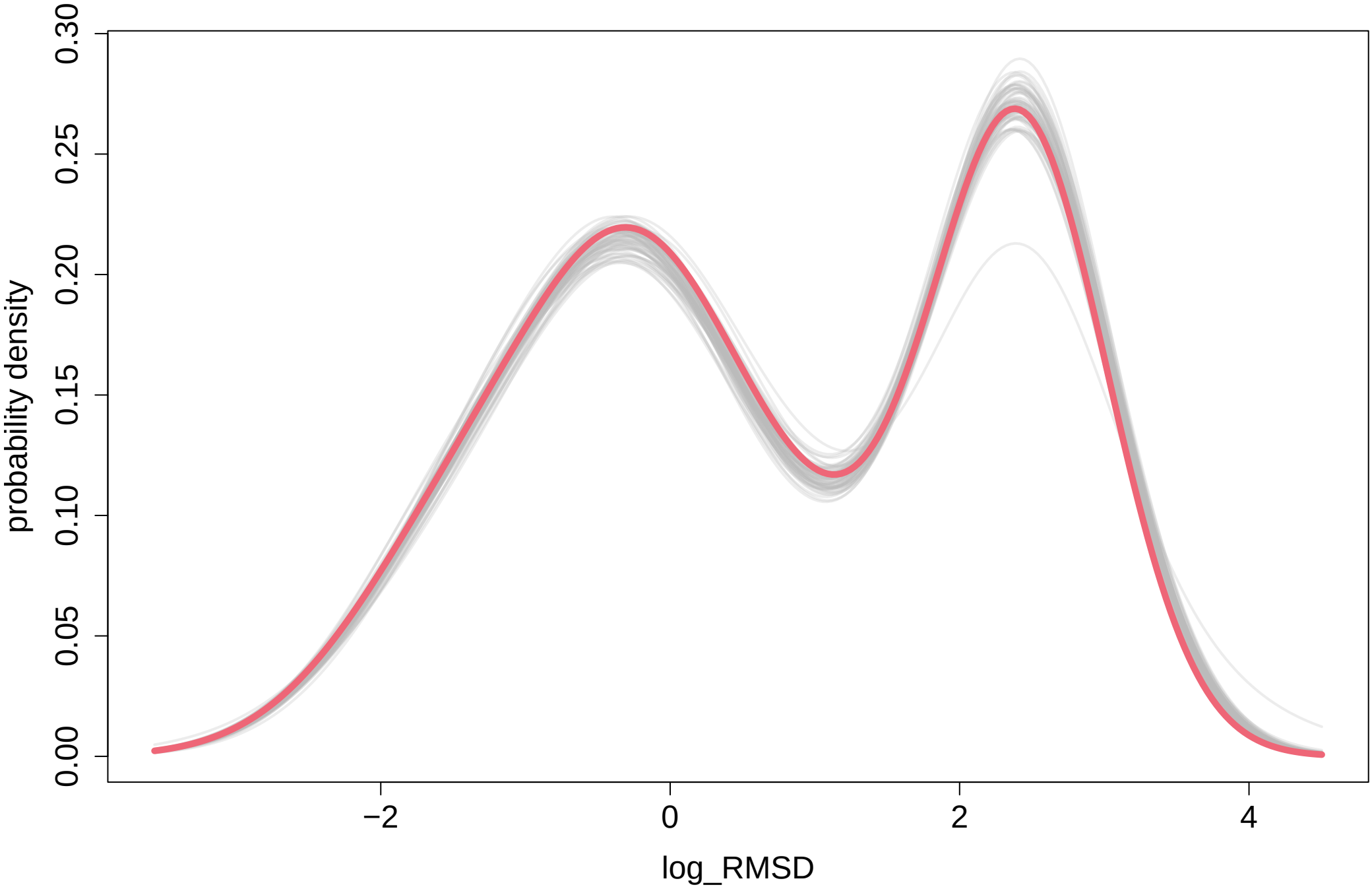
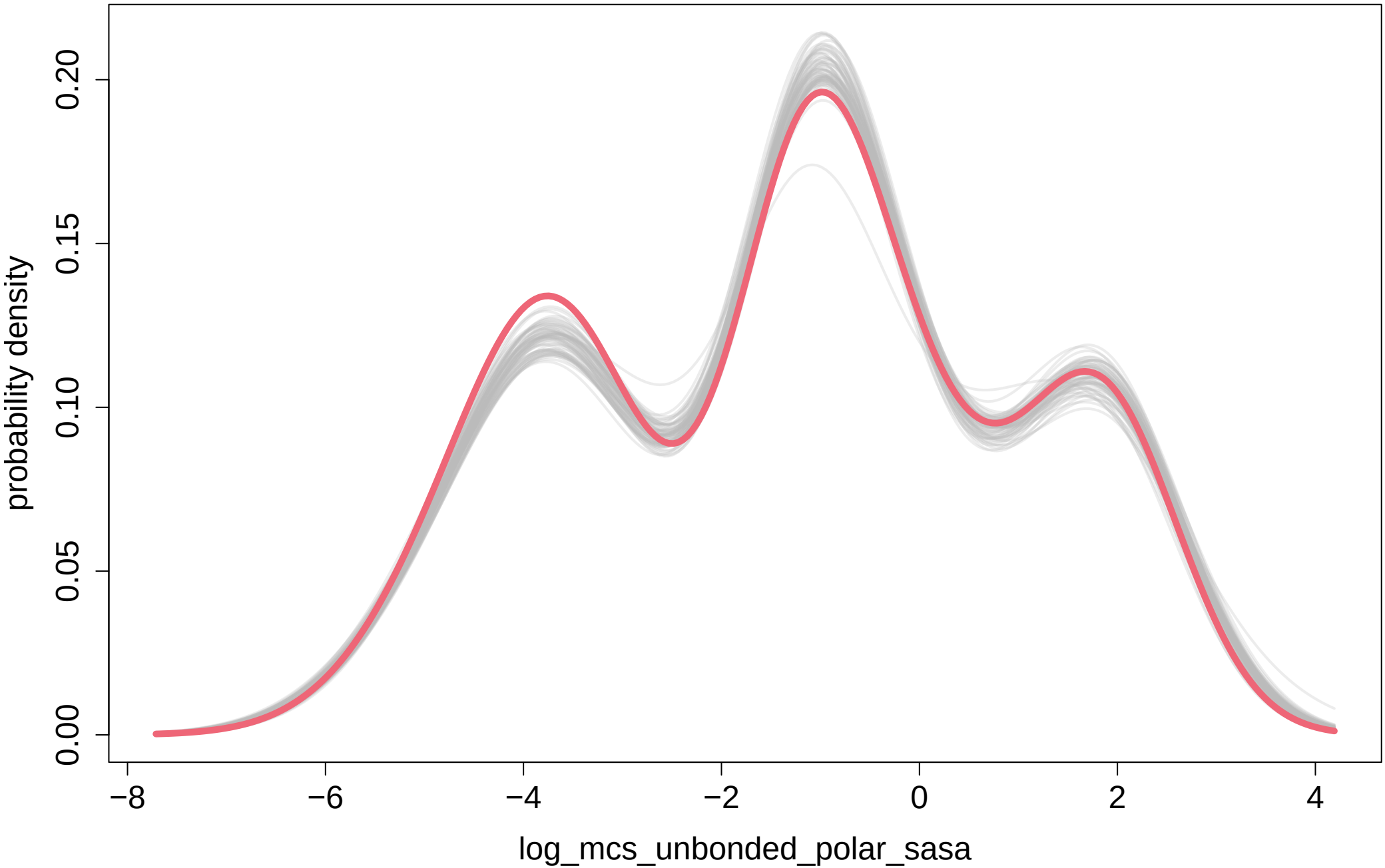
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.691608944706779
max MCSE = 16.4808899036598
all stationary: FALSE
burn: 306
max rel.err.: 1.77948333961391

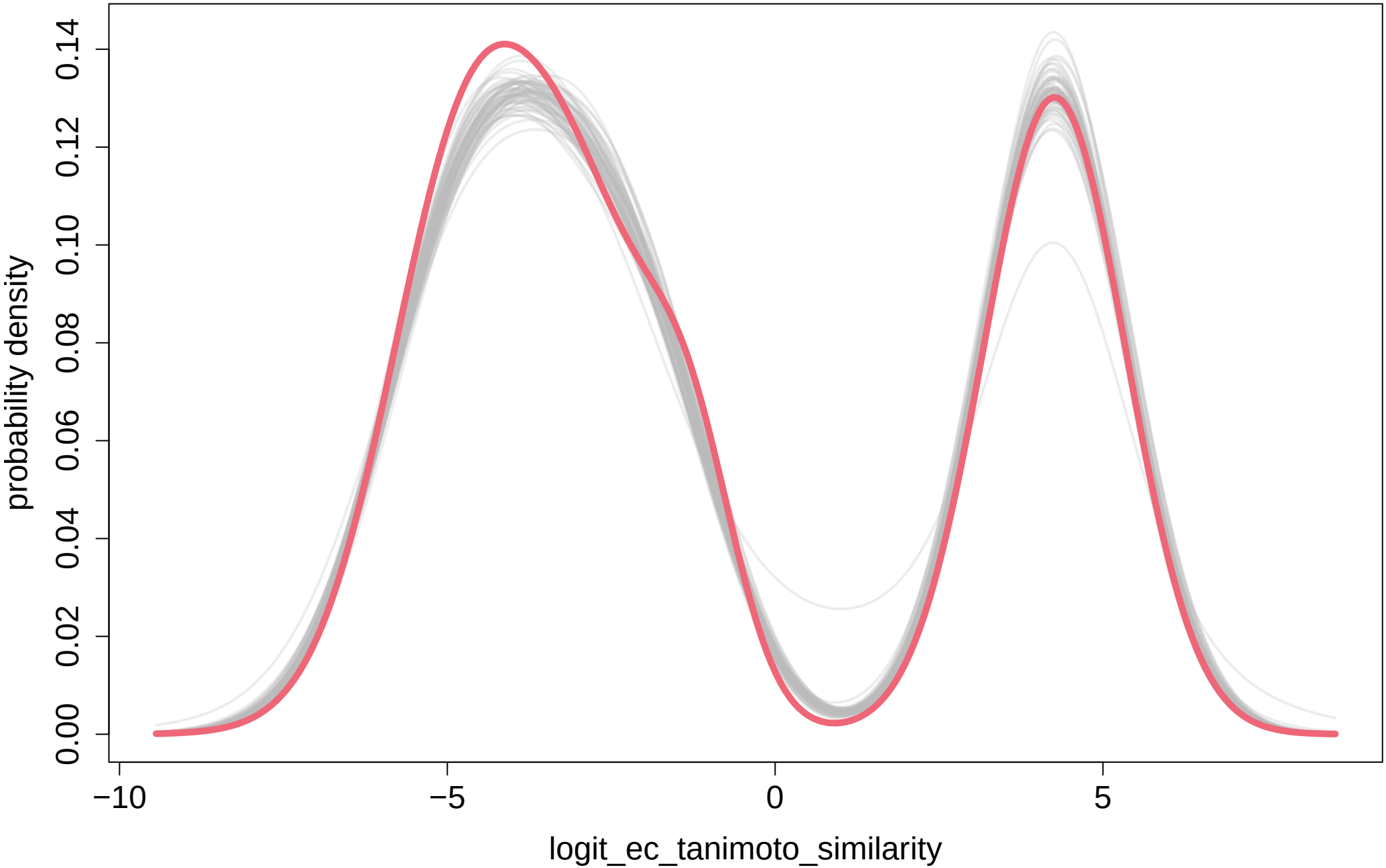
−− STATS 2D −−
min ESS = 872.104836385351
max BMK = 0.071582052579329 7
max MCSE = 4.09253988275022
all stationary: TRUE
burn: 0
max rel.err.: 2.16655180631787

−− STATS 1D −−
min ESS = 48.7494571389437
max BMK = 0.230930666898704
max MCSE = 8.06642434120884
all stationary: FALSE
burn: 0
max rel.err.: 2.70010931626478

Occupied clusters: 9 of 64
LL: −62600 +− 129


probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−2
0
2
4
log_RMSD


probability density
0.00
0.05
0.10
0.15
0.20
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa


probability density
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0.02
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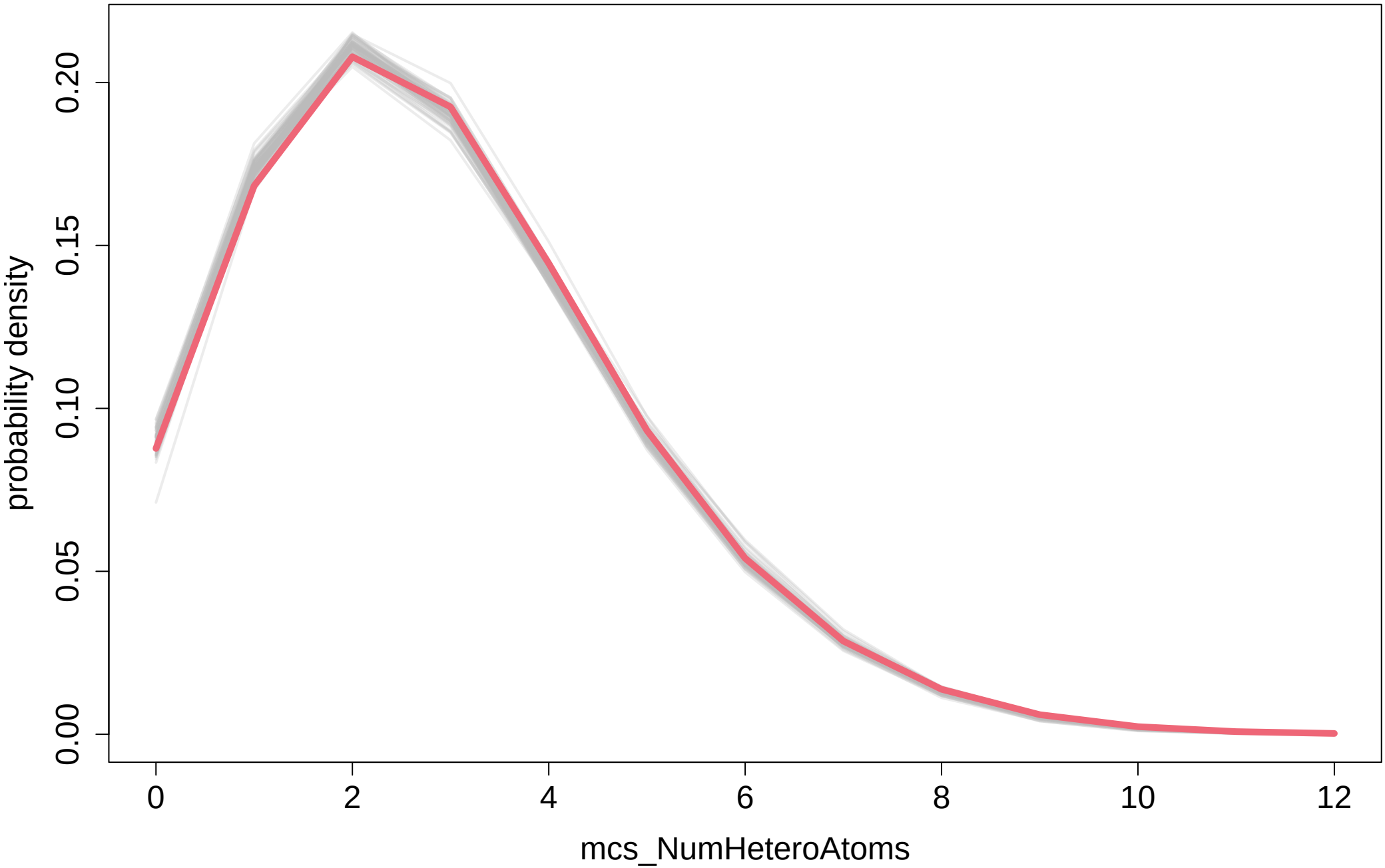
0.06
0.08
0.10
0.12
0.14
−10
−5
0
5
logit_ec_tanimoto_similarity


probability density
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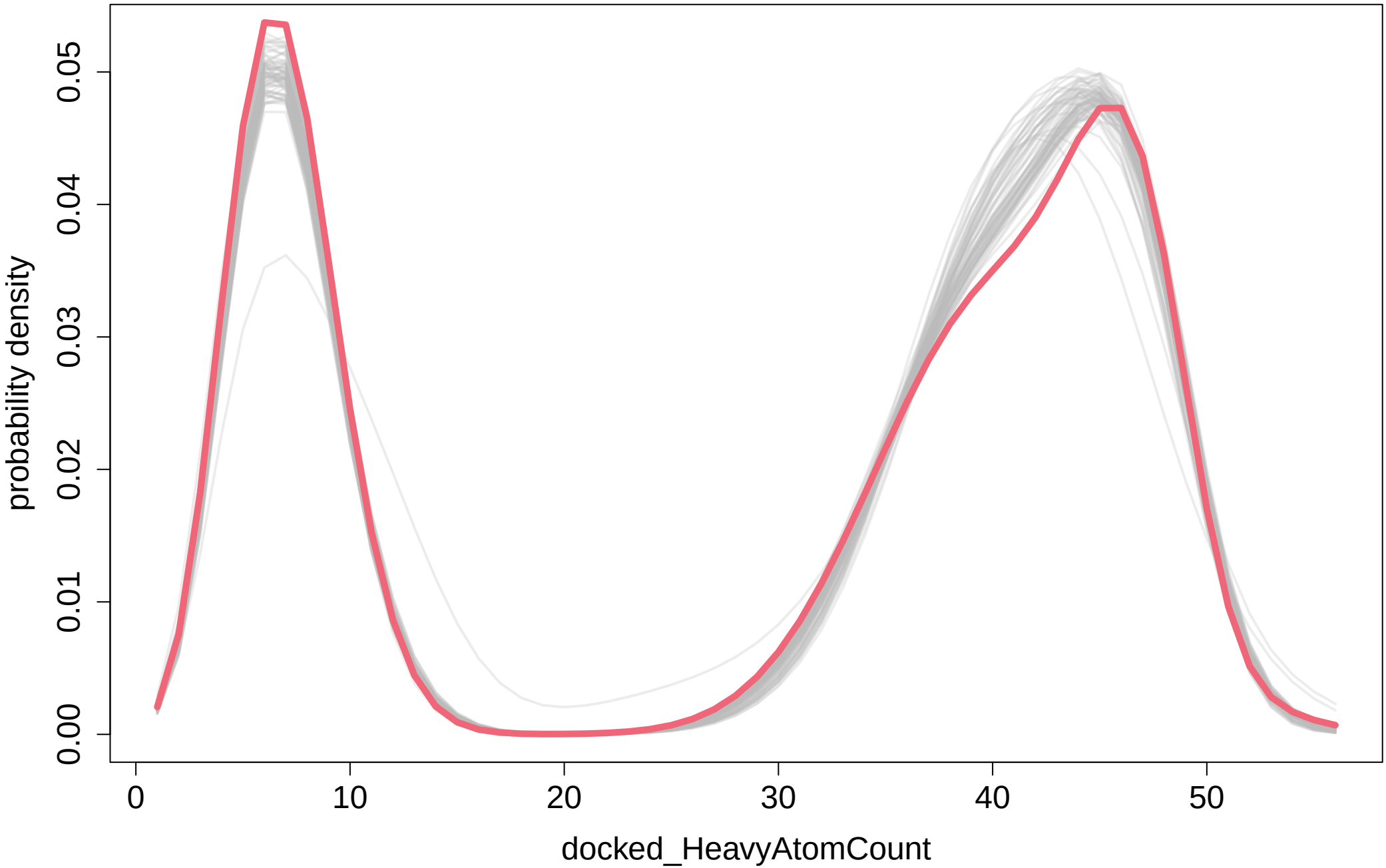
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms


probability density
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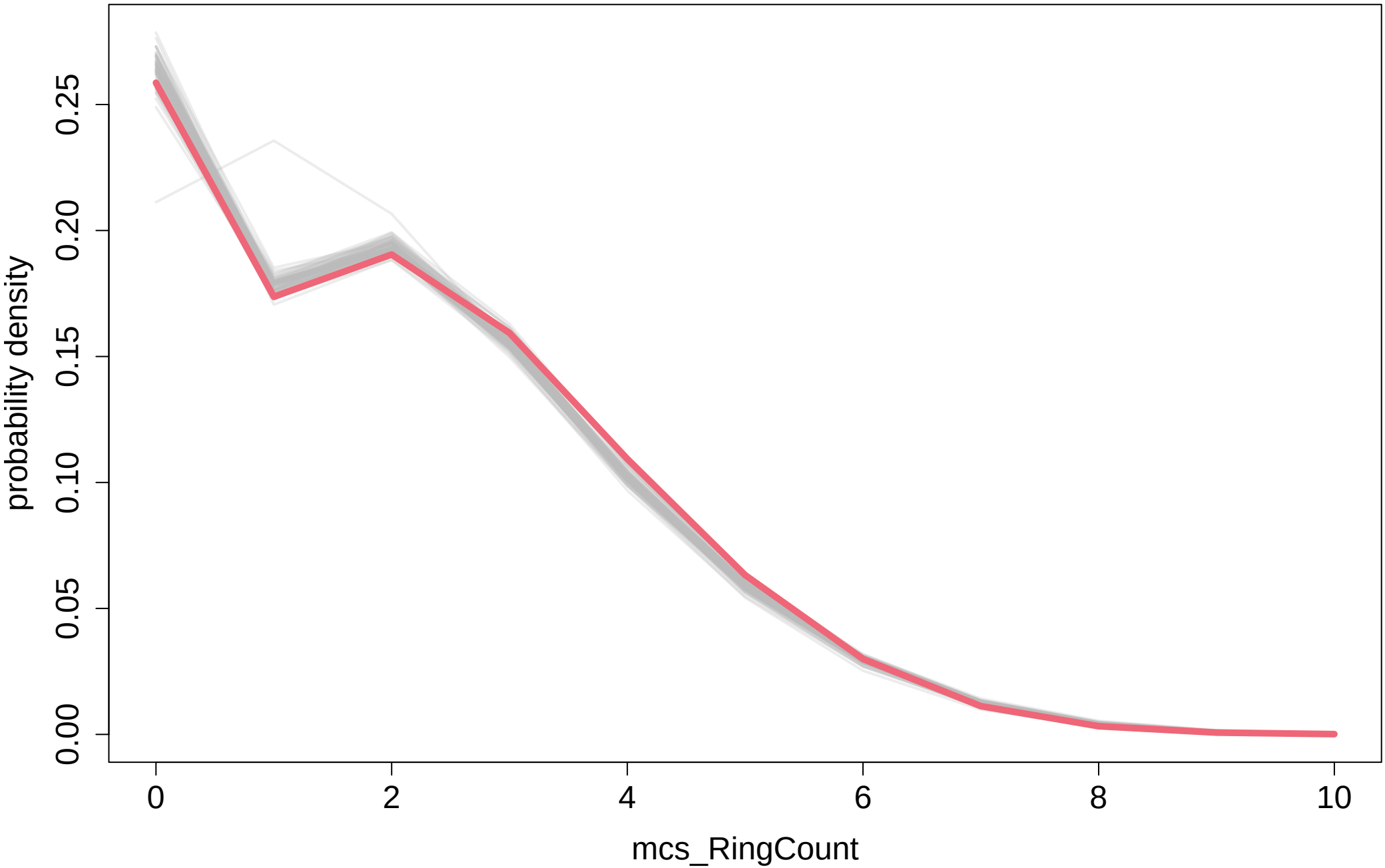
0.01
0.02
0.03
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount


probability density
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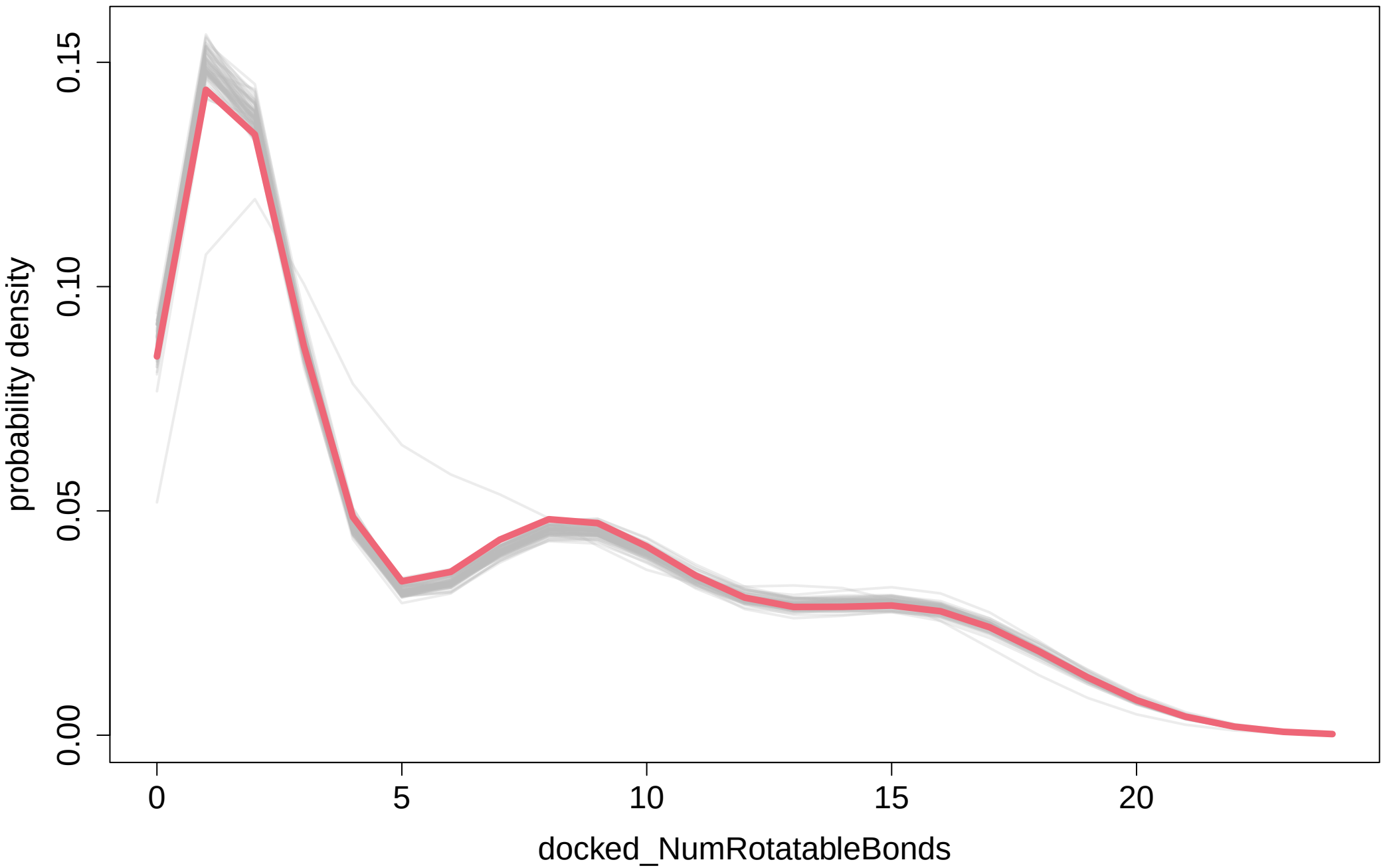
0.05
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount


probability density
0.00
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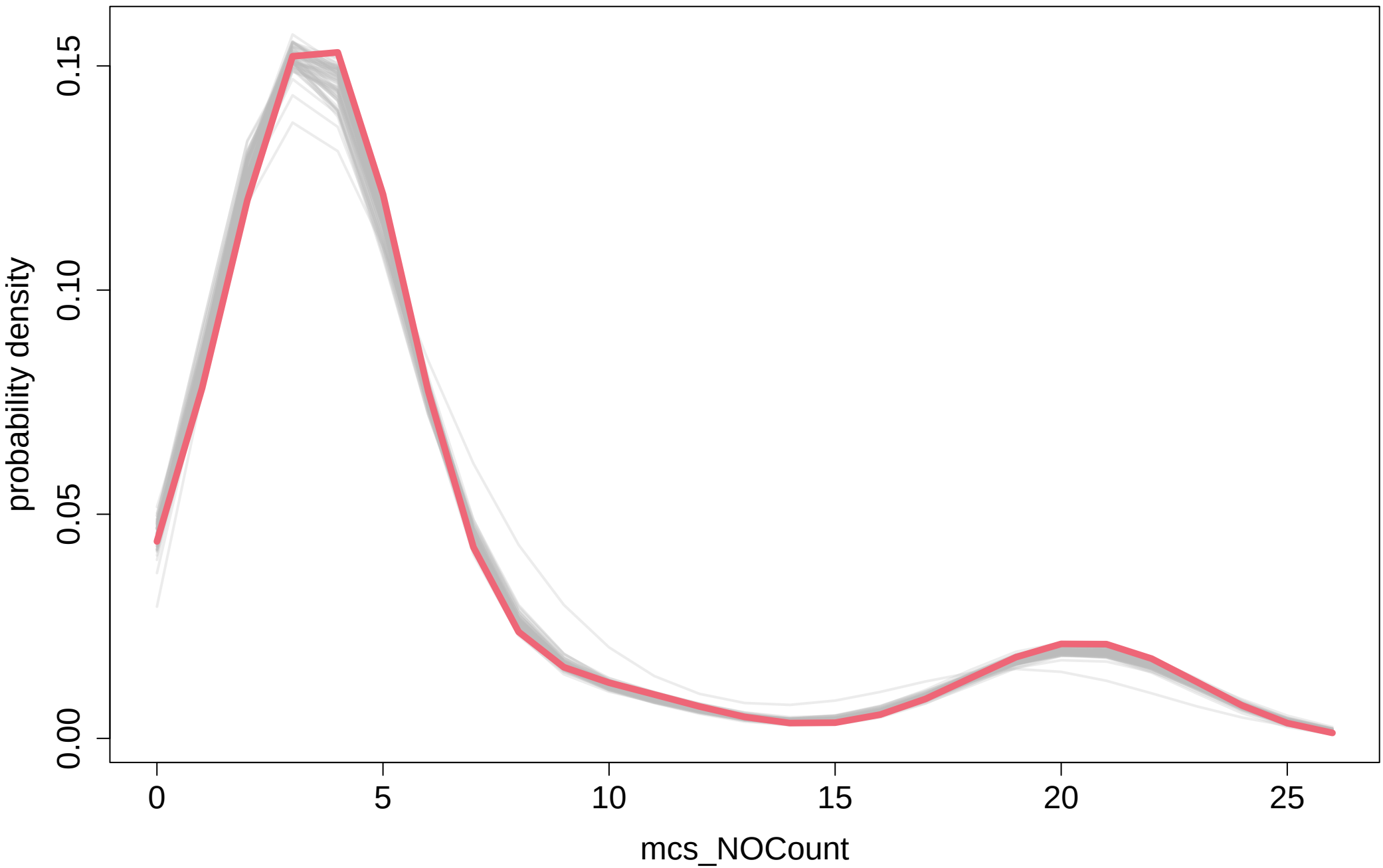
0.10
0.15
0
5
10
15
20
docked_NumRotatableBonds


probability density
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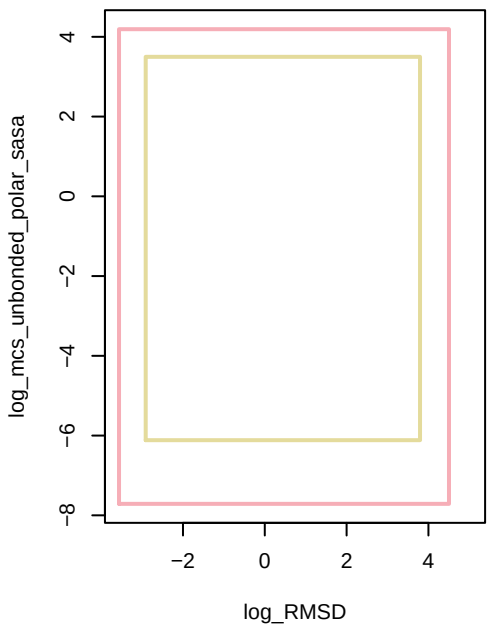
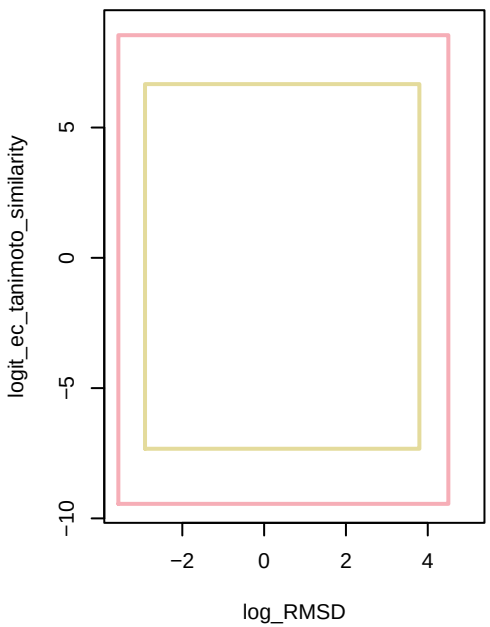
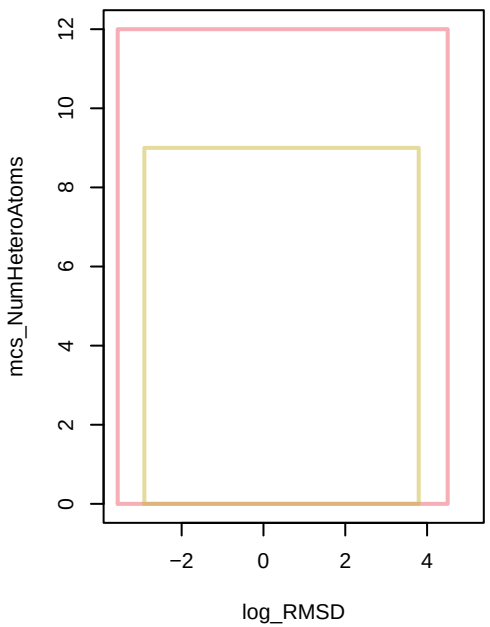
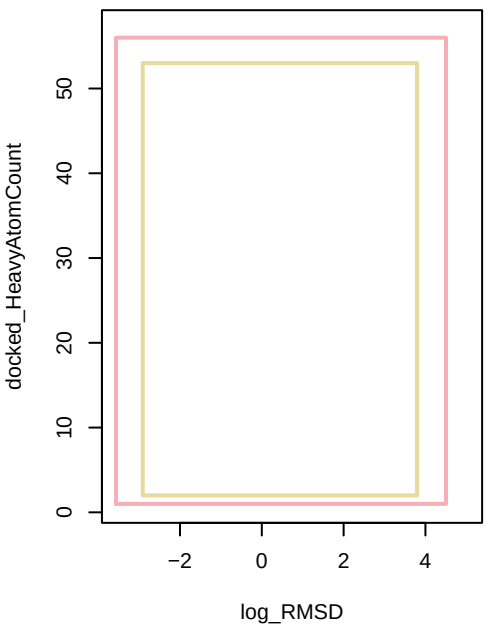
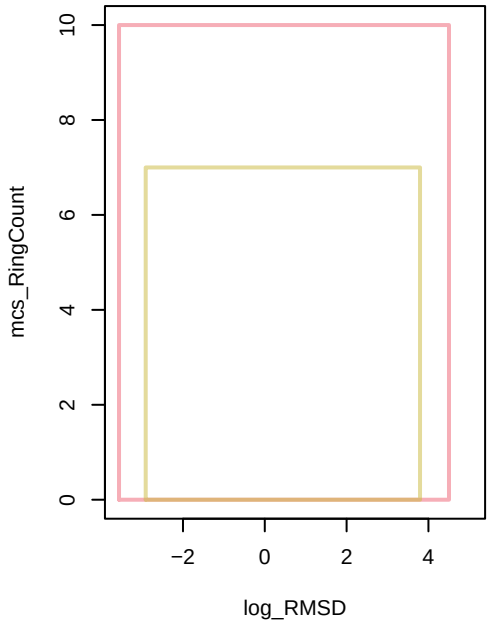
0.05
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

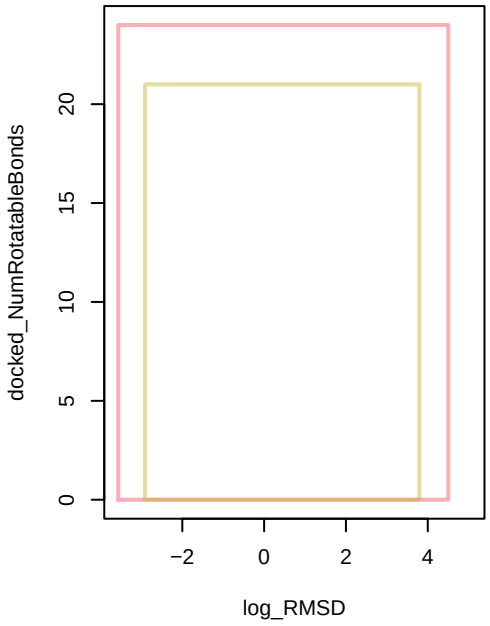

log_mcs_unbonded_polar_sasa
log_RMSD

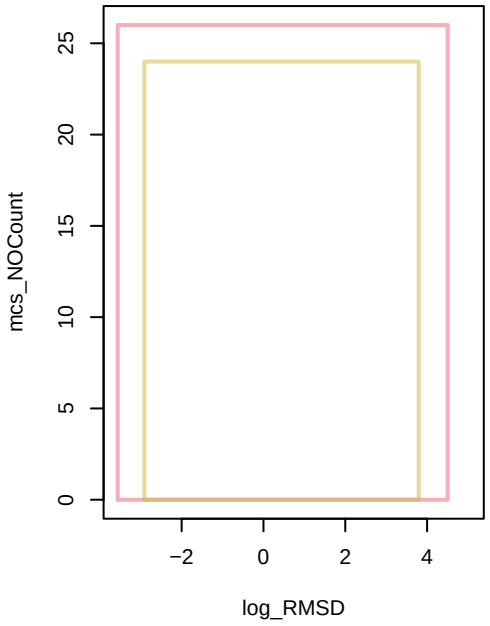

logit_ec_tanimoto_similarity
log_RMSD

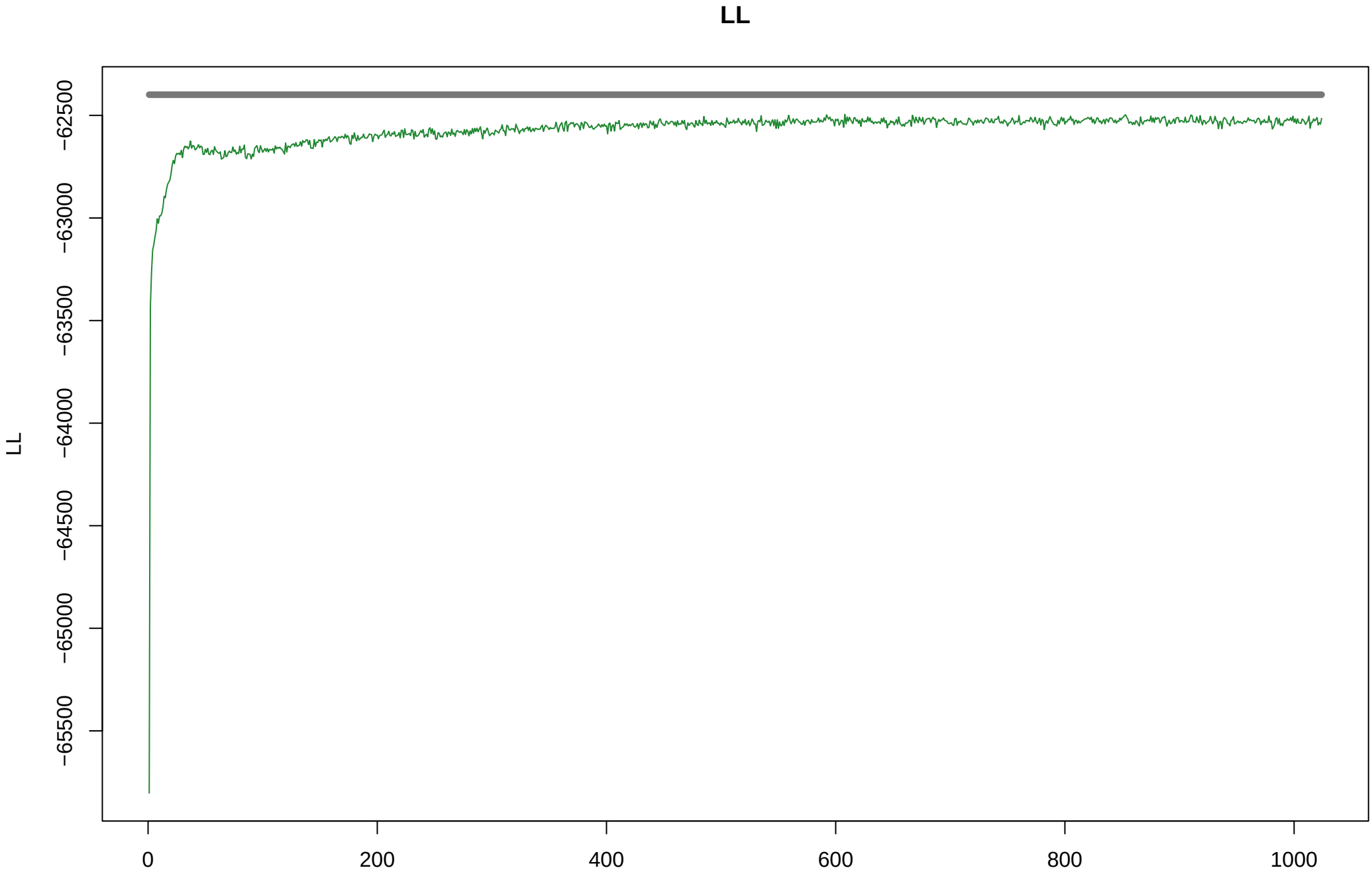

mcs_NumHeteroAtoms
log_RMSD

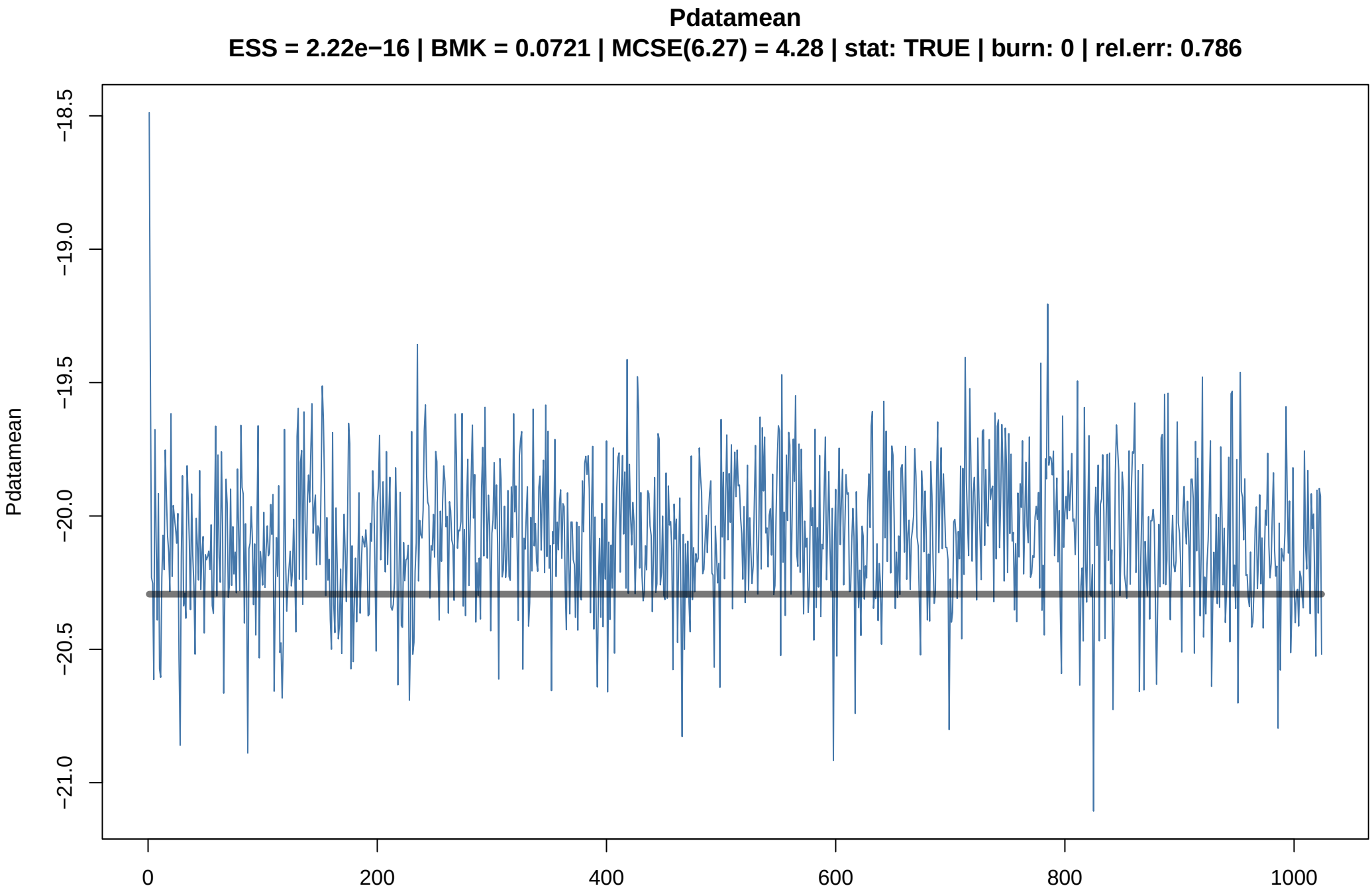

docked_HeavyAtomCount
log_RMSD

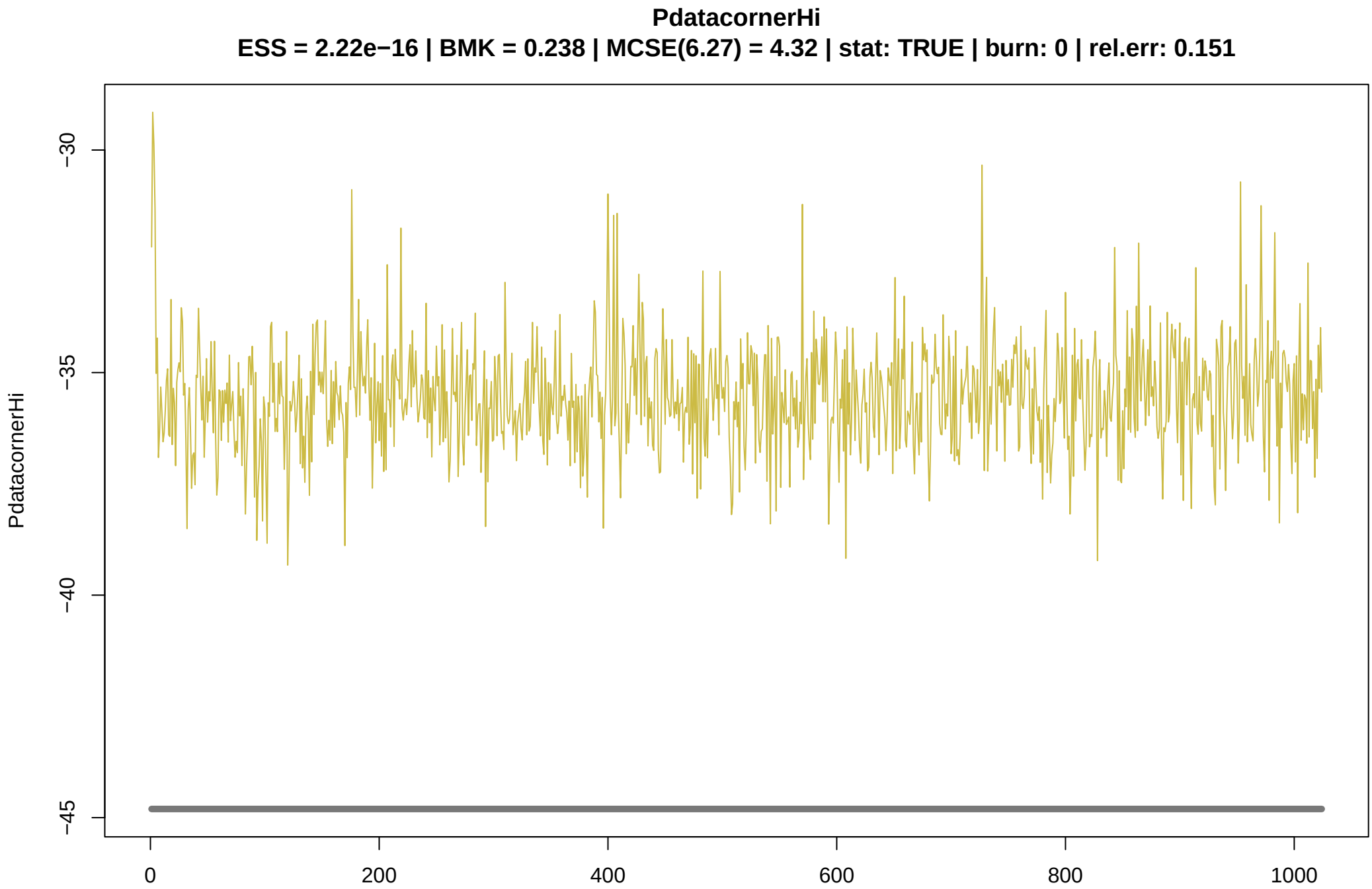

mcs_RingCount
log_RMSD

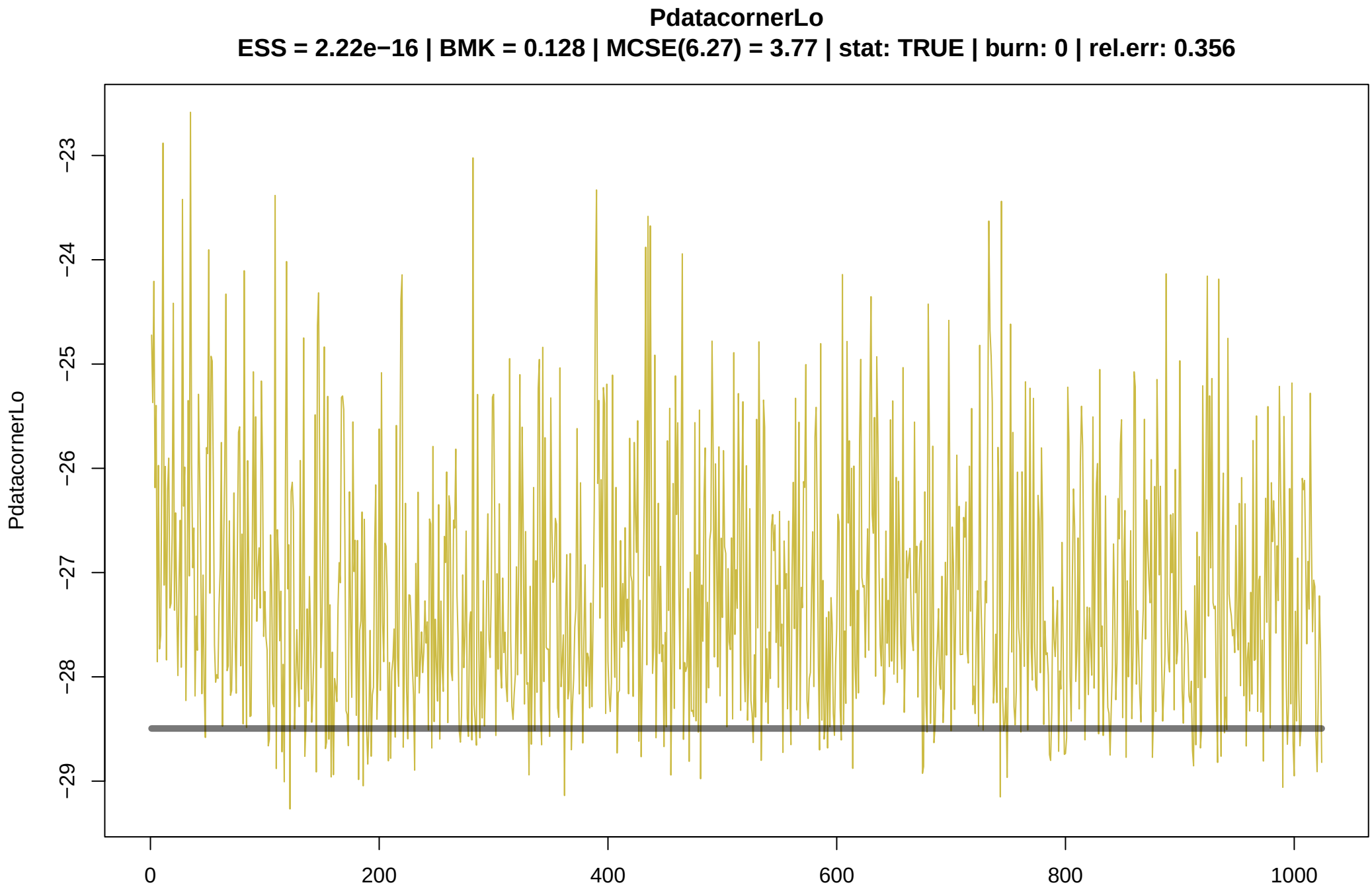

docked_NumRotatableBonds
log_RMSD

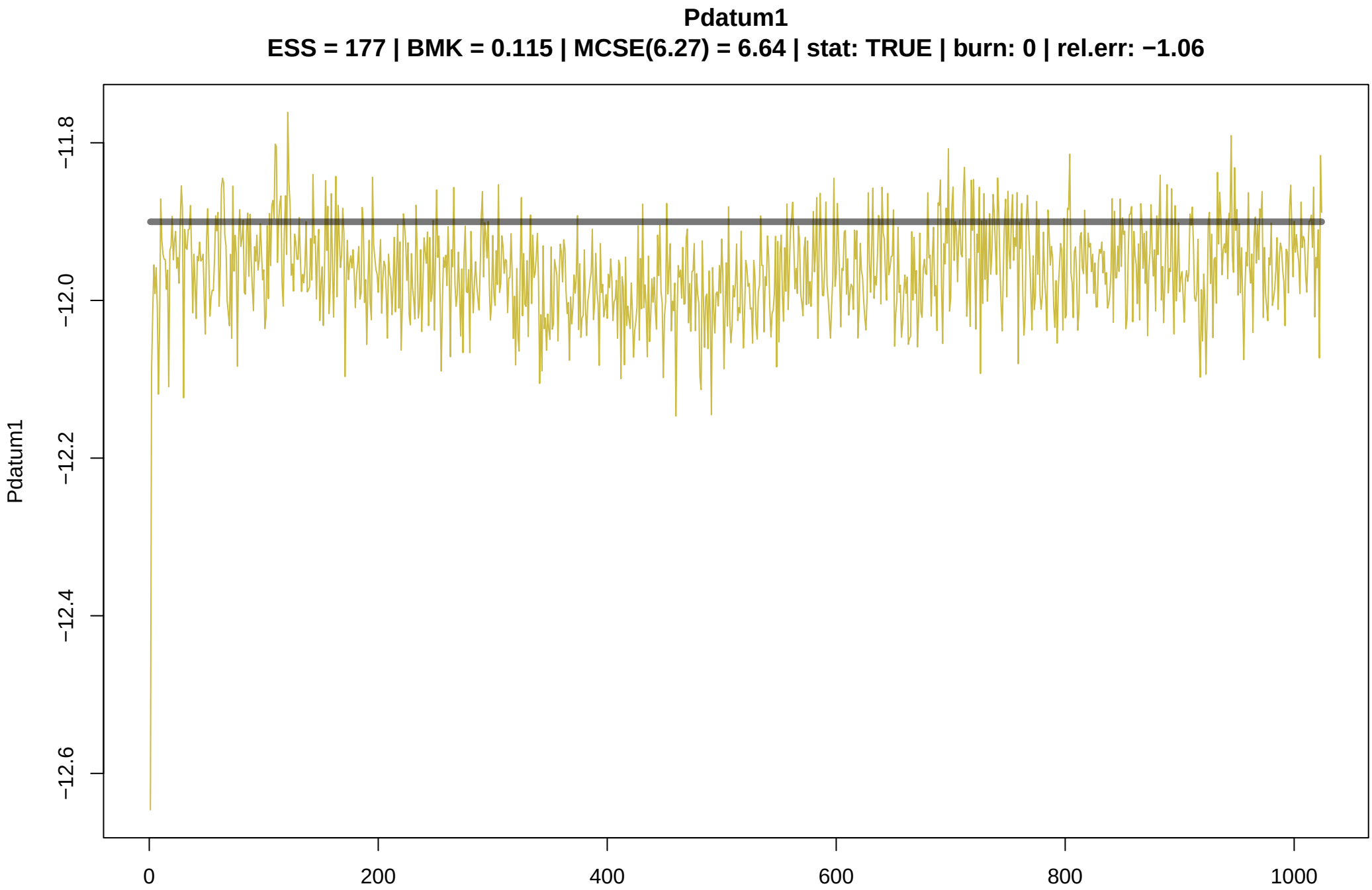

mcs_NOCount
log_RMSD

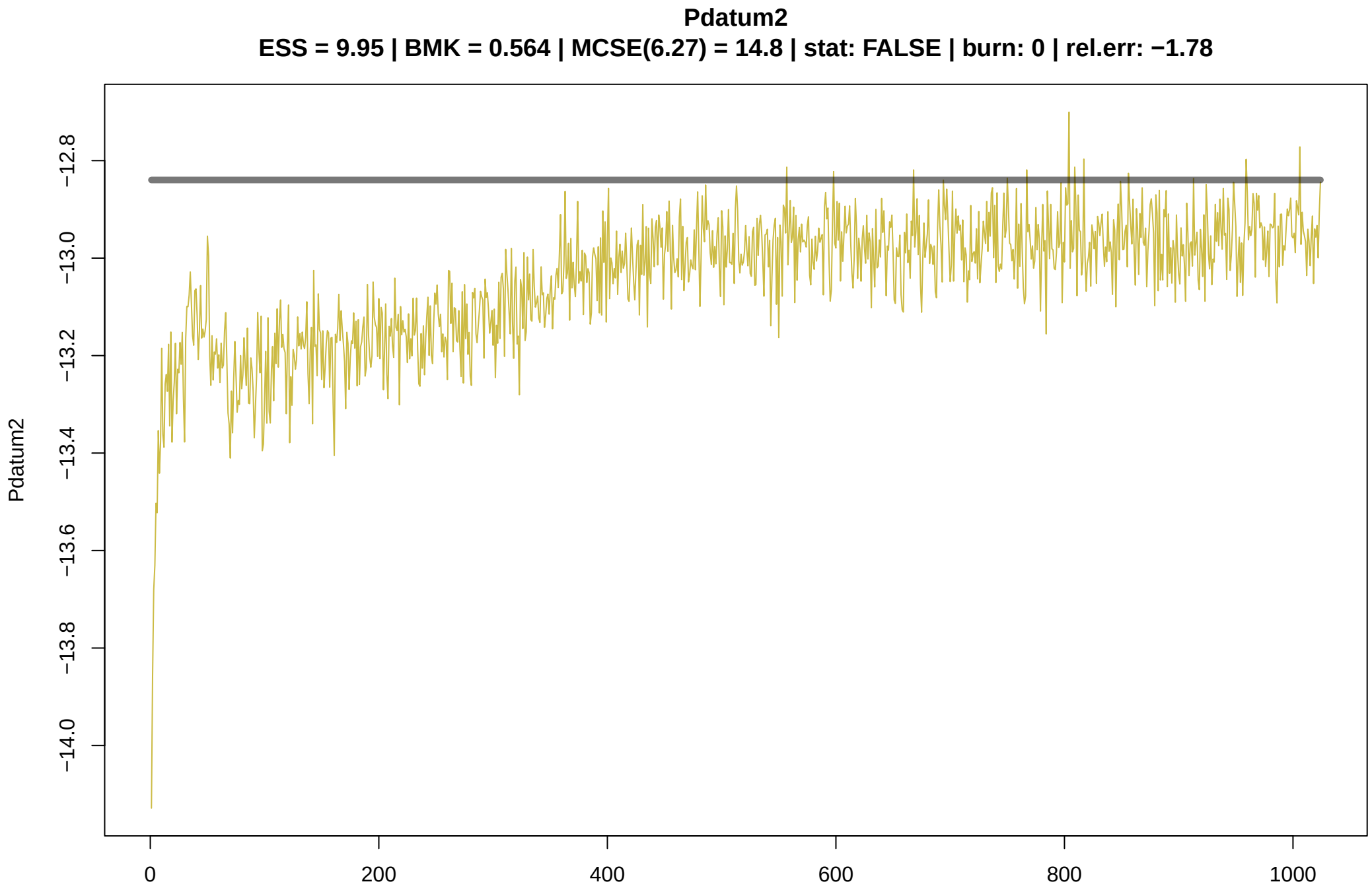

LL
LL
−62500
−63000
−63500
−64000
−64500
−65000
−65500
0
200
400
600
800
1000

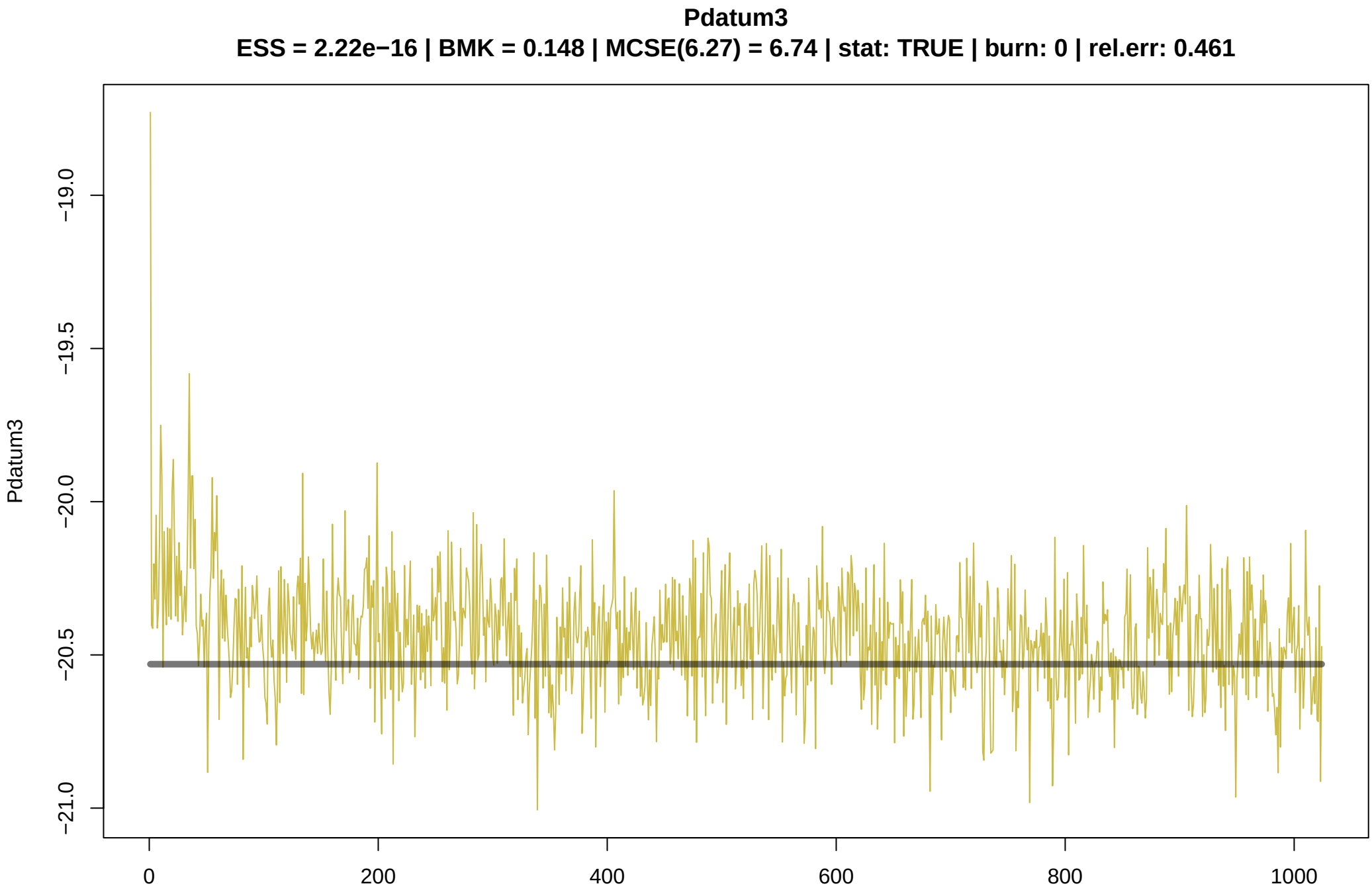

Pdatamean
ESS = 2.22e−16 | BMK = 0.0721 | MCSE(6.27) = 4.28 | stat: TRUE | burn: 0 | rel.err: 0.786
Pdatamean
−18.5
−19.0
−19.5
−20.0
−20.5
−21.0
0
200
400
600
800
1000

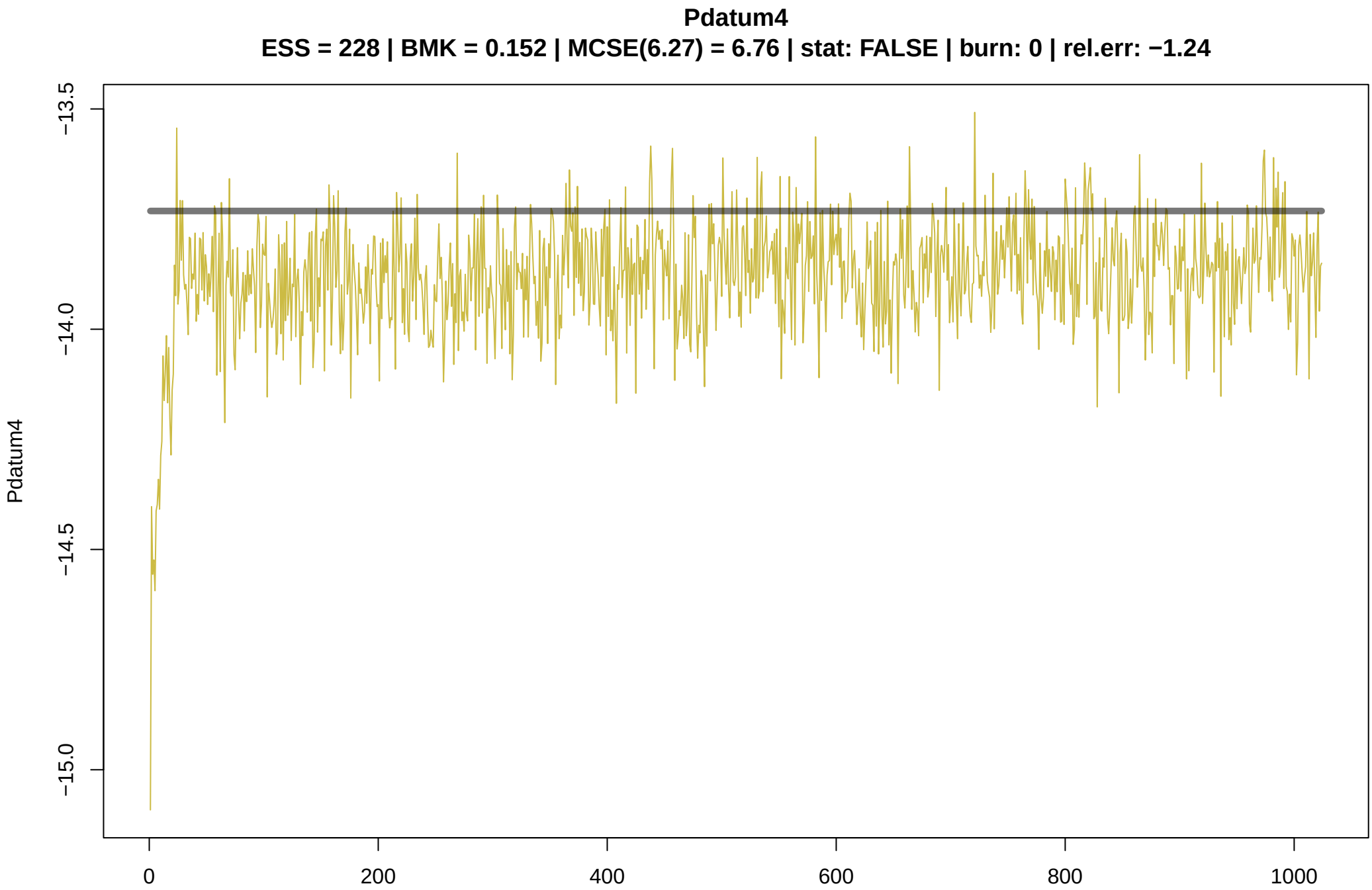

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.238 | MCSE(6.27) = 4.32 | stat: TRUE | burn: 0 | rel.err: 0.151
PdatacornerHi
−30
−35
−40
−45
0
200
400
600
800
1000

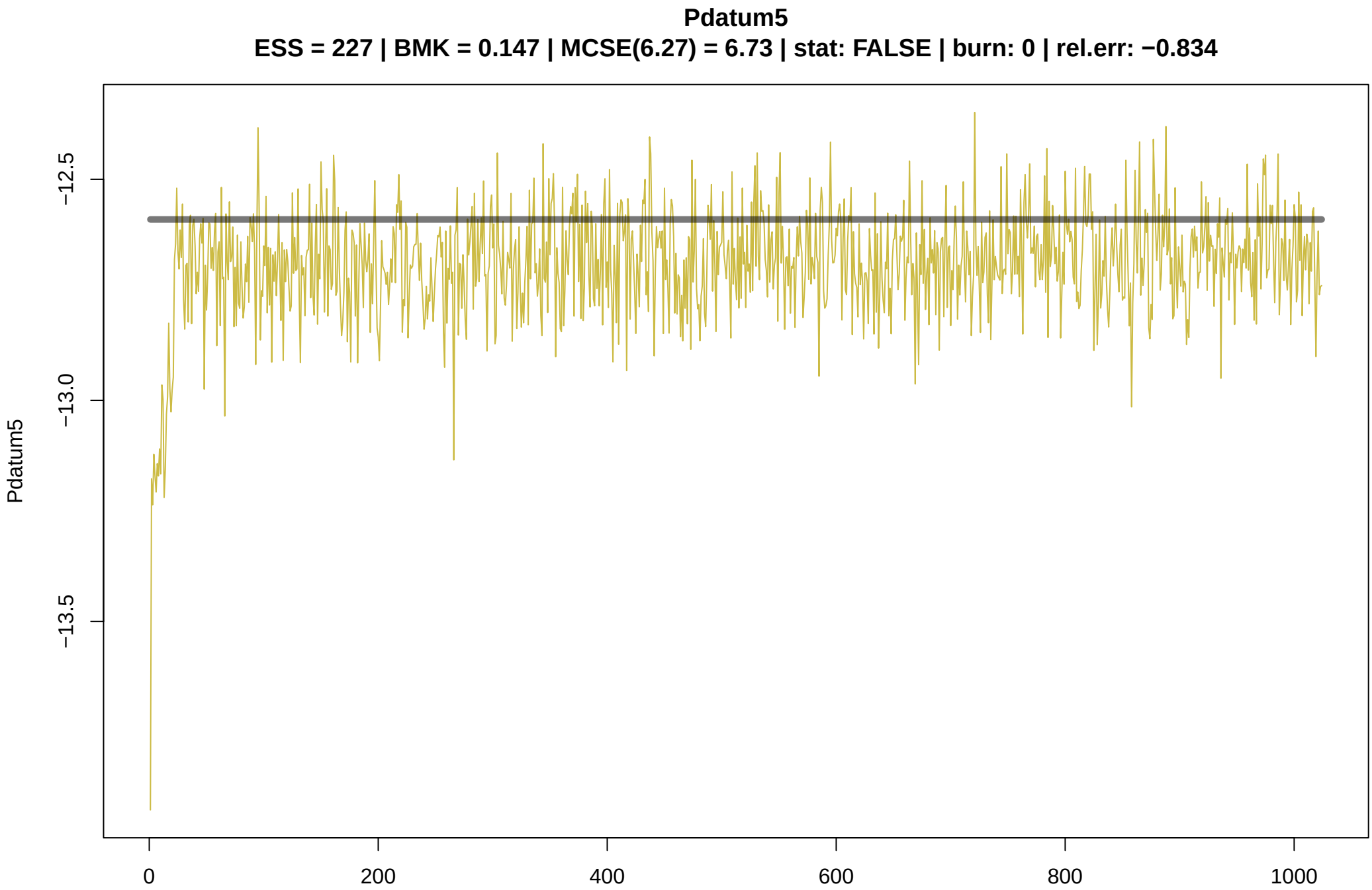

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.128 | MCSE(6.27) = 3.77 | stat: TRUE | burn: 0 | rel.err: 0.356
PdatacornerLo
−23
−24
−25
−26
−27
−28
−29
0
200
400
600
800
1000

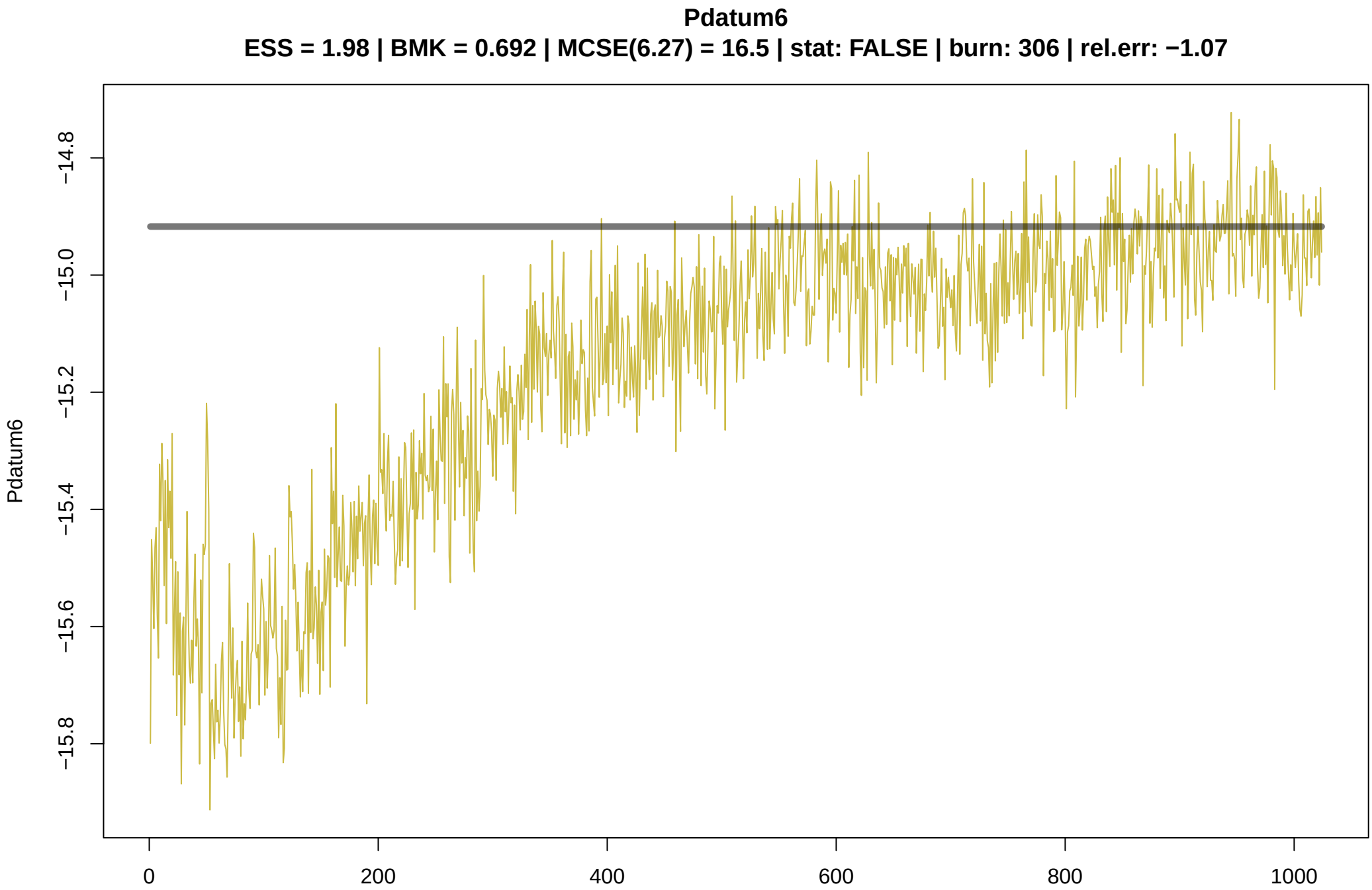

Pdatum1
ESS = 177 | BMK = 0.115 | MCSE(6.27) = 6.64 | stat: TRUE | burn: 0 | rel.err: −1.06
Pdatum1
−11.8
−12.0
−12.2
−12.4
−12.6
0
200
400
600
800
1000

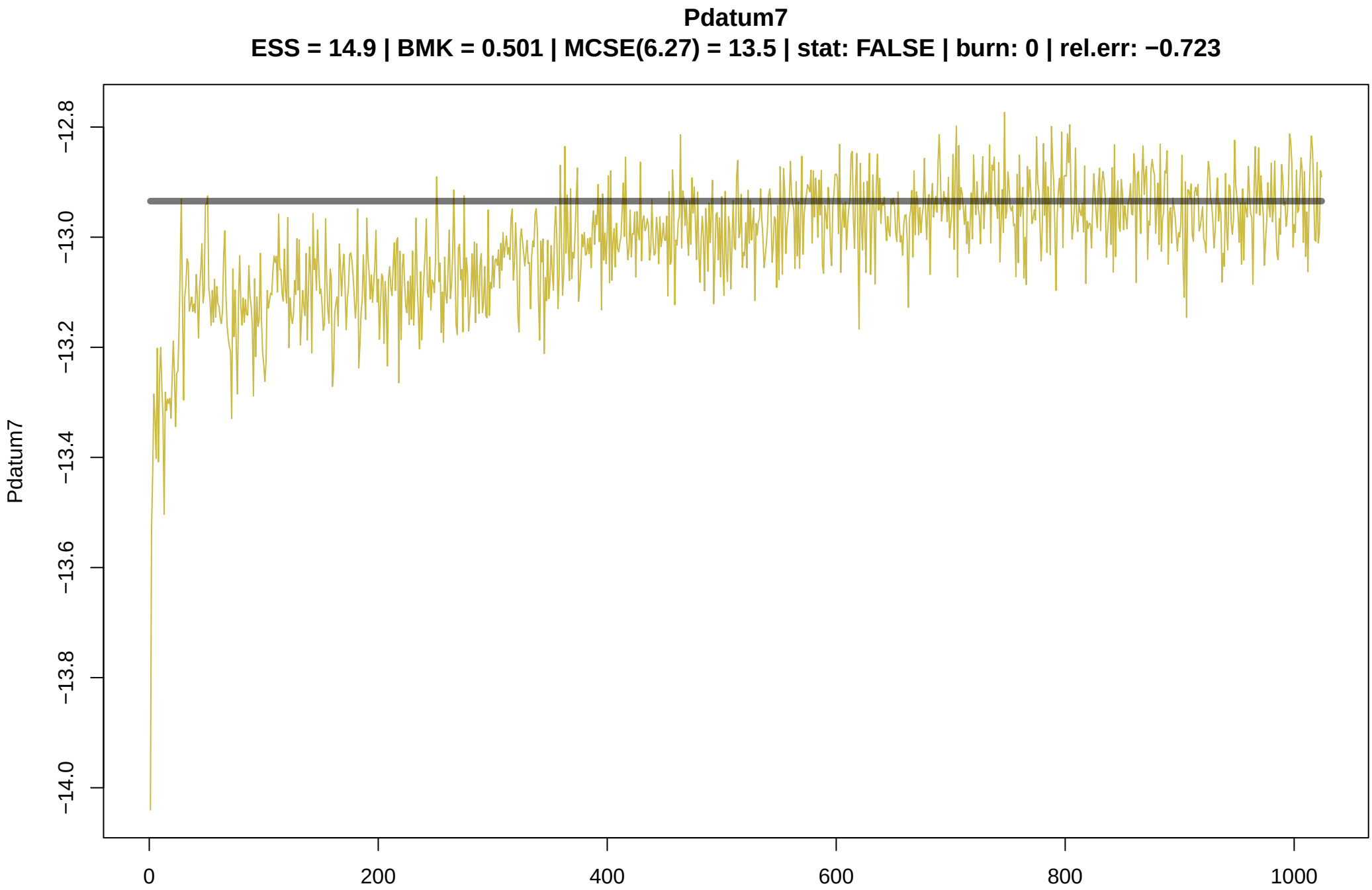

Pdatum2
ESS = 9.95 | BMK = 0.564 | MCSE(6.27) = 14.8 | stat: FALSE | burn: 0 | rel.err: −1.78
Pdatum2
−12.8
−13.0
−13.2
−13.4
−13.6
−13.8
−14.0
0
200
400
600
800
1000

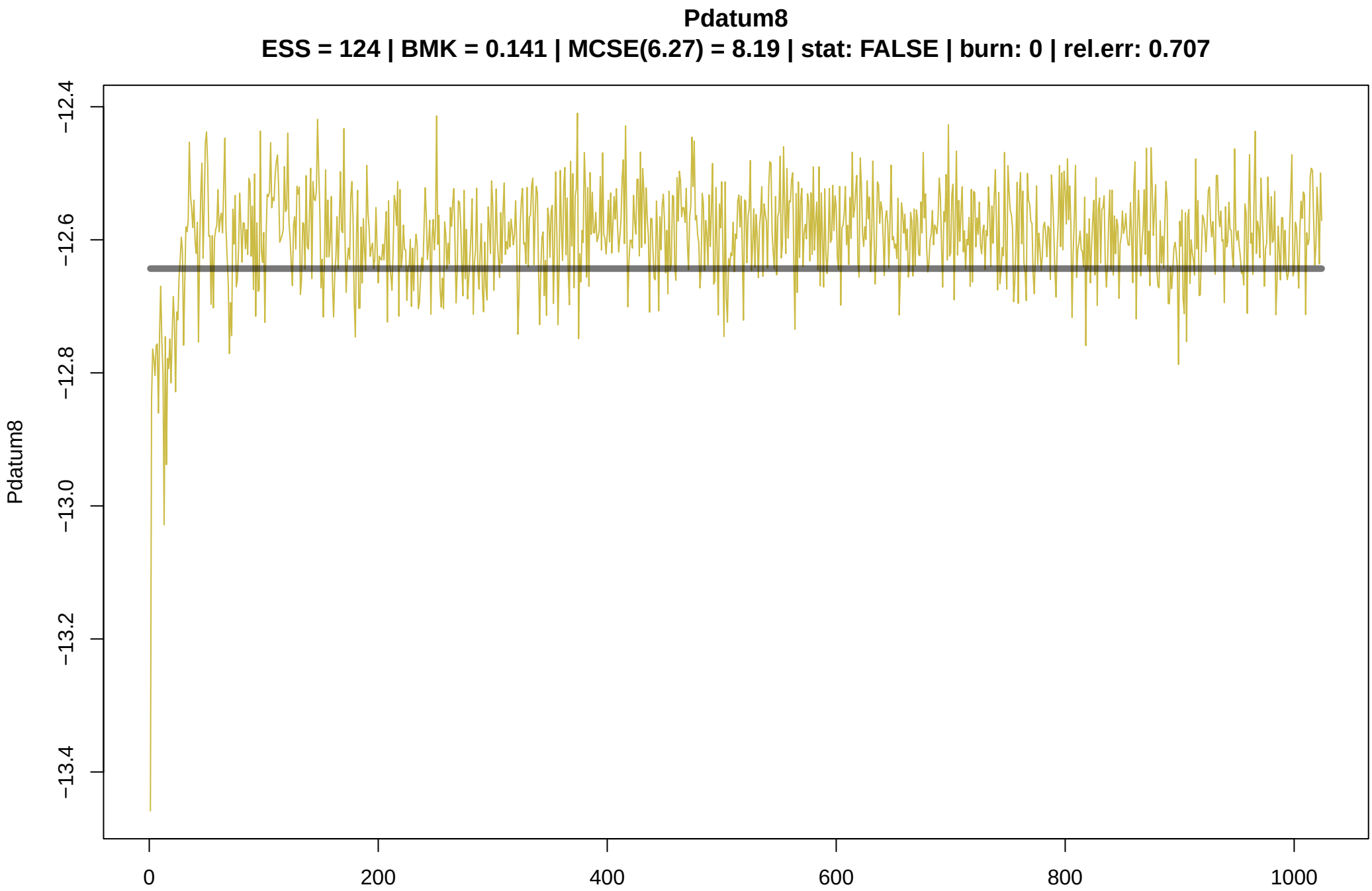

Pdatum3
ESS = 2.22e−16 | BMK = 0.148 | MCSE(6.27) = 6.74 | stat: TRUE | burn: 0 | rel.err: 0.461
Pdatum3
−19.0
−19.5
−20.0
−20.5
−21.0
0
200
400
600
800
1000

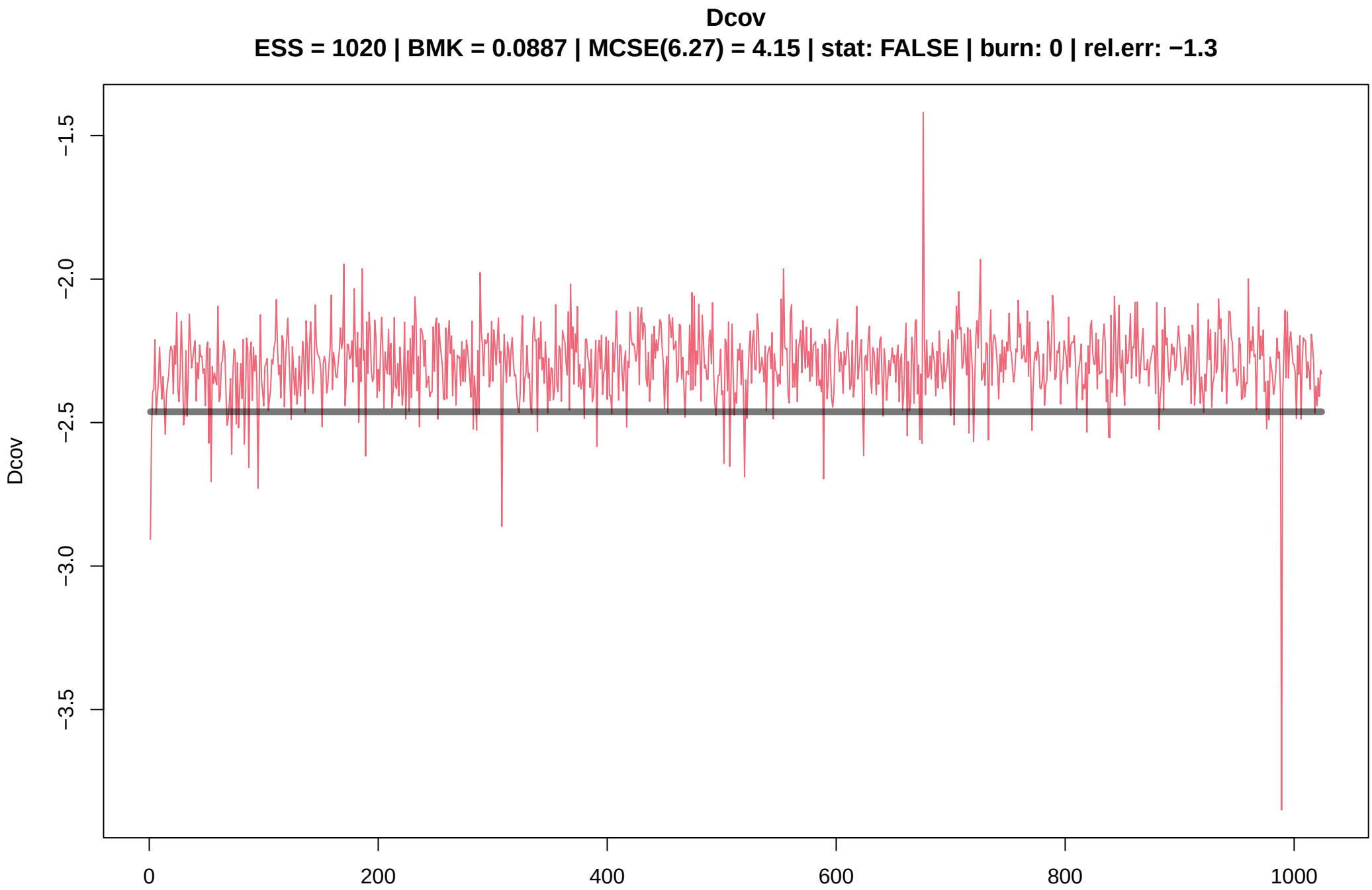

Pdatum4
ESS = 228 | BMK = 0.152 | MCSE(6.27) = 6.76 | stat: FALSE | burn: 0 | rel.err: −1.24
Pdatum4
−13.5
−14.0
−14.5
−15.0
0
200
400
600
800
1000

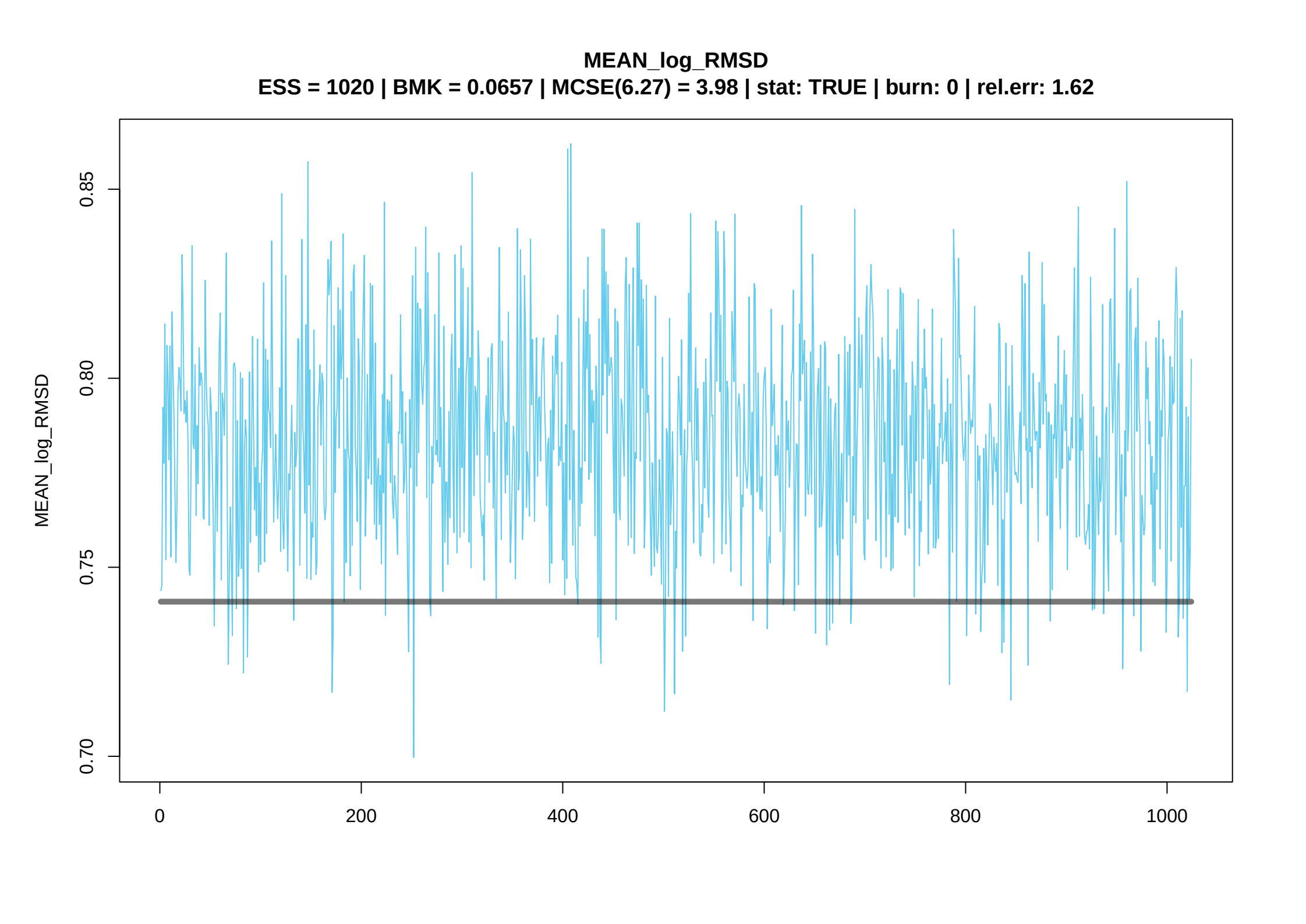

Pdatum5
ESS = 227 | BMK = 0.147 | MCSE(6.27) = 6.73 | stat: FALSE | burn: 0 | rel.err: −0.834
Pdatum5
−12.5
−13.0
−13.5
0
200
400
600
800
1000

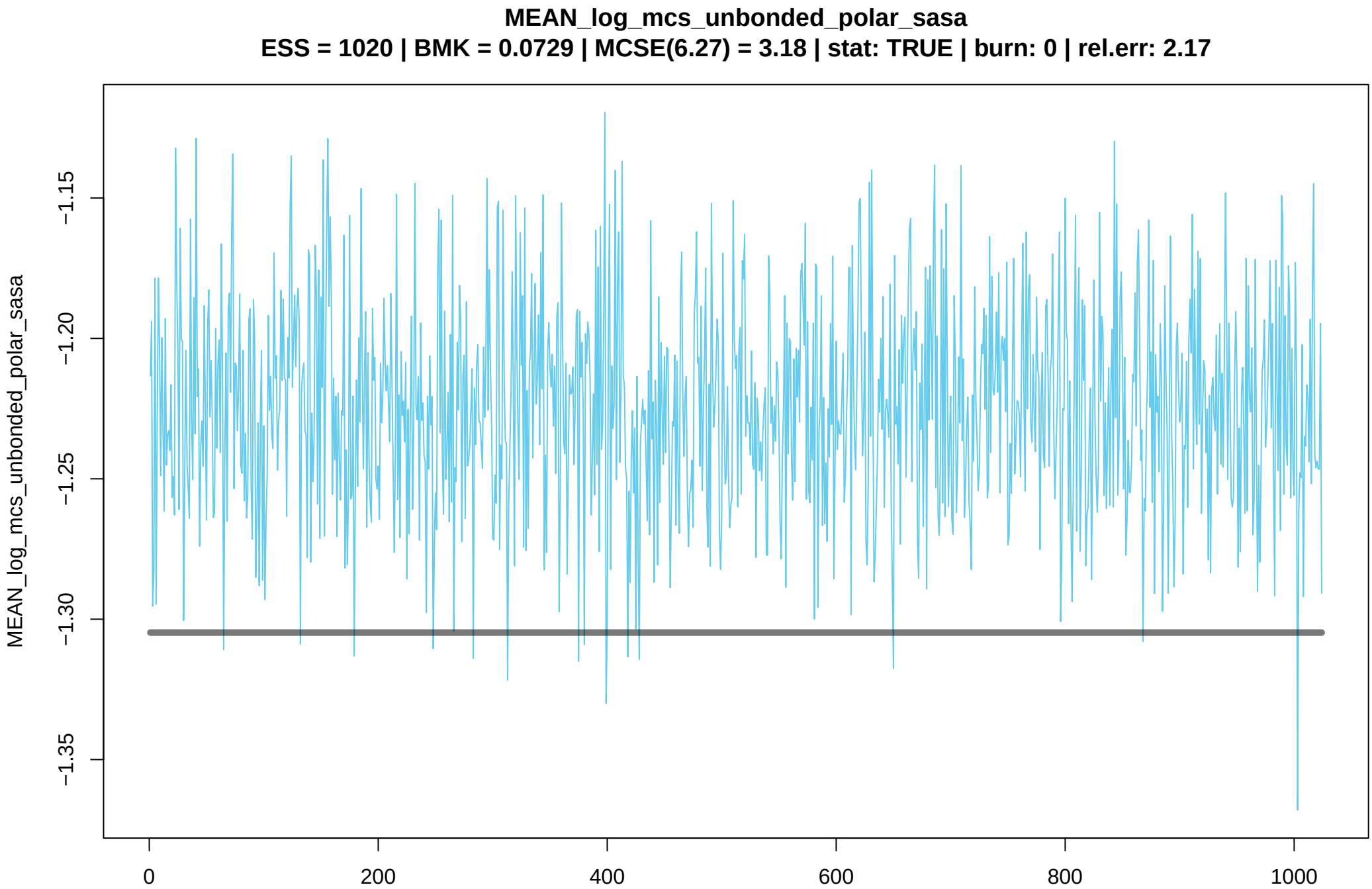

Pdatum6
ESS = 1.98 | BMK = 0.692 | MCSE(6.27) = 16.5 | stat: FALSE | burn: 306 | rel.err: −1.07
Pdatum6
−14.8
−15.0
−15.2
−15.4
−15.6
−15.8
0
200
400
600
800
1000

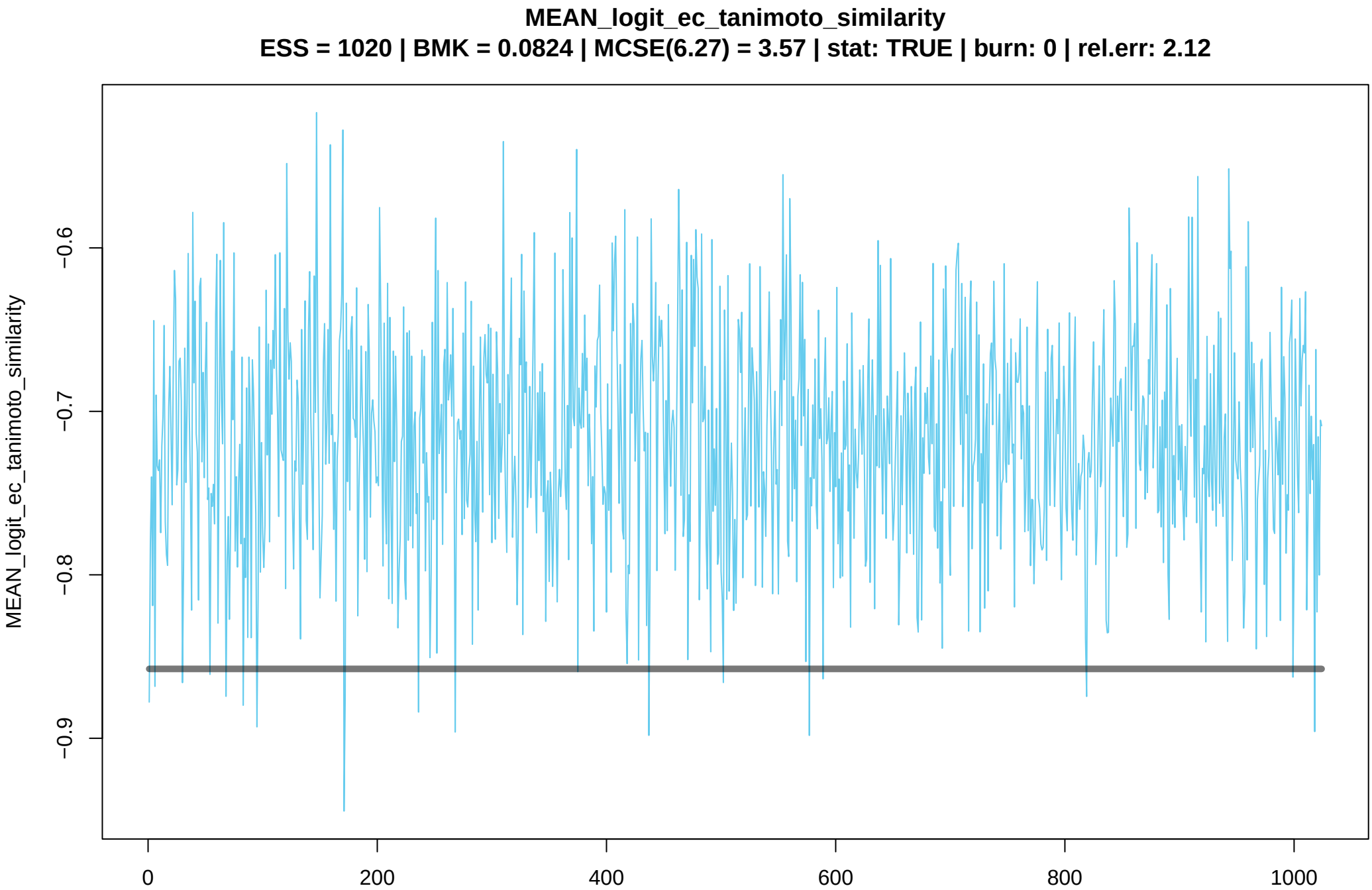

Pdatum7
ESS = 14.9 | BMK = 0.501 | MCSE(6.27) = 13.5 | stat: FALSE | burn: 0 | rel.err: −0.723
Pdatum7
−12.8
−13.0
−13.2
−13.4
−13.6
−13.8
−14.0
0
200
400
600
800
1000

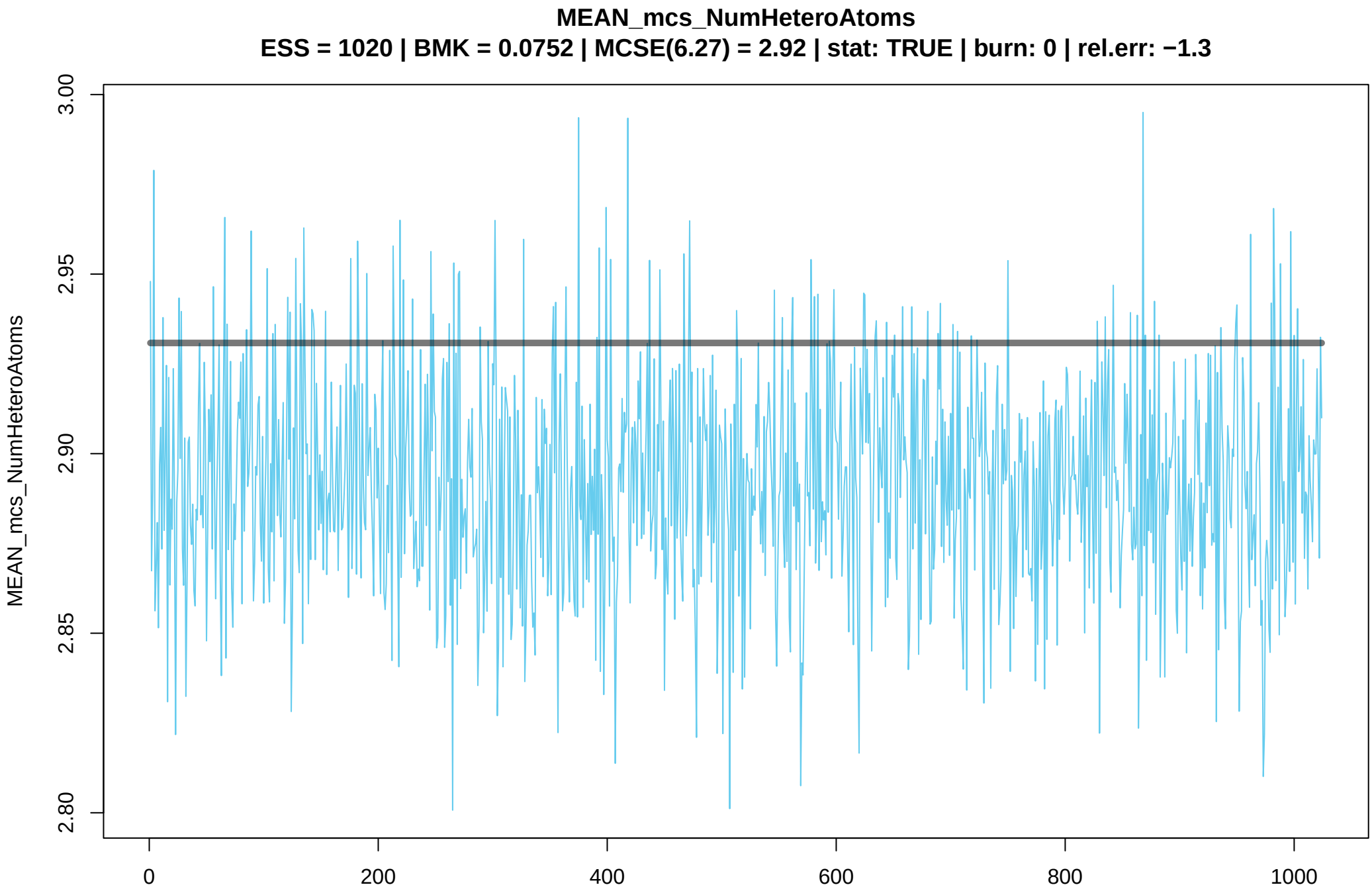

Pdatum8
ESS = 124 | BMK = 0.141 | MCSE(6.27) = 8.19 | stat: FALSE | burn: 0 | rel.err: 0.707
Pdatum8
−12.4
−12.6
−12.8
−13.0
−13.2
−13.4
0
200
400
600
800
1000

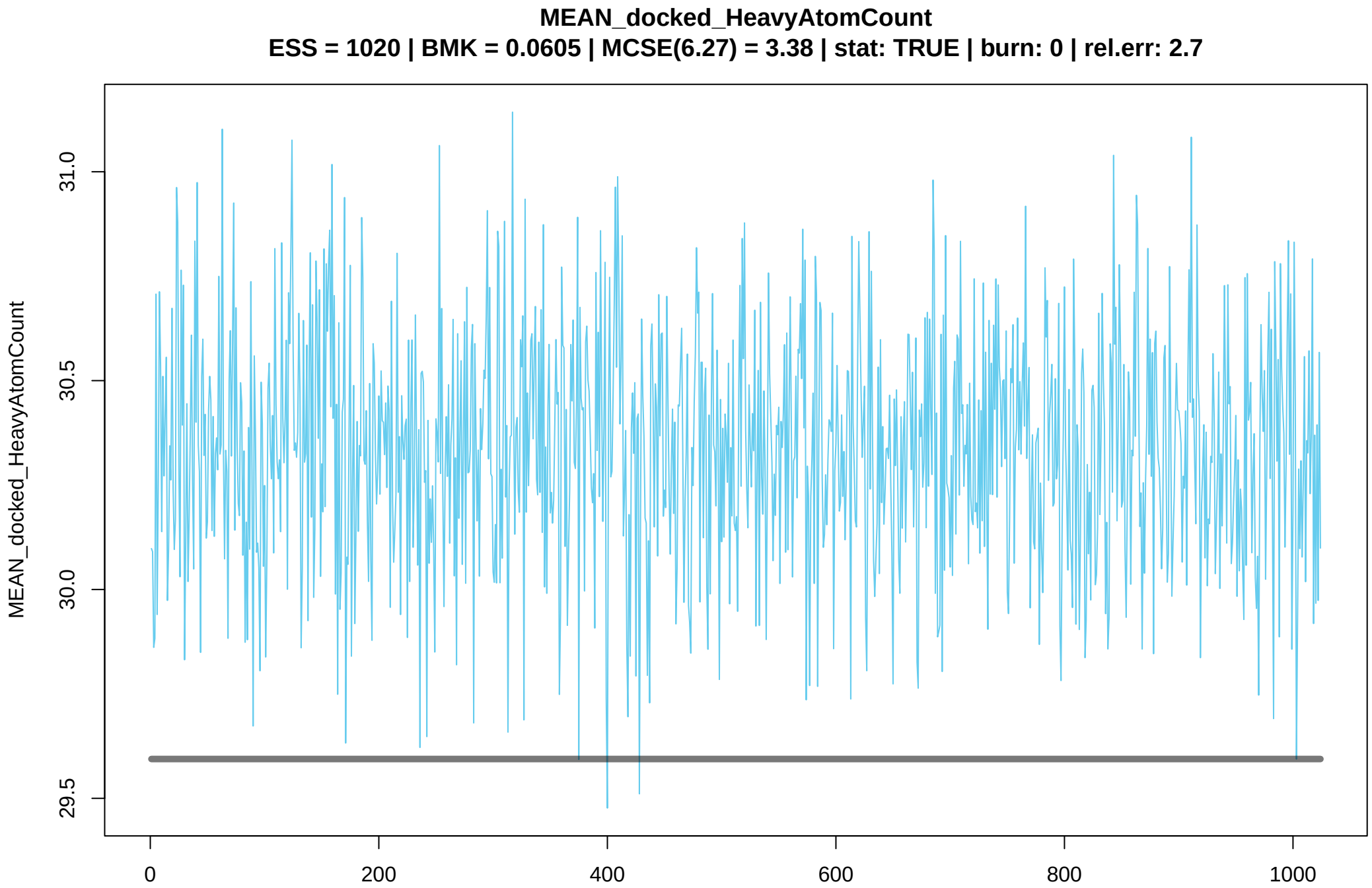

Dcov
ESS = 1020 | BMK = 0.0887 | MCSE(6.27) = 4.15 | stat: FALSE | burn: 0 | rel.err: −1.3
Dcov
−1.5
−2.0
−2.5
−3.0
−3.5
0
200
400
600
800
1000

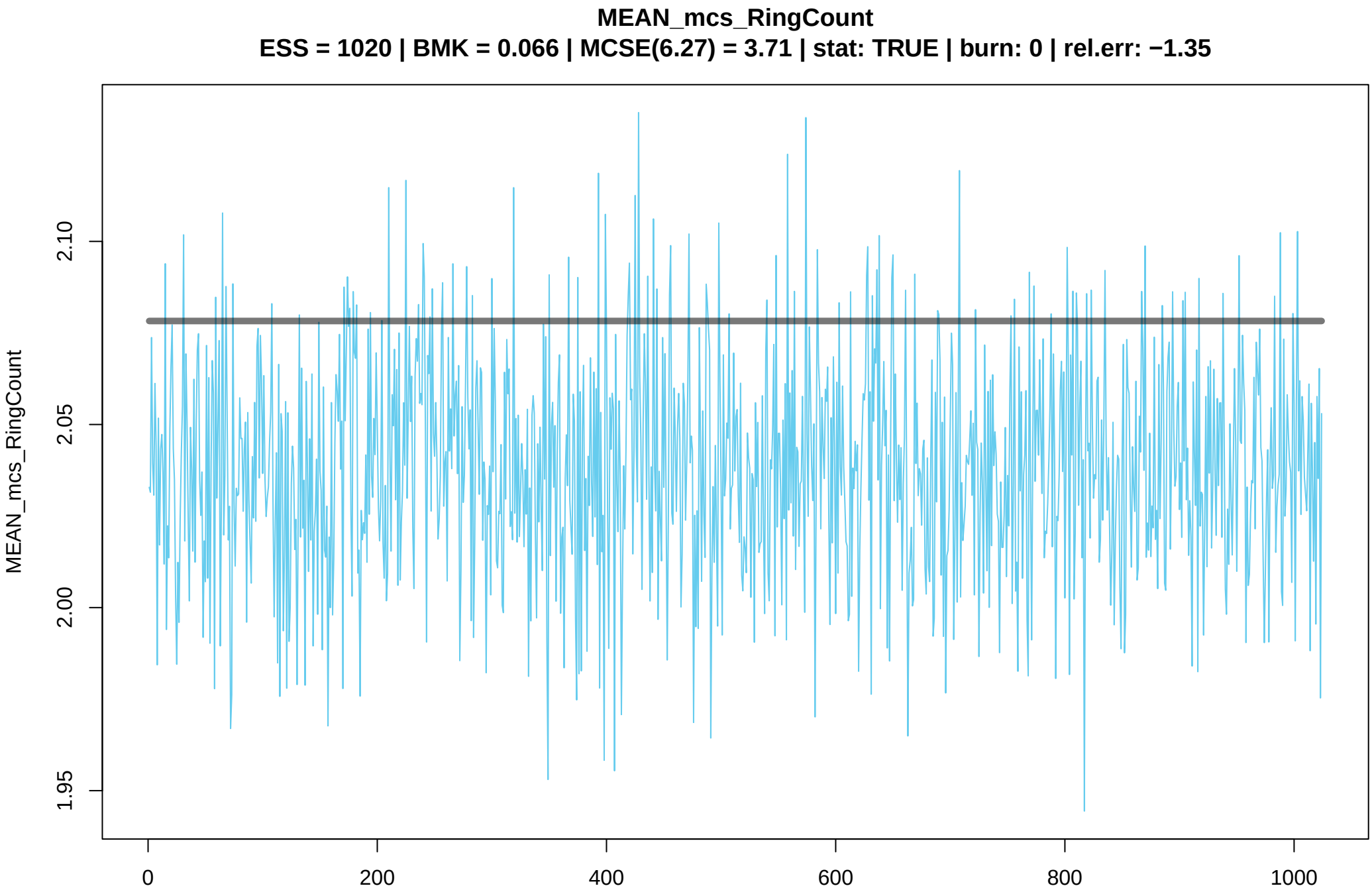

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0657 | MCSE(6.27) = 3.98 | stat: TRUE | burn: 0 | rel.err: 1.62
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

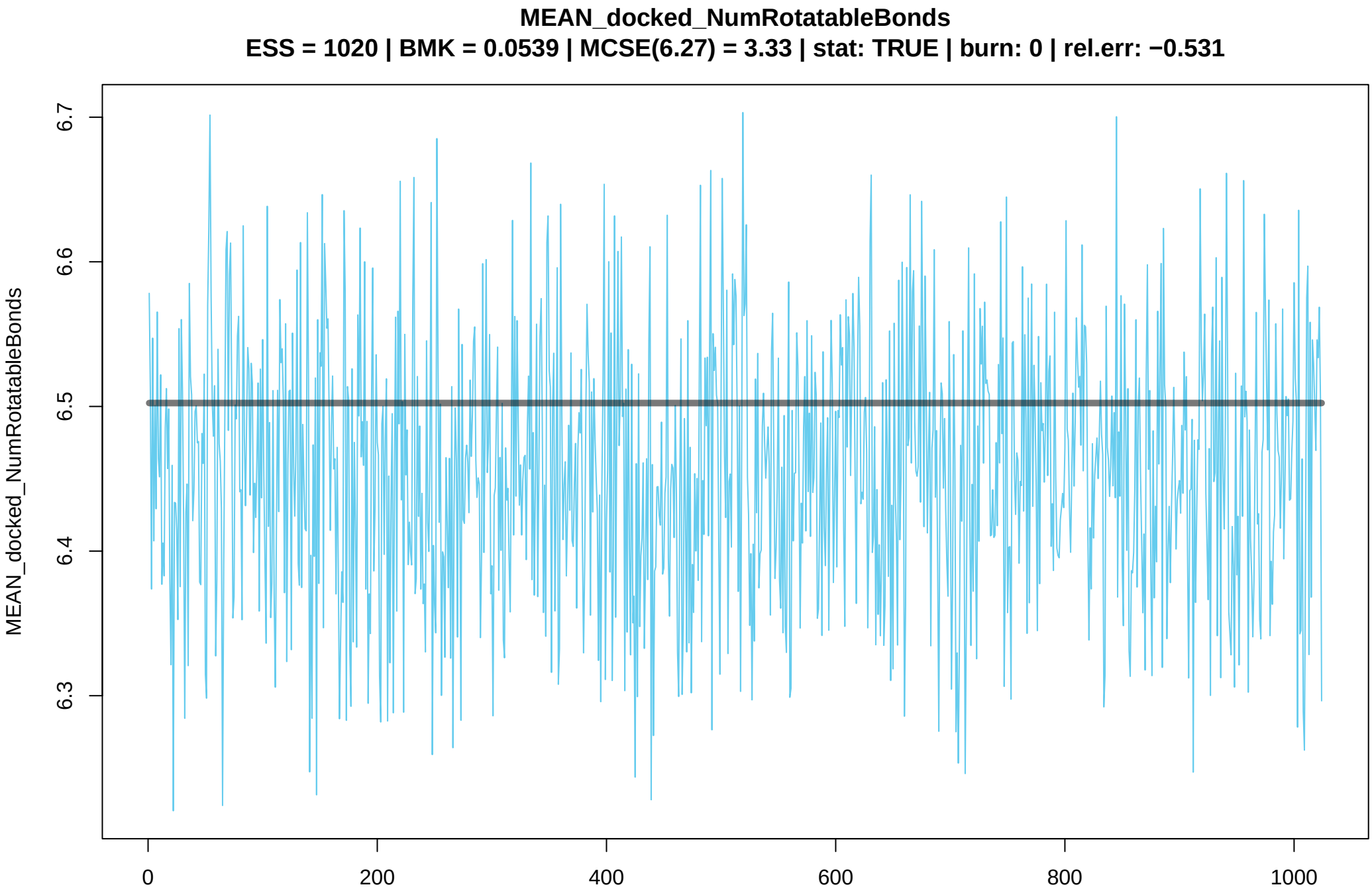

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0729 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | rel.err: 2.17
MEAN_log_mcs_unbonded_polar_sasa
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

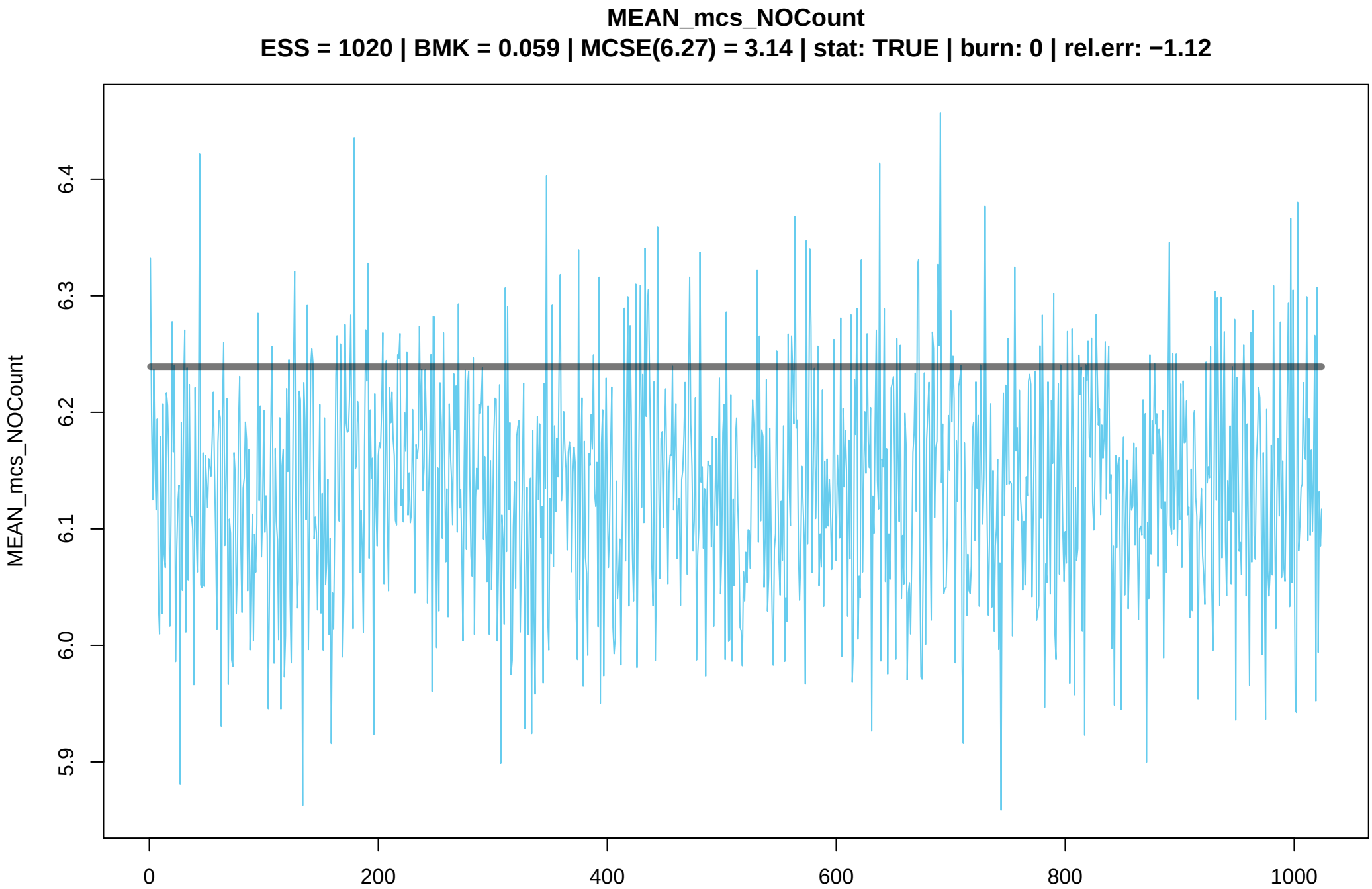

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0824 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | rel.err: 2.12
MEAN_logit_ec_tanimoto_similarity
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

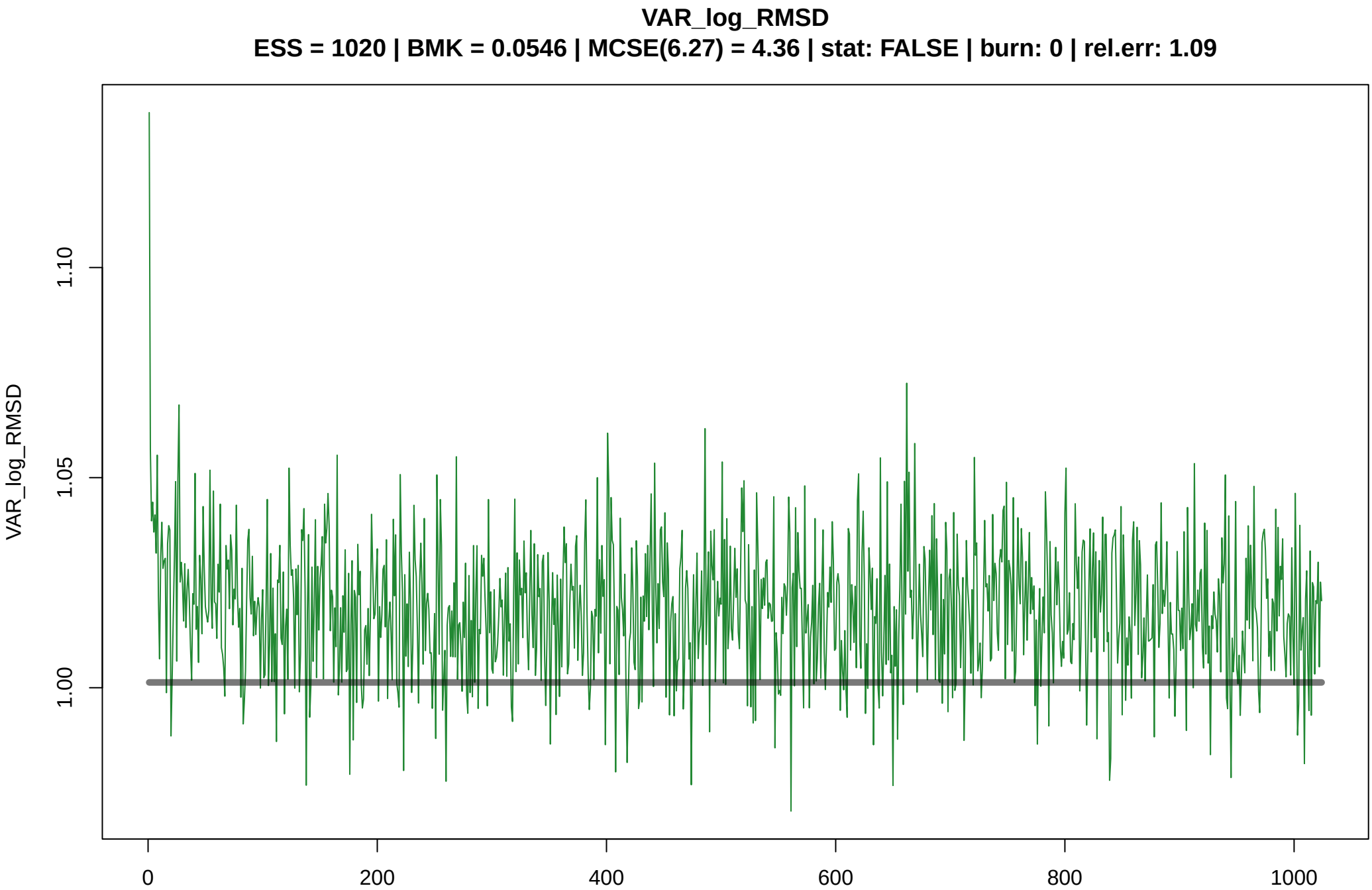

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0752 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0 | rel.err: −1.3
MEAN_mcs_NumHeteroAtoms
3.00
2.95
2.90
2.85
2.80
0
200
400
600
800
1000

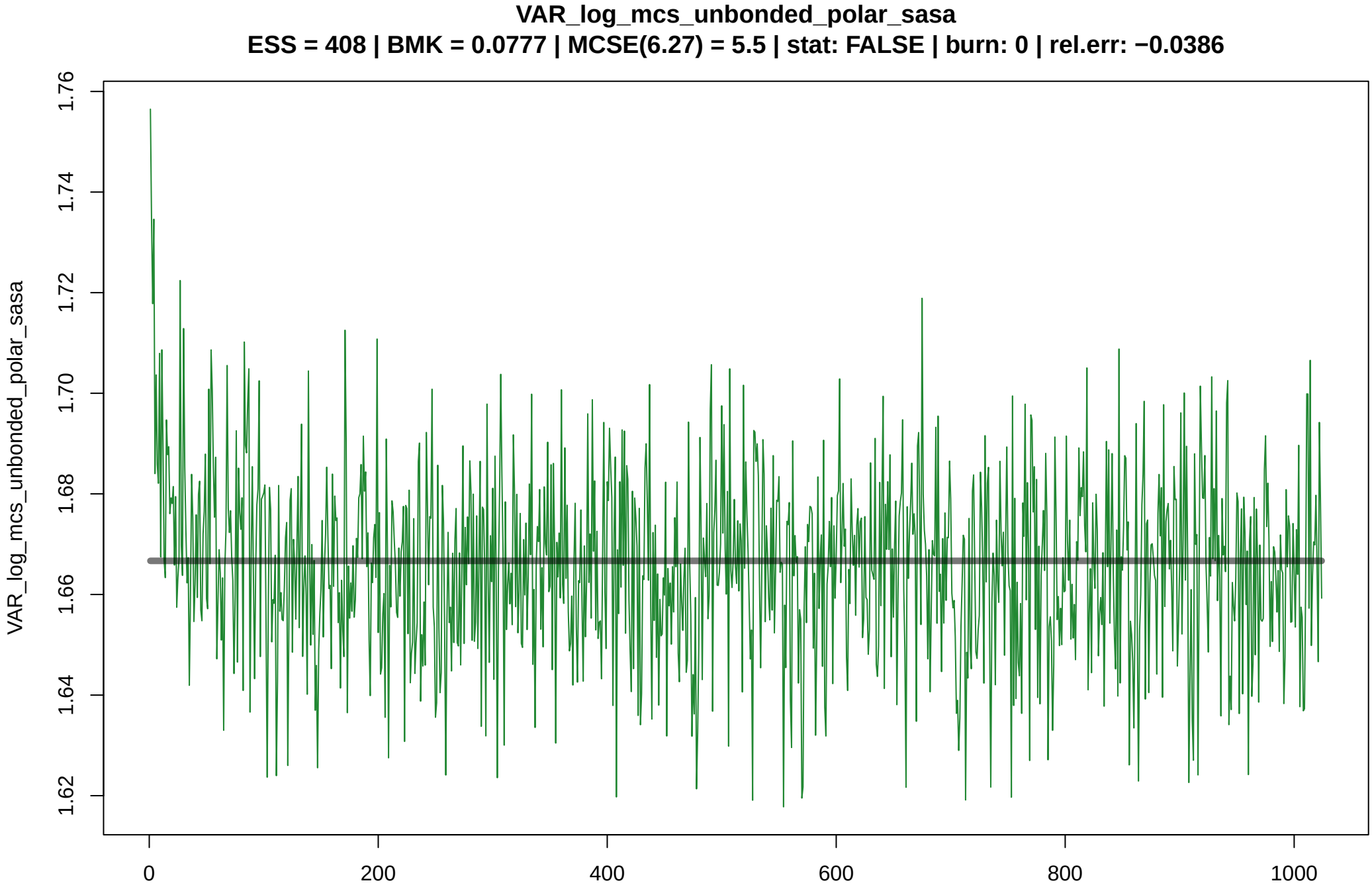

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0605 | MCSE(6.27) = 3.38 | stat: TRUE | burn: 0 | rel.err: 2.7
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
31.0
0
200
400
600
800
1000

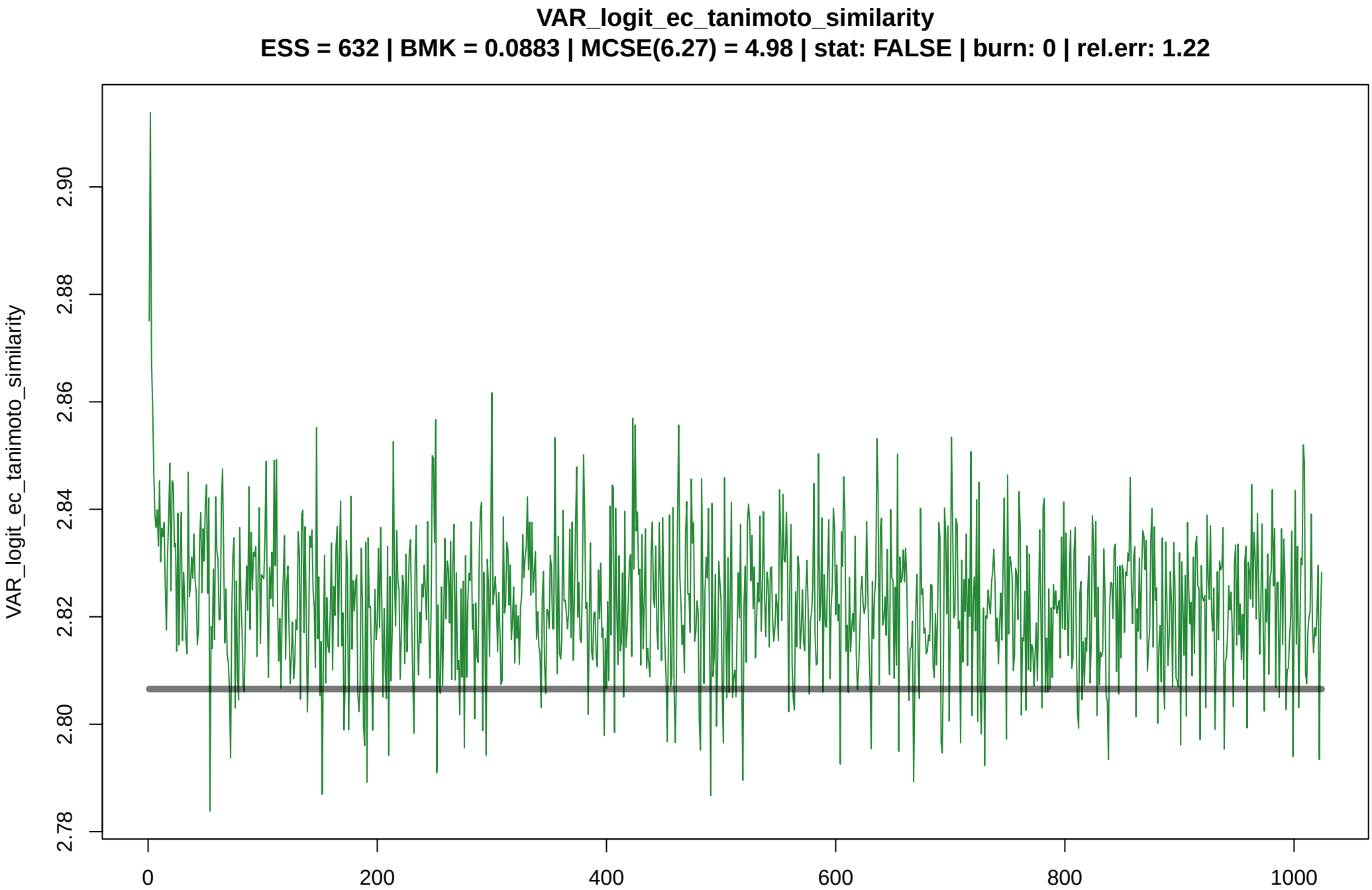

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.066 | MCSE(6.27) = 3.71 | stat: TRUE | burn: 0 | rel.err: −1.35
MEAN_mcs_RingCount
1.95
2.00
2.05
2.10
0
200
400
600
800
1000

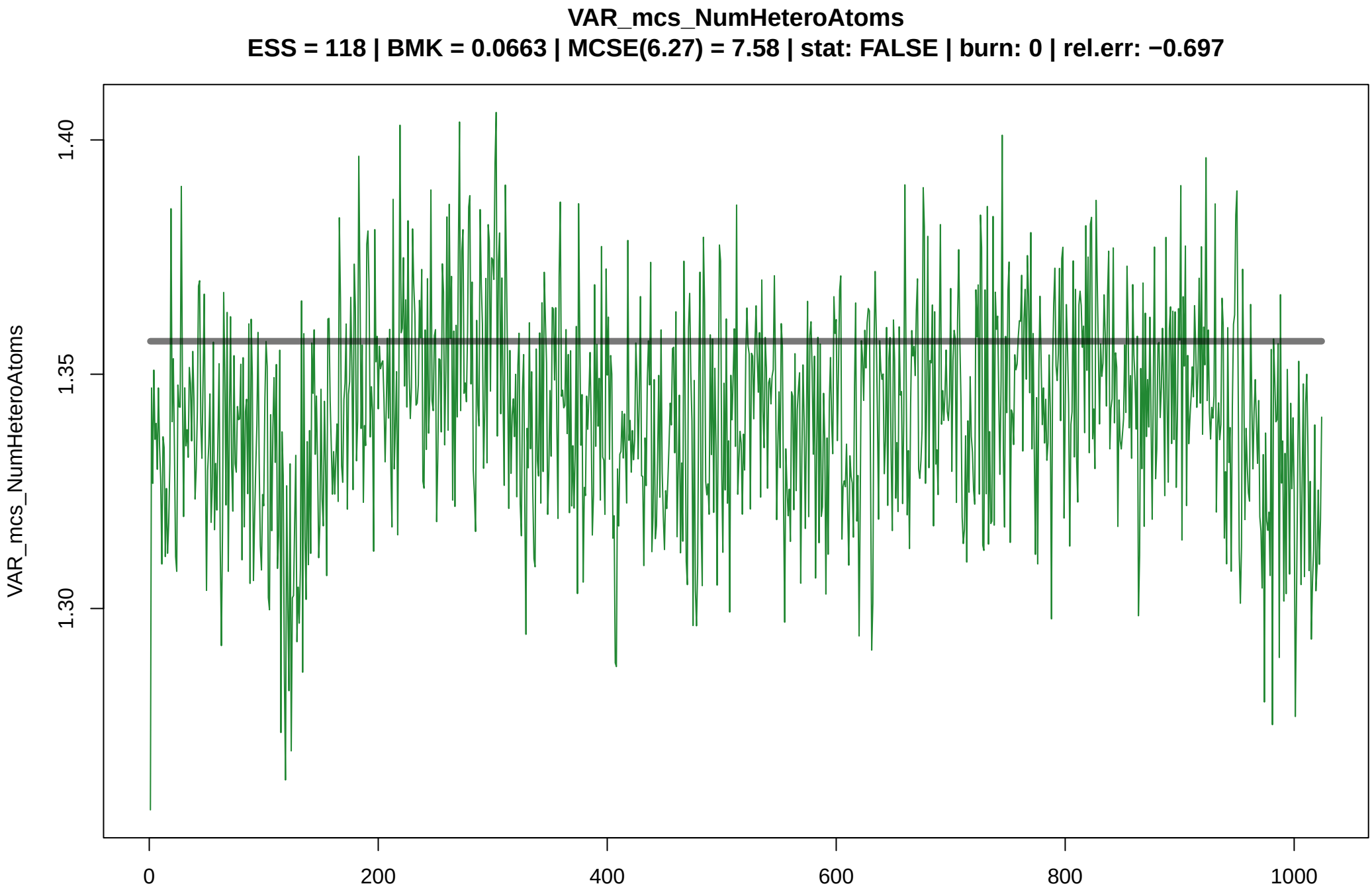

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0539 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0 | rel.err: −0.531
MEAN_docked_NumRotatableBonds
6.3
6.4
6.5
6.6
6.7
0
200
400
600
800
1000

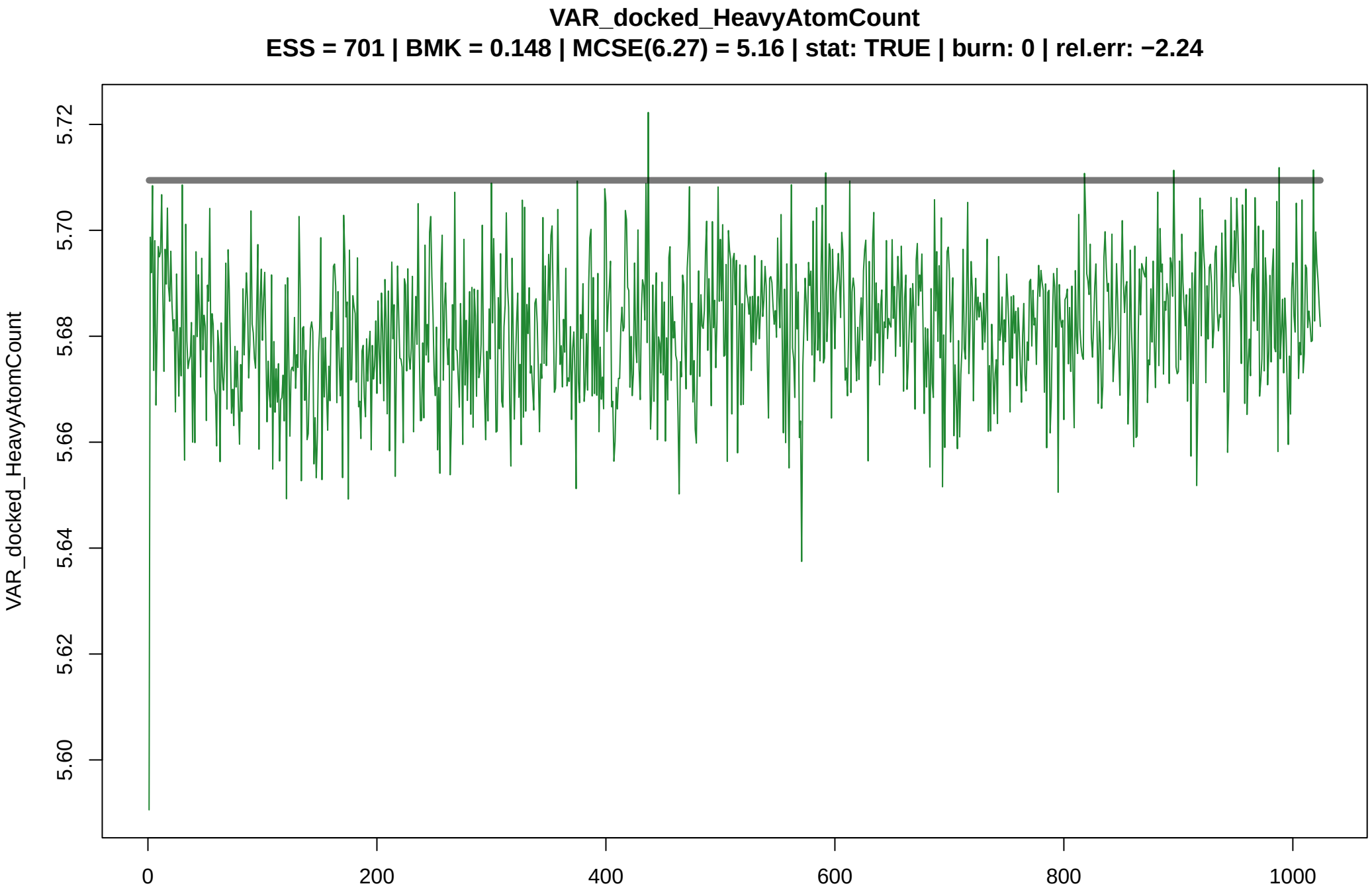

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.059 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | rel.err: −1.12
MEAN_mcs_NOCount
6.4
6.3
6.2
6.1
6.0
5.9
0
200
400
600
800
1000

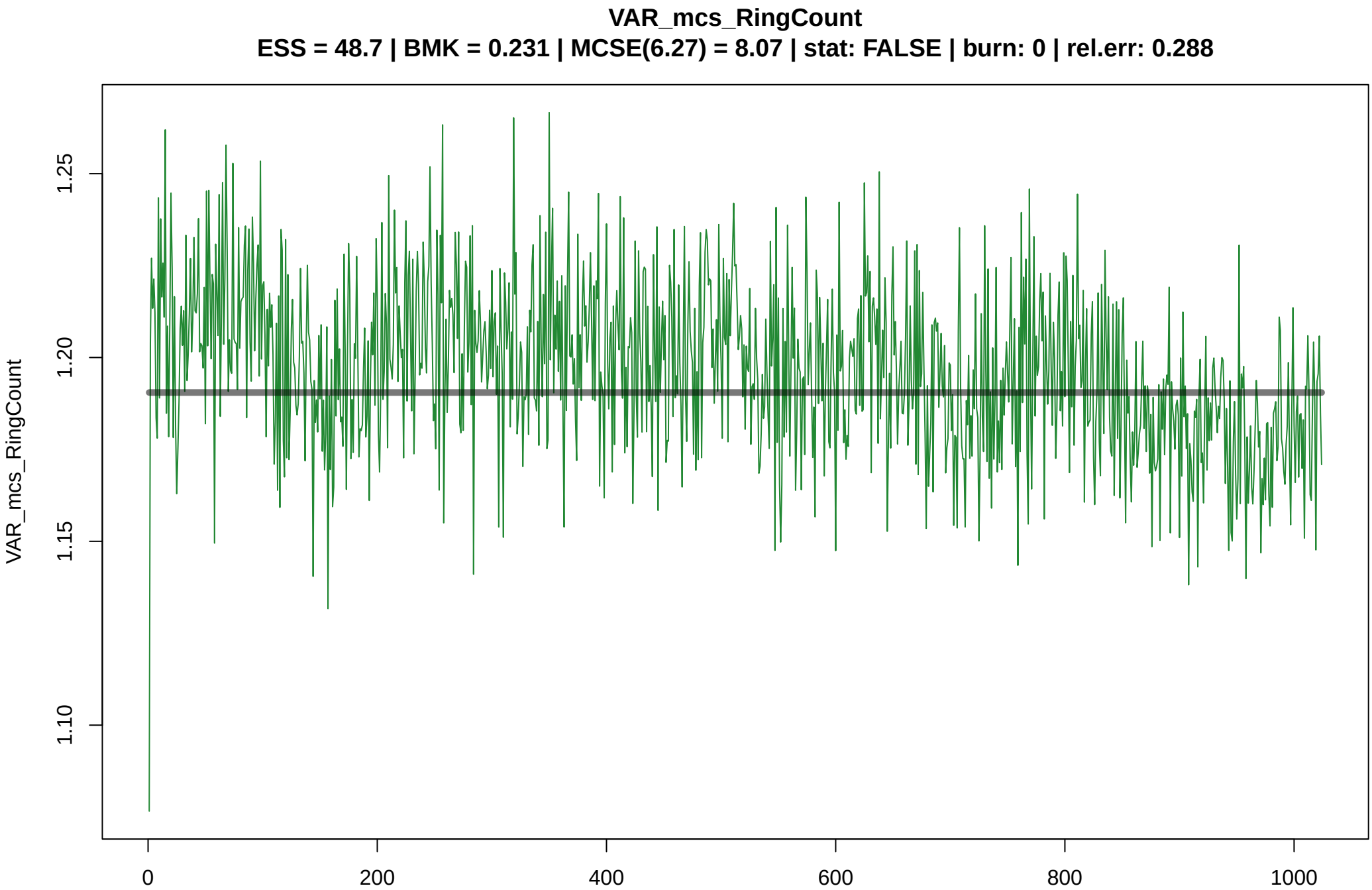

VAR_log_RMSD
ESS = 1020 | BMK = 0.0546 | MCSE(6.27) = 4.36 | stat: FALSE | burn: 0 | rel.err: 1.09
VAR_log_RMSD
1.00
1.05
1.10
0
200
400
600
800
1000

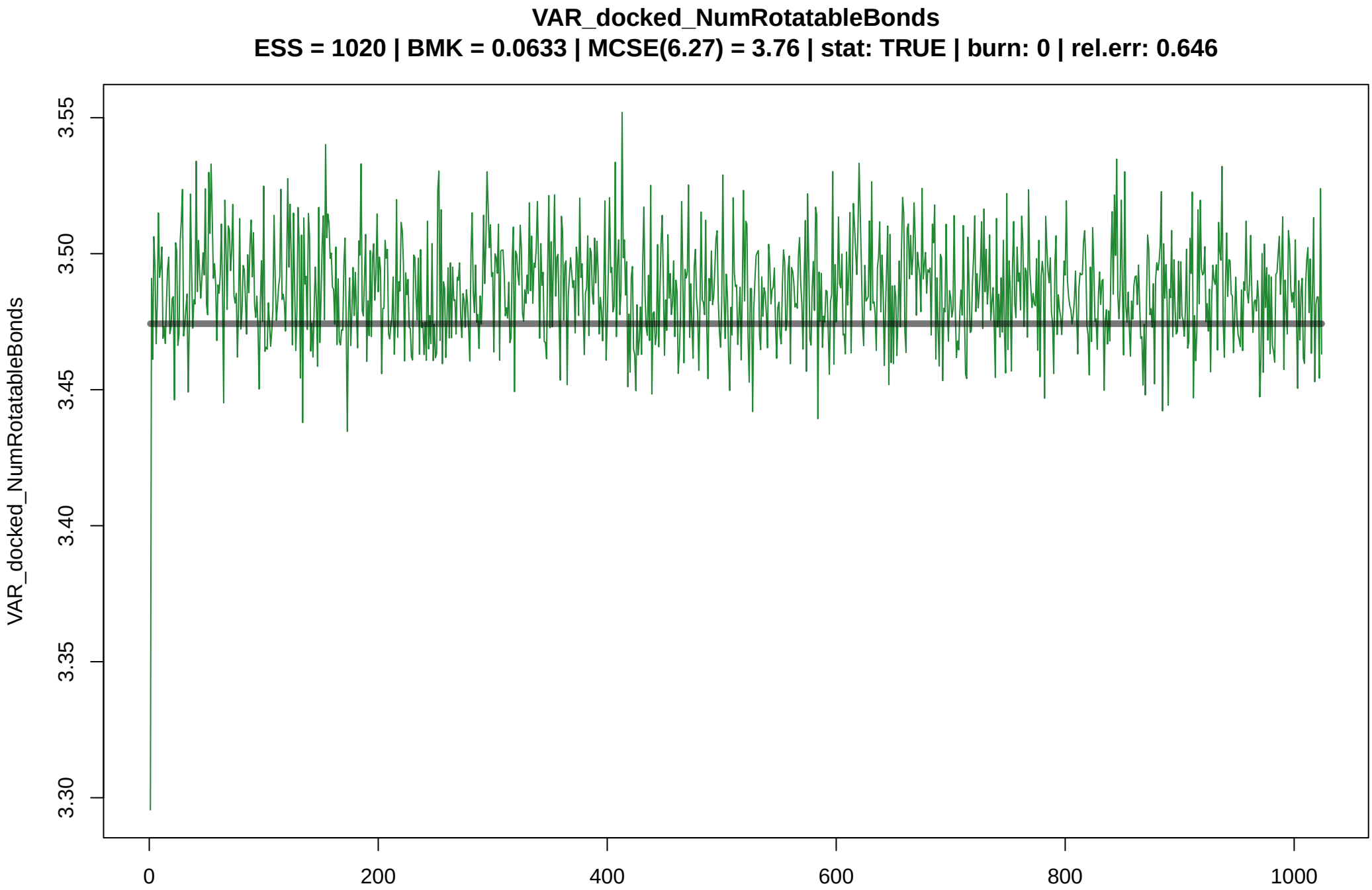

VAR_log_mcs_unbonded_polar_sasa
ESS = 408 | BMK = 0.0777 | MCSE(6.27) = 5.5 | stat: FALSE | burn: 0 | rel.err: −0.0386
VAR_log_mcs_unbonded_polar_sasa
1.76
1.74
1.72
1.70
1.68
1.66
1.64
1.62
0
200
400
600
800
1000

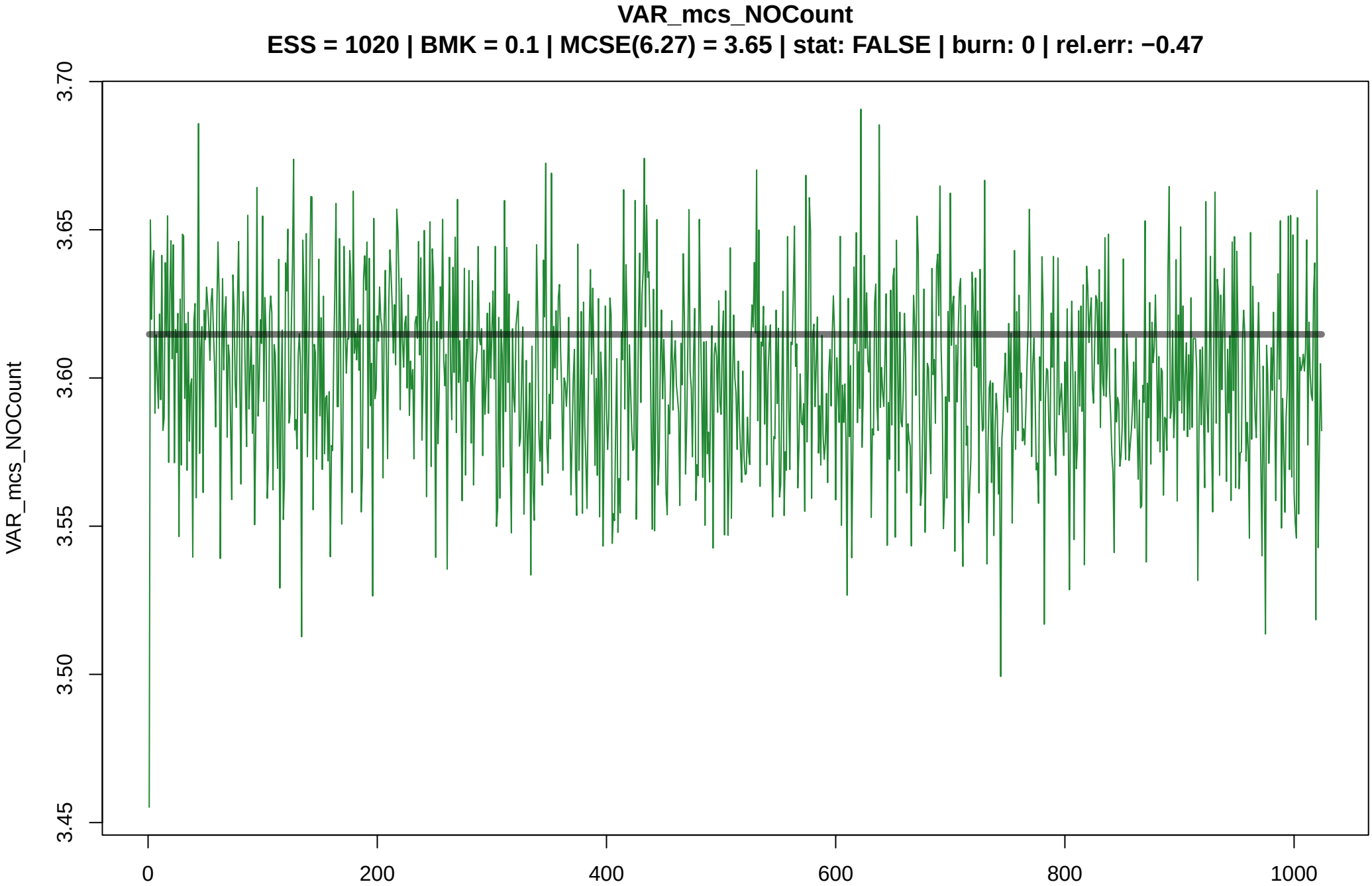

VAR_logit_ec_tanimoto_similarity
ESS = 632 | BMK = 0.0883 | MCSE(6.27) = 4.98 | stat: FALSE | burn: 0 | rel.err: 1.22
VAR_logit_ec_tanimoto_similarity
2.78
2.80
2.82
2.84
2.86
2.88
2.90
0
200
400
600
800
1000

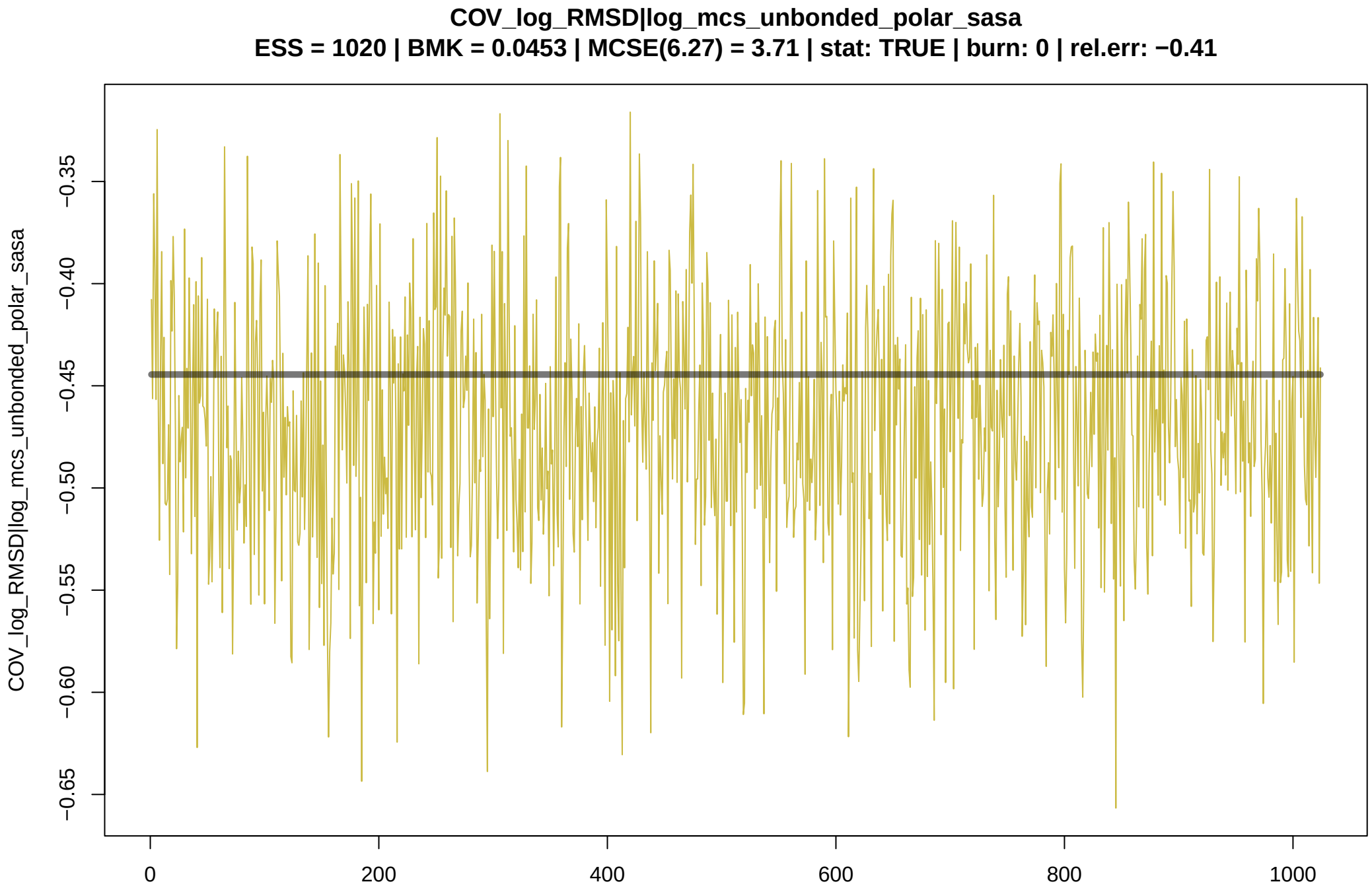

VAR_mcs_NumHeteroAtoms
ESS = 118 | BMK = 0.0663 | MCSE(6.27) = 7.58 | stat: FALSE | burn: 0 | rel.err: −0.697
VAR_mcs_NumHeteroAtoms
1.40
1.35
1.30
0
200
400
600
800
1000

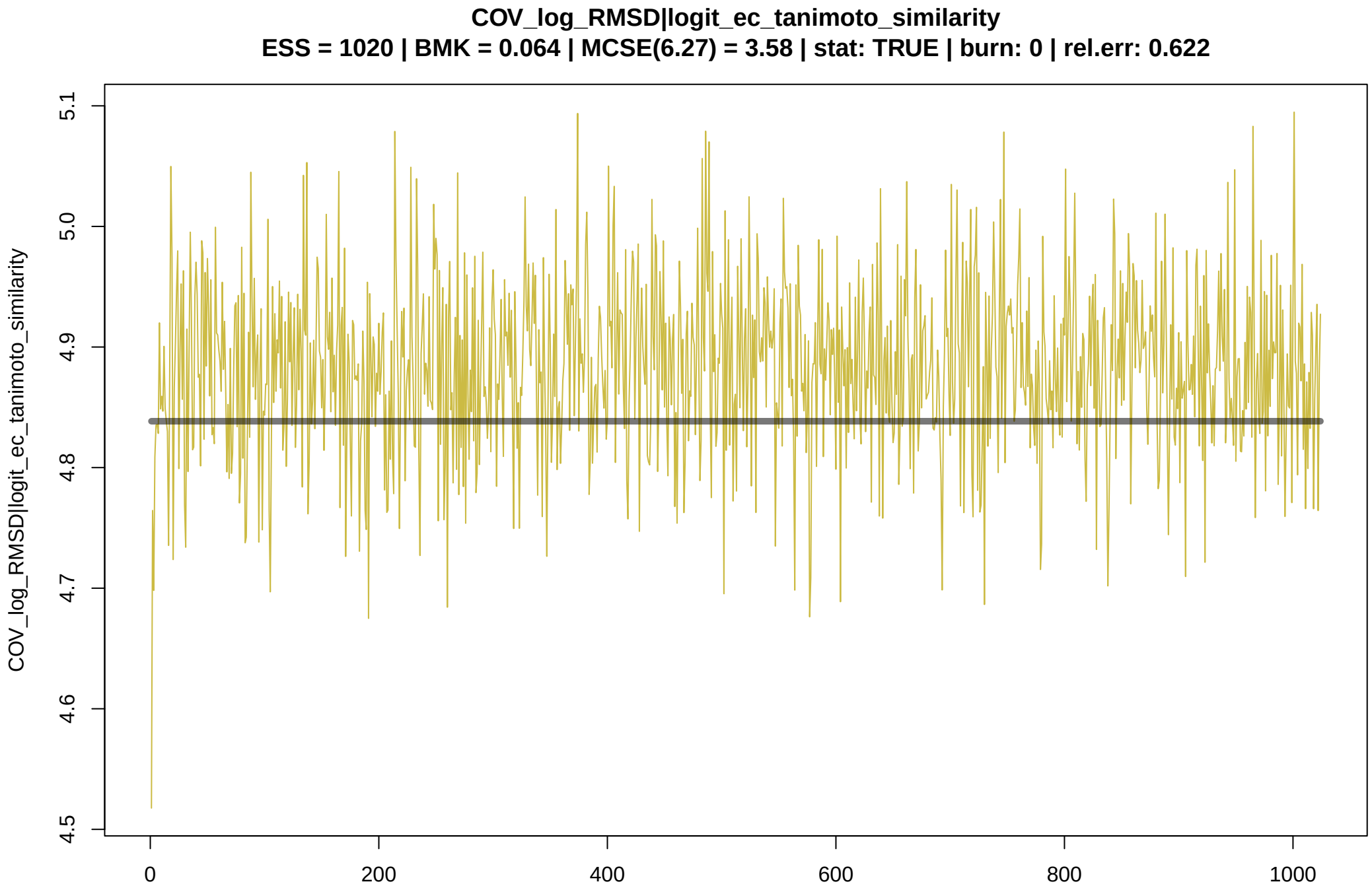

VAR_docked_HeavyAtomCount
ESS = 701 | BMK = 0.148 | MCSE(6.27) = 5.16 | stat: TRUE | burn: 0 | rel.err: −2.24
VAR_docked_HeavyAtomCount
5.60
5.62
5.64
5.66
5.68
5.70
5.72
0
200
400
600
800
1000

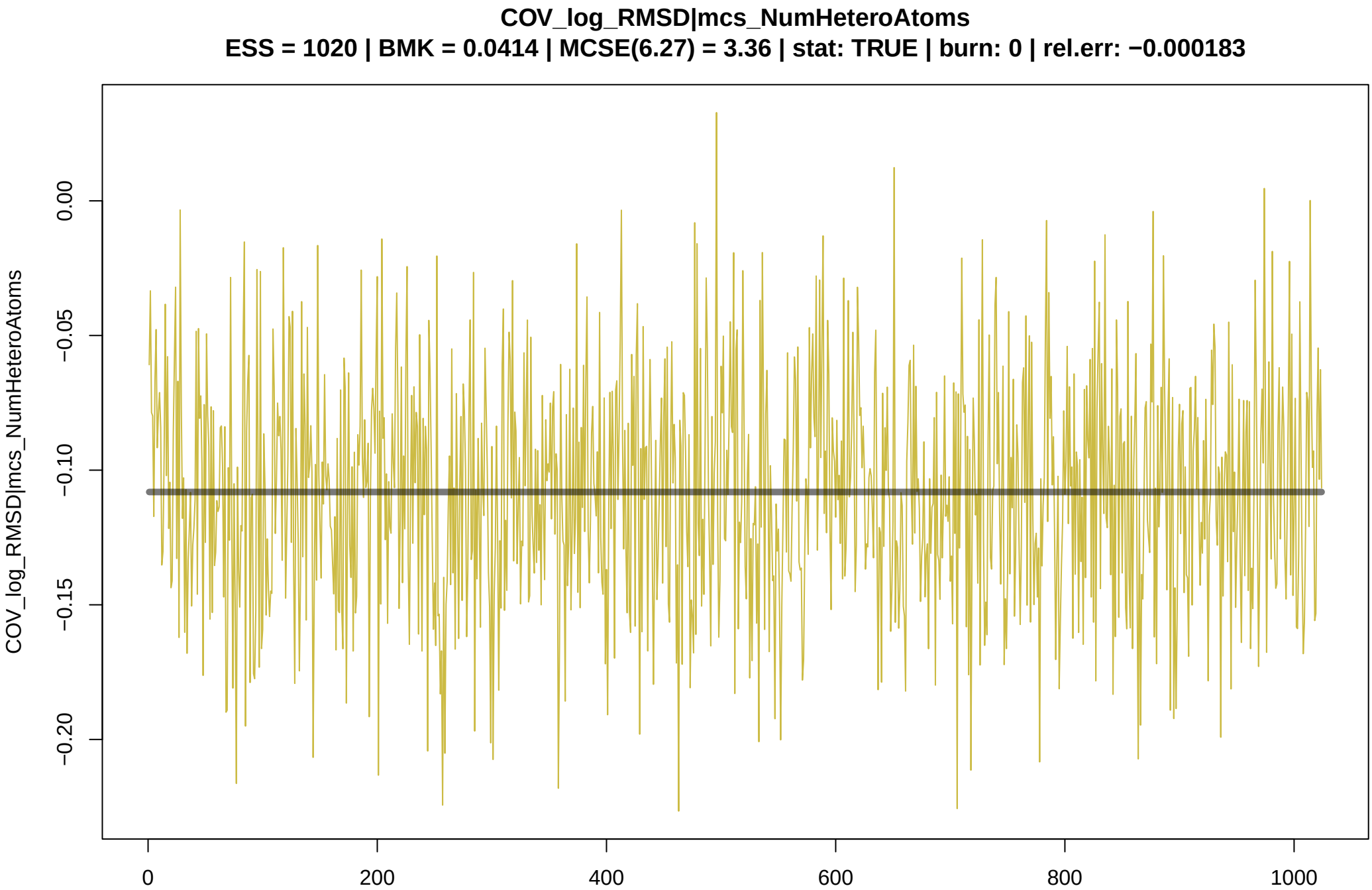

VAR_mcs_RingCount
ESS = 48.7 | BMK = 0.231 | MCSE(6.27) = 8.07 | stat: FALSE | burn: 0 | rel.err: 0.288
VAR_mcs_RingCount
1.10
1.15
1.20
1.25
0
200
400
600
800
1000

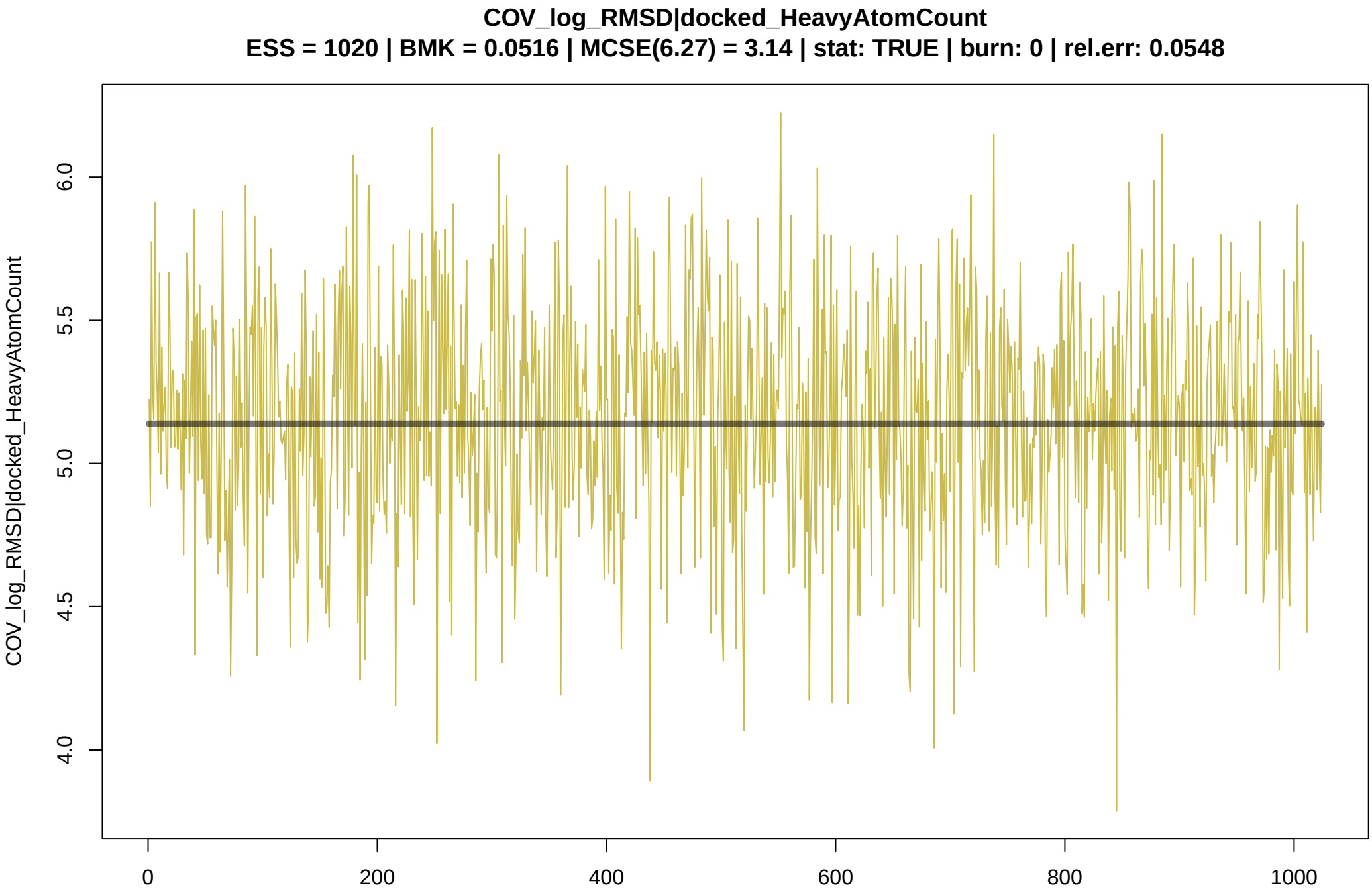

VAR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0633 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0 | rel.err: 0.646
VAR_docked_NumRotatableBonds
3.30
3.35
3.40
3.45
3.50
3.55
0
200
400
600
800
1000

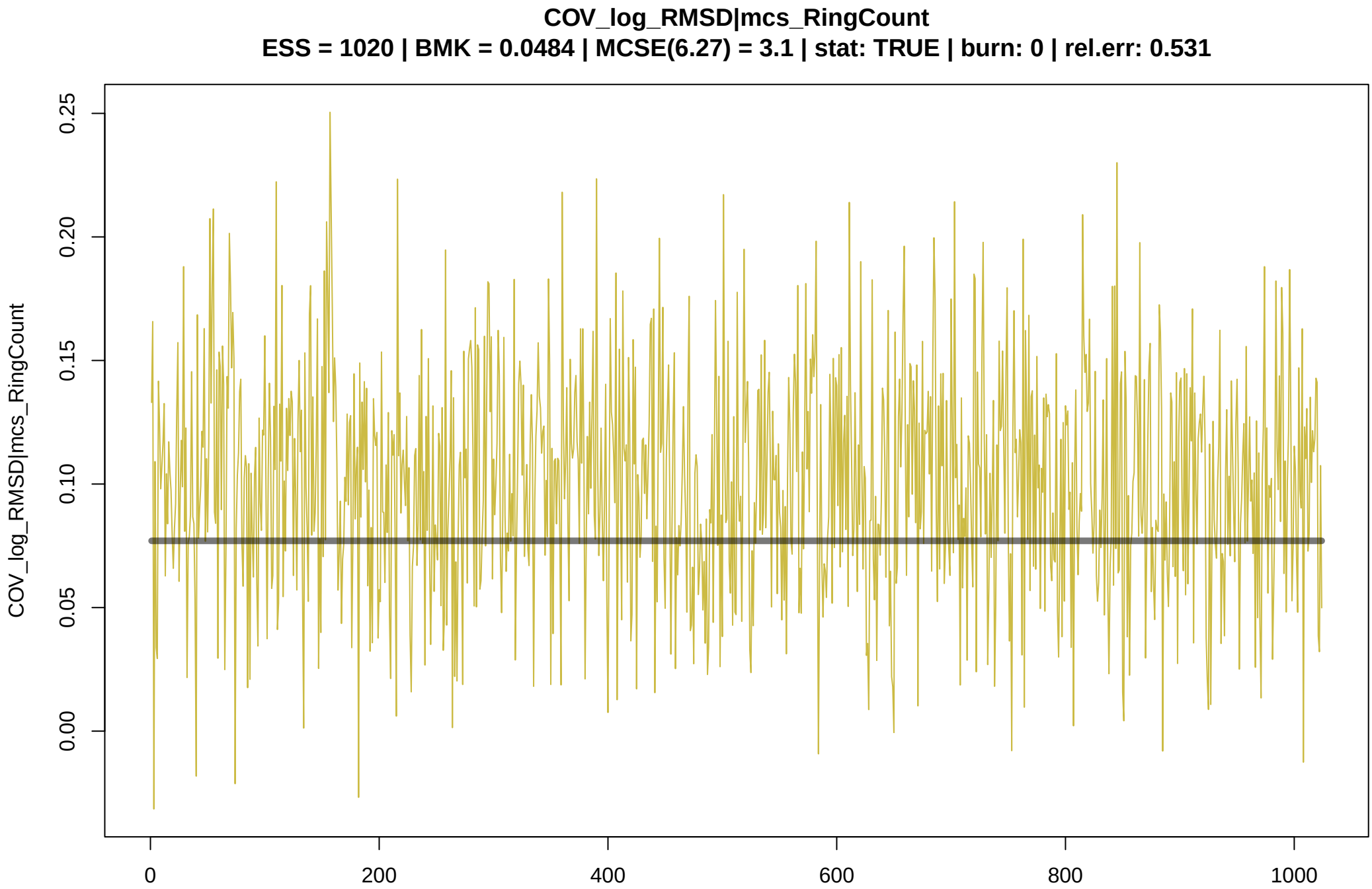

VAR_mcs_NOCount
ESS = 1020 | BMK = 0.1 | MCSE(6.27) = 3.65 | stat: FALSE | burn: 0 | rel.err: −0.47
VAR_mcs_NOCount
3.70
3.65
3.60
3.55
3.50
3.45
0
200
400
600
800
1000

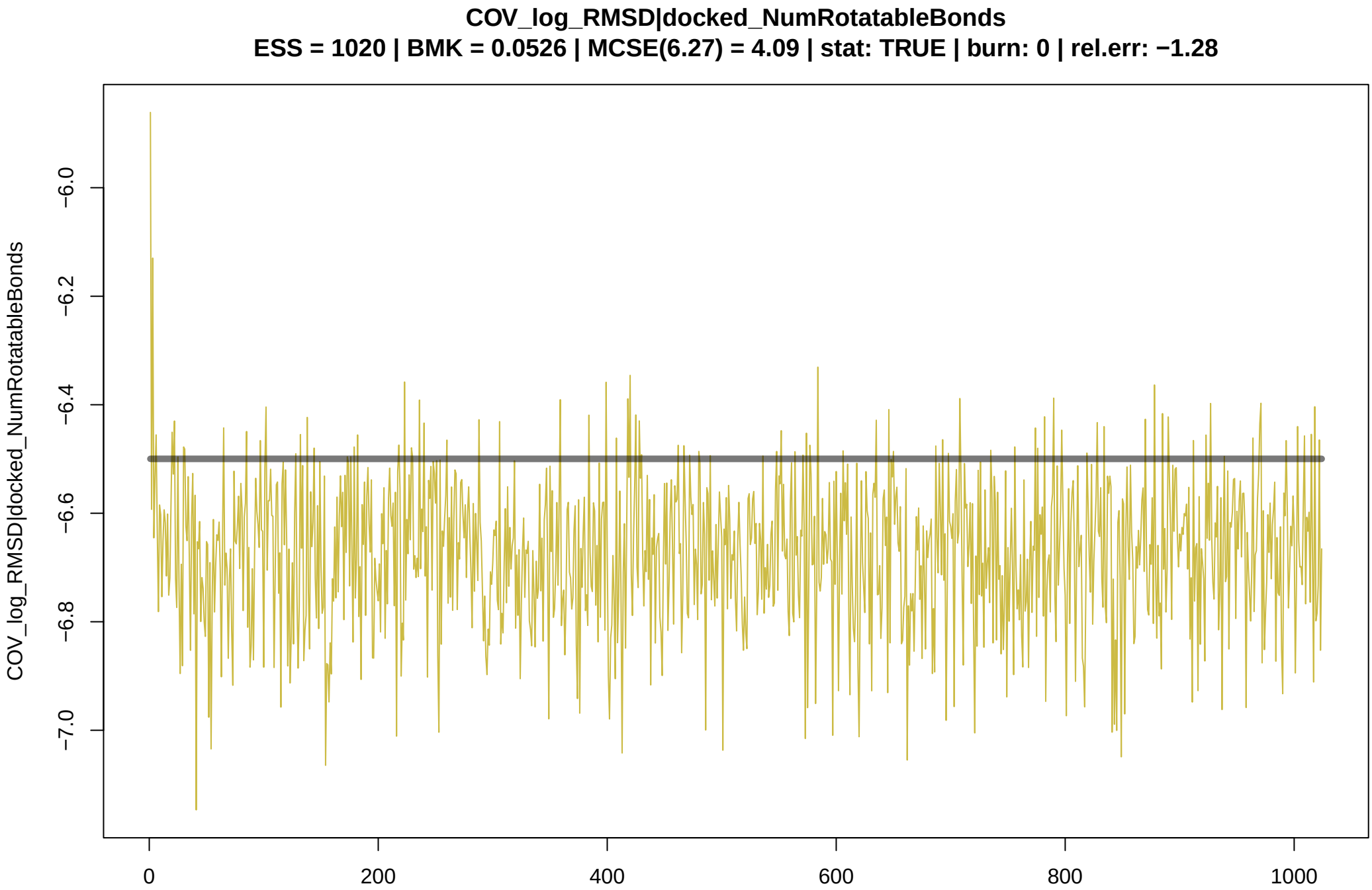

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0453 | MCSE(6.27) = 3.71 | stat: TRUE | burn: 0 | rel.err: −0.41
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.35
−0.40
−0.45
−0.50
−0.55
−0.60
−0.65
0
200
400
600
800
1000

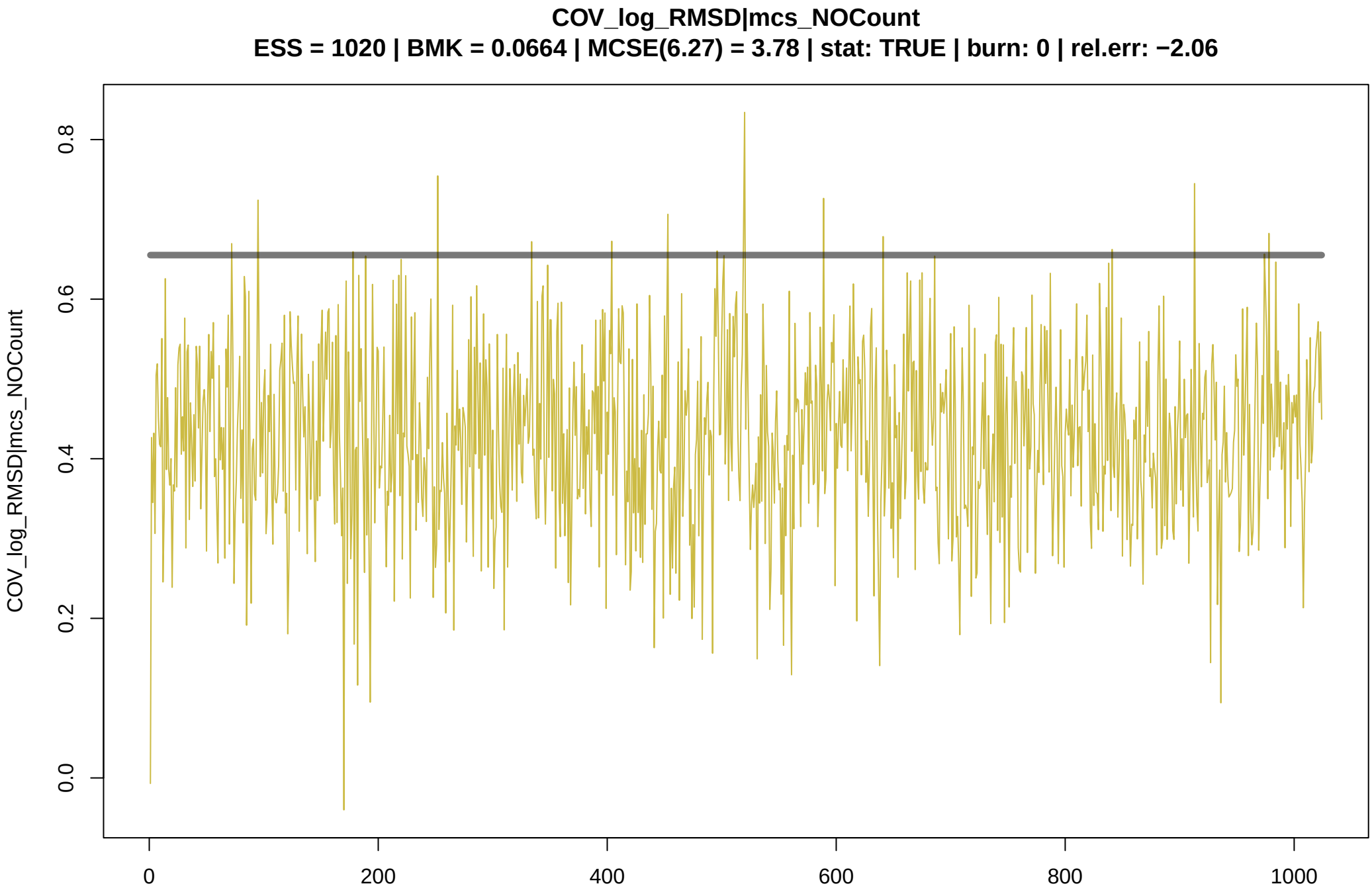

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.064 | MCSE(6.27) = 3.58 | stat: TRUE | burn: 0 | rel.err: 0.622
COV_log_RMSD|logit_ec_tanimoto_similarity
5.1
5.0
4.9
4.8
4.7
4.6
4.5
0
200
400
600
800
1000

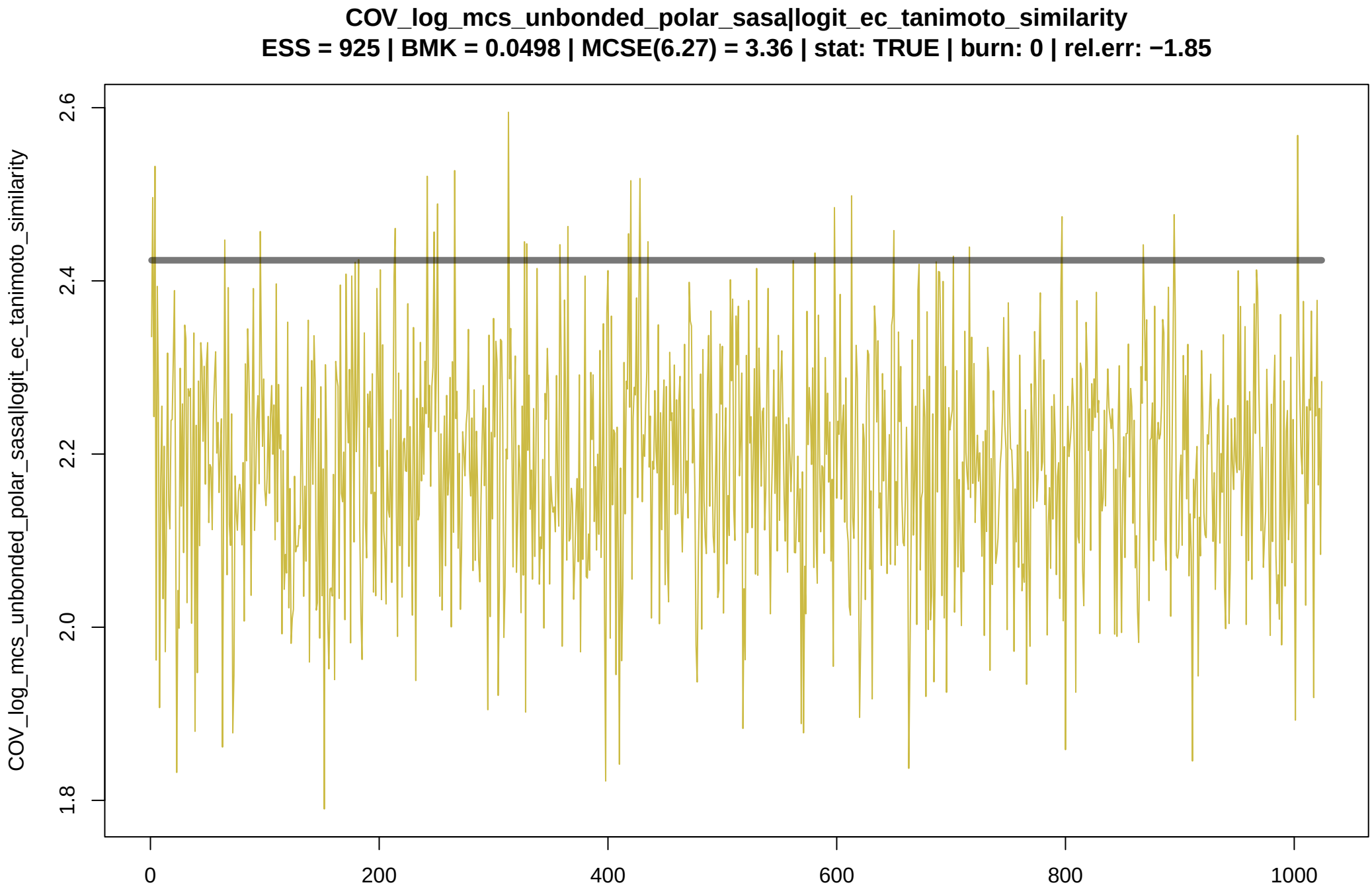

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0414 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | rel.err: −0.000183
COV_log_RMSD|mcs_NumHeteroAtoms
0.00
−0.05
−0.10
−0.15
−0.20
0
200
400
600
800
1000

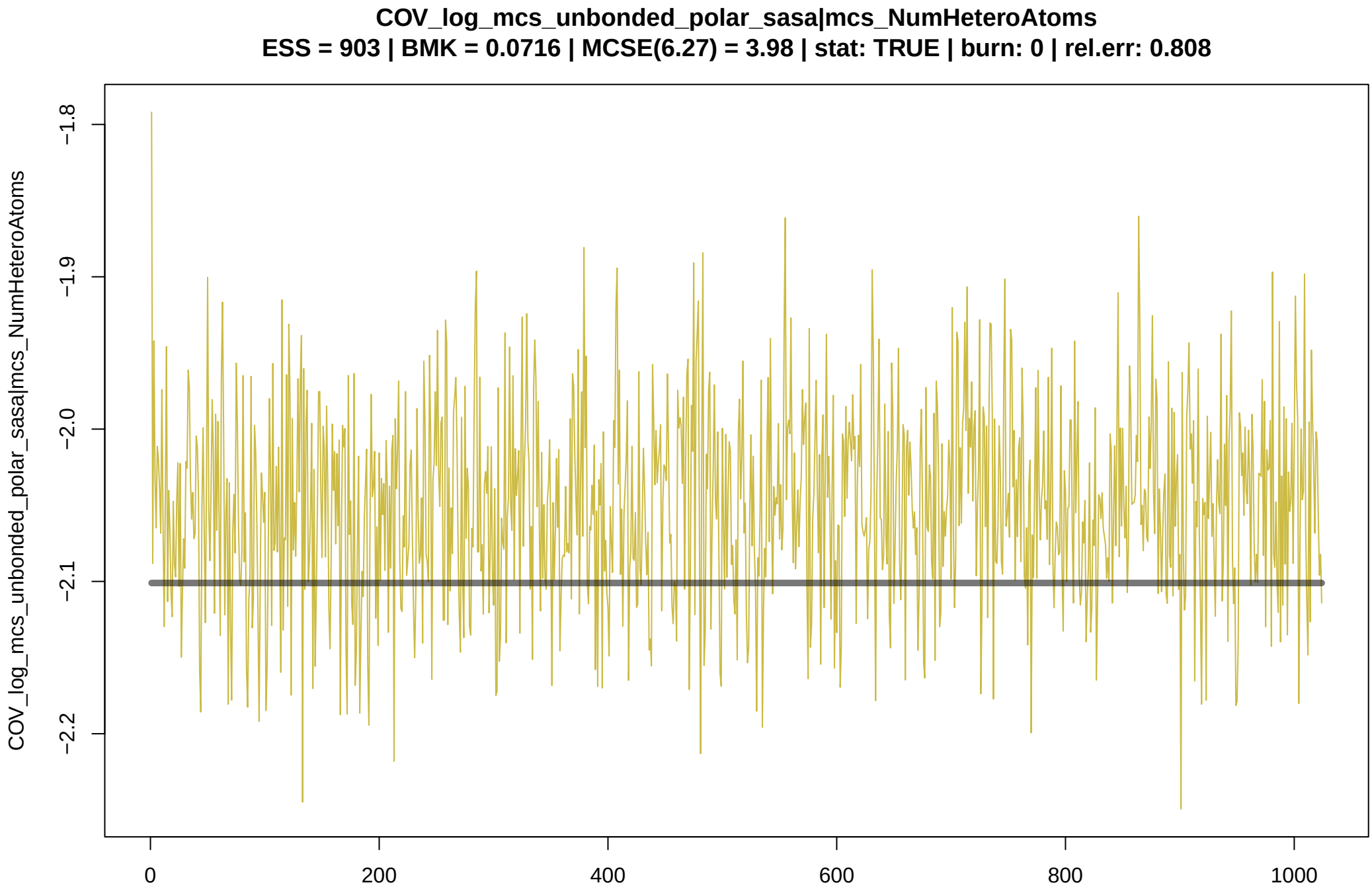

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0516 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | rel.err: 0.0548
COV_log_RMSD|docked_HeavyAtomCount
4.0
4.5
5.0
5.5
6.0
0
200
400
600
800
1000

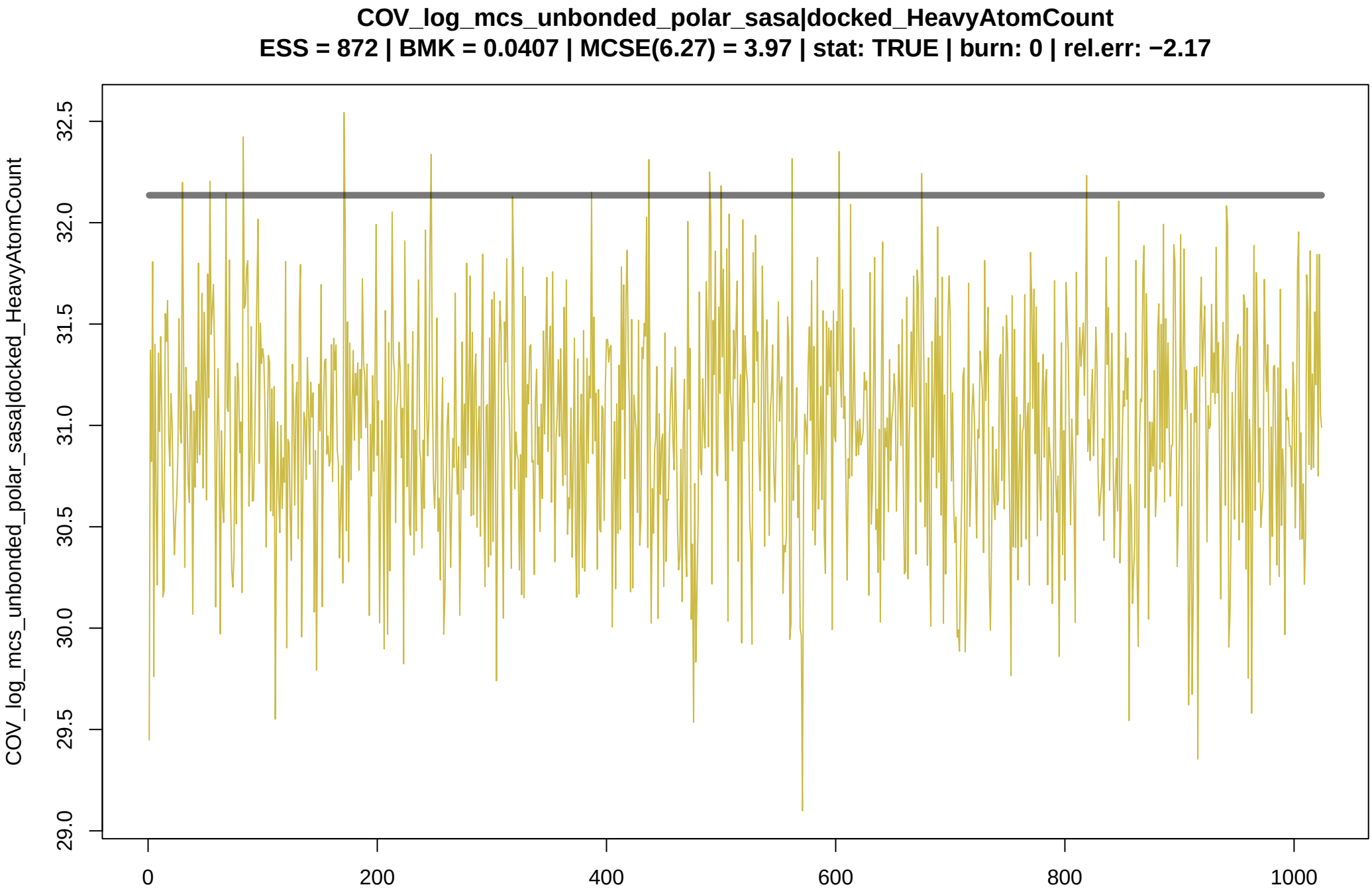

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0484 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | rel.err: 0.531
COV_log_RMSD|mcs_RingCount
0.00
0.05
0.10
0.15
0.20
0.25
0
200
400
600
800
1000

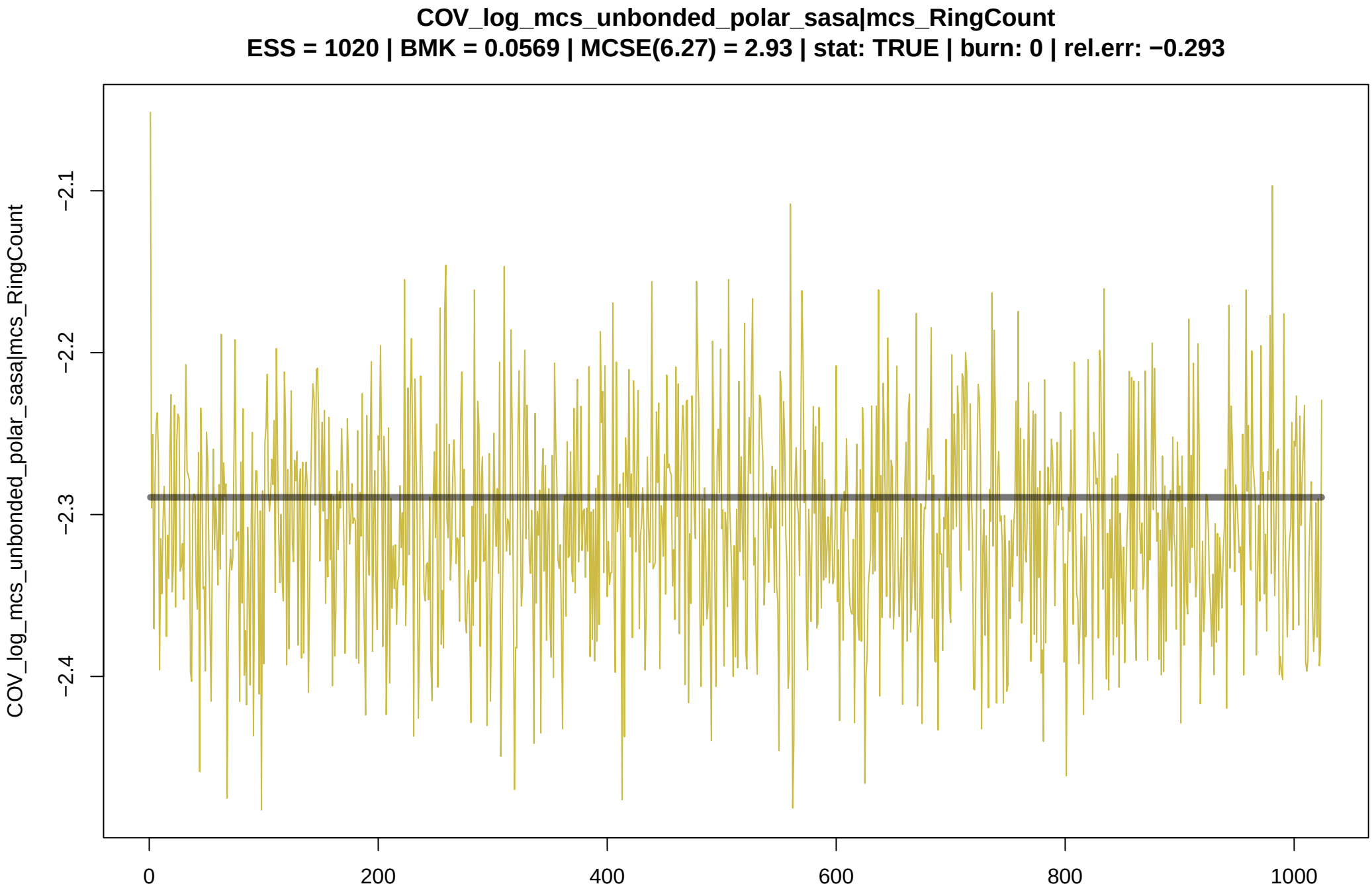

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0526 | MCSE(6.27) = 4.09 | stat: TRUE | burn: 0 | rel.err: −1.28
COV_log_RMSD|docked_NumRotatableBonds
−6.0
−6.2
−6.4
−6.6
−6.8
−7.0
0
200
400
600
800
1000

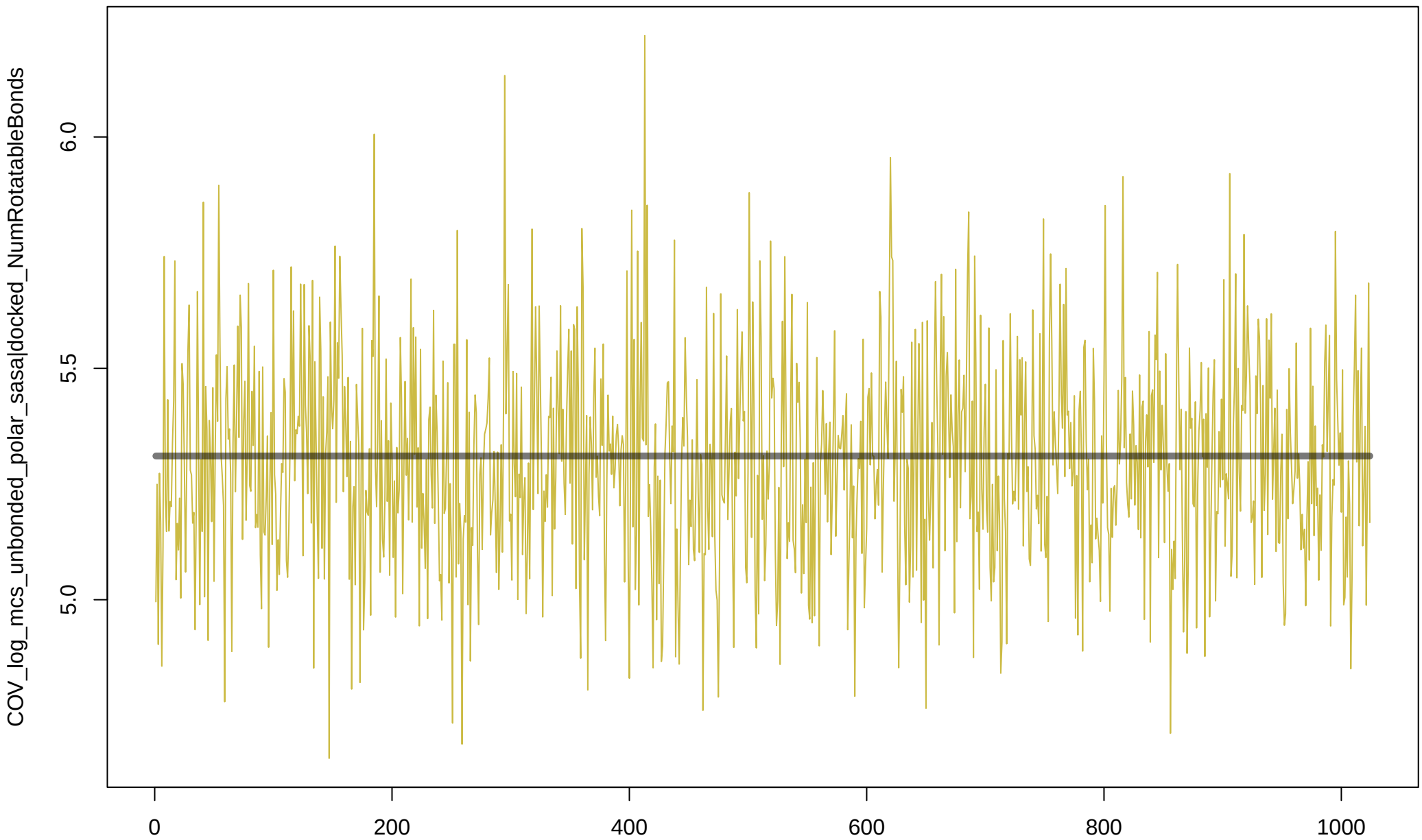

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0664 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0 | rel.err: −2.06
COV_log_RMSD|mcs_NOCount
0.0
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

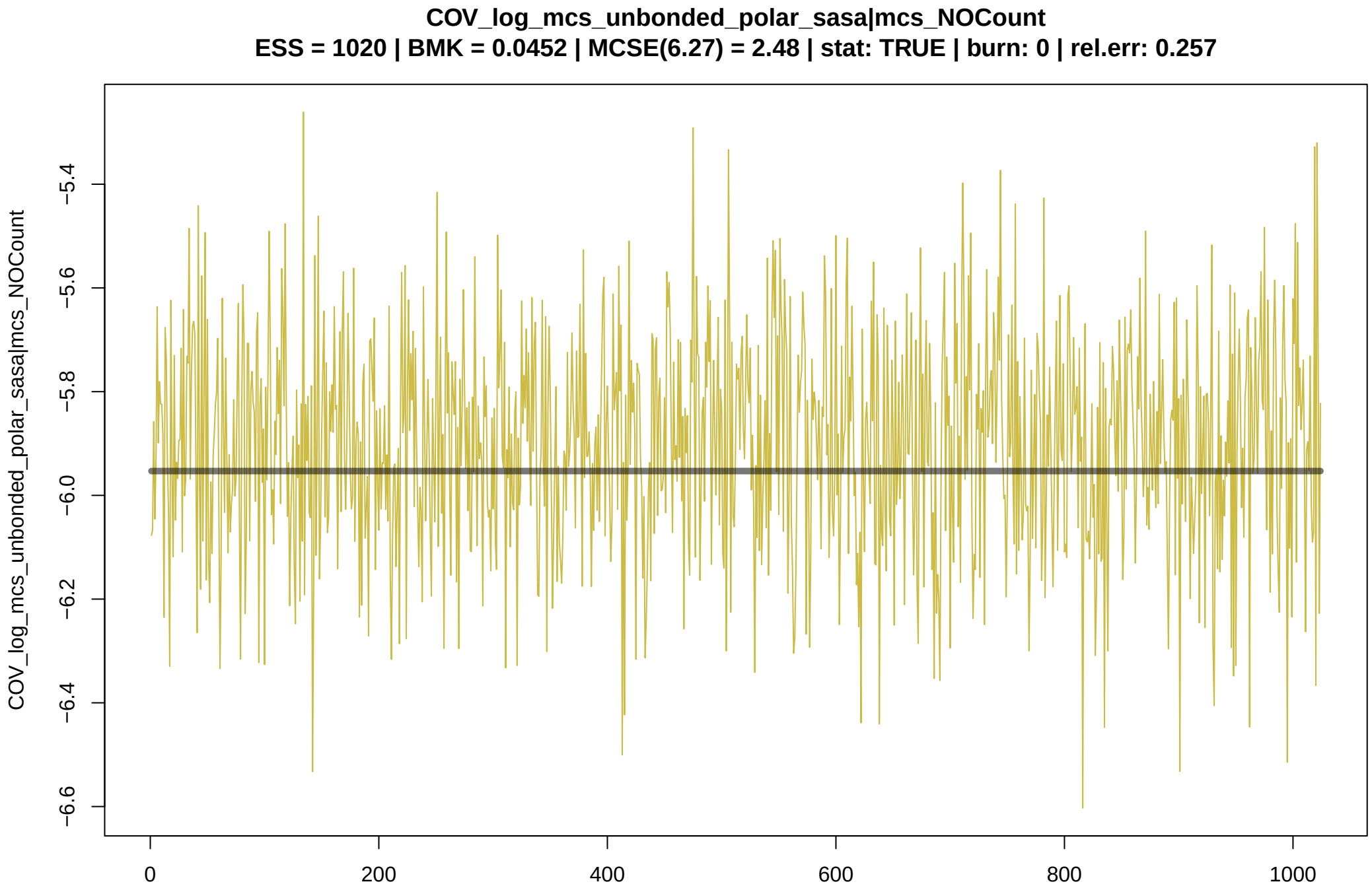

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 925 | BMK = 0.0498 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | rel.err: −1.85
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2.6
2.4
2.2
2.0
1.8
0
200
400
600
800
1000

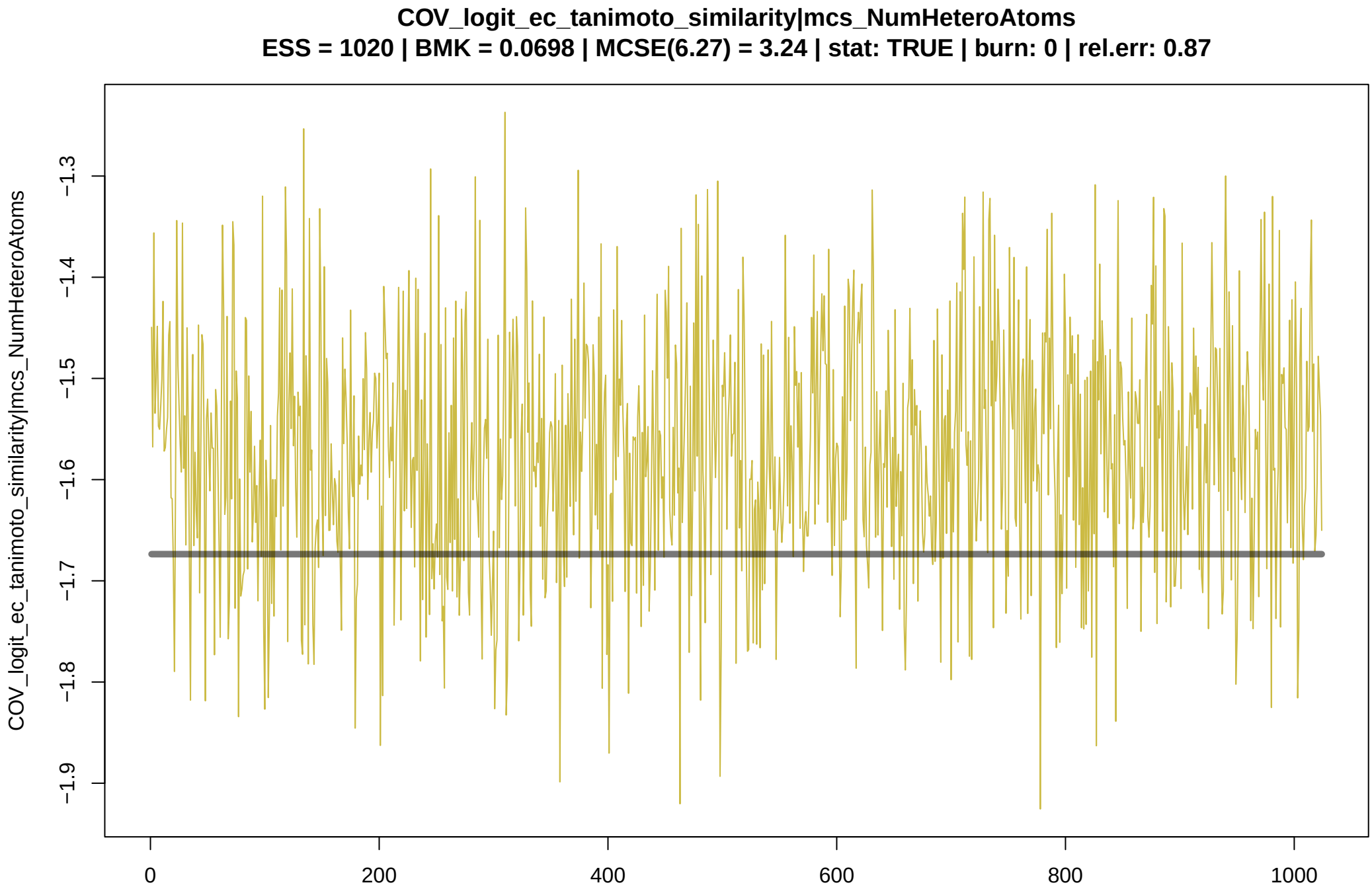

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 903 | BMK = 0.0716 | MCSE(6.27) = 3.98 | stat: TRUE | burn: 0 | rel.err: 0.808
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.8
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

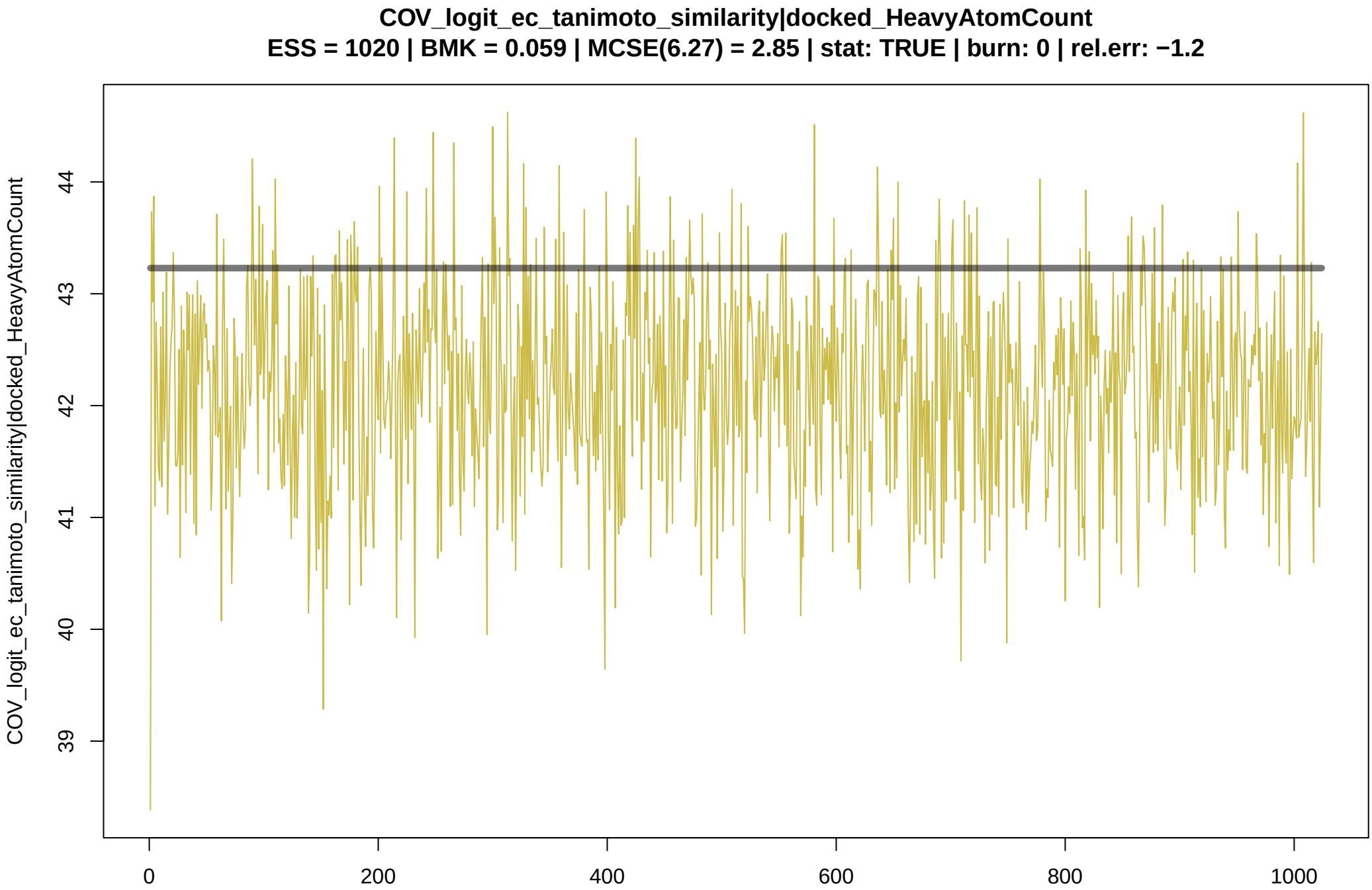

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 872 | BMK = 0.0407 | MCSE(6.27) = 3.97 | stat: TRUE | burn: 0 | rel.err: −2.17
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
29.0
29.5
30.0
30.5
31.0
31.5
32.0
32.5
0
200
400
600
800
1000

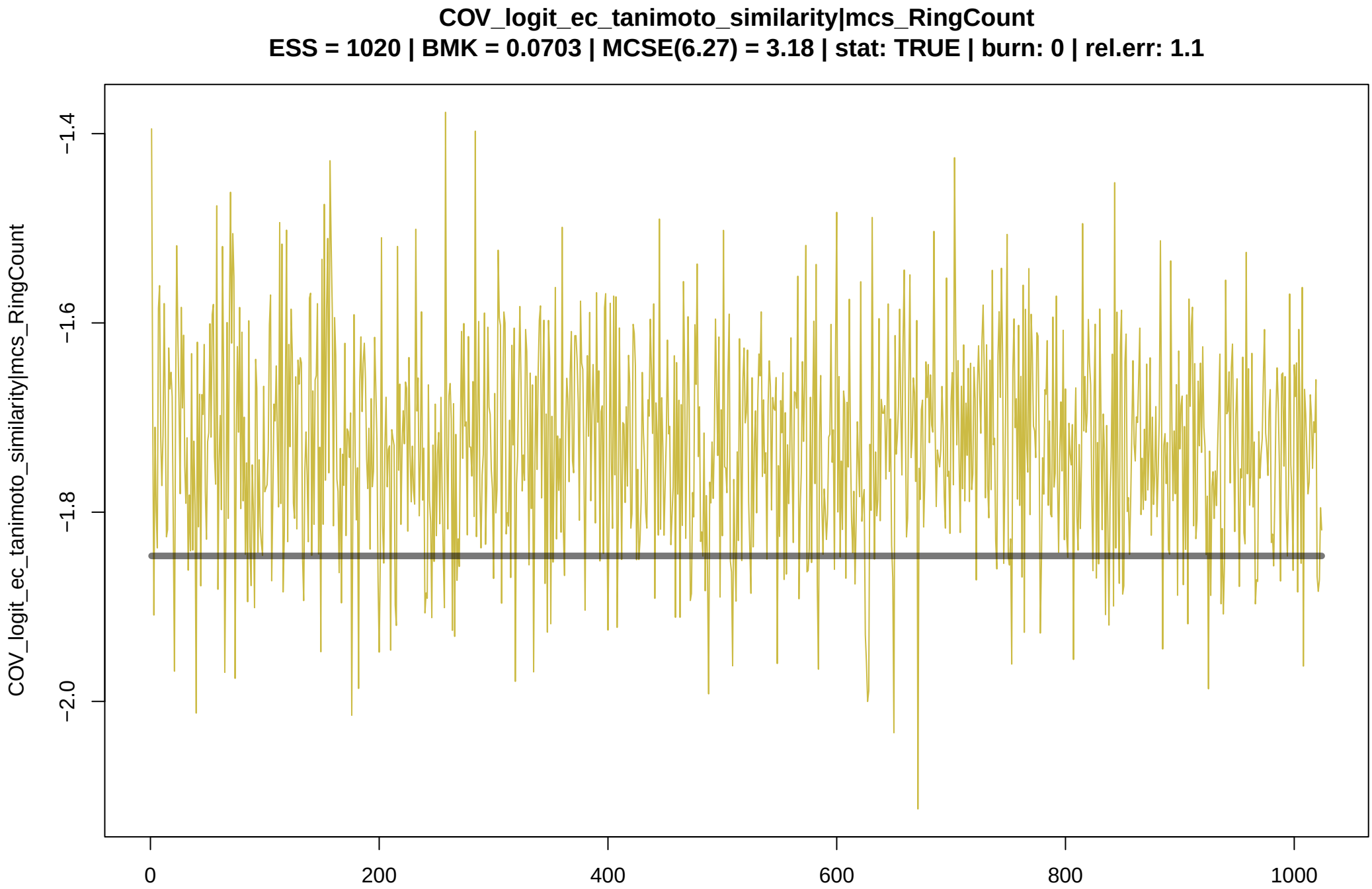

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0569 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | rel.err: −0.293
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.1
−2.2
−2.3
−2.4
0
200
400
600
800
1000

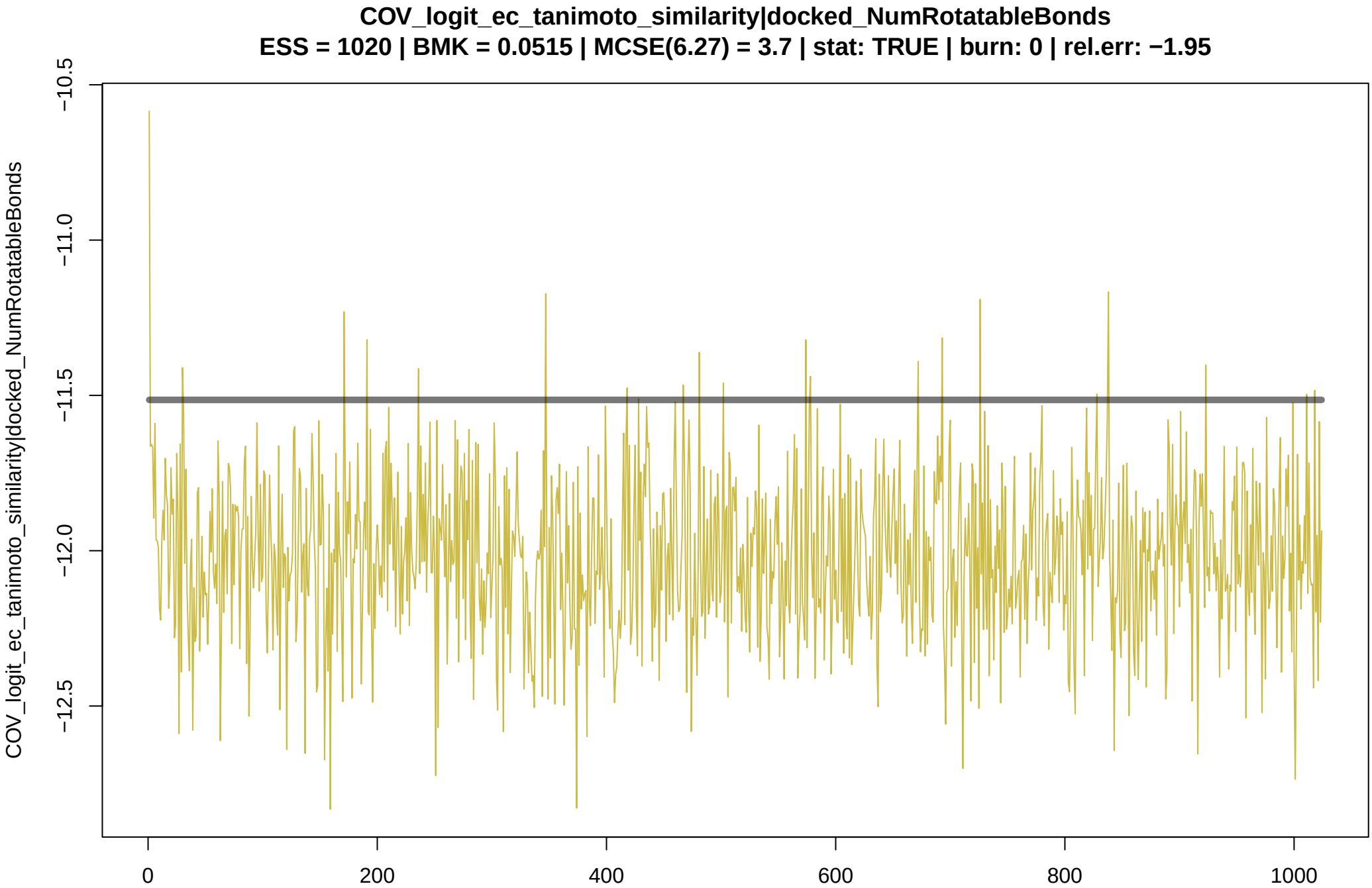

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 913 | BMK = 0.0539 | MCSE(6.27) = 3.67 | stat: TRUE | burn: 0 | rel.err: −0.0616
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
6.0
5.5
5.0
0
200
400
600
800
1000

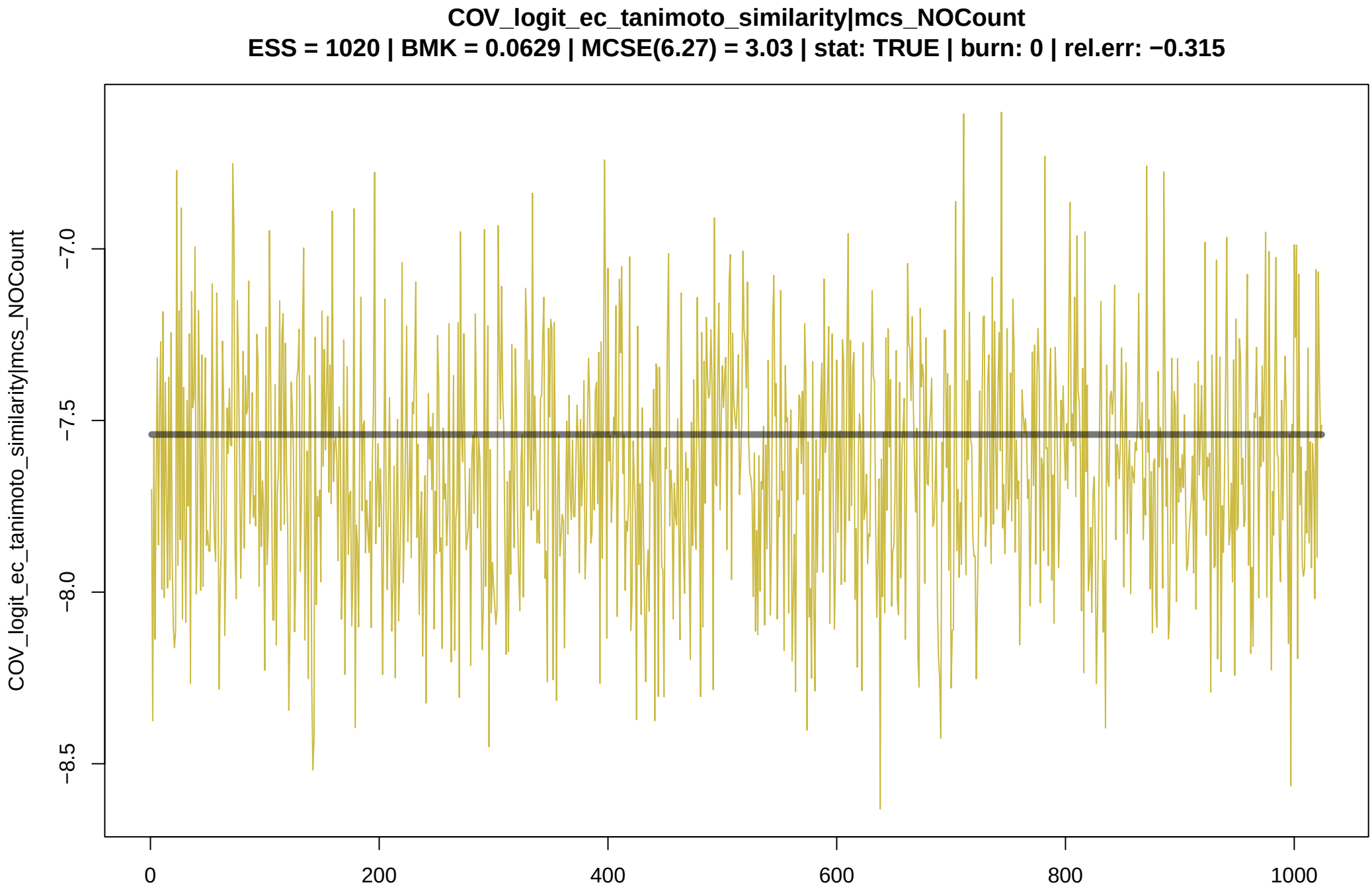

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0452 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0 | rel.err: 0.257
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.4
−5.6
−5.8
−6.0
−6.2
−6.4
−6.6
0
200
400
600
800
1000

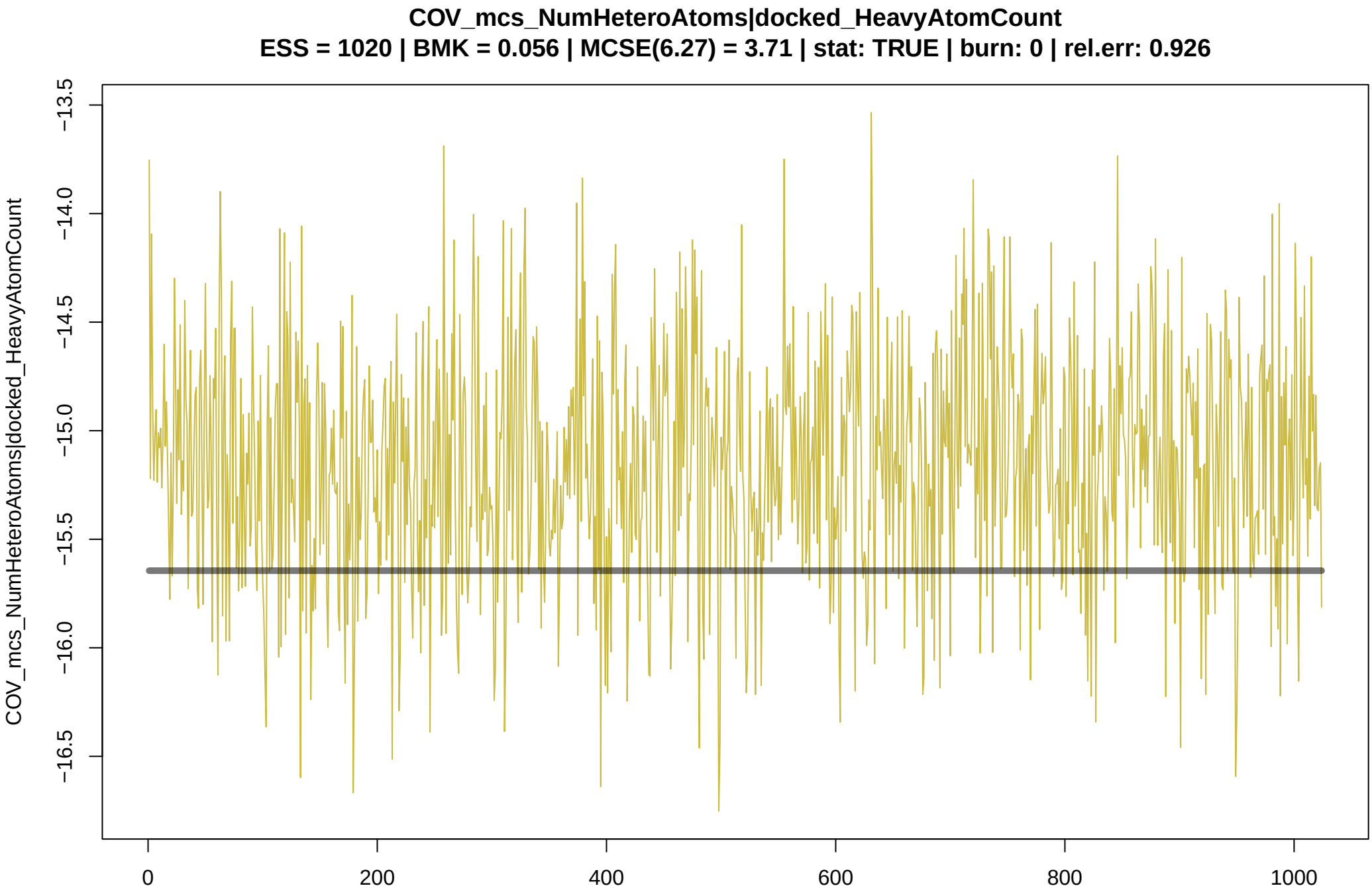

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0698 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | rel.err: 0.87
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.3
−1.4
−1.5
−1.6
−1.7
−1.8
−1.9
0
200
400
600
800
1000

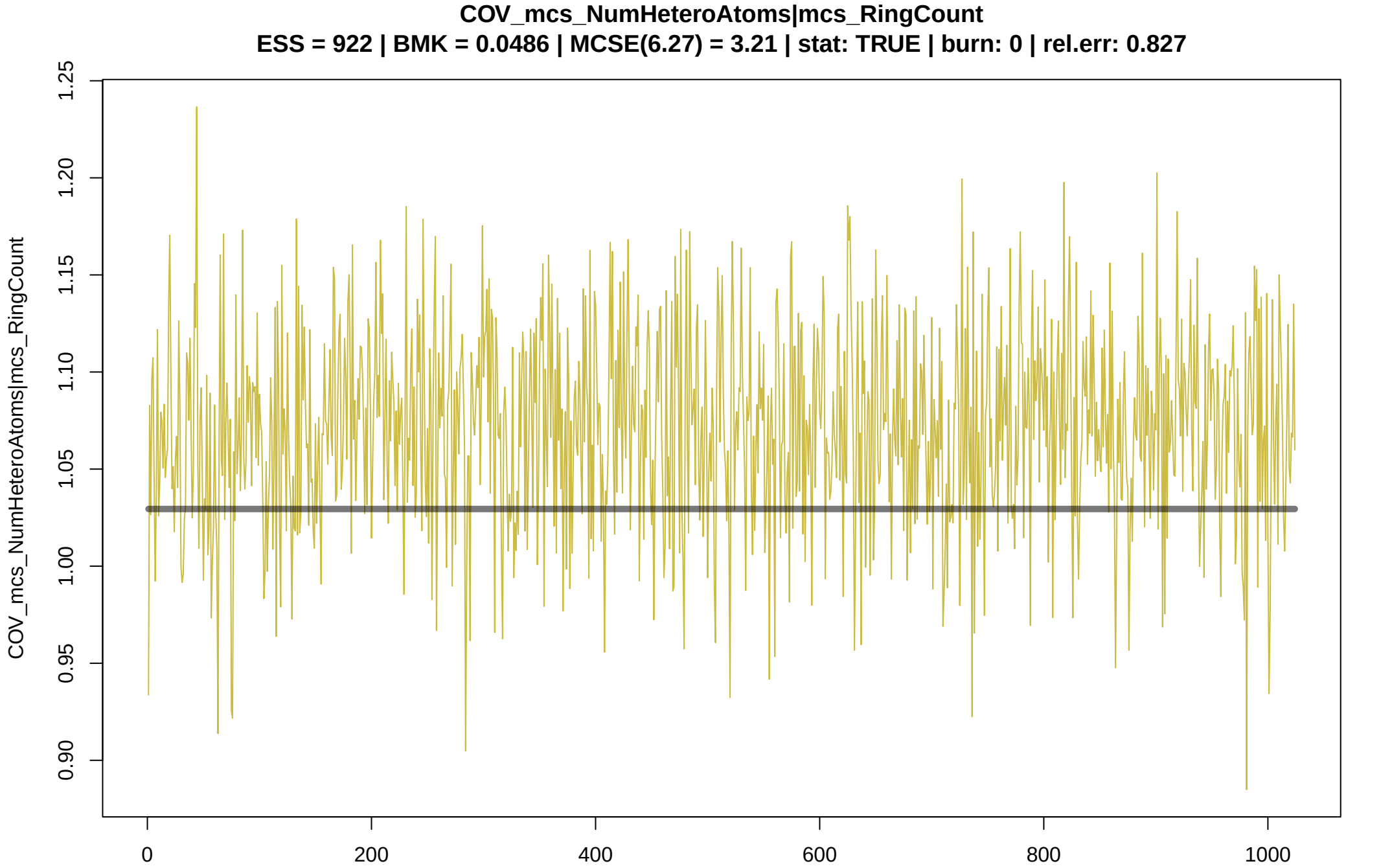

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.059 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | rel.err: −1.2
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
39
40
41
42
43
44
0
200
400
600
800
1000

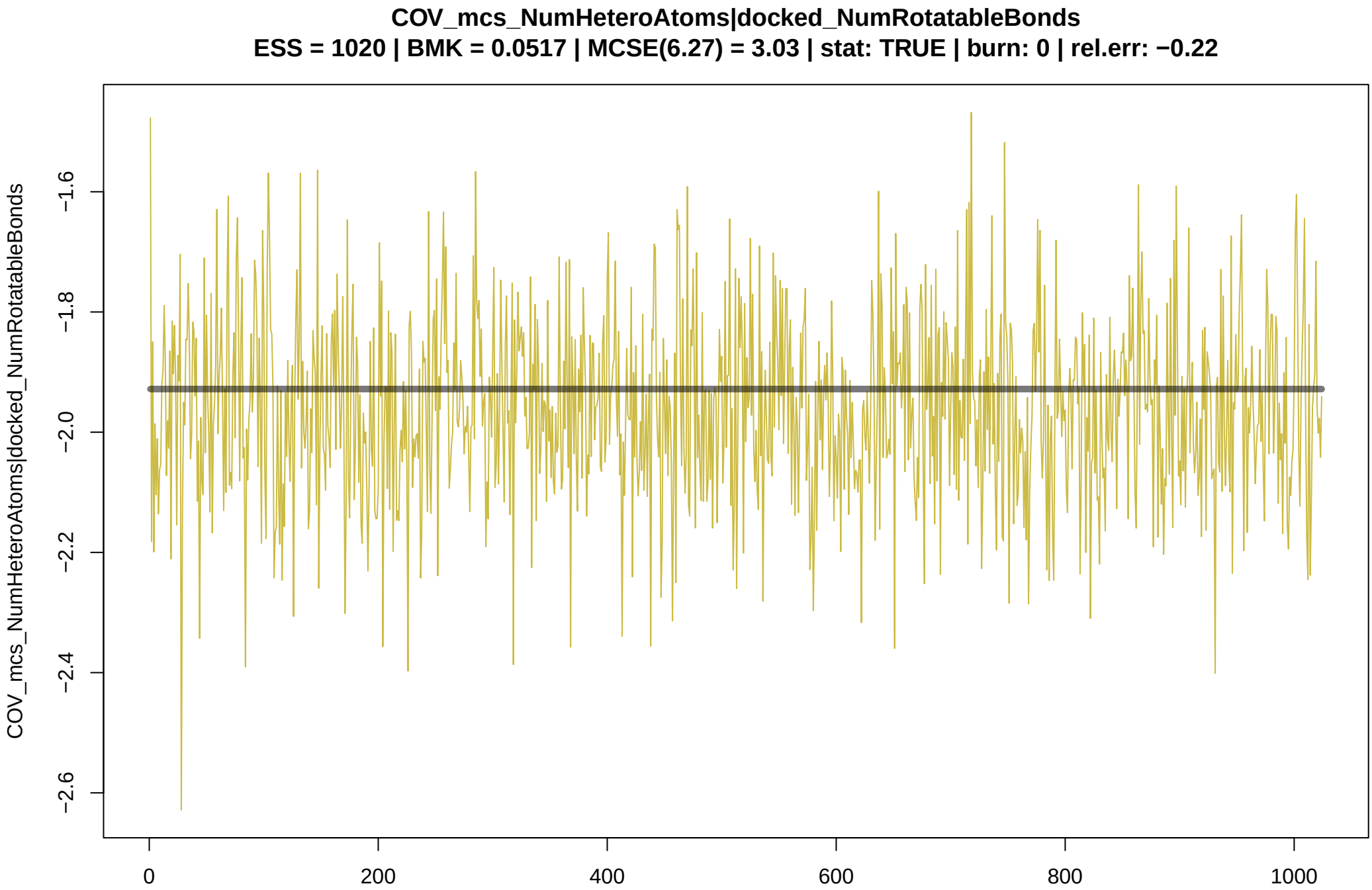

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0703 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | rel.err: 1.1
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

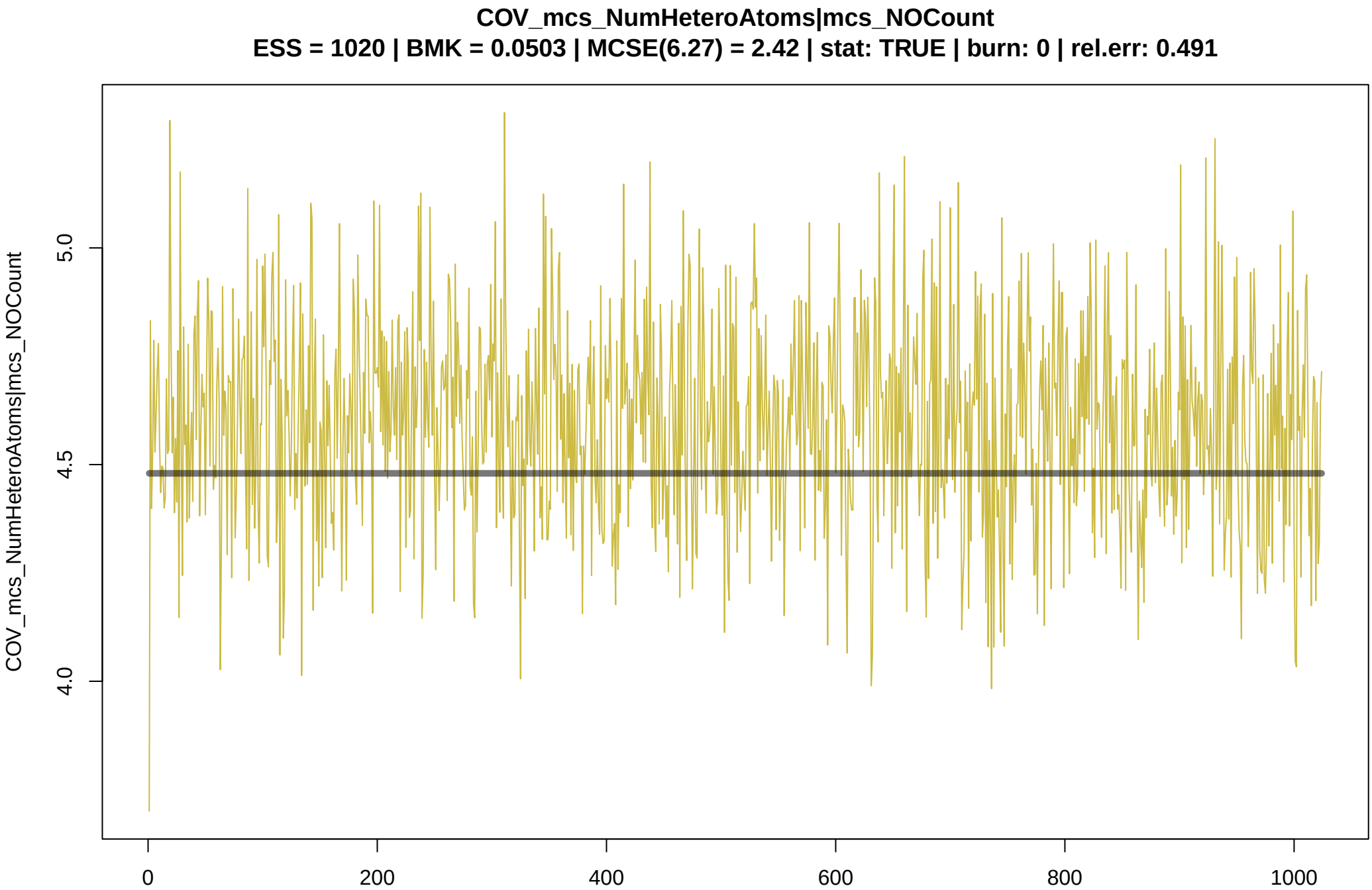

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0515 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | rel.err: −1.95
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−10.5
−11.0
−11.5
−12.0
−12.5
0
200
400
600
800
1000

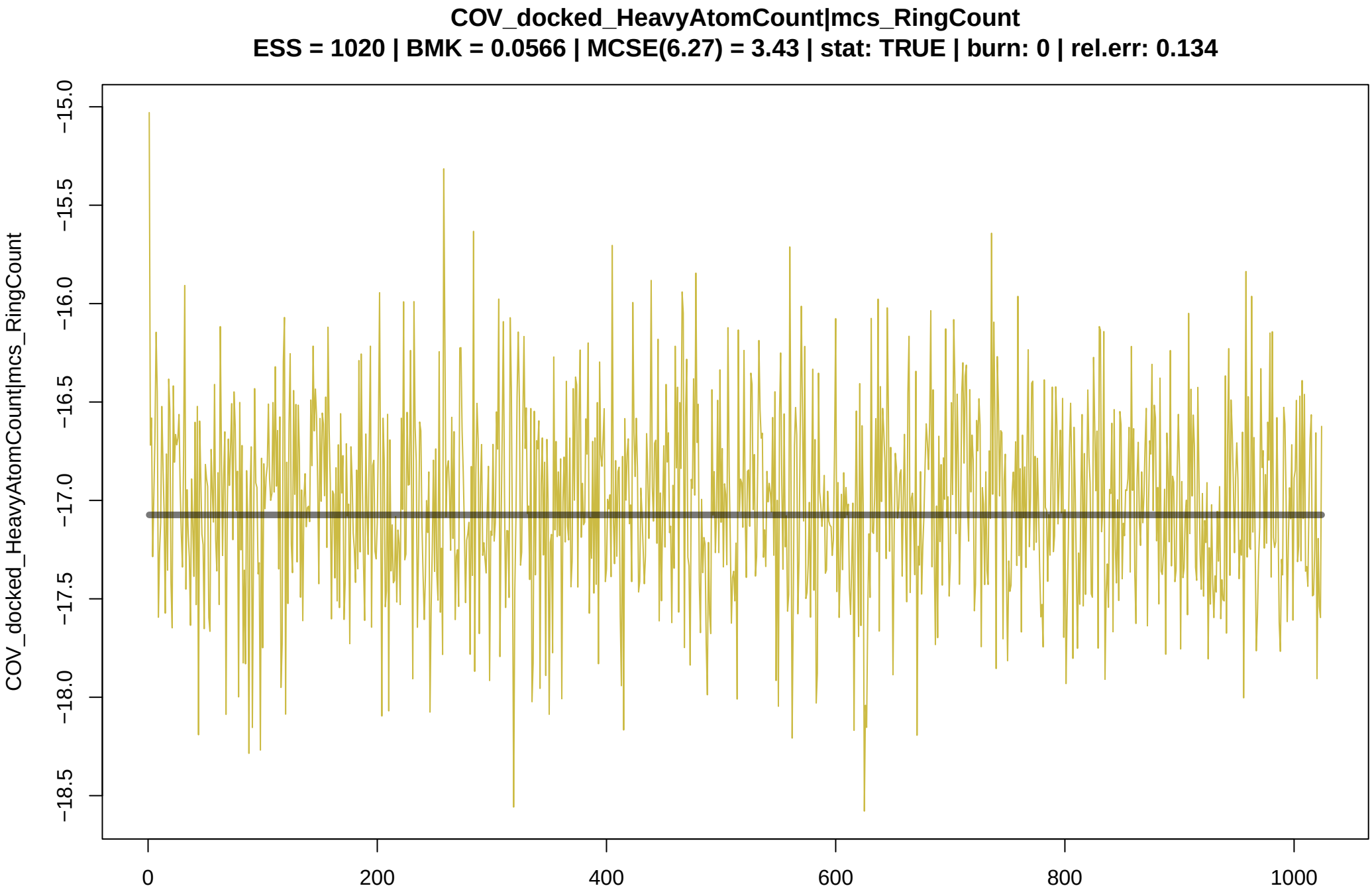

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0629 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | rel.err: −0.315
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−7.0
−7.5
−8.0
−8.5
0
200
400
600
800
1000

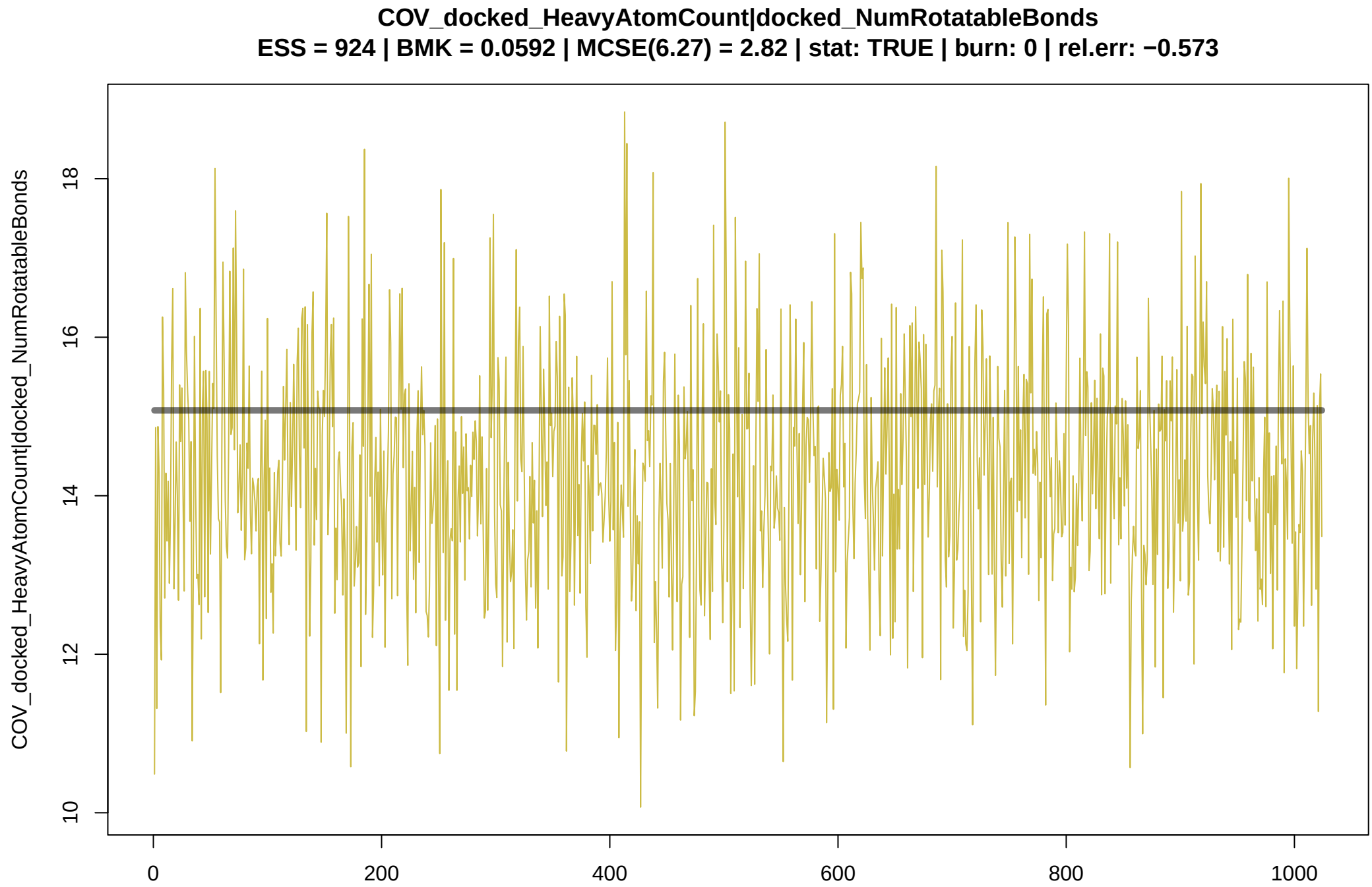

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.056 | MCSE(6.27) = 3.71 | stat: TRUE | burn: 0 | rel.err: 0.926
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−13.5
−14.0
−14.5
−15.0
−15.5
−16.0
−16.5
0
200
400
600
800
1000

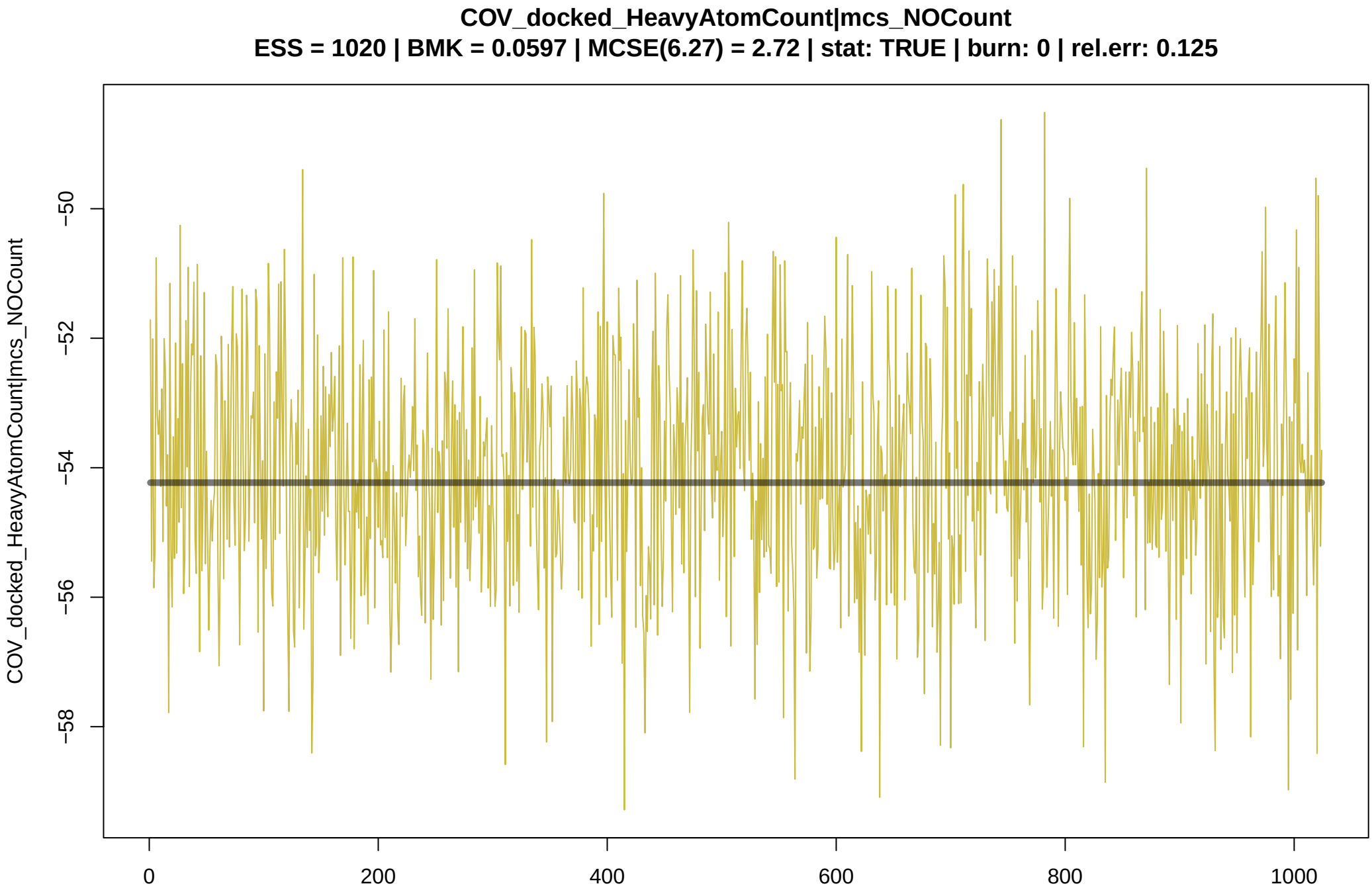

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 922 | BMK = 0.0486 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | rel.err: 0.827
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.90
0.95
1.00
1.05
1.10
1.15
1.20
1.25
0
200
400
600
800
1000

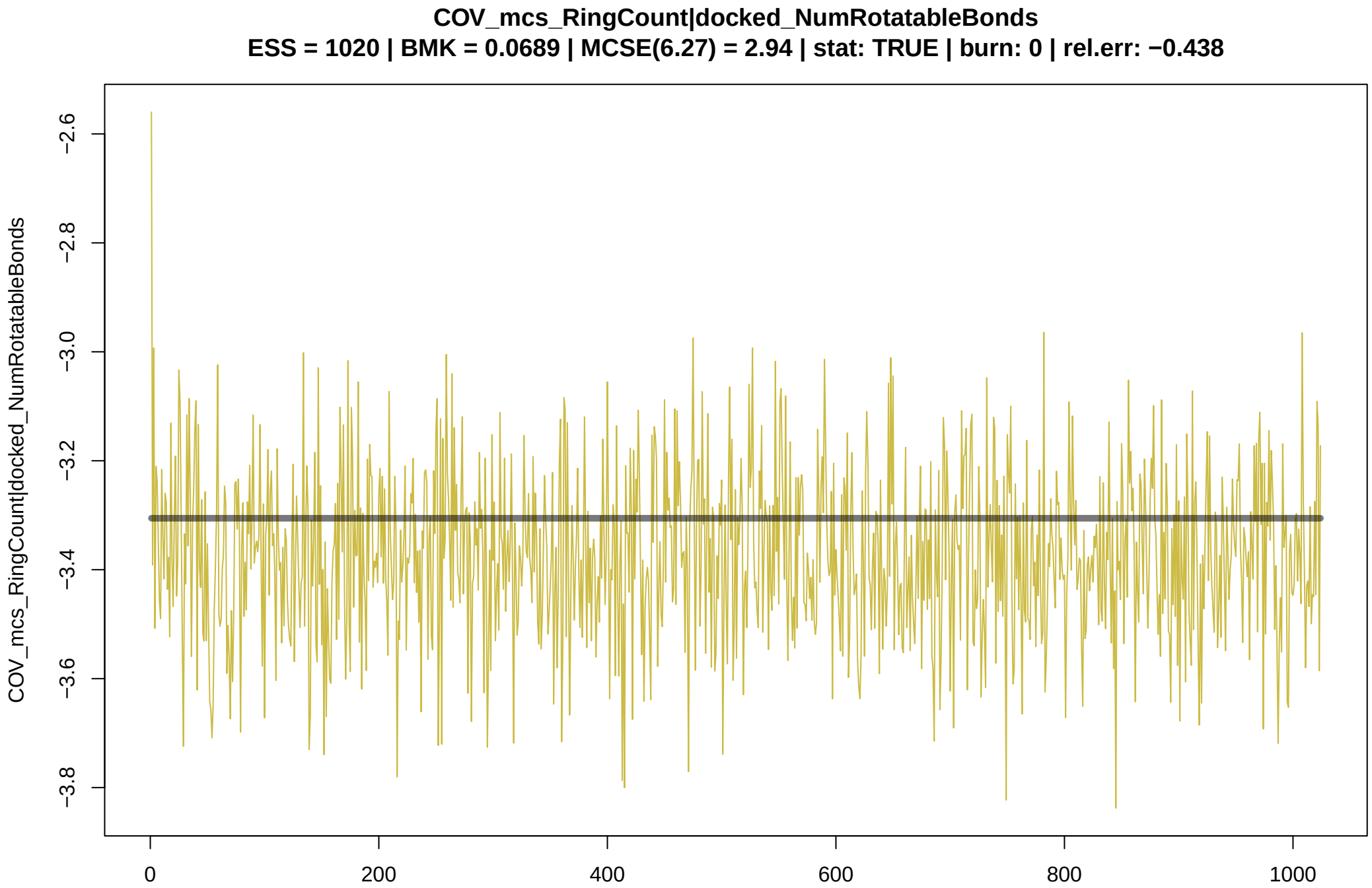

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0517 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | rel.err: −0.22
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.6
−1.8
−2.0
−2.2
−2.4
−2.6
0
200
400
600
800
1000

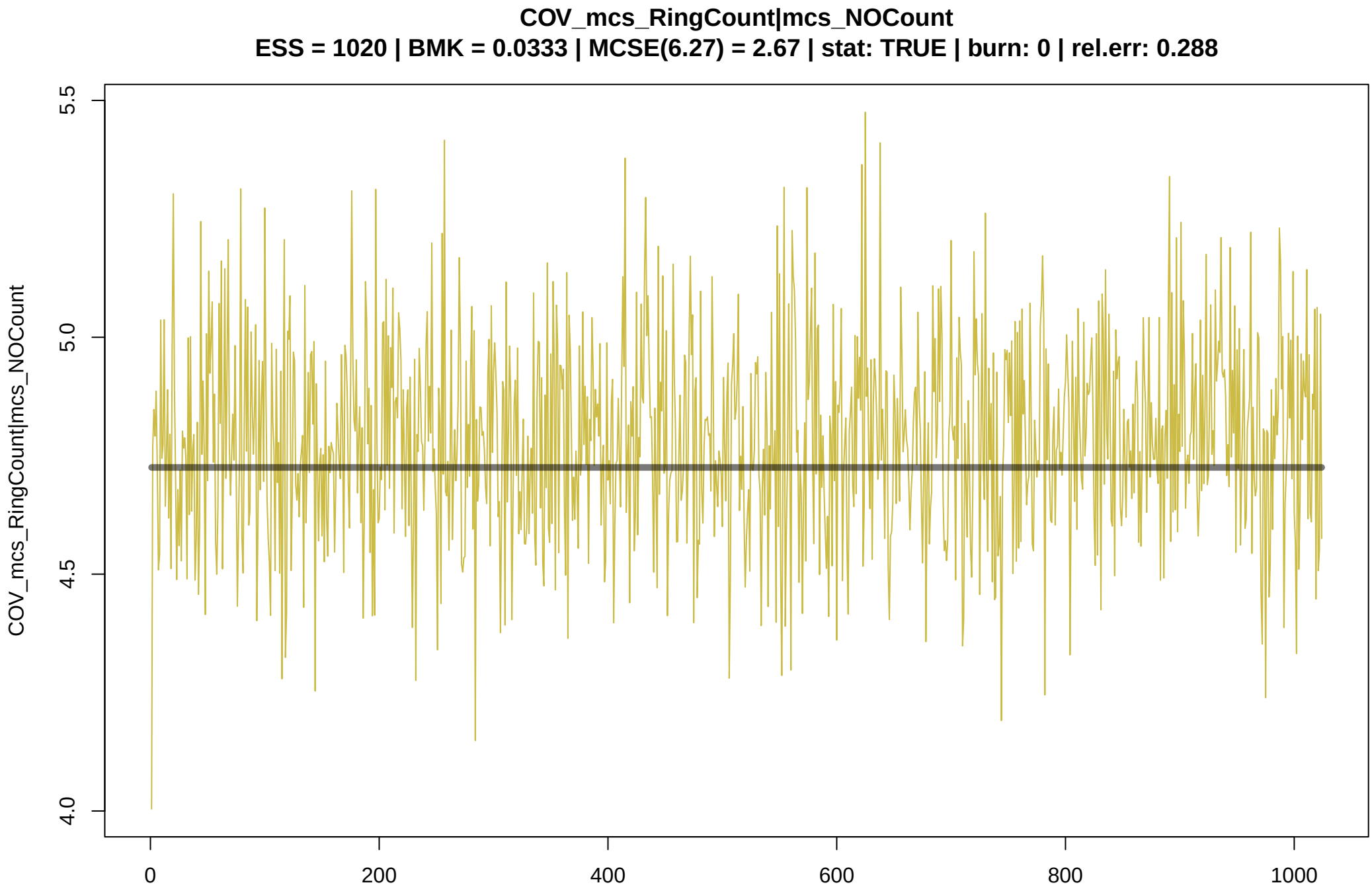

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0503 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 0.491
COV_mcs_NumHeteroAtoms|mcs_NOCount
4.0
4.5
5.0
0
200
400
600
800
1000

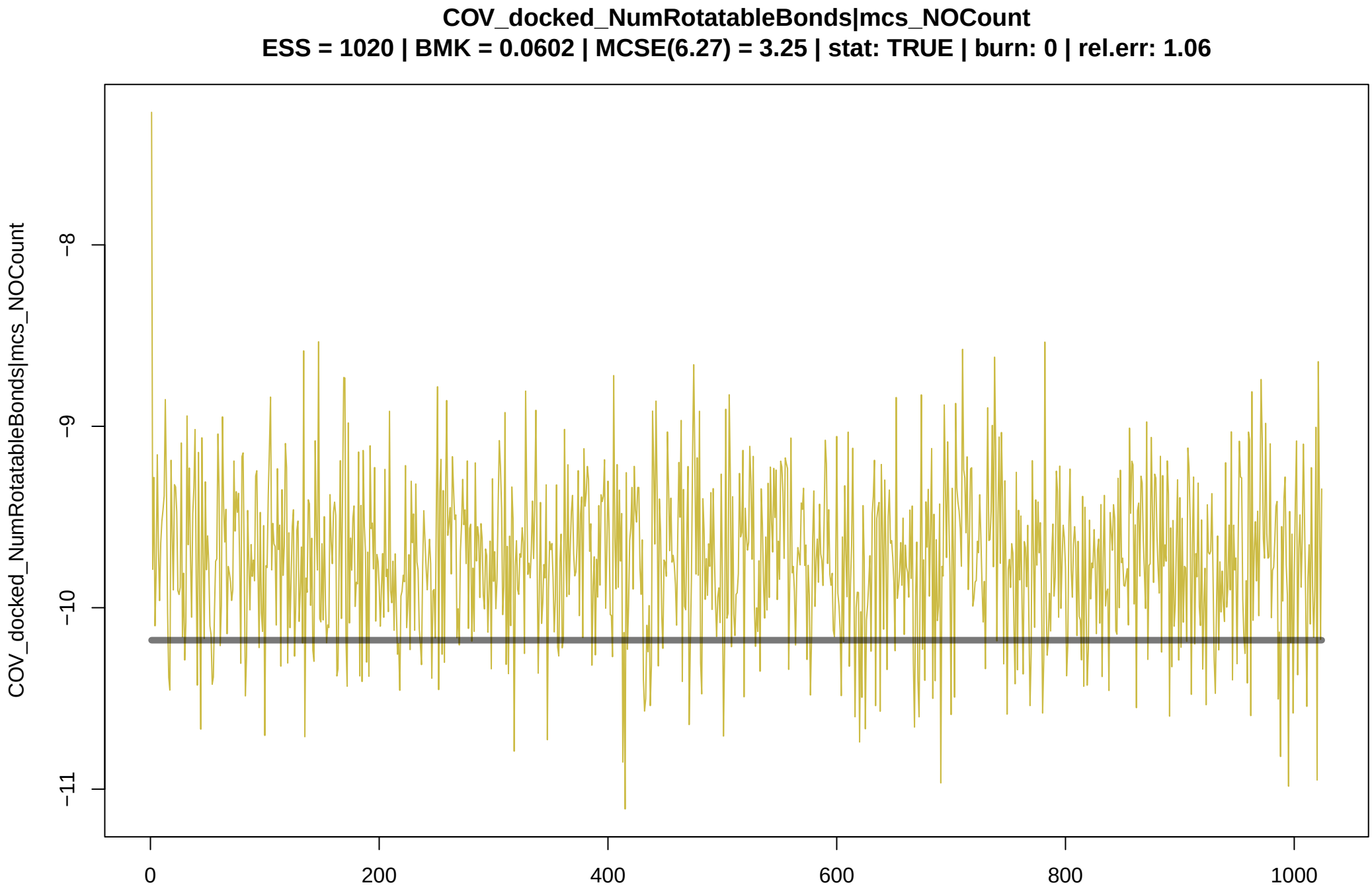

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0566 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0 | rel.err: 0.134
COV_docked_HeavyAtomCount|mcs_RingCount
−15.0
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 924 | BMK = 0.0592 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: −0.573
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0597 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: 0.125
COV_docked_HeavyAtomCount|mcs_NOCount
−50
−52
−54
−56
−58
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0689 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | rel.err: −0.438
COV_mcs_RingCount|docked_NumRotatableBonds
−2.6
−2.8
−3.0
−3.2
−3.4
−3.6
−3.8
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0333 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0 | rel.err: 0.288
COV_mcs_RingCount|mcs_NOCount
5.5
5.0
4.5
4.0
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0602 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | rel.err: 1.06
COV_docked_NumRotatableBonds|mcs_NOCount
−8
−9
−10
−11
0
200
400
600
800
1000