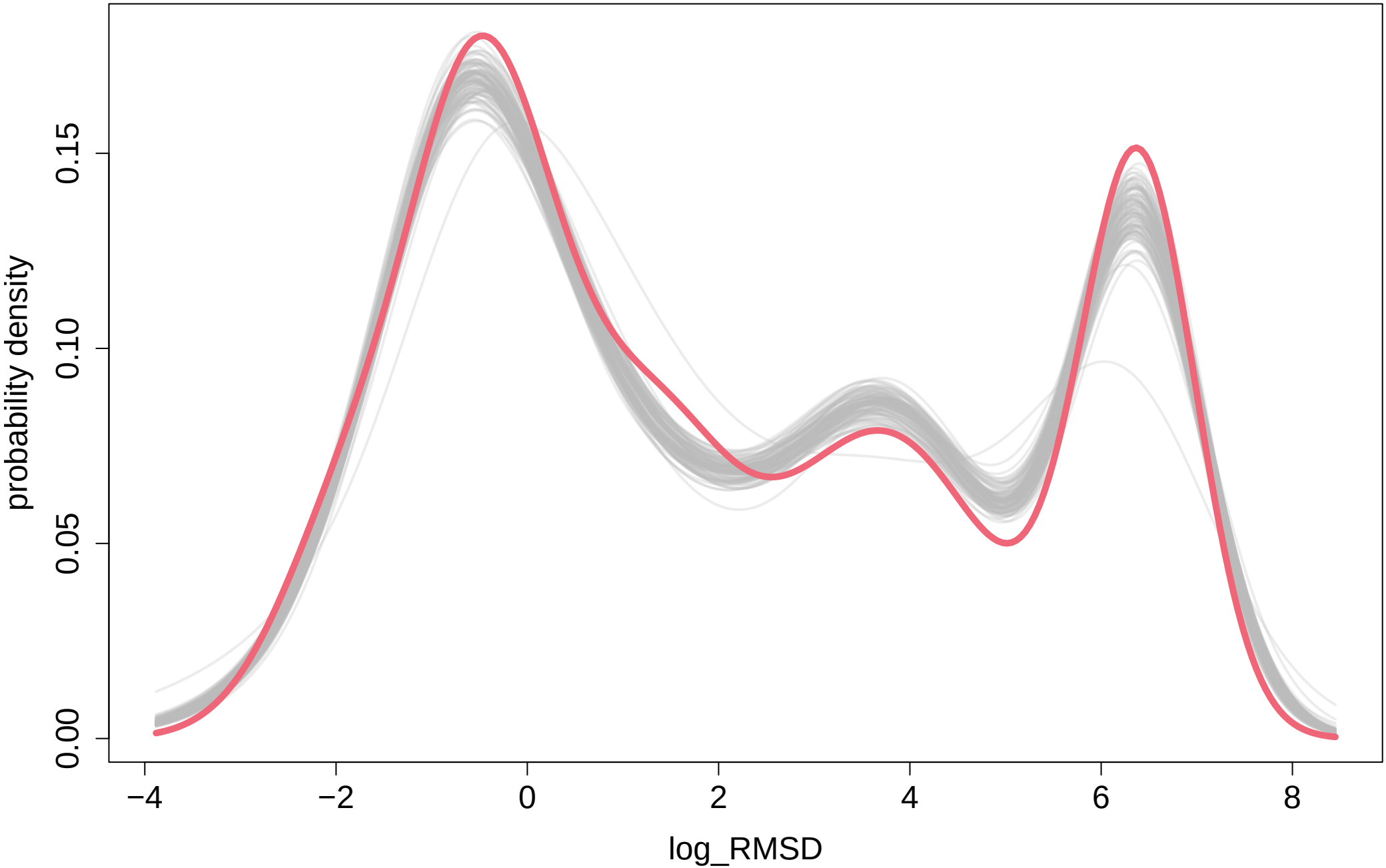
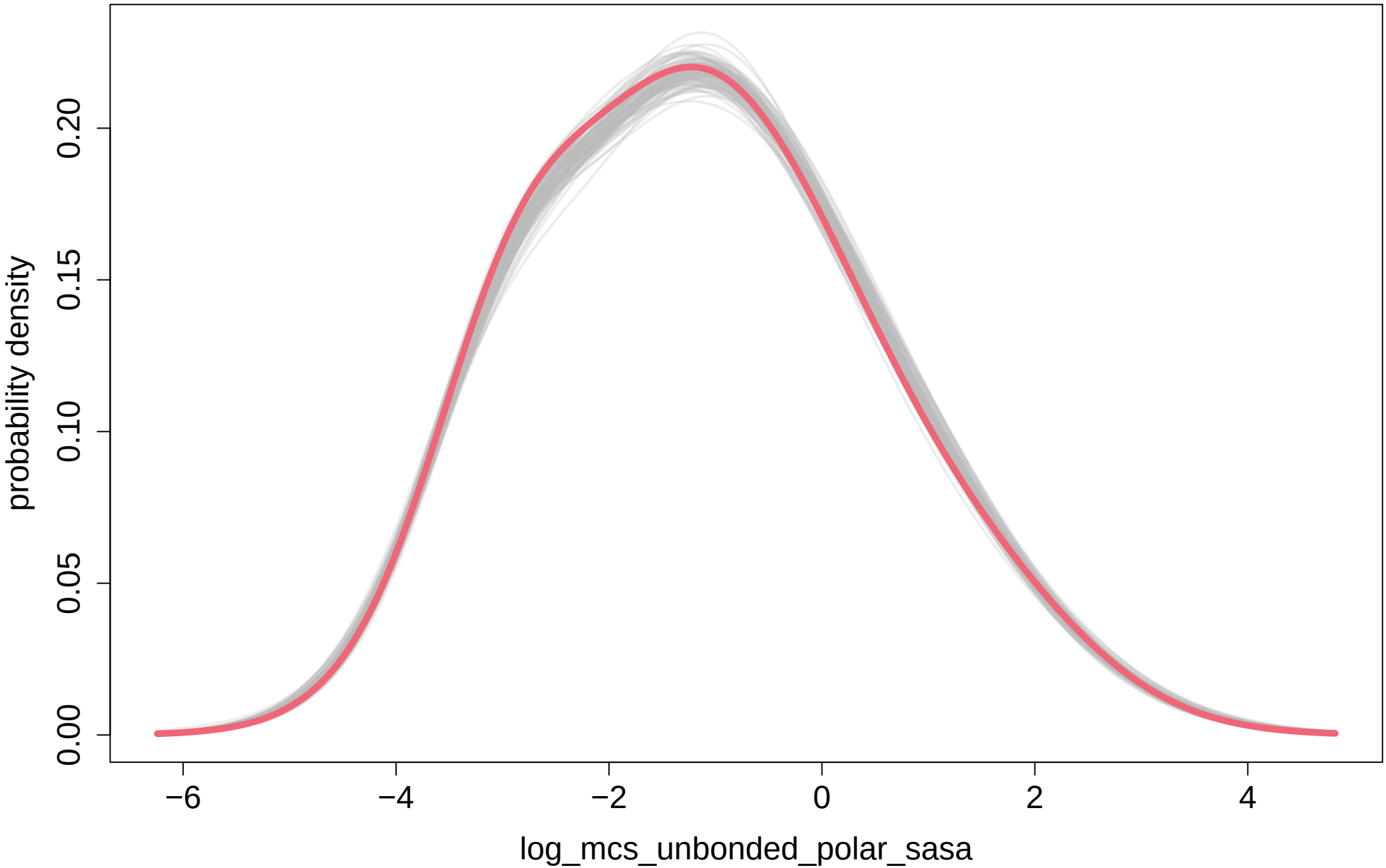
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.411885344902715
max MCSE = 12.6164529563501
all stationary: FALSE
burn: 1020
max rel.err.: 3.41273010759547

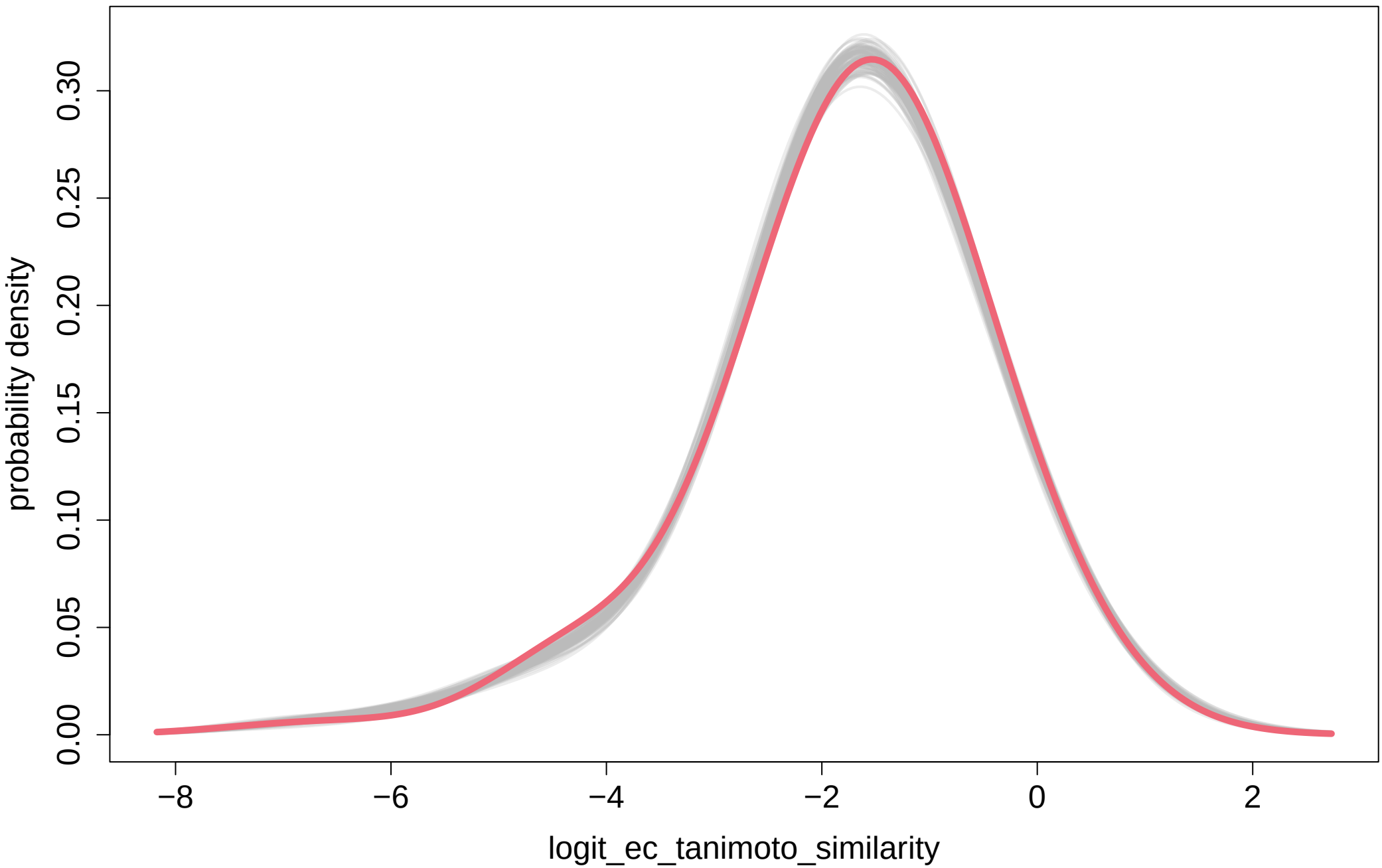
−− STATS 2D −−
min ESS = 16.2008981124193
max BMK = 0.205508469235429
max MCSE = 9.87542332784068
all stationary: FALSE
burn: 0
max rel.err.: 2.12912695975099

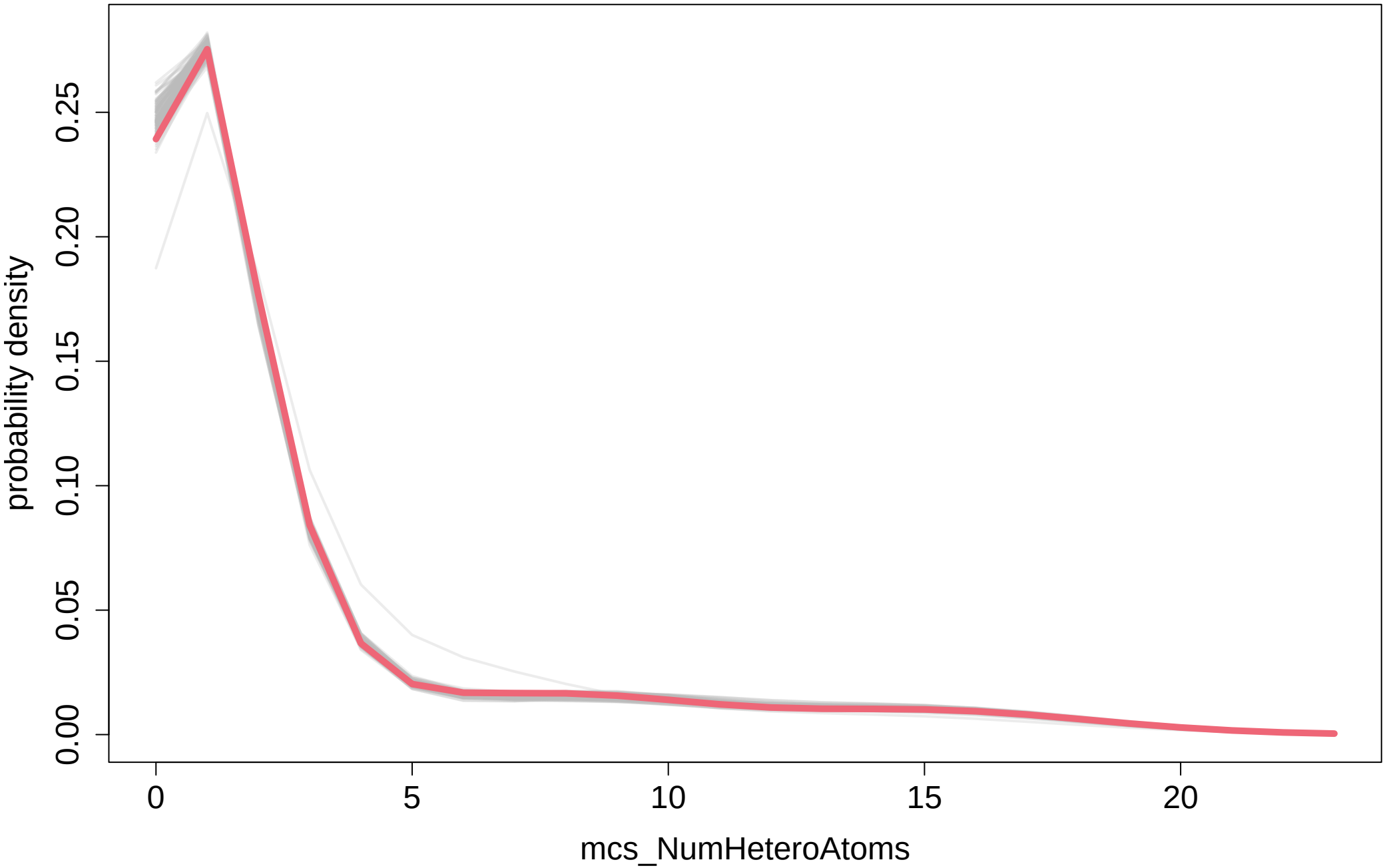
−− STATS 1D −−
min ESS = 90.6707462558497
max BMK = 0.117180654655456
max MCSE = 6.90041844912789
all stationary: TRUE
burn: 0
max rel.err.: 1.82017902160798

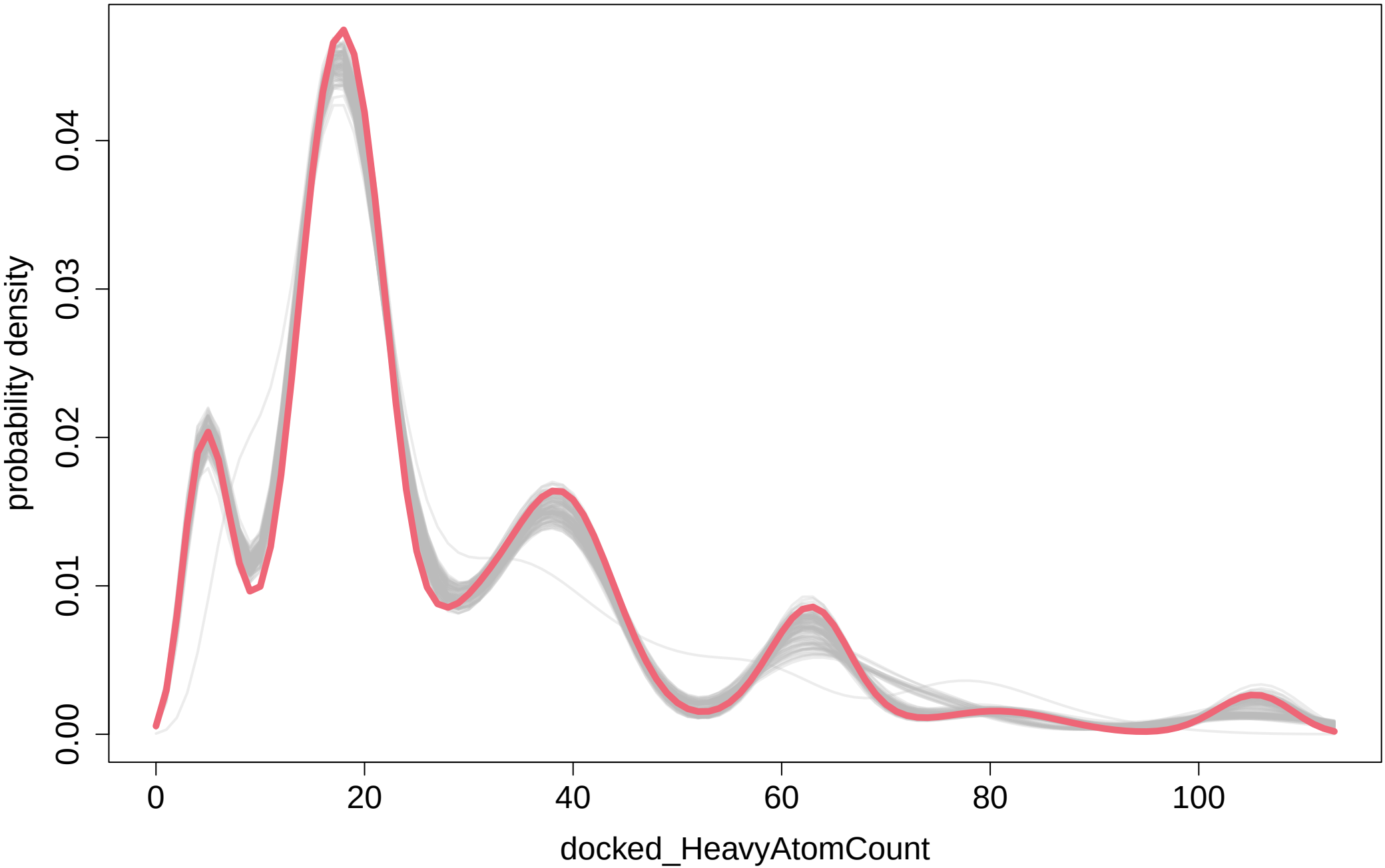
Occupied clusters: 25 of 64
LL: −64300 +− 240

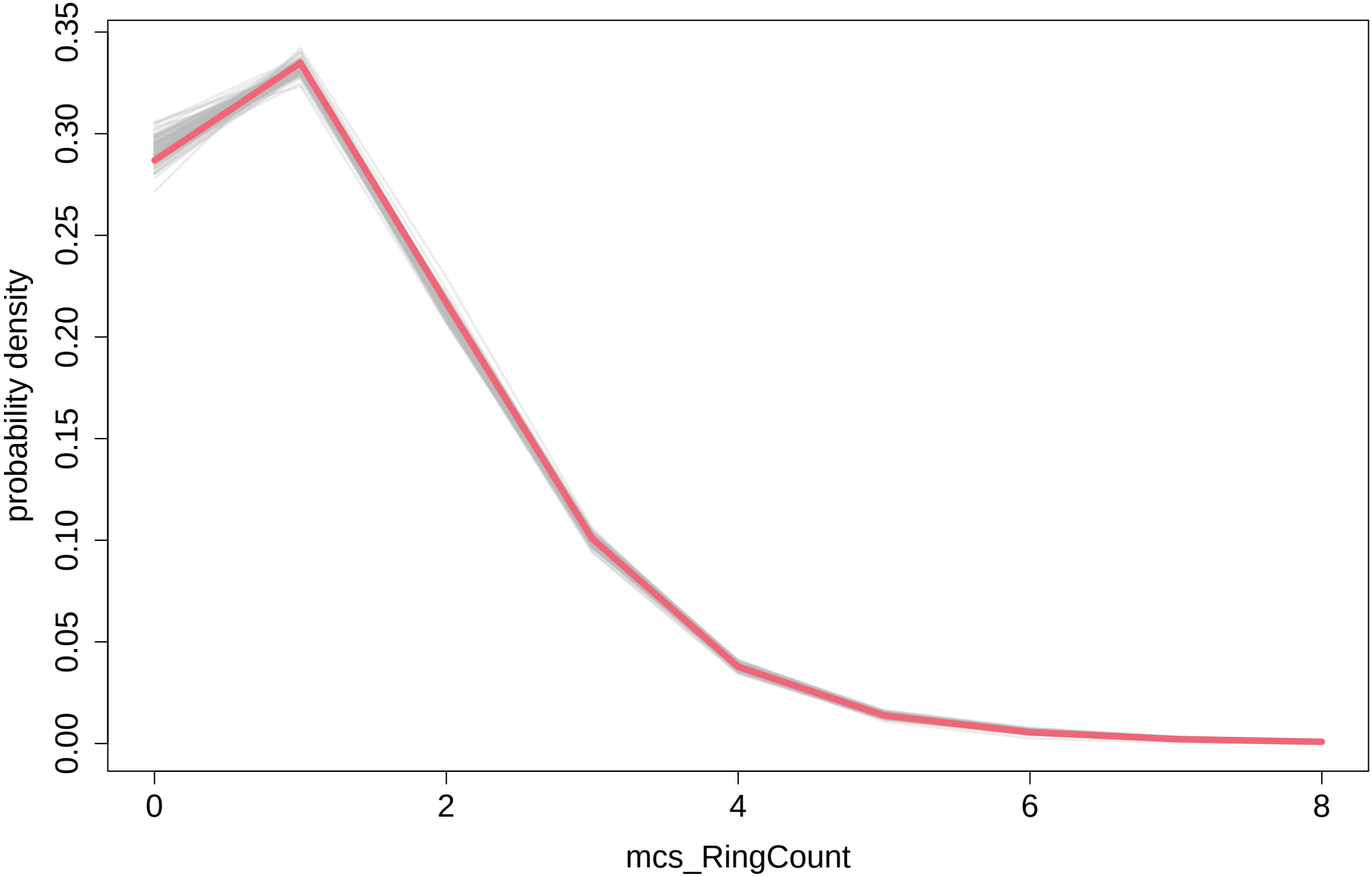

probability density
0.00
0.05
0.10
0.15
−4
−2
0
2
4
6
8
log_RMSD

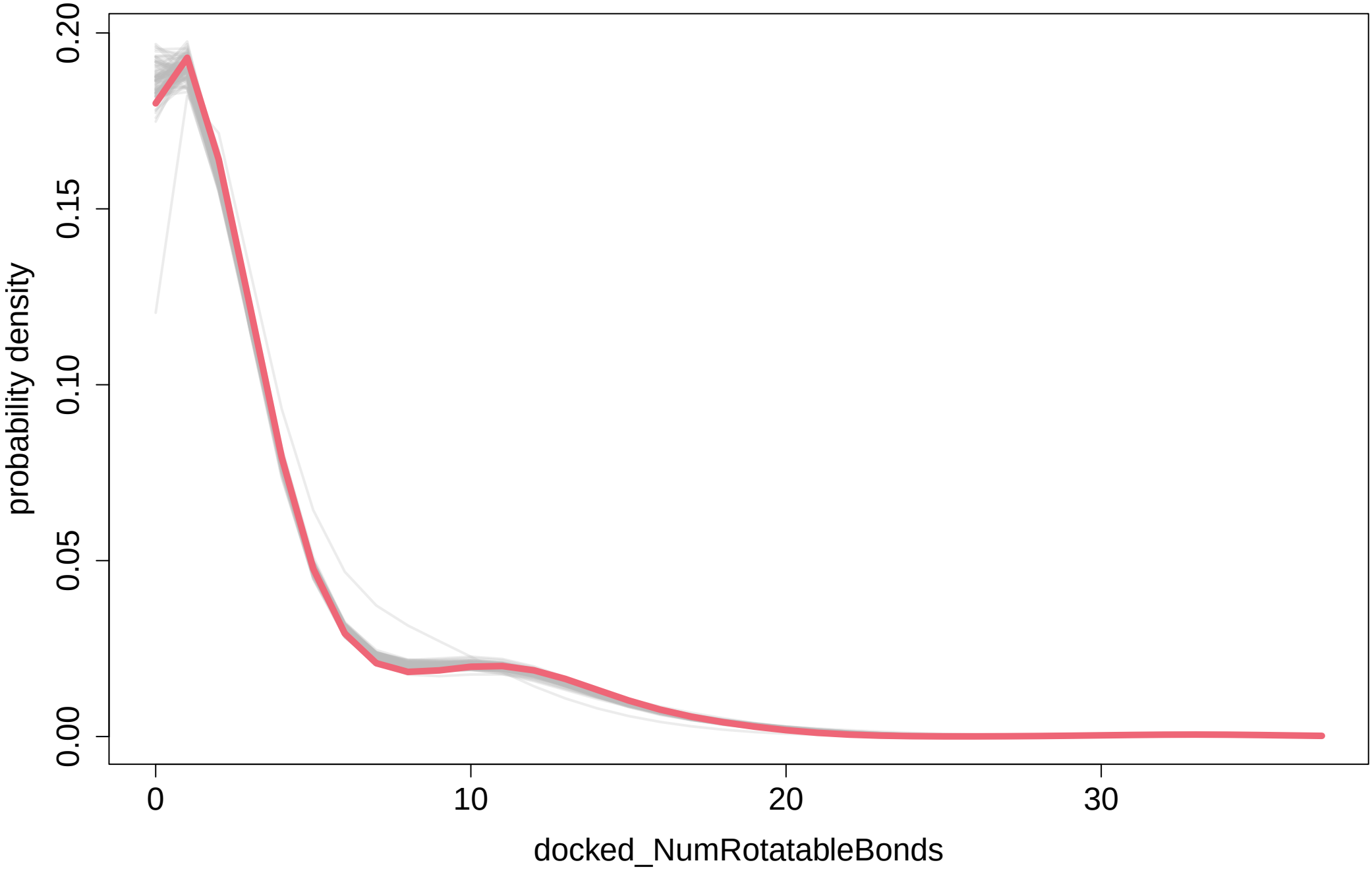

probability density
0.00
0.05
0.10
0.15
0.20
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

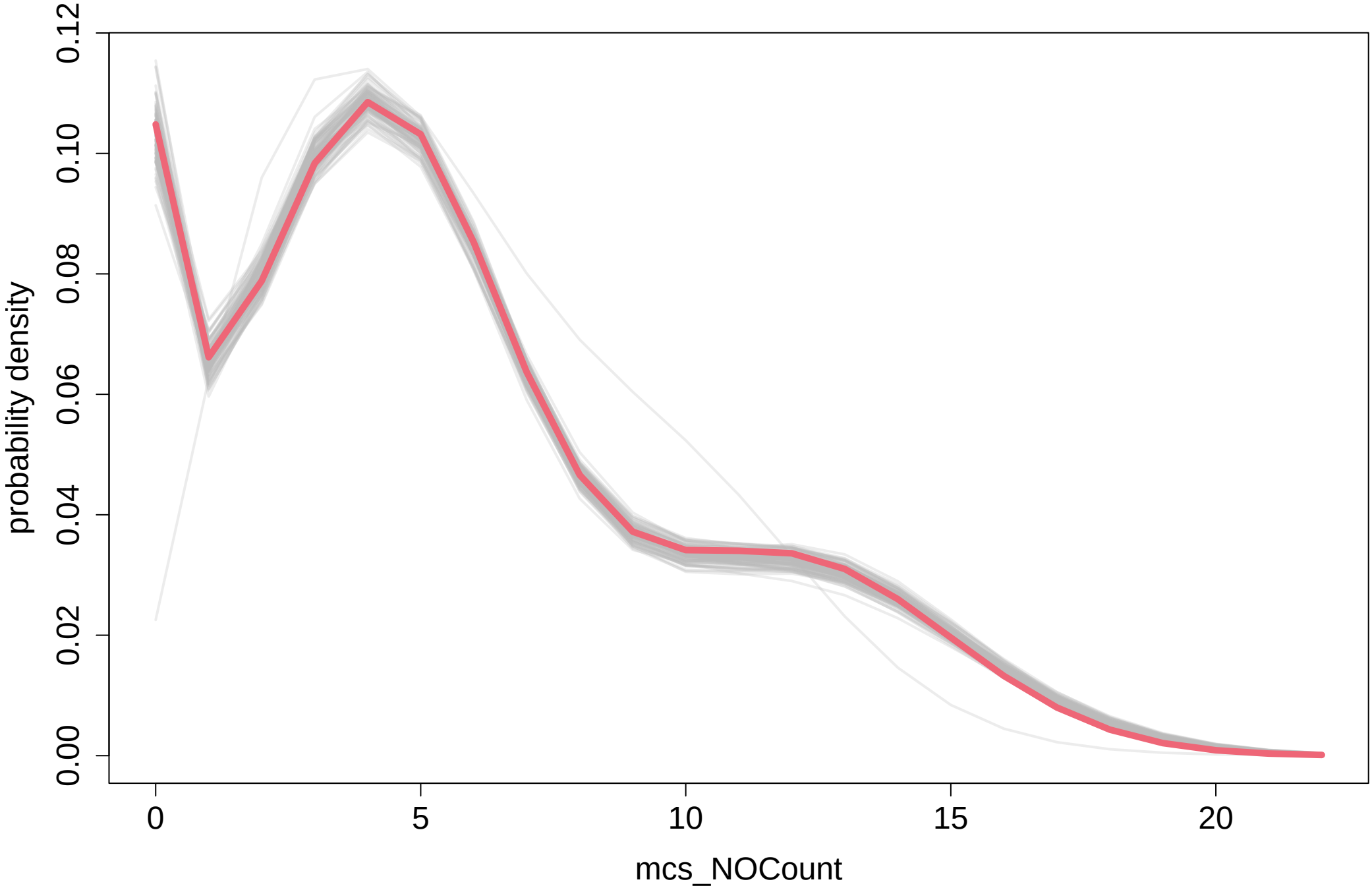

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−8
−6
−4
−2
0
2
logit_ec_tanimoto_similarity

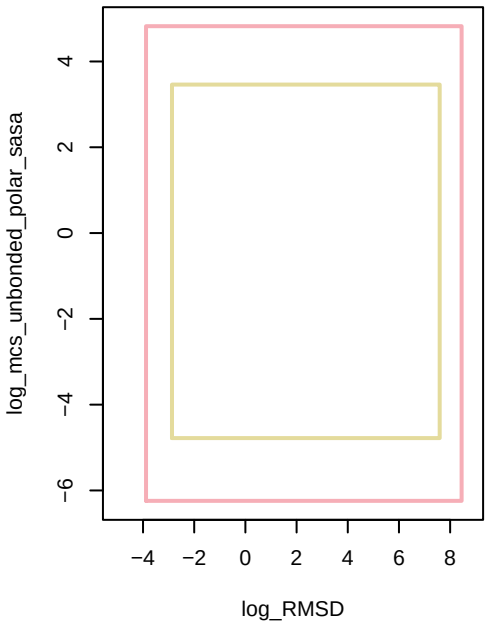

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
20
mcs_NumHeteroAtoms

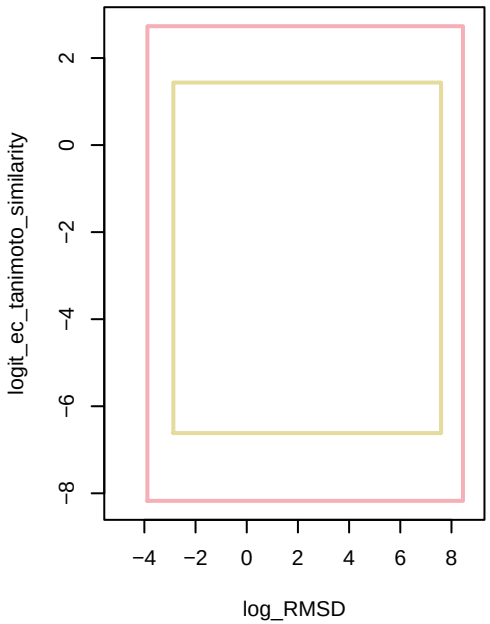

probability density
0.00
0.01
0.02
0.03
0.04
0
20
40
60
80
100
docked_HeavyAtomCount

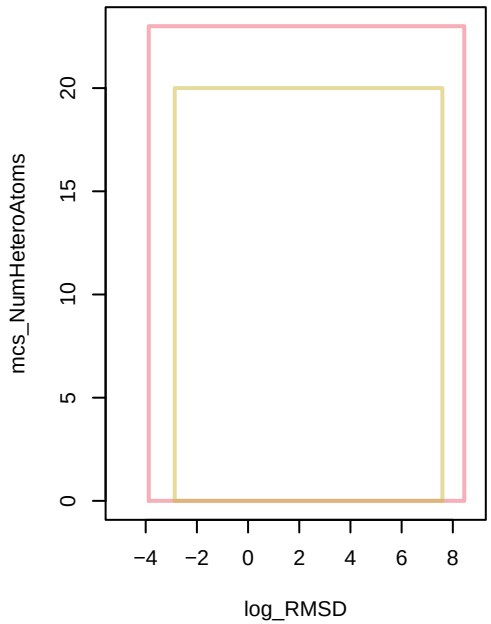

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0
2
4
6
8
mcs_RingCount

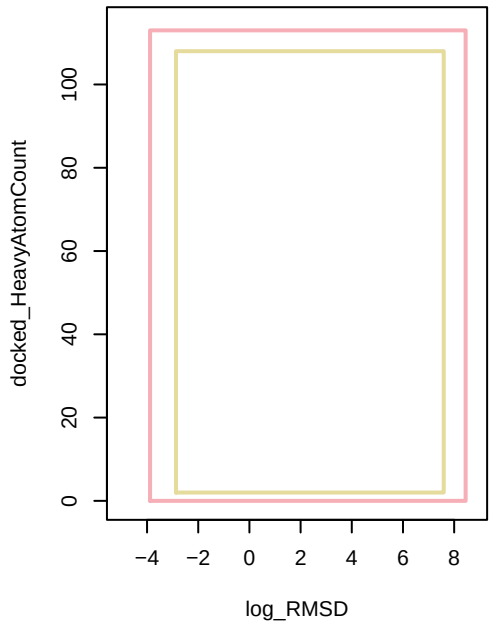

probability density
0.00
0.05
0.10
0.15
0.20
0
10
20
30
docked_NumRotatableBonds

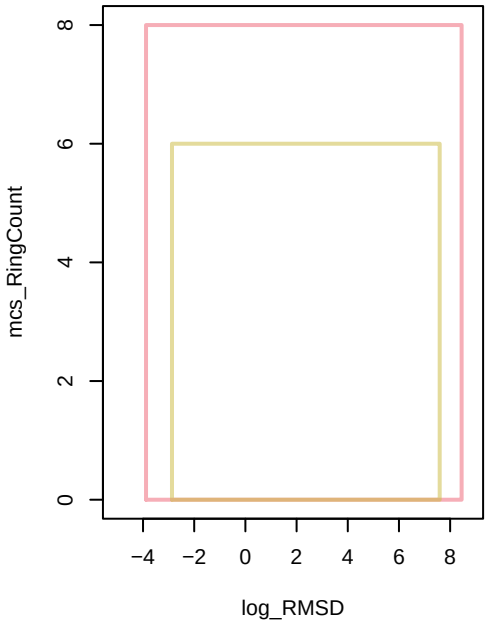

probability density
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0
5
10
15
20
mcs_NOCount

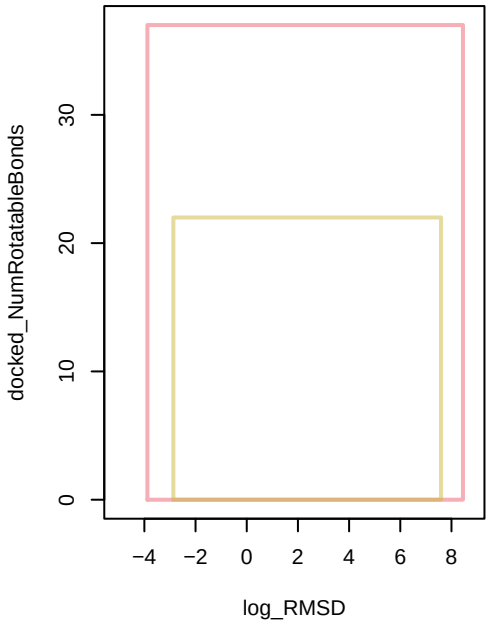

log_mcs_unbonded_polar_sasa
log_RMSD

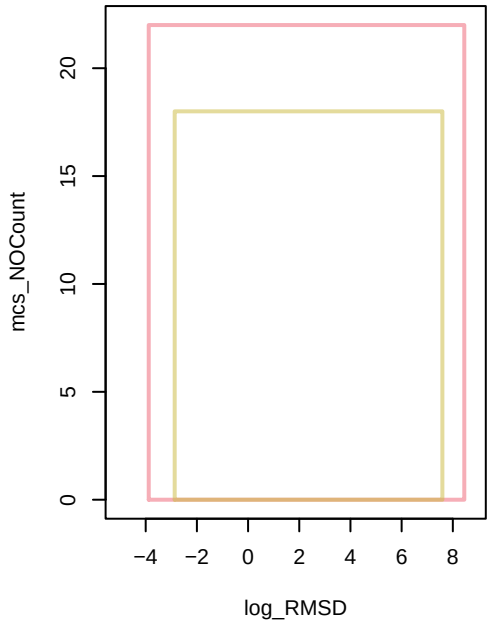

logit_ec_tanimoto_similarity
log_RMSD

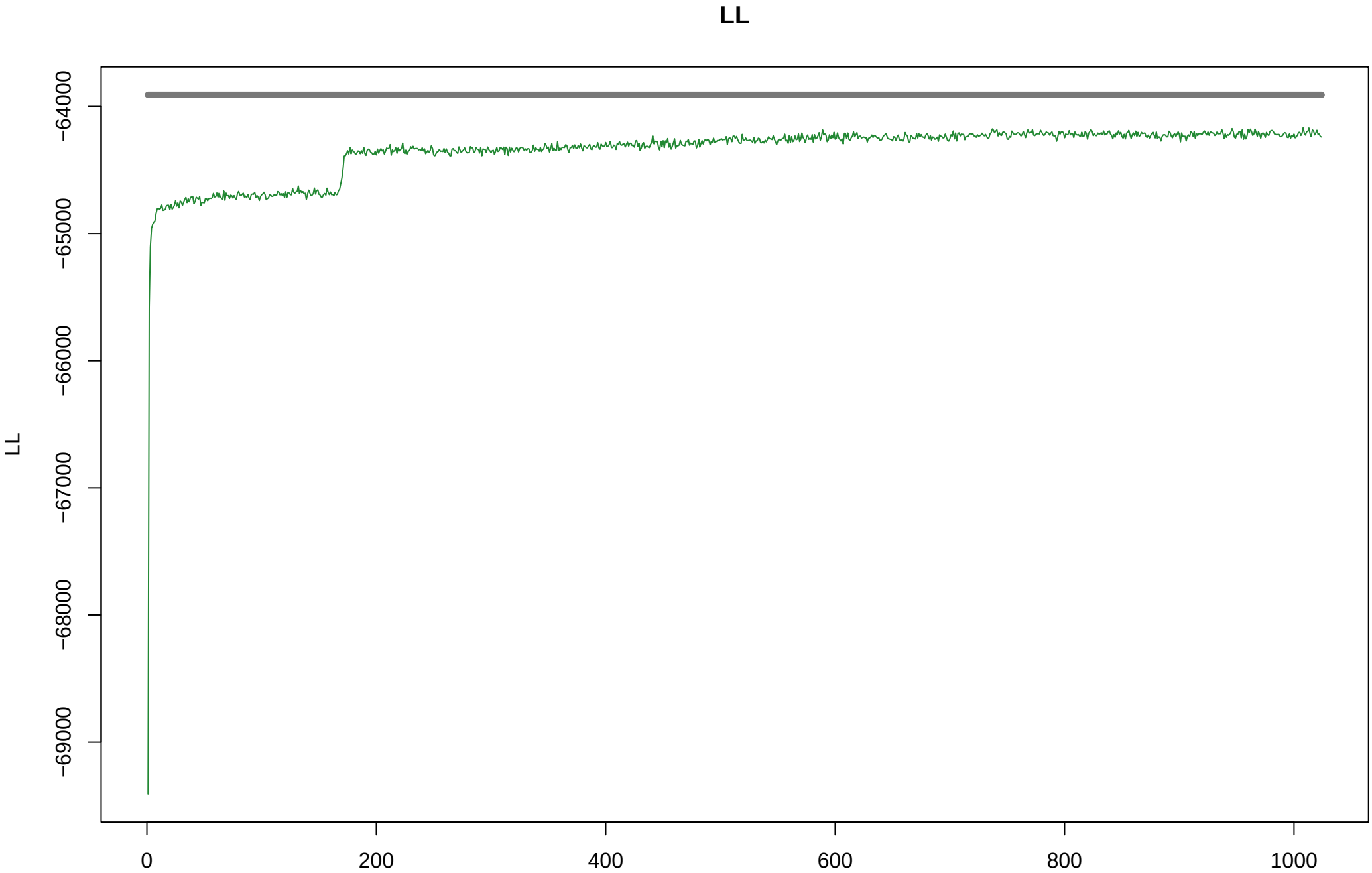

mcs_NumHeteroAtoms
log_RMSD

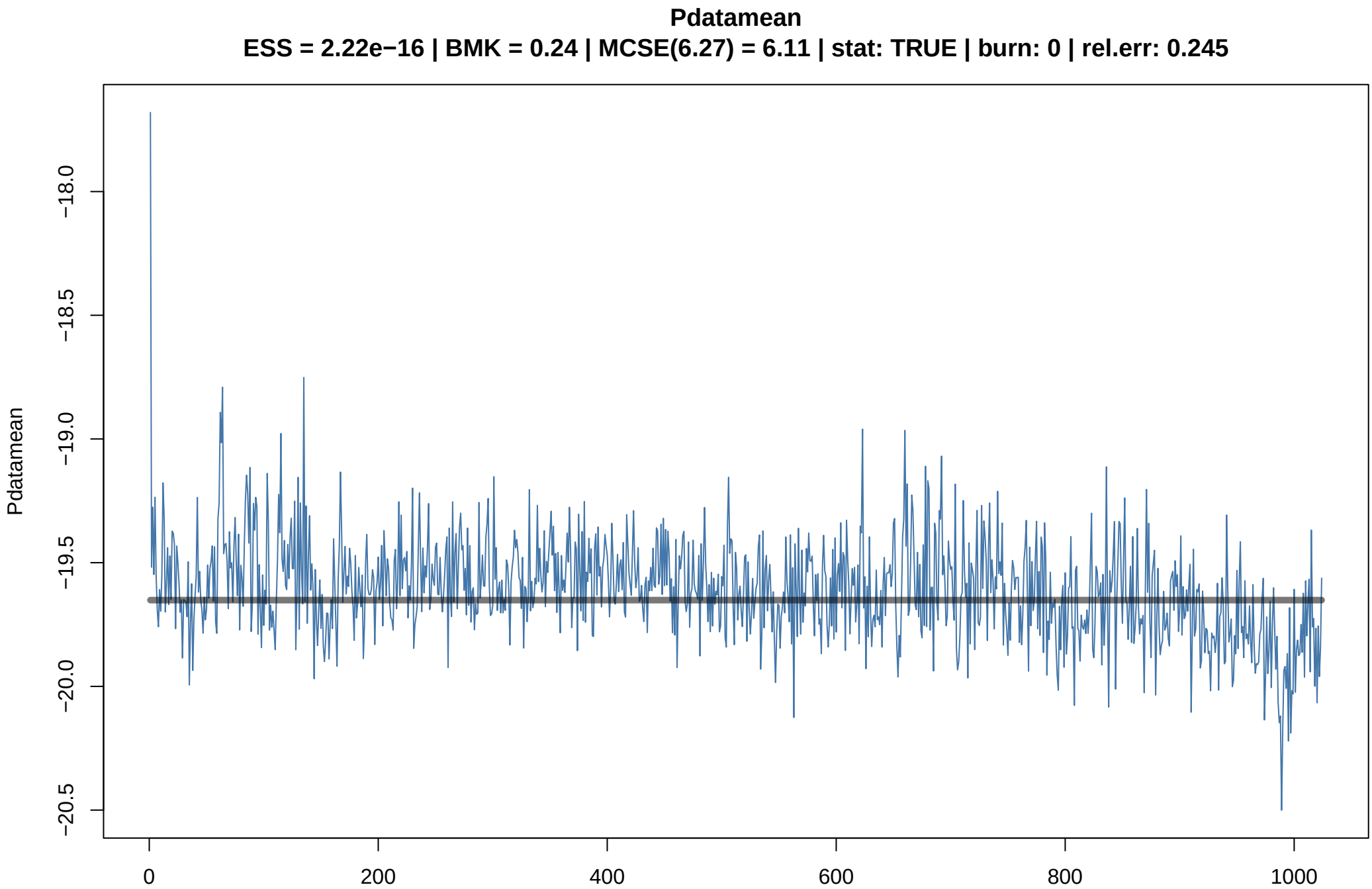

docked_HeavyAtomCount
log_RMSD

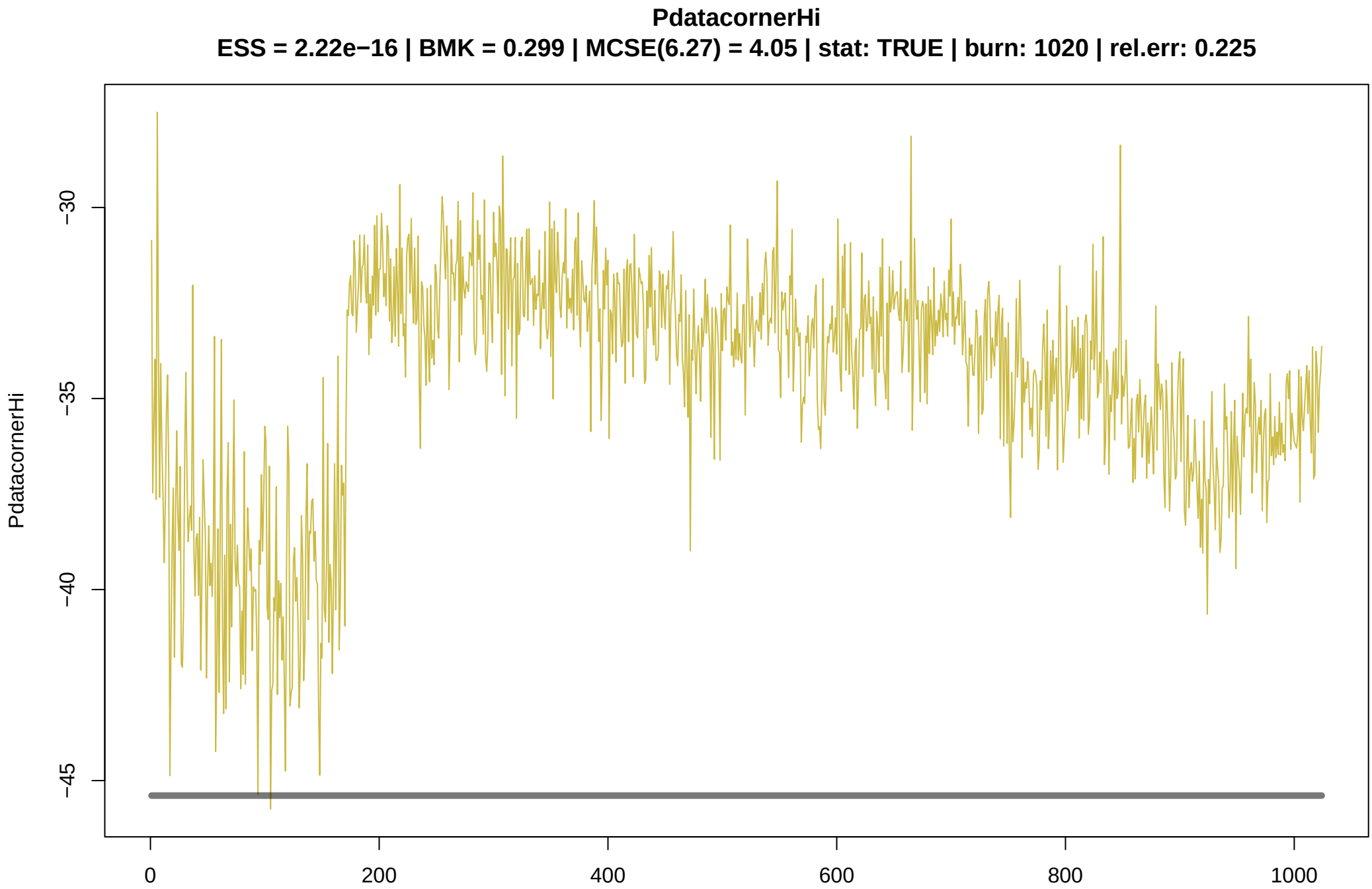

mcs_RingCount
log_RMSD

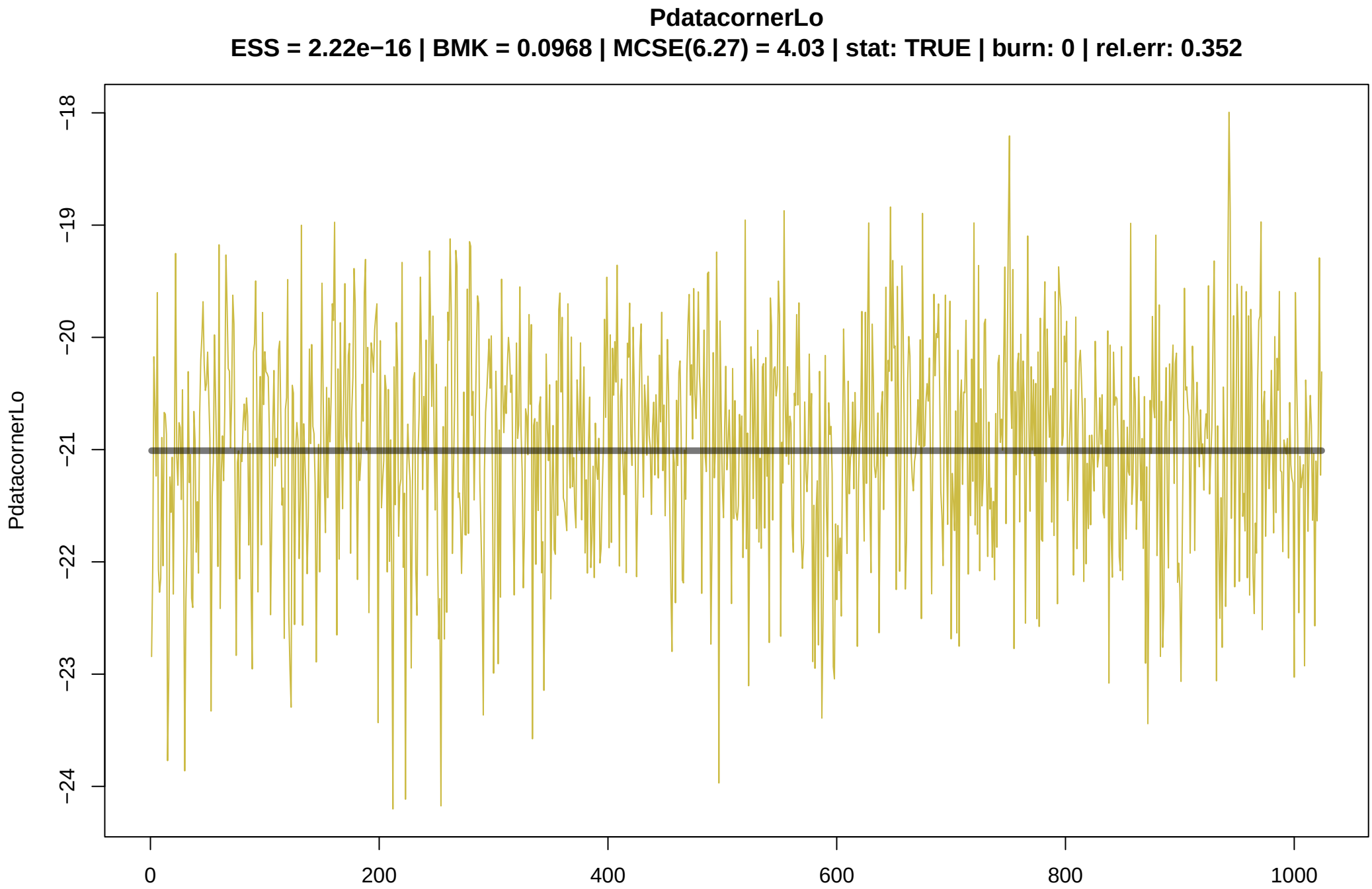

docked_NumRotatableBonds
log_RMSD

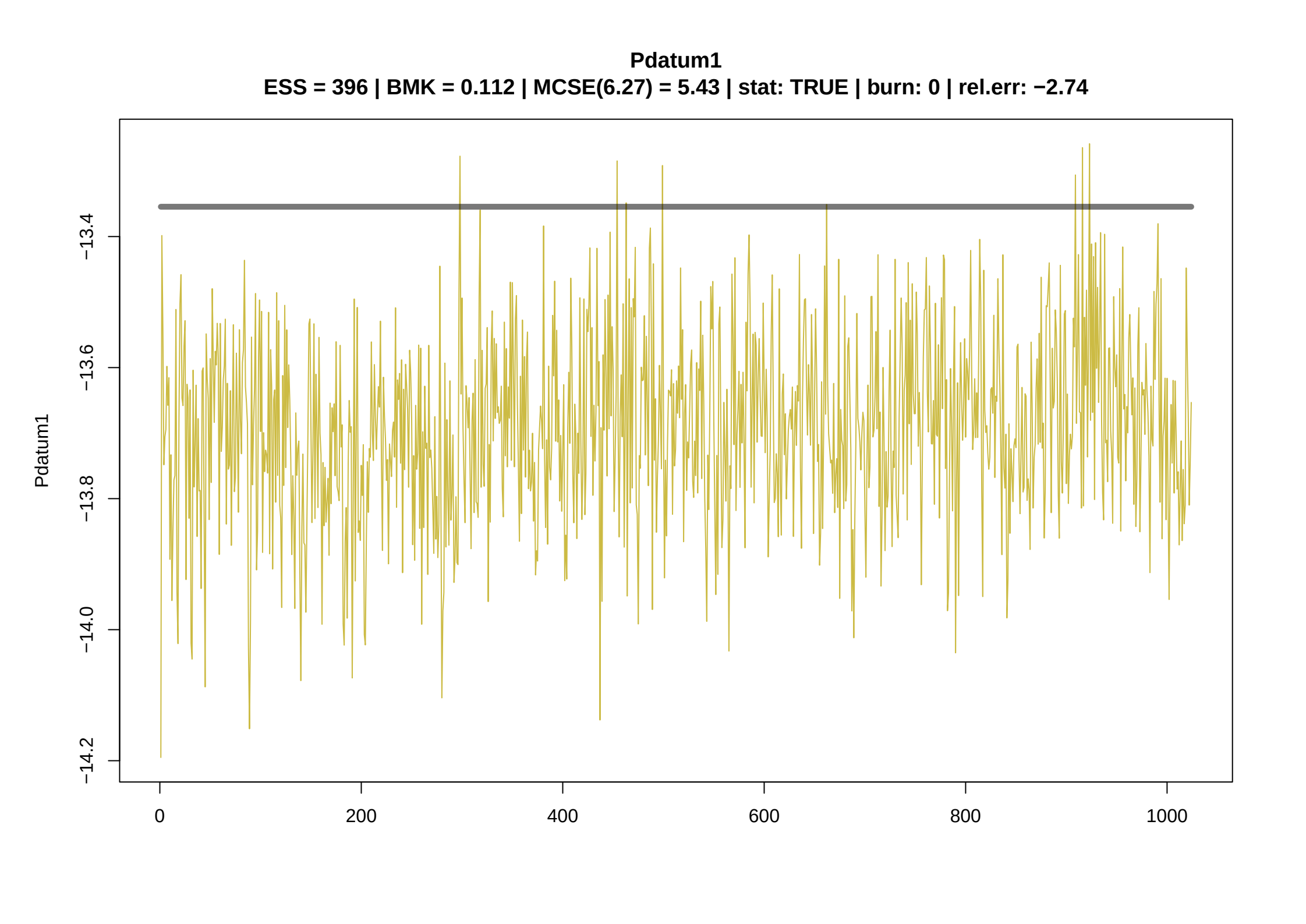

mcs_NOCount
log_RMSD

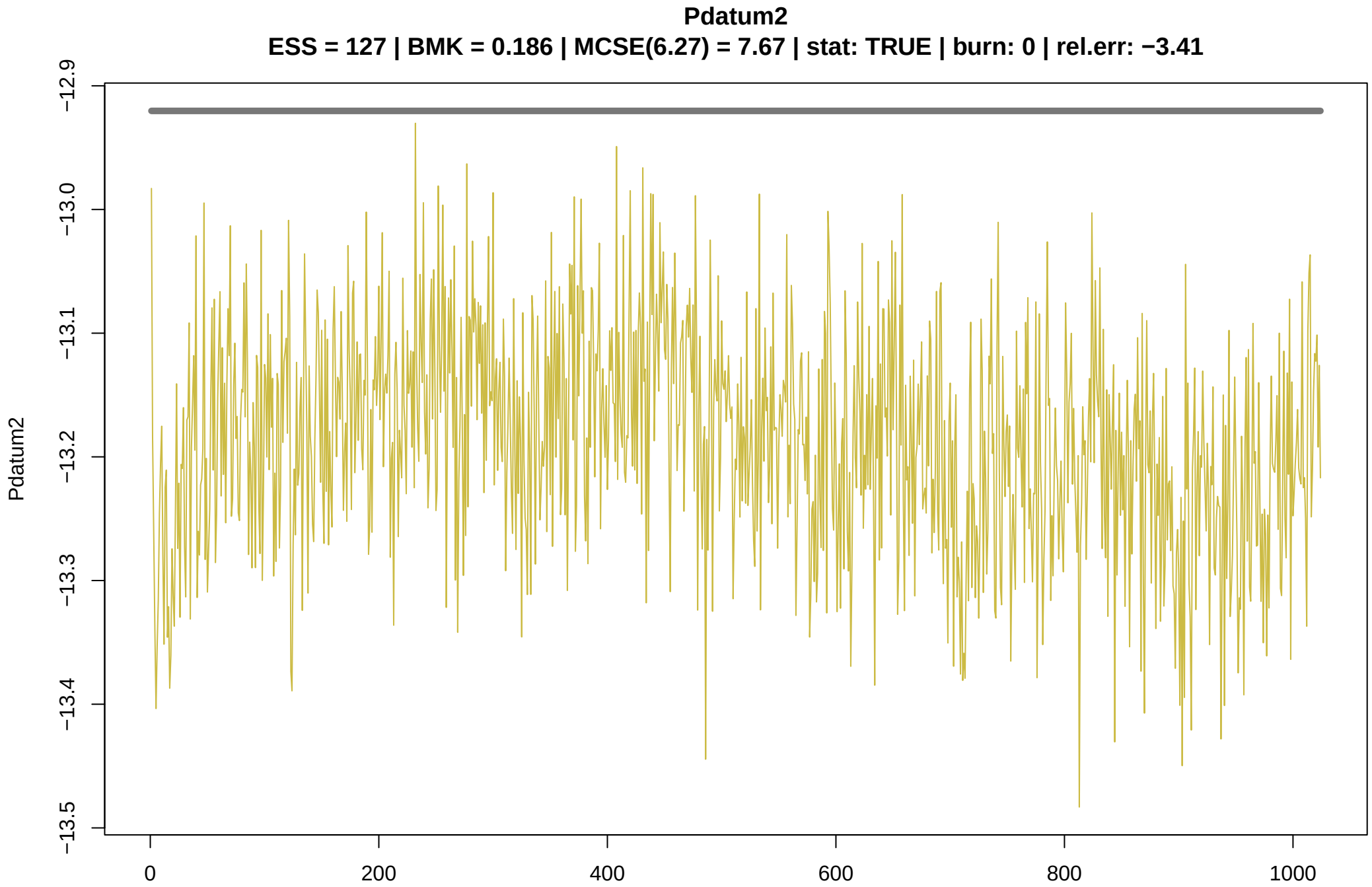

LL
LL
−64000
−65000
−66000
−67000
−68000
−69000
0
200
400
600
800
1000

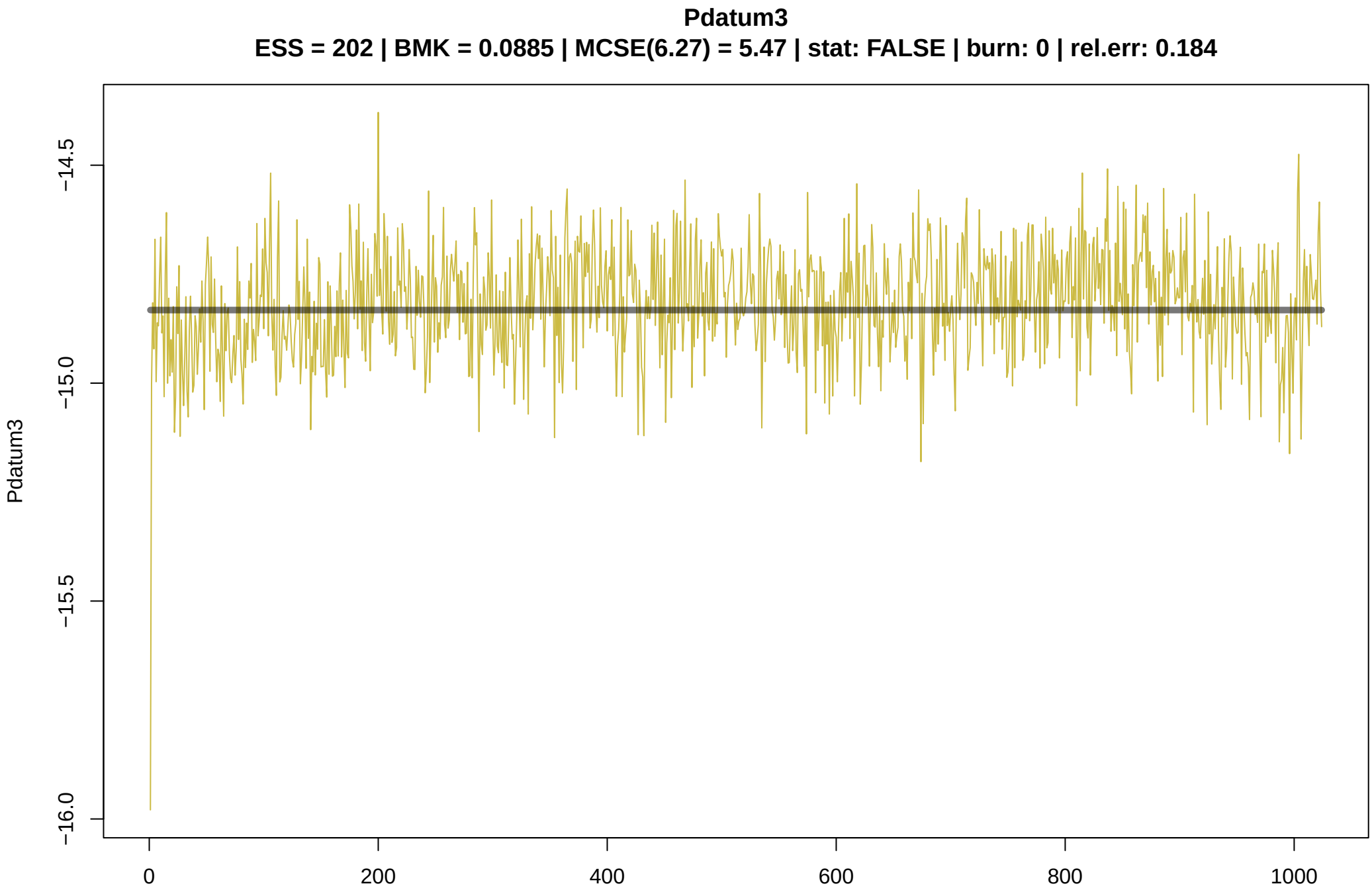

Pdatamean
ESS = 2.22e−16 | BMK = 0.24 | MCSE(6.27) = 6.11 | stat: TRUE | burn: 0 | rel.err: 0.245
Pdatamean
−18.0
−18.5
−19.0
−19.5
−20.0
−20.5
0
200
400
600
800
1000

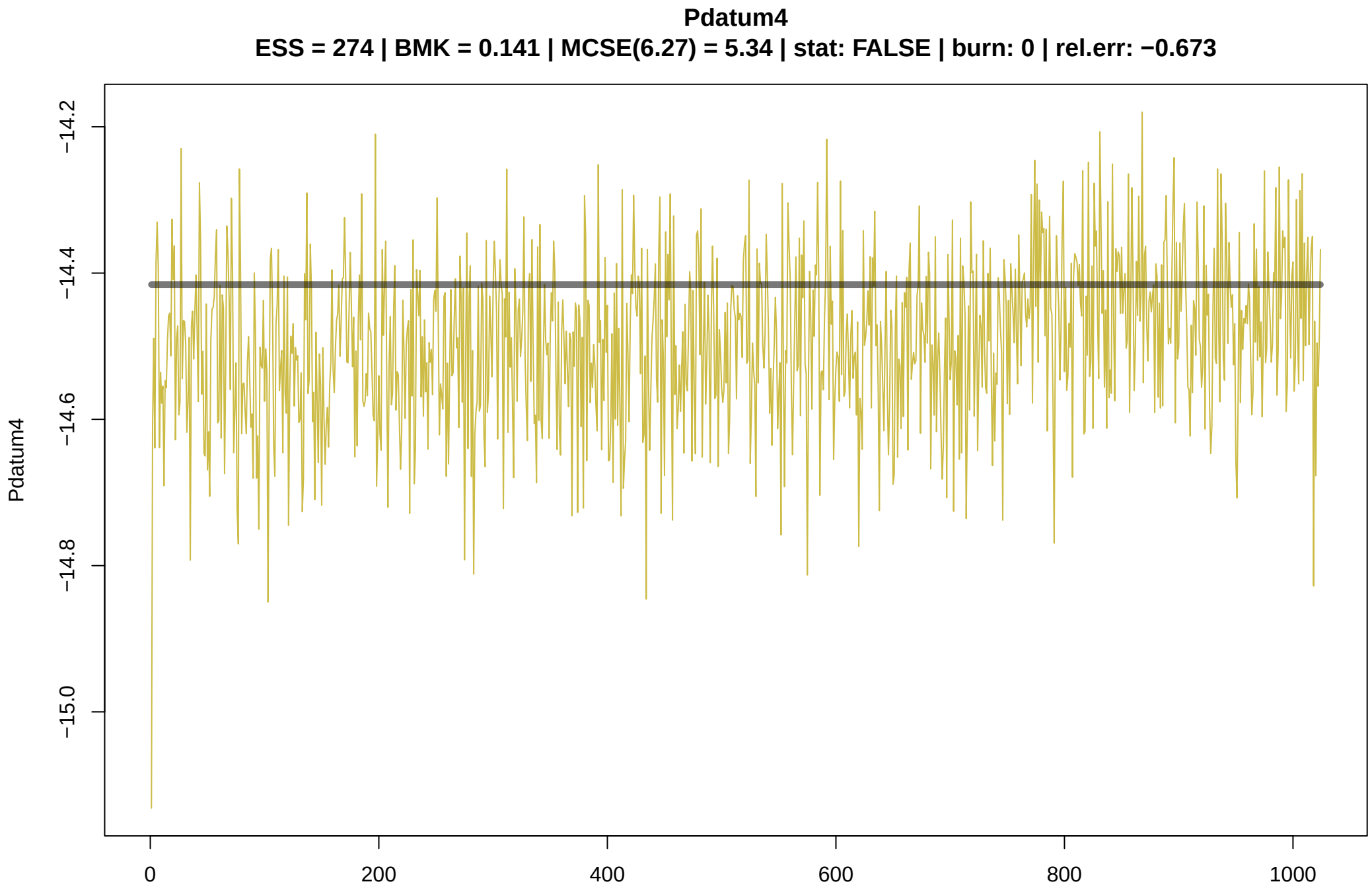

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.299 | MCSE(6.27) = 4.05 | stat: TRUE | burn: 1020 | rel.err: 0.225
PdatacornerHi
−30
−35
−40
−45
0
200
400
600
800
1000

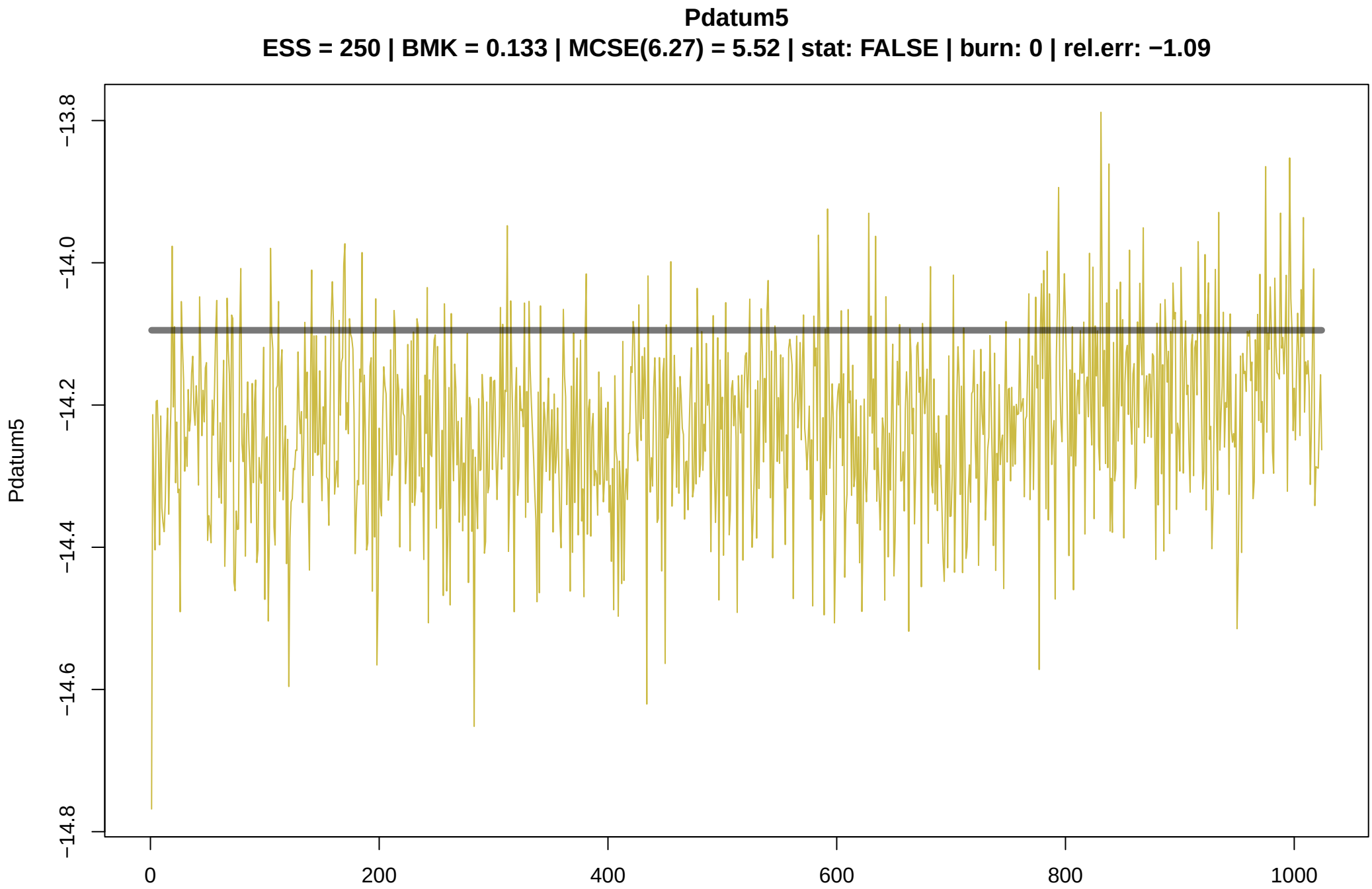

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.0968 | MCSE(6.27) = 4.03 | stat: TRUE | burn: 0 | rel.err: 0.352
PdatacornerLo
−18
−19
−20
−21
−22
−23
−24
0
200
400
600
800
1000

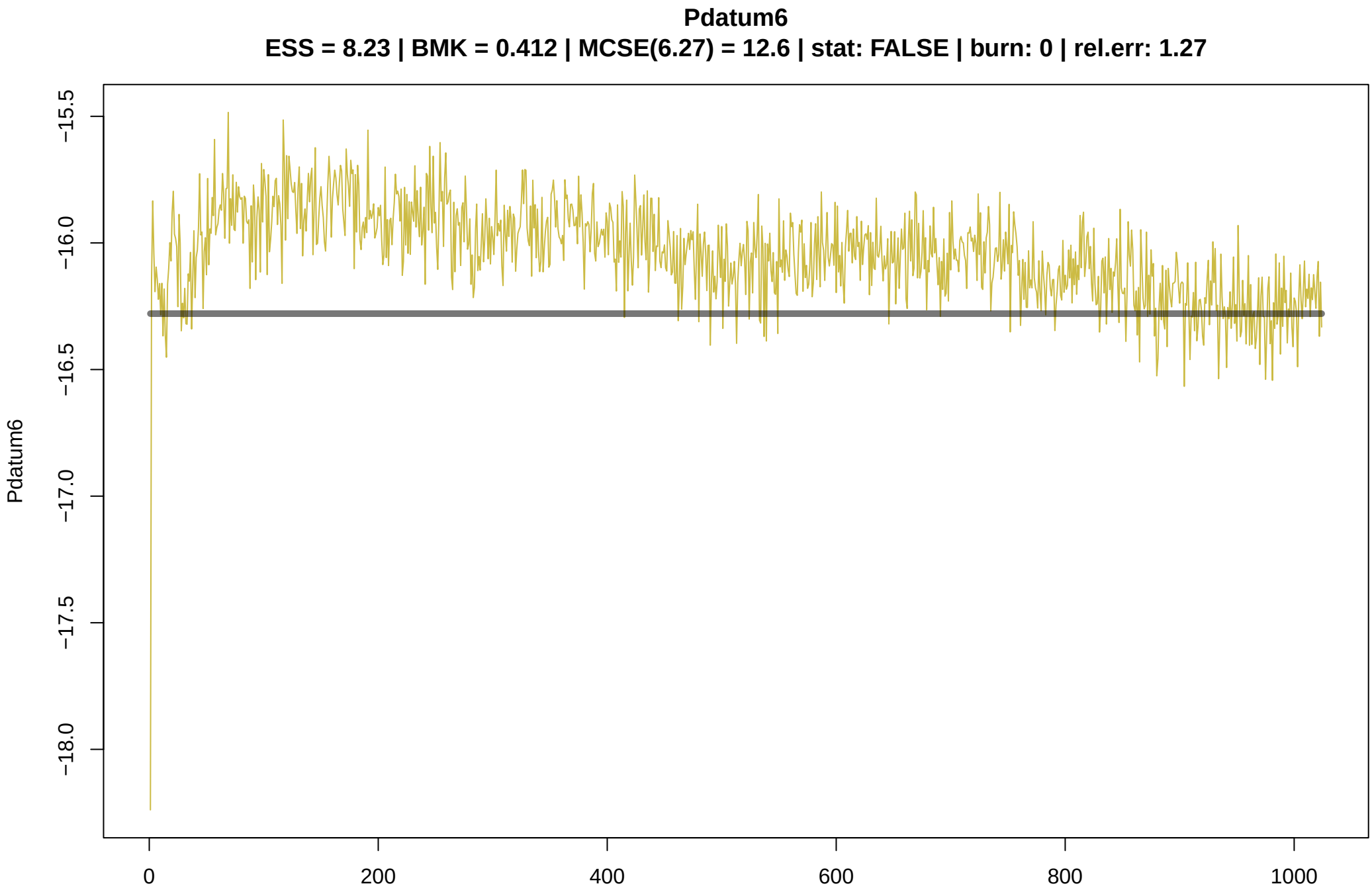

Pdatum1
ESS = 396 | BMK = 0.112 | MCSE(6.27) = 5.43 | stat: TRUE | burn: 0 | rel.err: −2.74
Pdatum1
−13.4
−13.6
−13.8
−14.0
−14.2
0
200
400
600
800
1000

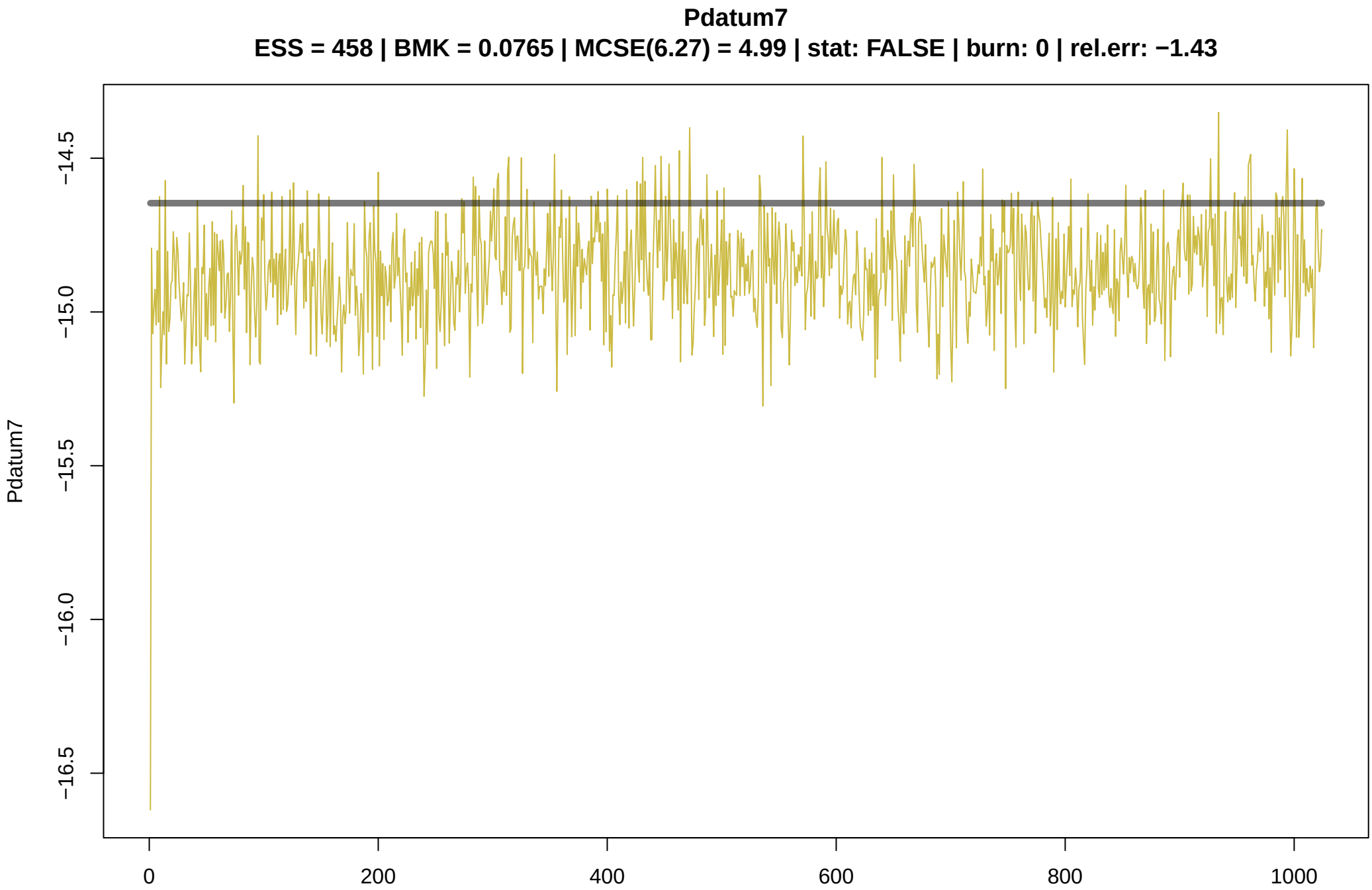

Pdatum2
ESS = 127 | BMK = 0.186 | MCSE(6.27) = 7.67 | stat: TRUE | burn: 0 | rel.err: −3.41
Pdatum2
−12.9
−13.0
−13.1
−13.2
−13.3
−13.4
−13.5
0
200
400
600
800
1000

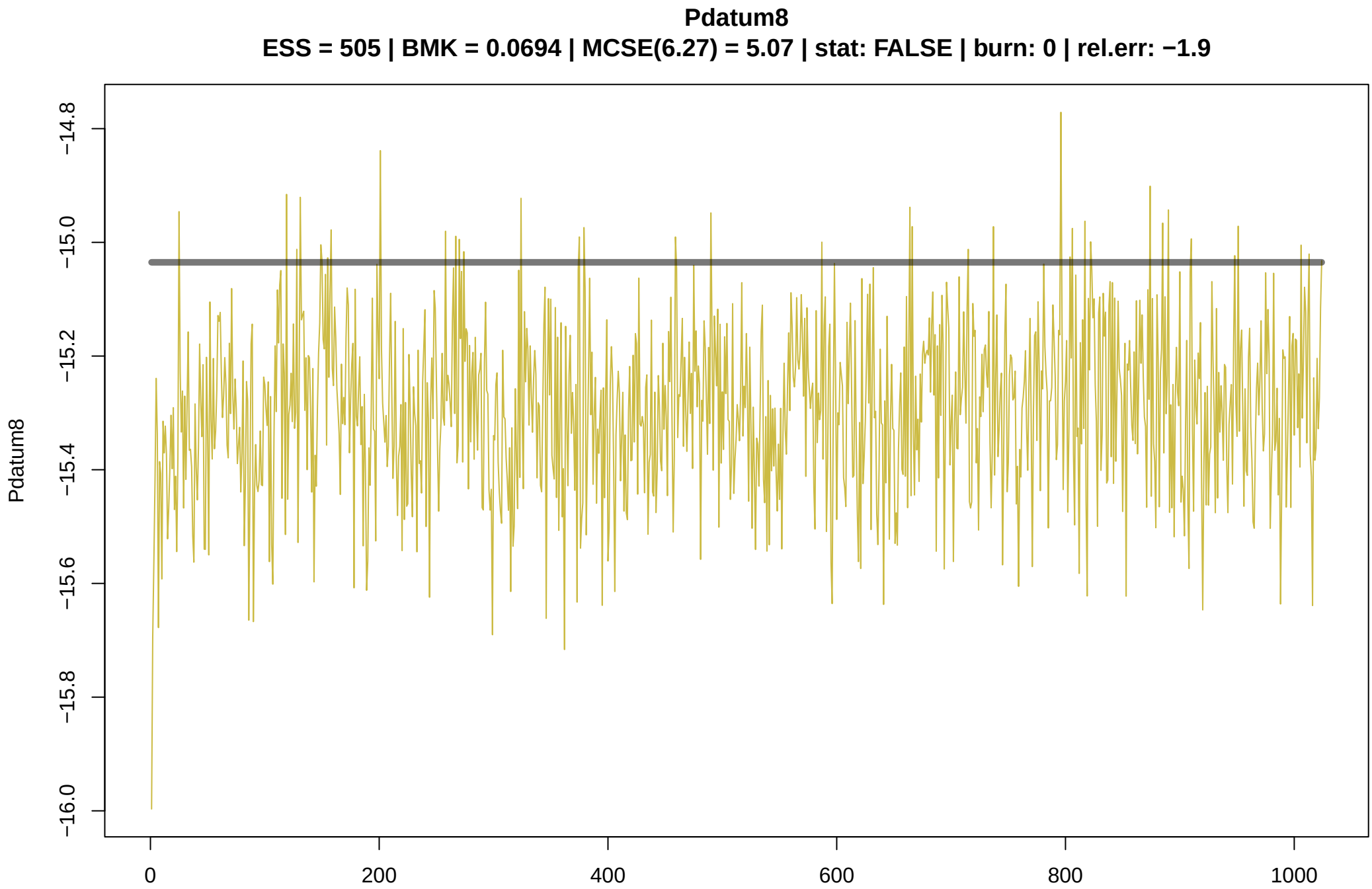

Pdatum3
ESS = 202 | BMK = 0.0885 | MCSE(6.27) = 5.47 | stat: FALSE | burn: 0 | rel.err: 0.184
Pdatum3
−14.5
−15.0
−15.5
−16.0
0
200
400
600
800
1000

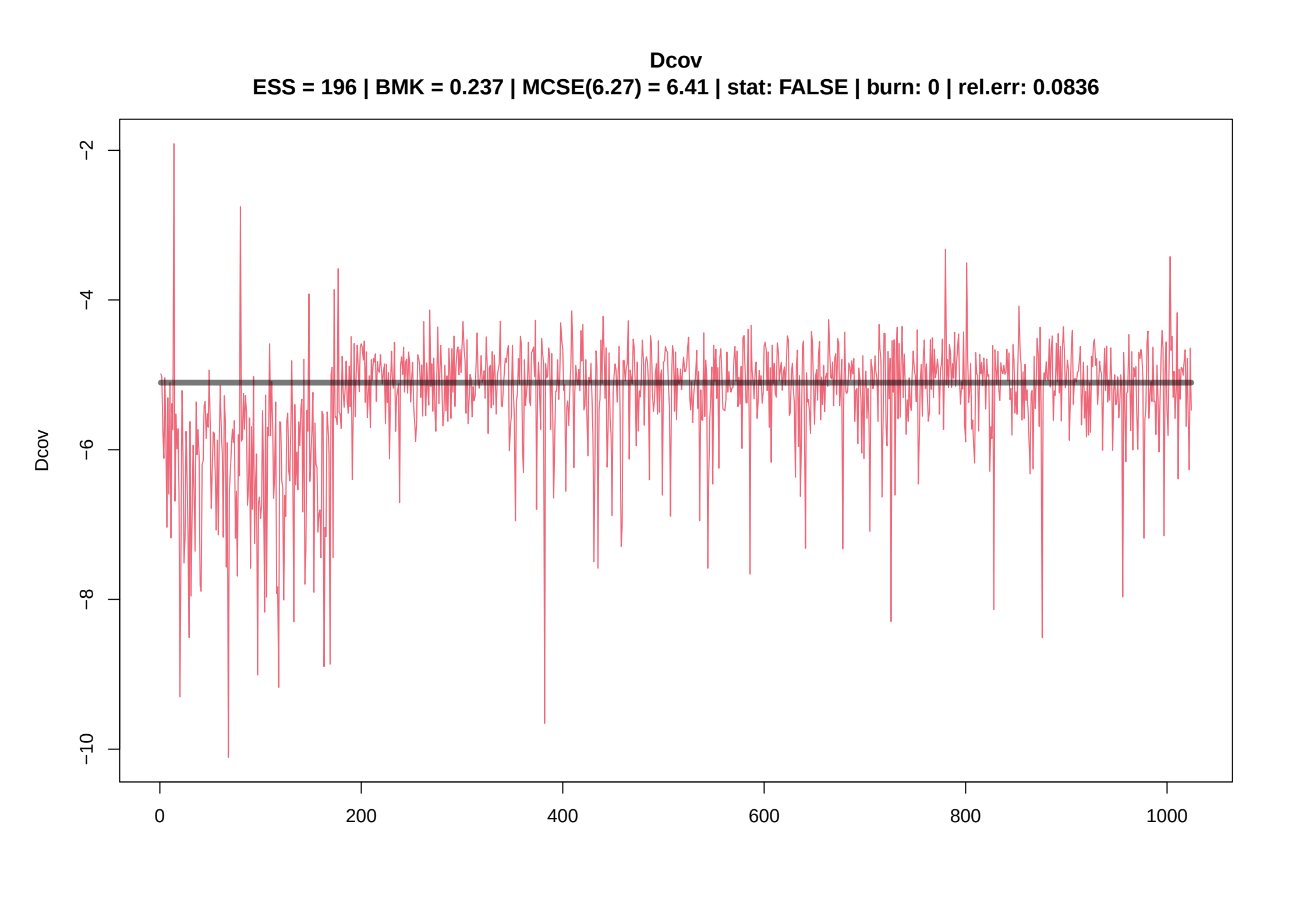

Pdatum4
ESS = 274 | BMK = 0.141 | MCSE(6.27) = 5.34 | stat: FALSE | burn: 0 | rel.err: −0.673
Pdatum4
−14.2
−14.4
−14.6
−14.8
−15.0
0
200
400
600
800
1000

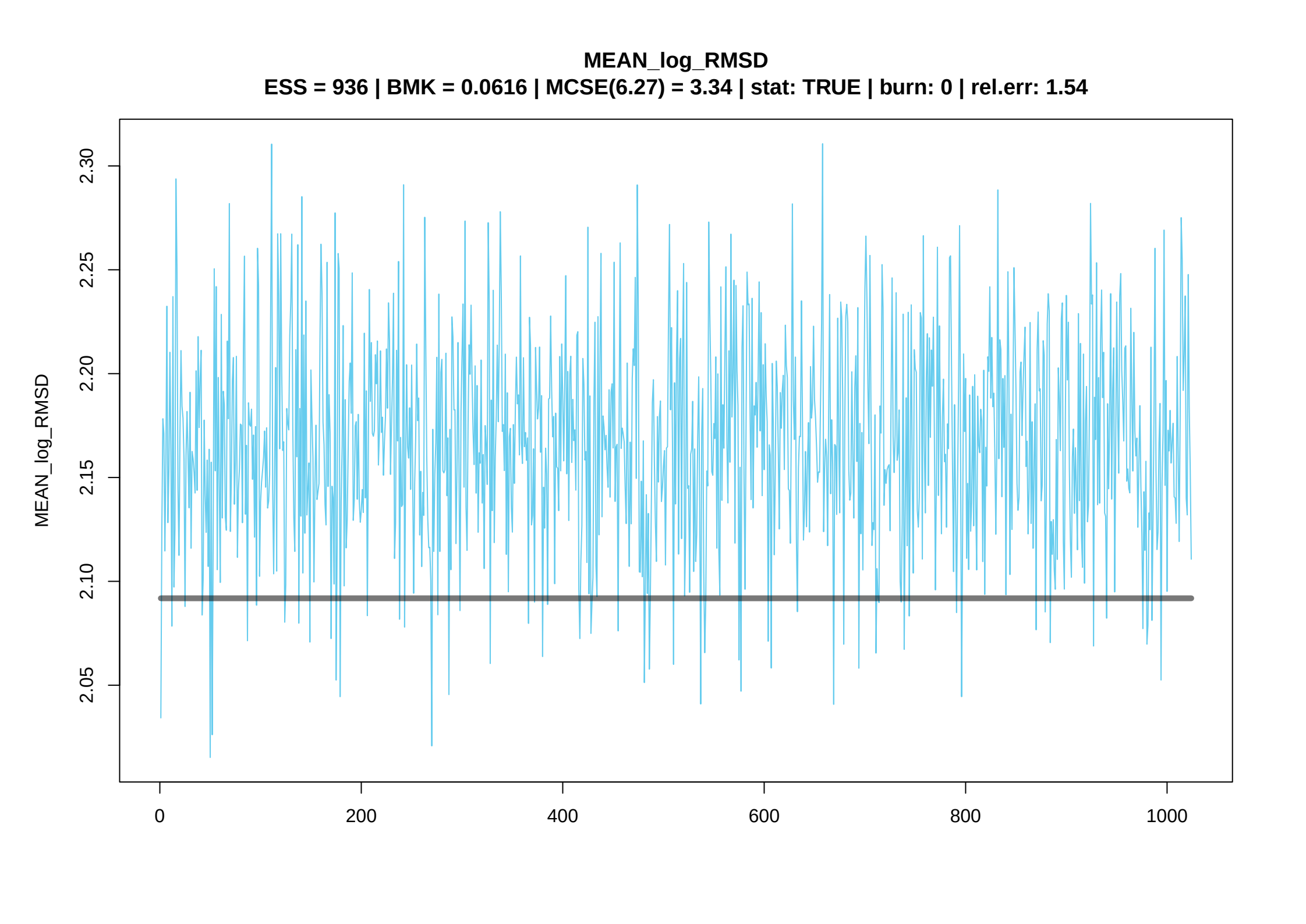

Pdatum5
ESS = 250 | BMK = 0.133 | MCSE(6.27) = 5.52 | stat: FALSE | burn: 0 | rel.err: −1.09
Pdatum5
−13.8
−14.0
−14.2
−14.4
−14.6
−14.8
0
200
400
600
800
1000

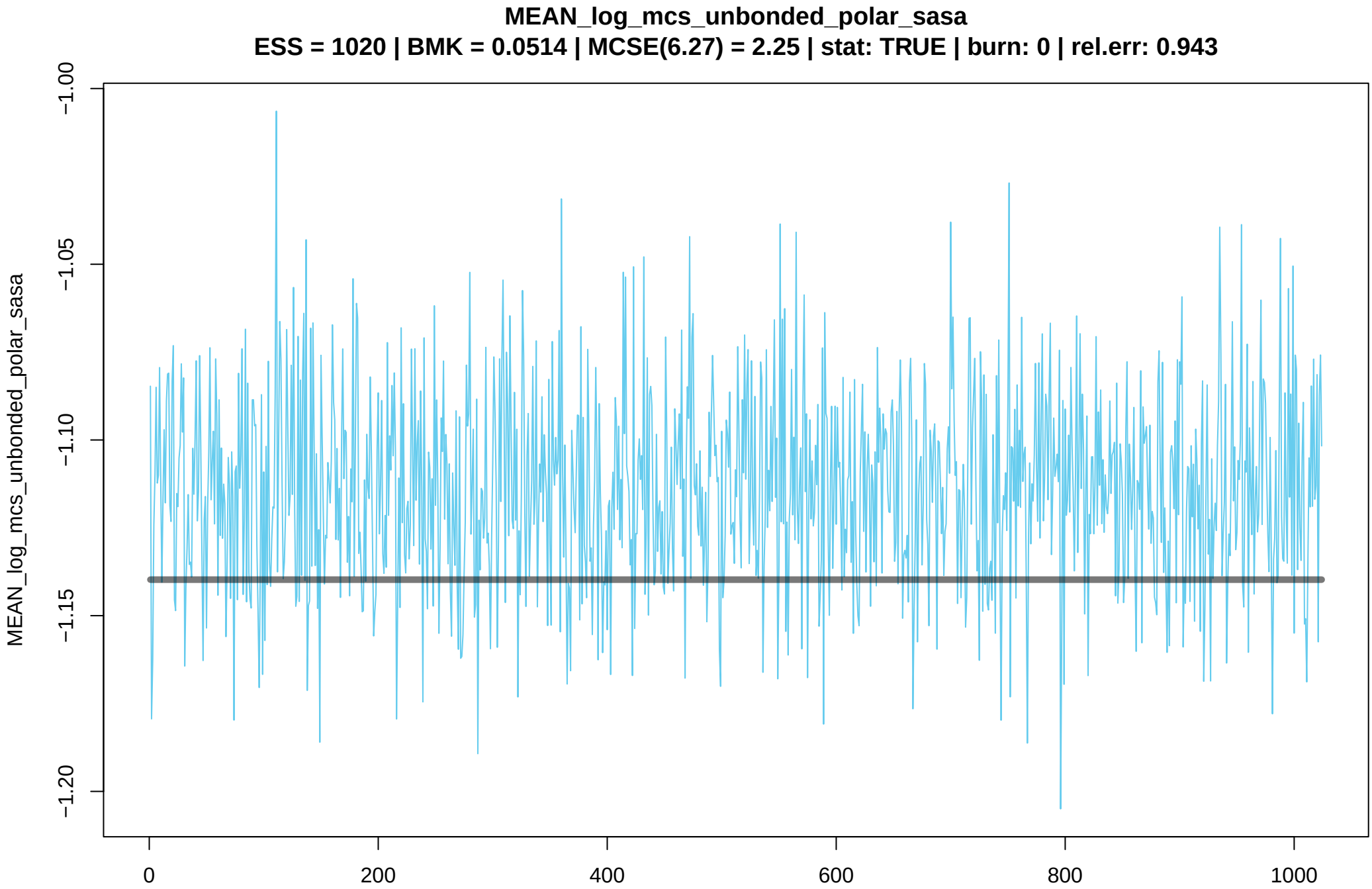

Pdatum6
ESS = 8.23 | BMK = 0.412 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 0 | rel.err: 1.27
Pdatum6
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
0
200
400
600
800
1000

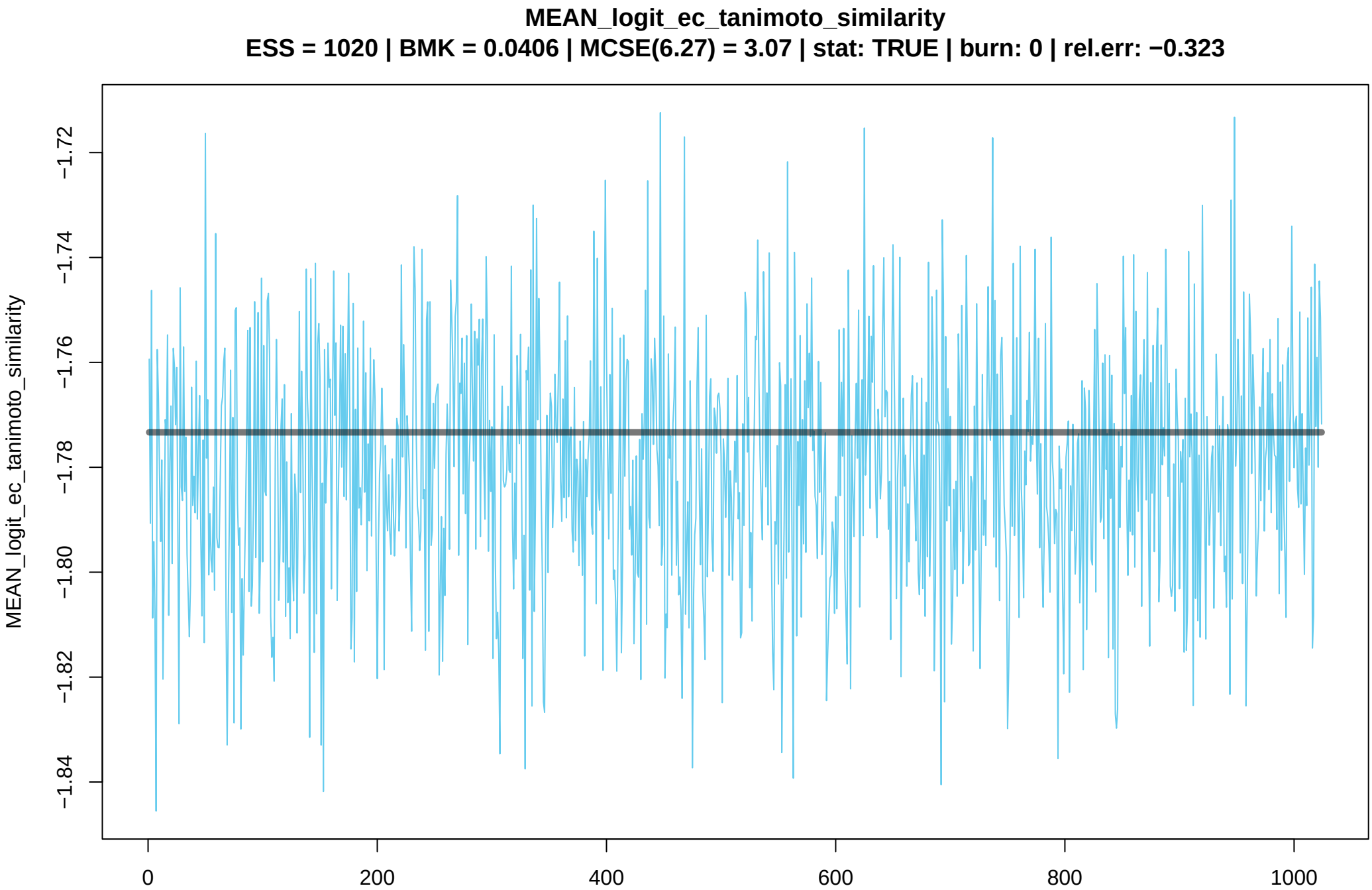

Pdatum7
ESS = 458 | BMK = 0.0765 | MCSE(6.27) = 4.99 | stat: FALSE | burn: 0 | rel.err: −1.43
Pdatum7
−14.5
−15.0
−15.5
−16.0
−16.5
0
200
400
600
800
1000

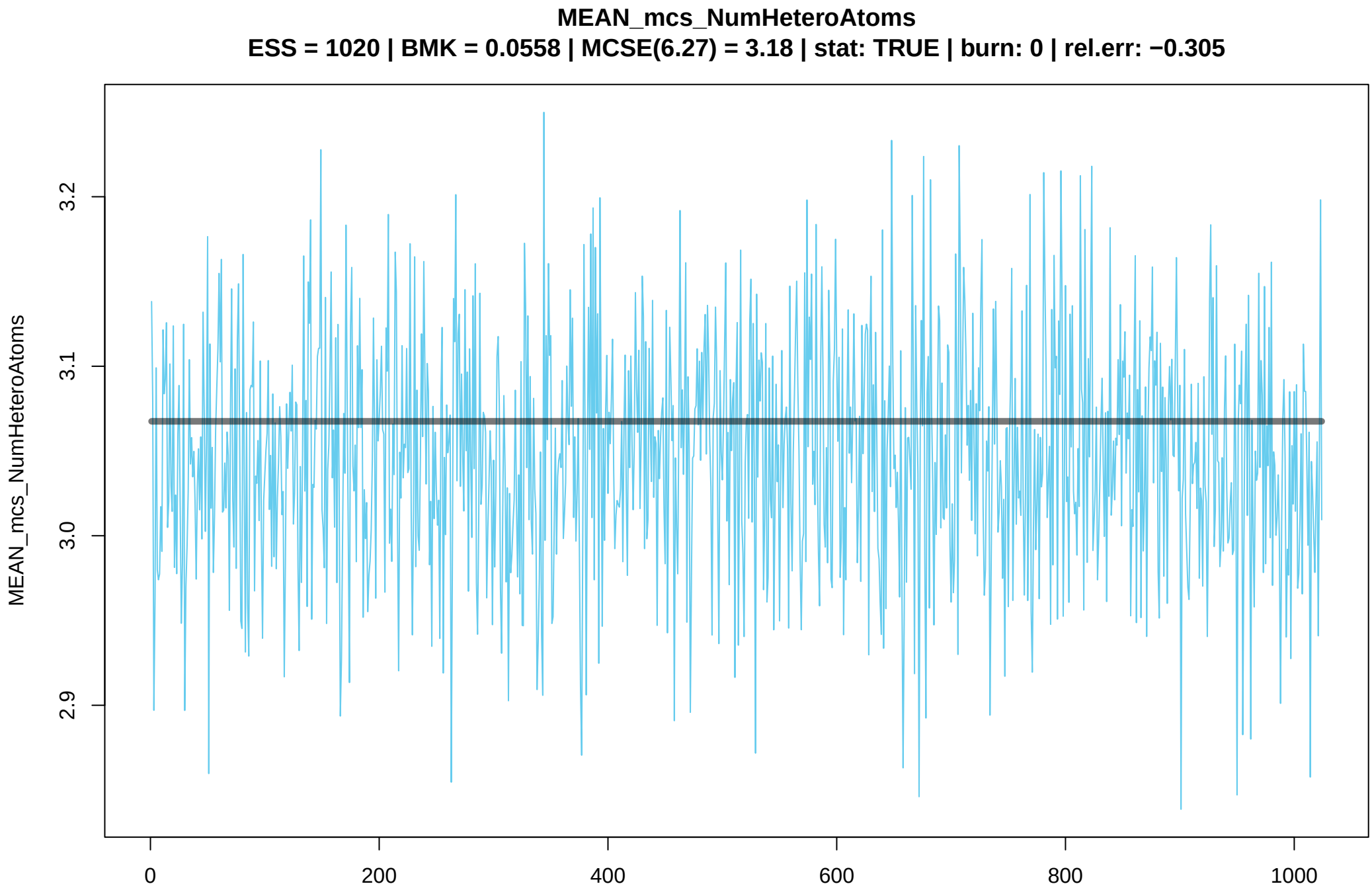

Pdatum8
ESS = 505 | BMK = 0.0694 | MCSE(6.27) = 5.07 | stat: FALSE | burn: 0 | rel.err: −1.9
Pdatum8
−14.8
−15.0
−15.2
−15.4
−15.6
−15.8
−16.0
0
200
400
600
800
1000

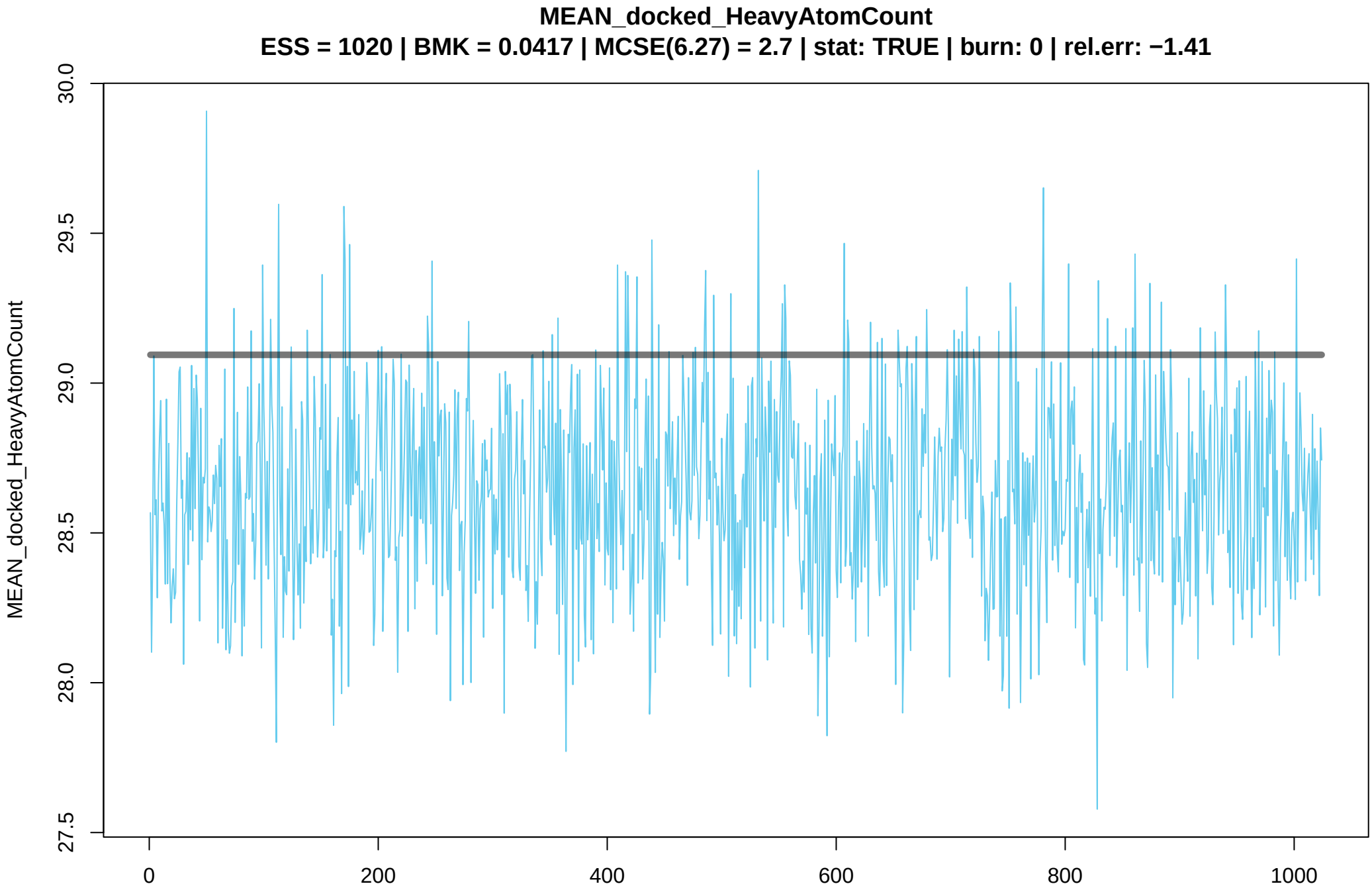

Dcov
ESS = 196 | BMK = 0.237 | MCSE(6.27) = 6.41 | stat: FALSE | burn: 0 | rel.err: 0.0836
Dcov
−2
−4
−6
−8
−10
0
200
400
600
800
1000

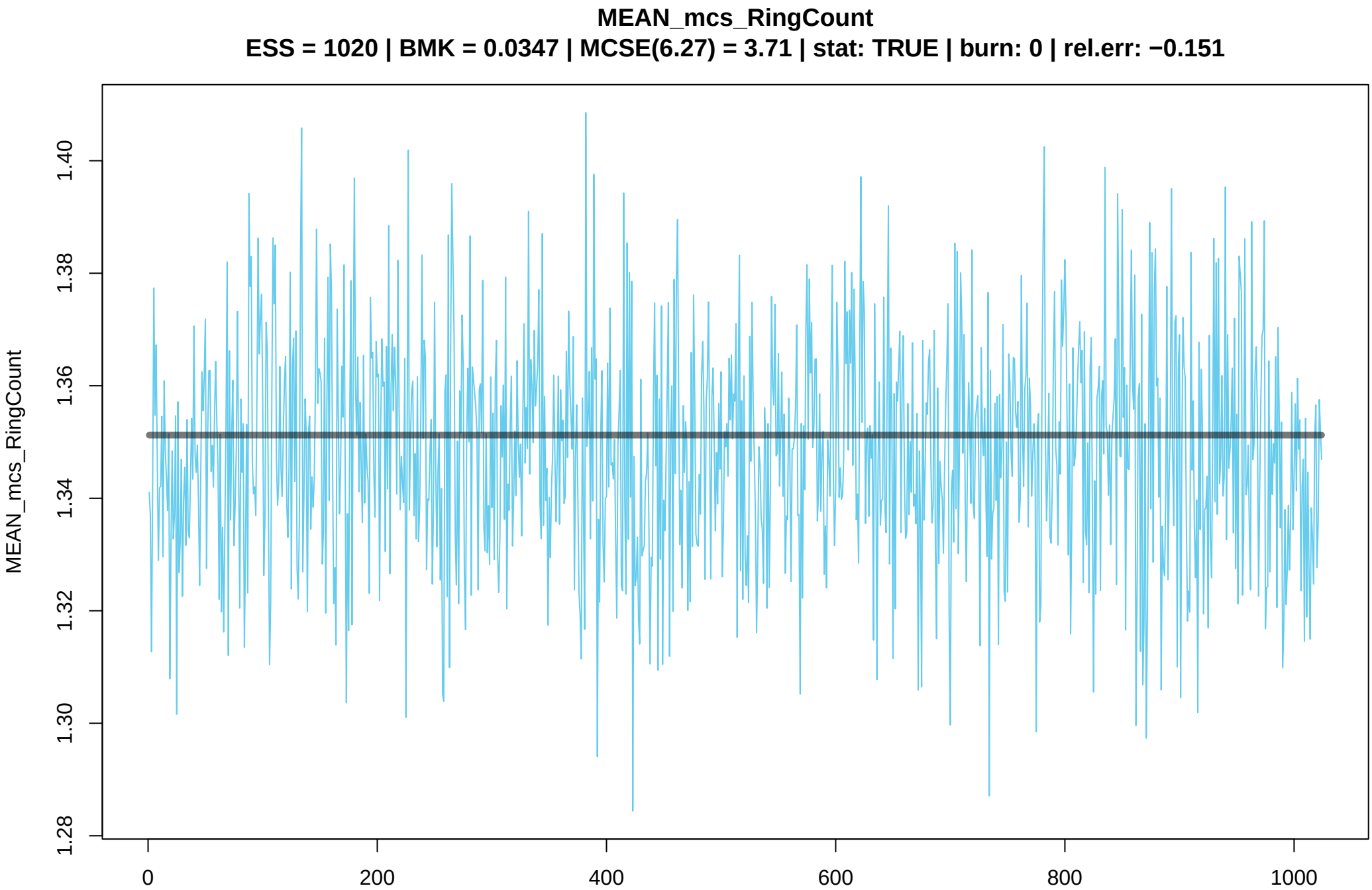

MEAN_log_RMSD
ESS = 936 | BMK = 0.0616 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0 | rel.err: 1.54
MEAN_log_RMSD
2.05
2.10
2.15
2.20
2.25
2.30
0
200
400
600
800
1000

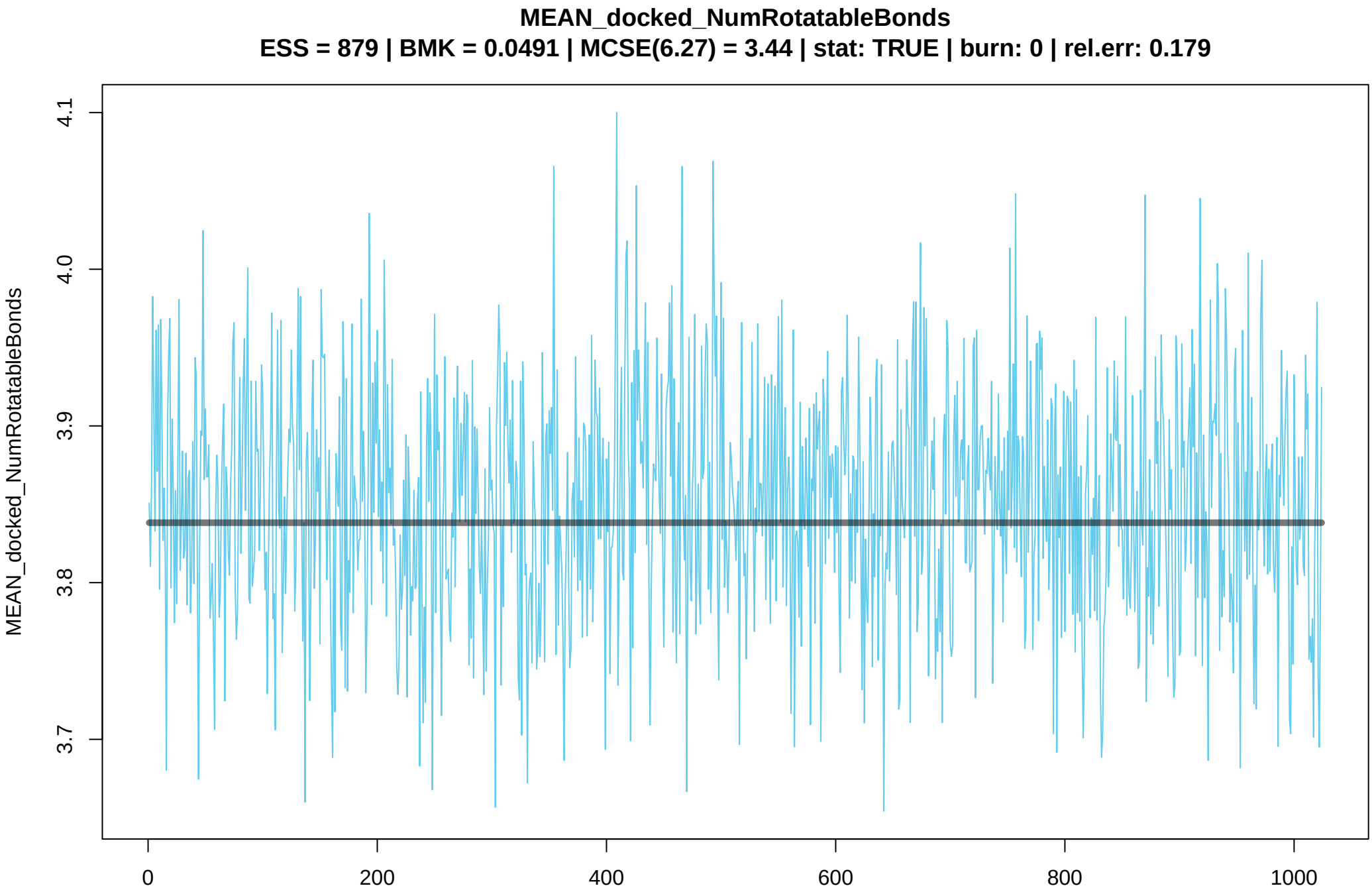

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0514 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | rel.err: 0.943
MEAN_log_mcs_unbonded_polar_sasa
−1.00
−1.05
−1.10
−1.15
−1.20
0
200
400
600
800
1000

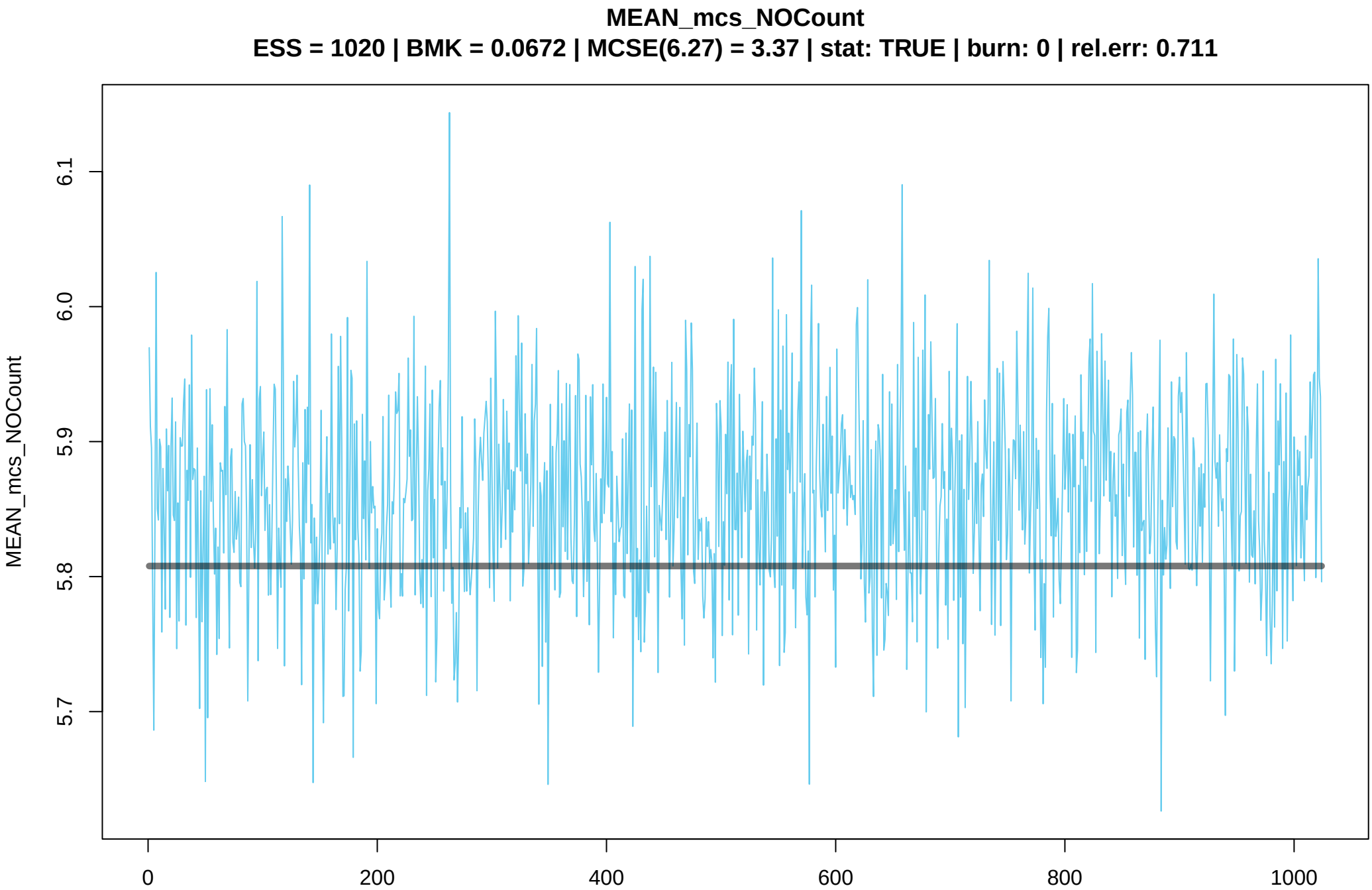

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0406 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | rel.err: −0.323
MEAN_logit_ec_tanimoto_similarity
−1.72
−1.74
−1.76
−1.78
−1.80
−1.82
−1.84
0
200
400
600
800
1000

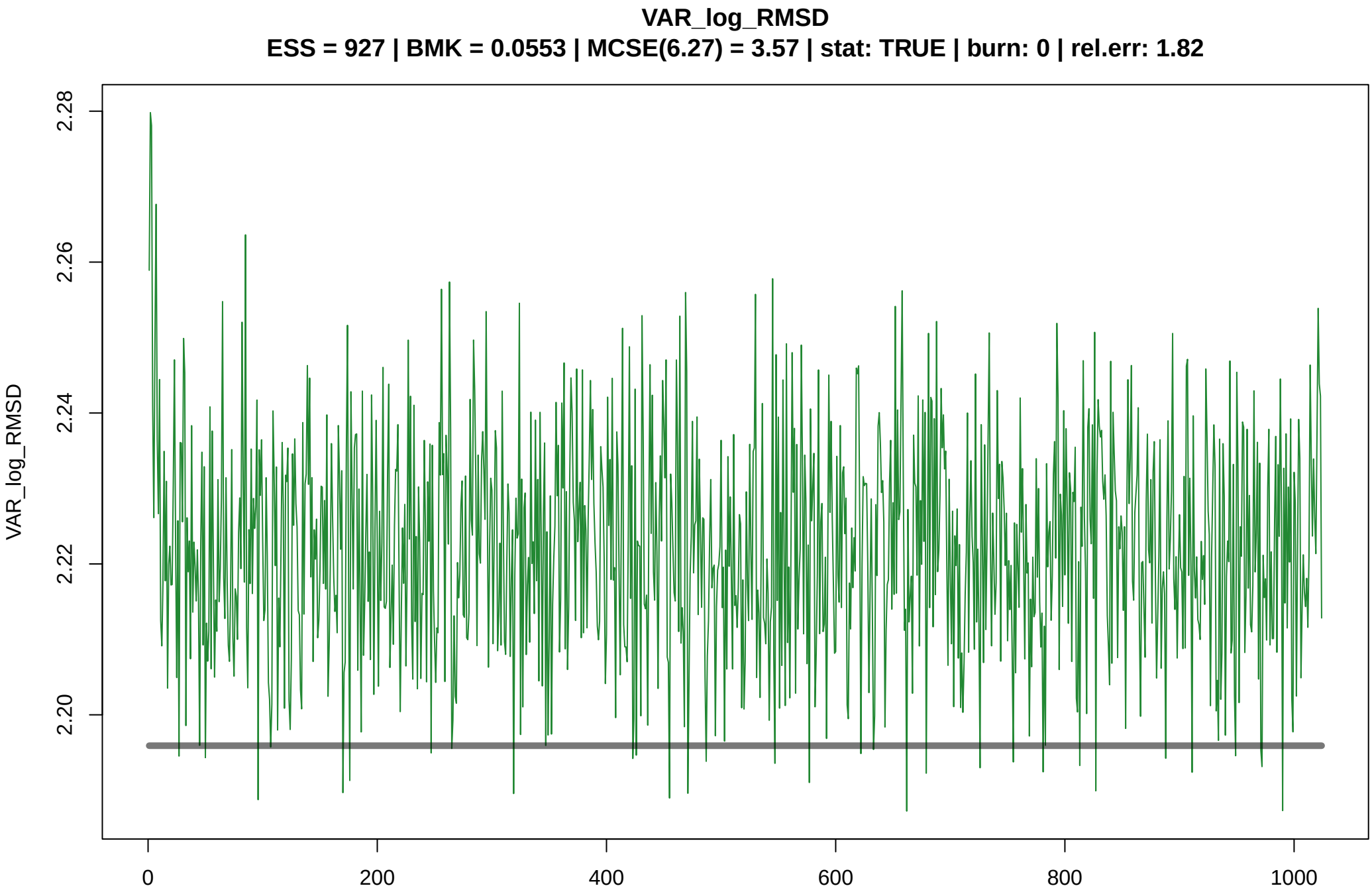

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0558 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | rel.err: −0.305
MEAN_mcs_NumHeteroAtoms
2.9
3.0
3.1
3.2
0
200
400
600
800
1000

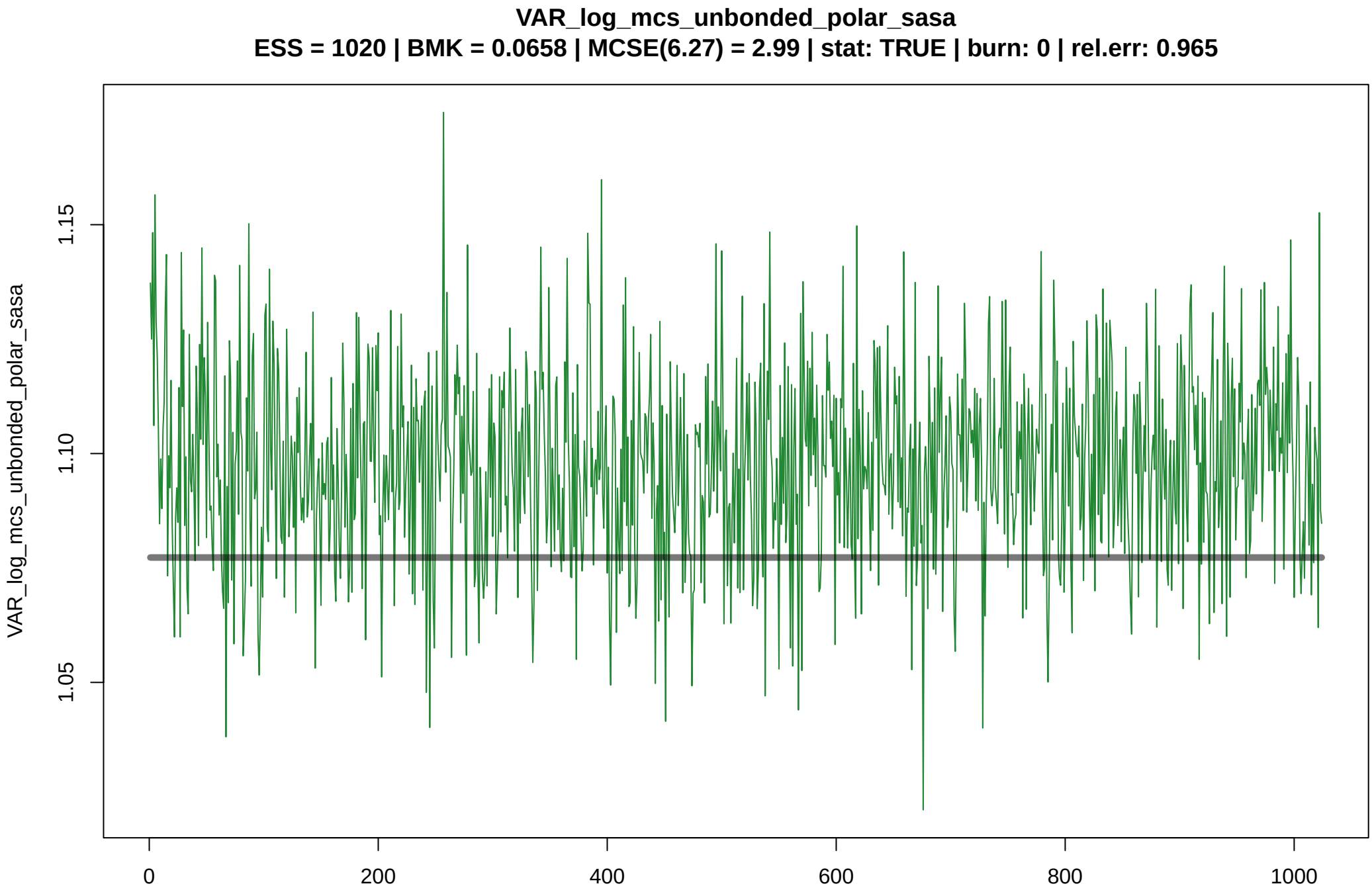

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0417 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | rel.err: −1.41
MEAN_docked_HeavyAtomCount
30.0
29.5
29.0
28.5
28.0
27.5
0
200
400
600
800
1000

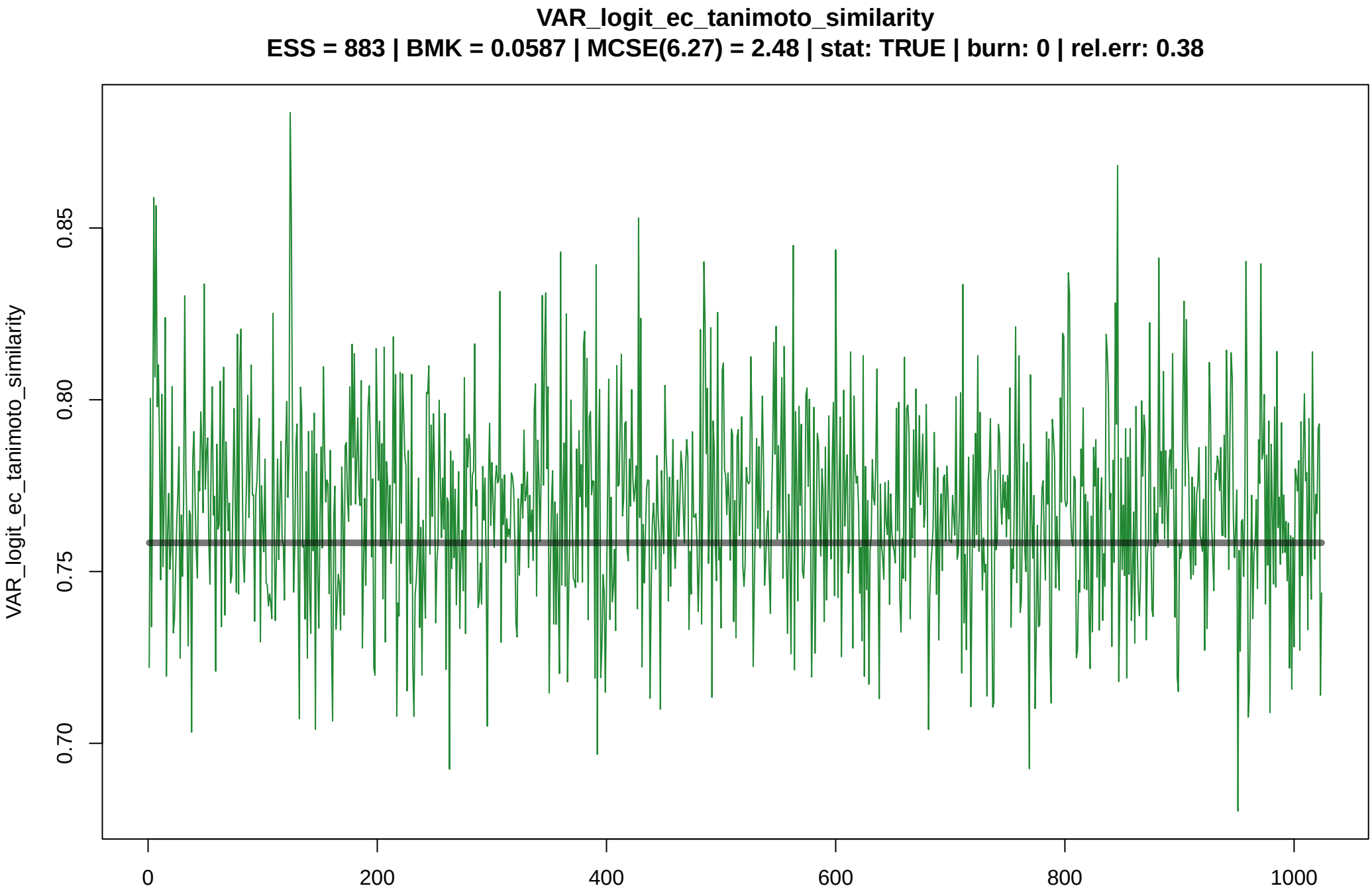

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0347 | MCSE(6.27) = 3.71 | stat: TRUE | burn: 0 | rel.err: −0.151
MEAN_mcs_RingCount
1.28
1.30
1.32
1.34
1.36
1.38
1.40
0
200
400
600
800
1000

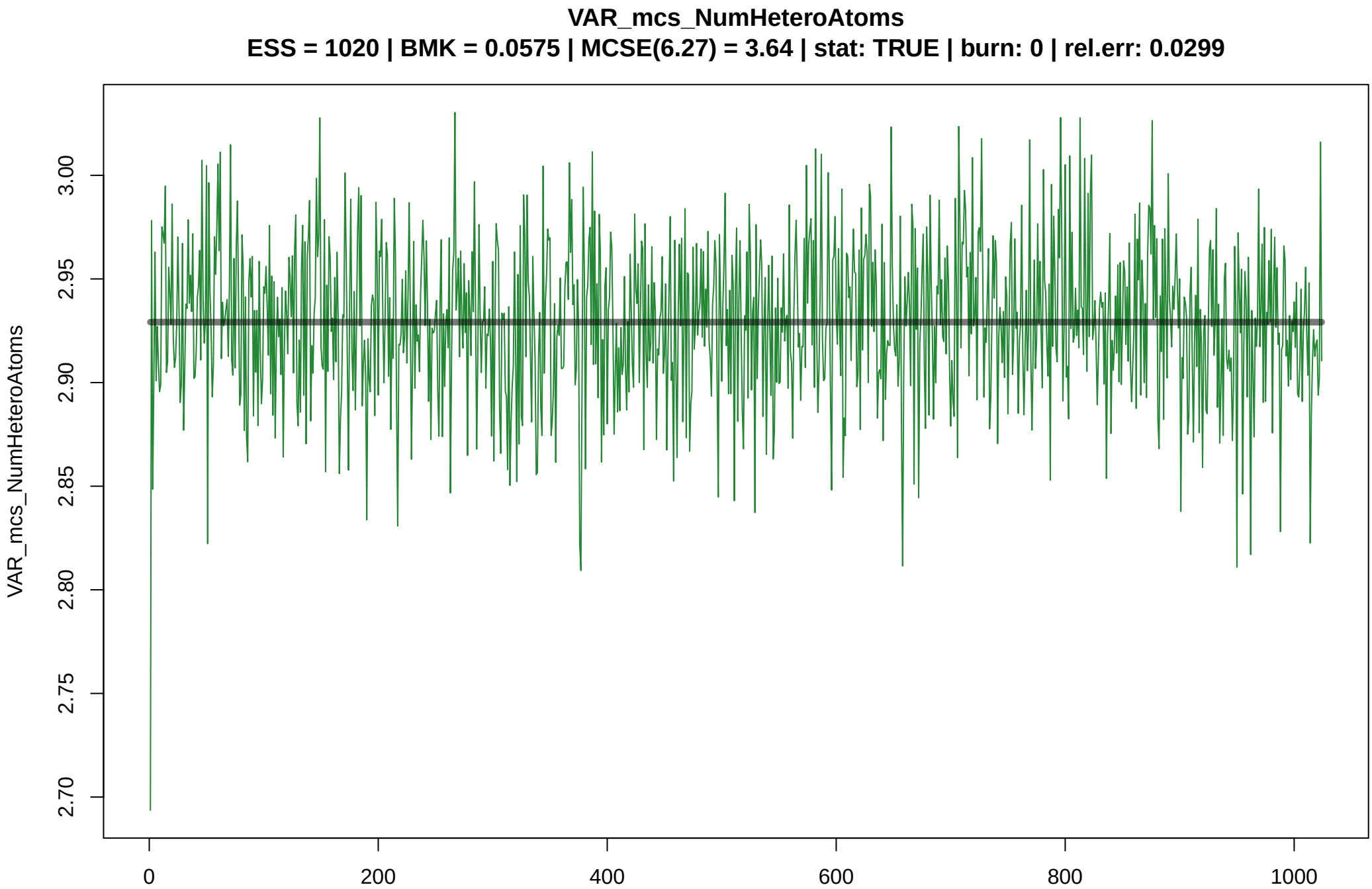

MEAN_docked_NumRotatableBonds
ESS = 879 | BMK = 0.0491 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | rel.err: 0.179
MEAN_docked_NumRotatableBonds
4.1
4.0
3.9
3.8
3.7
0
200
400
600
800
1000

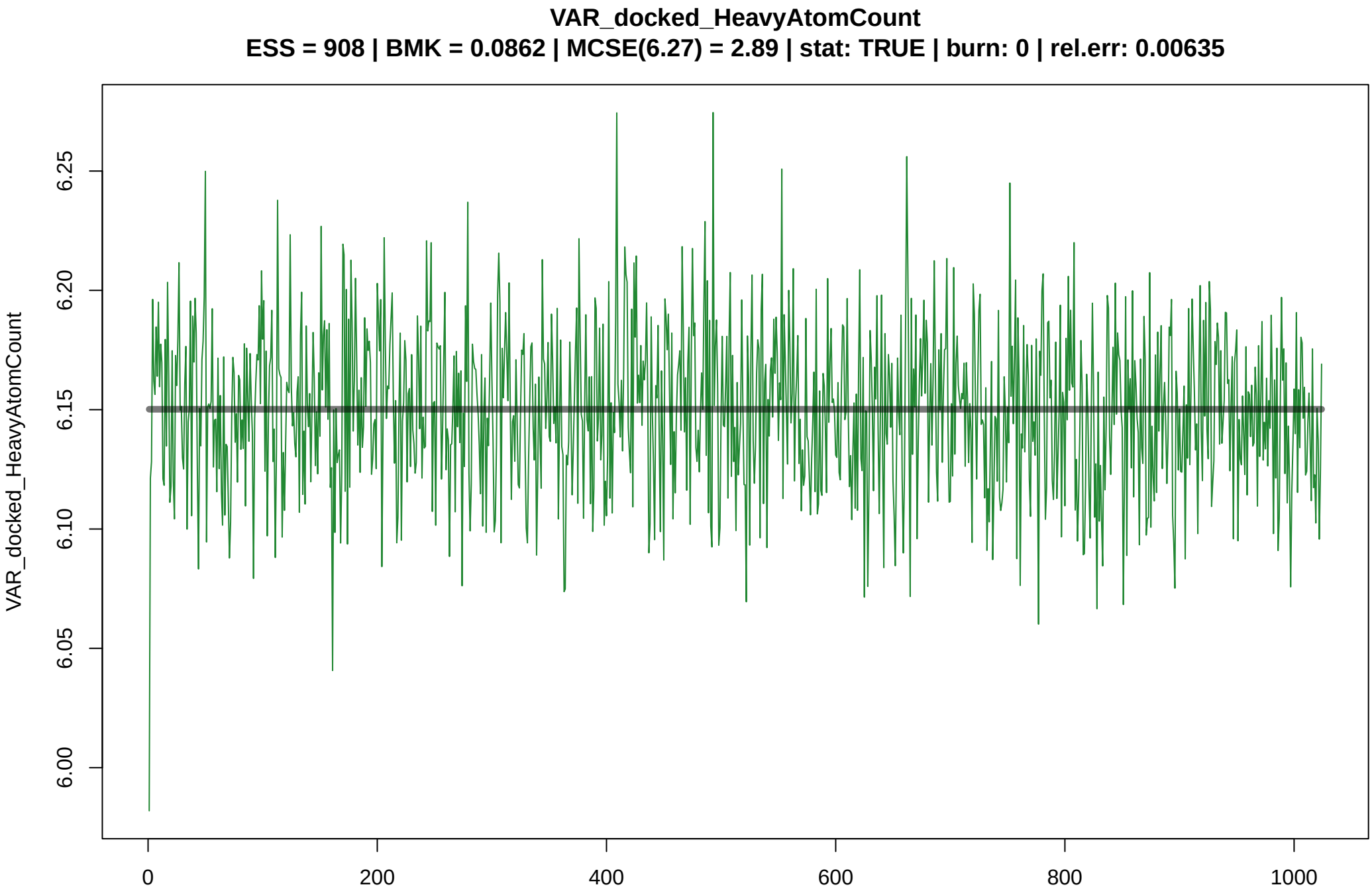

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0672 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | rel.err: 0.711
MEAN_mcs_NOCount
6.1
6.0
5.9
5.8
5.7
0
200
400
600
800
1000

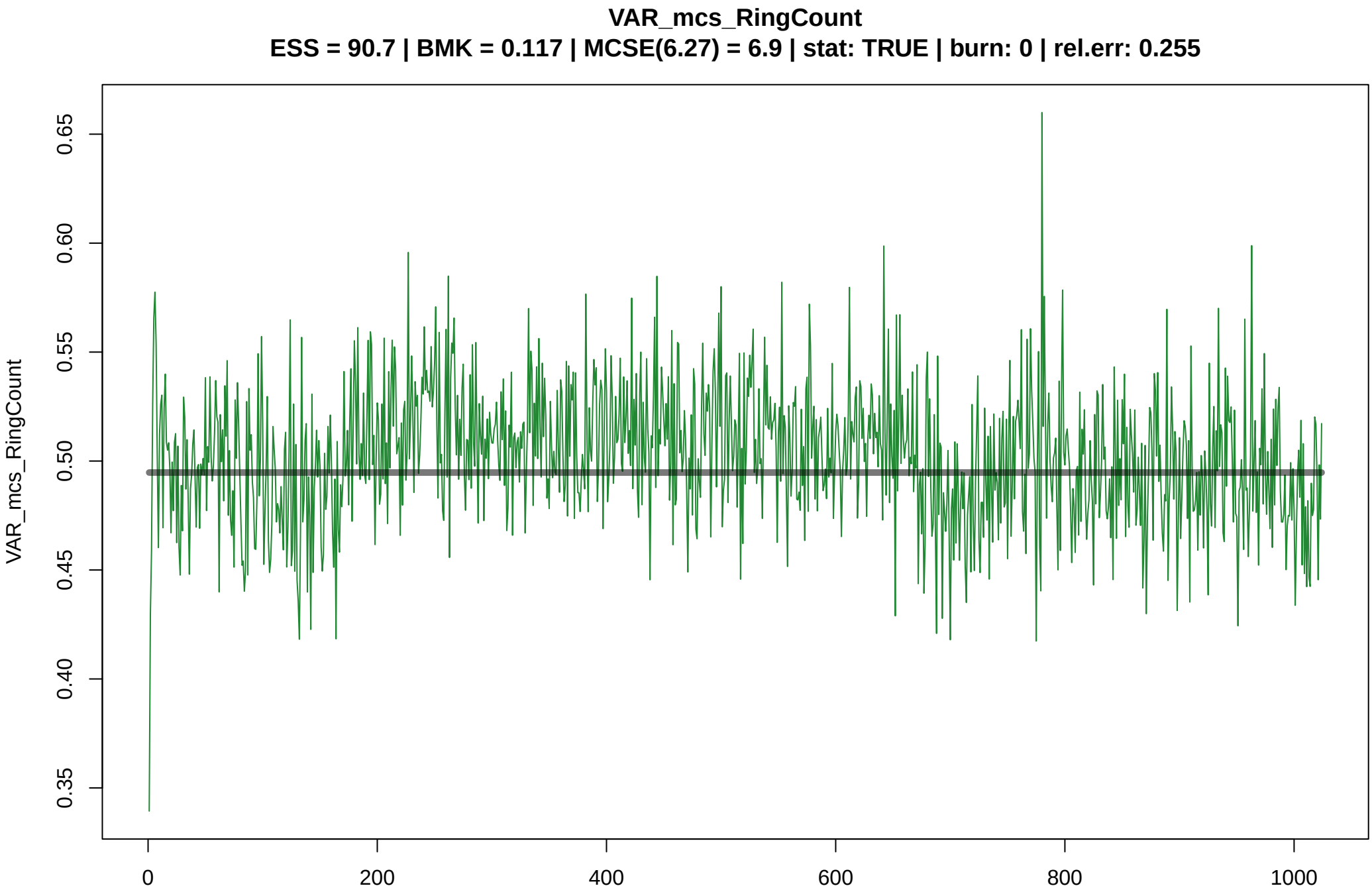

VAR_log_RMSD
ESS = 927 | BMK = 0.0553 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | rel.err: 1.82
VAR_log_RMSD
2.20
2.22
2.24
2.26
2.28
0
200
400
600
800
1000

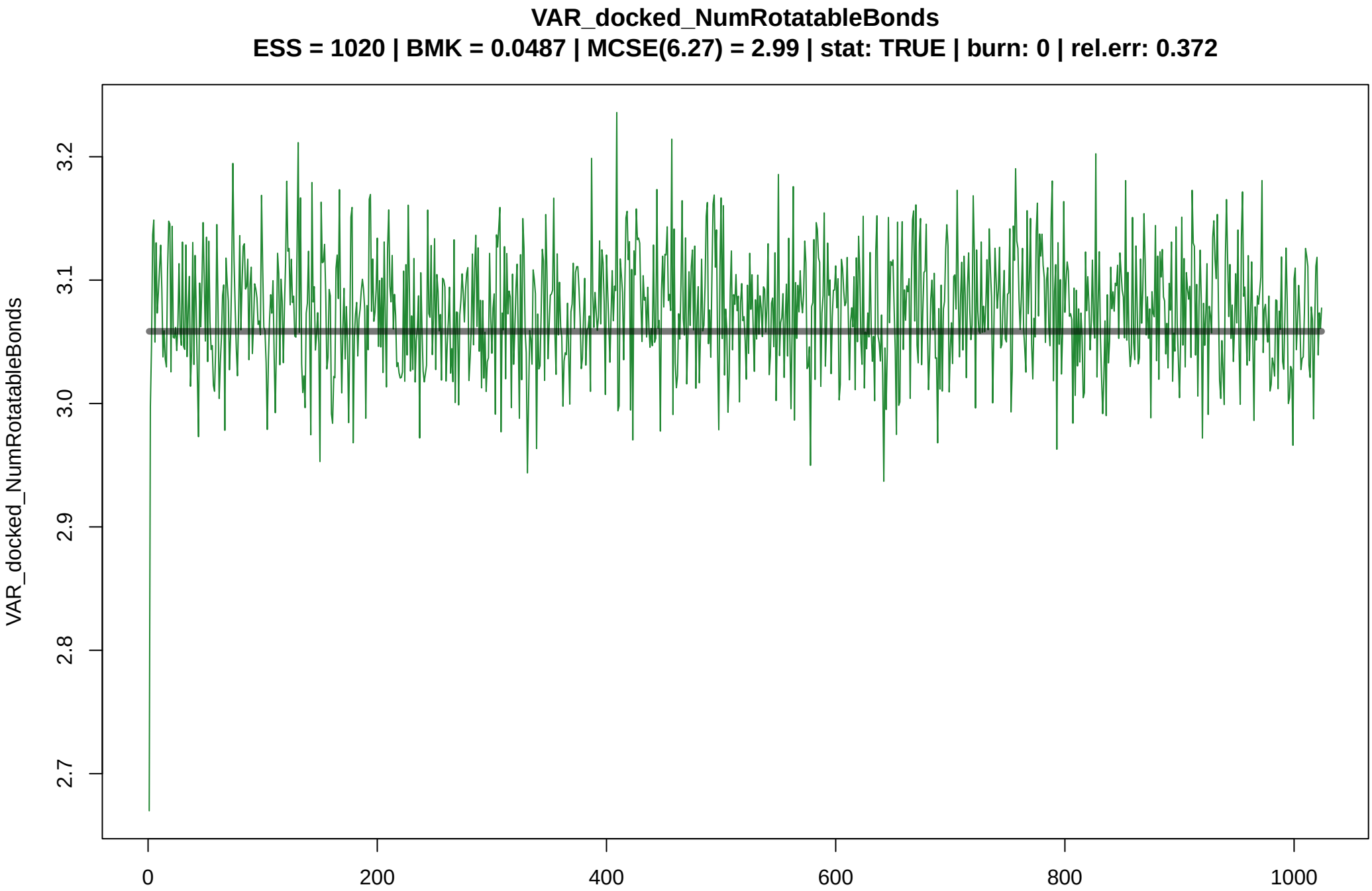

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0658 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | rel.err: 0.965
VAR_log_mcs_unbonded_polar_sasa
1.05
1.10
1.15
0
200
400
600
800
1000

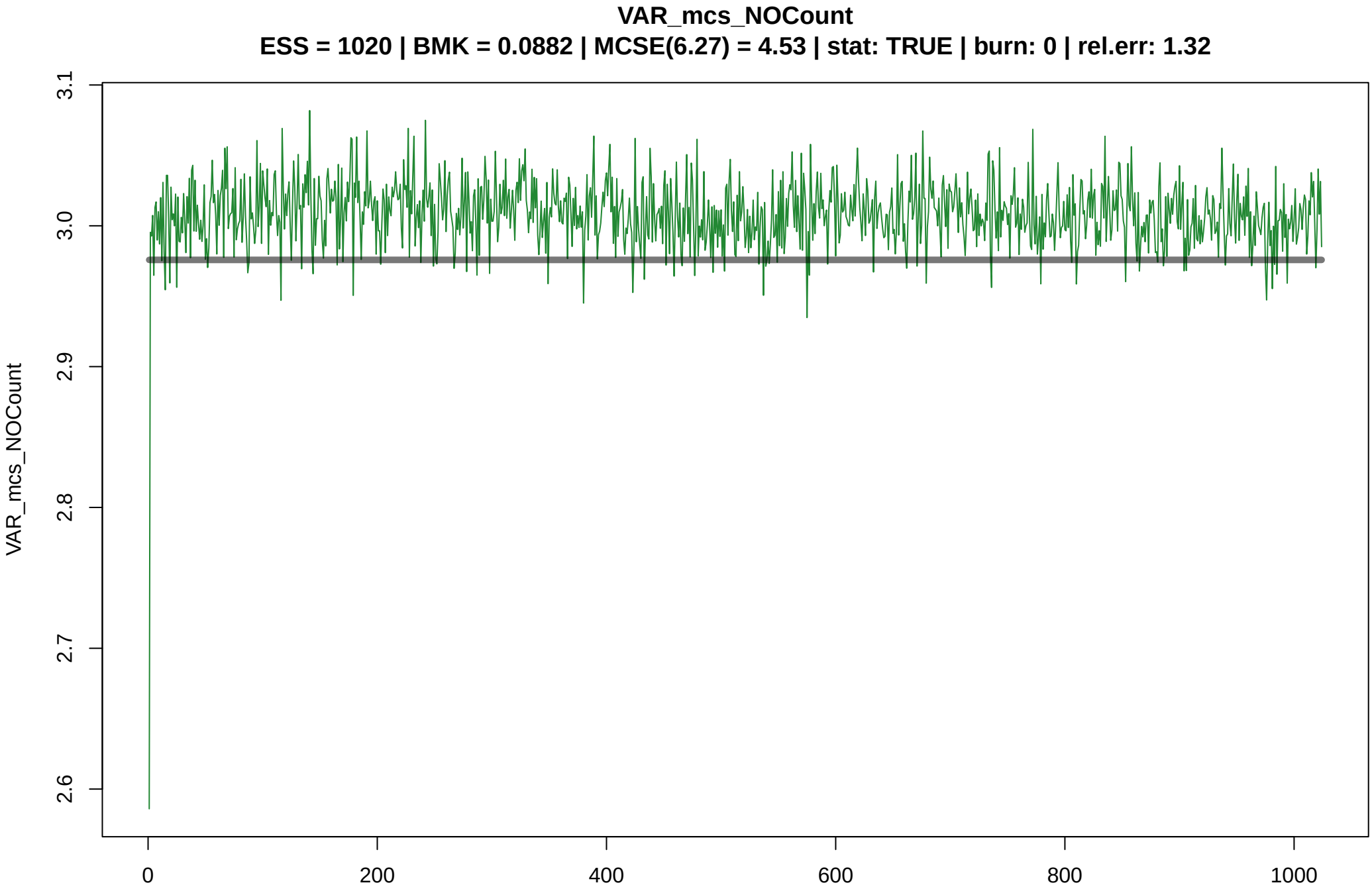

VAR_logit_ec_tanimoto_similarity
ESS = 883 | BMK = 0.0587 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0 | rel.err: 0.38
VAR_logit_ec_tanimoto_similarity
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

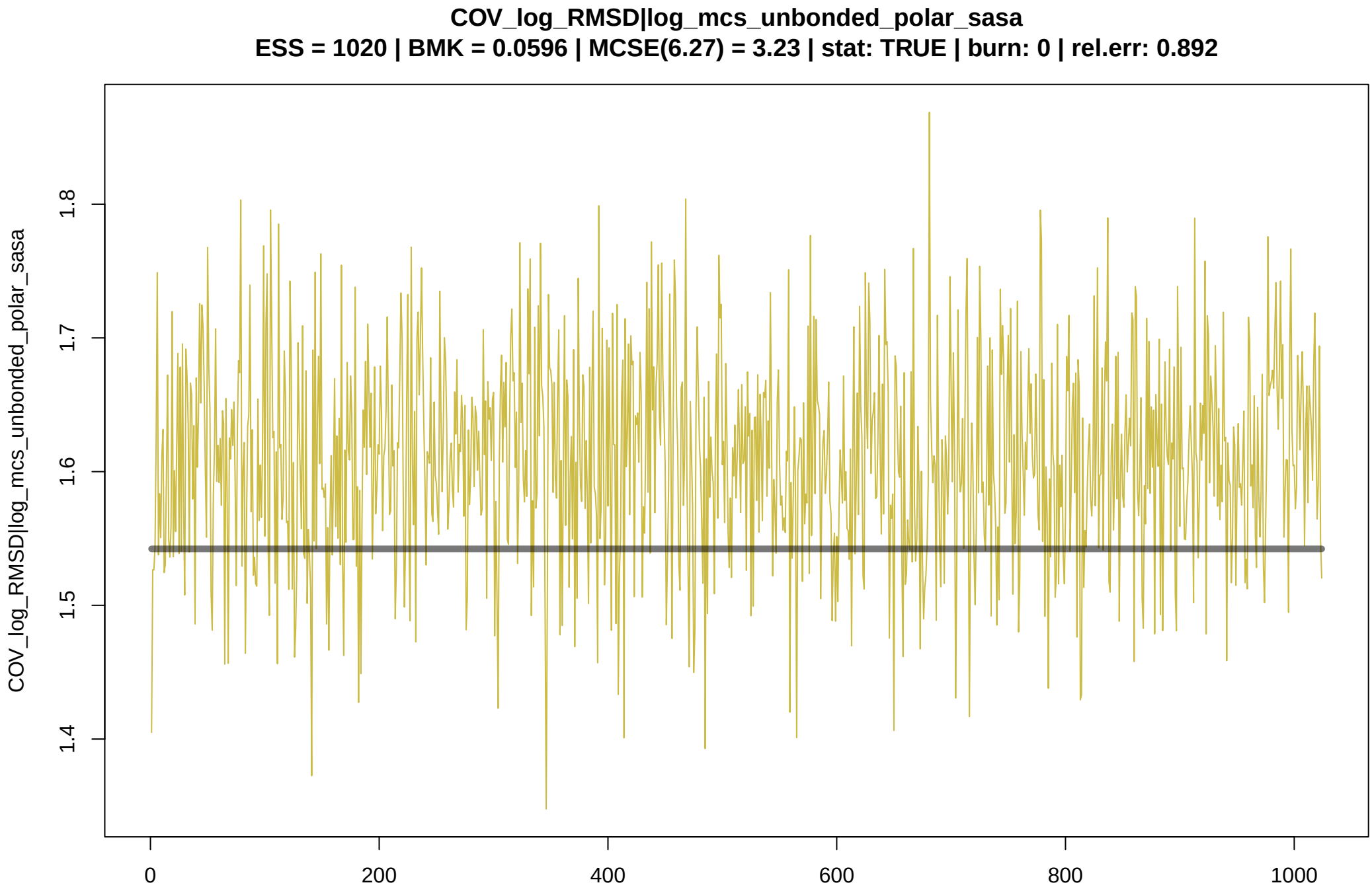

VAR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0575 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 0 | rel.err: 0.0299
VAR_mcs_NumHeteroAtoms
2.70
2.75
2.80
2.85
2.90
2.95
3.00
0
200
400
600
800
1000

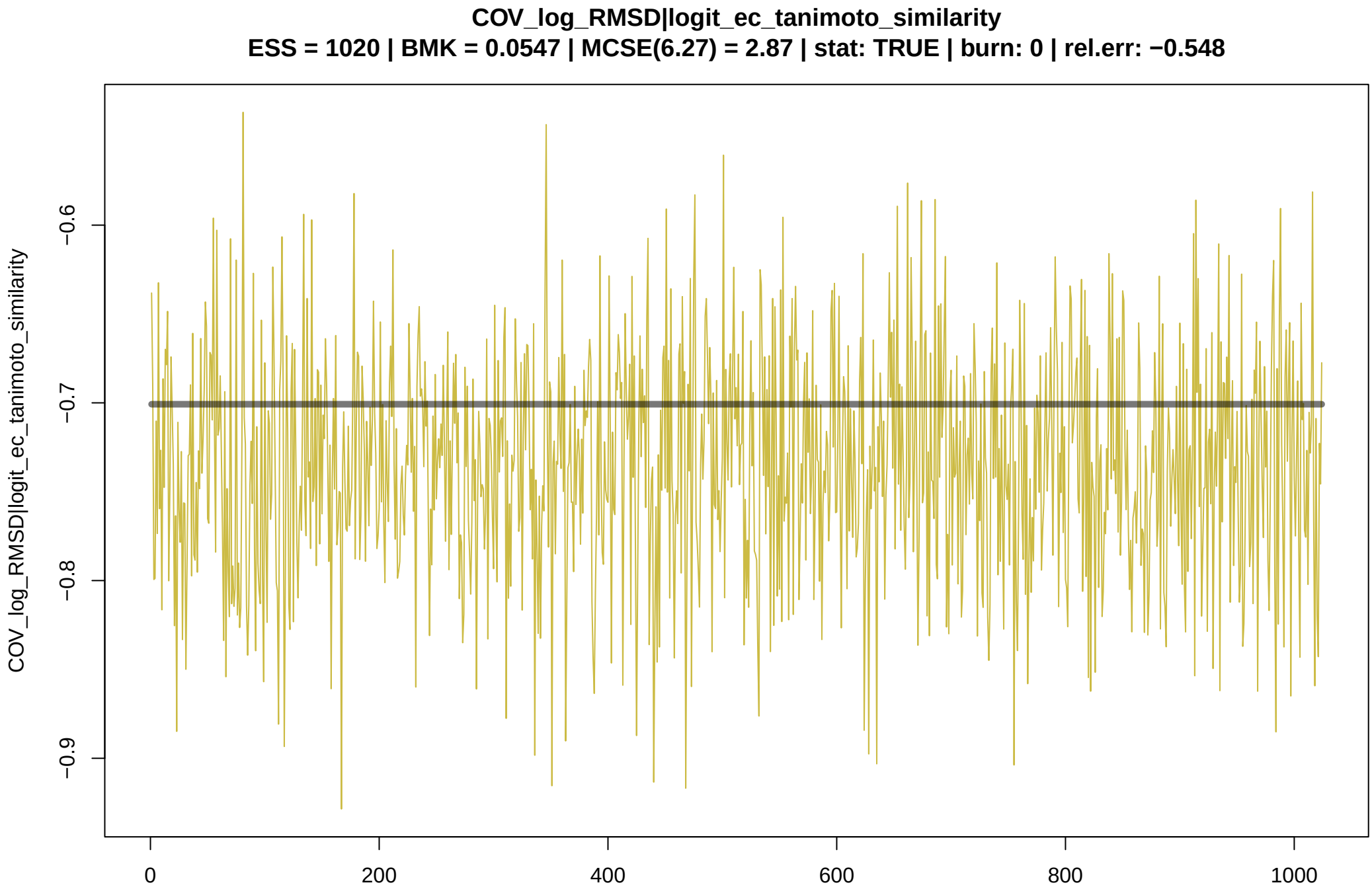

VAR_docked_HeavyAtomCount
ESS = 908 | BMK = 0.0862 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | rel.err: 0.00635
VAR_docked_HeavyAtomCount
6.00
6.05
6.10
6.15
6.20
6.25
0
200
400
600
800
1000

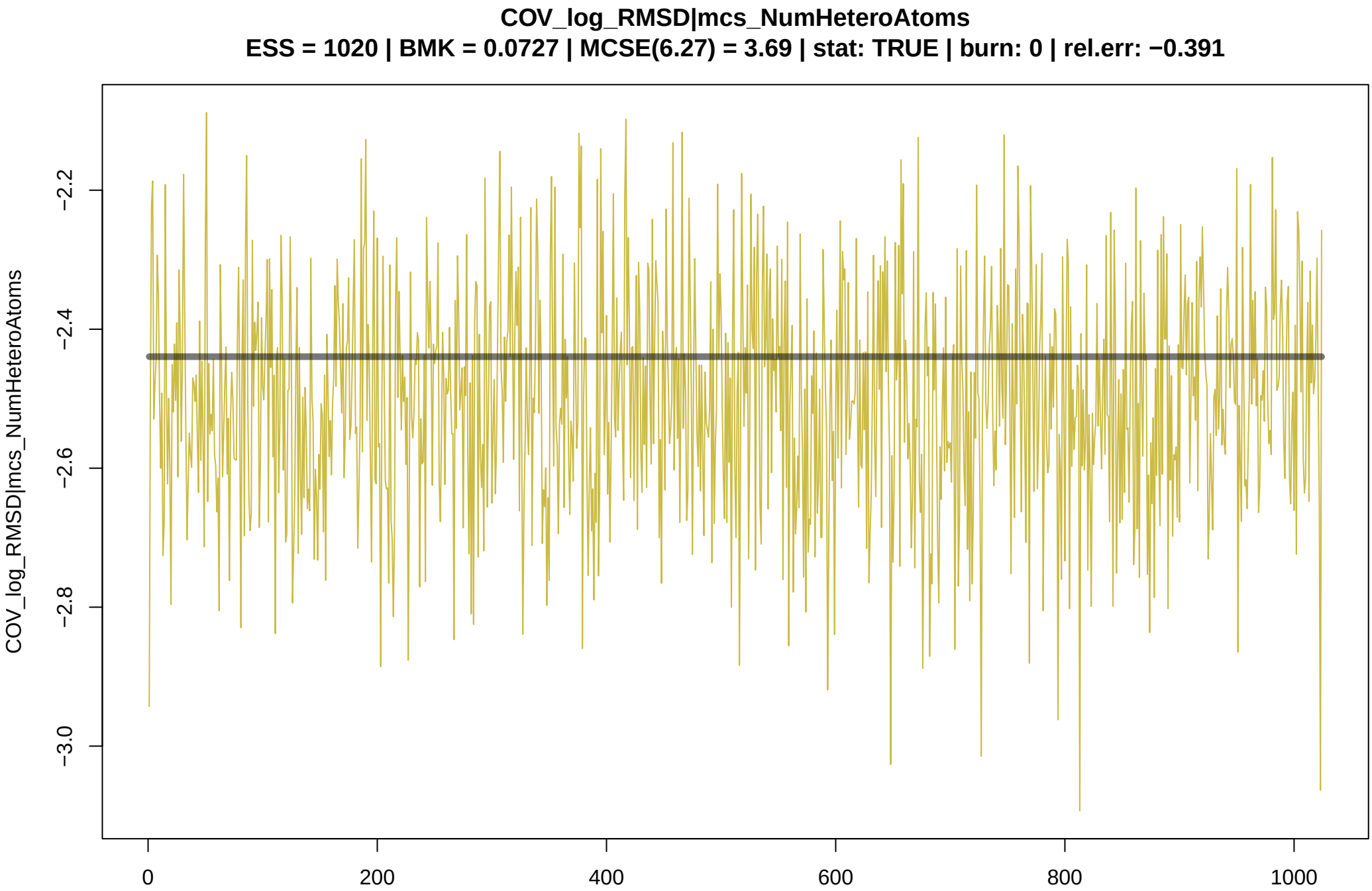

VAR_mcs_RingCount
ESS = 90.7 | BMK = 0.117 | MCSE(6.27) = 6.9 | stat: TRUE | burn: 0 | rel.err: 0.255
VAR_mcs_RingCount
0.35
0.40
0.45
0.50
0.55
0.60
0.65
0
200
400
600
800
1000

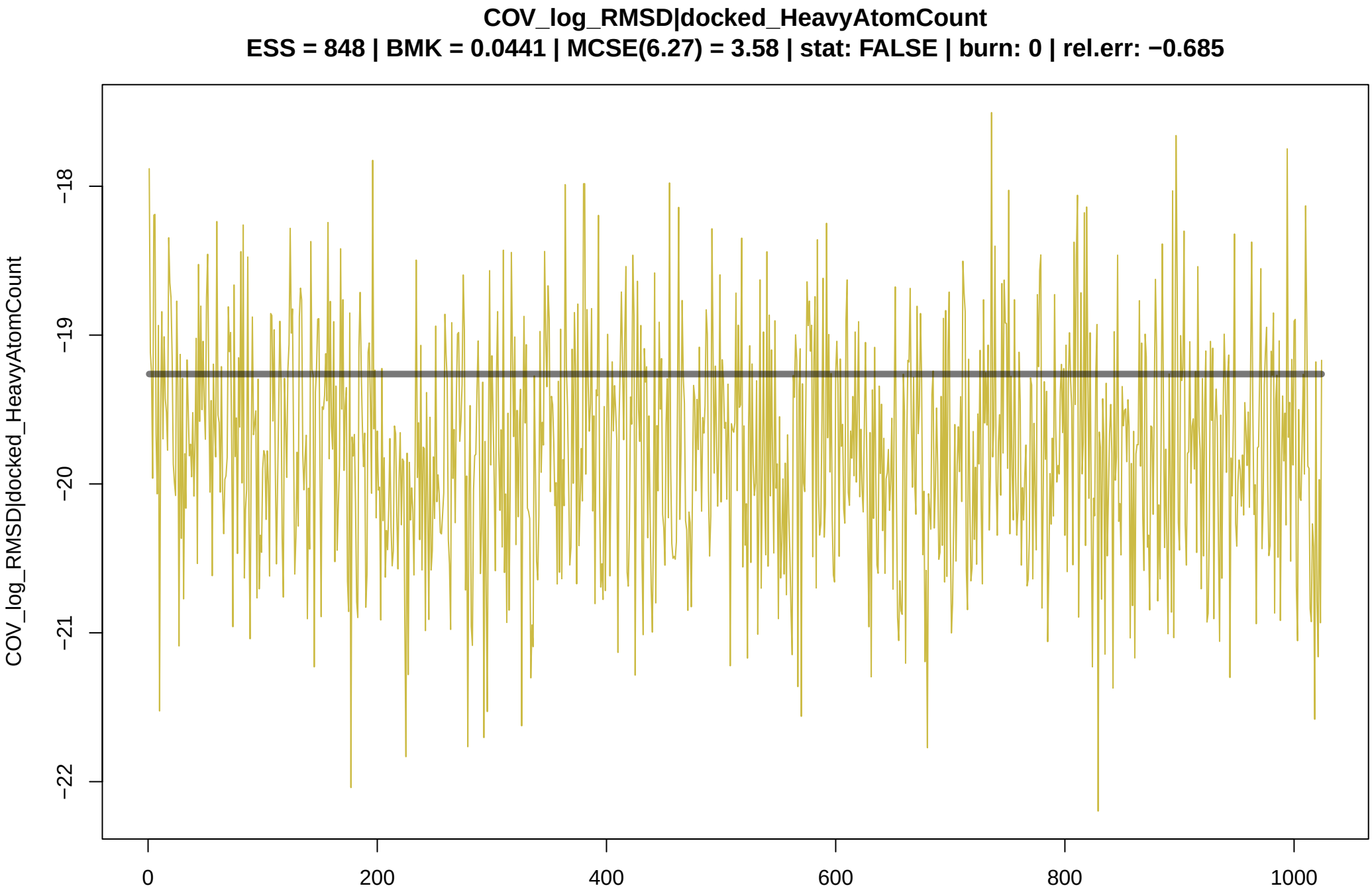

VAR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0487 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | rel.err: 0.372
VAR_docked_NumRotatableBonds
2.7
2.8
2.9
3.0
3.1
3.2
0
200
400
600
800
1000

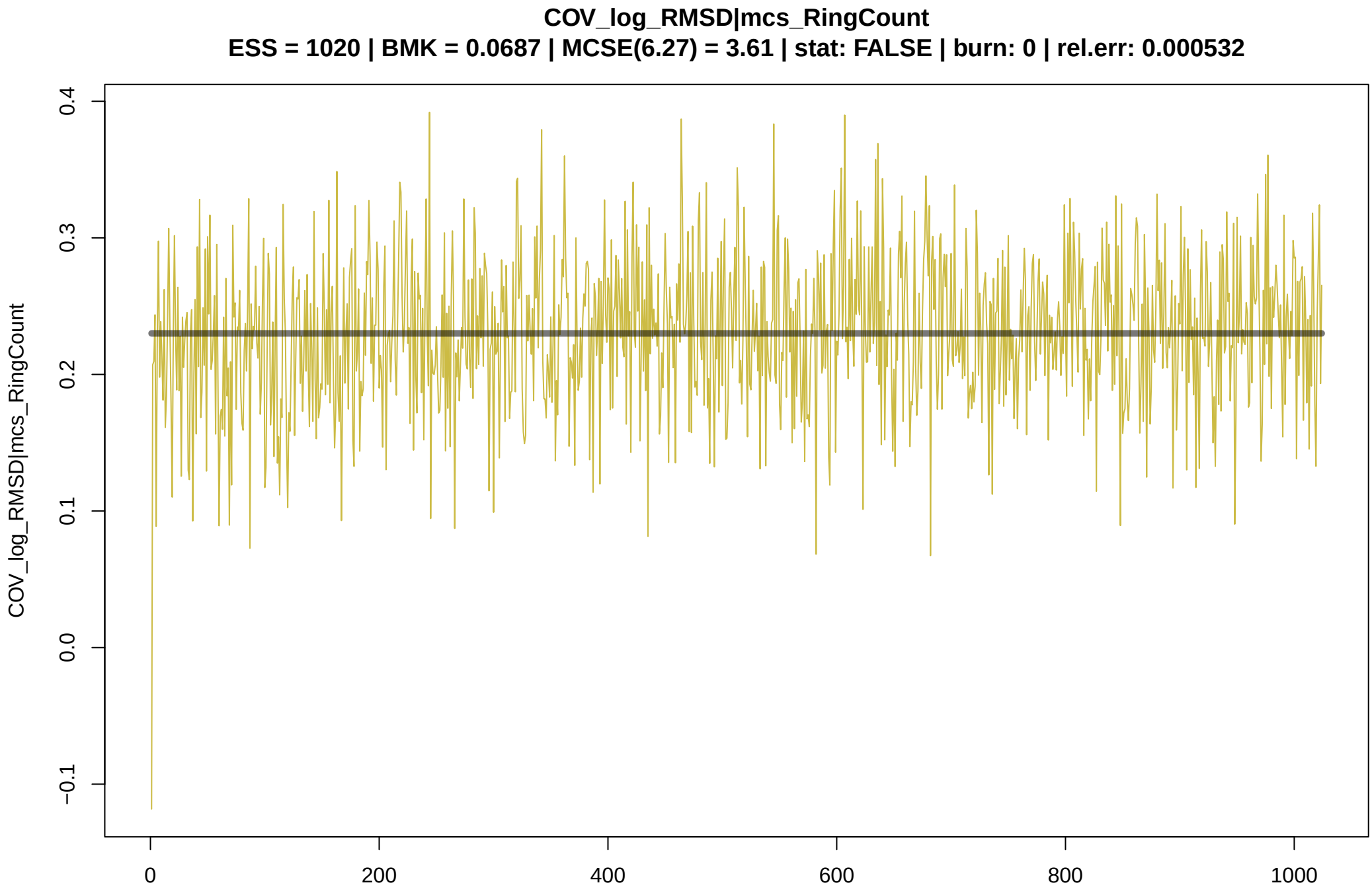

VAR_mcs_NOCount
ESS = 1020 | BMK = 0.0882 | MCSE(6.27) = 4.53 | stat: TRUE | burn: 0 | rel.err: 1.32
VAR_mcs_NOCount
3.1
3.0
2.9
2.8
2.7
2.6
0
200
400
600
800
1000

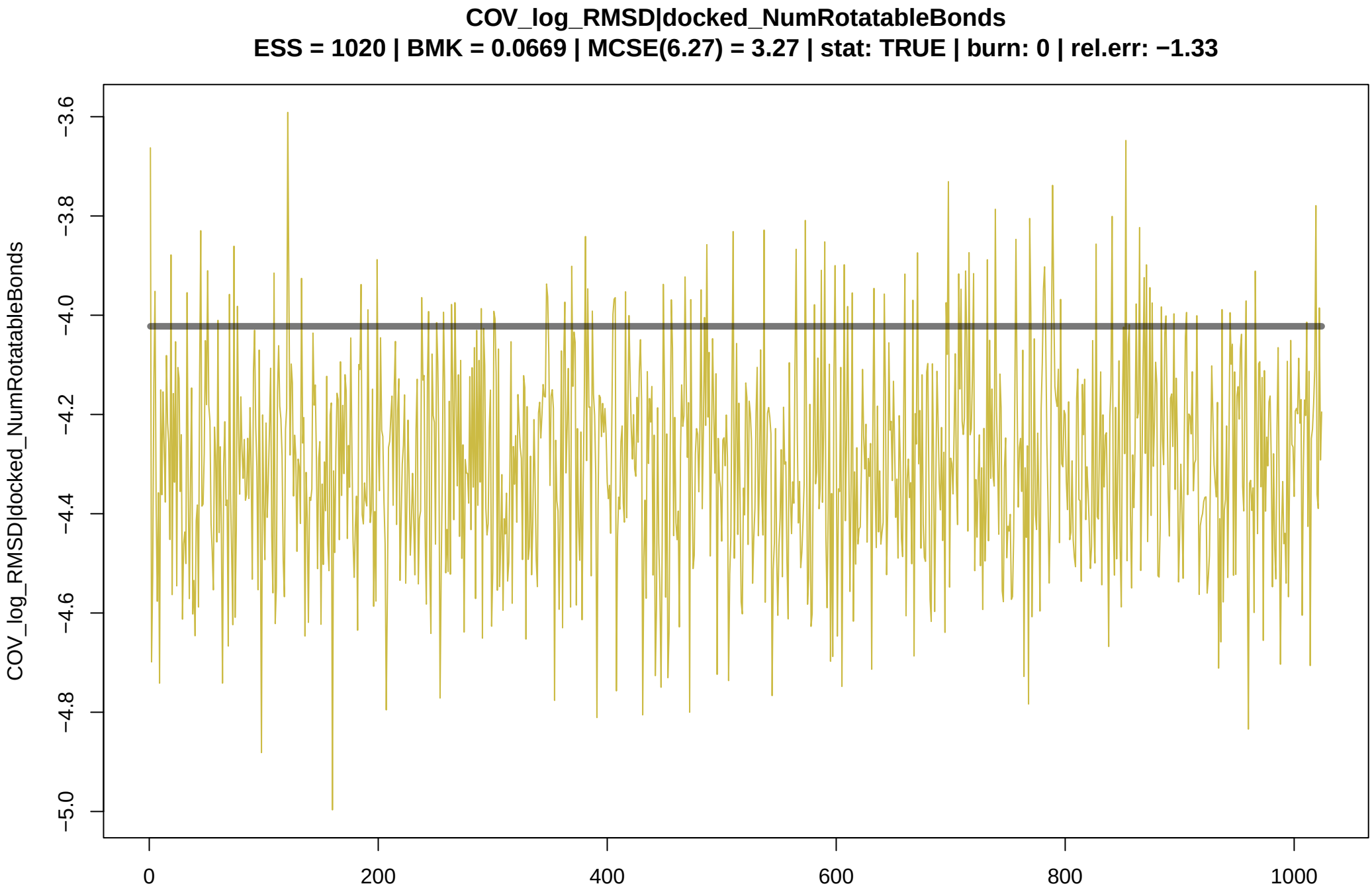

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0596 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | rel.err: 0.892
COV_log_RMSD|log_mcs_unbonded_polar_sasa
1.4
1.5
1.6
1.7
1.8
0
200
400
600
800
1000

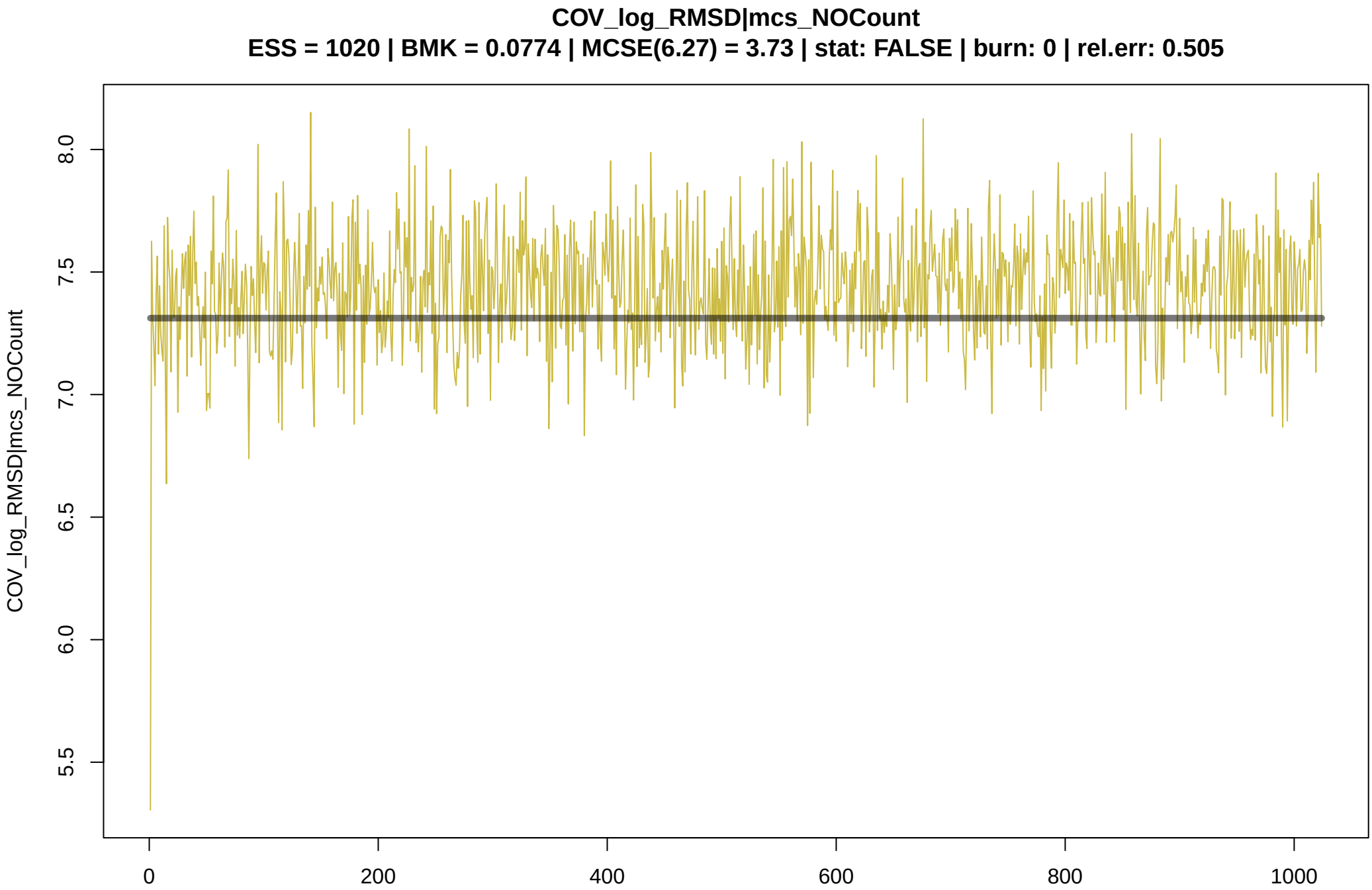

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0547 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0 | rel.err: −0.548
COV_log_RMSD|logit_ec_tanimoto_similarity
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

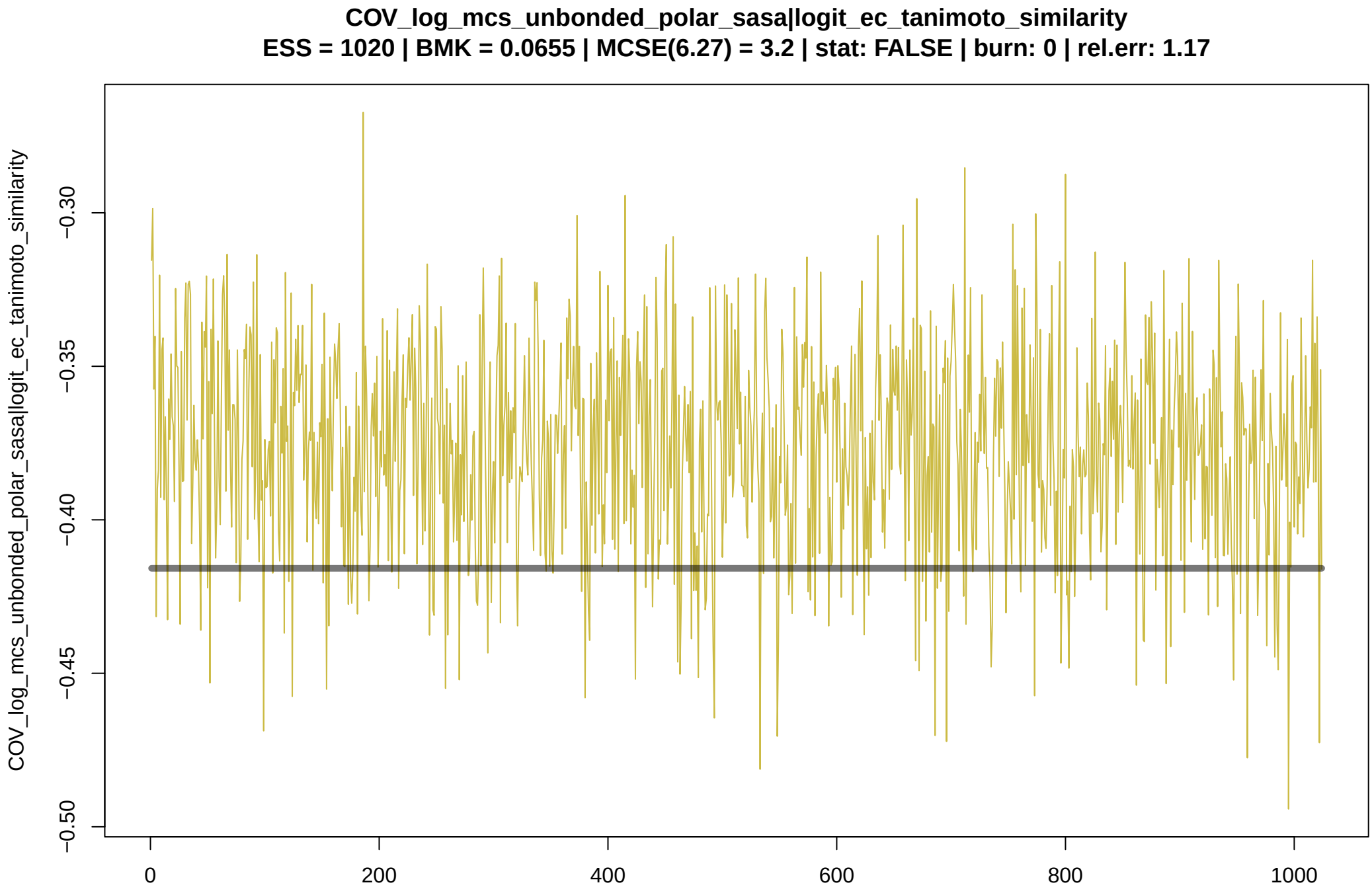

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0727 | MCSE(6.27) = 3.69 | stat: TRUE | burn: 0 | rel.err: −0.391
COV_log_RMSD|mcs_NumHeteroAtoms
−2.2
−2.4
−2.6
−2.8
−3.0
0
200
400
600
800
1000

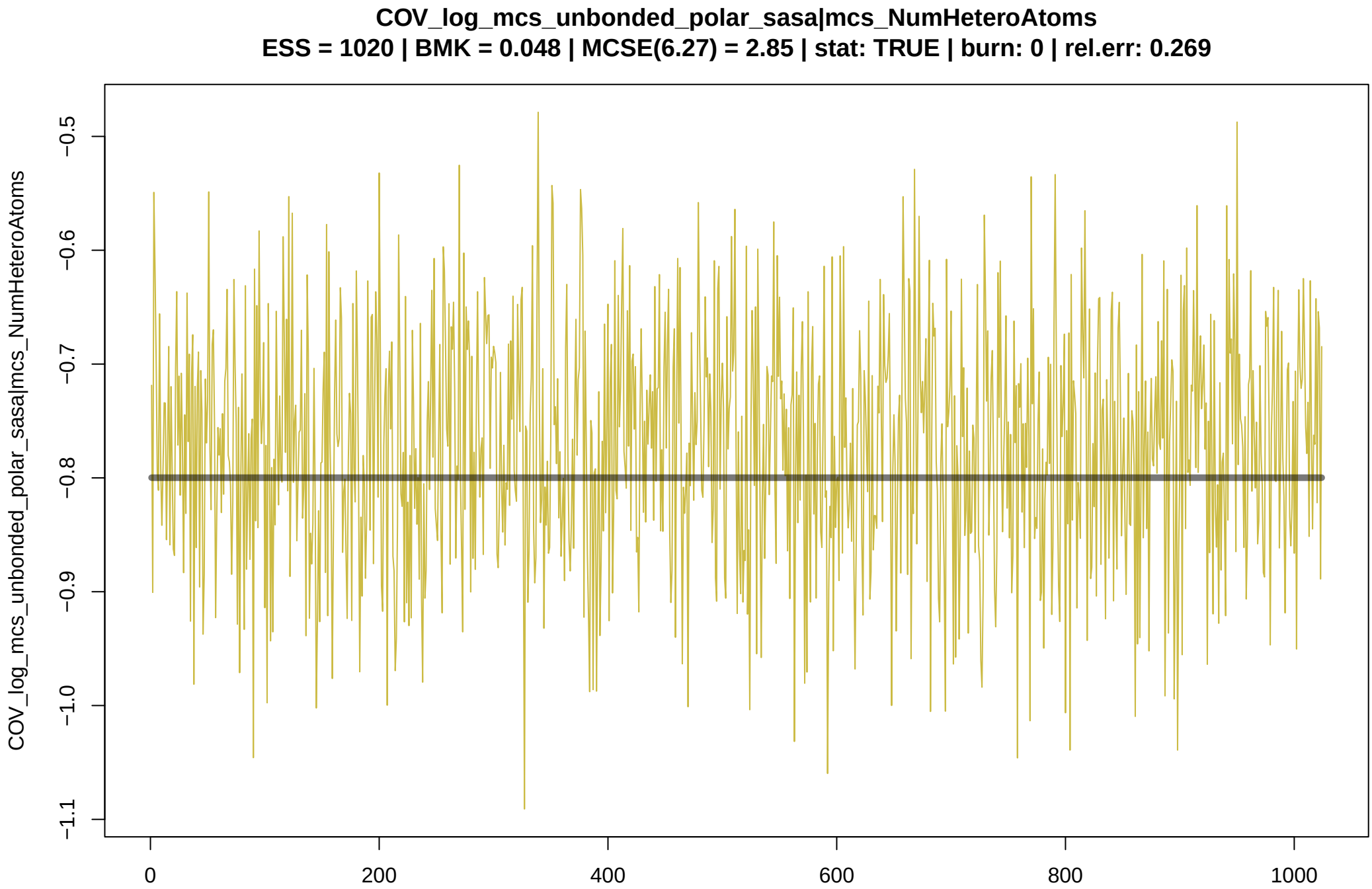

COV_log_RMSD|docked_HeavyAtomCount
ESS = 848 | BMK = 0.0441 | MCSE(6.27) = 3.58 | stat: FALSE | burn: 0 | rel.err: −0.685
COV_log_RMSD|docked_HeavyAtomCount
−18
−19
−20
−21
−22
0
200
400
600
800
1000

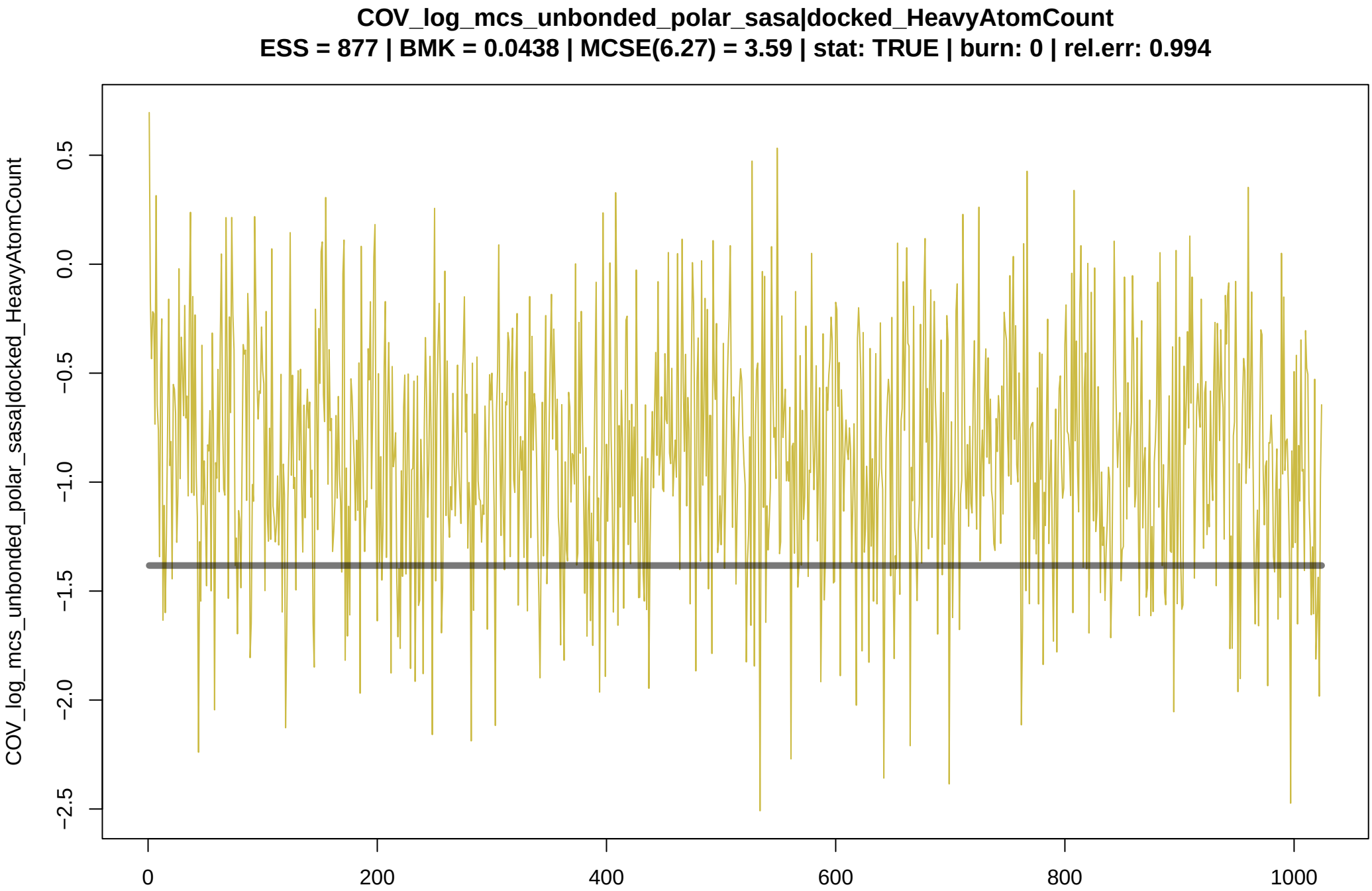

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0687 | MCSE(6.27) = 3.61 | stat: FALSE | burn: 0 | rel.err: 0.000532
COV_log_RMSD|mcs_RingCount
0.4
0.3
0.2
0.1
0.0
−0.1
0
200
400
600
800
1000

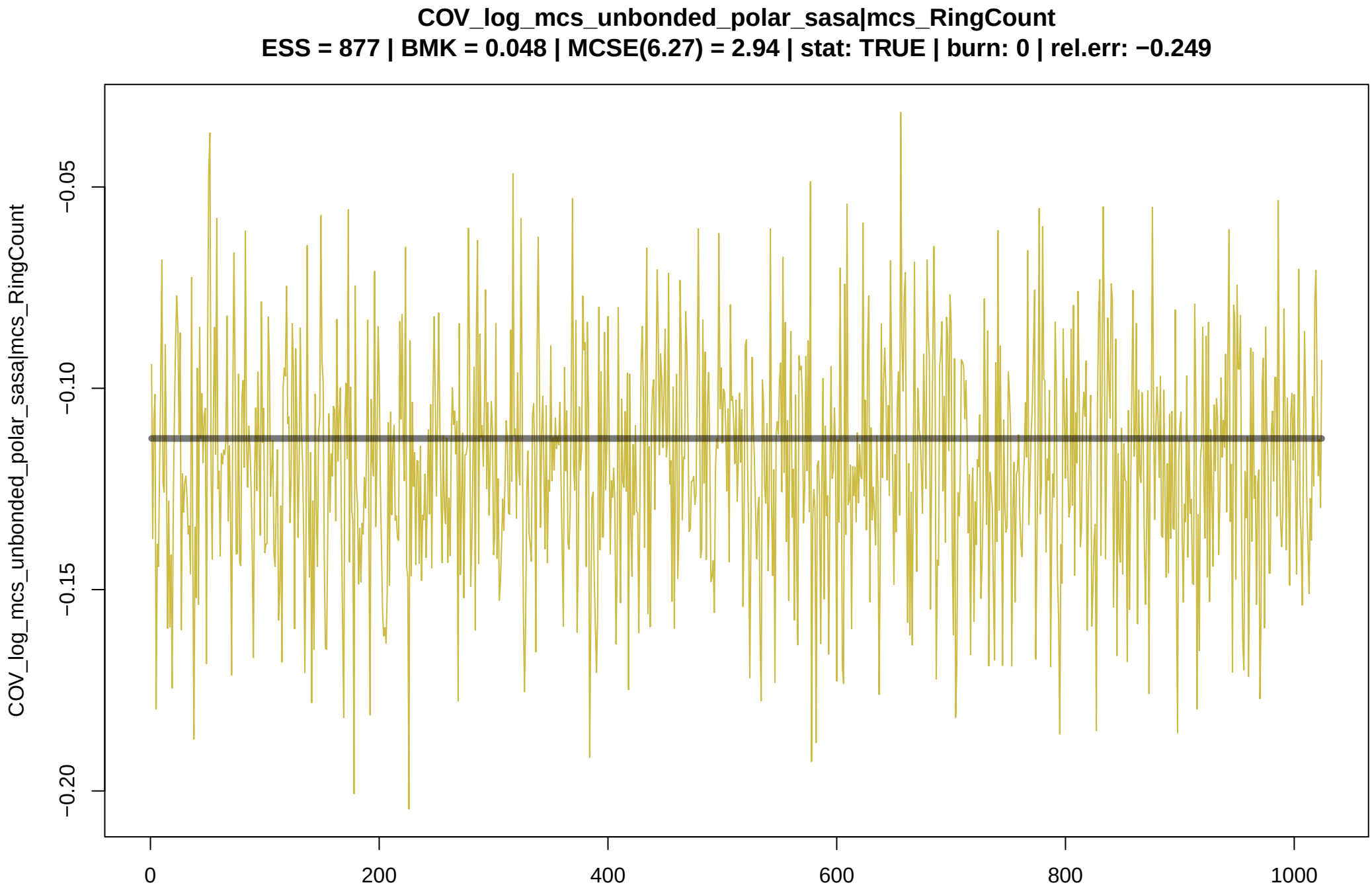

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0669 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | rel.err: −1.33
COV_log_RMSD|docked_NumRotatableBonds
−3.6
−3.8
−4.0
−4.2
−4.4
−4.6
−4.8
−5.0
0
200
400
600
800
1000

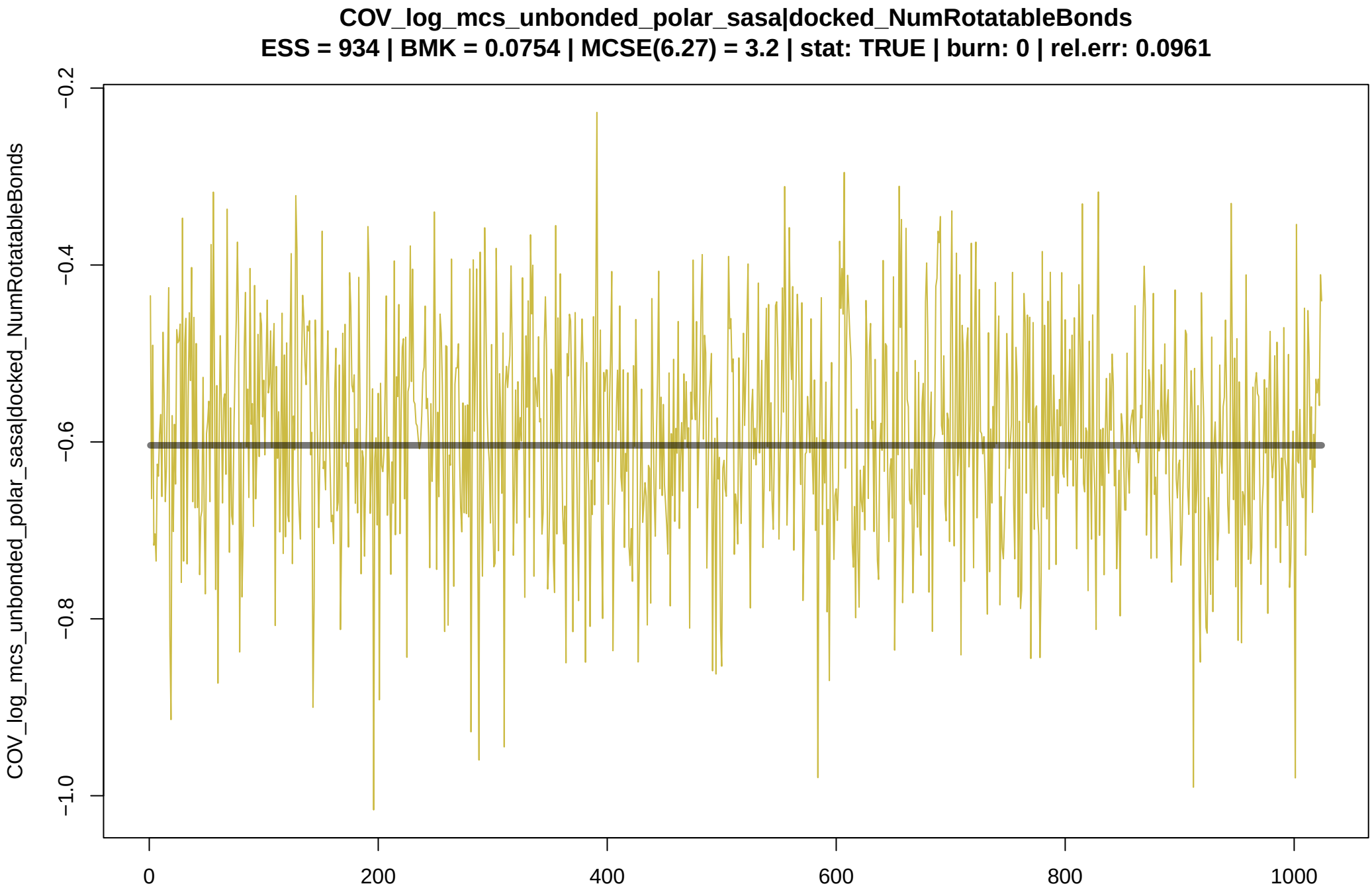

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0774 | MCSE(6.27) = 3.73 | stat: FALSE | burn: 0 | rel.err: 0.505
COV_log_RMSD|mcs_NOCount
5.5
6.0
6.5
7.0
7.5
8.0
0
200
400
600
800
1000

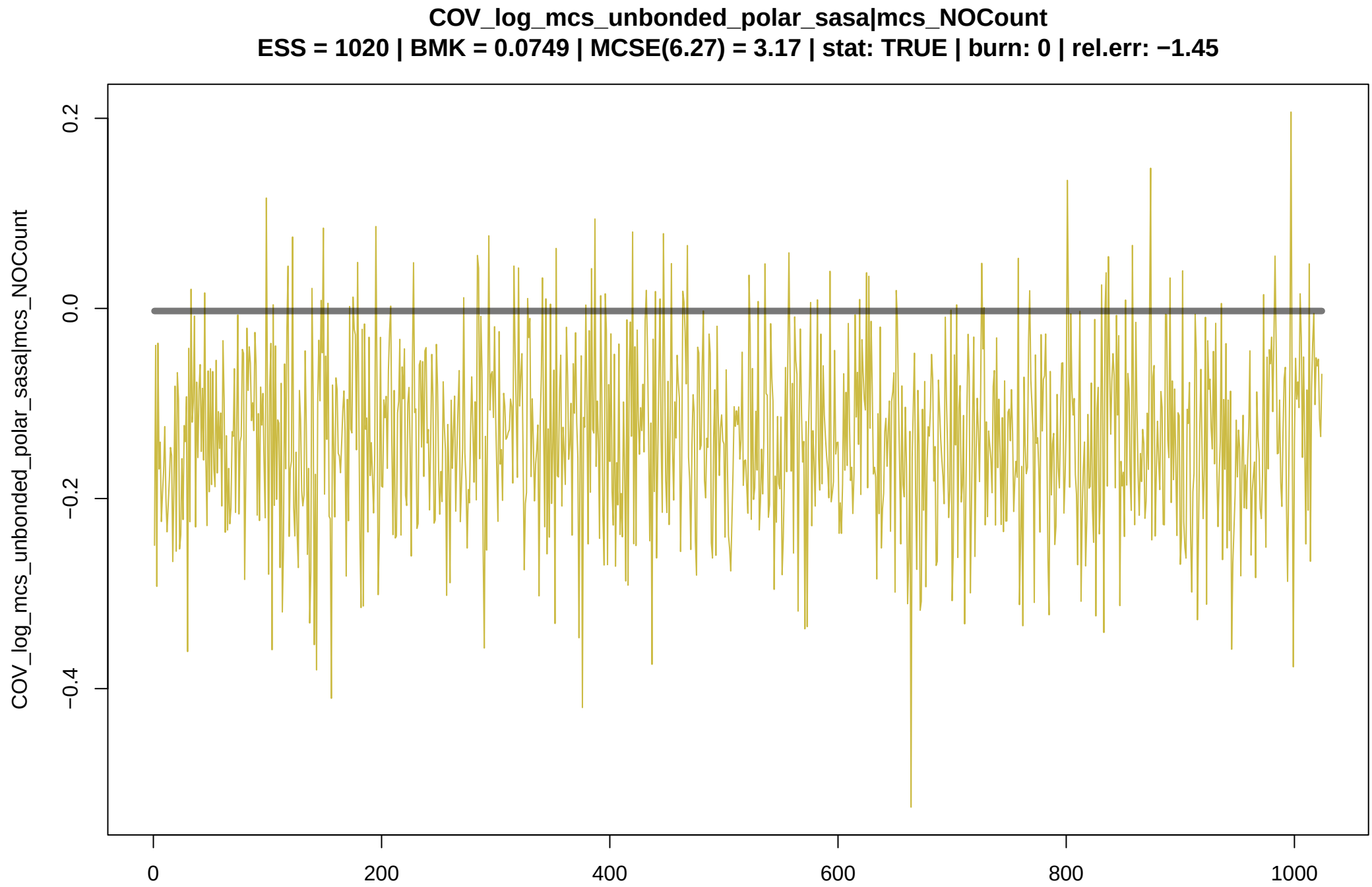

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0655 | MCSE(6.27) = 3.2 | stat: FALSE | burn: 0 | rel.err: 1.17
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
−0.30
−0.35
−0.40
−0.45
−0.50
0
200
400
600
800
1000

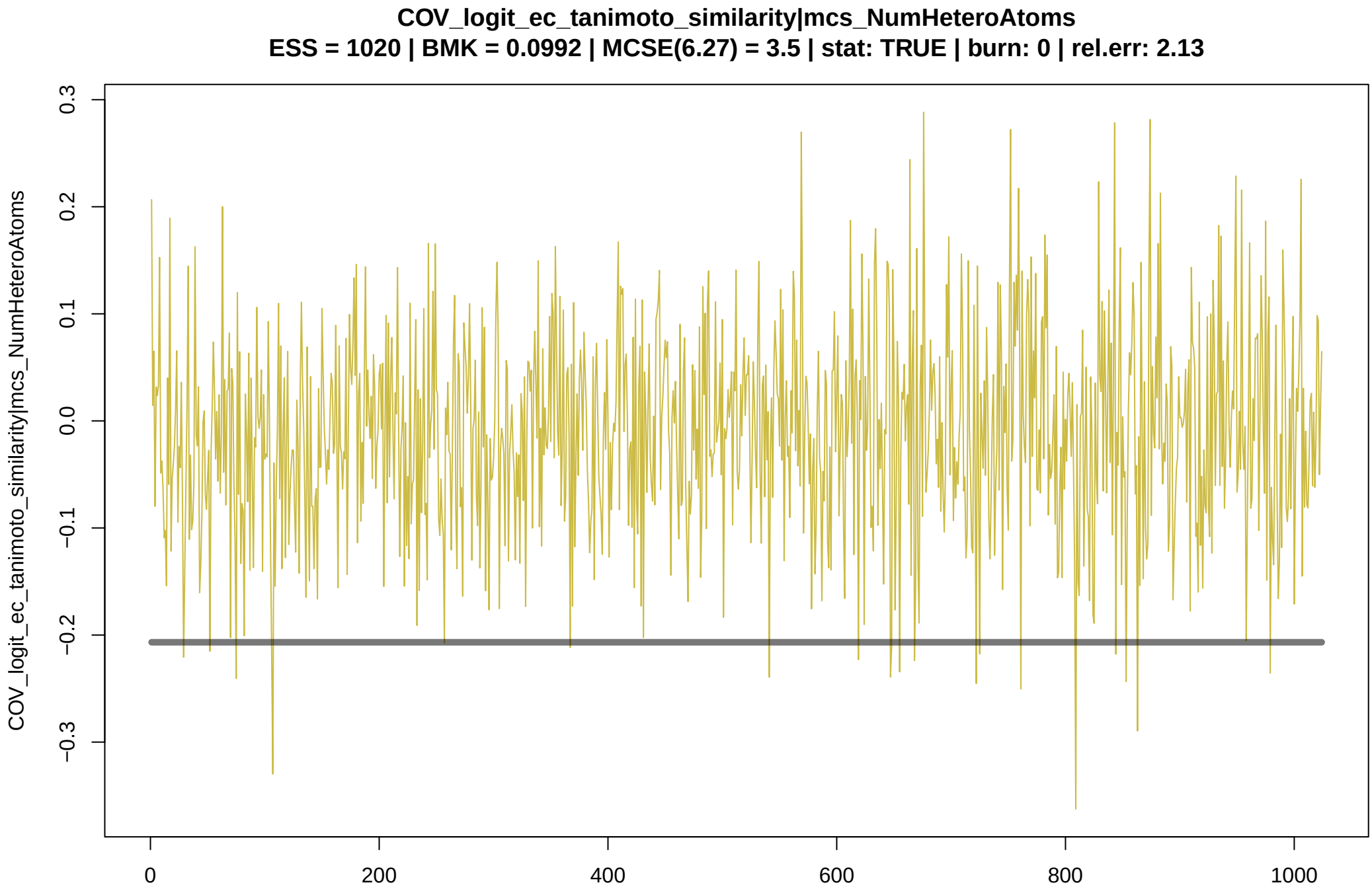

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.048 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | rel.err: 0.269
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−0.5
−0.6
−0.7
−0.8
−0.9
−1.0
−1.1
0
200
400
600
800
1000

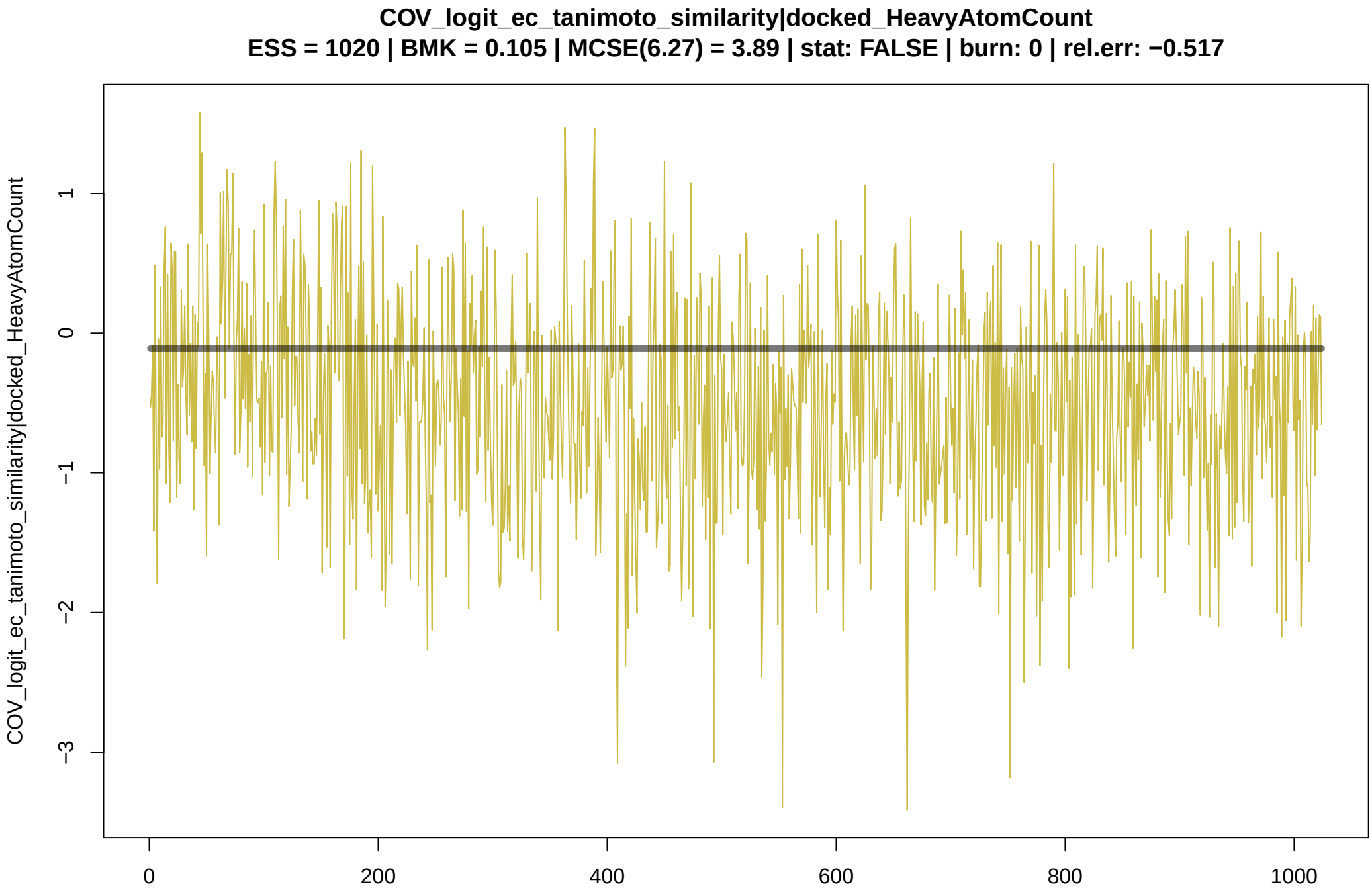

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 877 | BMK = 0.0438 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | rel.err: 0.994
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
0
200
400
600
800
1000

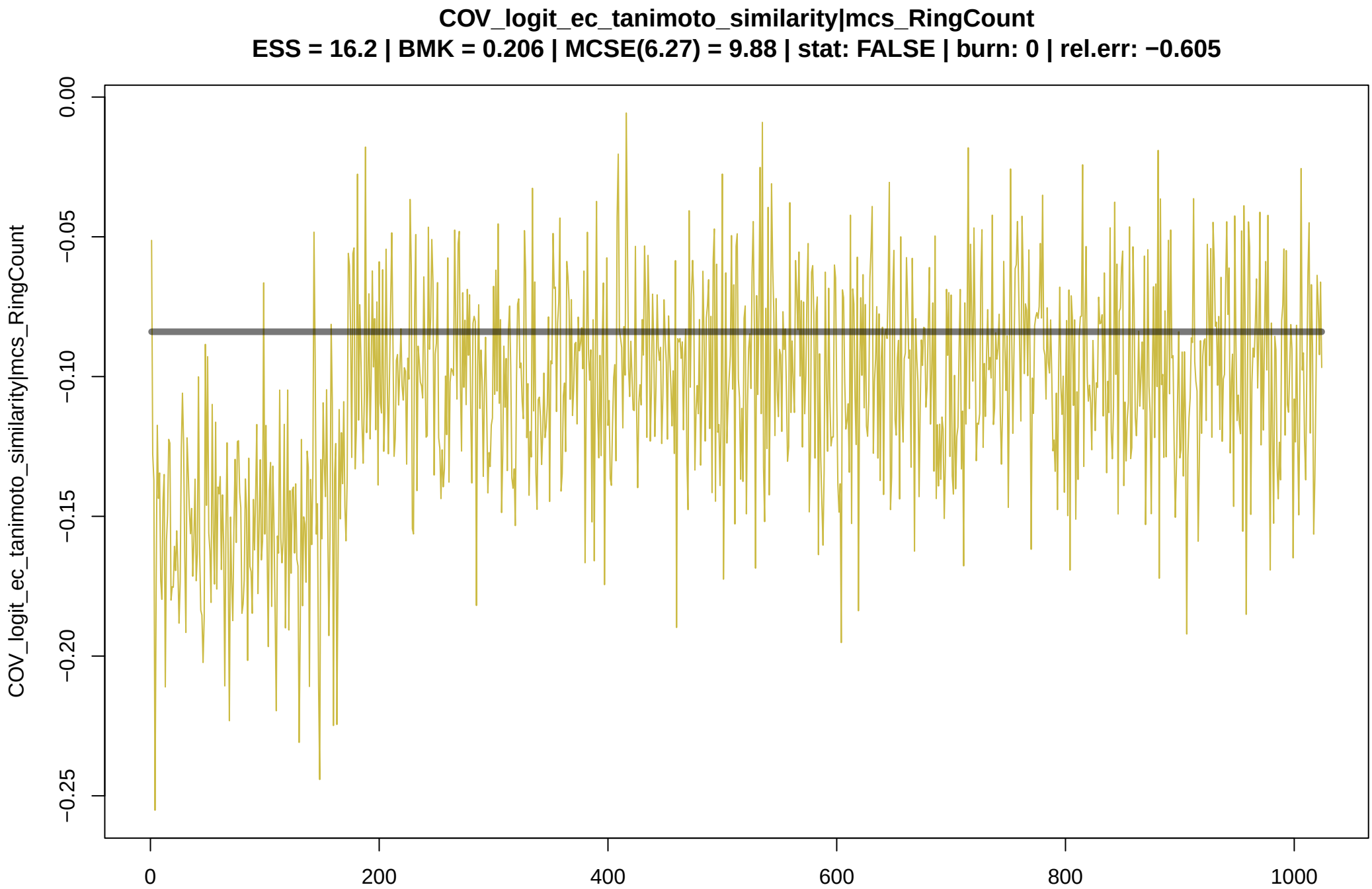

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 877 | BMK = 0.048 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | rel.err: −0.249
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−0.05
−0.10
−0.15
−0.20
0
200
400
600
800
1000

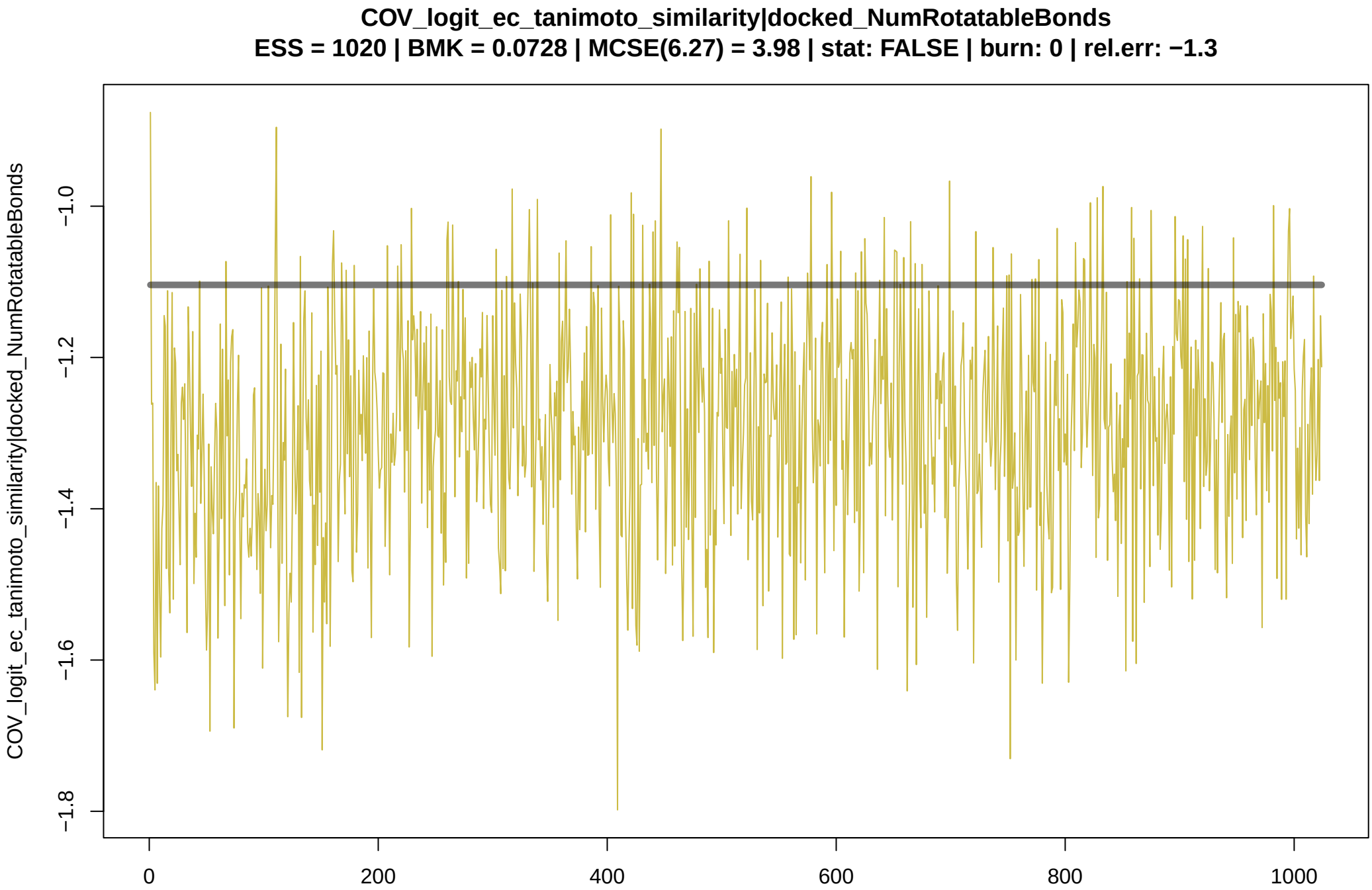

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 934 | BMK = 0.0754 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: 0.0961
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
−0.2
−0.4
−0.6
−0.8
−1.0
0
200
400
600
800
1000

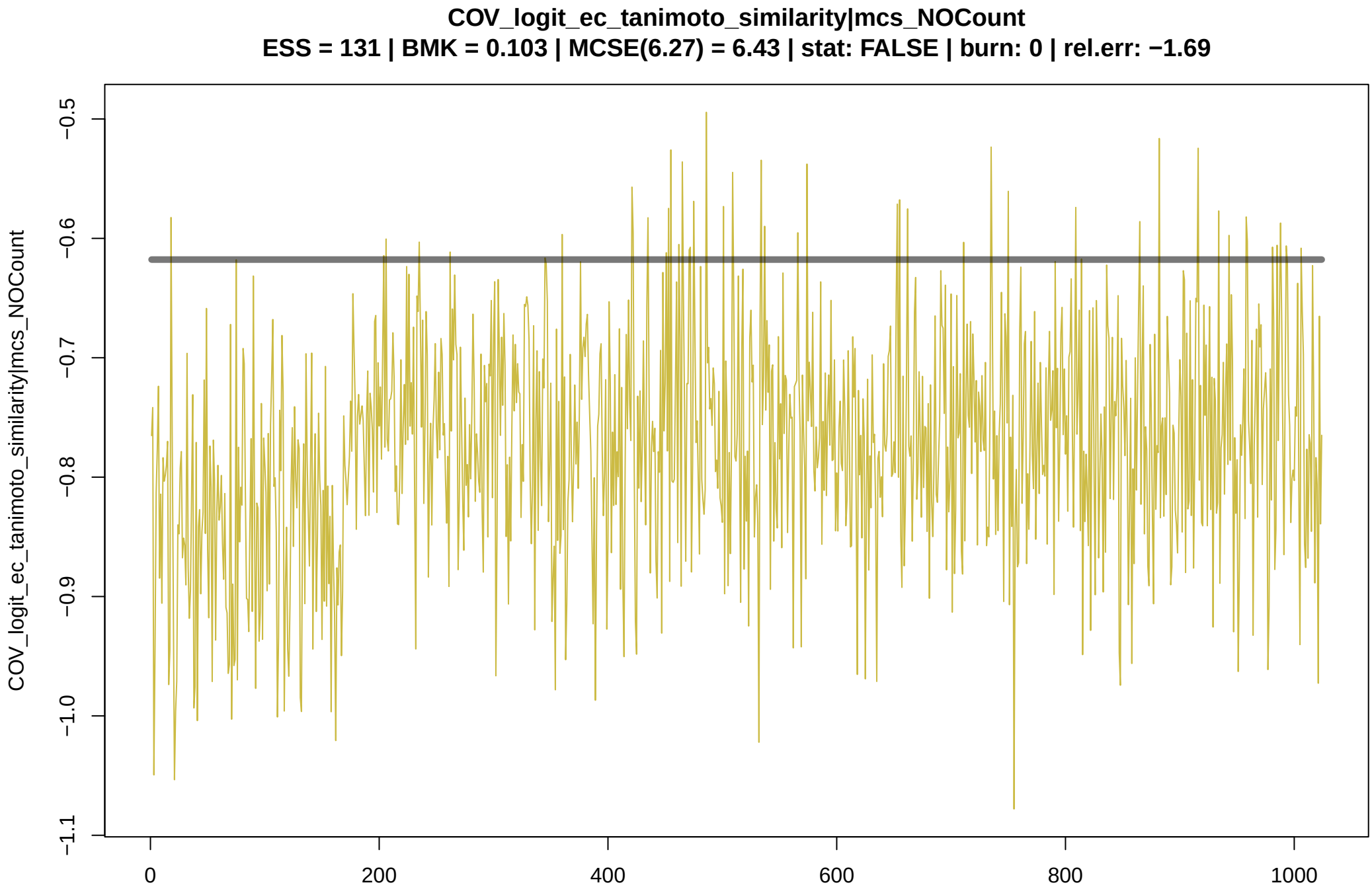

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0749 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | rel.err: −1.45
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
0.2
0.0
−0.2
−0.4
0
200
400
600
800
1000

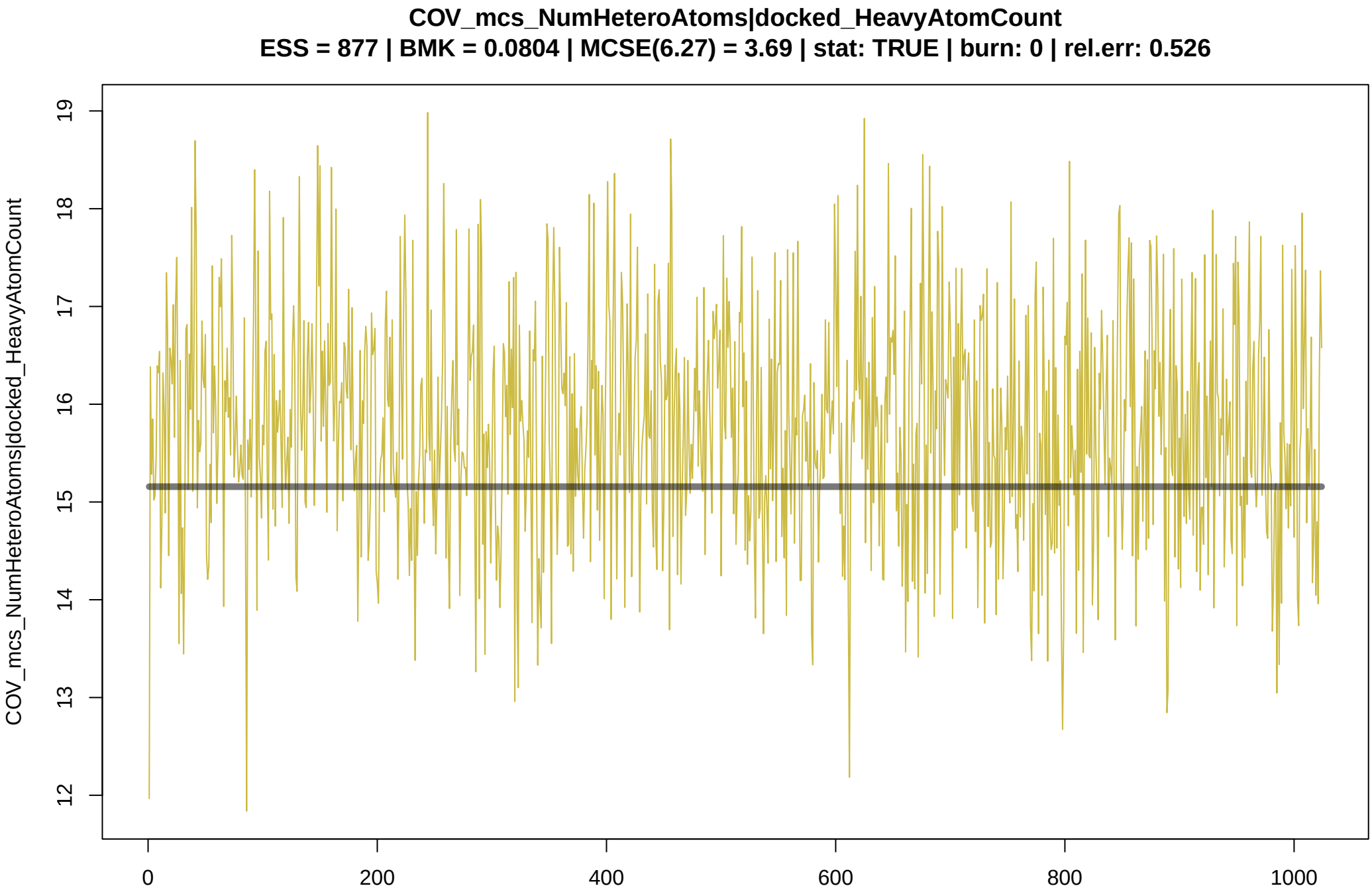

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0992 | MCSE(6.27) = 3.5 | stat: TRUE | burn: 0 | rel.err: 2.13
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
0
200
400
600
800
1000

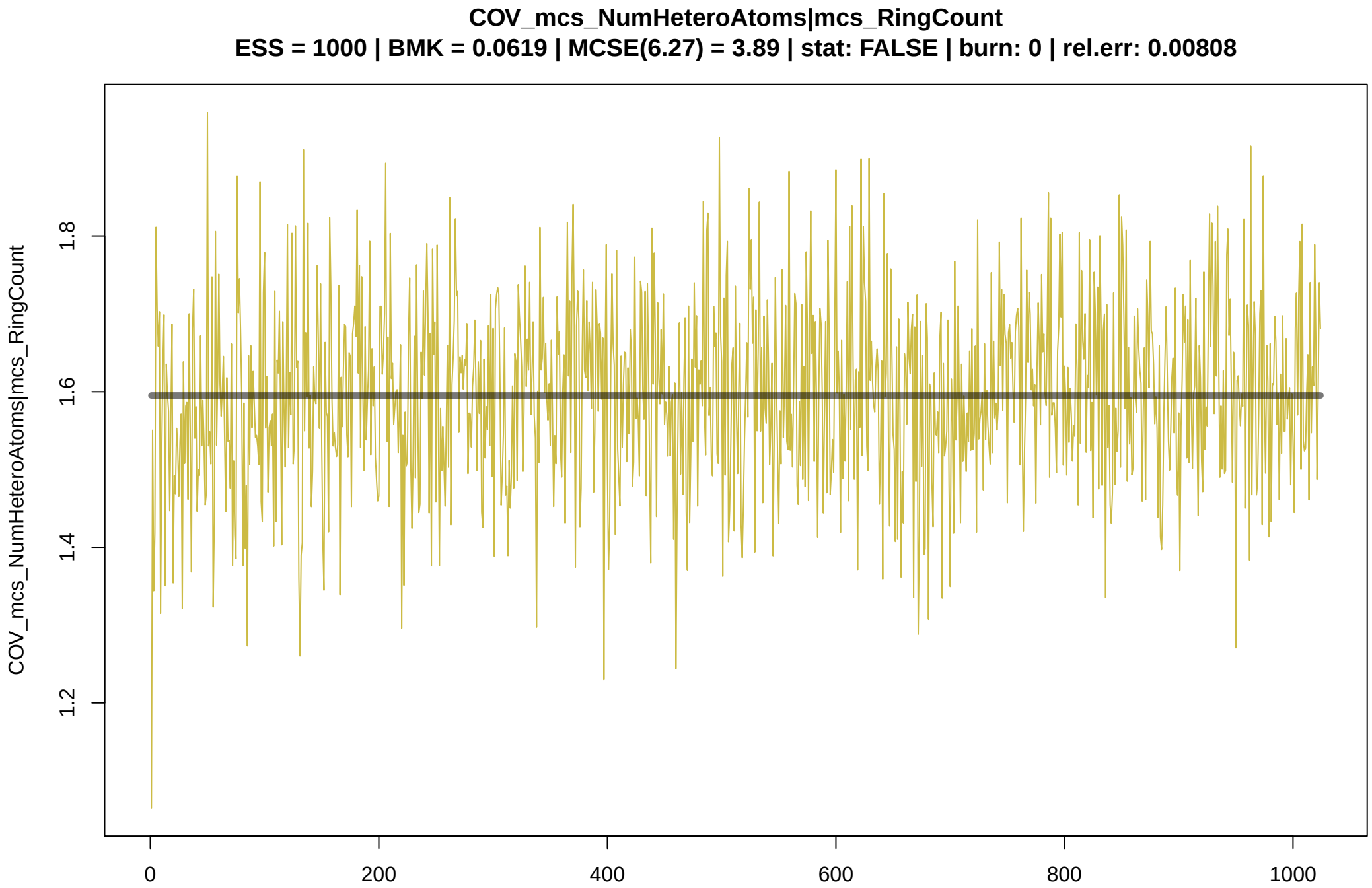

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.105 | MCSE(6.27) = 3.89 | stat: FALSE | burn: 0 | rel.err: −0.517
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
1
0
−1
−2
−3
0
200
400
600
800
1000

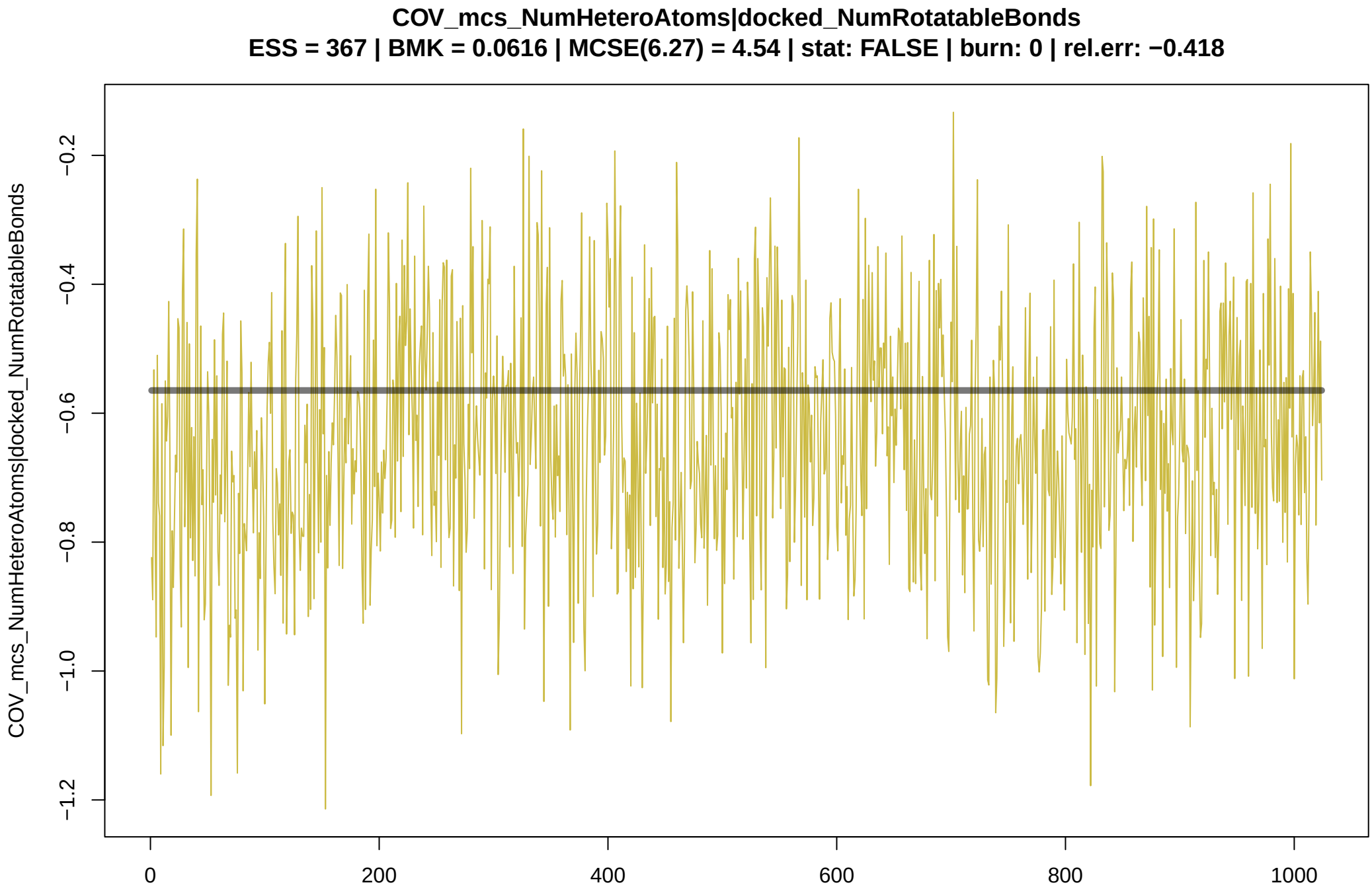

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 16.2 | BMK = 0.206 | MCSE(6.27) = 9.88 | stat: FALSE | burn: 0 | rel.err: −0.605
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
200
400
600
800
1000

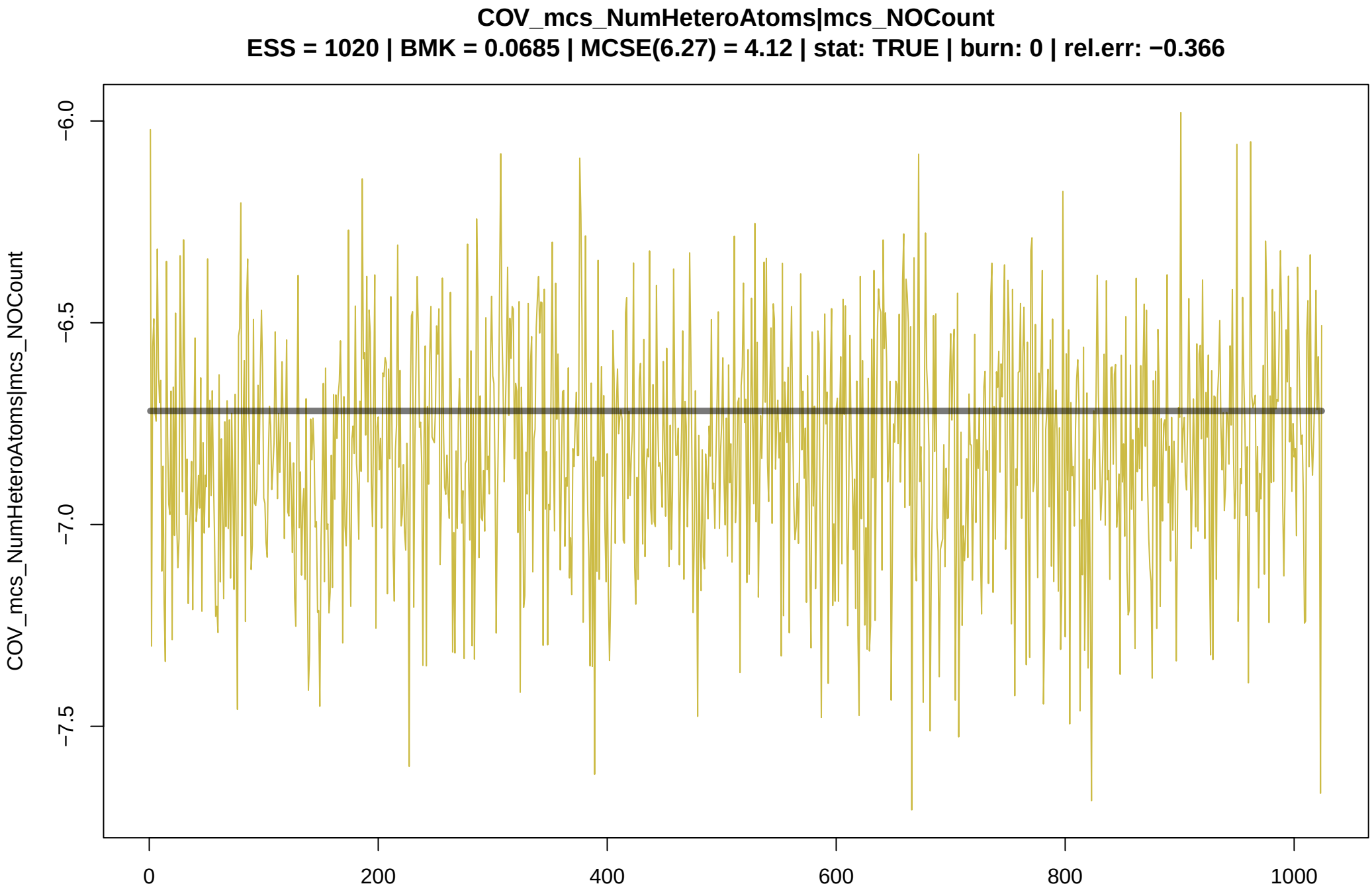

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0728 | MCSE(6.27) = 3.98 | stat: FALSE | burn: 0 | rel.err: −1.3
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−1.0
−1.2
−1.4
−1.6
−1.8
0
200
400
600
800
1000

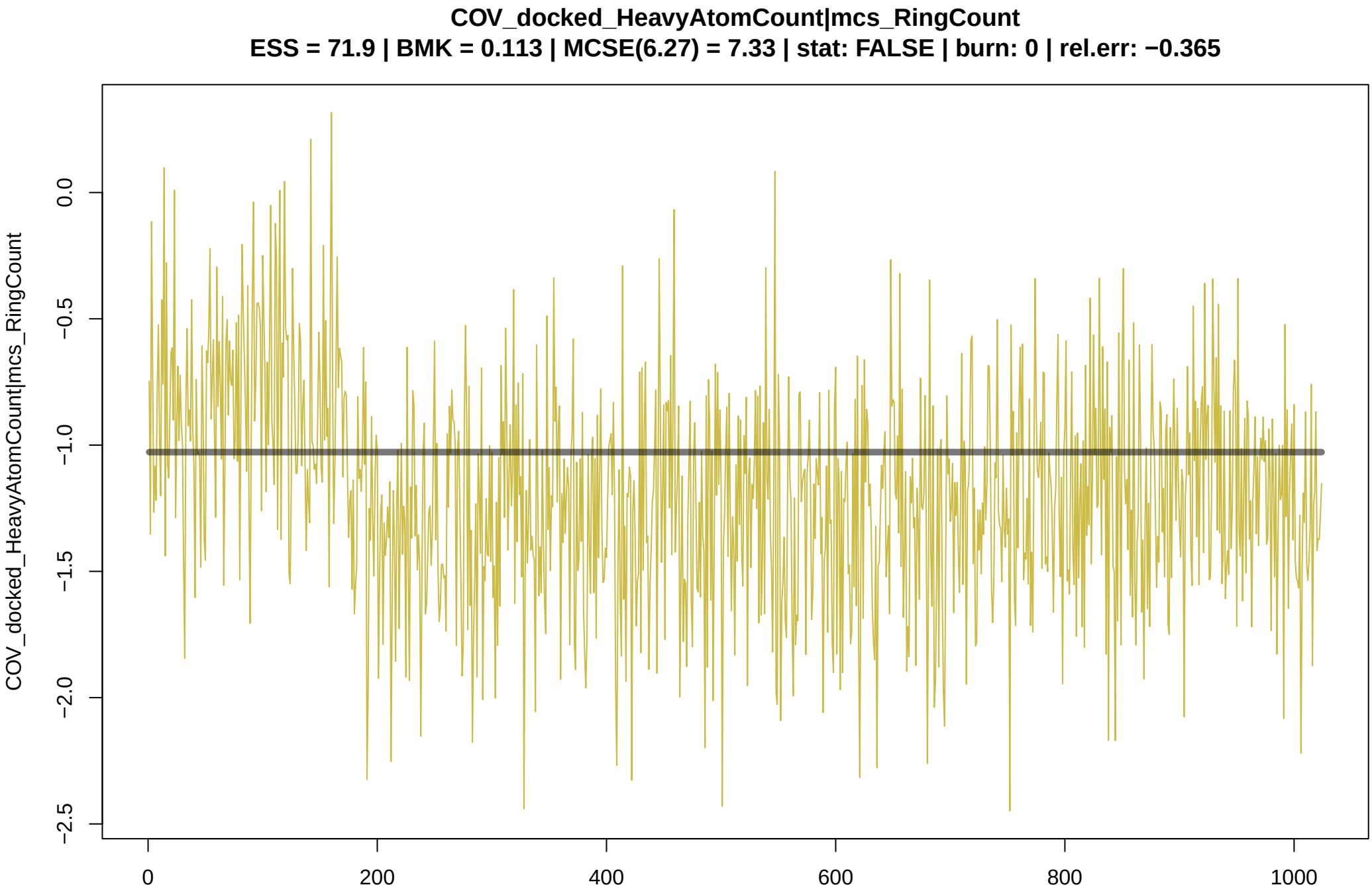

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 131 | BMK = 0.103 | MCSE(6.27) = 6.43 | stat: FALSE | burn: 0 | rel.err: −1.69
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−0.5
−0.6
−0.7
−0.8
−0.9
−1.0
−1.1
0
200
400
600
800
1000

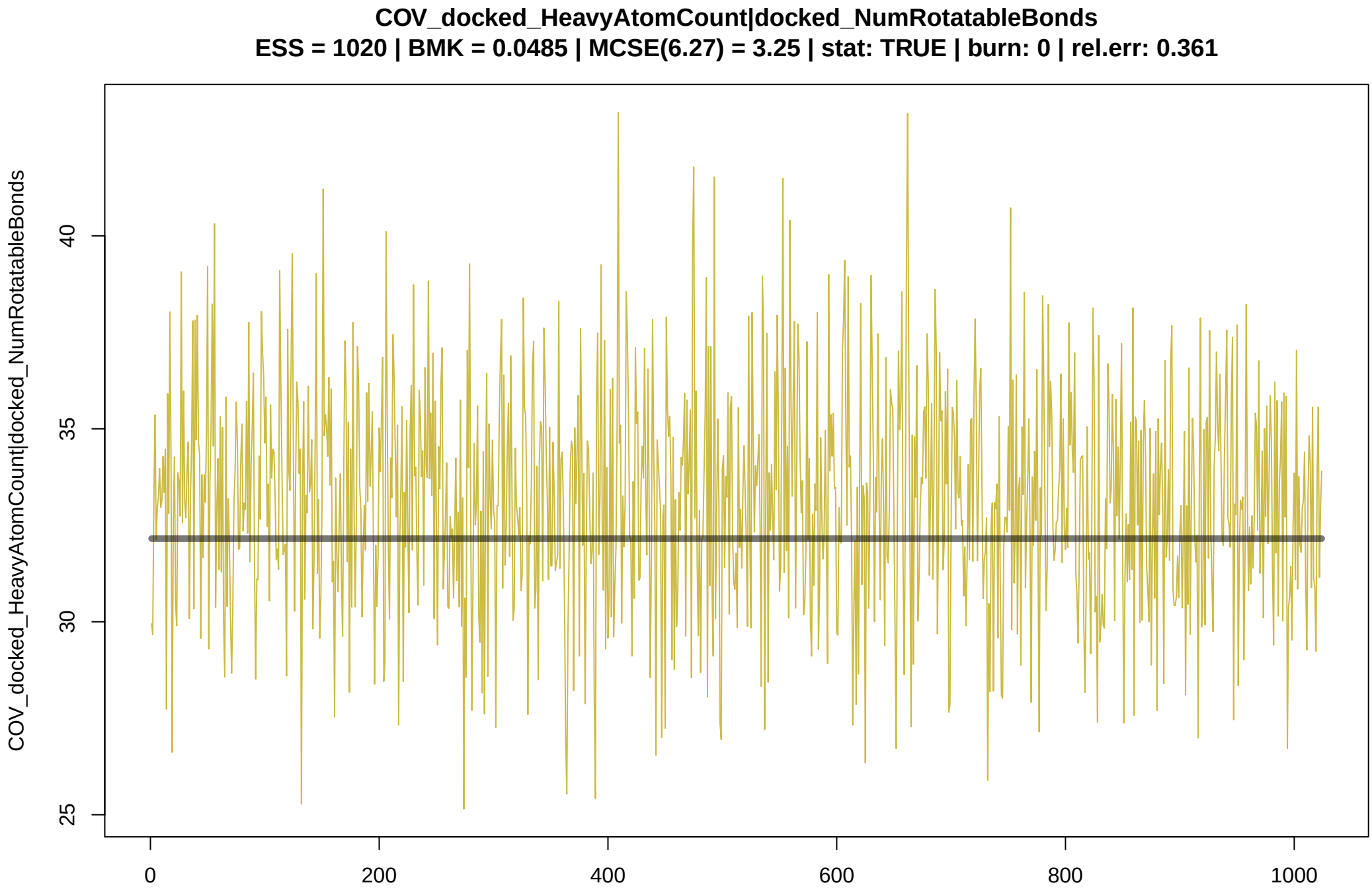

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 877 | BMK = 0.0804 | MCSE(6.27) = 3.69 | stat: TRUE | burn: 0 | rel.err: 0.526
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
12
13
14
15
16
17
18
19
0
200
400
600
800
1000

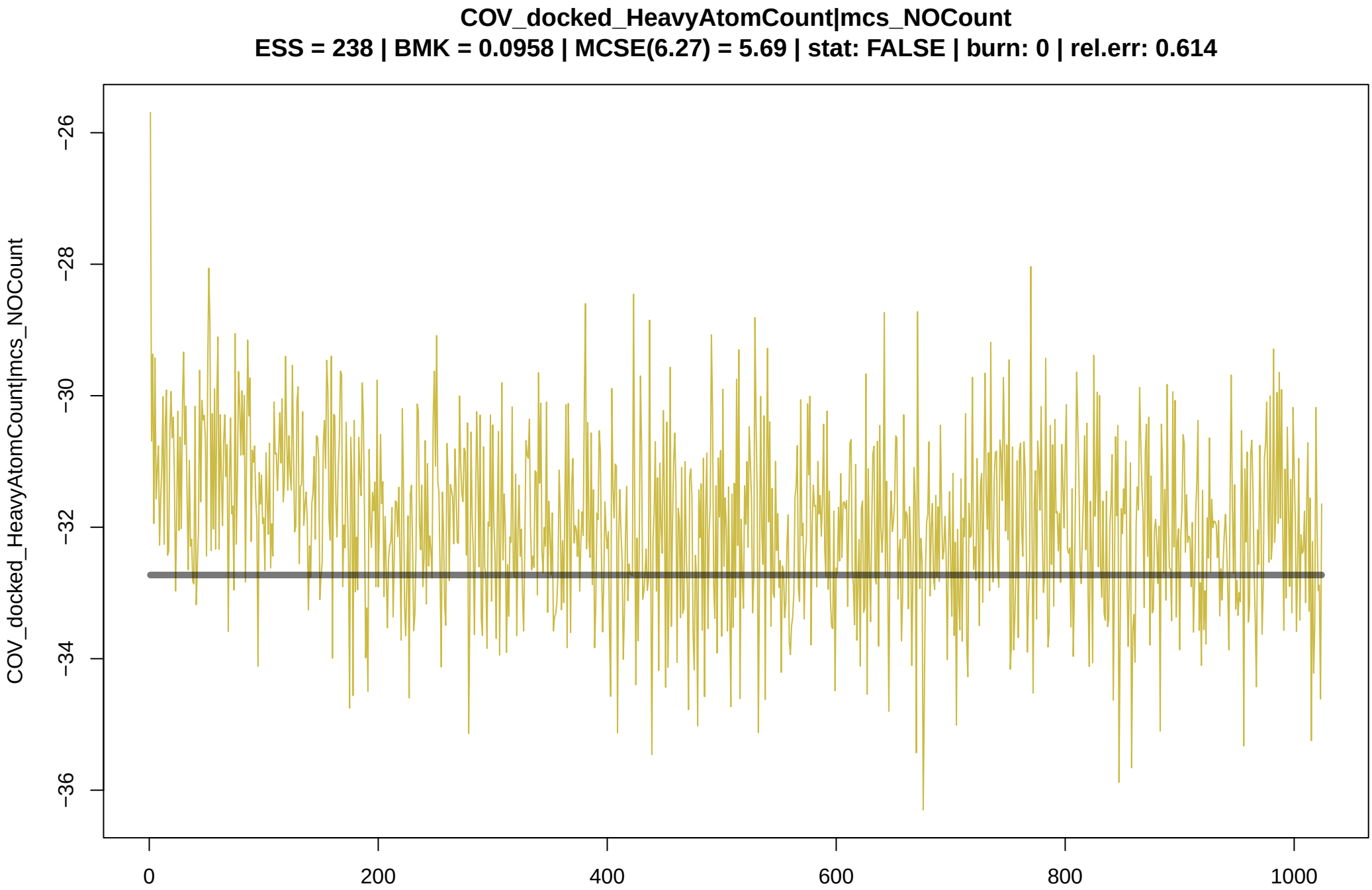

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1000 | BMK = 0.0619 | MCSE(6.27) = 3.89 | stat: FALSE | burn: 0 | rel.err: 0.00808
COV_mcs_NumHeteroAtoms|mcs_RingCount
1.2
1.4
1.6
1.8
0
200
400
600
800
1000

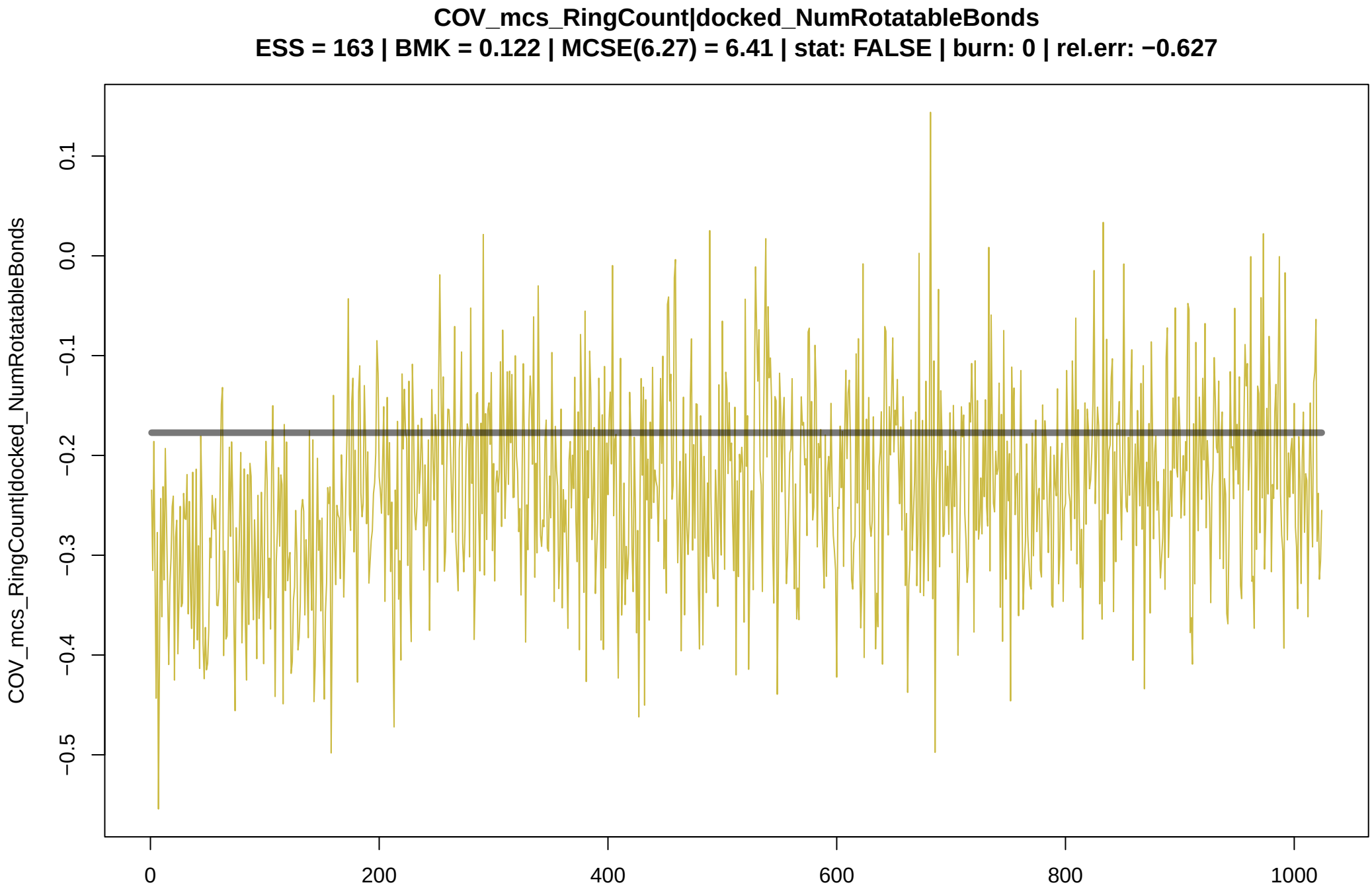

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 367 | BMK = 0.0616 | MCSE(6.27) = 4.54 | stat: FALSE | burn: 0 | rel.err: −0.418
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
0
200
400
600
800
1000

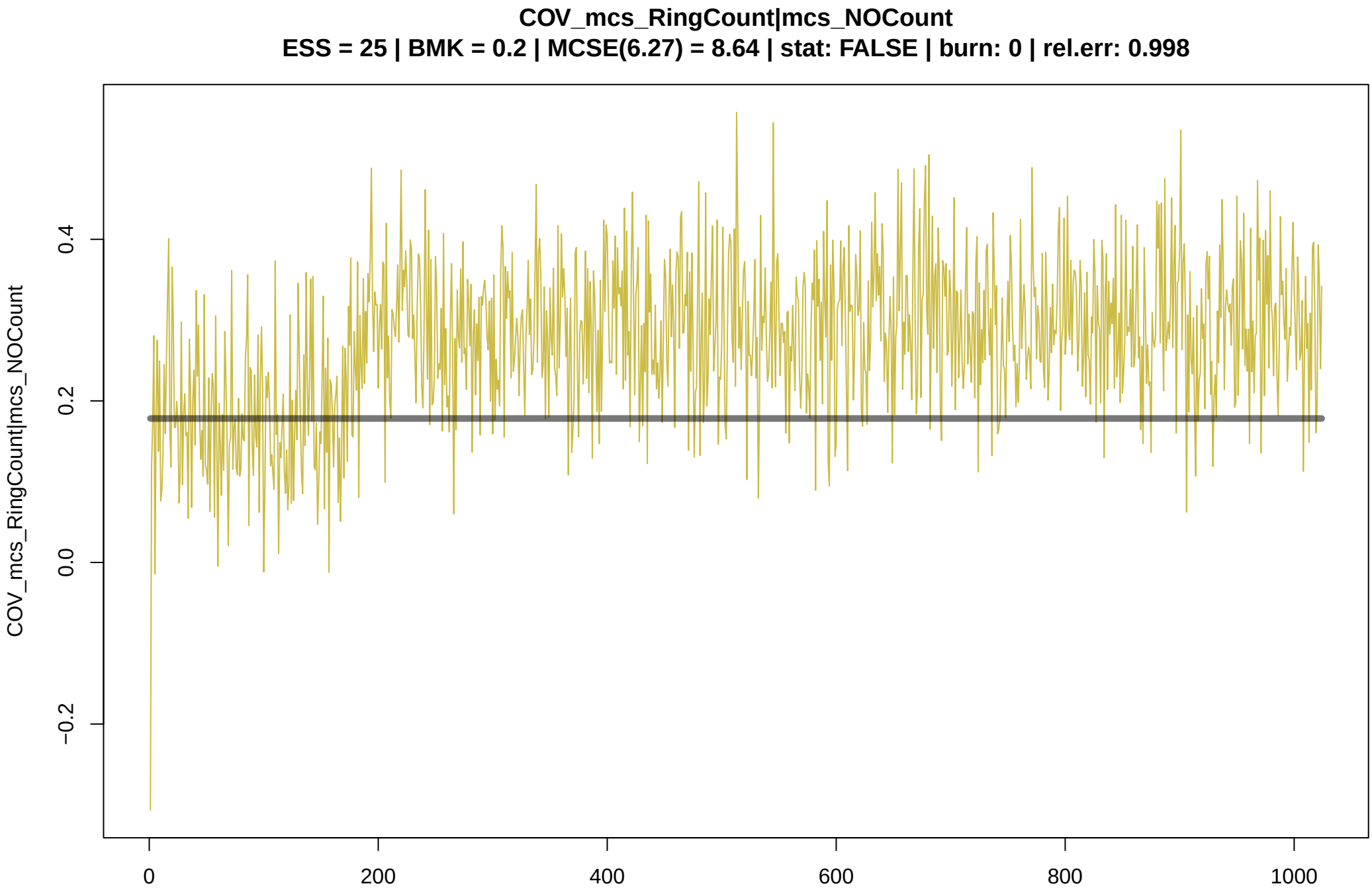

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0685 | MCSE(6.27) = 4.12 | stat: TRUE | burn: 0 | rel.err: −0.366
COV_mcs_NumHeteroAtoms|mcs_NOCount
−6.0
−6.5
−7.0
−7.5
0
200
400
600
800
1000

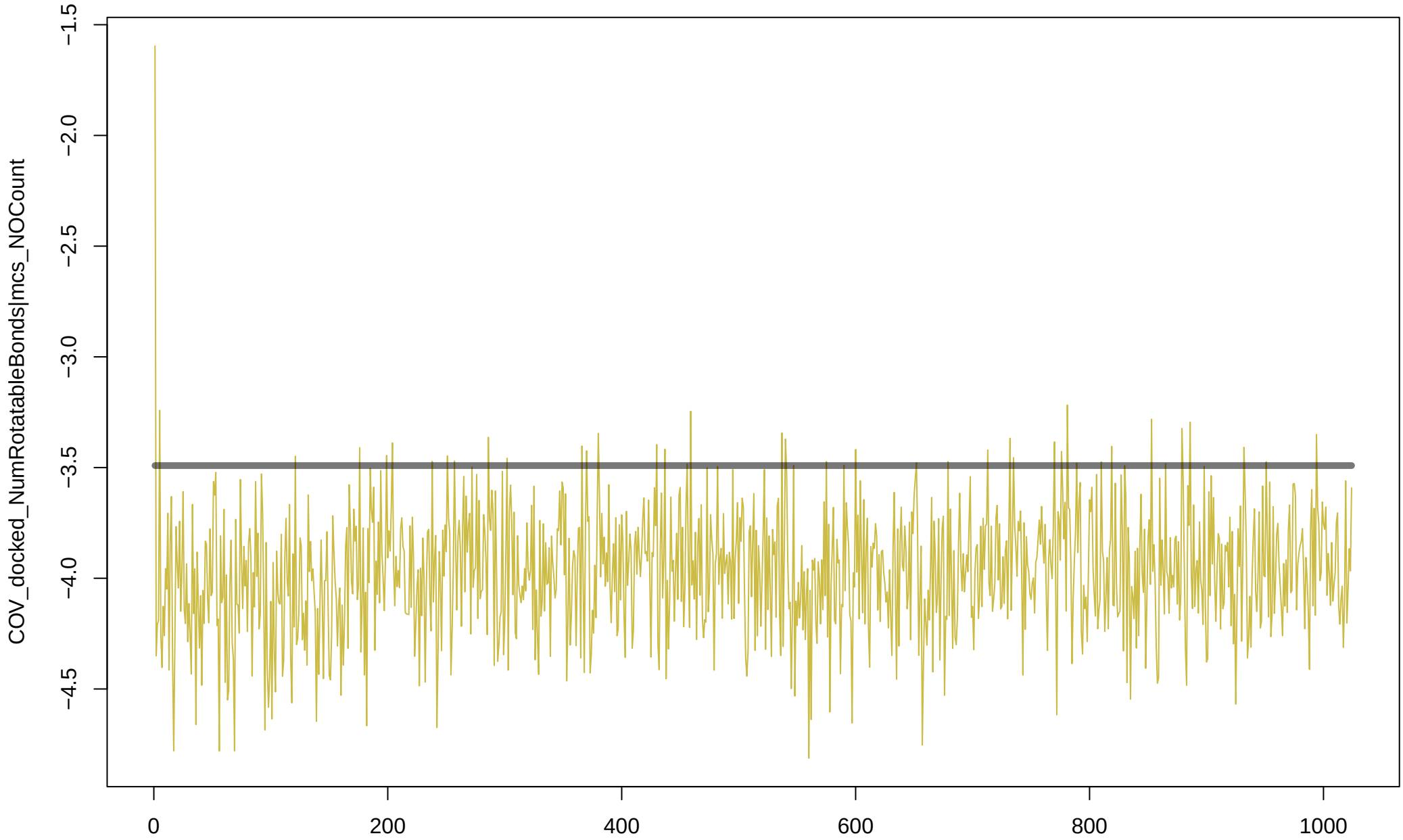

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 71.9 | BMK = 0.113 | MCSE(6.27) = 7.33 | stat: FALSE | burn: 0 | rel.err: −0.365
COV_docked_HeavyAtomCount|mcs_RingCount
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0485 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | rel.err: 0.361
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
25
30
35
40
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 238 | BMK = 0.0958 | MCSE(6.27) = 5.69 | stat: FALSE | burn: 0 | rel.err: 0.614
COV_docked_HeavyAtomCount|mcs_NOCount
−26
−28
−30
−32
−34
−36
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 163 | BMK = 0.122 | MCSE(6.27) = 6.41 | stat: FALSE | burn: 0 | rel.err: −0.627
COV_mcs_RingCount|docked_NumRotatableBonds
0.1
0.0
−0.1
−0.2
−0.3
−0.4
−0.5
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 25 | BMK = 0.2 | MCSE(6.27) = 8.64 | stat: FALSE | burn: 0 | rel.err: 0.998
COV_mcs_RingCount|mcs_NOCount
0.4
0.2
0.0
−0.2
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0666 | MCSE(6.27) = 4.2 | stat: FALSE | burn: 0 | rel.err: −1.71
COV_docked_NumRotatableBonds|mcs_NOCount
−1.5
−2.0
−2.5
−3.0
−3.5
−4.0
−4.5
0
200
400
600
800
1000