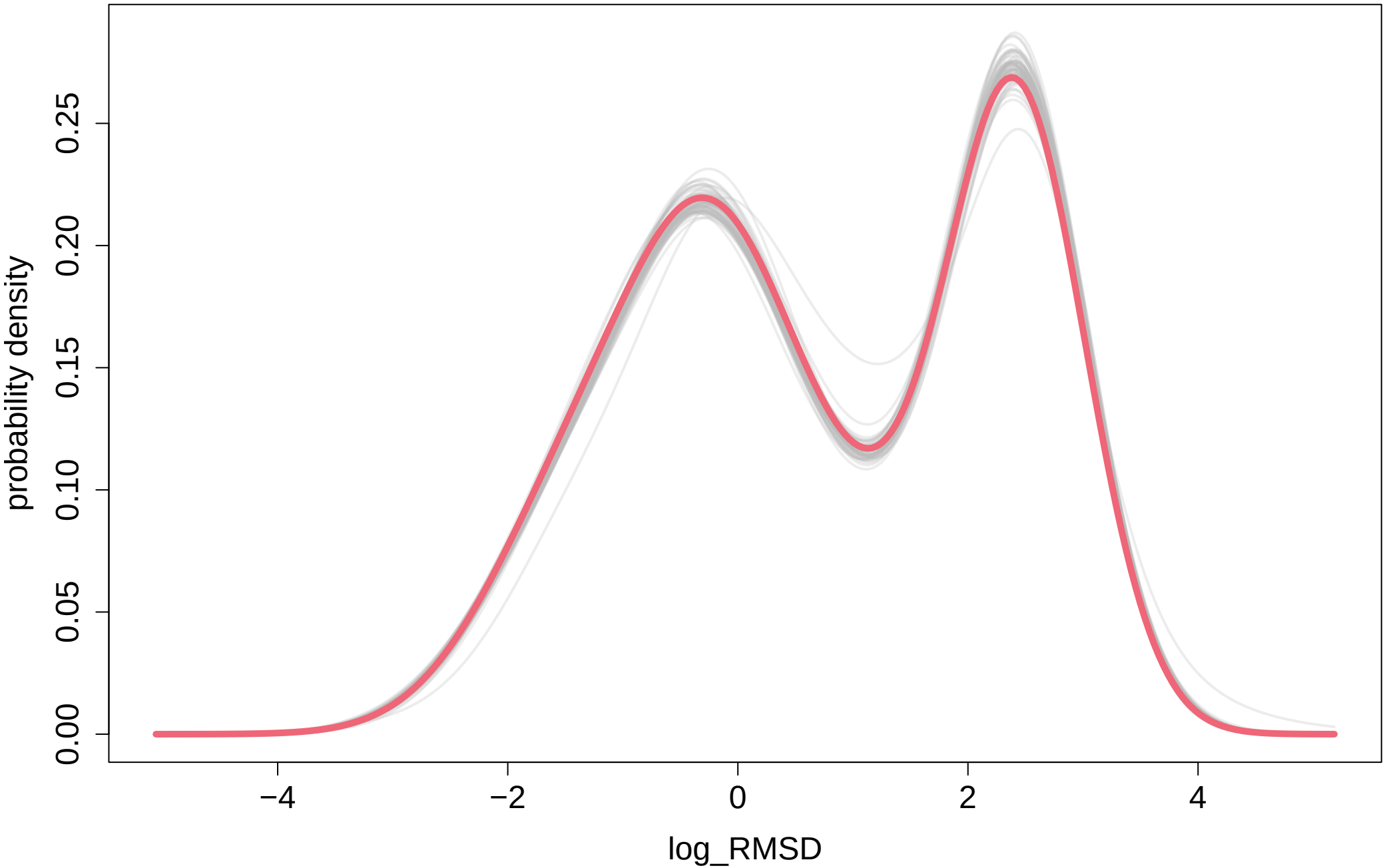
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 1
max MCSE = 14.3427173187412
all stationary: FALSE
burn: 1020
min percent.: 0

−− STATS 2D −−
min ESS = 849.861302935628
max BMK = 0.086346644542095
max MCSE = 4.35055481808116
all stationary: FALSE
burn: 0
min percent.: 0.78125

−− STATS 1D −−
min ESS = 2.2044604925031e−16
max BMK = 0.617285837943499
max MCSE = NaN
all stationary: FALSE
burn: 102
min percent.: 0

Occupied clusters: 11 of 64
LL: −125000 +− 332


probability density
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0.15
0.20
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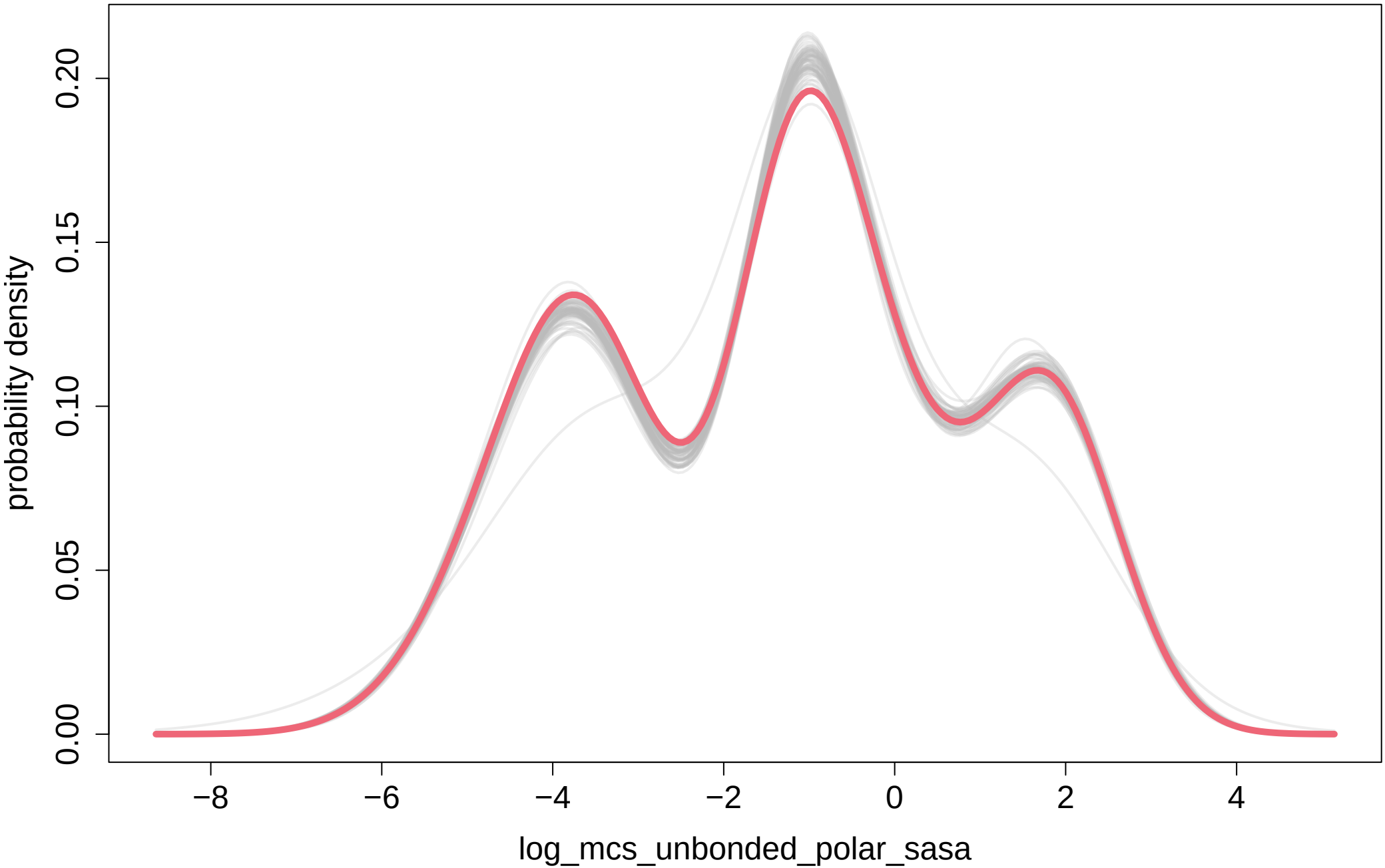
−4
−2
0
2
4
log_RMSD


probability density
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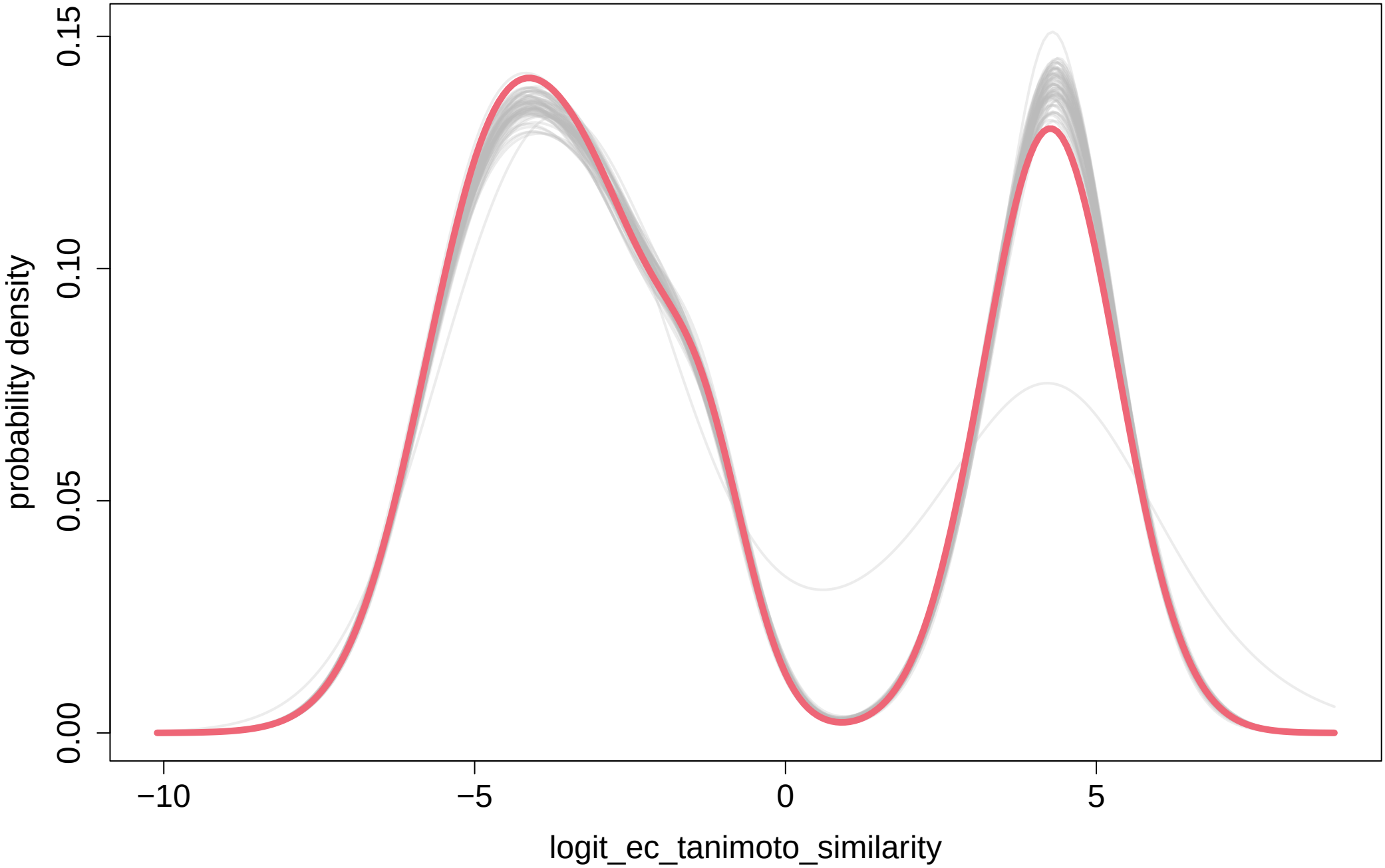
2
4
log_mcs_unbonded_polar_sasa


probability density
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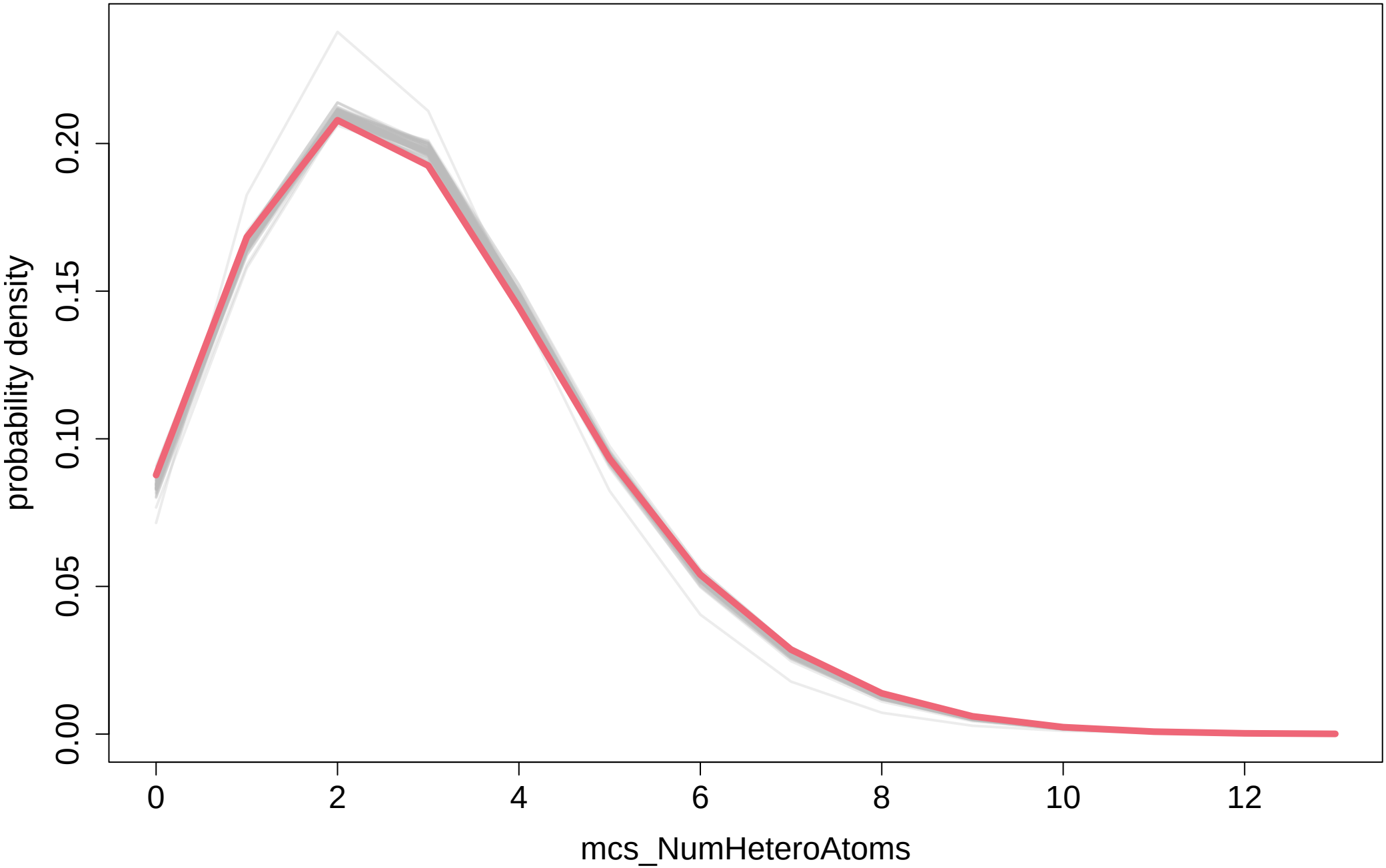
5
logit_ec_tanimoto_similarity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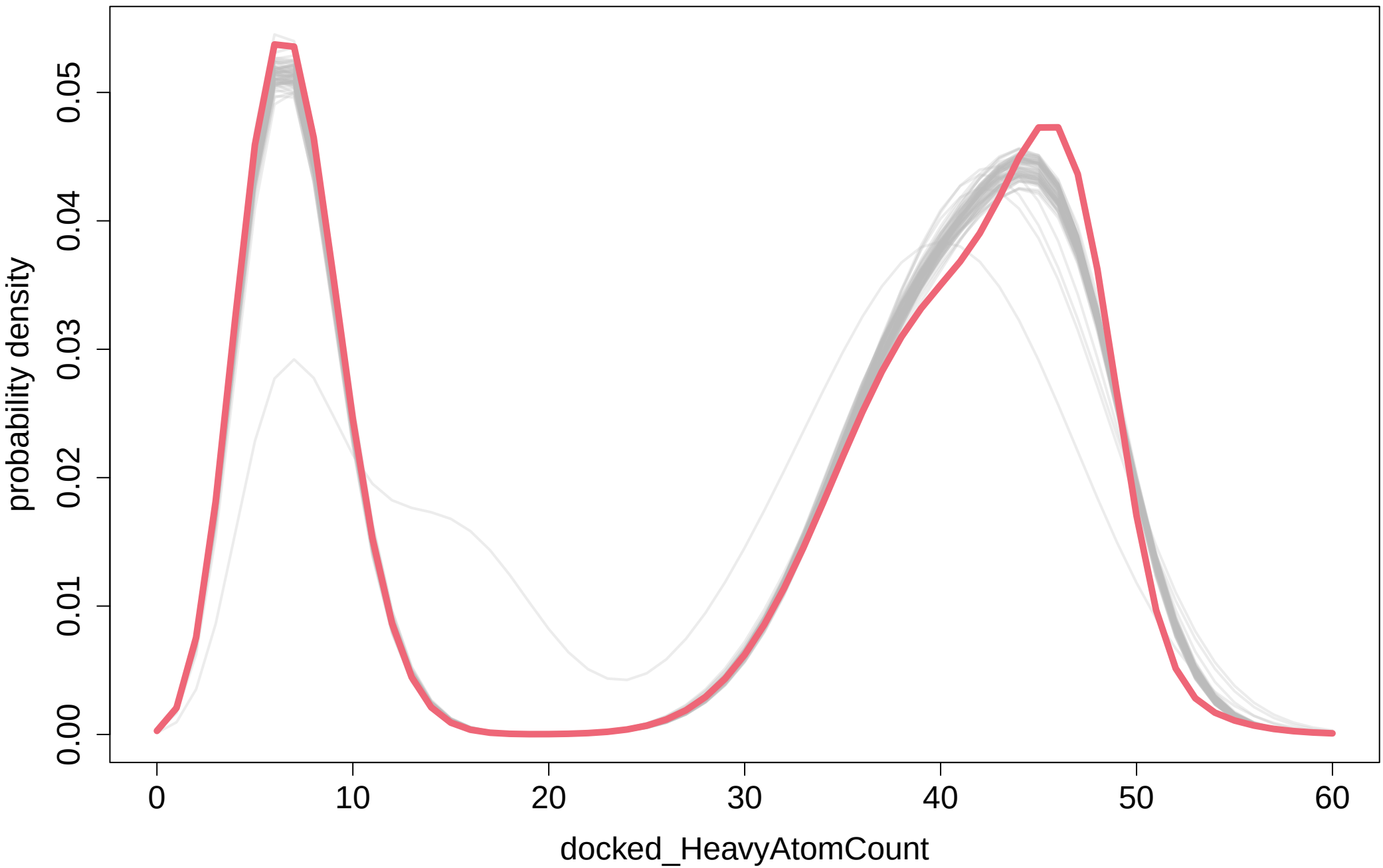
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms


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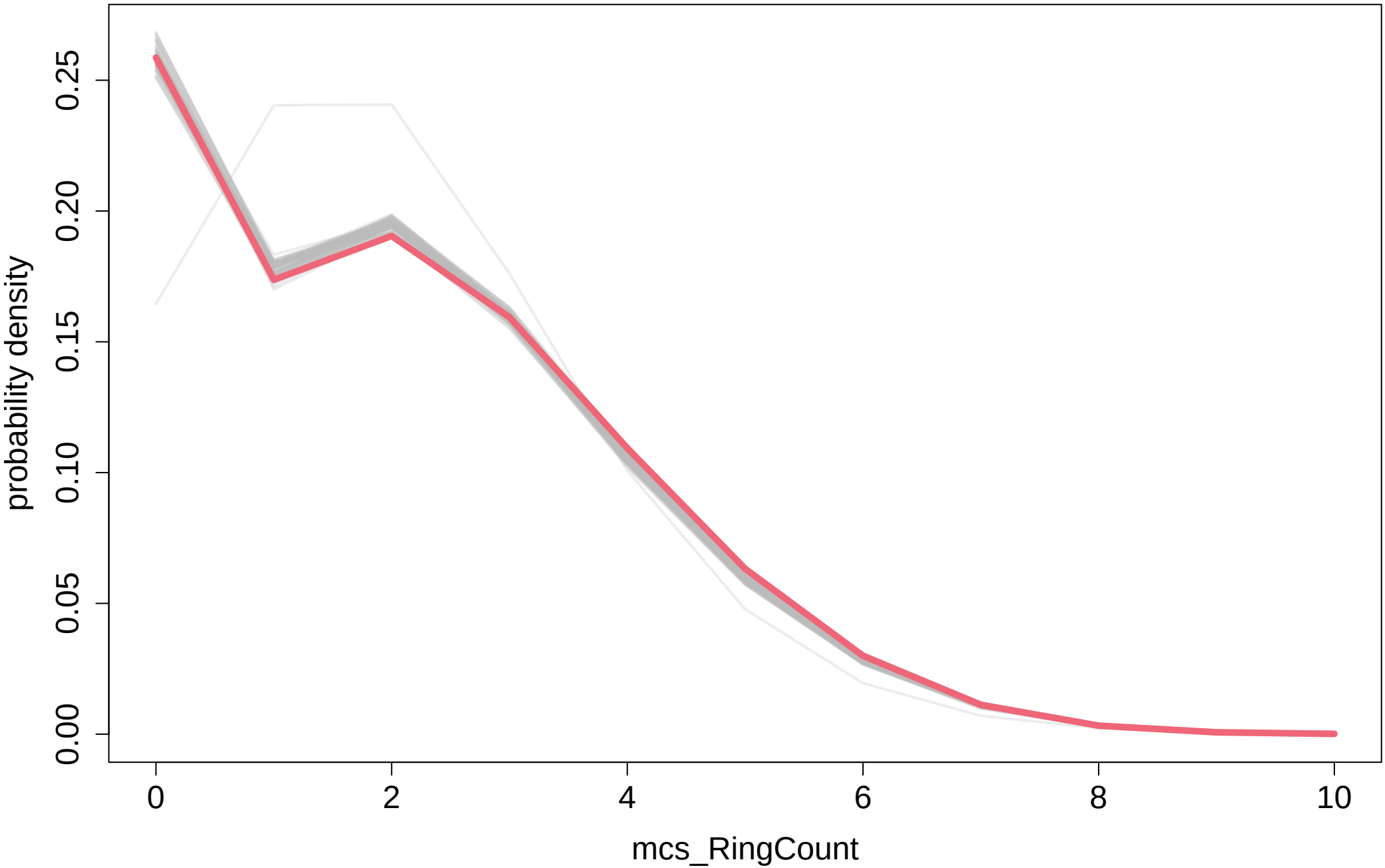
0.03
0.04
0.05
0
10
20
30
40
50
60
docked_HeavyAtomCount


probability density
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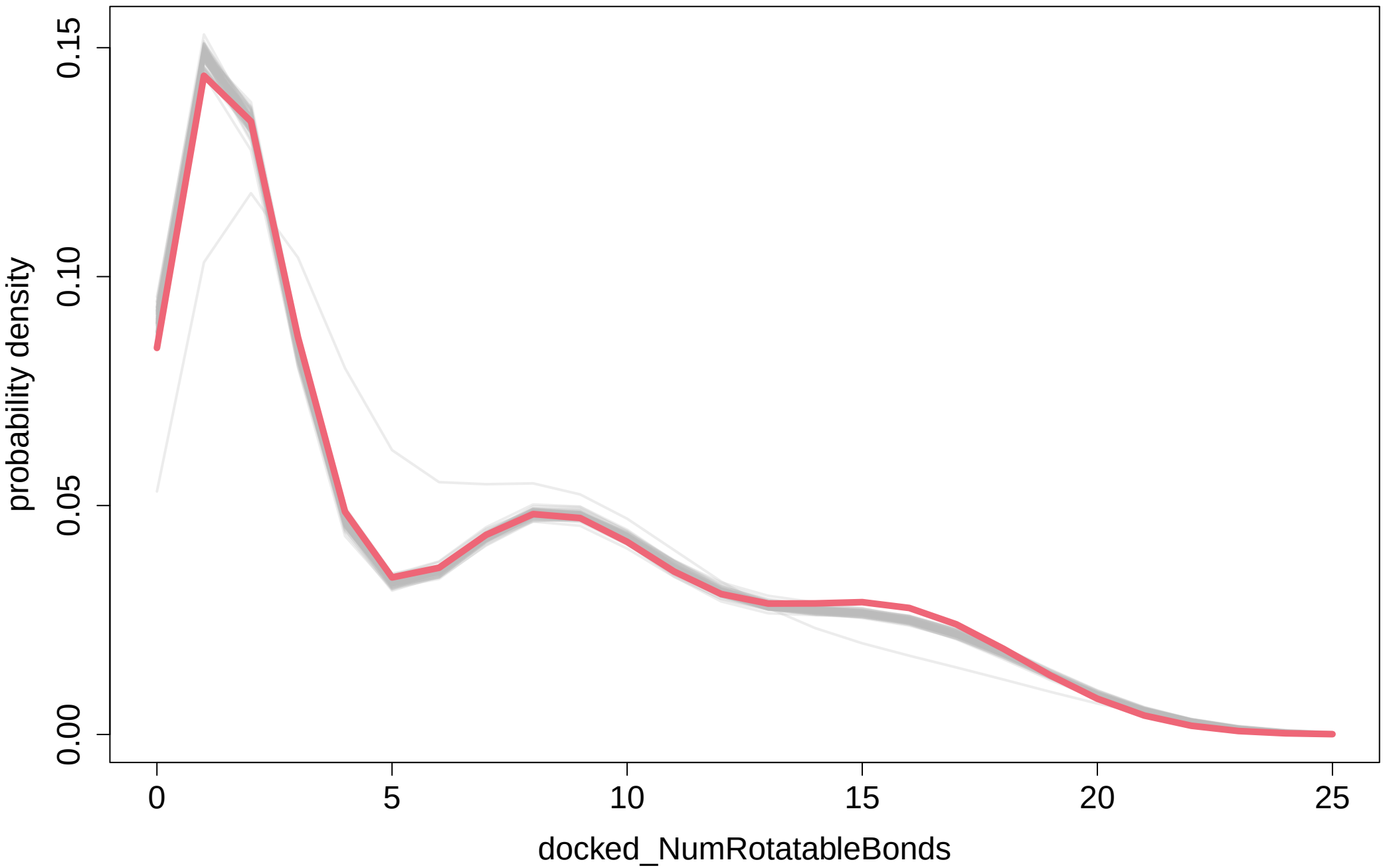
0
2
4
6
8
10
mcs_RingCount


probability density
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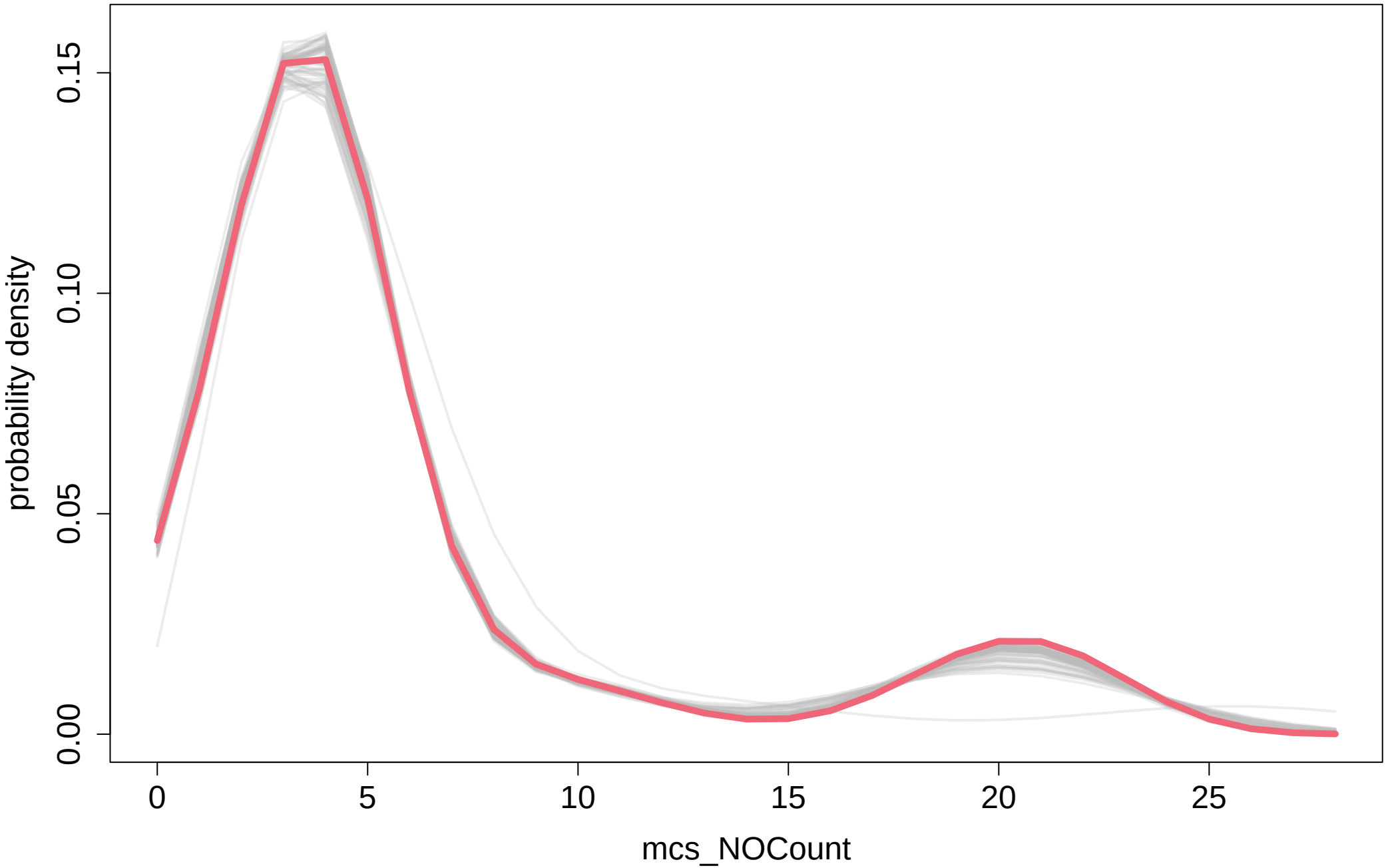
0.15
0
5
10
15
20
25
docked_NumRotatableBonds


probability density
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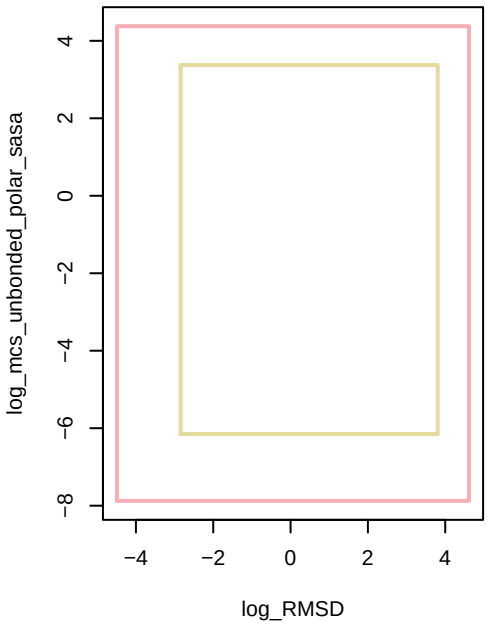
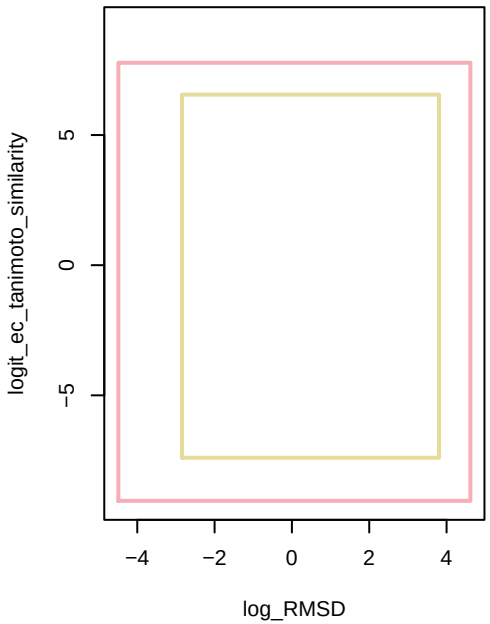
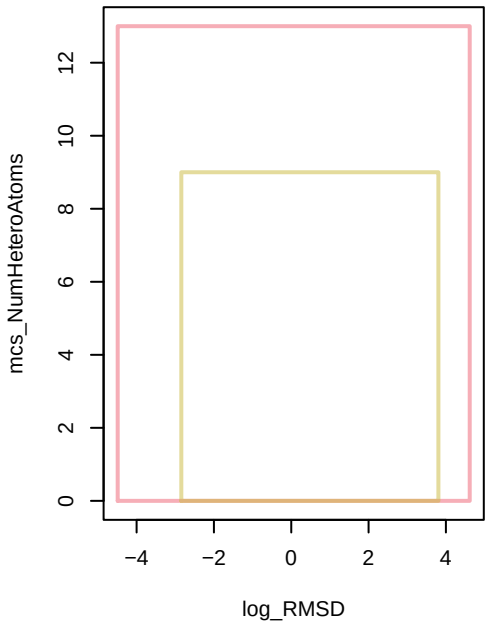
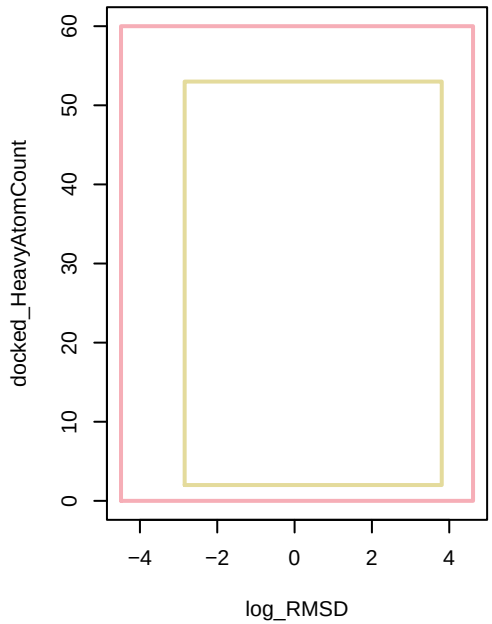
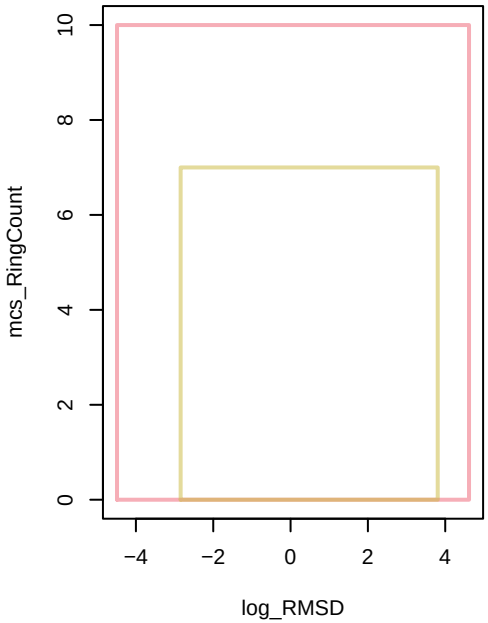
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

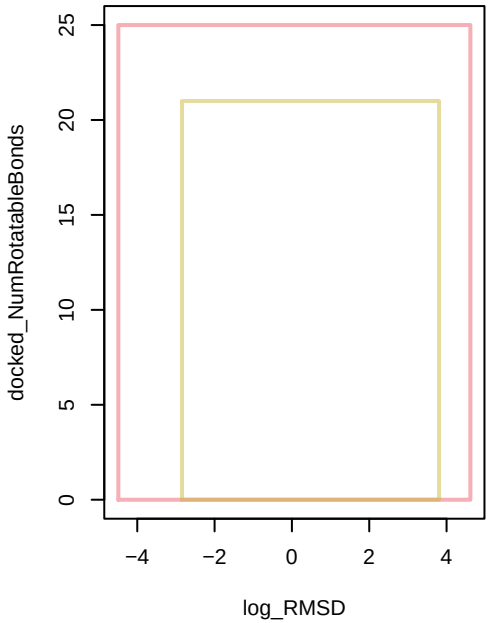

log_mcs_unbonded_polar_sasa
log_RMSD

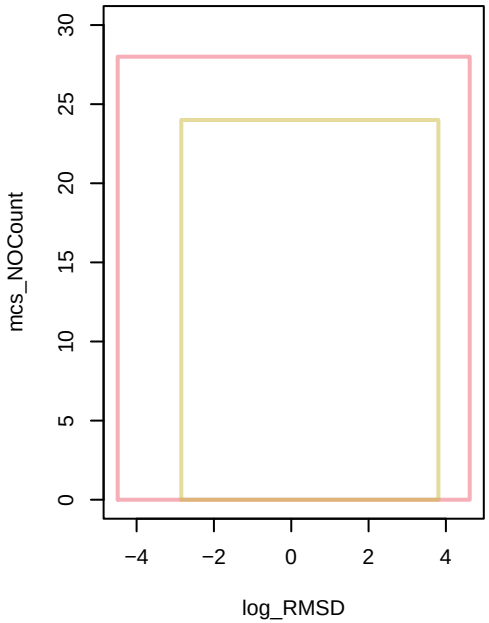

logit_ec_tanimoto_similarity
log_RMSD

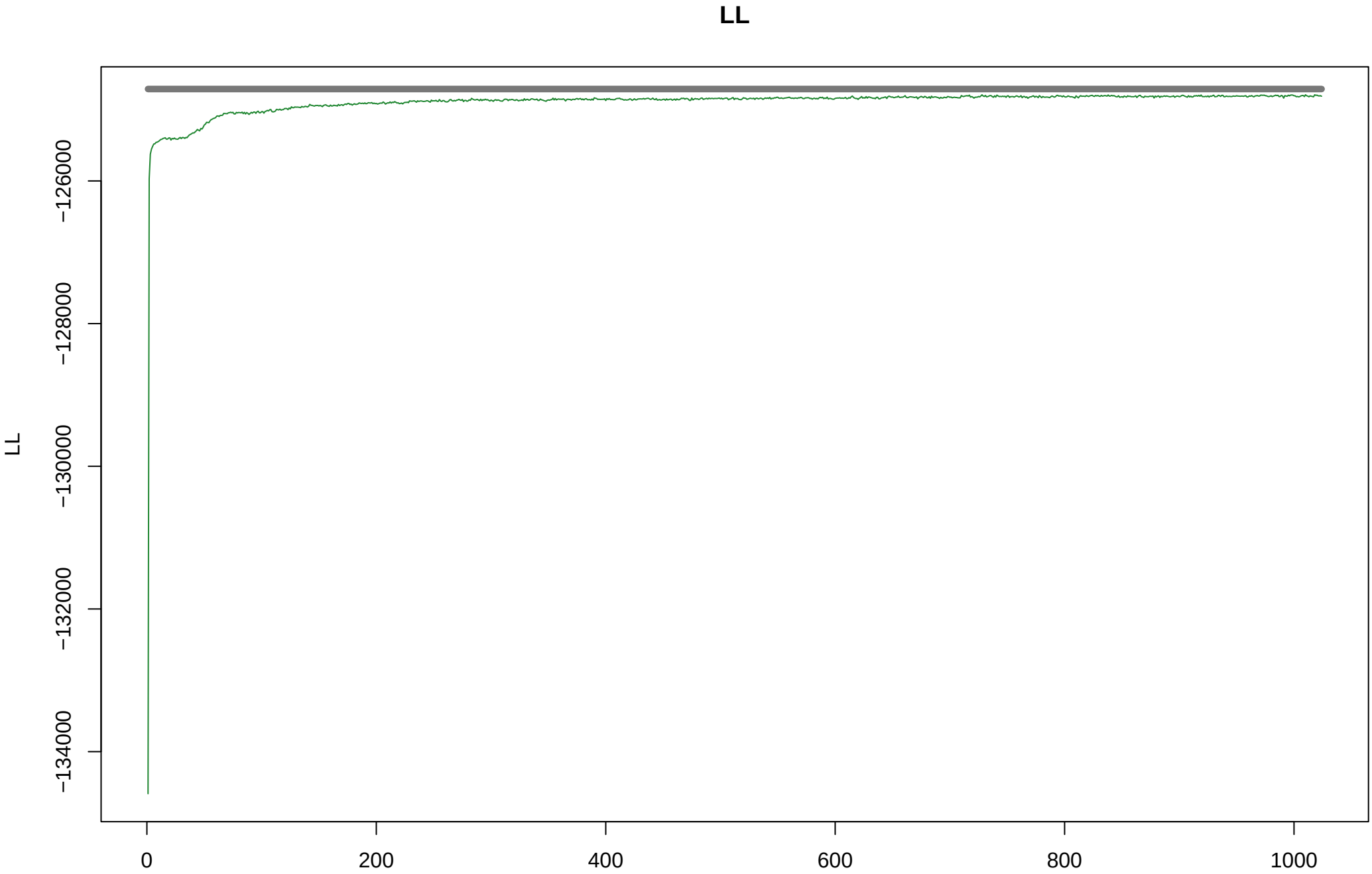

mcs_NumHeteroAtoms
log_RMSD

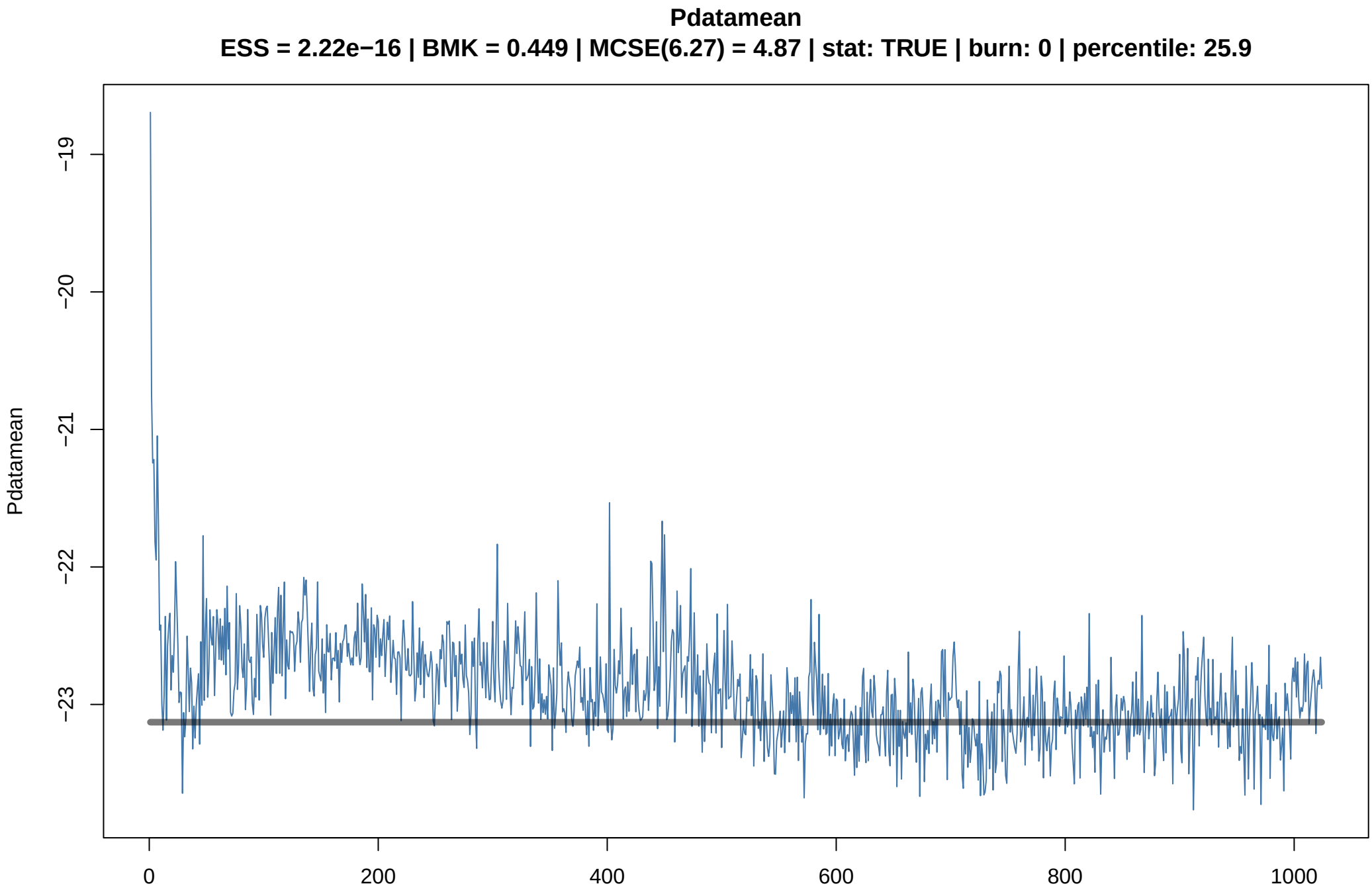

docked_HeavyAtomCount
log_RMSD

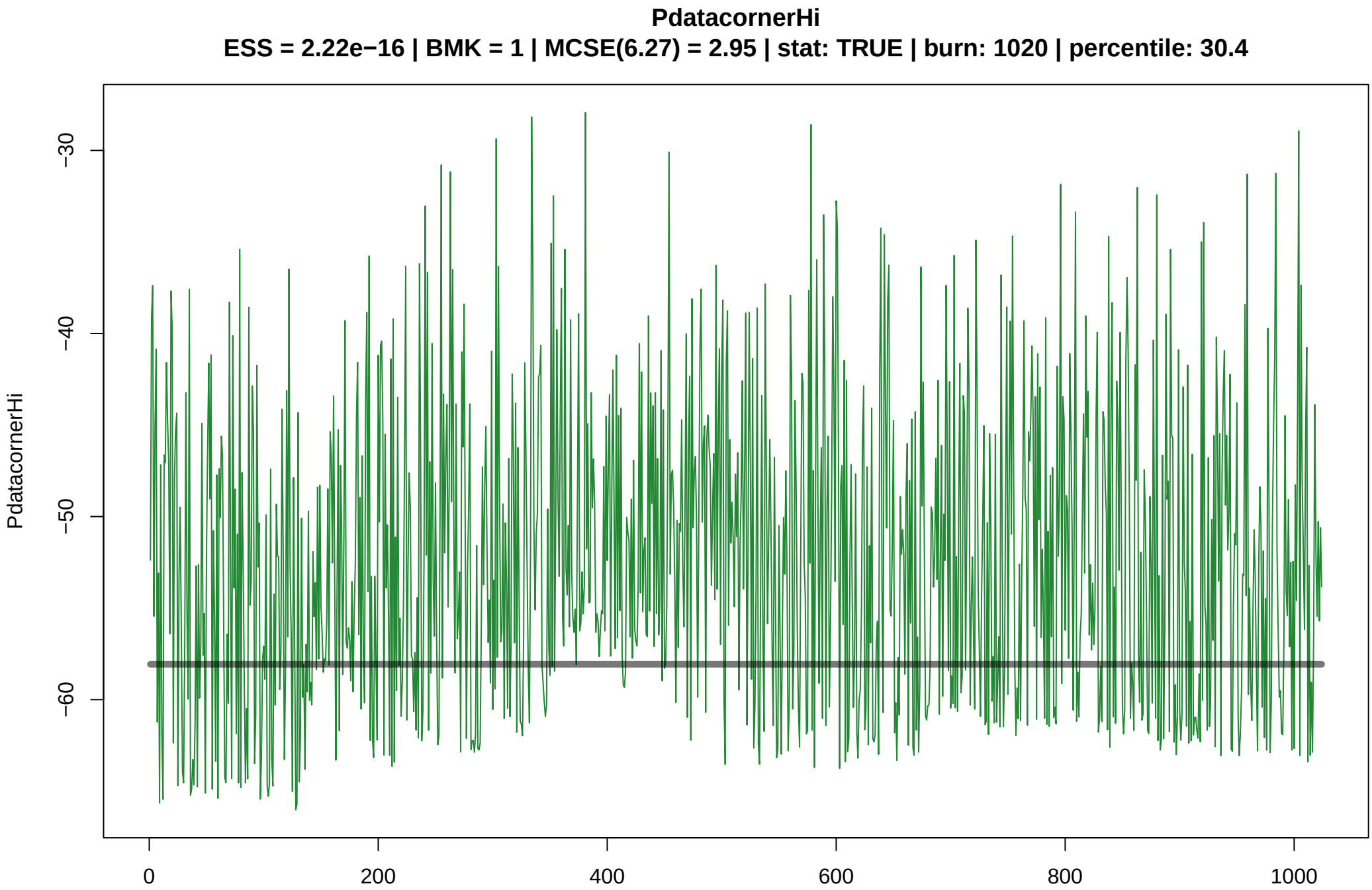

mcs_RingCount
log_RMSD

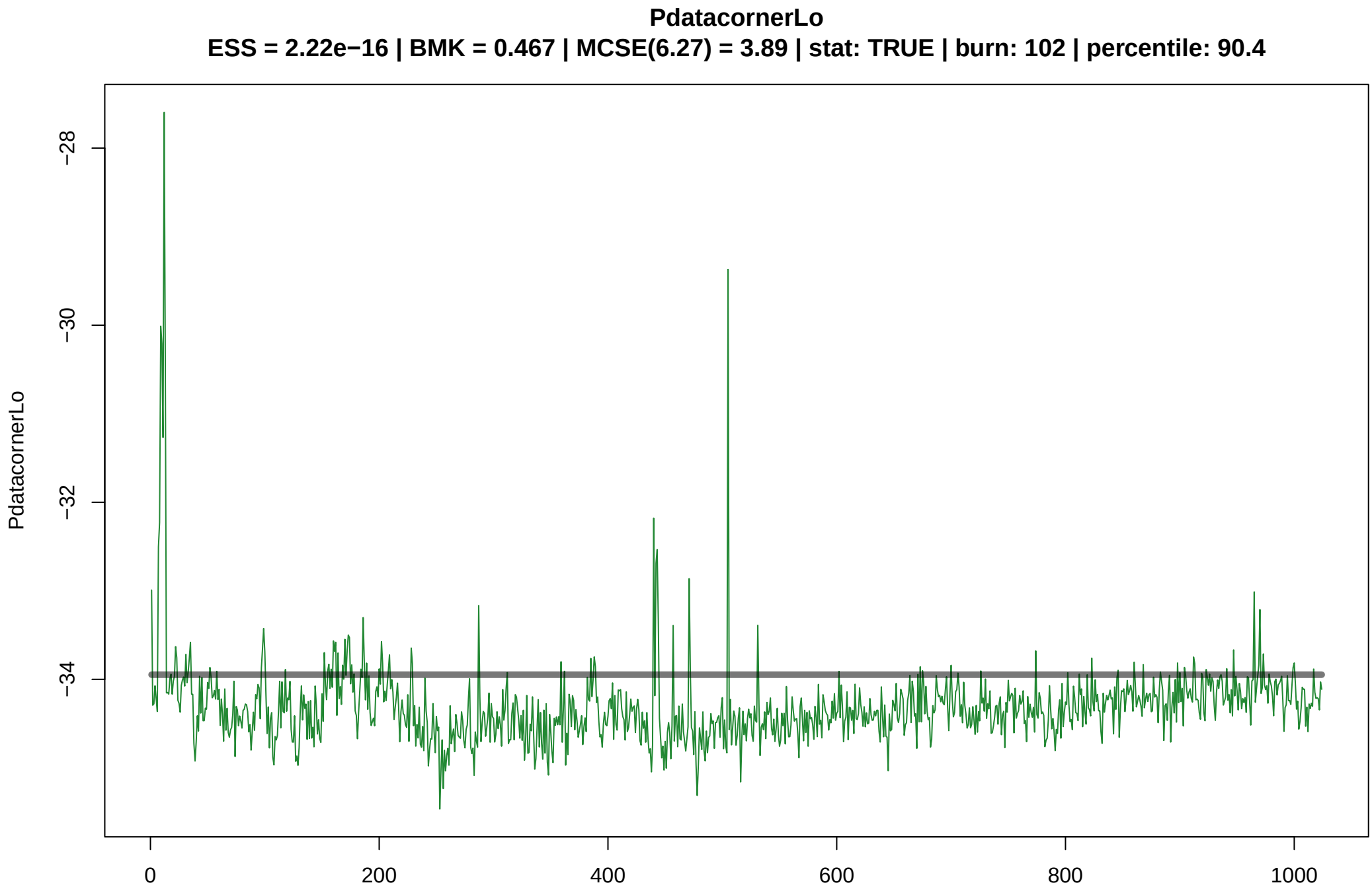

docked_NumRotatableBonds
log_RMSD

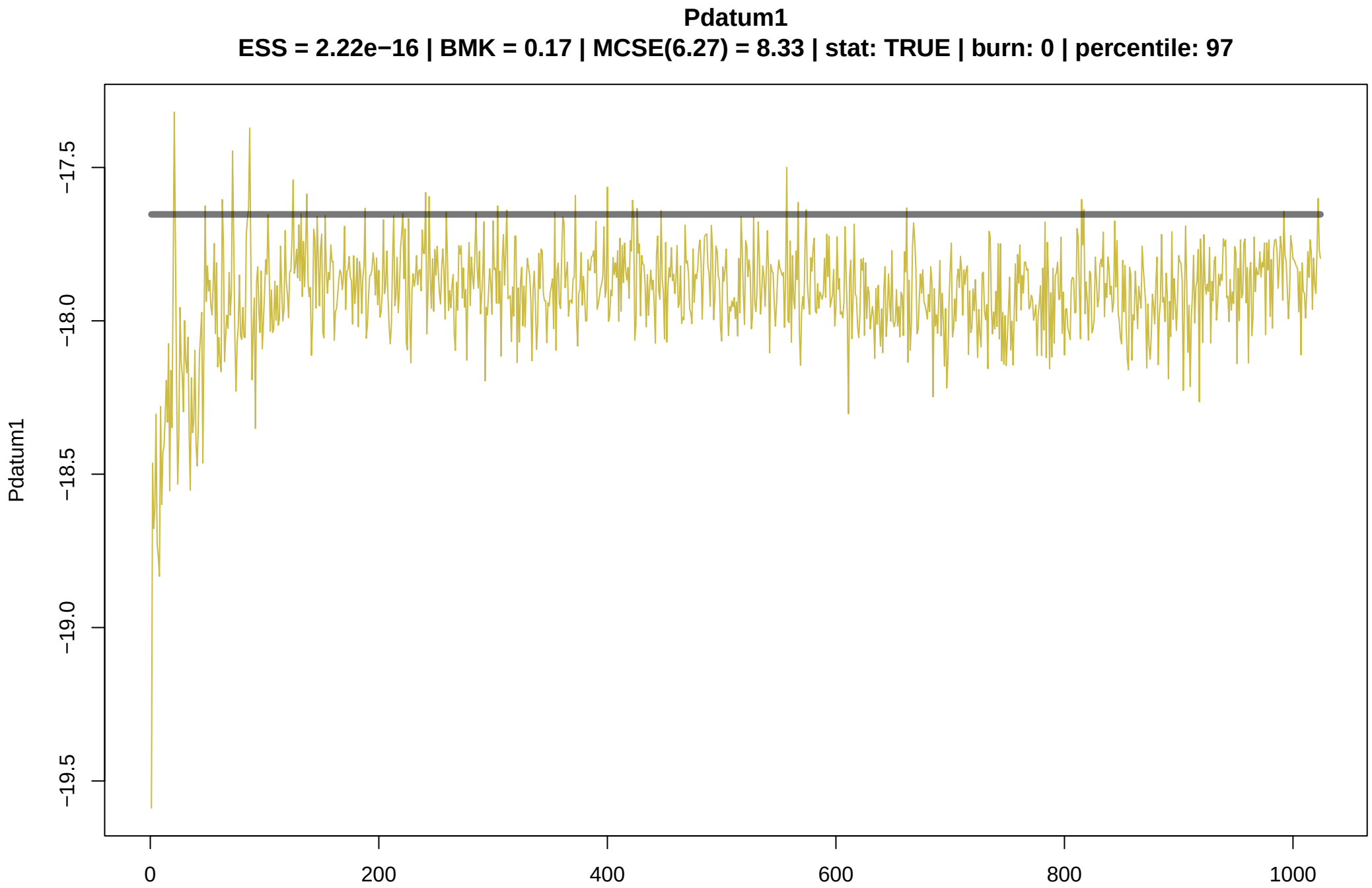

mcs_NOCount
log_RMSD

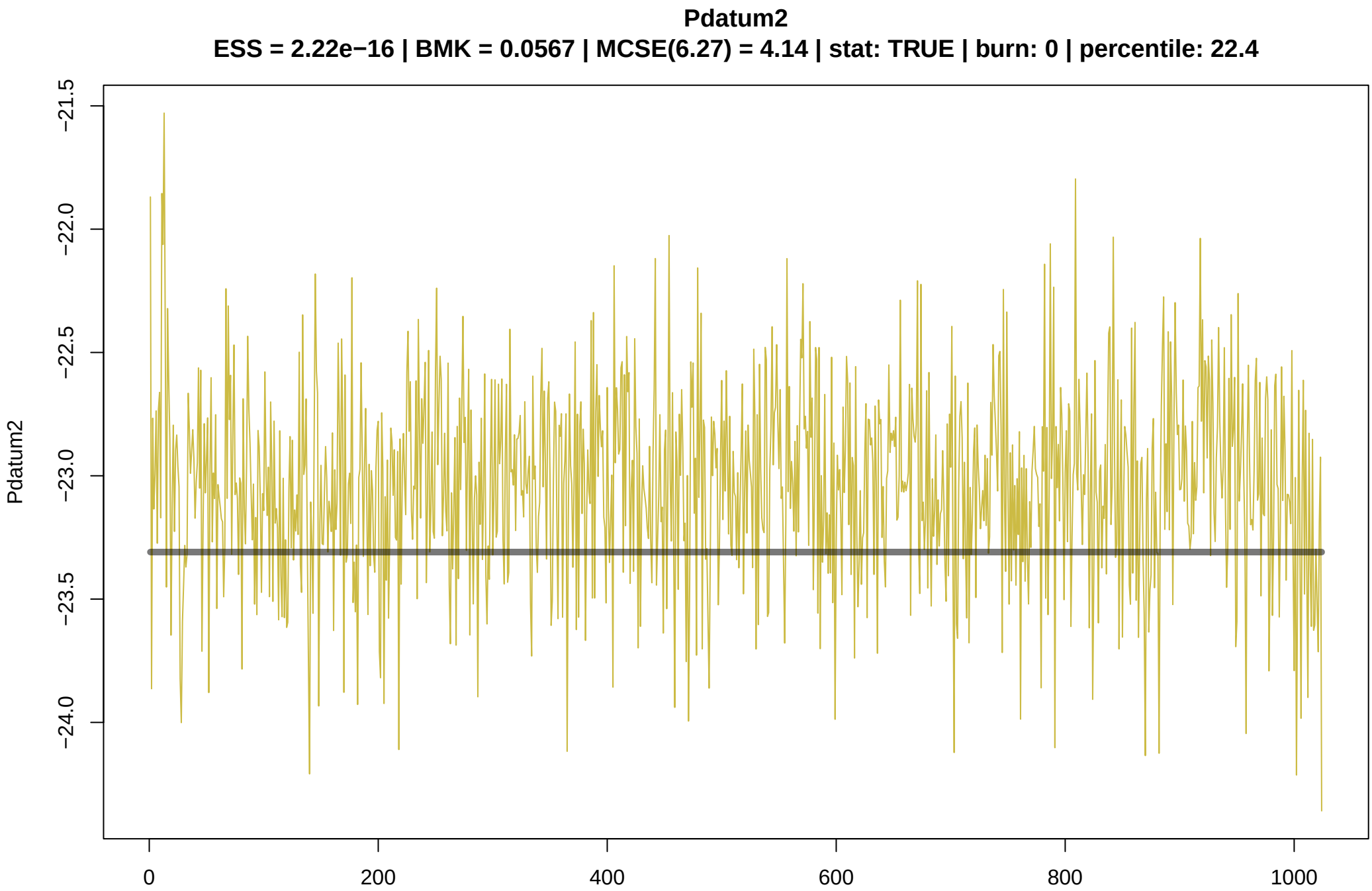

LL
LL
−126000
−128000
−130000
−132000
−134000
0
200
400
600
800
1000

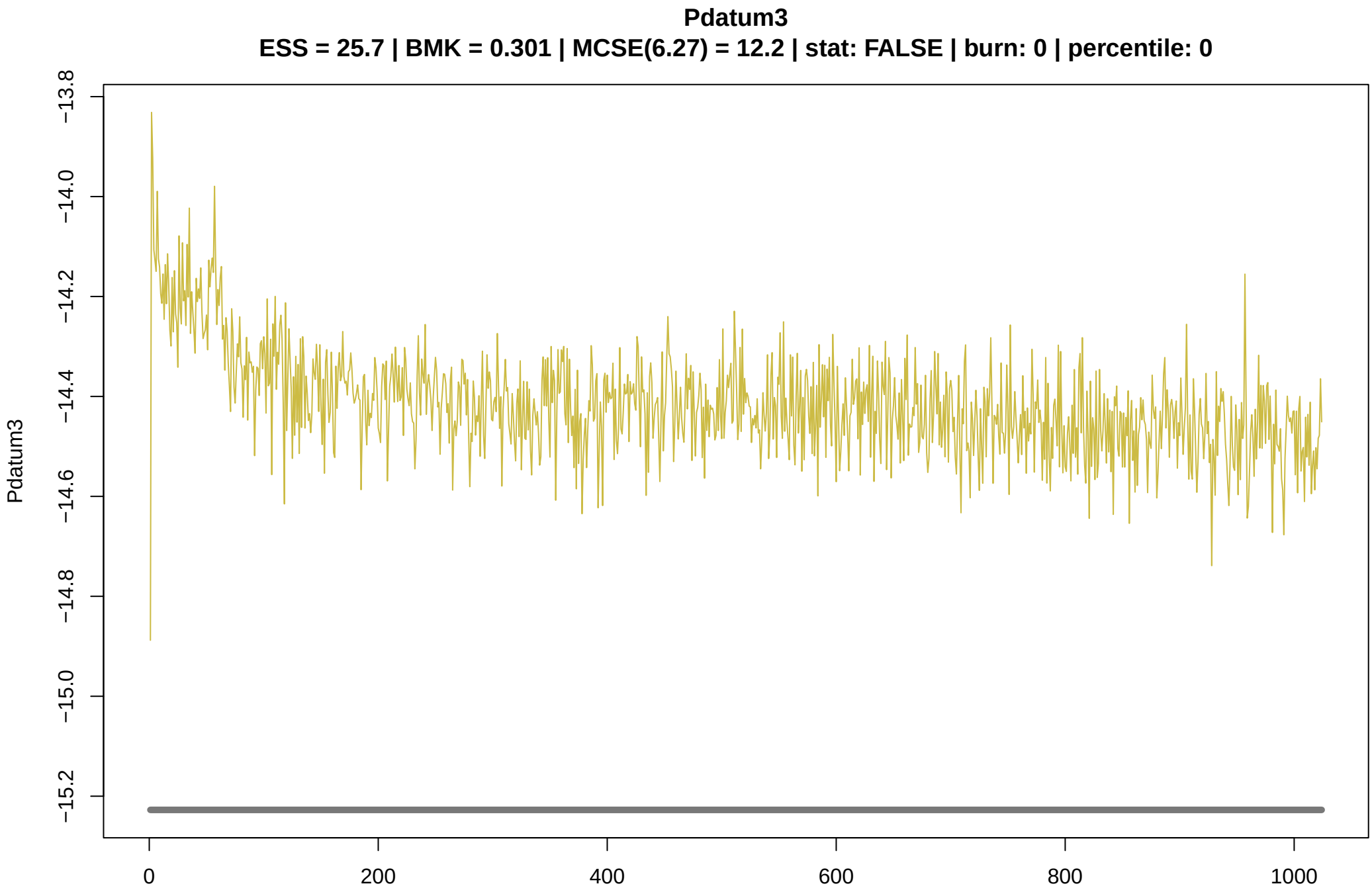

Pdatamean
ESS = 2.22e−16 | BMK = 0.449 | MCSE(6.27) = 4.87 | stat: TRUE | burn: 0 | percentile: 25.9
Pdatamean
−19
−20
−21
−22
−23
0
200
400
600
800
1000

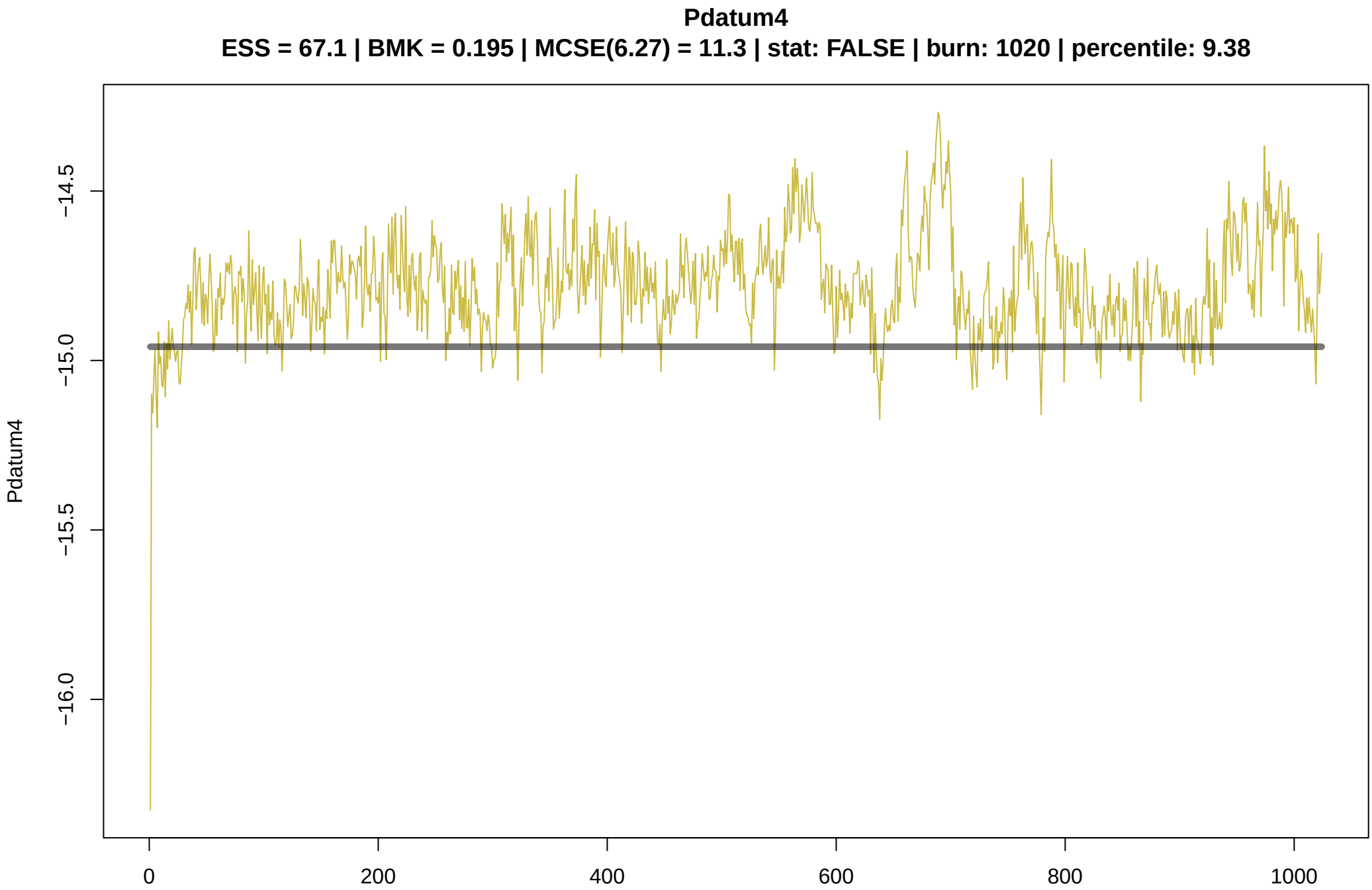

PdatacornerHi
ESS = 2.22e−16 | BMK = 1 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 1020 | percentile: 30.4
PdatacornerHi
−30
−40
−50
−60
0
200
400
600
800
1000

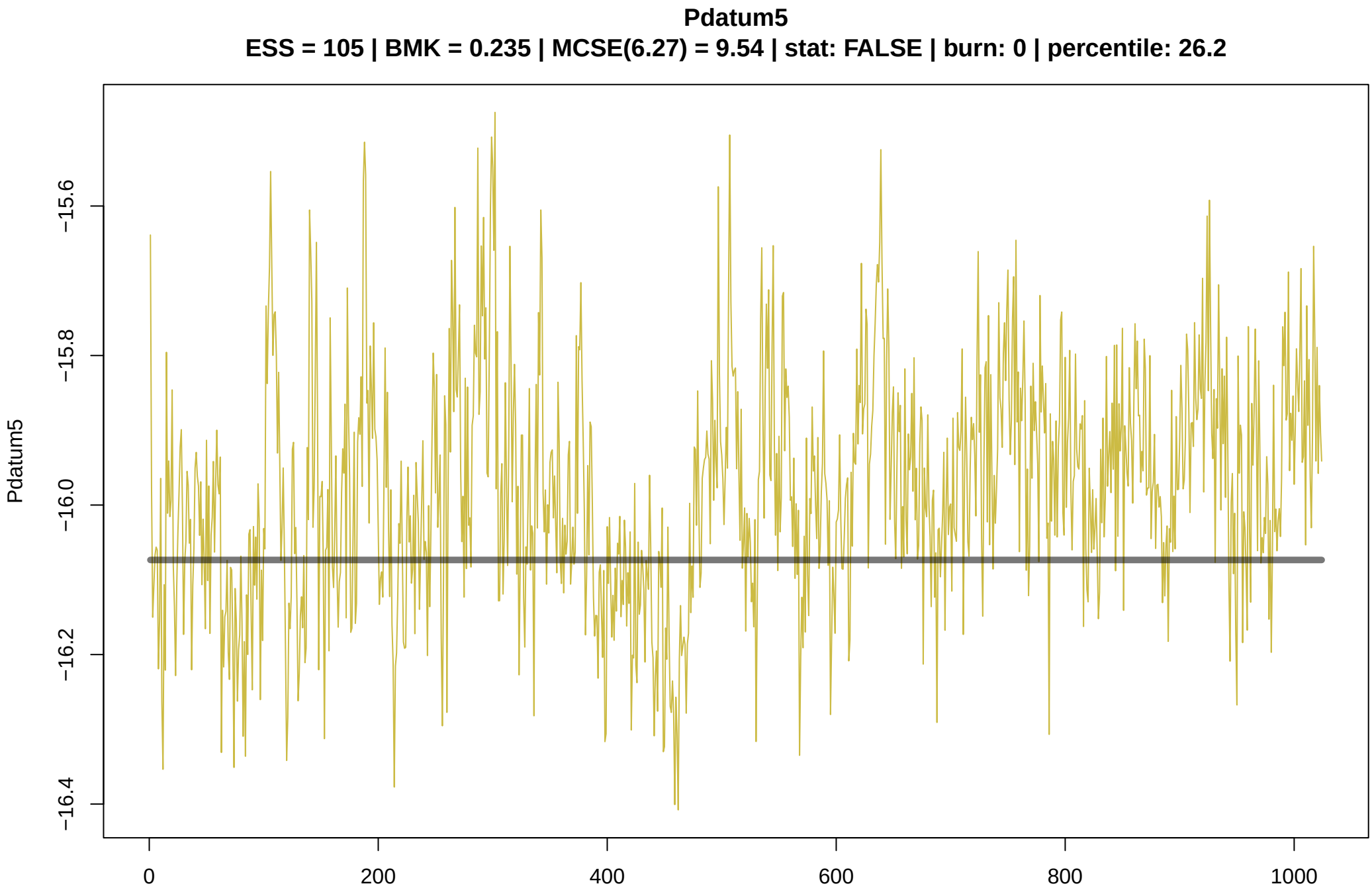

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.467 | MCSE(6.27) = 3.89 | stat: TRUE | burn: 102 | percentile: 90.4
PdatacornerLo
−28
−30
−32
−34
0
200
400
600
800
1000

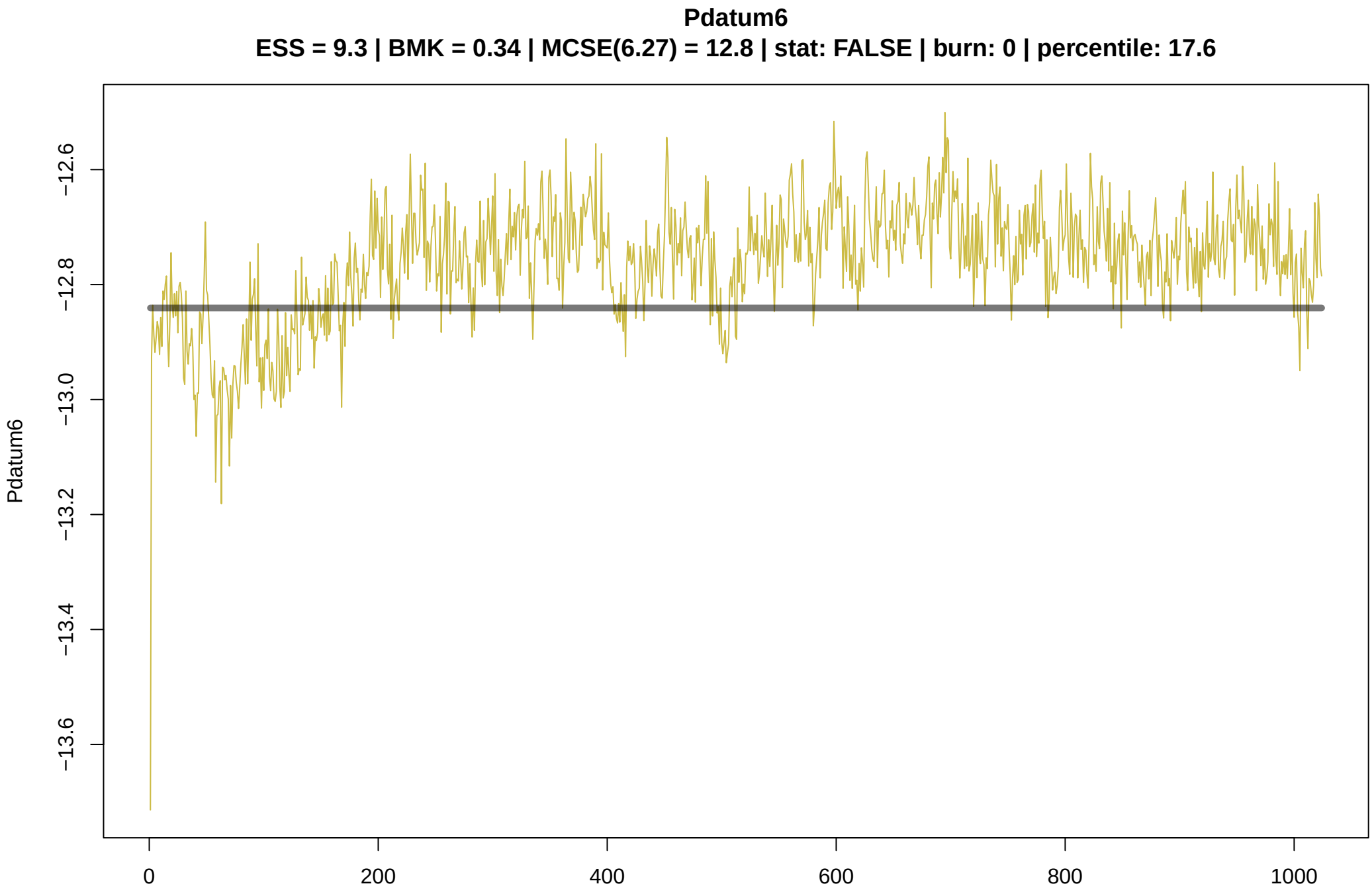

Pdatum1
ESS = 2.22e−16 | BMK = 0.17 | MCSE(6.27) = 8.33 | stat: TRUE | burn: 0 | percentile: 97
Pdatum1
−17.5
−18.0
−18.5
−19.0
−19.5
0
200
400
600
800
1000

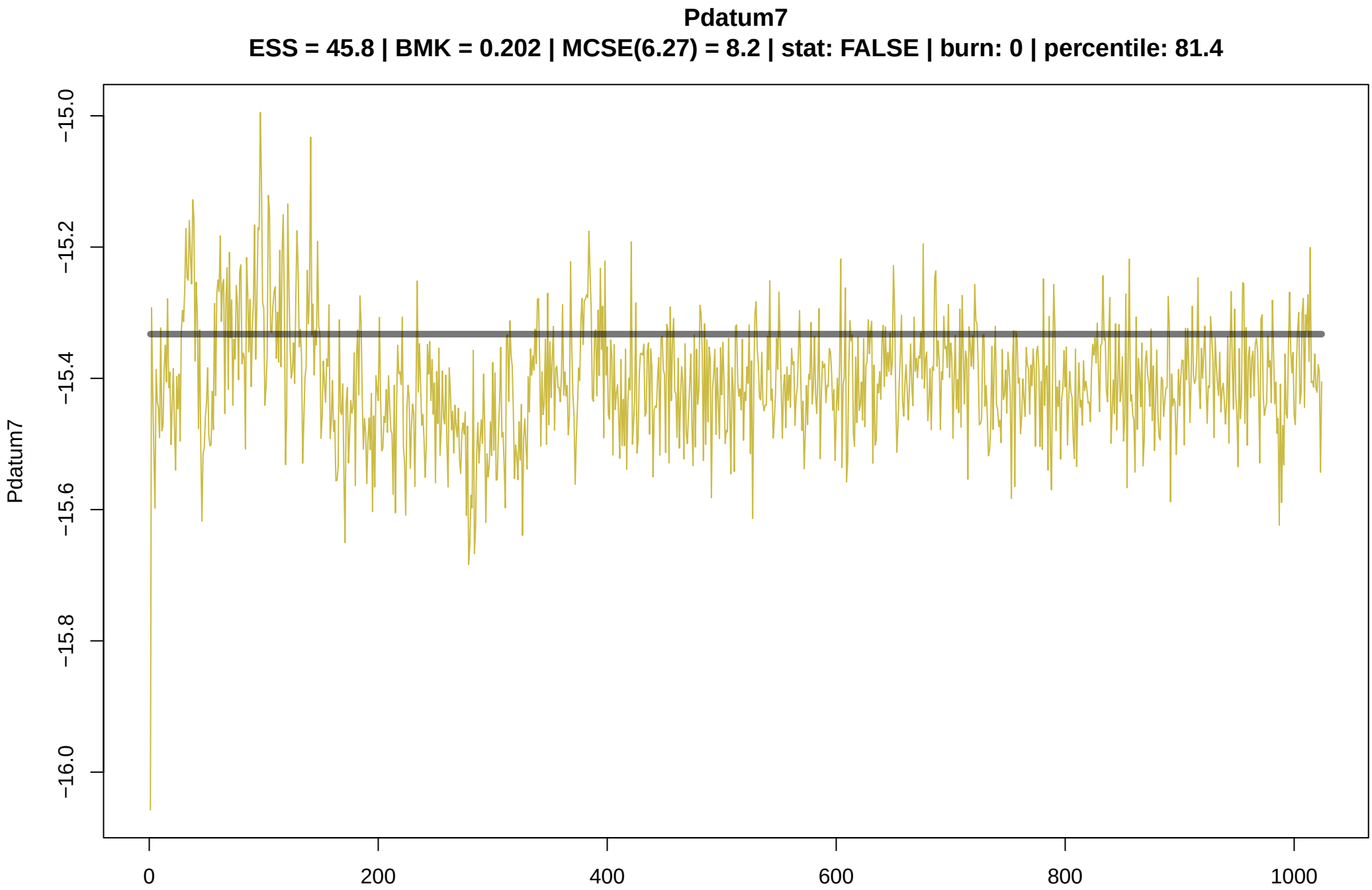

Pdatum2
ESS = 2.22e−16 | BMK = 0.0567 | MCSE(6.27) = 4.14 | stat: TRUE | burn: 0 | percentile: 22.4
Pdatum2
−21.5
−22.0
−22.5
−23.0
−23.5
−24.0
0
200
400
600
800
1000

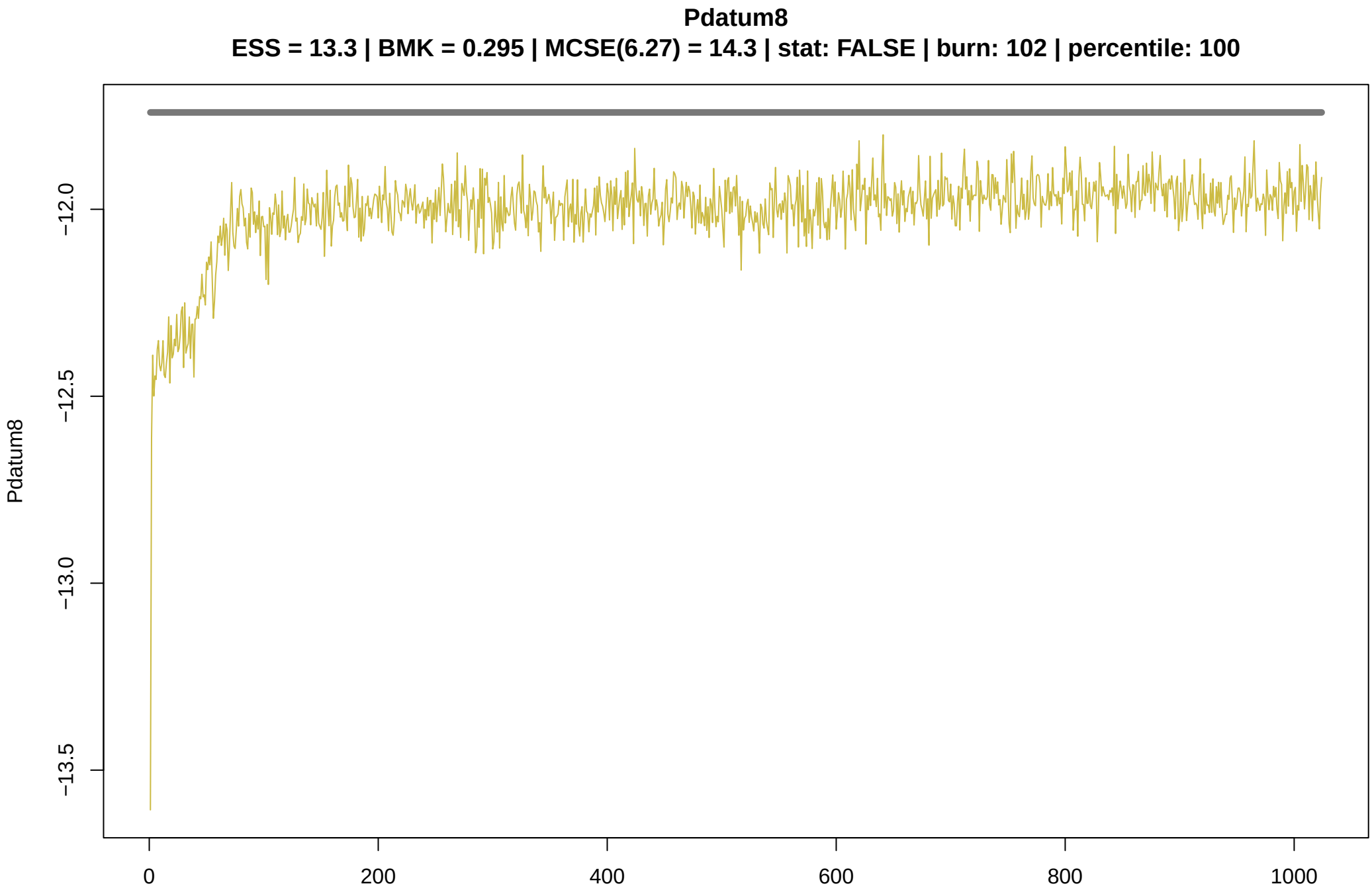

Pdatum3
ESS = 25.7 | BMK = 0.301 | MCSE(6.27) = 12.2 | stat: FALSE | burn: 0 | percentile: 0
Pdatum3
−13.8
−14.0
−14.2
−14.4
−14.6
−14.8
−15.0
−15.2
0
200
400
600
800
1000

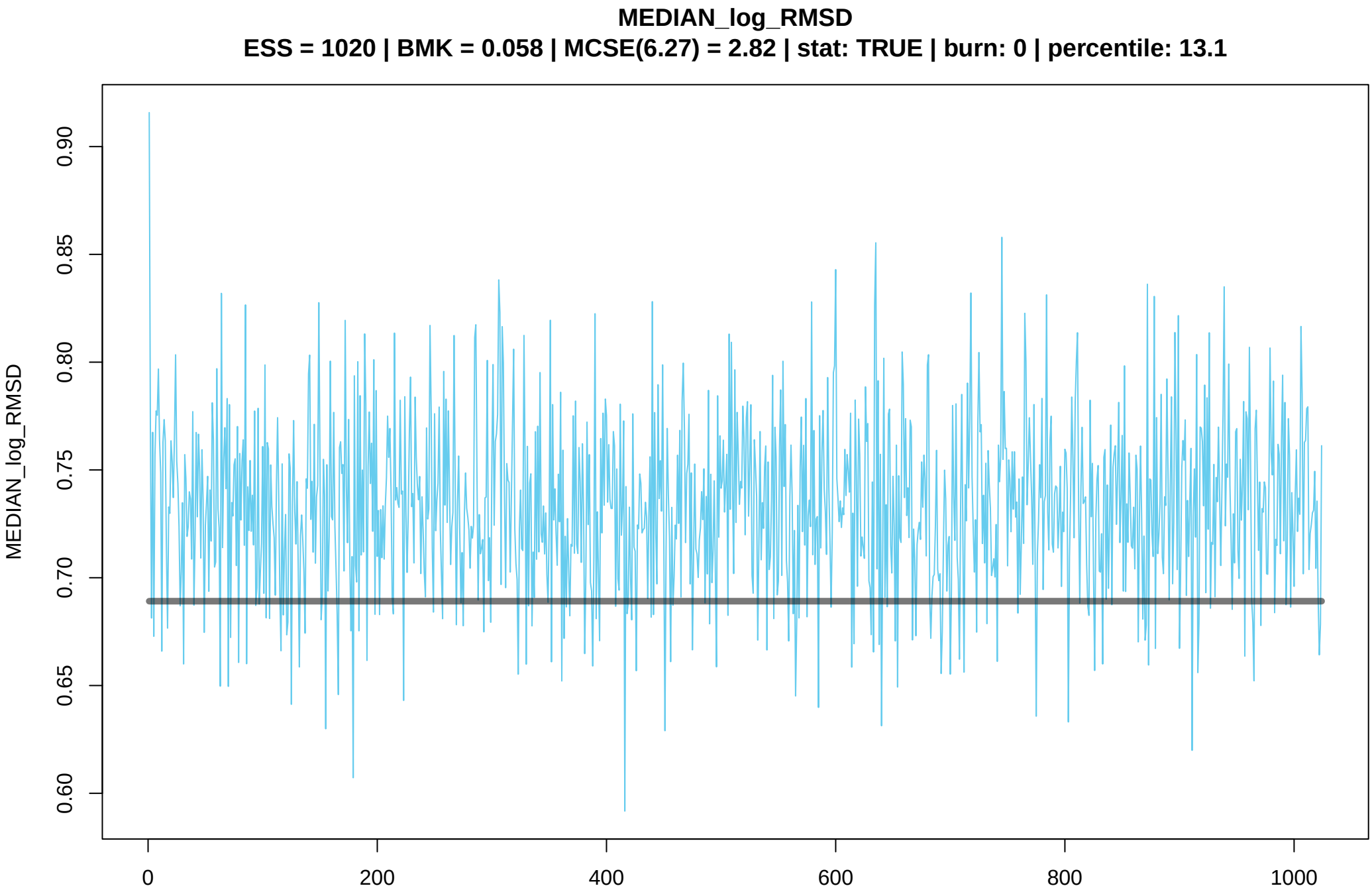

Pdatum4
ESS = 67.1 | BMK = 0.195 | MCSE(6.27) = 11.3 | stat: FALSE | burn: 1020 | percentile: 9.38
Pdatum4
−14.5
−15.0
−15.5
−16.0
0
200
400
600
800
1000

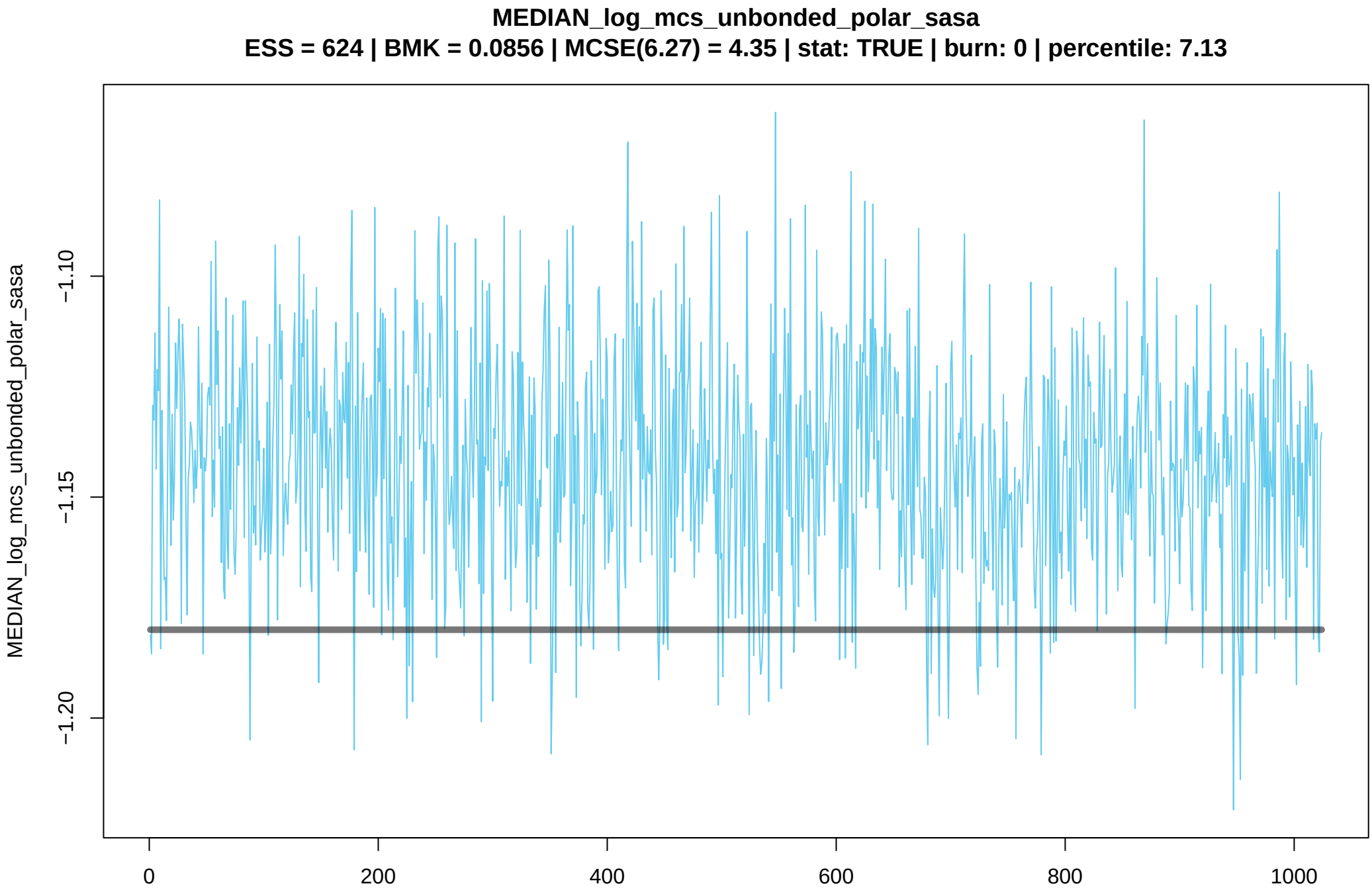

Pdatum5
ESS = 105 | BMK = 0.235 | MCSE(6.27) = 9.54 | stat: FALSE | burn: 0 | percentile: 26.2
Pdatum5
−15.6
−15.8
−16.0
−16.2
−16.4
0
200
400
600
800
1000

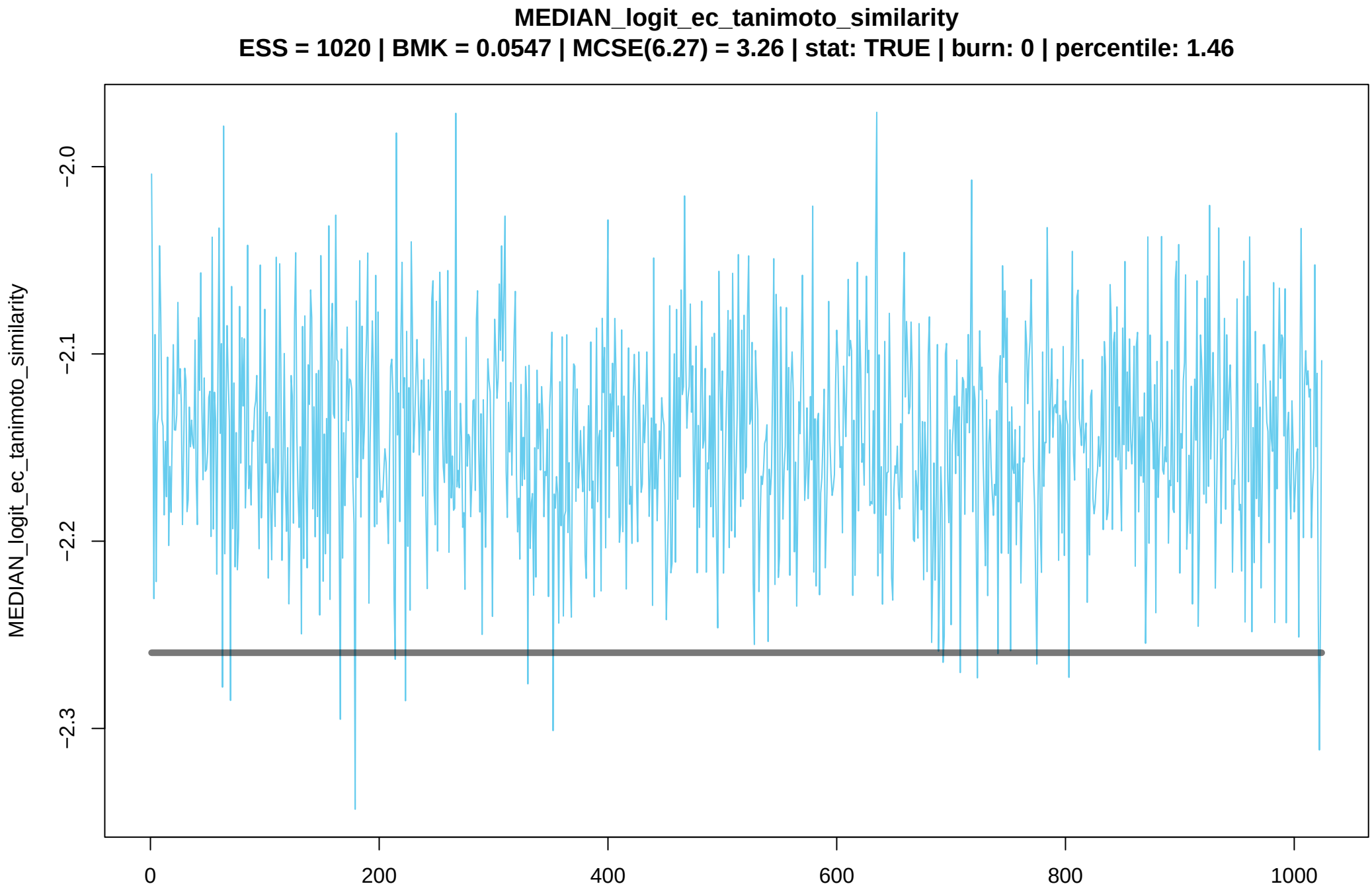

Pdatum6
ESS = 9.3 | BMK = 0.34 | MCSE(6.27) = 12.8 | stat: FALSE | burn: 0 | percentile: 17.6
Pdatum6
−12.6
−12.8
−13.0
−13.2
−13.4
−13.6
0
200
400
600
800
1000

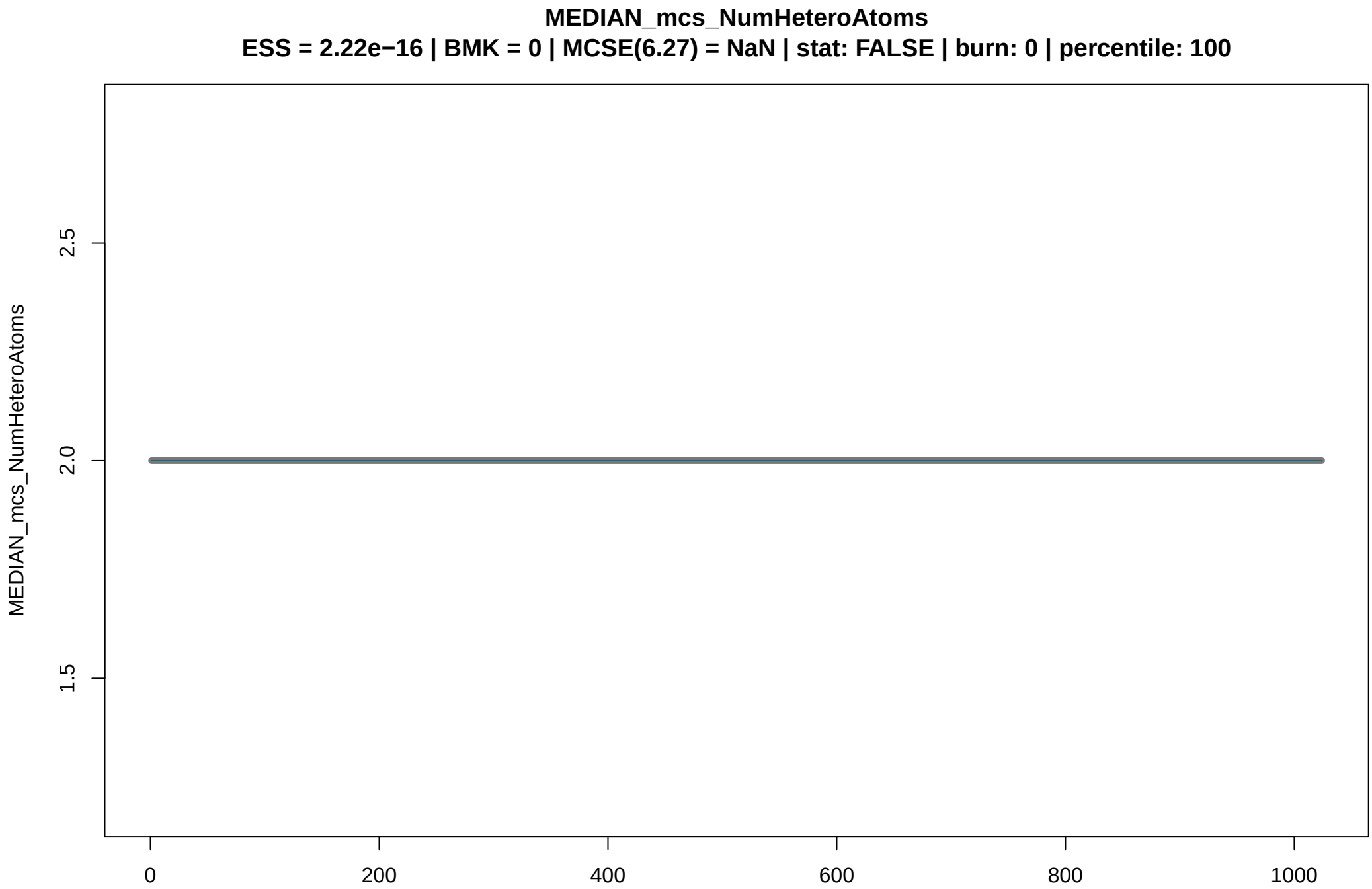

Pdatum7
ESS = 45.8 | BMK = 0.202 | MCSE(6.27) = 8.2 | stat: FALSE | burn: 0 | percentile: 81.4
Pdatum7
−15.0
−15.2
−15.4
−15.6
−15.8
−16.0
0
200
400
600
800
1000

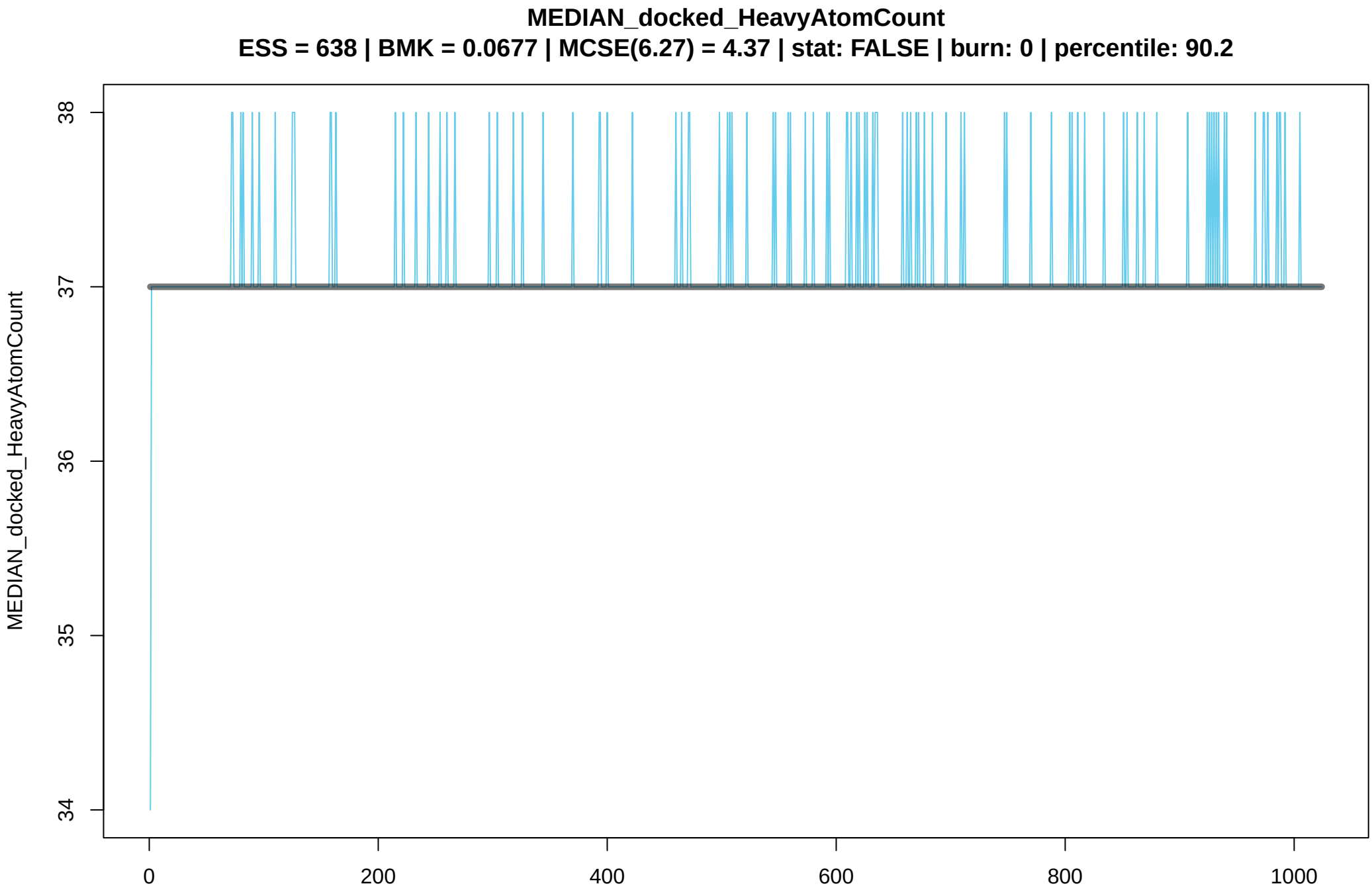

Pdatum8
ESS = 13.3 | BMK = 0.295 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 102 | percentile: 100
Pdatum8
−12.0
−12.5
−13.0
−13.5
0
200
400
600
800
1000

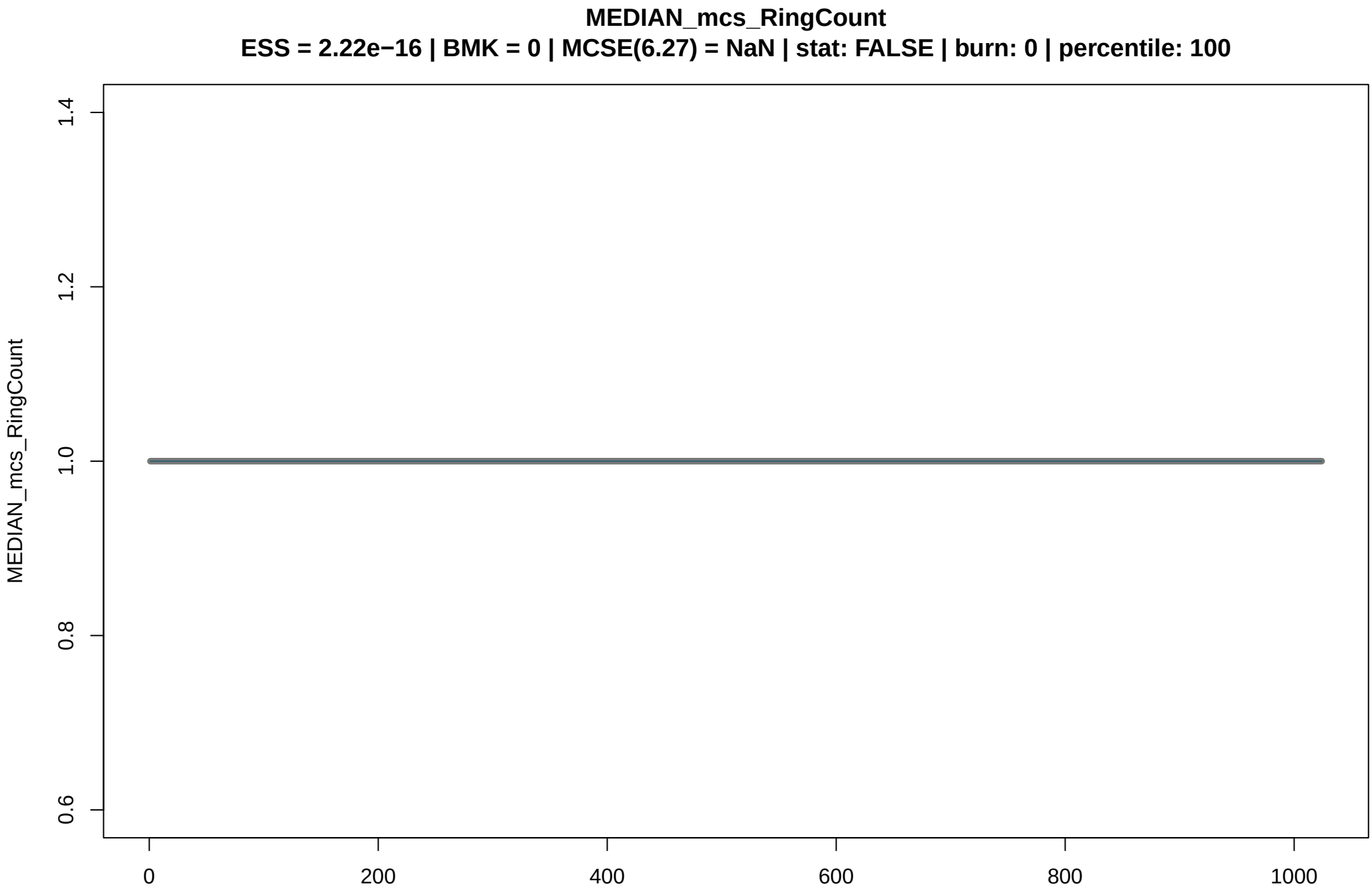

MEDIAN_log_RMSD
ESS = 1020 | BMK = 0.058 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | percentile: 13.1
MEDIAN_log_RMSD
0.60
0.65
0.70
0.75
0.80
0.85
0.90
0
200
400
600
800
1000

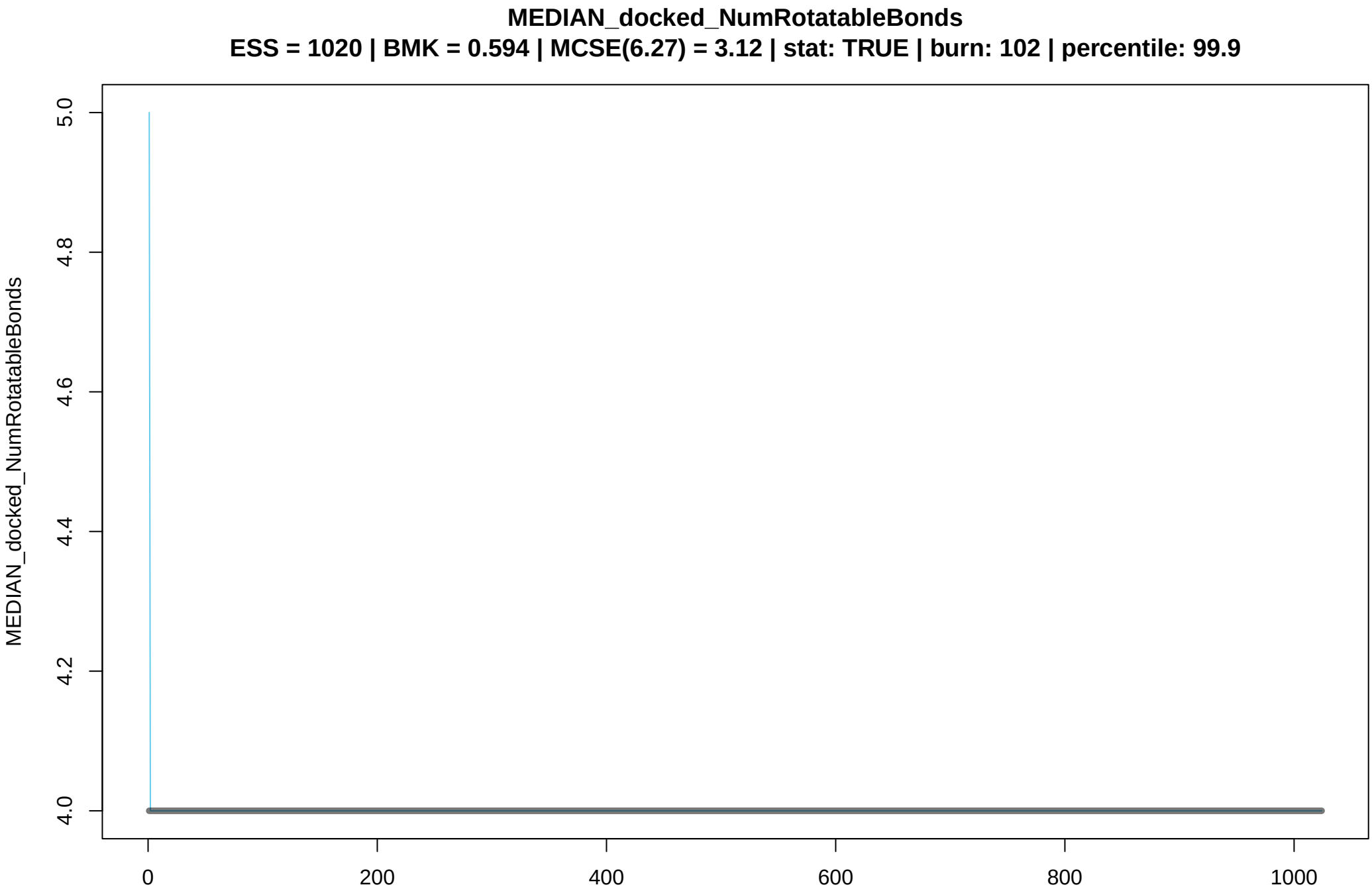

MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 624 | BMK = 0.0856 | MCSE(6.27) = 4.35 | stat: TRUE | burn: 0 | percentile: 7.13
MEDIAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
0
200
400
600
800
1000

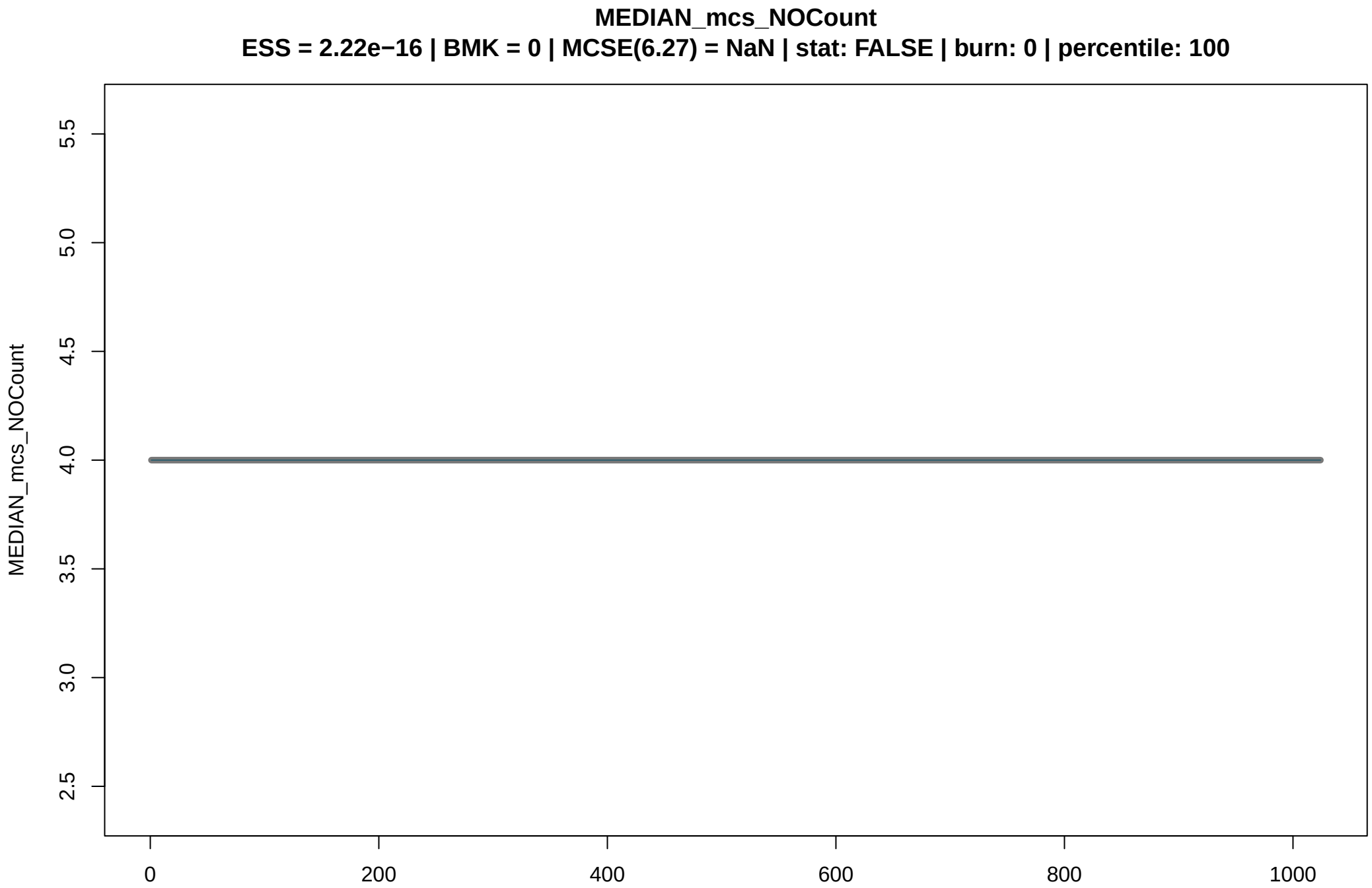

MEDIAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0547 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0 | percentile: 1.46
MEDIAN_logit_ec_tanimoto_similarity
−2.0
−2.1
−2.2
−2.3
0
200
400
600
800
1000

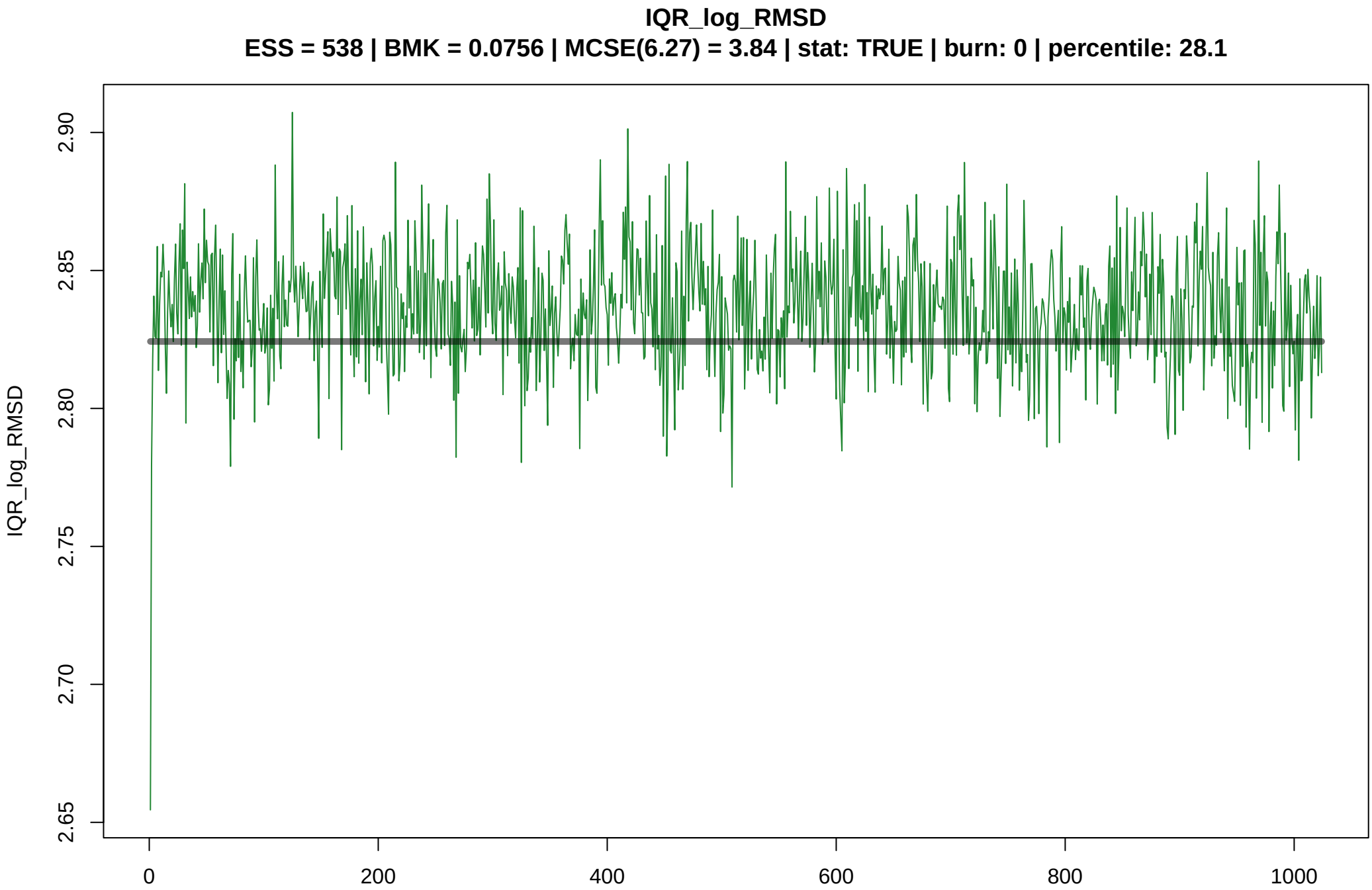

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
MEDIAN_mcs_NumHeteroAtoms
2.5
2.0
1.5
0
200
400
600
800
1000

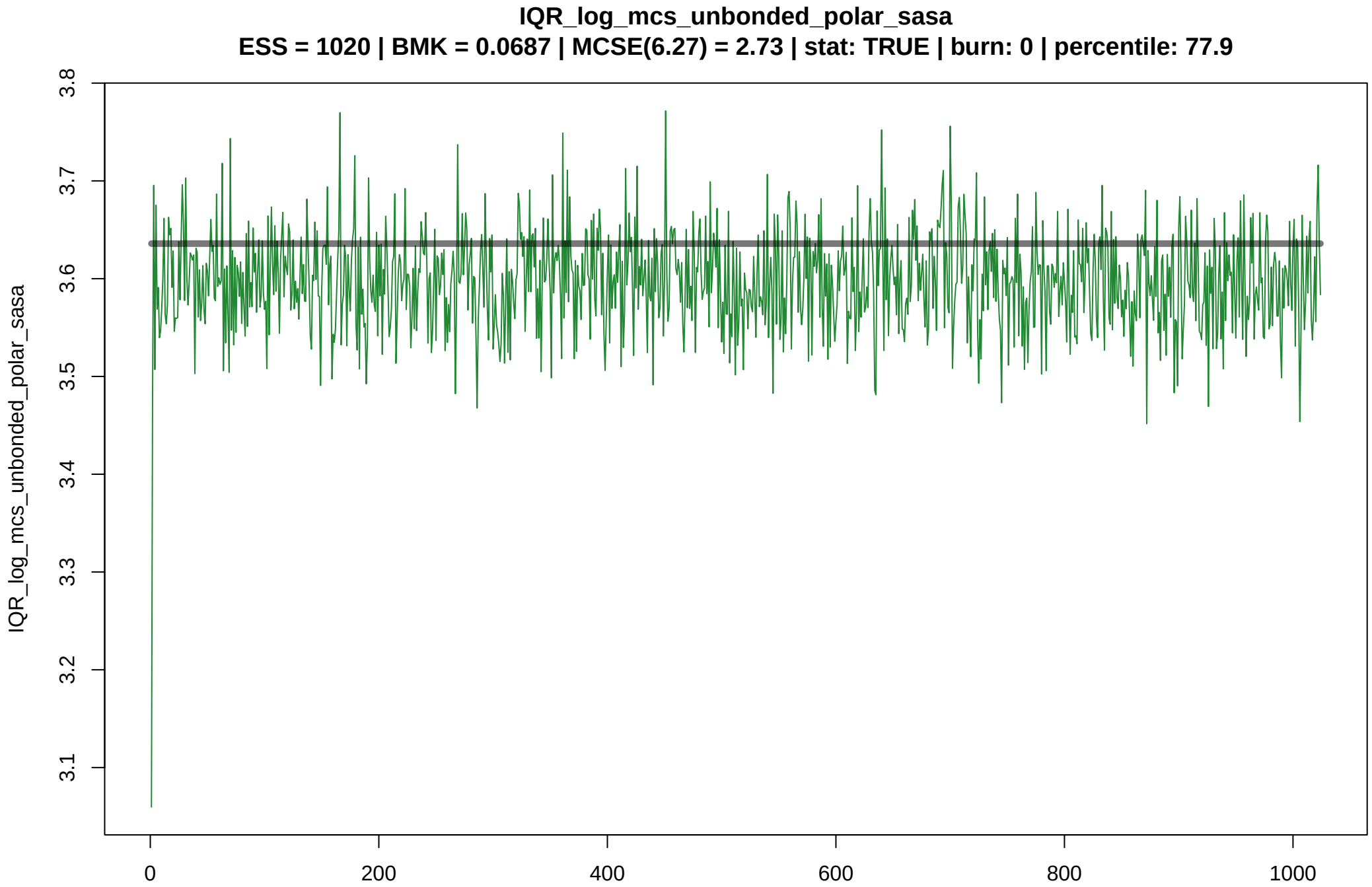

MEDIAN_docked_HeavyAtomCount
ESS = 638 | BMK = 0.0677 | MCSE(6.27) = 4.37 | stat: FALSE | burn: 0 | percentile: 90.2
MEDIAN_docked_HeavyAtomCount
38
37
36
35
34
0
200
400
600
800
1000

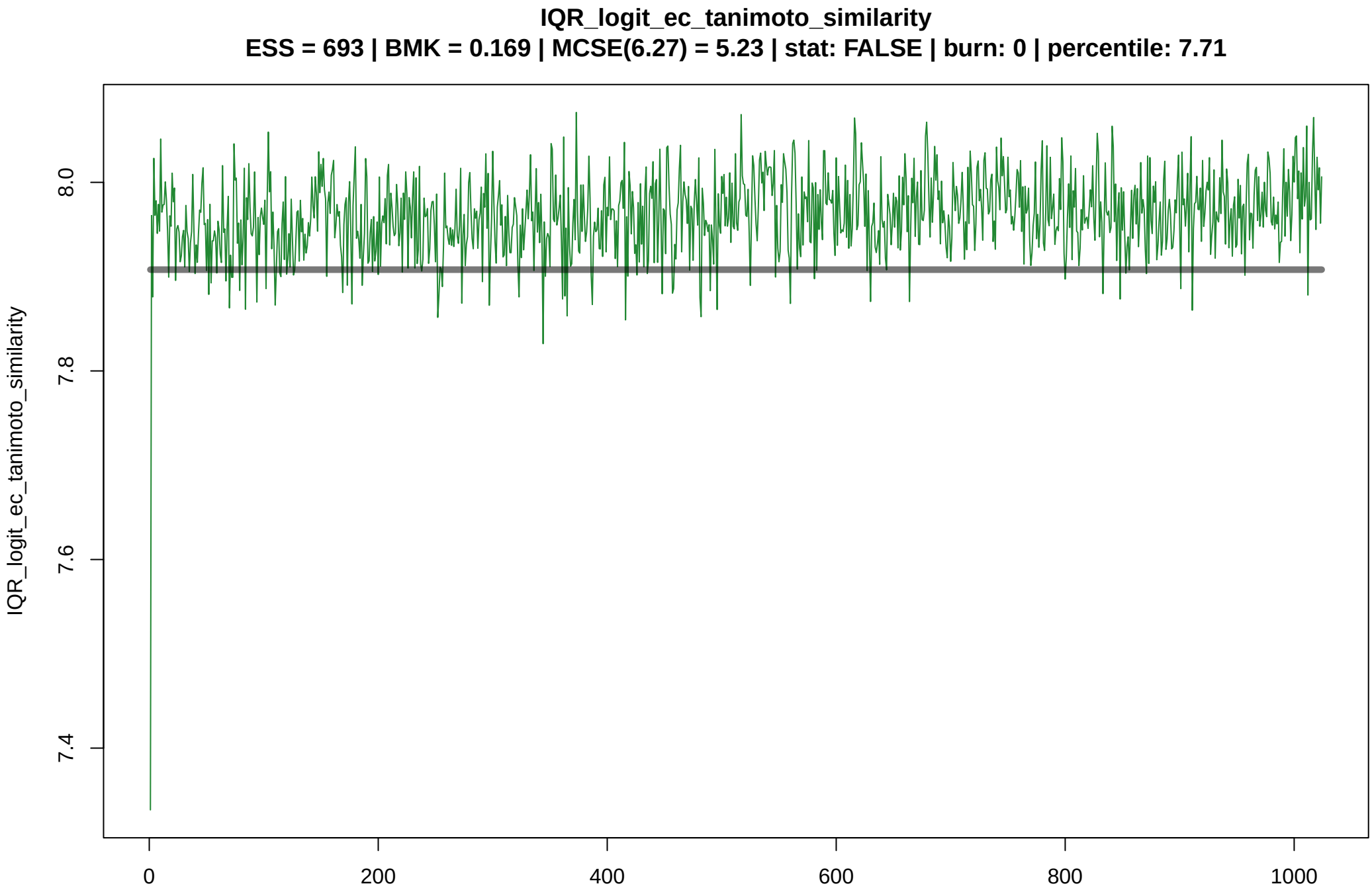

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
MEDIAN_mcs_RingCount
1.4
1.2
1.0
0.8
0.6
0
200
400
600
800
1000

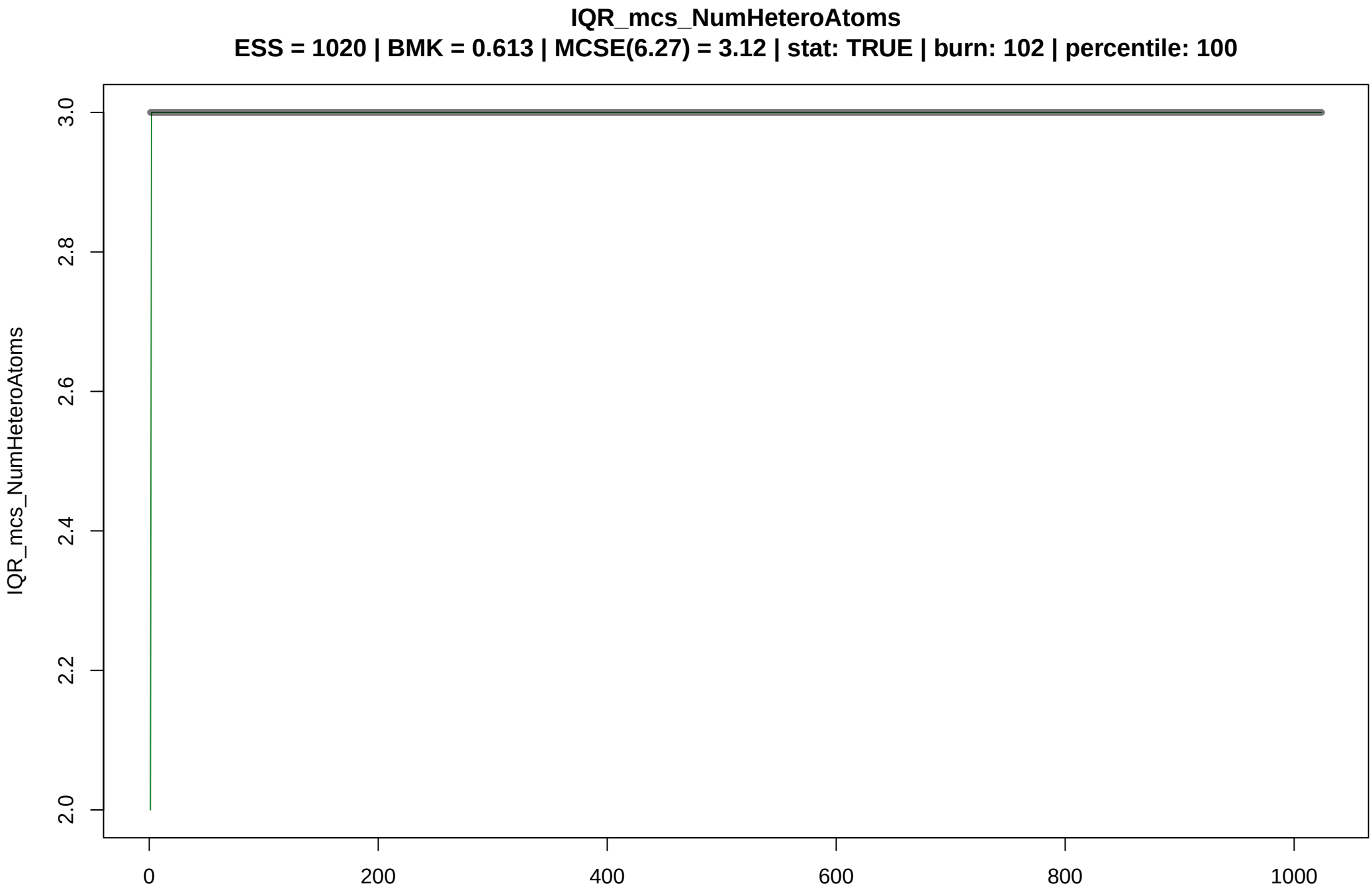

MEDIAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.594 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 99.9
MEDIAN_docked_NumRotatableBonds
5.0
4.8
4.6
4.4
4.2
4.0
0
200
400
600
800
1000

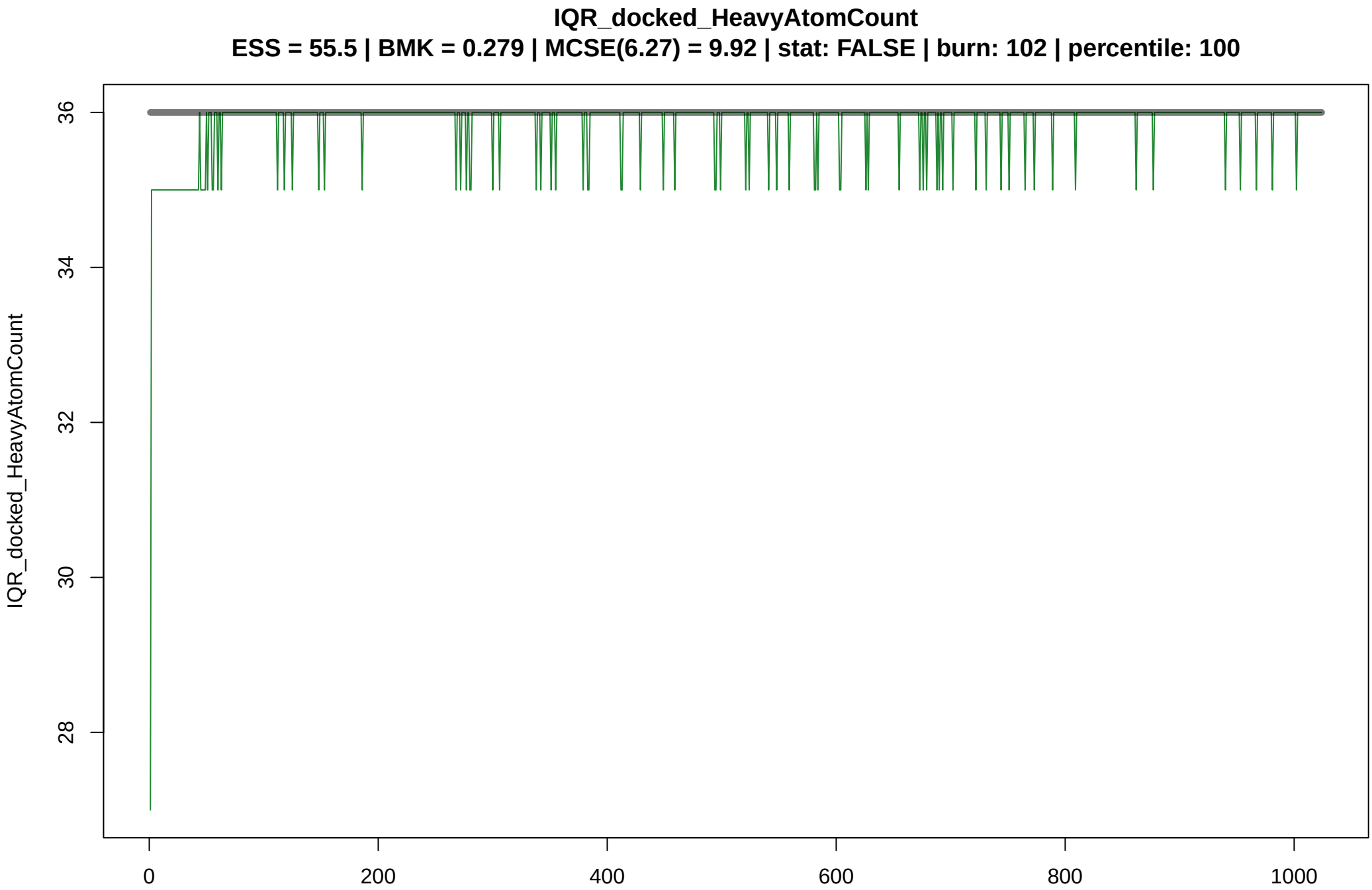

MEDIAN_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
MEDIAN_mcs_NOCount
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
200
400
600
800
1000

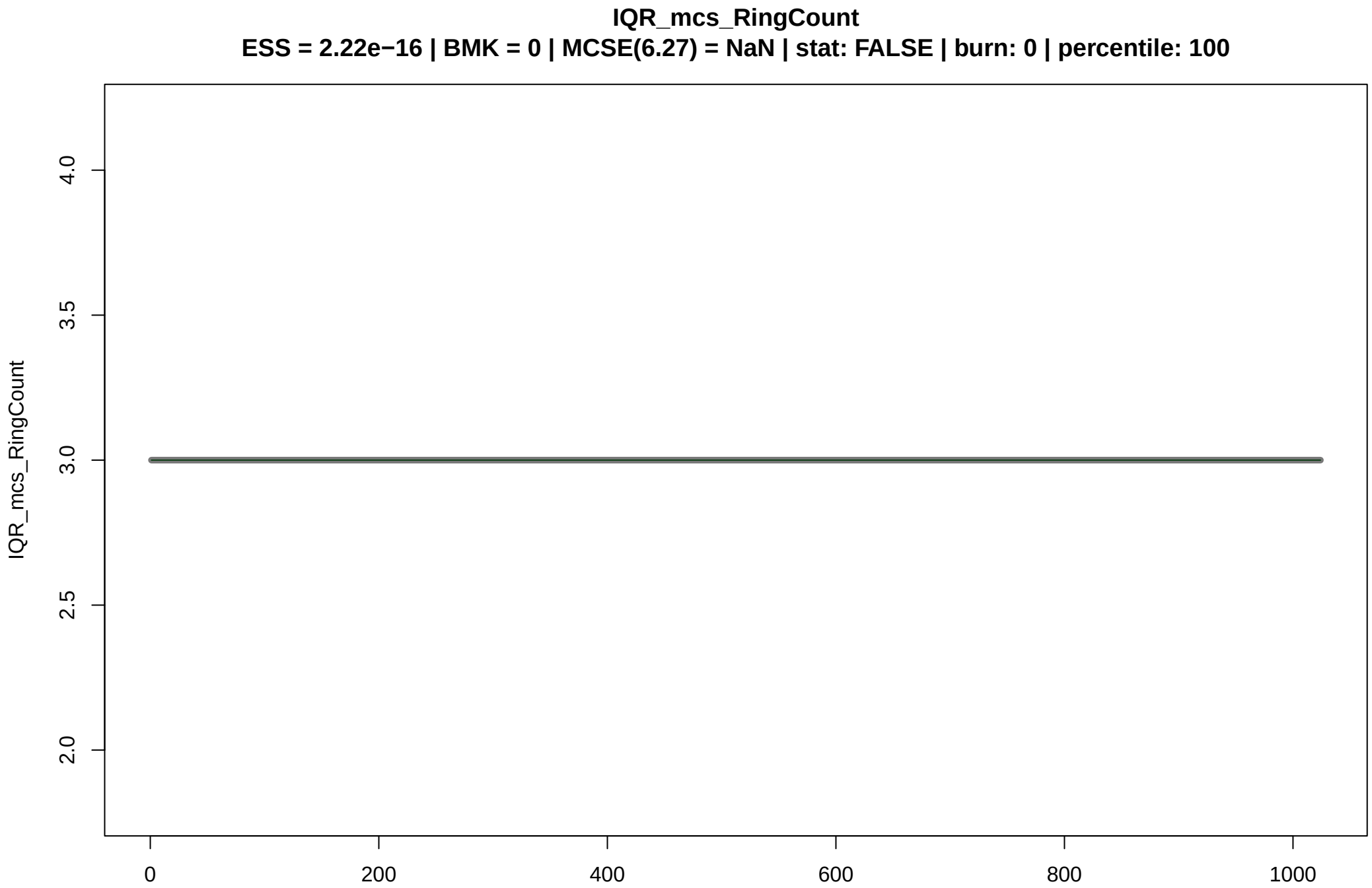

IQR_log_RMSD
ESS = 538 | BMK = 0.0756 | MCSE(6.27) = 3.84 | stat: TRUE | burn: 0 | percentile: 28.1
IQR_log_RMSD
2.65
2.70
2.75
2.80
2.85
2.90
0
200
400
600
800
1000

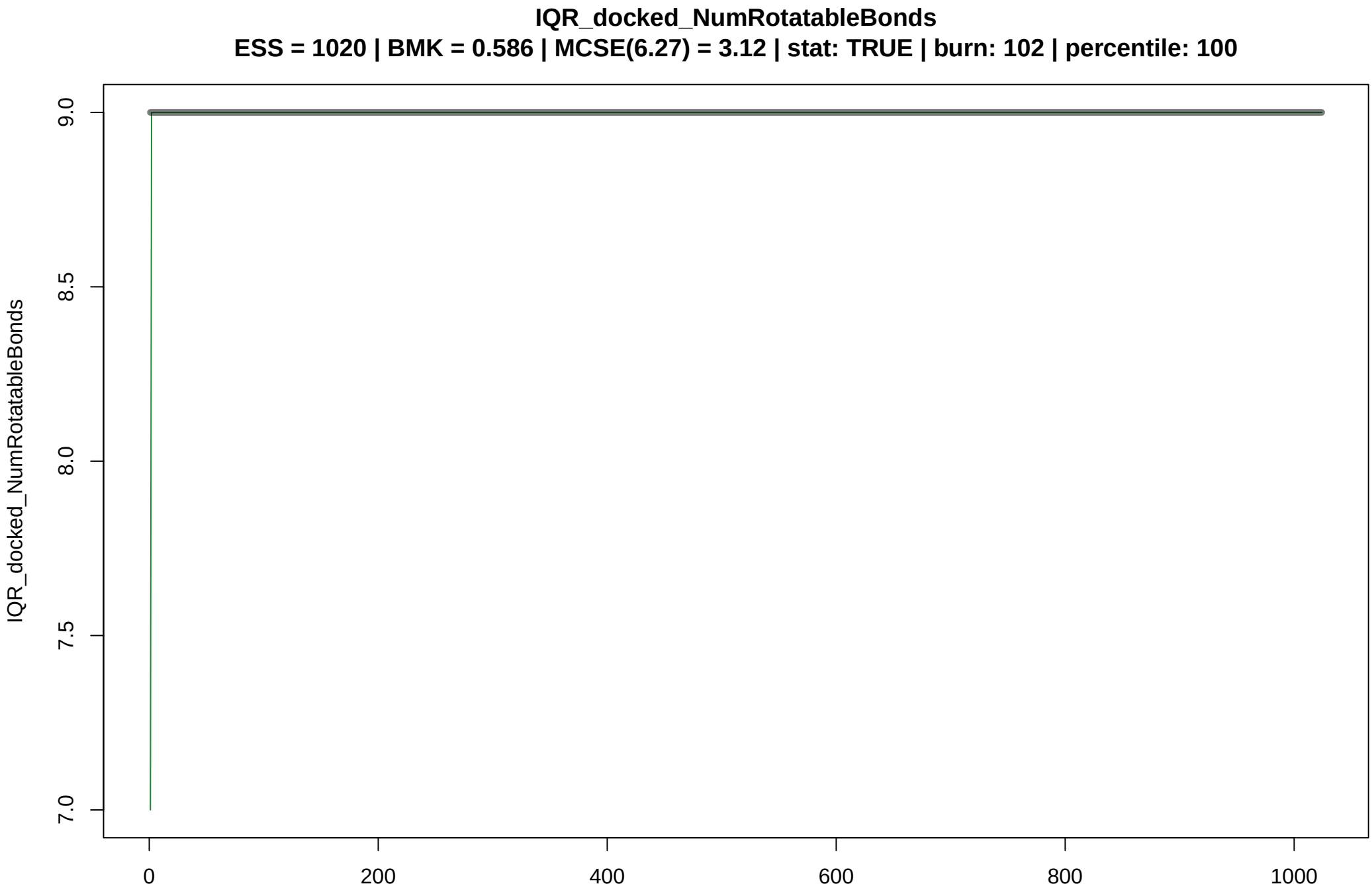

IQR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0687 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | percentile: 77.9
IQR_log_mcs_unbonded_polar_sasa
3.8
3.7
3.6
3.5
3.4
3.3
3.2
3.1
0
200
400
600
800
1000

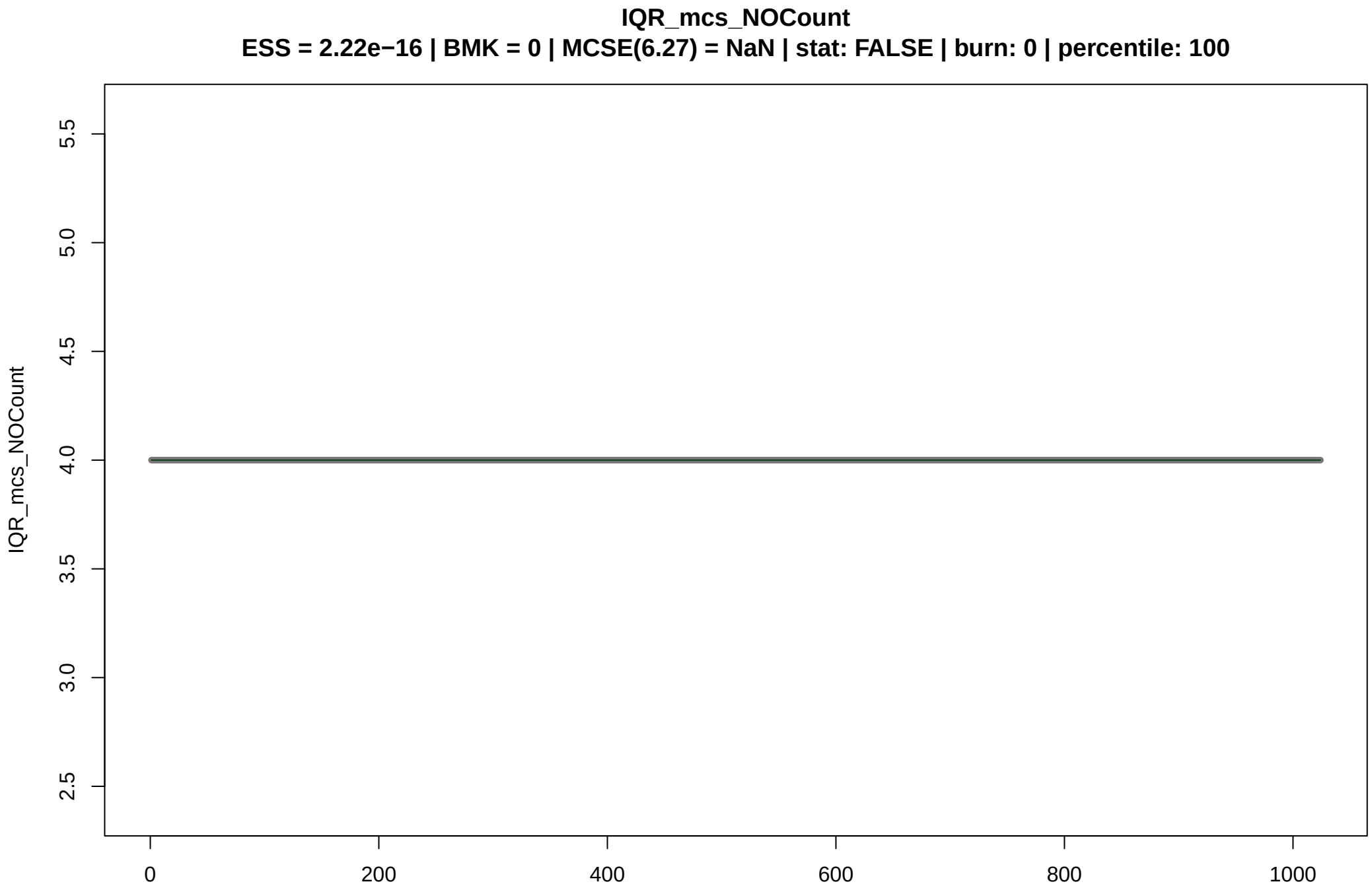

IQR_logit_ec_tanimoto_similarity
ESS = 693 | BMK = 0.169 | MCSE(6.27) = 5.23 | stat: FALSE | burn: 0 | percentile: 7.71
IQR_logit_ec_tanimoto_similarity
7.4
7.6
7.8
8.0
0
200
400
600
800
1000

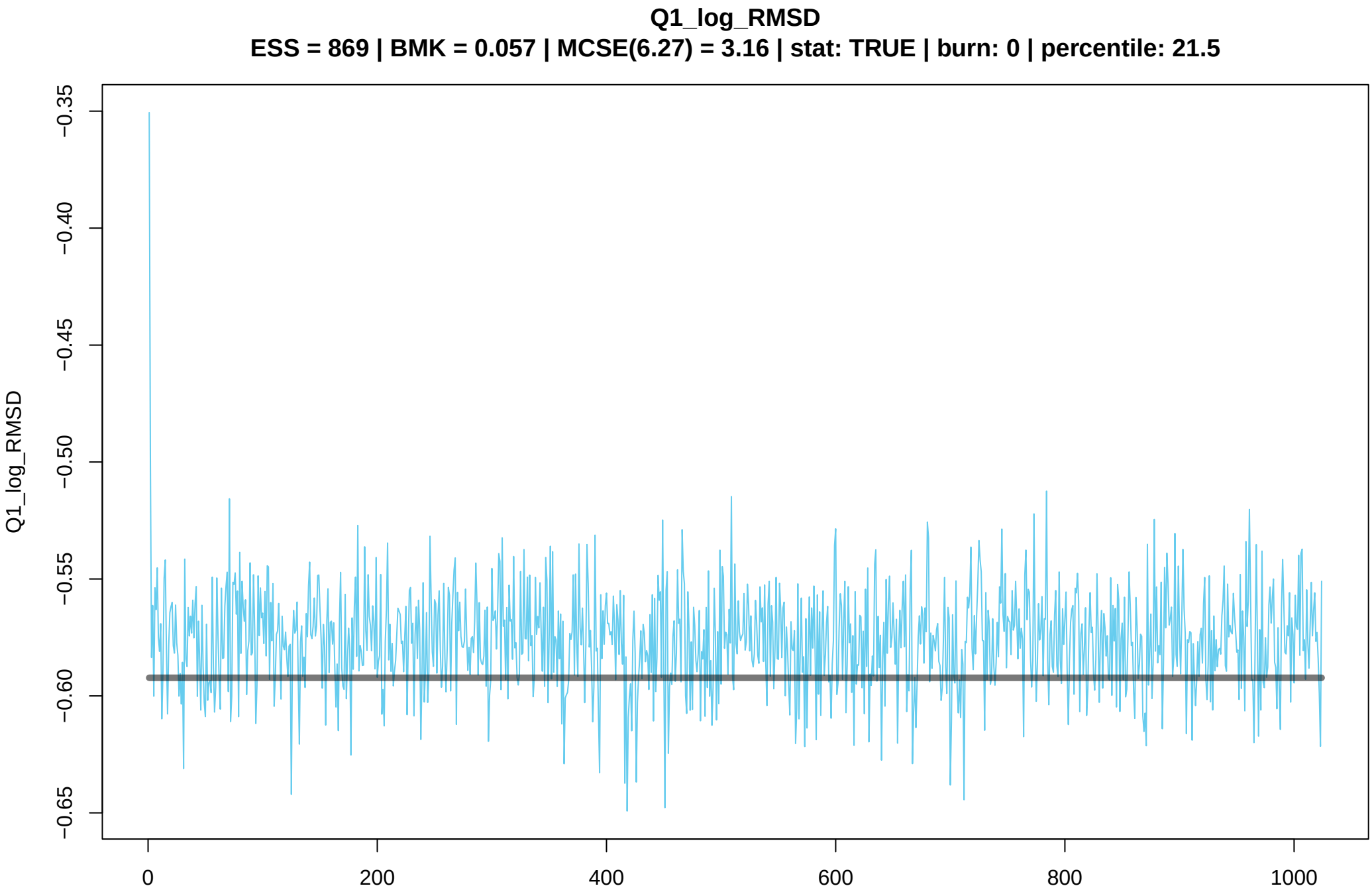

IQR_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.613 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 100
IQR_mcs_NumHeteroAtoms
2.0
2.2
2.4
2.6
2.8
3.0
0
200
400
600
800
1000

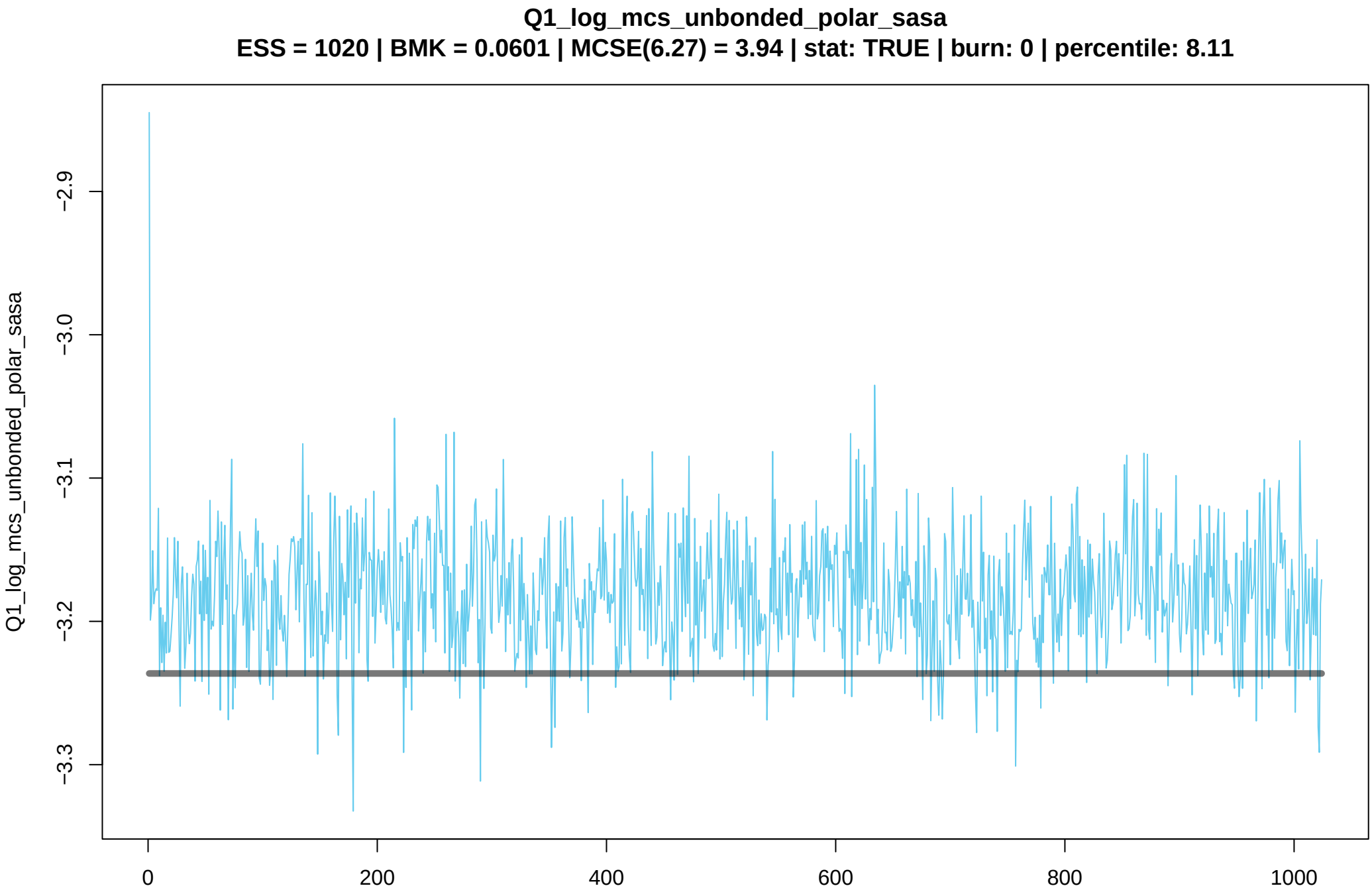

IQR_docked_HeavyAtomCount
ESS = 55.5 | BMK = 0.279 | MCSE(6.27) = 9.92 | stat: FALSE | burn: 102 | percentile: 100
IQR_docked_HeavyAtomCount
28
30
32
34
36
0
200
400
600
800
1000

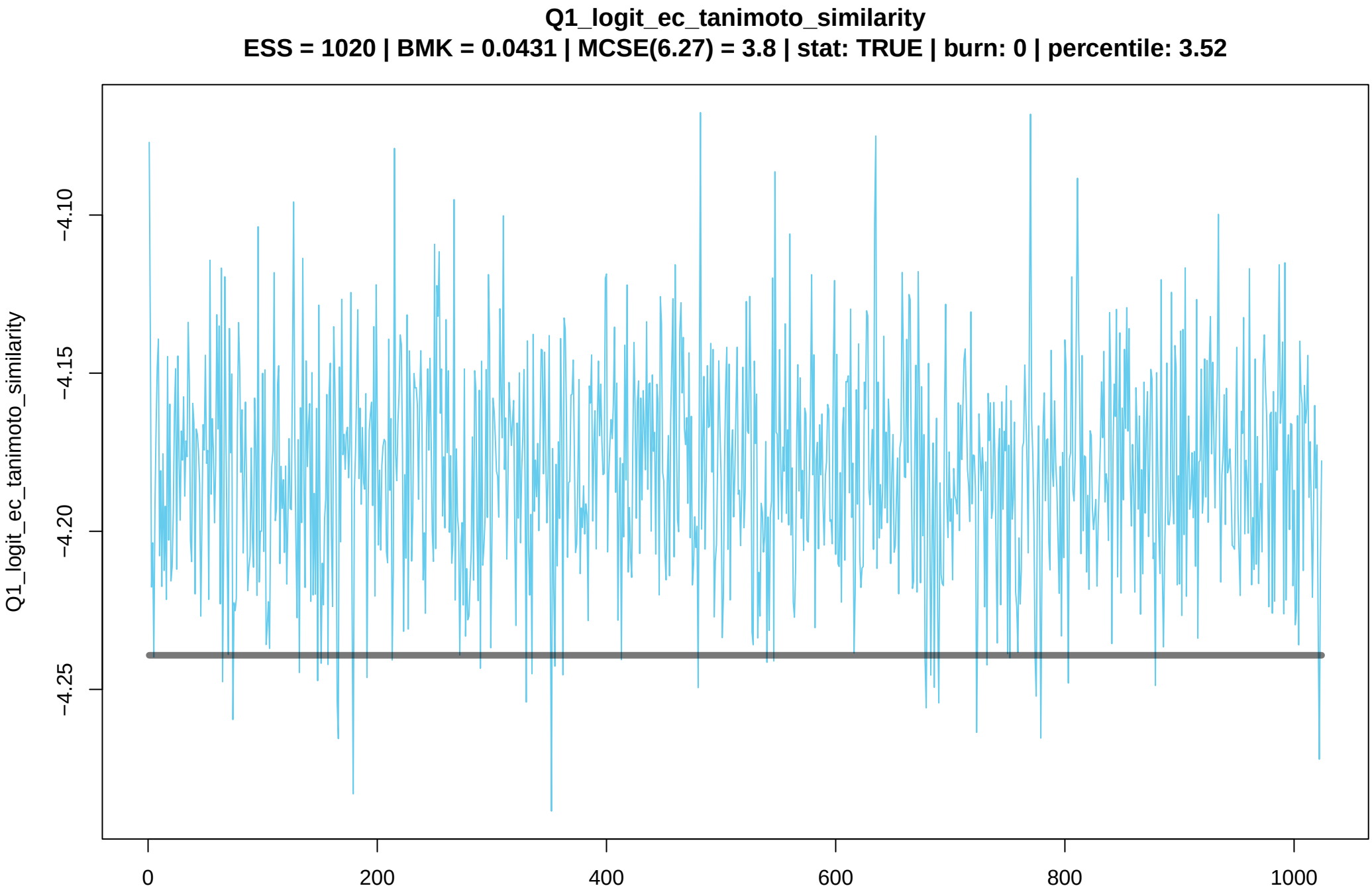

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
IQR_mcs_RingCount
2.0
2.5
3.0
3.5
4.0
0
200
400
600
800
1000

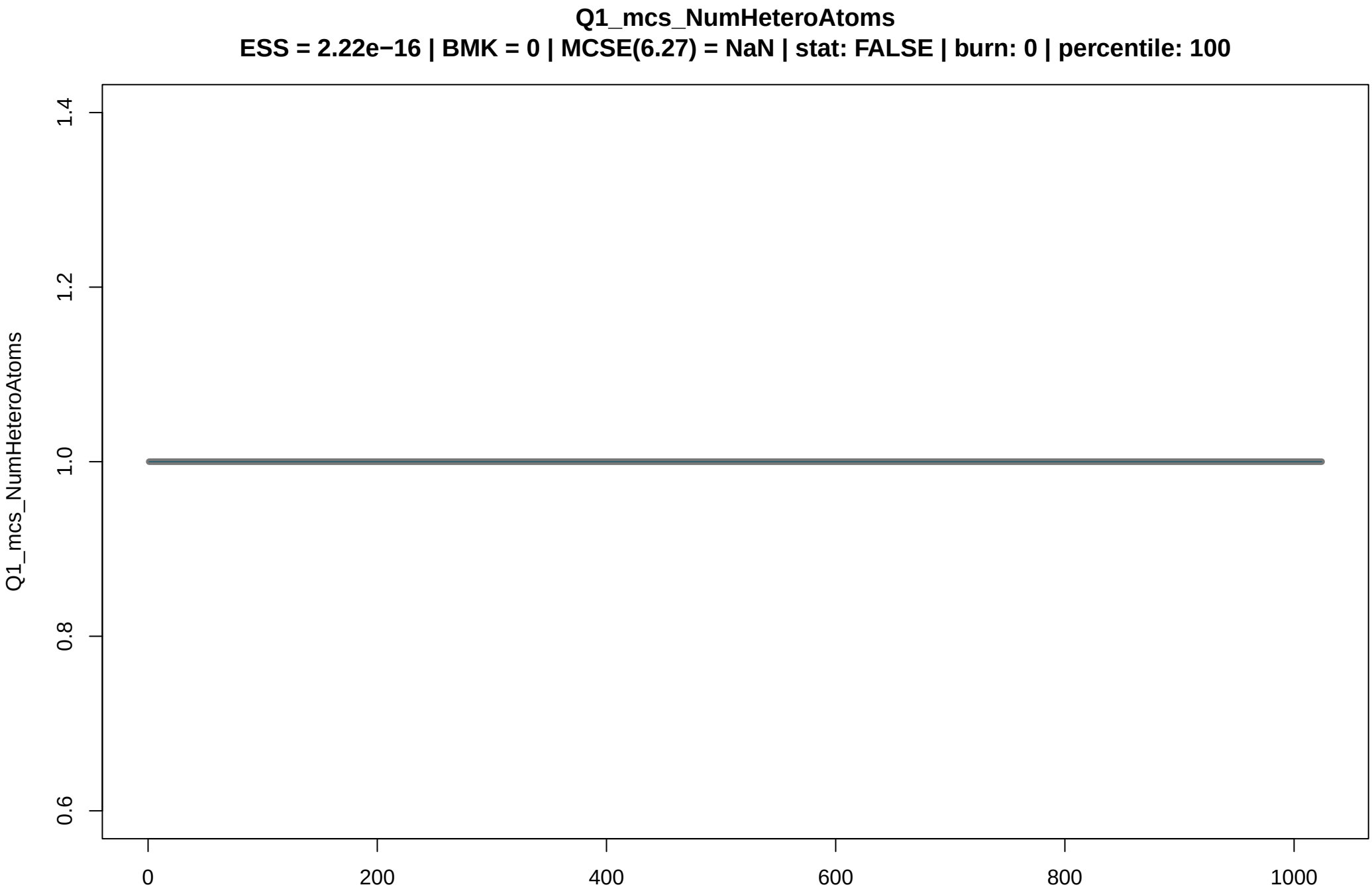

IQR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.586 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 100
IQR_docked_NumRotatableBonds
9.0
8.5
8.0
7.5
7.0
0
200
400
600
800
1000

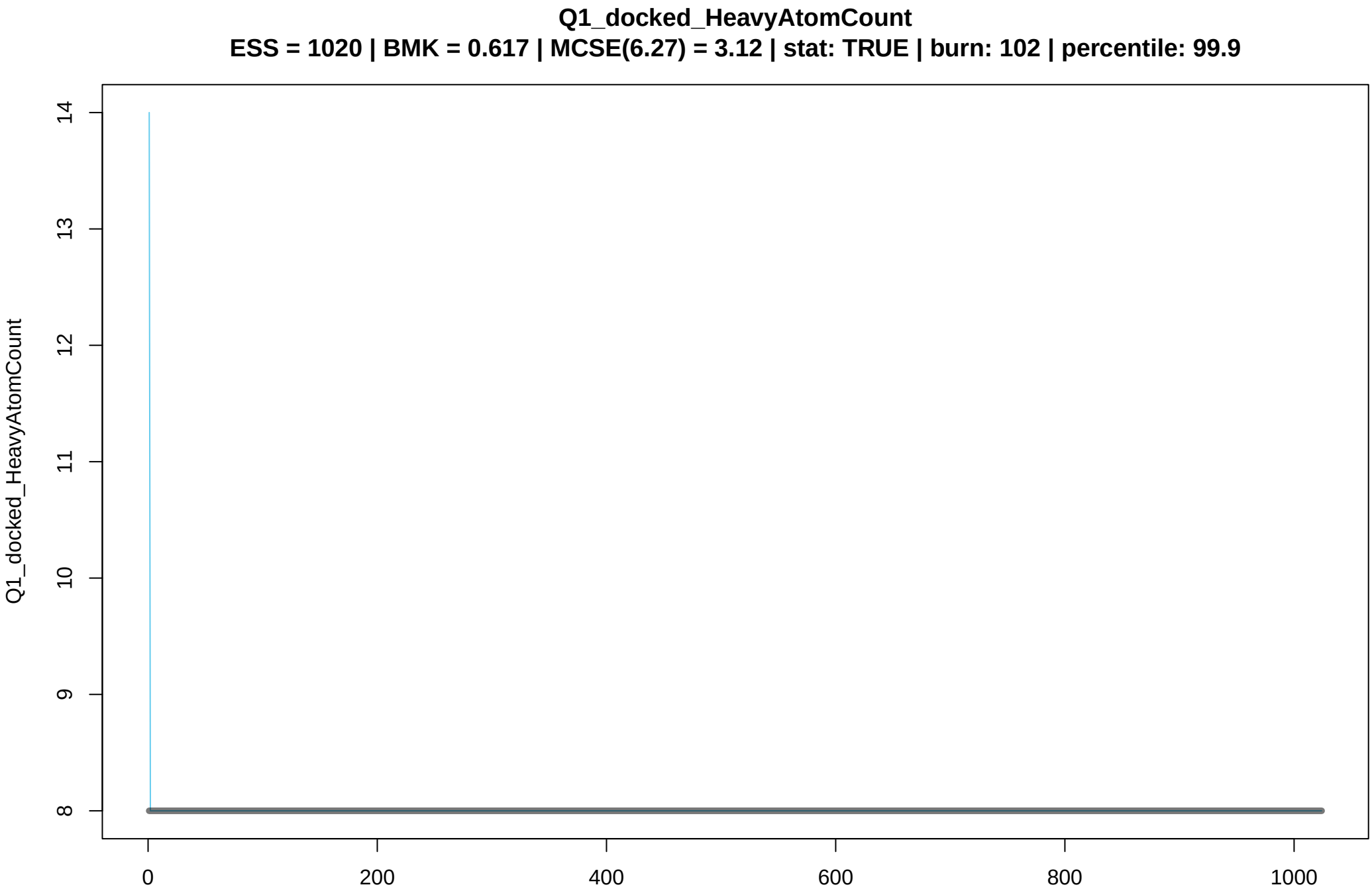

IQR_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
IQR_mcs_NOCount
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
200
400
600
800
1000

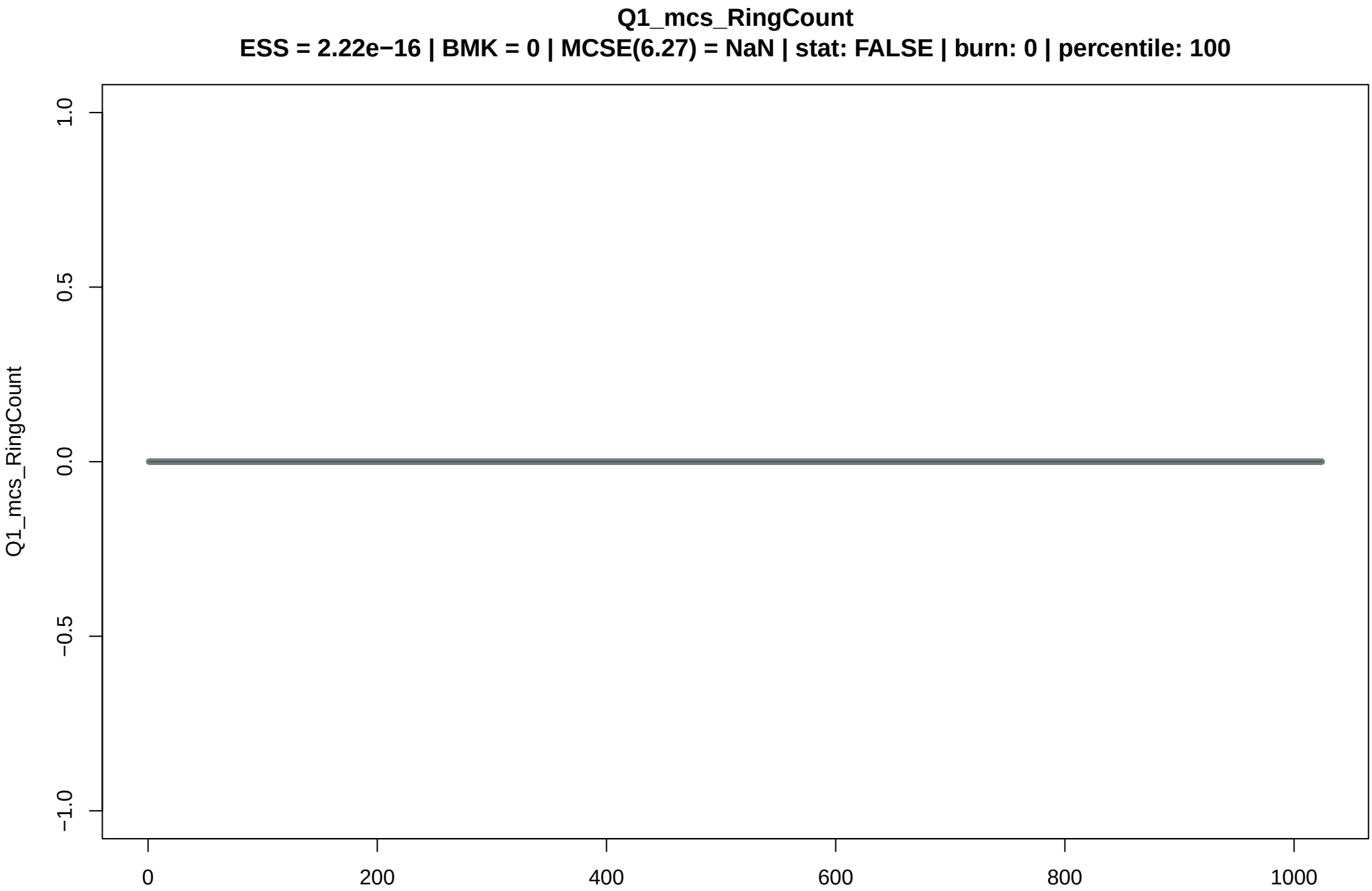

Q1_log_RMSD
ESS = 869 | BMK = 0.057 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | percentile: 21.5
Q1_log_RMSD
−0.35
−0.40
−0.45
−0.50
−0.55
−0.60
−0.65
0
200
400
600
800
1000

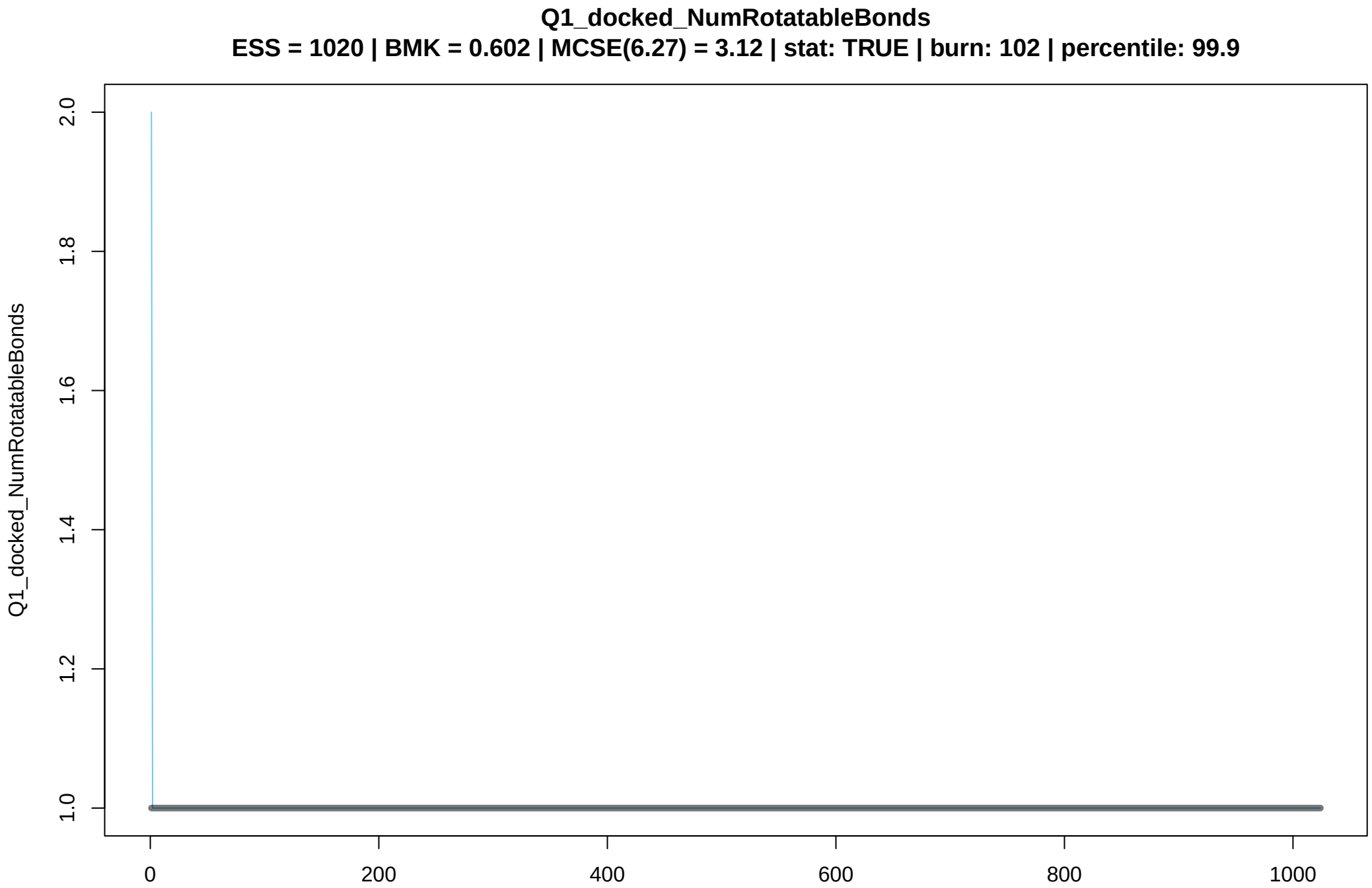

Q1_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0601 | MCSE(6.27) = 3.94 | stat: TRUE | burn: 0 | percentile: 8.11
Q1_log_mcs_unbonded_polar_sasa
−2.9
−3.0
−3.1
−3.2
−3.3
0
200
400
600
800
1000

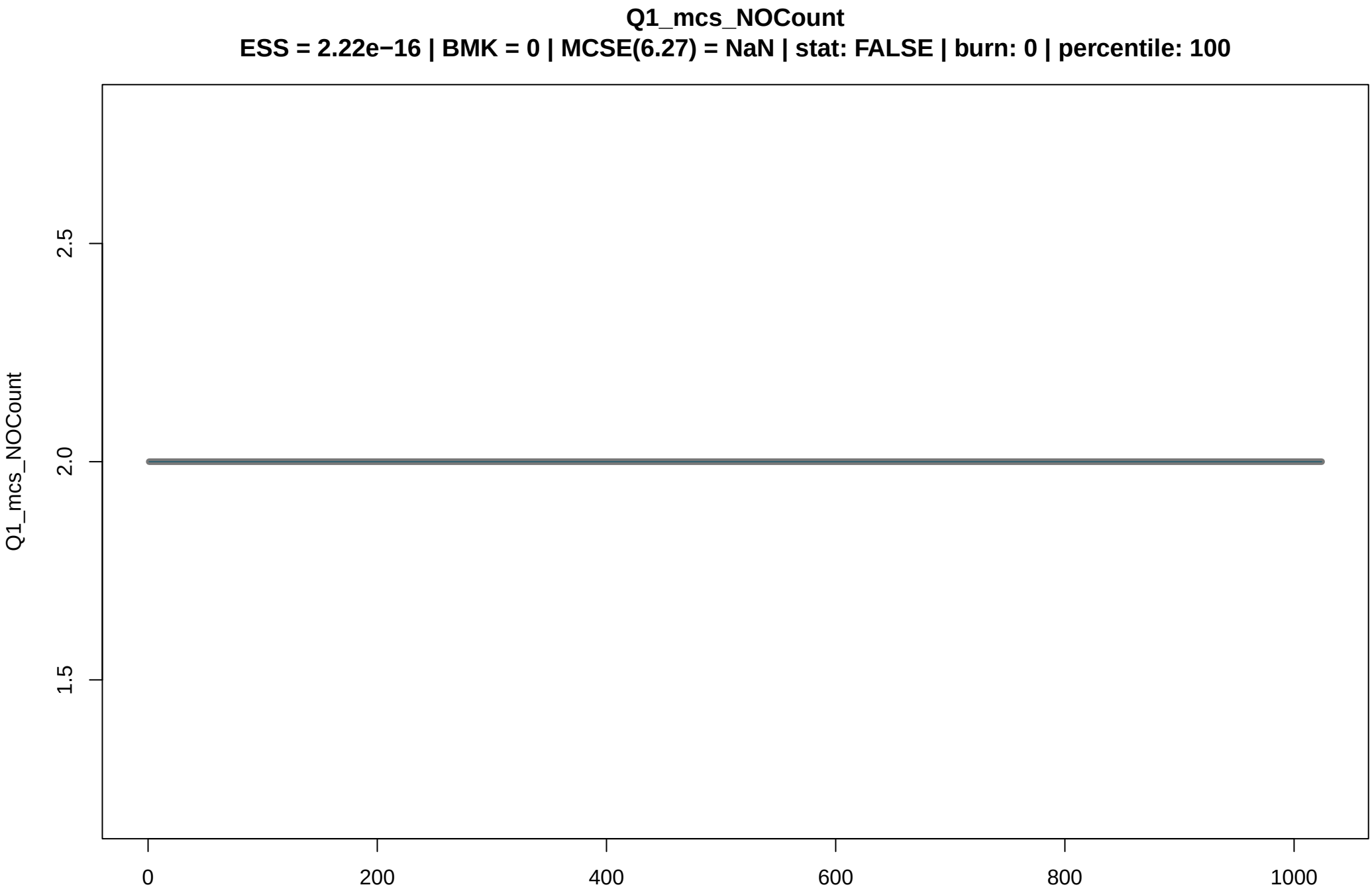

Q1_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0431 | MCSE(6.27) = 3.8 | stat: TRUE | burn: 0 | percentile: 3.52
Q1_logit_ec_tanimoto_similarity
−4.10
−4.15
−4.20
−4.25
0
200
400
600
800
1000

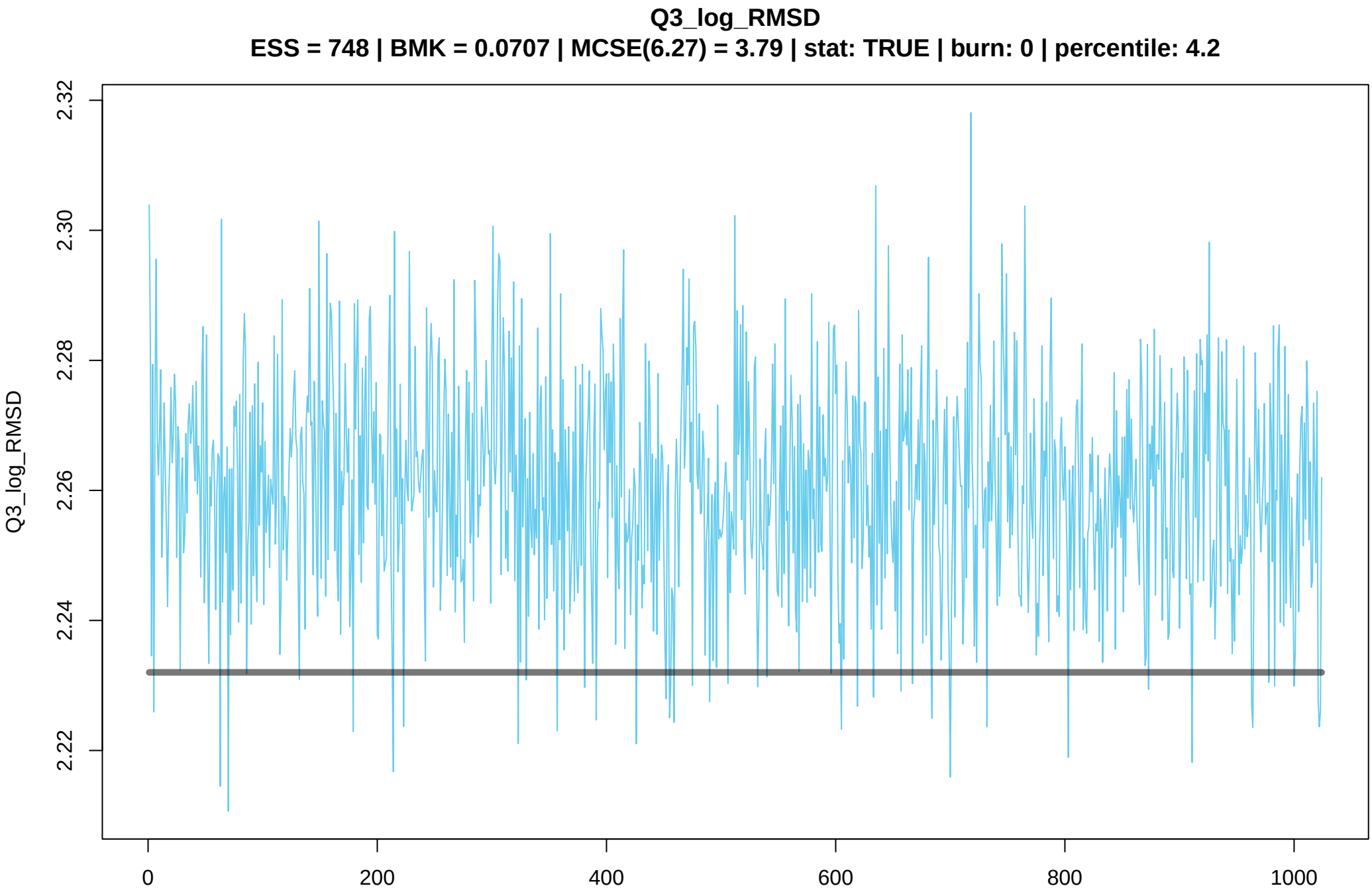

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
200
400
600
800
1000

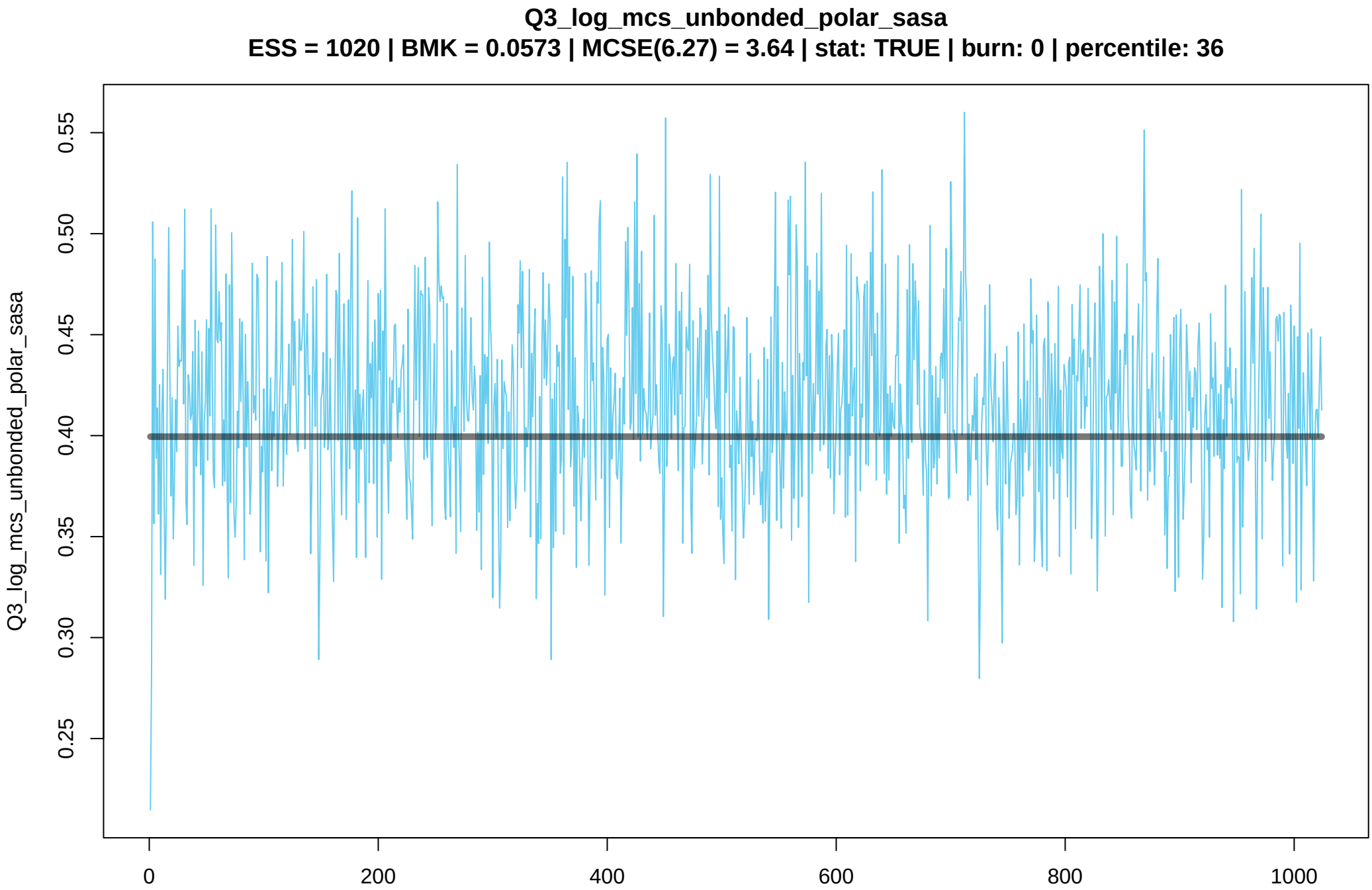

Q1_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.617 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 99.9
Q1_docked_HeavyAtomCount
8
9
10
11
12
13
14
0
200
400
600
800
1000

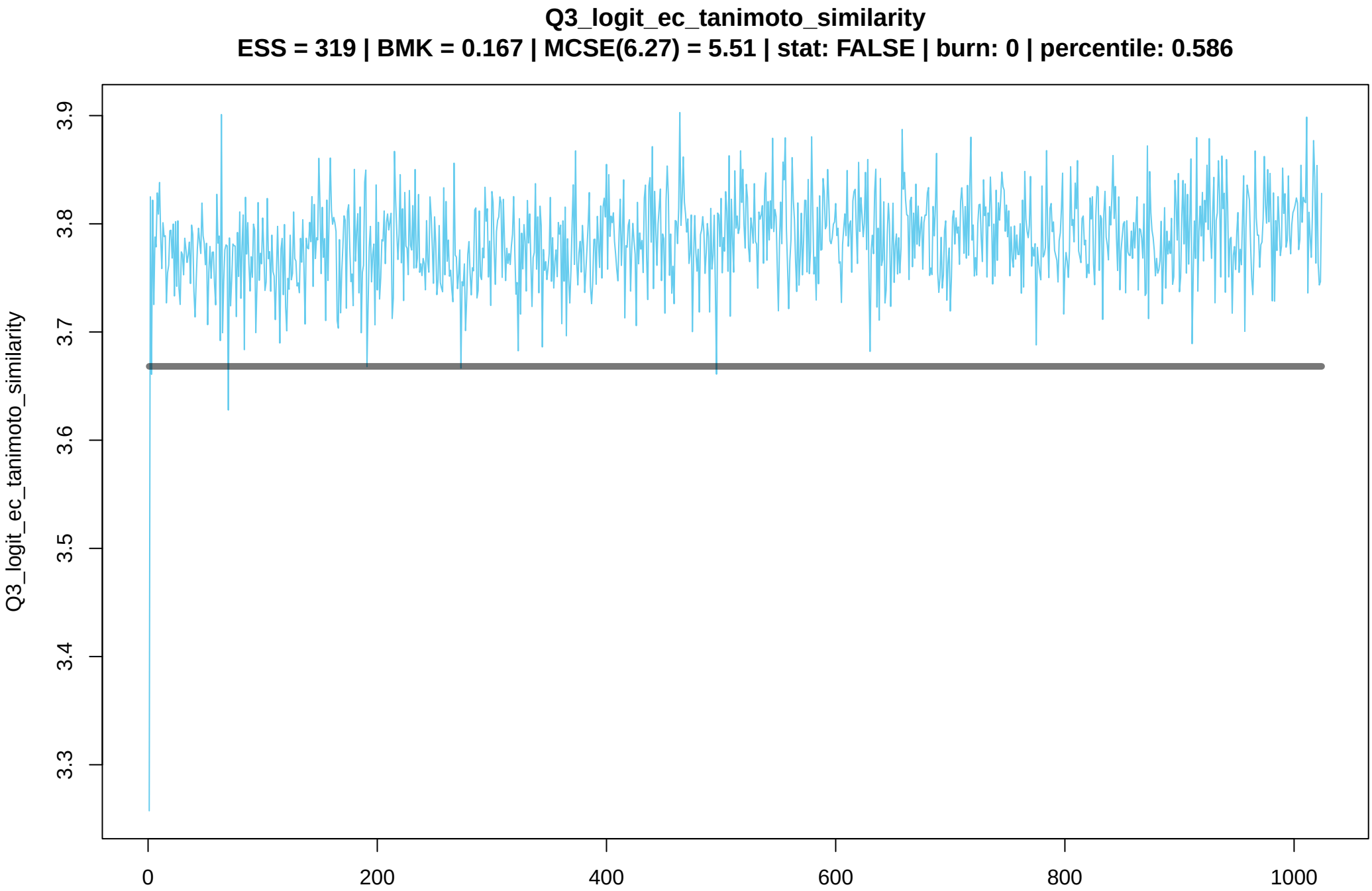

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
200
400
600
800
1000

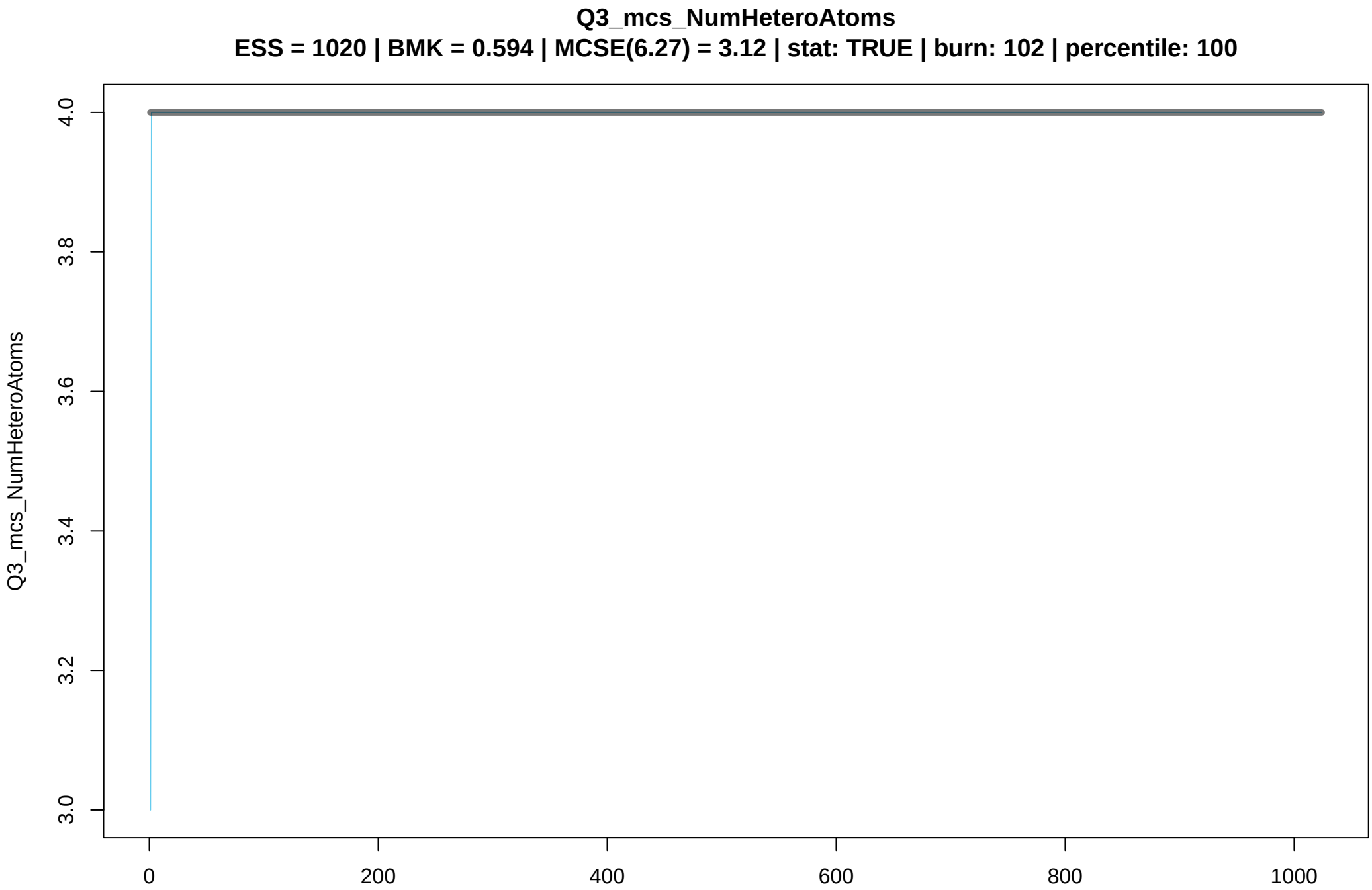

Q1_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.602 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 99.9
Q1_docked_NumRotatableBonds
1.0
1.2
1.4
1.6
1.8
2.0
0
200
400
600
800
1000

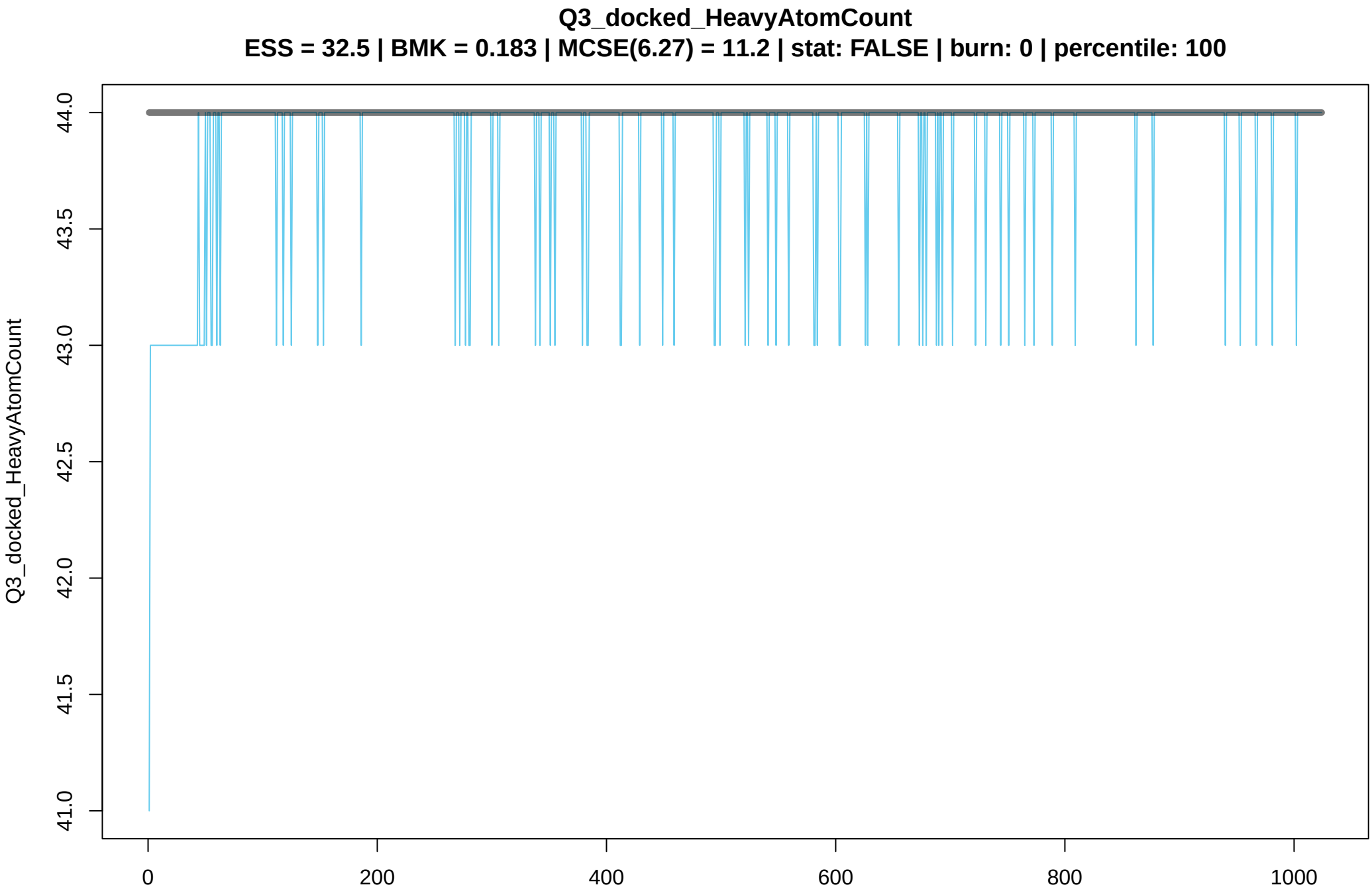

Q1_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q1_mcs_NOCount
2.5
2.0
1.5
0
200
400
600
800
1000

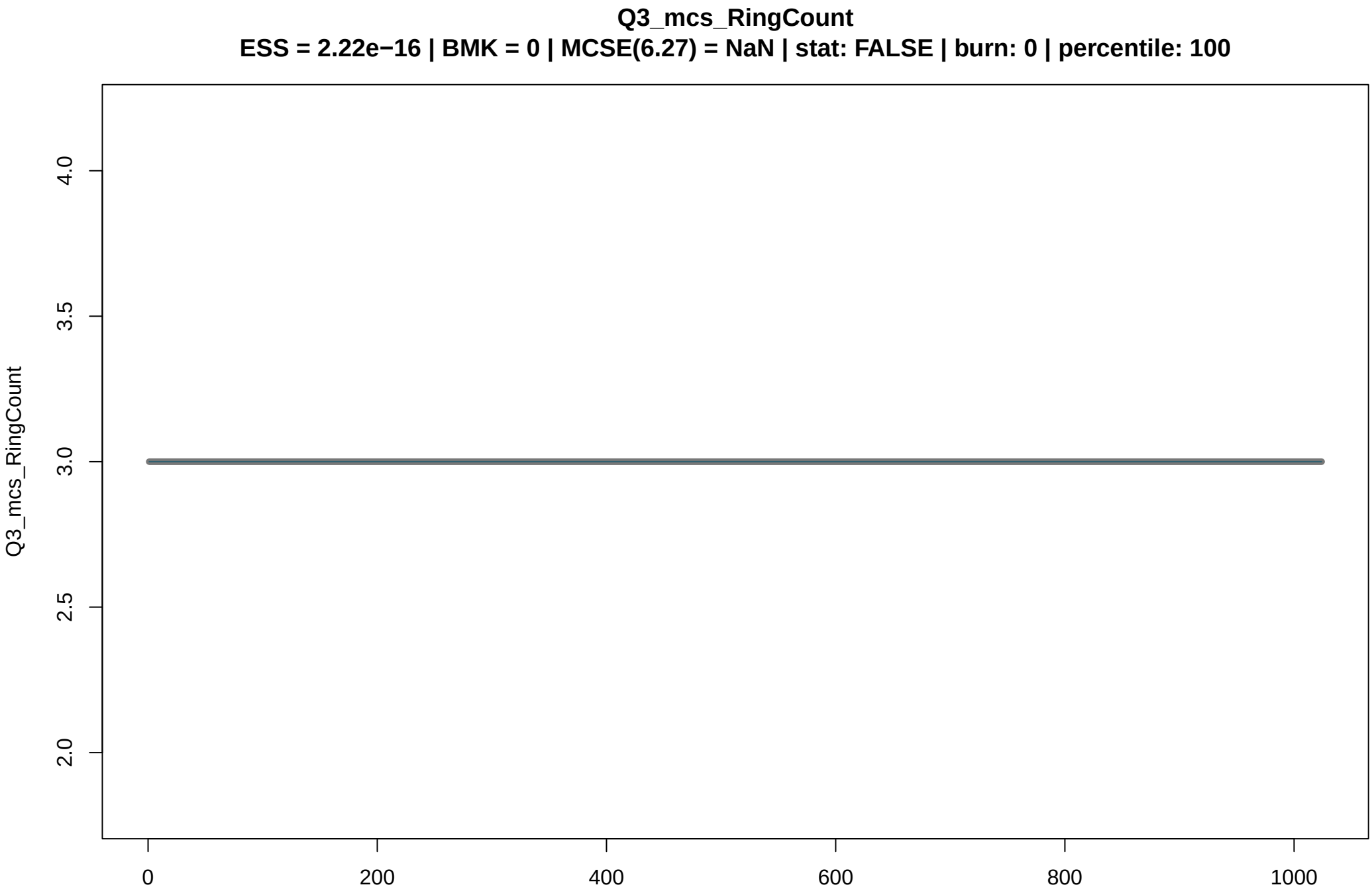

Q3_log_RMSD
ESS = 748 | BMK = 0.0707 | MCSE(6.27) = 3.79 | stat: TRUE | burn: 0 | percentile: 4.2
Q3_log_RMSD
2.22
2.24
2.26
2.28
2.30
2.32
0
200
400
600
800
1000

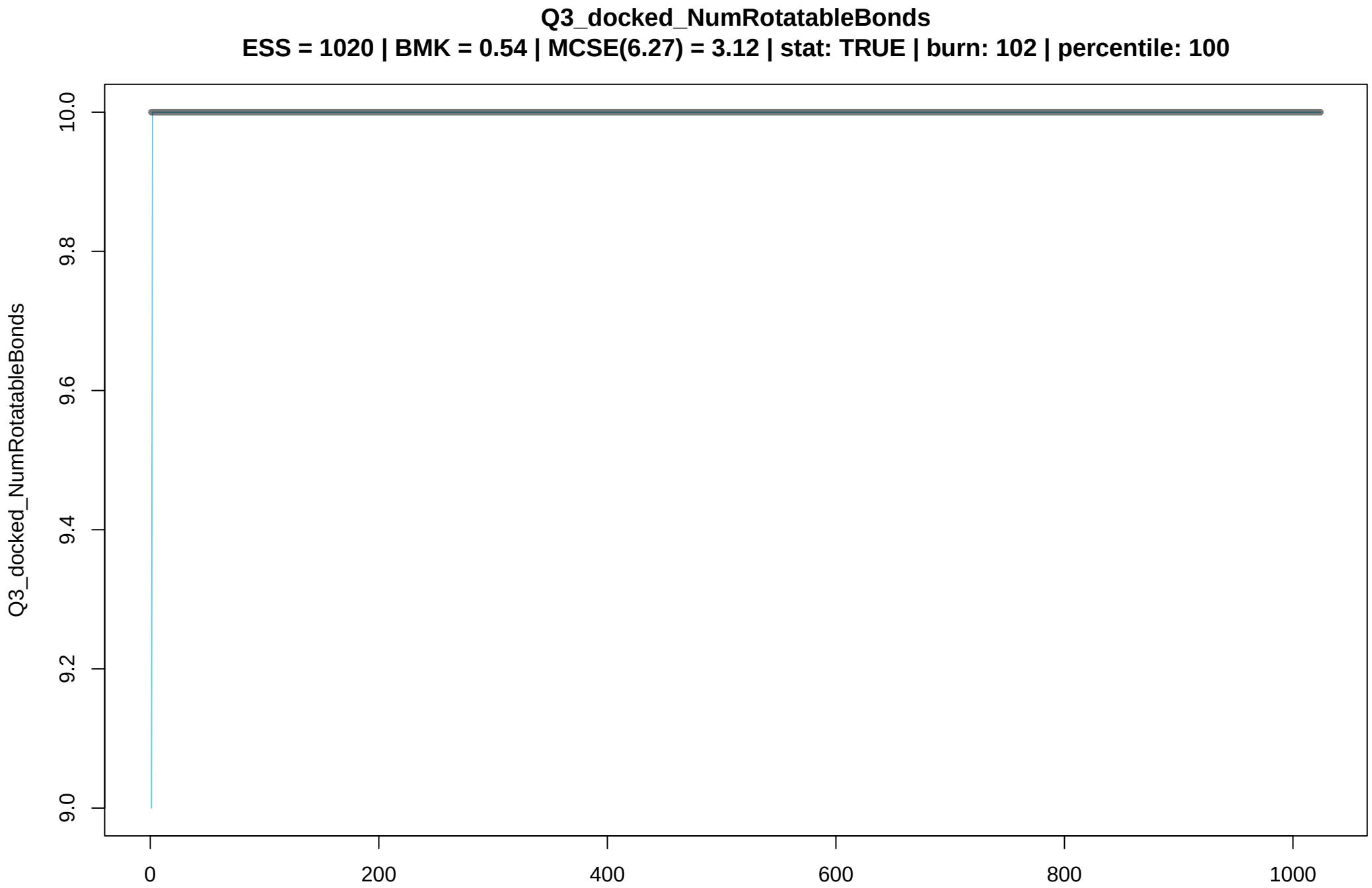

Q3_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0573 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 0 | percentile: 36
Q3_log_mcs_unbonded_polar_sasa
0.25
0.30
0.35
0.40
0.45
0.50
0.55
0
200
400
600
800
1000

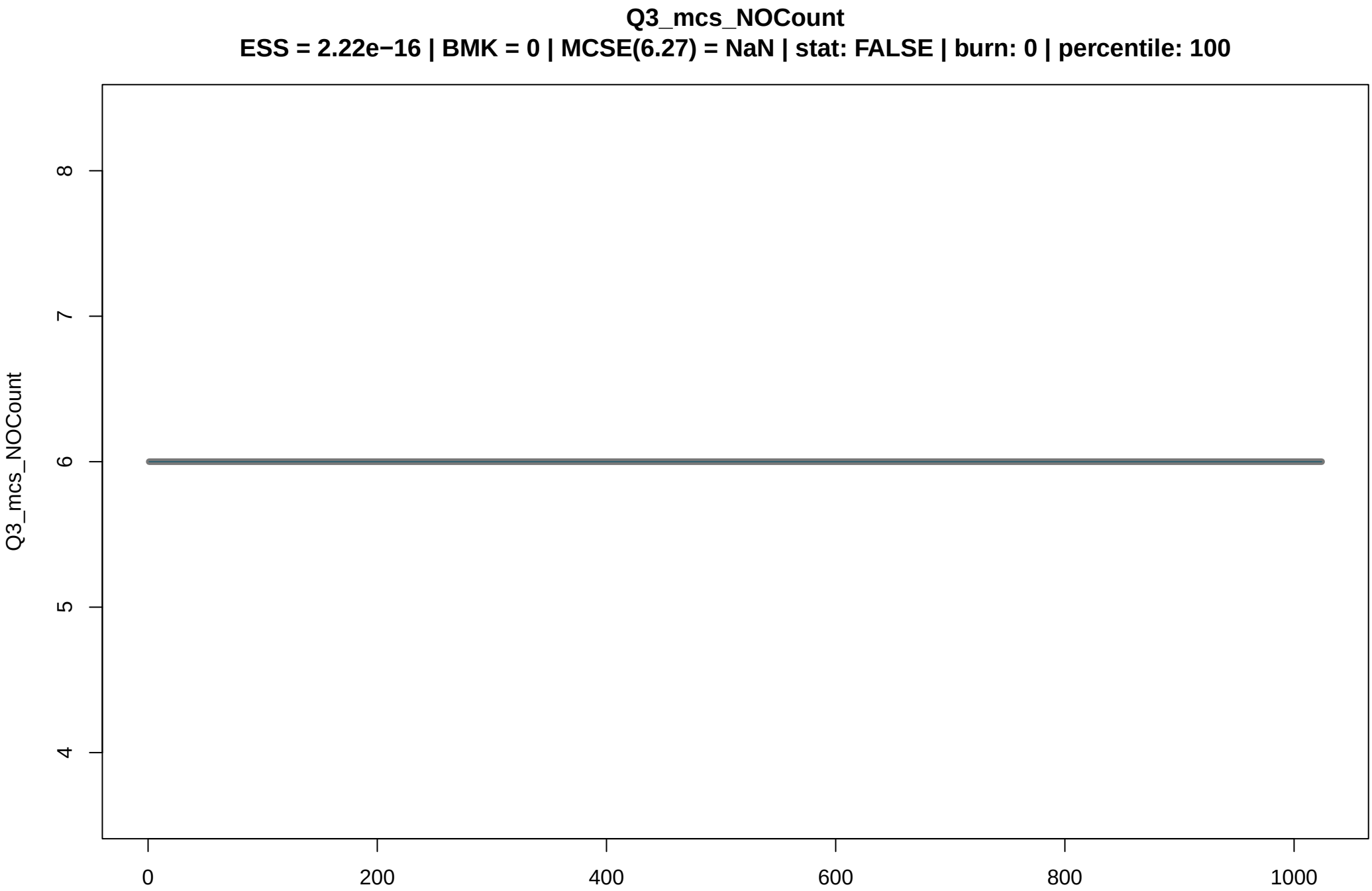

Q3_logit_ec_tanimoto_similarity
ESS = 319 | BMK = 0.167 | MCSE(6.27) = 5.51 | stat: FALSE | burn: 0 | percentile: 0.586
Q3_logit_ec_tanimoto_similarity
3.3
3.4
3.5
3.6
3.7
3.8
3.9
0
200
400
600
800
1000

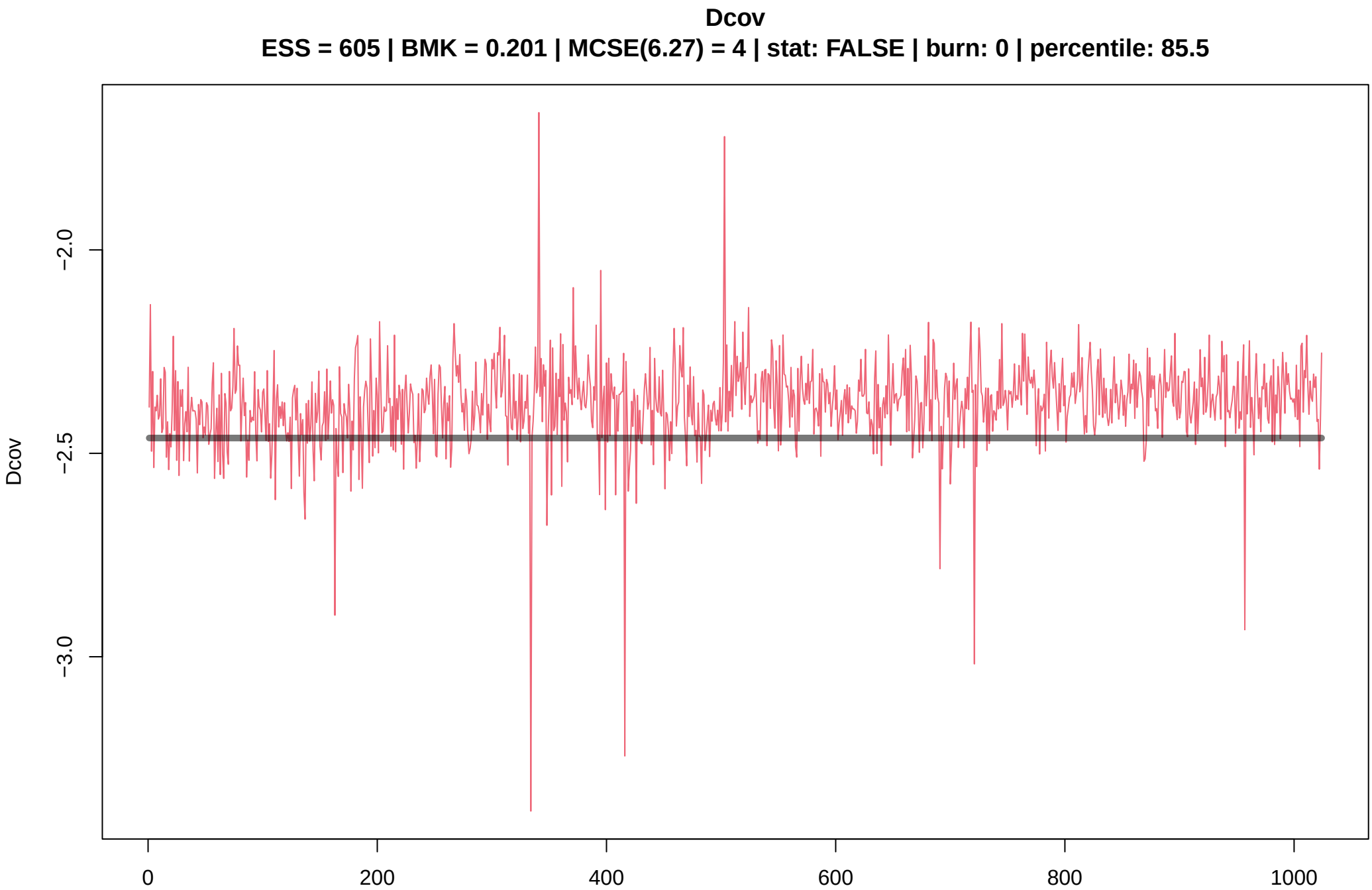

Q3_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.594 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 100
Q3_mcs_NumHeteroAtoms
4.0
3.8
3.6
3.4
3.2
3.0
0
200
400
600
800
1000

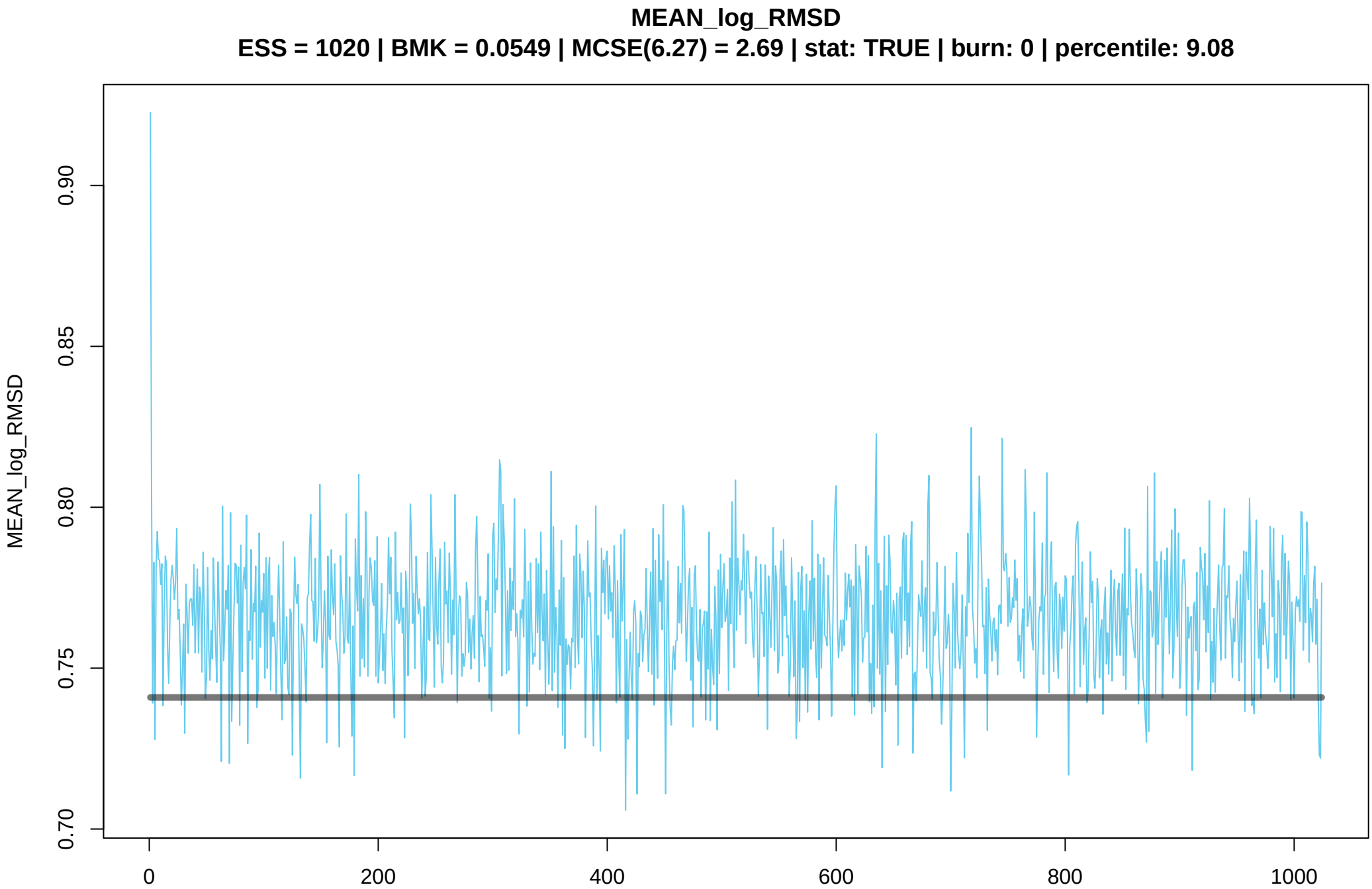

Q3_docked_HeavyAtomCount
ESS = 32.5 | BMK = 0.183 | MCSE(6.27) = 11.2 | stat: FALSE | burn: 0 | percentile: 100
Q3_docked_HeavyAtomCount
41.0
41.5
42.0
42.5
43.0
43.5
44.0
0
200
400
600
800
1000

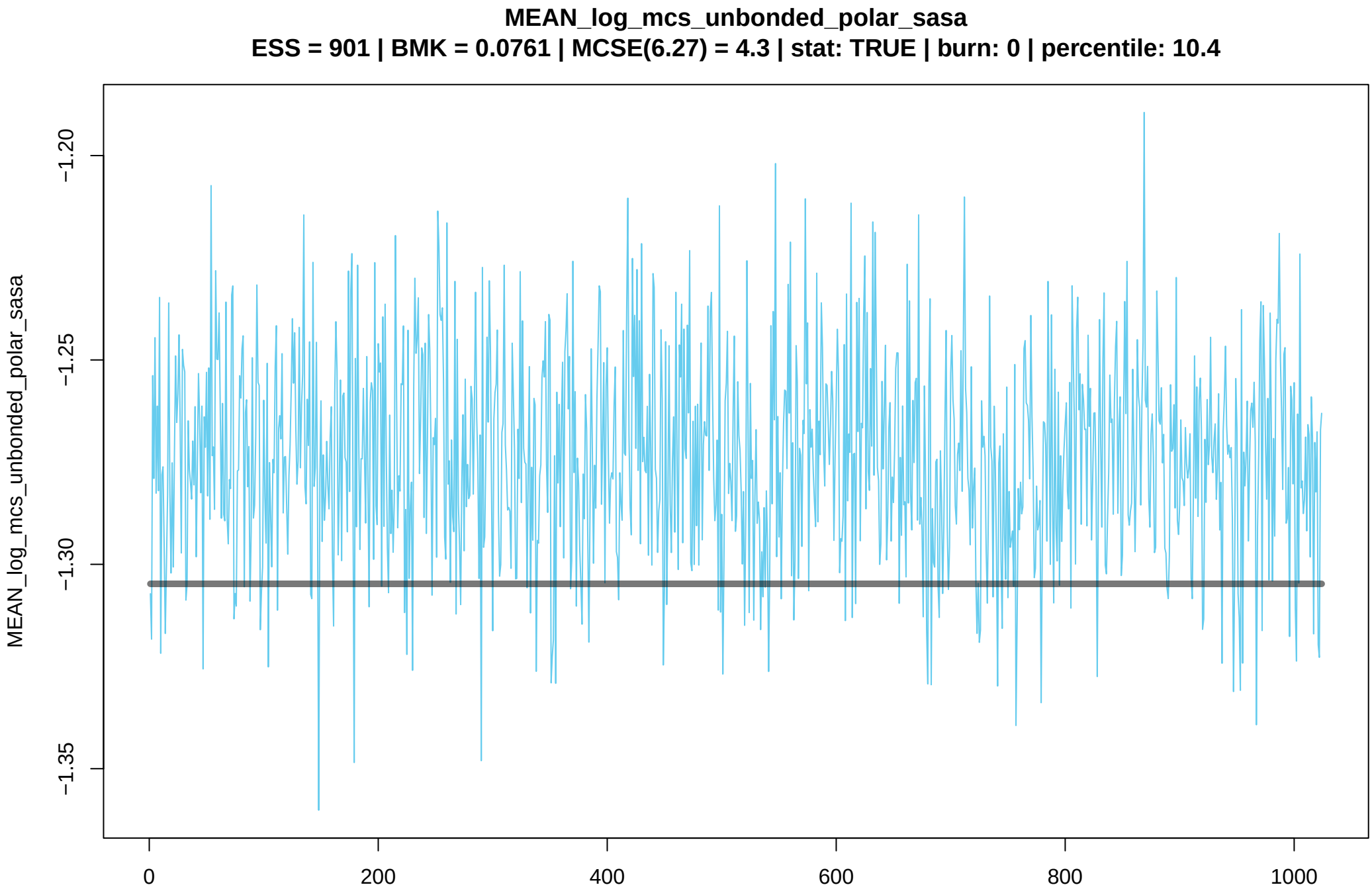

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q3_mcs_RingCount
4.0
3.5
3.0
2.5
2.0
0
200
400
600
800
1000

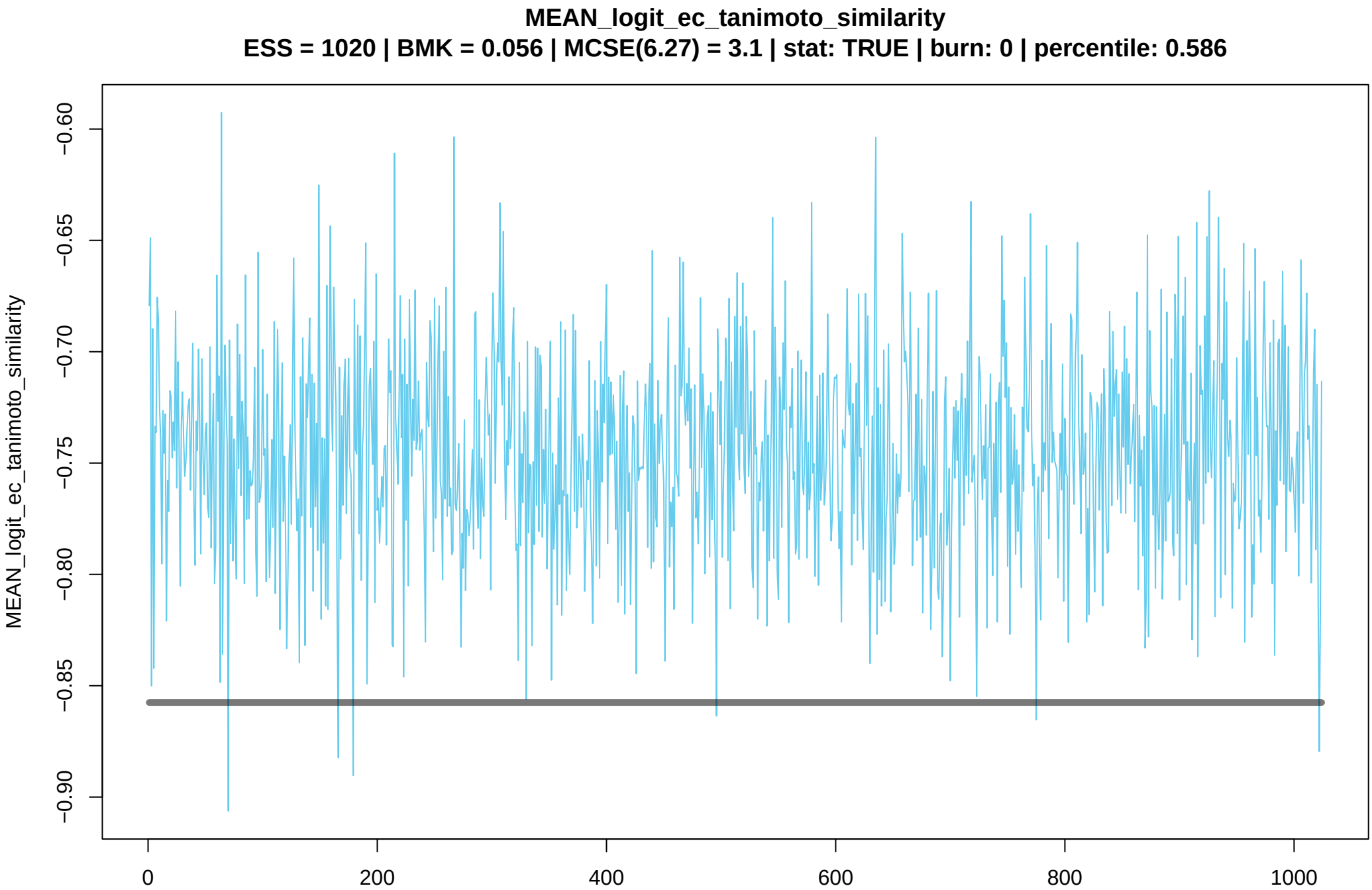

Q3_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.54 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 102 | percentile: 100
Q3_docked_NumRotatableBonds
10.0
9.8
9.6
9.4
9.2
9.0
0
200
400
600
800
1000

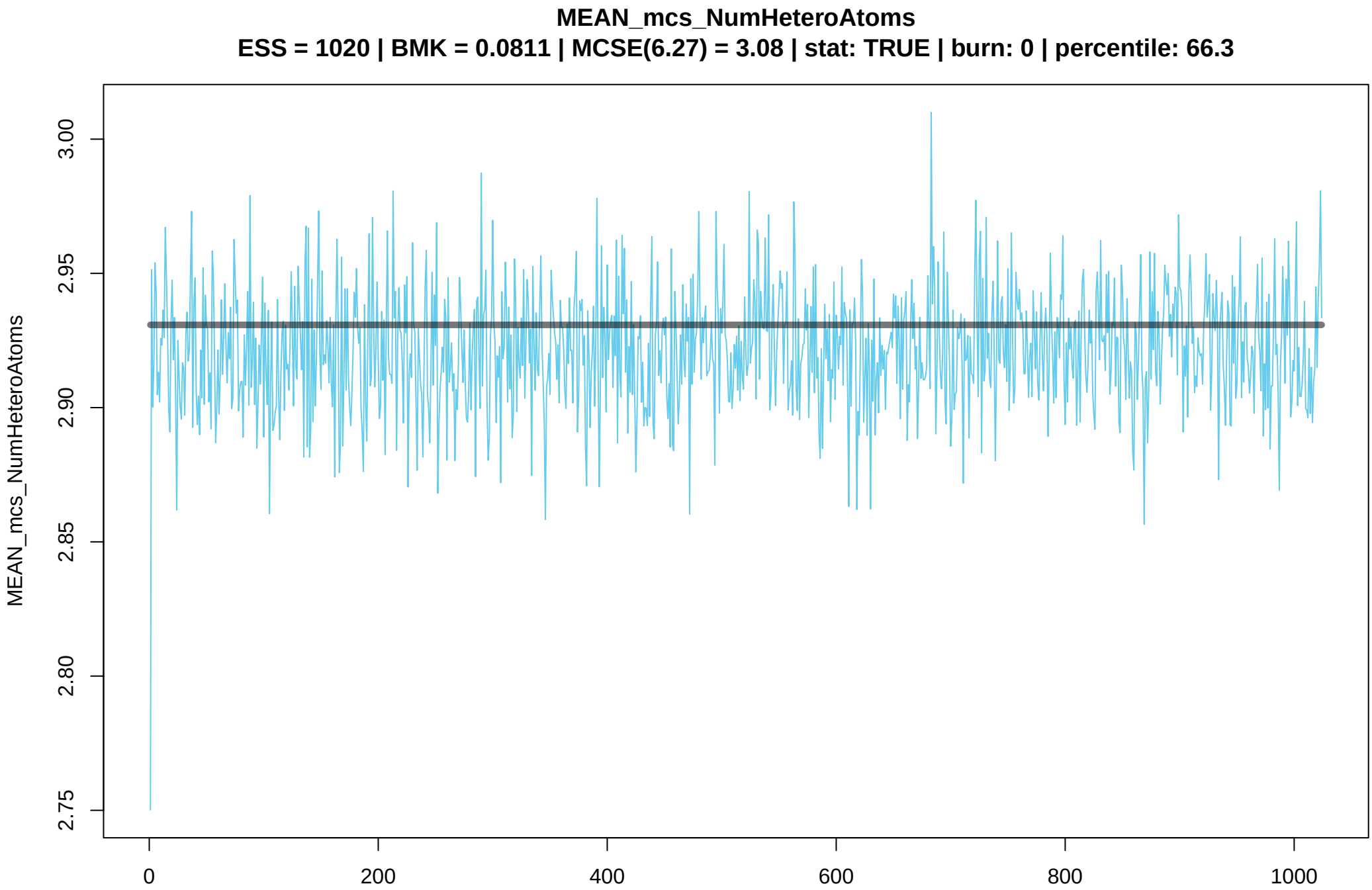

Q3_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q3_mcs_NOCount
4
5
6
7
8
0
200
400
600
800
1000

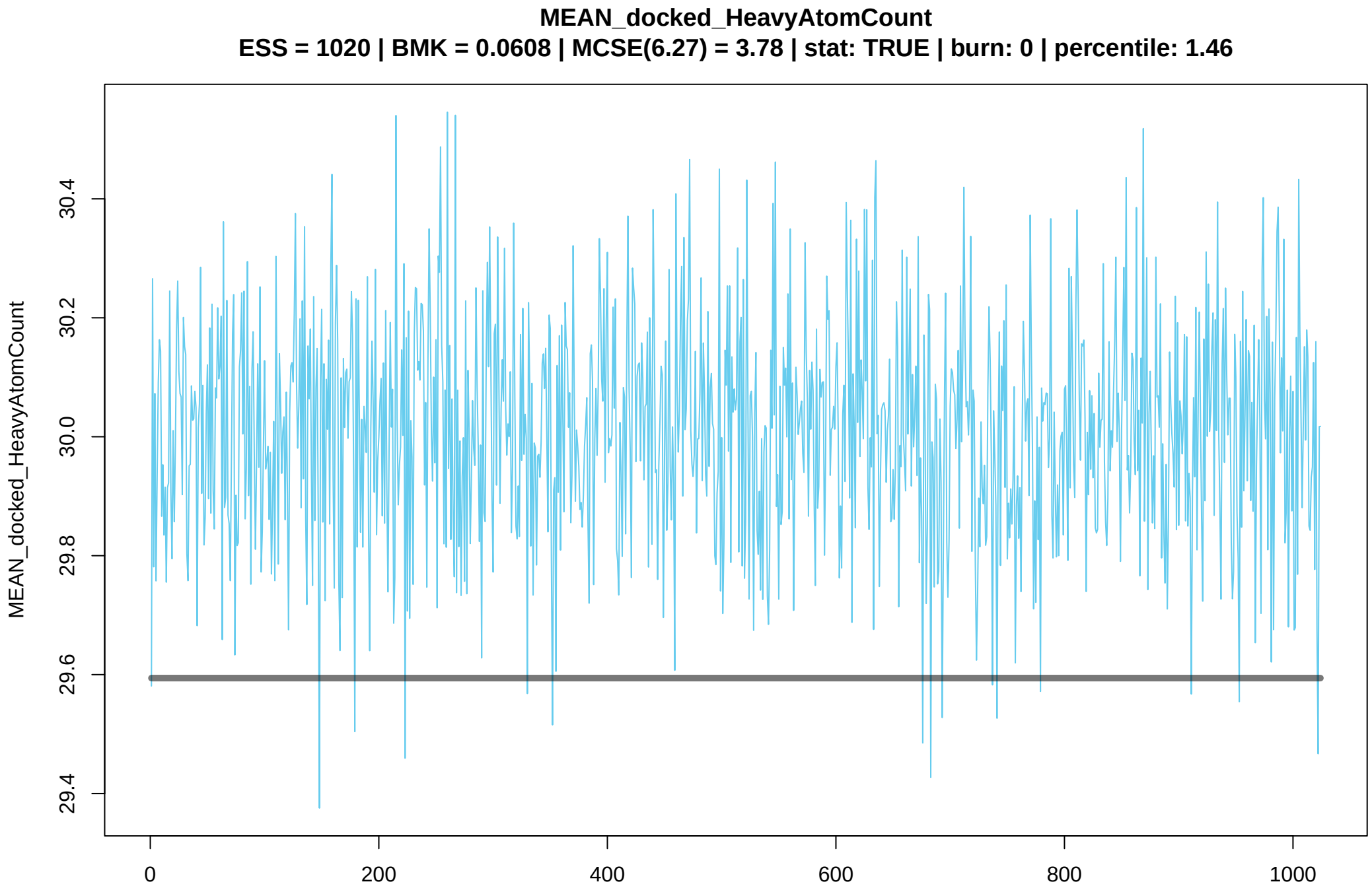

Dcov
ESS = 605 | BMK = 0.201 | MCSE(6.27) = 4 | stat: FALSE | burn: 0 | percentile: 85.5
Dcov
−2.0
−2.5
−3.0
0
200
400
600
800
1000

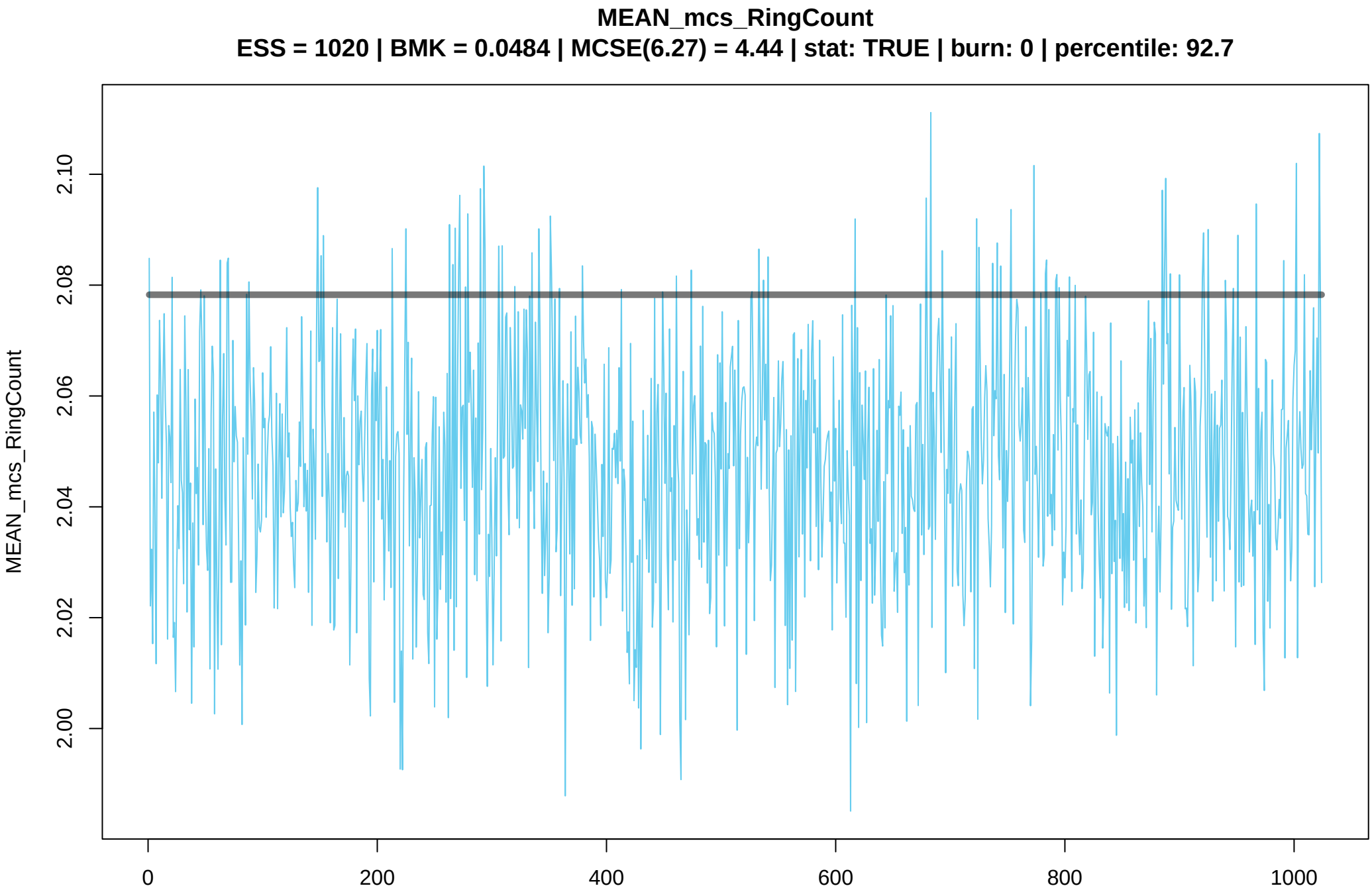

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0549 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | percentile: 9.08
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0.90
0
200
400
600
800
1000

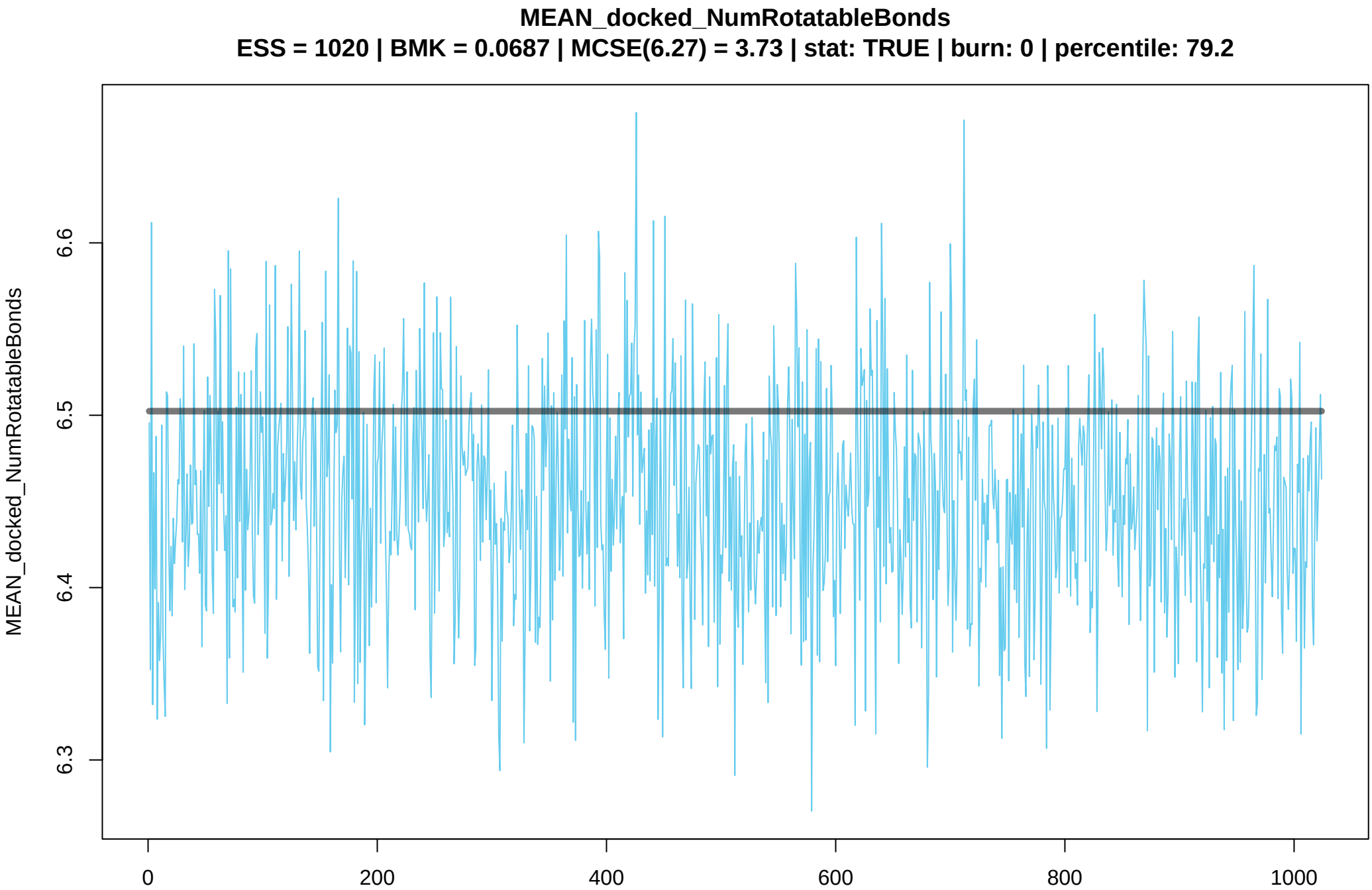

MEAN_log_mcs_unbonded_polar_sasa
ESS = 901 | BMK = 0.0761 | MCSE(6.27) = 4.3 | stat: TRUE | burn: 0 | percentile: 10.4
MEAN_log_mcs_unbonded_polar_sasa
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

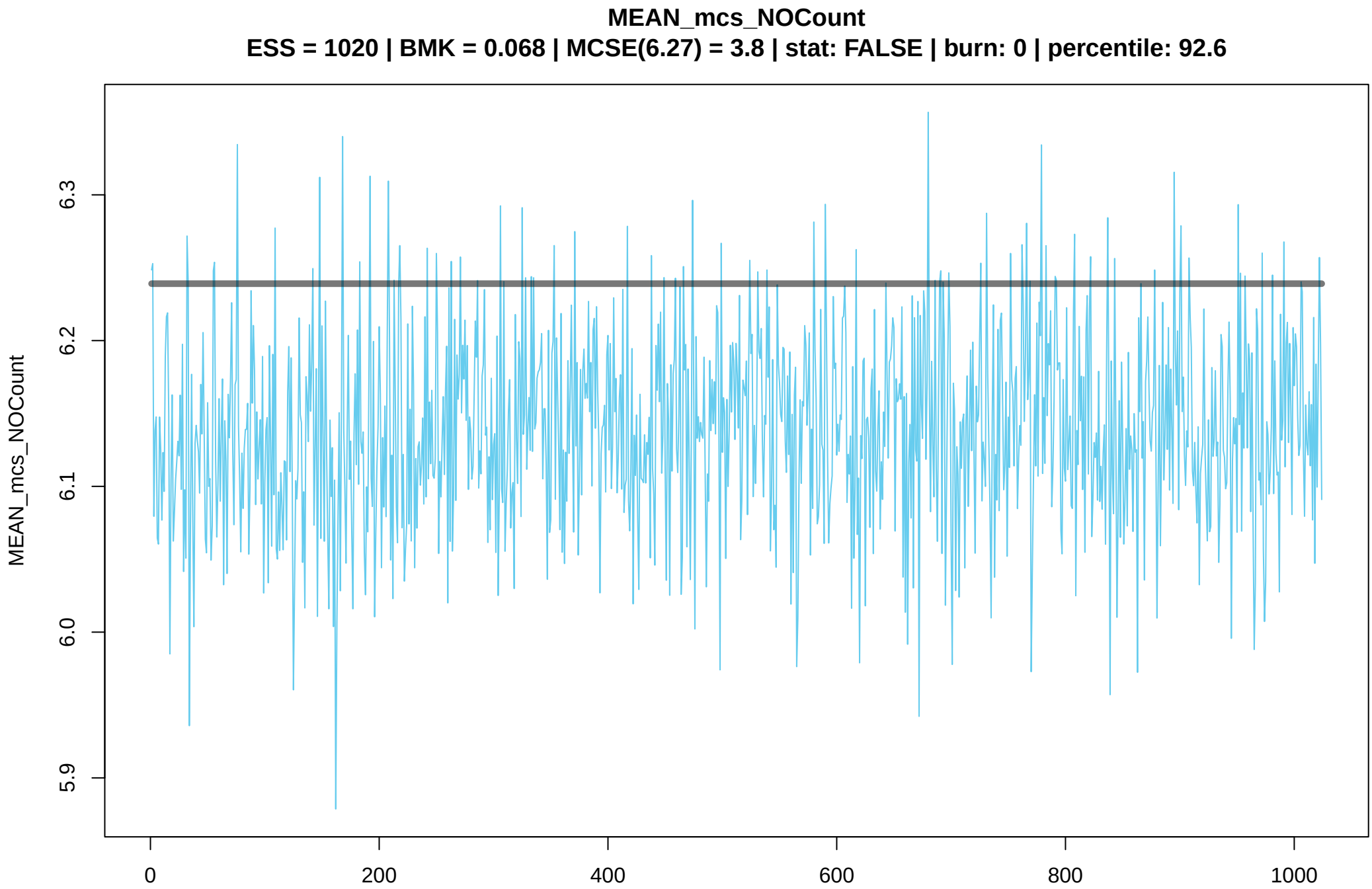

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.056 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | percentile: 0.586
MEAN_logit_ec_tanimoto_similarity
−0.60
−0.65
−0.70
−0.75
−0.80
−0.85
−0.90
0
200
400
600
800
1000

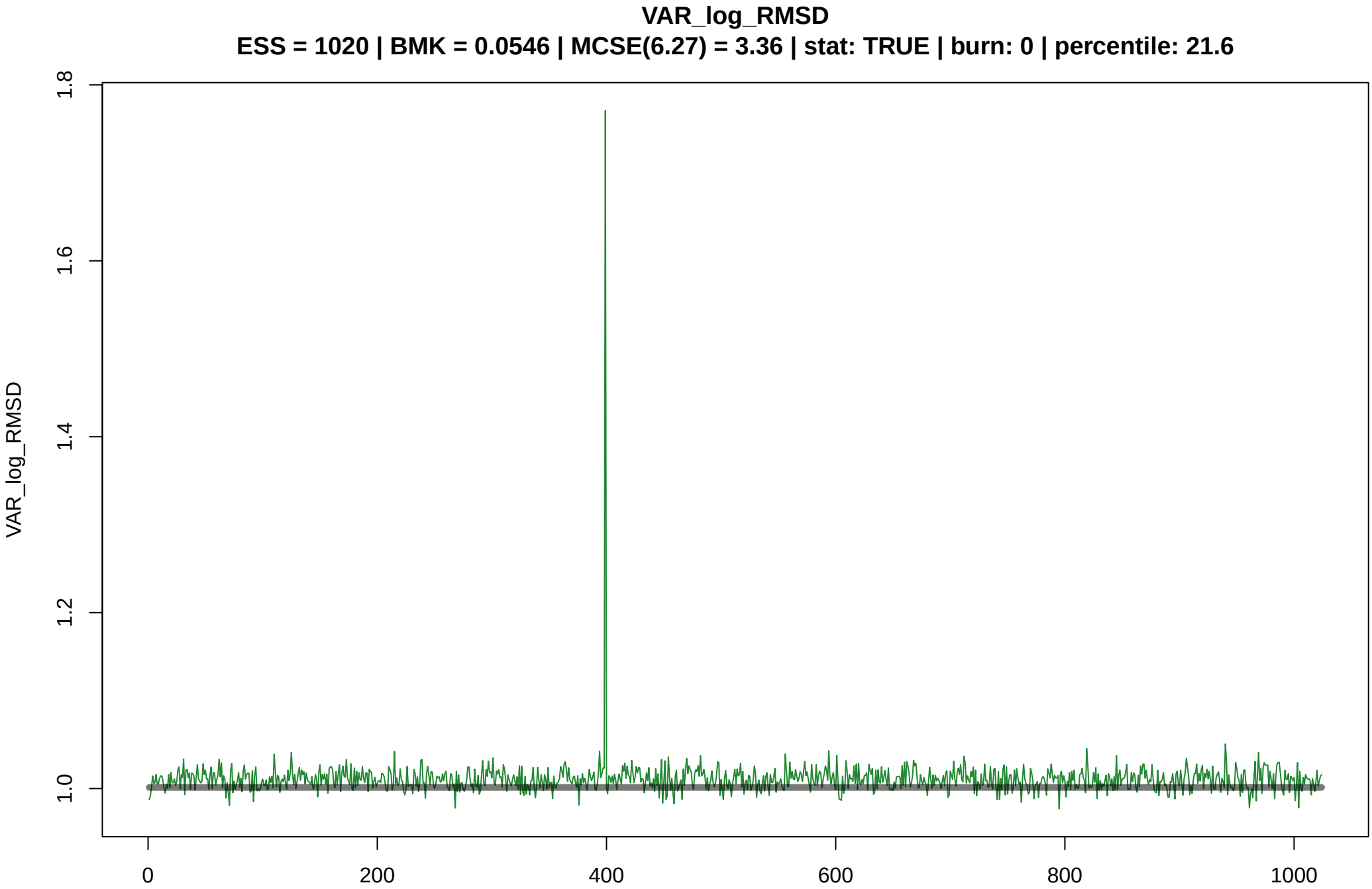

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0811 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | percentile: 66.3
MEAN_mcs_NumHeteroAtoms
2.75
2.80
2.85
2.90
2.95
3.00
0
200
400
600
800
1000

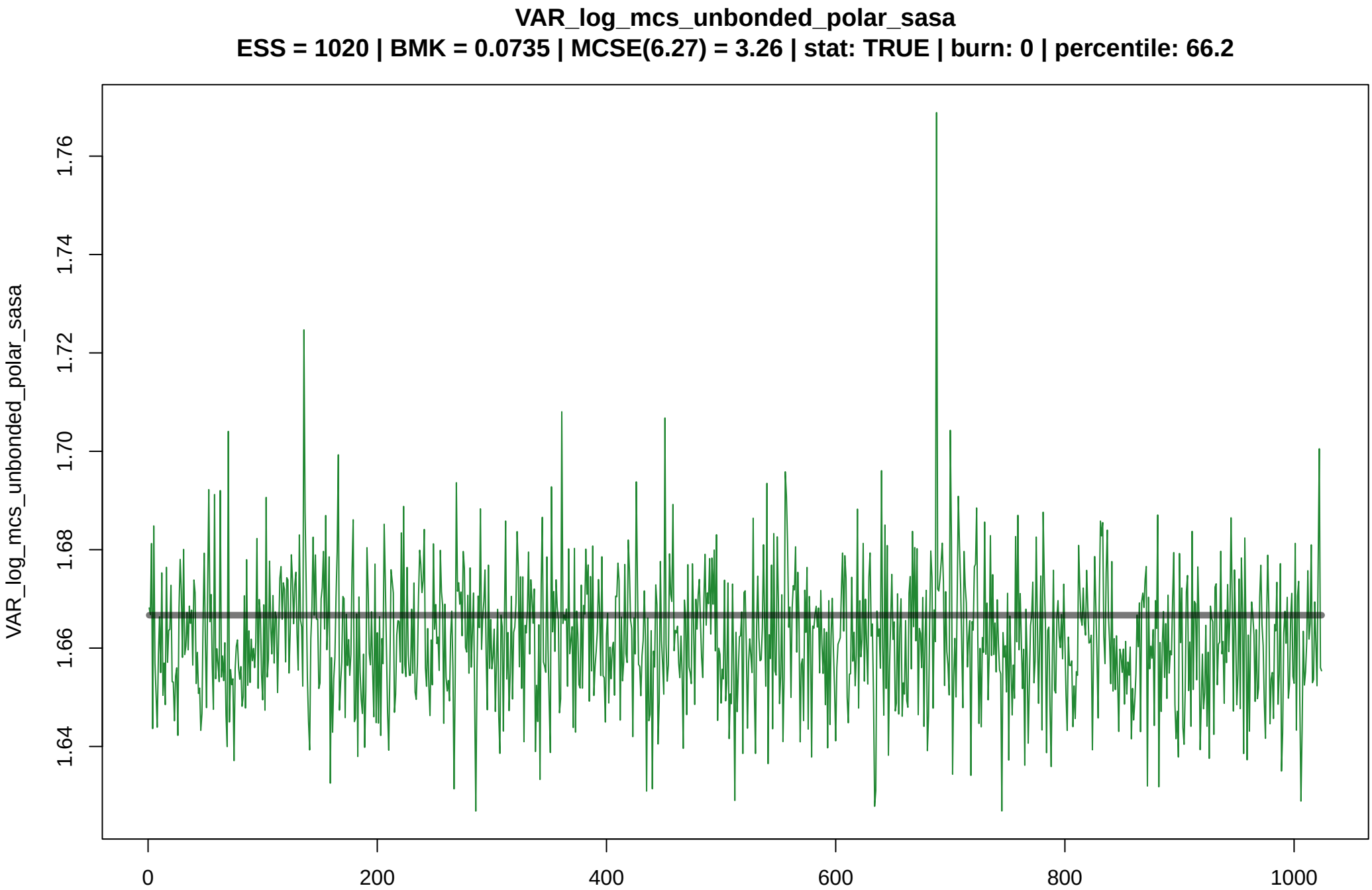

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0608 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0 | percentile: 1.46
MEAN_docked_HeavyAtomCount
29.4
29.6
29.8
30.0
30.2
30.4
0
200
400
600
800
1000

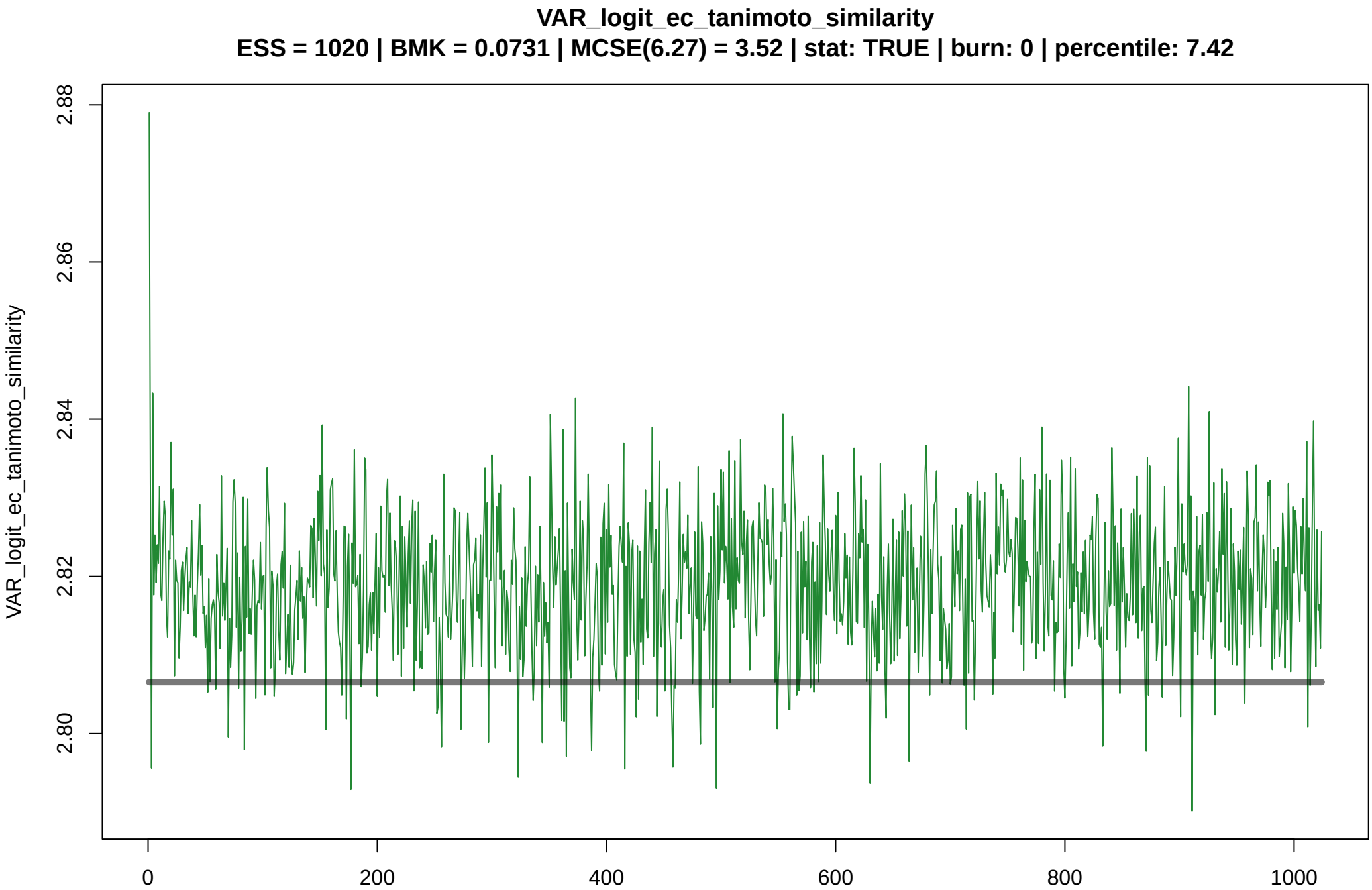

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0484 | MCSE(6.27) = 4.44 | stat: TRUE | burn: 0 | percentile: 92.7
MEAN_mcs_RingCount
2.00
2.02
2.04
2.06
2.08
2.10
0
200
400
600
800
1000

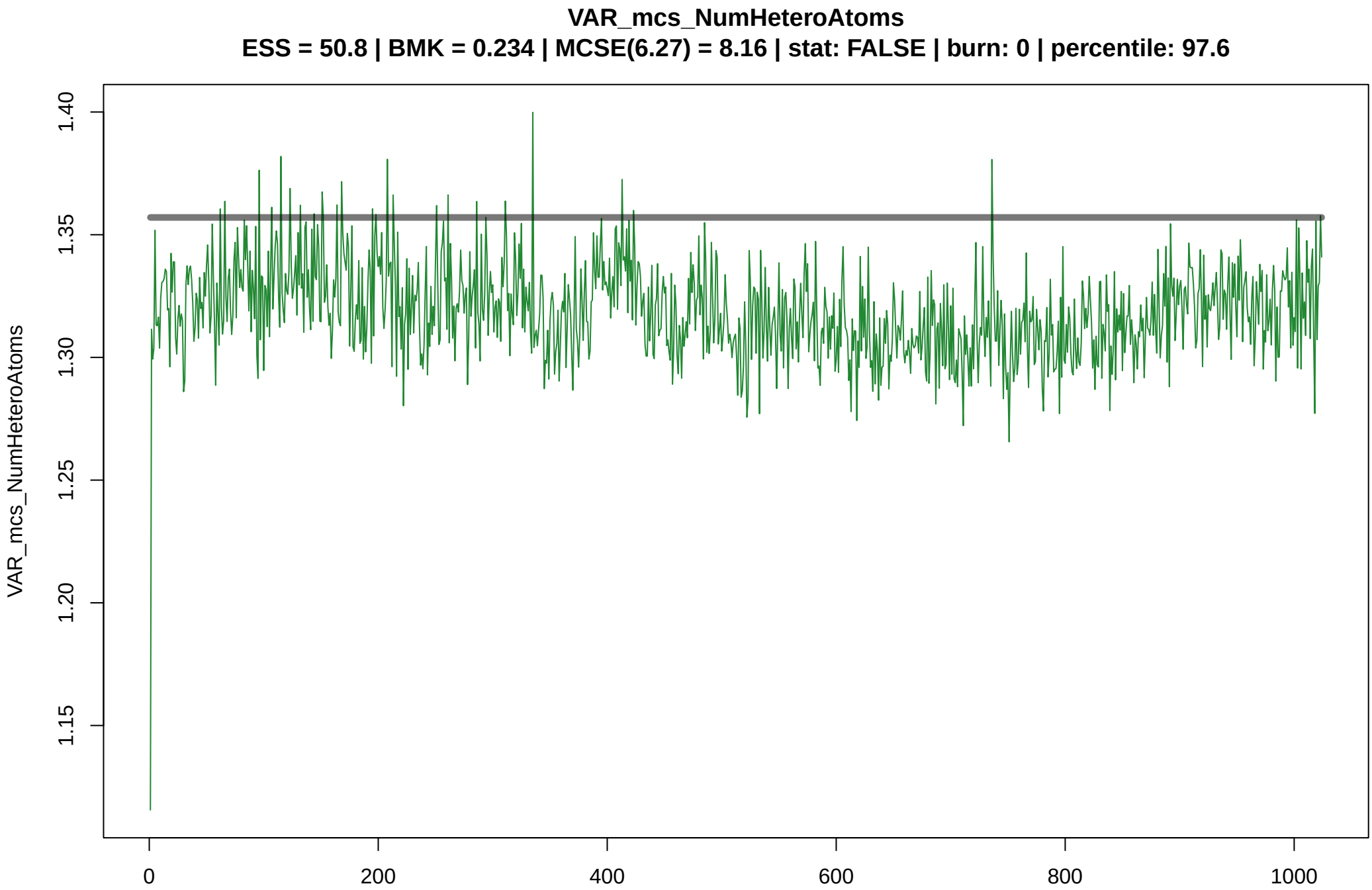

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0687 | MCSE(6.27) = 3.73 | stat: TRUE | burn: 0 | percentile: 79.2
MEAN_docked_NumRotatableBonds
6.3
6.4
6.5
6.6
0
200
400
600
800
1000

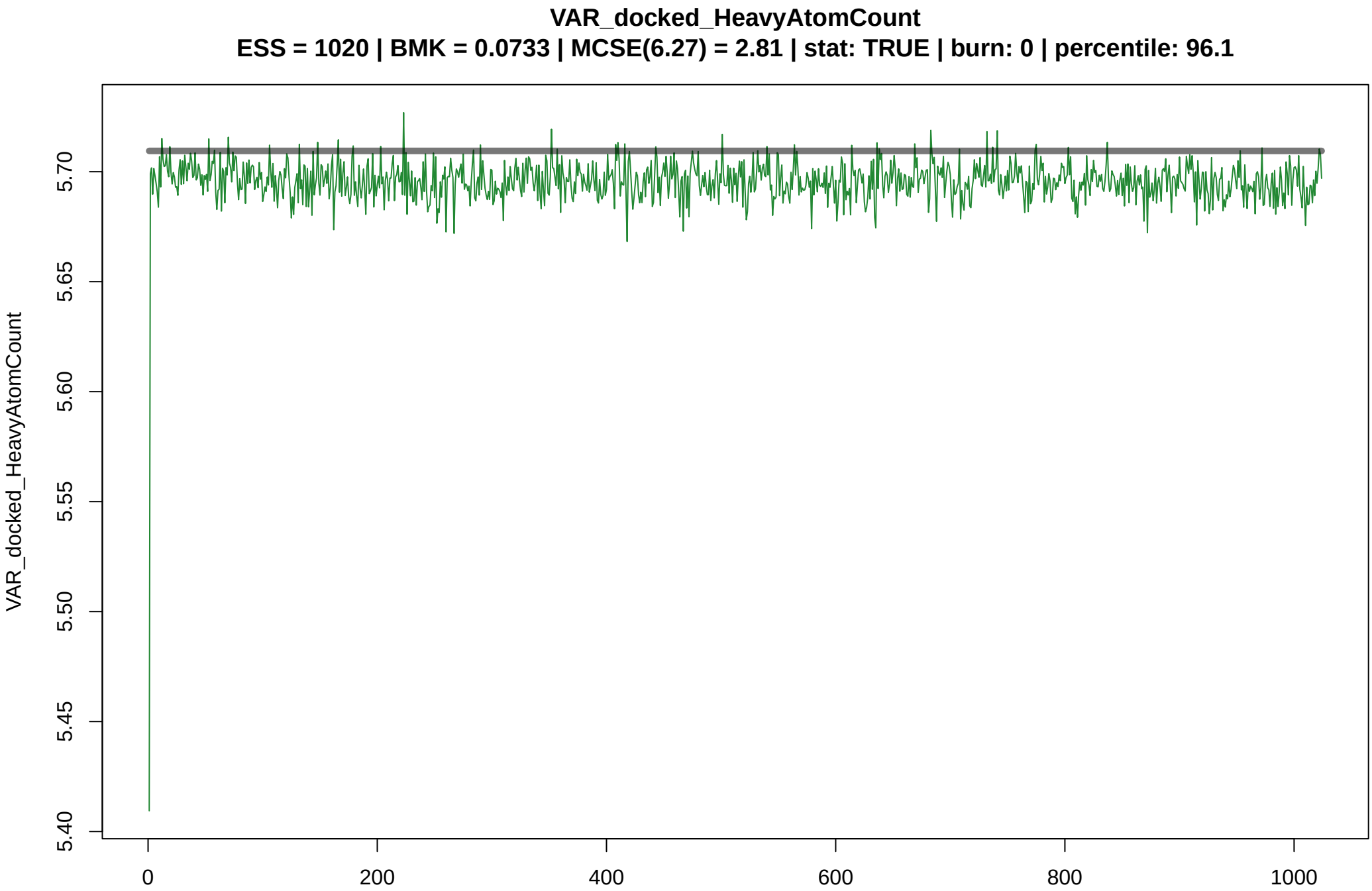

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.068 | MCSE(6.27) = 3.8 | stat: FALSE | burn: 0 | percentile: 92.6
MEAN_mcs_NOCount
6.3
6.2
6.1
6.0
5.9
0
200
400
600
800
1000

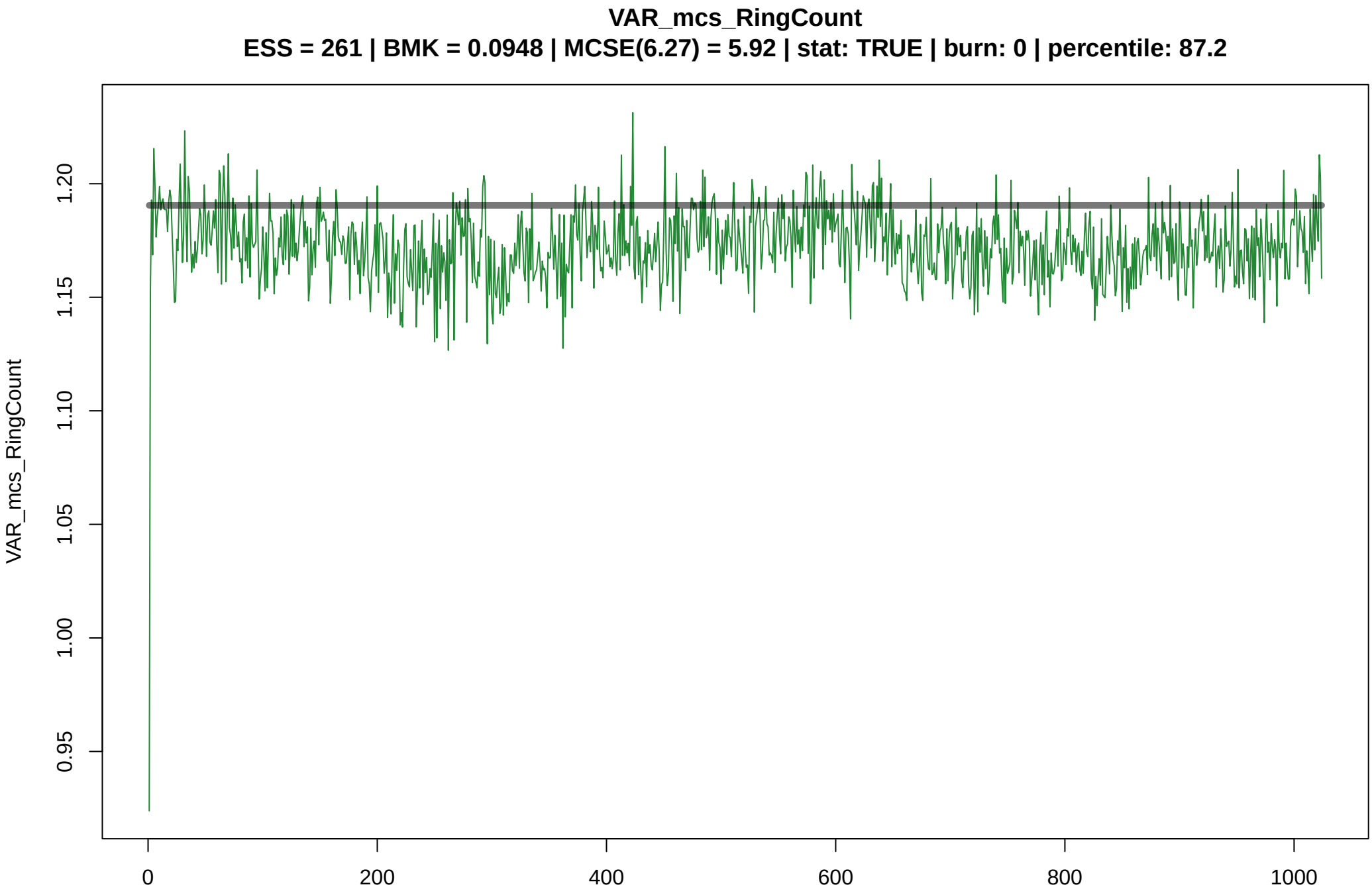

VAR_log_RMSD
ESS = 1020 | BMK = 0.0546 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | percentile: 21.6
VAR_log_RMSD
1.0
1.2
1.4
1.6
1.8
0
200
400
600
800
1000

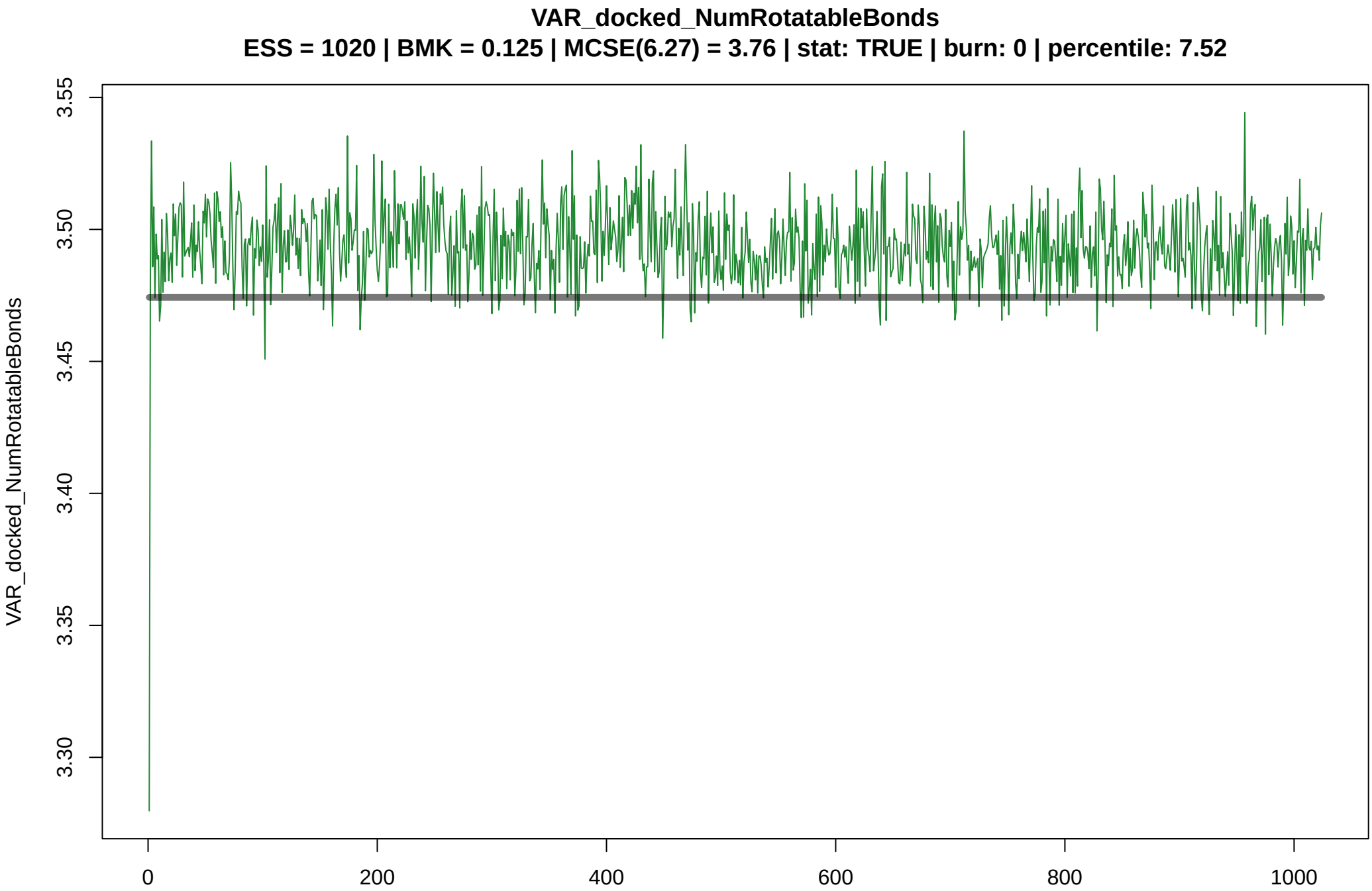

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0735 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0 | percentile: 66.2
VAR_log_mcs_unbonded_polar_sasa
1.64
1.66
1.68
1.70
1.72
1.74
1.76
0
200
400
600
800
1000

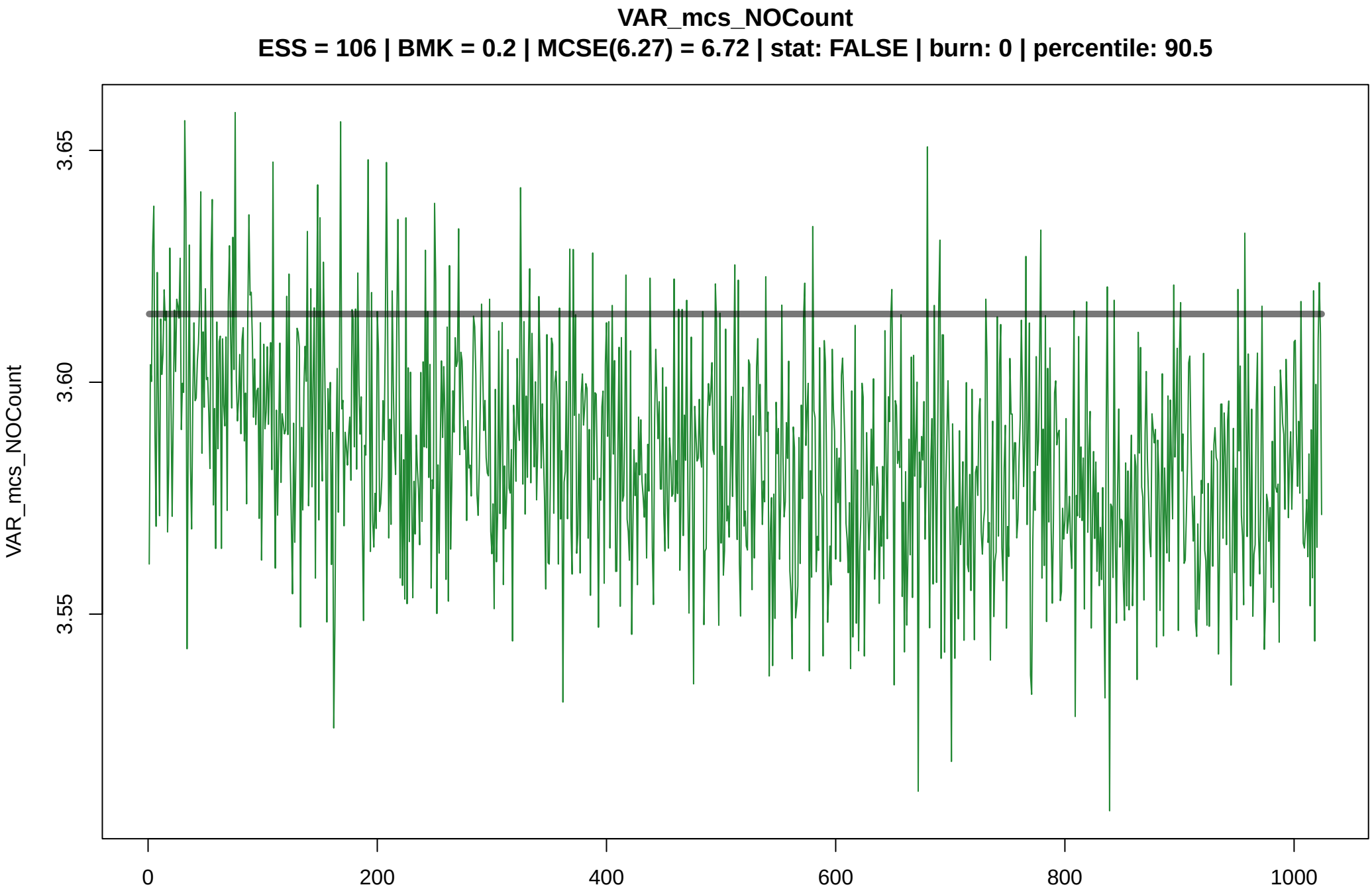

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0731 | MCSE(6.27) = 3.52 | stat: TRUE | burn: 0 | percentile: 7.42
VAR_logit_ec_tanimoto_similarity
2.88
2.86
2.84
2.82
2.80
0
200
400
600
800
1000

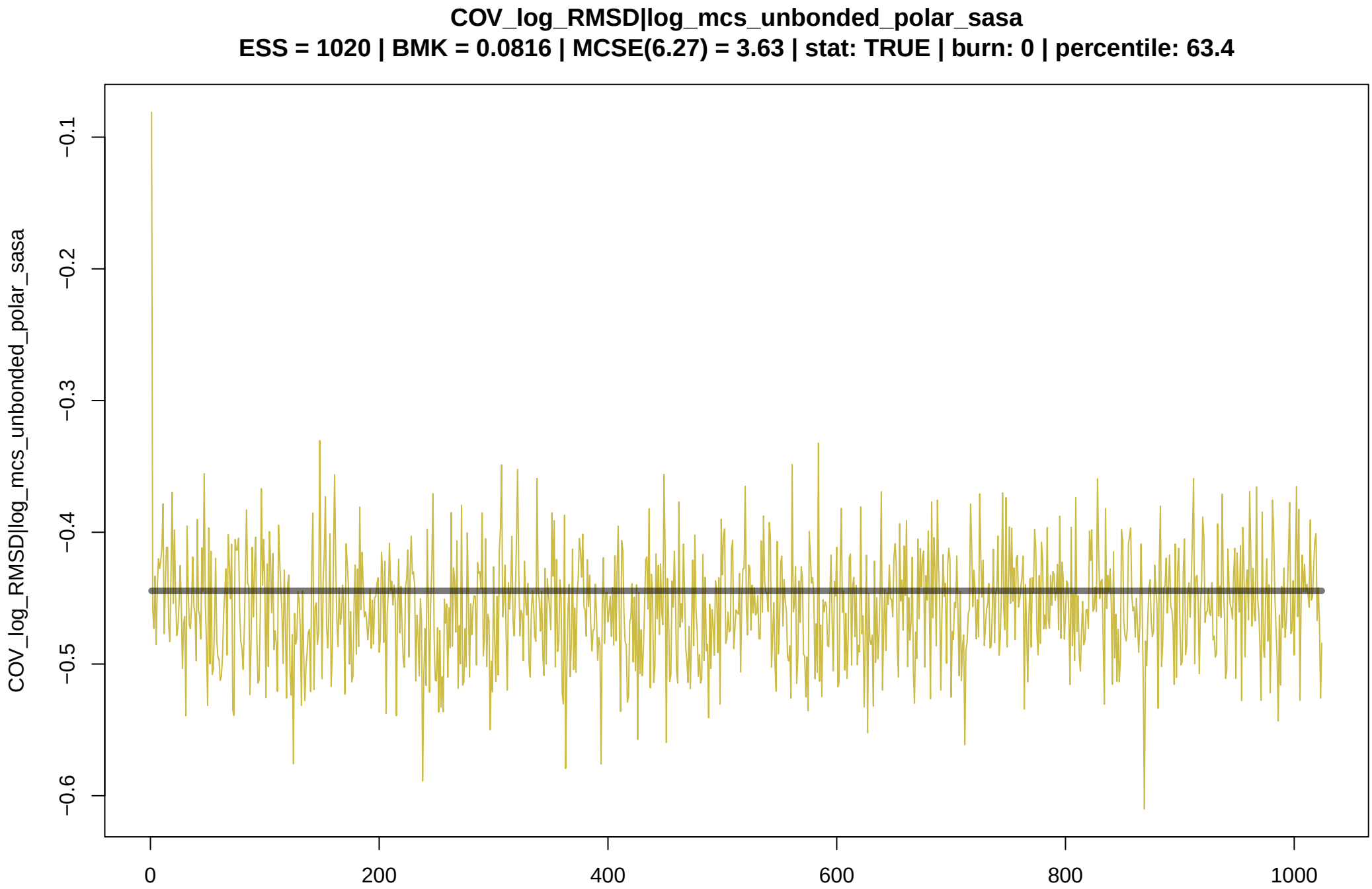

VAR_mcs_NumHeteroAtoms
ESS = 50.8 | BMK = 0.234 | MCSE(6.27) = 8.16 | stat: FALSE | burn: 0 | percentile: 97.6
VAR_mcs_NumHeteroAtoms
1.15
1.20
1.25
1.30
1.35
1.40
0
200
400
600
800
1000

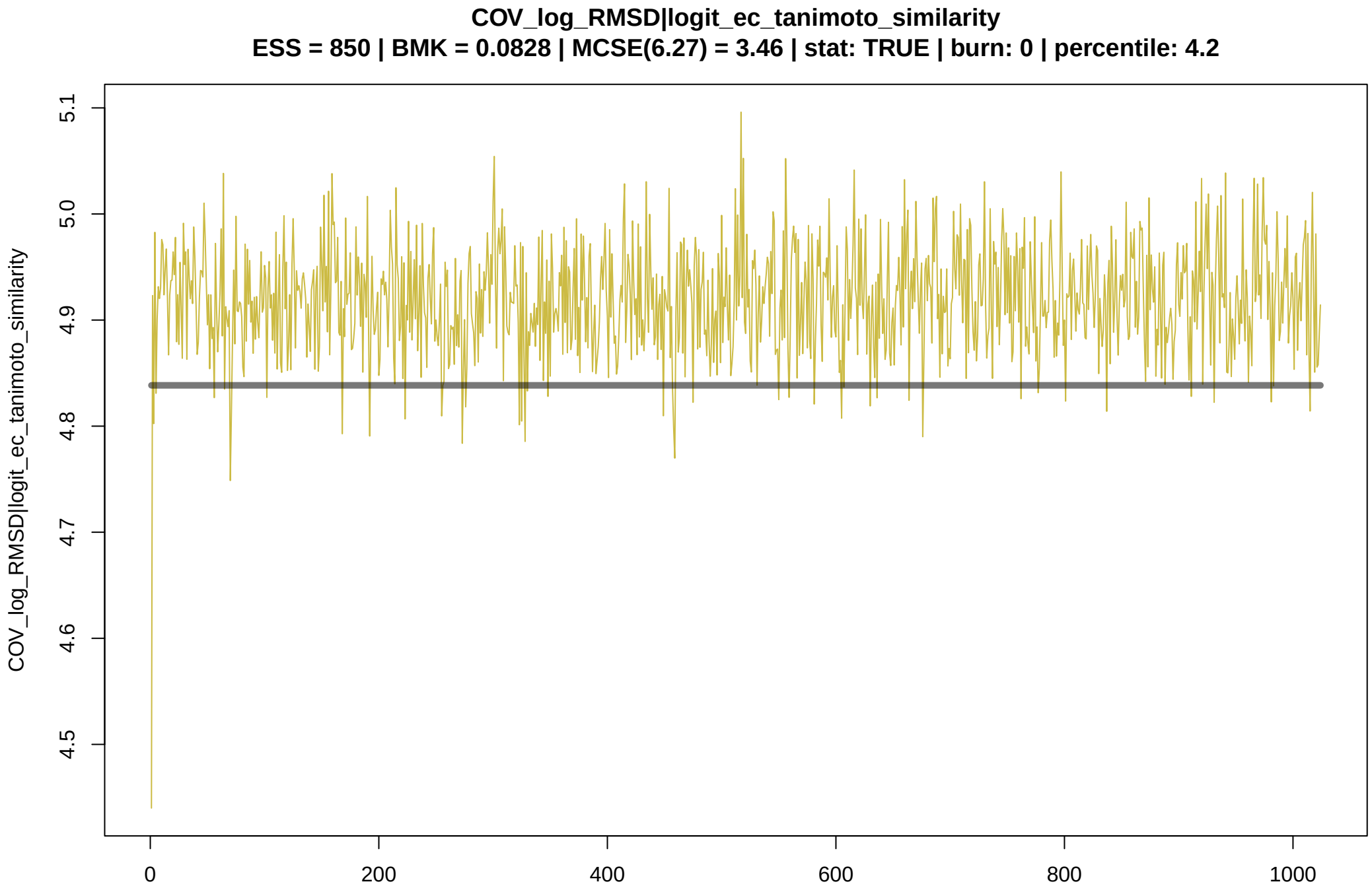

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0733 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | percentile: 96.1
VAR_docked_HeavyAtomCount
5.40
5.45
5.50
5.55
5.60
5.65
5.70
0
200
400
600
800
1000

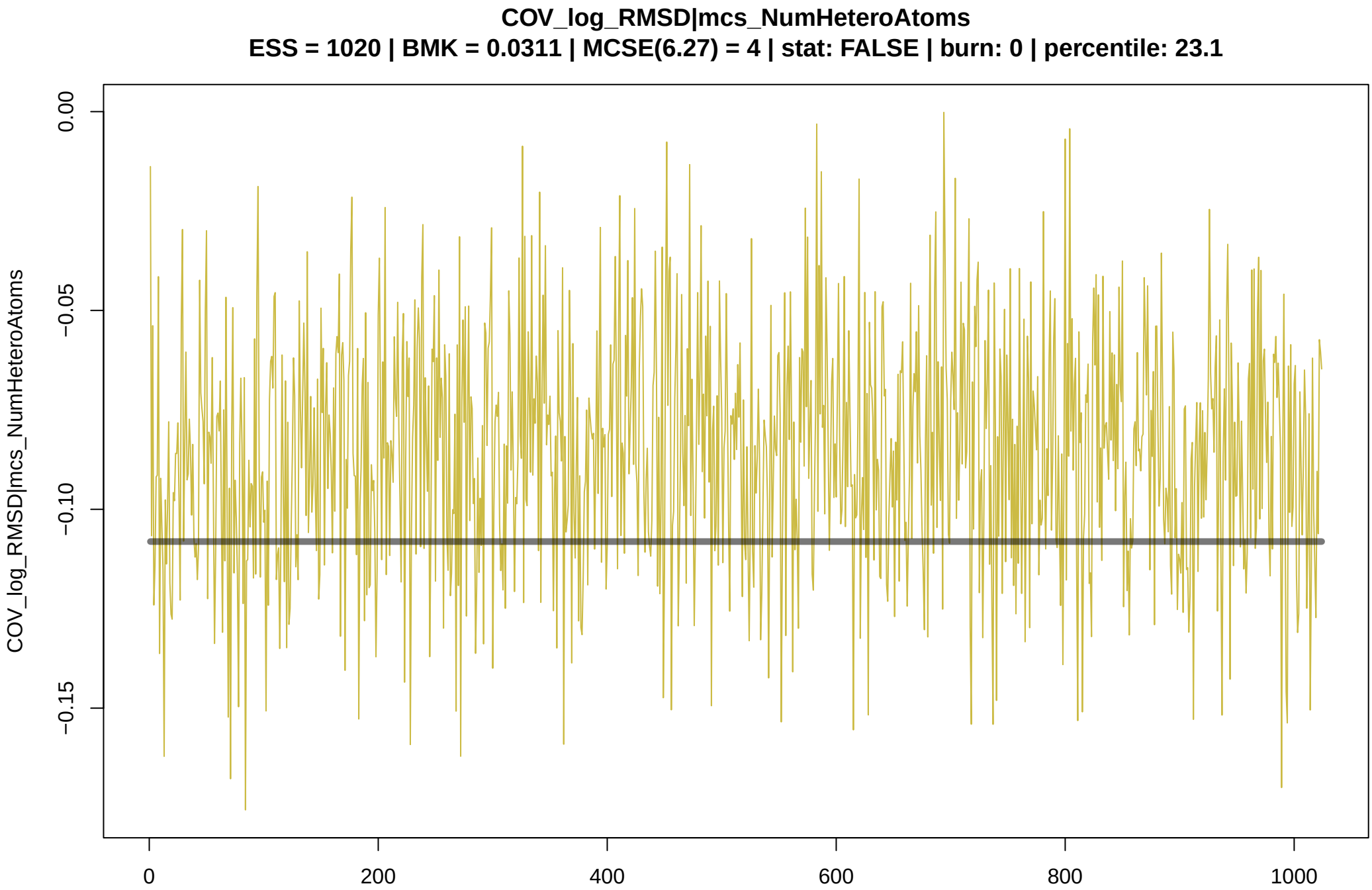

VAR_mcs_RingCount
ESS = 261 | BMK = 0.0948 | MCSE(6.27) = 5.92 | stat: TRUE | burn: 0 | percentile: 87.2
VAR_mcs_RingCount
0.95
1.00
1.05
1.10
1.15
1.20
0
200
400
600
800
1000

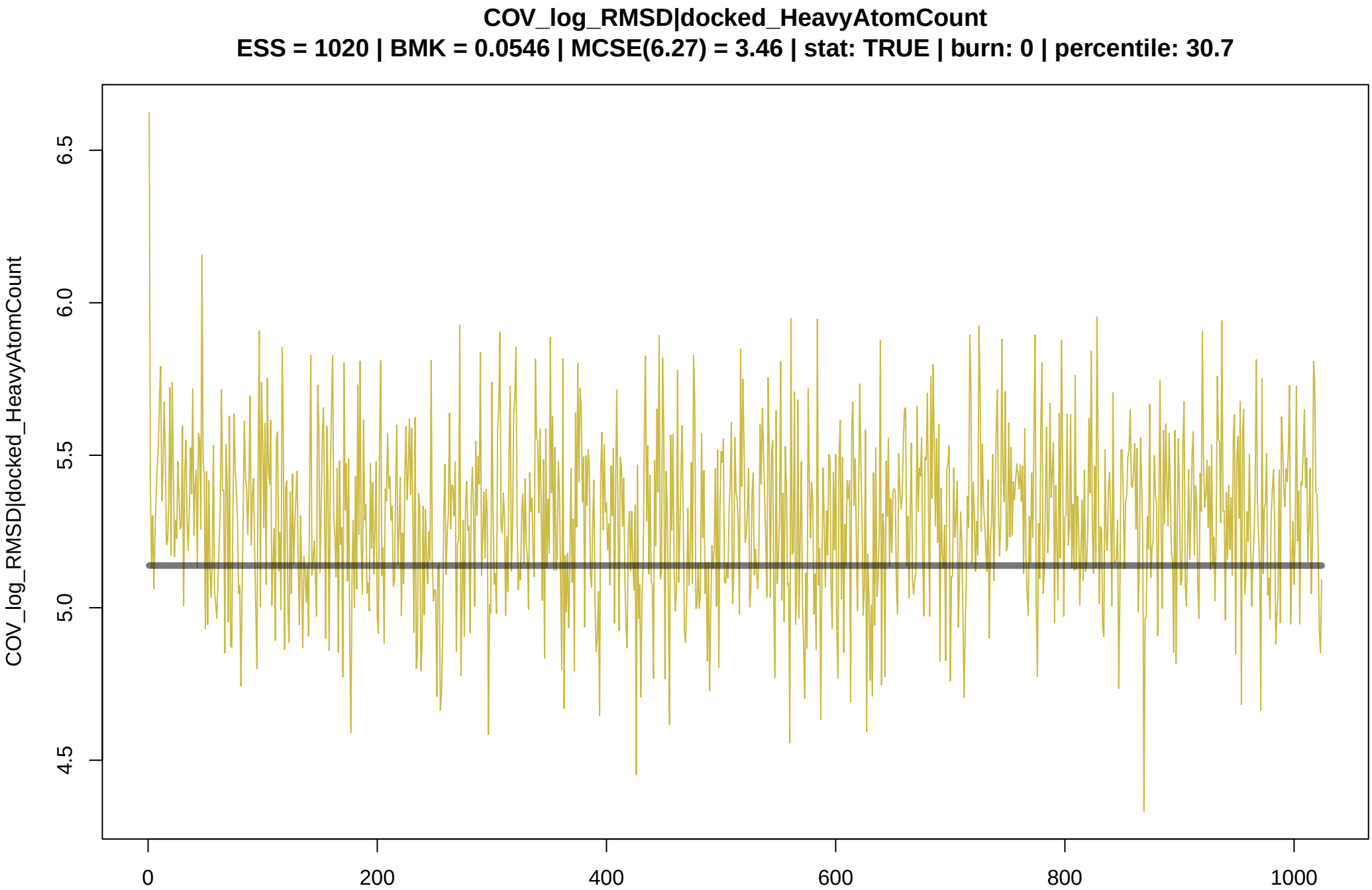

VAR_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.125 | MCSE(6.27) = 3.76 | stat: TRUE | burn: 0 | percentile: 7.52
VAR_docked_NumRotatableBonds
3.30
3.35
3.40
3.45
3.50
3.55
0
200
400
600
800
1000

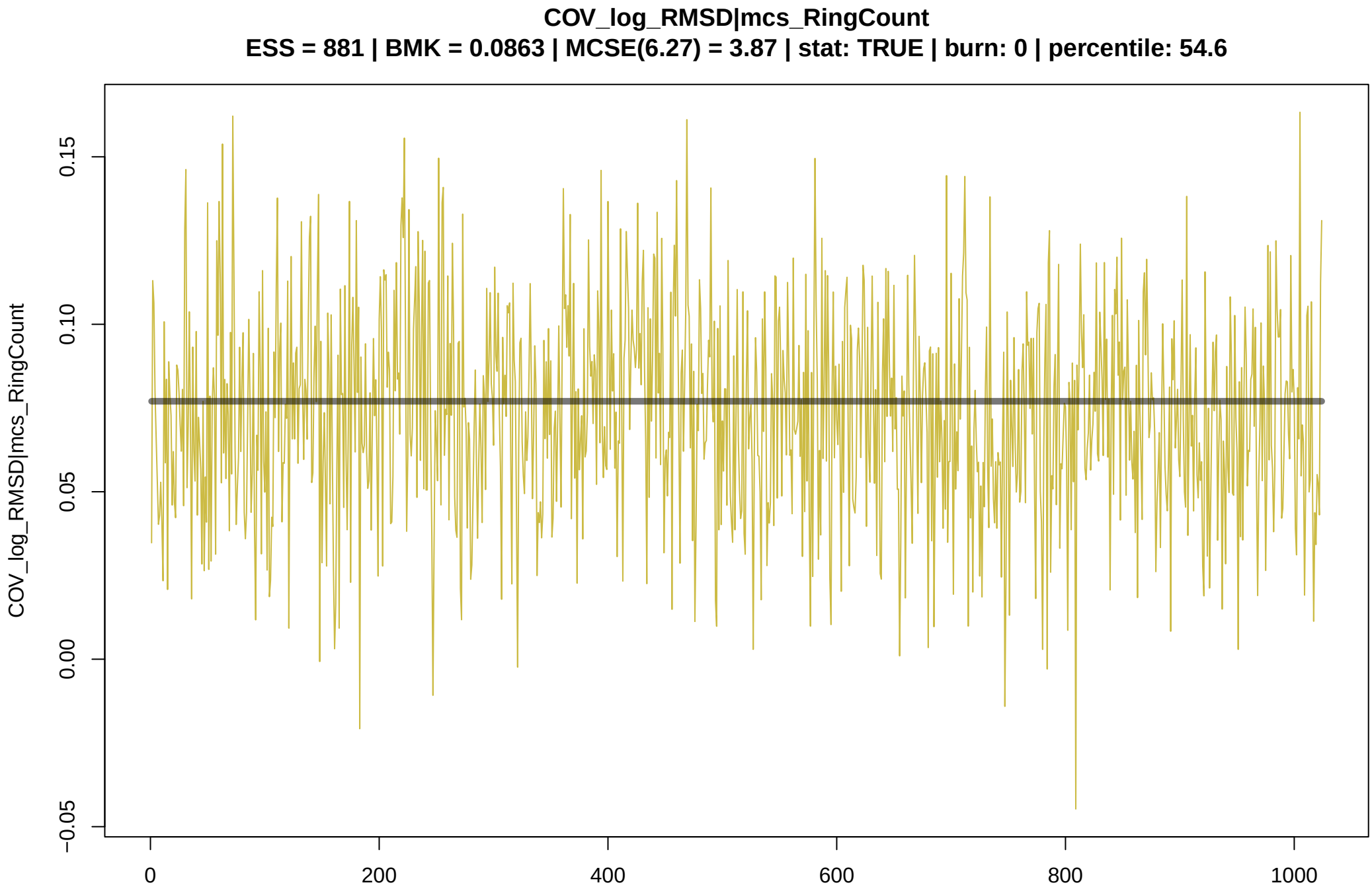

VAR_mcs_NOCount
ESS = 106 | BMK = 0.2 | MCSE(6.27) = 6.72 | stat: FALSE | burn: 0 | percentile: 90.5
VAR_mcs_NOCount
3.65
3.60
3.55
0
200
400
600
800
1000

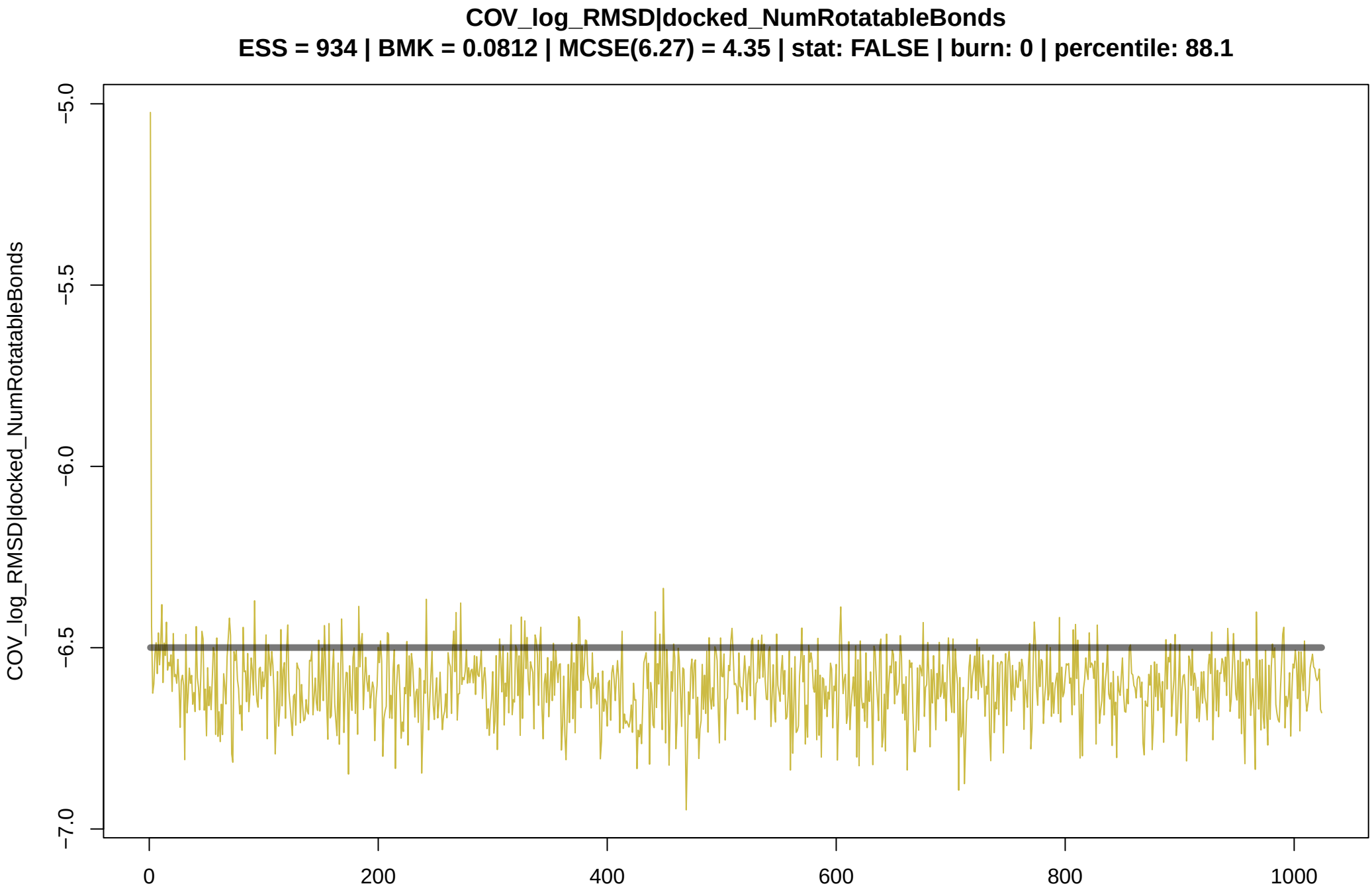

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0816 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | percentile: 63.4
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
0
200
400
600
800
1000

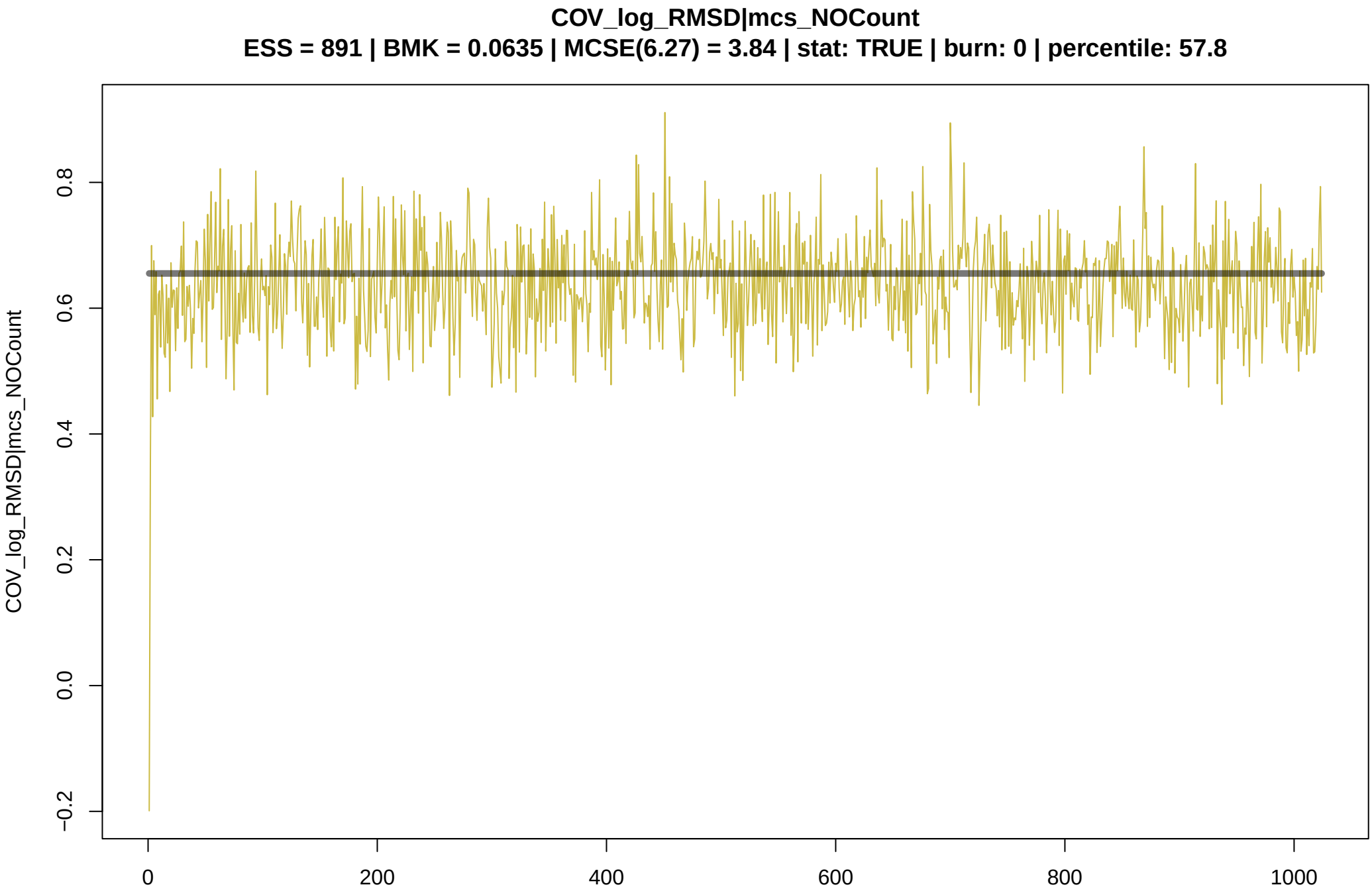

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 850 | BMK = 0.0828 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | percentile: 4.2
COV_log_RMSD|logit_ec_tanimoto_similarity
5.1
5.0
4.9
4.8
4.7
4.6
4.5
0
200
400
600
800
1000

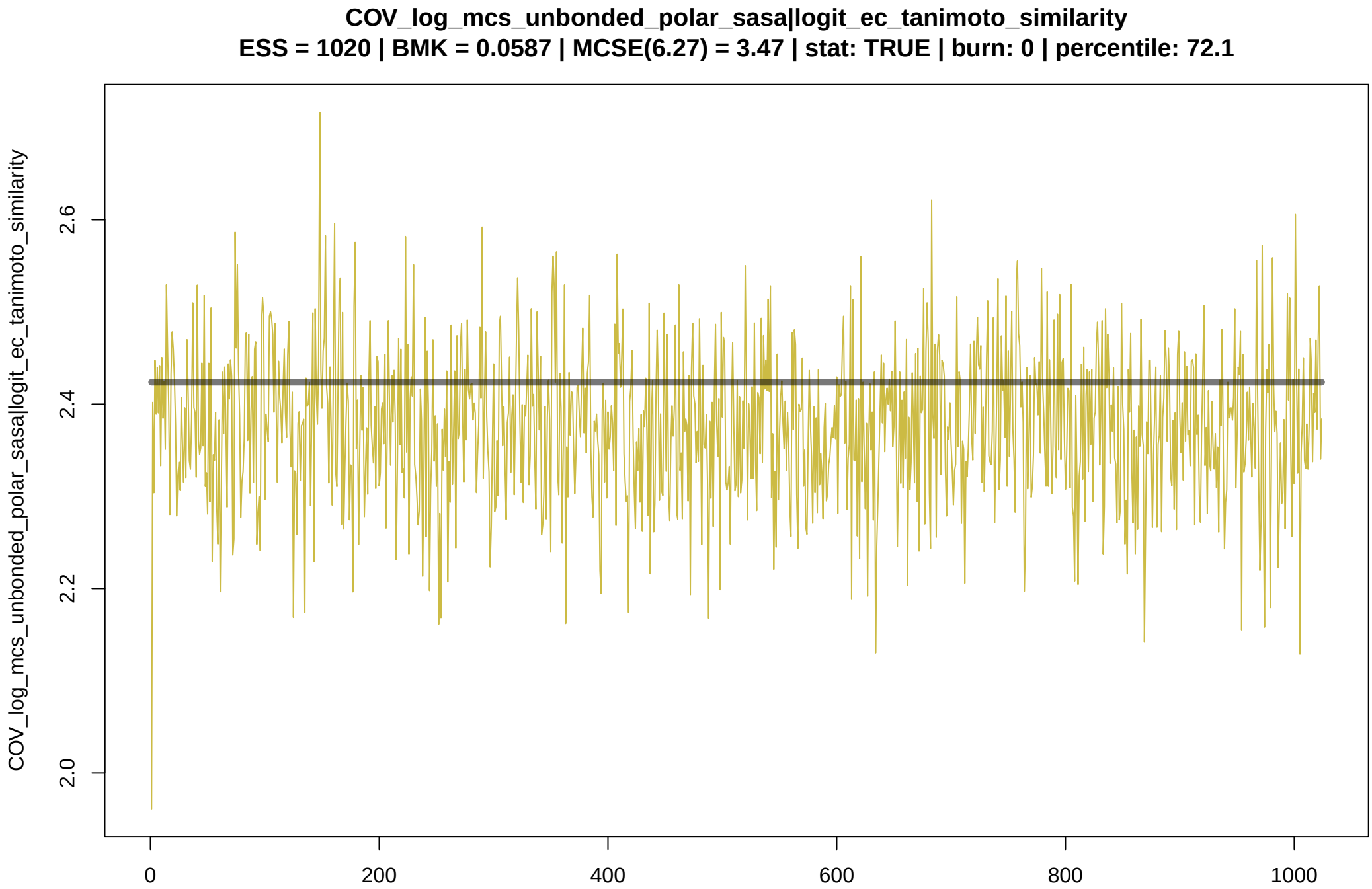

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0311 | MCSE(6.27) = 4 | stat: FALSE | burn: 0 | percentile: 23.1
COV_log_RMSD|mcs_NumHeteroAtoms
0.00
−0.05
−0.10
−0.15
0
200
400
600
800
1000

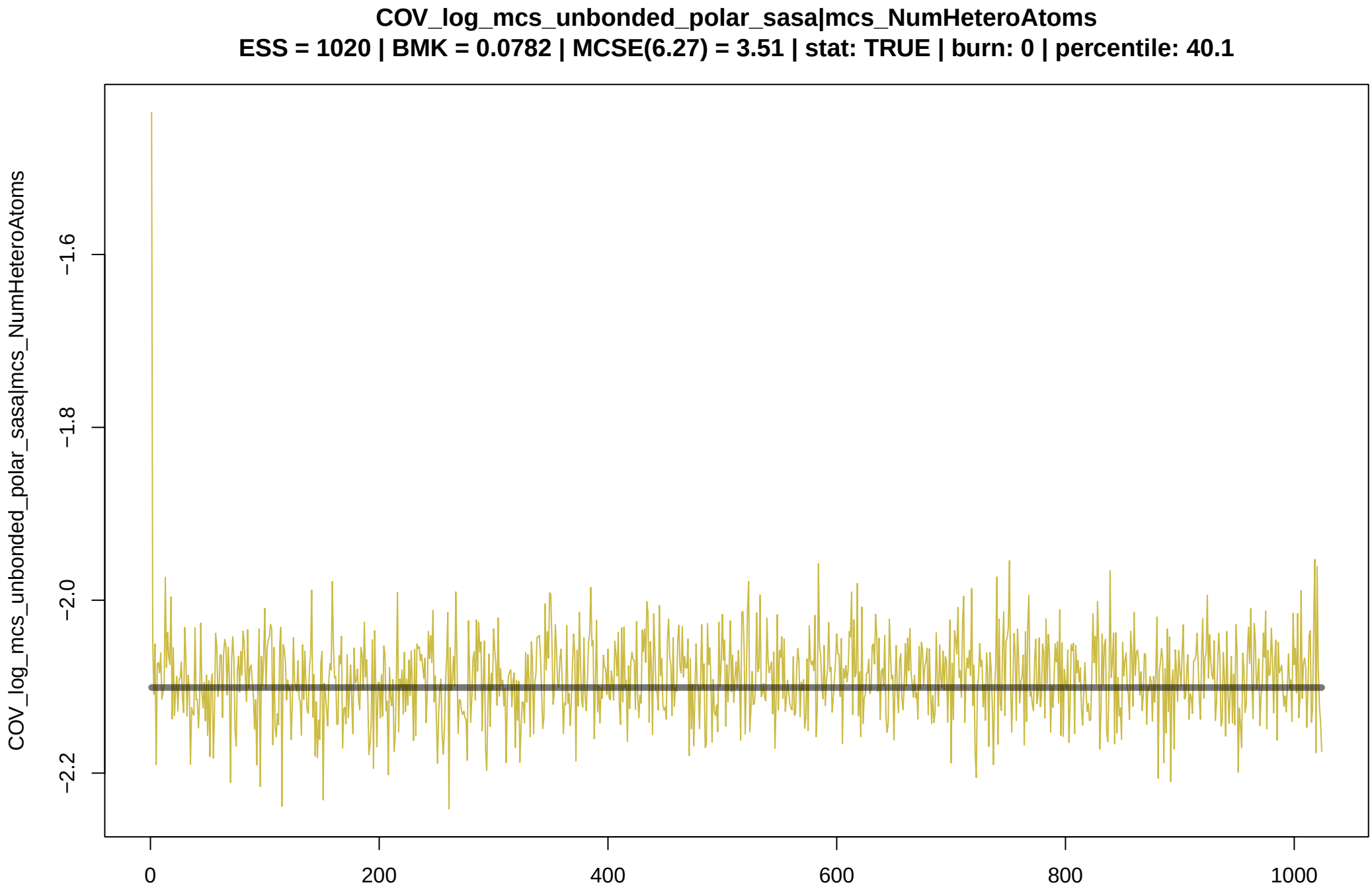

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0546 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | percentile: 30.7
COV_log_RMSD|docked_HeavyAtomCount
6.5
6.0
5.5
5.0
4.5
0
200
400
600
800
1000

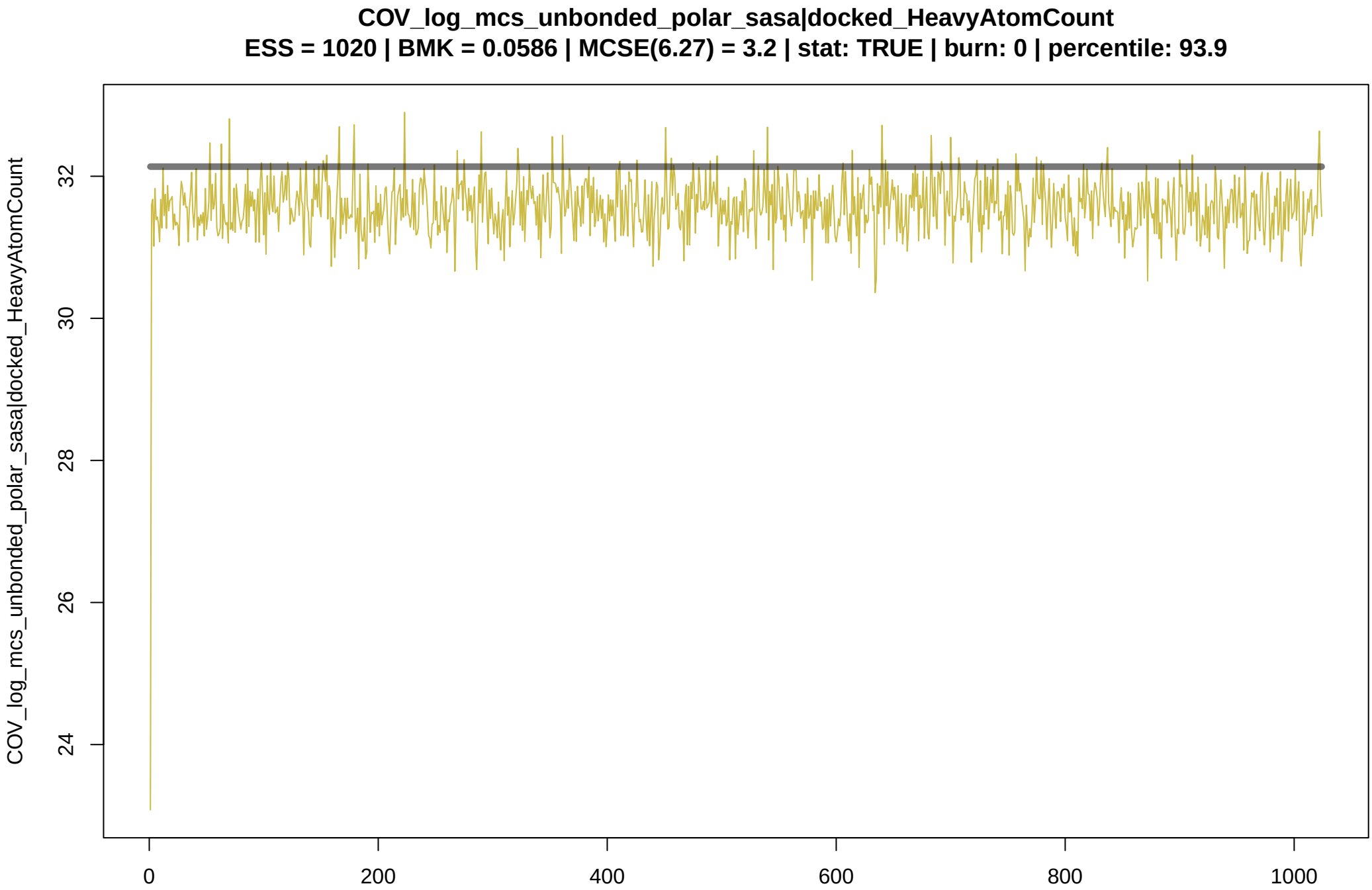

COV_log_RMSD|mcs_RingCount
ESS = 881 | BMK = 0.0863 | MCSE(6.27) = 3.87 | stat: TRUE | burn: 0 | percentile: 54.6
COV_log_RMSD|mcs_RingCount
0.15
0.10
0.05
0.00
−0.05
0
200
400
600
800
1000

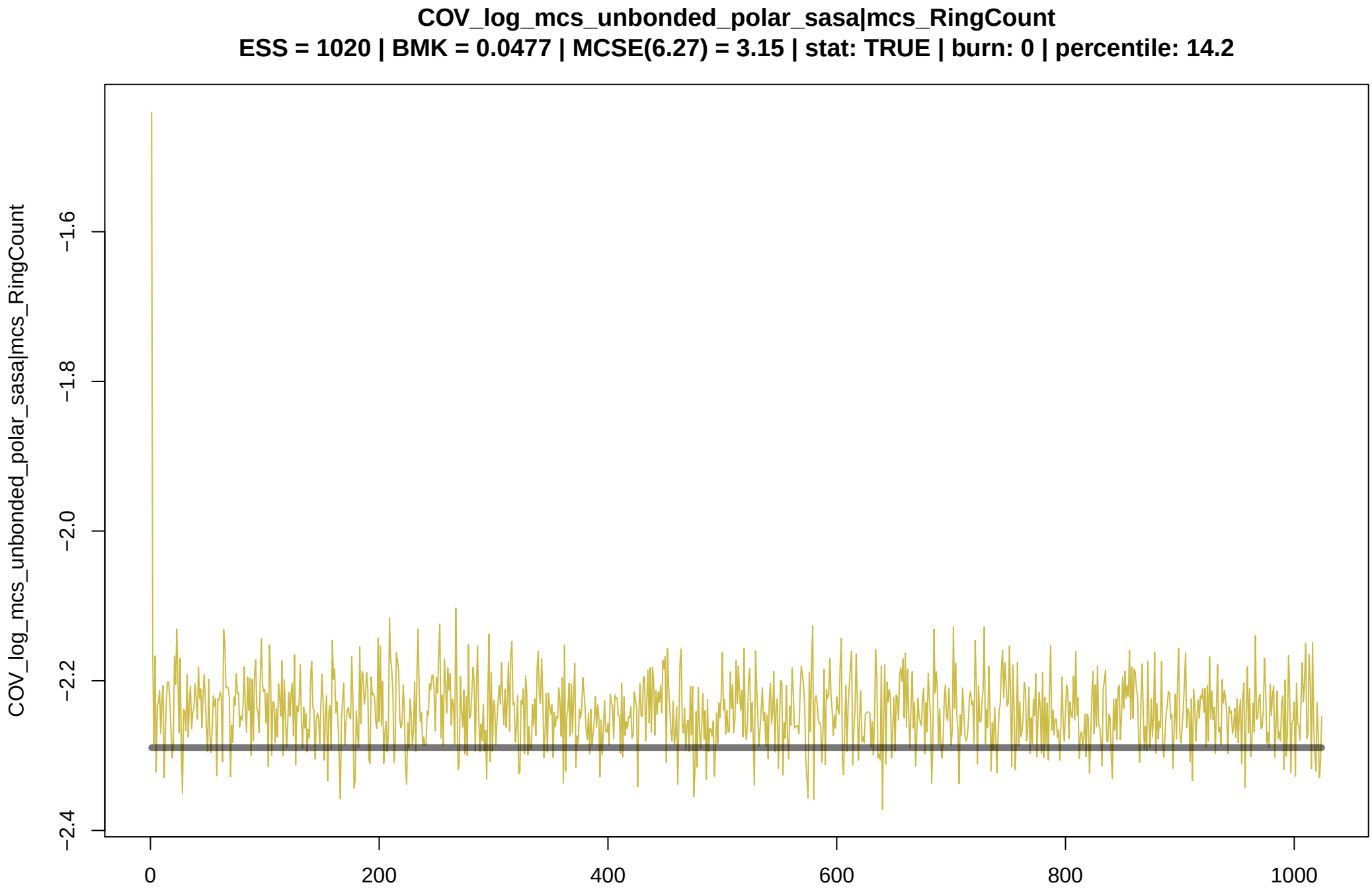

COV_log_RMSD|docked_NumRotatableBonds
ESS = 934 | BMK = 0.0812 | MCSE(6.27) = 4.35 | stat: FALSE | burn: 0 | percentile: 88.1
COV_log_RMSD|docked_NumRotatableBonds
−5.0
−5.5
−6.0
−6.5
−7.0
0
200
400
600
800
1000

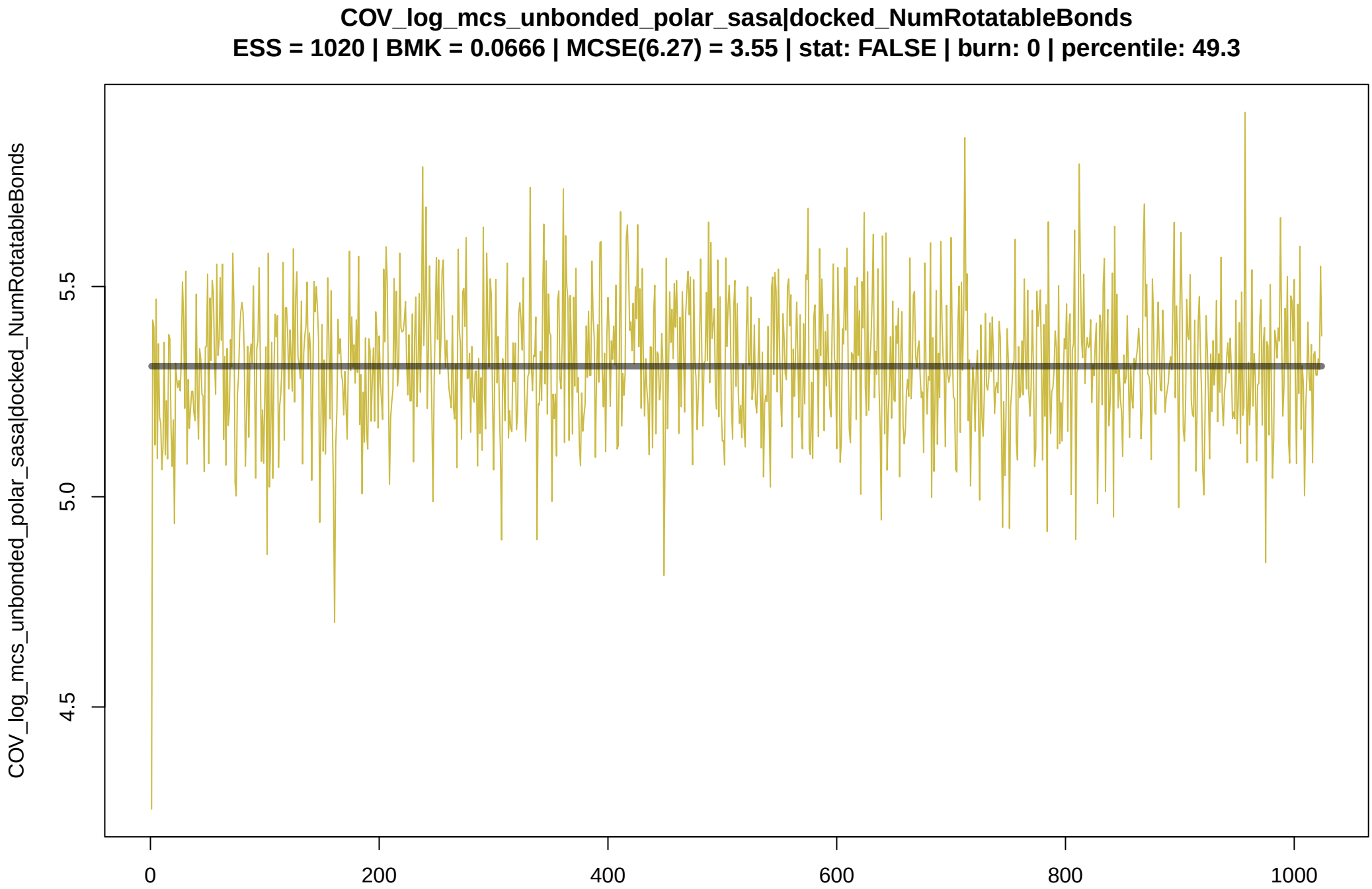

COV_log_RMSD|mcs_NOCount
ESS = 891 | BMK = 0.0635 | MCSE(6.27) = 3.84 | stat: TRUE | burn: 0 | percentile: 57.8
COV_log_RMSD|mcs_NOCount
−0.2
0.0
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

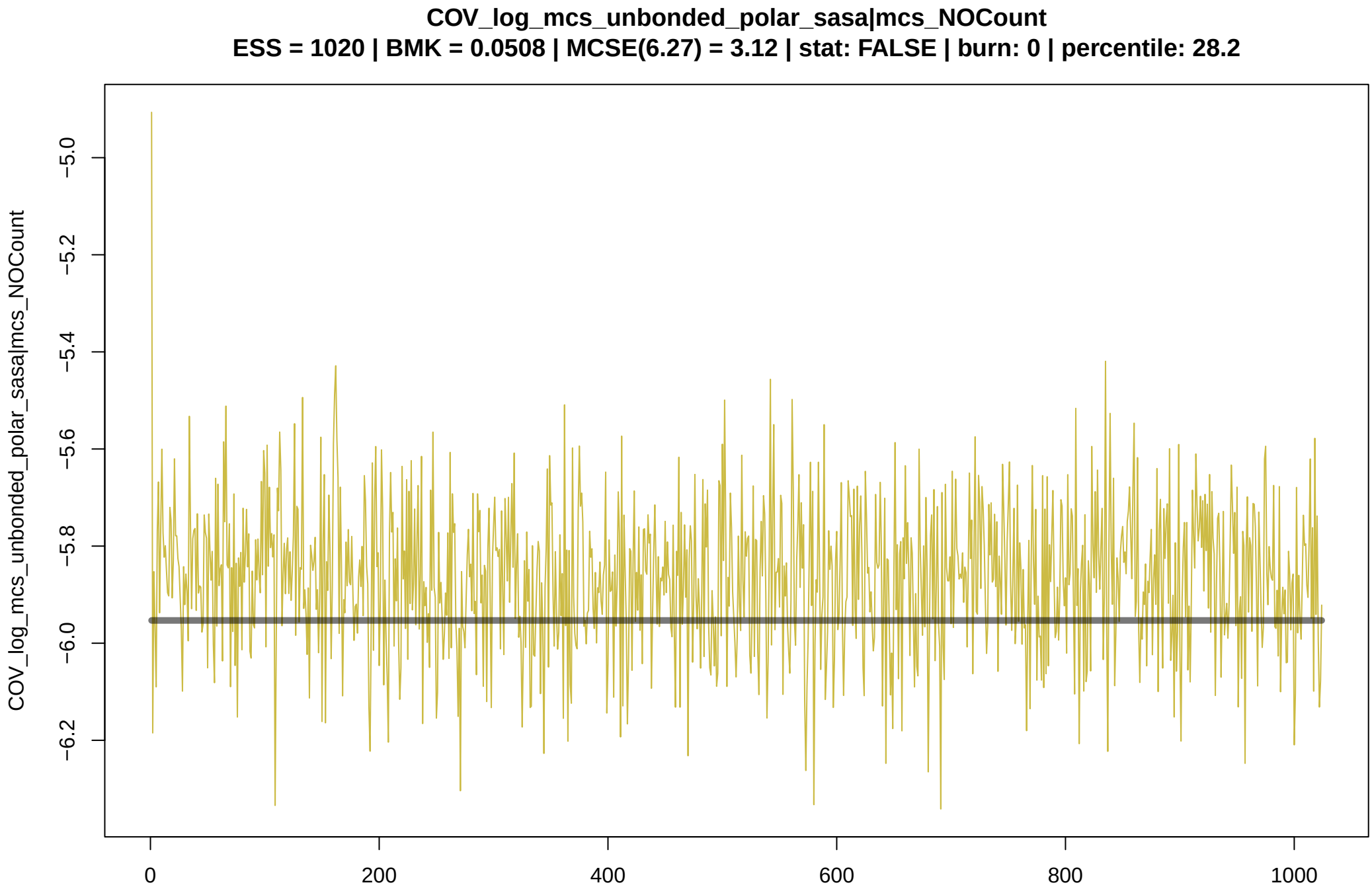

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0587 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | percentile: 72.1
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2.0
2.2
2.4
2.6
0
200
400
600
800
1000

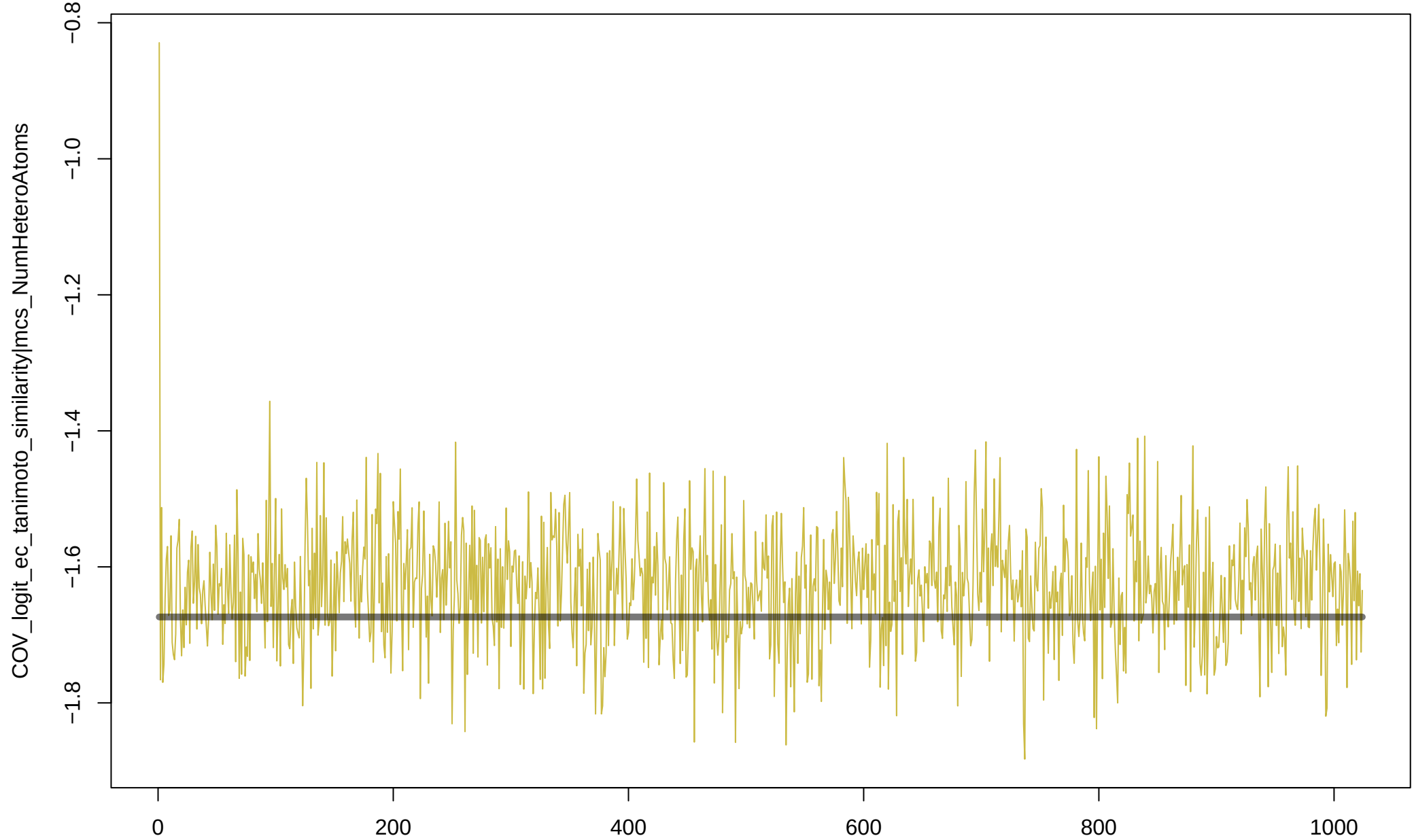

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0782 | MCSE(6.27) = 3.51 | stat: TRUE | burn: 0 | percentile: 40.1
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.6
−1.8
−2.0
−2.2
0
200
400
600
800
1000

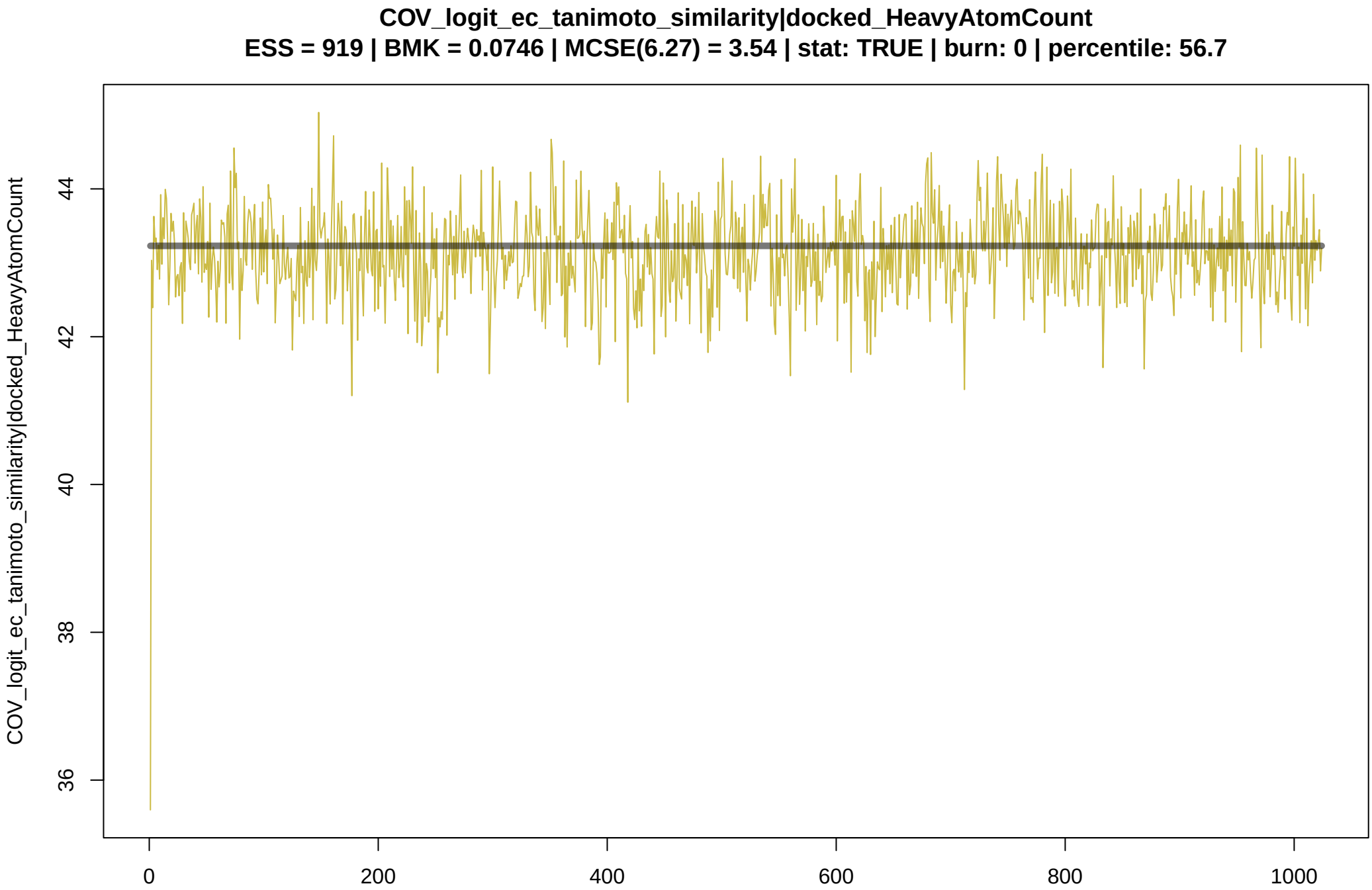

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0586 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | percentile: 93.9
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
24
26
28
30
32
0
200
400
600
800
1000

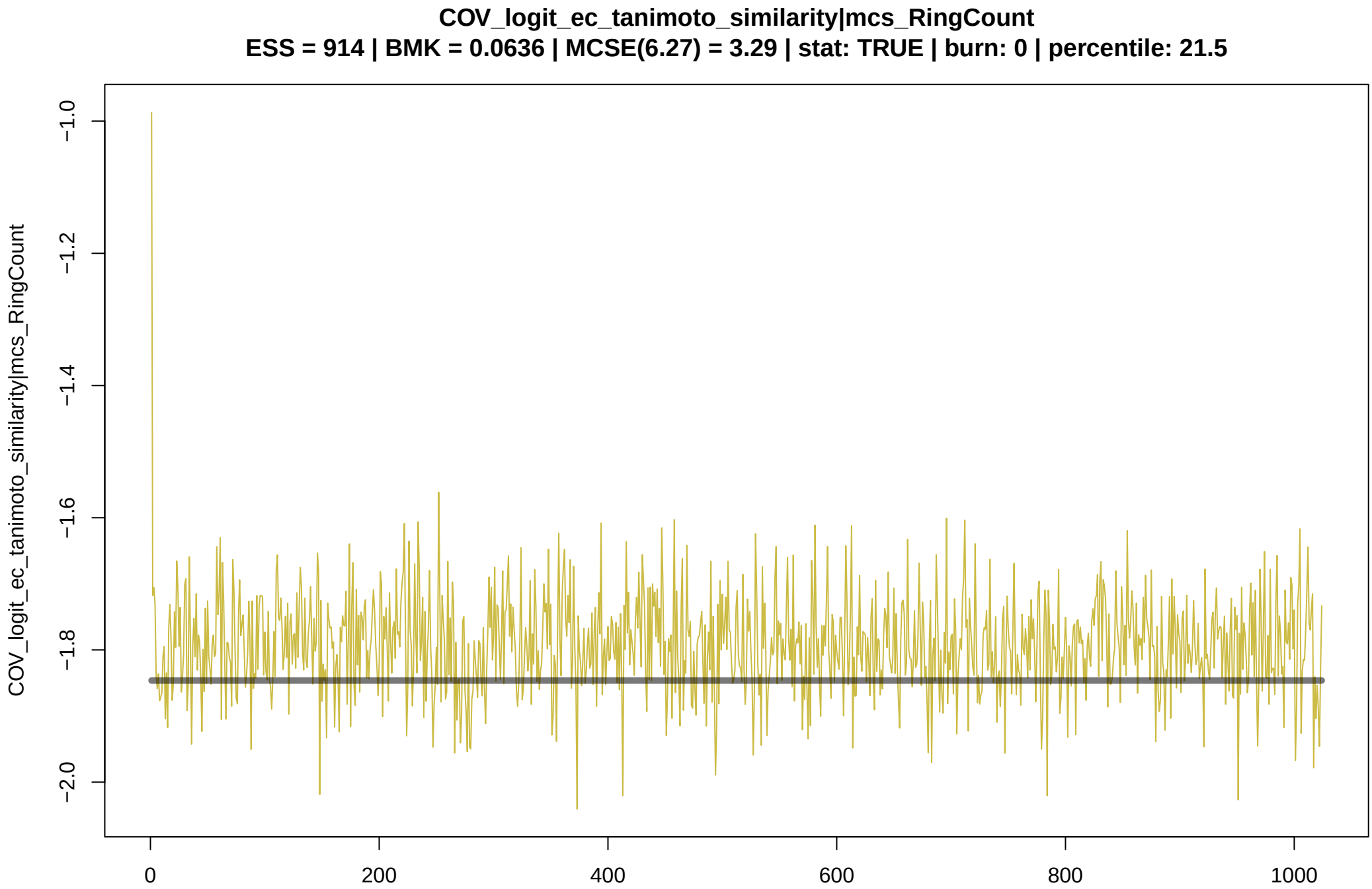

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0477 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | percentile: 14.2
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−1.6
−1.8
−2.0
−2.2
−2.4
0
200
400
600
800
1000

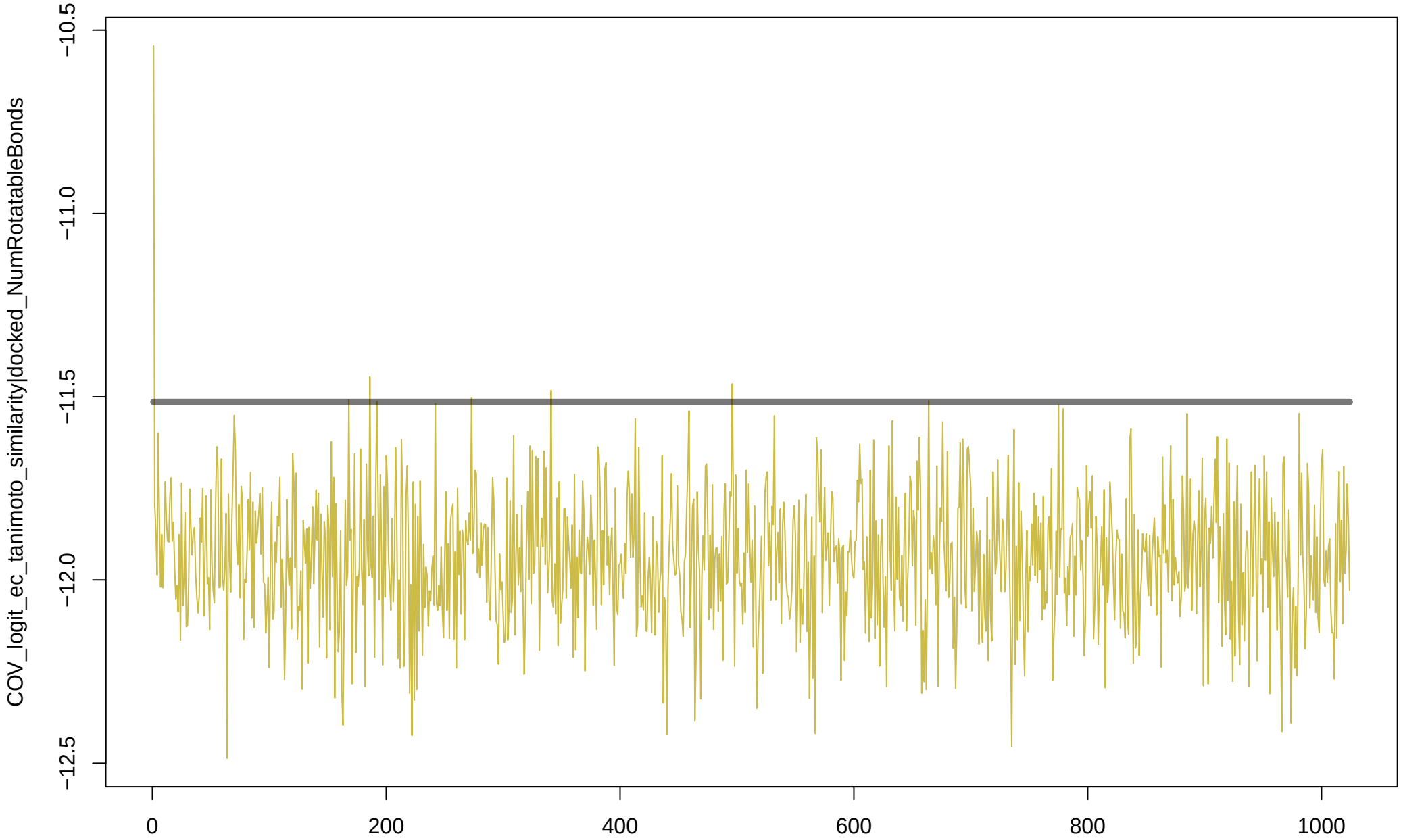

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0666 | MCSE(6.27) = 3.55 | stat: FALSE | burn: 0 | percentile: 49.3
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
4.5
5.0
5.5
0
200
400
600
800
1000

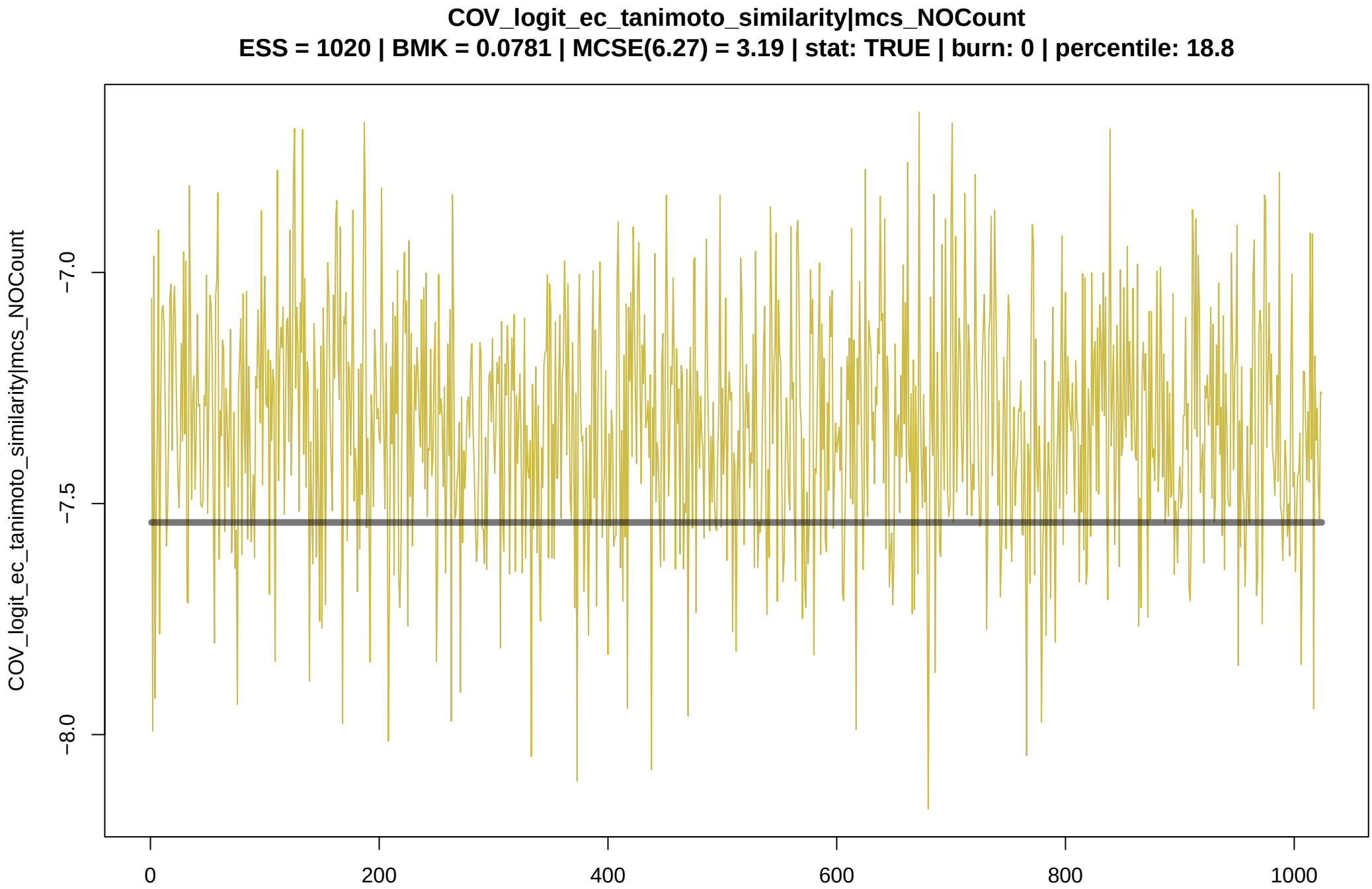

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0508 | MCSE(6.27) = 3.12 | stat: FALSE | burn: 0 | percentile: 28.2
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.0
−5.2
−5.4
−5.6
−5.8
−6.0
−6.2
0
200
400
600
800
1000

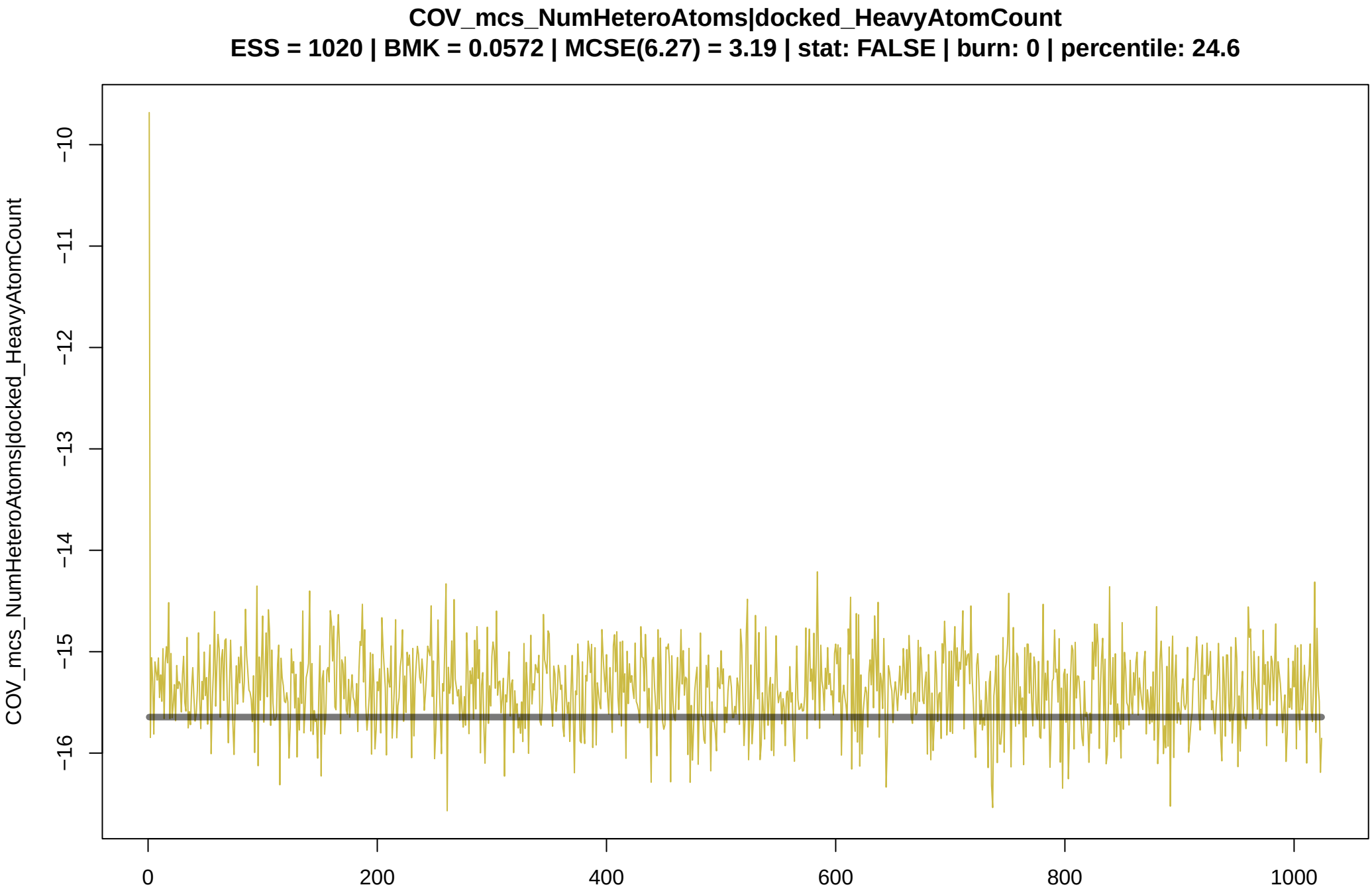

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.059 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0 | percentile: 29.7
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−0.8
−1.0
−1.2
−1.4
−1.6
−1.8
0
200
400
600
800
1000

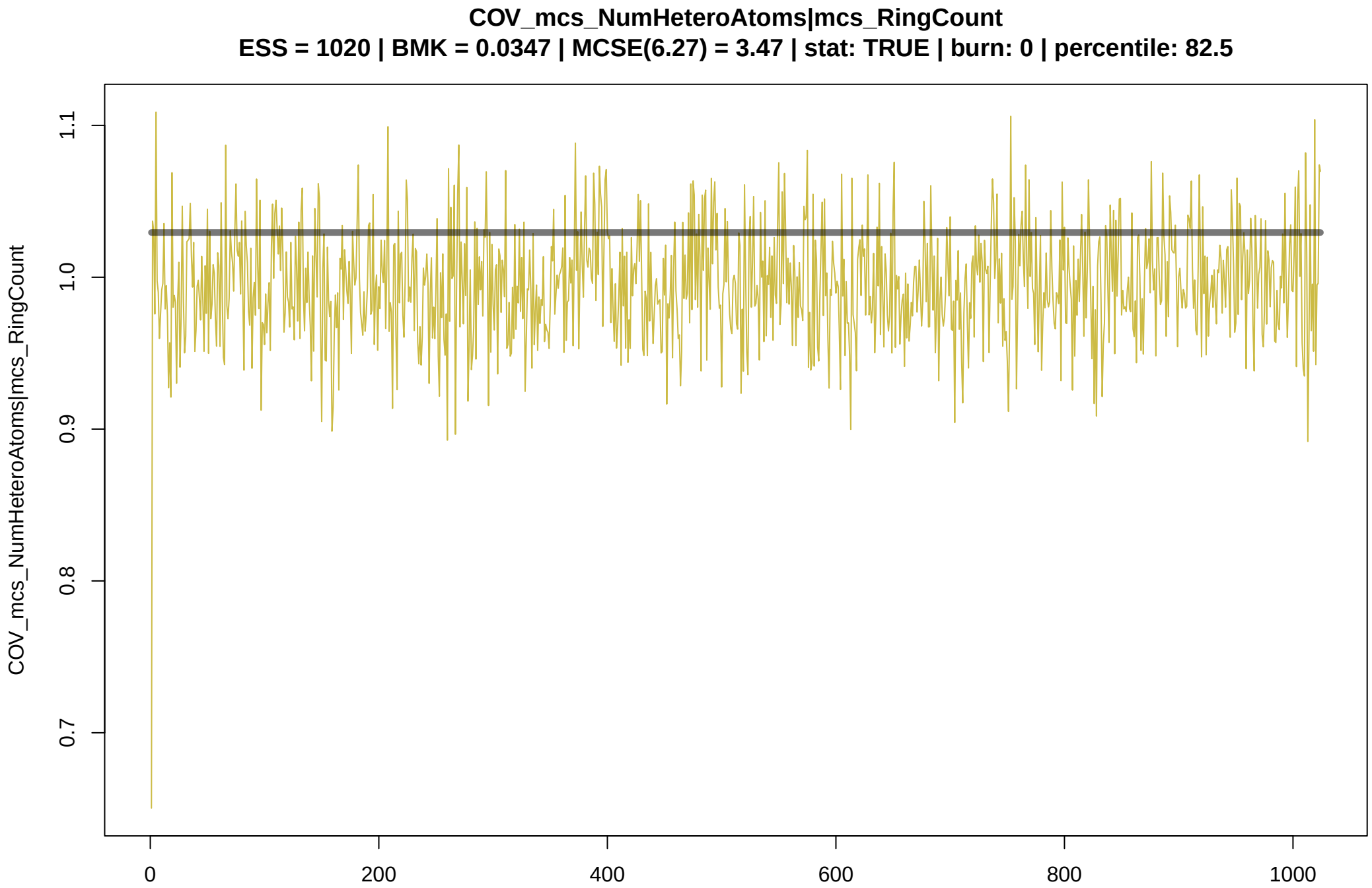

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 919 | BMK = 0.0746 | MCSE(6.27) = 3.54 | stat: TRUE | burn: 0 | percentile: 56.7
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
36
38
40
42
44
0
200
400
600
800
1000

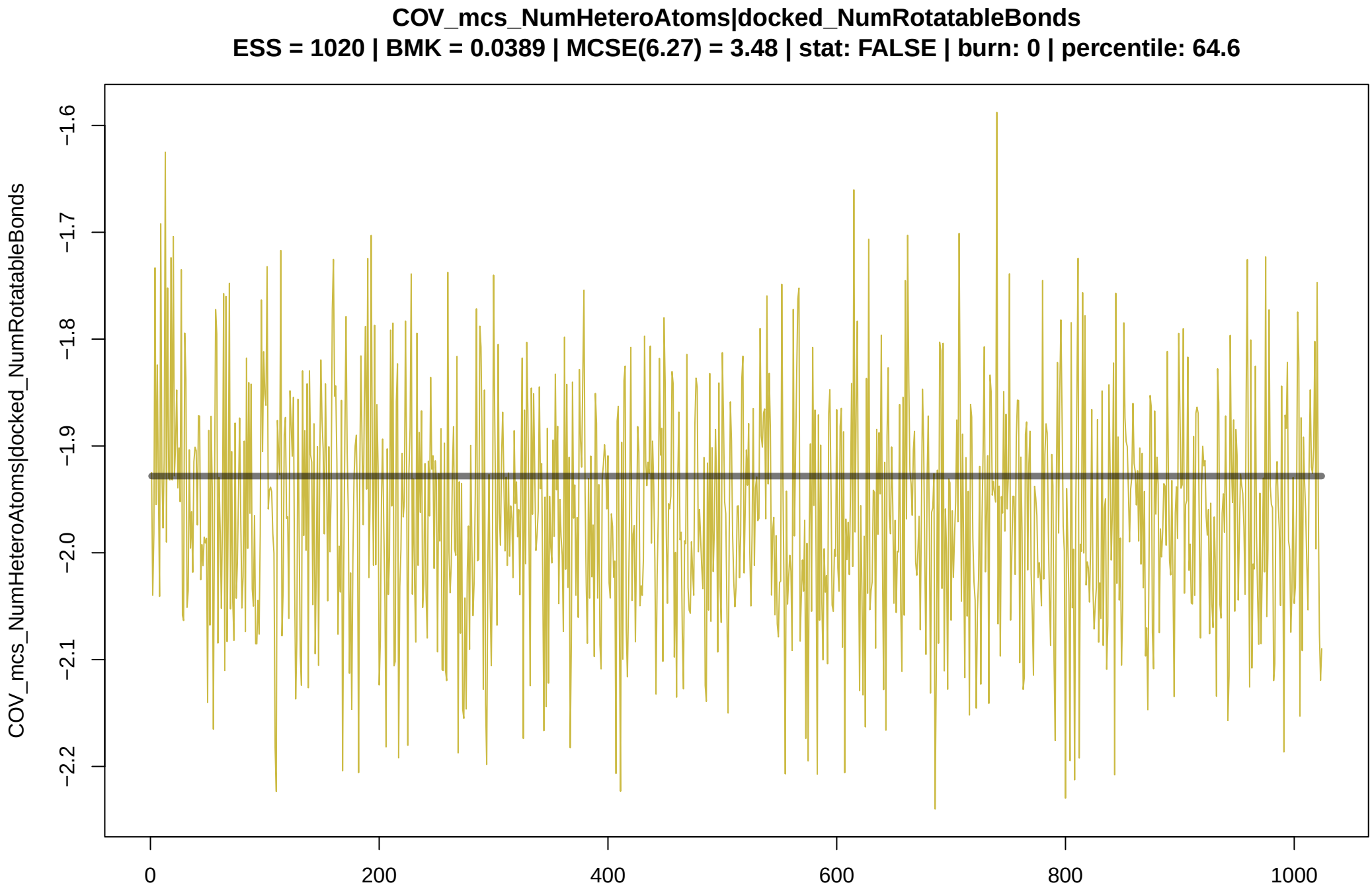

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 914 | BMK = 0.0636 | MCSE(6.27) = 3.29 | stat: TRUE | burn: 0 | percentile: 21.5
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.0
−1.2
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

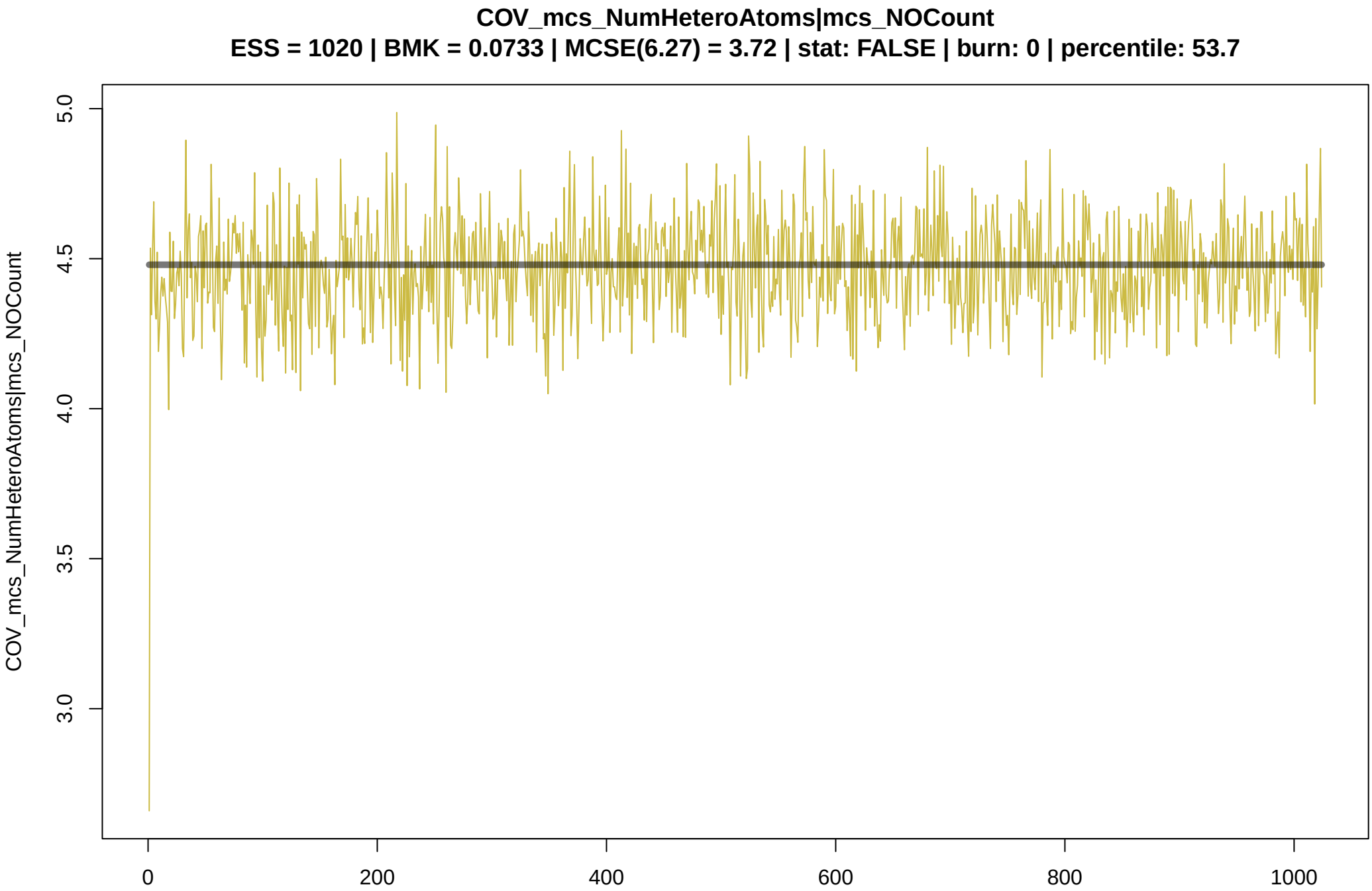

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0525 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | percentile: 99.2
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−10.5
−11.0
−11.5
−12.0
−12.5
0
200
400
600
800
1000

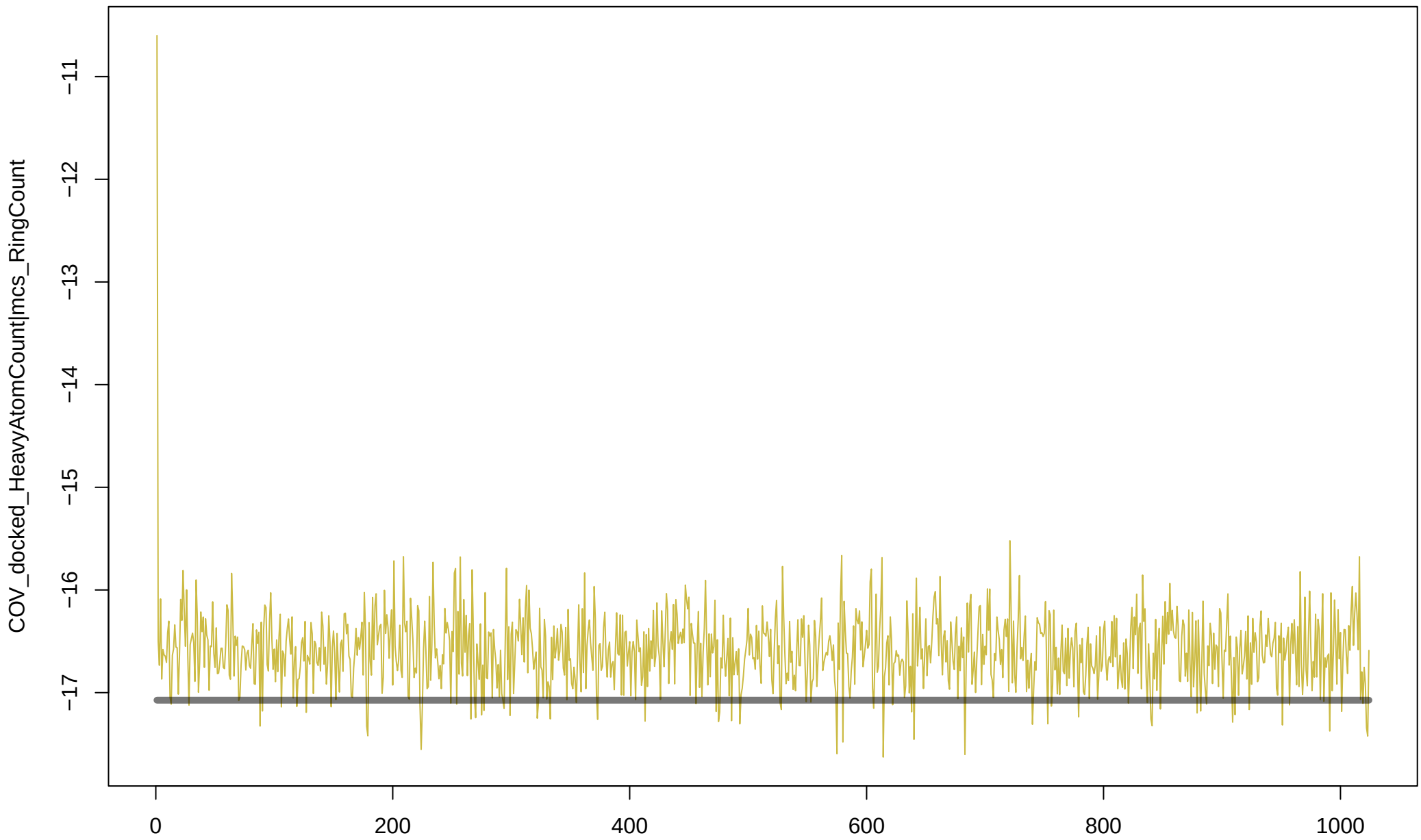

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0781 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 18.8
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−7.0
−7.5
−8.0
0
200
400
600
800
1000

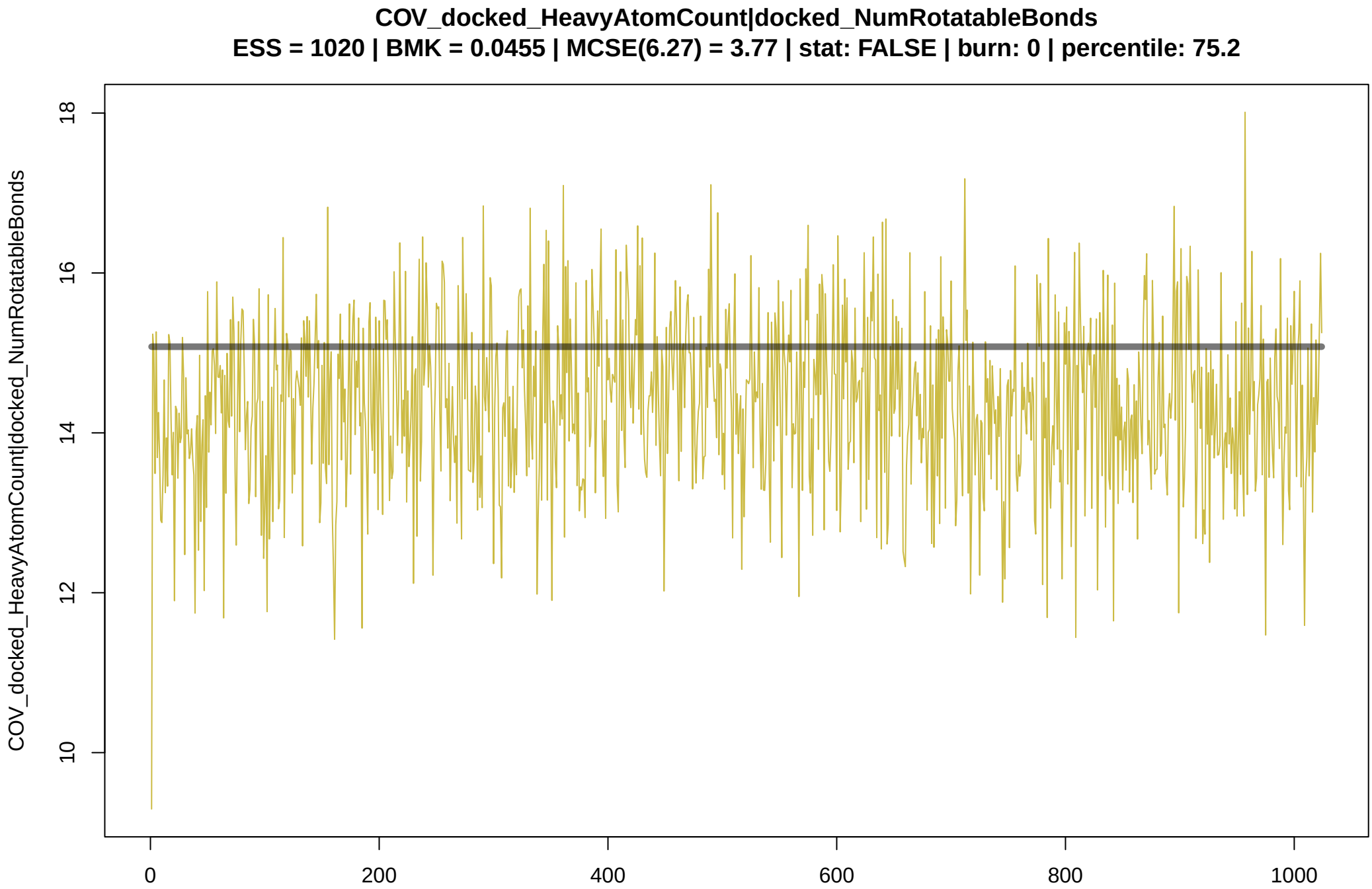

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0572 | MCSE(6.27) = 3.19 | stat: FALSE | burn: 0 | percentile: 24.6
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−10
−11
−12
−13
−14
−15
−16
0
200
400
600
800
1000

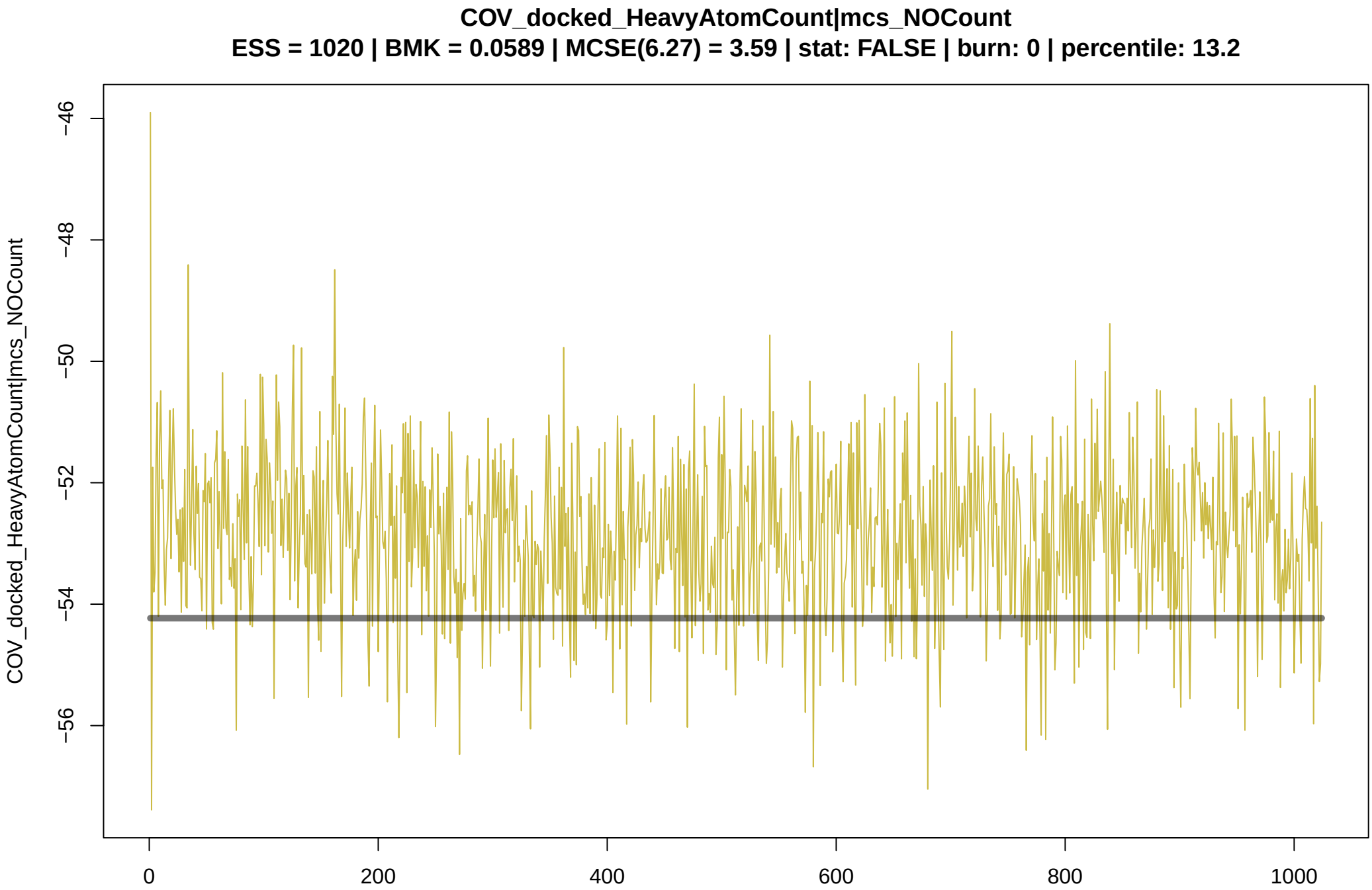

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 1020 | BMK = 0.0347 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | percentile: 82.5
COV_mcs_NumHeteroAtoms|mcs_RingCount
1.1
1.0
0.9
0.8
0.7
0
200
400
600
800
1000

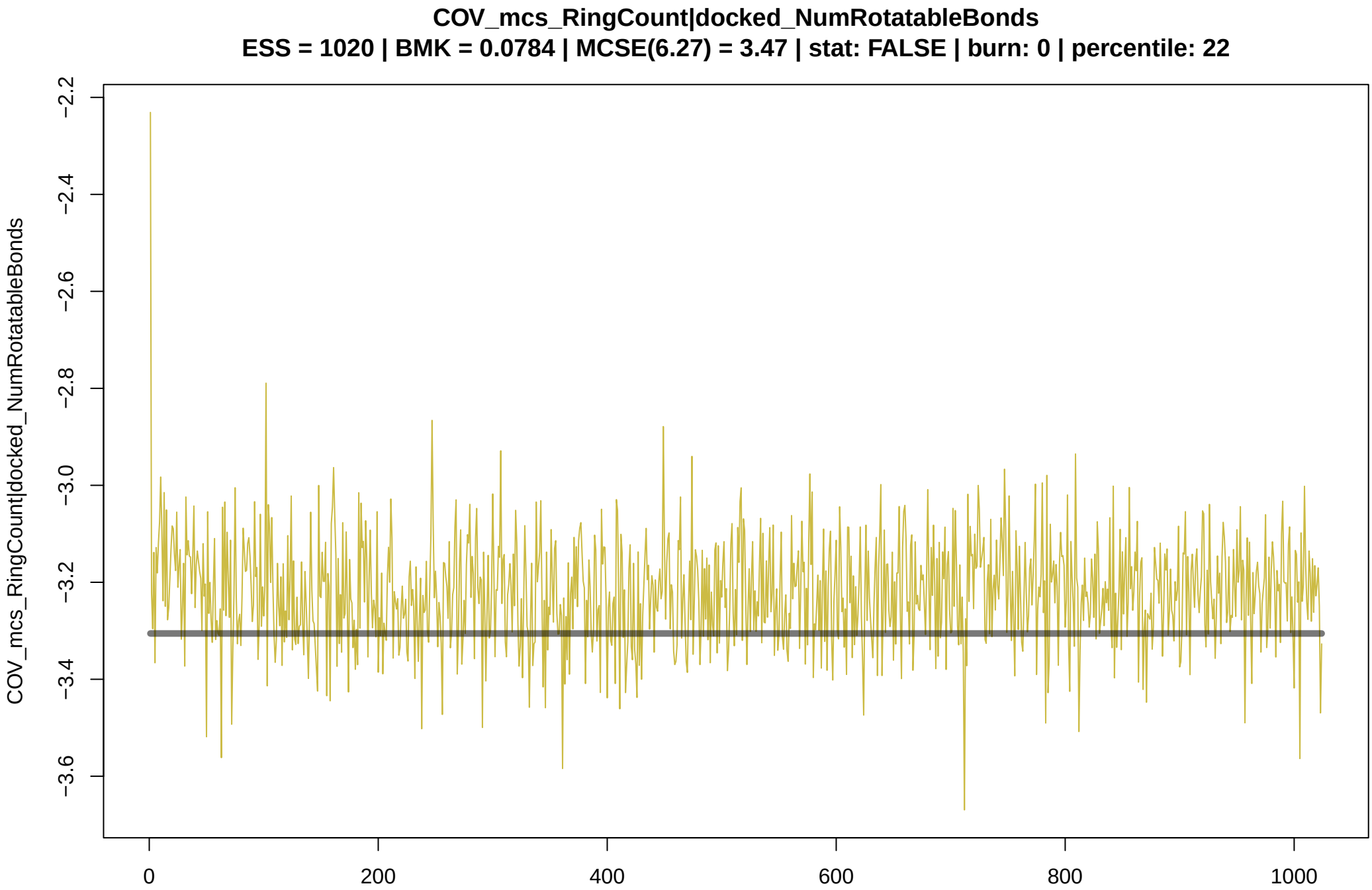

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0389 | MCSE(6.27) = 3.48 | stat: FALSE | burn: 0 | percentile: 64.6
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.6
−1.7
−1.8
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

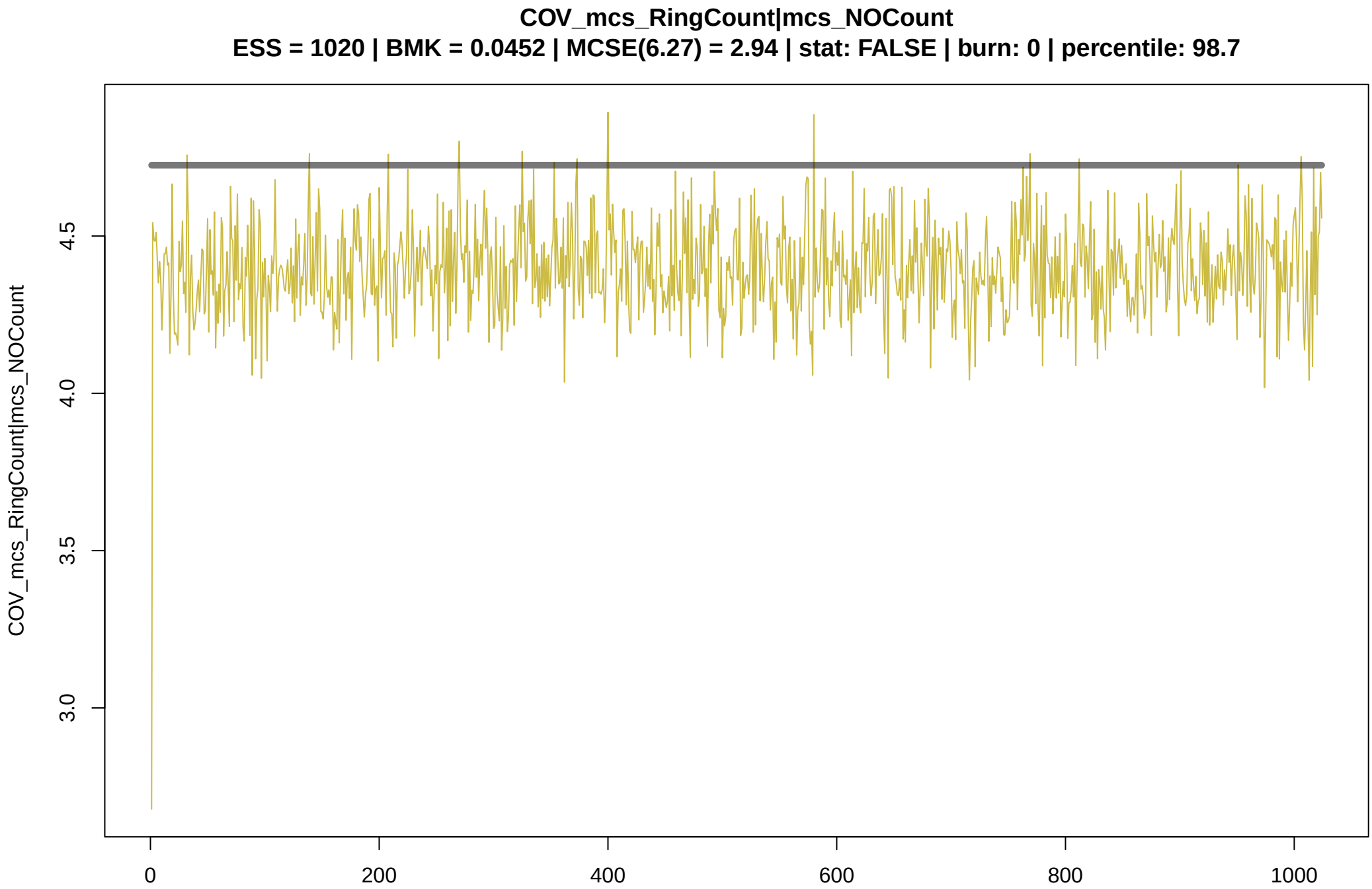

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0733 | MCSE(6.27) = 3.72 | stat: FALSE | burn: 0 | percentile: 53.7
COV_mcs_NumHeteroAtoms|mcs_NOCount
5.0
4.5
4.0
3.5
3.0
0
200
400
600
800
1000

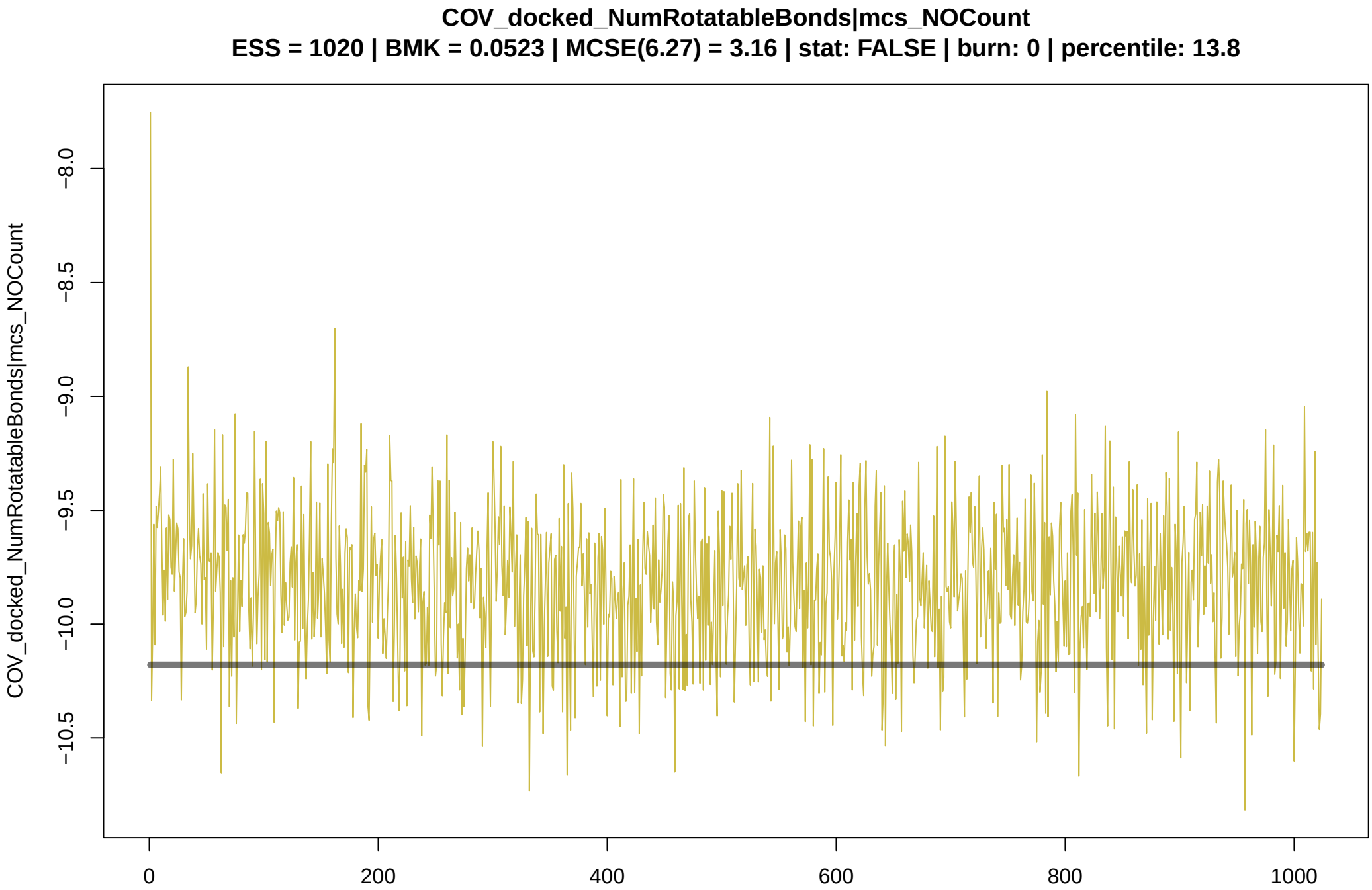

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0529 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0 | percentile: 6.74
COV_docked_HeavyAtomCount|mcs_RingCount
−11
−12
−13
−14
−15
−16
−17
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0455 | MCSE(6.27) = 3.77 | stat: FALSE | burn: 0 | percentile: 75.2
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0589 | MCSE(6.27) = 3.59 | stat: FALSE | burn: 0 | percentile: 13.2
COV_docked_HeavyAtomCount|mcs_NOCount
−46
−48
−50
−52
−54
−56
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0784 | MCSE(6.27) = 3.47 | stat: FALSE | burn: 0 | percentile: 22
COV_mcs_RingCount|docked_NumRotatableBonds
−2.2
−2.4
−2.6
−2.8
−3.0
−3.2
−3.4
−3.6
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.0452 | MCSE(6.27) = 2.94 | stat: FALSE | burn: 0 | percentile: 98.7
COV_mcs_RingCount|mcs_NOCount
3.0
3.5
4.0
4.5
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0523 | MCSE(6.27) = 3.16 | stat: FALSE | burn: 0 | percentile: 13.8
COV_docked_NumRotatableBonds|mcs_NOCount
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
200
400
600
800
1000