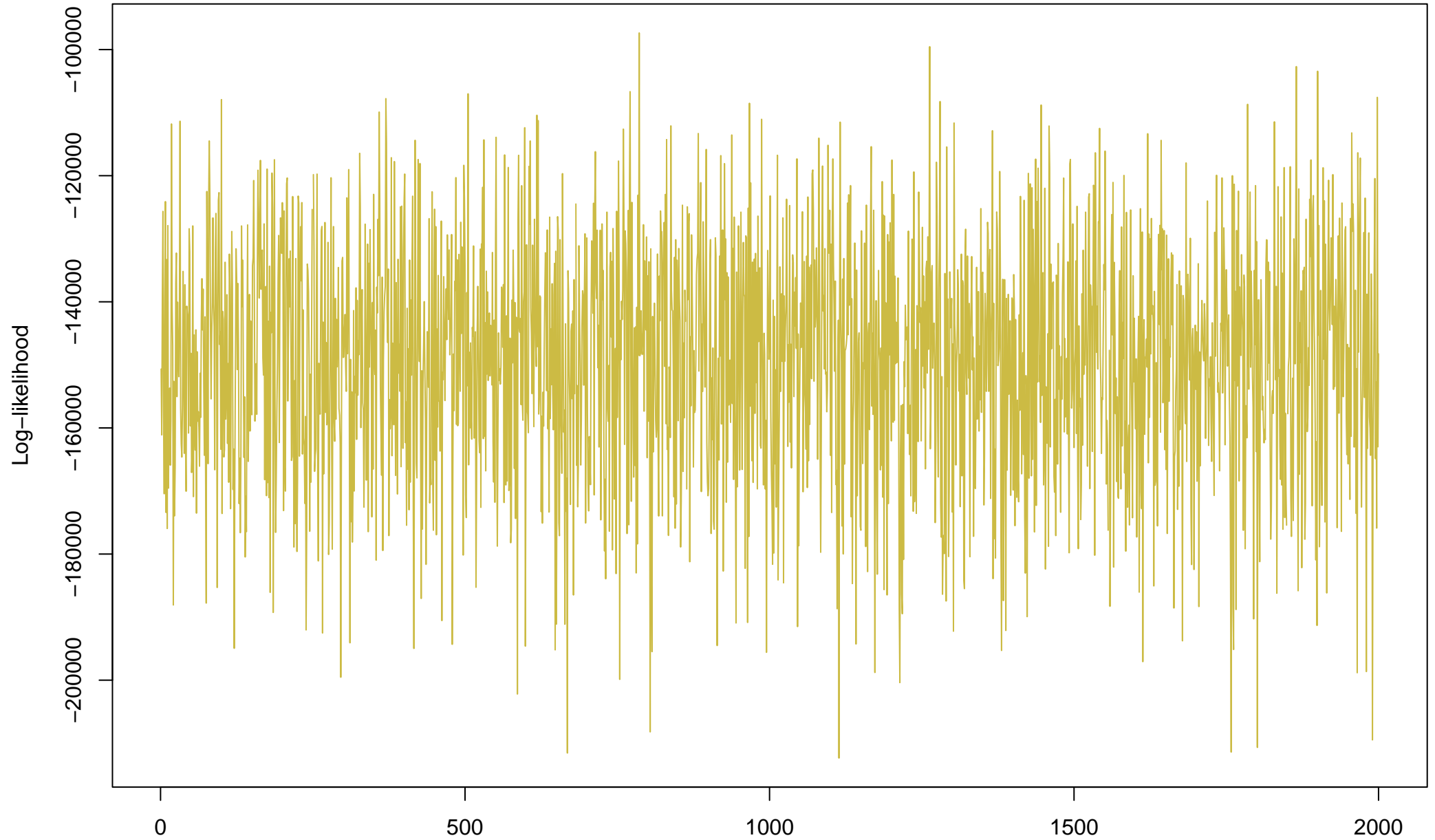**Stats**

min ESS = 1446.38696964171
max BMK = 0.114837801201167
max MCSE = 2.53829012117836
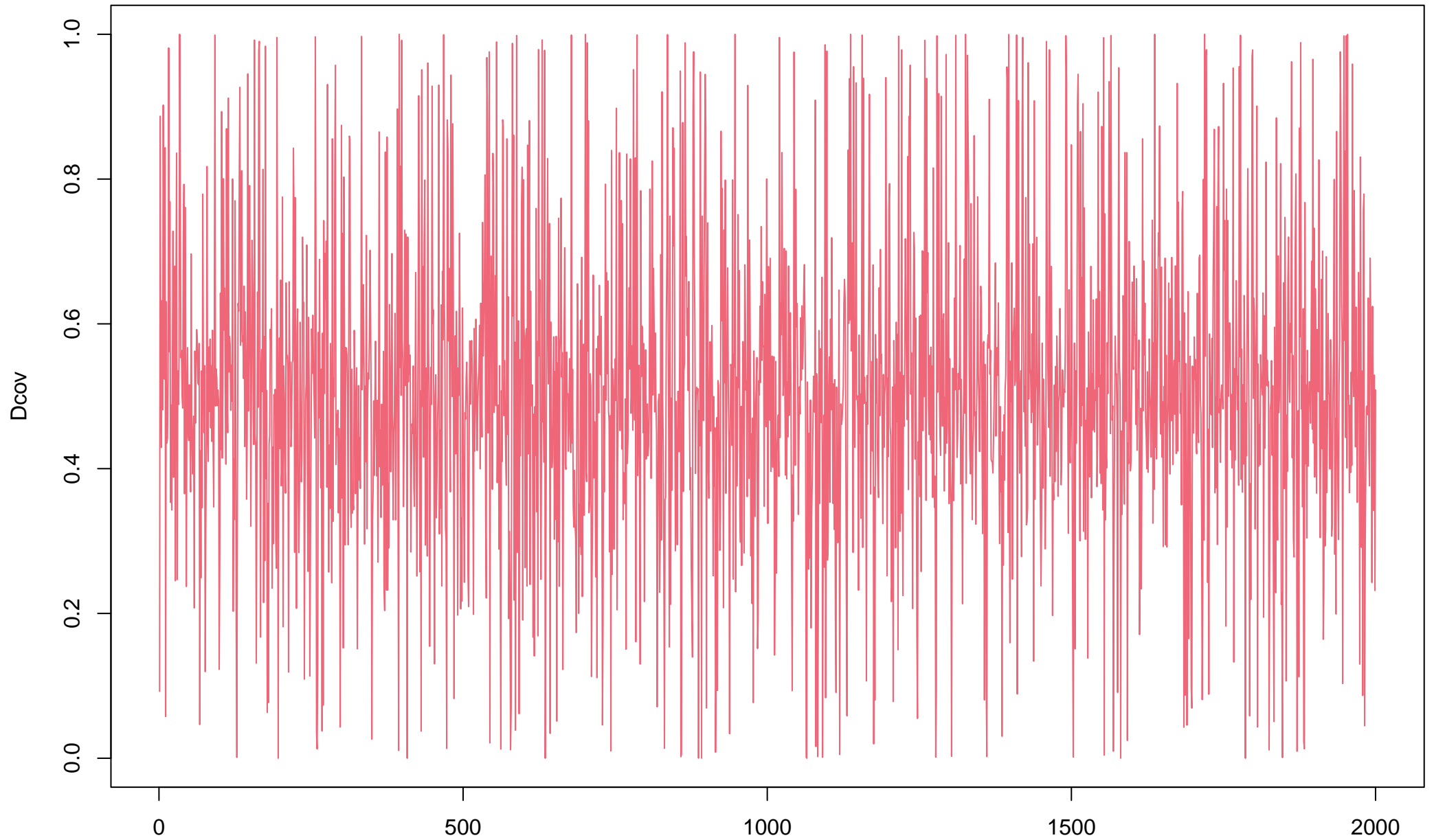all stationary: FALSE

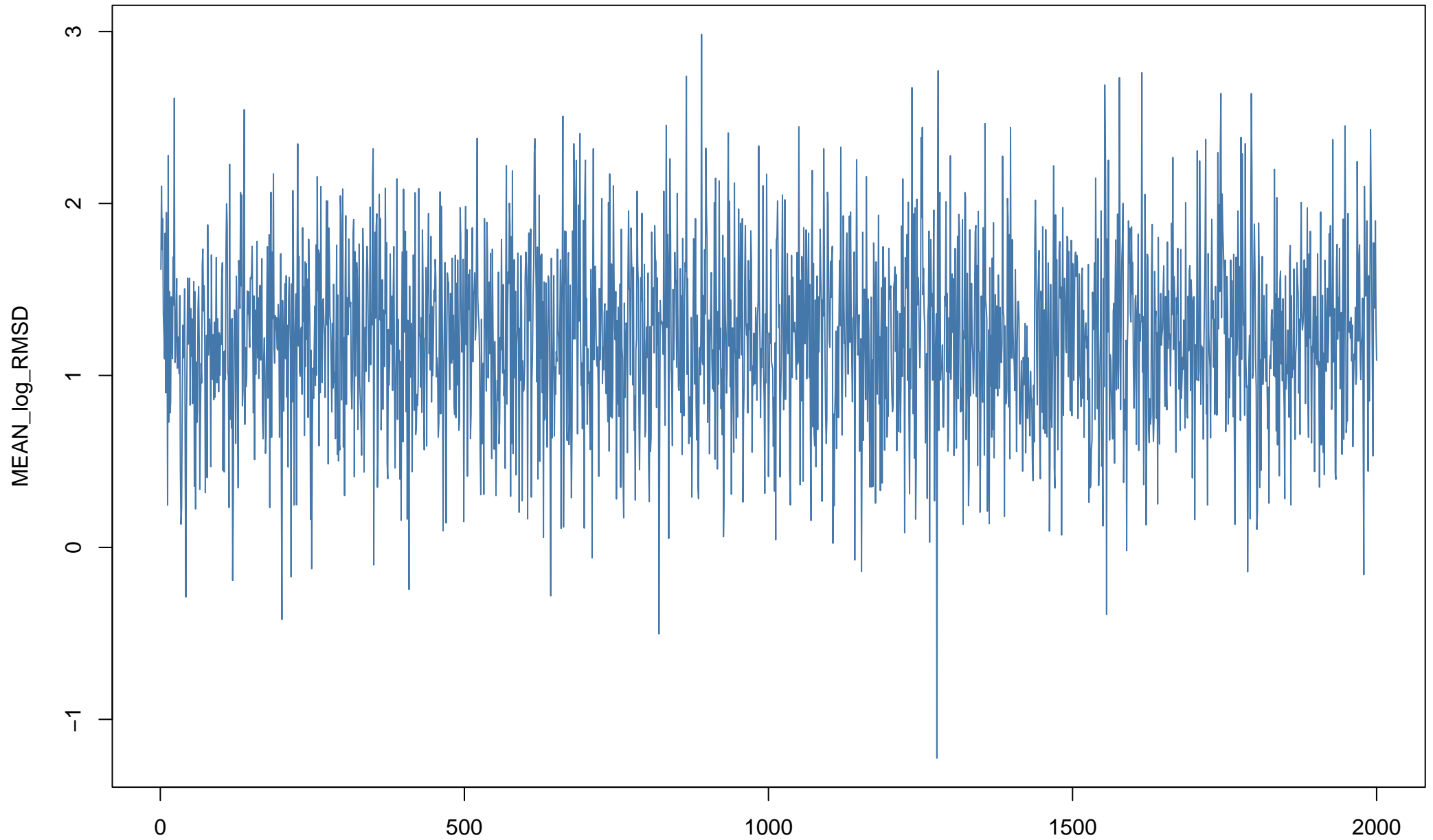**Log−likelihood**
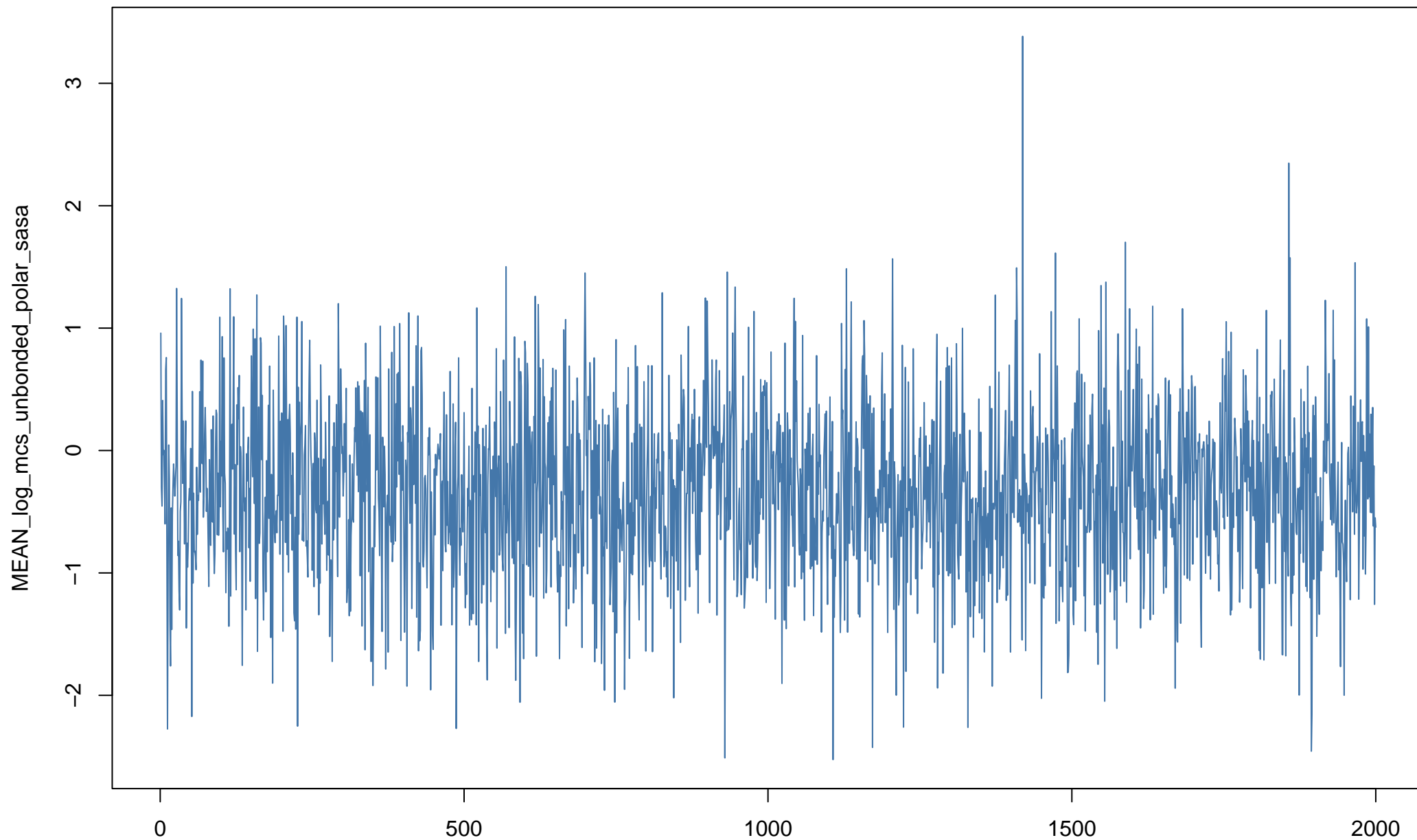**ESS = NA | BMK = 0.0873 | MCSE(6.27) = 2.2 | stat: FALSE**

Dcov
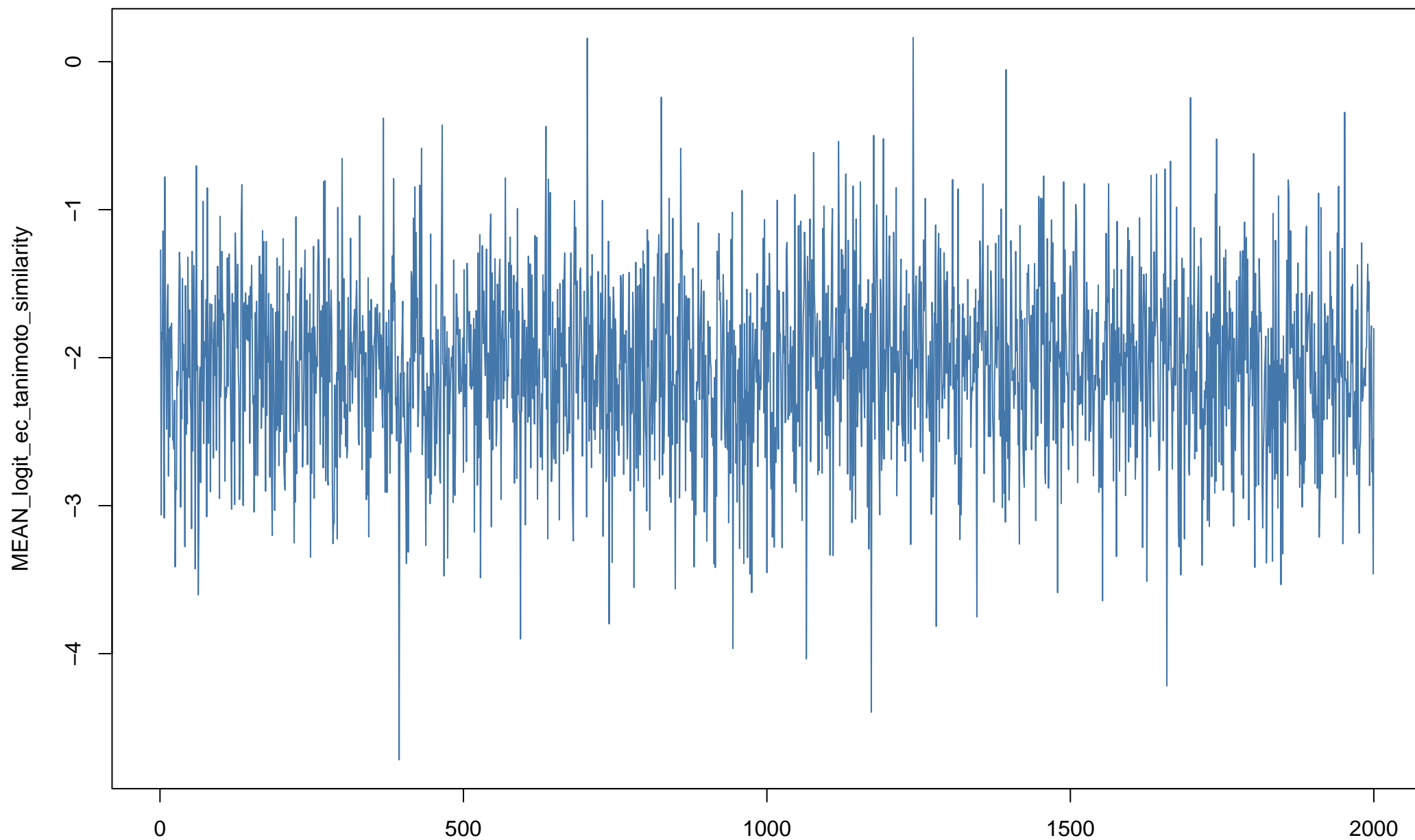**ESS = 2000 | BMK = 0.0616 | MCSE(6.27) = 2.38 | stat: TRUE**

MEAN_log_RMSD
ESS = 2000 | BMK = 0.0426 | MCSE(6.27) = 2.24 | stat: TRUE
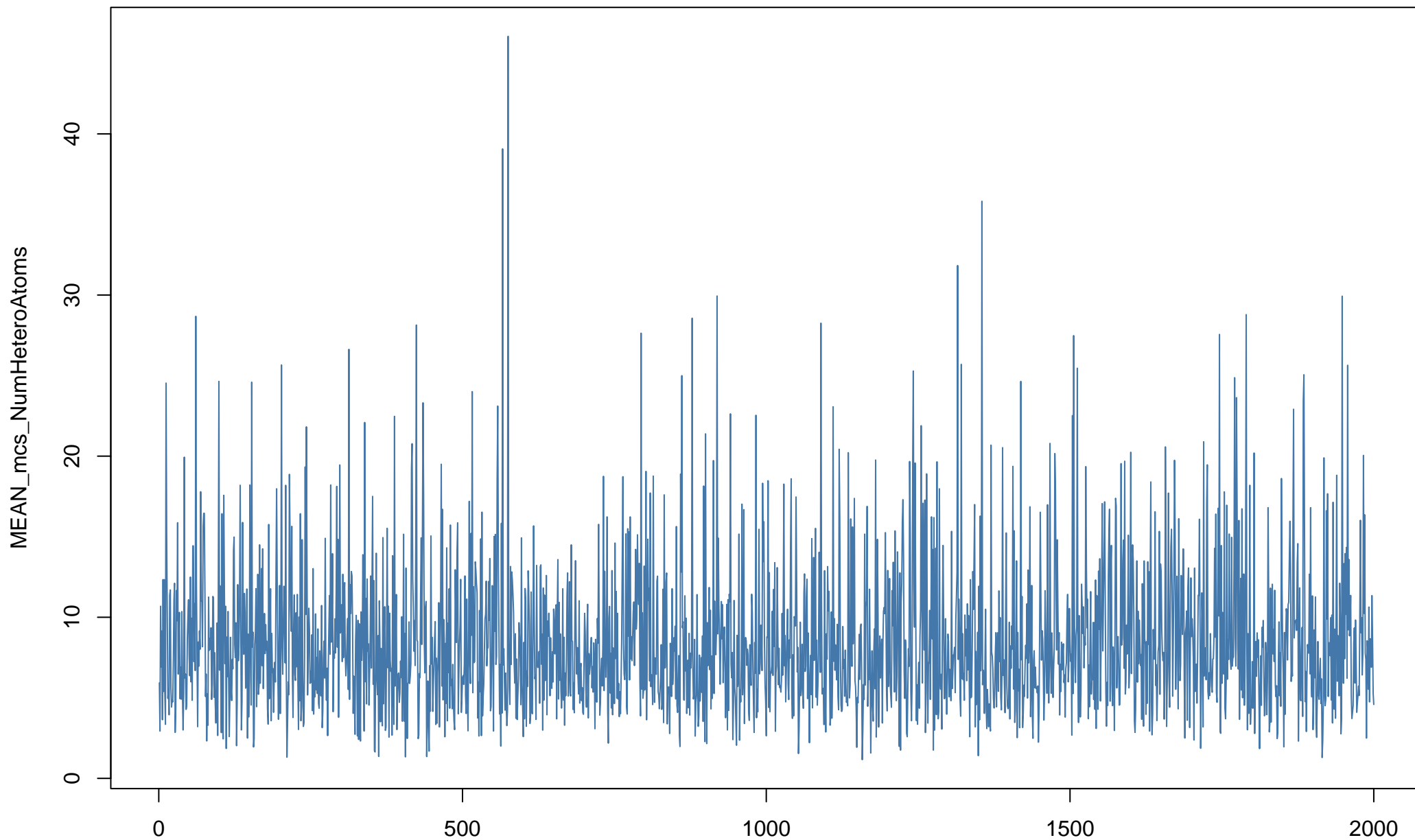
MEAN_log_mcs_unbonded_polar_sasa
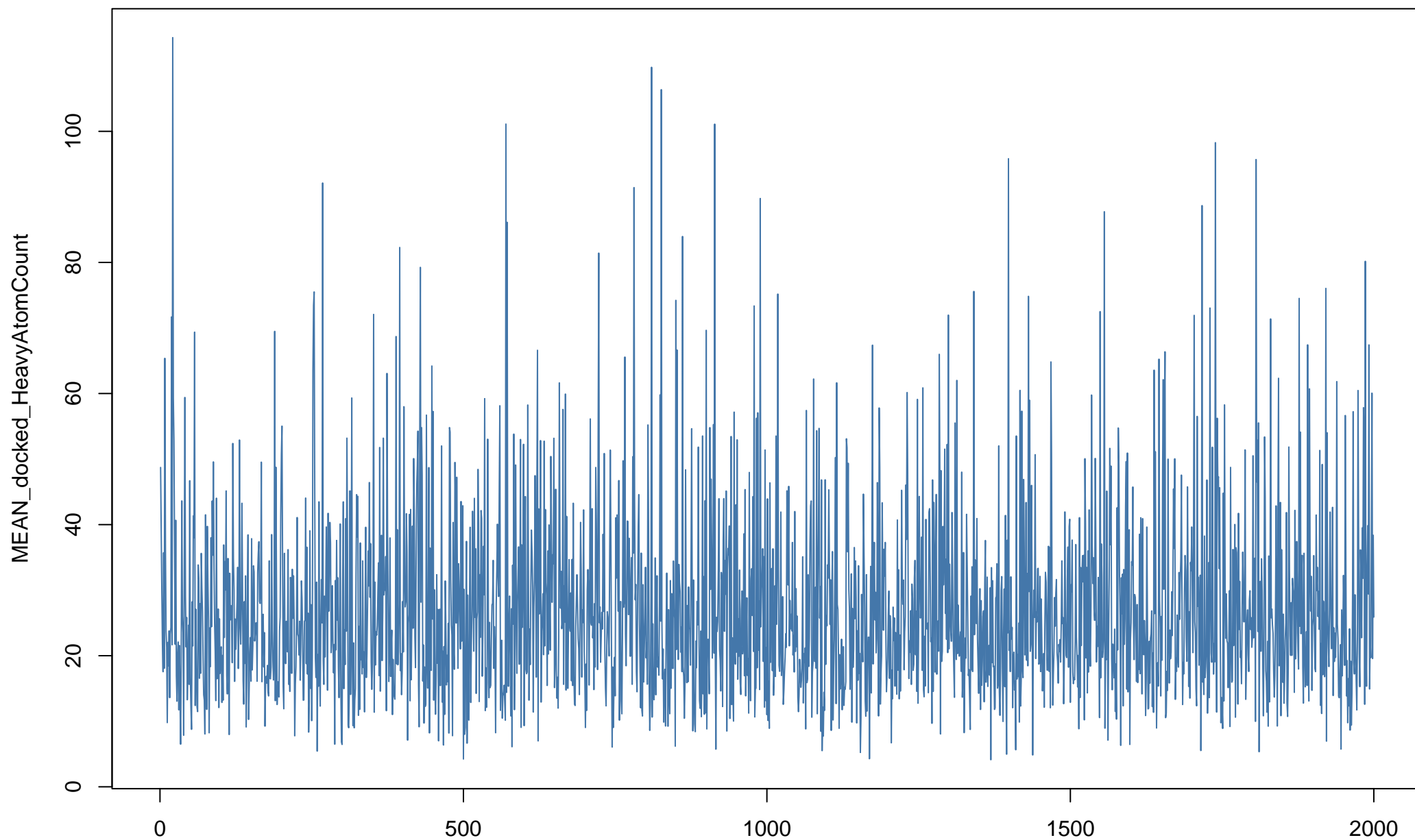**ESS = 1860 | BMK = 0.0583 | MCSE(6.27) = 2.38 | stat: TRUE**

MEAN_logit_ec_tanimoto_similarity
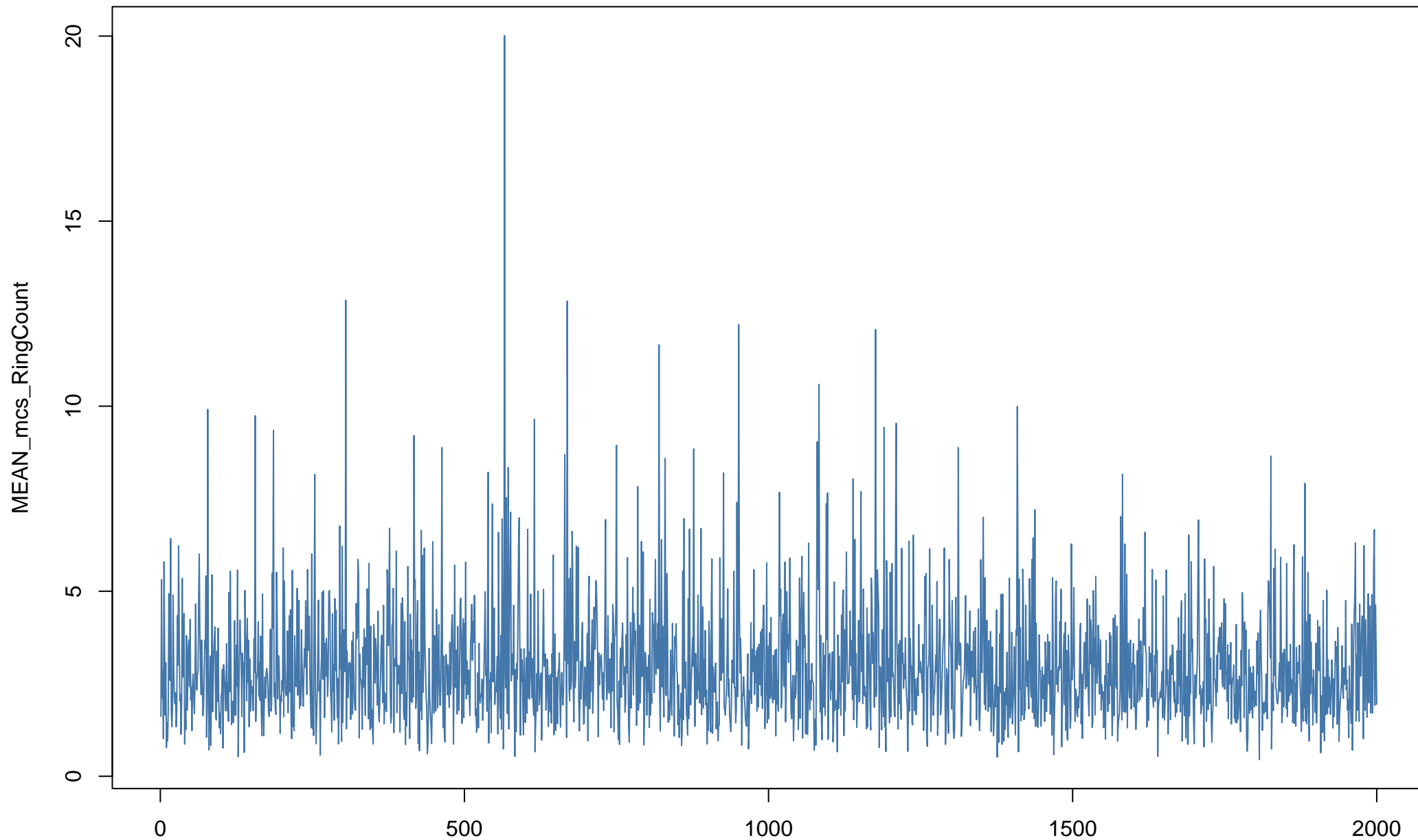**ESS = 2000 | BMK = 0.0442 | MCSE(6.27) = 2.19 | stat: TRUE**

MEAN_mcs_NumHeteroAtoms
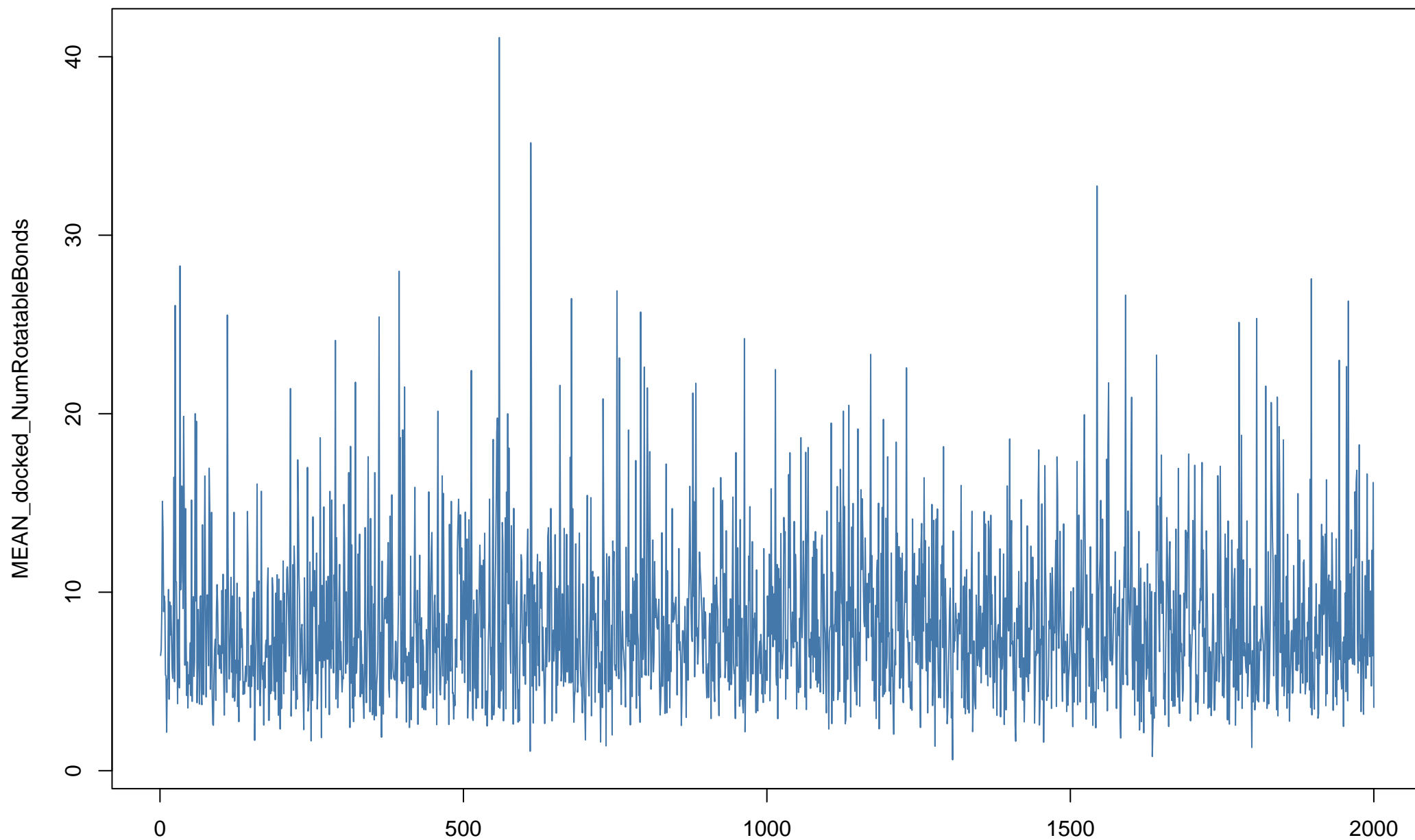**ESS = 2000 | BMK = 0.0587 | MCSE(6.27) = 2.28 | stat: TRUE**

MEAN_docked_HeavyAtomCount
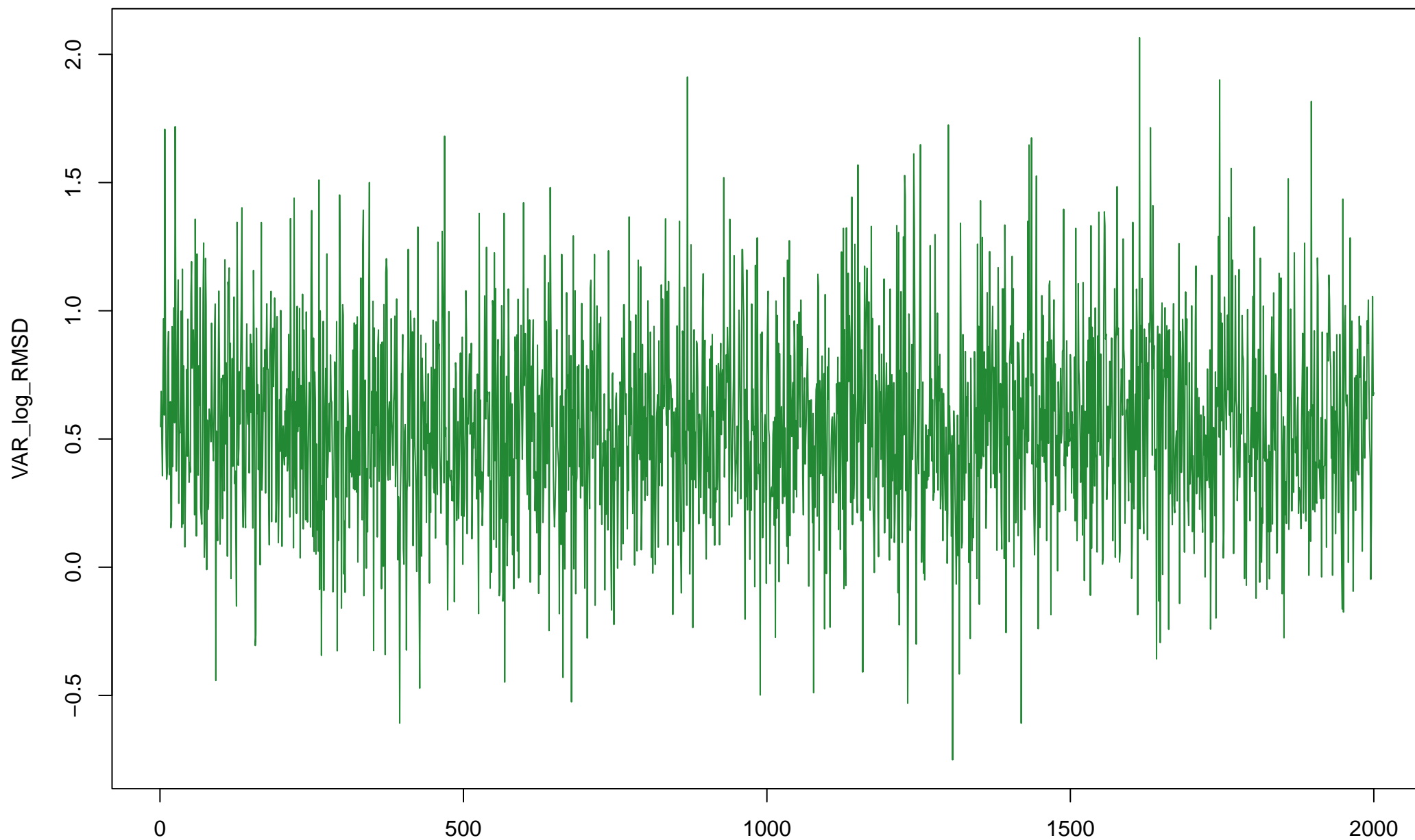**ESS = 1910 | BMK = 0.0628 | MCSE(6.27) = 2.23 | stat: TRUE**

MEAN_mcs_RingCount
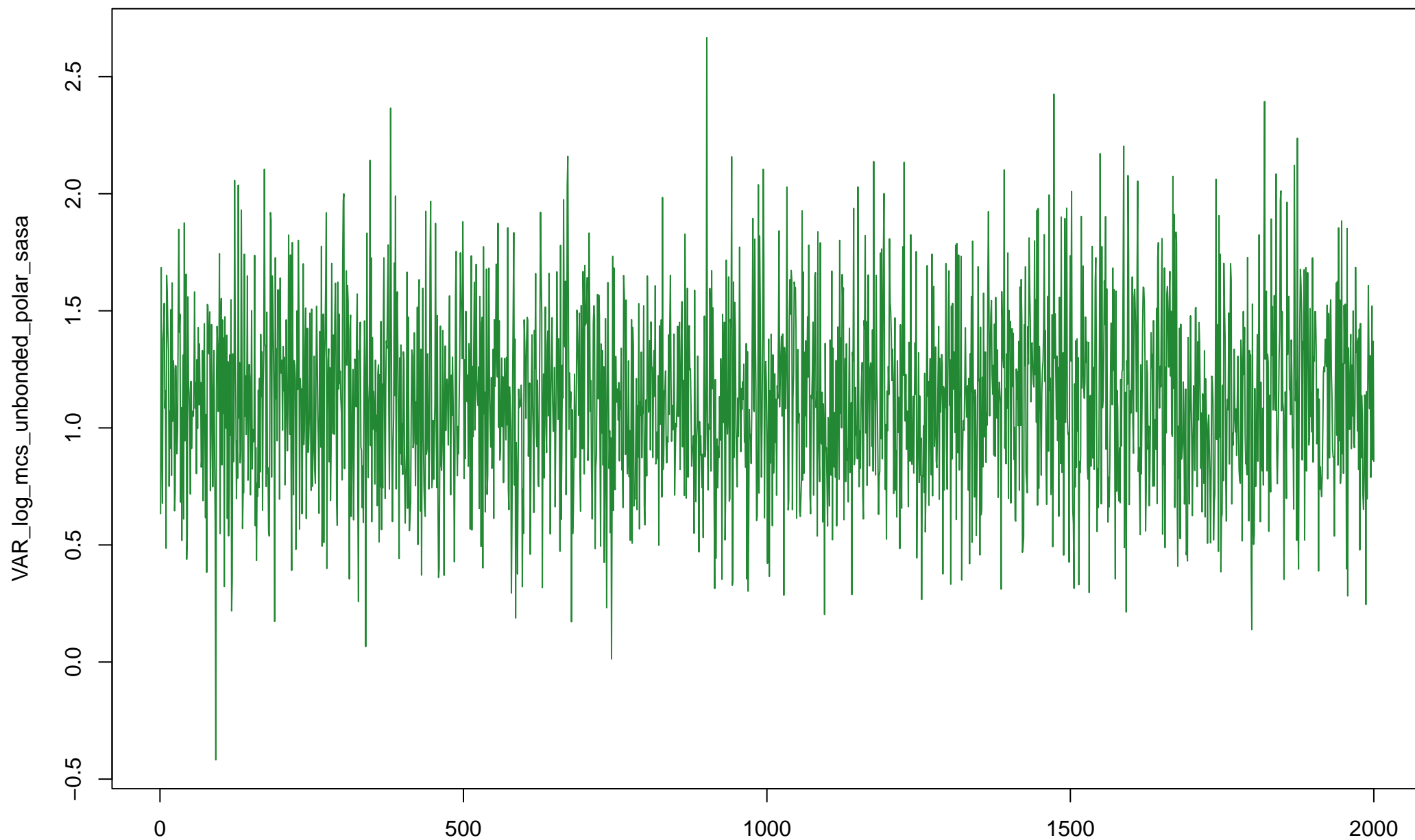**ESS = 1980 | BMK = 0.0454 | MCSE(6.27) = 2.23 | stat: TRUE**

MEAN_docked_NumRotatableBonds
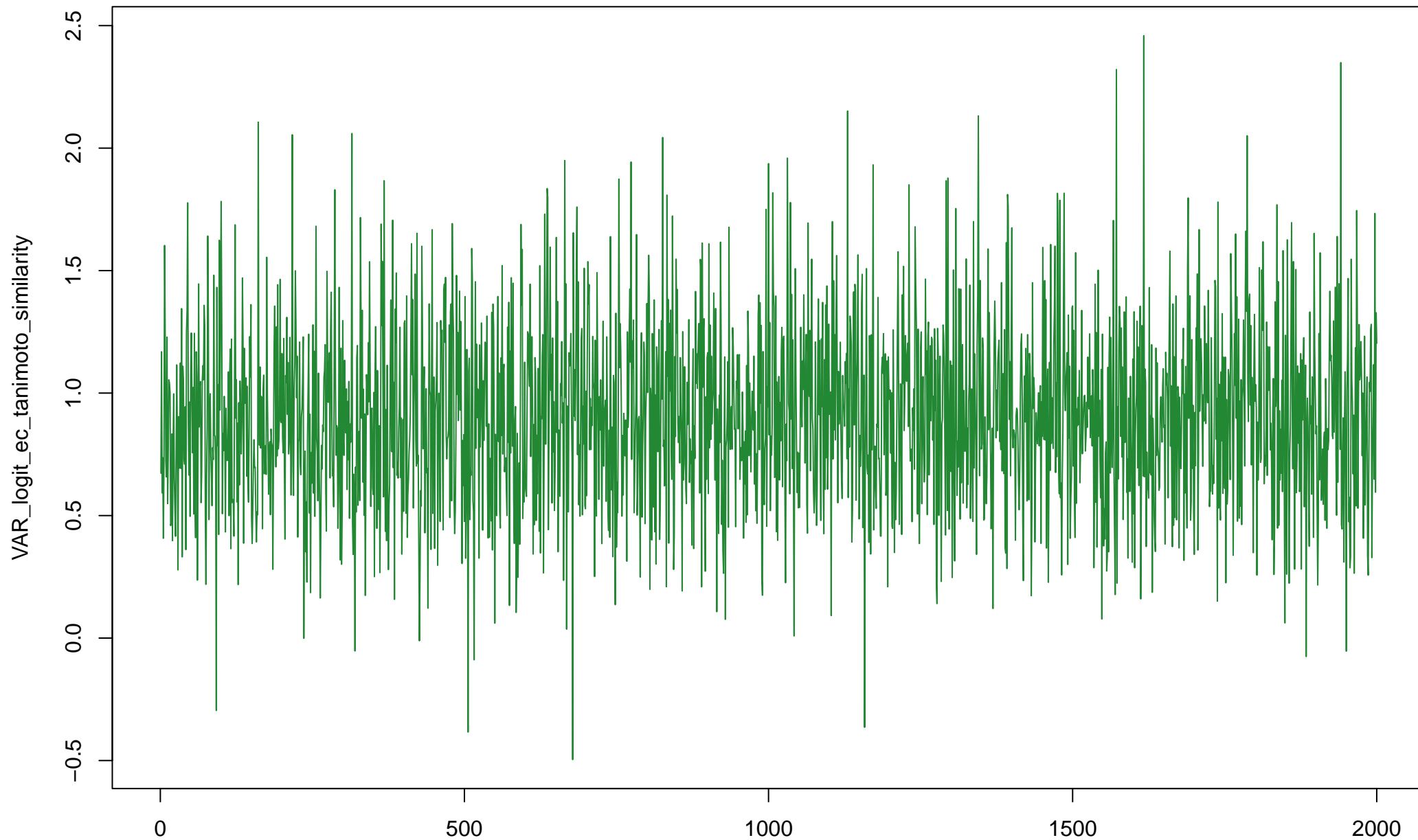**ESS = 2000 | BMK = 0.0552 | MCSE(6.27) = 2.23 | stat: TRUE**

VAR_log_RMSD
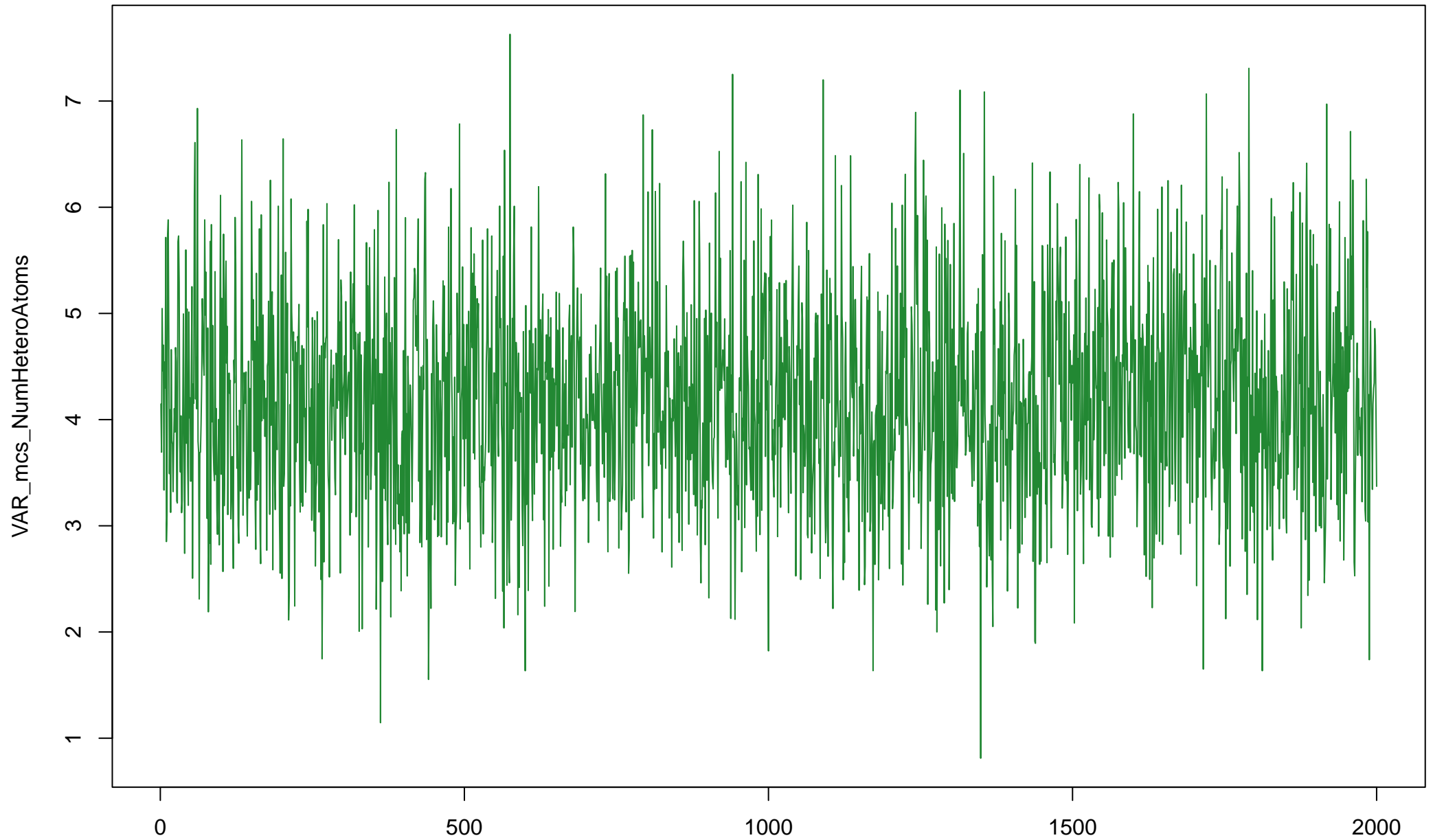**ESS = 2000 | BMK = 0.0342 | MCSE(6.27) = 2.16 | stat: TRUE**

VAR_log_mcs_unbonded_polar_sasa
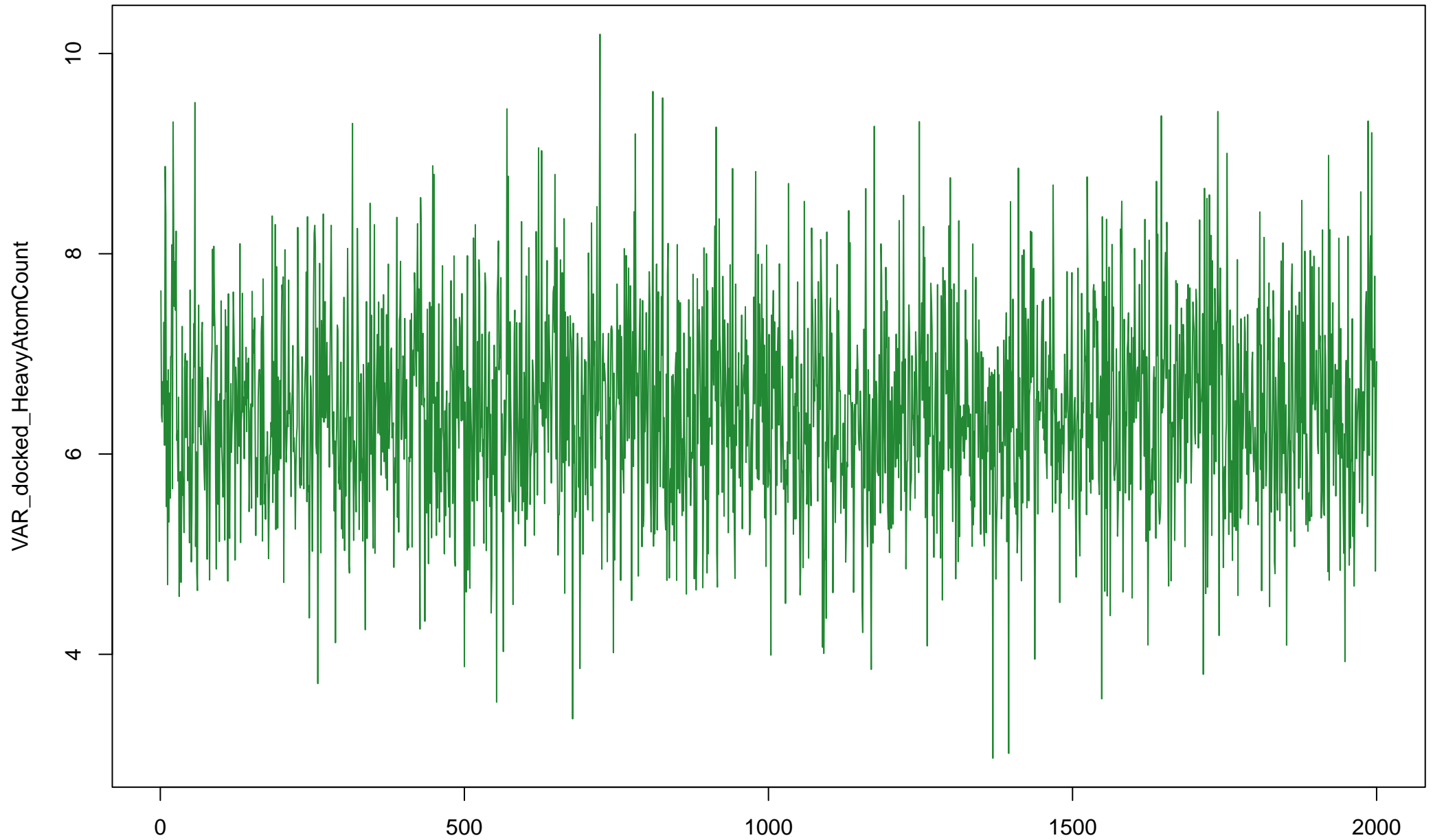**ESS = 2000 | BMK = 0.0444 | MCSE(6.27) = 2.27 | stat: TRUE**

VAR_logit_ec_tanimoto_similarity
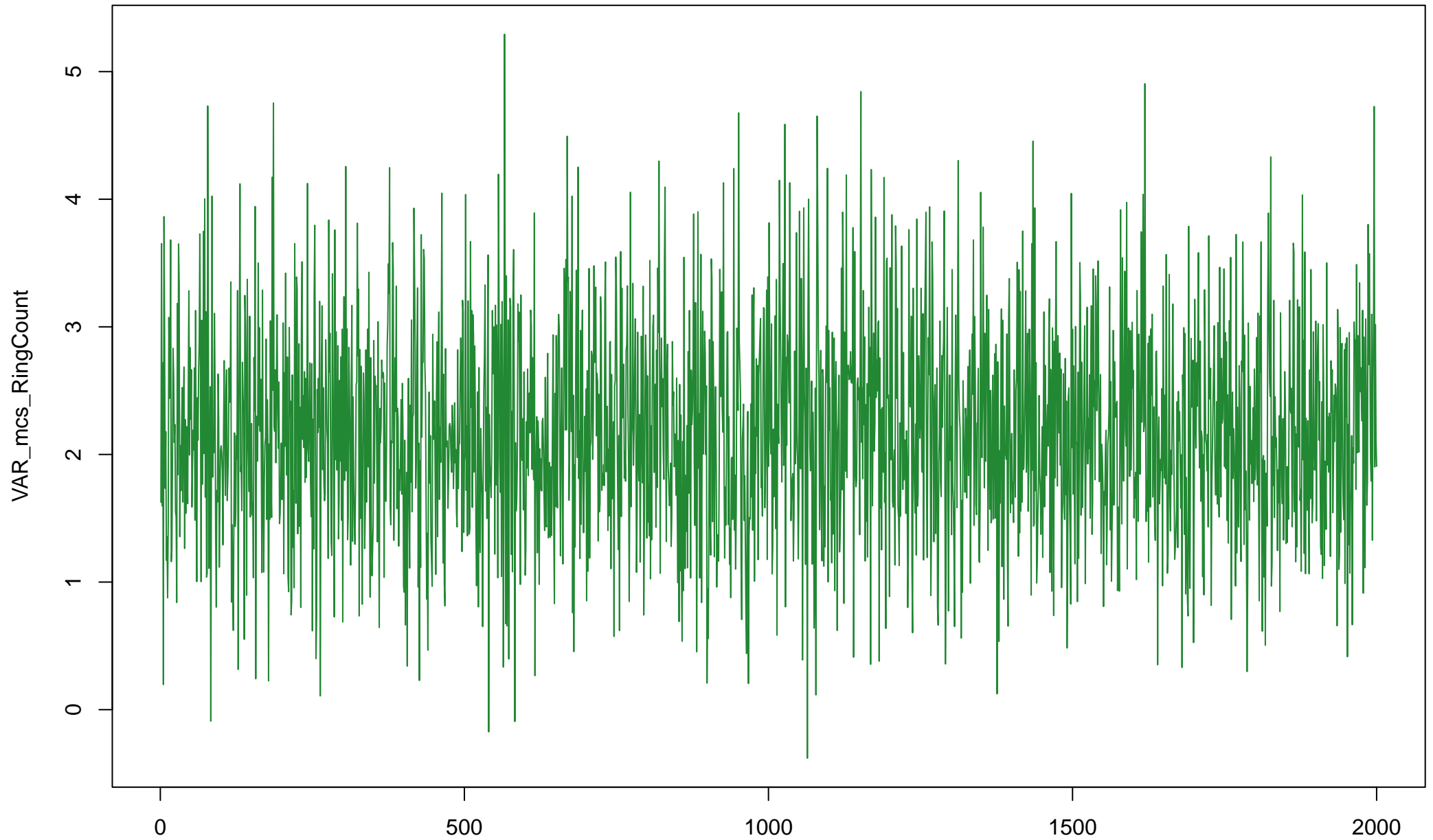**ESS = 2000 | BMK = 0.0433 | MCSE(6.27) = 2.21 | stat: TRUE**

VAR_mcs_NumHeteroAtoms
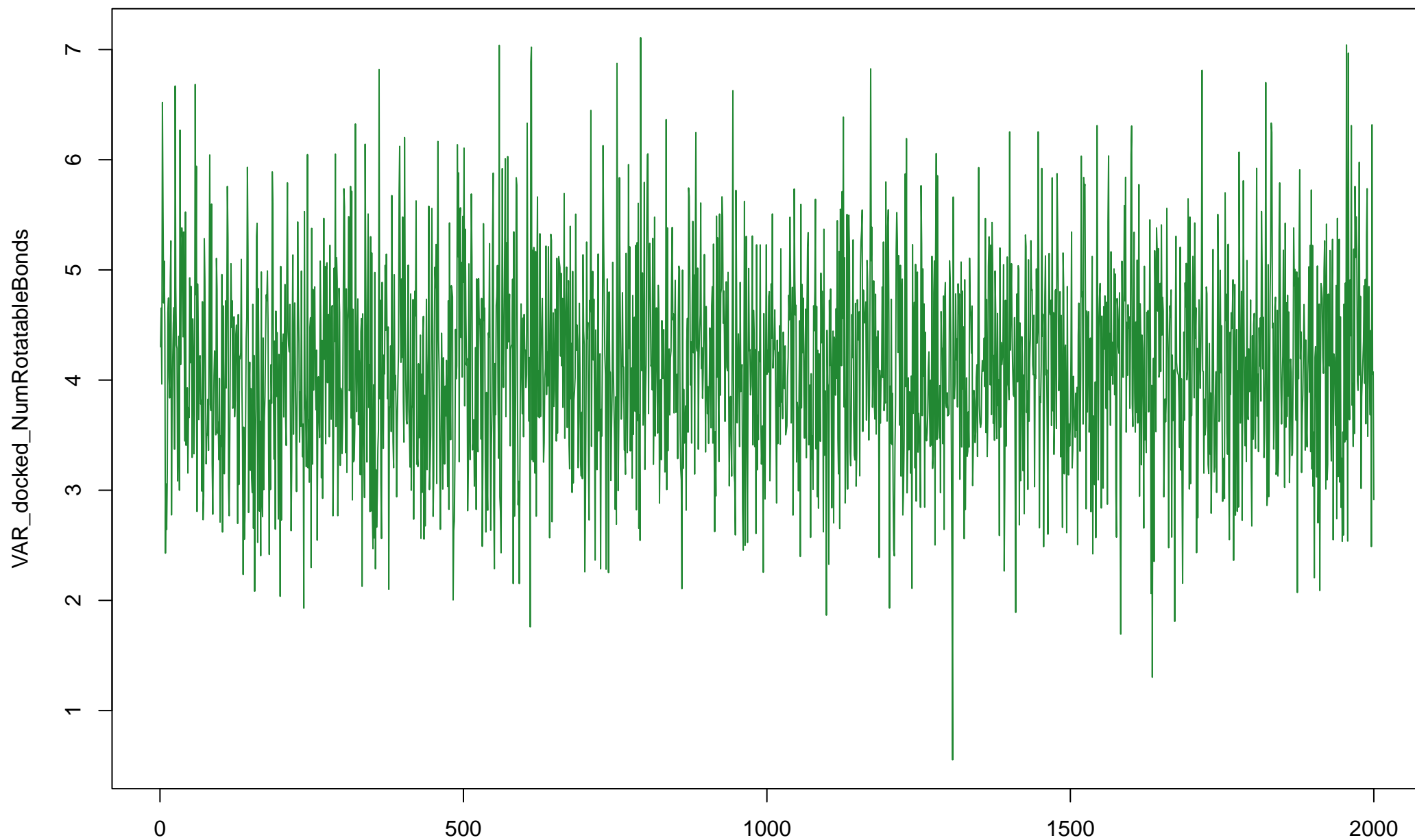**ESS = 2000 | BMK = 0.041 | MCSE(6.27) = 2.35 | stat: TRUE**

VAR_docked_HeavyAtomCount
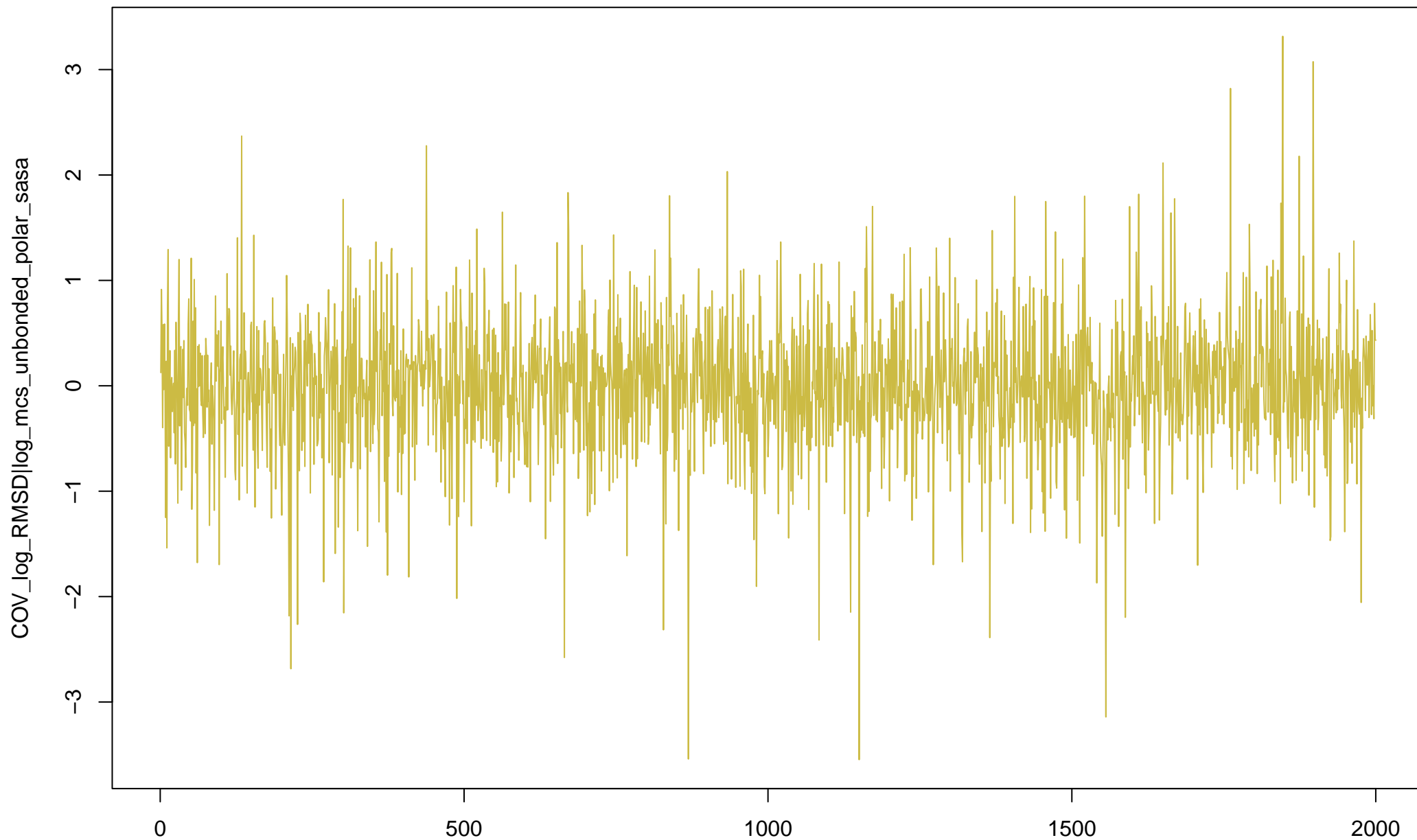**ESS = 2000 | BMK = 0.0376 | MCSE(6.27) = 2.3 | stat: TRUE**

VAR_mcs_RingCount
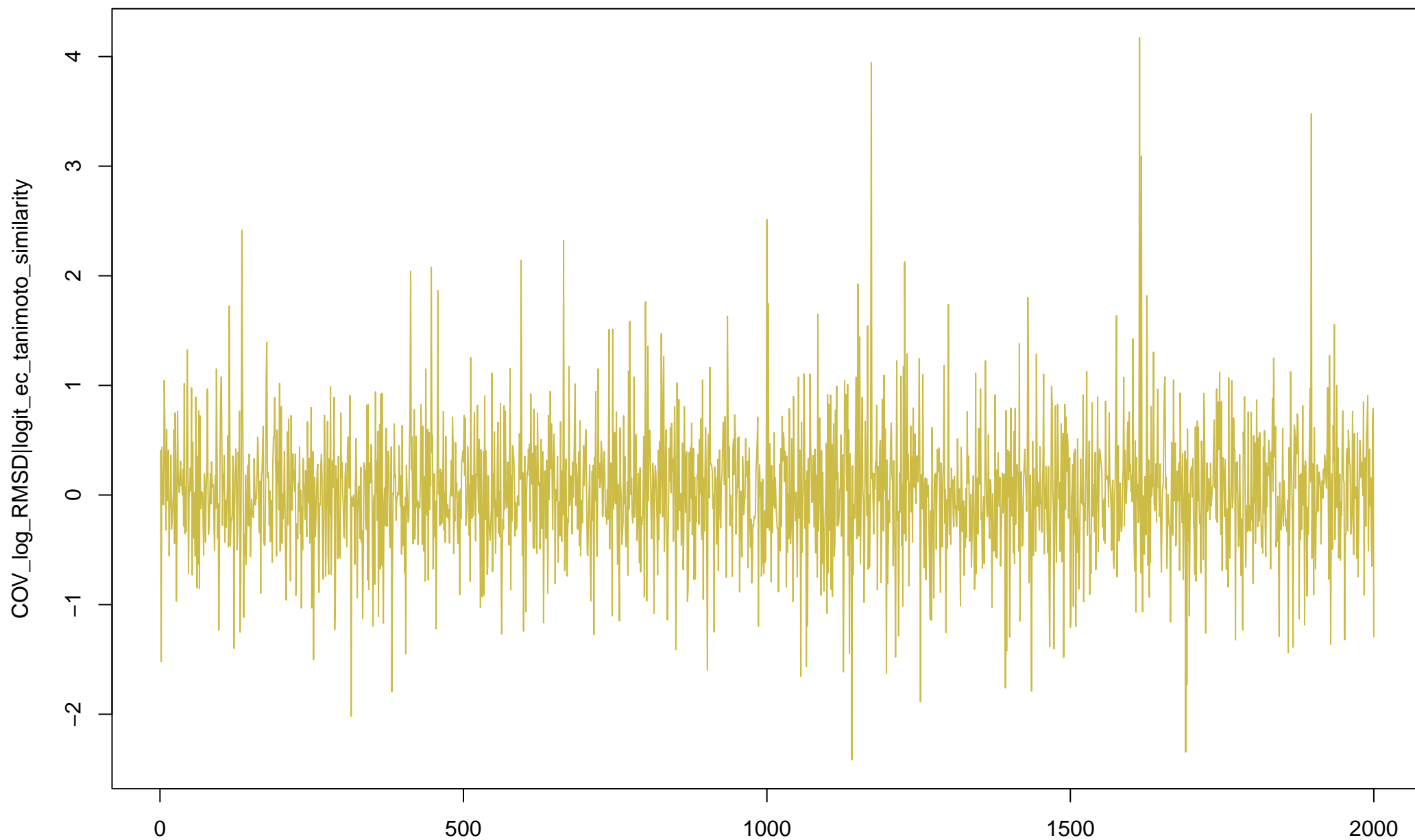**ESS = 2000 | BMK = 0.0374 | MCSE(6.27) = 2.17 | stat: TRUE**

VAR_docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0469 | MCSE(6.27) = 2.34 | stat: TRUE
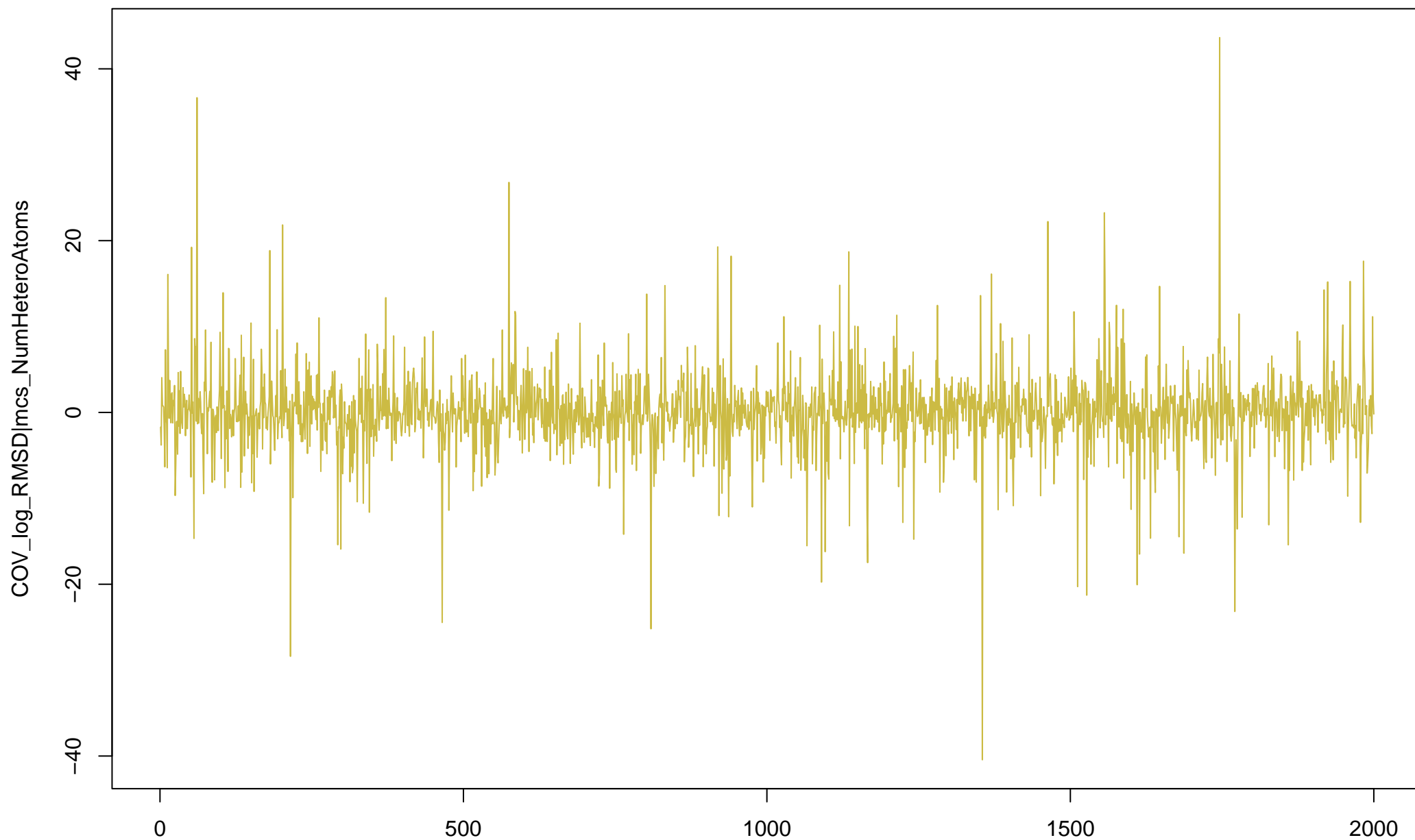
COV_log_RMSD|log_mcs_unbonded_polar_sasa
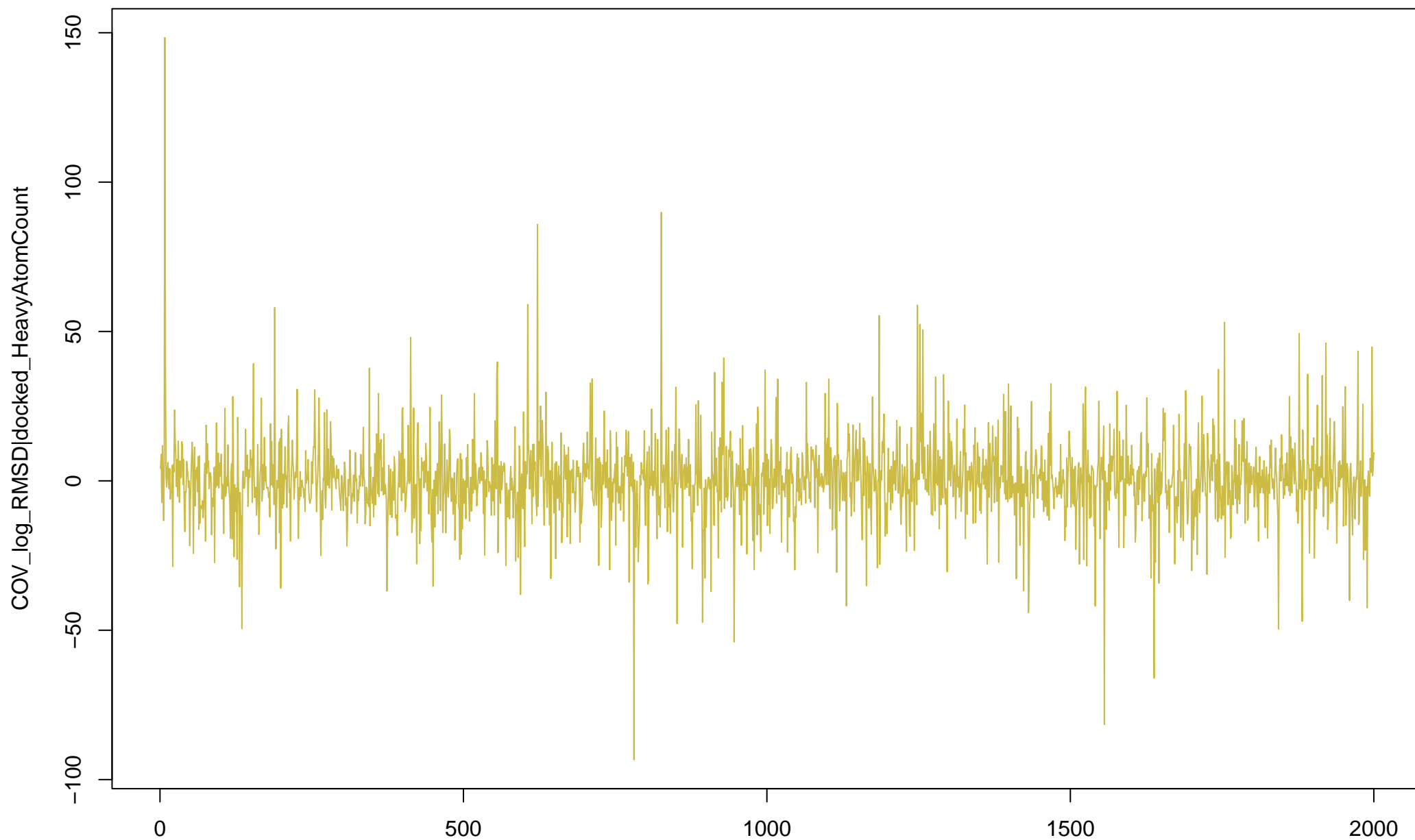**ESS = 2000 | BMK = 0.0661 | MCSE(6.27) = 2.21 | stat: TRUE**

COV_log_RMSD|logit_ec_tanimoto_similarity
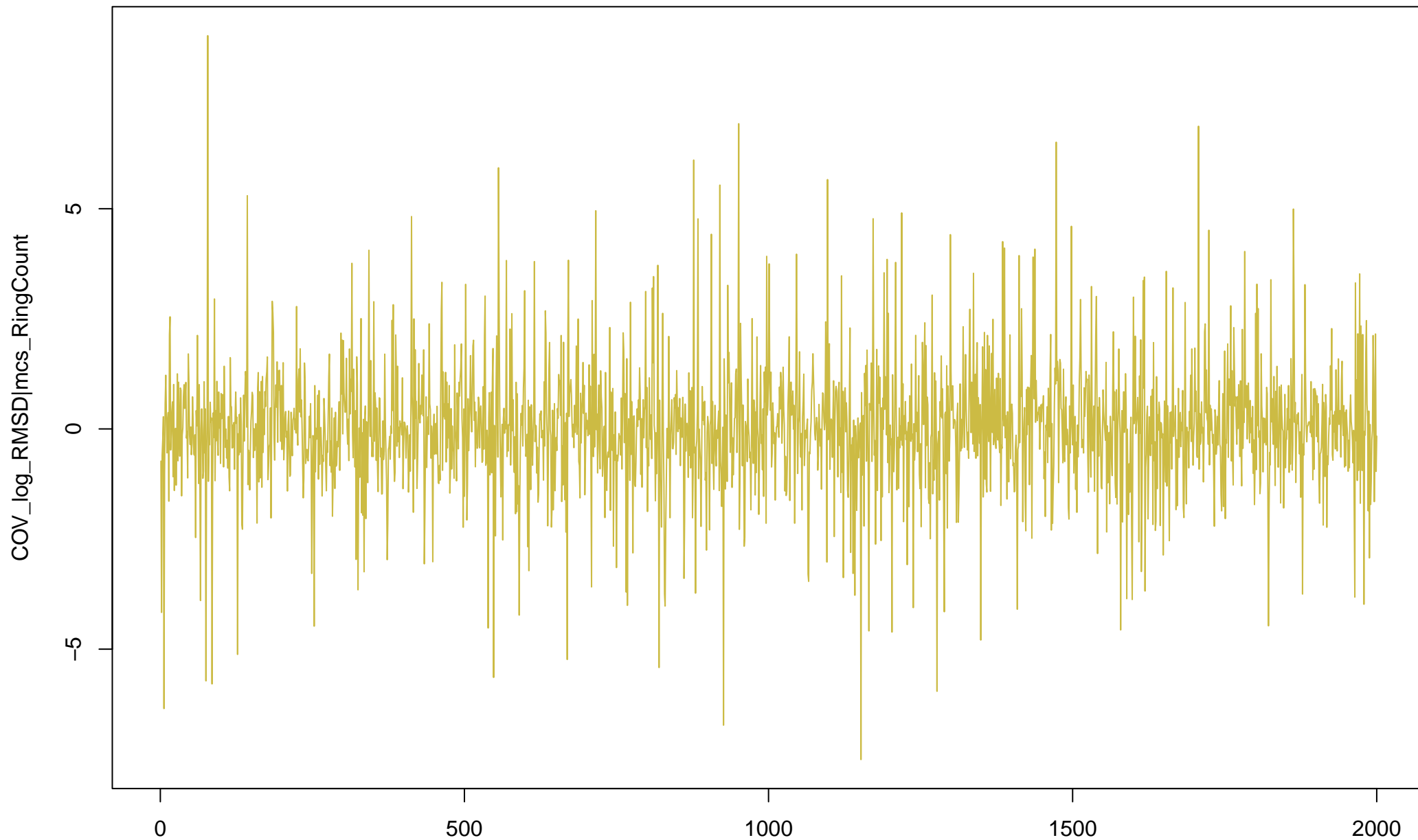**ESS = 2000 | BMK = 0.0757 | MCSE(6.27) = 2.13 | stat: TRUE**

COV_log_RMSD|mcs_NumHeteroAtoms
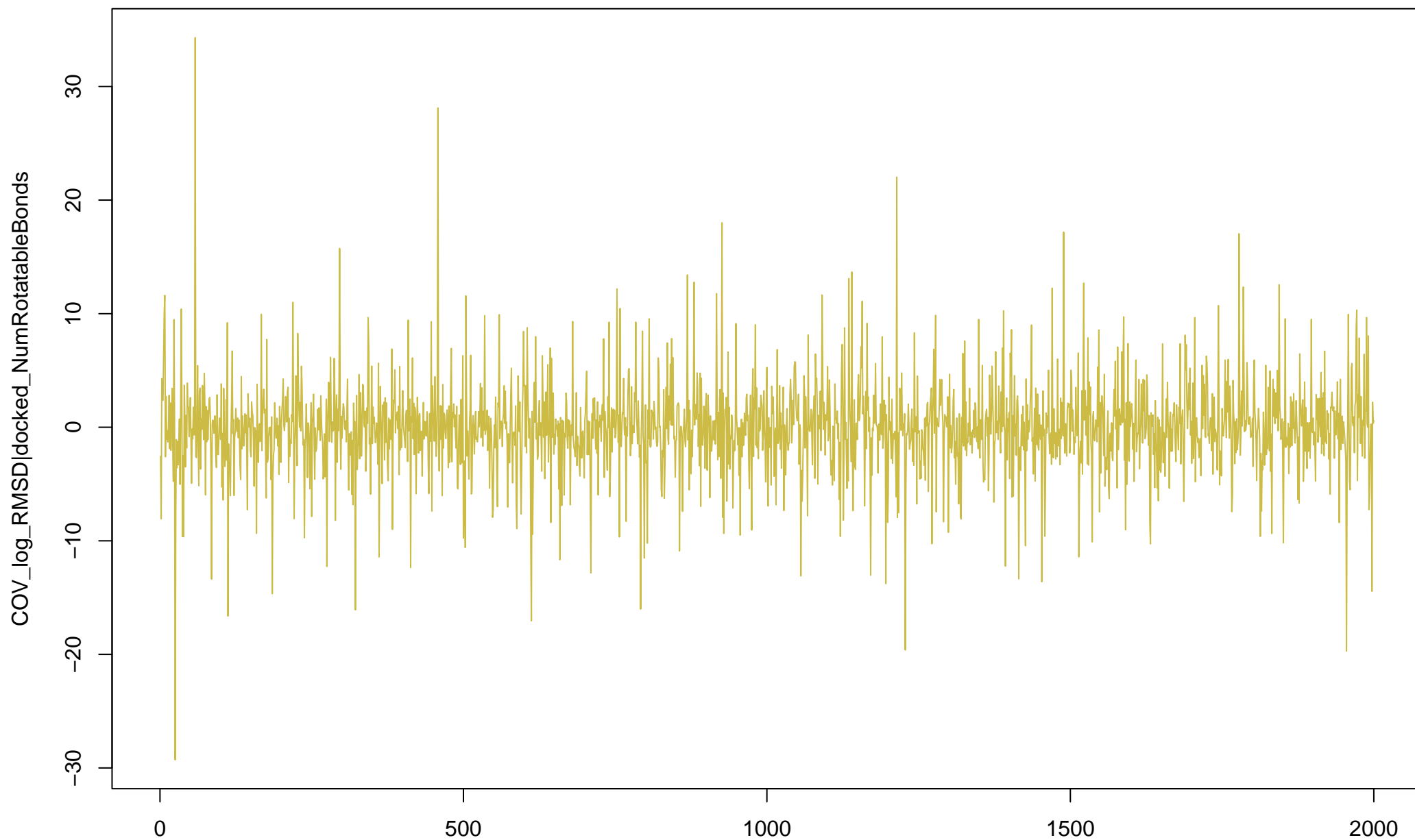**ESS = 2000 | BMK = 0.106 | MCSE(6.27) = 2.31 | stat: TRUE**

COV_log_RMSD|docked_HeavyAtomCount
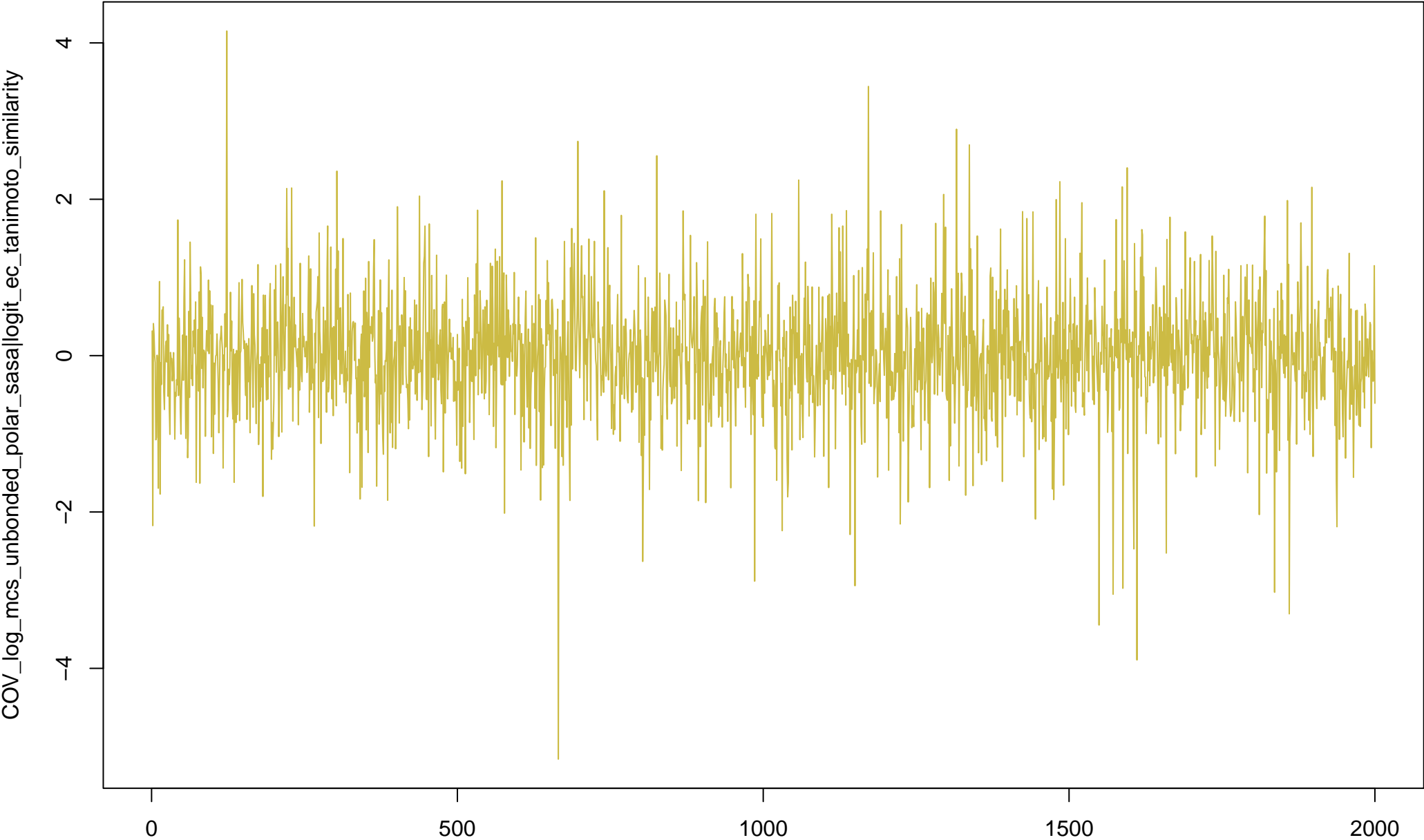**ESS = 1860 | BMK = 0.0879 | MCSE(6.27) = 2.42 | stat: TRUE**

COV_log_RMSD|mcs_RingCount
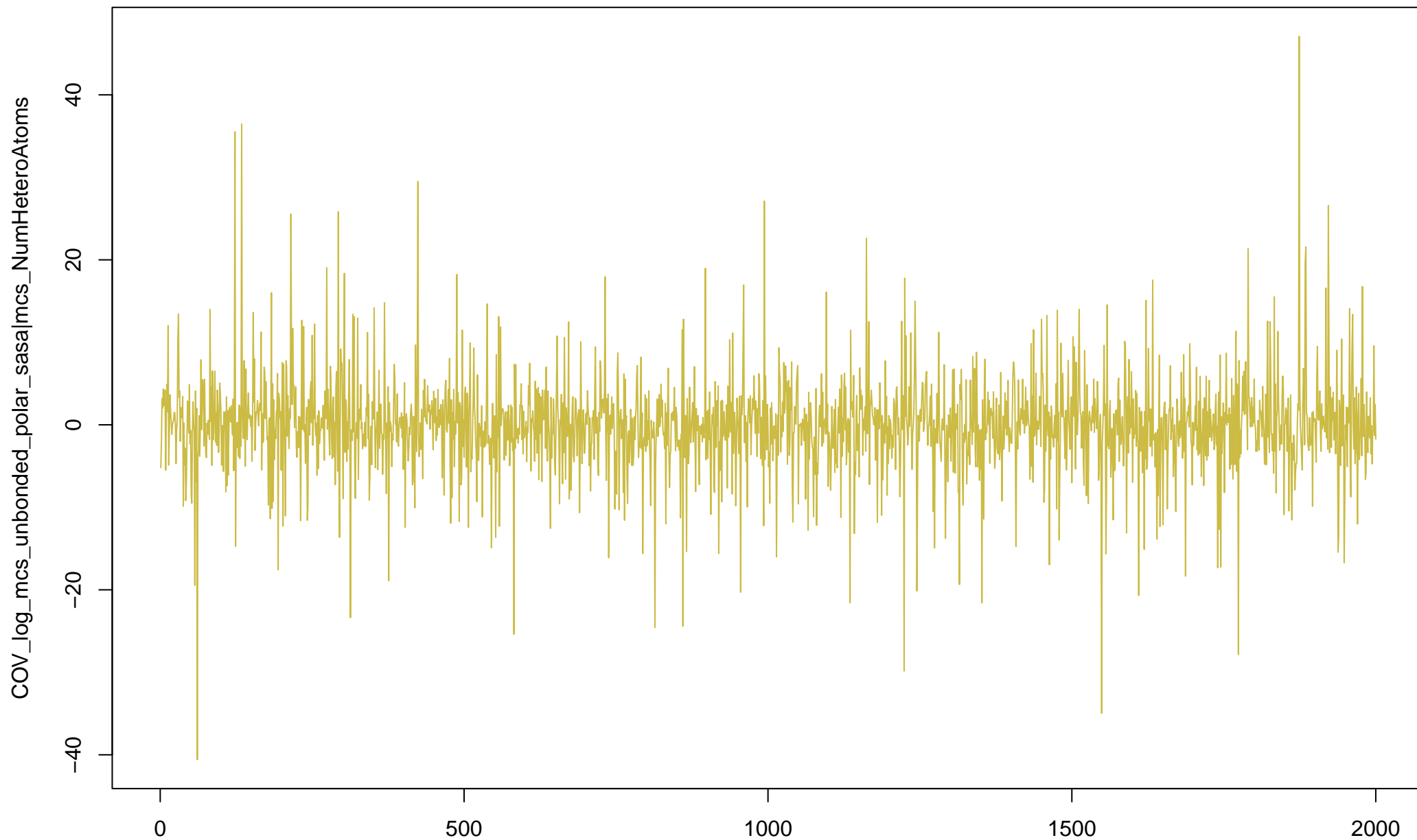**ESS = 2000 | BMK = 0.0792 | MCSE(6.27) = 2.42 | stat: TRUE**

COV_log_RMSD|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0871 | MCSE(6.27) = 2.29 | stat: TRUE
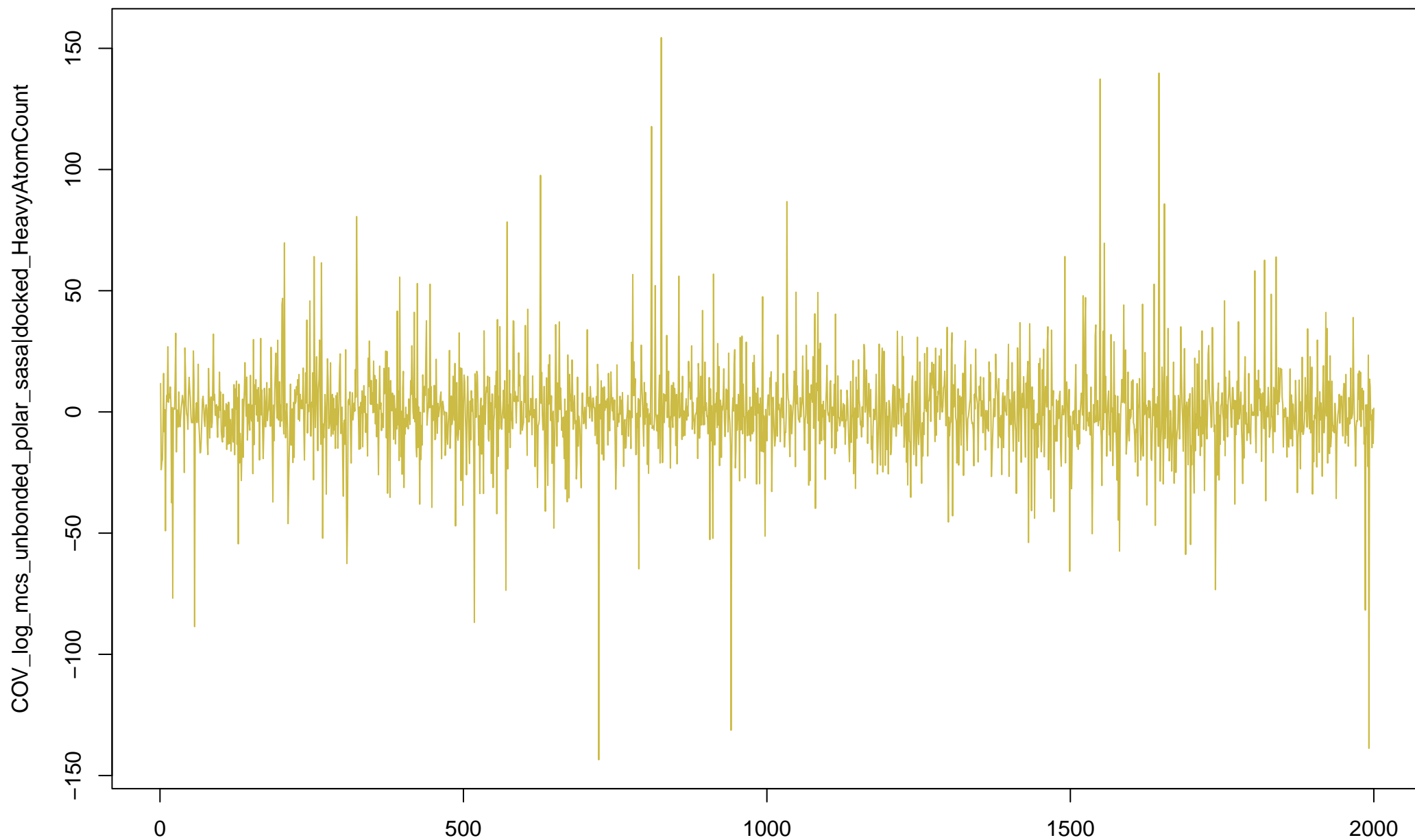
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
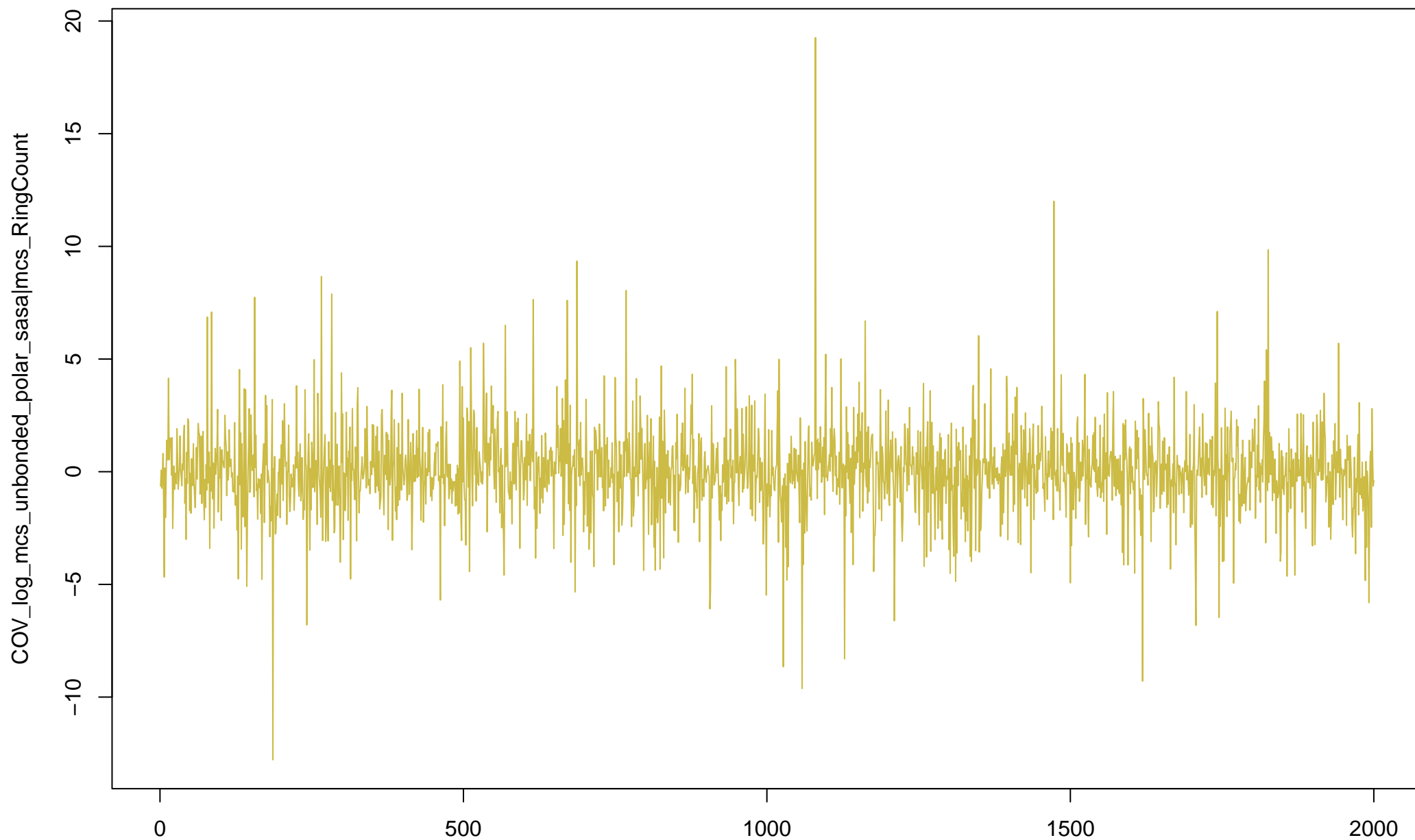**ESS = 2000 | BMK = 0.0683 | MCSE(6.27) = 2.33 | stat: TRUE**

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
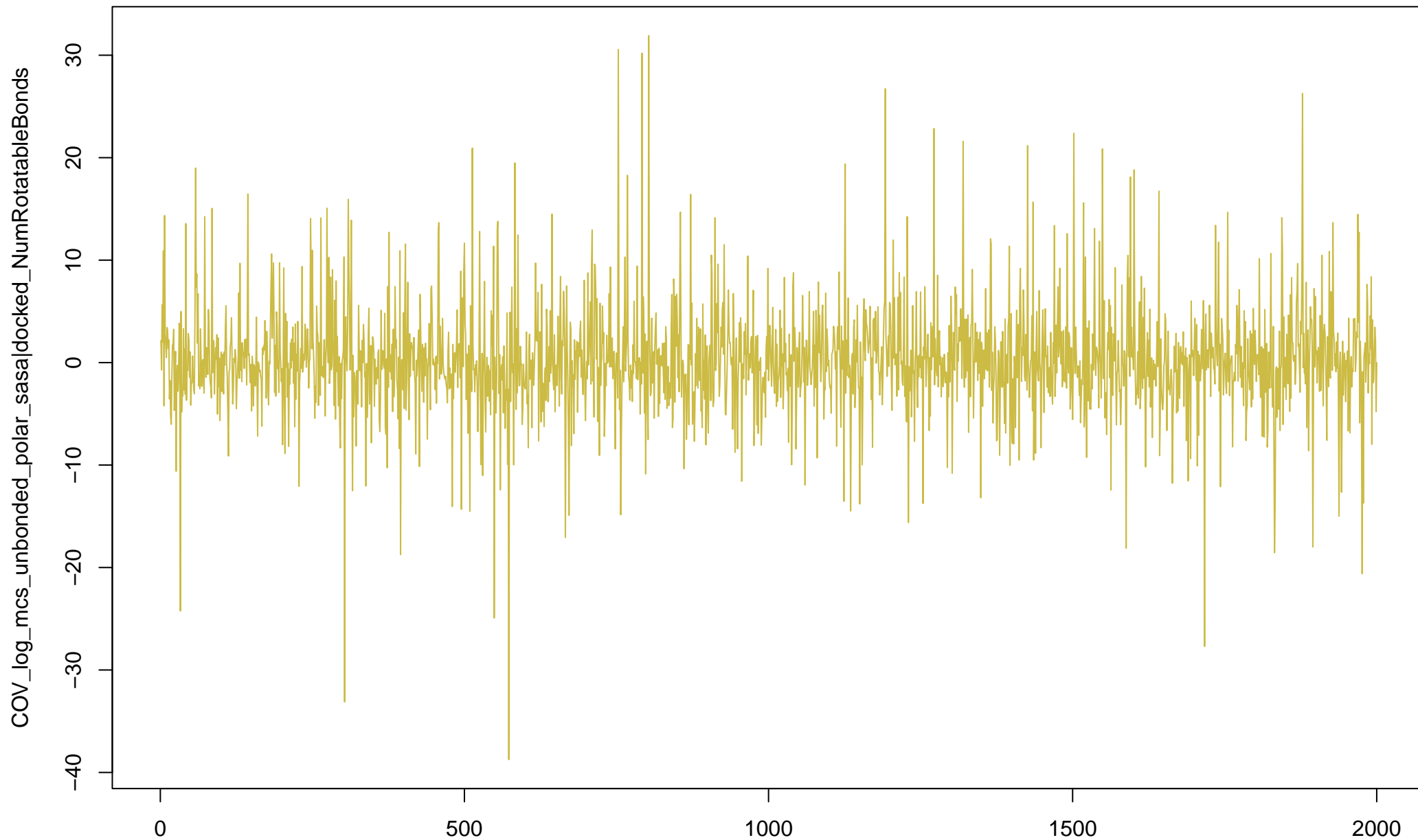**ESS = 2000 | BMK = 0.0947 | MCSE(6.27) = 2.15 | stat: TRUE**

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
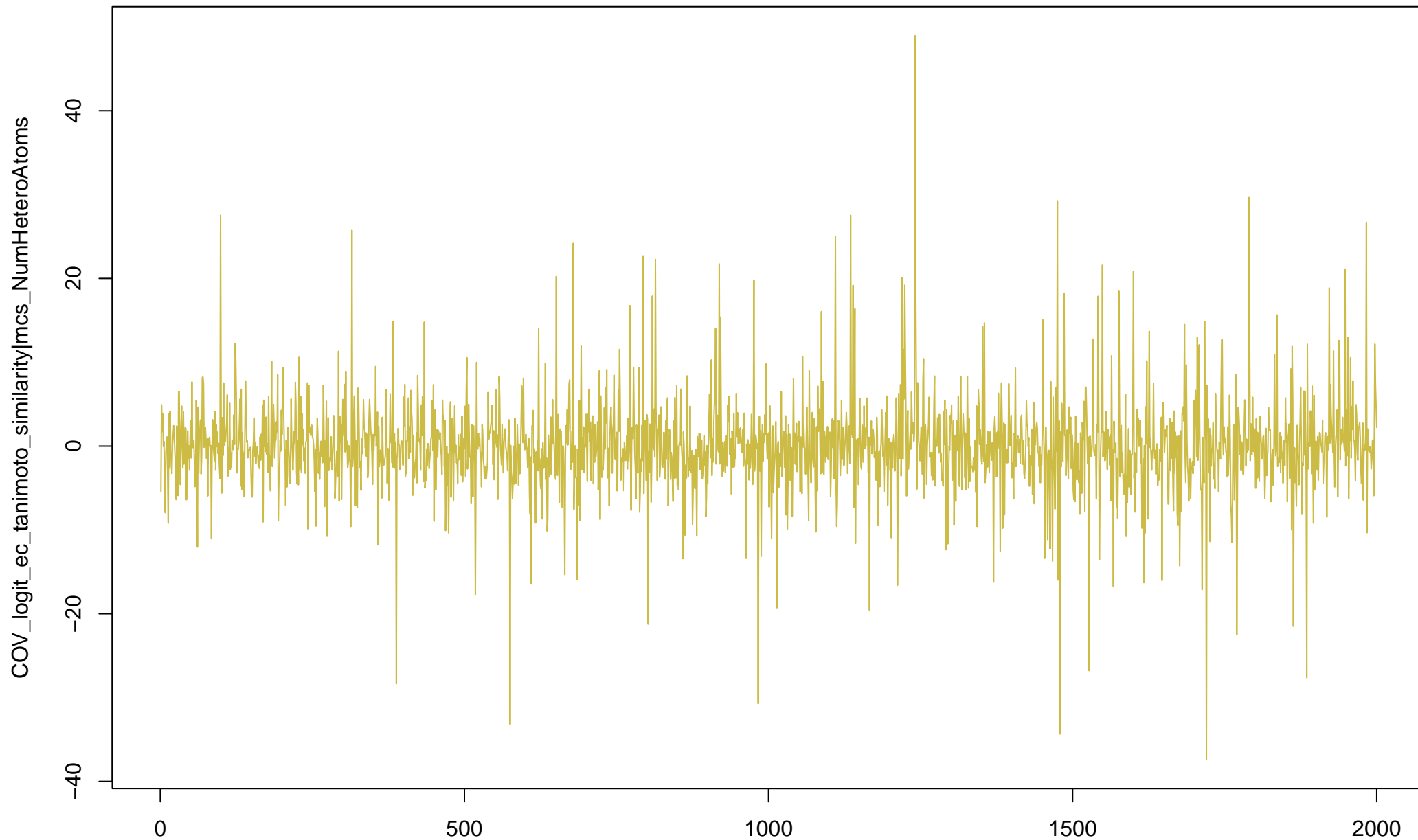**ESS = 2000 | BMK = 0.0844 | MCSE(6.27) = 2.19 | stat: TRUE**

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
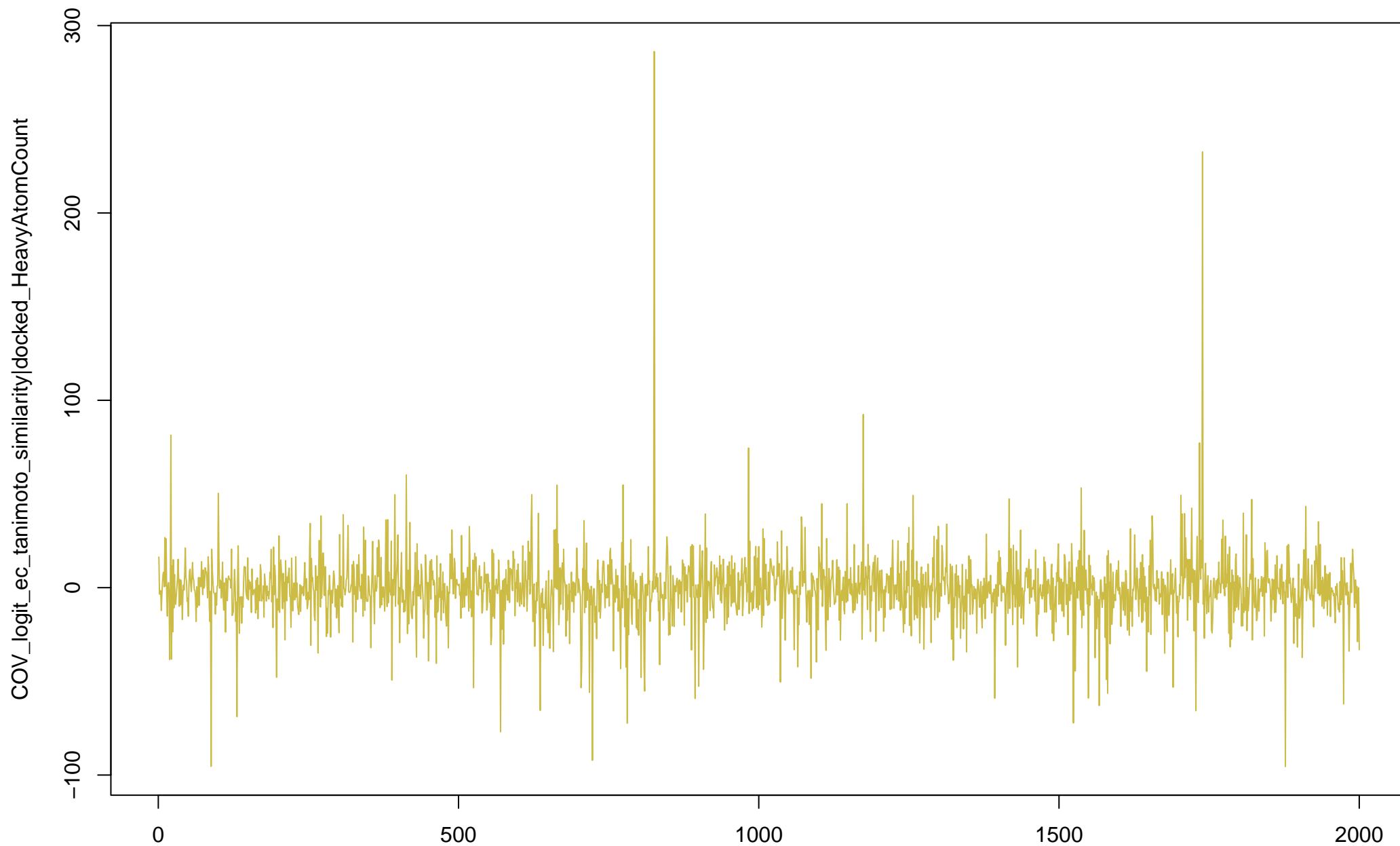**ESS = 2000 | BMK = 0.0919 | MCSE(6.27) = 2.27 | stat: TRUE**

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
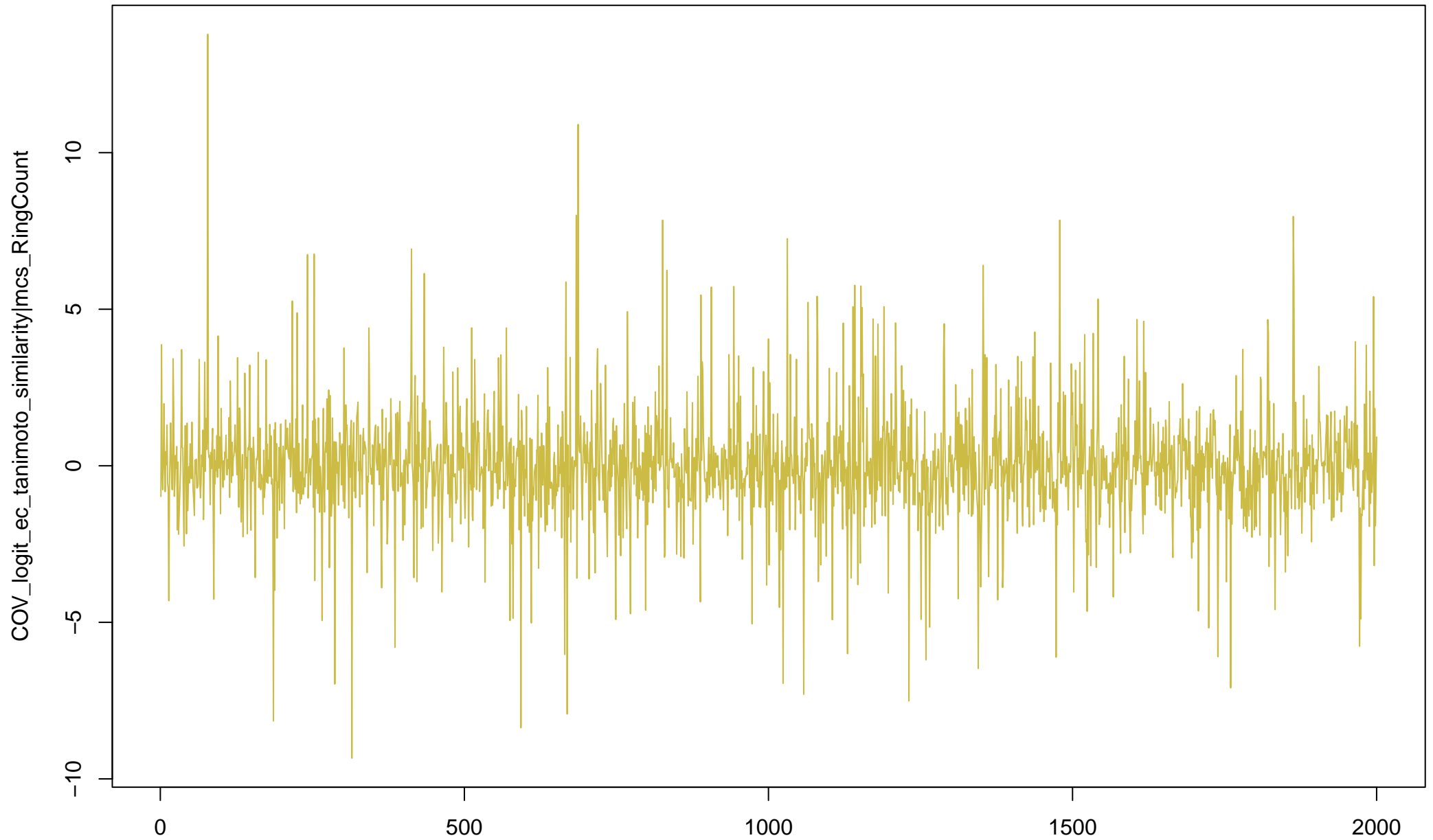**ESS = 2000 | BMK = 0.0943 | MCSE(6.27) = 2.42 | stat: TRUE**

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
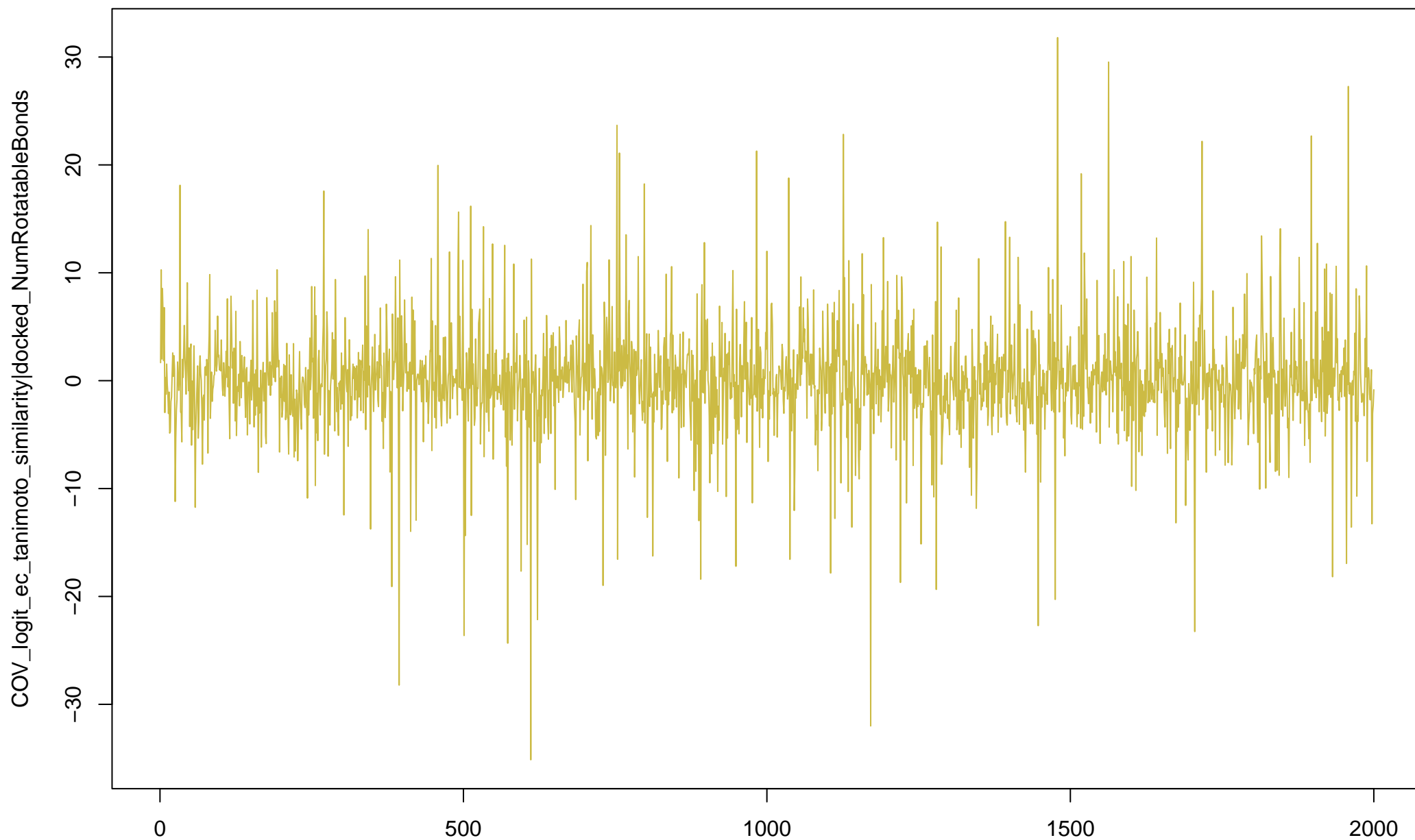**ESS = 2000 | BMK = 0.0924 | MCSE(6.27) = 2.24 | stat: TRUE**

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
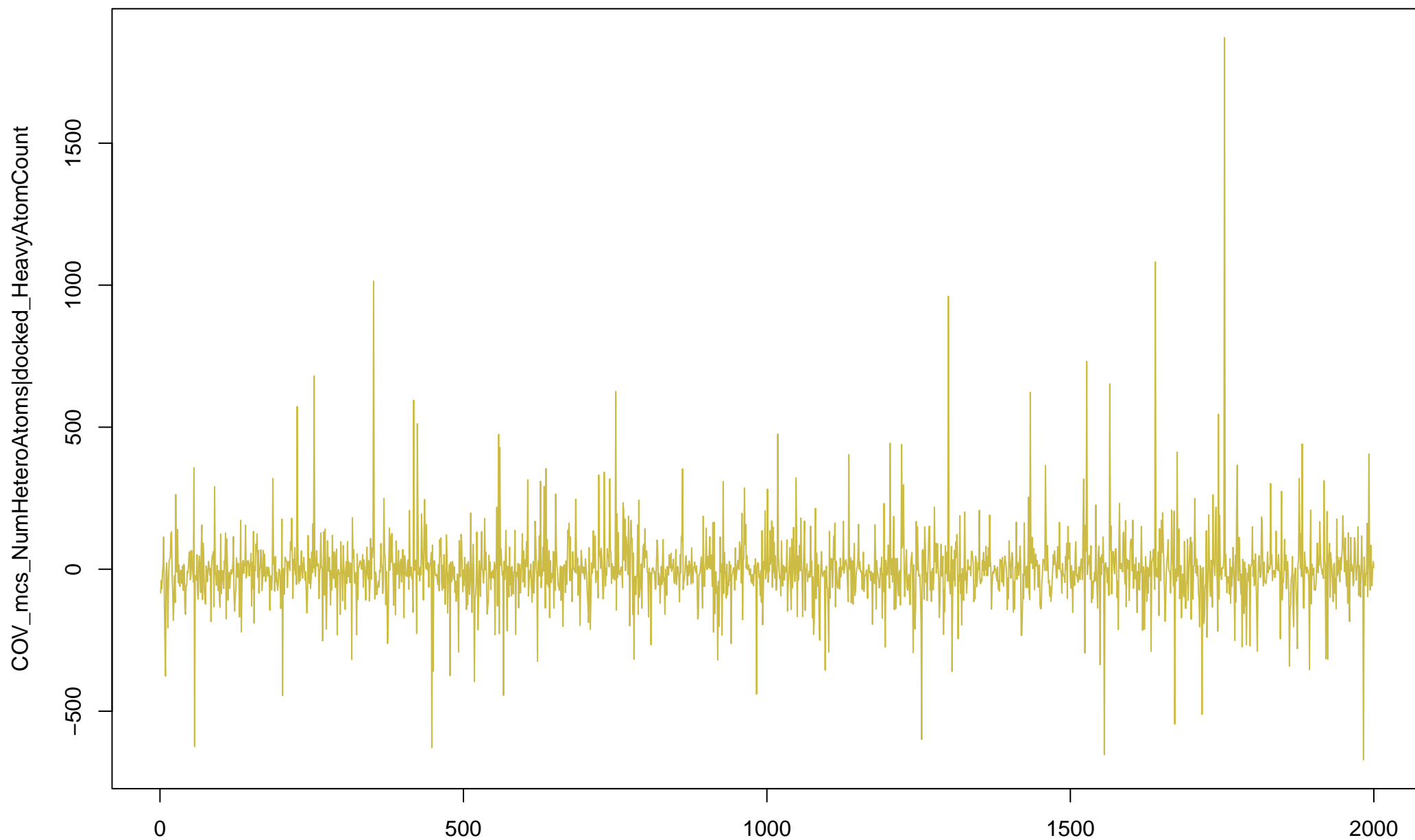**ESS = 2000 | BMK = 0.0729 | MCSE(6.27) = 2.31 | stat: TRUE**

COV_logit_ec_tanimoto_similarity|mcs_RingCount
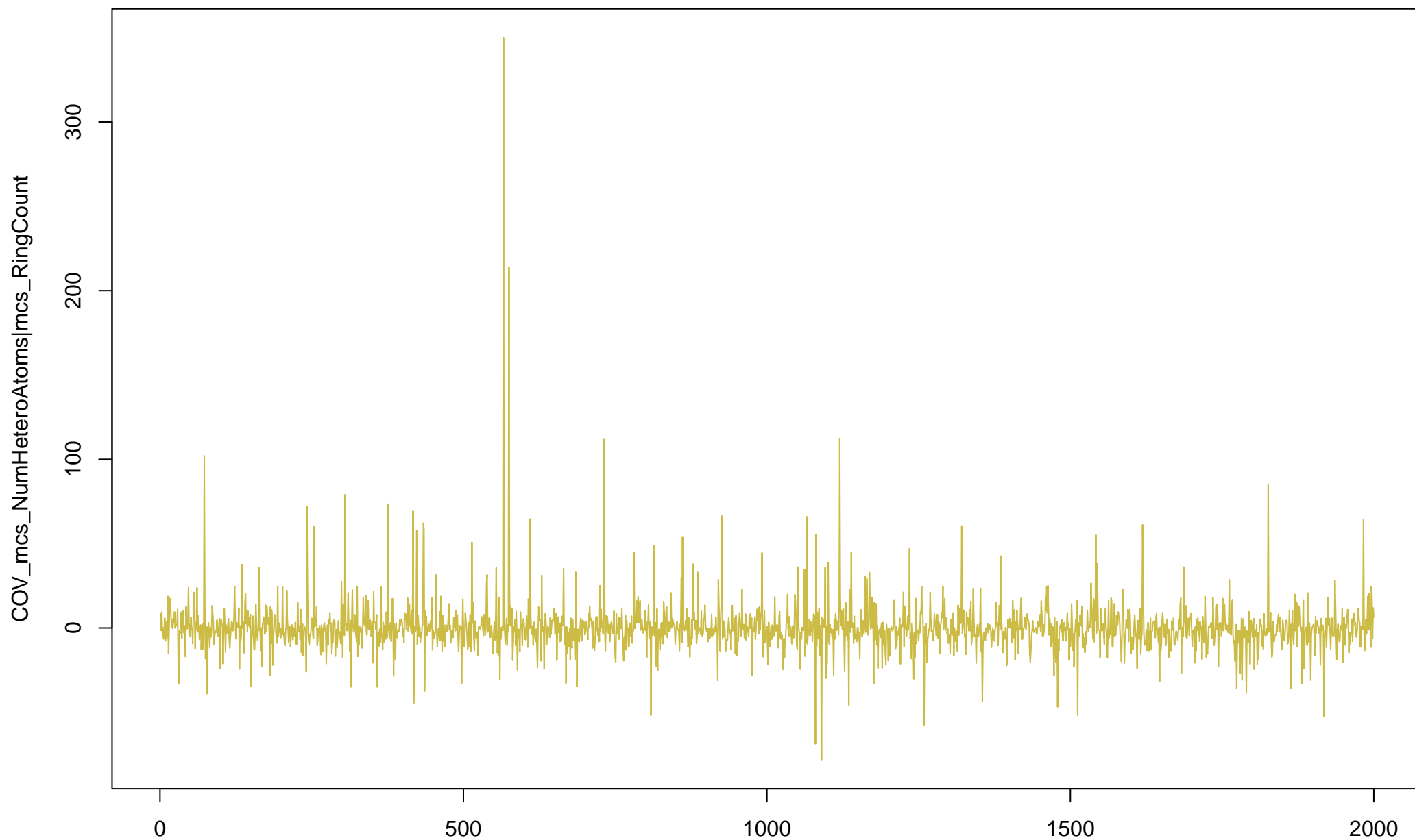**ESS = 2000 | BMK = 0.082 | MCSE(6.27) = 2.28 | stat: TRUE**

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
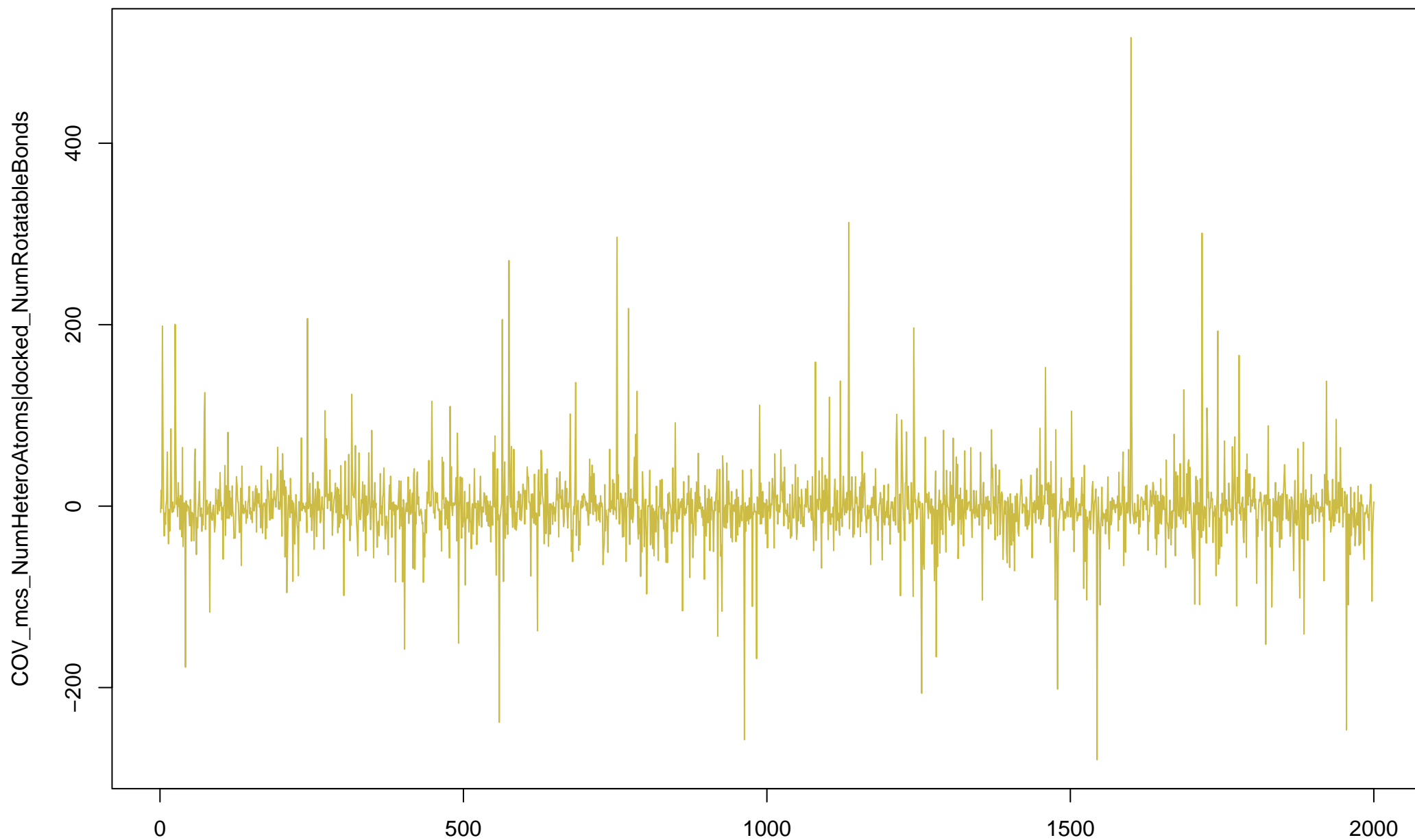**ESS = 2000 | BMK = 0.0817 | MCSE(6.27) = 2.17 | stat: TRUE**

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
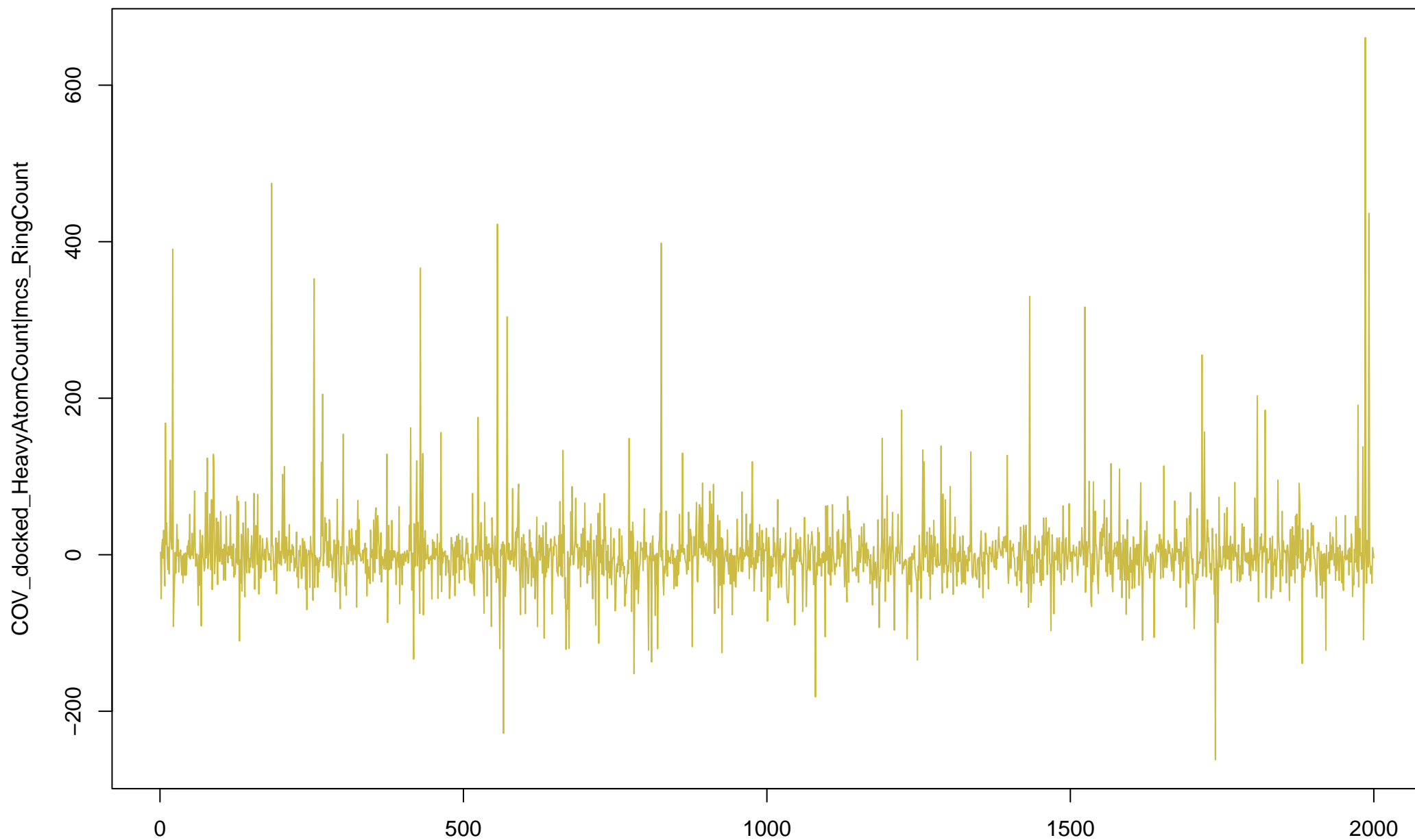**ESS = 2000 | BMK = 0.106 | MCSE(6.27) = 2.23 | stat: FALSE**

COV_mcs_NumHeteroAtoms|mcs_RingCount
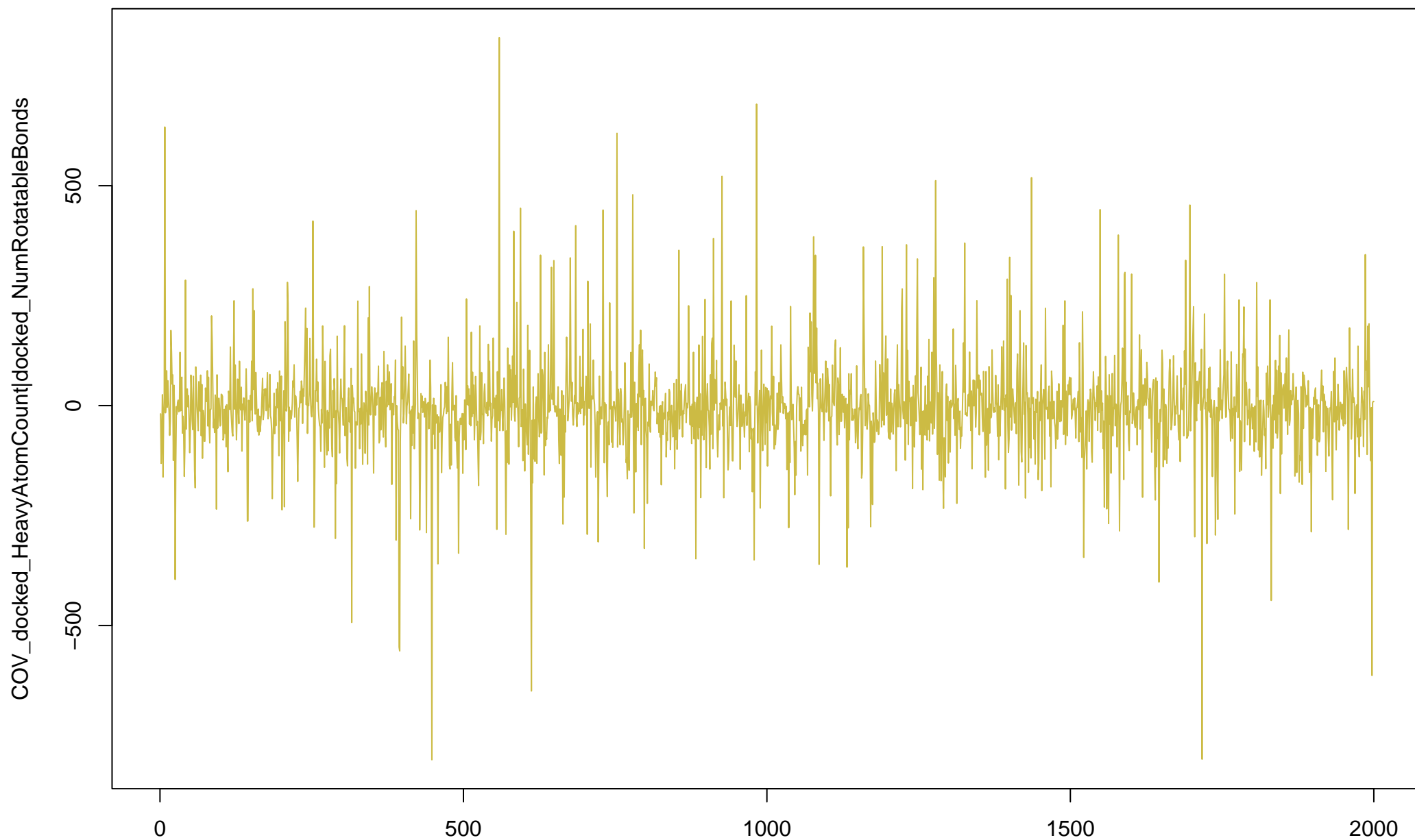ESS = 1450 | BMK = 0.0903 | MCSE(6.27) = 2.27 | stat: TRUE

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1860 | BMK = 0.103 | MCSE(6.27) = 2.35 | stat: TRUE

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1970 | BMK = 0.115 | MCSE(6.27) = 2.22 | stat: TRUE

COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1770 | BMK = 0.088 | MCSE(6.27) = 2.54 | stat: TRUE

COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0974 | MCSE(6.27) = 2.26 | stat: TRUE