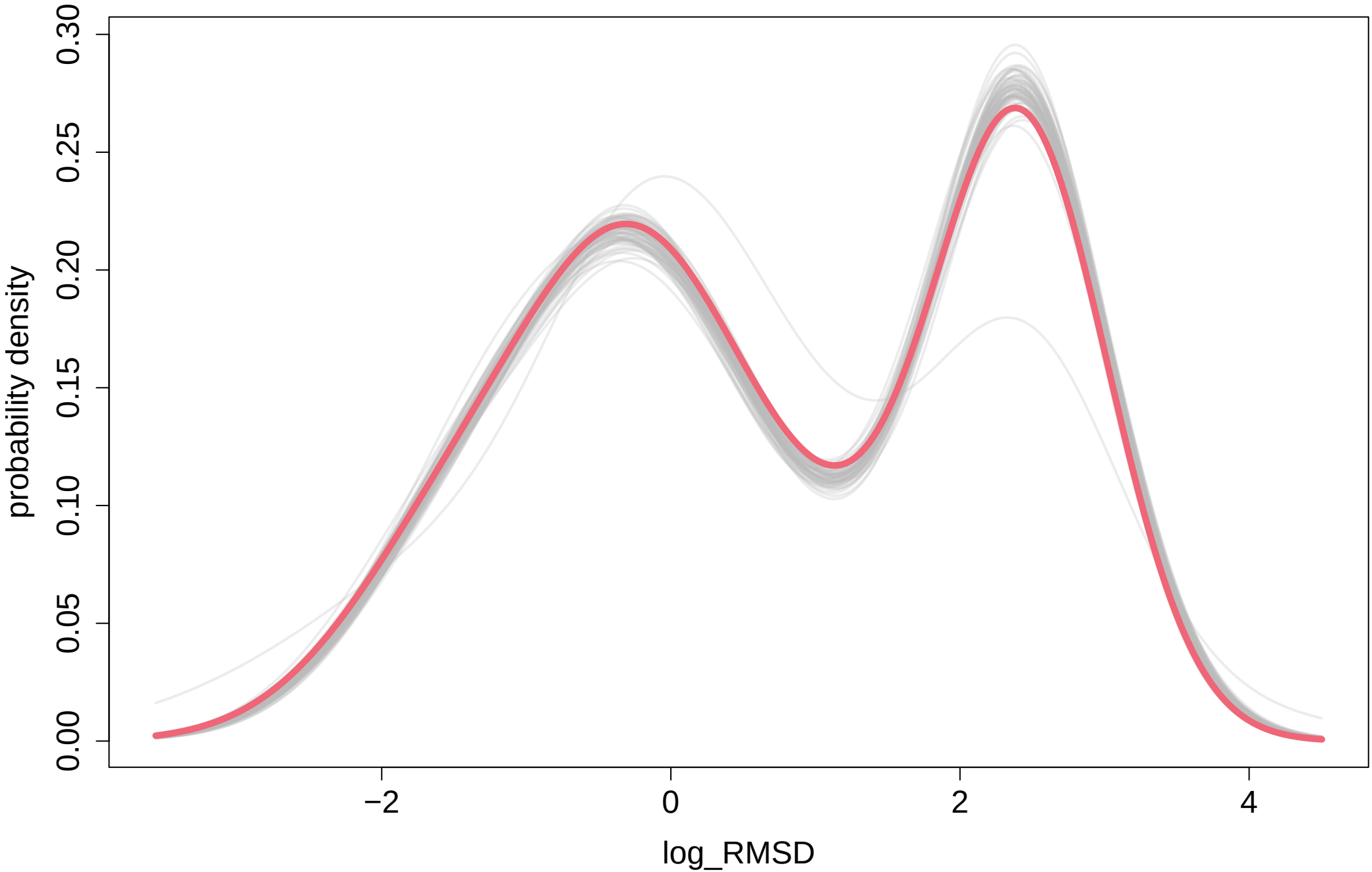
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.683858290180893
max MCSE = 13.7624126949477
all stationary: FALSE
burn: 306
min percent.: 0.390625

−− STATS 2D −−
min ESS = 13.6410707563279
max BMK = 0.474051879958858
max MCSE = 10.3022551966334
all stationary: FALSE
burn: 0
min percent.: 0.87890625

−− STATS 1D −−
min ESS = 4.87721066397992
max BMK = 1
max MCSE = 14.3192089607895
all stationary: FALSE
burn: 1020
min percent.: 0.29296875

Occupied clusters: 23 of 64
LL: −62600 +− 166


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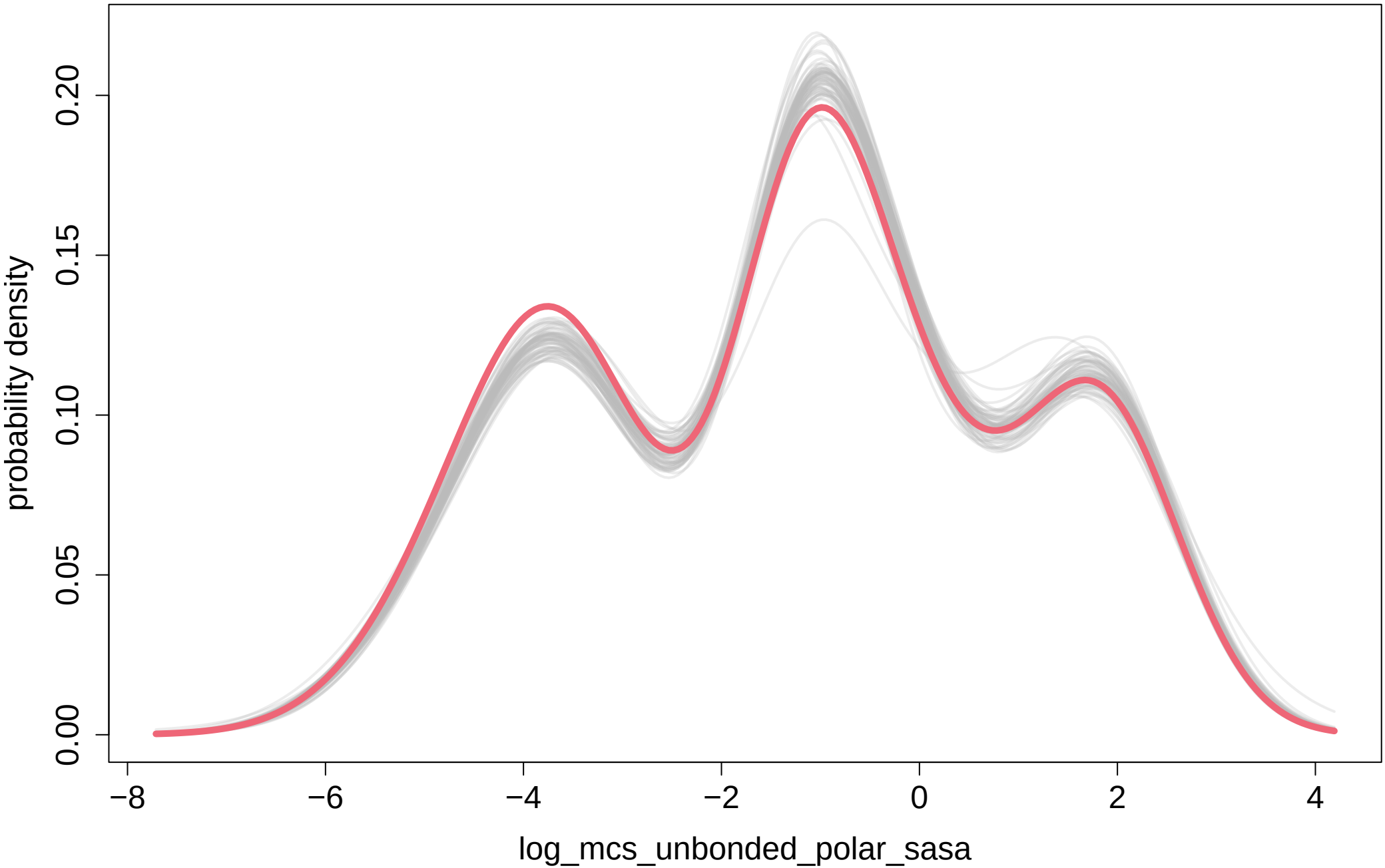
0.10
0.15
0.20
0.25
0.30
−2
0
2
4
log_RMSD


probability density
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−4
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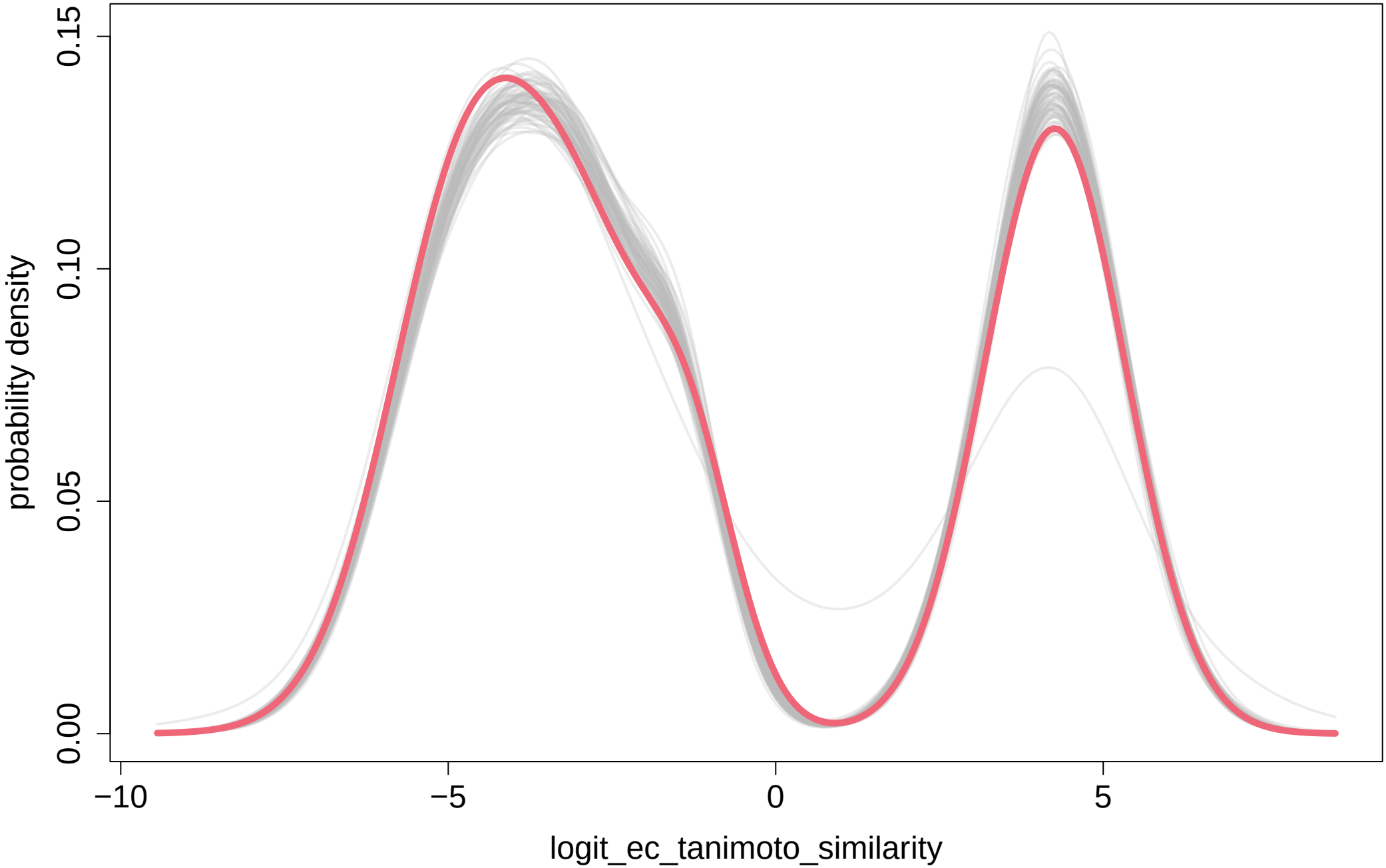
0
2
4
log_mcs_unbonded_polar_sasa


probability density
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−5
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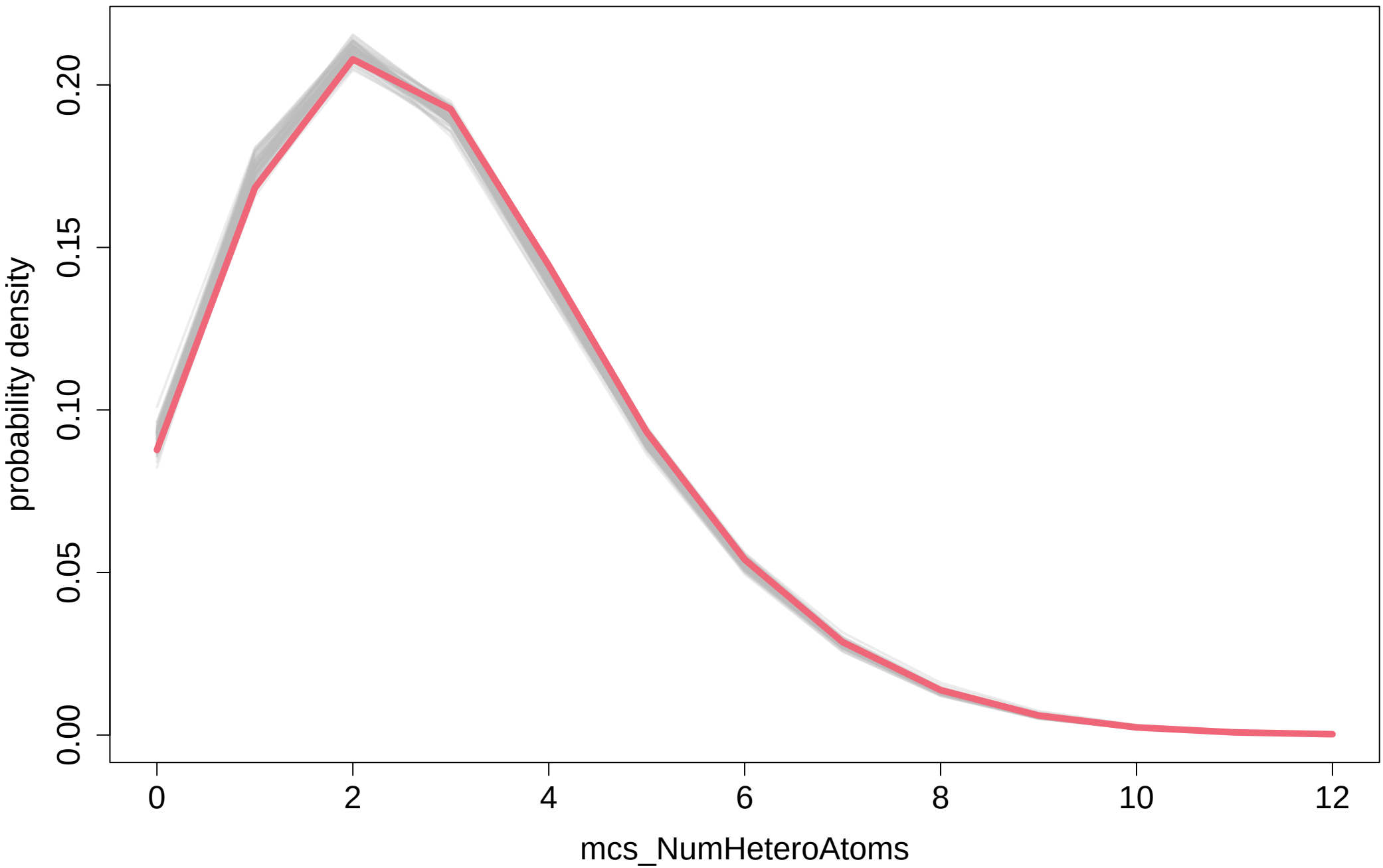
5
logit_ec_tanimoto_similarity


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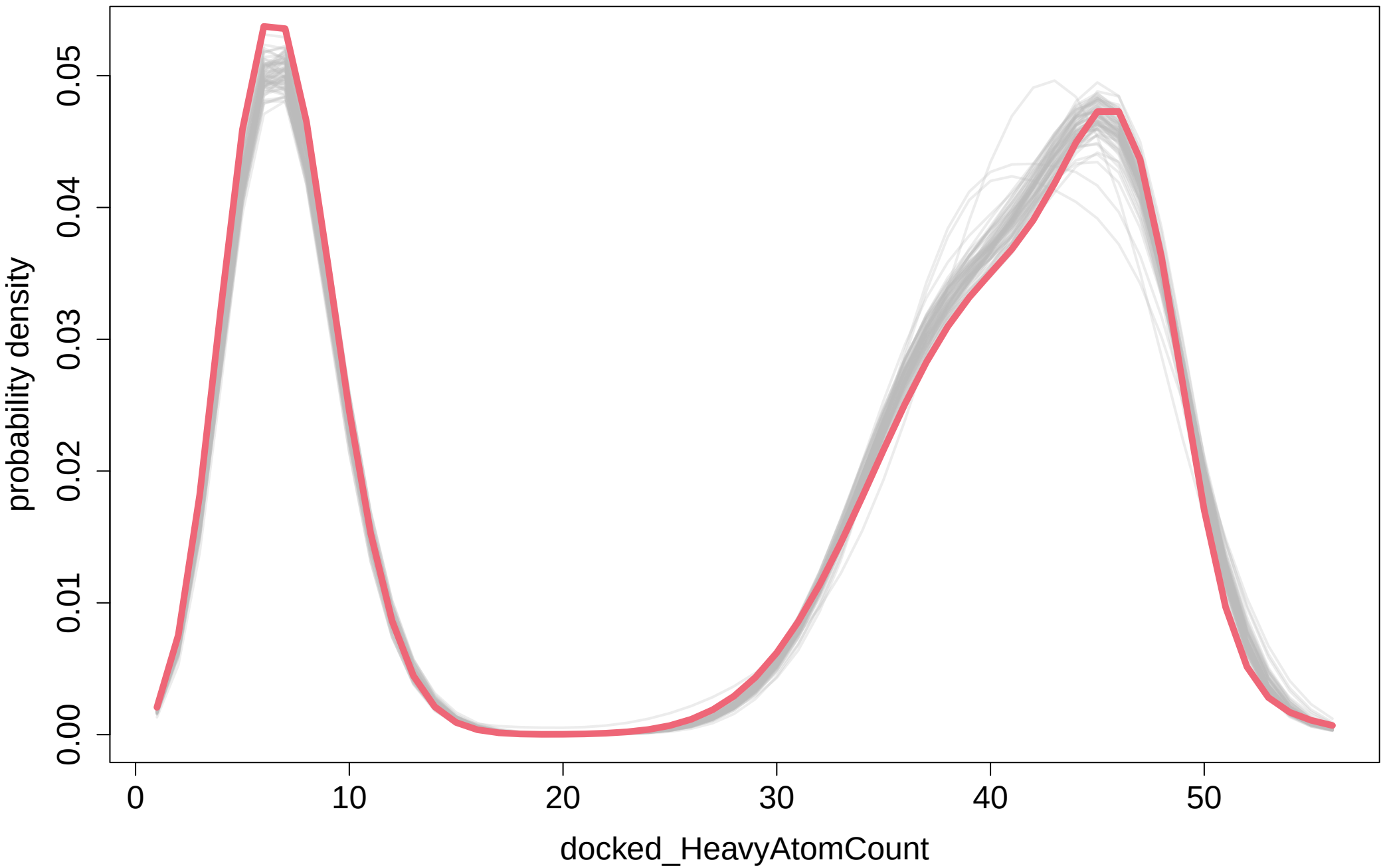
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms


probability density
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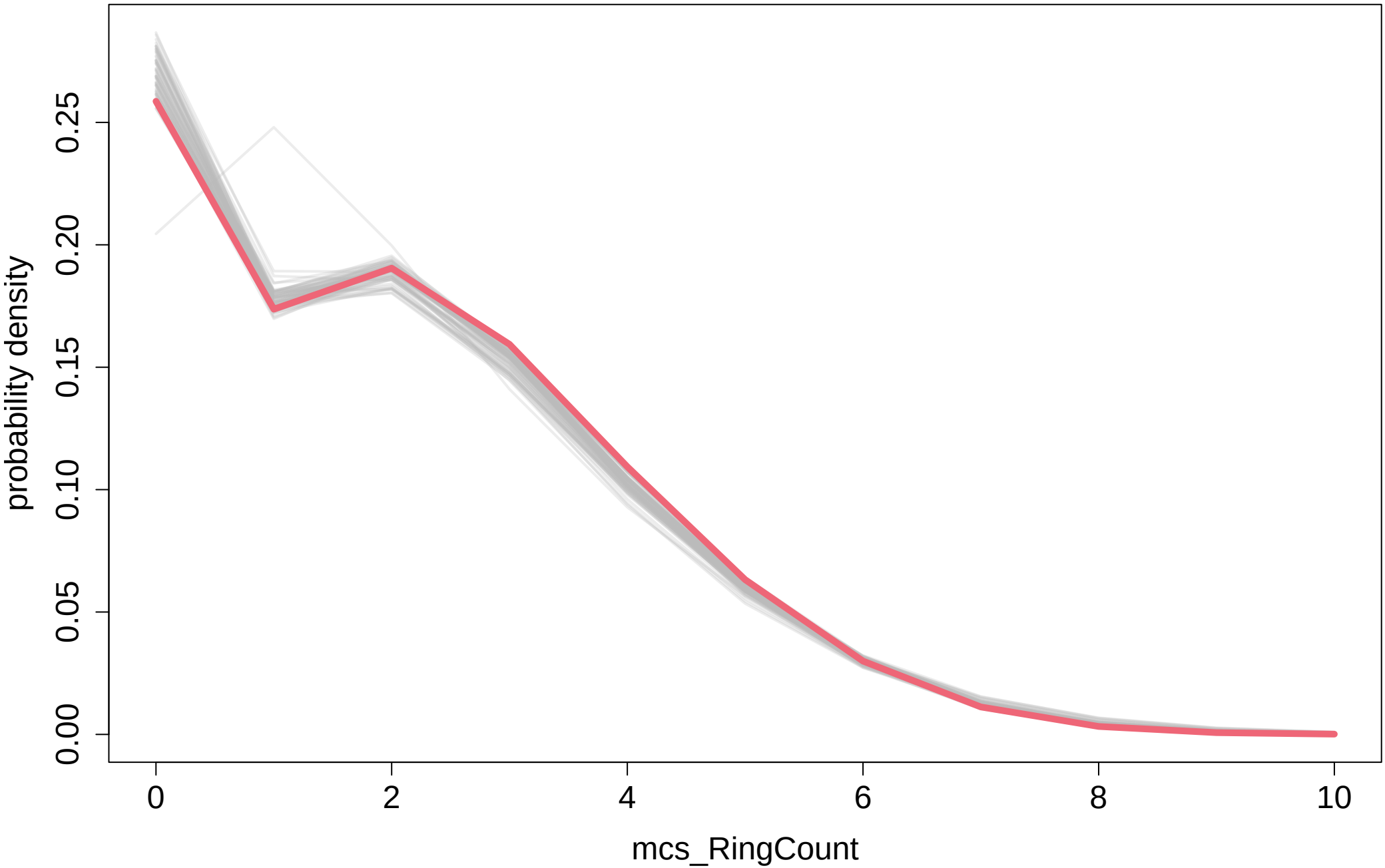
0.02
0.03
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount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0.15
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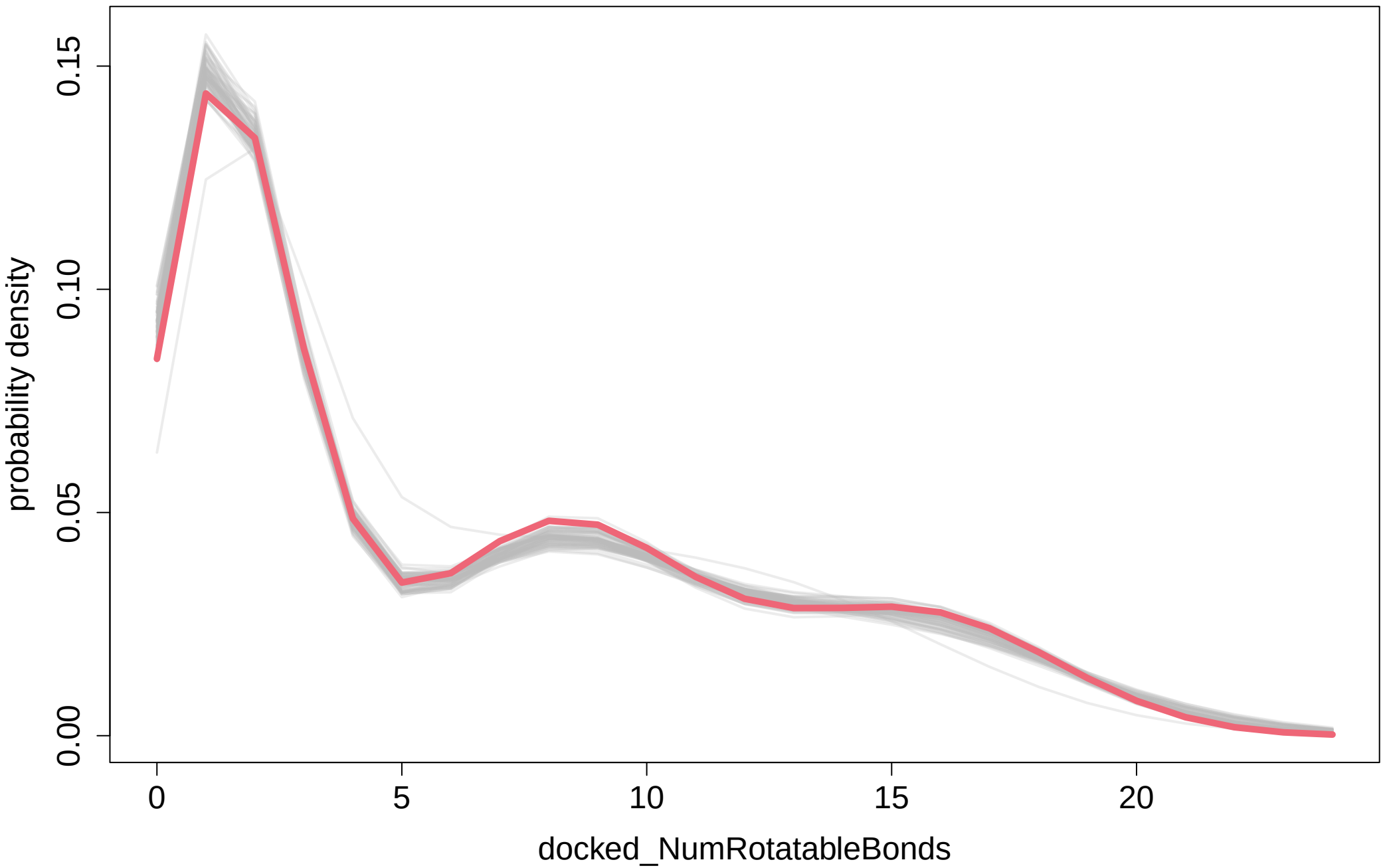
0
2
4
6
8
10
mcs_RingCount


probability density
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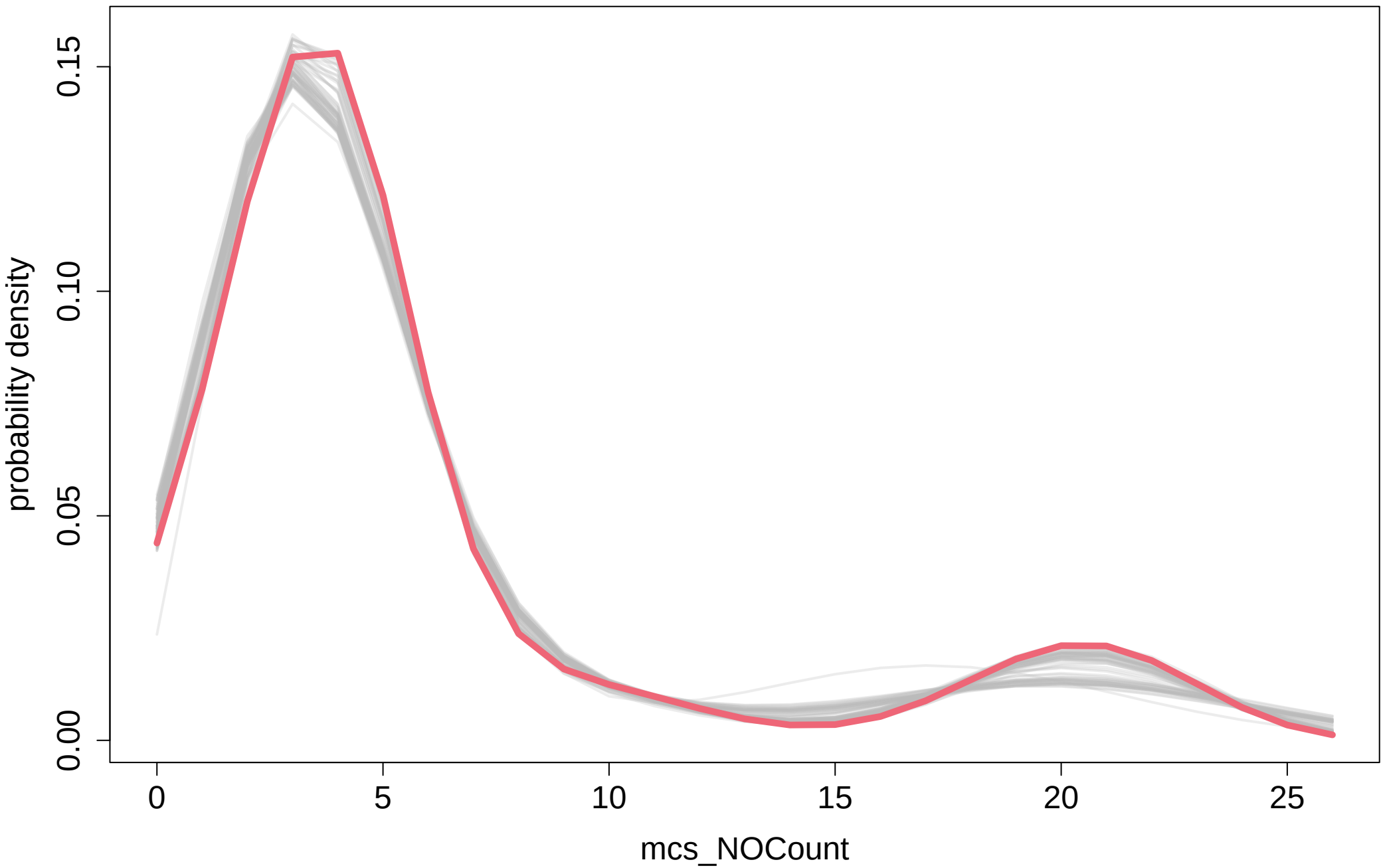
0
5
10
15
20
docked_NumRotatableBonds


probability density
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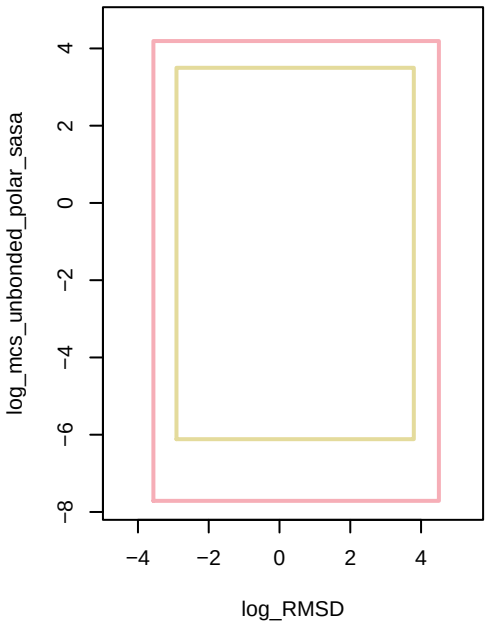
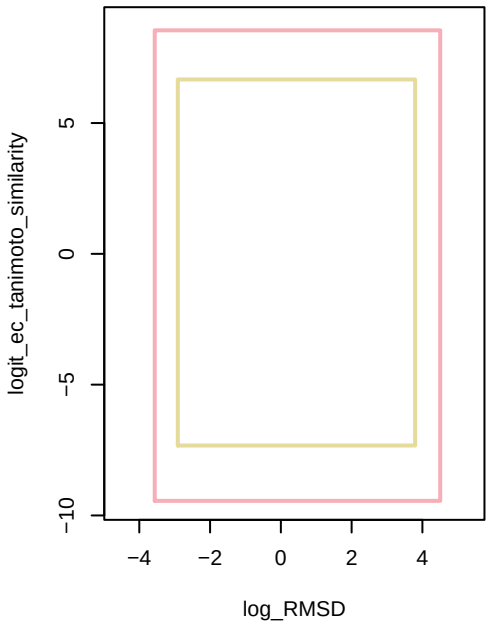
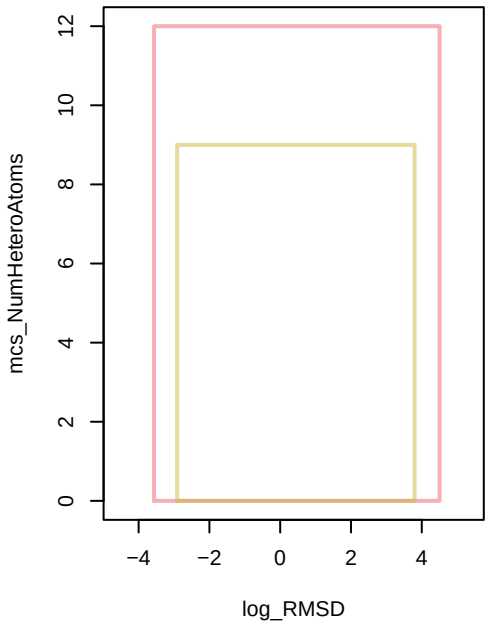
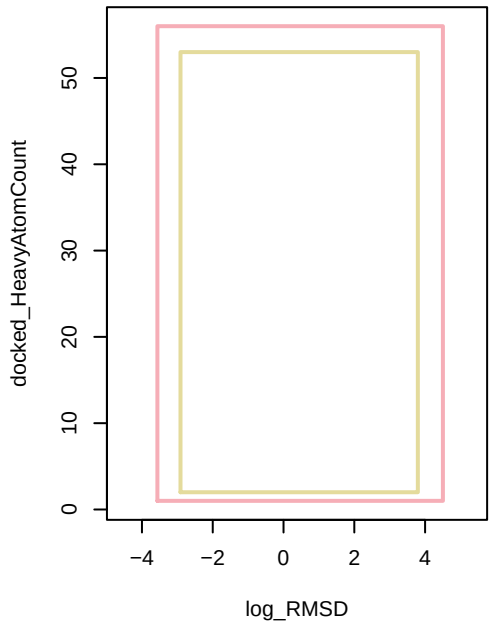
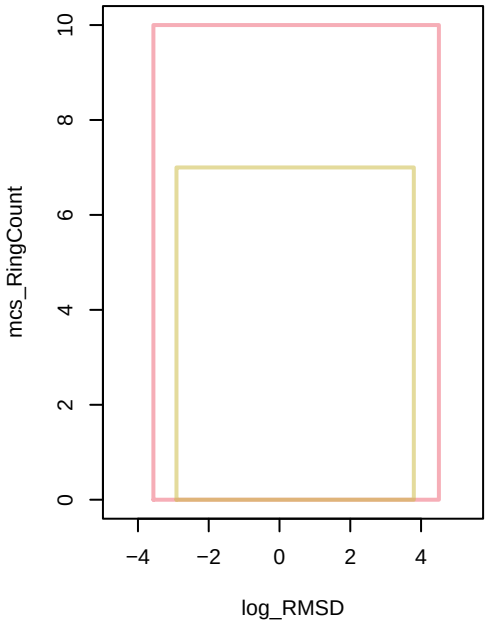
0.15
0
5
10
15
20
25
mcs_NOCount

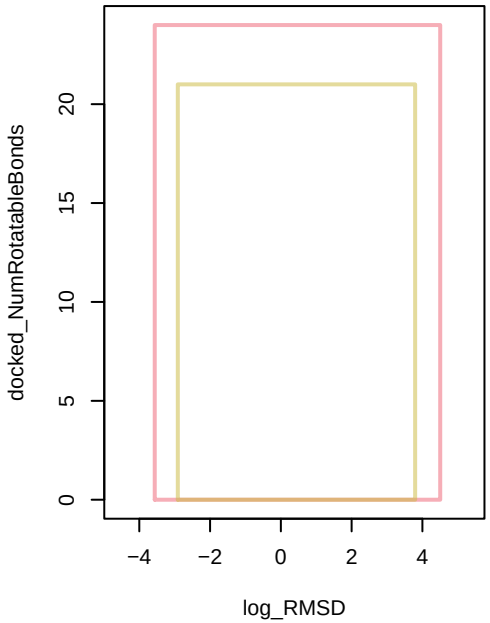

log_mcs_unbonded_polar_sasa
log_RMSD

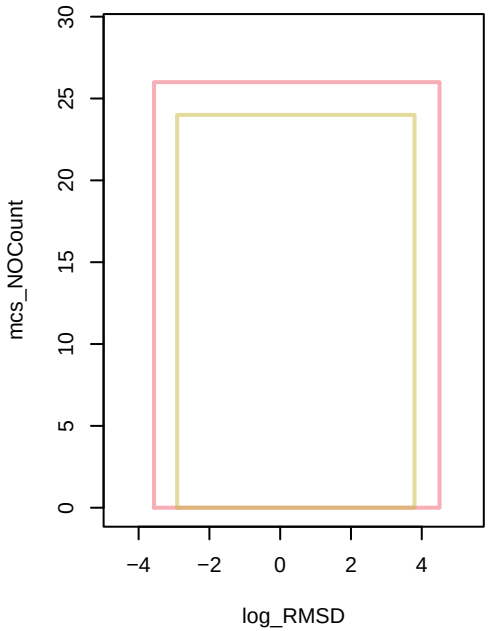

logit_ec_tanimoto_similarity
log_RMSD

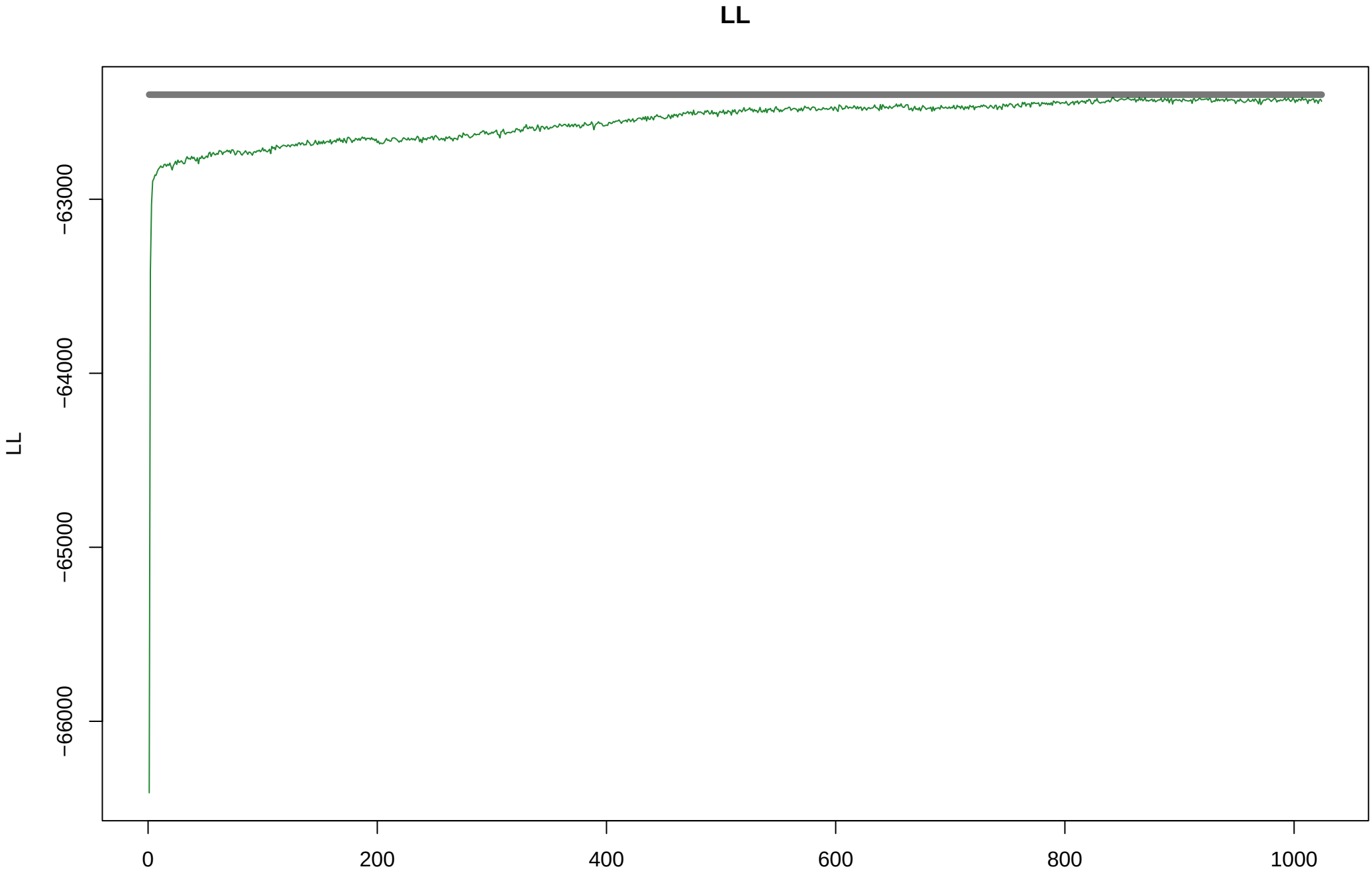

mcs_NumHeteroAtoms
log_RMSD

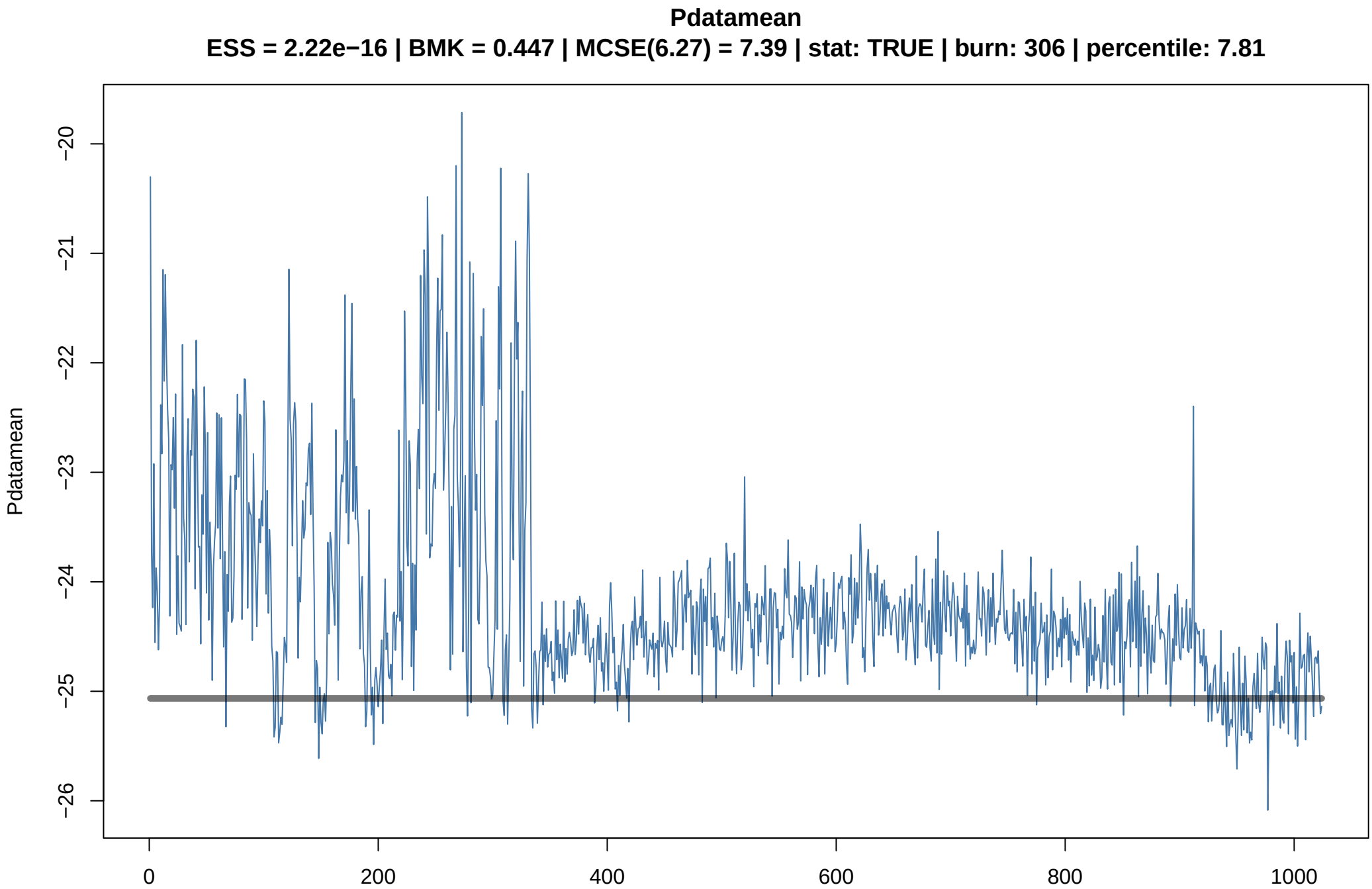

docked_HeavyAtomCount
log_RMSD

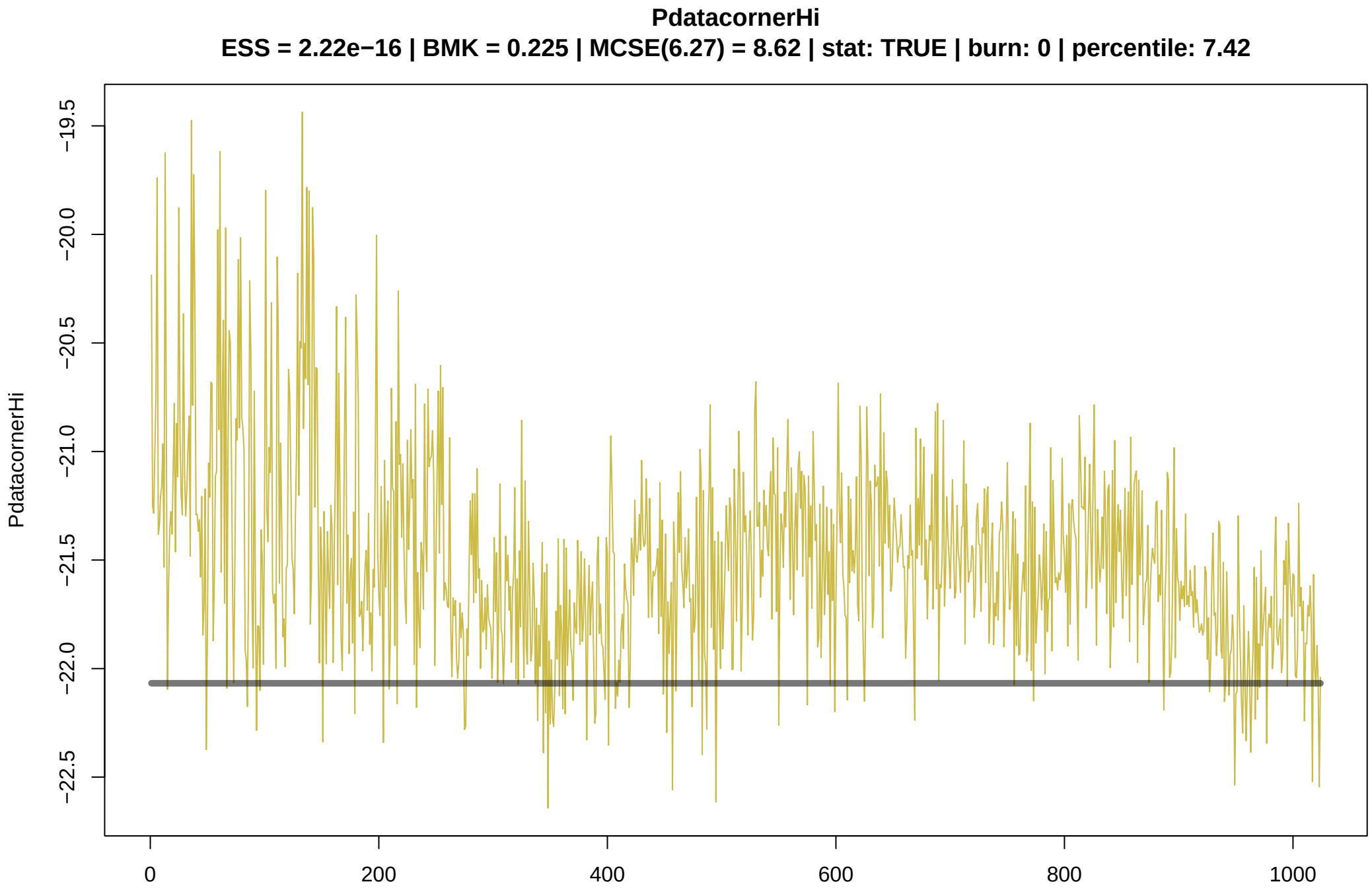

mcs_RingCount
log_RMSD

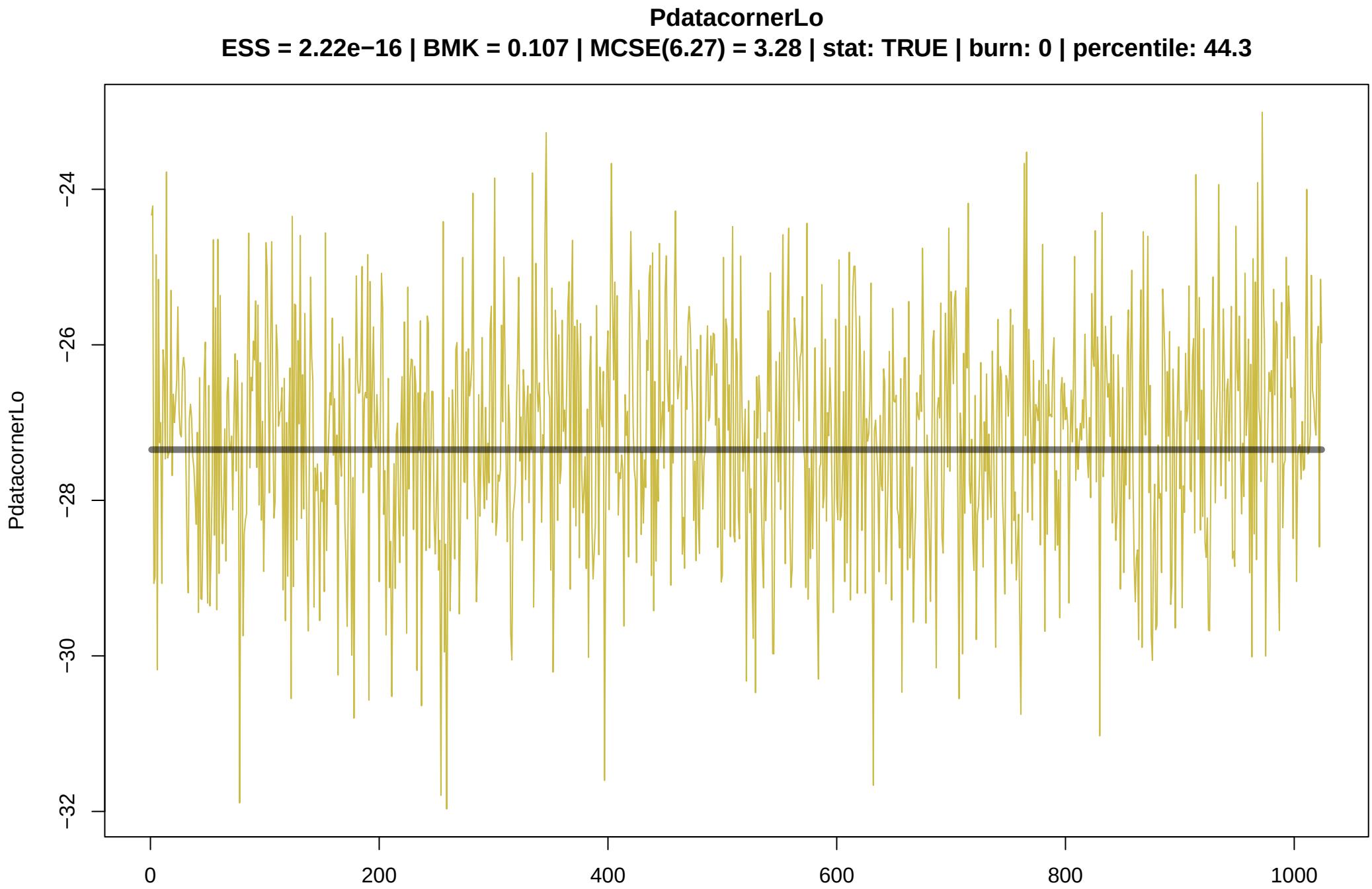

docked_NumRotatableBonds
log_RMSD

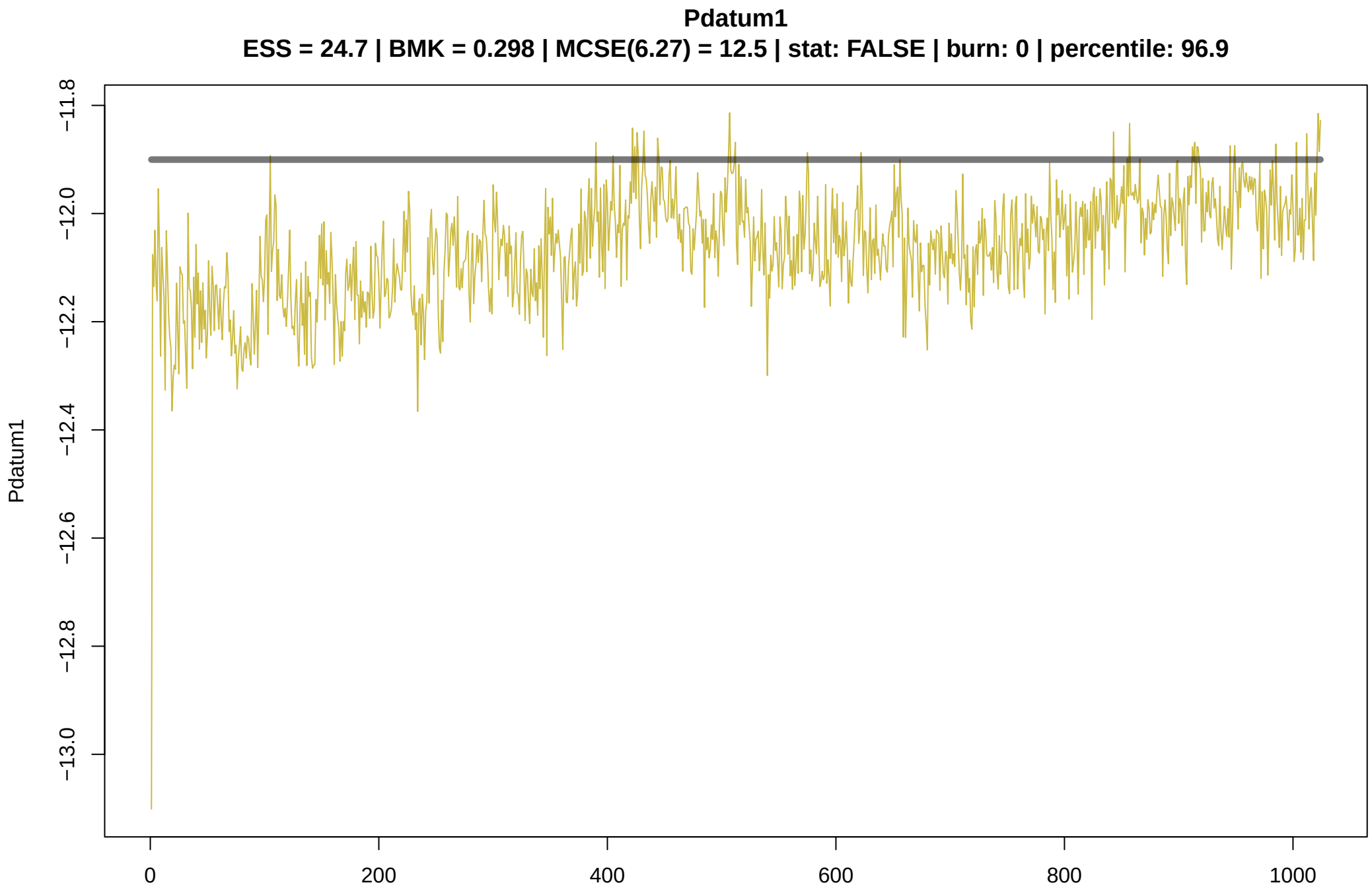

mcs_NOCount
log_RMSD

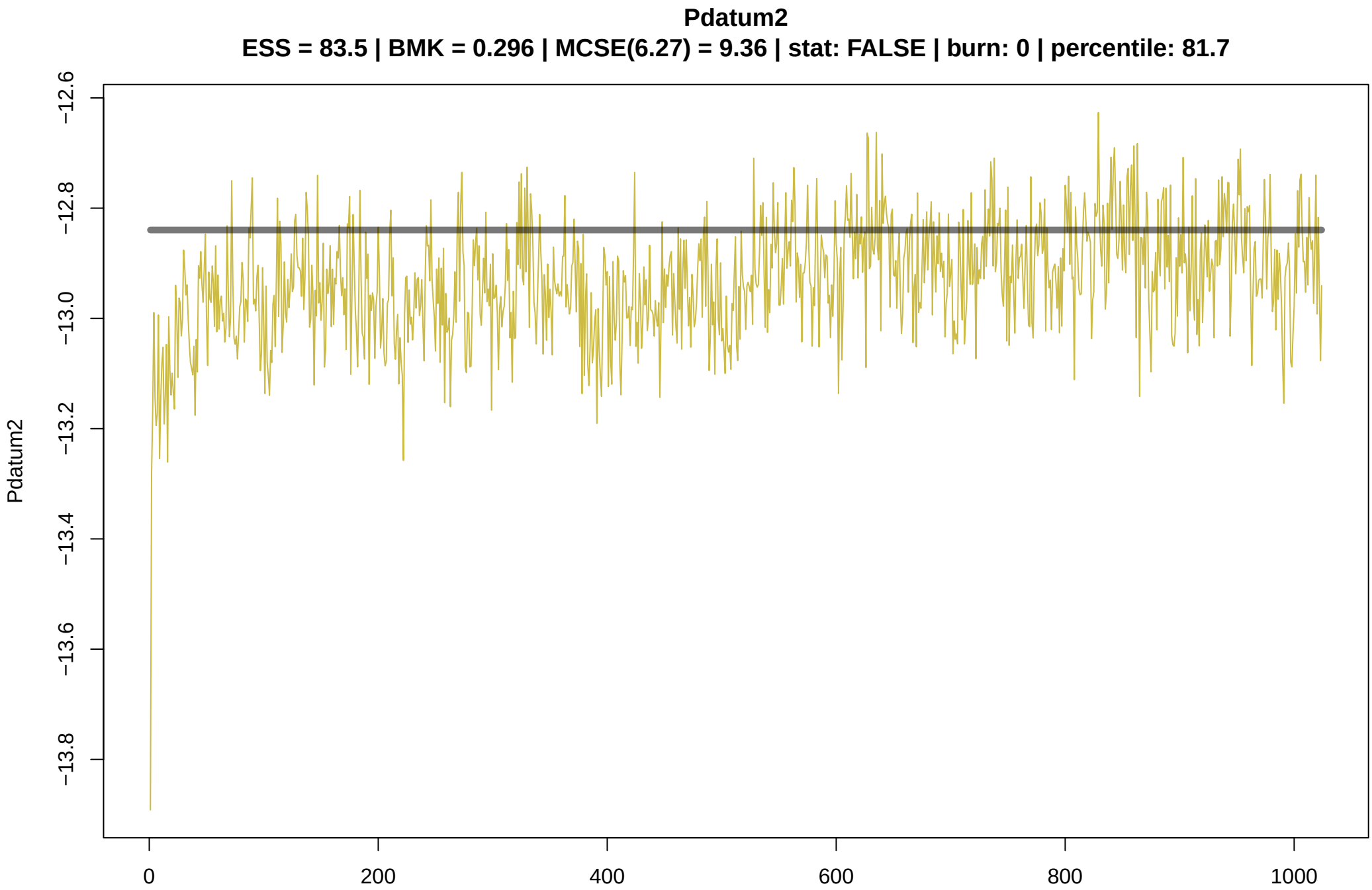

LL
LL
−63000
−64000
−65000
−66000
0
200
400
600
800
1000

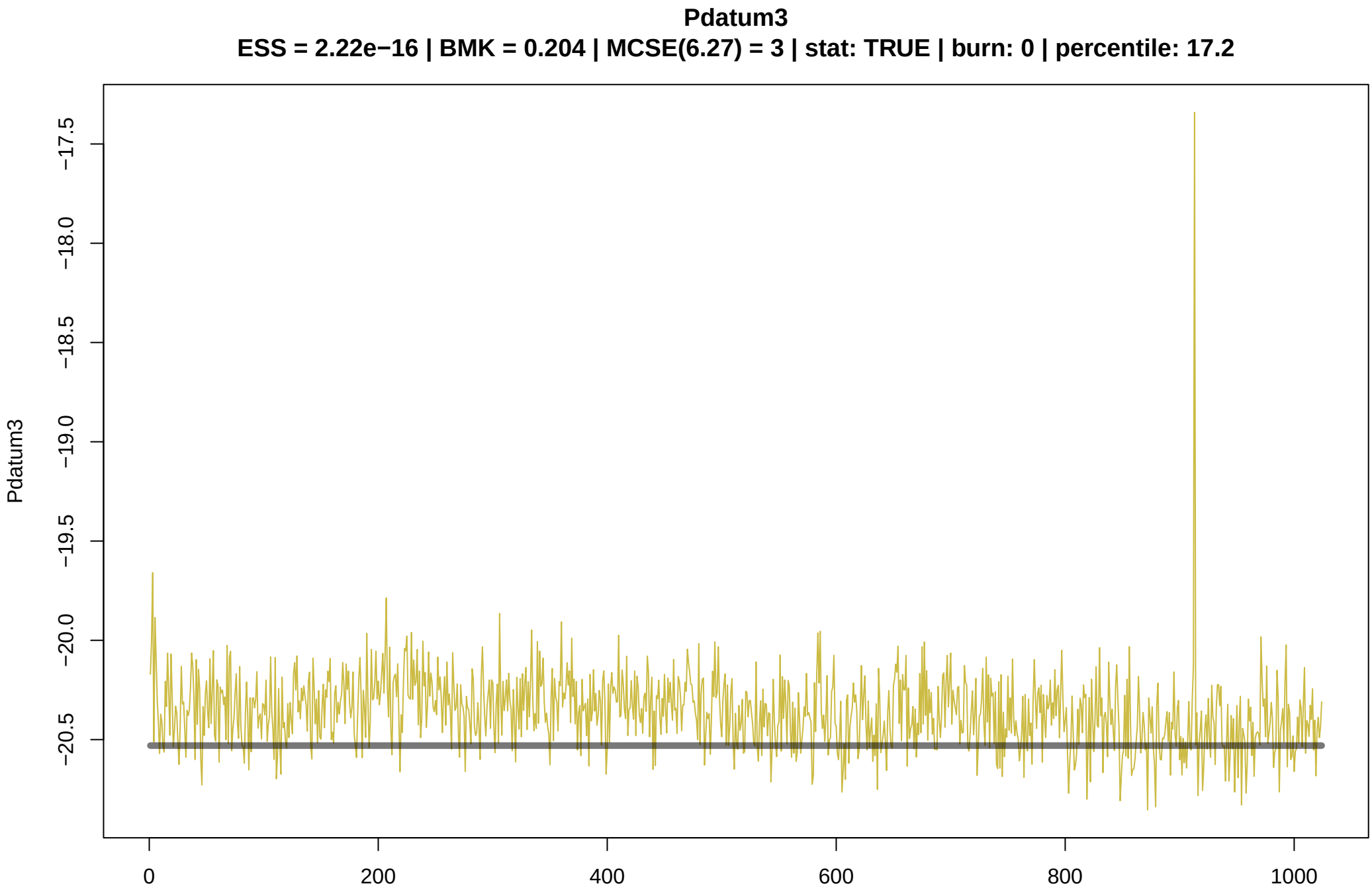

Pdatamean
ESS = 2.22e−16 | BMK = 0.447 | MCSE(6.27) = 7.39 | stat: TRUE | burn: 306 | percentile: 7.81
Pdatamean
−20
−21
−22
−23
−24
−25
−26
0
200
400
600
800
1000

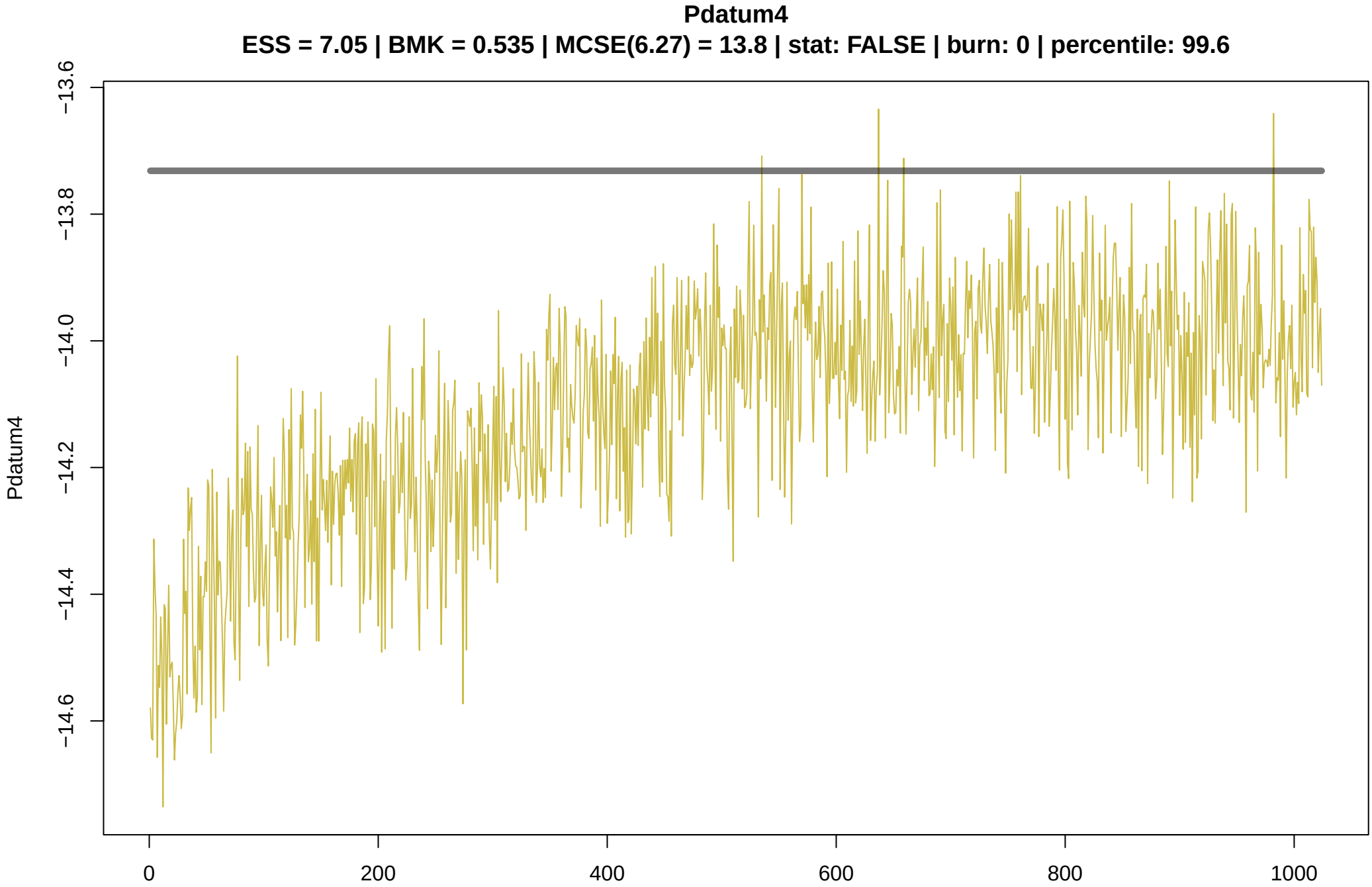

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.225 | MCSE(6.27) = 8.62 | stat: TRUE | burn: 0 | percentile: 7.42
PdatacornerHi
−19.5
−20.0
−20.5
−21.0
−21.5
−22.0
−22.5
0
200
400
600
800
1000

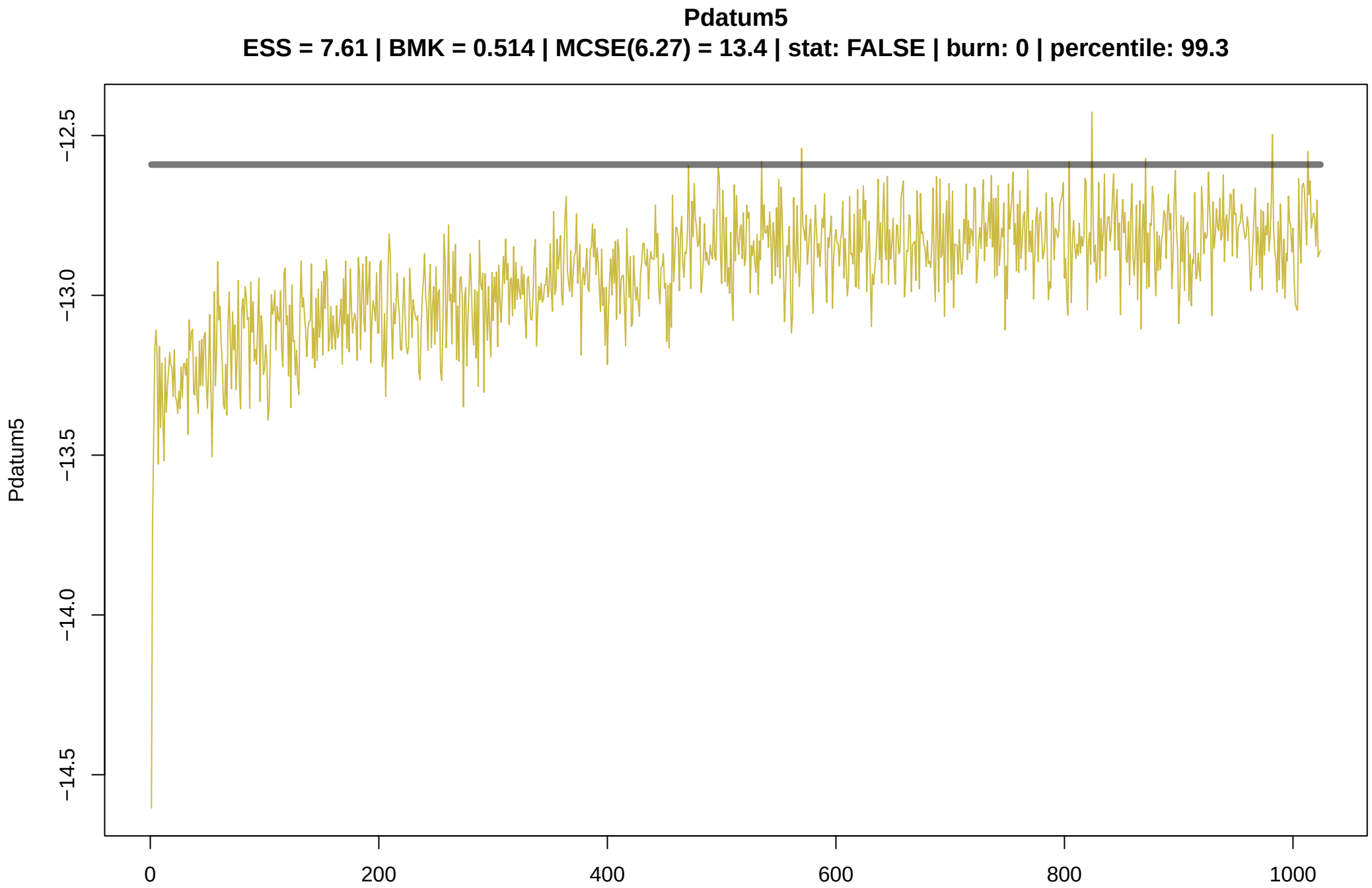

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.107 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | percentile: 44.3
PdatacornerLo
−24
−26
−28
−30
−32
0
200
400
600
800
1000

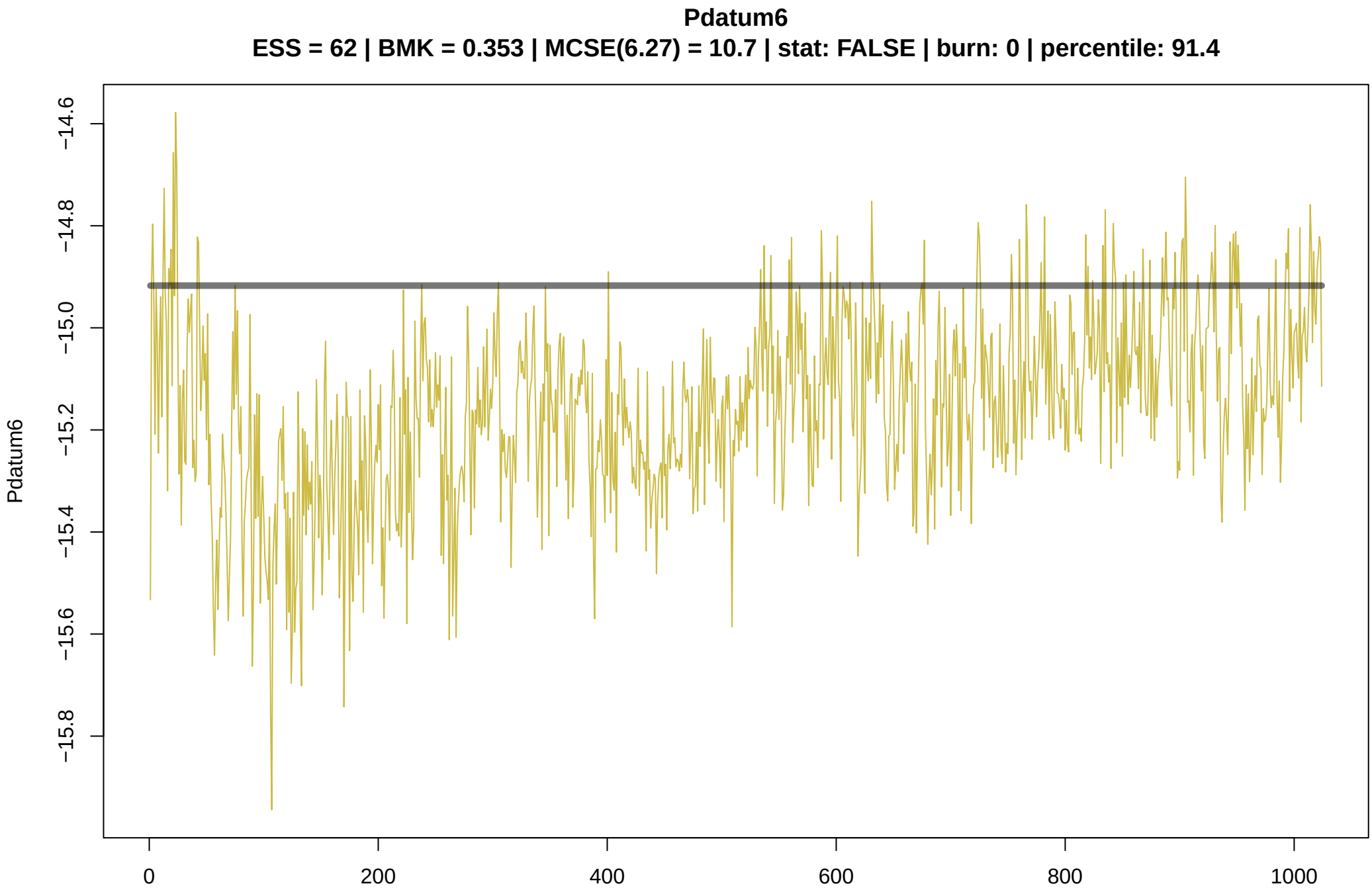

Pdatum1
ESS = 24.7 | BMK = 0.298 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 0 | percentile: 96.9
Pdatum1
−11.8
−12.0
−12.2
−12.4
−12.6
−12.8
−13.0
0
200
400
600
800
1000

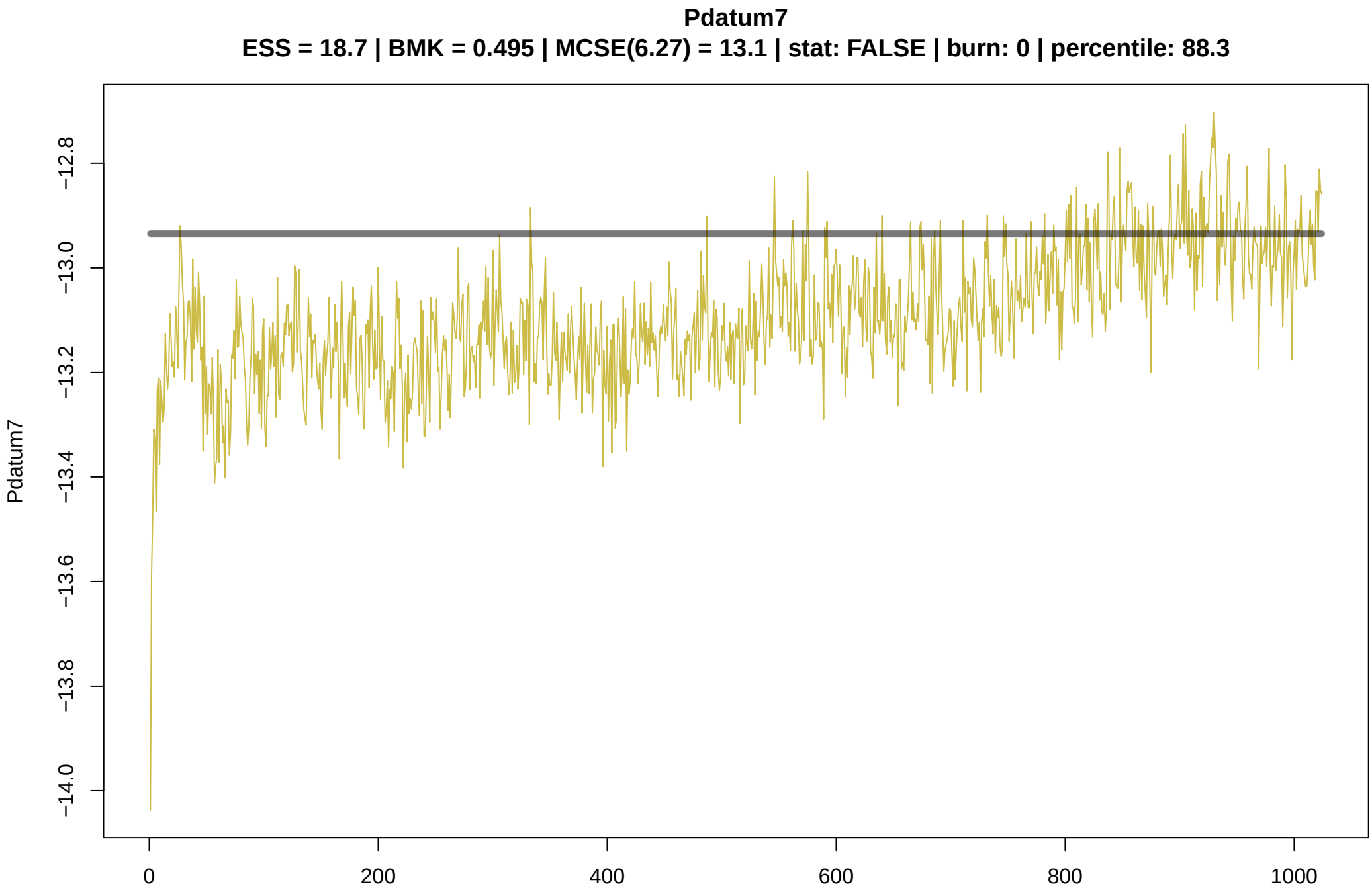

Pdatum2
ESS = 83.5 | BMK = 0.296 | MCSE(6.27) = 9.36 | stat: FALSE | burn: 0 | percentile: 81.7
Pdatum2
−12.6
−12.8
−13.0
−13.2
−13.4
−13.6
−13.8
0
200
400
600
800
1000

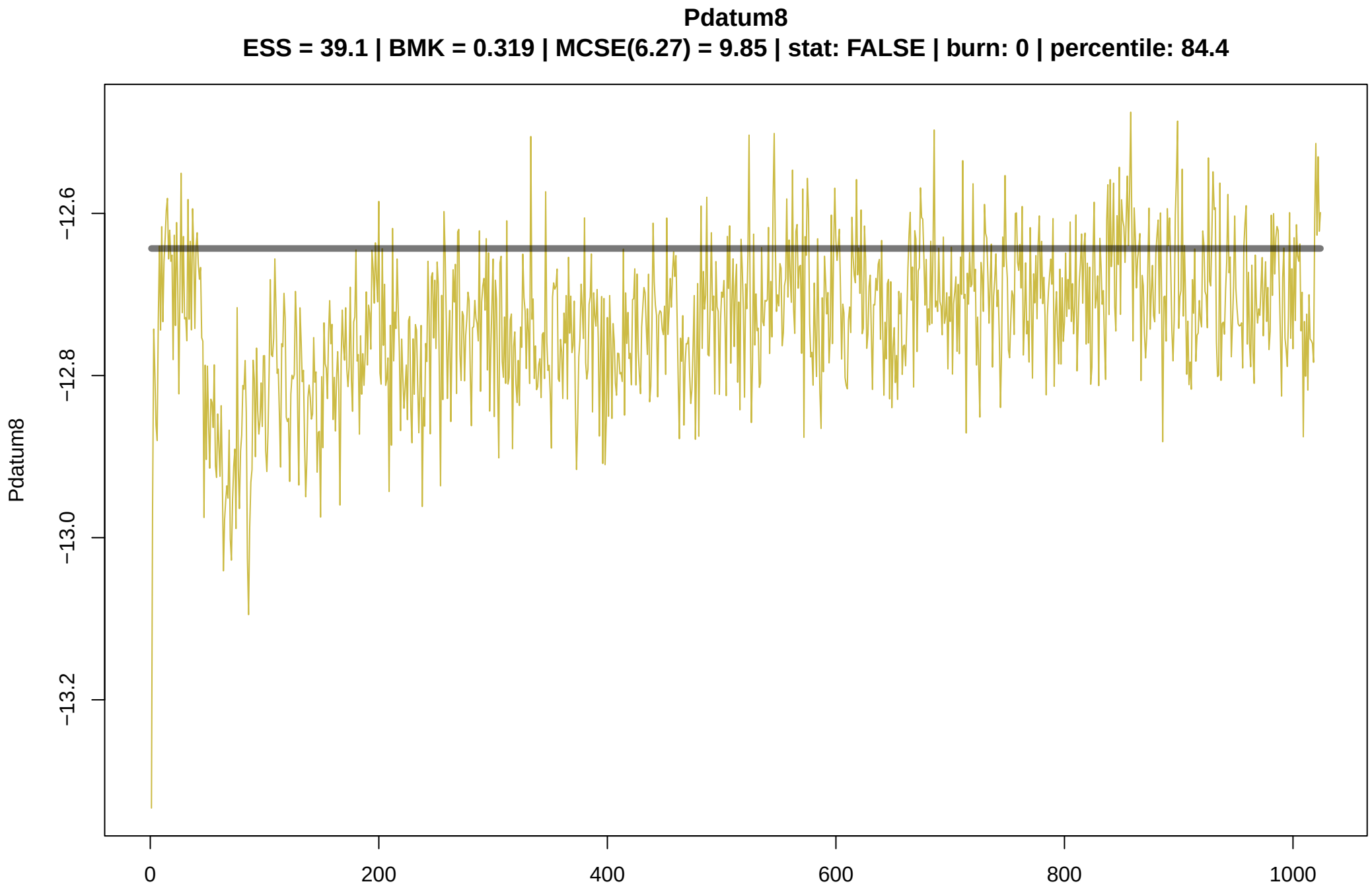

Pdatum3
ESS = 2.22e−16 | BMK = 0.204 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | percentile: 17.2
Pdatum3
−17.5
−18.0
−18.5
−19.0
−19.5
−20.0
−20.5
0
200
400
600
800
1000

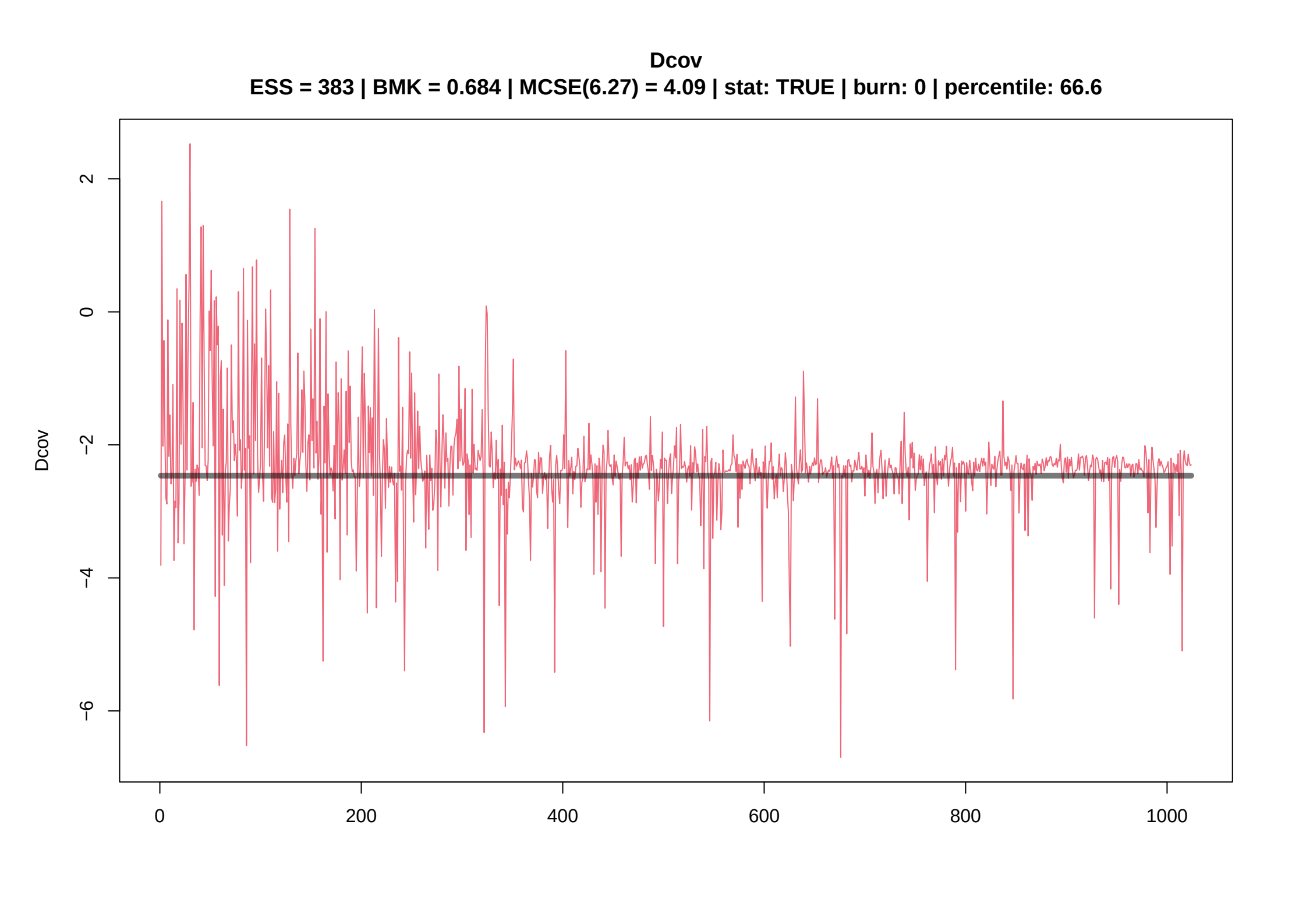

Pdatum4
ESS = 7.05 | BMK = 0.535 | MCSE(6.27) = 13.8 | stat: FALSE | burn: 0 | percentile: 99.6
Pdatum4
−13.6
−13.8
−14.0
−14.2
−14.4
−14.6
0
200
400
600
800
1000

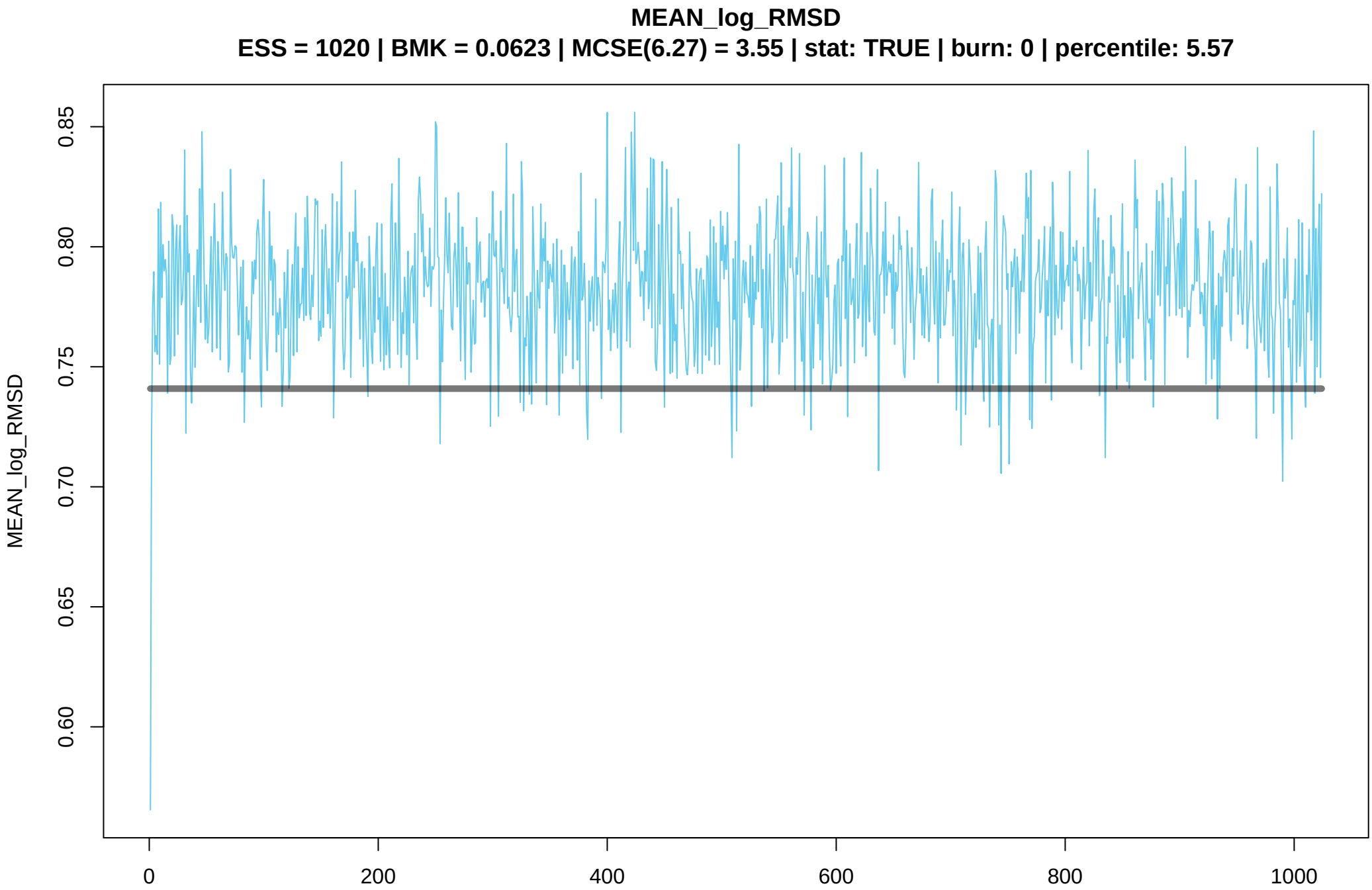

Pdatum5
ESS = 7.61 | BMK = 0.514 | MCSE(6.27) = 13.4 | stat: FALSE | burn: 0 | percentile: 99.3
Pdatum5
−12.5
−13.0
−13.5
−14.0
−14.5
0
200
400
600
800
1000

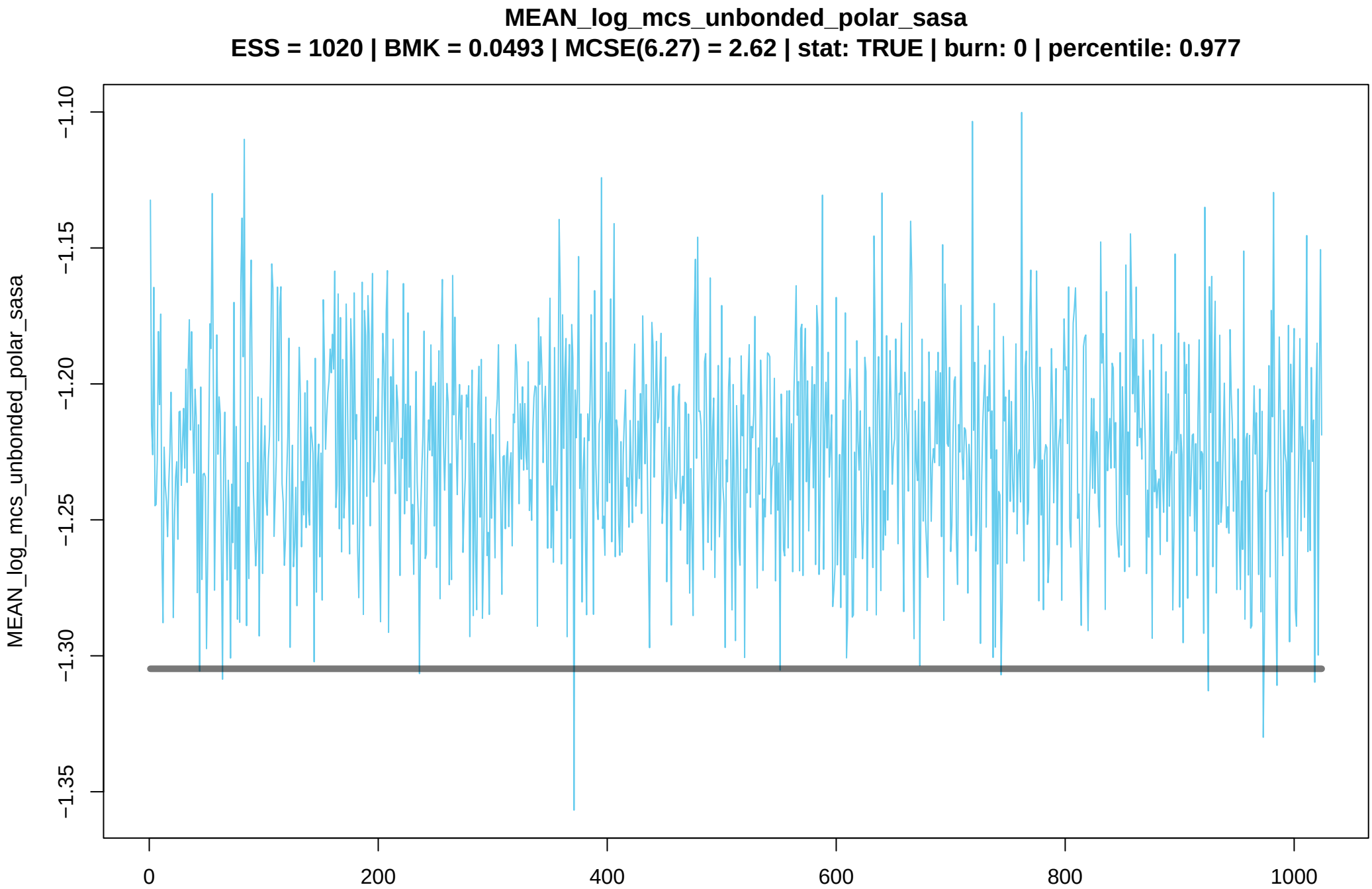

Pdatum6
ESS = 62 | BMK = 0.353 | MCSE(6.27) = 10.7 | stat: FALSE | burn: 0 | percentile: 91.4
Pdatum6
−14.6
−14.8
−15.0
−15.2
−15.4
−15.6
−15.8
0
200
400
600
800
1000

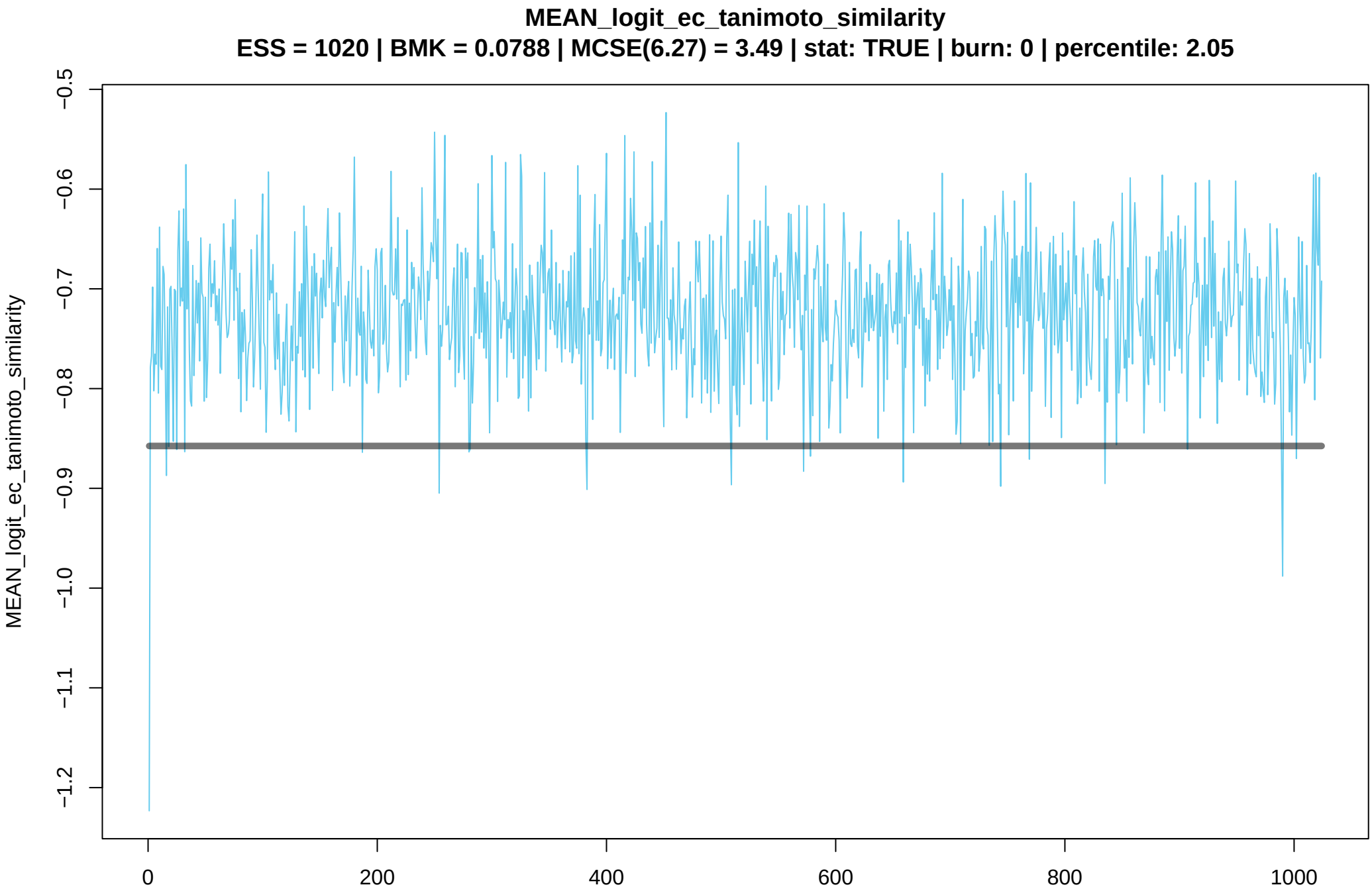

Pdatum7
ESS = 18.7 | BMK = 0.495 | MCSE(6.27) = 13.1 | stat: FALSE | burn: 0 | percentile: 88.3
Pdatum7
−12.8
−13.0
−13.2
−13.4
−13.6
−13.8
−14.0
0
200
400
600
800
1000

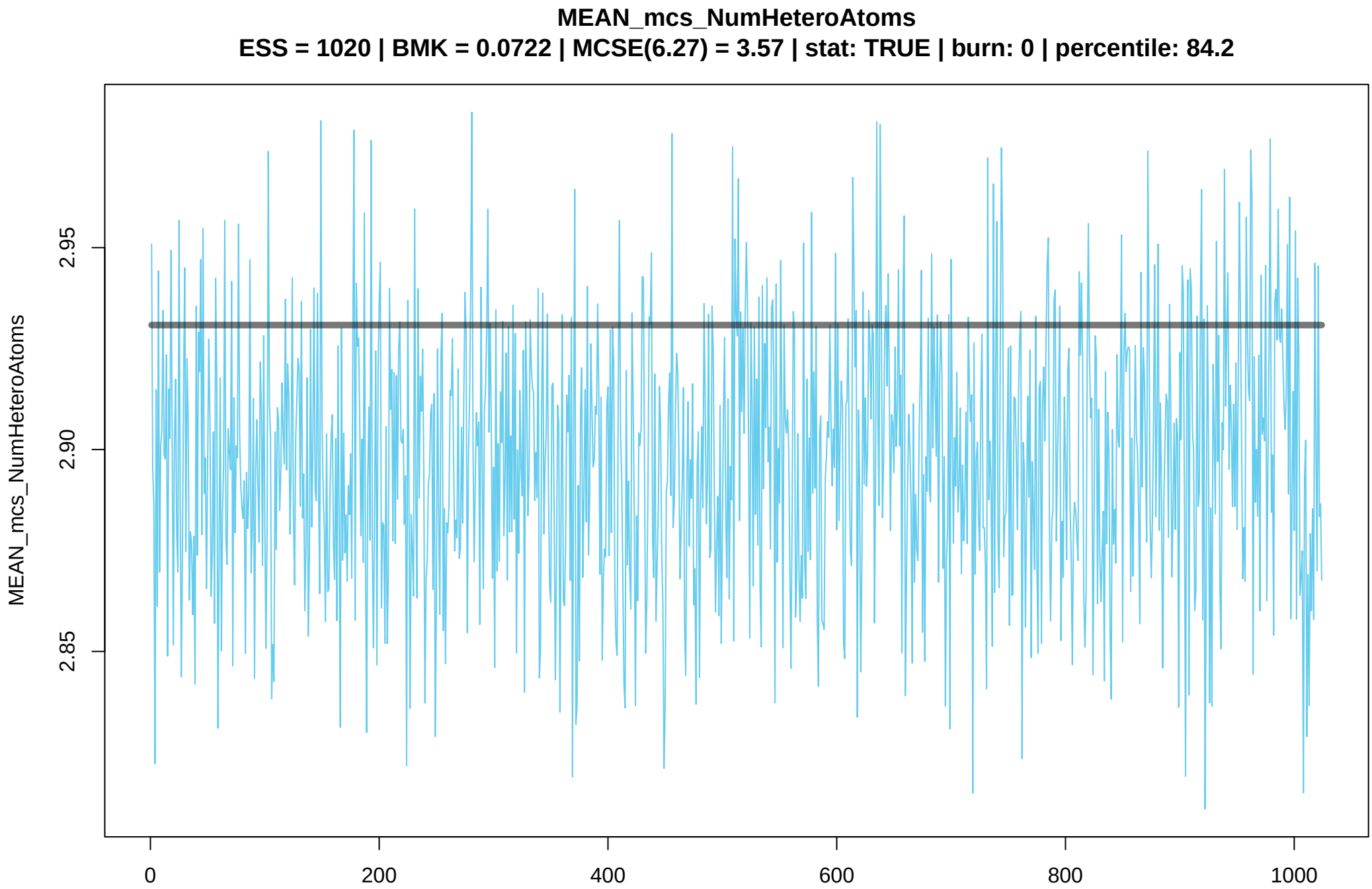

Pdatum8
ESS = 39.1 | BMK = 0.319 | MCSE(6.27) = 9.85 | stat: FALSE | burn: 0 | percentile: 84.4
Pdatum8
−12.6
−12.8
−13.0
−13.2
0
200
400
600
800
1000

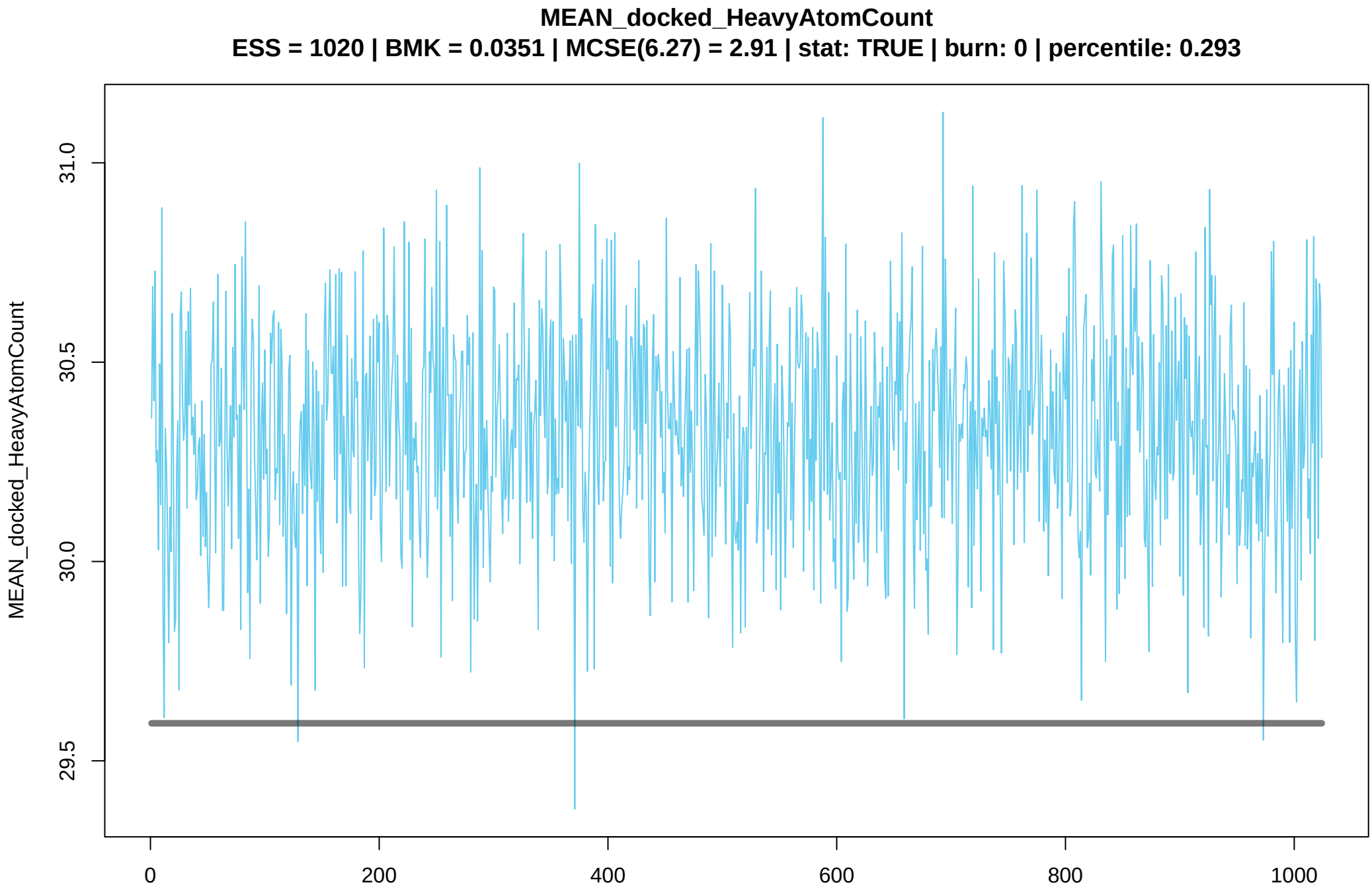

Dcov
ESS = 383 | BMK = 0.684 | MCSE(6.27) = 4.09 | stat: TRUE | burn: 0 | percentile: 66.6
Dcov
2
0
−2
−4
−6
0
200
400
600
800
1000

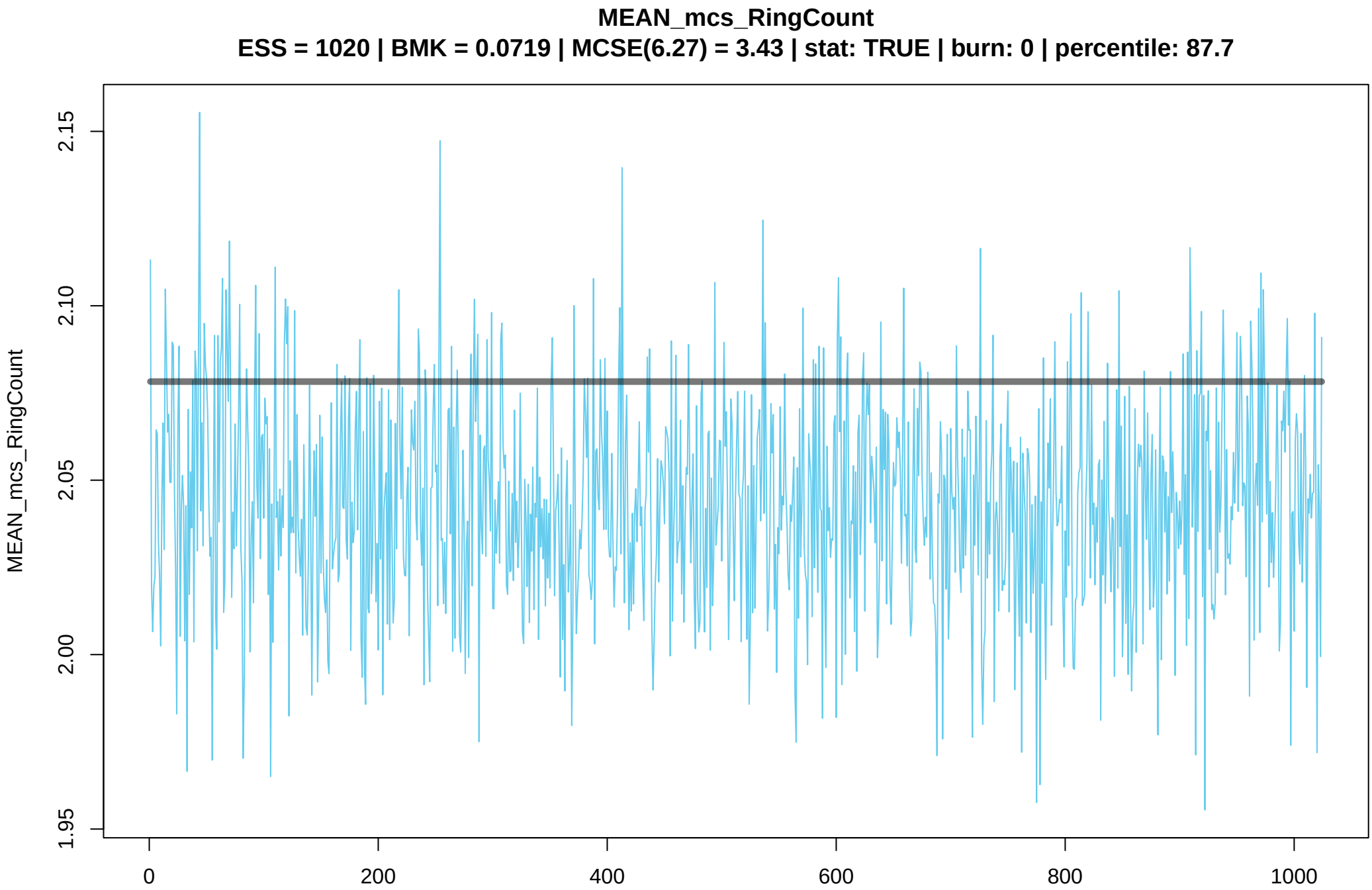

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0623 | MCSE(6.27) = 3.55 | stat: TRUE | burn: 0 | percentile: 5.57
MEAN_log_RMSD
0.60
0.65
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

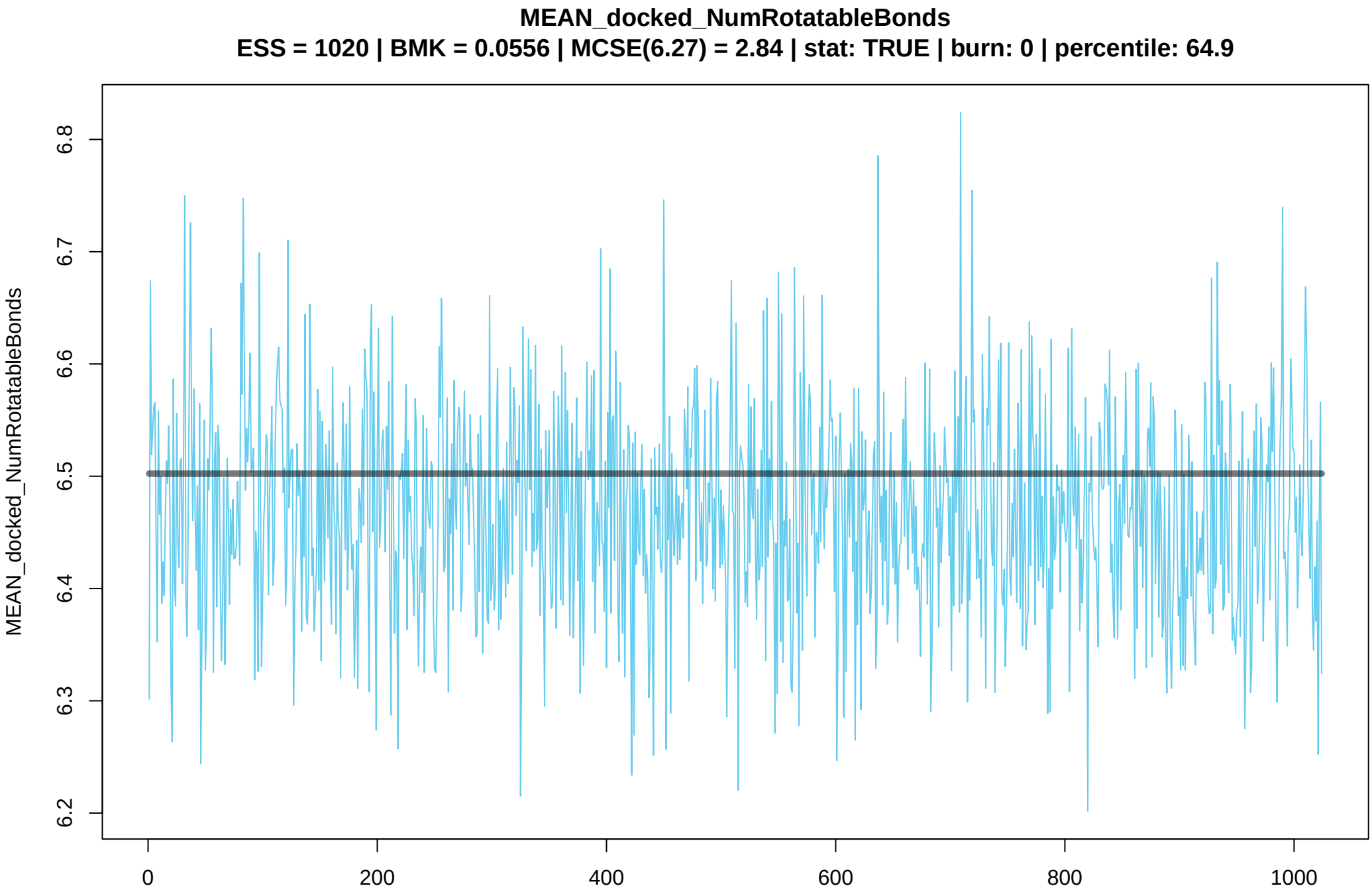

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0493 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | percentile: 0.977
MEAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

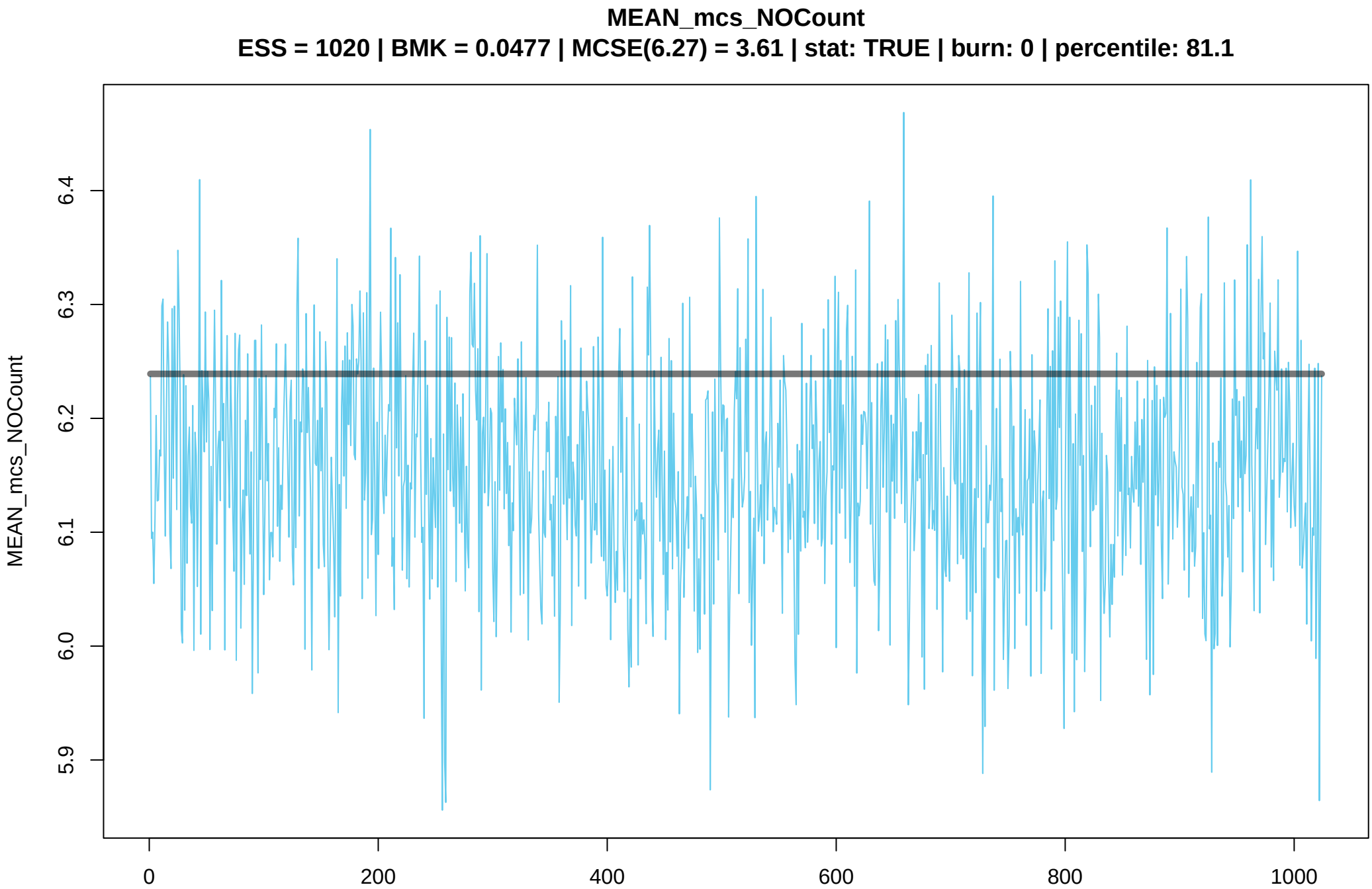

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0788 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0 | percentile: 2.05
MEAN_logit_ec_tanimoto_similarity
−0.5
−0.6
−0.7
−0.8
−0.9
−1.0
−1.1
−1.2
0
200
400
600
800
1000

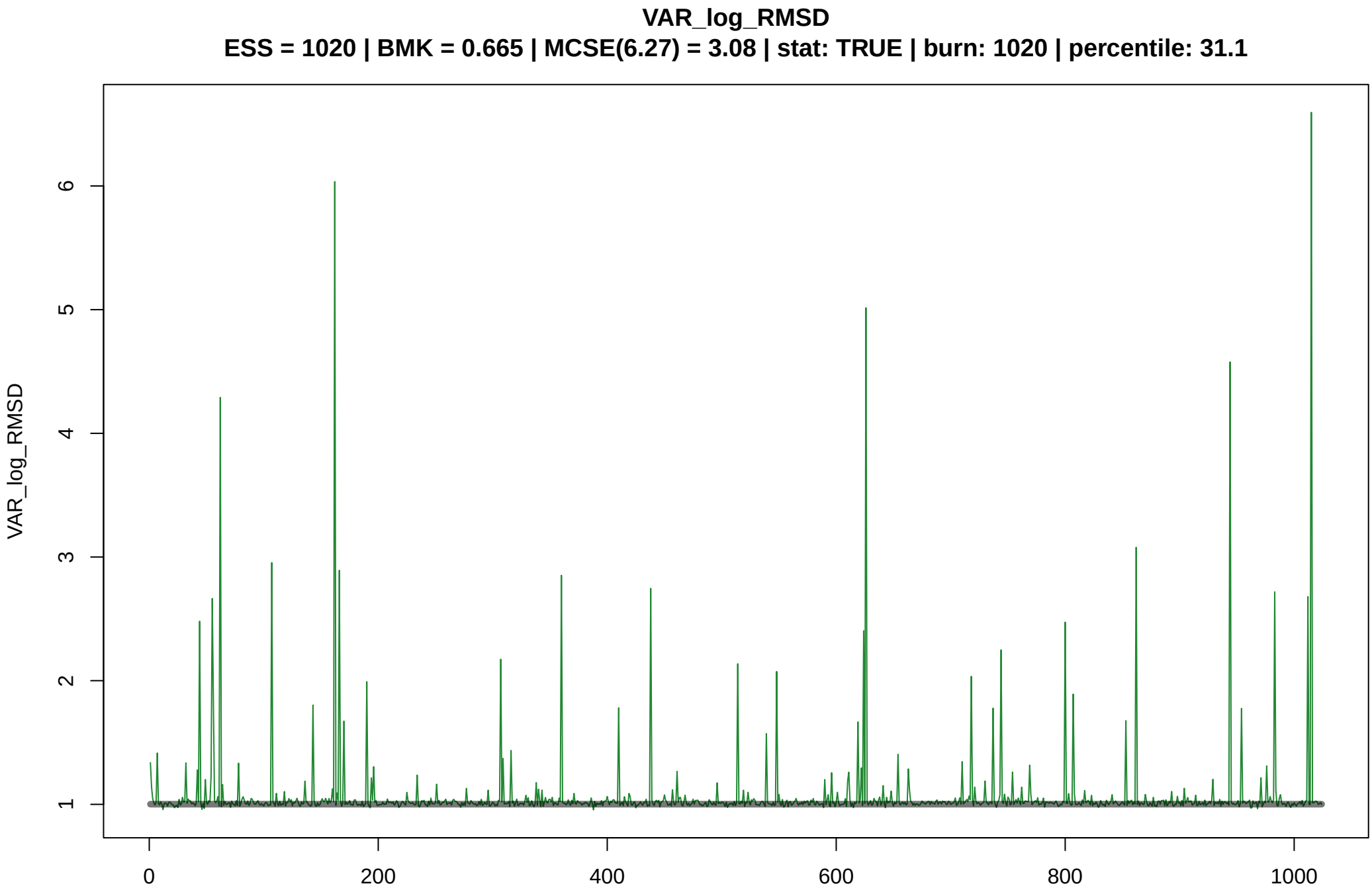

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0722 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | percentile: 84.2
MEAN_mcs_NumHeteroAtoms
2.85
2.90
2.95
0
200
400
600
800
1000

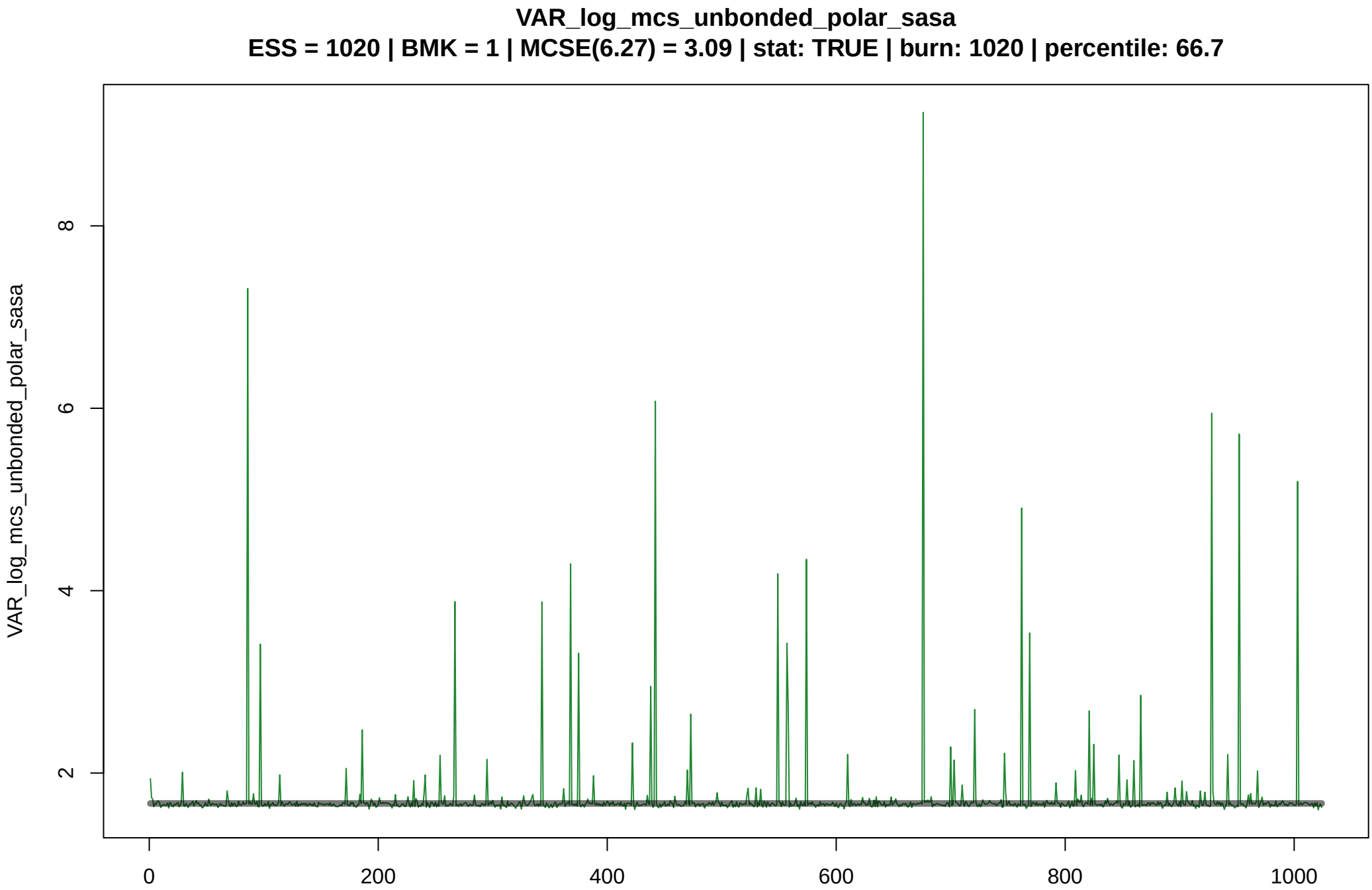

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0351 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | percentile: 0.293
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
31.0
0
200
400
600
800
1000

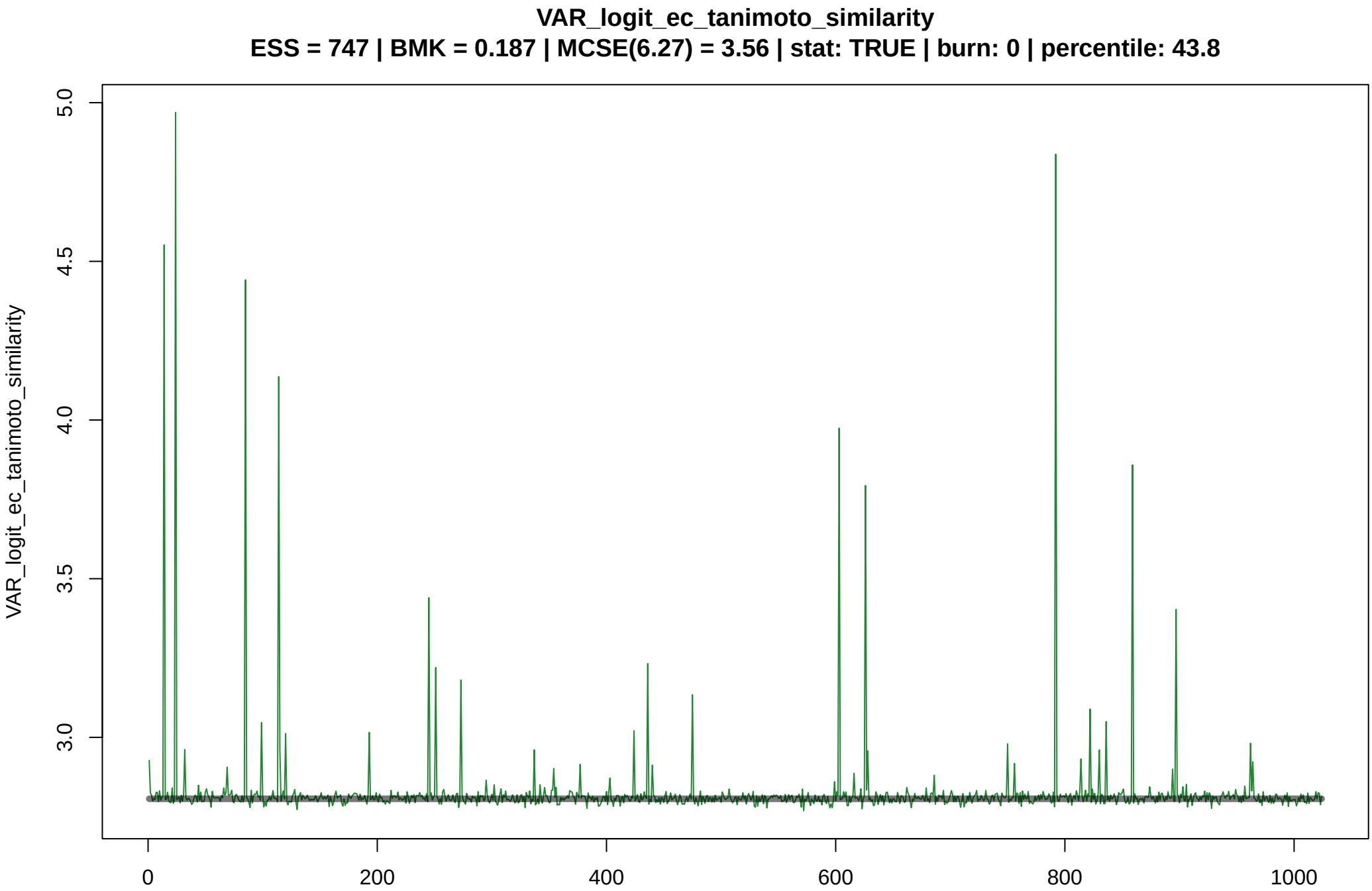

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0719 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0 | percentile: 87.7
MEAN_mcs_RingCount
2.15
2.10
2.05
2.00
1.95
0
200
400
600
800
1000

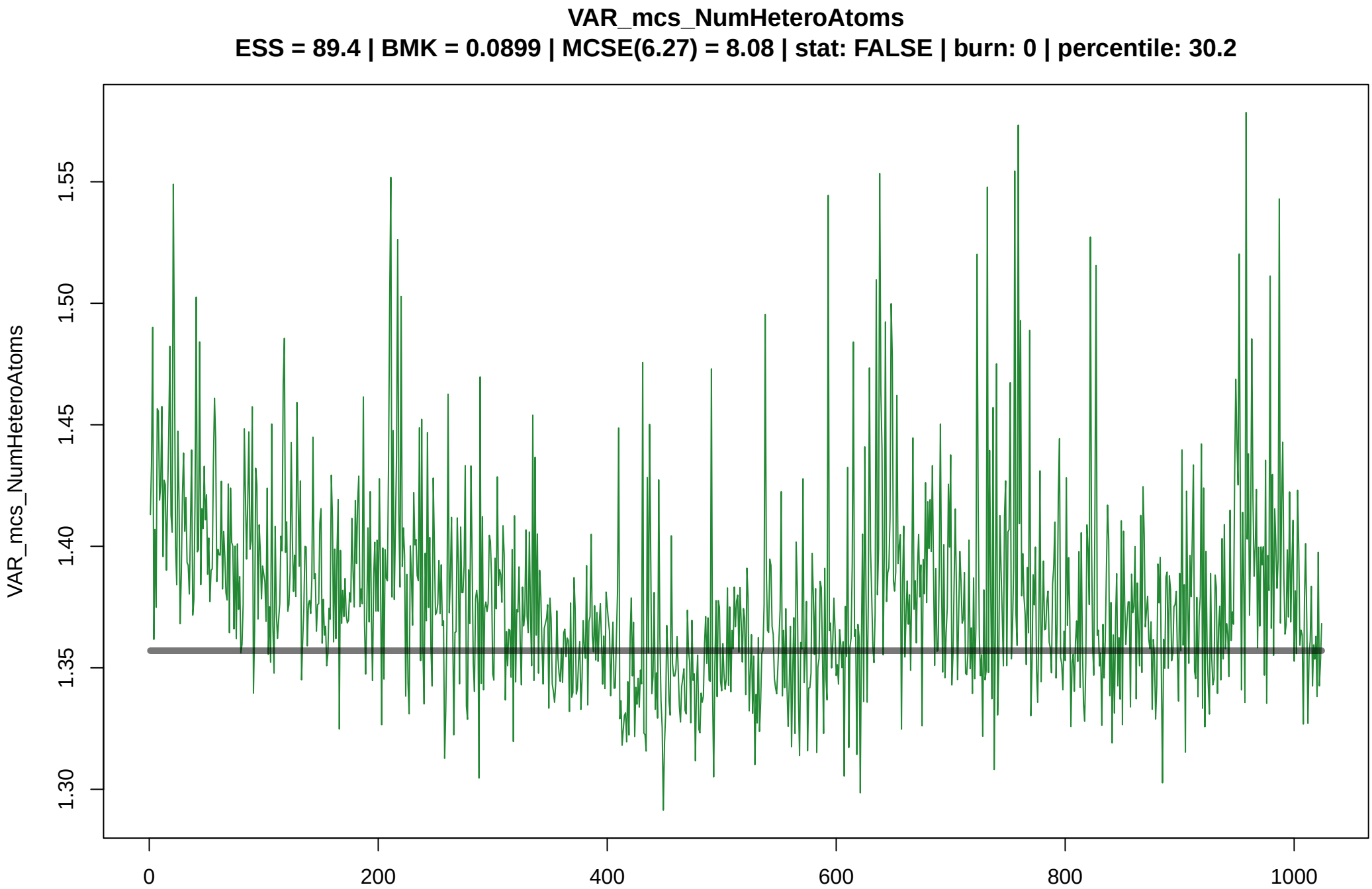

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0556 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0 | percentile: 64.9
MEAN_docked_NumRotatableBonds
6.2
6.3
6.4
6.5
6.6
6.7
6.8
0
200
400
600
800
1000

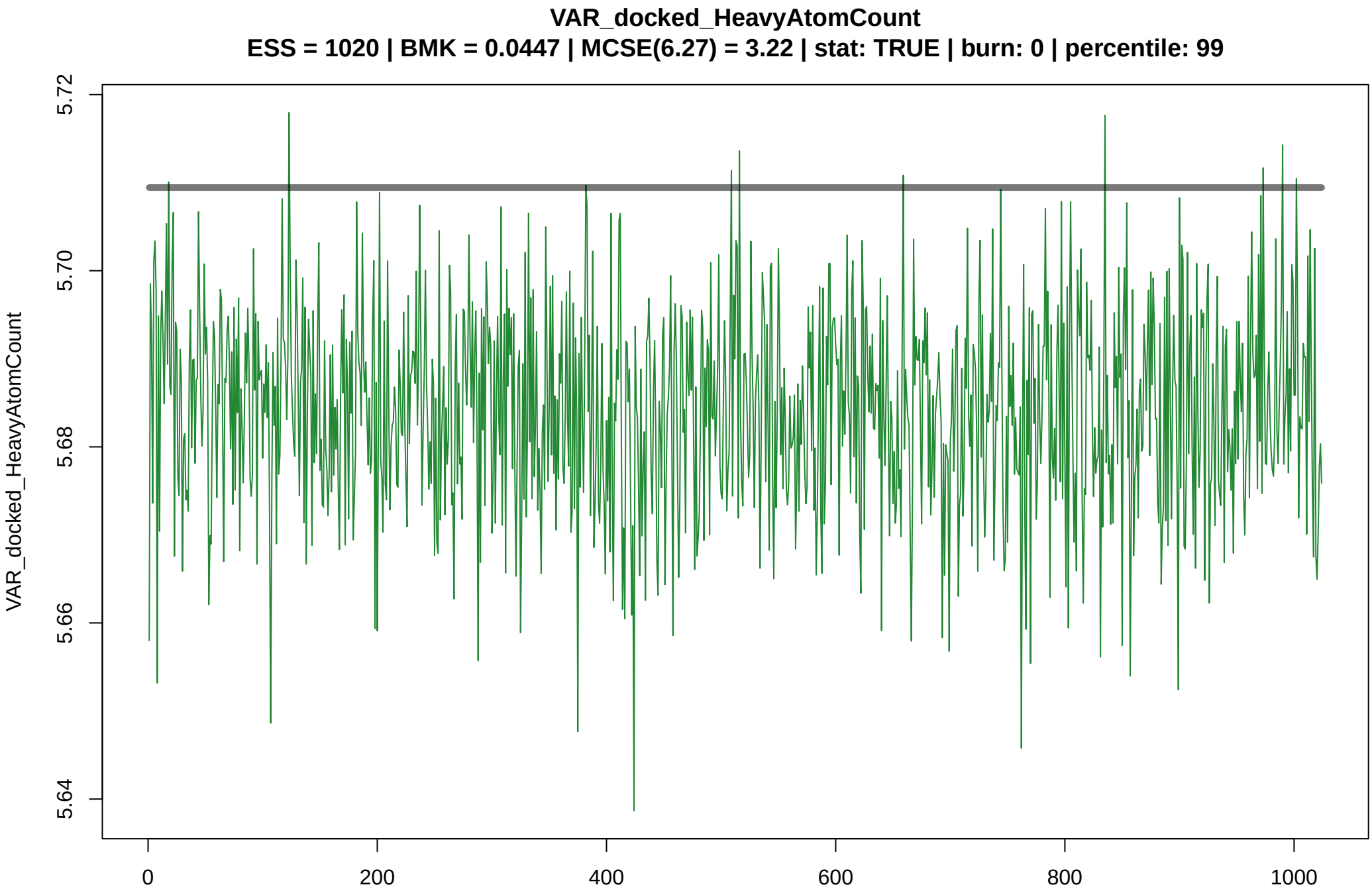

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0477 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0 | percentile: 81.1
MEAN_mcs_NOCount
6.4
6.3
6.2
6.1
6.0
5.9
0
200
400
600
800
1000

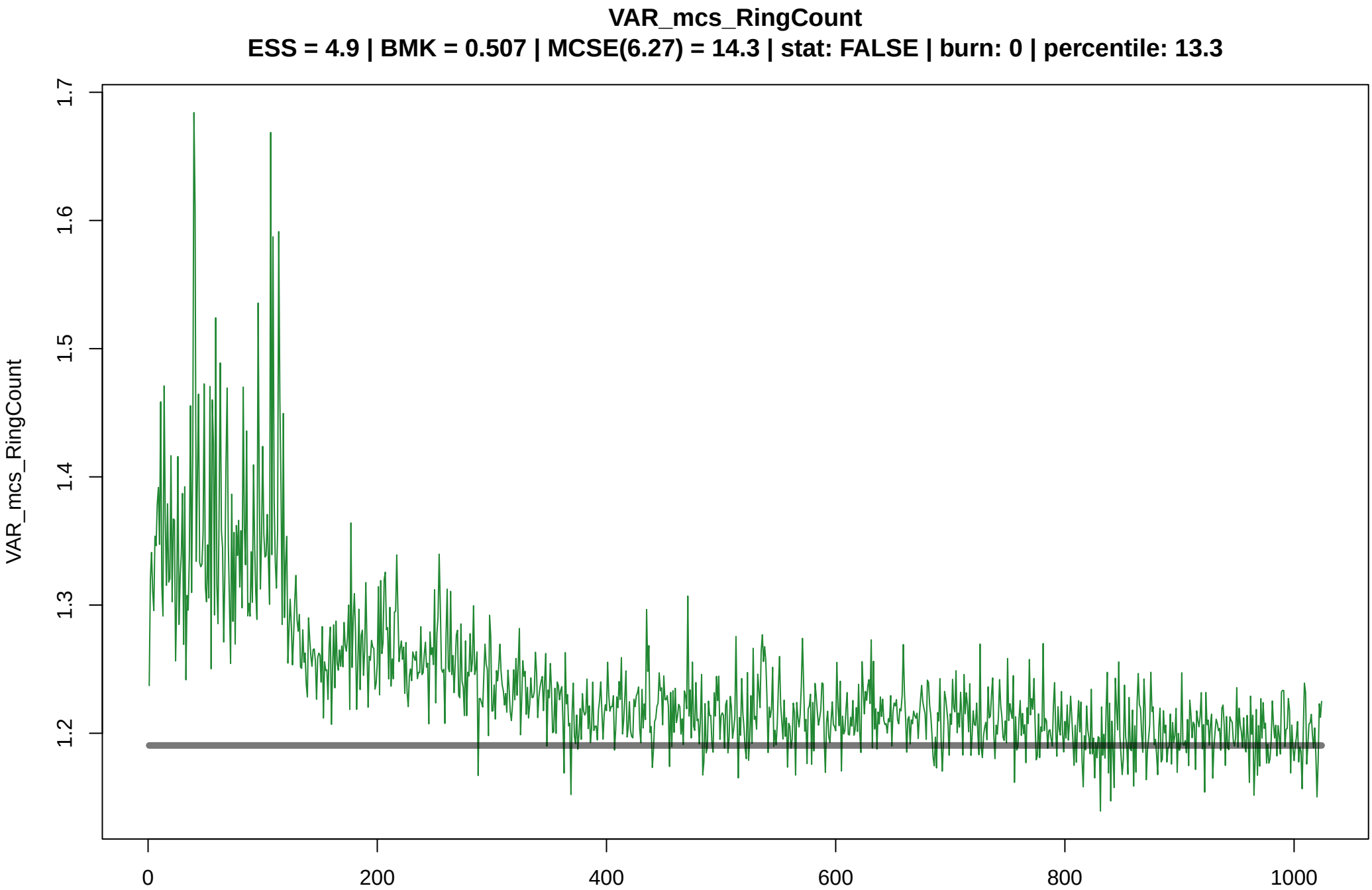

VAR_log_RMSD
ESS = 1020 | BMK = 0.665 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 1020 | percentile: 31.1
VAR_log_RMSD
1
2
3
4
5
6
0
200
400
600
800
1000

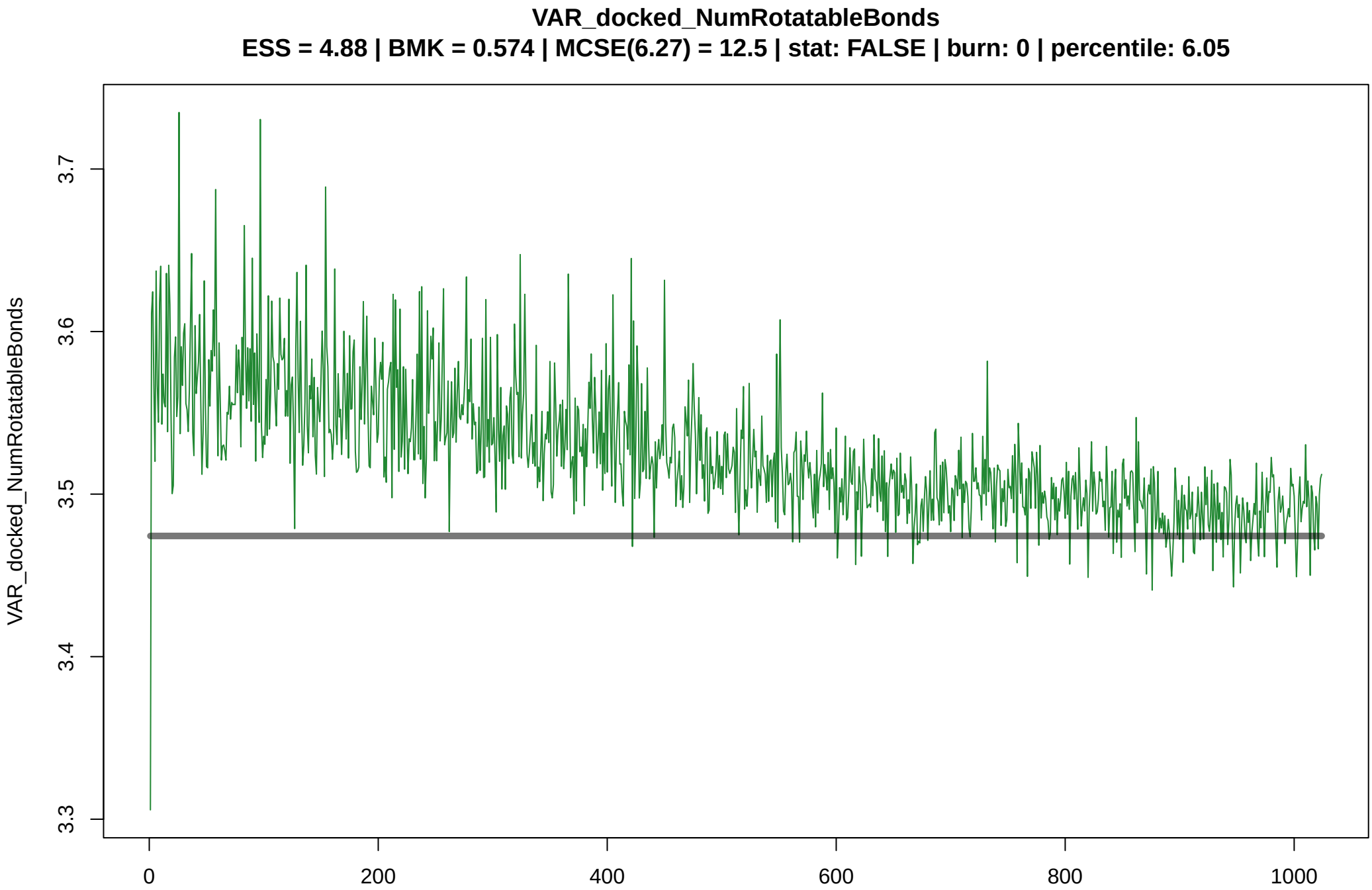

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 1020 | percentile: 66.7
VAR_log_mcs_unbonded_polar_sasa
2
4
6
8
0
200
400
600
800
1000

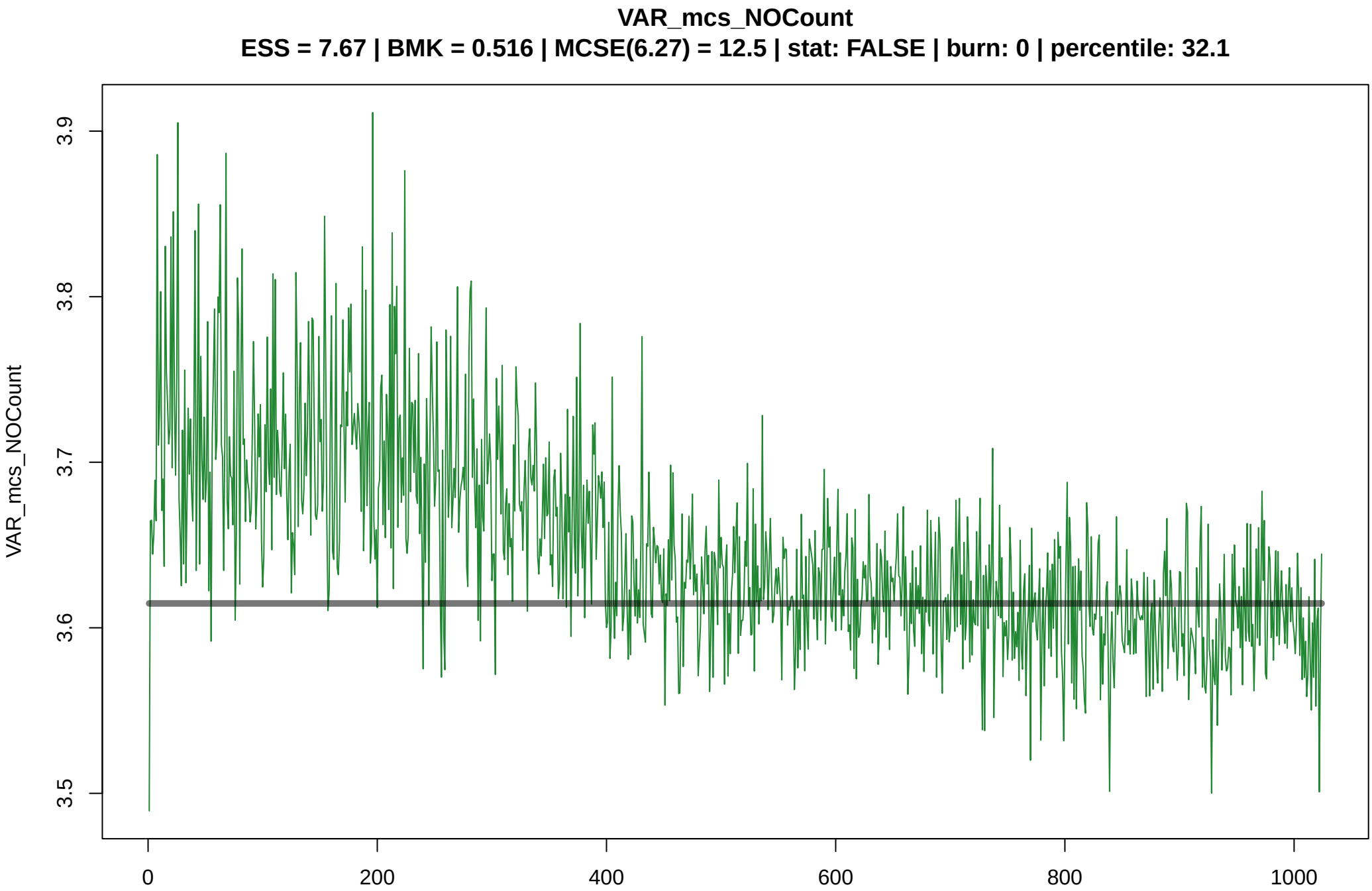

VAR_logit_ec_tanimoto_similarity
ESS = 747 | BMK = 0.187 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | percentile: 43.8
VAR_logit_ec_tanimoto_similarity
5.0
4.5
4.0
3.5
3.0
0
200
400
600
800
1000

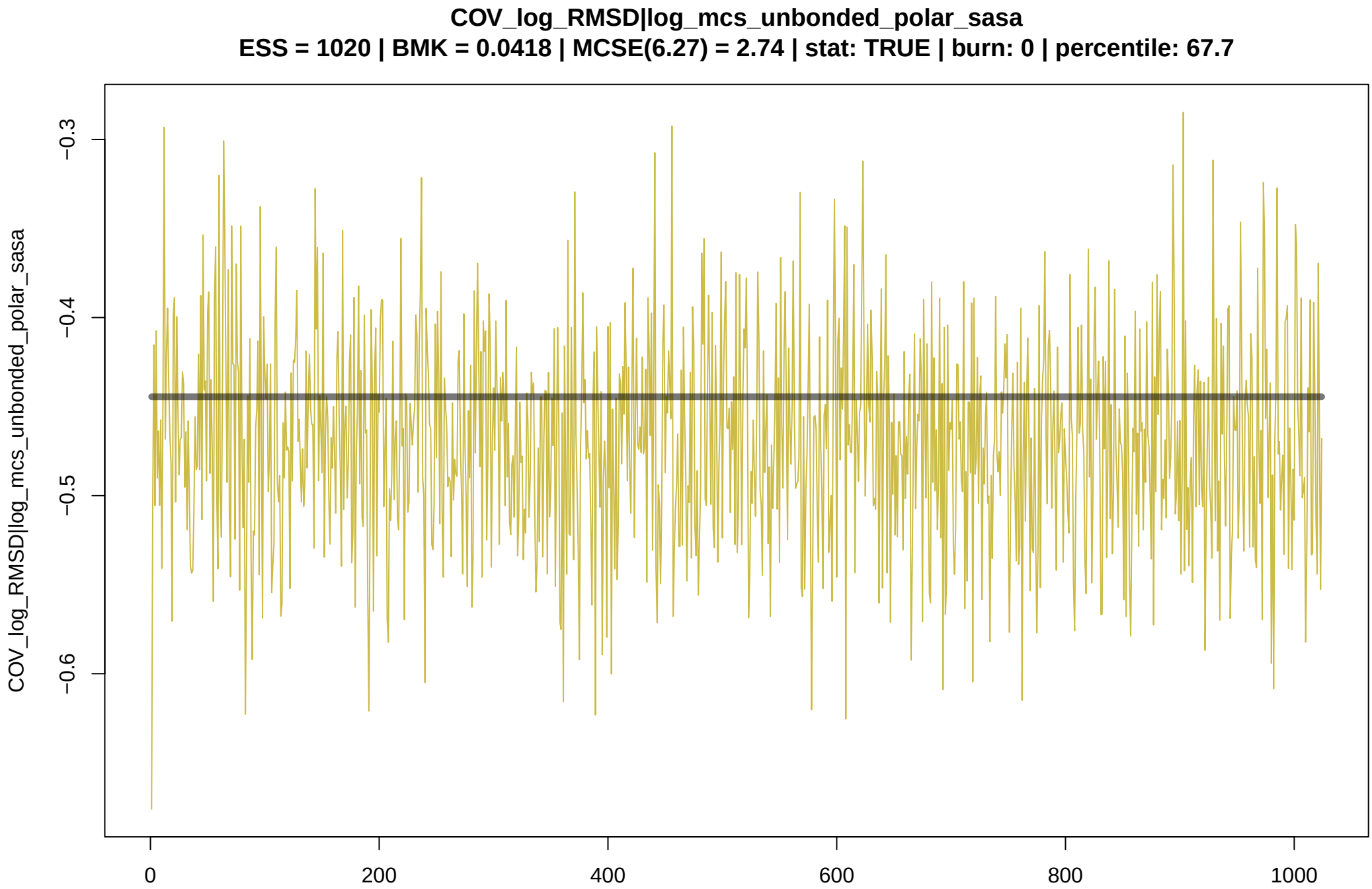

VAR_mcs_NumHeteroAtoms
ESS = 89.4 | BMK = 0.0899 | MCSE(6.27) = 8.08 | stat: FALSE | burn: 0 | percentile: 30.2
VAR_mcs_NumHeteroAtoms
1.30
1.35
1.40
1.45
1.50
1.55
0
200
400
600
800
1000

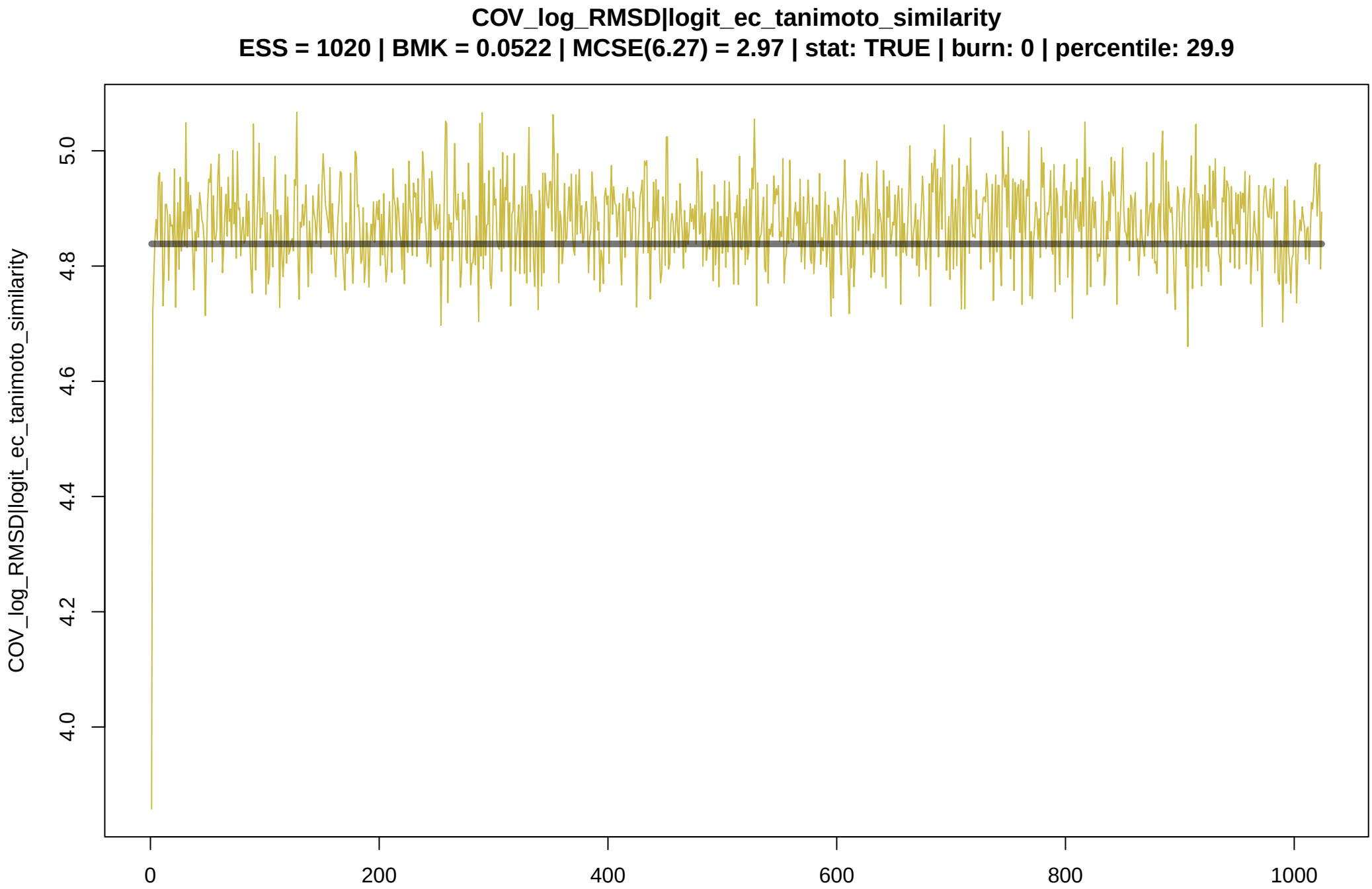

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0447 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0 | percentile: 99
VAR_docked_HeavyAtomCount
5.64
5.66
5.68
5.70
5.72
0
200
400
600
800
1000

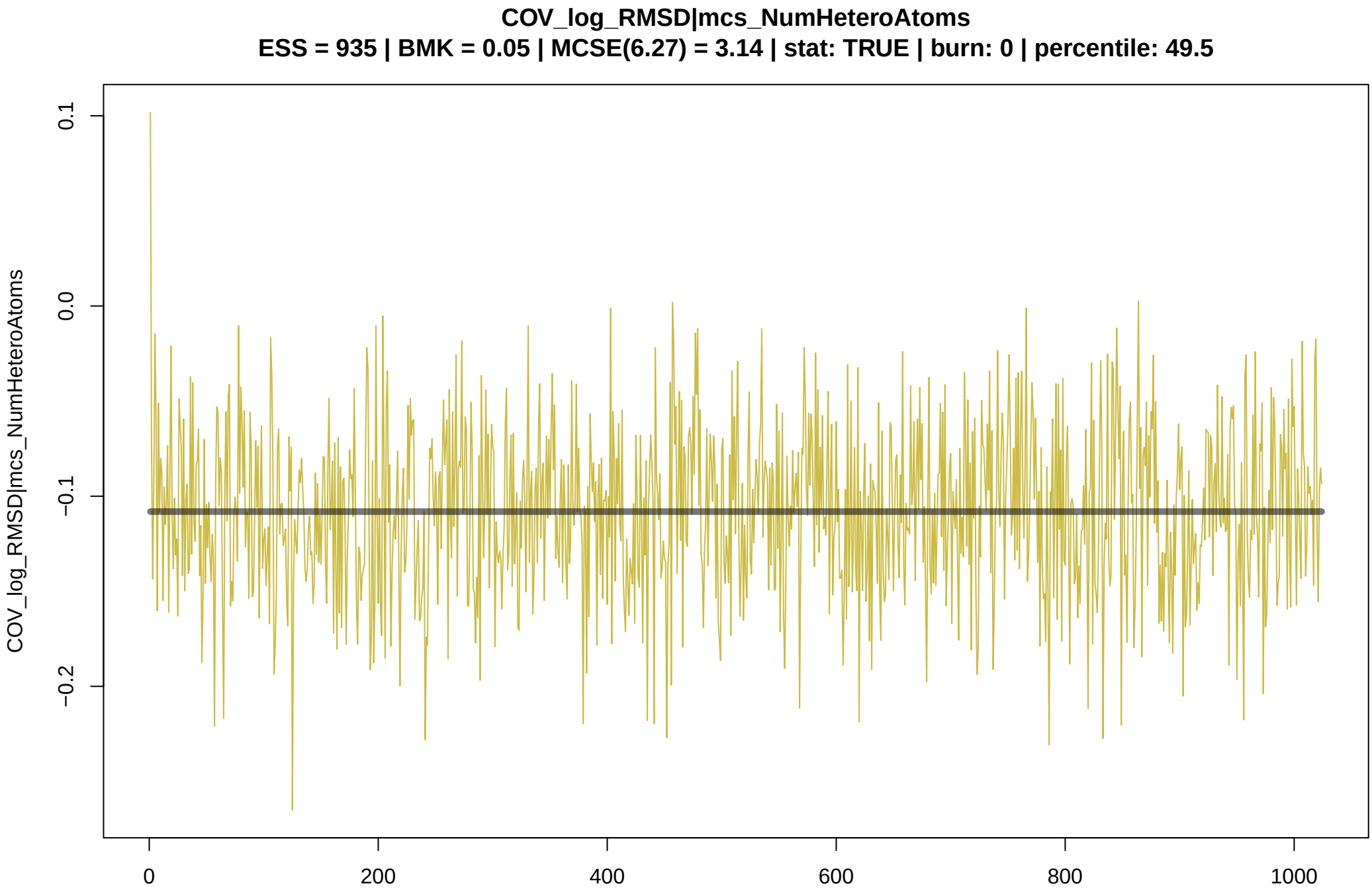

VAR_mcs_RingCount
ESS = 4.9 | BMK = 0.507 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 0 | percentile: 13.3
VAR_mcs_RingCount
1.2
1.3
1.4
1.5
1.6
1.7
0
200
400
600
800
1000

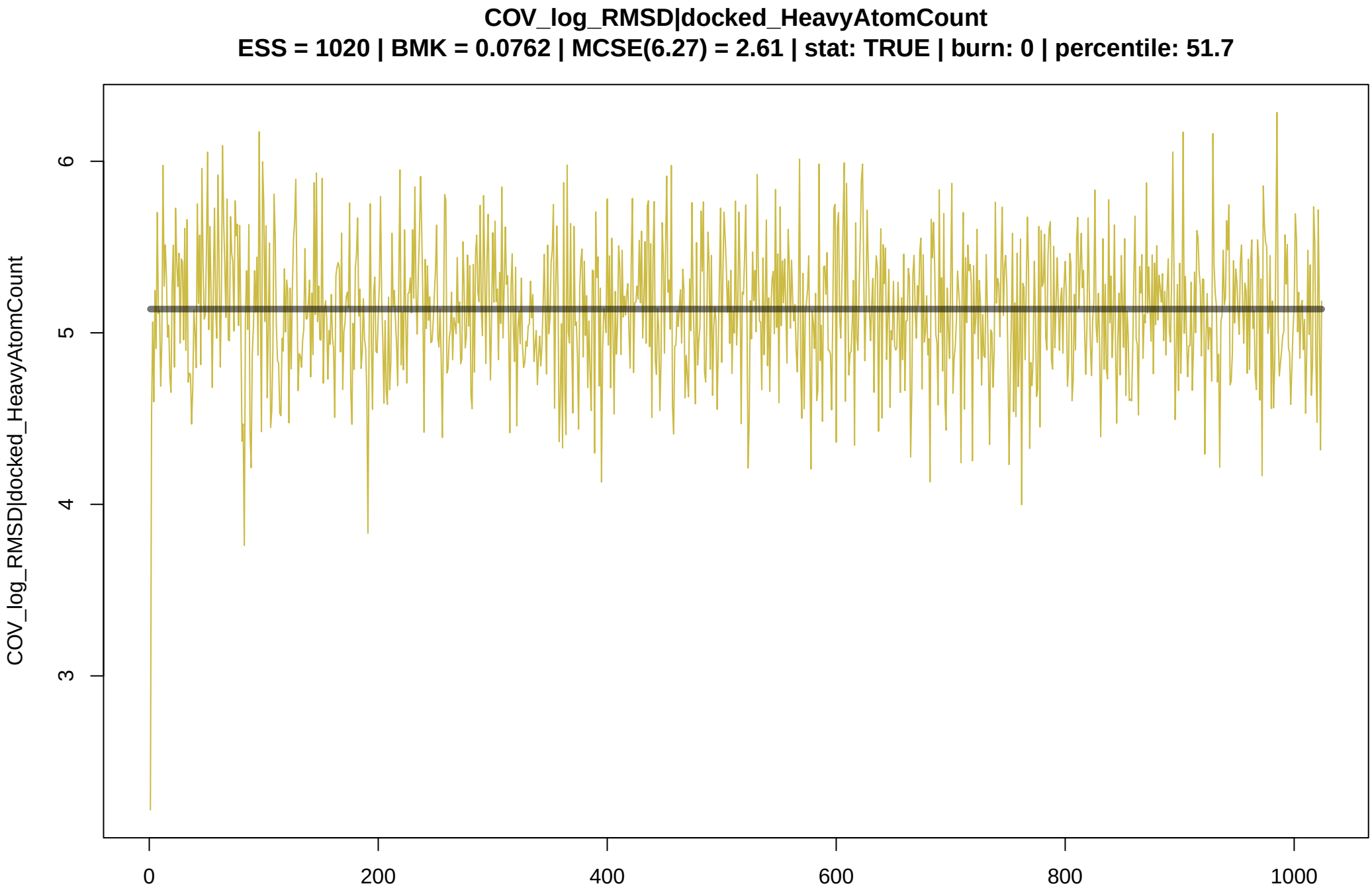

VAR_docked_NumRotatableBonds
ESS = 4.88 | BMK = 0.574 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 0 | percentile: 6.05
VAR_docked_NumRotatableBonds
3.3
3.4
3.5
3.6
3.7
0
200
400
600
800
1000

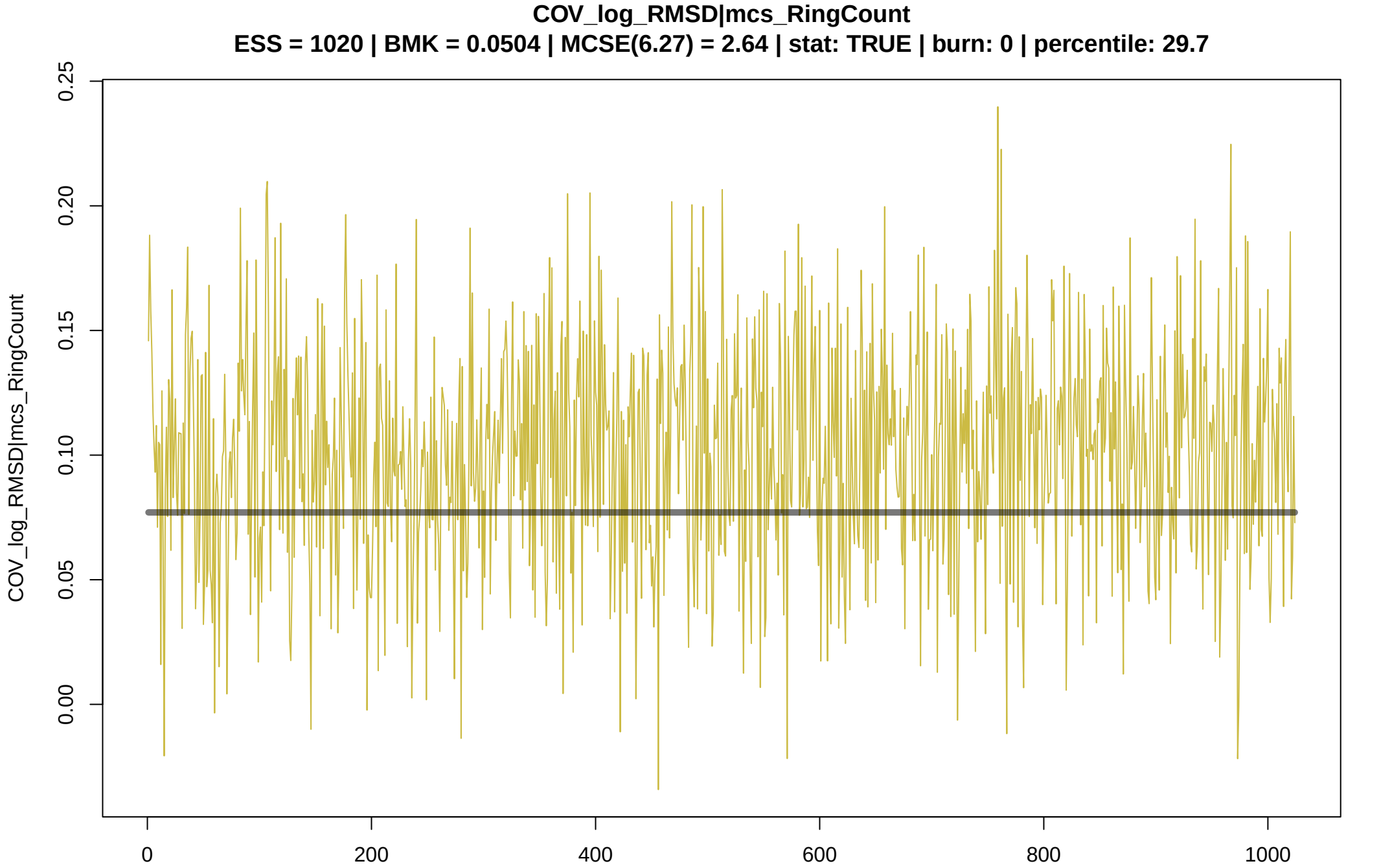

VAR_mcs_NOCount
ESS = 7.67 | BMK = 0.516 | MCSE(6.27) = 12.5 | stat: FALSE | burn: 0 | percentile: 32.1
VAR_mcs_NOCount
3.5
3.6
3.7
3.8
3.9
0
200
400
600
800
1000

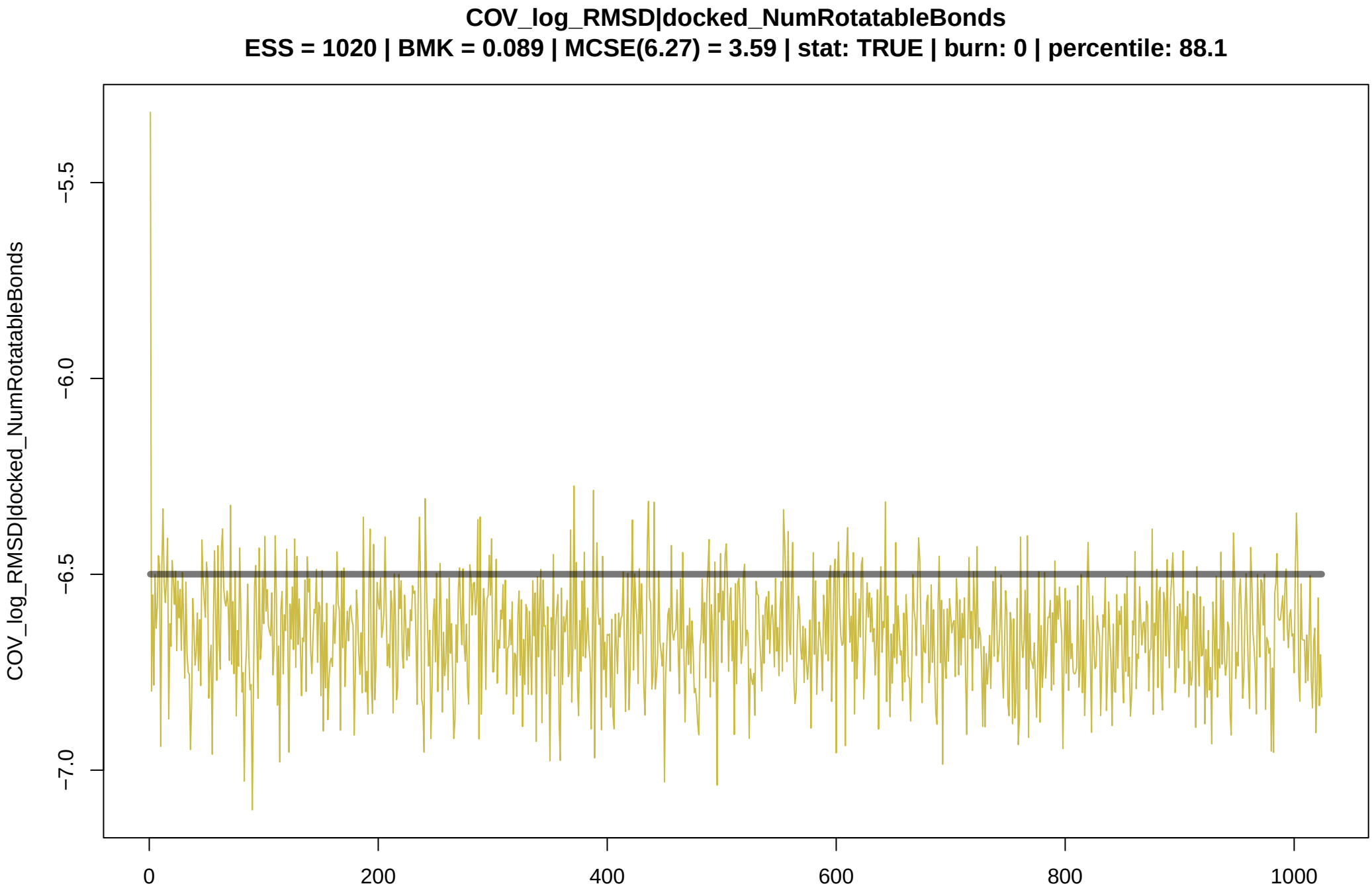

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0418 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | percentile: 67.7
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.3
−0.4
−0.5
−0.6
0
200
400
600
800
1000

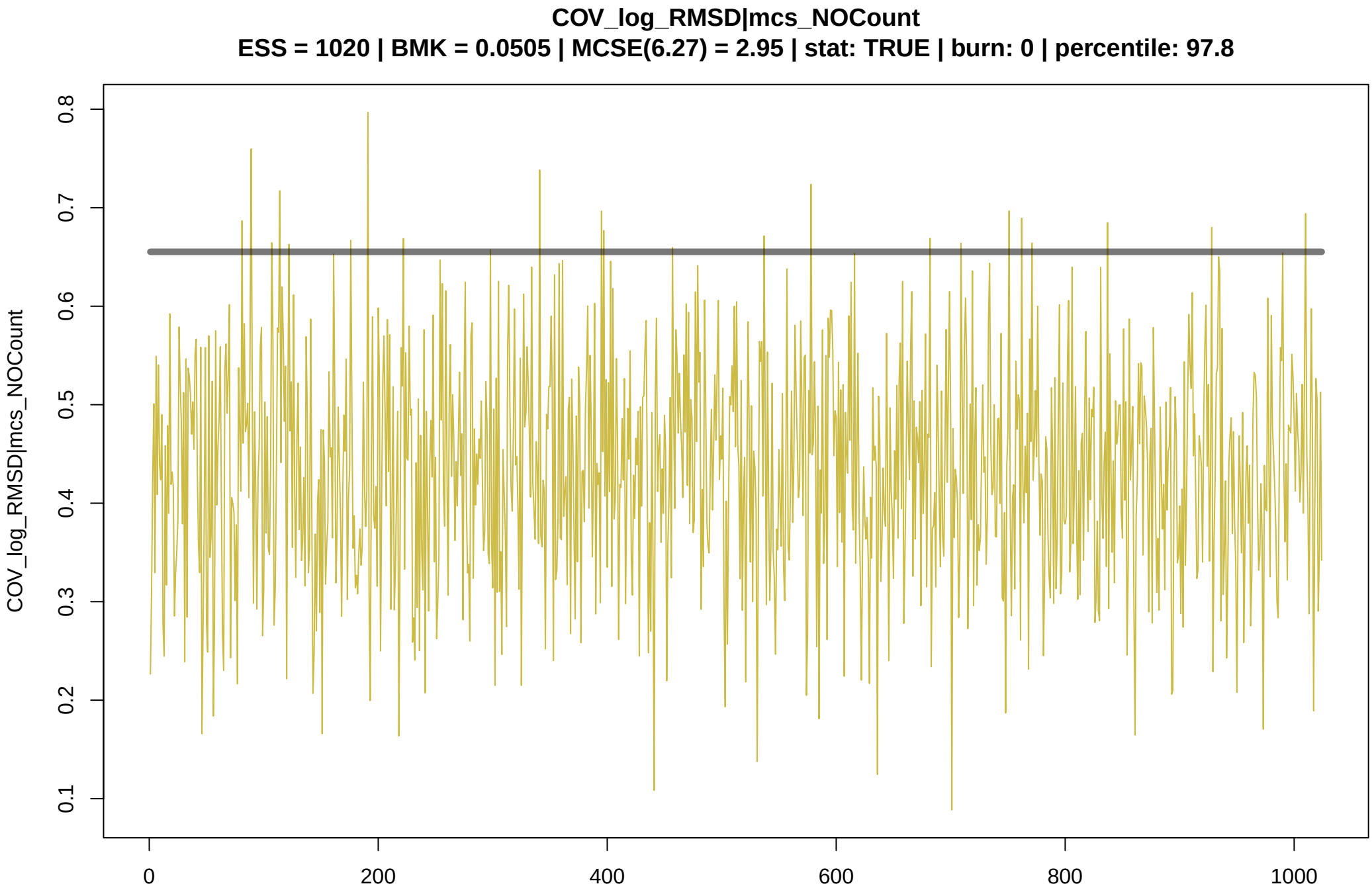

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0522 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0 | percentile: 29.9
COV_log_RMSD|logit_ec_tanimoto_similarity
4.0
4.2
4.4
4.6
4.8
5.0
0
200
400
600
800
1000

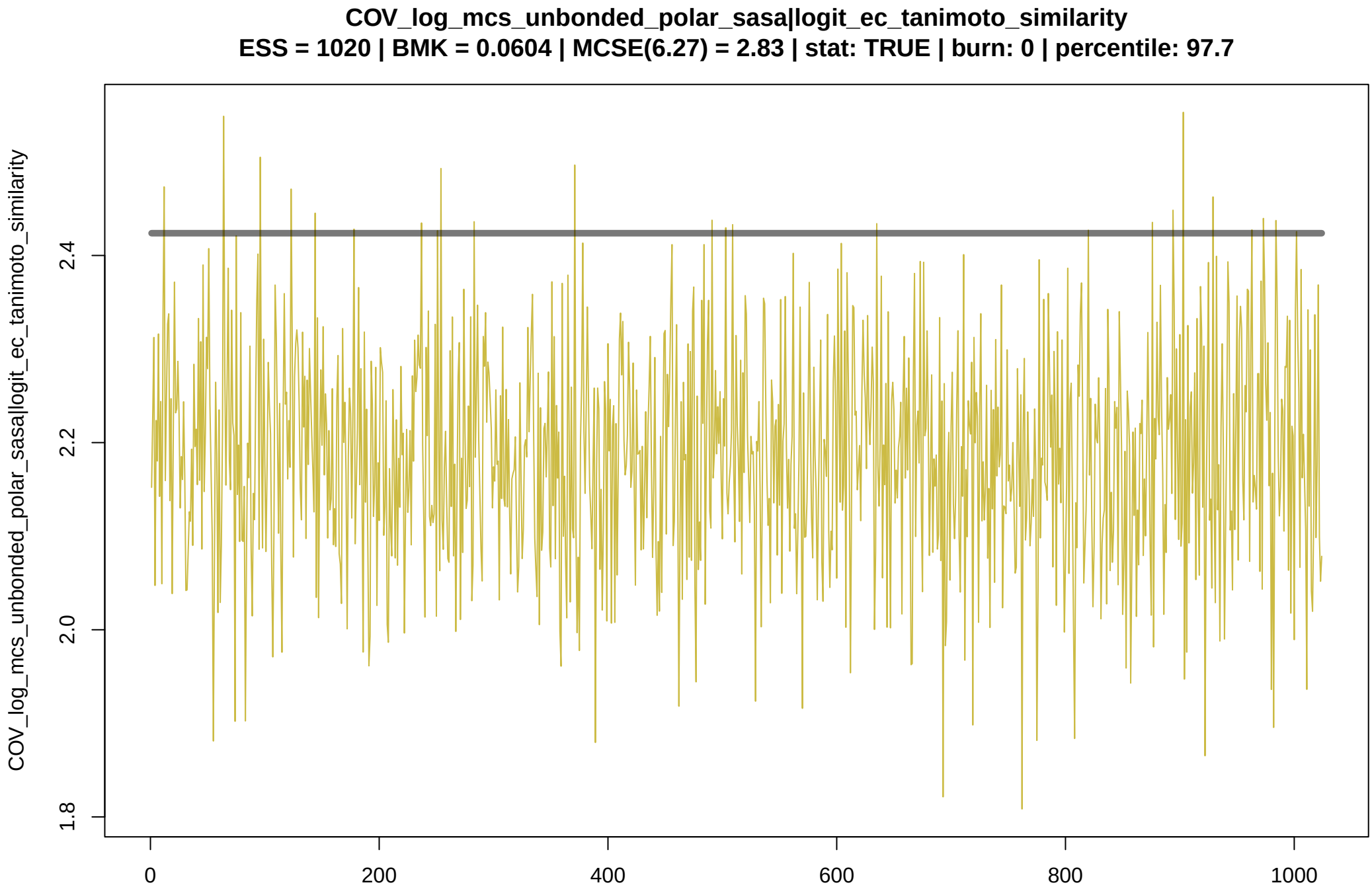

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 935 | BMK = 0.05 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | percentile: 49.5
COV_log_RMSD|mcs_NumHeteroAtoms
0.1
0.0
−0.1
−0.2
0
200
400
600
800
1000

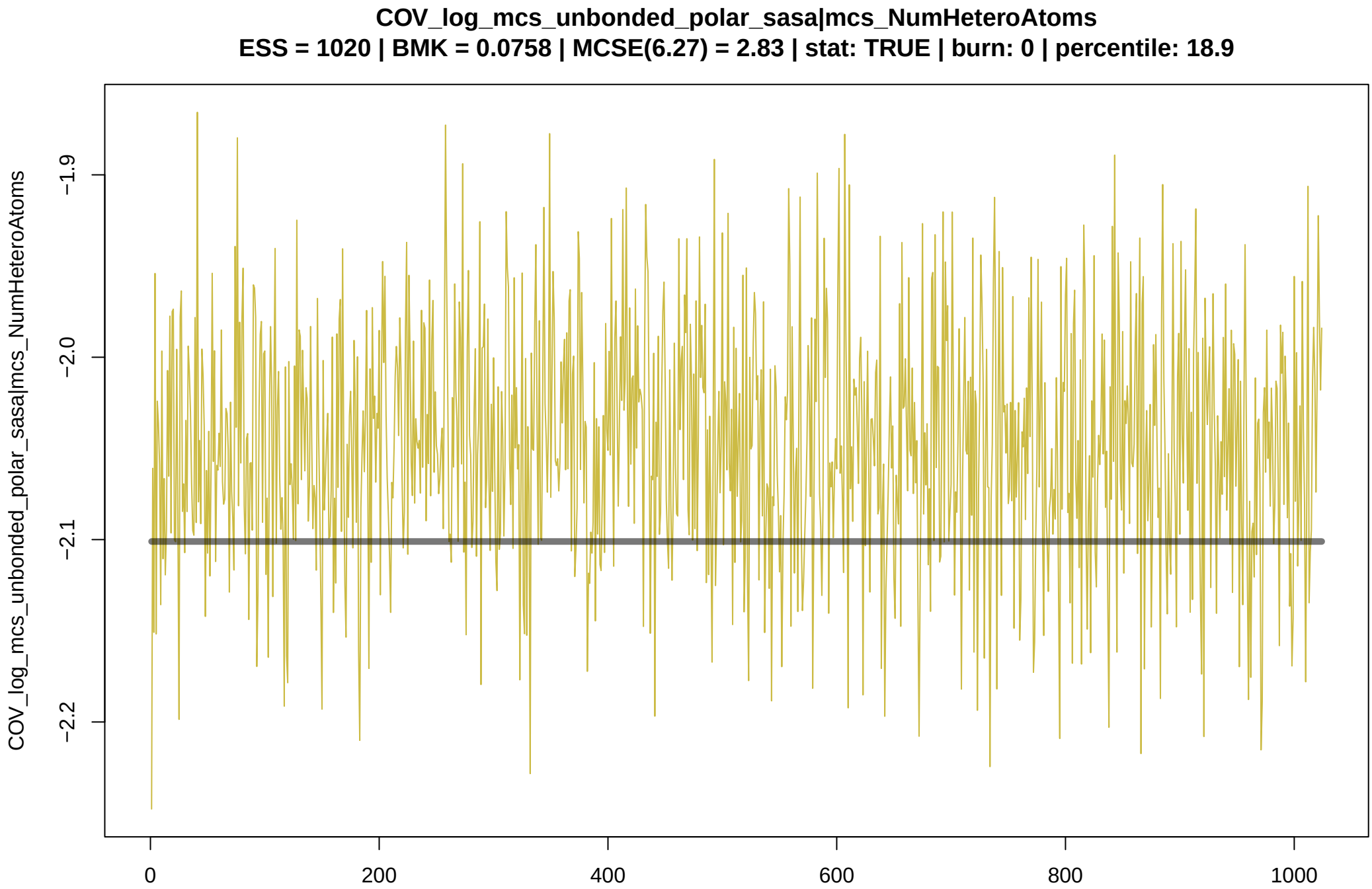

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0762 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | percentile: 51.7
COV_log_RMSD|docked_HeavyAtomCount
3
4
5
6
0
200
400
600
800
1000

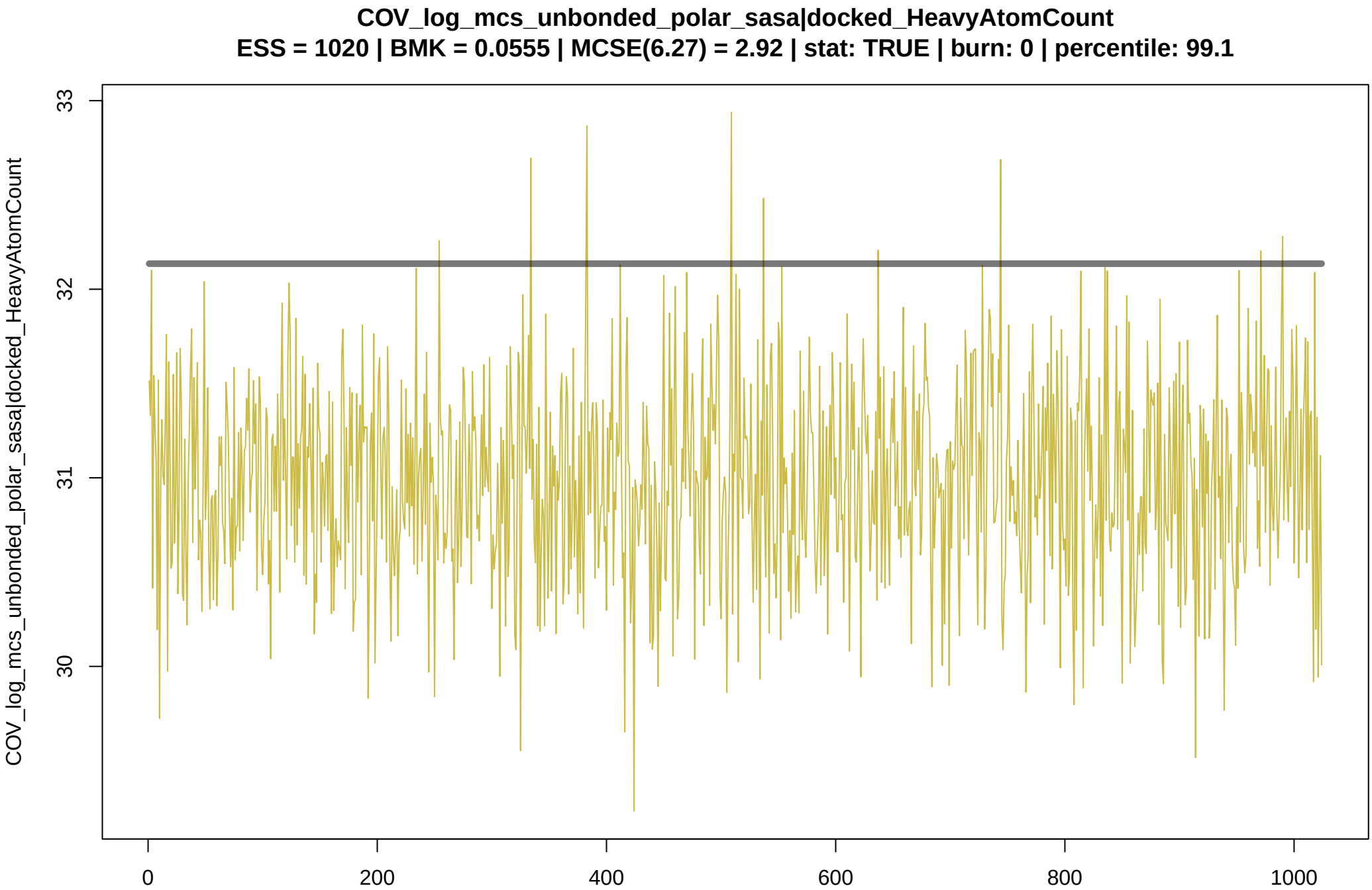

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0504 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | percentile: 29.7
COV_log_RMSD|mcs_RingCount
0.25
0.20
0.15
0.10
0.05
0.00
0
200
400
600
800
1000

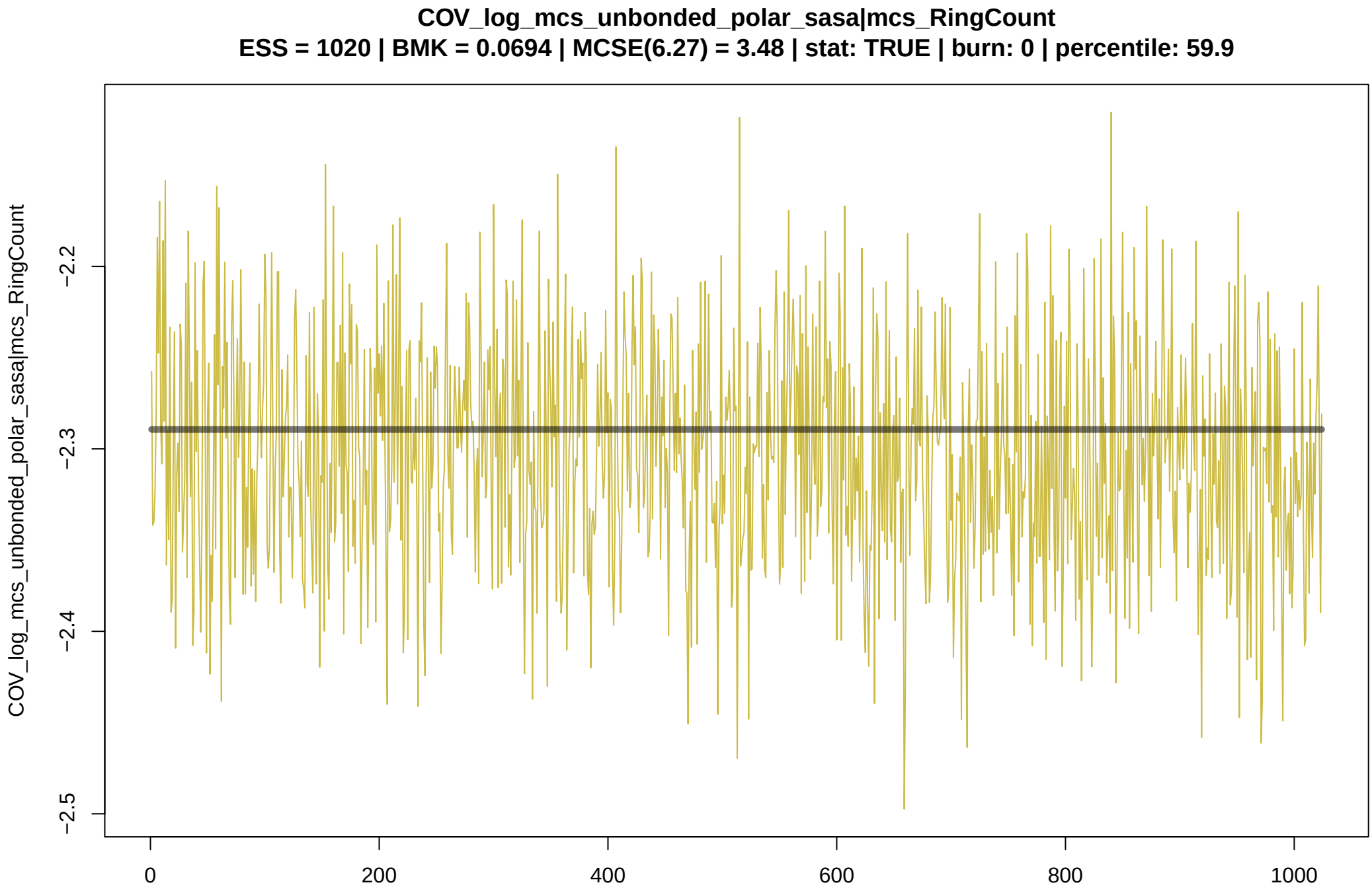

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.089 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | percentile: 88.1
COV_log_RMSD|docked_NumRotatableBonds
−5.5
−6.0
−6.5
−7.0
0
200
400
600
800
1000

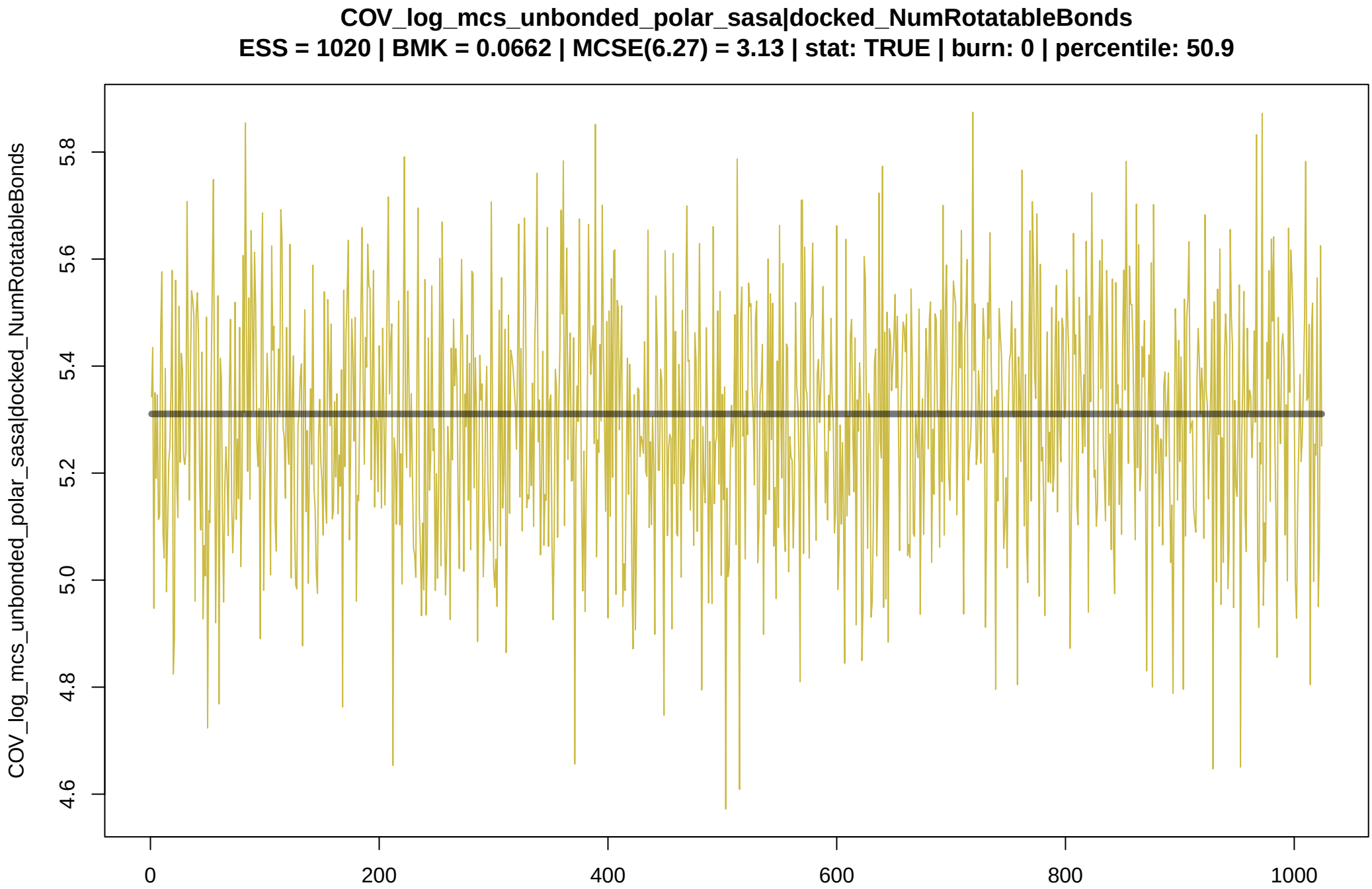

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0505 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | percentile: 97.8
COV_log_RMSD|mcs_NOCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
200
400
600
800
1000

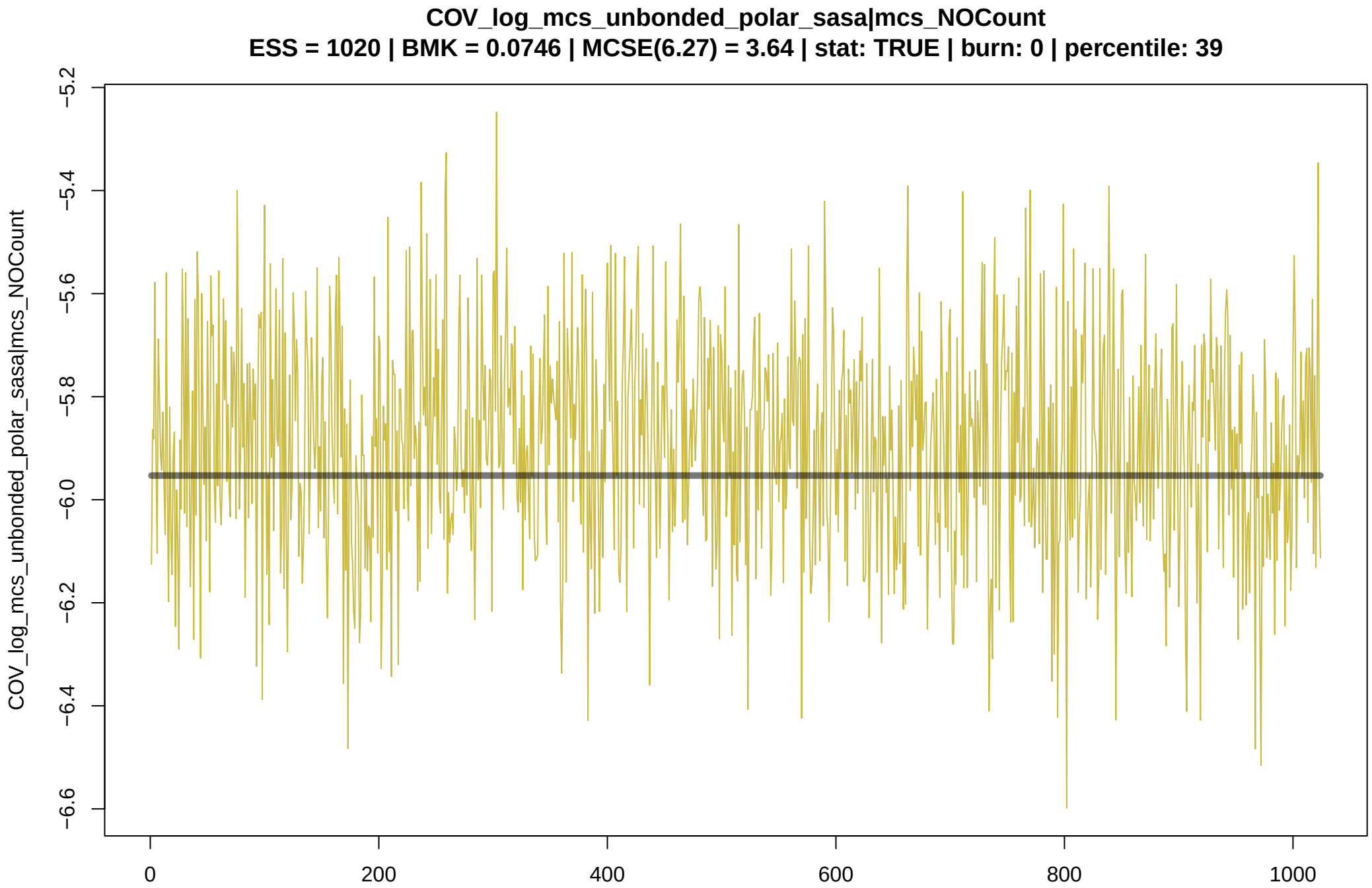

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0604 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | percentile: 97.7
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
1.8
2.0
2.2
2.4
0
200
400
600
800
1000

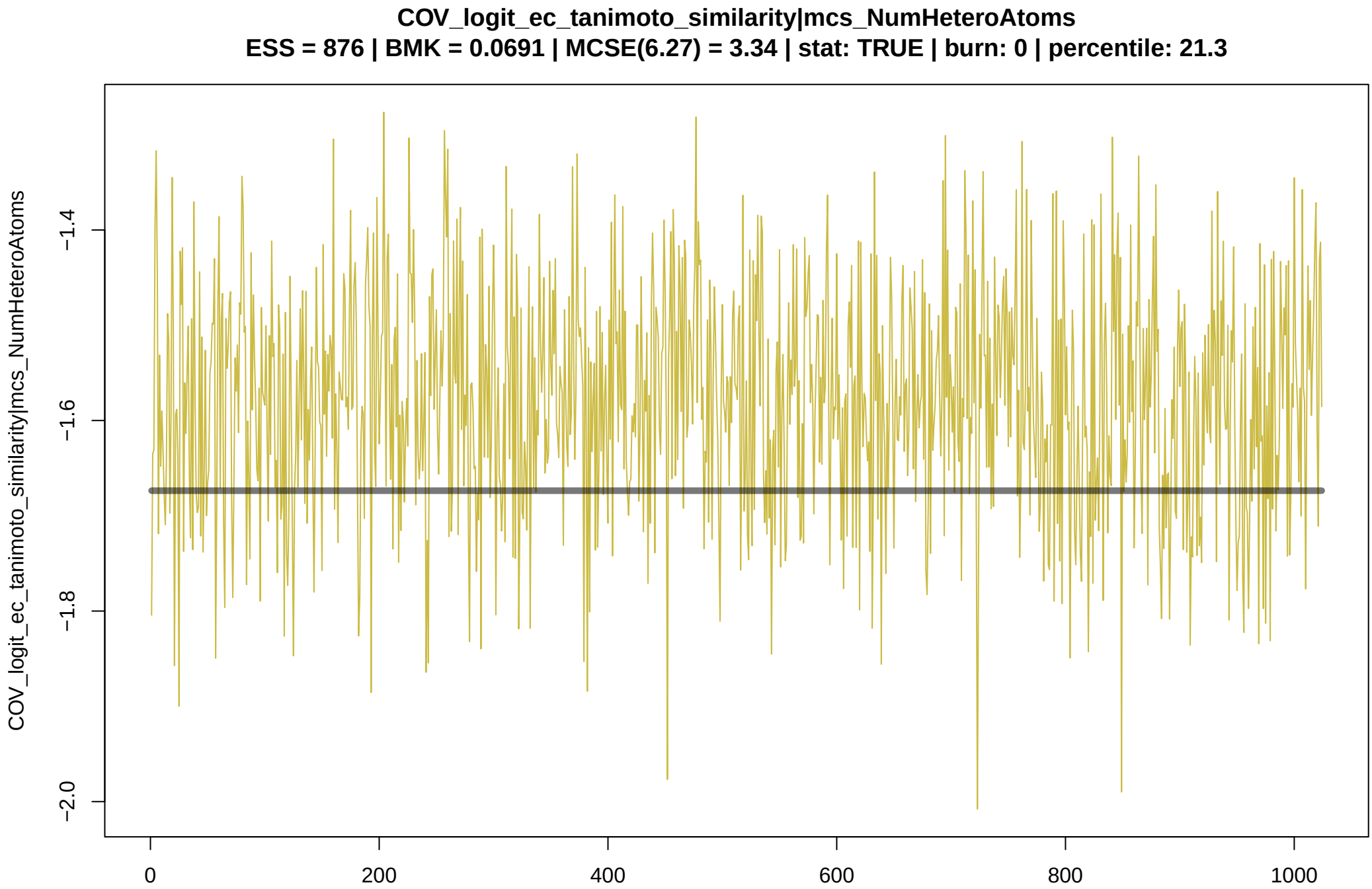

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0758 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | percentile: 18.9
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

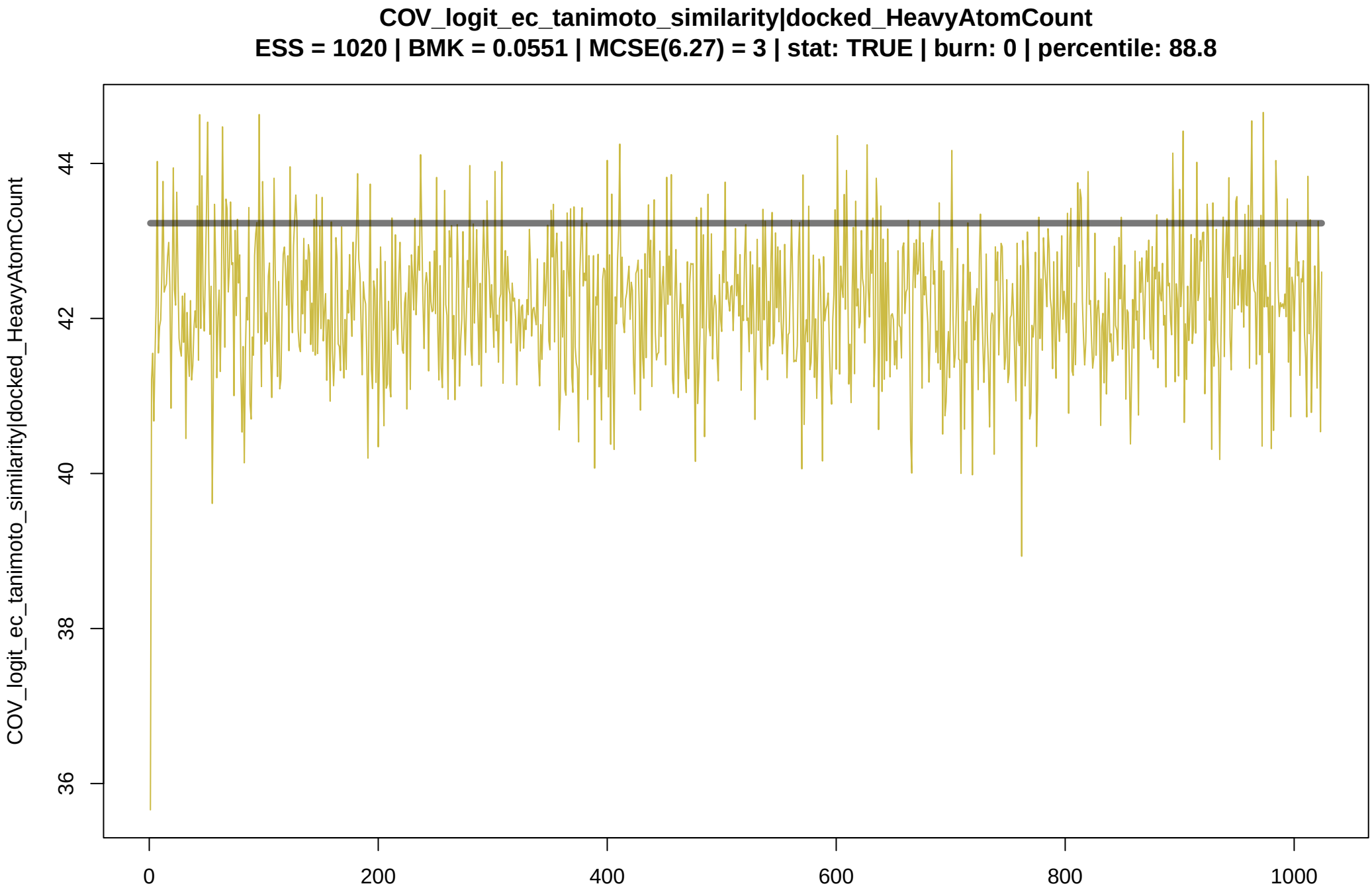

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0555 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0 | percentile: 99.1
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
33
32
31
30
0
200
400
600
800
1000

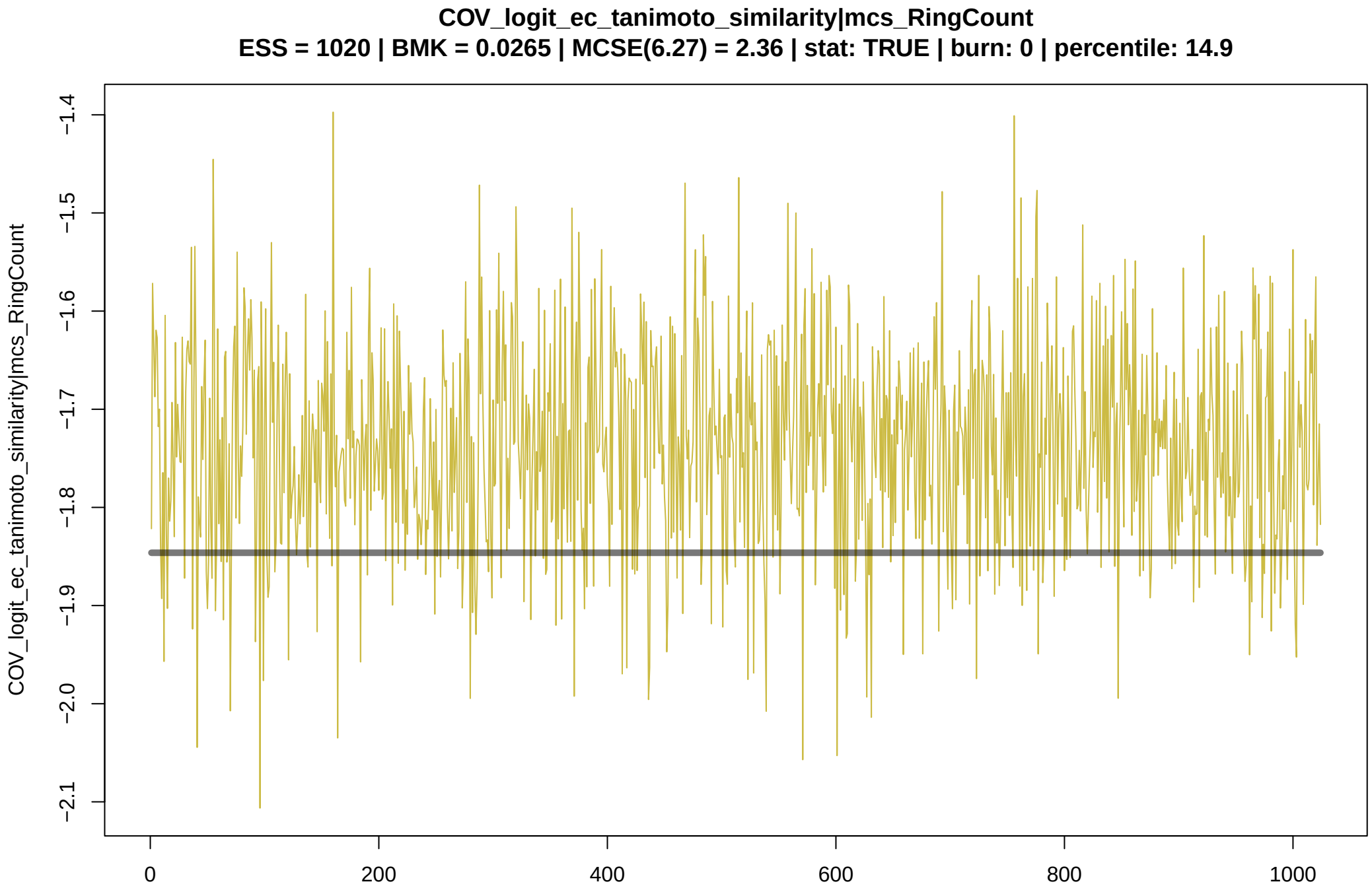

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0694 | MCSE(6.27) = 3.48 | stat: TRUE | burn: 0 | percentile: 59.9
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.2
−2.3
−2.4
−2.5
0
200
400
600
800
1000

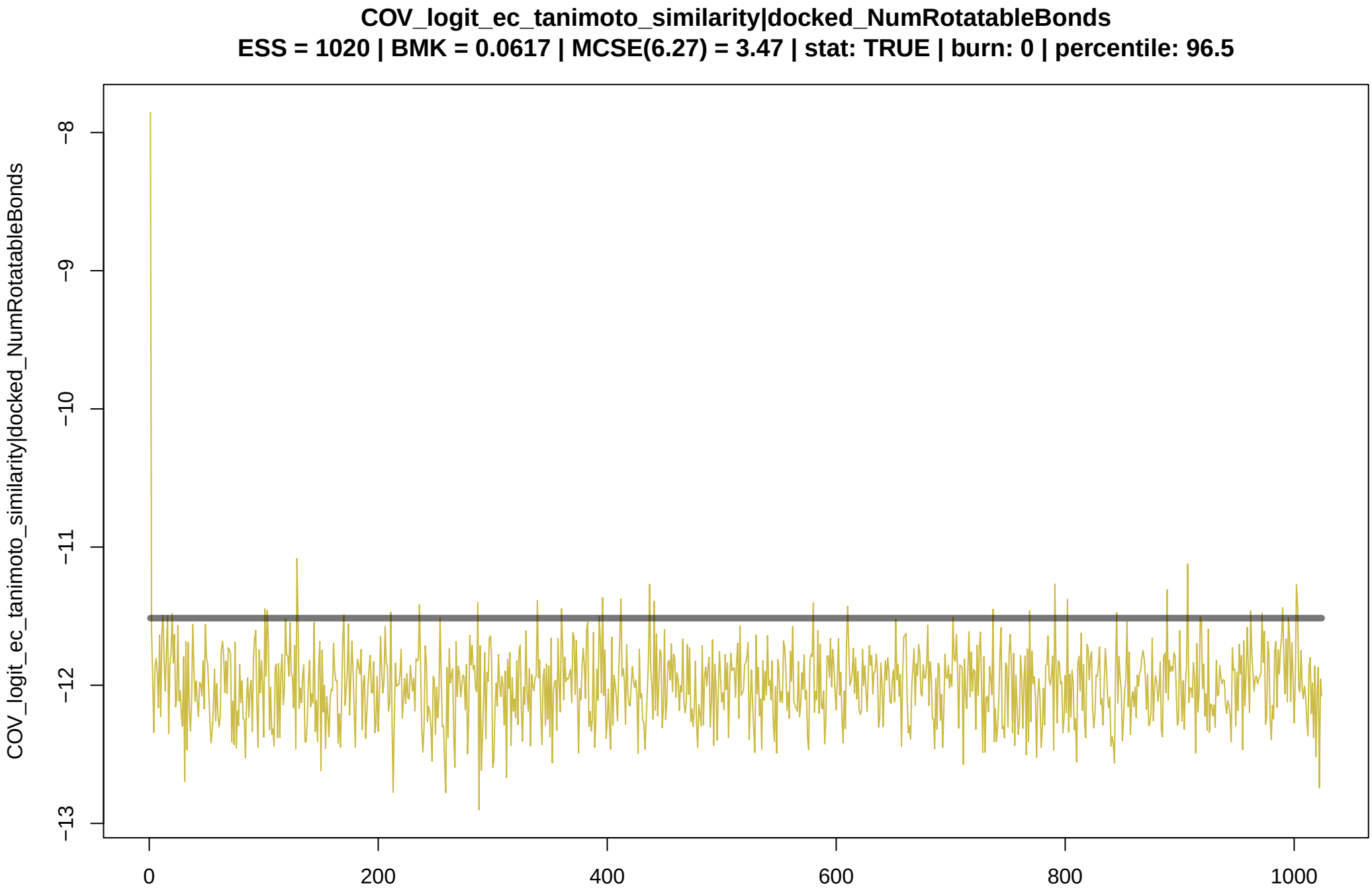

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0662 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0 | percentile: 50.9
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
4.6
4.8
5.0
5.2
5.4
5.6
5.8
0
200
400
600
800
1000

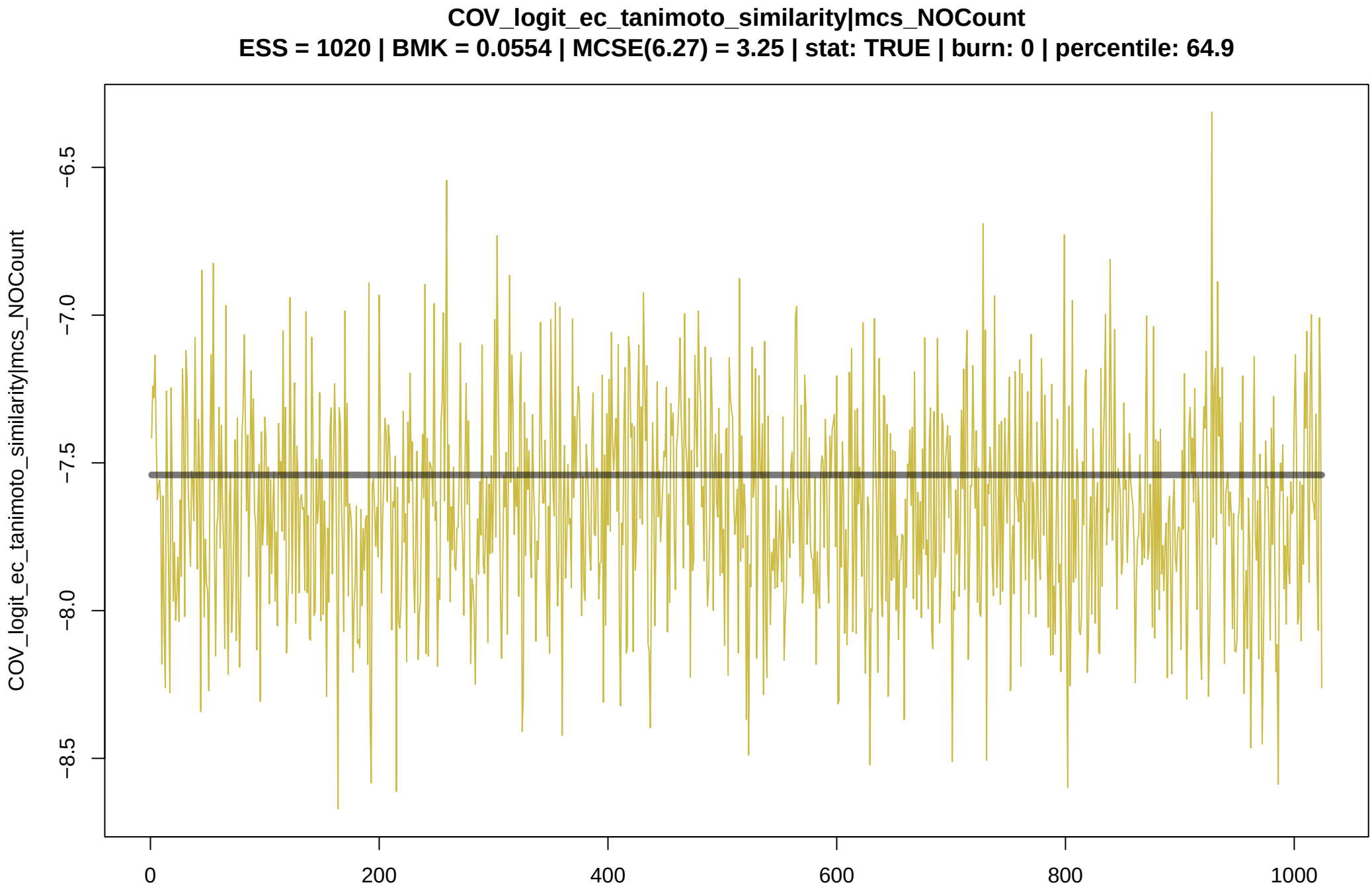

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0746 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 0 | percentile: 39
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.2
−5.4
−5.6
−5.8
−6.0
−6.2
−6.4
−6.6
0
200
400
600
800
1000

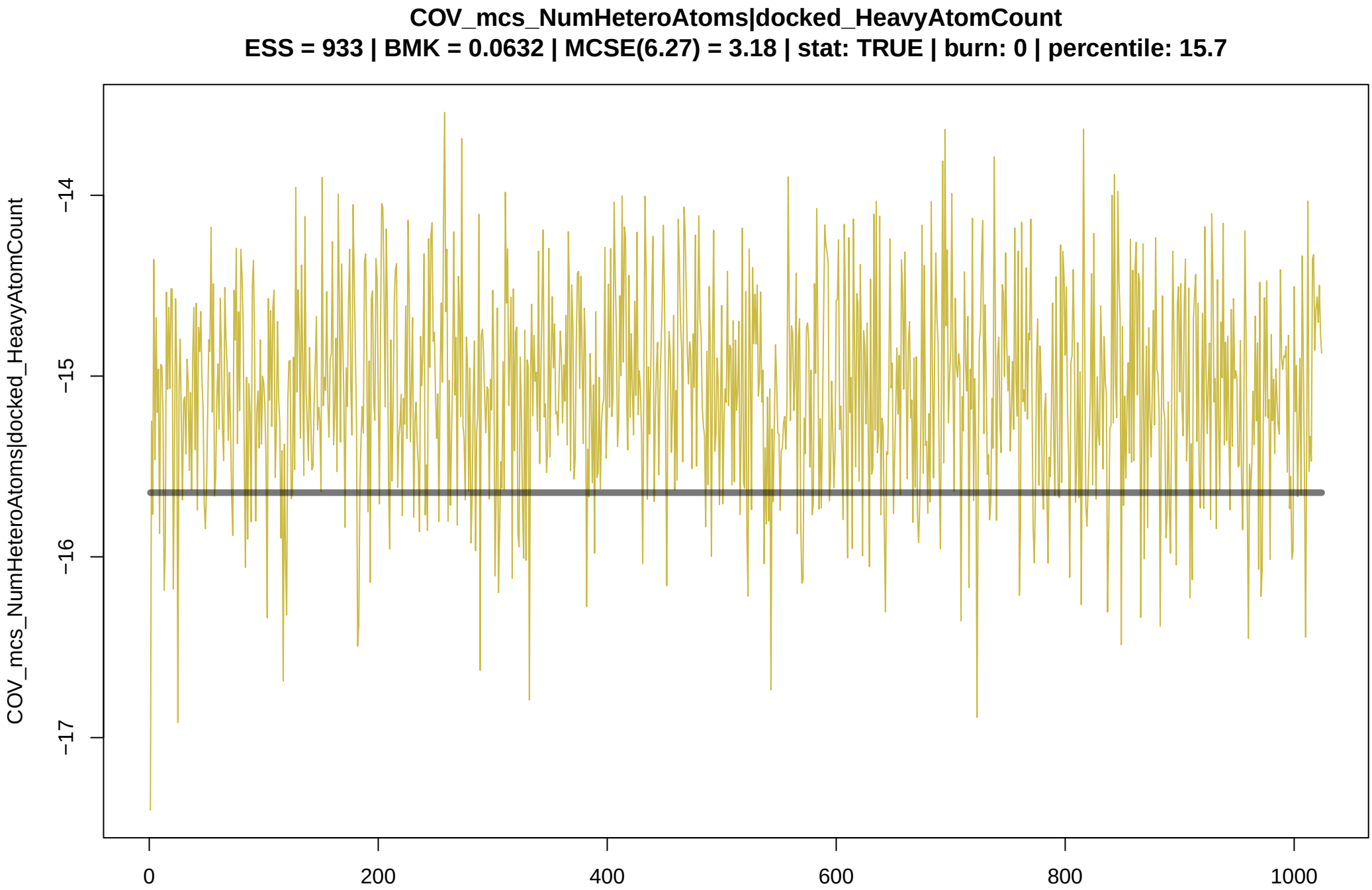

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 876 | BMK = 0.0691 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0 | percentile: 21.3
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

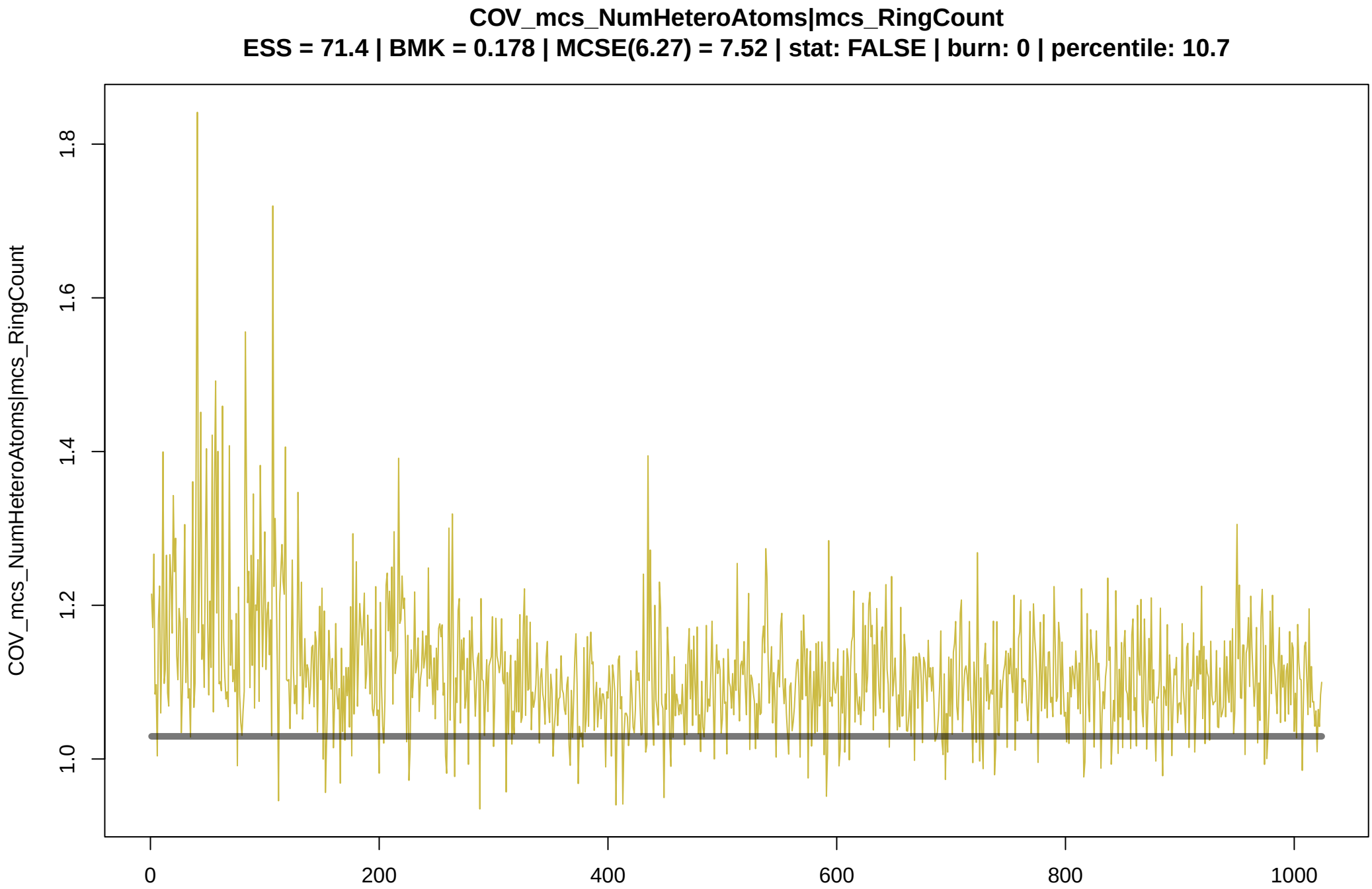

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0551 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | percentile: 88.8
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
36
38
40
42
44
0
200
400
600
800
1000

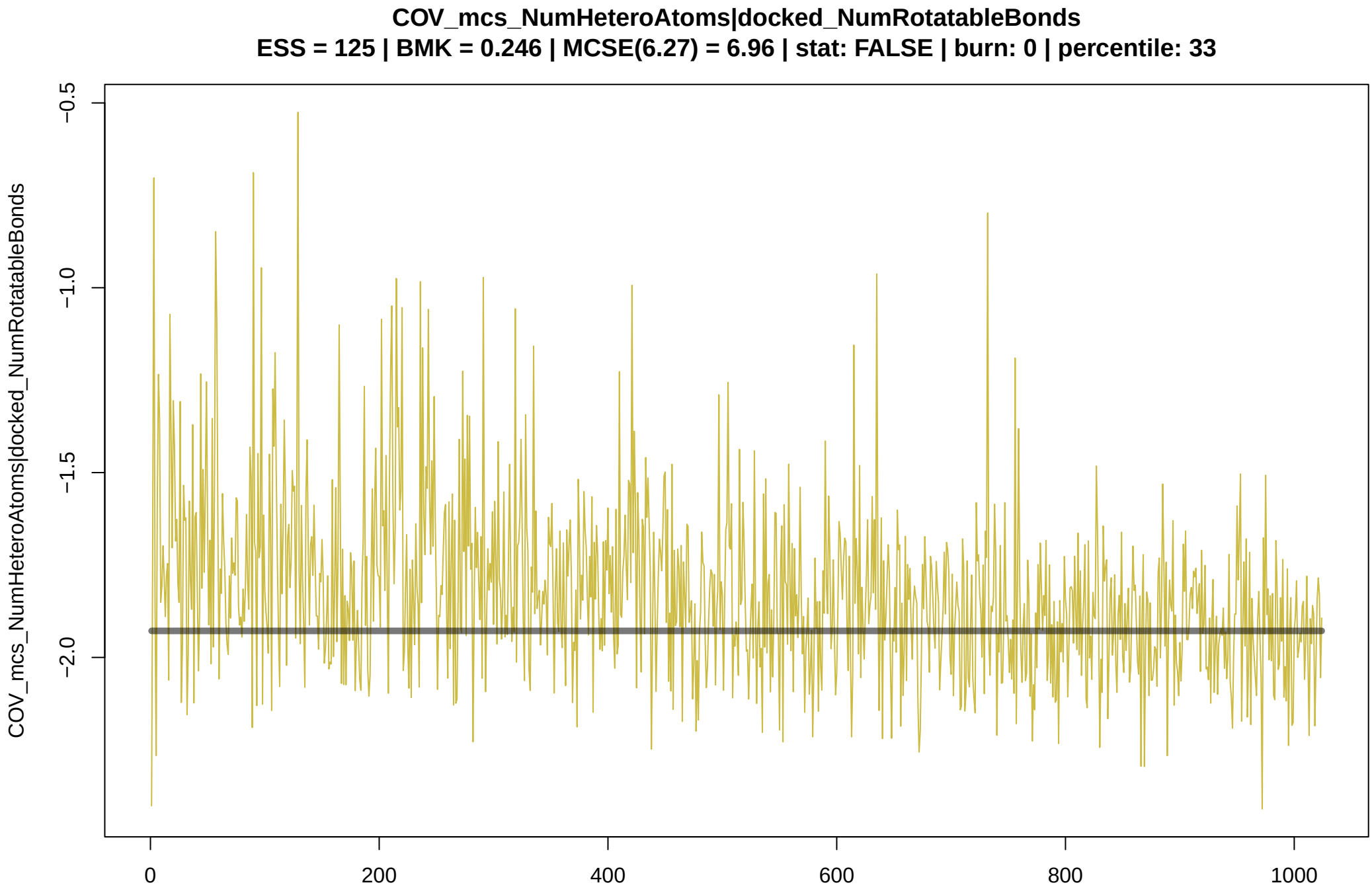

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0265 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0 | percentile: 14.9
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.4
−1.5
−1.6
−1.7
−1.8
−1.9
−2.0
−2.1
0
200
400
600
800
1000

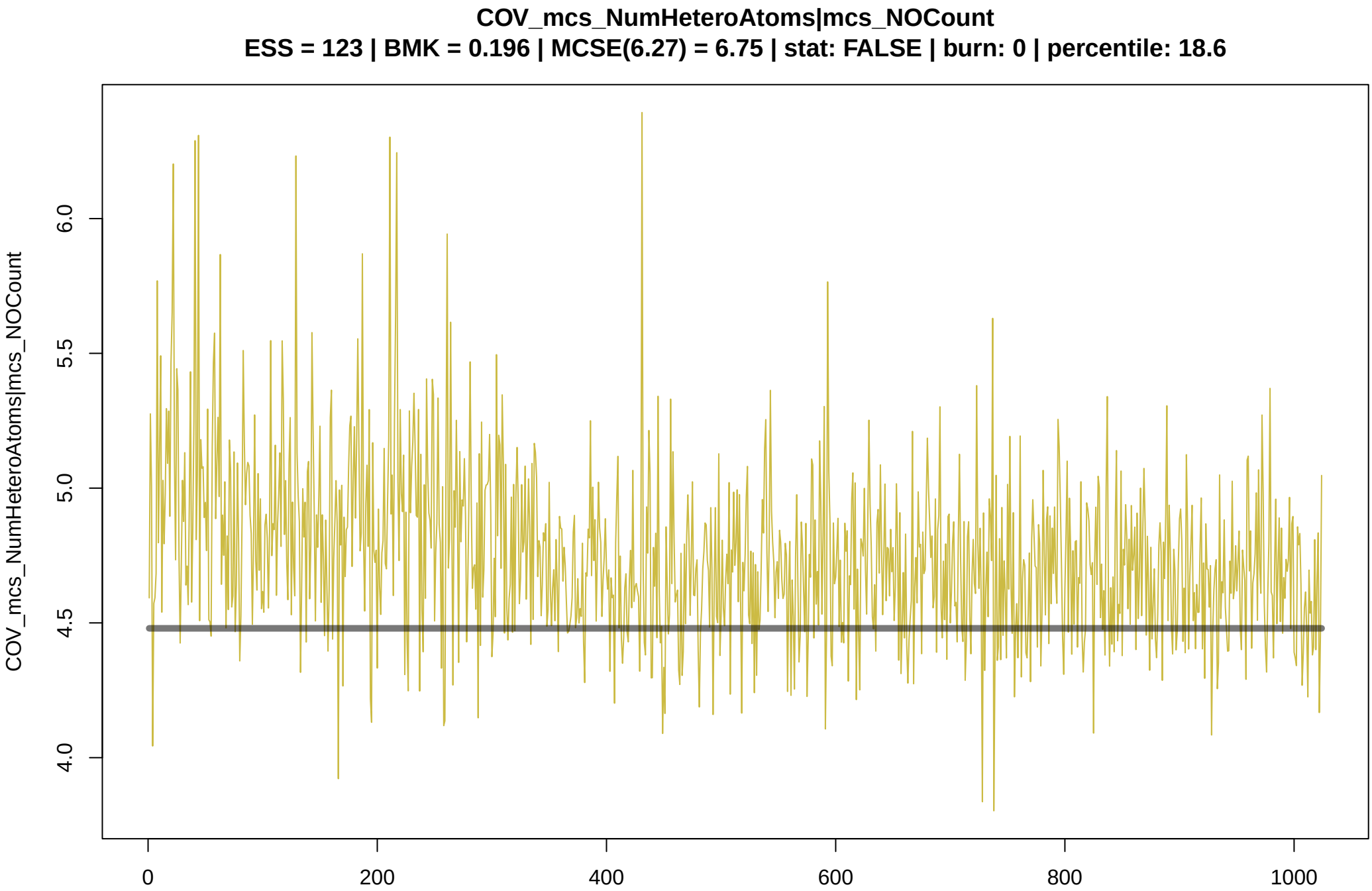

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0617 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | percentile: 96.5
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−8
−9
−10
−11
−12
−13
0
200
400
600
800
1000

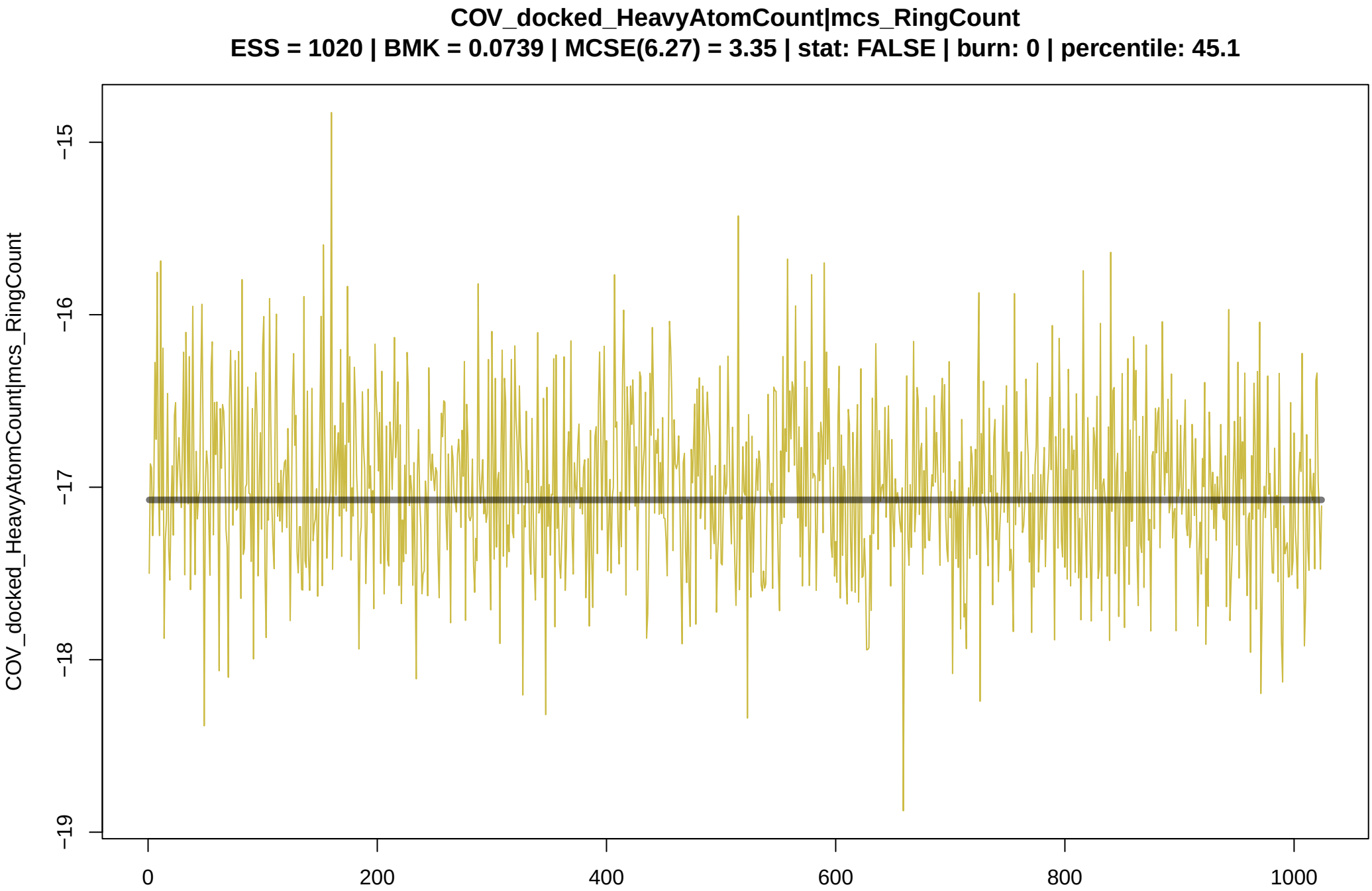

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0554 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | percentile: 64.9
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−6.5
−7.0
−7.5
−8.0
−8.5
0
200
400
600
800
1000

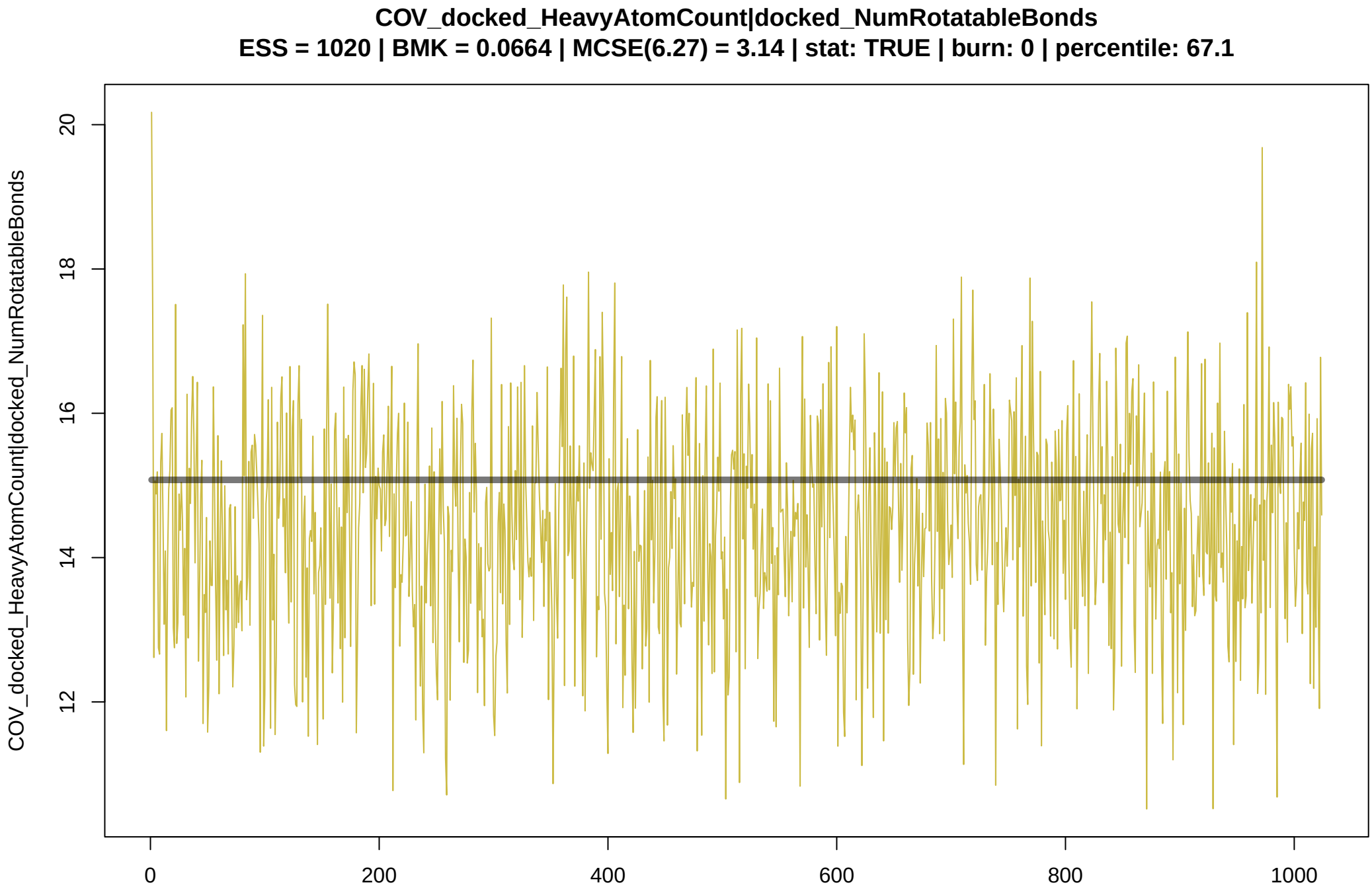

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 933 | BMK = 0.0632 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | percentile: 15.7
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−14
−15
−16
−17
0
200
400
600
800
1000

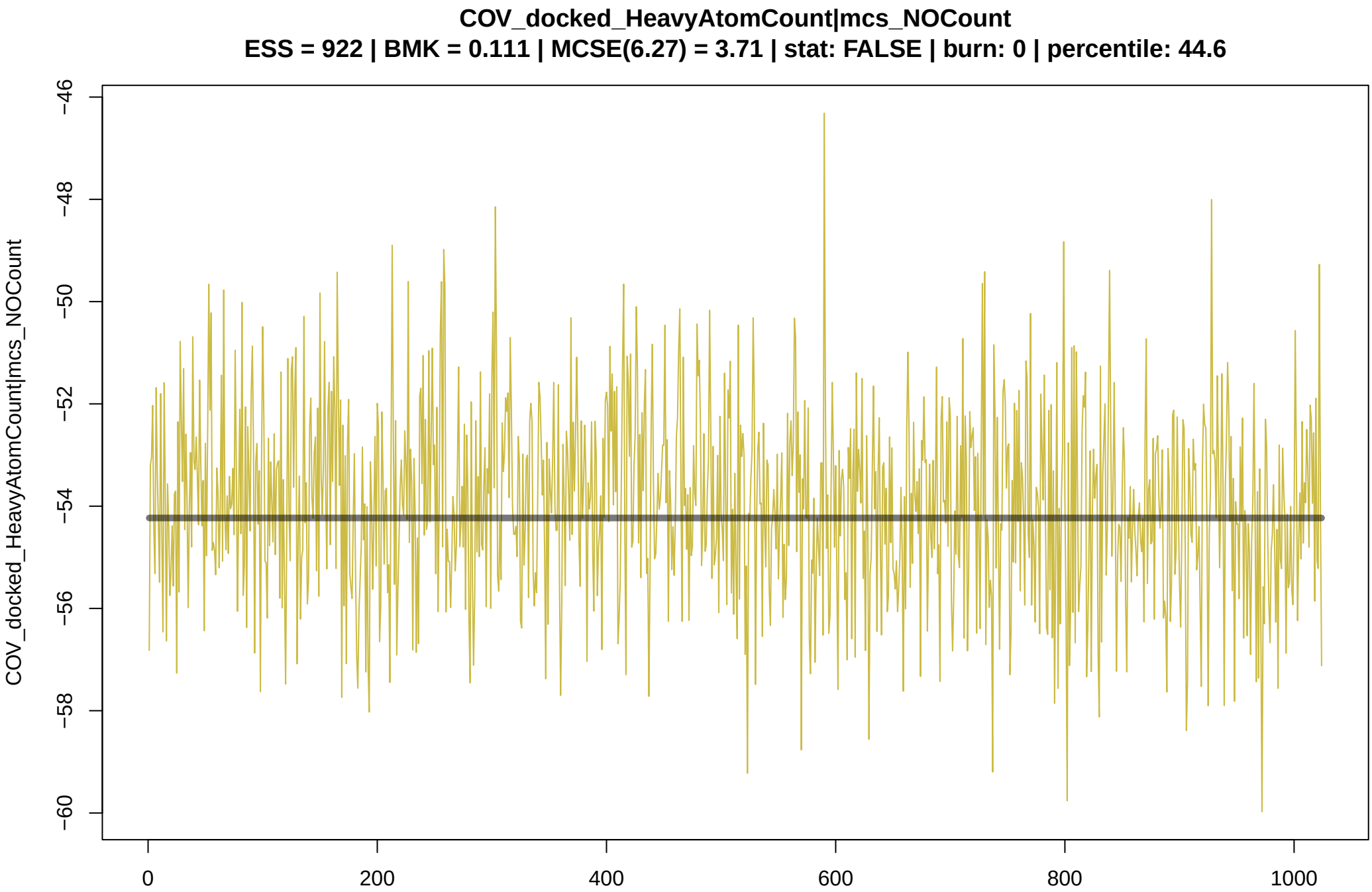

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 71.4 | BMK = 0.178 | MCSE(6.27) = 7.52 | stat: FALSE | burn: 0 | percentile: 10.7
COV_mcs_NumHeteroAtoms|mcs_RingCount
1.0
1.2
1.4
1.6
1.8
0
200
400
600
800
1000

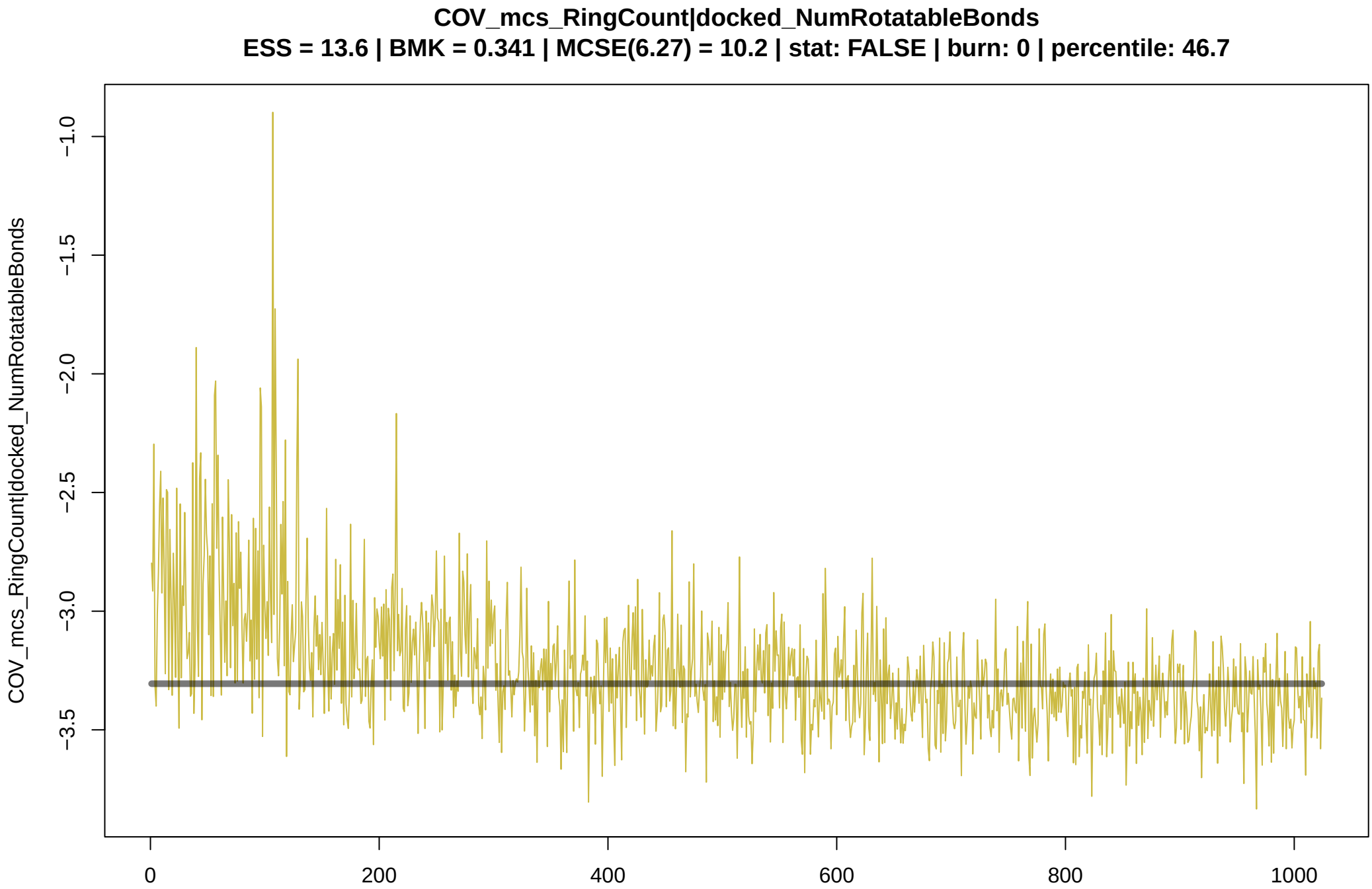

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 125 | BMK = 0.246 | MCSE(6.27) = 6.96 | stat: FALSE | burn: 0 | percentile: 33
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−0.5
−1.0
−1.5
−2.0
0
200
400
600
800
1000

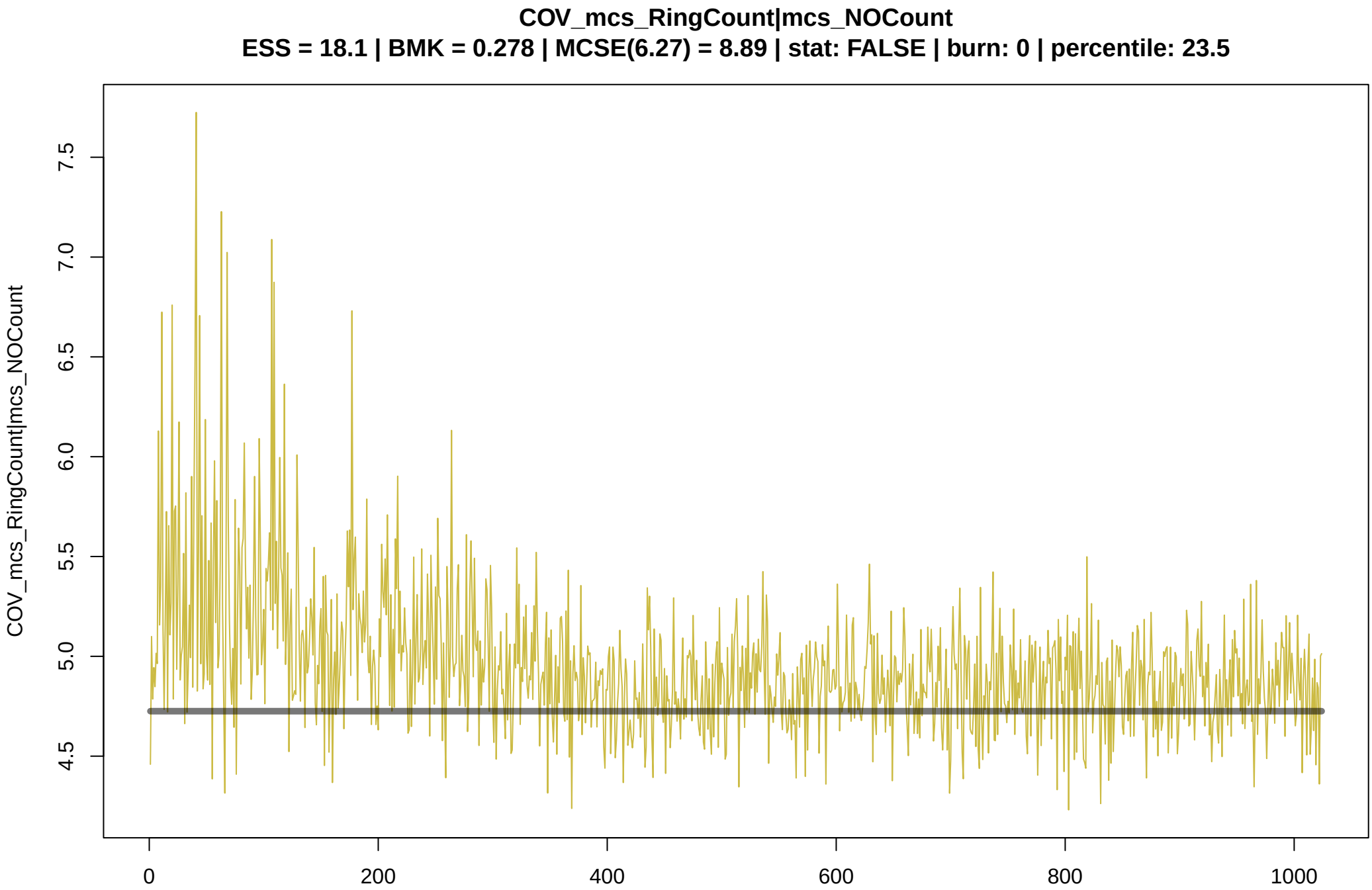

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 123 | BMK = 0.196 | MCSE(6.27) = 6.75 | stat: FALSE | burn: 0 | percentile: 18.6
COV_mcs_NumHeteroAtoms|mcs_NOCount
4.0
4.5
5.0
5.5
6.0
0
200
400
600
800
1000

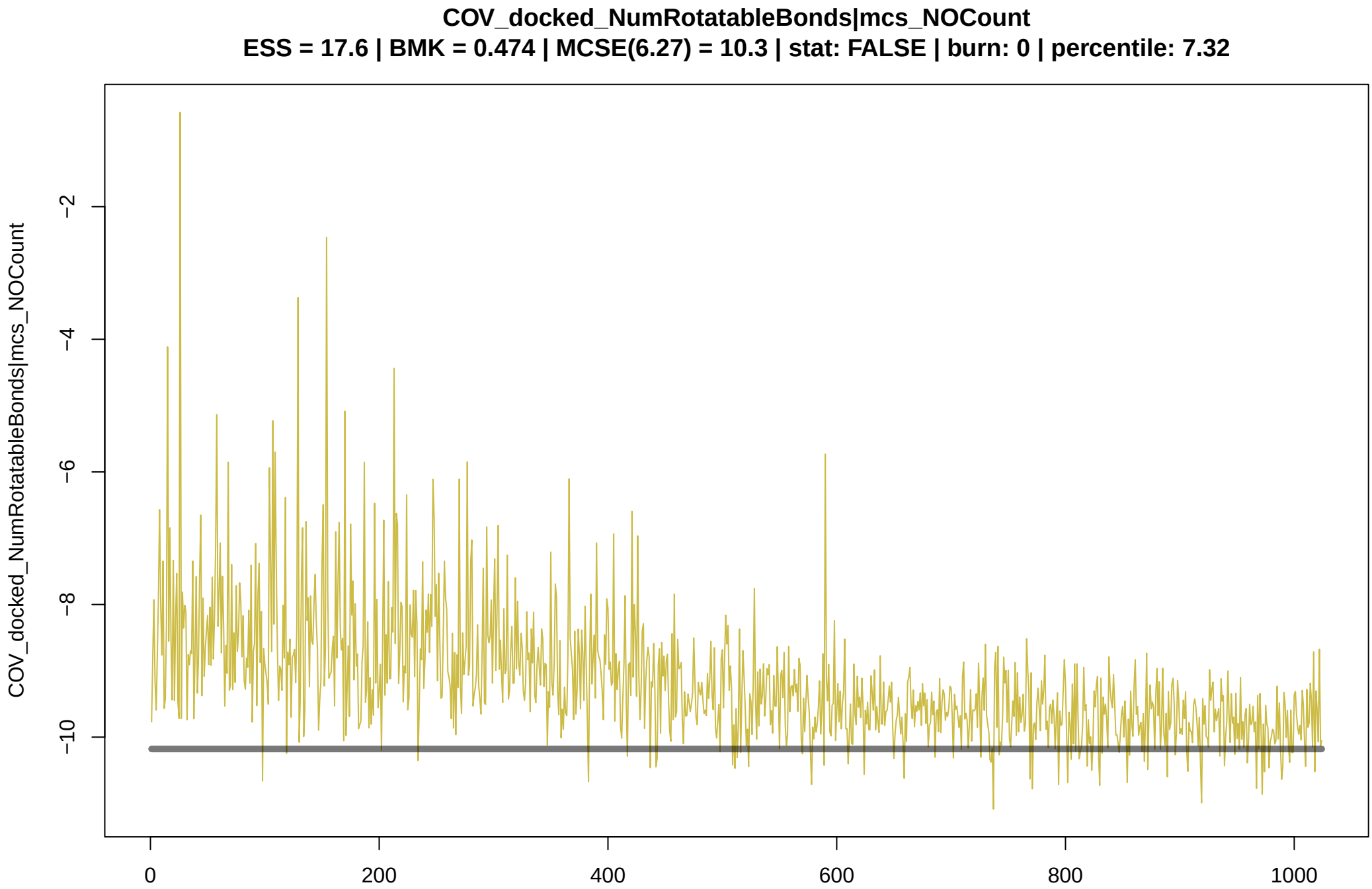

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0739 | MCSE(6.27) = 3.35 | stat: FALSE | burn: 0 | percentile: 45.1
COV_docked_HeavyAtomCount|mcs_RingCount
−15
−16
−17
−18
−19
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0664 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | percentile: 67.1
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
12
14
16
18
20
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 922 | BMK = 0.111 | MCSE(6.27) = 3.71 | stat: FALSE | burn: 0 | percentile: 44.6
COV_docked_HeavyAtomCount|mcs_NOCount
−46
−48
−50
−52
−54
−56
−58
−60
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 13.6 | BMK = 0.341 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 0 | percentile: 46.7
COV_mcs_RingCount|docked_NumRotatableBonds
−1.0
−1.5
−2.0
−2.5
−3.0
−3.5
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 18.1 | BMK = 0.278 | MCSE(6.27) = 8.89 | stat: FALSE | burn: 0 | percentile: 23.5
COV_mcs_RingCount|mcs_NOCount
4.5
5.0
5.5
6.0
6.5
7.0
7.5
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 17.6 | BMK = 0.474 | MCSE(6.27) = 10.3 | stat: FALSE | burn: 0 | percentile: 7.32
COV_docked_NumRotatableBonds|mcs_NOCount
−2
−4
−6
−8
−10
0
200
400
600
800
1000