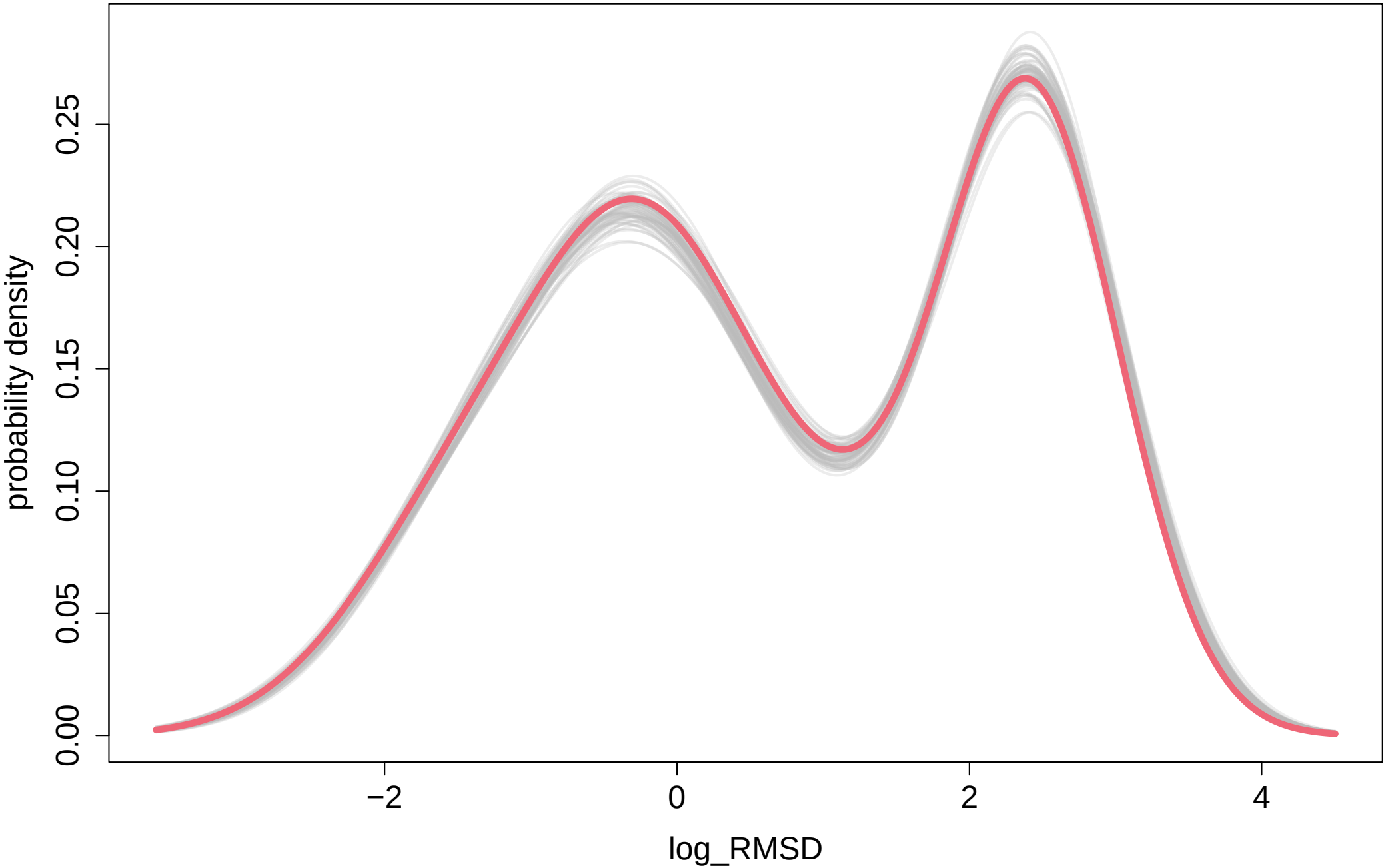
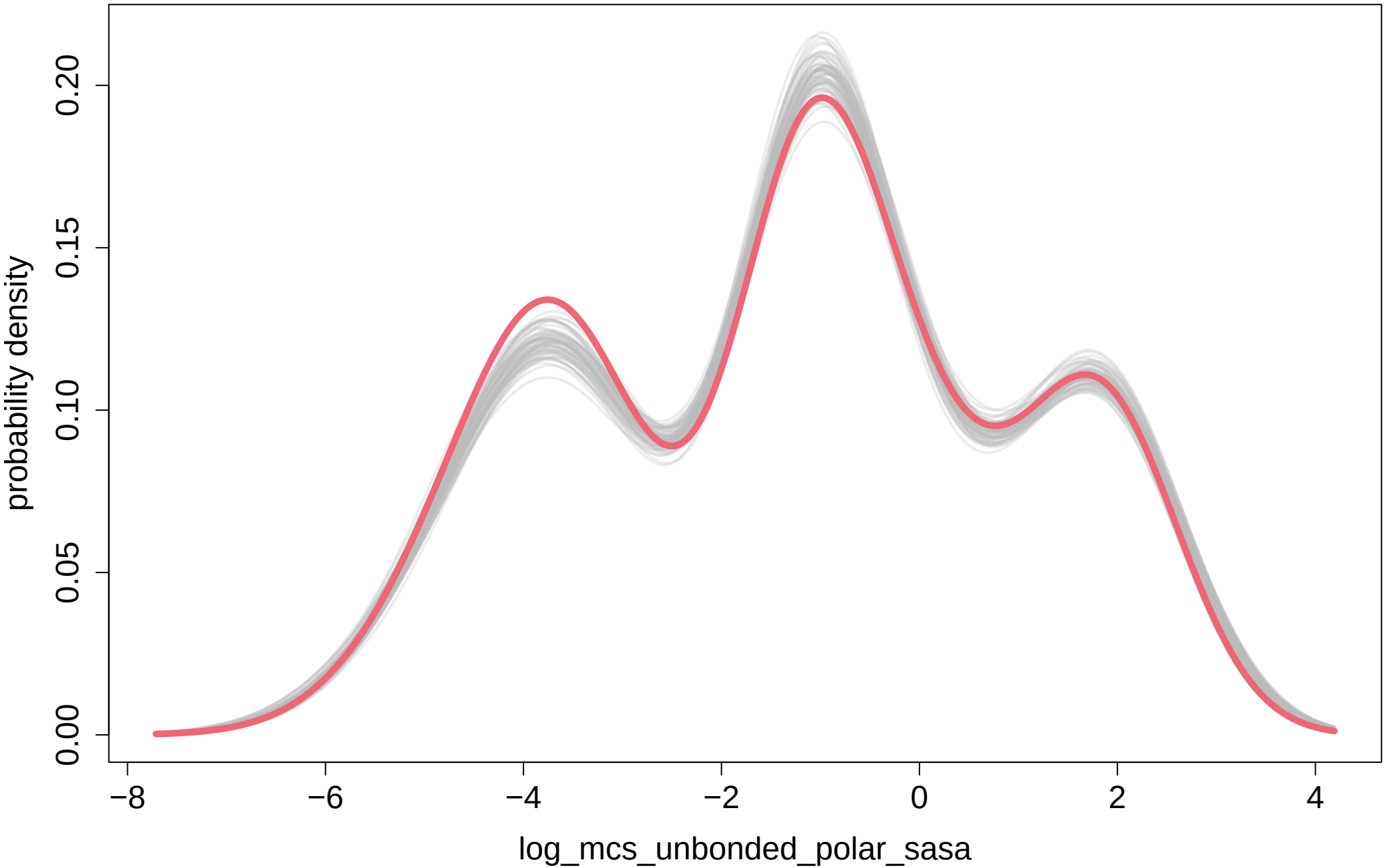
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.228831786348289
max MCSE = 7.20003635342419
all stationary: FALSE
burn: 0
max rel.err.: 1.32478256433726

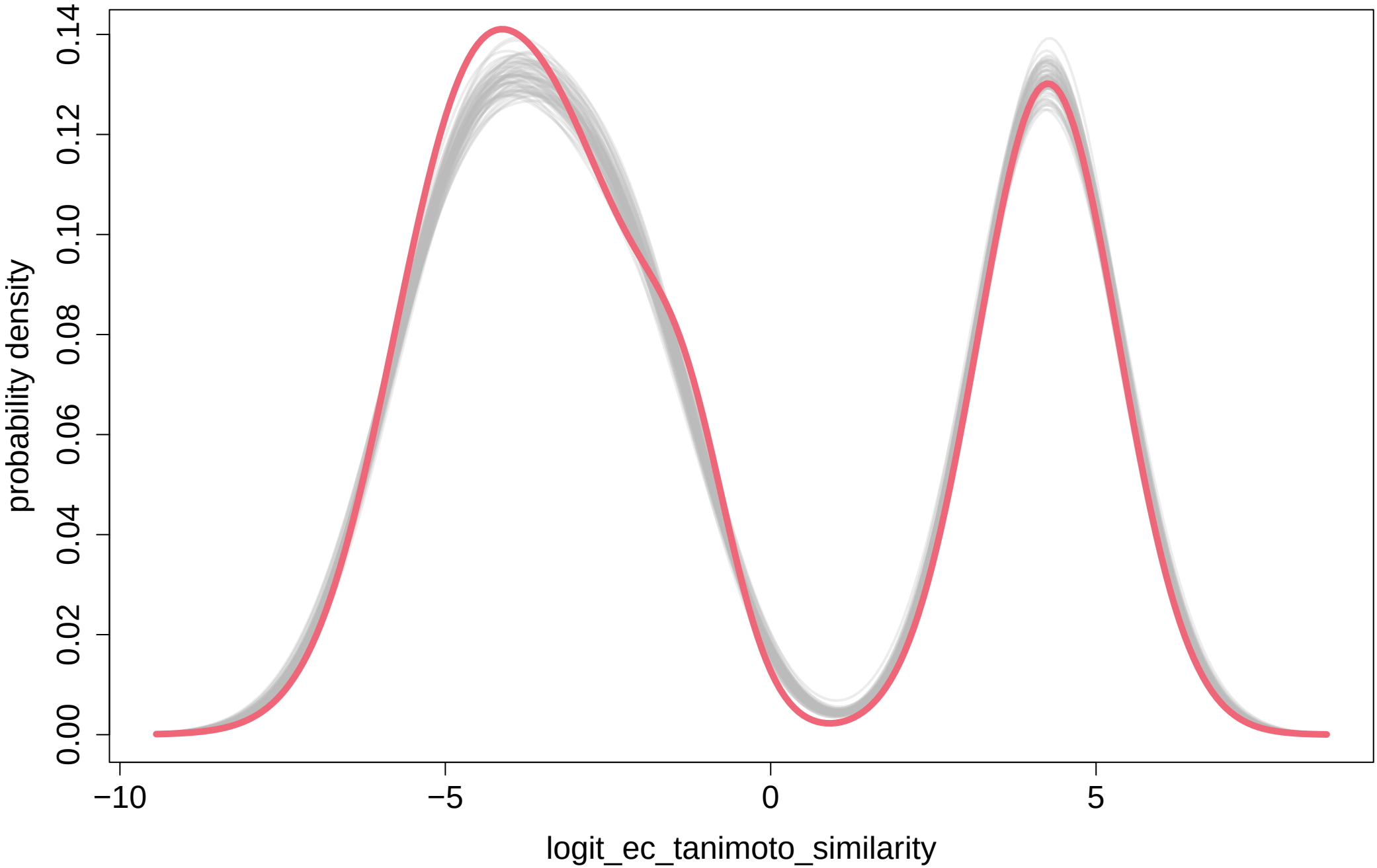
−− STATS 2D −−
min ESS = 855.901029925204
max BMK = 0.077566144009065
max MCSE = 3.83867973386277
all stationary: TRUE
burn: 0
max rel.err.: 2.16154353607516

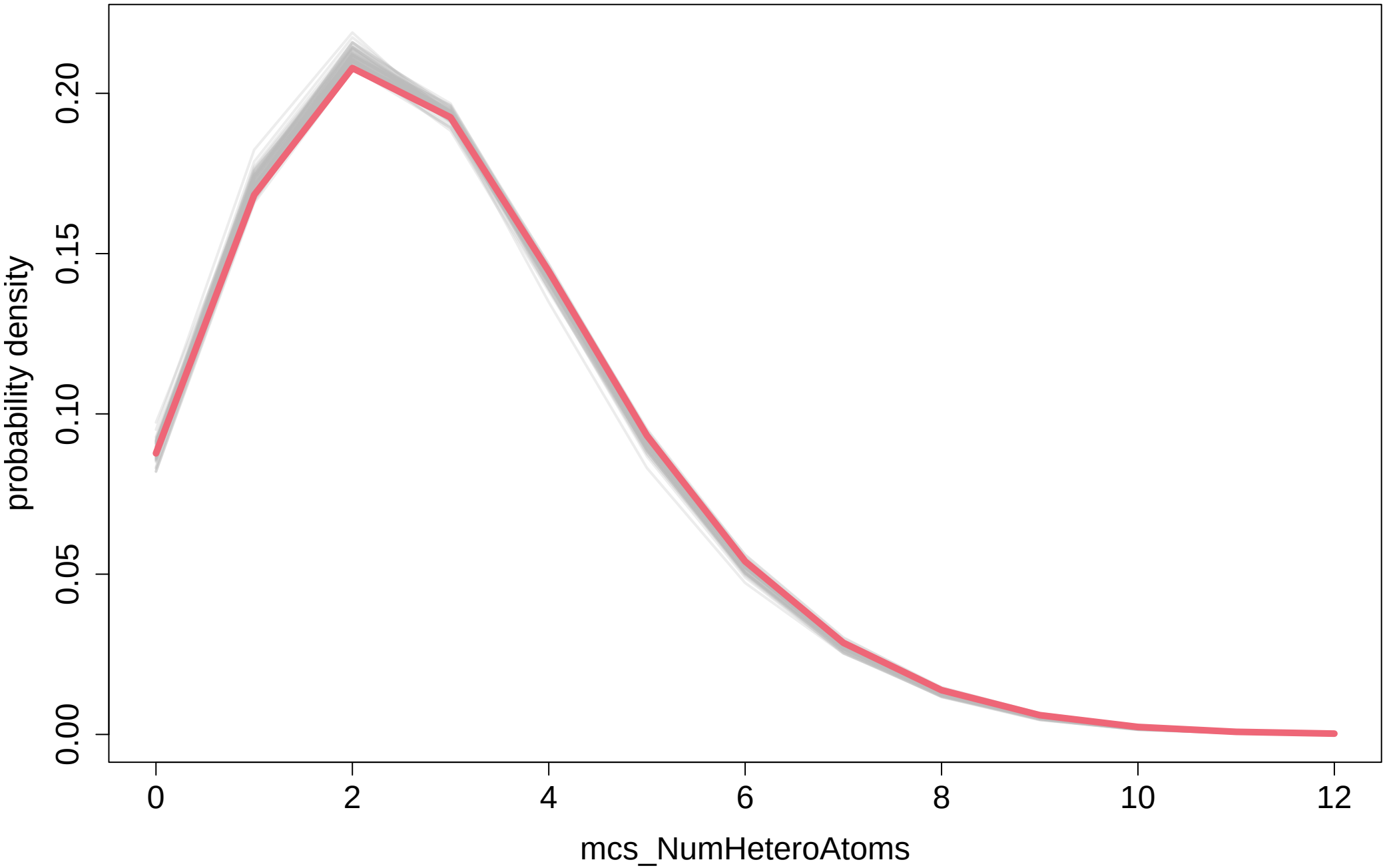
−− STATS 1D −−
min ESS = 26.7239528830038
max BMK = 0.272650816878395
max MCSE = 8.51273555989701
all stationary: FALSE
burn: 0
max rel.err.: 2.68437850589777

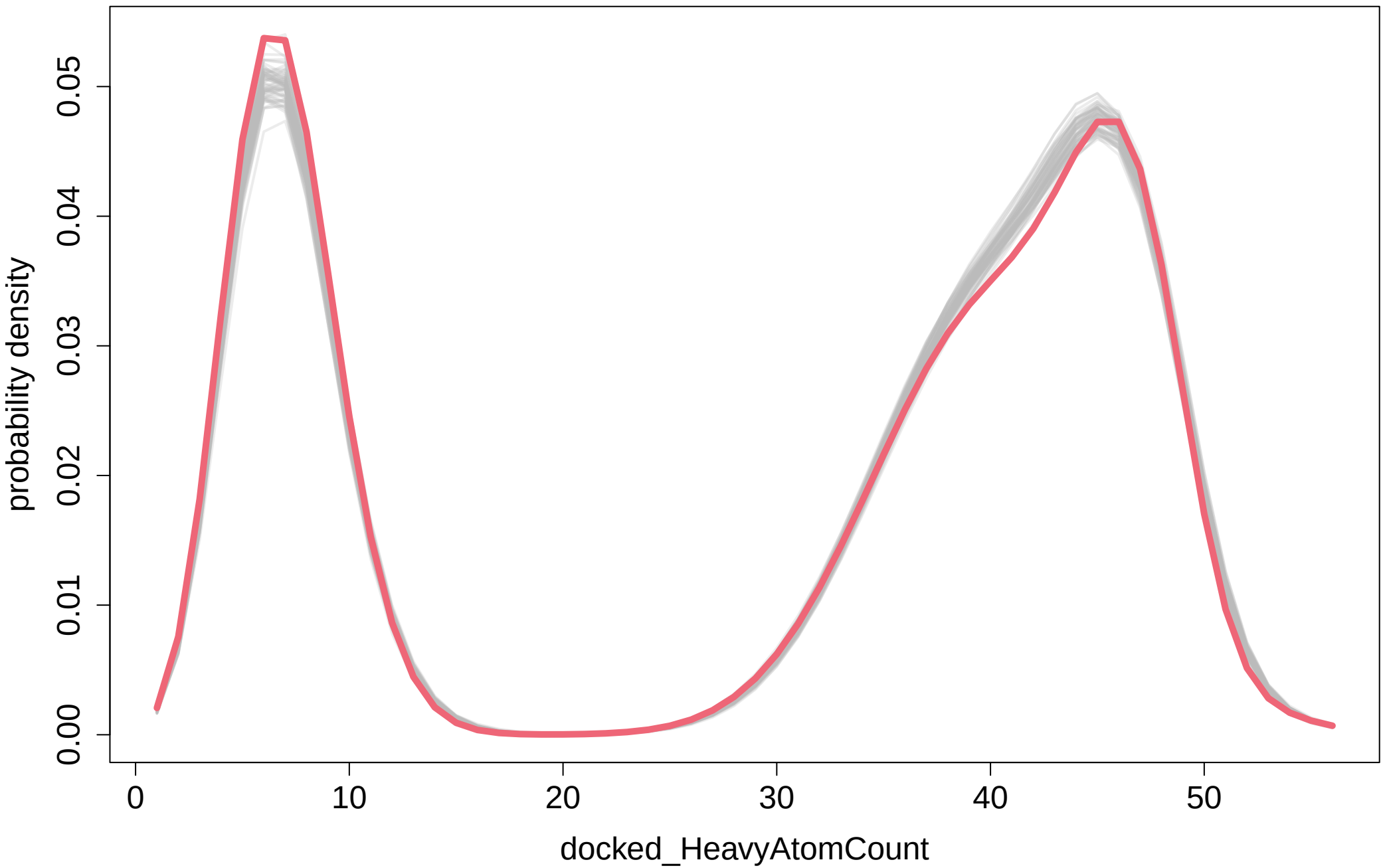
Occupied clusters: 8 of 64
LL: −62500 +− 13.4

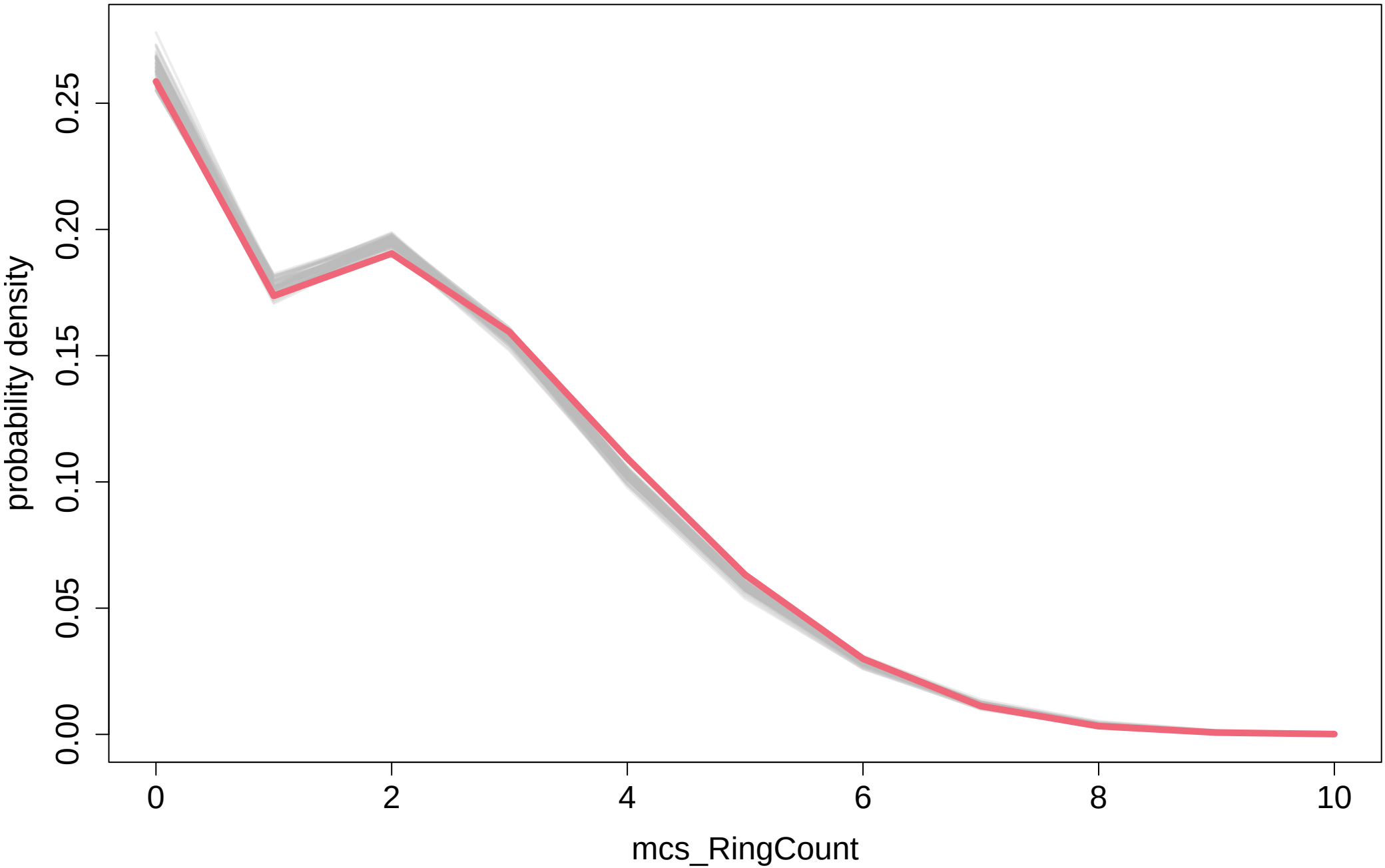

probability density
0.00
0.05
0.10
0.15
0.20
0.25
−2
0
2
4
log_RMSD

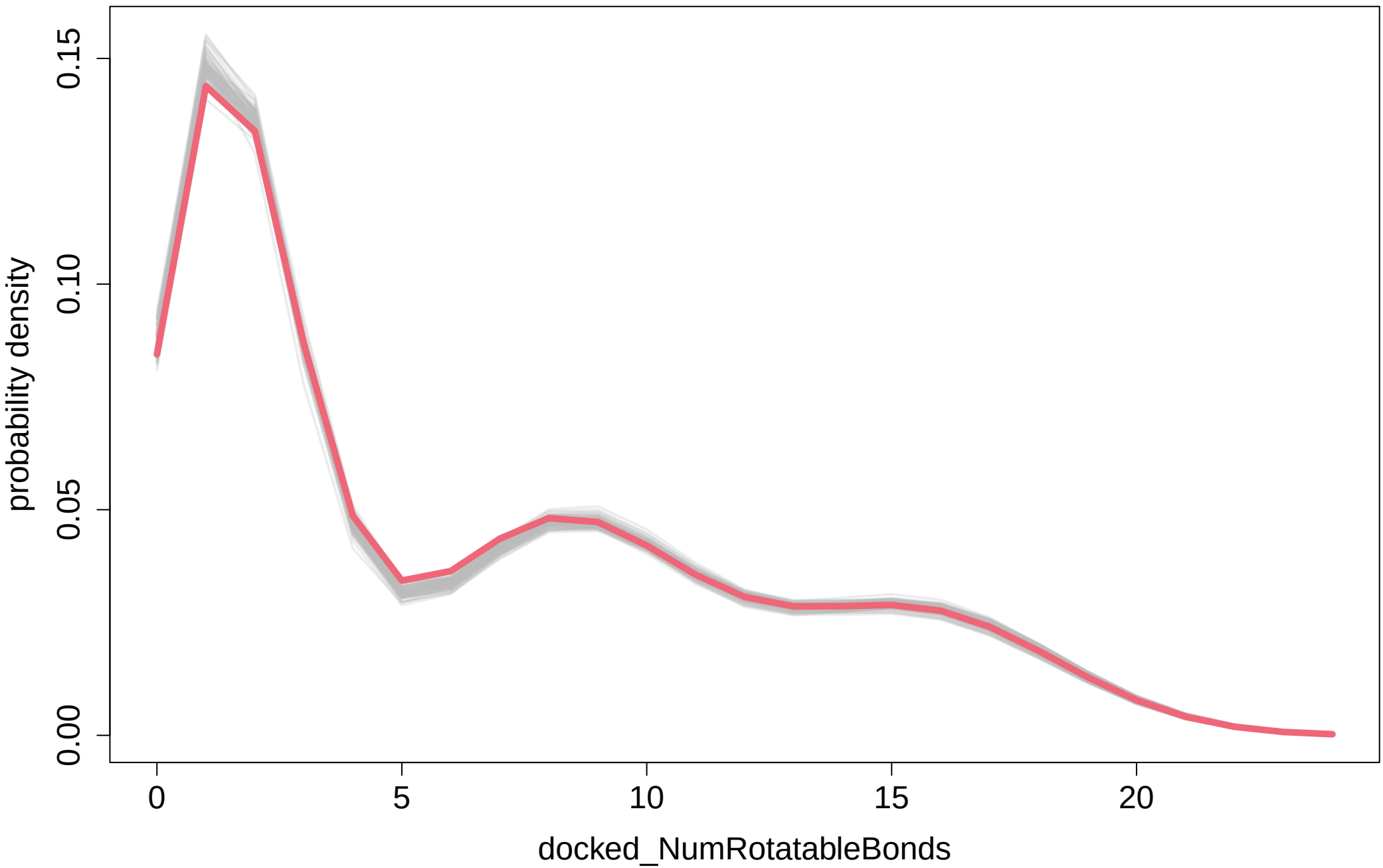

probability density
0.00
0.05
0.10
0.15
0.20
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

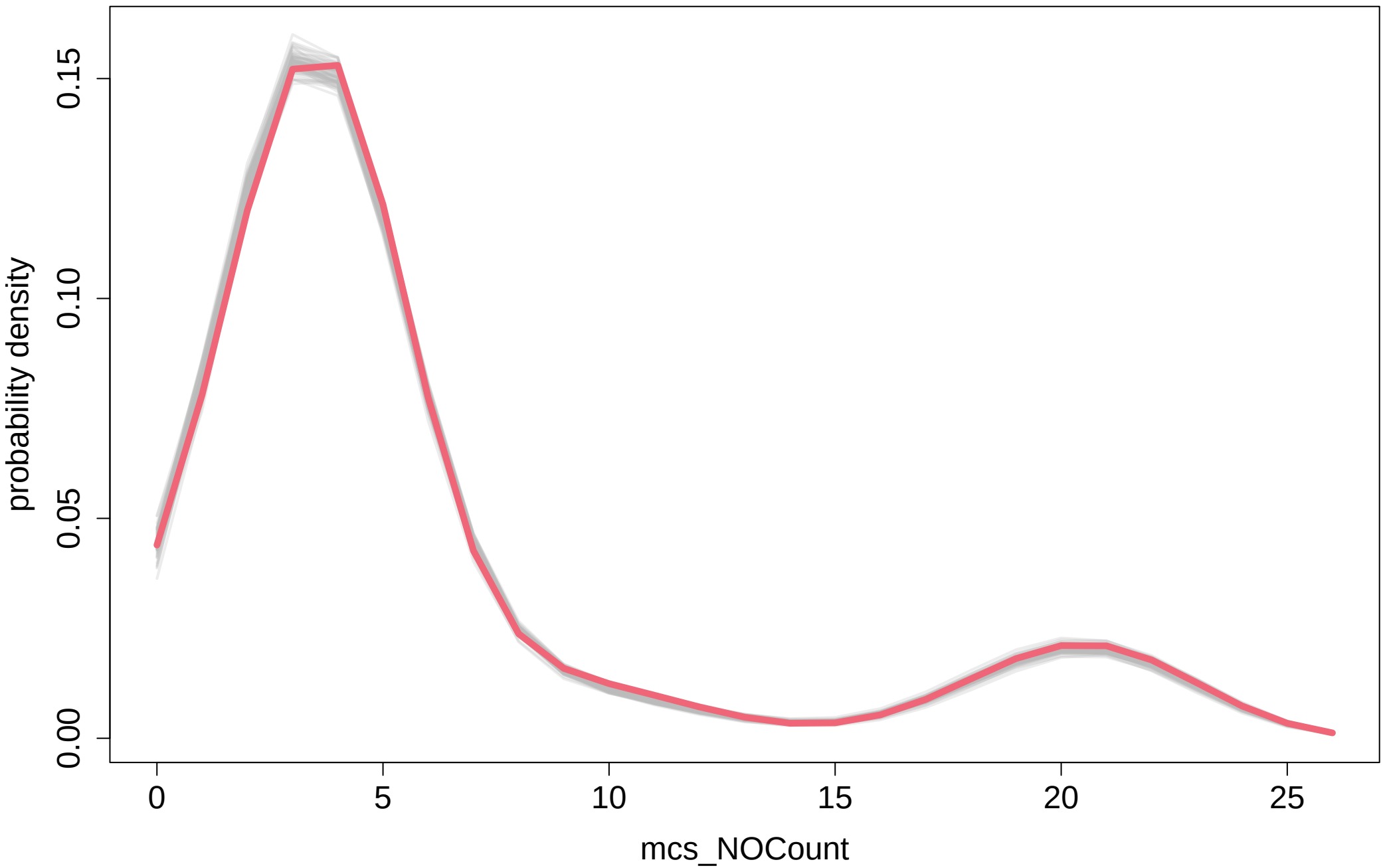

probability density
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
−10
−5
0
5
logit_ec_tanimoto_similarity

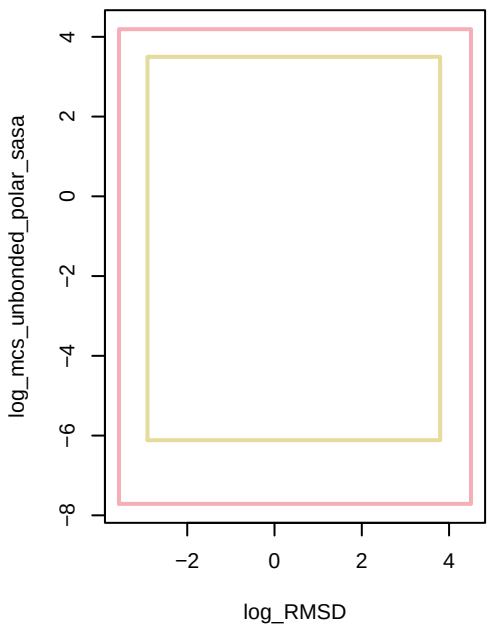

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms

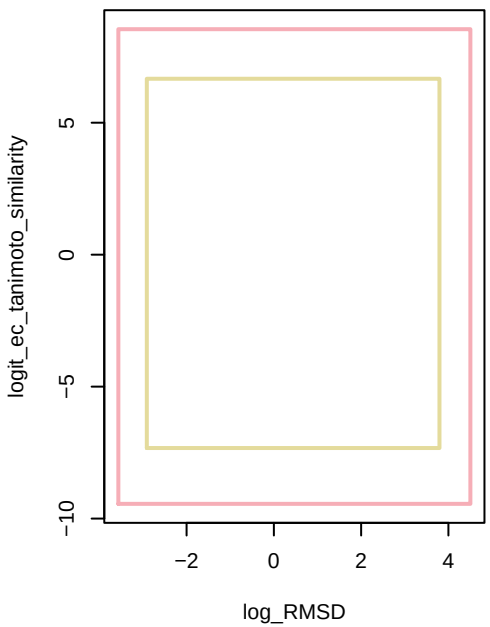

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount

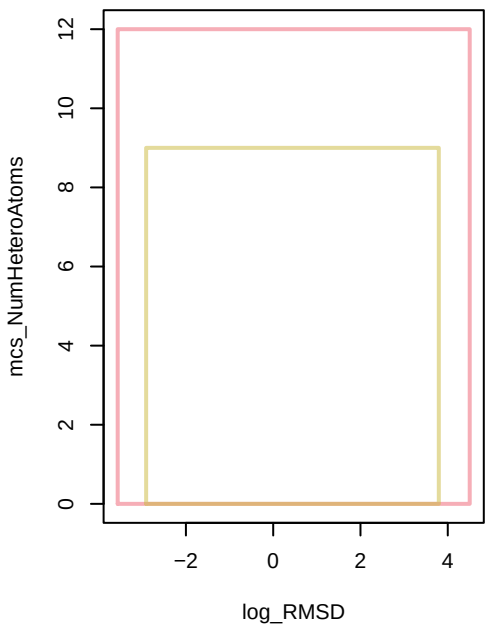

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount

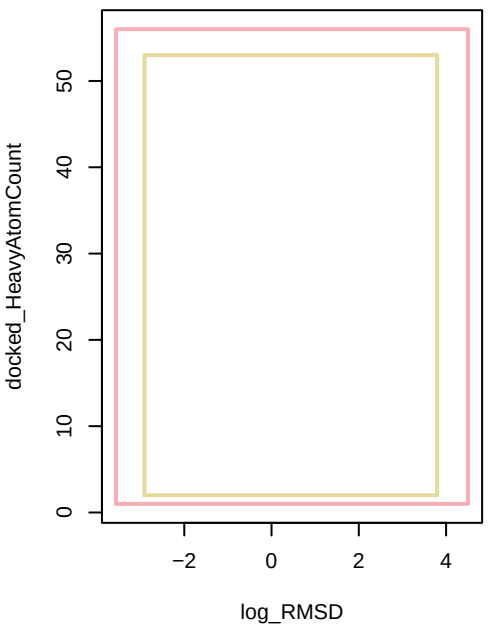

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
docked_NumRotatableBonds

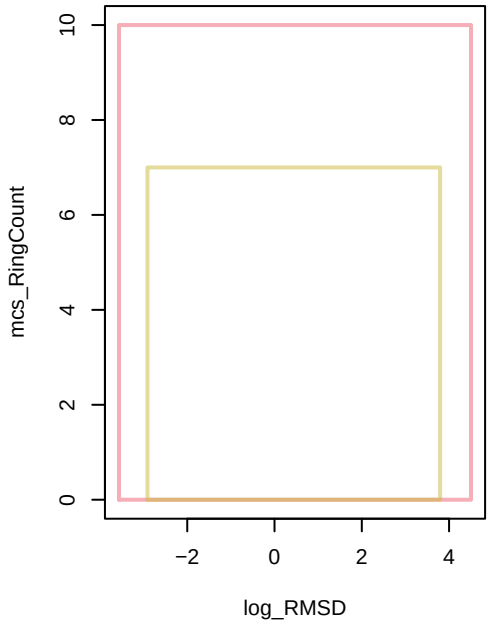

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

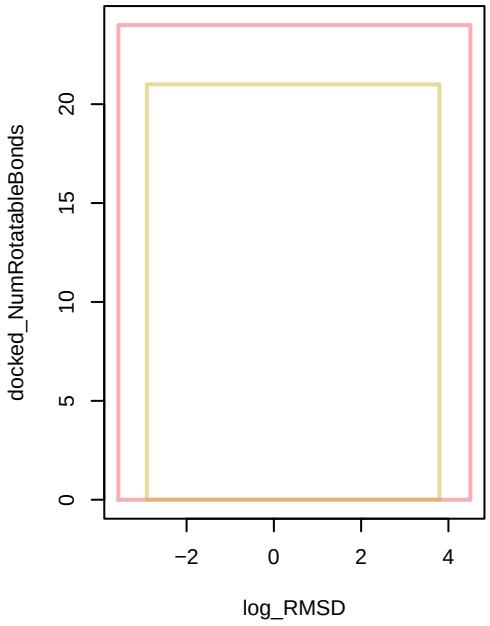

log_mcs_unbonded_polar_sasa
log_RMSD

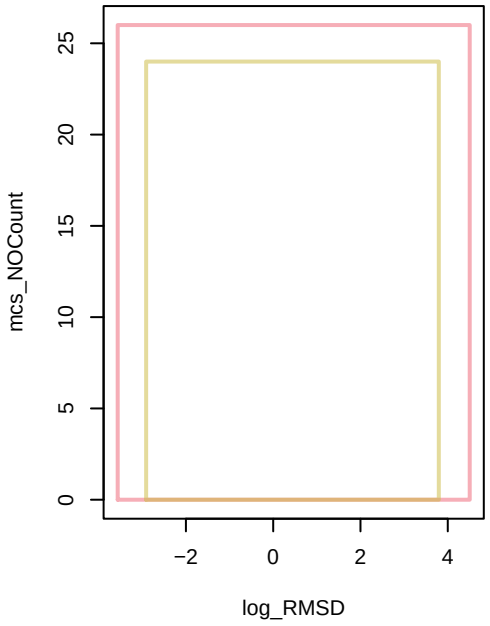

logit_ec_tanimoto_similarity
log_RMSD

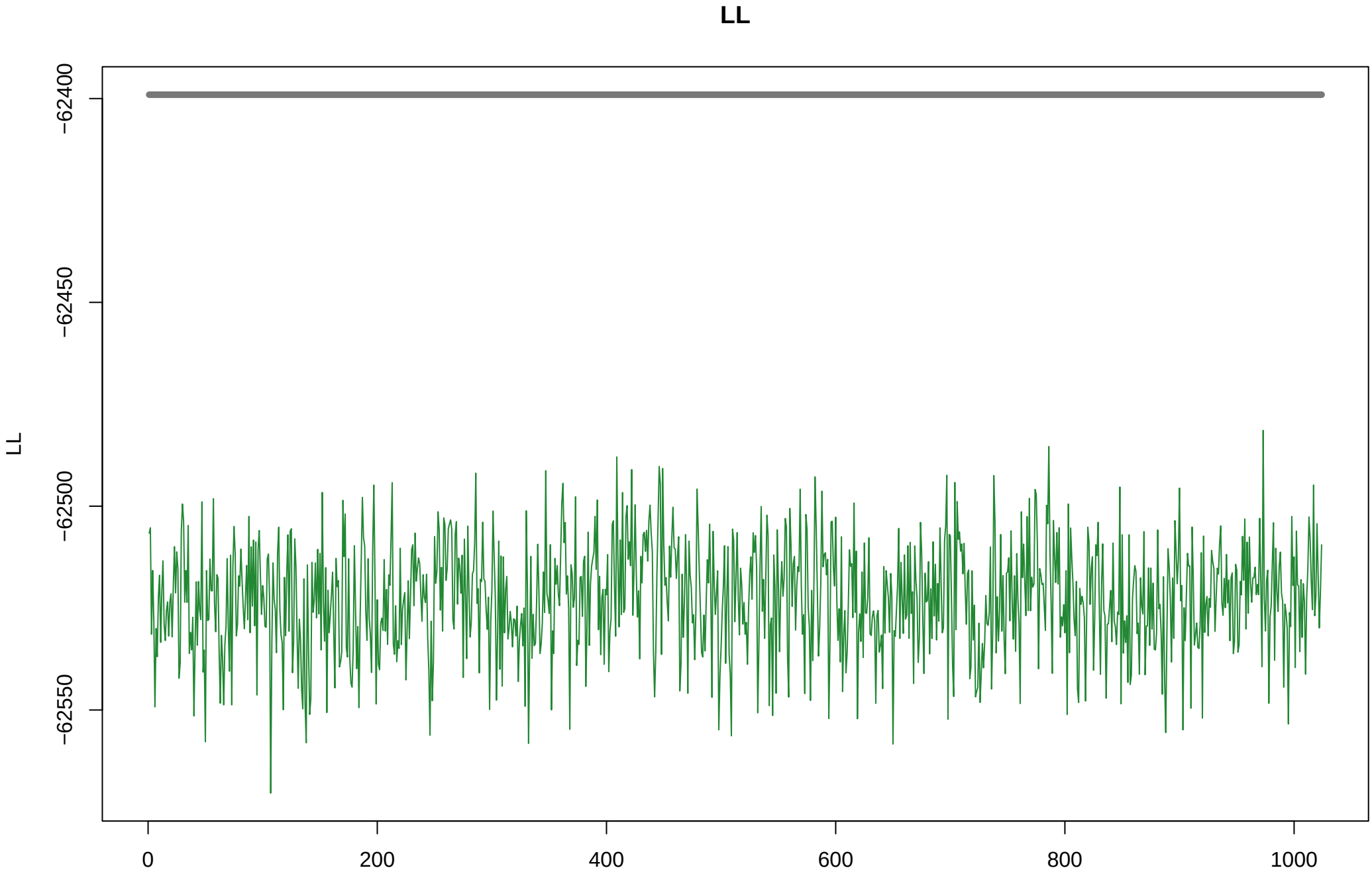

mcs_NumHeteroAtoms
log_RMSD

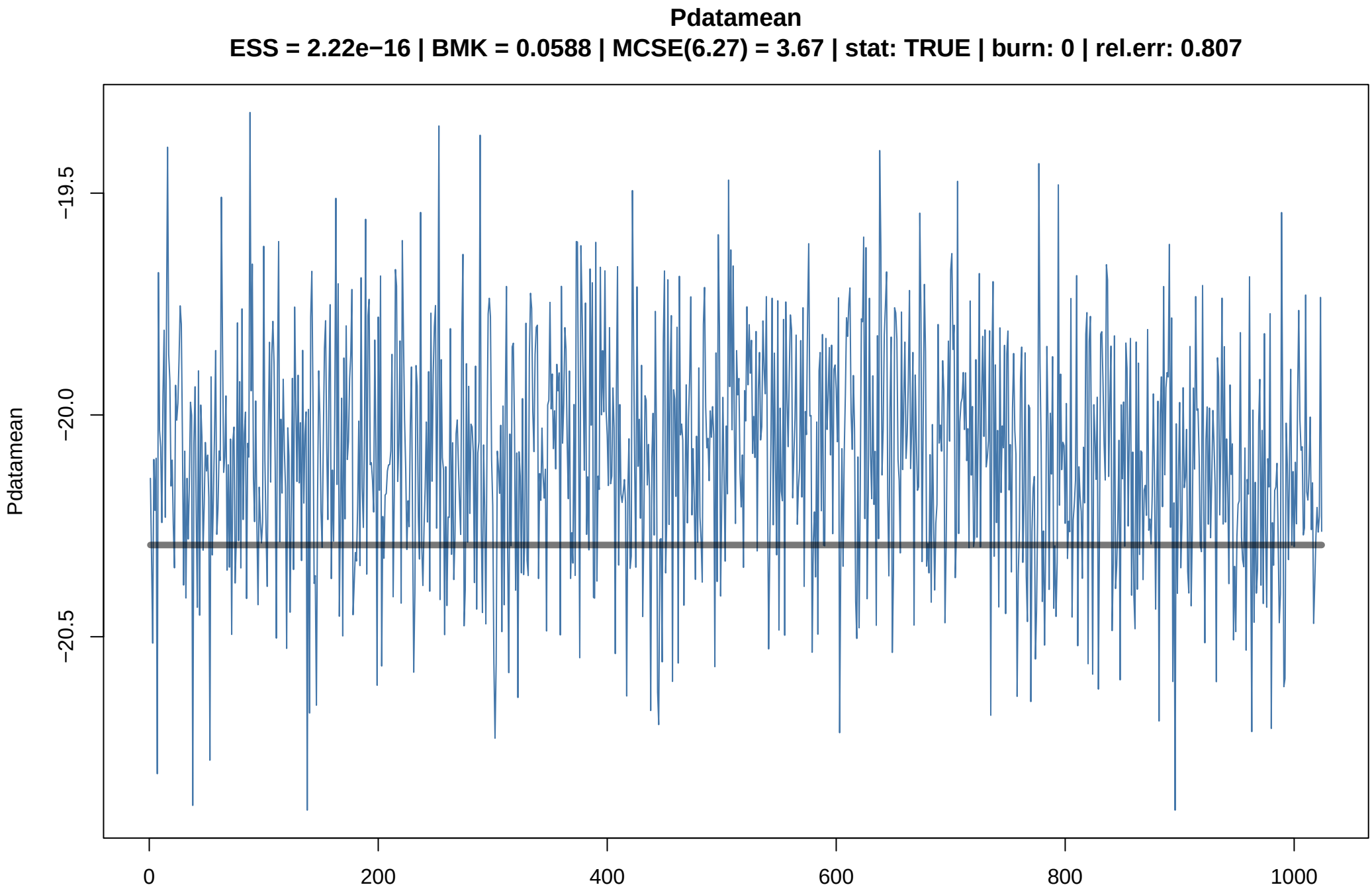

docked_HeavyAtomCount
log_RMSD

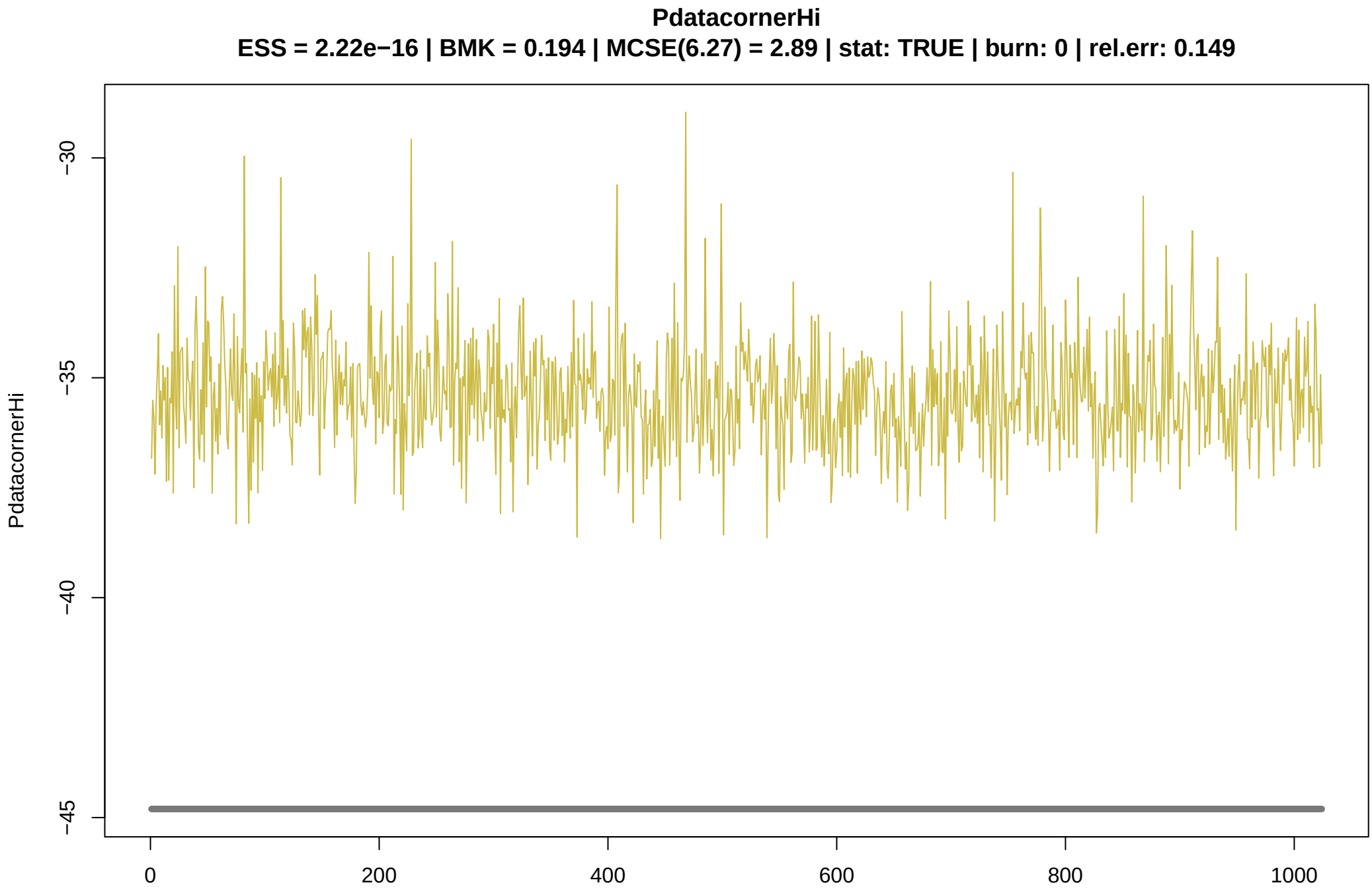

mcs_RingCount
log_RMSD

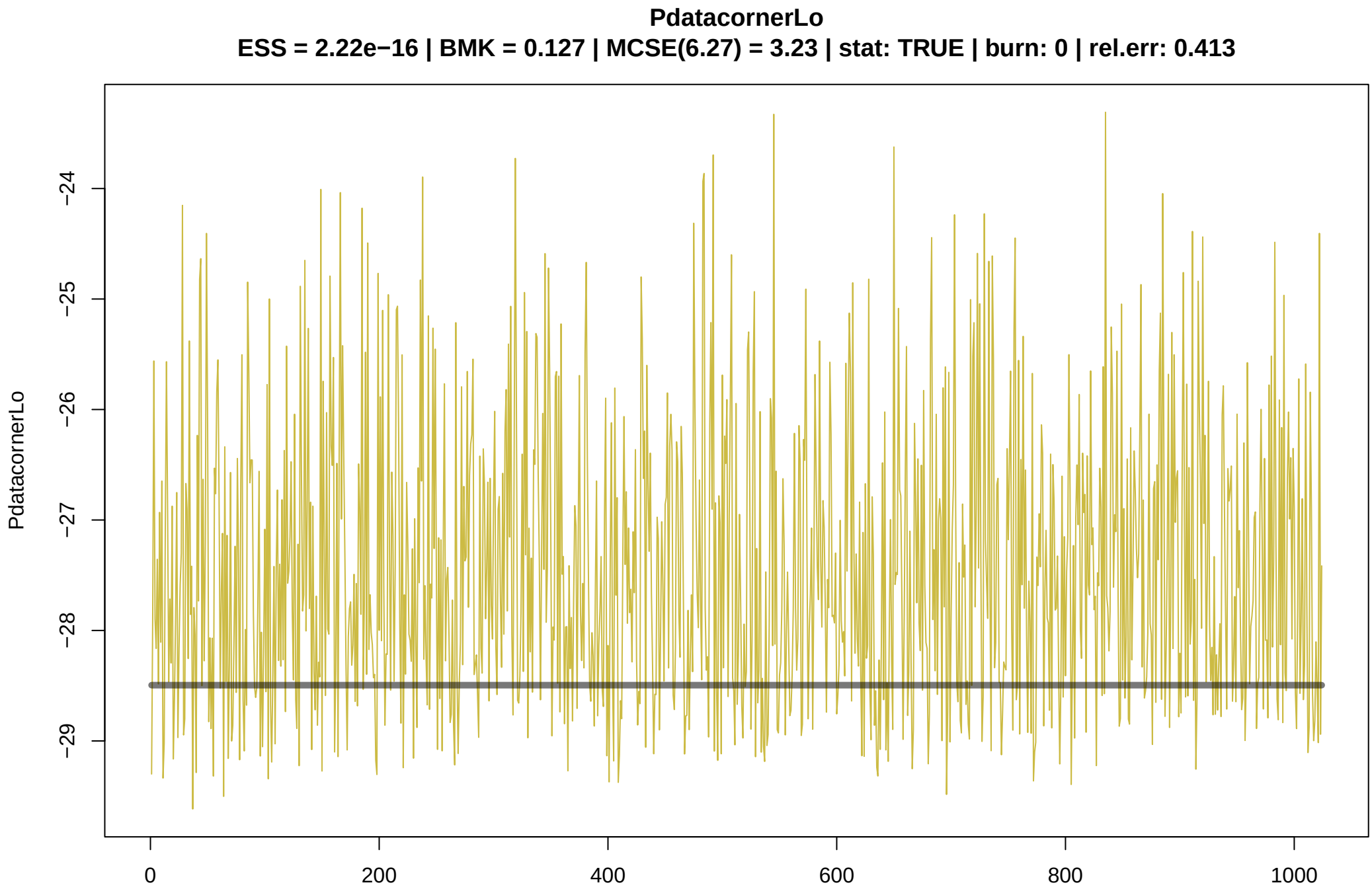

docked_NumRotatableBonds
log_RMSD

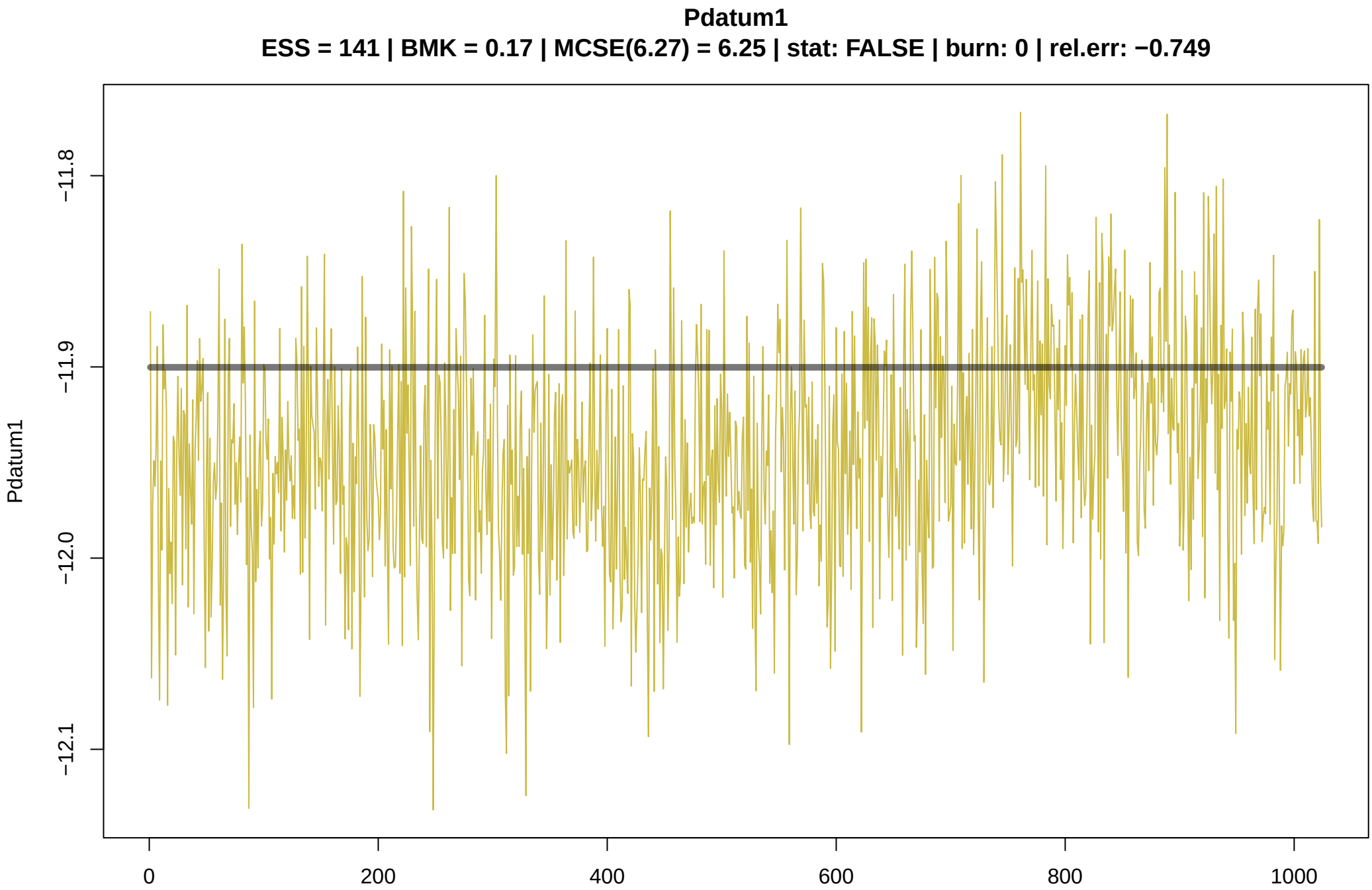

mcs_NOCount
log_RMSD

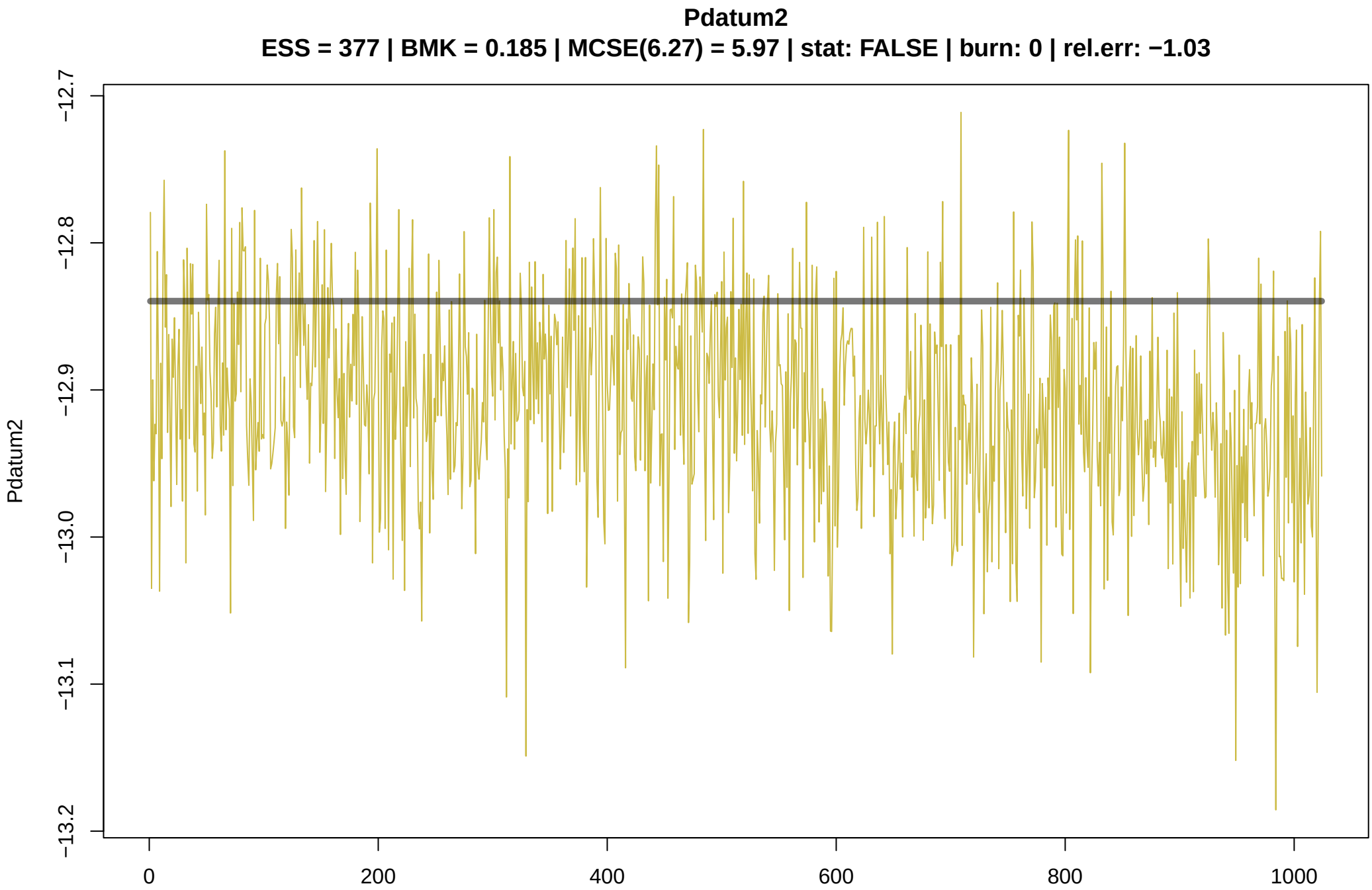

LL
LL
−62400
−62450
−62500
−62550
0
200
400
600
800
1000

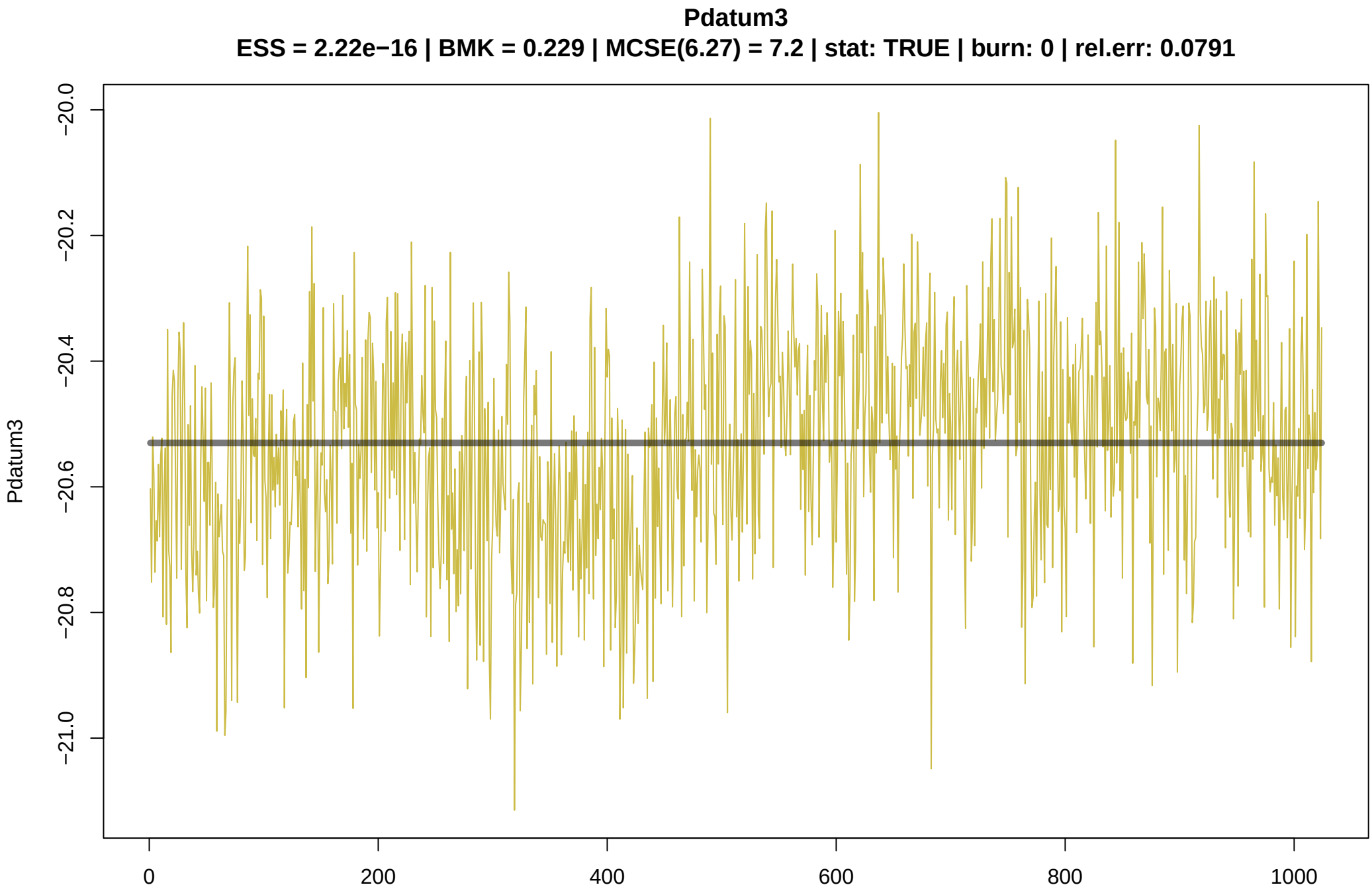

Pdatamean
ESS = 2.22e−16 | BMK = 0.0588 | MCSE(6.27) = 3.67 | stat: TRUE | burn: 0 | rel.err: 0.807
Pdatamean
−19.5
−20.0
−20.5
0
200
400
600
800
1000

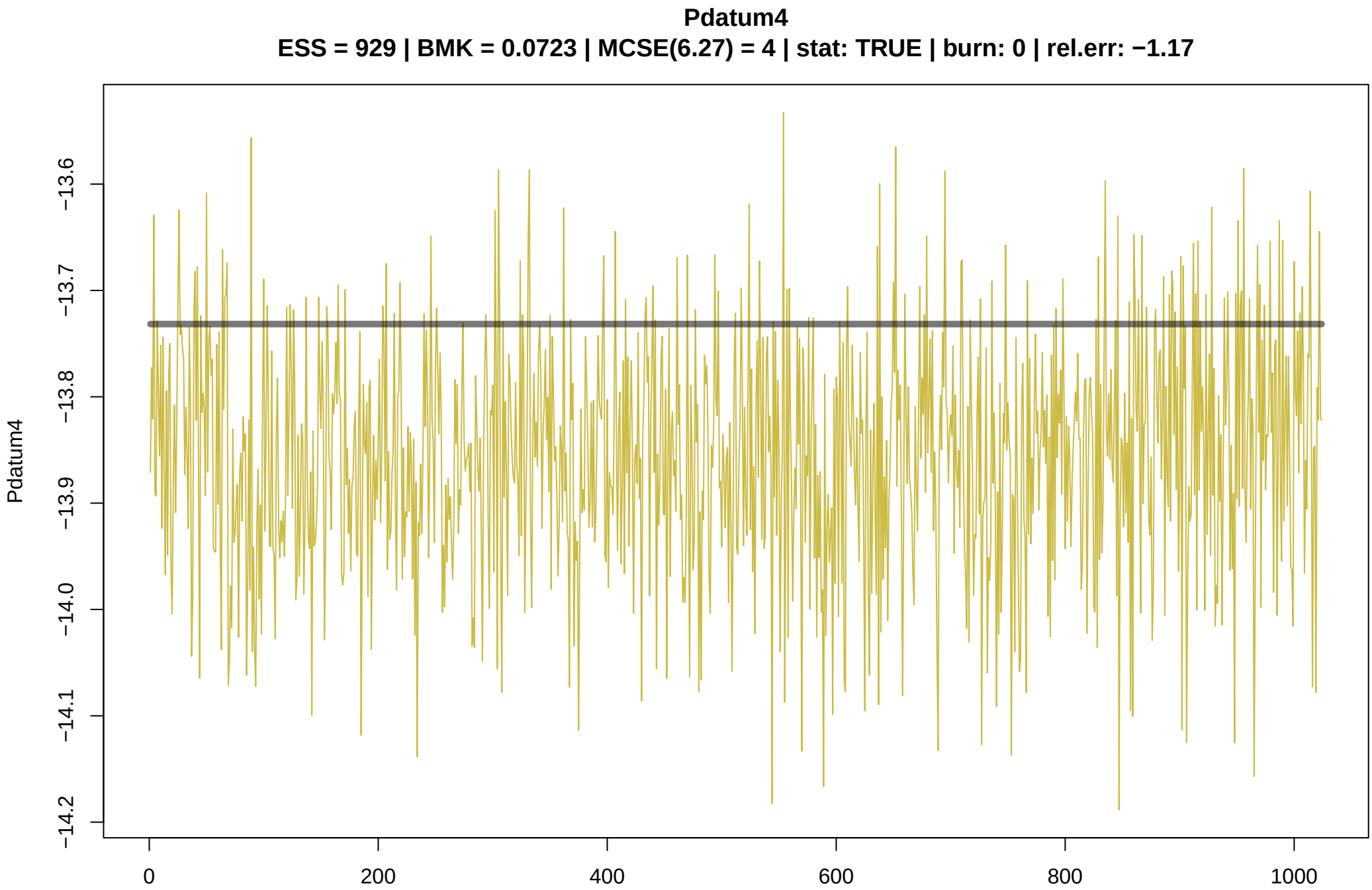

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.194 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | rel.err: 0.149
PdatacornerHi
−30
−35
−40
−45
0
200
400
600
800
1000

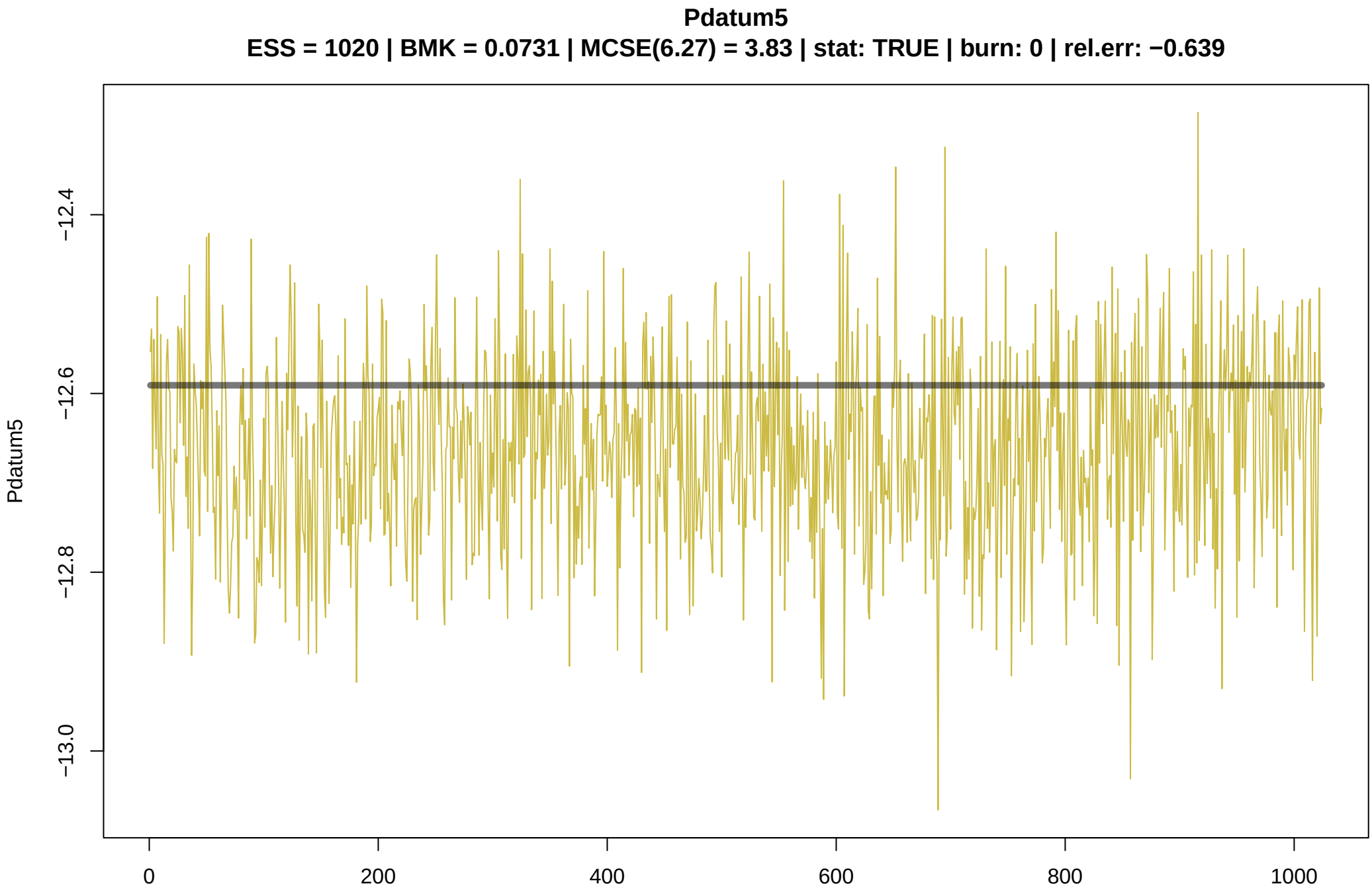

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.127 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | rel.err: 0.413
PdatacornerLo
−24
−25
−26
−27
−28
−29
0
200
400
600
800
1000

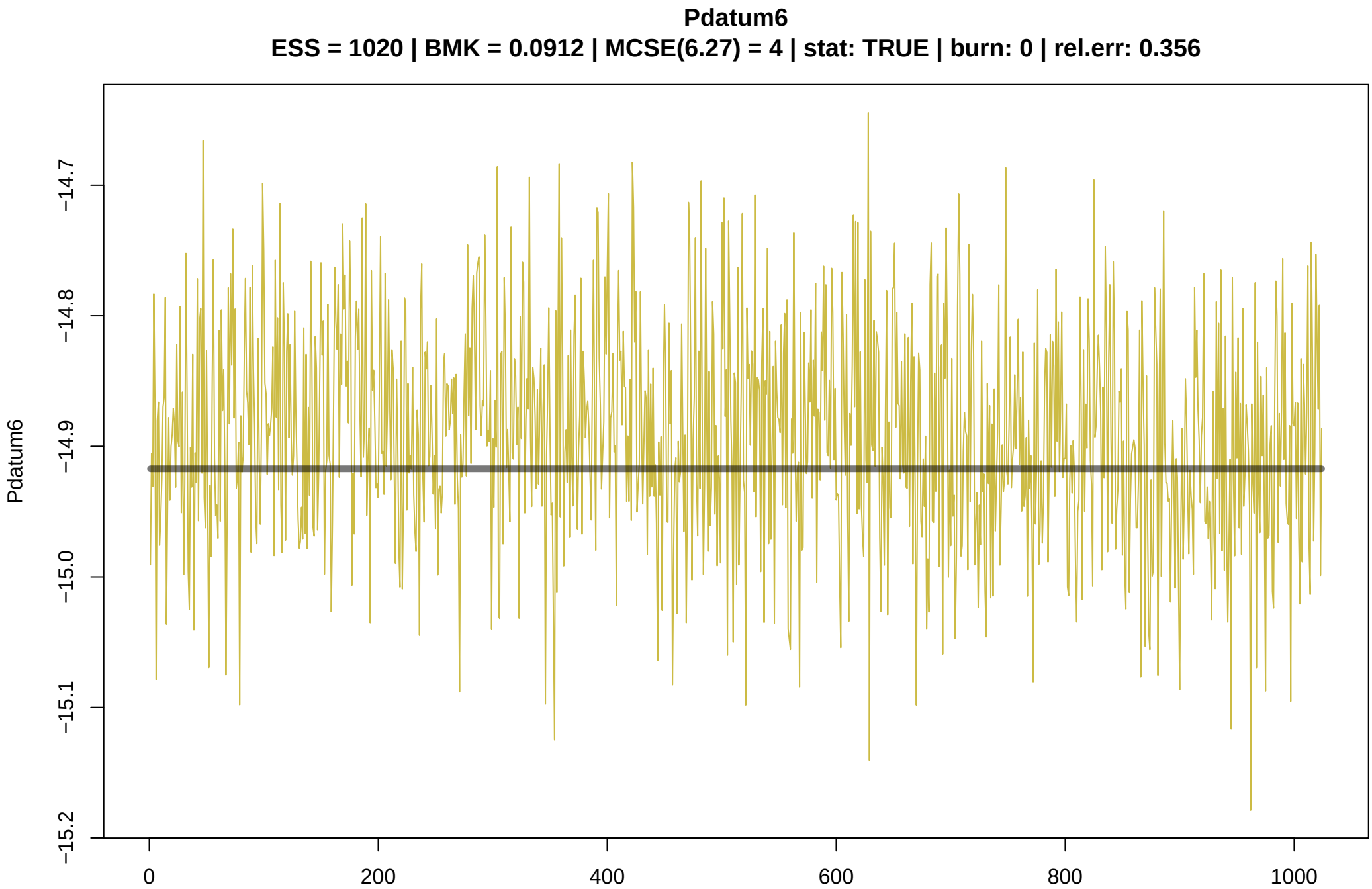

Pdatum1
ESS = 141 | BMK = 0.17 | MCSE(6.27) = 6.25 | stat: FALSE | burn: 0 | rel.err: −0.749
Pdatum1
−11.8
−11.9
−12.0
−12.1
0
200
400
600
800
1000

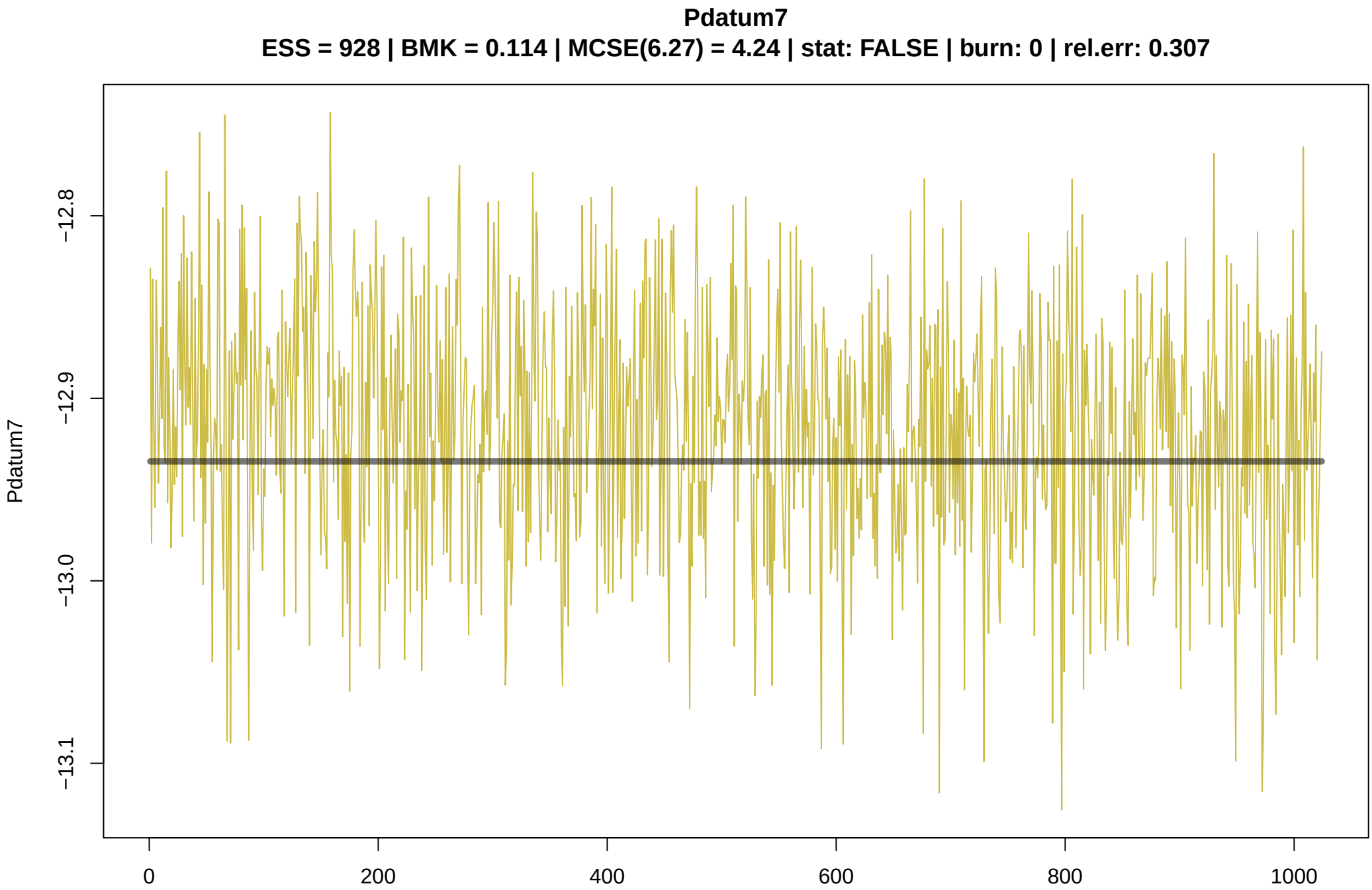

Pdatum2
ESS = 377 | BMK = 0.185 | MCSE(6.27) = 5.97 | stat: FALSE | burn: 0 | rel.err: −1.03
Pdatum2
−12.7
−12.8
−12.9
−13.0
−13.1
−13.2
0
200
400
600
800
1000

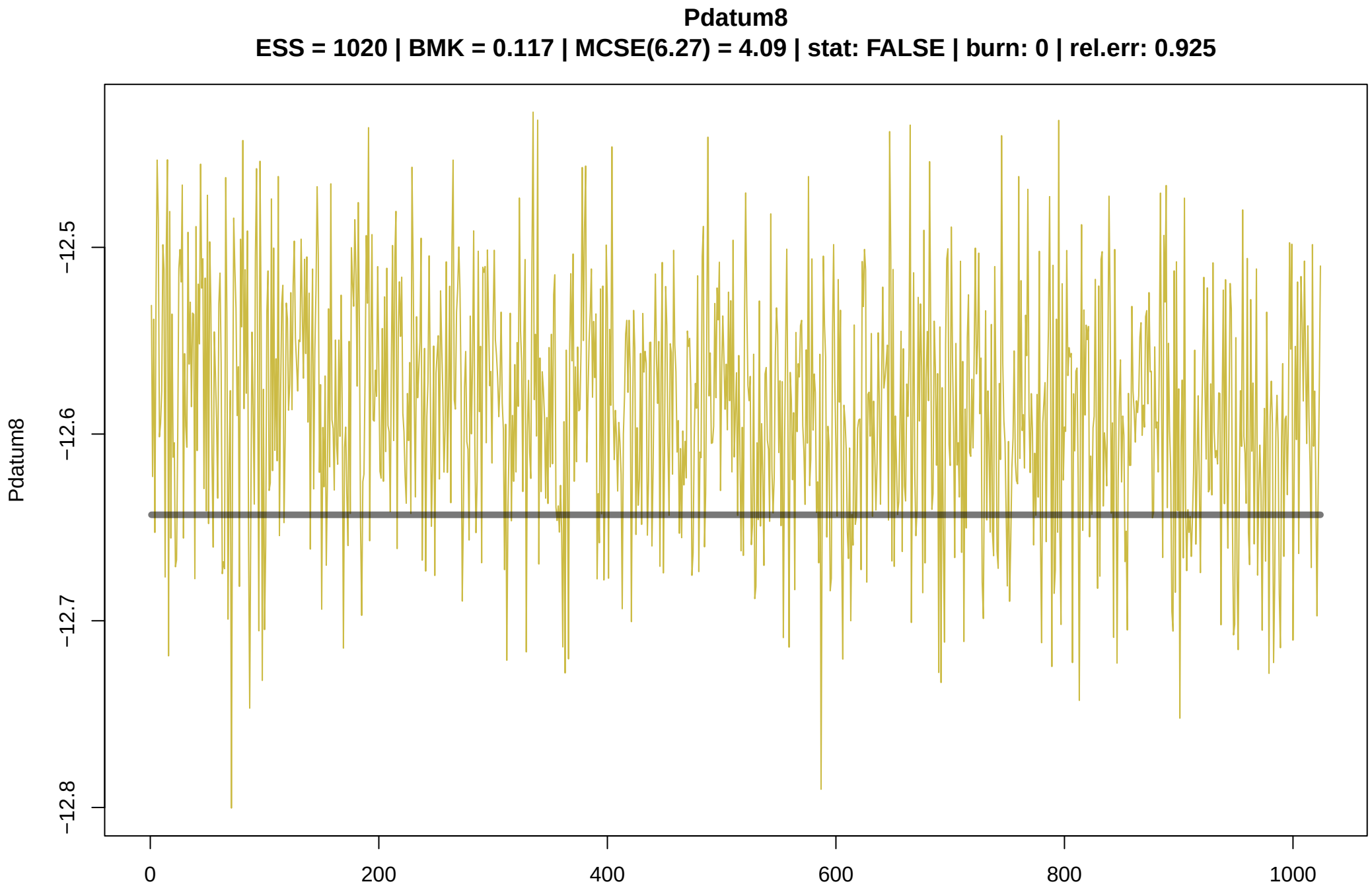

Pdatum3
ESS = 2.22e−16 | BMK = 0.229 | MCSE(6.27) = 7.2 | stat: TRUE | burn: 0 | rel.err: 0.0791
Pdatum3
−20.0
−20.2
−20.4
−20.6
−20.8
−21.0
0
200
400
600
800
1000

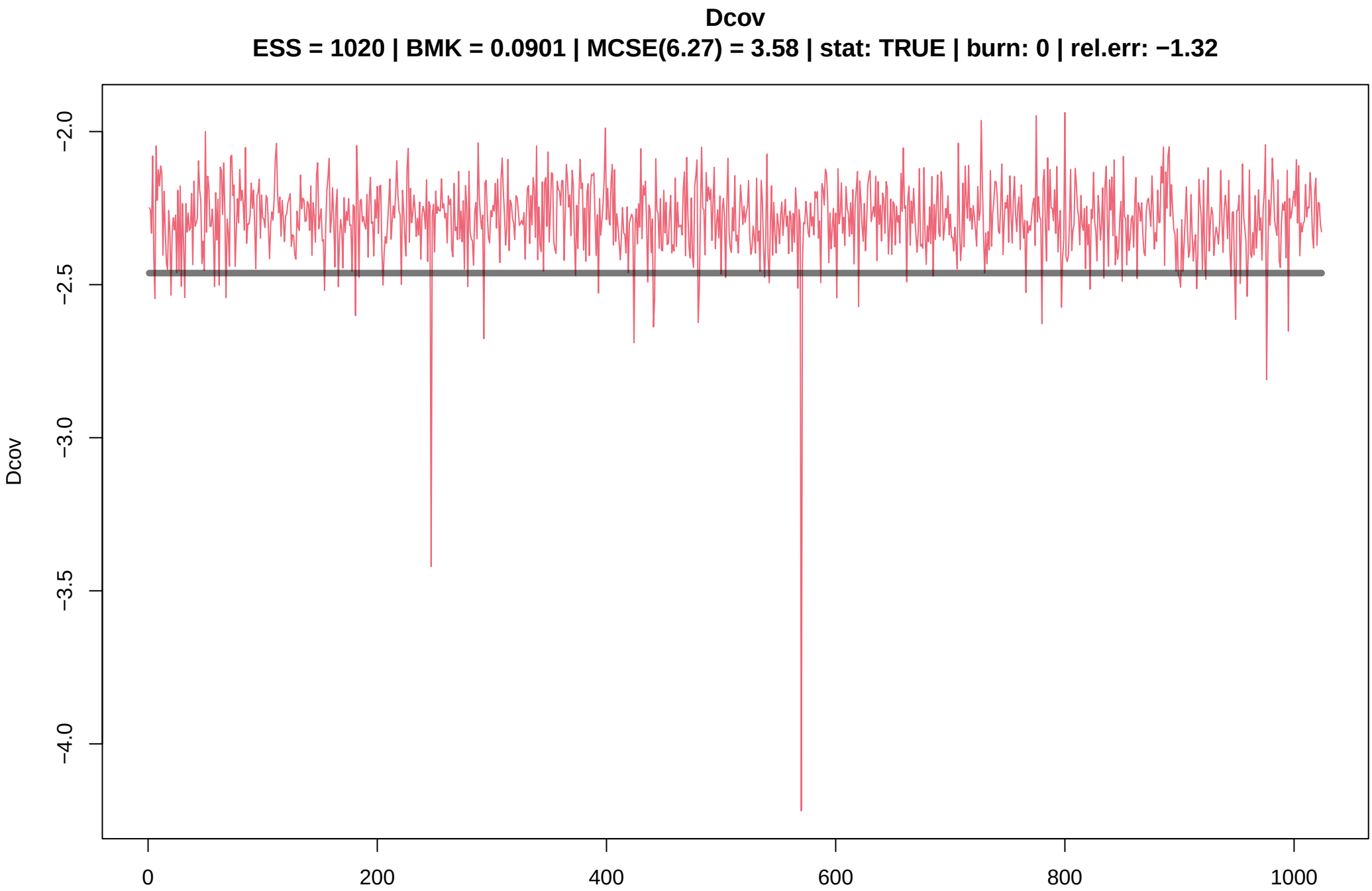

Pdatum4
ESS = 929 | BMK = 0.0723 | MCSE(6.27) = 4 | stat: TRUE | burn: 0 | rel.err: −1.17
Pdatum4
−13.6
−13.7
−13.8
−13.9
−14.0
−14.1
−14.2
0
200
400
600
800
1000

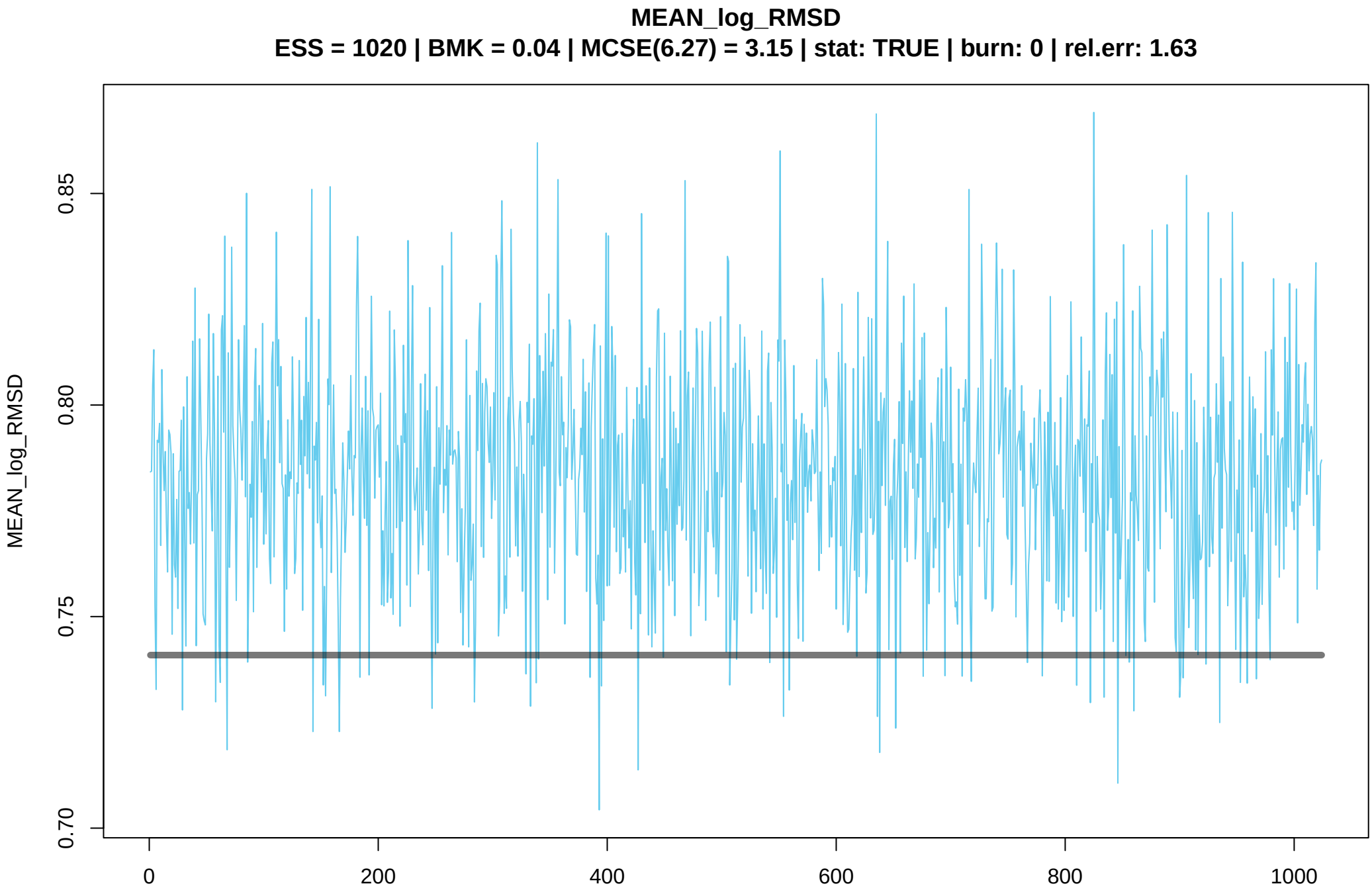

Pdatum5
ESS = 1020 | BMK = 0.0731 | MCSE(6.27) = 3.83 | stat: TRUE | burn: 0 | rel.err: −0.639
Pdatum5
−12.4
−12.6
−12.8
−13.0
0
200
400
600
800
1000

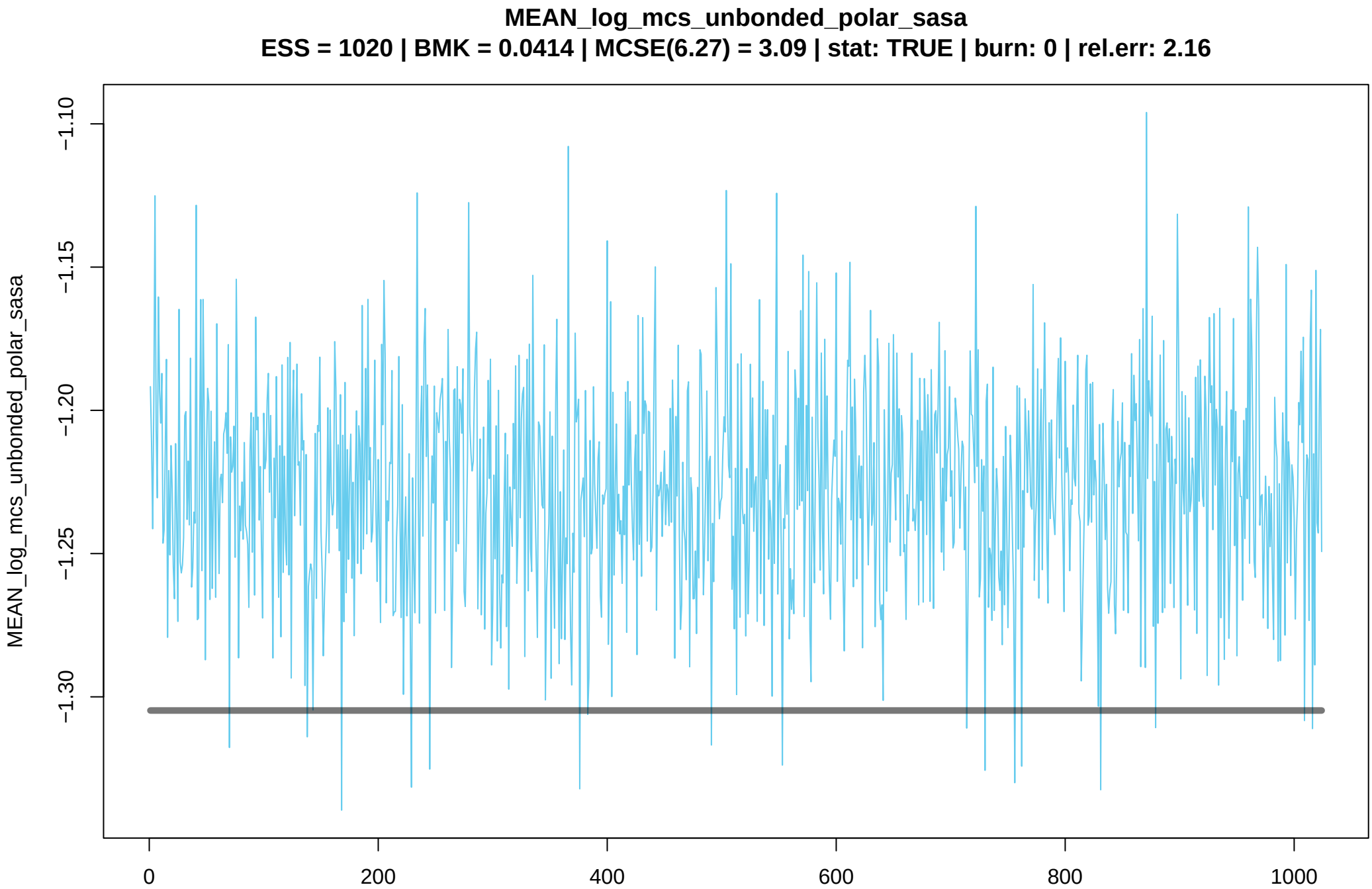

Pdatum6
ESS = 1020 | BMK = 0.0912 | MCSE(6.27) = 4 | stat: TRUE | burn: 0 | rel.err: 0.356
Pdatum6
−14.7
−14.8
−14.9
−15.0
−15.1
−15.2
0
200
400
600
800
1000

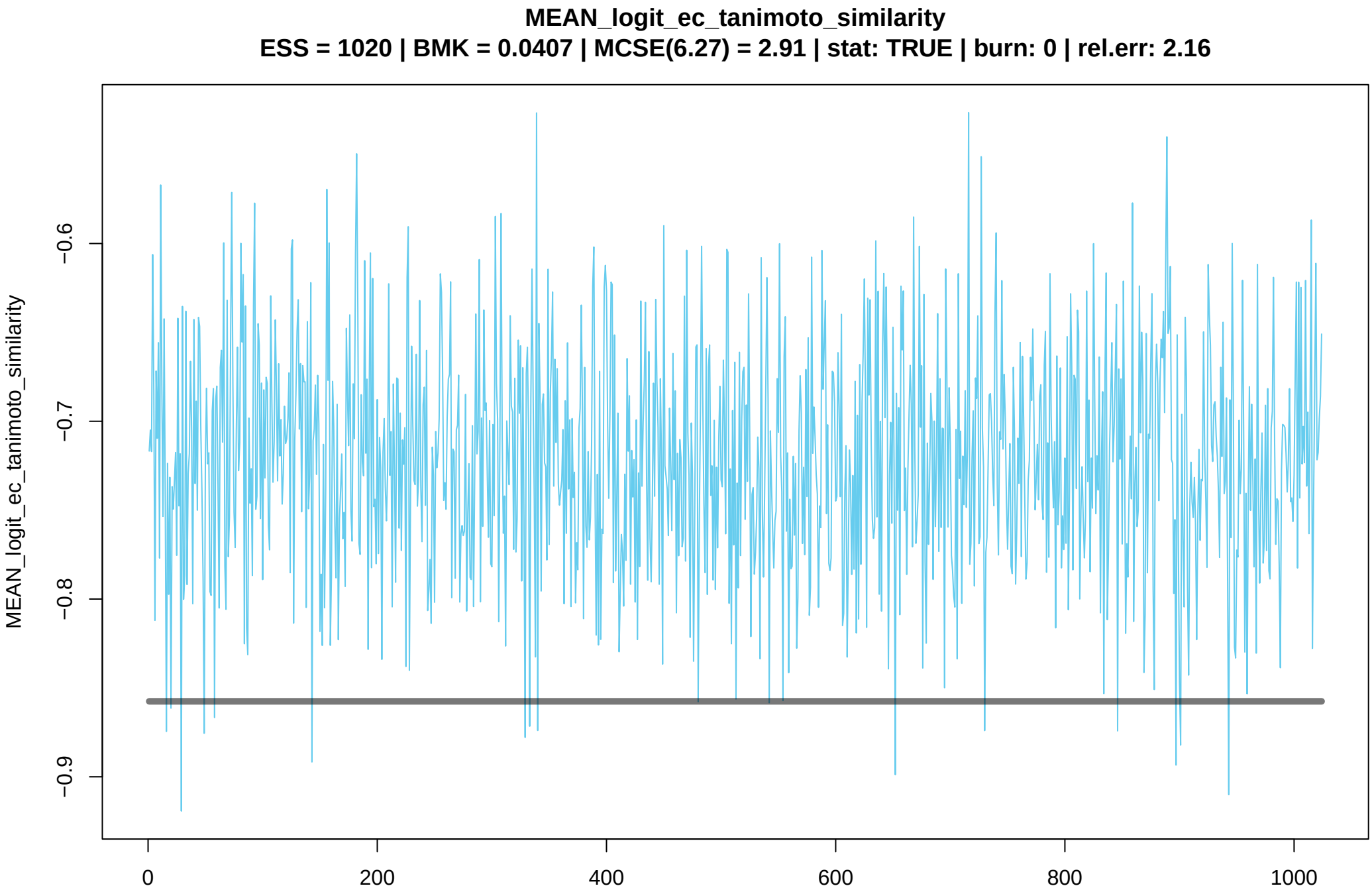

Pdatum7
ESS = 928 | BMK = 0.114 | MCSE(6.27) = 4.24 | stat: FALSE | burn: 0 | rel.err: 0.307
Pdatum7
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

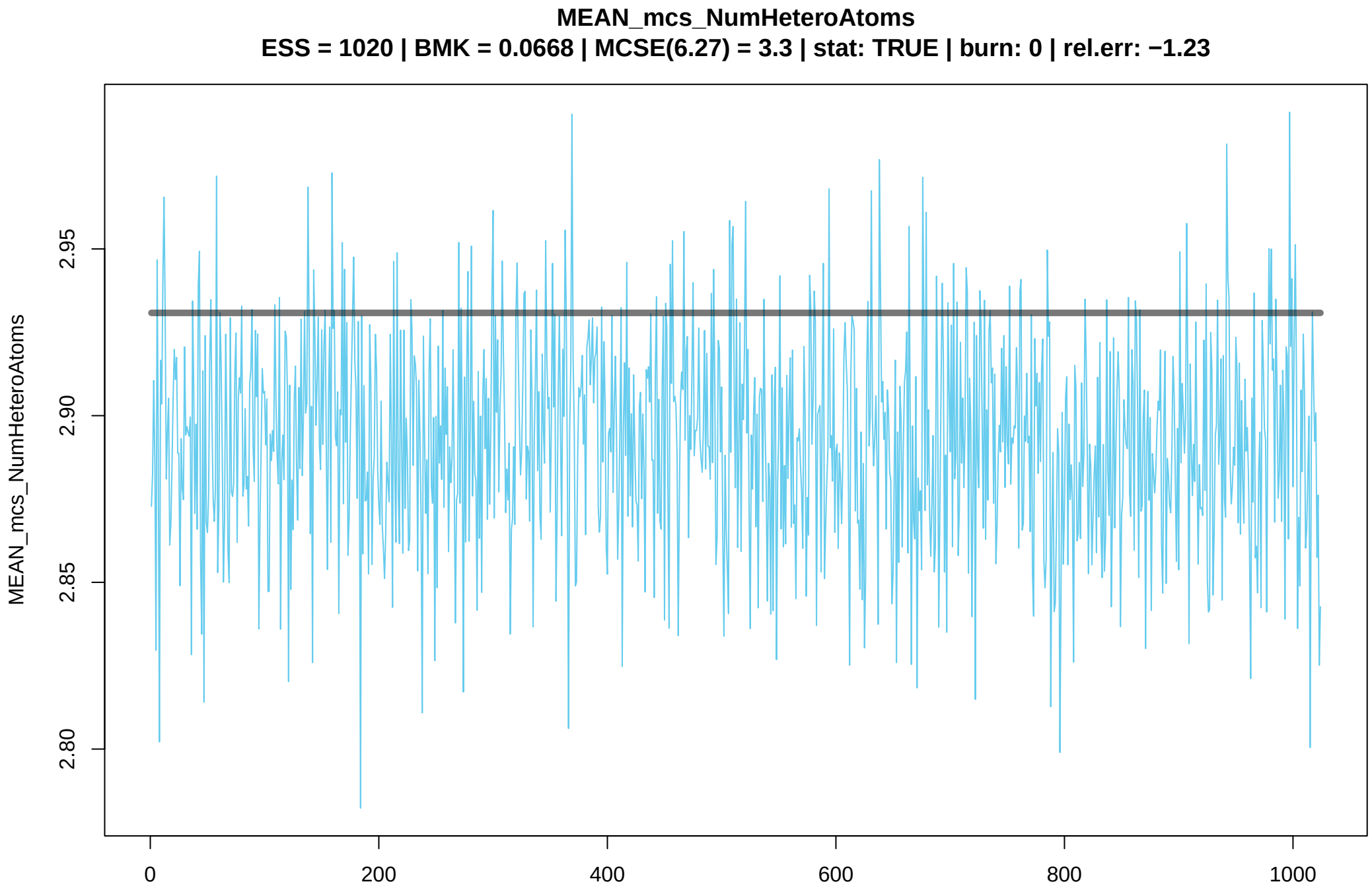

Pdatum8
ESS = 1020 | BMK = 0.117 | MCSE(6.27) = 4.09 | stat: FALSE | burn: 0 | rel.err: 0.925
Pdatum8
−12.5
−12.6
−12.7
−12.8
0
200
400
600
800
1000

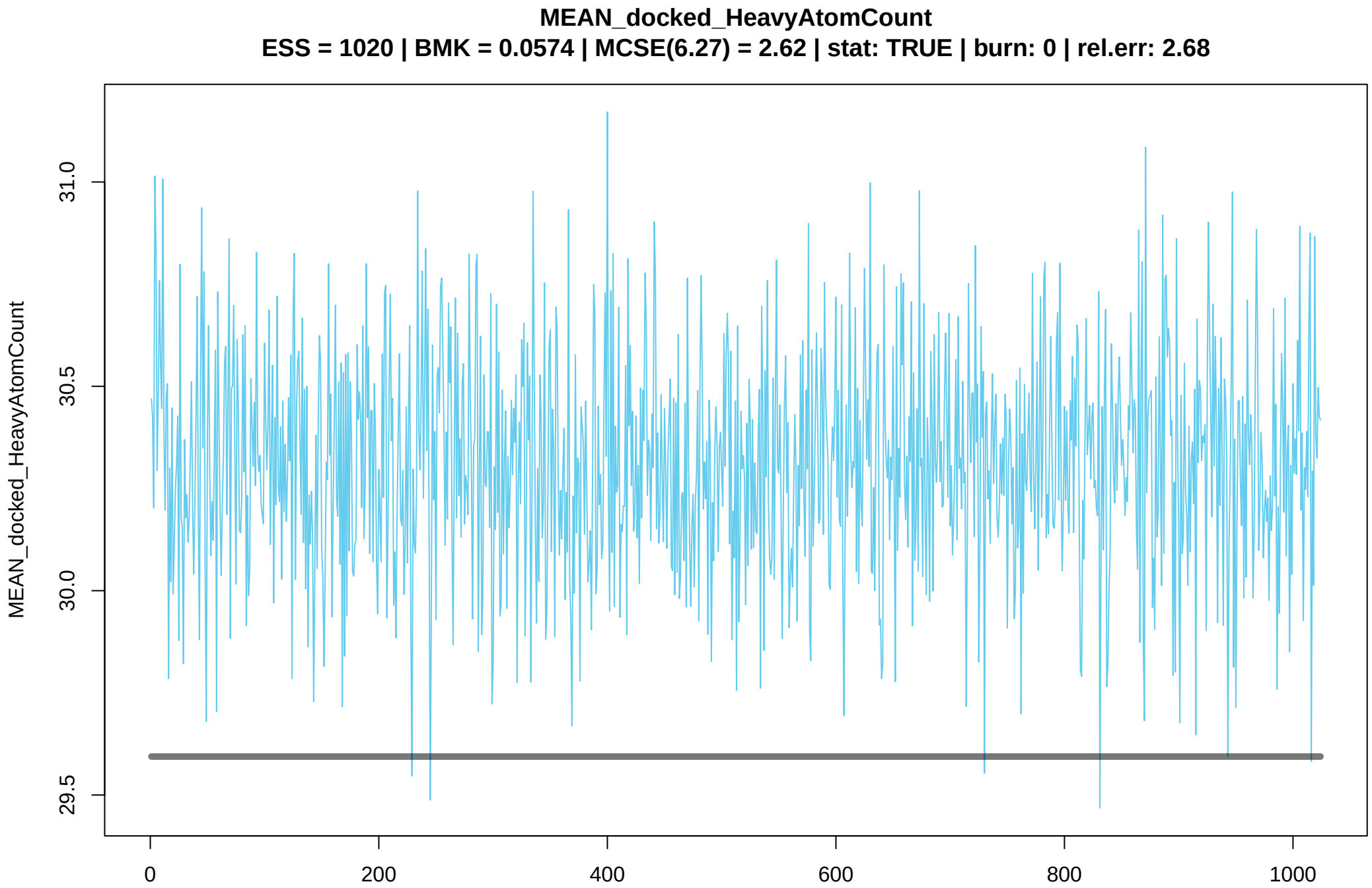

Dcov
ESS = 1020 | BMK = 0.0901 | MCSE(6.27) = 3.58 | stat: TRUE | burn: 0 | rel.err: −1.32
Dcov
−2.0
−2.5
−3.0
−3.5
−4.0
0
200
400
600
800
1000

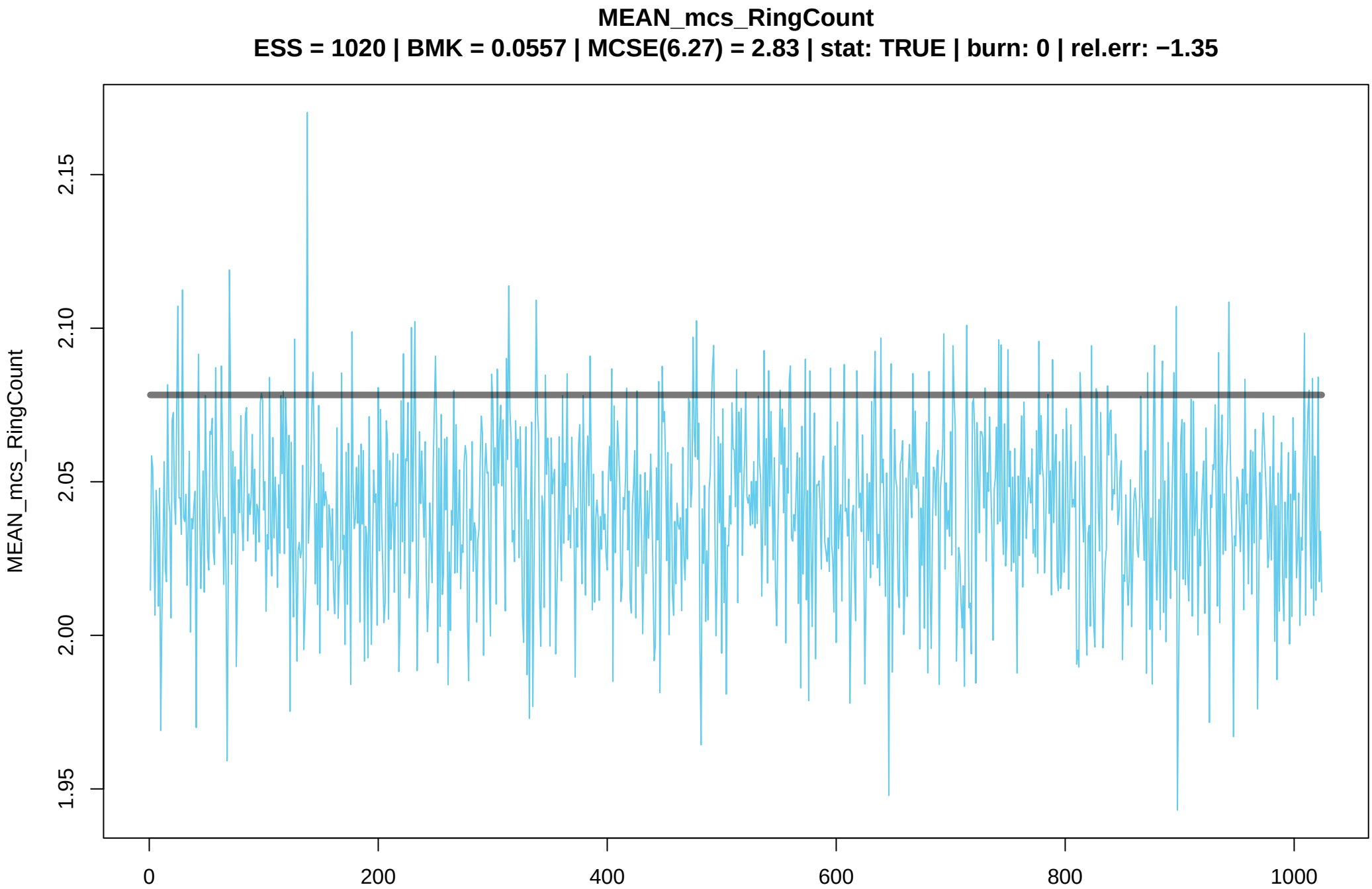

MEAN_log_RMSD
ESS = 1020 | BMK = 0.04 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | rel.err: 1.63
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

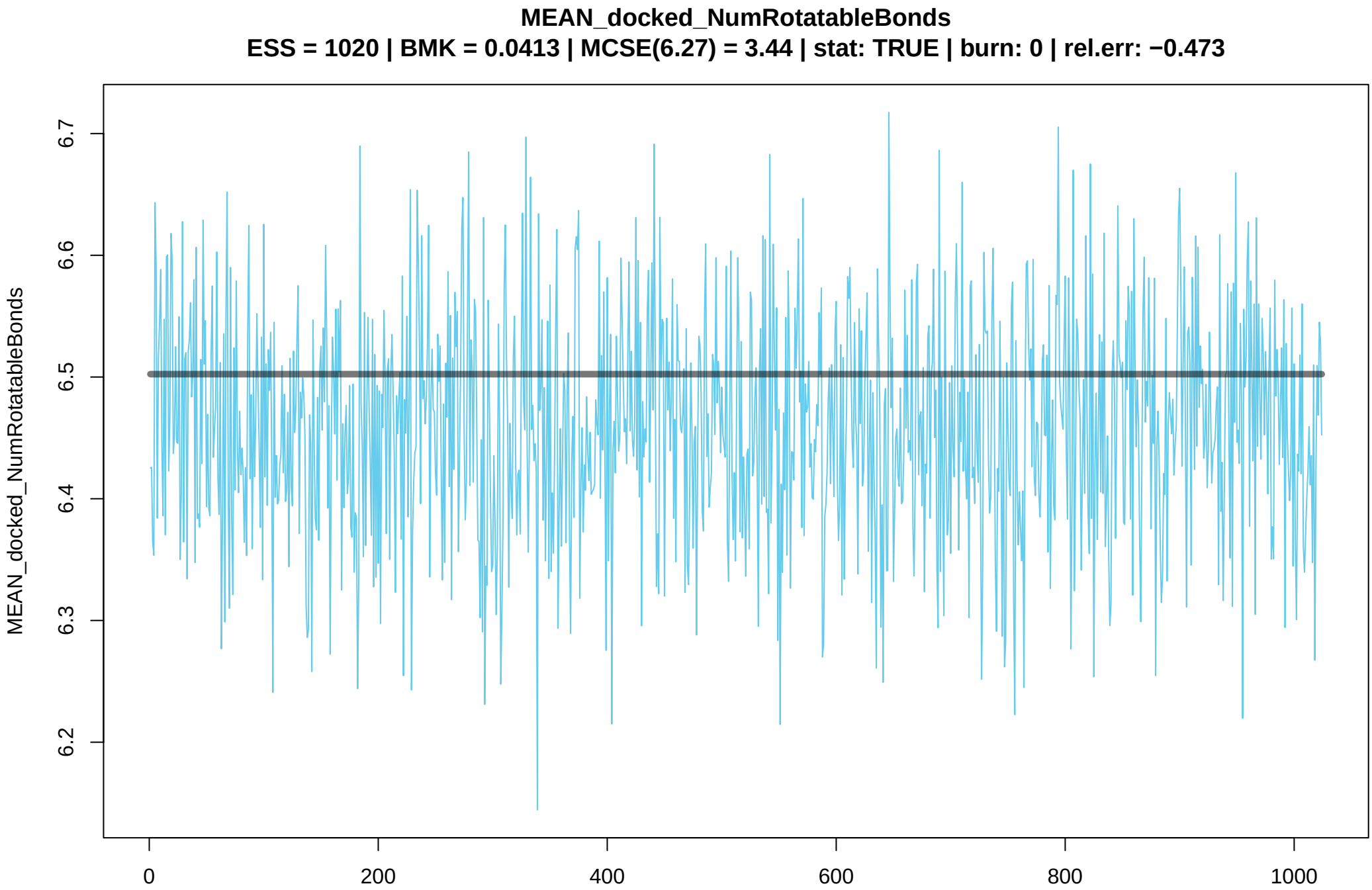

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0414 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | rel.err: 2.16
MEAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
−1.25
−1.30
0
200
400
600
800
1000

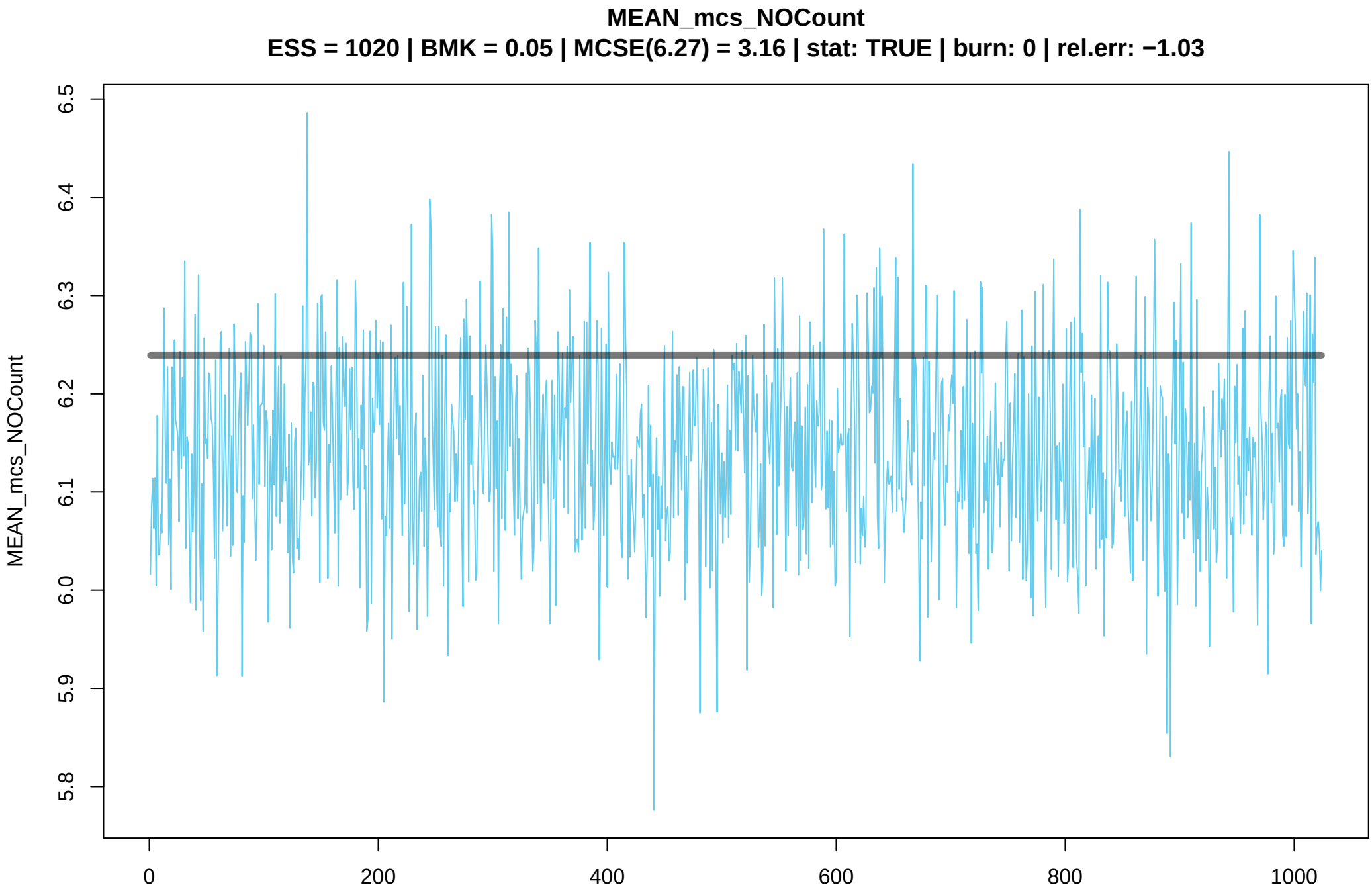

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0407 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | rel.err: 2.16
MEAN_logit_ec_tanimoto_similarity
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

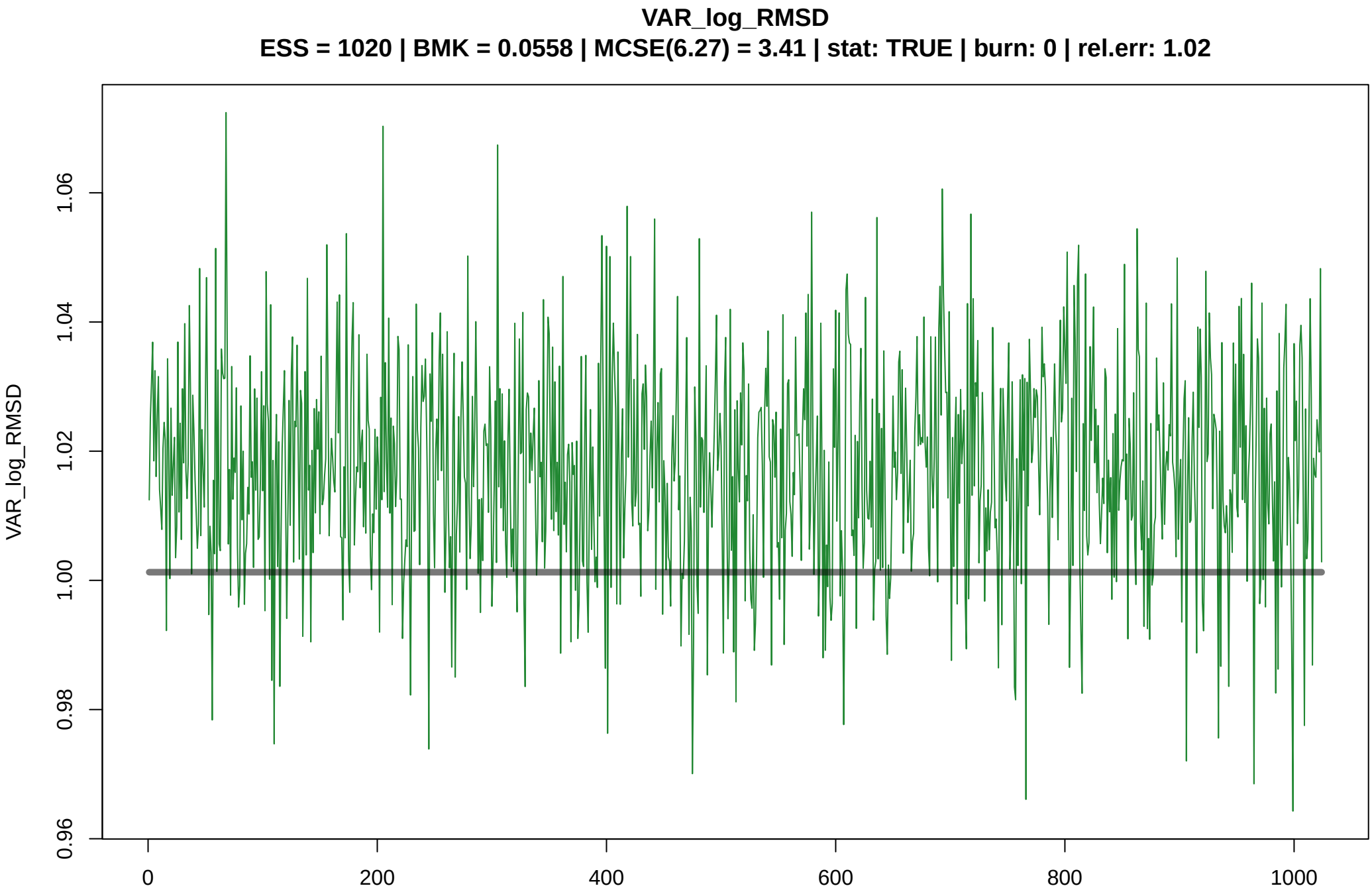

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0668 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0 | rel.err: −1.23
MEAN_mcs_NumHeteroAtoms
2.80
2.85
2.90
2.95
0
200
400
600
800
1000

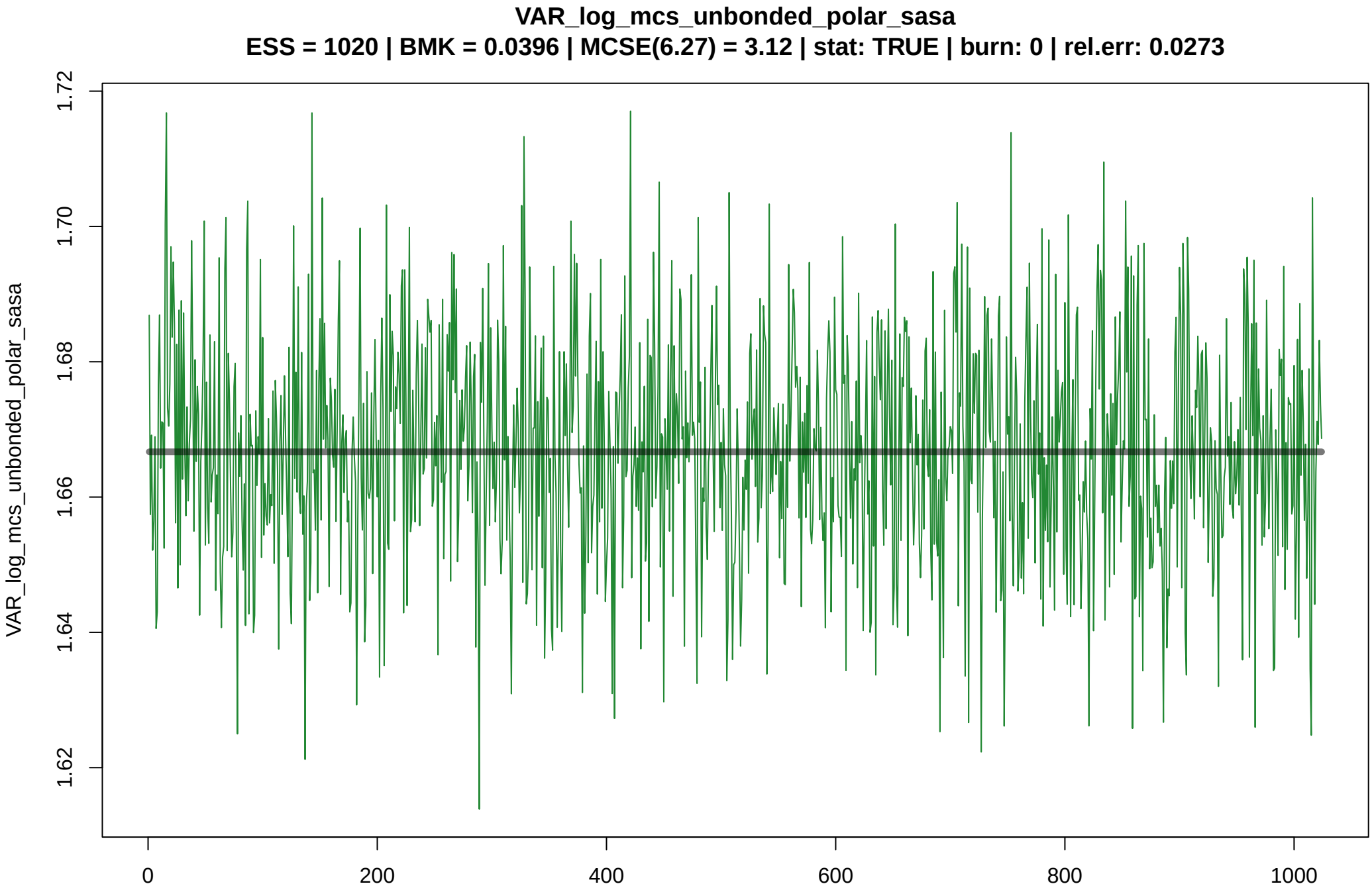

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0574 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | rel.err: 2.68
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
31.0
0
200
400
600
800
1000

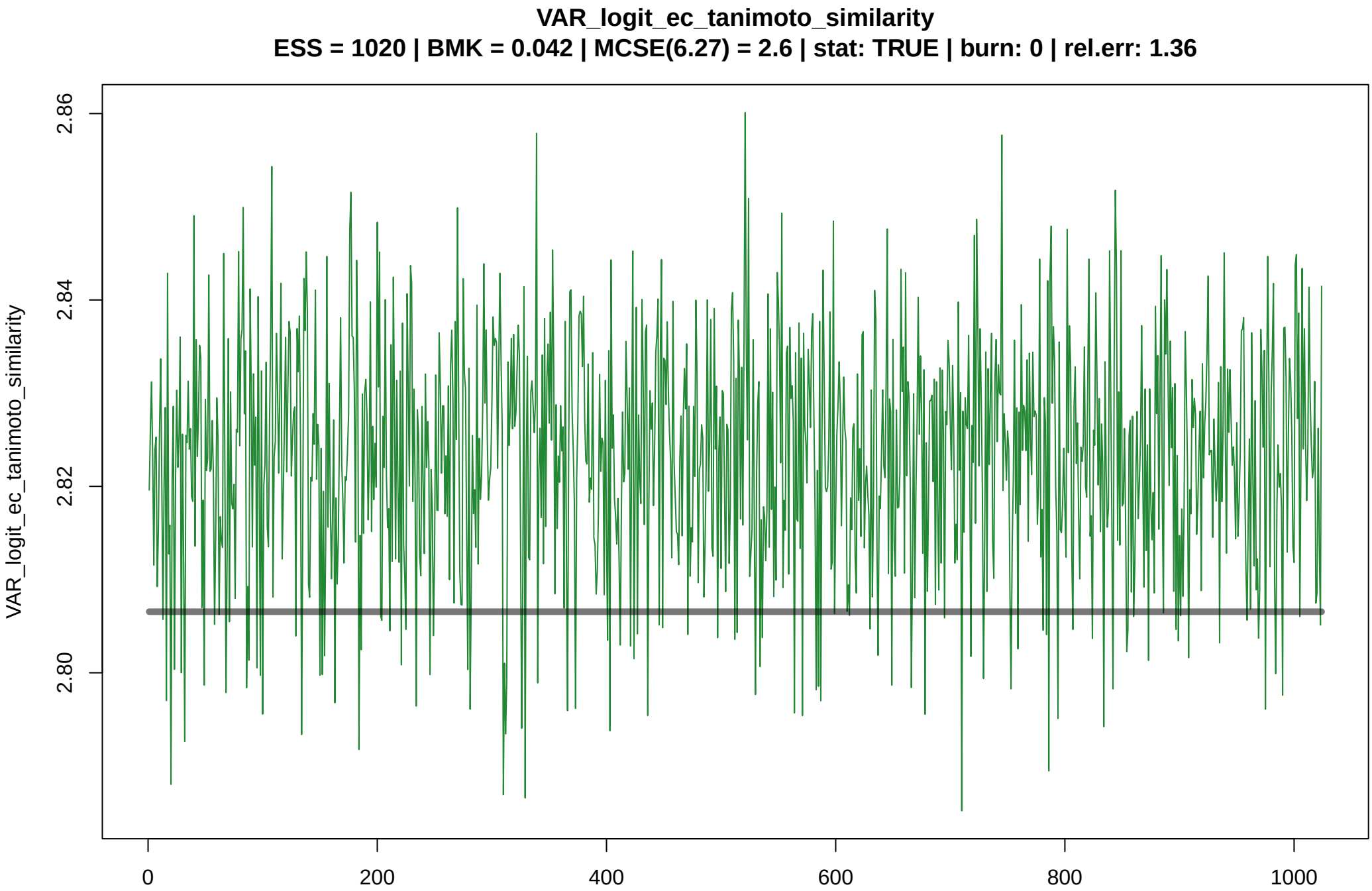

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0557 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | rel.err: −1.35
MEAN_mcs_RingCount
1.95
2.00
2.05
2.10
2.15
0
200
400
600
800
1000

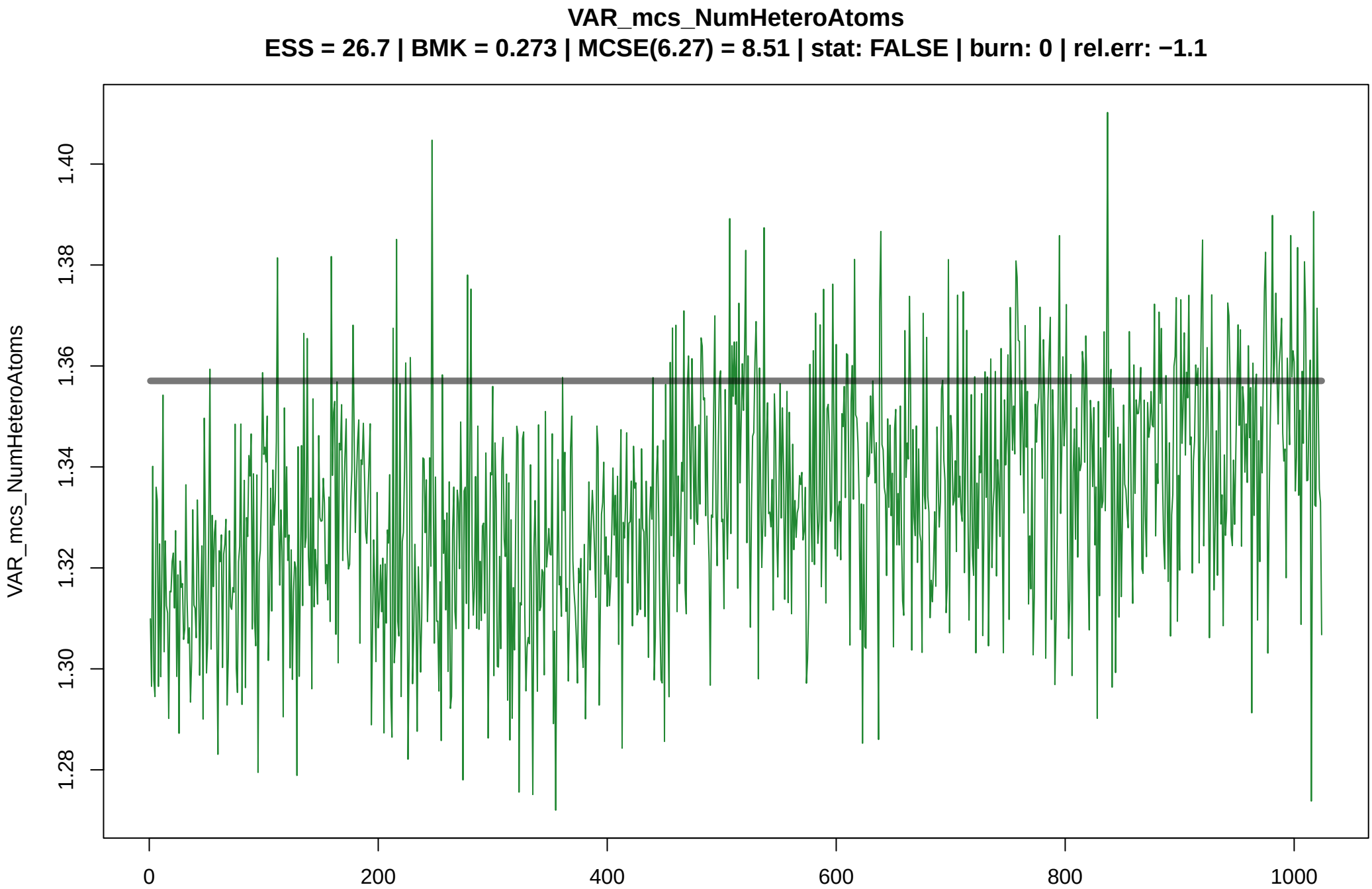

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0413 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | rel.err: −0.473
MEAN_docked_NumRotatableBonds
6.2
6.3
6.4
6.5
6.6
6.7
0
200
400
600
800
1000

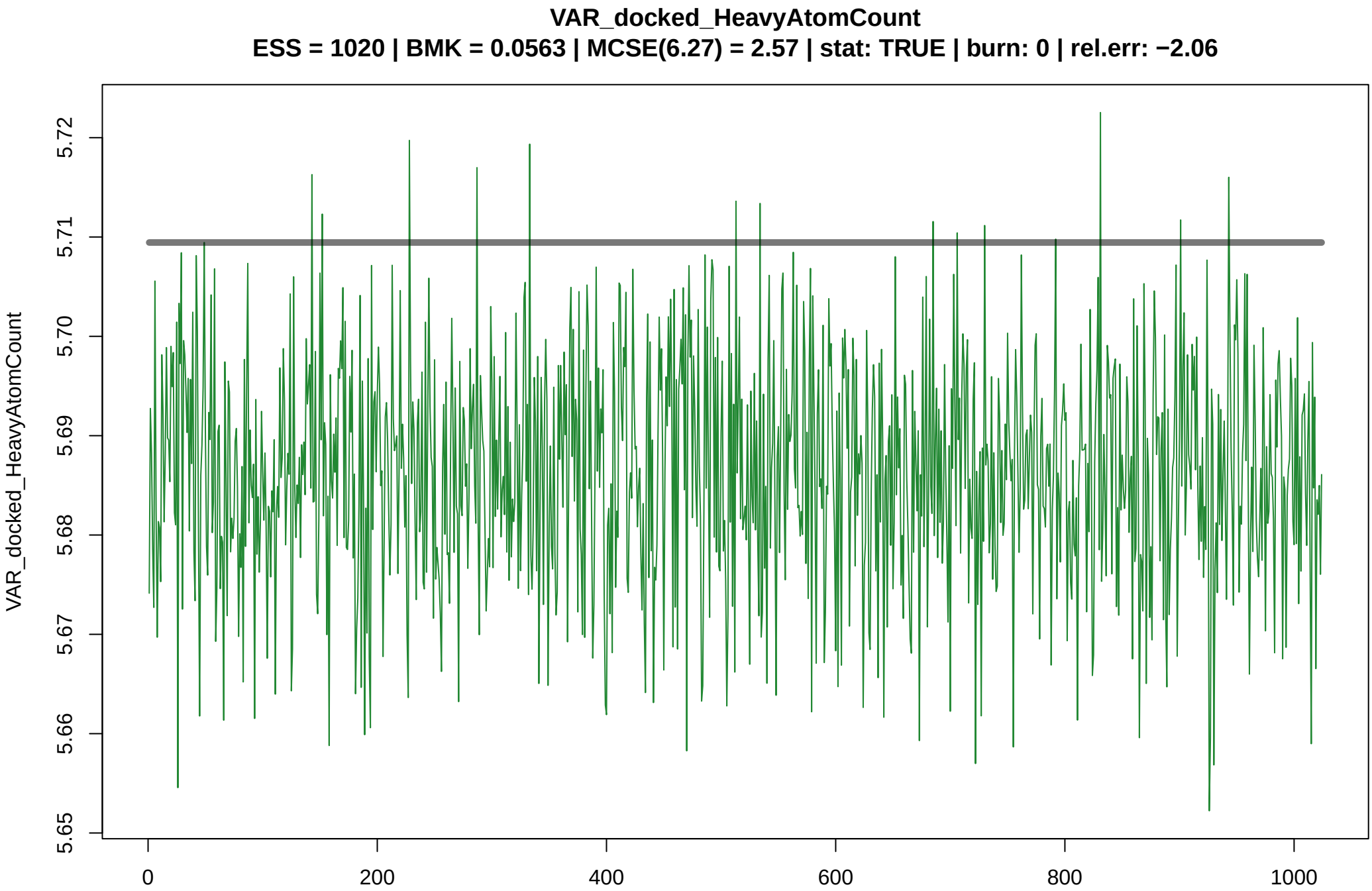

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.05 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | rel.err: −1.03
MEAN_mcs_NOCount
6.5
6.4
6.3
6.2
6.1
6.0
5.9
5.8
0
200
400
600
800
1000

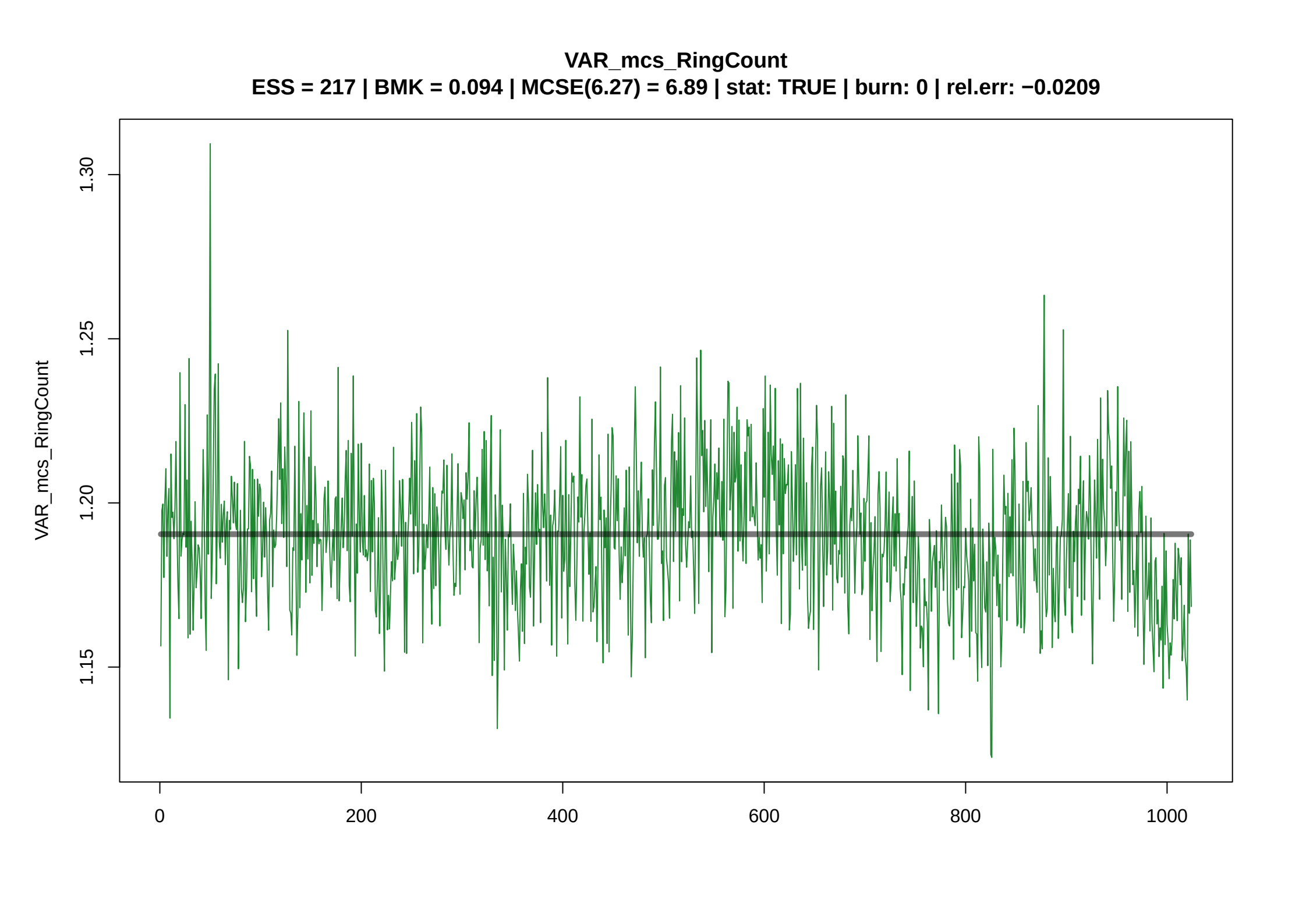

VAR_log_RMSD
ESS = 1020 | BMK = 0.0558 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0 | rel.err: 1.02
VAR_log_RMSD
0.96
0.98
1.00
1.02
1.04
1.06
0
200
400
600
800
1000

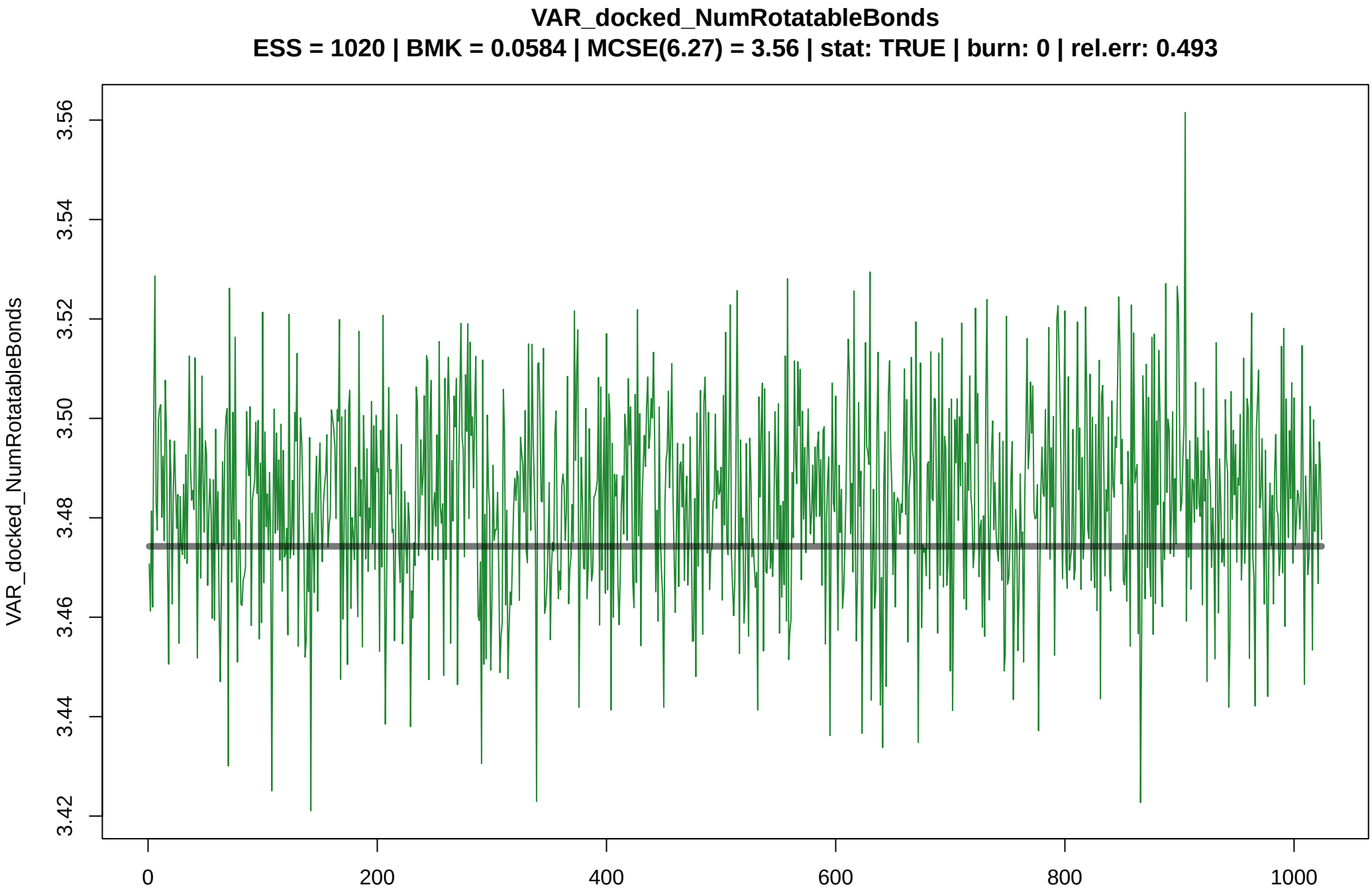

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0396 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | rel.err: 0.0273
VAR_log_mcs_unbonded_polar_sasa
1.72
1.70
1.68
1.66
1.64
1.62
0
200
400
600
800
1000

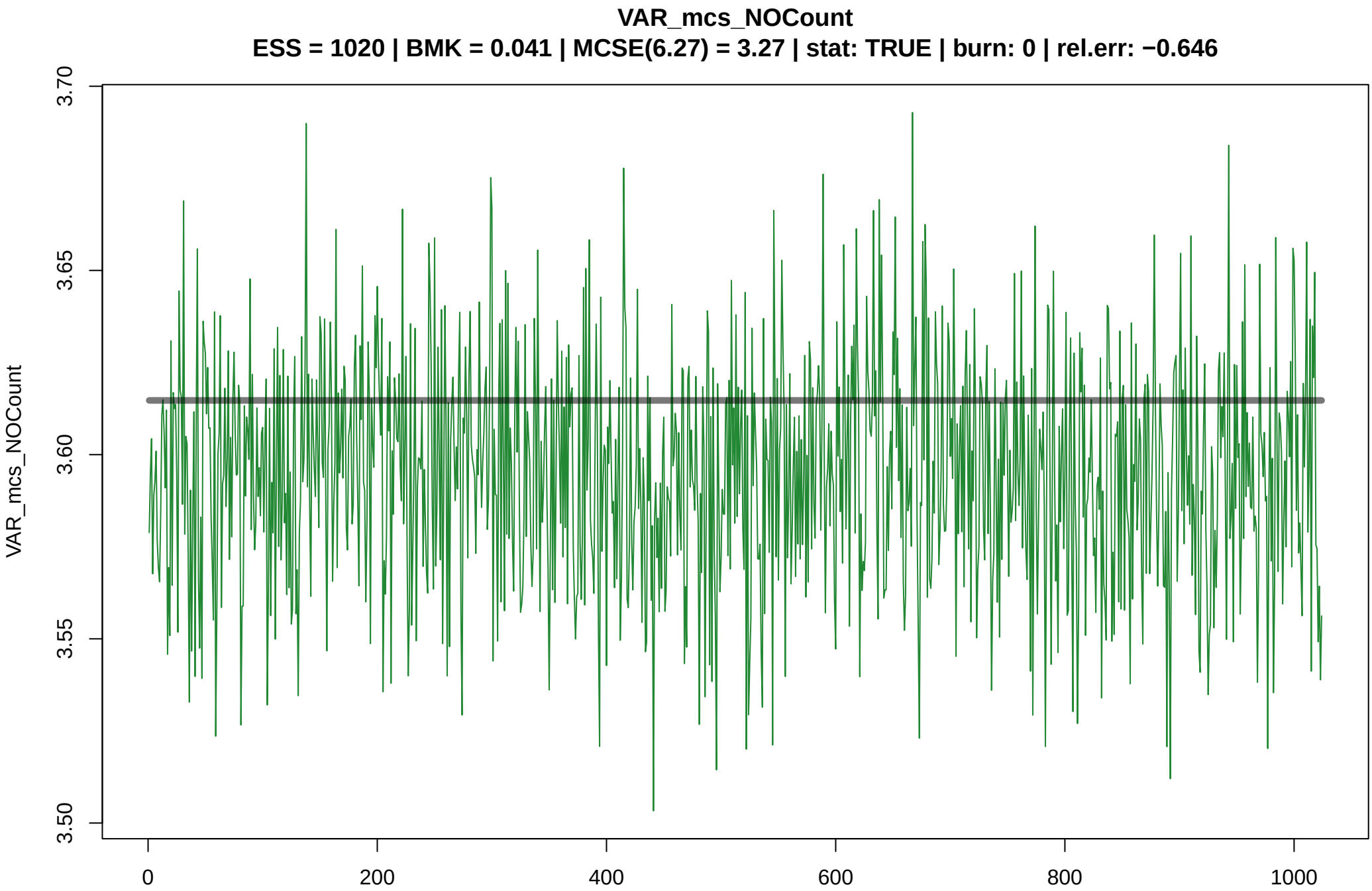

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.042 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: 1.36
VAR_logit_ec_tanimoto_similarity
2.86
2.84
2.82
2.80
0
200
400
600
800
1000

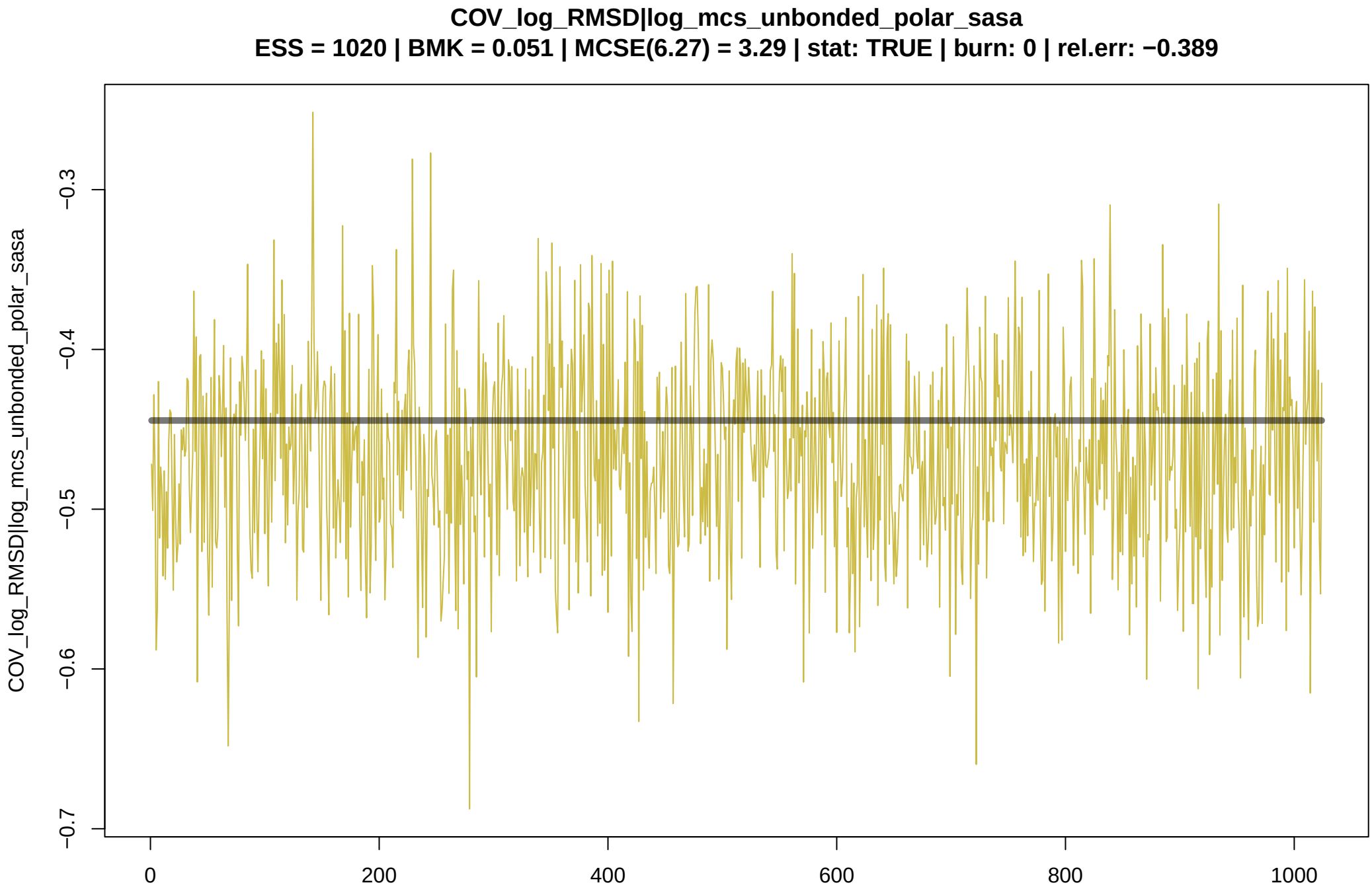

VAR_mcs_NumHeteroAtoms
ESS = 26.7 | BMK = 0.273 | MCSE(6.27) = 8.51 | stat: FALSE | burn: 0 | rel.err: −1.1
VAR_mcs_NumHeteroAtoms
1.28
1.30
1.32
1.34
1.36
1.38
1.40
0
200
400
600
800
1000

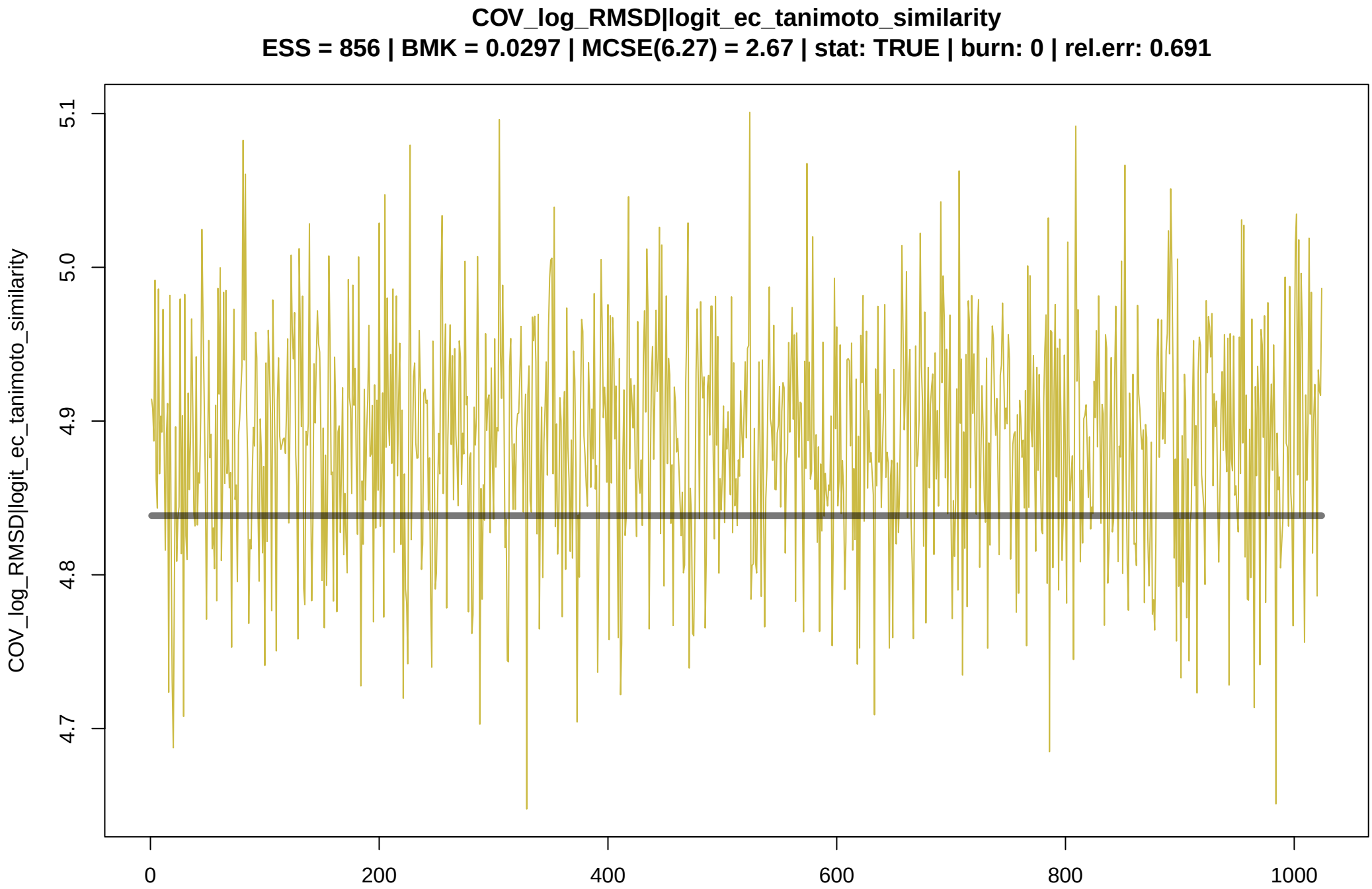

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0563 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: −2.06
VAR_docked_HeavyAtomCount
5.65
5.66
5.67
5.68
5.69
5.70
5.71
5.72
0
200
400
600
800
1000

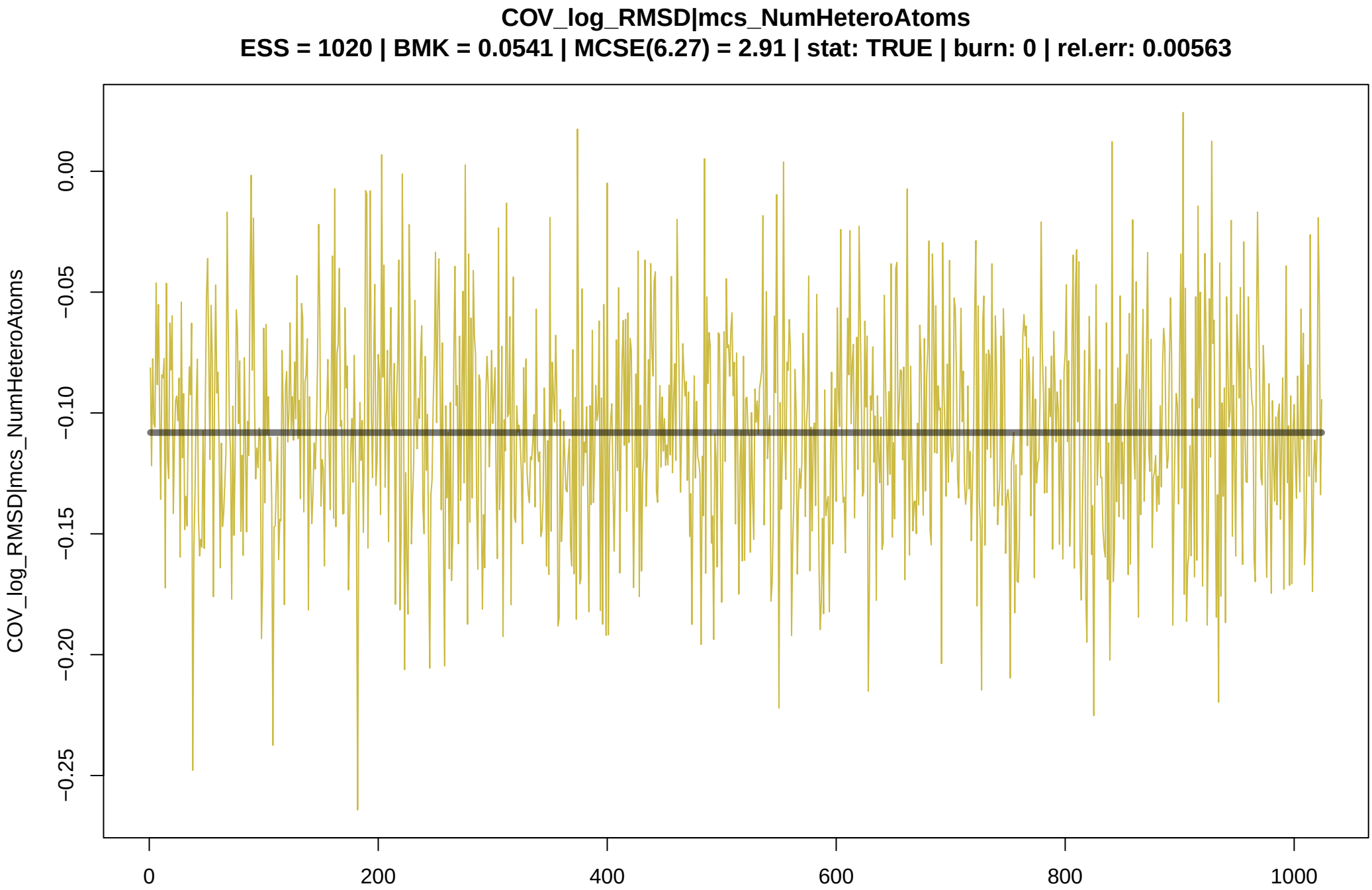

VAR_mcs_RingCount
ESS = 217 | BMK = 0.094 | MCSE(6.27) = 6.89 | stat: TRUE | burn: 0 | rel.err: −0.0209
VAR_mcs_RingCount
1.15
1.20
1.25
1.30
0
200
400
600
800
1000

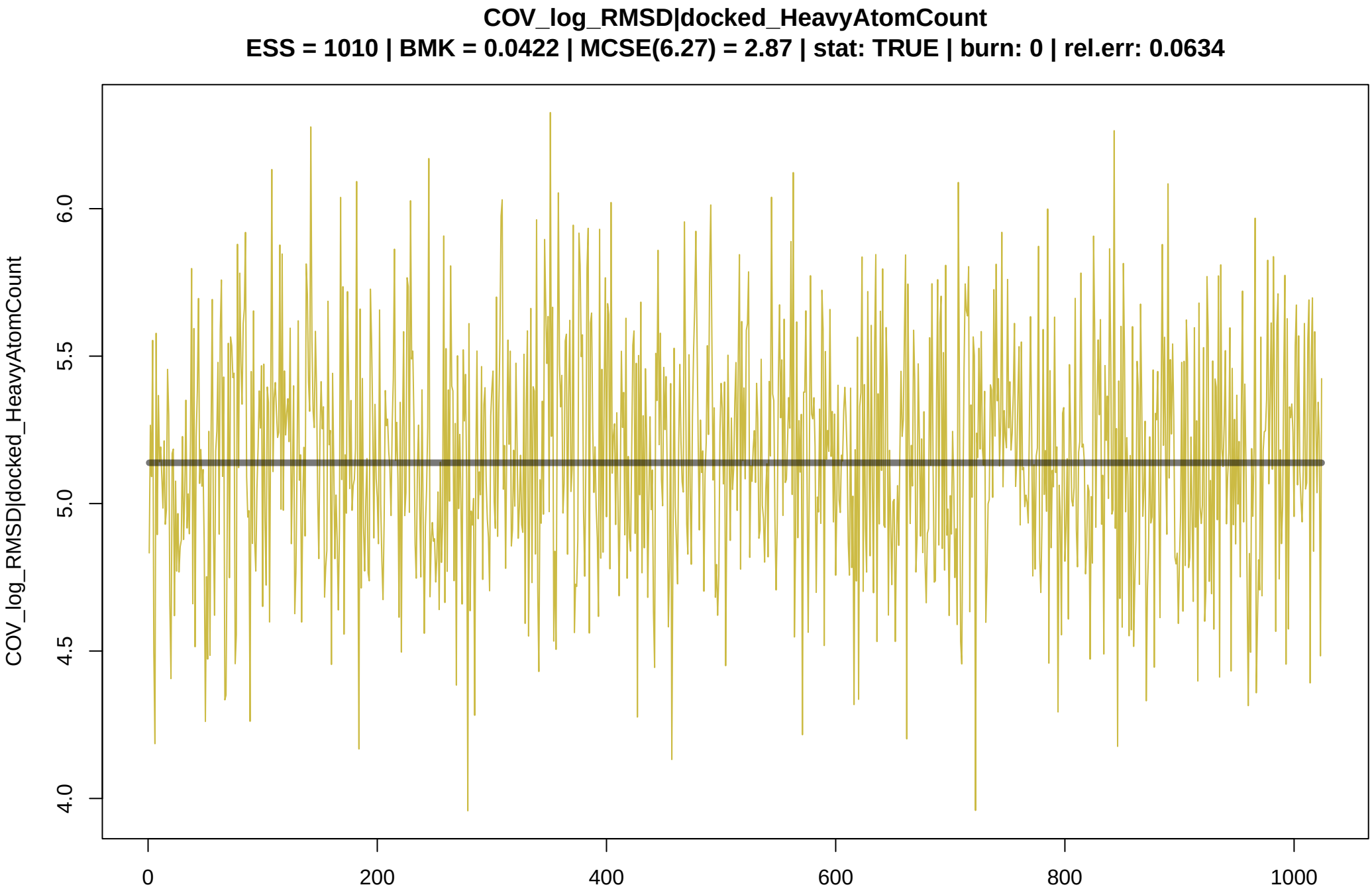

VAR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0584 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | rel.err: 0.493
VAR_docked_NumRotatableBonds
3.42
3.44
3.46
3.48
3.50
3.52
3.54
3.56
0
200
400
600
800
1000

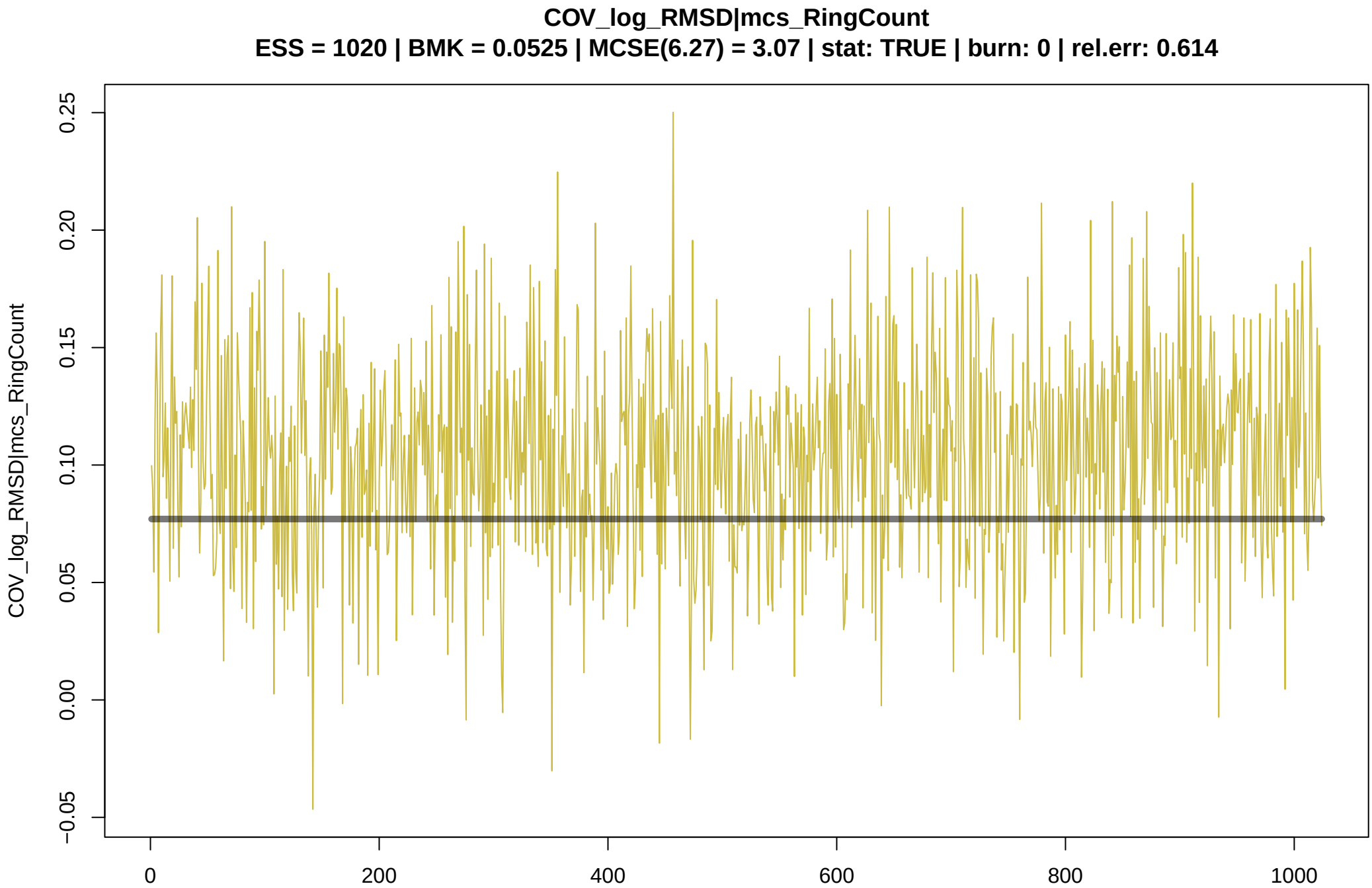

VAR_mcs_NOCount
ESS = 1020 | BMK = 0.041 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | rel.err: −0.646
VAR_mcs_NOCount
3.70
3.65
3.60
3.55
3.50
0
200
400
600
800
1000

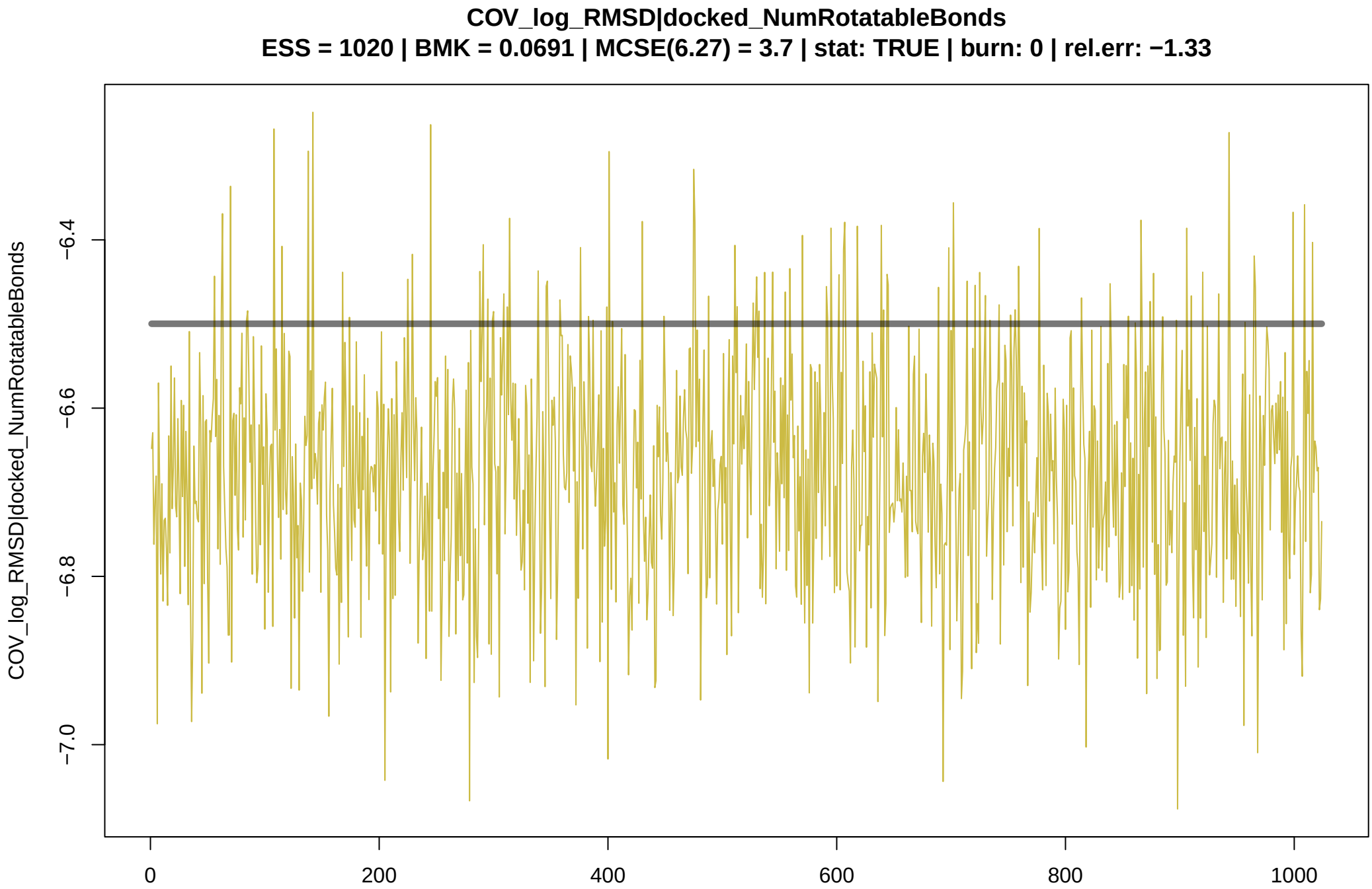

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.051 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0 | rel.err: −0.389
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.3
−0.4
−0.5
−0.6
−0.7
0
200
400
600
800
1000

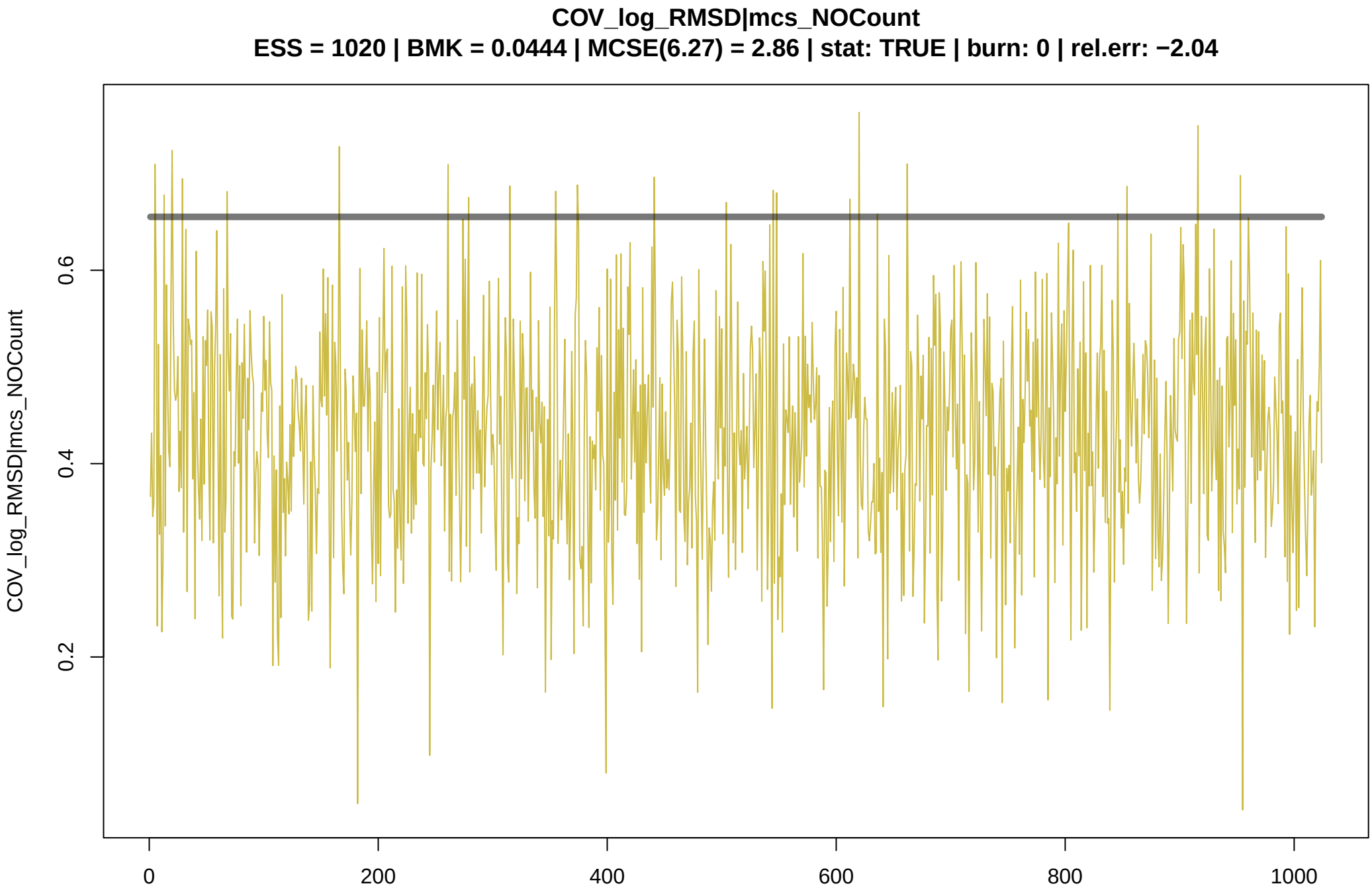

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 856 | BMK = 0.0297 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0 | rel.err: 0.691
COV_log_RMSD|logit_ec_tanimoto_similarity
5.1
5.0
4.9
4.8
4.7
0
200
400
600
800
1000

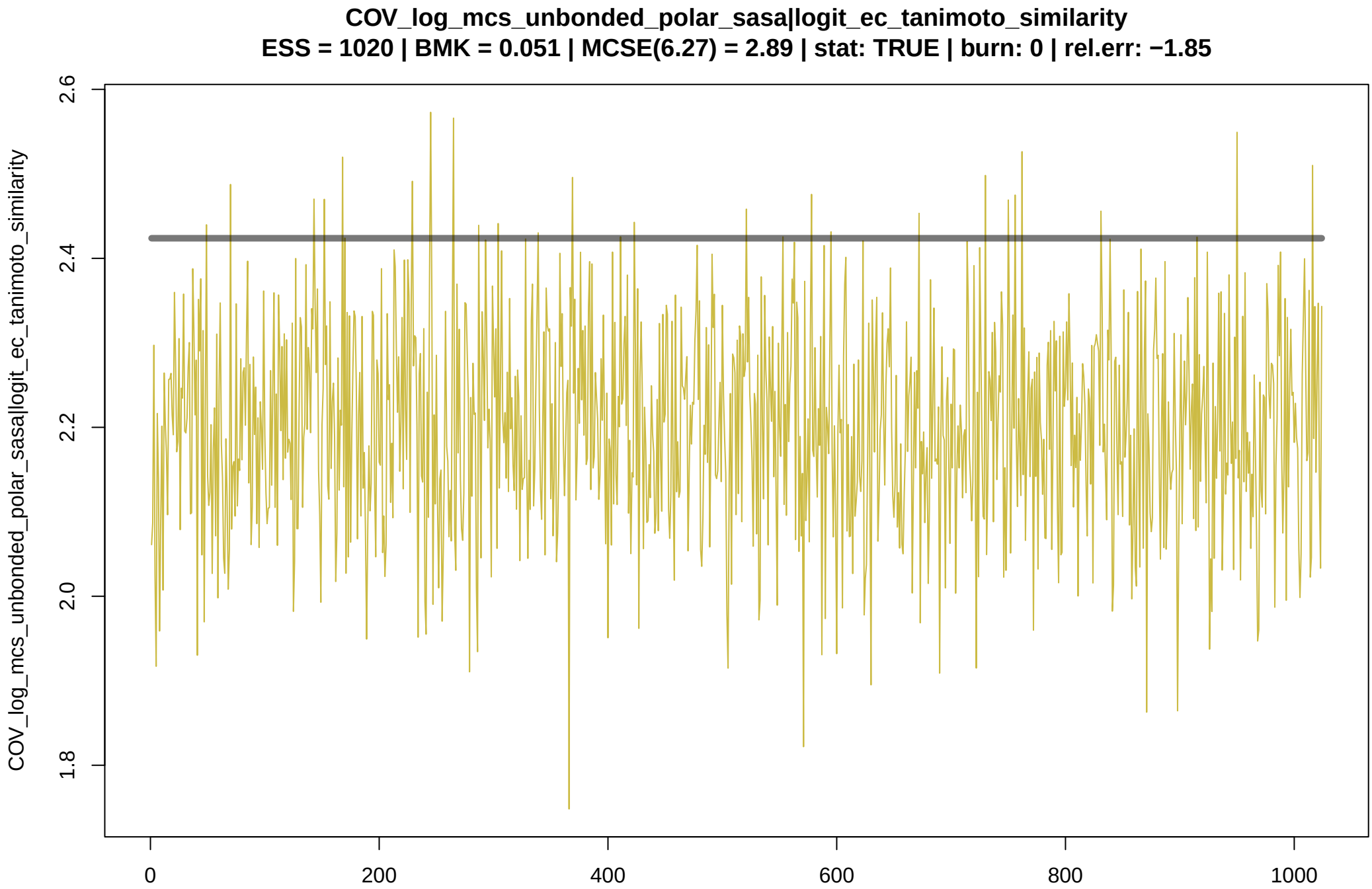

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0541 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | rel.err: 0.00563
COV_log_RMSD|mcs_NumHeteroAtoms
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
200
400
600
800
1000

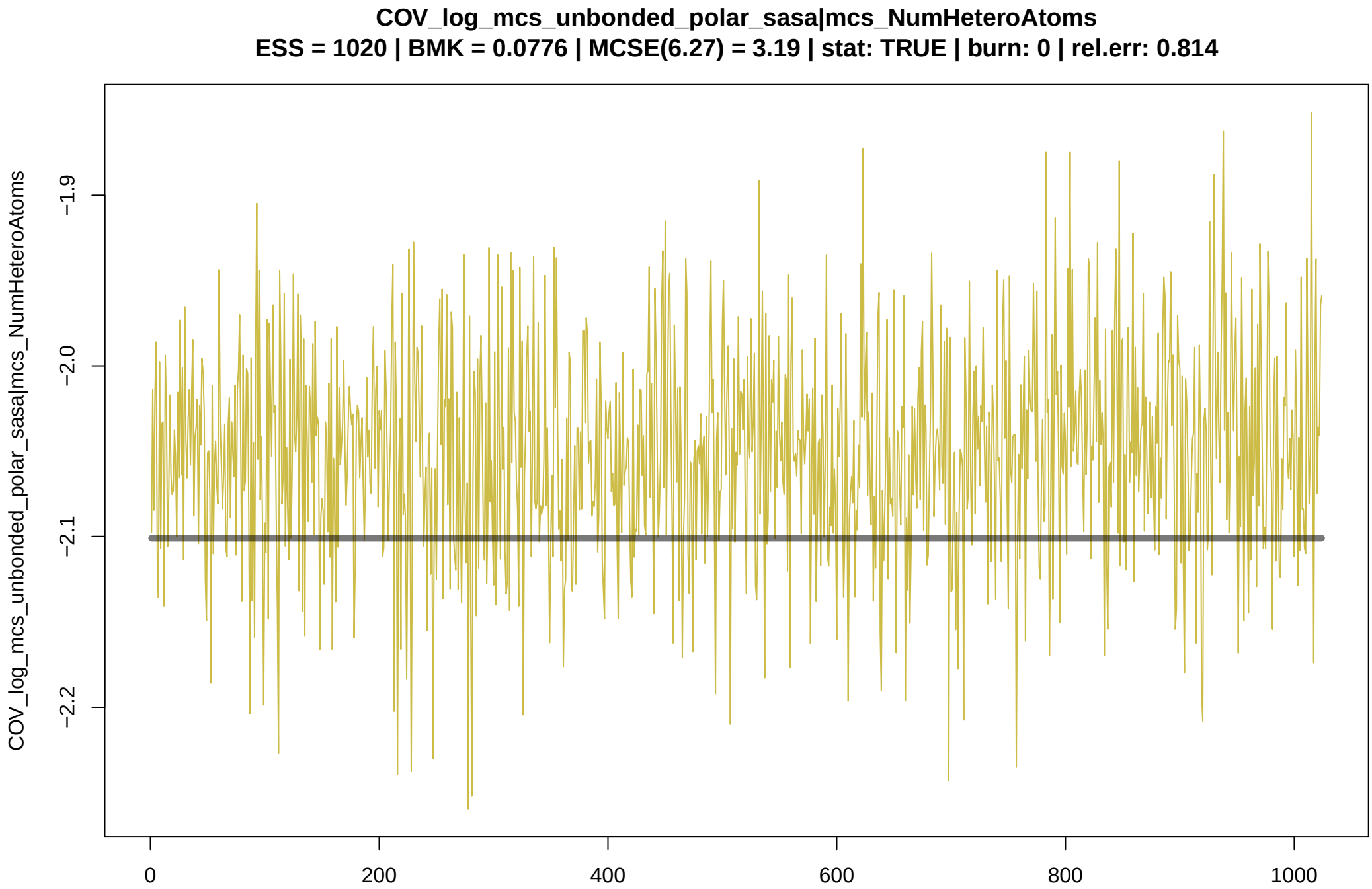

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1010 | BMK = 0.0422 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0 | rel.err: 0.0634
COV_log_RMSD|docked_HeavyAtomCount
4.0
4.5
5.0
5.5
6.0
0
200
400
600
800
1000

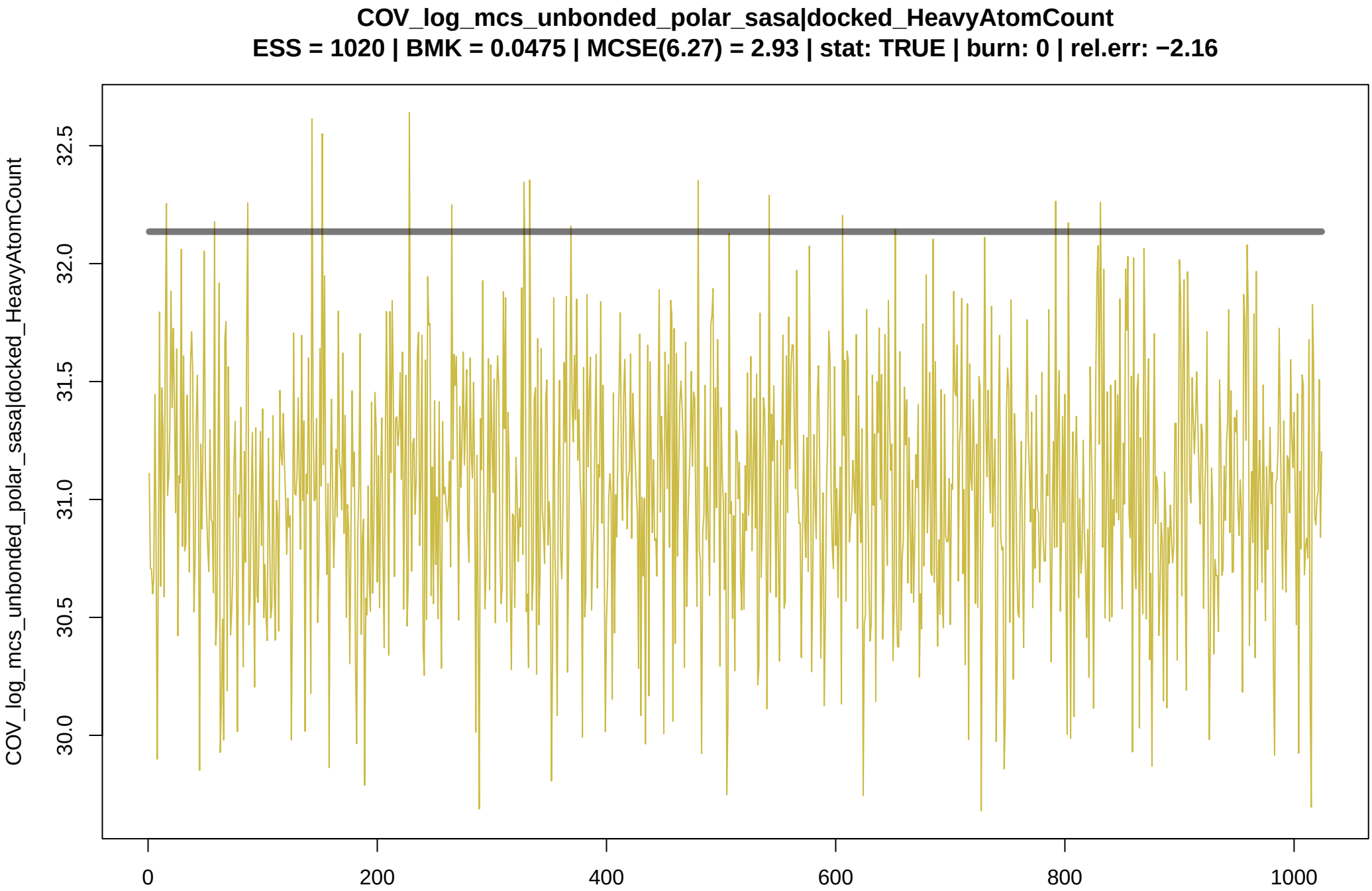

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0525 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | rel.err: 0.614
COV_log_RMSD|mcs_RingCount
0.25
0.20
0.15
0.10
0.05
0.00
−0.05
0
200
400
600
800
1000

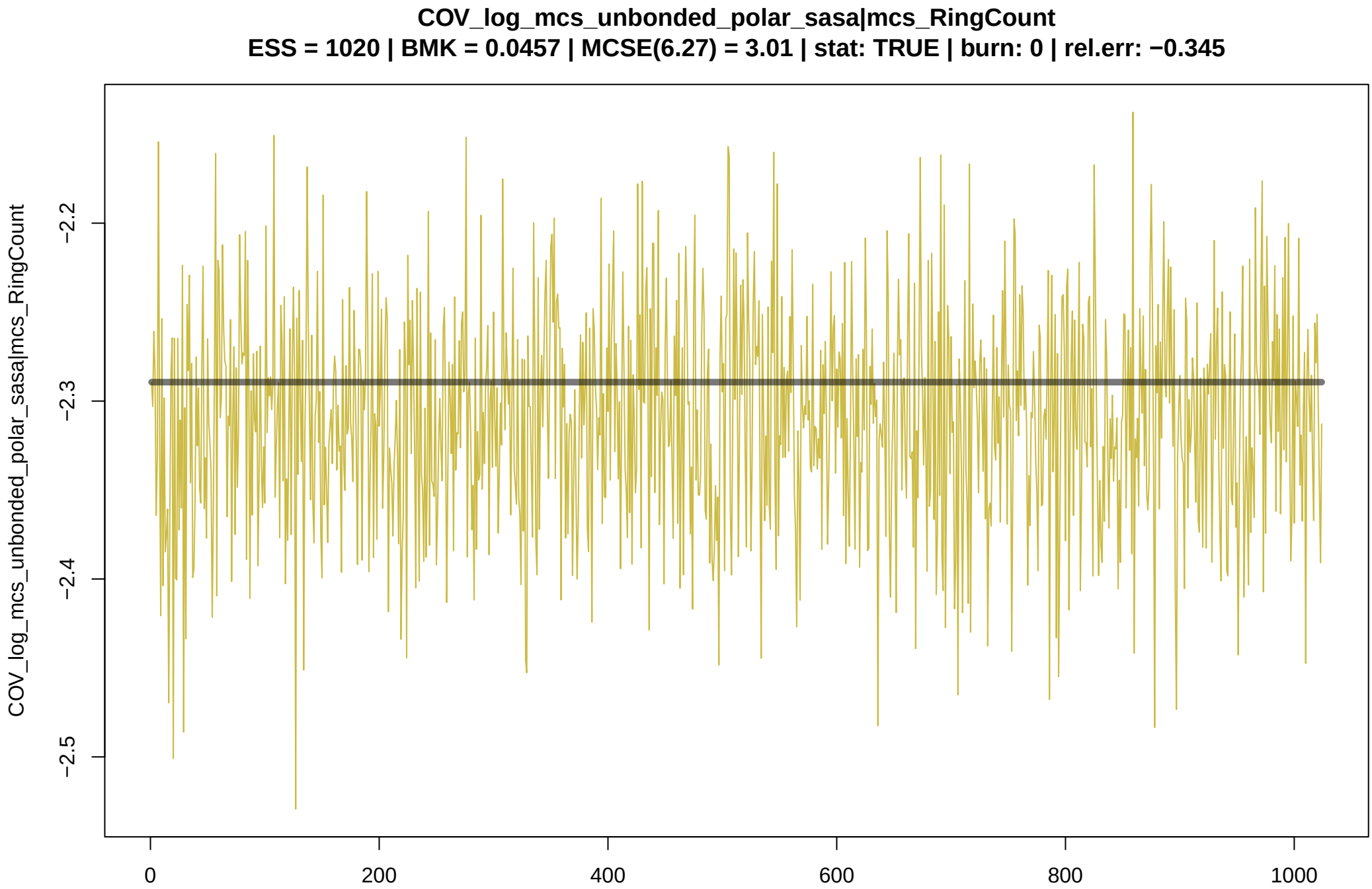

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0691 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | rel.err: −1.33
COV_log_RMSD|docked_NumRotatableBonds
−6.4
−6.6
−6.8
−7.0
0
200
400
600
800
1000

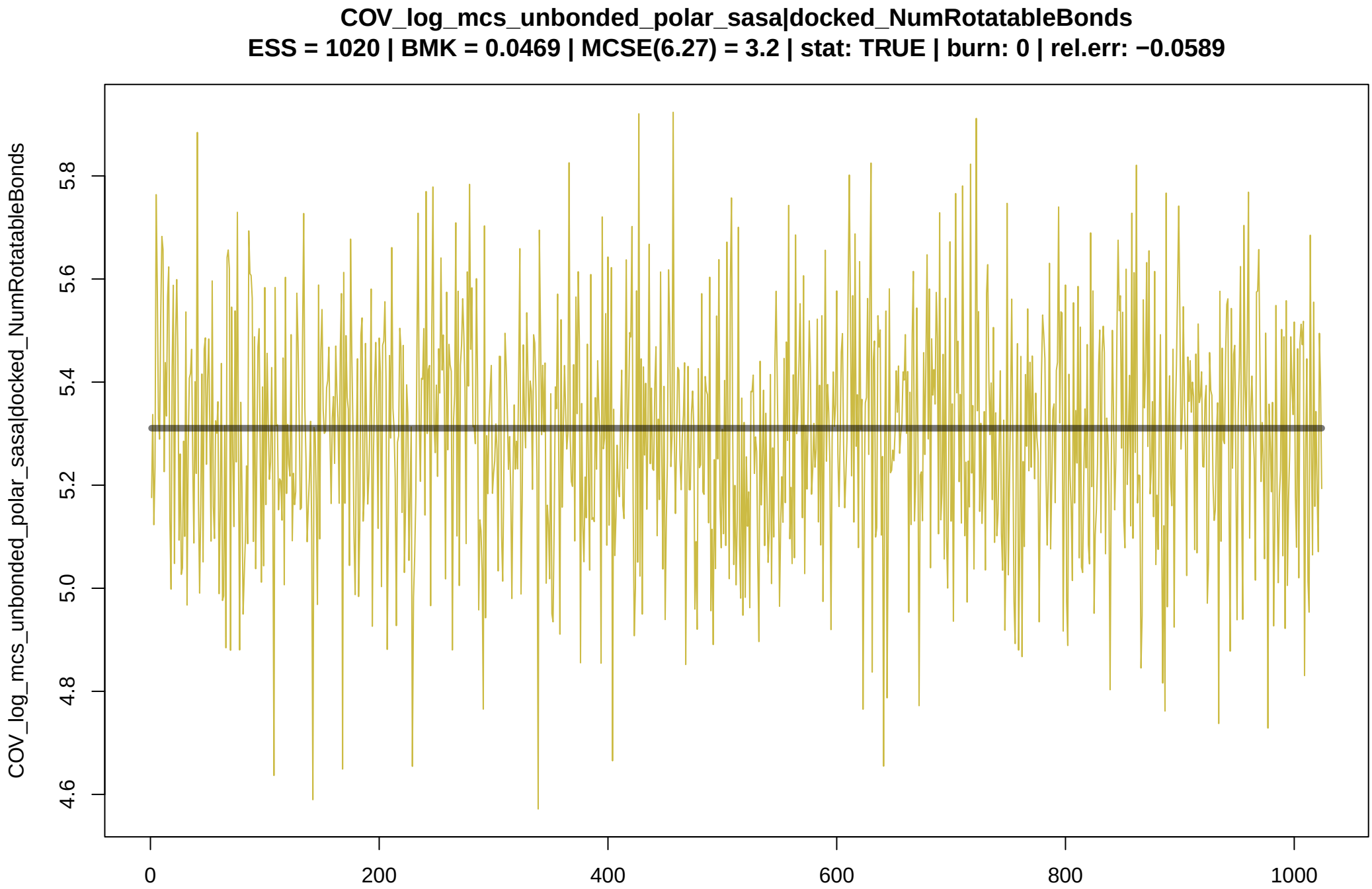

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0444 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | rel.err: −2.04
COV_log_RMSD|mcs_NOCount
0.2
0.4
0.6
0
200
400
600
800
1000

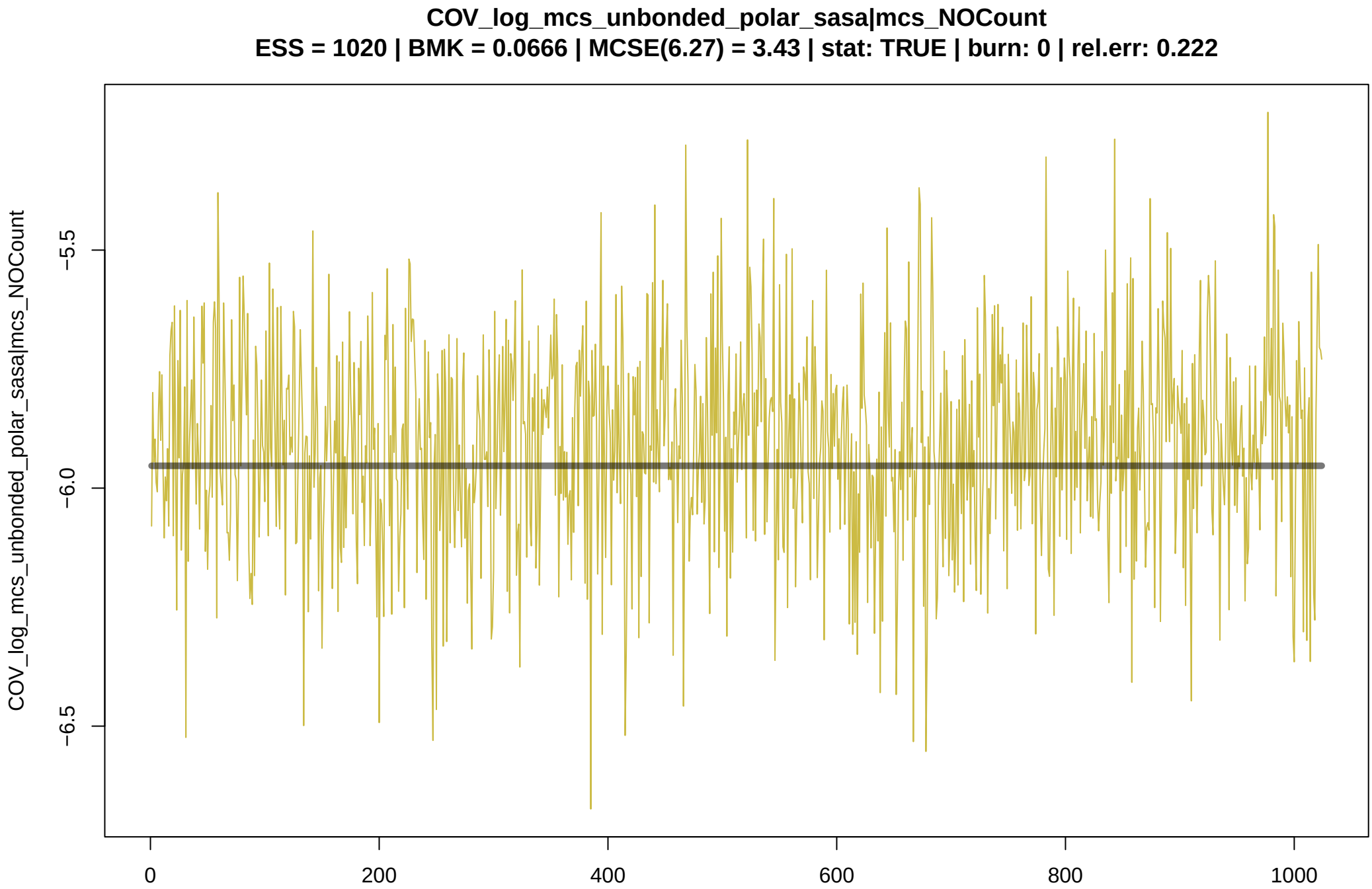

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.051 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | rel.err: −1.85
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2.6
2.4
2.2
2.0
1.8
0
200
400
600
800
1000

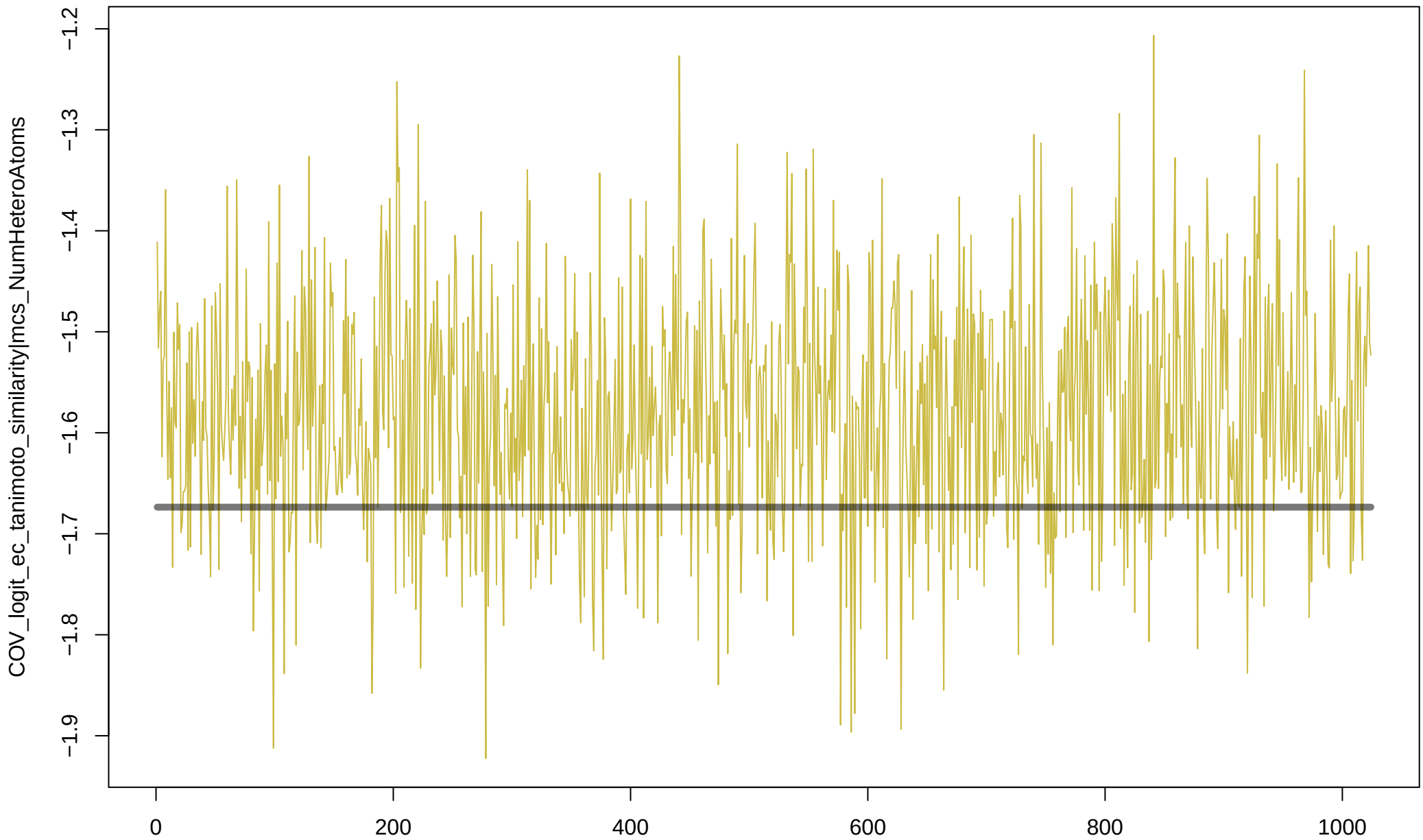

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0776 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | rel.err: 0.814
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

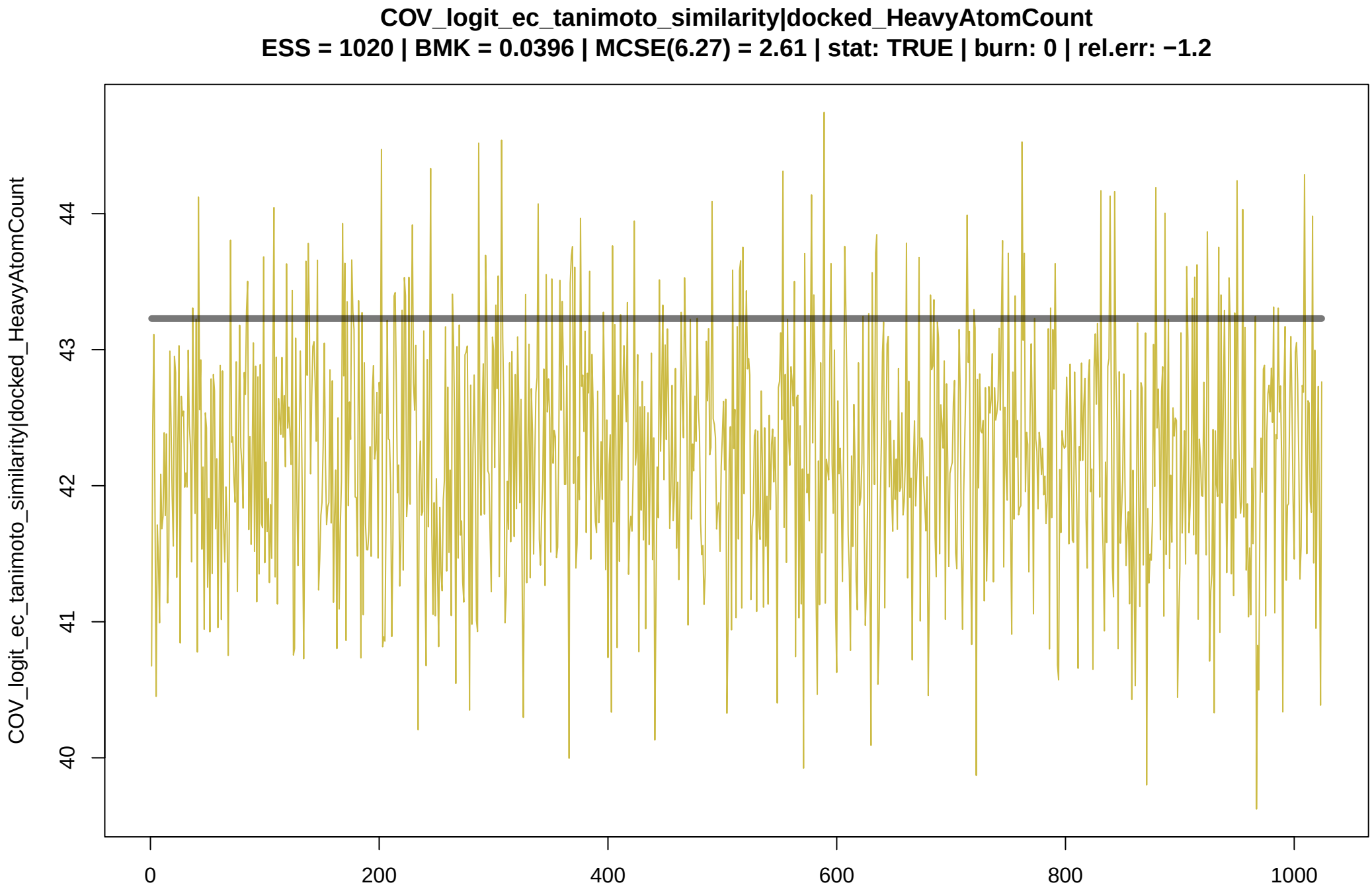

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0475 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | rel.err: −2.16
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
30.0
30.5
31.0
31.5
32.0
32.5
0
200
400
600
800
1000

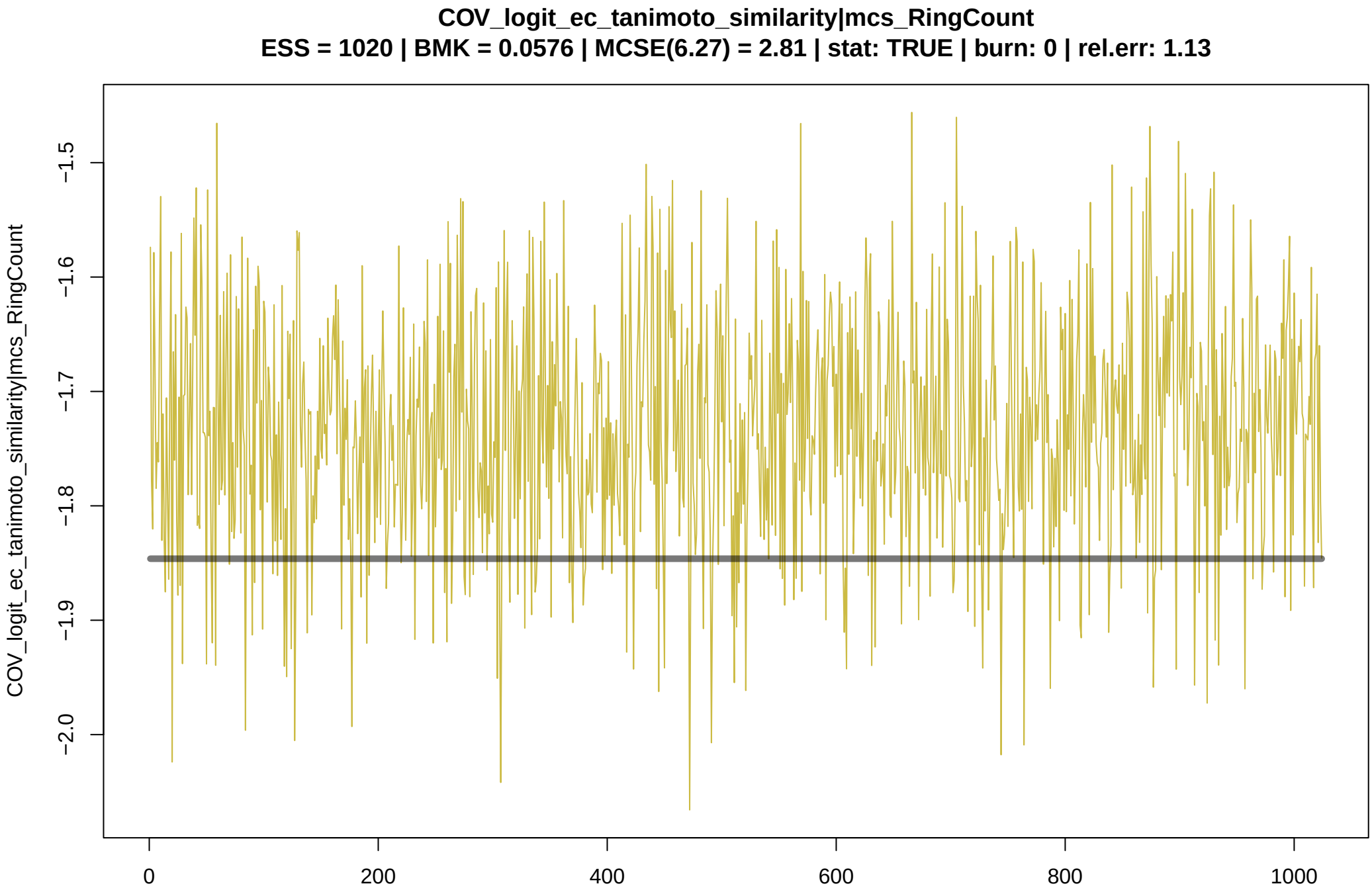

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0457 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | rel.err: −0.345
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.2
−2.3
−2.4
−2.5
0
200
400
600
800
1000

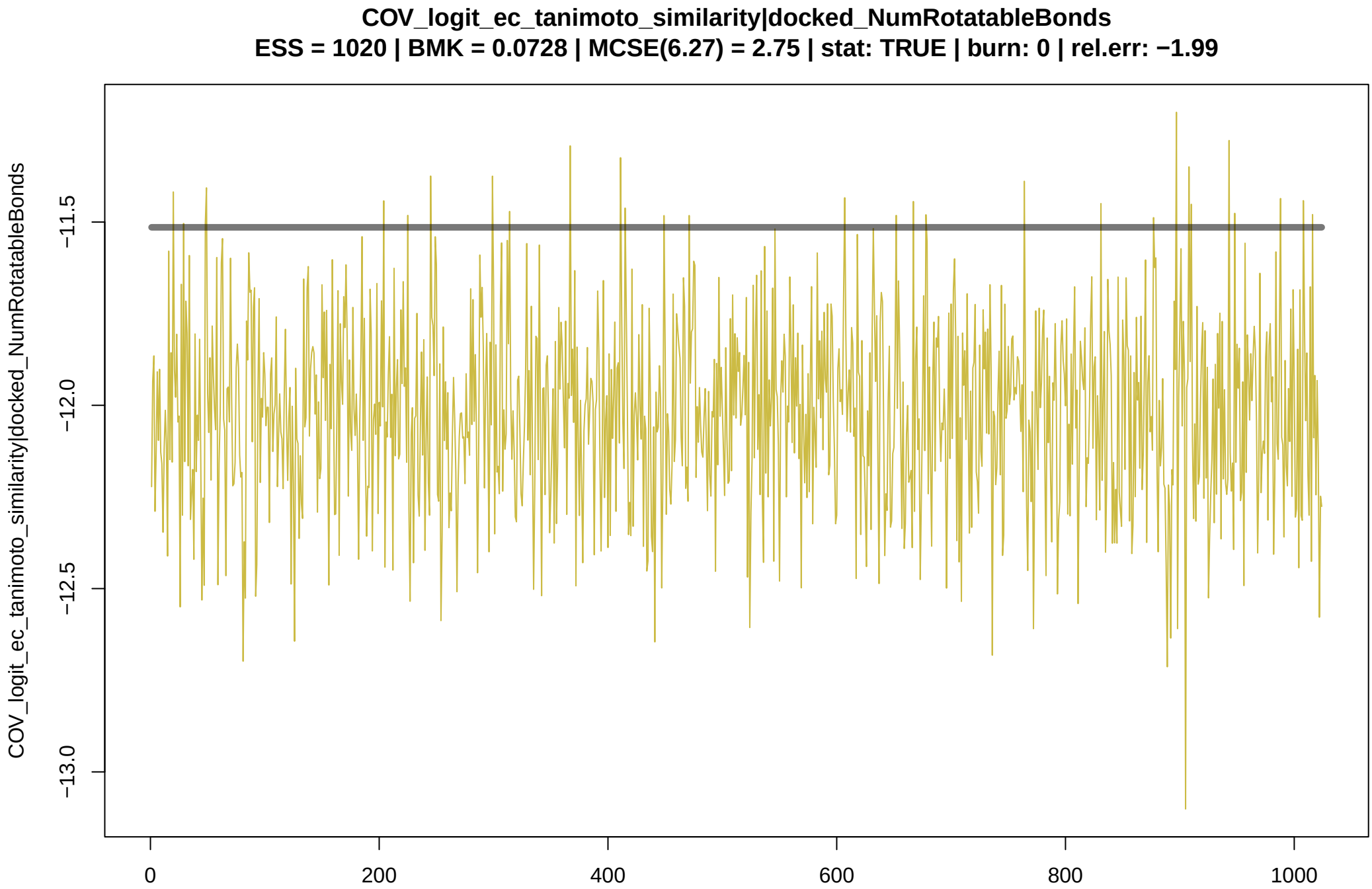

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0469 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: −0.0589
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
4.6
4.8
5.0
5.2
5.4
5.6
5.8
0
200
400
600
800
1000

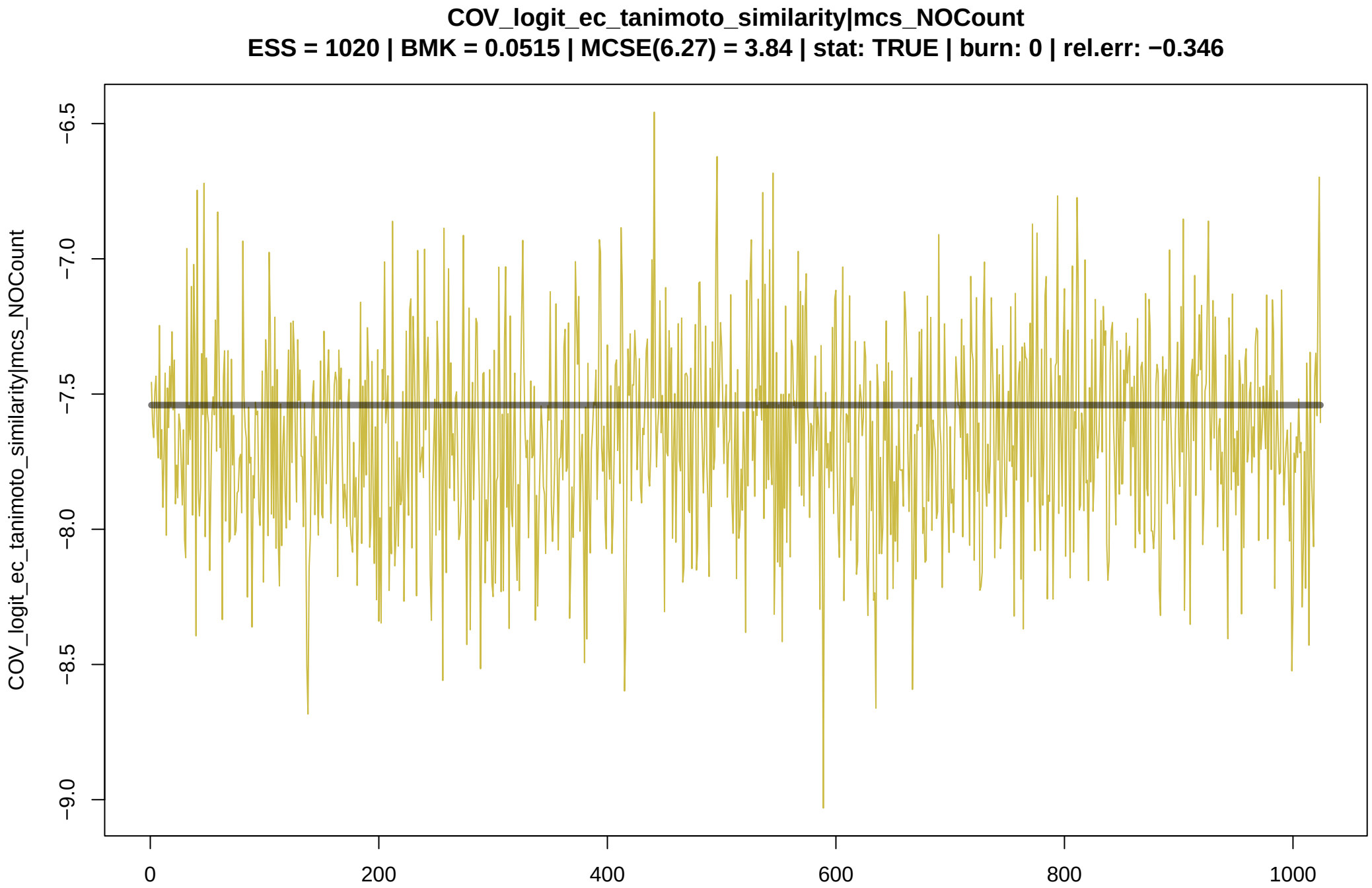

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0666 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0 | rel.err: 0.222
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.5
−6.0
−6.5
0
200
400
600
800
1000

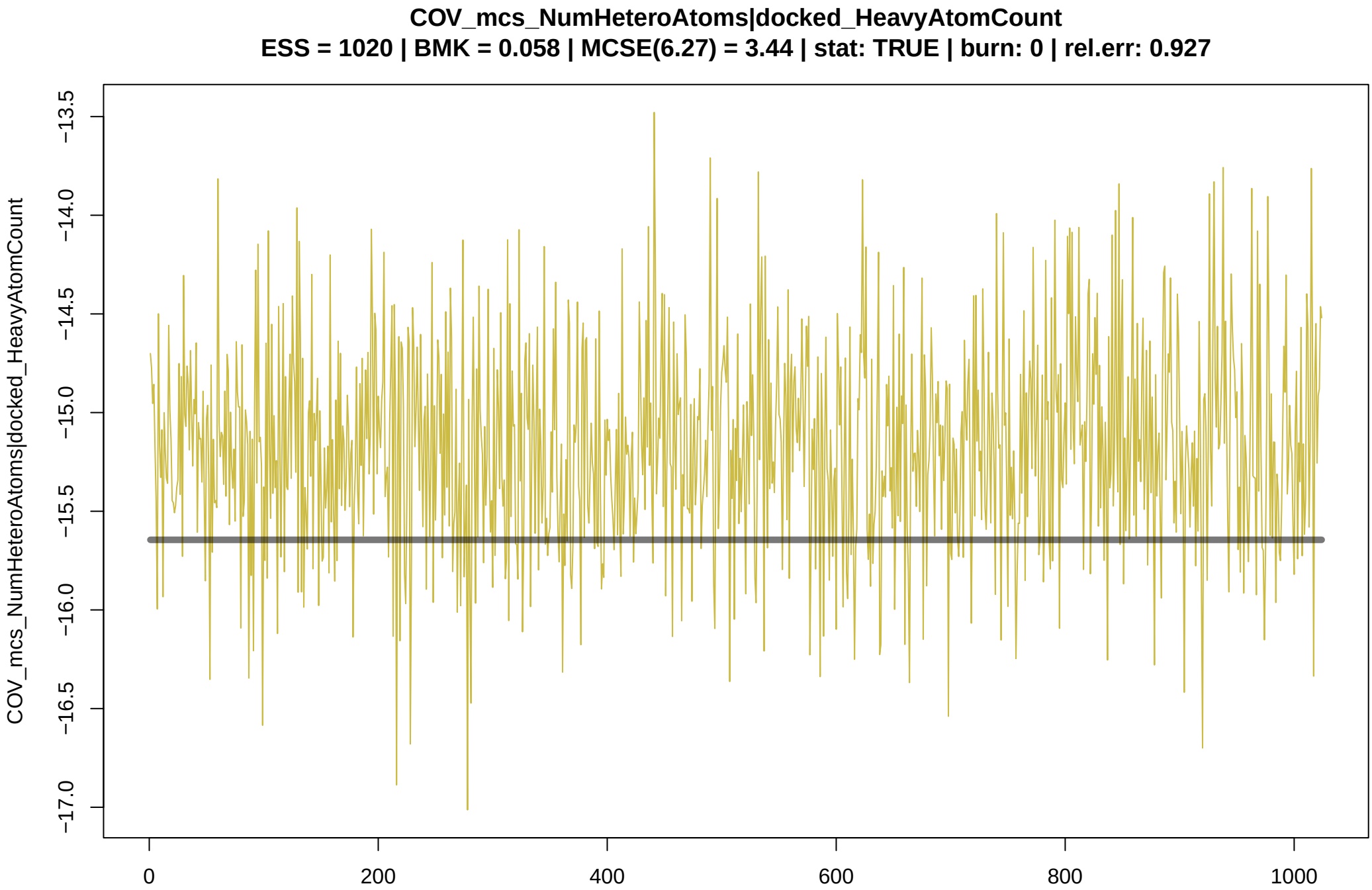

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0506 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0 | rel.err: 0.84
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.2
−1.3
−1.4
−1.5
−1.6
−1.7
−1.8
−1.9
0
200
400
600
800
1000

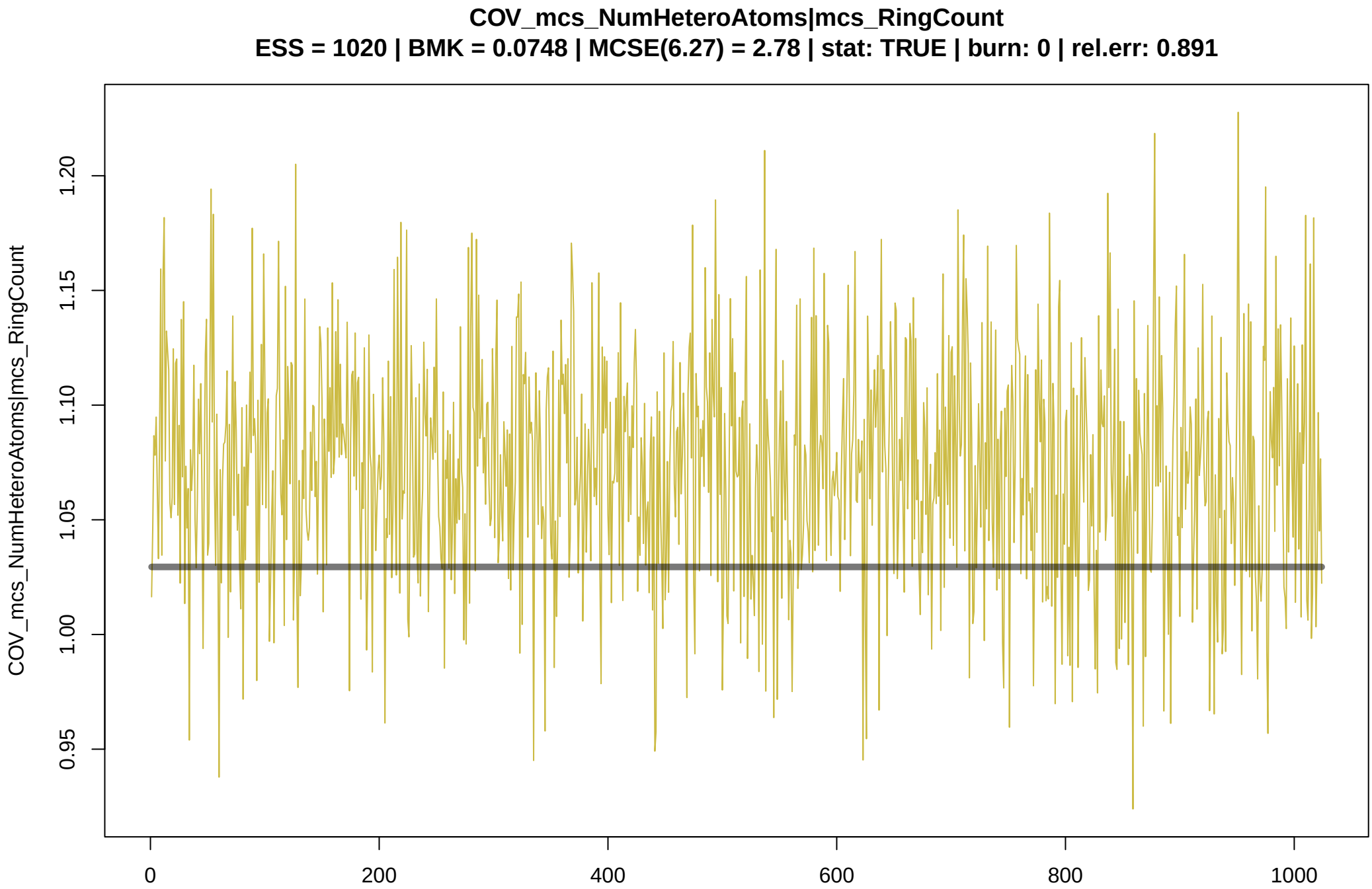

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0396 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: −1.2
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
40
41
42
43
44
0
200
400
600
800
1000

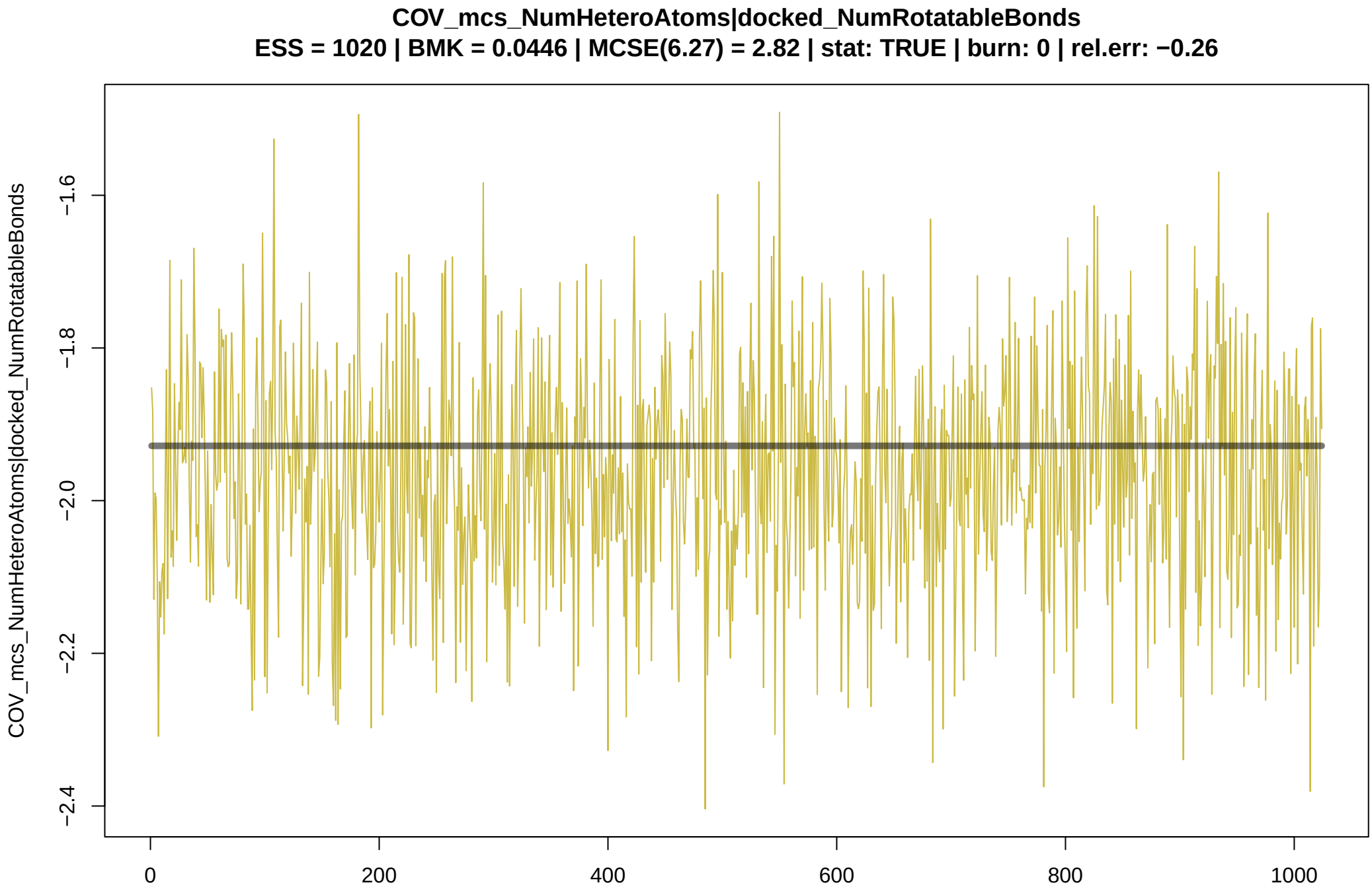

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0576 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | rel.err: 1.13
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.5
−1.6
−1.7
−1.8
−1.9
−2.0
0
200
400
600
800
1000

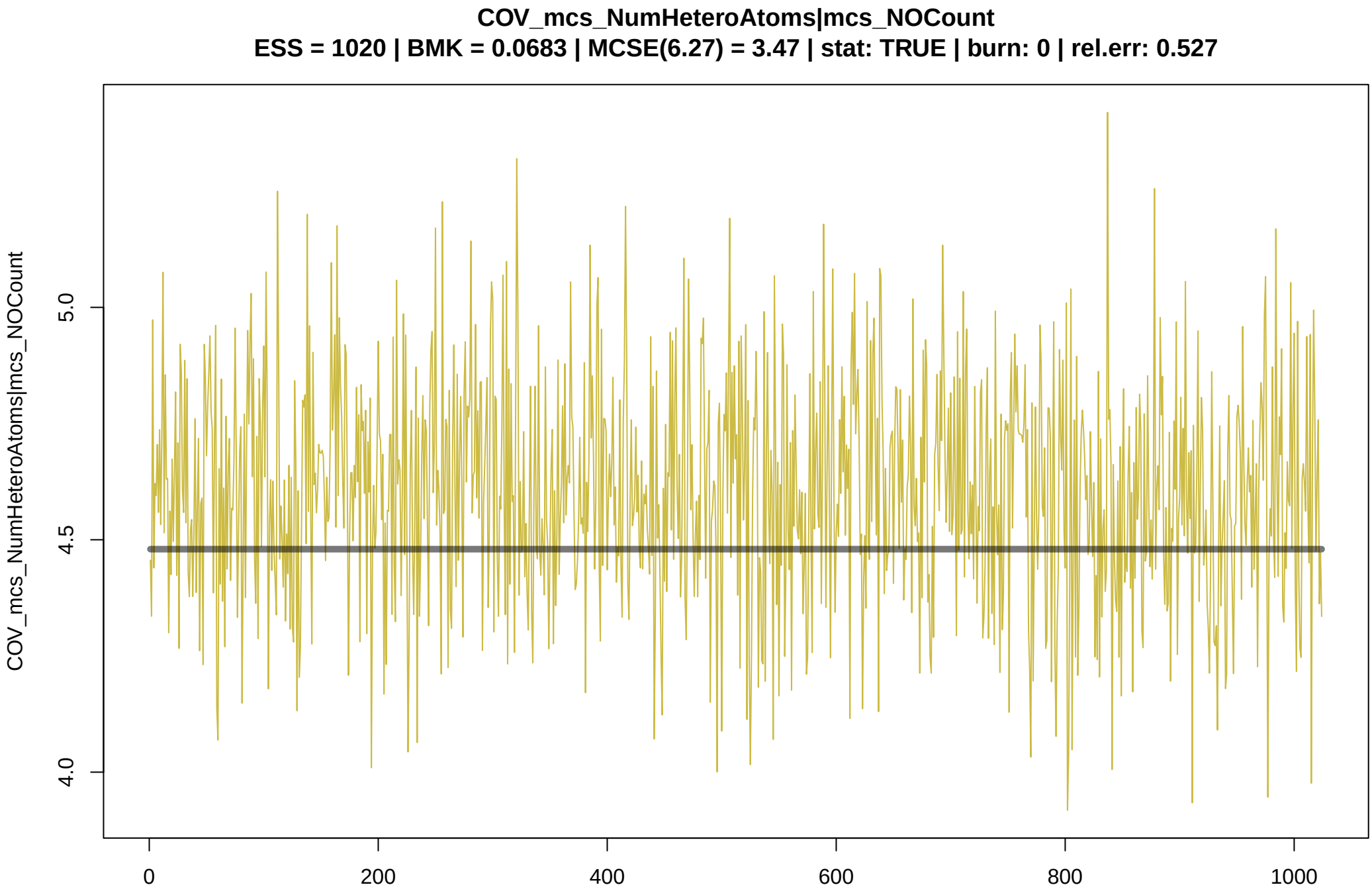

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0728 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0 | rel.err: −1.99
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−11.5
−12.0
−12.5
−13.0
0
200
400
600
800
1000

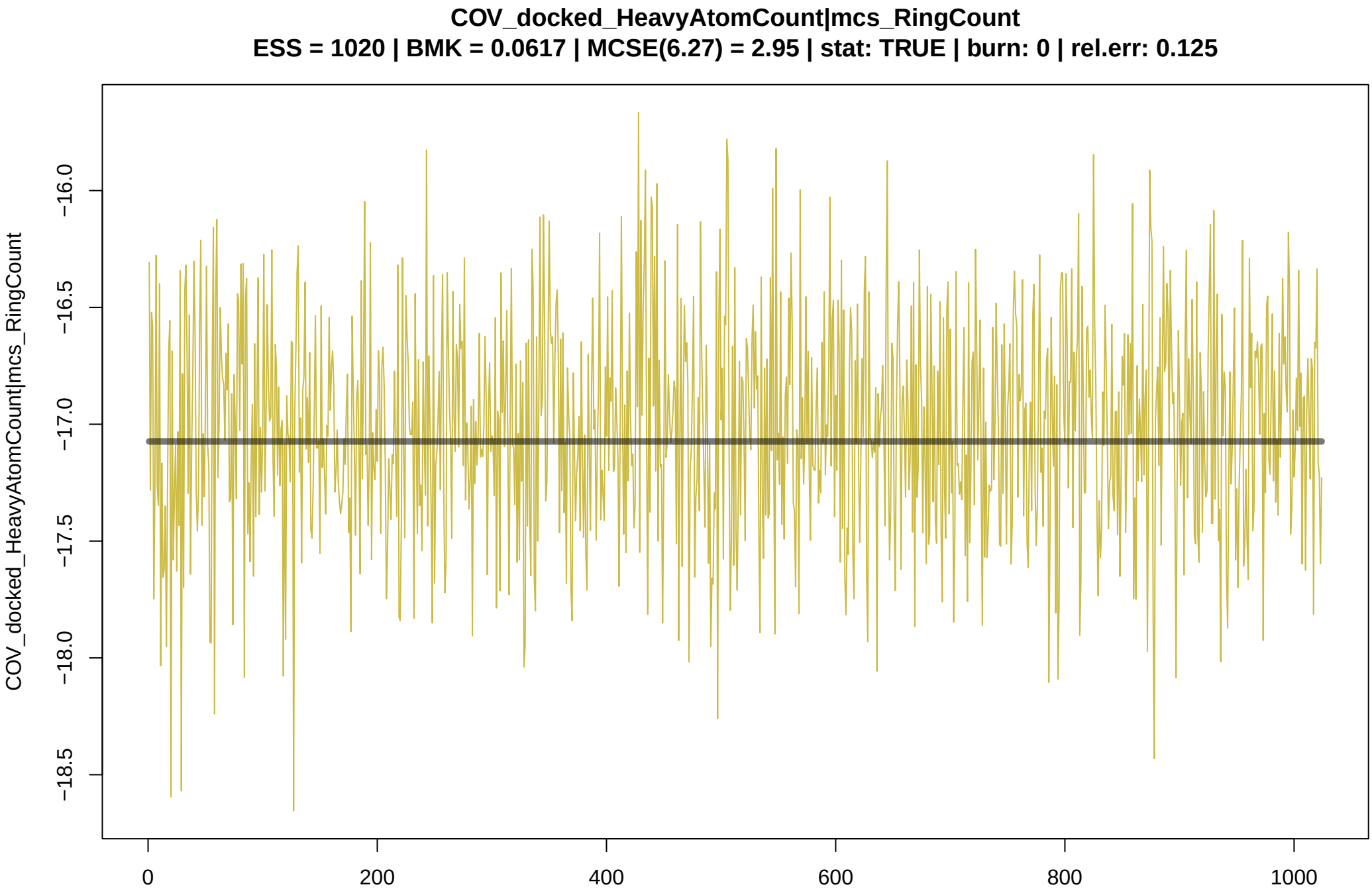

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0515 | MCSE(6.27) = 3.84 | stat: TRUE | burn: 0 | rel.err: −0.346
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−6.5
−7.0
−7.5
−8.0
−8.5
−9.0
0
200
400
600
800
1000

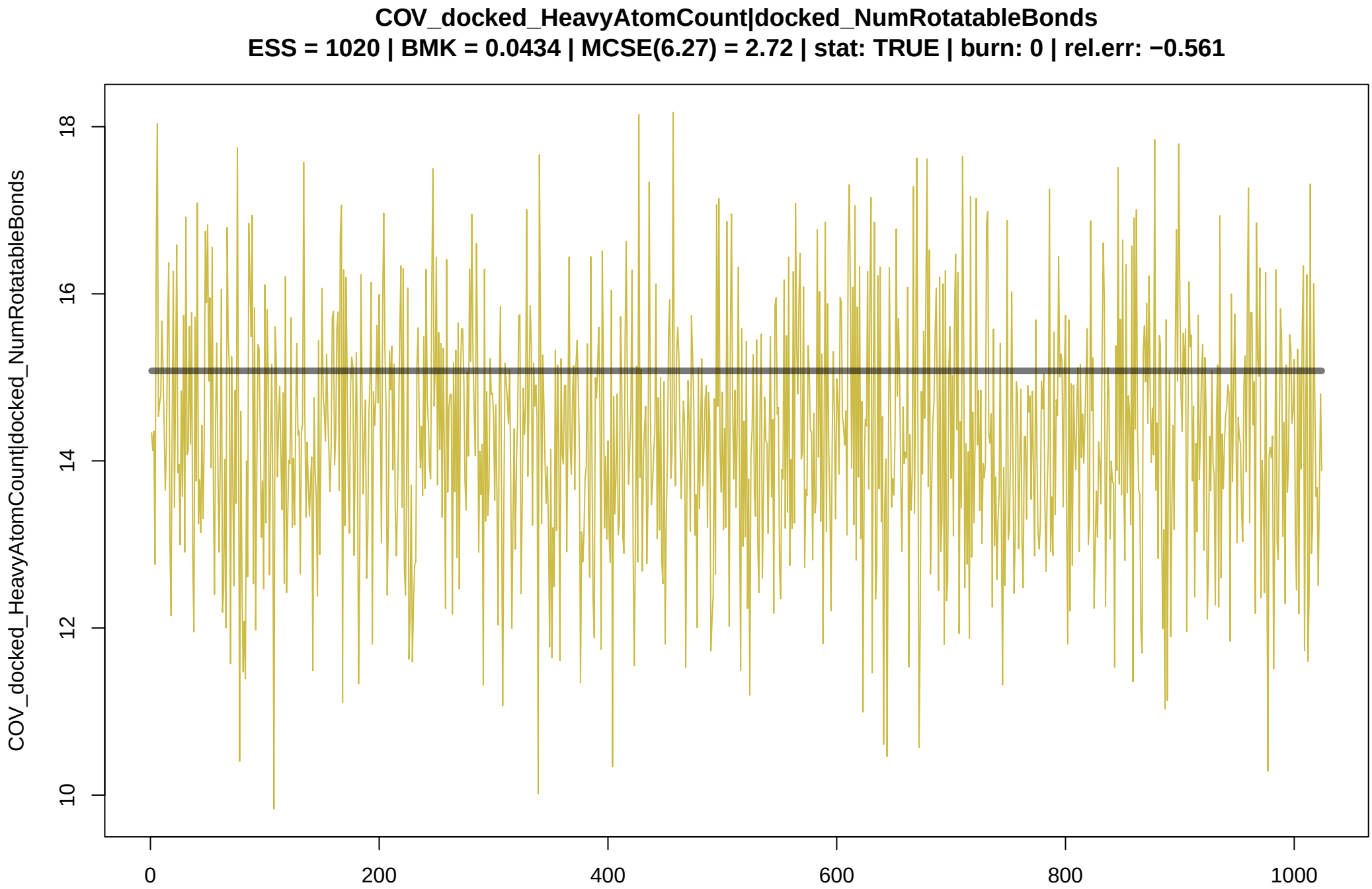

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.058 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | rel.err: 0.927
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−13.5
−14.0
−14.5
−15.0
−15.5
−16.0
−16.5
−17.0
0
200
400
600
800
1000

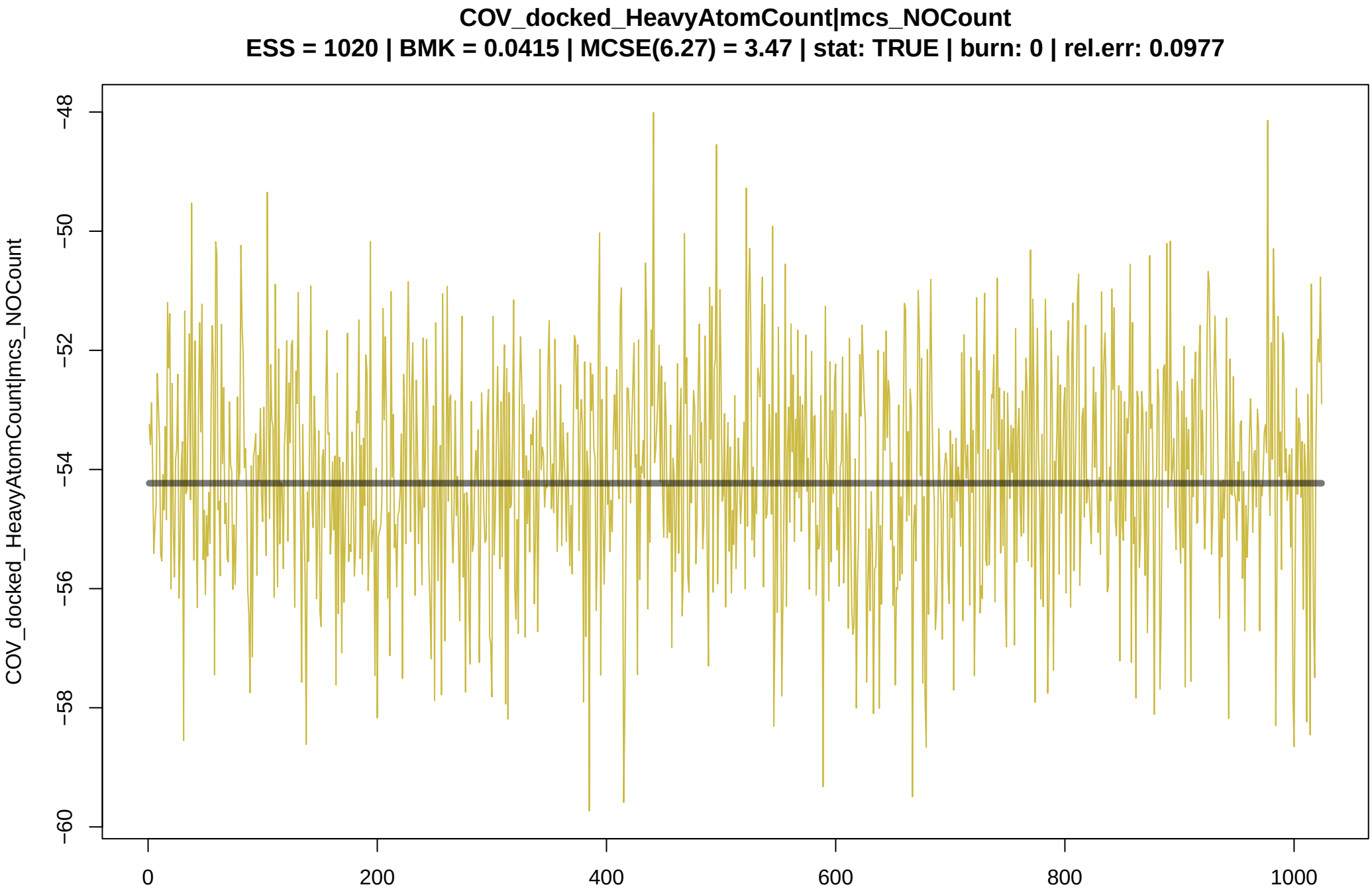

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0748 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: 0.891
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.95
1.00
1.05
1.10
1.15
1.20
0
200
400
600
800
1000

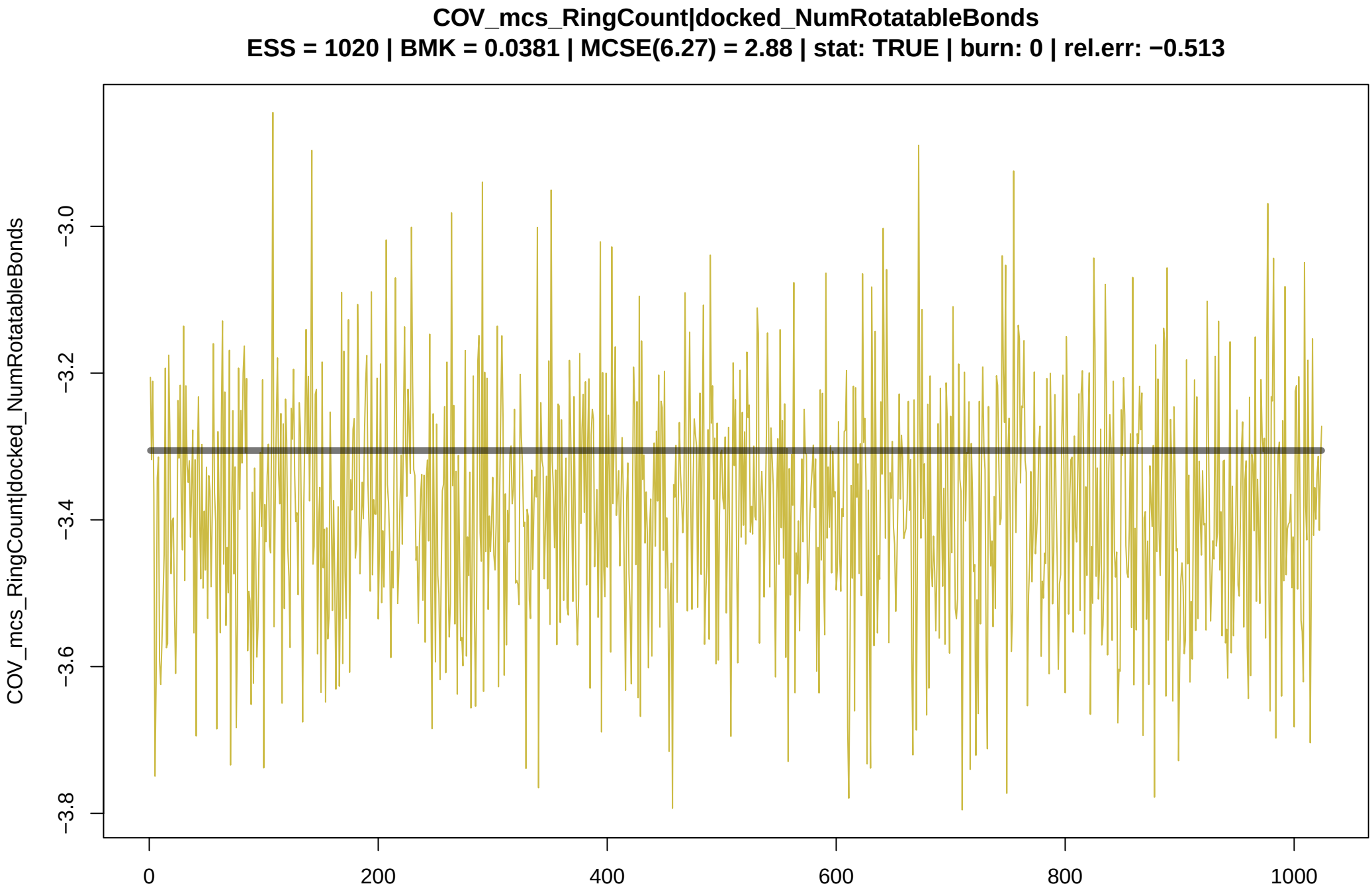

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0446 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: −0.26
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.6
−1.8
−2.0
−2.2
−2.4
0
200
400
600
800
1000

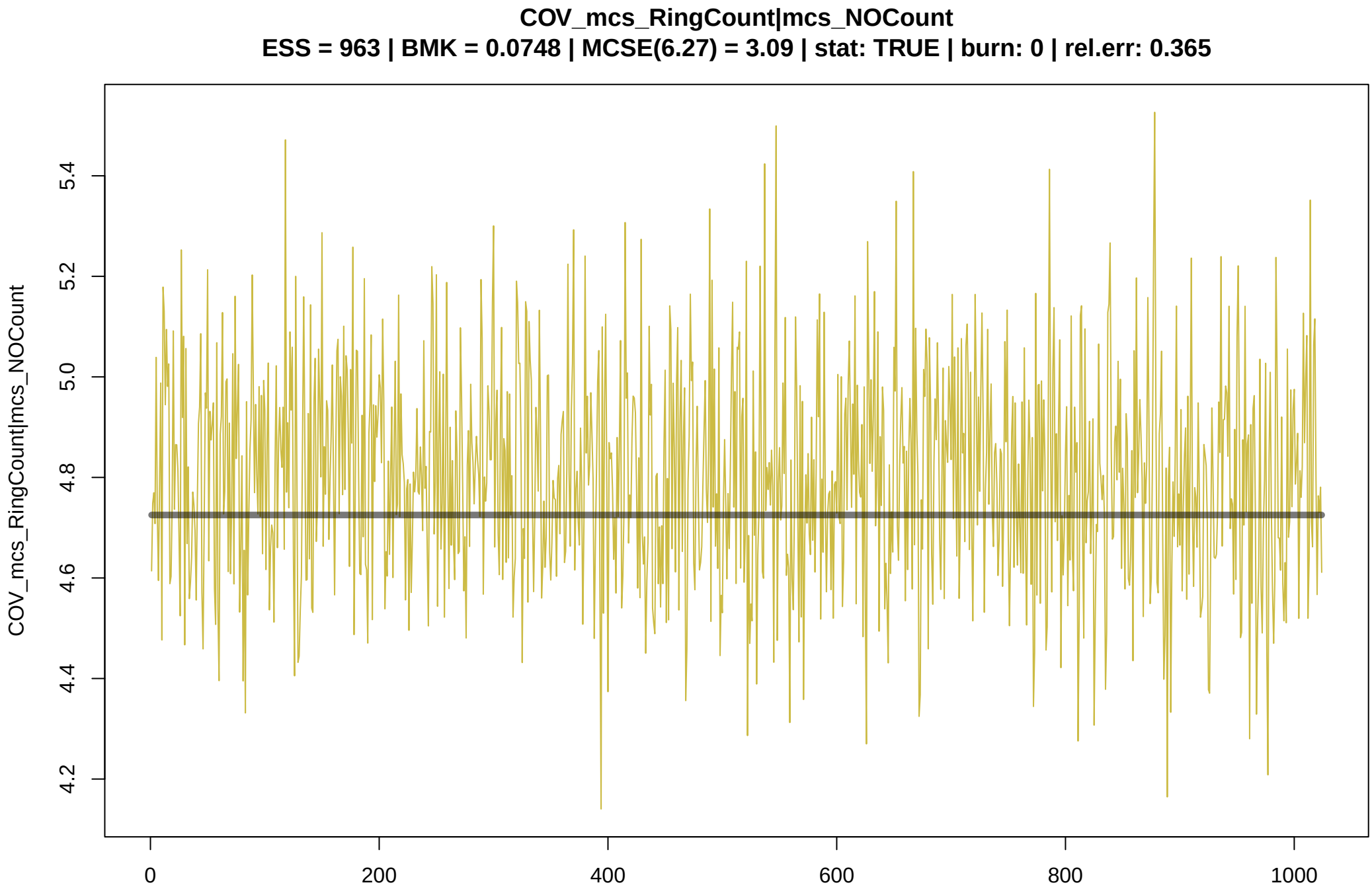

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0683 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | rel.err: 0.527
COV_mcs_NumHeteroAtoms|mcs_NOCount
4.0
4.5
5.0
0
200
400
600
800
1000

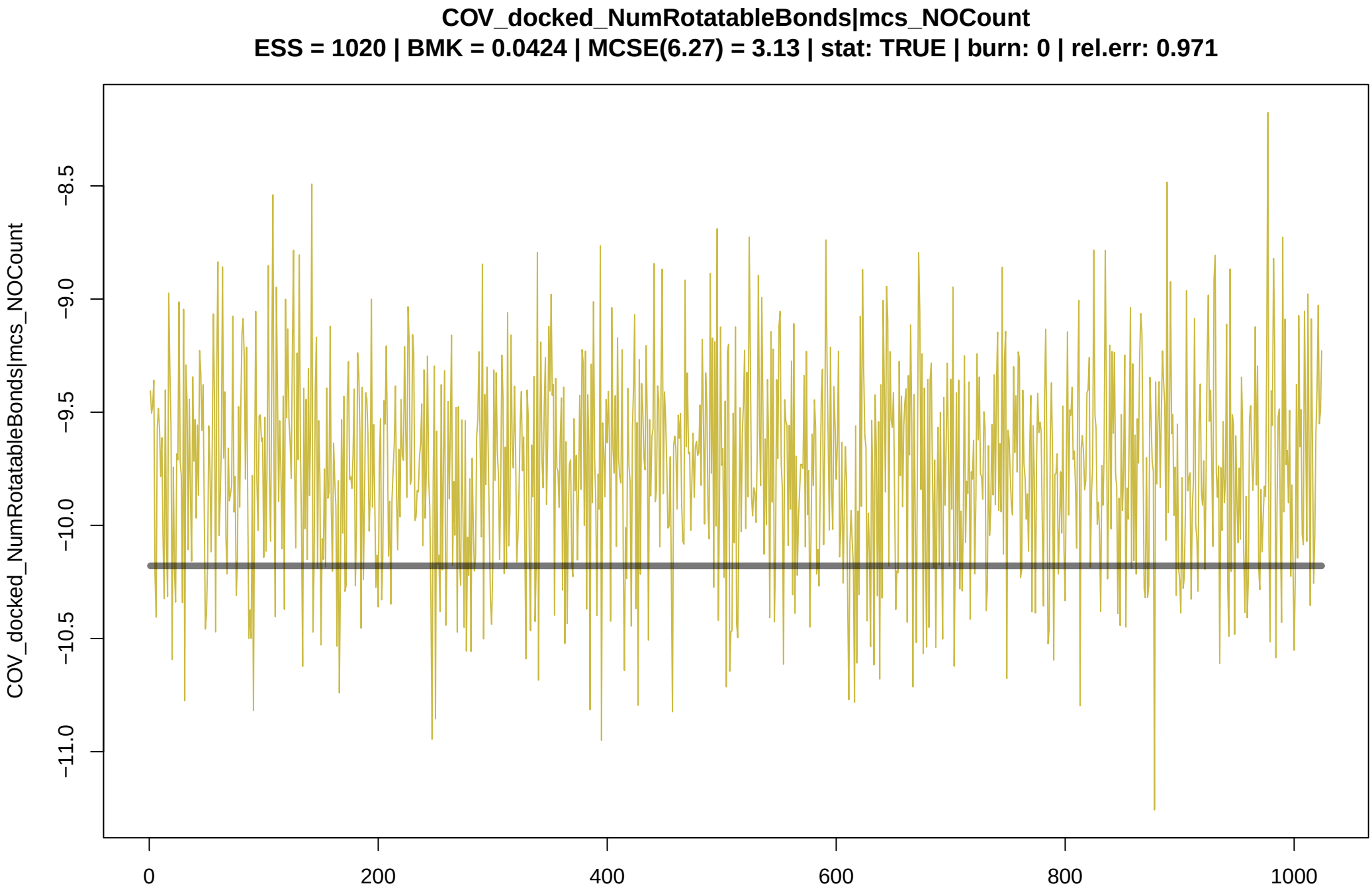

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0617 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: 0.125
COV_docked_HeavyAtomCount|mcs_RingCount
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0434 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: −0.561
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0415 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | rel.err: 0.0977
COV_docked_HeavyAtomCount|mcs_NOCount
−48
−50
−52
−54
−56
−58
−60
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0381 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: −0.513
COV_mcs_RingCount|docked_NumRotatableBonds
−3.0
−3.2
−3.4
−3.6
−3.8
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 963 | BMK = 0.0748 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | rel.err: 0.365
COV_mcs_RingCount|mcs_NOCount
4.2
4.4
4.6
4.8
5.0
5.2
5.4
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0424 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | rel.err: 0.971
COV_docked_NumRotatableBonds|mcs_NOCount
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
0
200
400
600
800
1000