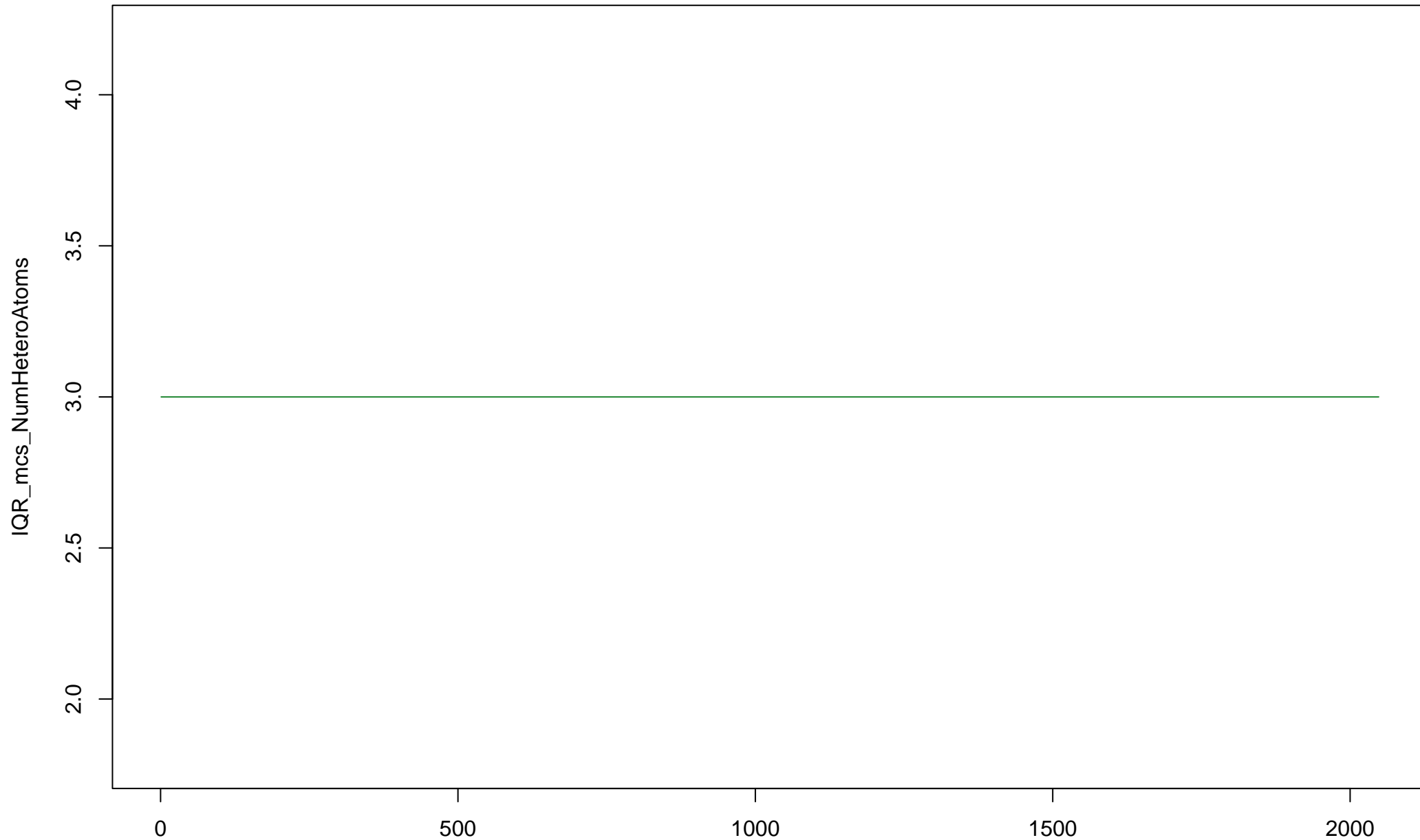
IQR_mcs_docked_NumHAcceptors
ESS = 624 | BMK = 0.264 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 2040



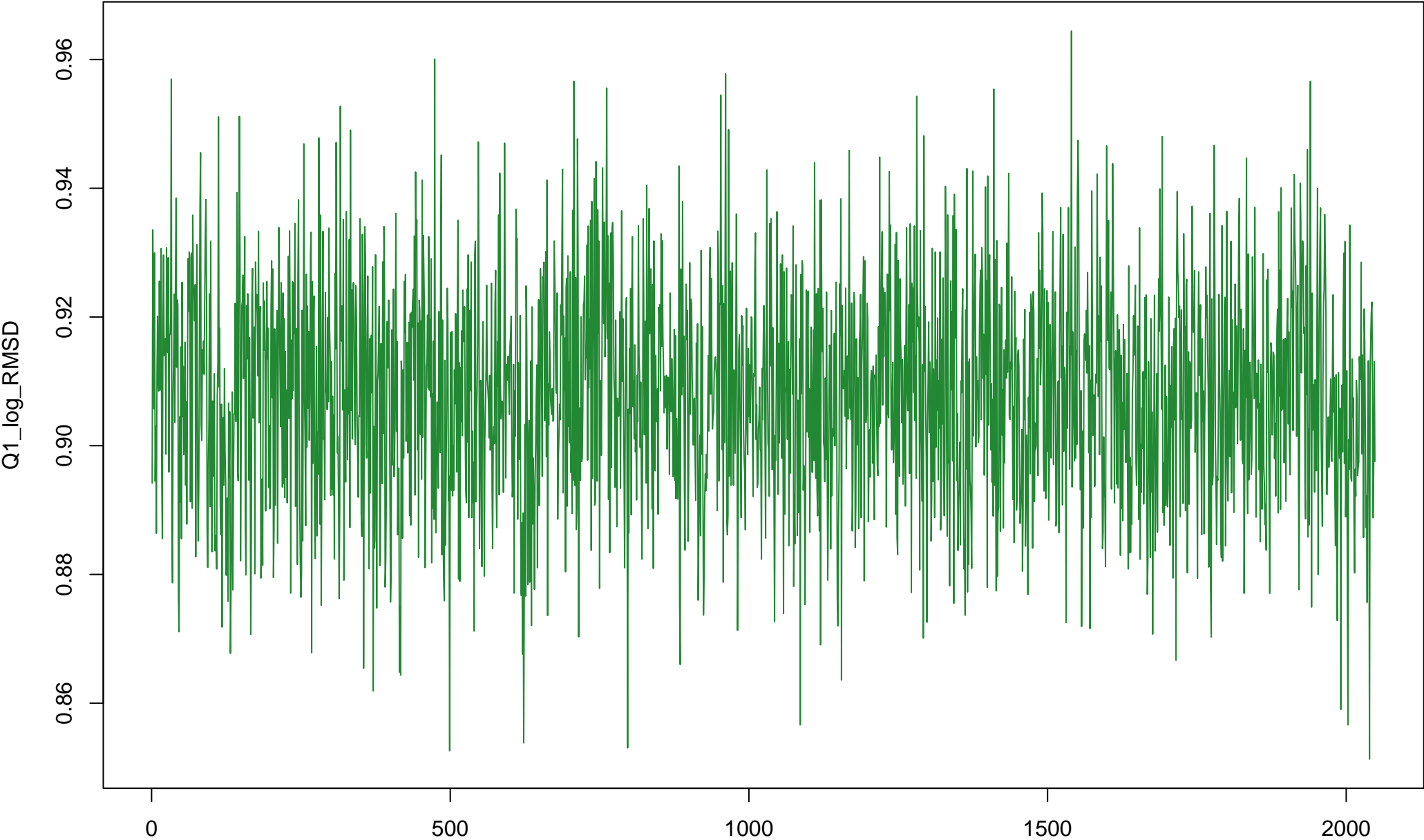
IQR_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



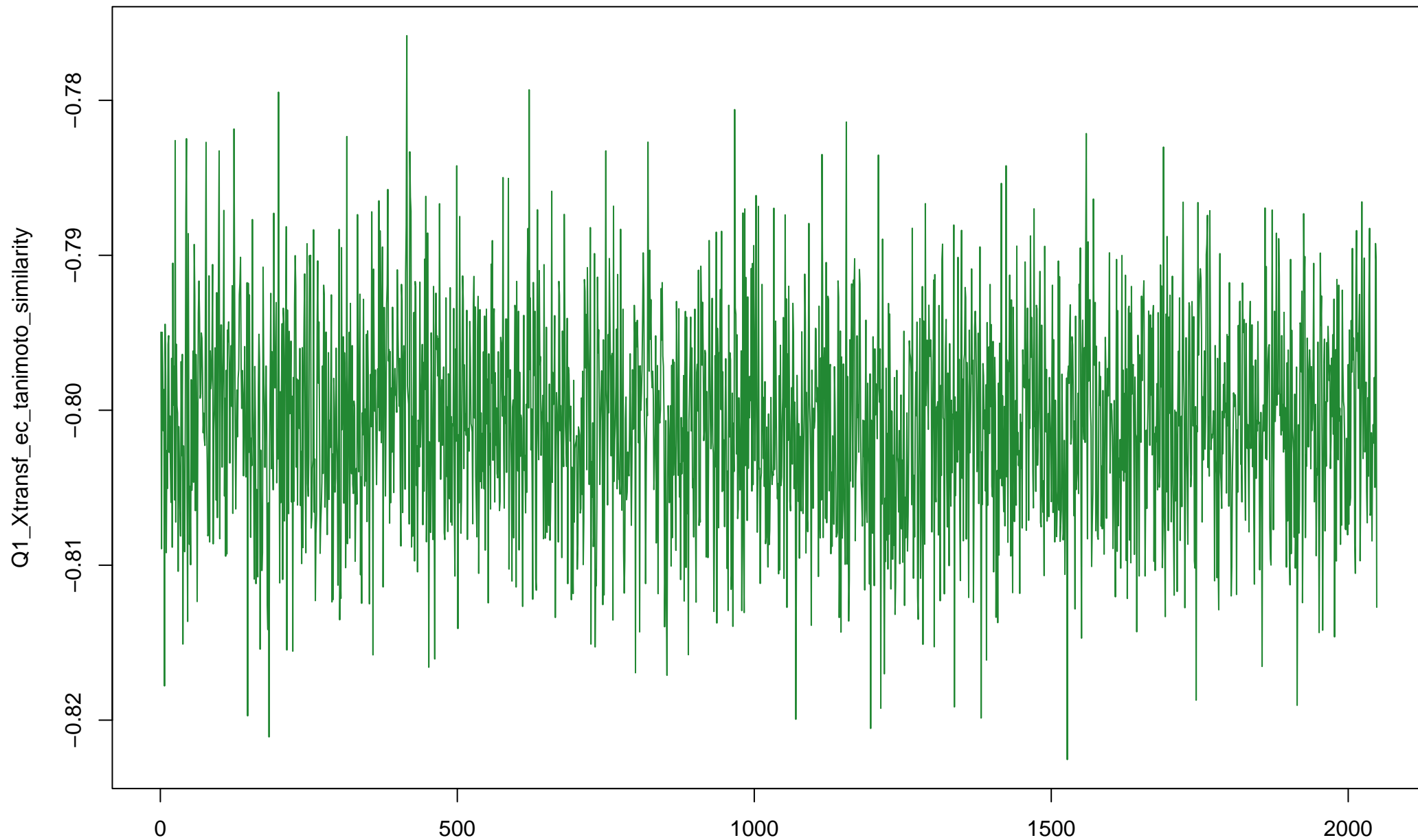
IQR_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



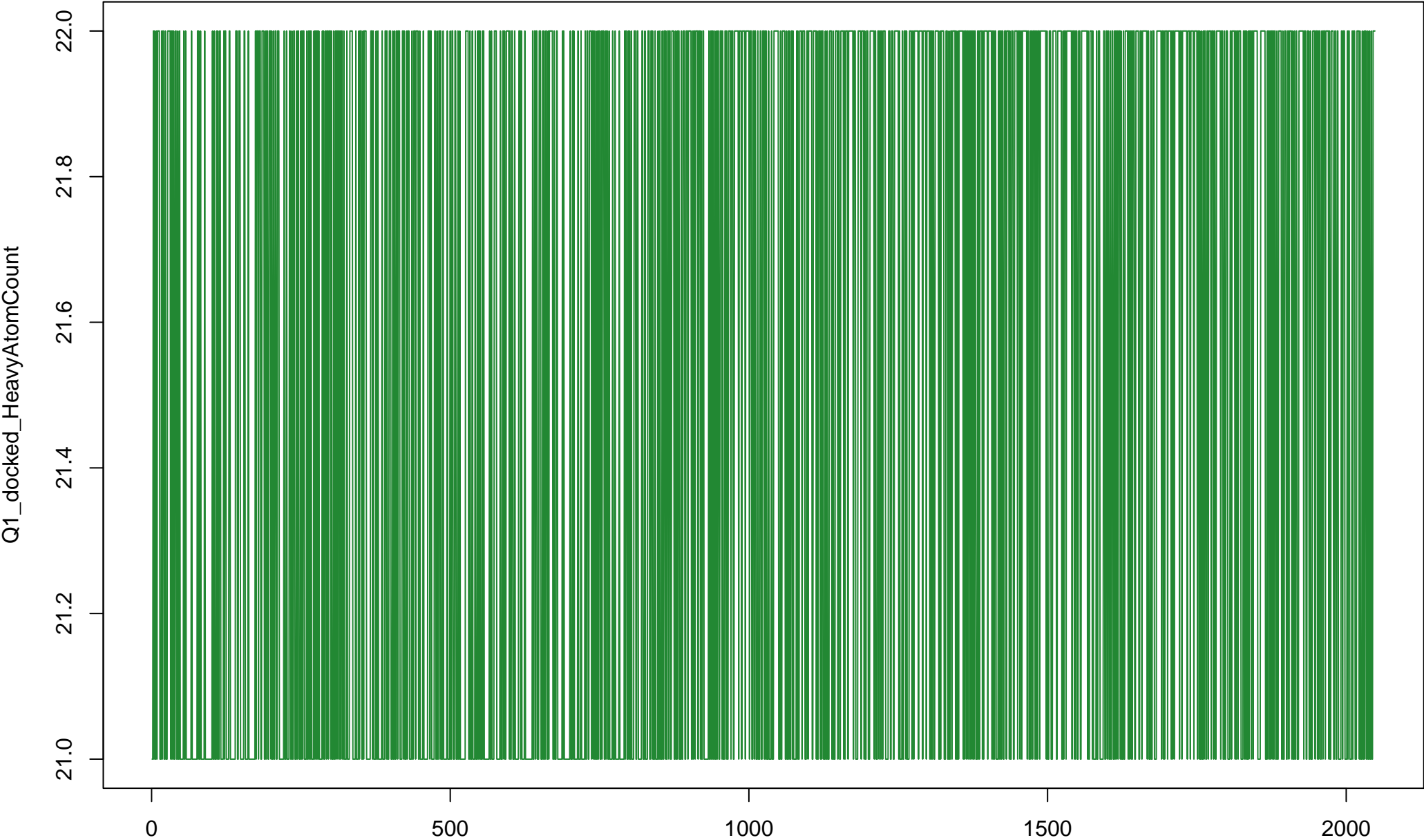
Q1_log_RMSD
ESS = 855 | BMK = 0.0473 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0



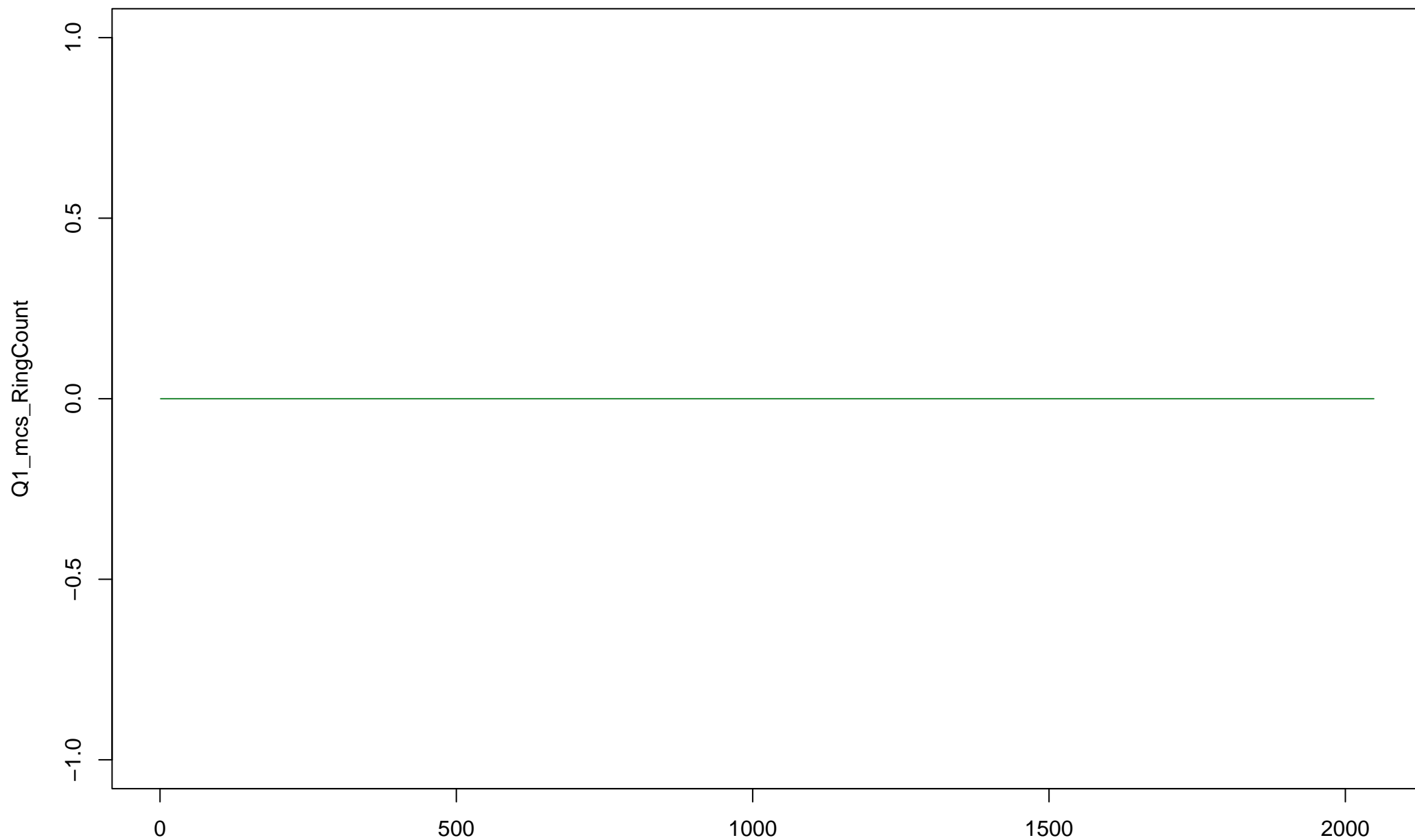
Q1_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.05 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0



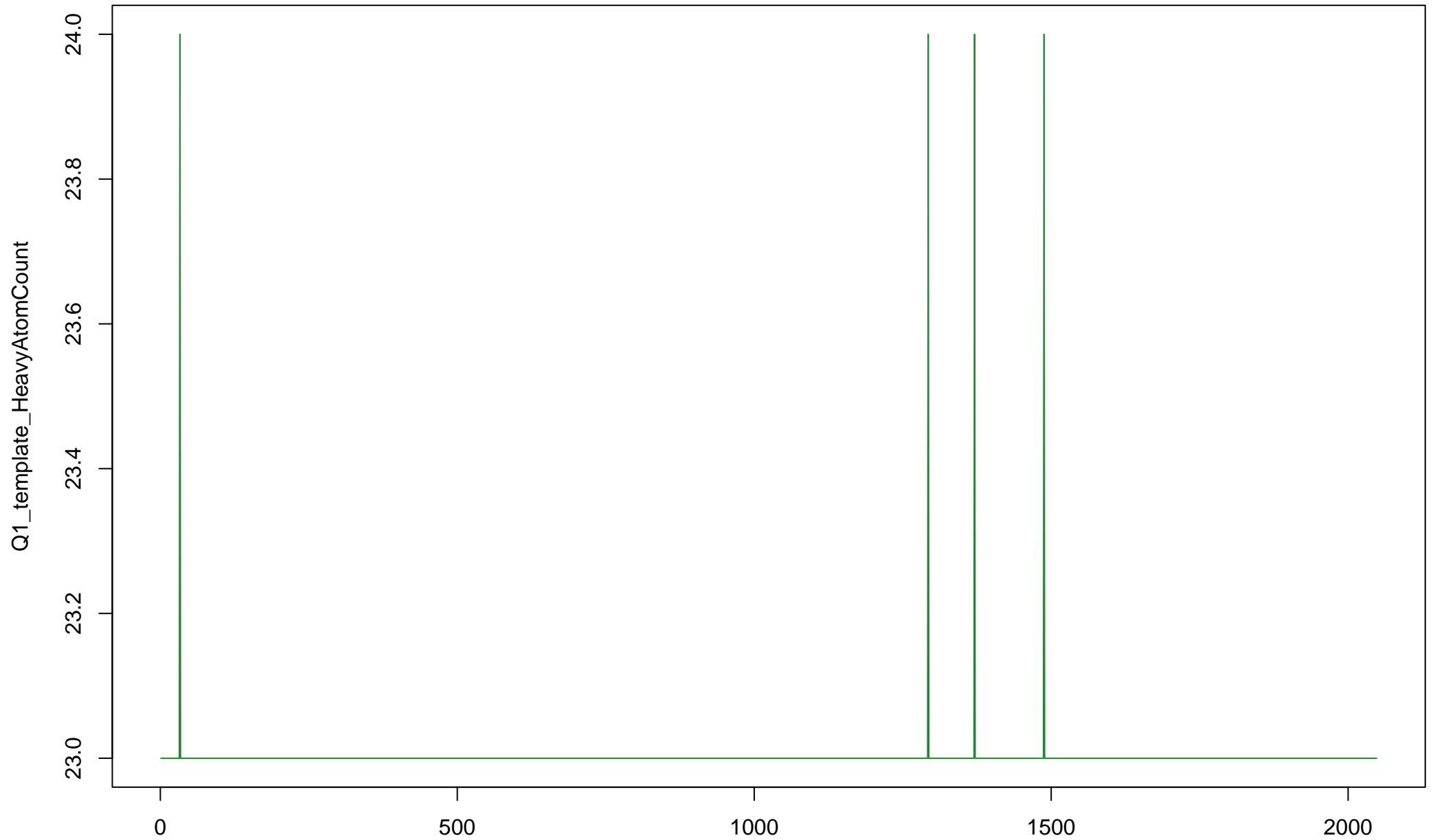
Q1_docked_HeavyAtomCount
ESS = 257 | BMK = 0.116 | MCSE(6.27) = 4.72 | stat: FALSE | burn: 0



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



Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1632



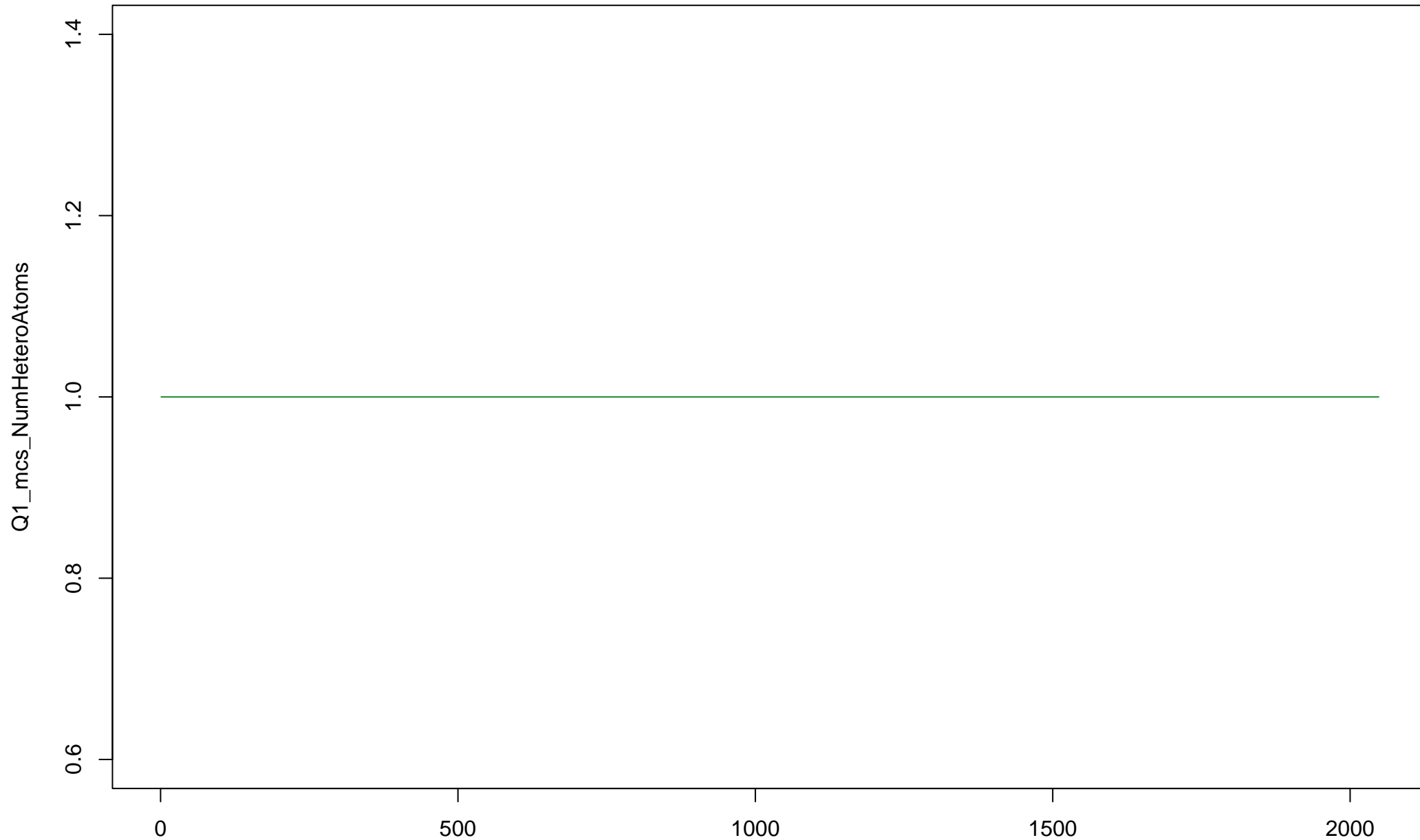
Q1_mcs_docked_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



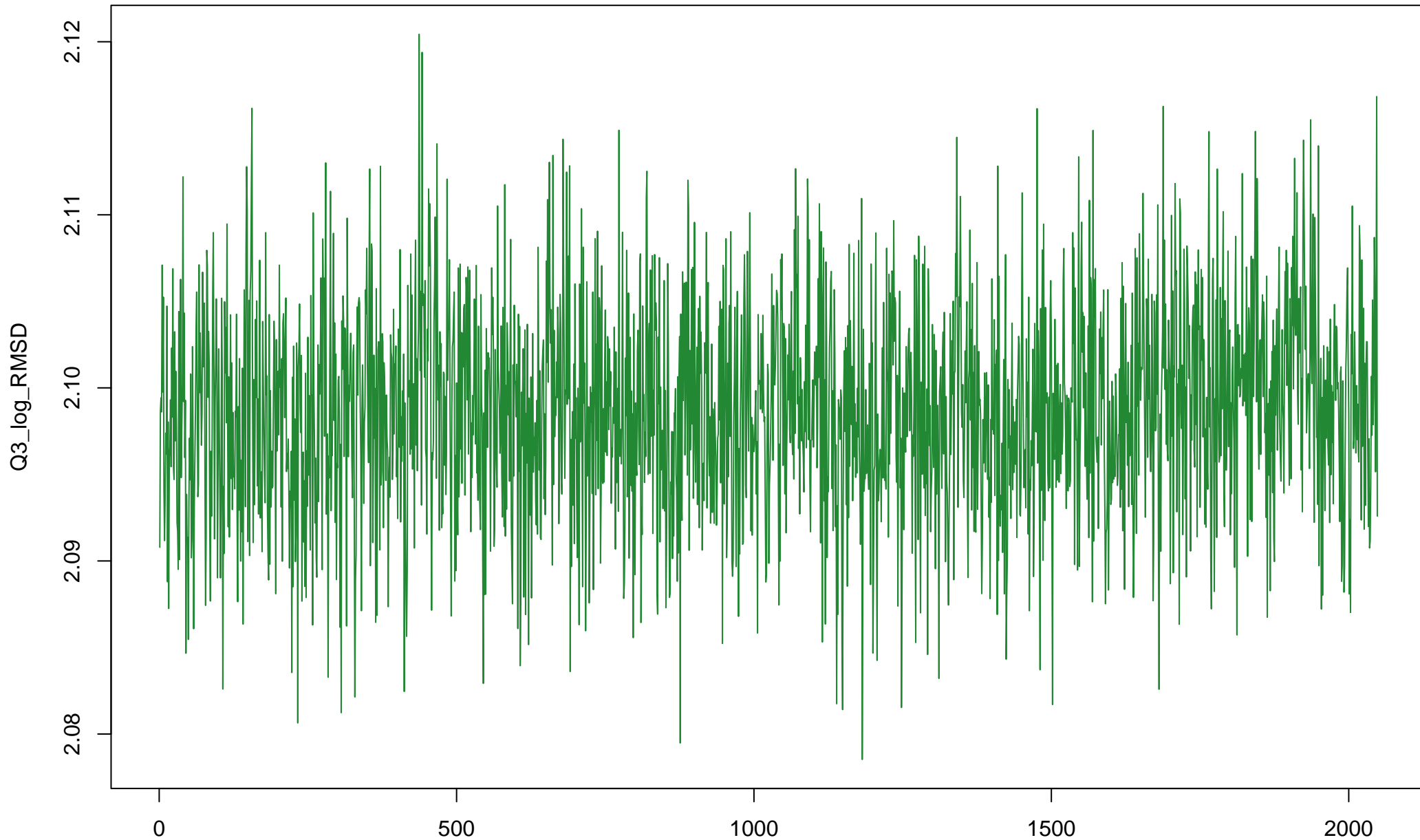
Q1_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



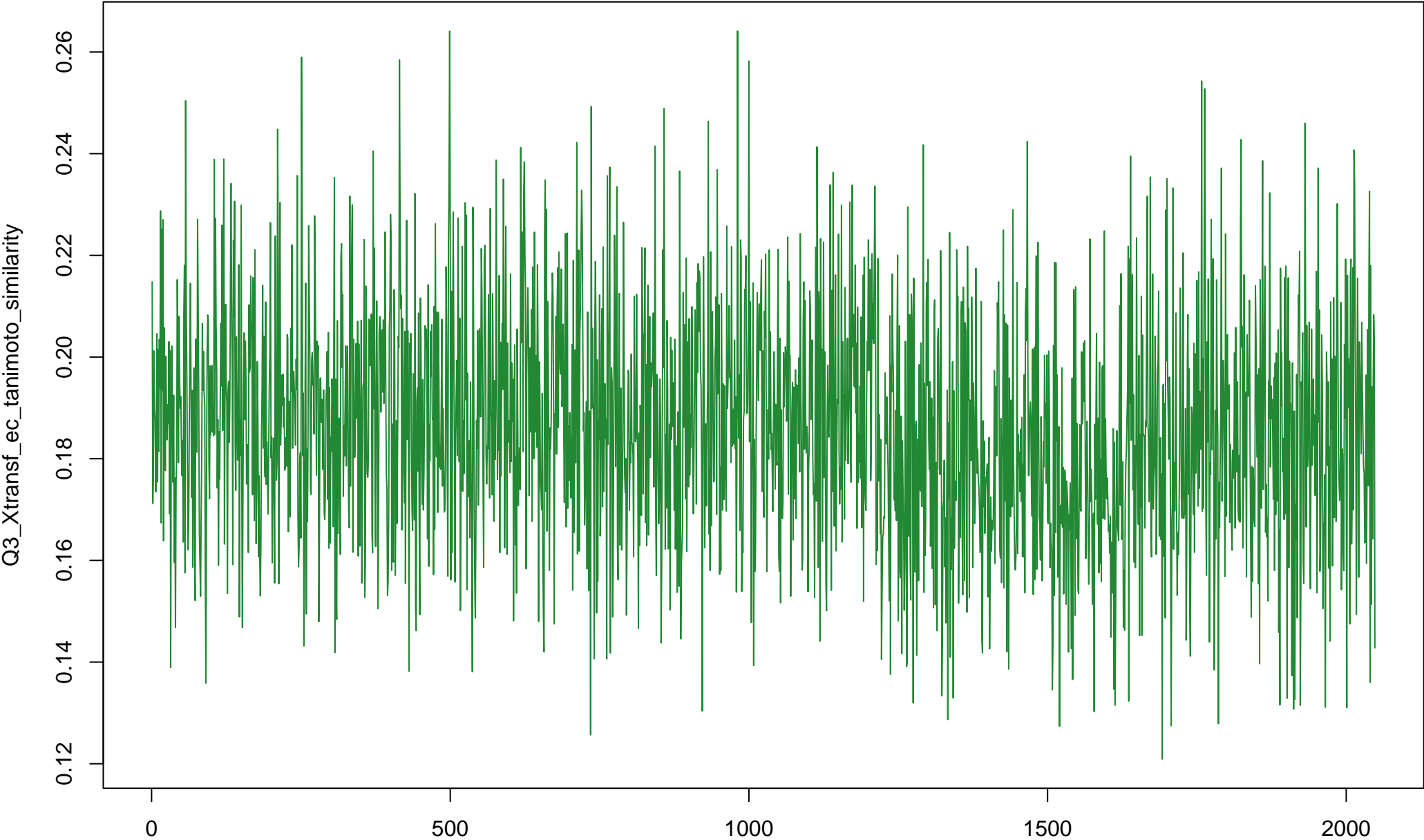
Q1_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



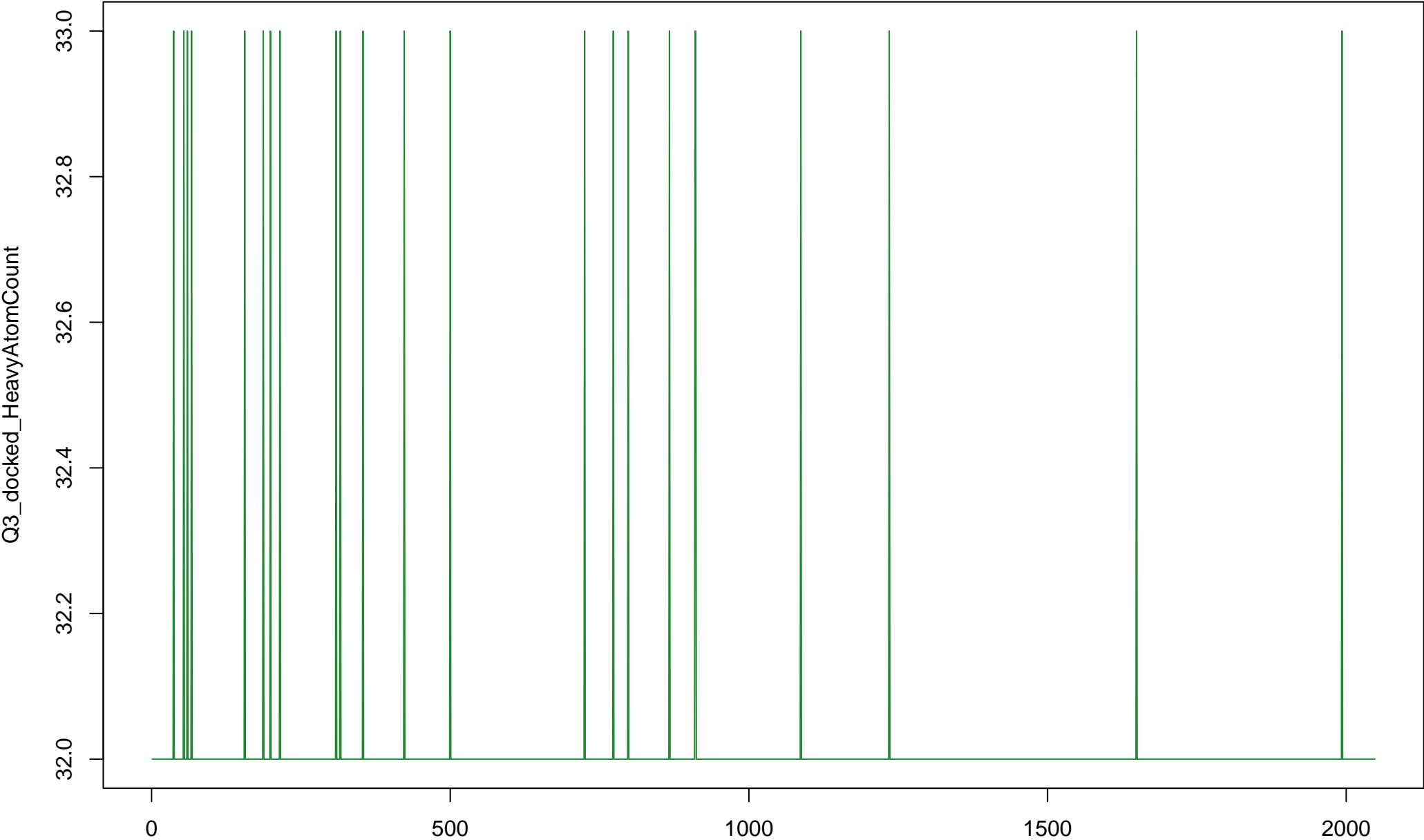
Q3_log_RMSD
ESS = 963 | BMK = 0.0532 | MCSE(6.27) = 3.19 | stat: FALSE | burn: 0



Q3_Xtransf_ec_tanimoto_similarity
ESS = 738 | BMK = 0.121 | MCSE(6.27) = 3.73 | stat: FALSE | burn: 0



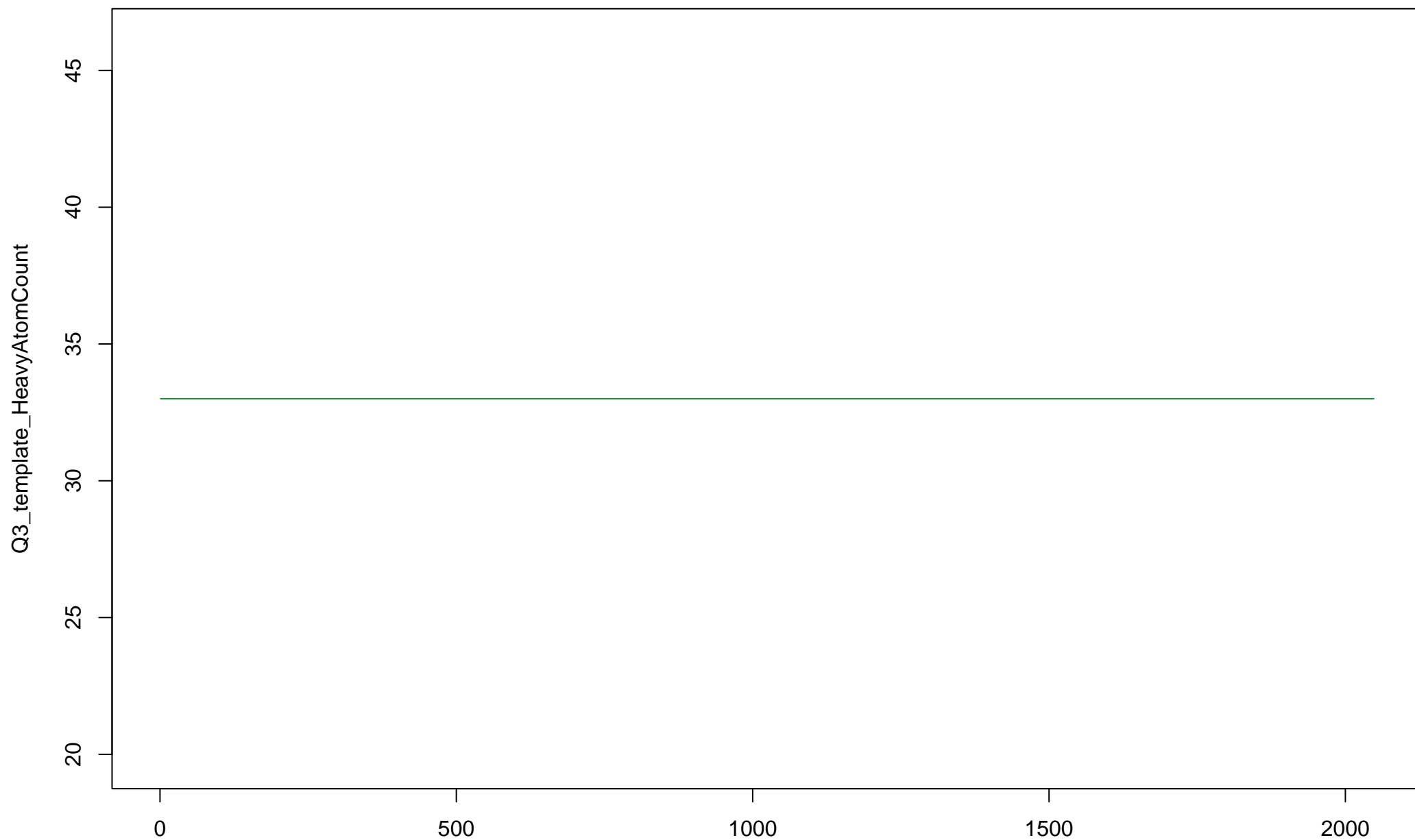
Q3_docked_HeavyAtomCount
ESS = 1690 | BMK = 0.256 | MCSE(6.27) = 2.55 | stat: FALSE | burn: 1632



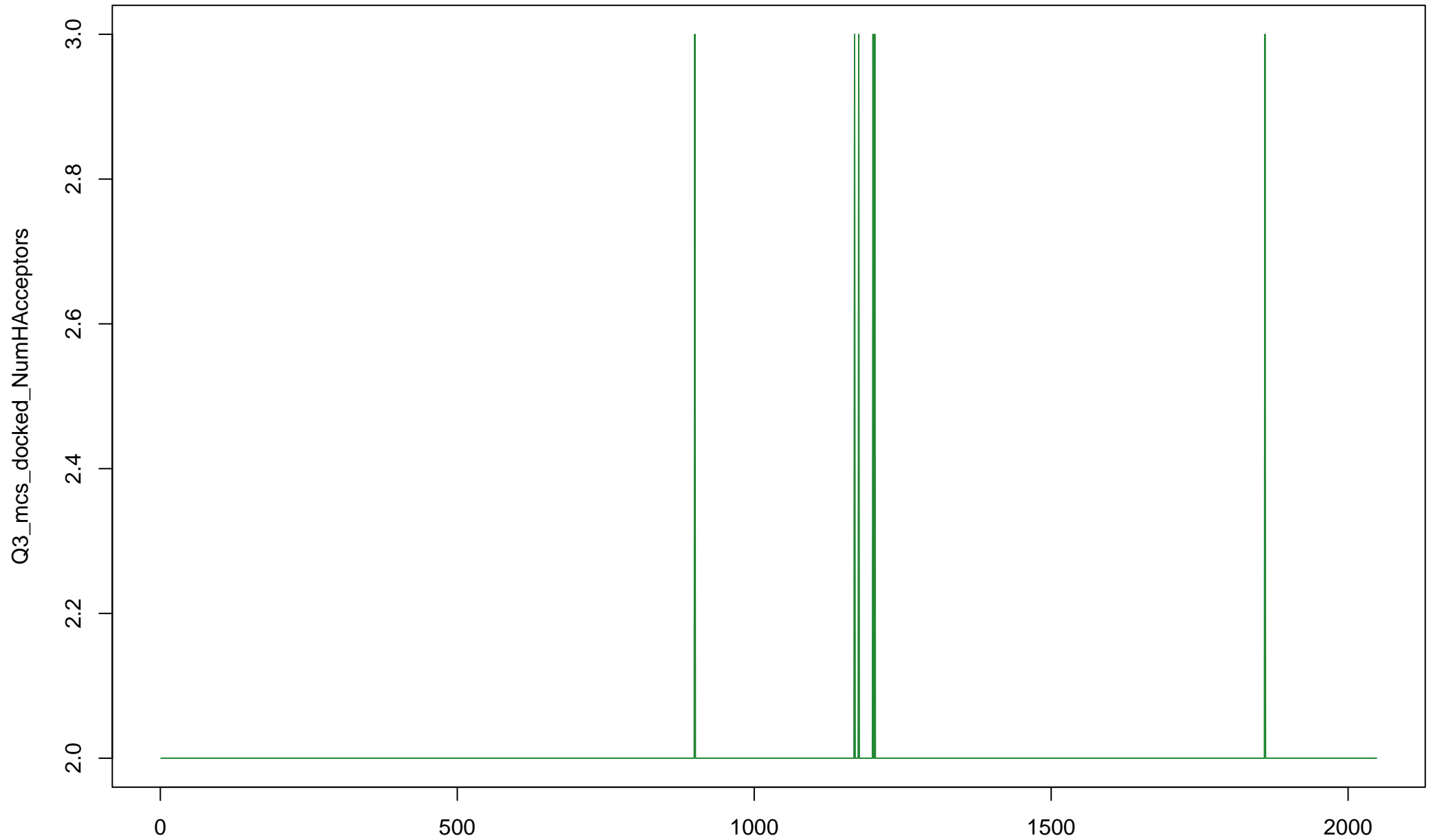
Q3_mcs_RingCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



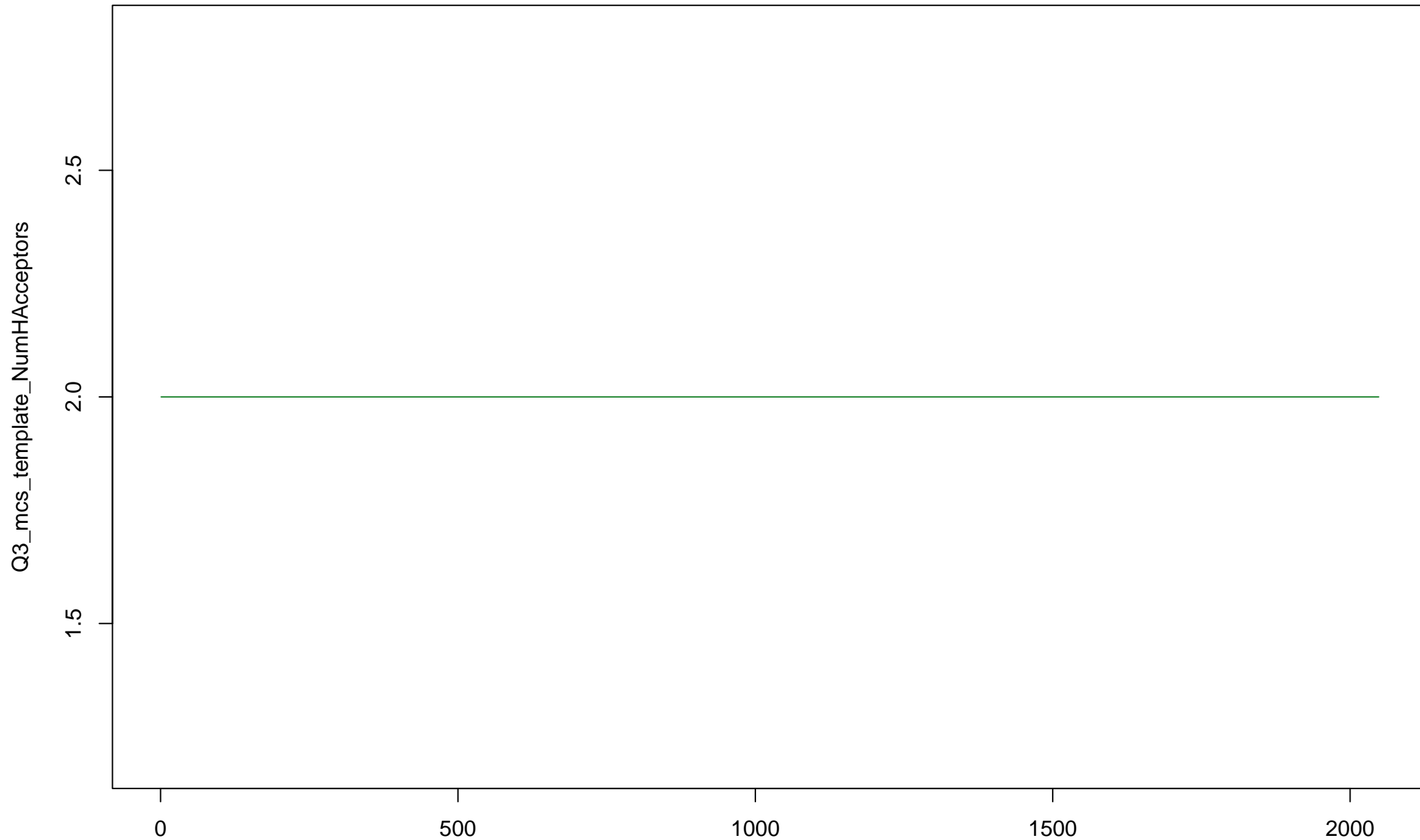
Q3_template_HeavyAtomCount
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



Q3_mcs_docked_NumHAcceptors
ESS = 624 | BMK = 0.264 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 2040



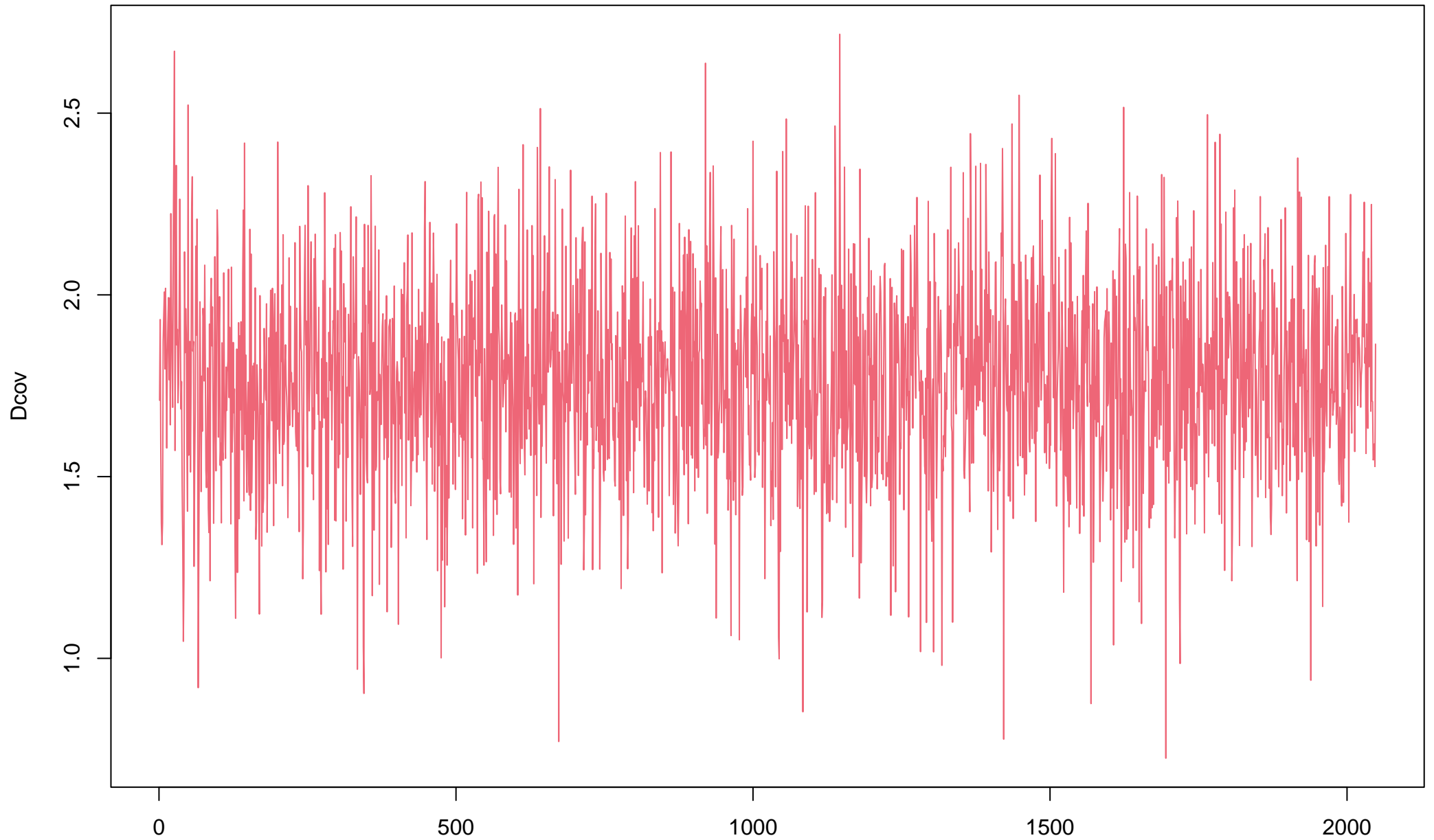
Q3_mcs_template_NumHAcceptors
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



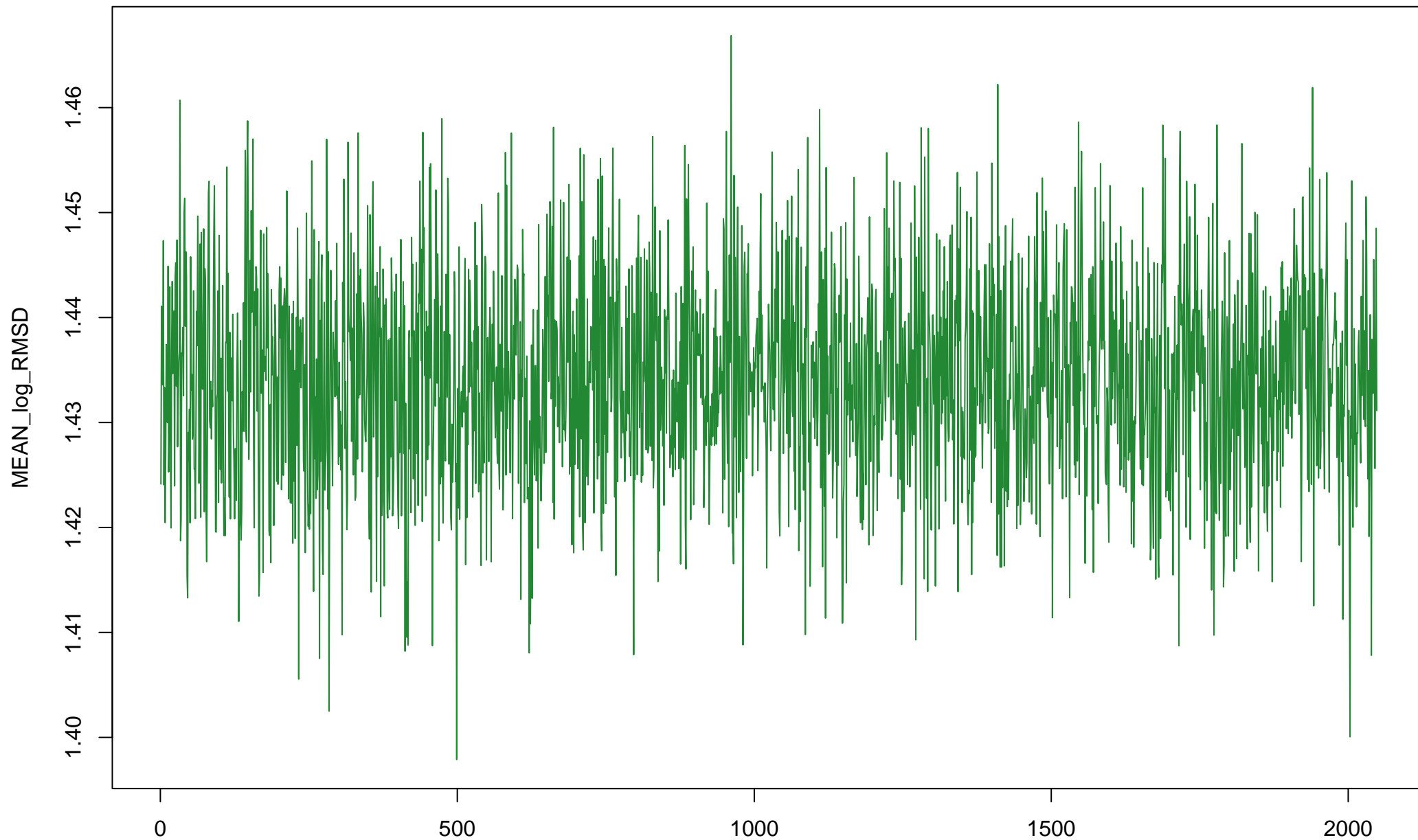
Q3_mcs_NumHeteroAtoms
ESS = 2.22e-16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0



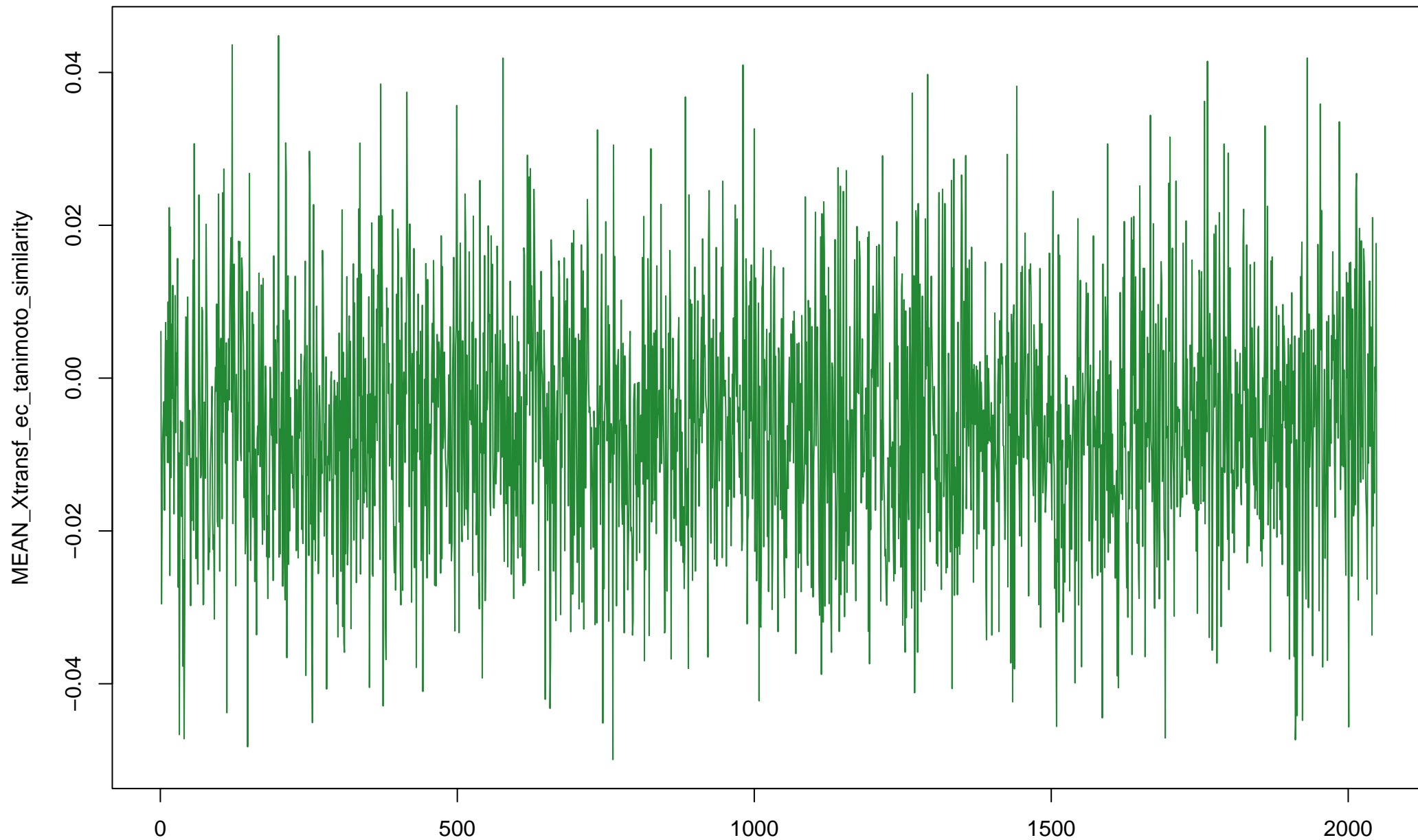
Dcov
ESS = 2050 | BMK = 0.0494 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0



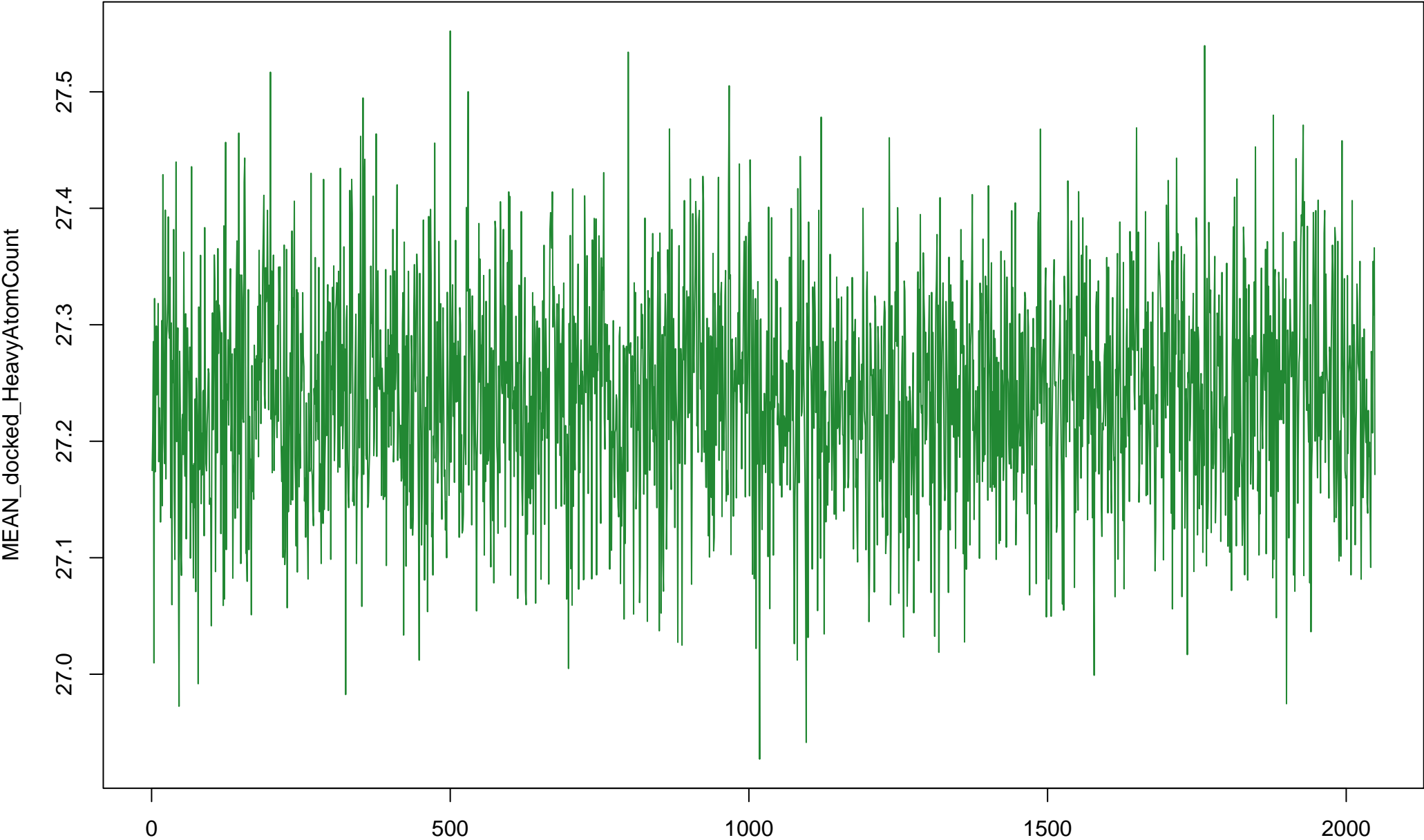
MEAN_log_RMSD
ESS = 2050 | BMK = 0.0404 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0



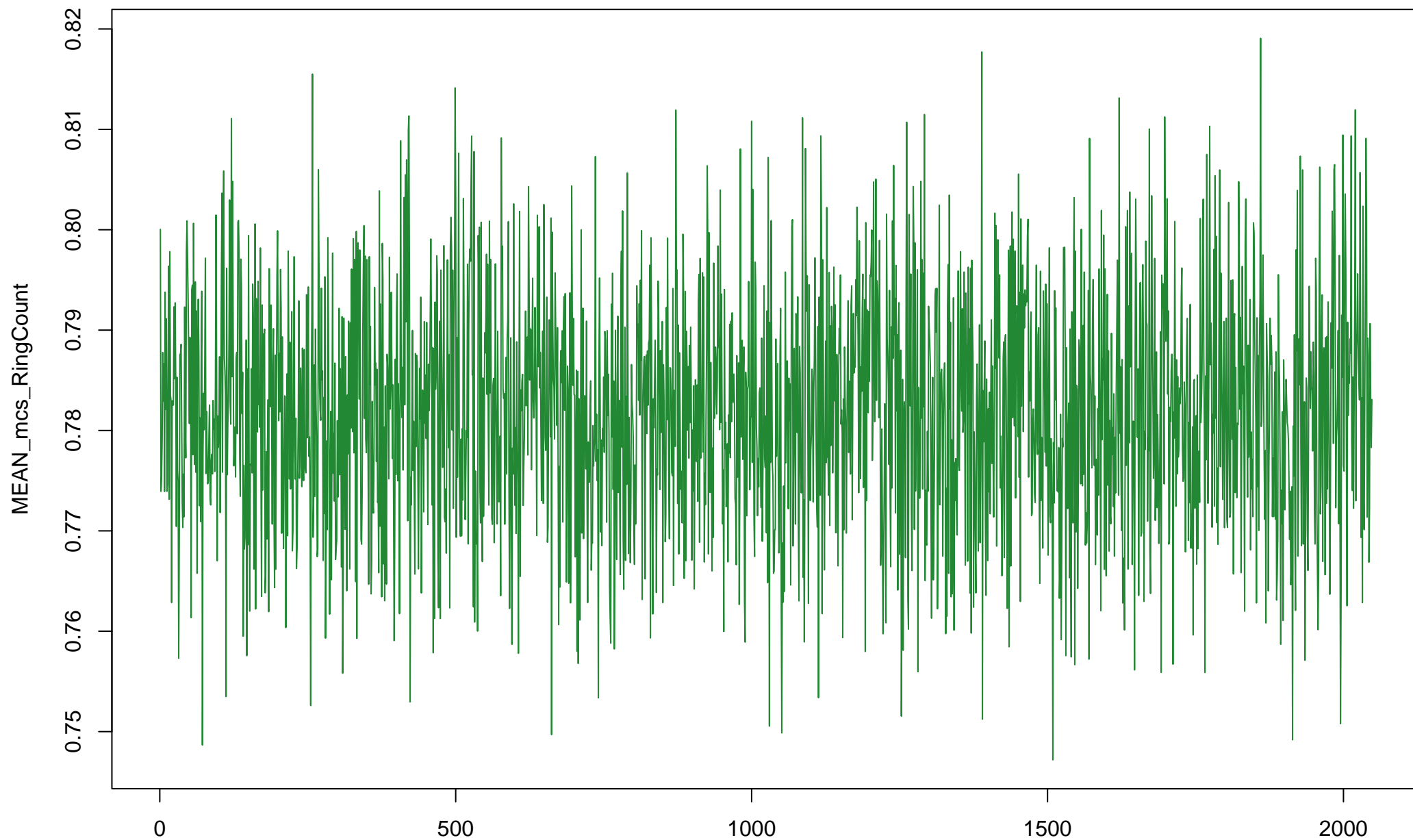
MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0322 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0



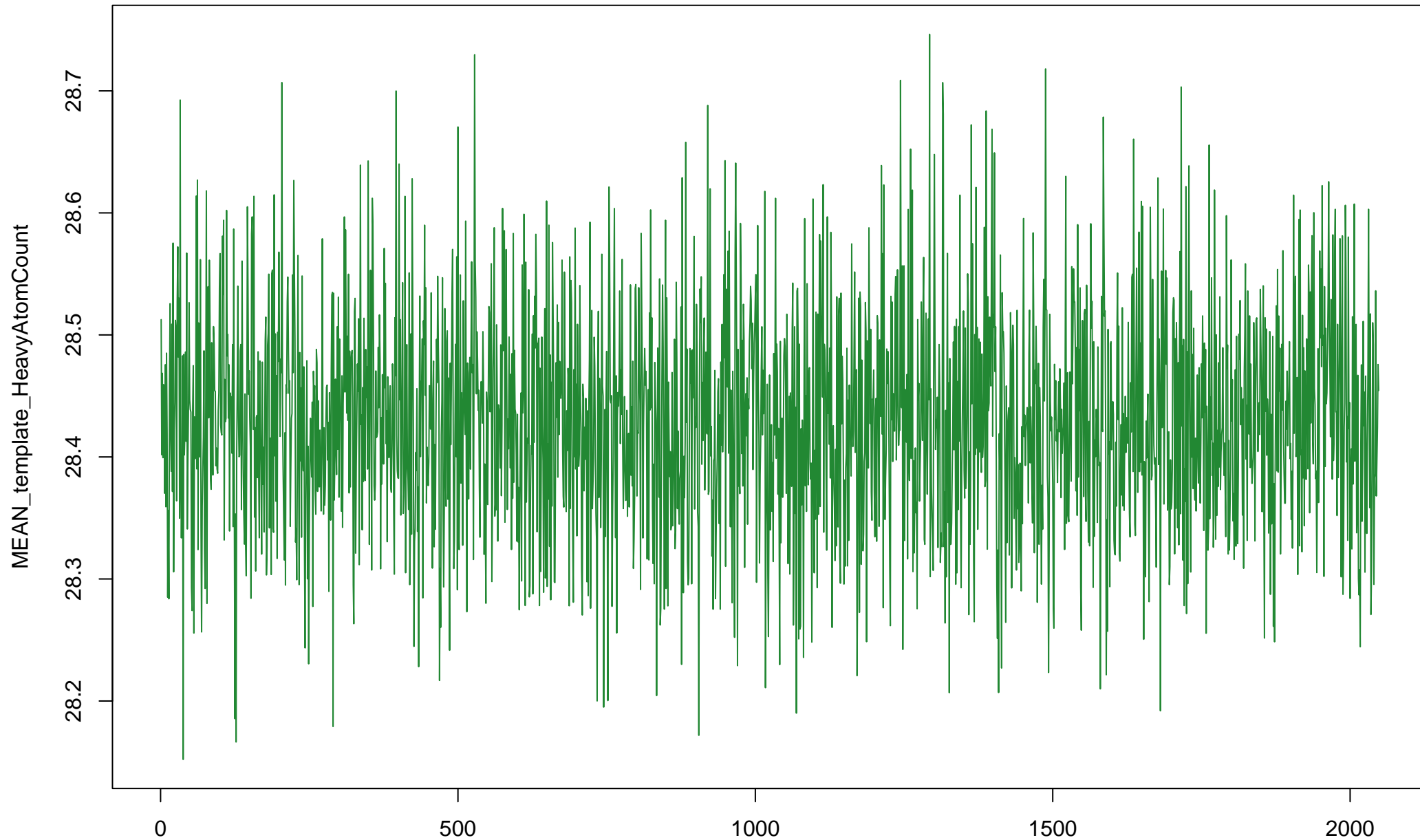
MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0366 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0



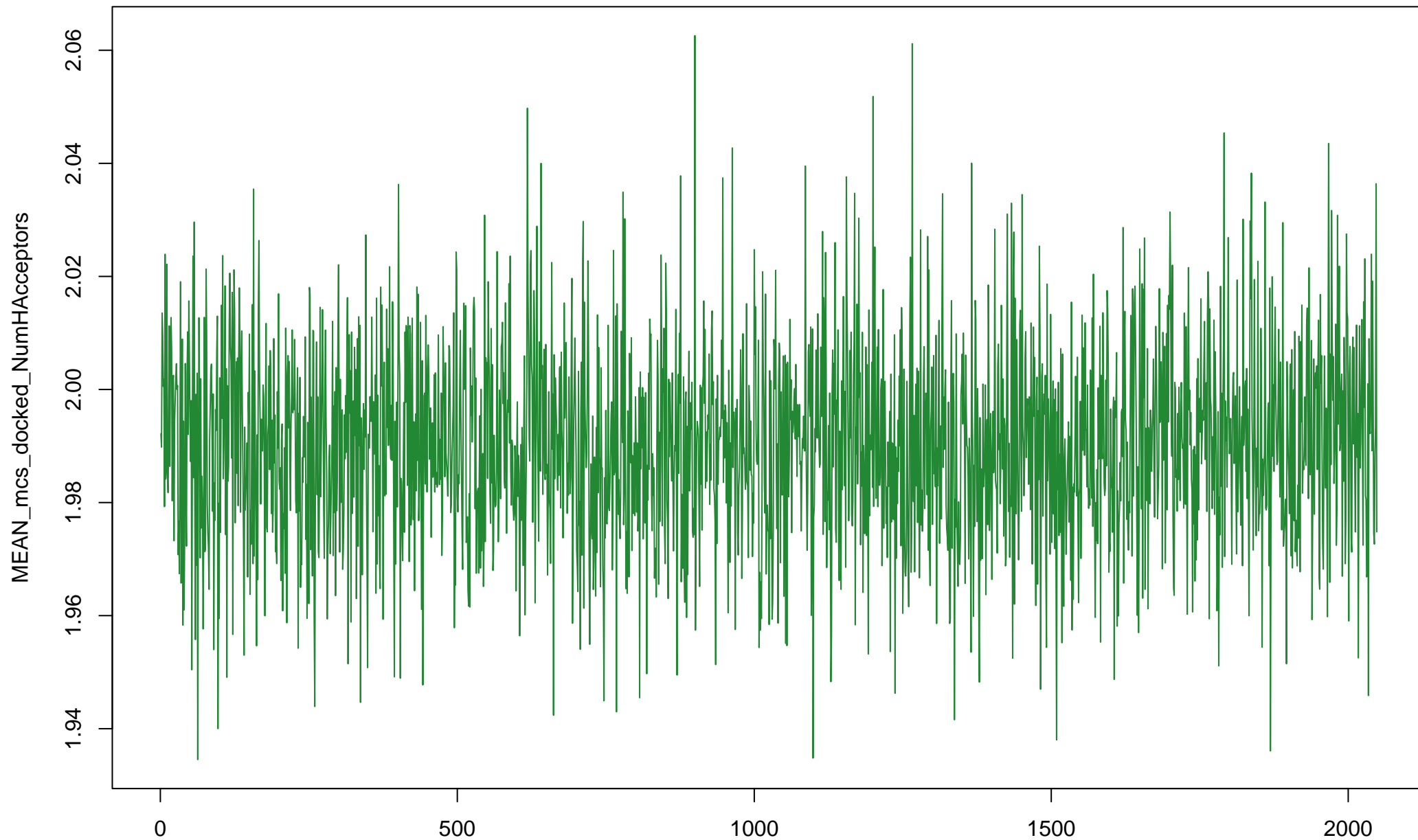
MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0438 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0



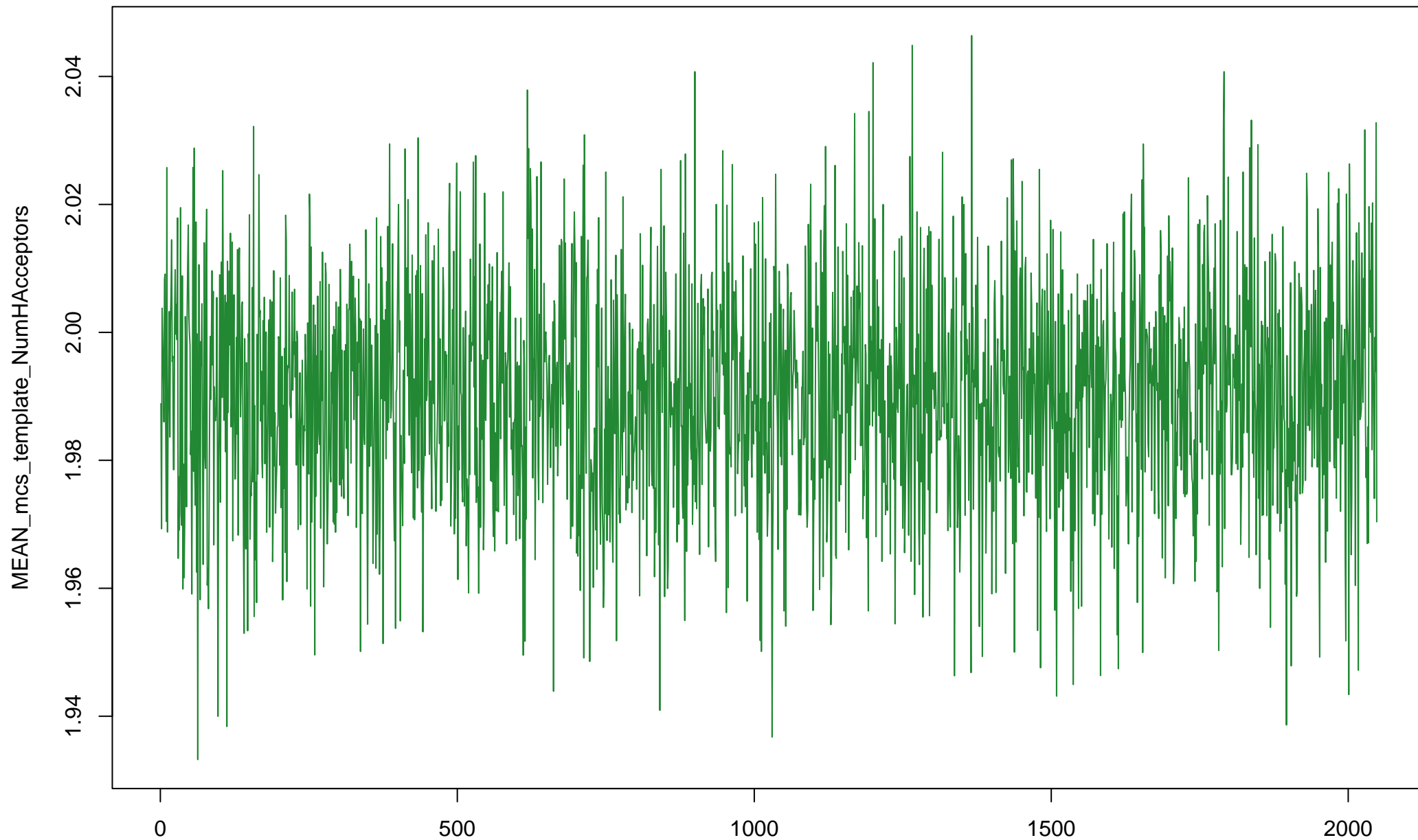
MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0514 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0



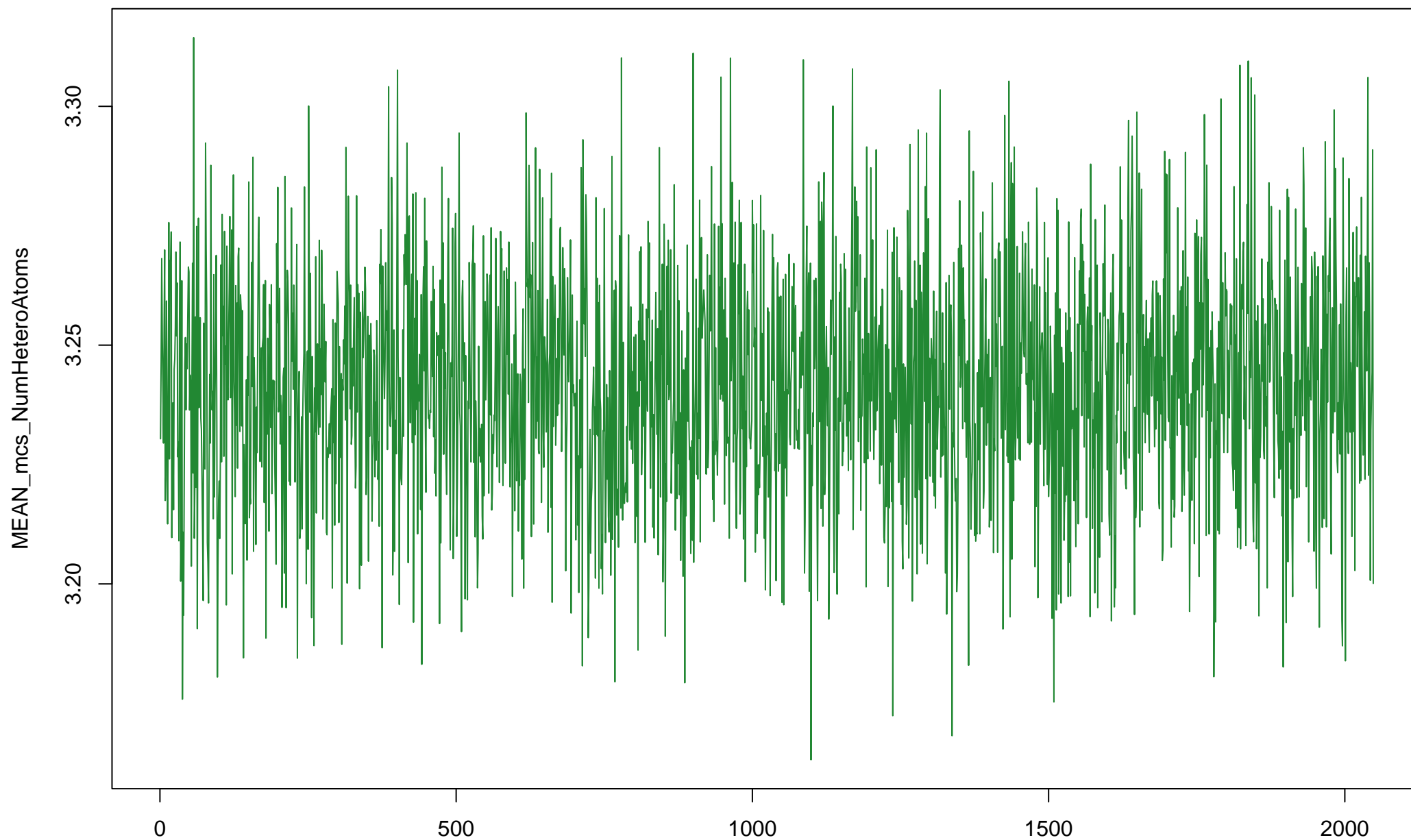
MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0333 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0



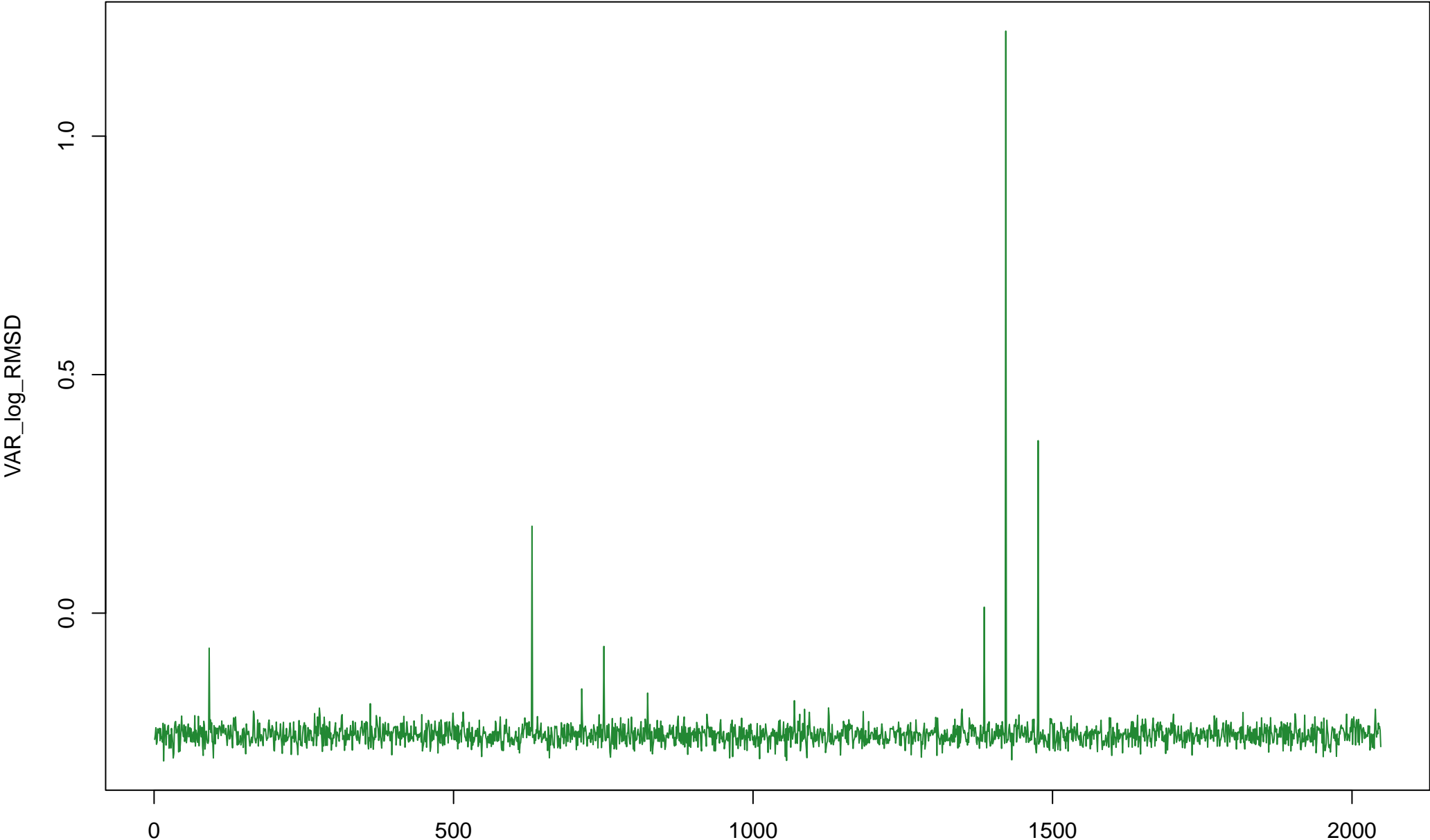
MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0429 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



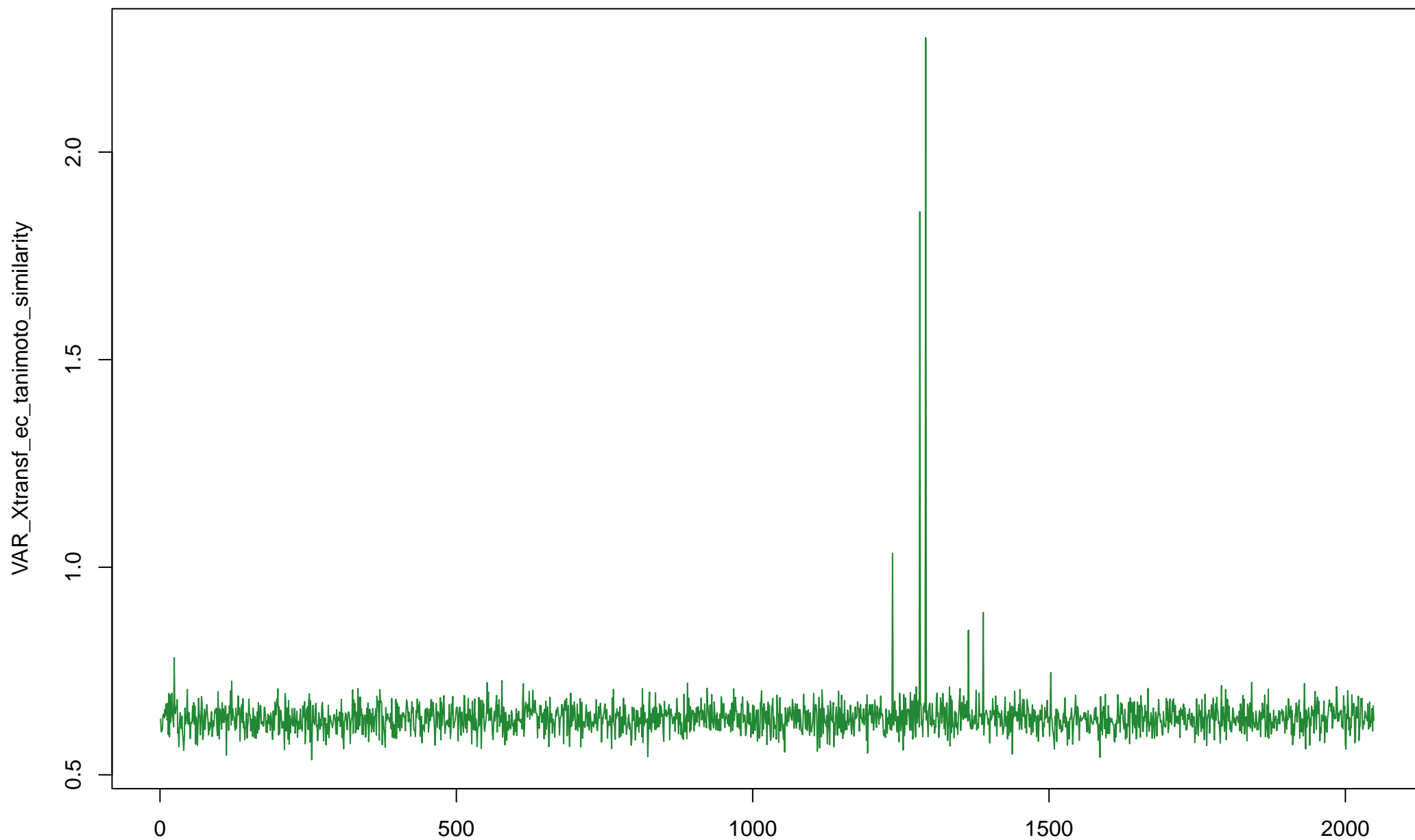
MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0465 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0



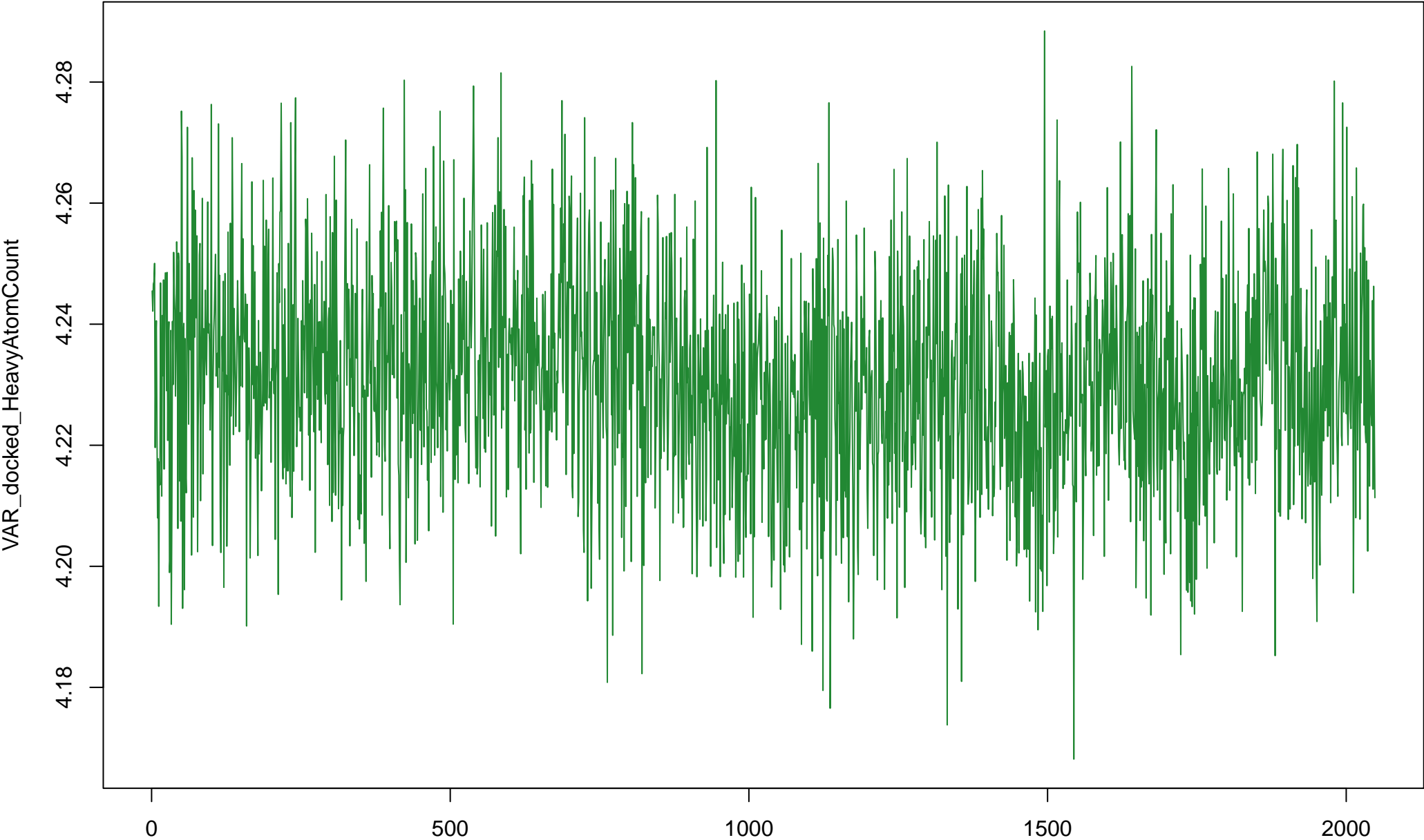
VAR_log_RMSD
ESS = 2050 | BMK = 0.0692 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0



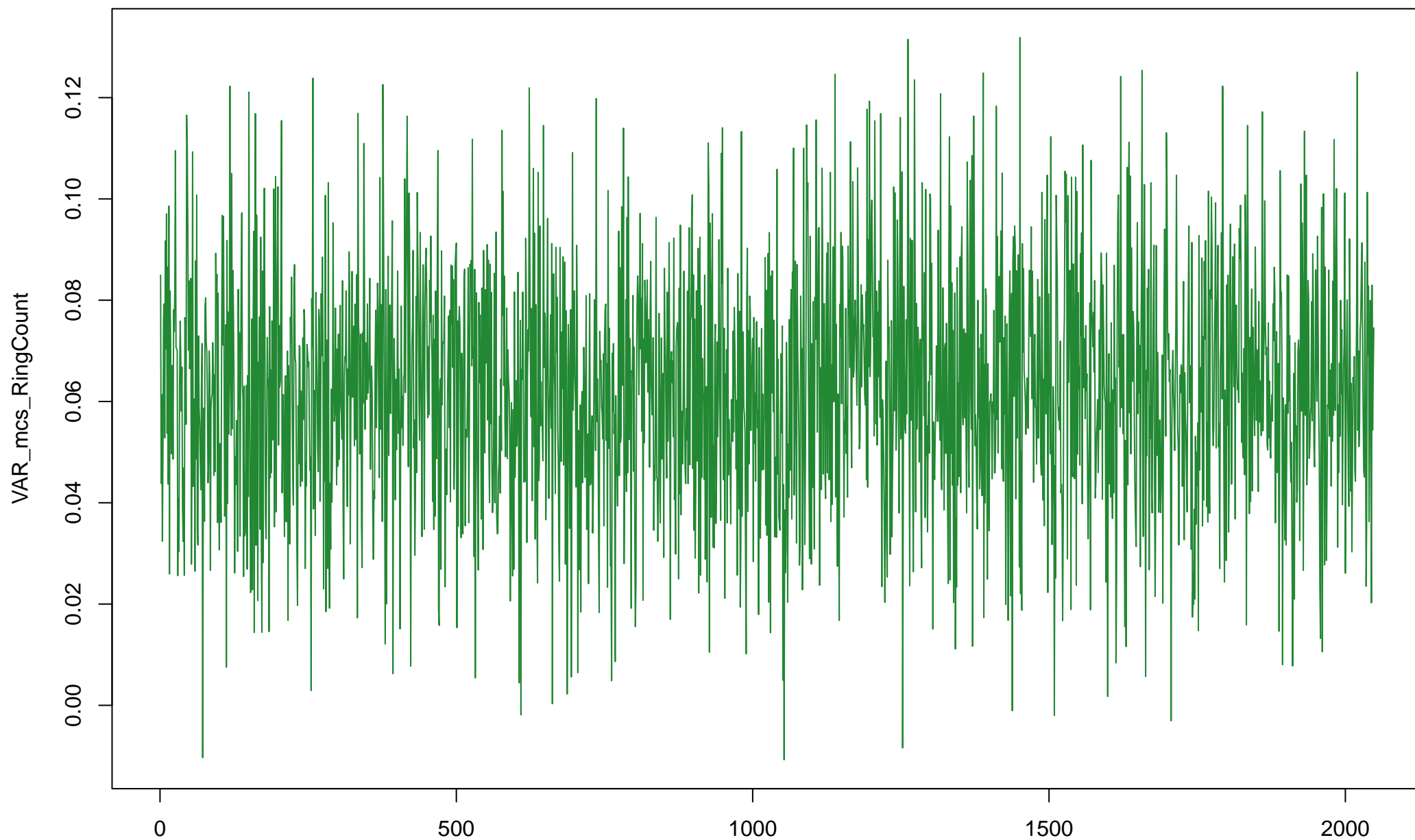
VAR_Xtransf_ec_tanimoto_similarity
ESS = 1180 | BMK = 0.0605 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0



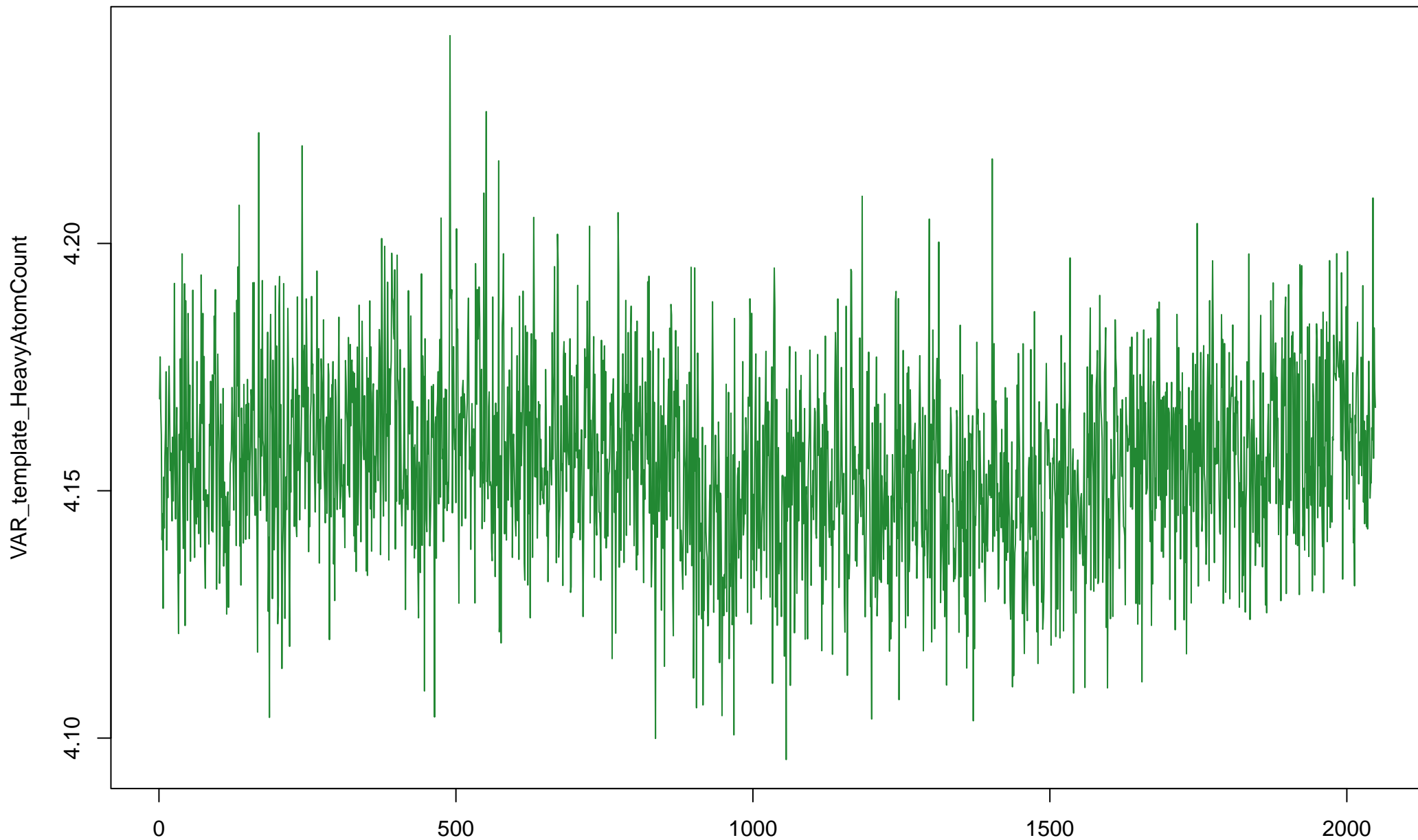
VAR_docked_HeavyAtomCount
ESS = 483 | BMK = 0.106 | MCSE(6.27) = 4.03 | stat: FALSE | burn: 0



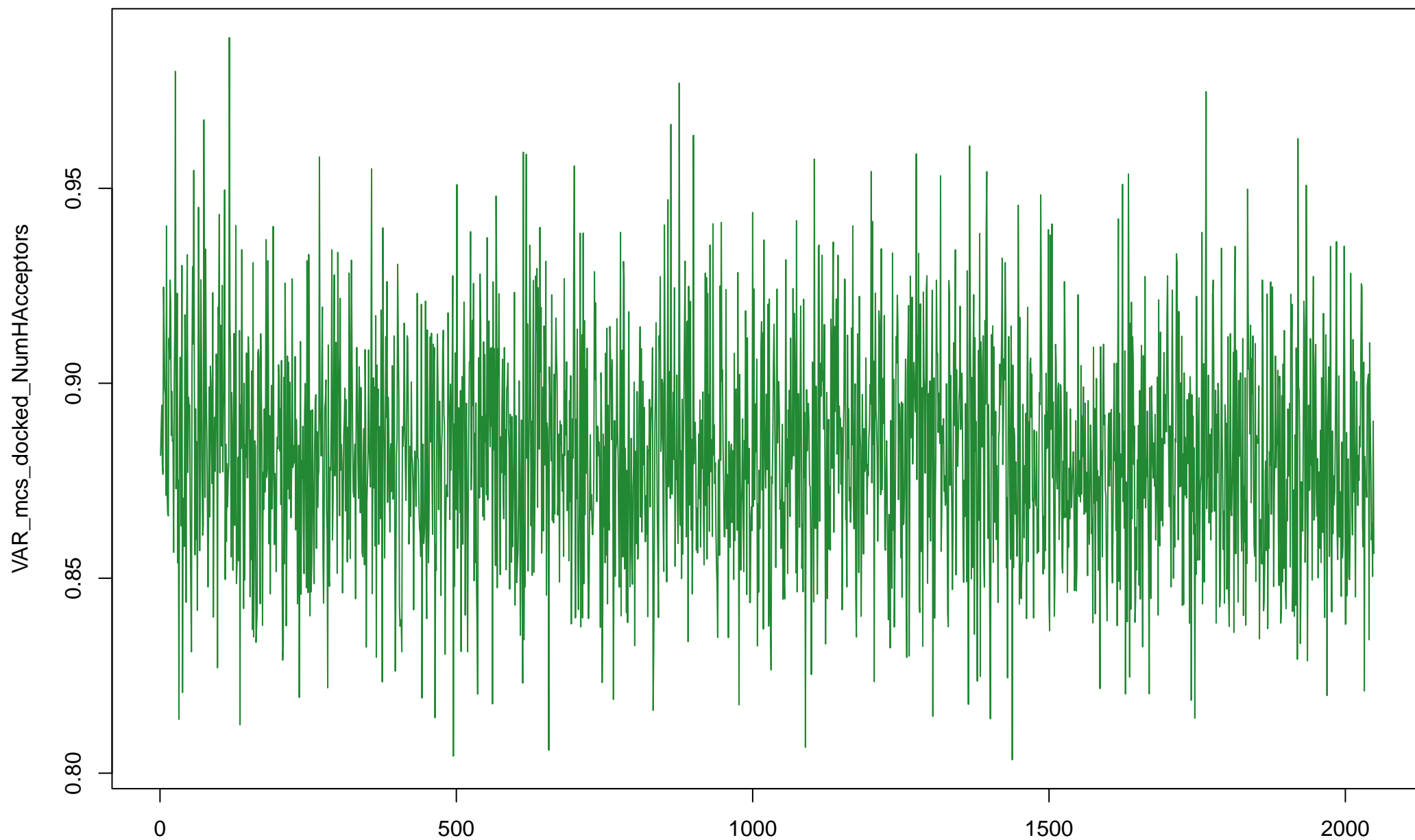
VAR_mcs_RingCount
ESS = 1890 | BMK = 0.0538 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0



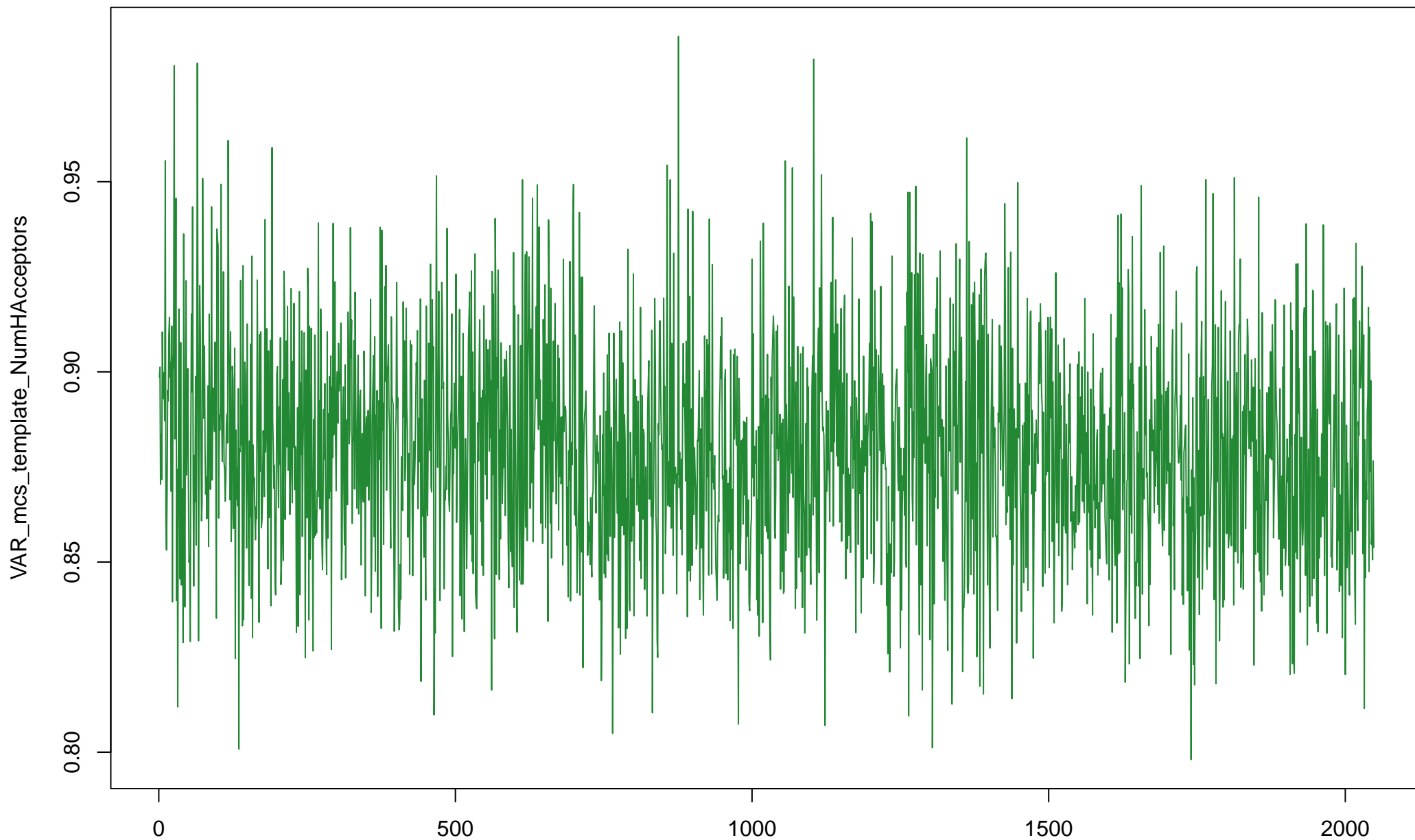
VAR_template_HeavyAtomCount
ESS = 176 | BMK = 0.0881 | MCSE(6.27) = 4.72 | stat: FALSE | burn: 0



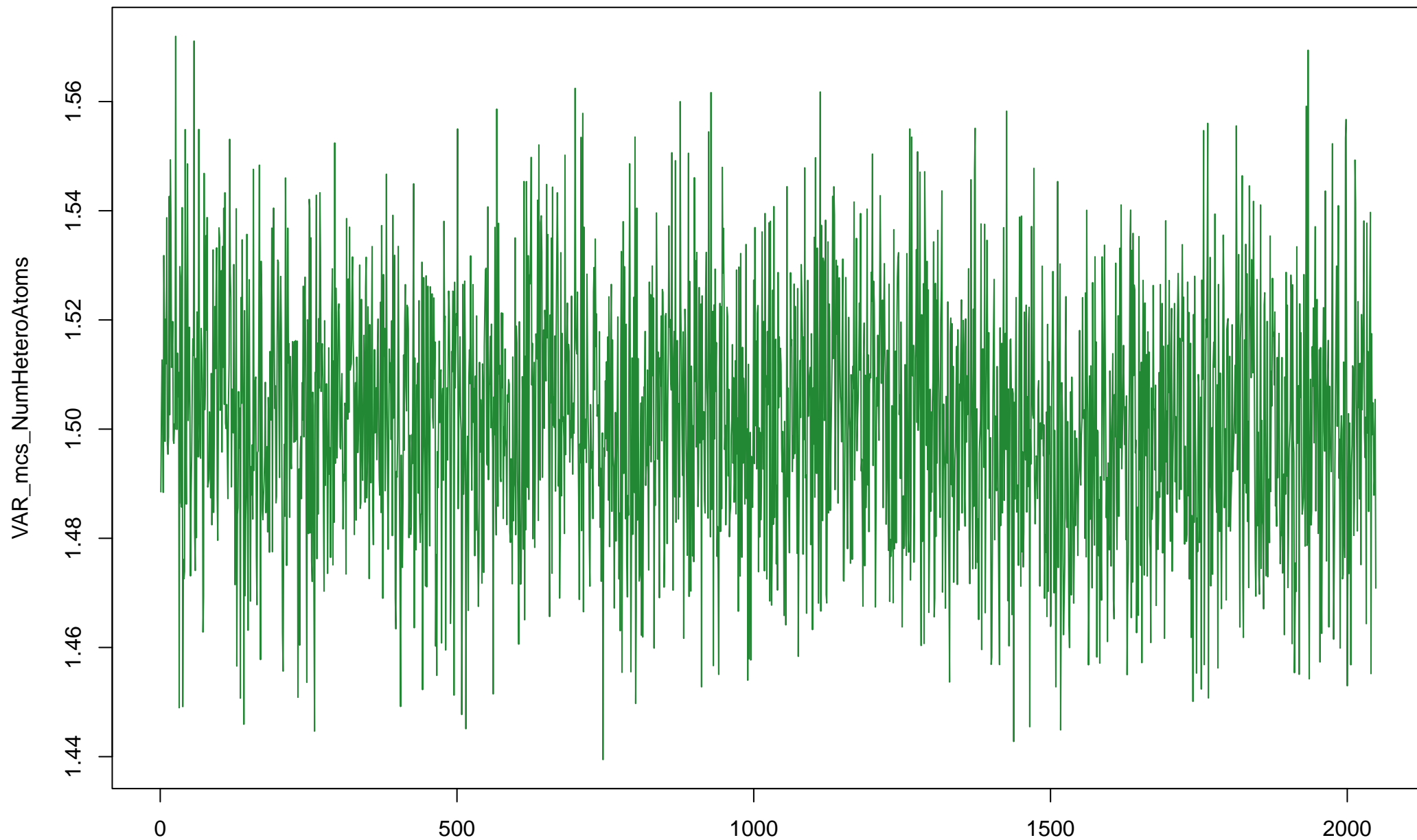
VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0353 | MCSE(6.27) = 2.39 | stat: FALSE | burn: 0



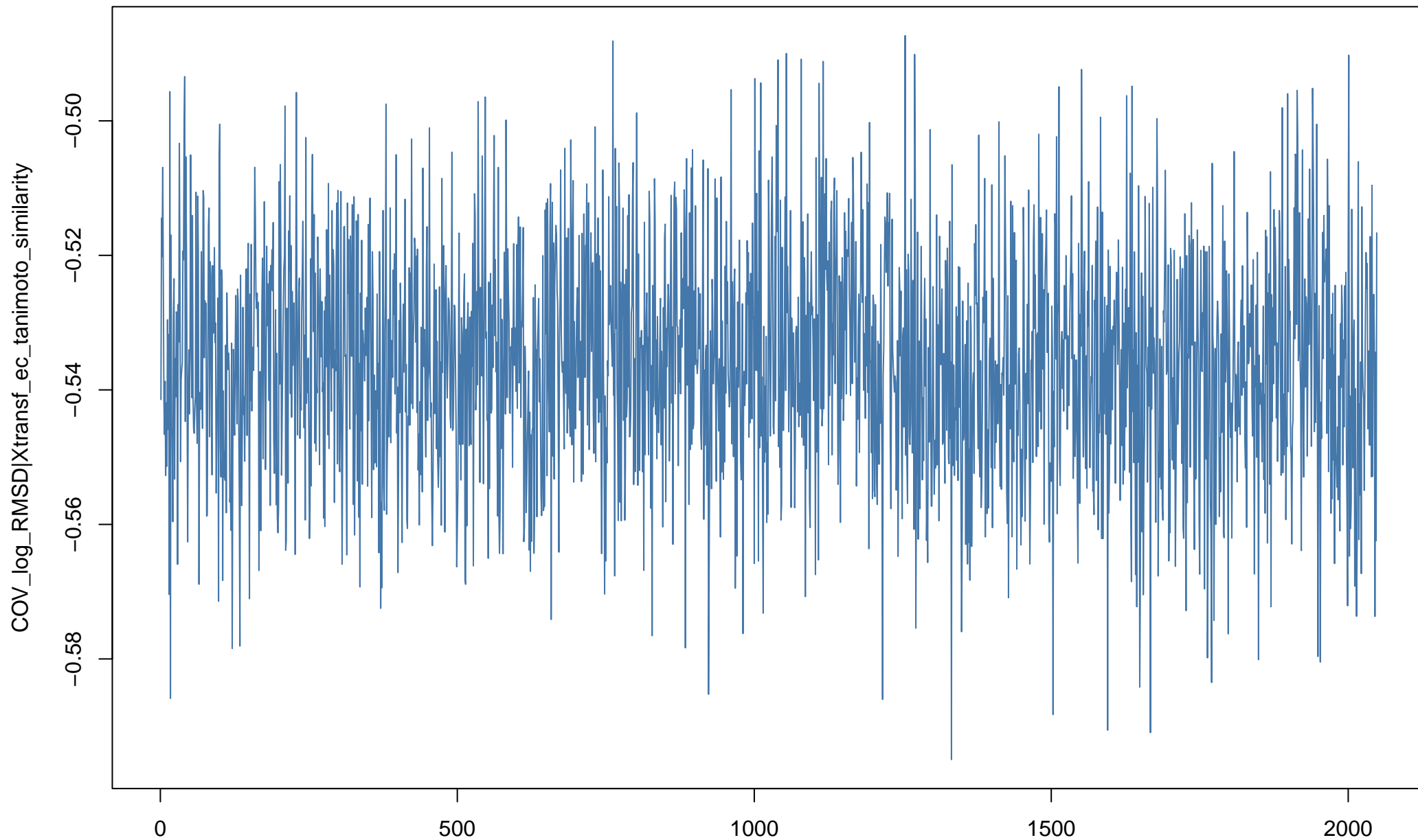
VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0444 | MCSE(6.27) = 2.75 | stat: FALSE | burn: 0



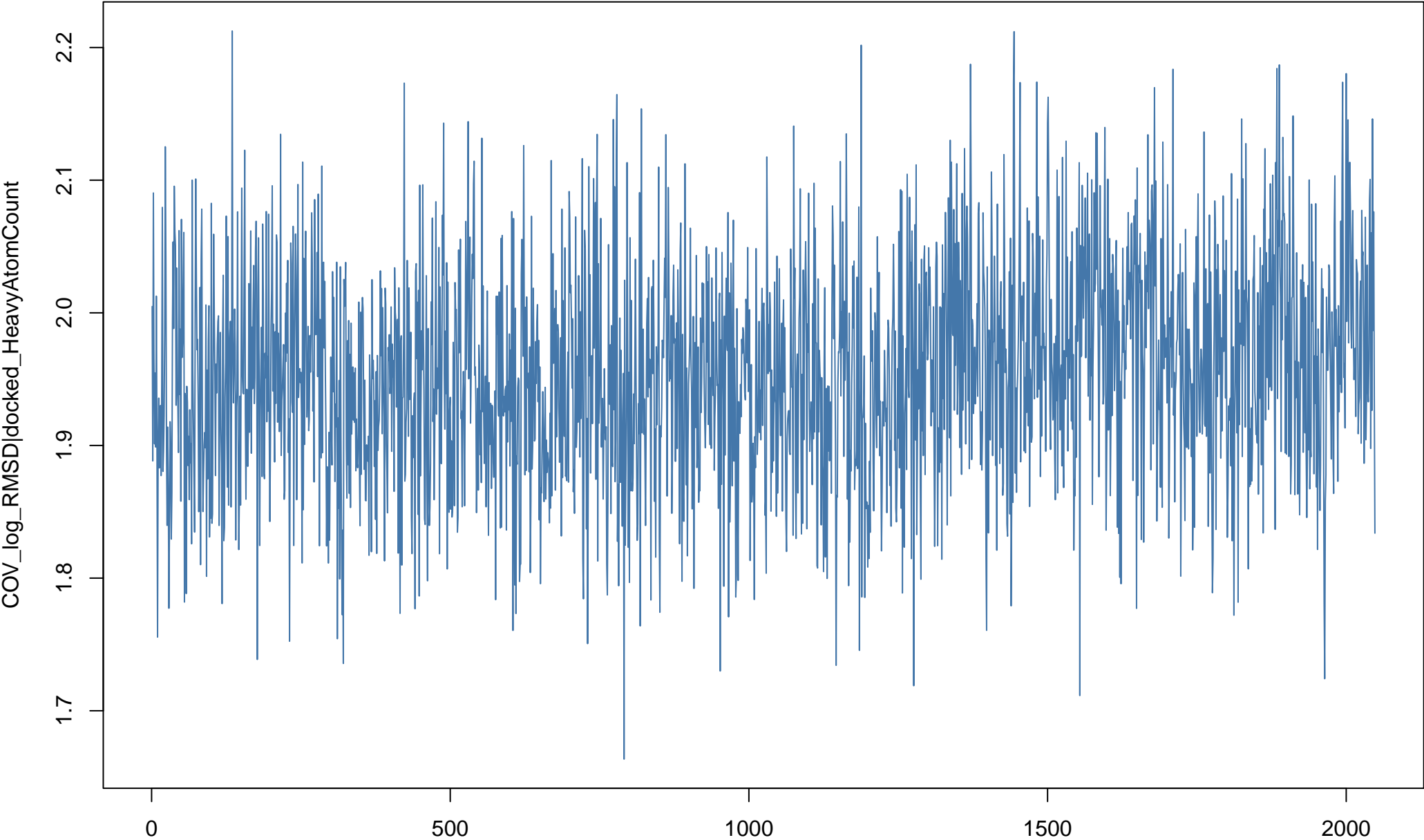
VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0677 | MCSE(6.27) = 2.83 | stat: FALSE | burn: 0



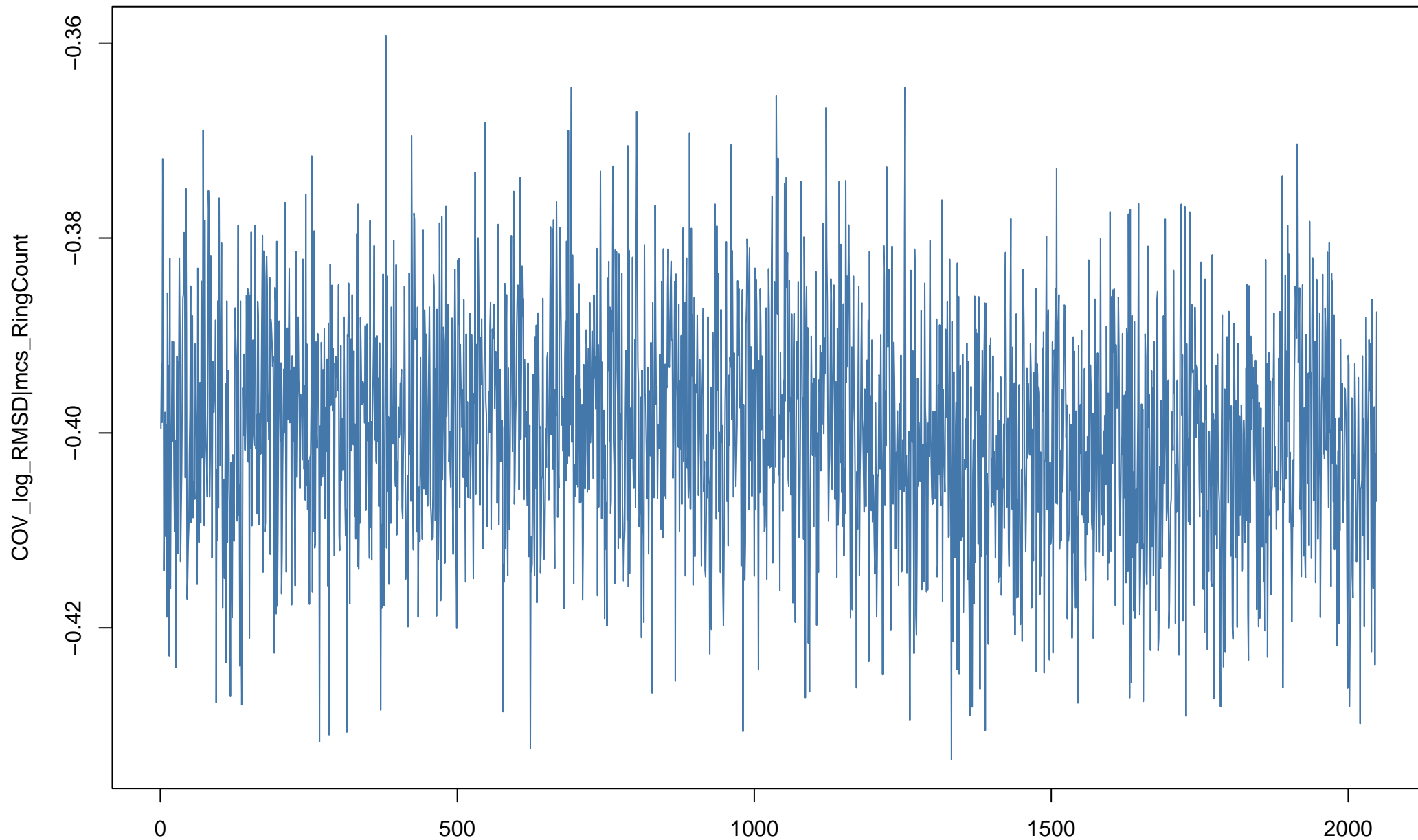
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0482 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0



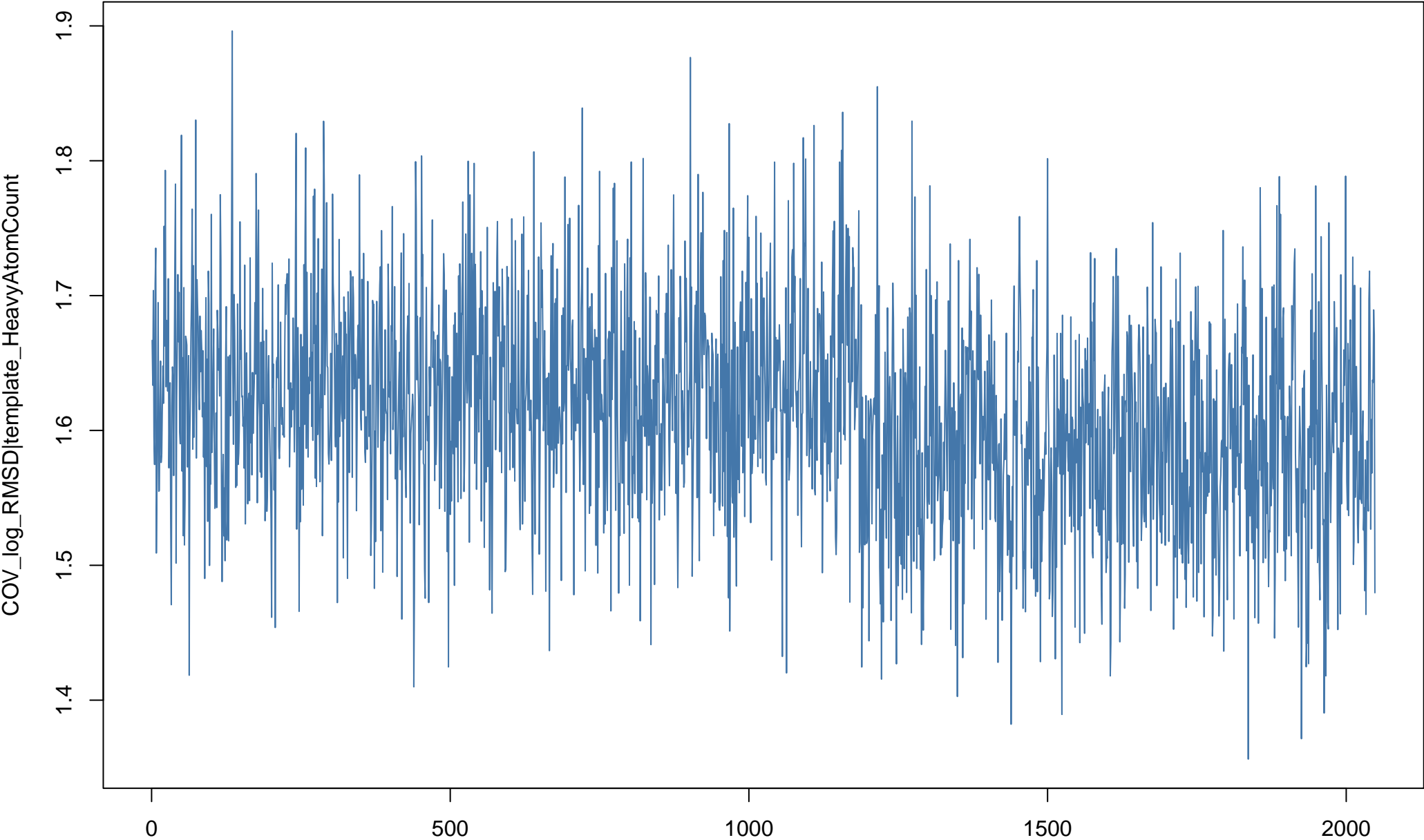
COV_log_RMSD|docked_HeavyAtomCount
ESS = 774 | BMK = 0.113 | MCSE(6.27) = 3.97 | stat: FALSE | burn: 0



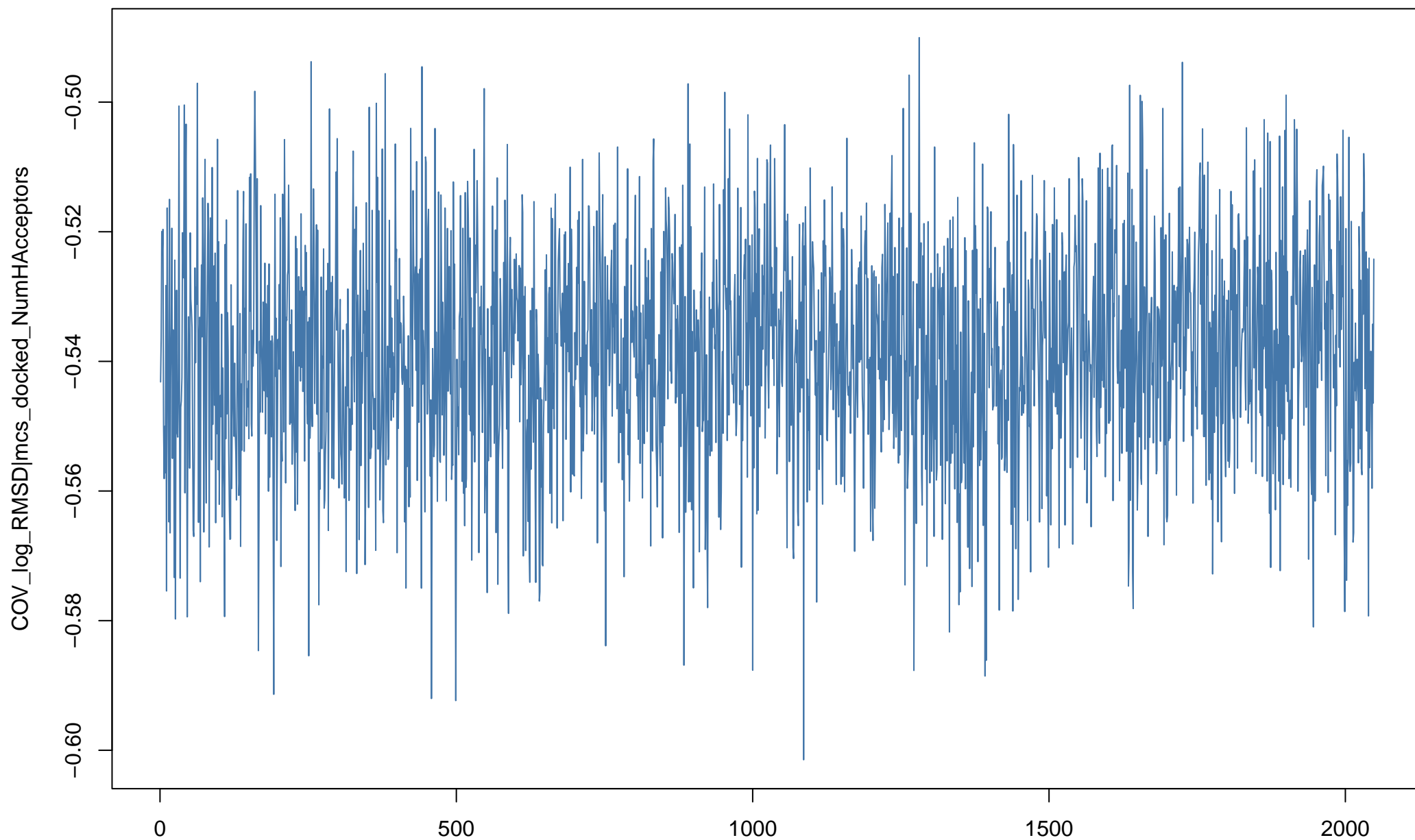
COV_log_RMSD|mcs_RingCount
ESS = 799 | BMK = 0.102 | MCSE(6.27) = 3.64 | stat: FALSE | burn: 0



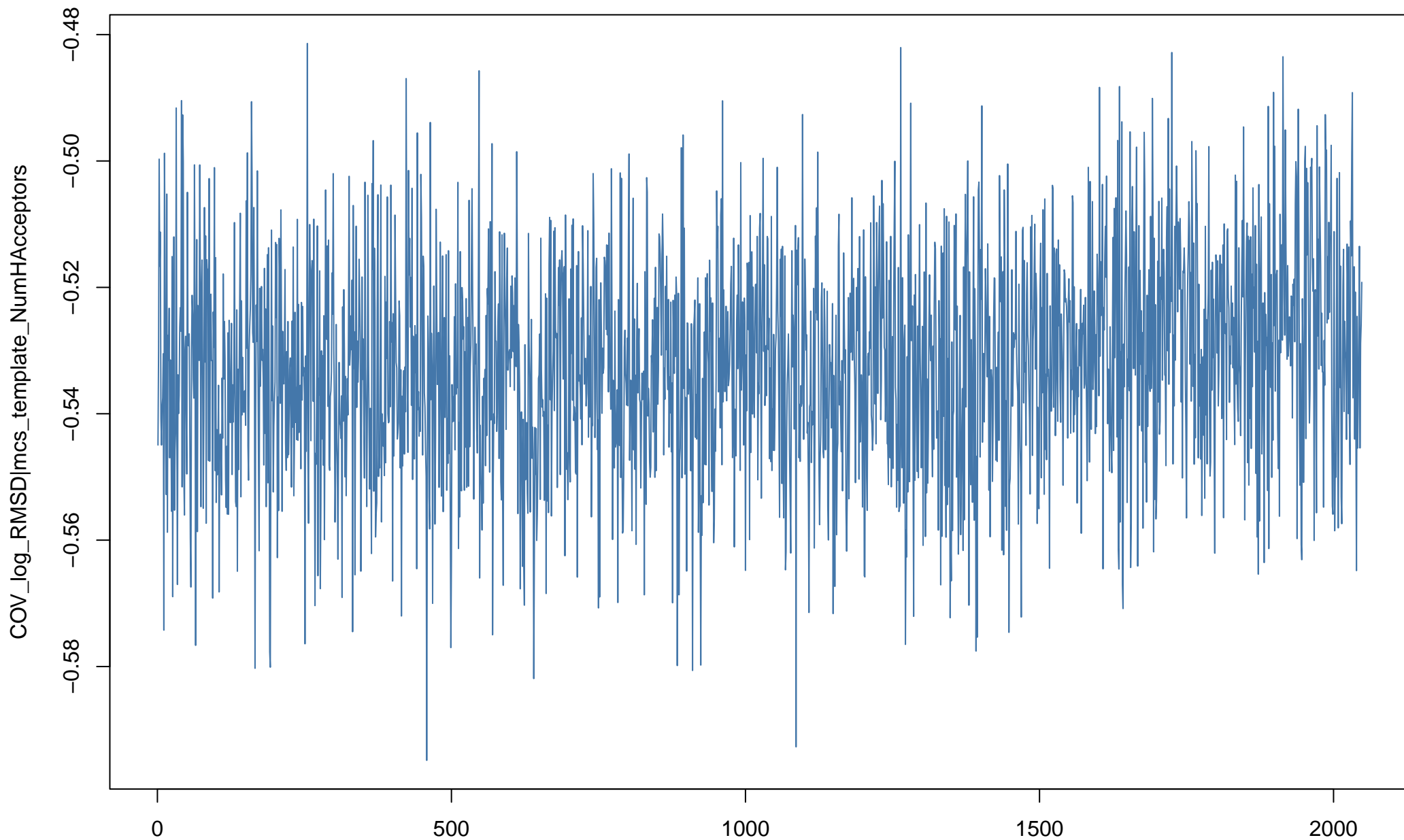
COV_log_RMSD|template_HeavyAtomCount
ESS = 217 | BMK = 0.172 | MCSE(6.27) = 4.83 | stat: FALSE | burn: 0



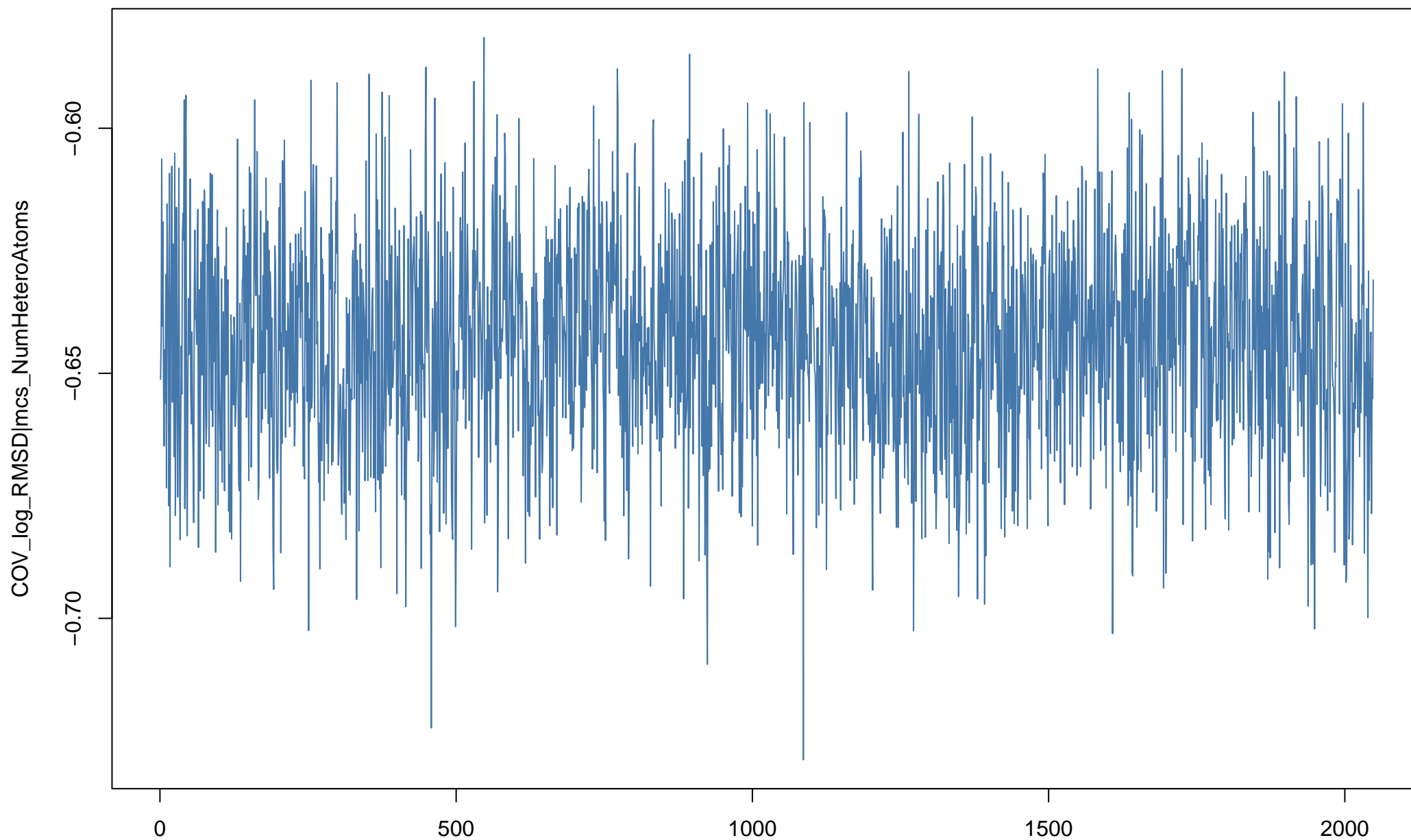
COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0401 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0



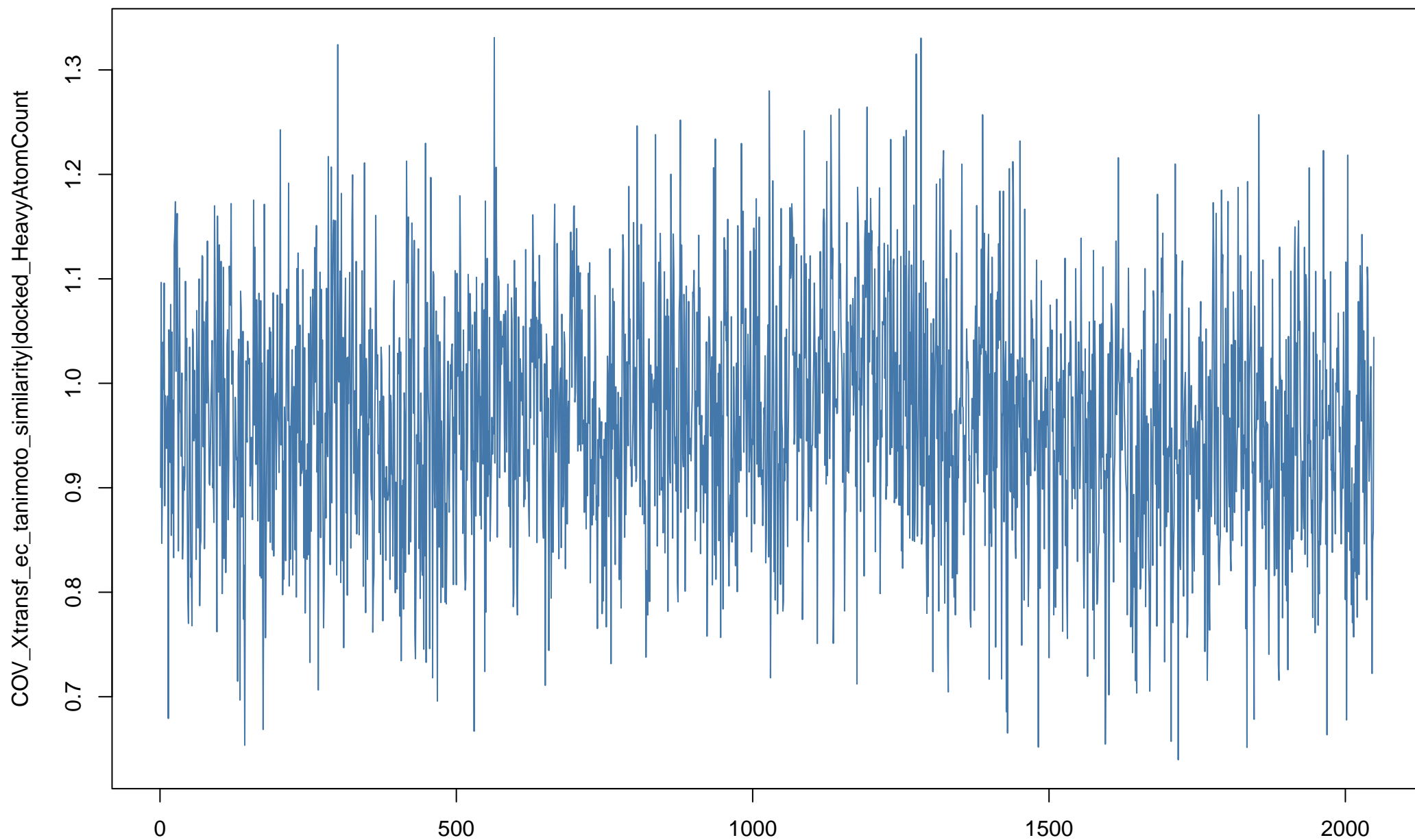
COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 801 | BMK = 0.0935 | MCSE(6.27) = 3.64 | stat: FALSE | burn: 0



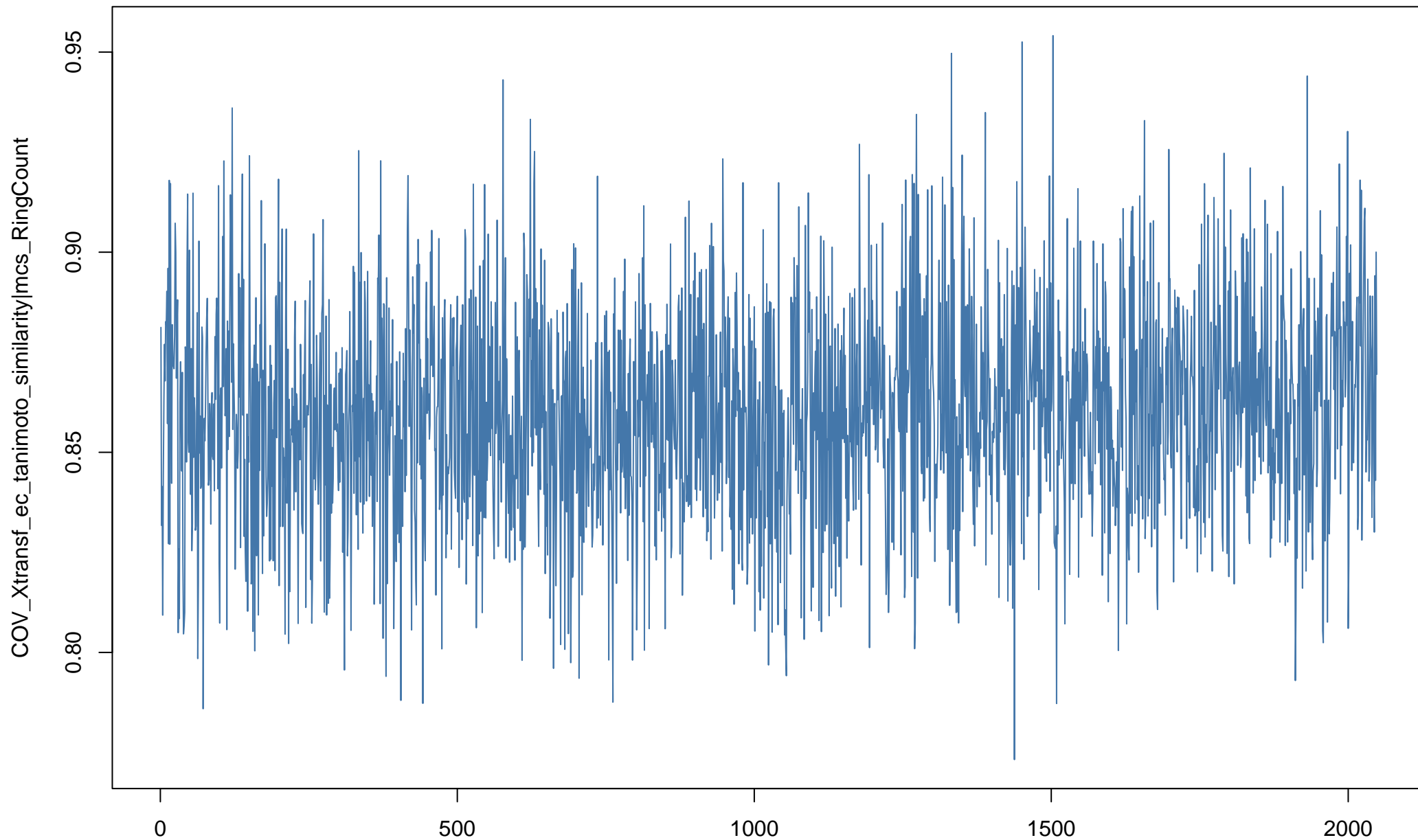
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0354 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0



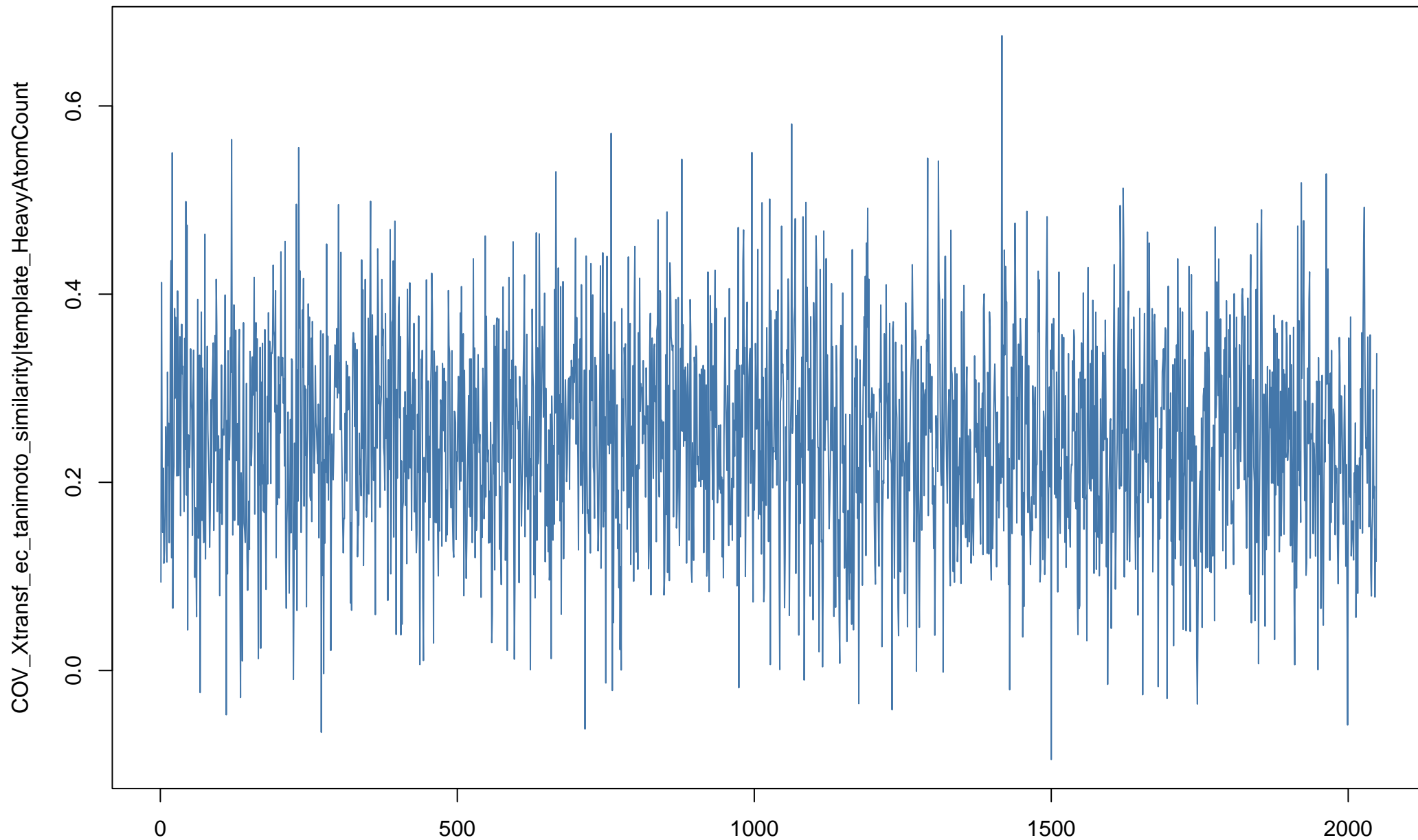
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1070 | BMK = 0.0458 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0



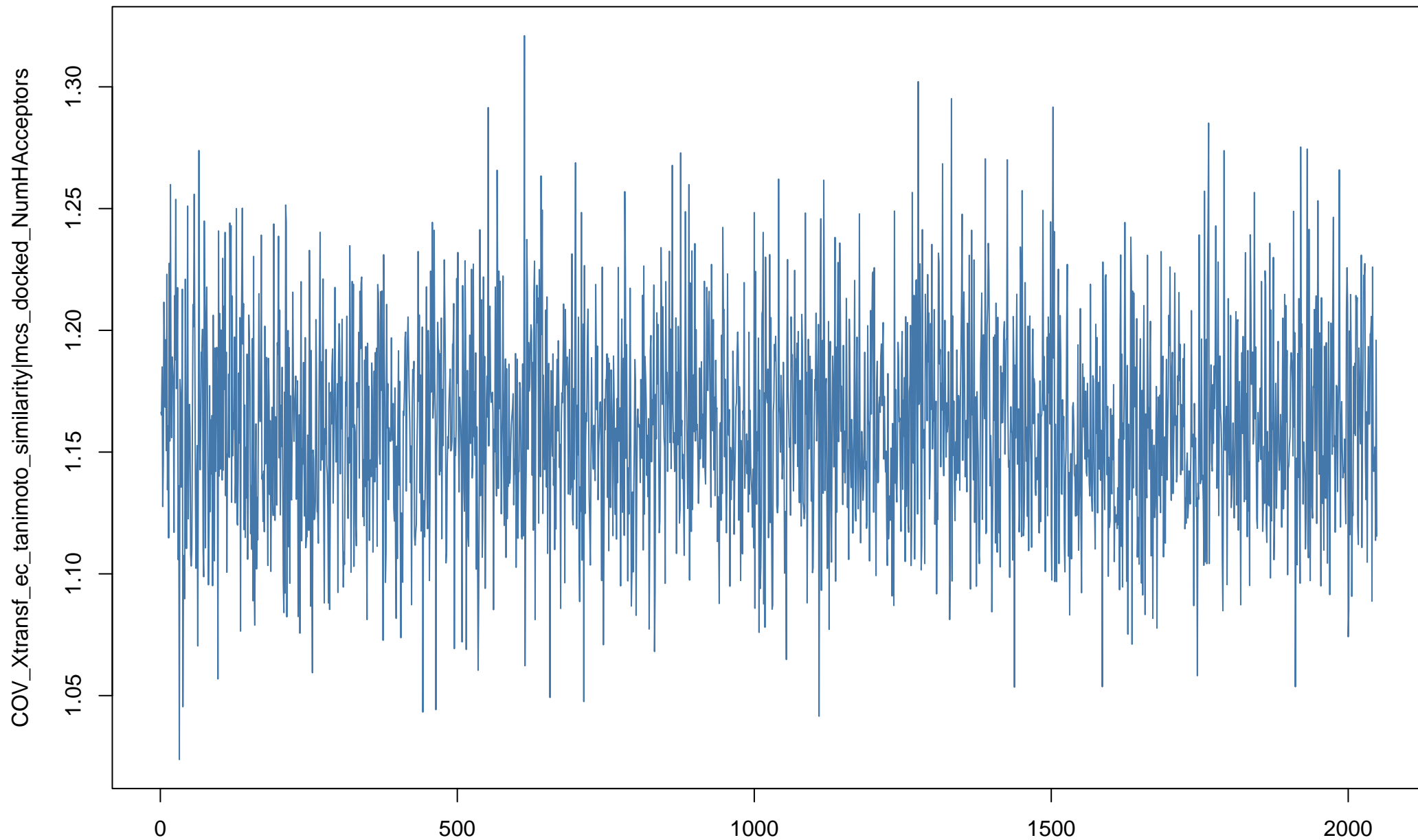
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1760 | BMK = 0.0684 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0



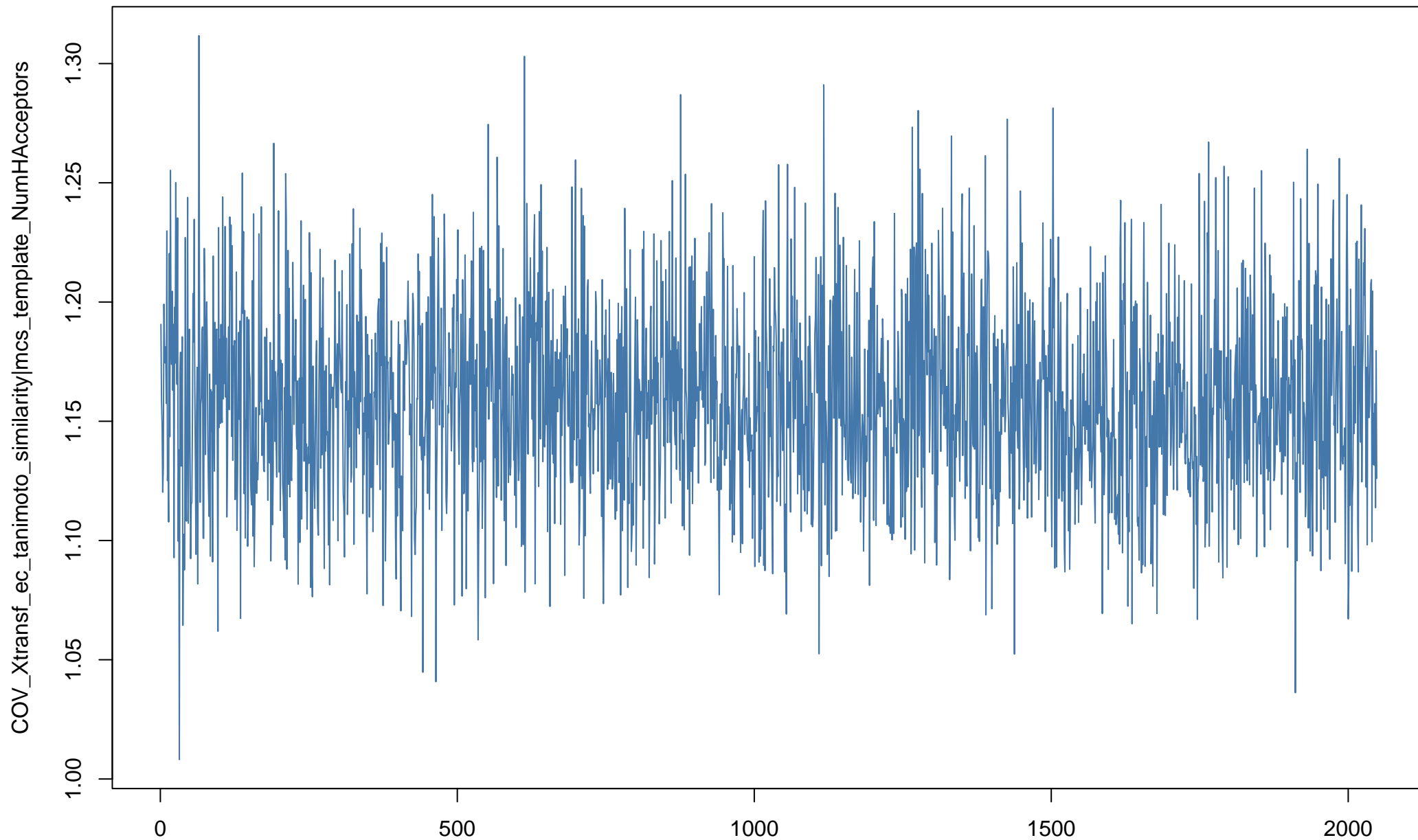
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1640 | BMK = 0.0454 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0



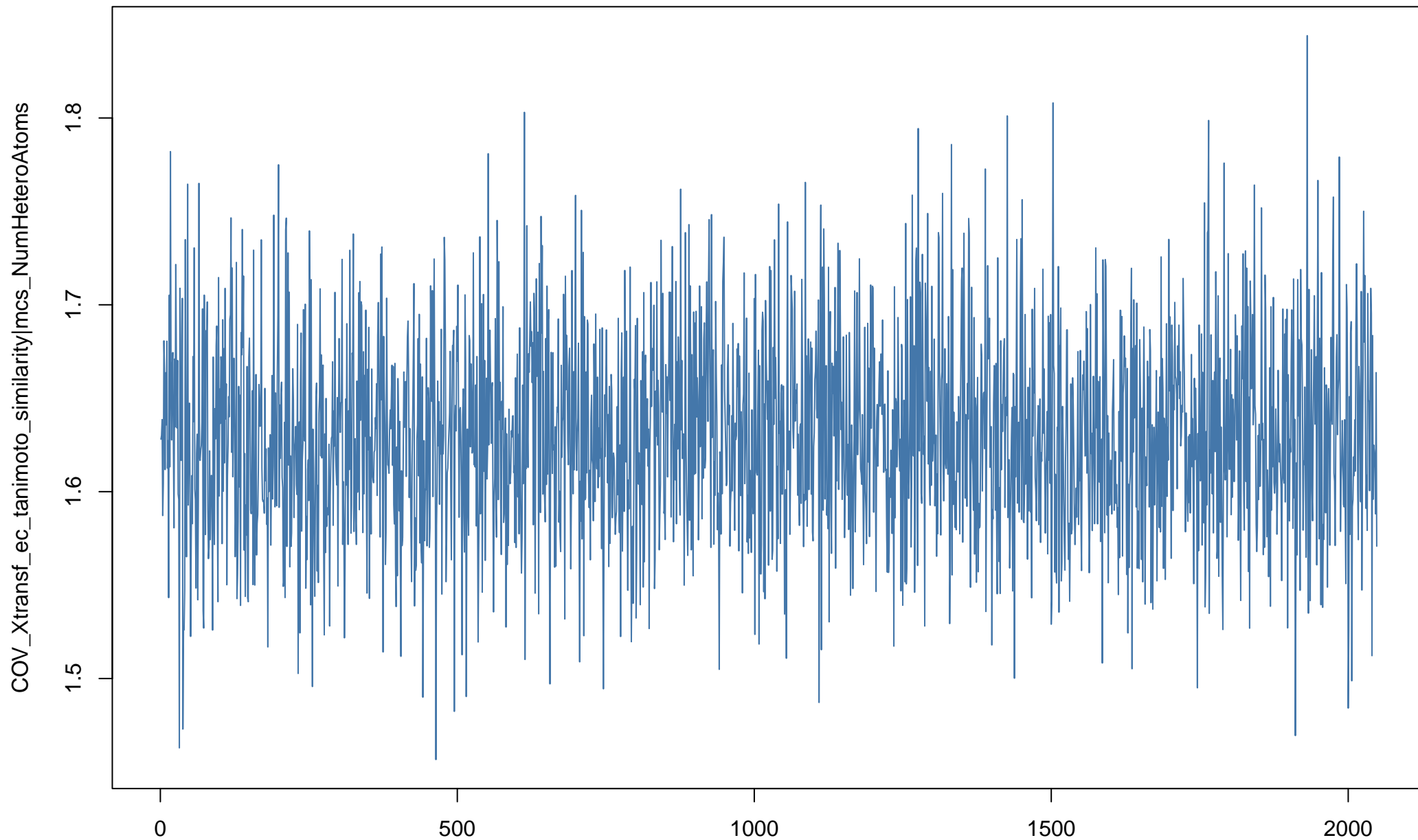
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0452 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0



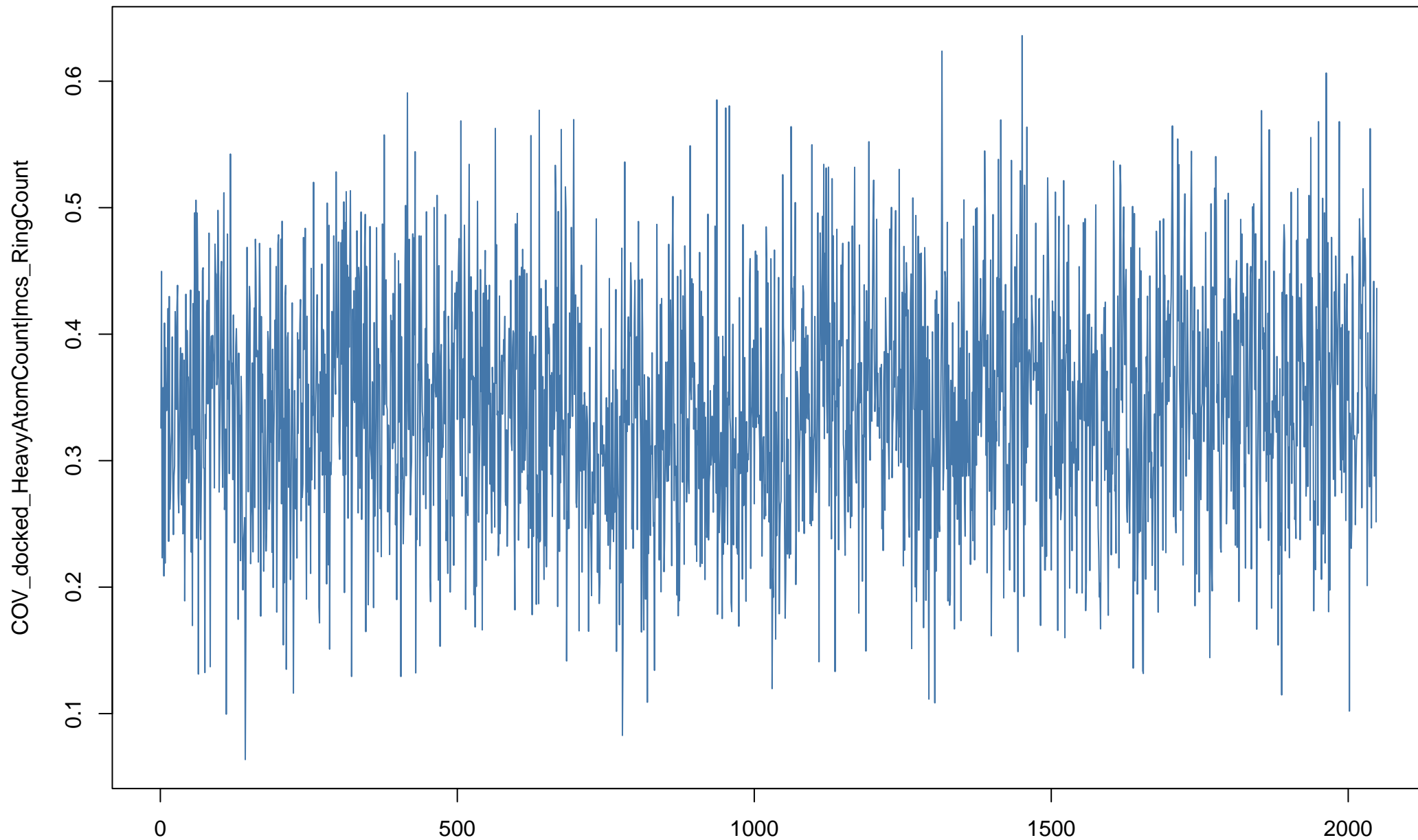
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0534 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0



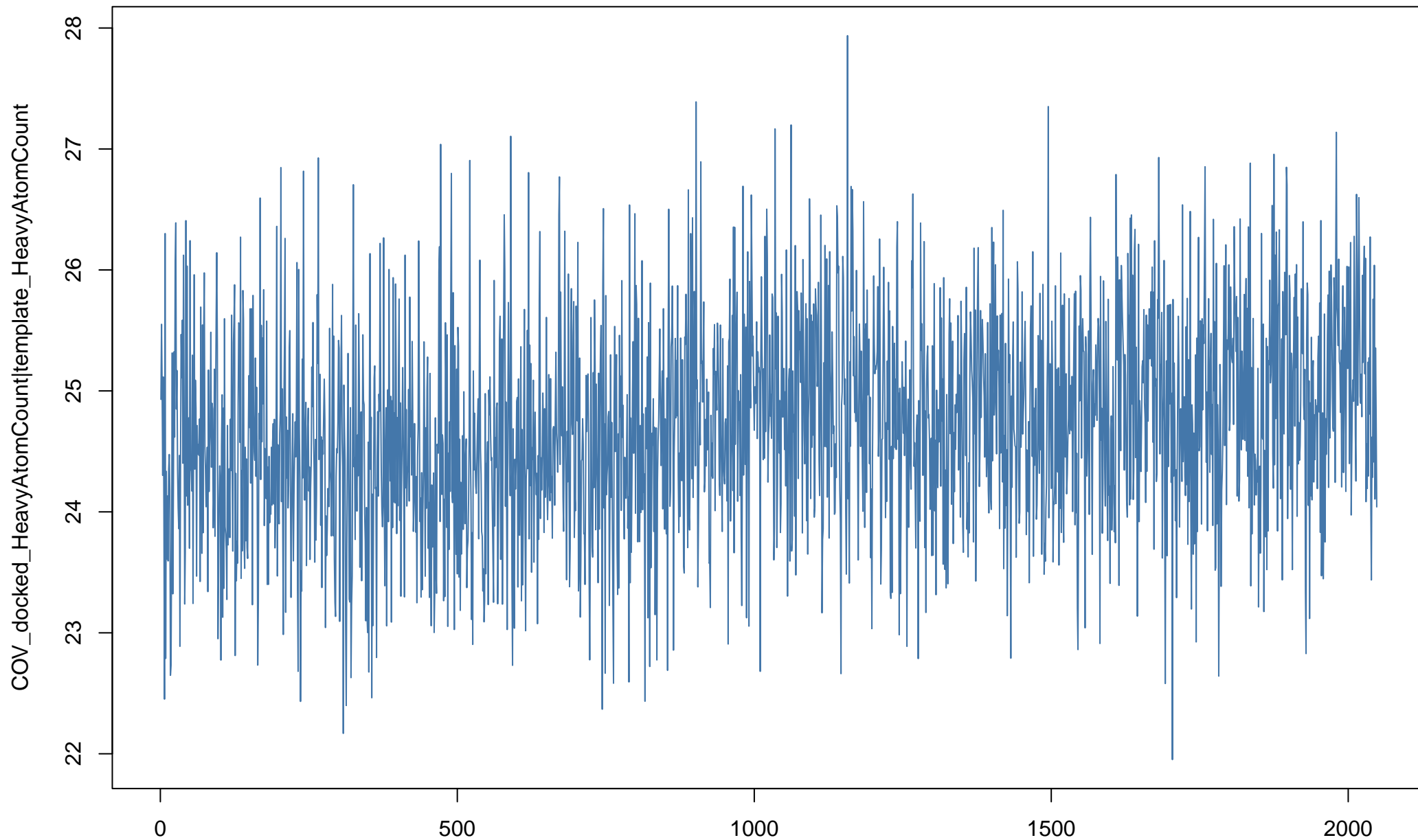
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0365 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0



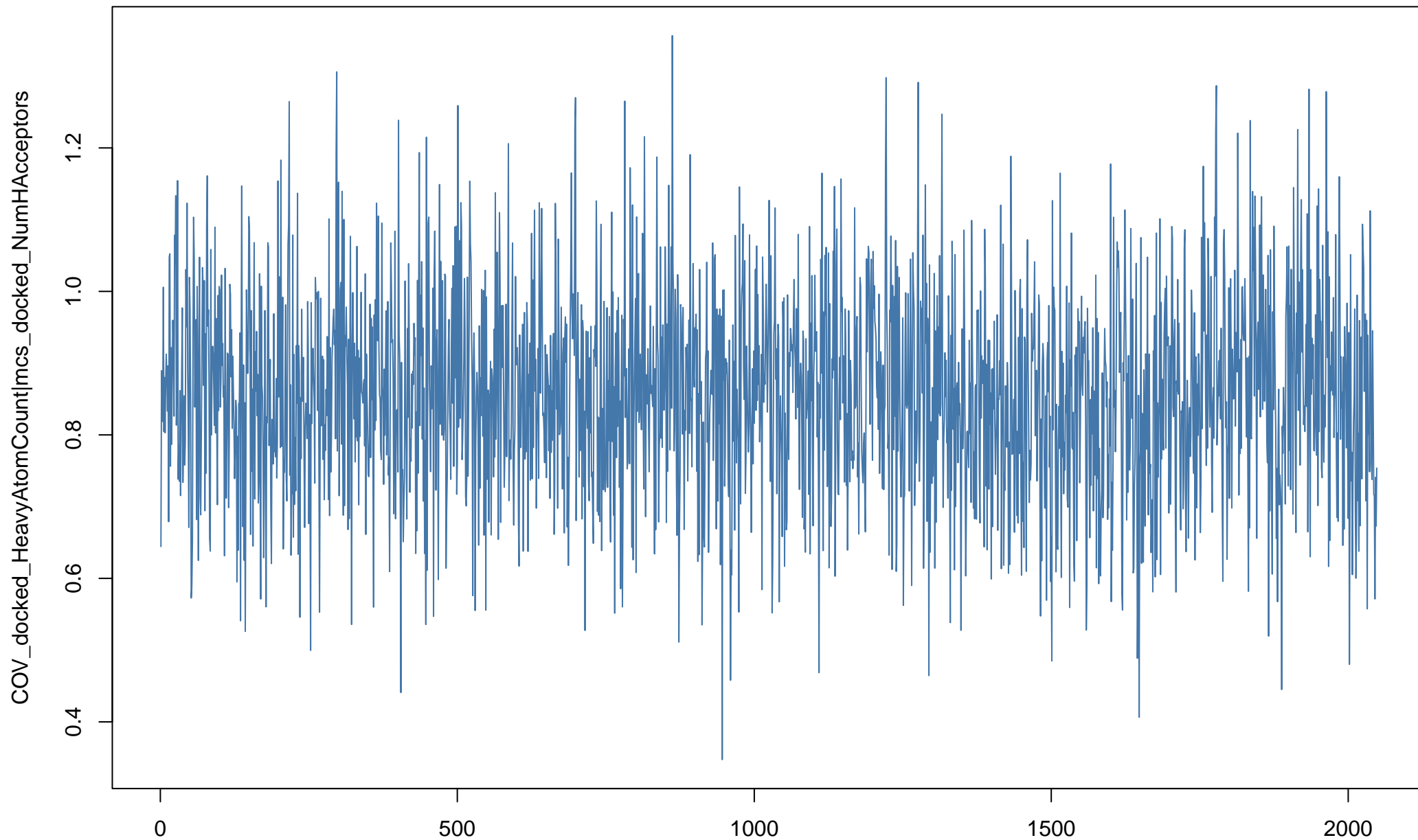
COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1630 | BMK = 0.0586 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0



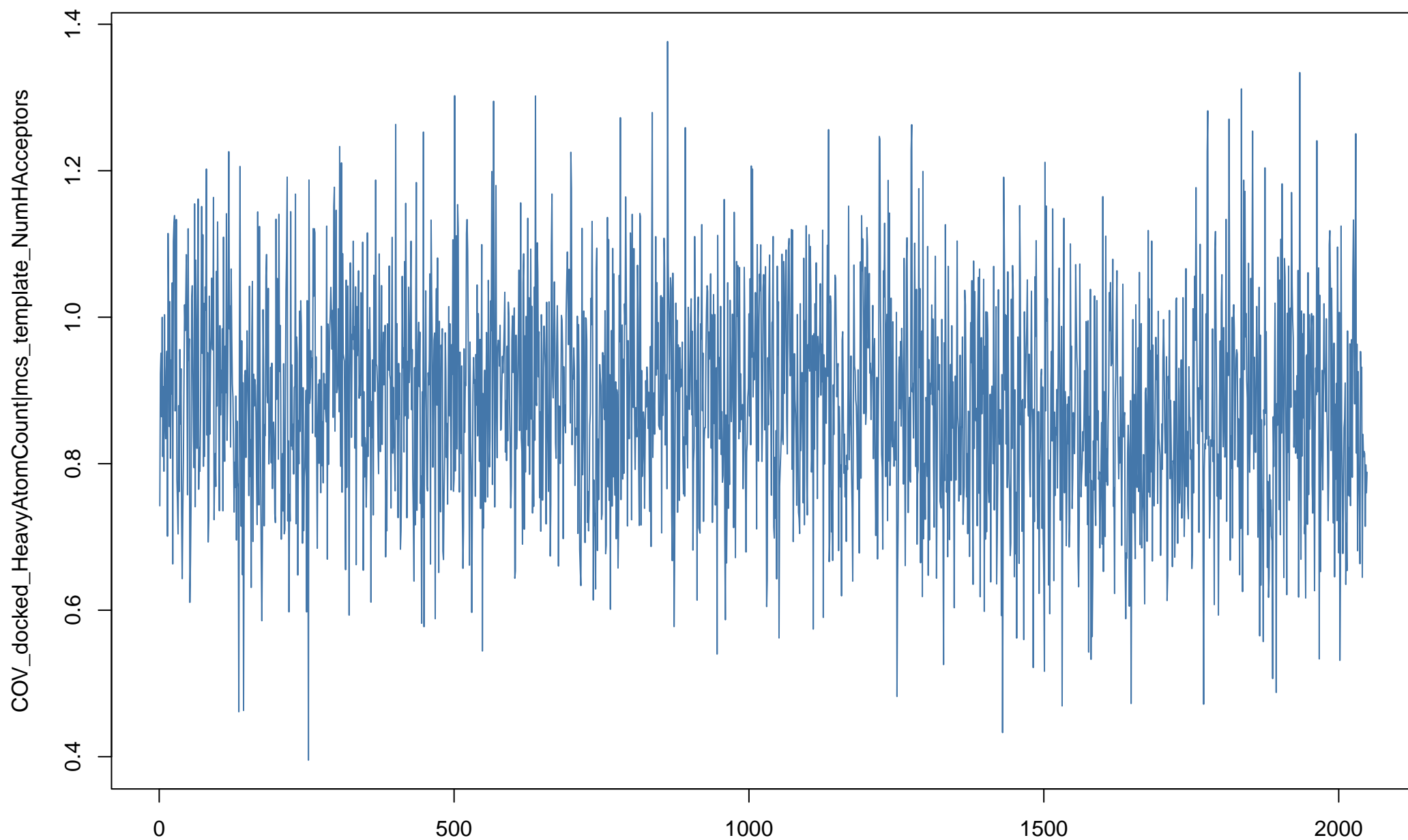
COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 388 | BMK = 0.158 | MCSE(6.27) = 4.26 | stat: FALSE | burn: 0



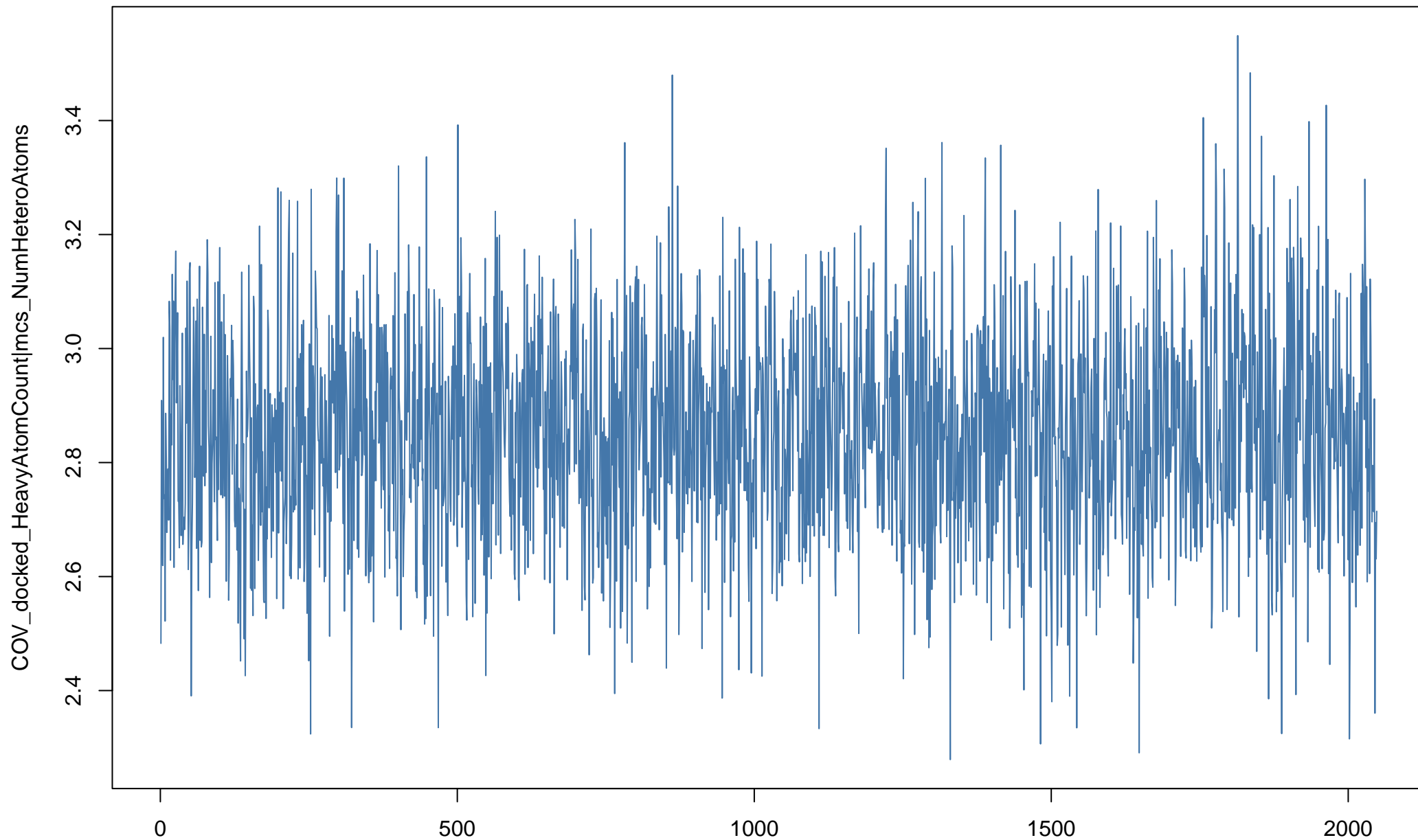
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1860 | BMK = 0.0479 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0



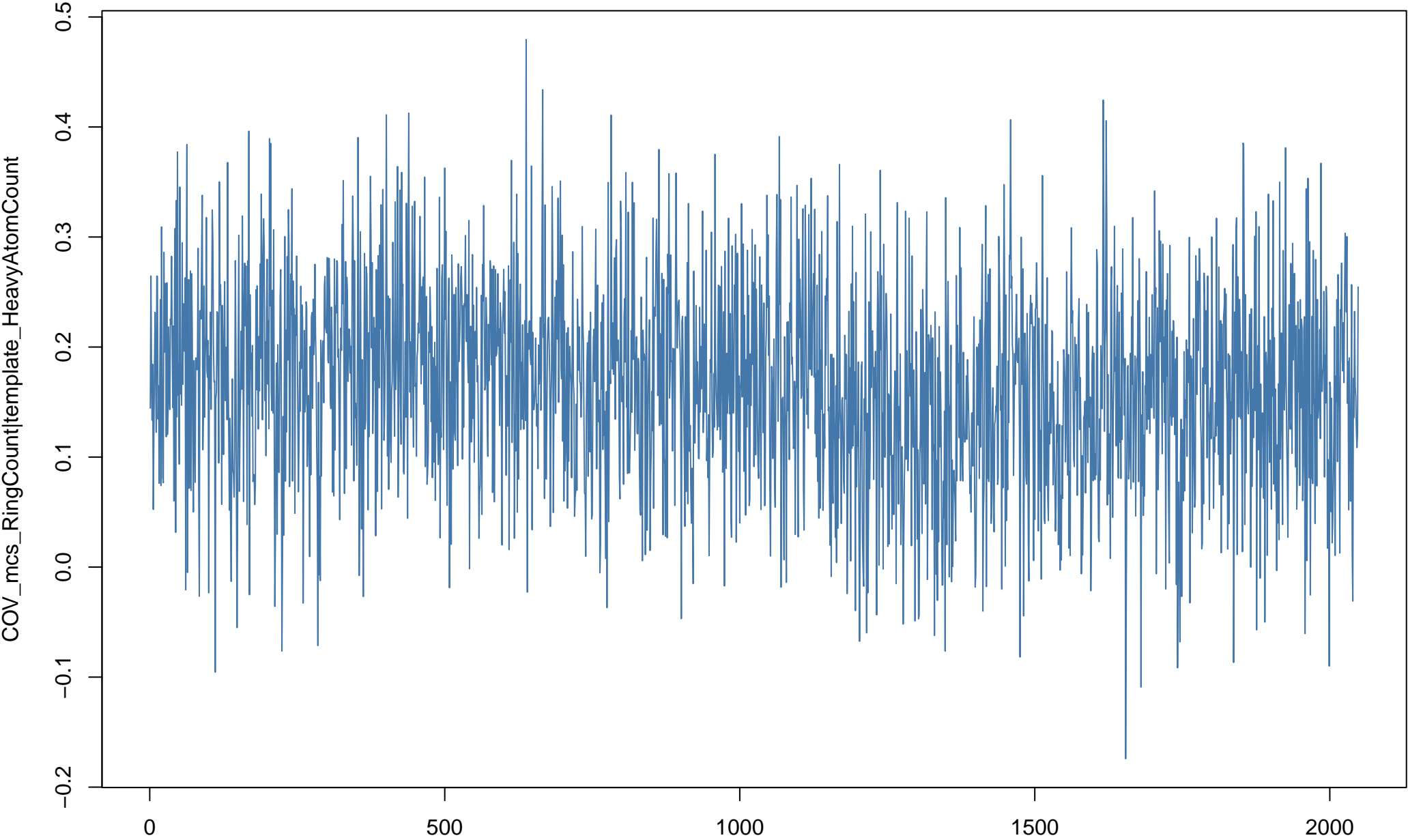
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 925 | BMK = 0.0906 | MCSE(6.27) = 3.06 | stat: FALSE | burn: 0



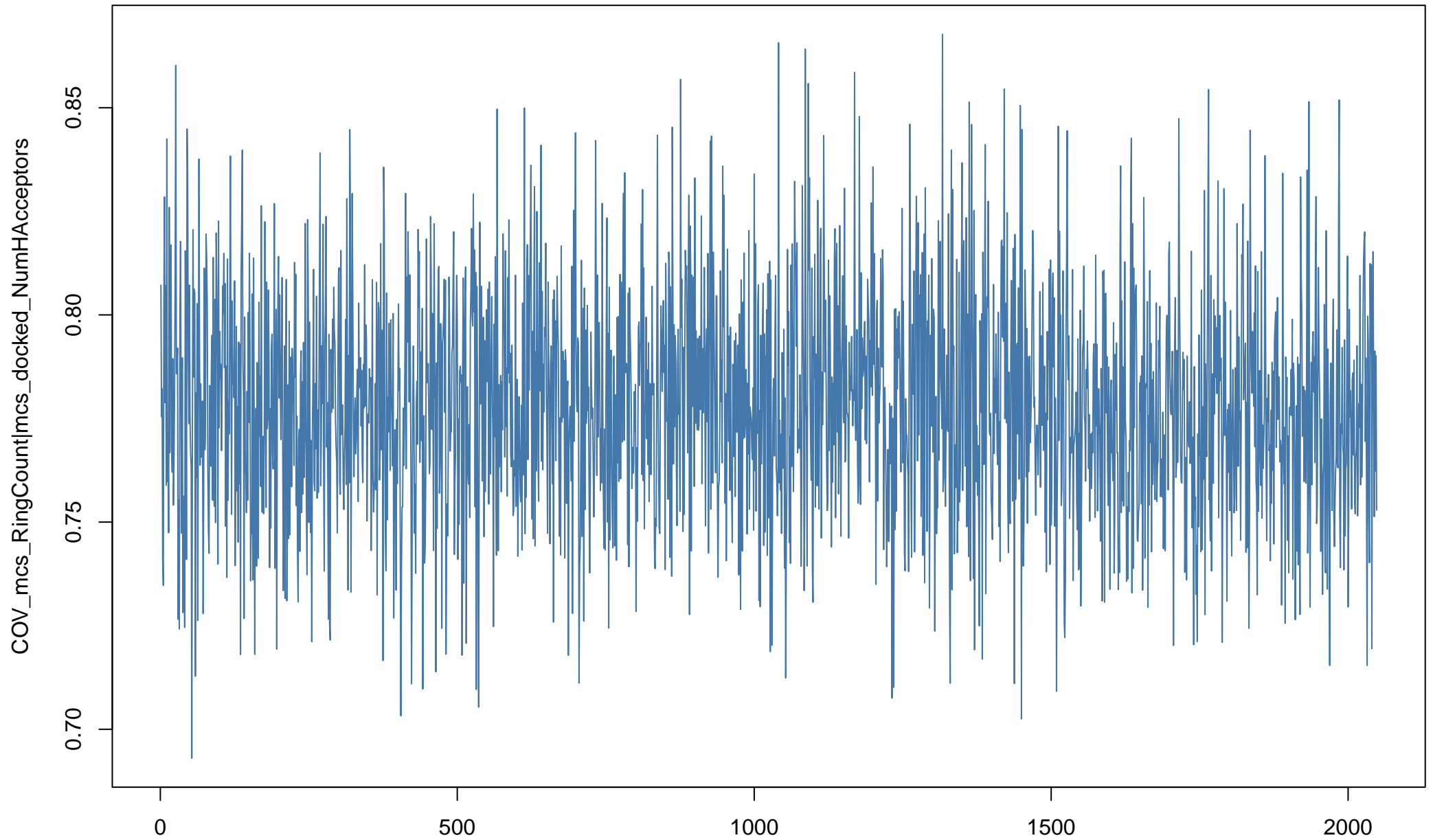
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0438 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0



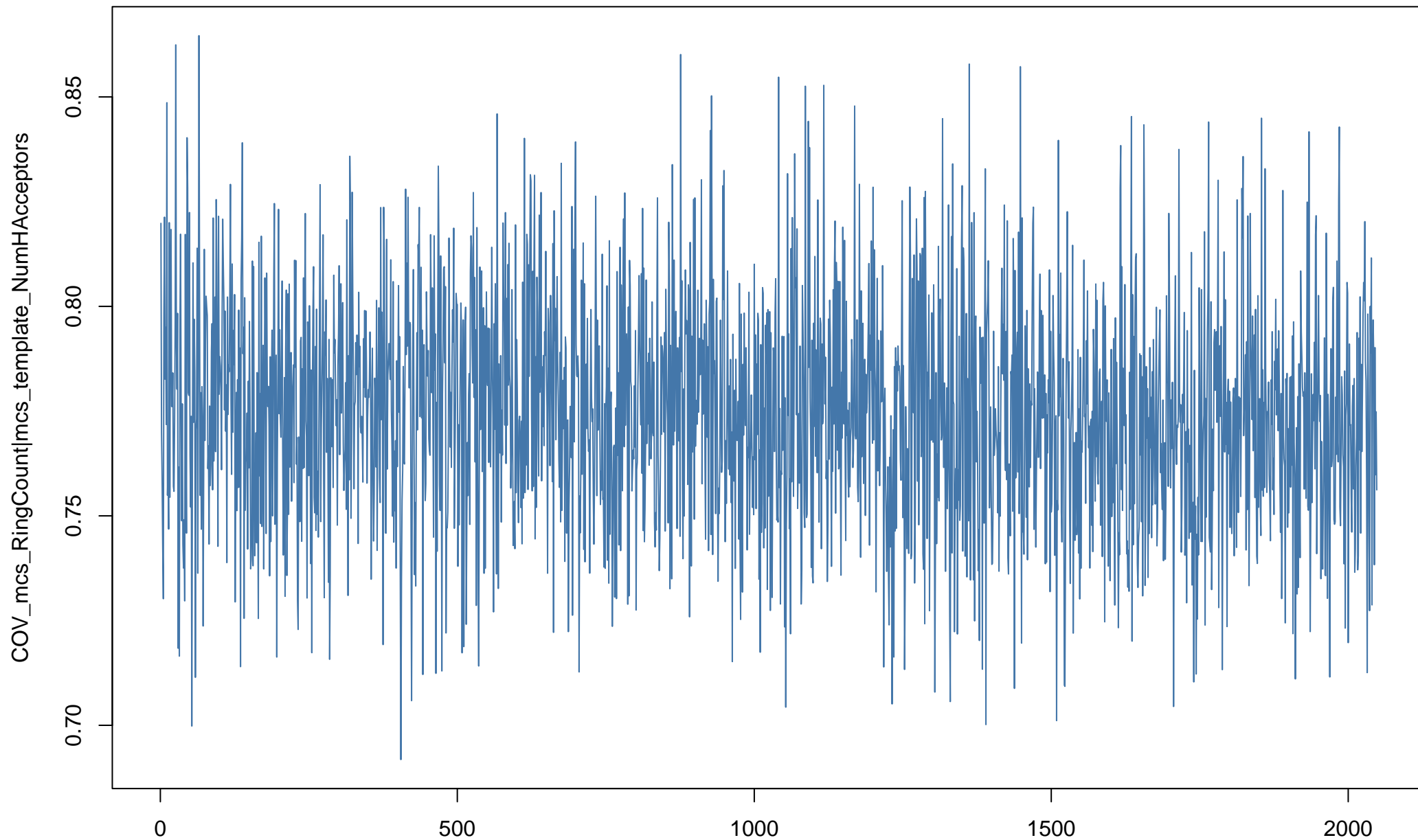
COV_mcs_RingCount|template_HeavyAtomCount
ESS = 846 | BMK = 0.118 | MCSE(6.27) = 3.65 | stat: FALSE | burn: 0



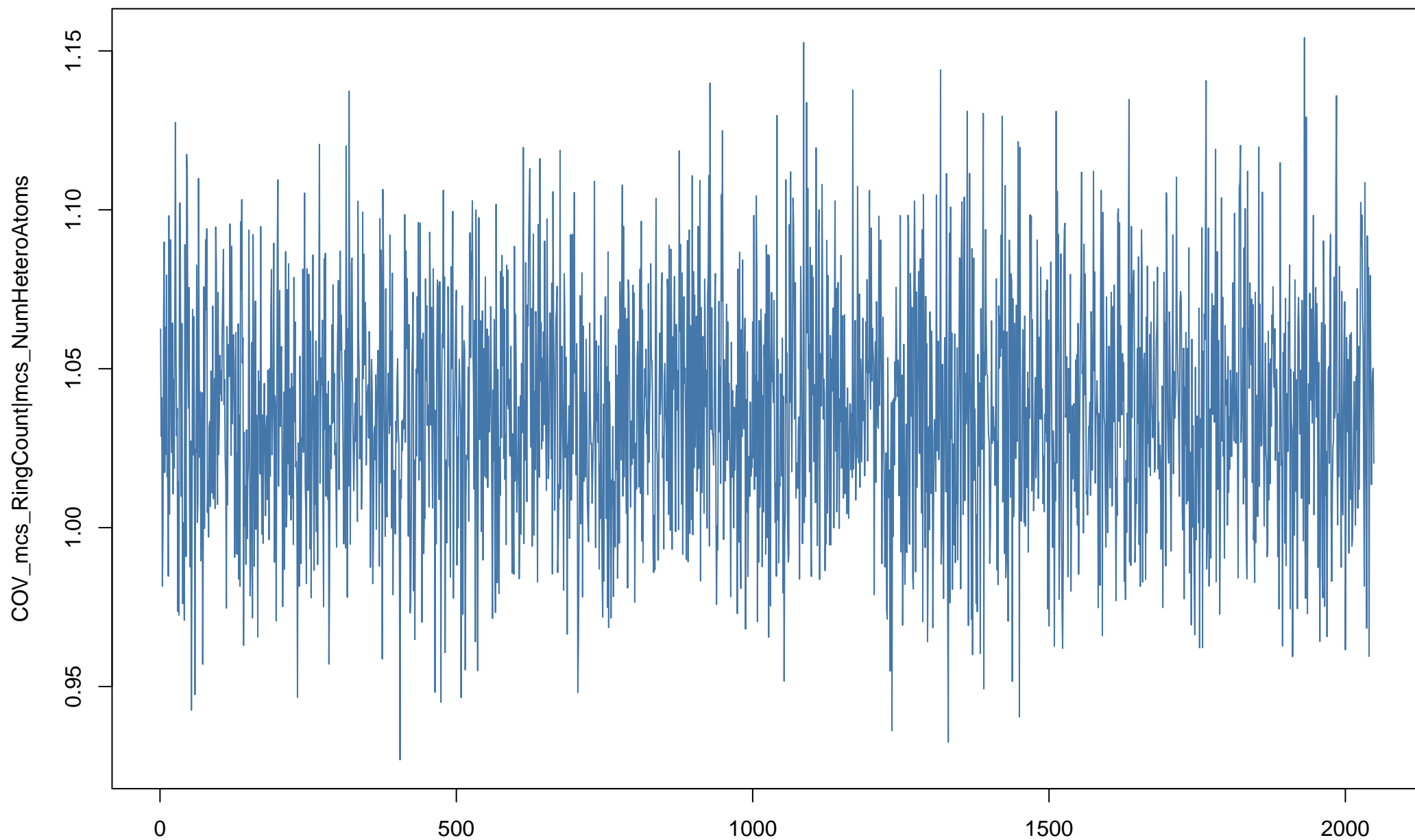
COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0481 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0



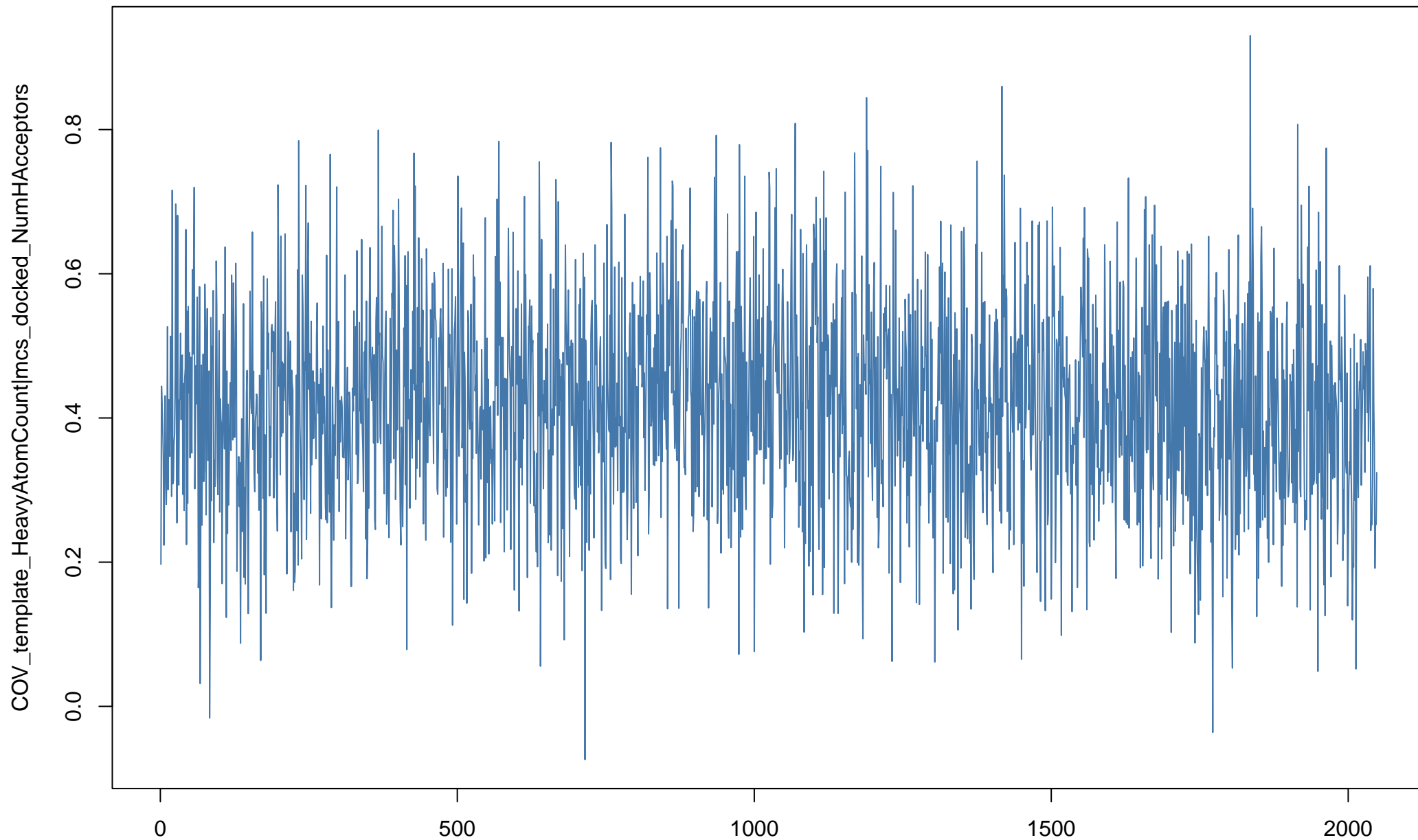
COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0763 | MCSE(6.27) = 2.75 | stat: FALSE | burn: 0



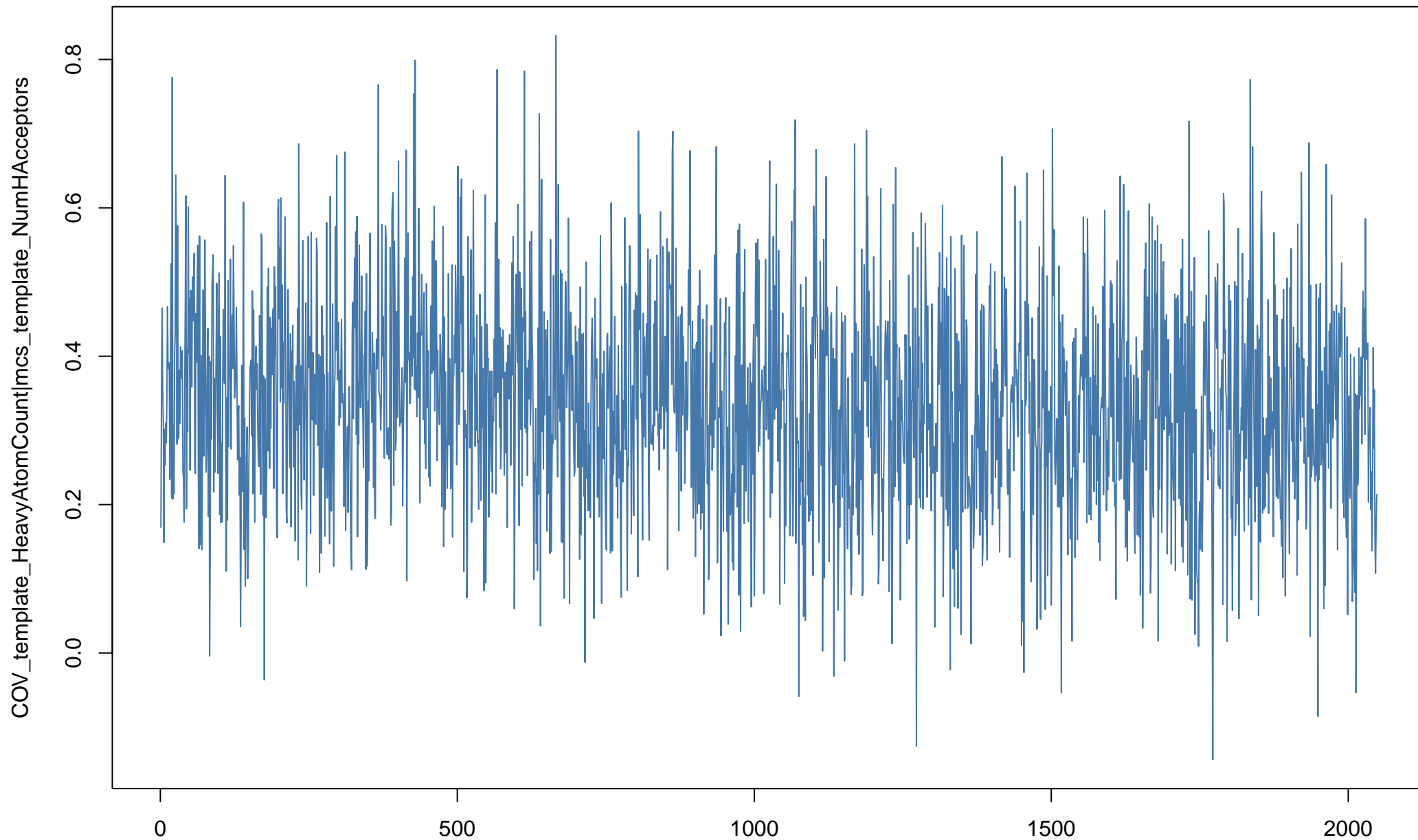
COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0429 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0



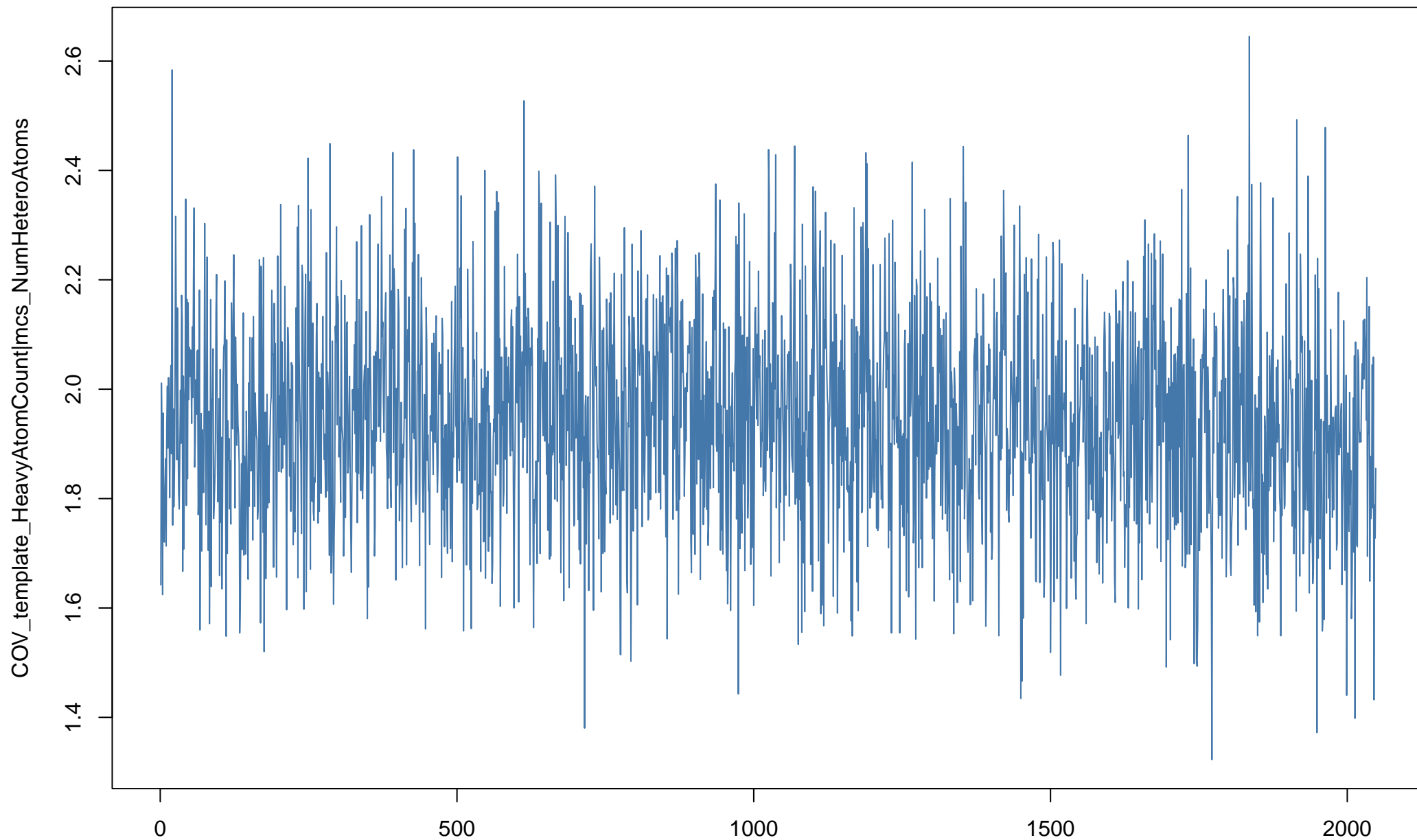
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.056 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0



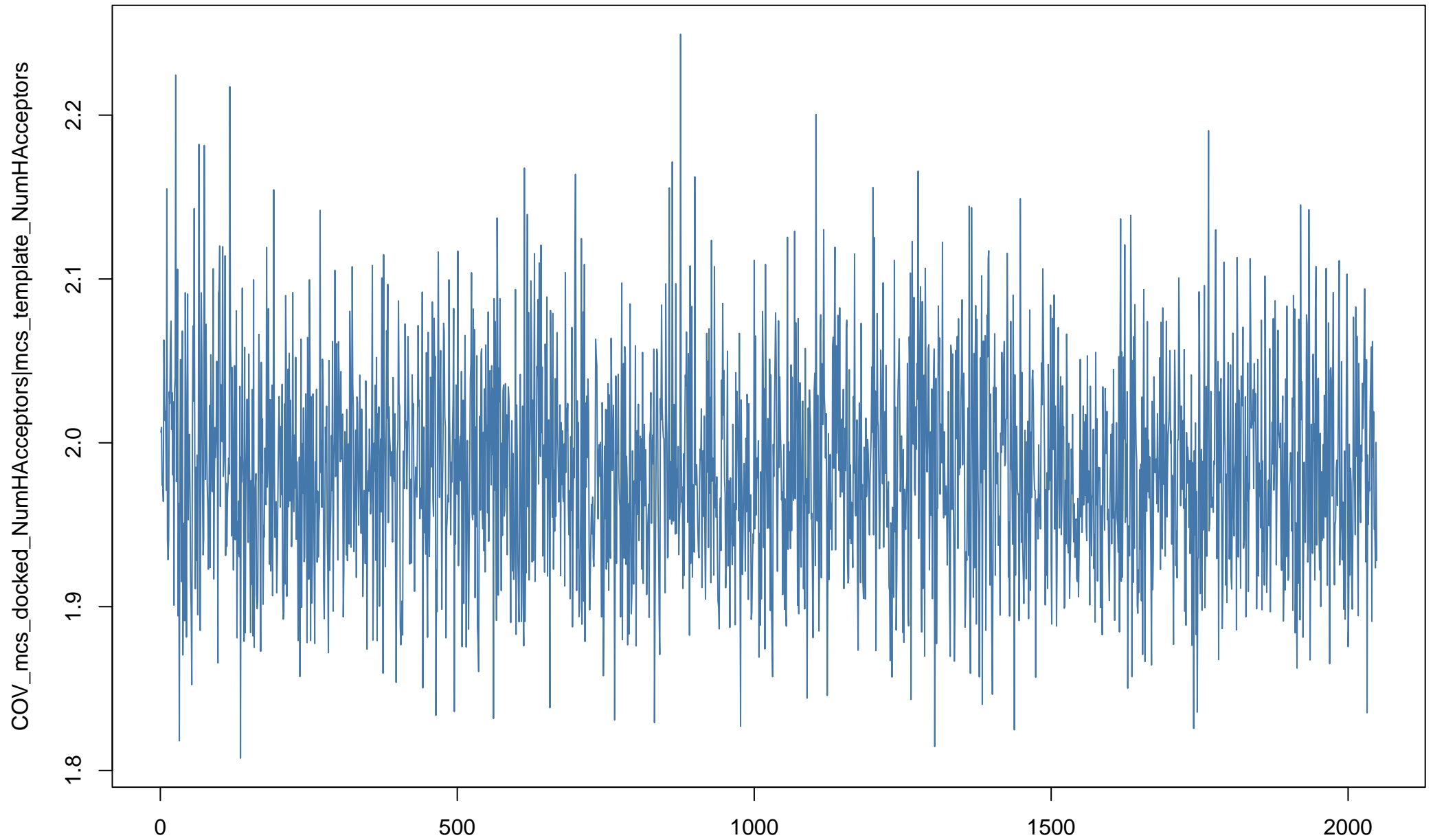
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1310 | BMK = 0.102 | MCSE(6.27) = 3.11 | stat: FALSE | burn: 0



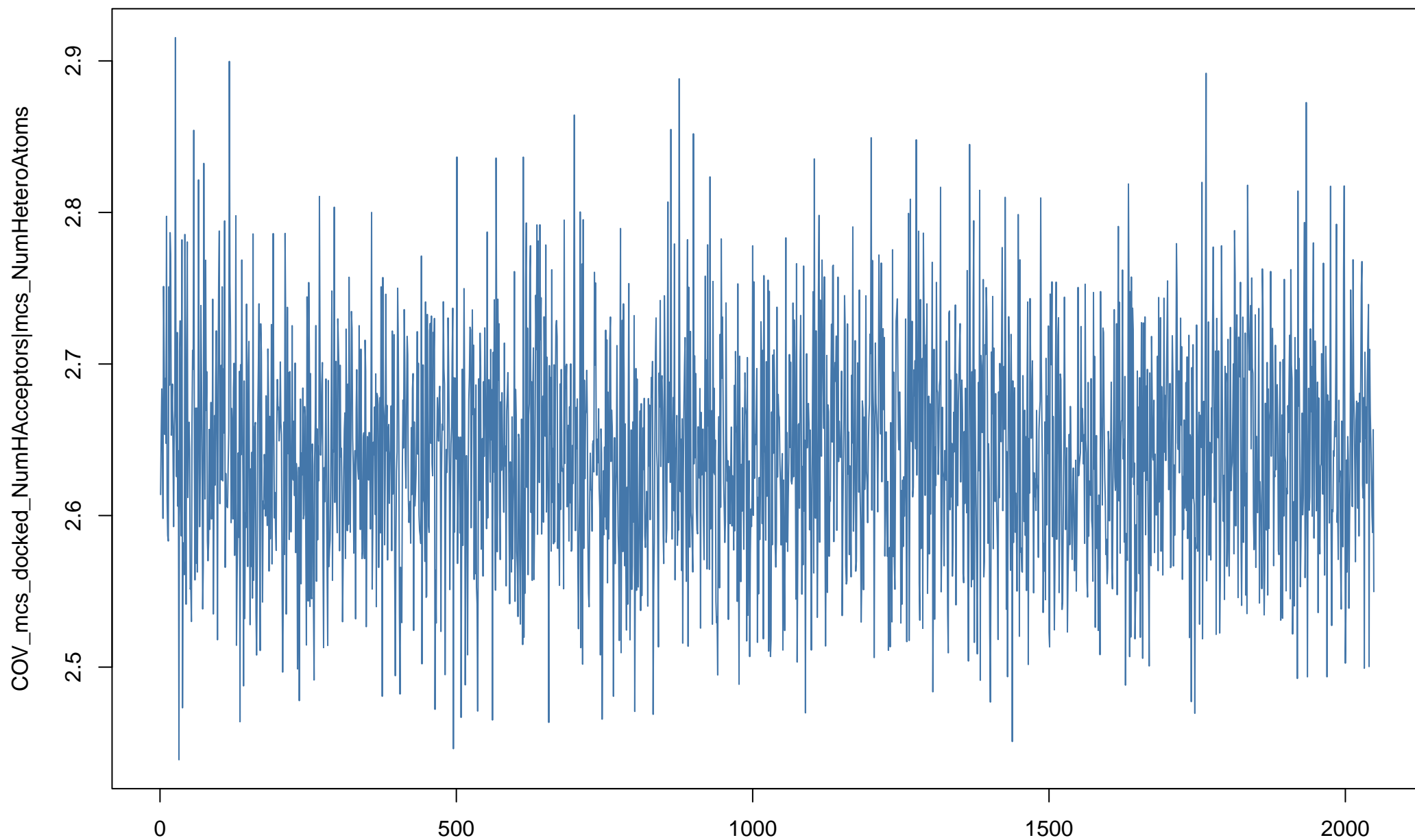
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1500 | BMK = 0.0539 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0414 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0



COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0464 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0



COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0632 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0

