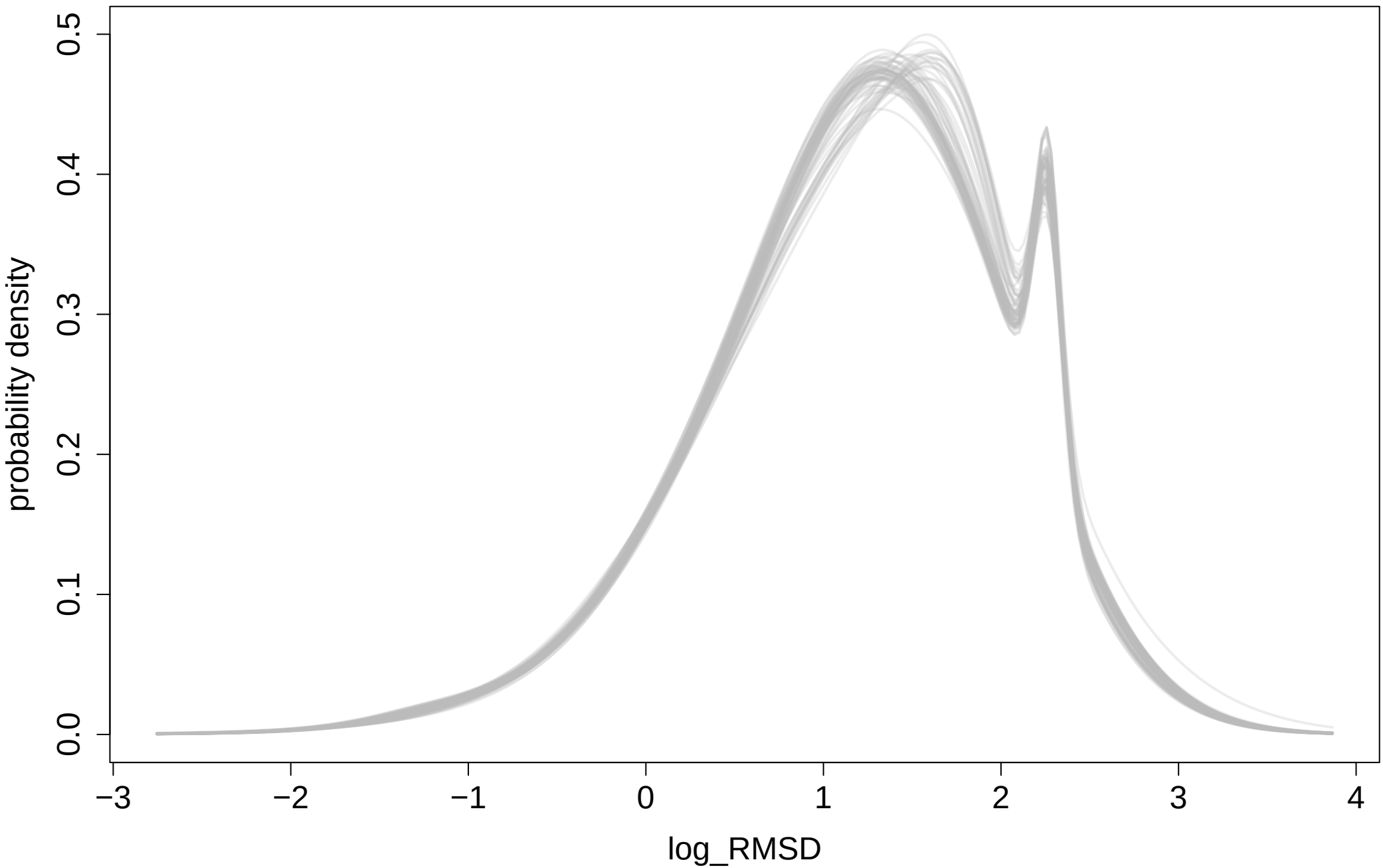
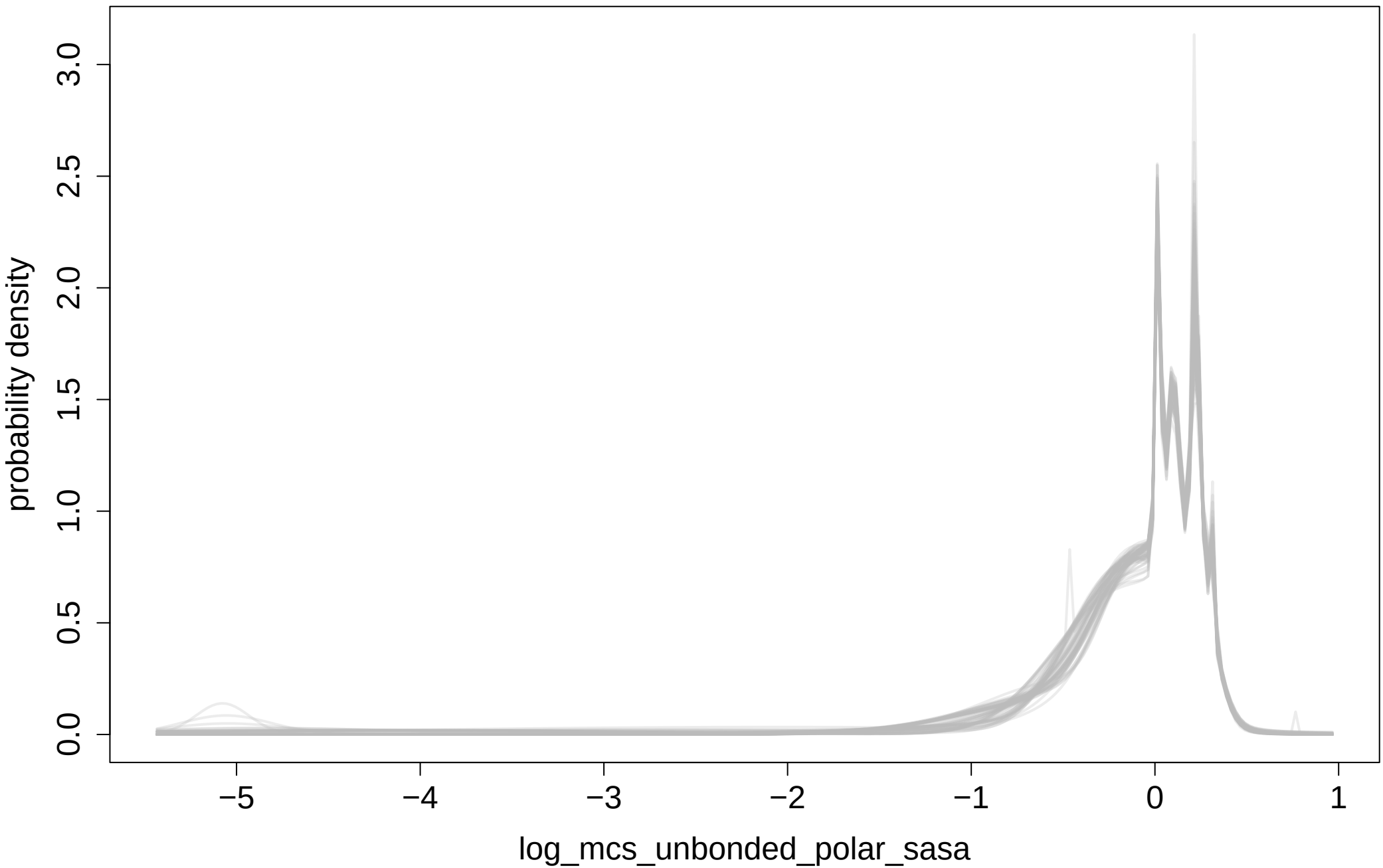
−− STATS maxD −−
min ESS = 3.21583958236453
max BMK = 0.76246478184438
max MCSE = 14.5791694768574
all stationary: FALSE
burn: 2040

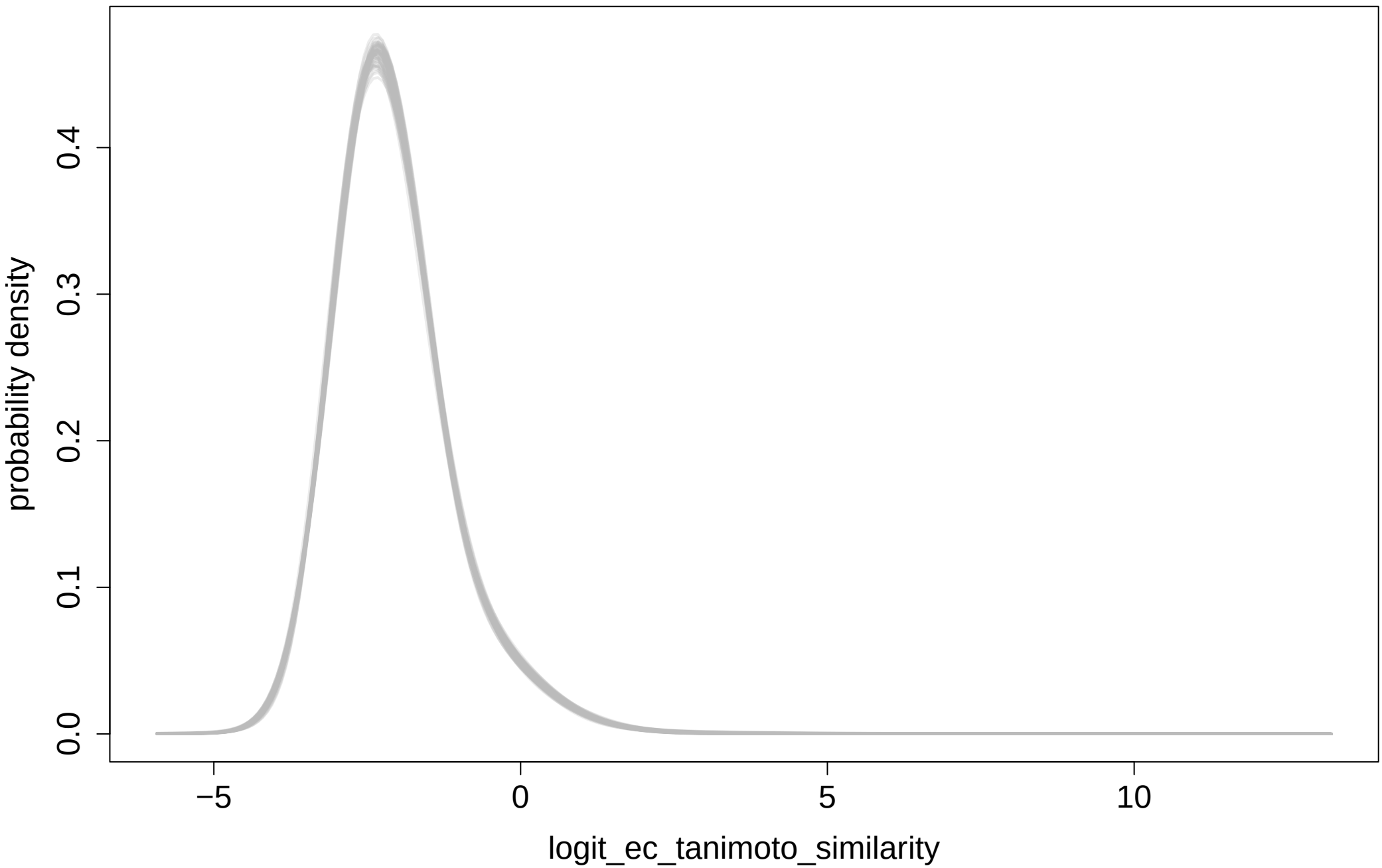
−− STATS 2D −−
min ESS = 5.5568429543
max BMK = 0.637434481890428
max MCSE = 13.9935317979071
all stationary: FALSE
burn: 1632

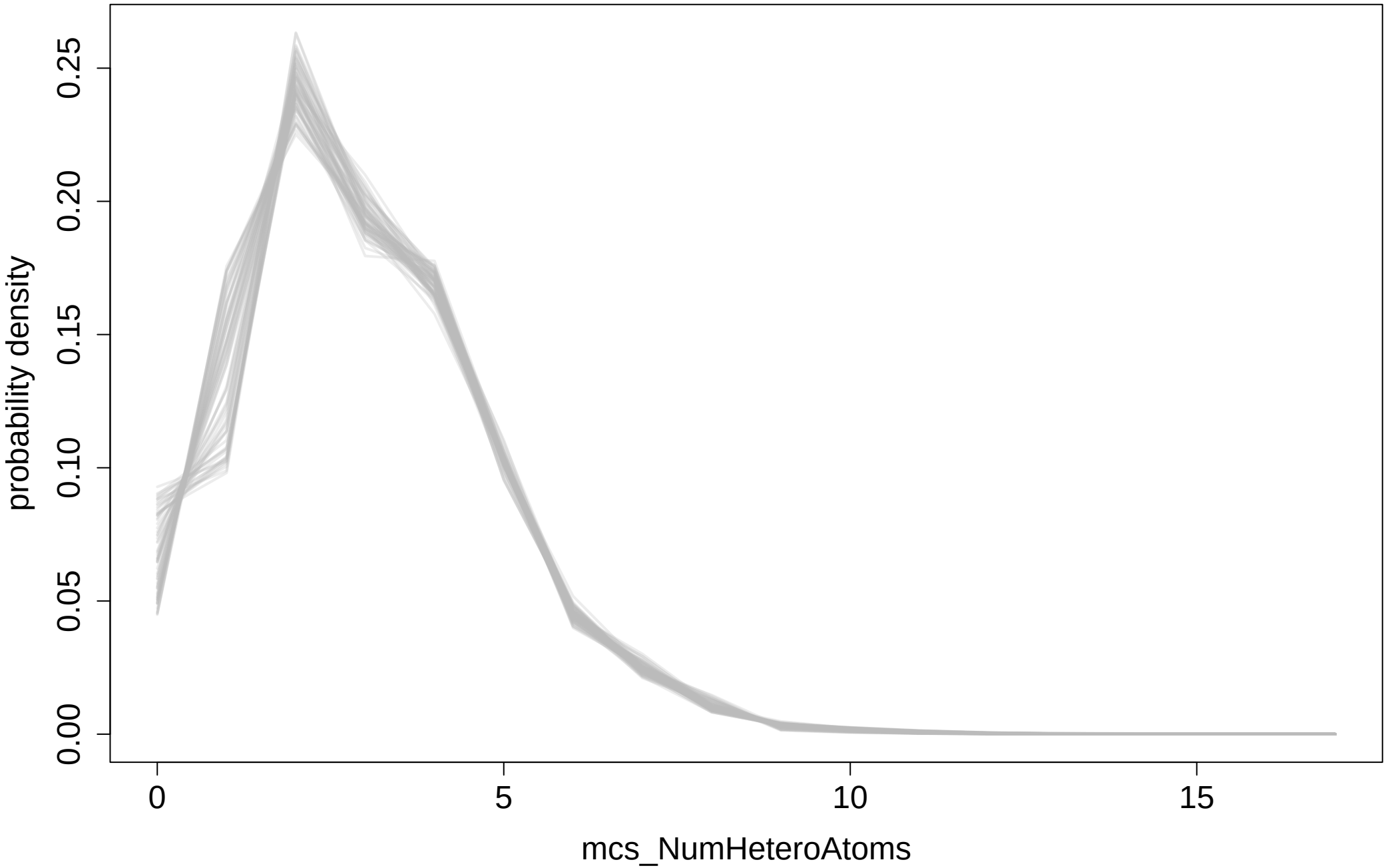
−− STATS 1D −−
min ESS = 2.2204604925031e−16
max BMK = 1
max MCSE = NaN
all stationary: FALSE
burn: 2040

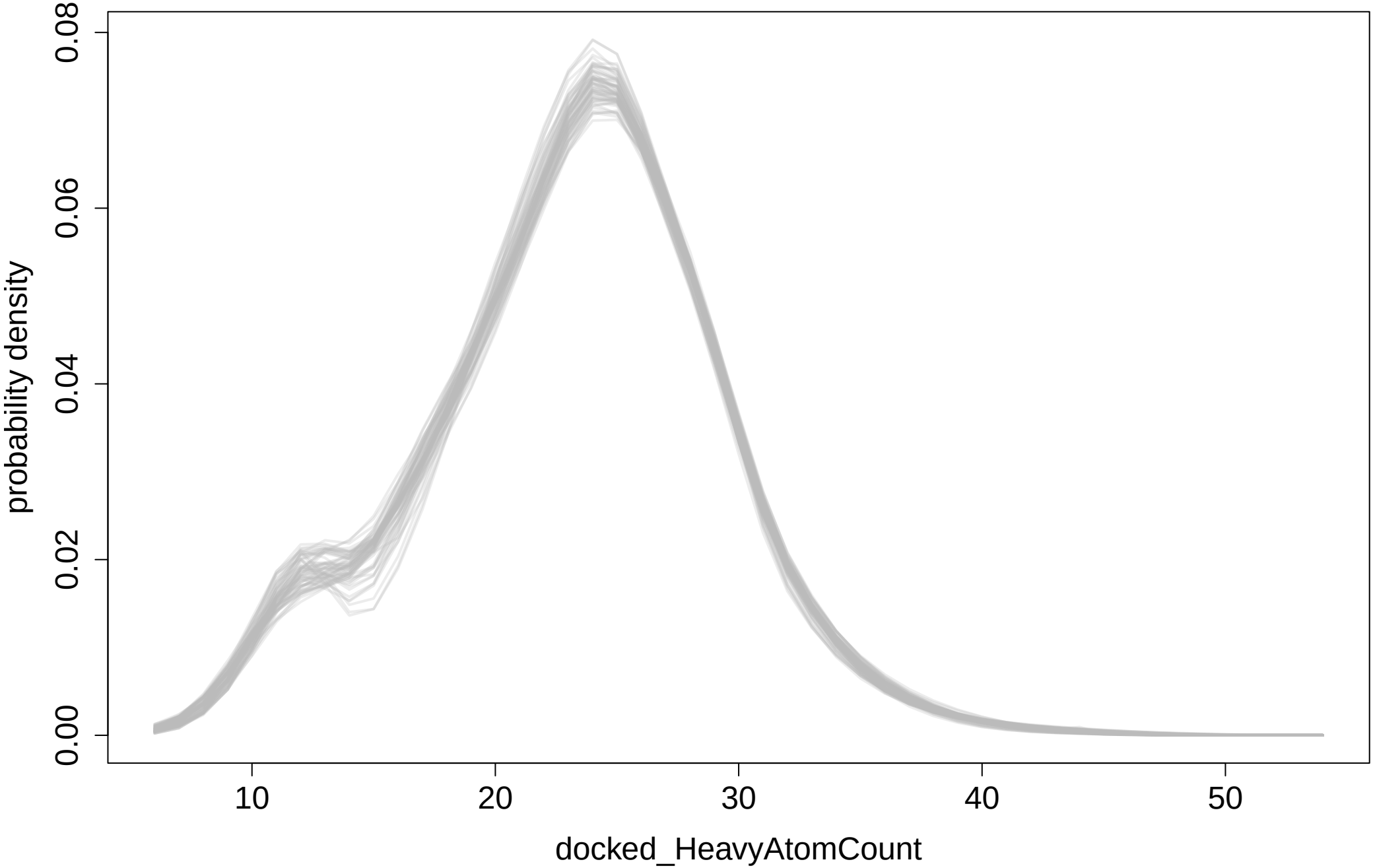
Occupied clusters: 33 of 64
LL: −77700 +− 7250

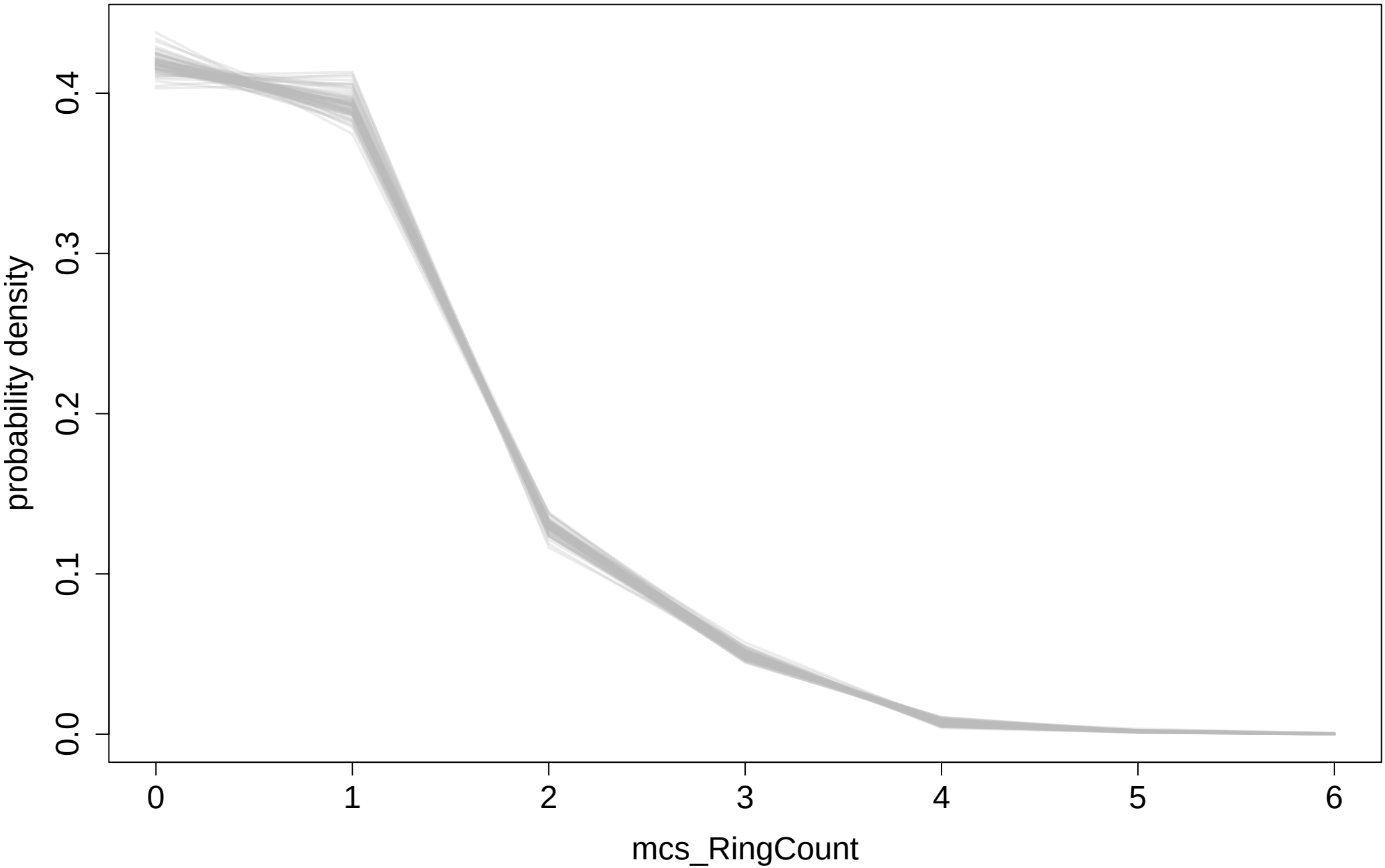

probability density
0.0
0.1
0.2
0.3
0.4
0.5
−3
−2
−1
0
1
2
3
4
log_RMSD

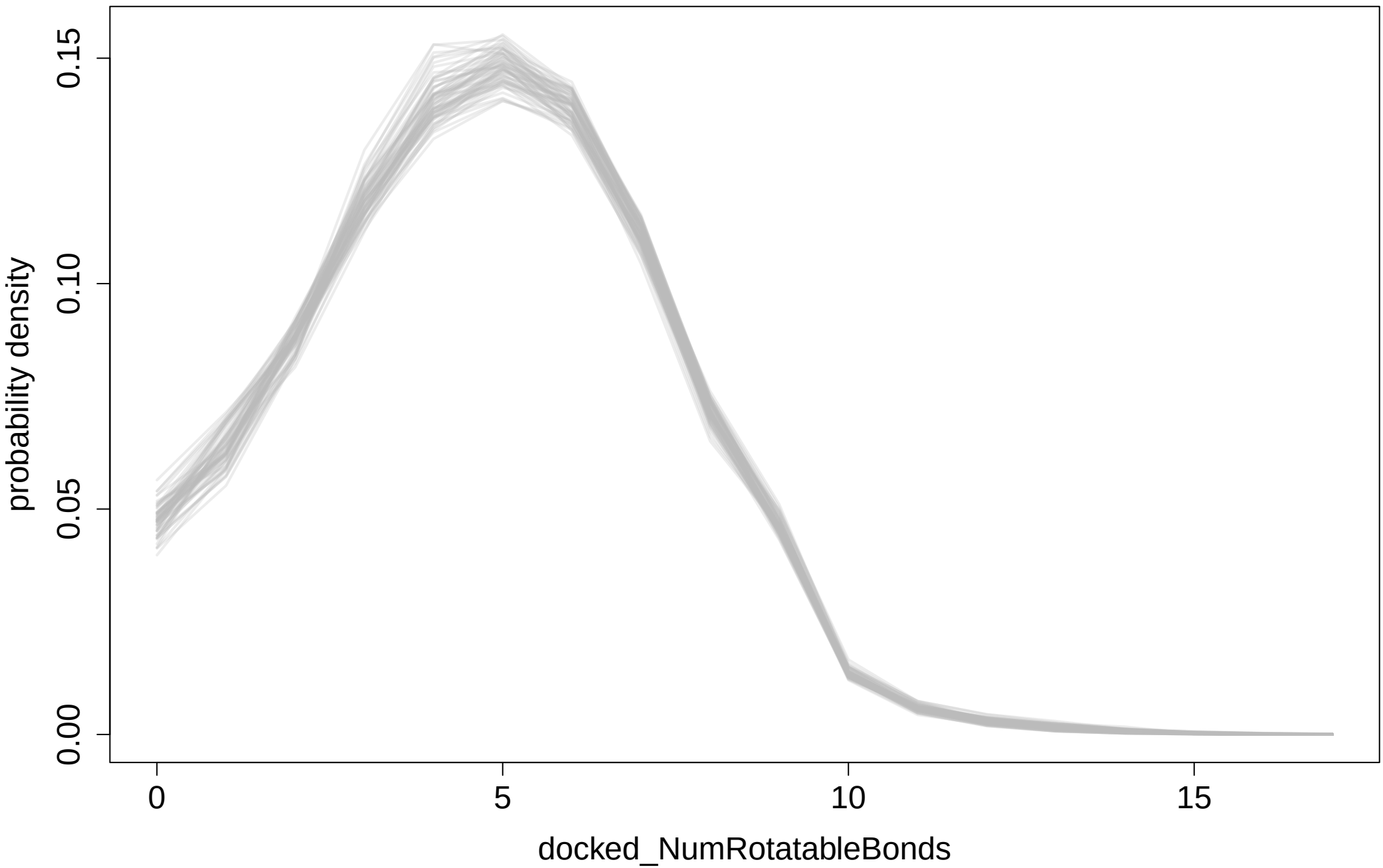

probability density
0.0
0.5
1.0
1.5
2.0
2.5
3.0
−5
−4
−3
−2
−1
0
1
log_mcs_unbonded_polar_sasa

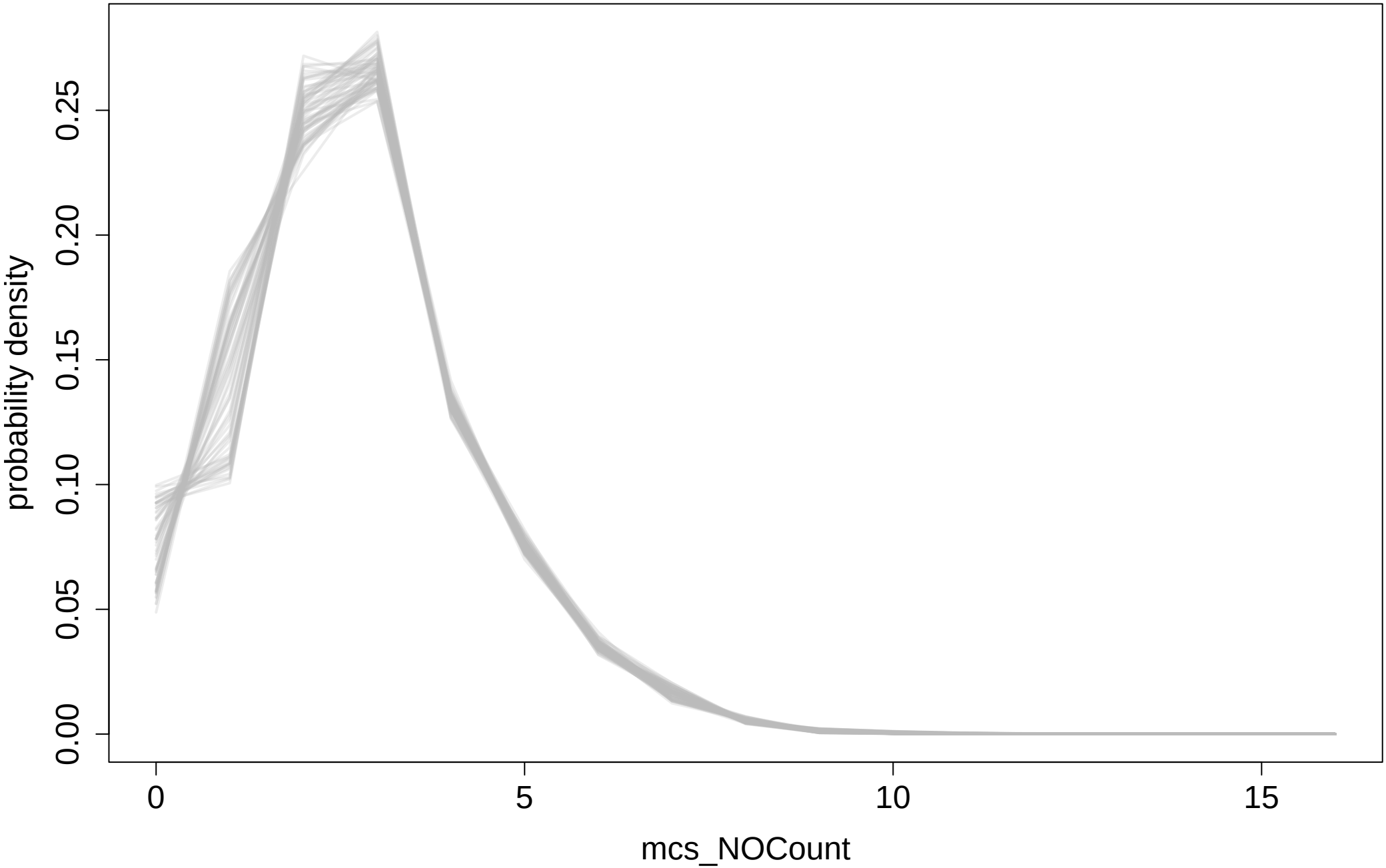

probability density
0.0
0.1
0.2
0.3
0.4
−5
0
5
10
logit_ec_tanimoto_similarity

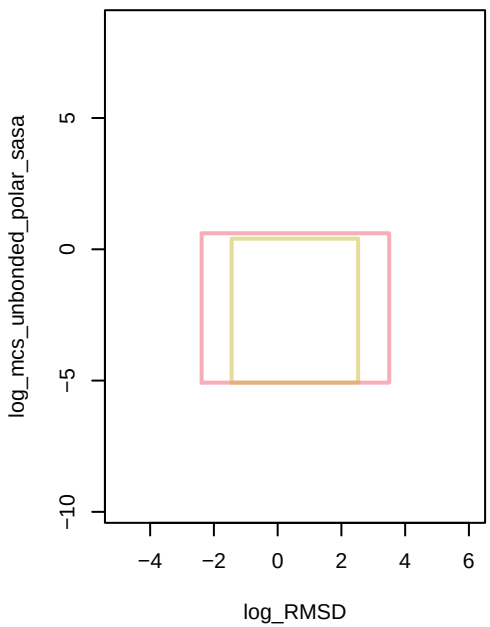

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms

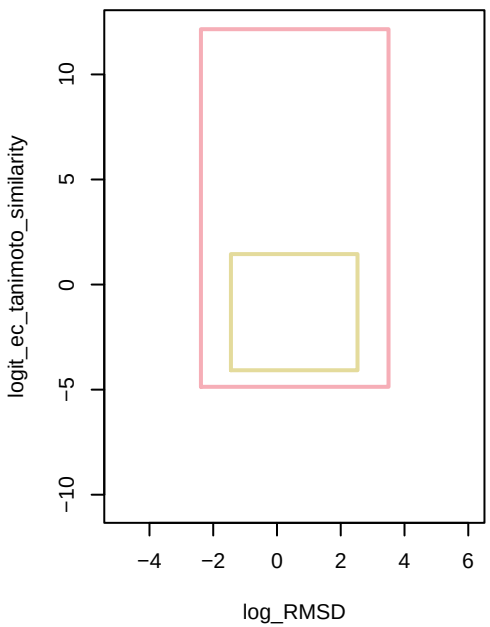

probability density
0.00
0.02
0.04
0.06
0.08
10
20
30
40
50
docked_HeavyAtomCount

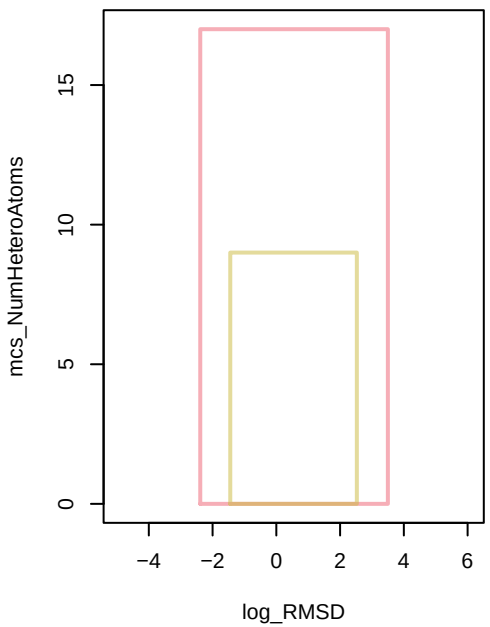

probability density
0.0
0.1
0.2
0.3
0.4
0
1
2
3
4
5
6
mcs_RingCount

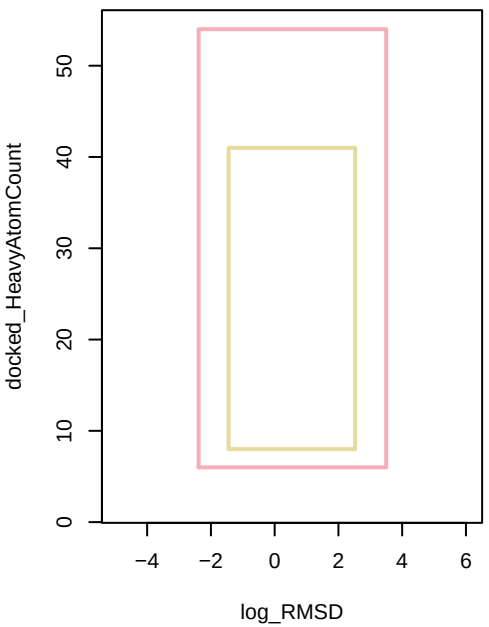

probability density
0.00
0.05
0.10
0.15
0
5
10
15
docked_NumRotatableBonds

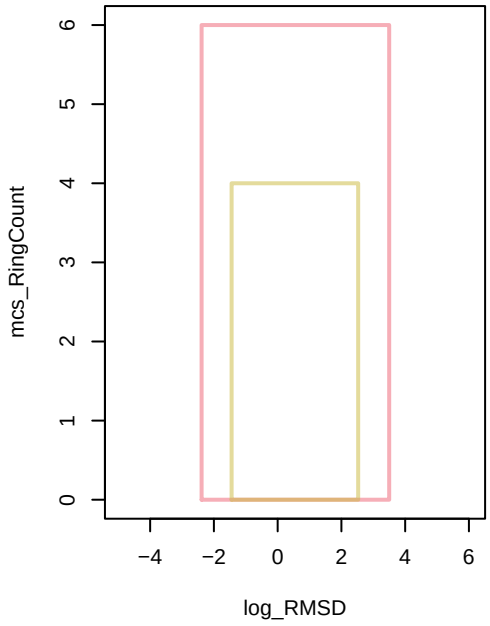

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NOCount

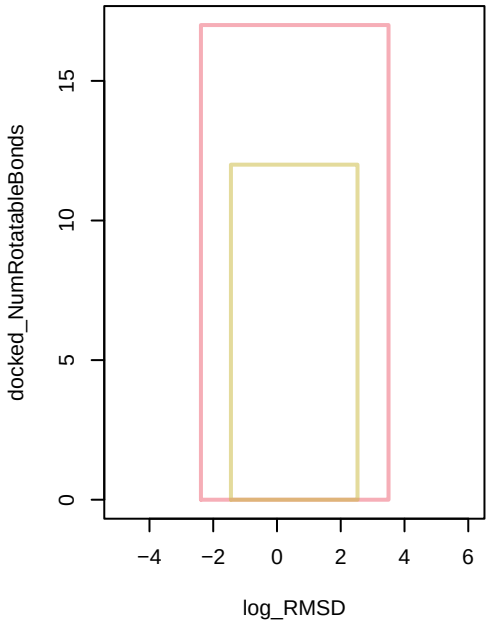

log_mcs_unbonded_polar_sasa
log_RMSD

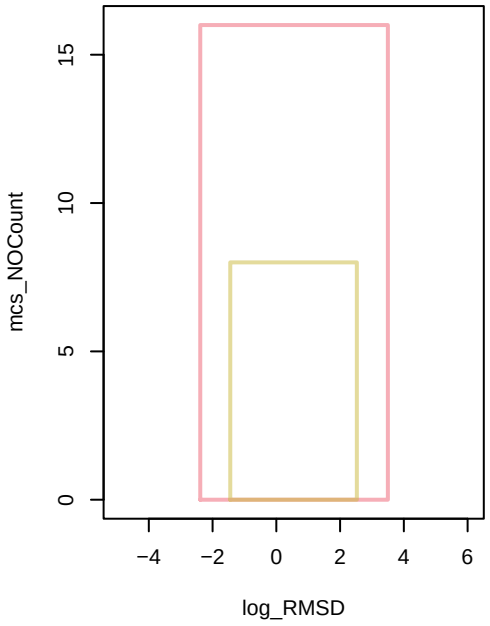

logit_ec_tanimoto_similarity
log_RMSD

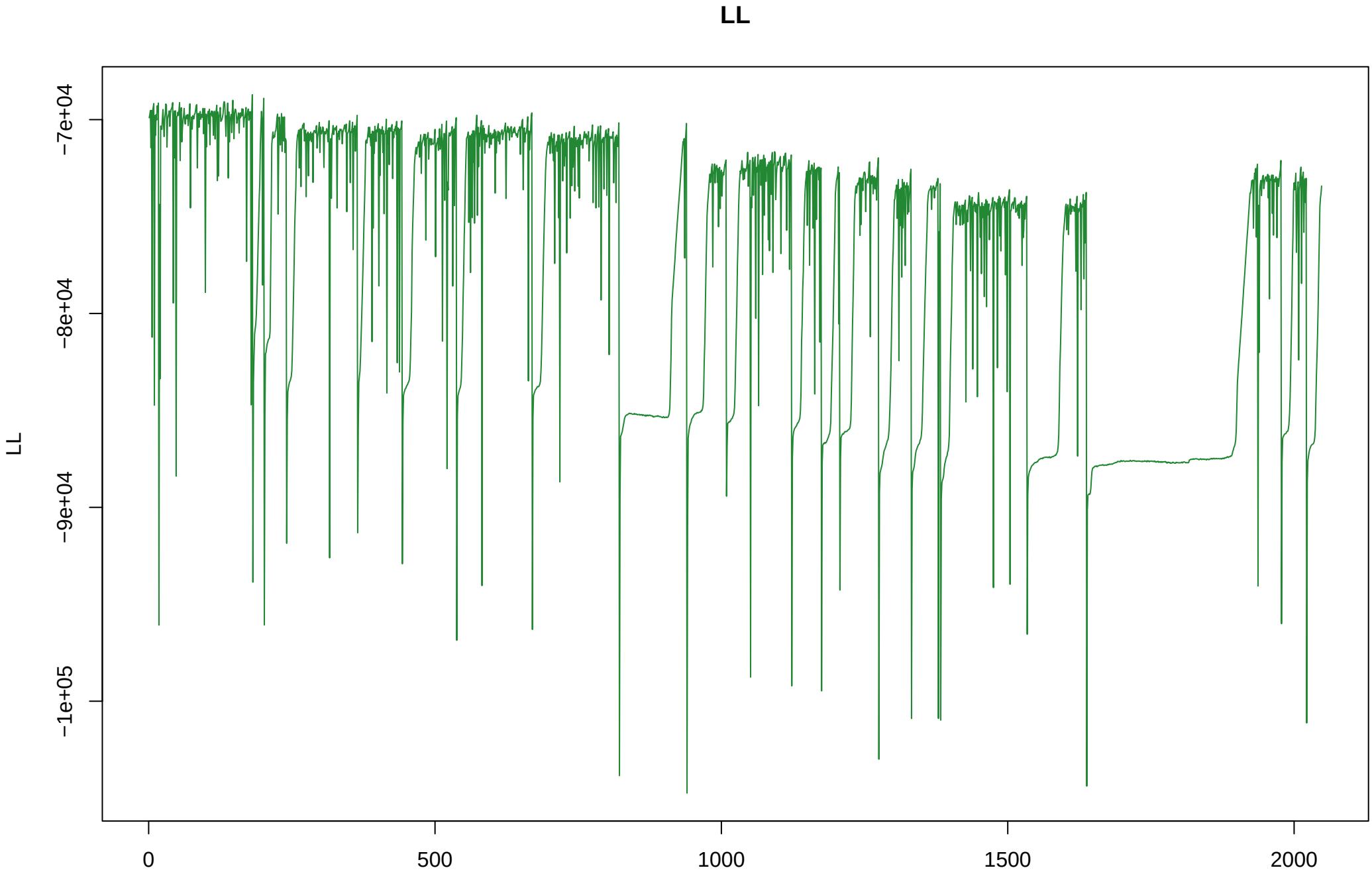

mcs_NumHeteroAtoms
log_RMSD

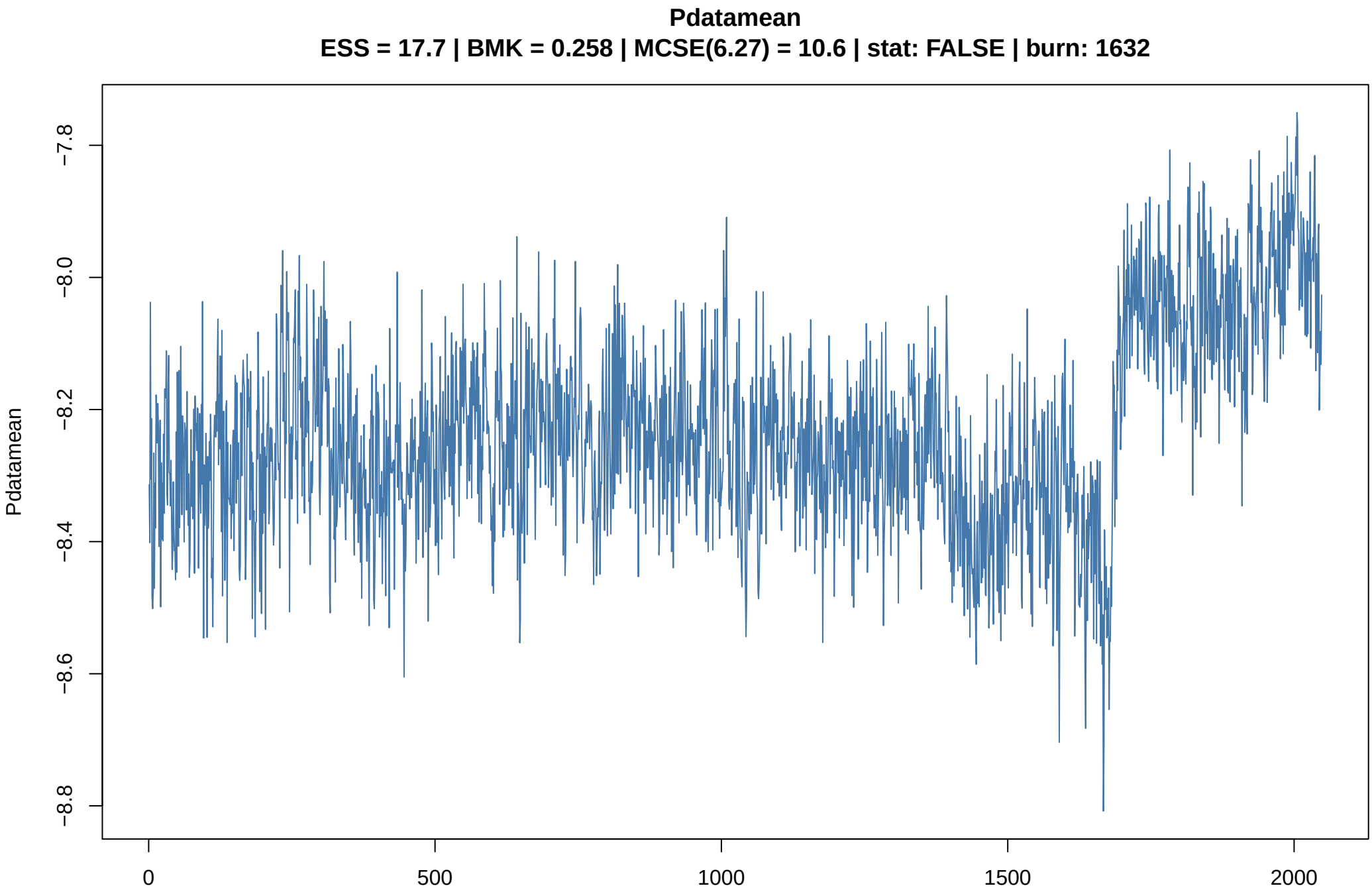

docked_HeavyAtomCount
log_RMSD

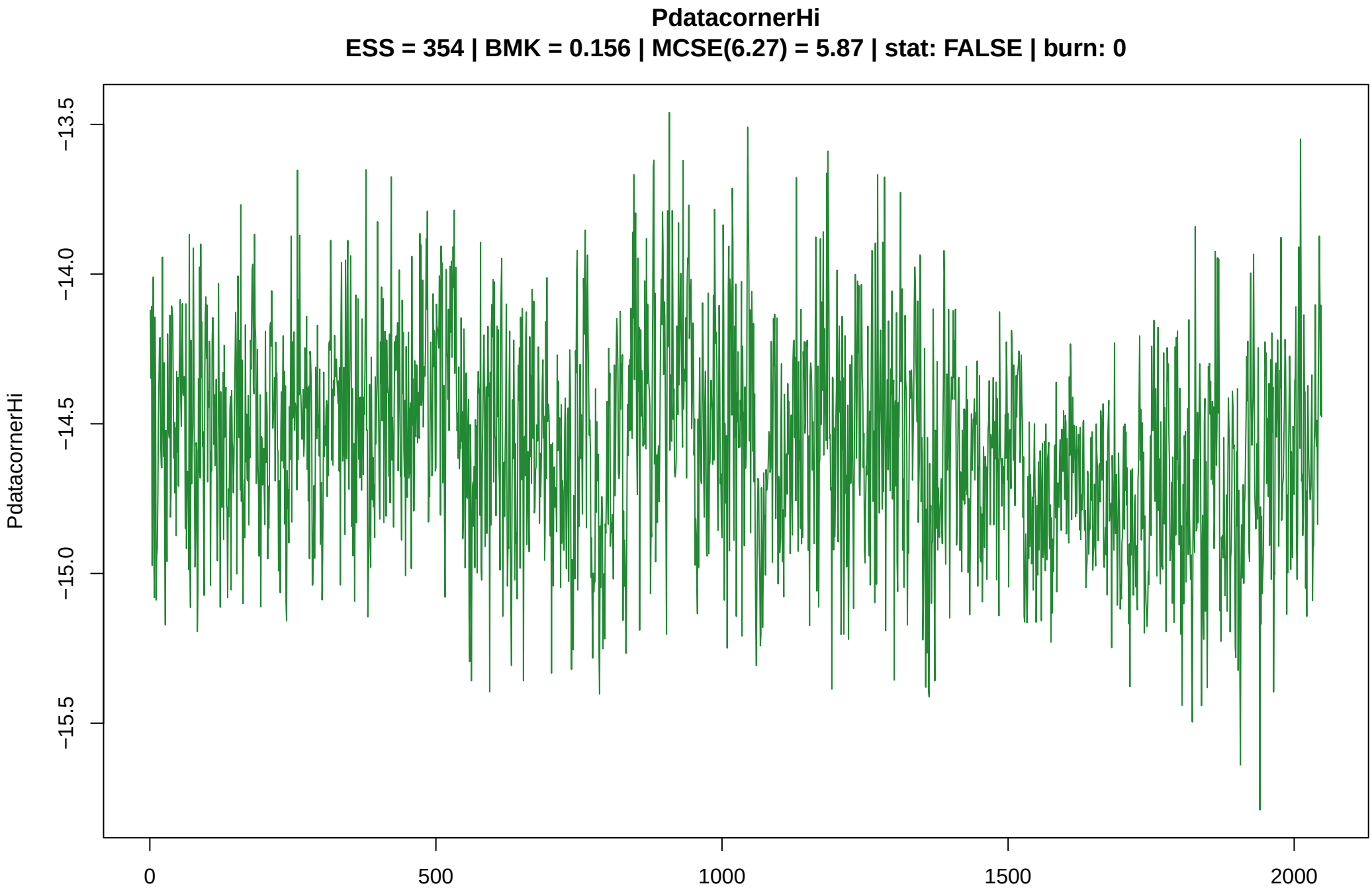

mcs_RingCount
log_RMSD

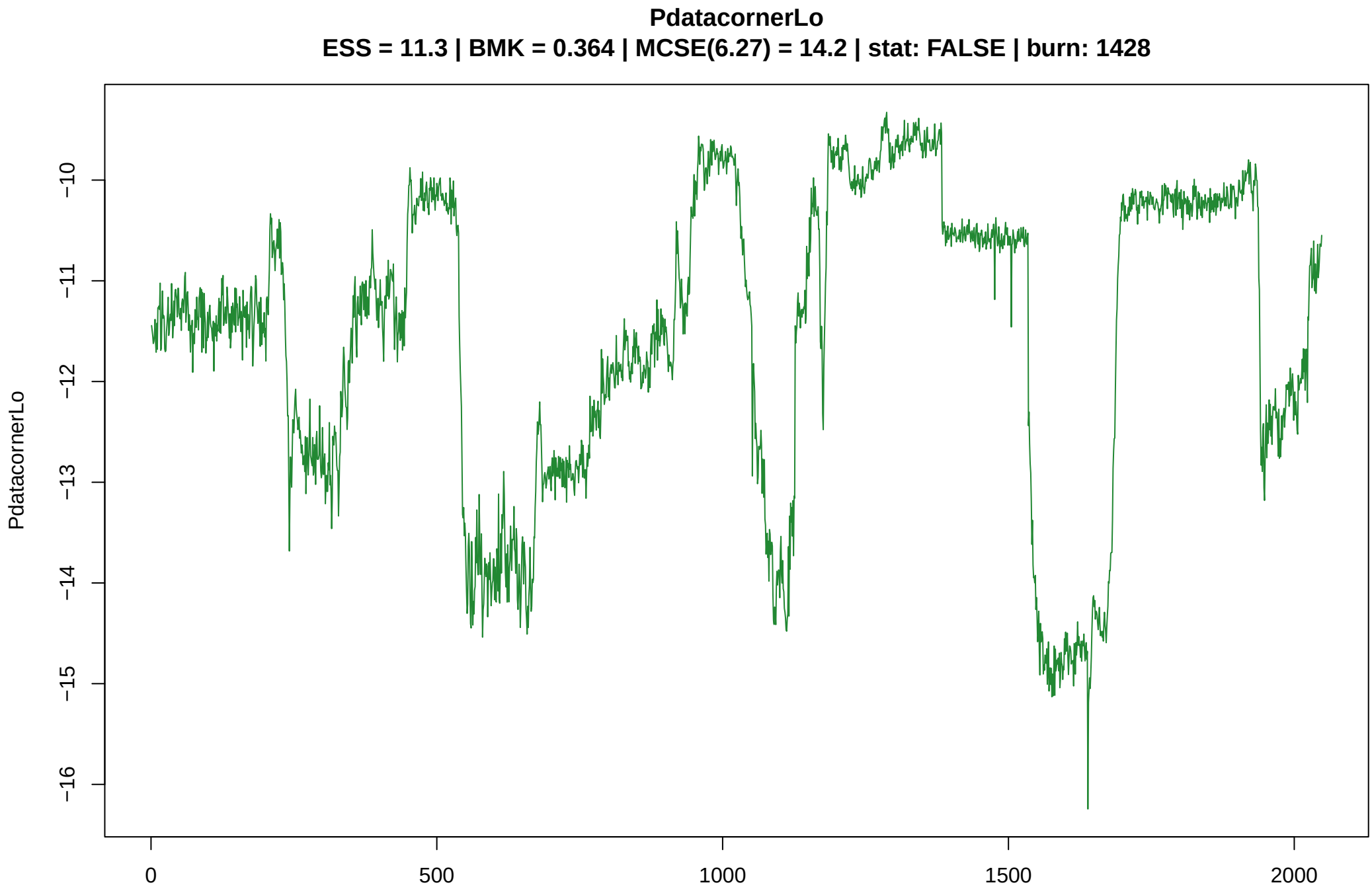

docked_NumRotatableBonds
log_RMSD

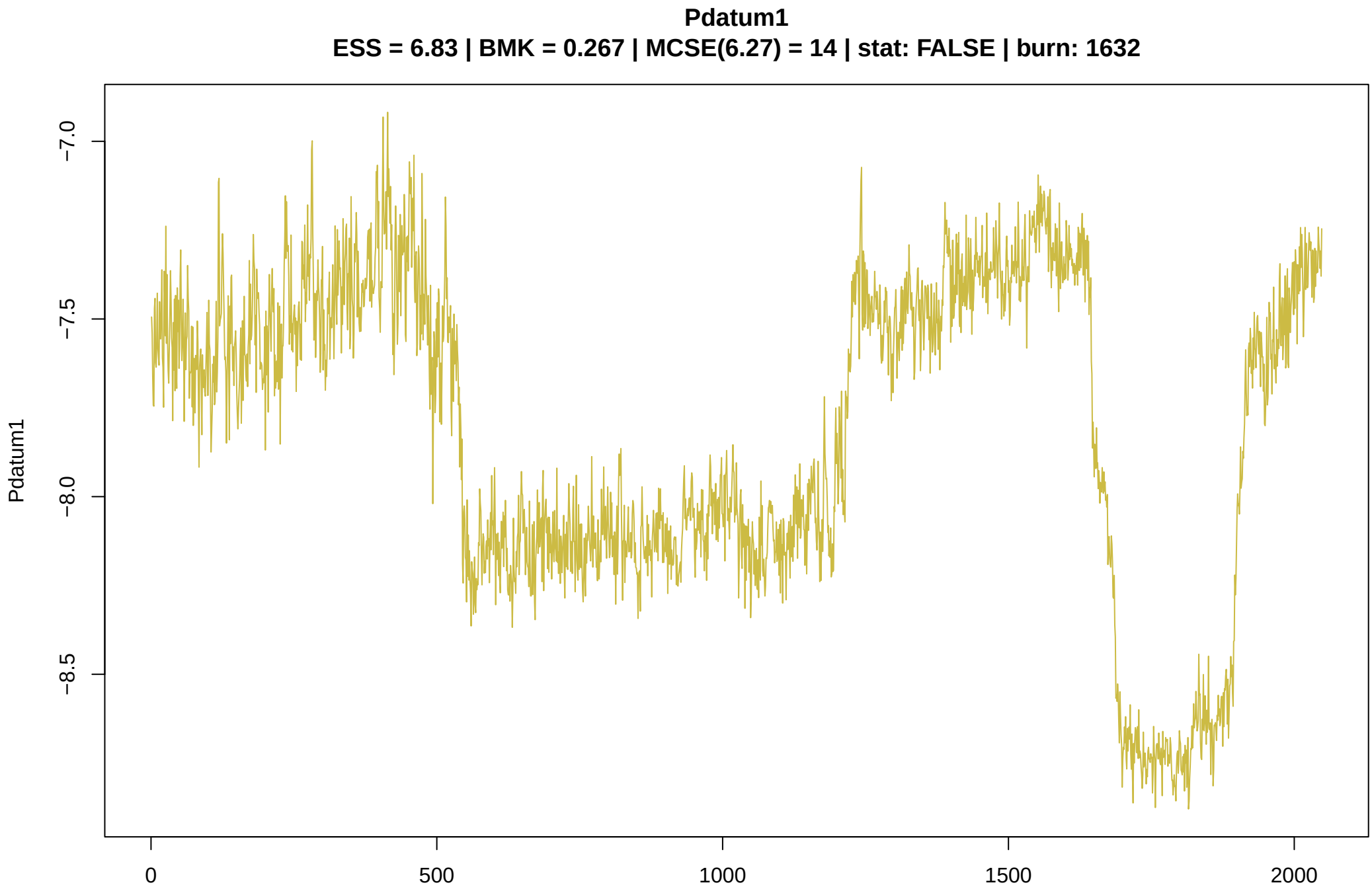

mcs_NOCount
log_RMSD

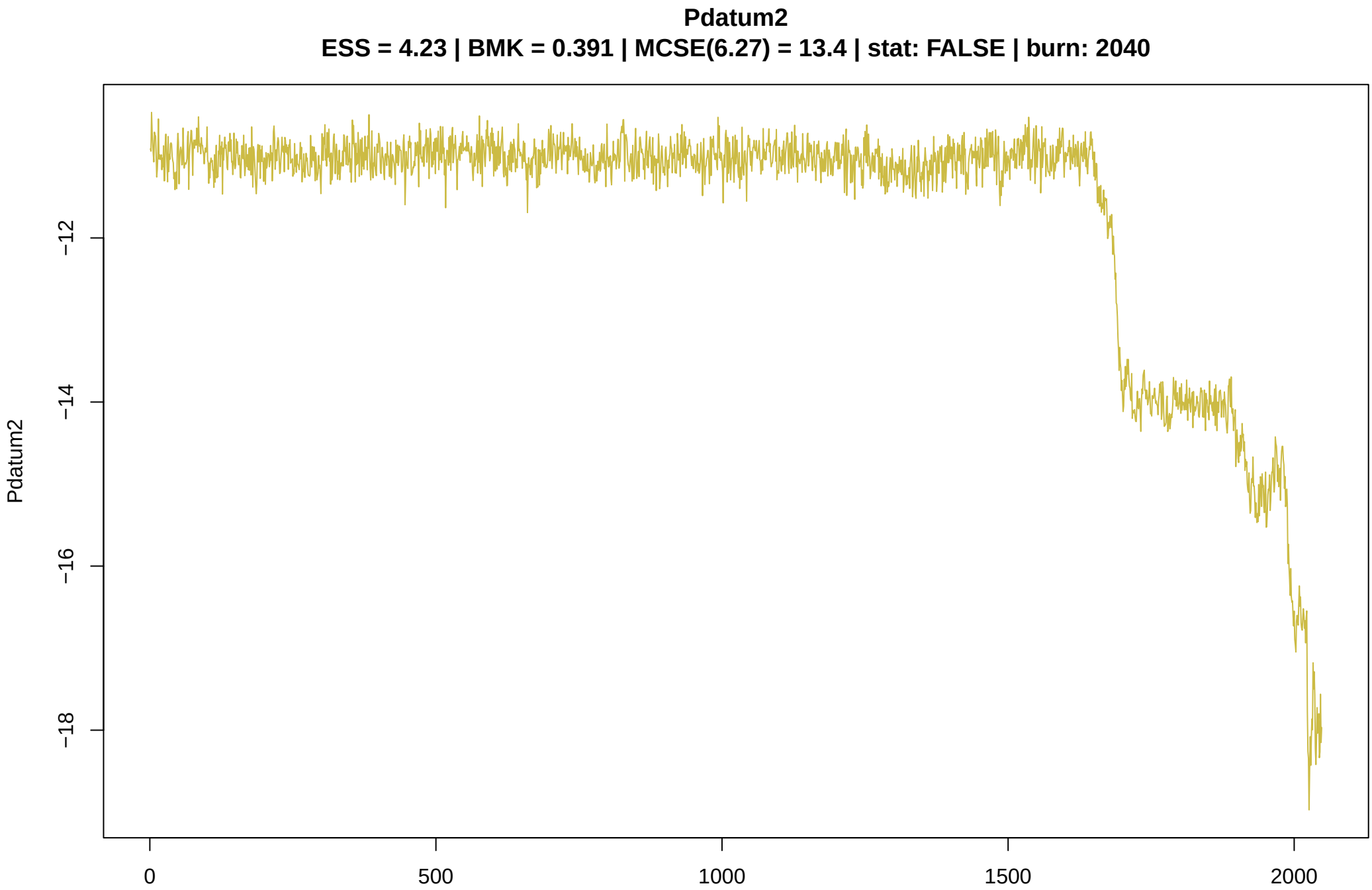

LL
LL
−7e+04
−8e+04
−9e+04
−1e+05
0
500
1000
1500
2000

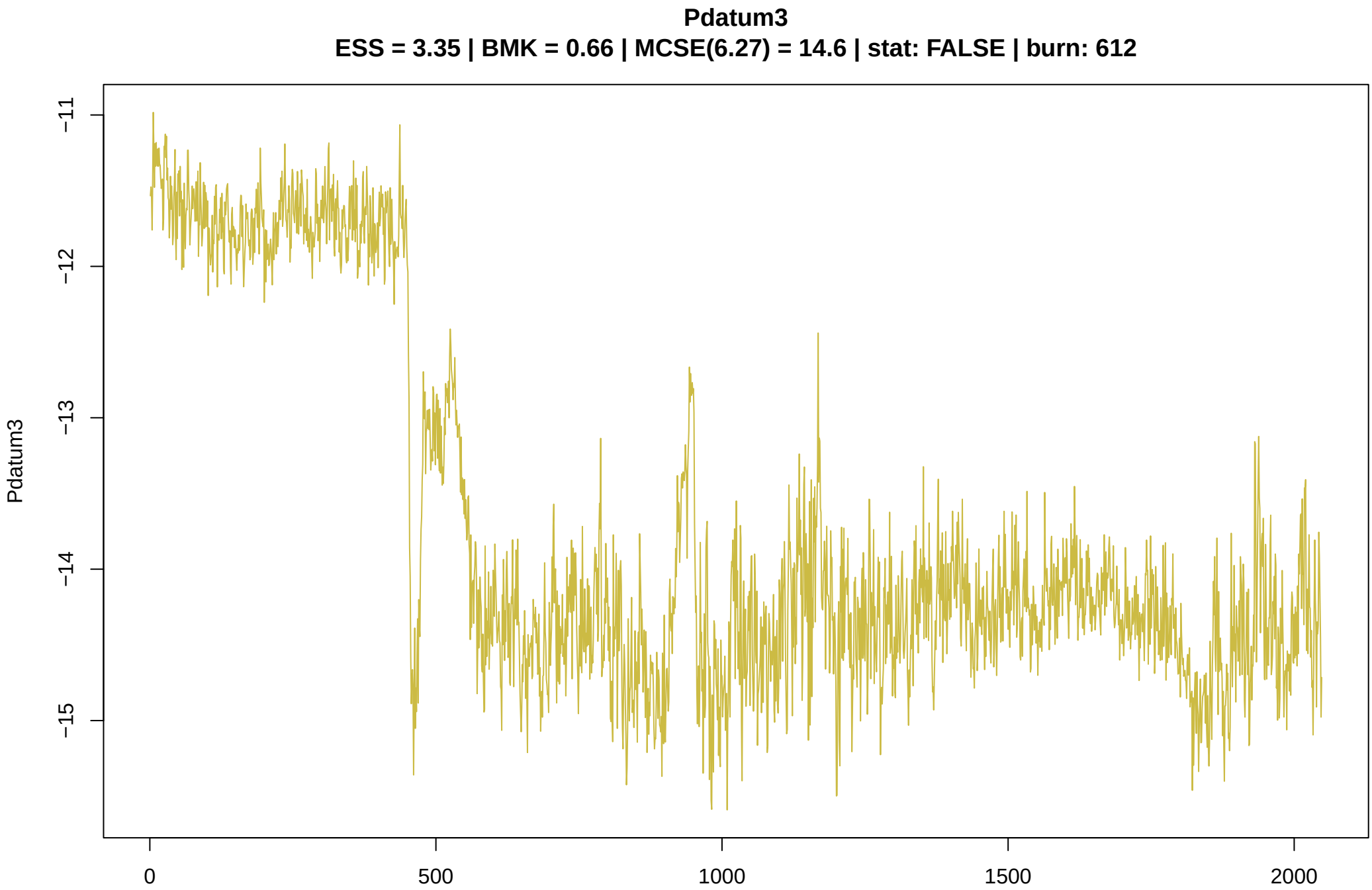

Pdatamean
ESS = 17.7 | BMK = 0.258 | MCSE(6.27) = 10.6 | stat: FALSE | burn: 1632
Pdatamean
−7.8
−8.0
−8.2
−8.4
−8.6
−8.8
0
500
1000
1500
2000

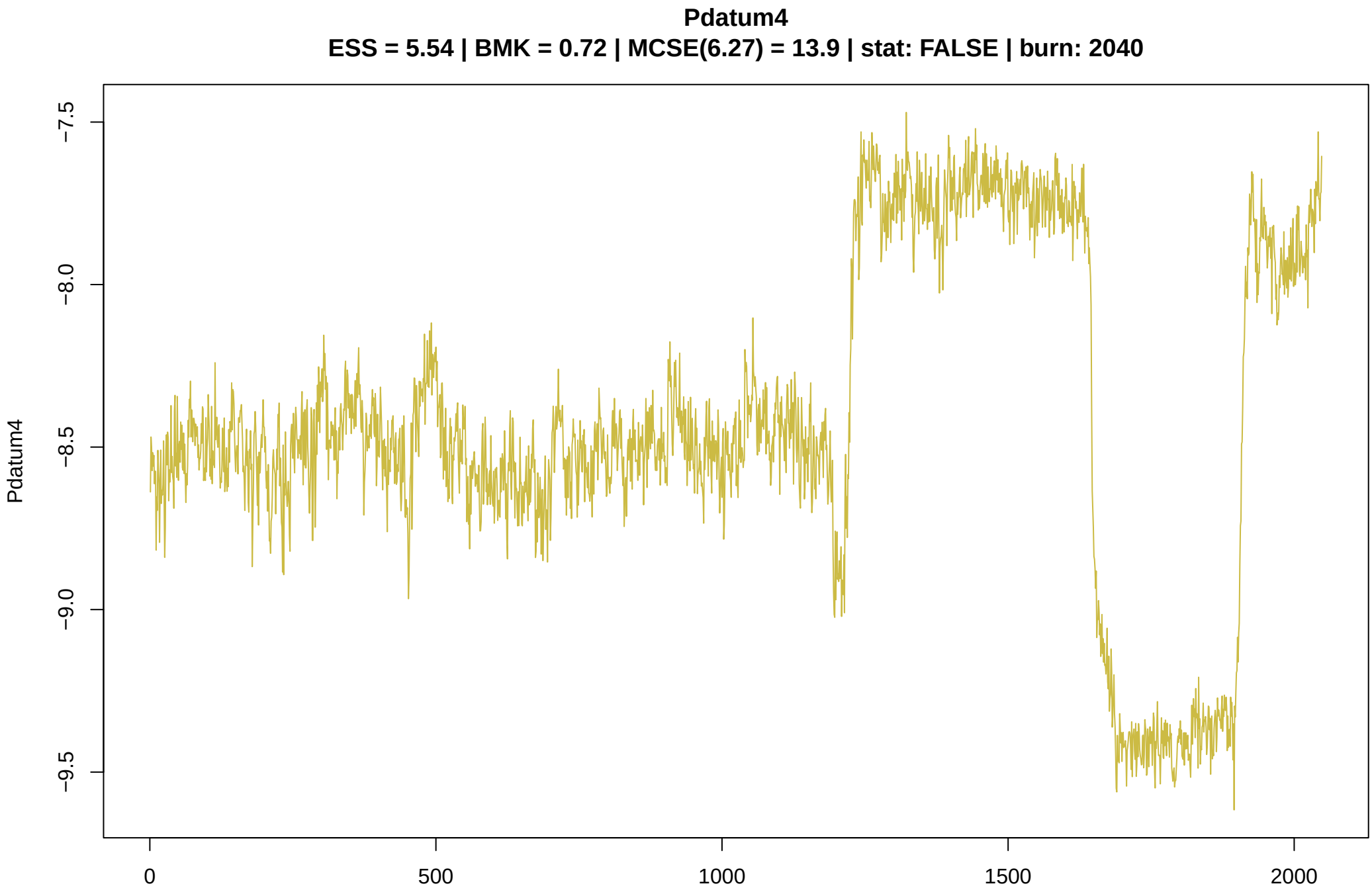

PdatacornerHi
ESS = 354 | BMK = 0.156 | MCSE(6.27) = 5.87 | stat: FALSE | burn: 0
PdatacornerHi
−13.5
−14.0
−14.5
−15.0
−15.5
0
500
1000
1500
2000

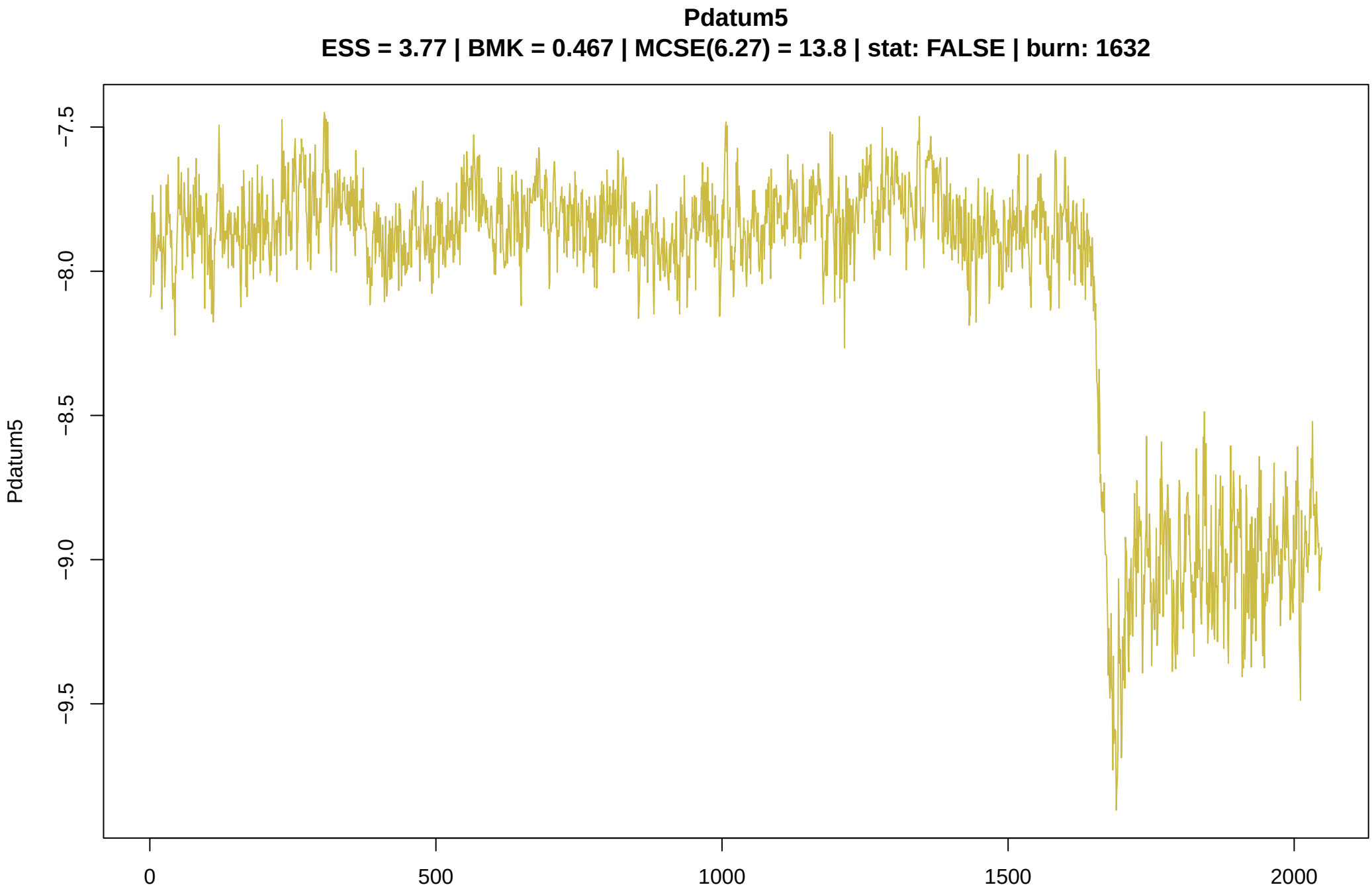

PdatacornerLo
ESS = 11.3 | BMK = 0.364 | MCSE(6.27) = 14.2 | stat: FALSE | burn: 1428
PdatacornerLo
−10
−11
−12
−13
−14
−15
−16
0
500
1000
1500
2000

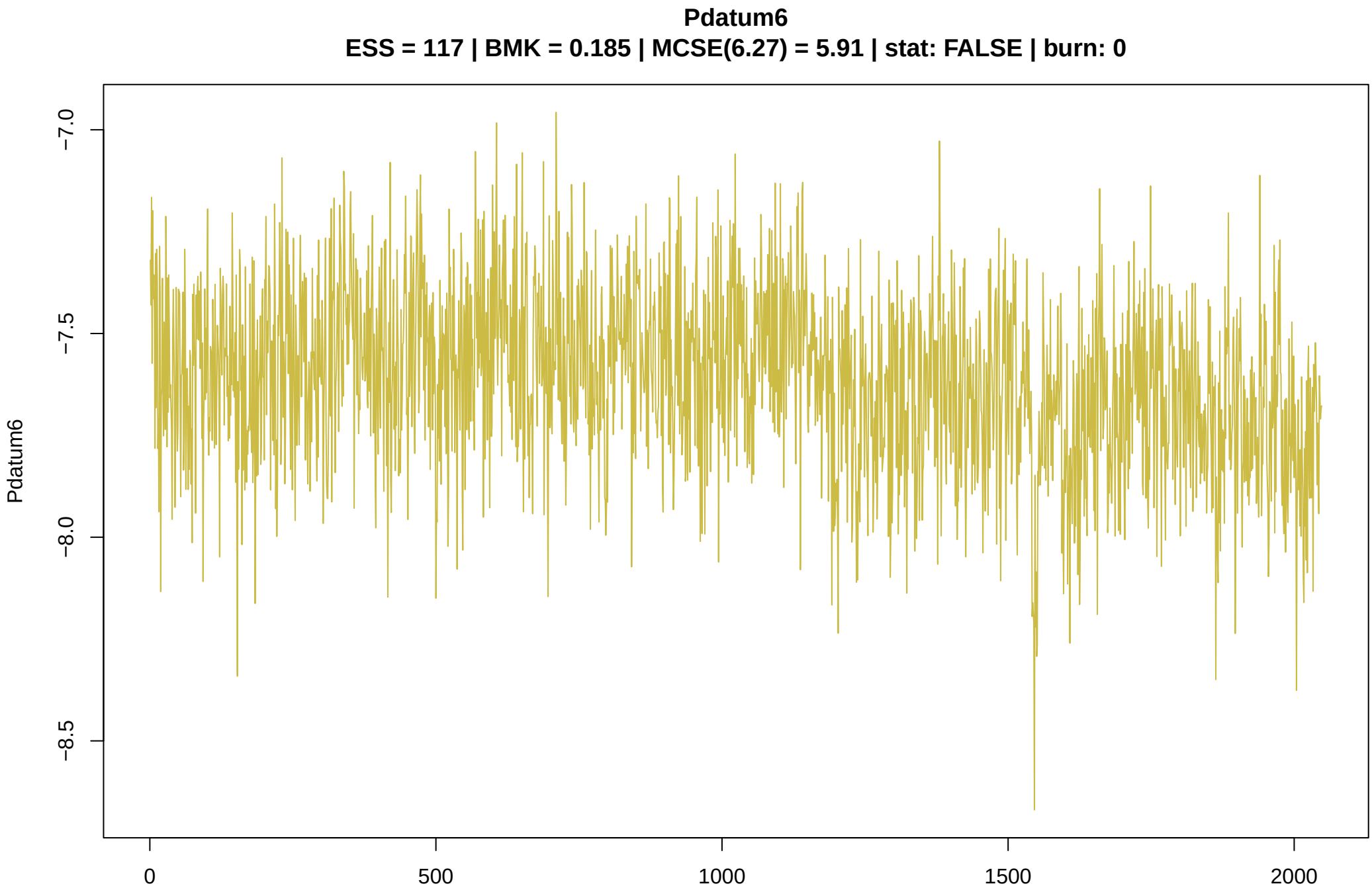

Pdatum1
ESS = 6.83 | BMK = 0.267 | MCSE(6.27) = 14 | stat: FALSE | burn: 1632
Pdatum1
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

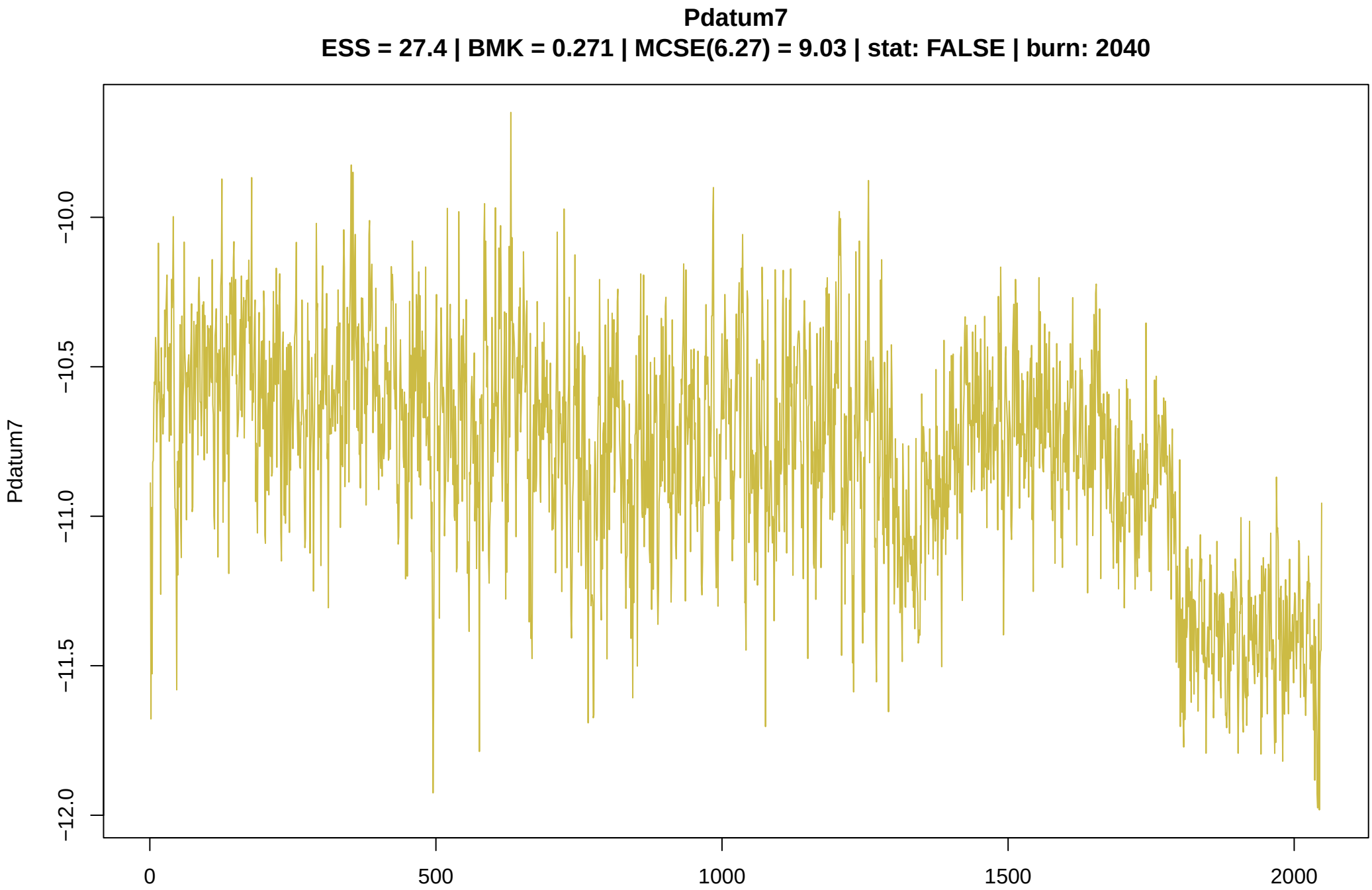

Pdatum2
ESS = 4.23 | BMK = 0.391 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 2040
Pdatum2
−12
−14
−16
−18
0
500
1000
1500
2000

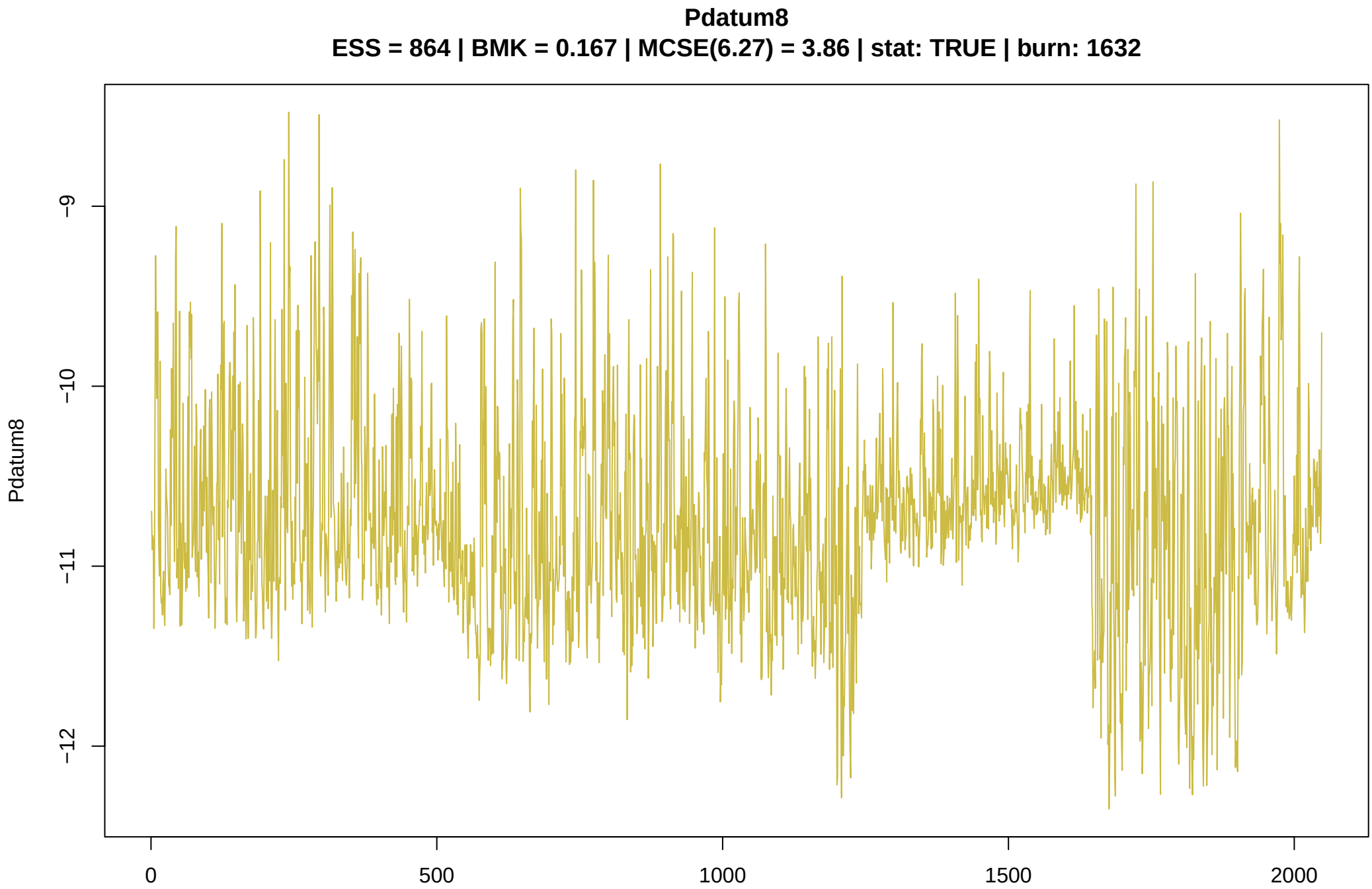

Pdatum3
ESS = 3.35 | BMK = 0.66 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 612
Pdatum3
−11
−12
−13
−14
−15
0
500
1000
1500
2000

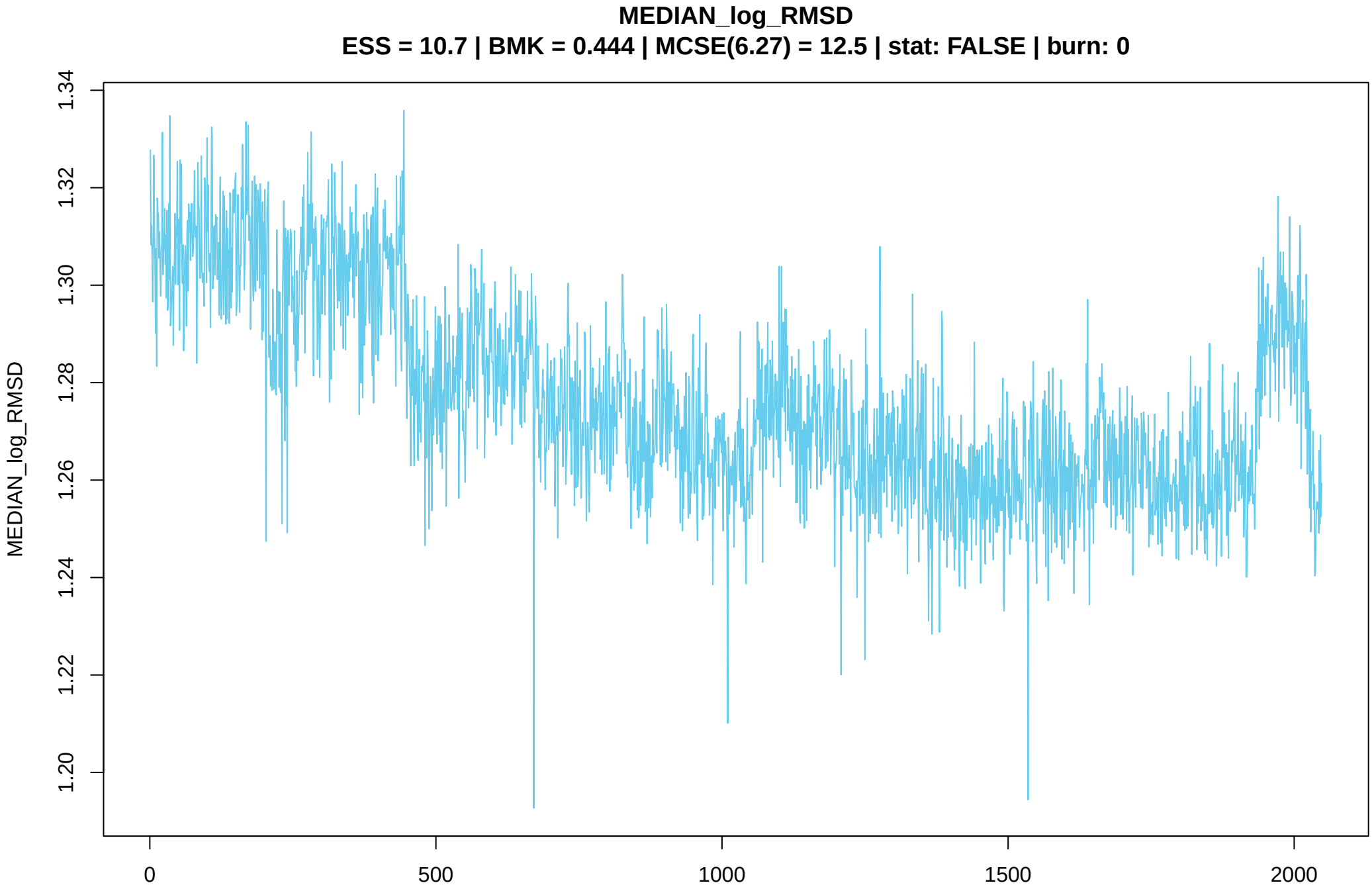

Pdatum4
ESS = 5.54 | BMK = 0.72 | MCSE(6.27) = 13.9 | stat: FALSE | burn: 2040
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

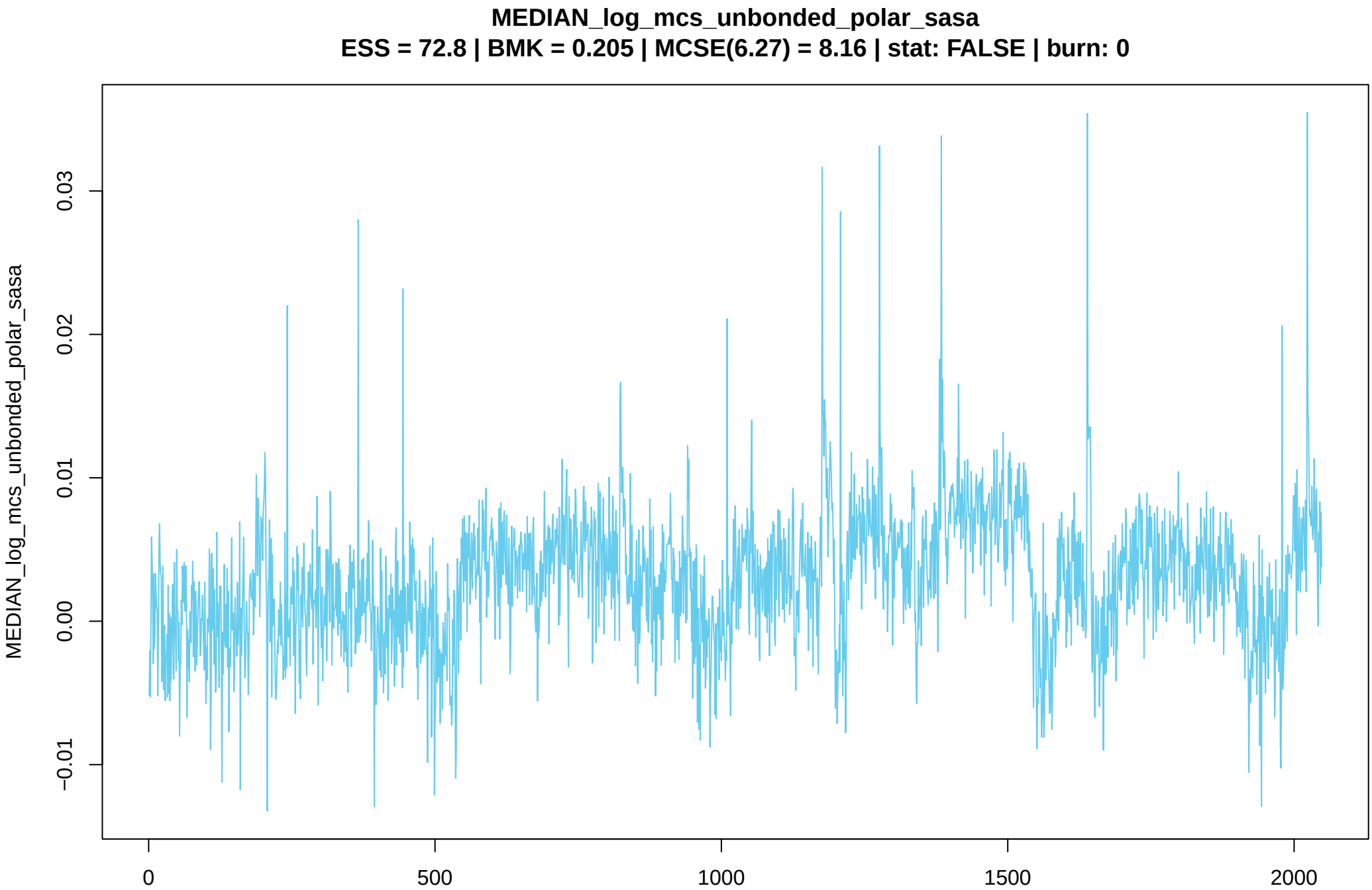

Pdatum5
ESS = 3.77 | BMK = 0.467 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 1632
Pdatum5
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

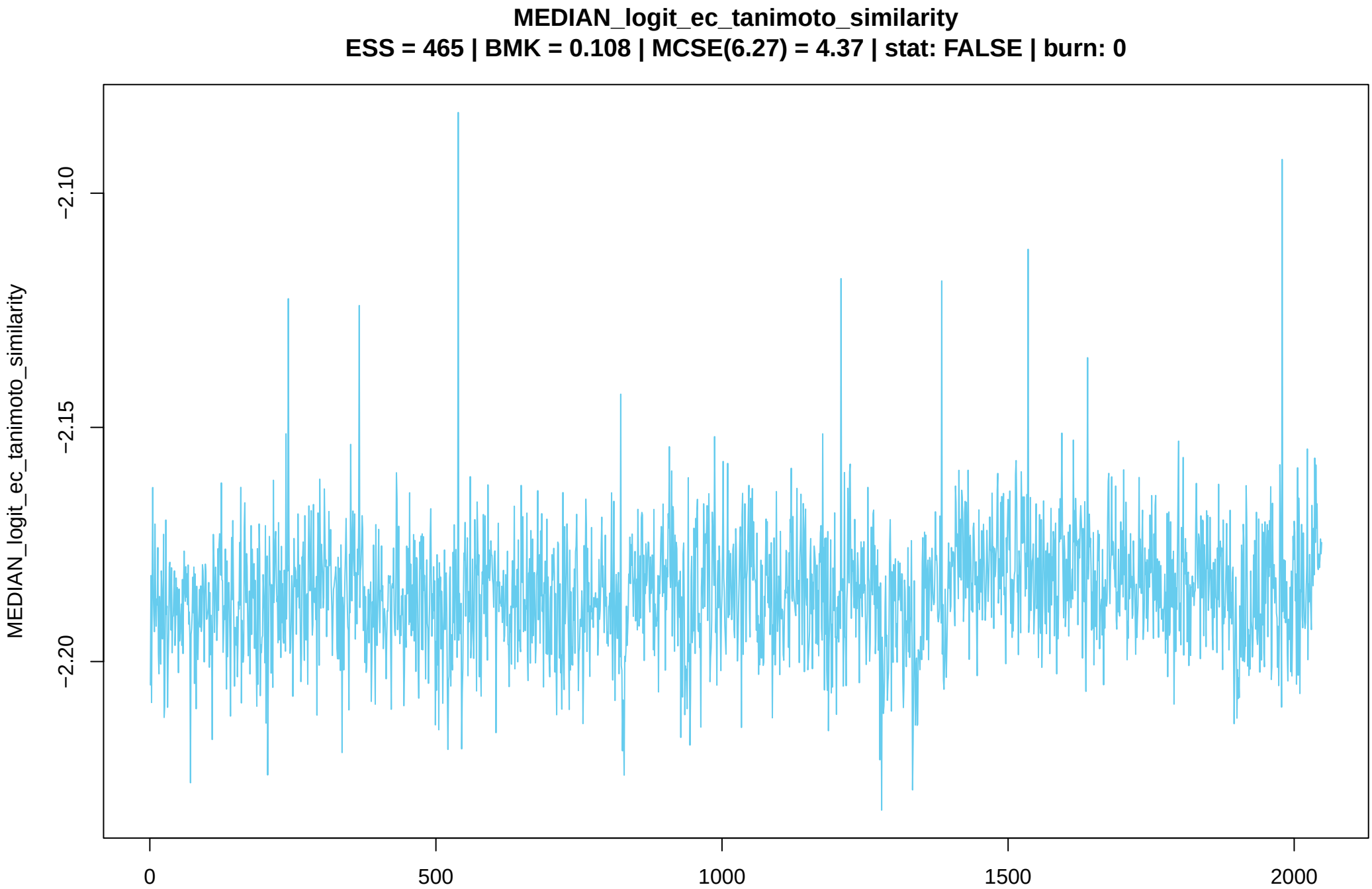

Pdatum6
ESS = 117 | BMK = 0.185 | MCSE(6.27) = 5.91 | stat: FALSE | burn: 0
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

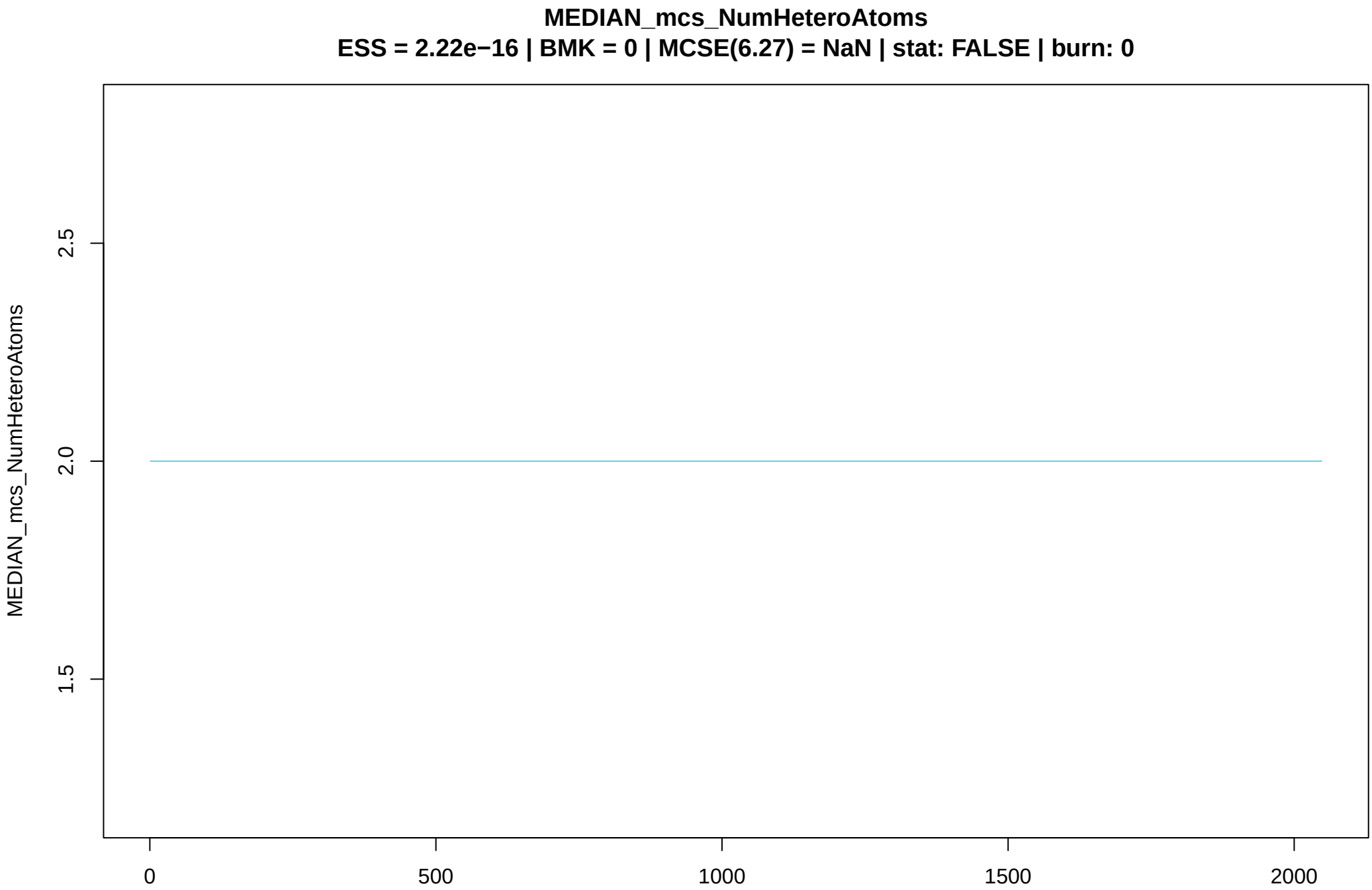

Pdatum7
ESS = 27.4 | BMK = 0.271 | MCSE(6.27) = 9.03 | stat: FALSE | burn: 2040
Pdatum7
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

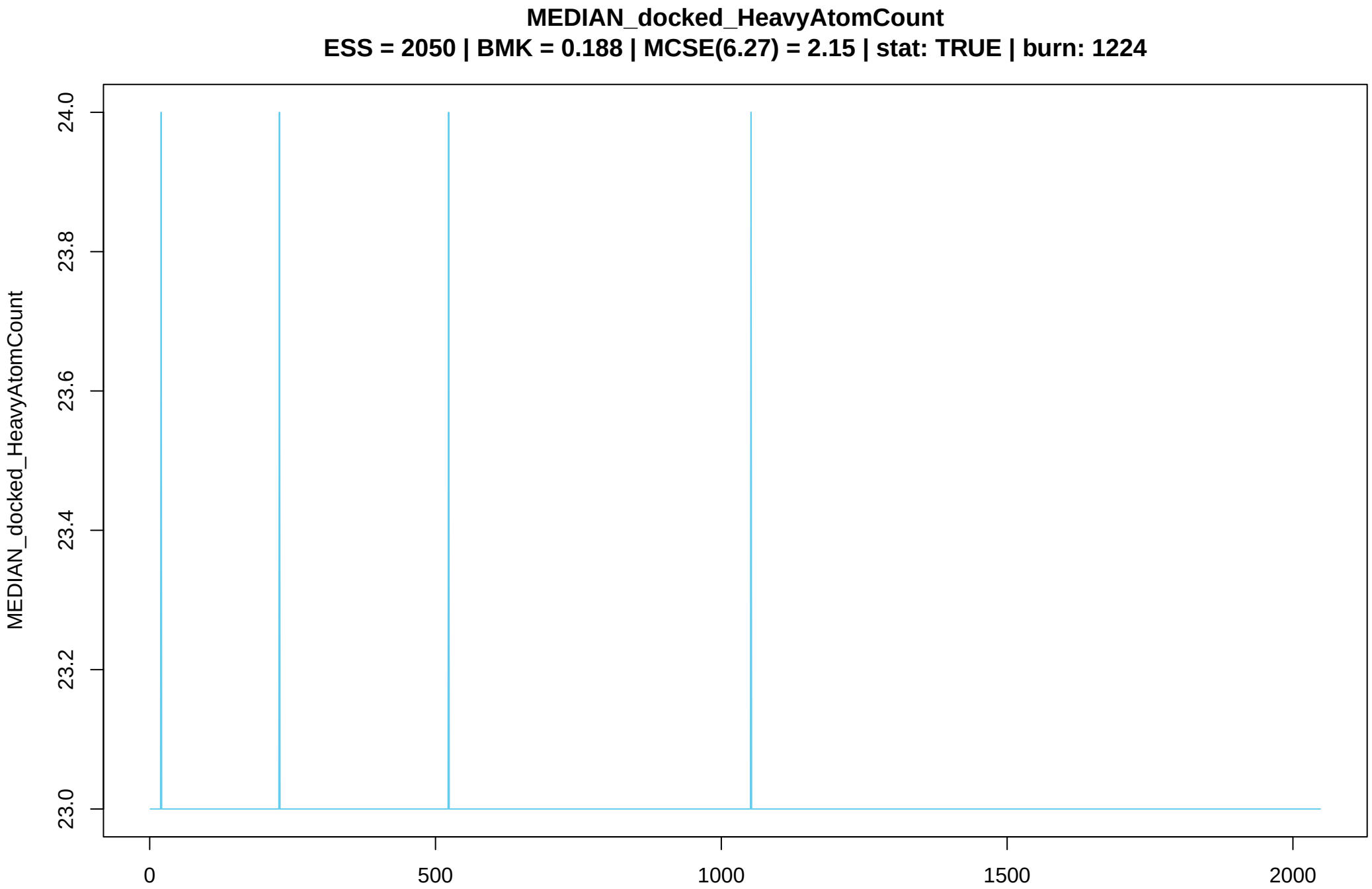

Pdatum8
ESS = 864 | BMK = 0.167 | MCSE(6.27) = 3.86 | stat: TRUE | burn: 1632
Pdatum8
−9
−10
−11
−12
0
500
1000
1500
2000

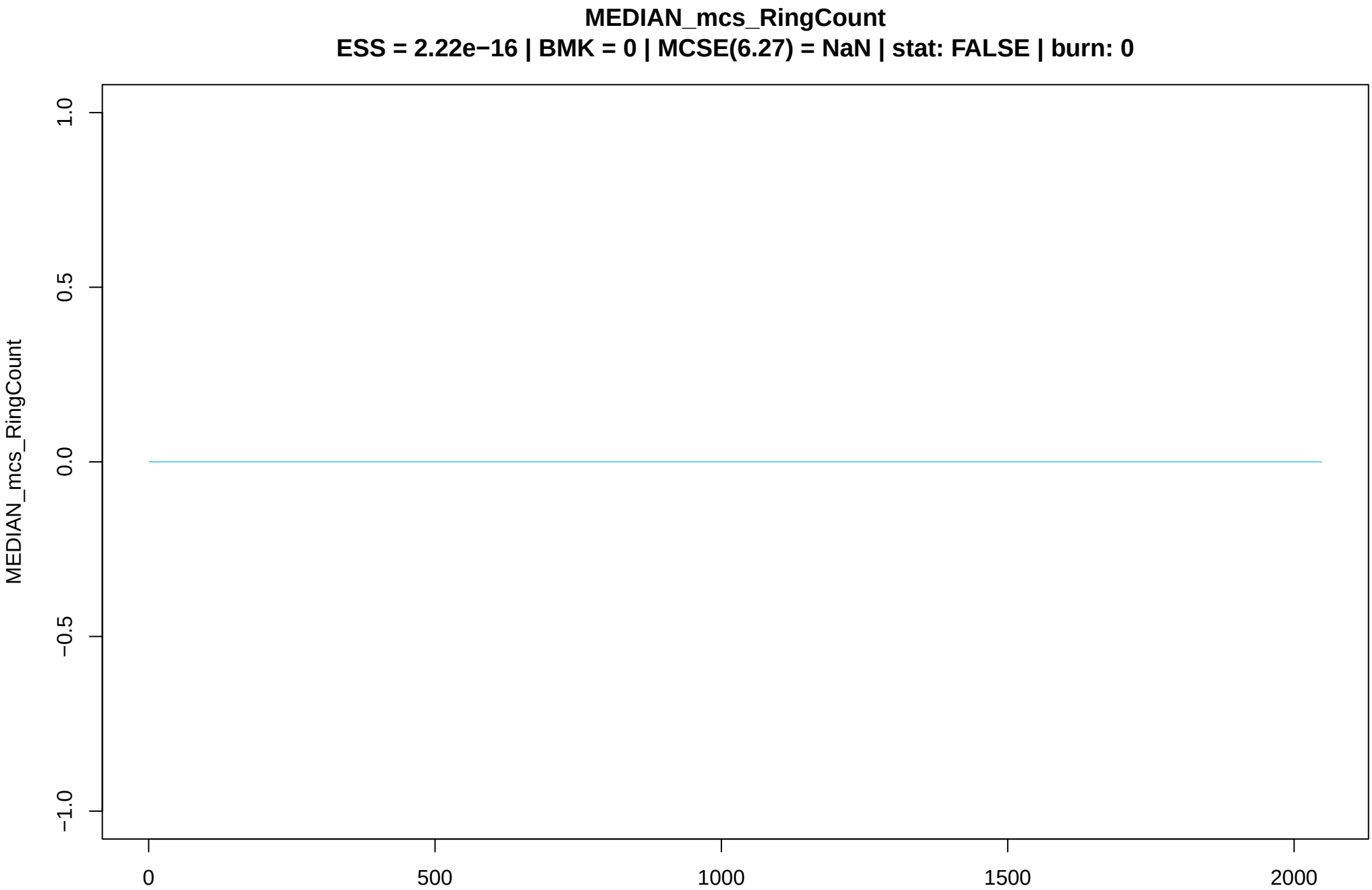

MEDIAN_log_RMSD
ESS = 10.7 | BMK = 0.444 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 0
MEDIAN_log_RMSD
1.20
1.22
1.24
1.26
1.28
1.30
1.32
1.34
0
500
1000
1500
2000

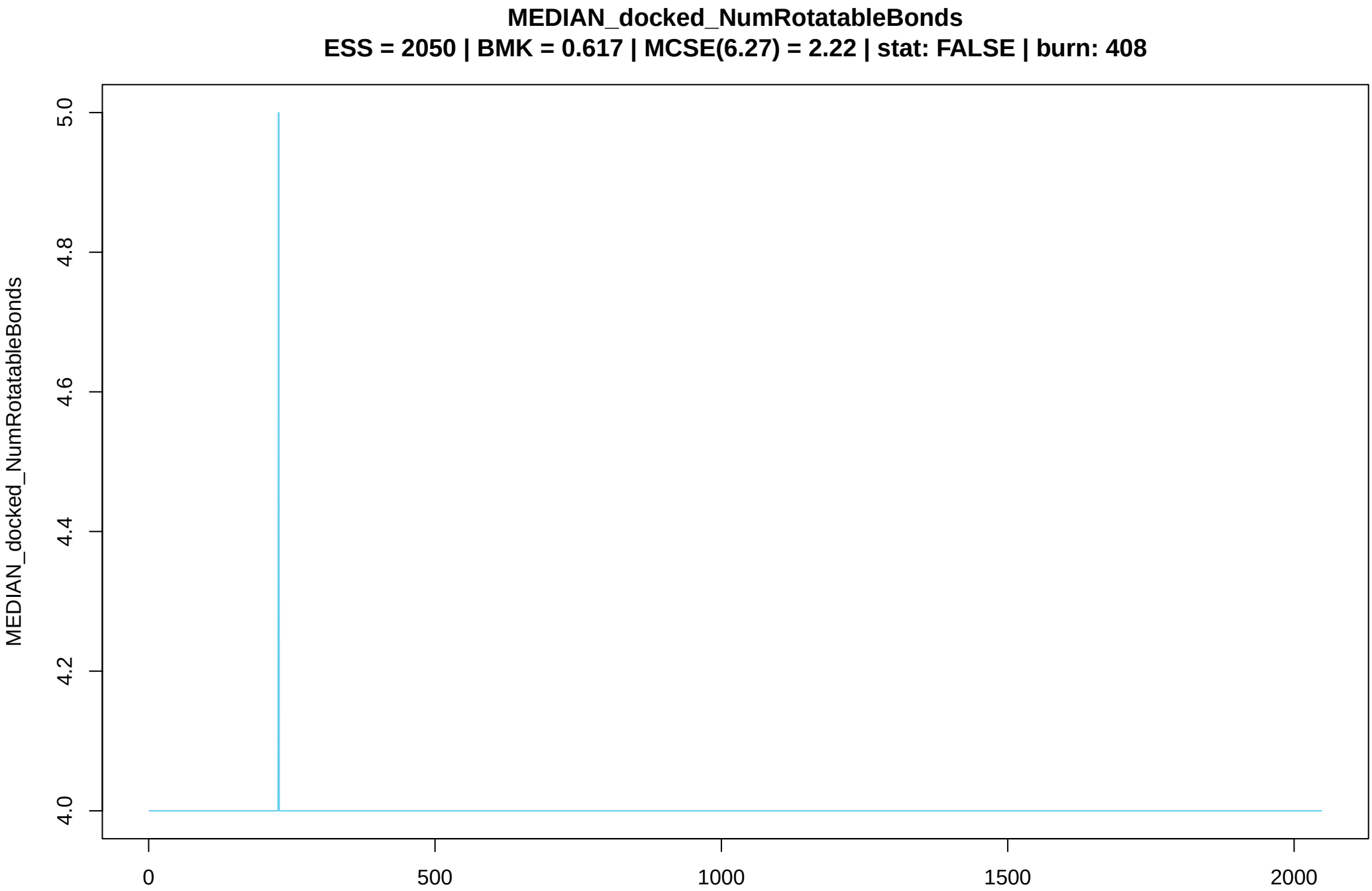

MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 72.8 | BMK = 0.205 | MCSE(6.27) = 8.16 | stat: FALSE | burn: 0
MEDIAN_log_mcs_unbonded_polar_sasa
0.03
0.02
0.01
0.00
−0.01
0
500
1000
1500
2000

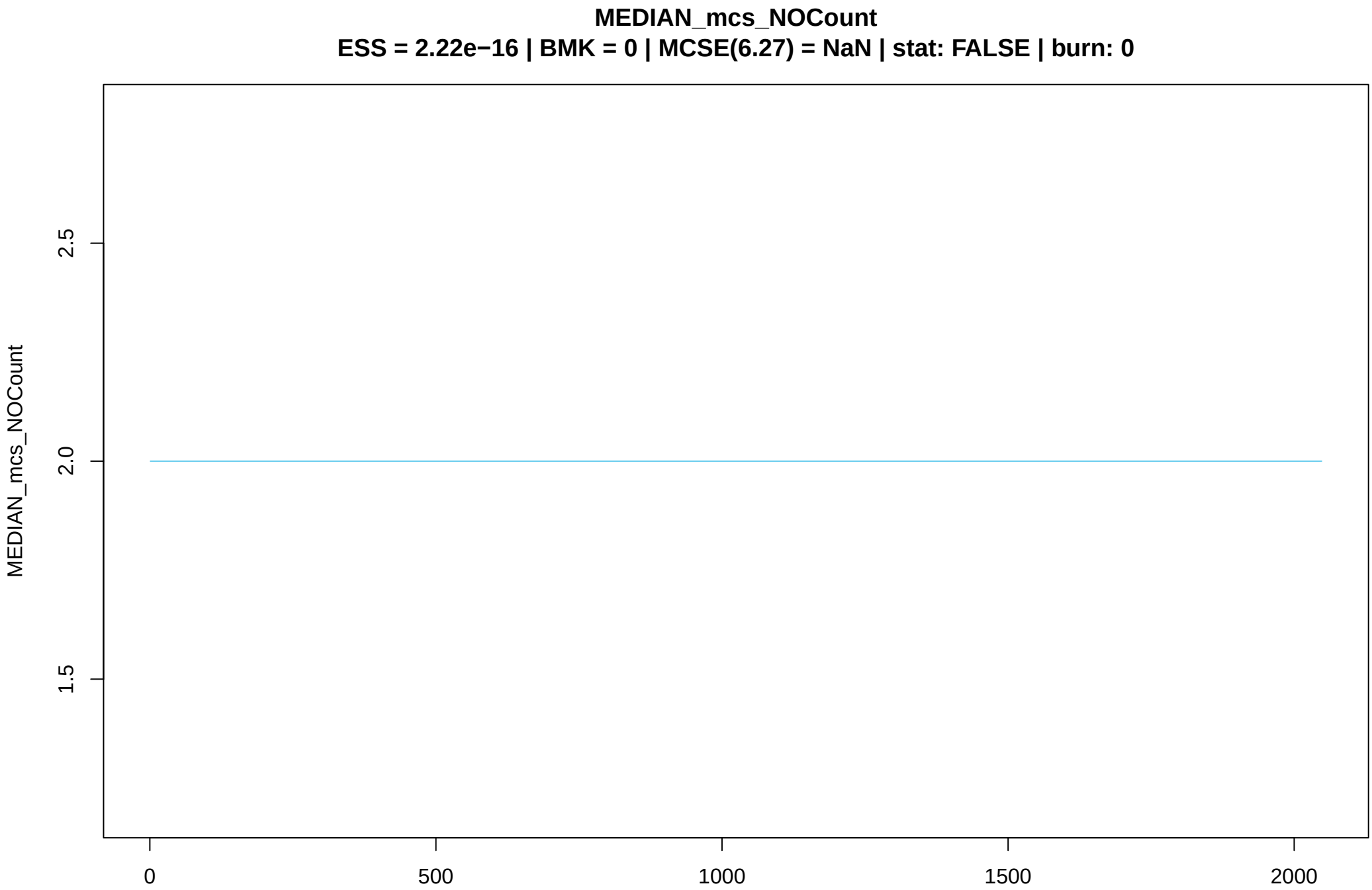

MEDIAN_logit_ec_tanimoto_similarity
ESS = 465 | BMK = 0.108 | MCSE(6.27) = 4.37 | stat: FALSE | burn: 0
MEDIAN_logit_ec_tanimoto_similarity
−2.10
−2.15
−2.20
0
500
1000
1500
2000

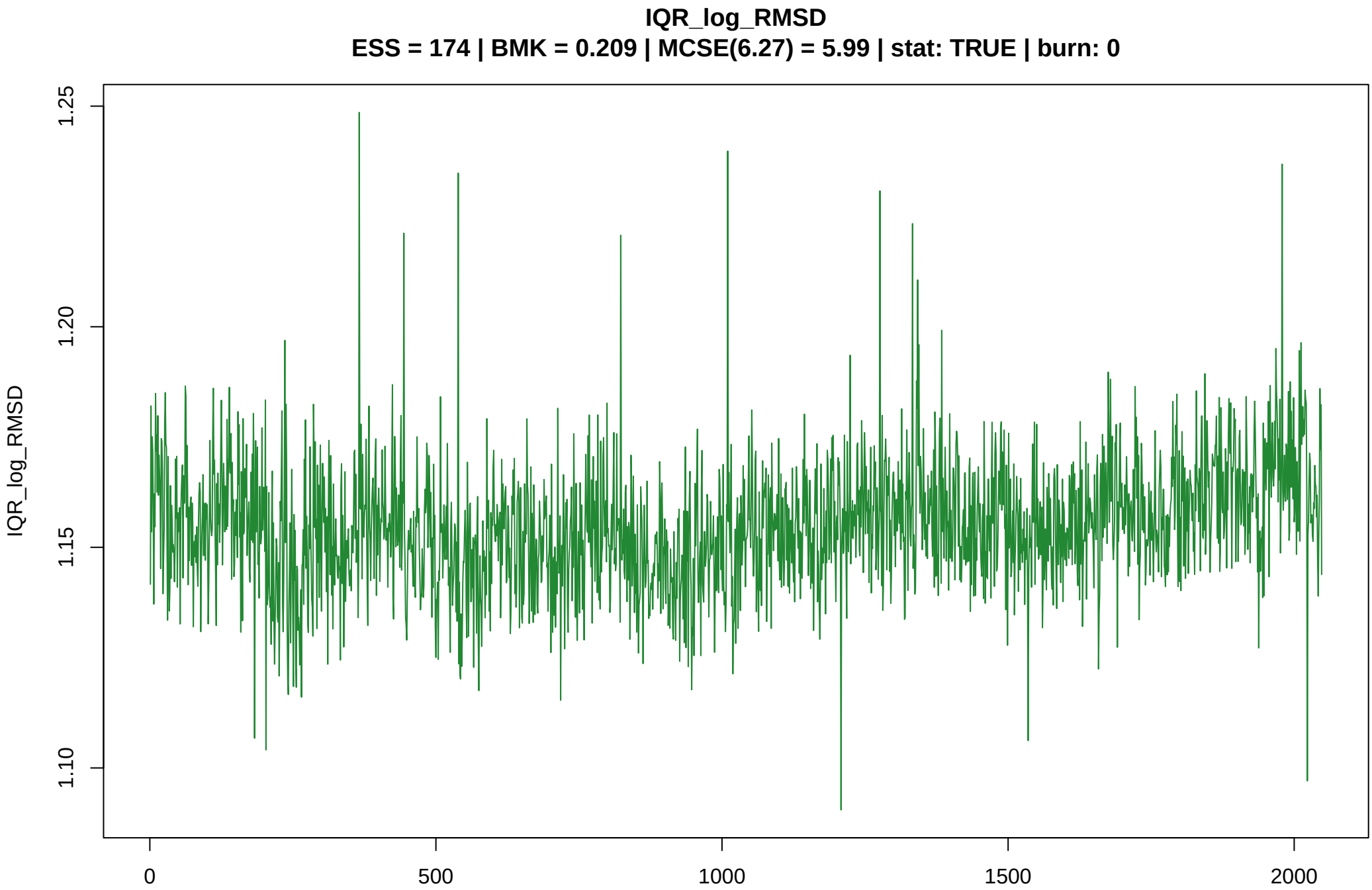

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

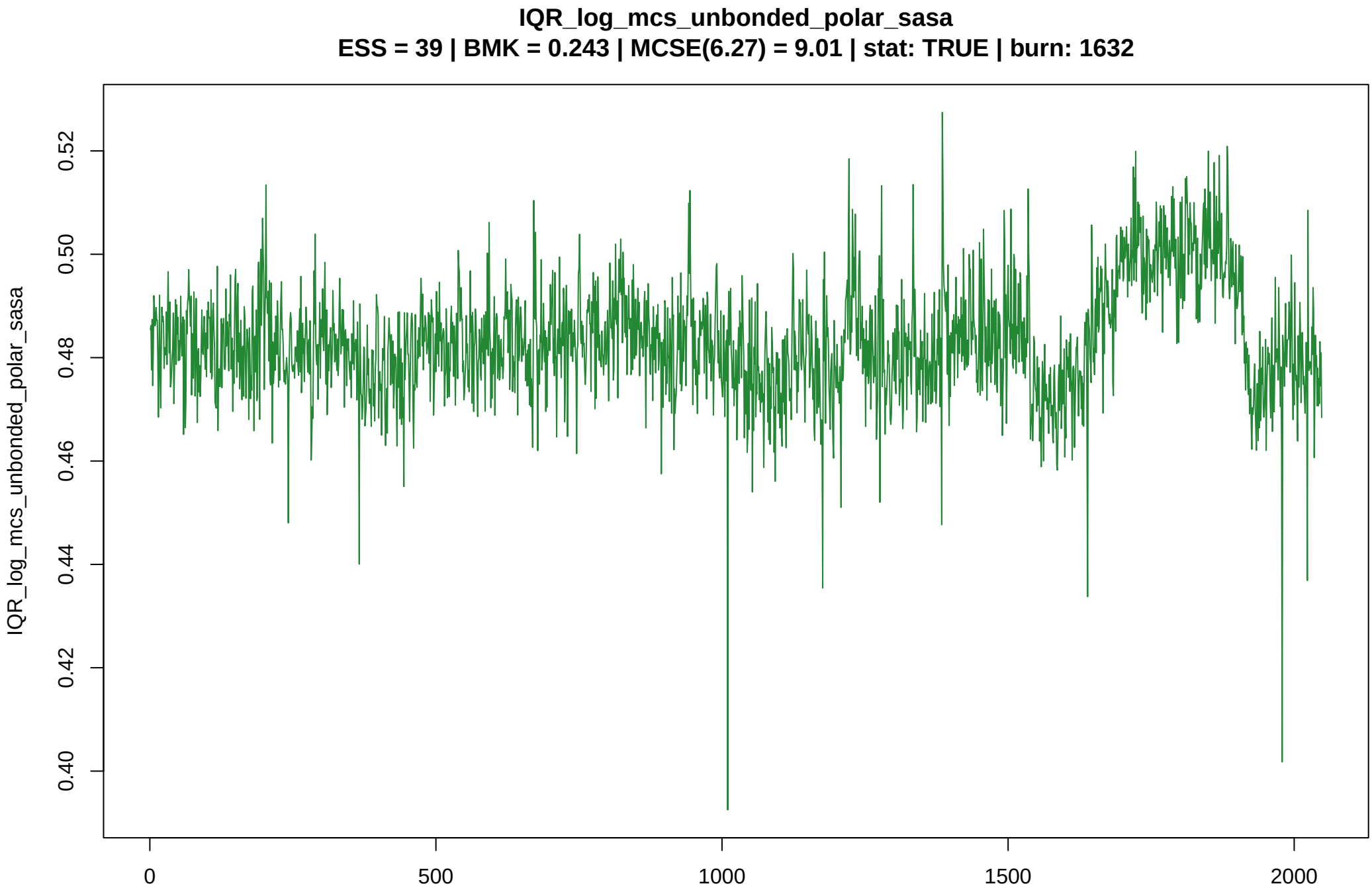

MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1224
MEDIAN_docked_HeavyAtomCount
24.0
23.8
23.6
23.4
23.2
23.0
0
500
1000
1500
2000

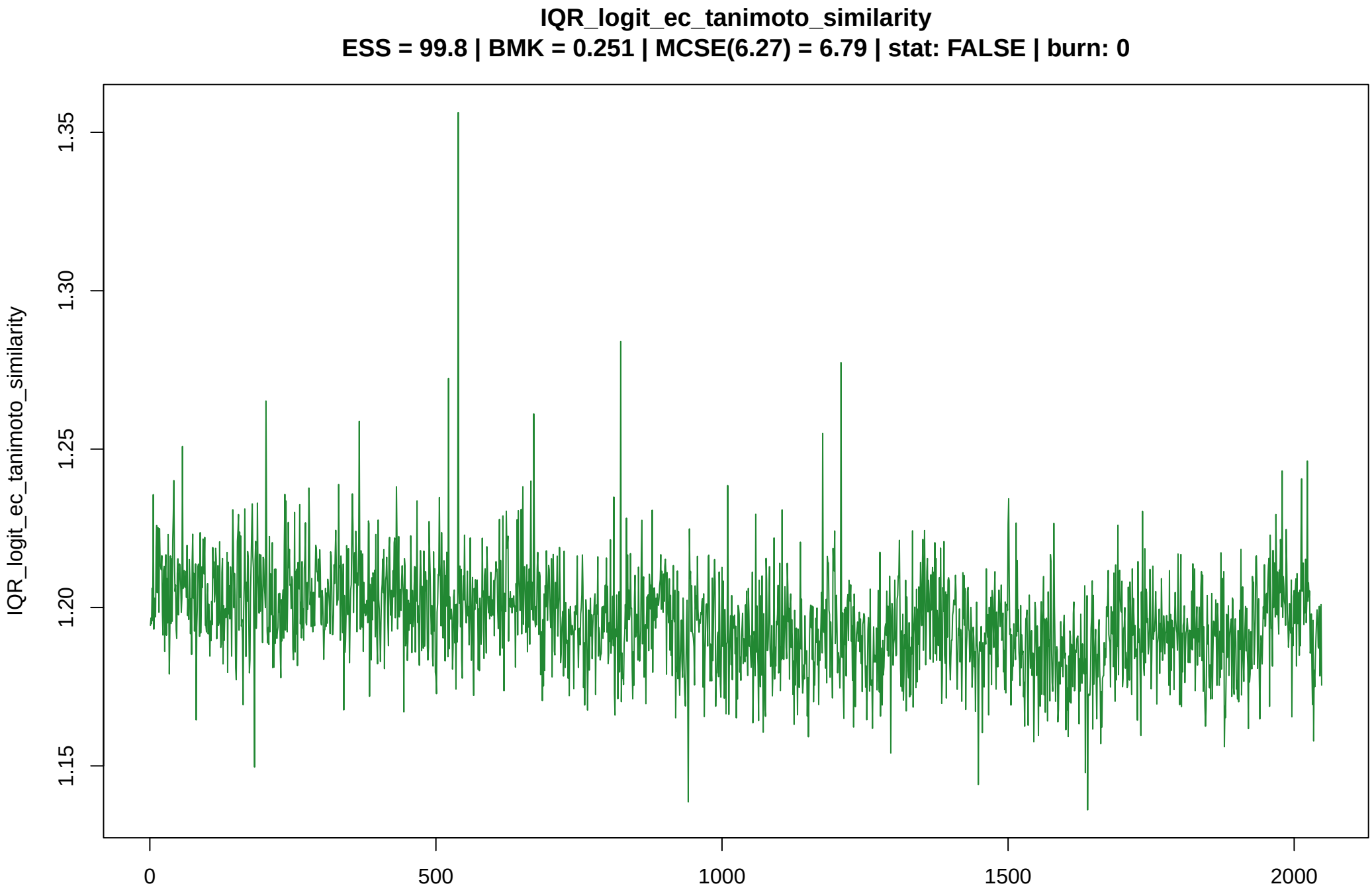

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

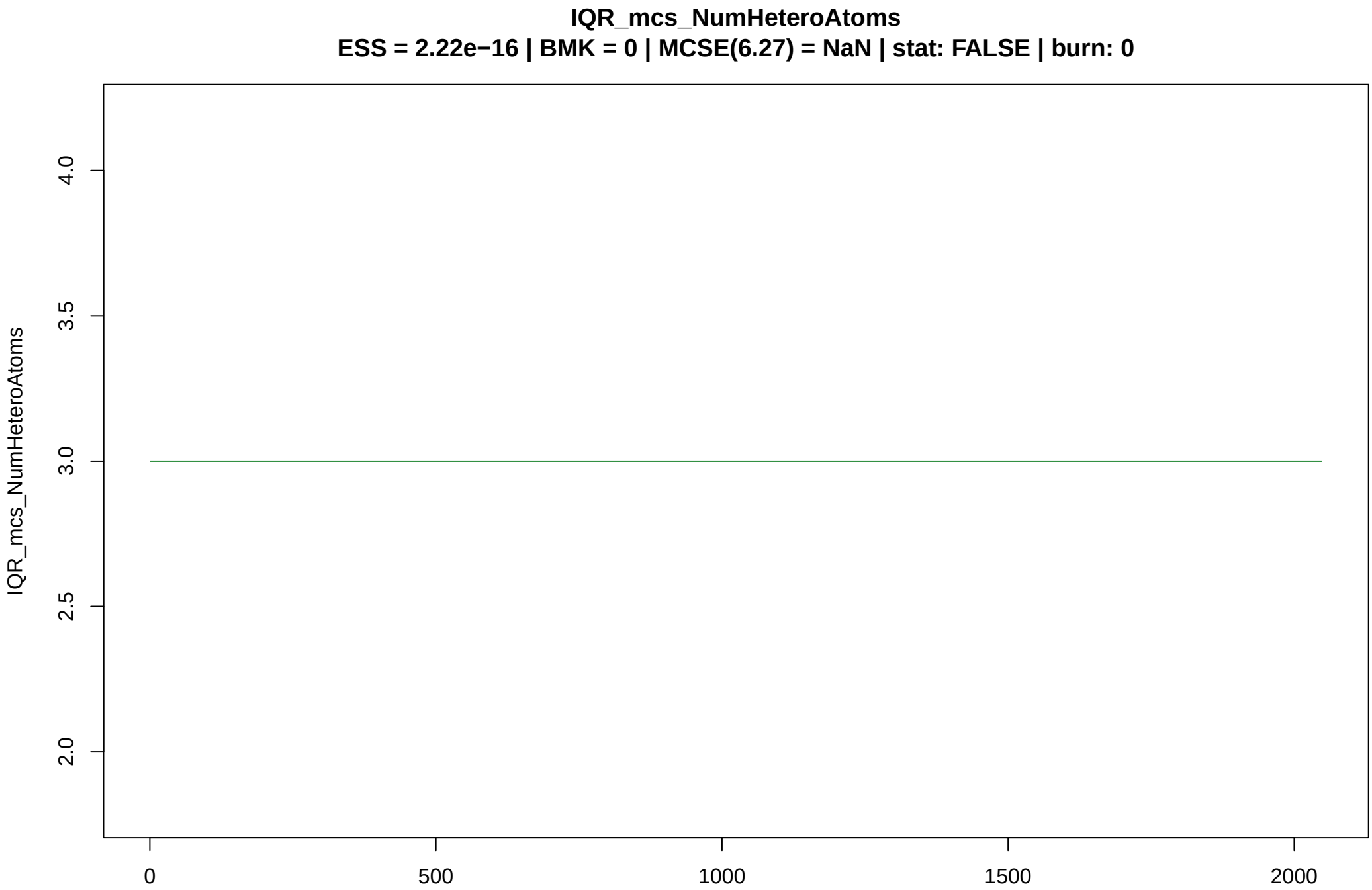

MEDIAN_docked_NumRotatableBonds
ESS = 2050 | BMK = 0.617 | MCSE(6.27) = 2.22 | stat: FALSE | burn: 408
MEDIAN_docked_NumRotatableBonds
5.0
4.8
4.6
4.4
4.2
4.0
0
500
1000
1500
2000

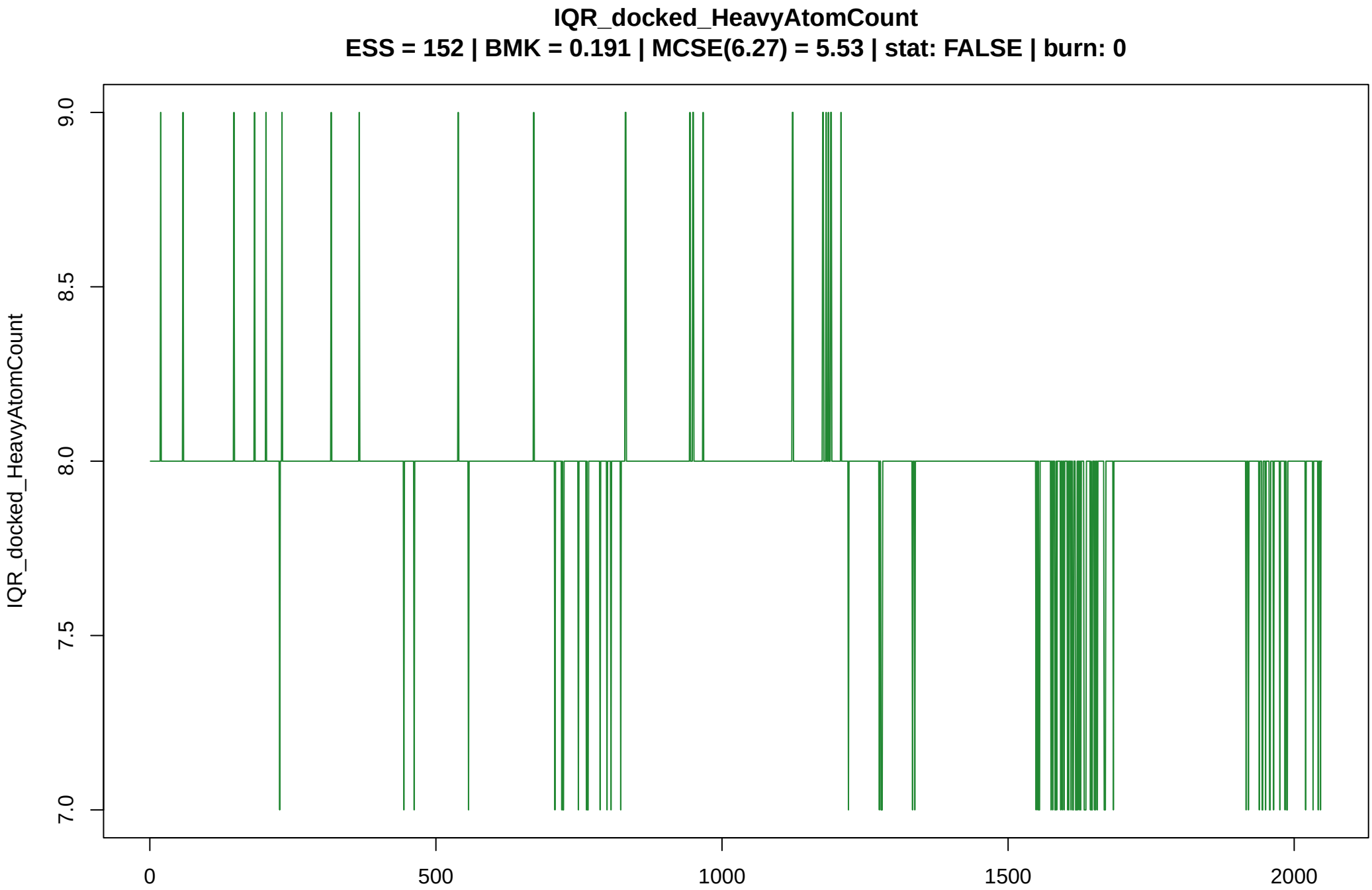

MEDIAN_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NOCount
2.5
2.0
1.5
0
500
1000
1500
2000

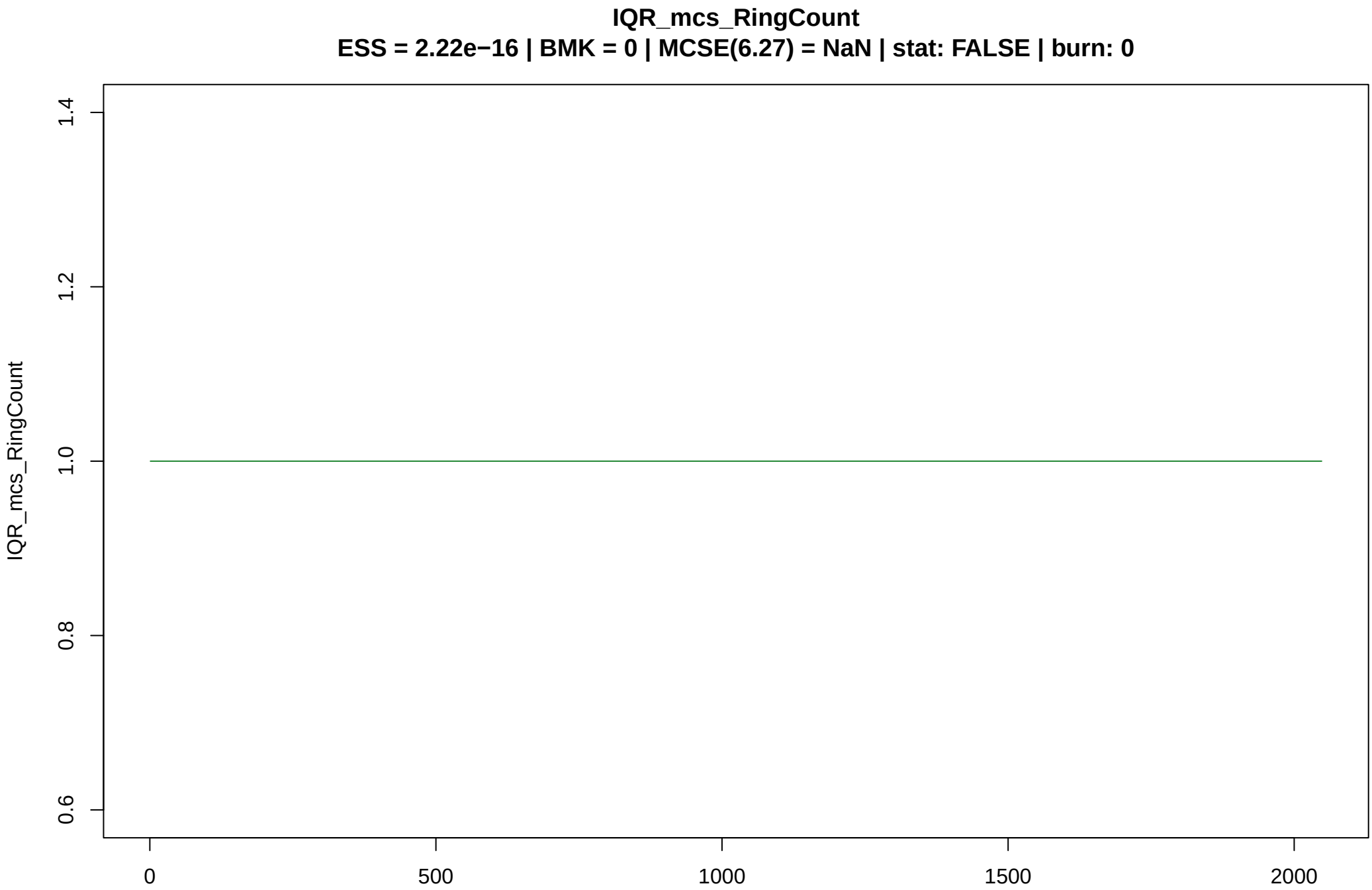

IQR_log_RMSD
ESS = 174 | BMK = 0.209 | MCSE(6.27) = 5.99 | stat: TRUE | burn: 0
IQR_log_RMSD
1.10
1.15
1.20
1.25
0
500
1000
1500
2000

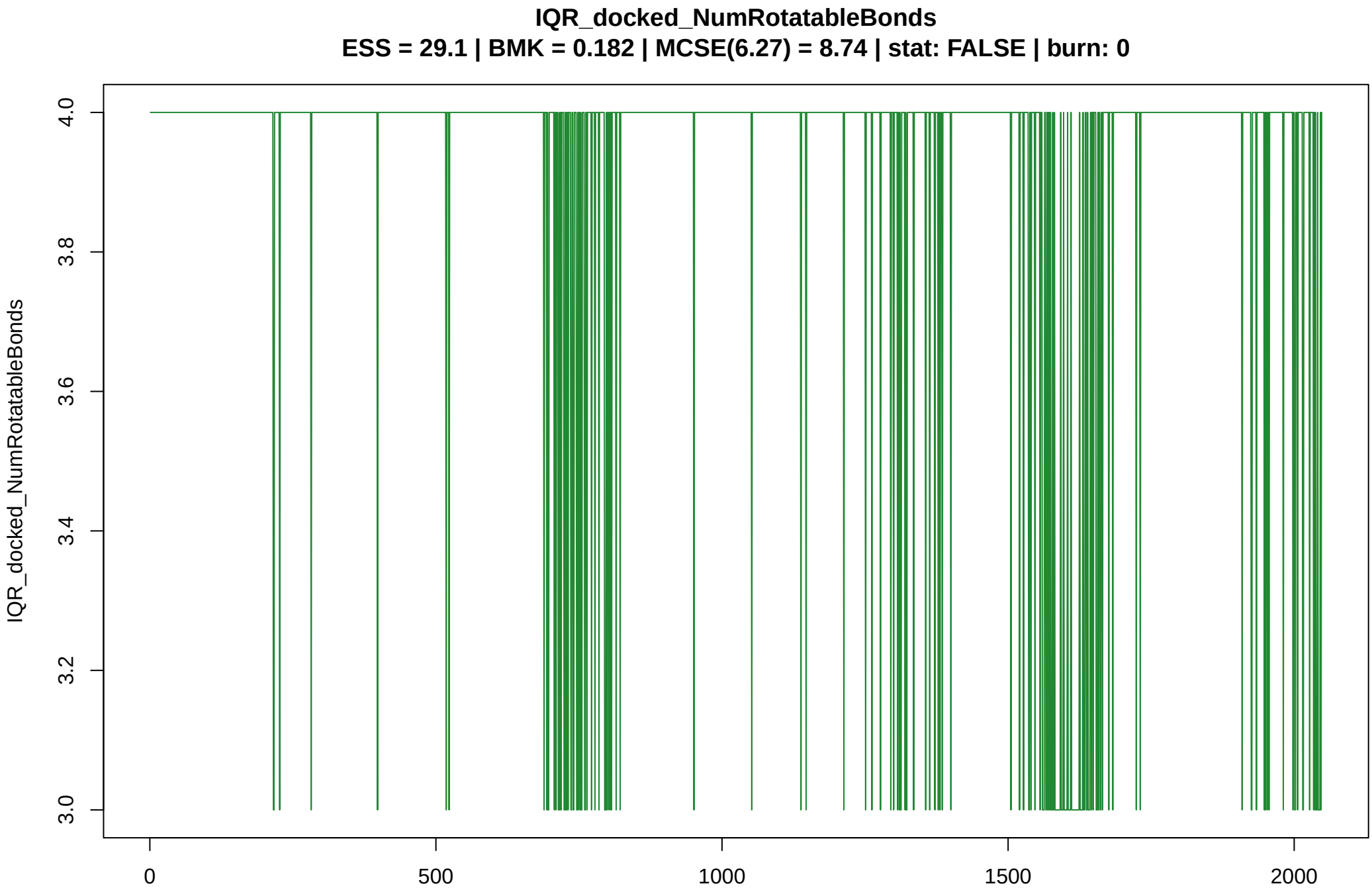

IQR_log_mcs_unbonded_polar_sasa
ESS = 39 | BMK = 0.243 | MCSE(6.27) = 9.01 | stat: TRUE | burn: 1632
IQR_log_mcs_unbonded_polar_sasa
0.40
0.42
0.44
0.46
0.48
0.50
0.52
0
500
1000
1500
2000

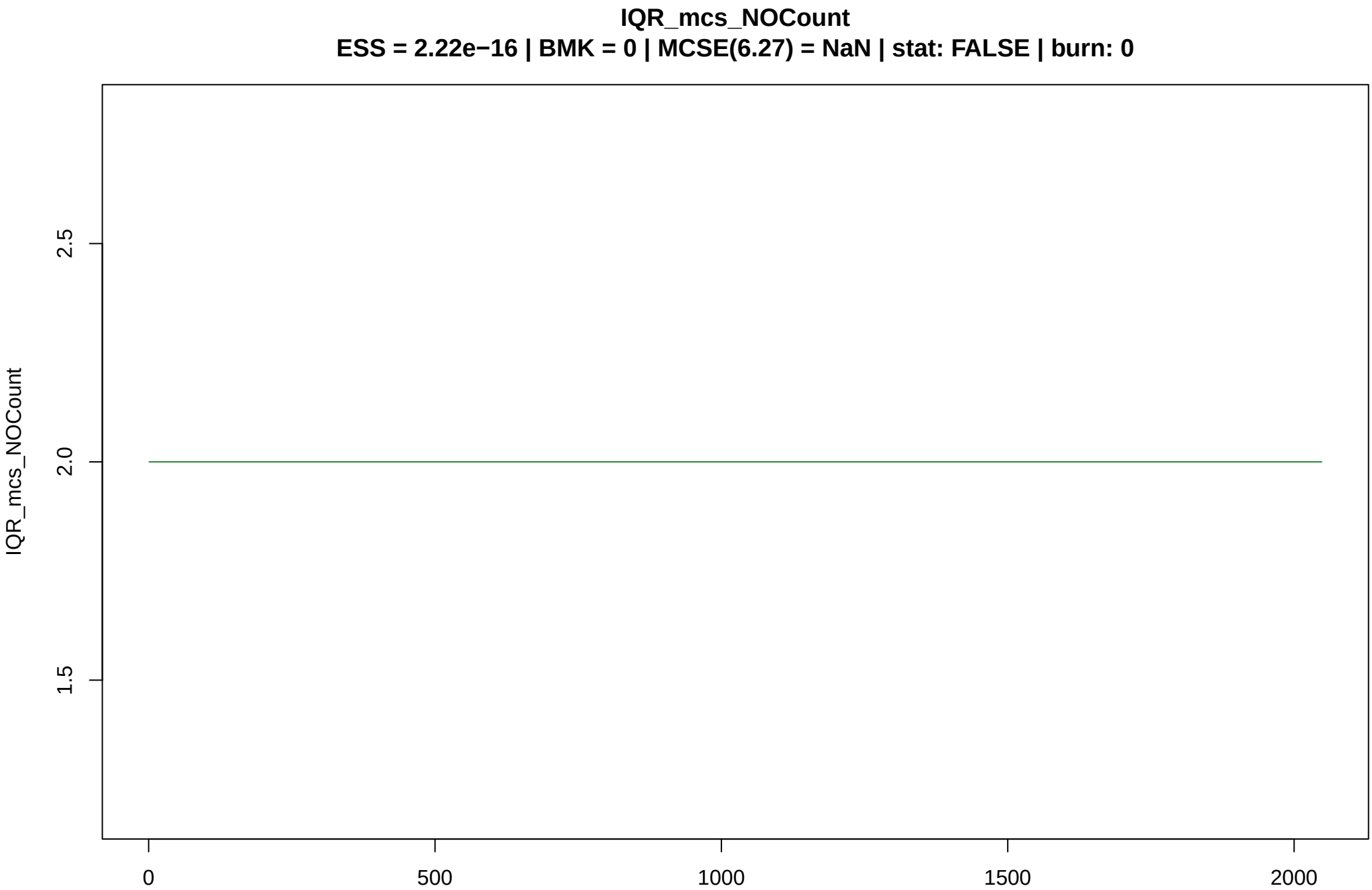

IQR_logit_ec_tanimoto_similarity
ESS = 99.8 | BMK = 0.251 | MCSE(6.27) = 6.79 | stat: FALSE | burn: 0
IQR_logit_ec_tanimoto_similarity
1.35
1.30
1.25
1.20
1.15
0
500
1000
1500
2000

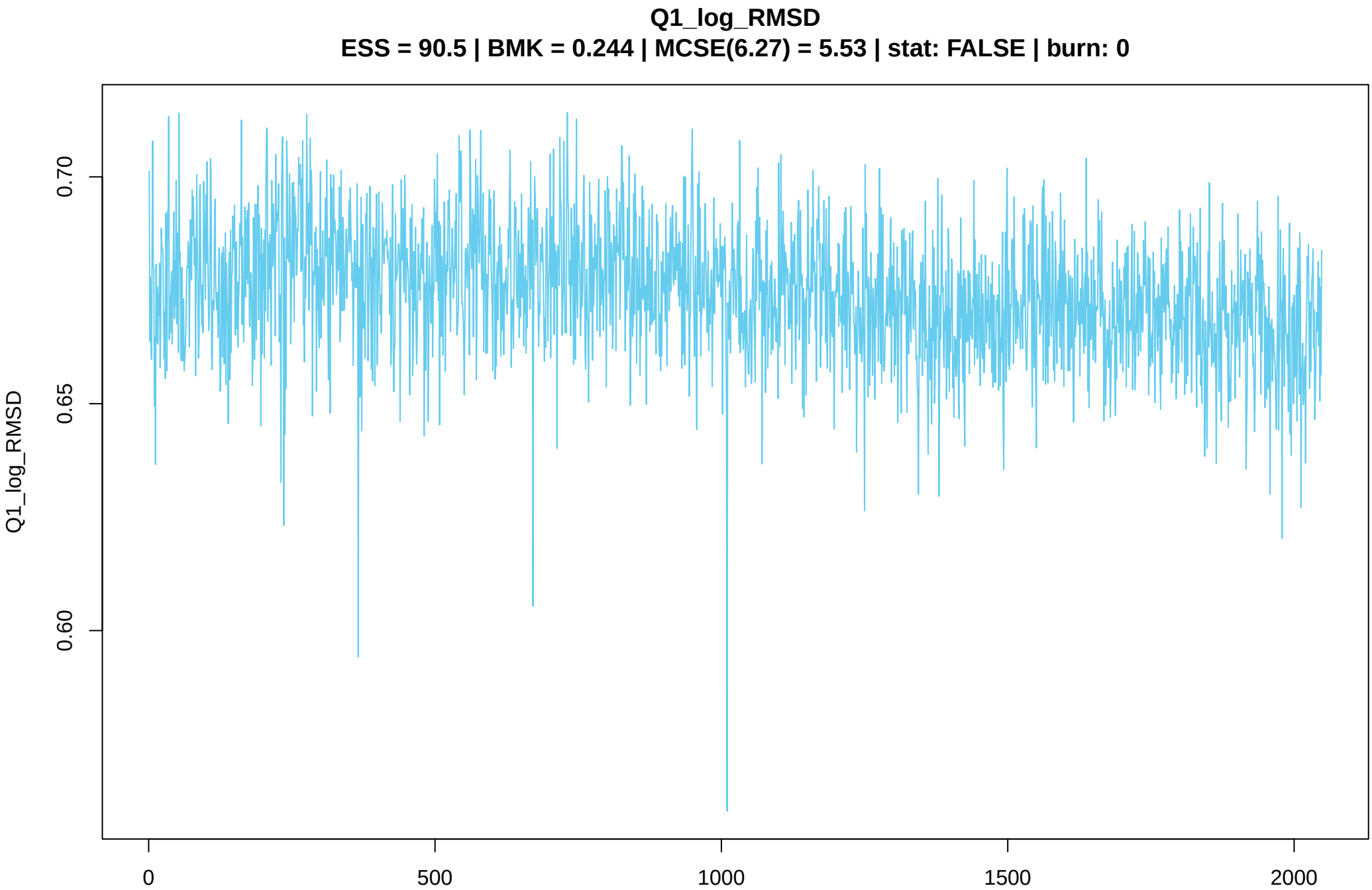

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

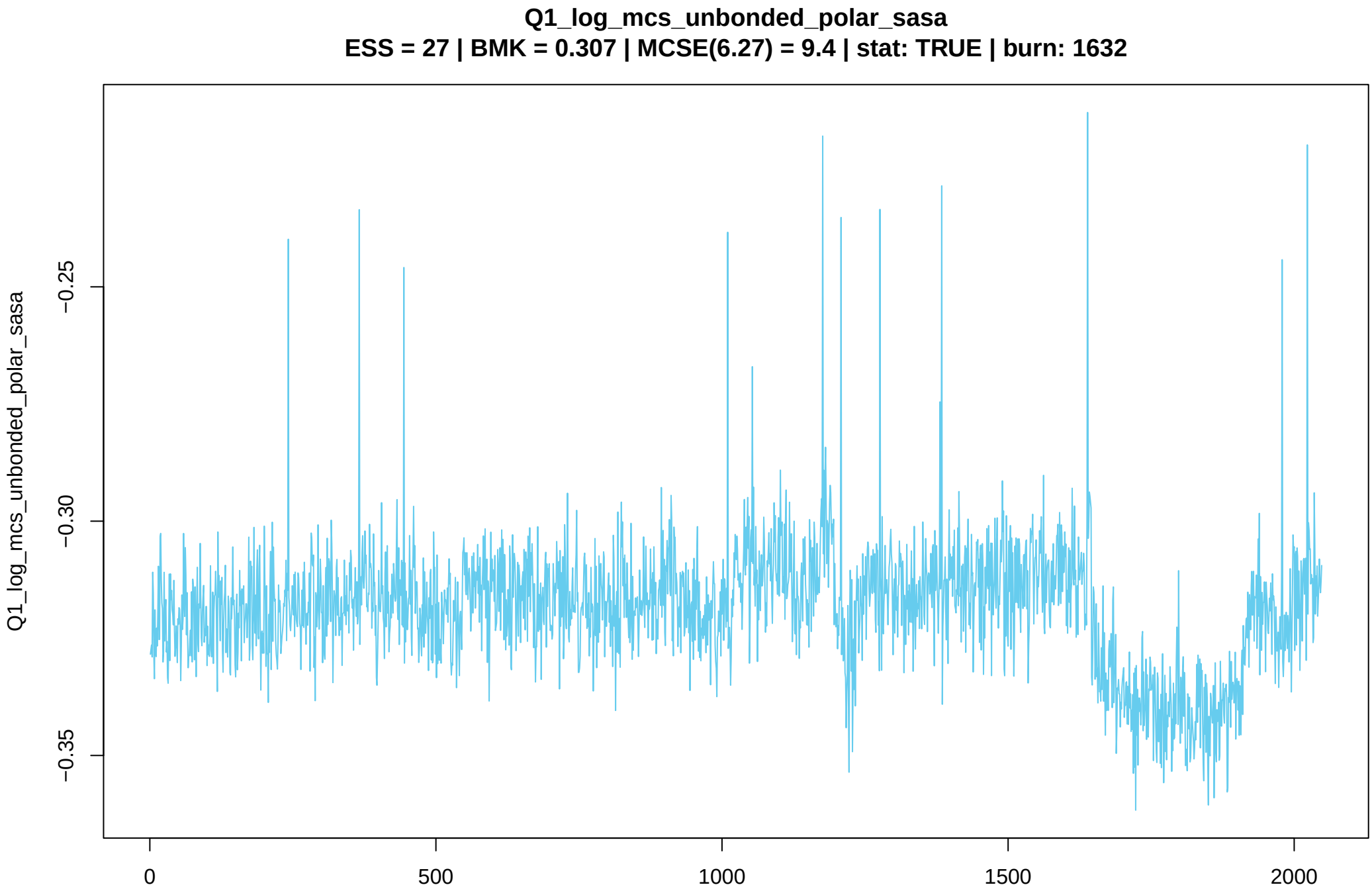

IQR_docked_HeavyAtomCount
ESS = 152 | BMK = 0.191 | MCSE(6.27) = 5.53 | stat: FALSE | burn: 0
IQR_docked_HeavyAtomCount
9.0
8.5
8.0
7.5
7.0
0
500
1000
1500
2000

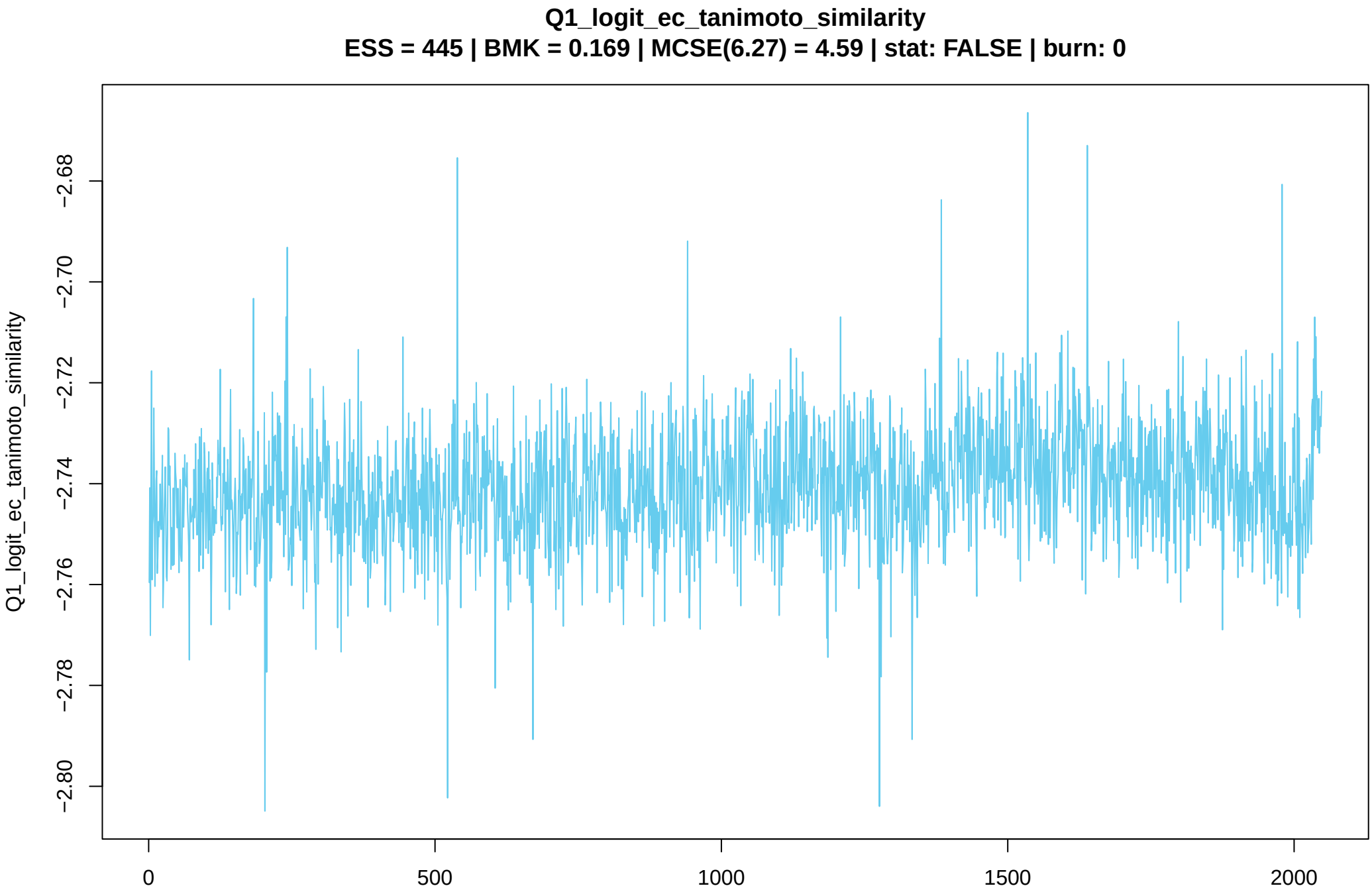

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

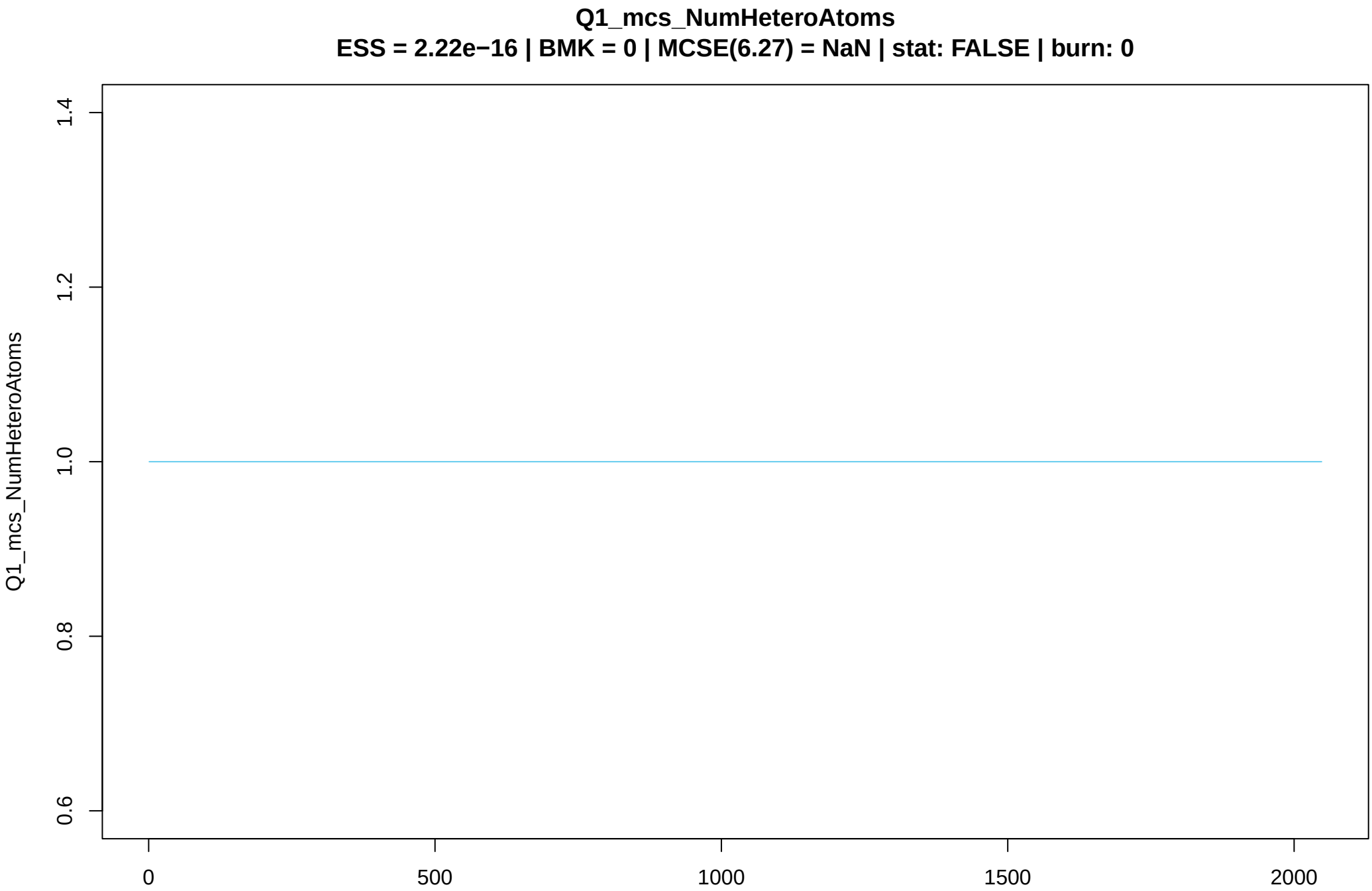

IQR_docked_NumRotatableBonds
ESS = 29.1 | BMK = 0.182 | MCSE(6.27) = 8.74 | stat: FALSE | burn: 0
IQR_docked_NumRotatableBonds
4.0
3.8
3.6
3.4
3.2
3.0
0
500
1000
1500
2000

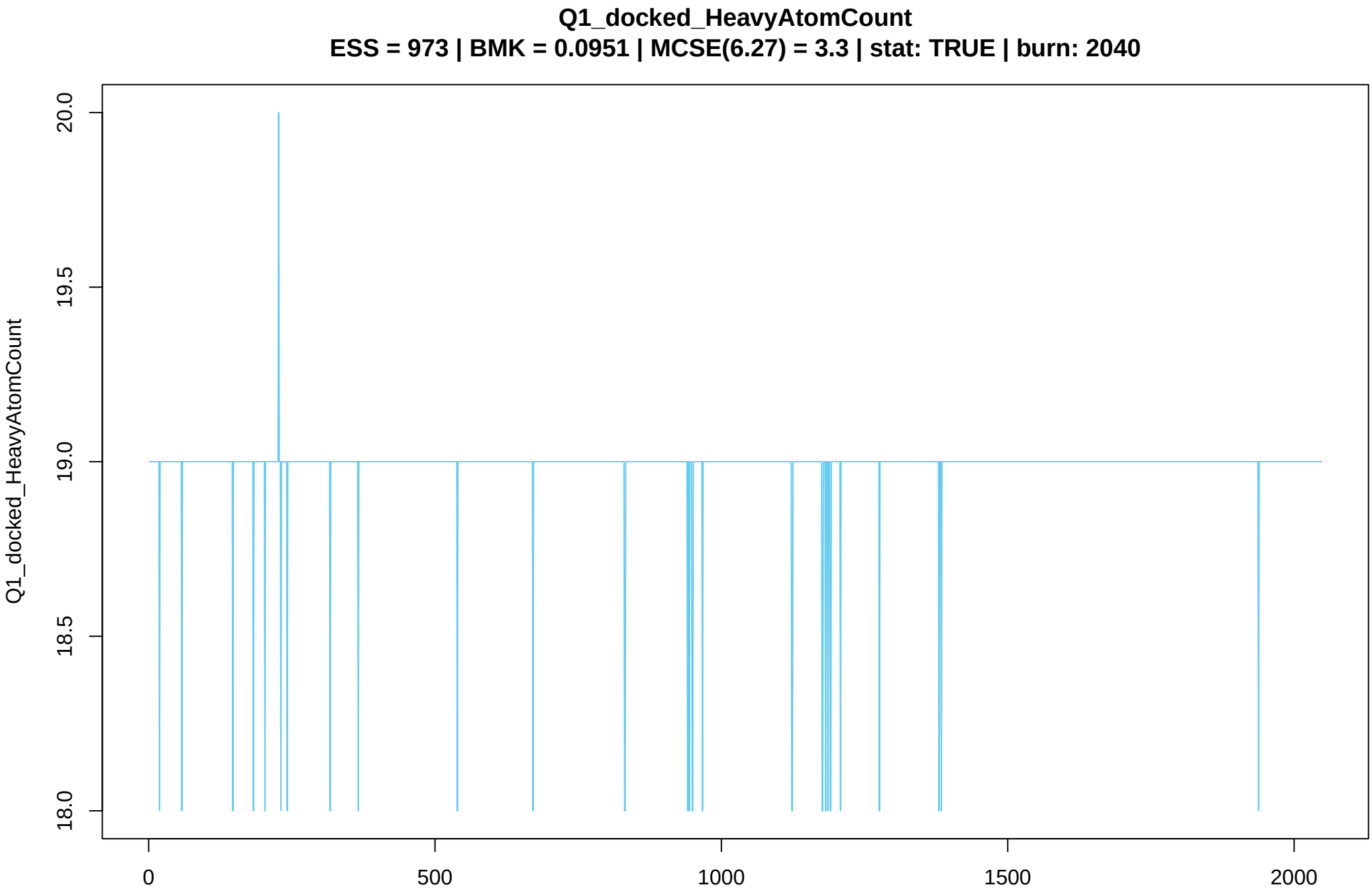

IQR_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NOCount
2.5
2.0
1.5
0
500
1000
1500
2000

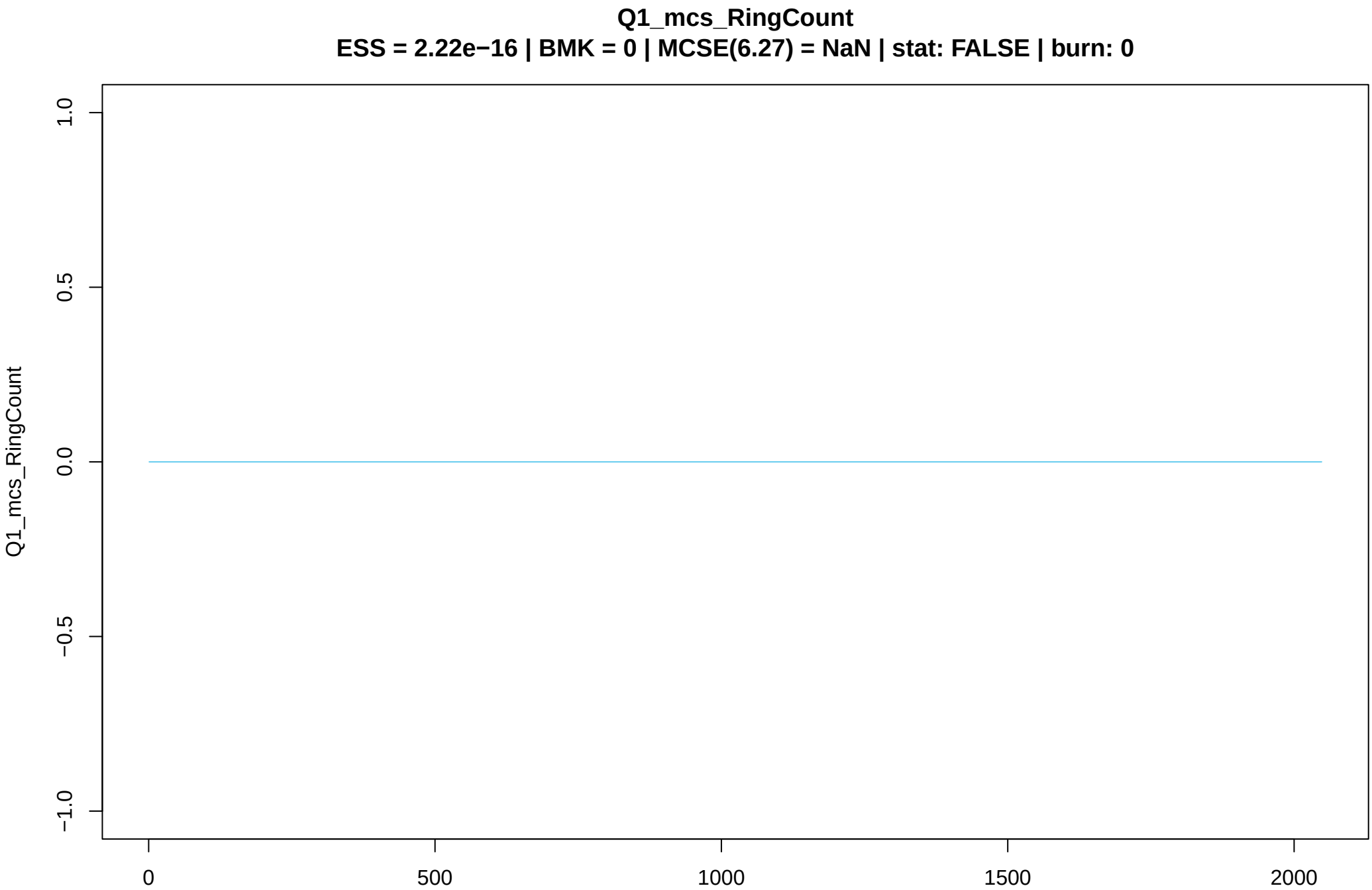

Q1_log_RMSD
ESS = 90.5 | BMK = 0.244 | MCSE(6.27) = 5.53 | stat: FALSE | burn: 0
Q1_log_RMSD
0.70
0.65
0.60
0
500
1000
1500
2000

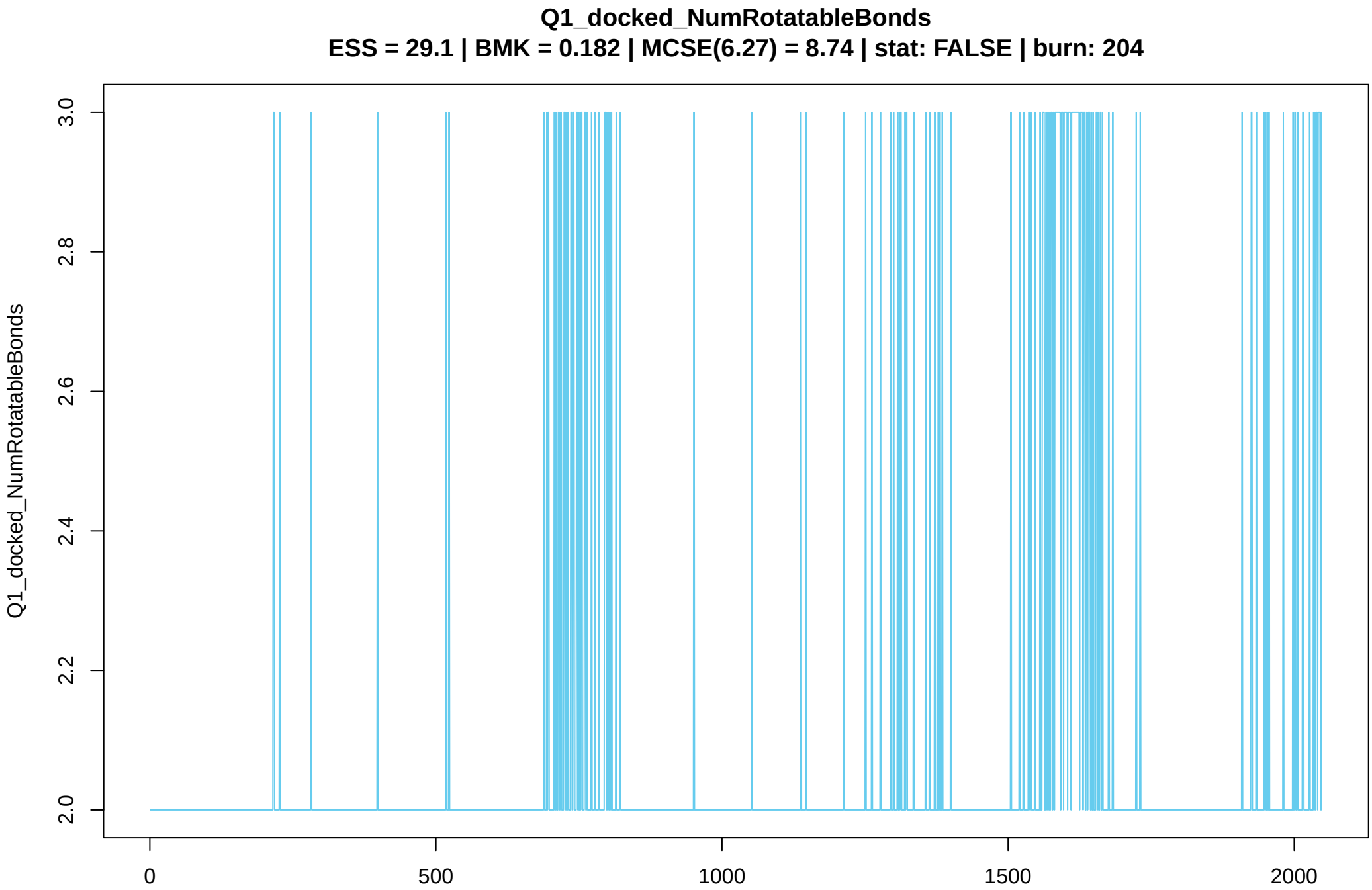

Q1_log_mcs_unbonded_polar_sasa
ESS = 27 | BMK = 0.307 | MCSE(6.27) = 9.4 | stat: TRUE | burn: 1632
Q1_log_mcs_unbonded_polar_sasa
−0.25
−0.30
−0.35
0
500
1000
1500
2000

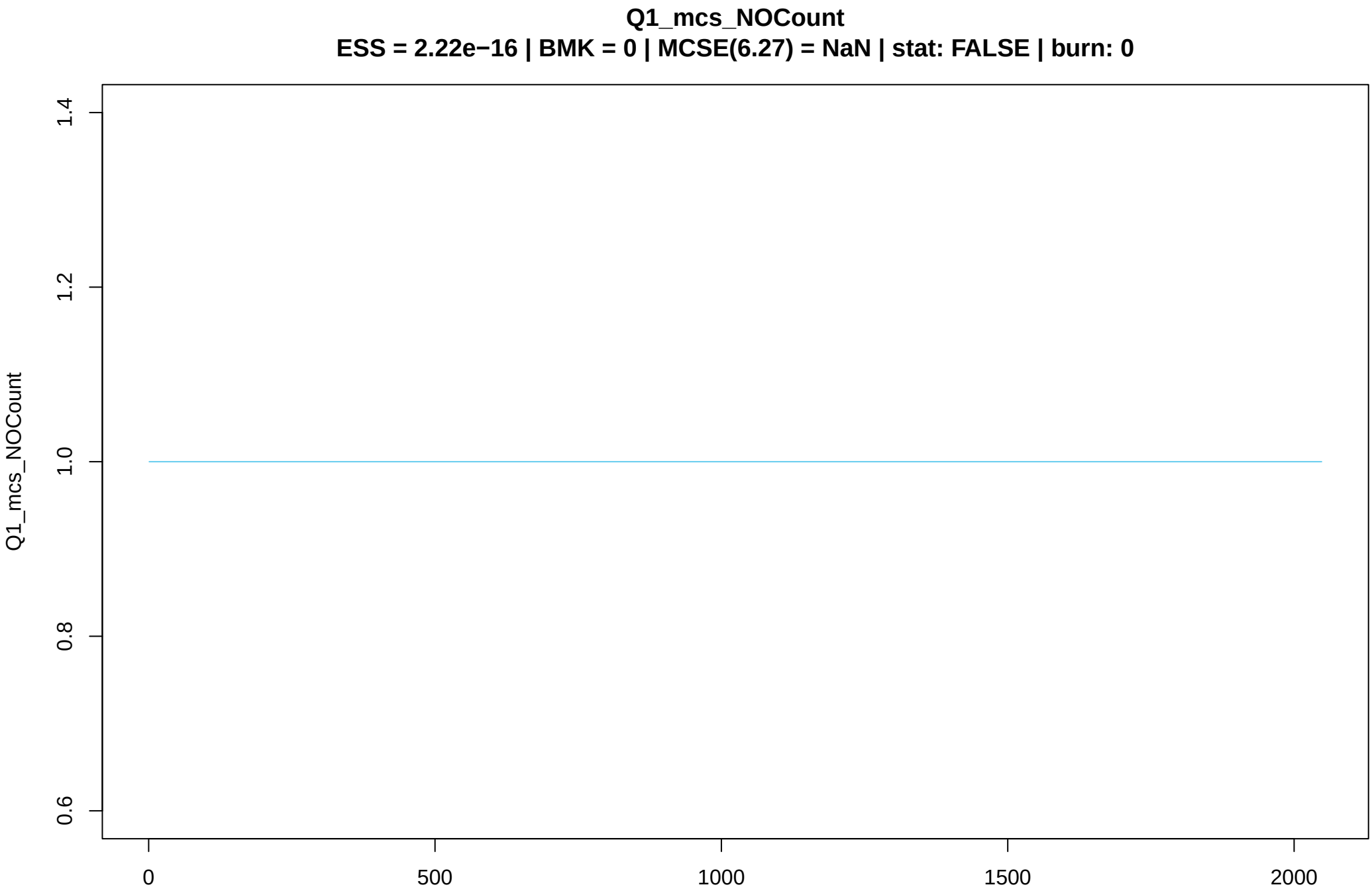

Q1_logit_ec_tanimoto_similarity
ESS = 445 | BMK = 0.169 | MCSE(6.27) = 4.59 | stat: FALSE | burn: 0
Q1_logit_ec_tanimoto_similarity
−2.68
−2.70
−2.72
−2.74
−2.76
−2.78
−2.80
0
500
1000
1500
2000

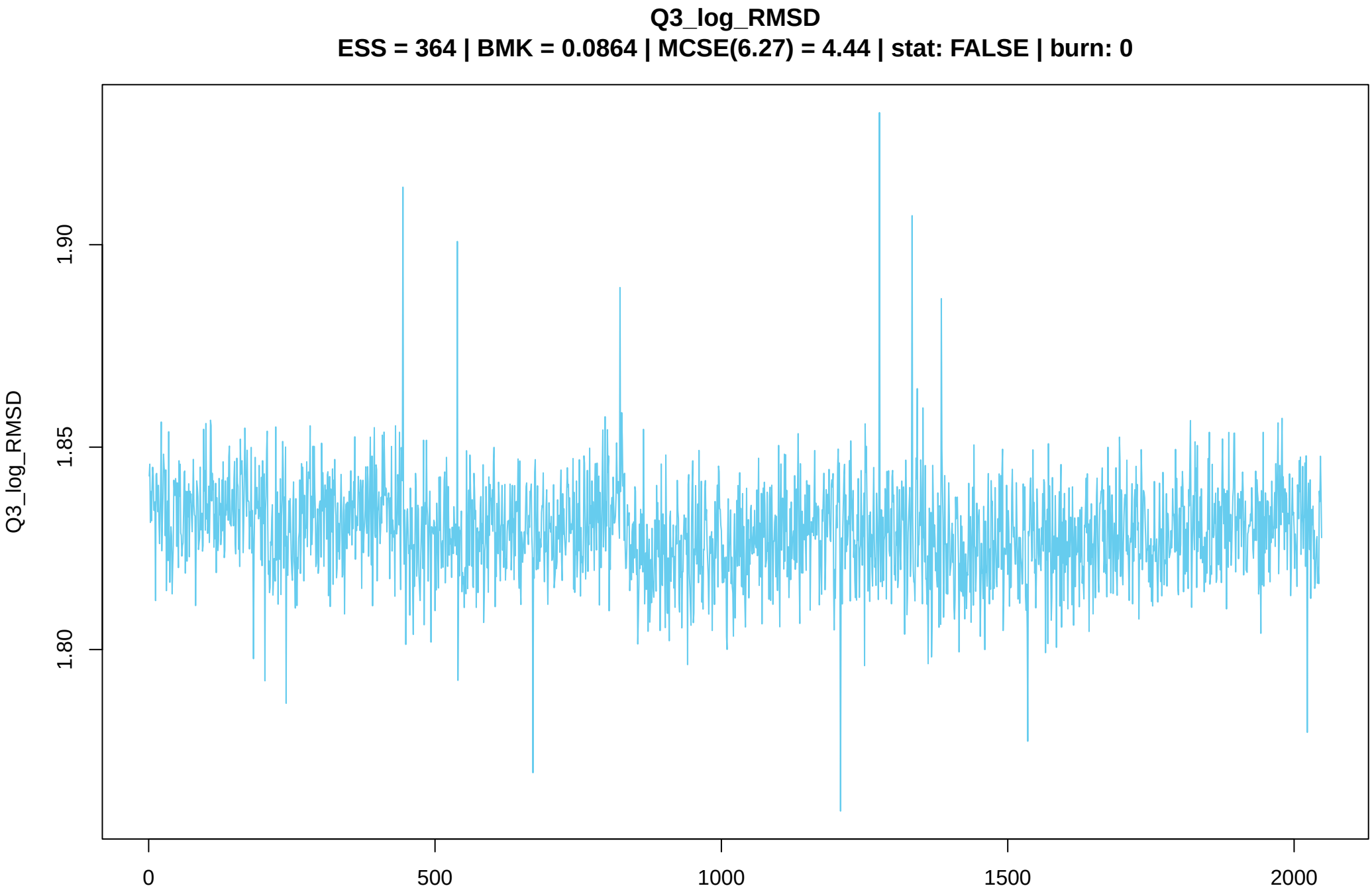

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

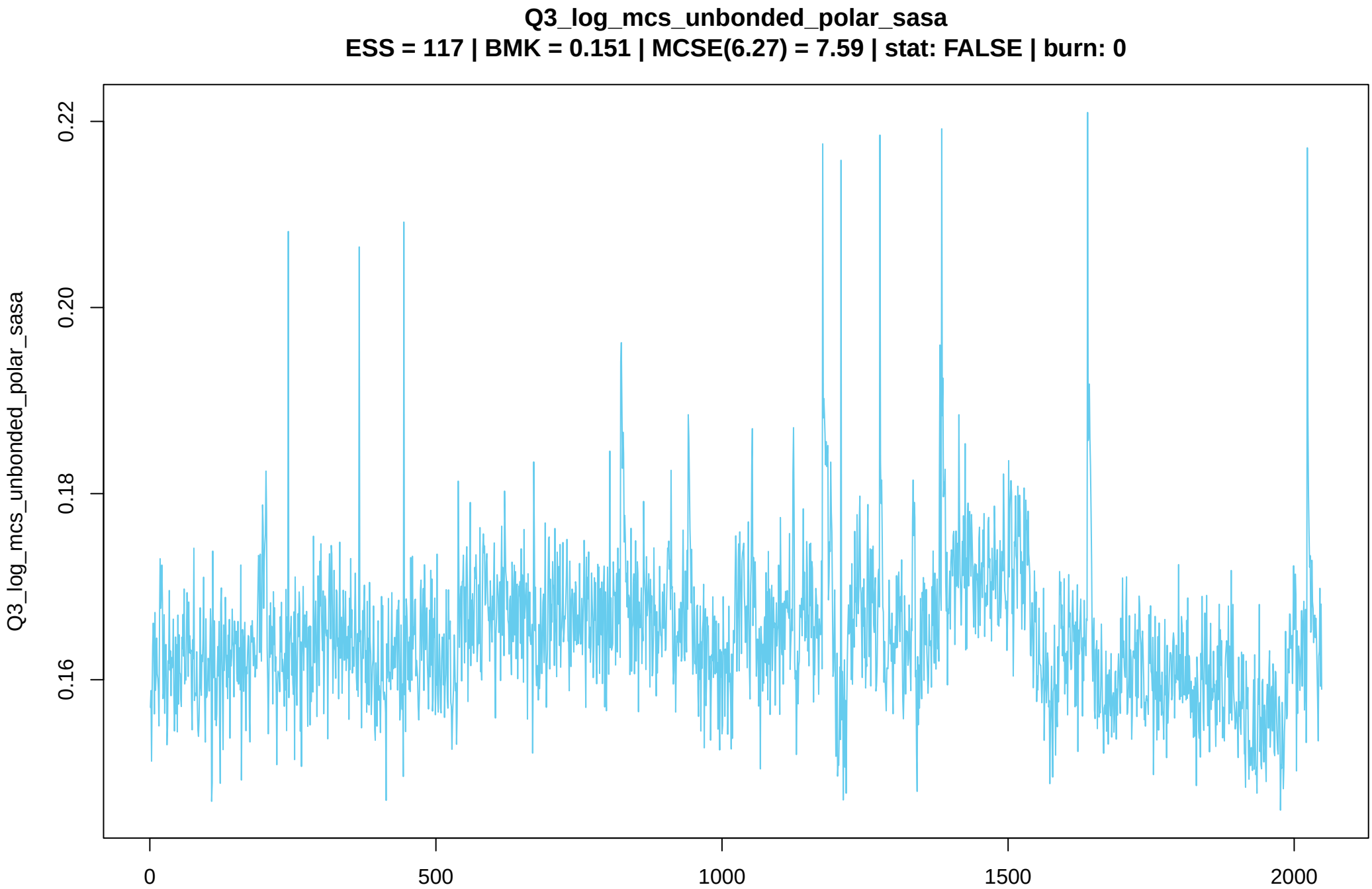

Q1_docked_HeavyAtomCount
ESS = 973 | BMK = 0.0951 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 2040
Q1_docked_HeavyAtomCount
20.0
19.5
19.0
18.5
18.0
0
500
1000
1500
2000

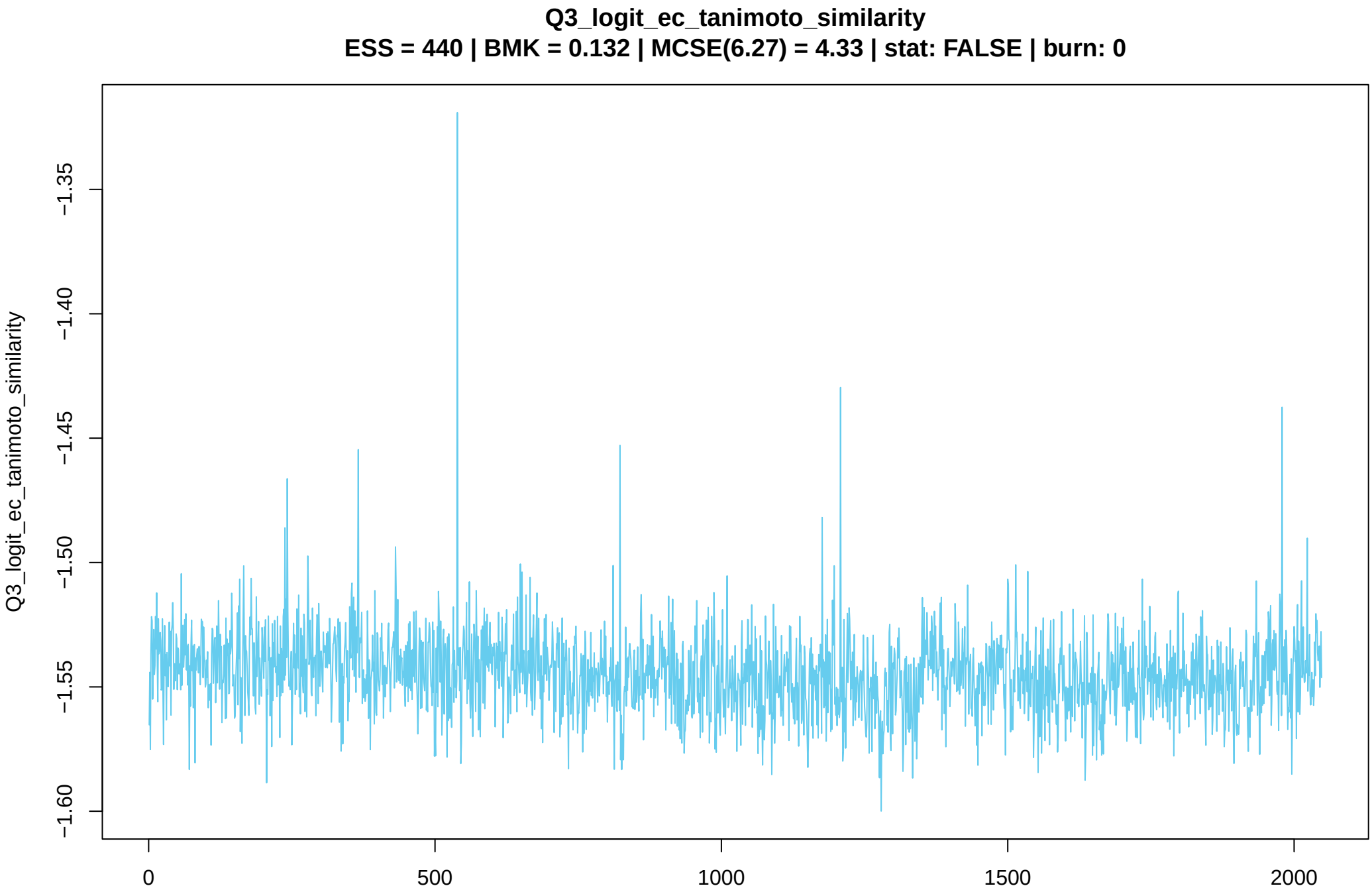

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

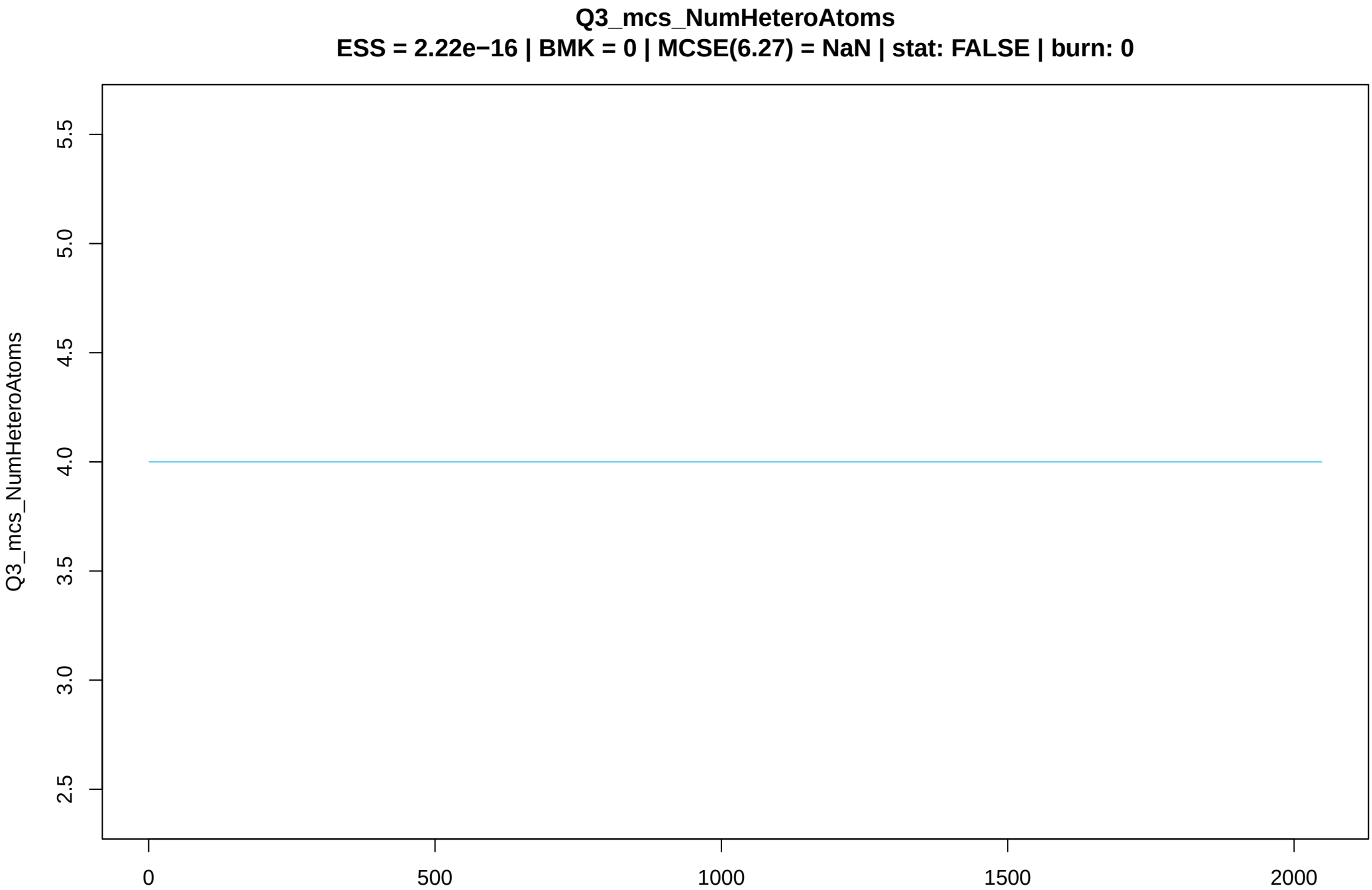

Q1_docked_NumRotatableBonds
ESS = 29.1 | BMK = 0.182 | MCSE(6.27) = 8.74 | stat: FALSE | burn: 204
Q1_docked_NumRotatableBonds
2.0
2.2
2.4
2.6
2.8
3.0
0
500
1000
1500
2000

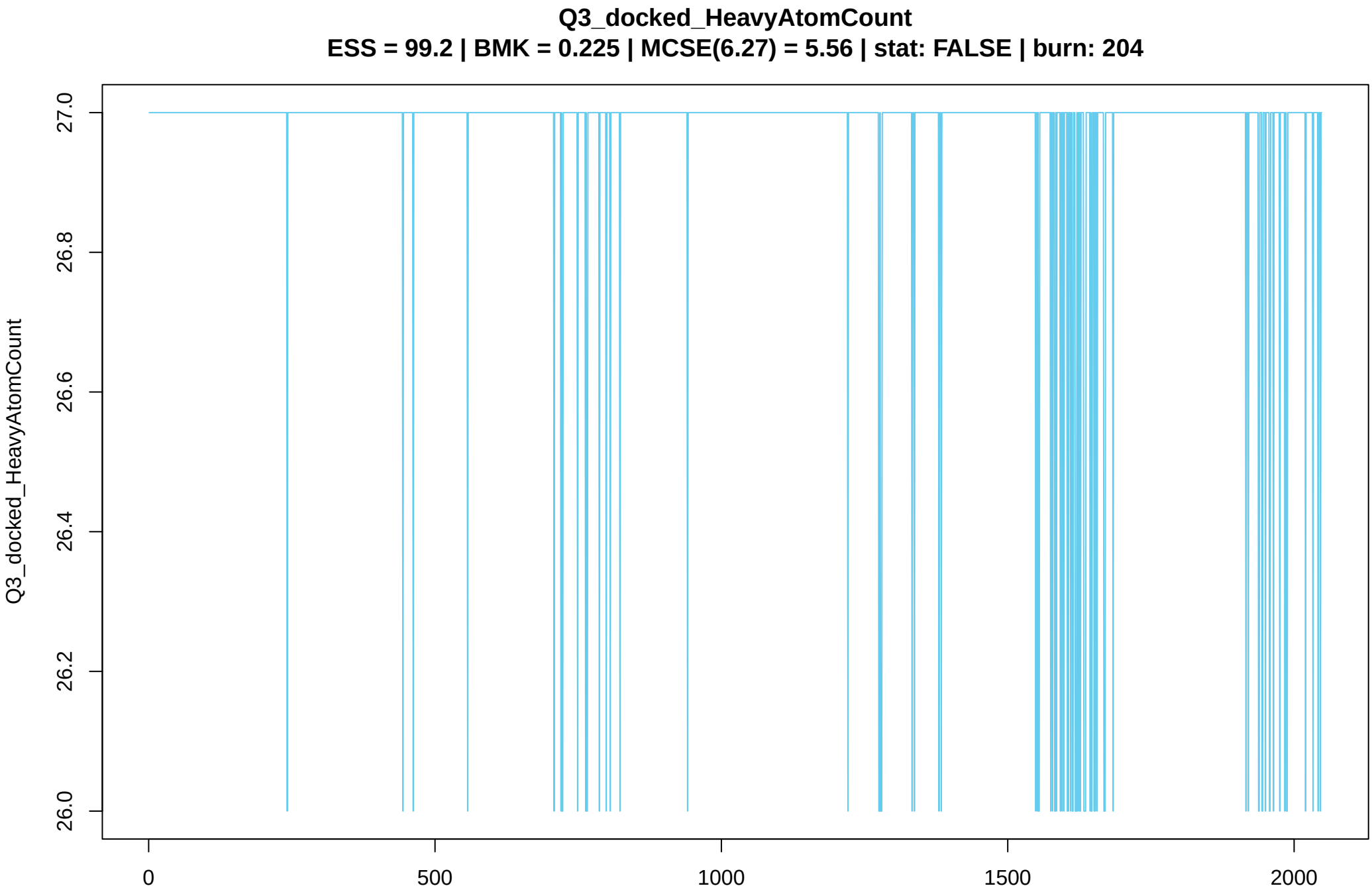

Q1_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NOCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

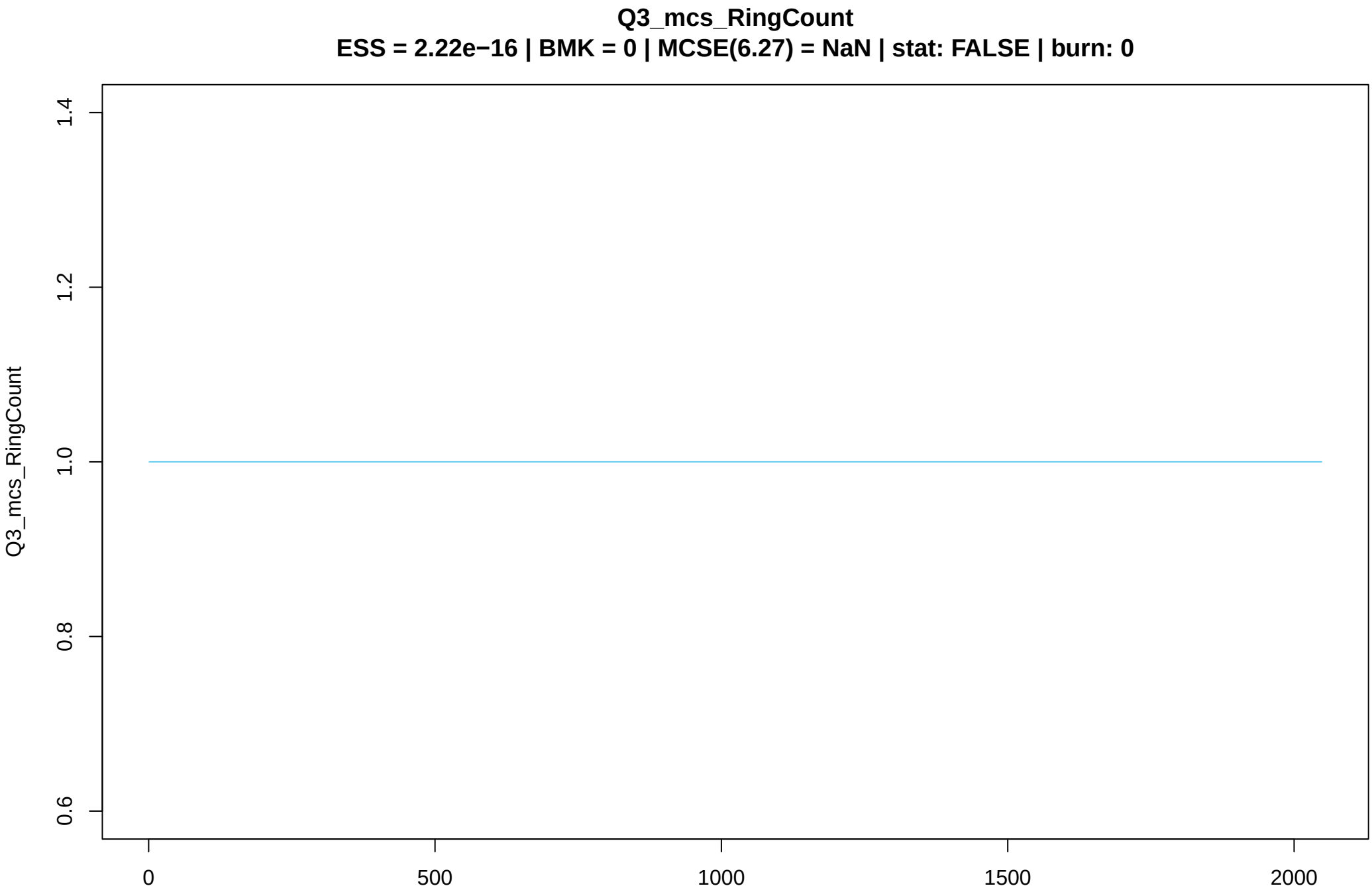

Q3_log_RMSD
ESS = 364 | BMK = 0.0864 | MCSE(6.27) = 4.44 | stat: FALSE | burn: 0
Q3_log_RMSD
1.80
1.85
1.90
0
500
1000
1500
2000

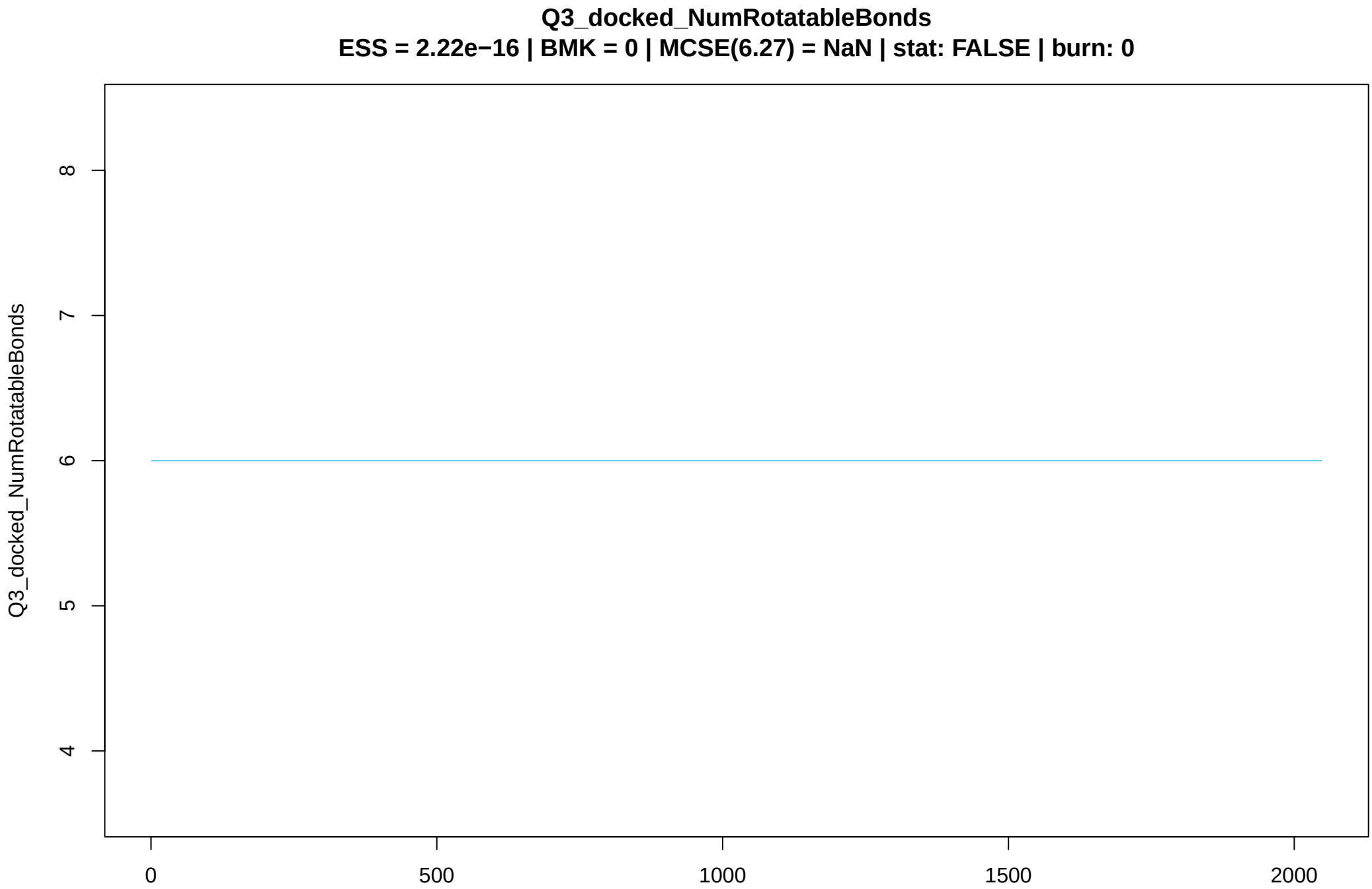

Q3_log_mcs_unbonded_polar_sasa
ESS = 117 | BMK = 0.151 | MCSE(6.27) = 7.59 | stat: FALSE | burn: 0
Q3_log_mcs_unbonded_polar_sasa
0.16
0.18
0.20
0.22
0
500
1000
1500
2000

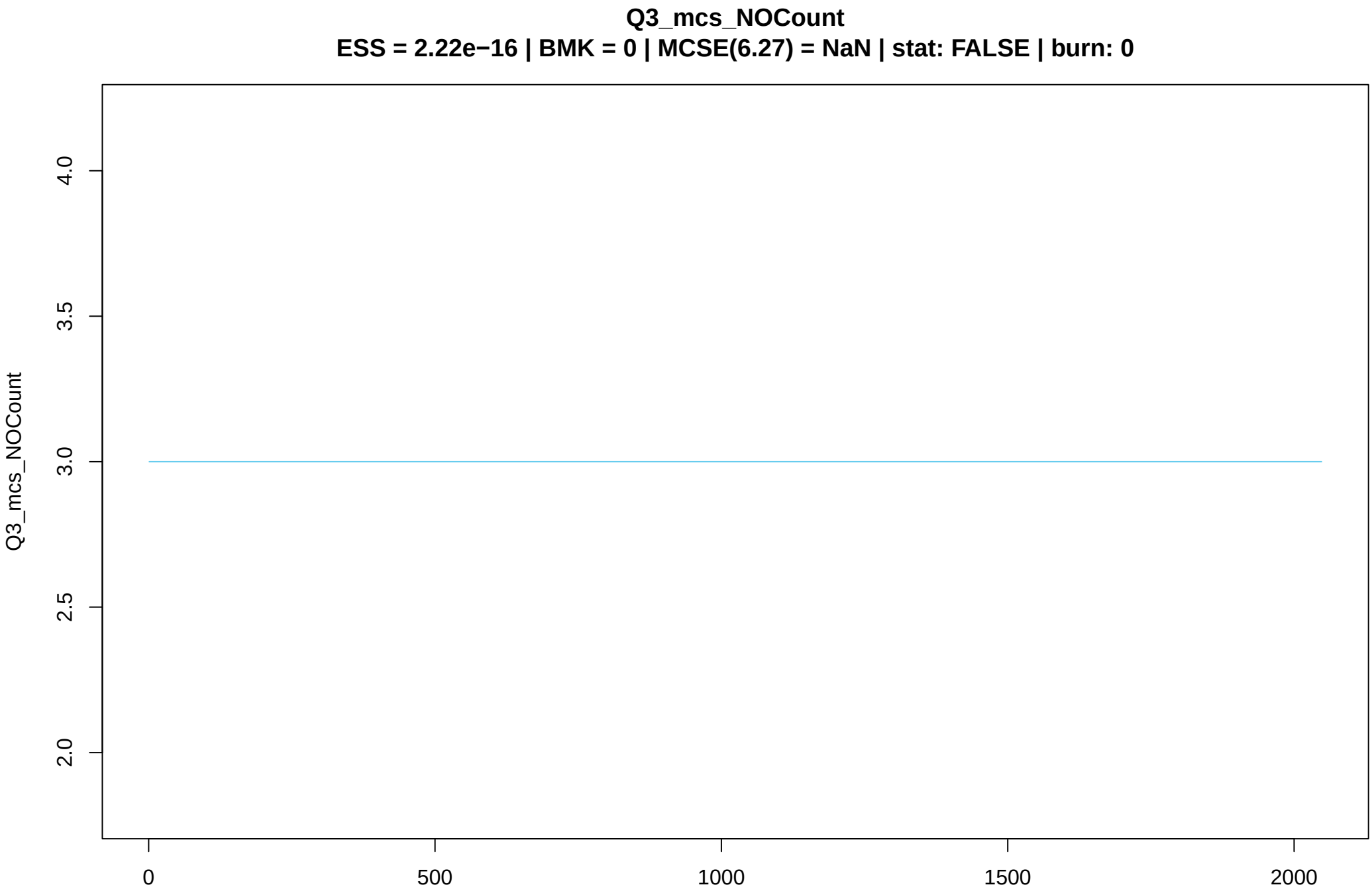

Q3_logit_ec_tanimoto_similarity
ESS = 440 | BMK = 0.132 | MCSE(6.27) = 4.33 | stat: FALSE | burn: 0
Q3_logit_ec_tanimoto_similarity
−1.35
−1.40
−1.45
−1.50
−1.55
−1.60
0
500
1000
1500
2000

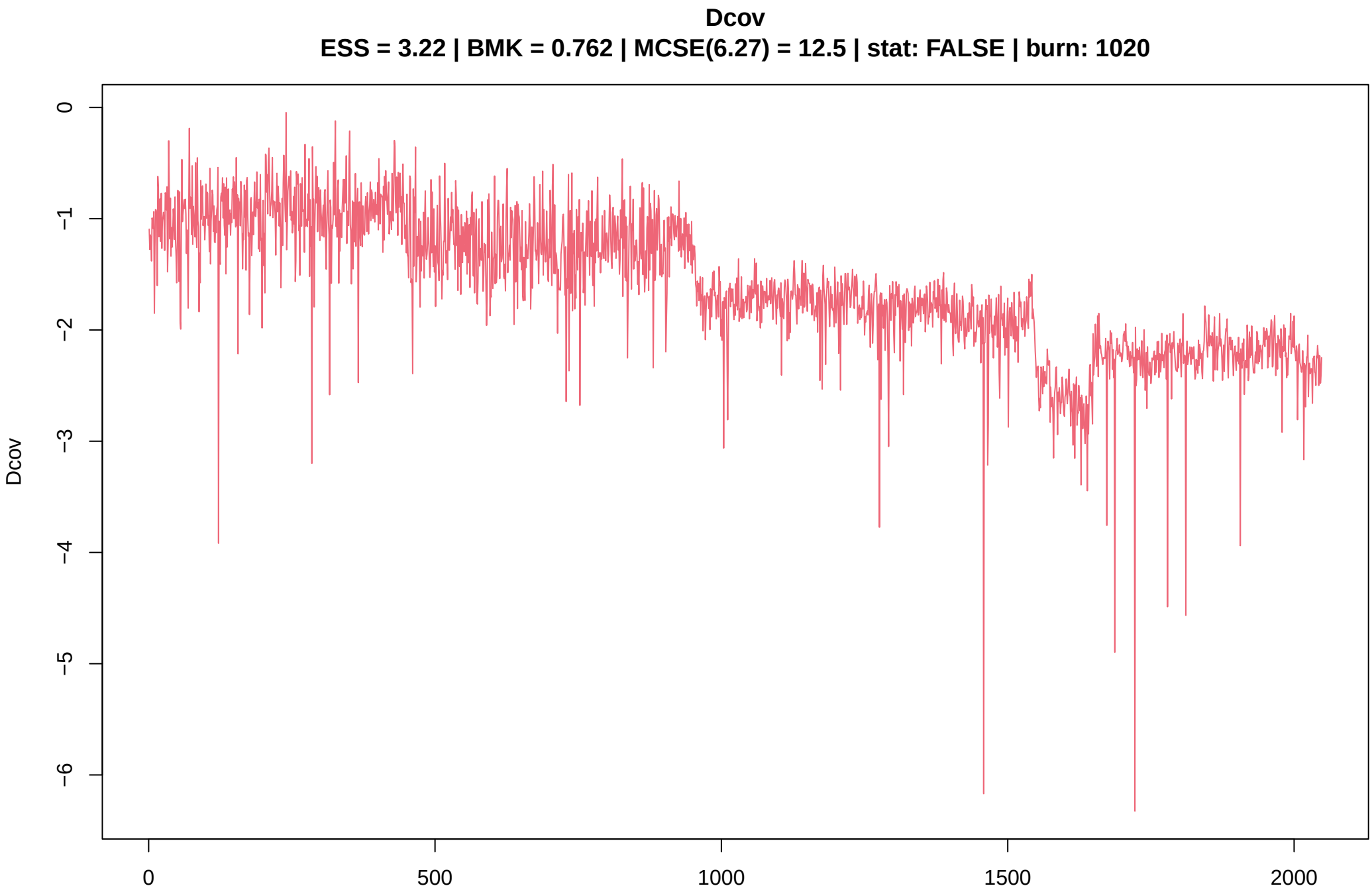

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

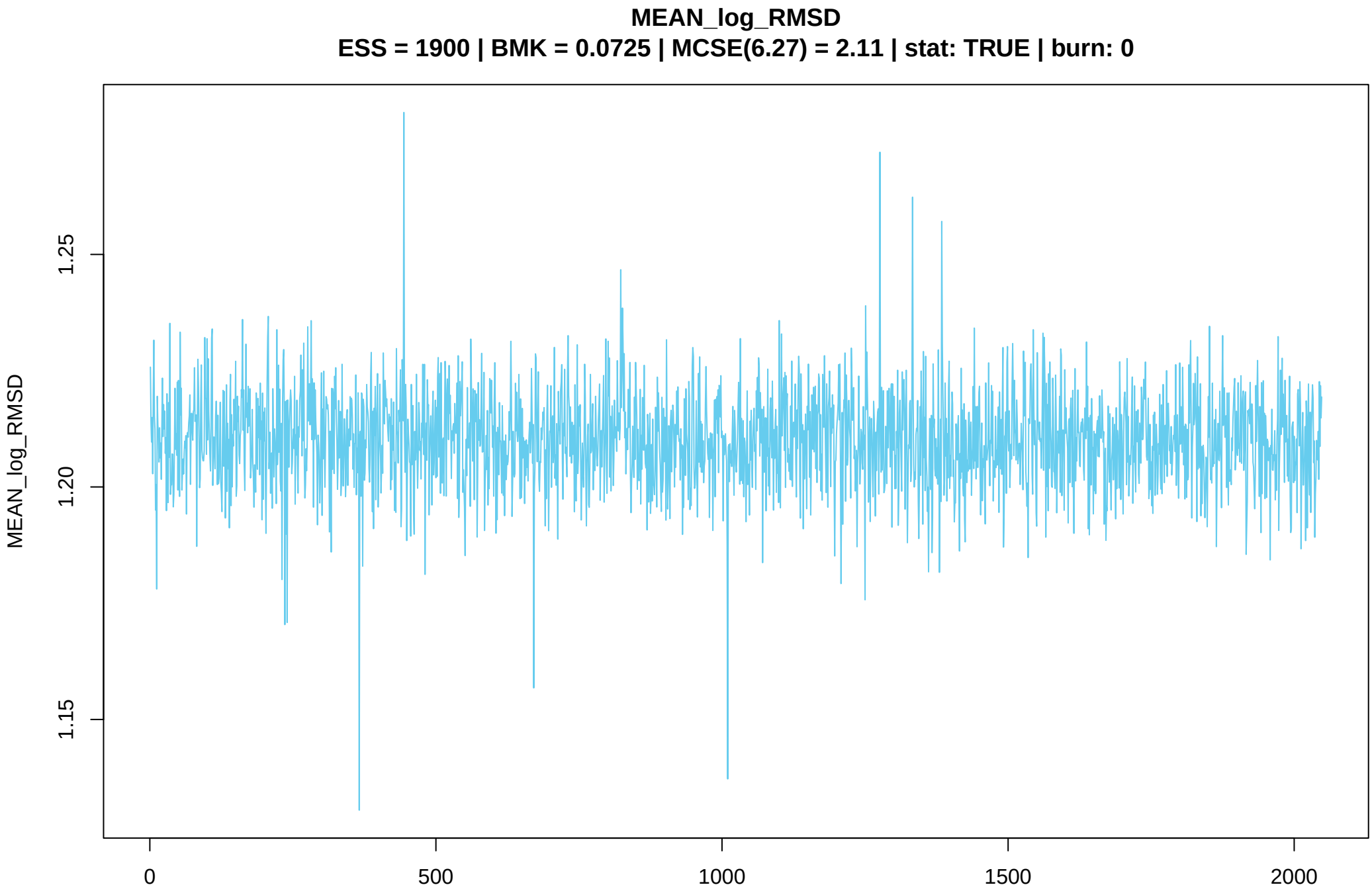

Q3_docked_HeavyAtomCount
ESS = 99.2 | BMK = 0.225 | MCSE(6.27) = 5.56 | stat: FALSE | burn: 204
Q3_docked_HeavyAtomCount
27.0
26.8
26.6
26.4
26.2
26.0
0
500
1000
1500
2000

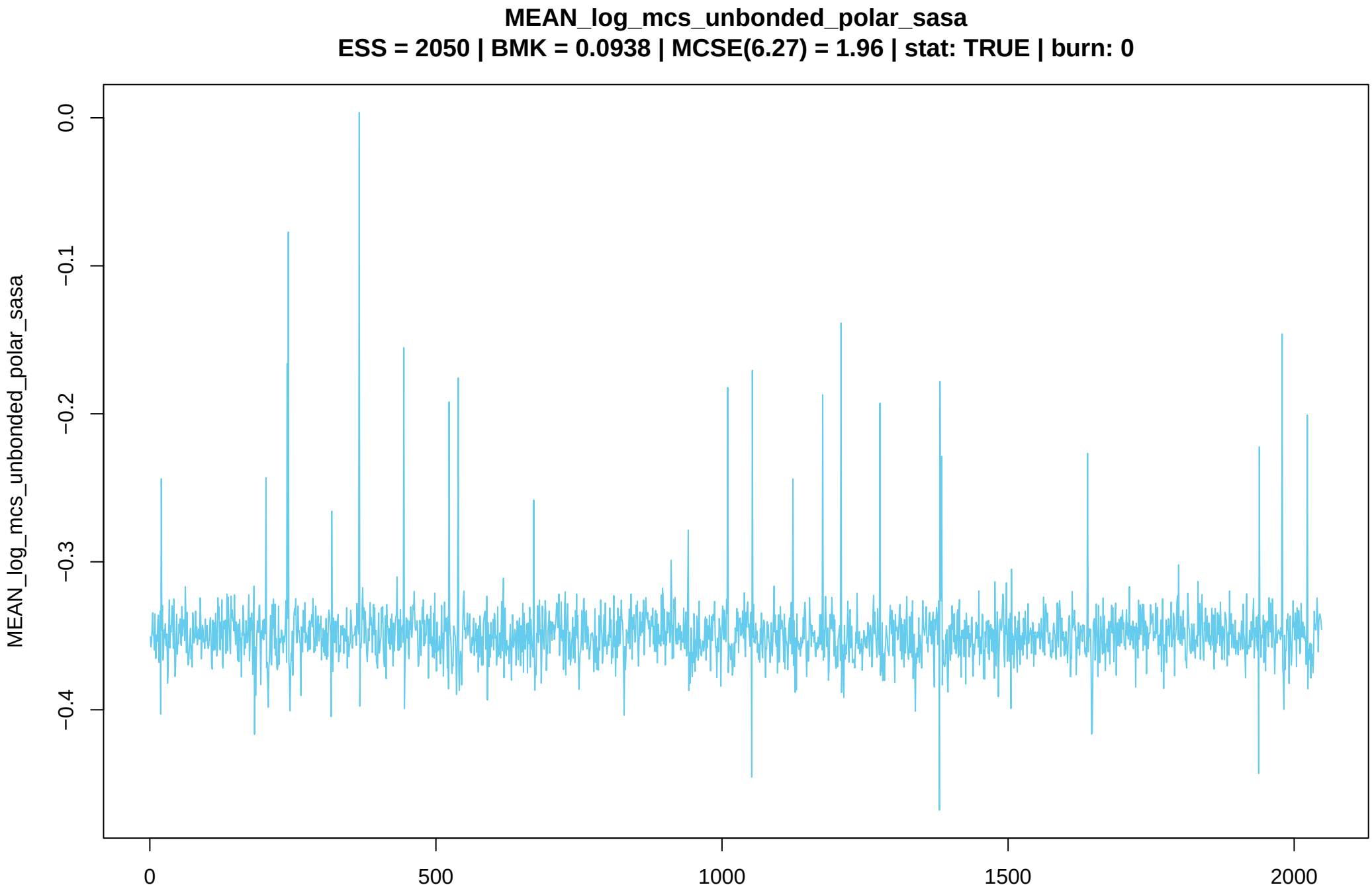

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

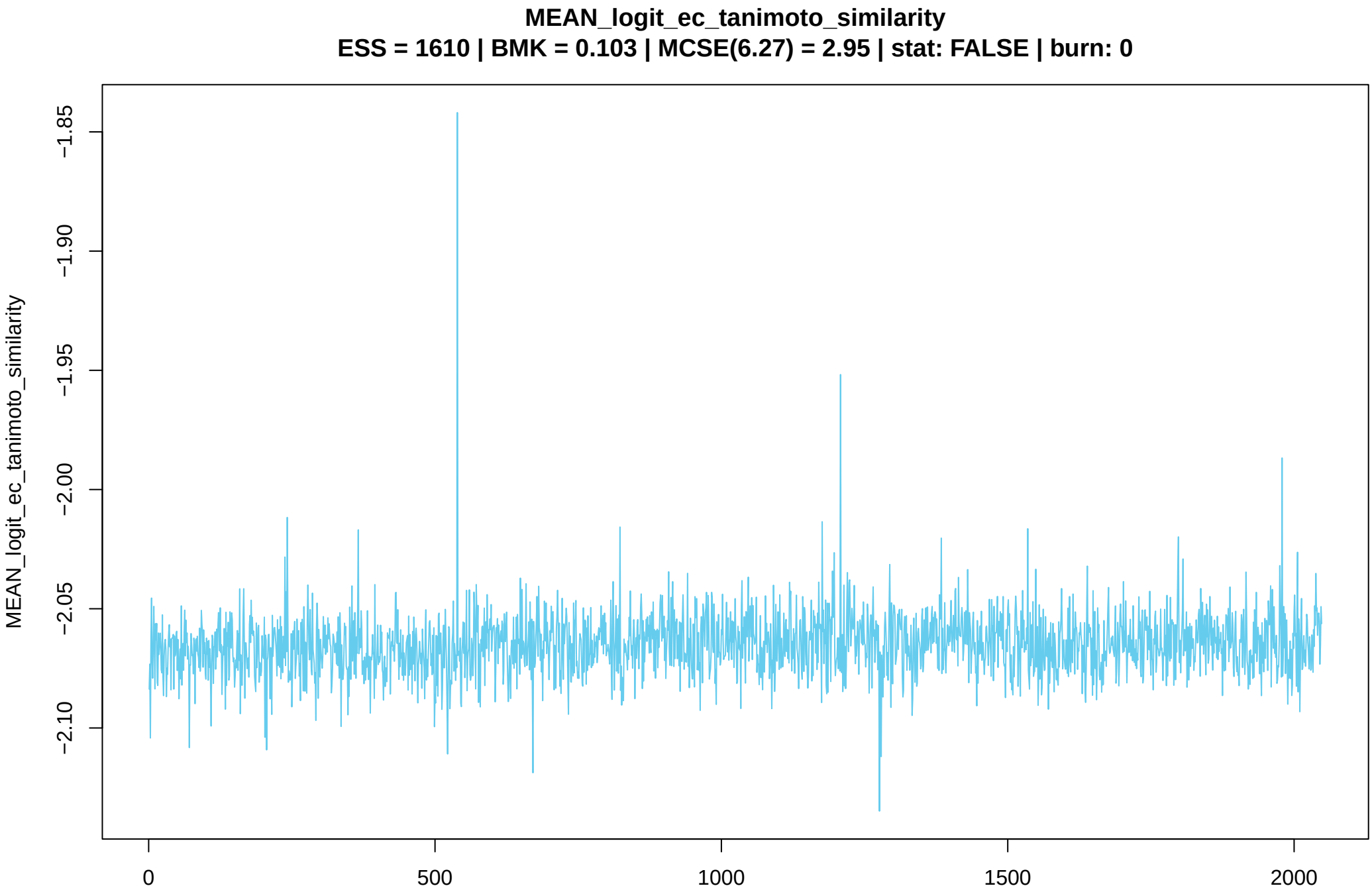

Q3_docked_NumRotatableBonds
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_docked_NumRotatableBonds
4
5
6
7
8
0
500
1000
1500
2000

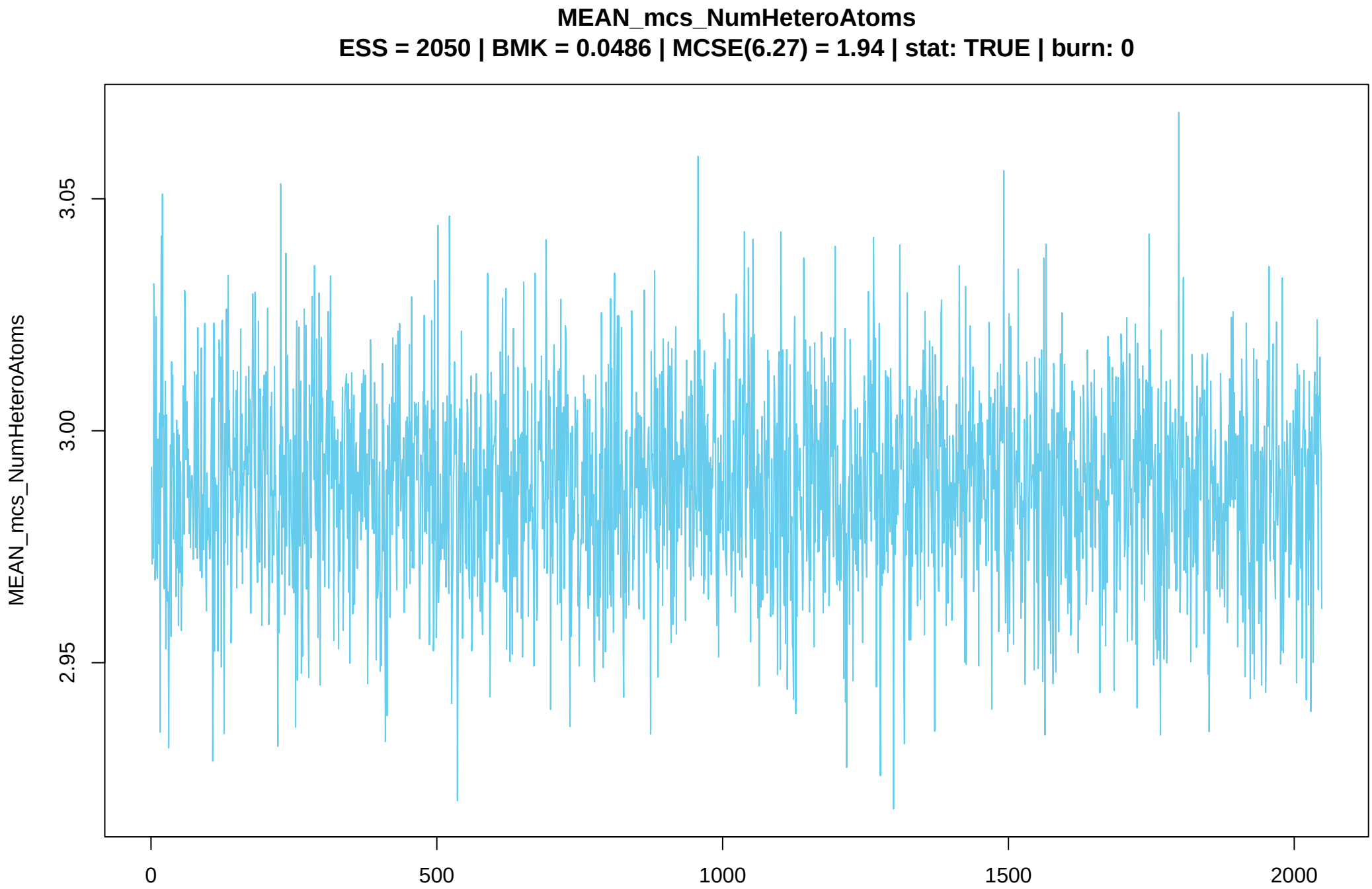

Q3_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NOCount
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

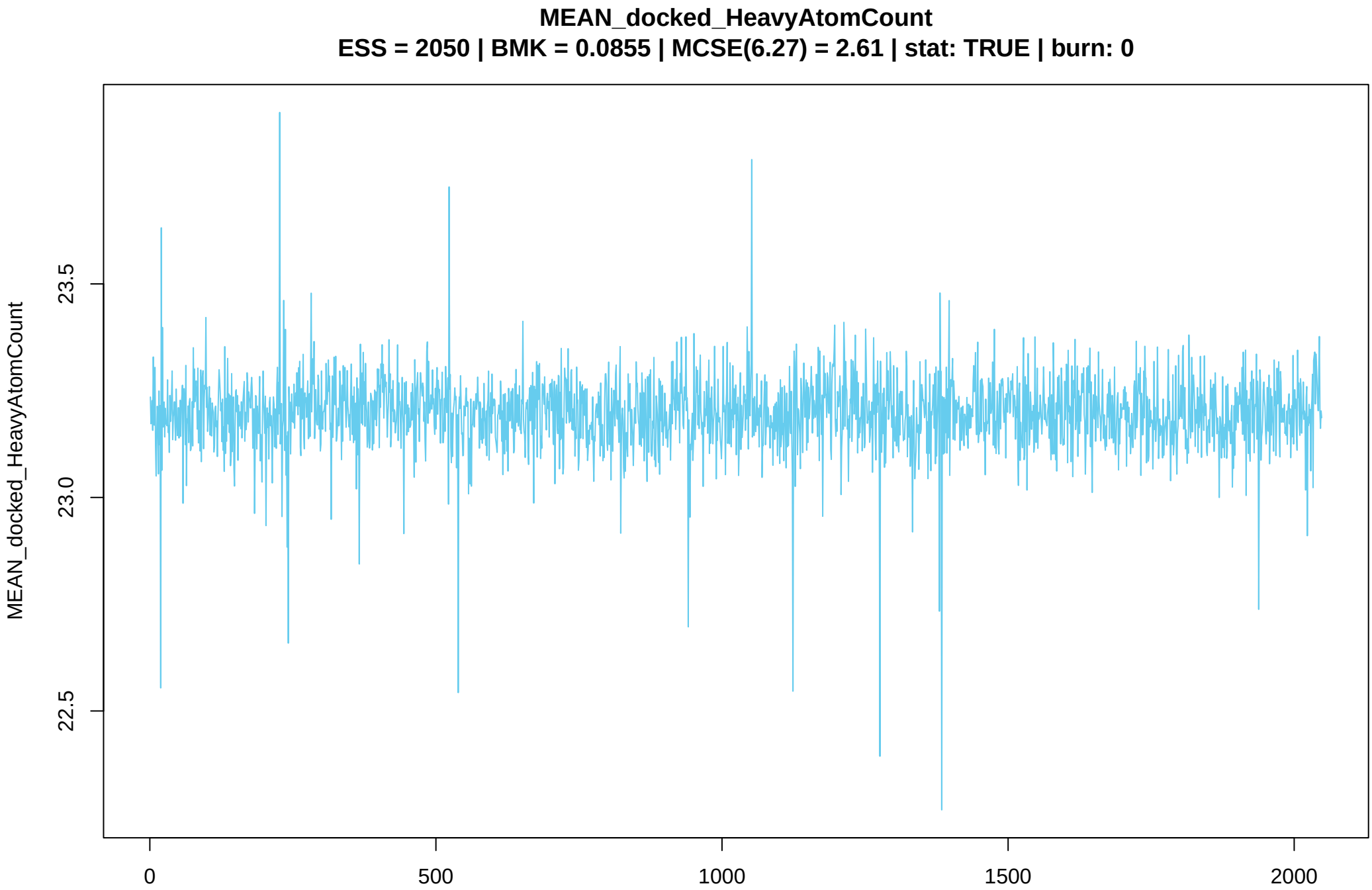

Dcov
ESS = 3.22 | BMK = 0.762 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 1020
Dcov
0
−1
−2
−3
−4
−5
−6
0
500
1000
1500
2000

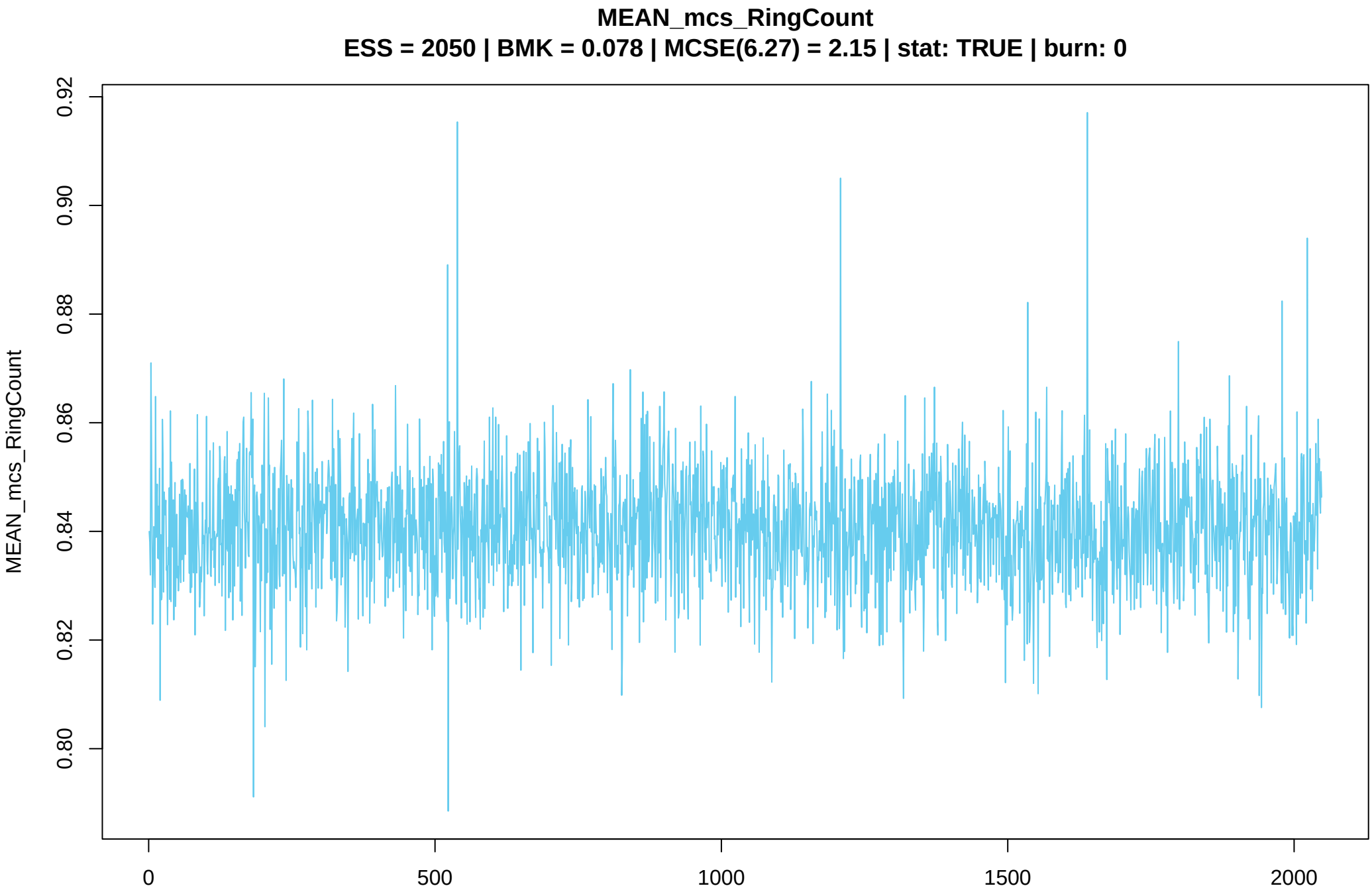

MEAN_log_RMSD
ESS = 1900 | BMK = 0.0725 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.25
1.20
1.15
0
500
1000
1500
2000

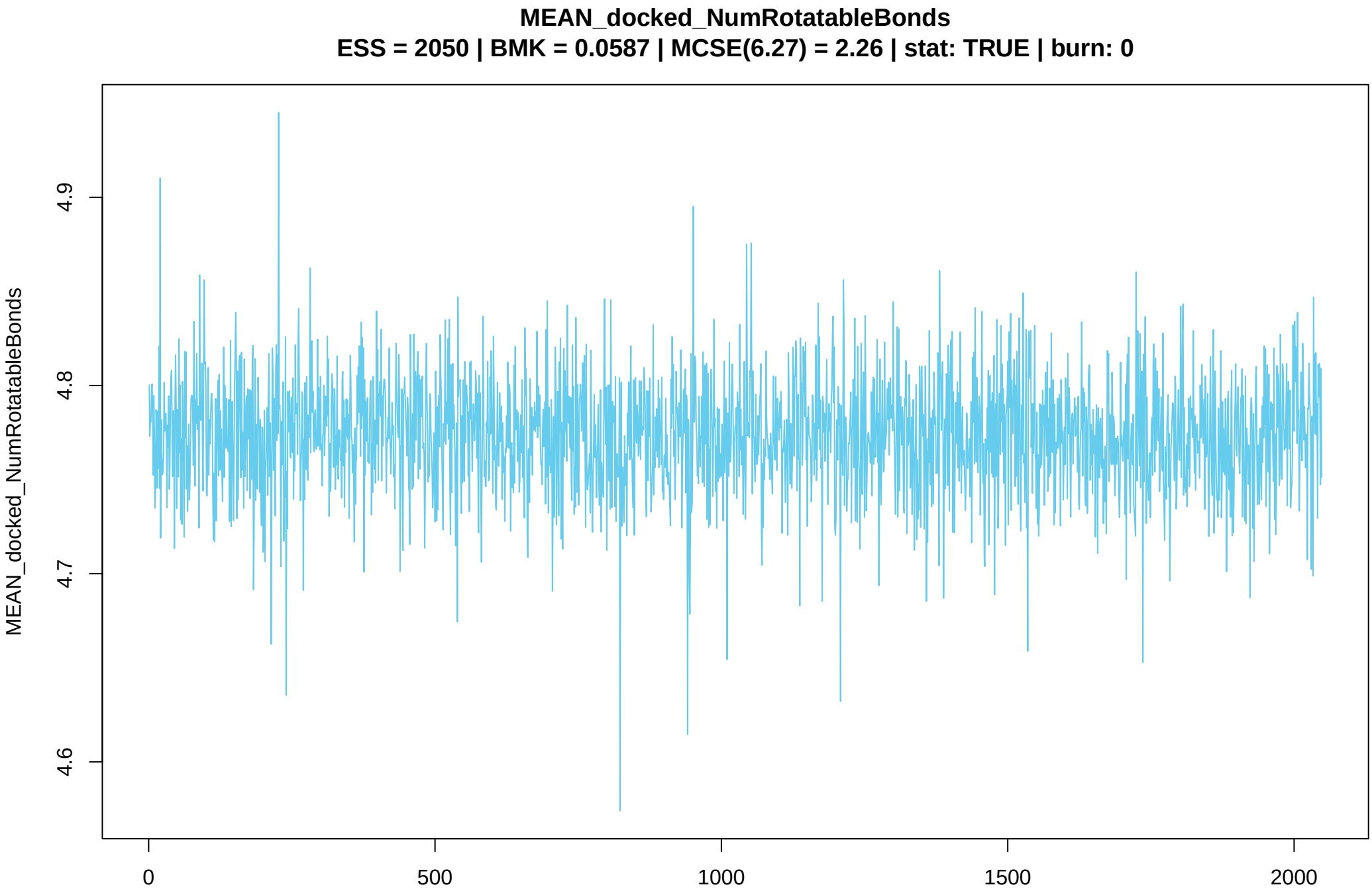

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0938 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0
MEAN_log_mcs_unbonded_polar_sasa
0.0
−0.1
−0.2
−0.3
−0.4
0
500
1000
1500
2000

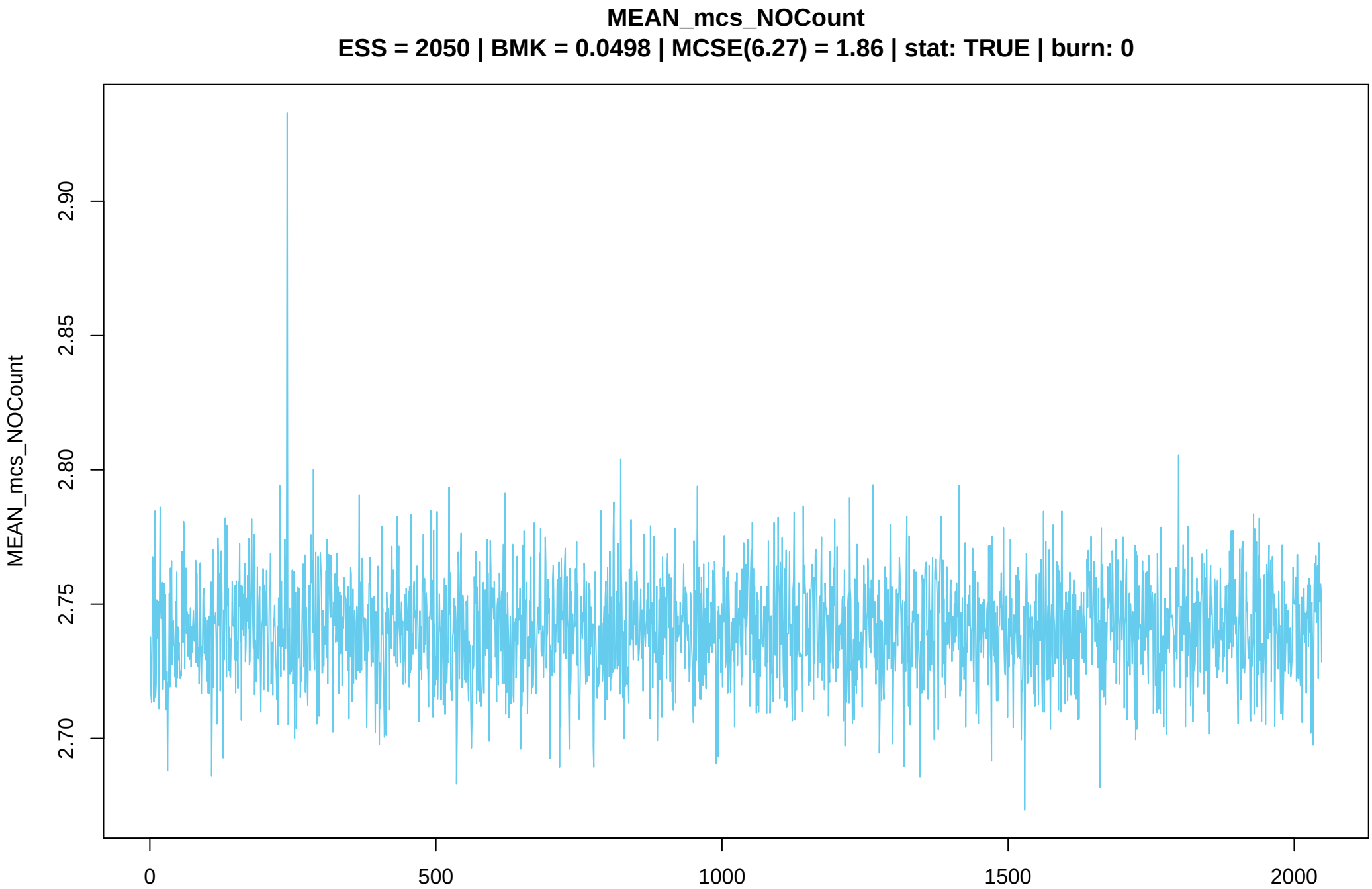

MEAN_logit_ec_tanimoto_similarity
ESS = 1610 | BMK = 0.103 | MCSE(6.27) = 2.95 | stat: FALSE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−1.85
−1.90
−1.95
−2.00
−2.05
−2.10
0
500
1000
1500
2000

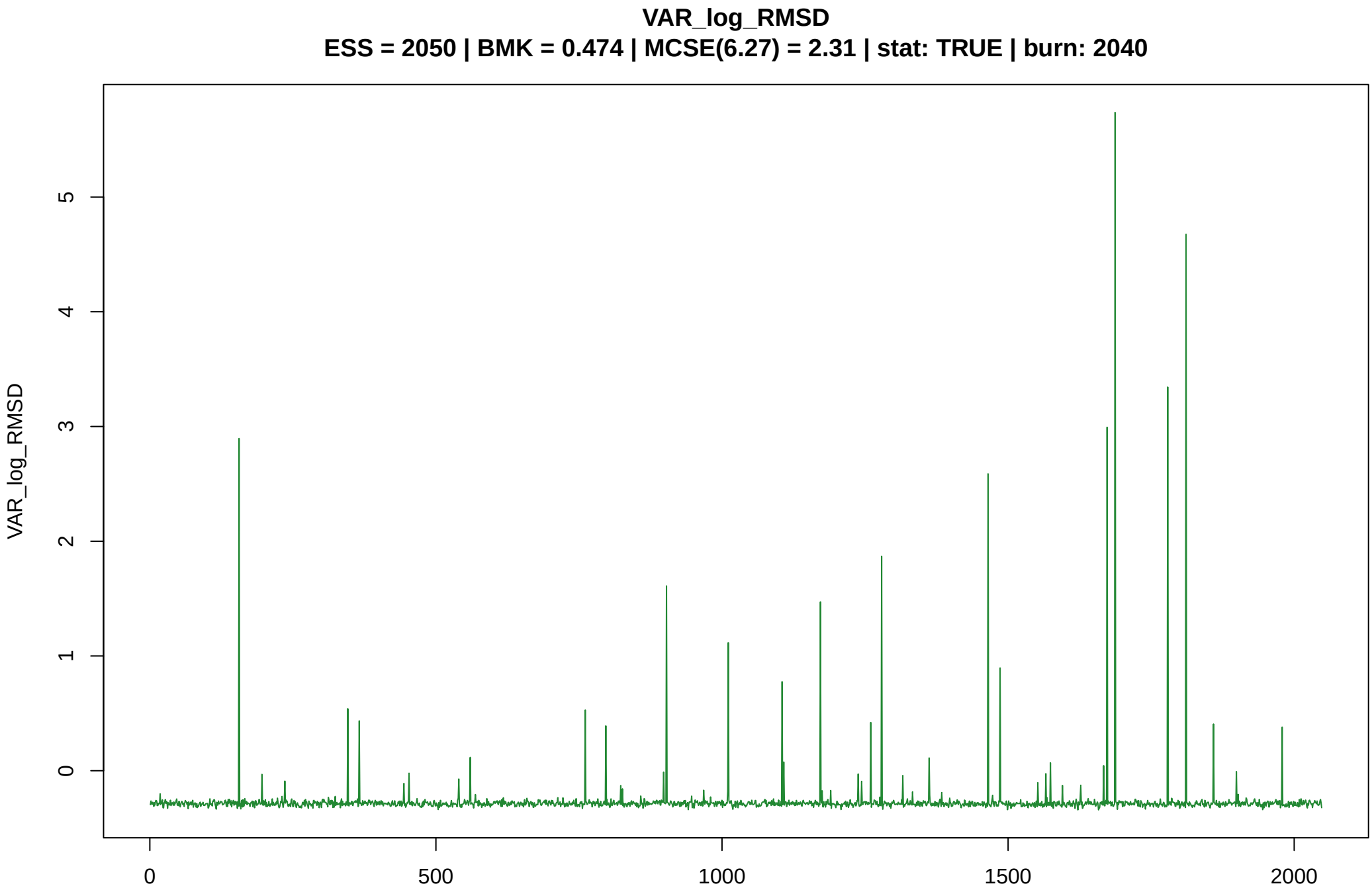

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0486 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.05
3.00
2.95
0
500
1000
1500
2000

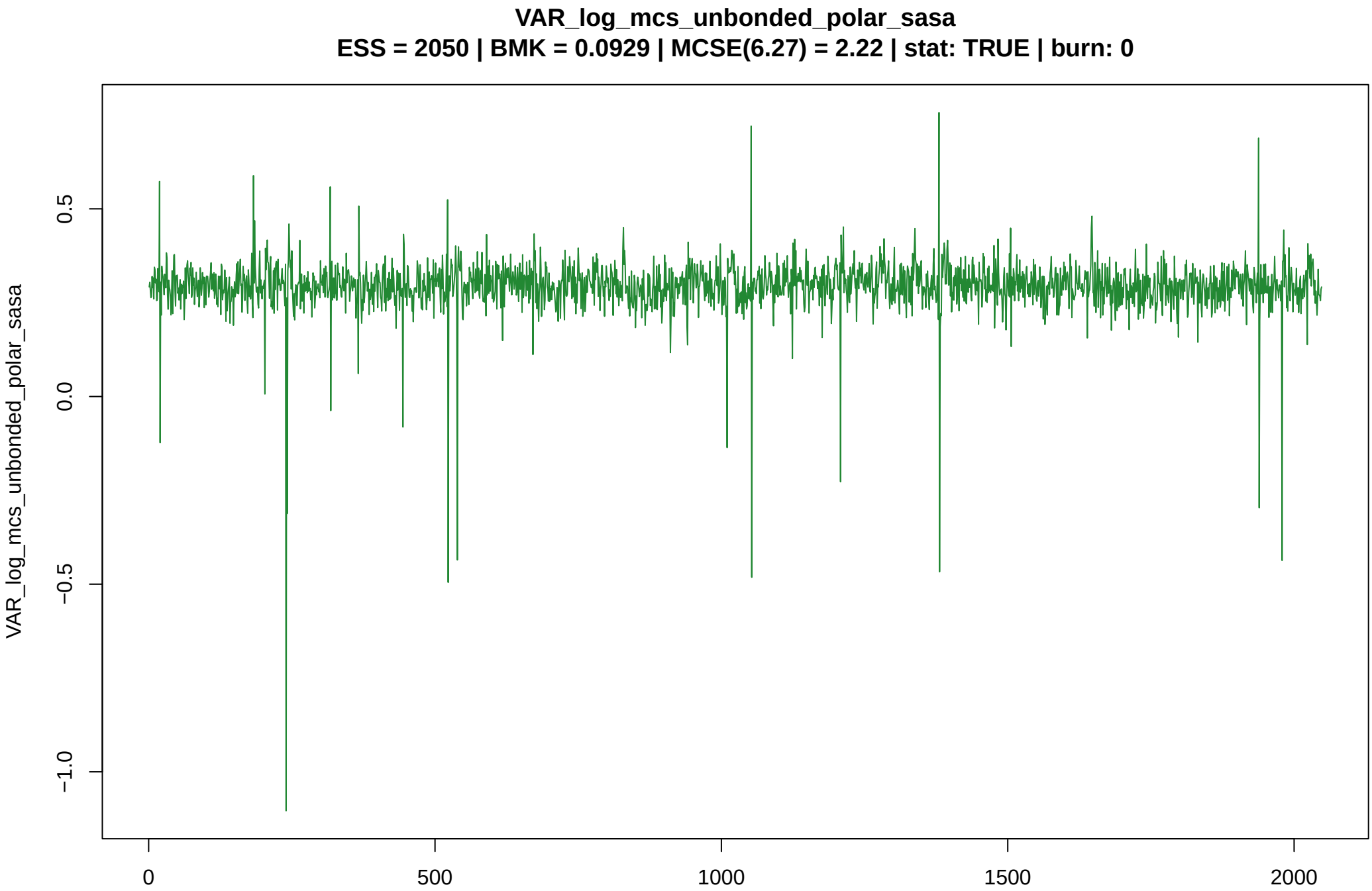

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0855 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
22.5
23.0
23.5
0
500
1000
1500
2000

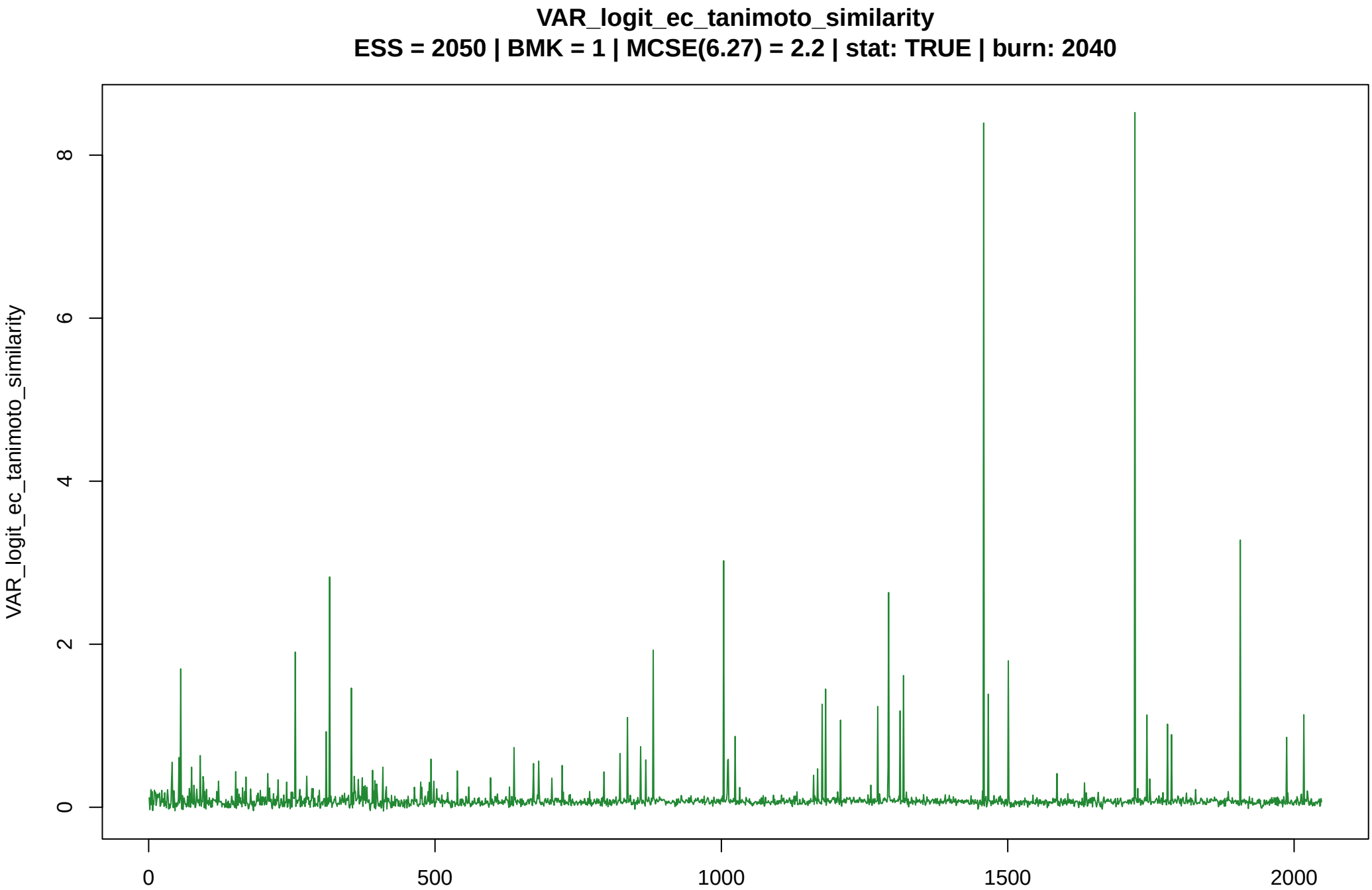

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.078 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.80
0.82
0.84
0.86
0.88
0.90
0.92
0
500
1000
1500
2000

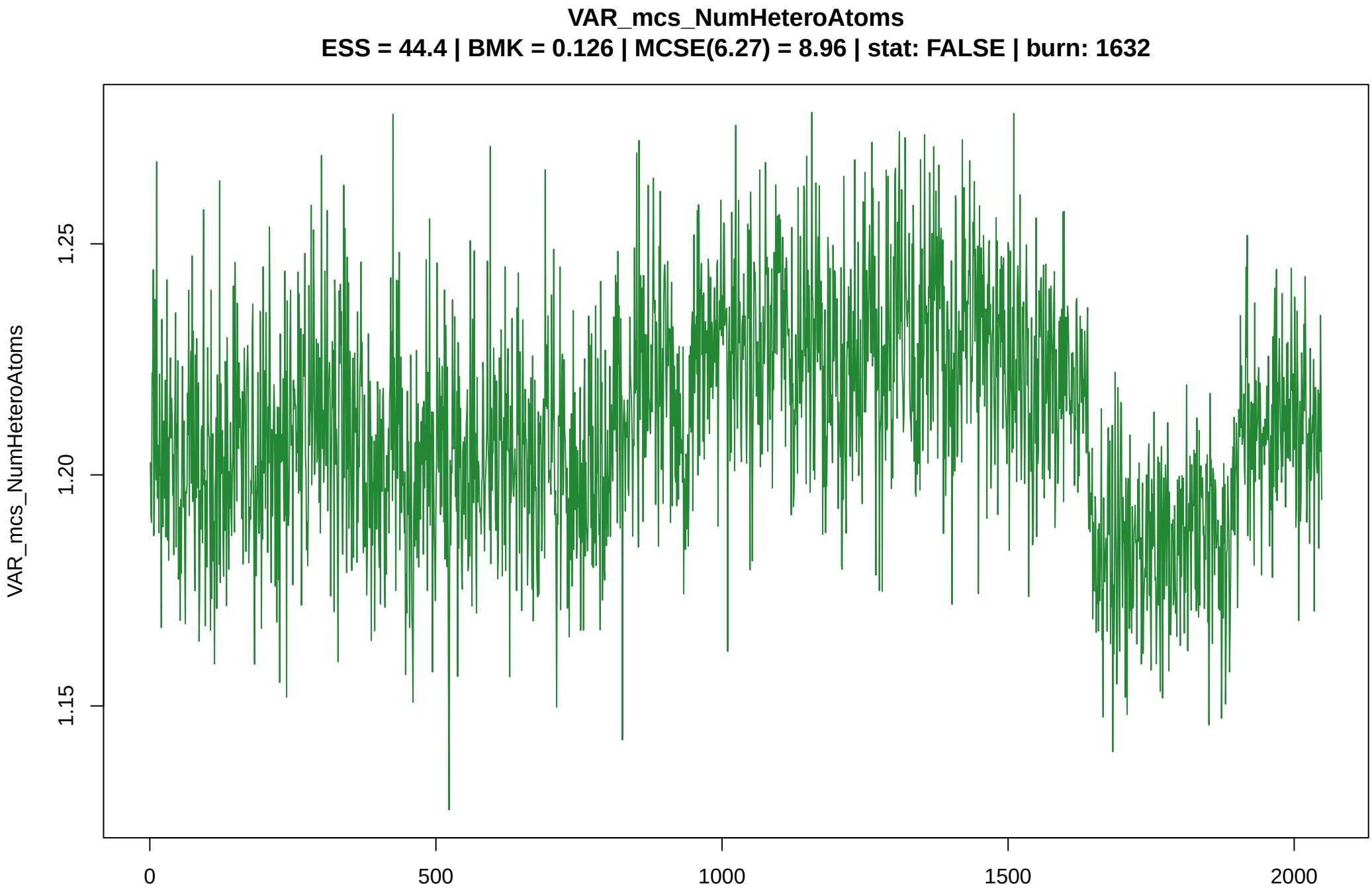

MEAN_docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0587 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
4.6
4.7
4.8
4.9
0
500
1000
1500
2000

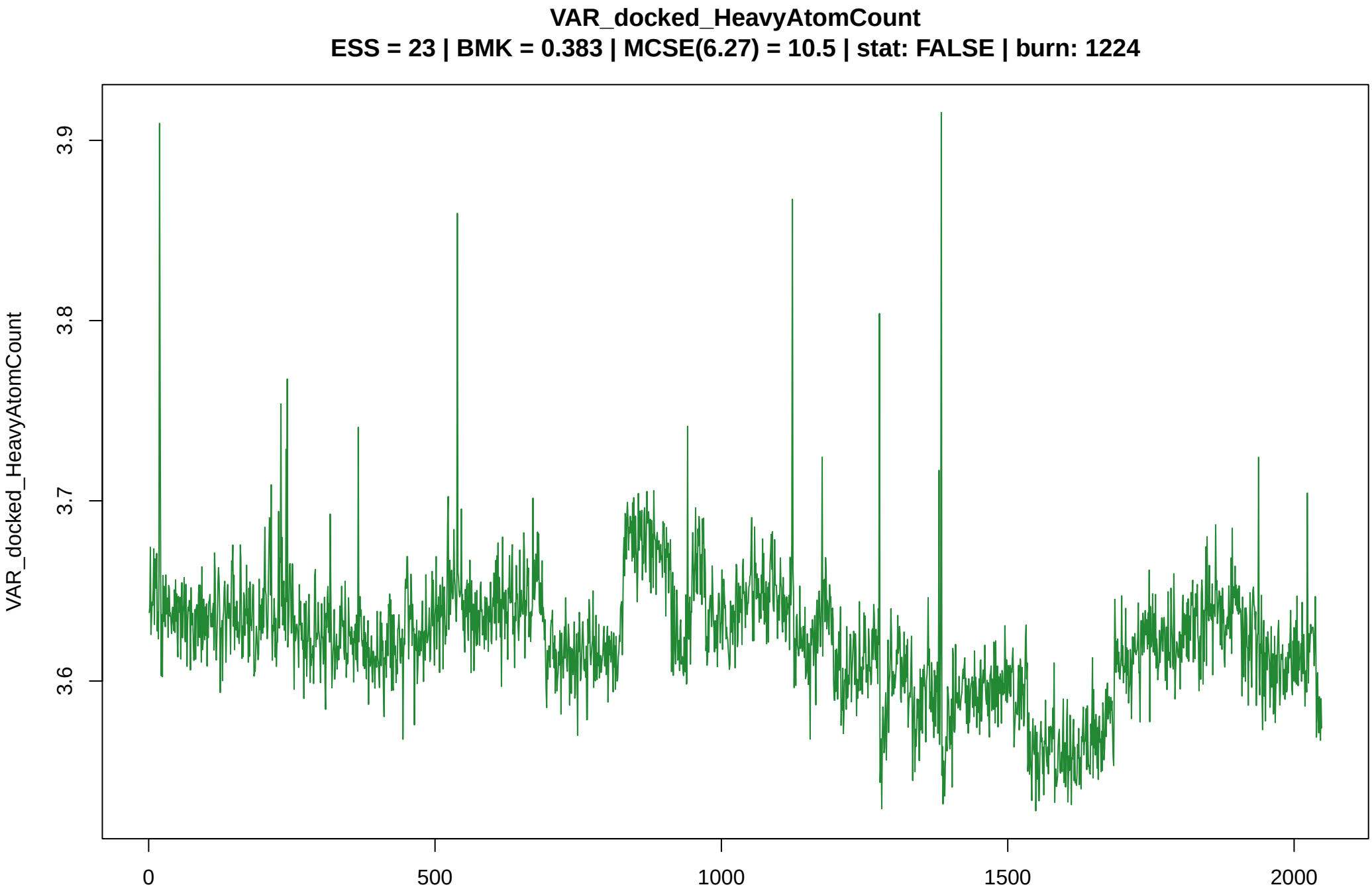

MEAN_mcs_NOCount
ESS = 2050 | BMK = 0.0498 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0
MEAN_mcs_NOCount
2.70
2.75
2.80
2.85
2.90
0
500
1000
1500
2000

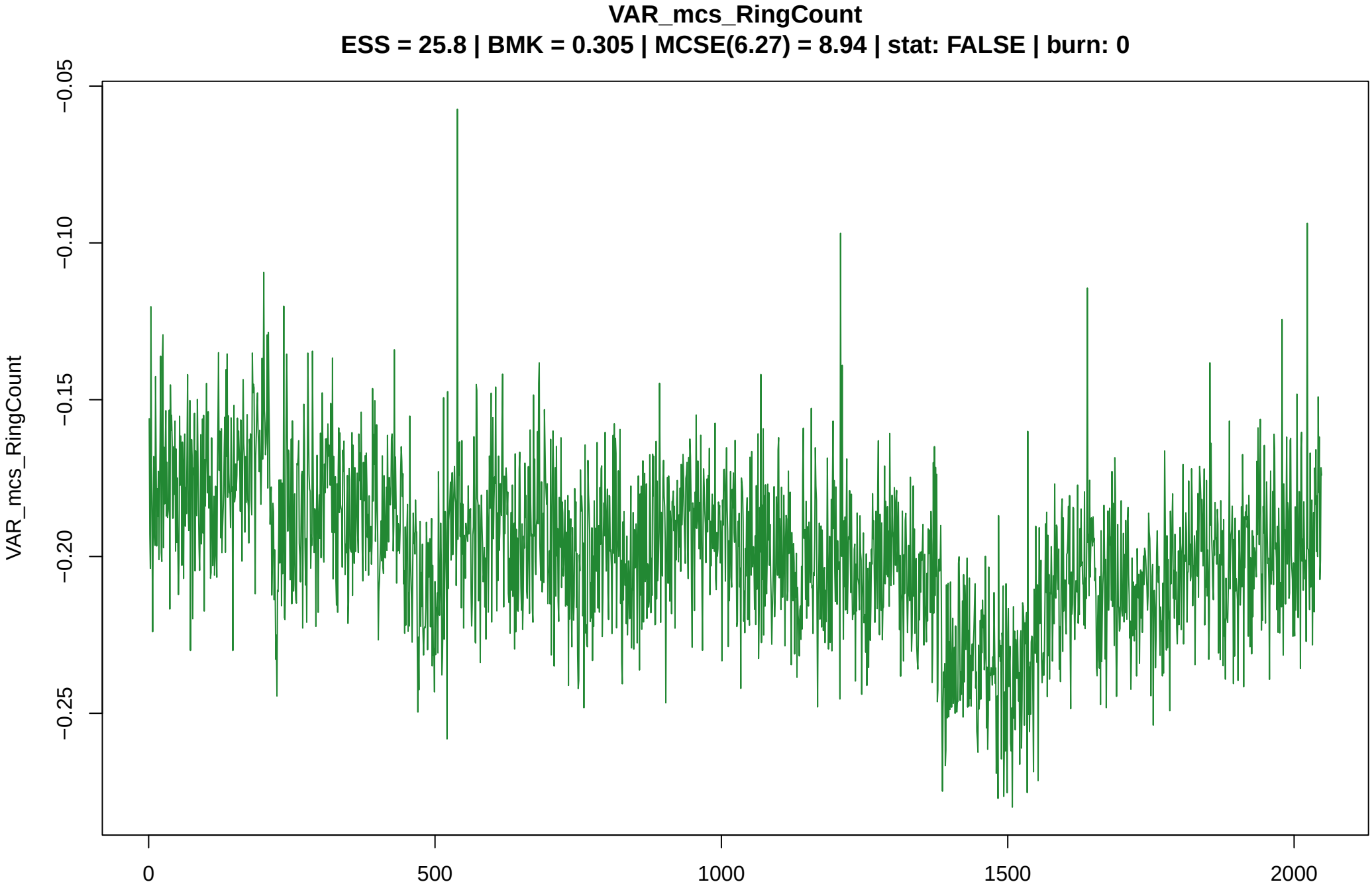

VAR_log_RMSD
ESS = 2050 | BMK = 0.474 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 2040
VAR_log_RMSD
0
1
2
3
4
5
0
500
1000
1500
2000

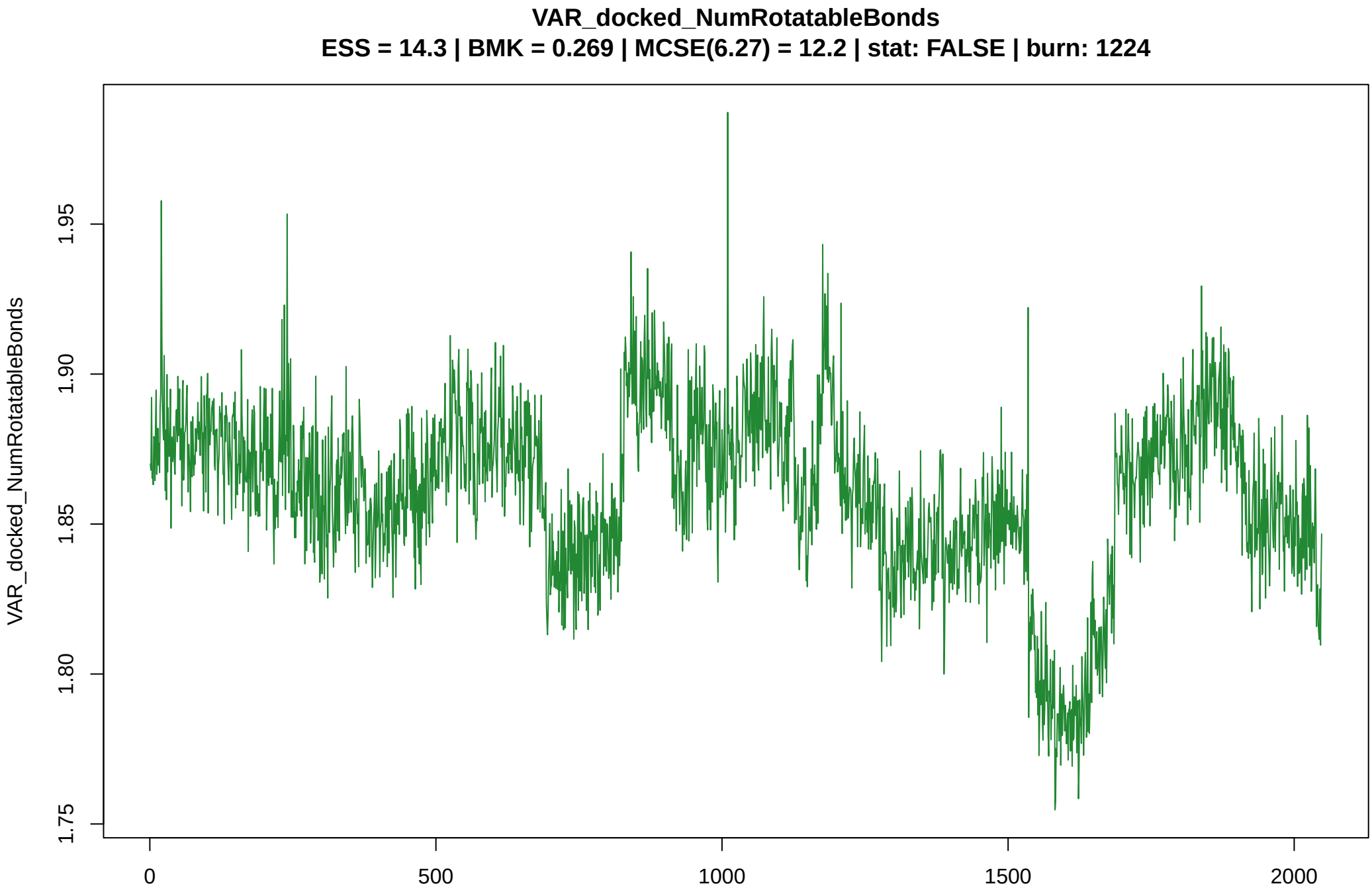

VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0929 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
VAR_log_mcs_unbonded_polar_sasa
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

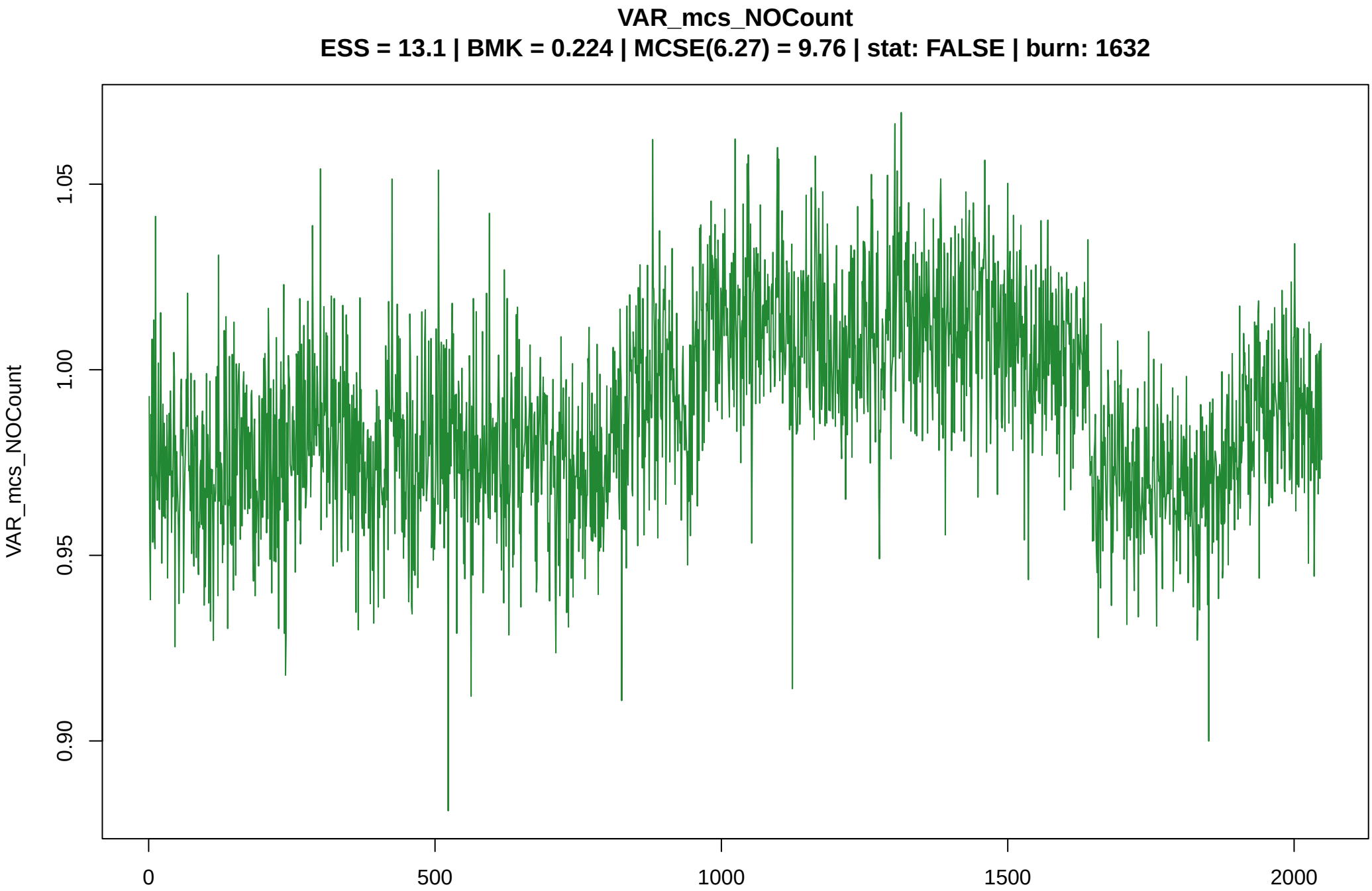

VAR_logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 1 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 2040
VAR_logit_ec_tanimoto_similarity
0
2
4
6
8
0
500
1000
1500
2000

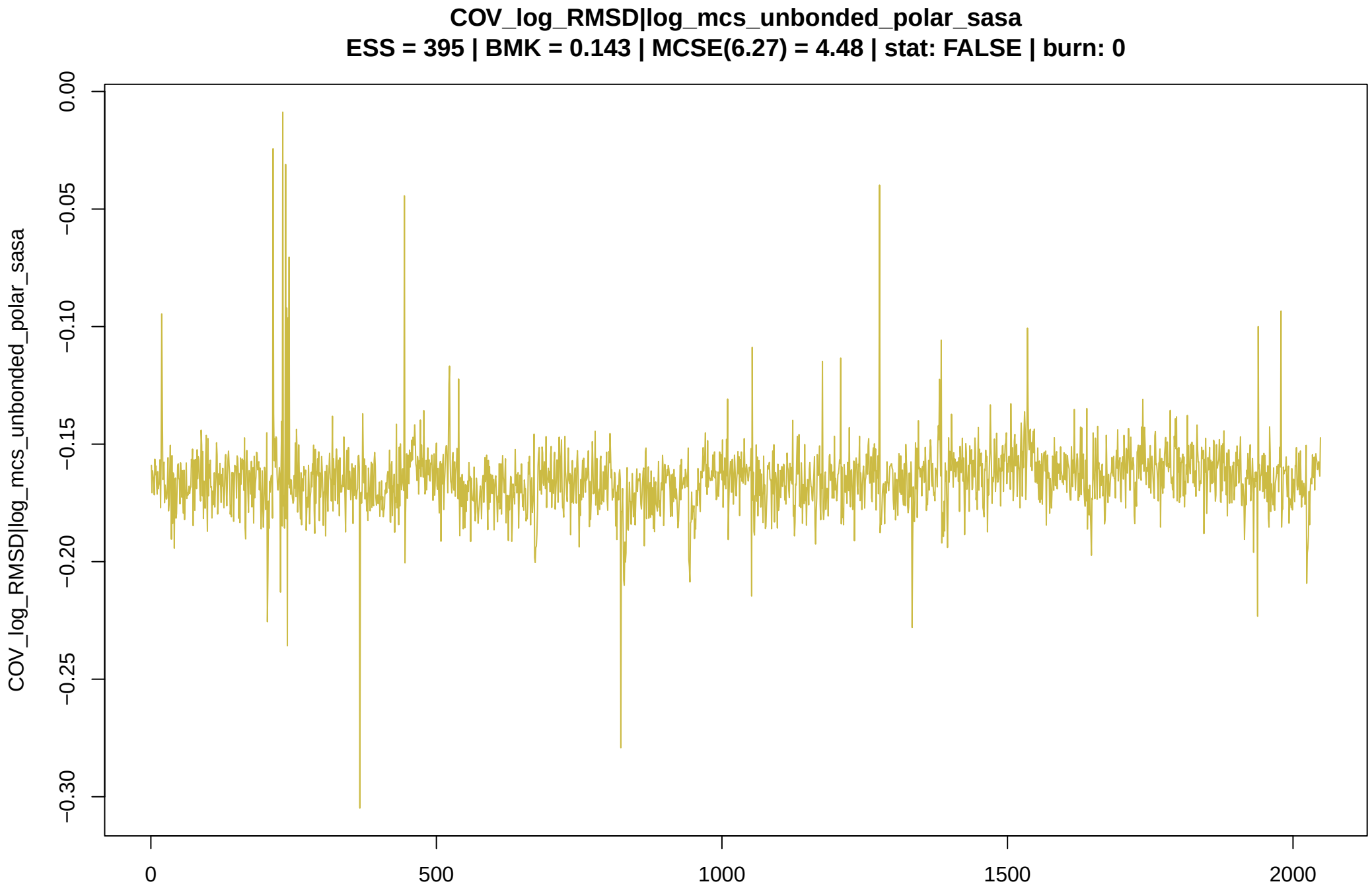

VAR_mcs_NumHeteroAtoms
ESS = 44.4 | BMK = 0.126 | MCSE(6.27) = 8.96 | stat: FALSE | burn: 1632
VAR_mcs_NumHeteroAtoms
1.15
1.20
1.25
0
500
1000
1500
2000

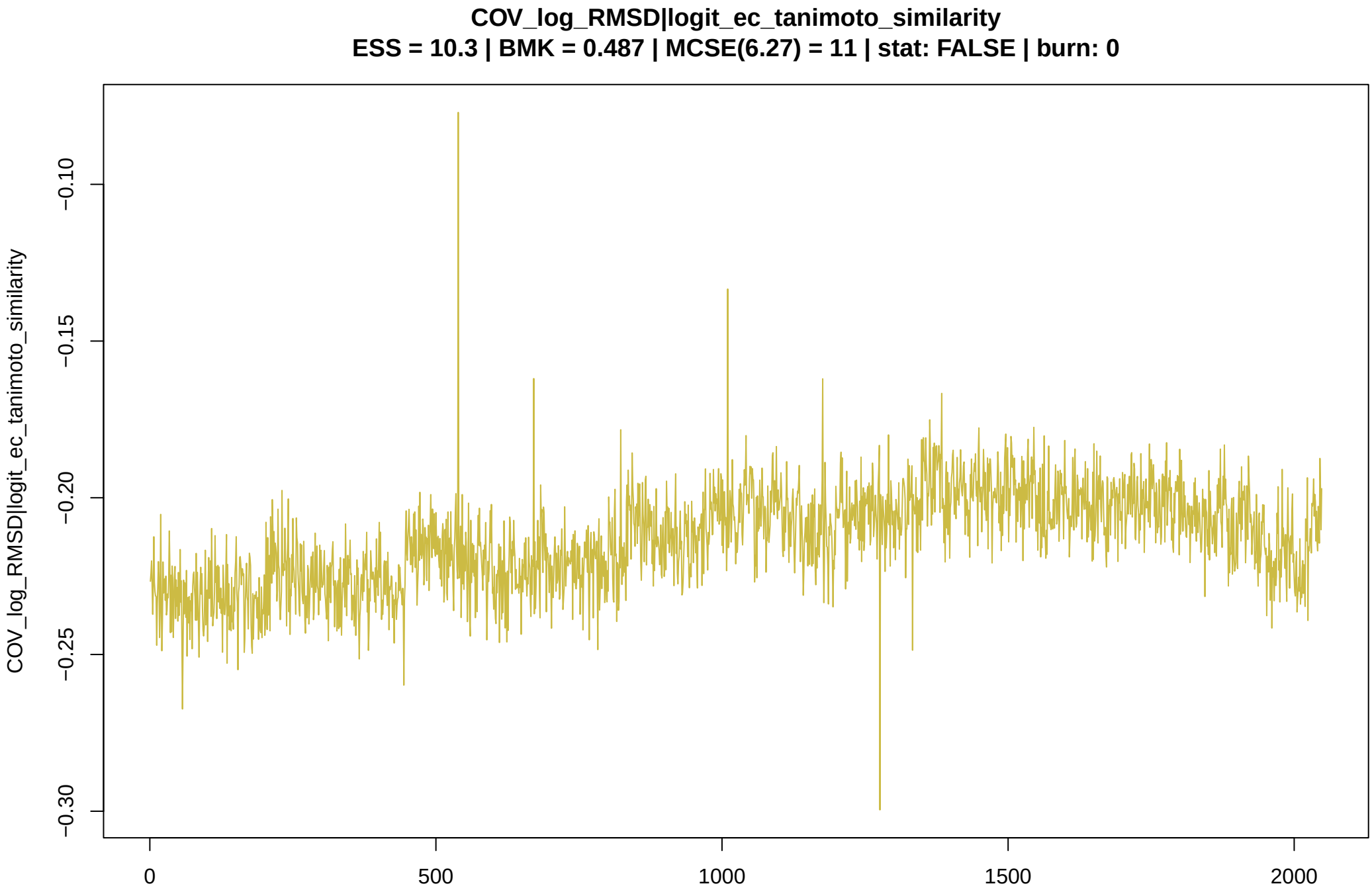

VAR_docked_HeavyAtomCount
ESS = 23 | BMK = 0.383 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 1224
VAR_docked_HeavyAtomCount
3.6
3.7
3.8
3.9
0
500
1000
1500
2000

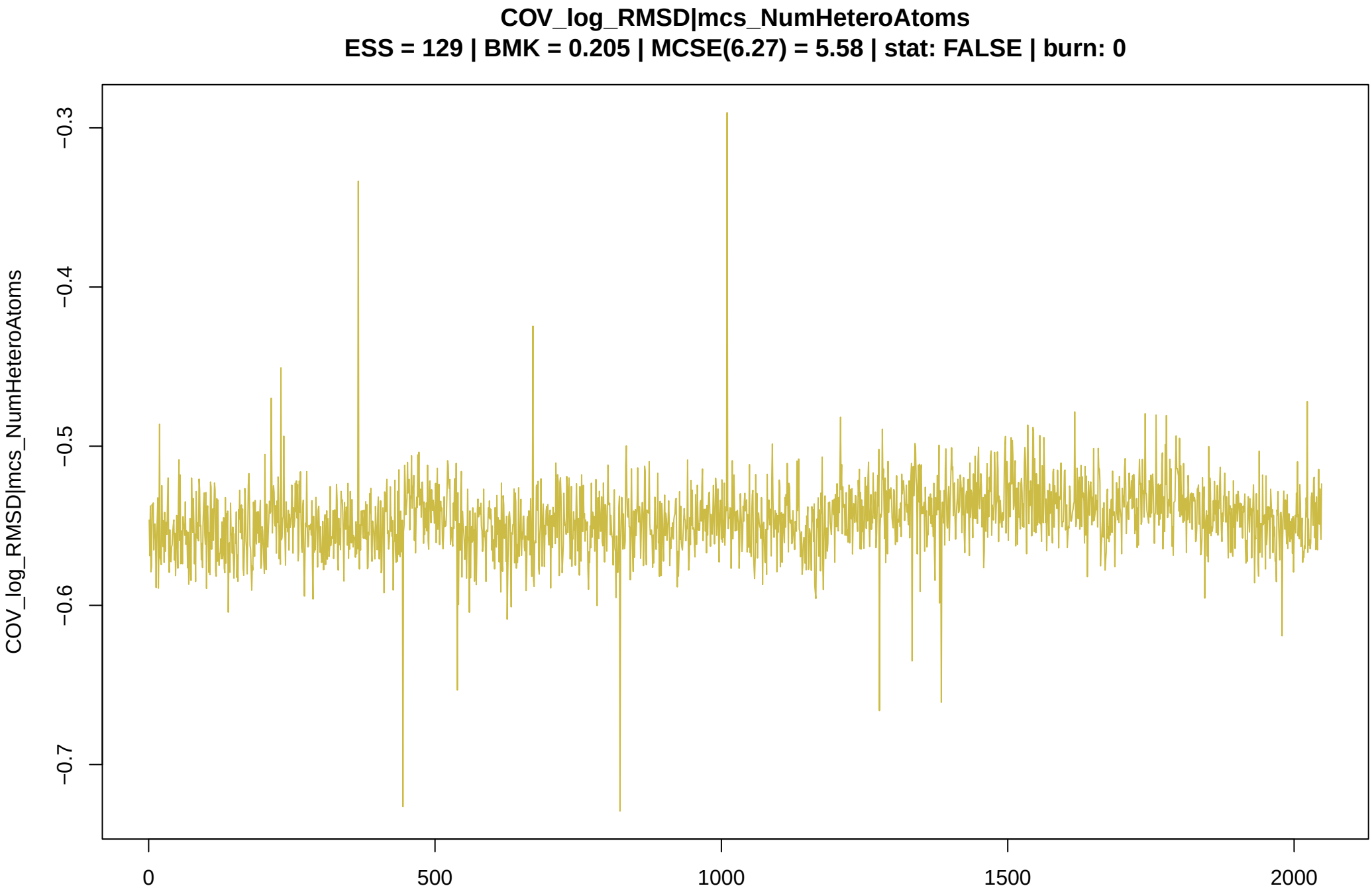

VAR_mcs_RingCount
ESS = 25.8 | BMK = 0.305 | MCSE(6.27) = 8.94 | stat: FALSE | burn: 0
VAR_mcs_RingCount
−0.05
−0.10
−0.15
−0.20
−0.25
0
500
1000
1500
2000

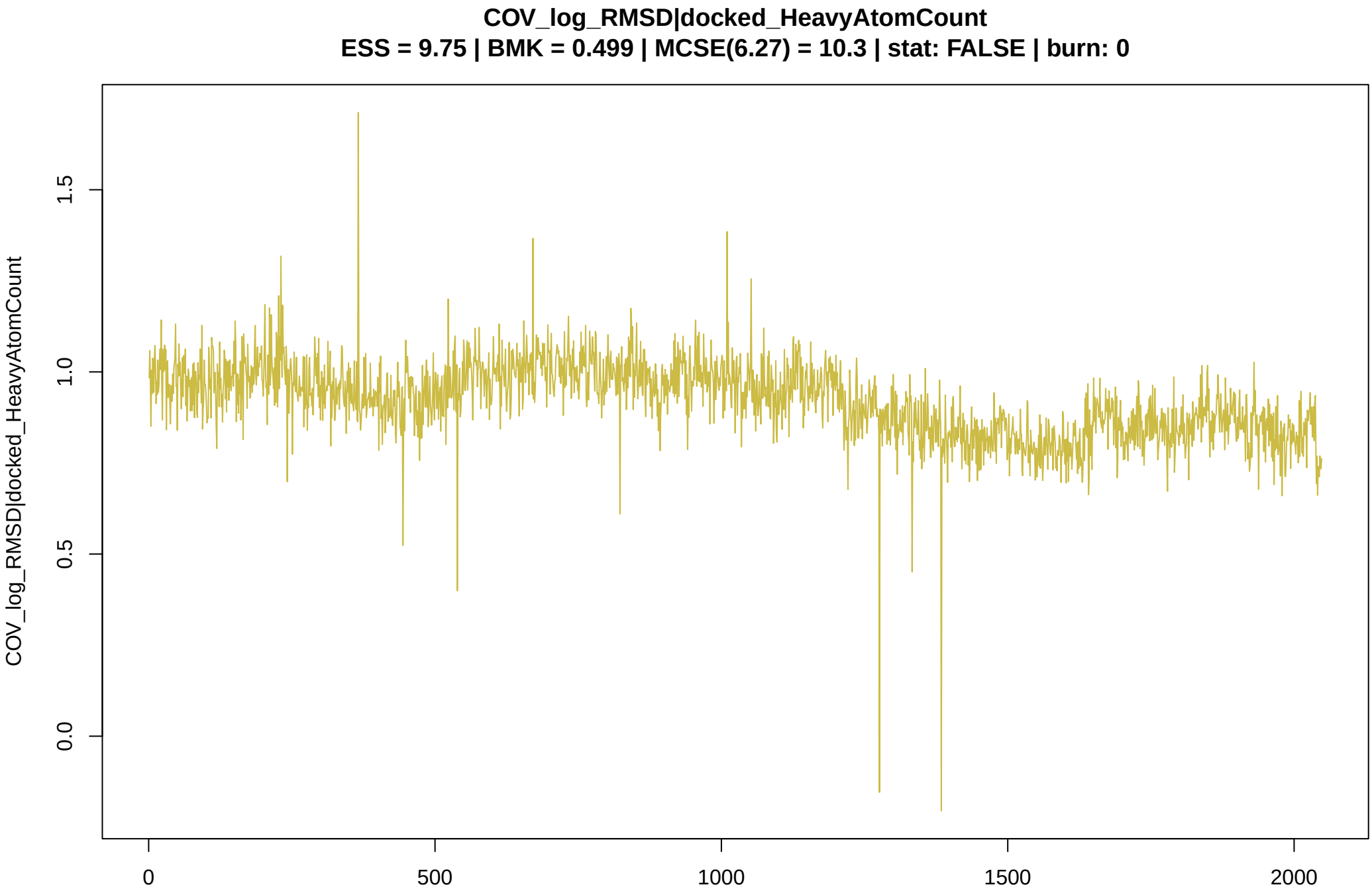

VAR_docked_NumRotatableBonds
ESS = 14.3 | BMK = 0.269 | MCSE(6.27) = 12.2 | stat: FALSE | burn: 1224
VAR_docked_NumRotatableBonds
1.75
1.80
1.85
1.90
1.95
0
500
1000
1500
2000

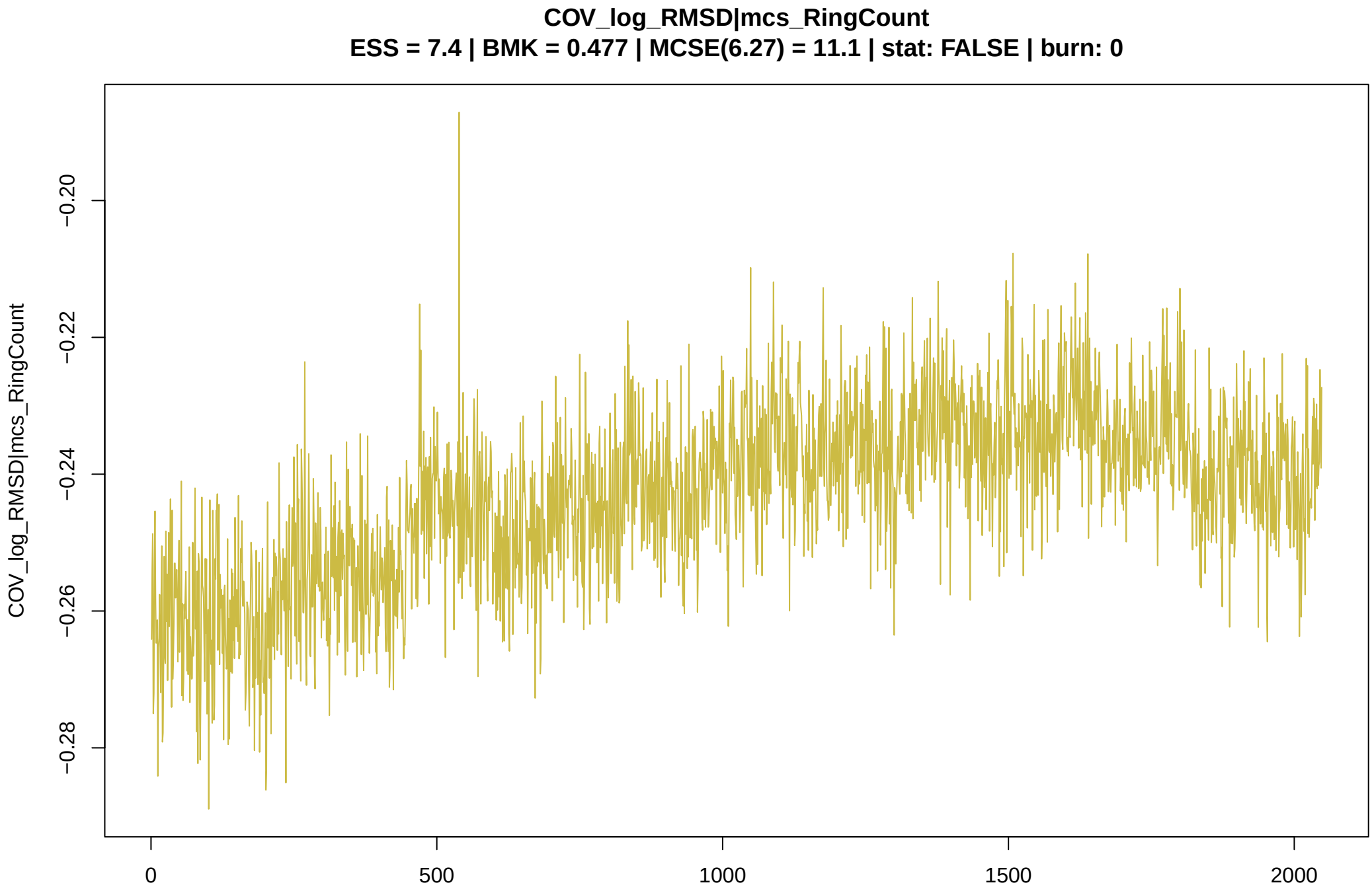

VAR_mcs_NOCount
ESS = 13.1 | BMK = 0.224 | MCSE(6.27) = 9.76 | stat: FALSE | burn: 1632
VAR_mcs_NOCount
0.90
0.95
1.00
1.05
0
500
1000
1500
2000

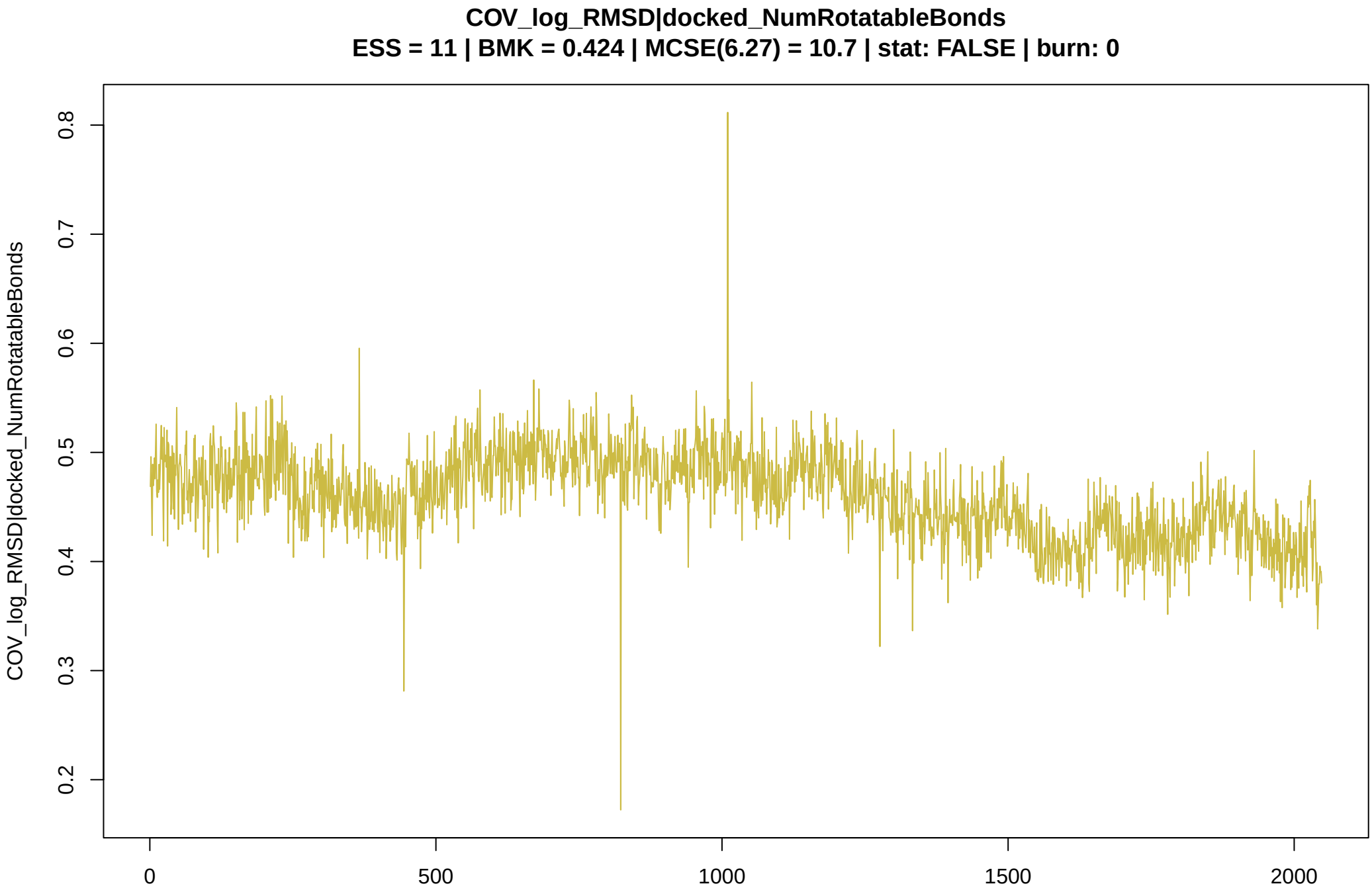

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 395 | BMK = 0.143 | MCSE(6.27) = 4.48 | stat: FALSE | burn: 0
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
−0.30
0
500
1000
1500
2000

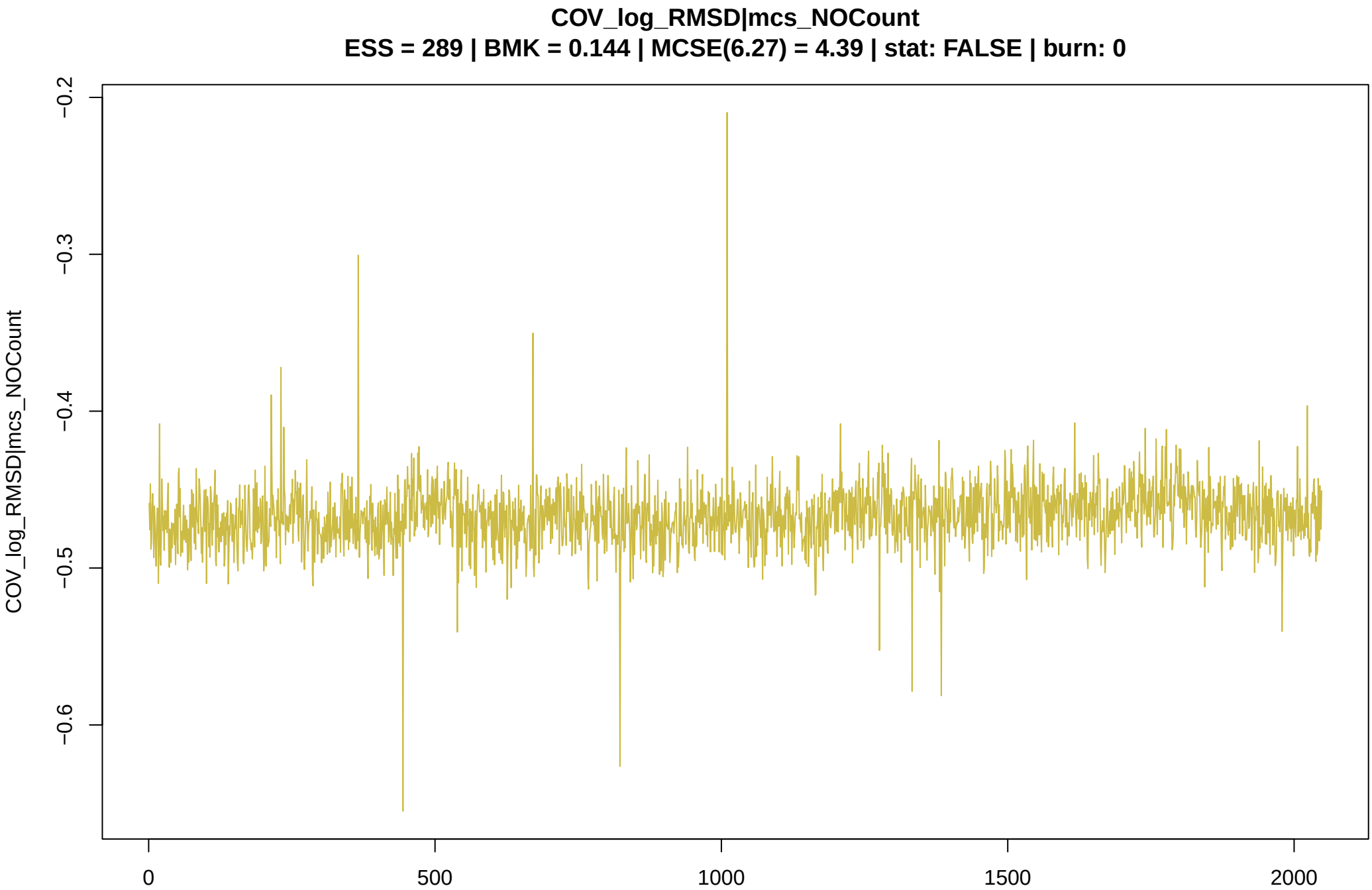

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 10.3 | BMK = 0.487 | MCSE(6.27) = 11 | stat: FALSE | burn: 0
COV_log_RMSD|logit_ec_tanimoto_similarity
−0.10
−0.15
−0.20
−0.25
−0.30
0
500
1000
1500
2000

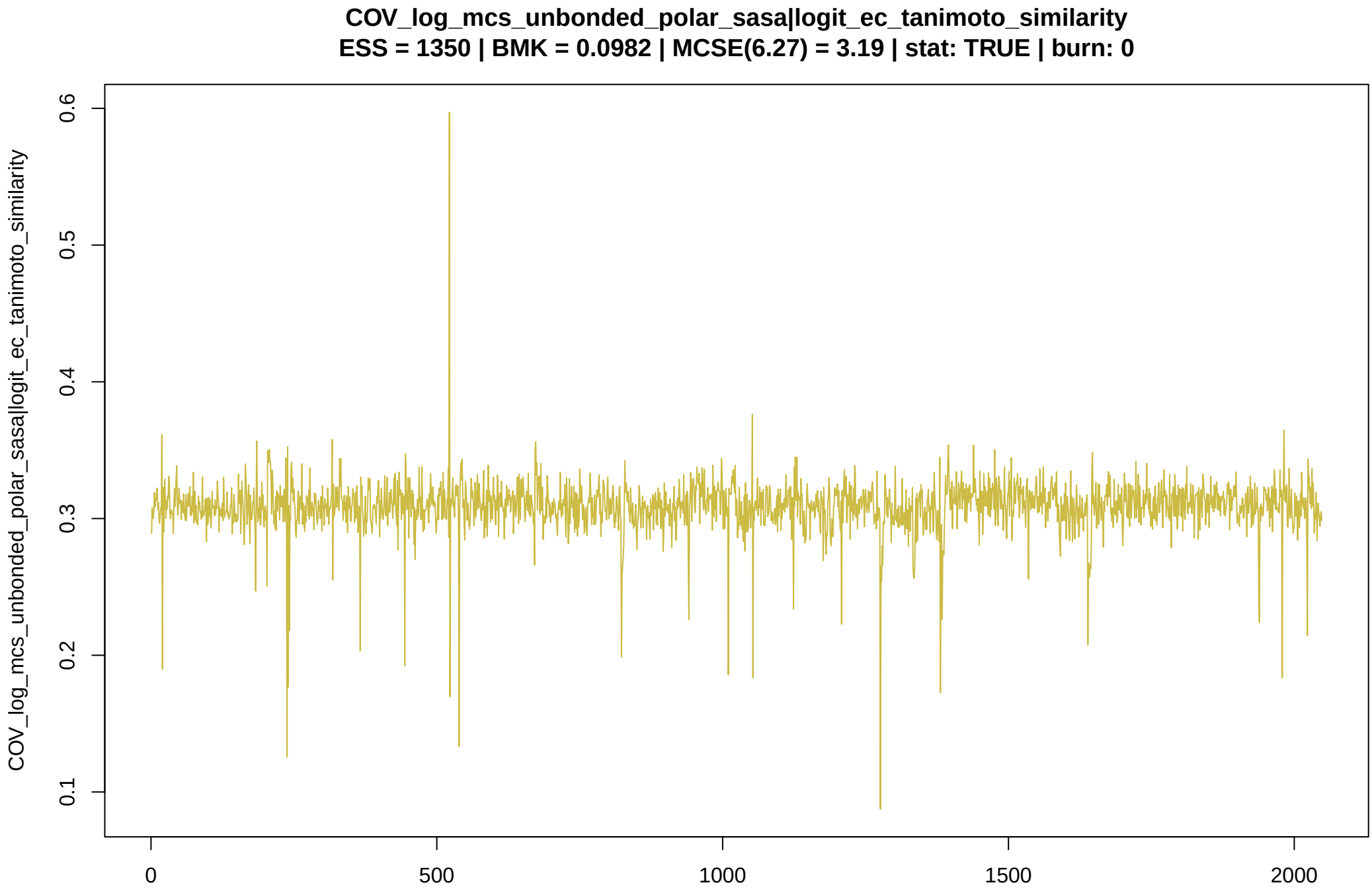

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 129 | BMK = 0.205 | MCSE(6.27) = 5.58 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.3
−0.4
−0.5
−0.6
−0.7
0
500
1000
1500
2000

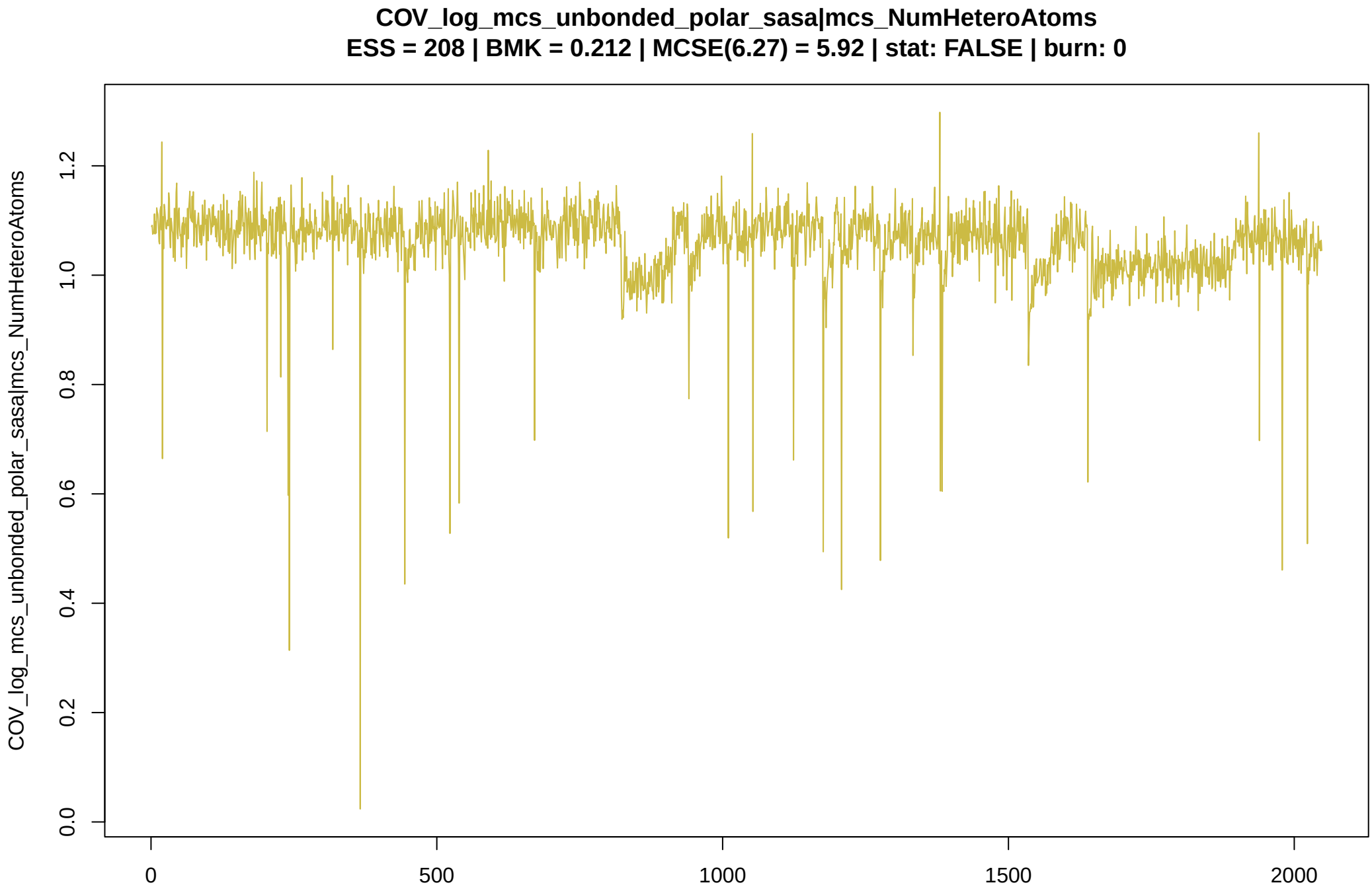

COV_log_RMSD|docked_HeavyAtomCount
ESS = 9.75 | BMK = 0.499 | MCSE(6.27) = 10.3 | stat: FALSE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
0.0
0.5
1.0
1.5
0
500
1000
1500
2000

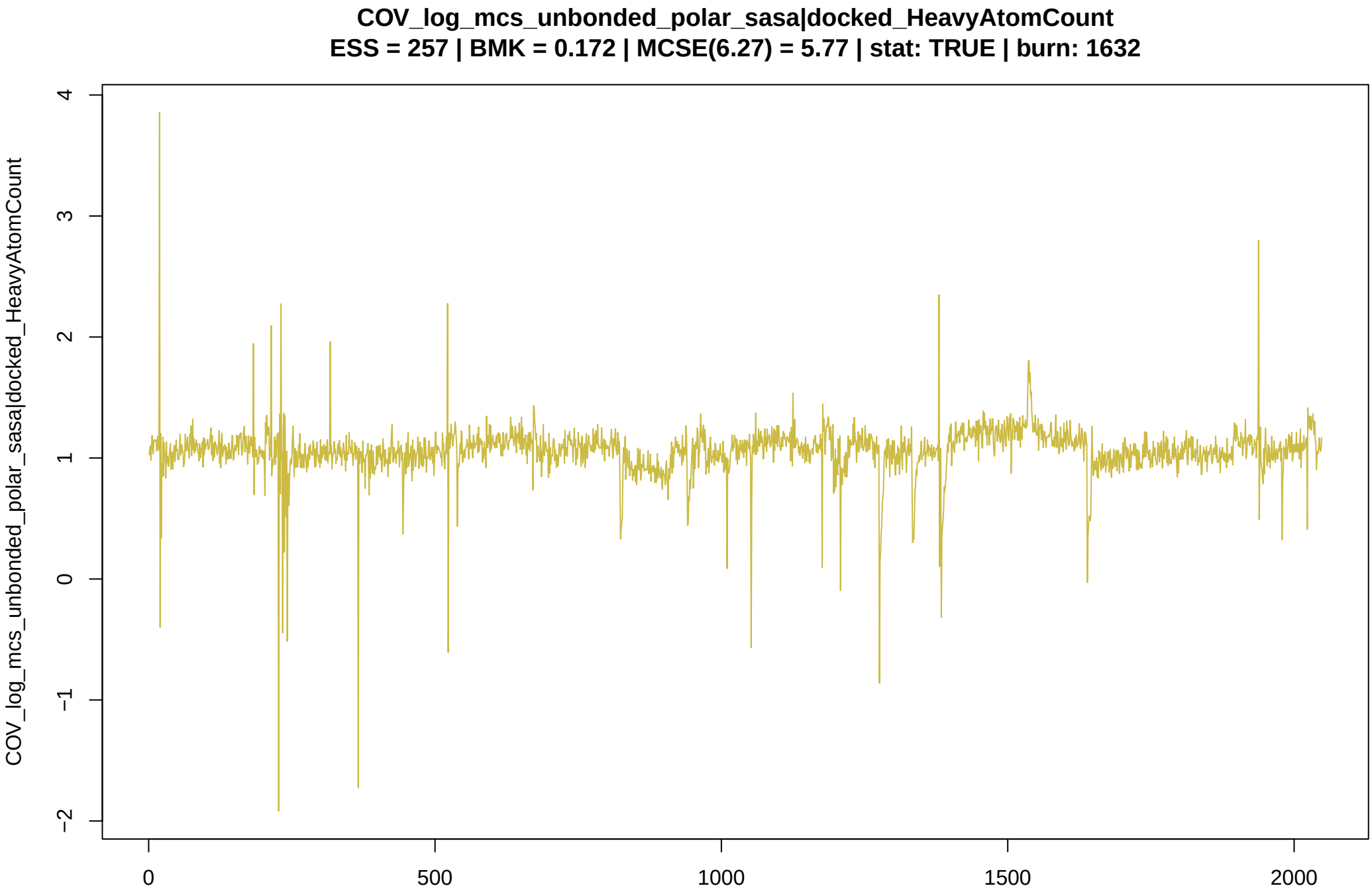

COV_log_RMSD|mcs_RingCount
ESS = 7.4 | BMK = 0.477 | MCSE(6.27) = 11.1 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.20
−0.22
−0.24
−0.26
−0.28
0
500
1000
1500
2000

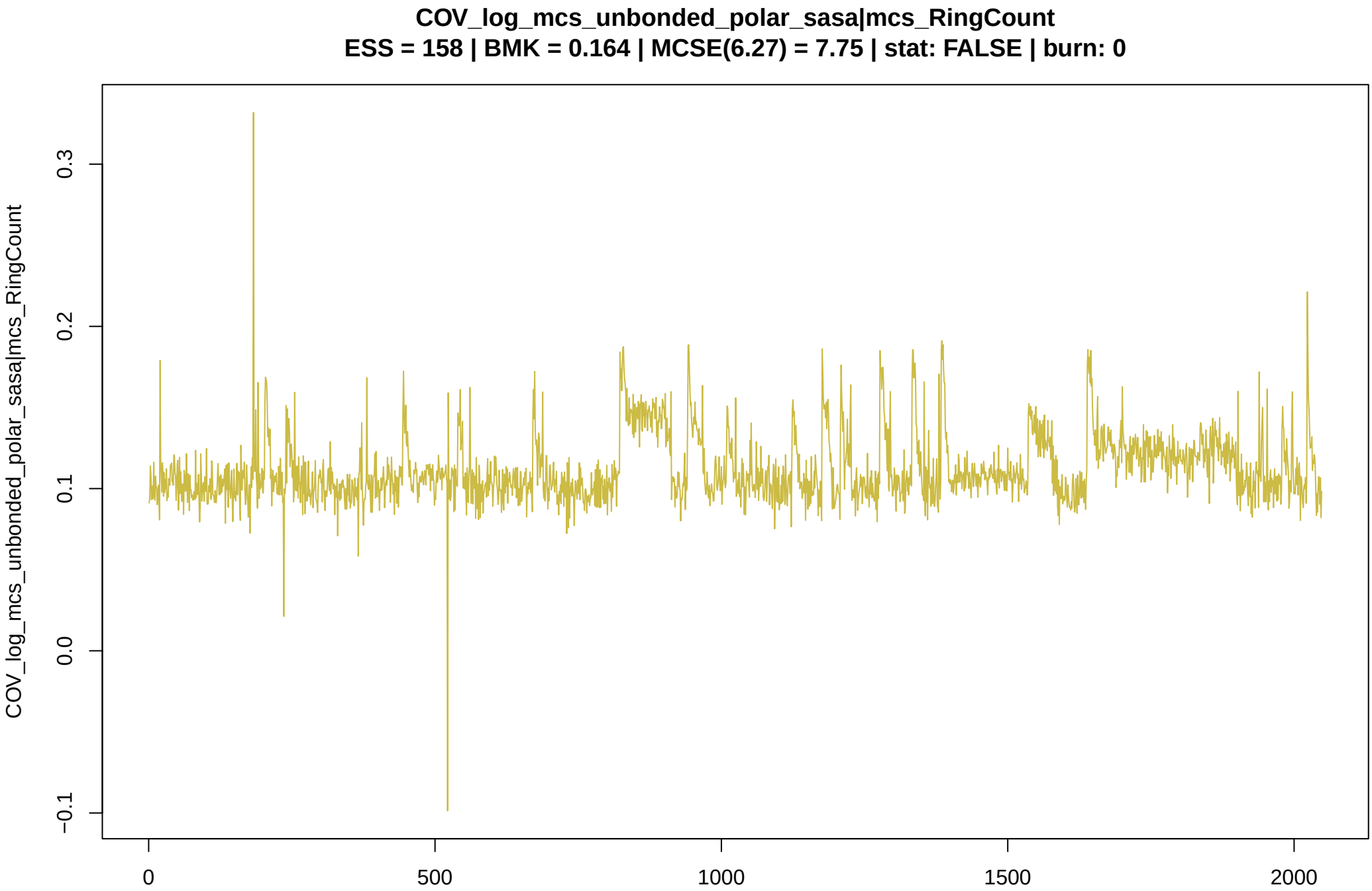

COV_log_RMSD|docked_NumRotatableBonds
ESS = 11 | BMK = 0.424 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 0
COV_log_RMSD|docked_NumRotatableBonds
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
500
1000
1500
2000

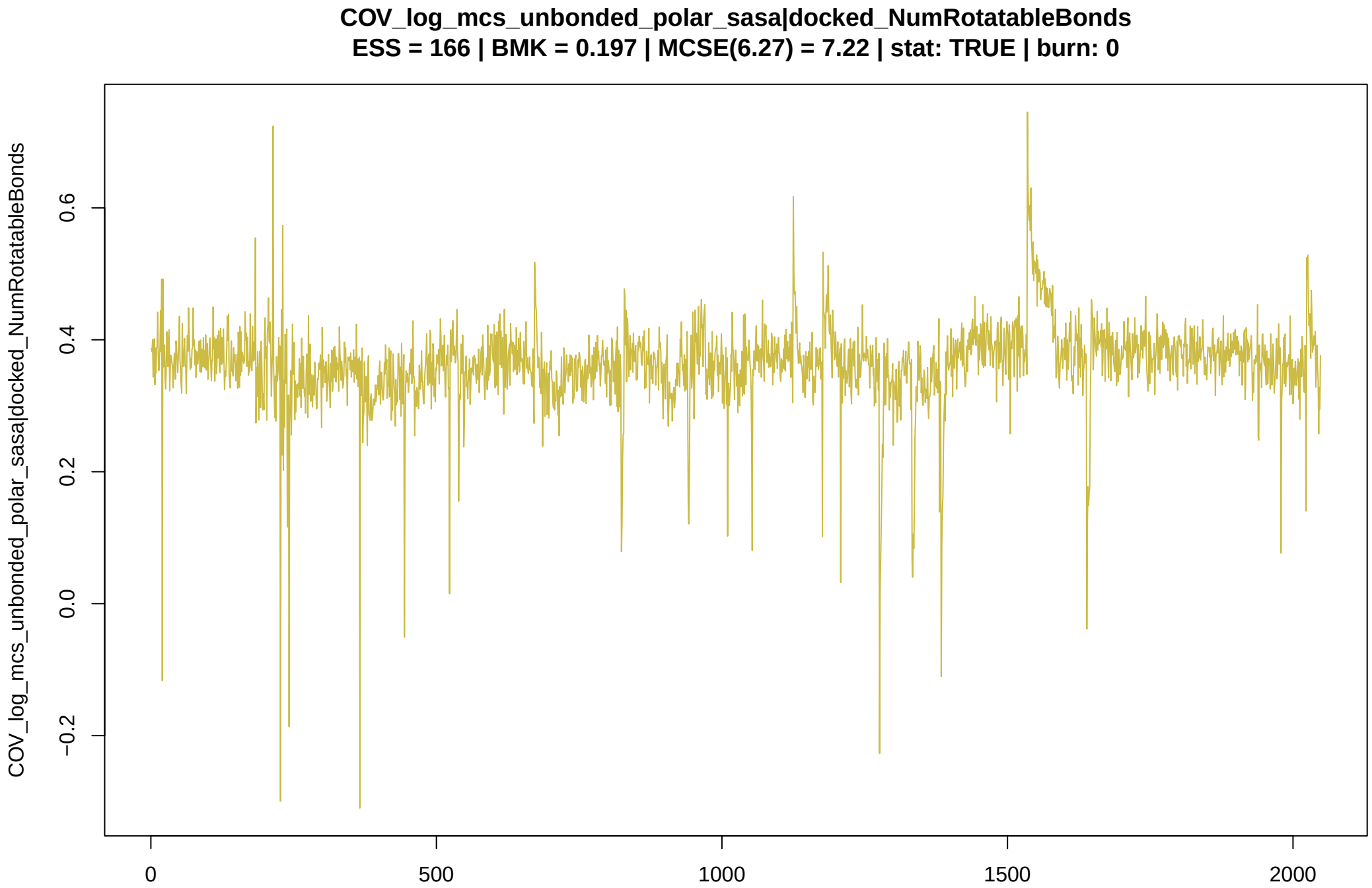

COV_log_RMSD|mcs_NOCount
ESS = 289 | BMK = 0.144 | MCSE(6.27) = 4.39 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_NOCount
−0.2
−0.3
−0.4
−0.5
−0.6
0
500
1000
1500
2000

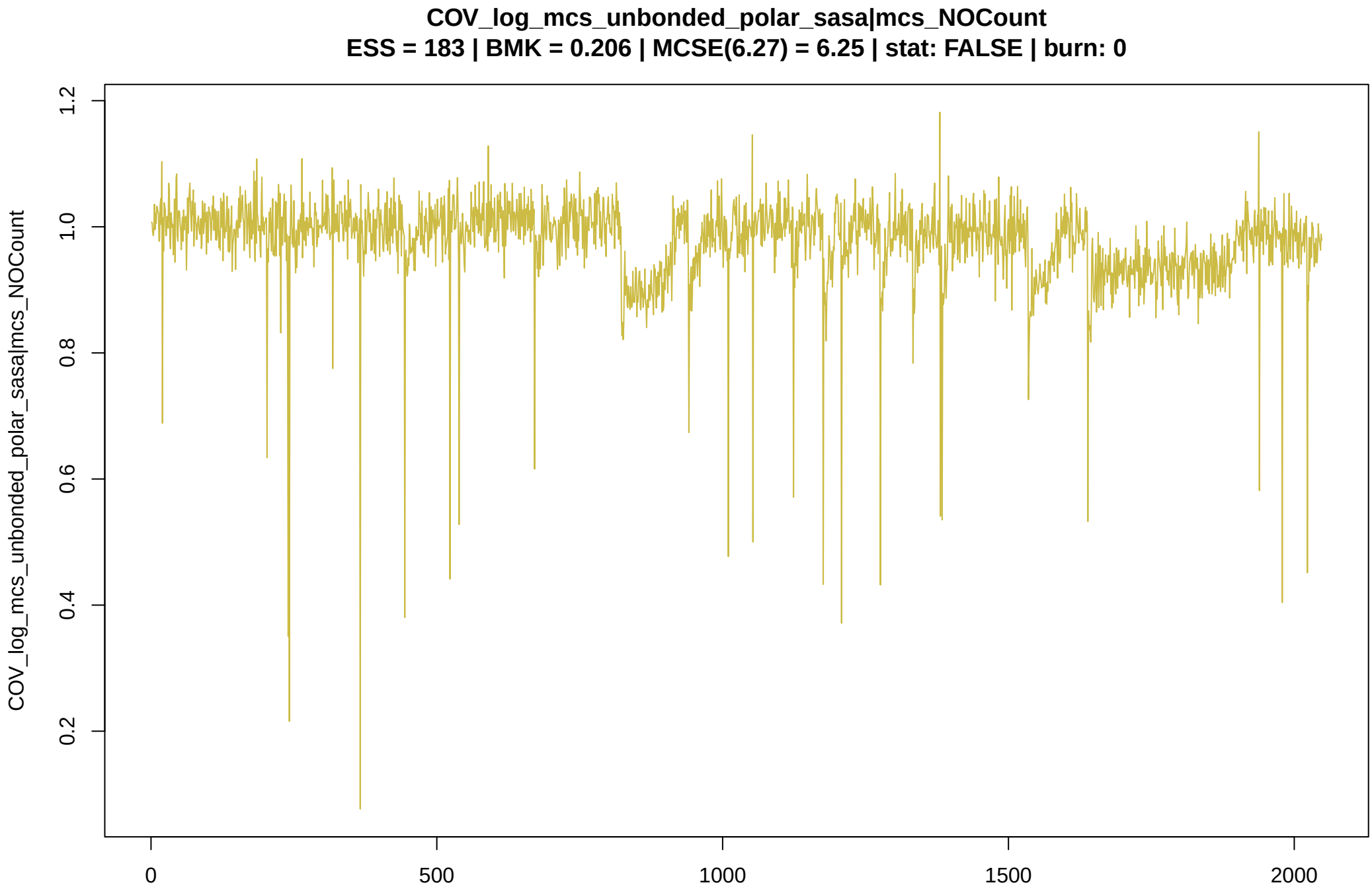

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1350 | BMK = 0.0982 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.1
0.2
0.3
0.4
0.5
0.6
0
500
1000
1500
2000

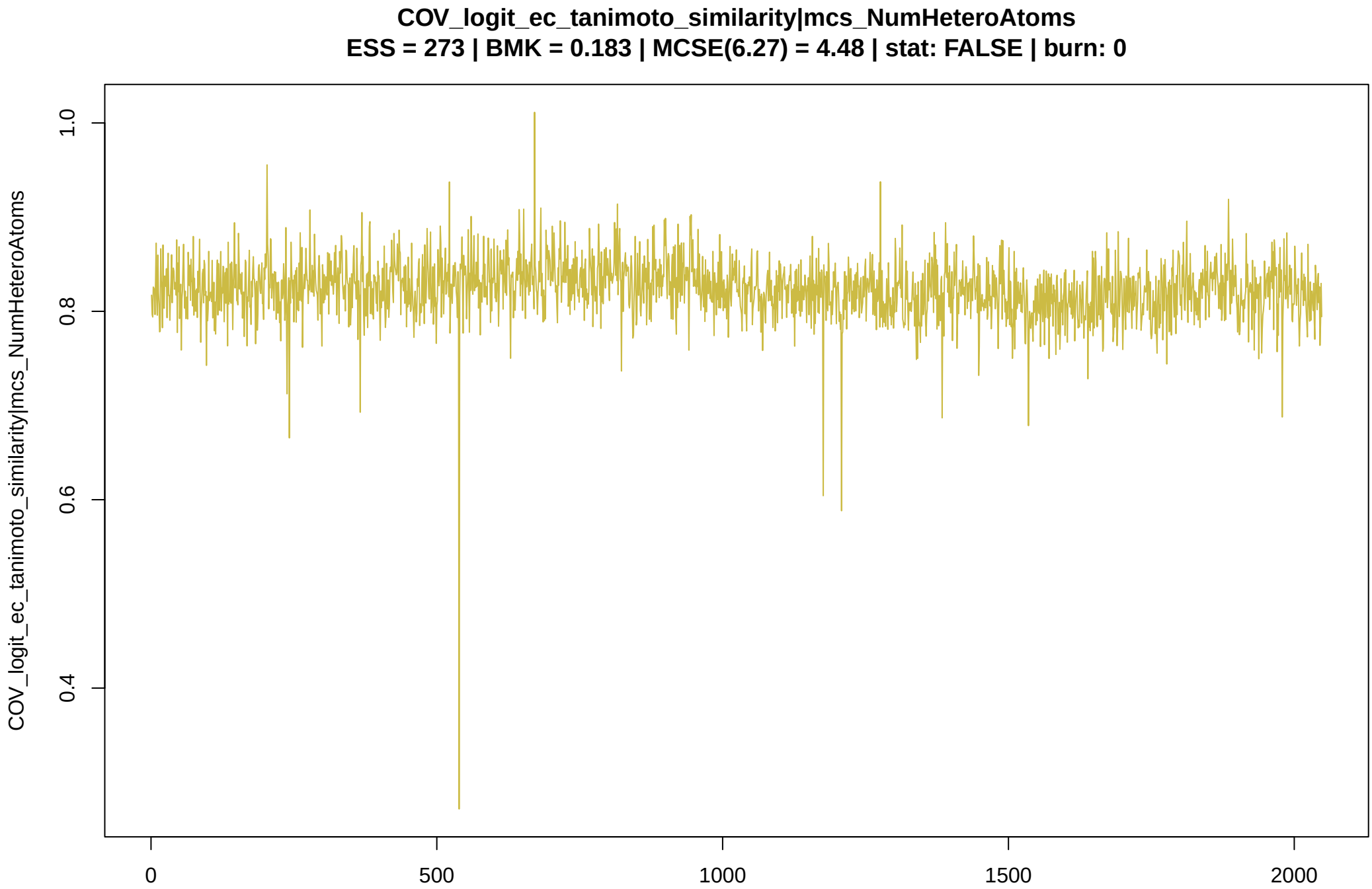

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 208 | BMK = 0.212 | MCSE(6.27) = 5.92 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

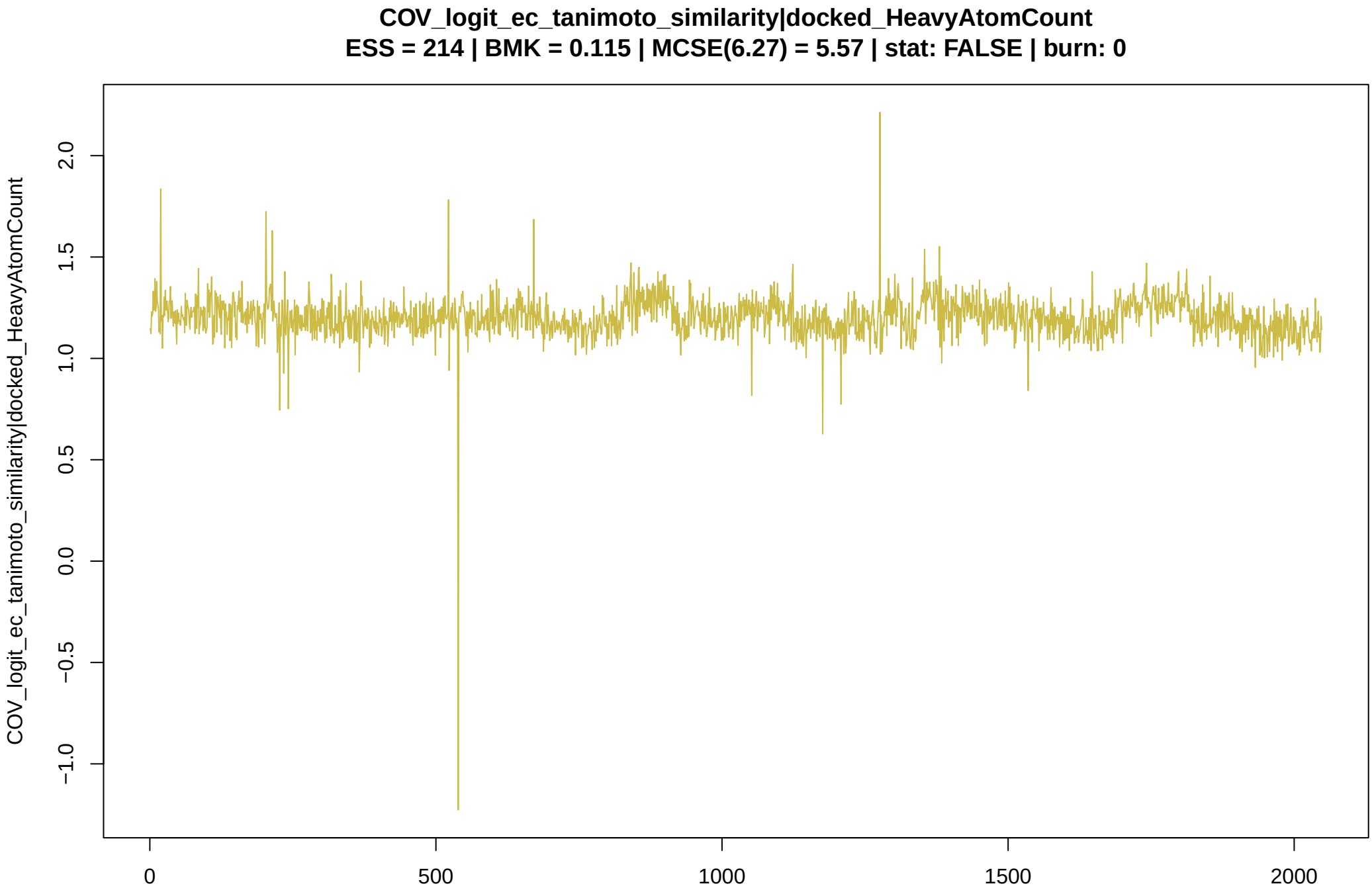

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 257 | BMK = 0.172 | MCSE(6.27) = 5.77 | stat: TRUE | burn: 1632
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
4
3
2
1
0
−1
−2
0
500
1000
1500
2000

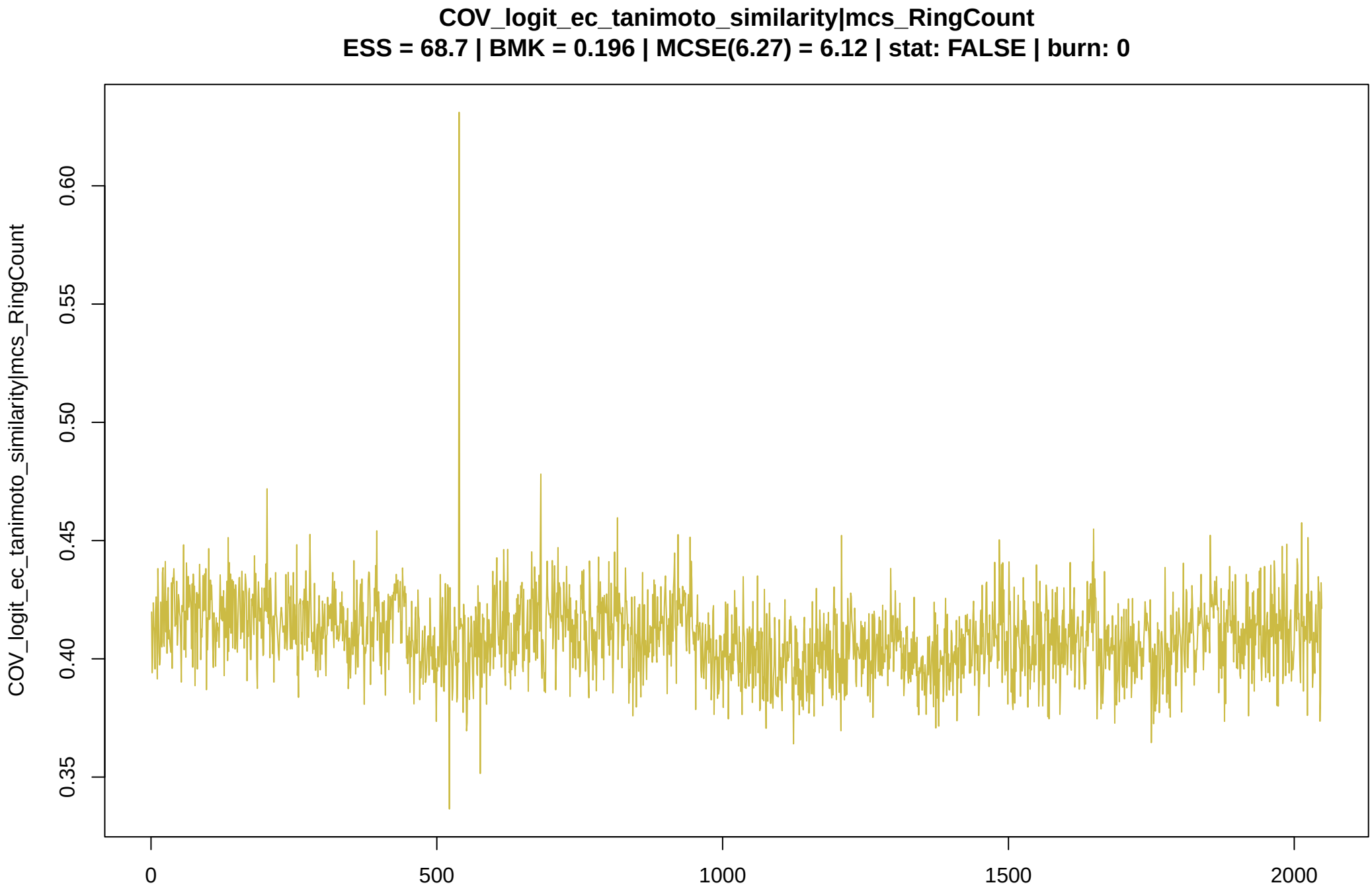

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 158 | BMK = 0.164 | MCSE(6.27) = 7.75 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−0.1
0.0
0.1
0.2
0.3
0
500
1000
1500
2000

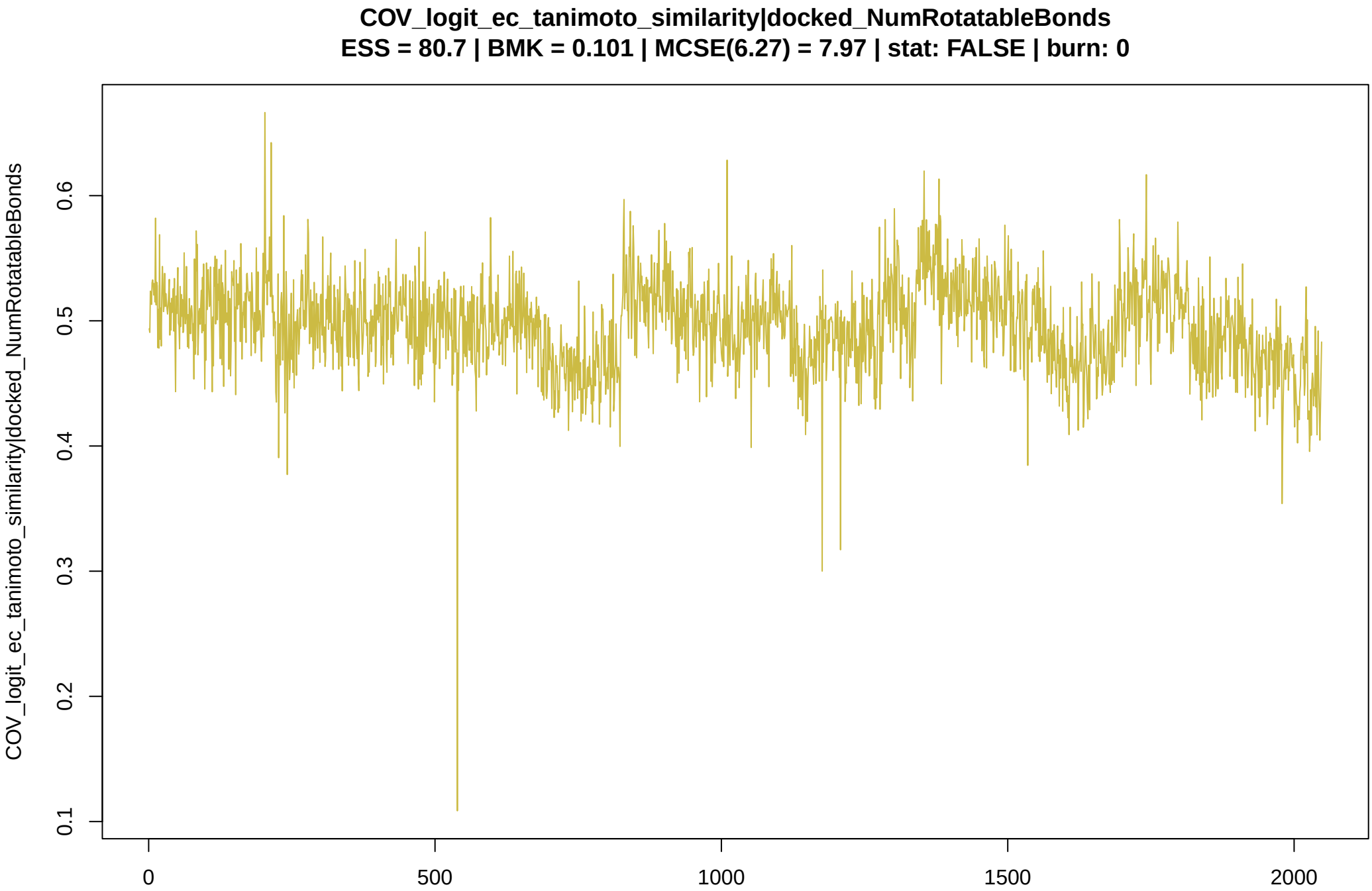

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 166 | BMK = 0.197 | MCSE(6.27) = 7.22 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
−0.2
0.0
0.2
0.4
0.6
0
500
1000
1500
2000

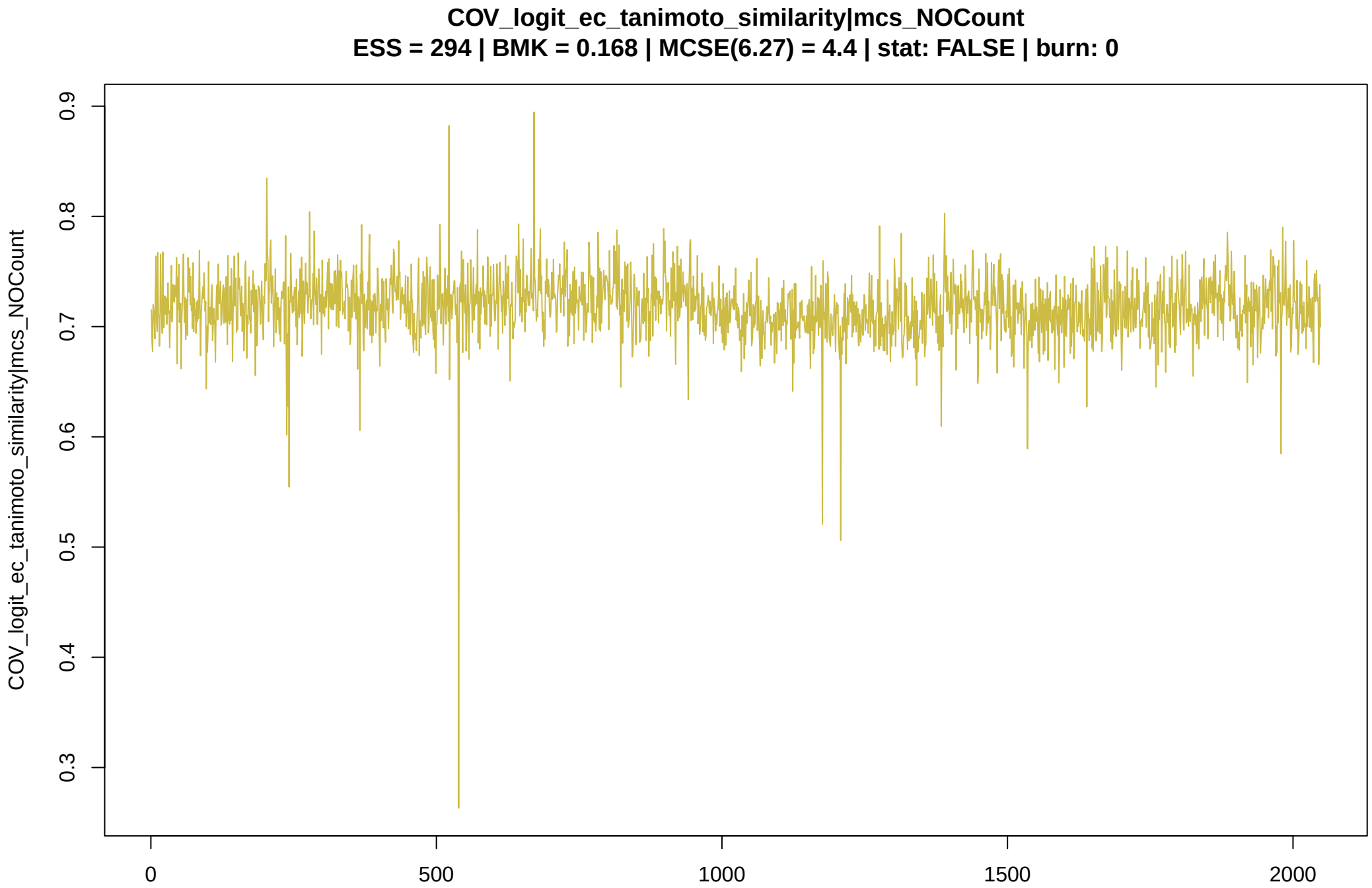

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 183 | BMK = 0.206 | MCSE(6.27) = 6.25 | stat: FALSE | burn: 0
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
0.2
0.4
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

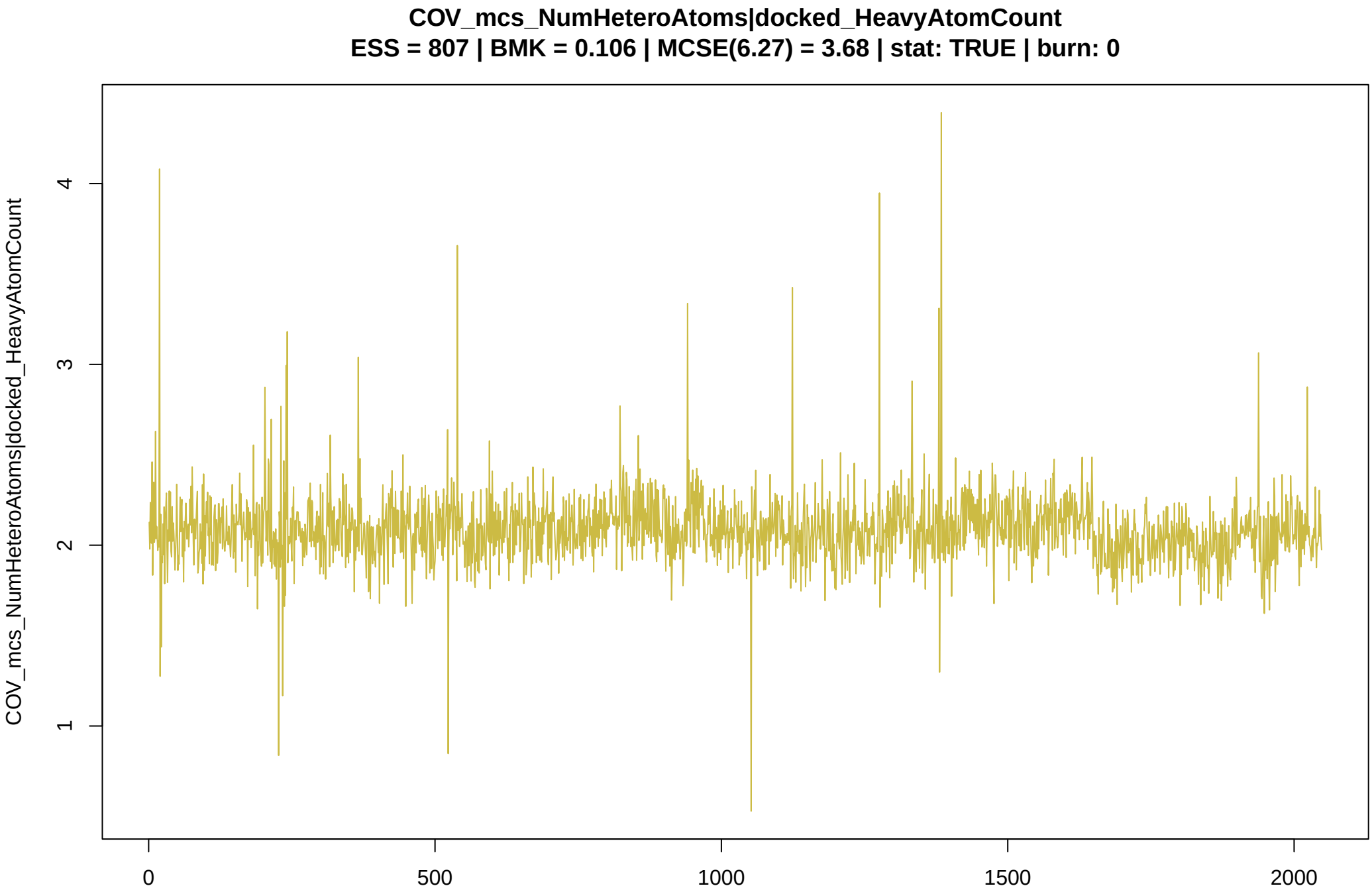

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 273 | BMK = 0.183 | MCSE(6.27) = 4.48 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.0
0.8
0.6
0.4
0
500
1000
1500
2000

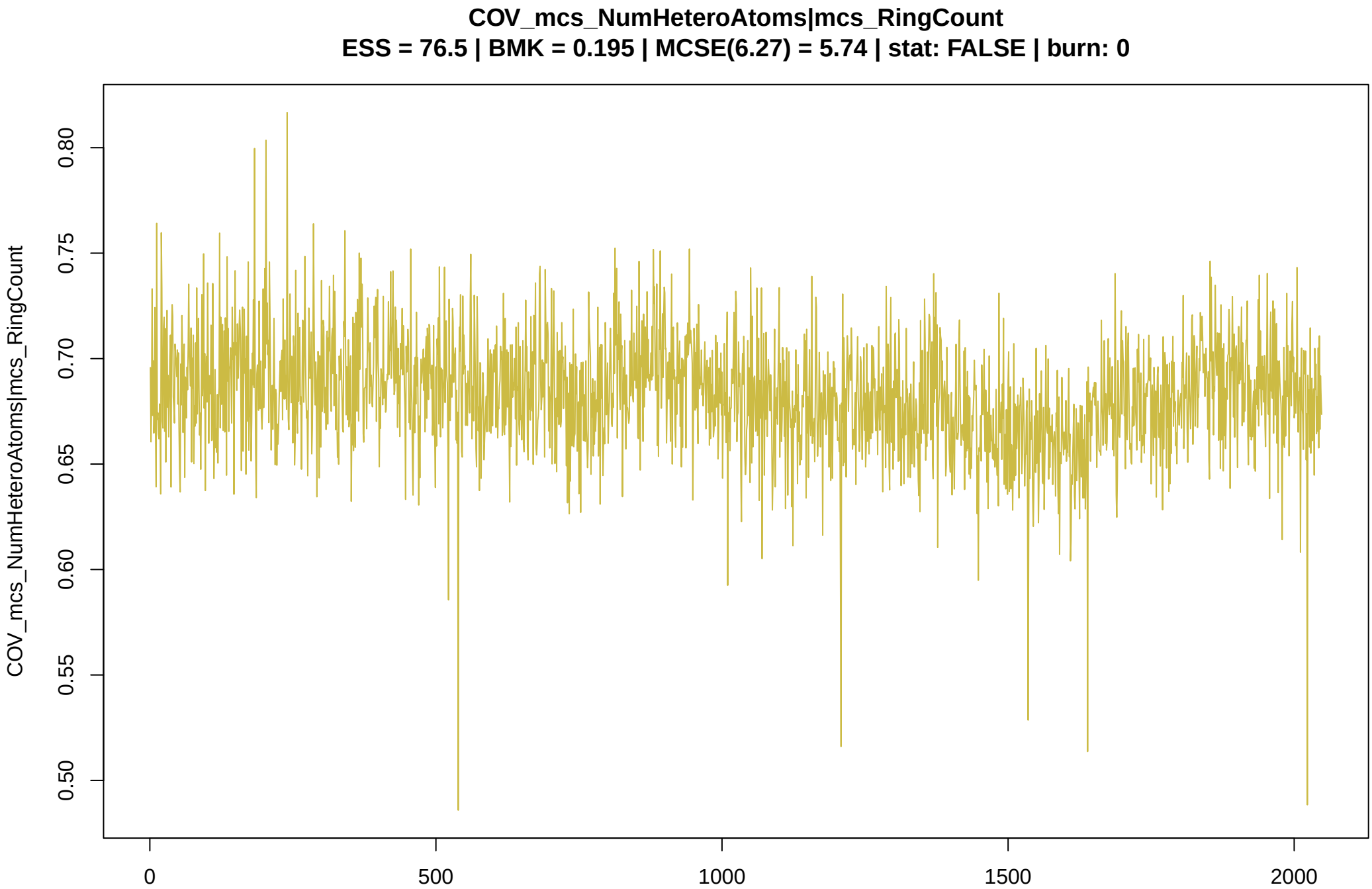

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 214 | BMK = 0.115 | MCSE(6.27) = 5.57 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

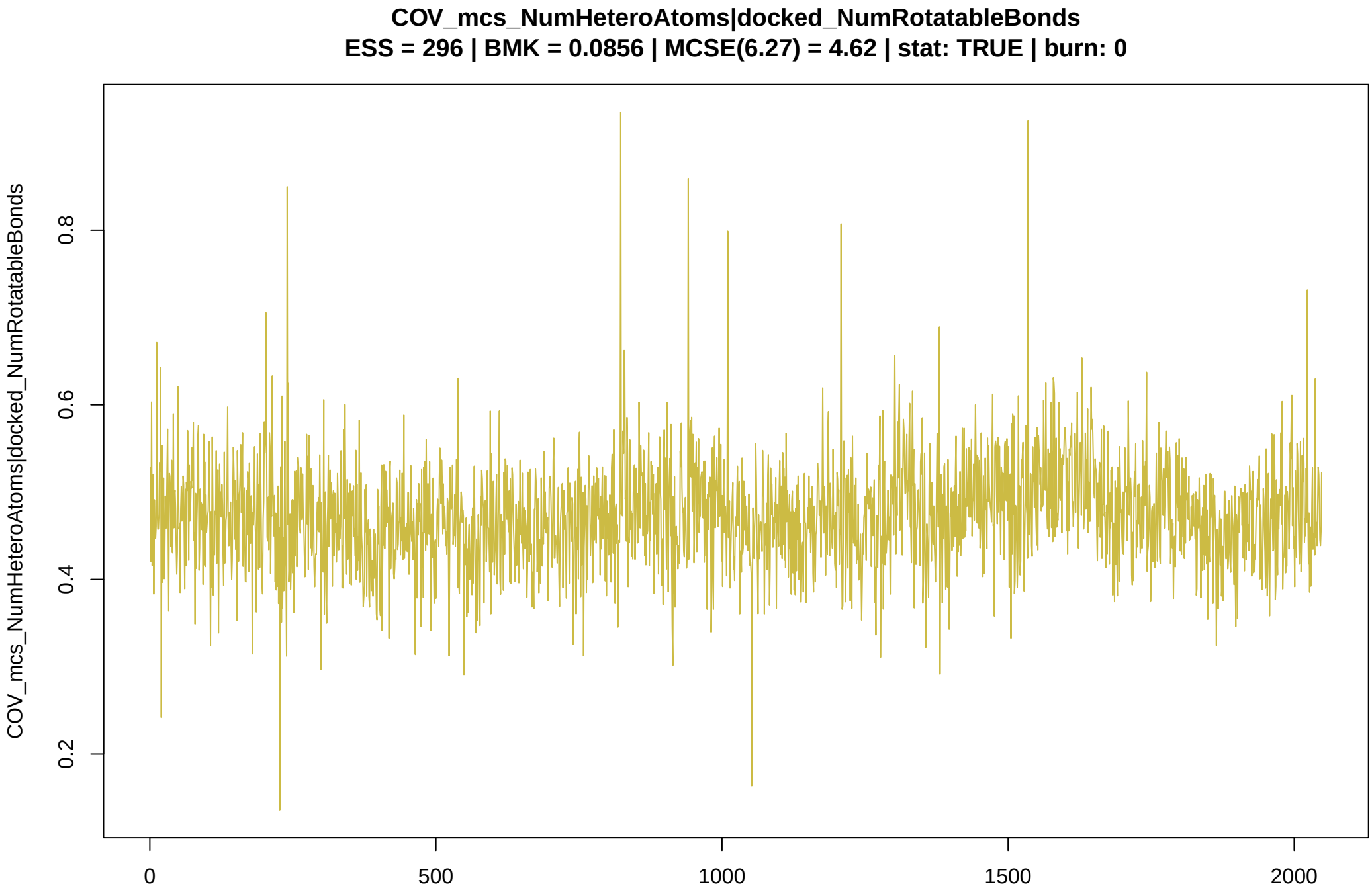

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 68.7 | BMK = 0.196 | MCSE(6.27) = 6.12 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.35
0.40
0.45
0.50
0.55
0.60
0
500
1000
1500
2000

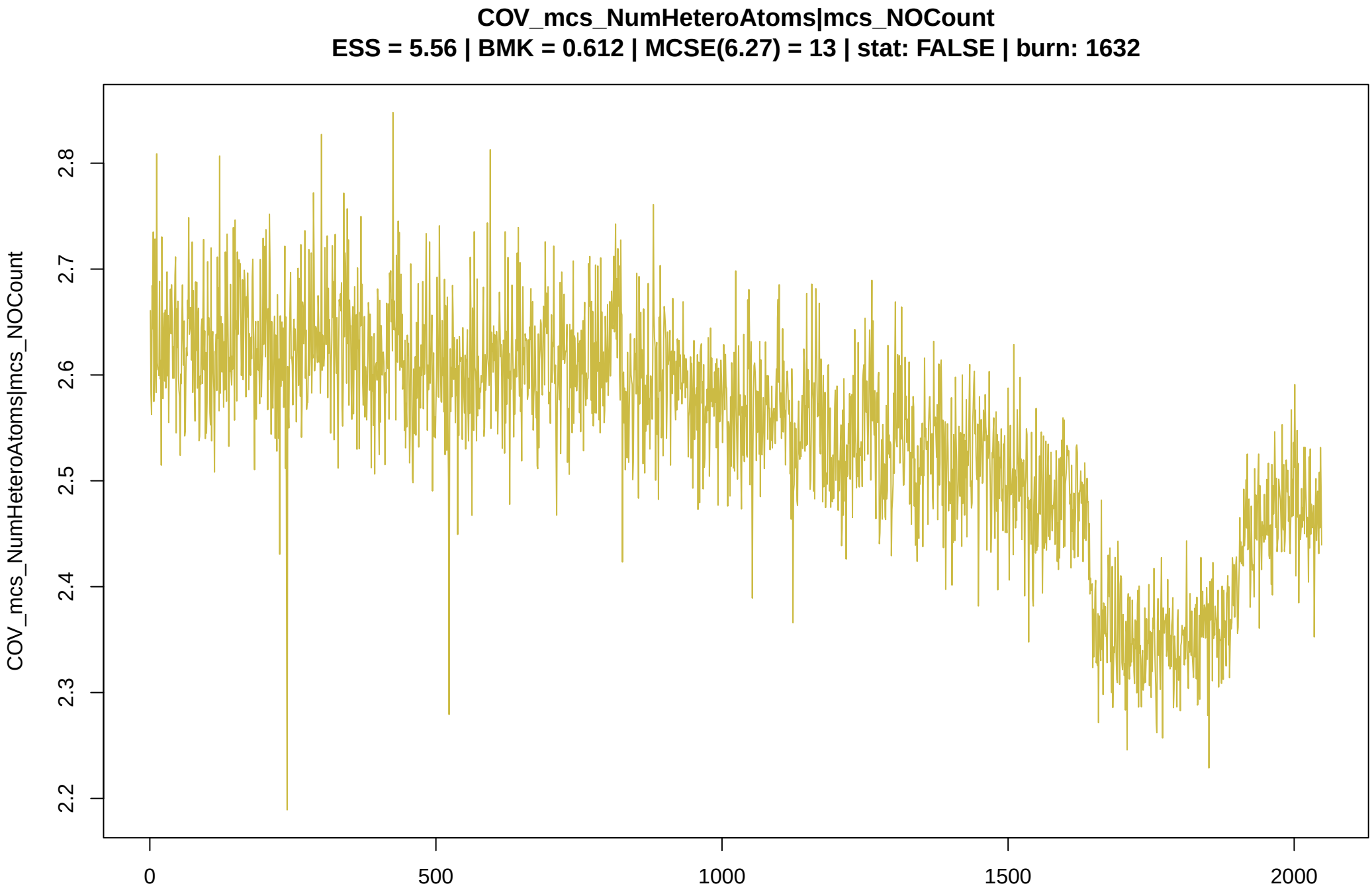

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 80.7 | BMK = 0.101 | MCSE(6.27) = 7.97 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
0.1
0.2
0.3
0.4
0.5
0.6
0
500
1000
1500
2000

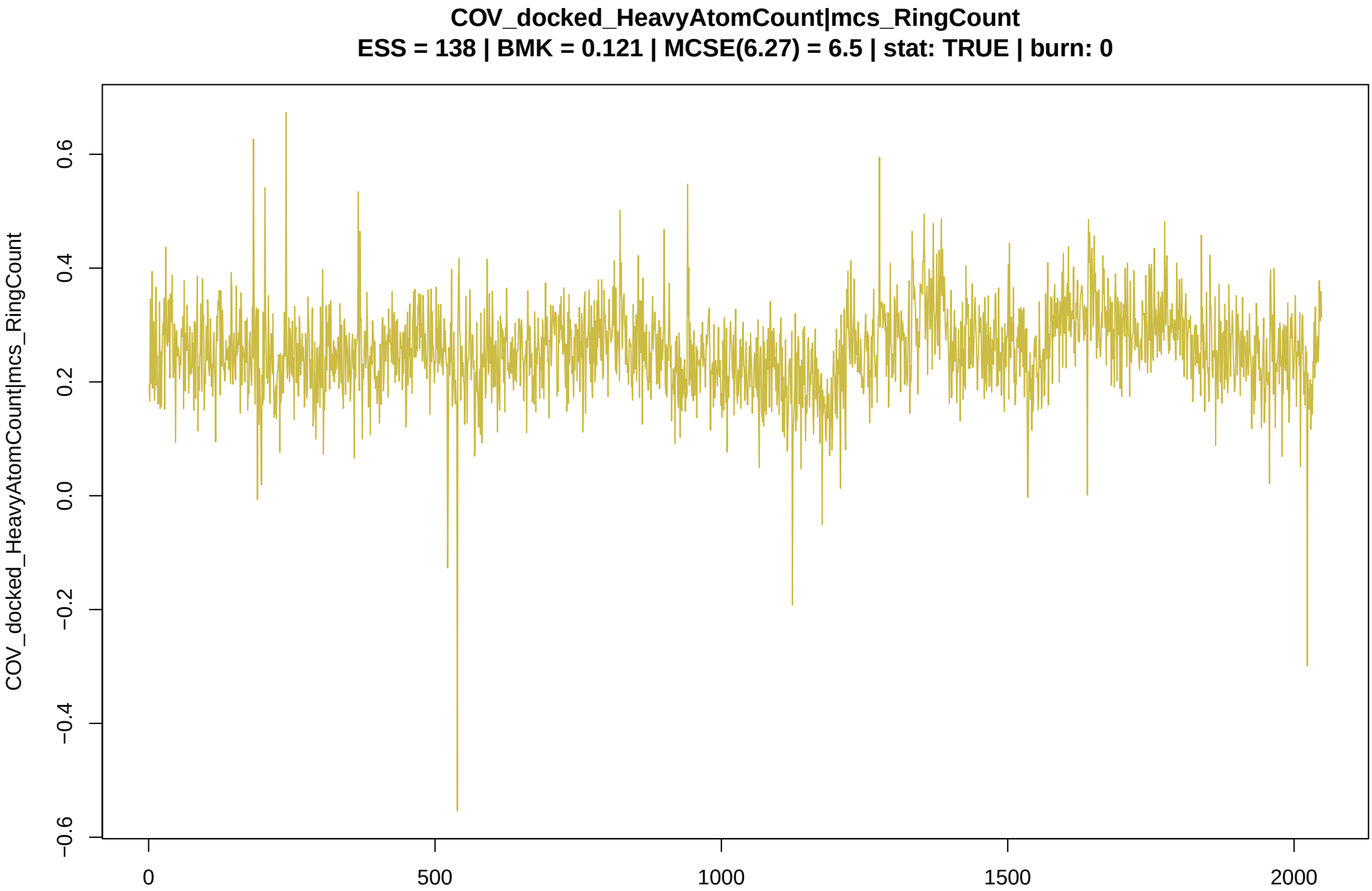

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 294 | BMK = 0.168 | MCSE(6.27) = 4.4 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NOCount
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0
500
1000
1500
2000

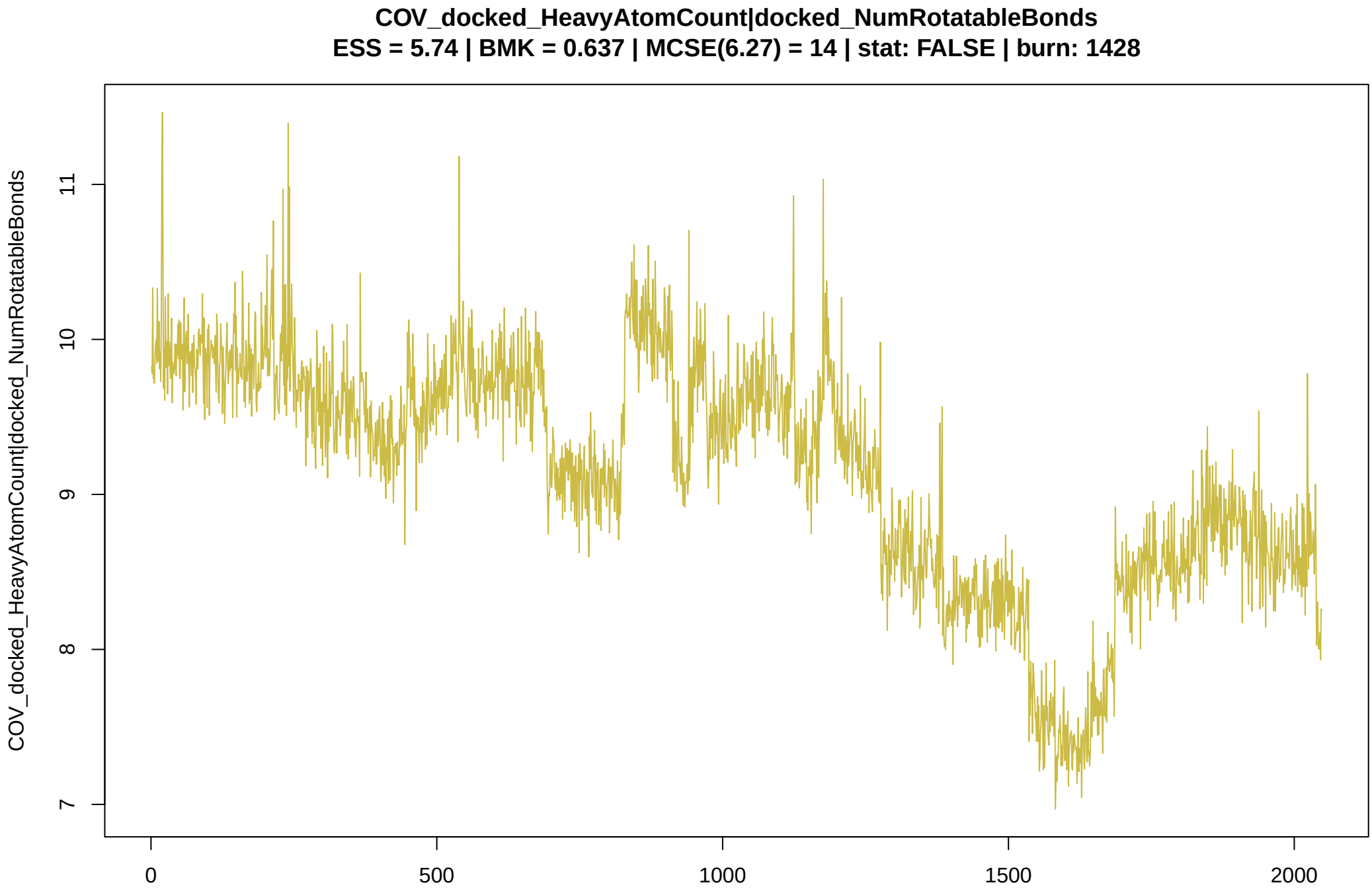

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 807 | BMK = 0.106 | MCSE(6.27) = 3.68 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
1
2
3
4
0
500
1000
1500
2000

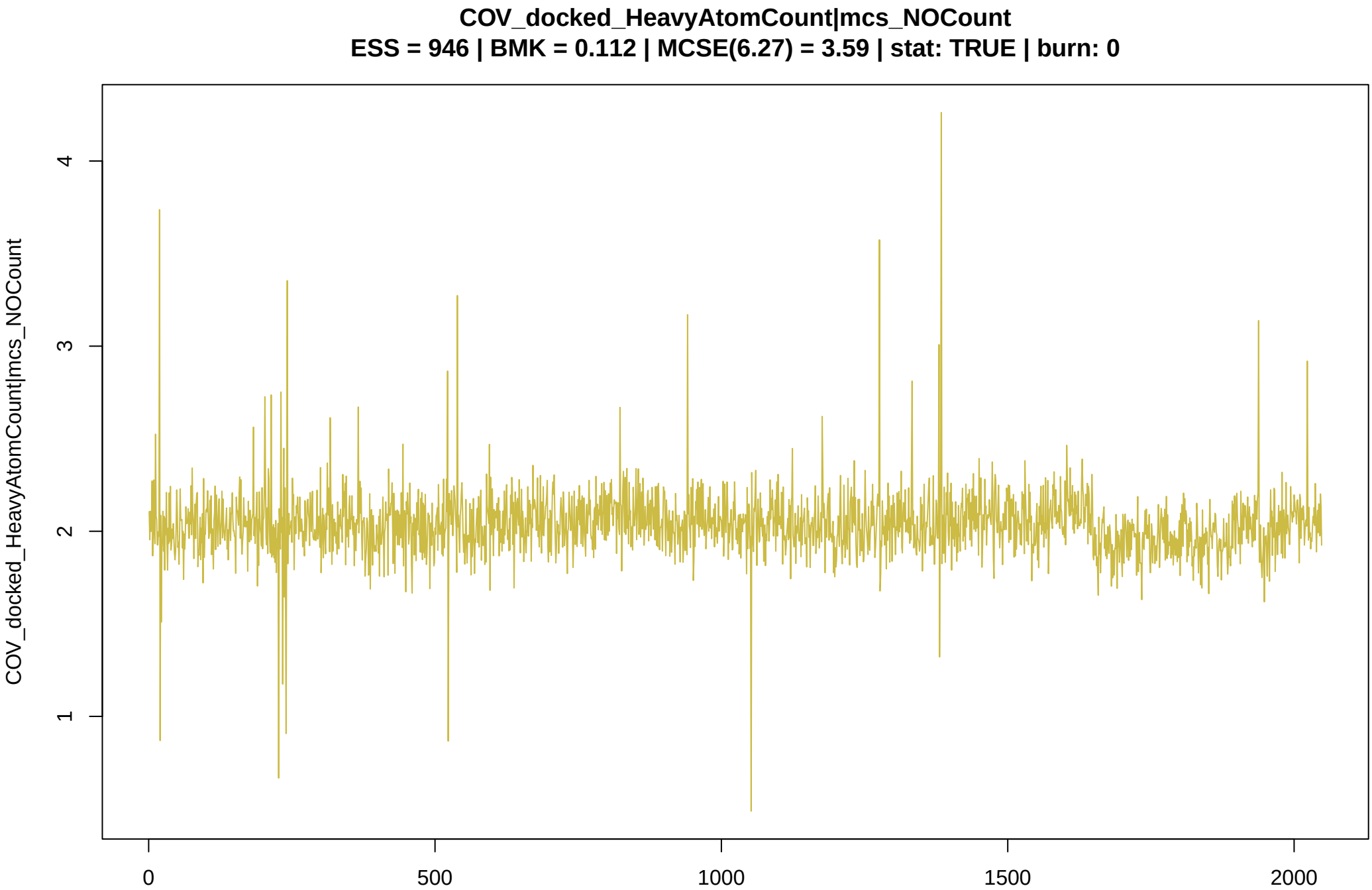

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 76.5 | BMK = 0.195 | MCSE(6.27) = 5.74 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.50
0.55
0.60
0.65
0.70
0.75
0.80
0
500
1000
1500
2000

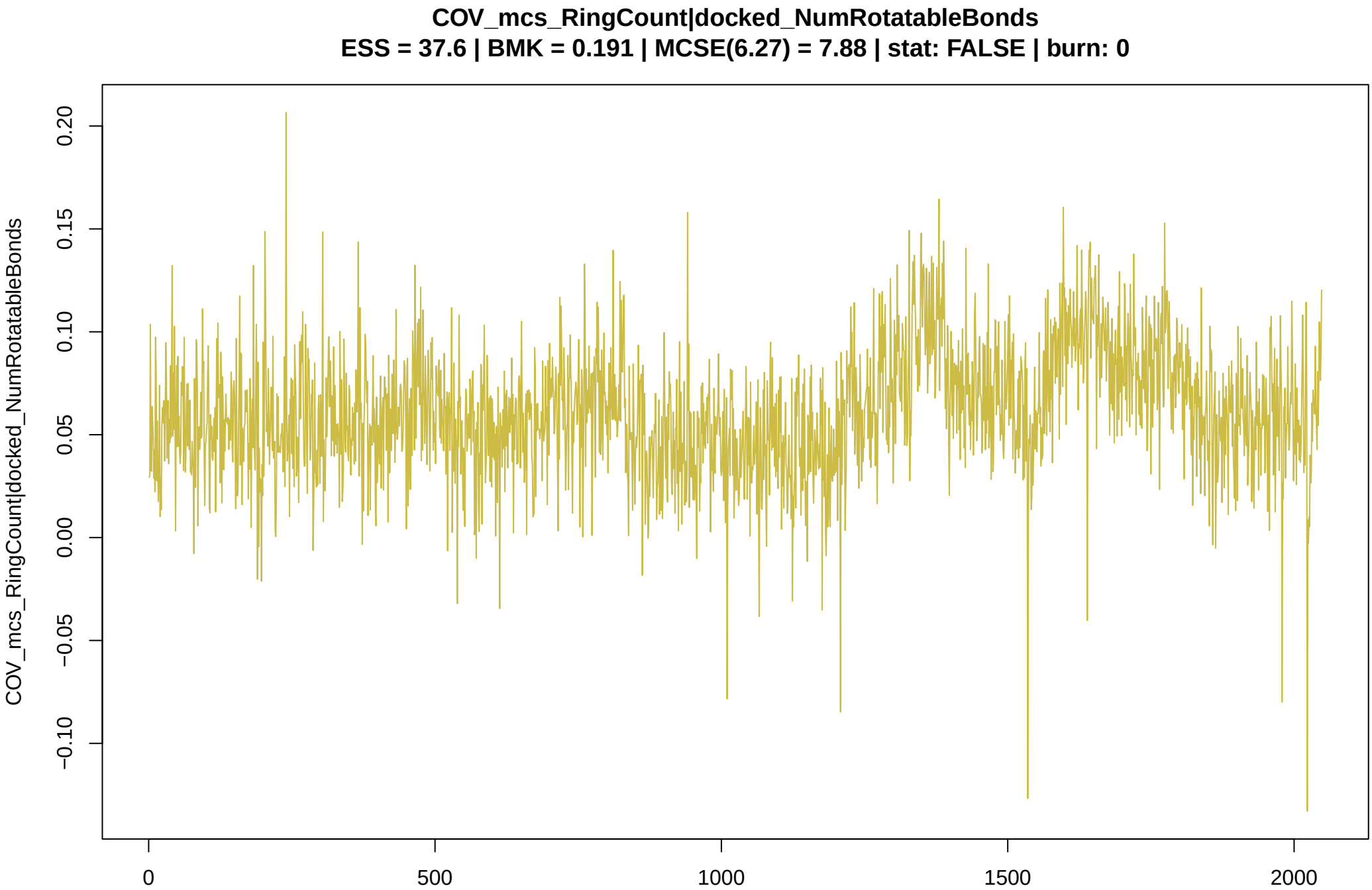

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 296 | BMK = 0.0856 | MCSE(6.27) = 4.62 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
0.2
0.4
0.6
0.8
0
500
1000
1500
2000

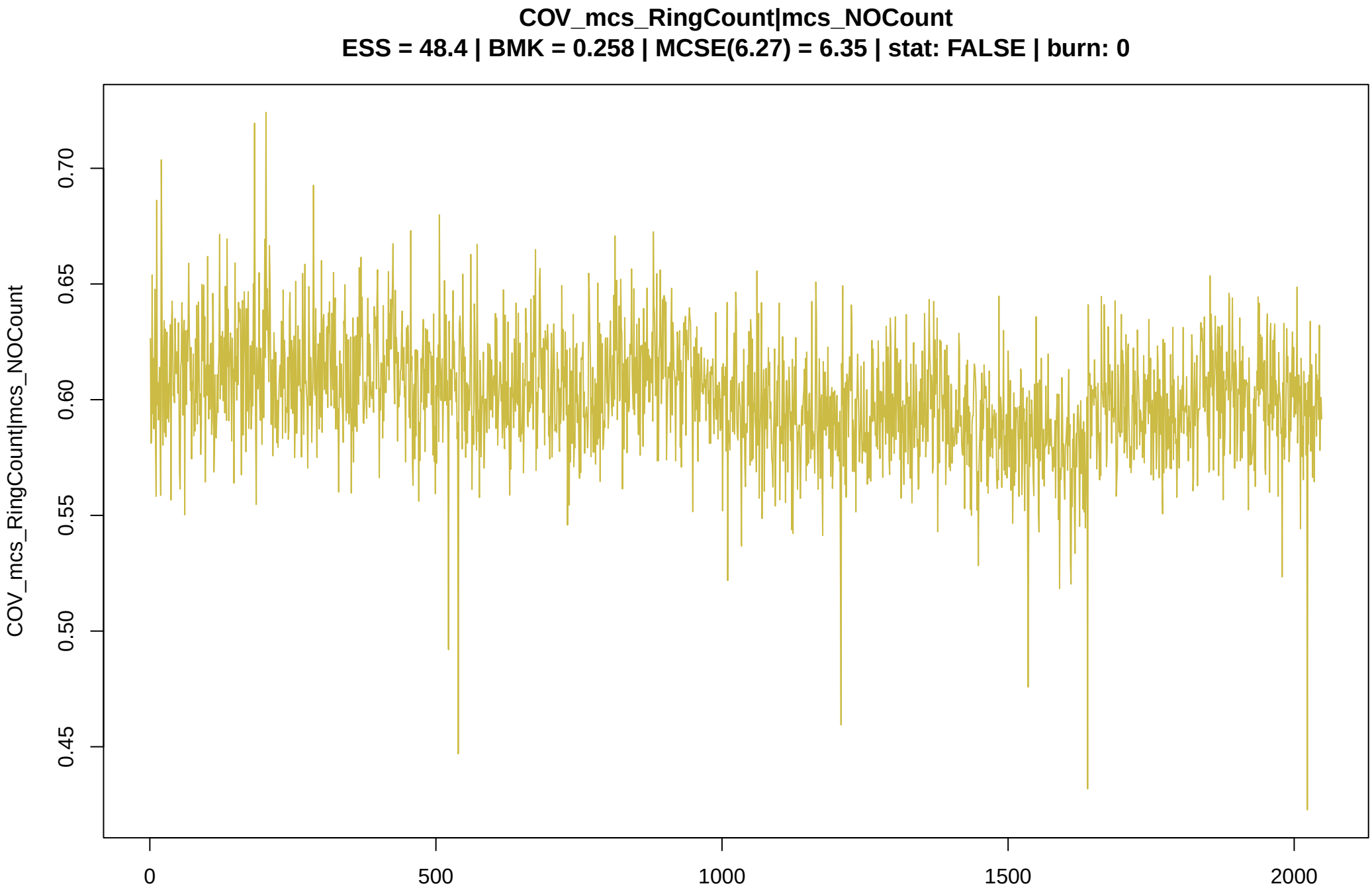

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 5.56 | BMK = 0.612 | MCSE(6.27) = 13 | stat: FALSE | burn: 1632
COV_mcs_NumHeteroAtoms|mcs_NOCount
2.2
2.3
2.4
2.5
2.6
2.7
2.8
0
500
1000
1500
2000

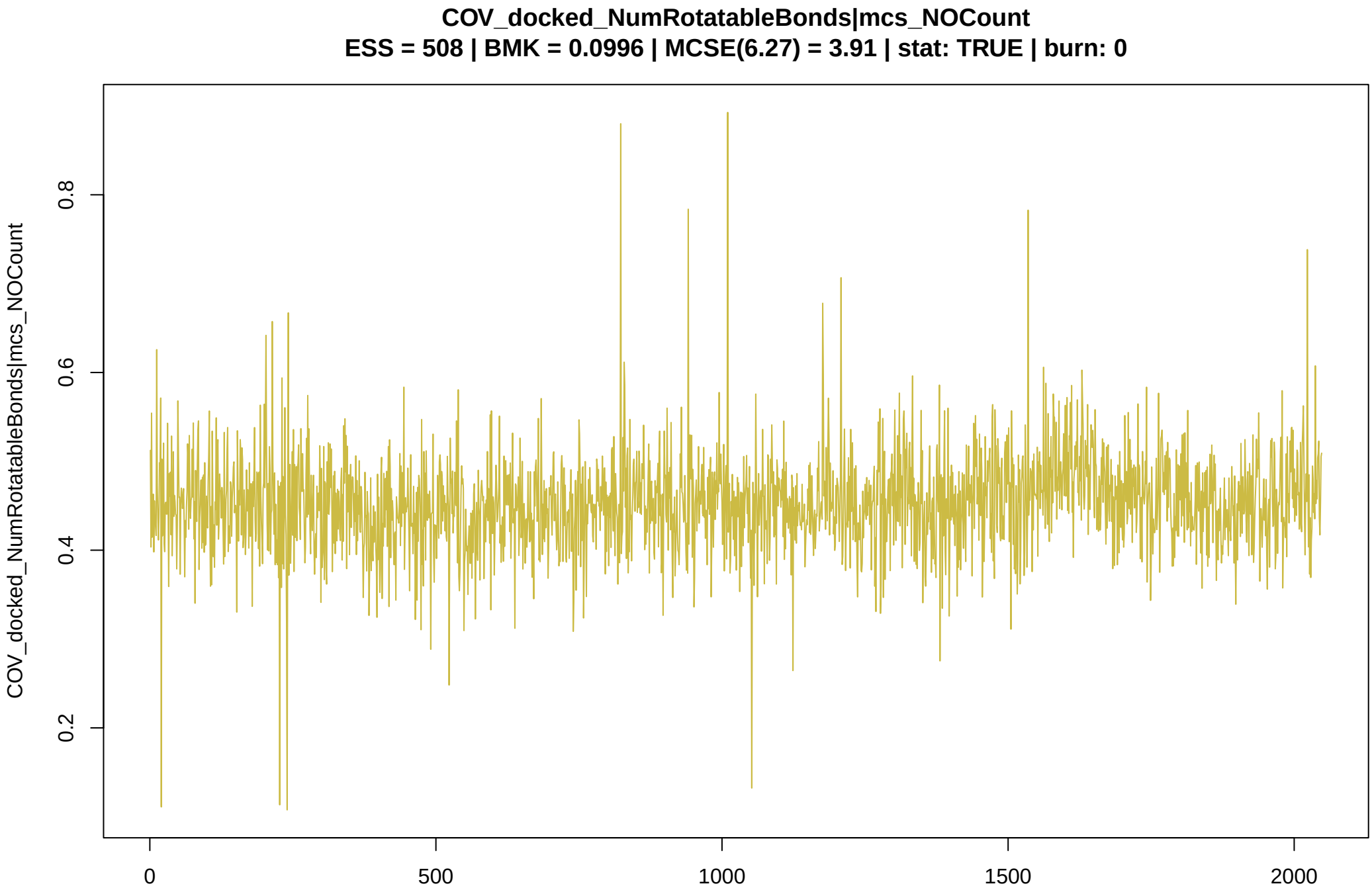

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 138 | BMK = 0.121 | MCSE(6.27) = 6.5 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 5.74 | BMK = 0.637 | MCSE(6.27) = 14 | stat: FALSE | burn: 1428
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
7
8
9
10
11
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 946 | BMK = 0.112 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NOCount
1
2
3
4
0
500
1000
1500
2000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 37.6 | BMK = 0.191 | MCSE(6.27) = 7.88 | stat: FALSE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
0.20
0.15
0.10
0.05
0.00
−0.05
−0.10
0
500
1000
1500
2000


COV_mcs_RingCount|mcs_NOCount
ESS = 48.4 | BMK = 0.258 | MCSE(6.27) = 6.35 | stat: FALSE | burn: 0
COV_mcs_RingCount|mcs_NOCount
0.45
0.50
0.55
0.60
0.65
0.70
0
500
1000
1500
2000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 508 | BMK = 0.0996 | MCSE(6.27) = 3.91 | stat: TRUE | burn: 0
COV_docked_NumRotatableBonds|mcs_NOCount
0.2
0.4
0.6
0.8
0
500
1000
1500
2000