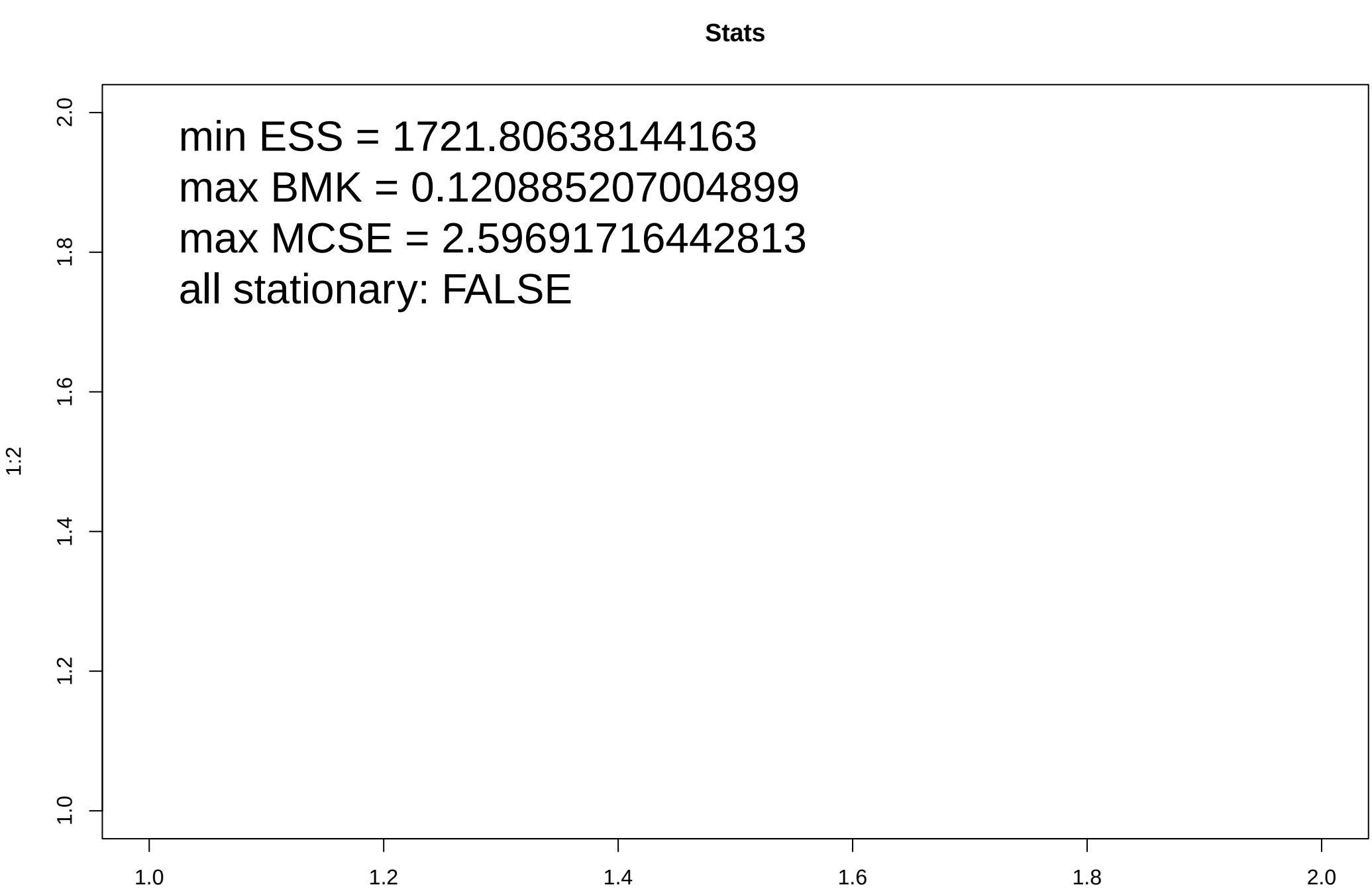
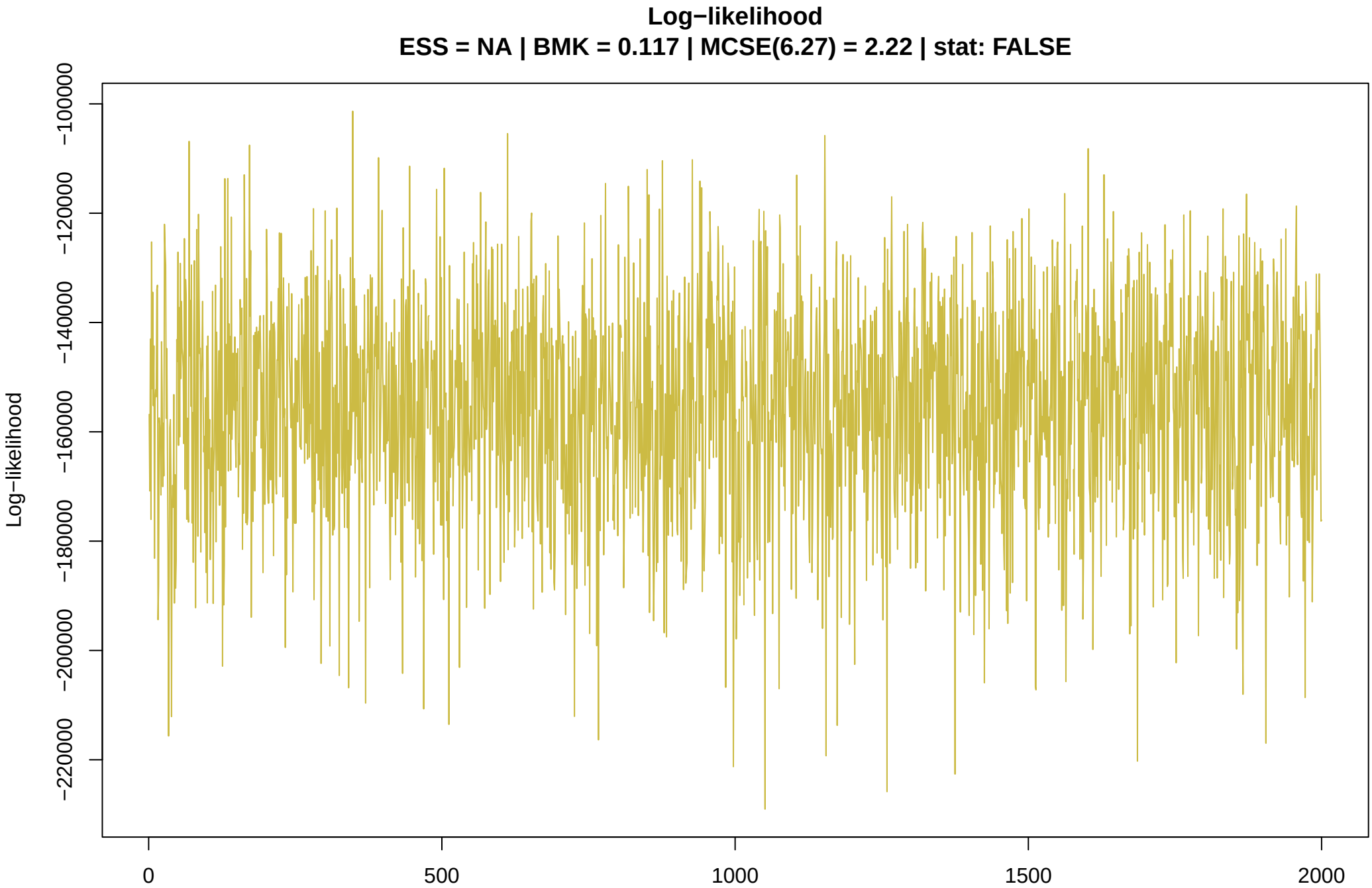
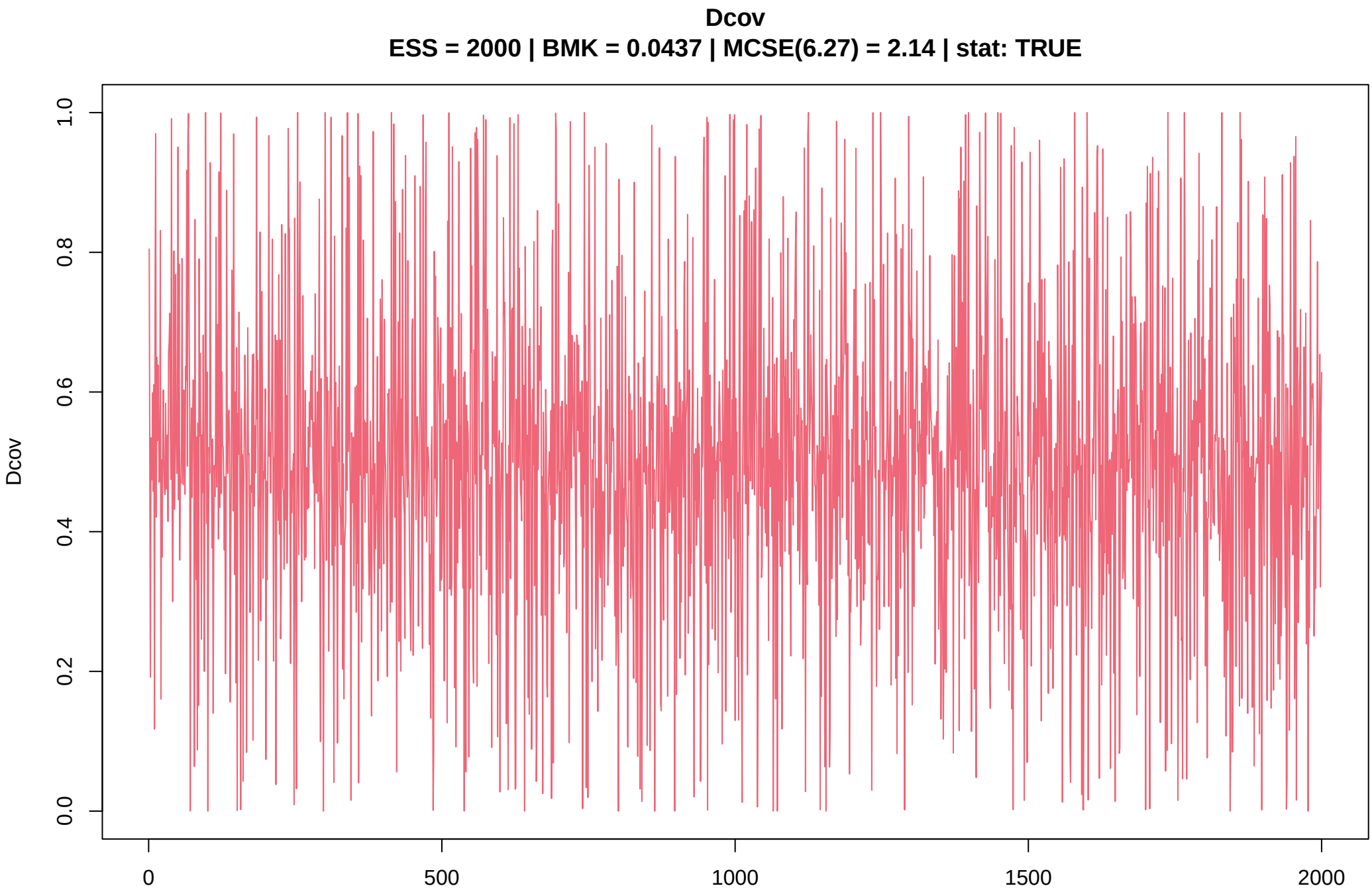
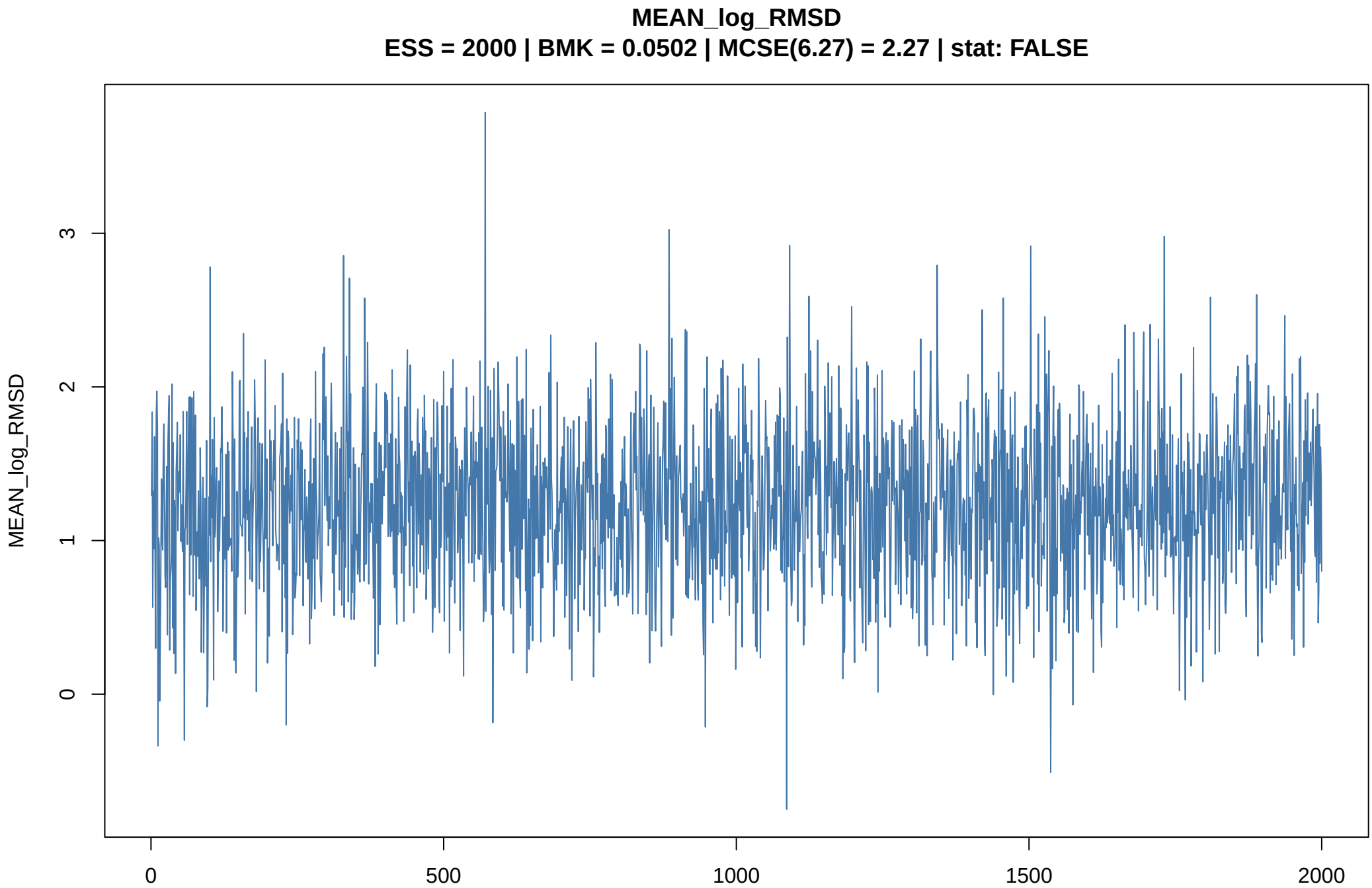
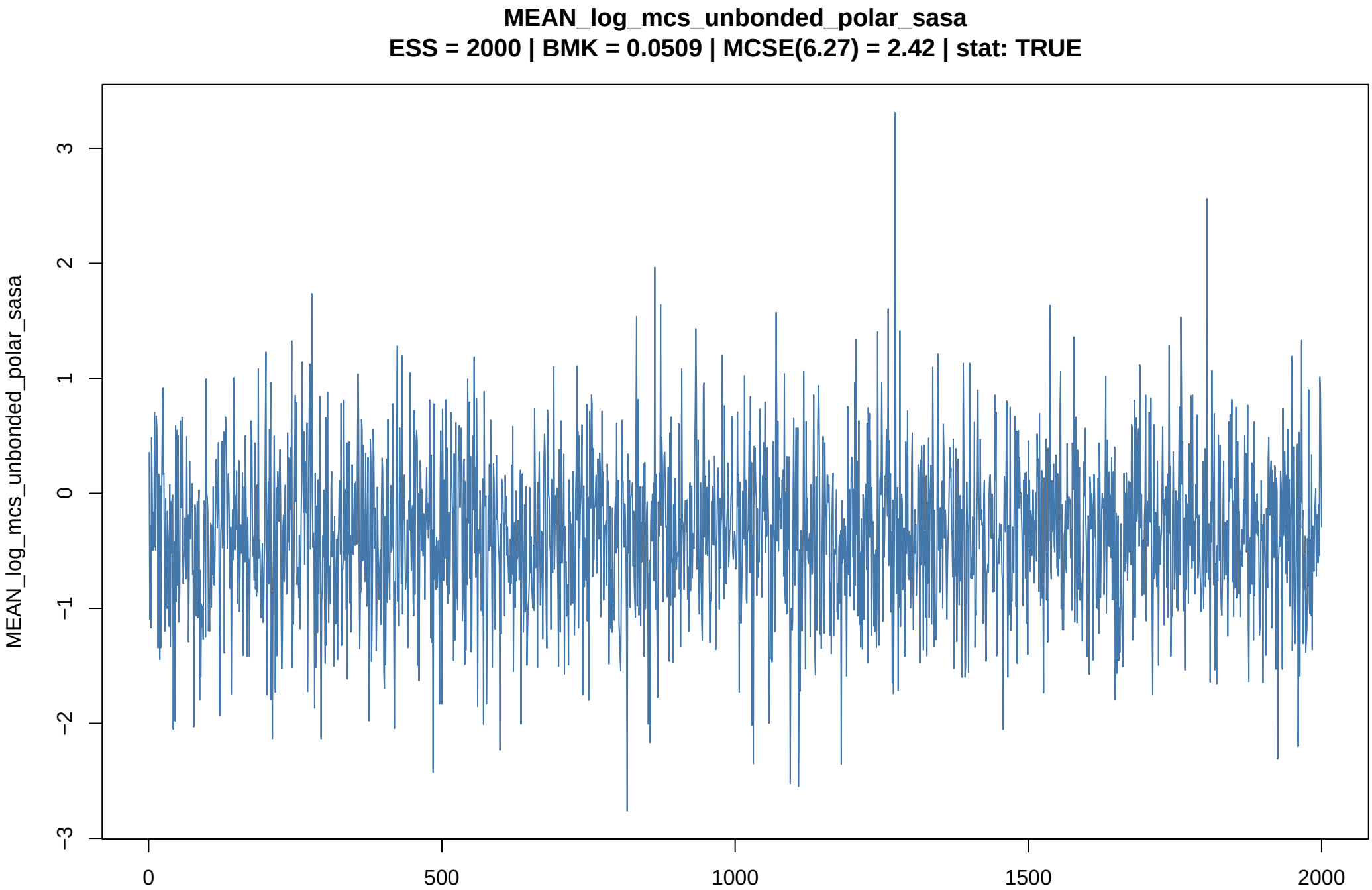
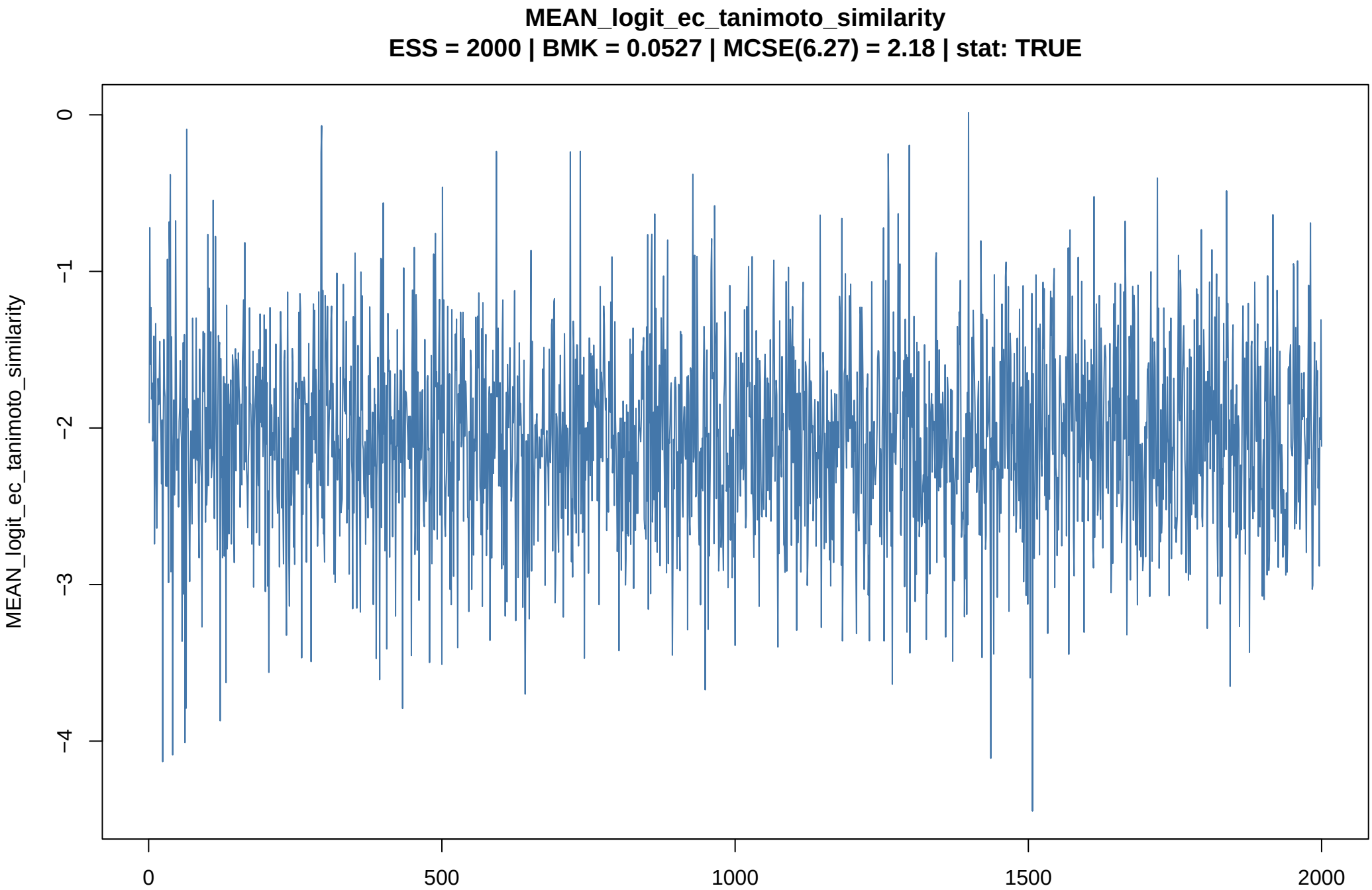

Stats
min ESS = 1721.80638144163
max BMK = 0.120885207004899
max MCSE = 2.59691716442813
all stationary: FALSE
1:2
1.0
1.2
1.4
1.6
1.8
2.0
1.0
1.2
1.4
1.6
1.8
2.0

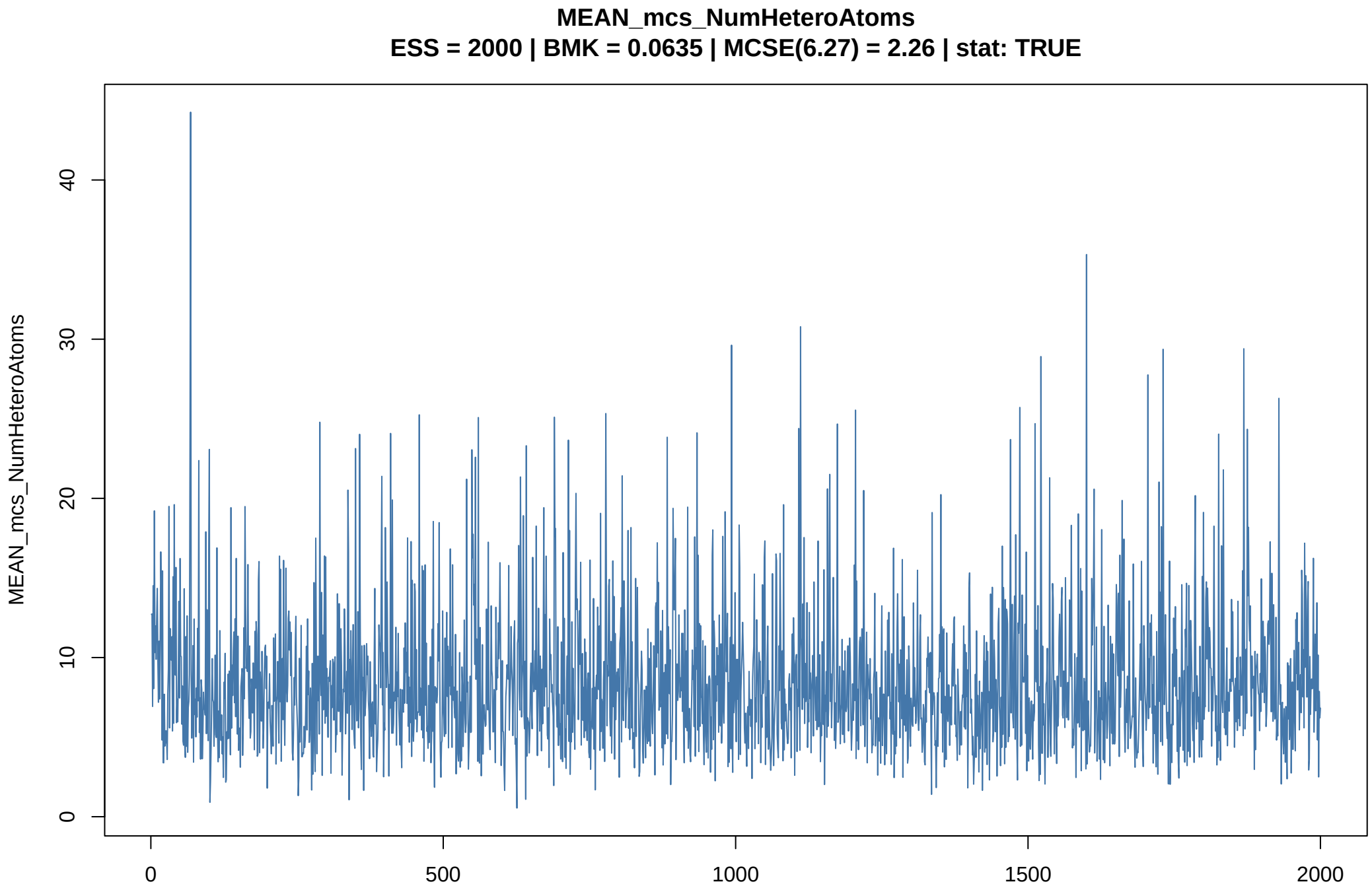

Log−likelihood
ESS = NA | BMK = 0.117 | MCSE(6.27) = 2.22 | stat: FALSE
Log−likelihood
−100000
−120000
−140000
−160000
−180000
−200000
−220000
0
500
1000
1500
2000

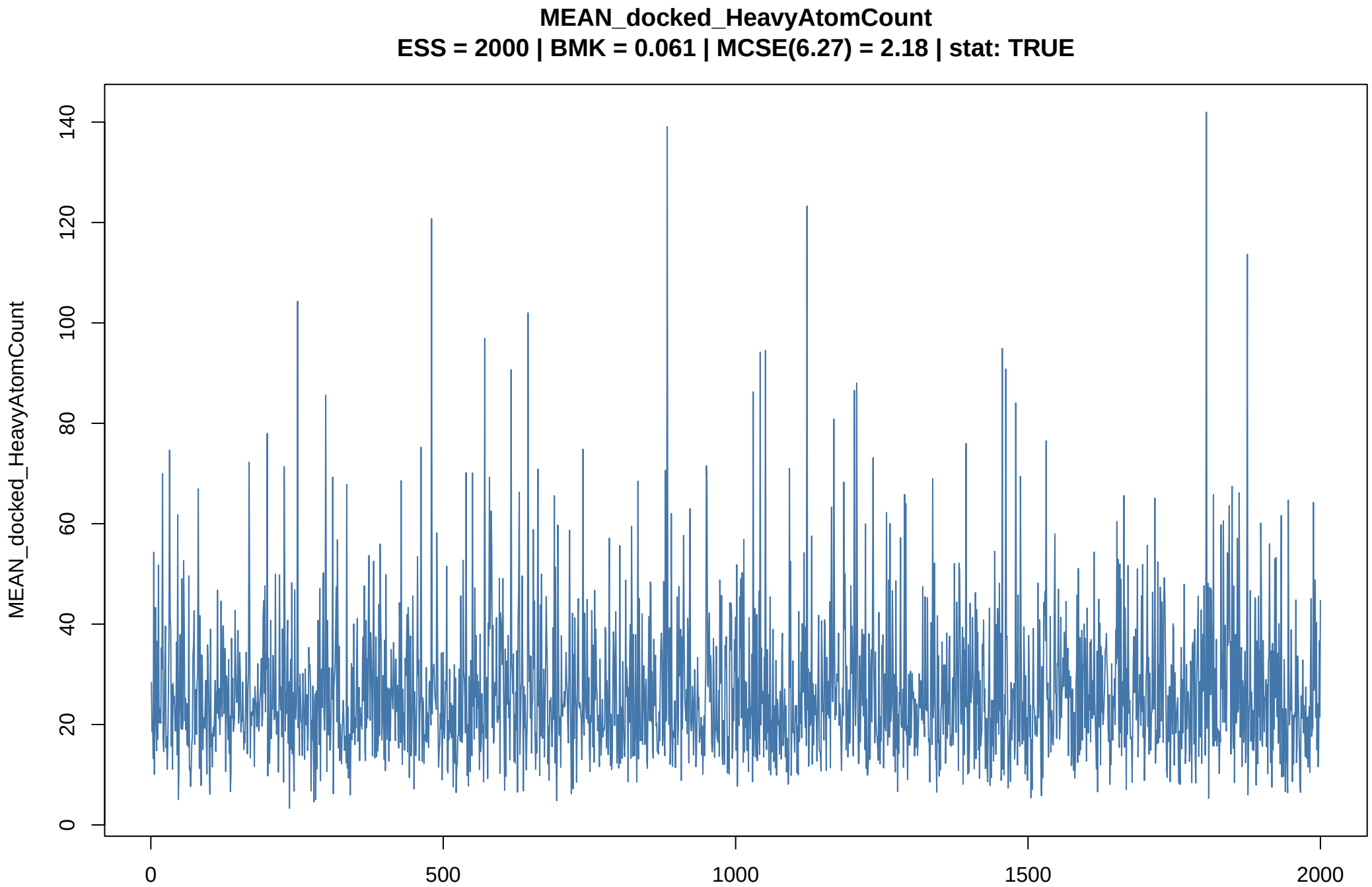

Dcov
ESS = 2000 | BMK = 0.0437 | MCSE(6.27) = 2.14 | stat: TRUE
Dcov
0.0
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

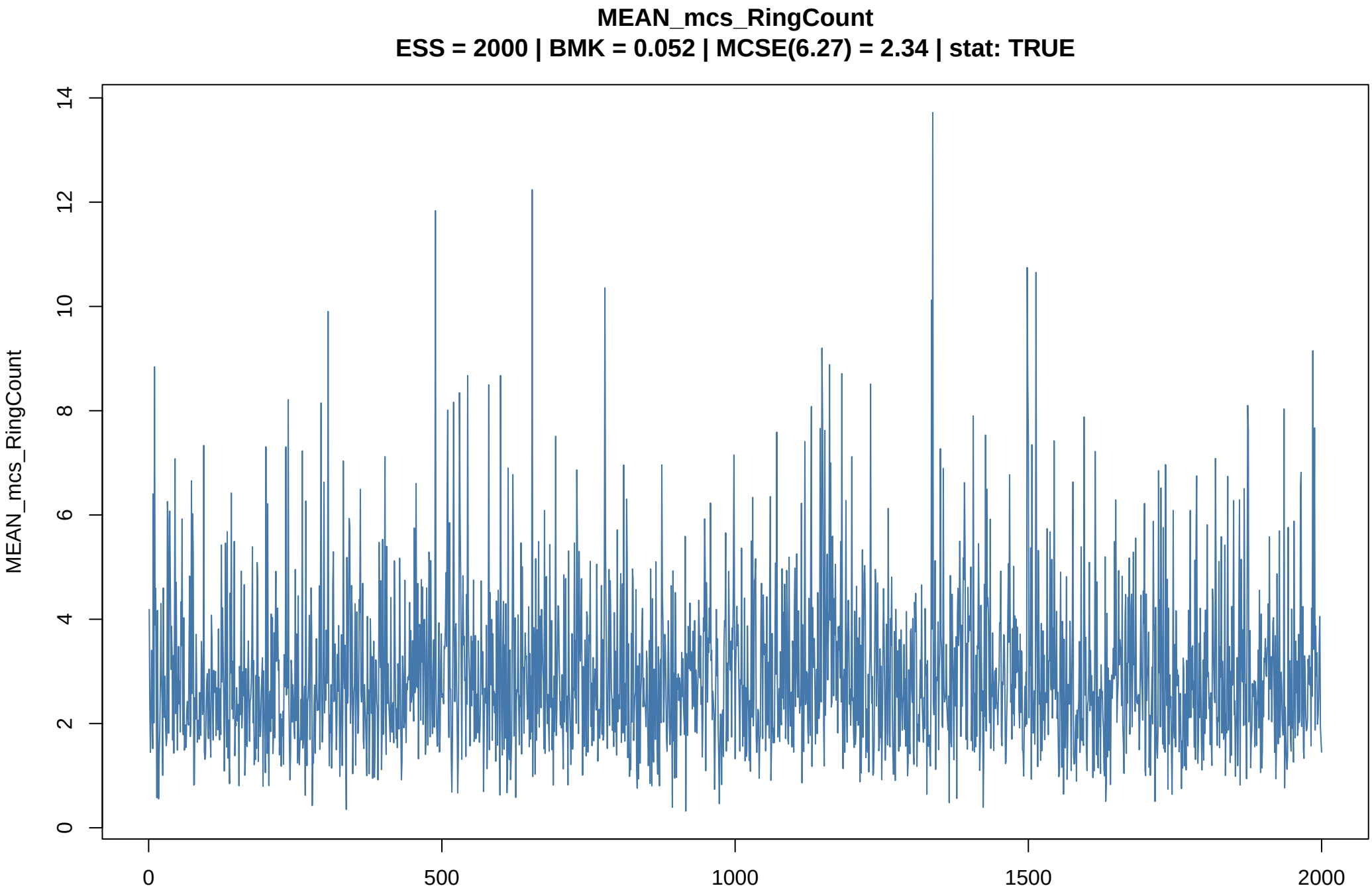

MEAN_log_RMSD
ESS = 2000 | BMK = 0.0502 | MCSE(6.27) = 2.27 | stat: FALSE
MEAN_log_RMSD
0
1
2
3
0
500
1000
1500
2000

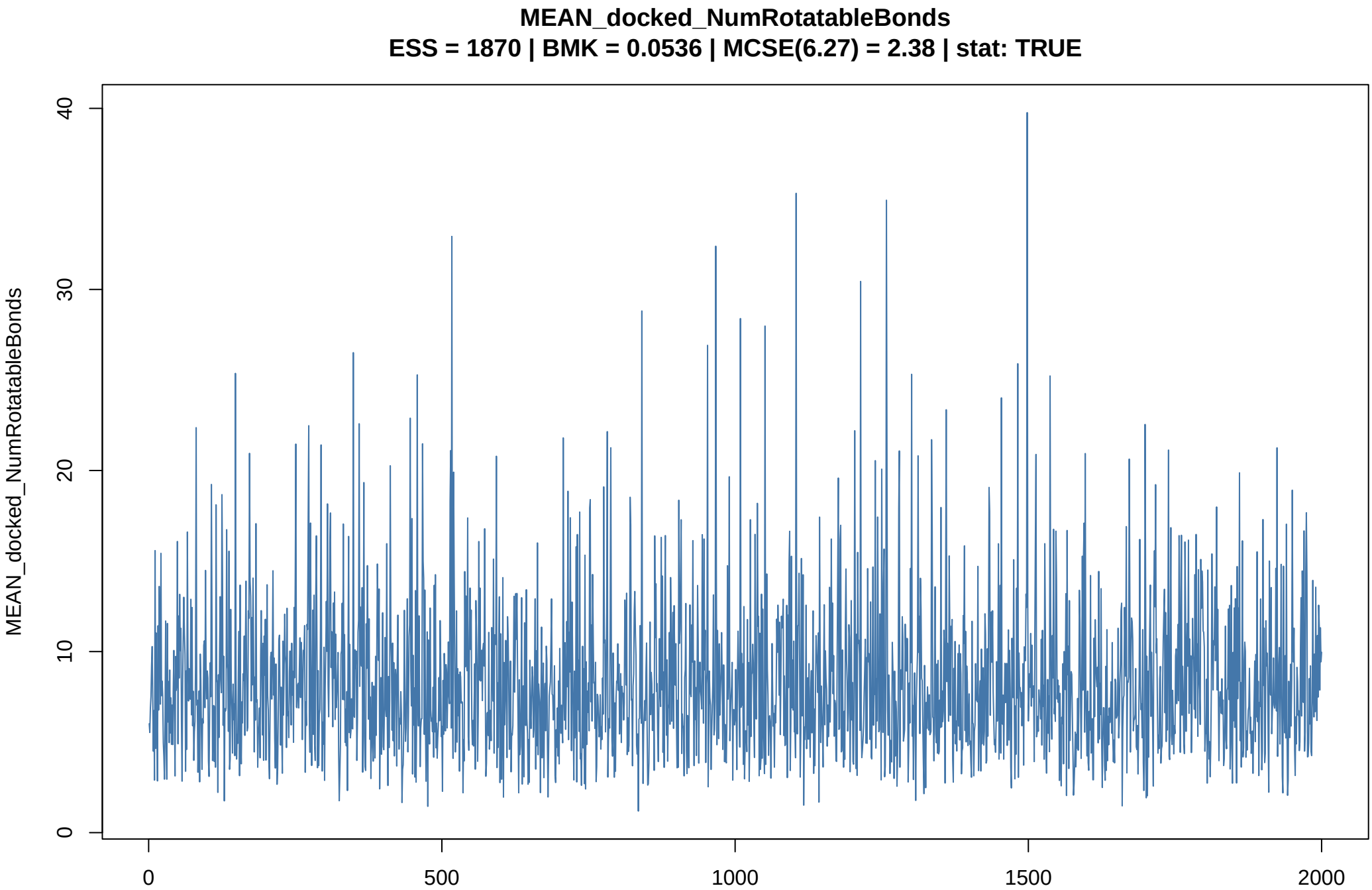

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0509 | MCSE(6.27) = 2.42 | stat: TRUE
MEAN_log_mcs_unbonded_polar_sasa
3
2
1
0
−1
−2
−3
0
500
1000
1500
2000

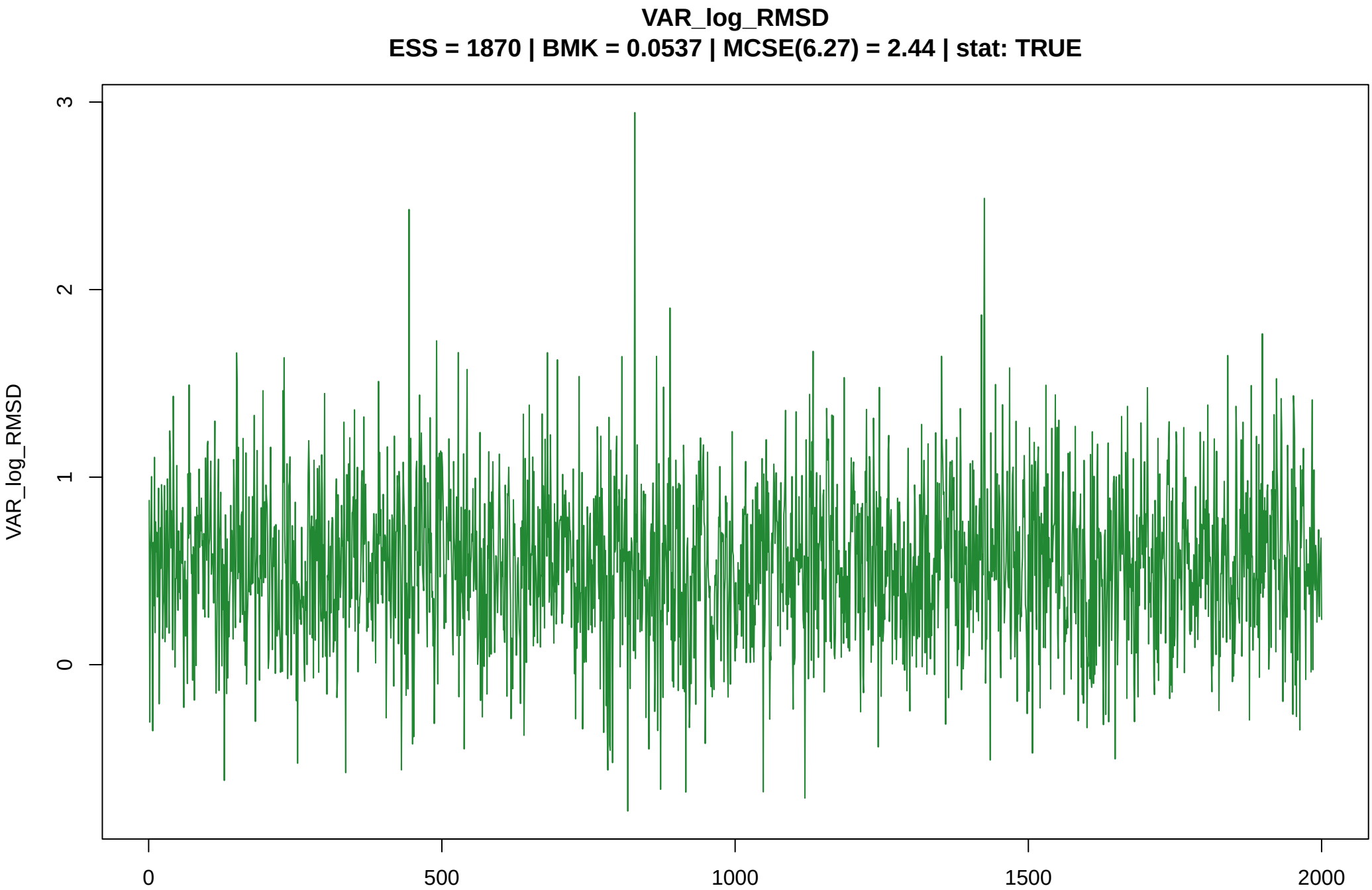

MEAN_logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.0527 | MCSE(6.27) = 2.18 | stat: TRUE
MEAN_logit_ec_tanimoto_similarity
0
−1
−2
−3
−4
0
500
1000
1500
2000

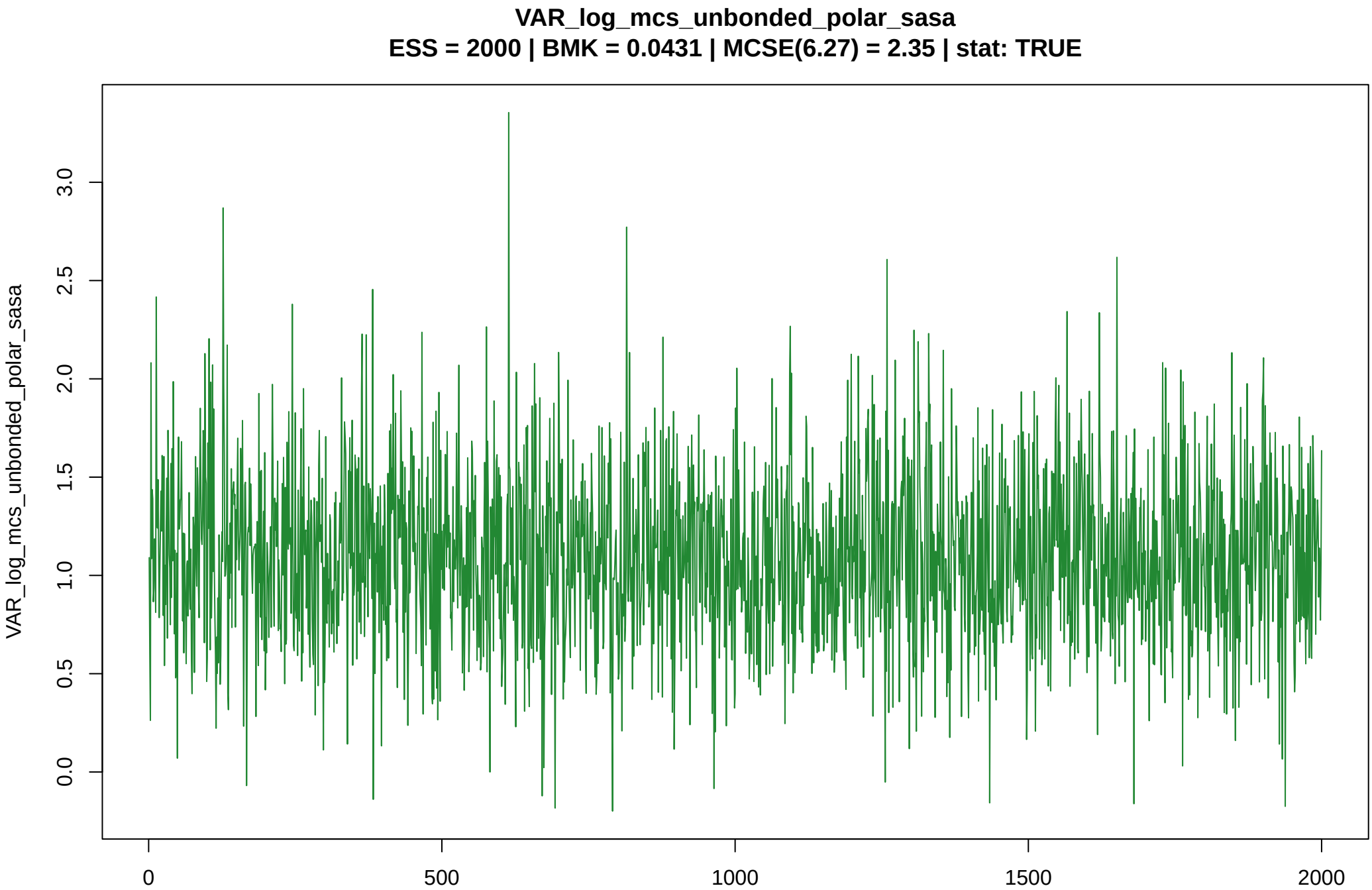

MEAN_mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0635 | MCSE(6.27) = 2.26 | stat: TRUE
MEAN_mcs_NumHeteroAtoms
0
10
20
30
40
0
500
1000
1500
2000

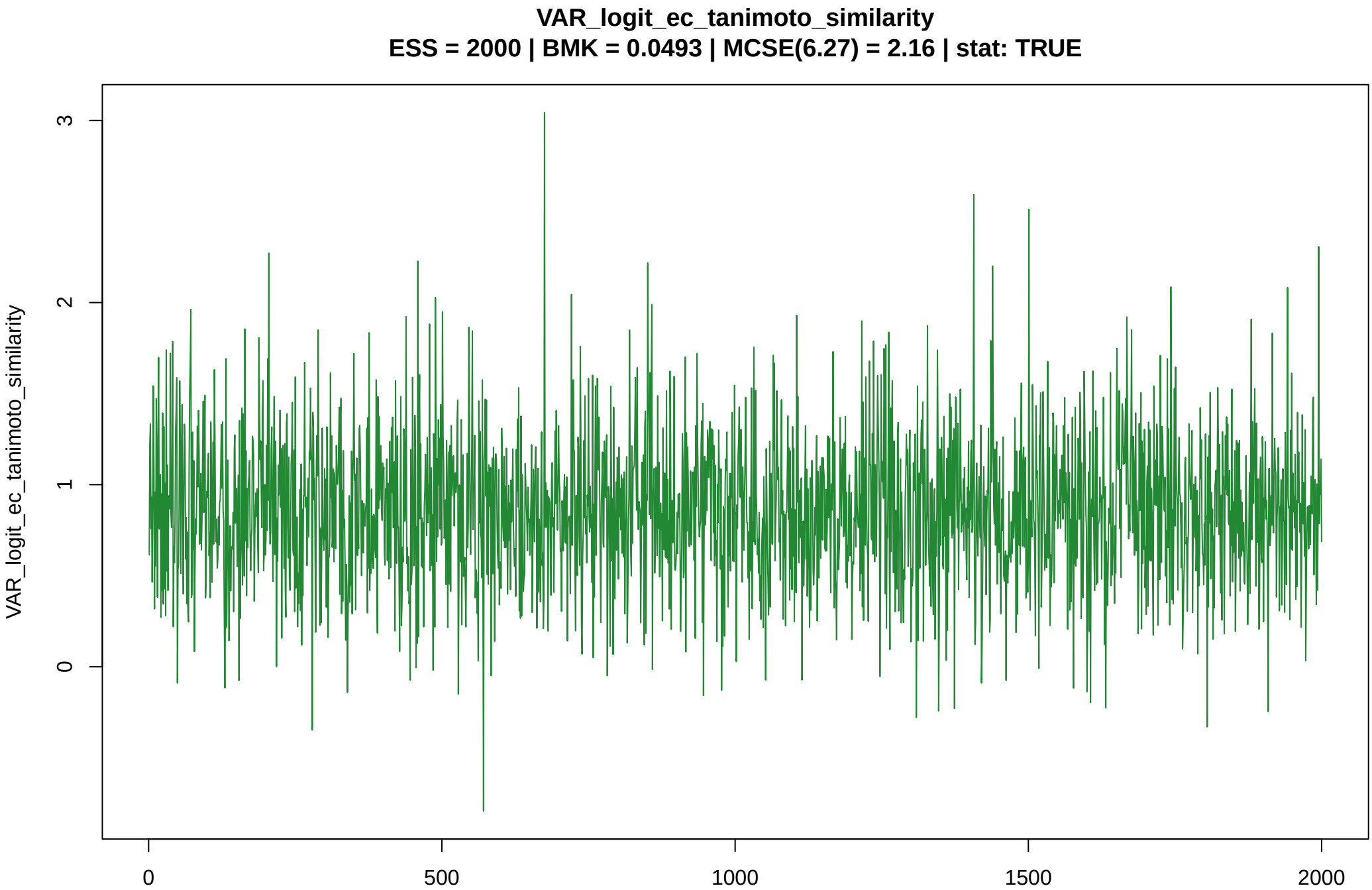

MEAN_docked_HeavyAtomCount
ESS = 2000 | BMK = 0.061 | MCSE(6.27) = 2.18 | stat: TRUE
MEAN_docked_HeavyAtomCount
0
20
40
60
80
100
120
140
0
500
1000
1500
2000

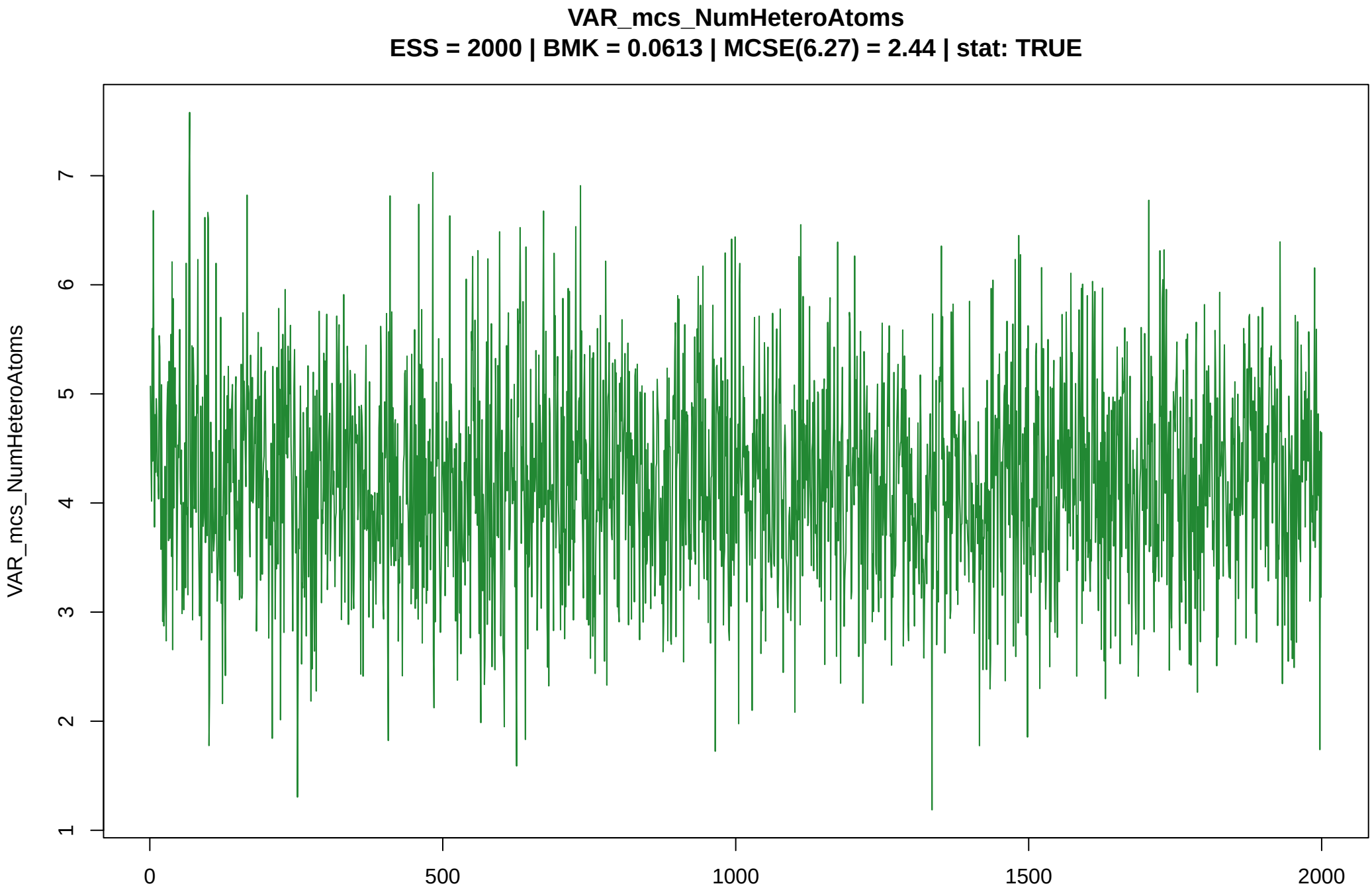

MEAN_mcs_RingCount
ESS = 2000 | BMK = 0.052 | MCSE(6.27) = 2.34 | stat: TRUE
MEAN_mcs_RingCount
0
2
4
6
8
10
12
14
0
500
1000
1500
2000

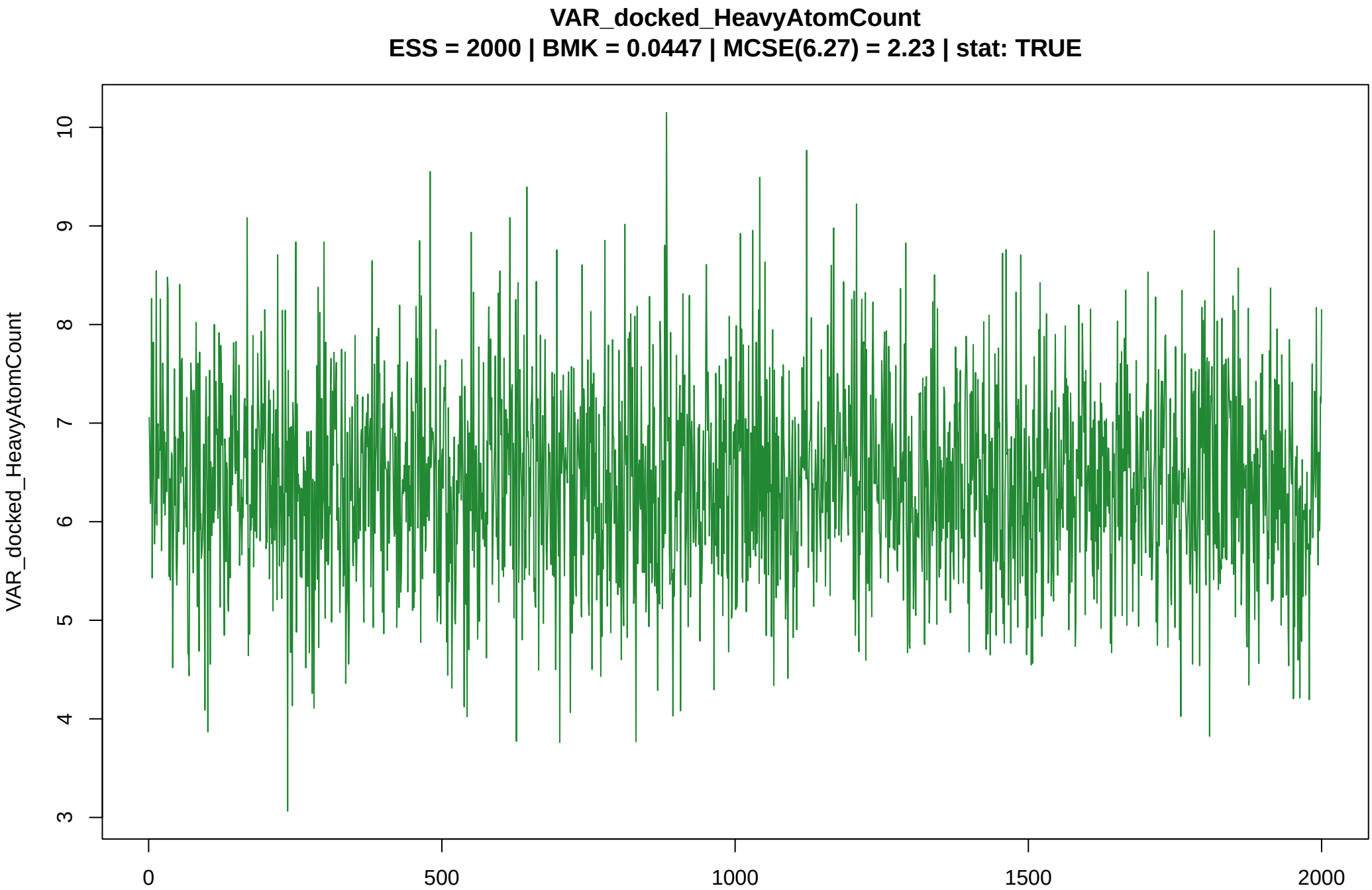

MEAN_docked_NumRotatableBonds
ESS = 1870 | BMK = 0.0536 | MCSE(6.27) = 2.38 | stat: TRUE
MEAN_docked_NumRotatableBonds
0
10
20
30
40
0
500
1000
1500
2000

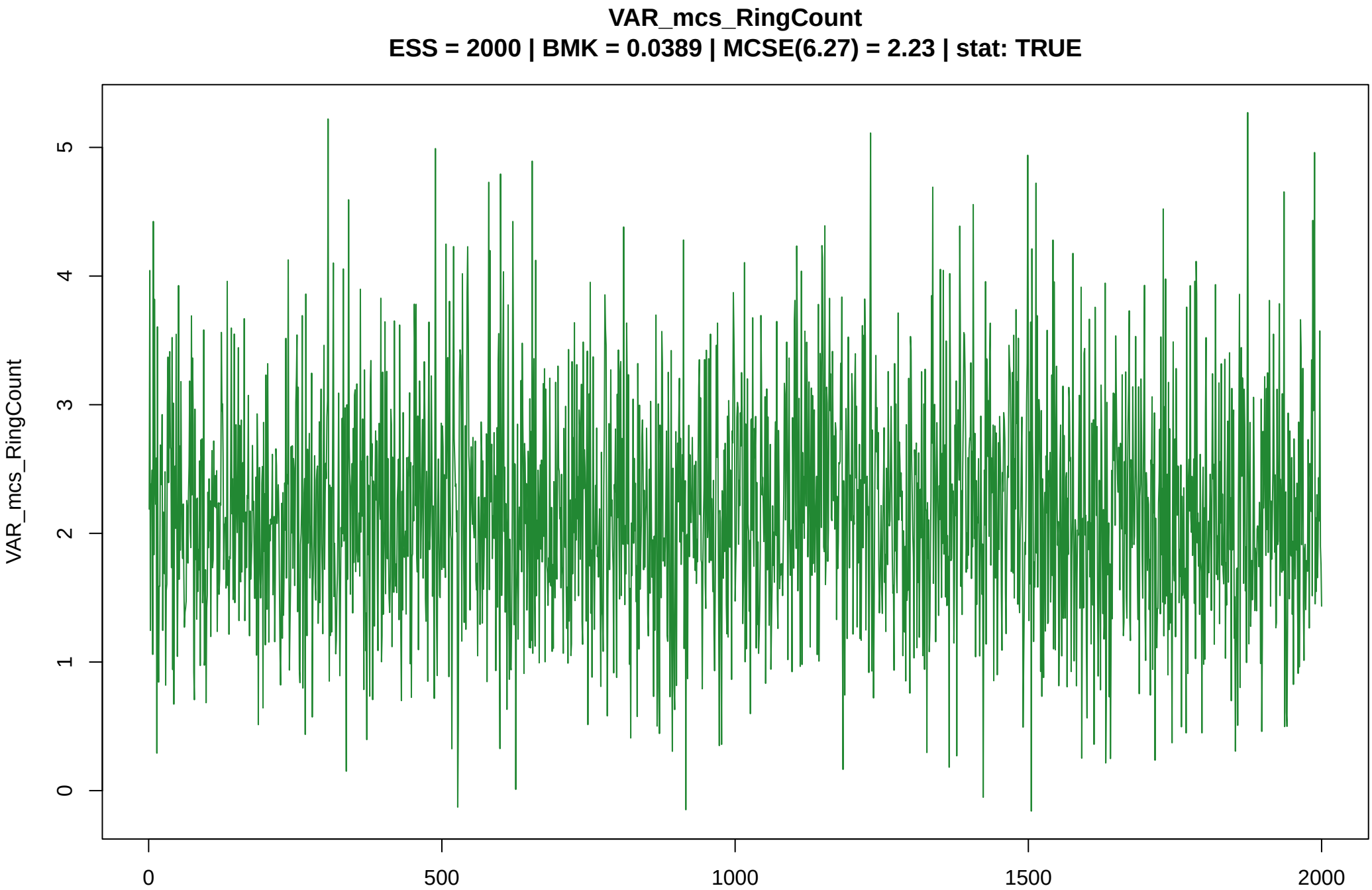

VAR_log_RMSD
ESS = 1870 | BMK = 0.0537 | MCSE(6.27) = 2.44 | stat: TRUE
VAR_log_RMSD
0
1
2
3
0
500
1000
1500
2000

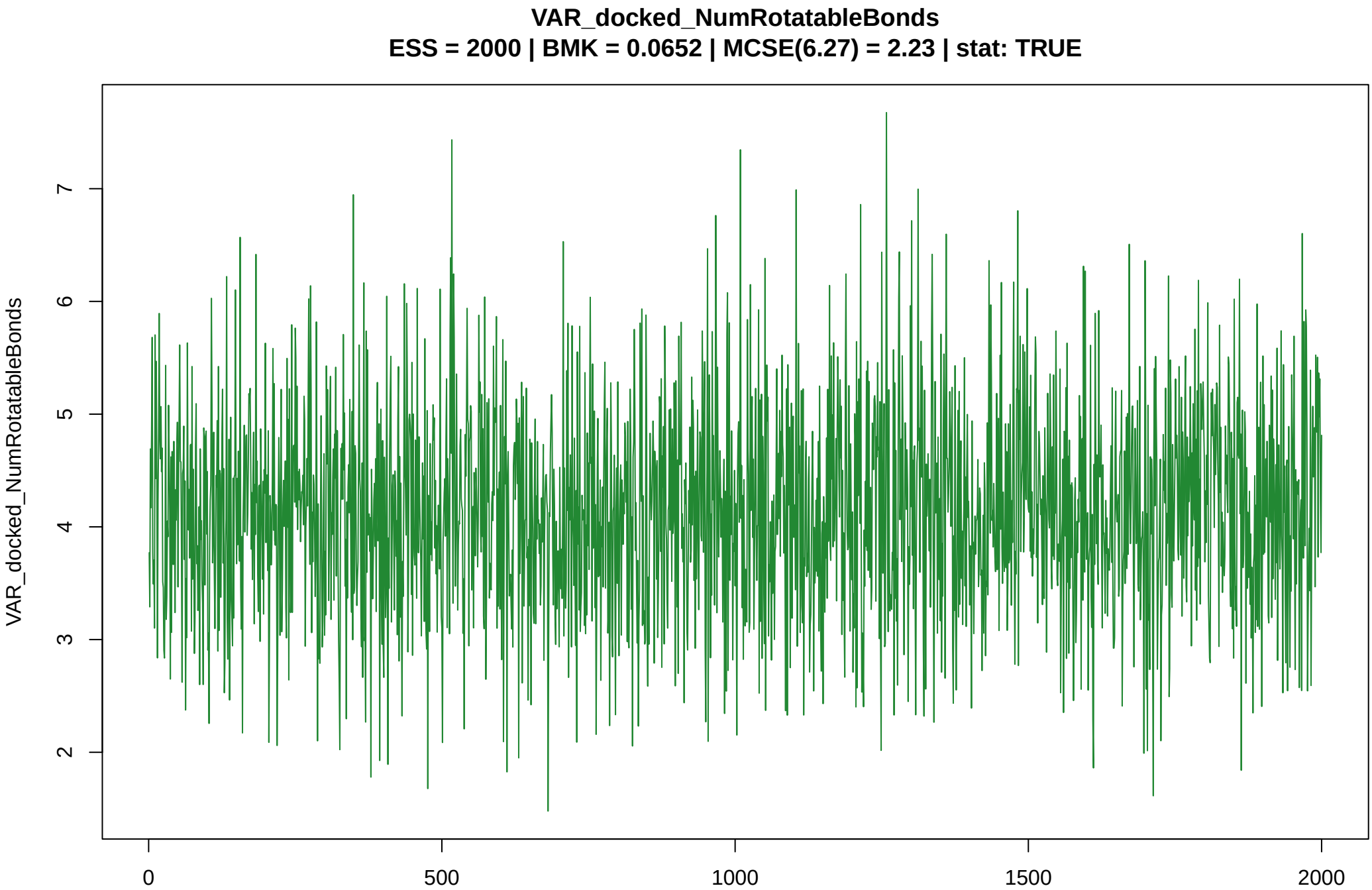

VAR_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0431 | MCSE(6.27) = 2.35 | stat: TRUE
VAR_log_mcs_unbonded_polar_sasa
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
500
1000
1500
2000

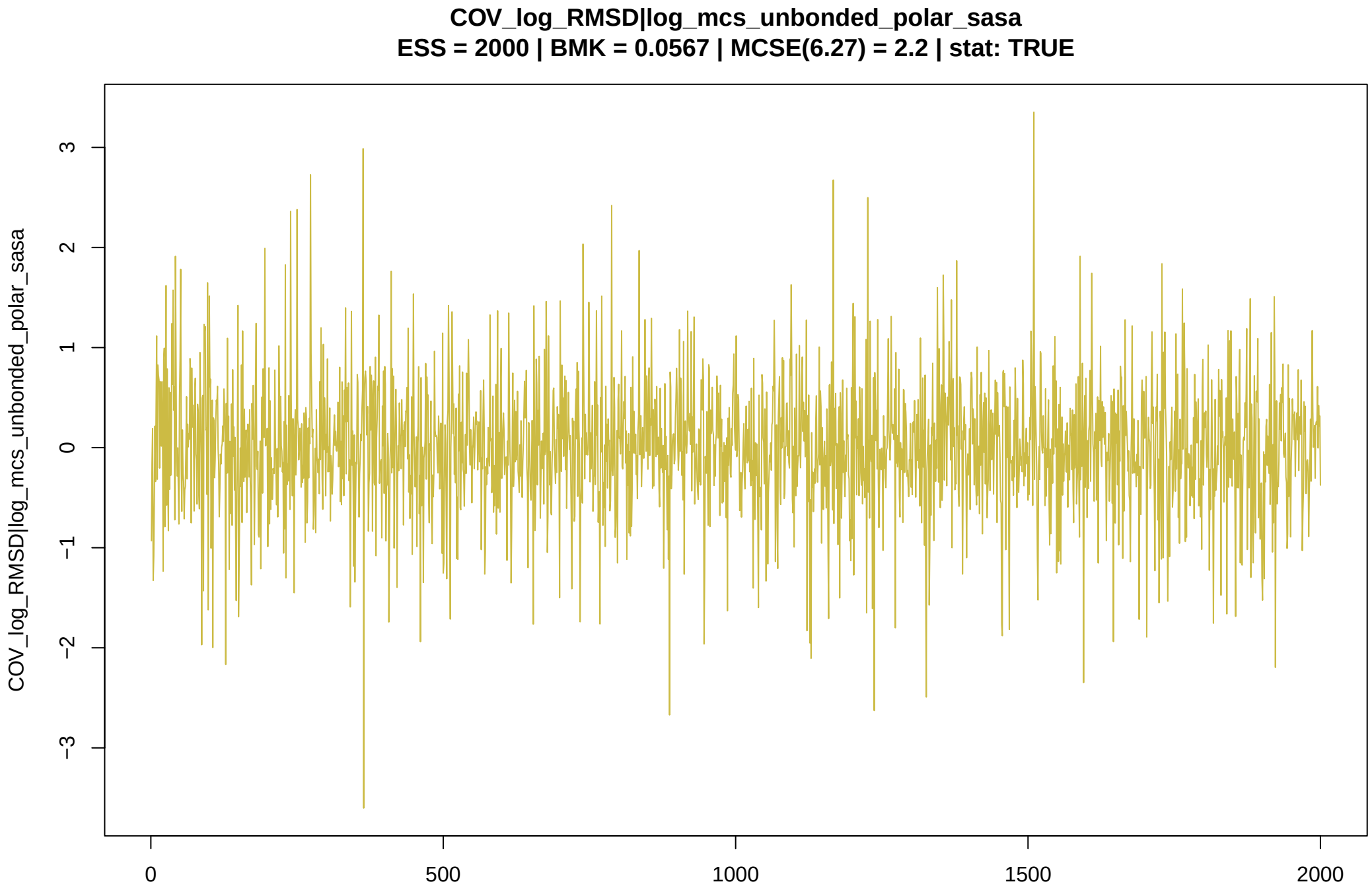

VAR_logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.0493 | MCSE(6.27) = 2.16 | stat: TRUE
VAR_logit_ec_tanimoto_similarity
0
1
2
3
0
500
1000
1500
2000

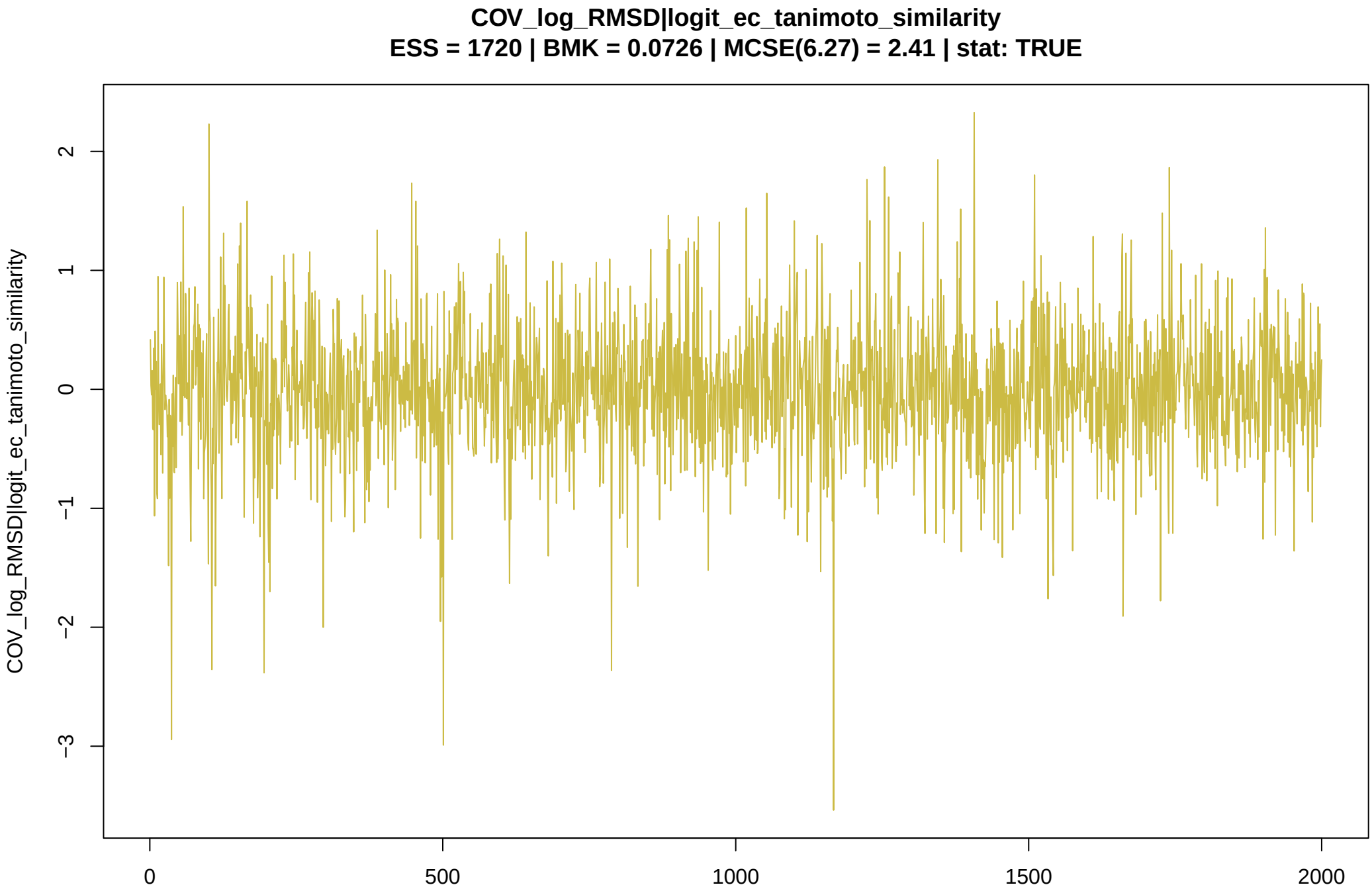

VAR_mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0613 | MCSE(6.27) = 2.44 | stat: TRUE
VAR_mcs_NumHeteroAtoms
1
2
3
4
5
6
7
0
500
1000
1500
2000

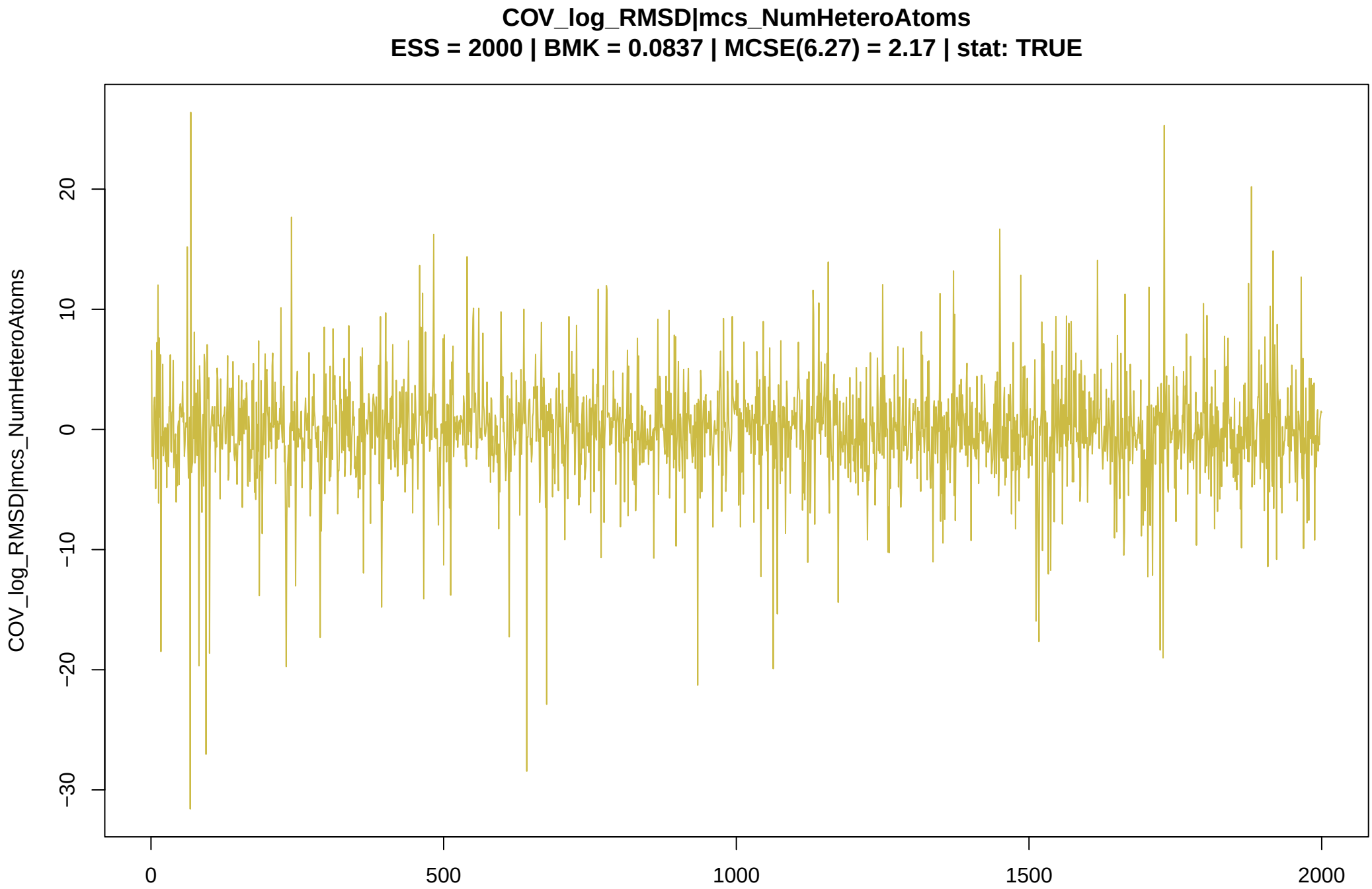

VAR_docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0447 | MCSE(6.27) = 2.23 | stat: TRUE
VAR_docked_HeavyAtomCount
3
4
5
6
7
8
9
10
0
500
1000
1500
2000

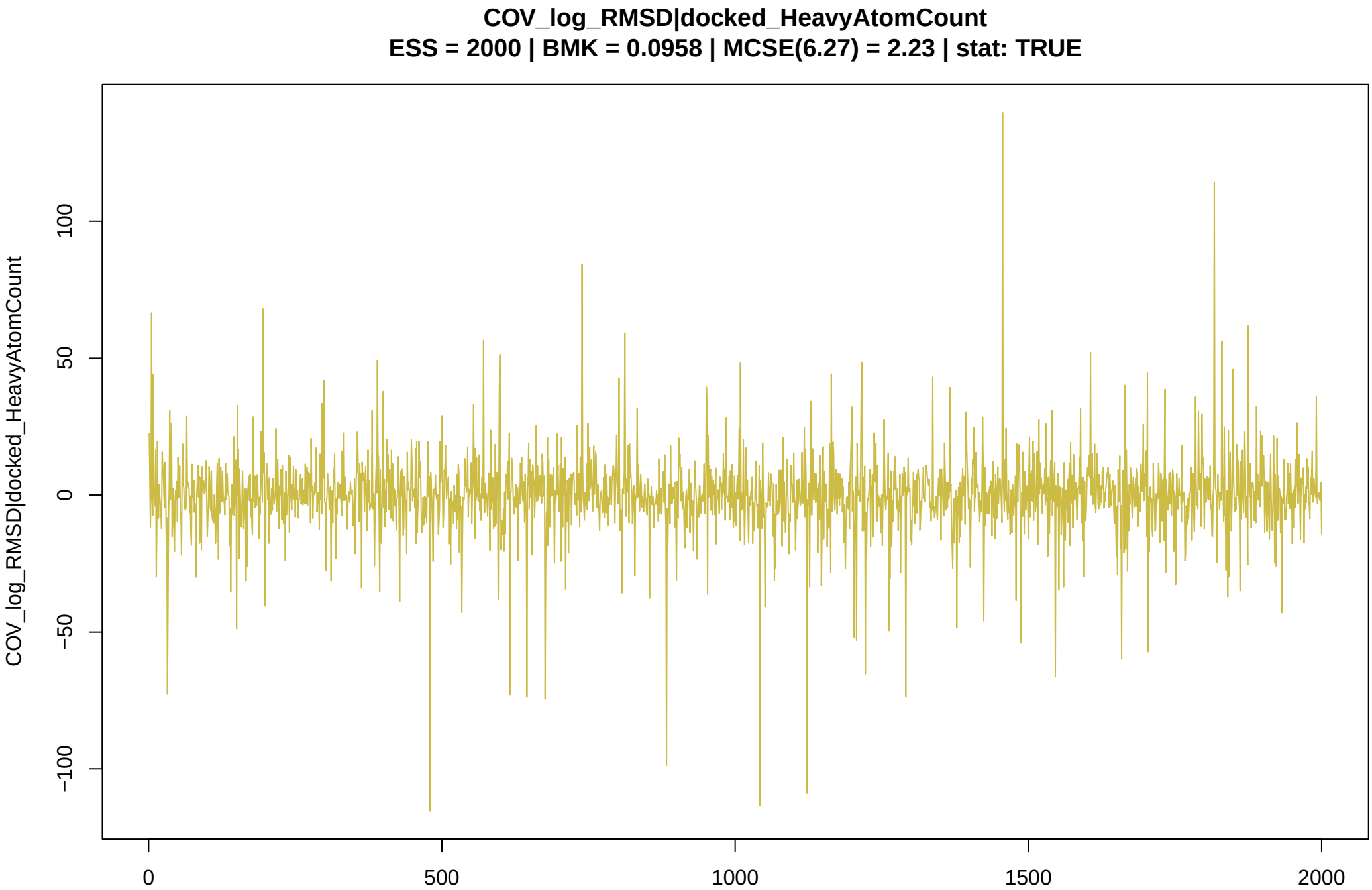

VAR_mcs_RingCount
ESS = 2000 | BMK = 0.0389 | MCSE(6.27) = 2.23 | stat: TRUE
VAR_mcs_RingCount
0
1
2
3
4
5
0
500
1000
1500
2000

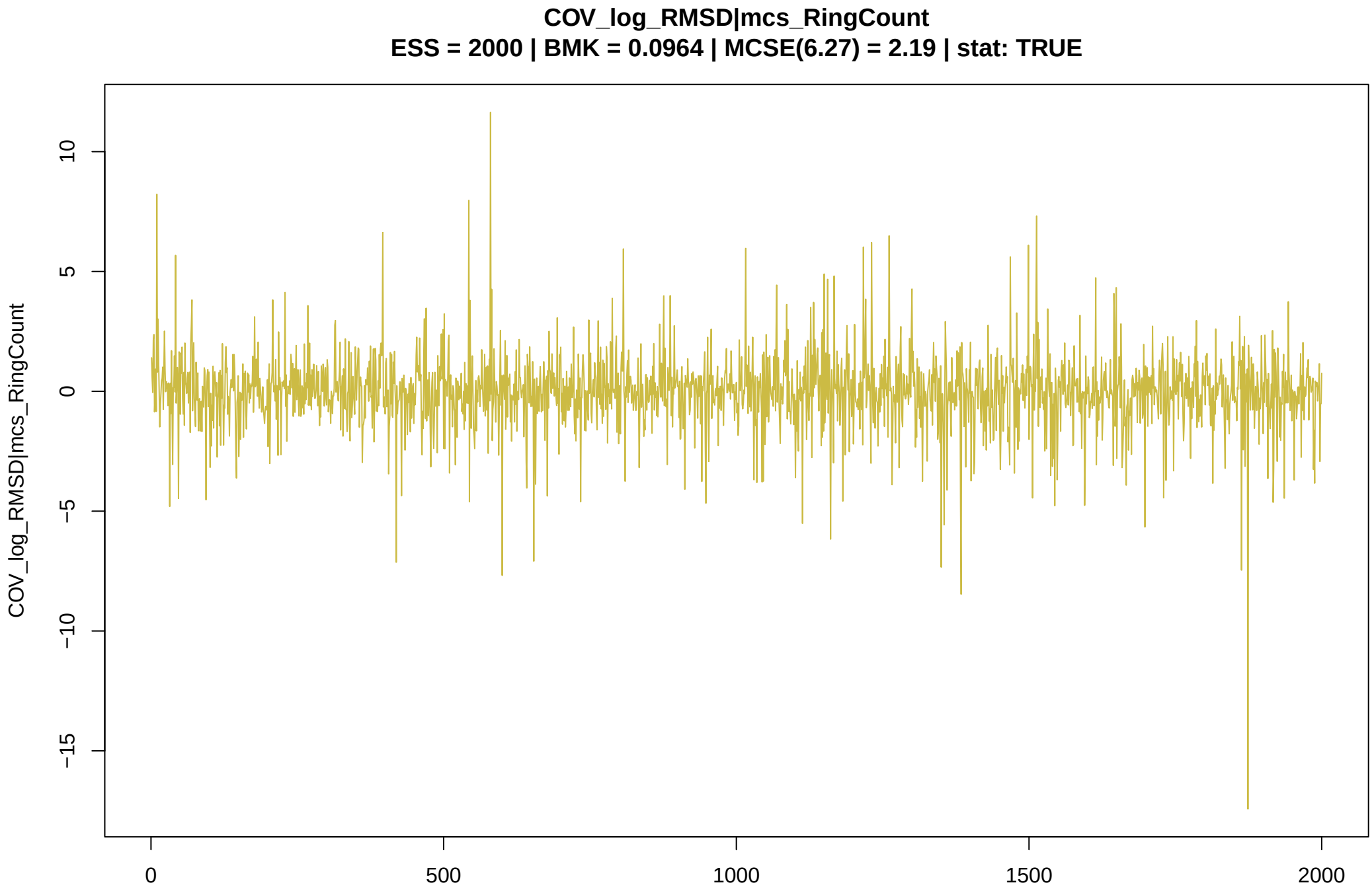

VAR_docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0652 | MCSE(6.27) = 2.23 | stat: TRUE
VAR_docked_NumRotatableBonds
2
3
4
5
6
7
0
500
1000
1500
2000

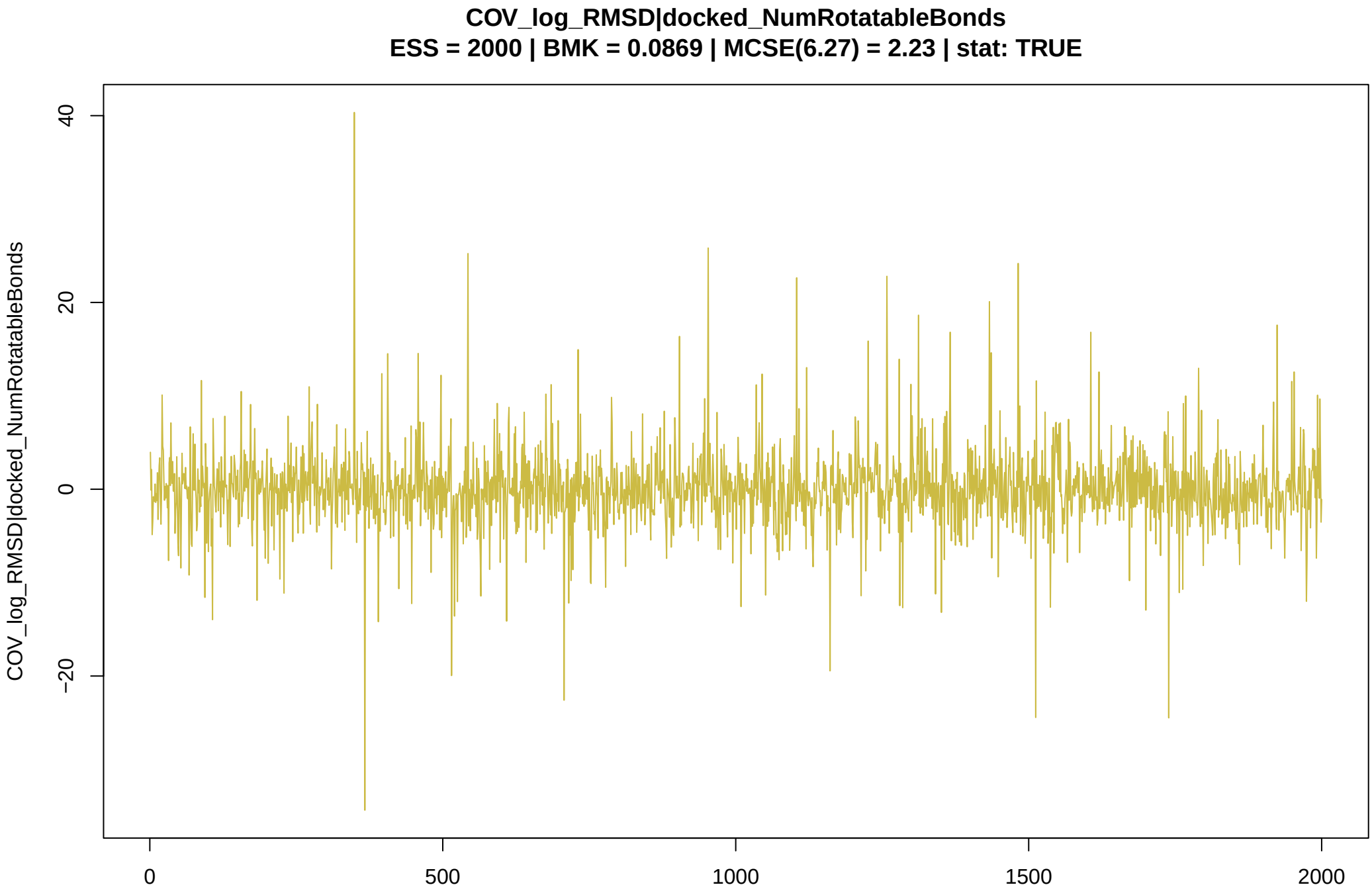

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0567 | MCSE(6.27) = 2.2 | stat: TRUE
COV_log_RMSD|log_mcs_unbonded_polar_sasa
3
2
1
0
−1
−2
−3
0
500
1000
1500
2000

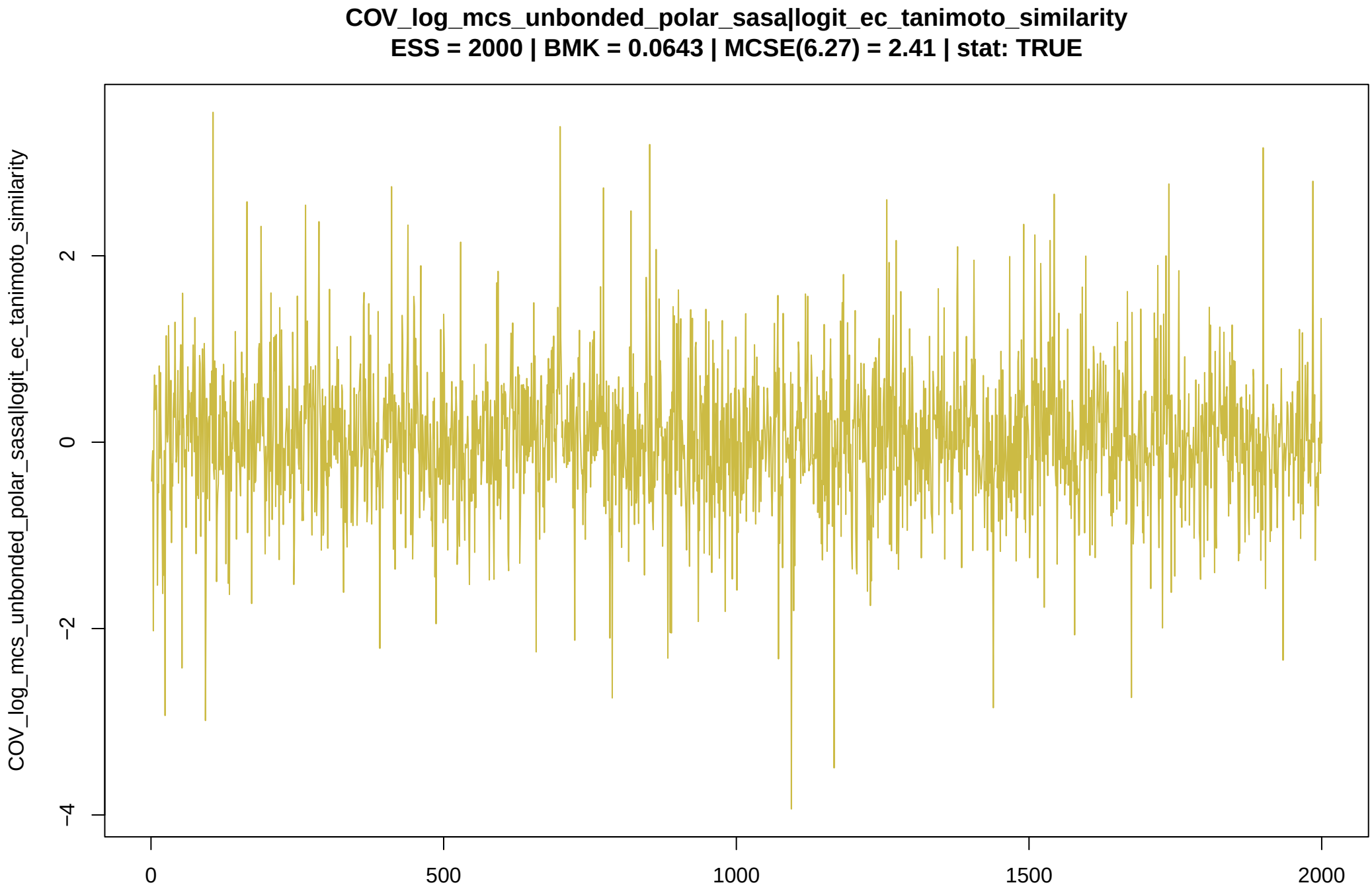

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1720 | BMK = 0.0726 | MCSE(6.27) = 2.41 | stat: TRUE
COV_log_RMSD|logit_ec_tanimoto_similarity
2
1
0
−1
−2
−3
0
500
1000
1500
2000

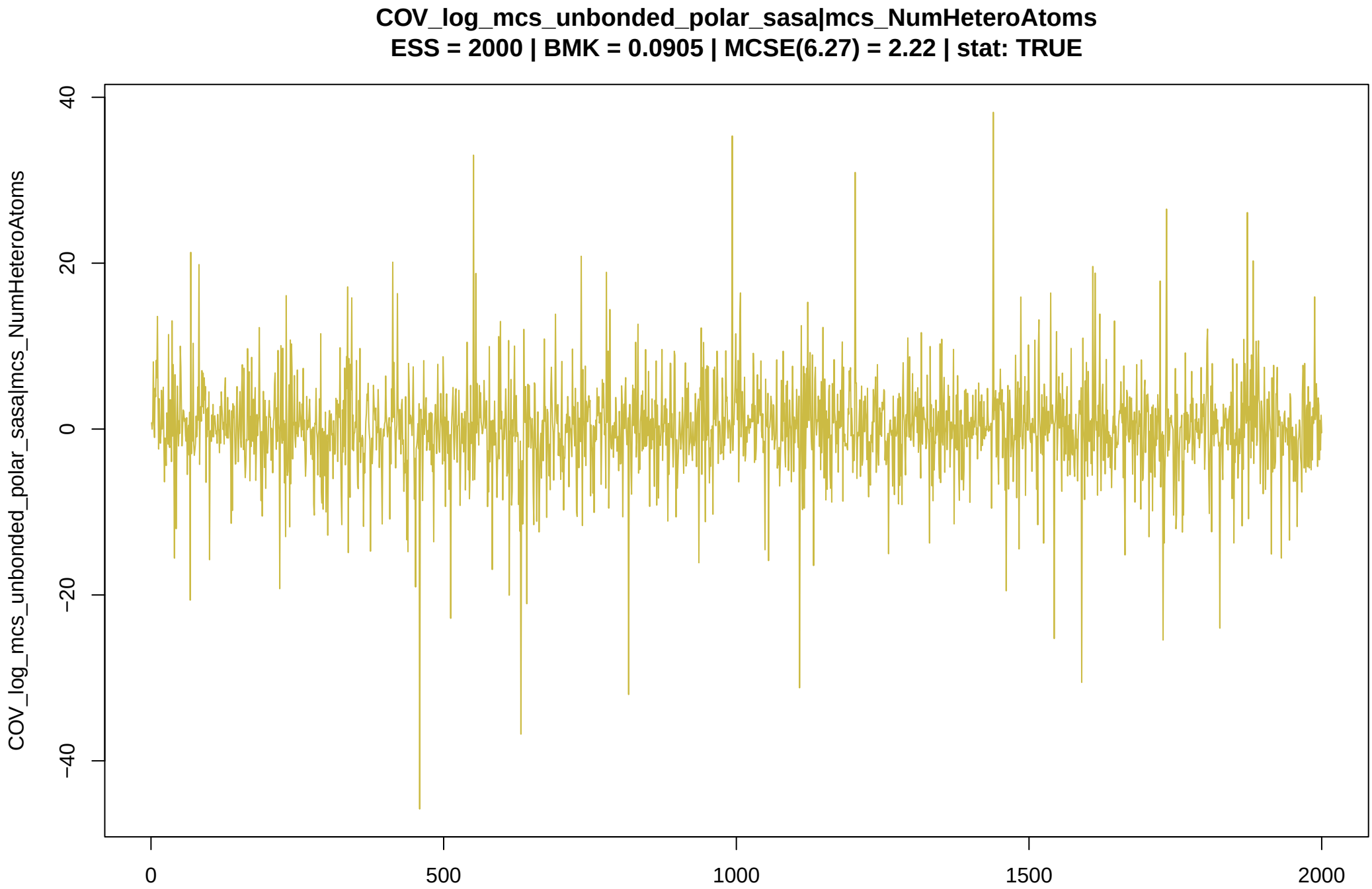

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0837 | MCSE(6.27) = 2.17 | stat: TRUE
COV_log_RMSD|mcs_NumHeteroAtoms
20
10
0
−10
−20
−30
0
500
1000
1500
2000

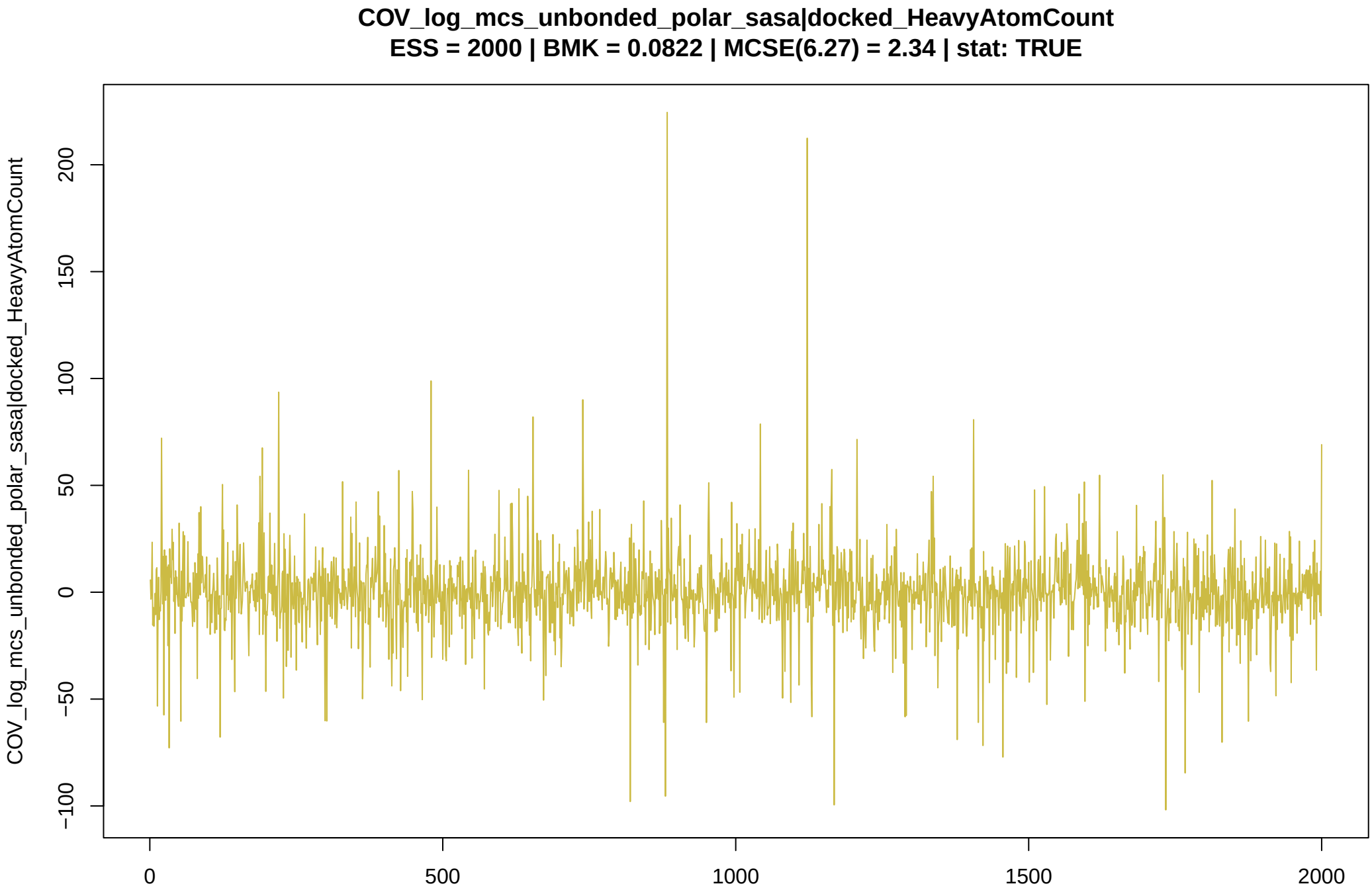

COV_log_RMSD|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0958 | MCSE(6.27) = 2.23 | stat: TRUE
COV_log_RMSD|docked_HeavyAtomCount
100
50
0
−50
−100
0
500
1000
1500
2000

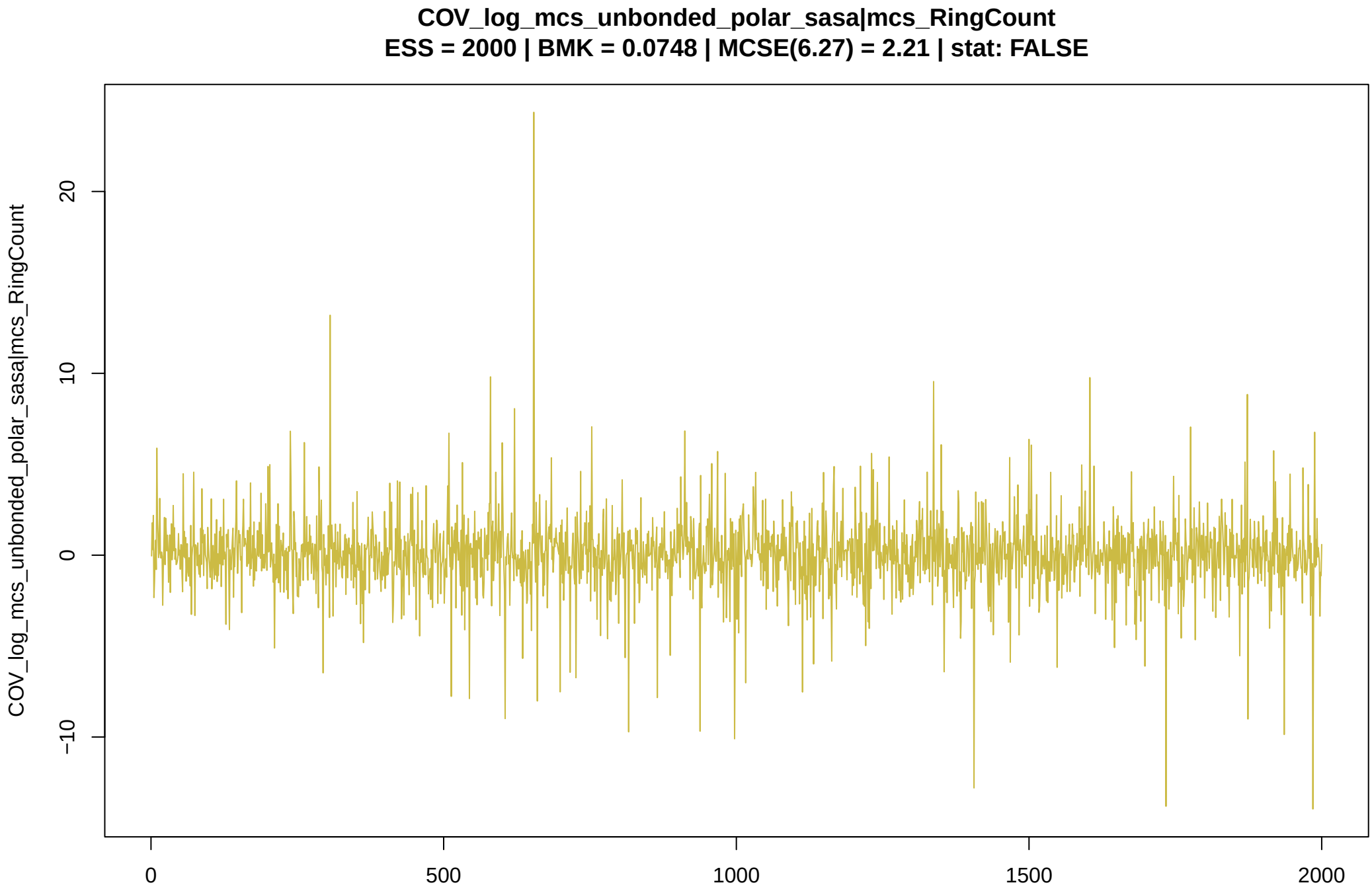

COV_log_RMSD|mcs_RingCount
ESS = 2000 | BMK = 0.0964 | MCSE(6.27) = 2.19 | stat: TRUE
COV_log_RMSD|mcs_RingCount
10
5
0
−5
−10
−15
0
500
1000
1500
2000

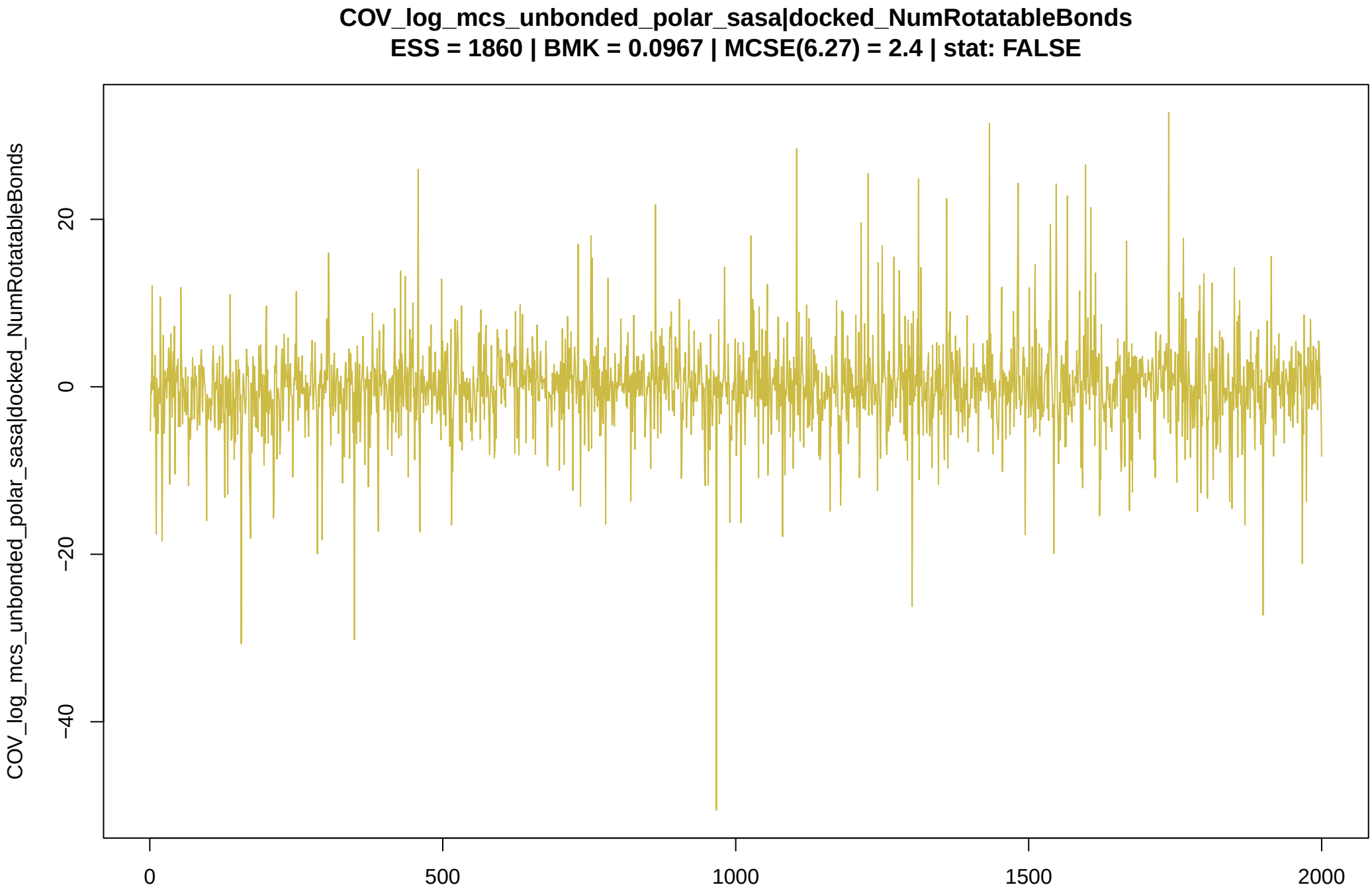

COV_log_RMSD|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0869 | MCSE(6.27) = 2.23 | stat: TRUE
COV_log_RMSD|docked_NumRotatableBonds
40
20
0
−20
0
500
1000
1500
2000

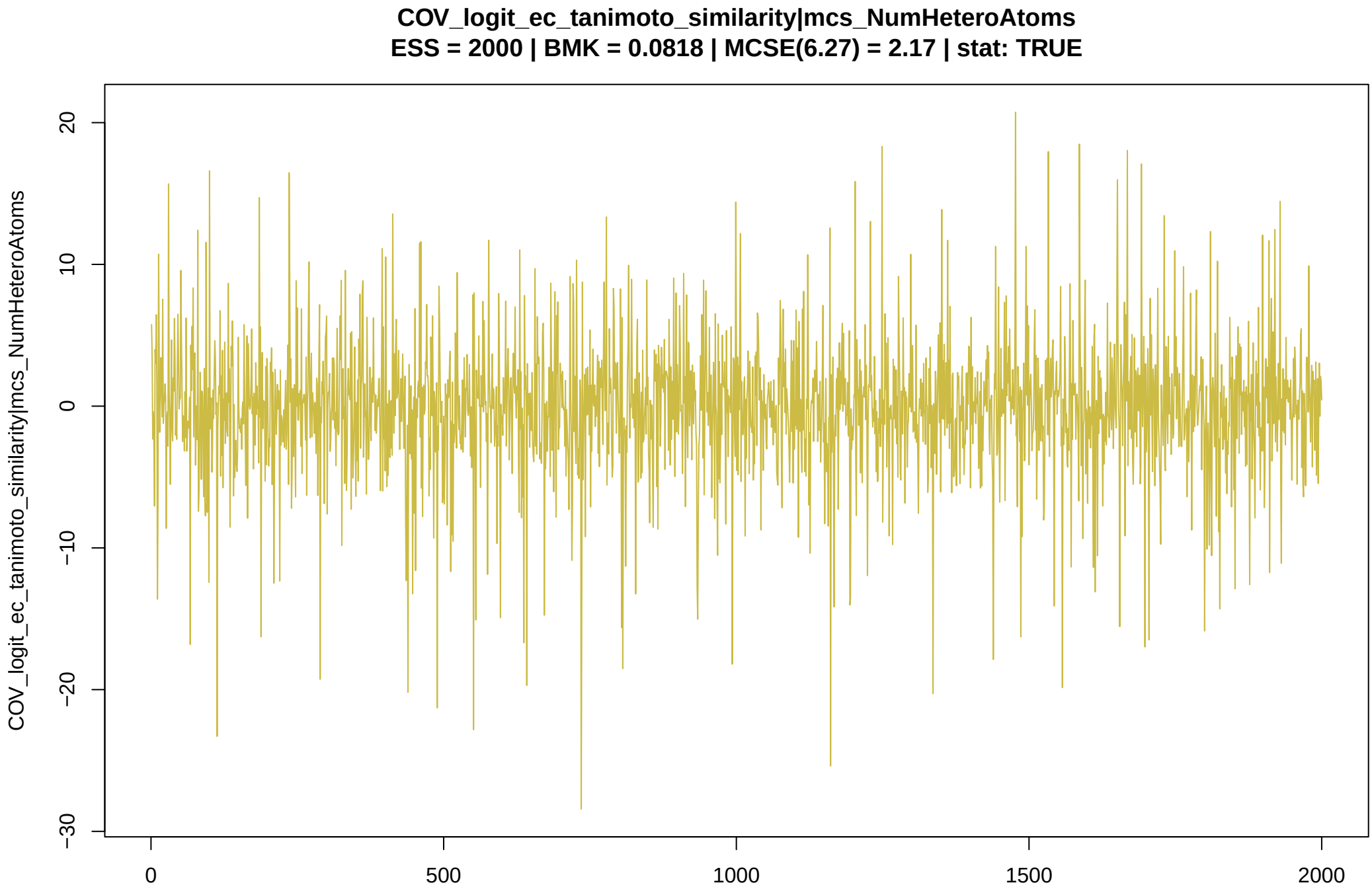

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 2000 | BMK = 0.0643 | MCSE(6.27) = 2.41 | stat: TRUE
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2
0
−2
−4
0
500
1000
1500
2000

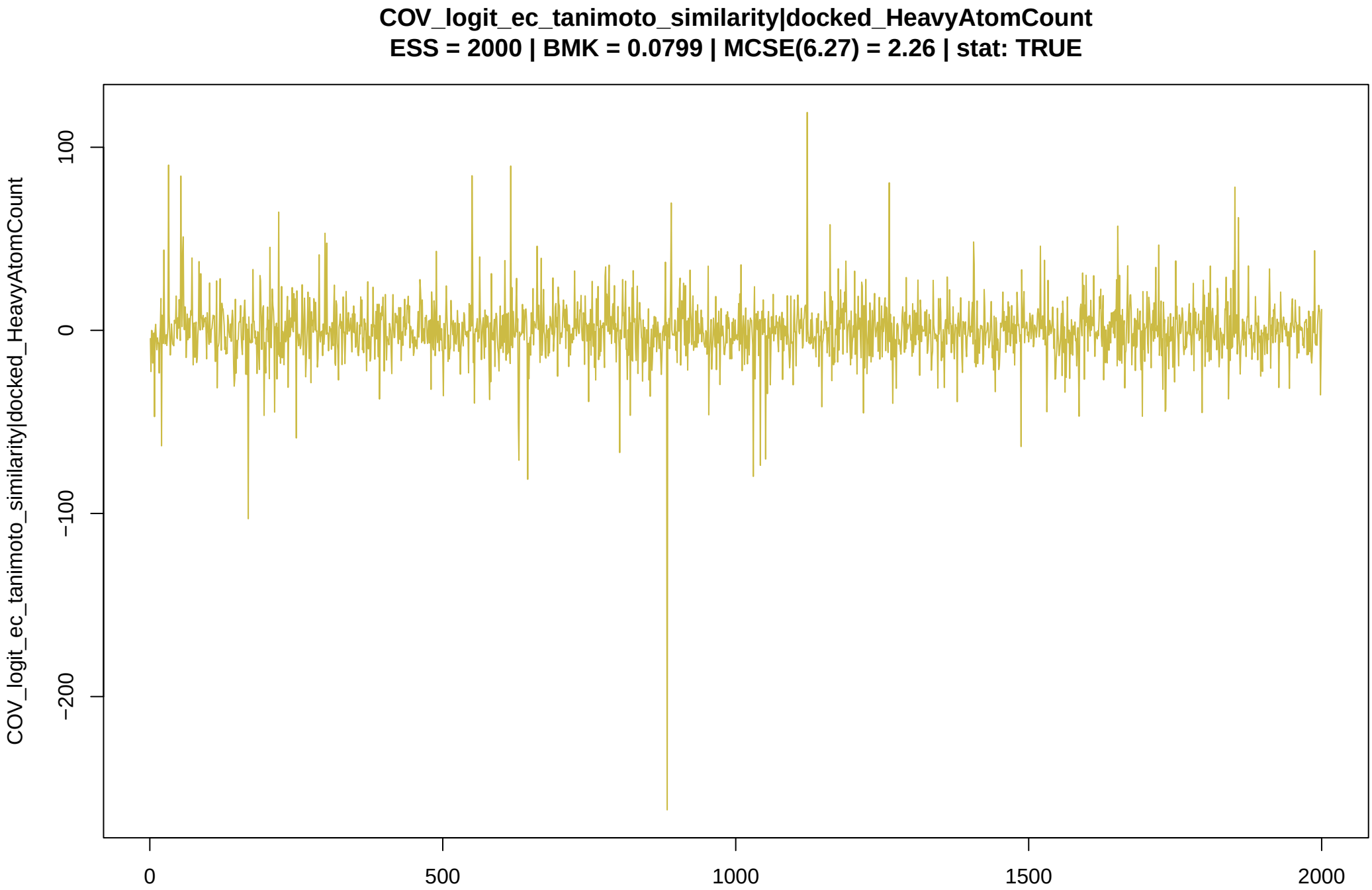

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0905 | MCSE(6.27) = 2.22 | stat: TRUE
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
40
20
0
−20
−40
0
500
1000
1500
2000

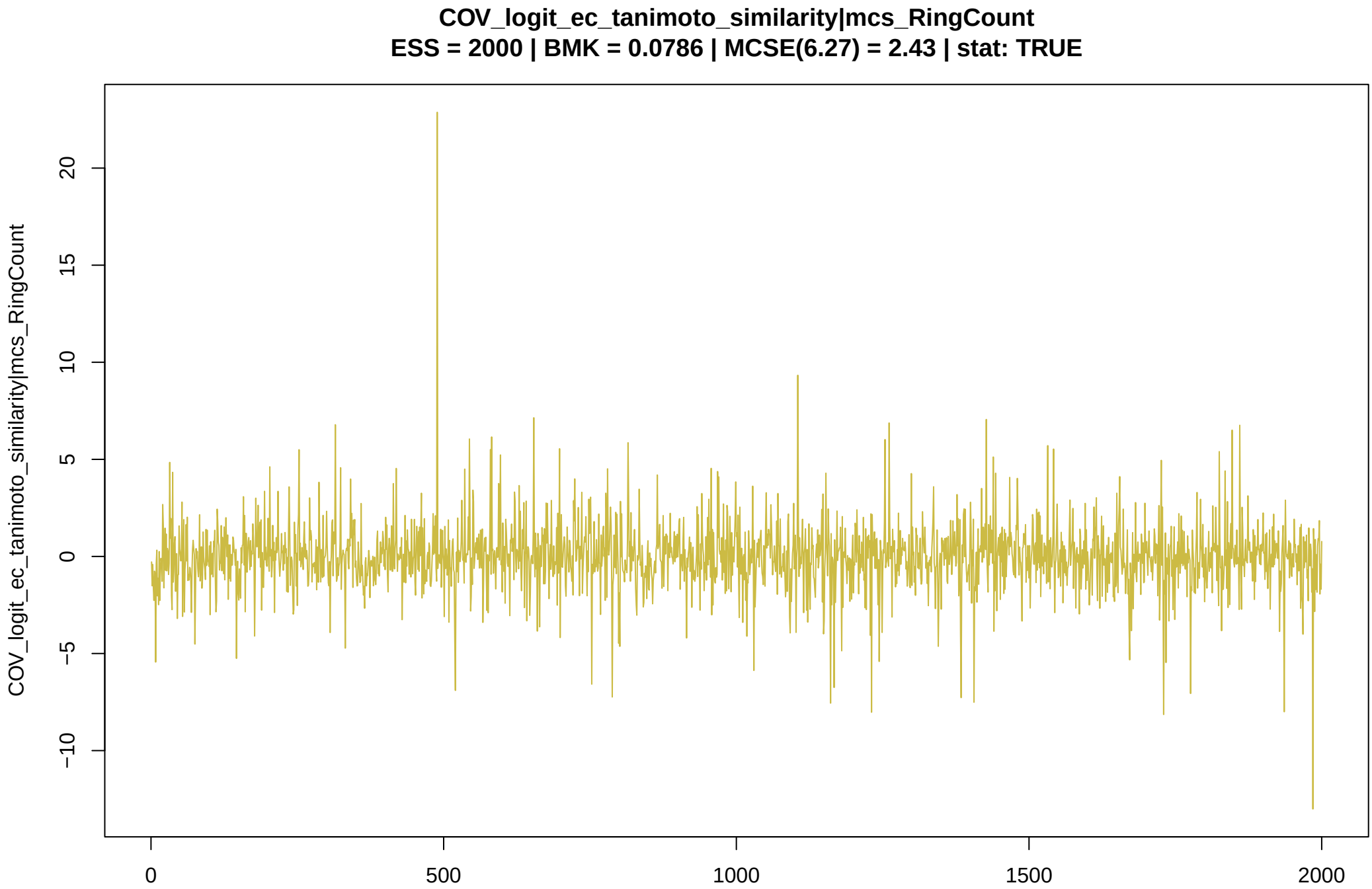

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0822 | MCSE(6.27) = 2.34 | stat: TRUE
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
−100
−50
0
50
100
150
200
0
500
1000
1500
2000

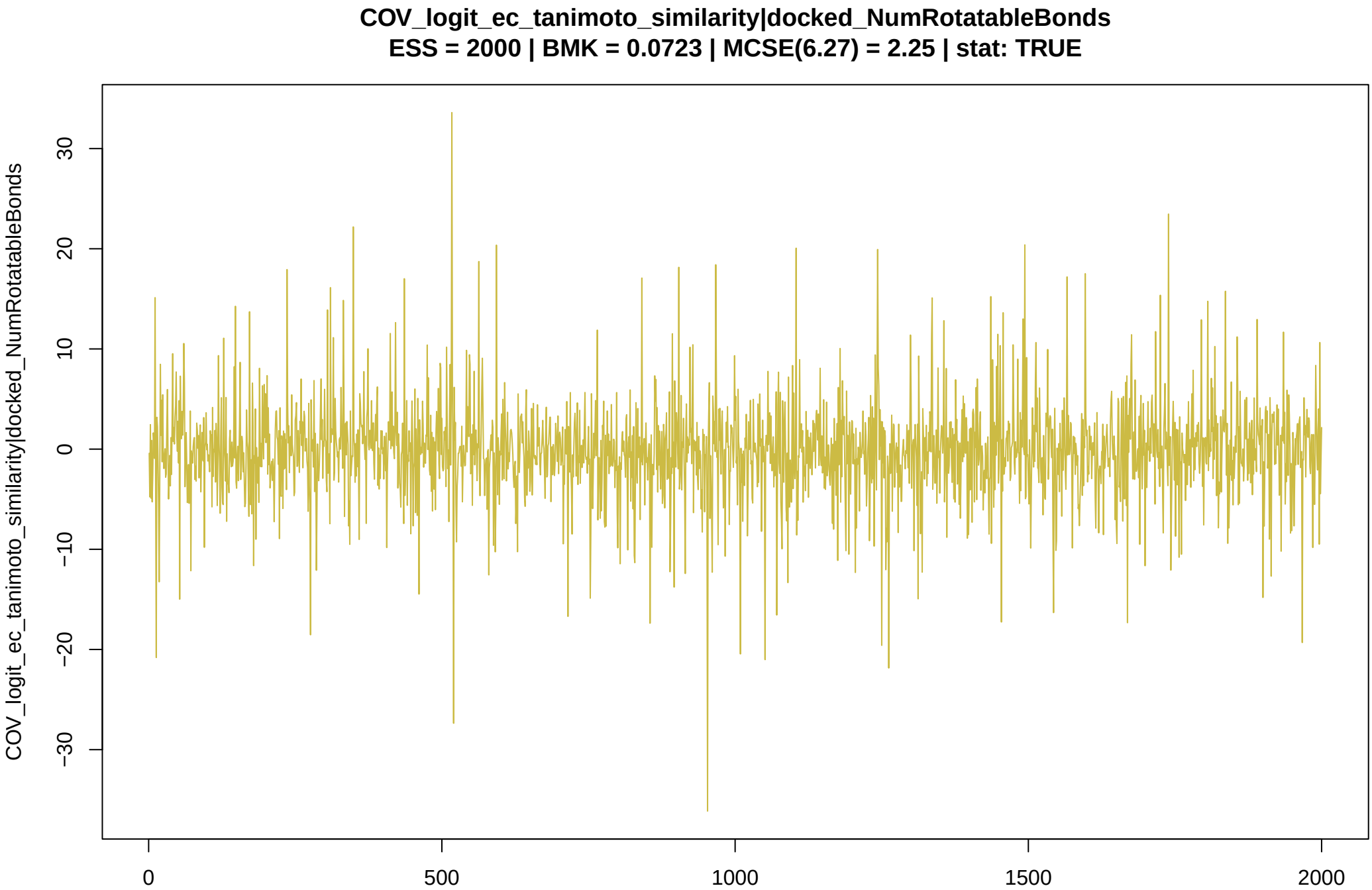

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 2000 | BMK = 0.0748 | MCSE(6.27) = 2.21 | stat: FALSE
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
20
10
0
−10
0
500
1000
1500
2000

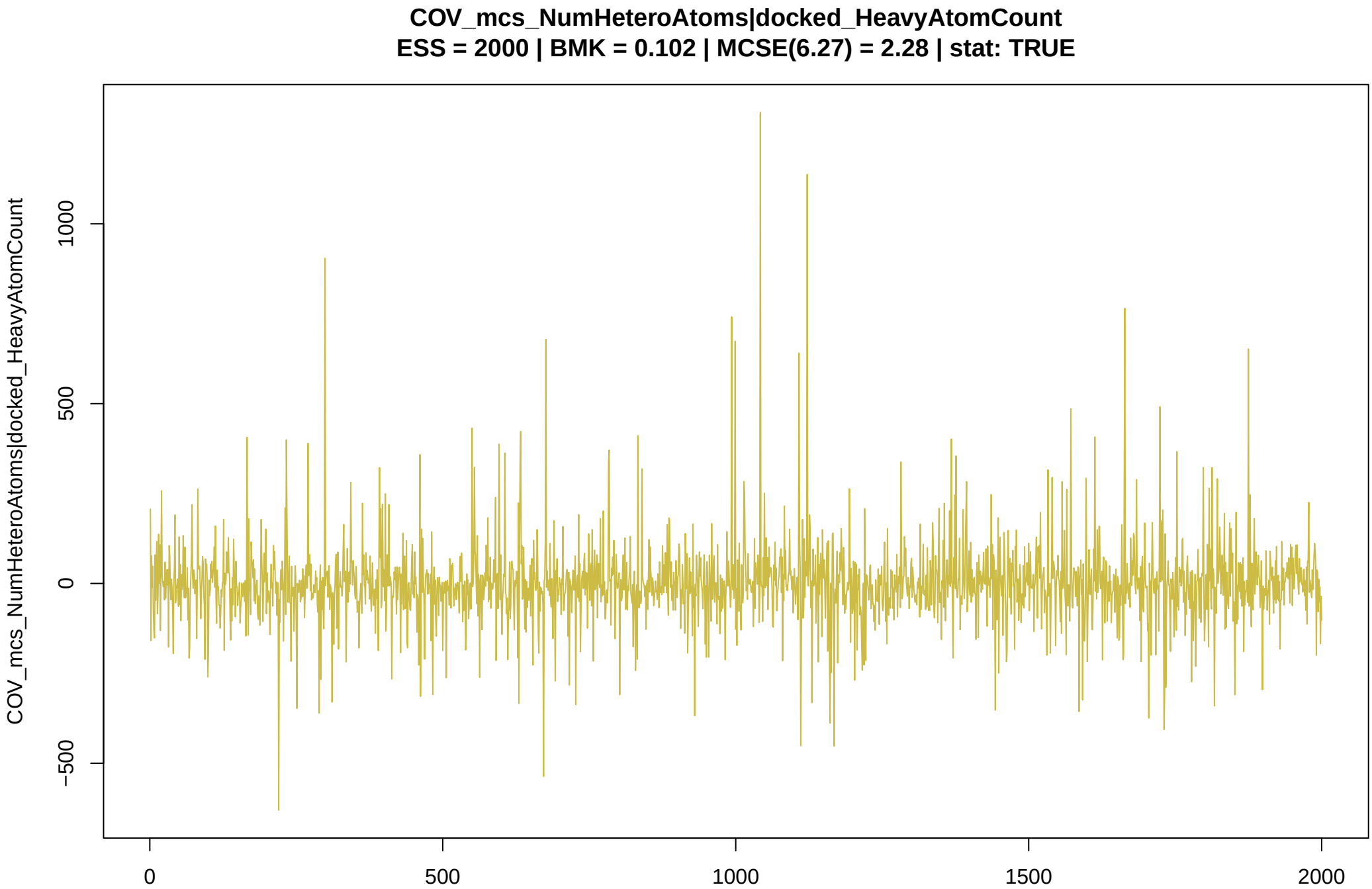

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1860 | BMK = 0.0967 | MCSE(6.27) = 2.4 | stat: FALSE
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
20
0
−20
−40
0
500
1000
1500
2000

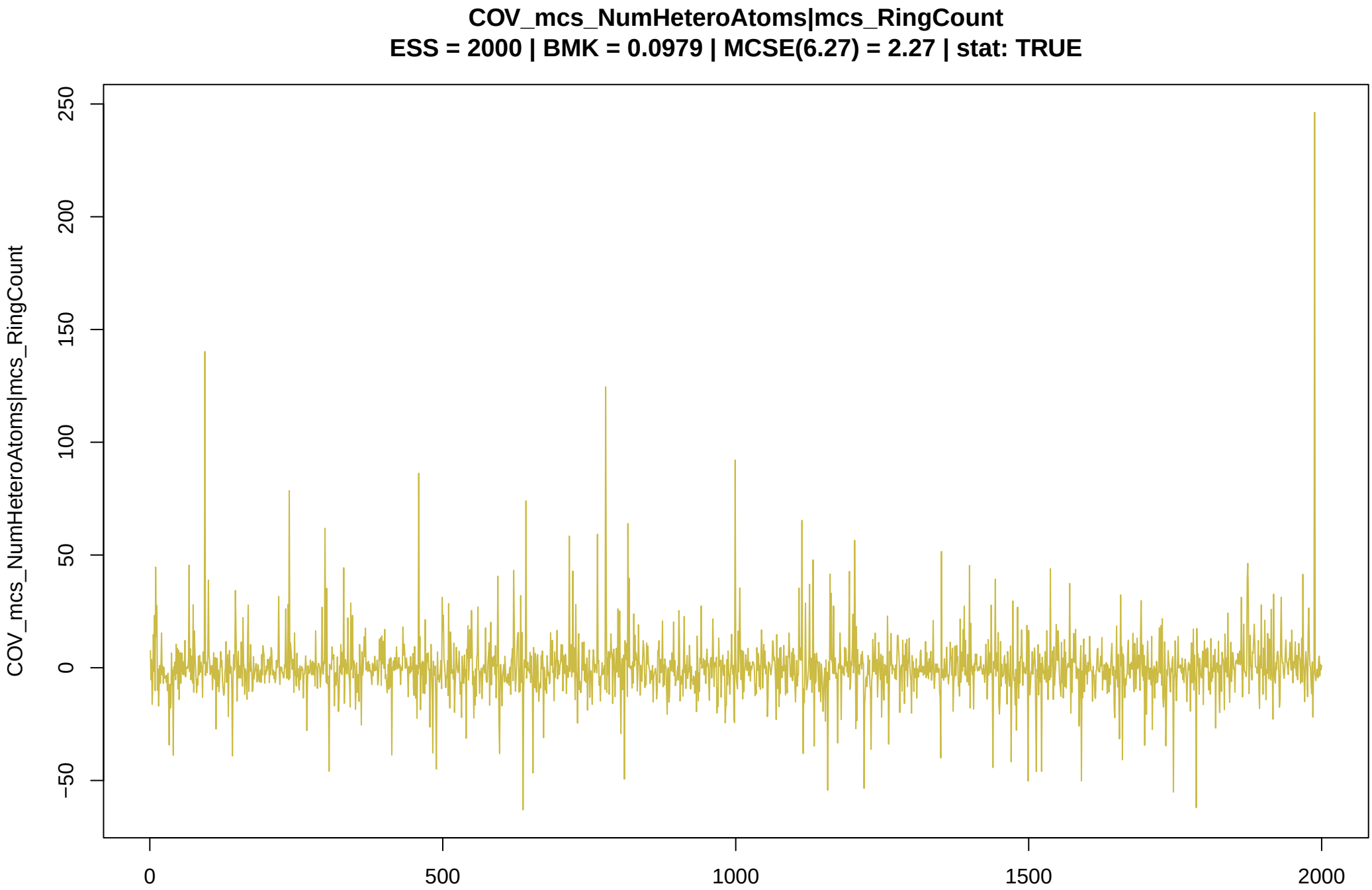

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2000 | BMK = 0.0818 | MCSE(6.27) = 2.17 | stat: TRUE
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
20
10
0
−10
−20
−30
0
500
1000
1500
2000

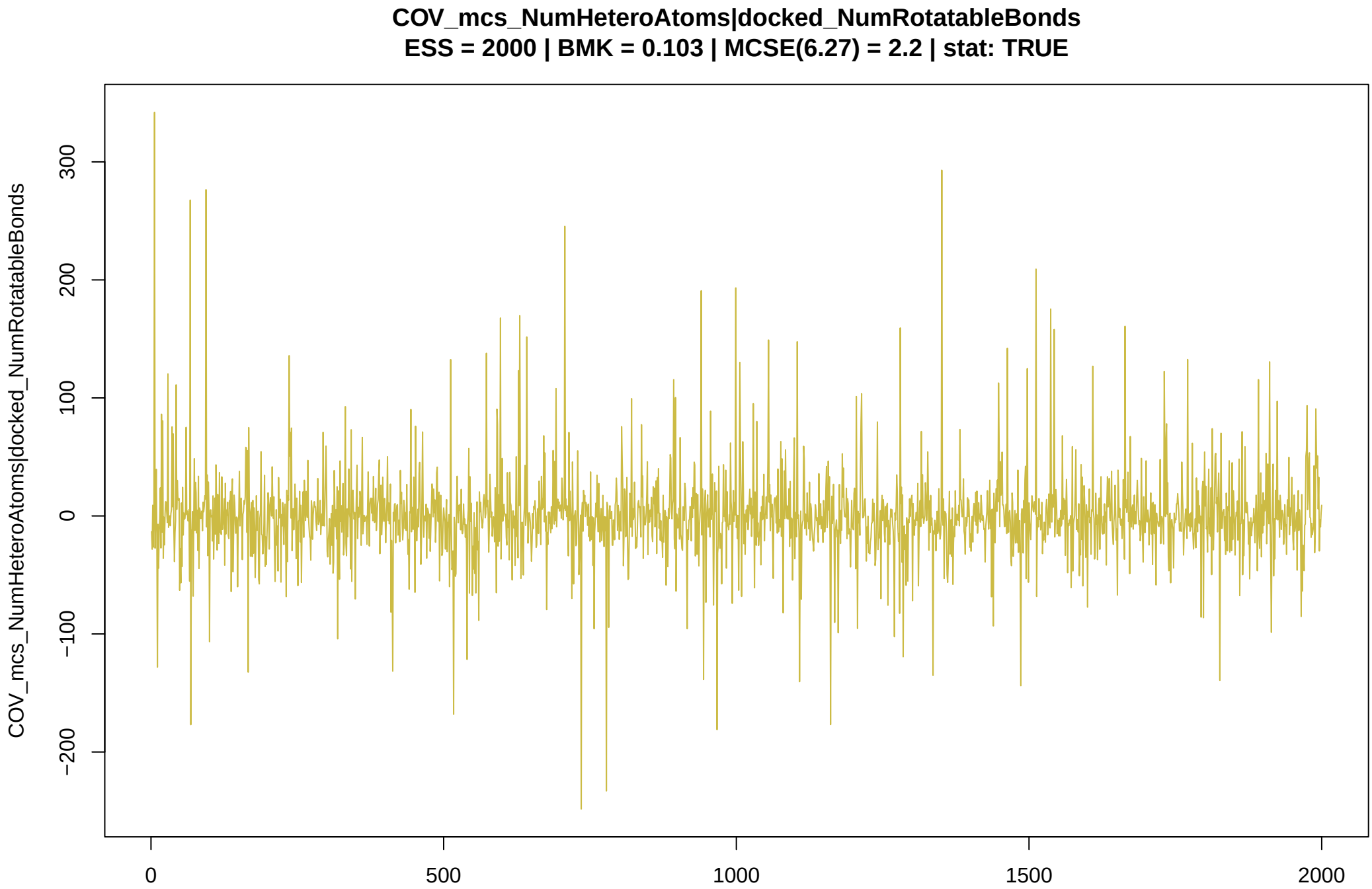

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.0799 | MCSE(6.27) = 2.26 | stat: TRUE
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
100
0
−100
−200
0
500
1000
1500
2000

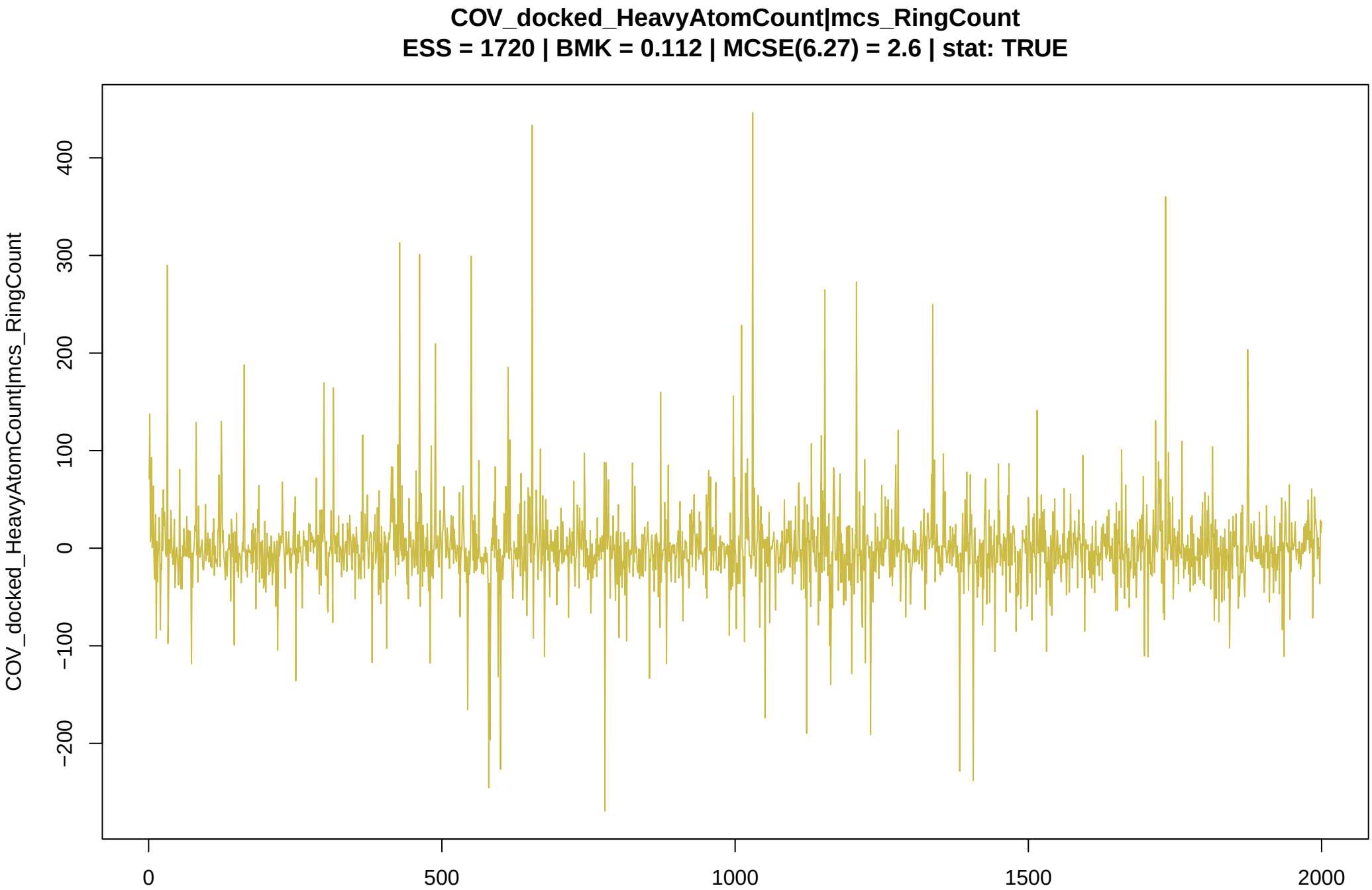

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 2000 | BMK = 0.0786 | MCSE(6.27) = 2.43 | stat: TRUE
COV_logit_ec_tanimoto_similarity|mcs_RingCount
20
15
10
5
0
−5
−10
0
500
1000
1500
2000

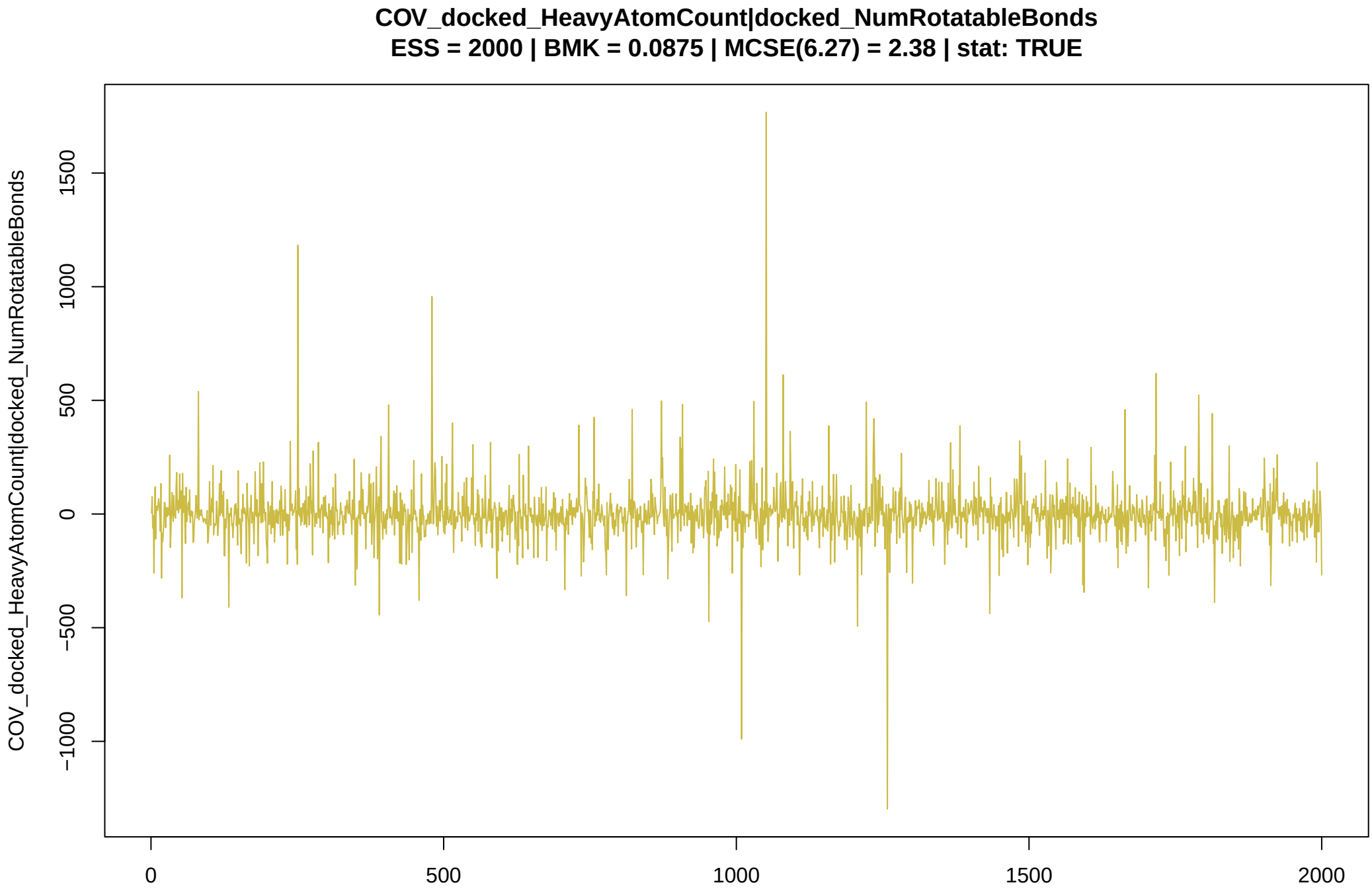

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0723 | MCSE(6.27) = 2.25 | stat: TRUE
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
30
20
10
0
−10
−20
−30
0
500
1000
1500
2000

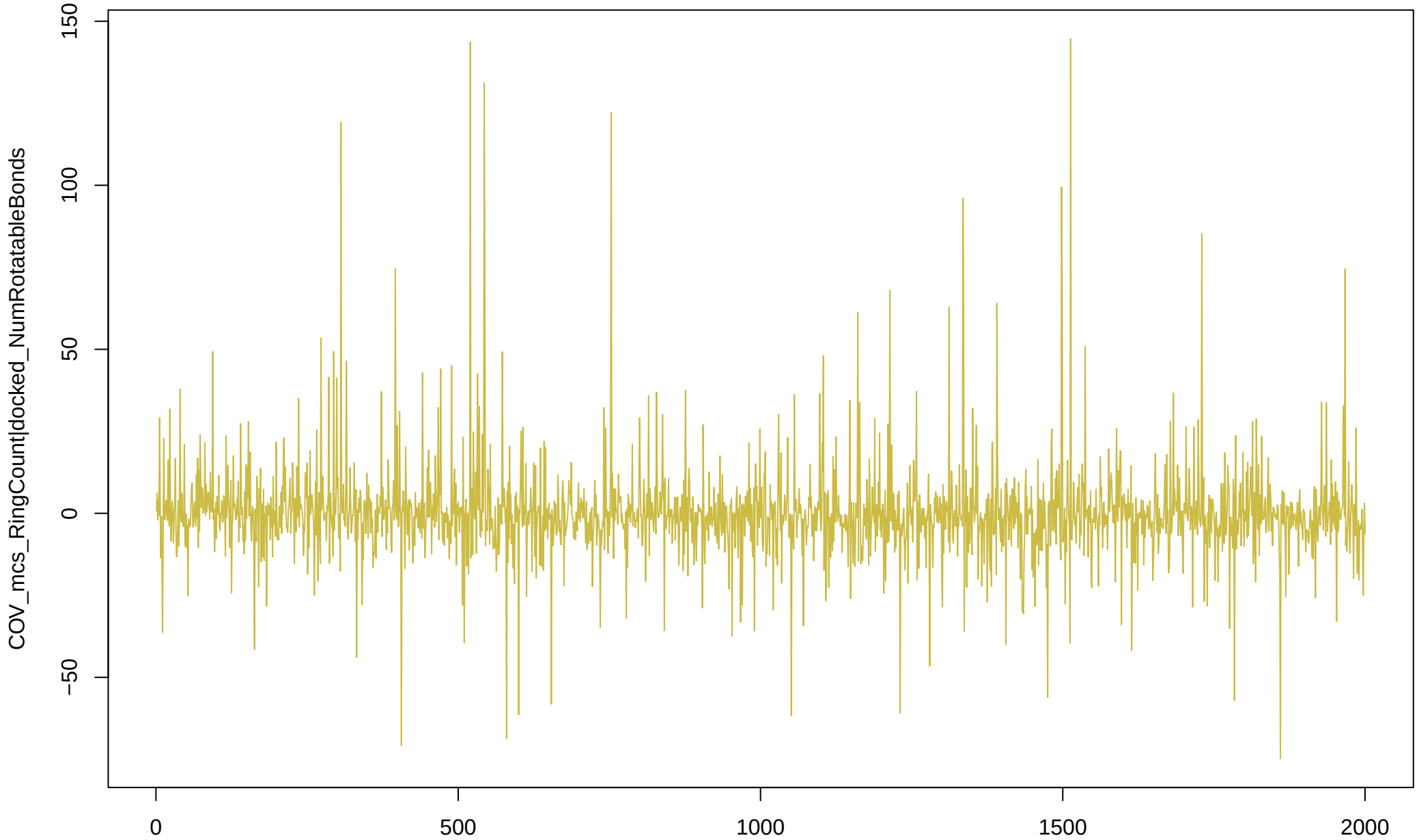

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2000 | BMK = 0.102 | MCSE(6.27) = 2.28 | stat: TRUE
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−500
0
500
1000
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 2000 | BMK = 0.0979 | MCSE(6.27) = 2.27 | stat: TRUE
COV_mcs_NumHeteroAtoms|mcs_RingCount
250
200
150
100
50
0
−50
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.103 | MCSE(6.27) = 2.2 | stat: TRUE
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
300
200
100
0
−100
−200
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1720 | BMK = 0.112 | MCSE(6.27) = 2.6 | stat: TRUE
COV_docked_HeavyAtomCount|mcs_RingCount
400
300
200
100
0
−100
−200
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.0875 | MCSE(6.27) = 2.38 | stat: TRUE
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
1500
1000
500
0
−500
−1000
0
500
1000
1500
2000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 2000 | BMK = 0.121 | MCSE(6.27) = 2.31 | stat: TRUE
COV_mcs_RingCount|docked_NumRotatableBonds
150
100
50
0
−50
0
500
1000
1500
2000