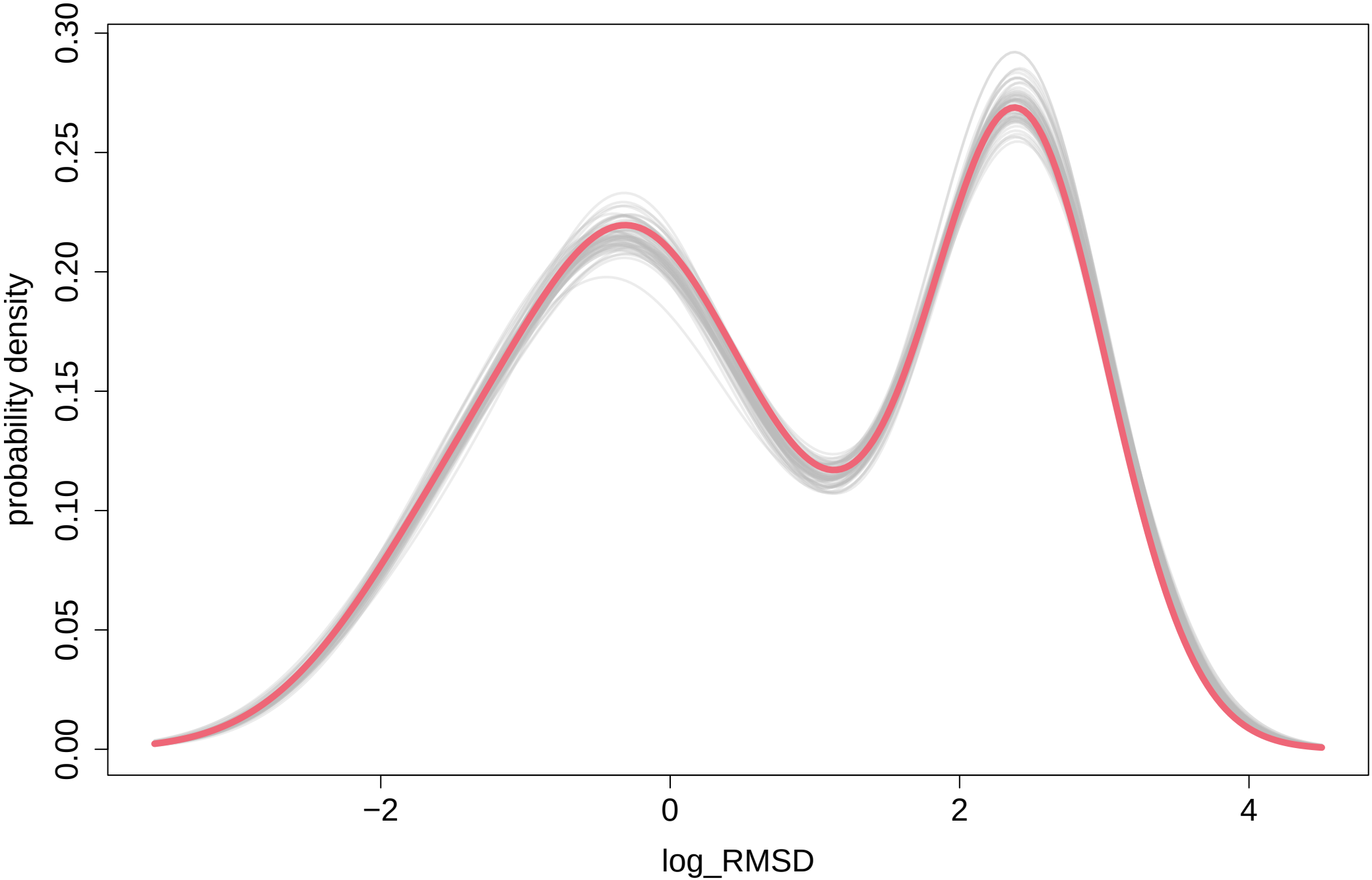
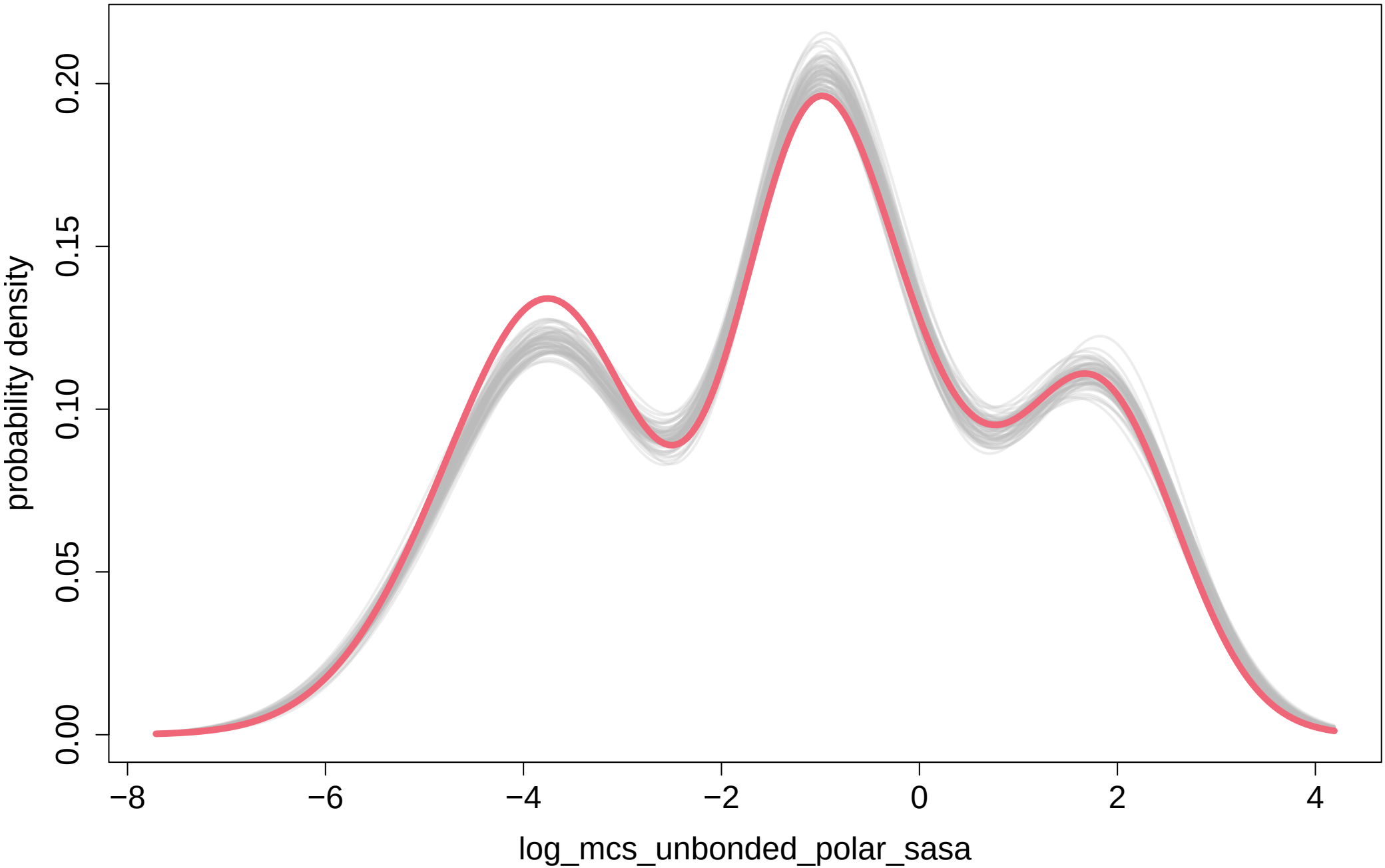
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.170477800990135
max MCSE = 7.69242922720397
all stationary: FALSE
burn: 0
max rel.err.: 1.3642577557353

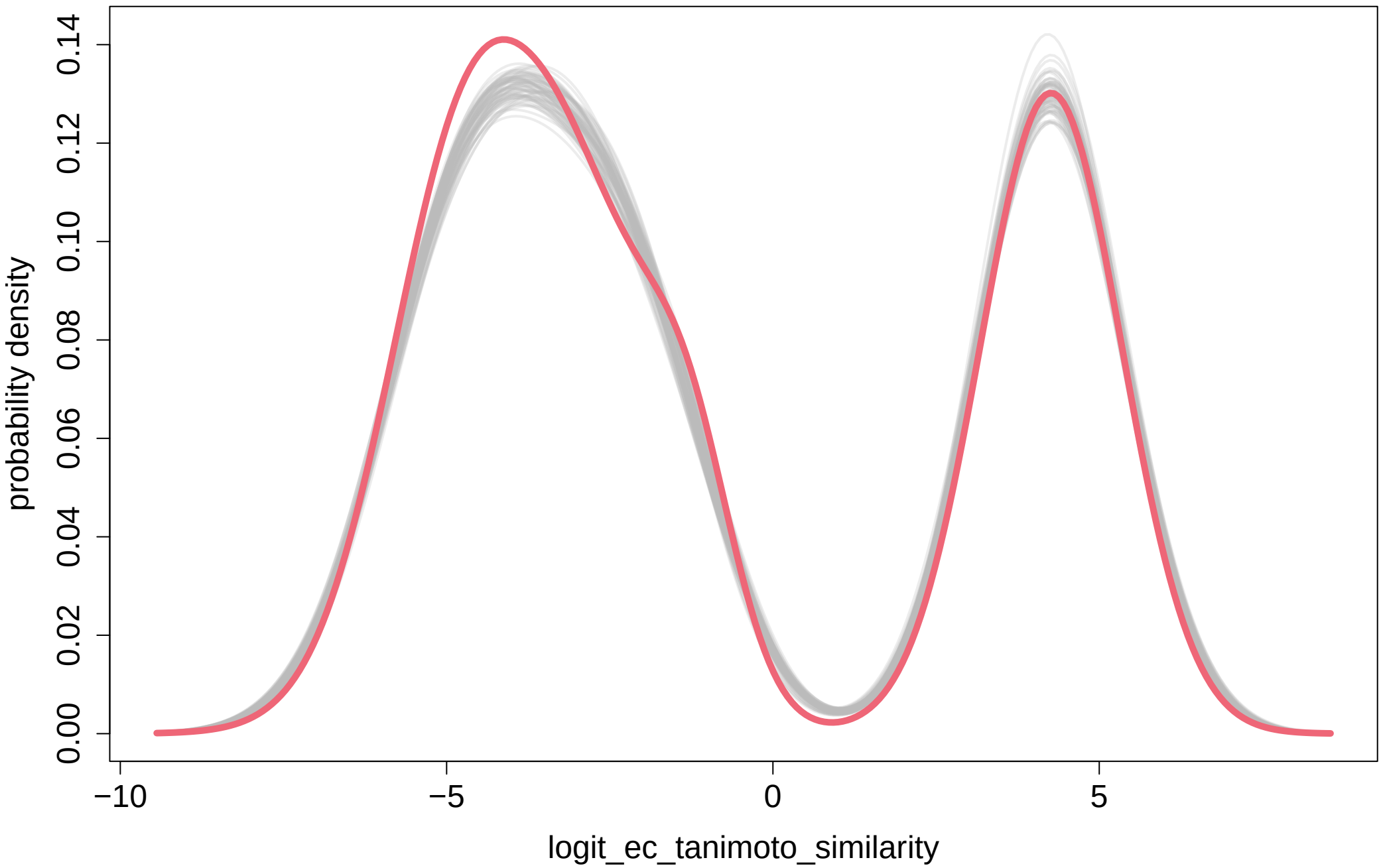
−− STATS 2D −−
min ESS = 888.542930726395
max BMK = 0.0936652446565228
max MCSE = 3.65274339208525
all stationary: FALSE
burn: 0
max rel.err.: 2.17752176608784

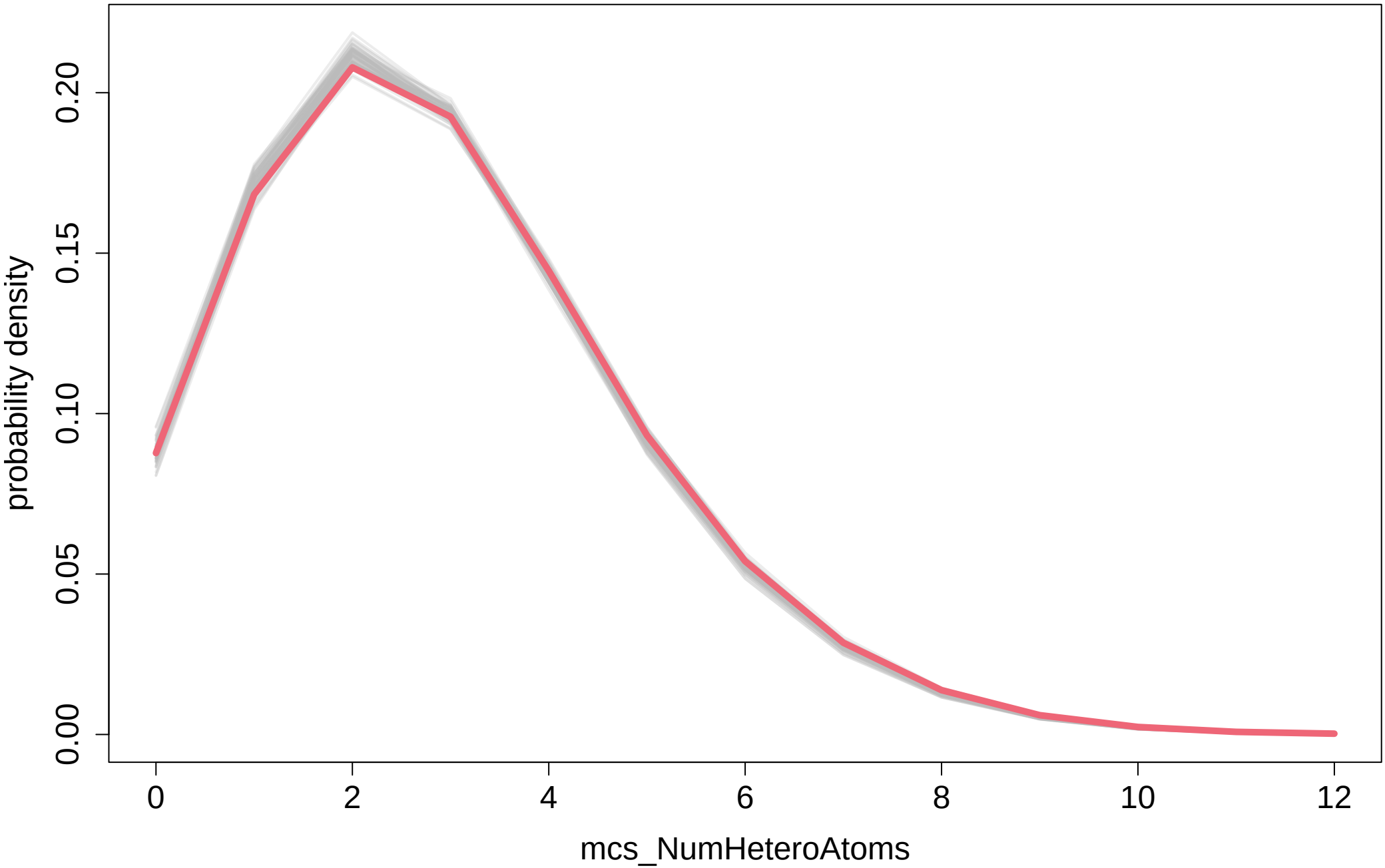
−− STATS 1D −−
min ESS = 119.314594812765
max BMK = 0.197153307454581
max MCSE = 7.1457667956898
all stationary: FALSE
burn: 0
max rel.err.: 2.7366884330593

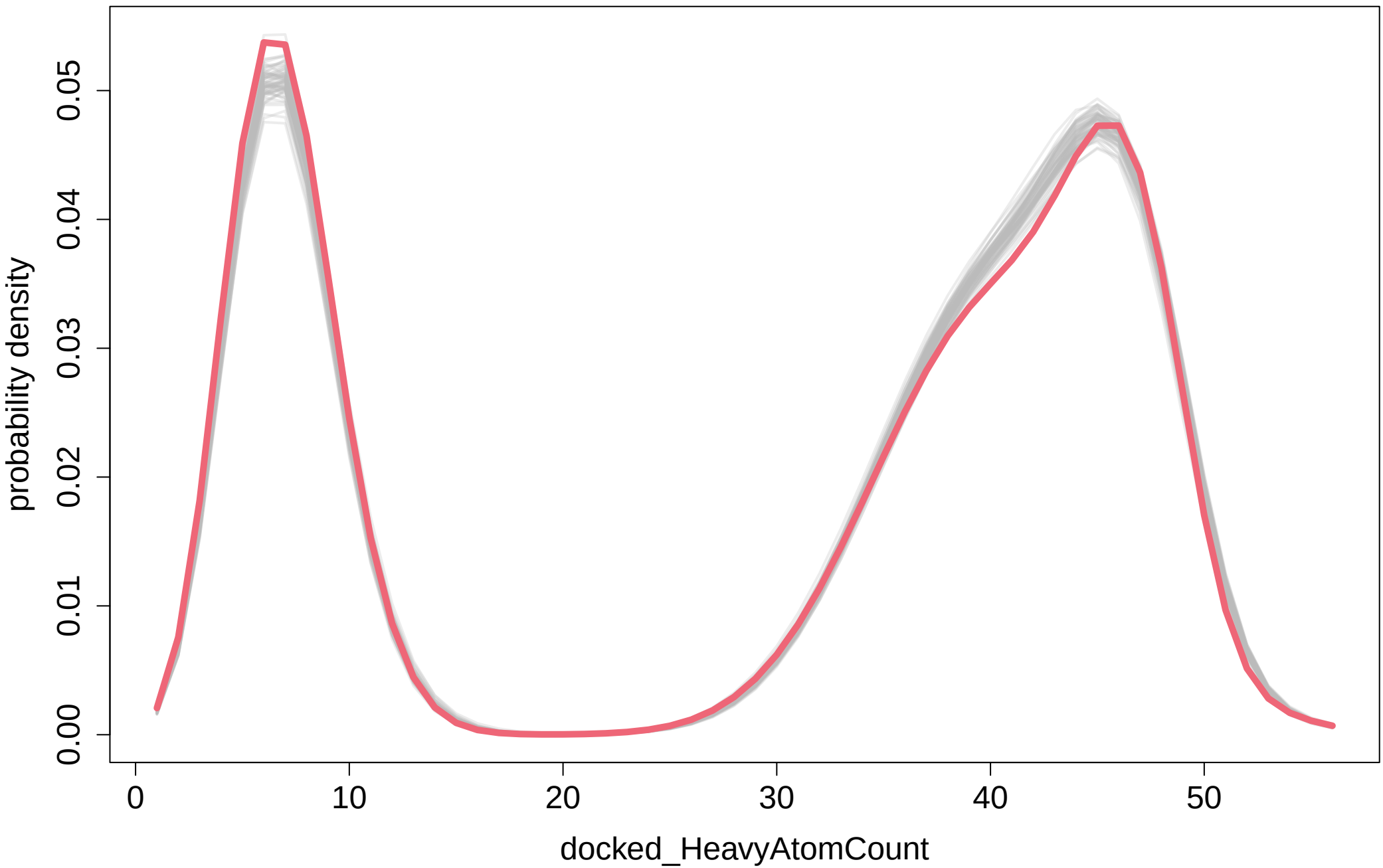
Occupied clusters: 9 of 64
LL: −62500 +− 12.8

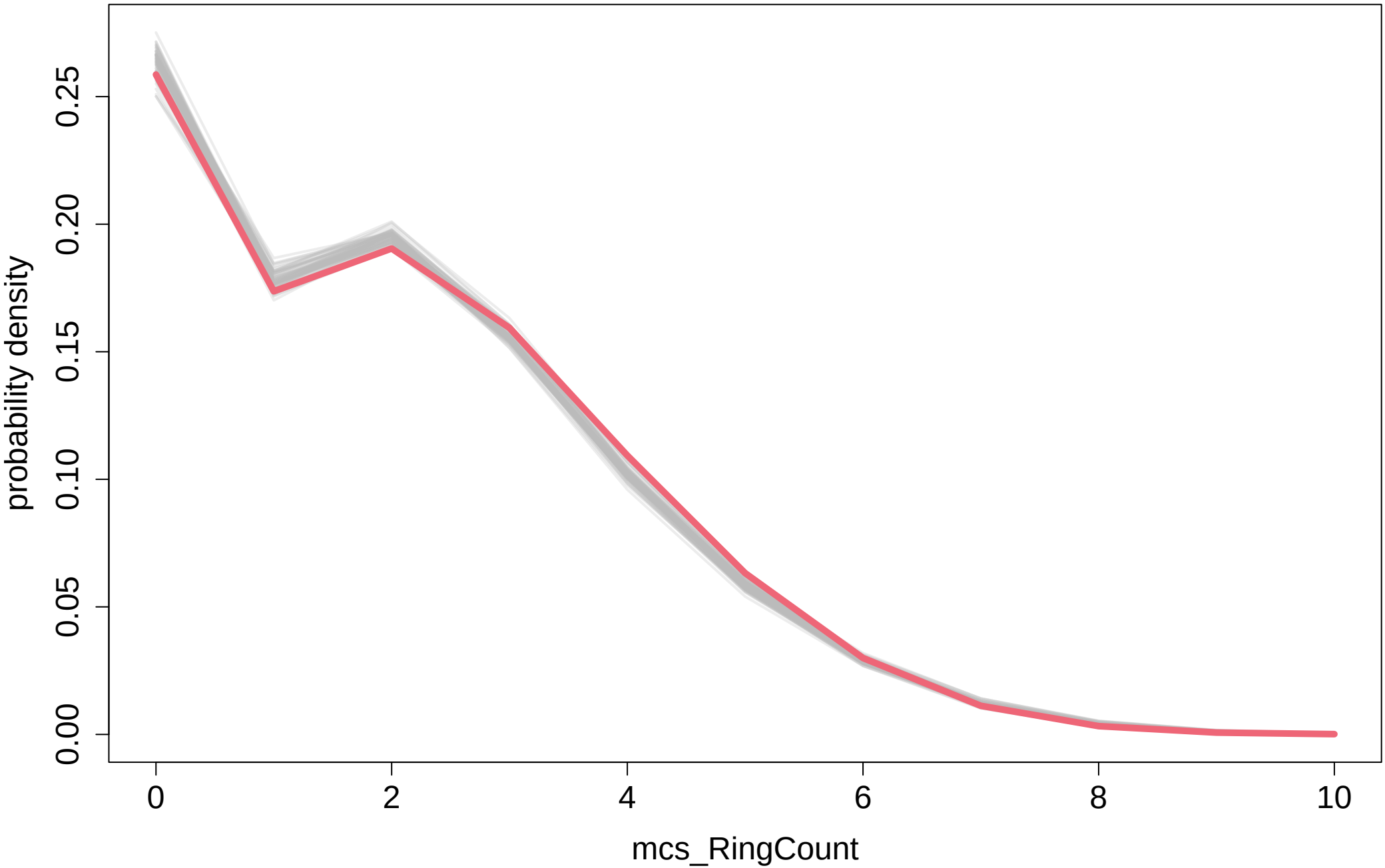

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−2
0
2
4
log_RMSD

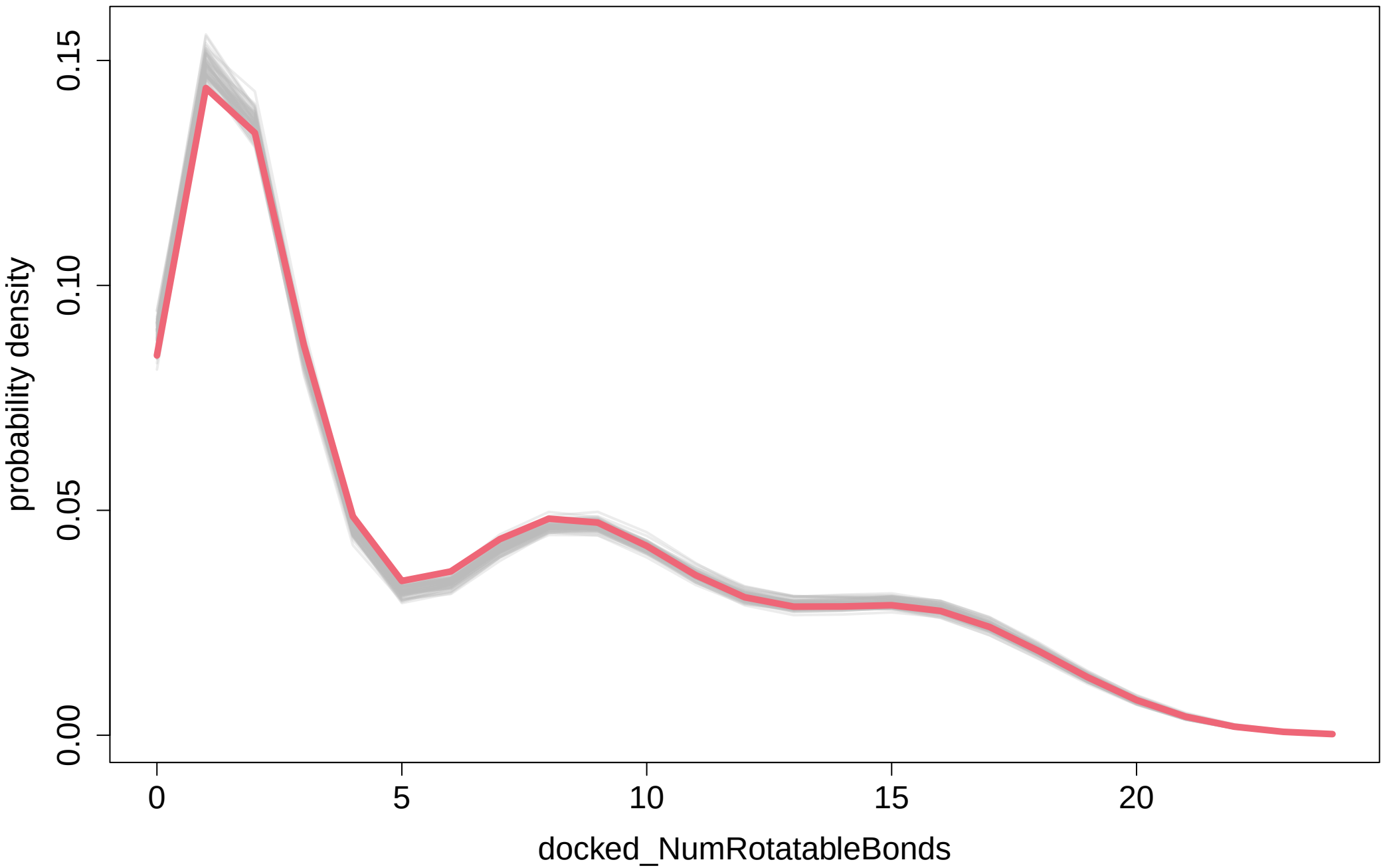

probability density
0.00
0.05
0.10
0.15
0.20
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

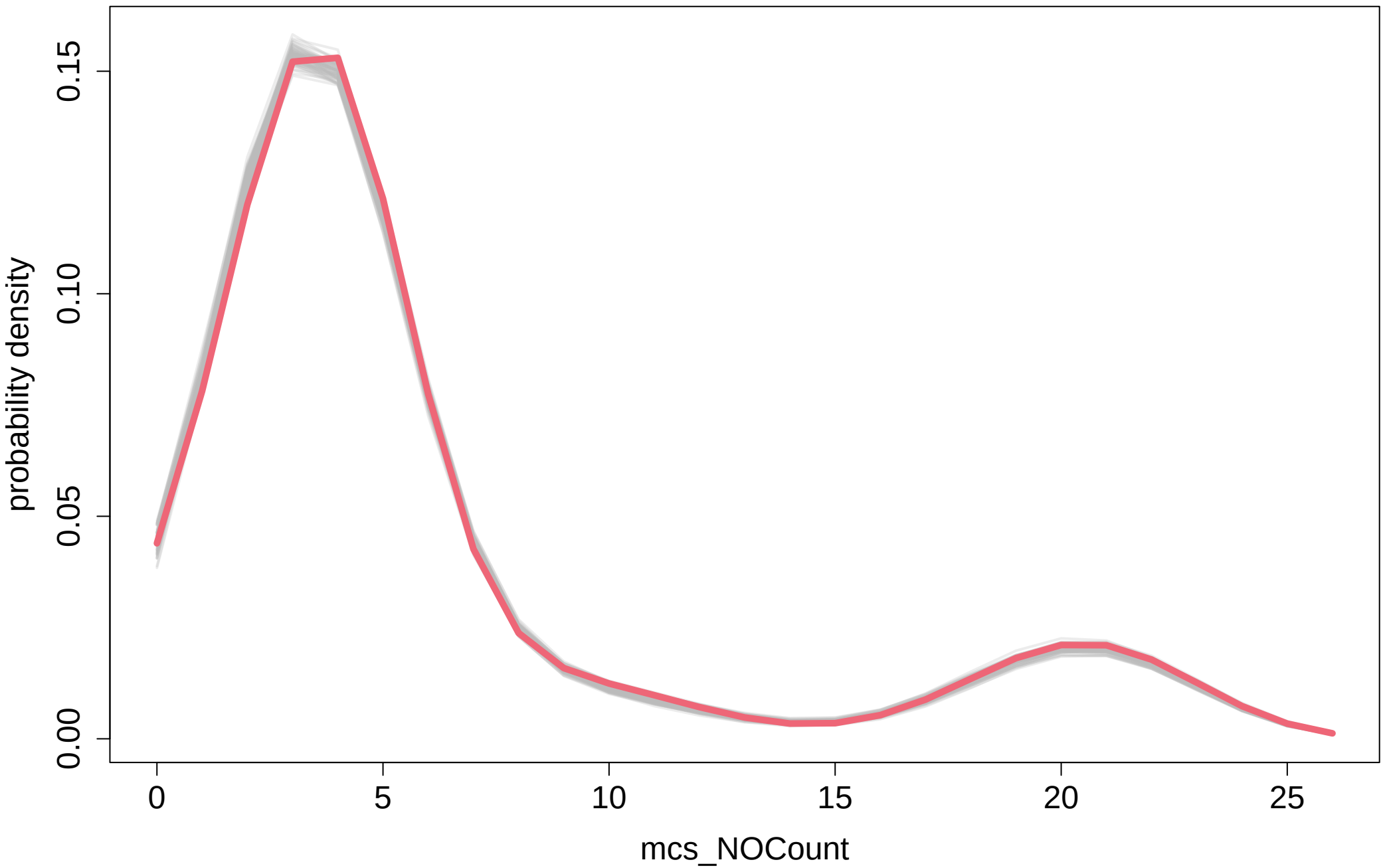

probability density
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
−10
−5
0
5
logit_ec_tanimoto_similarity

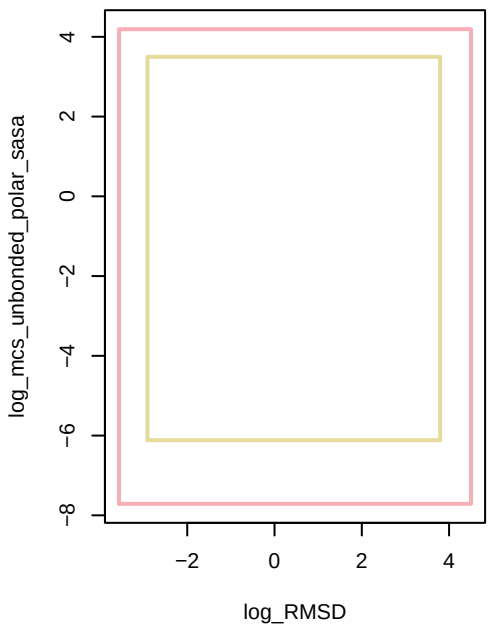

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms

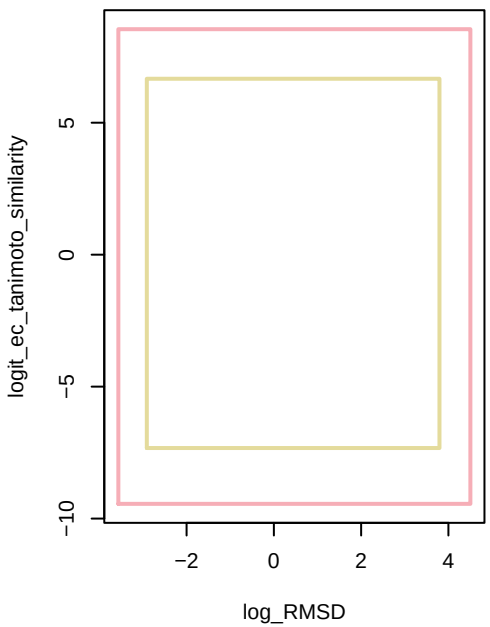

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount

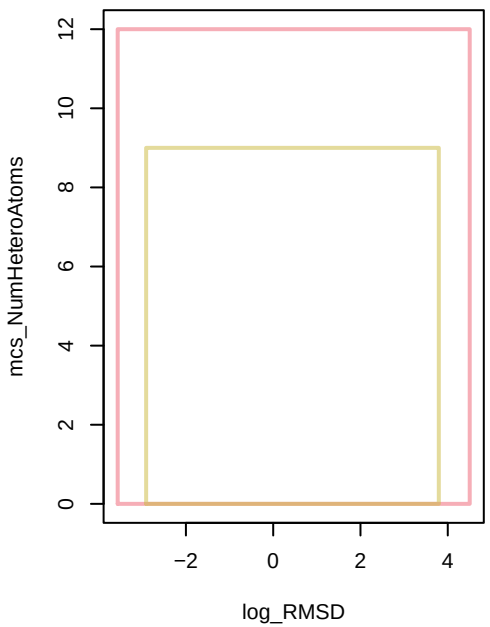

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount

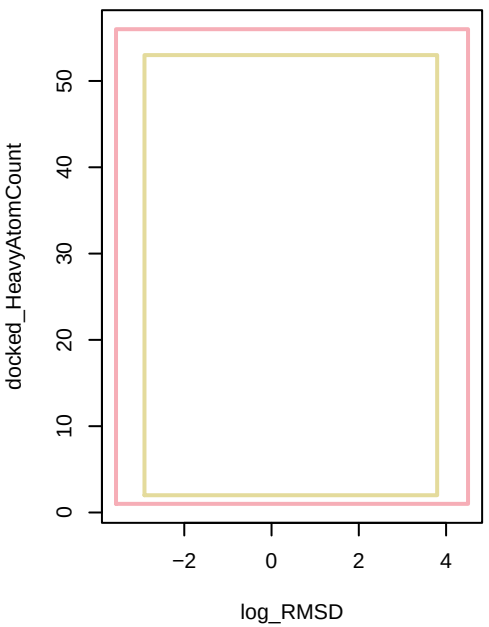

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
docked_NumRotatableBonds

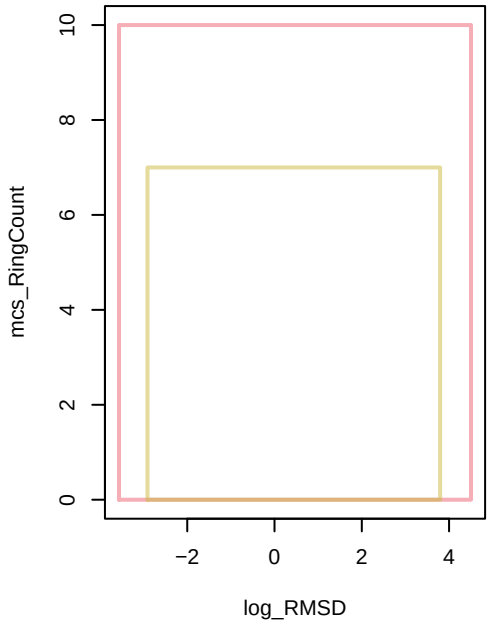

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

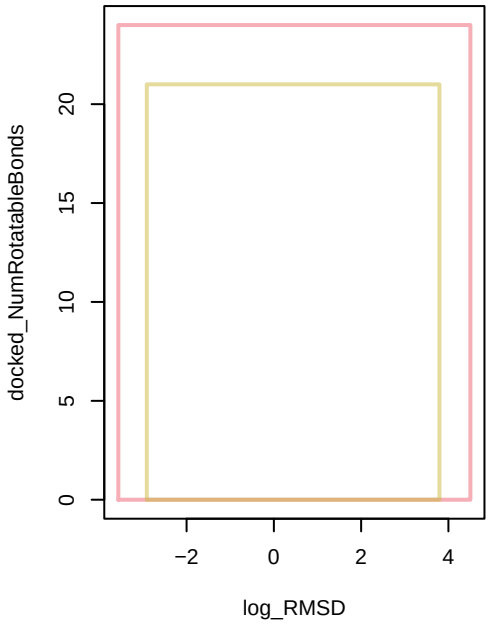

log_mcs_unbonded_polar_sasa
log_RMSD

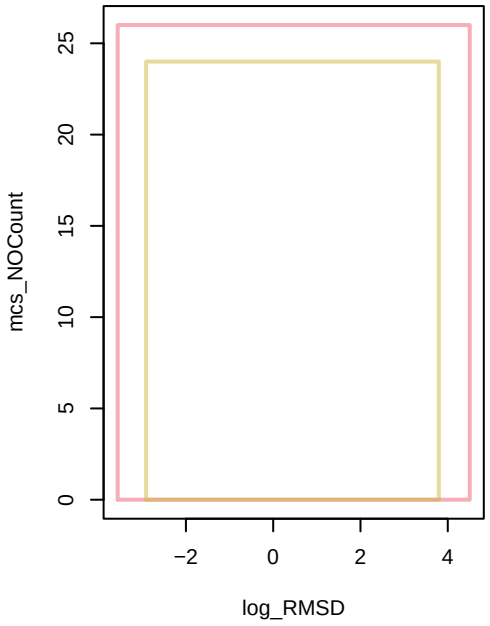

logit_ec_tanimoto_similarity
log_RMSD

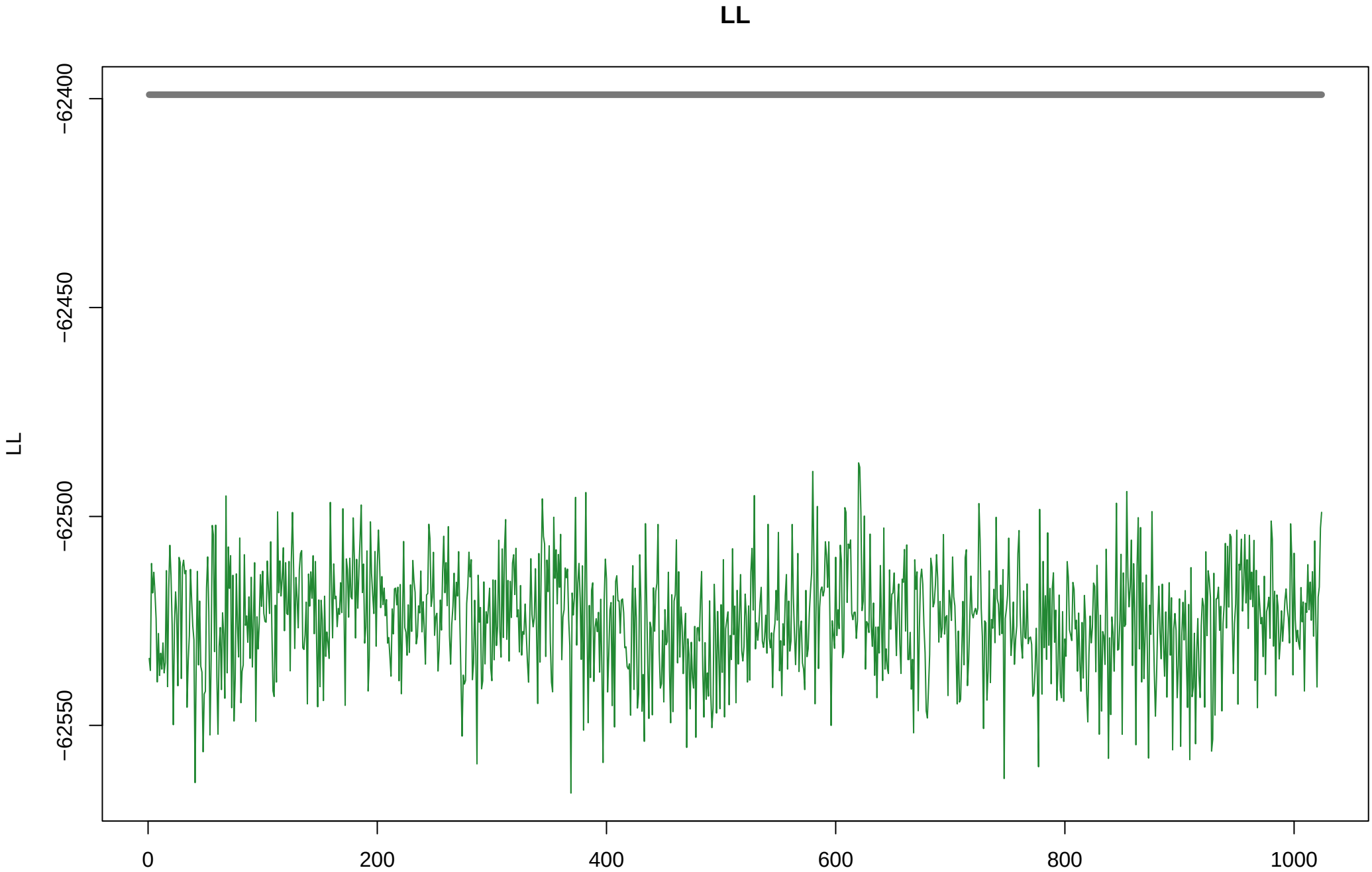

mcs_NumHeteroAtoms
log_RMSD

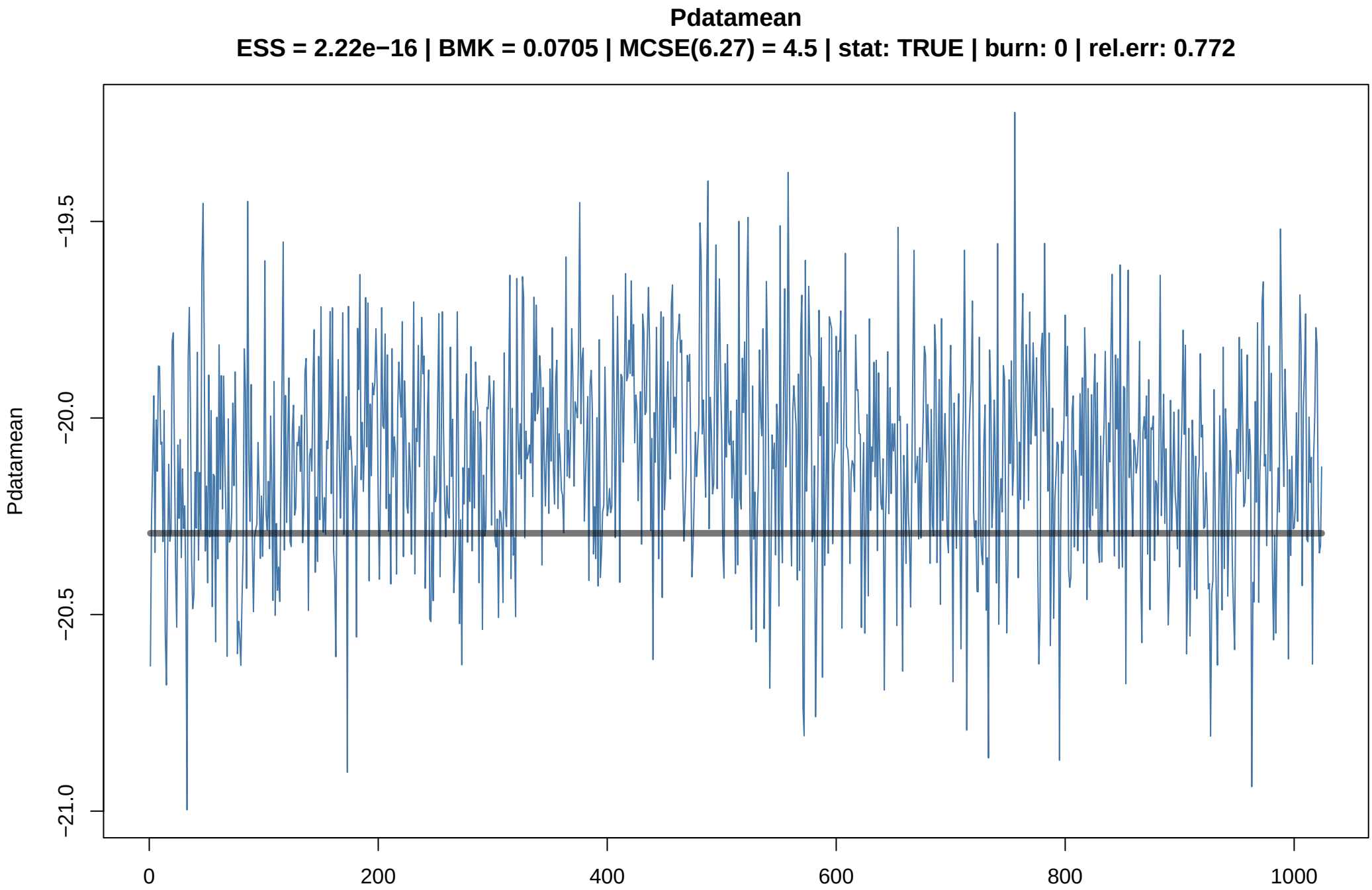

docked_HeavyAtomCount
log_RMSD

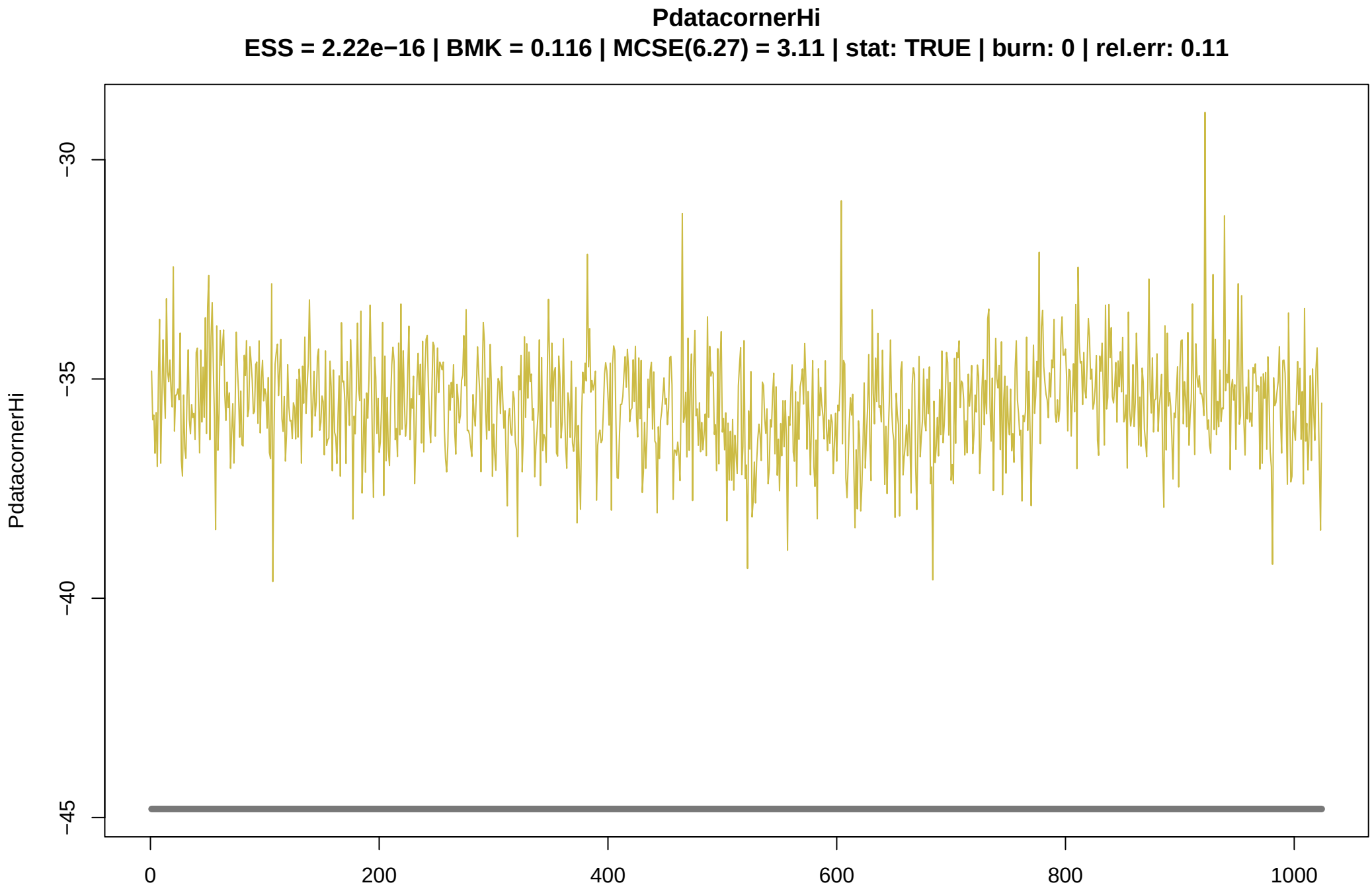

mcs_RingCount
log_RMSD

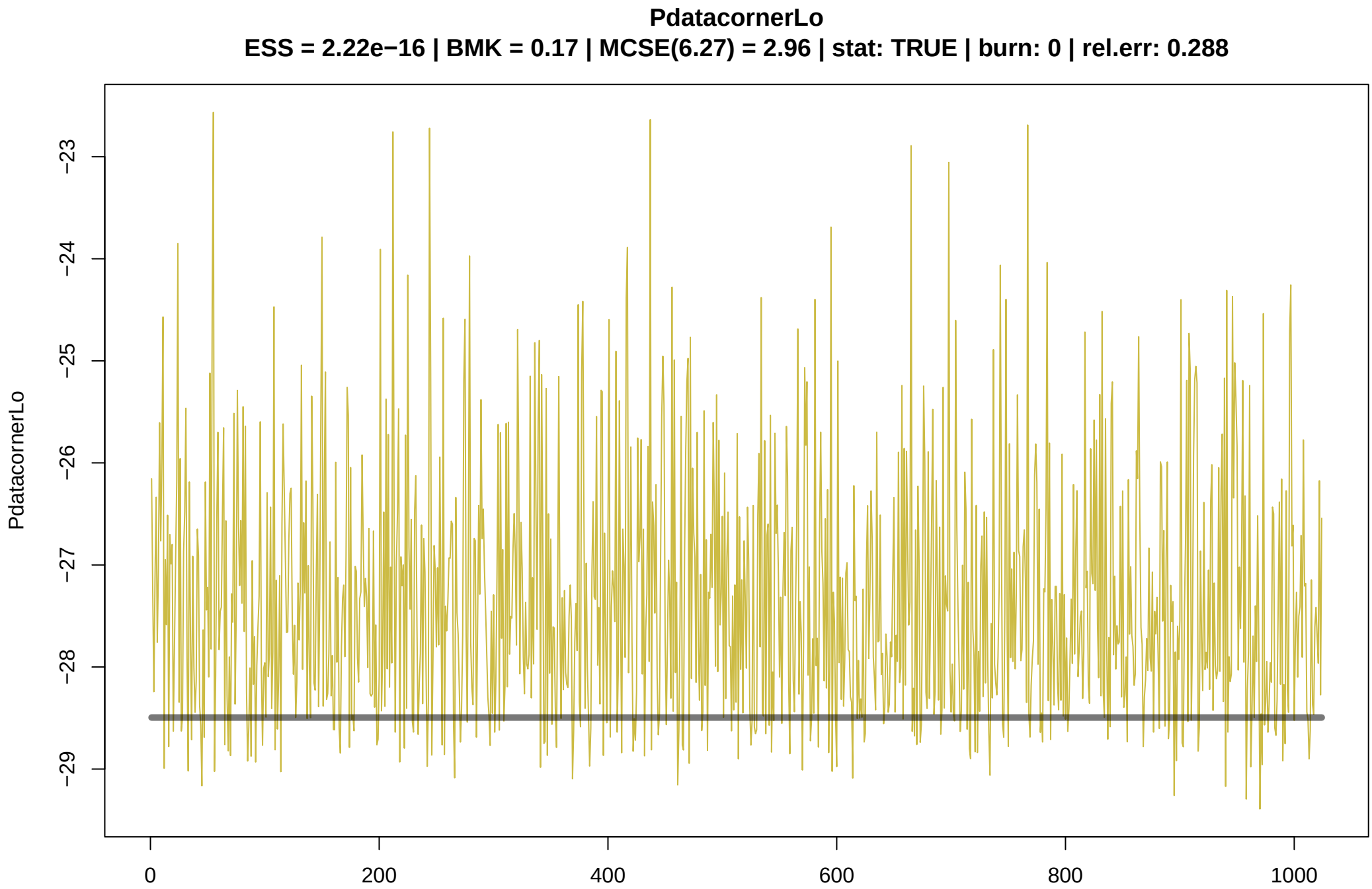

docked_NumRotatableBonds
log_RMSD

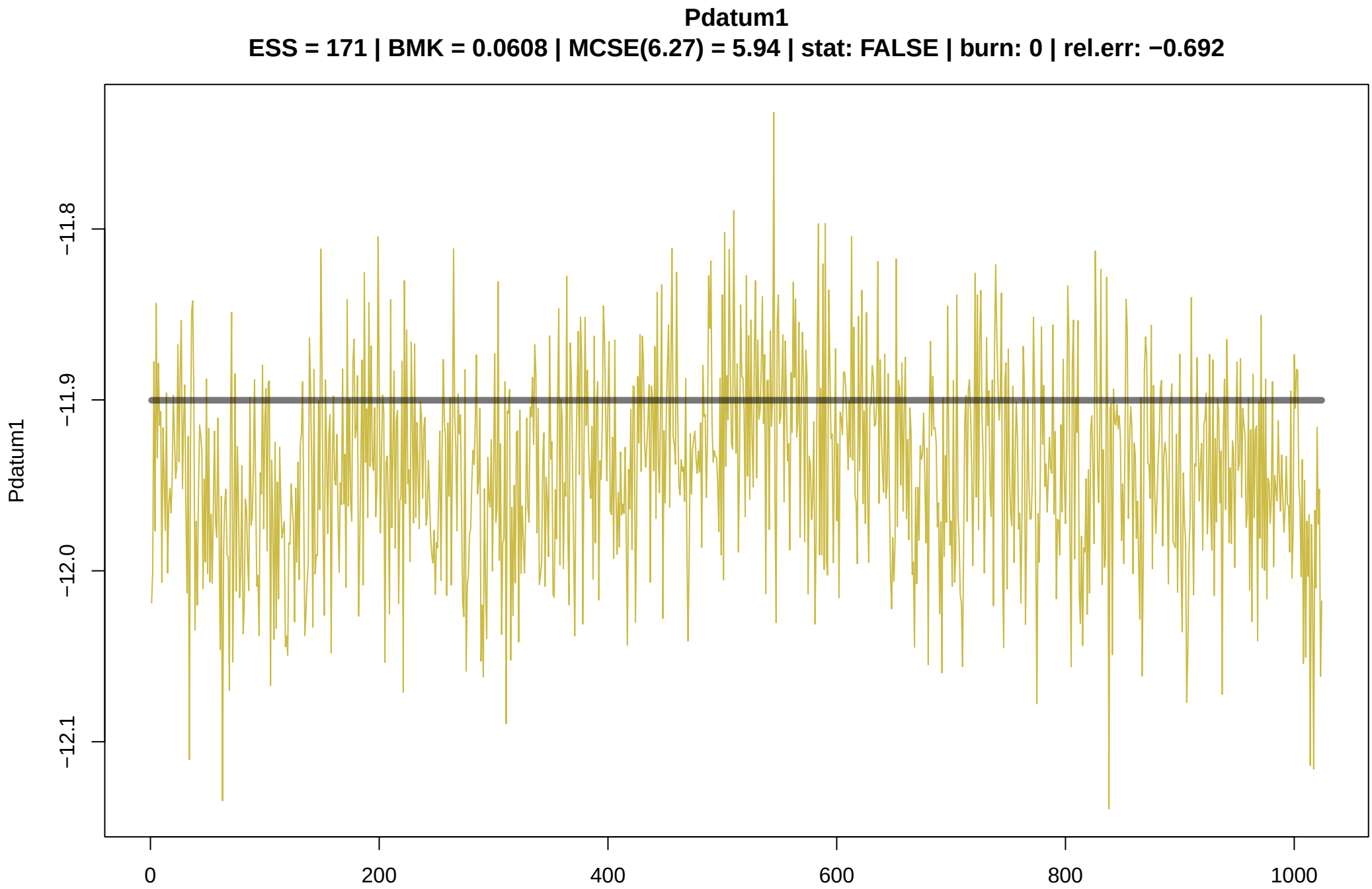

mcs_NOCount
log_RMSD

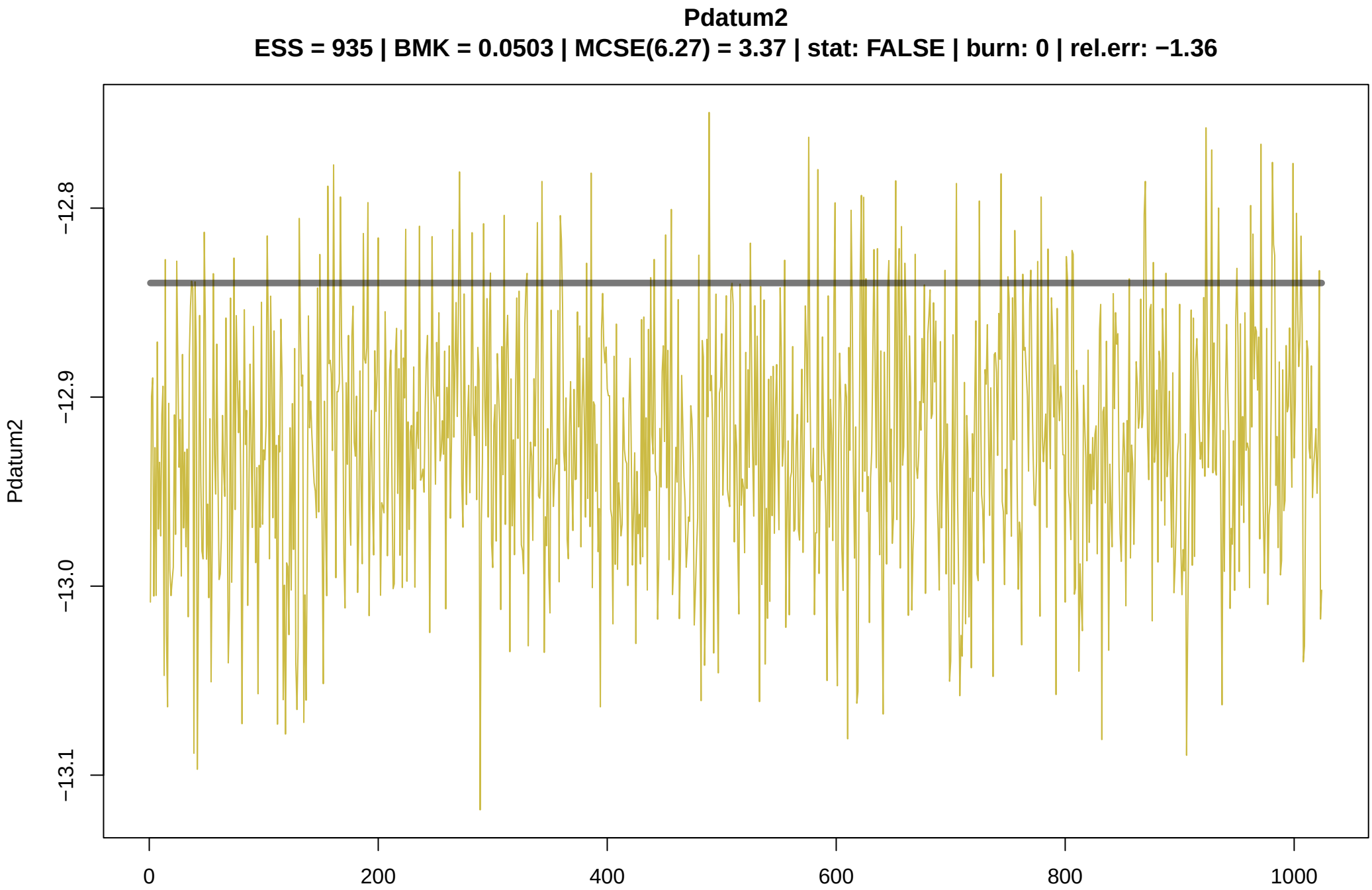

LL
LL
−62400
−62450
−62500
−62550
0
200
400
600
800
1000

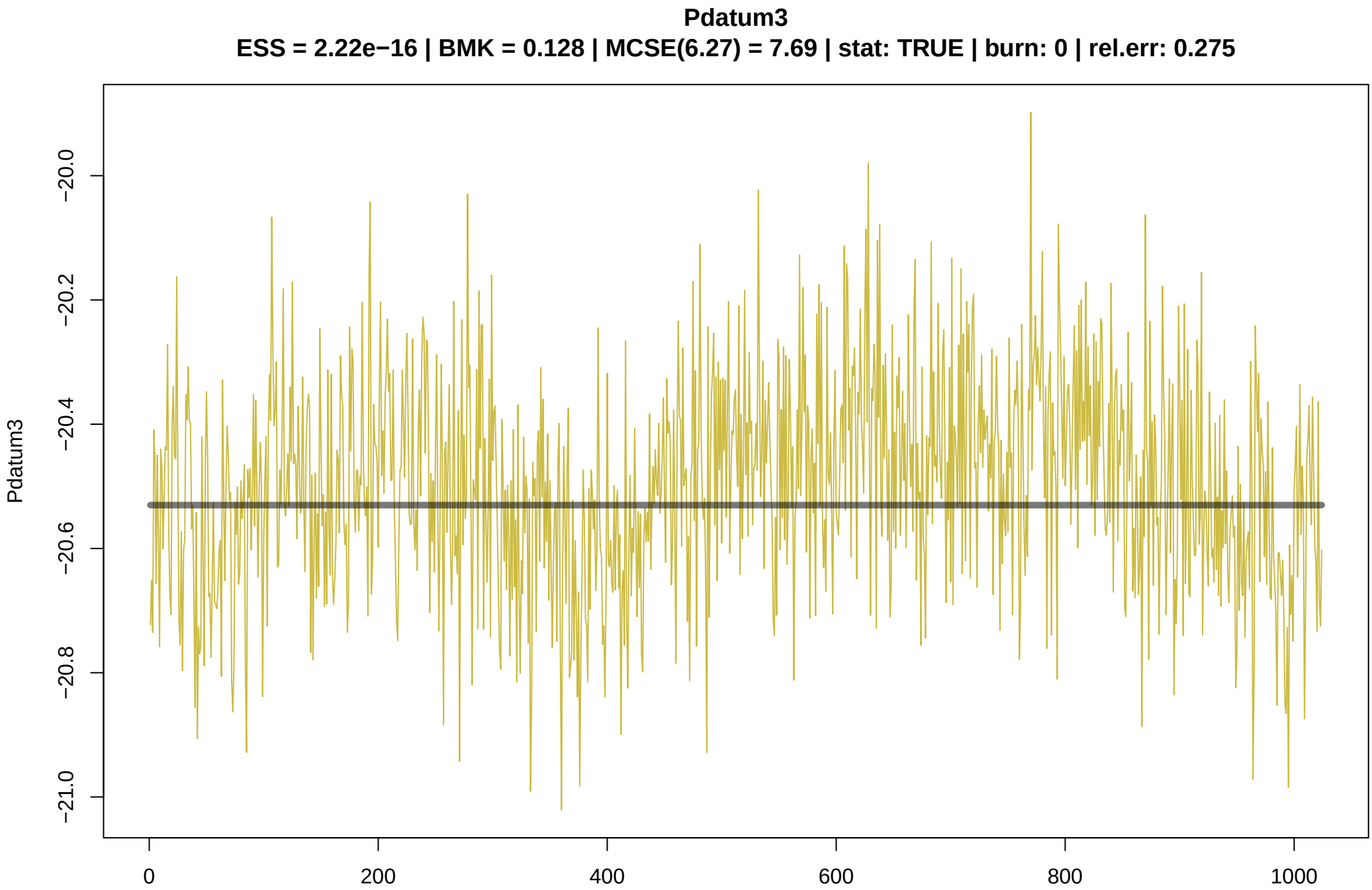

Pdatamean
ESS = 2.22e−16 | BMK = 0.0705 | MCSE(6.27) = 4.5 | stat: TRUE | burn: 0 | rel.err: 0.772
Pdatamean
−19.5
−20.0
−20.5
−21.0
0
200
400
600
800
1000

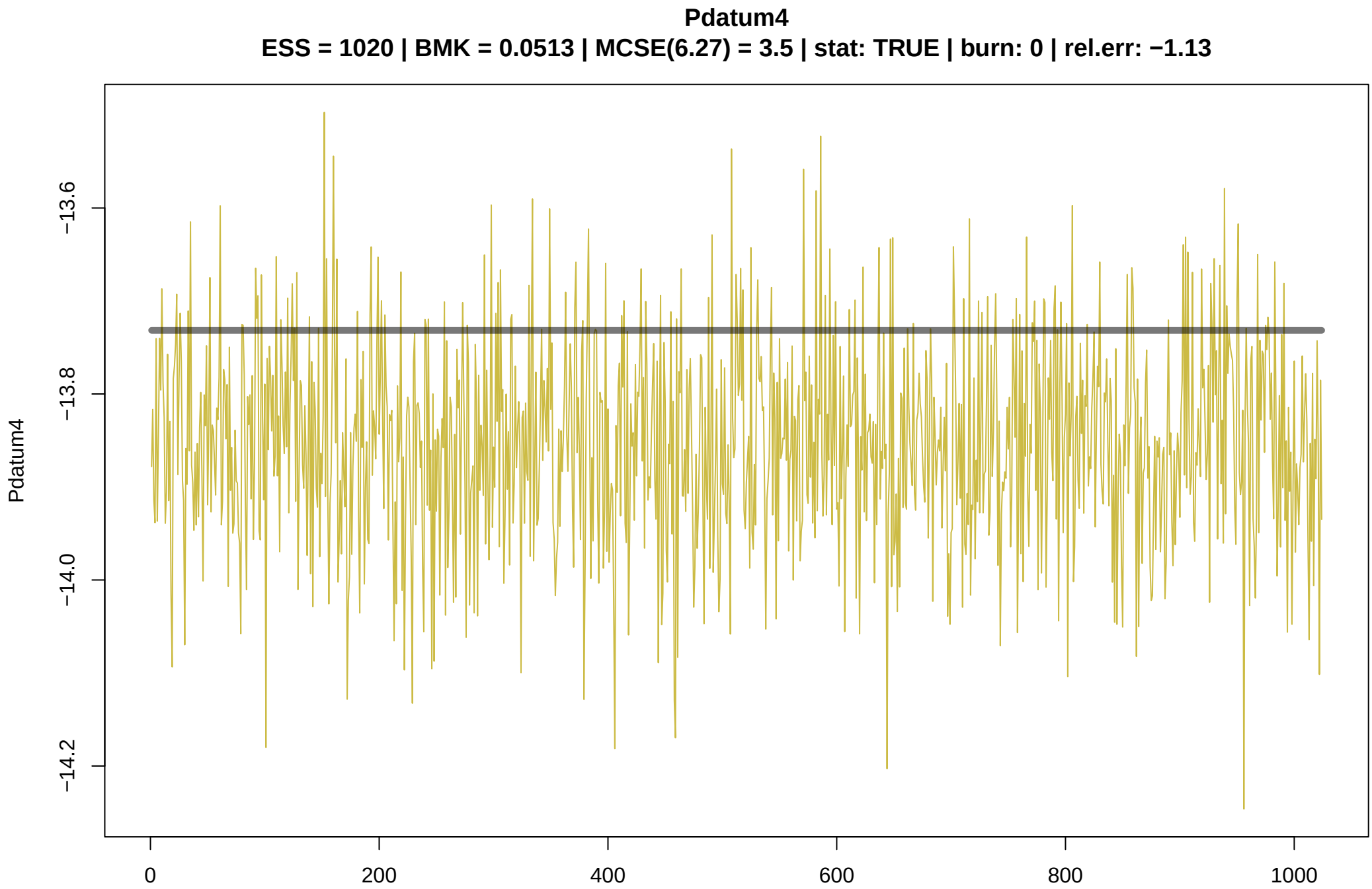

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.116 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0 | rel.err: 0.11
PdatacornerHi
−30
−35
−40
−45
0
200
400
600
800
1000

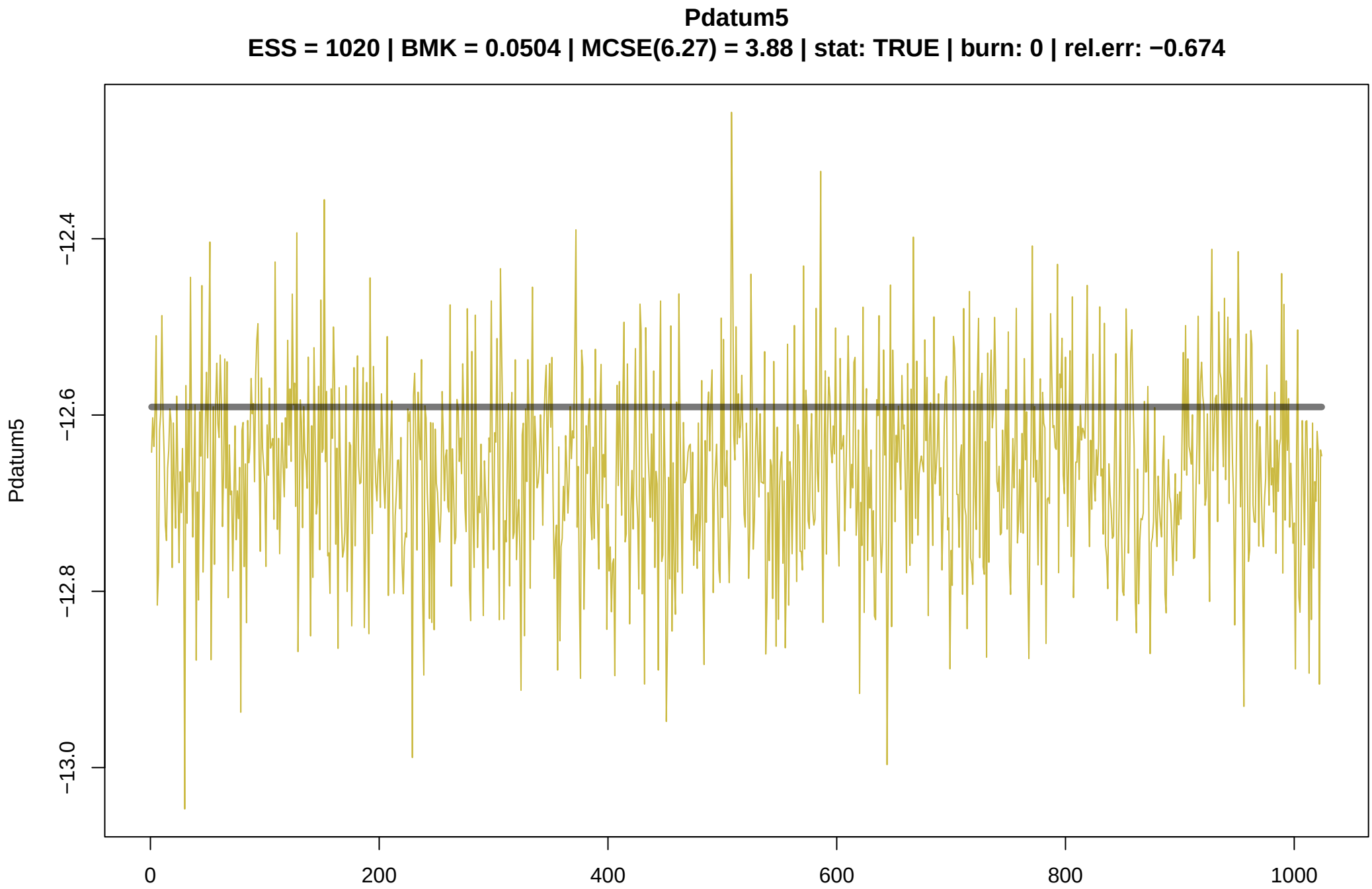

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.17 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0 | rel.err: 0.288
PdatacornerLo
−23
−24
−25
−26
−27
−28
−29
0
200
400
600
800
1000

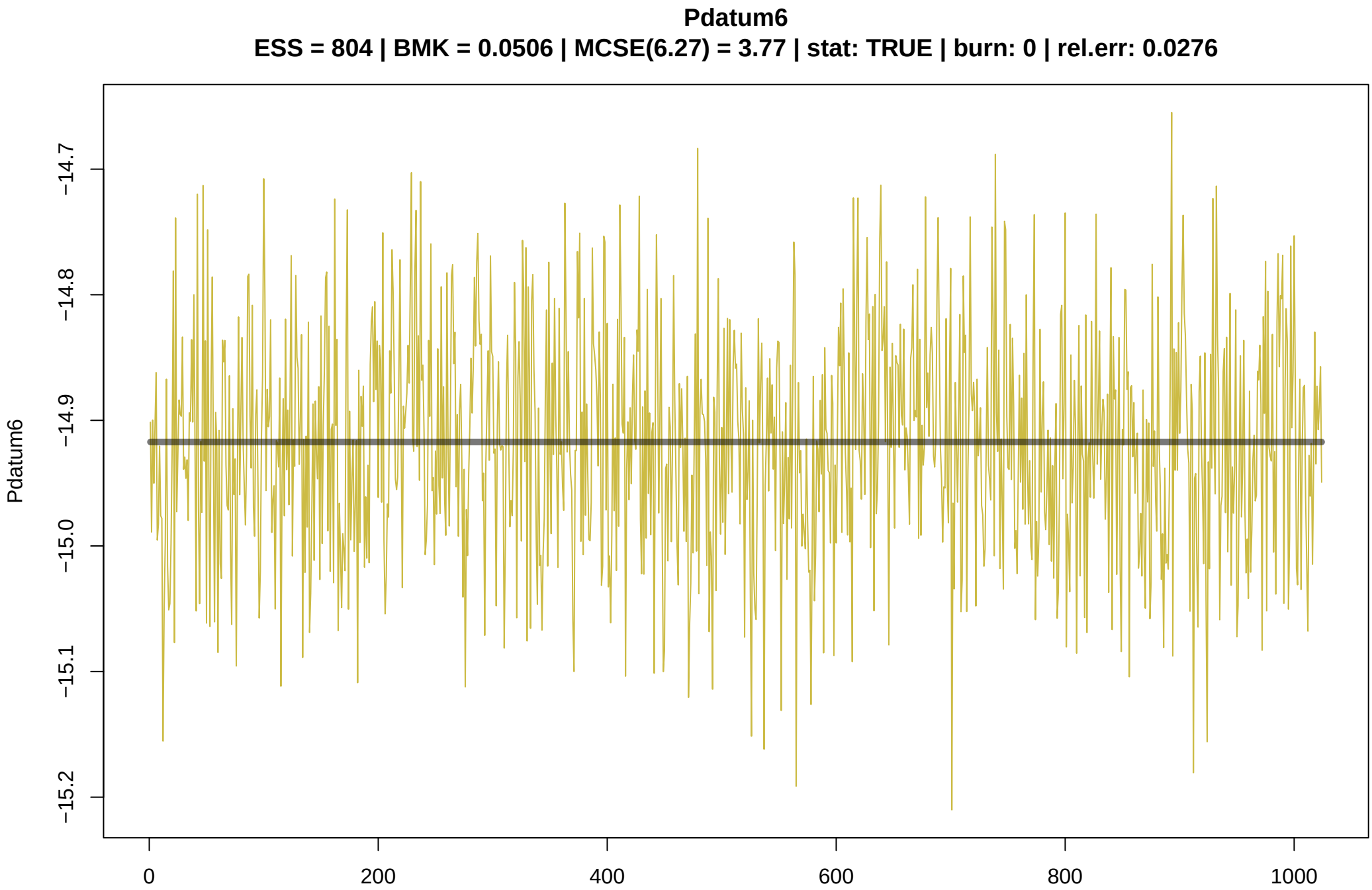

Pdatum1
ESS = 171 | BMK = 0.0608 | MCSE(6.27) = 5.94 | stat: FALSE | burn: 0 | rel.err: −0.692
Pdatum1
−11.8
−11.9
−12.0
−12.1
0
200
400
600
800
1000

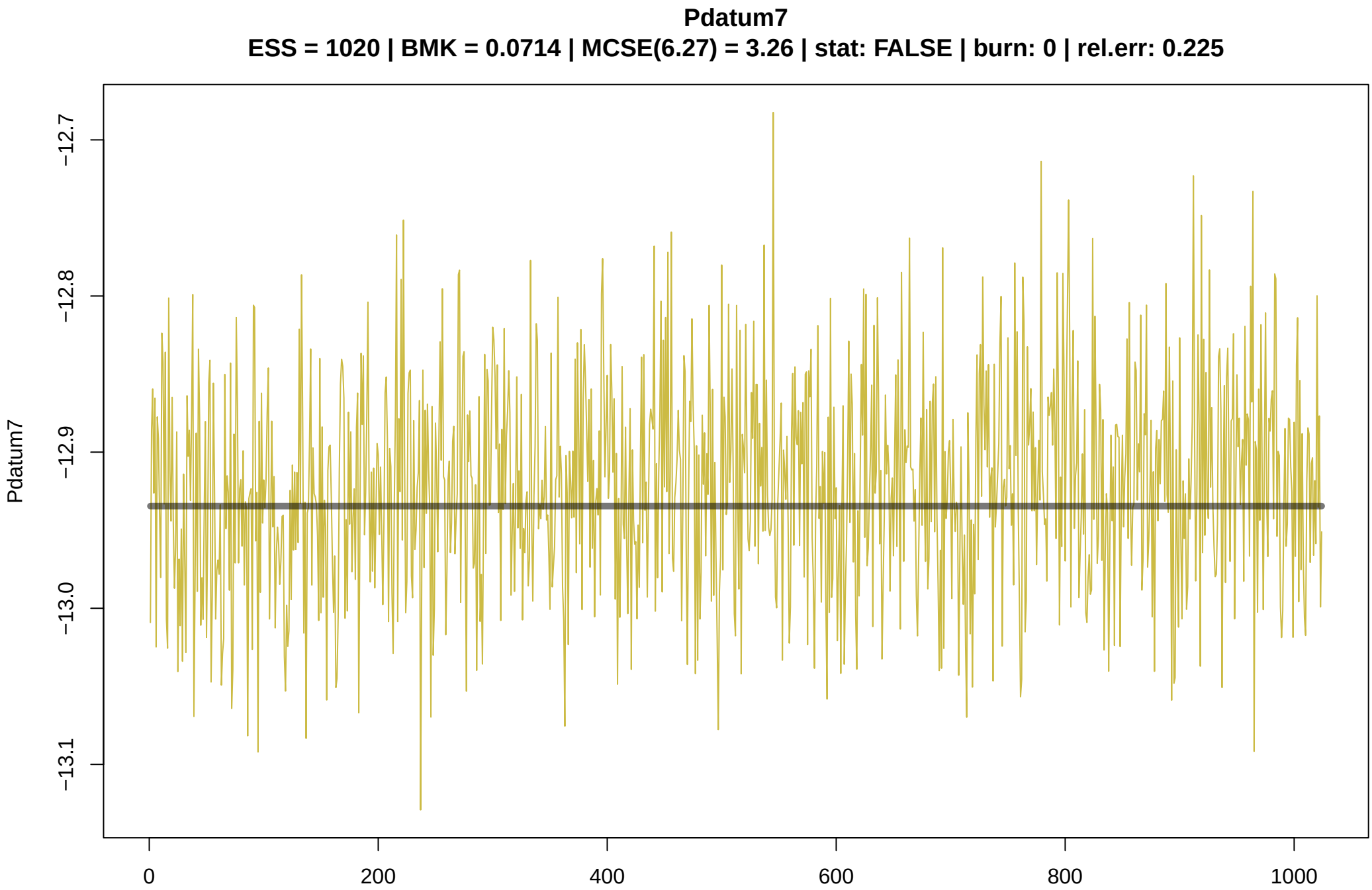

Pdatum2
ESS = 935 | BMK = 0.0503 | MCSE(6.27) = 3.37 | stat: FALSE | burn: 0 | rel.err: −1.36
Pdatum2
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

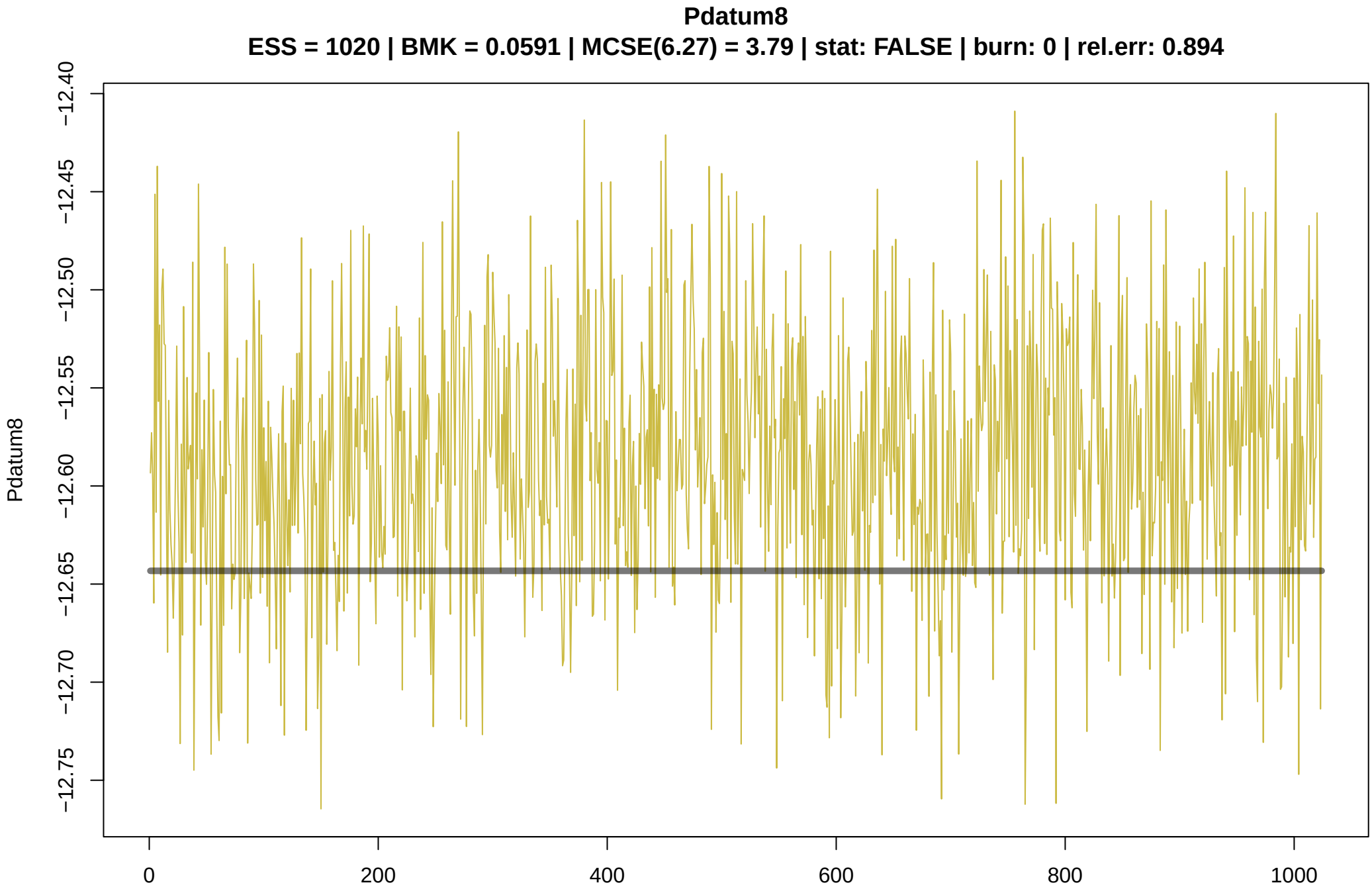

Pdatum3
ESS = 2.22e−16 | BMK = 0.128 | MCSE(6.27) = 7.69 | stat: TRUE | burn: 0 | rel.err: 0.275
Pdatum3
−20.0
−20.2
−20.4
−20.6
−20.8
−21.0
0
200
400
600
800
1000

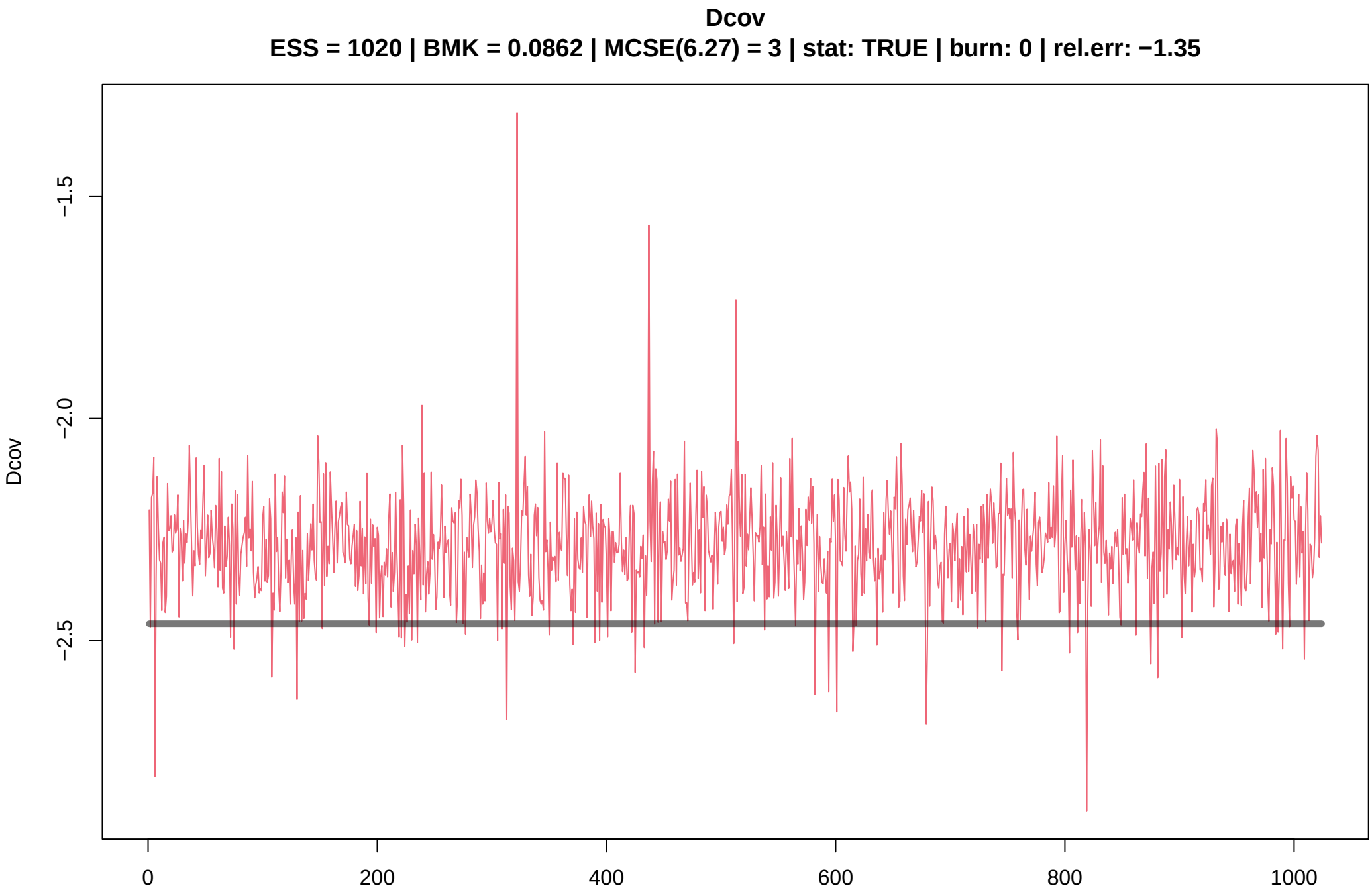

Pdatum4
ESS = 1020 | BMK = 0.0513 | MCSE(6.27) = 3.5 | stat: TRUE | burn: 0 | rel.err: −1.13
Pdatum4
−13.6
−13.8
−14.0
−14.2
0
200
400
600
800
1000

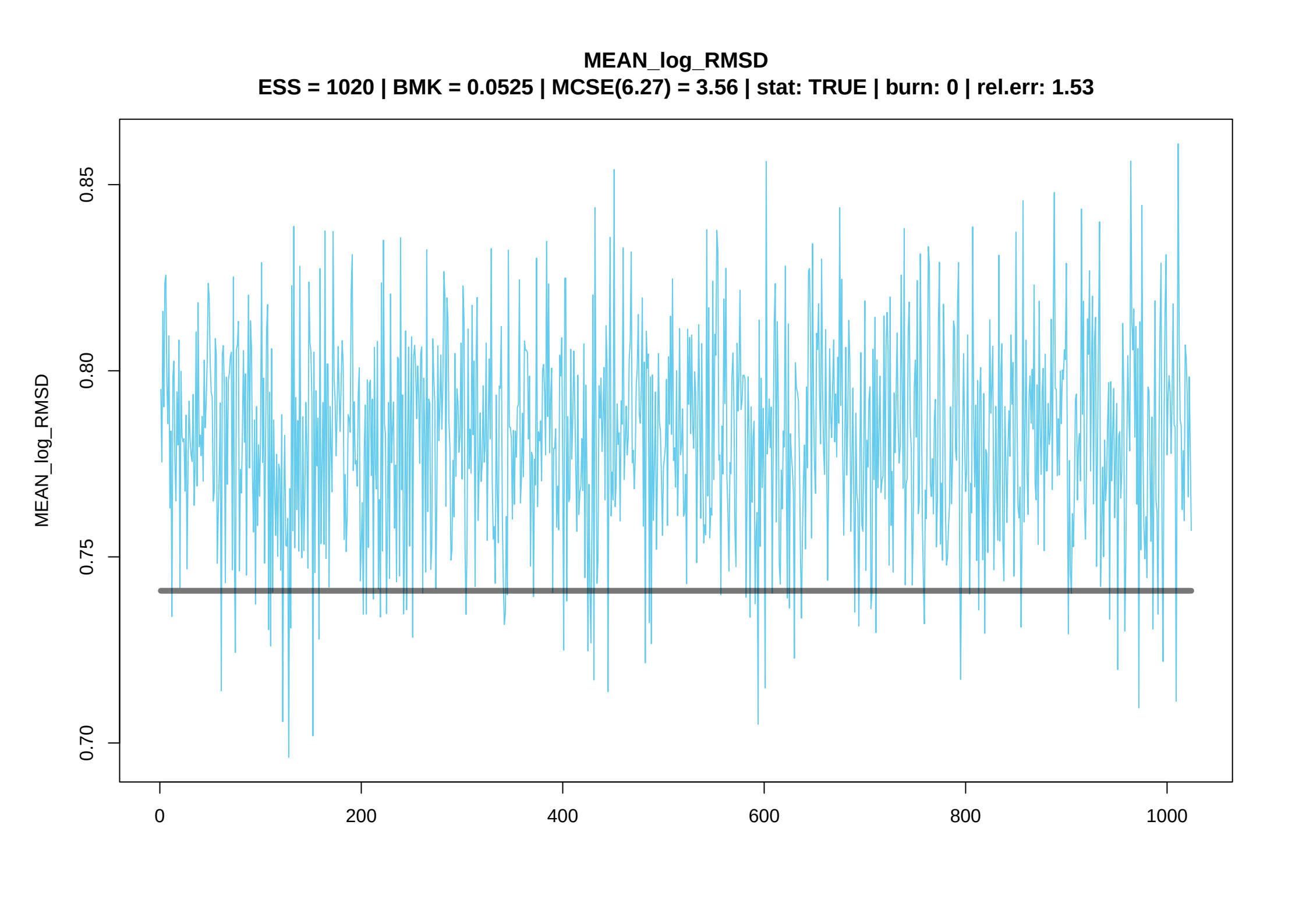

Pdatum5
ESS = 1020 | BMK = 0.0504 | MCSE(6.27) = 3.88 | stat: TRUE | burn: 0 | rel.err: −0.674
Pdatum5
−12.4
−12.6
−12.8
−13.0
0
200
400
600
800
1000

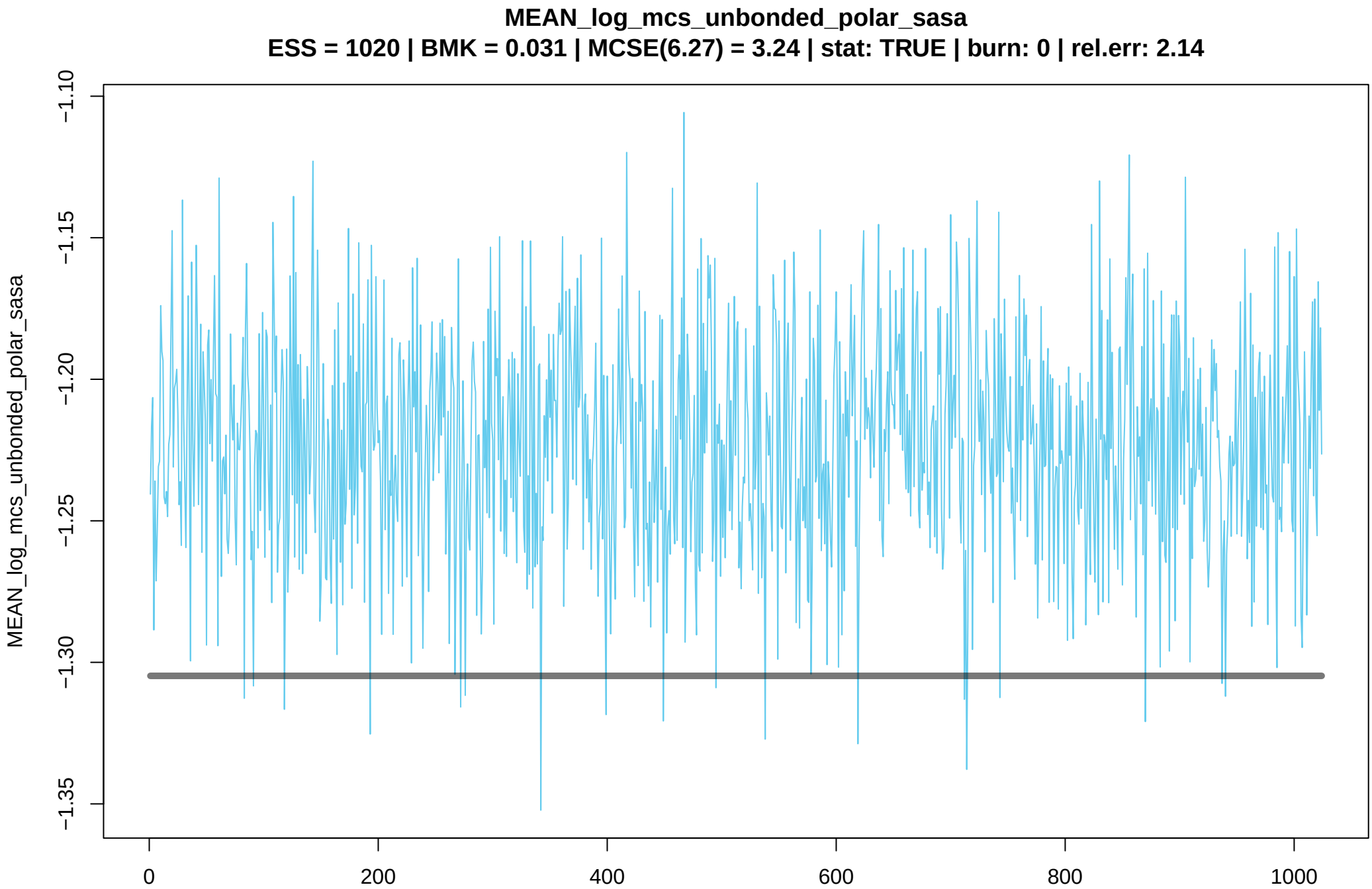

Pdatum6
ESS = 804 | BMK = 0.0506 | MCSE(6.27) = 3.77 | stat: TRUE | burn: 0 | rel.err: 0.0276
Pdatum6
−14.7
−14.8
−14.9
−15.0
−15.1
−15.2
0
200
400
600
800
1000

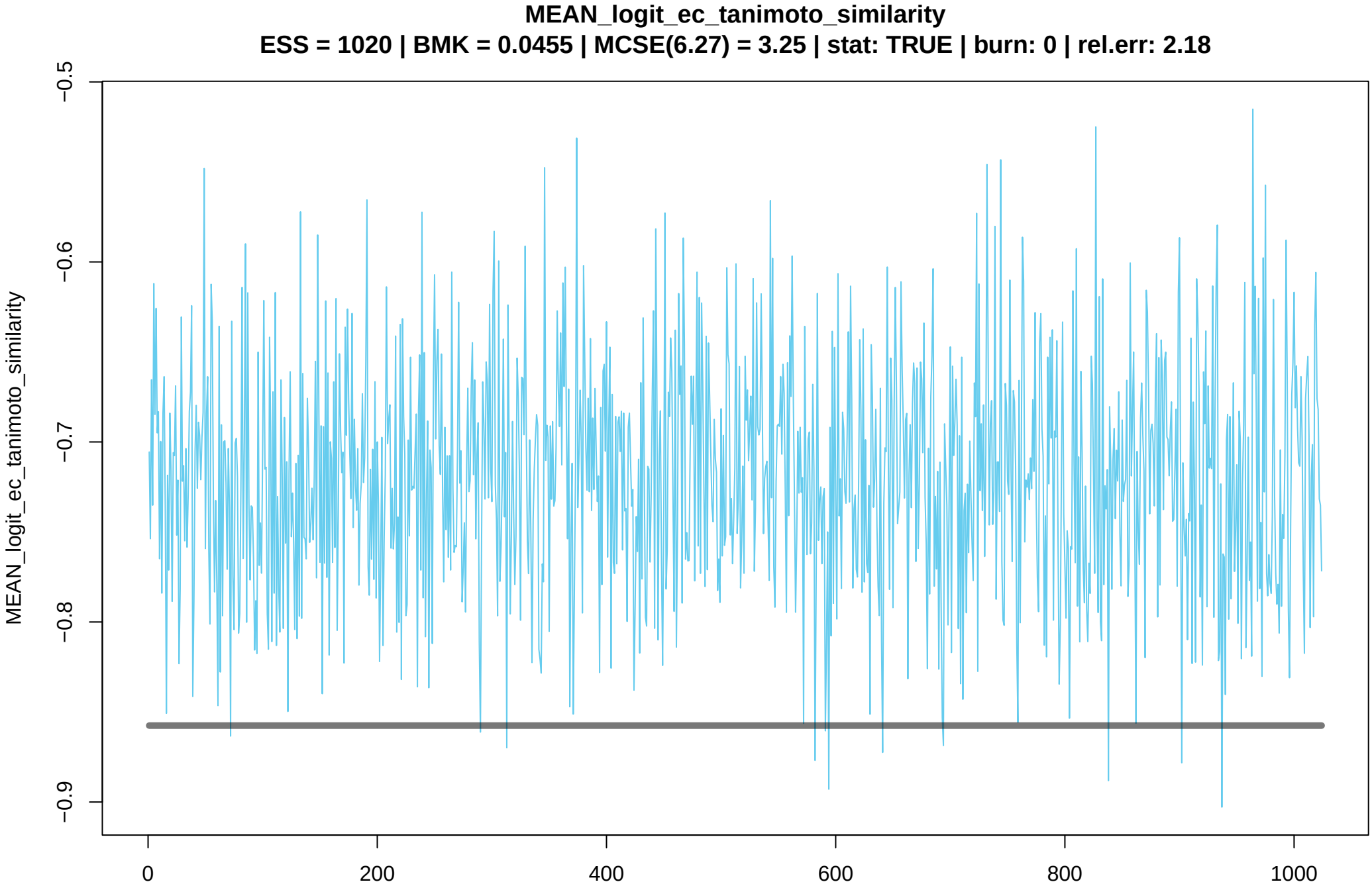

Pdatum7
ESS = 1020 | BMK = 0.0714 | MCSE(6.27) = 3.26 | stat: FALSE | burn: 0 | rel.err: 0.225
Pdatum7
−12.7
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

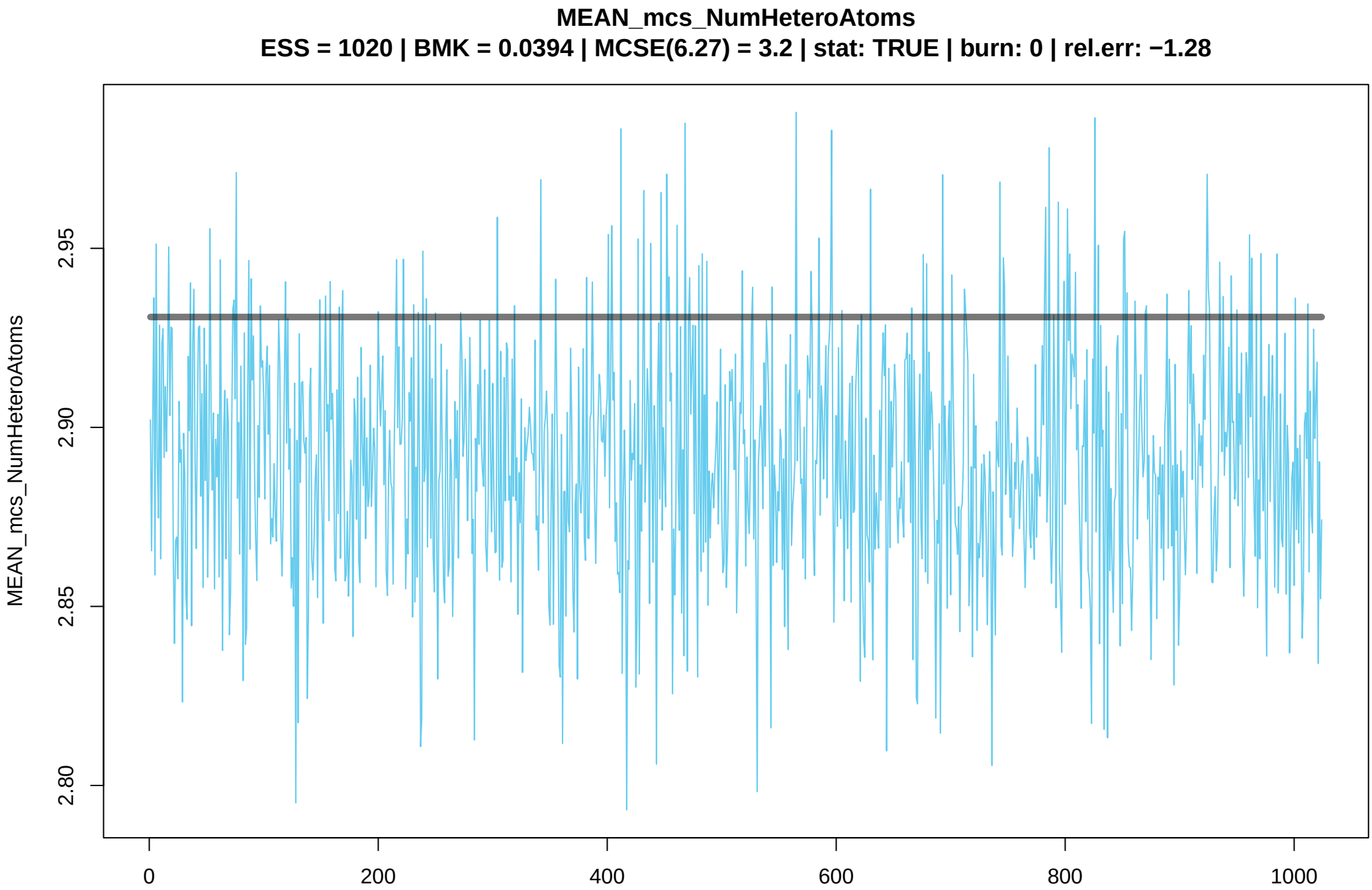

Pdatum8
ESS = 1020 | BMK = 0.0591 | MCSE(6.27) = 3.79 | stat: FALSE | burn: 0 | rel.err: 0.894
Pdatum8
−12.40
−12.45
−12.50
−12.55
−12.60
−12.65
−12.70
−12.75
0
200
400
600
800
1000

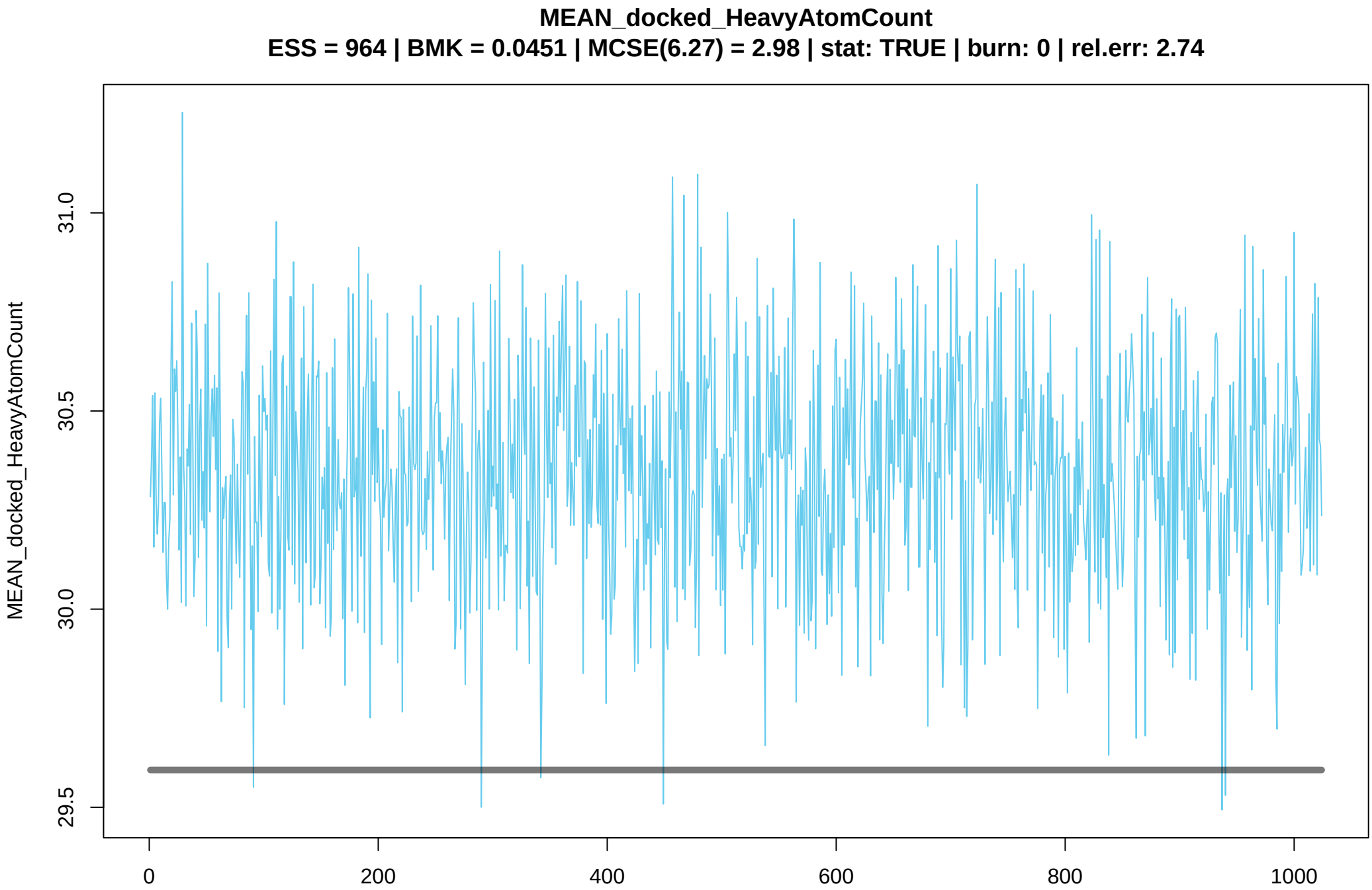

Dcov
ESS = 1020 | BMK = 0.0862 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | rel.err: −1.35
Dcov
−1.5
−2.0
−2.5
0
200
400
600
800
1000

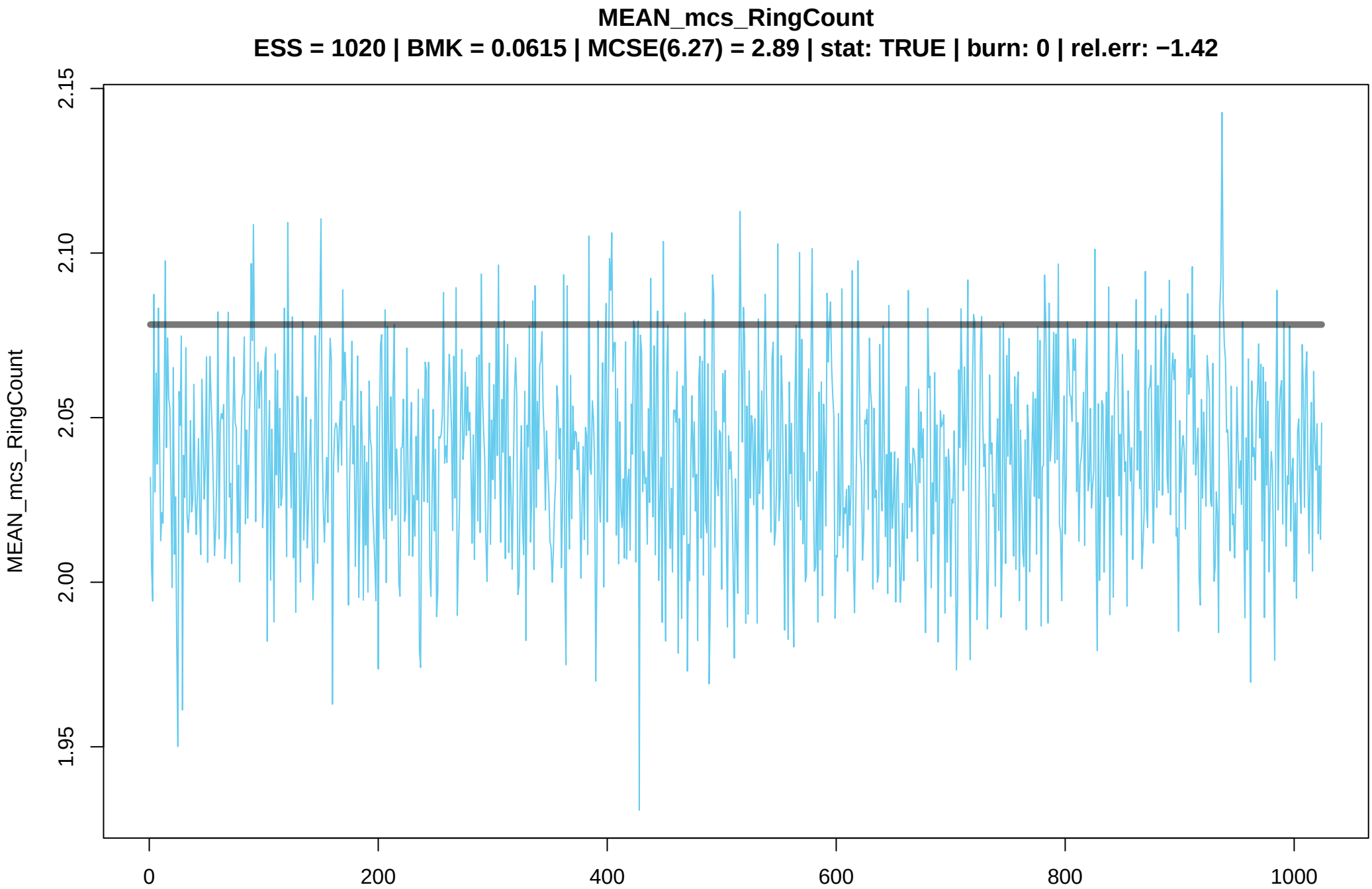

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0525 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | rel.err: 1.53
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

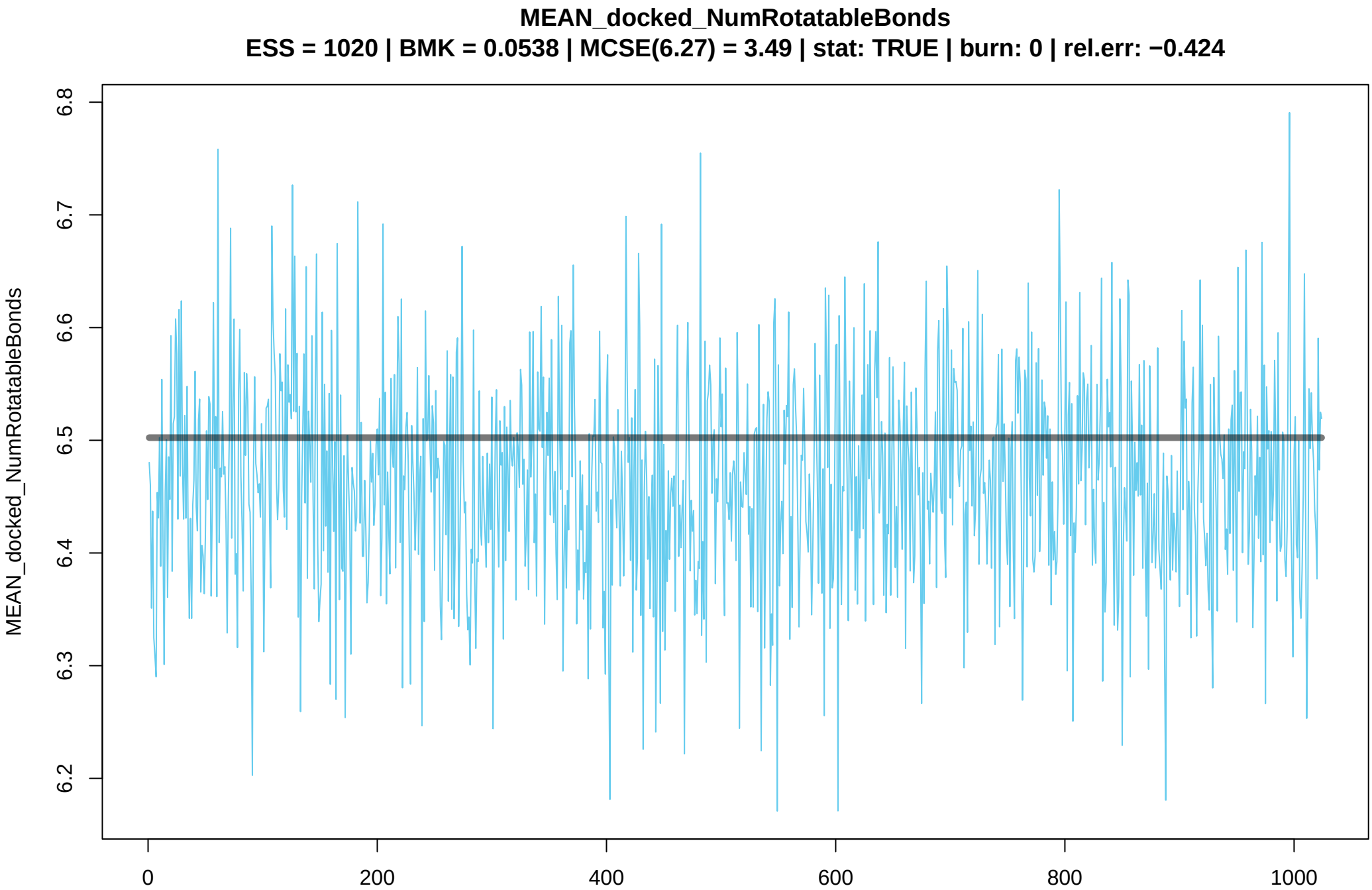

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.031 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | rel.err: 2.14
MEAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

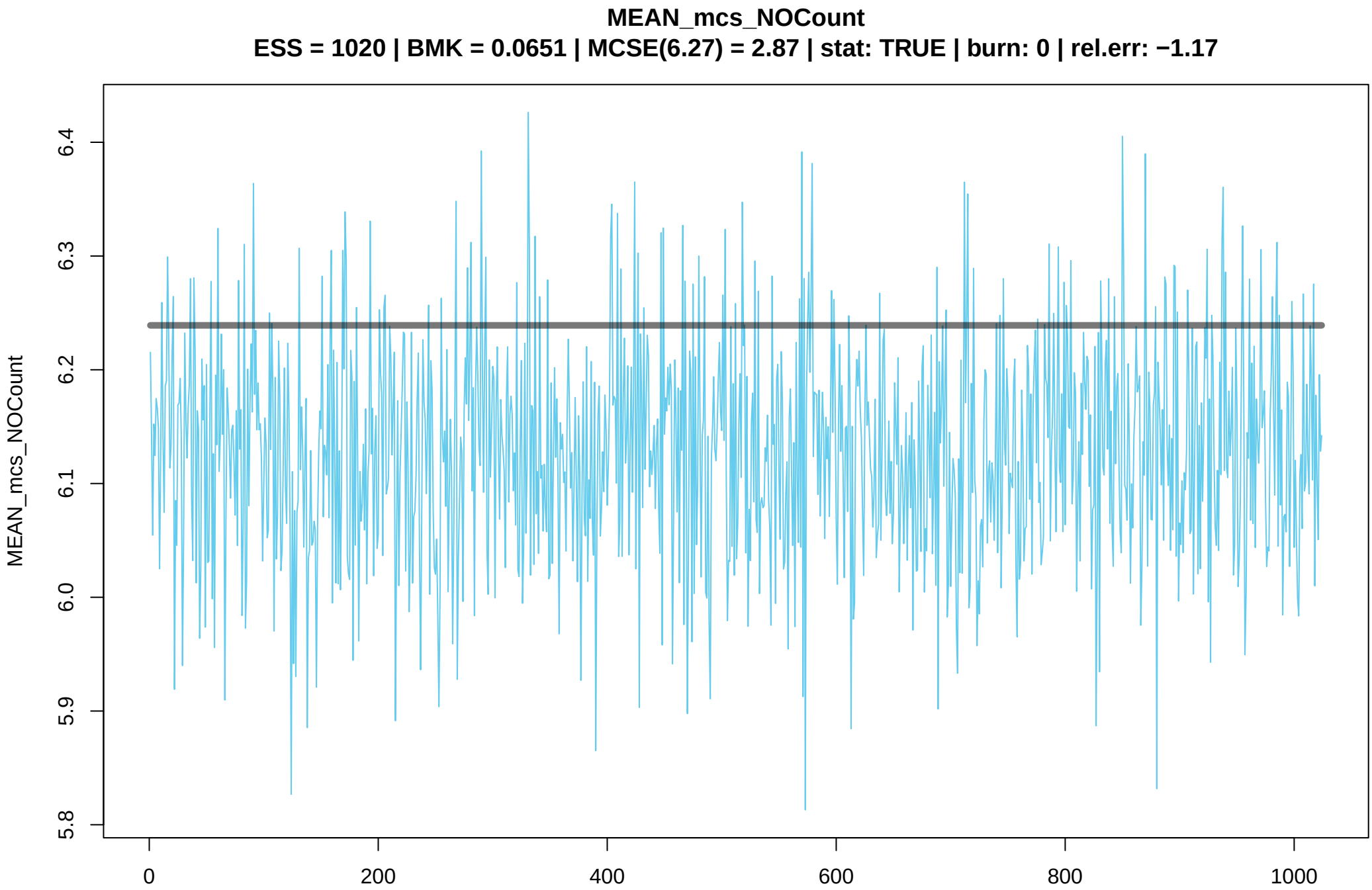

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0455 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | rel.err: 2.18
MEAN_logit_ec_tanimoto_similarity
−0.5
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

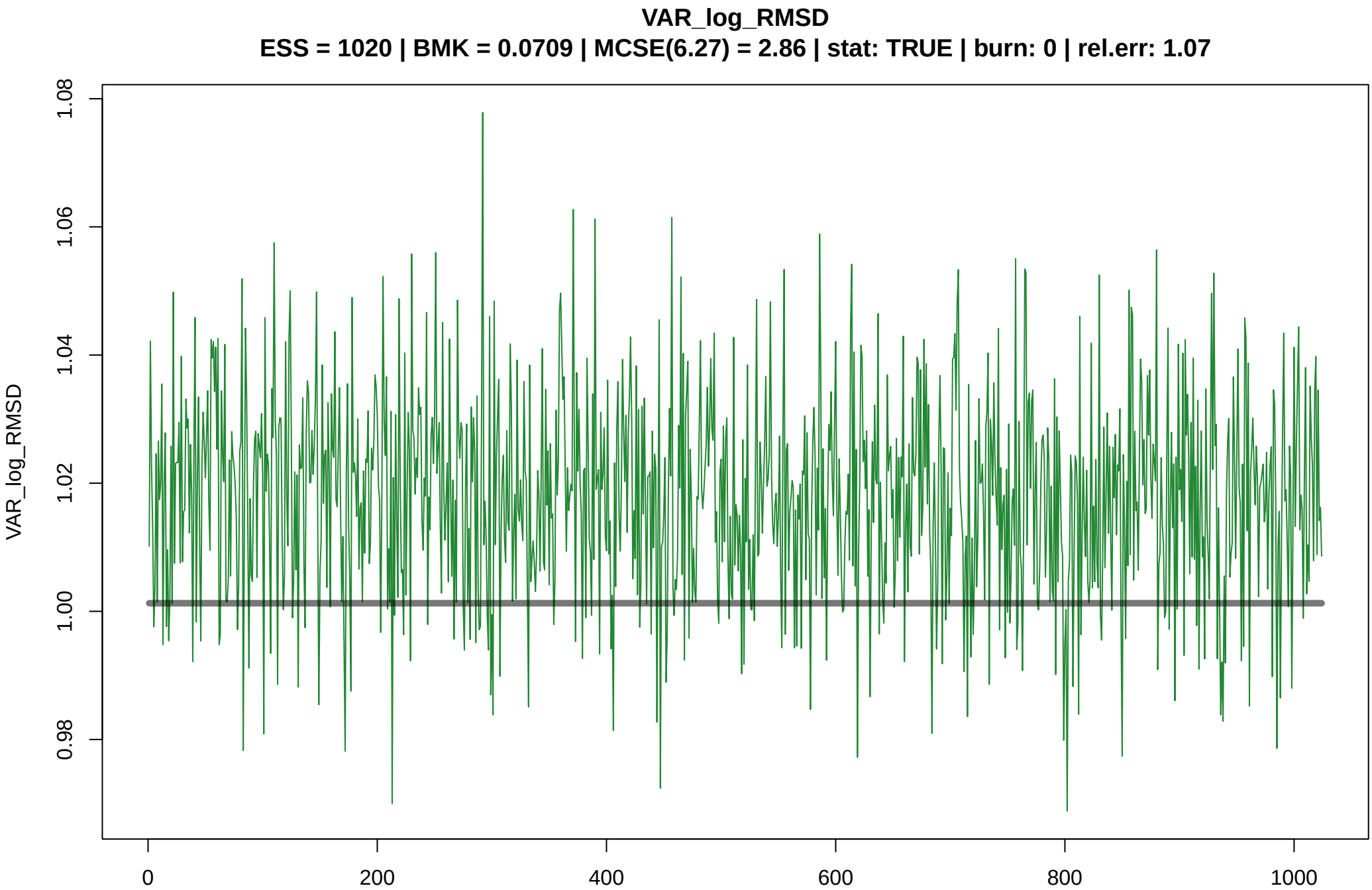

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0394 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: −1.28
MEAN_mcs_NumHeteroAtoms
2.80
2.85
2.90
2.95
0
200
400
600
800
1000

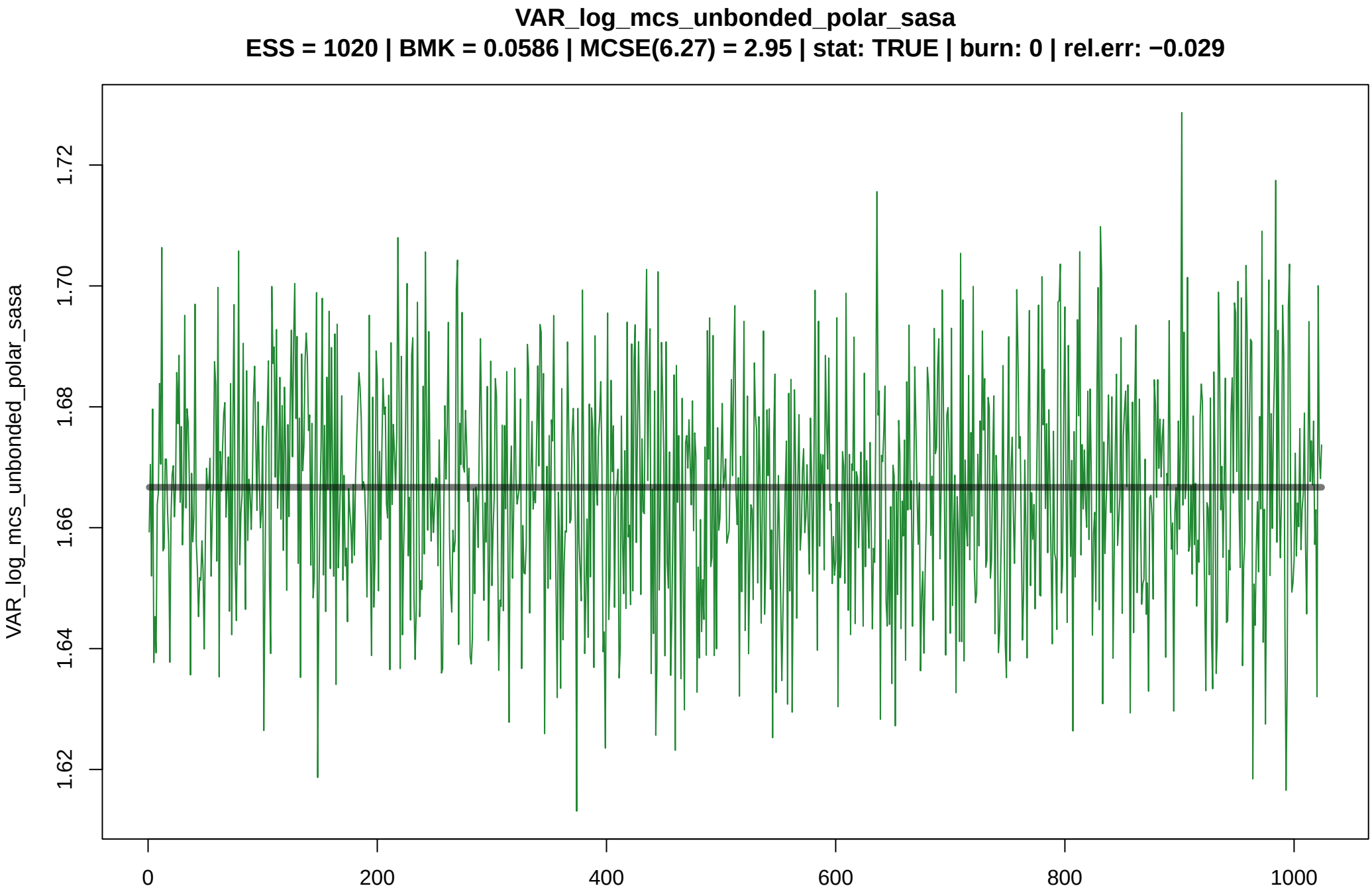

MEAN_docked_HeavyAtomCount
ESS = 964 | BMK = 0.0451 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | rel.err: 2.74
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
31.0
0
200
400
600
800
1000

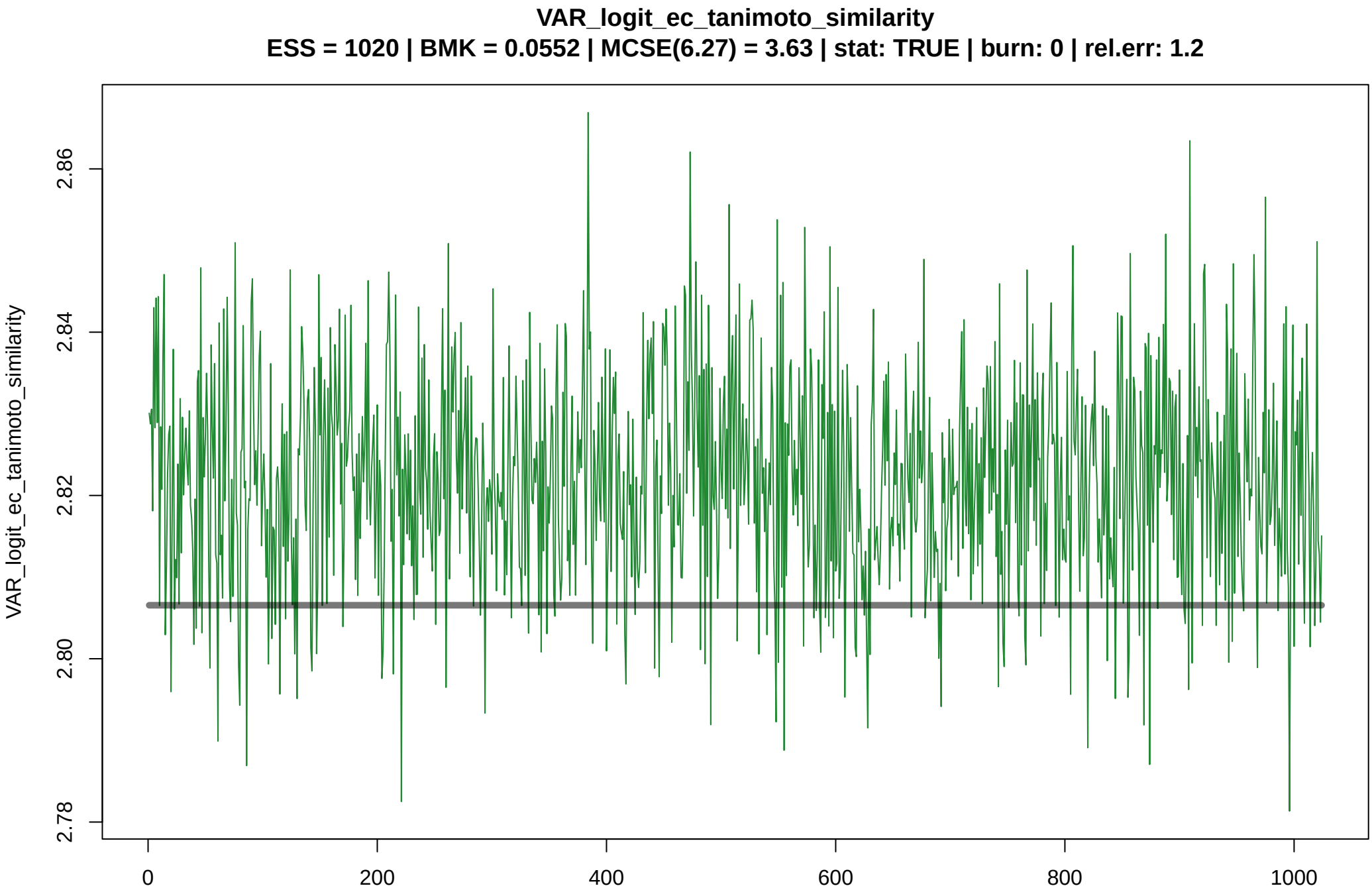

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0615 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | rel.err: −1.42
MEAN_mcs_RingCount
2.15
2.10
2.05
2.00
1.95
0
200
400
600
800
1000

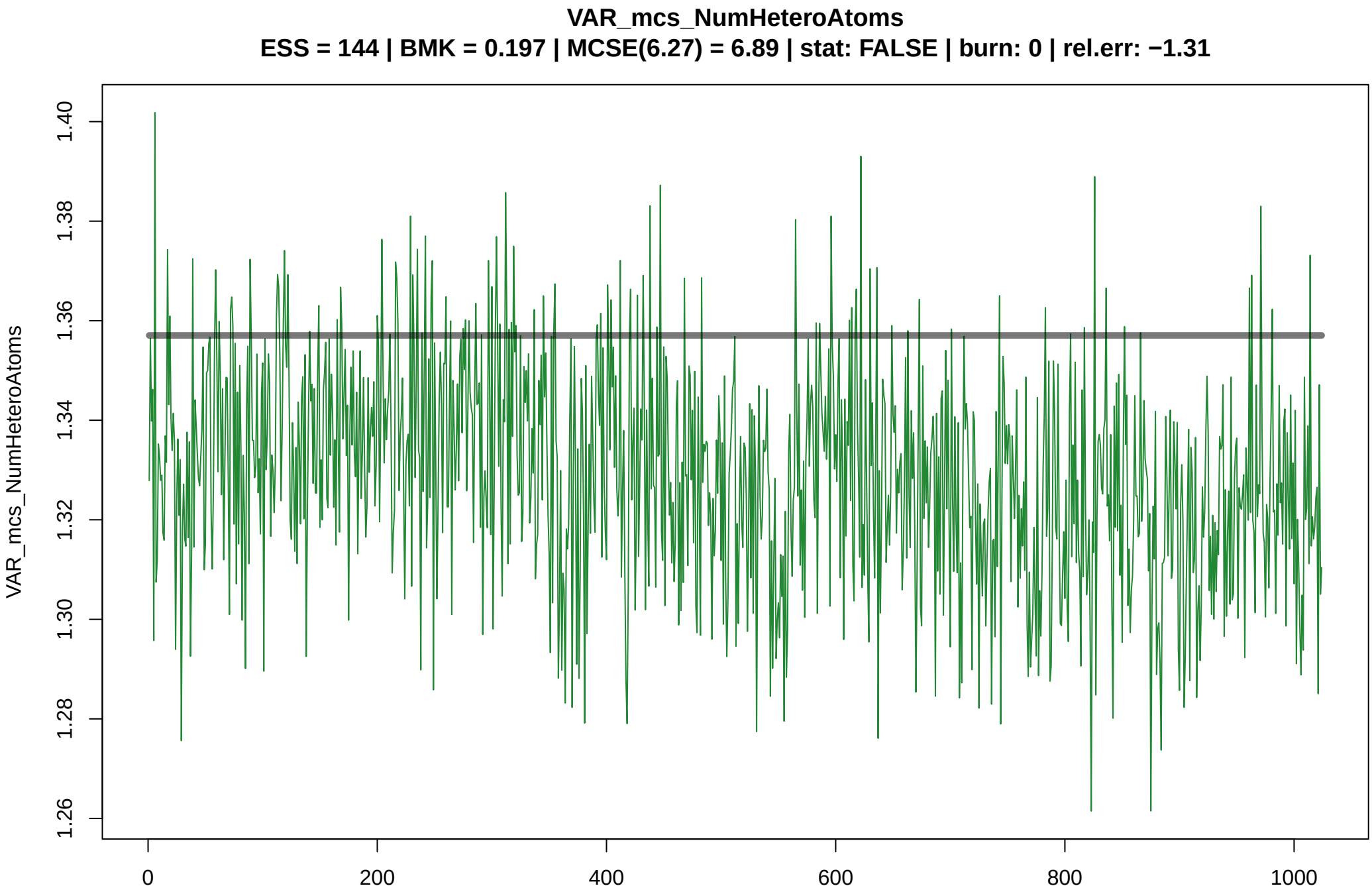

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0538 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0 | rel.err: −0.424
MEAN_docked_NumRotatableBonds
6.8
6.7
6.6
6.5
6.4
6.3
6.2
0
200
400
600
800
1000

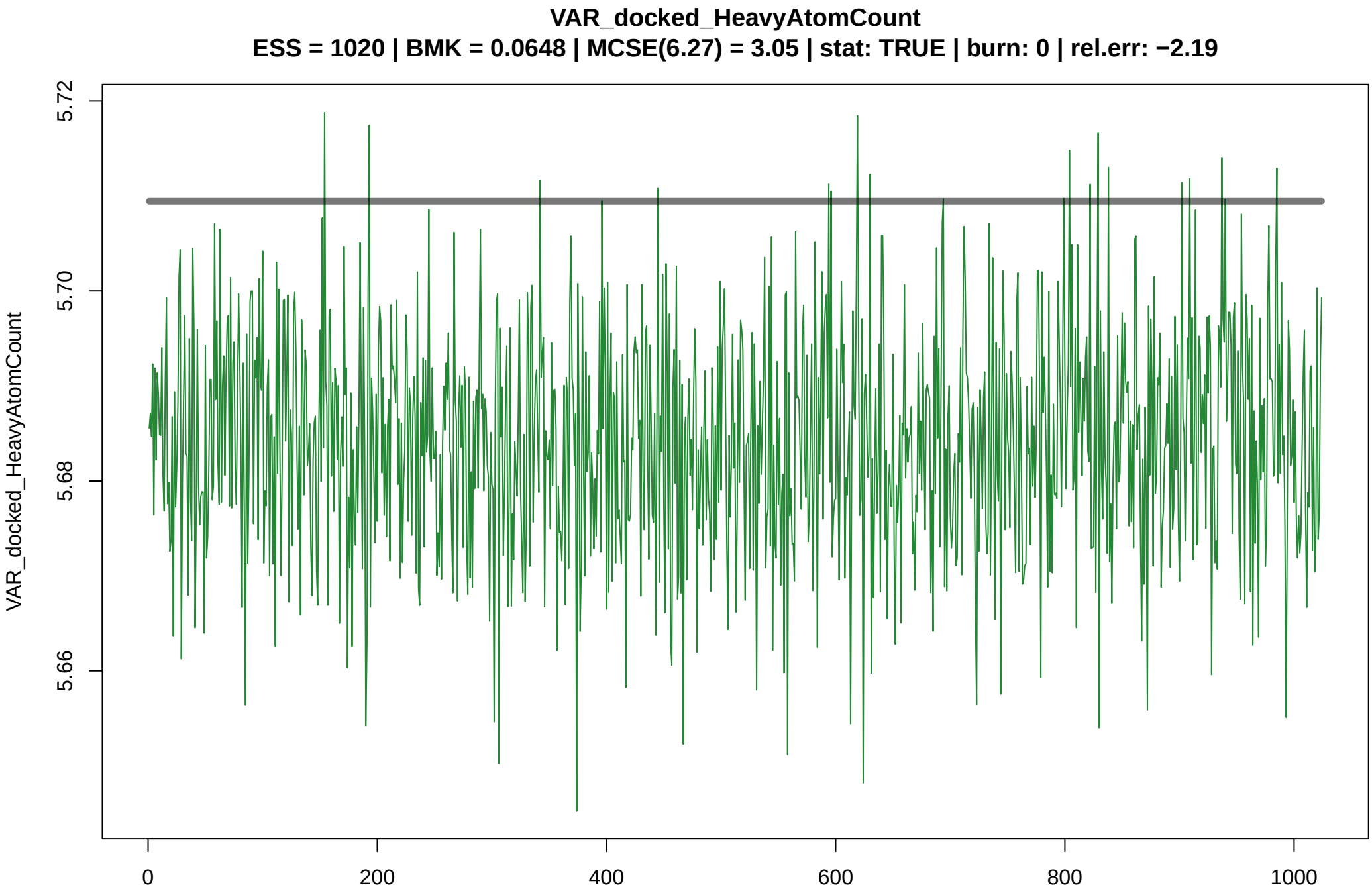

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0651 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0 | rel.err: −1.17
MEAN_mcs_NOCount
5.8
5.9
6.0
6.1
6.2
6.3
6.4
0
200
400
600
800
1000

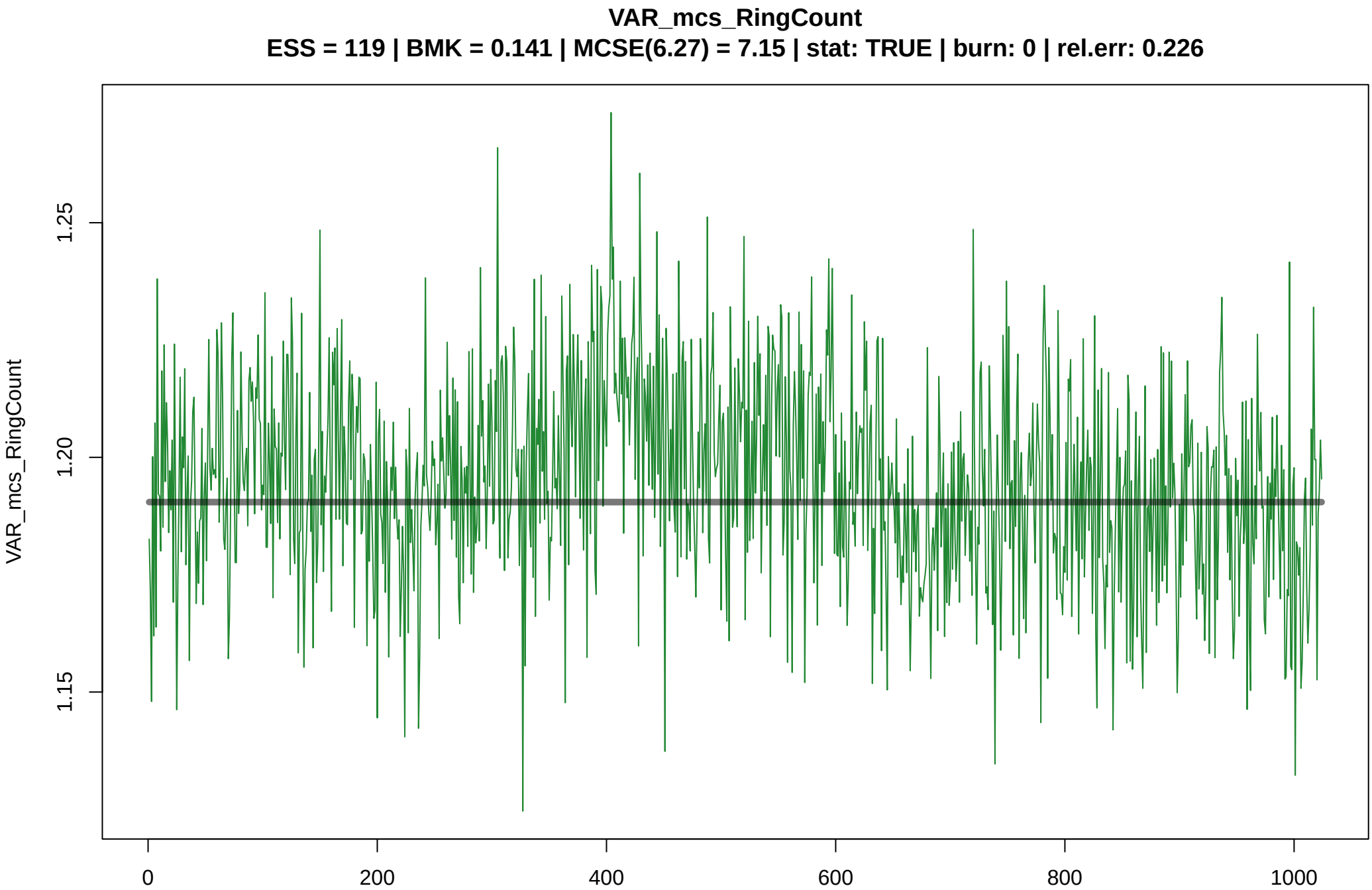

VAR_log_RMSD
ESS = 1020 | BMK = 0.0709 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | rel.err: 1.07
VAR_log_RMSD
1.08
1.06
1.04
1.02
1.00
0.98
0
200
400
600
800
1000

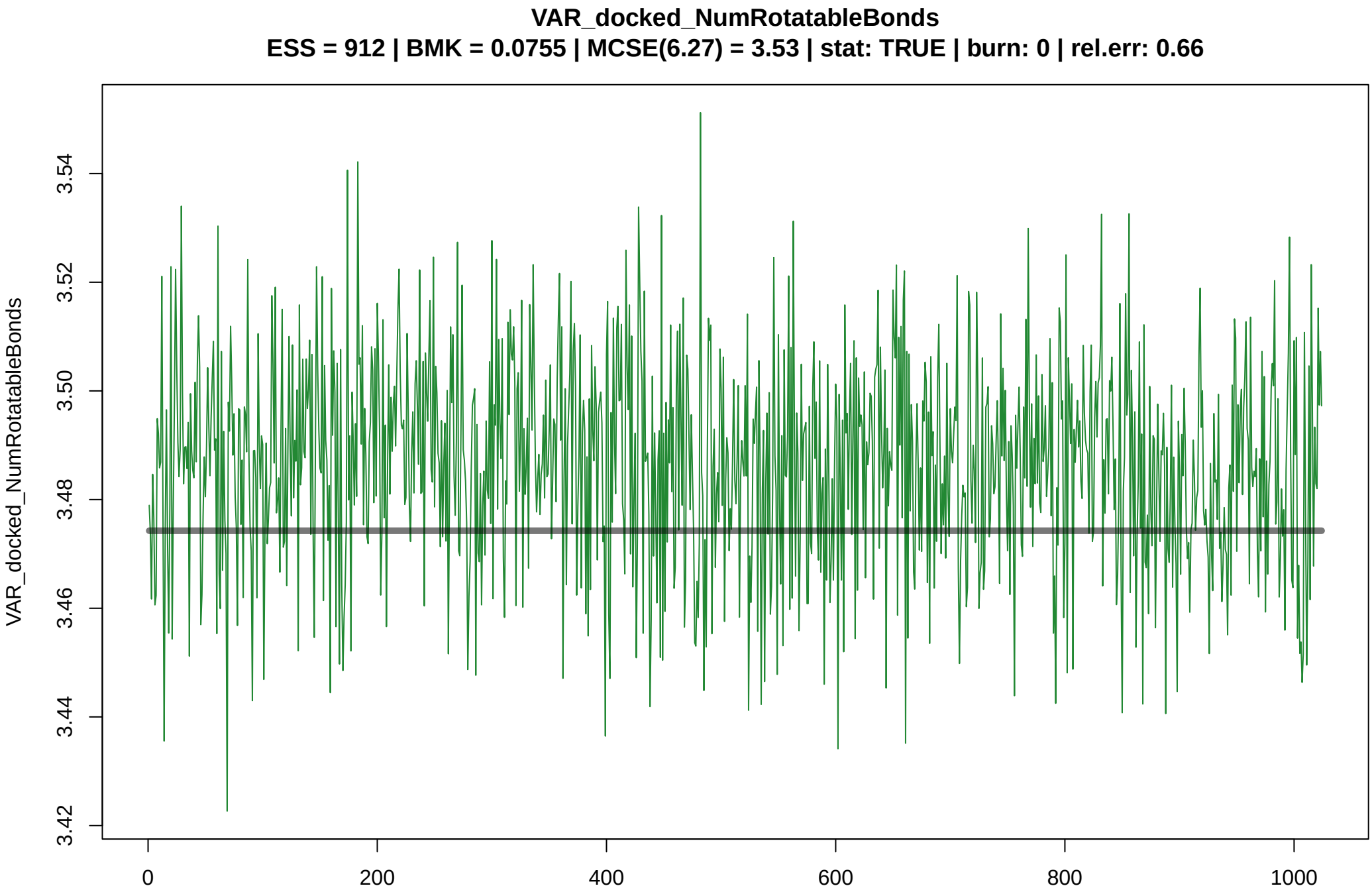

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0586 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: −0.029
VAR_log_mcs_unbonded_polar_sasa
1.62
1.64
1.66
1.68
1.70
1.72
0
200
400
600
800
1000

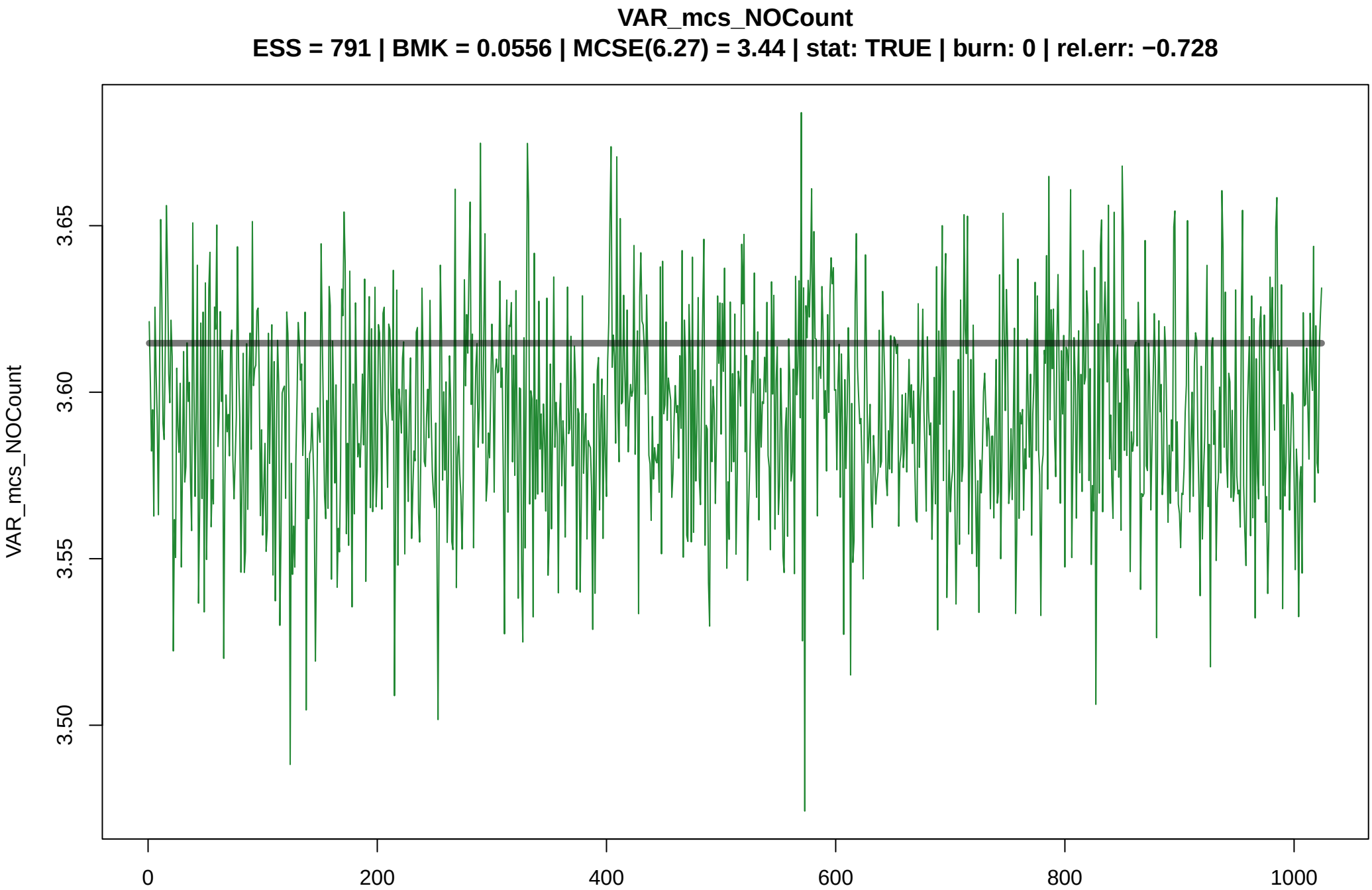

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0552 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | rel.err: 1.2
VAR_logit_ec_tanimoto_similarity
2.78
2.80
2.82
2.84
2.86
0
200
400
600
800
1000

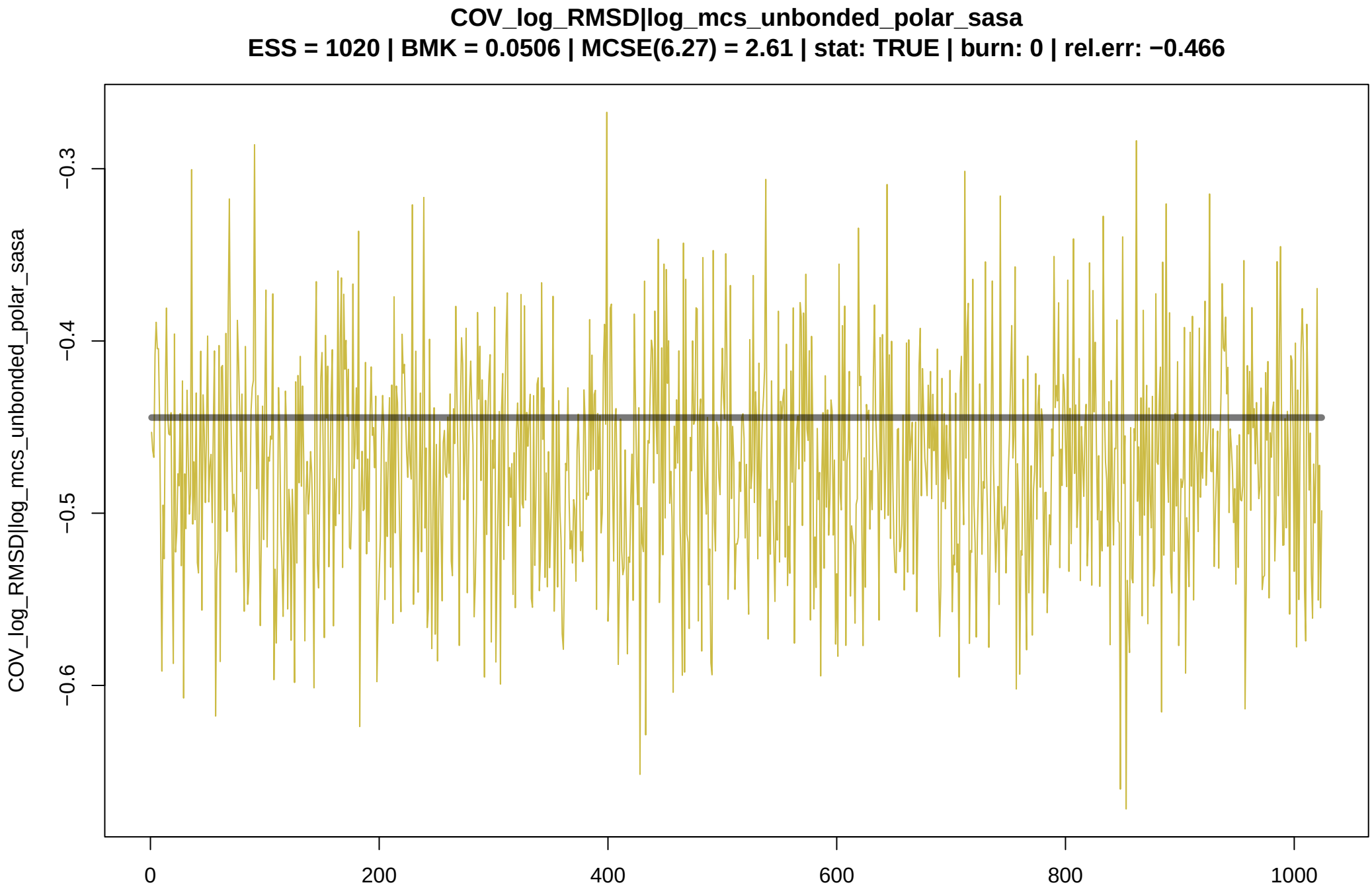

VAR_mcs_NumHeteroAtoms
ESS = 144 | BMK = 0.197 | MCSE(6.27) = 6.89 | stat: FALSE | burn: 0 | rel.err: −1.31
VAR_mcs_NumHeteroAtoms
1.26
1.28
1.30
1.32
1.34
1.36
1.38
1.40
0
200
400
600
800
1000

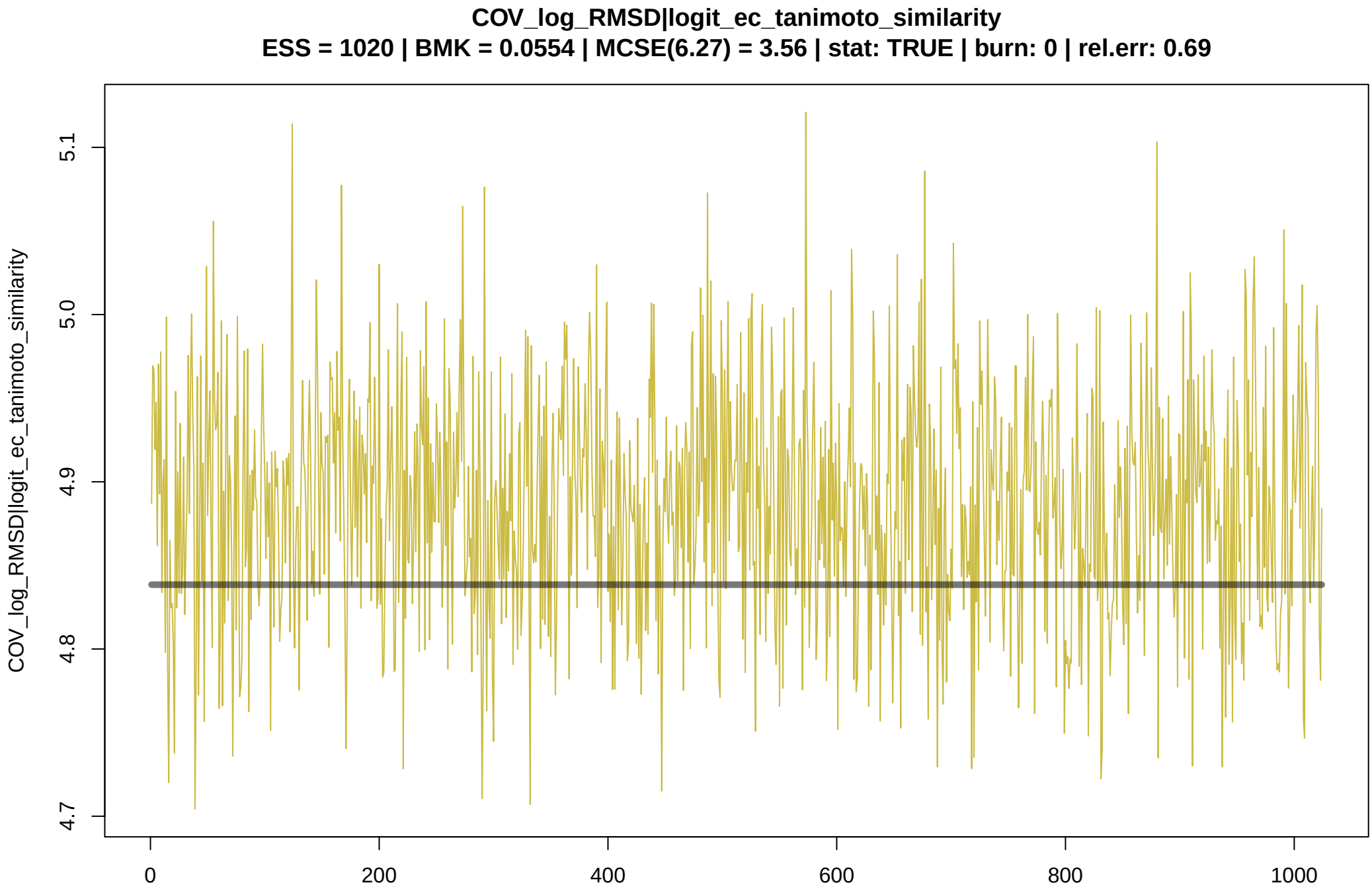

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0648 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | rel.err: −2.19
VAR_docked_HeavyAtomCount
5.72
5.70
5.68
5.66
0
200
400
600
800
1000

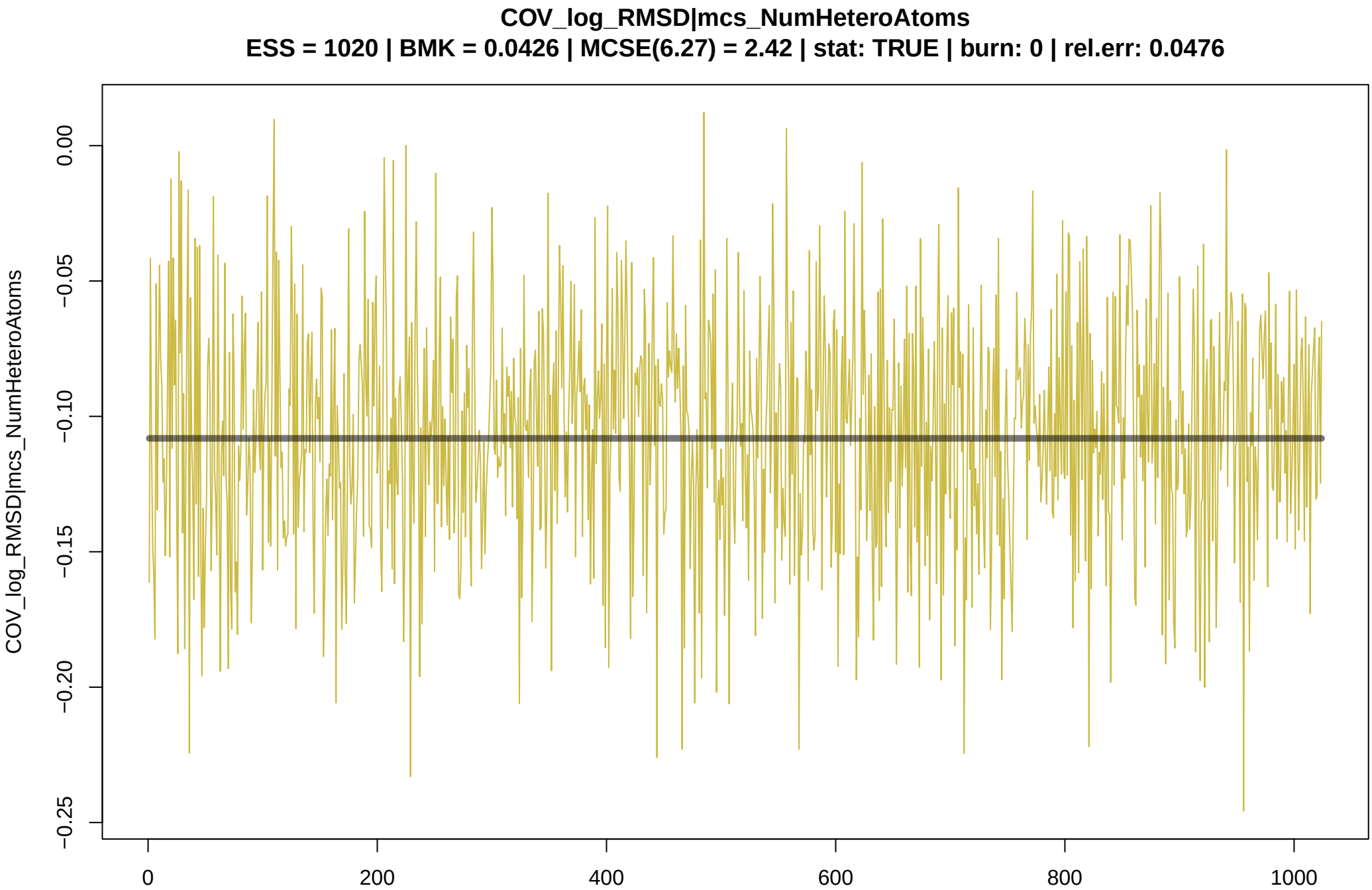

VAR_mcs_RingCount
ESS = 119 | BMK = 0.141 | MCSE(6.27) = 7.15 | stat: TRUE | burn: 0 | rel.err: 0.226
VAR_mcs_RingCount
1.15
1.20
1.25
0
200
400
600
800
1000

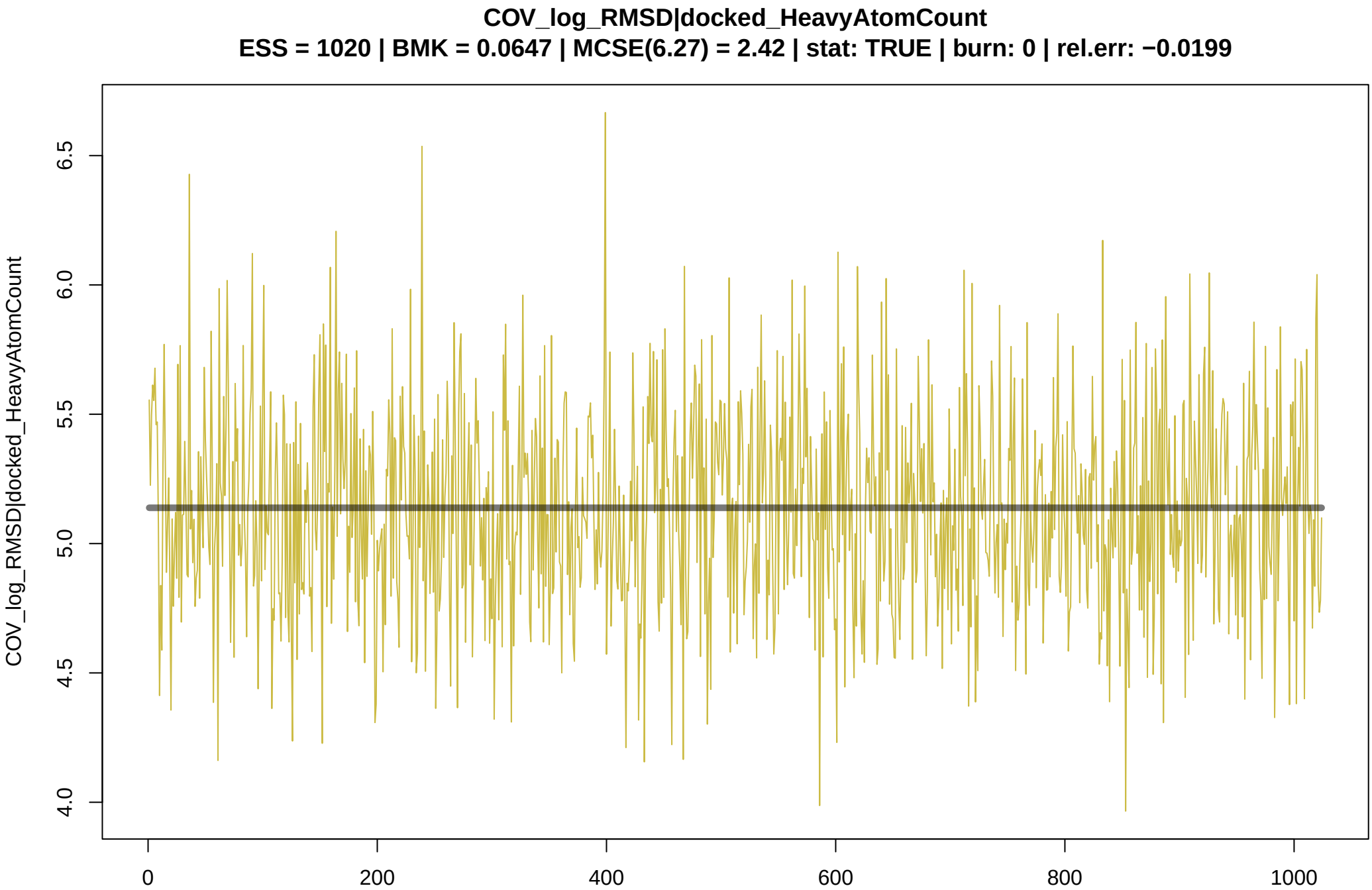

VAR_docked_NumRotatableBonds
ESS = 912 | BMK = 0.0755 | MCSE(6.27) = 3.53 | stat: TRUE | burn: 0 | rel.err: 0.66
VAR_docked_NumRotatableBonds
3.42
3.44
3.46
3.48
3.50
3.52
3.54
0
200
400
600
800
1000

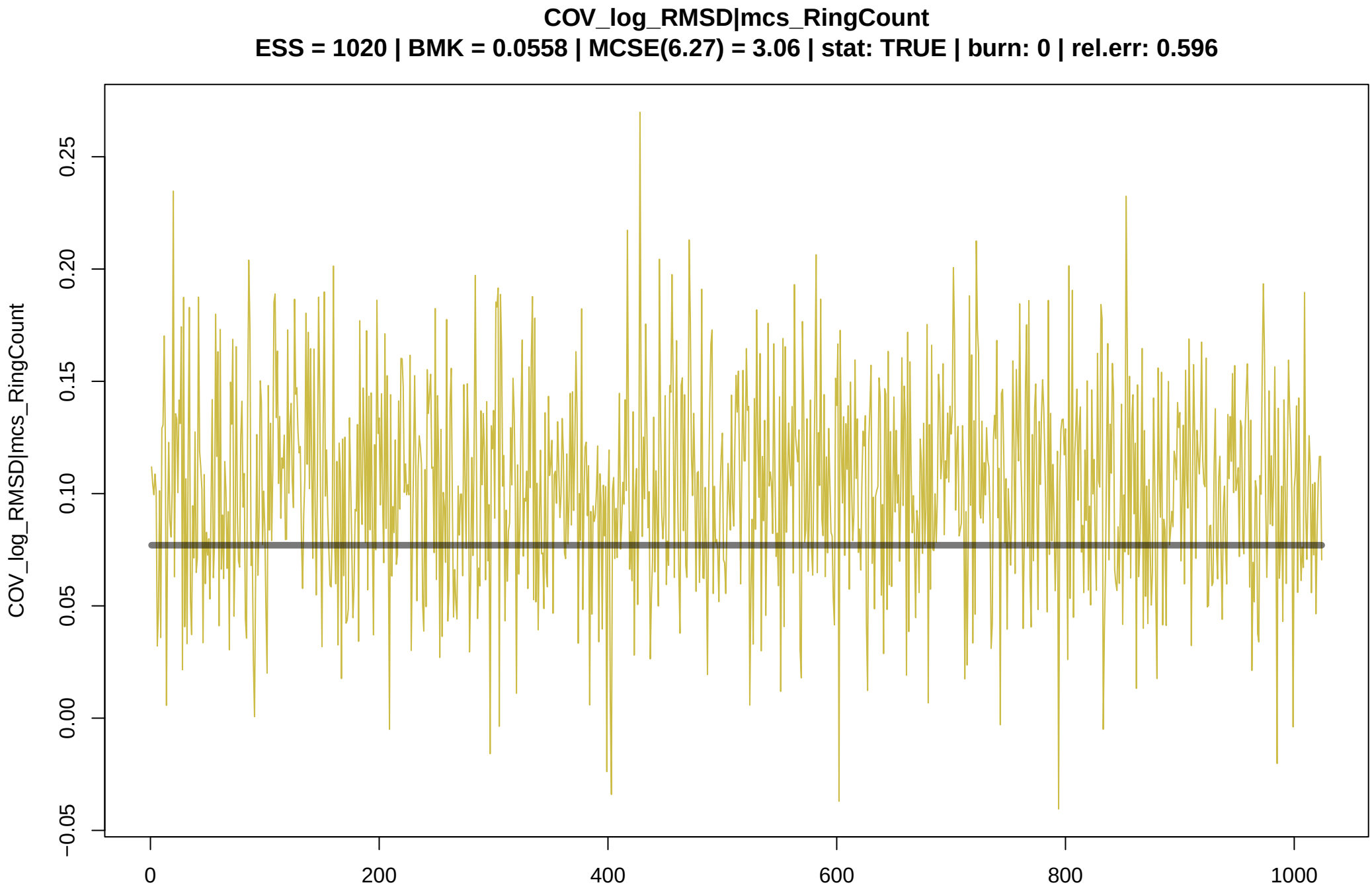

VAR_mcs_NOCount
ESS = 791 | BMK = 0.0556 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | rel.err: −0.728
VAR_mcs_NOCount
3.50
3.55
3.60
3.65
0
200
400
600
800
1000

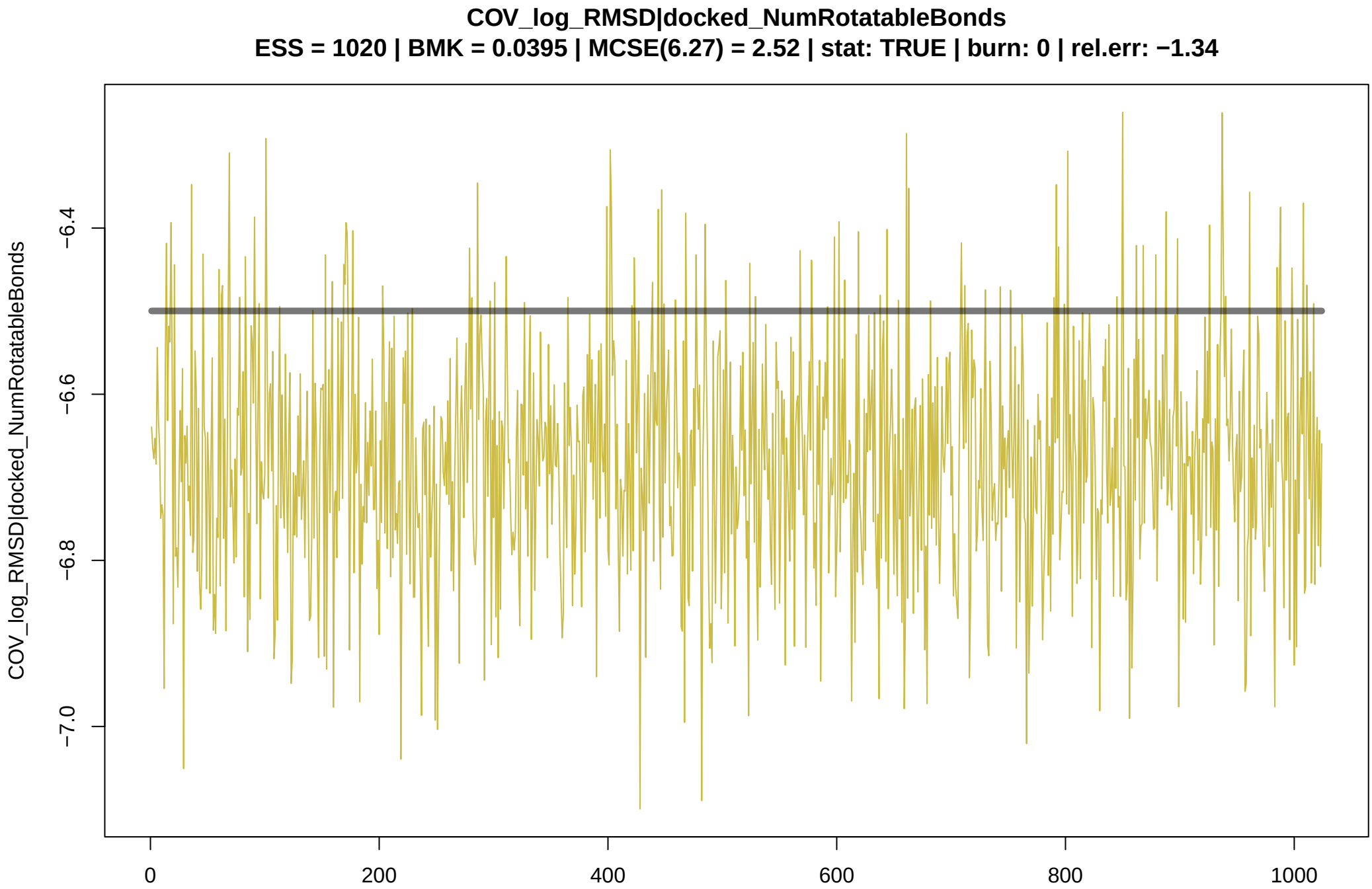

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0506 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: −0.466
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.3
−0.4
−0.5
−0.6
0
200
400
600
800
1000

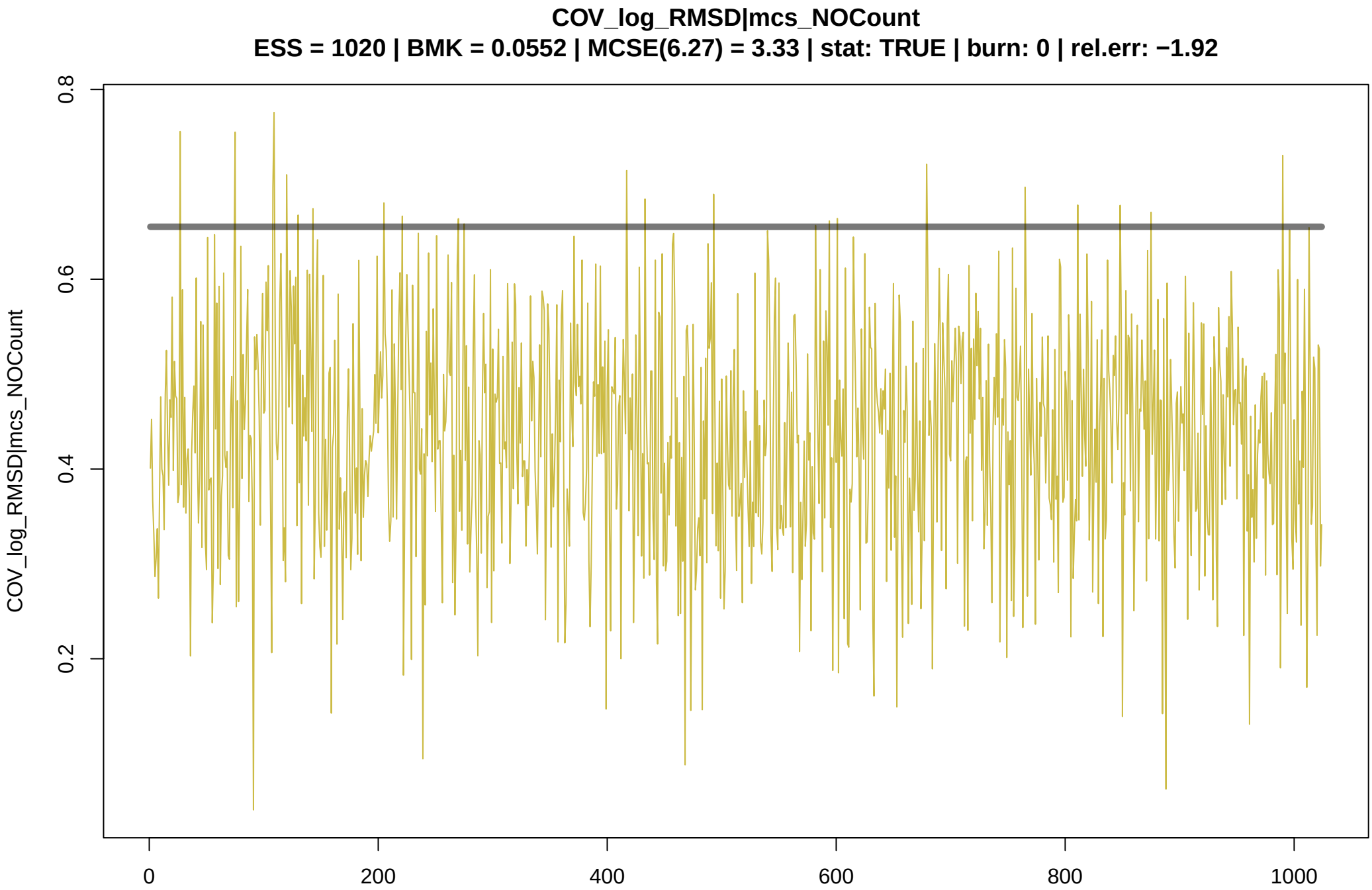

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0554 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | rel.err: 0.69
COV_log_RMSD|logit_ec_tanimoto_similarity
4.7
4.8
4.9
5.0
5.1
0
200
400
600
800
1000

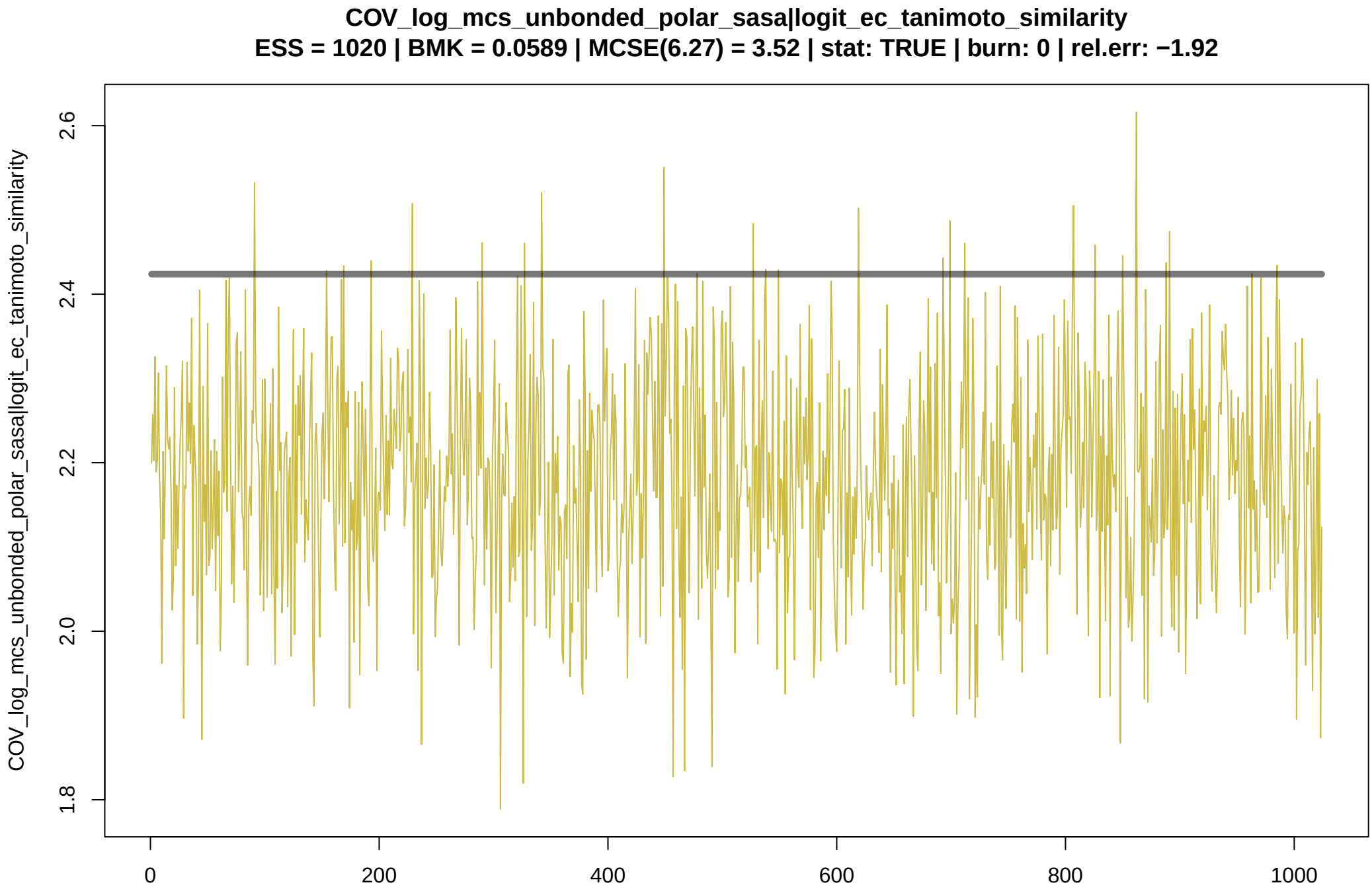

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0426 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 0.0476
COV_log_RMSD|mcs_NumHeteroAtoms
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
200
400
600
800
1000

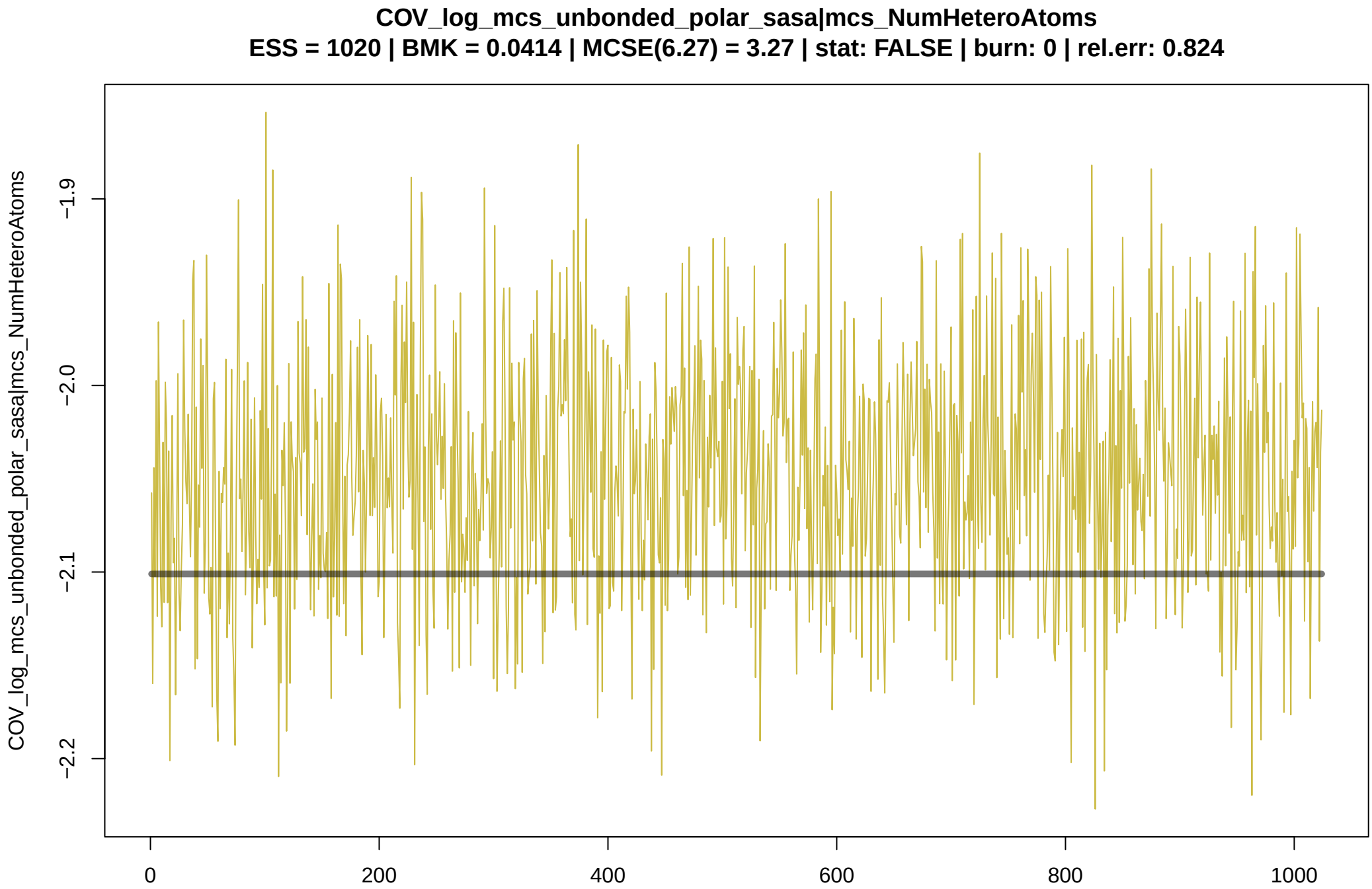

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0647 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: −0.0199
COV_log_RMSD|docked_HeavyAtomCount
4.0
4.5
5.0
5.5
6.0
6.5
0
200
400
600
800
1000

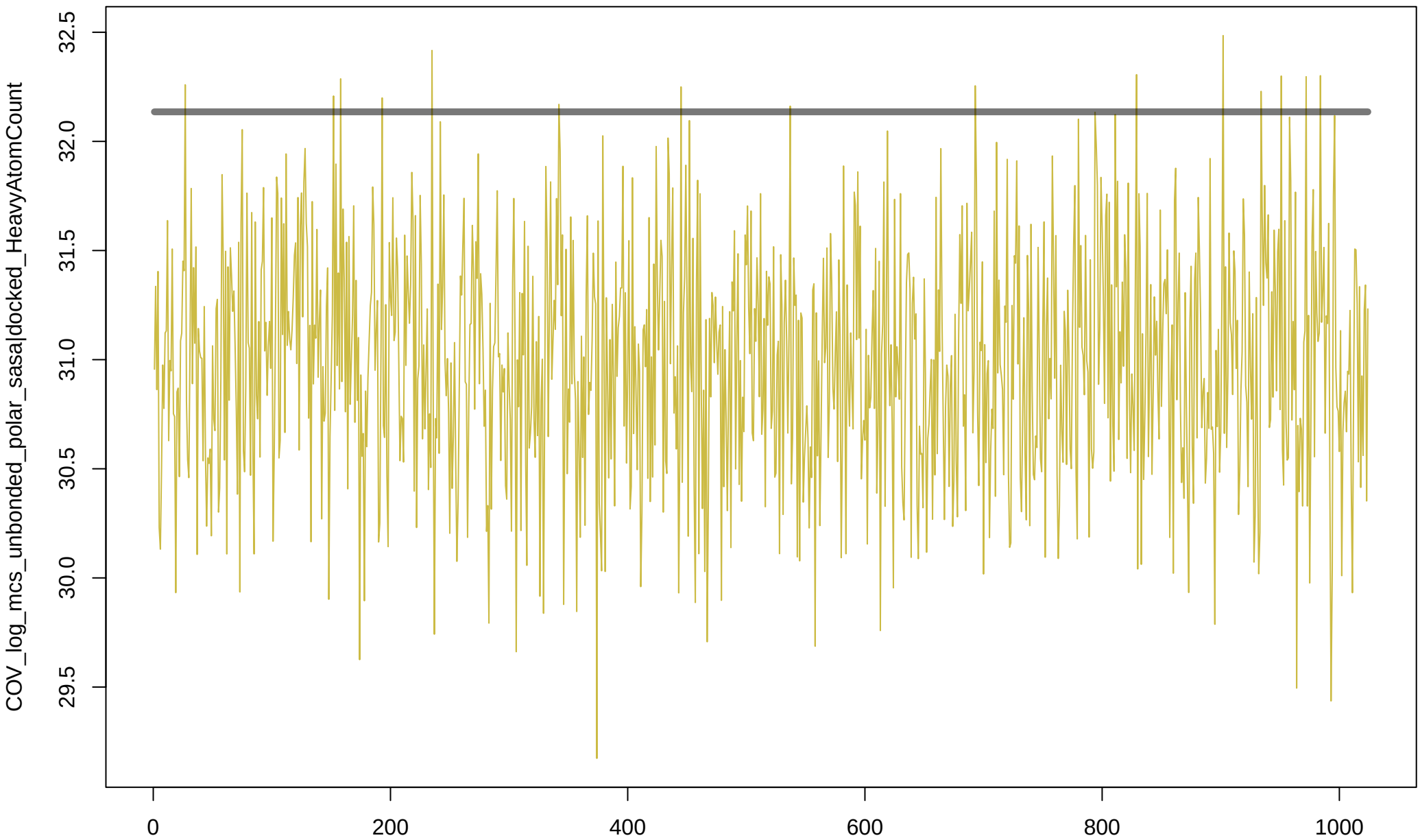

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0558 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | rel.err: 0.596
COV_log_RMSD|mcs_RingCount
0.25
0.20
0.15
0.10
0.05
0.00
−0.05
0
200
400
600
800
1000

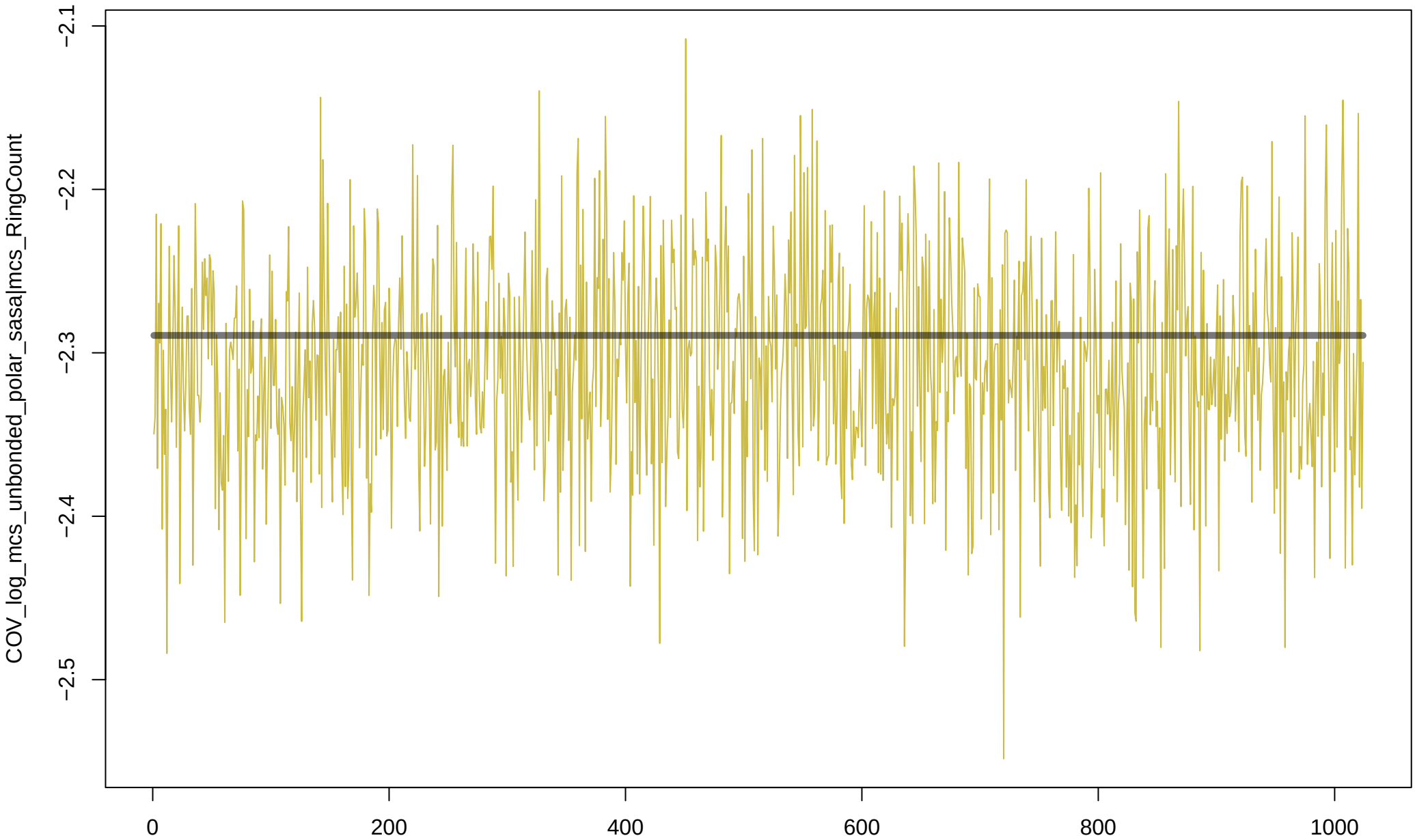

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0395 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | rel.err: −1.34
COV_log_RMSD|docked_NumRotatableBonds
−6.4
−6.6
−6.8
−7.0
0
200
400
600
800
1000

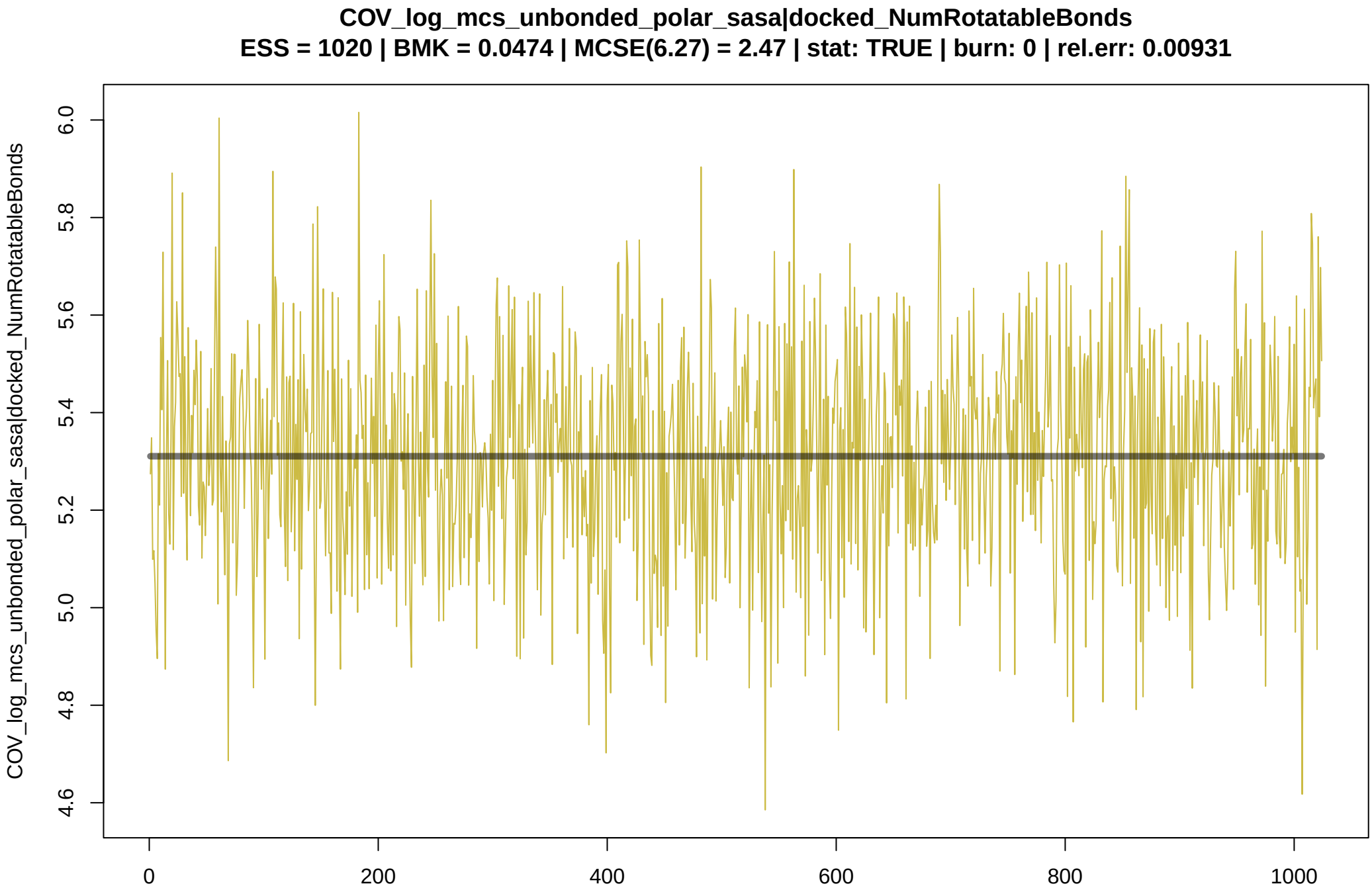

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0552 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0 | rel.err: −1.92
COV_log_RMSD|mcs_NOCount
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

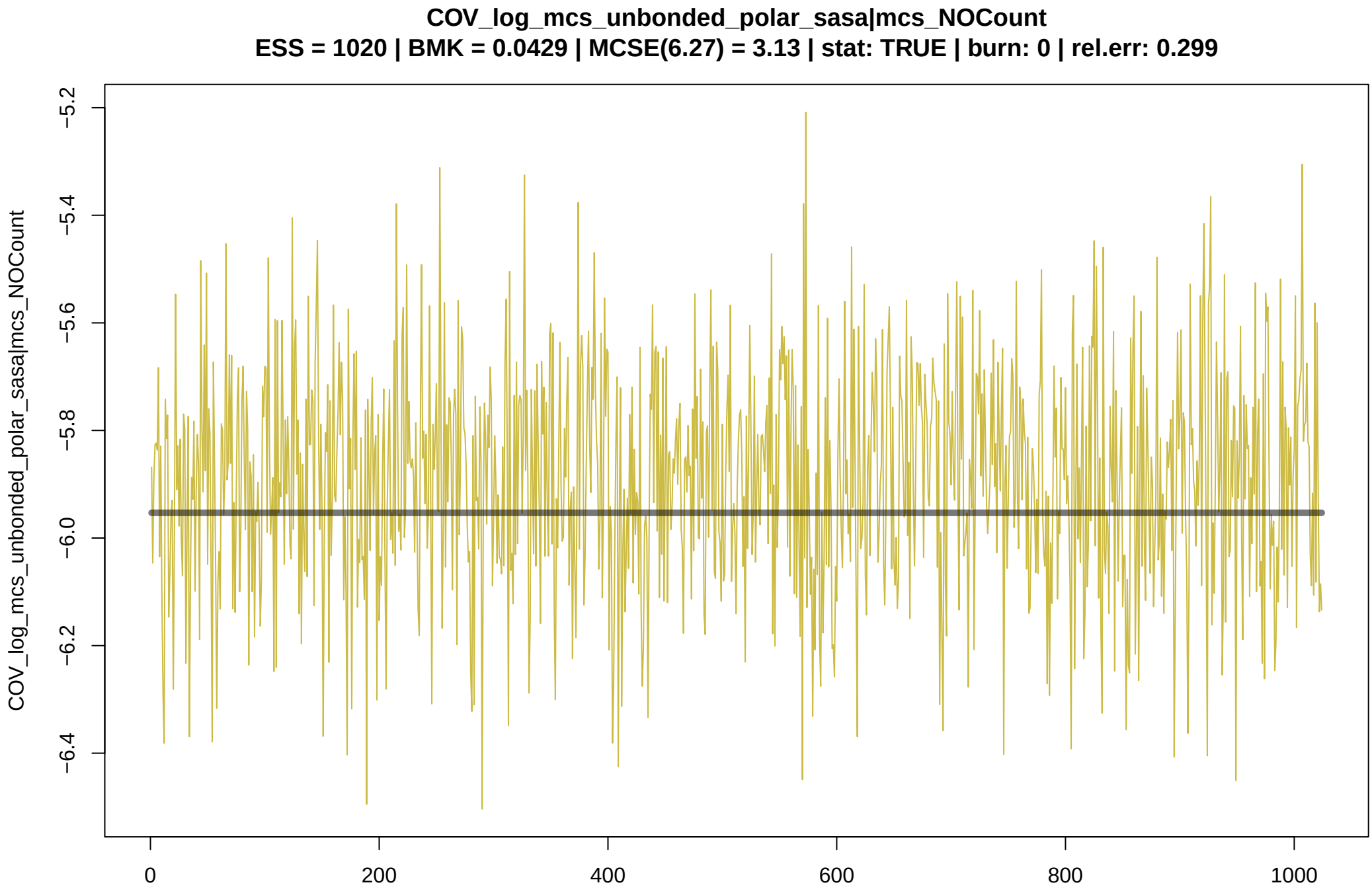

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0589 | MCSE(6.27) = 3.52 | stat: TRUE | burn: 0 | rel.err: −1.92
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
1.8
2.0
2.2
2.4
2.6
0
200
400
600
800
1000

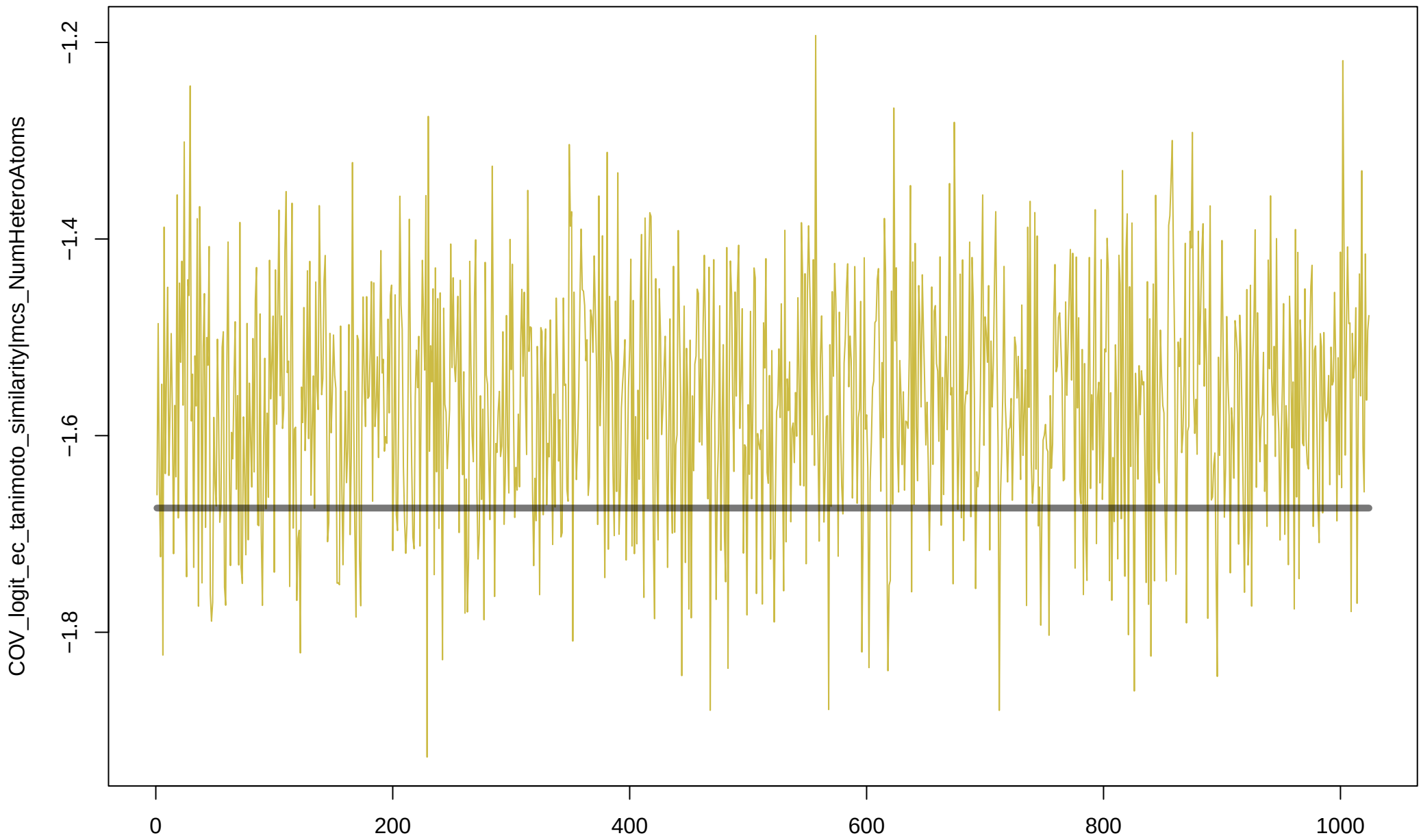

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0414 | MCSE(6.27) = 3.27 | stat: FALSE | burn: 0 | rel.err: 0.824
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

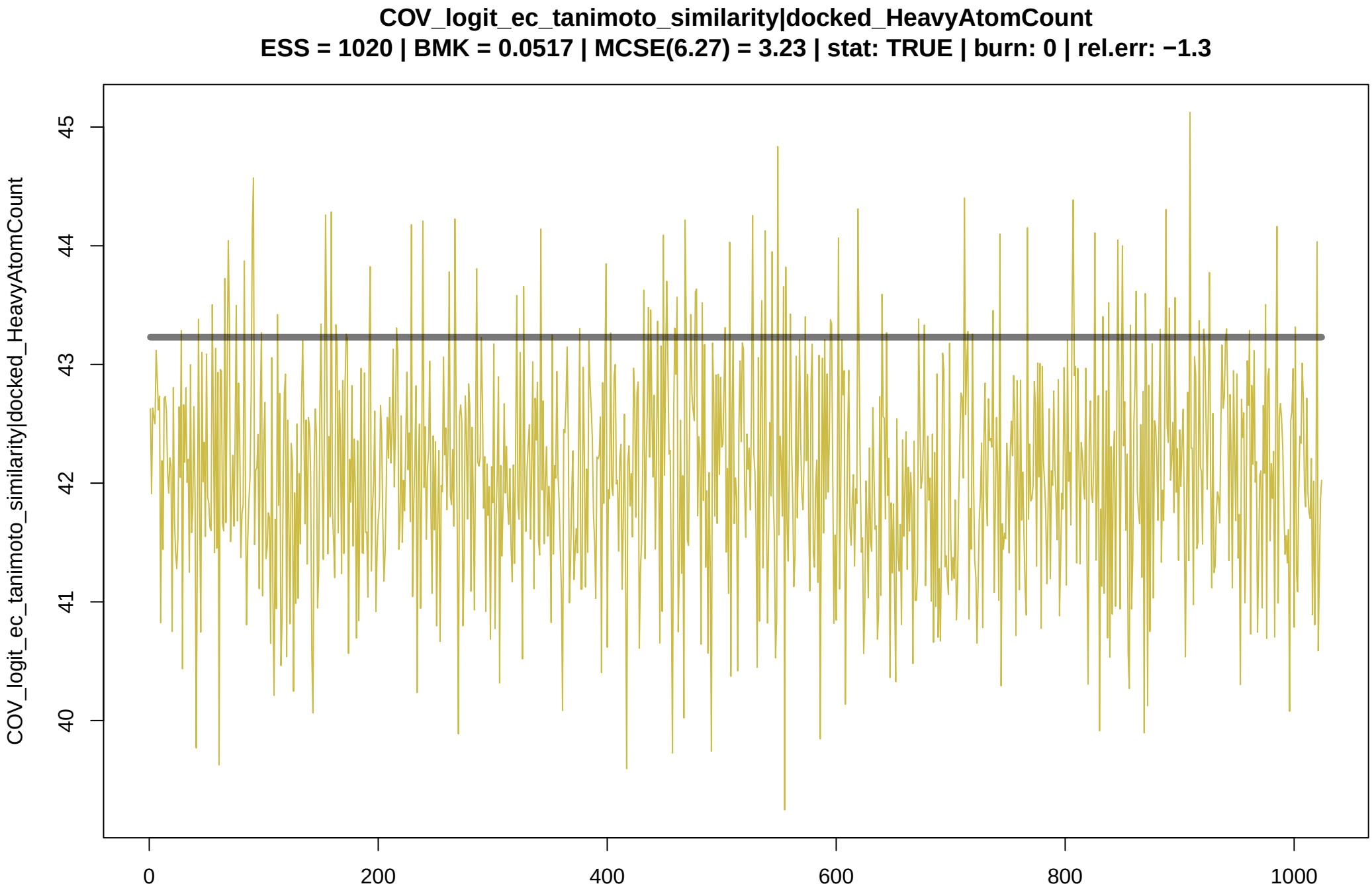

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0562 | MCSE(6.27) = 3.58 | stat: TRUE | burn: 0 | rel.err: −2.18
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
32.5
32.0
31.5
31.0
30.5
30.0
29.5
0
200
400
600
800
1000

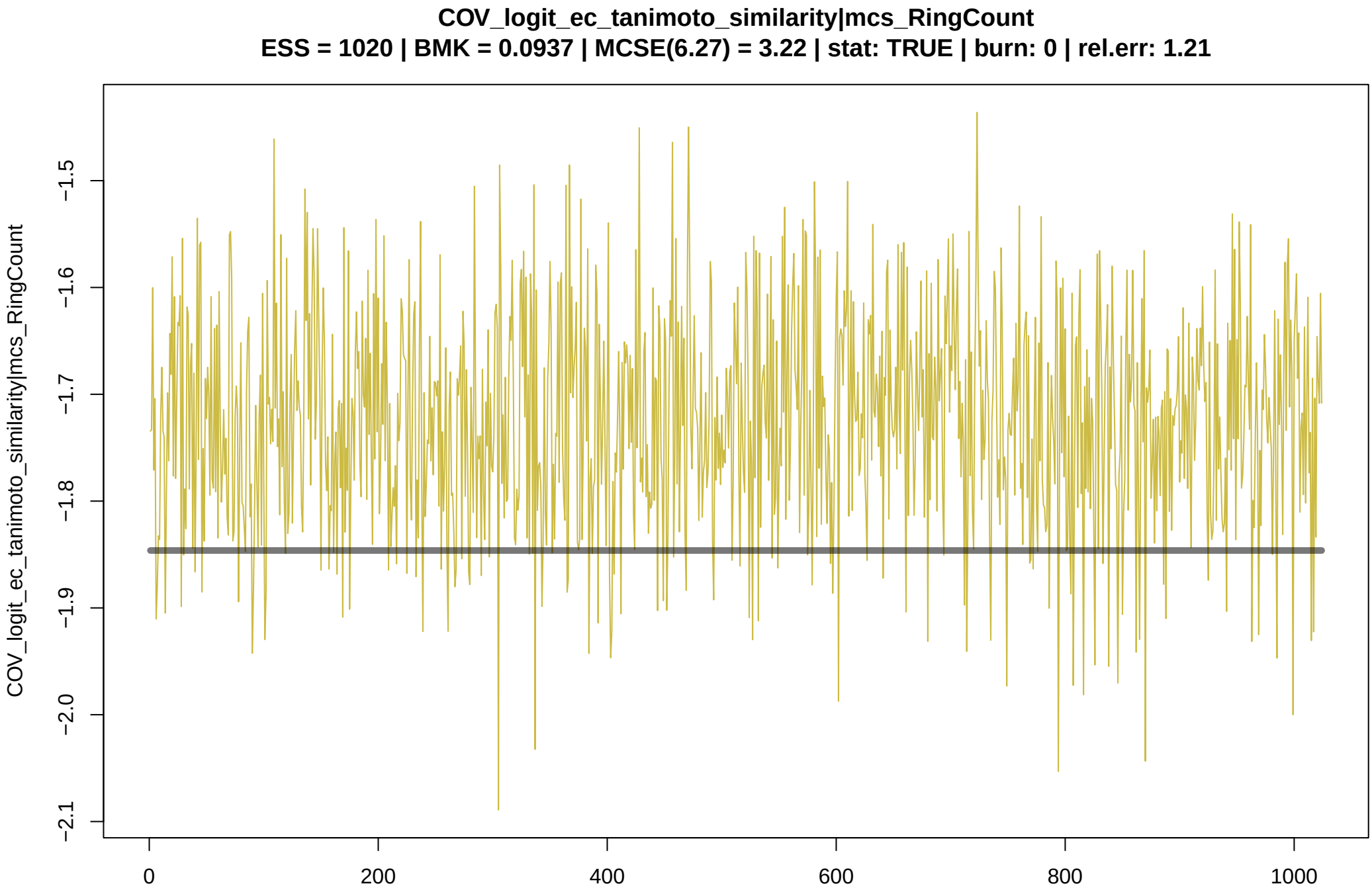

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0447 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | rel.err: −0.308
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.1
−2.2
−2.3
−2.4
−2.5
0
200
400
600
800
1000

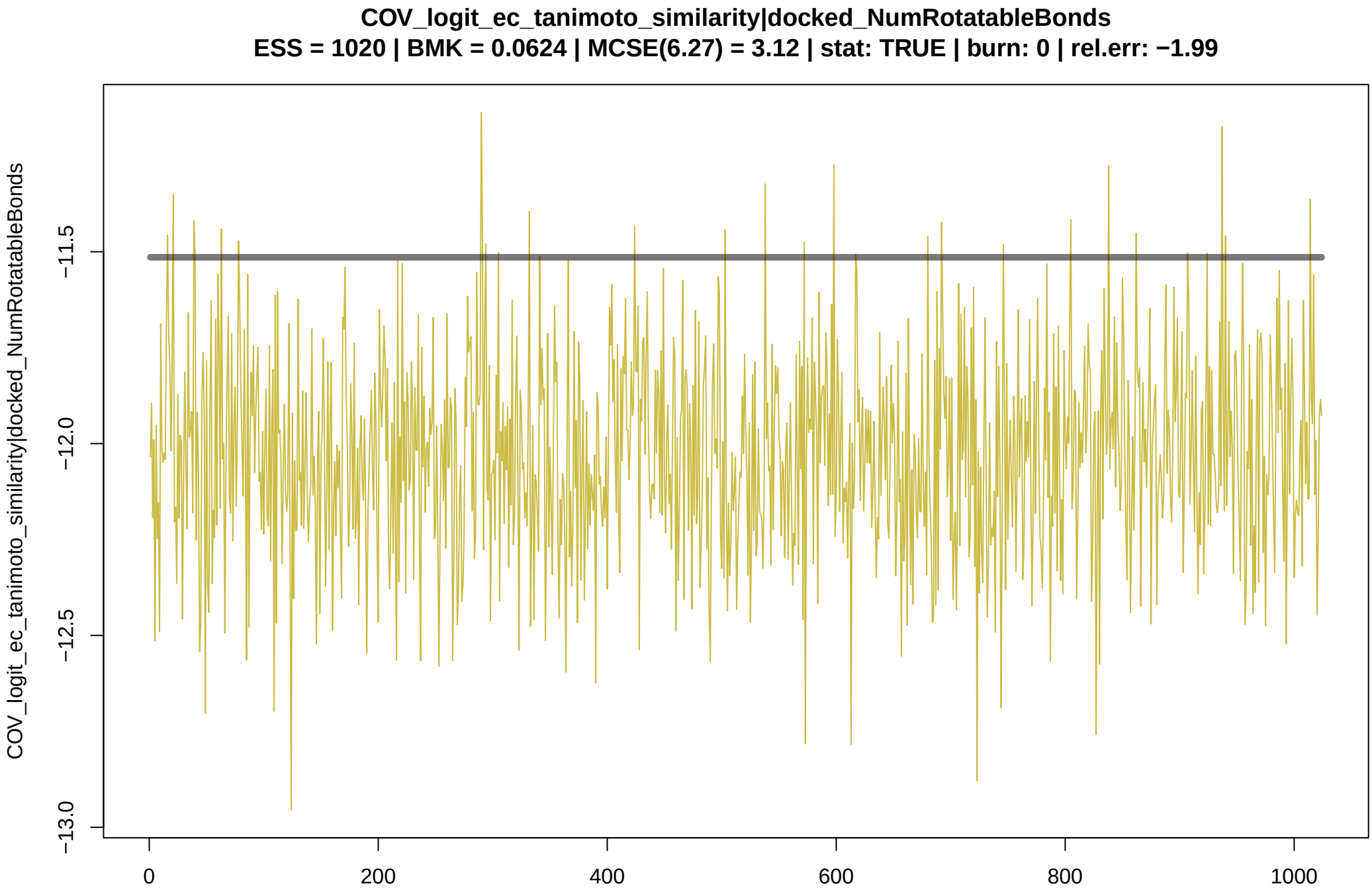

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0474 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0 | rel.err: 0.00931
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
4.6
4.8
5.0
5.2
5.4
5.6
5.8
6.0
0
200
400
600
800
1000

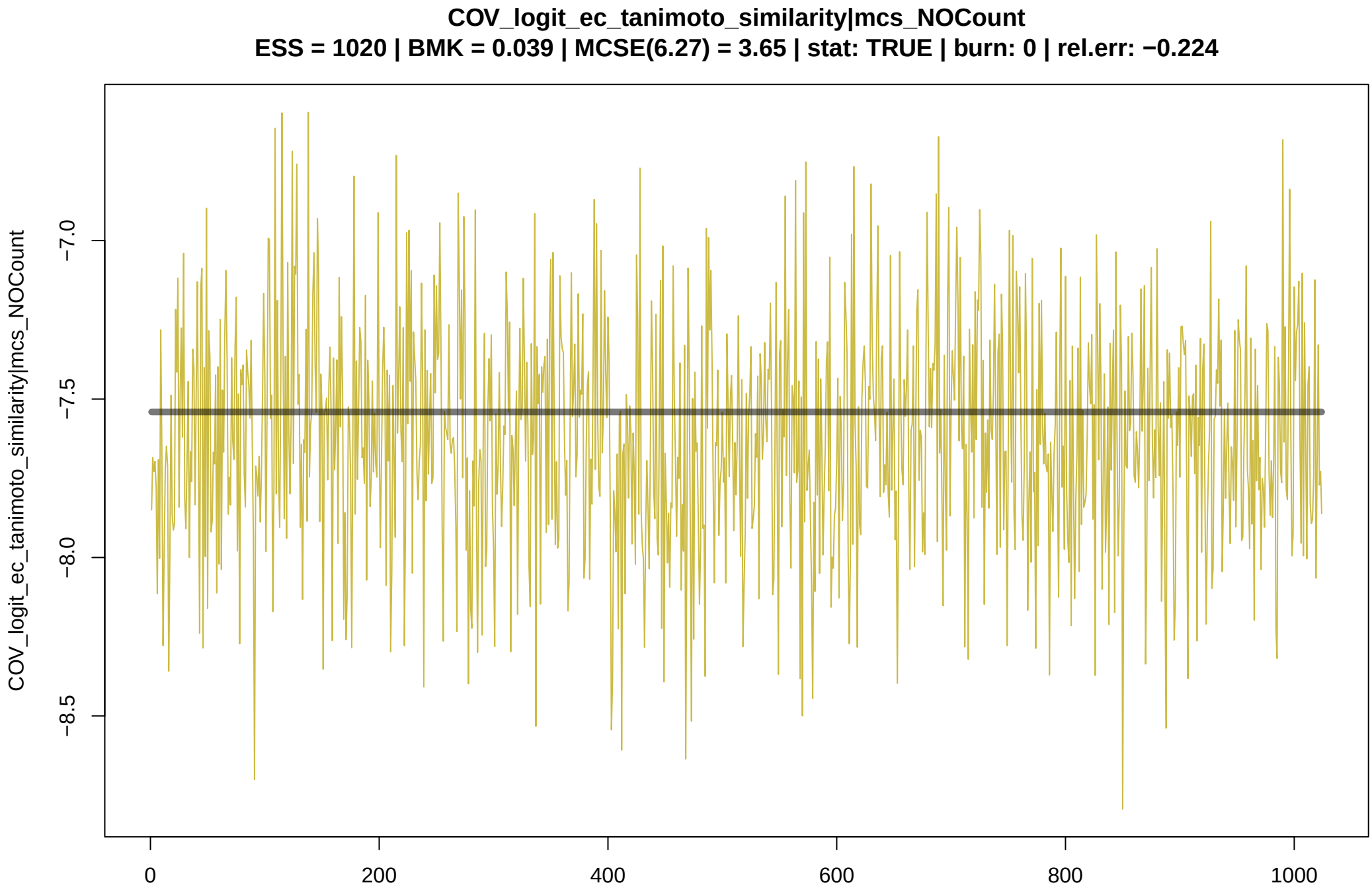

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0429 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | rel.err: 0.299
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.2
−5.4
−5.6
−5.8
−6.0
−6.2
−6.4
0
200
400
600
800
1000

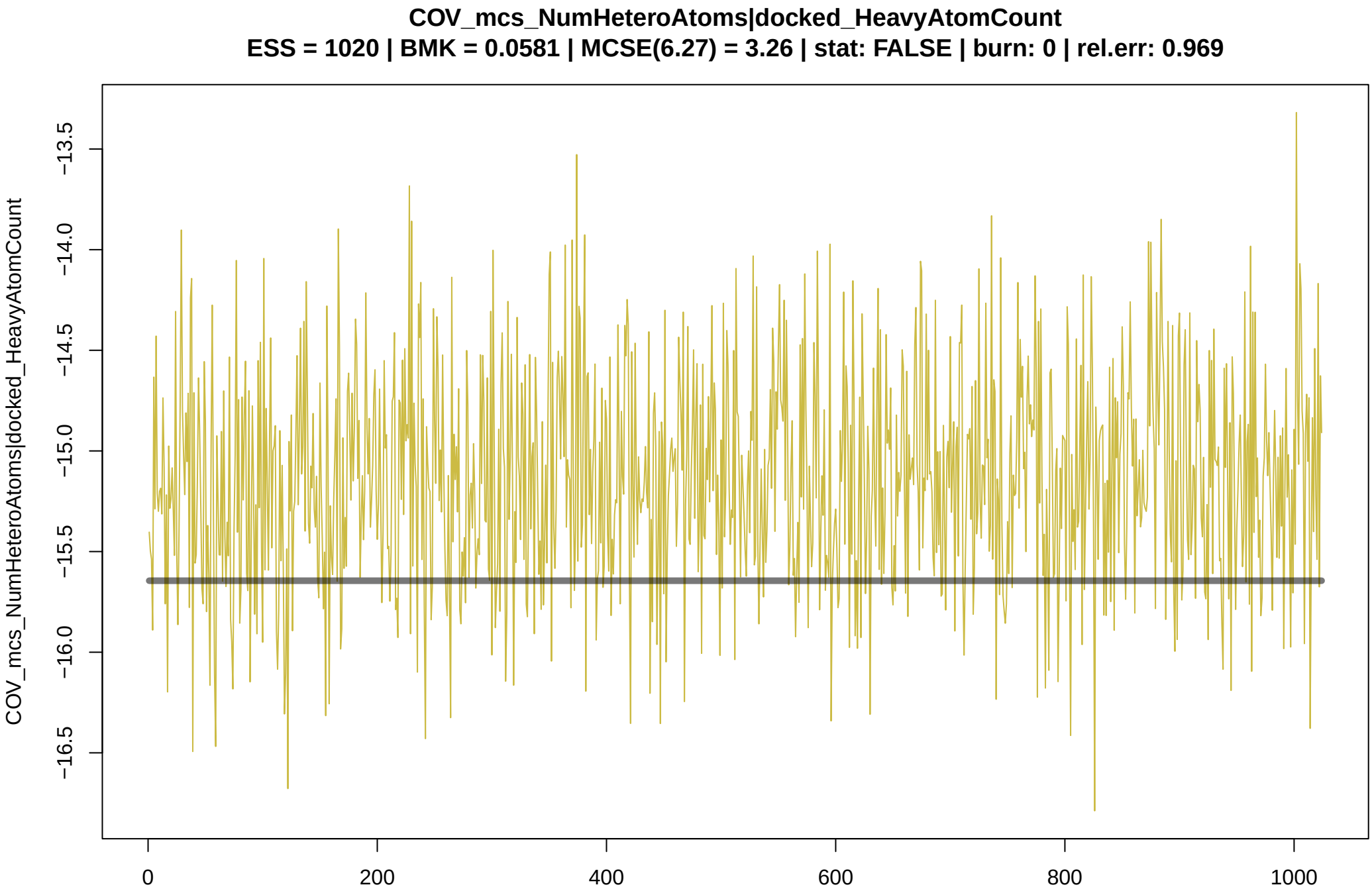

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0554 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | rel.err: 0.939
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.2
−1.4
−1.6
−1.8
0
200
400
600
800
1000

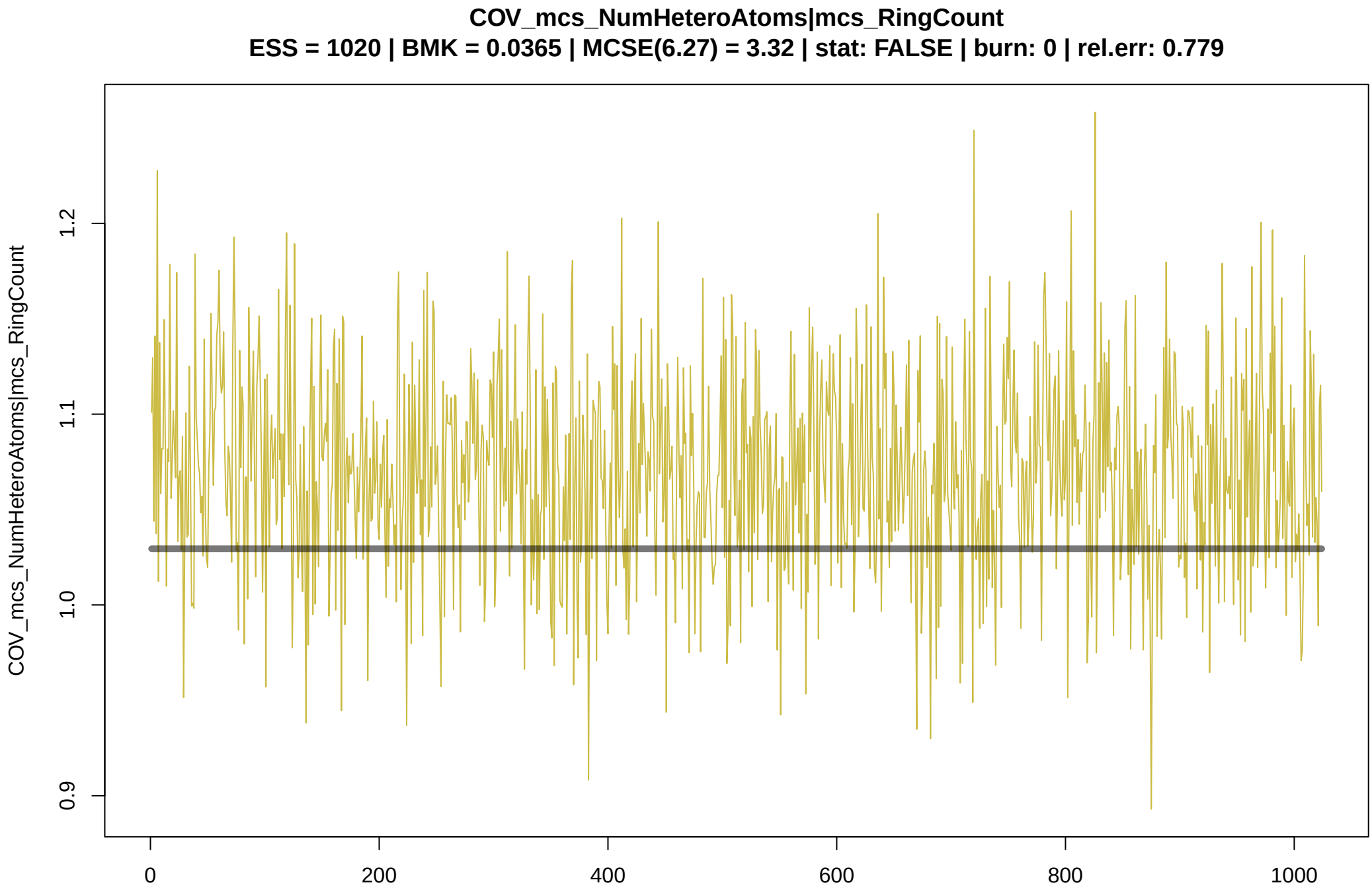

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0517 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | rel.err: −1.3
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
45
44
43
42
41
40
0
200
400
600
800
1000

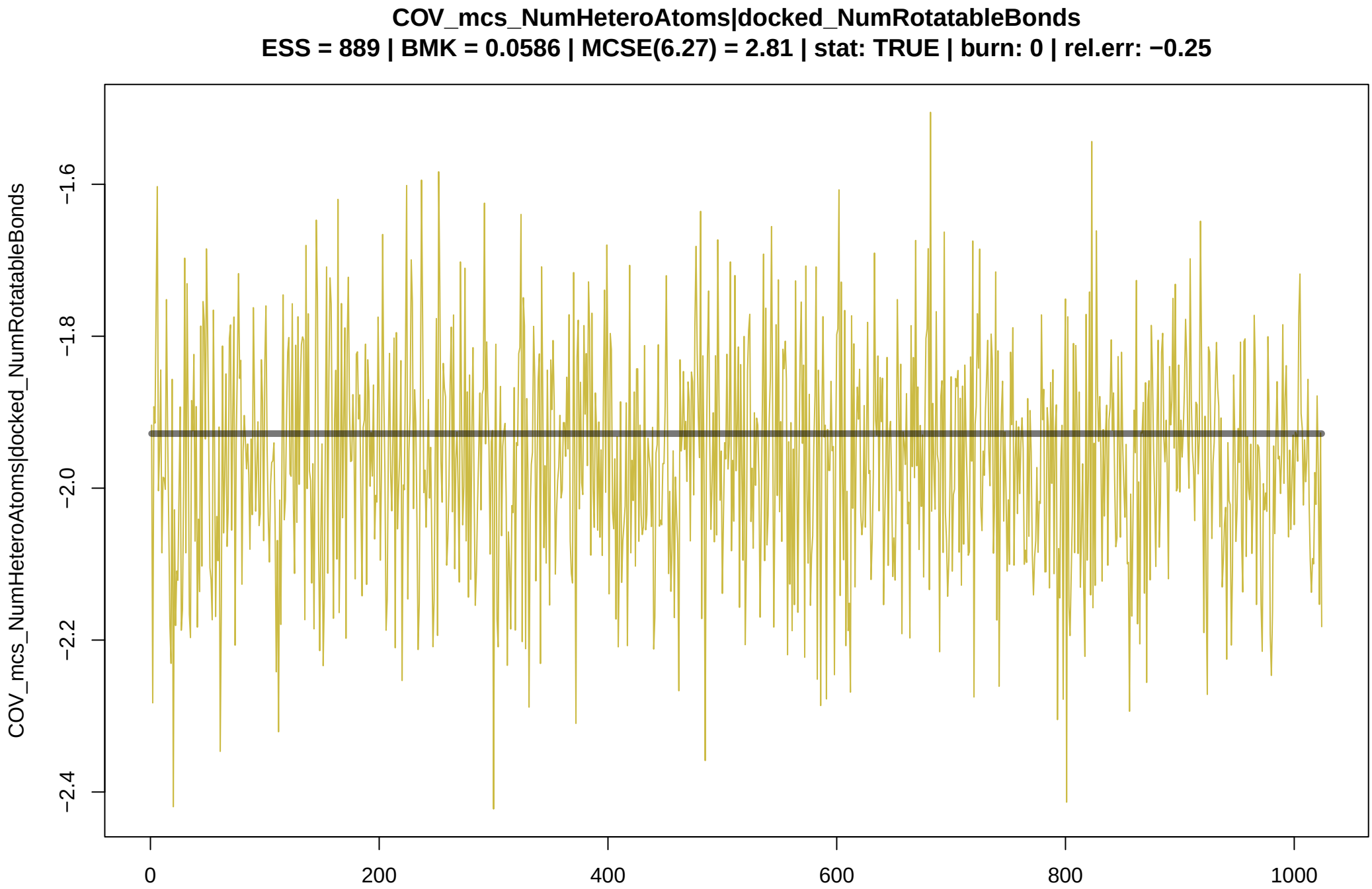

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0937 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0 | rel.err: 1.21
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.5
−1.6
−1.7
−1.8
−1.9
−2.0
−2.1
0
200
400
600
800
1000

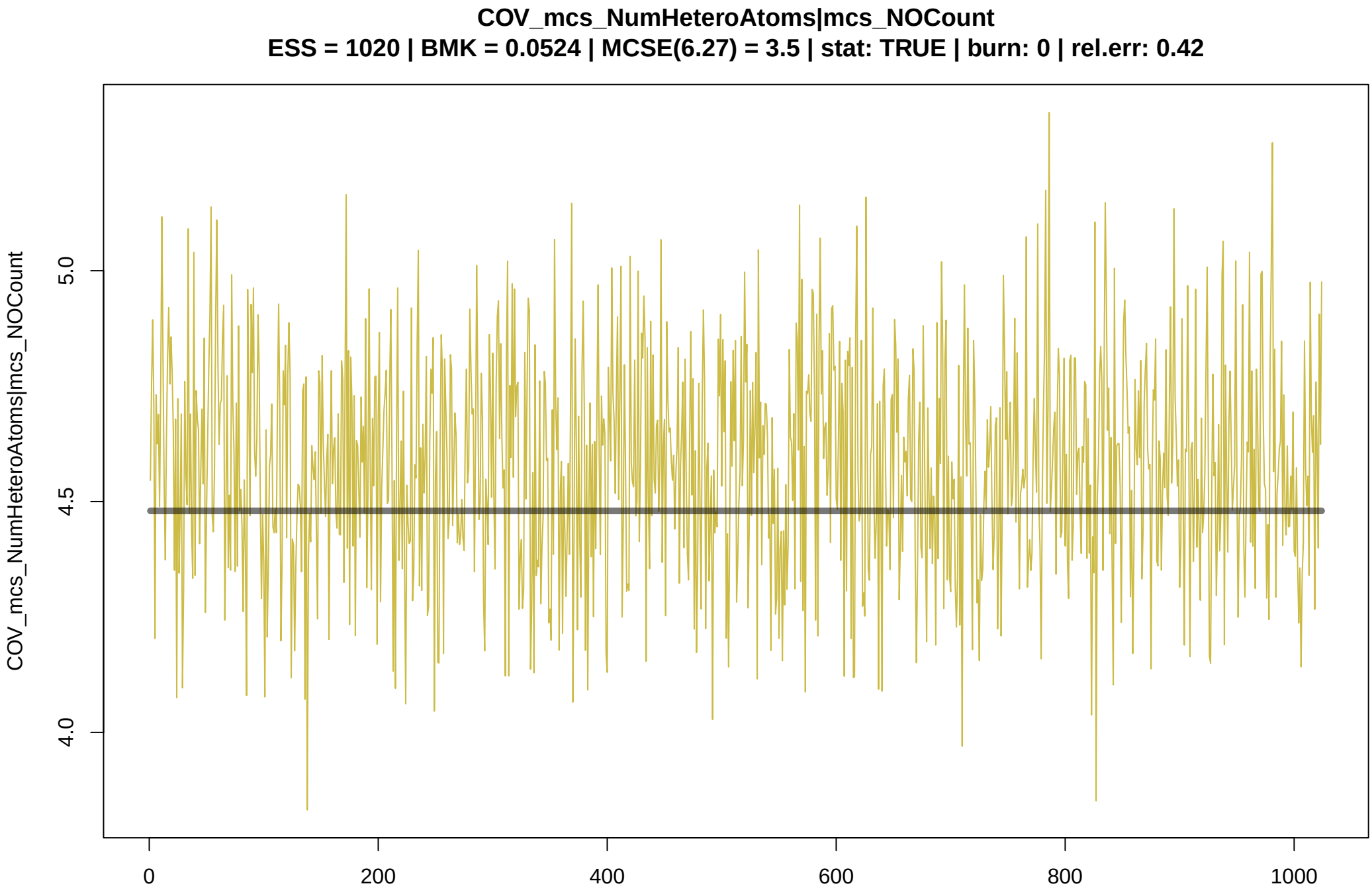

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0624 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | rel.err: −1.99
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−11.5
−12.0
−12.5
−13.0
0
200
400
600
800
1000

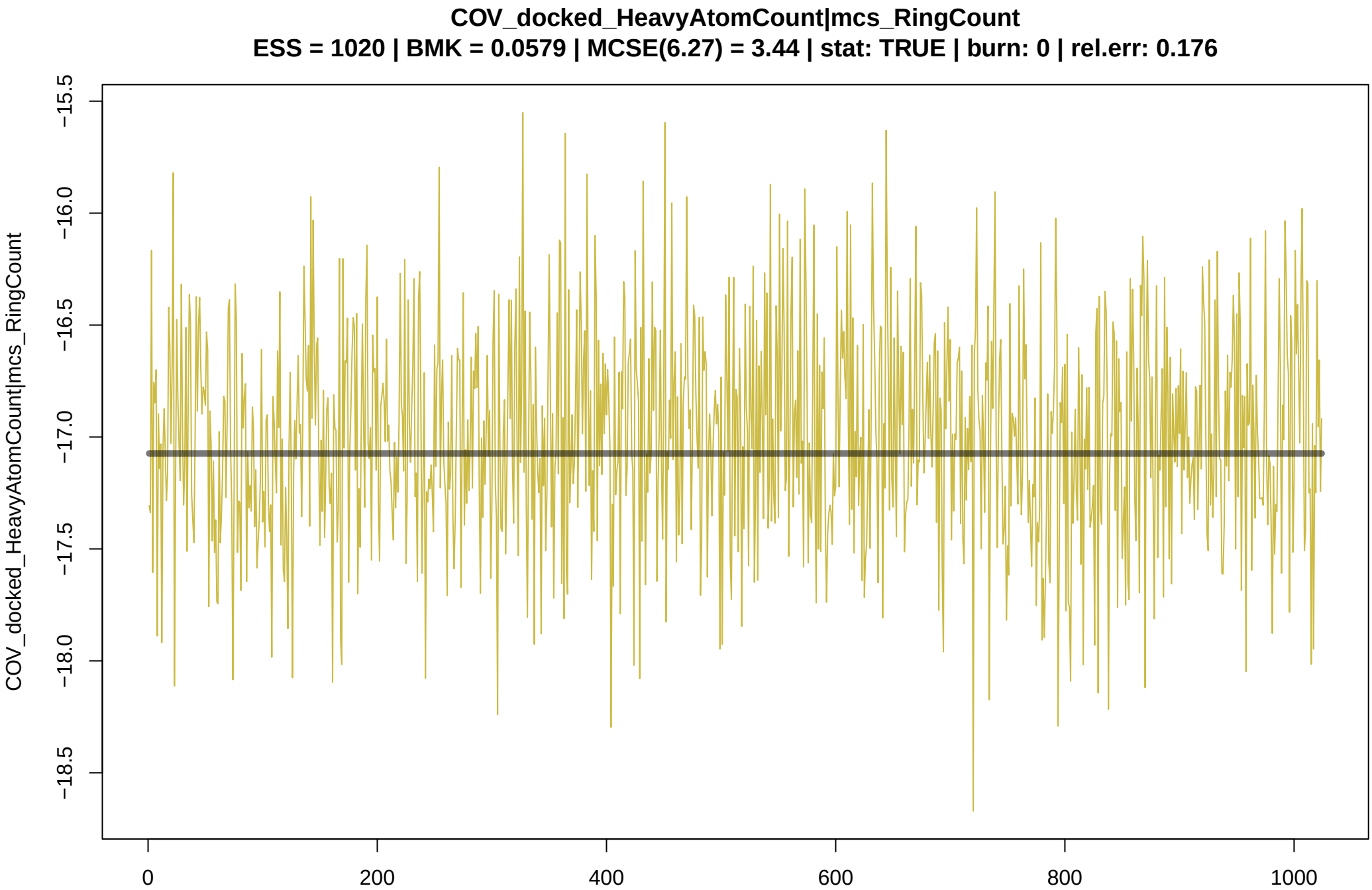

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.039 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0 | rel.err: −0.224
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−7.0
−7.5
−8.0
−8.5
0
200
400
600
800
1000

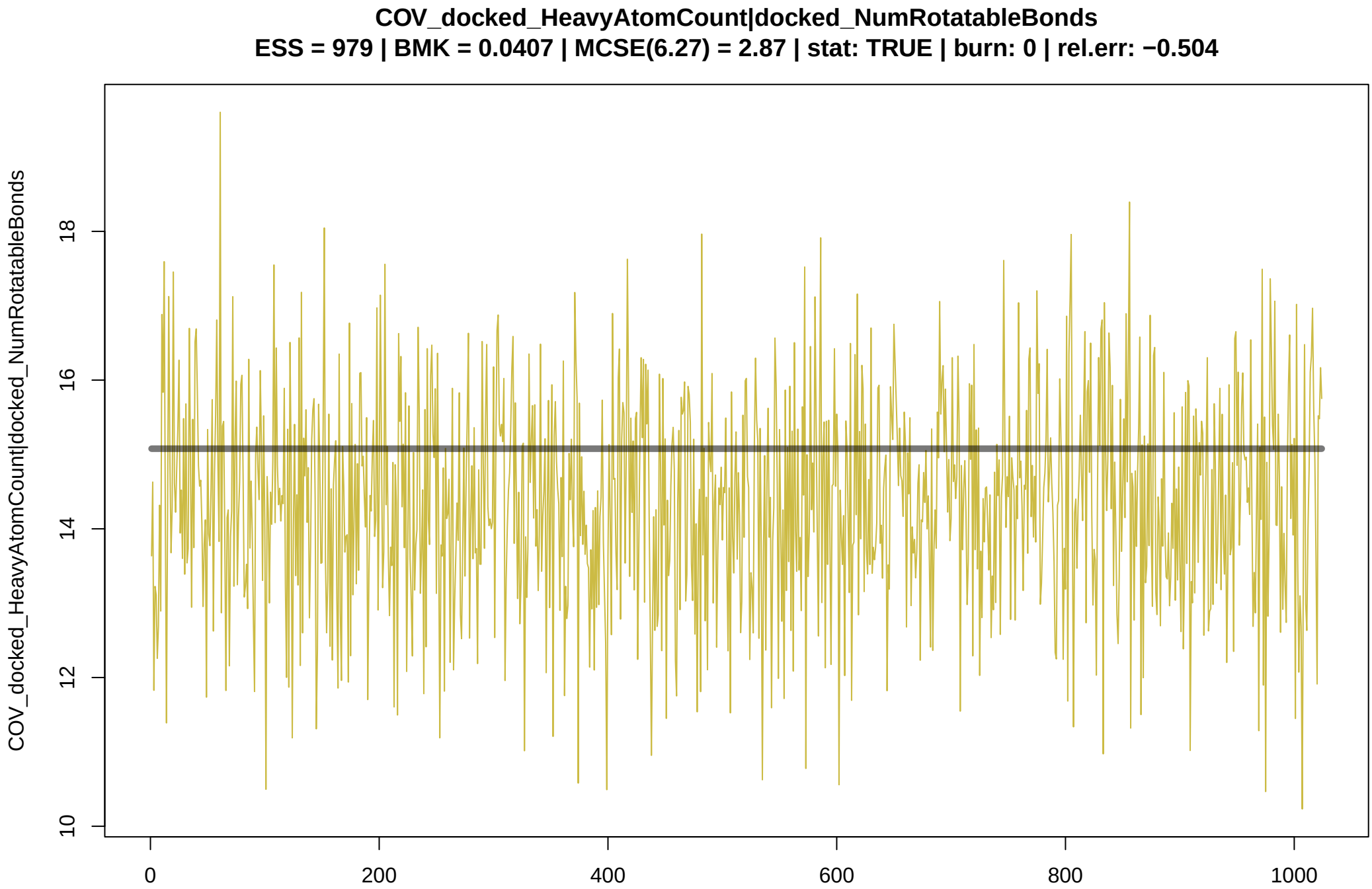

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0581 | MCSE(6.27) = 3.26 | stat: FALSE | burn: 0 | rel.err: 0.969
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−13.5
−14.0
−14.5
−15.0
−15.5
−16.0
−16.5
0
200
400
600
800
1000

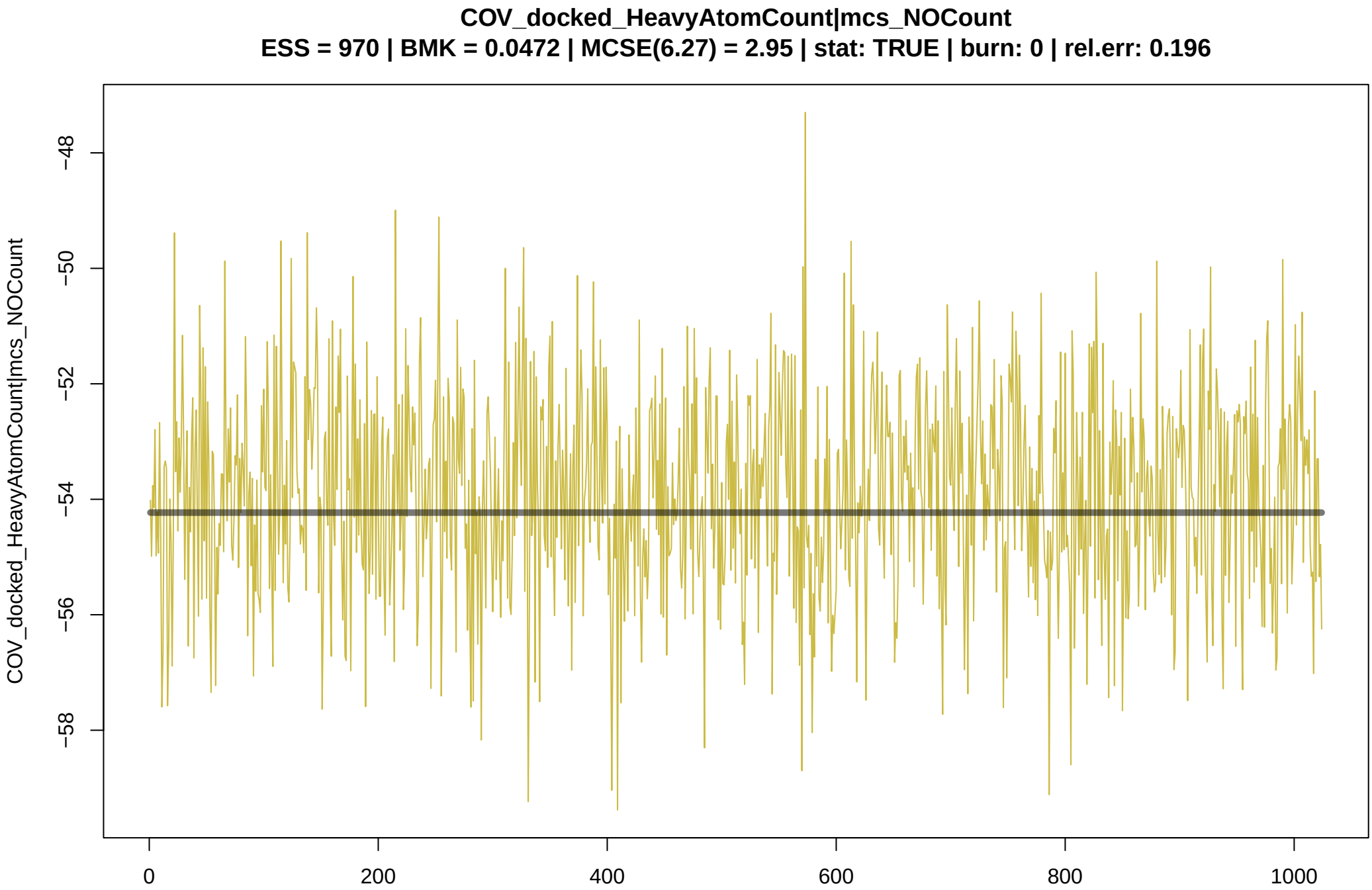

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0365 | MCSE(6.27) = 3.32 | stat: FALSE | burn: 0 | rel.err: 0.779
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.9
1.0
1.1
1.2
0
200
400
600
800
1000

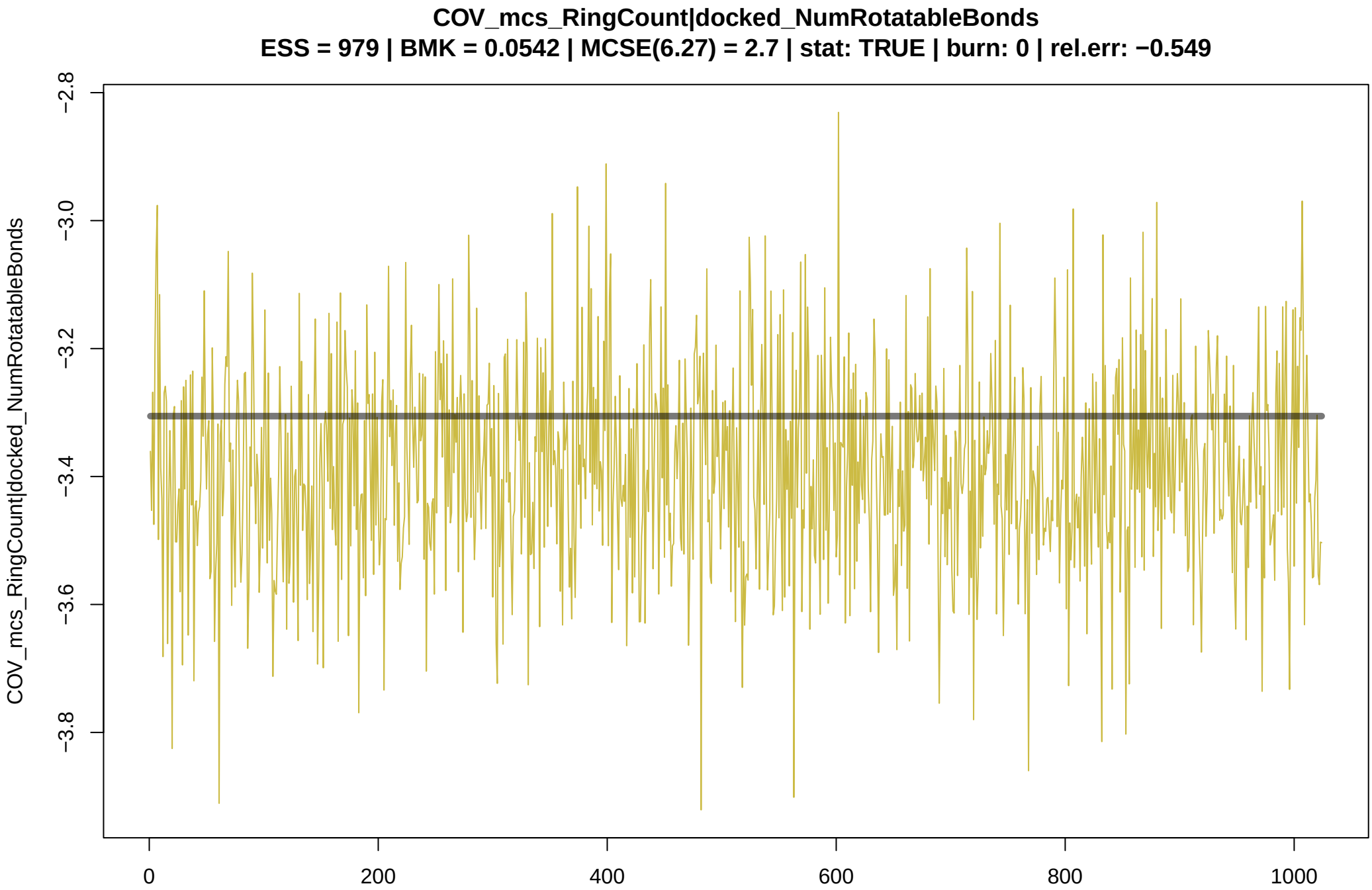

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 889 | BMK = 0.0586 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | rel.err: −0.25
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.6
−1.8
−2.0
−2.2
−2.4
0
200
400
600
800
1000

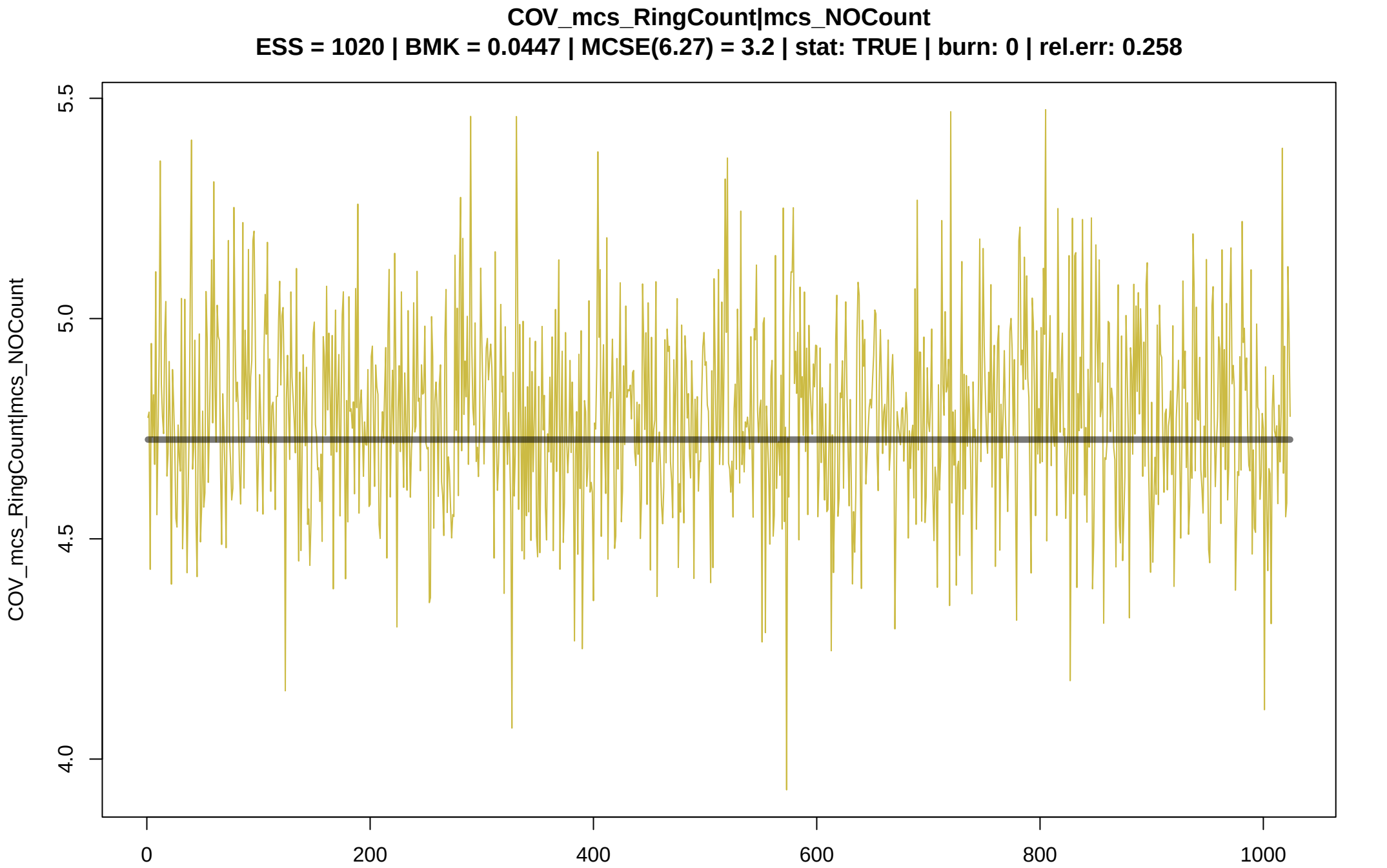

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0524 | MCSE(6.27) = 3.5 | stat: TRUE | burn: 0 | rel.err: 0.42
COV_mcs_NumHeteroAtoms|mcs_NOCount
5.0
4.5
4.0
0
200
400
600
800
1000

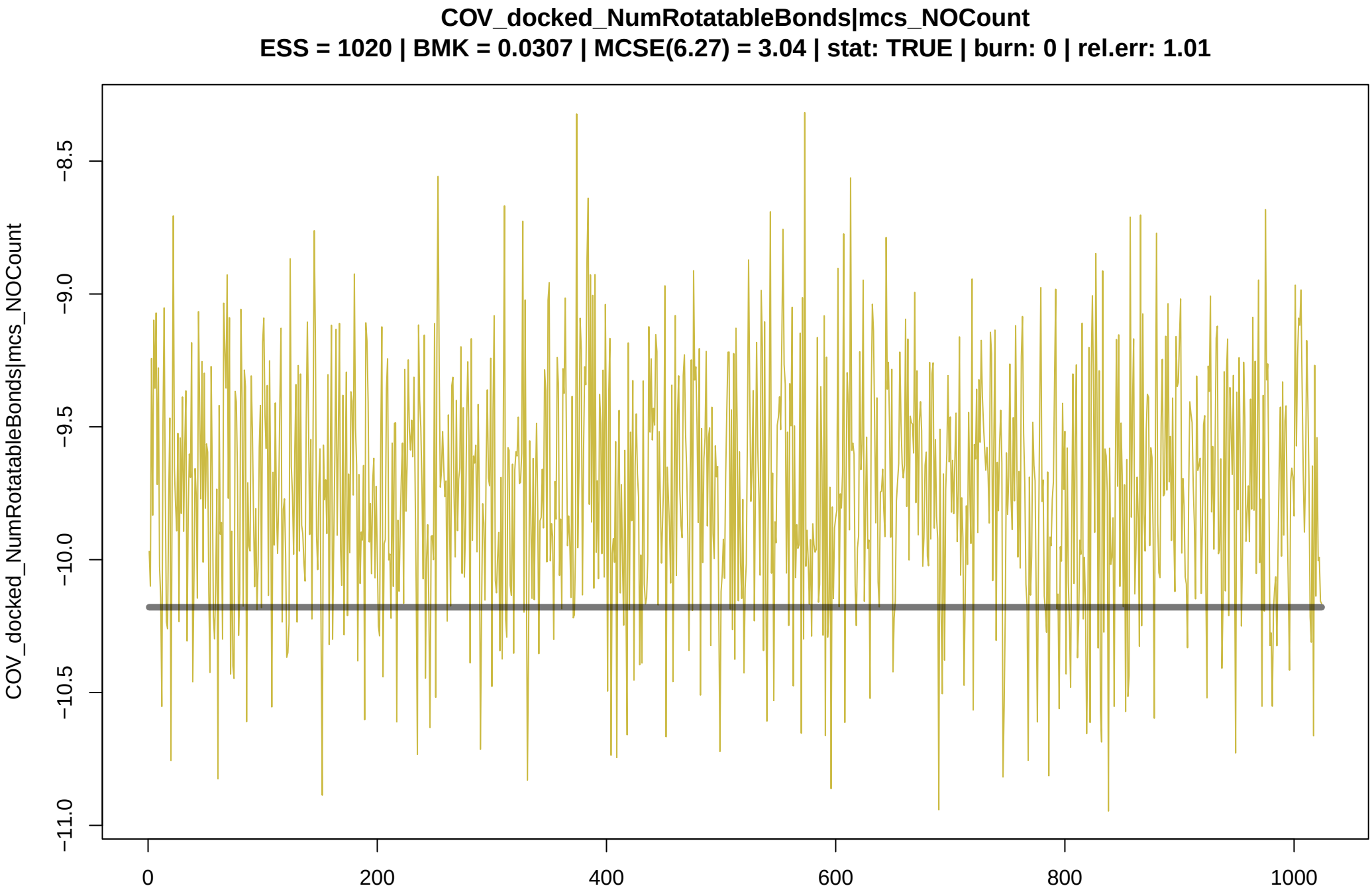

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0579 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | rel.err: 0.176
COV_docked_HeavyAtomCount|mcs_RingCount
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 979 | BMK = 0.0407 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0 | rel.err: −0.504
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 970 | BMK = 0.0472 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: 0.196
COV_docked_HeavyAtomCount|mcs_NOCount
−48
−50
−52
−54
−56
−58
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 979 | BMK = 0.0542 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | rel.err: −0.549
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 = 0.0447 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: 0.258
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 = 0.0307 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: 1.01
COV_docked_NumRotatableBonds|mcs_NOCount
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
0
200
400
600
800
1000