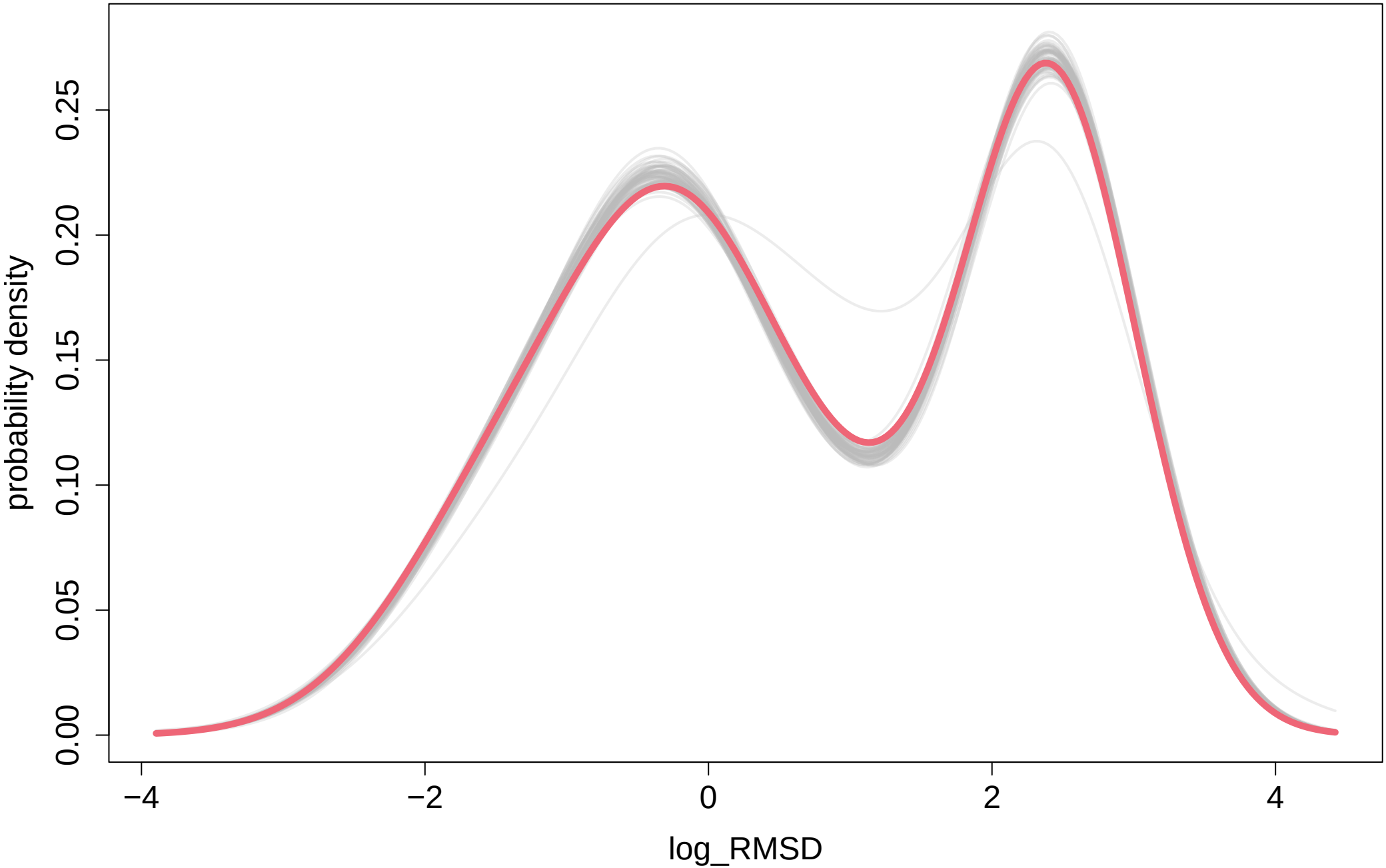
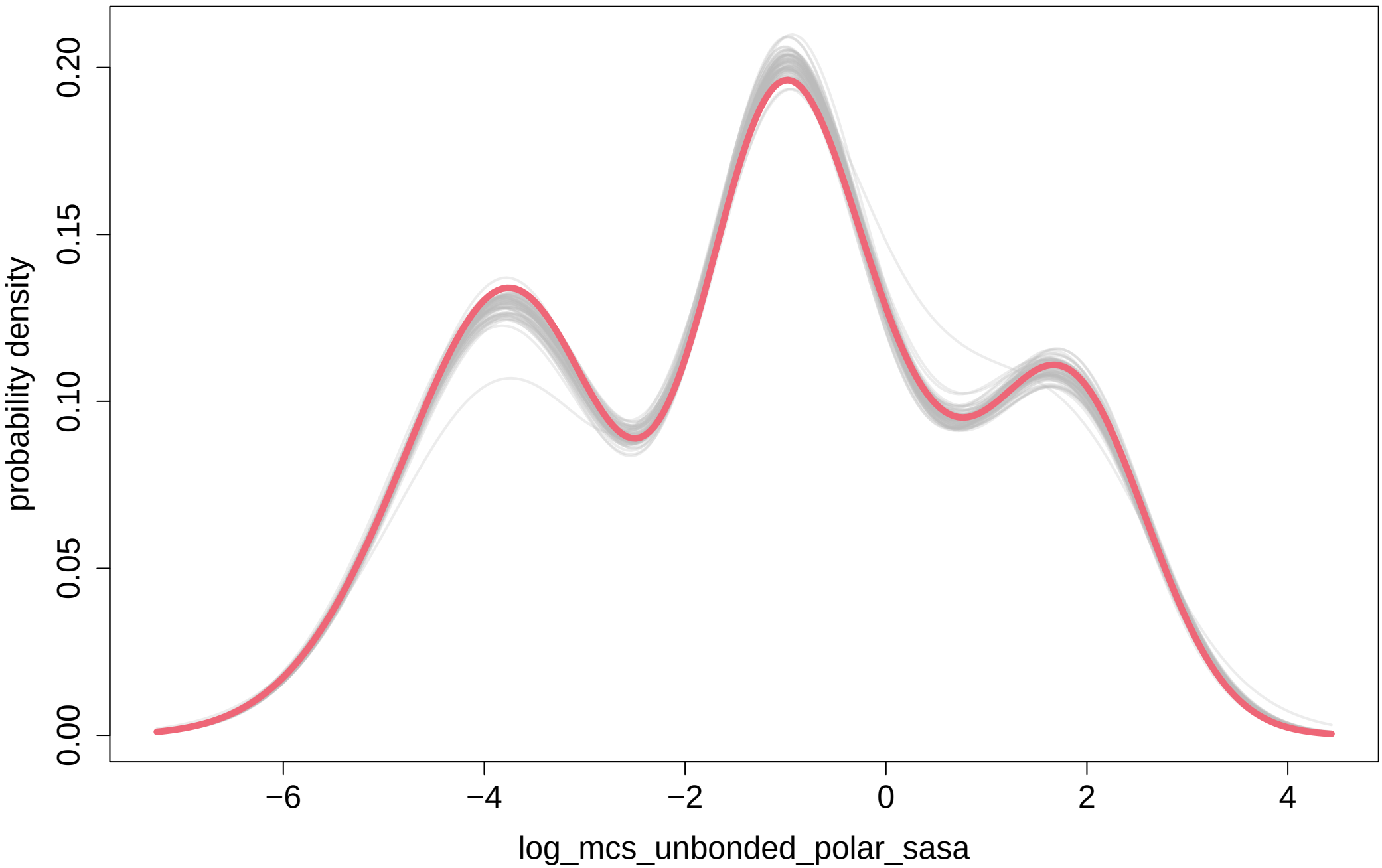
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 1
max MCSE = 14.8963594992563
all stationary: FALSE
burn: 1020
max rel.err.: 4.11409217408066

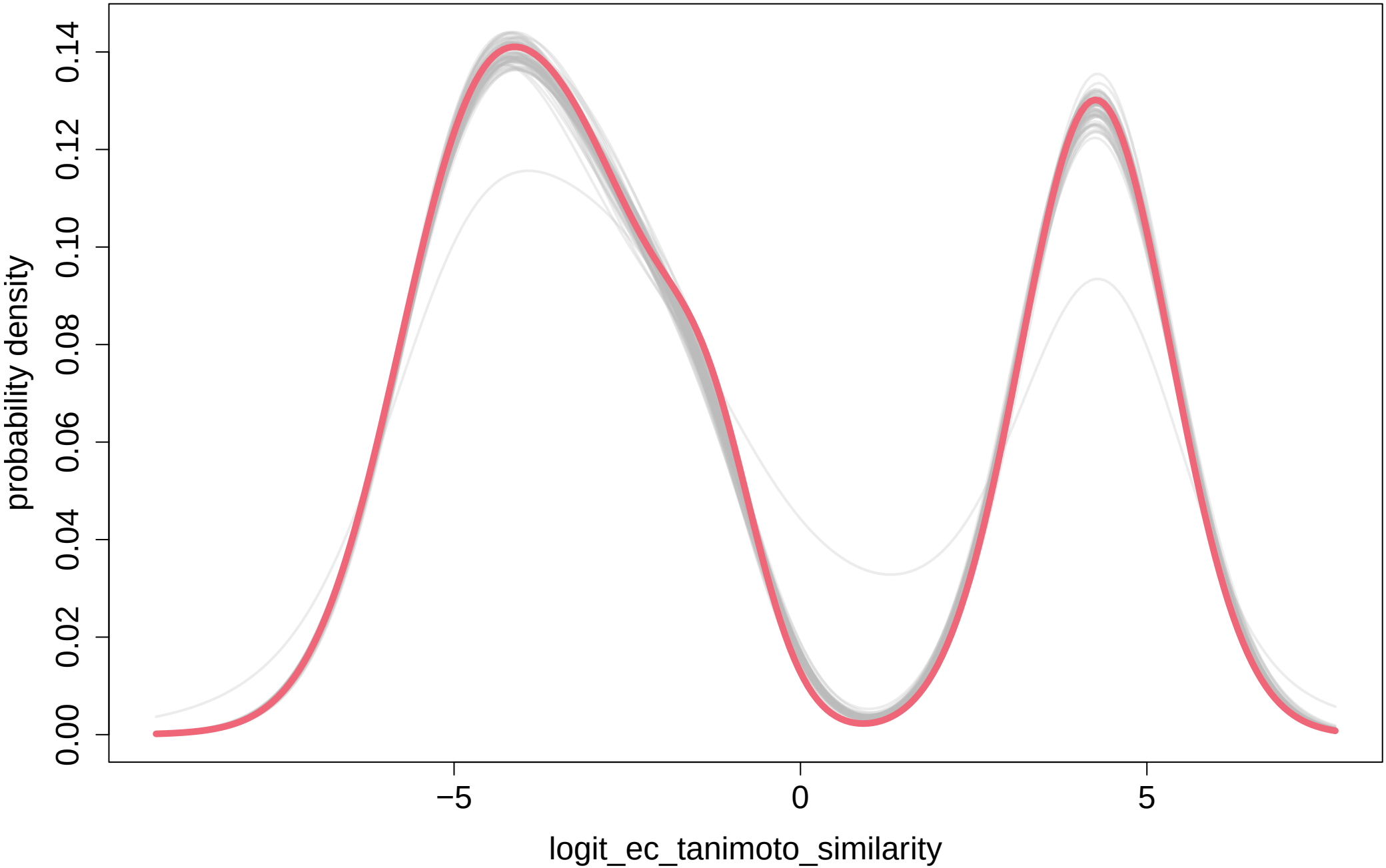
−− STATS 2D −−
min ESS = 769.451675575034
max BMK = 0.07768424292017 9
max MCSE = 3.95588997434827
all stationary: FALSE
burn: 0
max rel.err.: 1.41321100359497

−− STATS 1D −−
min ESS = 30.2057789584234
max BMK = 0.302005246427818
max MCSE = 9.36819534958588
all stationary: FALSE
burn: 0
max rel.err.: 1.61981048882467

Occupied clusters: 9 of 64
LL: −125000 +− 296


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


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


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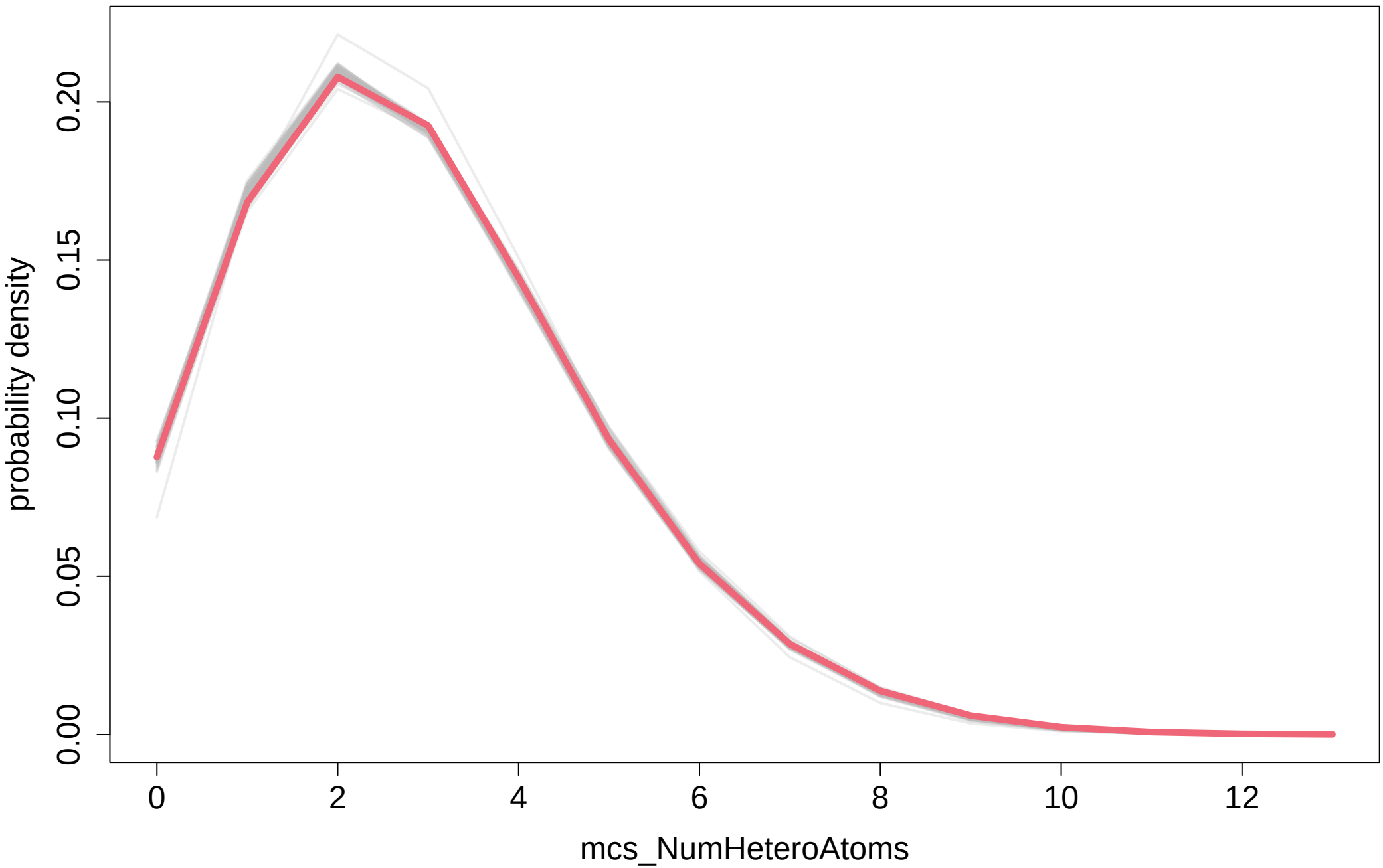
0.06
0.08
0.10
0.12
0.14
−5
0
5
logit_ec_tanimoto_similarity


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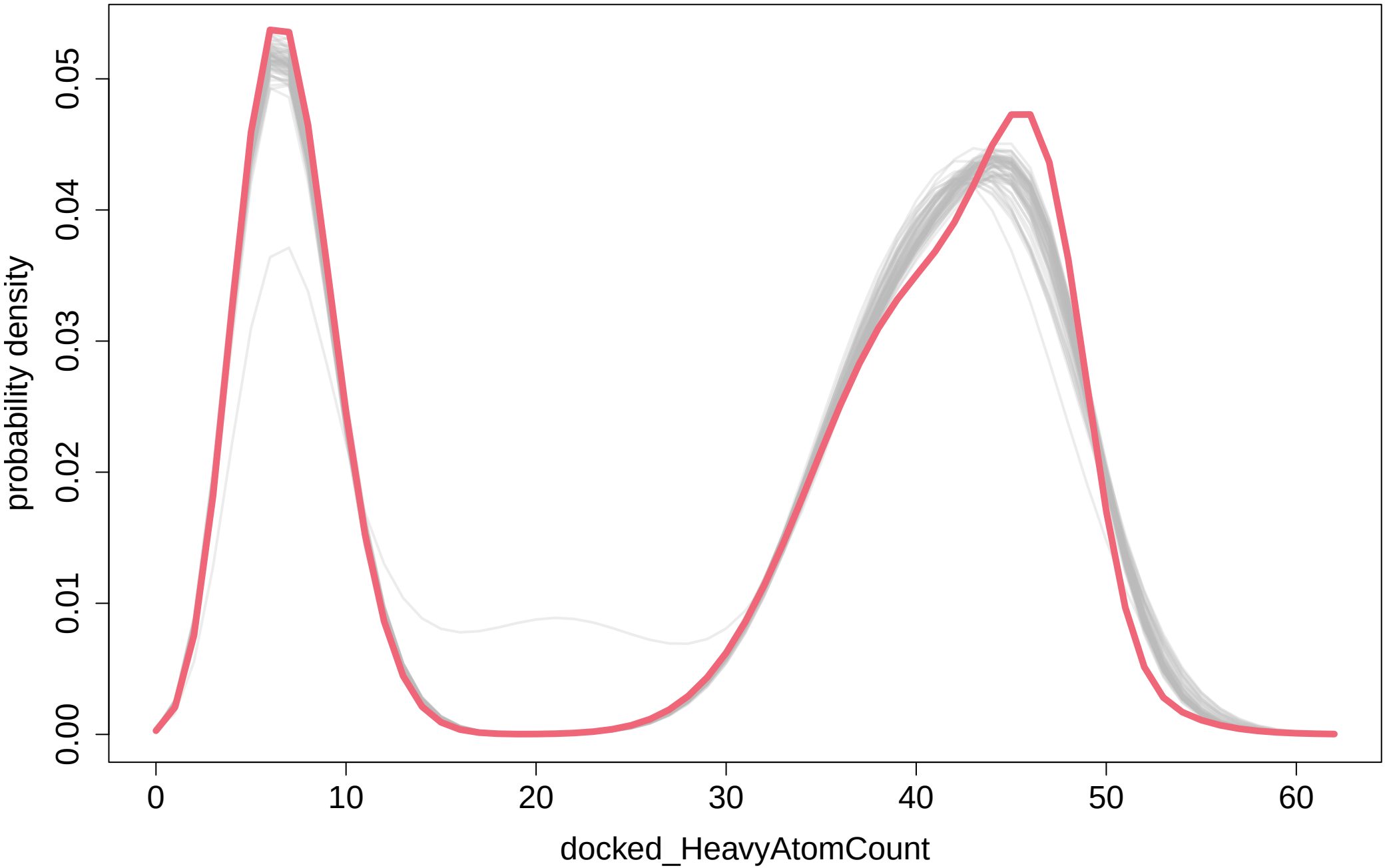
0.10
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms


probability density
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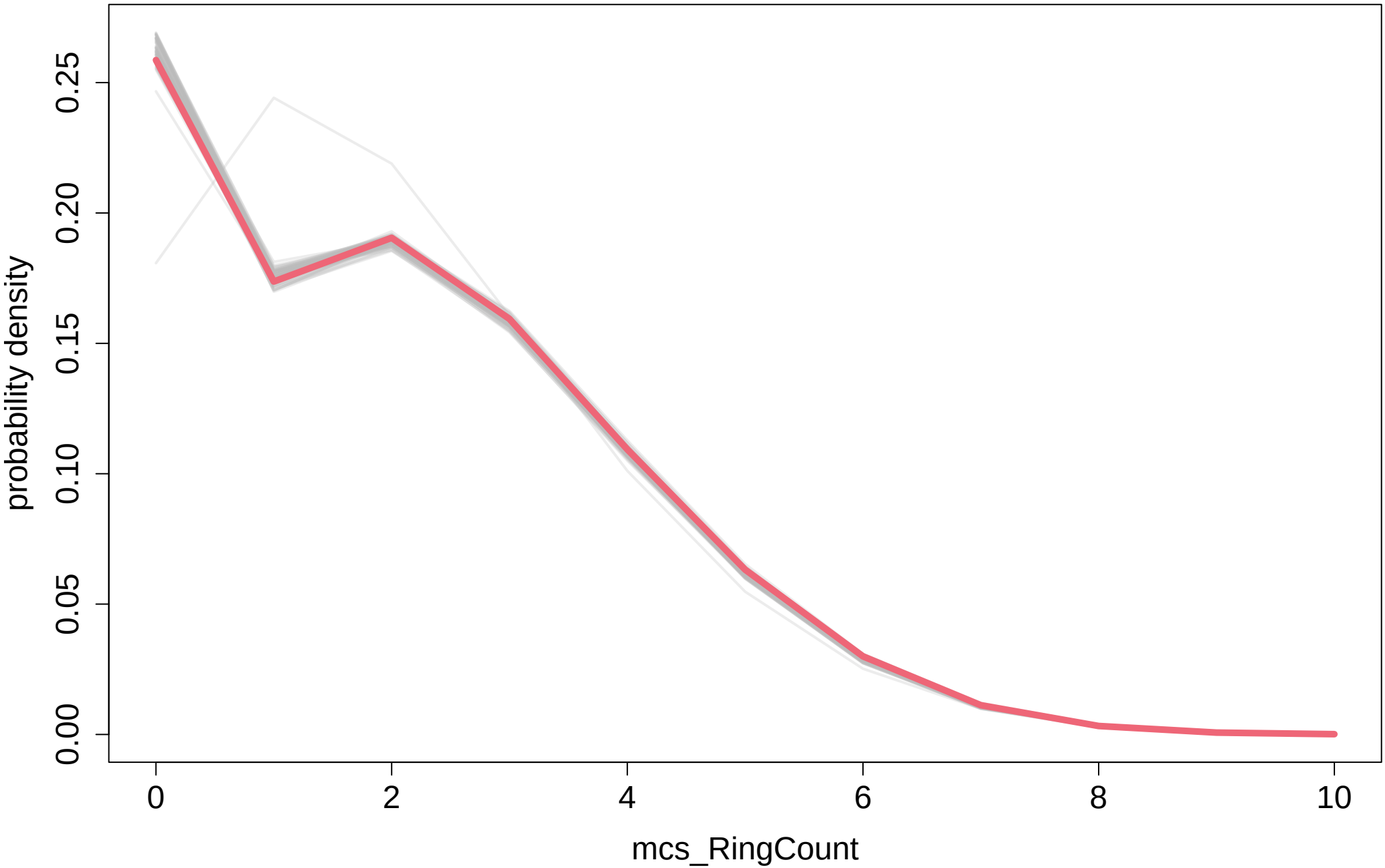
0.01
0.02
0.03
0.04
0.05
0
10
20
30
40
50
60
docked_HeavyAtomCount


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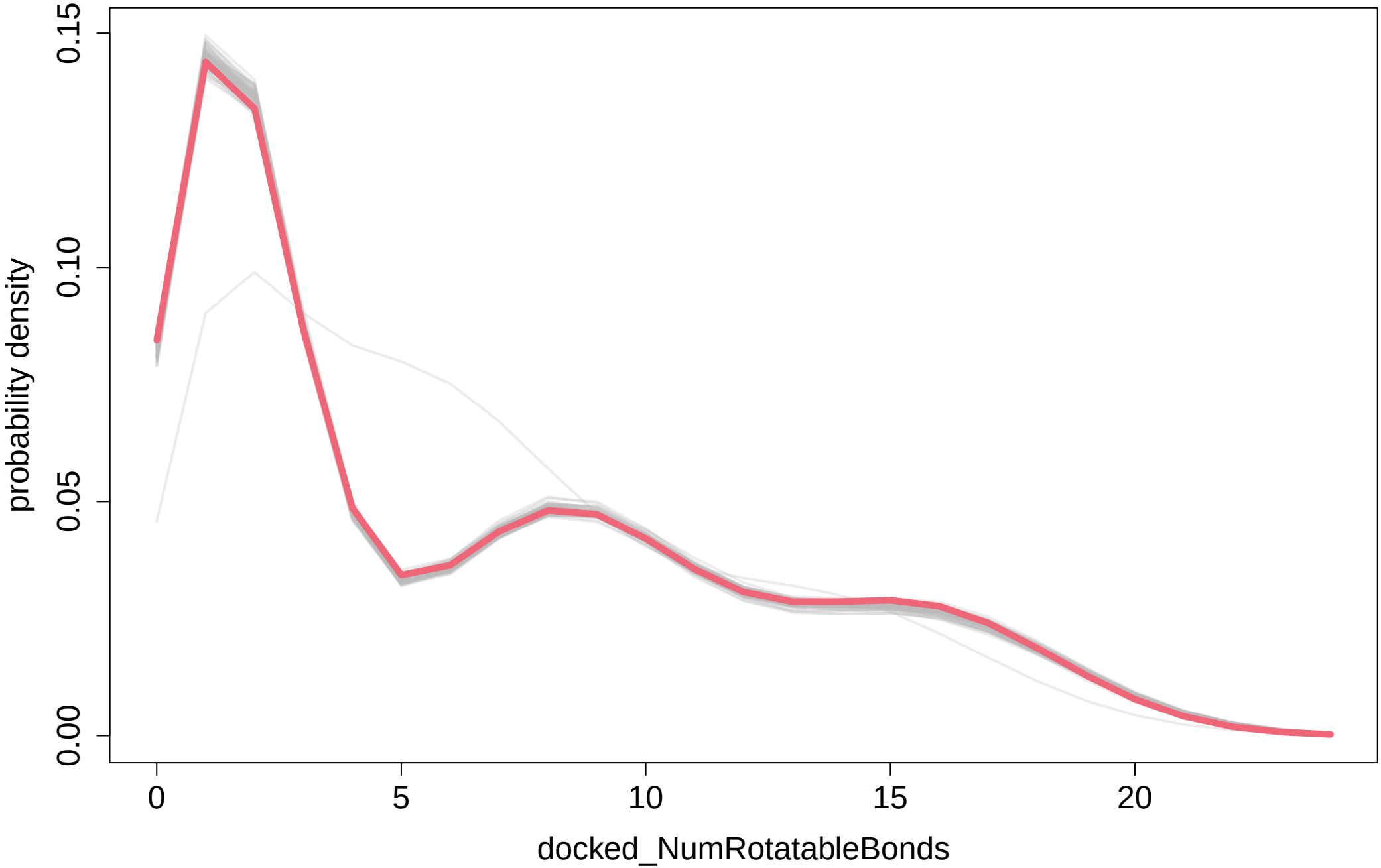
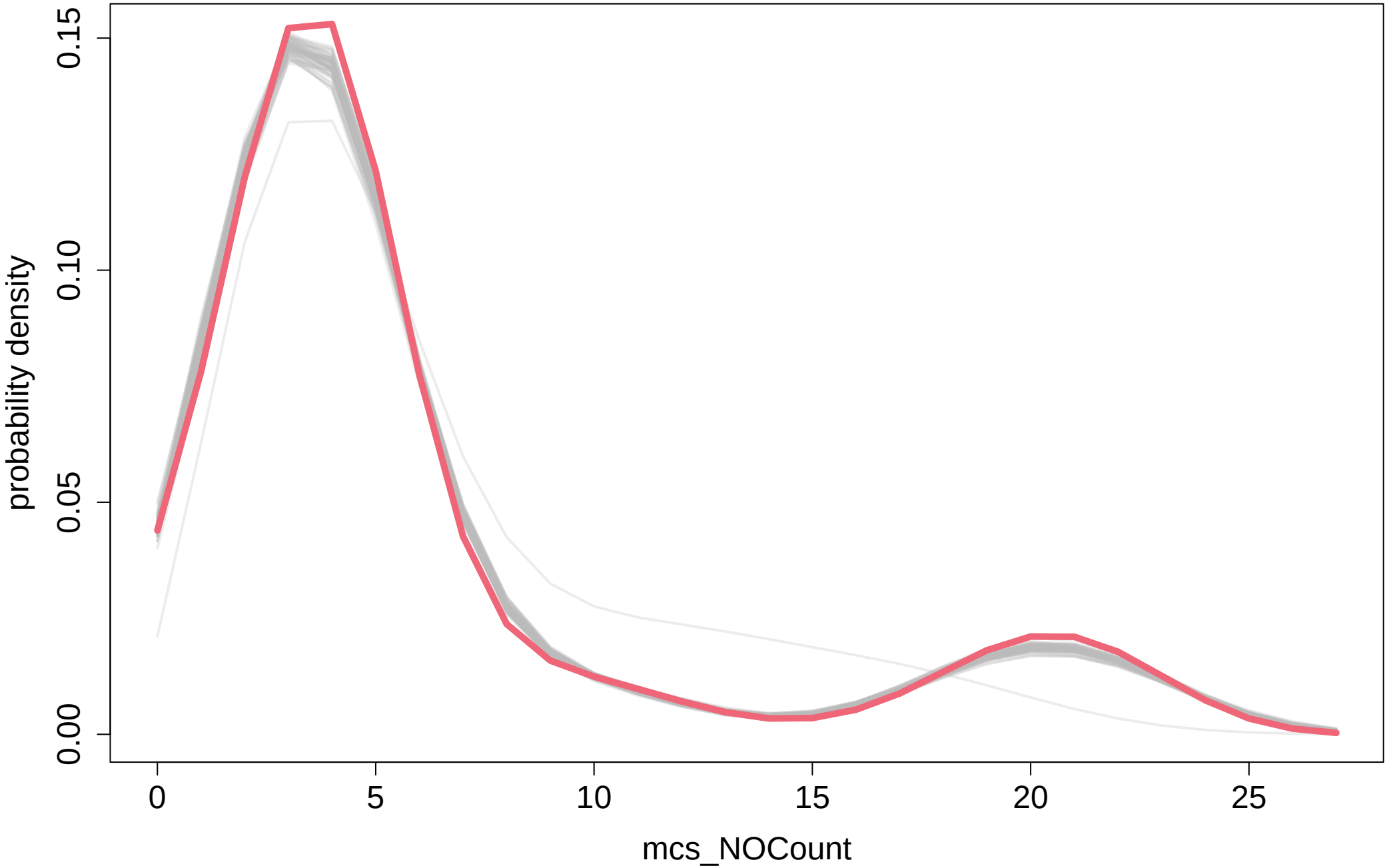
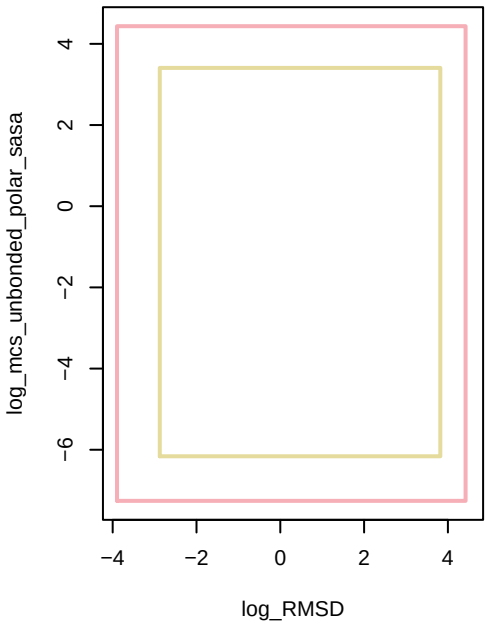
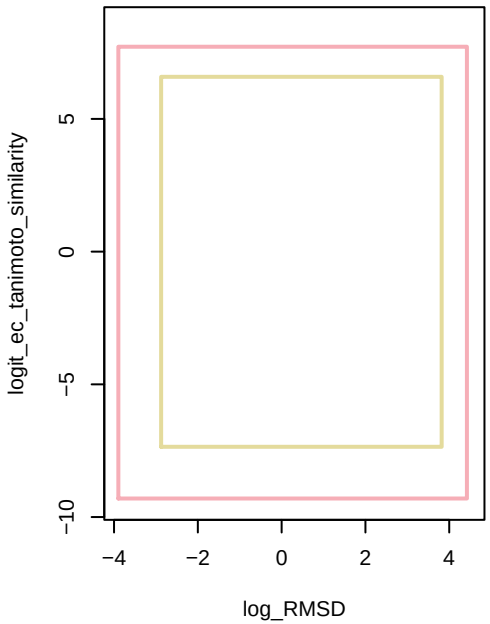
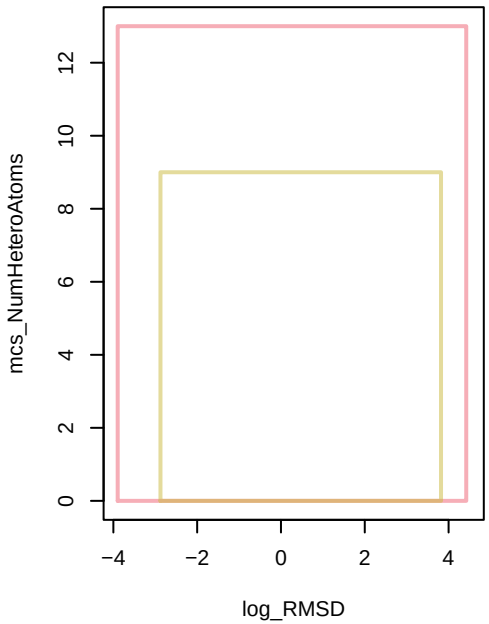
0.05
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount

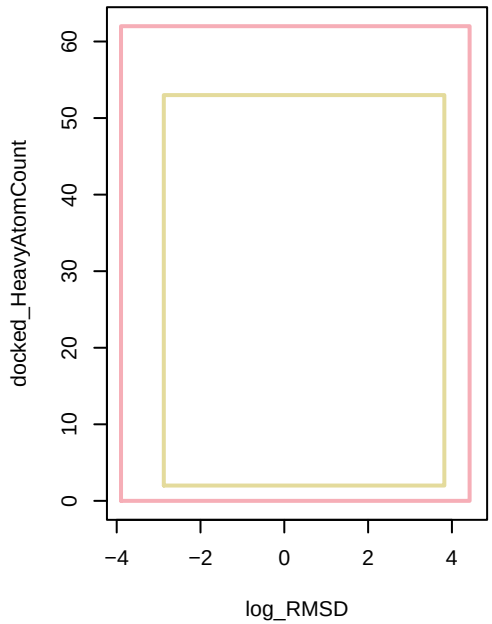

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
docked_NumRotatableBonds

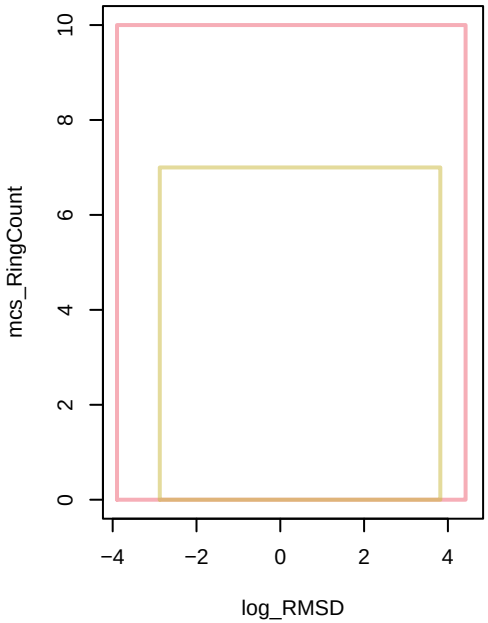

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

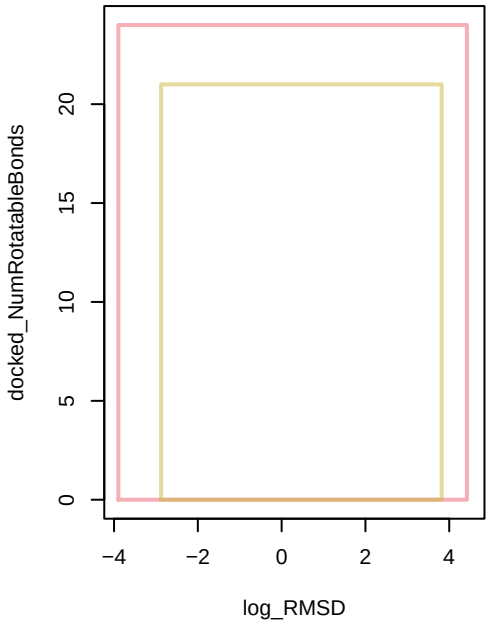

log_mcs_unbonded_polar_sasa
log_RMSD

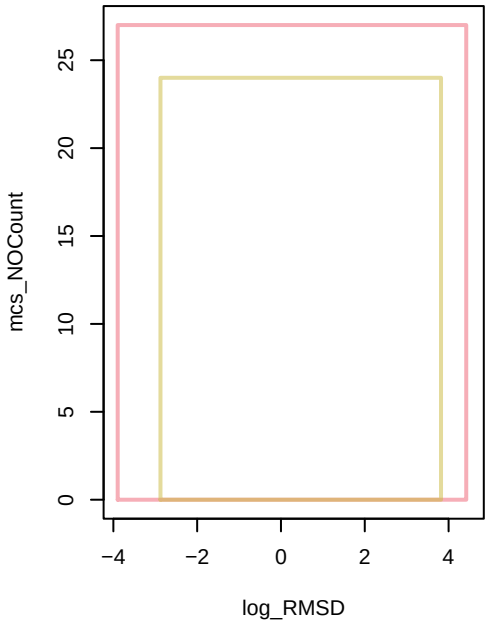

logit_ec_tanimoto_similarity
log_RMSD

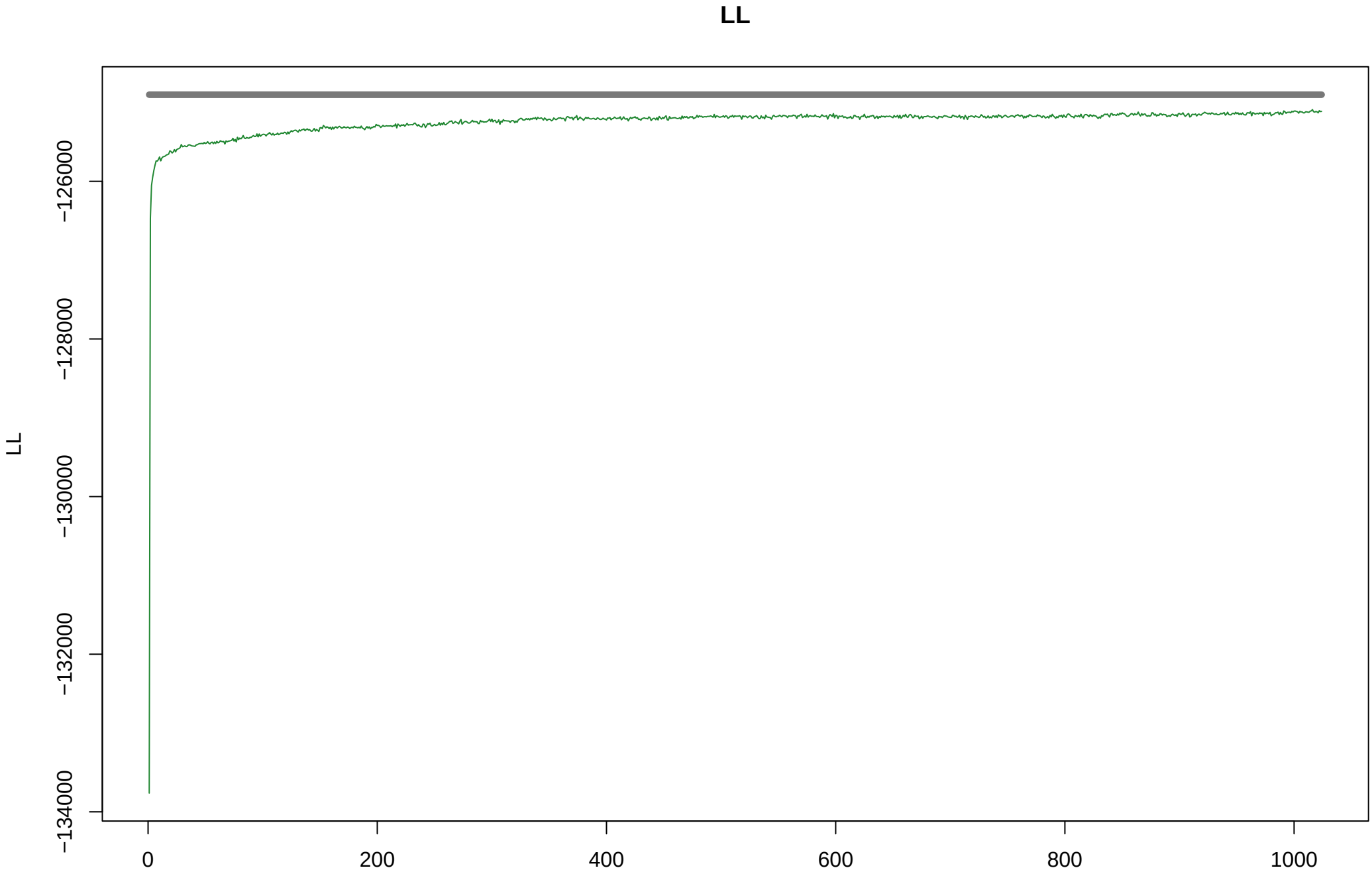

mcs_NumHeteroAtoms
log_RMSD

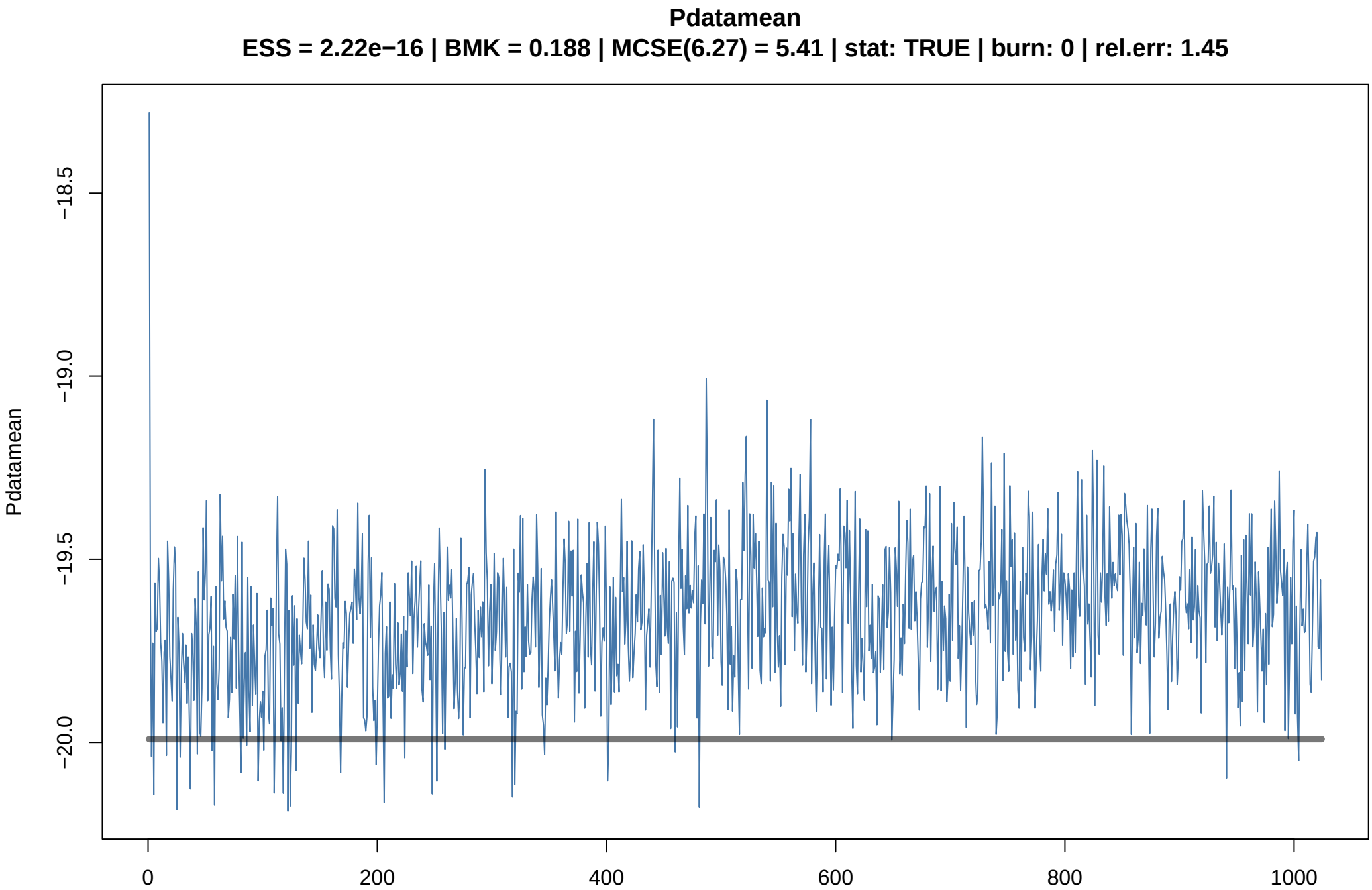

docked_HeavyAtomCount
log_RMSD

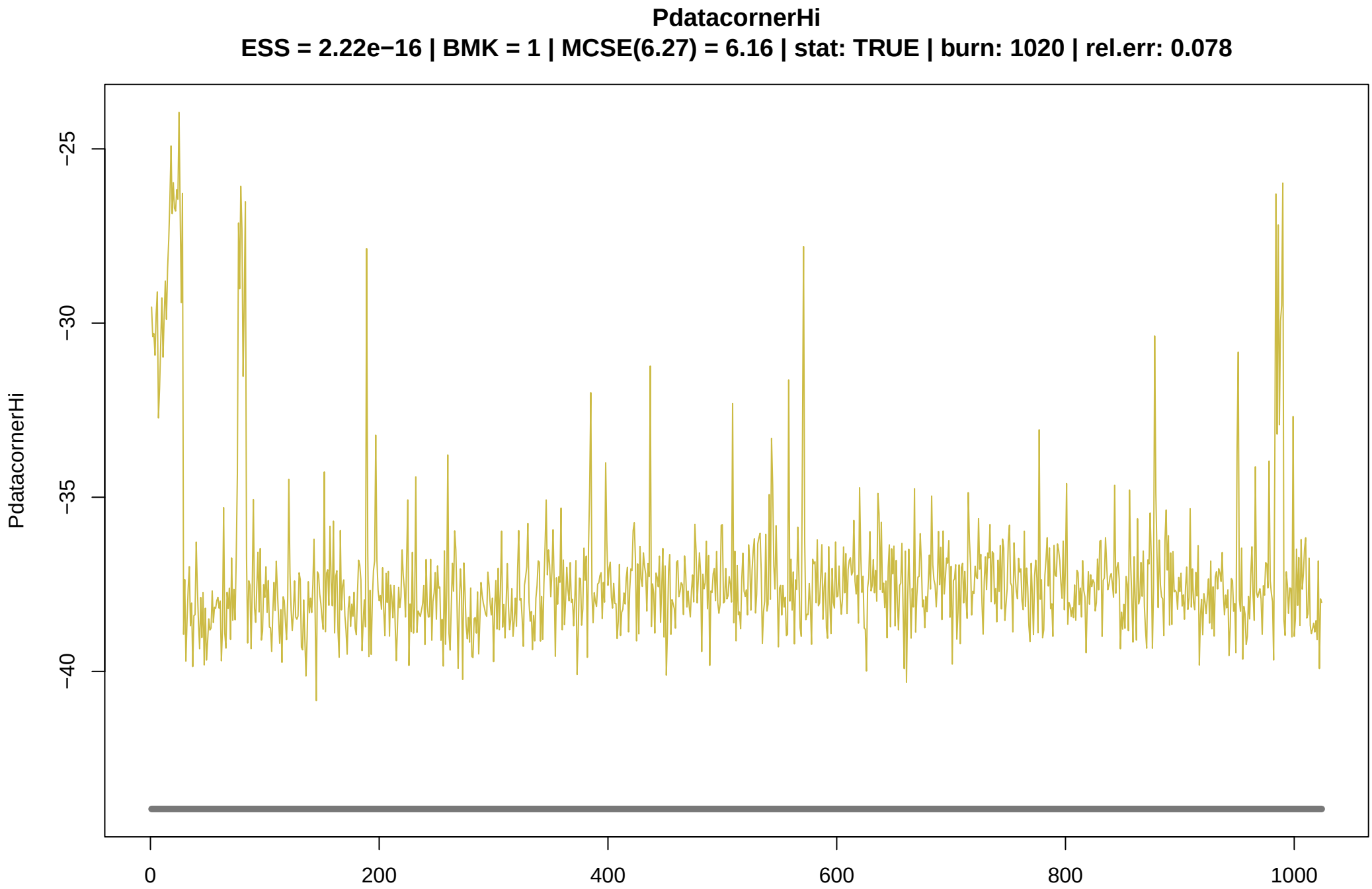

mcs_RingCount
log_RMSD

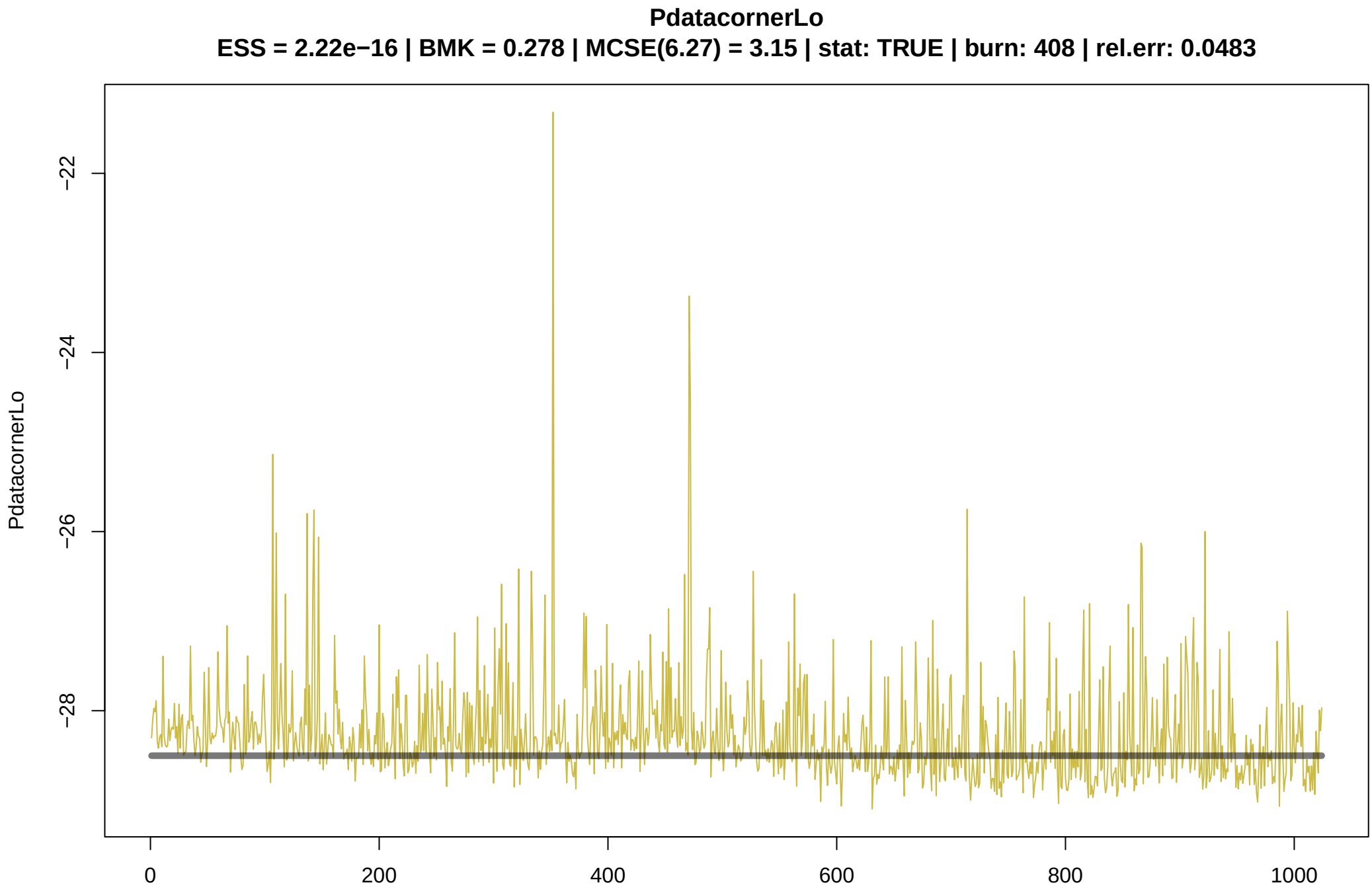

docked_NumRotatableBonds
log_RMSD

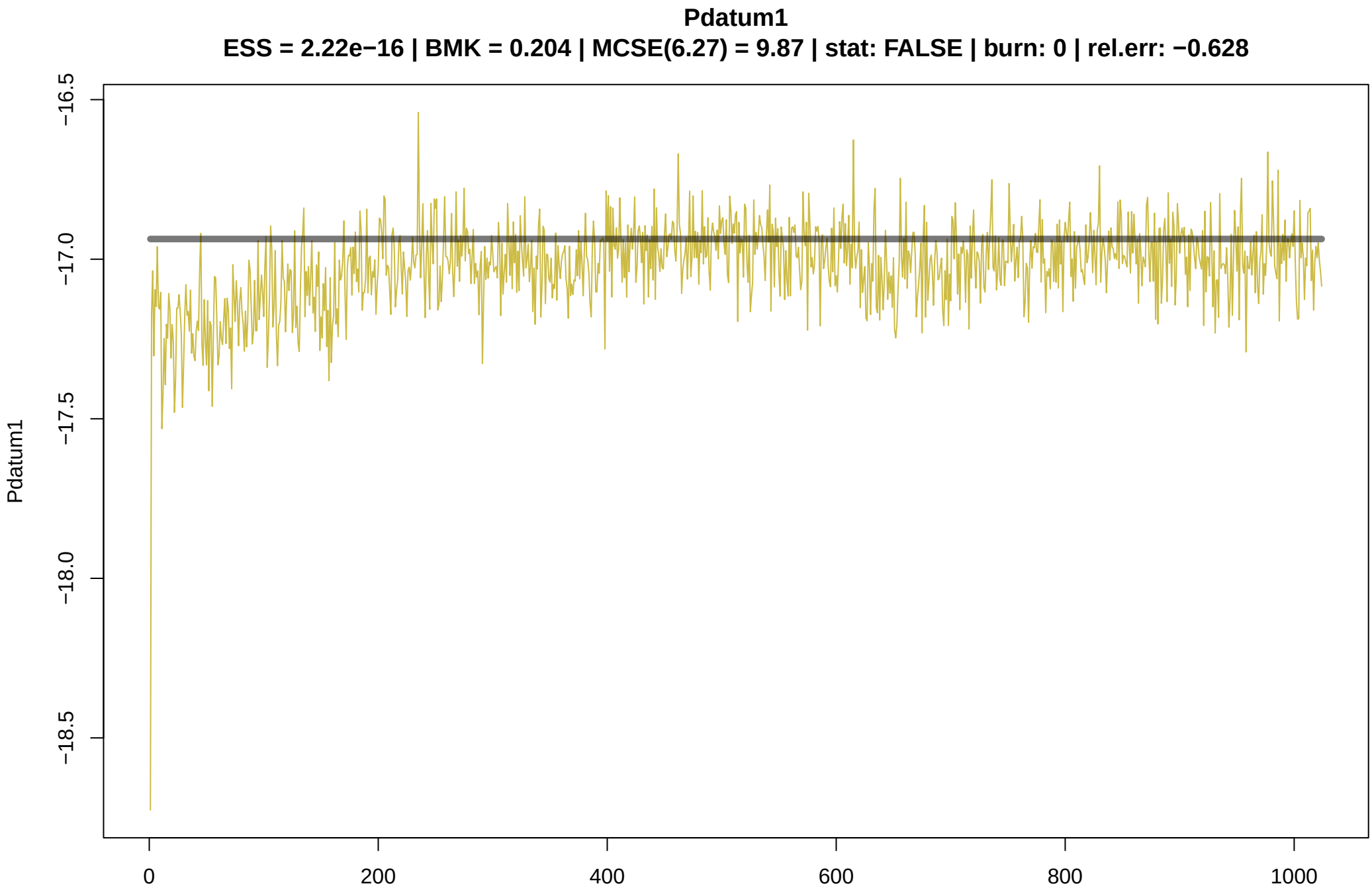

mcs_NOCount
log_RMSD

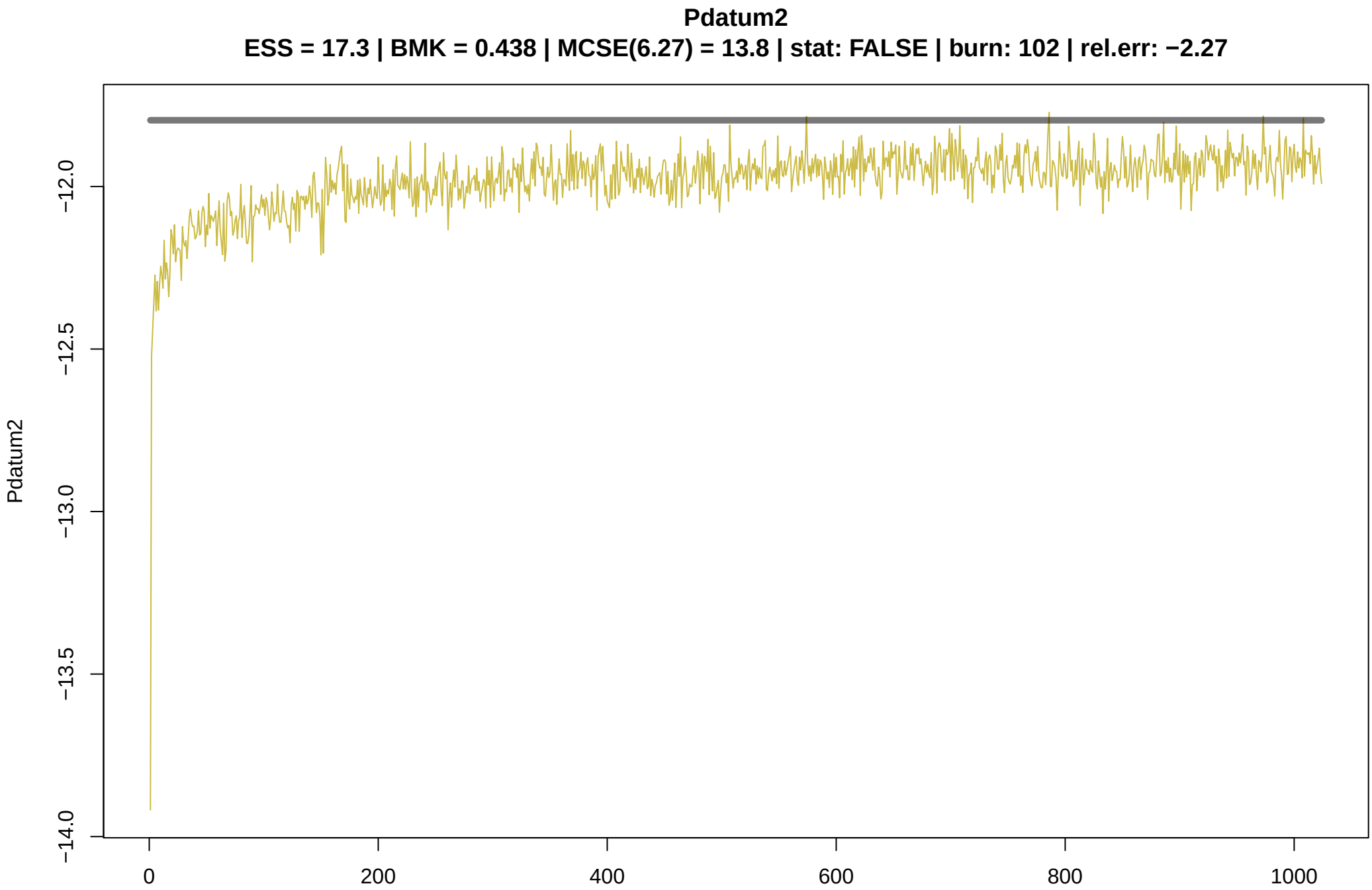

LL
LL
−126000
−128000
−130000
−132000
−134000
0
200
400
600
800
1000

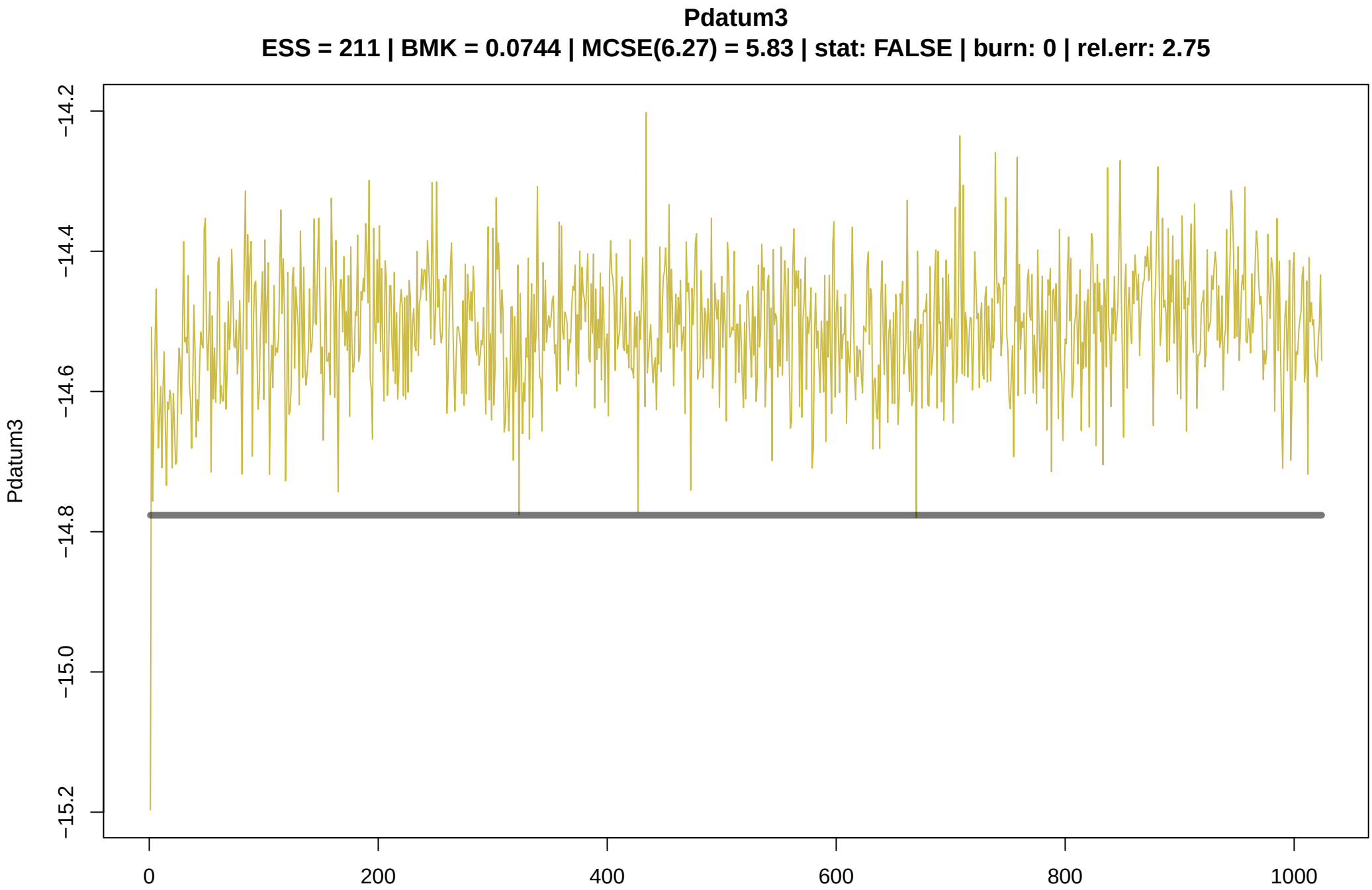

Pdatamean
ESS = 2.22e−16 | BMK = 0.188 | MCSE(6.27) = 5.41 | stat: TRUE | burn: 0 | rel.err: 1.45
Pdatamean
−18.5
−19.0
−19.5
−20.0
0
200
400
600
800
1000

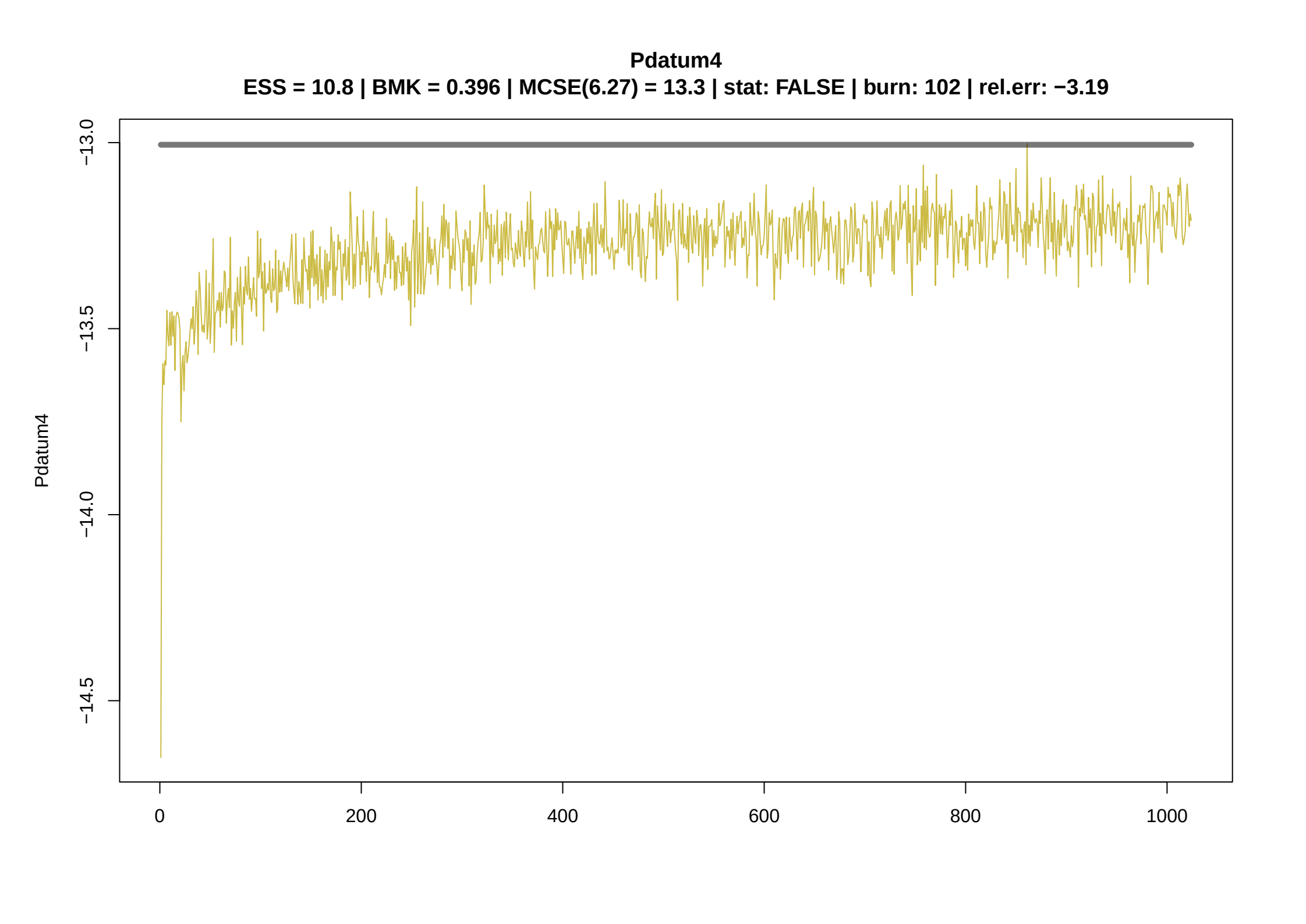

PdatacornerHi
ESS = 2.22e−16 | BMK = 1 | MCSE(6.27) = 6.16 | stat: TRUE | burn: 1020 | rel.err: 0.078
PdatacornerHi
−25
−30
−35
−40
0
200
400
600
800
1000

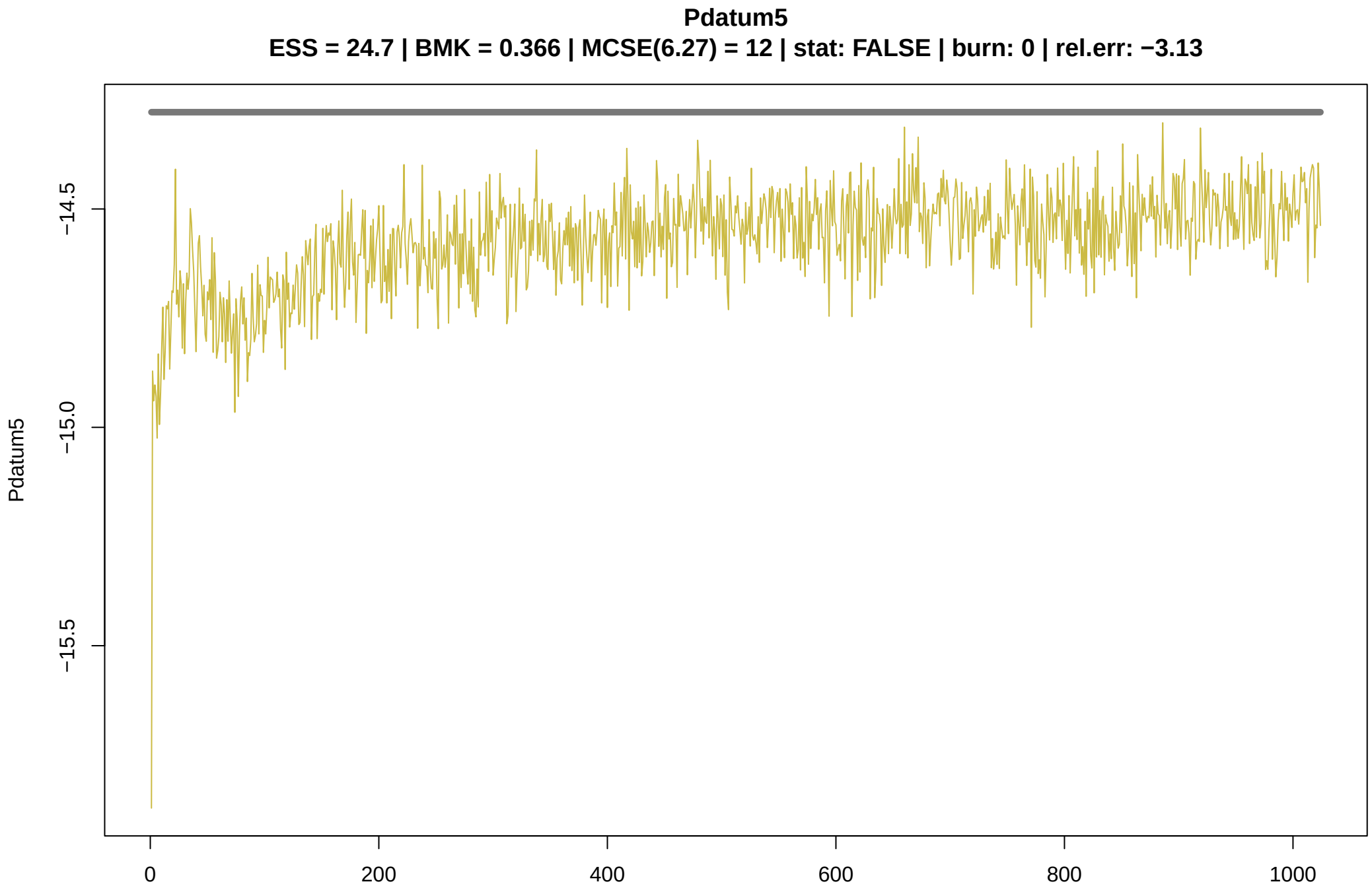

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.278 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 408 | rel.err: 0.0483
PdatacornerLo
−22
−24
−26
−28
0
200
400
600
800
1000

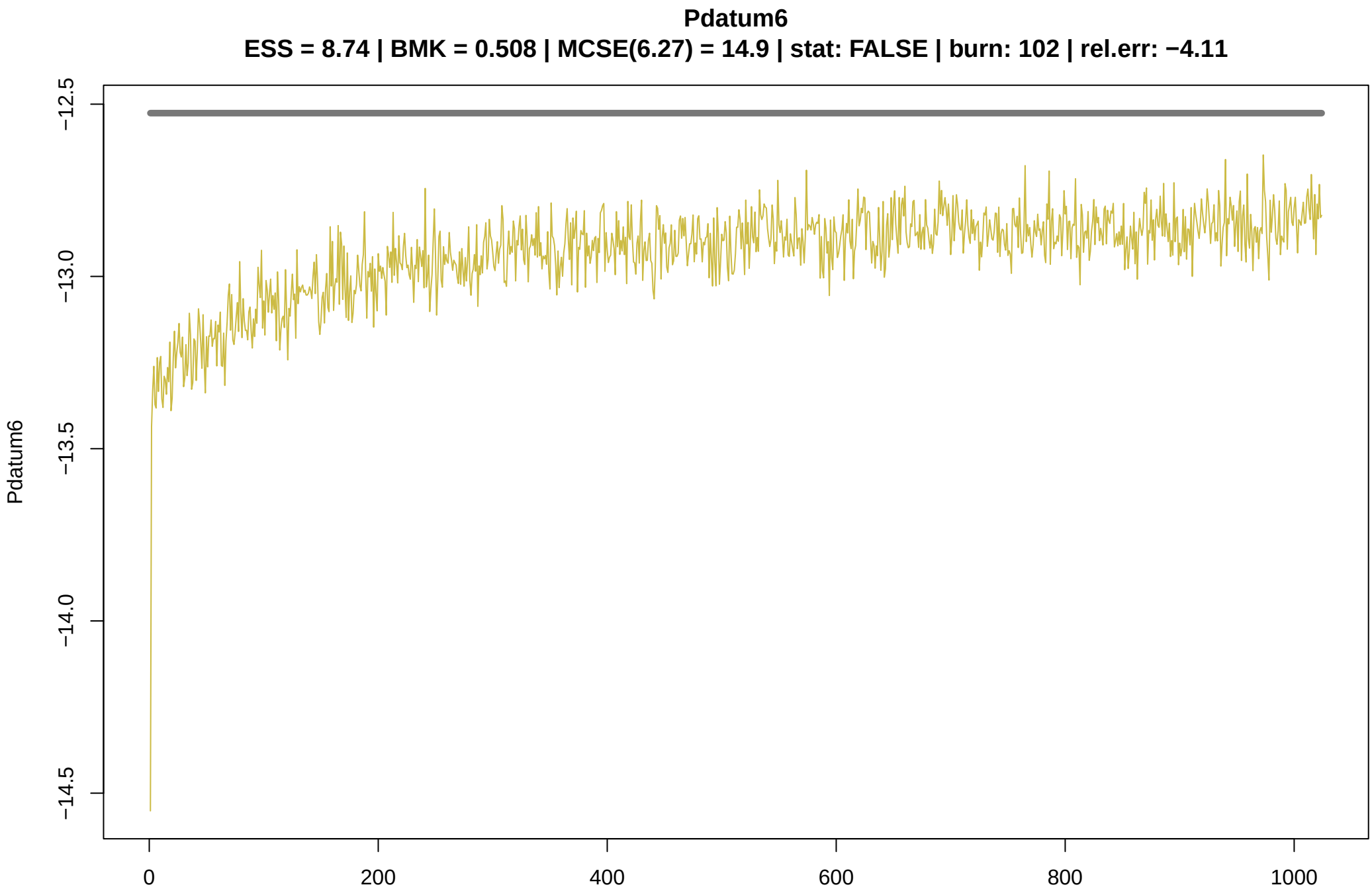

Pdatum1
ESS = 2.22e−16 | BMK = 0.204 | MCSE(6.27) = 9.87 | stat: FALSE | burn: 0 | rel.err: −0.628
Pdatum1
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000

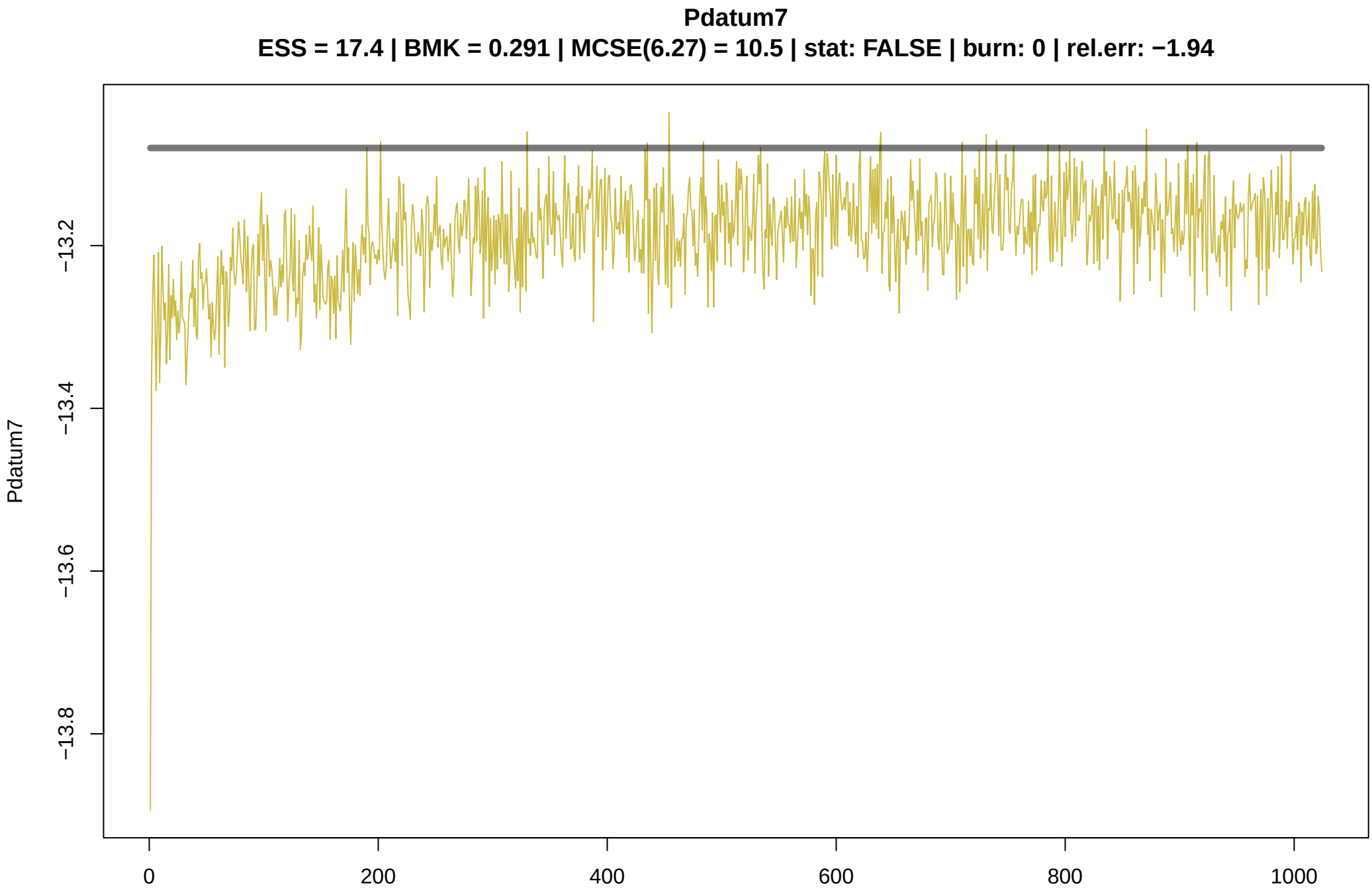

Pdatum2
ESS = 17.3 | BMK = 0.438 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 102 | rel.err: −2.27
Pdatum2
−12.0
−12.5
−13.0
−13.5
−14.0
0
200
400
600
800
1000

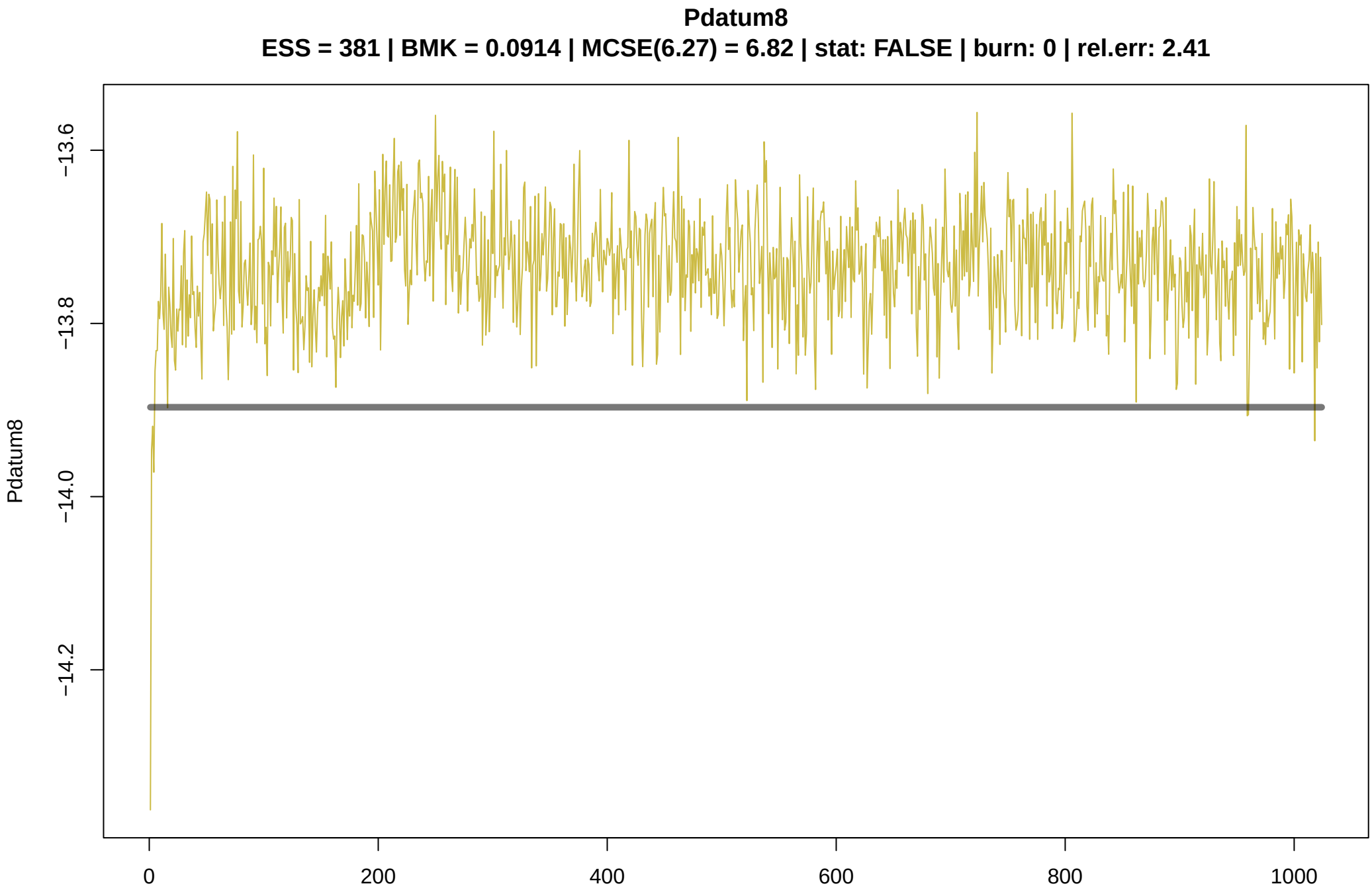

Pdatum3
ESS = 211 | BMK = 0.0744 | MCSE(6.27) = 5.83 | stat: FALSE | burn: 0 | rel.err: 2.75
Pdatum3
−14.2
−14.4
−14.6
−14.8
−15.0
−15.2
0
200
400
600
800
1000

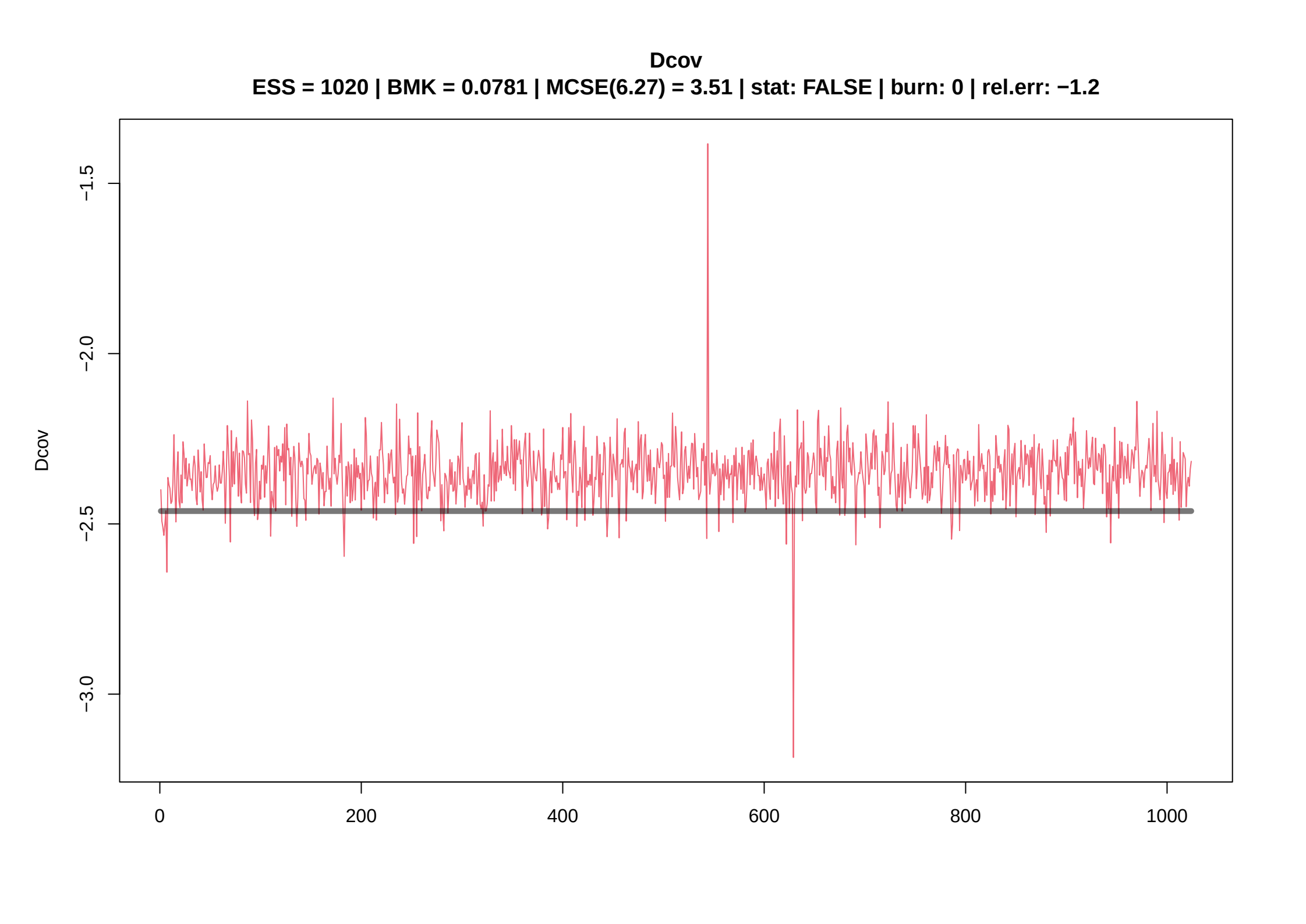

Pdatum4
ESS = 10.8 | BMK = 0.396 | MCSE(6.27) = 13.3 | stat: FALSE | burn: 102 | rel.err: −3.19
Pdatum4
−13.0
−13.5
−14.0
−14.5
0
200
400
600
800
1000

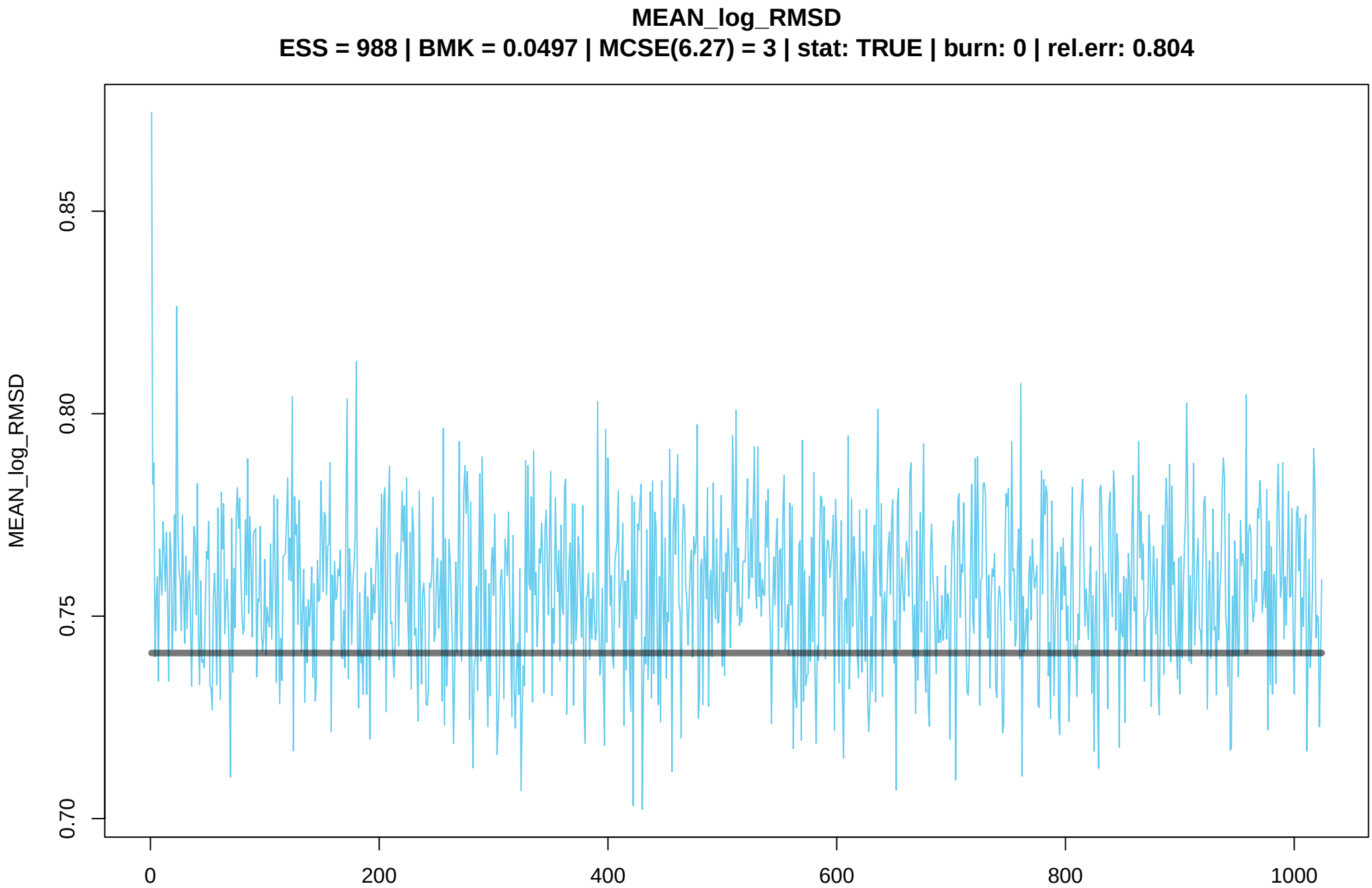

Pdatum5
ESS = 24.7 | BMK = 0.366 | MCSE(6.27) = 12 | stat: FALSE | burn: 0 | rel.err: −3.13
Pdatum5
−14.5
−15.0
−15.5
0
200
400
600
800
1000

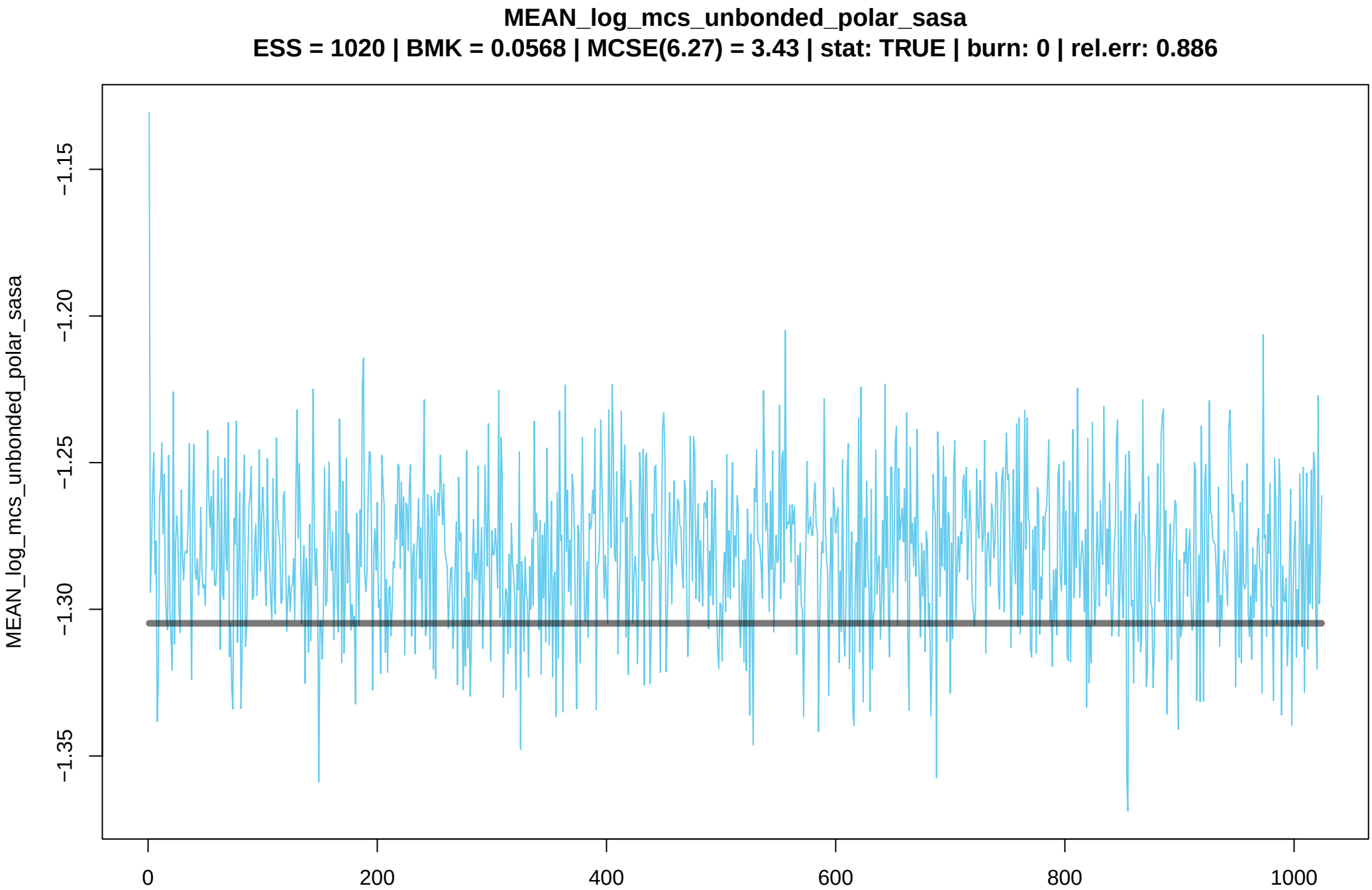

Pdatum6
ESS = 8.74 | BMK = 0.508 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 102 | rel.err: −4.11
Pdatum6
−12.5
−13.0
−13.5
−14.0
−14.5
0
200
400
600
800
1000

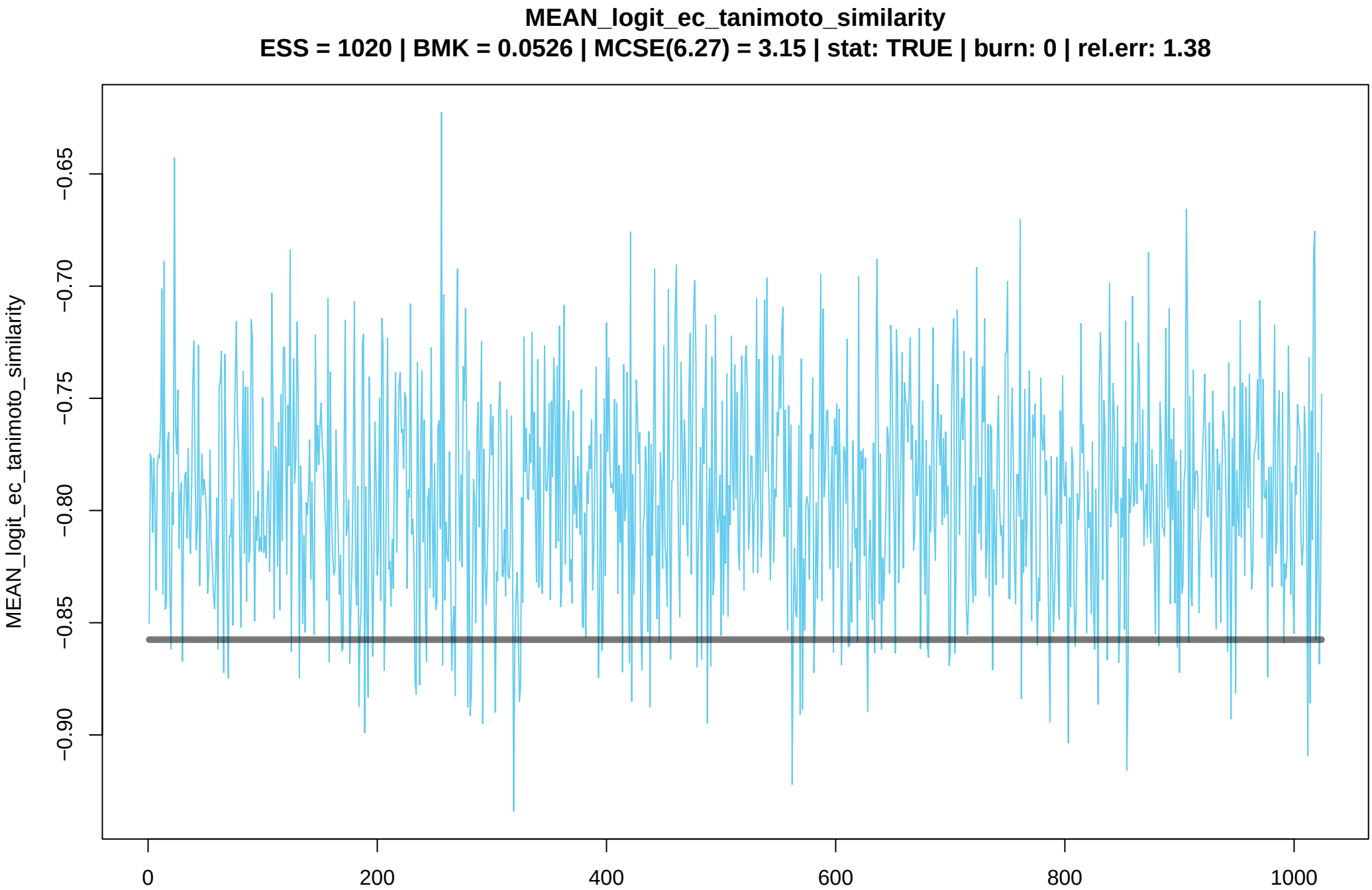

Pdatum7
ESS = 17.4 | BMK = 0.291 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 0 | rel.err: −1.94
Pdatum7
−13.2
−13.4
−13.6
−13.8
0
200
400
600
800
1000

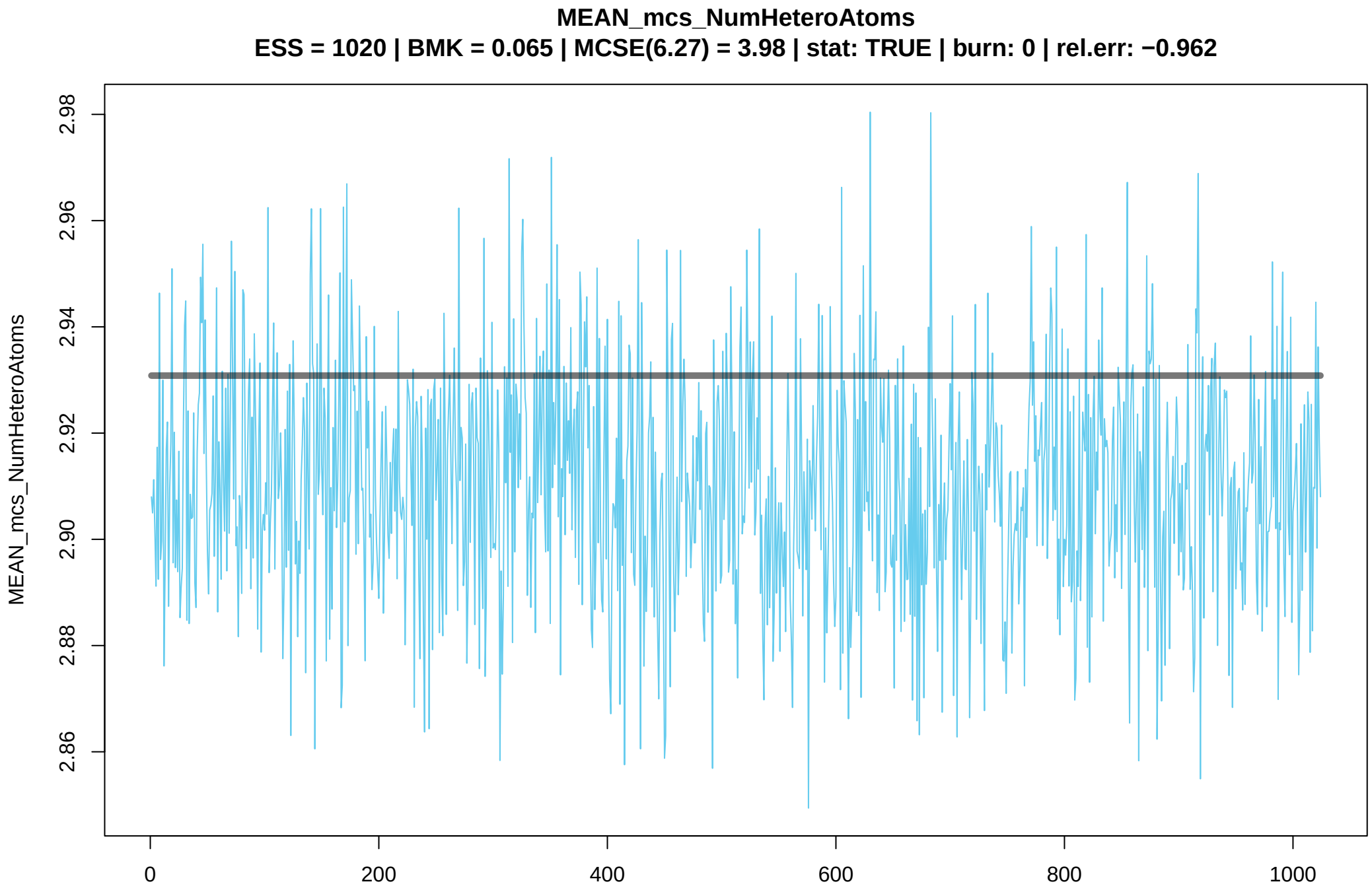

Pdatum8
ESS = 381 | BMK = 0.0914 | MCSE(6.27) = 6.82 | stat: FALSE | burn: 0 | rel.err: 2.41
Pdatum8
−13.6
−13.8
−14.0
−14.2
0
200
400
600
800
1000

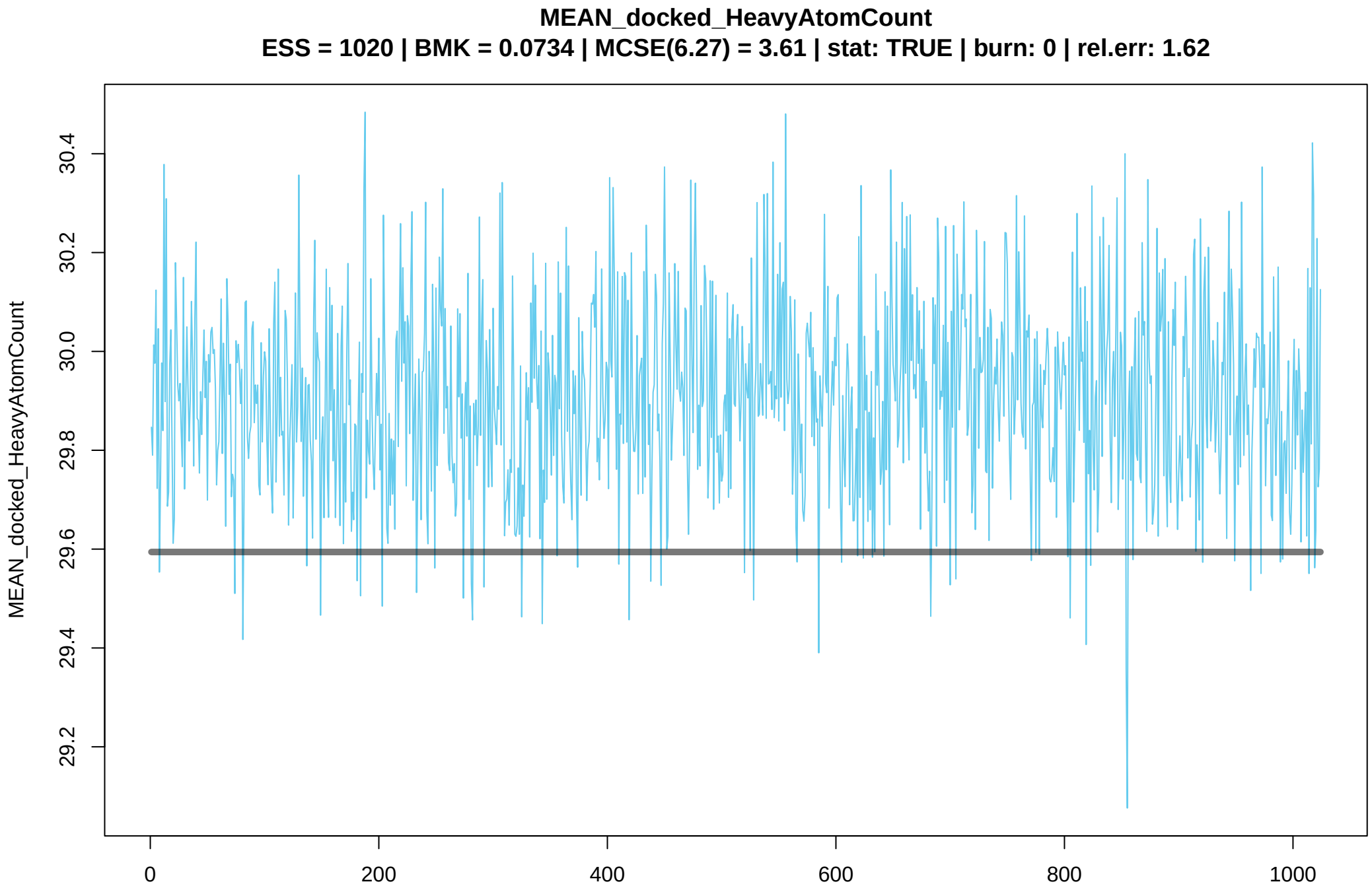

Dcov
ESS = 1020 | BMK = 0.0781 | MCSE(6.27) = 3.51 | stat: FALSE | burn: 0 | rel.err: −1.2
Dcov
−1.5
−2.0
−2.5
−3.0
0
200
400
600
800
1000

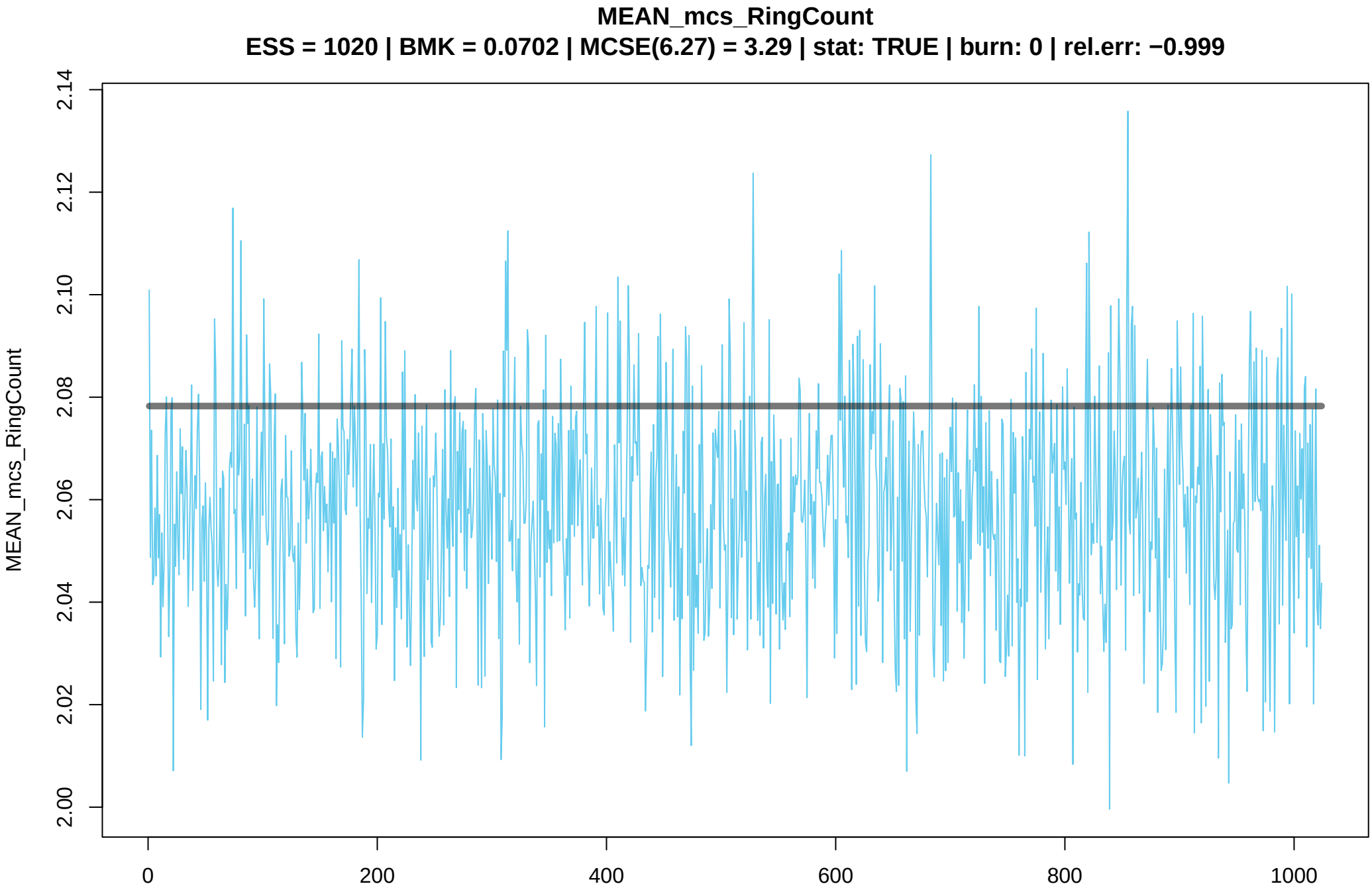

MEAN_log_RMSD
ESS = 988 | BMK = 0.0497 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | rel.err: 0.804
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

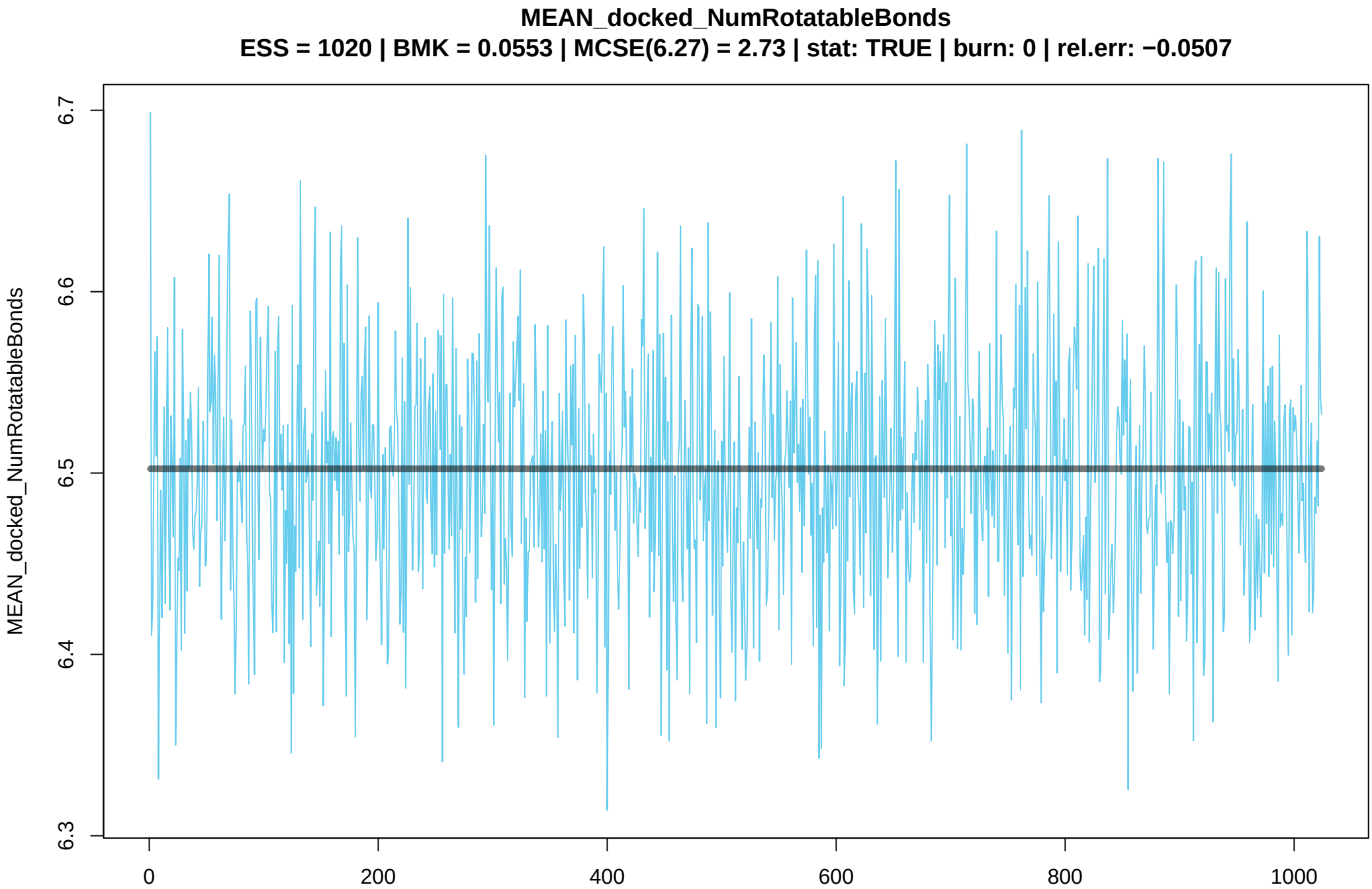

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0568 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0 | rel.err: 0.886
MEAN_log_mcs_unbonded_polar_sasa
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

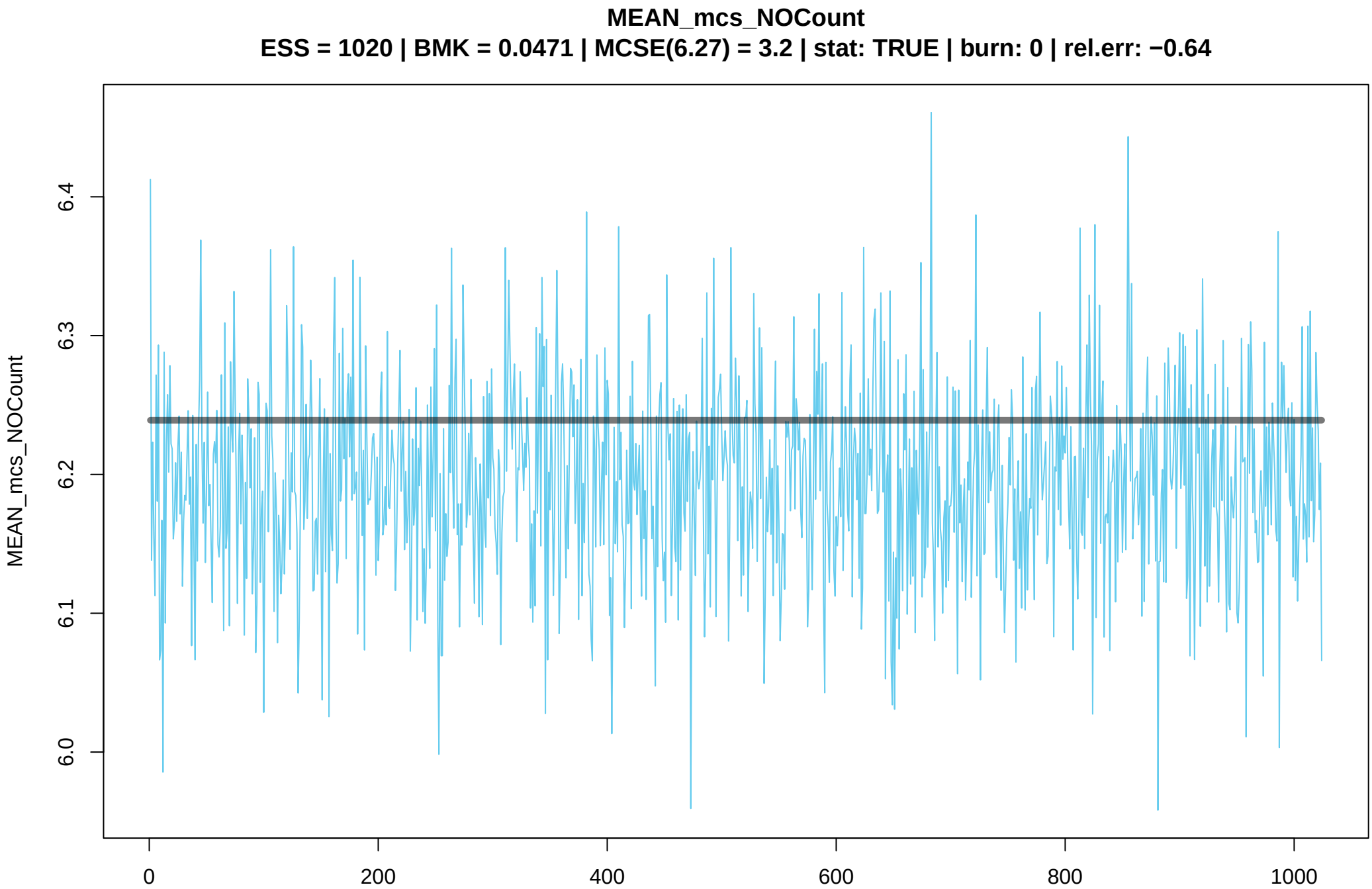

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0526 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | rel.err: 1.38
MEAN_logit_ec_tanimoto_similarity
−0.65
−0.70
−0.75
−0.80
−0.85
−0.90
0
200
400
600
800
1000

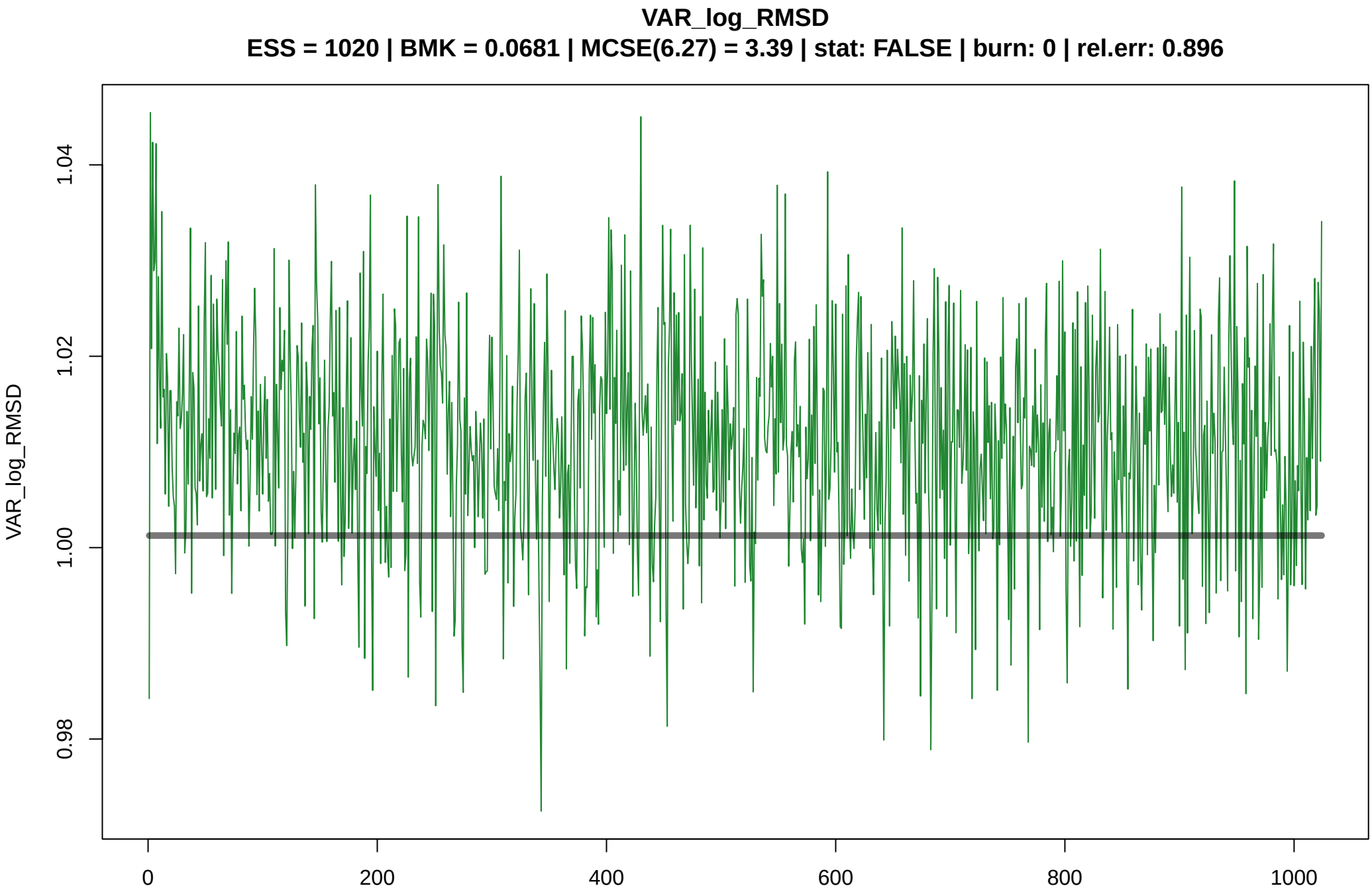

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.065 | MCSE(6.27) = 3.98 | stat: TRUE | burn: 0 | rel.err: −0.962
MEAN_mcs_NumHeteroAtoms
2.86
2.88
2.90
2.92
2.94
2.96
2.98
0
200
400
600
800
1000

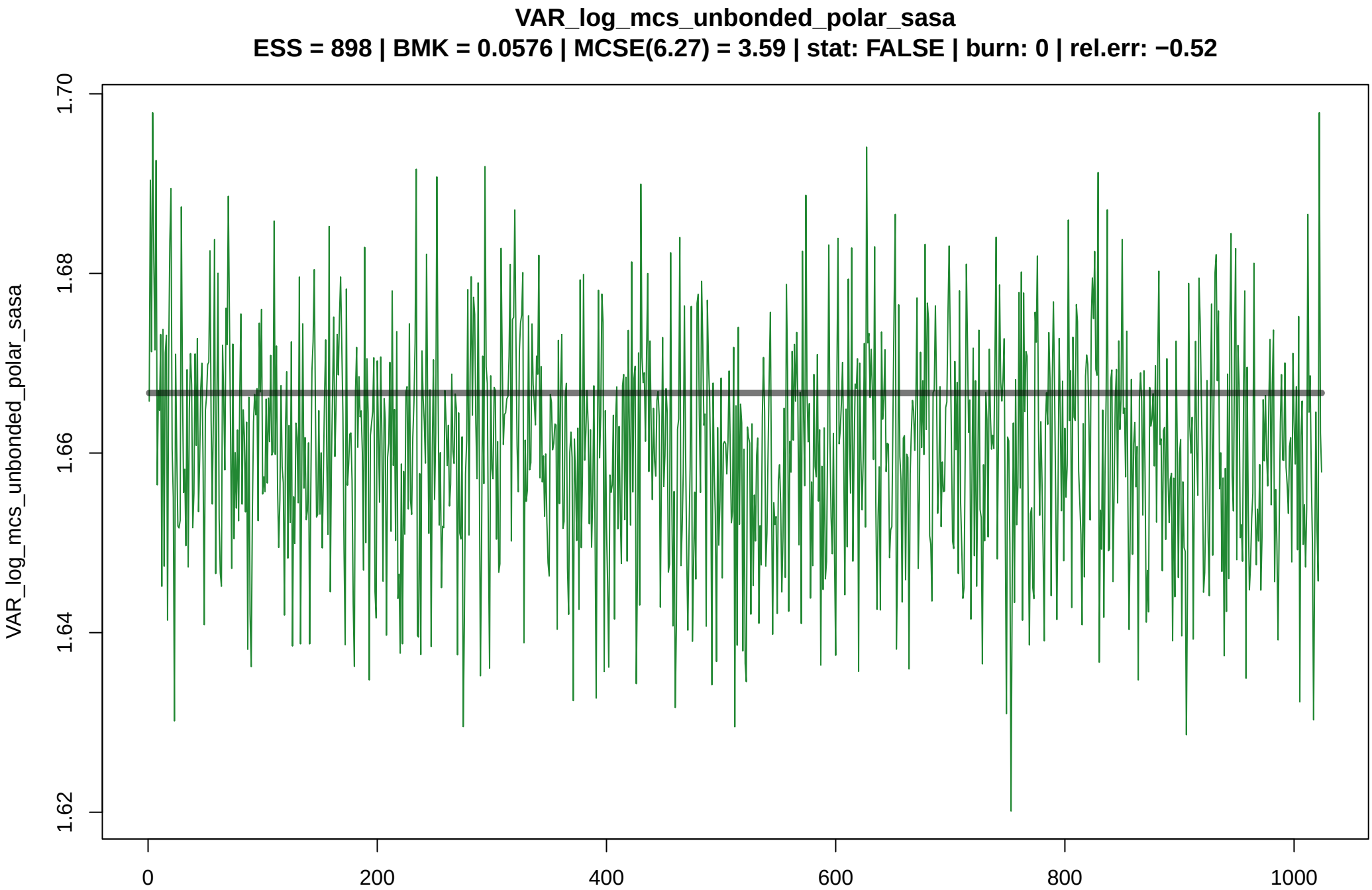

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0734 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0 | rel.err: 1.62
MEAN_docked_HeavyAtomCount
29.2
29.4
29.6
29.8
30.0
30.2
30.4
0
200
400
600
800
1000

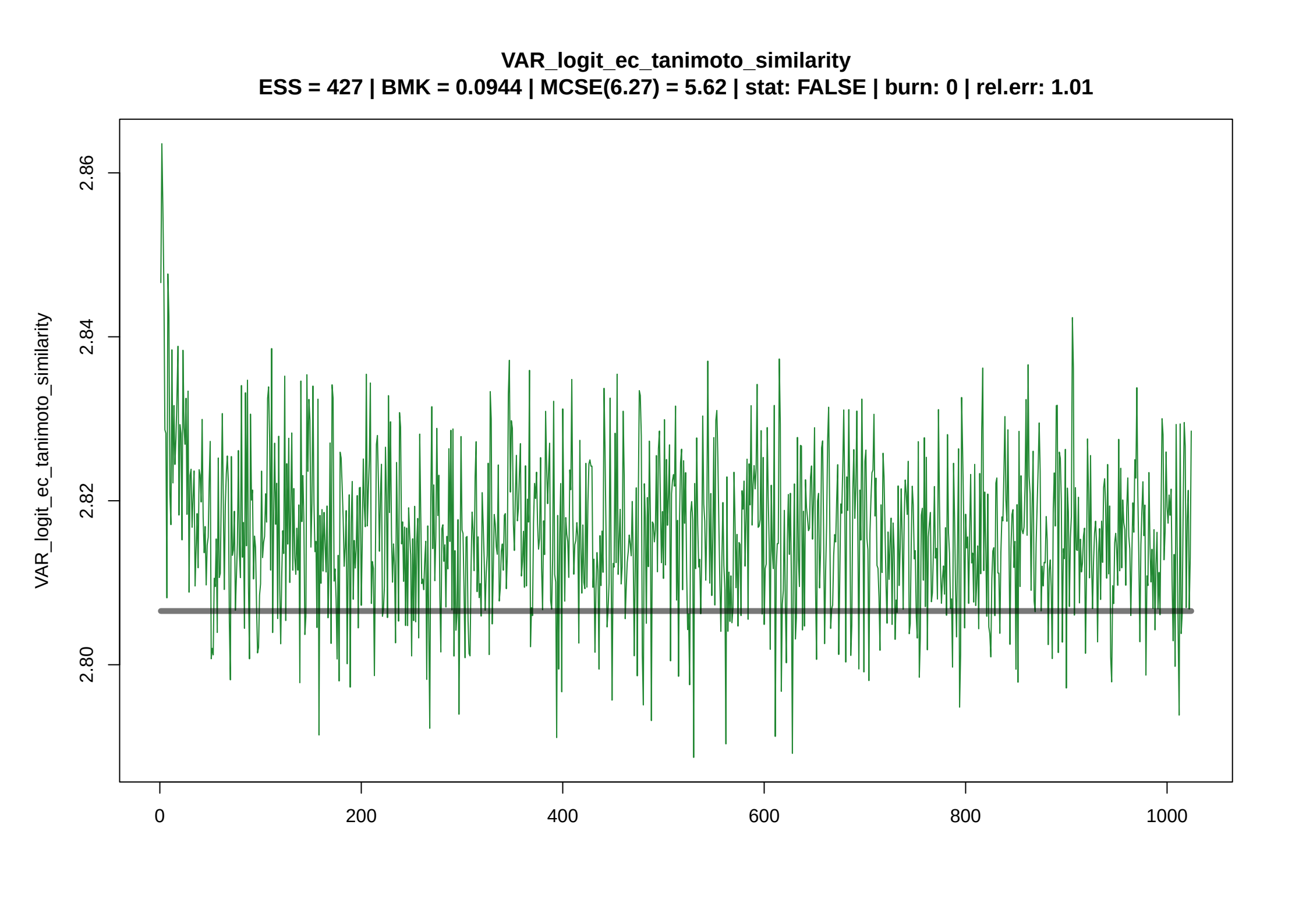

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0702 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0 | rel.err: −0.999
MEAN_mcs_RingCount
2.00
2.02
2.04
2.06
2.08
2.10
2.12
2.14
0
200
400
600
800
1000

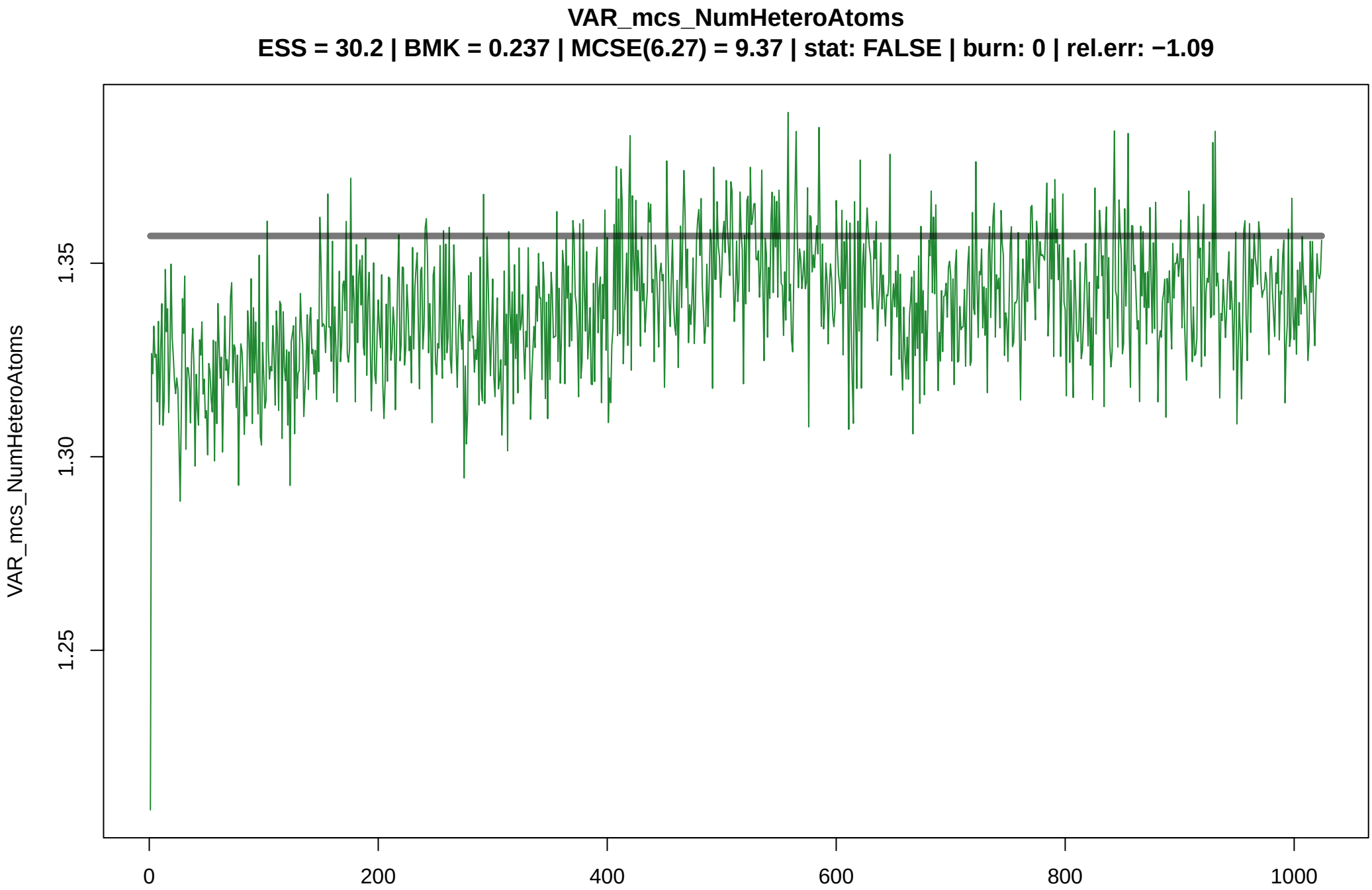

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0553 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | rel.err: −0.0507
MEAN_docked_NumRotatableBonds
6.7
6.6
6.5
6.4
6.3
0
200
400
600
800
1000

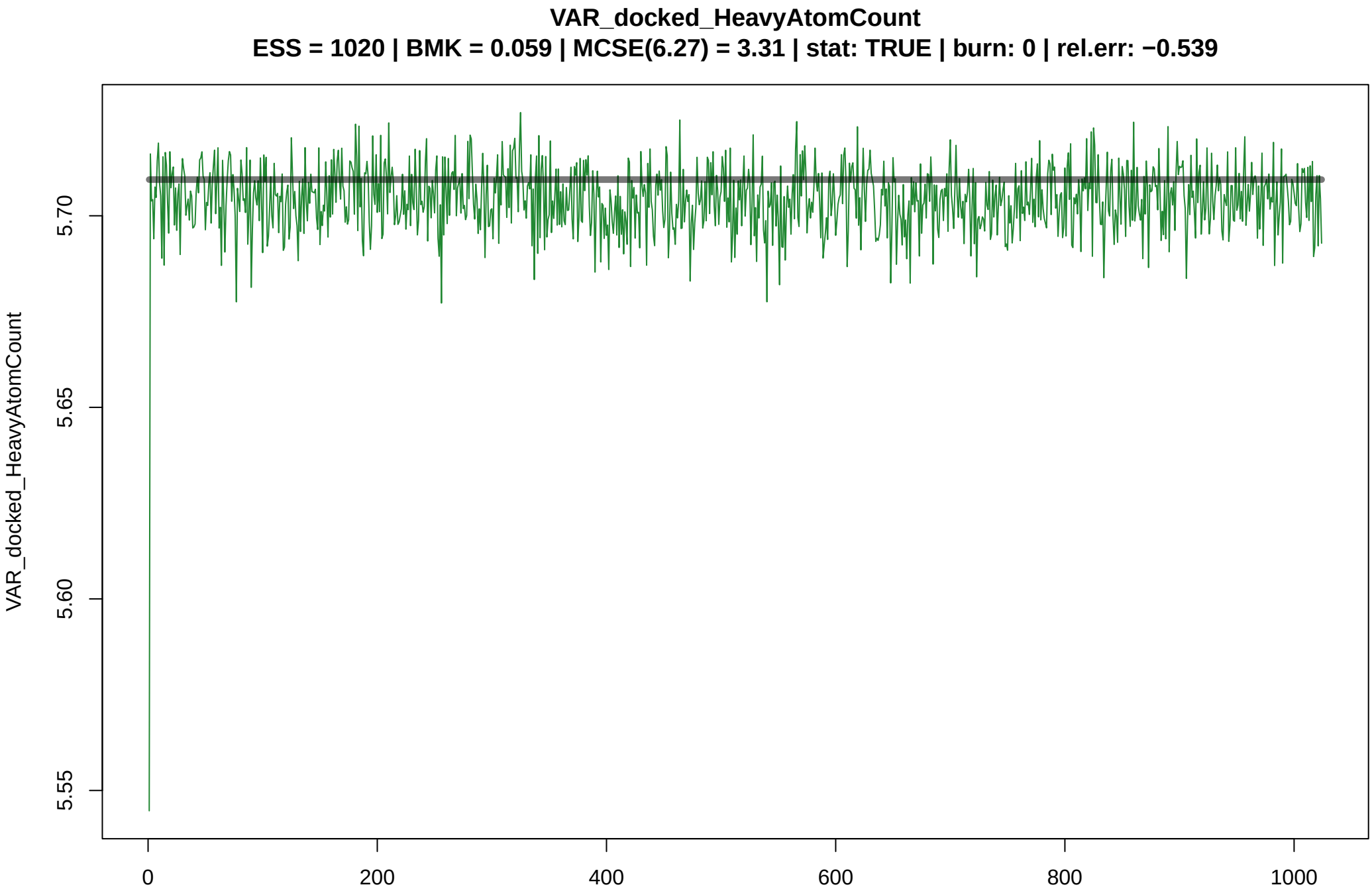

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0471 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: −0.64
MEAN_mcs_NOCount
6.0
6.1
6.2
6.3
6.4
0
200
400
600
800
1000

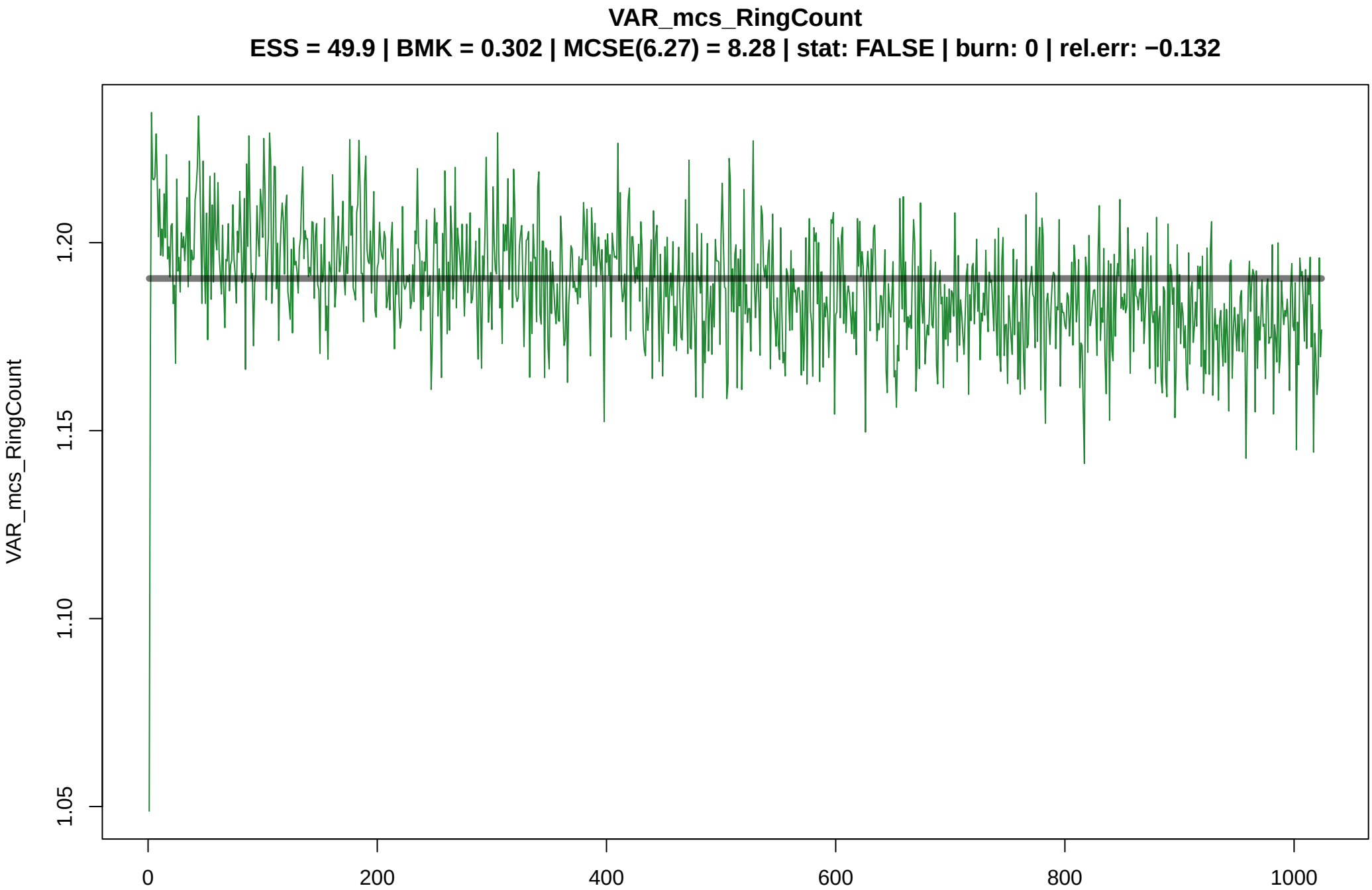

VAR_log_RMSD
ESS = 1020 | BMK = 0.0681 | MCSE(6.27) = 3.39 | stat: FALSE | burn: 0 | rel.err: 0.896
VAR_log_RMSD
1.04
1.02
1.00
0.98
0
200
400
600
800
1000

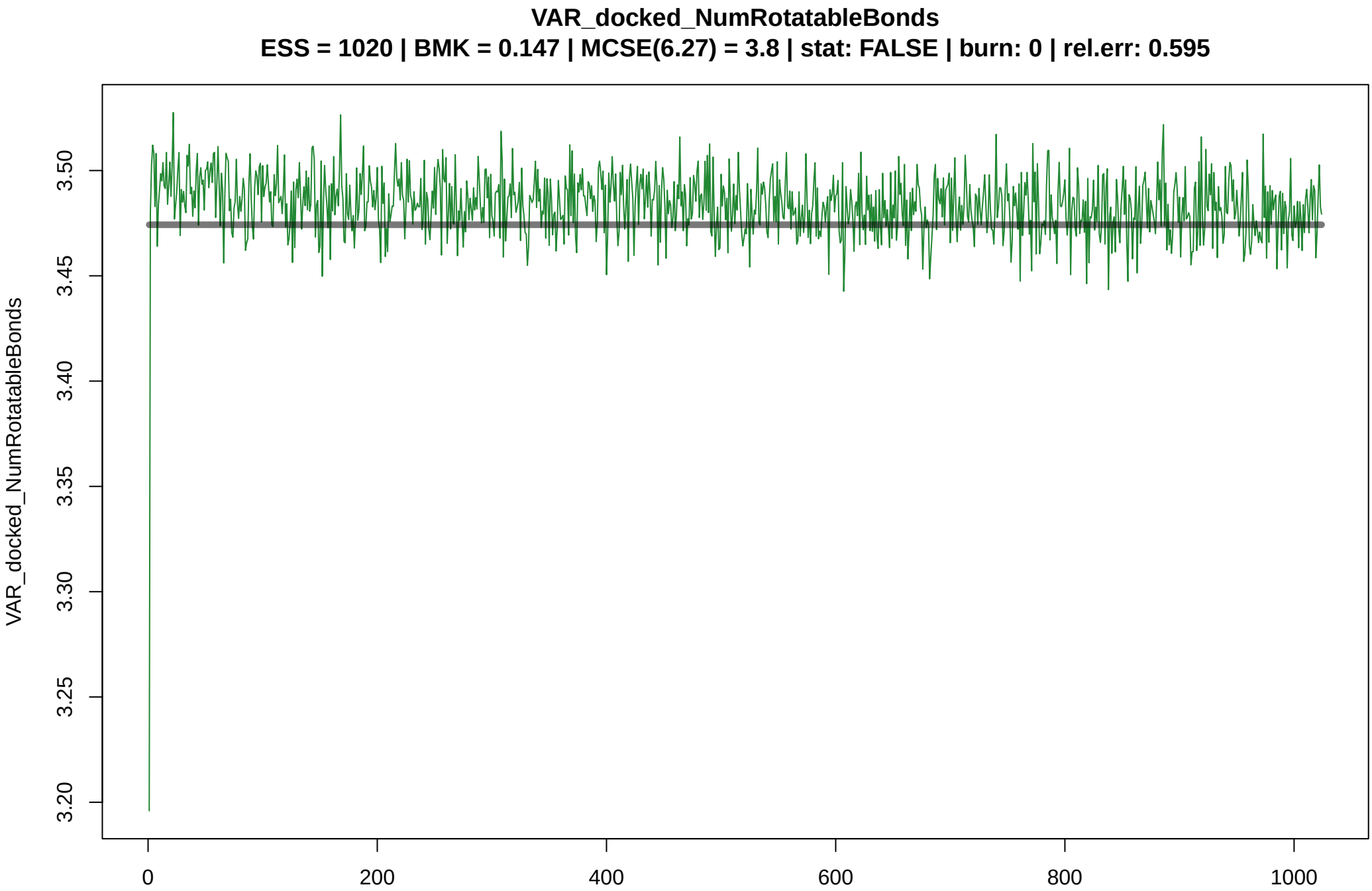

VAR_log_mcs_unbonded_polar_sasa
ESS = 898 | BMK = 0.0576 | MCSE(6.27) = 3.59 | stat: FALSE | burn: 0 | rel.err: −0.52
VAR_log_mcs_unbonded_polar_sasa
1.70
1.68
1.66
1.64
1.62
0
200
400
600
800
1000

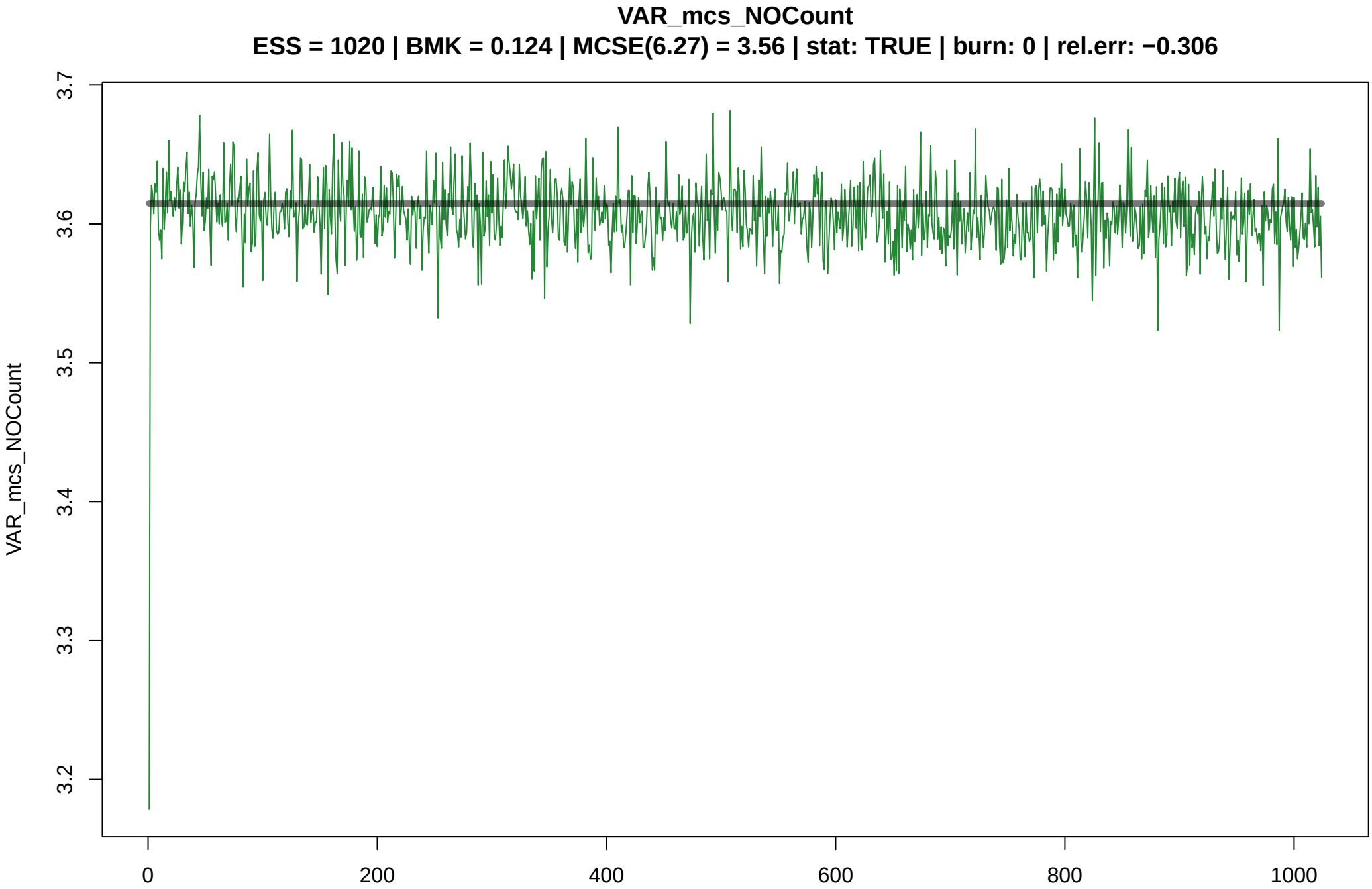

VAR_logit_ec_tanimoto_similarity
ESS = 427 | BMK = 0.0944 | MCSE(6.27) = 5.62 | stat: FALSE | burn: 0 | rel.err: 1.01
VAR_logit_ec_tanimoto_similarity
2.80
2.82
2.84
2.86
0
200
400
600
800
1000

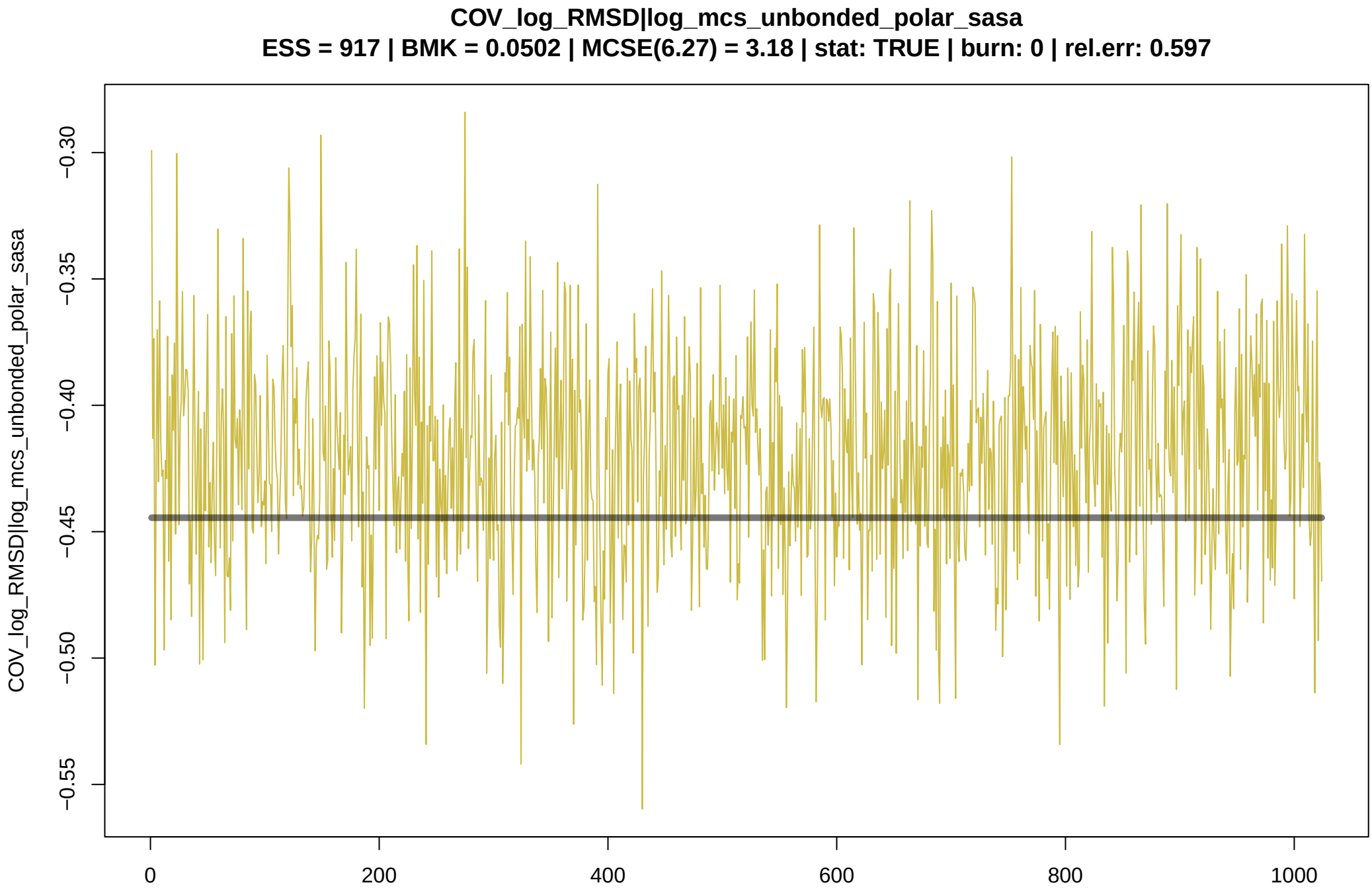

VAR_mcs_NumHeteroAtoms
ESS = 30.2 | BMK = 0.237 | MCSE(6.27) = 9.37 | stat: FALSE | burn: 0 | rel.err: −1.09
VAR_mcs_NumHeteroAtoms
1.25
1.30
1.35
0
200
400
600
800
1000

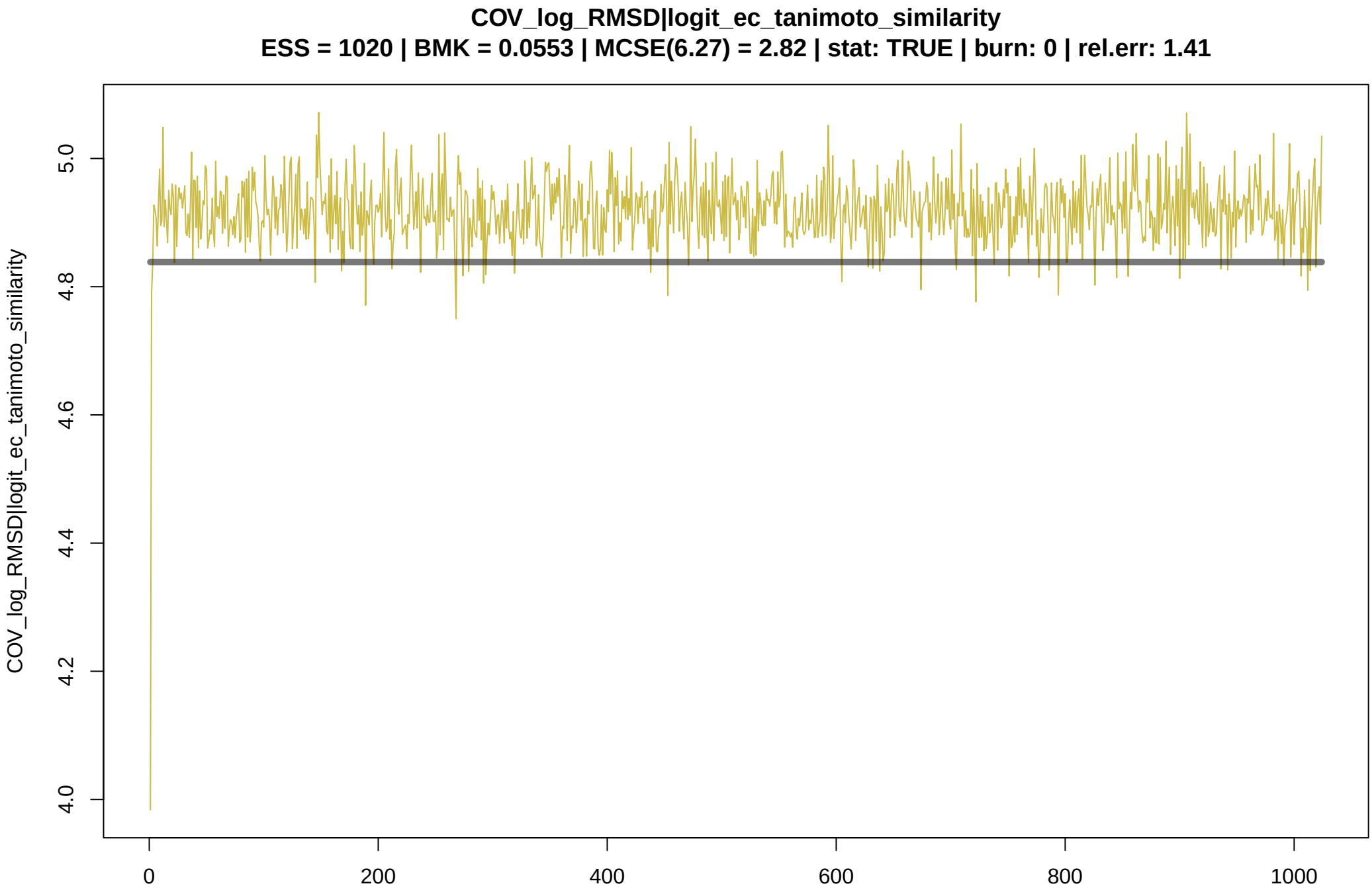

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.059 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0 | rel.err: −0.539
VAR_docked_HeavyAtomCount
5.55
5.60
5.65
5.70
0
200
400
600
800
1000

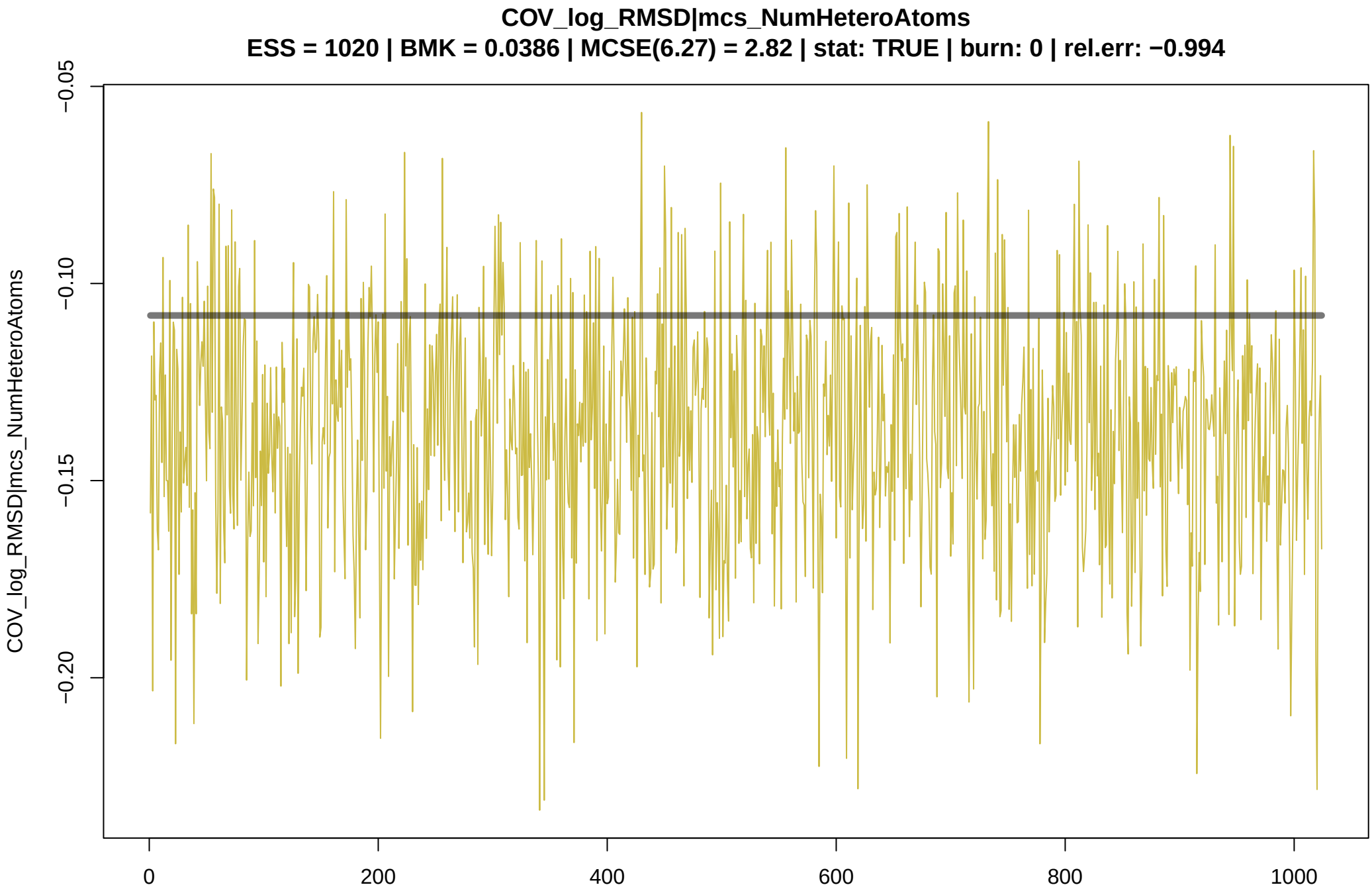

VAR_mcs_RingCount
ESS = 49.9 | BMK = 0.302 | MCSE(6.27) = 8.28 | stat: FALSE | burn: 0 | rel.err: −0.132
VAR_mcs_RingCount
1.05
1.10
1.15
1.20
0
200
400
600
800
1000

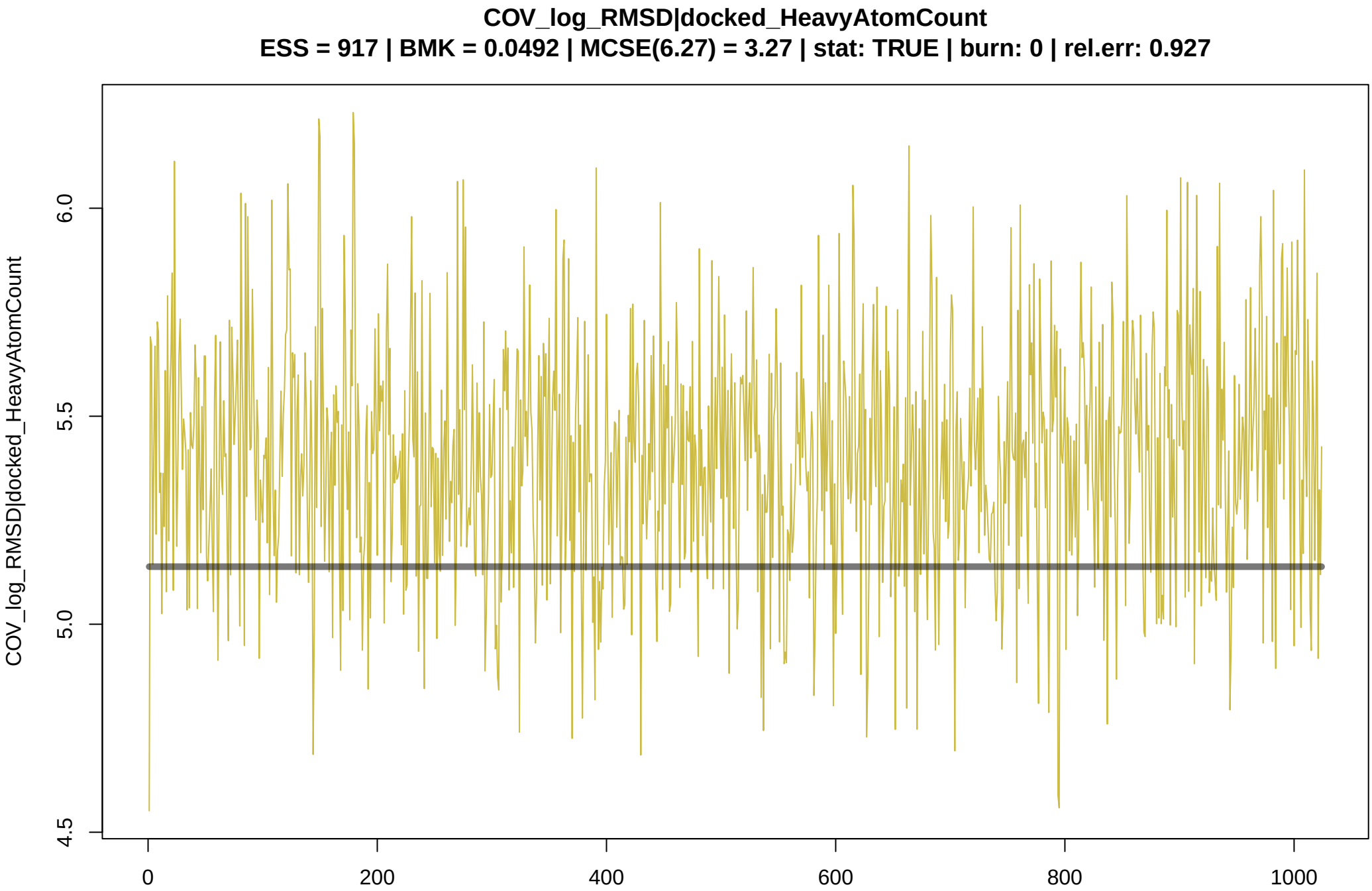

VAR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.147 | MCSE(6.27) = 3.8 | stat: FALSE | burn: 0 | rel.err: 0.595
VAR_docked_NumRotatableBonds
3.20
3.25
3.30
3.35
3.40
3.45
3.50
0
200
400
600
800
1000

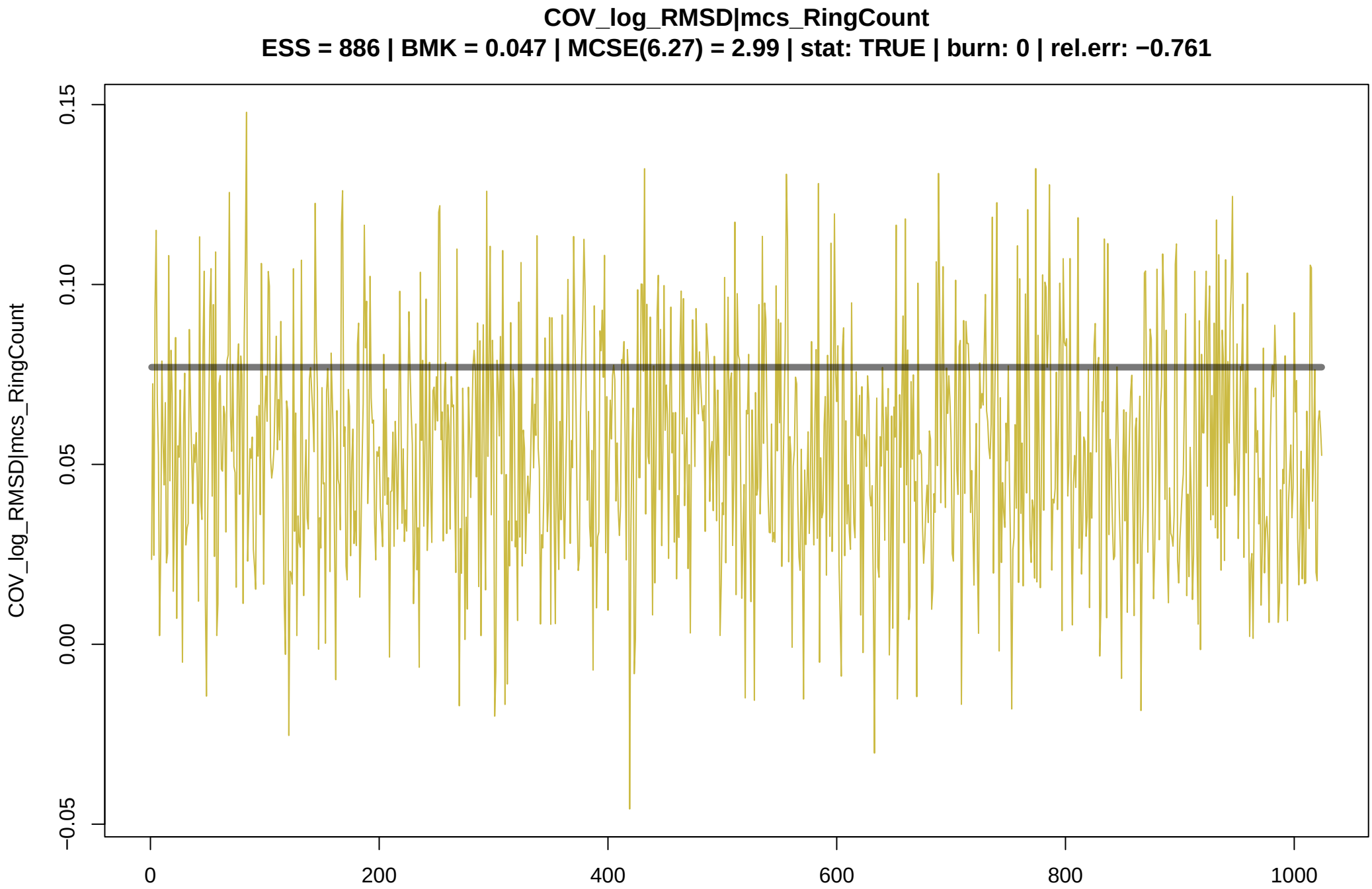

VAR_mcs_NOCount
ESS = 1020 | BMK = 0.124 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | rel.err: −0.306
VAR_mcs_NOCount
3.2
3.3
3.4
3.5
3.6
3.7
0
200
400
600
800
1000

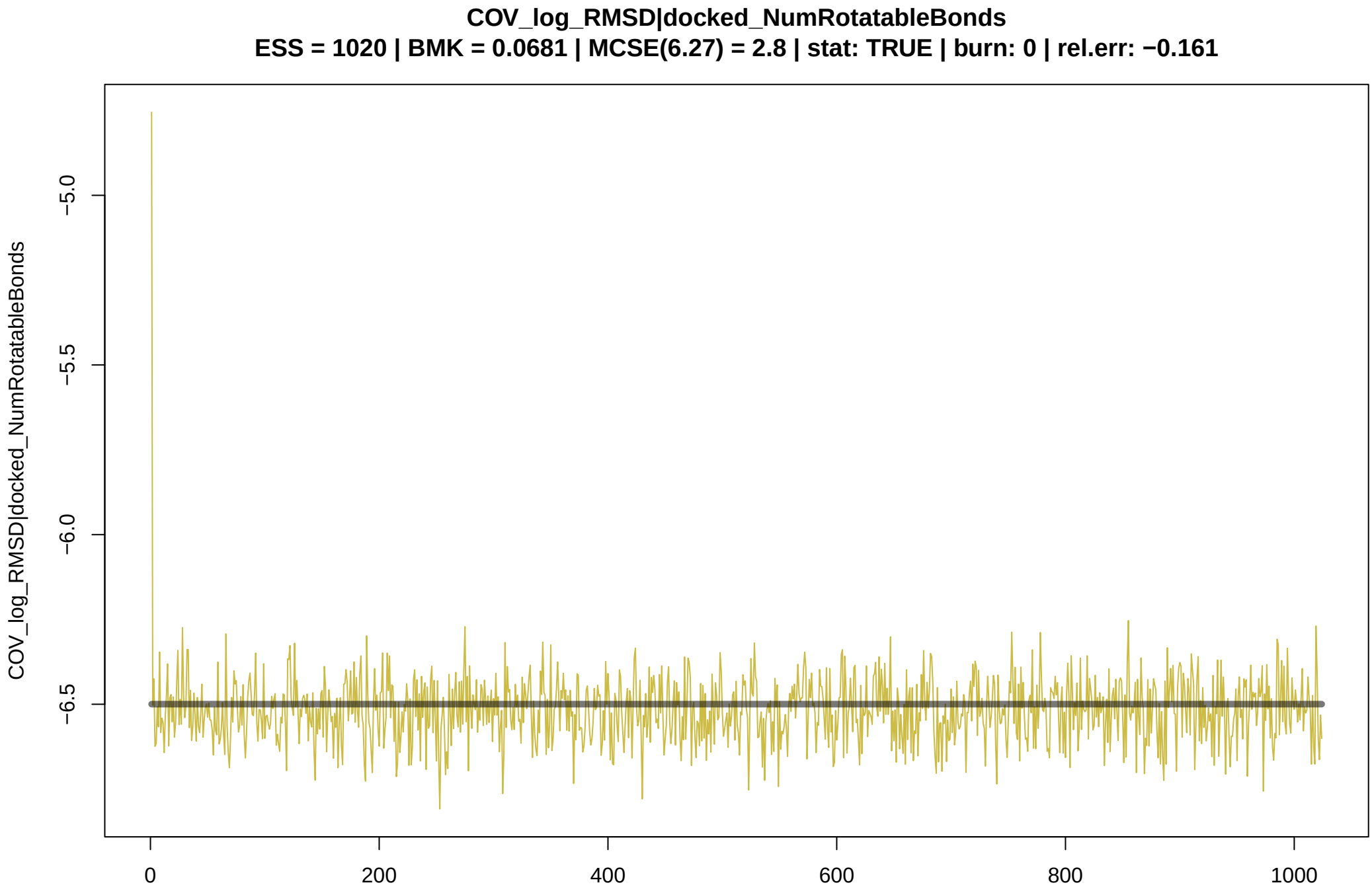

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 917 | BMK = 0.0502 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | rel.err: 0.597
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.30
−0.35
−0.40
−0.45
−0.50
−0.55
0
200
400
600
800
1000

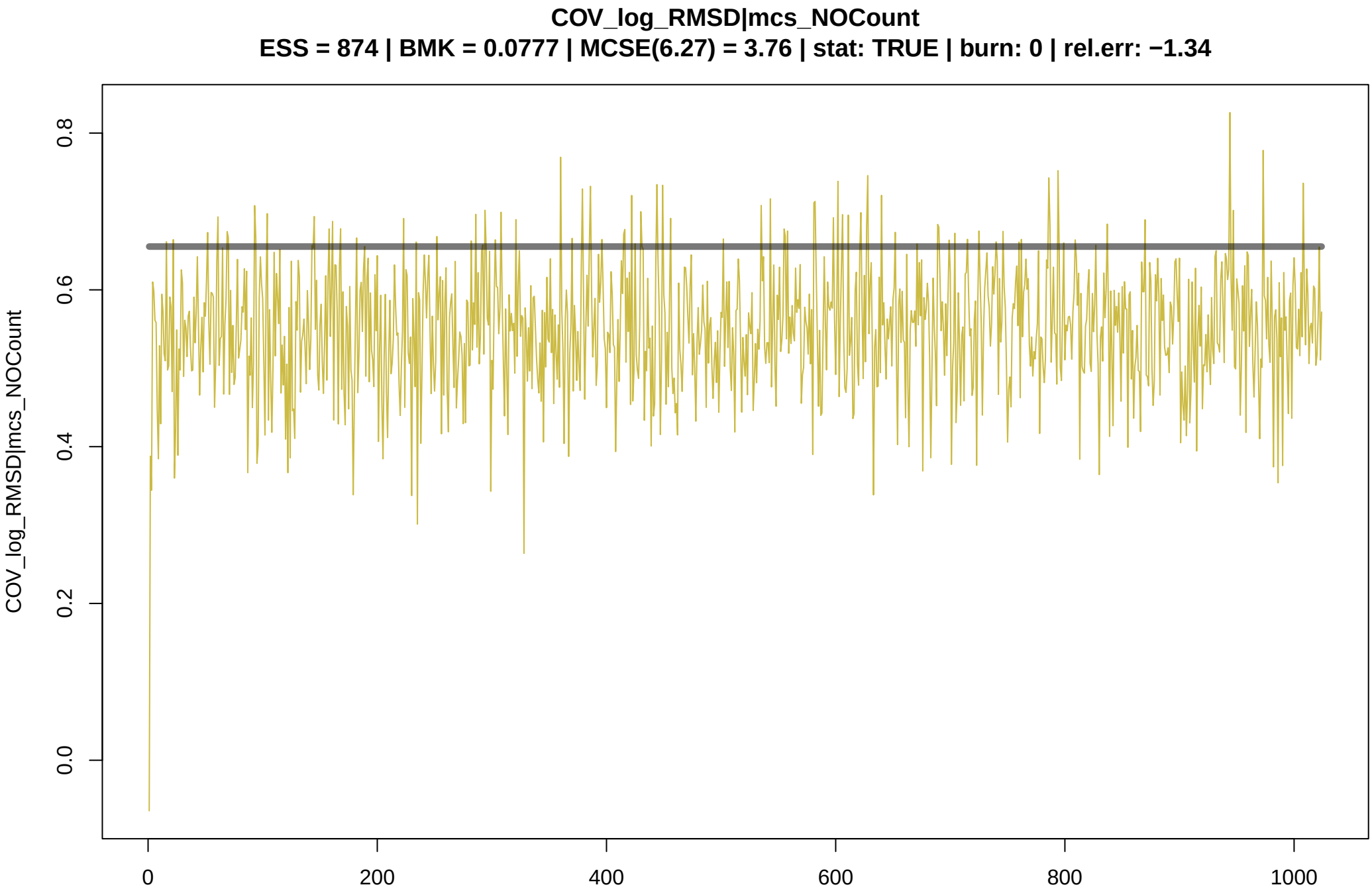

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0553 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: 1.41
COV_log_RMSD|logit_ec_tanimoto_similarity
4.0
4.2
4.4
4.6
4.8
5.0
0
200
400
600
800
1000

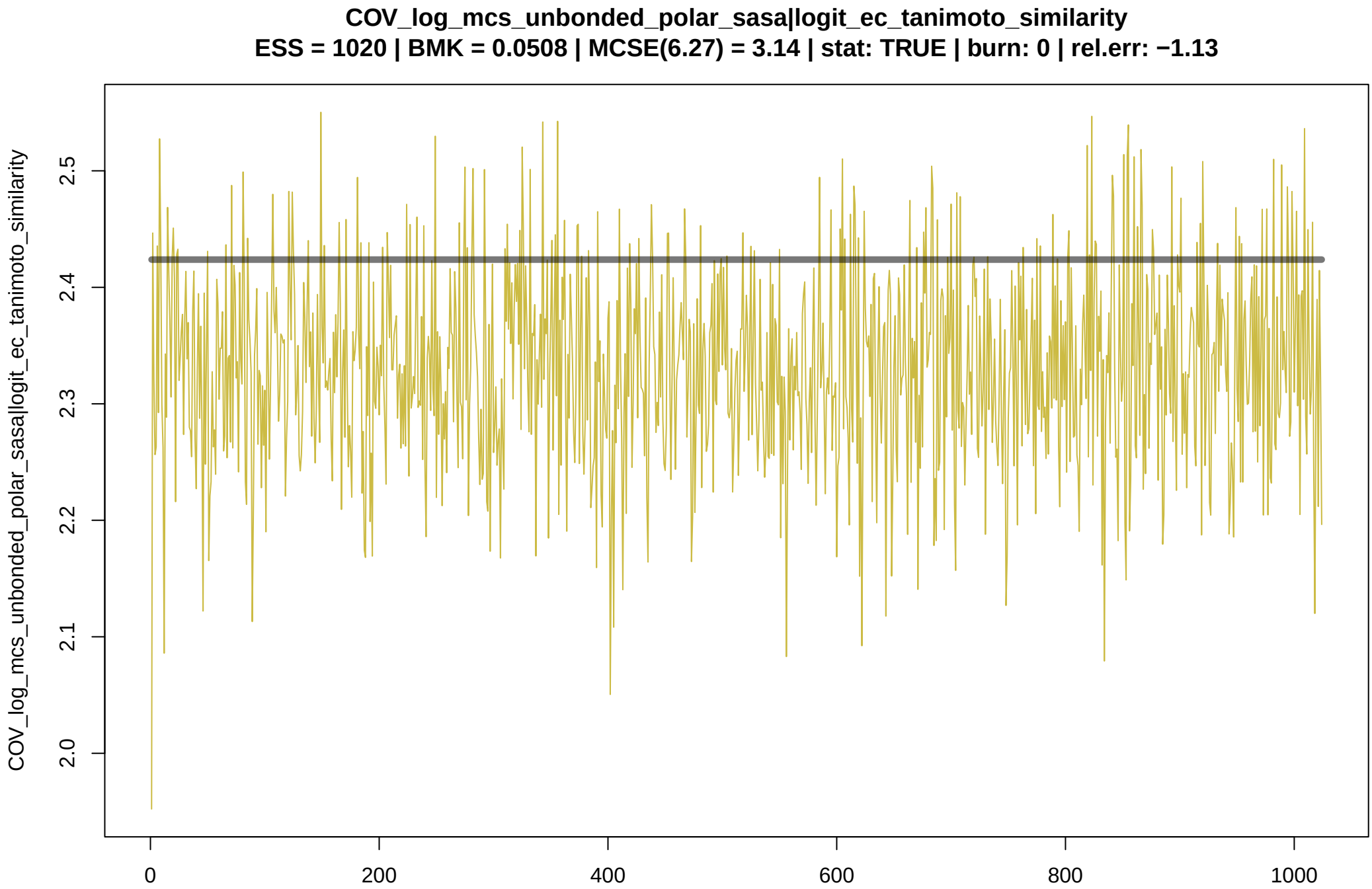

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0386 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: −0.994
COV_log_RMSD|mcs_NumHeteroAtoms
−0.05
−0.10
−0.15
−0.20
0
200
400
600
800
1000

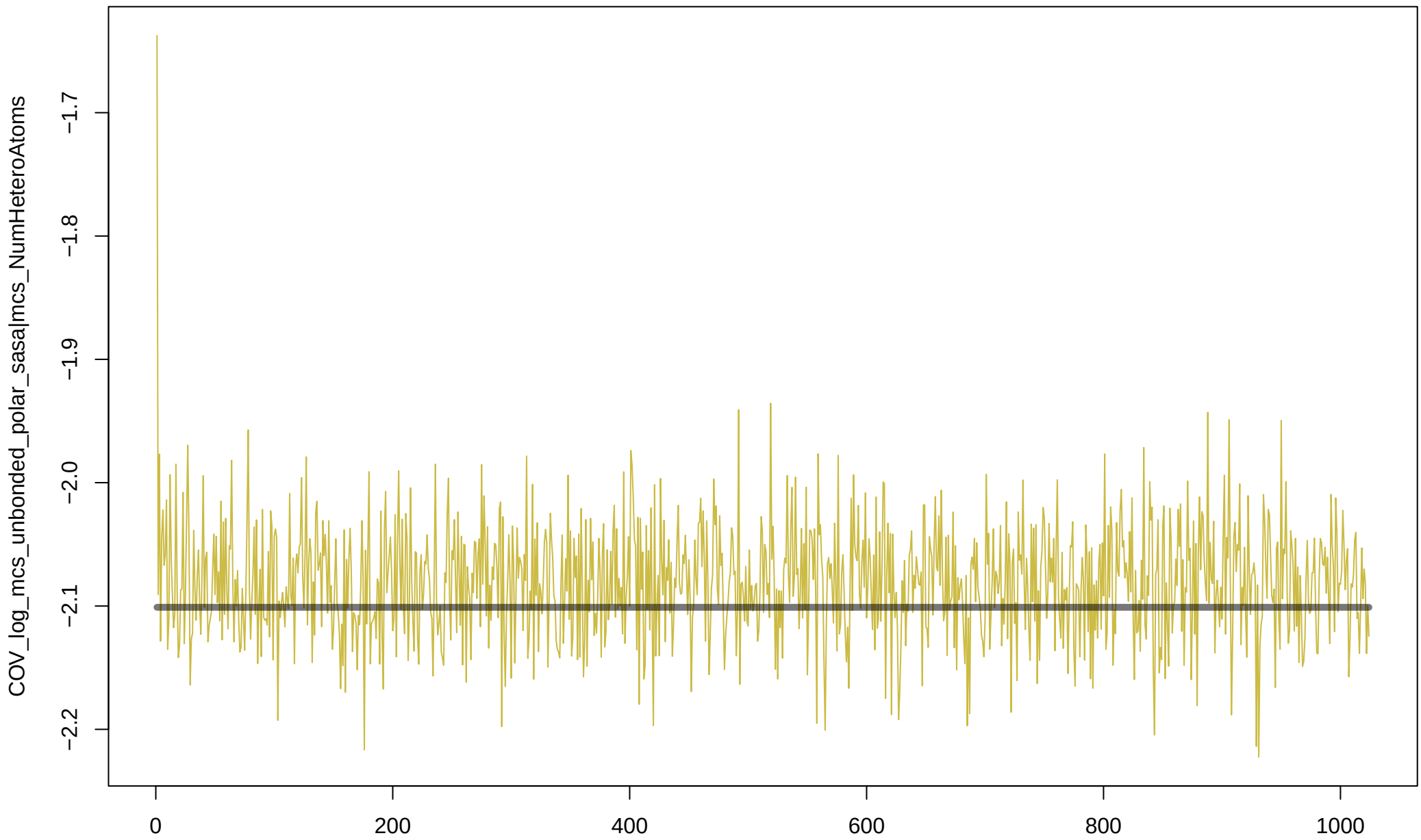

COV_log_RMSD|docked_HeavyAtomCount
ESS = 917 | BMK = 0.0492 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | rel.err: 0.927
COV_log_RMSD|docked_HeavyAtomCount
4.5
5.0
5.5
6.0
0
200
400
600
800
1000

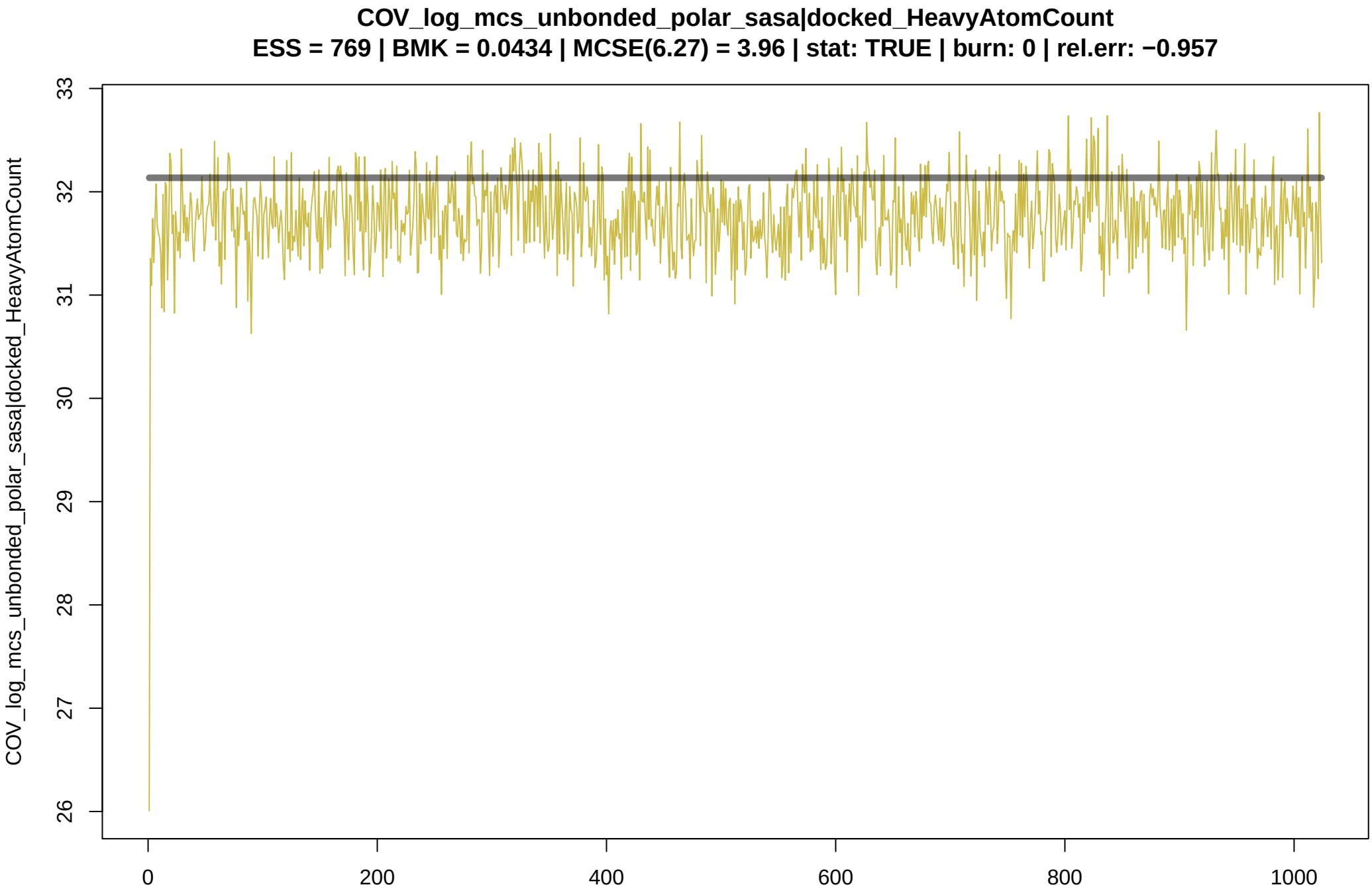

COV_log_RMSD|mcs_RingCount
ESS = 886 | BMK = 0.047 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | rel.err: −0.761
COV_log_RMSD|mcs_RingCount
0.15
0.10
0.05
0.00
−0.05
0
200
400
600
800
1000

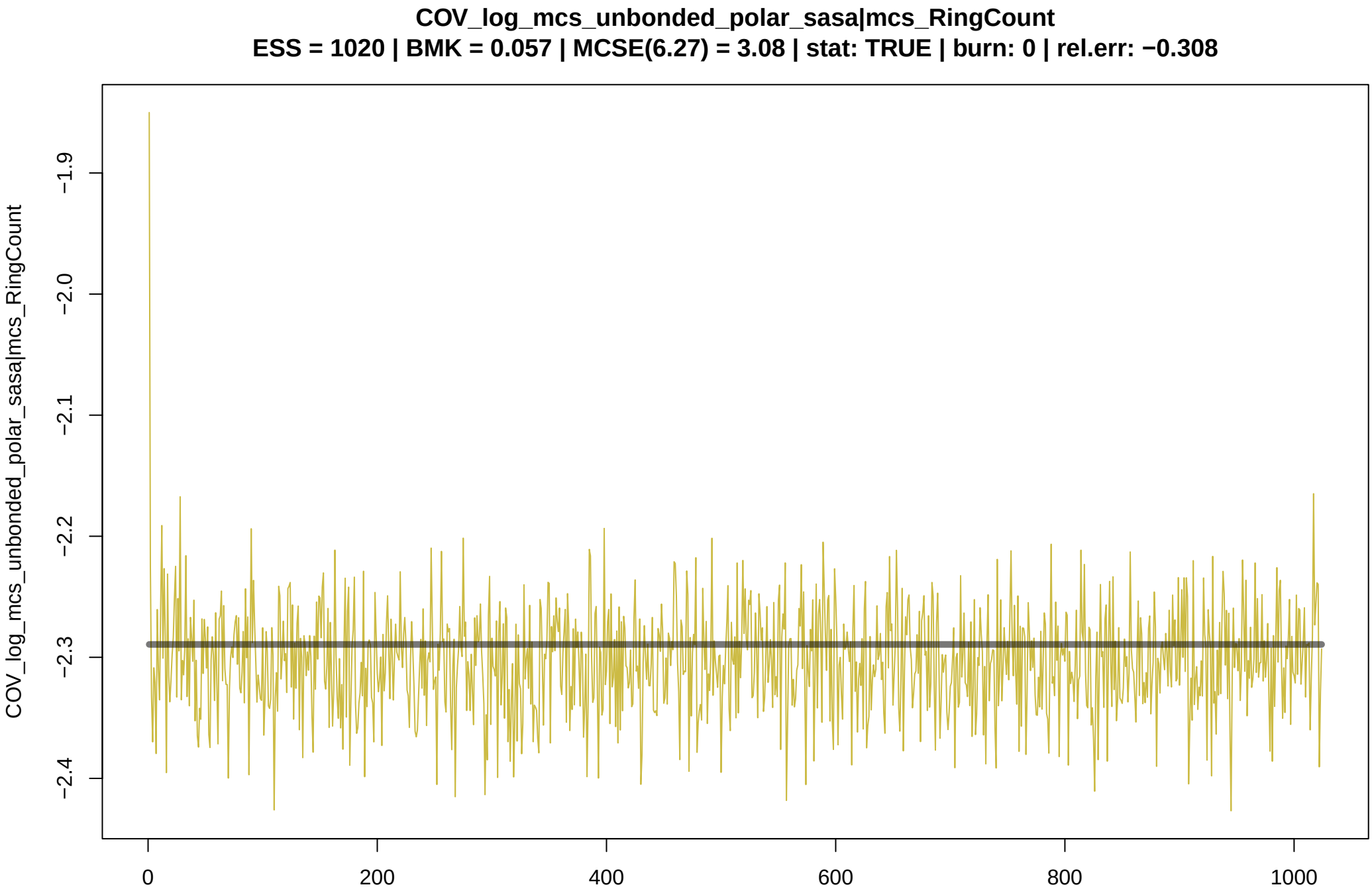

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0681 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0 | rel.err: −0.161
COV_log_RMSD|docked_NumRotatableBonds
−5.0
−5.5
−6.0
−6.5
0
200
400
600
800
1000

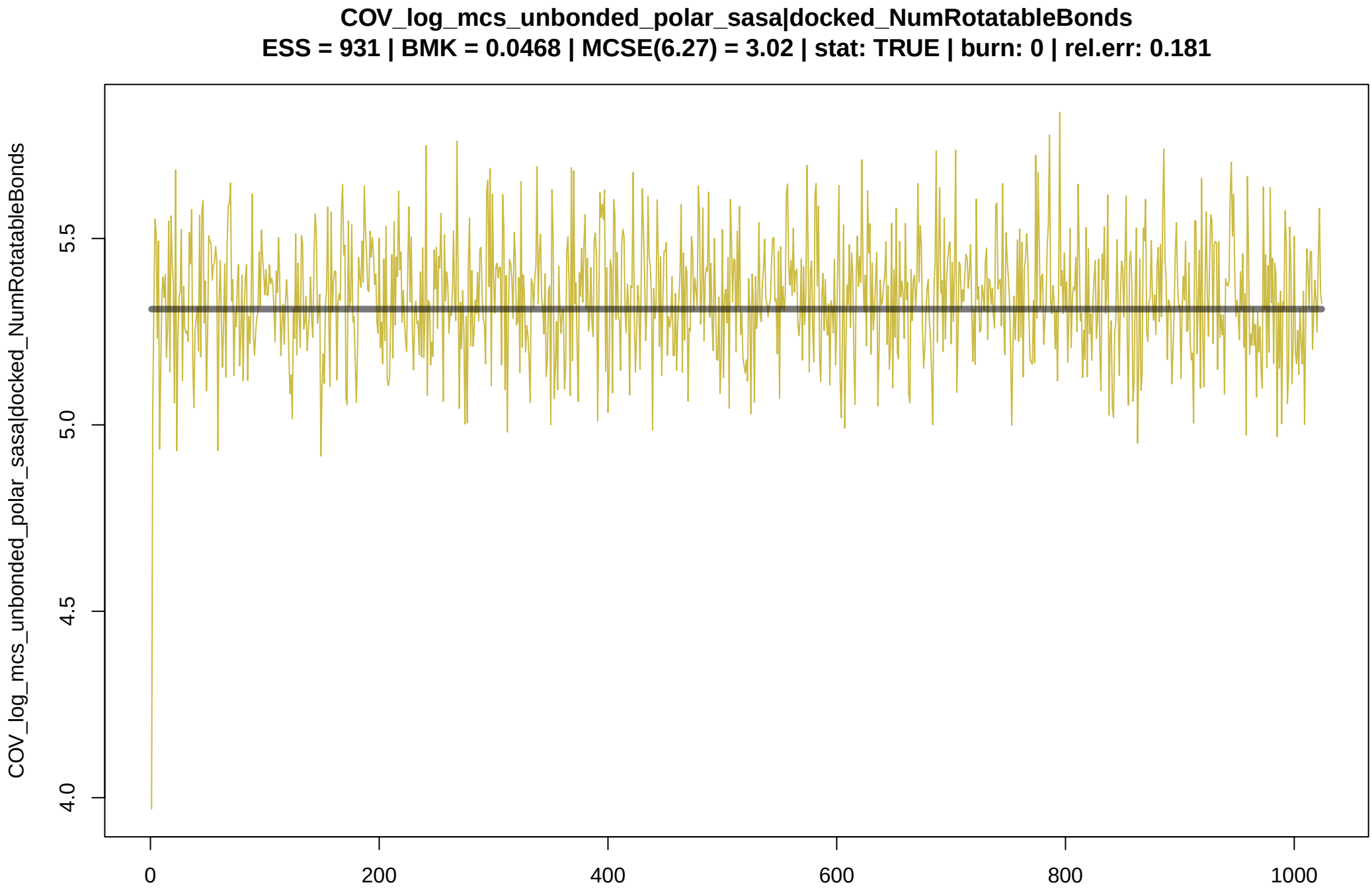

COV_log_RMSD|mcs_NOCount
ESS = 874 | BMK = 0.0777 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0 | rel.err: −1.34
COV_log_RMSD|mcs_NOCount
0.0
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

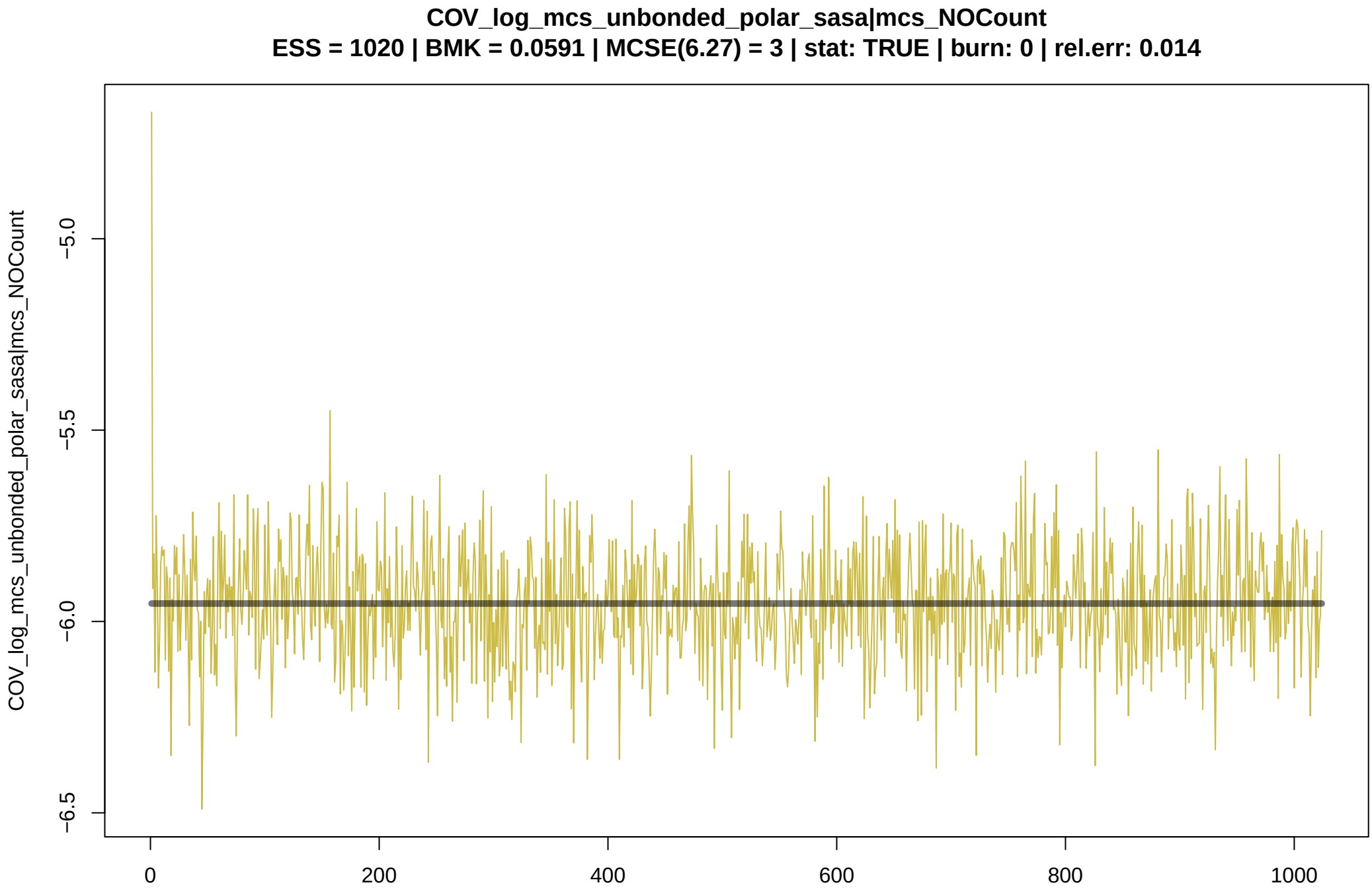

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0508 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | rel.err: −1.13
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2.0
2.1
2.2
2.3
2.4
2.5
0
200
400
600
800
1000

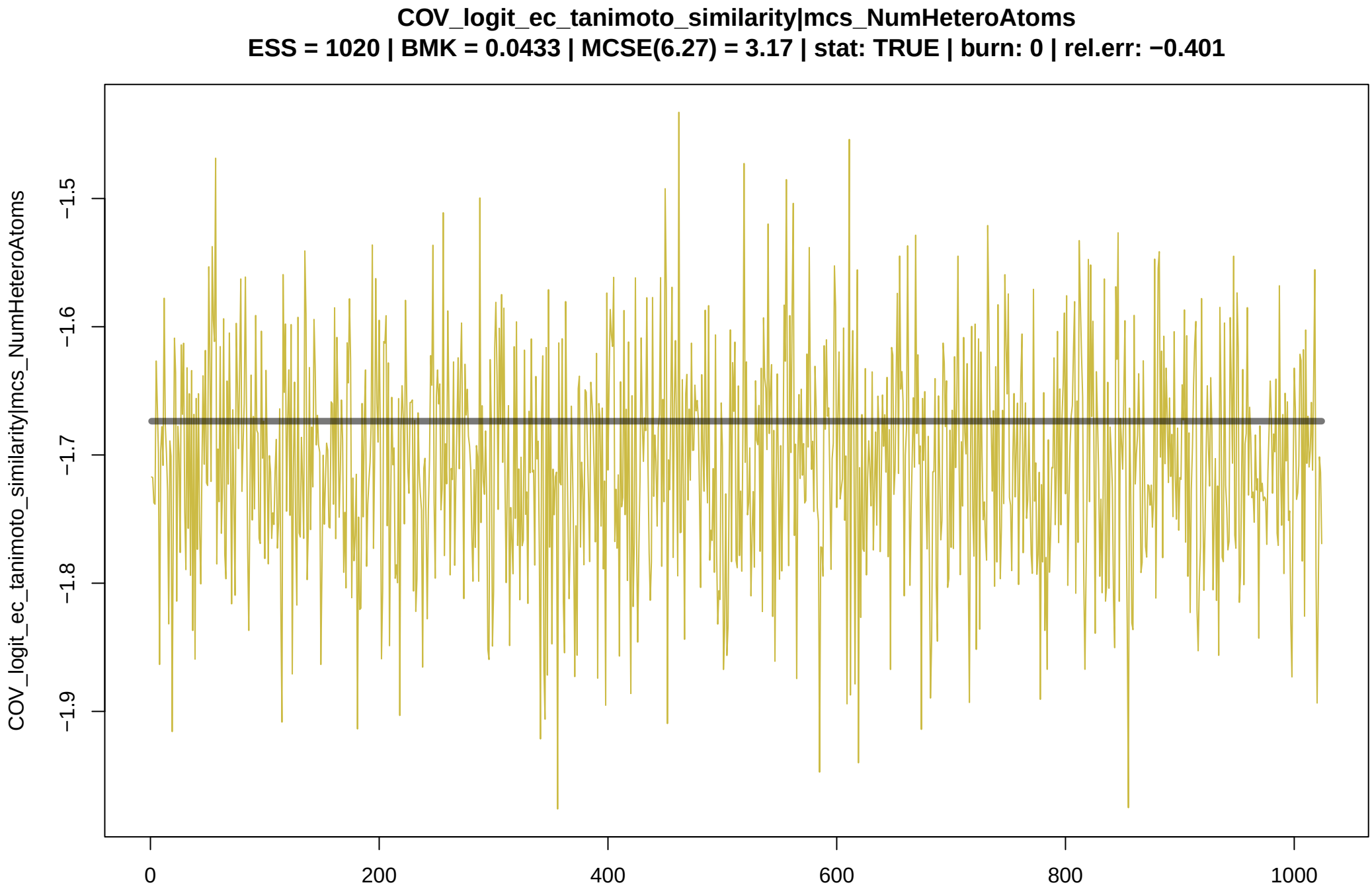

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0641 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | rel.err: 0.428
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.7
−1.8
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

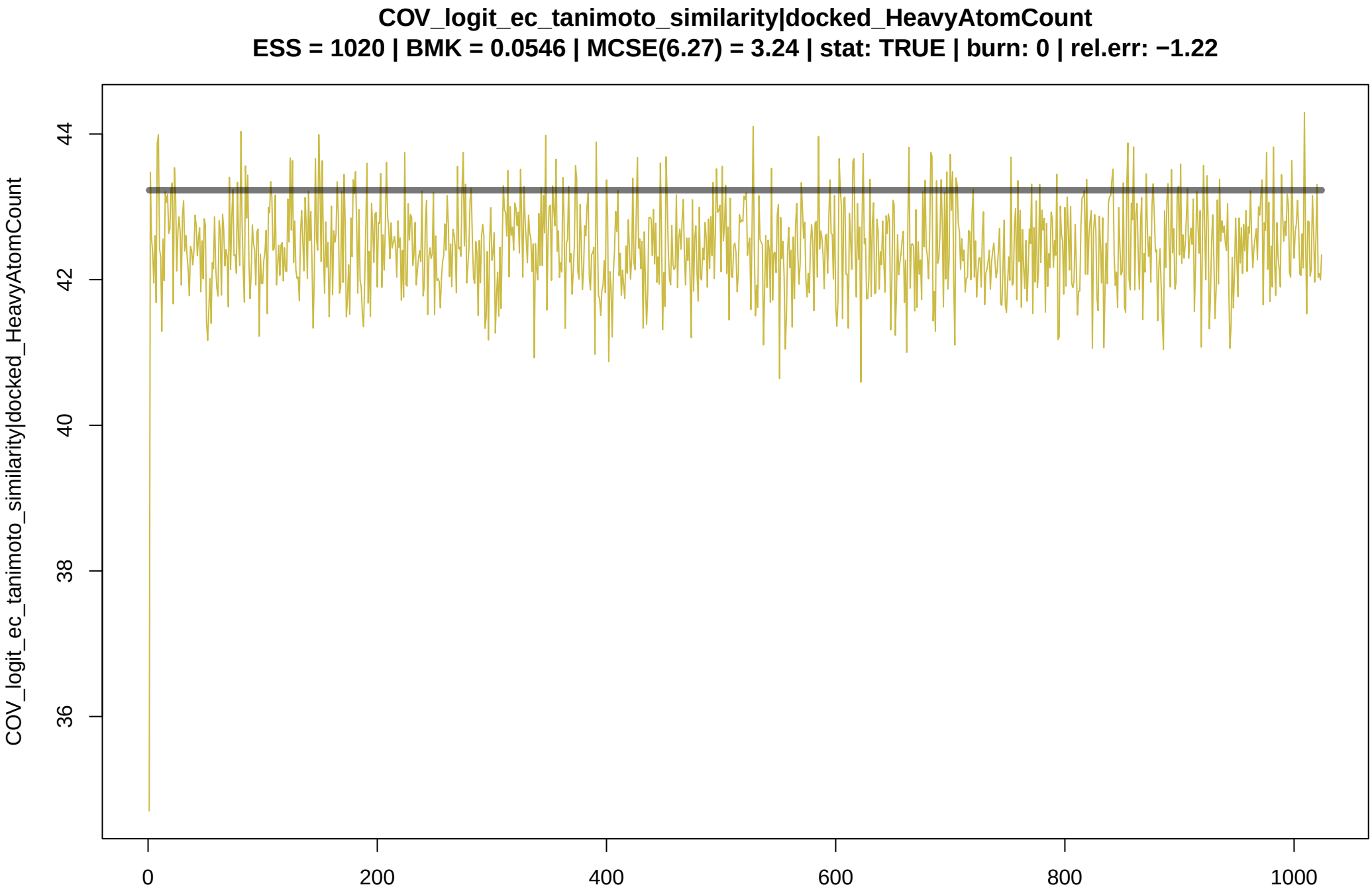

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 769 | BMK = 0.0434 | MCSE(6.27) = 3.96 | stat: TRUE | burn: 0 | rel.err: −0.957
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
26
27
28
29
30
31
32
33
0
200
400
600
800
1000

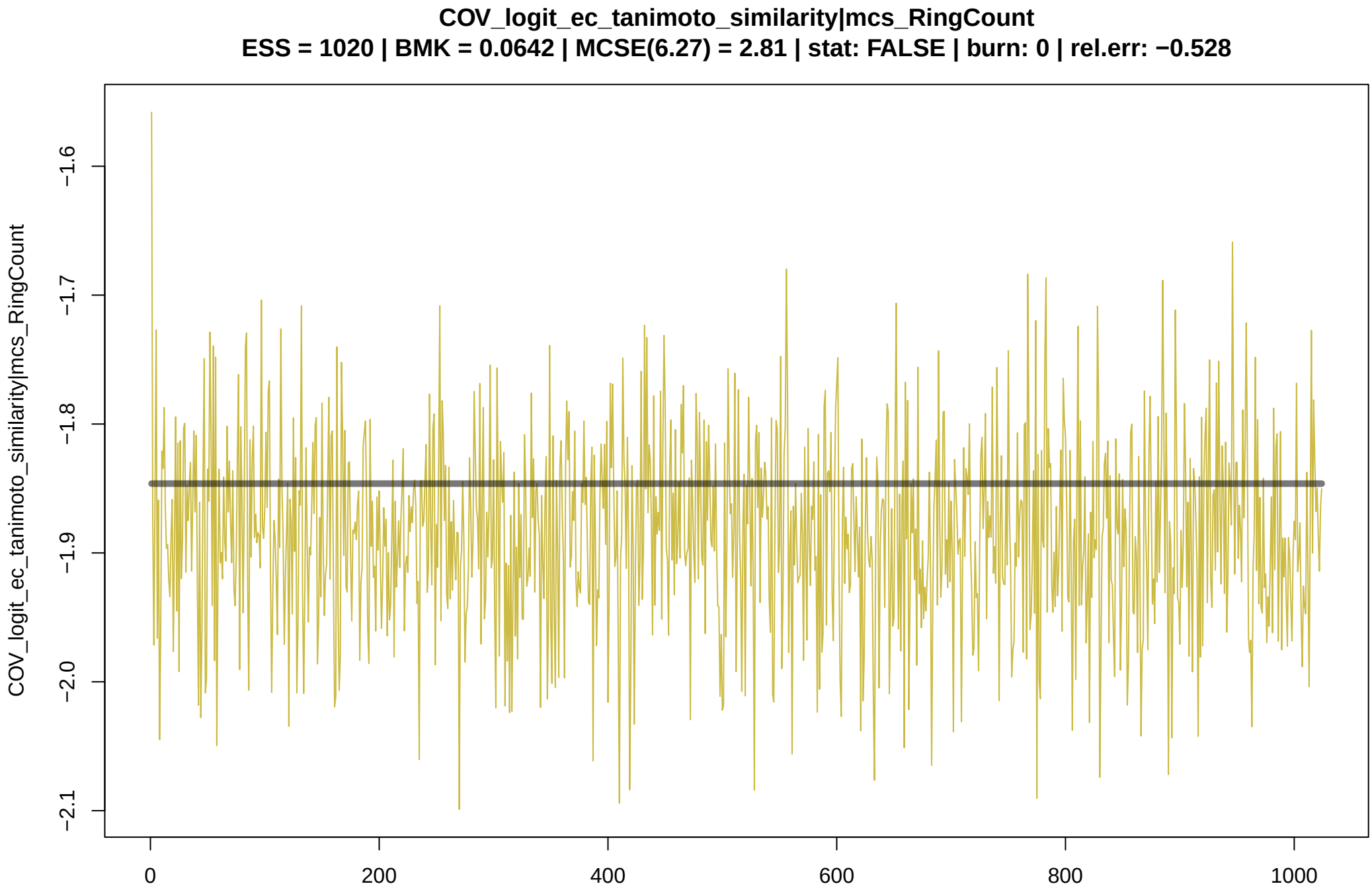

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.057 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | rel.err: −0.308
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−1.9
−2.0
−2.1
−2.2
−2.3
−2.4
0
200
400
600
800
1000

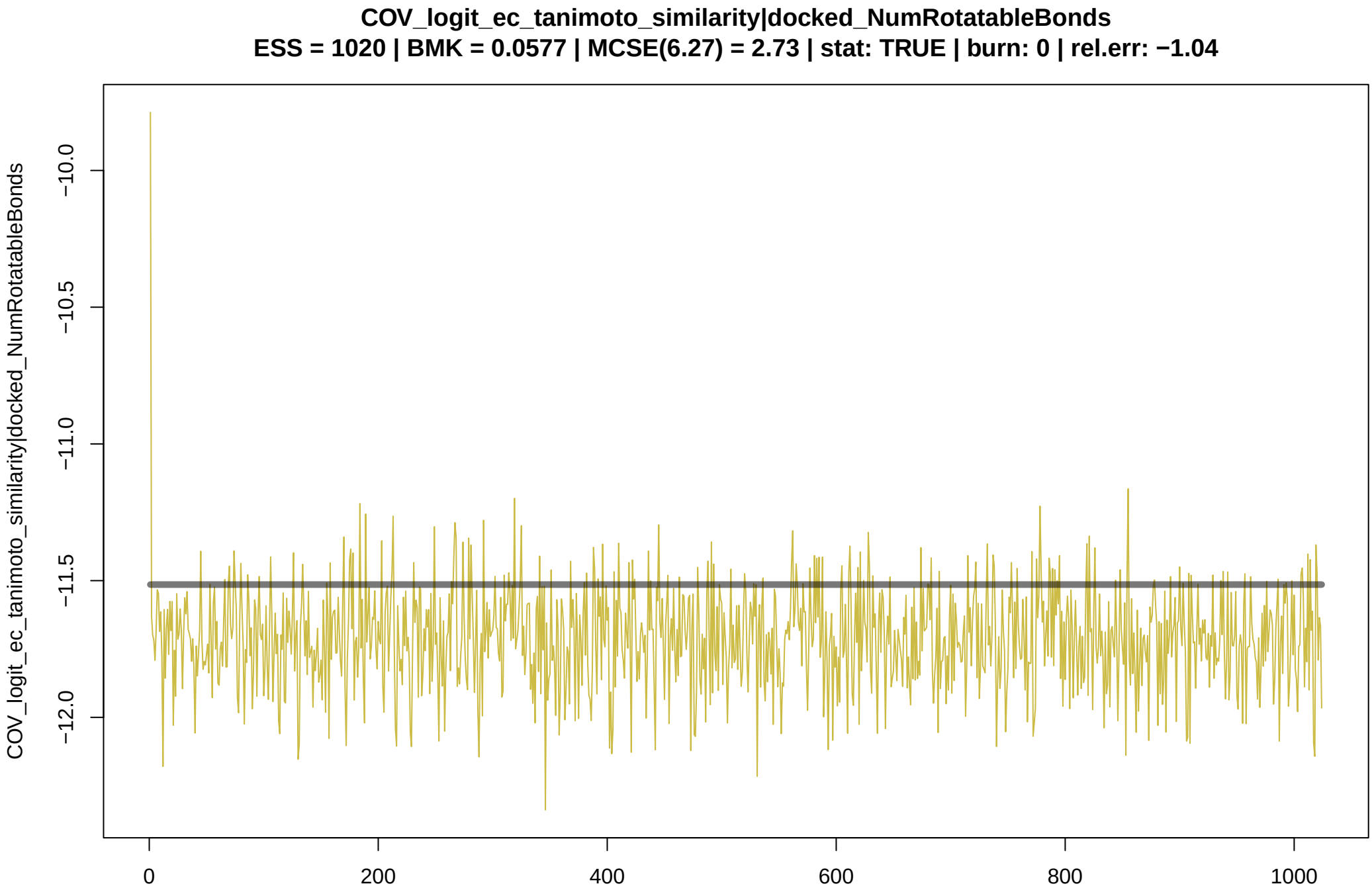

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 931 | BMK = 0.0468 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | rel.err: 0.181
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
4.0
4.5
5.0
5.5
0
200
400
600
800
1000

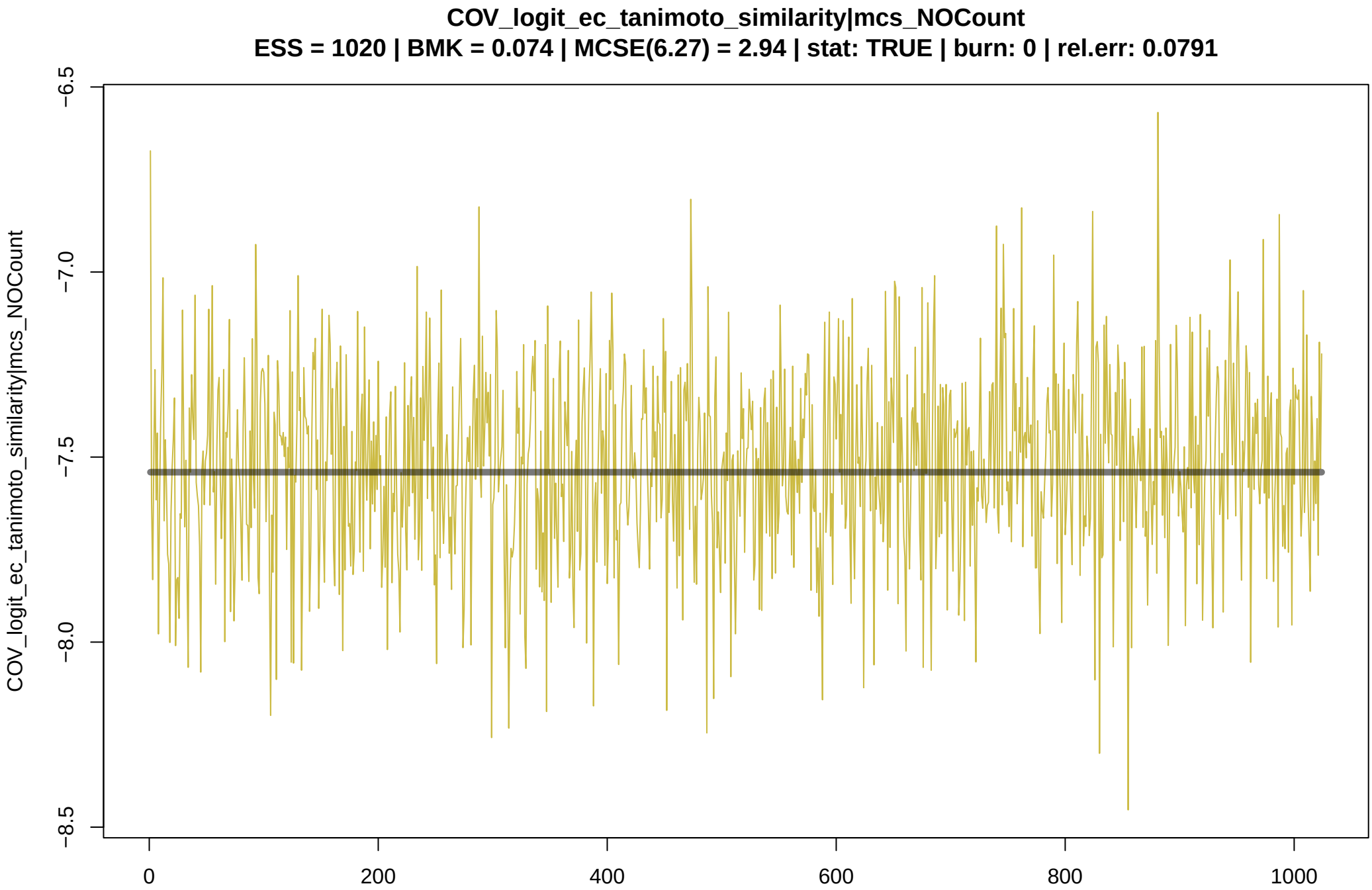

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0591 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | rel.err: 0.014
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.0
−5.5
−6.0
−6.5
0
200
400
600
800
1000

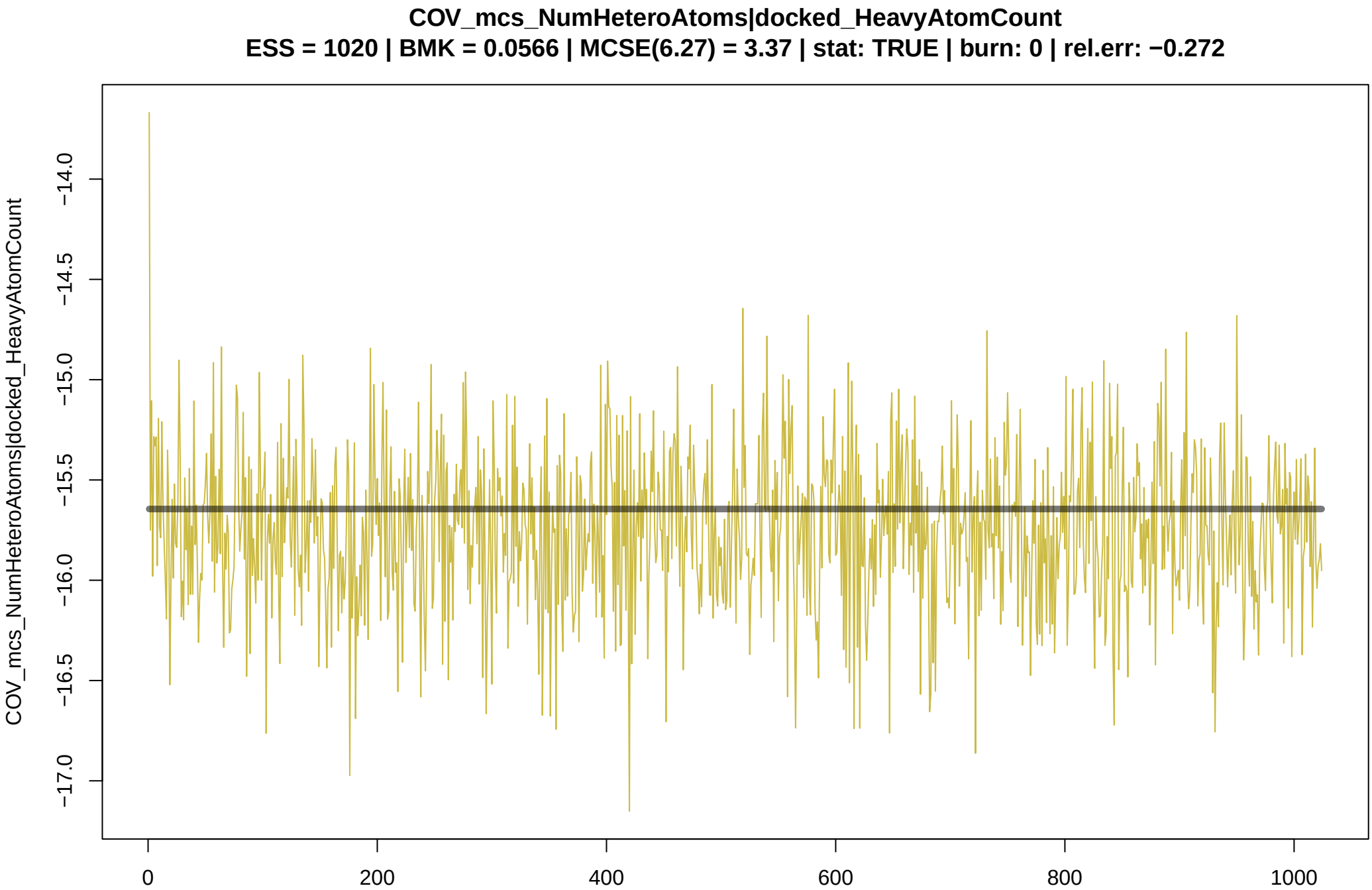

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0433 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | rel.err: −0.401
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.5
−1.6
−1.7
−1.8
−1.9
0
200
400
600
800
1000

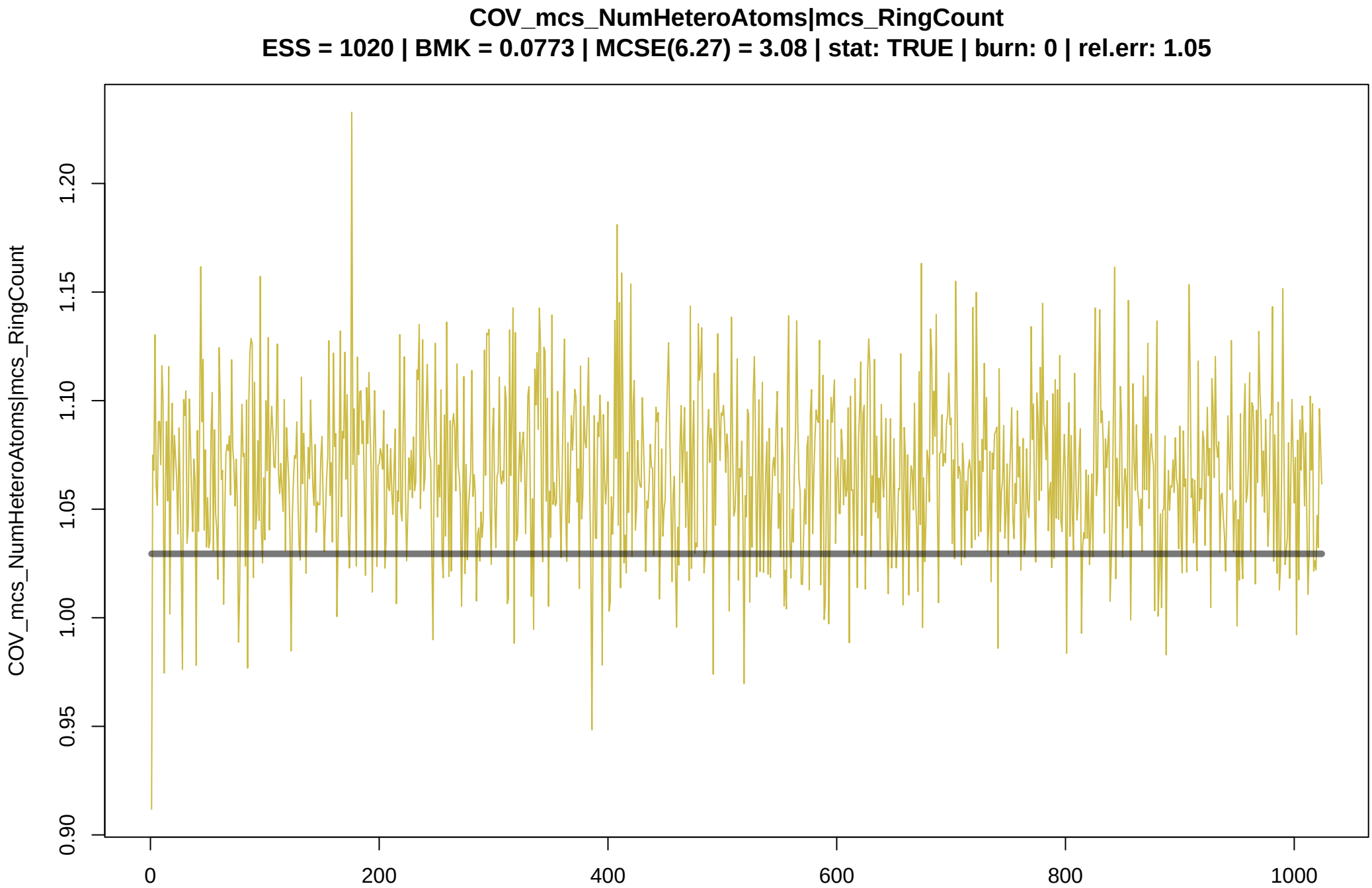

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0546 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | rel.err: −1.22
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
36
38
40
42
44
0
200
400
600
800
1000

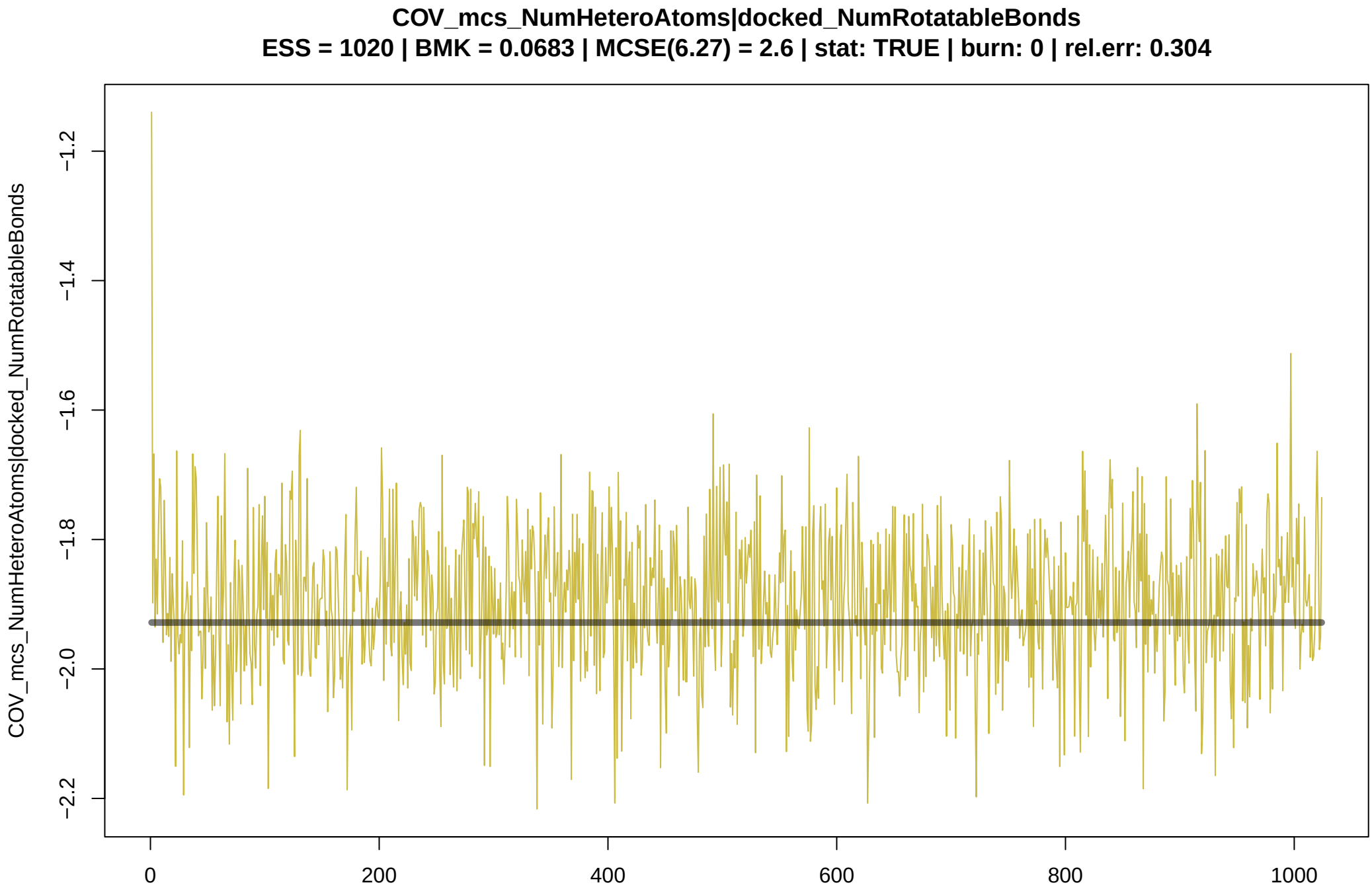

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0642 | MCSE(6.27) = 2.81 | stat: FALSE | burn: 0 | rel.err: −0.528
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.6
−1.7
−1.8
−1.9
−2.0
−2.1
0
200
400
600
800
1000

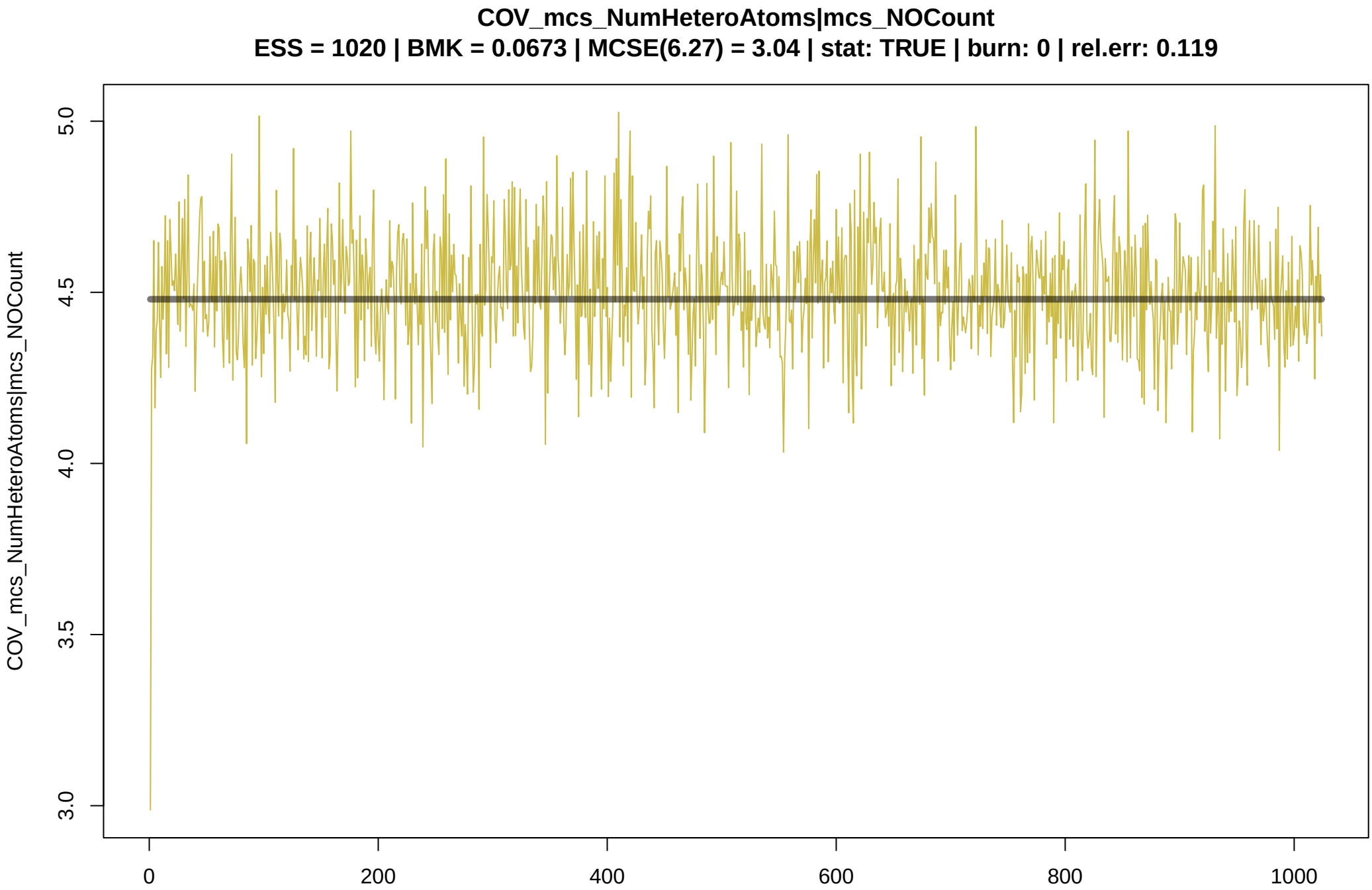

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0577 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | rel.err: −1.04
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−10.0
−10.5
−11.0
−11.5
−12.0
0
200
400
600
800
1000

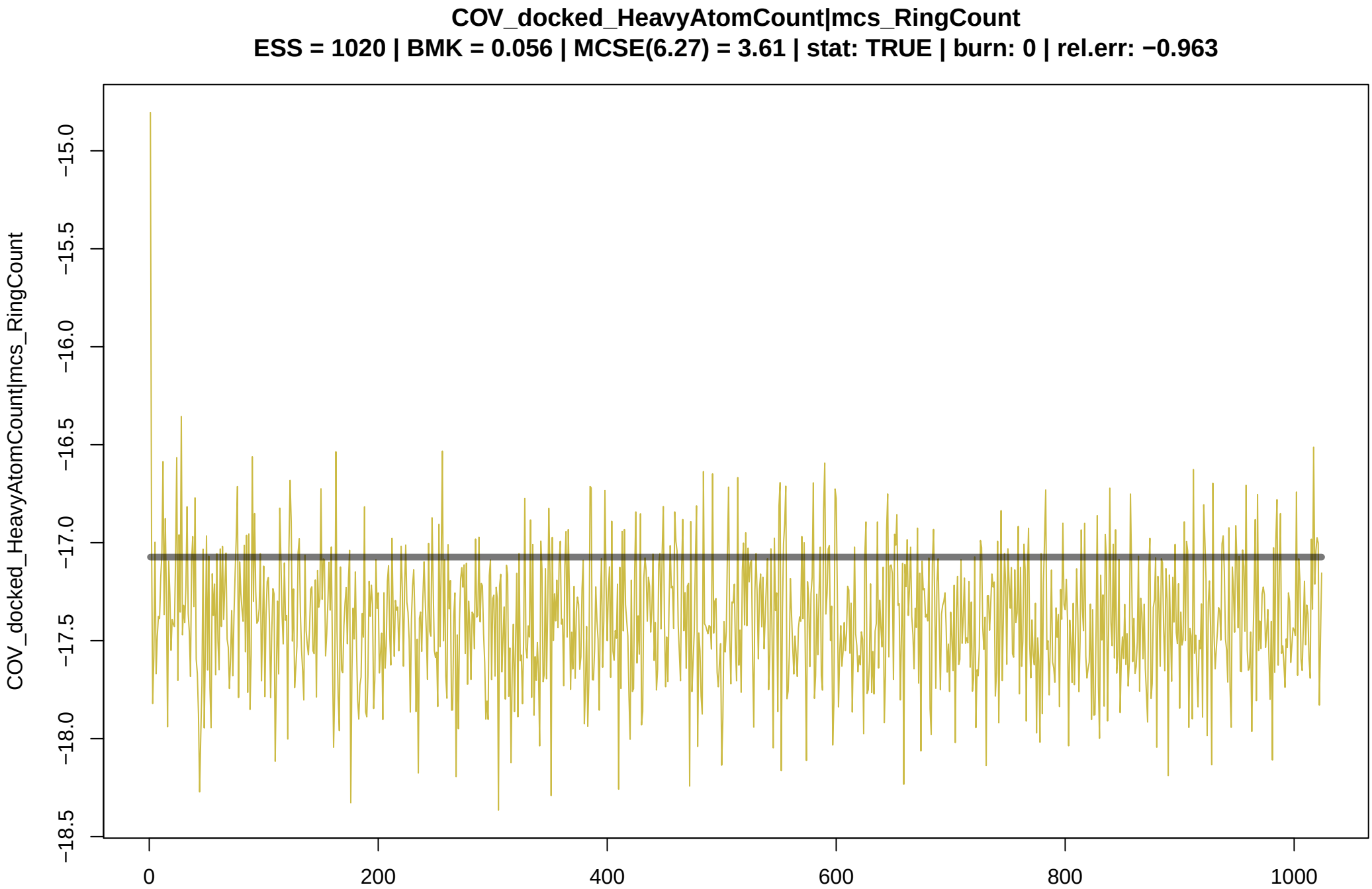

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.074 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | rel.err: 0.0791
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−6.5
−7.0
−7.5
−8.0
−8.5
0
200
400
600
800
1000

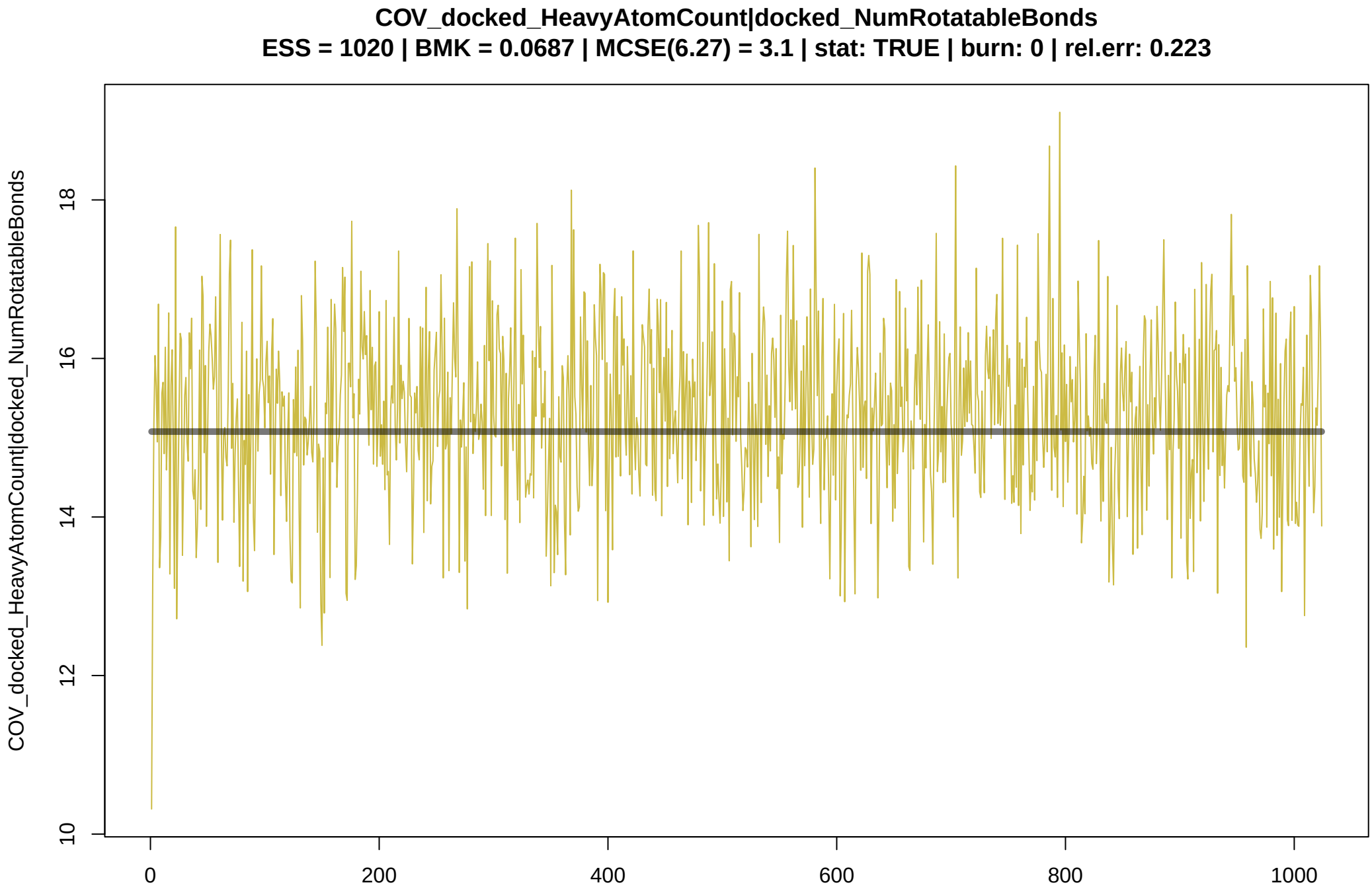

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0566 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | rel.err: −0.272
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−14.0
−14.5
−15.0
−15.5
−16.0
−16.5
−17.0
0
200
400
600
800
1000

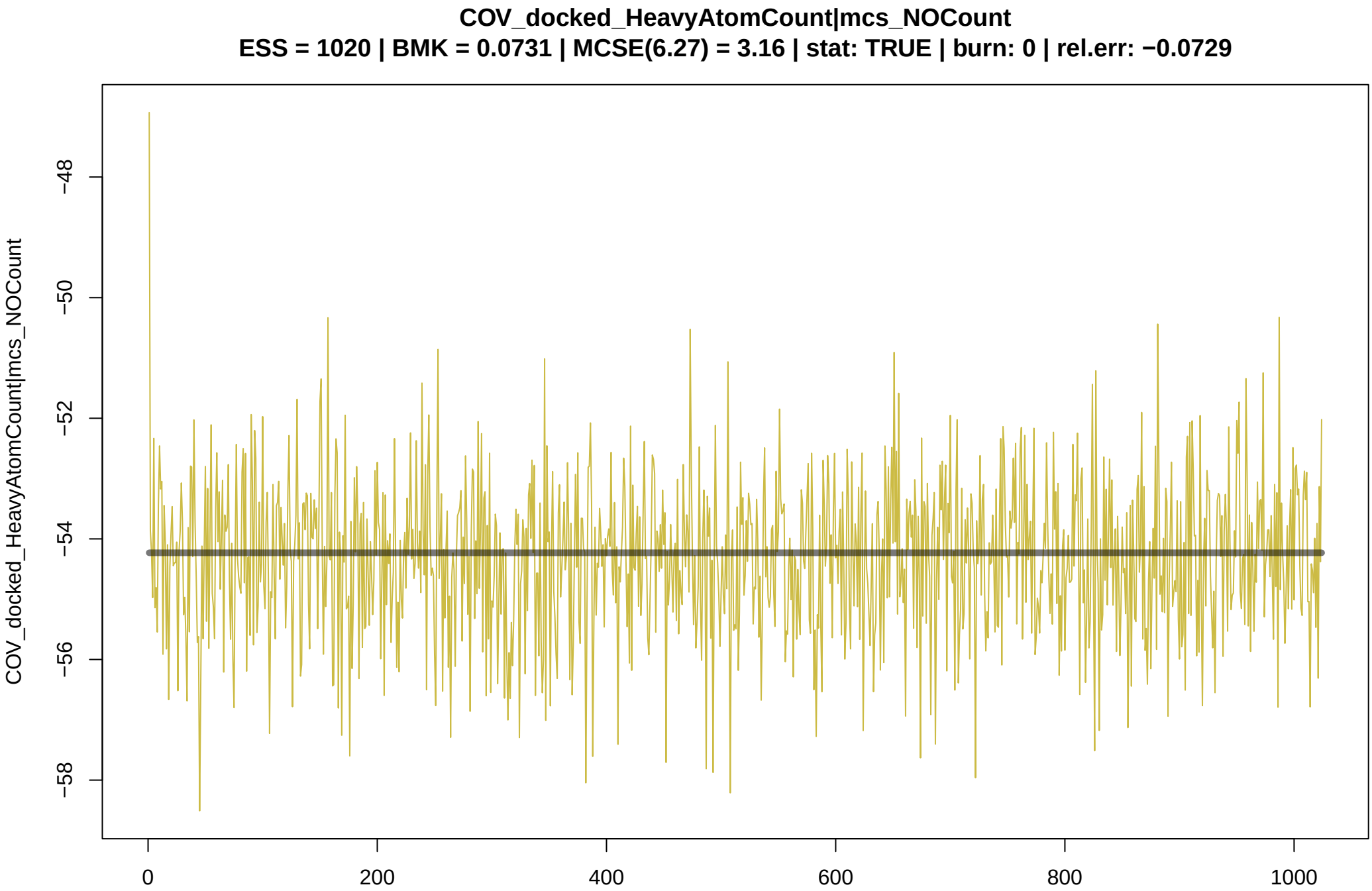

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0773 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | rel.err: 1.05
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.90
0.95
1.00
1.05
1.10
1.15
1.20
0
200
400
600
800
1000

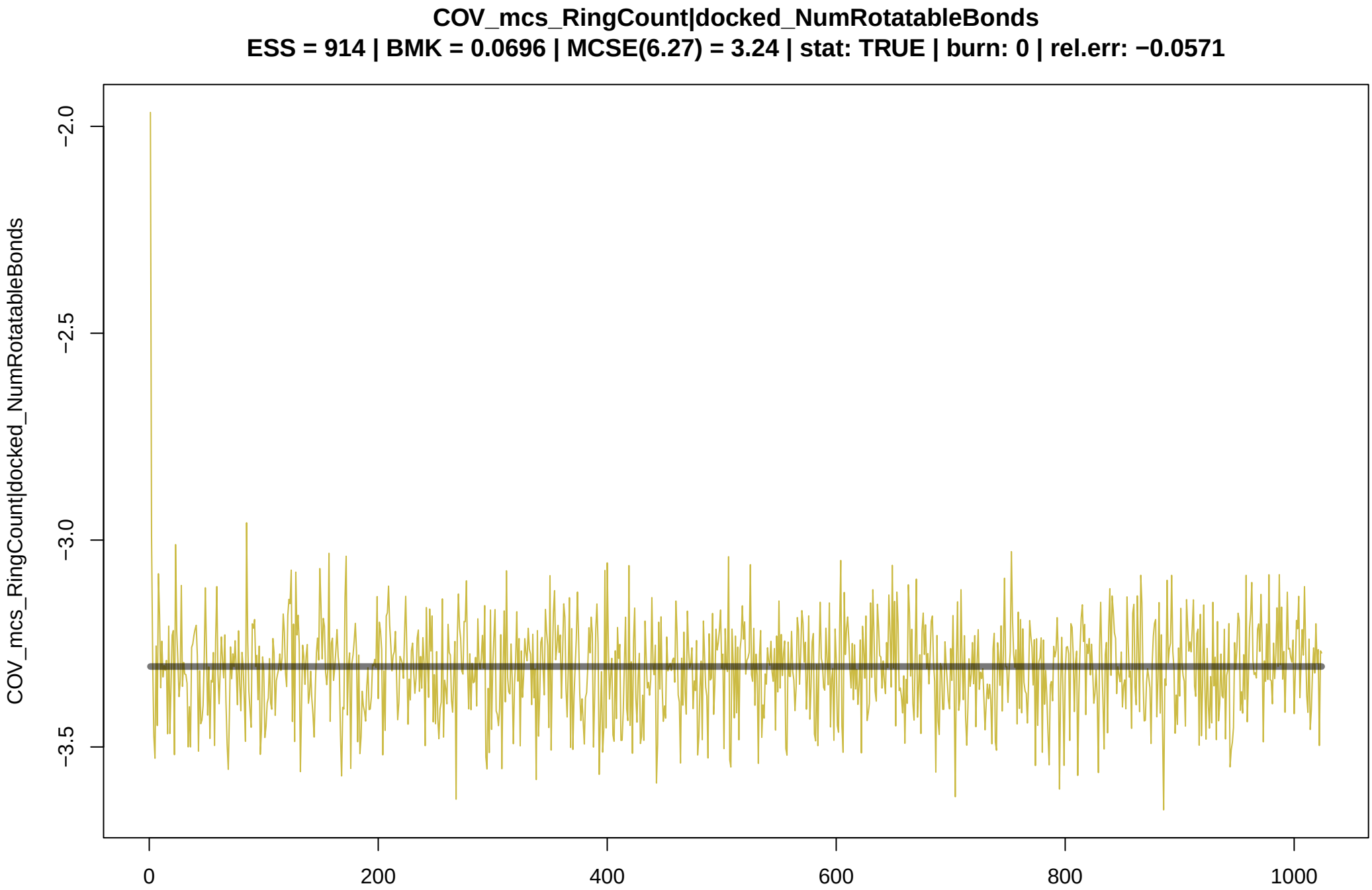

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0683 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: 0.304
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.2
−1.4
−1.6
−1.8
−2.0
−2.2
0
200
400
600
800
1000

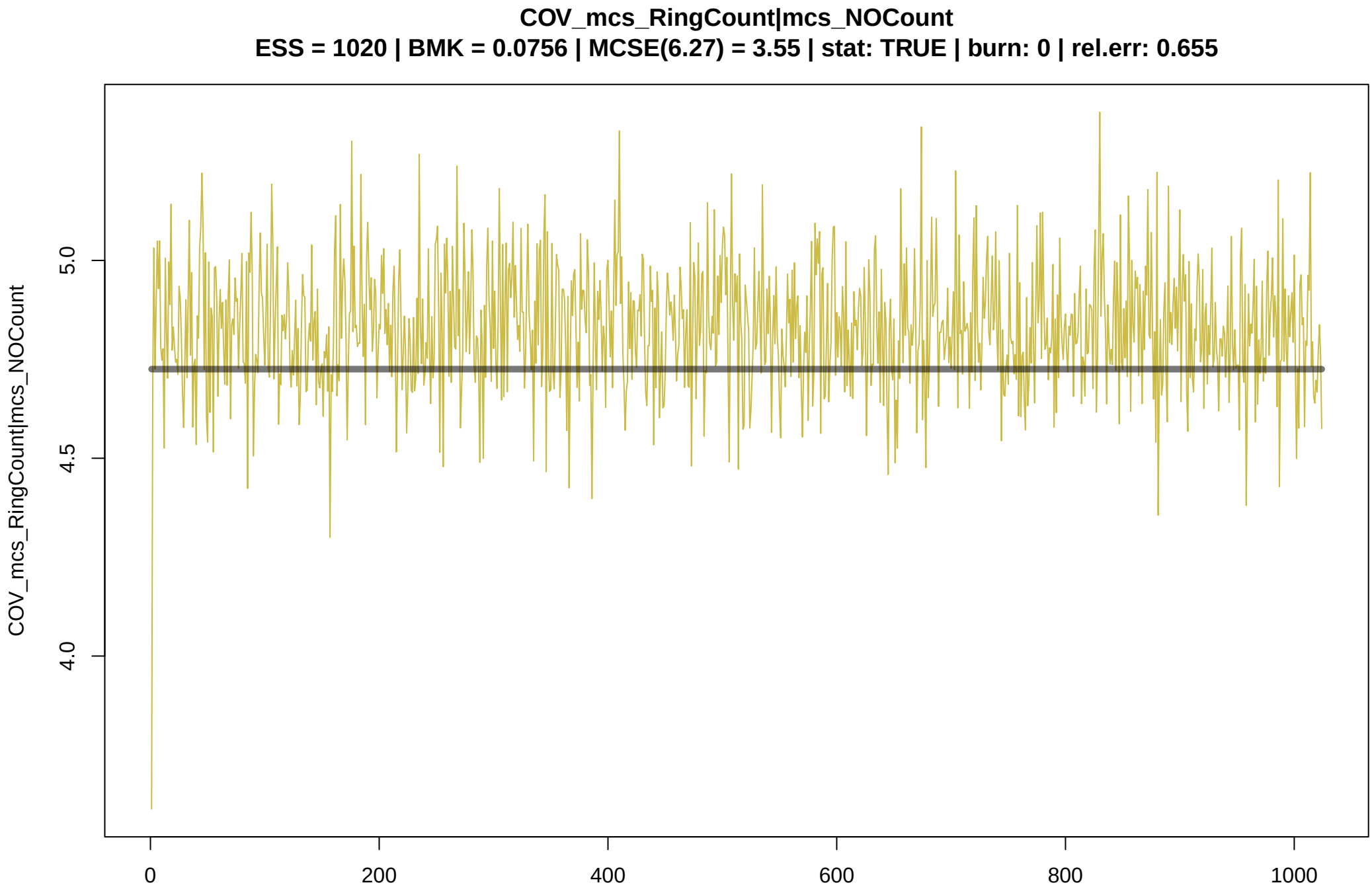

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0673 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: 0.119
COV_mcs_NumHeteroAtoms|mcs_NOCount
3.0
3.5
4.0
4.5
5.0
0
200
400
600
800
1000

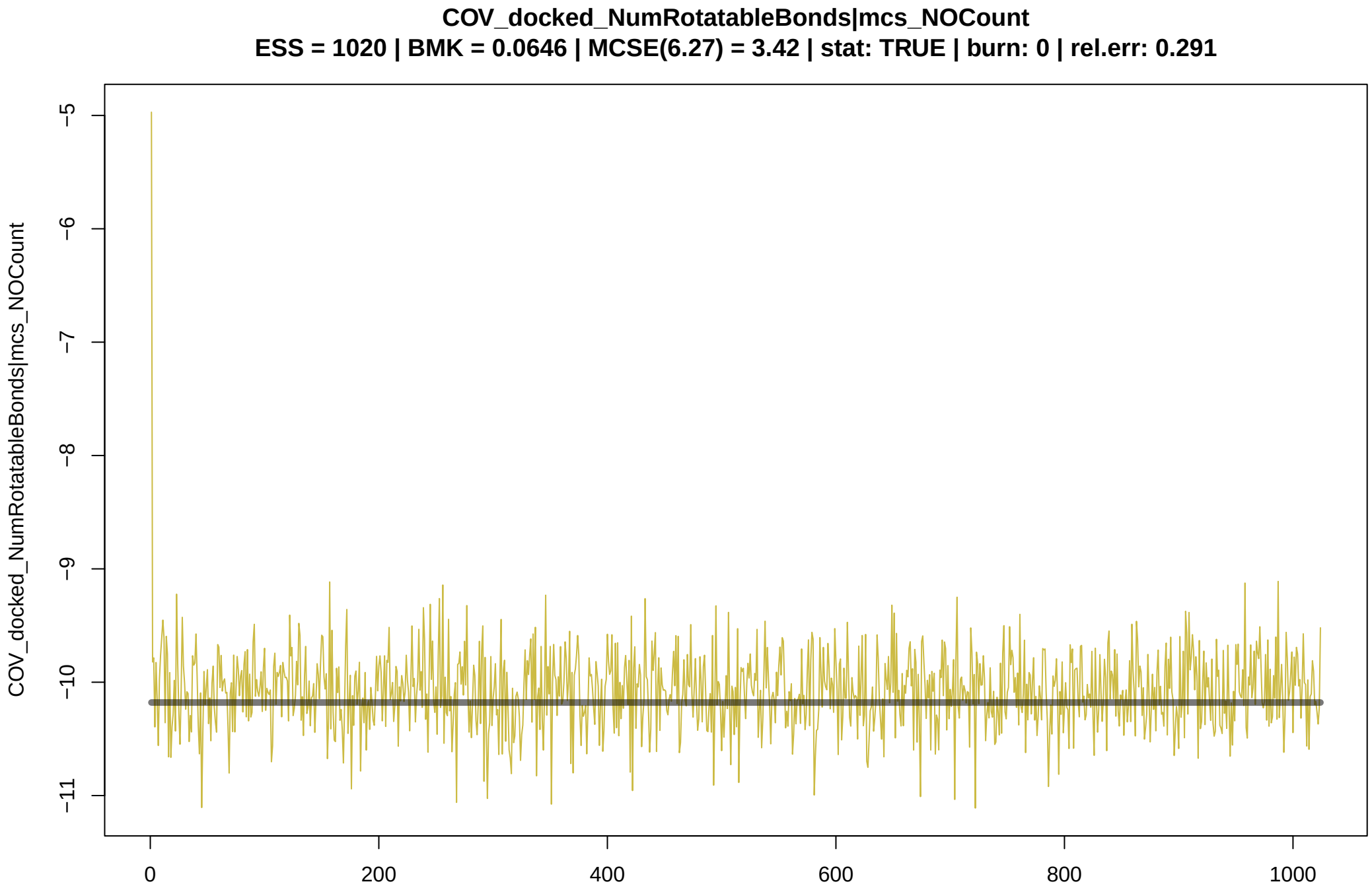

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.056 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0 | rel.err: −0.963
COV_docked_HeavyAtomCount|mcs_RingCount
−15.0
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0687 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | rel.err: 0.223
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0731 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | rel.err: −0.0729
COV_docked_HeavyAtomCount|mcs_NOCount
−48
−50
−52
−54
−56
−58
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 914 | BMK = 0.0696 | MCSE(6.27) = 3.24 | stat: TRUE | burn: 0 | rel.err: −0.0571
COV_mcs_RingCount|docked_NumRotatableBonds
−2.0
−2.5
−3.0
−3.5
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0756 | MCSE(6.27) = 3.55 | stat: TRUE | burn: 0 | rel.err: 0.655
COV_mcs_RingCount|mcs_NOCount
4.0
4.5
5.0
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0646 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | rel.err: 0.291
COV_docked_NumRotatableBonds|mcs_NOCount
−5
−6
−7
−8
−9
−10
−11
0
200
400
600
800
1000