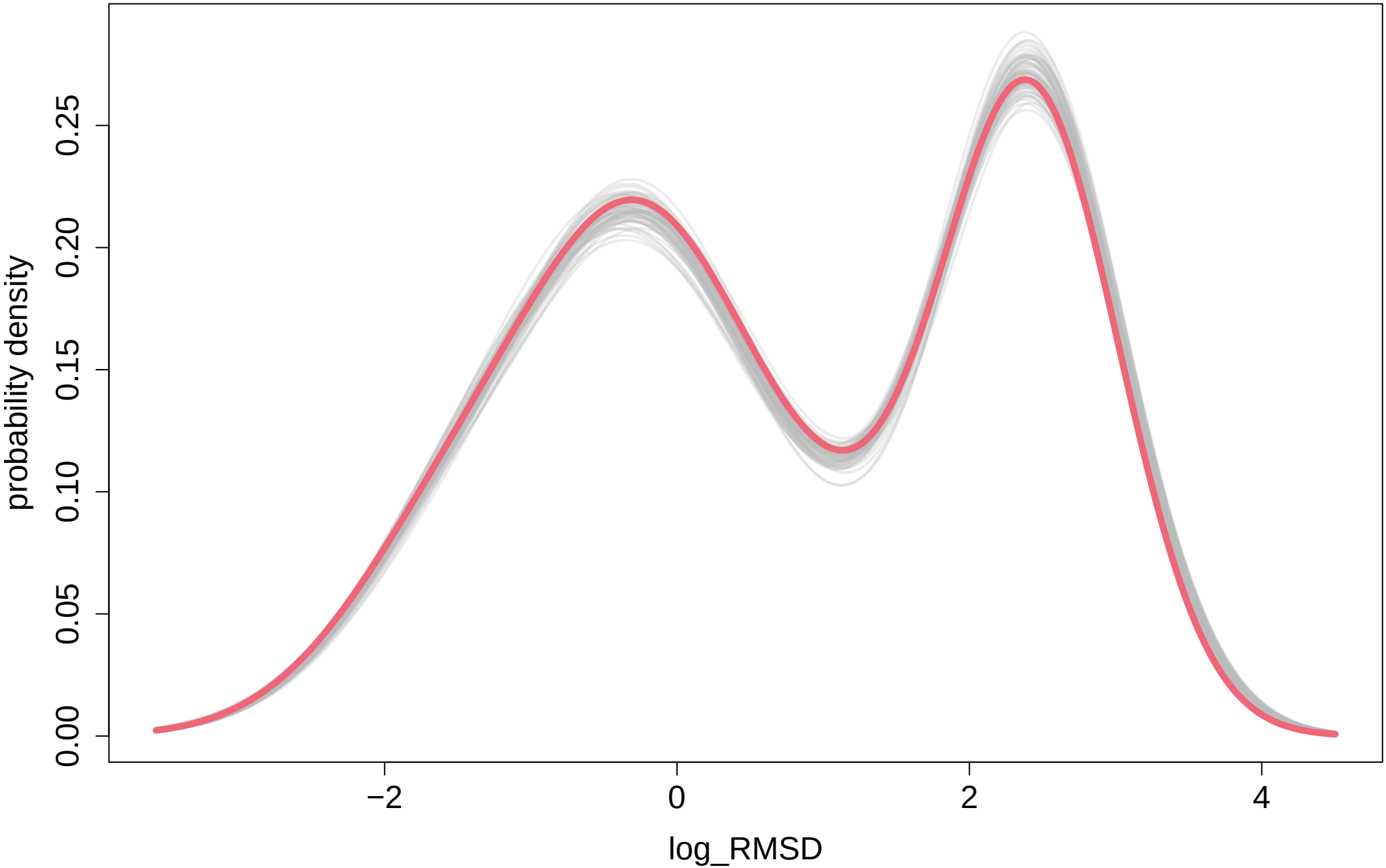
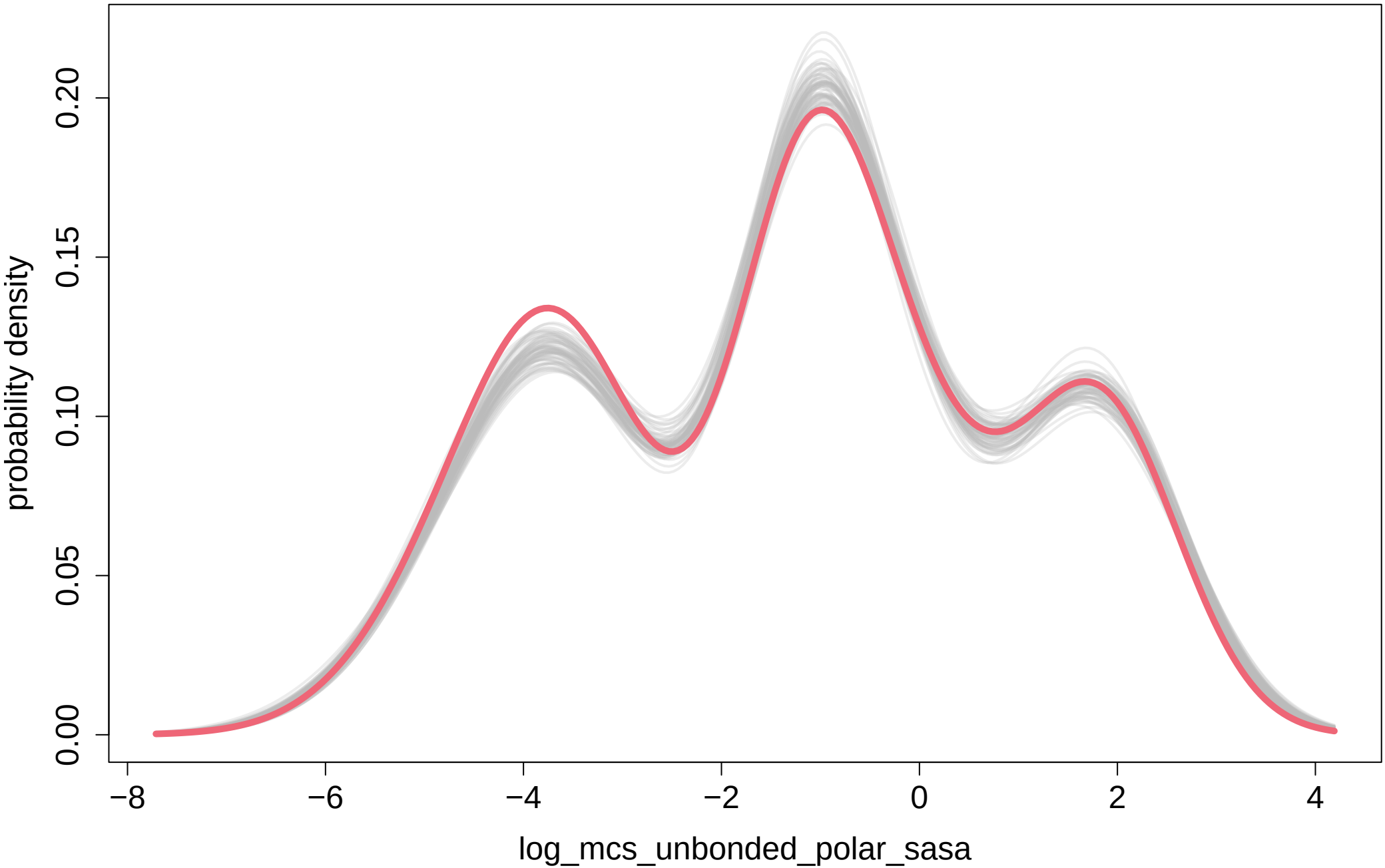
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.317964088502535
max MCSE = 9.90751678746672
all stationary: FALSE
burn: 714
max rel.err.: 1.49555561450031

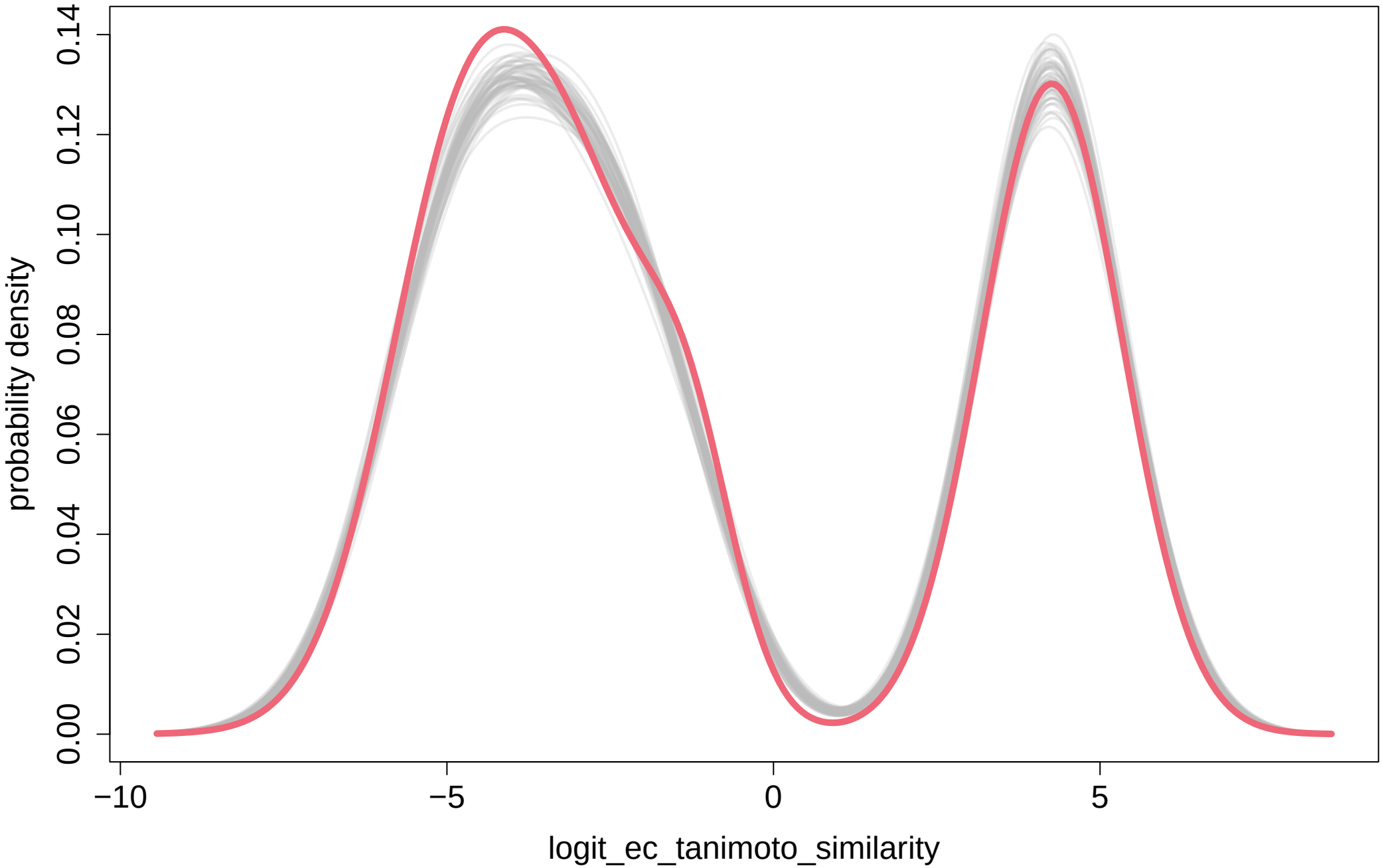
−− STATS 2D −−
min ESS = 1024
max BMK = 0.076301544919282 7
max MCSE = 4.19870939486683
all stationary: TRUE
burn: 0
max rel.err.: 2.18032297923413

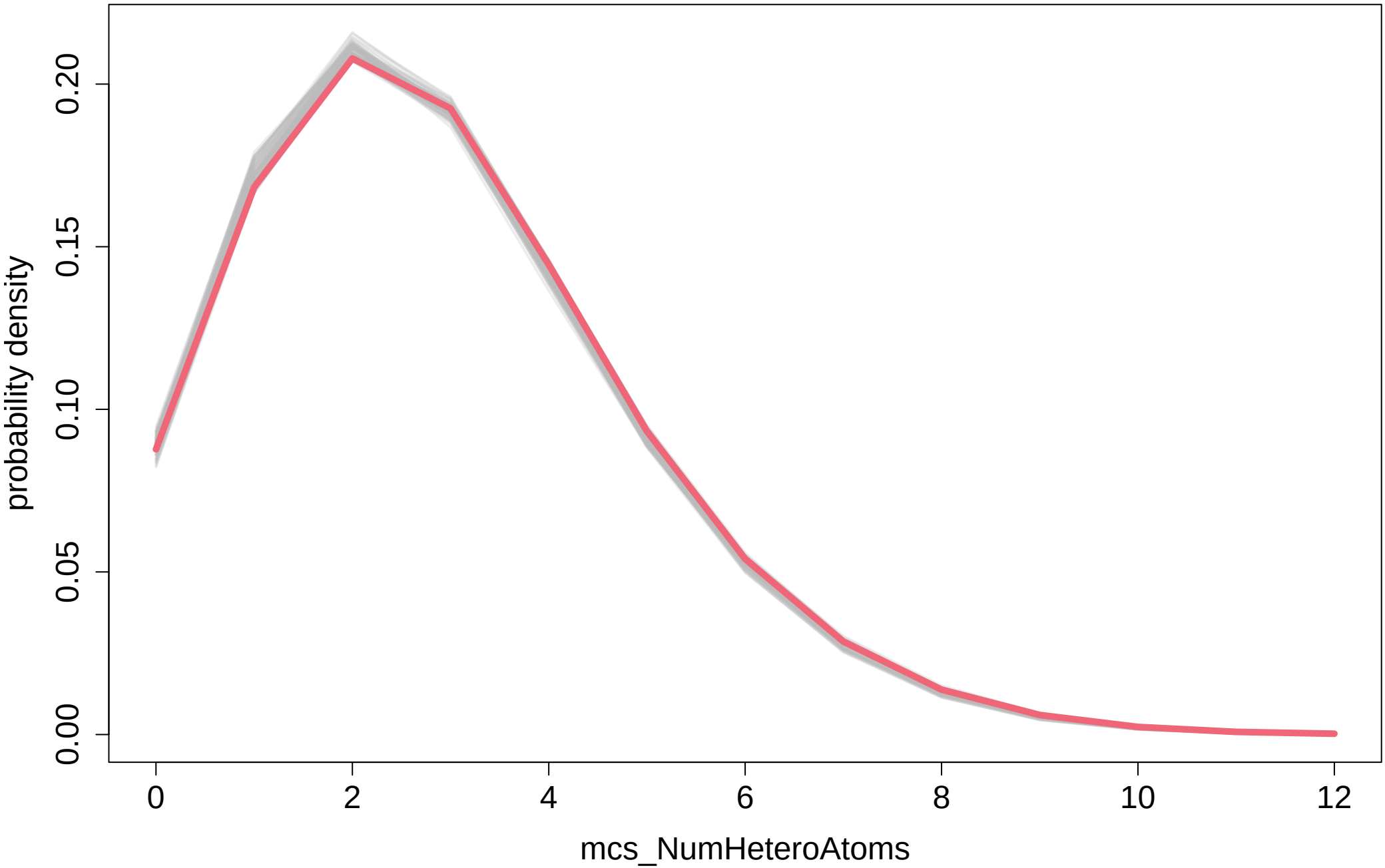
−− STATS 1D −−
min ESS = 29.9025132528866
max BMK = 0.136844050586569
max MCSE = 9.61138890162248
all stationary: FALSE
burn: 0
max rel.err.: 2.74944118601327

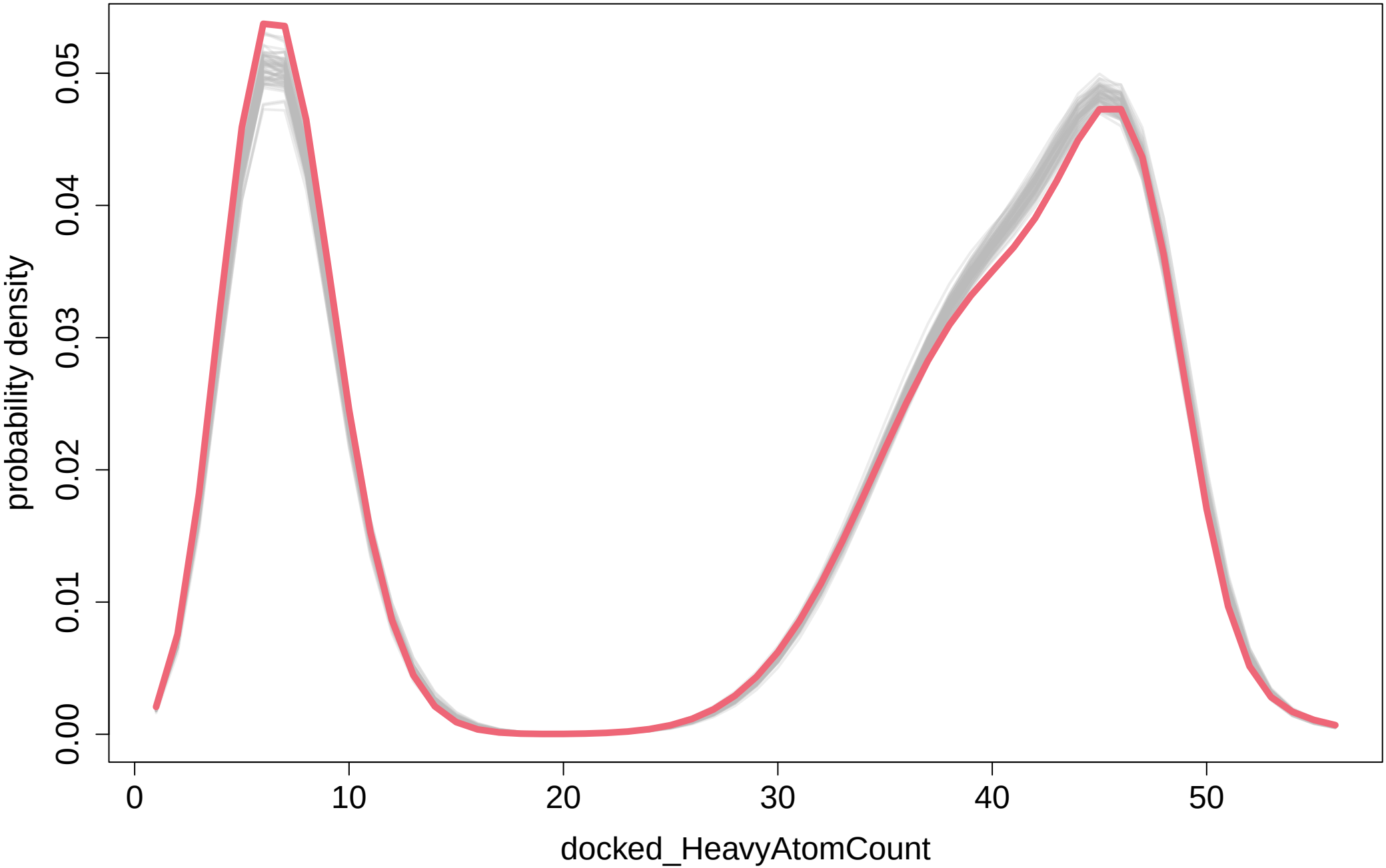
Occupied clusters: 9 of 64
LL: −62500 +− 13

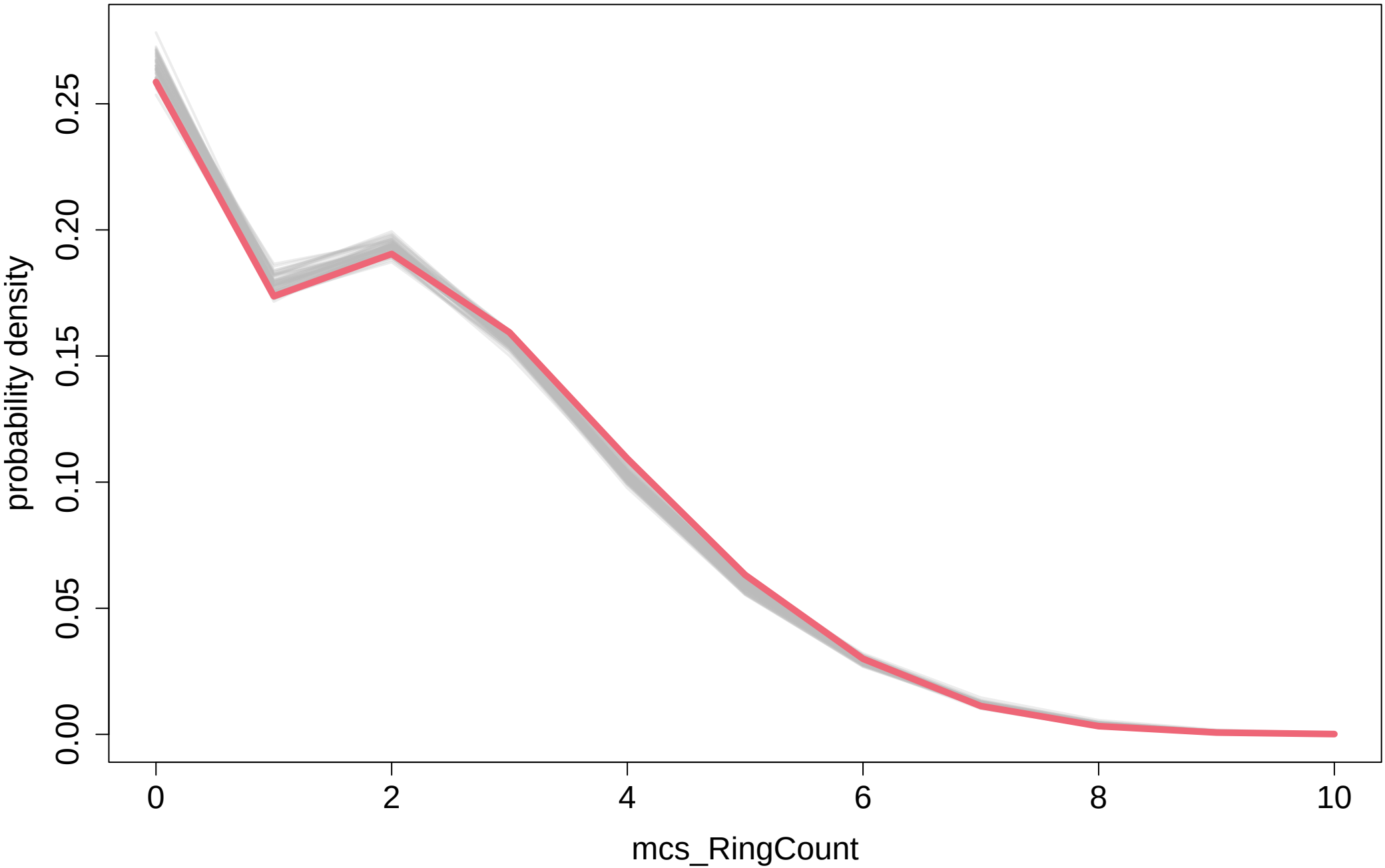

probability density
0.00
0.05
0.10
0.15
0.20
0.25
−2
0
2
4
log_RMSD

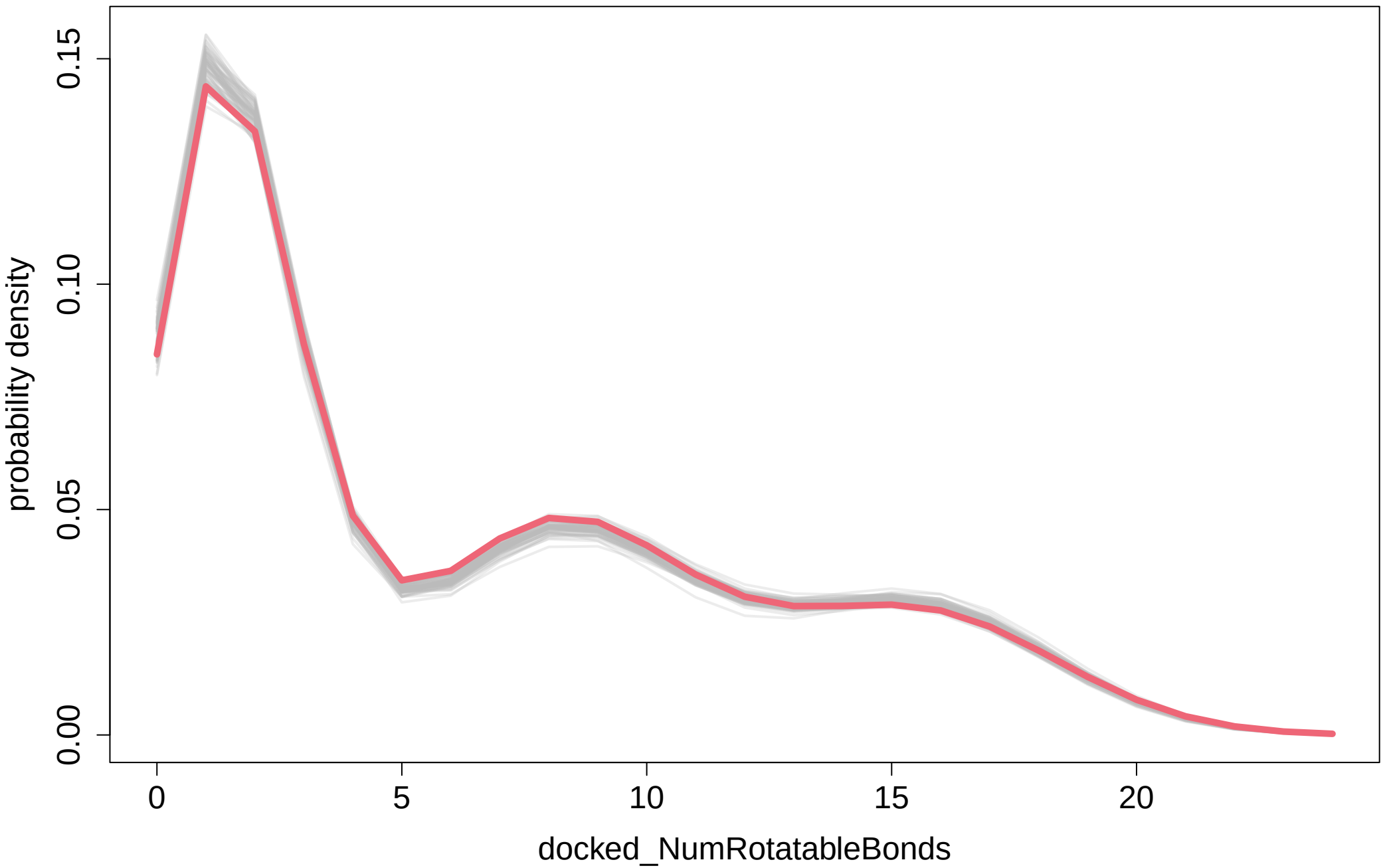

probability density
0.00
0.05
0.10
0.15
0.20
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

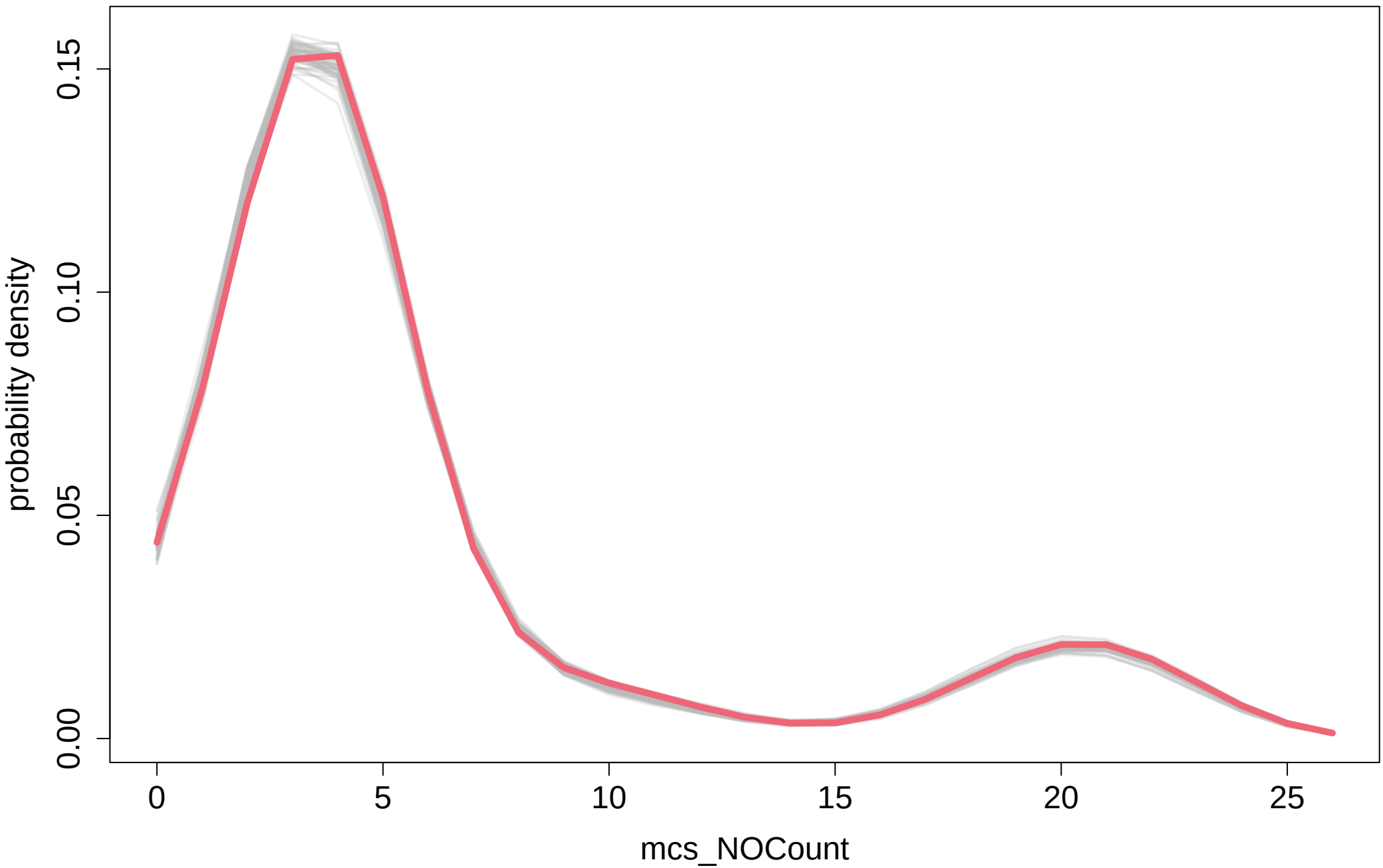

probability density
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
−10
−5
0
5
logit_ec_tanimoto_similarity

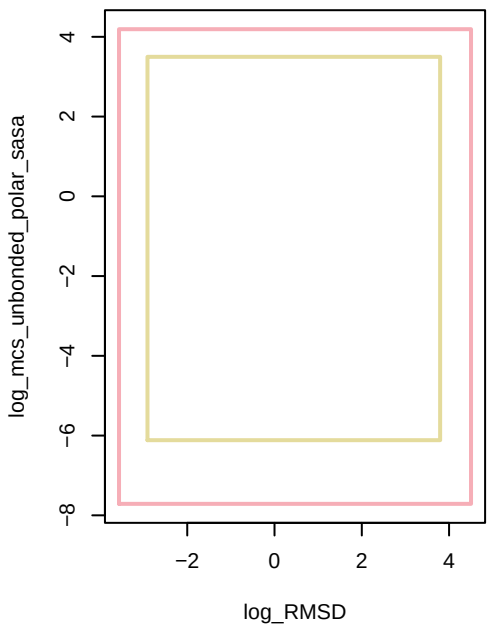

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms

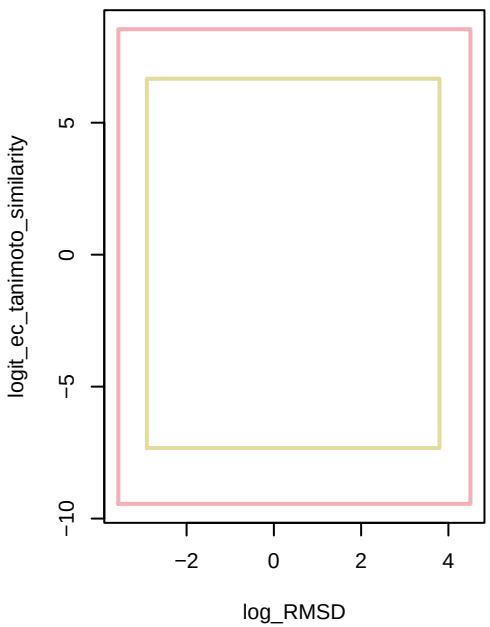

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount

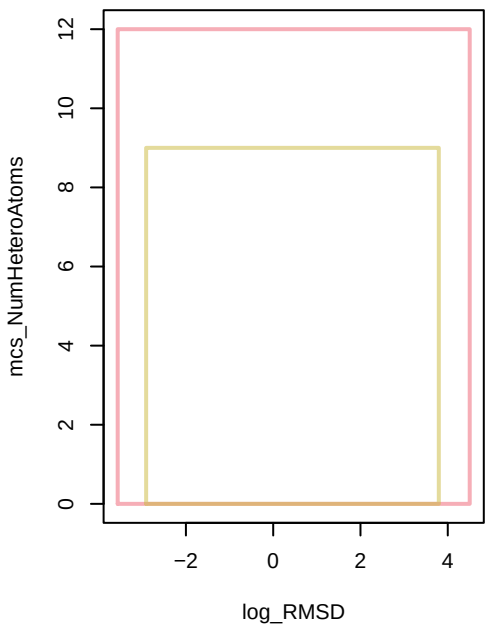

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount

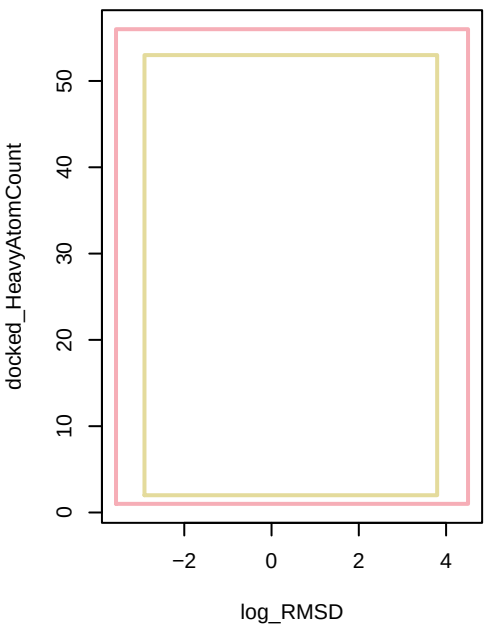

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
docked_NumRotatableBonds

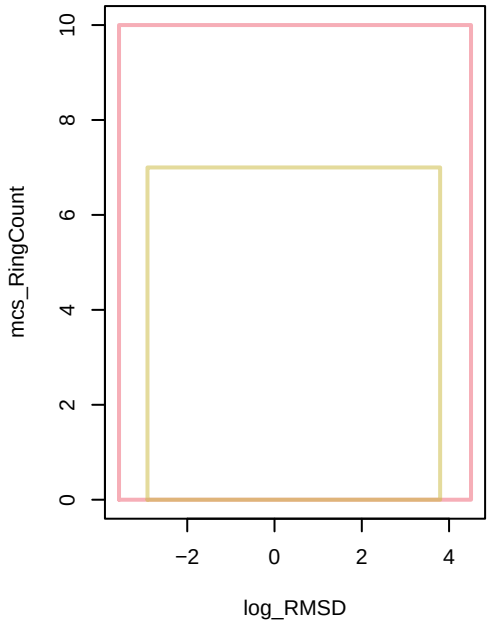

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

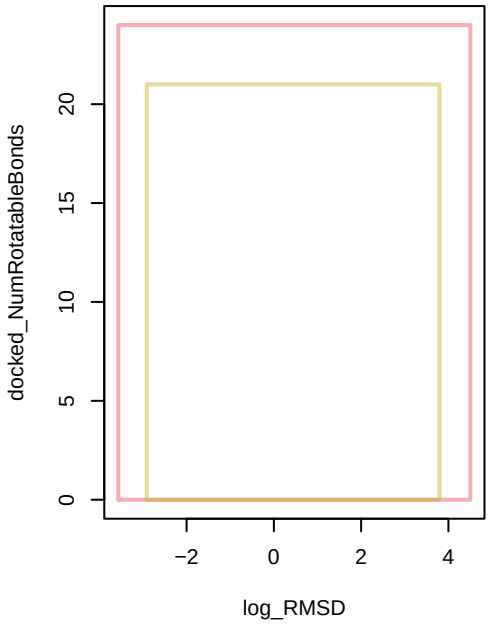

log_mcs_unbonded_polar_sasa
log_RMSD

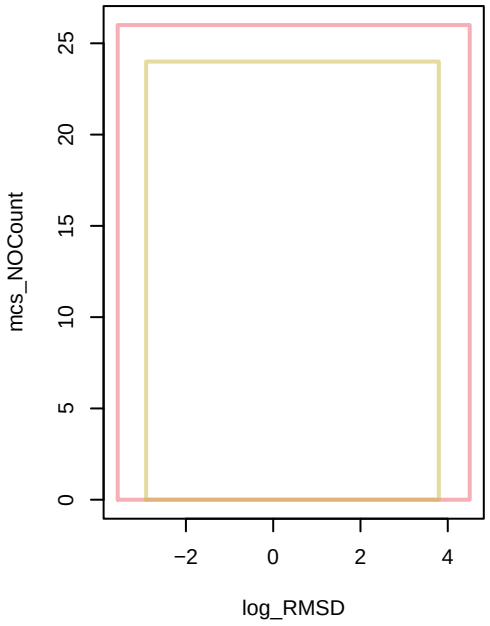

logit_ec_tanimoto_similarity
log_RMSD

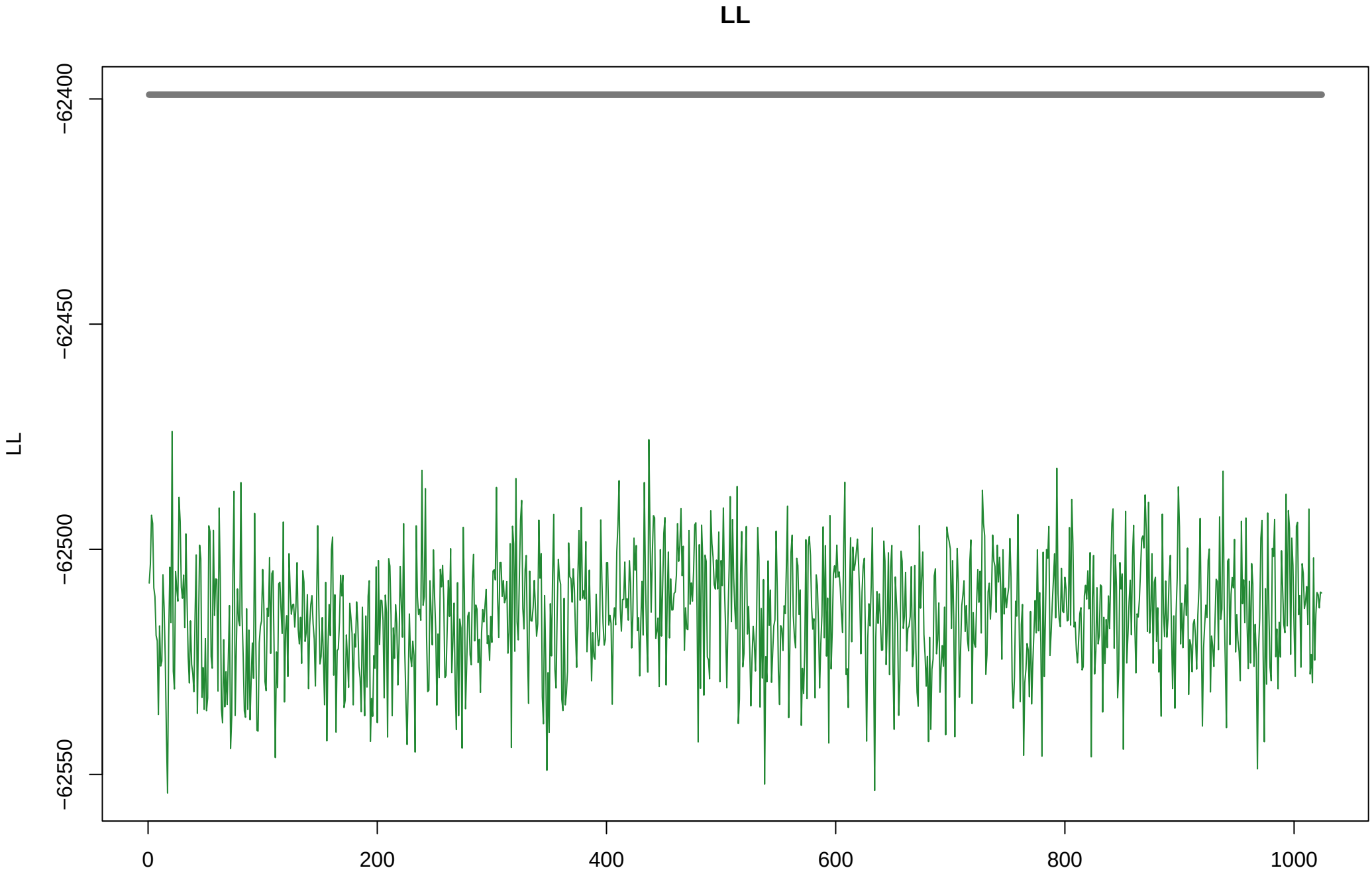

mcs_NumHeteroAtoms
log_RMSD

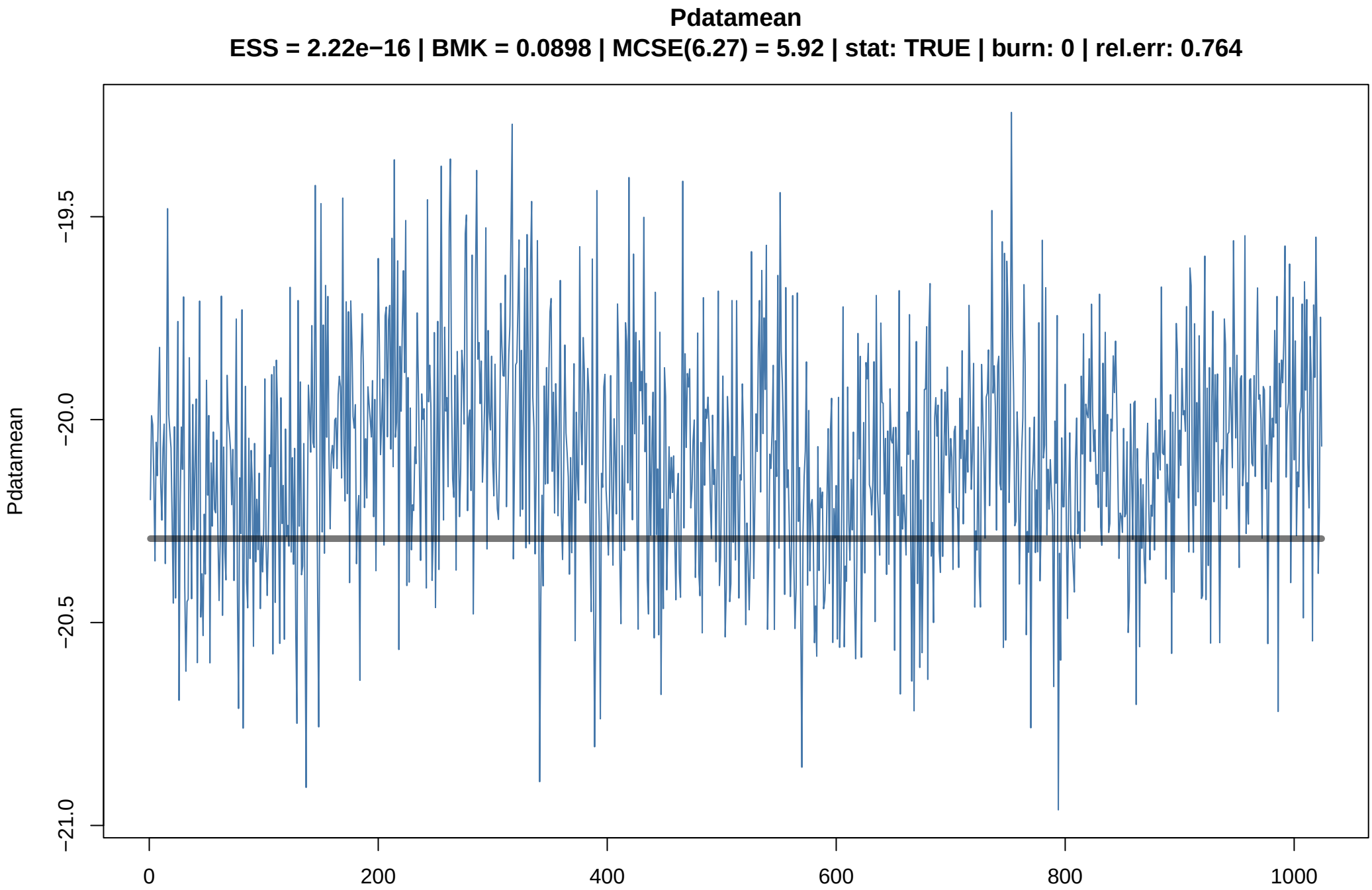

docked_HeavyAtomCount
log_RMSD

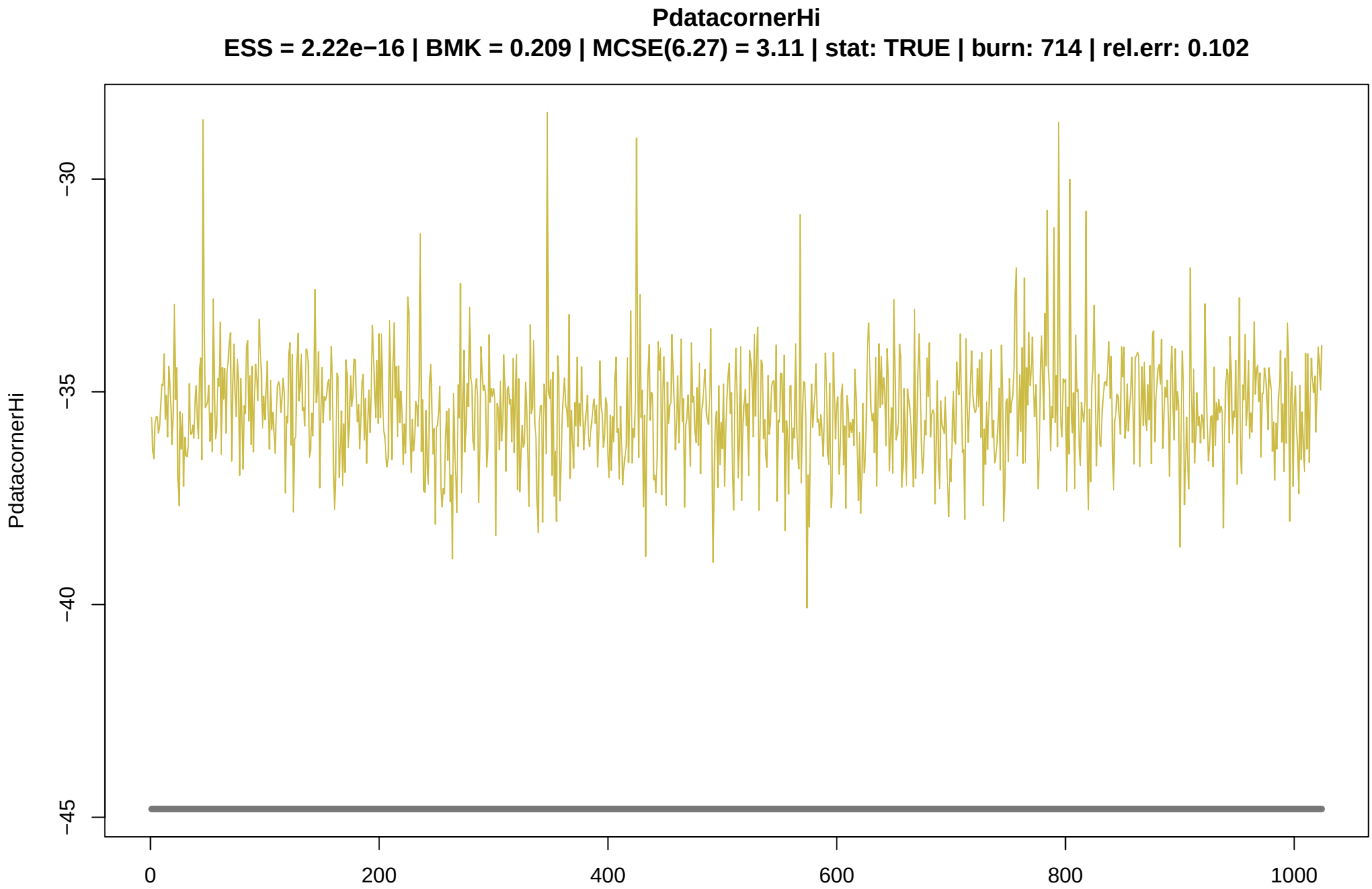

mcs_RingCount
log_RMSD

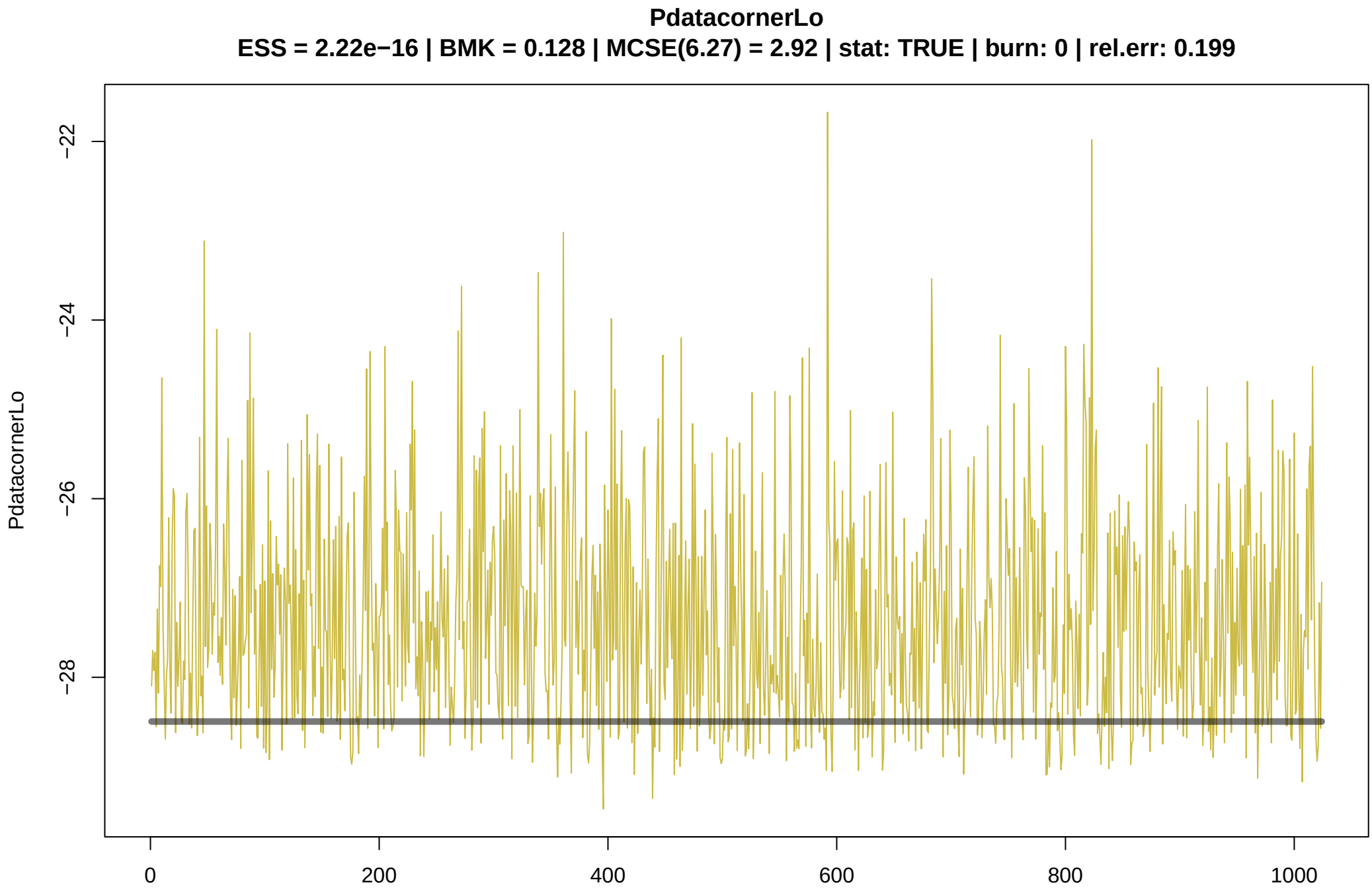

docked_NumRotatableBonds
log_RMSD

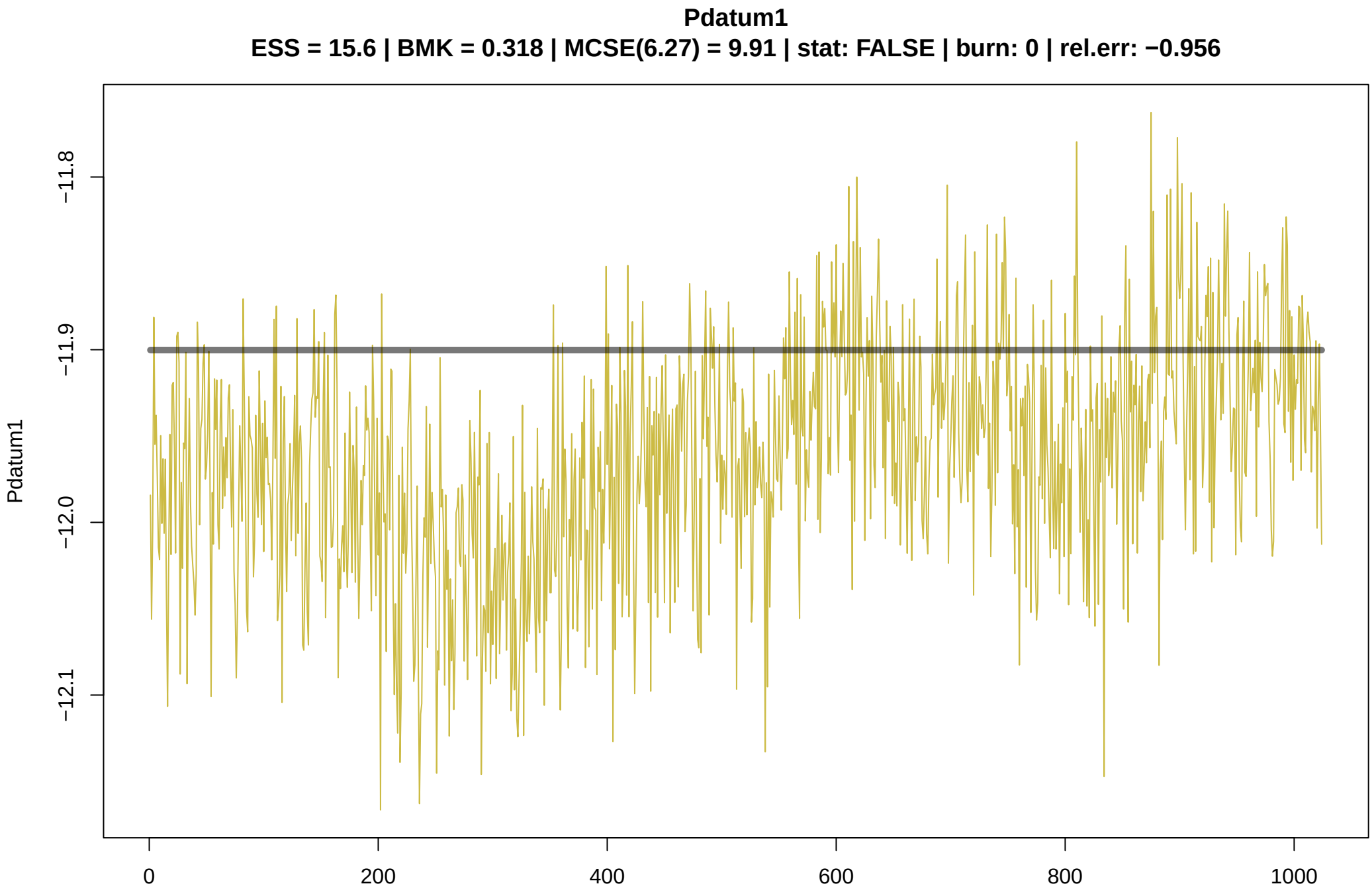

mcs_NOCount
log_RMSD

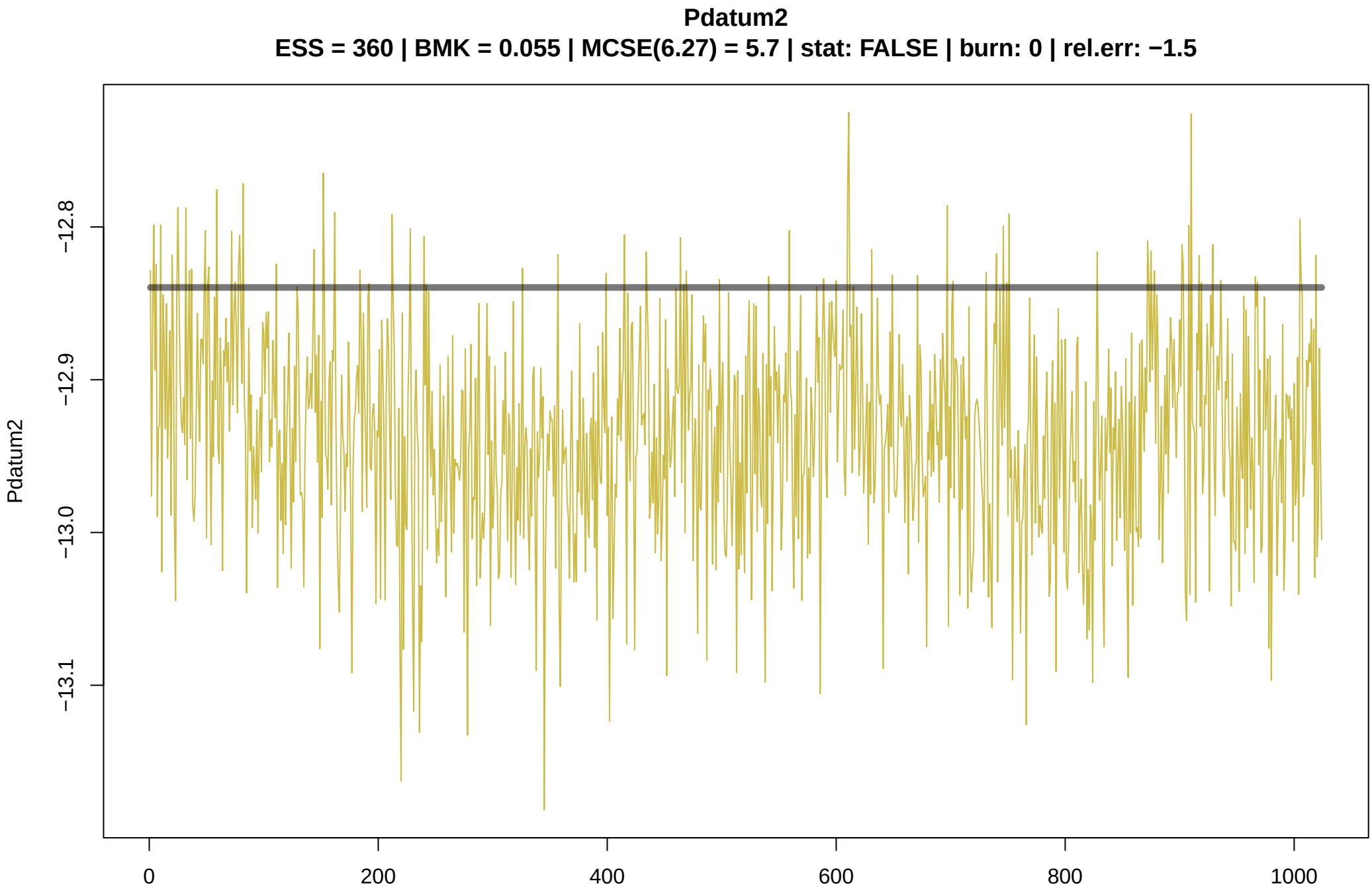

LL
LL
−62400
−62450
−62500
−62550
0
200
400
600
800
1000

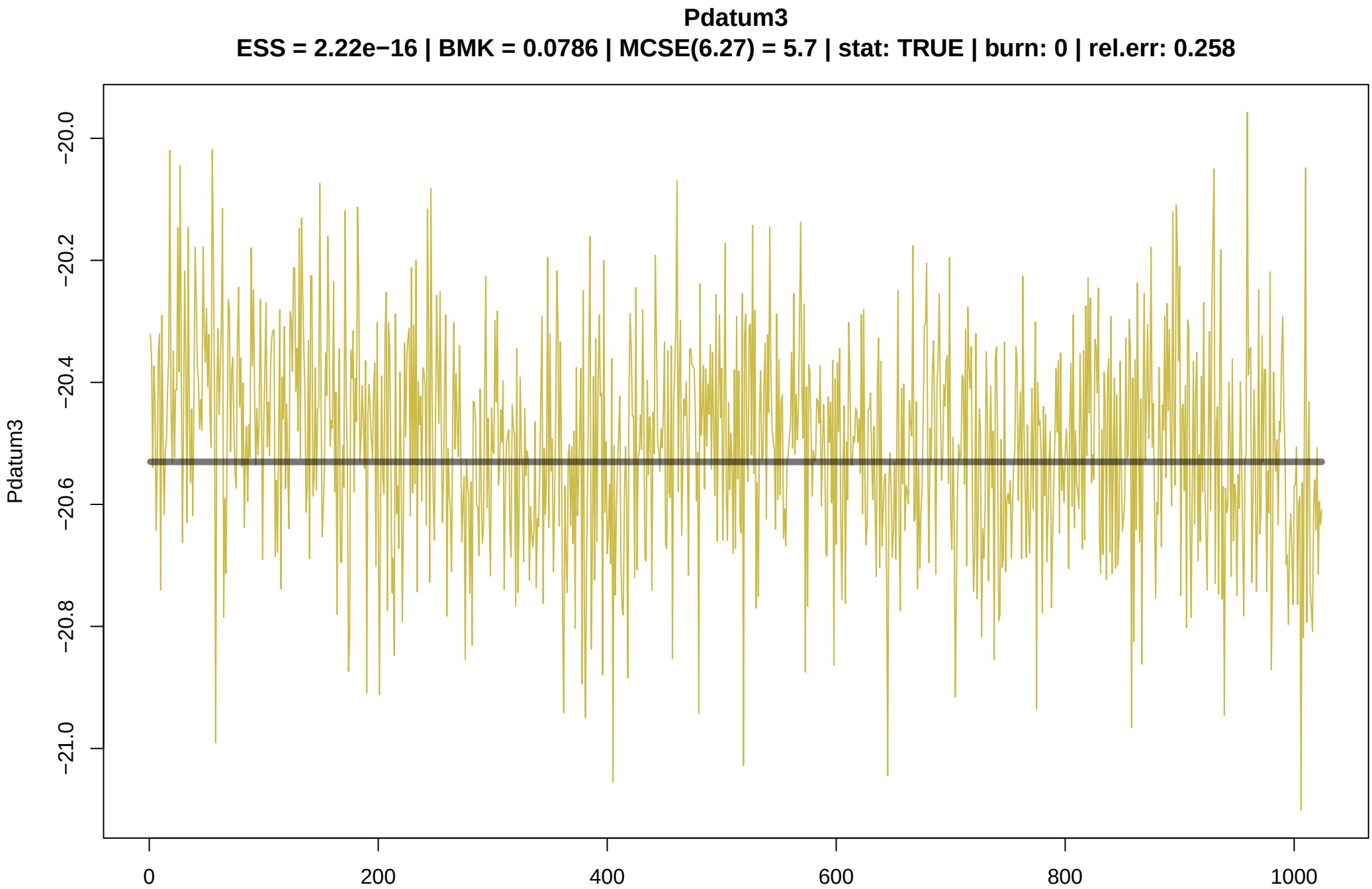

Pdatamean
ESS = 2.22e−16 | BMK = 0.0898 | MCSE(6.27) = 5.92 | stat: TRUE | burn: 0 | rel.err: 0.764
Pdatamean
−19.5
−20.0
−20.5
−21.0
0
200
400
600
800
1000

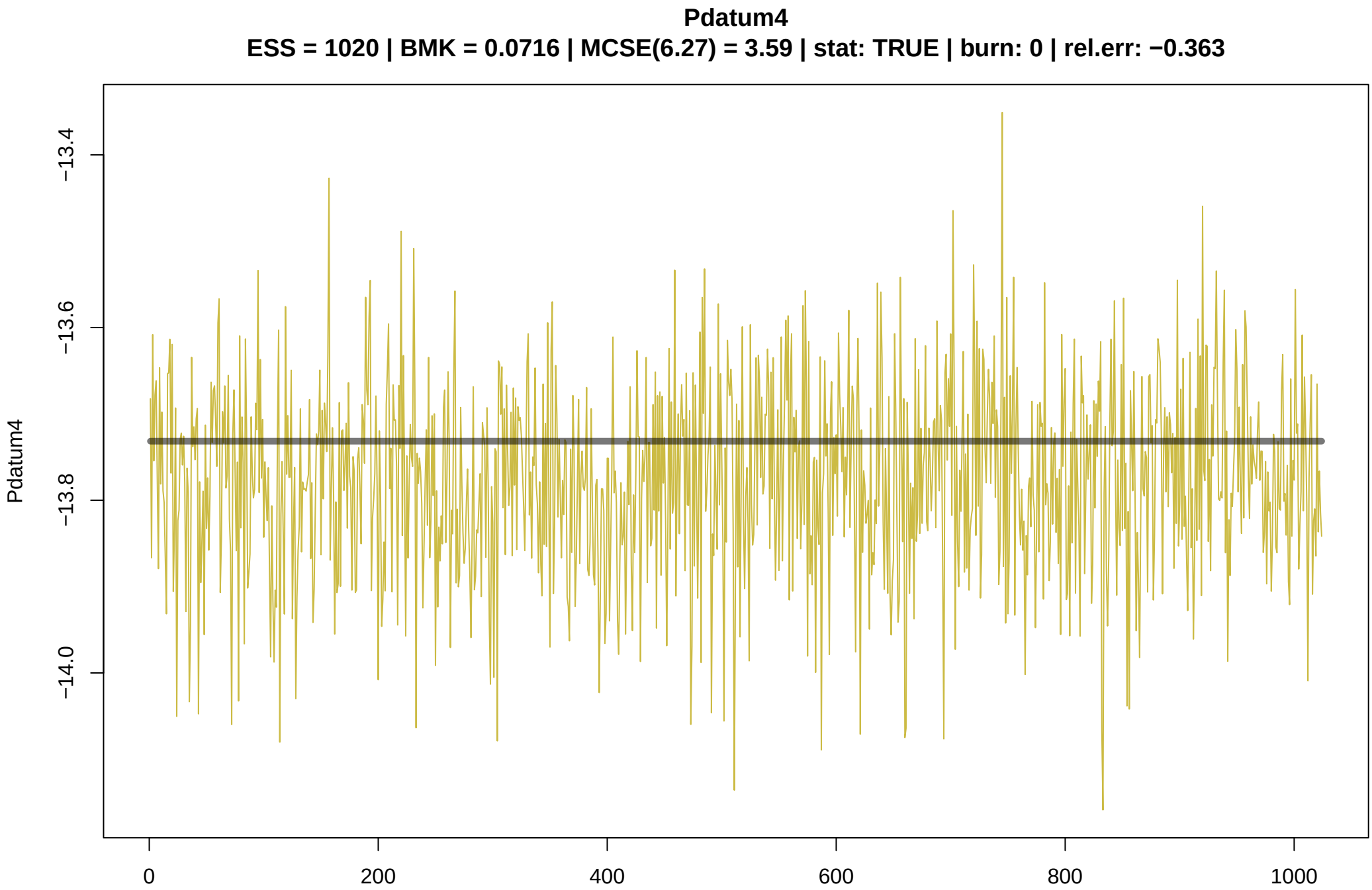

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.209 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 714 | rel.err: 0.102
PdatacornerHi
−30
−35
−40
−45
0
200
400
600
800
1000

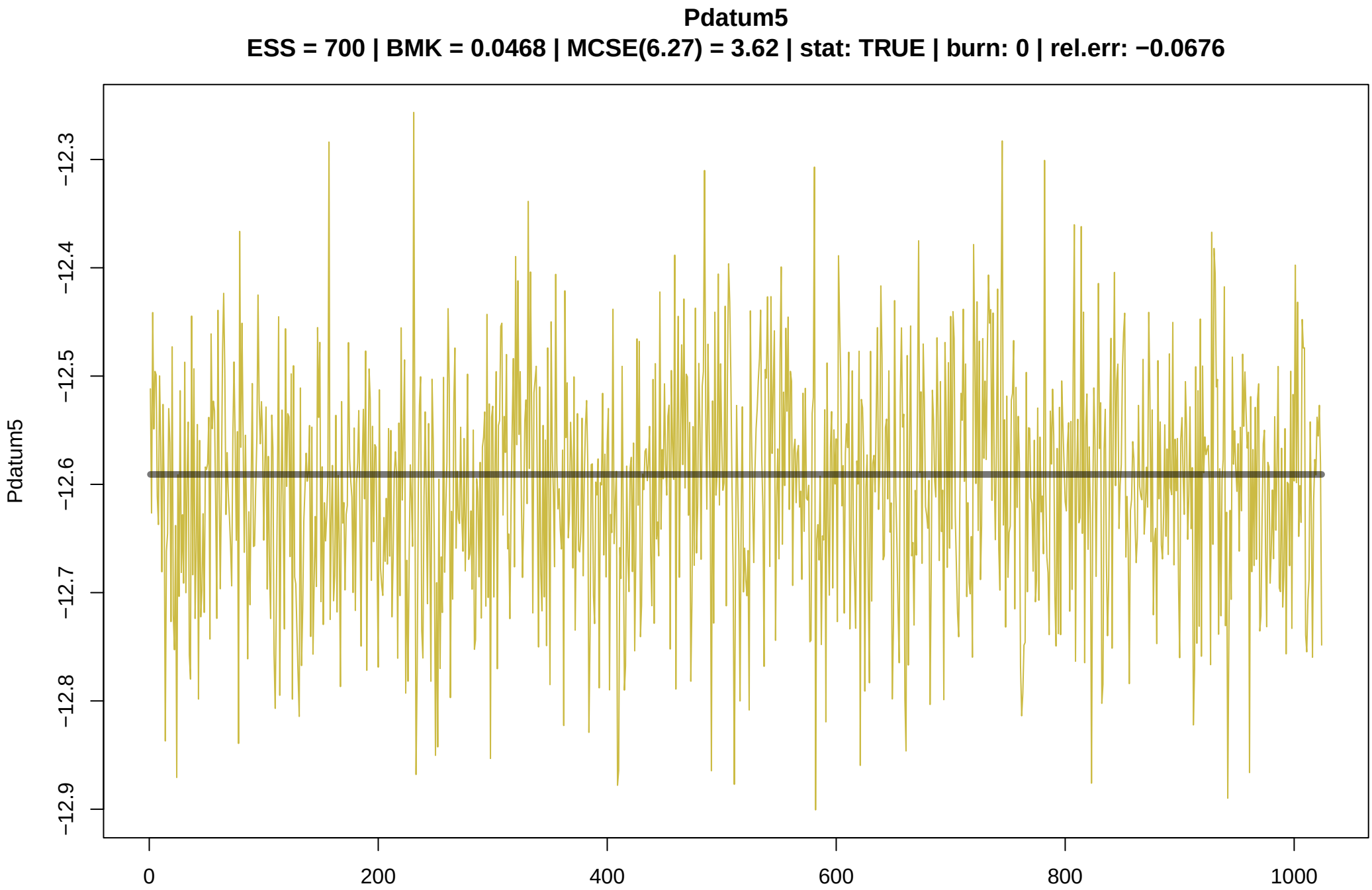

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.128 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0 | rel.err: 0.199
PdatacornerLo
−22
−24
−26
−28
0
200
400
600
800
1000

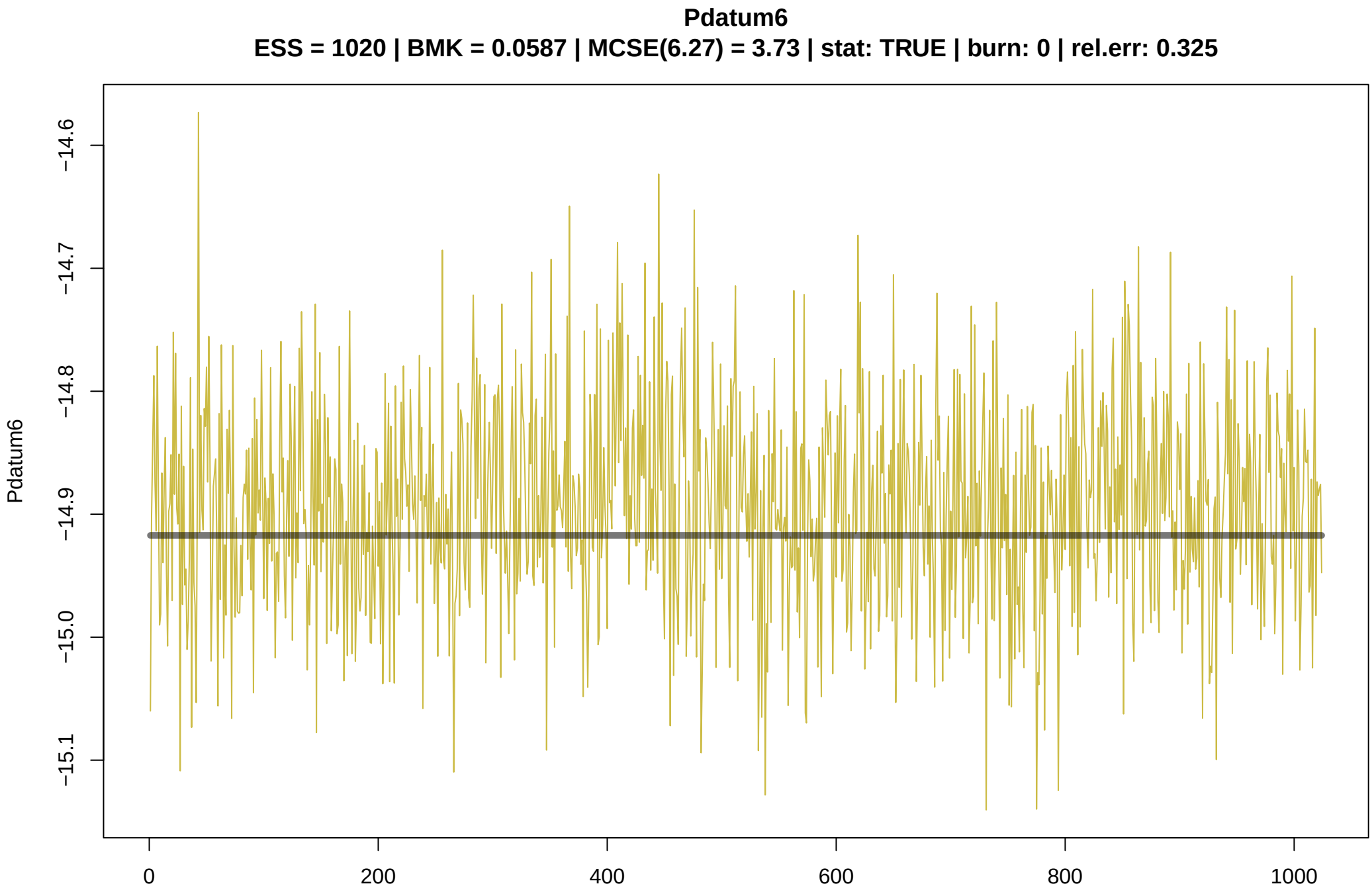

Pdatum1
ESS = 15.6 | BMK = 0.318 | MCSE(6.27) = 9.91 | stat: FALSE | burn: 0 | rel.err: −0.956
Pdatum1
−11.8
−11.9
−12.0
−12.1
0
200
400
600
800
1000

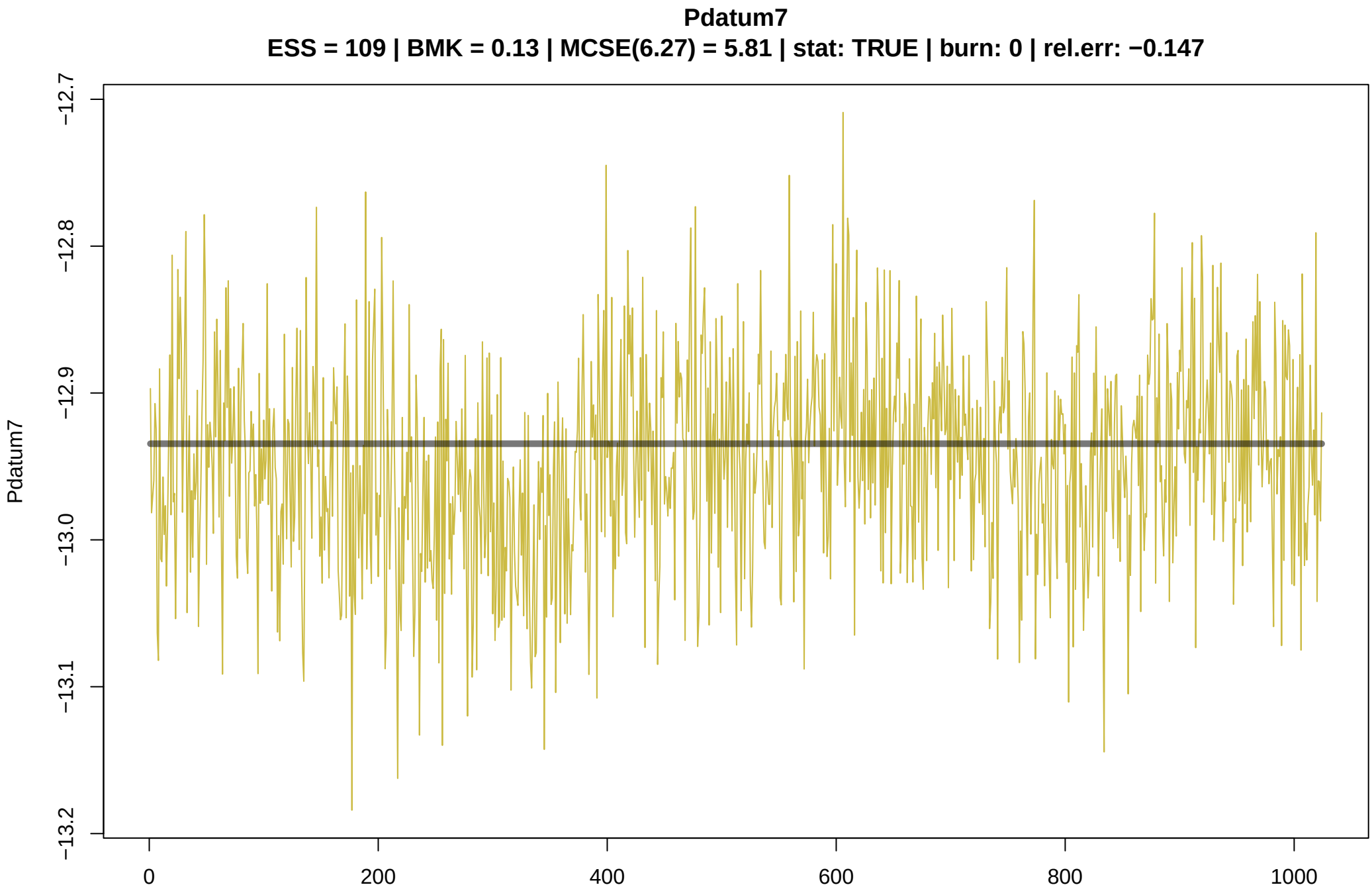

Pdatum2
ESS = 360 | BMK = 0.055 | MCSE(6.27) = 5.7 | stat: FALSE | burn: 0 | rel.err: −1.5
Pdatum2
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

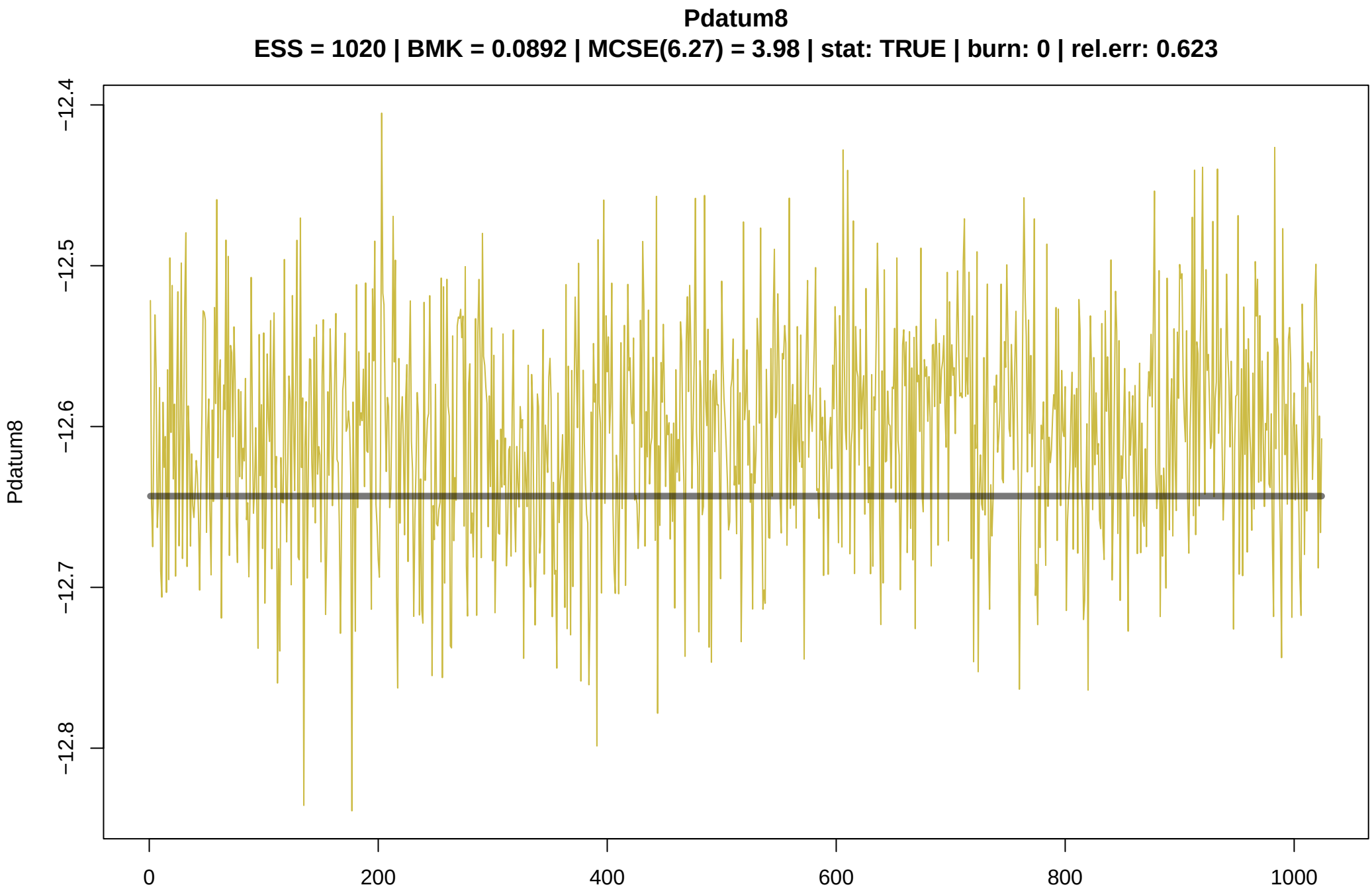

Pdatum3
ESS = 2.22e−16 | BMK = 0.0786 | MCSE(6.27) = 5.7 | stat: TRUE | burn: 0 | rel.err: 0.258
Pdatum3
−20.0
−20.2
−20.4
−20.6
−20.8
−21.0
0
200
400
600
800
1000

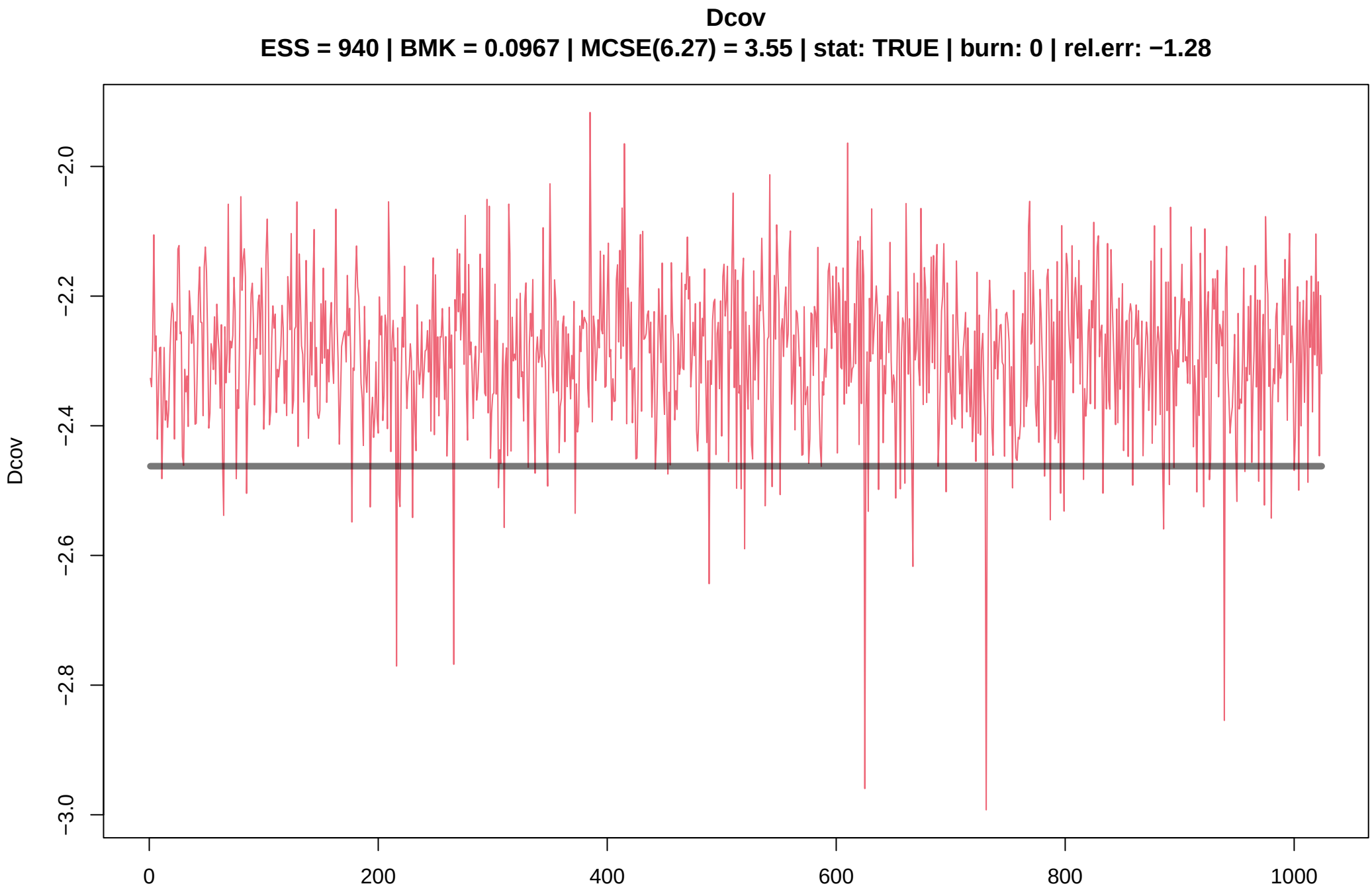

Pdatum4
ESS = 1020 | BMK = 0.0716 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | rel.err: −0.363
Pdatum4
−13.4
−13.6
−13.8
−14.0
0
200
400
600
800
1000

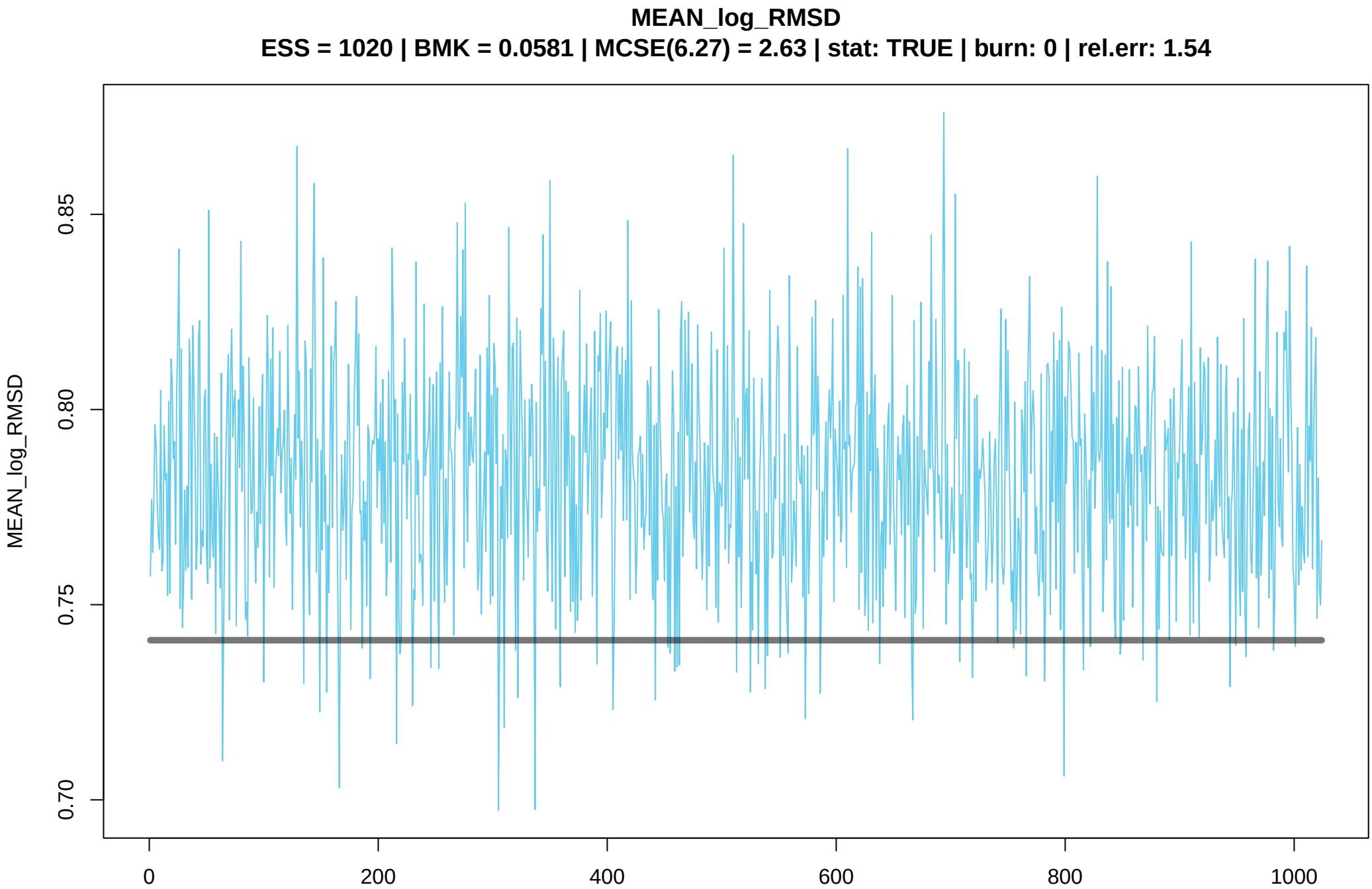

Pdatum5
ESS = 700 | BMK = 0.0468 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0 | rel.err: −0.0676
Pdatum5
−12.3
−12.4
−12.5
−12.6
−12.7
−12.8
−12.9
0
200
400
600
800
1000

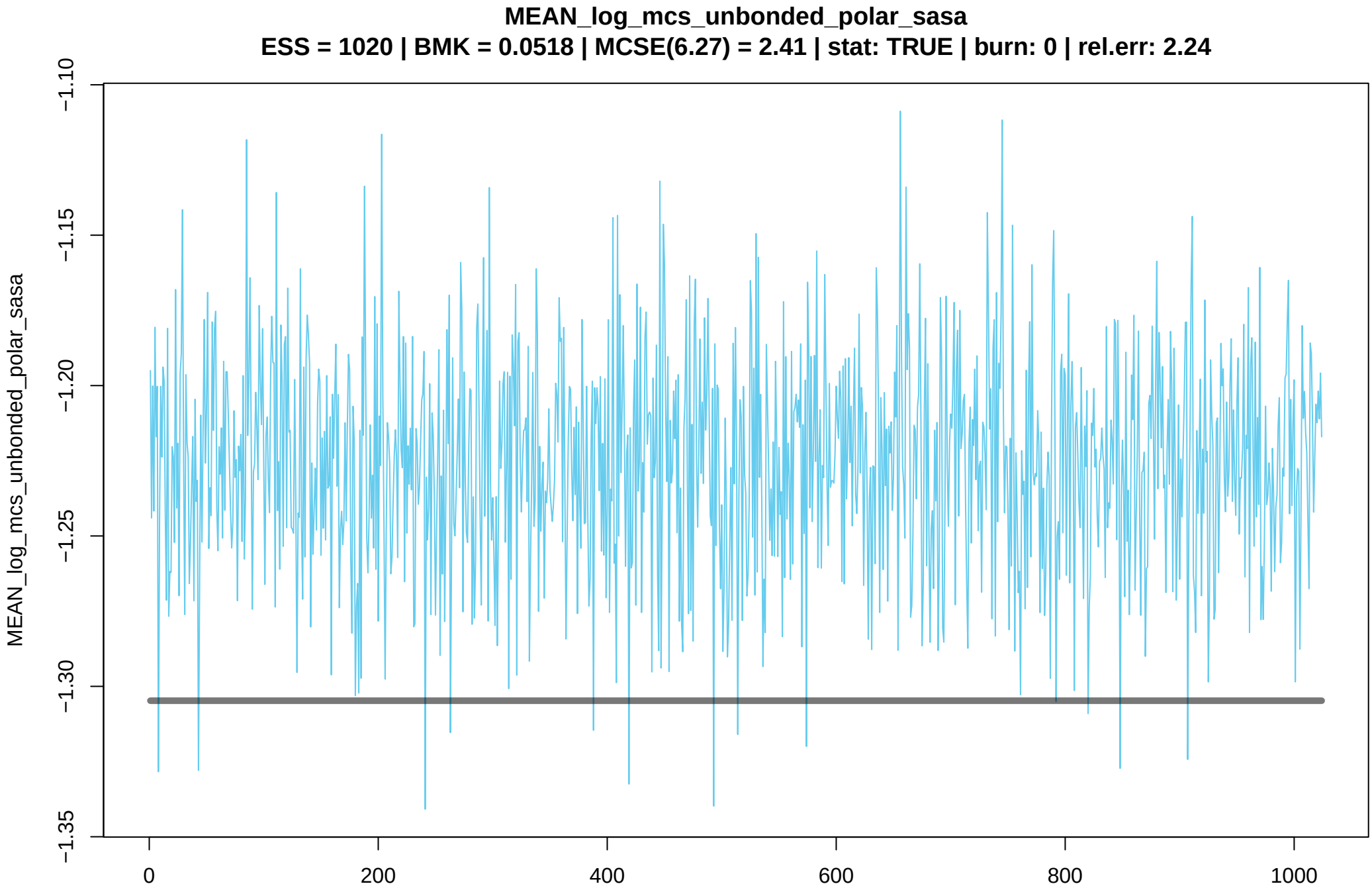

Pdatum6
ESS = 1020 | BMK = 0.0587 | MCSE(6.27) = 3.73 | stat: TRUE | burn: 0 | rel.err: 0.325
Pdatum6
−14.6
−14.7
−14.8
−14.9
−15.0
−15.1
0
200
400
600
800
1000

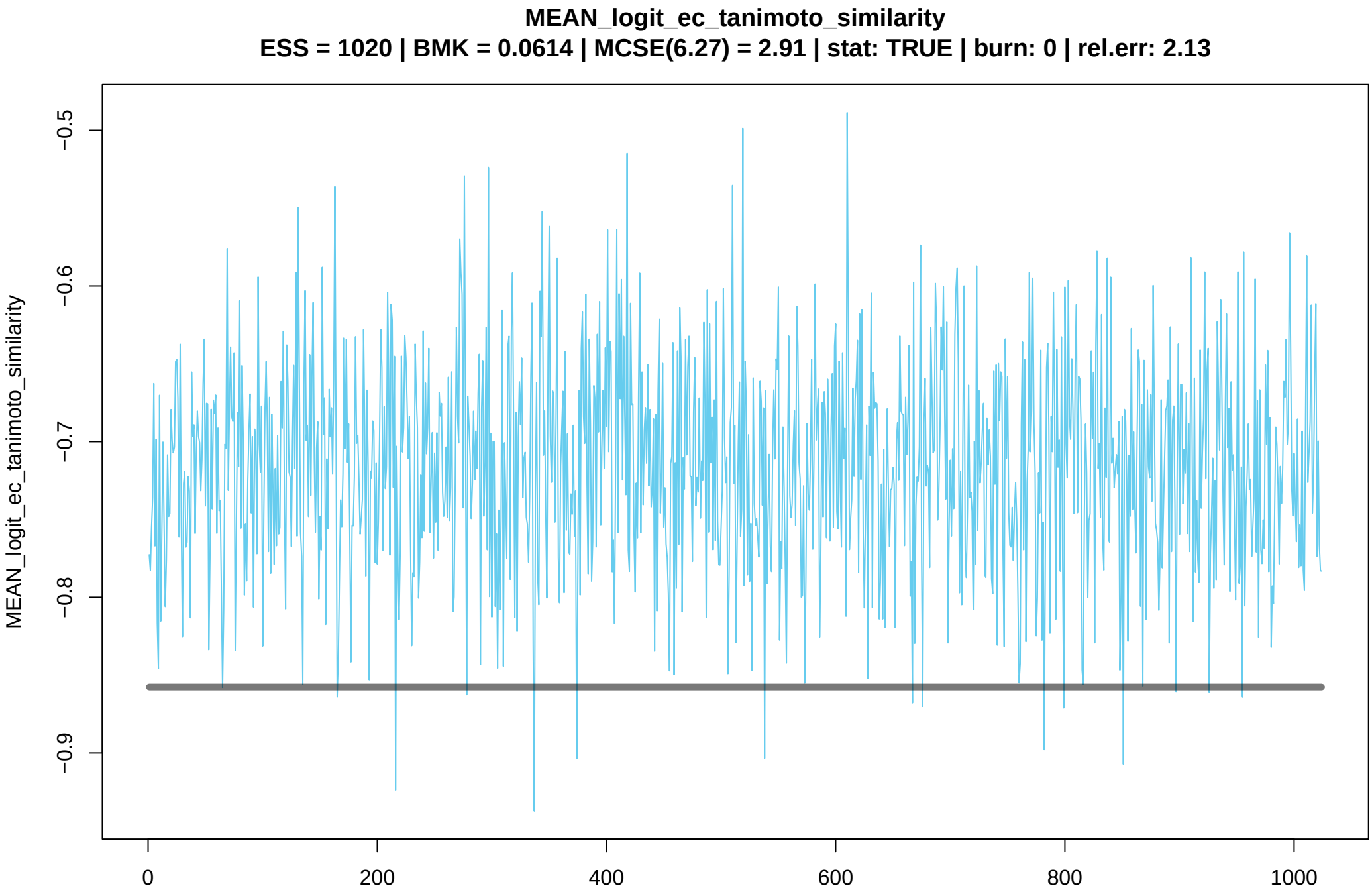

Pdatum7
ESS = 109 | BMK = 0.13 | MCSE(6.27) = 5.81 | stat: TRUE | burn: 0 | rel.err: −0.147
Pdatum7
−12.7
−12.8
−12.9
−13.0
−13.1
−13.2
0
200
400
600
800
1000

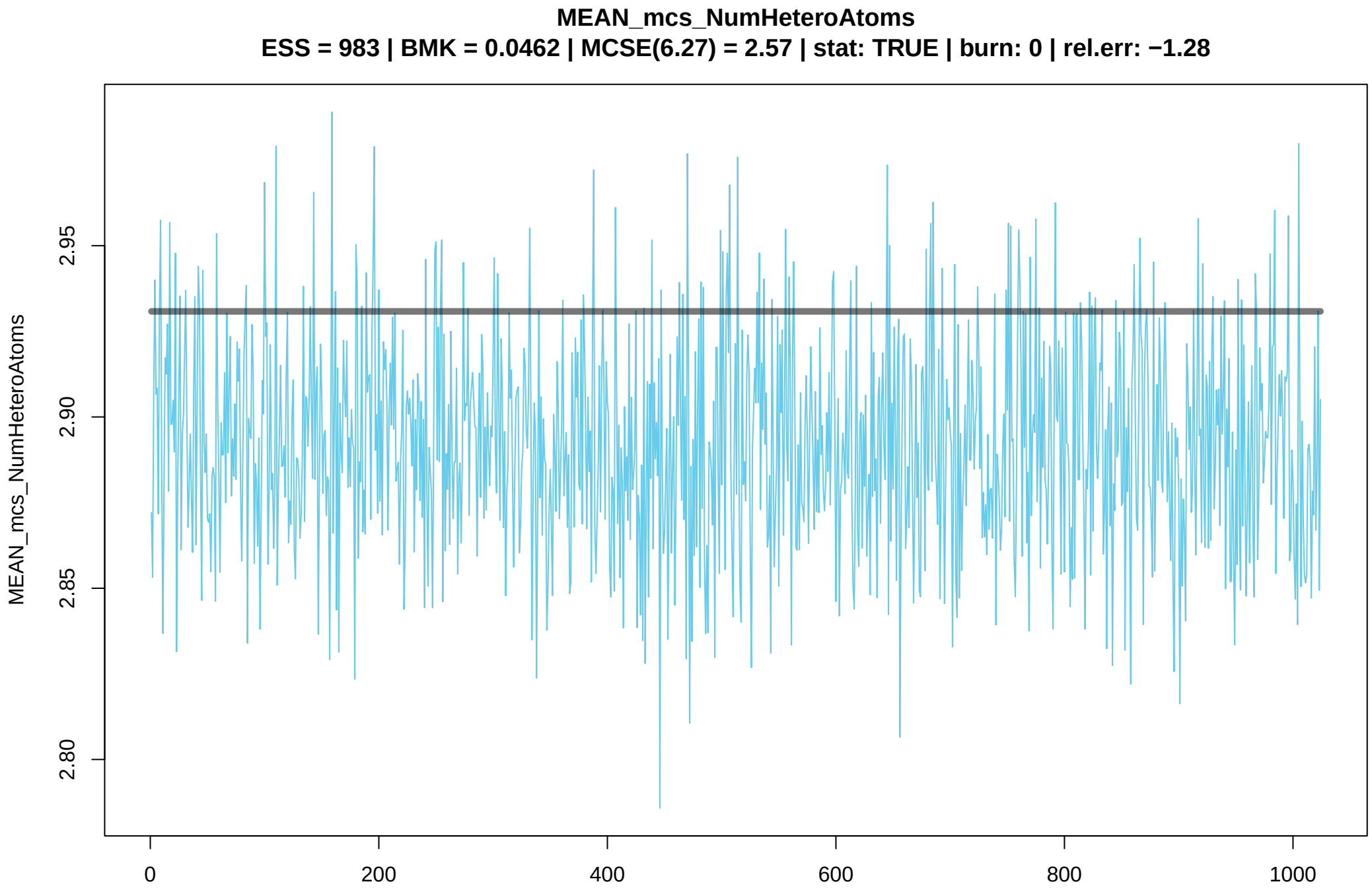

Pdatum8
ESS = 1020 | BMK = 0.0892 | MCSE(6.27) = 3.98 | stat: TRUE | burn: 0 | rel.err: 0.623
Pdatum8
−12.4
−12.5
−12.6
−12.7
−12.8
0
200
400
600
800
1000

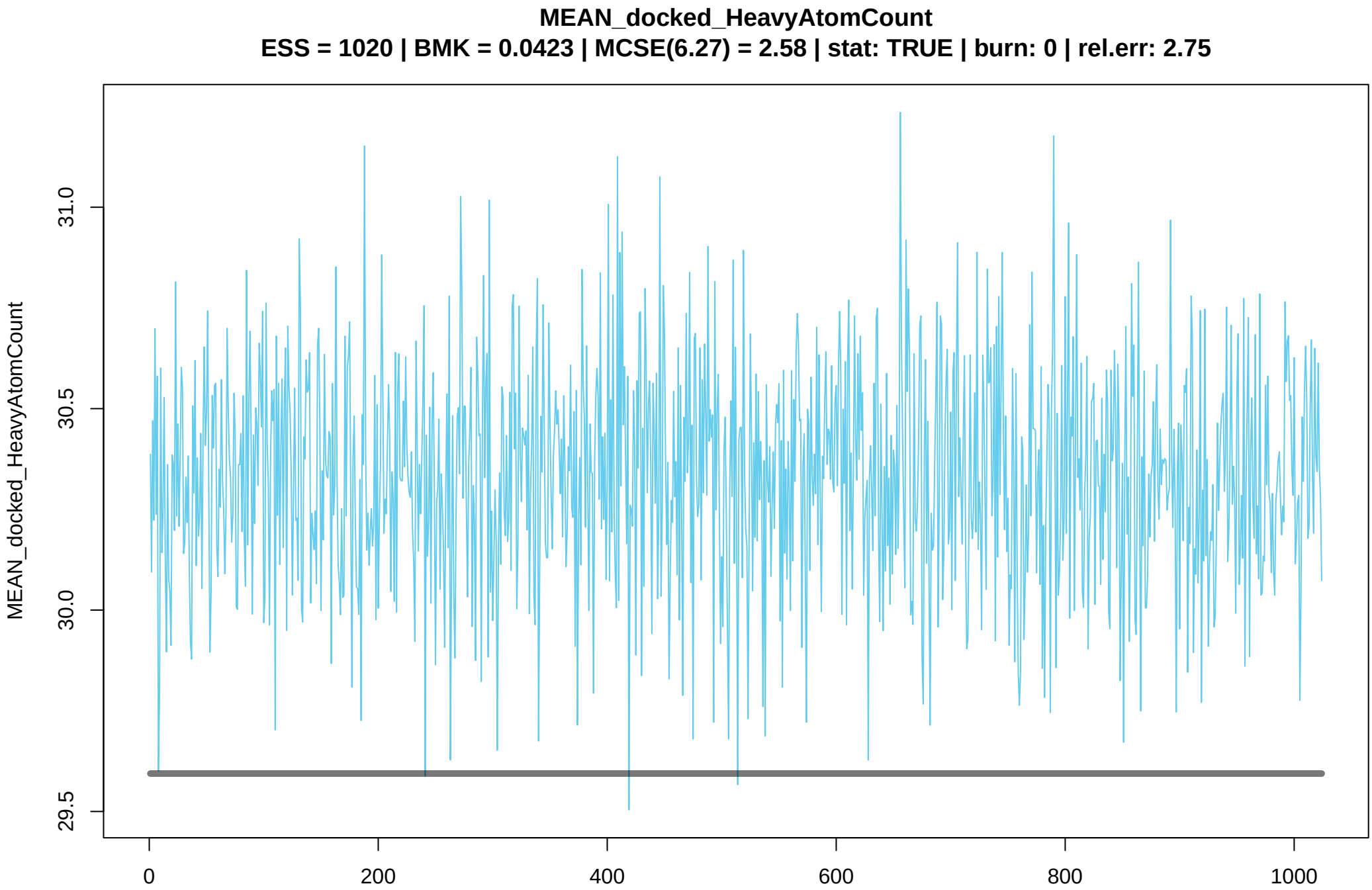

Dcov
ESS = 940 | BMK = 0.0967 | MCSE(6.27) = 3.55 | stat: TRUE | burn: 0 | rel.err: −1.28
Dcov
−2.0
−2.2
−2.4
−2.6
−2.8
−3.0
0
200
400
600
800
1000

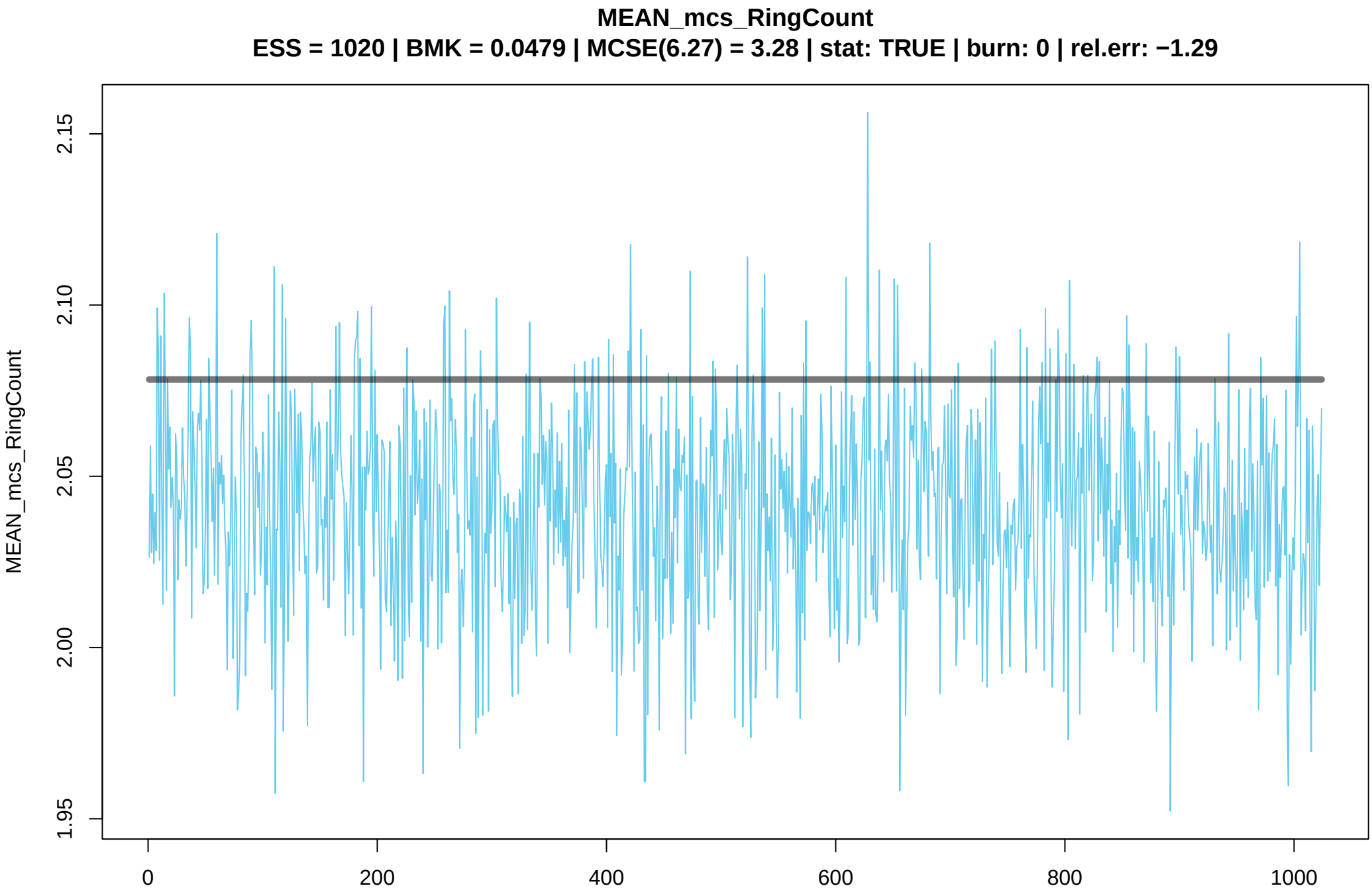

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0581 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | rel.err: 1.54
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

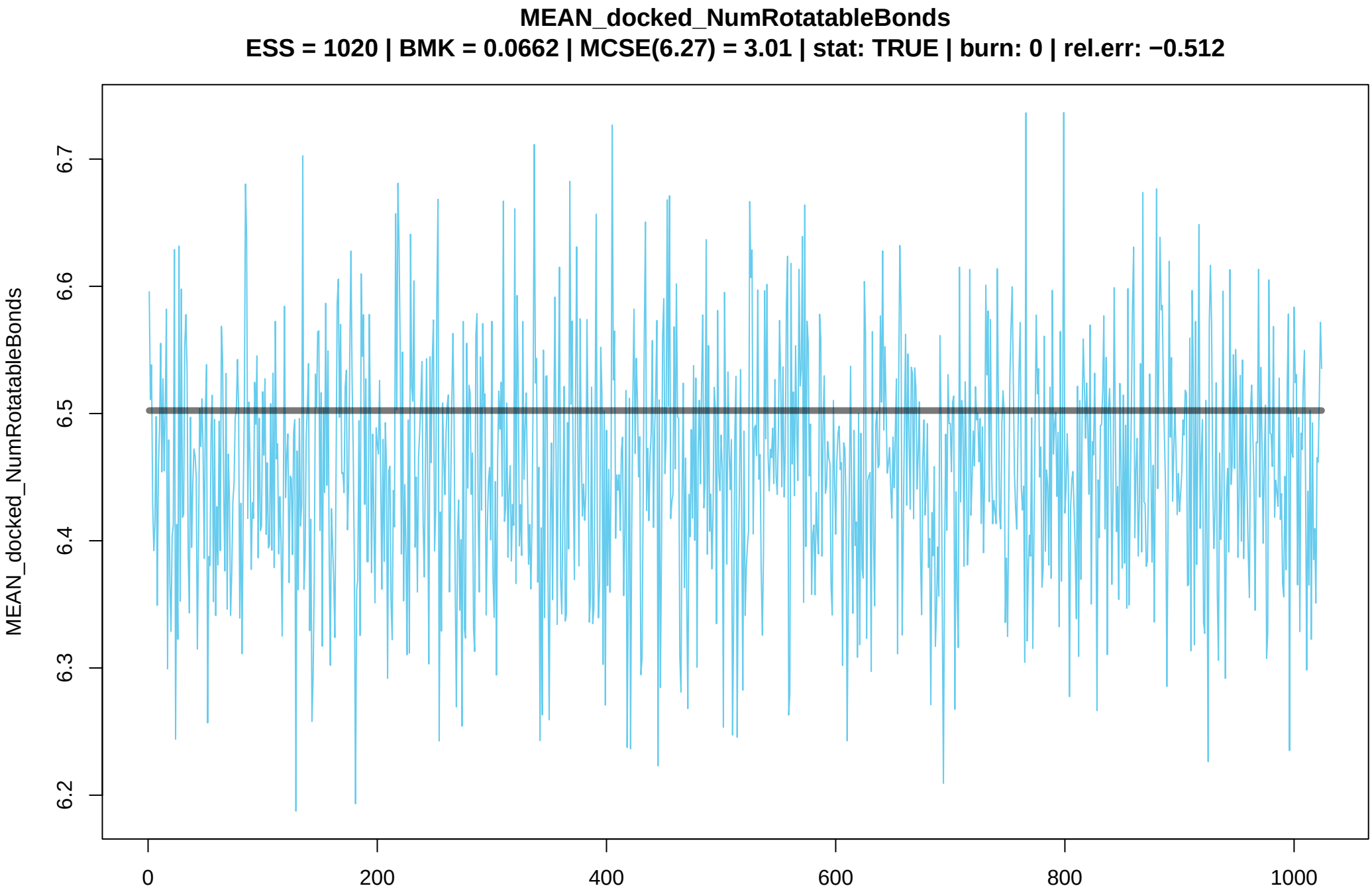

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0518 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0 | rel.err: 2.24
MEAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

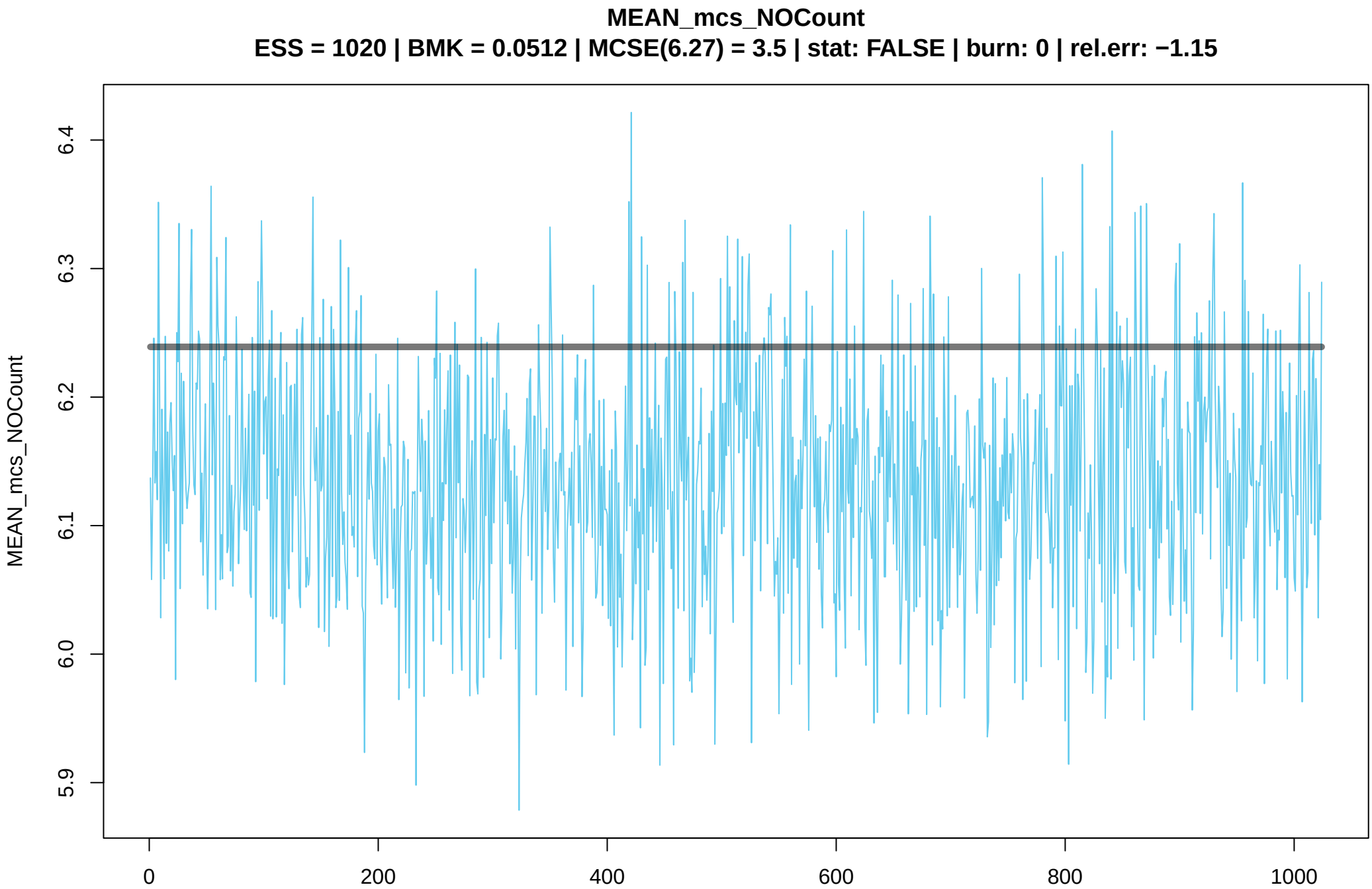

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0614 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | rel.err: 2.13
MEAN_logit_ec_tanimoto_similarity
−0.5
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

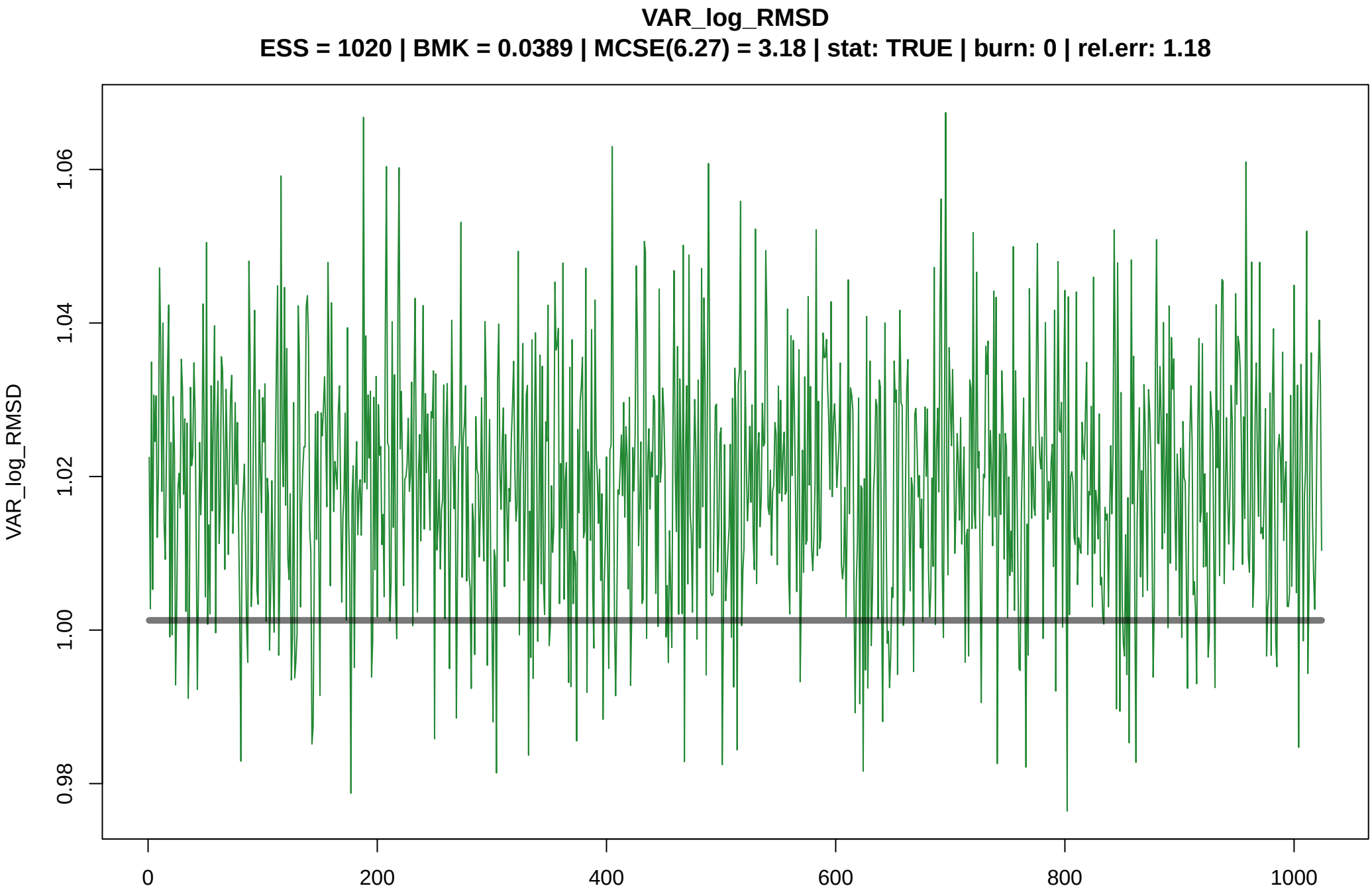

MEAN_mcs_NumHeteroAtoms
ESS = 983 | BMK = 0.0462 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: −1.28
MEAN_mcs_NumHeteroAtoms
2.80
2.85
2.90
2.95
0
200
400
600
800
1000

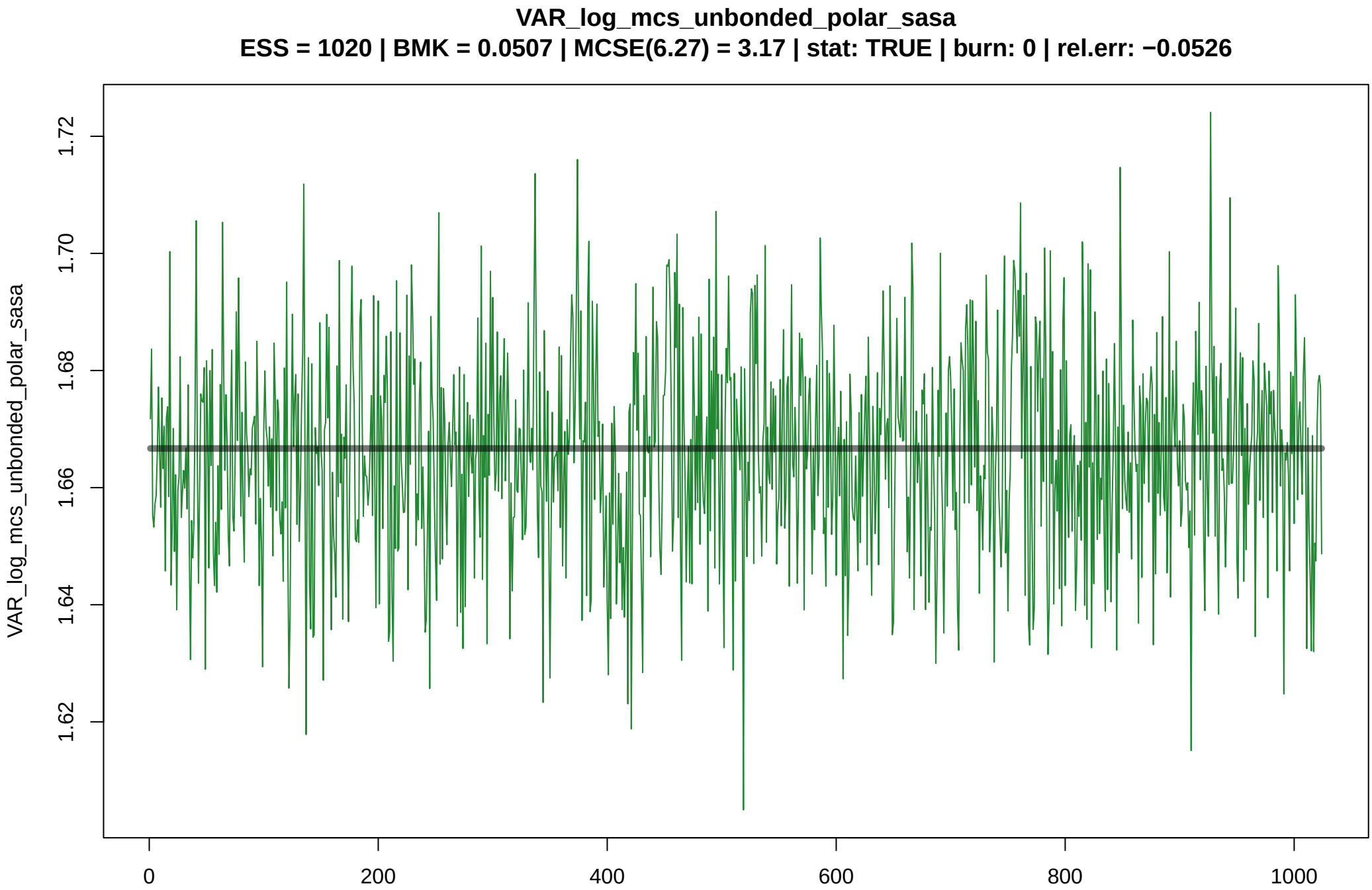

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0423 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0 | rel.err: 2.75
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
31.0
0
200
400
600
800
1000

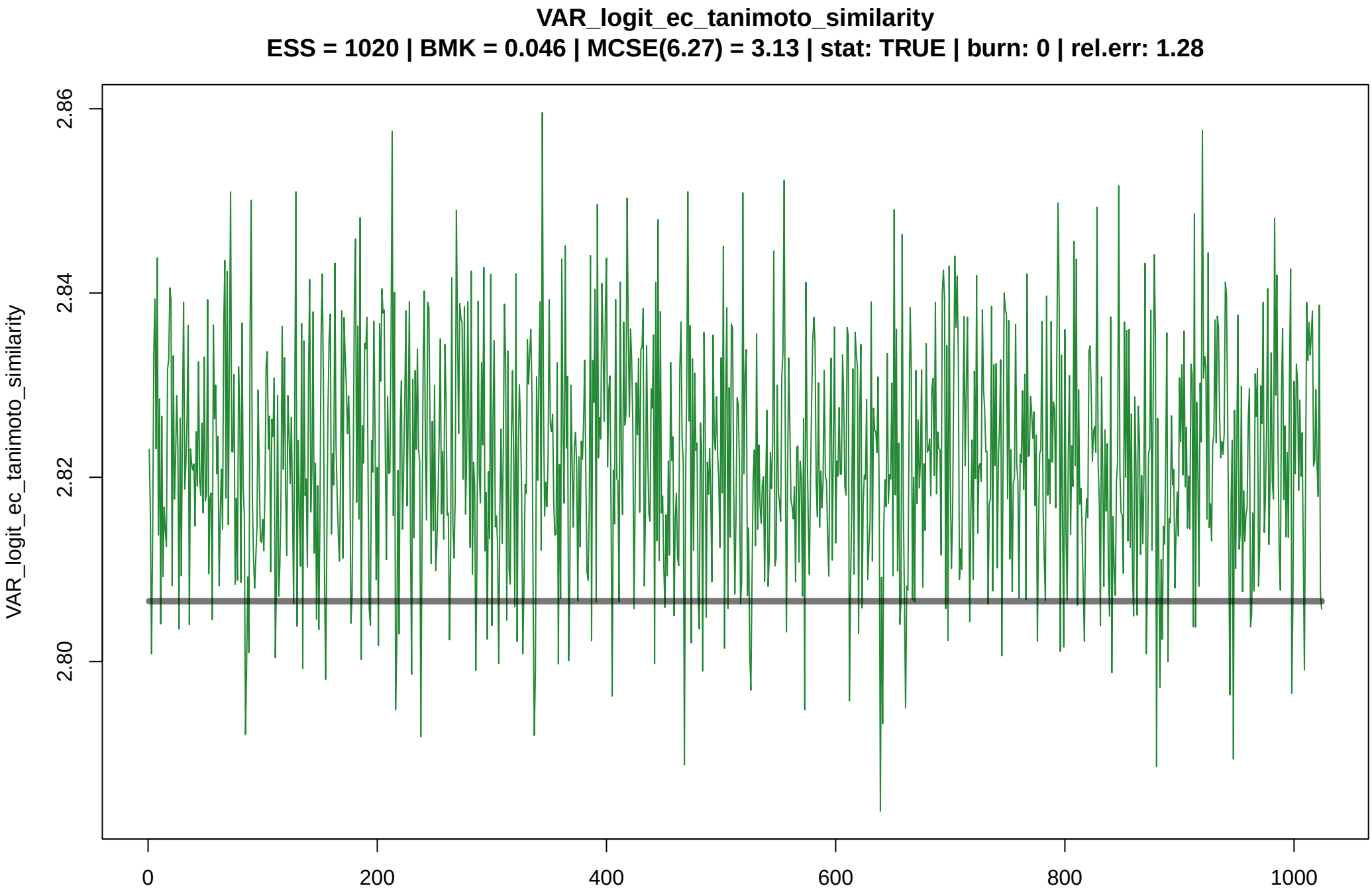

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0479 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | rel.err: −1.29
MEAN_mcs_RingCount
2.15
2.10
2.05
2.00
1.95
0
200
400
600
800
1000

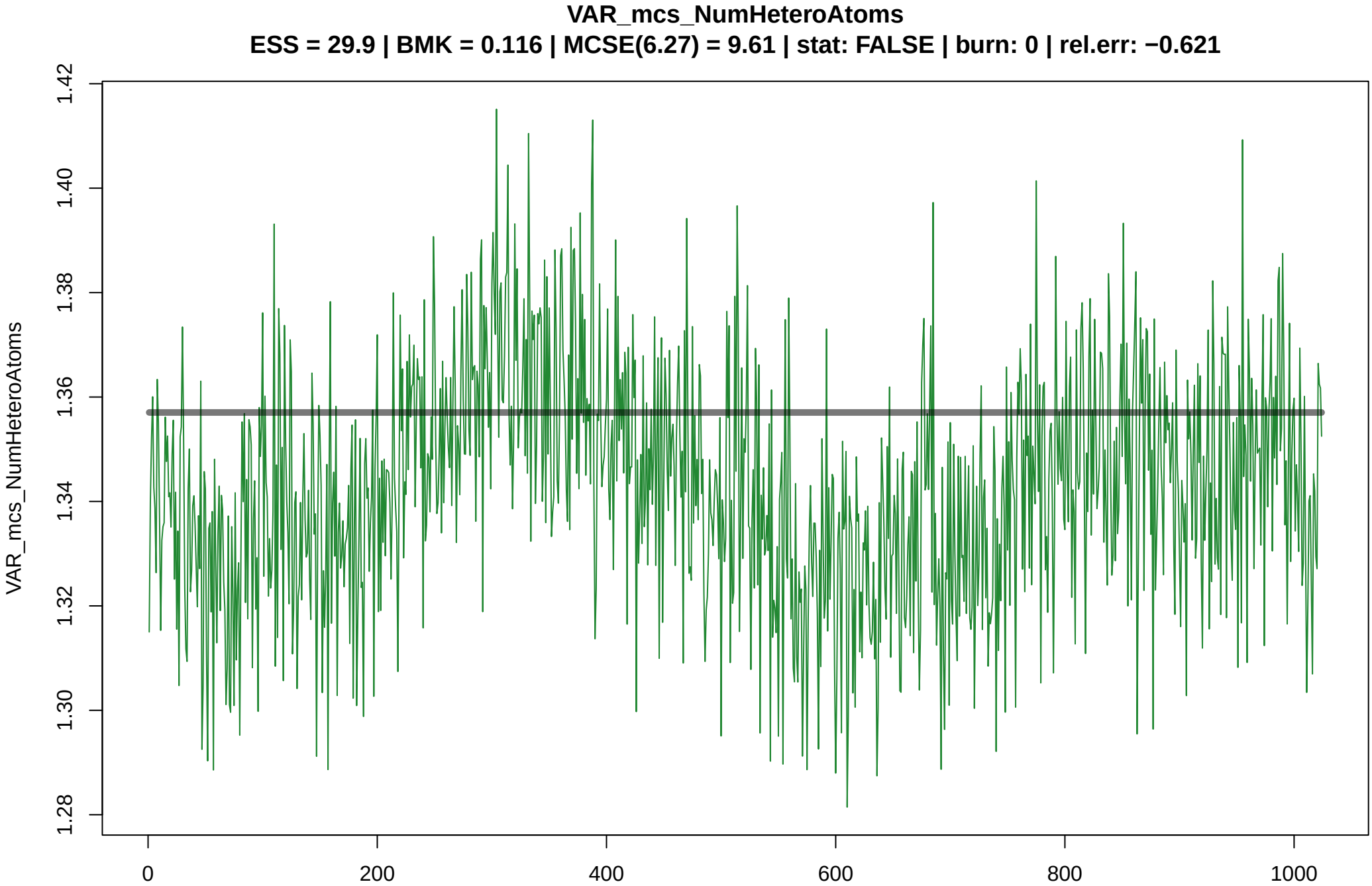

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0662 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | rel.err: −0.512
MEAN_docked_NumRotatableBonds
6.2
6.3
6.4
6.5
6.6
6.7
0
200
400
600
800
1000

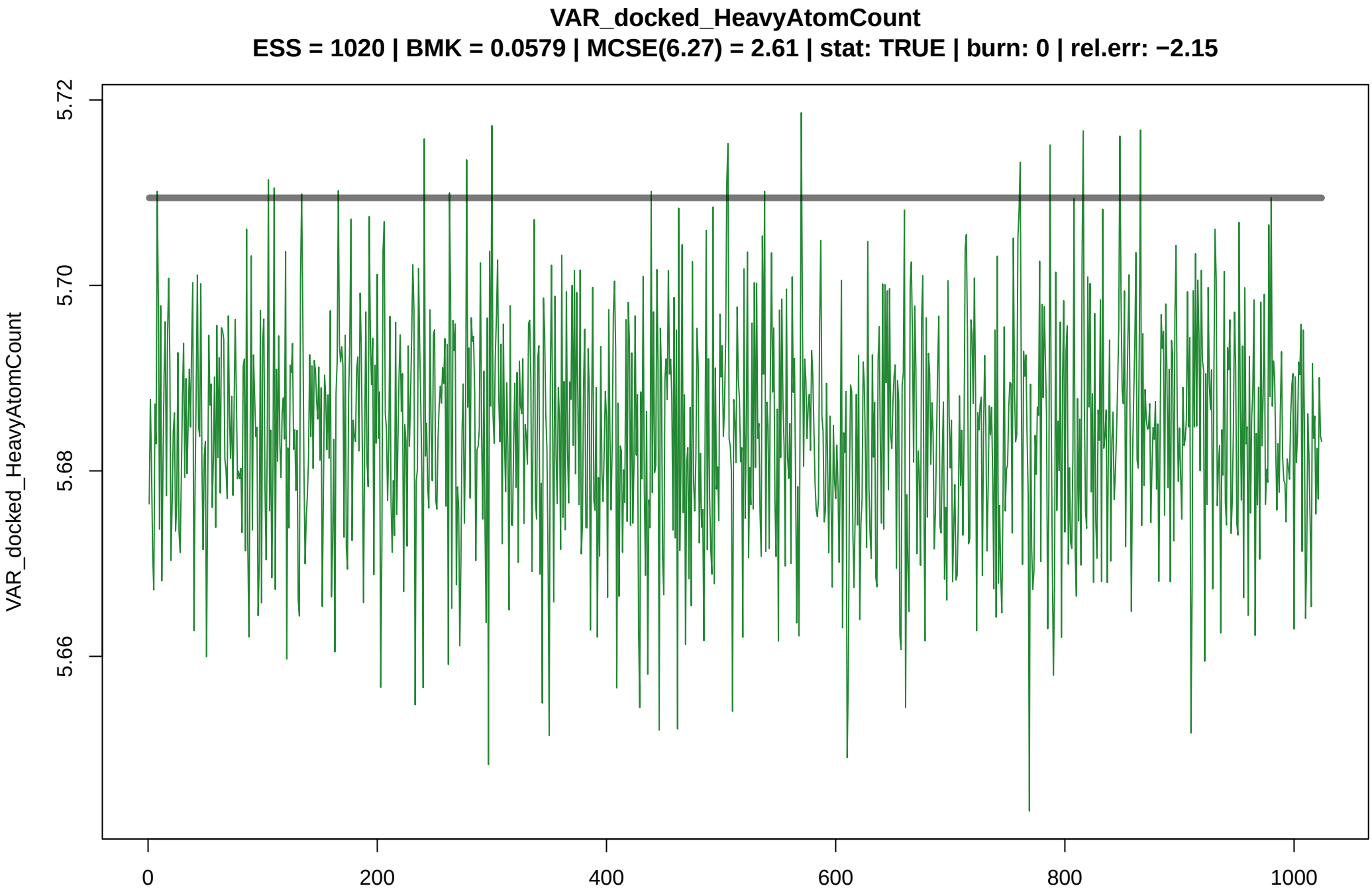

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0512 | MCSE(6.27) = 3.5 | stat: FALSE | burn: 0 | rel.err: −1.15
MEAN_mcs_NOCount
6.4
6.3
6.2
6.1
6.0
5.9
0
200
400
600
800
1000

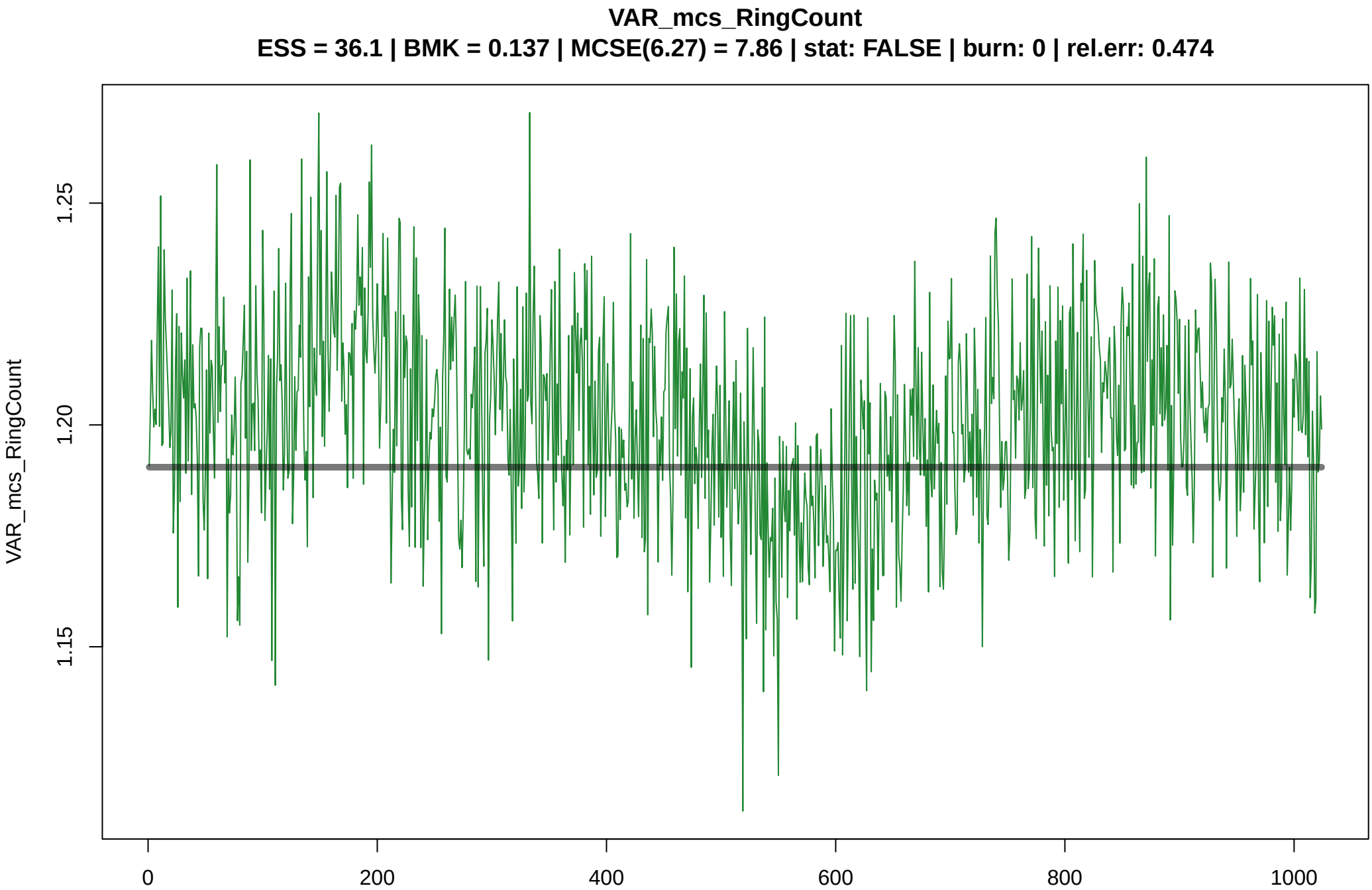

VAR_log_RMSD
ESS = 1020 | BMK = 0.0389 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | rel.err: 1.18
VAR_log_RMSD
0.98
1.00
1.02
1.04
1.06
0
200
400
600
800
1000

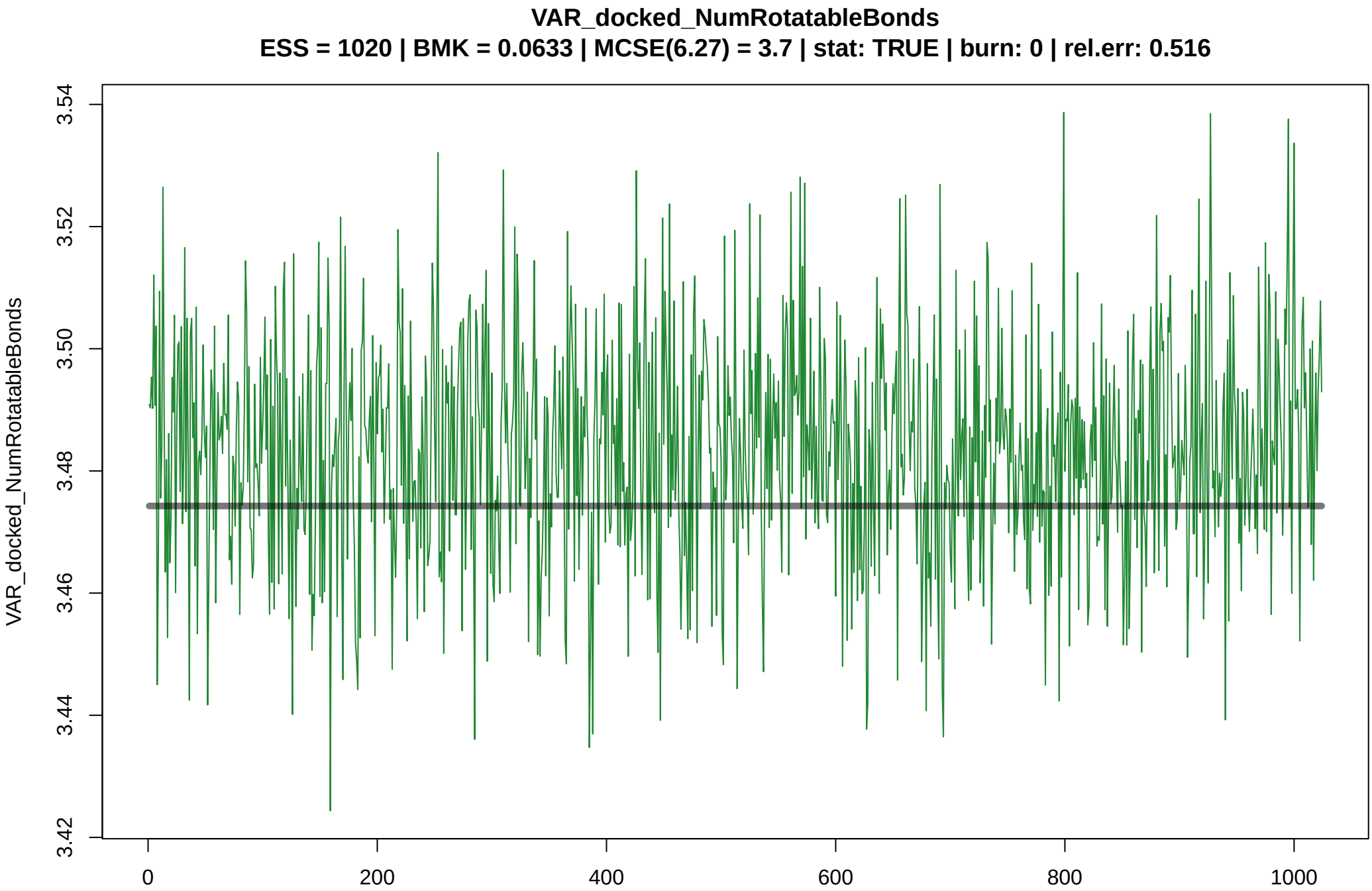

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0507 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | rel.err: −0.0526
VAR_log_mcs_unbonded_polar_sasa
1.72
1.70
1.68
1.66
1.64
1.62
0
200
400
600
800
1000

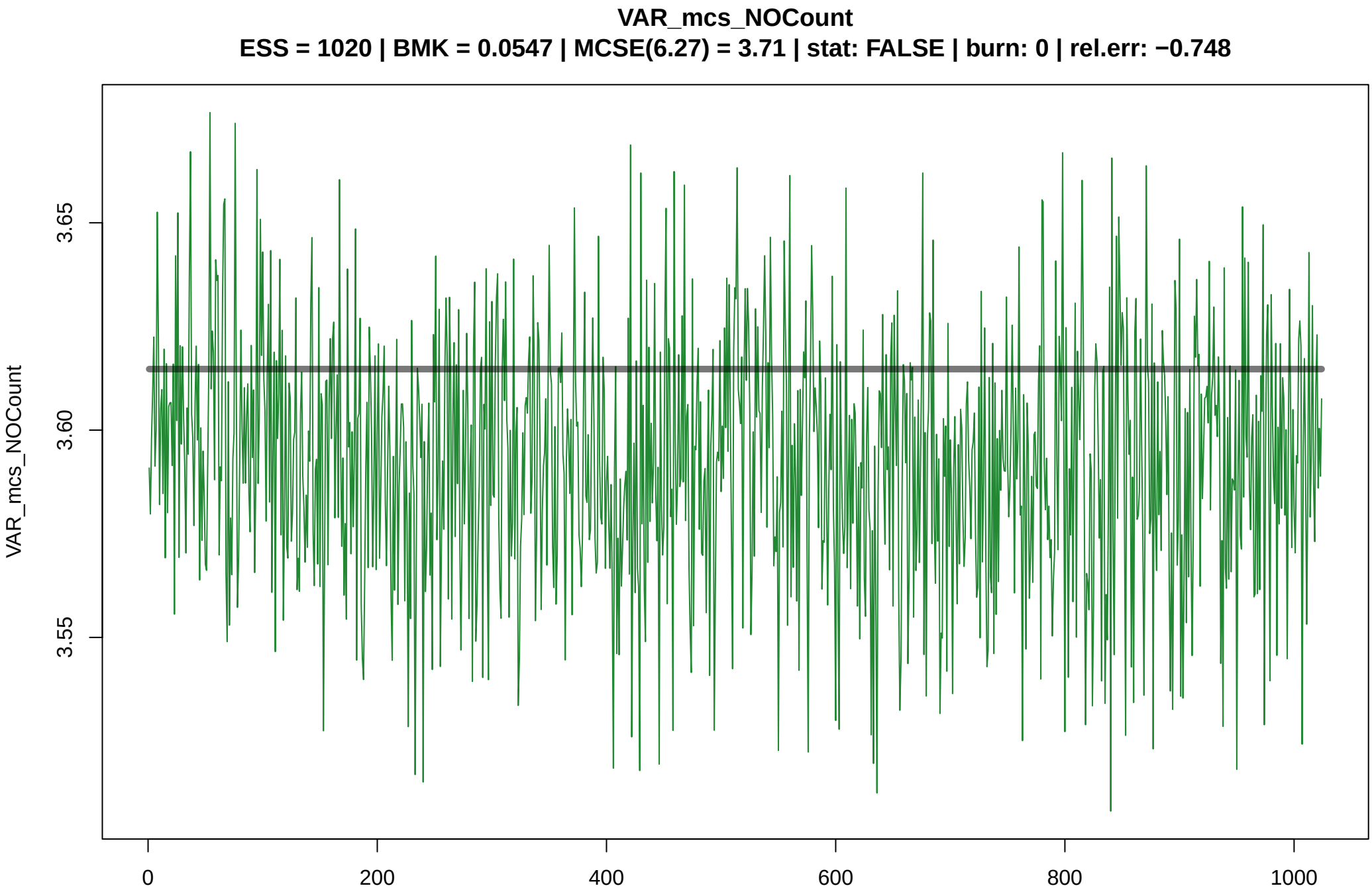

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.046 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | rel.err: 1.28
VAR_logit_ec_tanimoto_similarity
2.80
2.82
2.84
2.86
0
200
400
600
800
1000

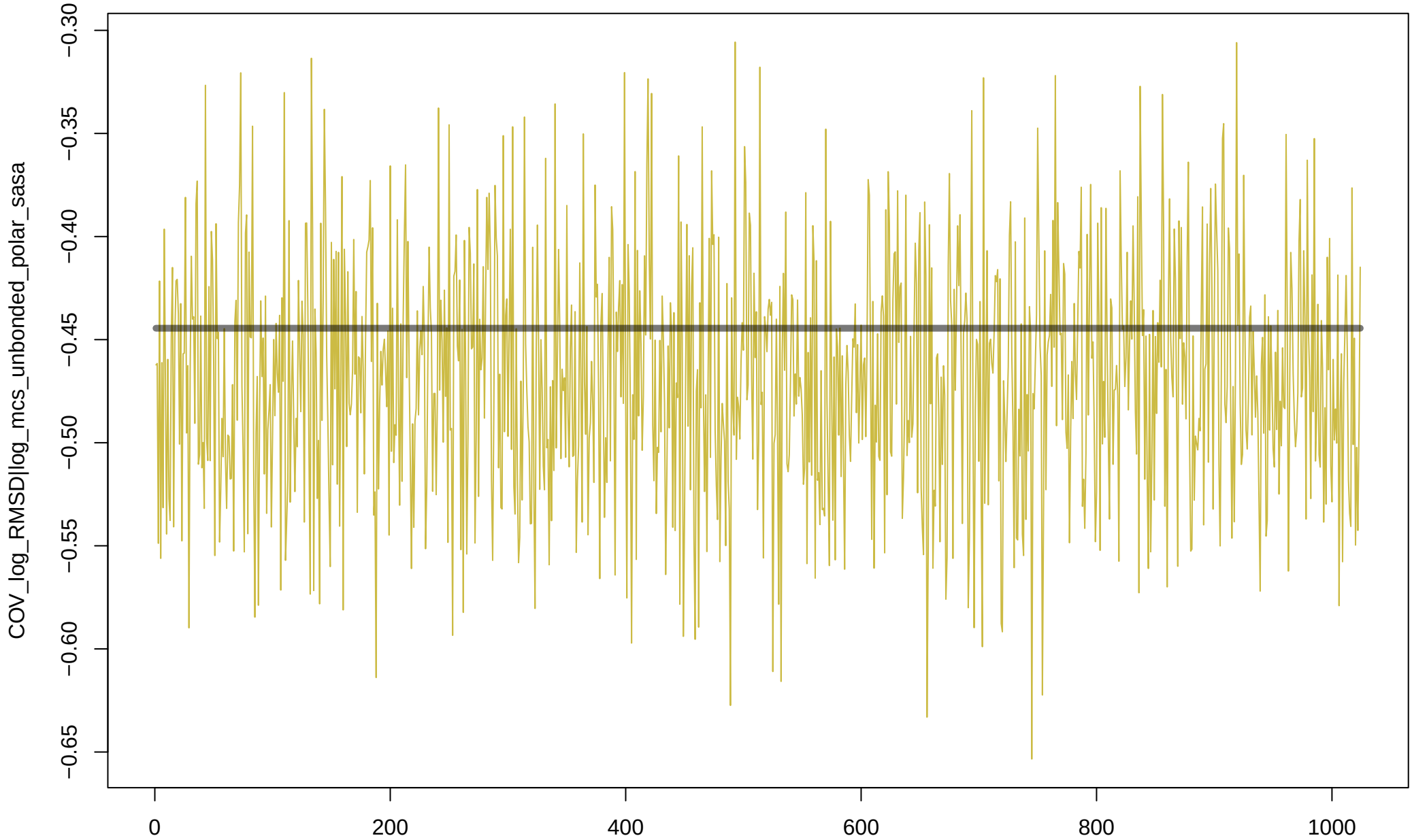

VAR_mcs_NumHeteroAtoms
ESS = 29.9 | BMK = 0.116 | MCSE(6.27) = 9.61 | stat: FALSE | burn: 0 | rel.err: −0.621
VAR_mcs_NumHeteroAtoms
1.28
1.30
1.32
1.34
1.36
1.38
1.40
1.42
0
200
400
600
800
1000

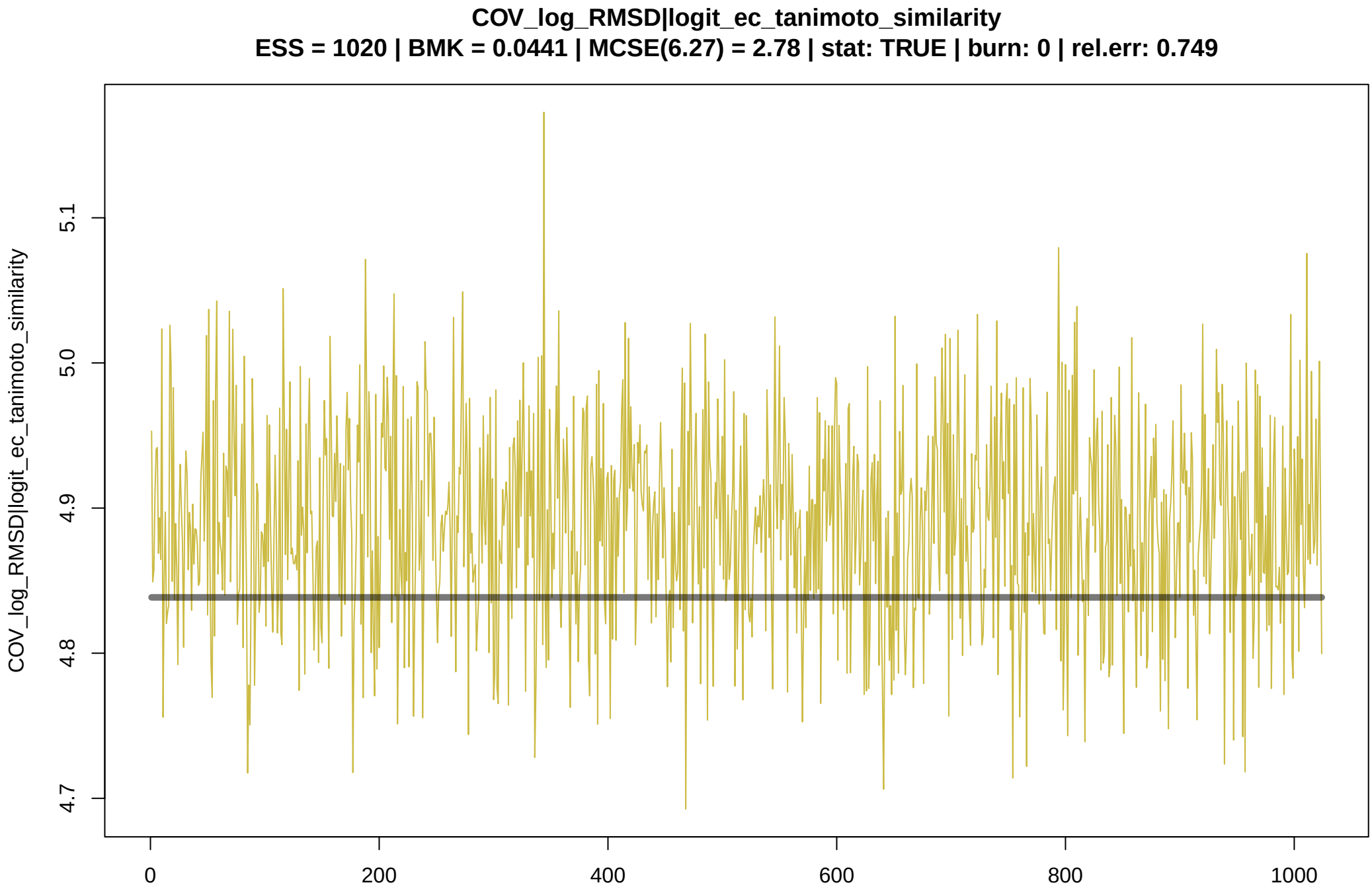

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0579 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: −2.15
VAR_docked_HeavyAtomCount
5.72
5.70
5.68
5.66
0
200
400
600
800
1000

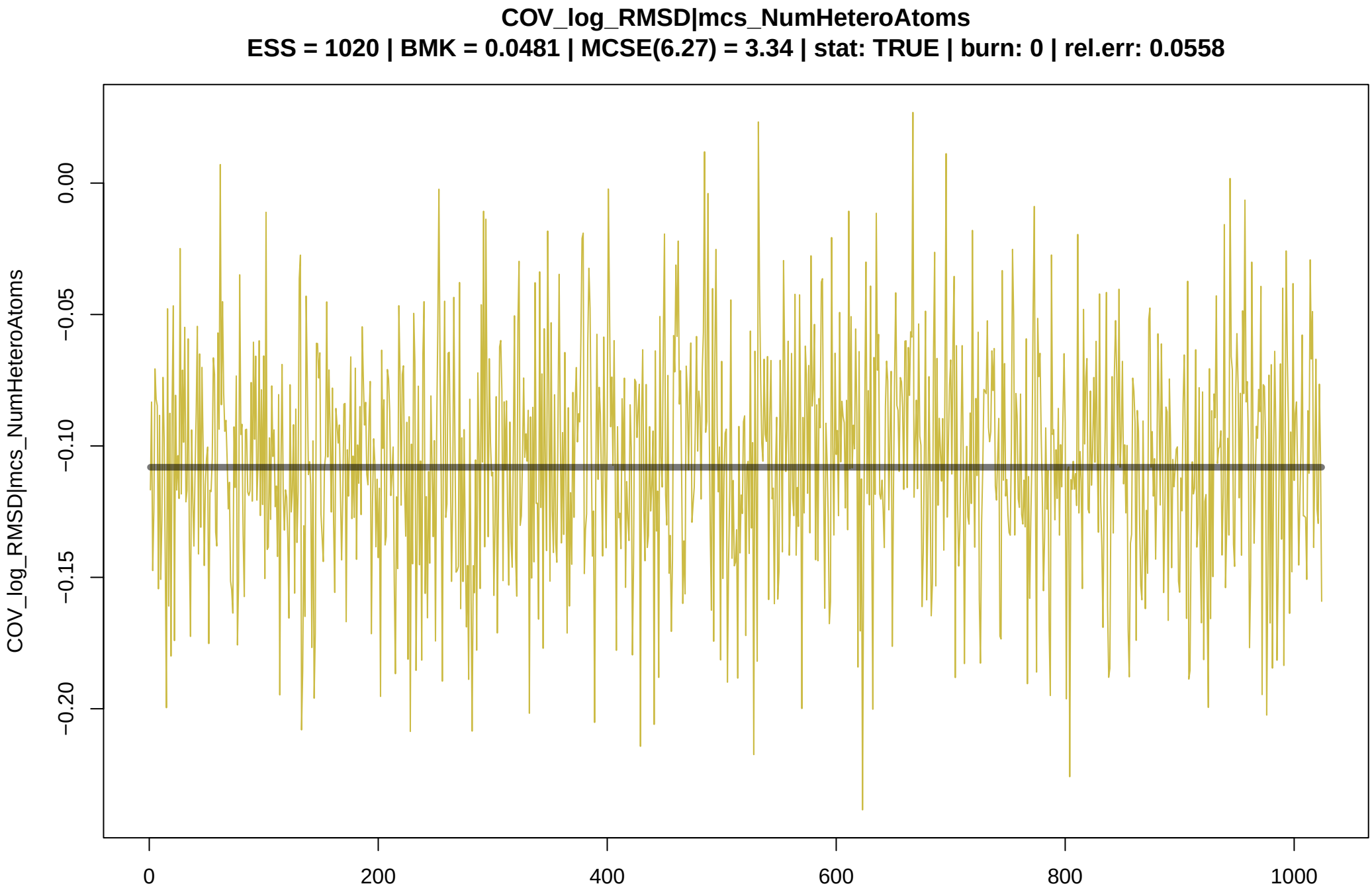

VAR_mcs_RingCount
ESS = 36.1 | BMK = 0.137 | MCSE(6.27) = 7.86 | stat: FALSE | burn: 0 | rel.err: 0.474
VAR_mcs_RingCount
1.15
1.20
1.25
0
200
400
600
800
1000

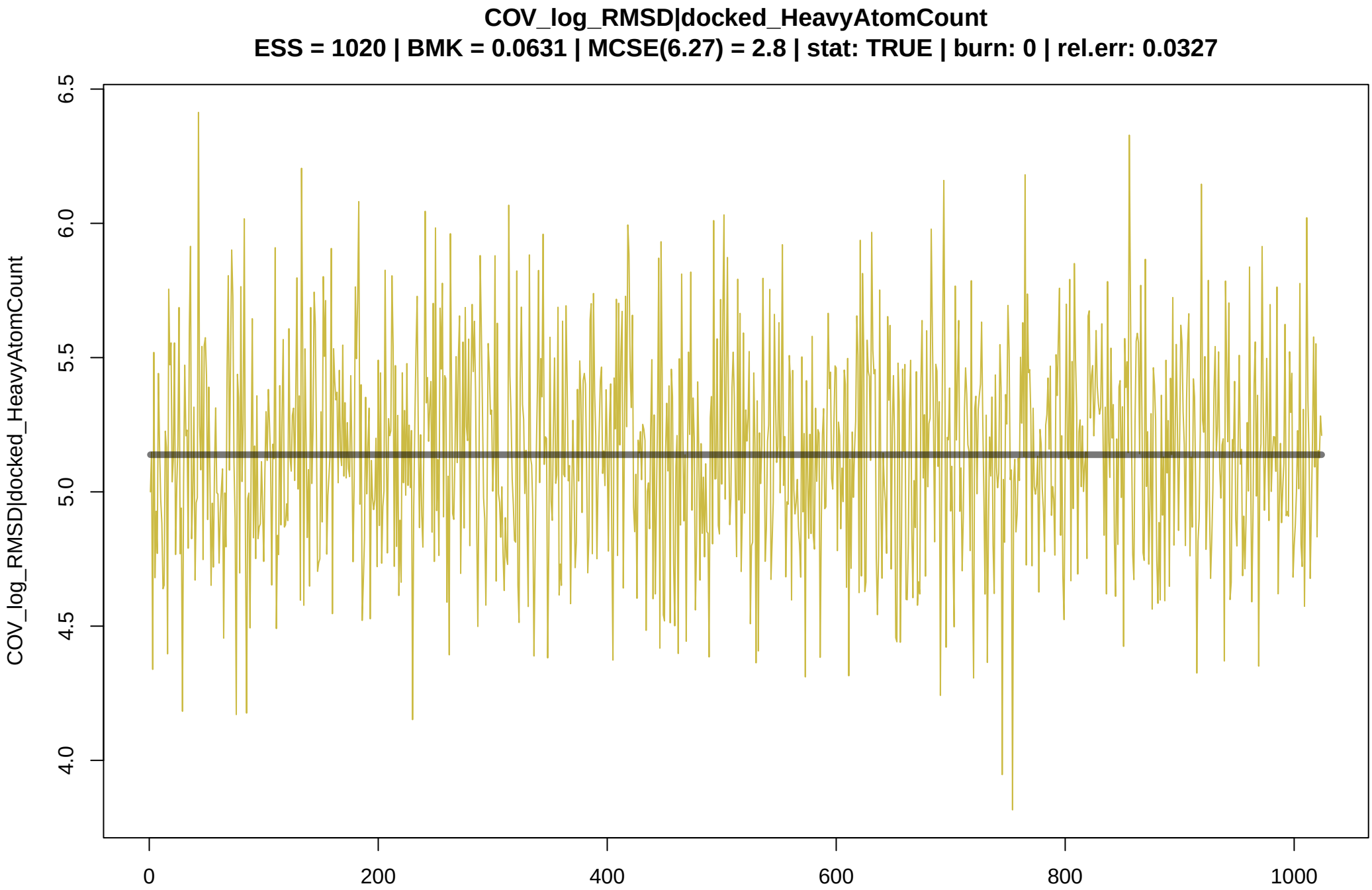

VAR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0633 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | rel.err: 0.516
VAR_docked_NumRotatableBonds
3.42
3.44
3.46
3.48
3.50
3.52
3.54
0
200
400
600
800
1000

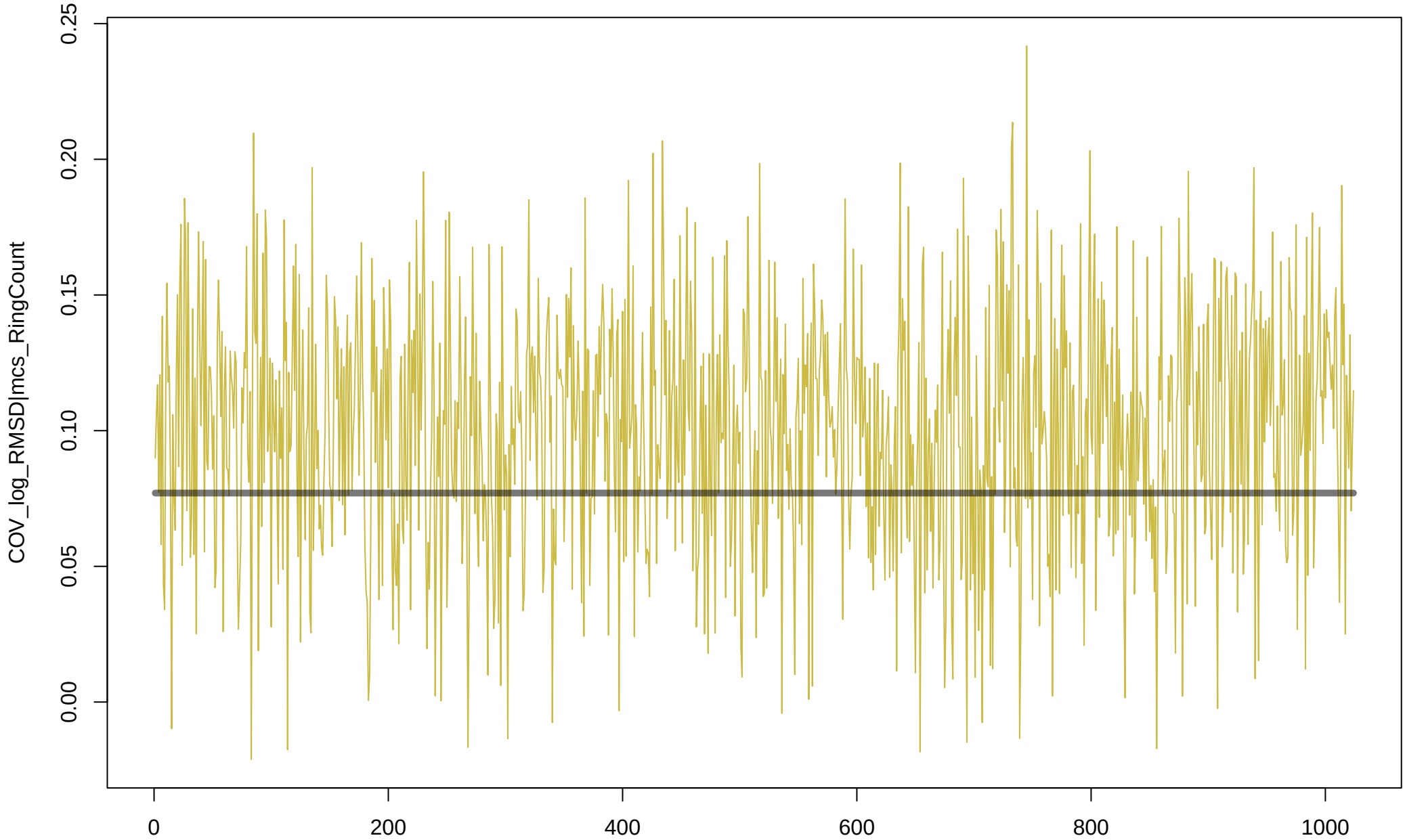

VAR_mcs_NOCount
ESS = 1020 | BMK = 0.0547 | MCSE(6.27) = 3.71 | stat: FALSE | burn: 0 | rel.err: −0.748
VAR_mcs_NOCount
3.55
3.60
3.65
0
200
400
600
800
1000

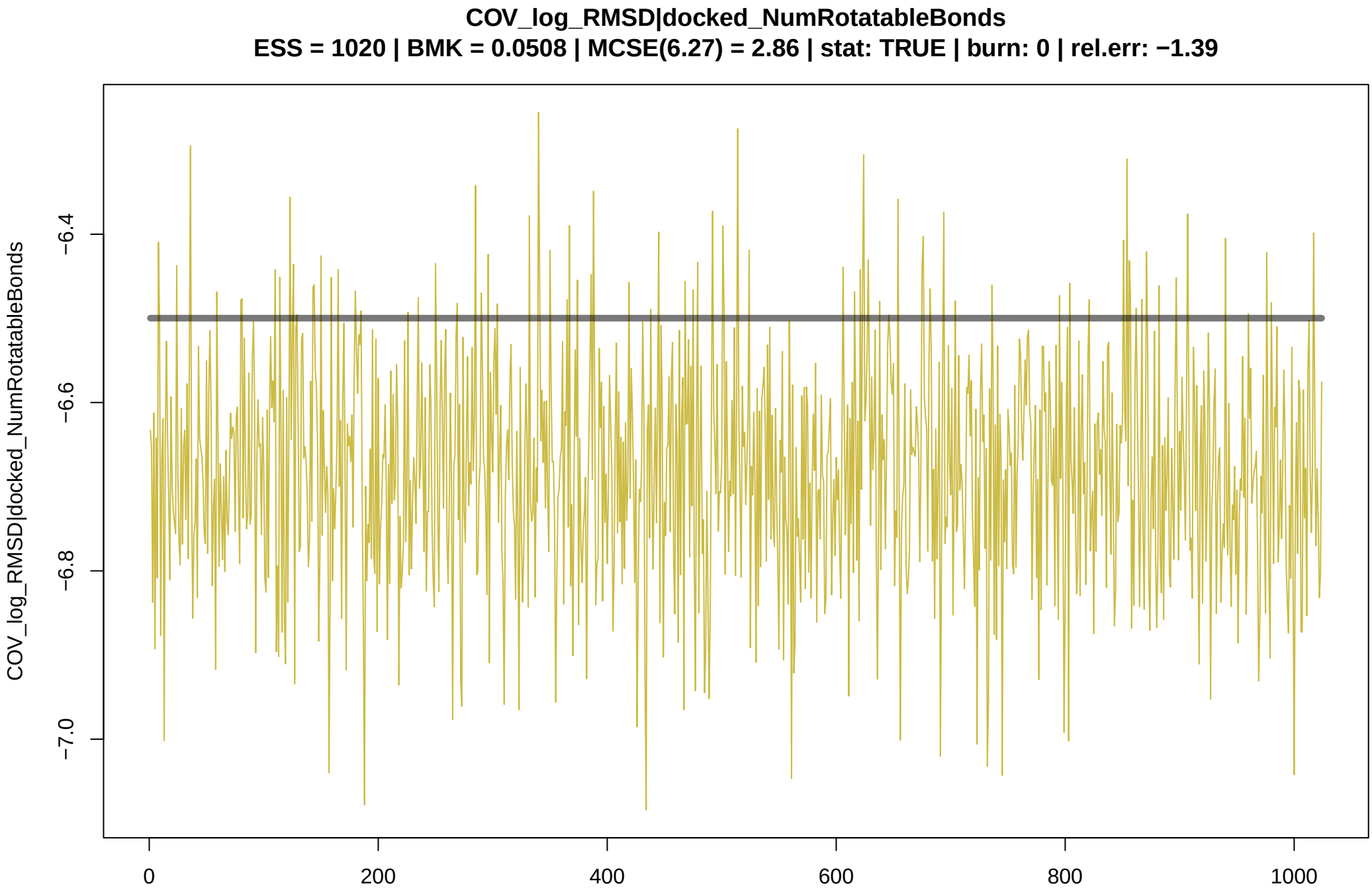

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0413 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | rel.err: −0.419
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.30
−0.35
−0.40
−0.45
−0.50
−0.55
−0.60
−0.65
0
200
400
600
800
1000

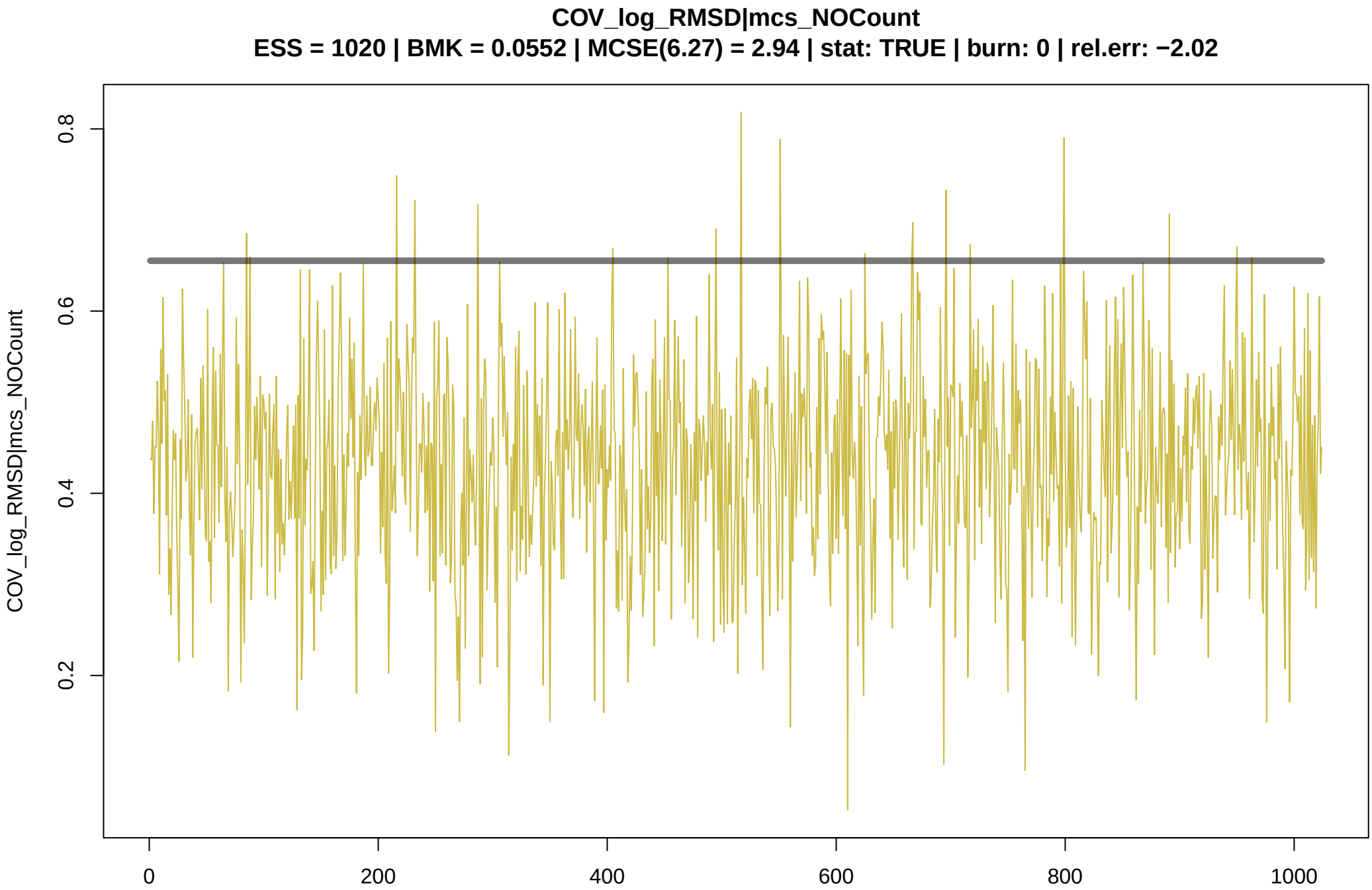

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0441 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: 0.749
COV_log_RMSD|logit_ec_tanimoto_similarity
4.7
4.8
4.9
5.0
5.1
0
200
400
600
800
1000

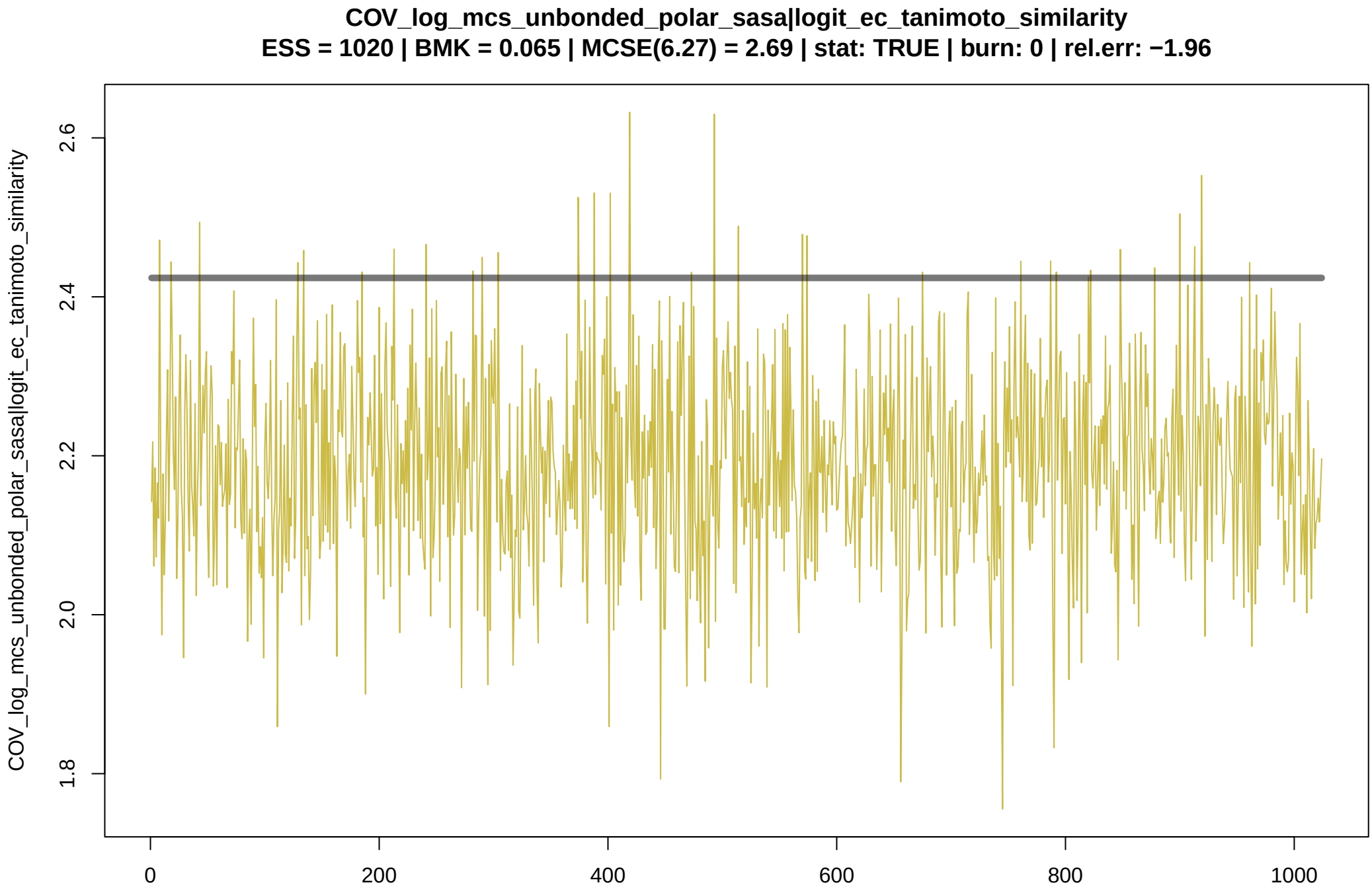

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0481 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0 | rel.err: 0.0558
COV_log_RMSD|mcs_NumHeteroAtoms
0.00
−0.05
−0.10
−0.15
−0.20
0
200
400
600
800
1000

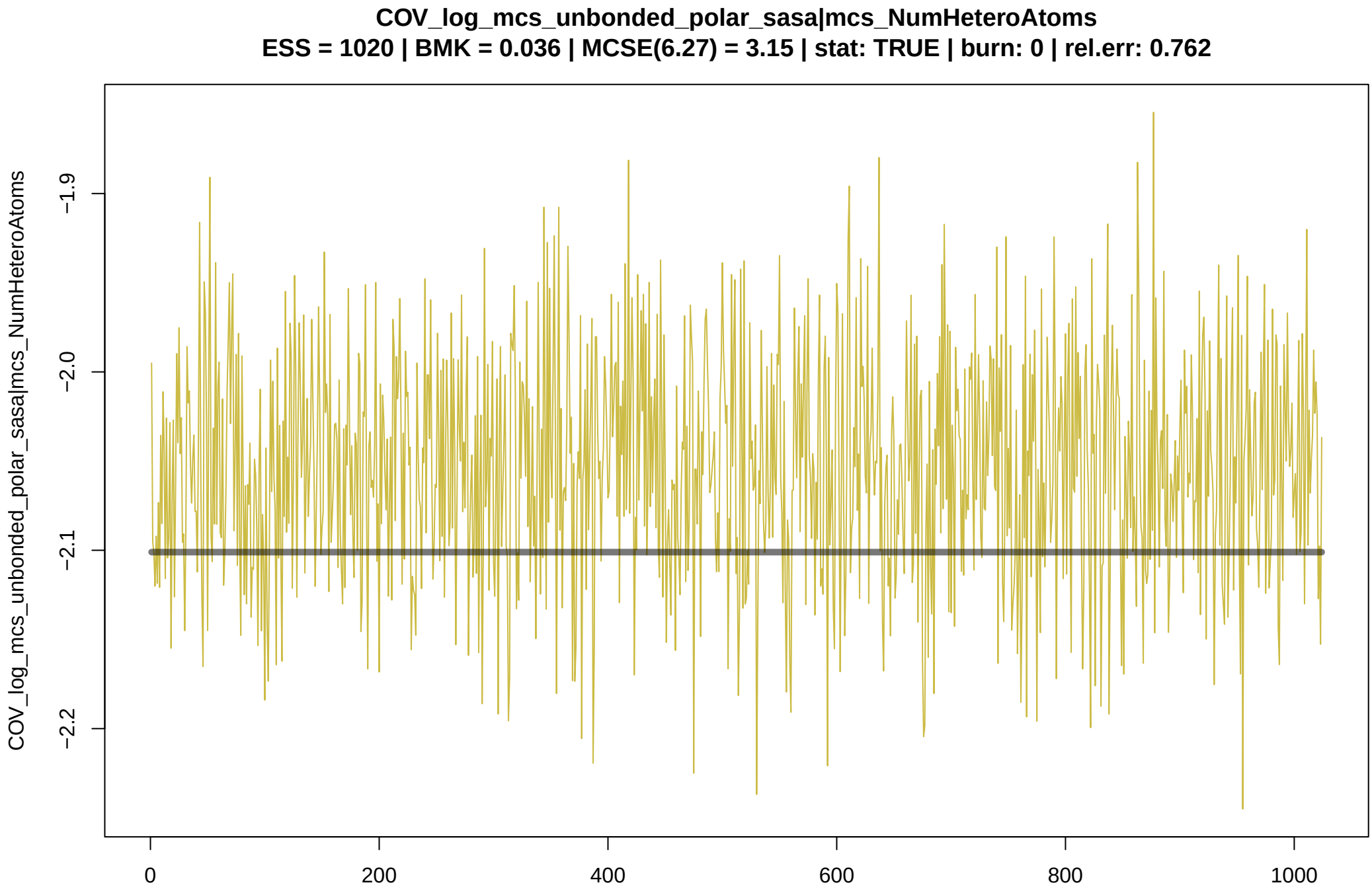

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0631 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0 | rel.err: 0.0327
COV_log_RMSD|docked_HeavyAtomCount
6.5
6.0
5.5
5.0
4.5
4.0
0
200
400
600
800
1000

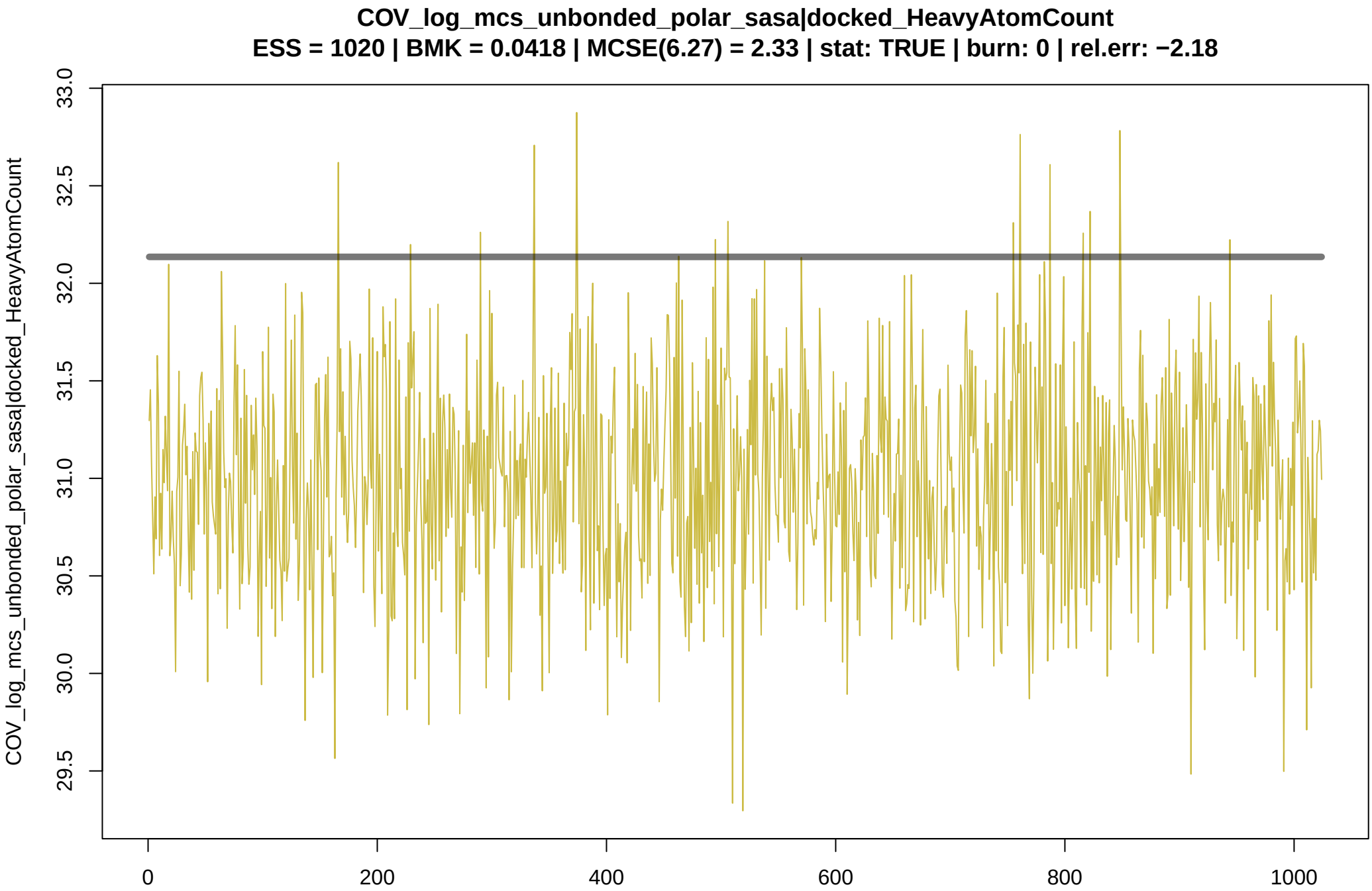

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0344 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0 | rel.err: 0.524
COV_log_RMSD|mcs_RingCount
0.00
0.05
0.10
0.15
0.20
0.25
0
200
400
600
800
1000

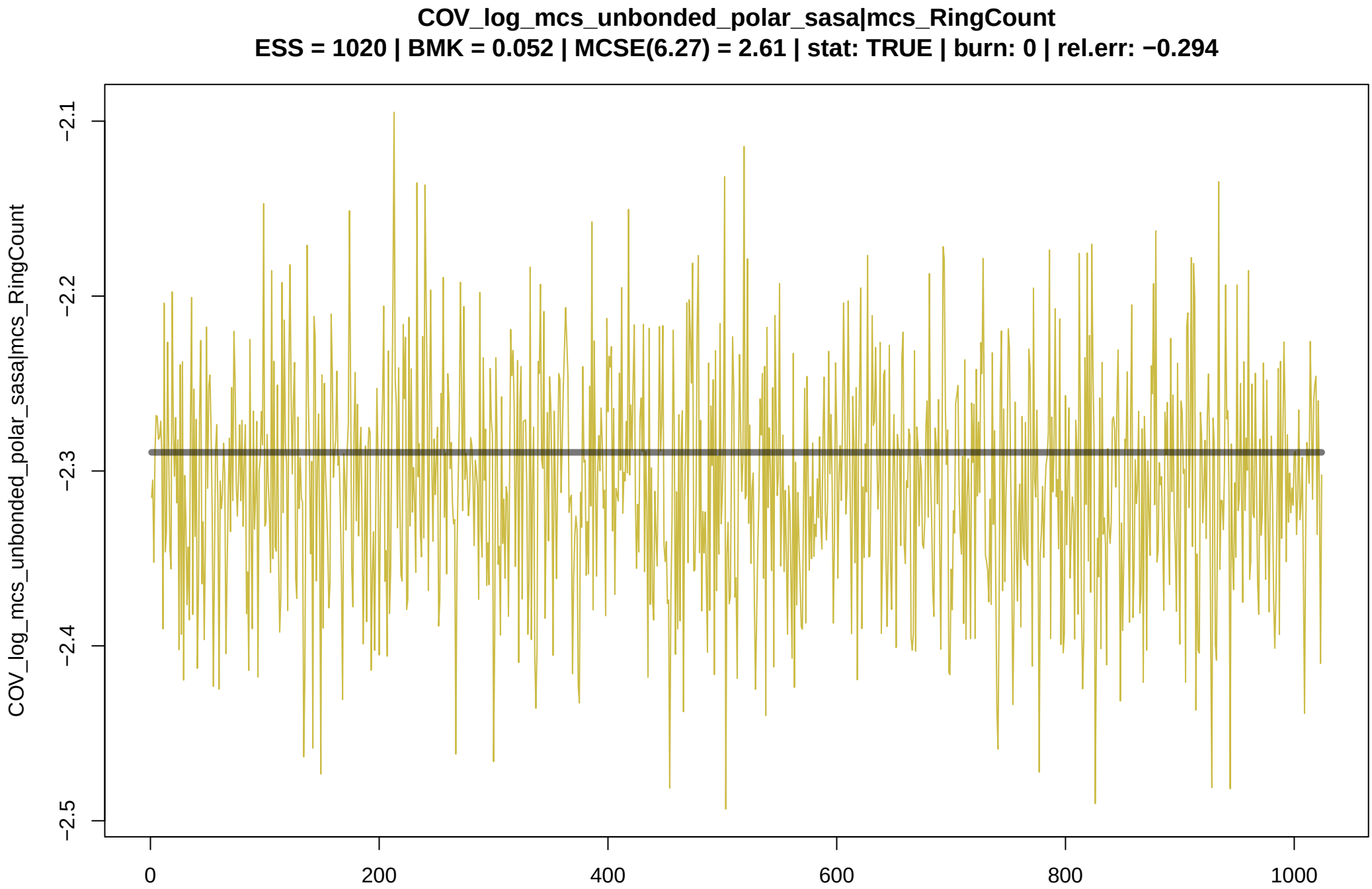

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0508 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | rel.err: −1.39
COV_log_RMSD|docked_NumRotatableBonds
−6.4
−6.6
−6.8
−7.0
0
200
400
600
800
1000

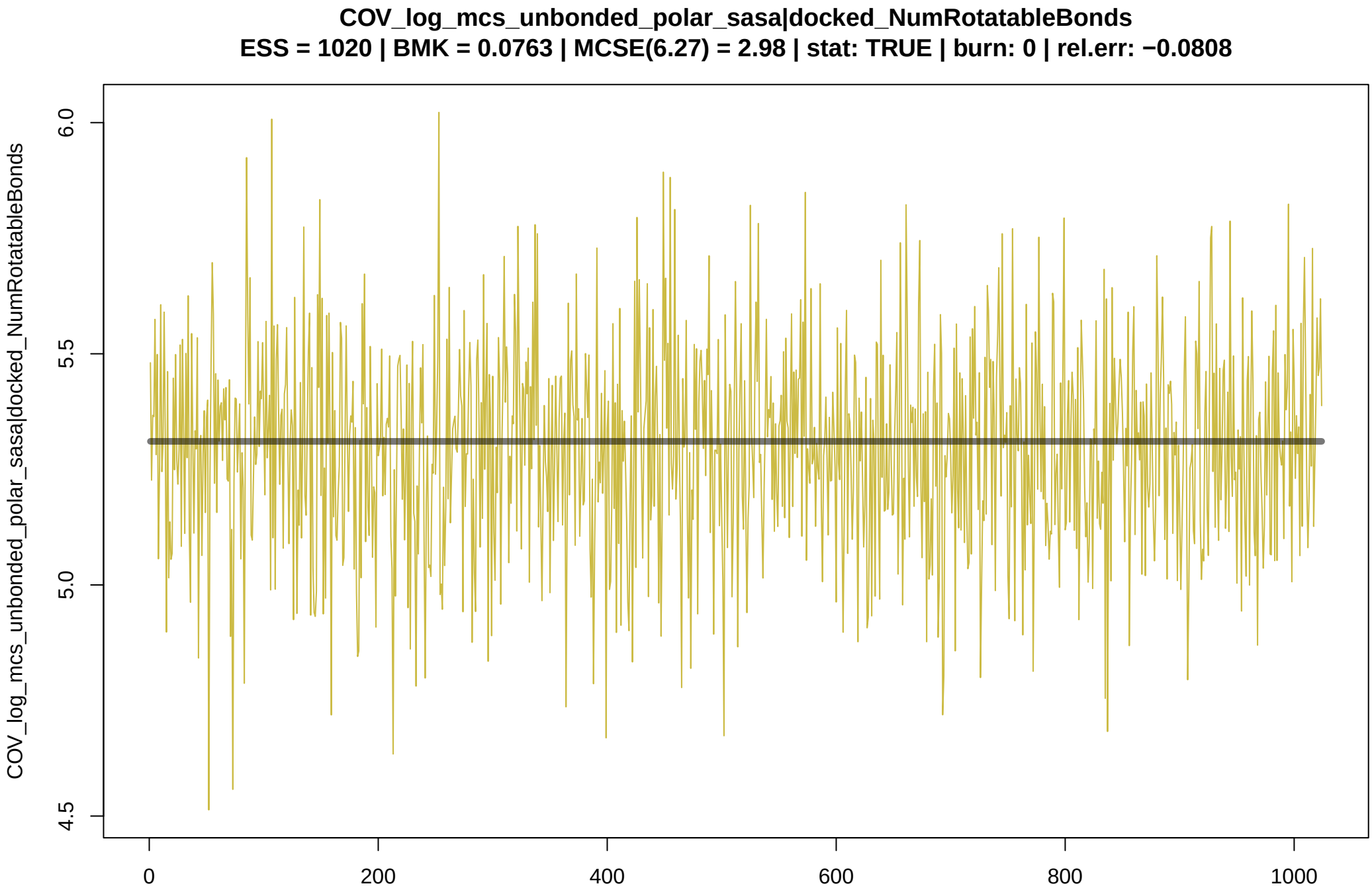

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0552 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | rel.err: −2.02
COV_log_RMSD|mcs_NOCount
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

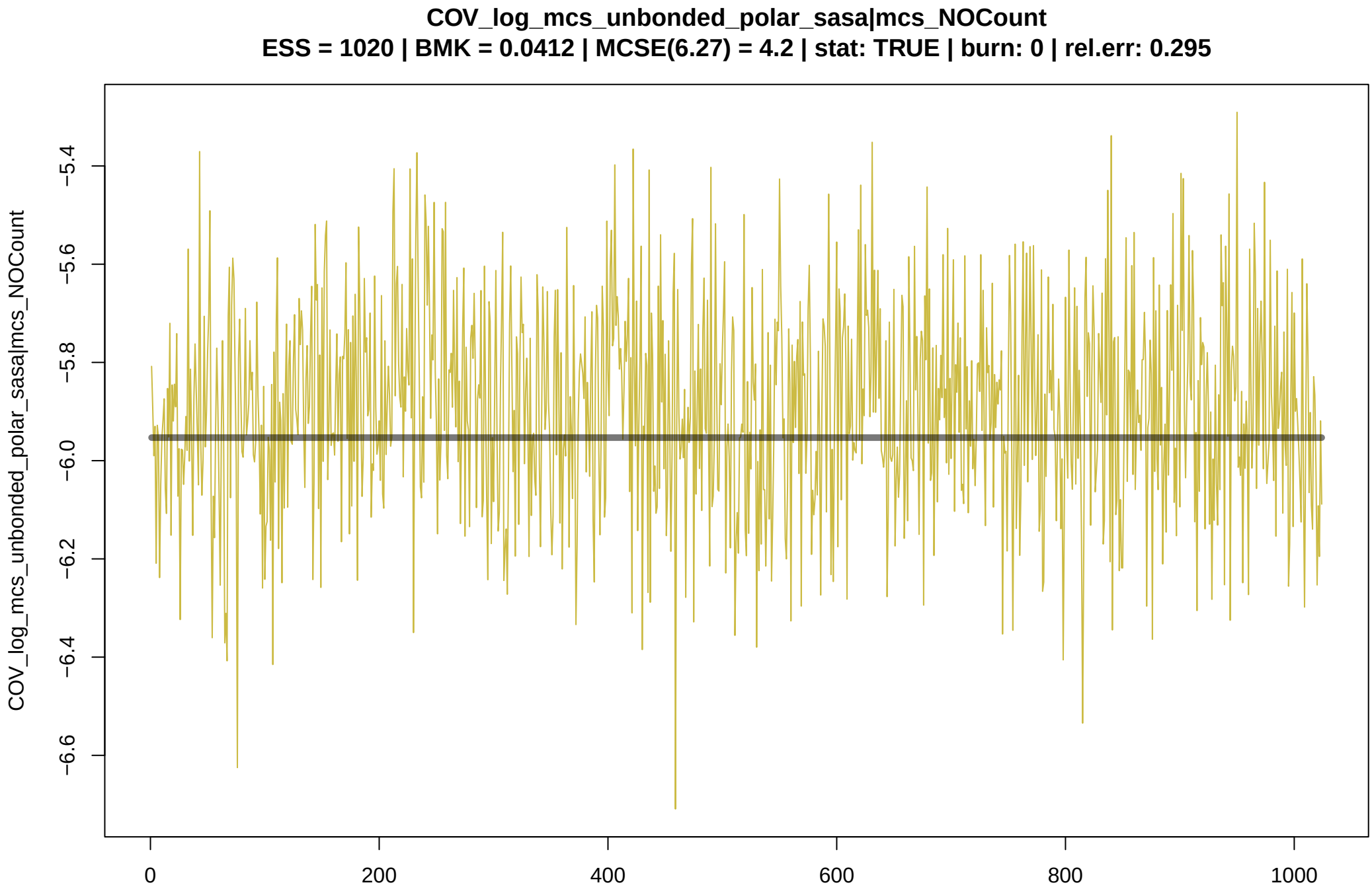

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.065 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | rel.err: −1.96
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
1.8
2.0
2.2
2.4
2.6
0
200
400
600
800
1000

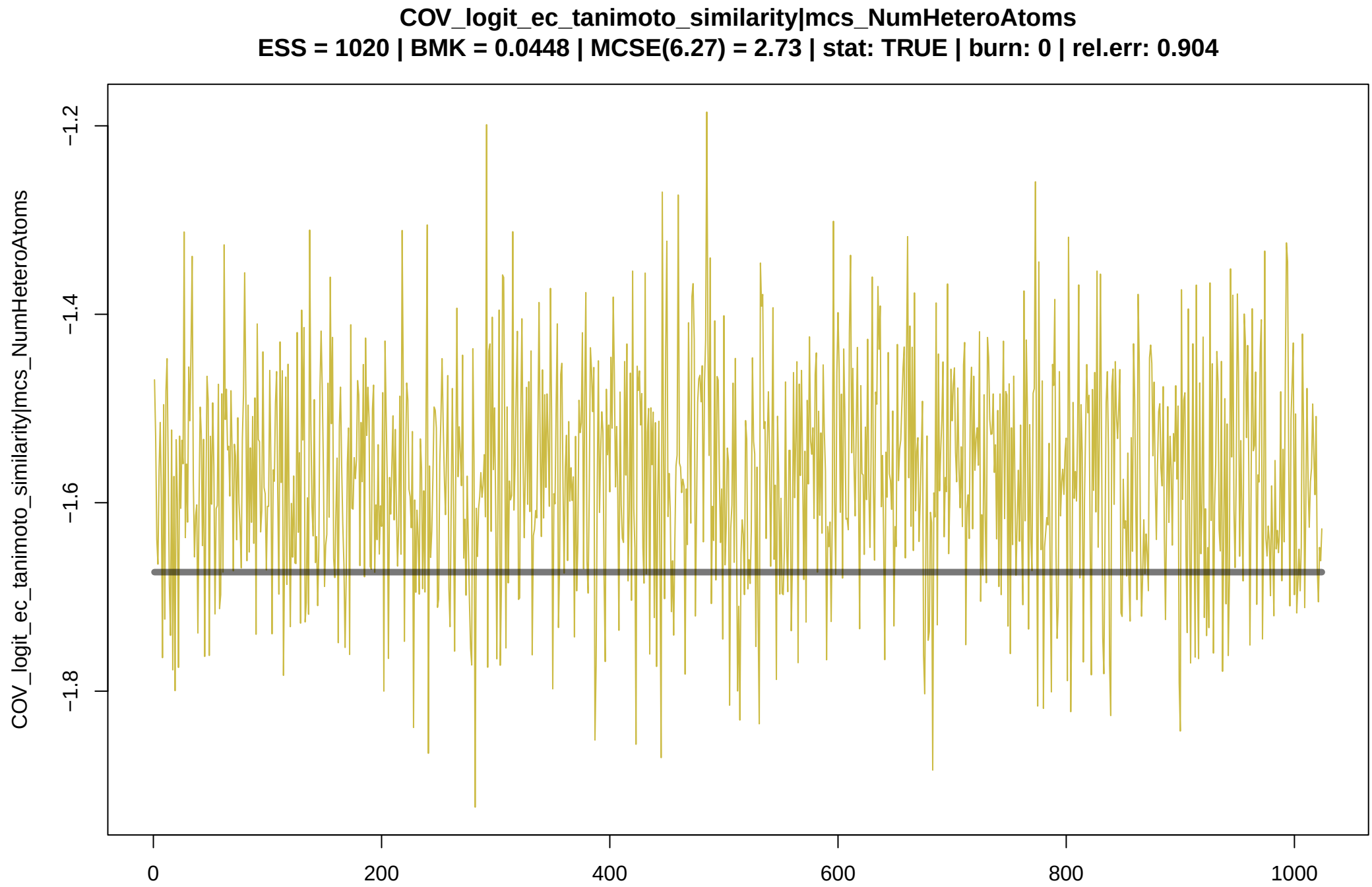

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.036 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | rel.err: 0.762
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

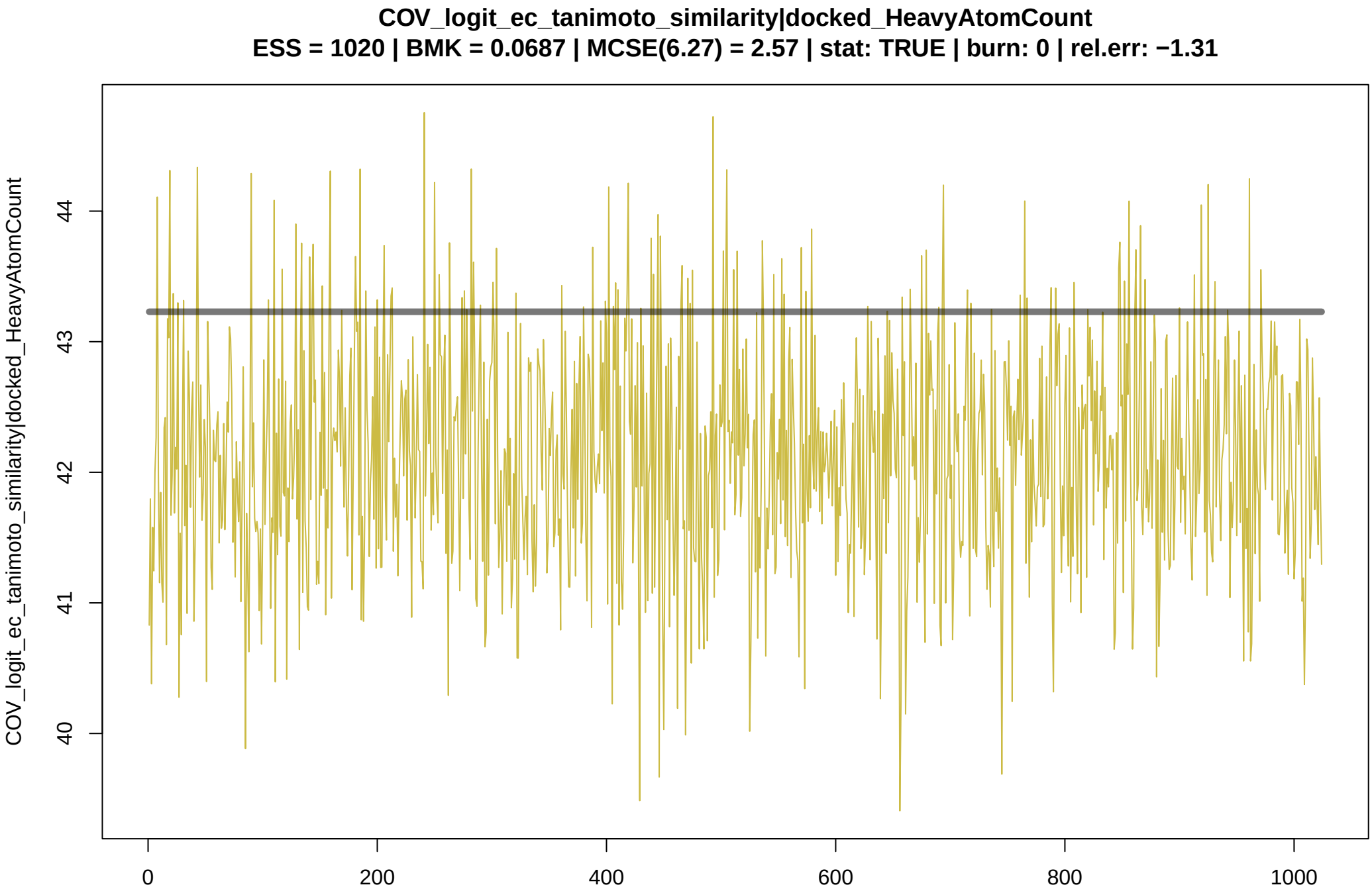

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0418 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: −2.18
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
33.0
32.5
32.0
31.5
31.0
30.5
30.0
29.5
0
200
400
600
800
1000

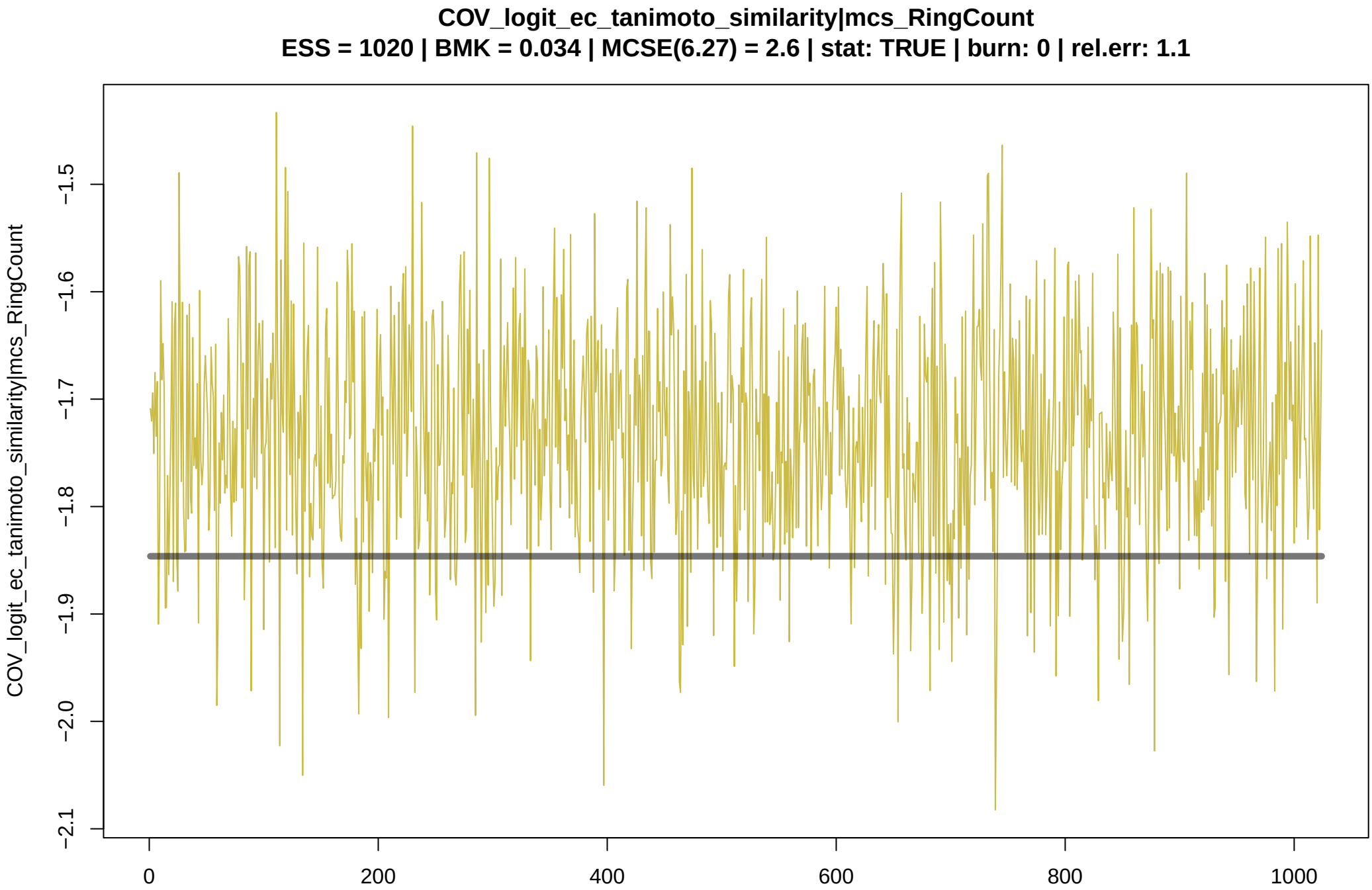

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.052 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: −0.294
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.1
−2.2
−2.3
−2.4
−2.5
0
200
400
600
800
1000

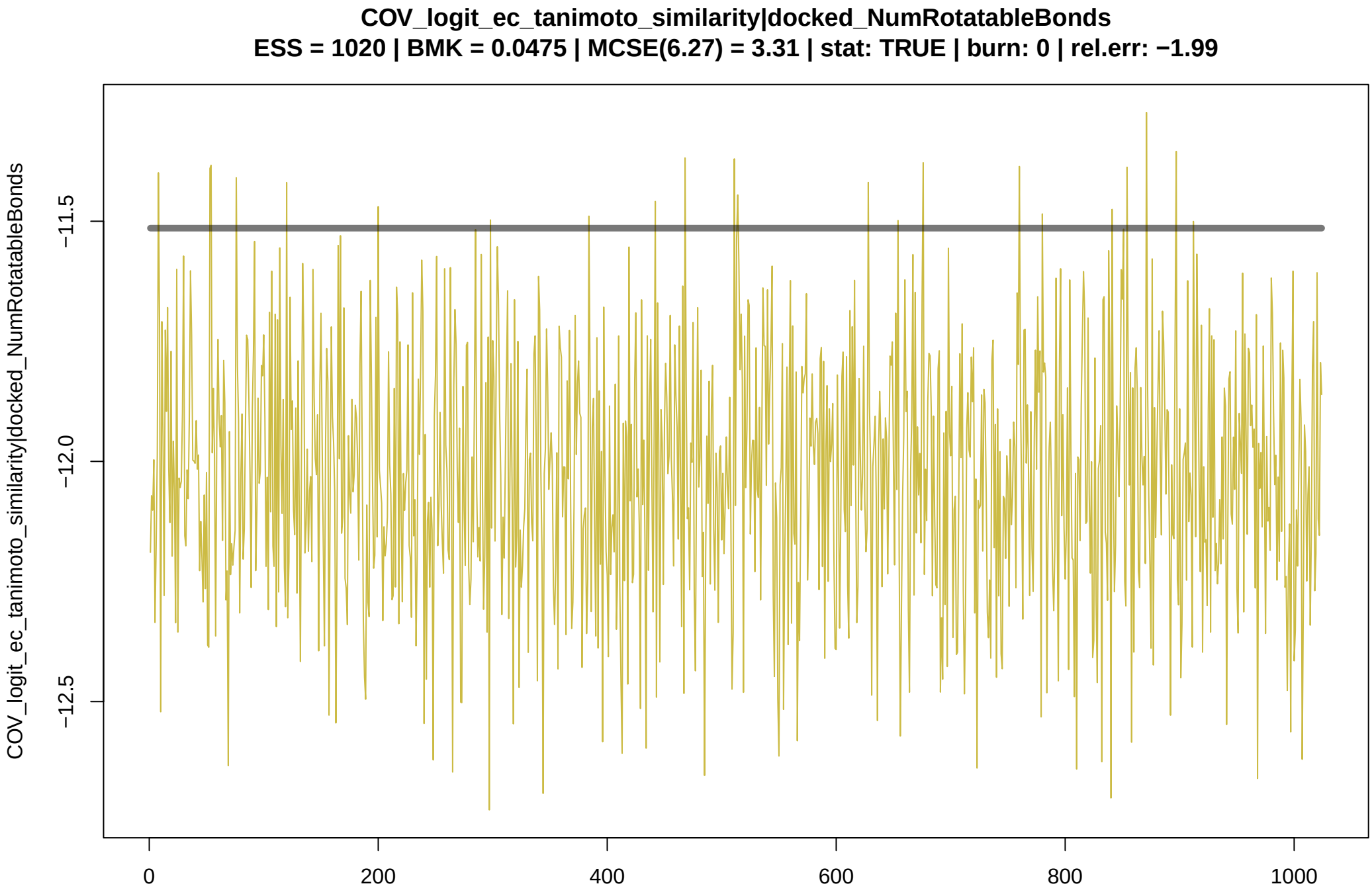

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0763 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | rel.err: −0.0808
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
6.0
5.5
5.0
4.5
0
200
400
600
800
1000

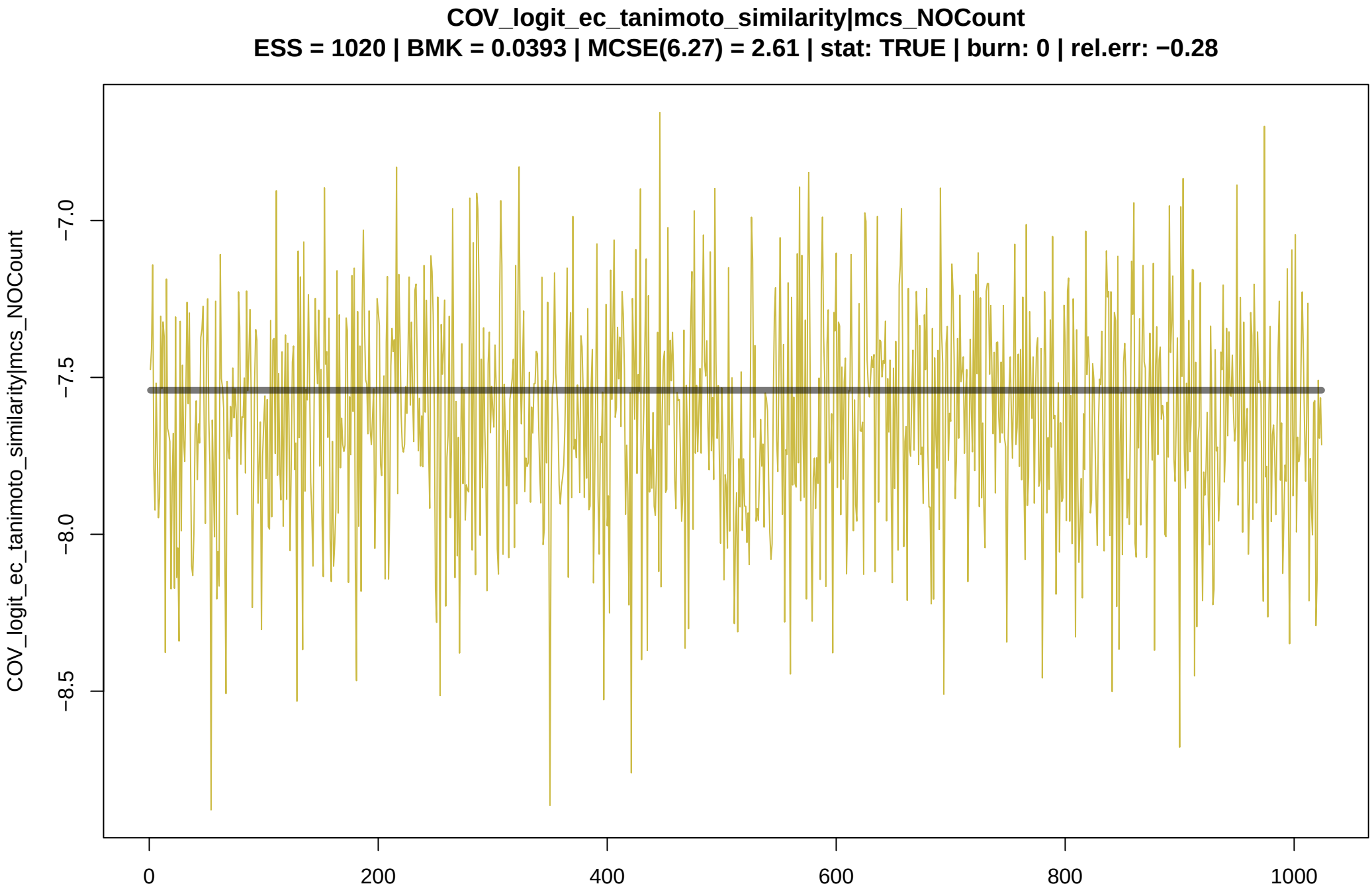

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0412 | MCSE(6.27) = 4.2 | stat: TRUE | burn: 0 | rel.err: 0.295
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.4
−5.6
−5.8
−6.0
−6.2
−6.4
−6.6
0
200
400
600
800
1000

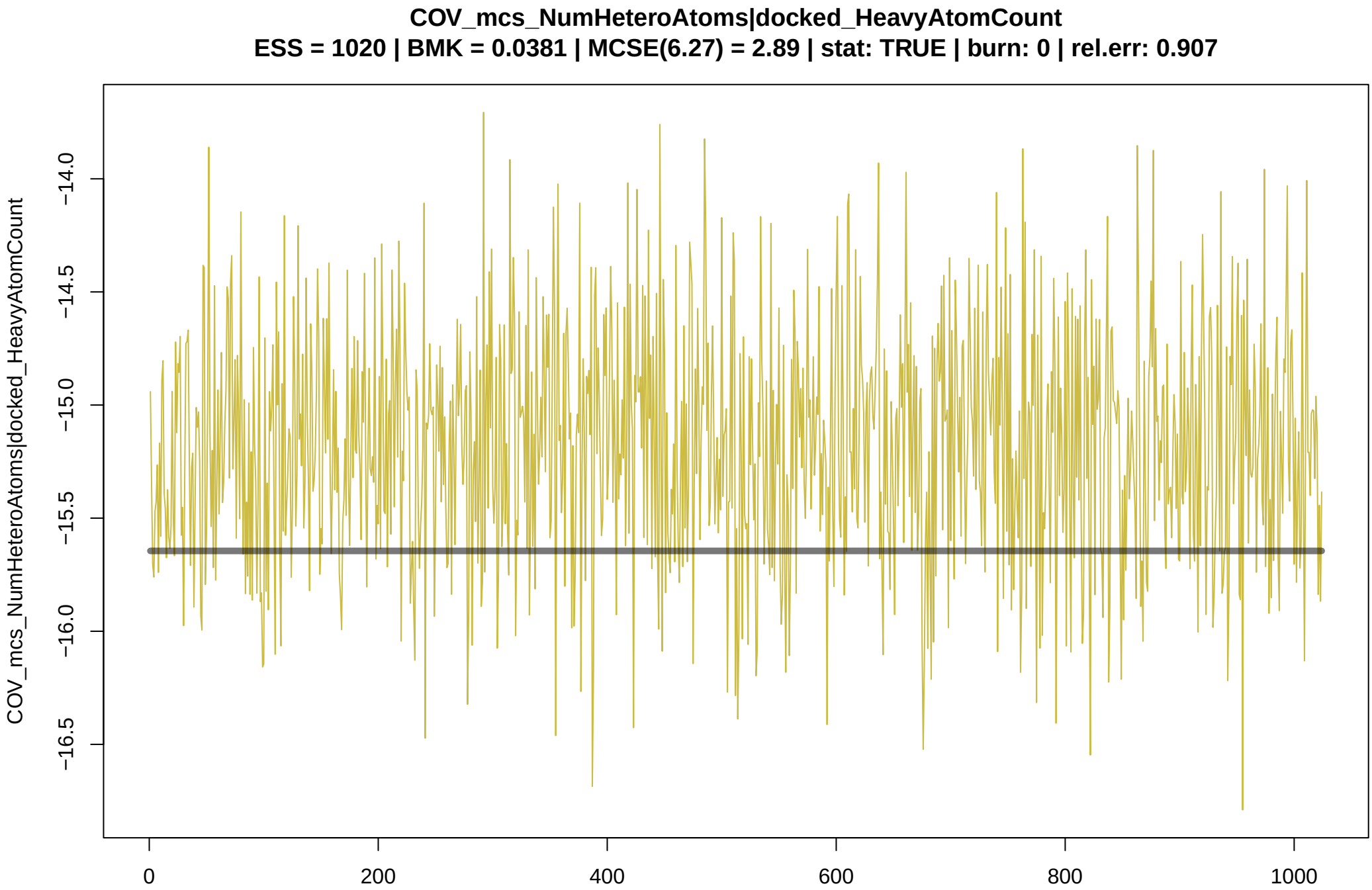

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0448 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | rel.err: 0.904
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.2
−1.4
−1.6
−1.8
0
200
400
600
800
1000

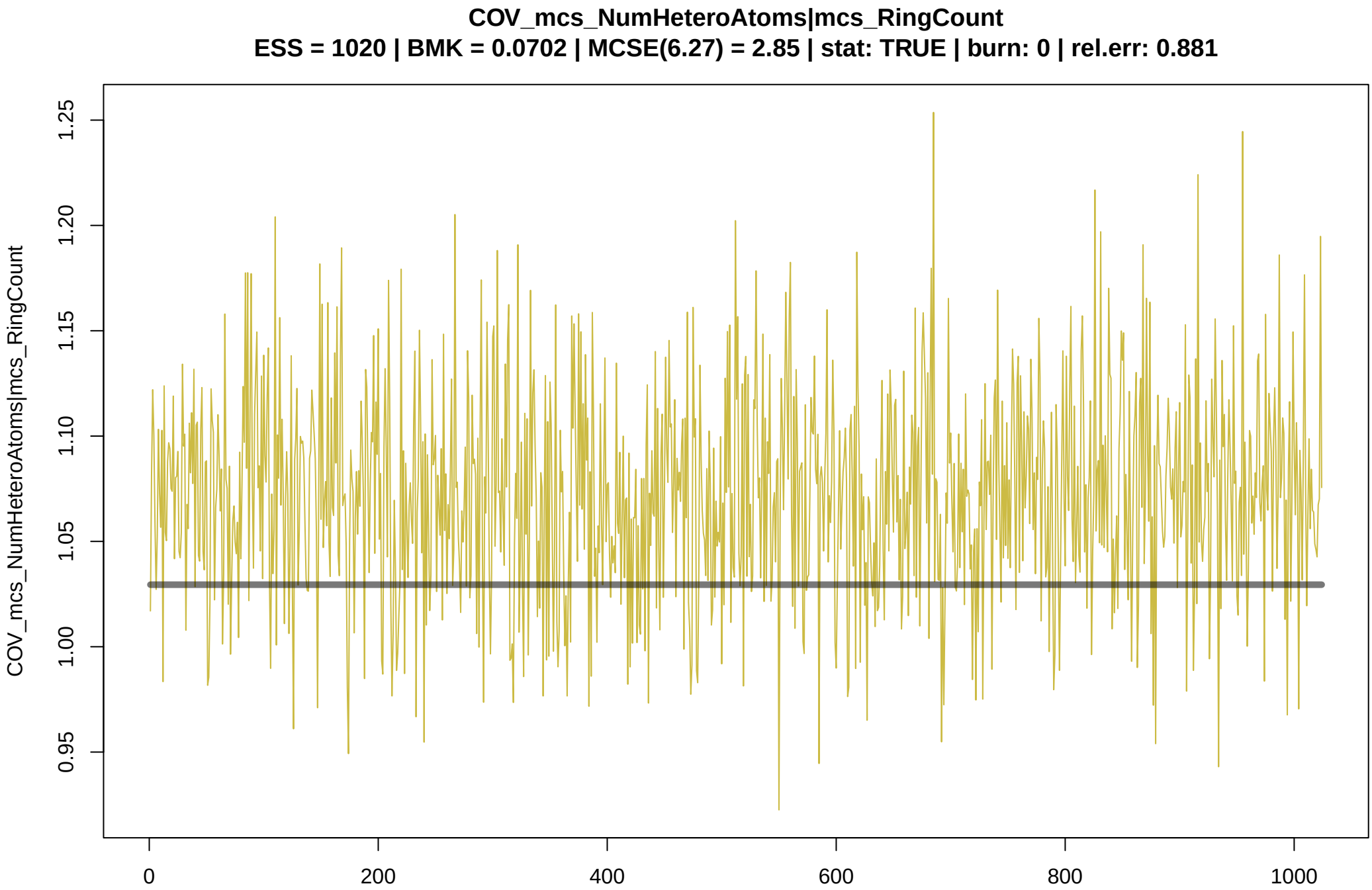

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0687 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: −1.31
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
40
41
42
43
44
0
200
400
600
800
1000

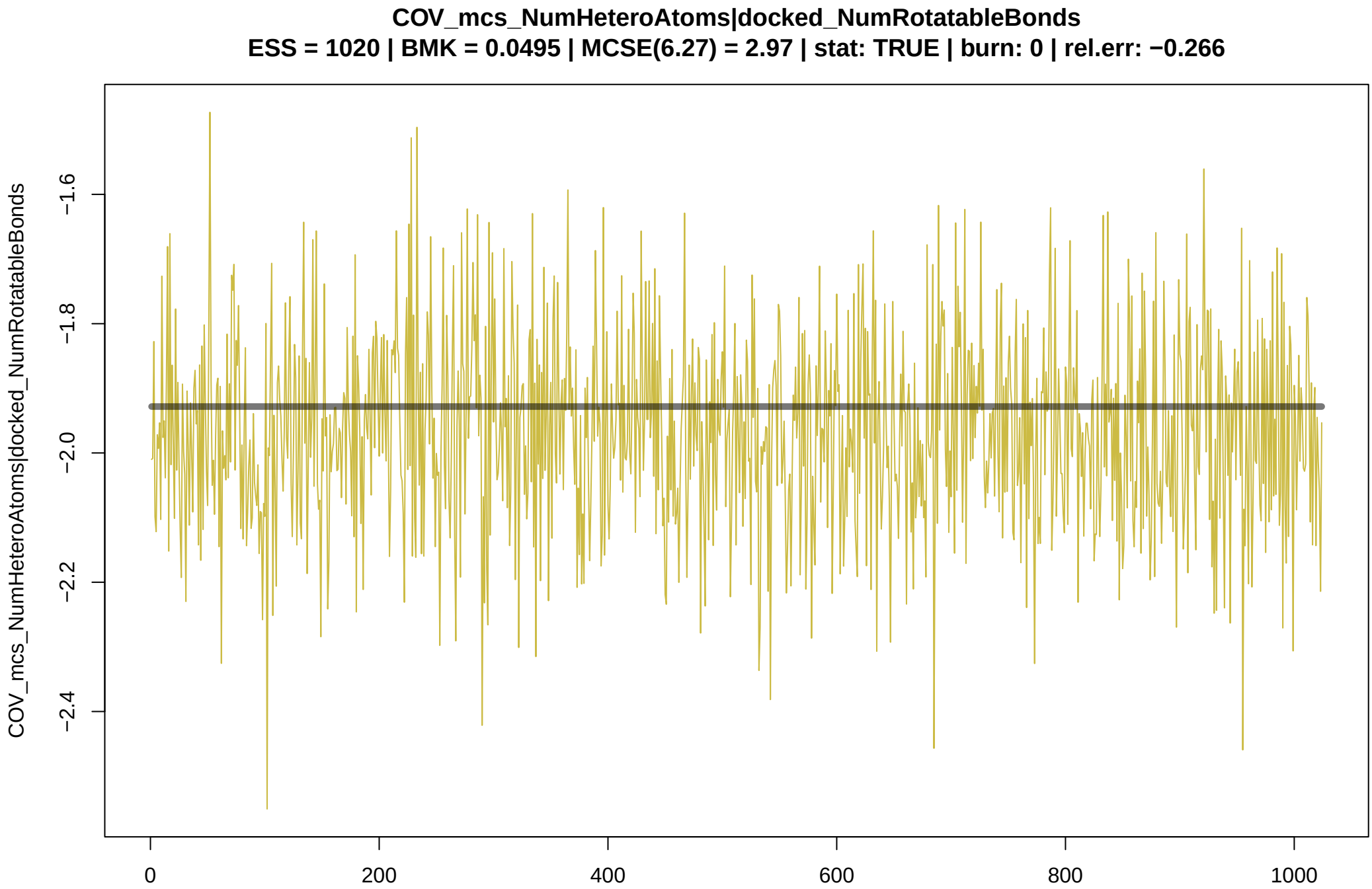

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.034 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: 1.1
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.5
−1.6
−1.7
−1.8
−1.9
−2.0
−2.1
0
200
400
600
800
1000

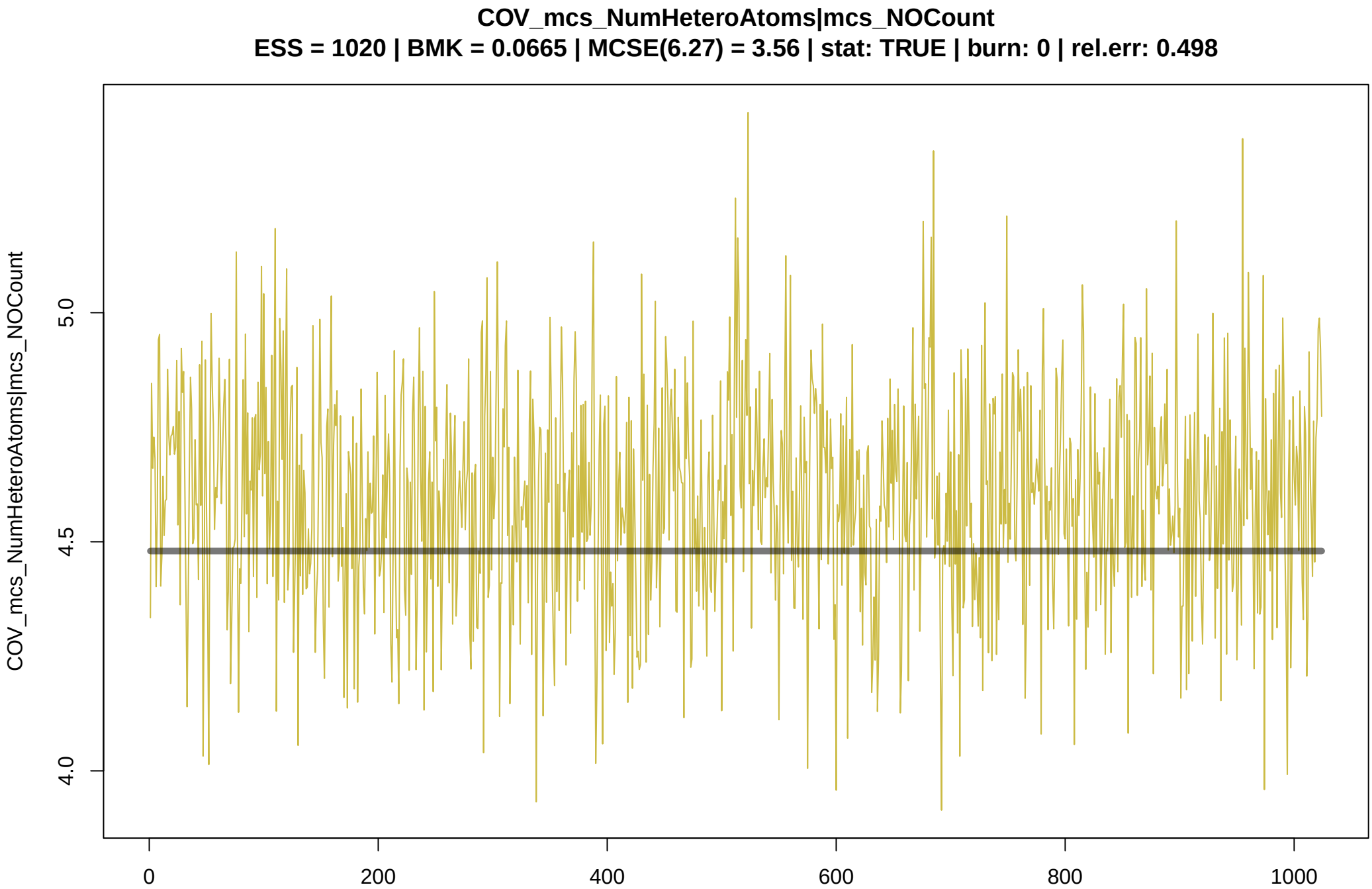

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0475 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0 | rel.err: −1.99
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−11.5
−12.0
−12.5
0
200
400
600
800
1000

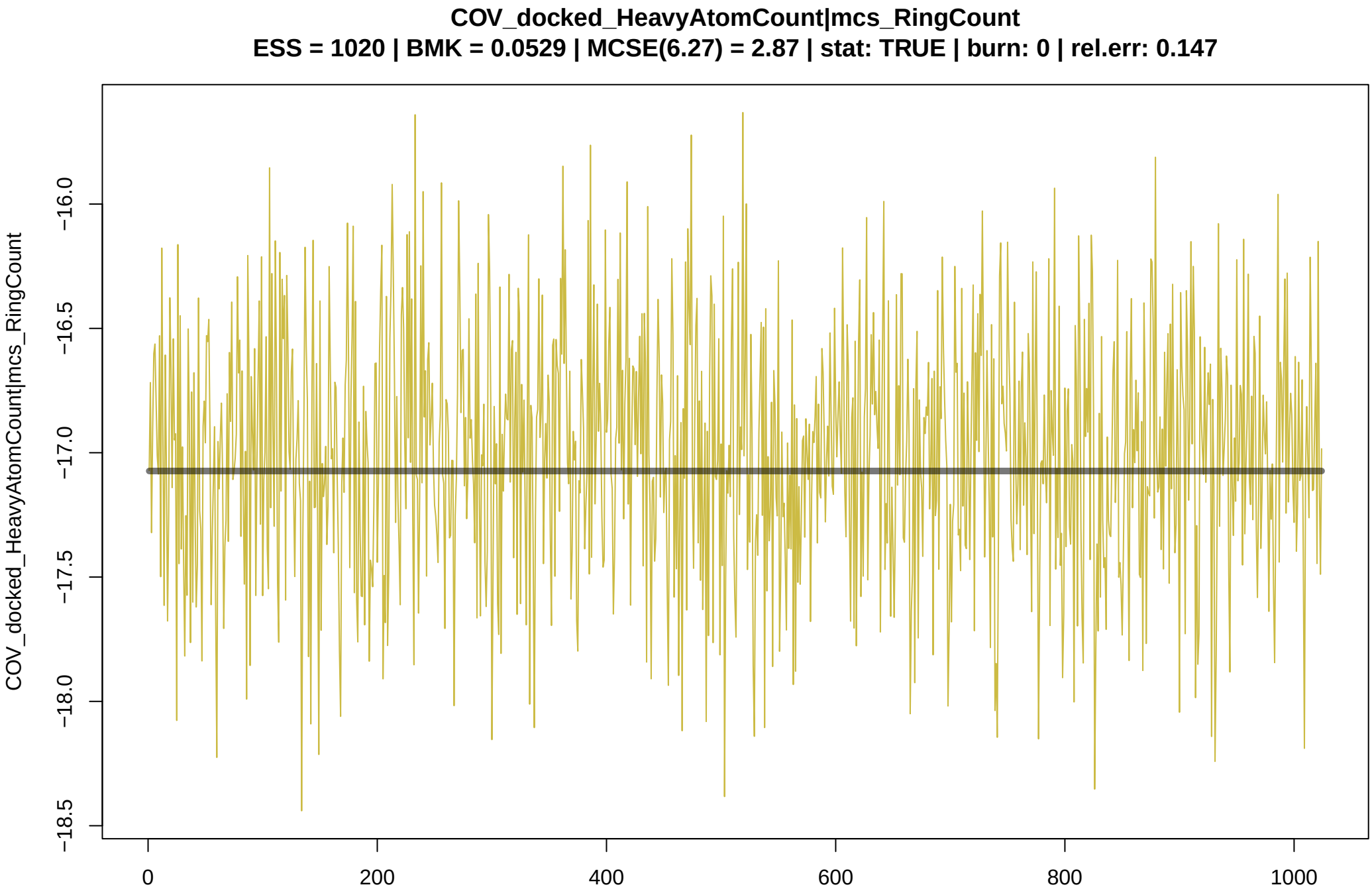

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0393 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: −0.28
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−7.0
−7.5
−8.0
−8.5
0
200
400
600
800
1000

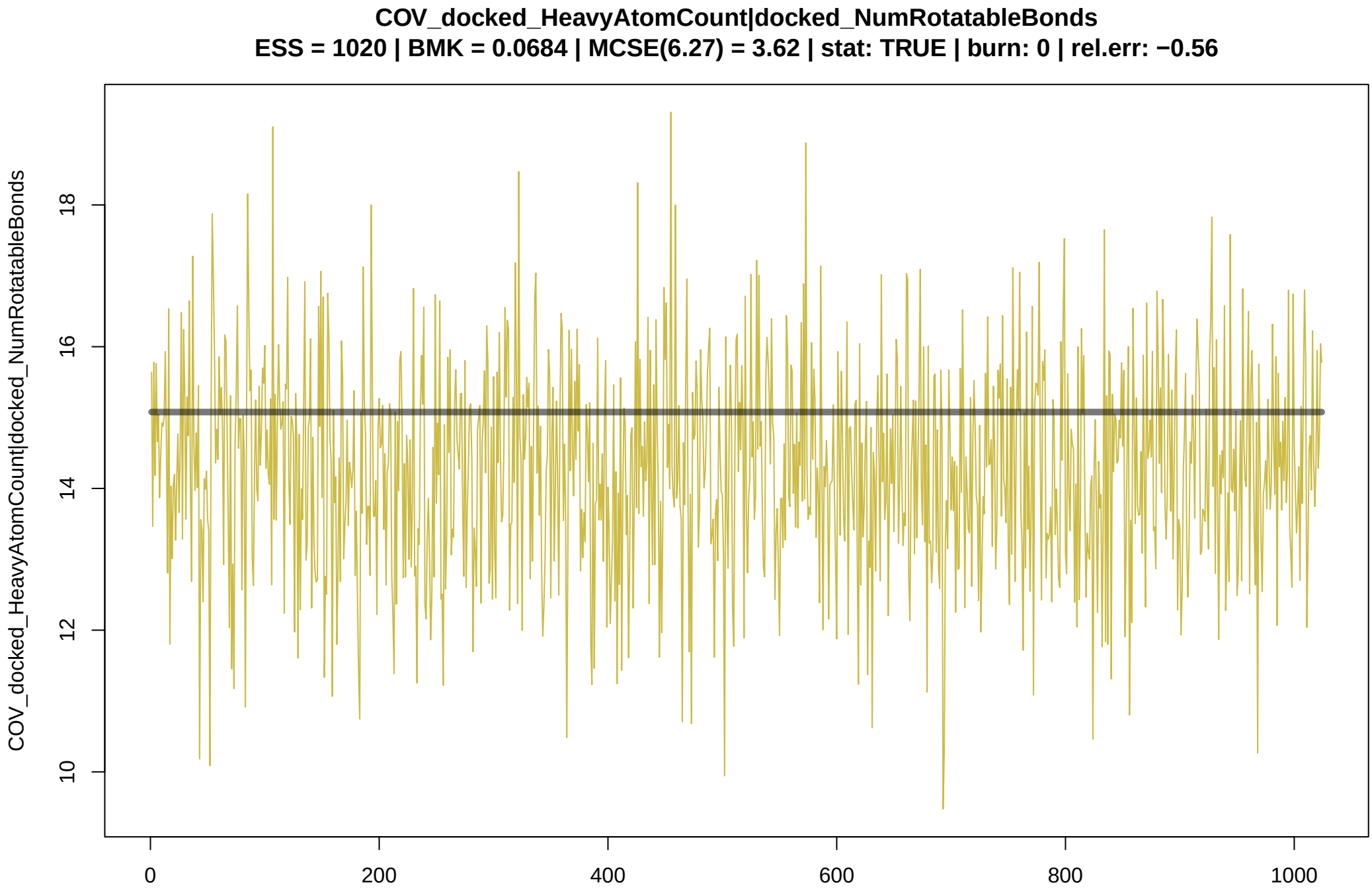

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0381 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | rel.err: 0.907
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−14.0
−14.5
−15.0
−15.5
−16.0
−16.5
0
200
400
600
800
1000

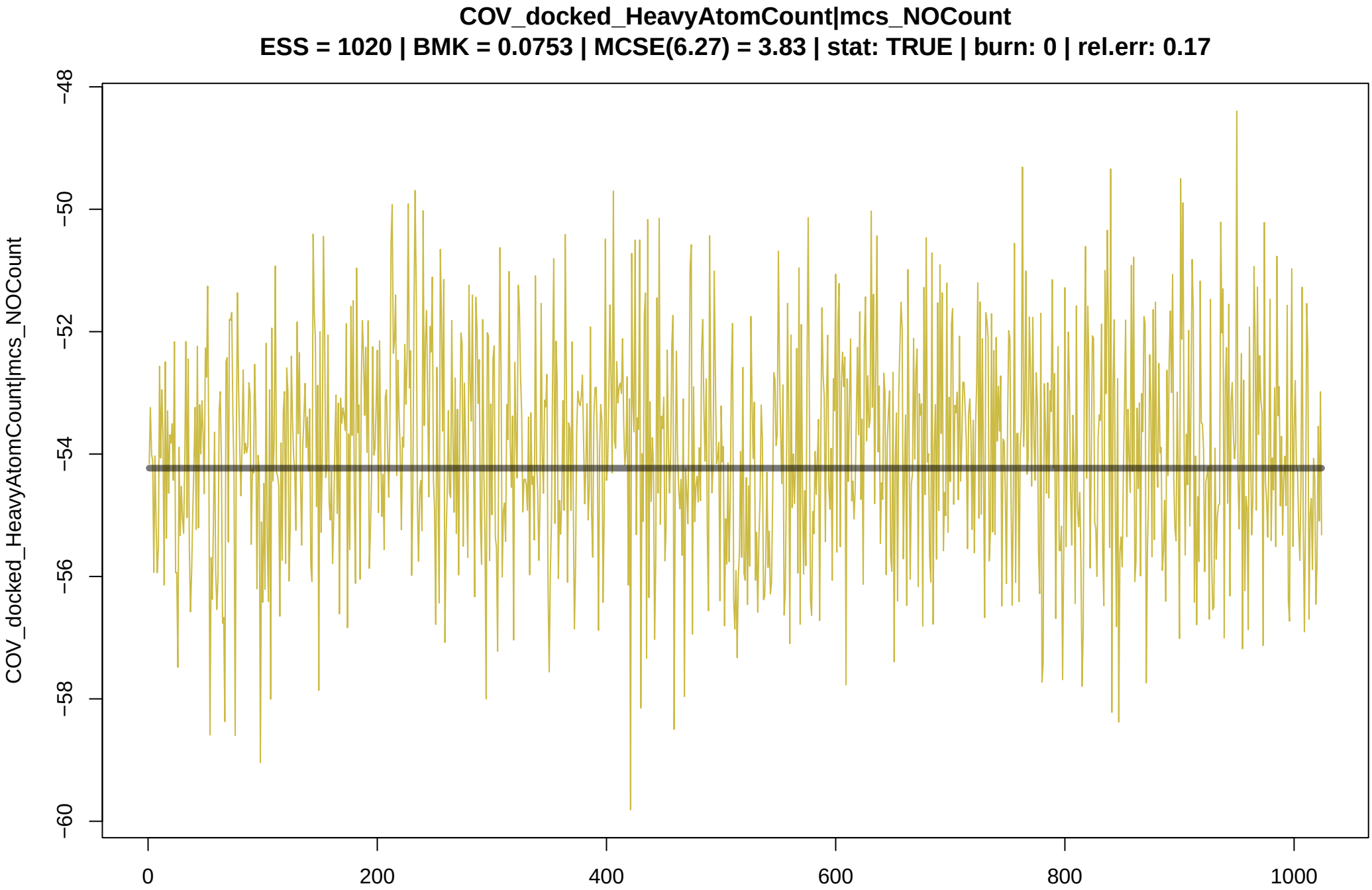

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0702 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | rel.err: 0.881
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.95
1.00
1.05
1.10
1.15
1.20
1.25
0
200
400
600
800
1000

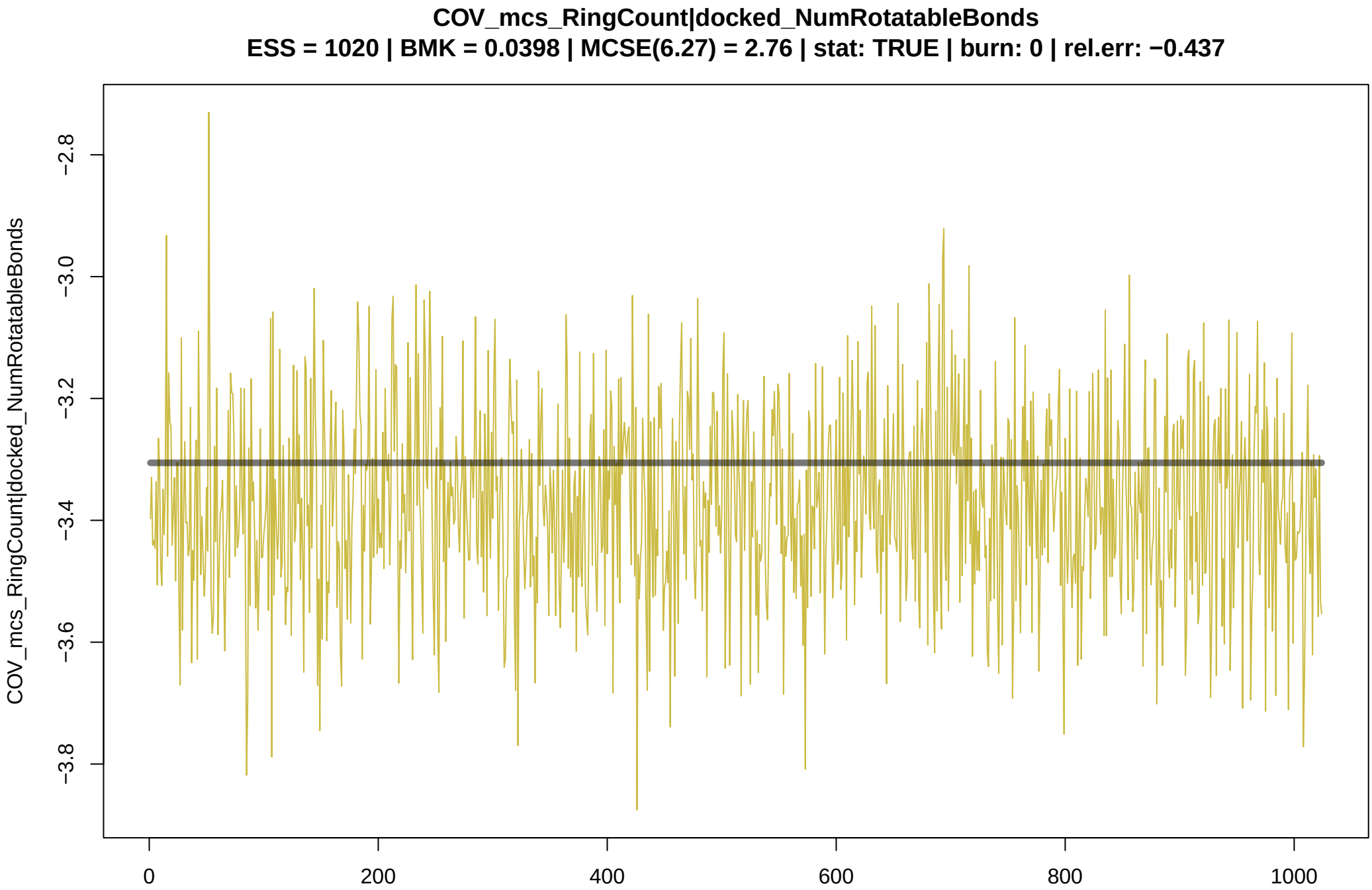

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0495 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0 | rel.err: −0.266
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.6
−1.8
−2.0
−2.2
−2.4
0
200
400
600
800
1000

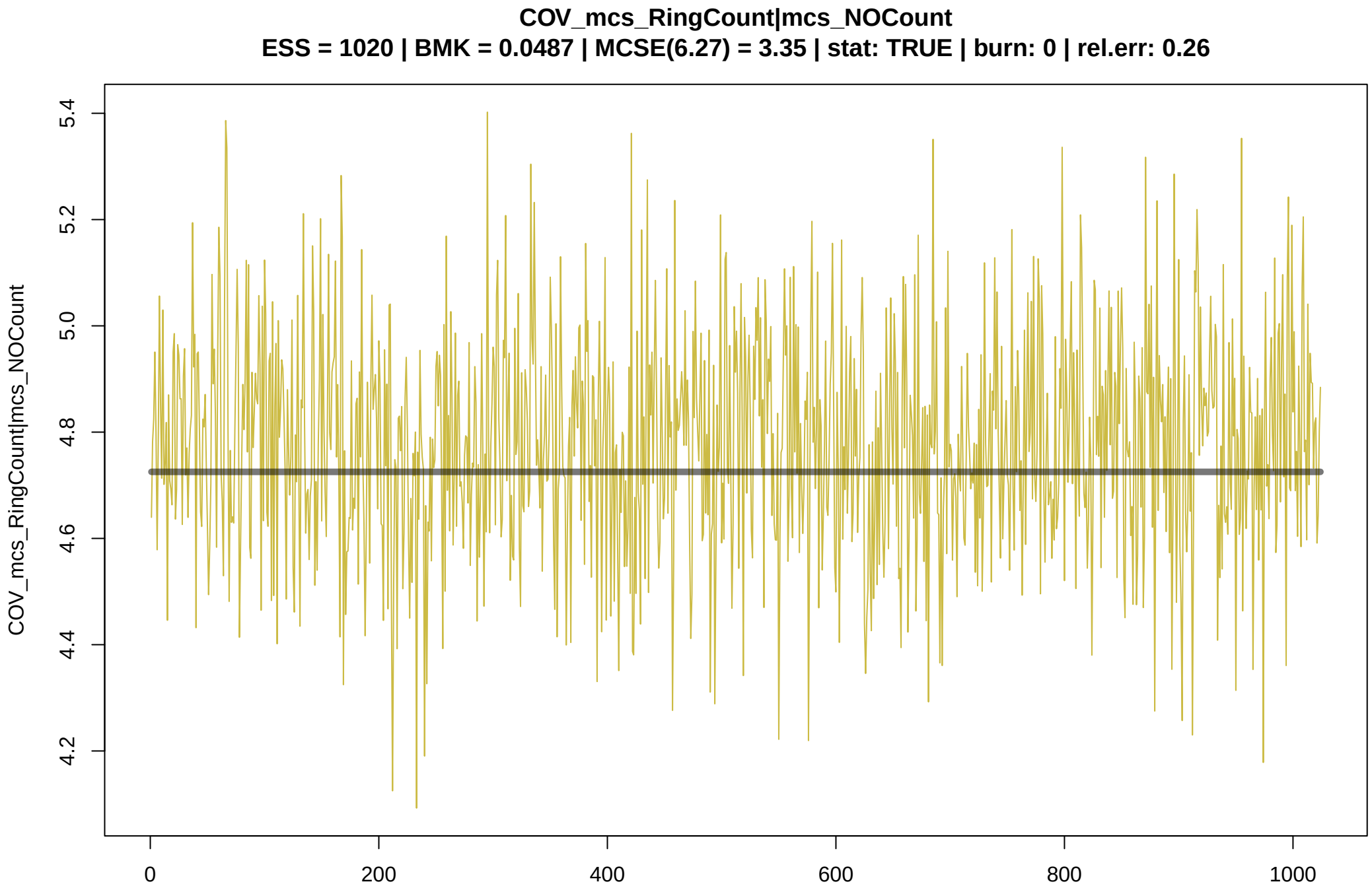

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0665 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | rel.err: 0.498
COV_mcs_NumHeteroAtoms|mcs_NOCount
4.0
4.5
5.0
0
200
400
600
800
1000

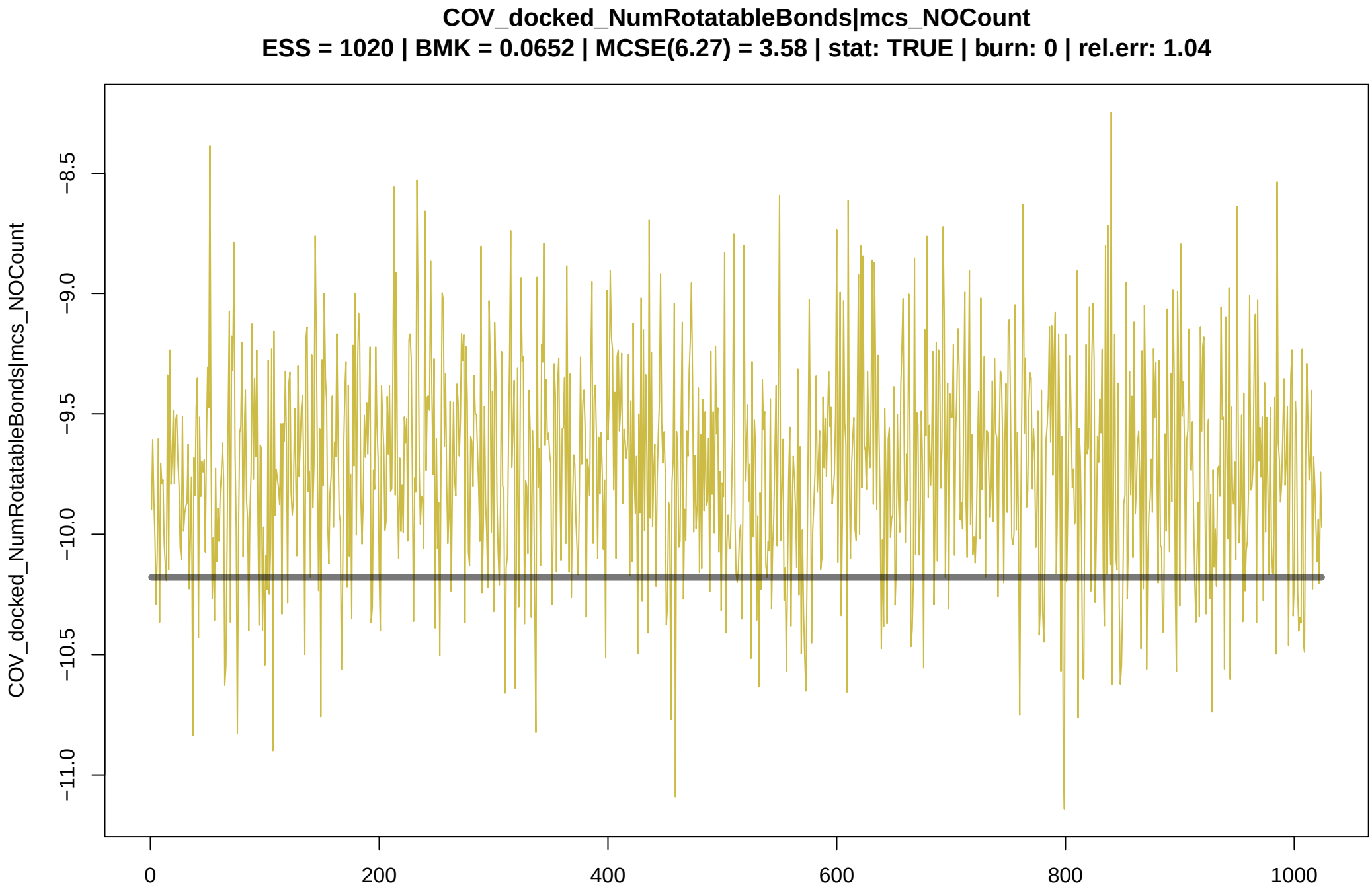

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0529 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0 | rel.err: 0.147
COV_docked_HeavyAtomCount|mcs_RingCount
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0684 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0 | rel.err: −0.56
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0753 | MCSE(6.27) = 3.83 | stat: TRUE | burn: 0 | rel.err: 0.17
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 = 0.0398 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | rel.err: −0.437
COV_mcs_RingCount|docked_NumRotatableBonds
−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 = 0.0487 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0 | rel.err: 0.26
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 = 0.0652 | MCSE(6.27) = 3.58 | stat: TRUE | burn: 0 | rel.err: 1.04
COV_docked_NumRotatableBonds|mcs_NOCount
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
0
200
400
600
800
1000