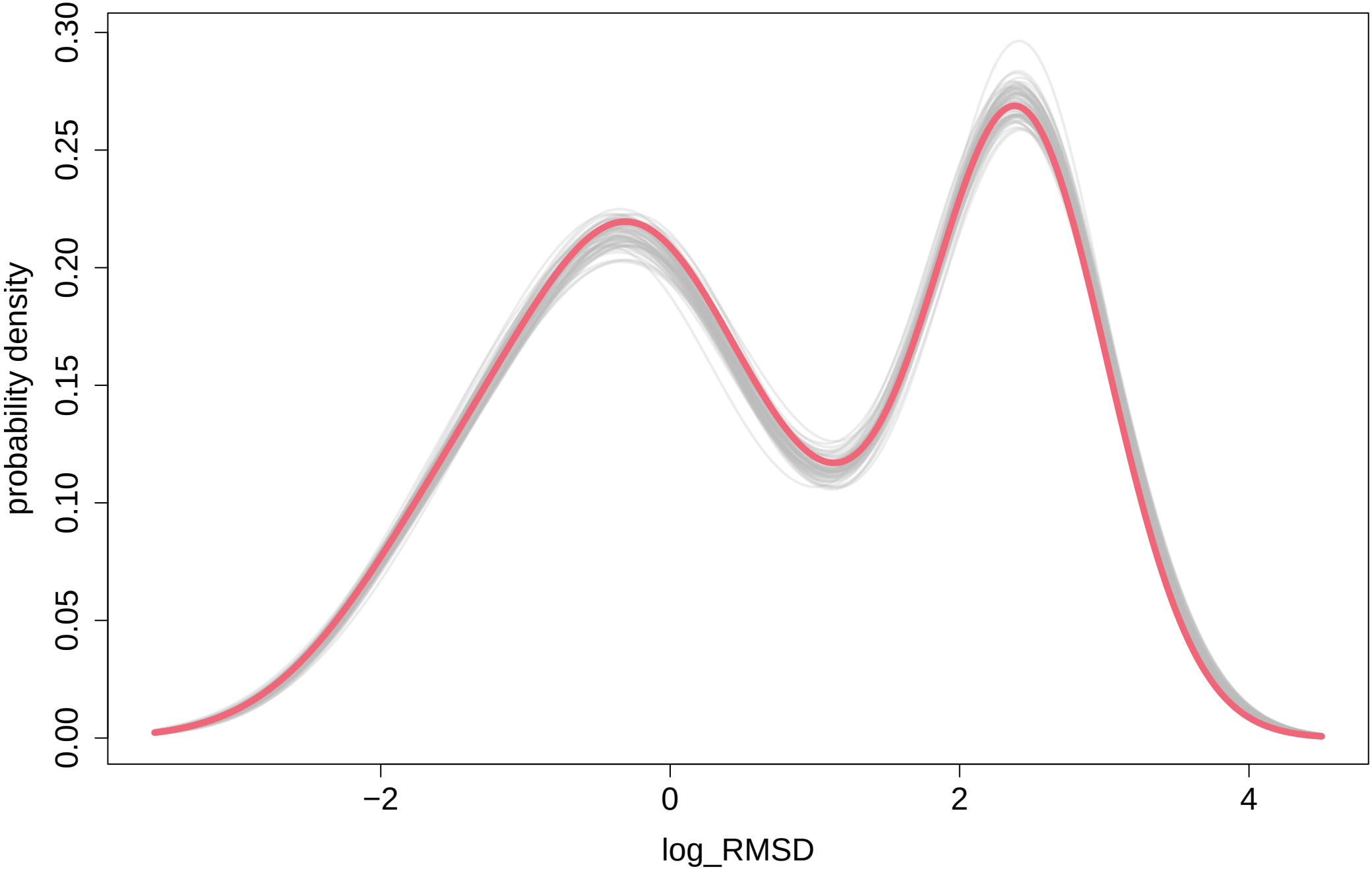
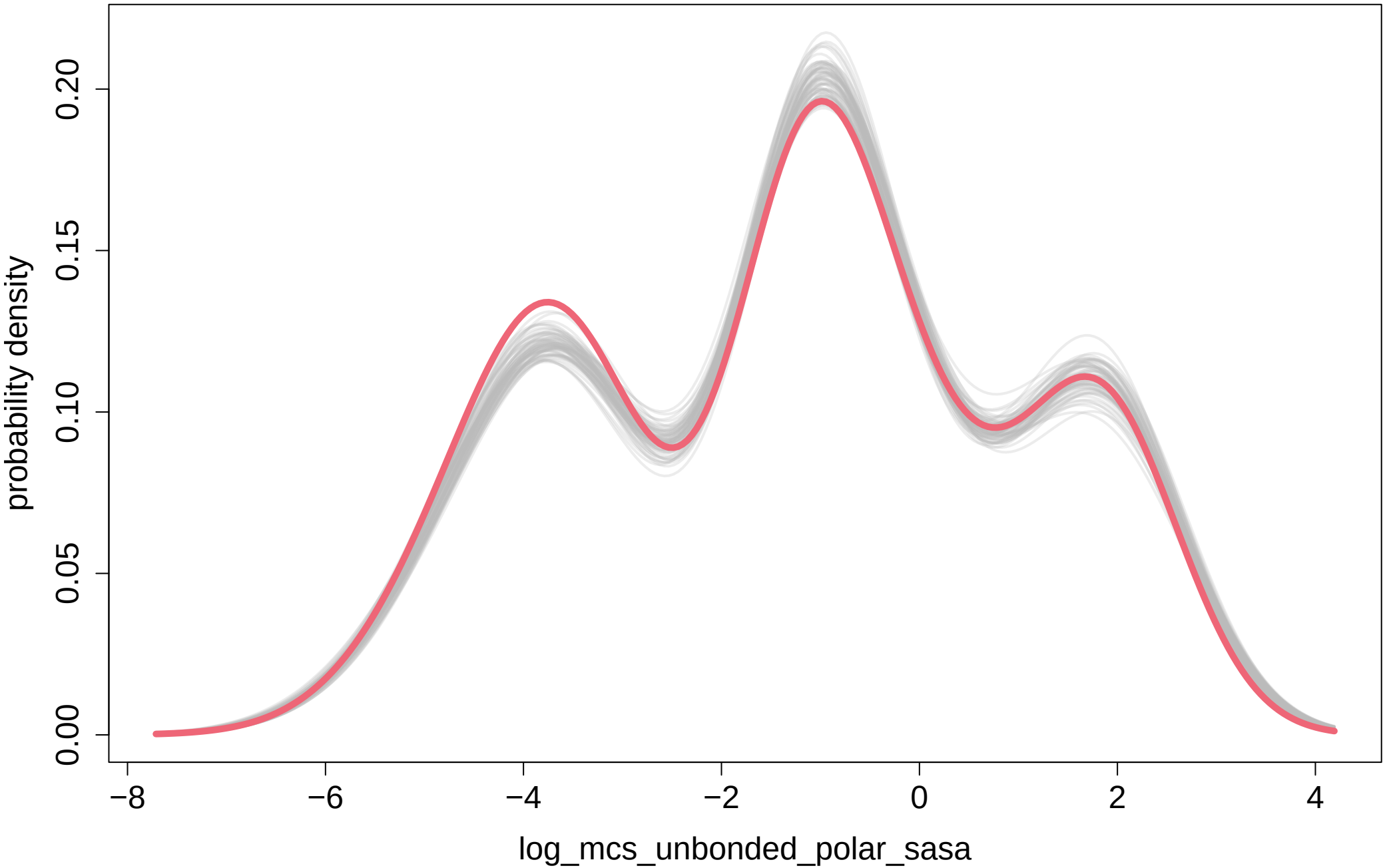
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.571254366282458
max MCSE = 10.776423512619
all stationary: FALSE
burn: 816
max rel.err.: 1.2693051932364

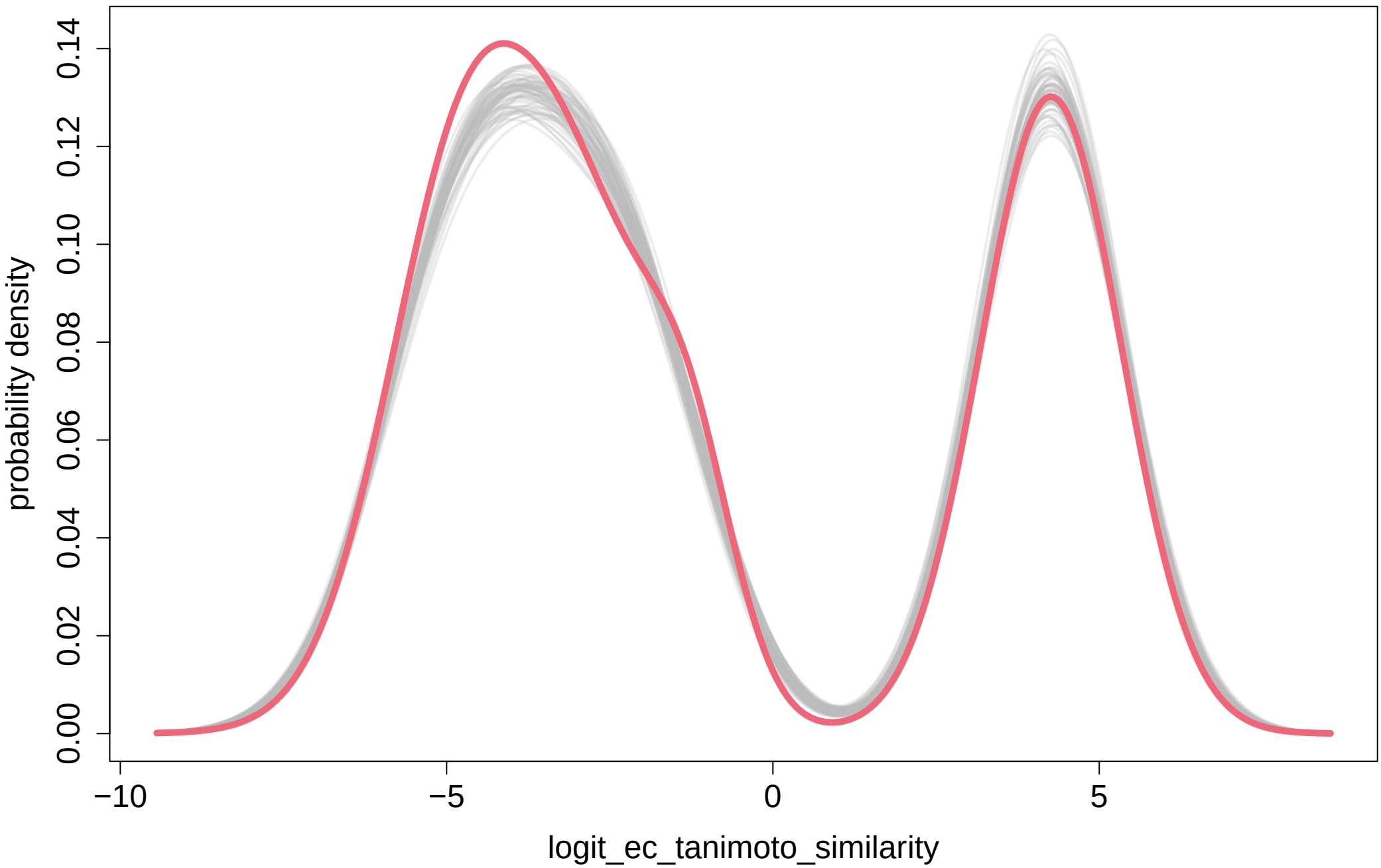
−− STATS 2D −−
min ESS = 727.342781379631
max BMK = 0.095438795550170 1
max MCSE = 3.7225805344764
all stationary: FALSE
burn: 0
max rel.err.: 2.1190290279689 3

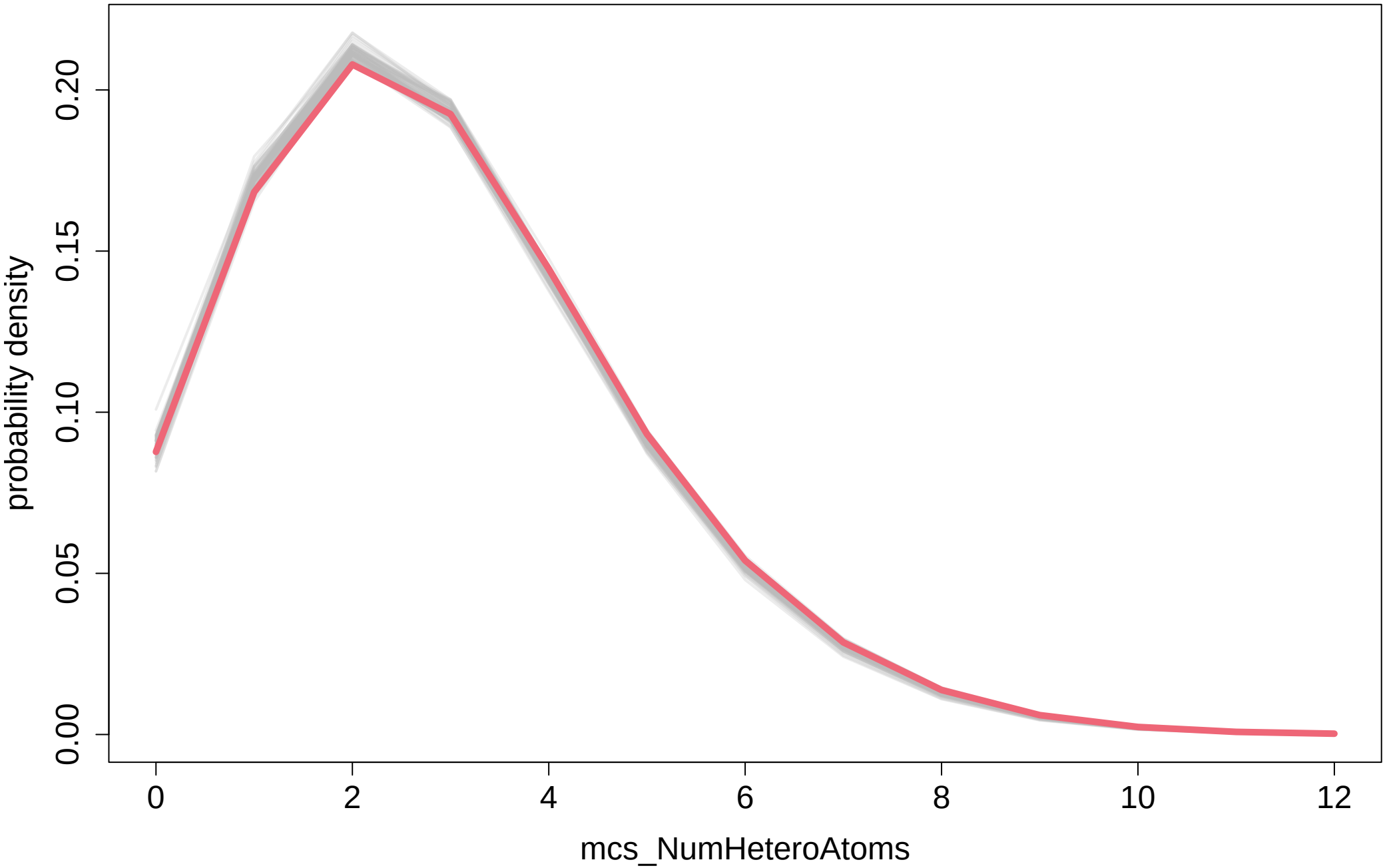
−− STATS 1D −−
min ESS = 33.0921407266511
max BMK = 0.200719489956277
max MCSE = 8.9762233291897
all stationary: FALSE
burn: 0
max rel.err.: 2.73473580460135

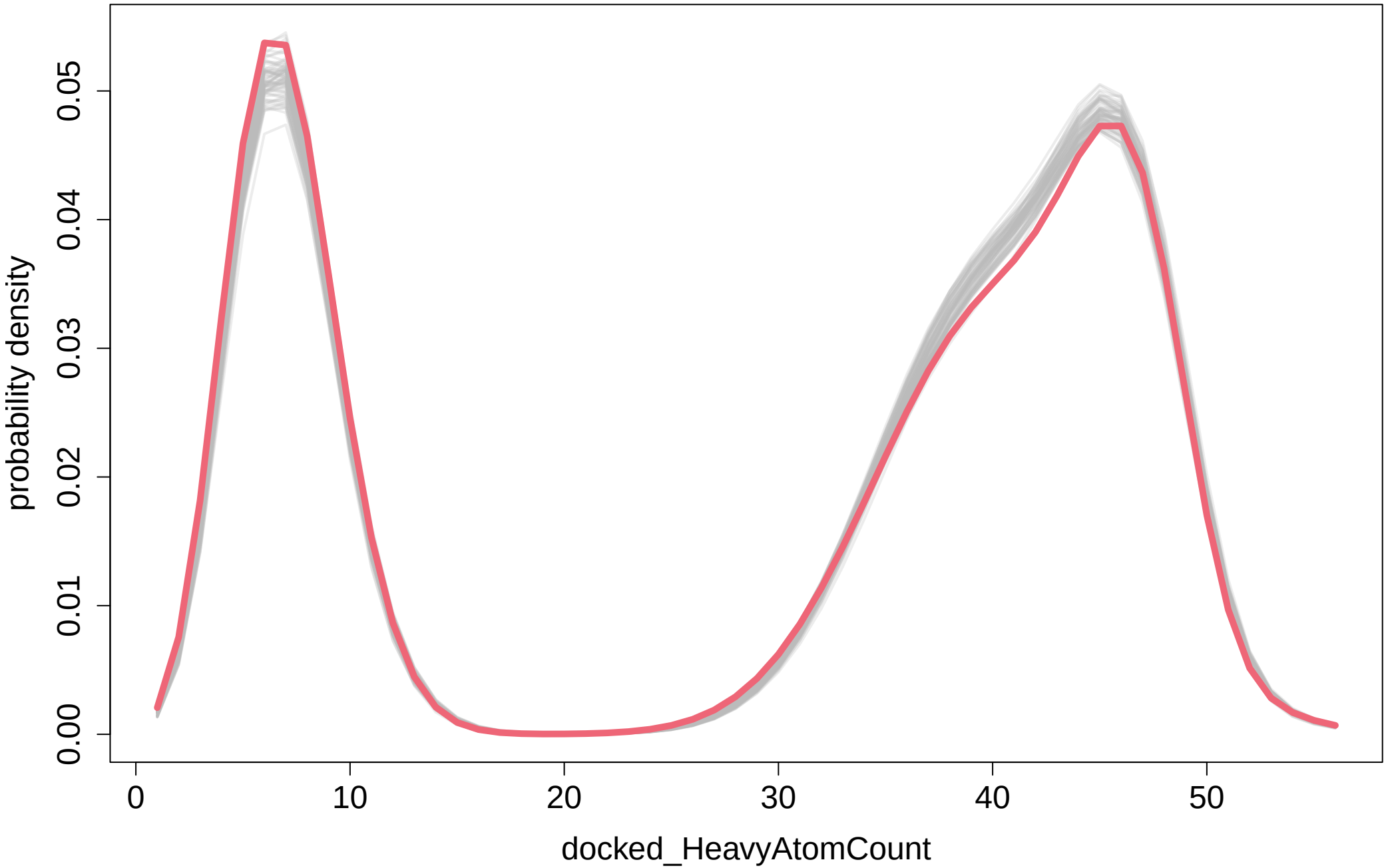
Occupied clusters: 9 of 64
LL: −62500 +− 12.9

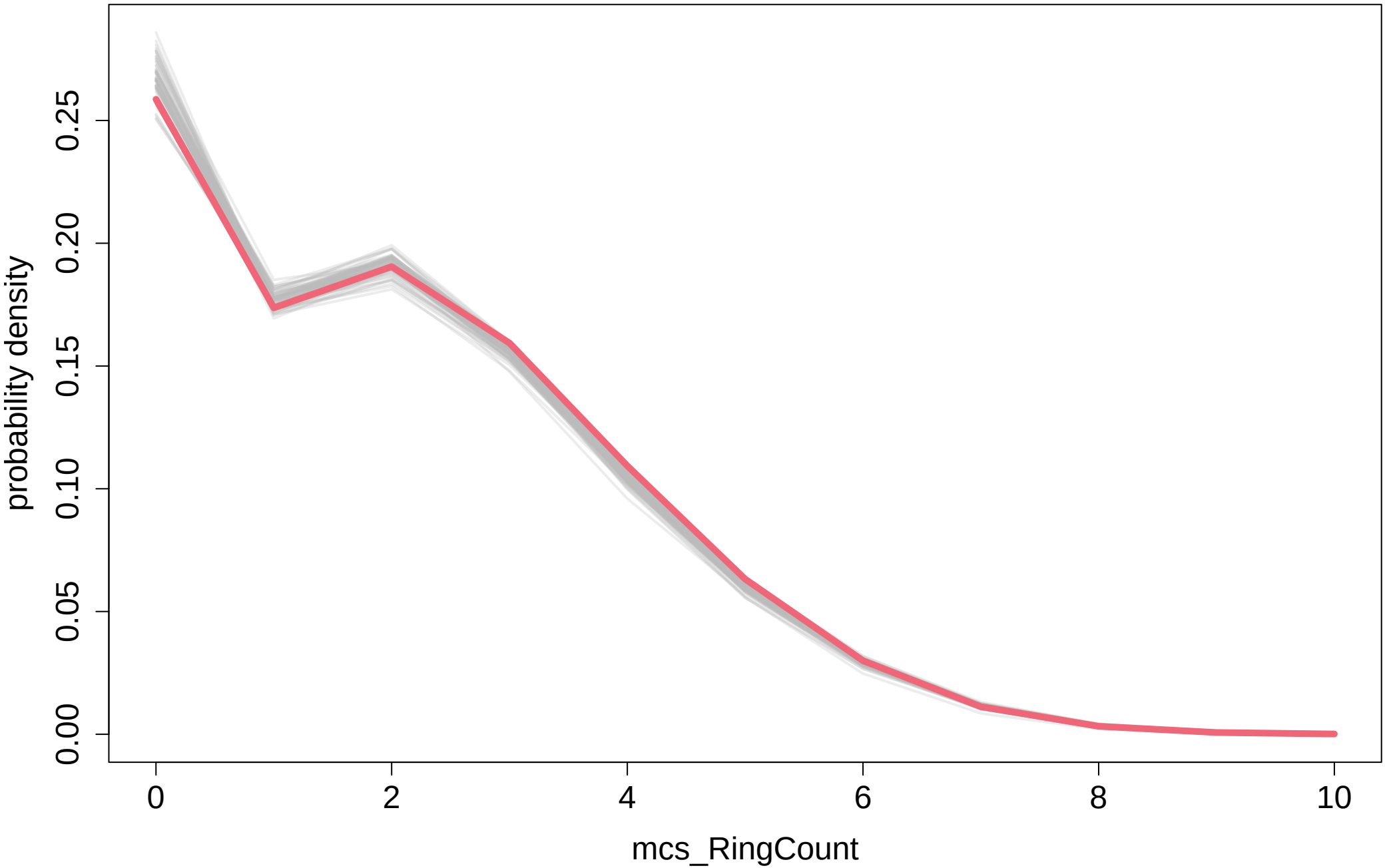

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−2
0
2
4
log_RMSD

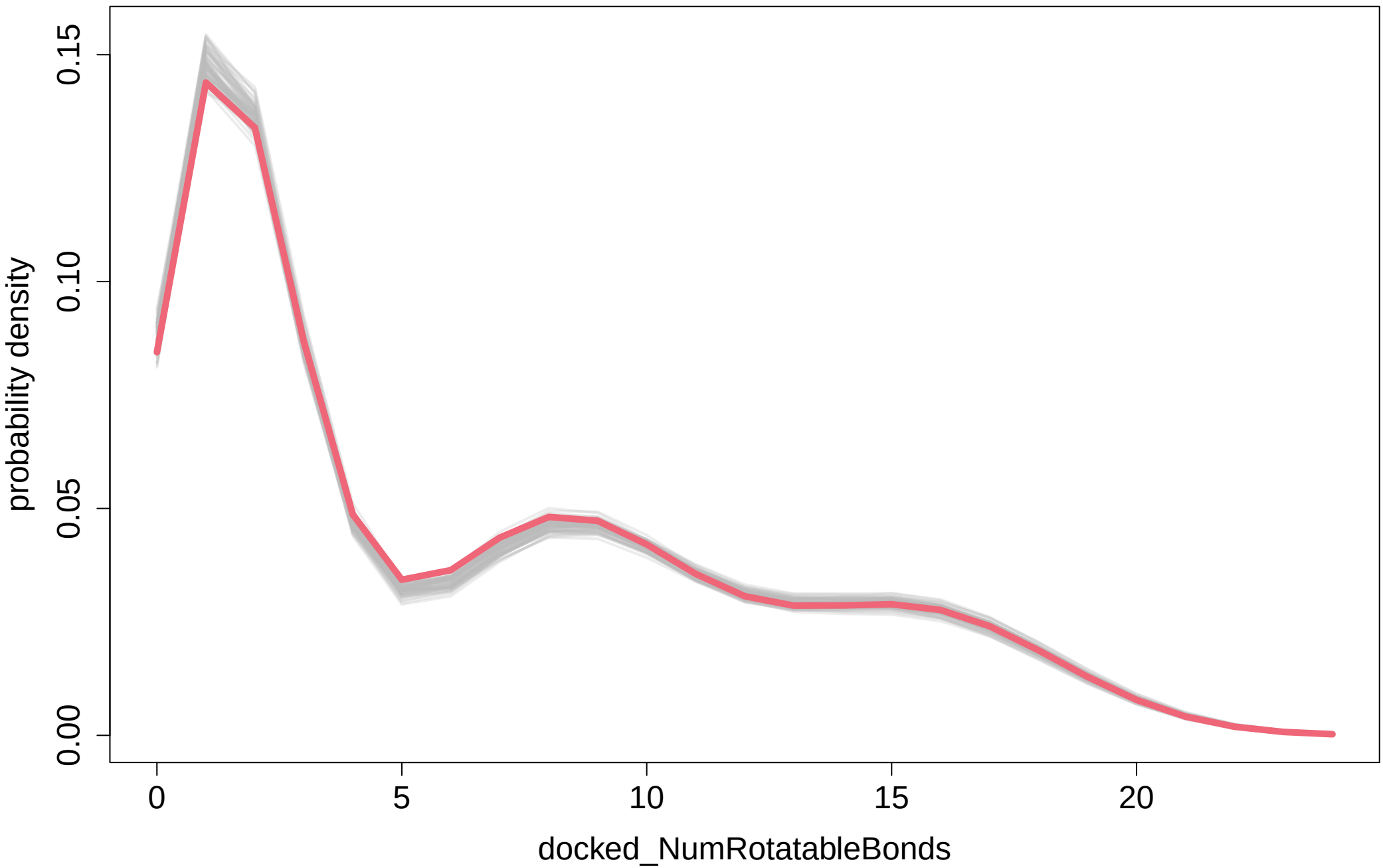

probability density
0.00
0.05
0.10
0.15
0.20
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

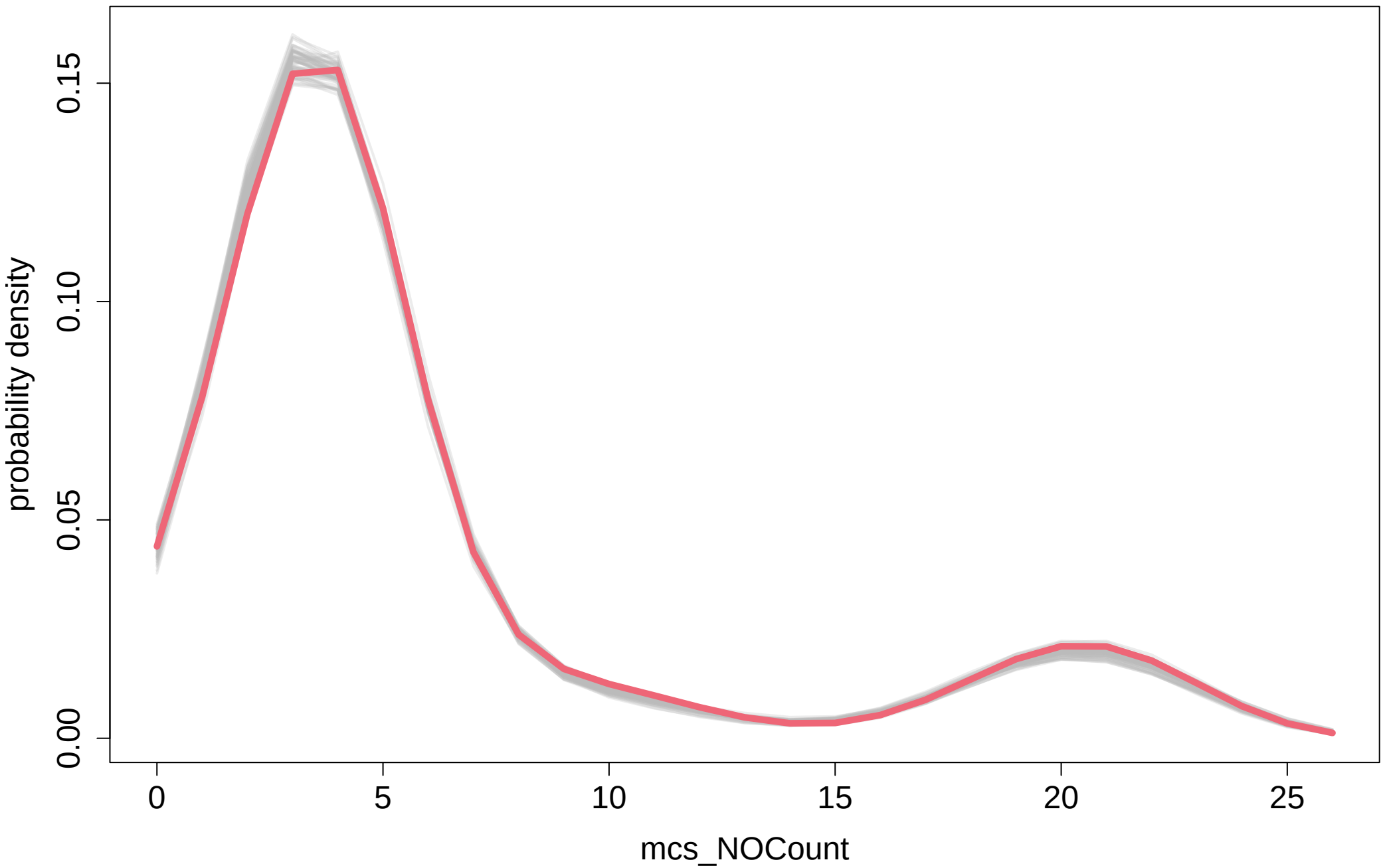

probability density
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
−10
−5
0
5
logit_ec_tanimoto_similarity

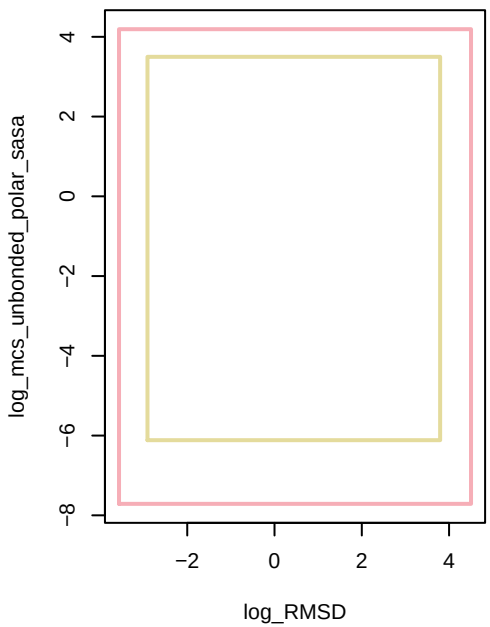

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms

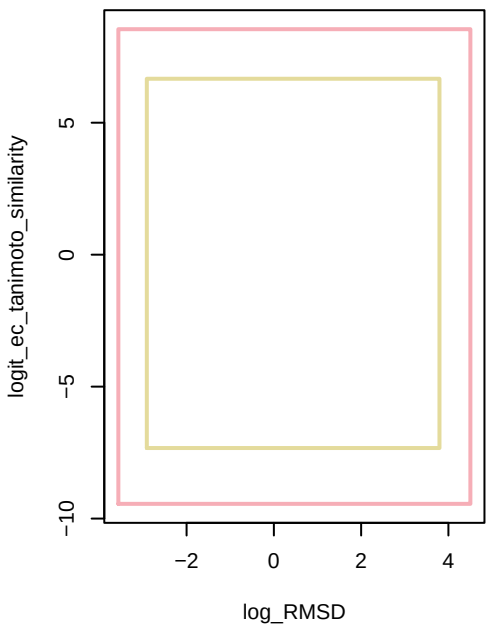

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount

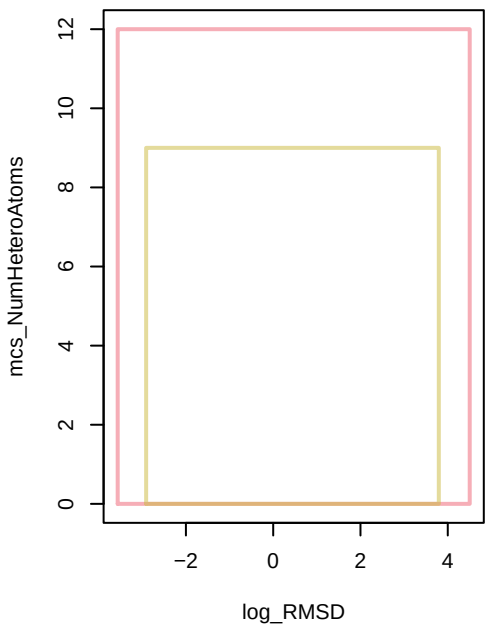

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount

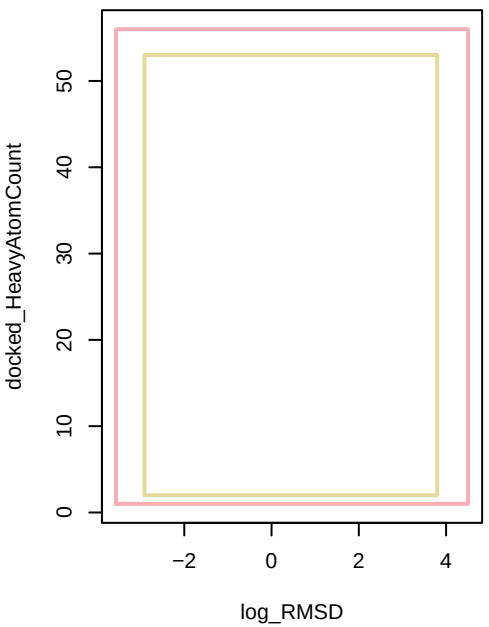

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
docked_NumRotatableBonds

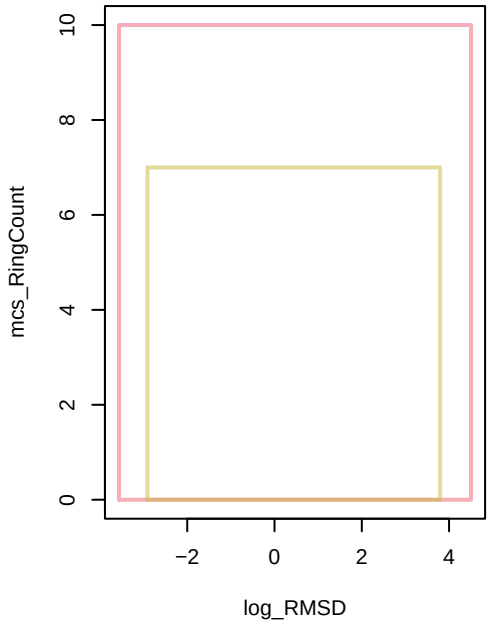

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

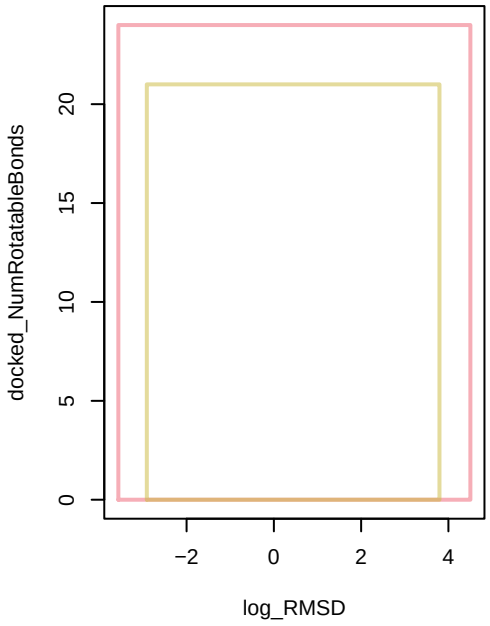

log_mcs_unbonded_polar_sasa
log_RMSD

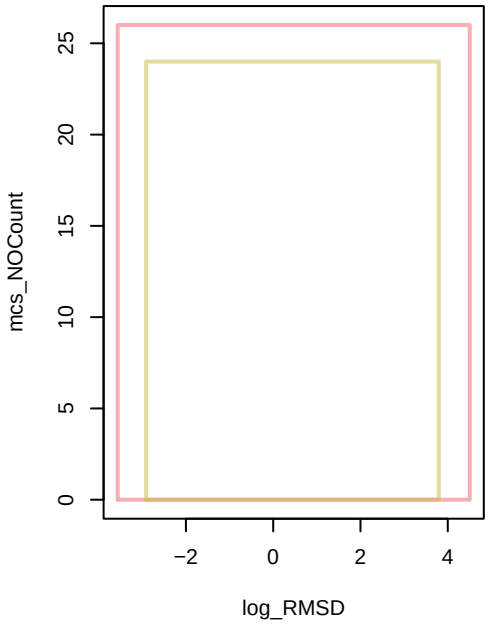

logit_ec_tanimoto_similarity
log_RMSD

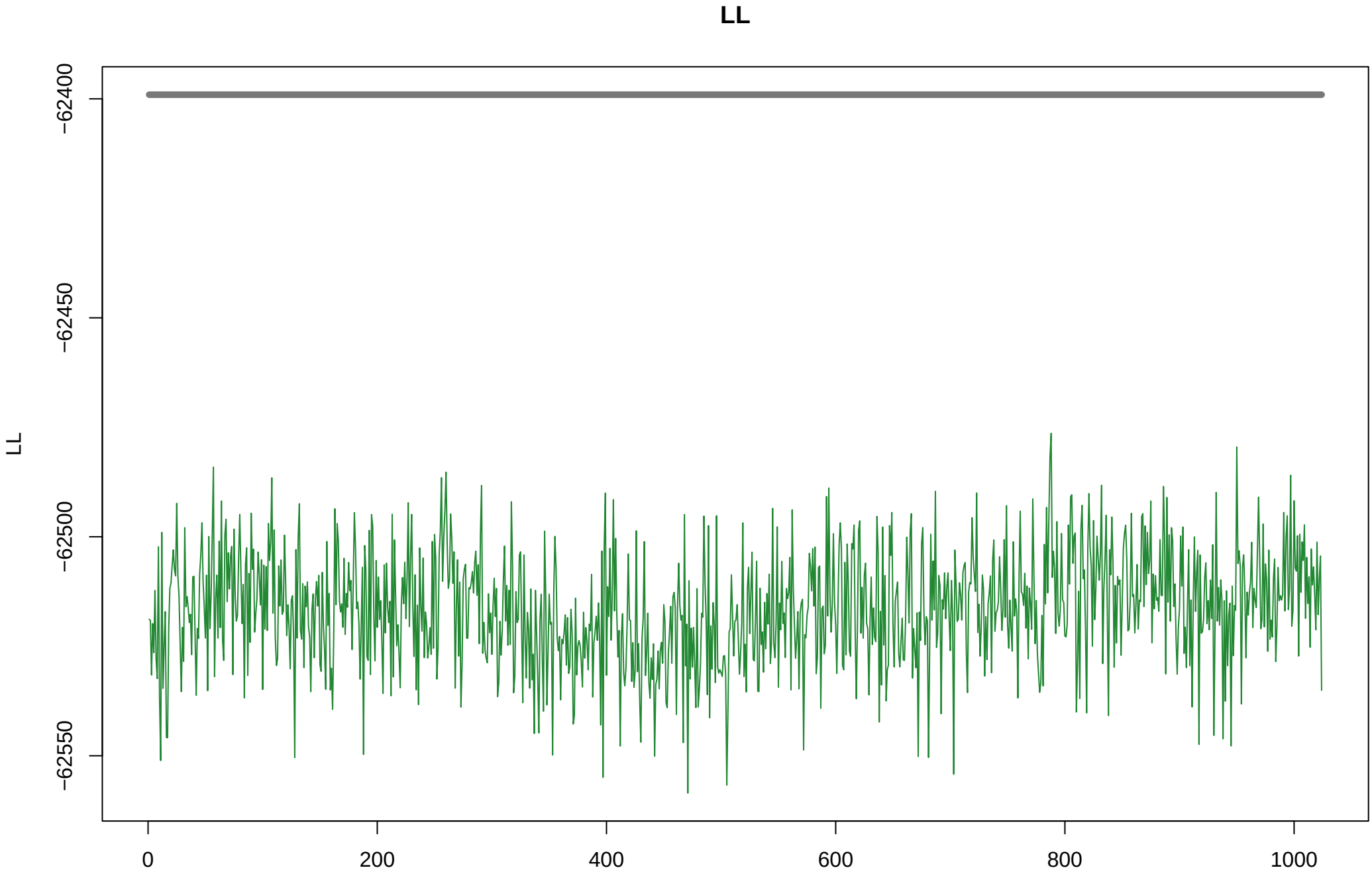

mcs_NumHeteroAtoms
log_RMSD

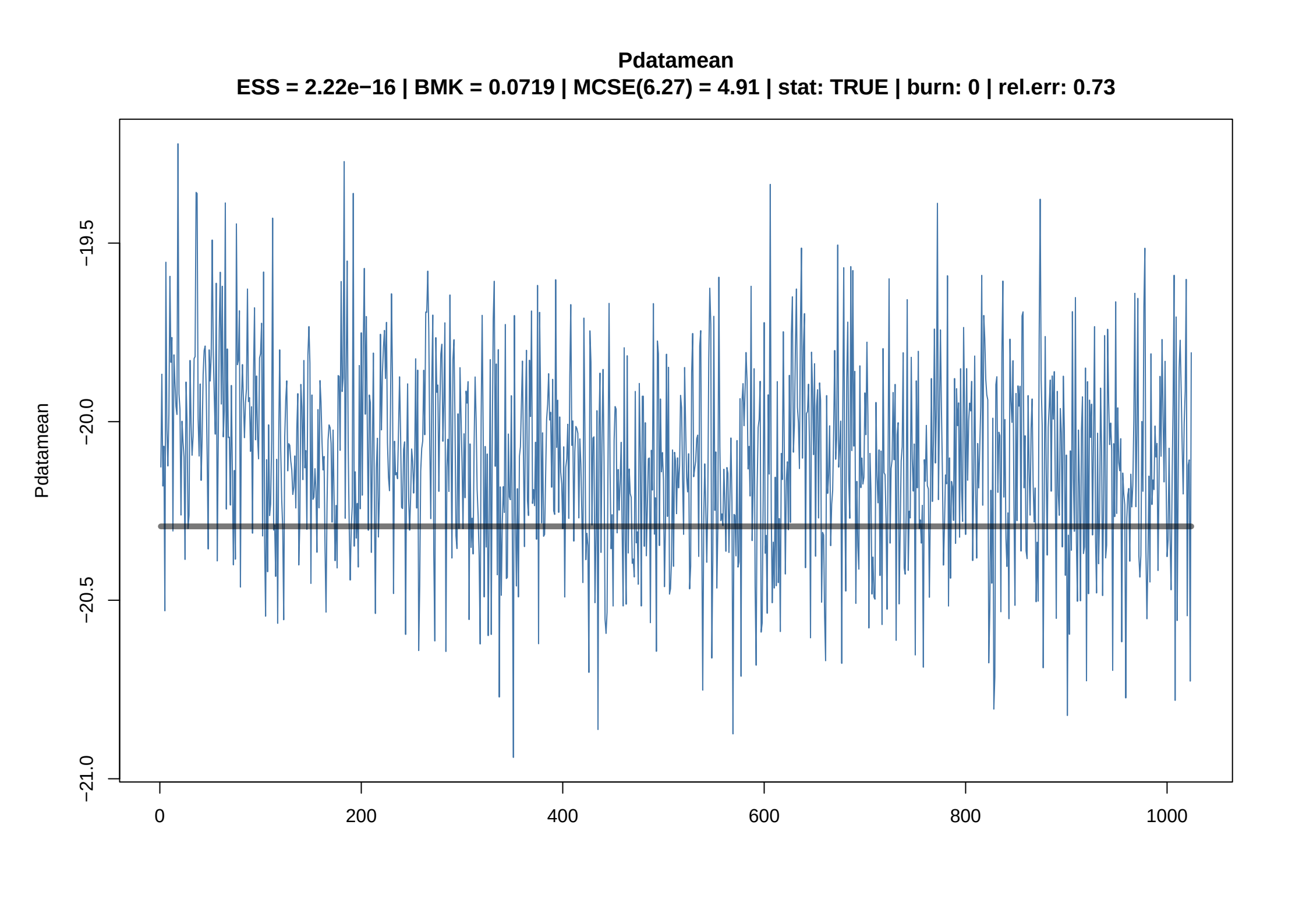

docked_HeavyAtomCount
log_RMSD

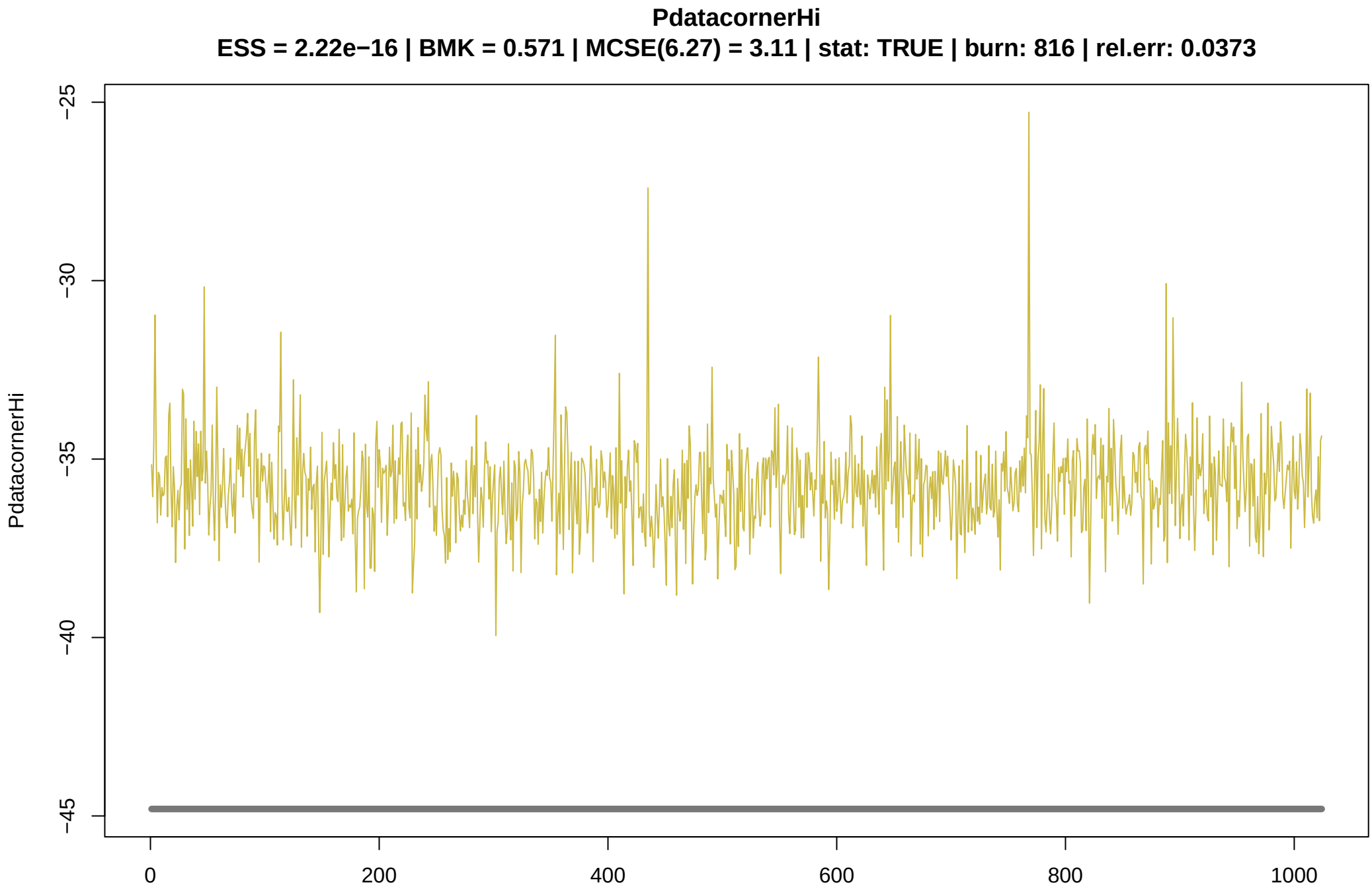

mcs_RingCount
log_RMSD

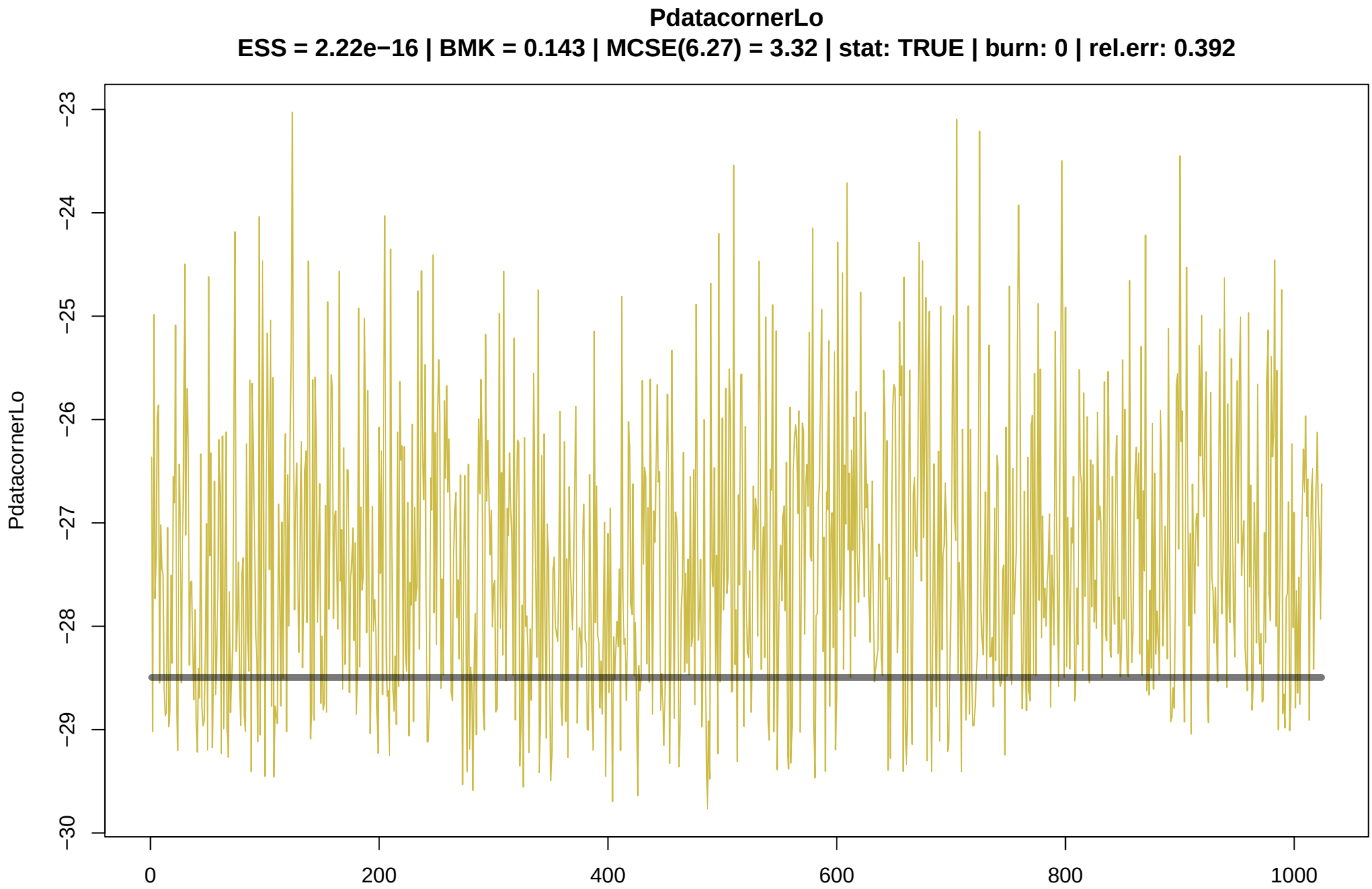

docked_NumRotatableBonds
log_RMSD

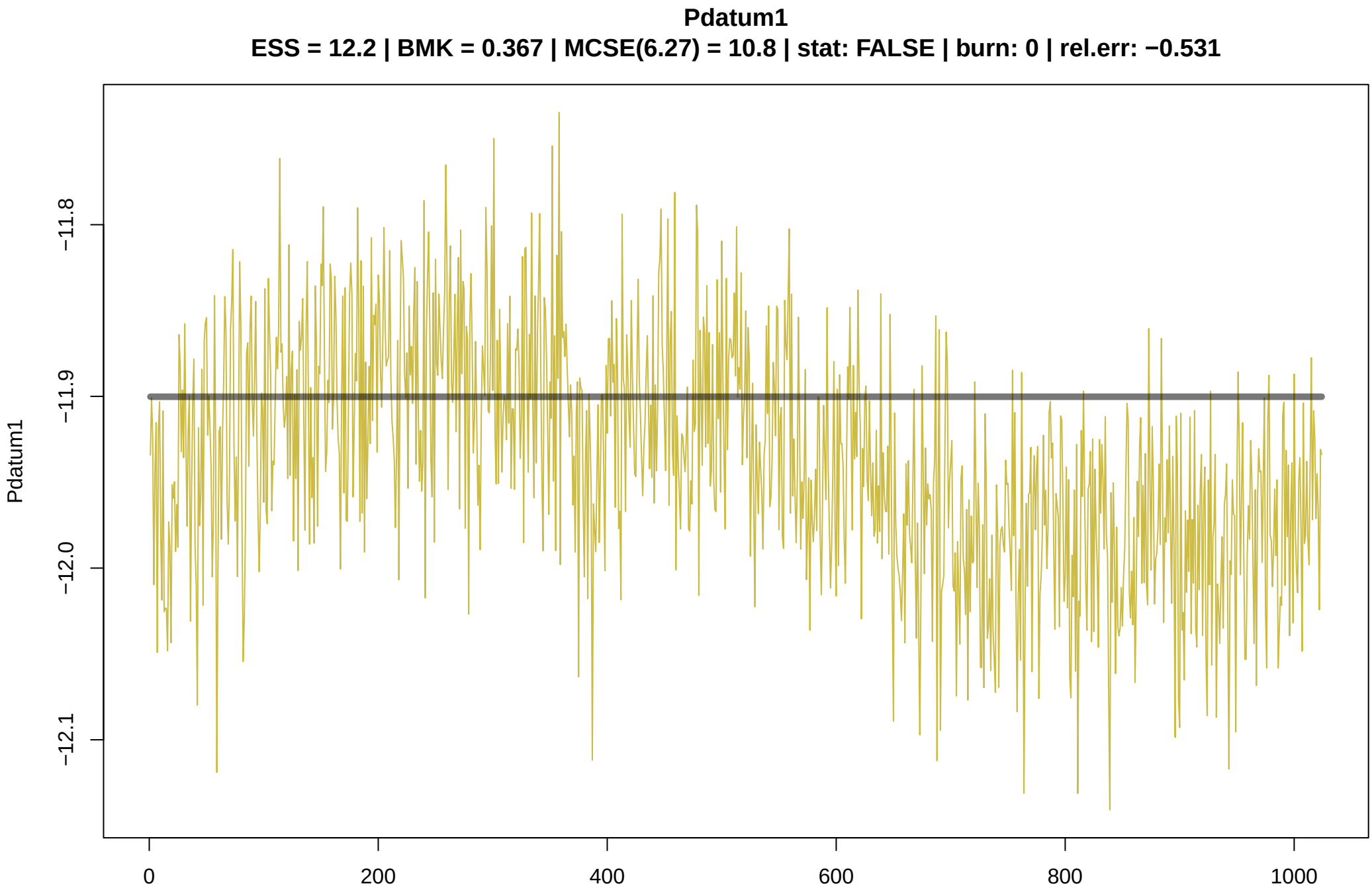

mcs_NOCount
log_RMSD

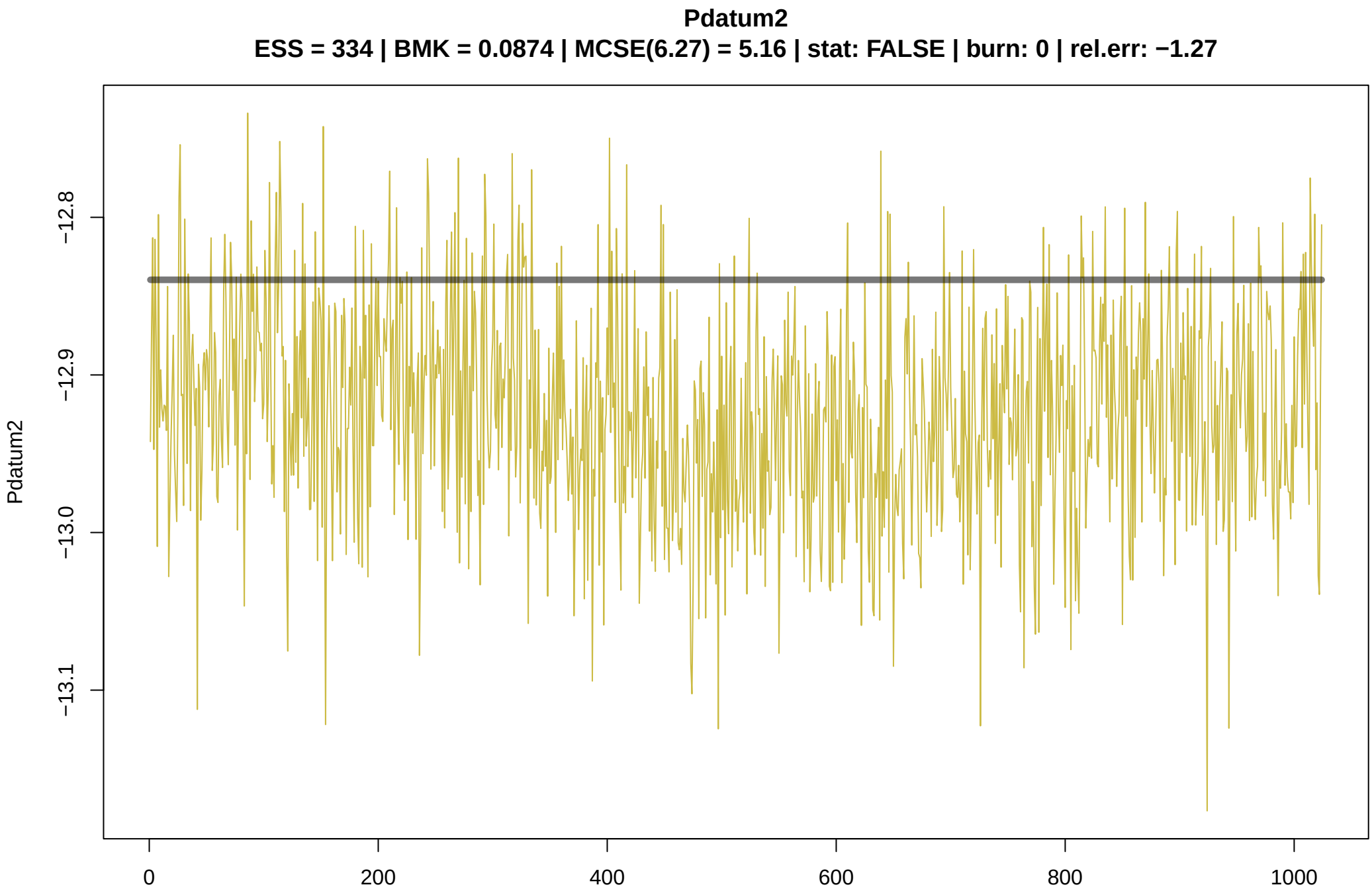

LL
LL
−62400
−62450
−62500
−62550
0
200
400
600
800
1000

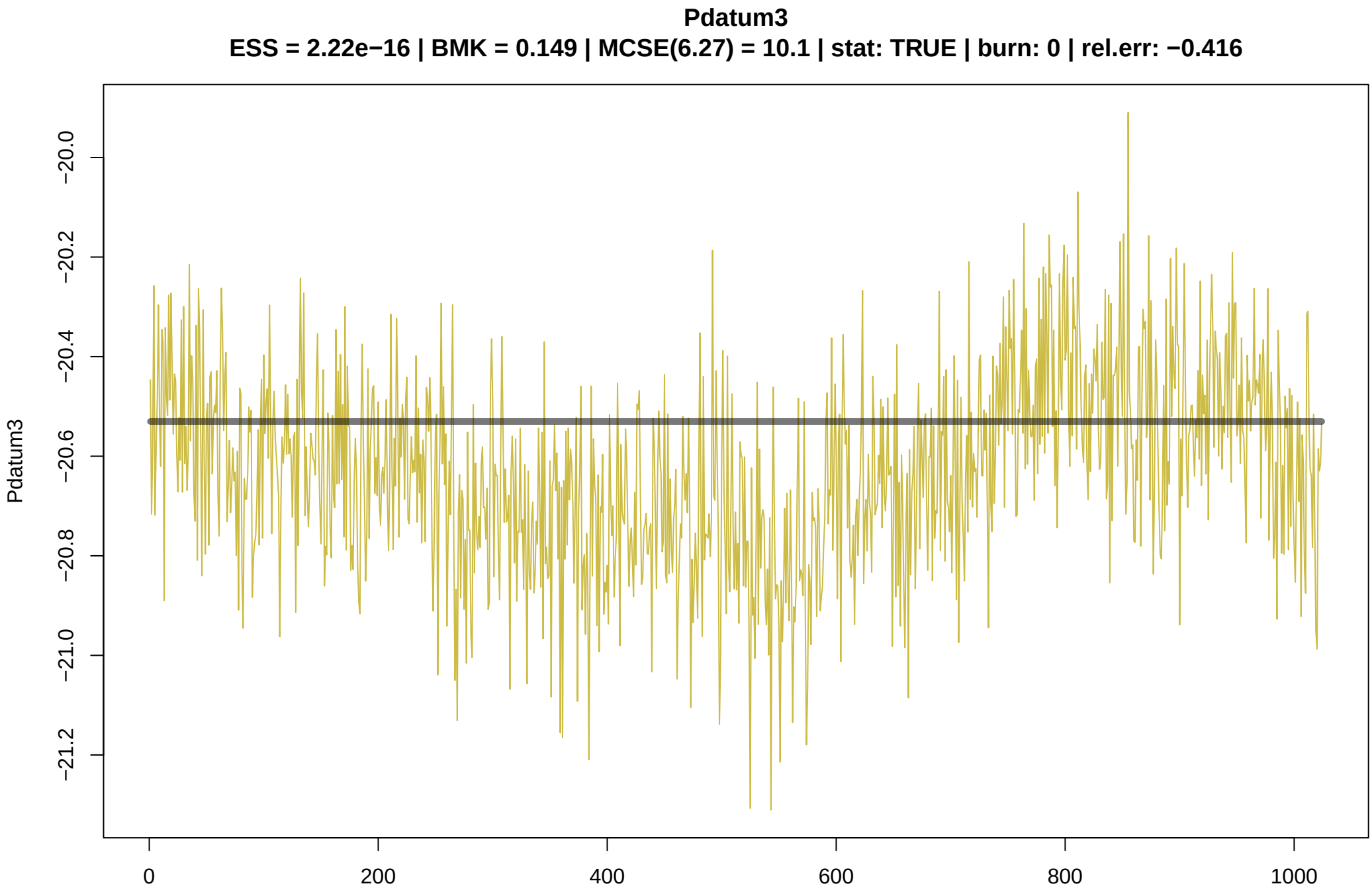

Pdatamean
ESS = 2.22e−16 | BMK = 0.0719 | MCSE(6.27) = 4.91 | stat: TRUE | burn: 0 | rel.err: 0.73
Pdatamean
−19.5
−20.0
−20.5
−21.0
0
200
400
600
800
1000

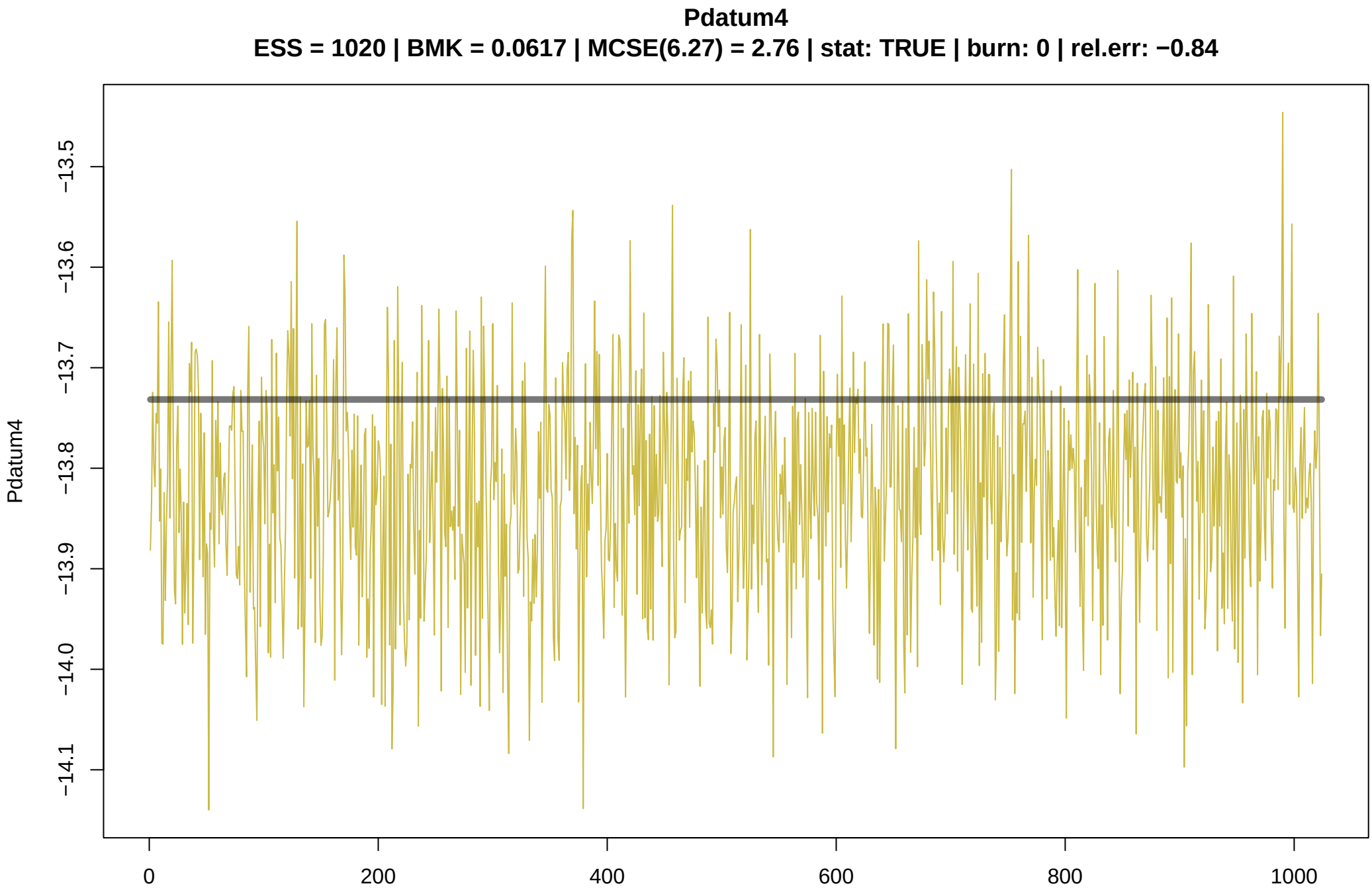

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.571 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 816 | rel.err: 0.0373
PdatacornerHi
−25
−30
−35
−40
−45
0
200
400
600
800
1000

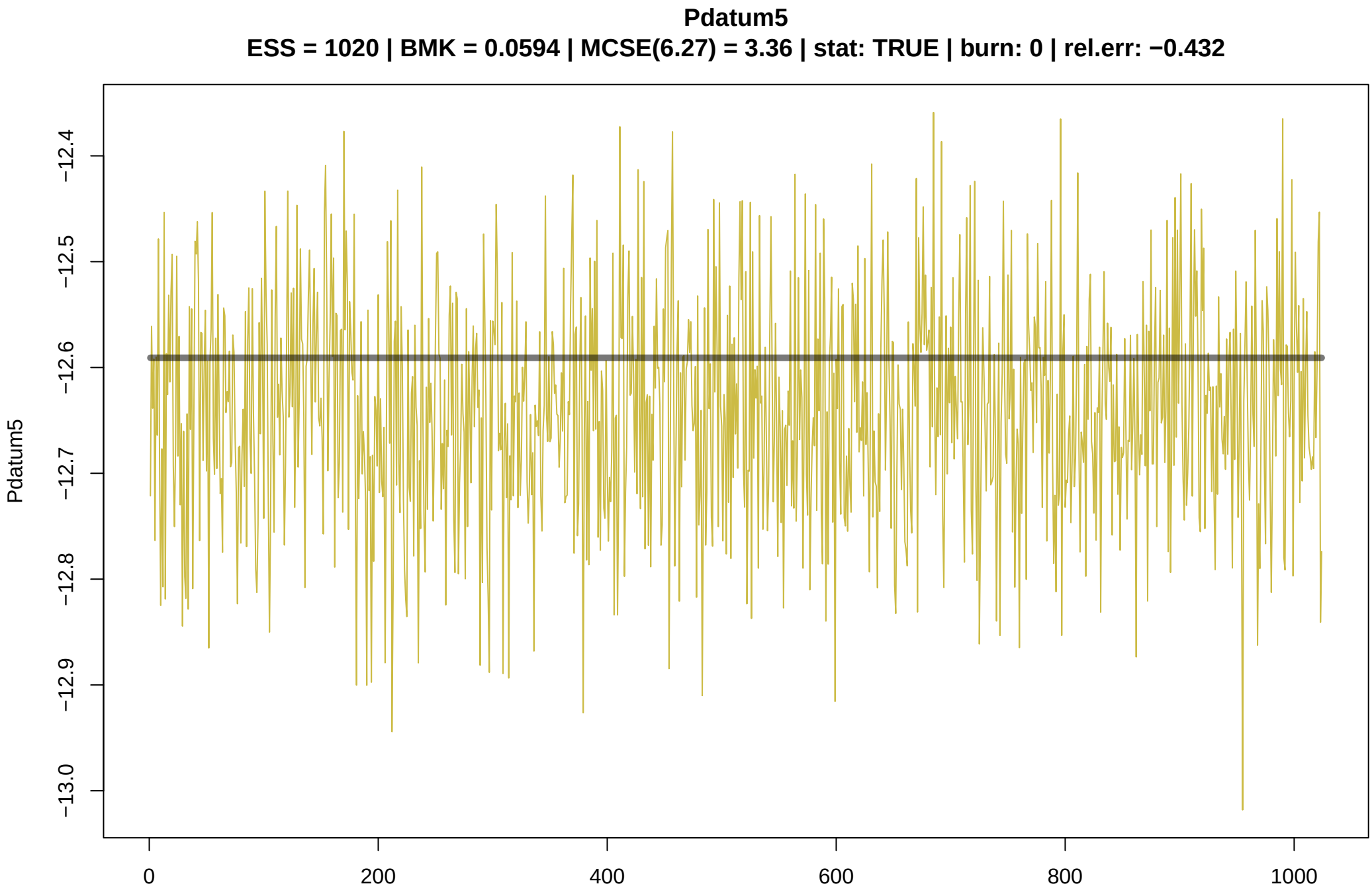

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.143 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0 | rel.err: 0.392
PdatacornerLo
−23
−24
−25
−26
−27
−28
−29
−30
0
200
400
600
800
1000

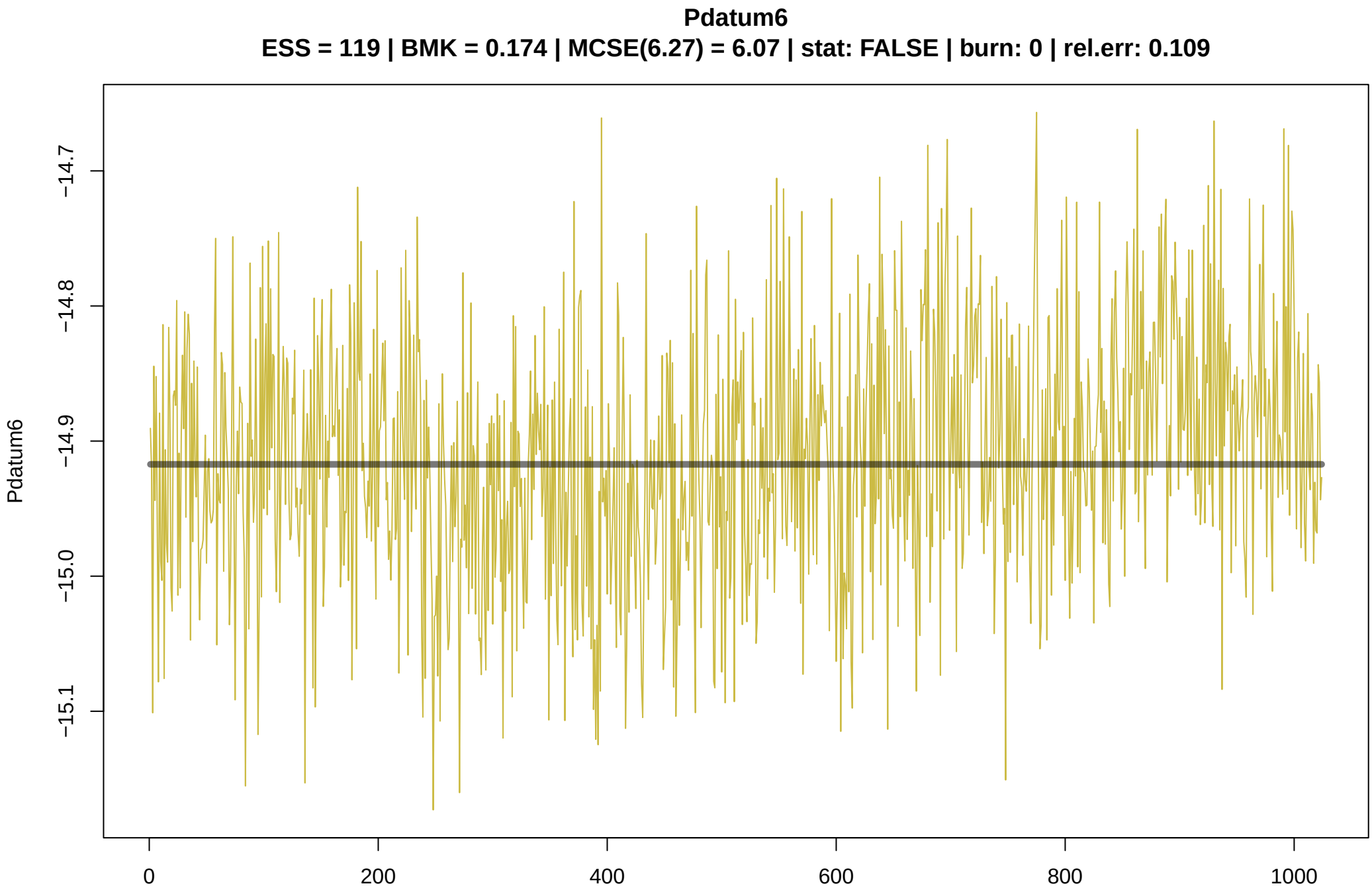

Pdatum1
ESS = 12.2 | BMK = 0.367 | MCSE(6.27) = 10.8 | stat: FALSE | burn: 0 | rel.err: −0.531
Pdatum1
−11.8
−11.9
−12.0
−12.1
0
200
400
600
800
1000

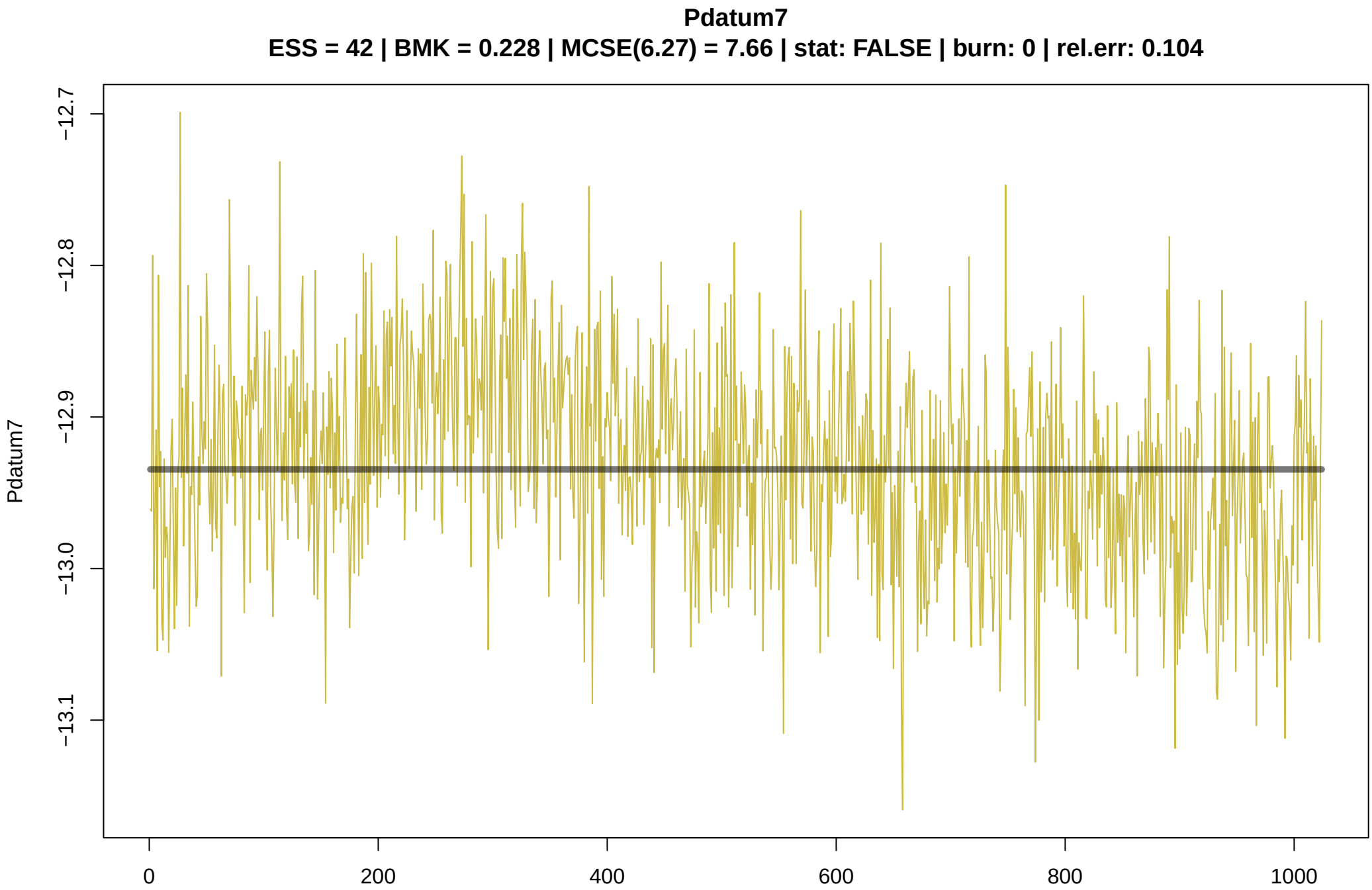

Pdatum2
ESS = 334 | BMK = 0.0874 | MCSE(6.27) = 5.16 | stat: FALSE | burn: 0 | rel.err: −1.27
Pdatum2
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

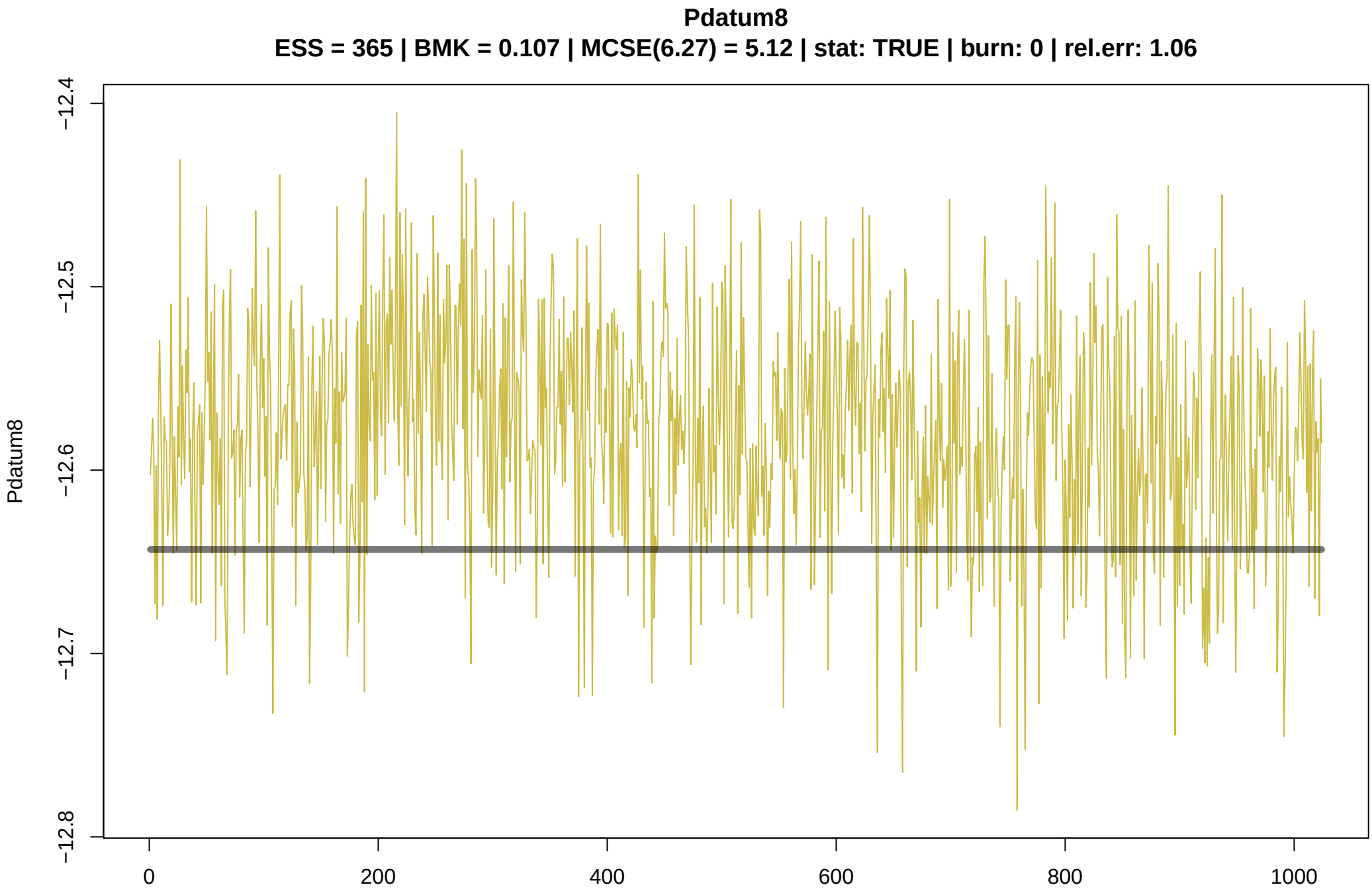

Pdatum3
ESS = 2.22e−16 | BMK = 0.149 | MCSE(6.27) = 10.1 | stat: TRUE | burn: 0 | rel.err: −0.416
Pdatum3
−20.0
−20.2
−20.4
−20.6
−20.8
−21.0
−21.2
0
200
400
600
800
1000

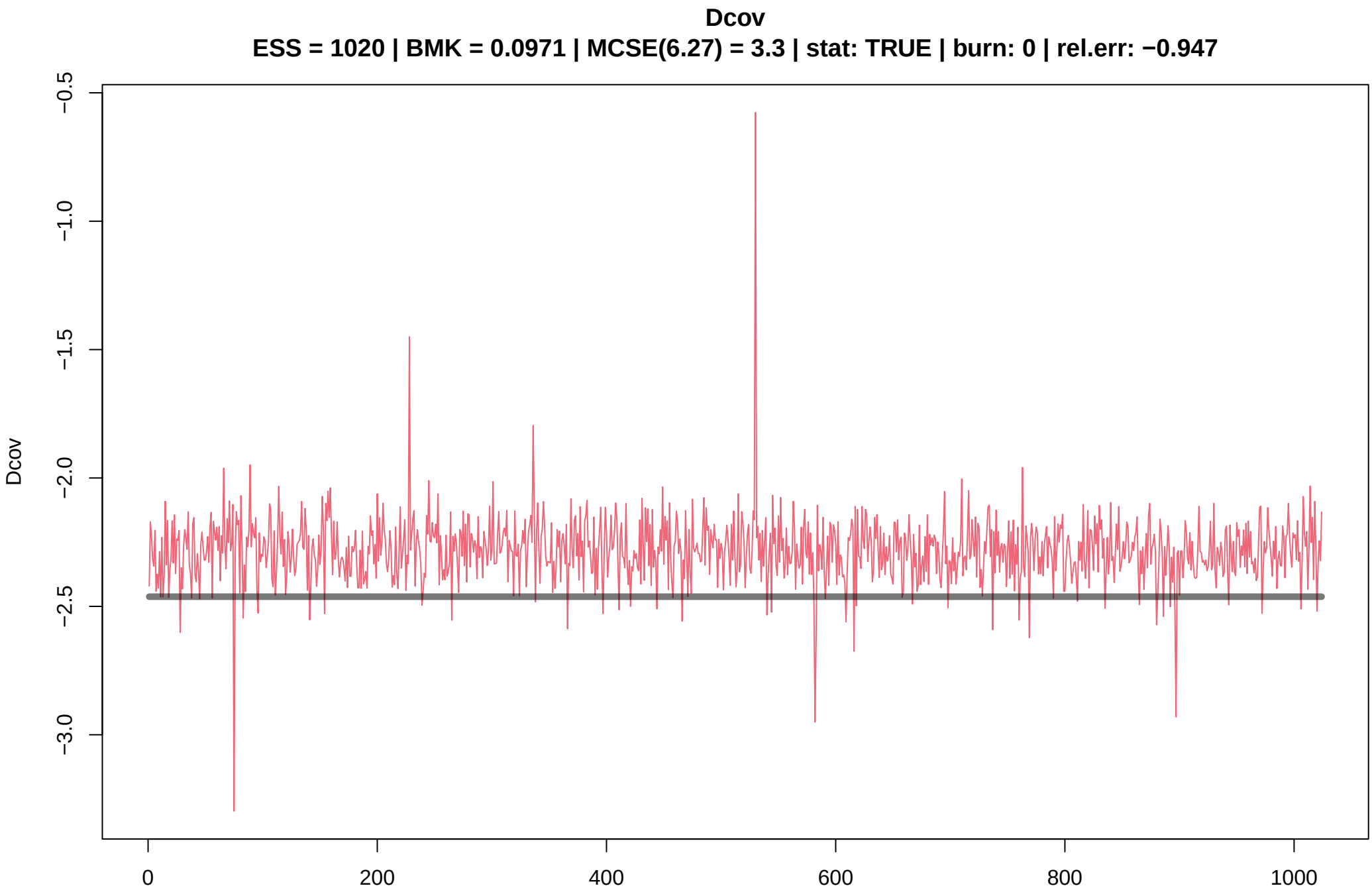

Pdatum4
ESS = 1020 | BMK = 0.0617 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | rel.err: −0.84
Pdatum4
−13.5
−13.6
−13.7
−13.8
−13.9
−14.0
−14.1
0
200
400
600
800
1000

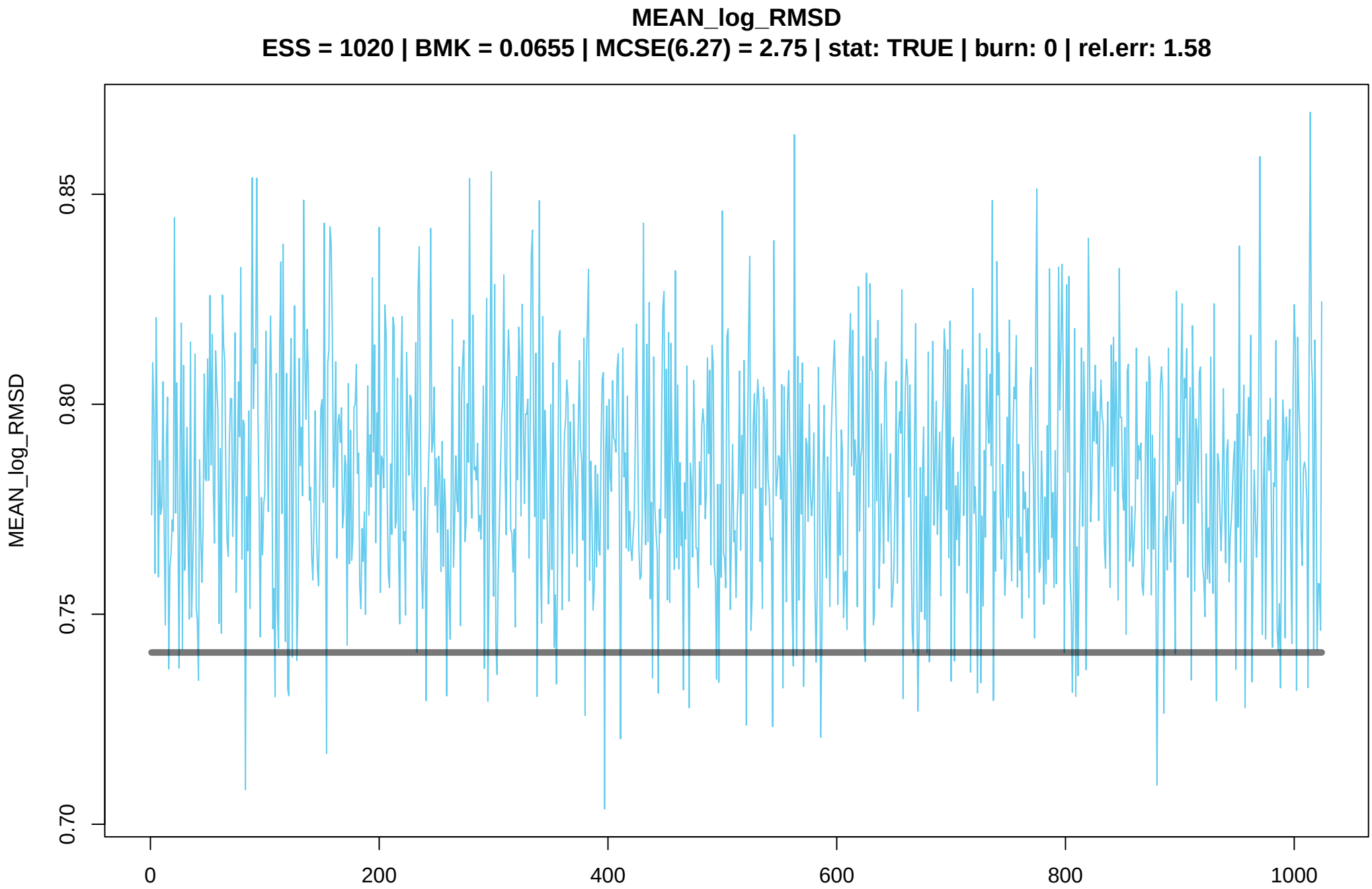

Pdatum5
ESS = 1020 | BMK = 0.0594 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | rel.err: −0.432
Pdatum5
−12.4
−12.5
−12.6
−12.7
−12.8
−12.9
−13.0
0
200
400
600
800
1000

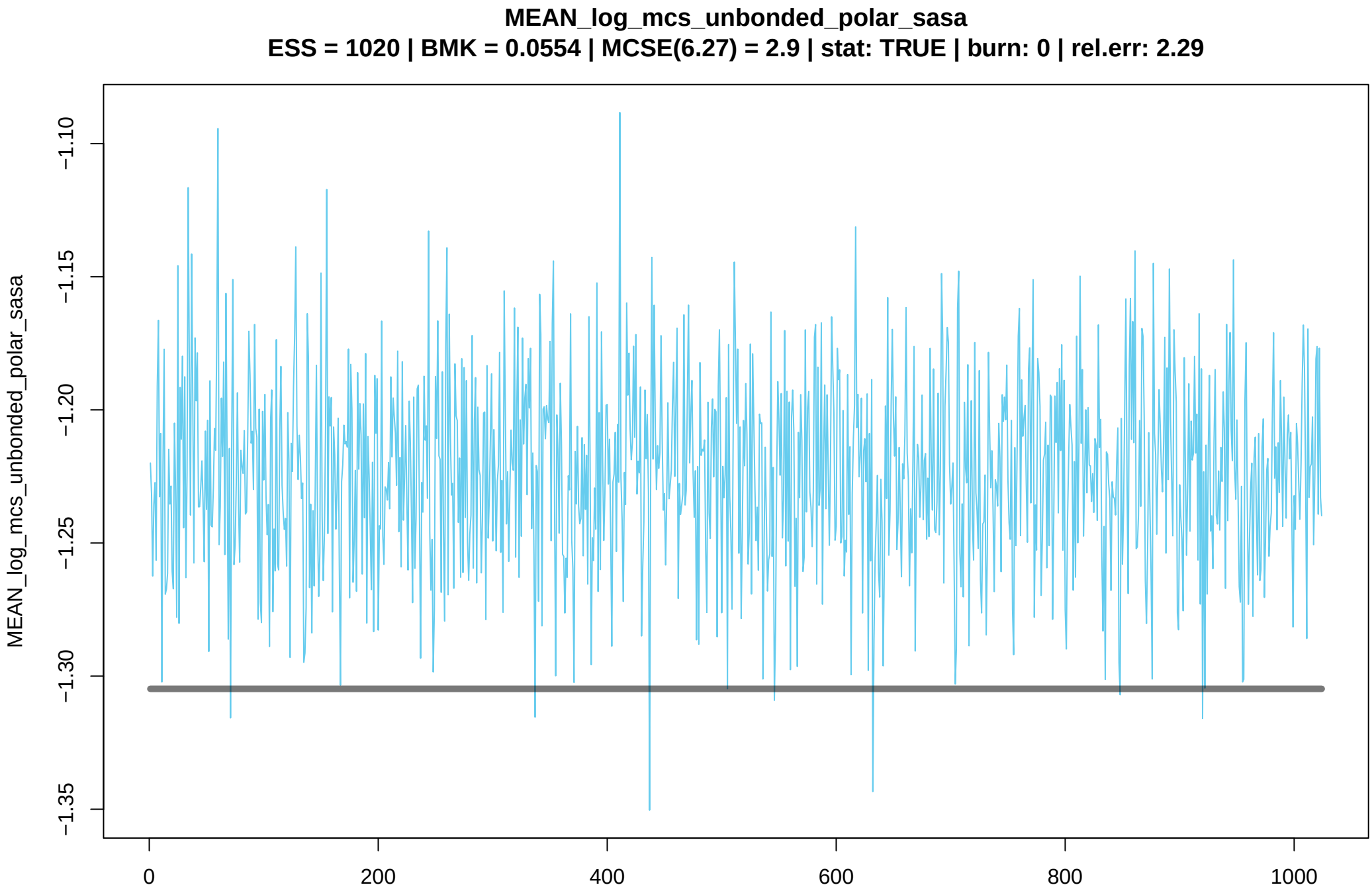

Pdatum6
ESS = 119 | BMK = 0.174 | MCSE(6.27) = 6.07 | stat: FALSE | burn: 0 | rel.err: 0.109
Pdatum6
−14.7
−14.8
−14.9
−15.0
−15.1
0
200
400
600
800
1000

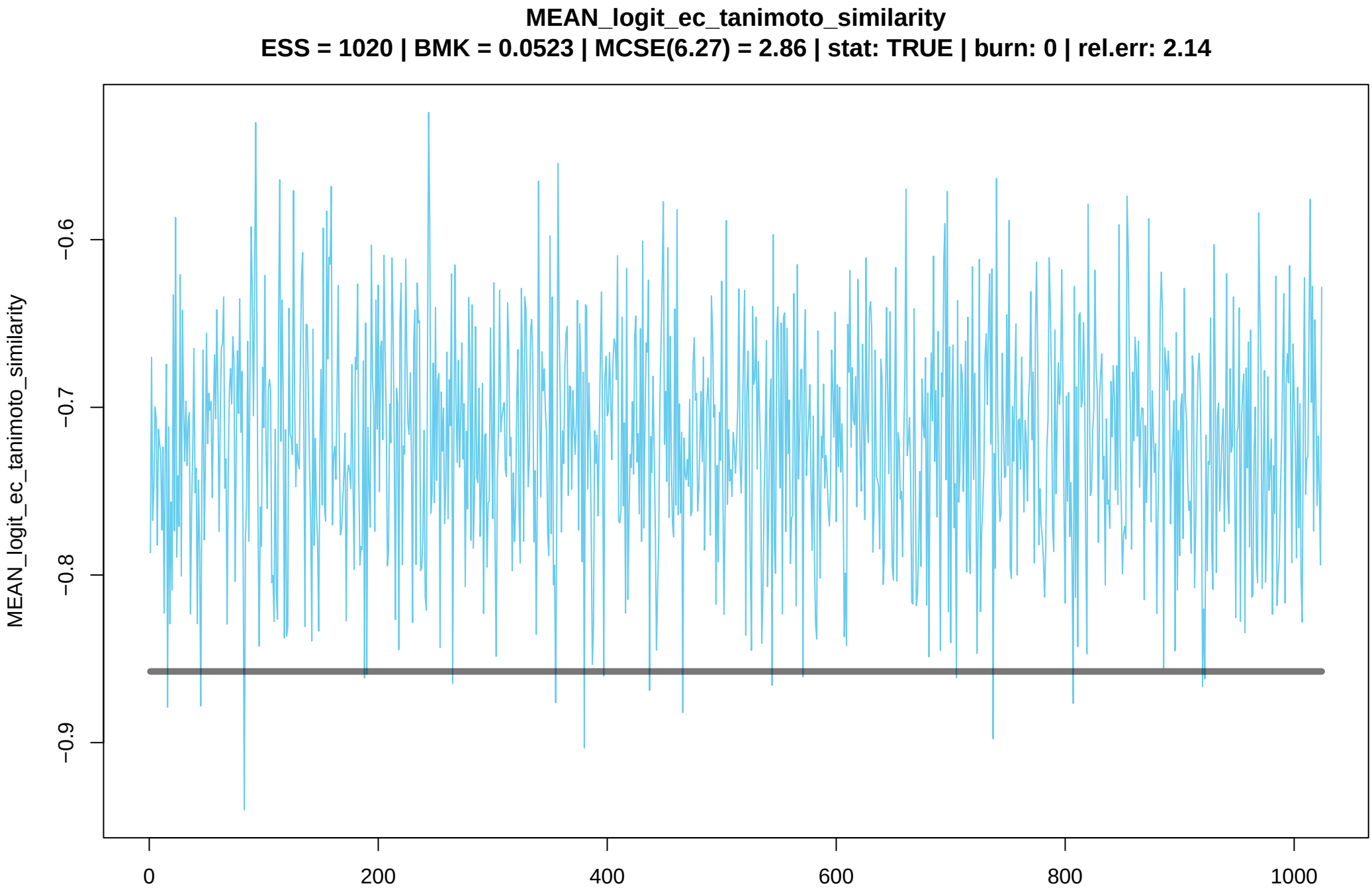

Pdatum7
ESS = 42 | BMK = 0.228 | MCSE(6.27) = 7.66 | stat: FALSE | burn: 0 | rel.err: 0.104
Pdatum7
−12.7
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

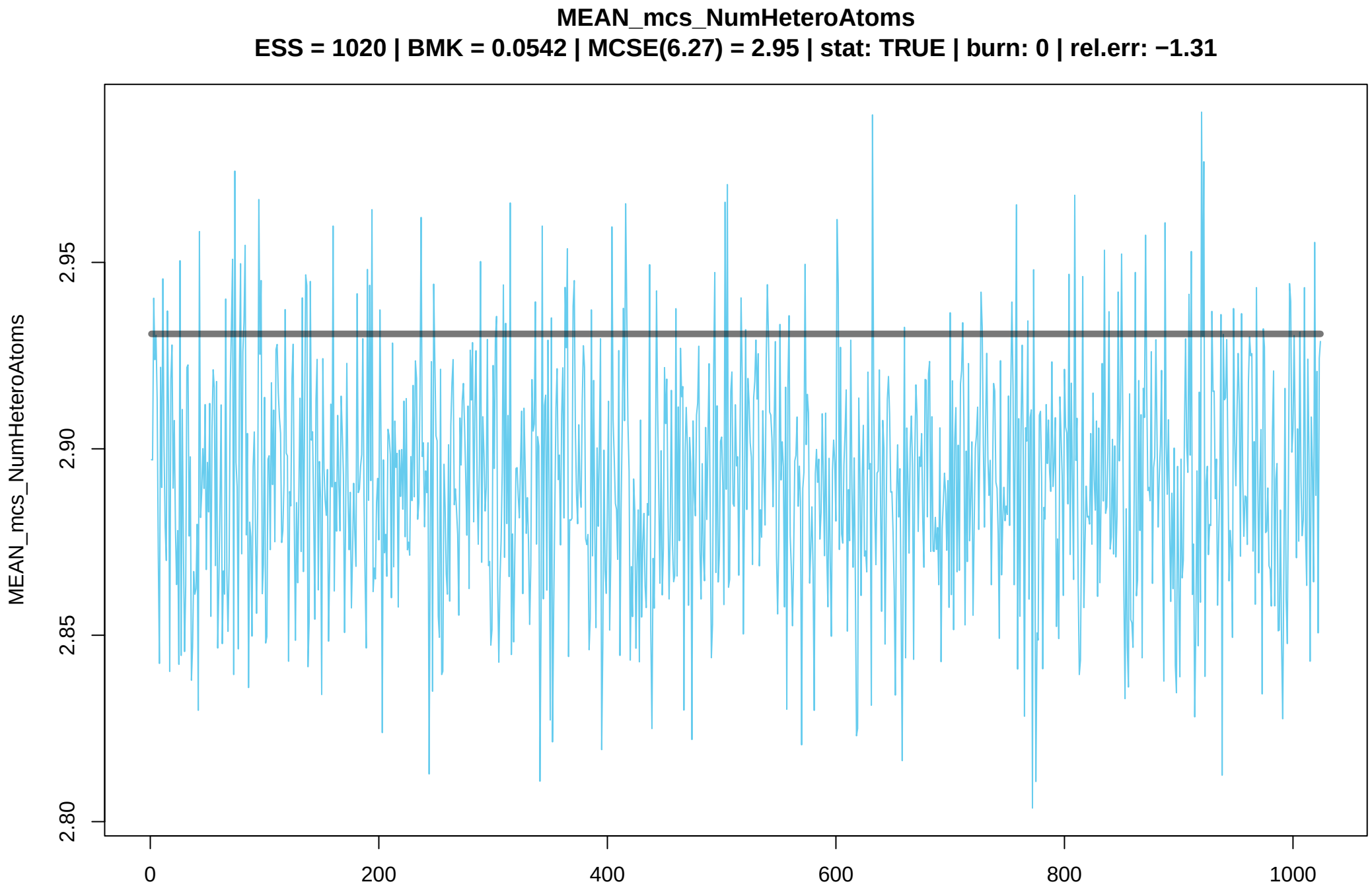

Pdatum8
ESS = 365 | BMK = 0.107 | MCSE(6.27) = 5.12 | stat: TRUE | burn: 0 | rel.err: 1.06
Pdatum8
−12.4
−12.5
−12.6
−12.7
−12.8
0
200
400
600
800
1000

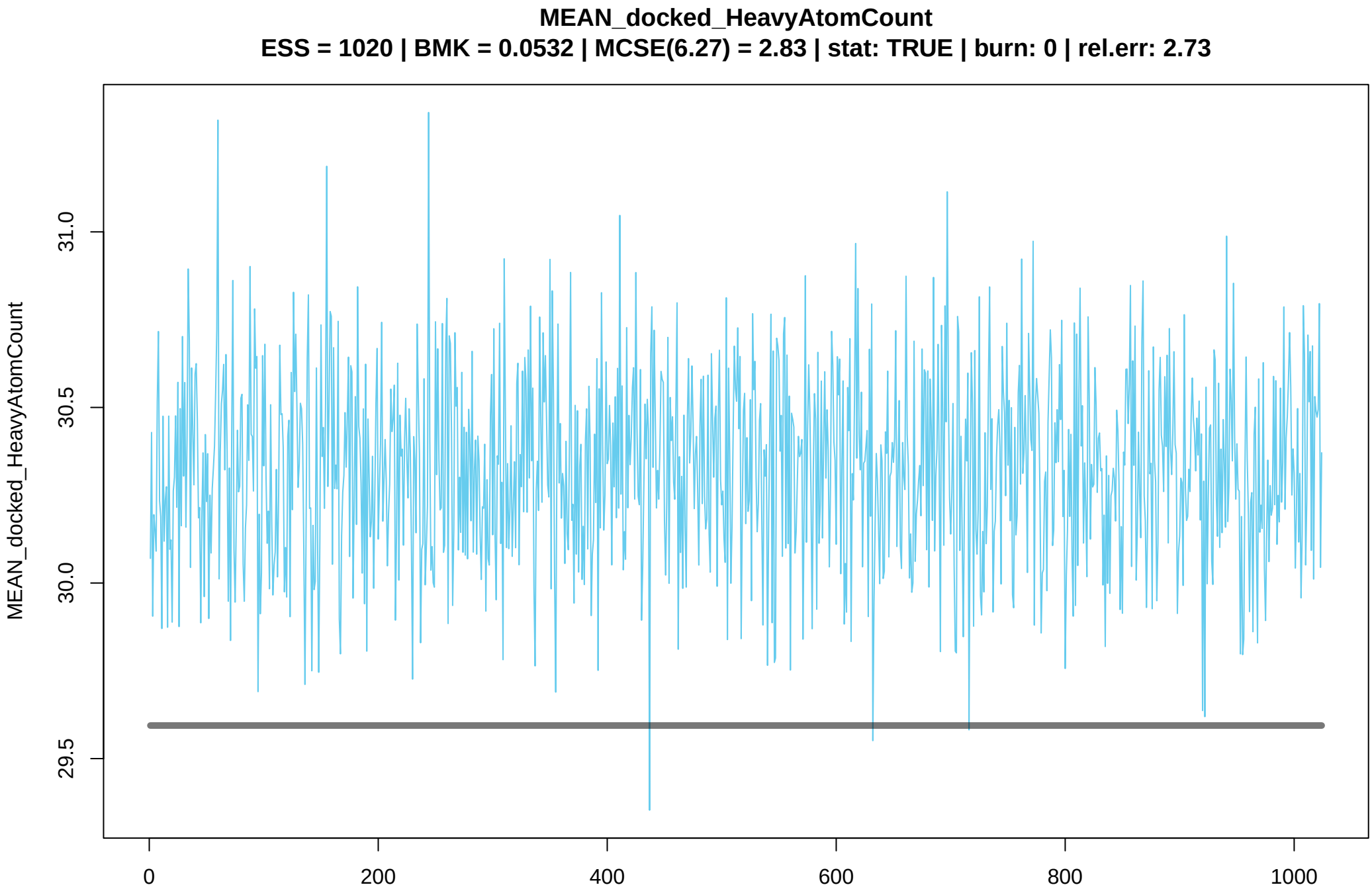

Dcov
ESS = 1020 | BMK = 0.0971 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0 | rel.err: −0.947
Dcov
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
0
200
400
600
800
1000

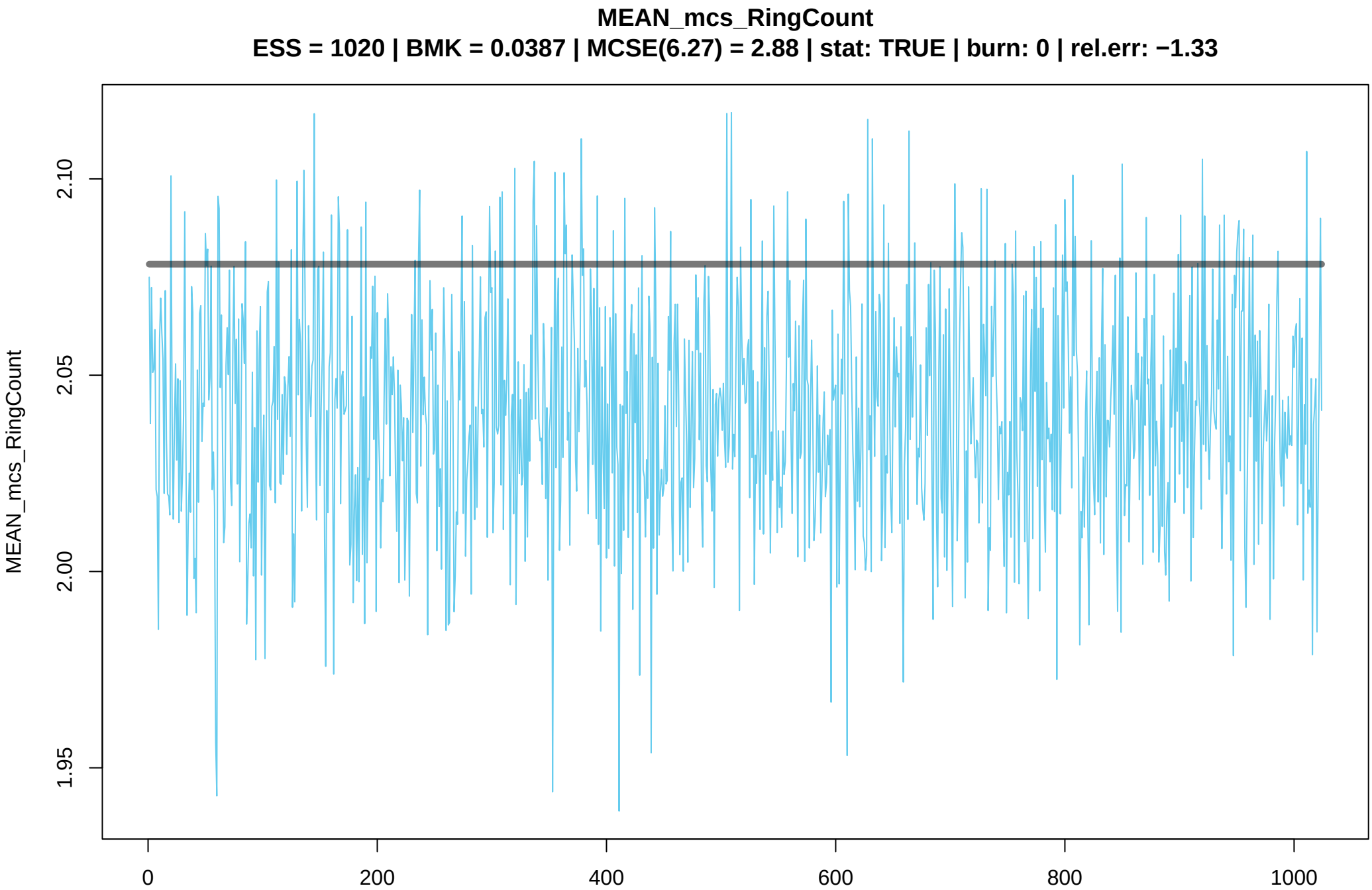

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0655 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0 | rel.err: 1.58
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

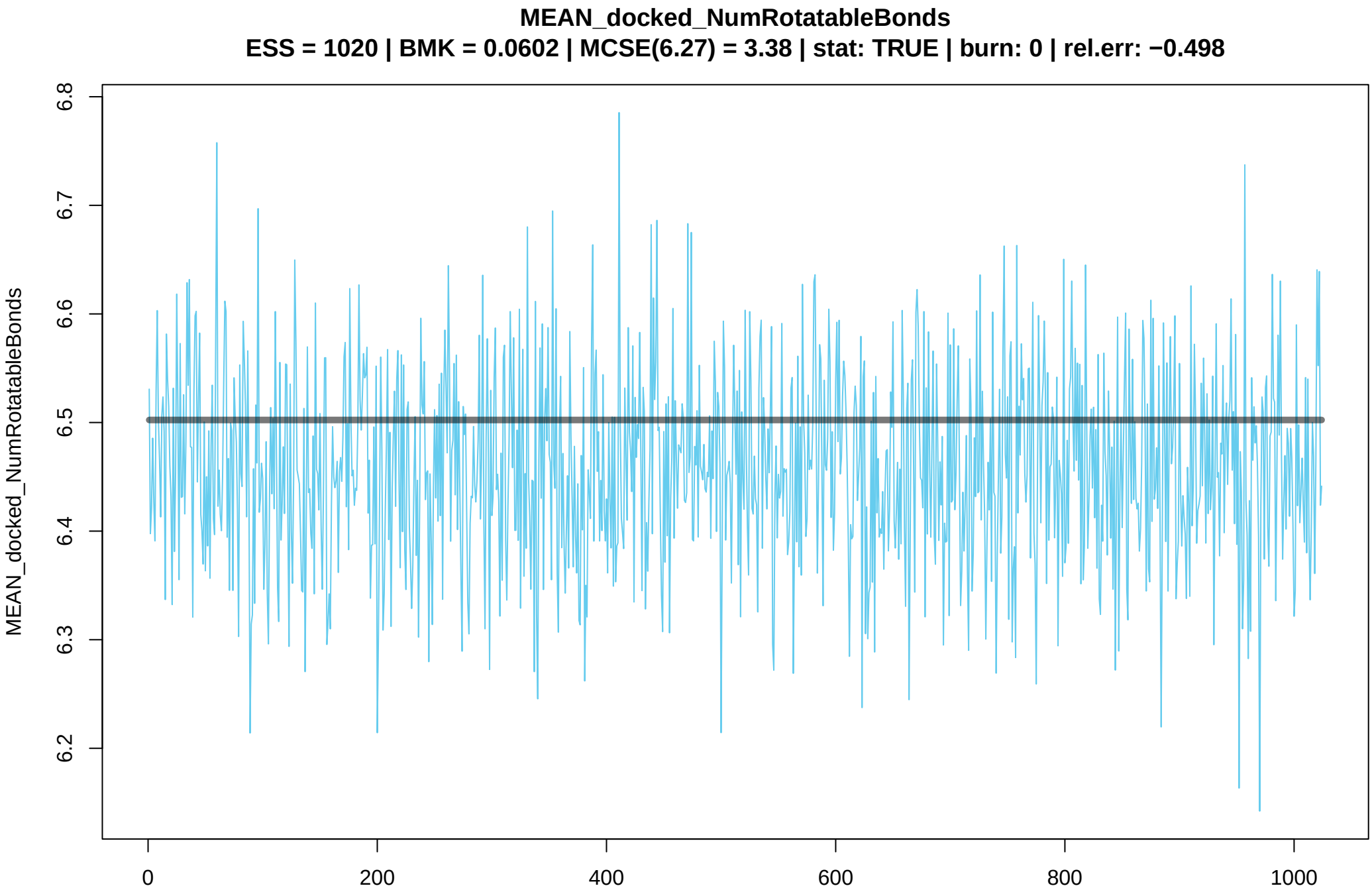

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0554 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0 | rel.err: 2.29
MEAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

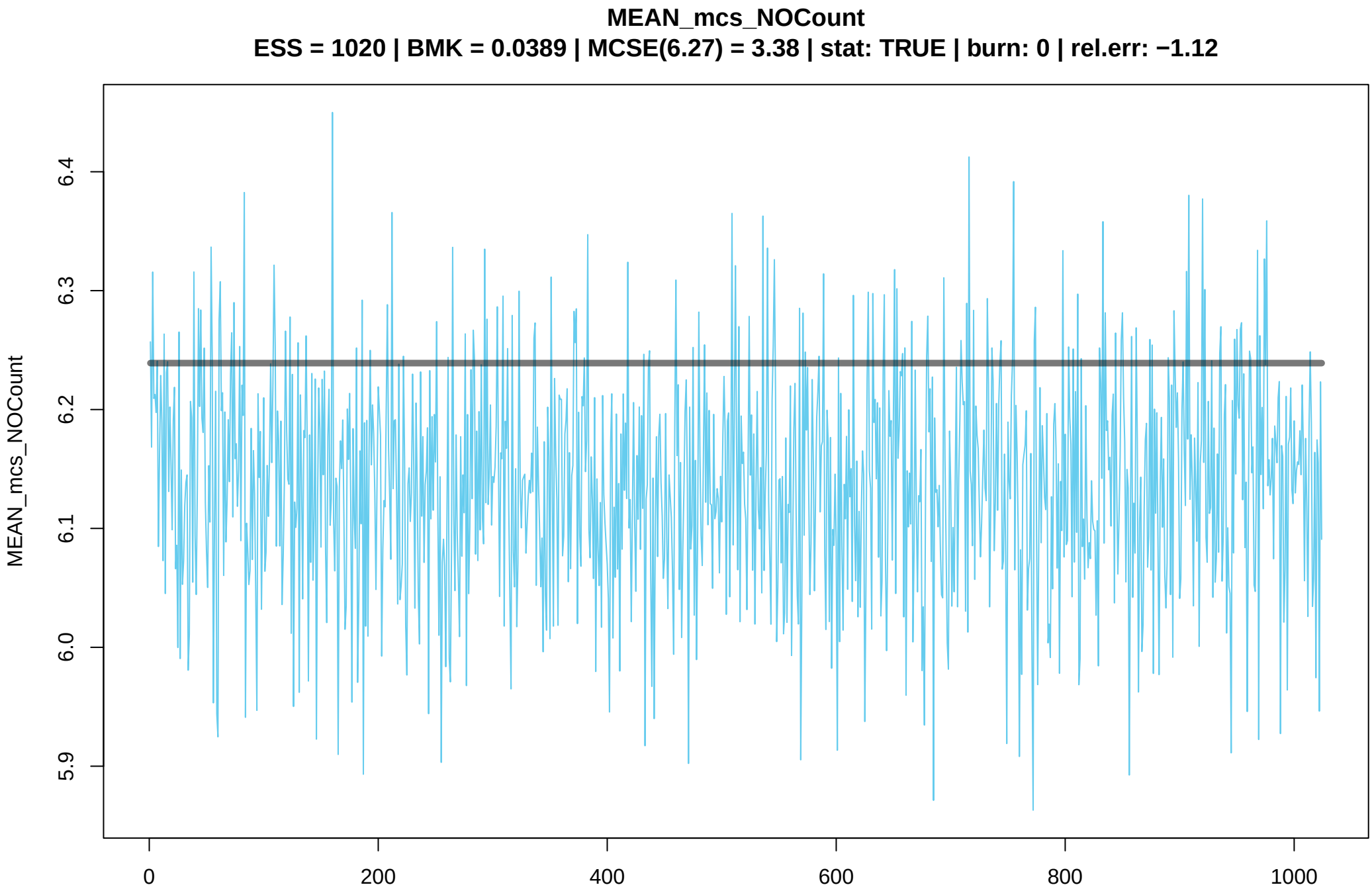

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0523 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | rel.err: 2.14
MEAN_logit_ec_tanimoto_similarity
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

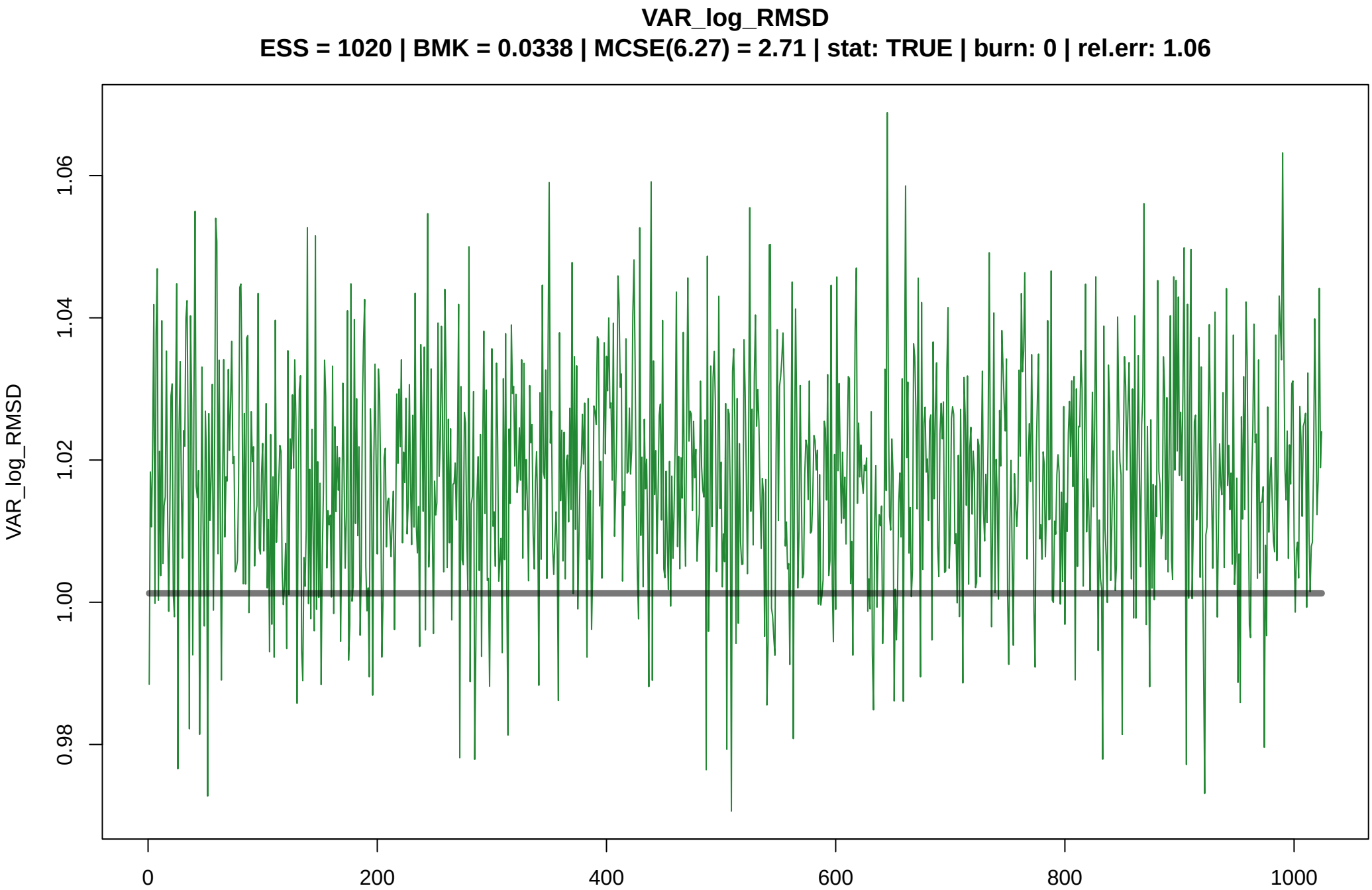

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0542 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: −1.31
MEAN_mcs_NumHeteroAtoms
2.80
2.85
2.90
2.95
0
200
400
600
800
1000

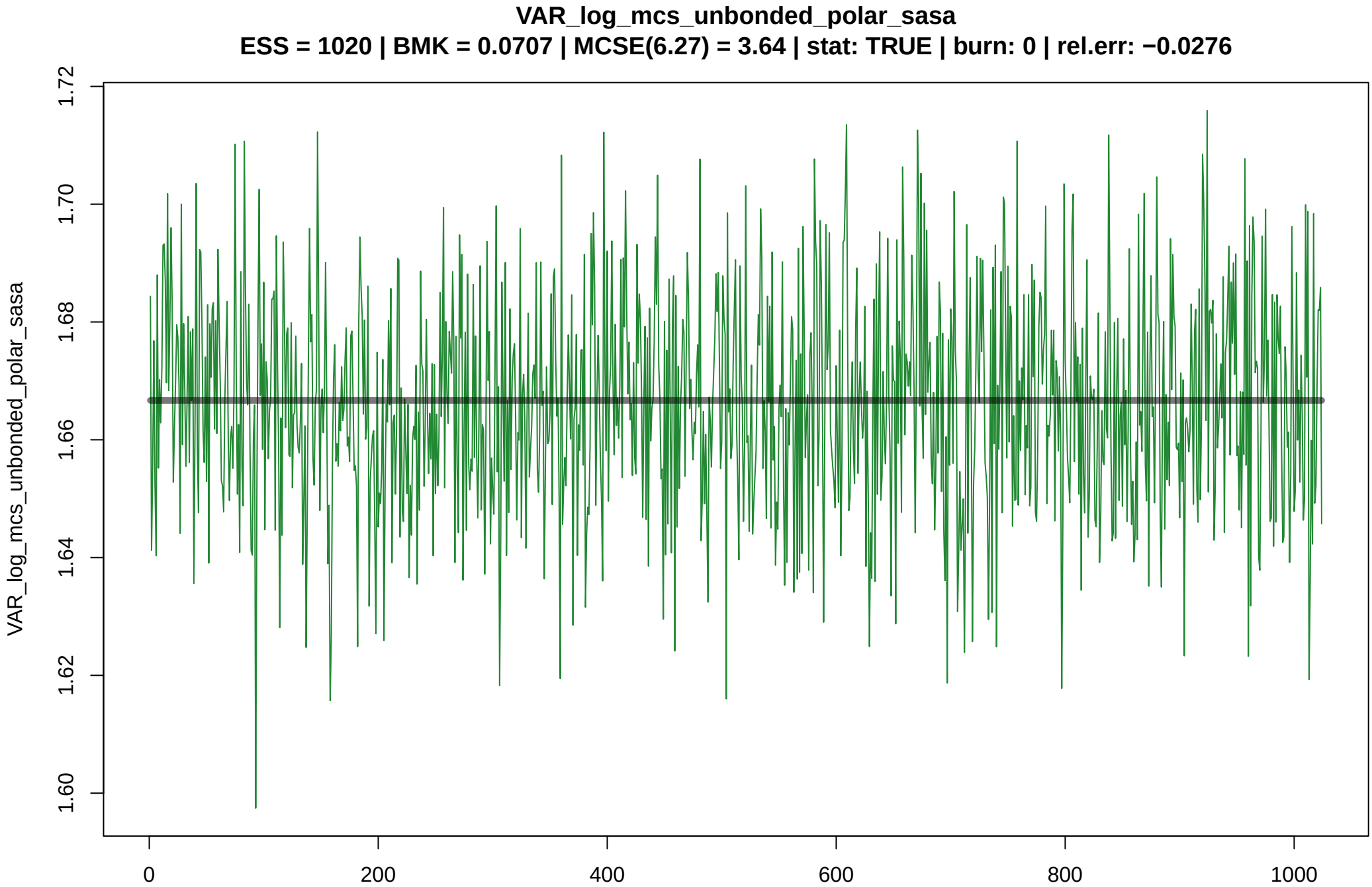

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0532 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | rel.err: 2.73
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
31.0
0
200
400
600
800
1000

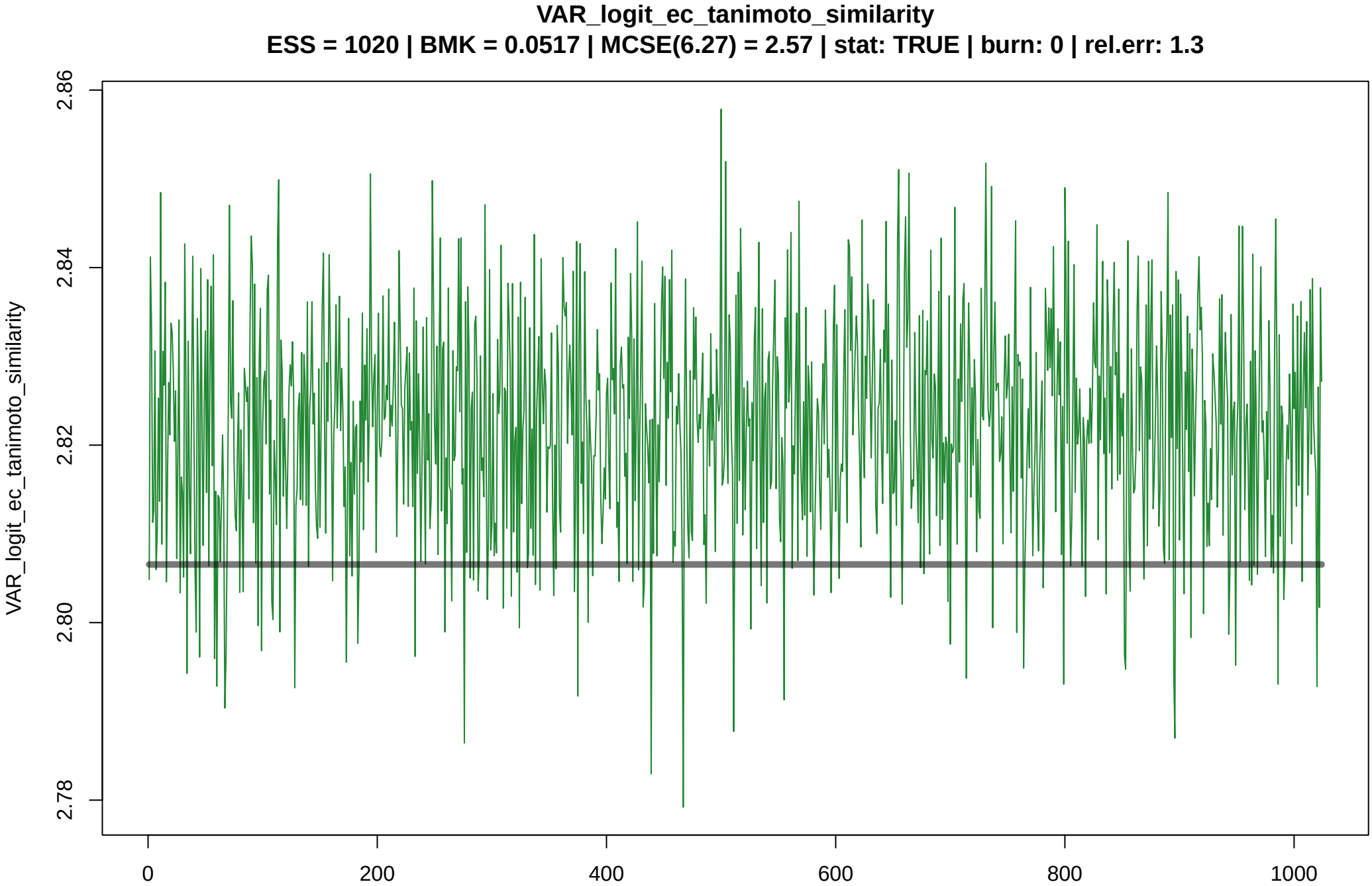

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0387 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: −1.33
MEAN_mcs_RingCount
1.95
2.00
2.05
2.10
0
200
400
600
800
1000

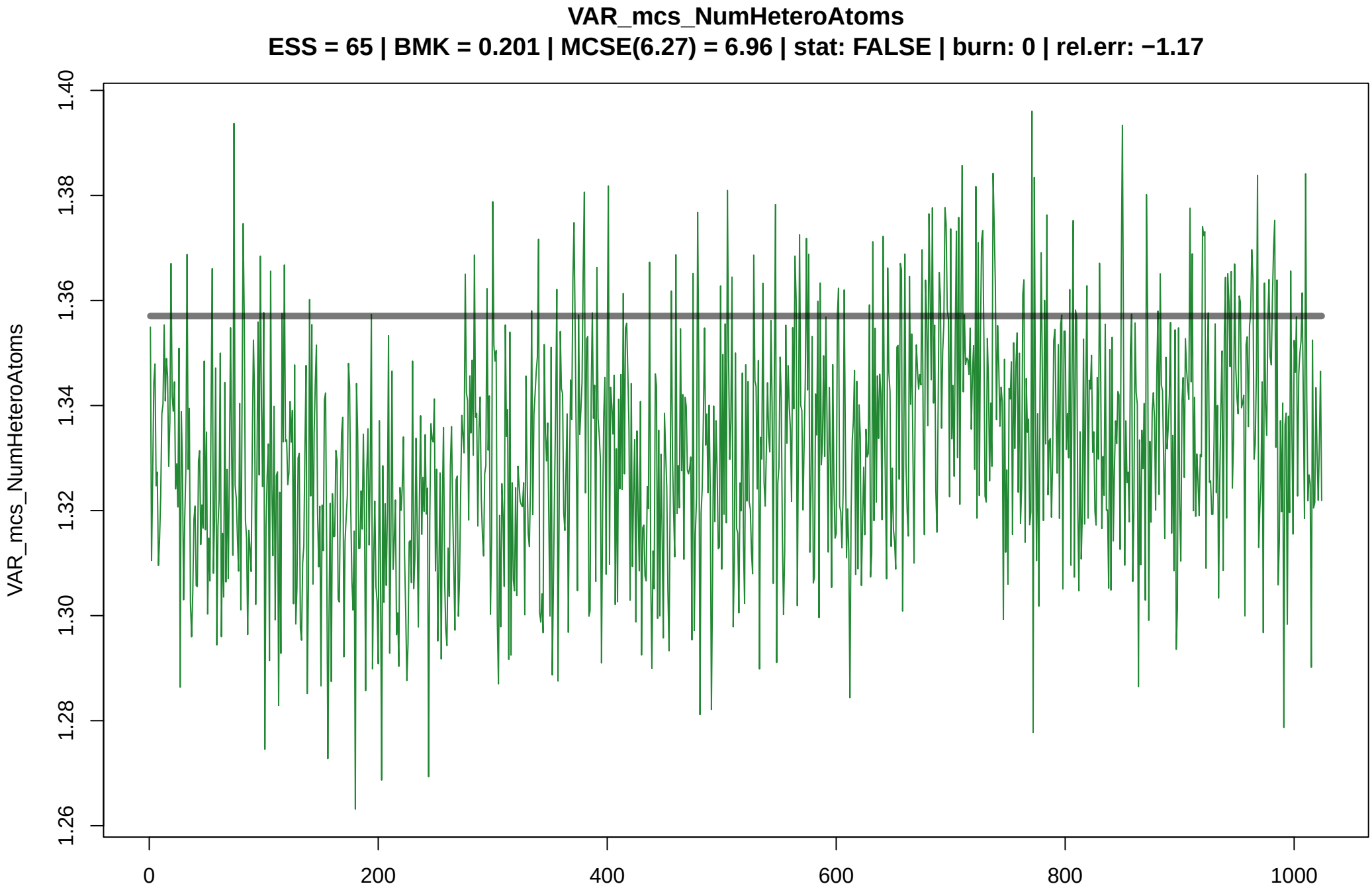

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0602 | MCSE(6.27) = 3.38 | stat: TRUE | burn: 0 | rel.err: −0.498
MEAN_docked_NumRotatableBonds
6.8
6.7
6.6
6.5
6.4
6.3
6.2
0
200
400
600
800
1000

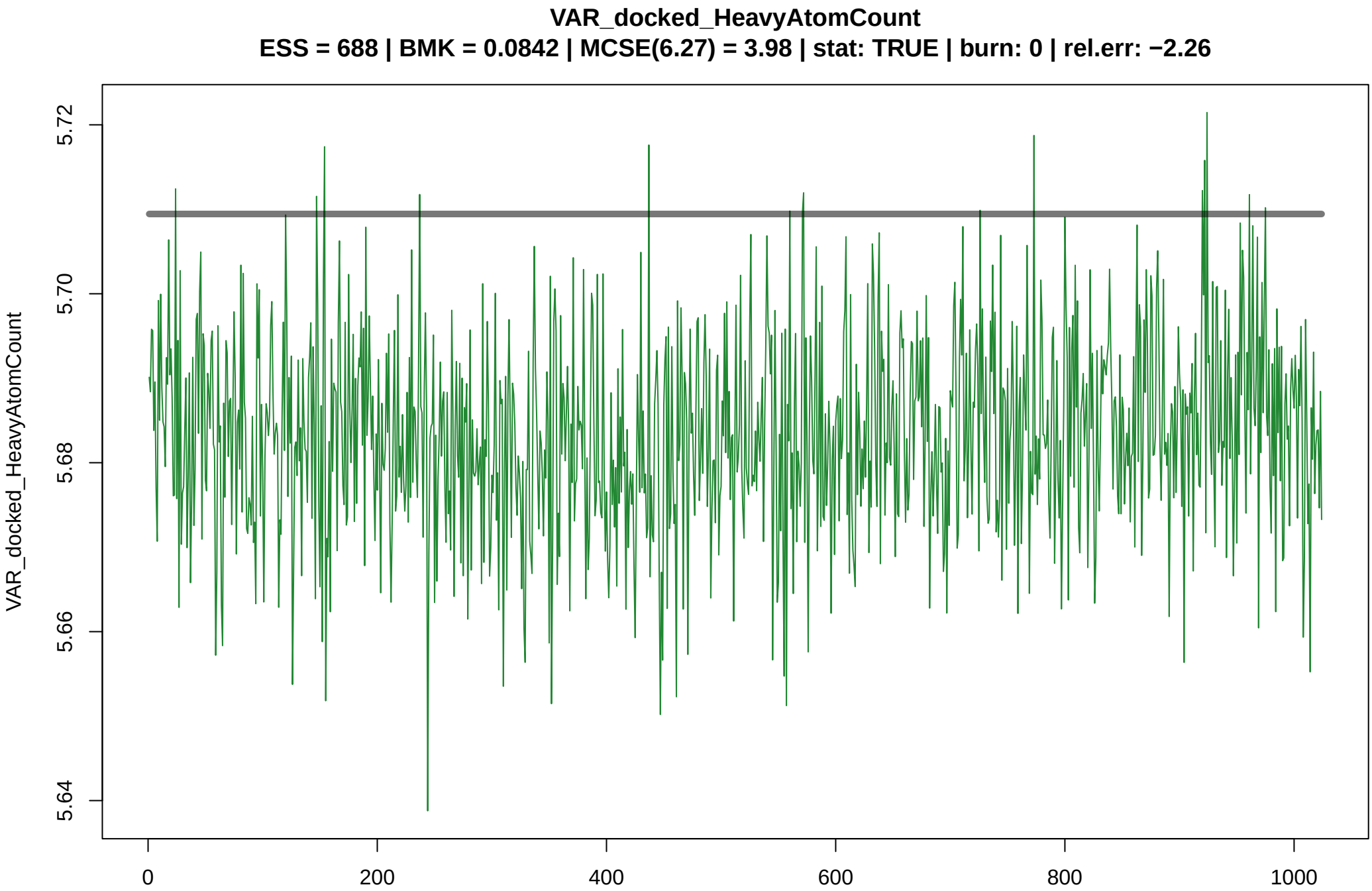

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0389 | MCSE(6.27) = 3.38 | stat: TRUE | burn: 0 | rel.err: −1.12
MEAN_mcs_NOCount
6.4
6.3
6.2
6.1
6.0
5.9
0
200
400
600
800
1000

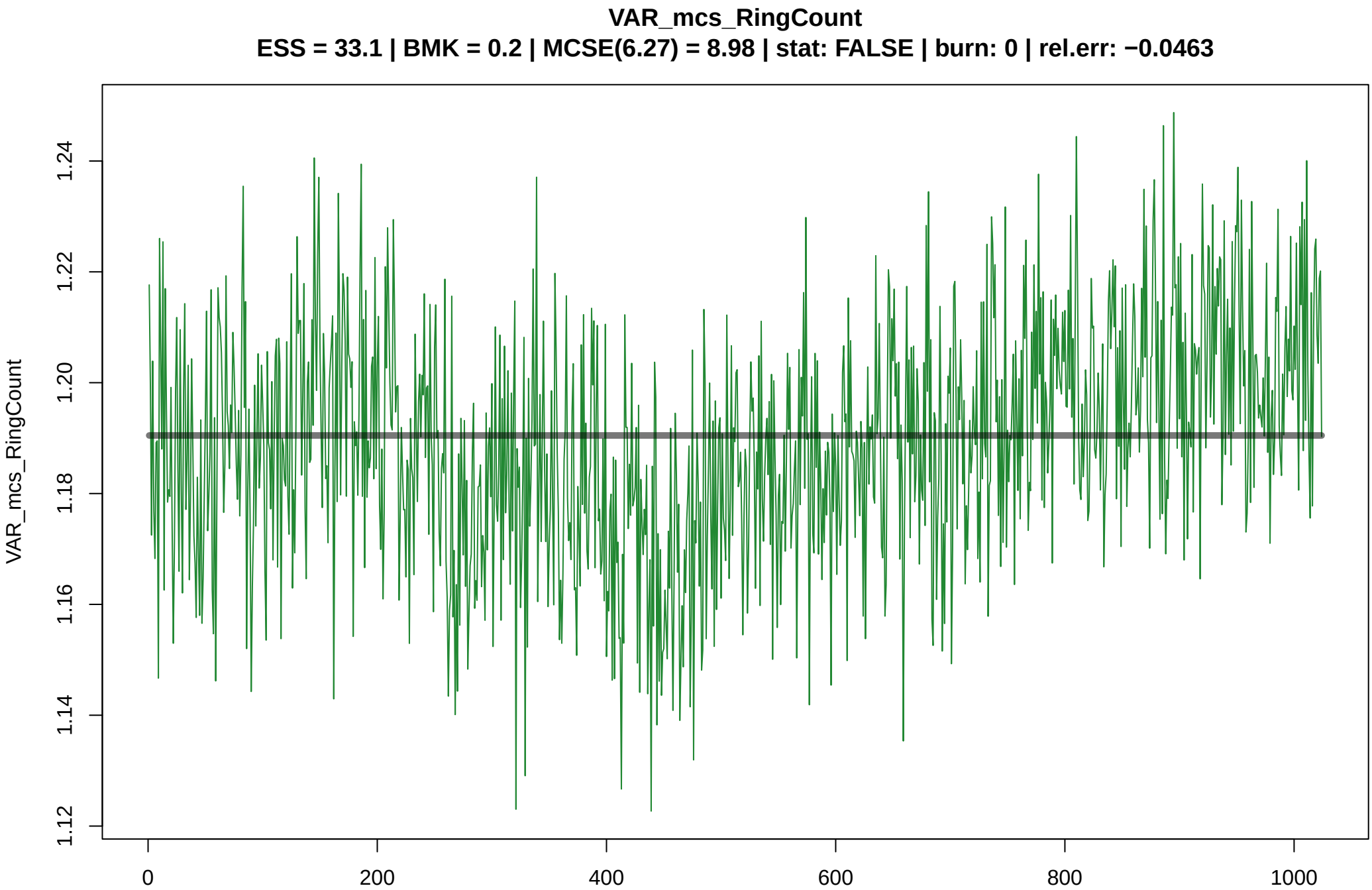

VAR_log_RMSD
ESS = 1020 | BMK = 0.0338 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | rel.err: 1.06
VAR_log_RMSD
0.98
1.00
1.02
1.04
1.06
0
200
400
600
800
1000

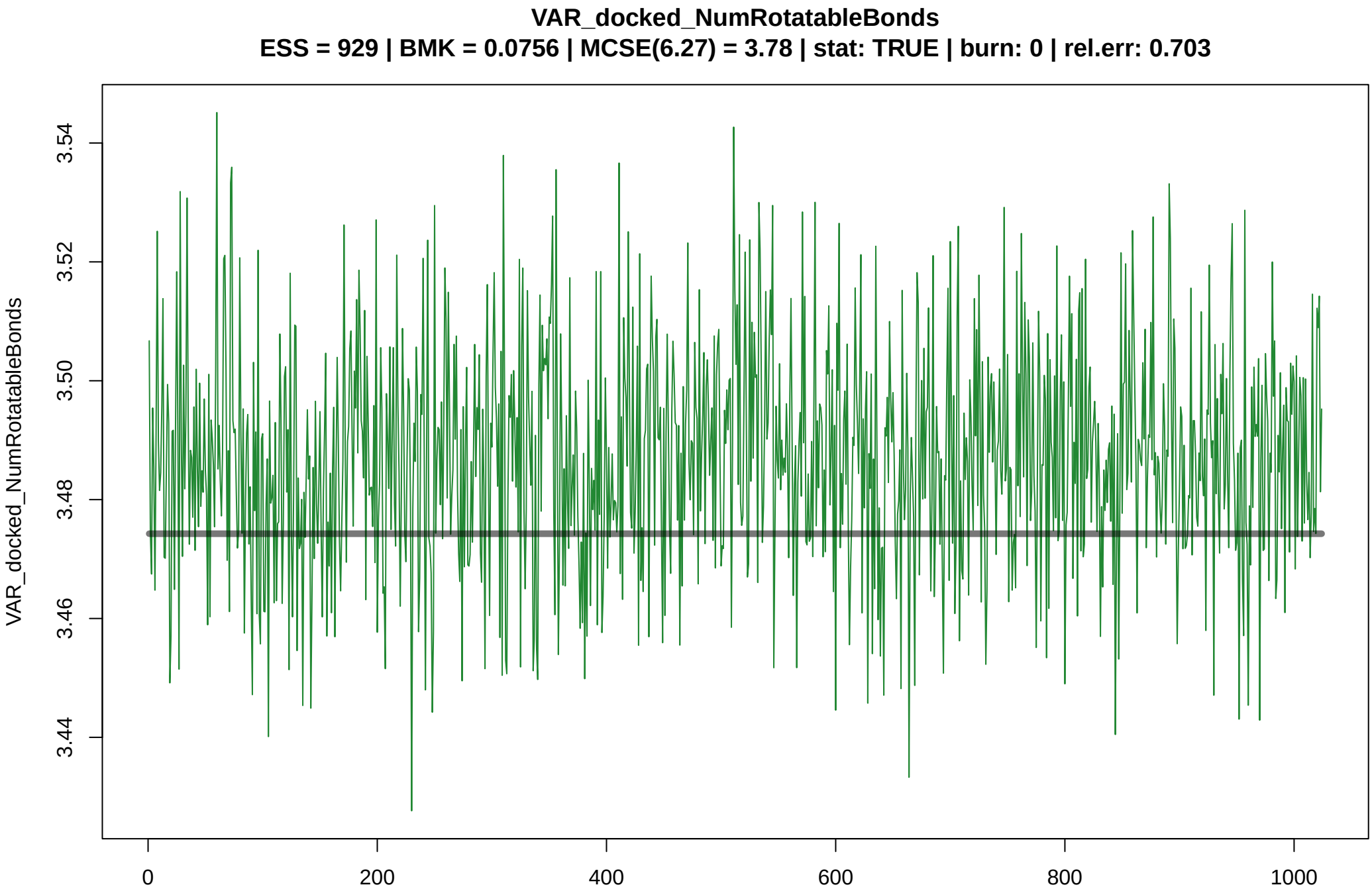

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0707 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 0 | rel.err: −0.0276
VAR_log_mcs_unbonded_polar_sasa
1.60
1.62
1.64
1.66
1.68
1.70
1.72
0
200
400
600
800
1000

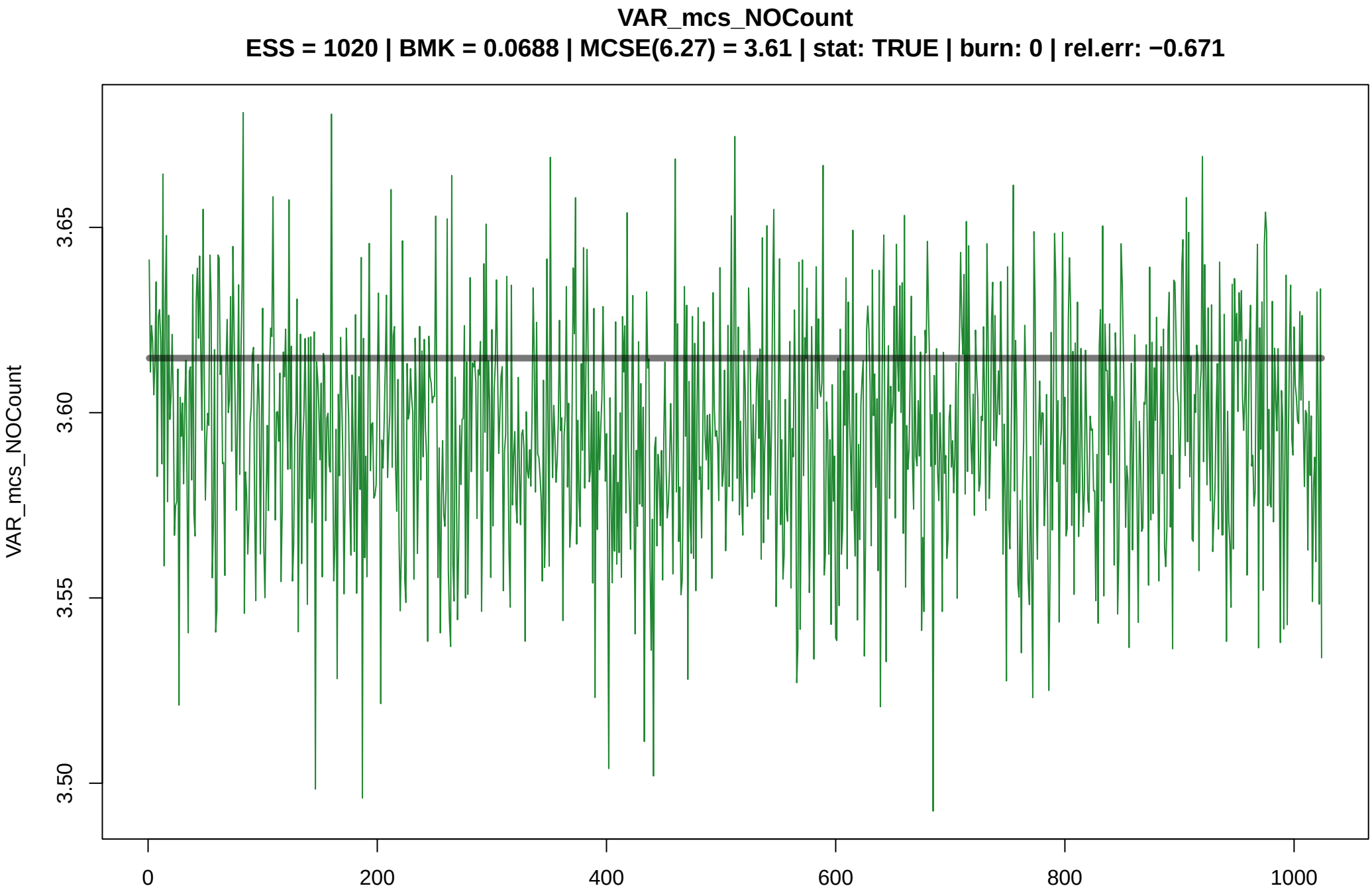

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0517 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: 1.3
VAR_logit_ec_tanimoto_similarity
2.86
2.84
2.82
2.80
2.78
0
200
400
600
800
1000

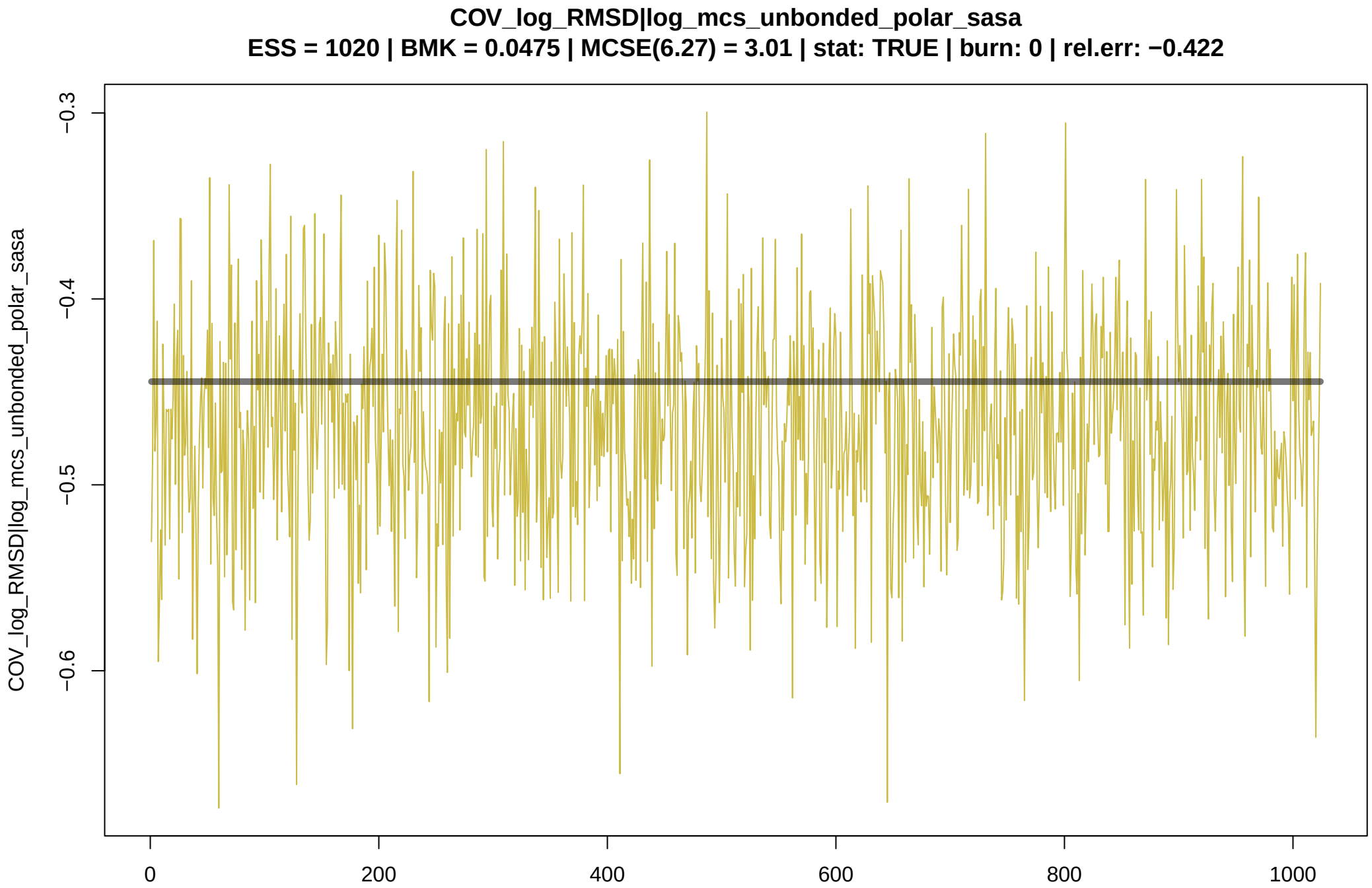

VAR_mcs_NumHeteroAtoms
ESS = 65 | BMK = 0.201 | MCSE(6.27) = 6.96 | stat: FALSE | burn: 0 | rel.err: −1.17
VAR_mcs_NumHeteroAtoms
1.26
1.28
1.30
1.32
1.34
1.36
1.38
1.40
0
200
400
600
800
1000

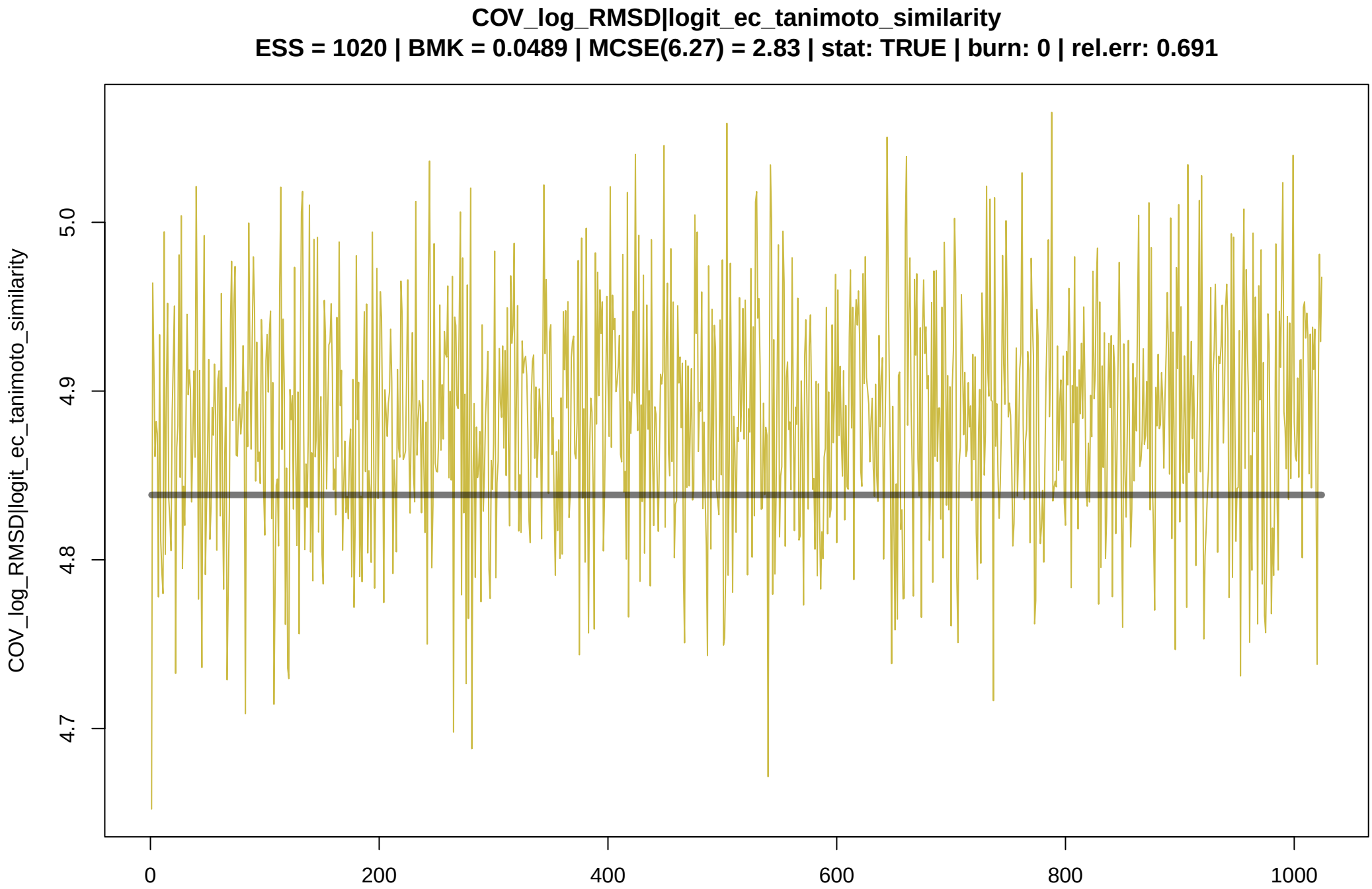

VAR_docked_HeavyAtomCount
ESS = 688 | BMK = 0.0842 | MCSE(6.27) = 3.98 | stat: TRUE | burn: 0 | rel.err: −2.26
VAR_docked_HeavyAtomCount
5.64
5.66
5.68
5.70
5.72
0
200
400
600
800
1000

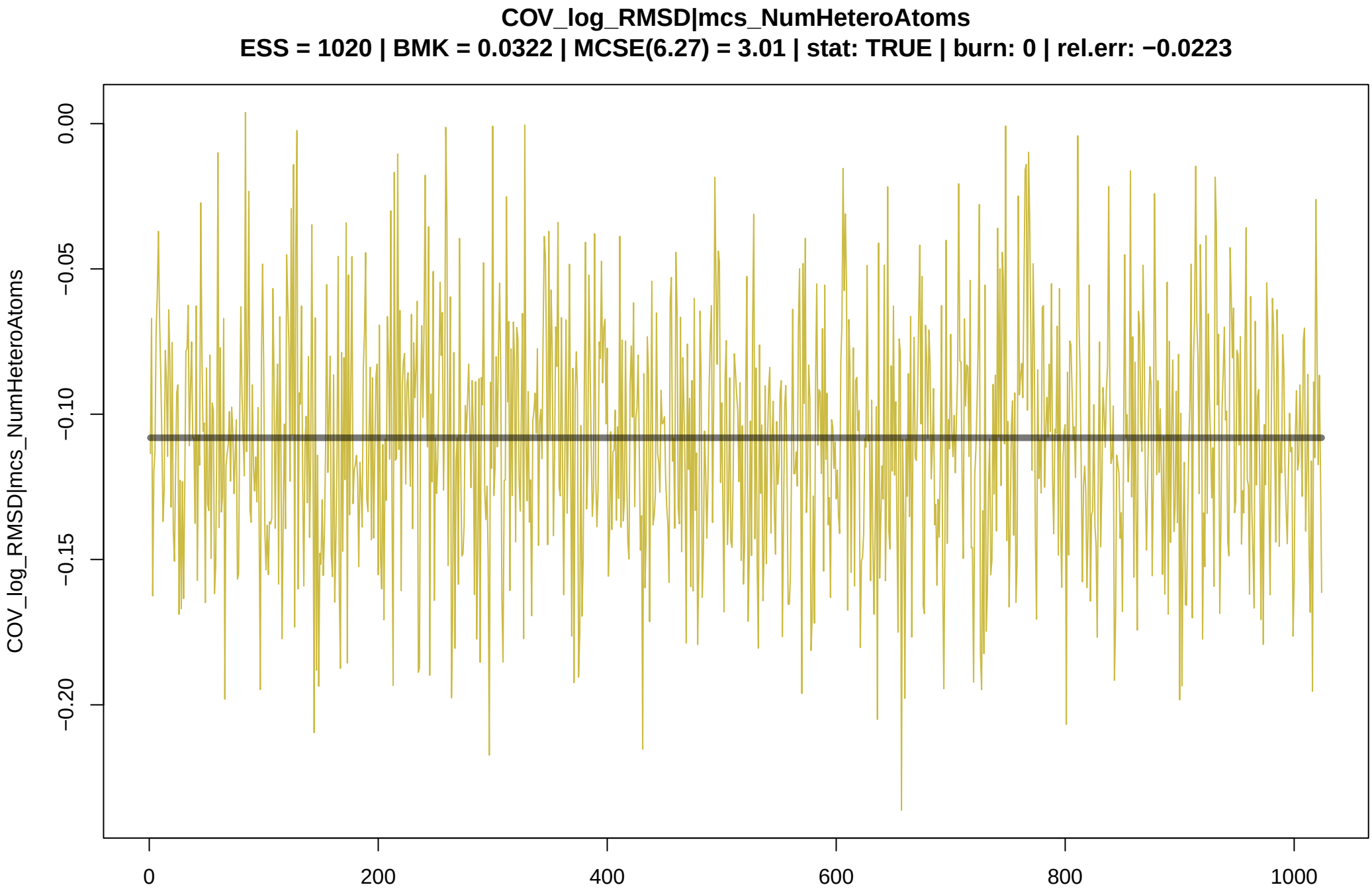

VAR_mcs_RingCount
ESS = 33.1 | BMK = 0.2 | MCSE(6.27) = 8.98 | stat: FALSE | burn: 0 | rel.err: −0.0463
VAR_mcs_RingCount
1.12
1.14
1.16
1.18
1.20
1.22
1.24
0
200
400
600
800
1000

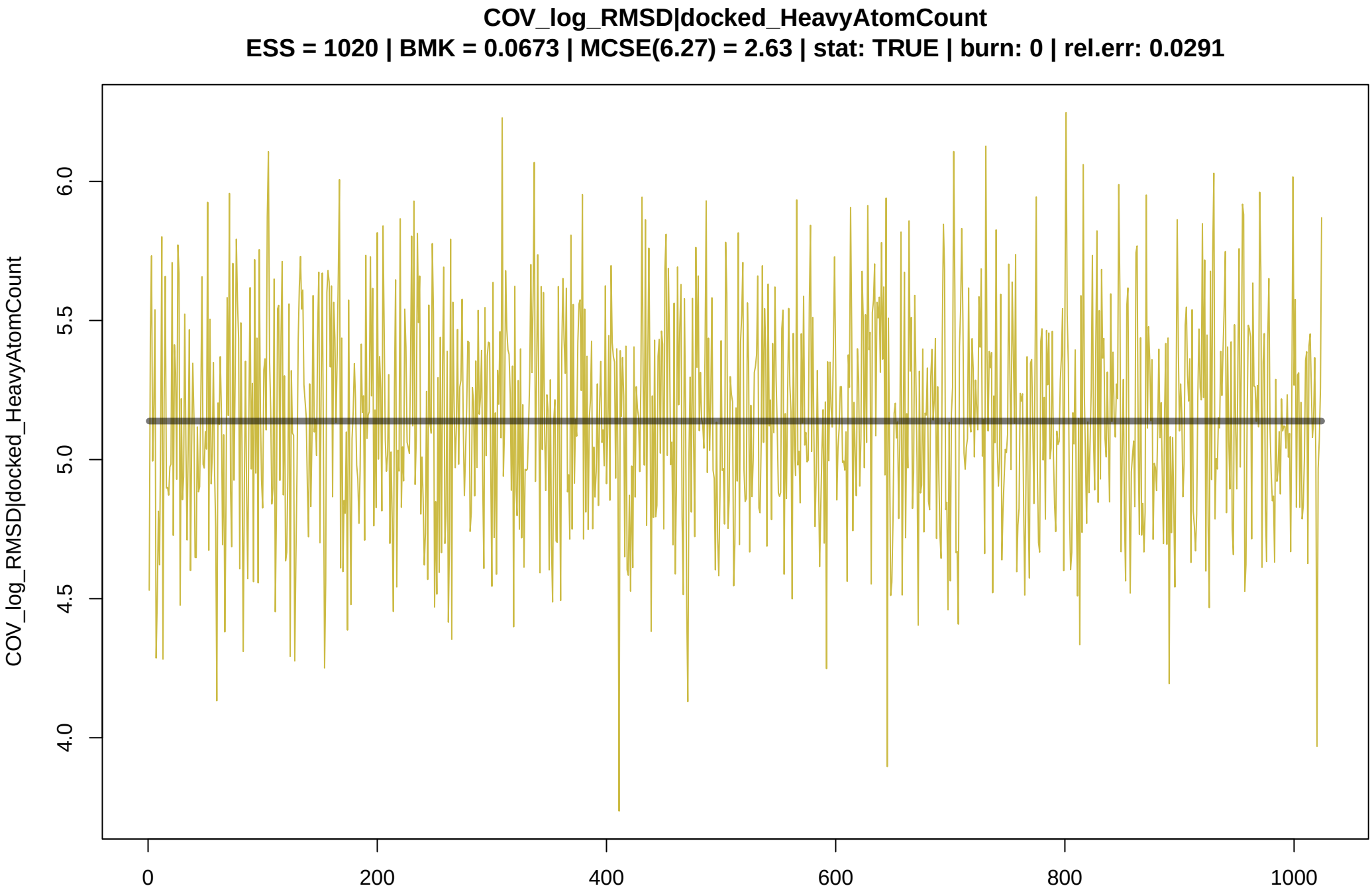

VAR_docked_NumRotatableBonds
ESS = 929 | BMK = 0.0756 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0 | rel.err: 0.703
VAR_docked_NumRotatableBonds
3.44
3.46
3.48
3.50
3.52
3.54
0
200
400
600
800
1000

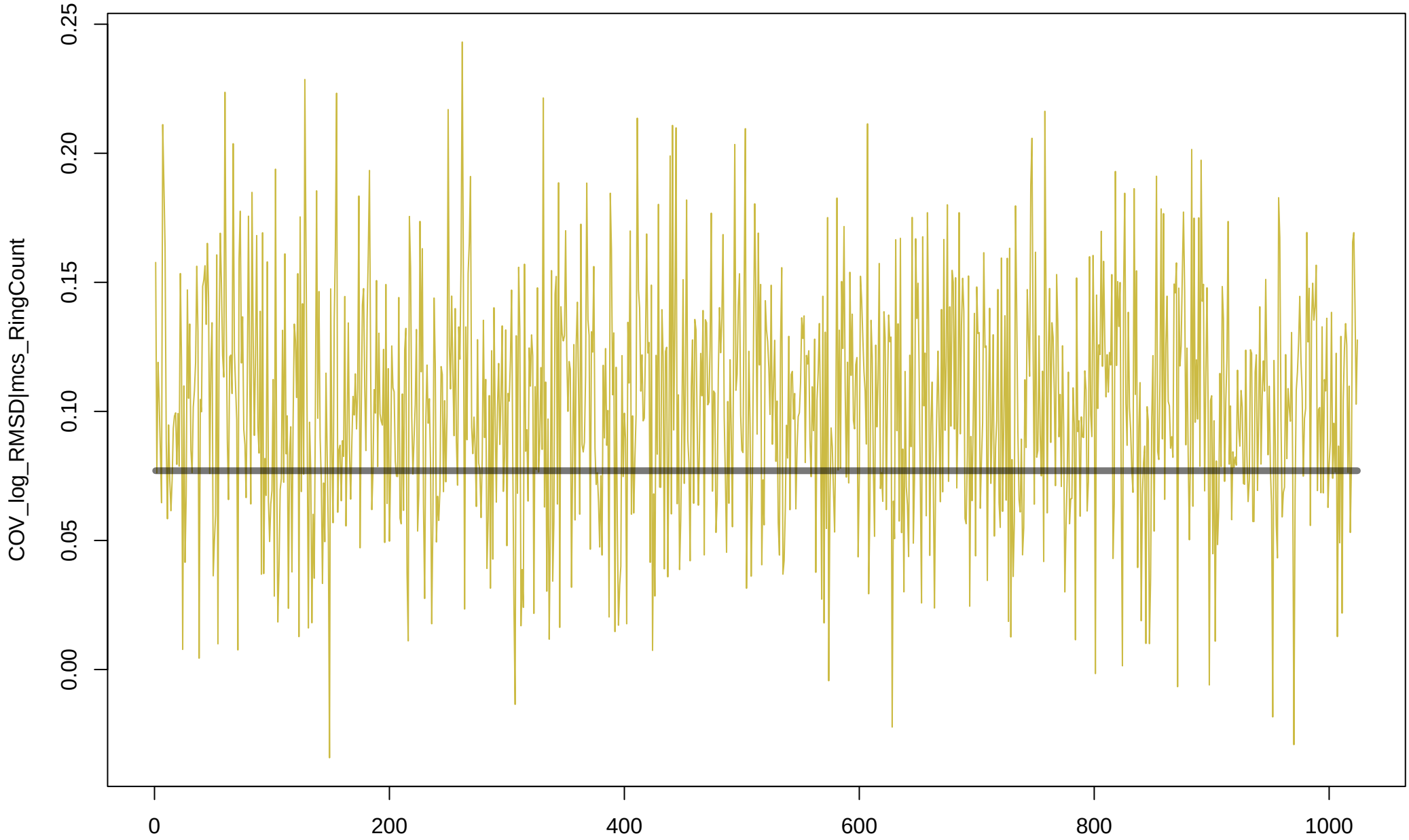

VAR_mcs_NOCount
ESS = 1020 | BMK = 0.0688 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0 | rel.err: −0.671
VAR_mcs_NOCount
3.50
3.55
3.60
3.65
0
200
400
600
800
1000

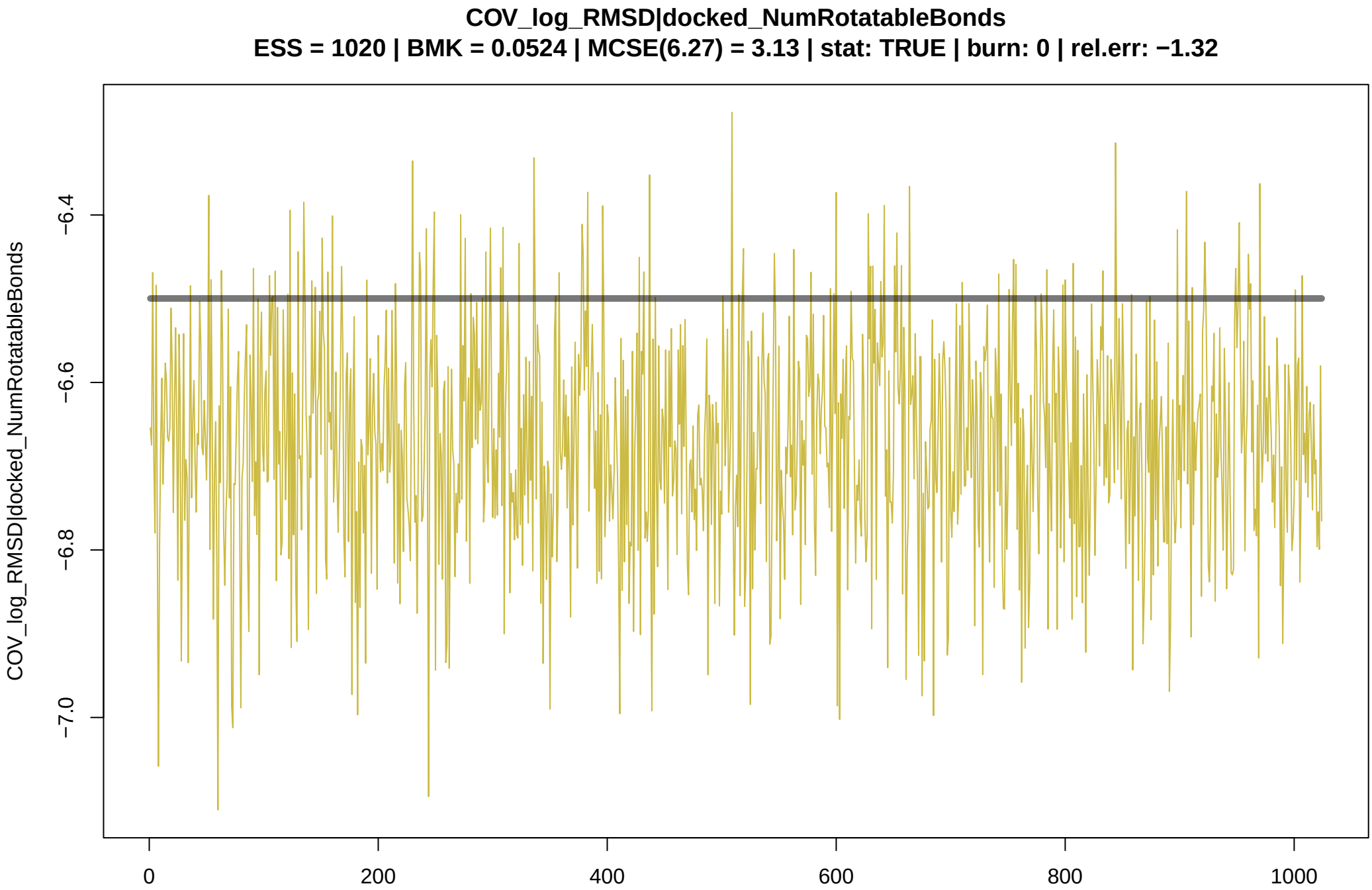

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0475 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | rel.err: −0.422
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.3
−0.4
−0.5
−0.6
0
200
400
600
800
1000

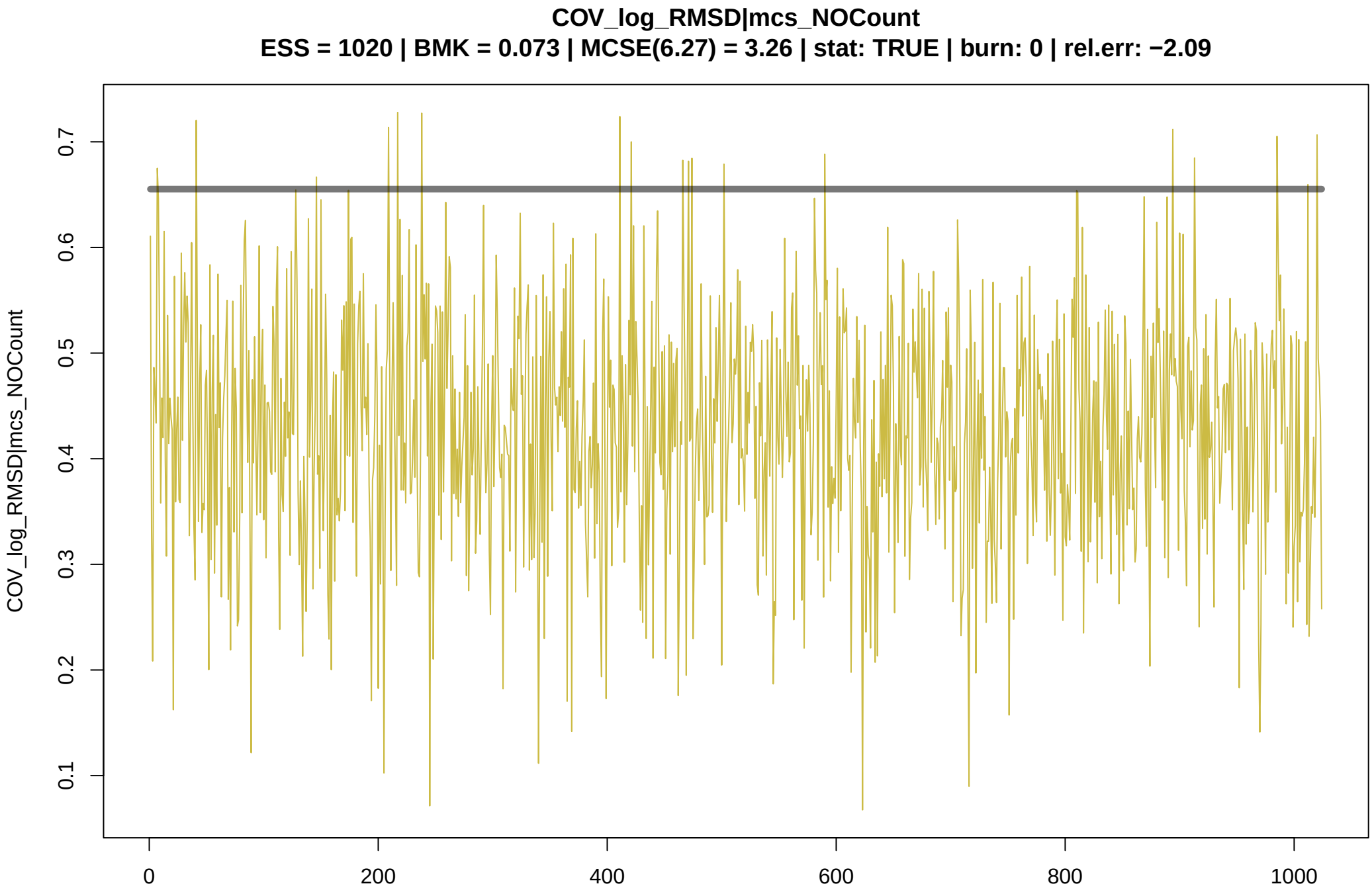

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0489 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | rel.err: 0.691
COV_log_RMSD|logit_ec_tanimoto_similarity
5.0
4.9
4.8
4.7
0
200
400
600
800
1000

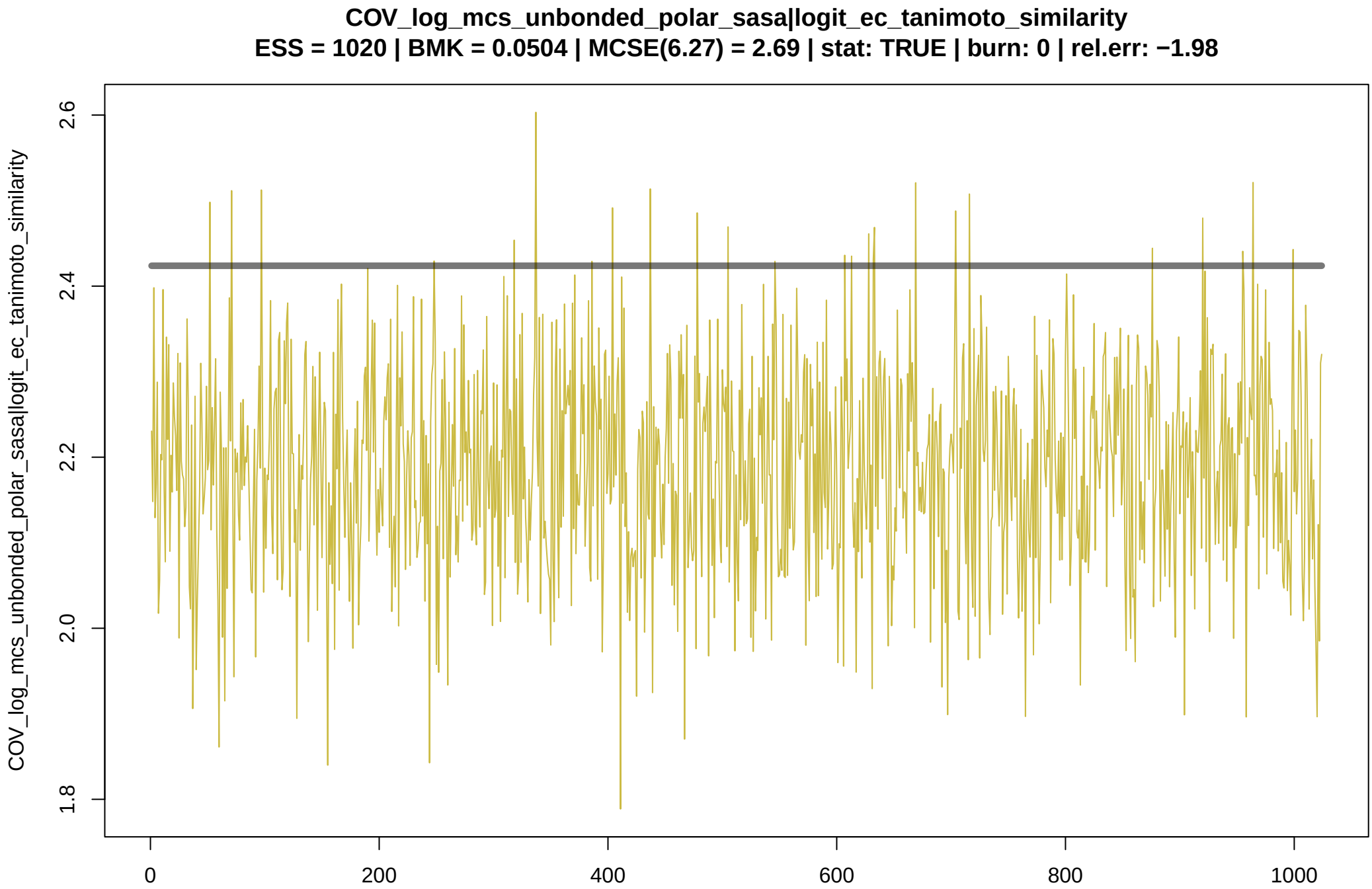

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0322 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | rel.err: −0.0223
COV_log_RMSD|mcs_NumHeteroAtoms
0.00
−0.05
−0.10
−0.15
−0.20
0
200
400
600
800
1000

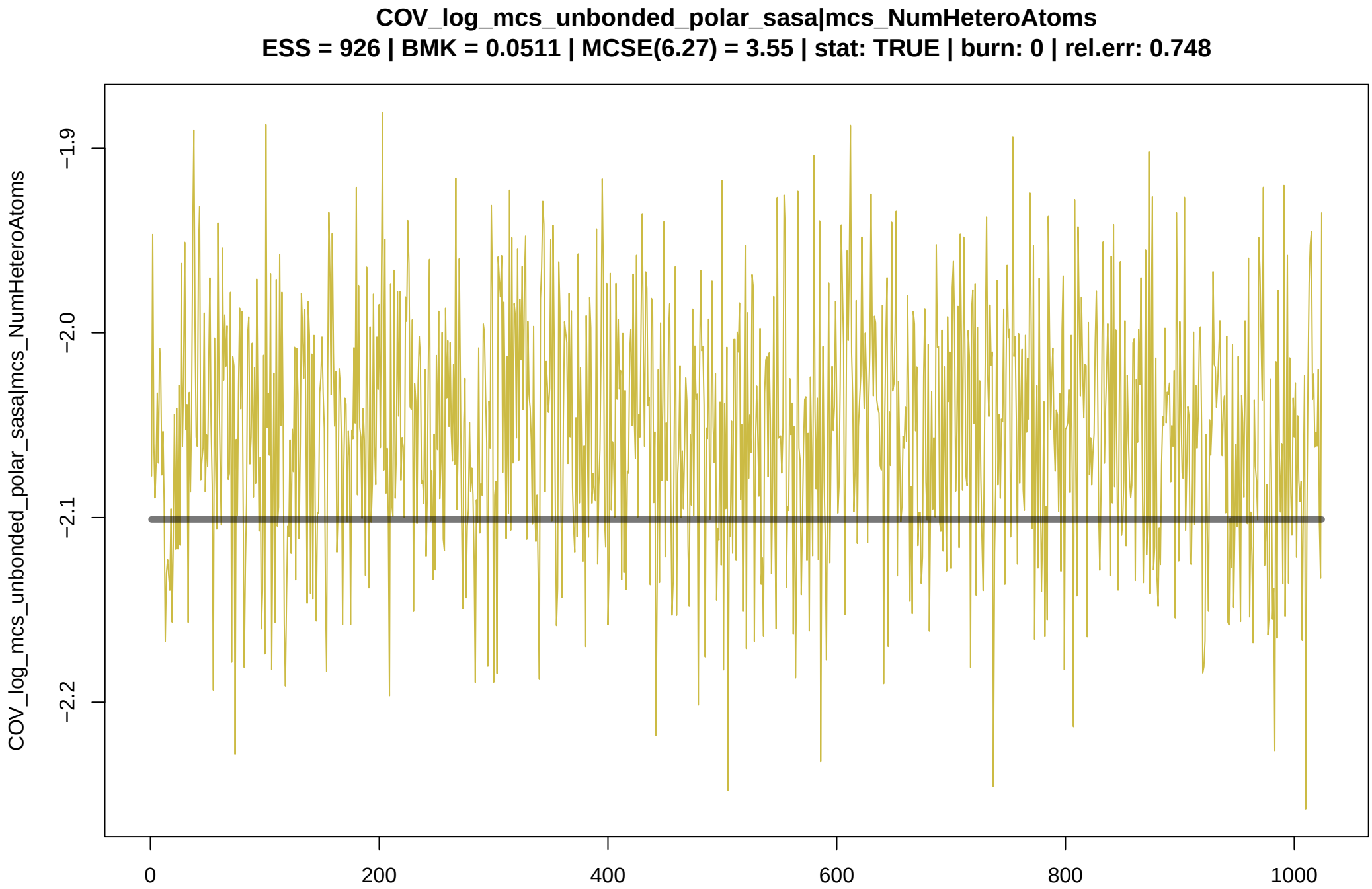

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0673 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | rel.err: 0.0291
COV_log_RMSD|docked_HeavyAtomCount
4.0
4.5
5.0
5.5
6.0
0
200
400
600
800
1000

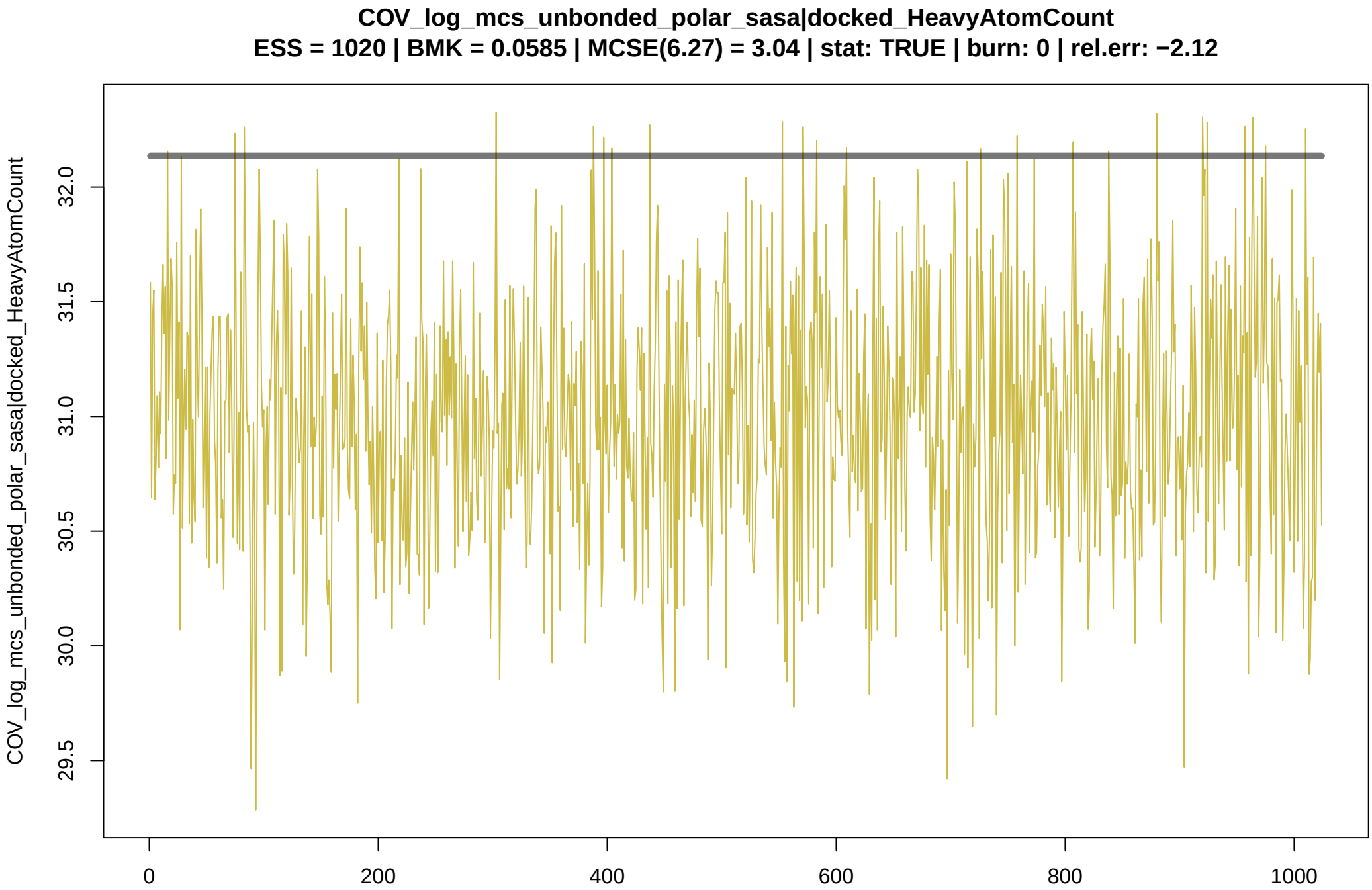

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0727 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0 | rel.err: 0.571
COV_log_RMSD|mcs_RingCount
0.00
0.05
0.10
0.15
0.20
0.25
0
200
400
600
800
1000

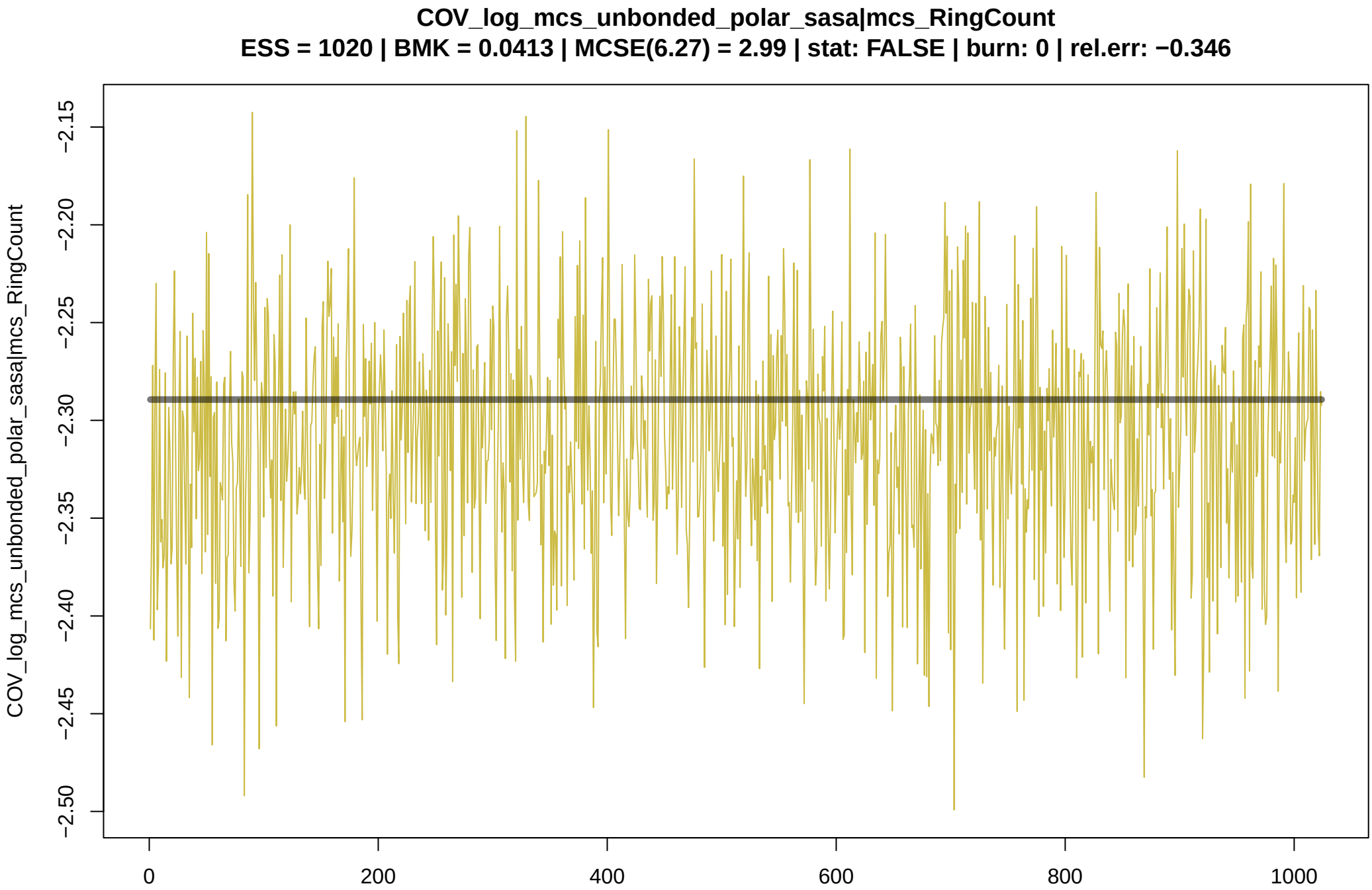

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0524 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | rel.err: −1.32
COV_log_RMSD|docked_NumRotatableBonds
−6.4
−6.6
−6.8
−7.0
0
200
400
600
800
1000

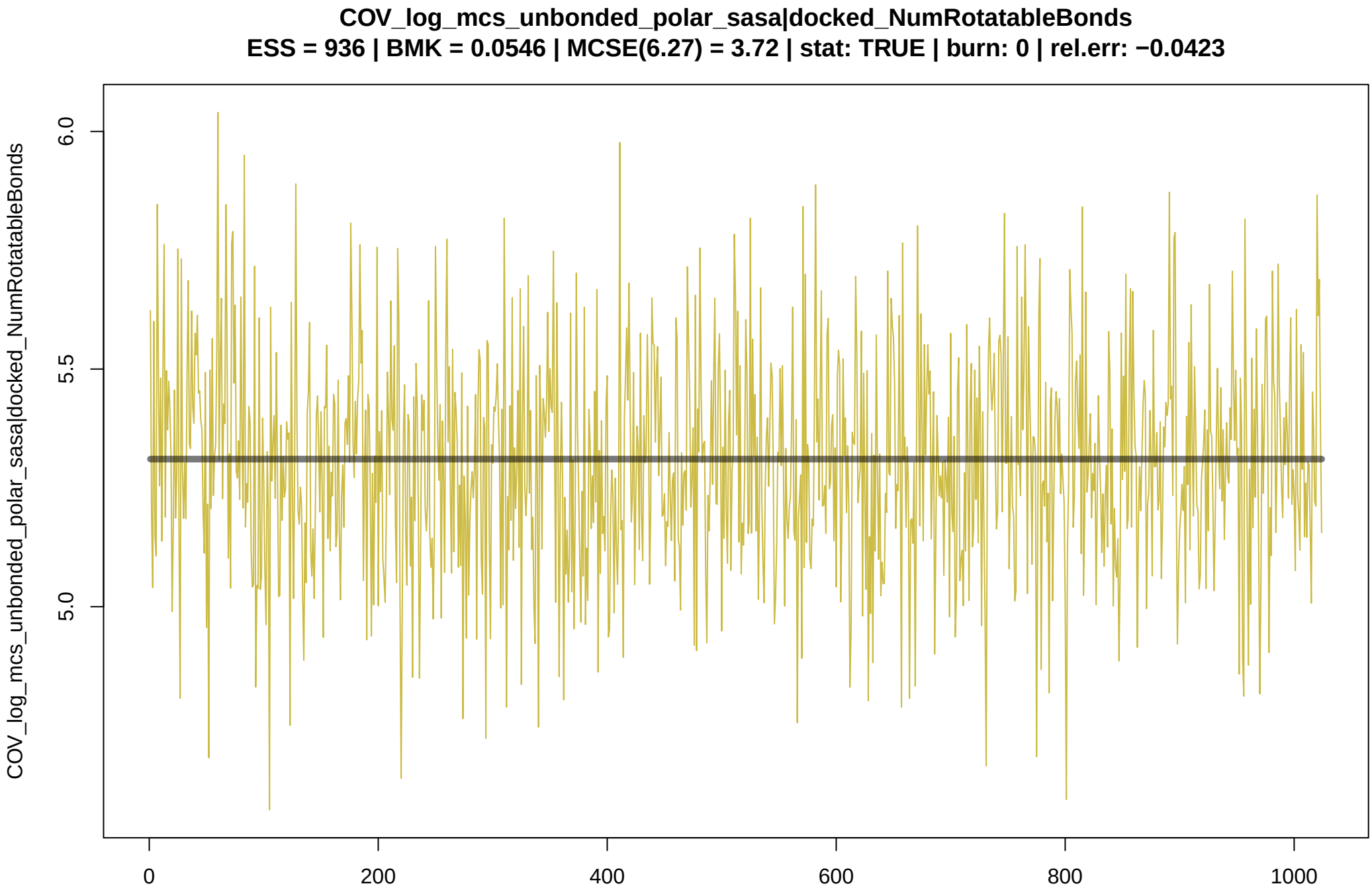

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.073 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0 | rel.err: −2.09
COV_log_RMSD|mcs_NOCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
200
400
600
800
1000

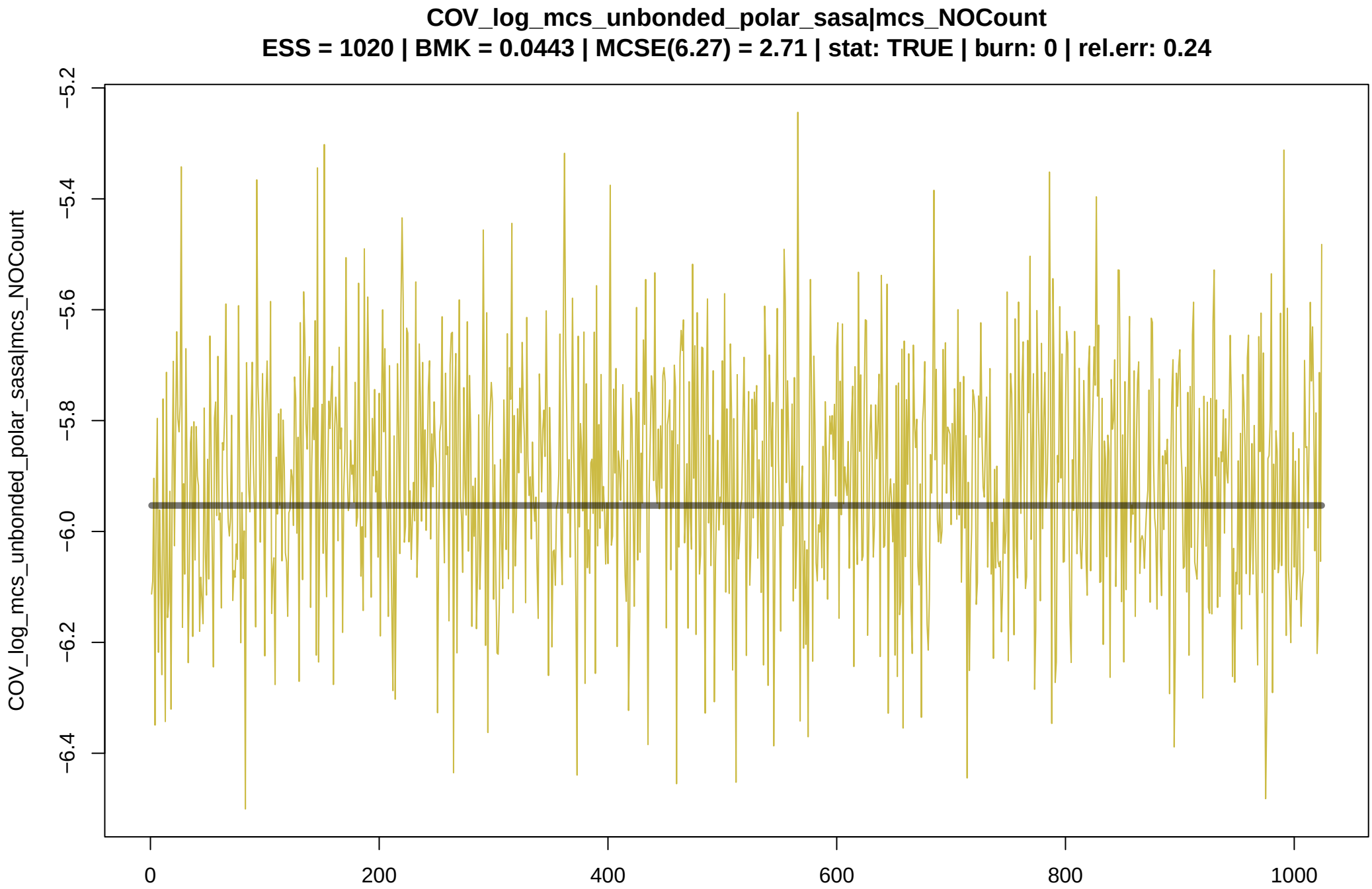

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0504 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | rel.err: −1.98
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2.6
2.4
2.2
2.0
1.8
0
200
400
600
800
1000

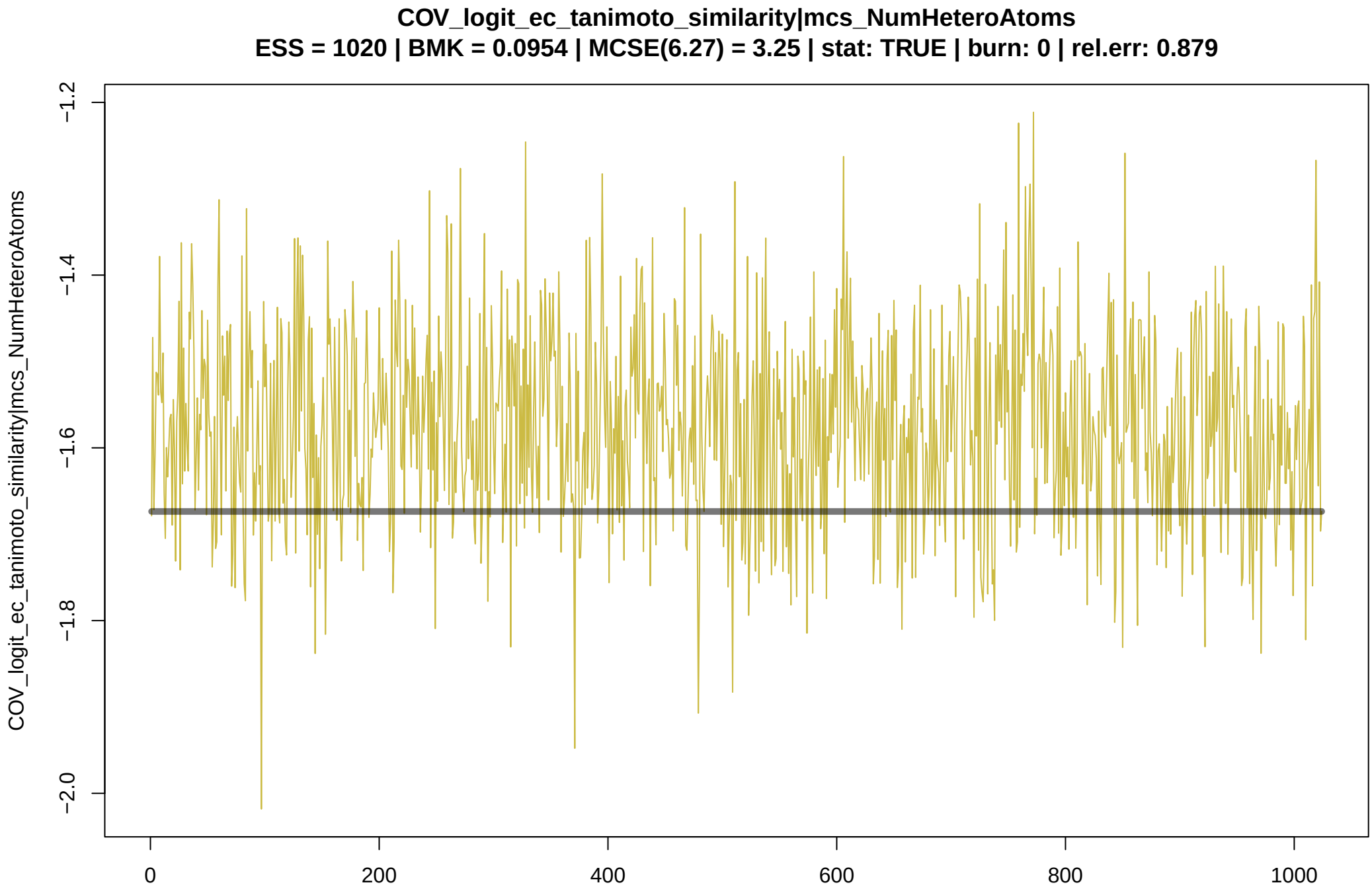

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 926 | BMK = 0.0511 | MCSE(6.27) = 3.55 | stat: TRUE | burn: 0 | rel.err: 0.748
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

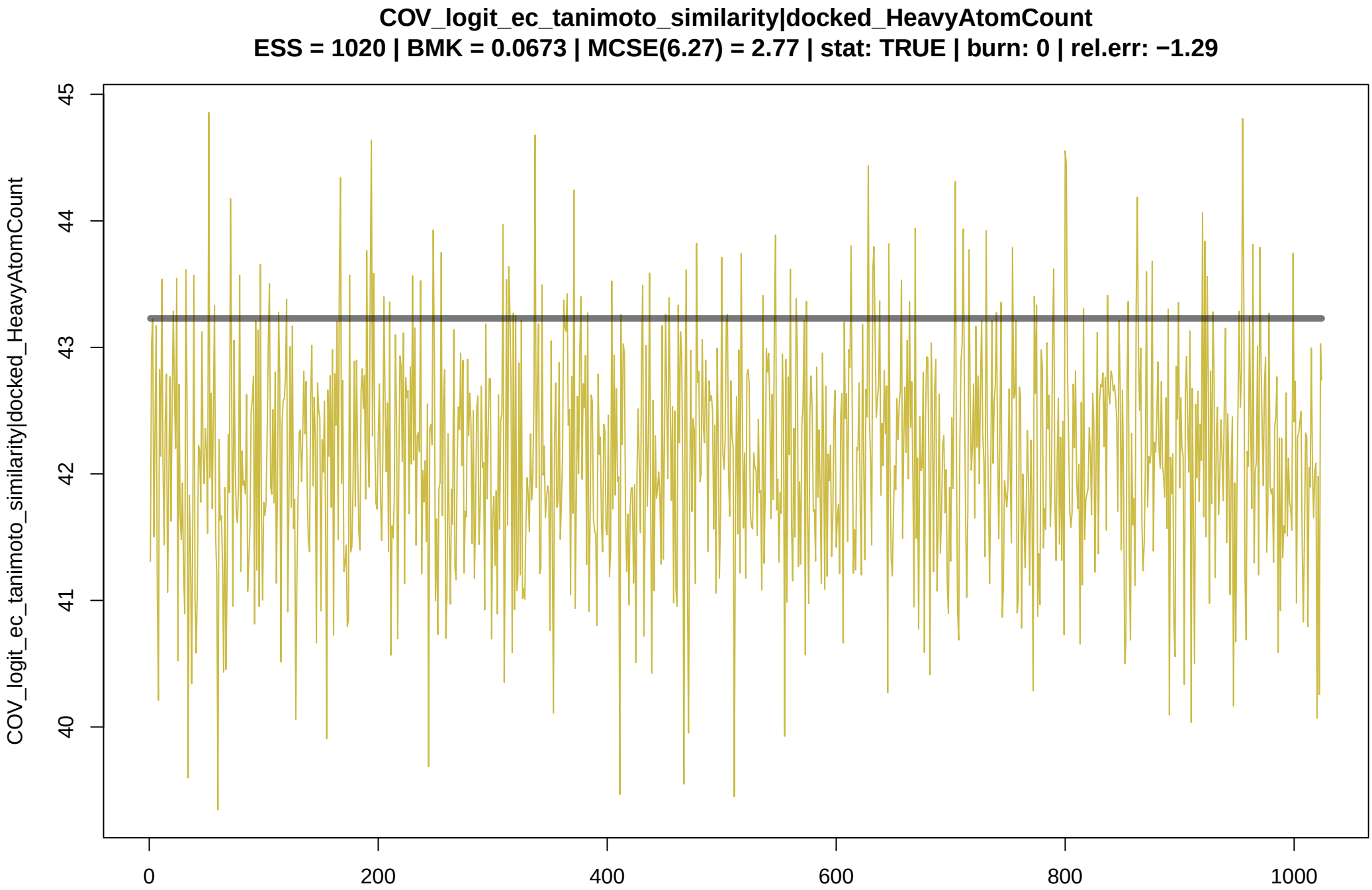

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0585 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: −2.12
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
29.5
30.0
30.5
31.0
31.5
32.0
0
200
400
600
800
1000

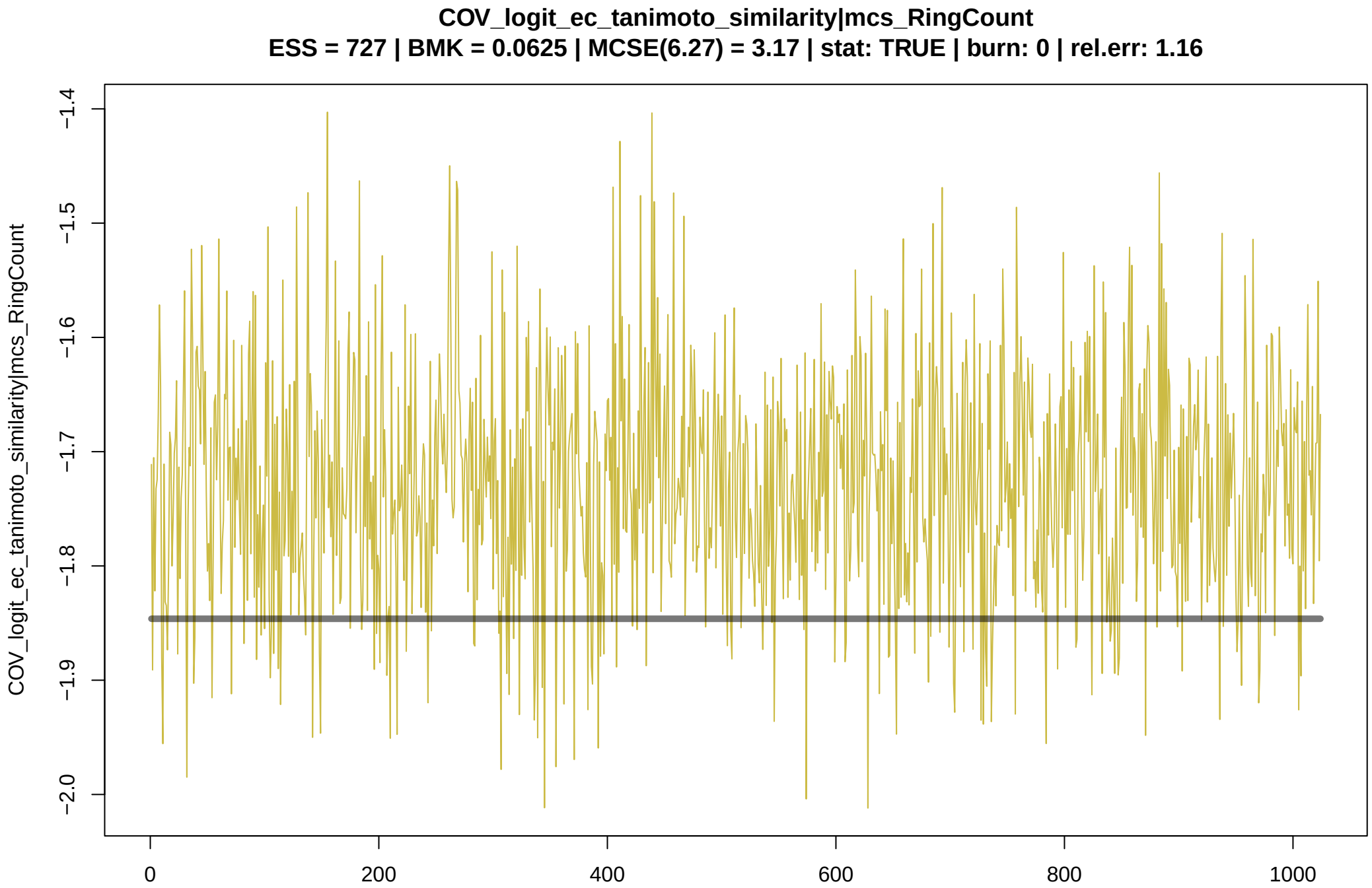

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0413 | MCSE(6.27) = 2.99 | stat: FALSE | burn: 0 | rel.err: −0.346
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.15
−2.20
−2.25
−2.30
−2.35
−2.40
−2.45
−2.50
0
200
400
600
800
1000

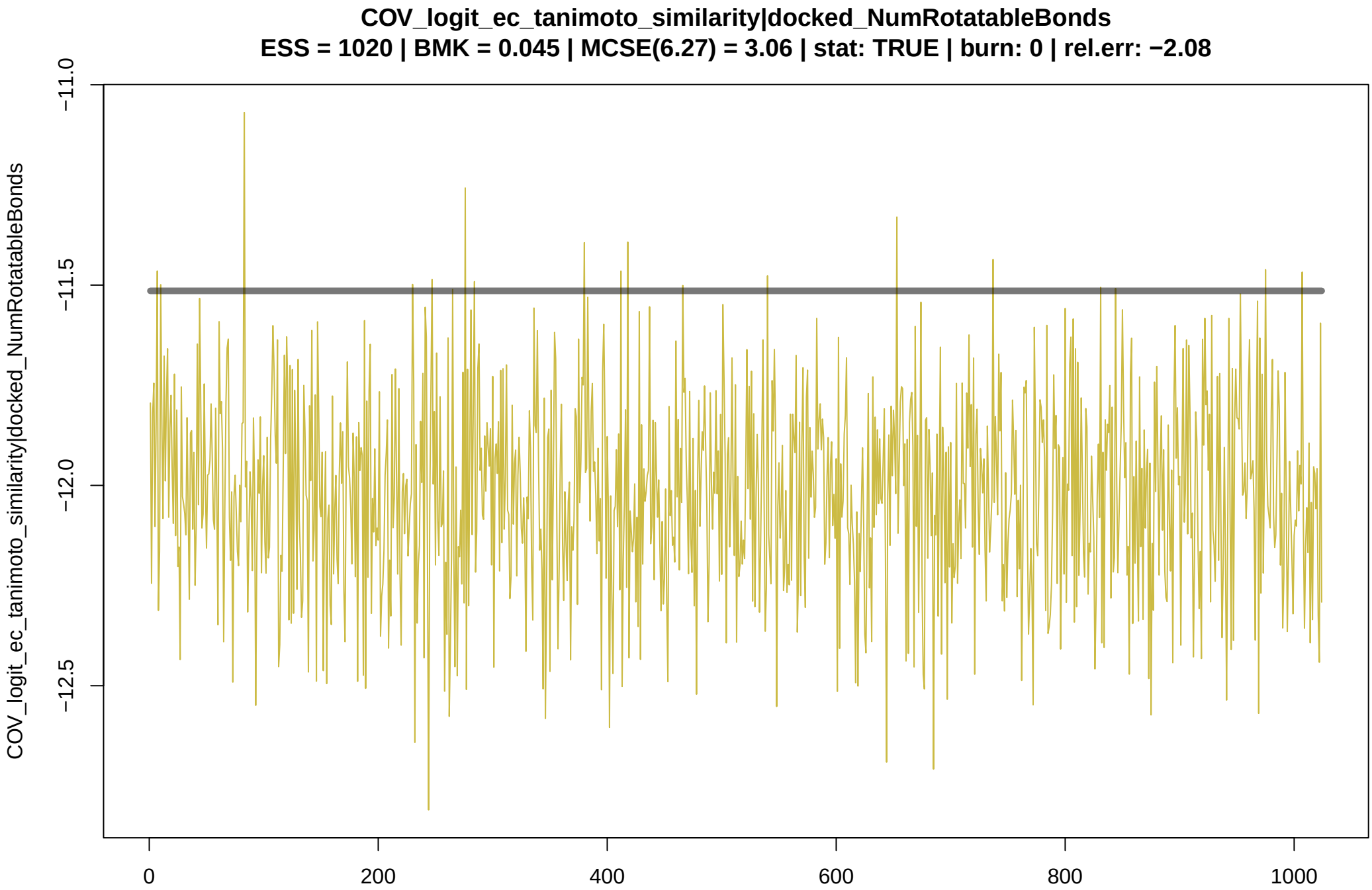

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 936 | BMK = 0.0546 | MCSE(6.27) = 3.72 | stat: TRUE | burn: 0 | rel.err: −0.0423
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
6.0
5.5
5.0
0
200
400
600
800
1000

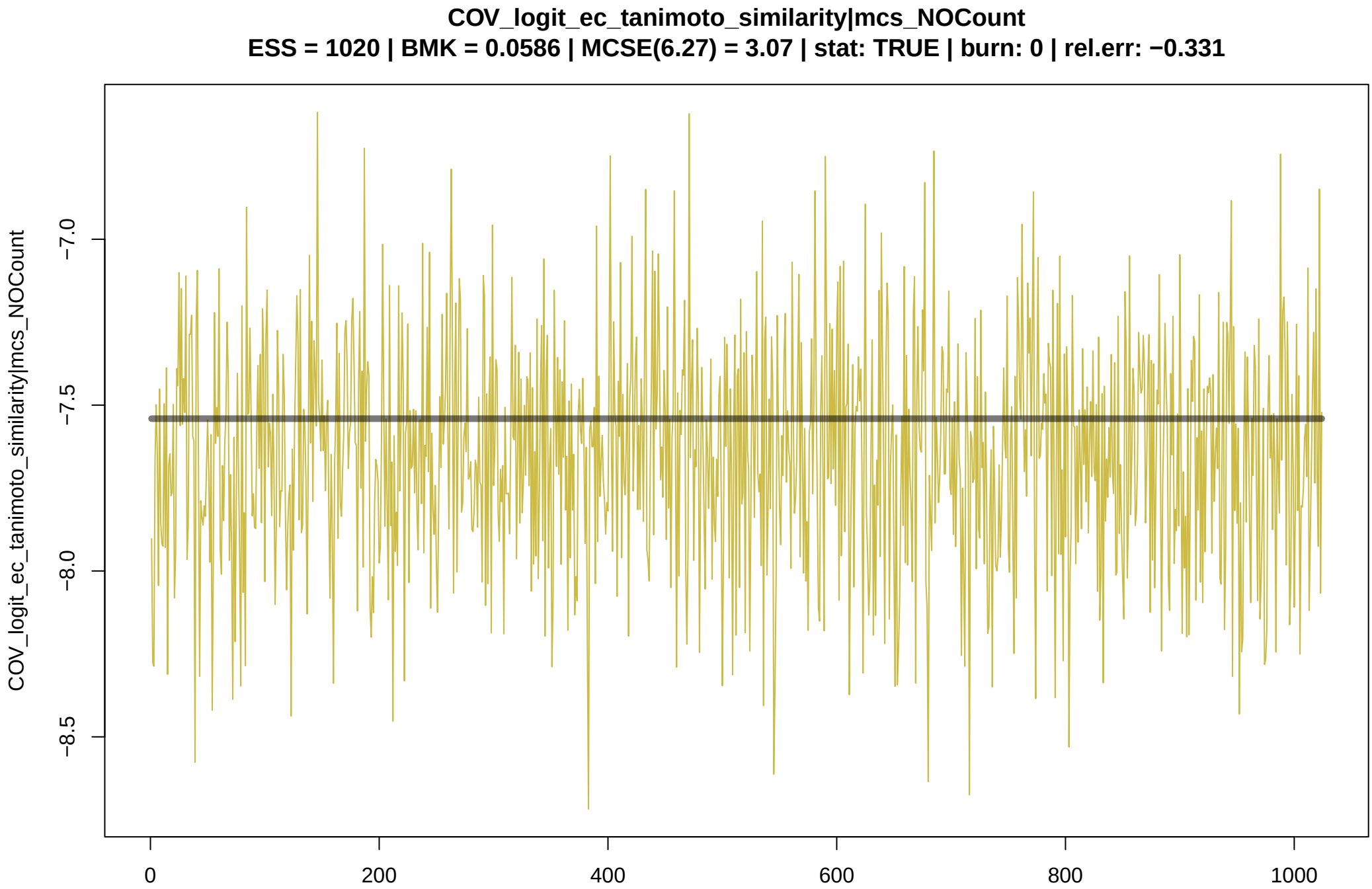

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0443 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | rel.err: 0.24
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.2
−5.4
−5.6
−5.8
−6.0
−6.2
−6.4
0
200
400
600
800
1000

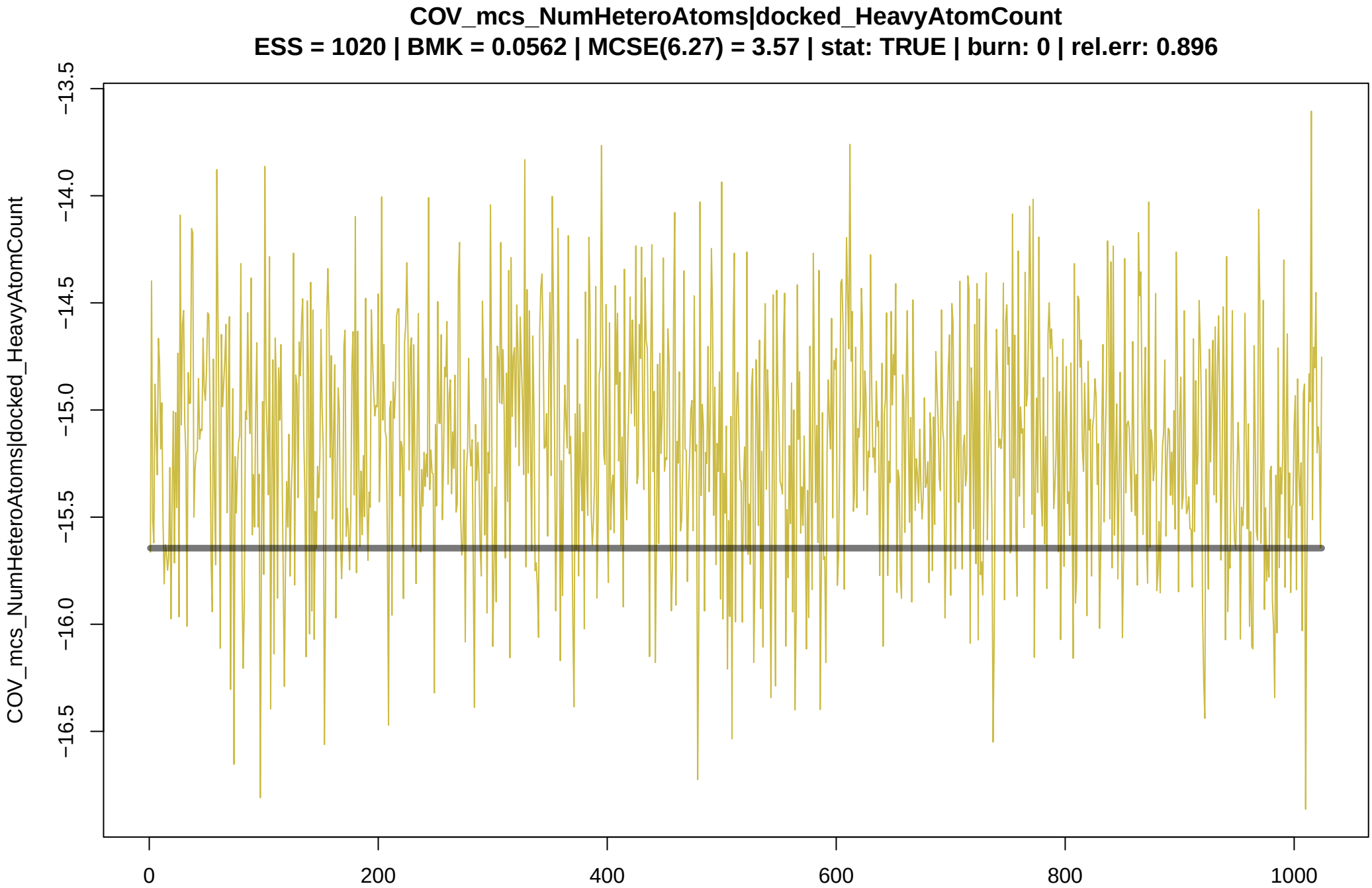

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0954 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | rel.err: 0.879
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.2
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

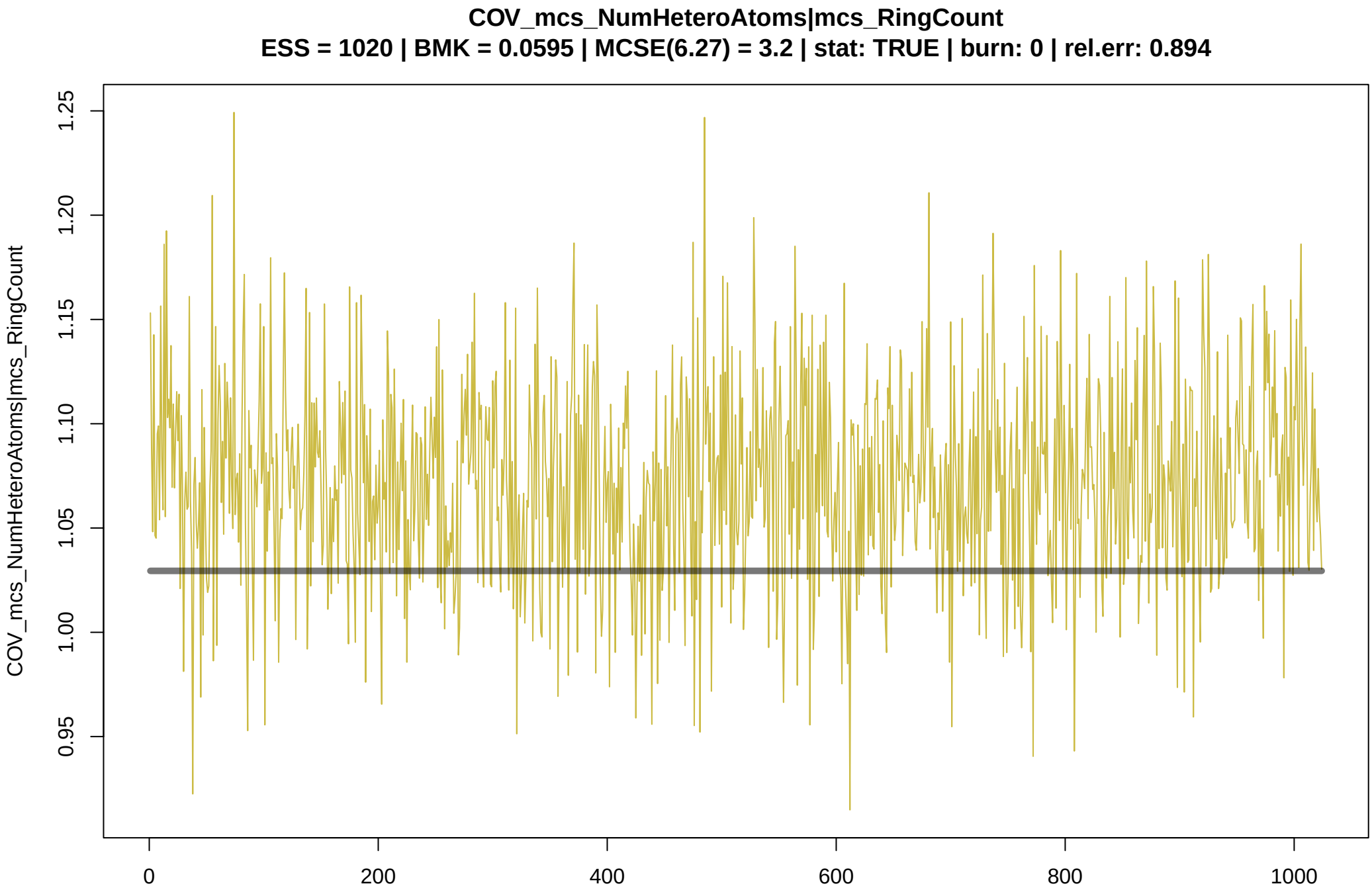

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0673 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0 | rel.err: −1.29
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
45
44
43
42
41
40
0
200
400
600
800
1000

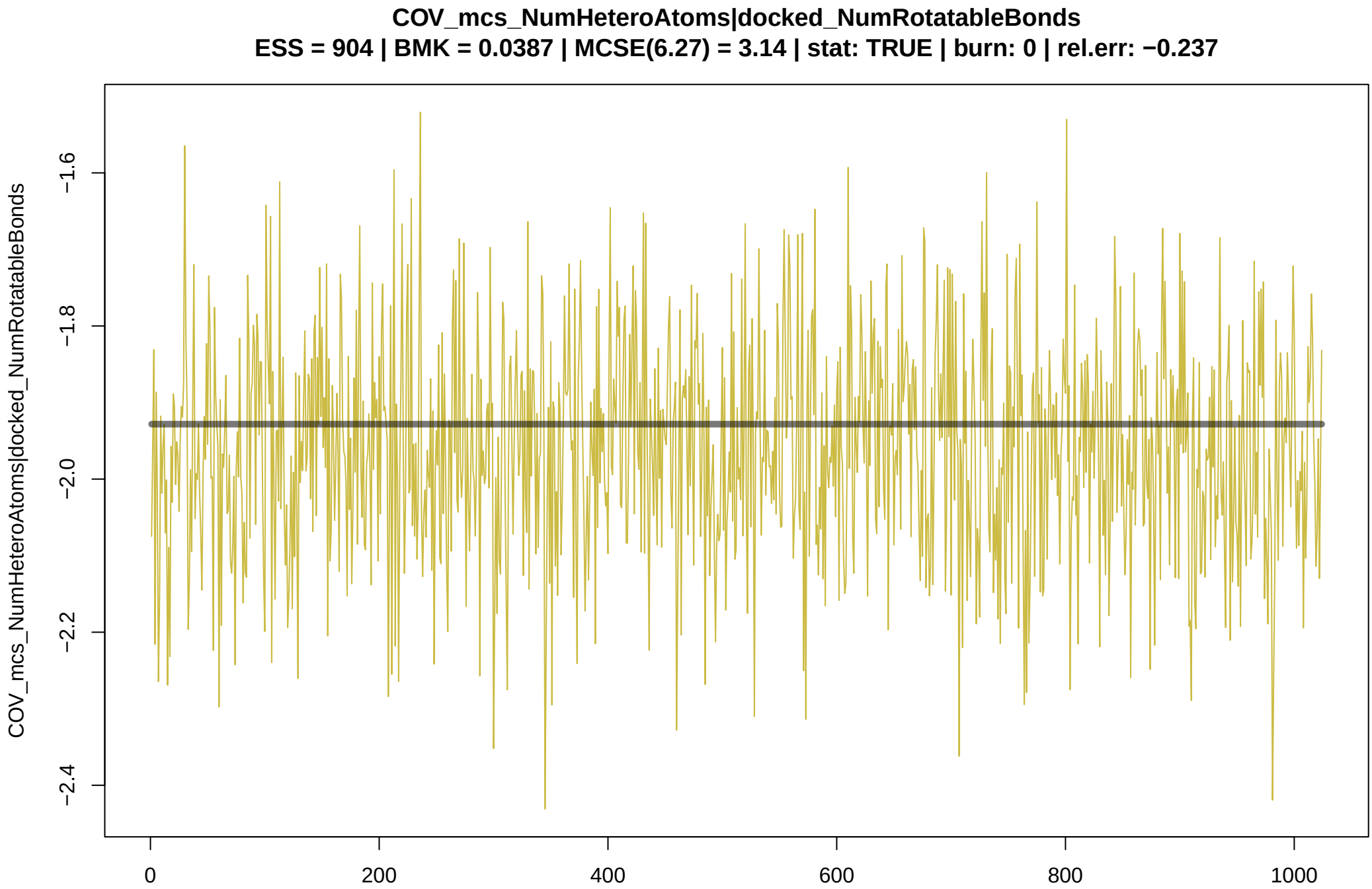

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 727 | BMK = 0.0625 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | rel.err: 1.16
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.4
−1.5
−1.6
−1.7
−1.8
−1.9
−2.0
0
200
400
600
800
1000

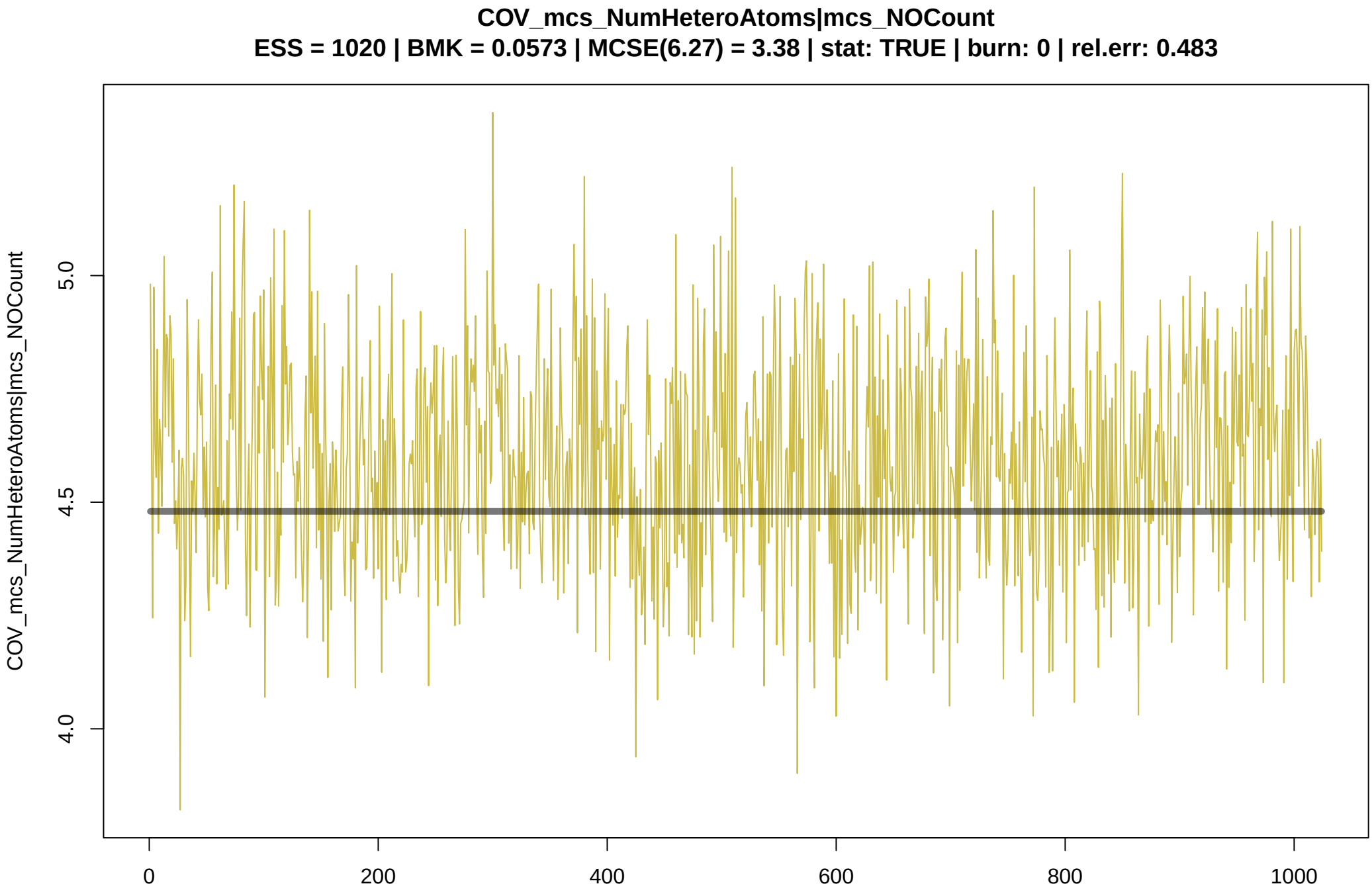

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.045 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | rel.err: −2.08
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−11.0
−11.5
−12.0
−12.5
0
200
400
600
800
1000

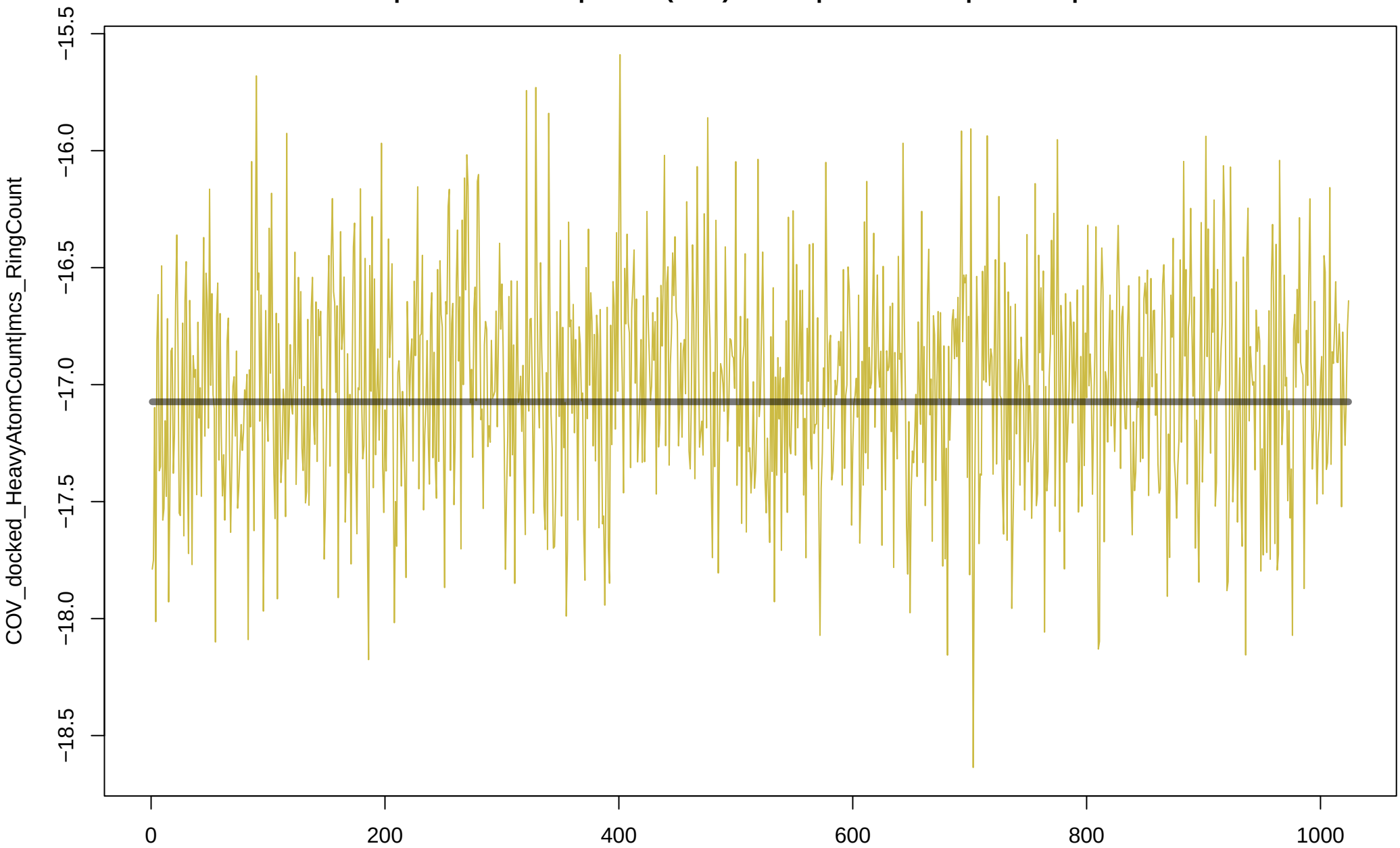

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0586 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | rel.err: −0.331
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−7.0
−7.5
−8.0
−8.5
0
200
400
600
800
1000

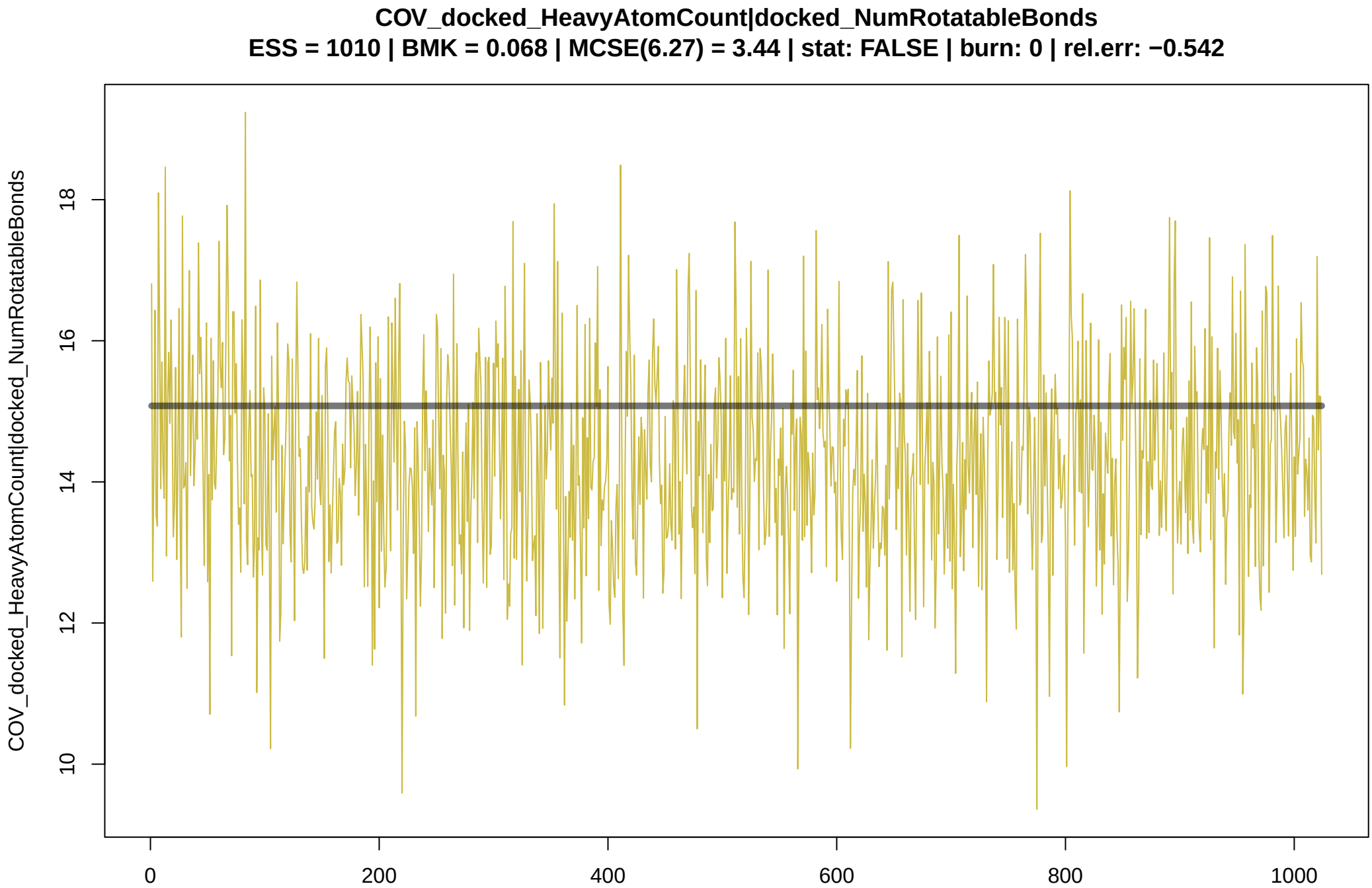

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0562 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | rel.err: 0.896
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−13.5
−14.0
−14.5
−15.0
−15.5
−16.0
−16.5
0
200
400
600
800
1000

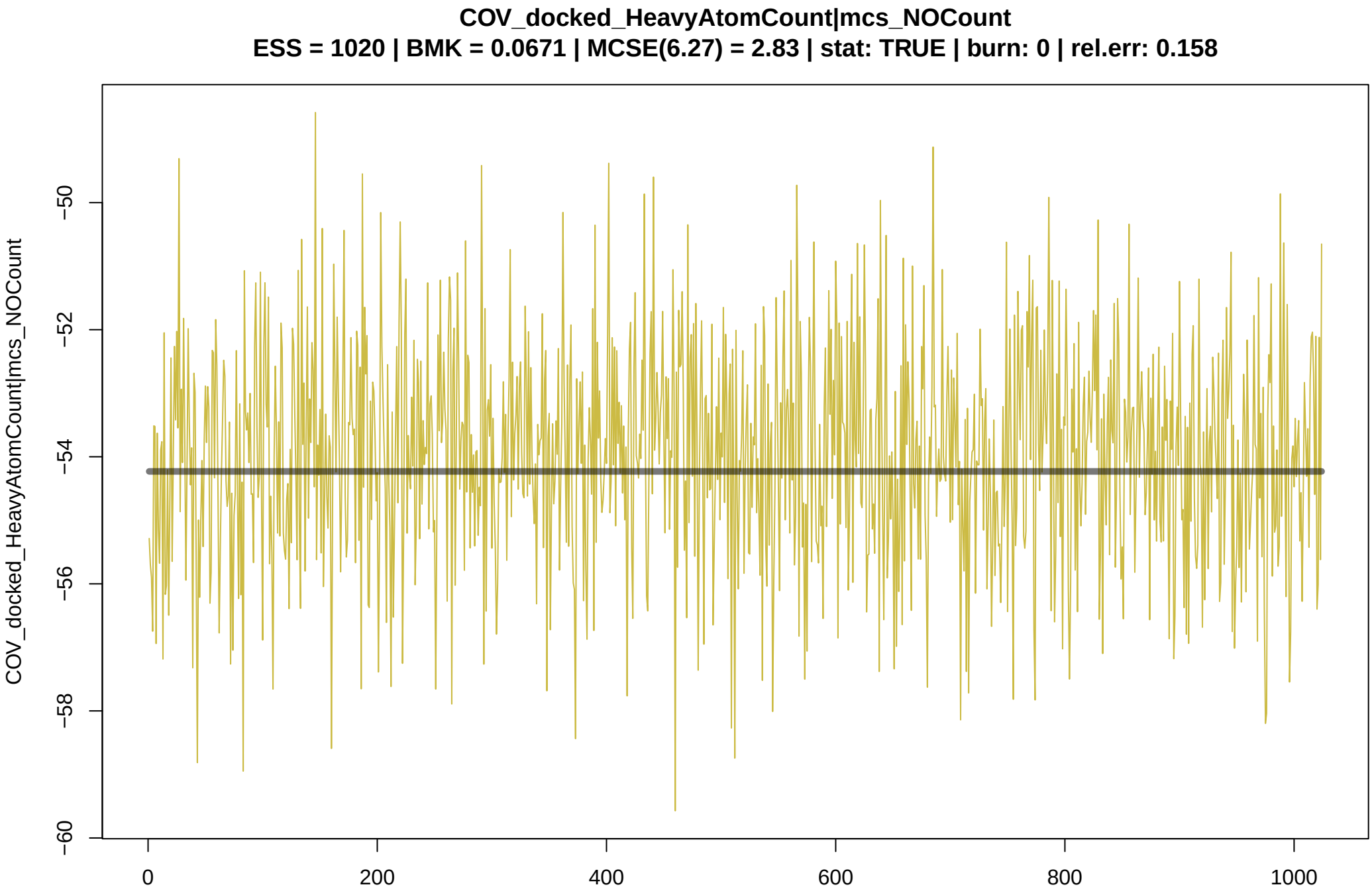

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0595 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: 0.894
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.95
1.00
1.05
1.10
1.15
1.20
1.25
0
200
400
600
800
1000

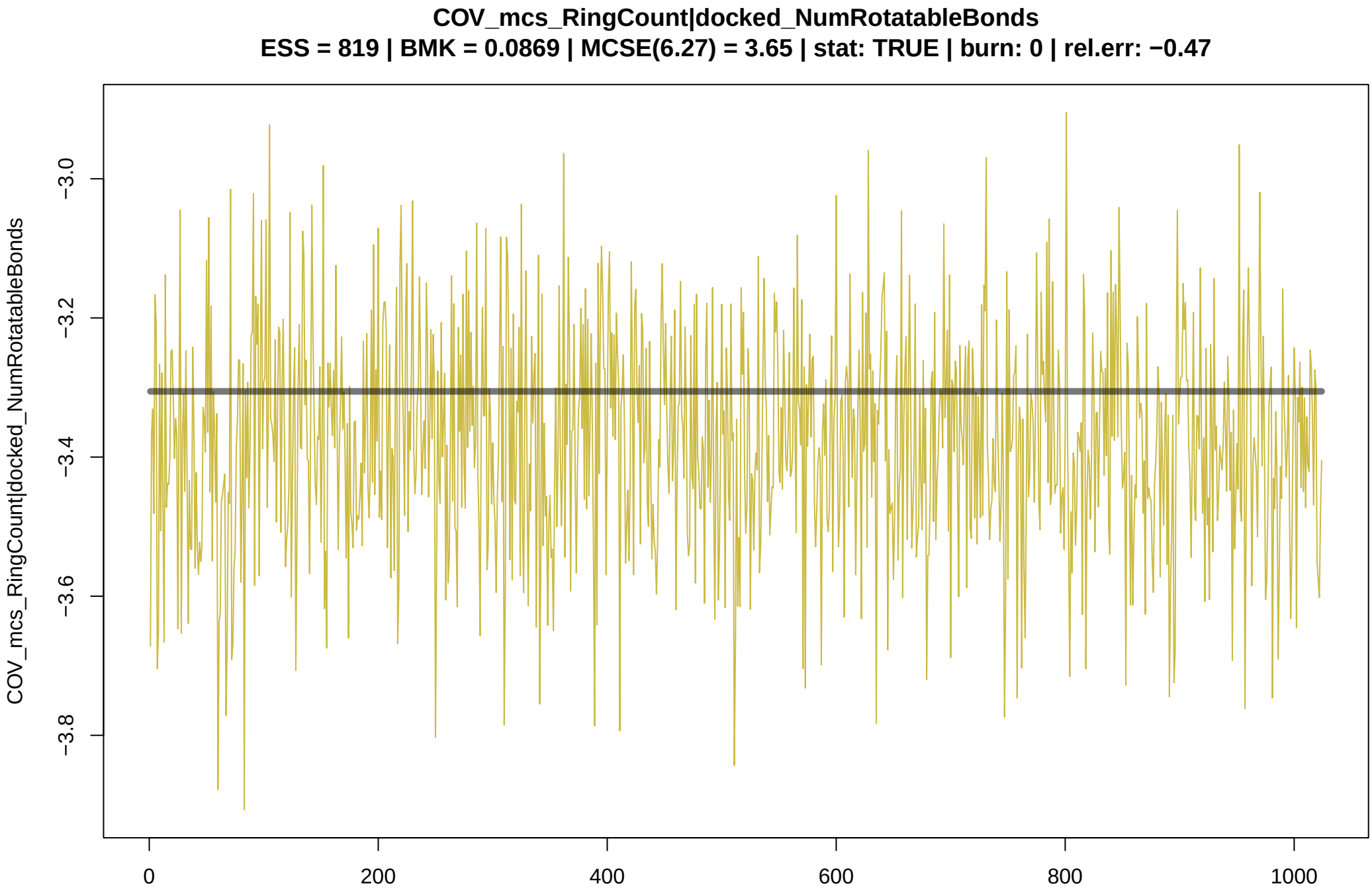

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 904 | BMK = 0.0387 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | rel.err: −0.237
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.6
−1.8
−2.0
−2.2
−2.4
0
200
400
600
800
1000

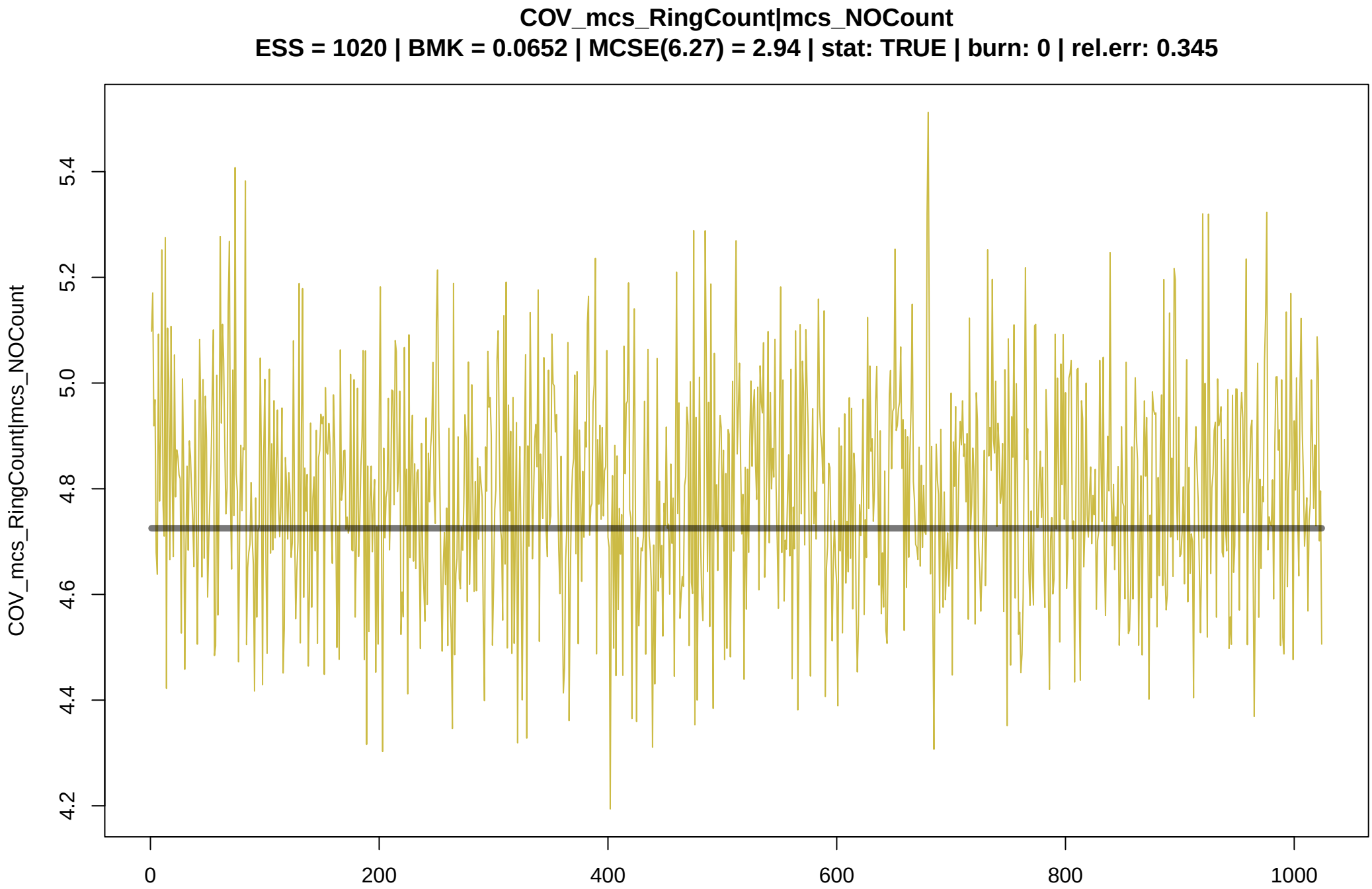

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0573 | MCSE(6.27) = 3.38 | stat: TRUE | burn: 0 | rel.err: 0.483
COV_mcs_NumHeteroAtoms|mcs_NOCount
4.0
4.5
5.0
0
200
400
600
800
1000

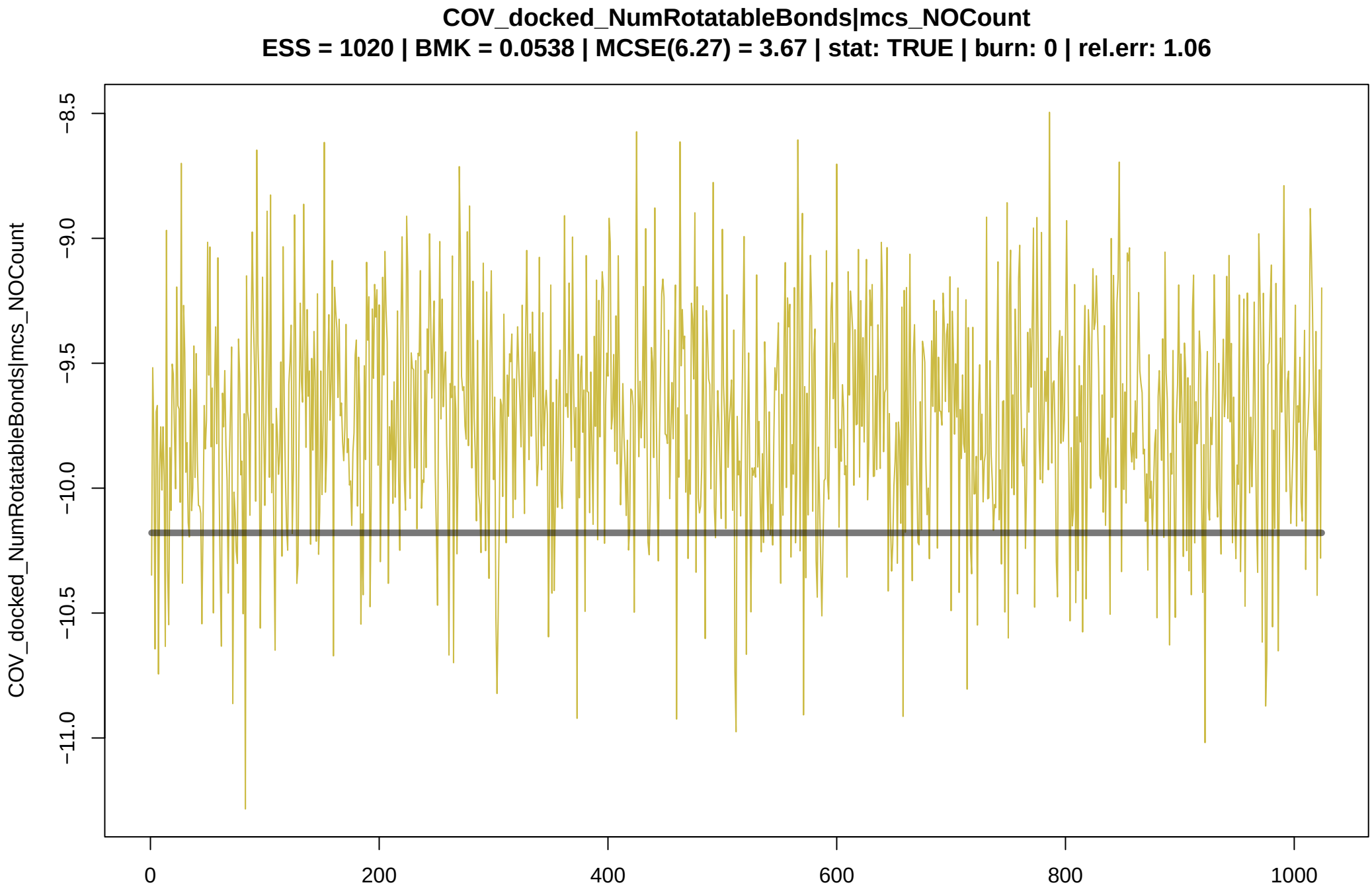

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 909 | BMK = 0.0512 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0 | rel.err: 0.166
COV_docked_HeavyAtomCount|mcs_RingCount
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1010 | BMK = 0.068 | MCSE(6.27) = 3.44 | stat: FALSE | burn: 0 | rel.err: −0.542
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0671 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | rel.err: 0.158
COV_docked_HeavyAtomCount|mcs_NOCount
−50
−52
−54
−56
−58
−60
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 819 | BMK = 0.0869 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0 | rel.err: −0.47
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 = 1020 | BMK = 0.0652 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | rel.err: 0.345
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 = 0.0538 | MCSE(6.27) = 3.67 | stat: TRUE | burn: 0 | rel.err: 1.06
COV_docked_NumRotatableBonds|mcs_NOCount
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
0
200
400
600
800
1000