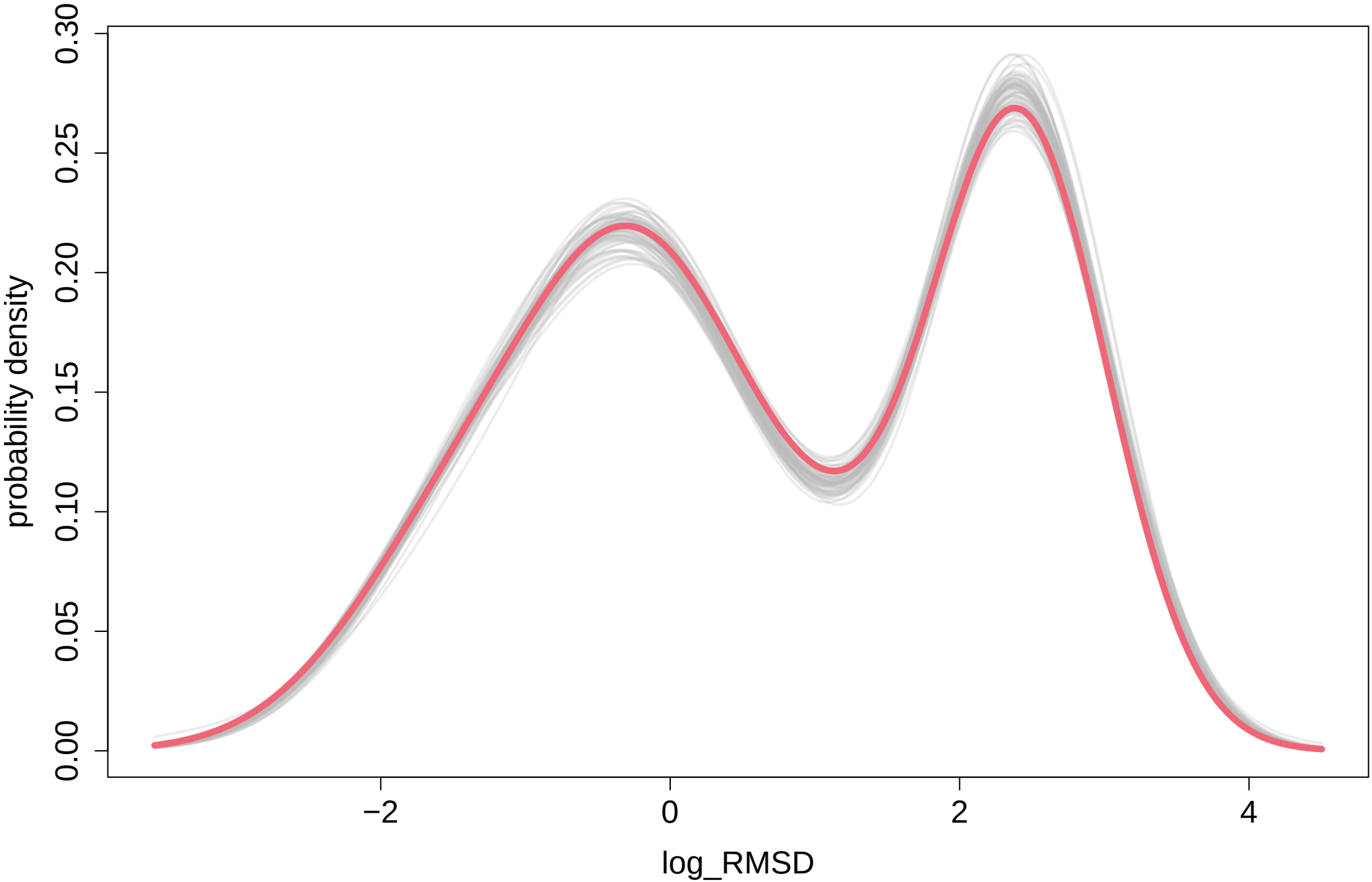
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.559465282174973
max MCSE = 12.3688544951282
all stationary: FALSE
burn: 0
min percent.: 0.9765625

−− STATS 2D −−
min ESS = 25.8360355336446
max BMK = 0.382397207508386
max MCSE = 9.50683682497285
all stationary: FALSE
burn: 0
min percent.: 1.66015625

−− STATS 1D −−
min ESS = 4.42365634296168
max BMK = 1
max MCSE = 12.8073646141644
all stationary: FALSE
burn: 1020
min percent.: 0.48828125

Occupied clusters: 23 of 64
LL: −62600 +− 121


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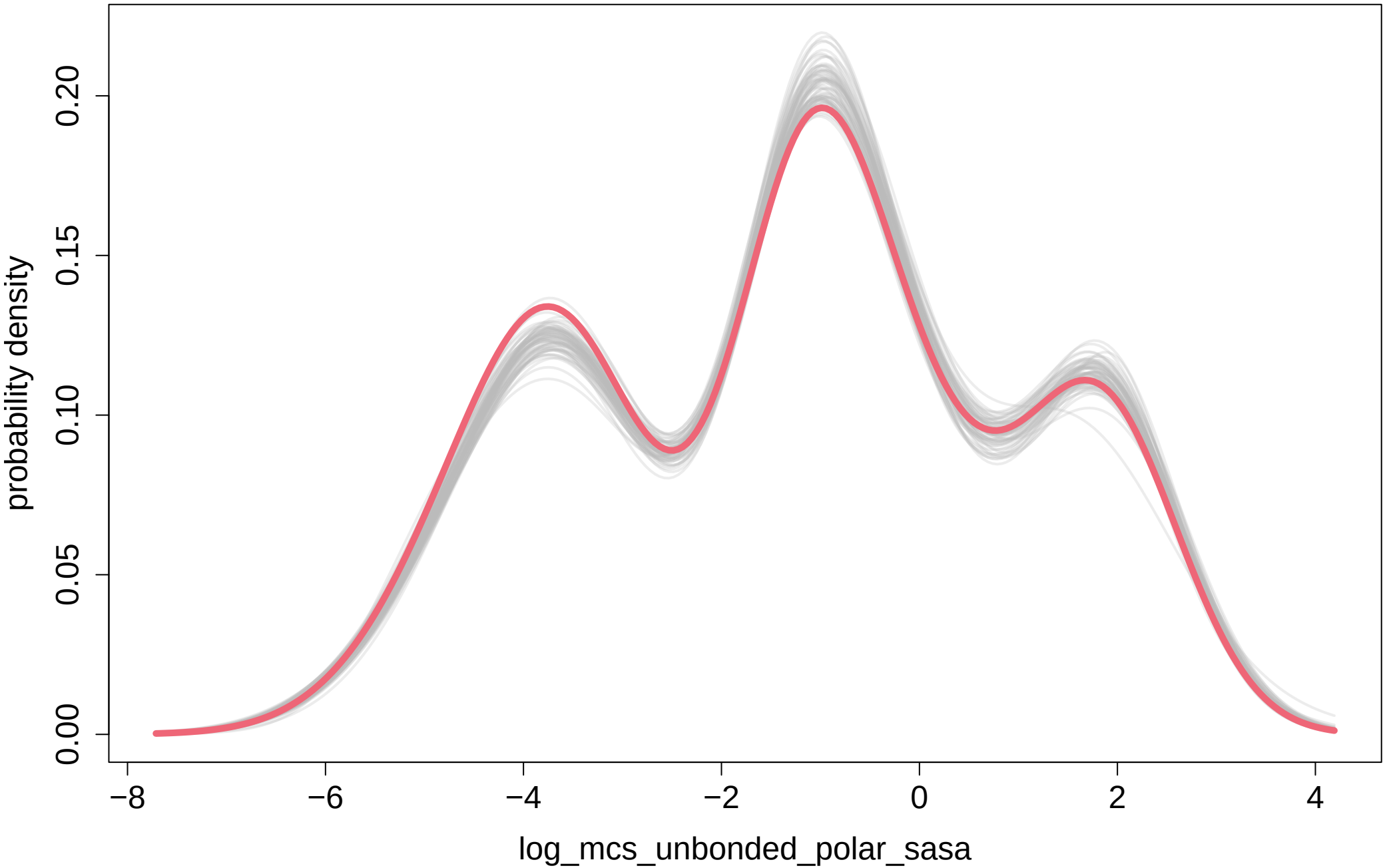
0.30
−2
0
2
4
log_RMSD


probability density
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0.20
−8
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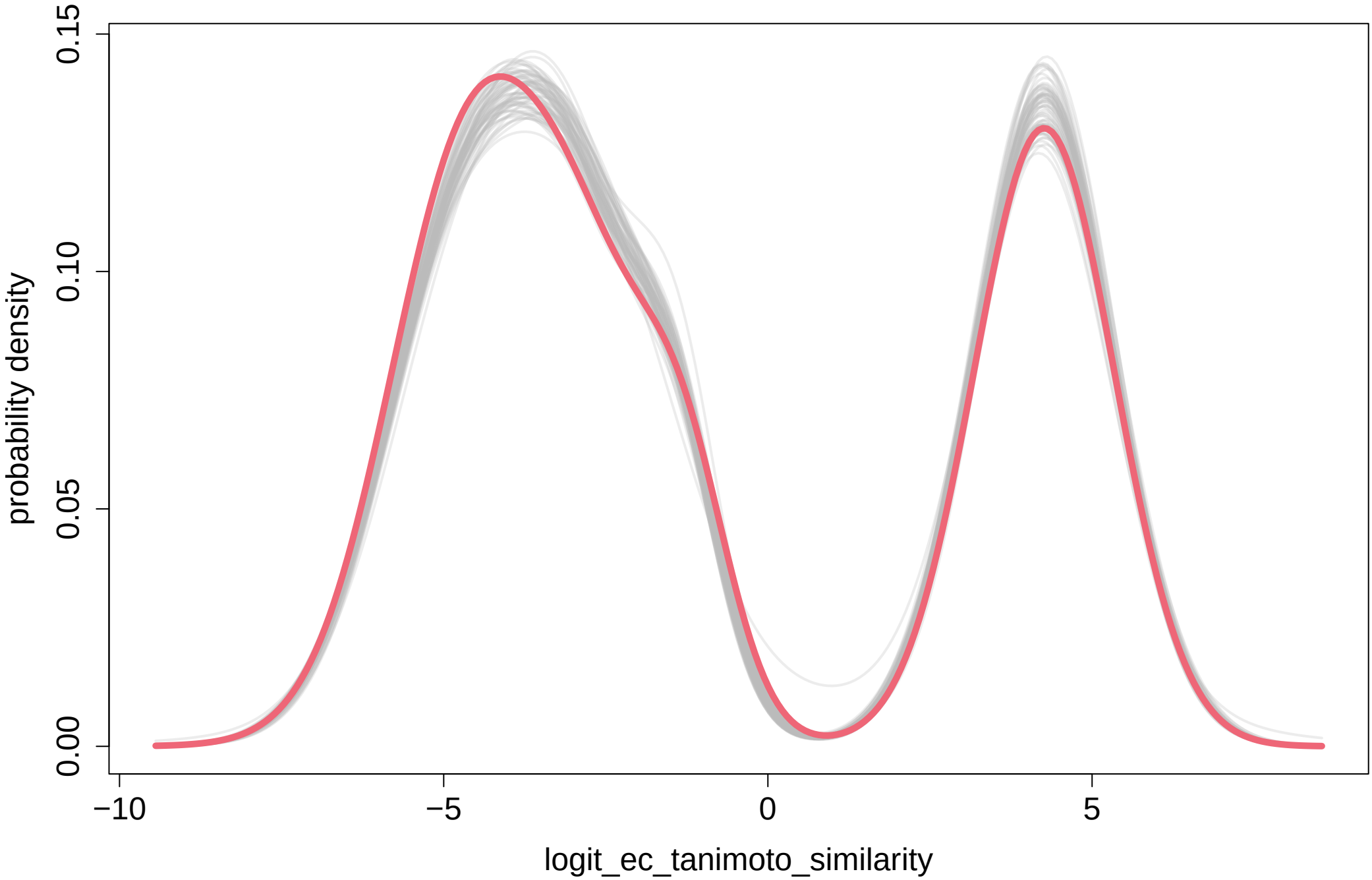
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa


probability density
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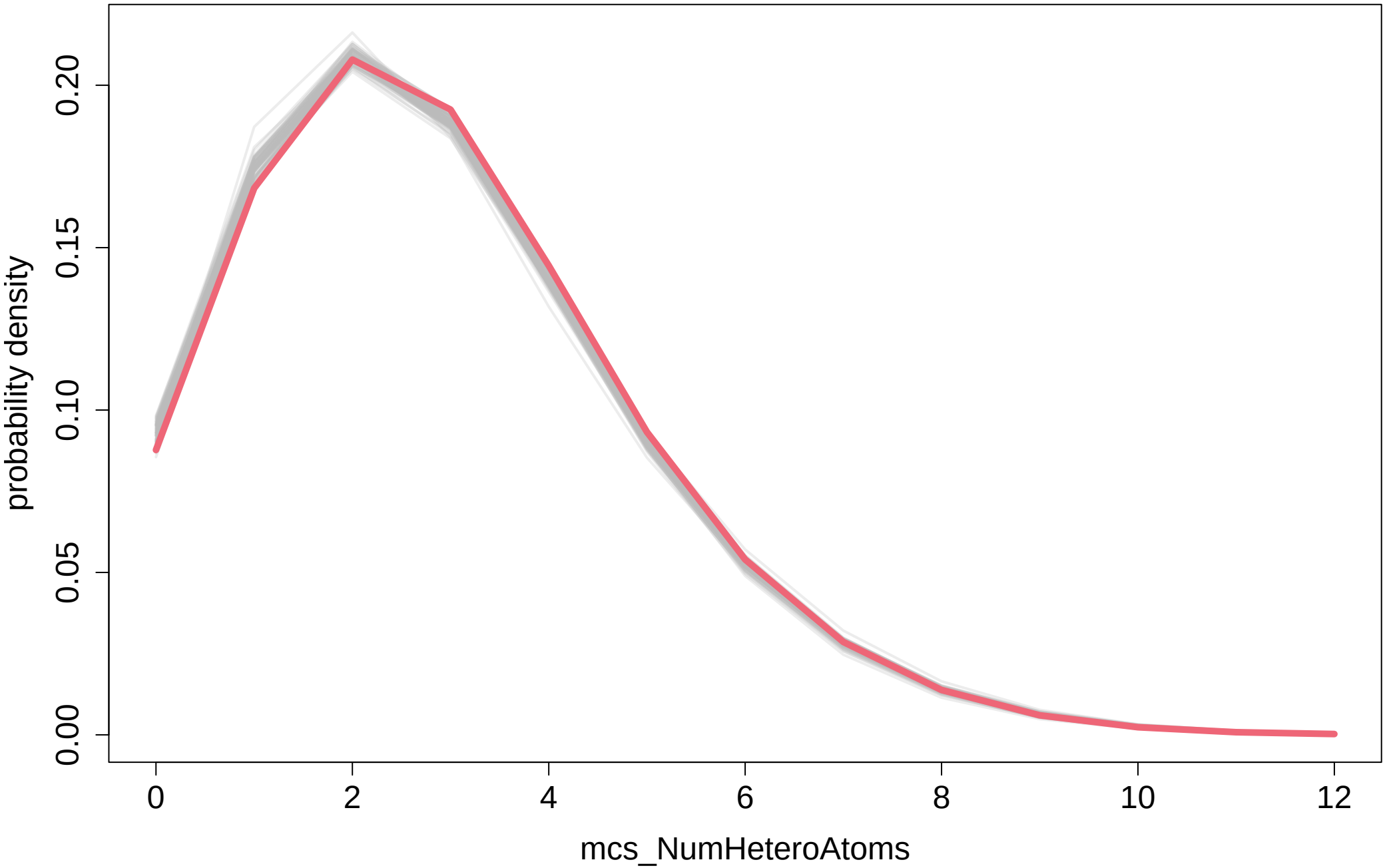
0.15
−10
−5
0
5
logit_ec_tanimoto_similarity


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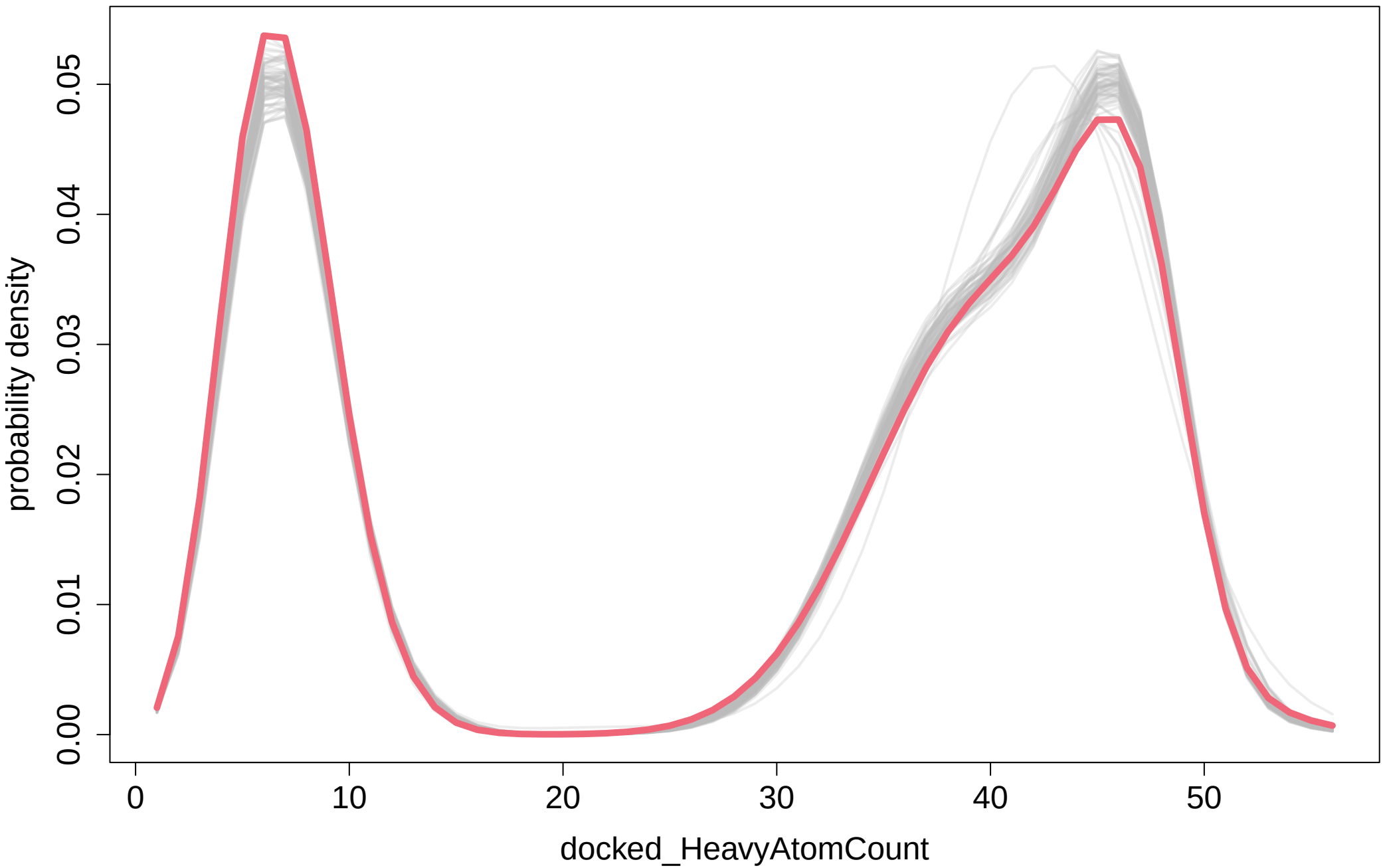
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms


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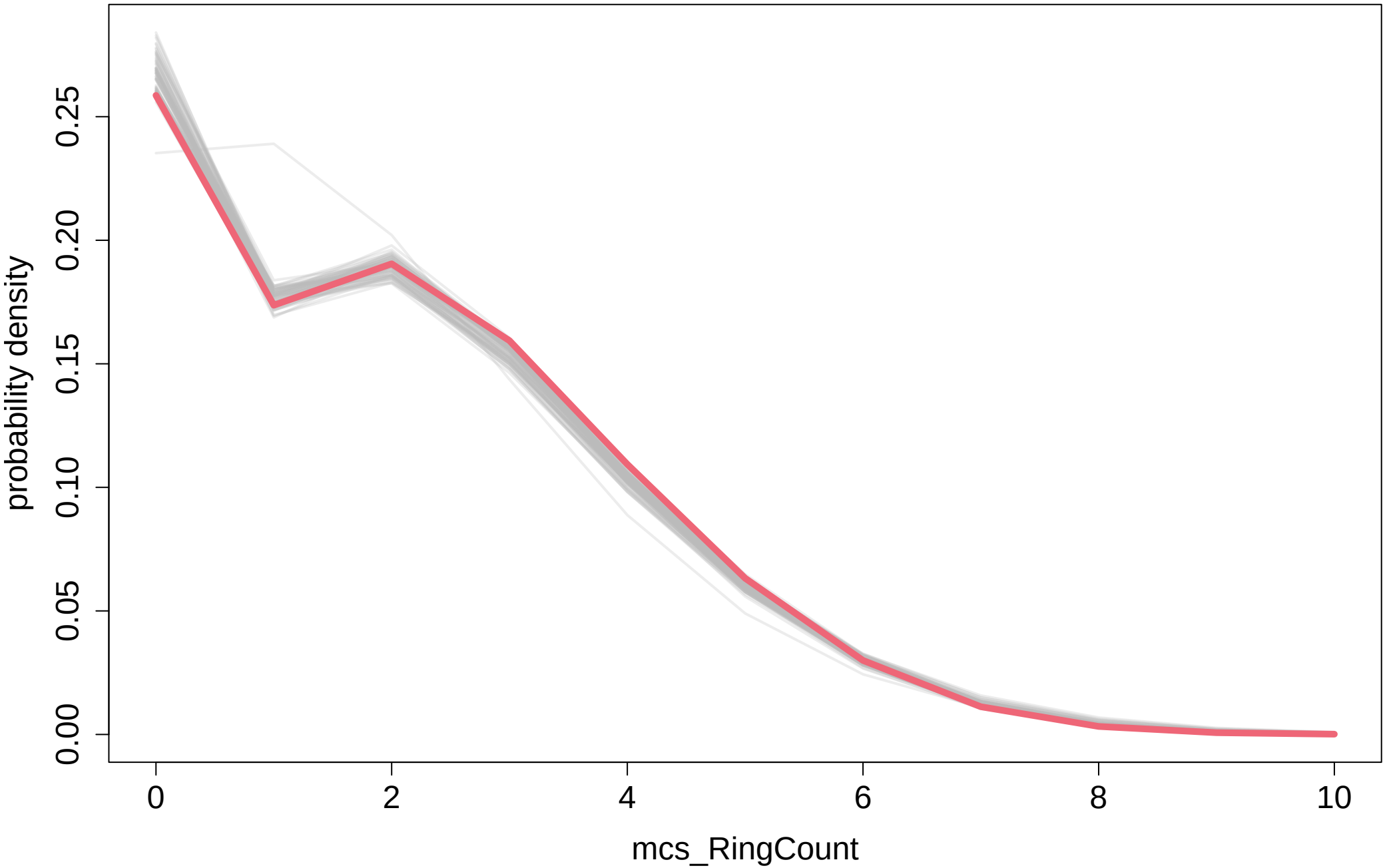
10
20
30
40
50
docked_HeavyAtomCount


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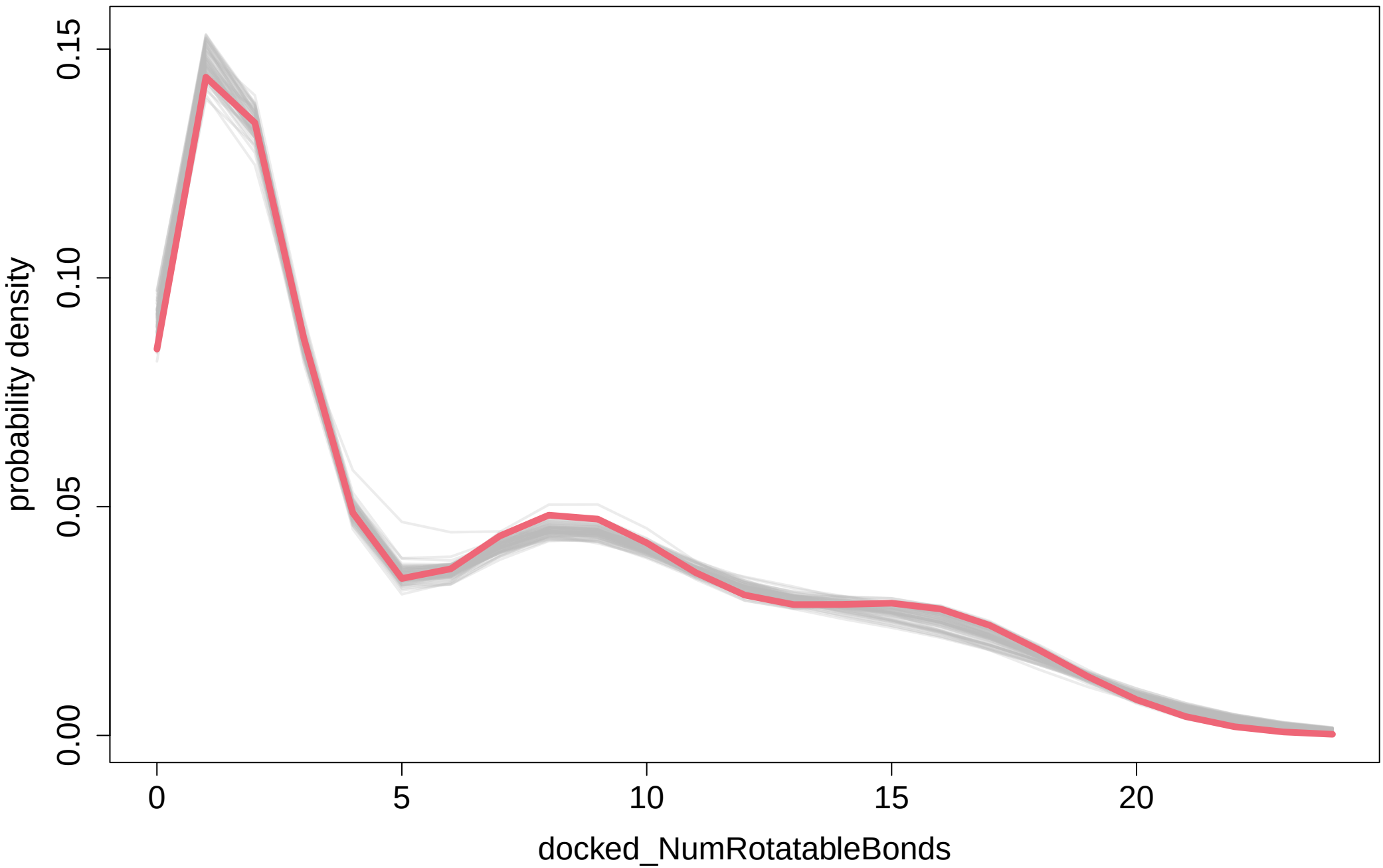
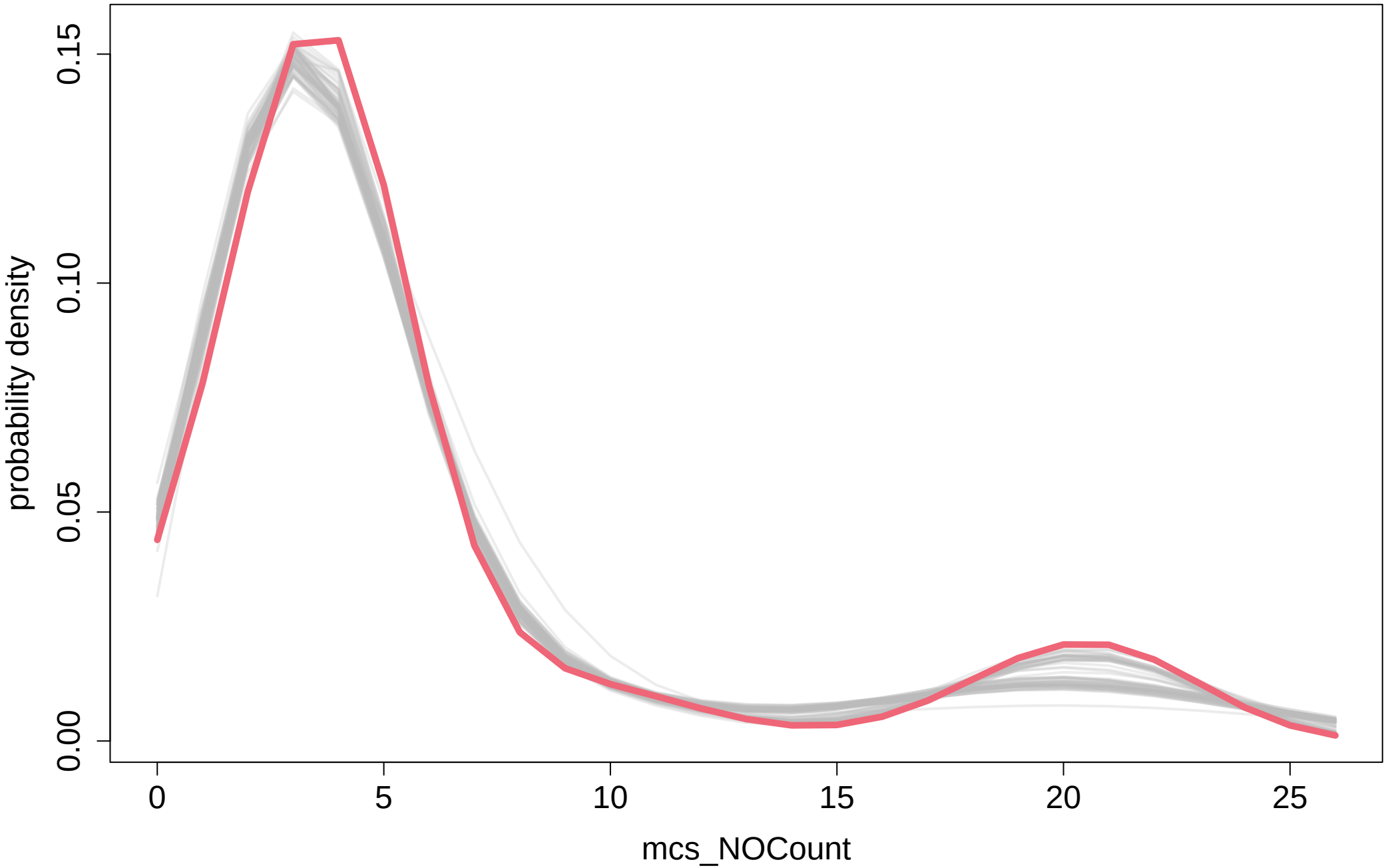
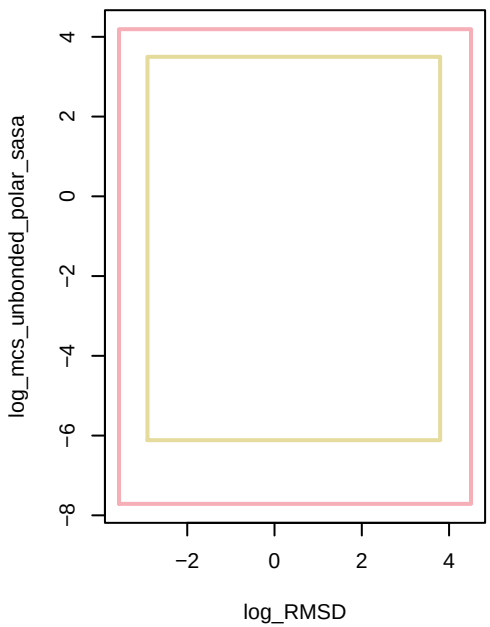
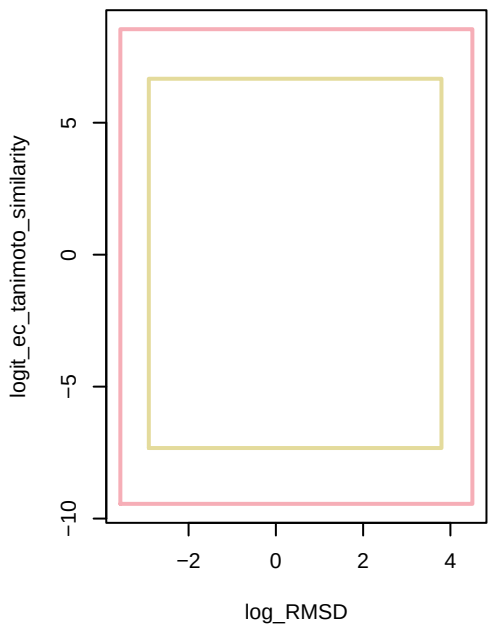
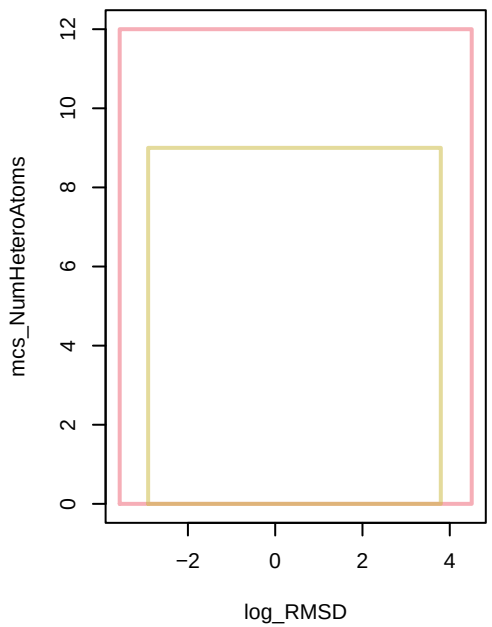
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount

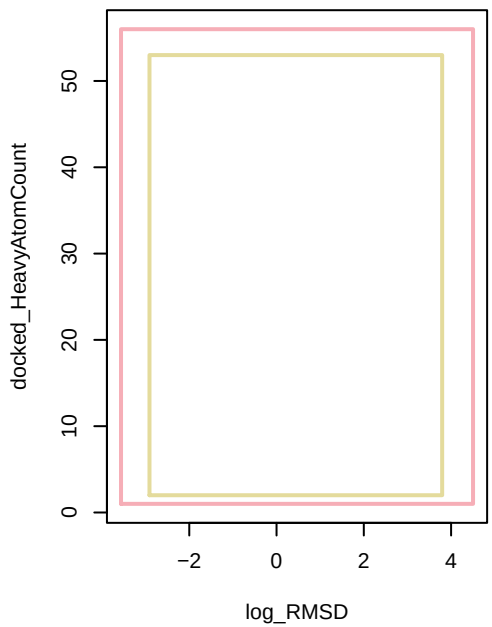

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
docked_NumRotatableBonds

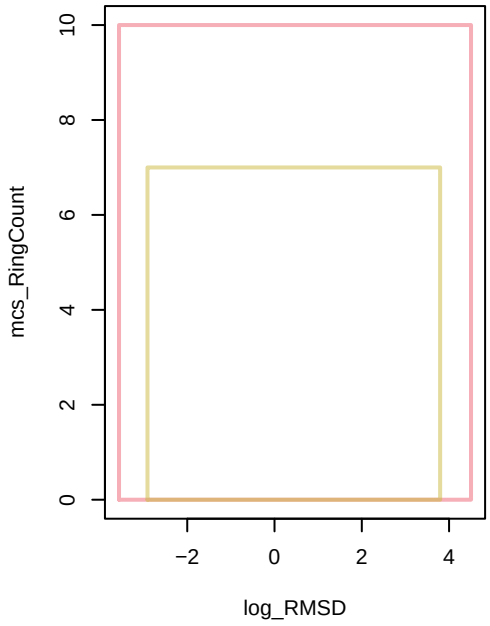

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

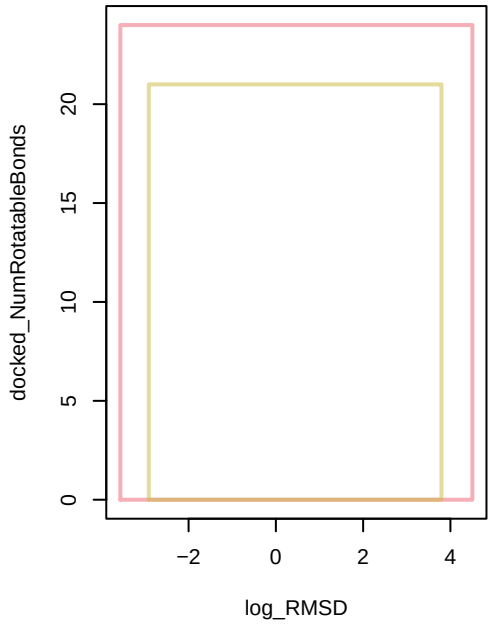

log_mcs_unbonded_polar_sasa
log_RMSD

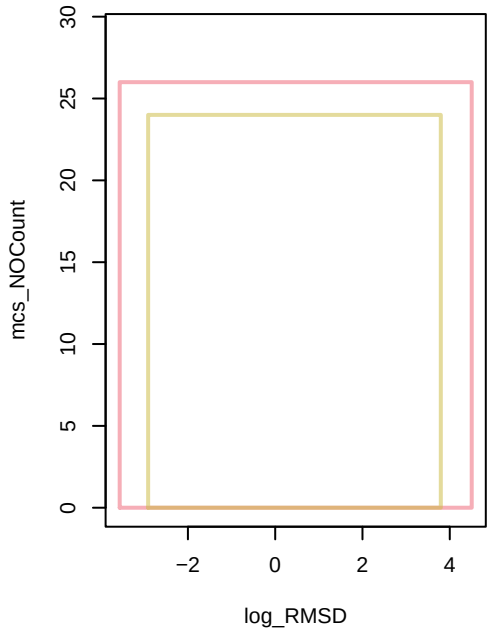

logit_ec_tanimoto_similarity
log_RMSD

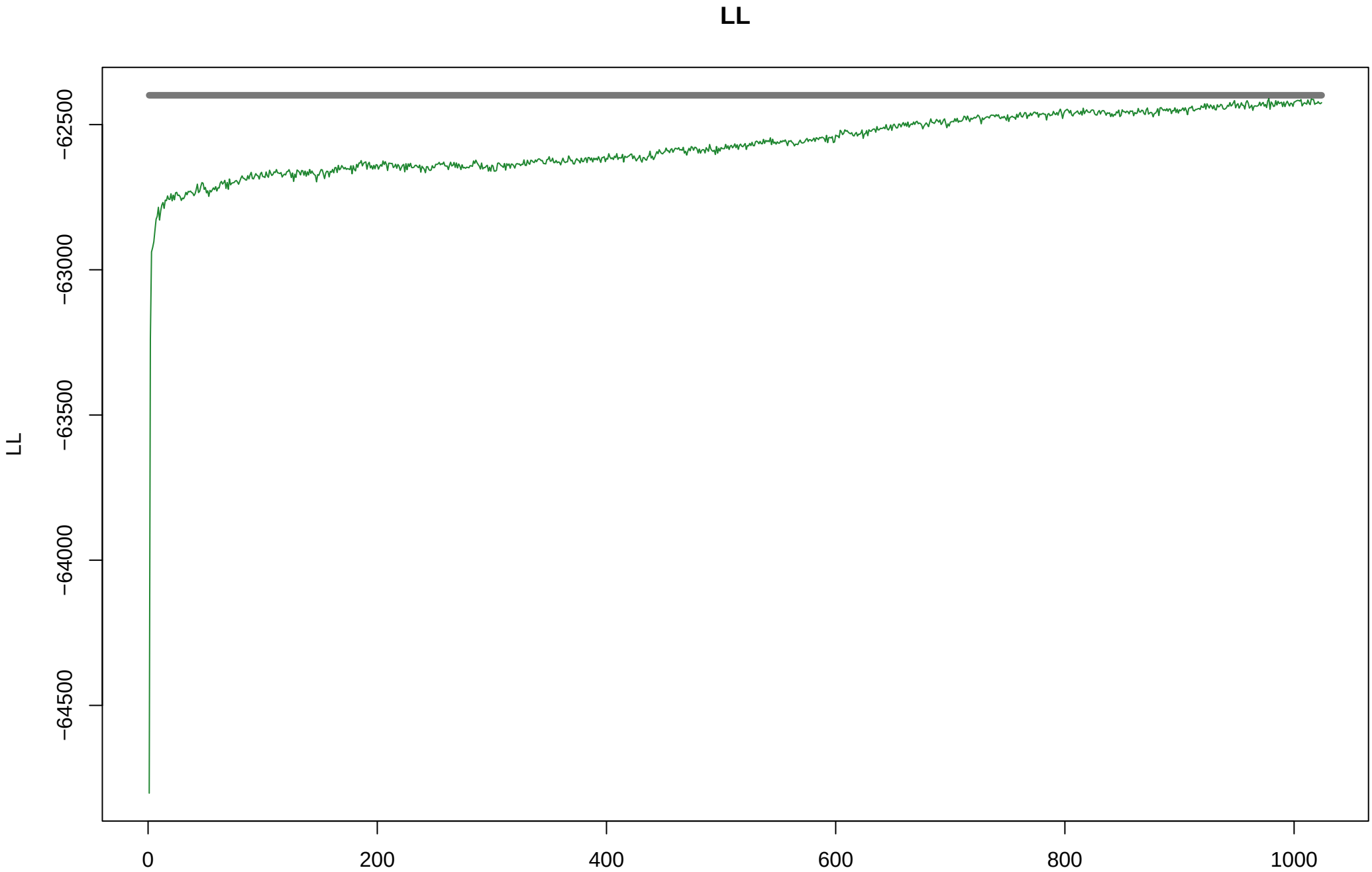

mcs_NumHeteroAtoms
log_RMSD

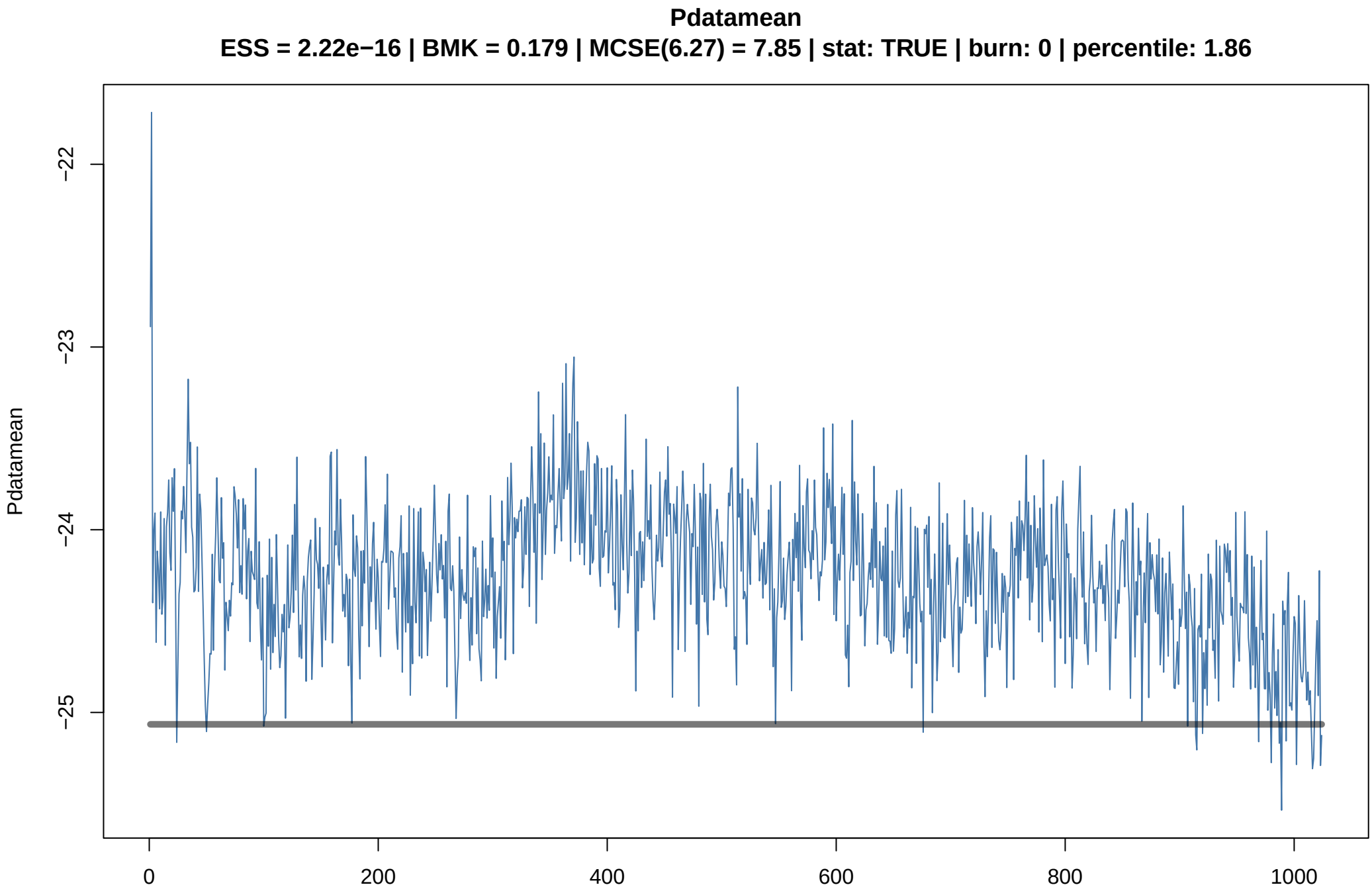

docked_HeavyAtomCount
log_RMSD

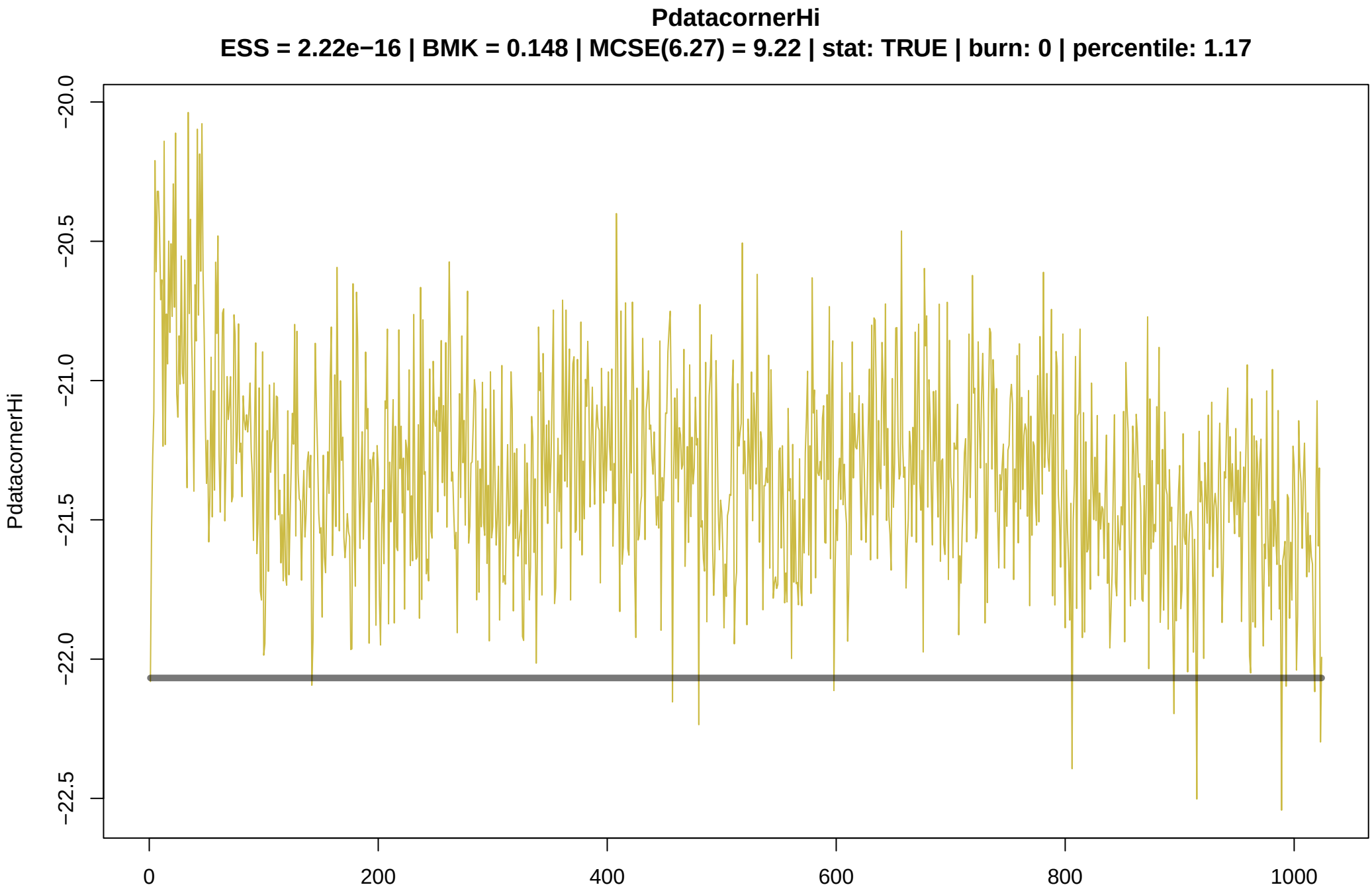

mcs_RingCount
log_RMSD

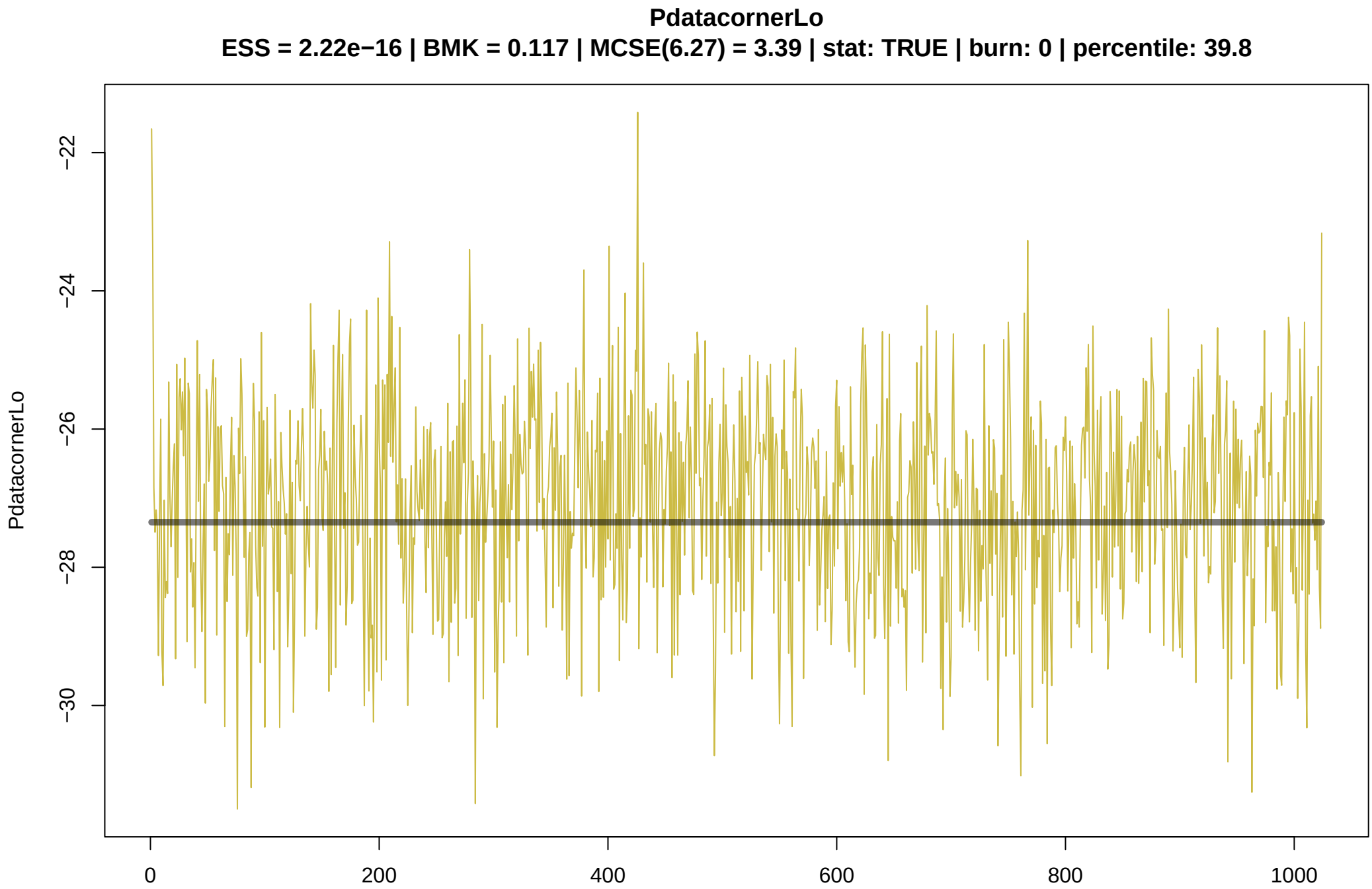

docked_NumRotatableBonds
log_RMSD

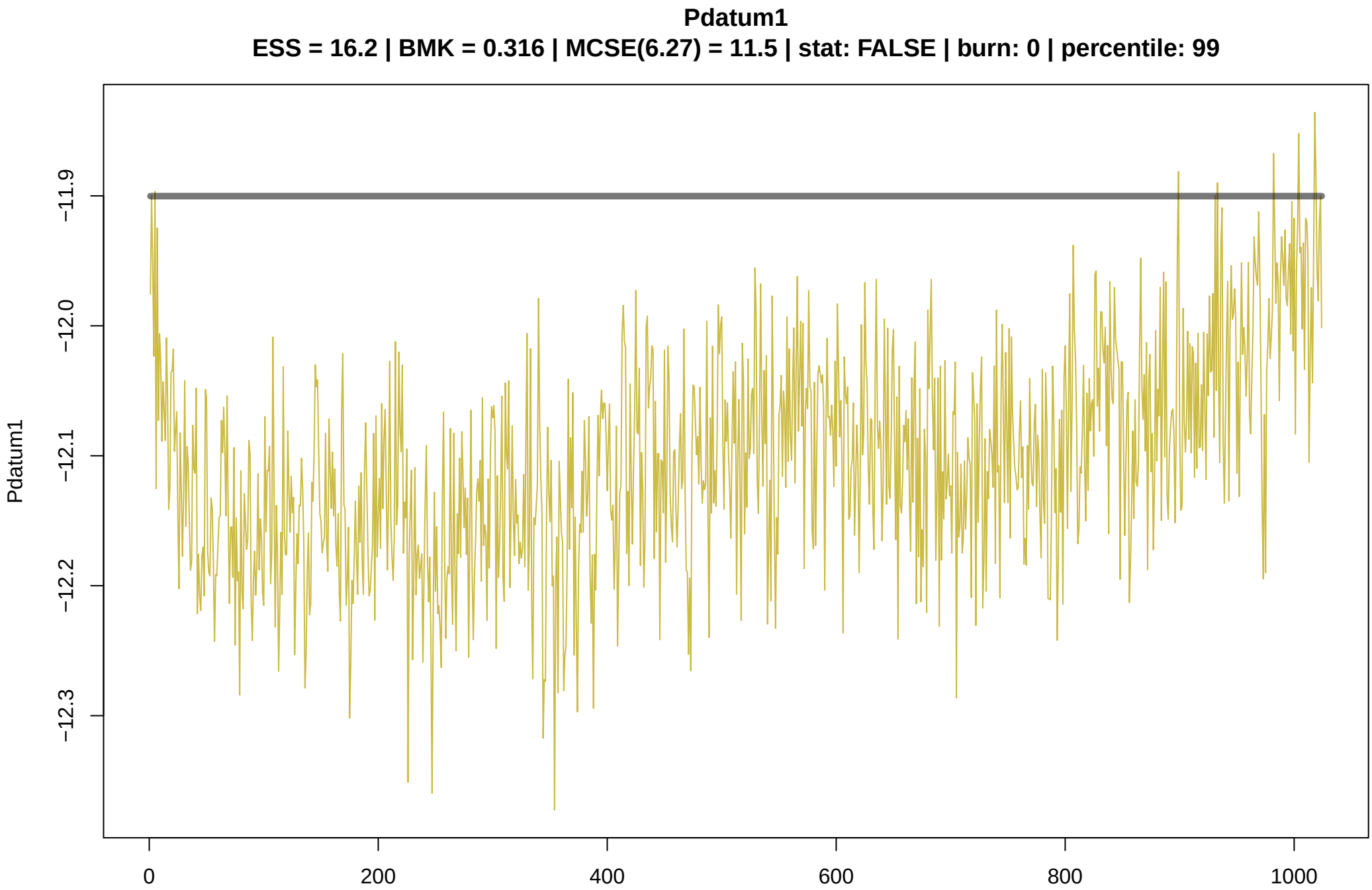

mcs_NOCount
log_RMSD

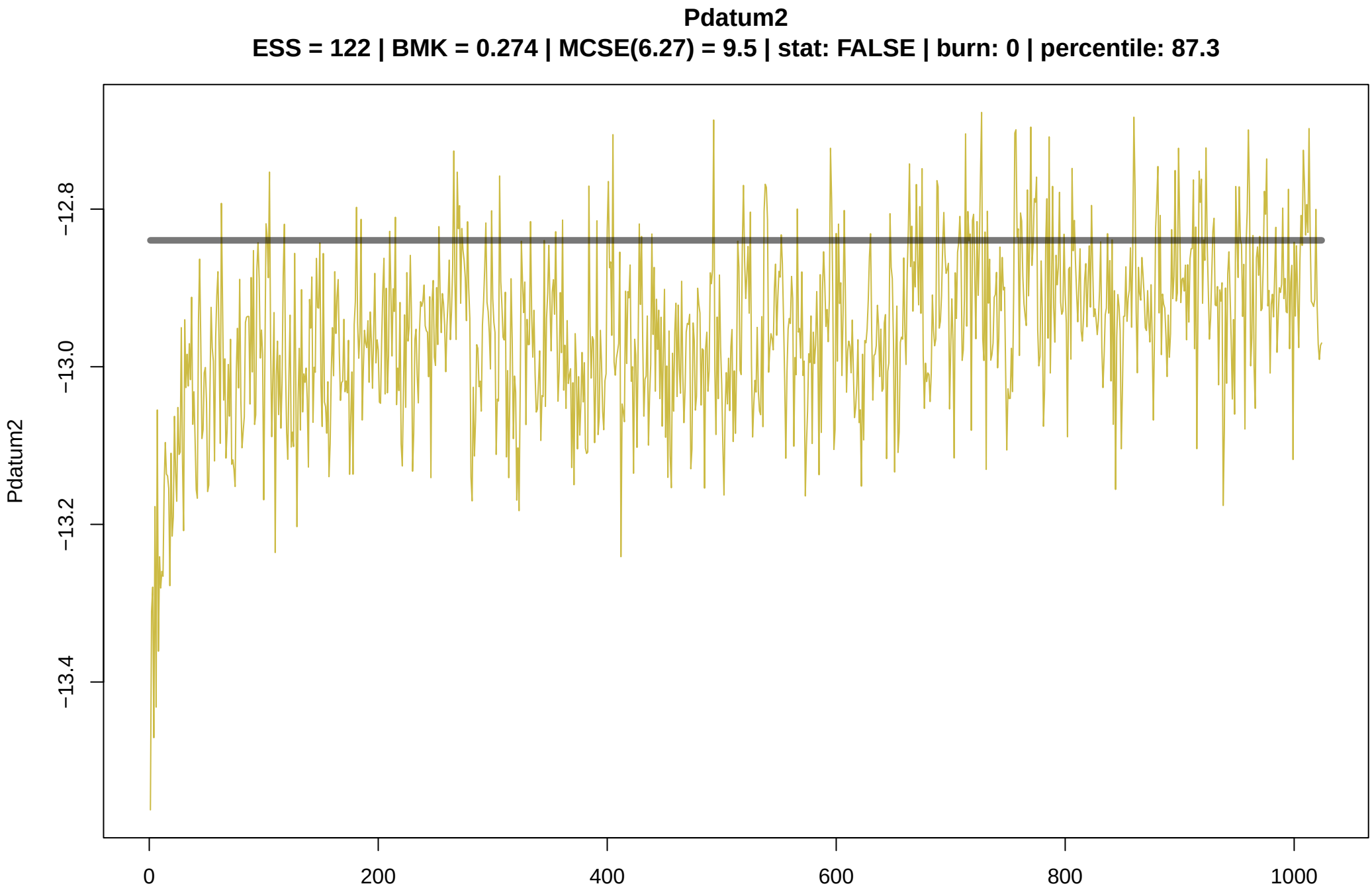

LL
LL
−62500
−63000
−63500
−64000
−64500
0
200
400
600
800
1000

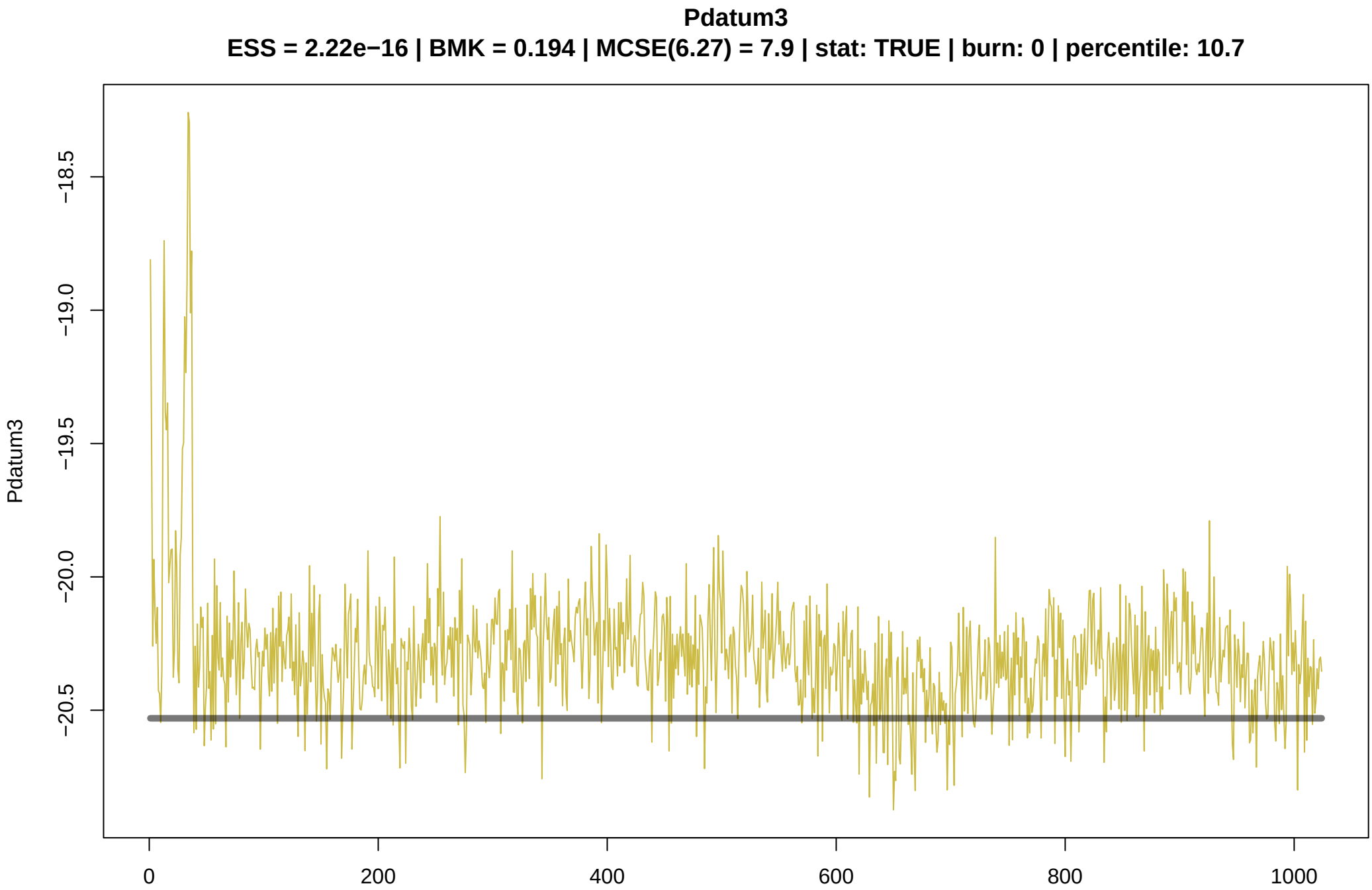

Pdatamean
ESS = 2.22e−16 | BMK = 0.179 | MCSE(6.27) = 7.85 | stat: TRUE | burn: 0 | percentile: 1.86
Pdatamean
−22
−23
−24
−25
0
200
400
600
800
1000

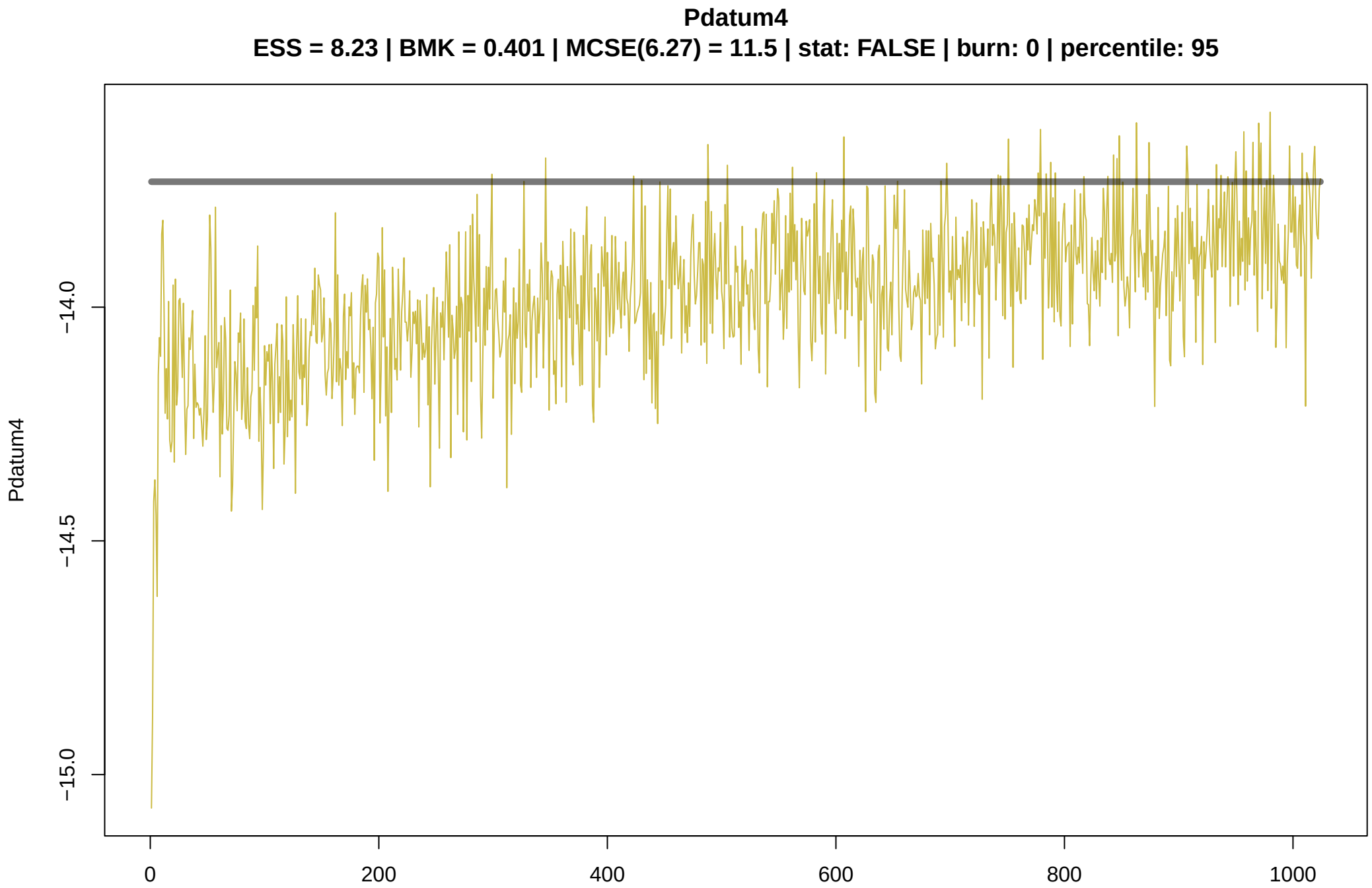

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.148 | MCSE(6.27) = 9.22 | stat: TRUE | burn: 0 | percentile: 1.17
PdatacornerHi
−20.0
−20.5
−21.0
−21.5
−22.0
−22.5
0
200
400
600
800
1000

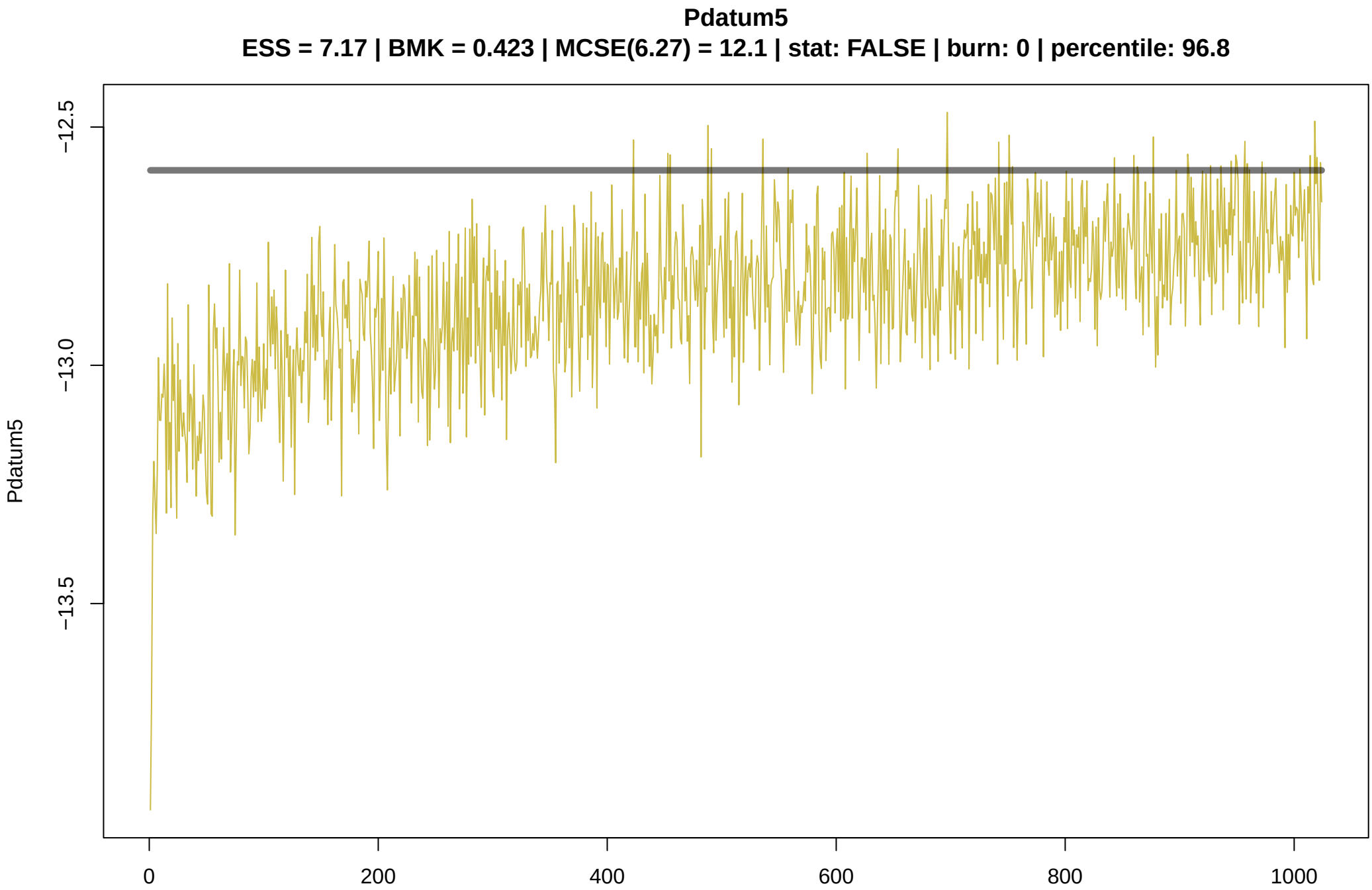

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.117 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | percentile: 39.8
PdatacornerLo
−22
−24
−26
−28
−30
0
200
400
600
800
1000

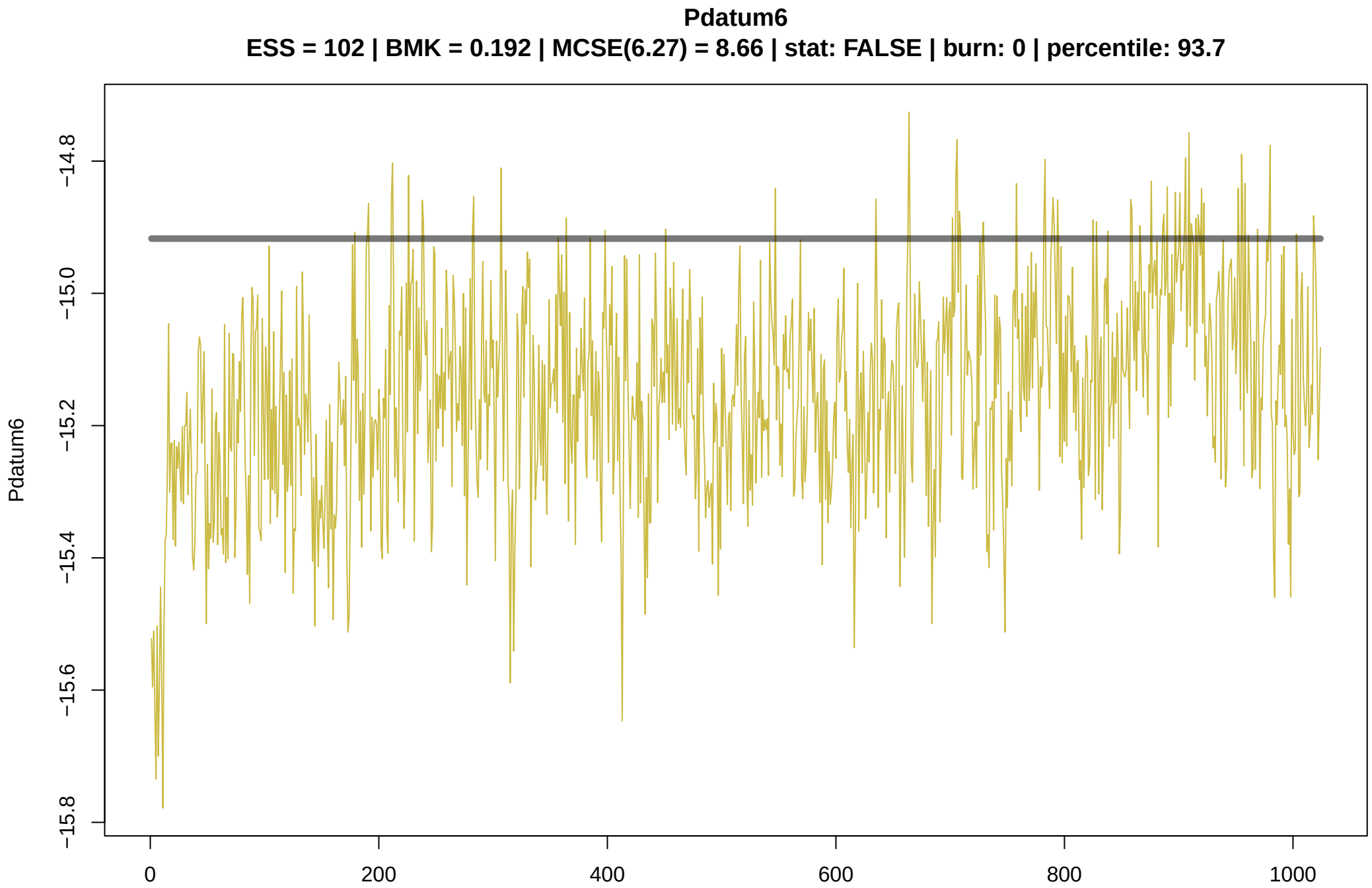

Pdatum1
ESS = 16.2 | BMK = 0.316 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 0 | percentile: 99
Pdatum1
−11.9
−12.0
−12.1
−12.2
−12.3
0
200
400
600
800
1000

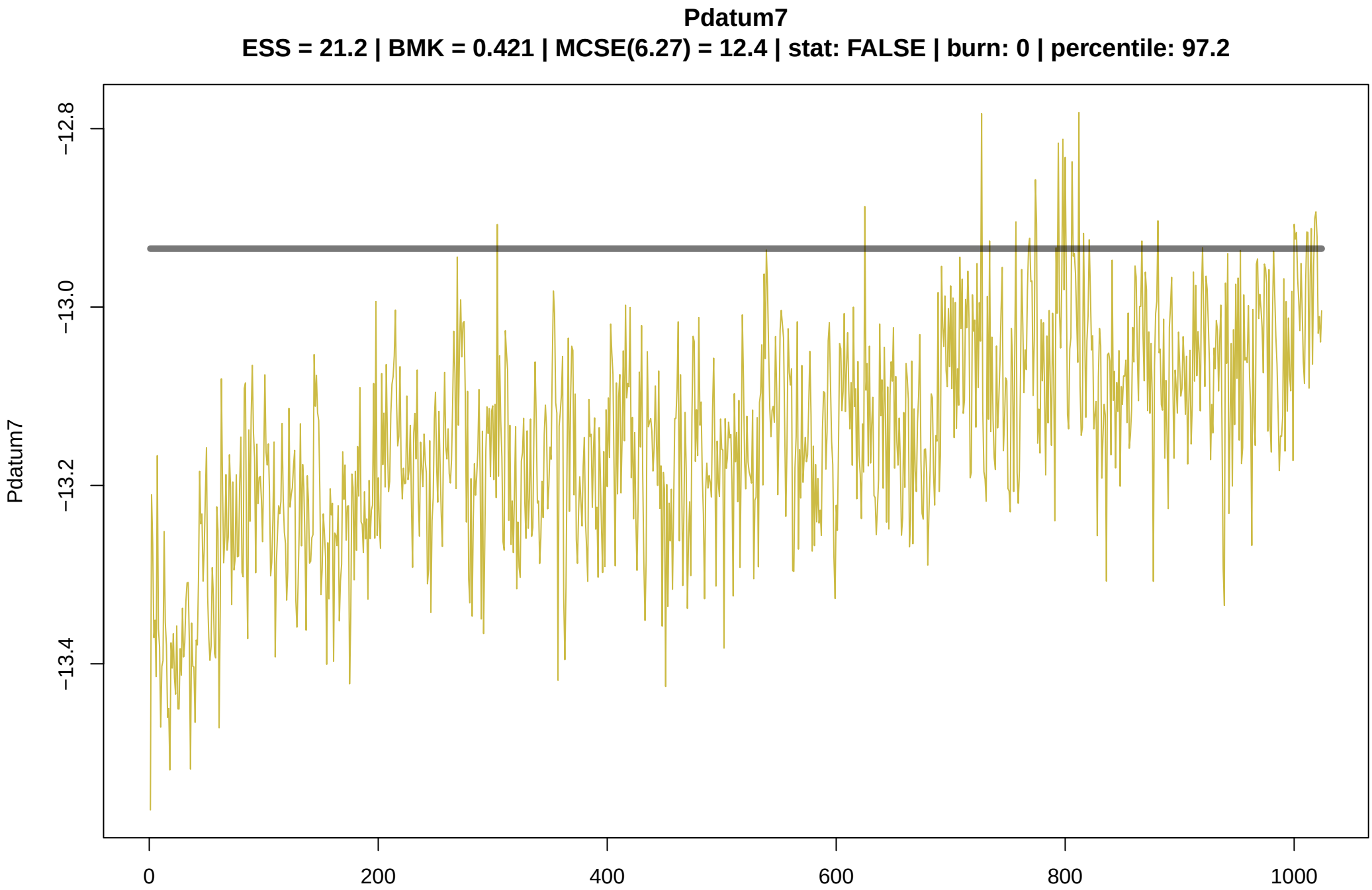

Pdatum2
ESS = 122 | BMK = 0.274 | MCSE(6.27) = 9.5 | stat: FALSE | burn: 0 | percentile: 87.3
Pdatum2
−12.8
−13.0
−13.2
−13.4
0
200
400
600
800
1000

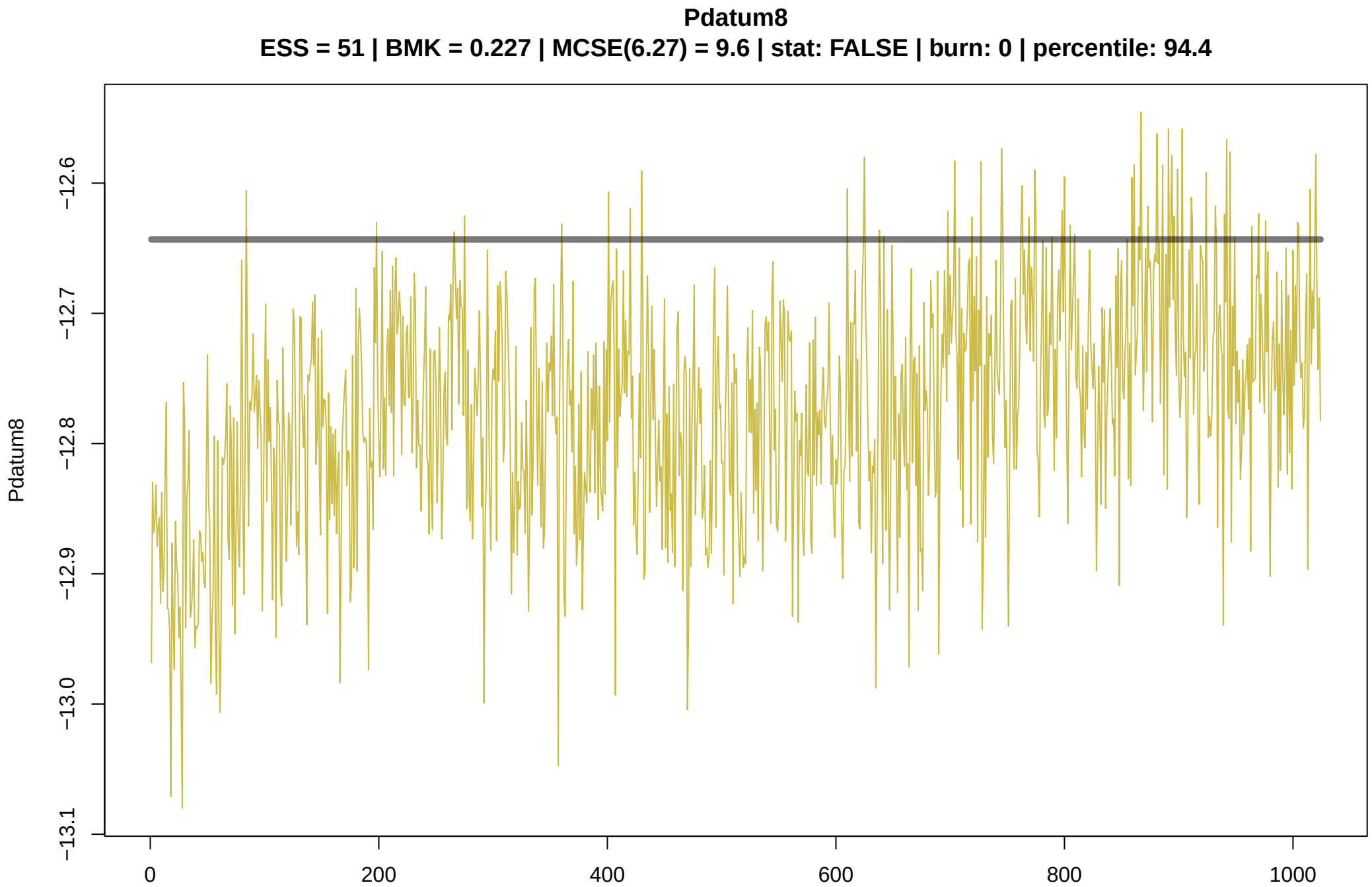

Pdatum3
ESS = 2.22e−16 | BMK = 0.194 | MCSE(6.27) = 7.9 | stat: TRUE | burn: 0 | percentile: 10.7
Pdatum3
−18.5
−19.0
−19.5
−20.0
−20.5
0
200
400
600
800
1000

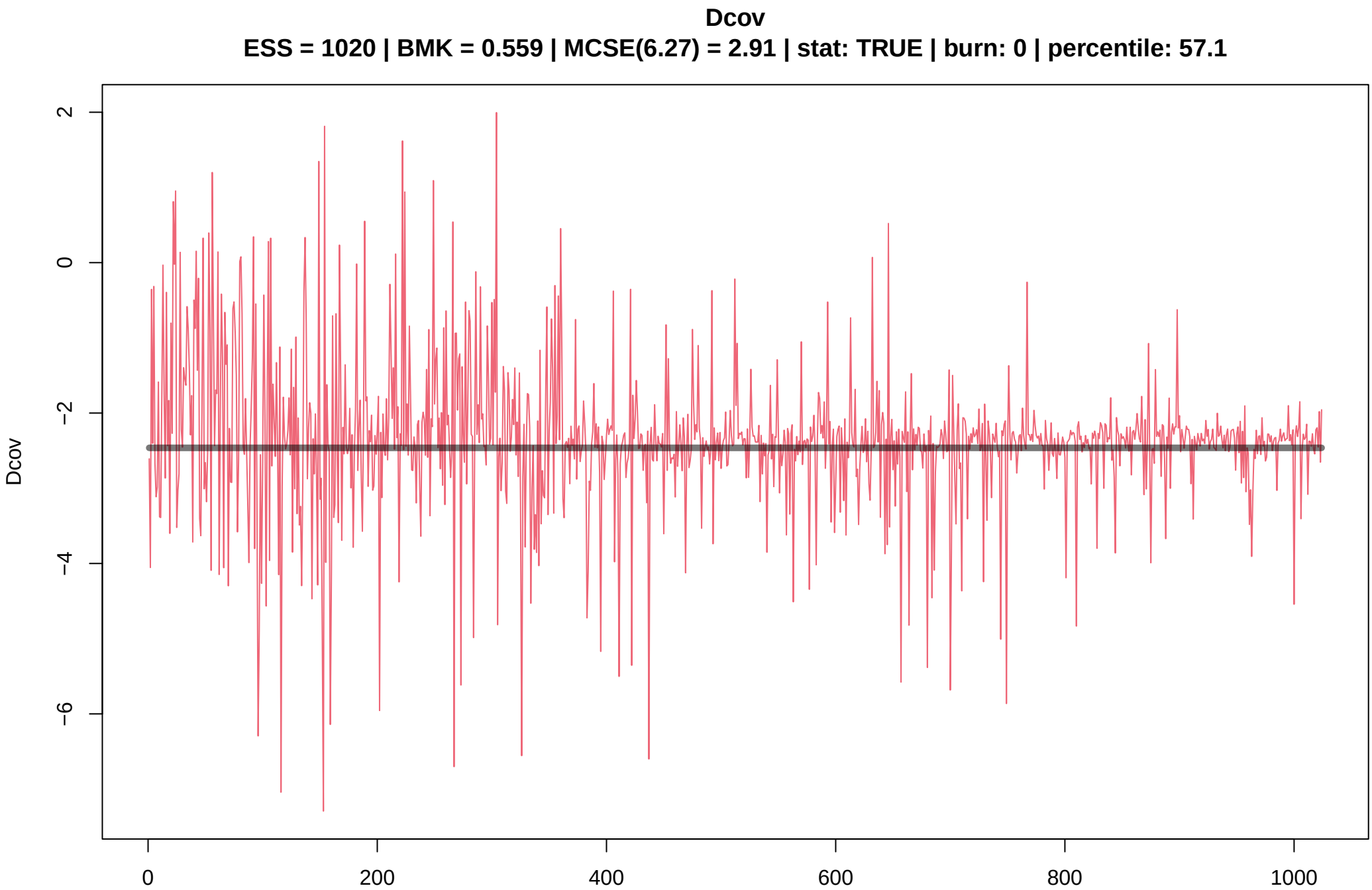

Pdatum4
ESS = 8.23 | BMK = 0.401 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 0 | percentile: 95
Pdatum4
−14.0
−14.5
−15.0
0
200
400
600
800
1000

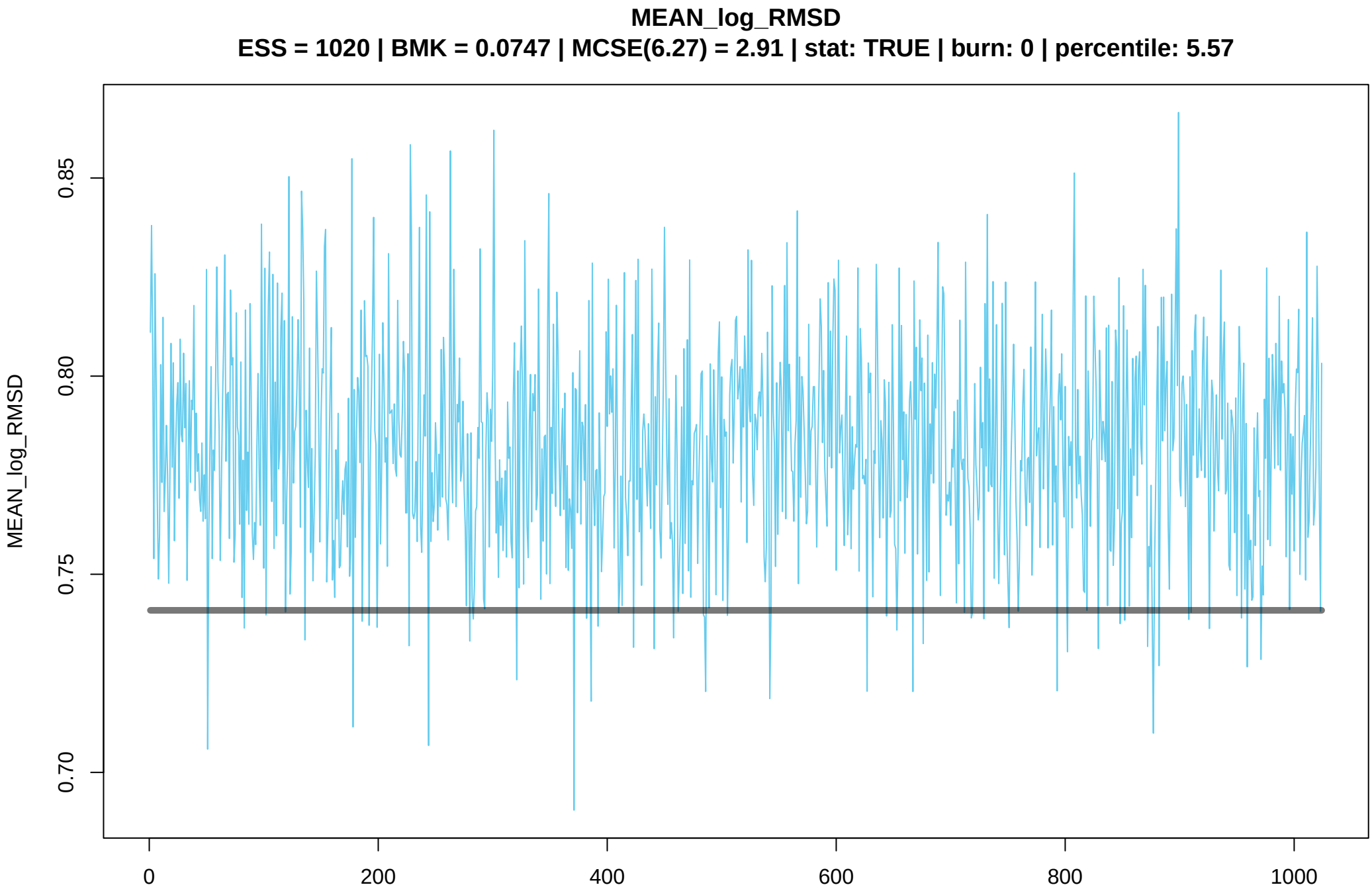

Pdatum5
ESS = 7.17 | BMK = 0.423 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0 | percentile: 96.8
Pdatum5
−12.5
−13.0
−13.5
0
200
400
600
800
1000

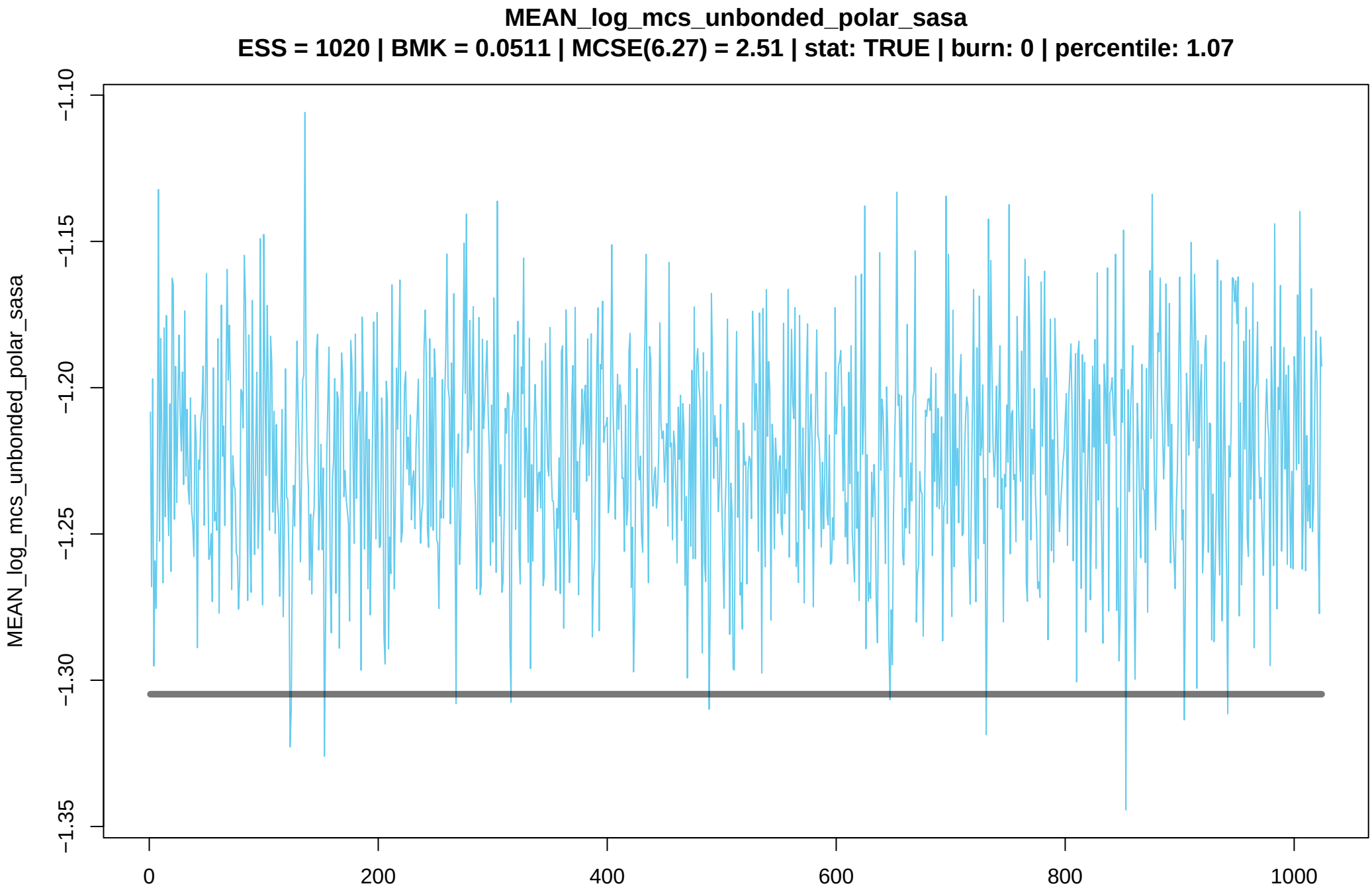

Pdatum6
ESS = 102 | BMK = 0.192 | MCSE(6.27) = 8.66 | stat: FALSE | burn: 0 | percentile: 93.7
Pdatum6
−14.8
−15.0
−15.2
−15.4
−15.6
−15.8
0
200
400
600
800
1000

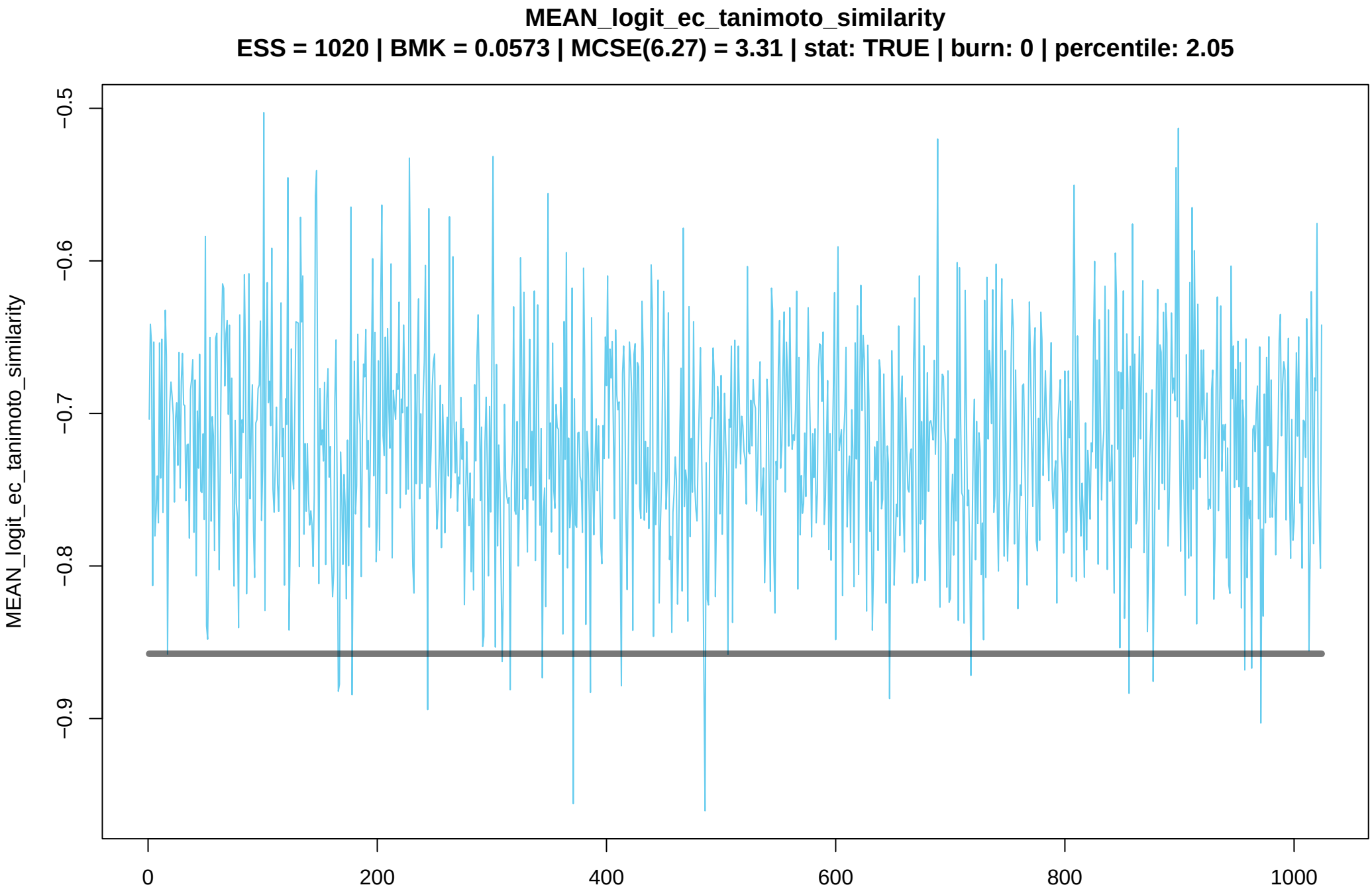

Pdatum7
ESS = 21.2 | BMK = 0.421 | MCSE(6.27) = 12.4 | stat: FALSE | burn: 0 | percentile: 97.2
Pdatum7
−12.8
−13.0
−13.2
−13.4
0
200
400
600
800
1000

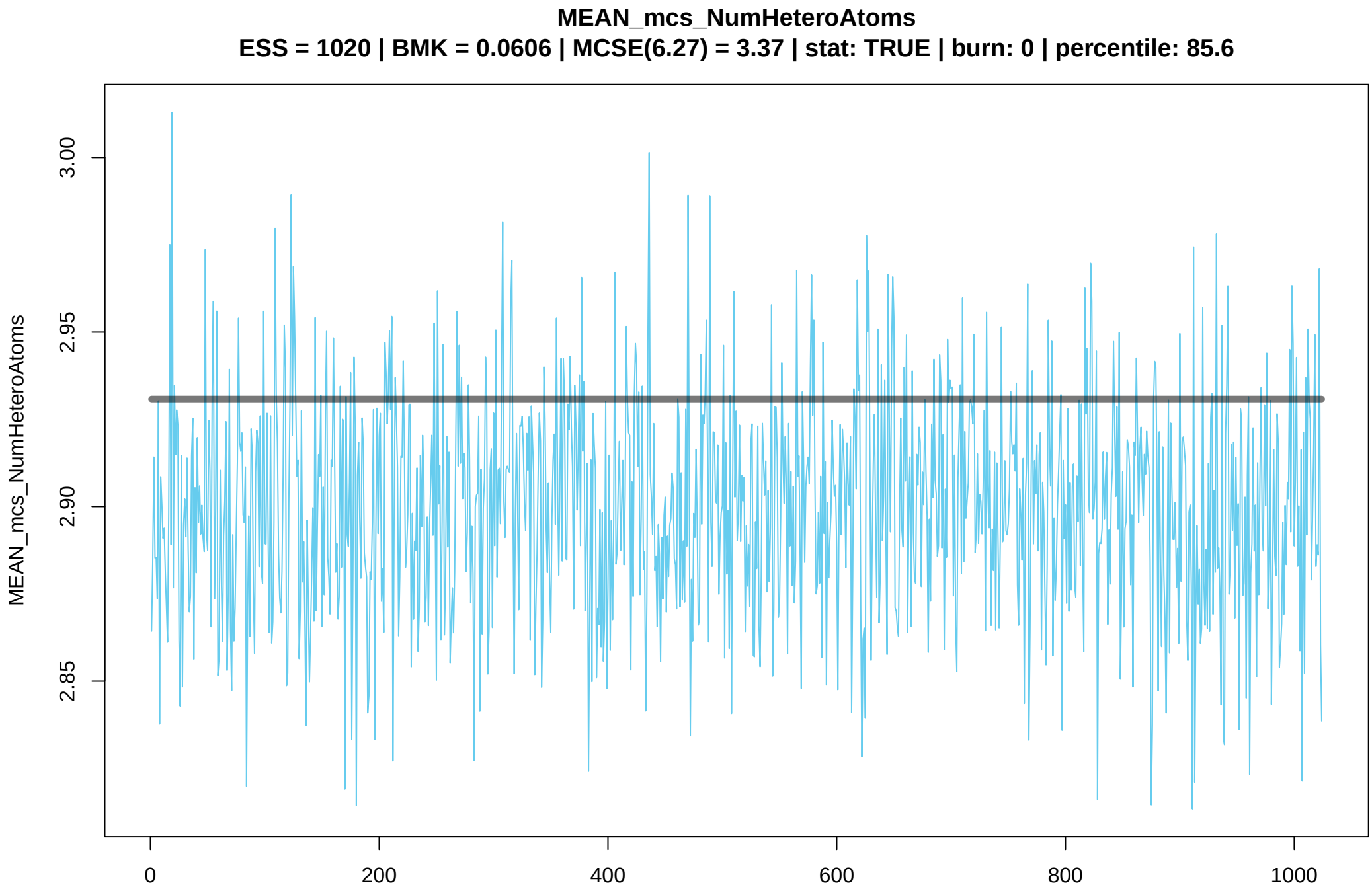

Pdatum8
ESS = 51 | BMK = 0.227 | MCSE(6.27) = 9.6 | stat: FALSE | burn: 0 | percentile: 94.4
Pdatum8
−12.6
−12.7
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

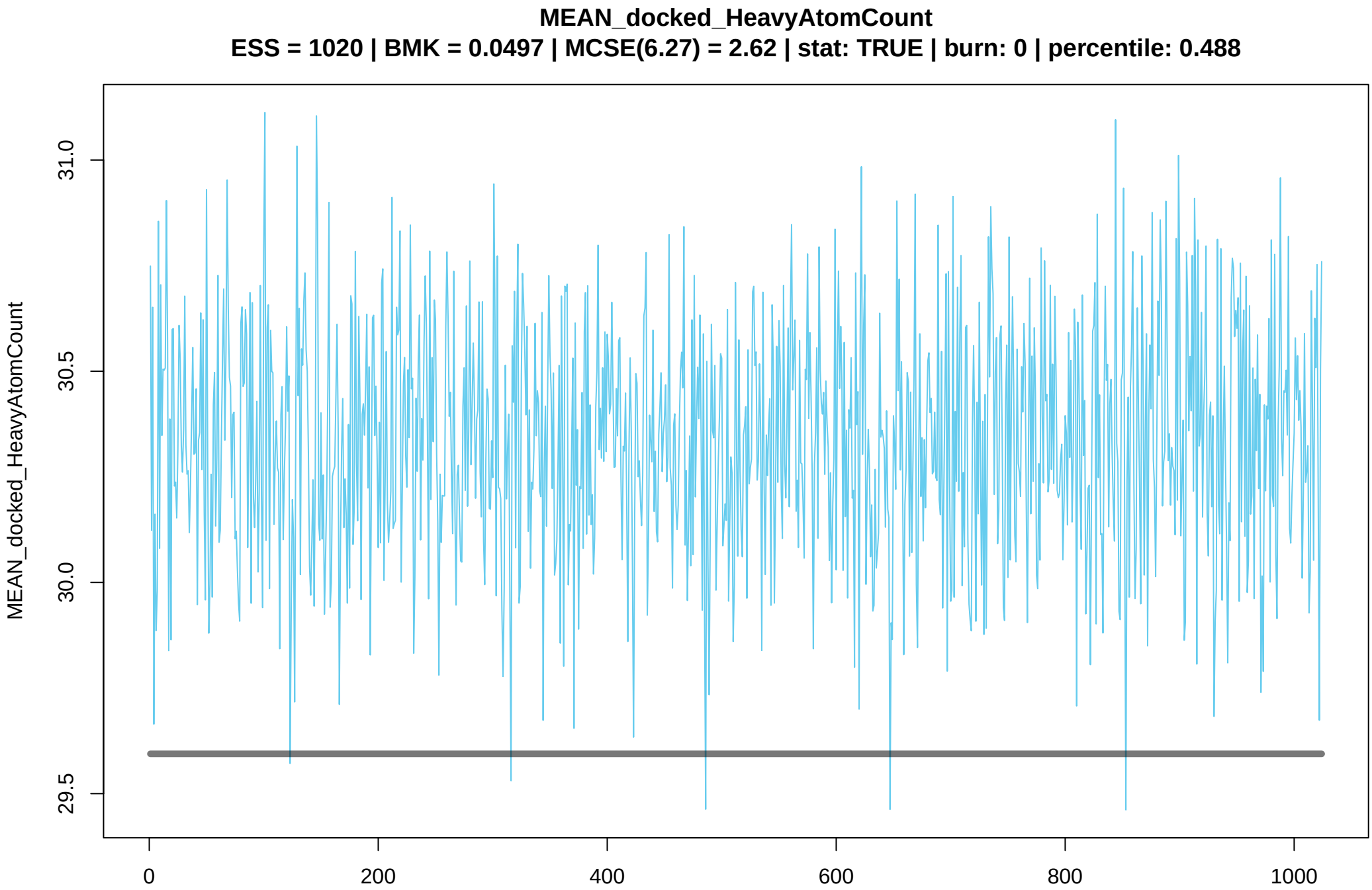

Dcov
ESS = 1020 | BMK = 0.559 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | percentile: 57.1
Dcov
2
0
−2
−4
−6
0
200
400
600
800
1000

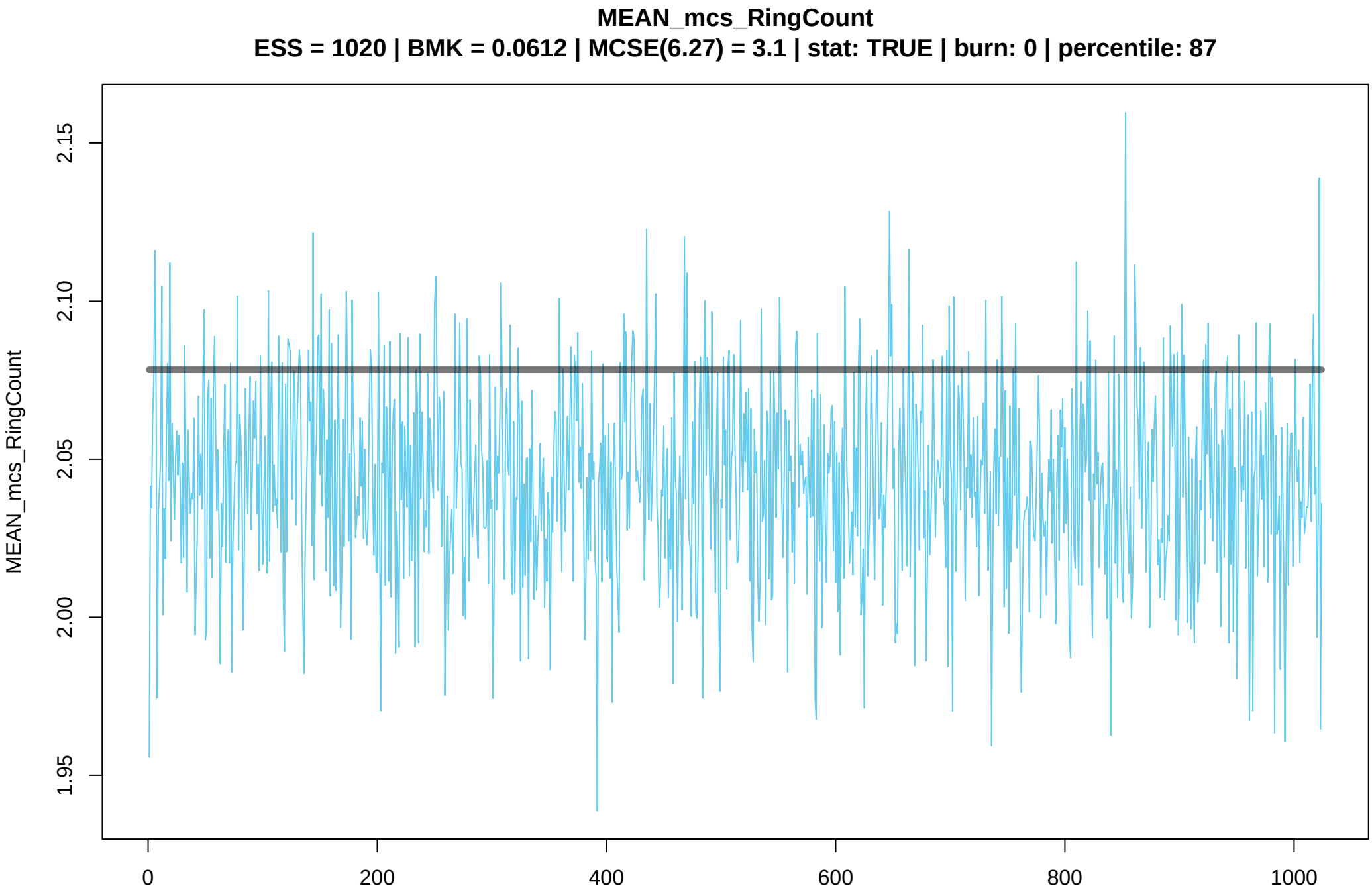

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0747 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | percentile: 5.57
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

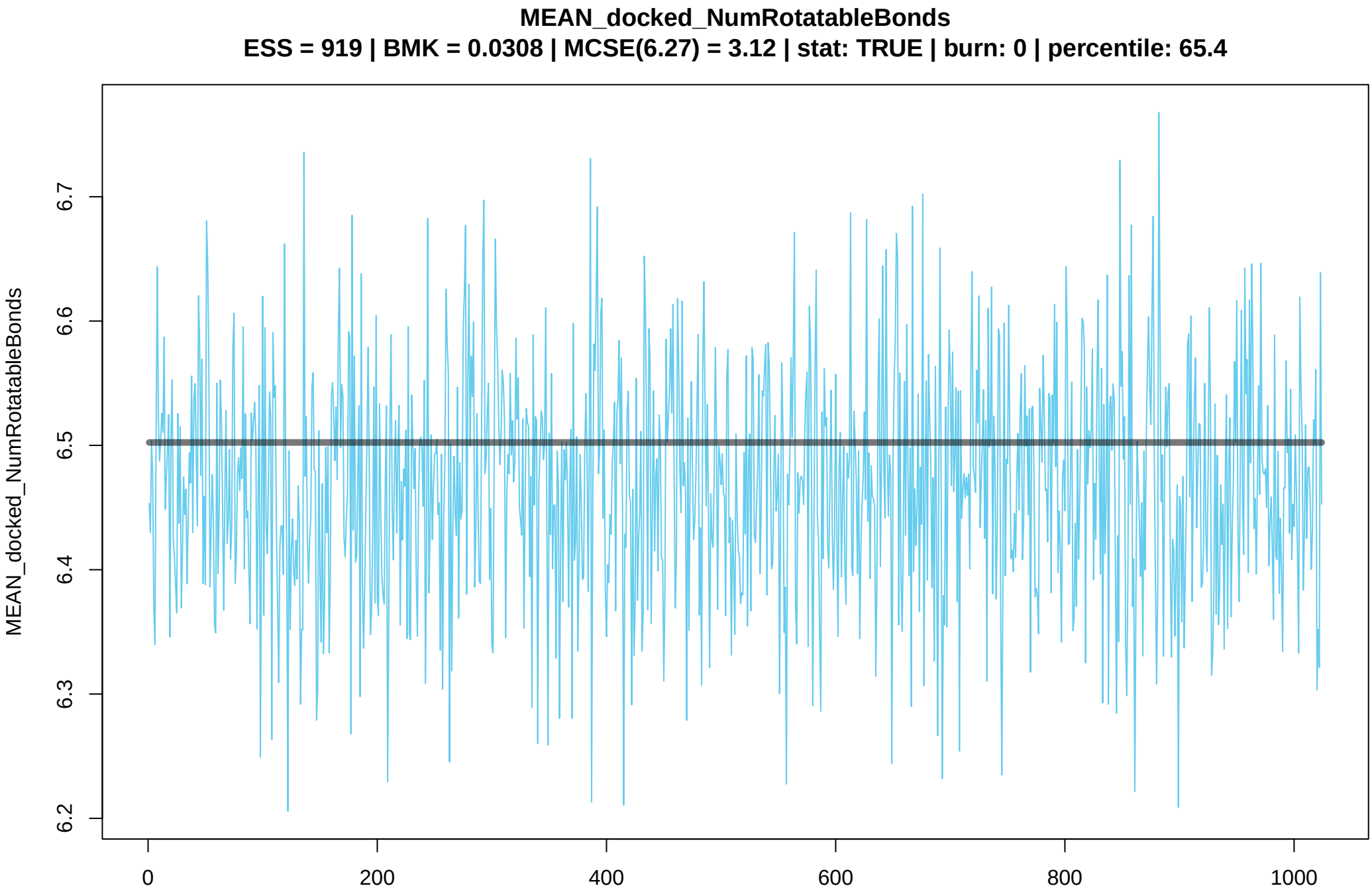

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0511 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | percentile: 1.07
MEAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

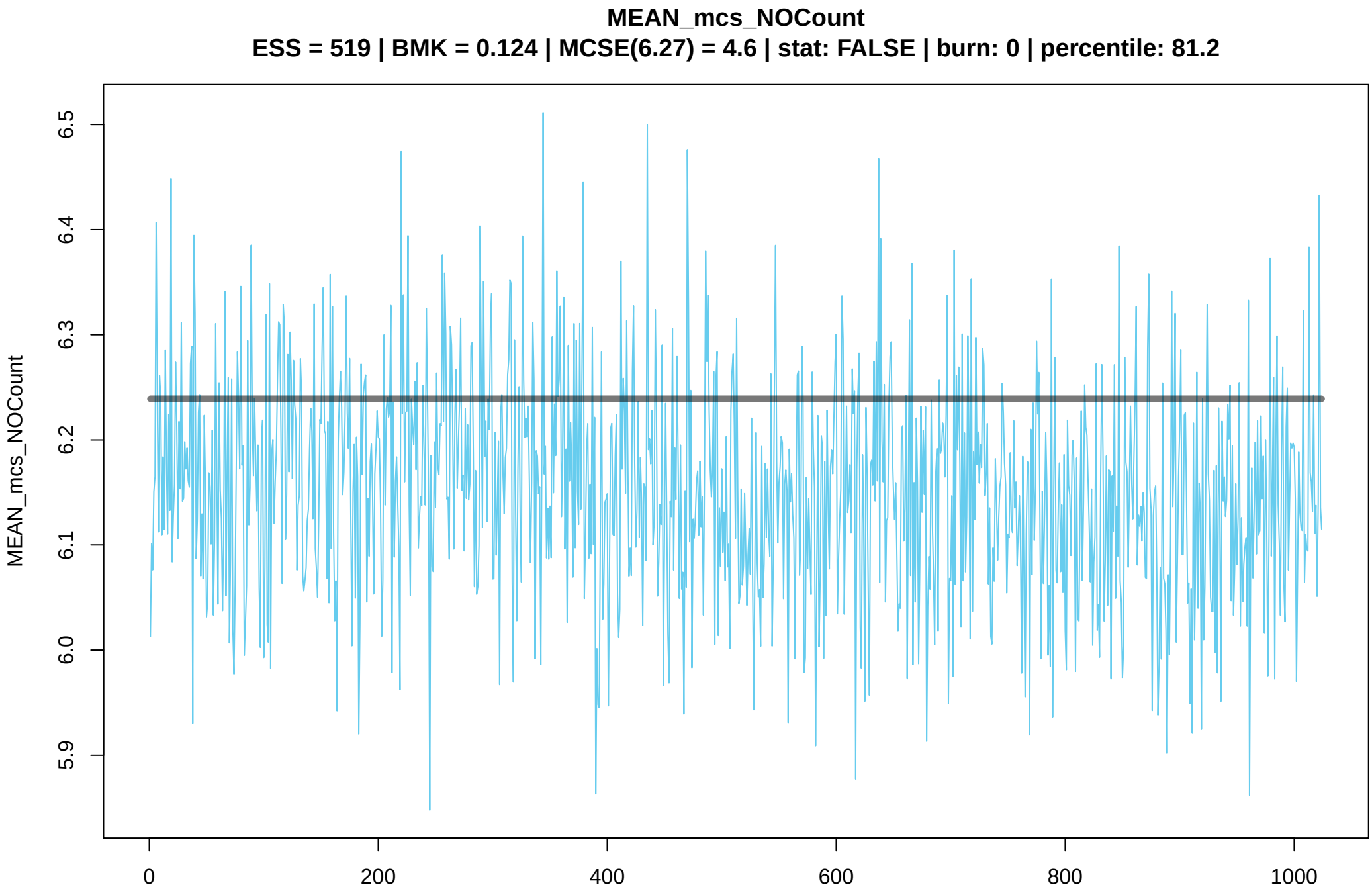

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0573 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0 | percentile: 2.05
MEAN_logit_ec_tanimoto_similarity
−0.5
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

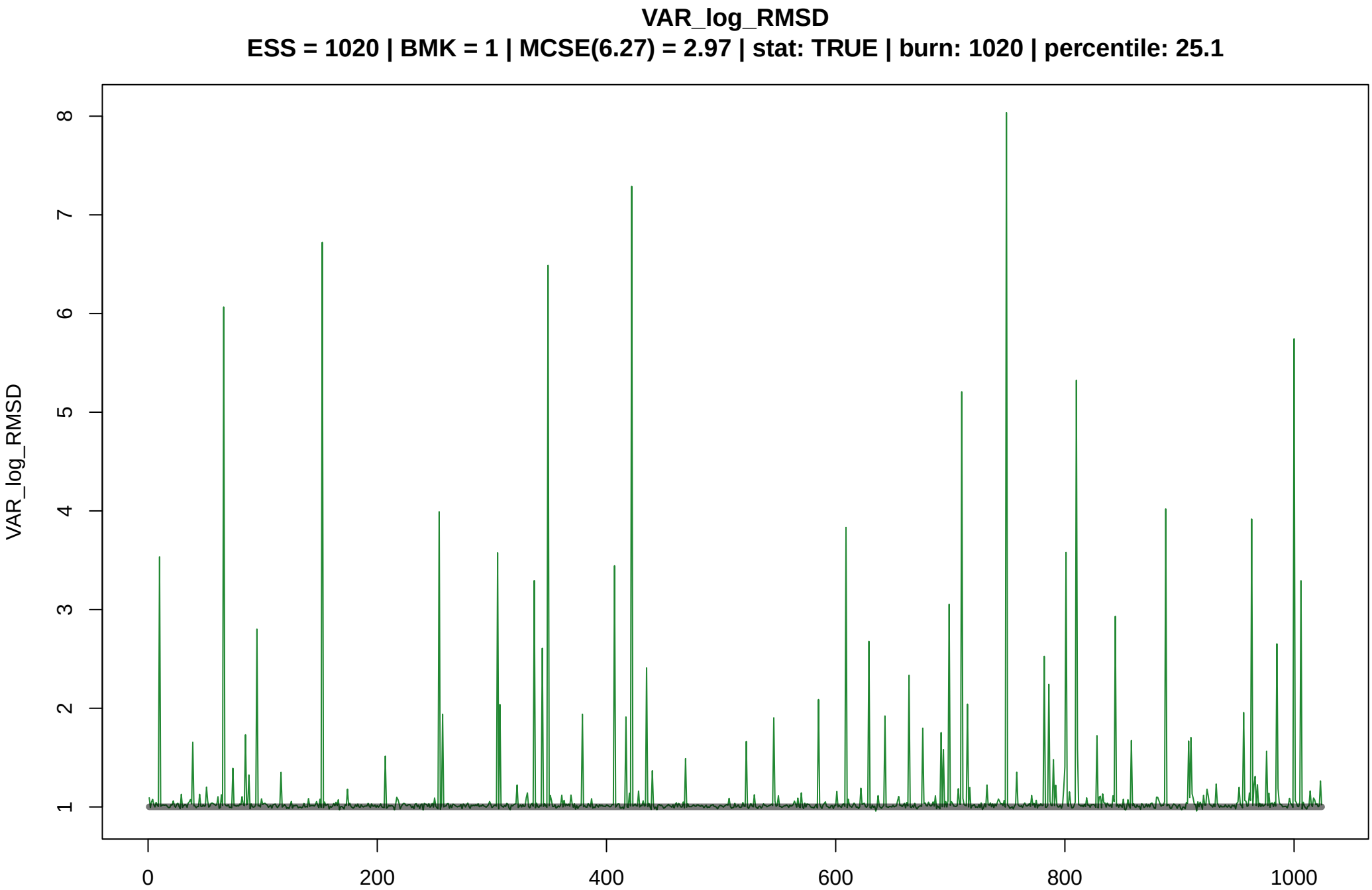

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0606 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | percentile: 85.6
MEAN_mcs_NumHeteroAtoms
3.00
2.95
2.90
2.85
0
200
400
600
800
1000

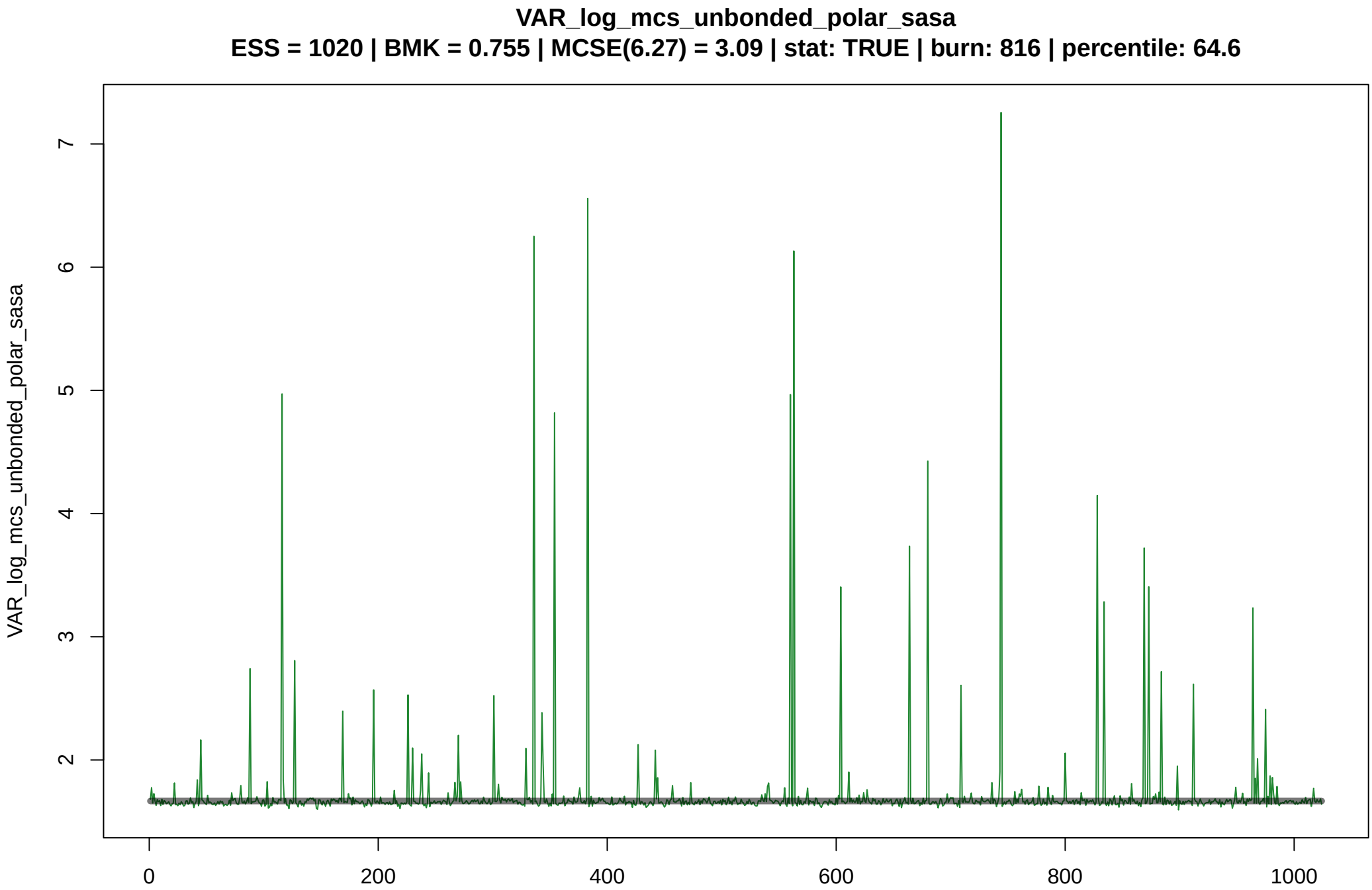

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0497 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | percentile: 0.488
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
31.0
0
200
400
600
800
1000

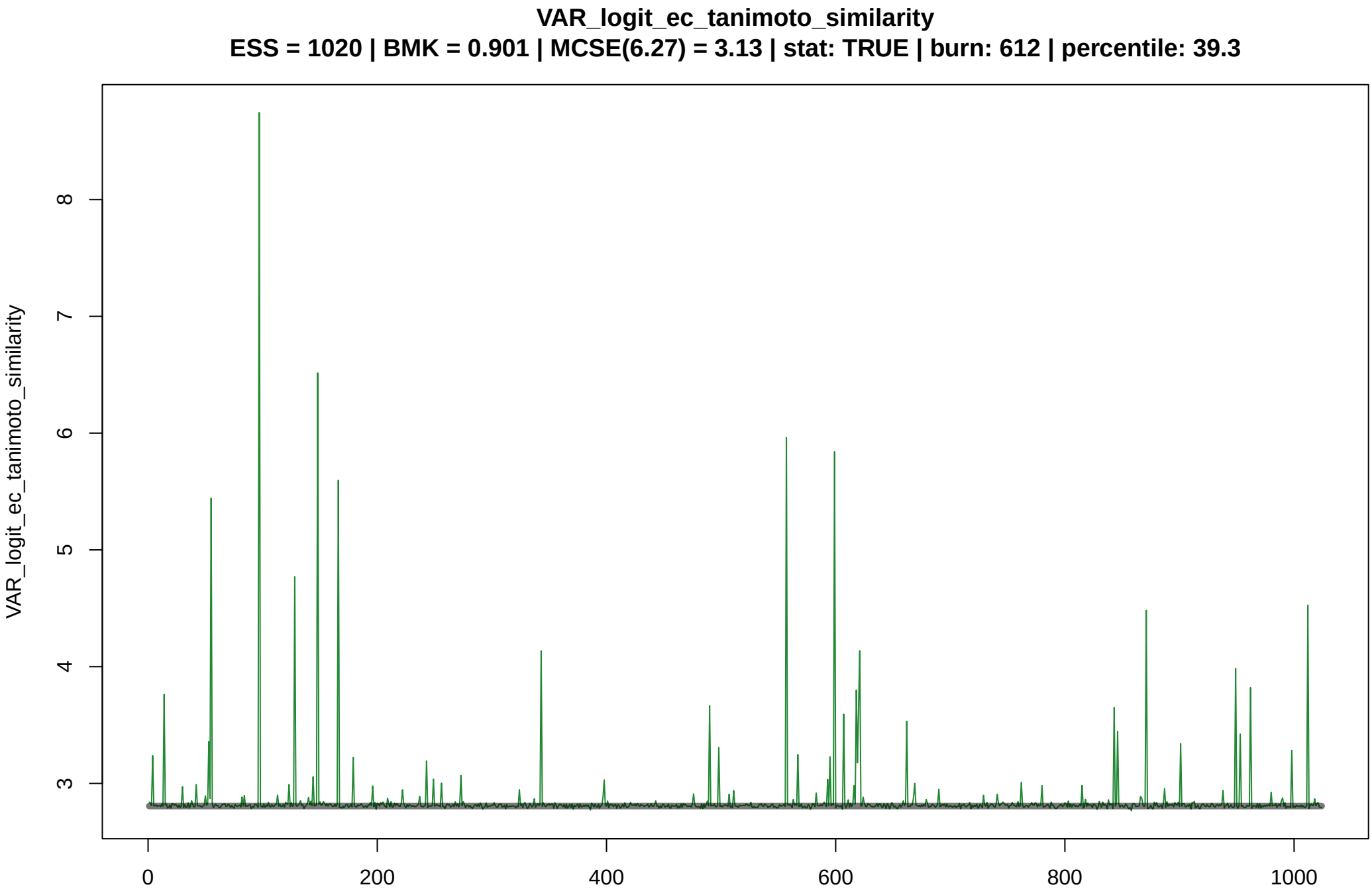

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0612 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | percentile: 87
MEAN_mcs_RingCount
2.15
2.10
2.05
2.00
1.95
0
200
400
600
800
1000

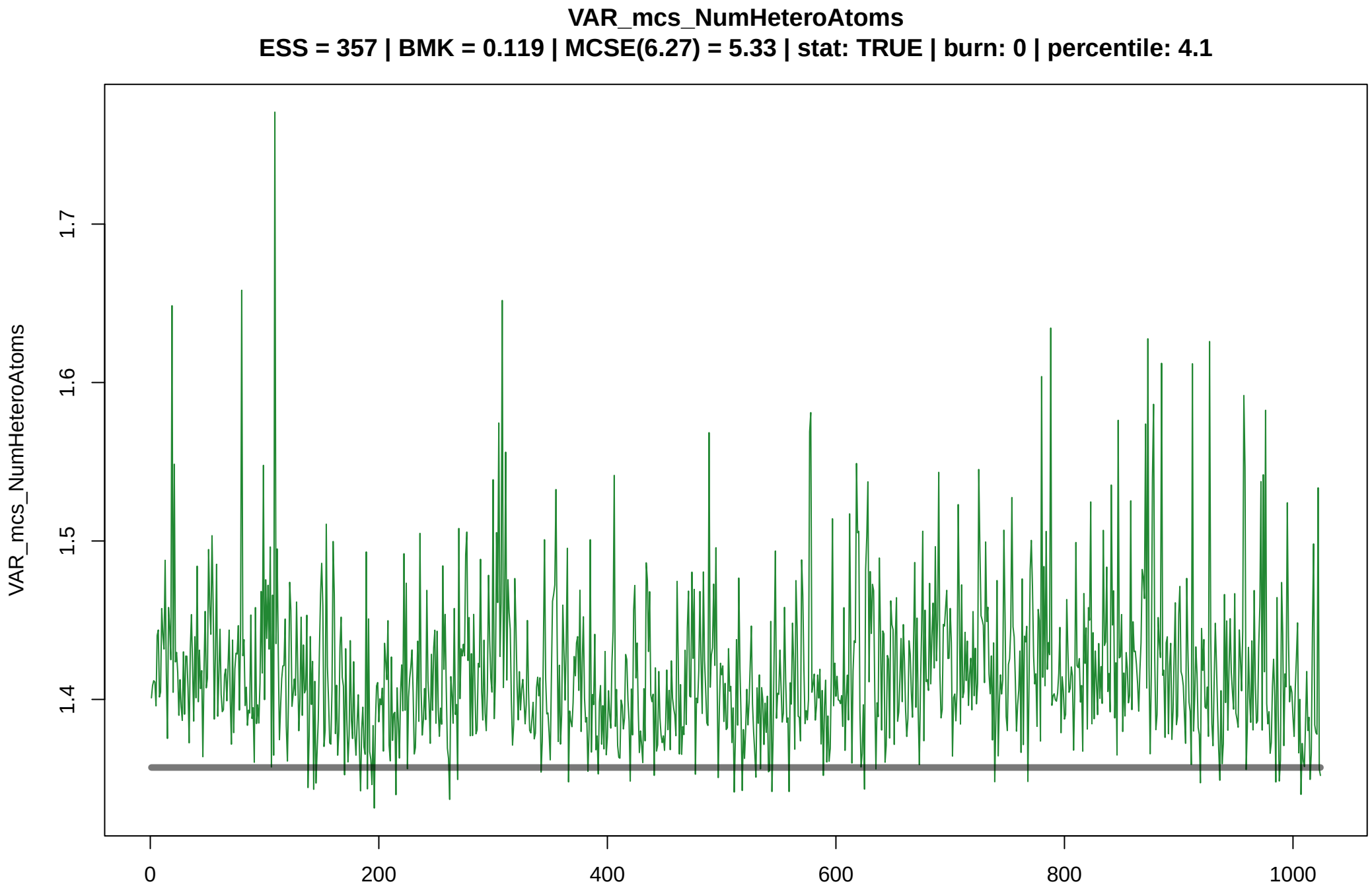

MEAN_docked_NumRotatableBonds
ESS = 919 | BMK = 0.0308 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | percentile: 65.4
MEAN_docked_NumRotatableBonds
6.2
6.3
6.4
6.5
6.6
6.7
0
200
400
600
800
1000

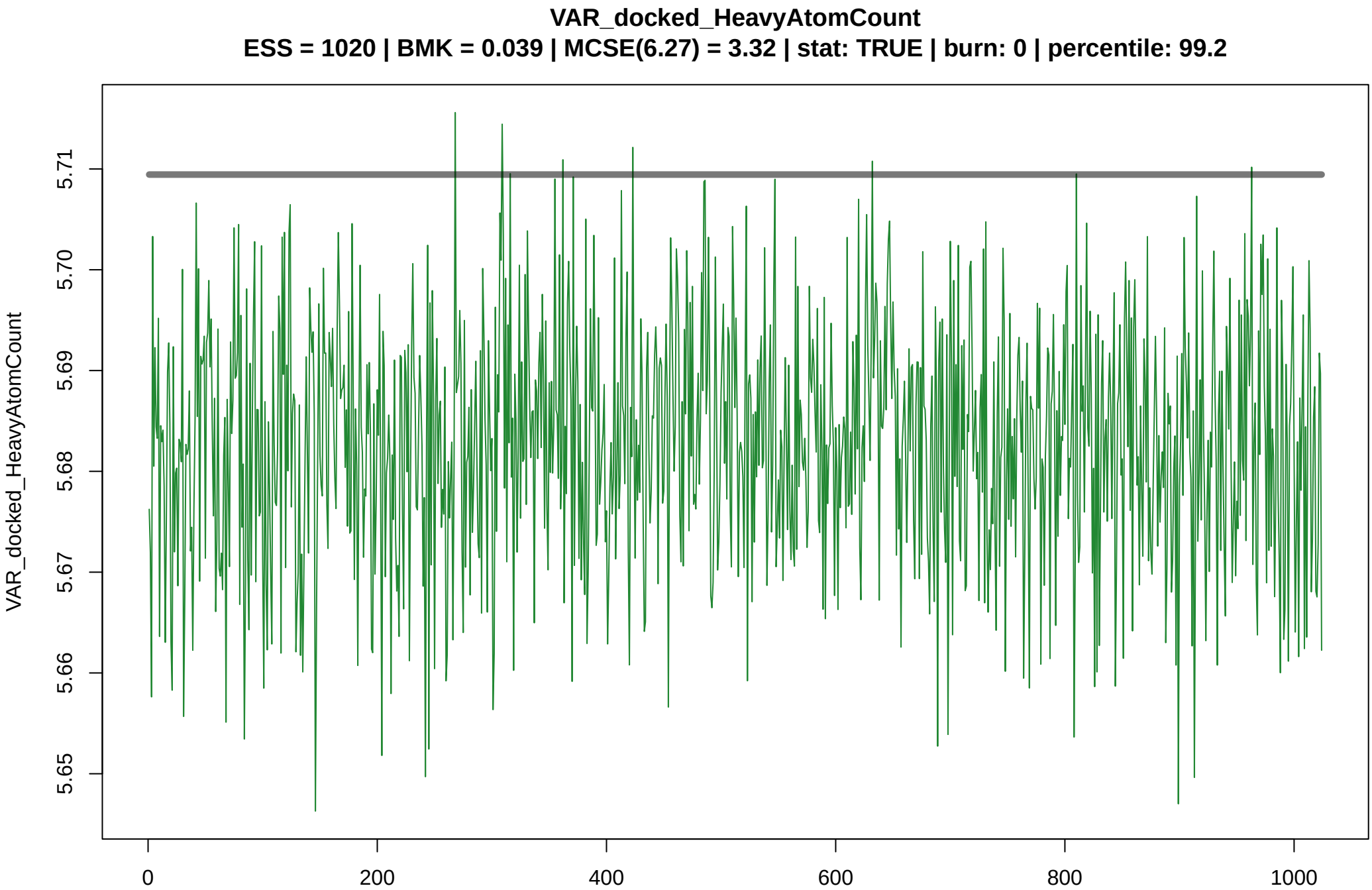

MEAN_mcs_NOCount
ESS = 519 | BMK = 0.124 | MCSE(6.27) = 4.6 | stat: FALSE | burn: 0 | percentile: 81.2
MEAN_mcs_NOCount
5.9
6.0
6.1
6.2
6.3
6.4
6.5
0
200
400
600
800
1000

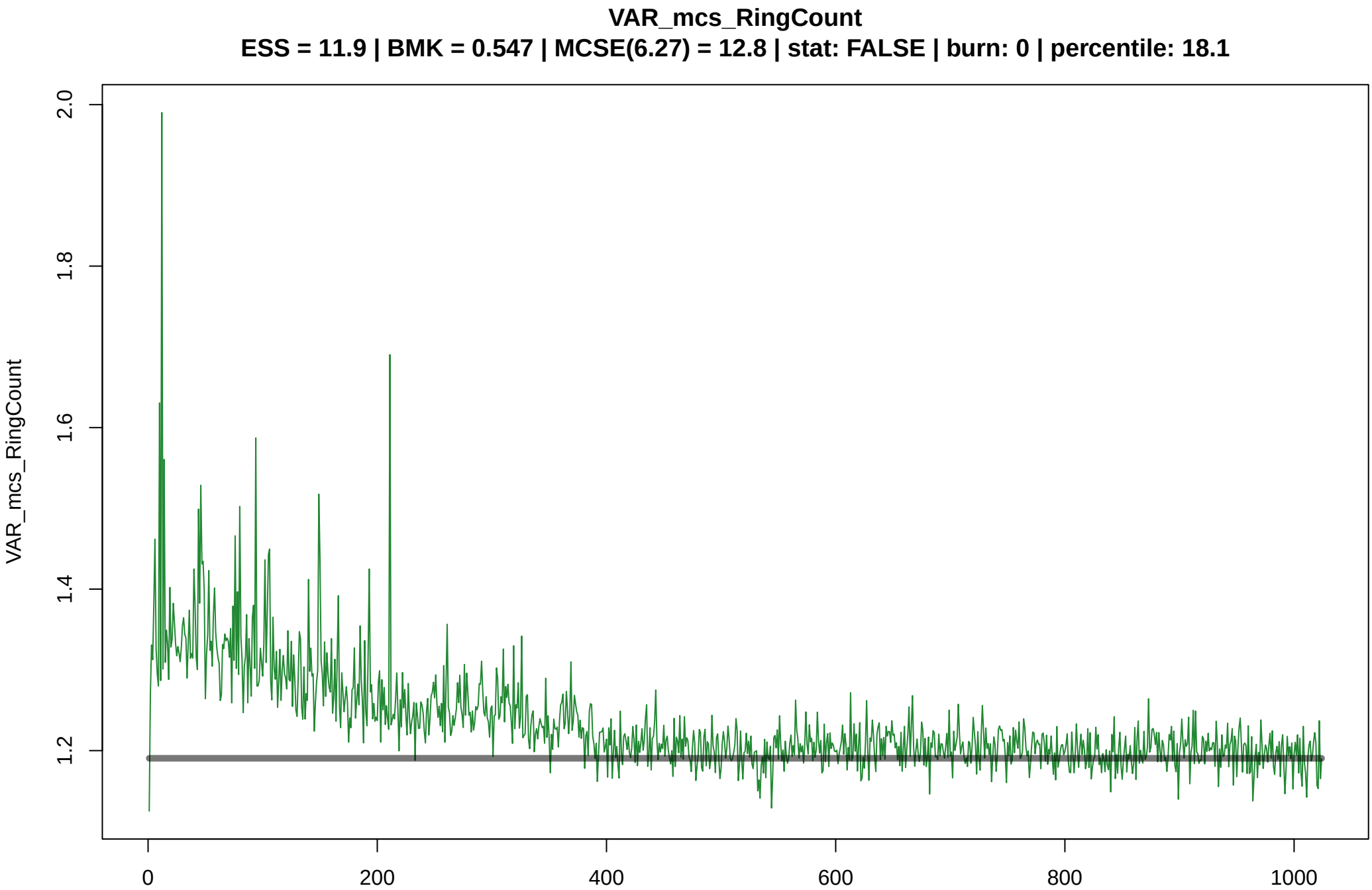

VAR_log_RMSD
ESS = 1020 | BMK = 1 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 1020 | percentile: 25.1
VAR_log_RMSD
1
2
3
4
5
6
7
8
0
200
400
600
800
1000

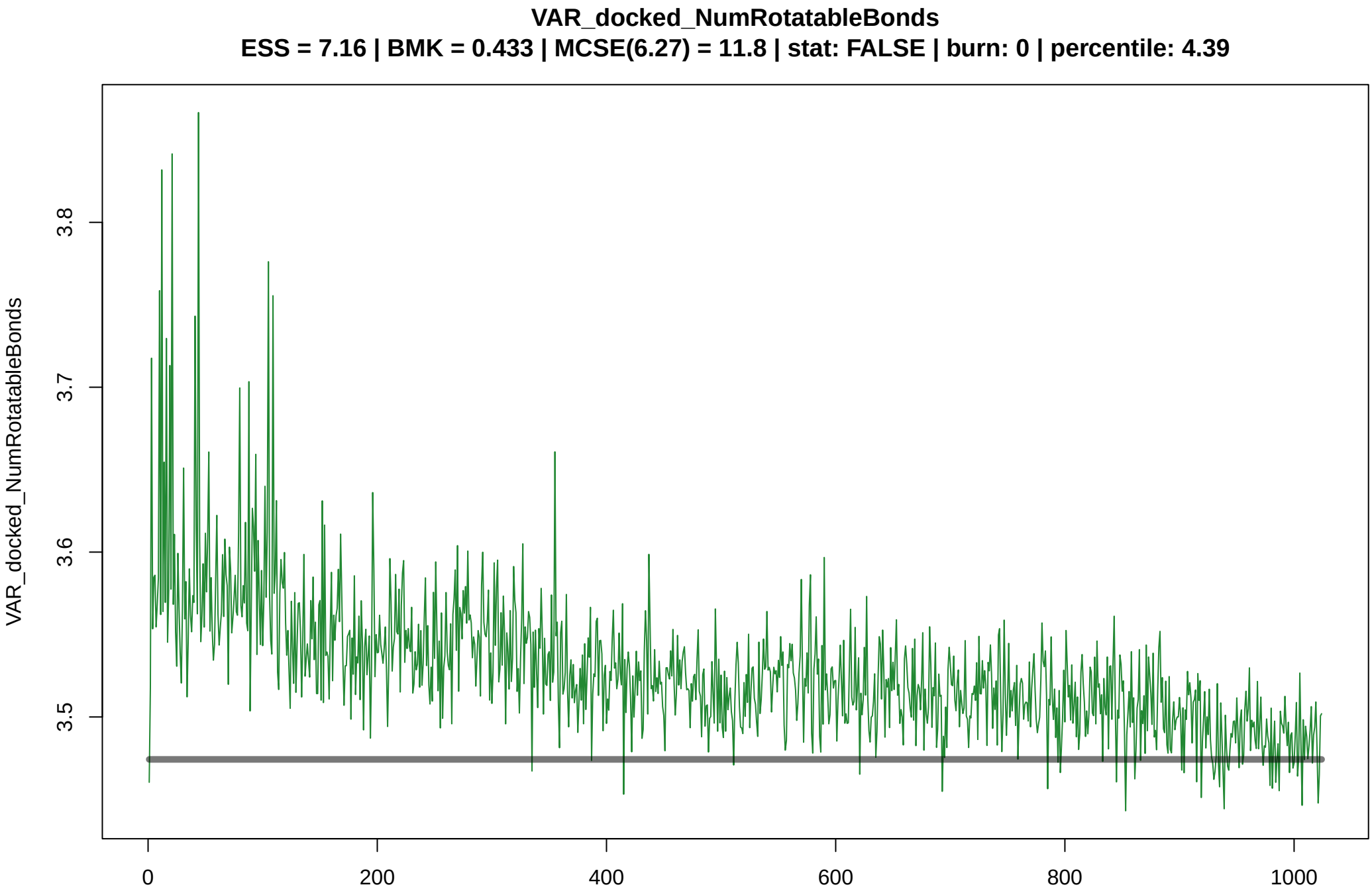

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.755 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 816 | percentile: 64.6
VAR_log_mcs_unbonded_polar_sasa
2
3
4
5
6
7
0
200
400
600
800
1000

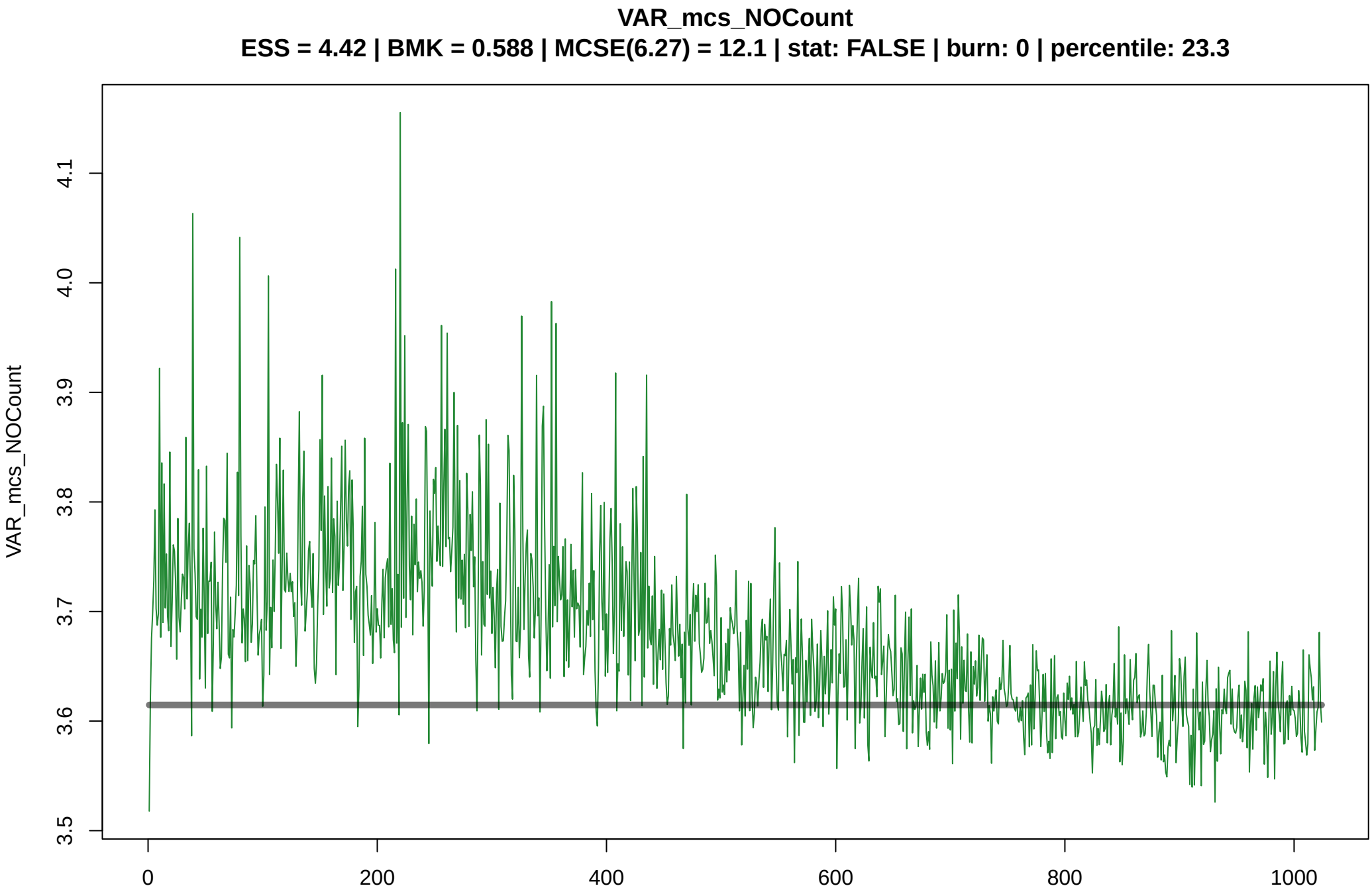

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.901 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 612 | percentile: 39.3
VAR_logit_ec_tanimoto_similarity
3
4
5
6
7
8
0
200
400
600
800
1000

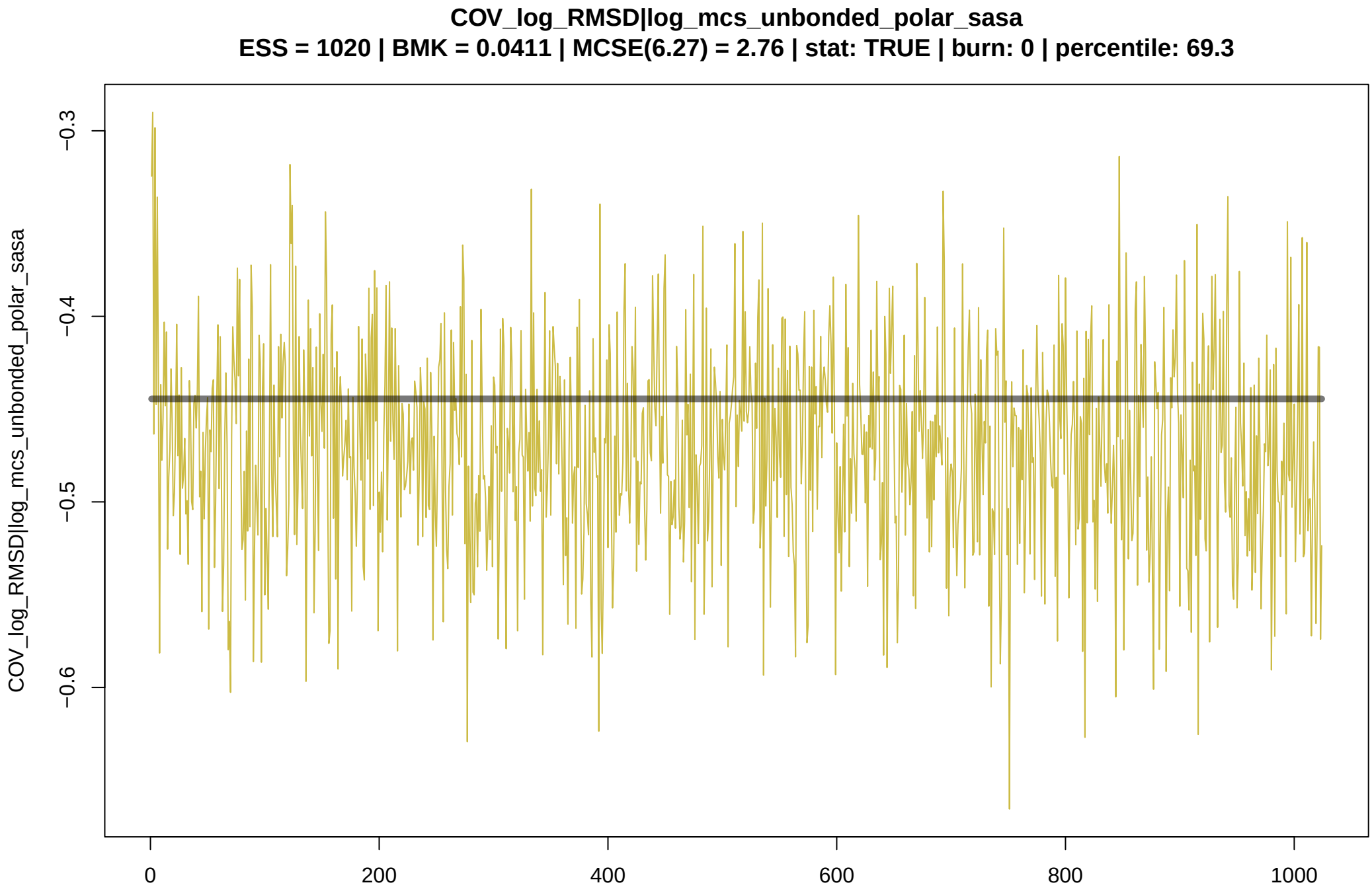

VAR_mcs_NumHeteroAtoms
ESS = 357 | BMK = 0.119 | MCSE(6.27) = 5.33 | stat: TRUE | burn: 0 | percentile: 4.1
VAR_mcs_NumHeteroAtoms
1.4
1.5
1.6
1.7
0
200
400
600
800
1000

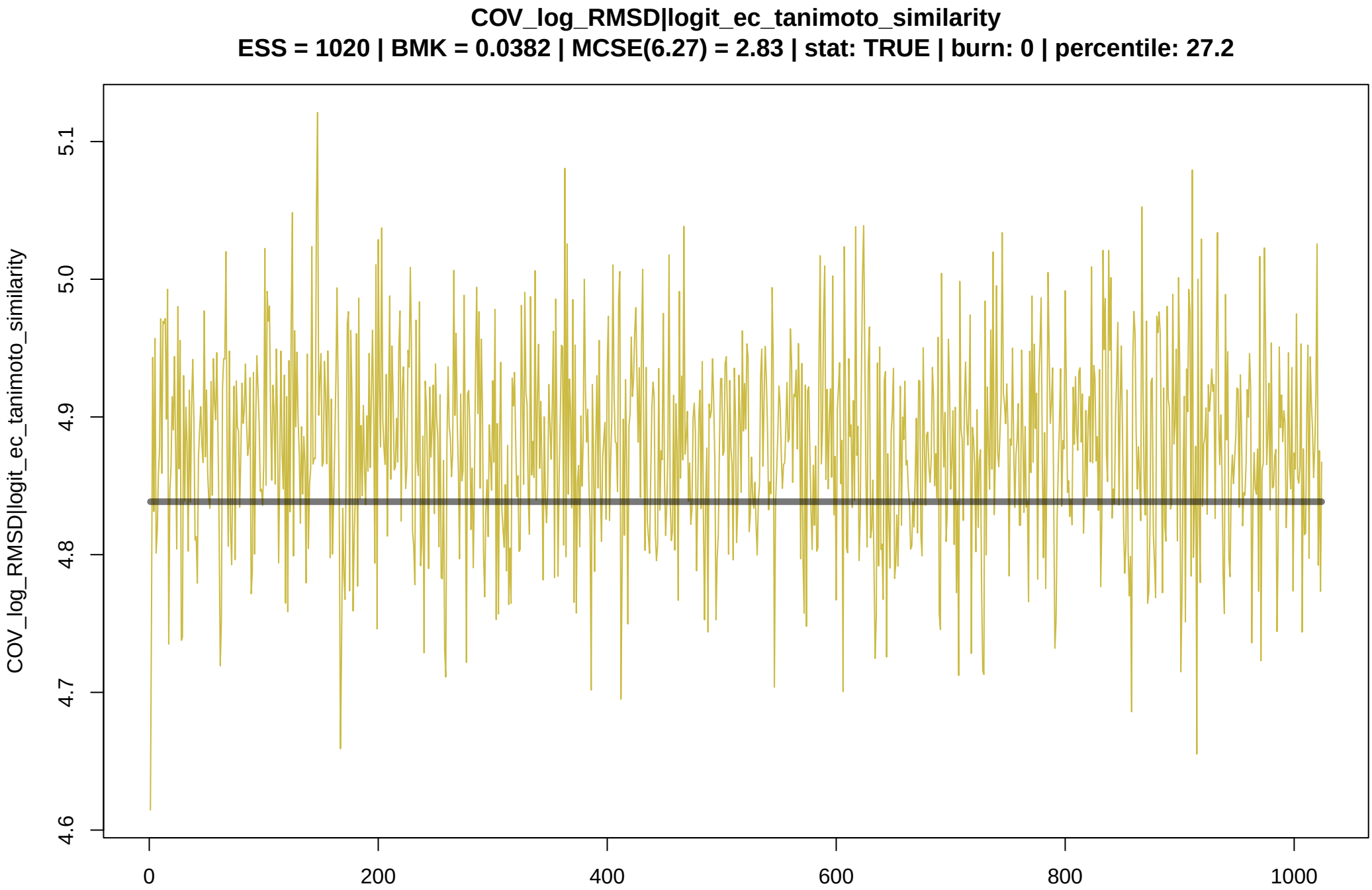

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.039 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0 | percentile: 99.2
VAR_docked_HeavyAtomCount
5.65
5.66
5.67
5.68
5.69
5.70
5.71
0
200
400
600
800
1000

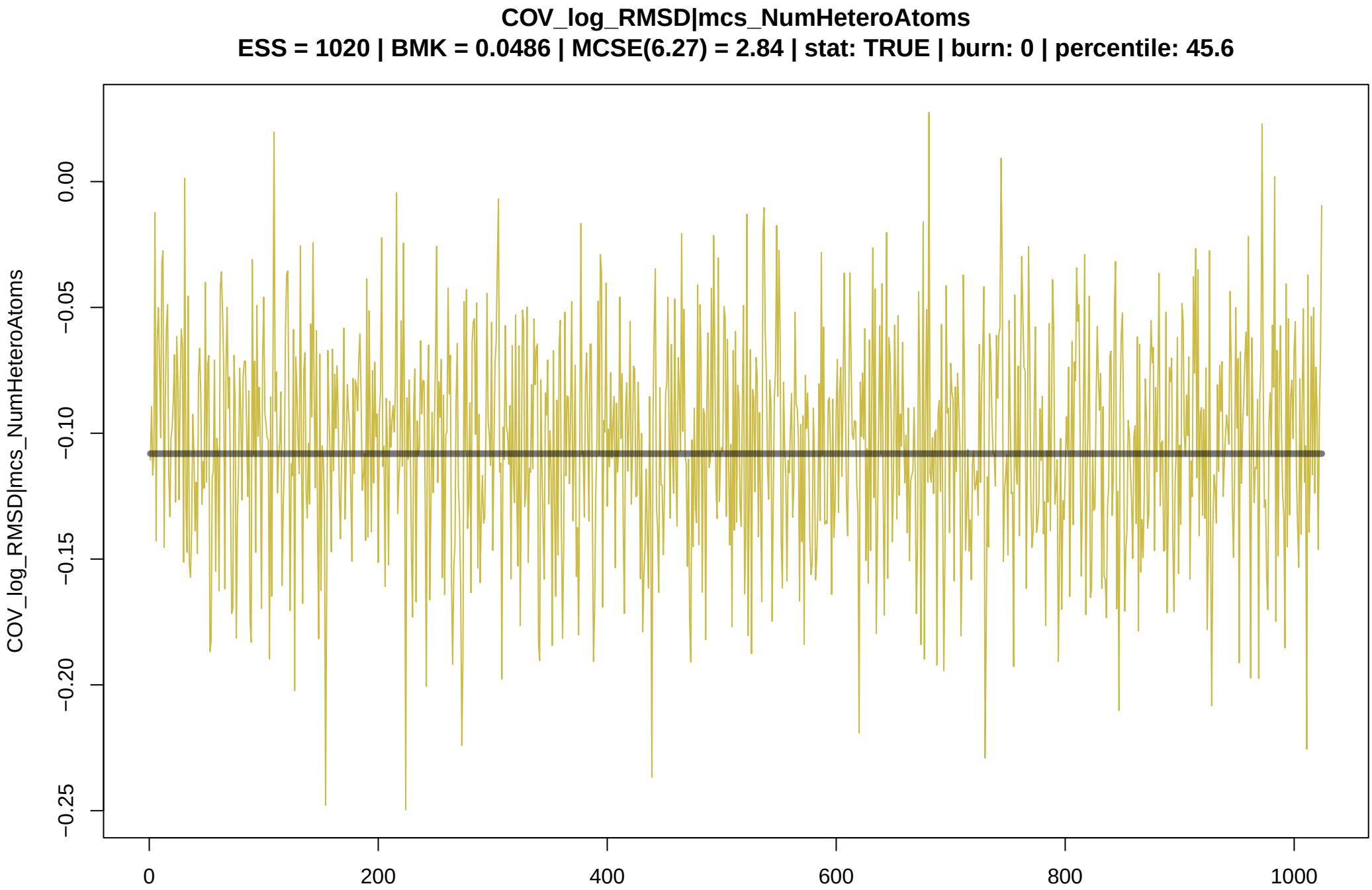

VAR_mcs_RingCount
ESS = 11.9 | BMK = 0.547 | MCSE(6.27) = 12.8 | stat: FALSE | burn: 0 | percentile: 18.1
VAR_mcs_RingCount
2.0
1.8
1.6
1.4
1.2
0
200
400
600
800
1000

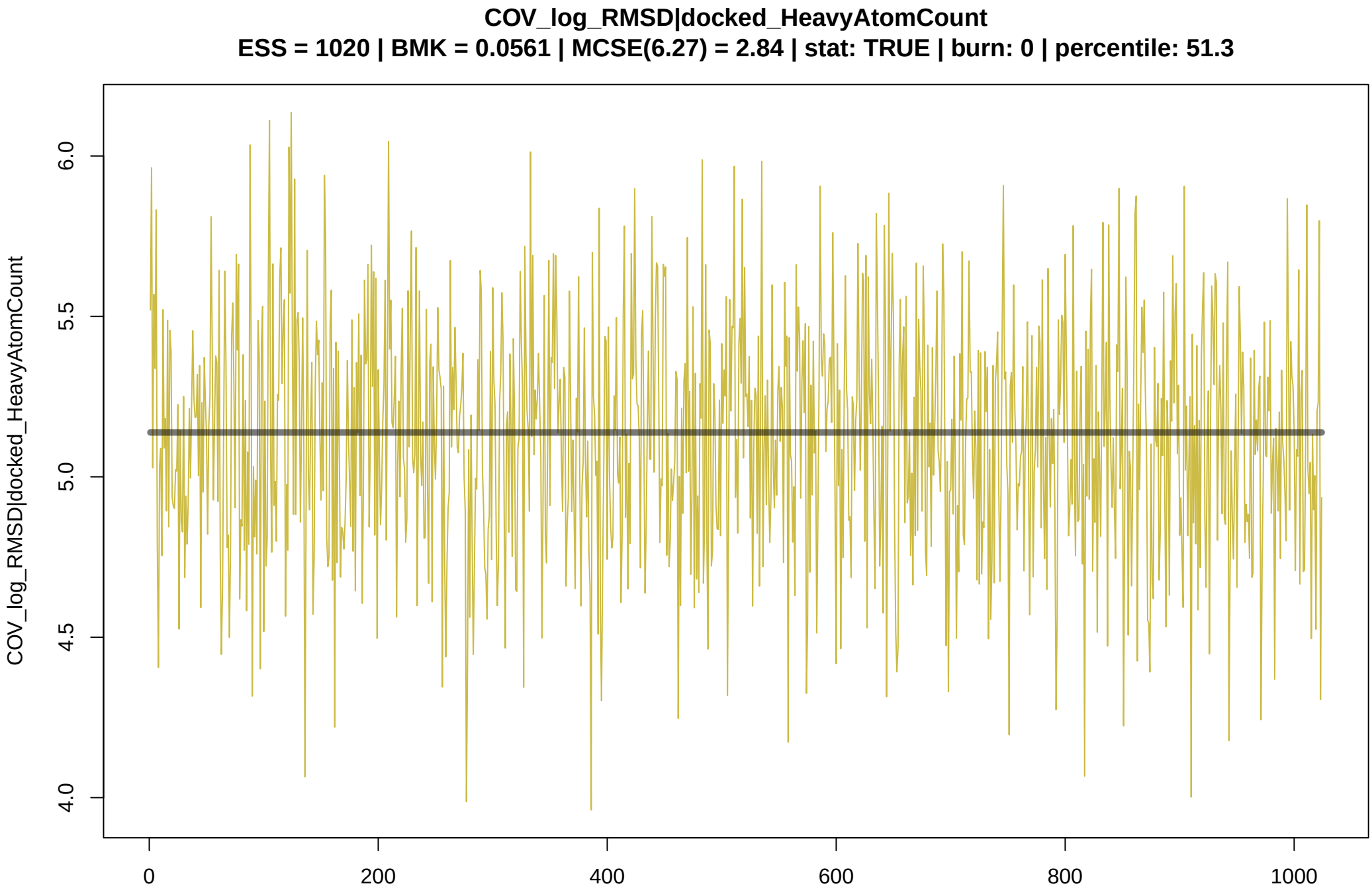

VAR_docked_NumRotatableBonds
ESS = 7.16 | BMK = 0.433 | MCSE(6.27) = 11.8 | stat: FALSE | burn: 0 | percentile: 4.39
VAR_docked_NumRotatableBonds
3.5
3.6
3.7
3.8
0
200
400
600
800
1000

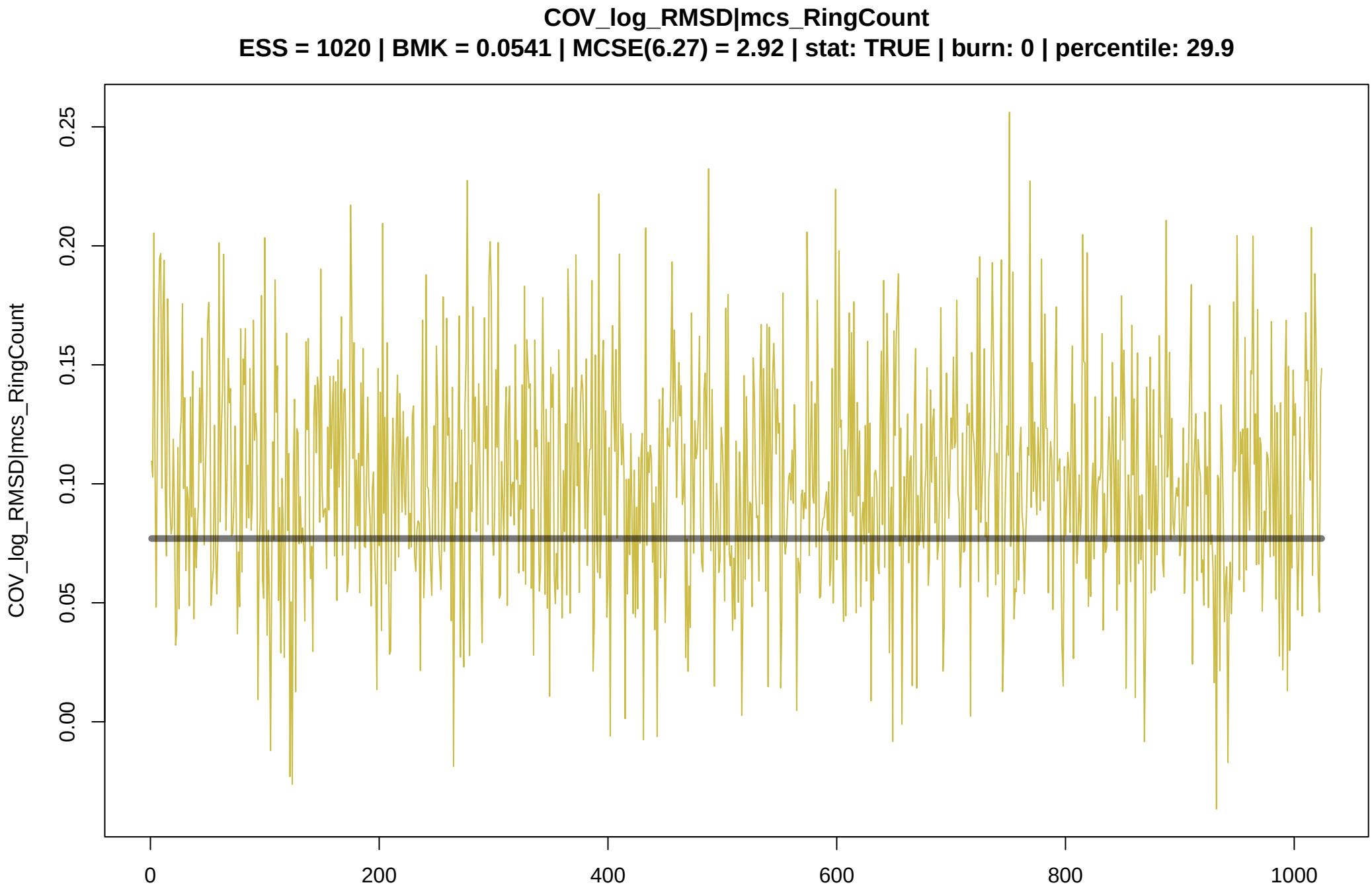

VAR_mcs_NOCount
ESS = 4.42 | BMK = 0.588 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 0 | percentile: 23.3
VAR_mcs_NOCount
3.5
3.6
3.7
3.8
3.9
4.0
4.1
0
200
400
600
800
1000

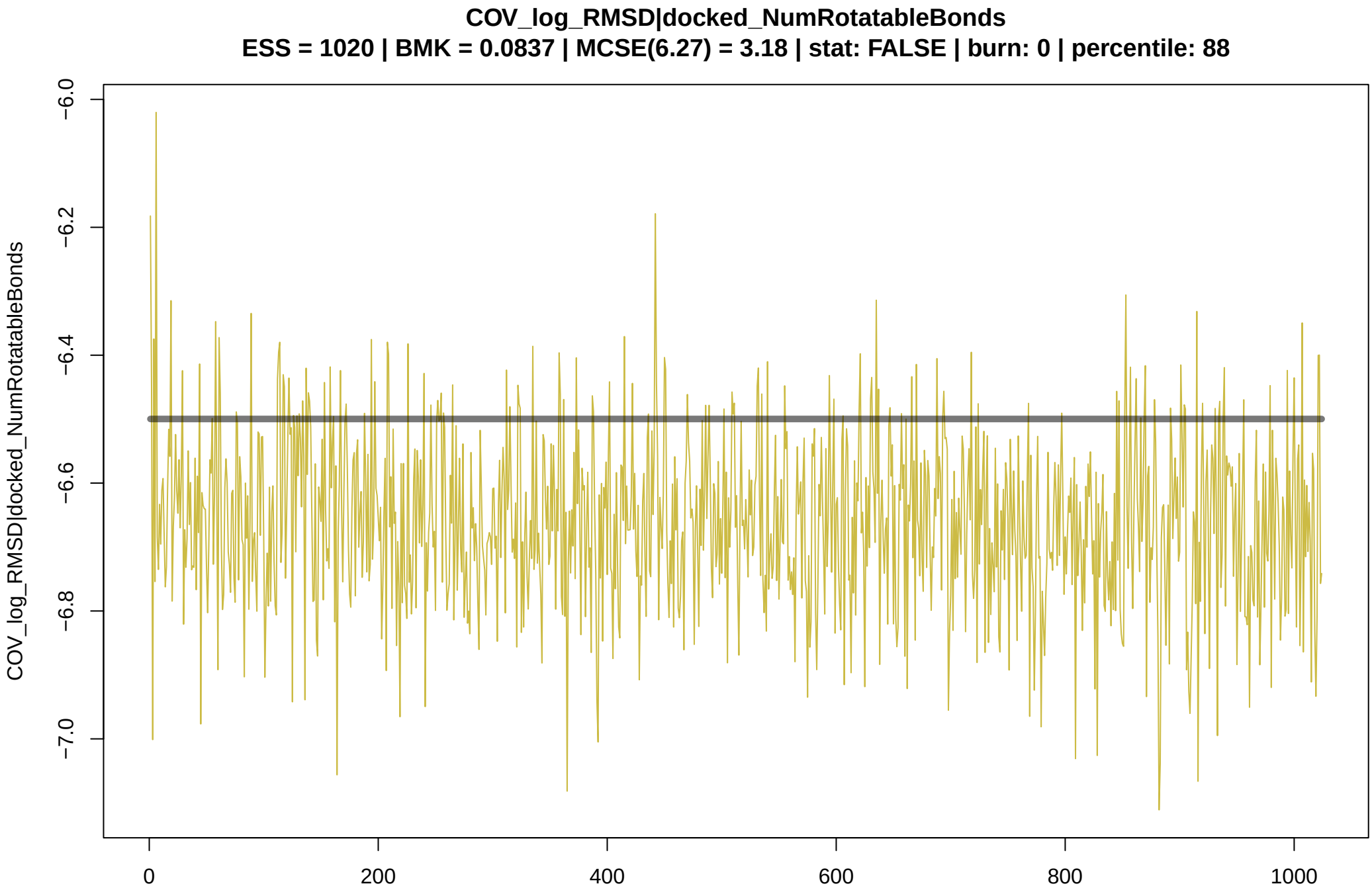

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0411 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | percentile: 69.3
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.3
−0.4
−0.5
−0.6
0
200
400
600
800
1000

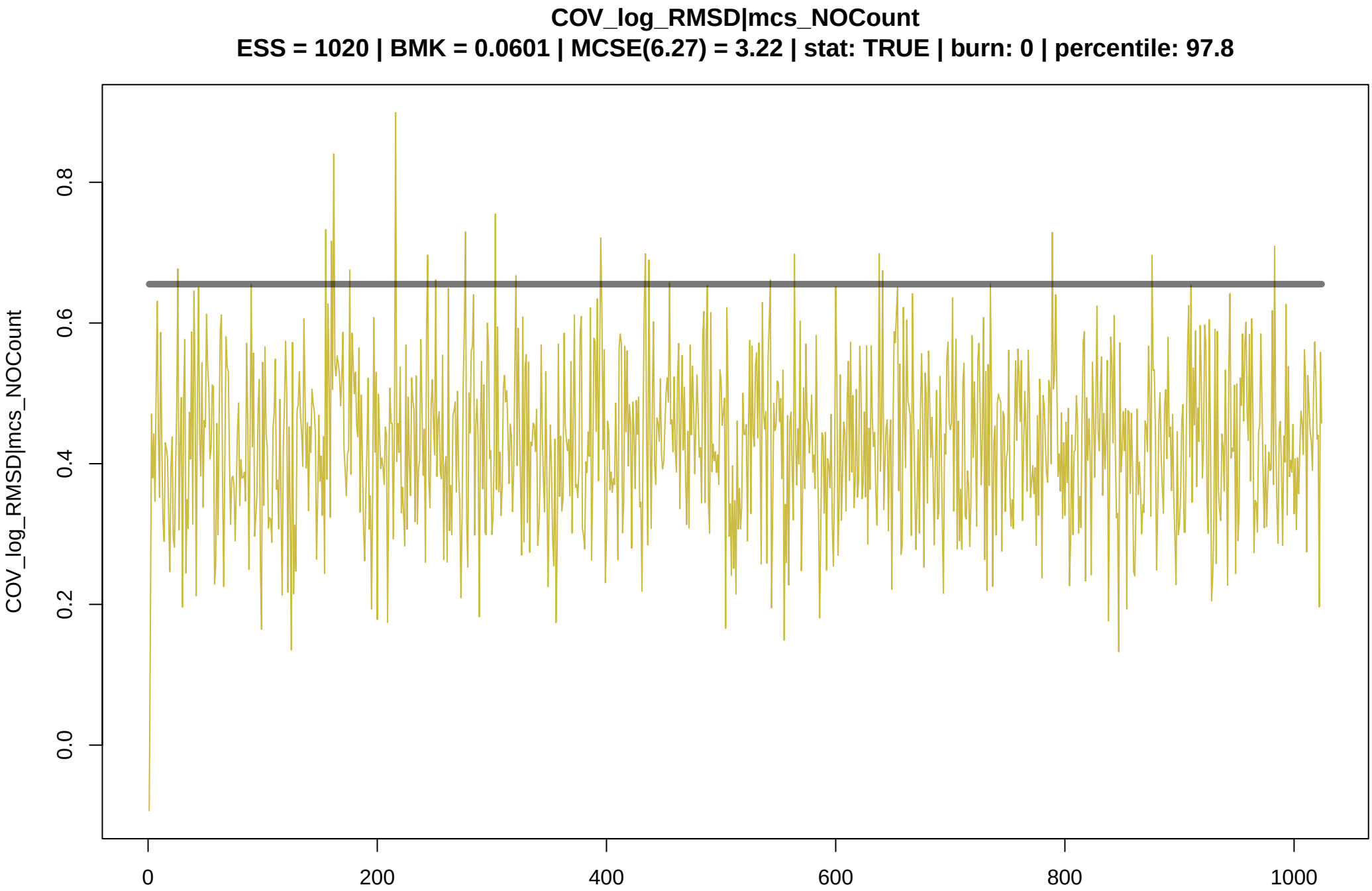

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0382 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | percentile: 27.2
COV_log_RMSD|logit_ec_tanimoto_similarity
4.6
4.7
4.8
4.9
5.0
5.1
0
200
400
600
800
1000

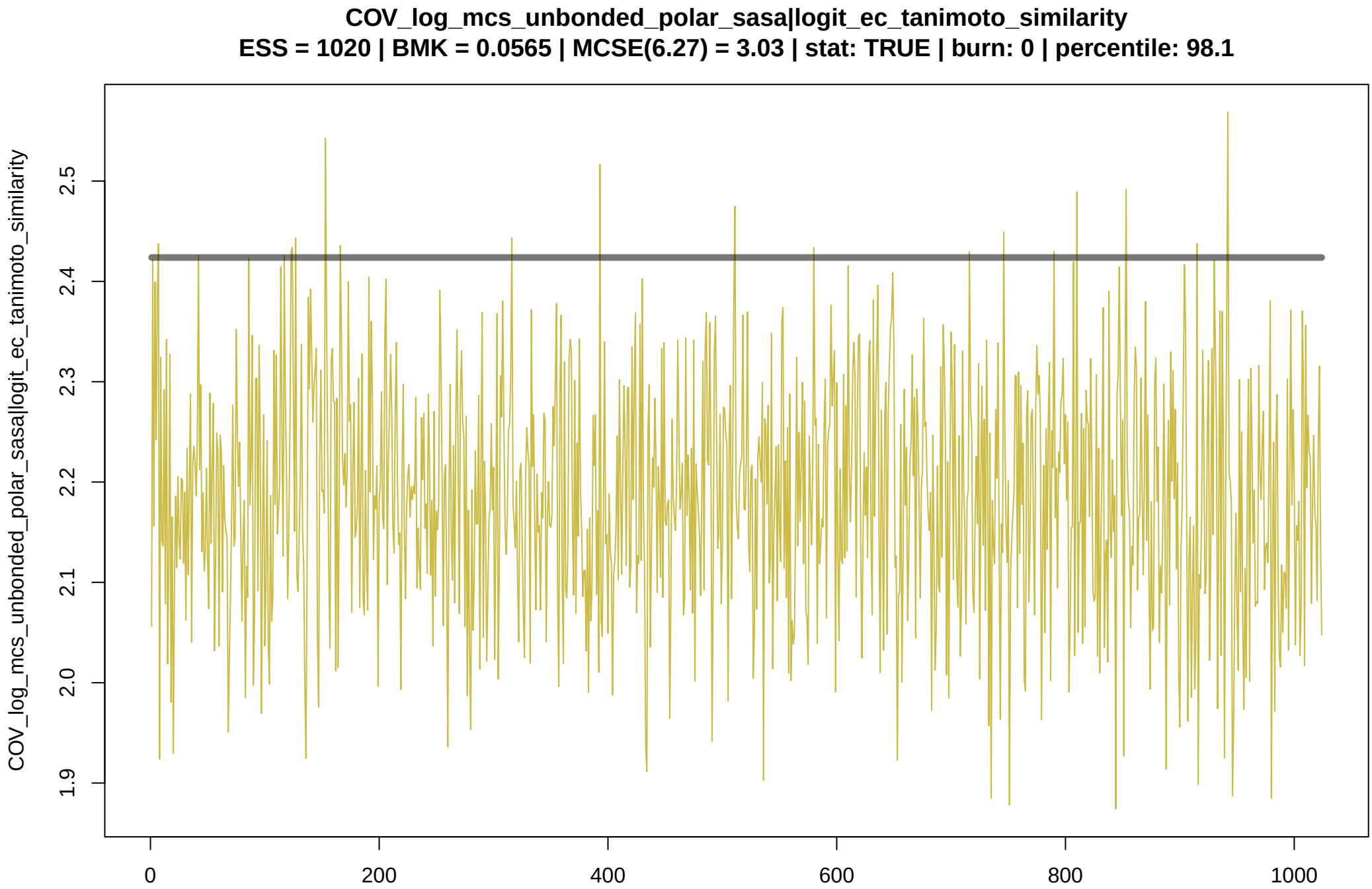

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0486 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0 | percentile: 45.6
COV_log_RMSD|mcs_NumHeteroAtoms
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
200
400
600
800
1000

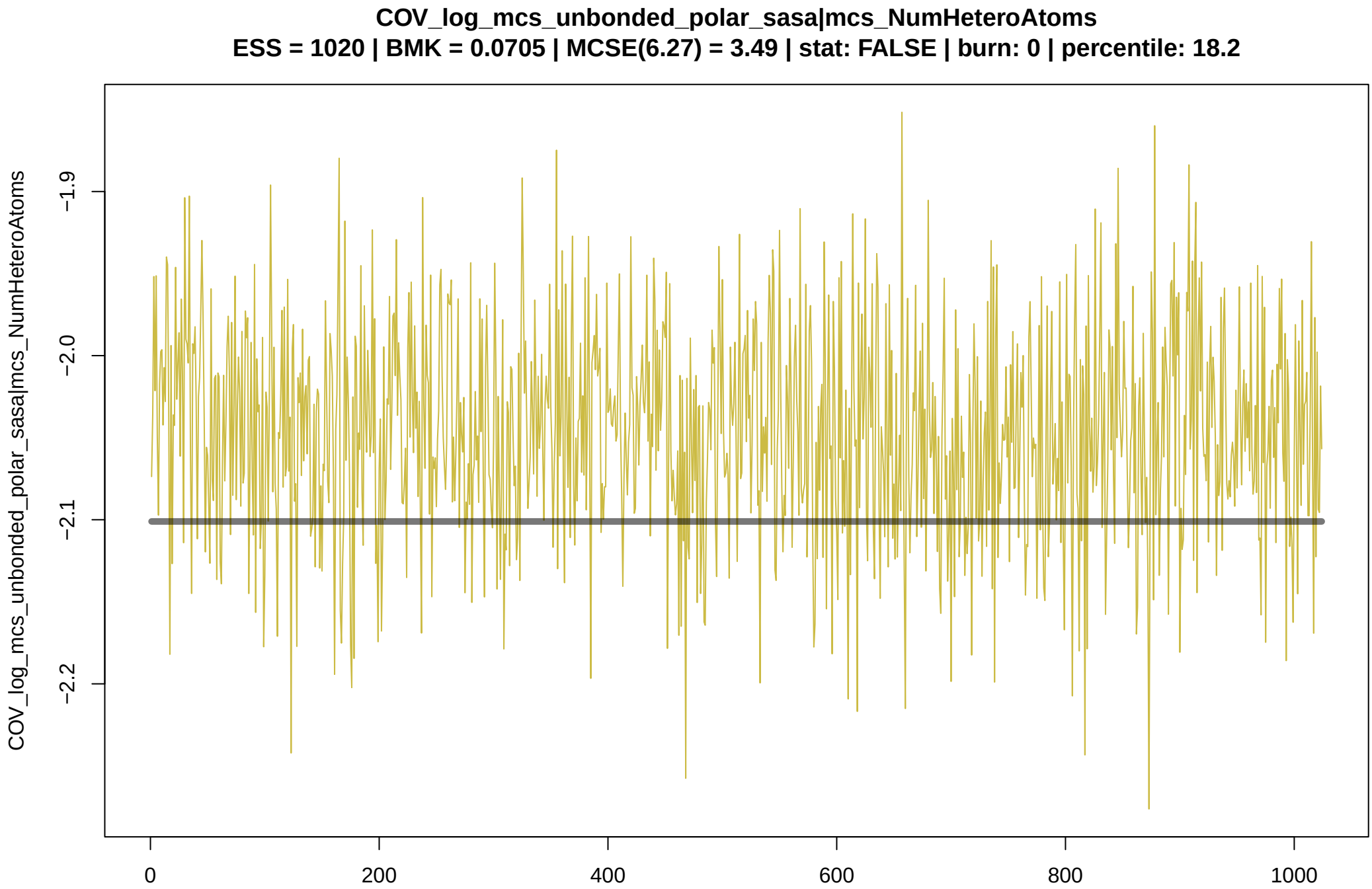

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0561 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0 | percentile: 51.3
COV_log_RMSD|docked_HeavyAtomCount
4.0
4.5
5.0
5.5
6.0
0
200
400
600
800
1000

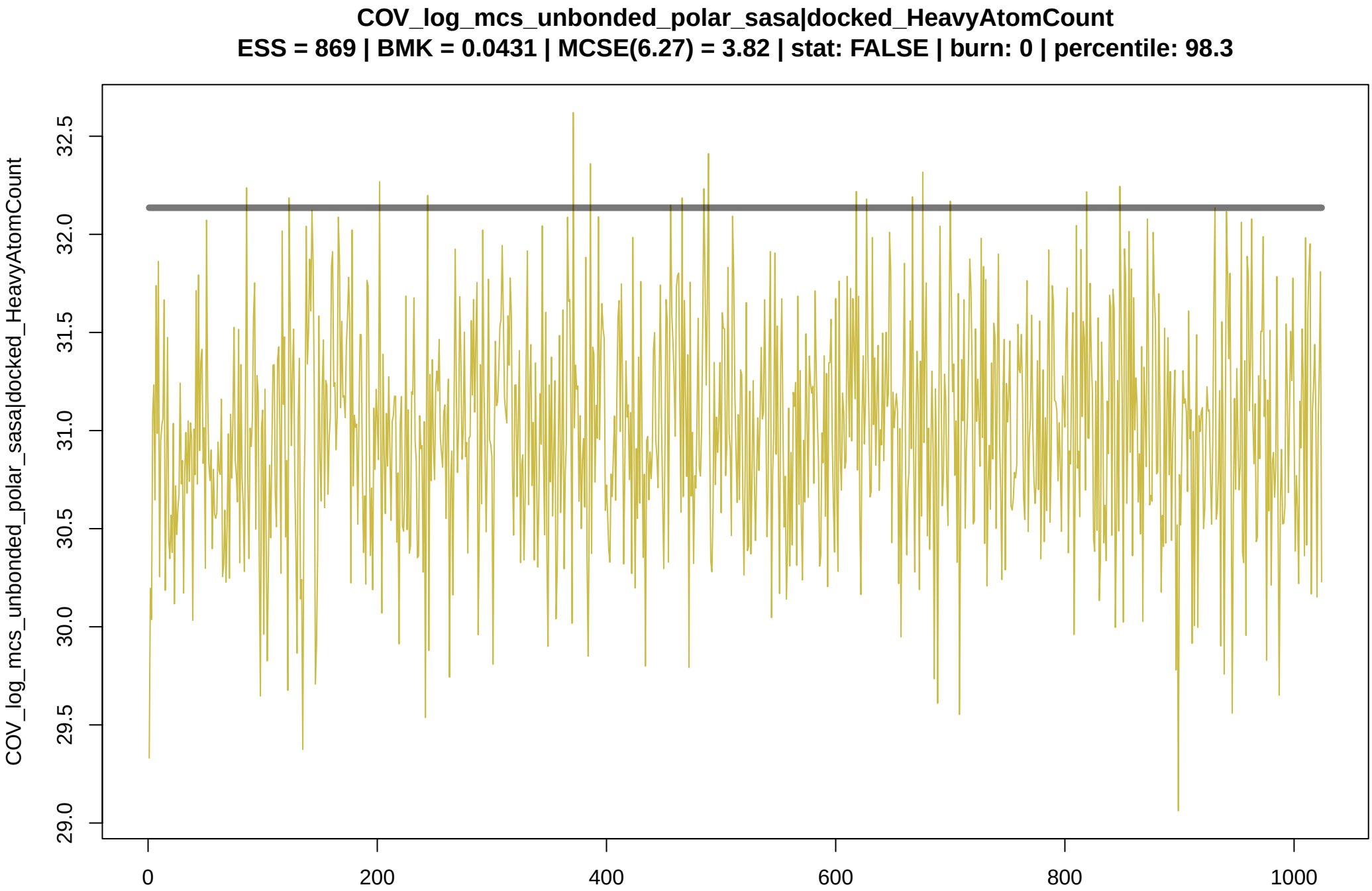

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0541 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0 | percentile: 29.9
COV_log_RMSD|mcs_RingCount
0.00
0.05
0.10
0.15
0.20
0.25
0
200
400
600
800
1000

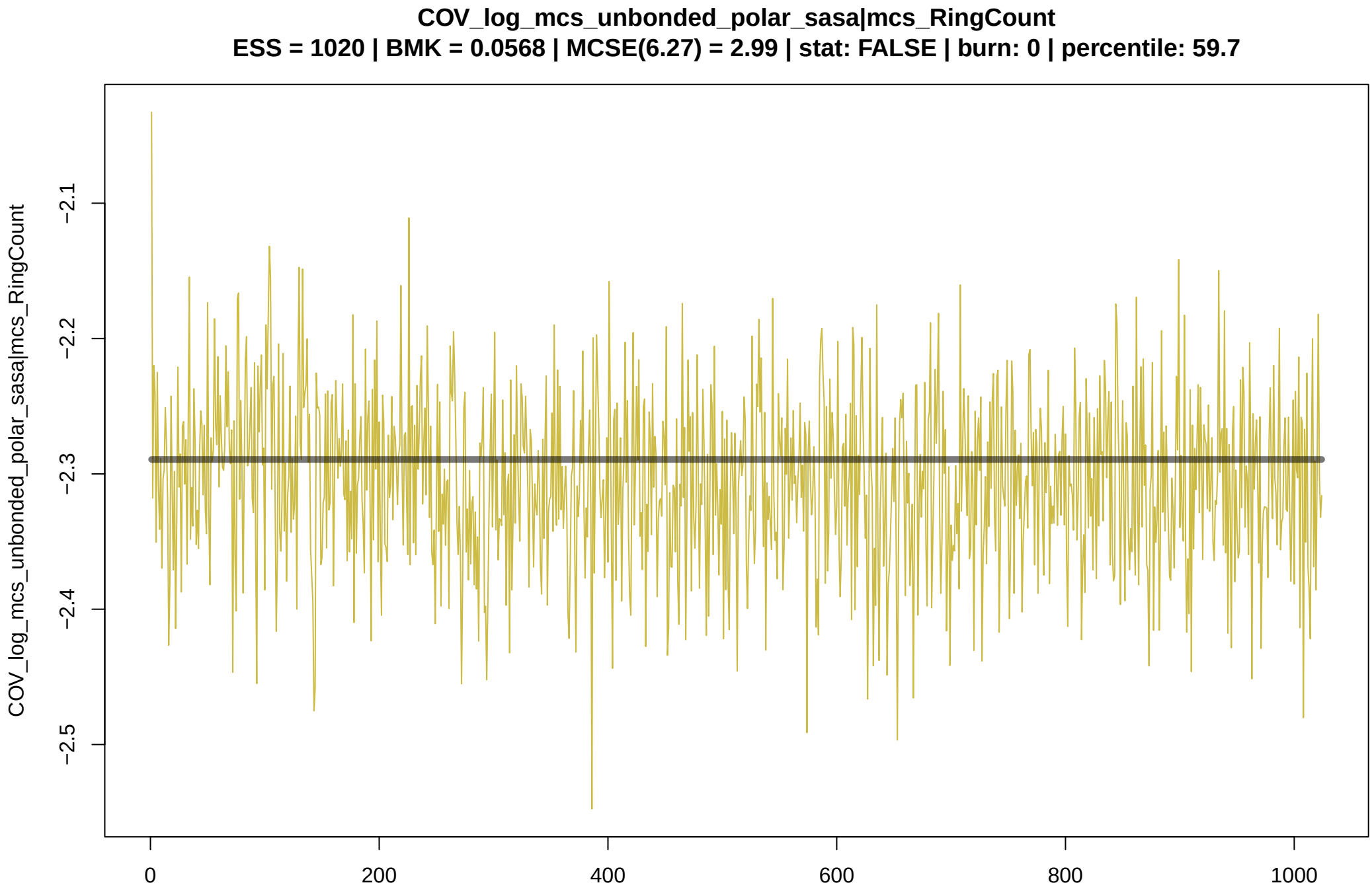

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0837 | MCSE(6.27) = 3.18 | stat: FALSE | burn: 0 | percentile: 88
COV_log_RMSD|docked_NumRotatableBonds
−6.0
−6.2
−6.4
−6.6
−6.8
−7.0
0
200
400
600
800
1000

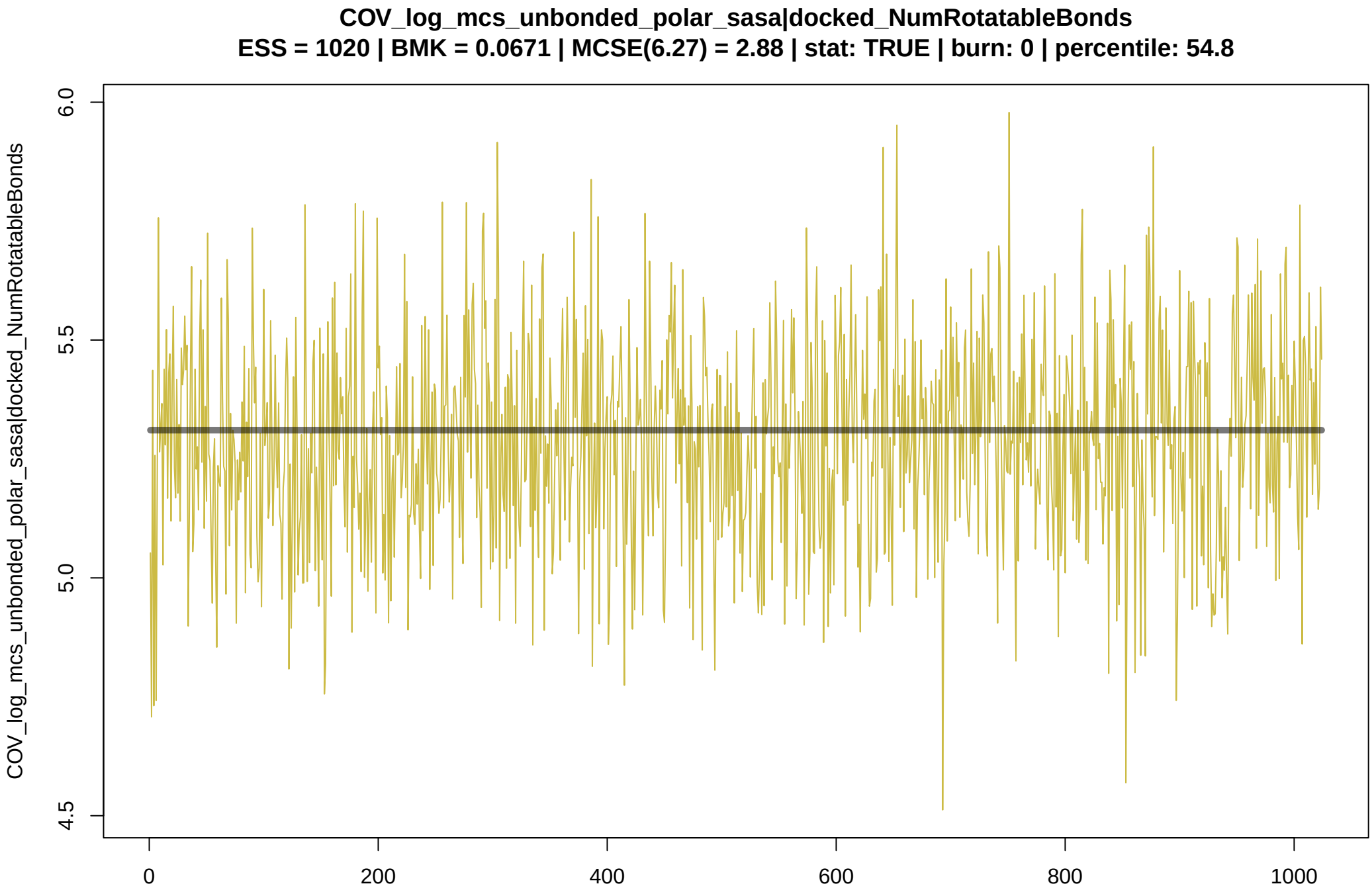

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0601 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0 | percentile: 97.8
COV_log_RMSD|mcs_NOCount
0.0
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

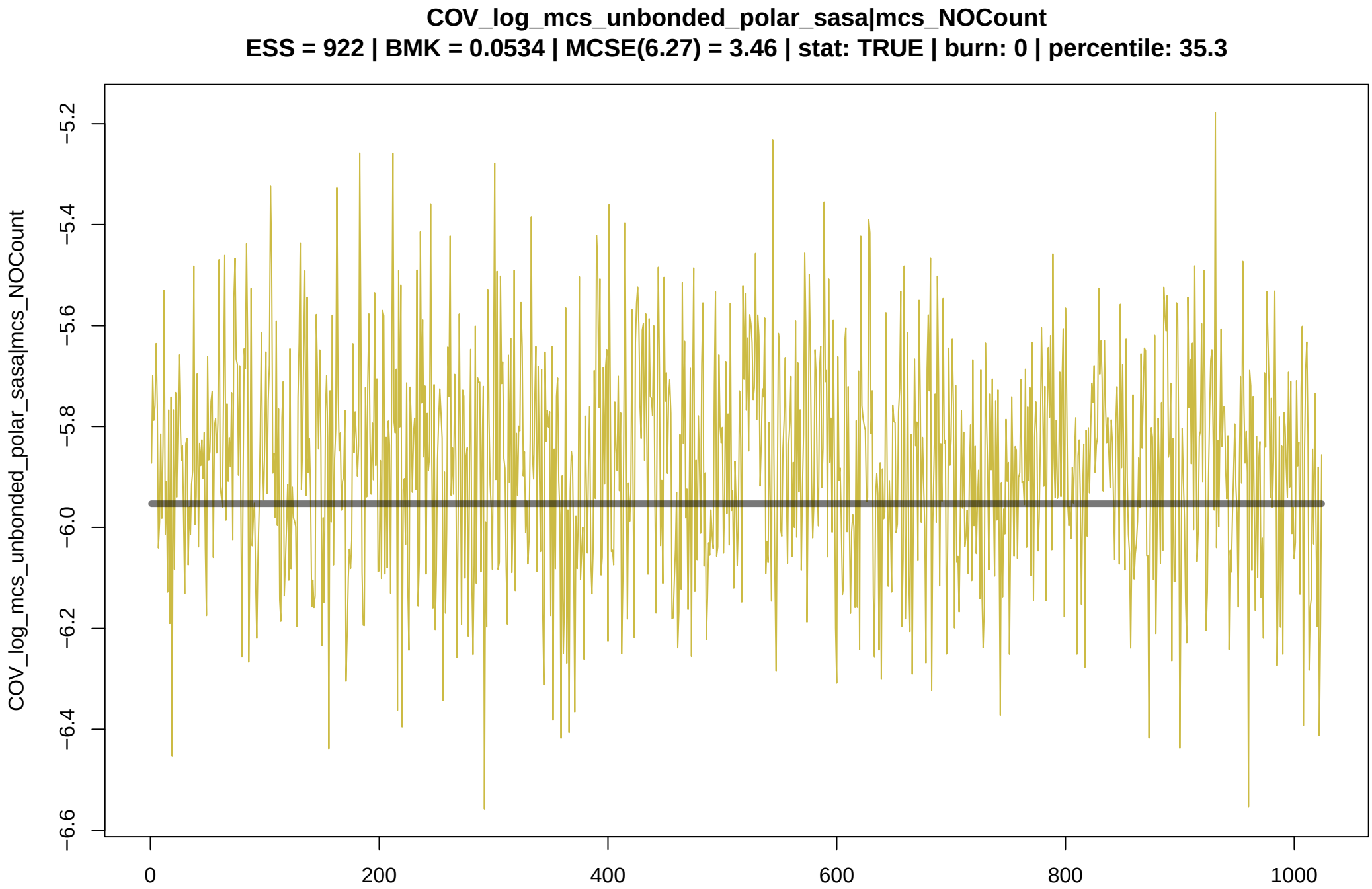

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0565 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | percentile: 98.1
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
1.9
2.0
2.1
2.2
2.3
2.4
2.5
0
200
400
600
800
1000

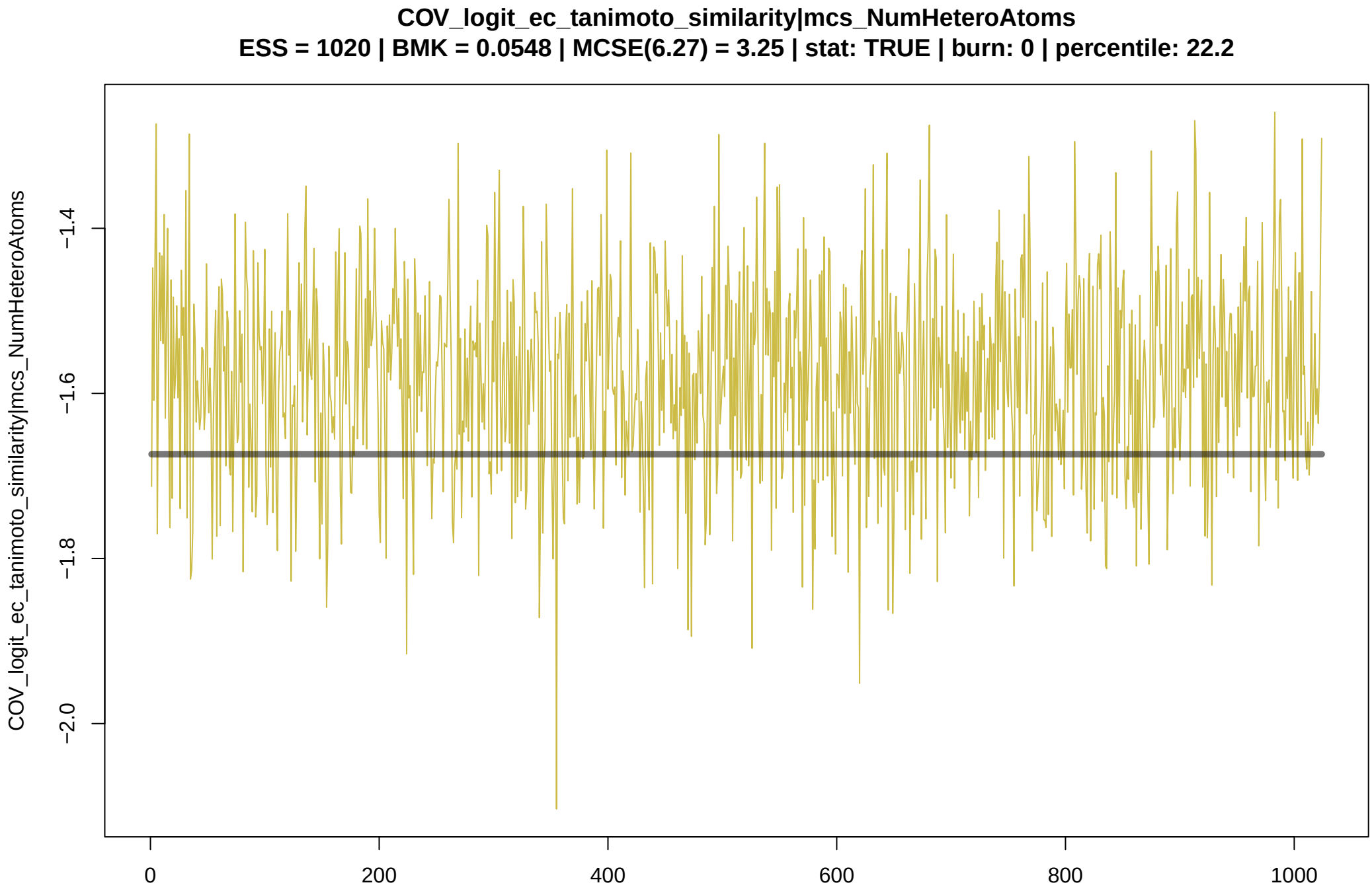

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0705 | MCSE(6.27) = 3.49 | stat: FALSE | burn: 0 | percentile: 18.2
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

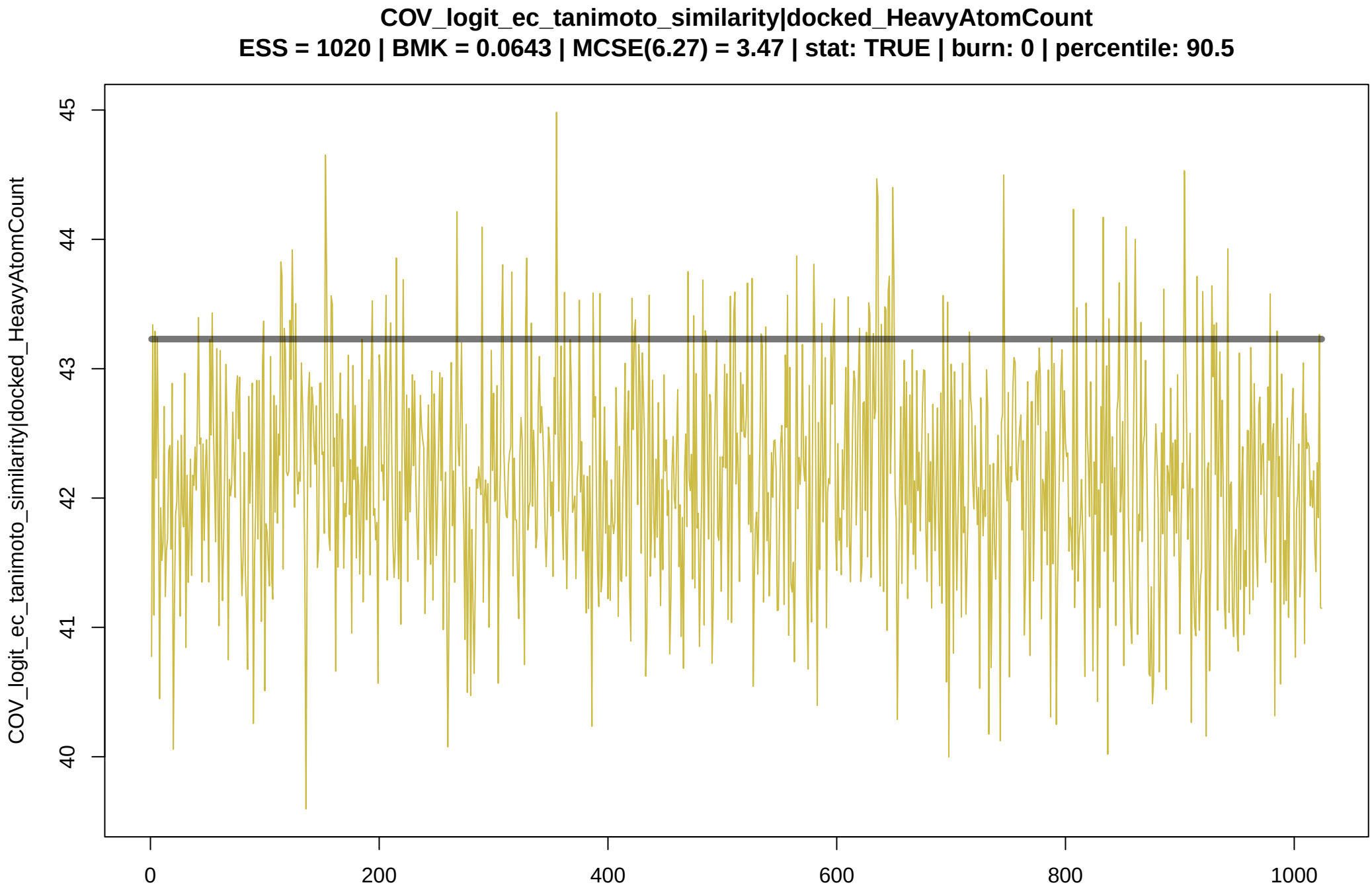

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 869 | BMK = 0.0431 | MCSE(6.27) = 3.82 | stat: FALSE | burn: 0 | percentile: 98.3
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
29.0
29.5
30.0
30.5
31.0
31.5
32.0
32.5
0
200
400
600
800
1000

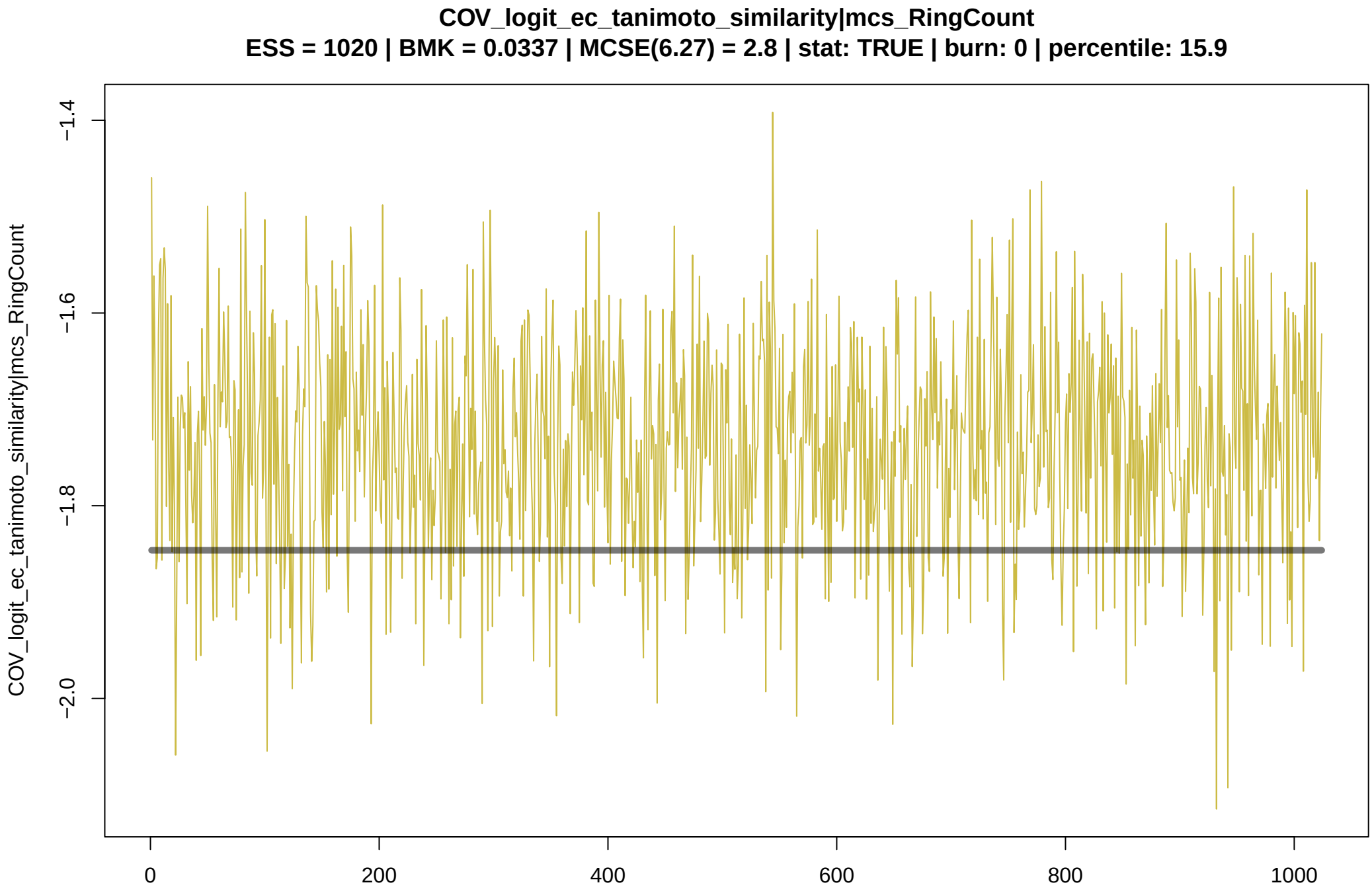

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0568 | MCSE(6.27) = 2.99 | stat: FALSE | burn: 0 | percentile: 59.7
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.1
−2.2
−2.3
−2.4
−2.5
0
200
400
600
800
1000

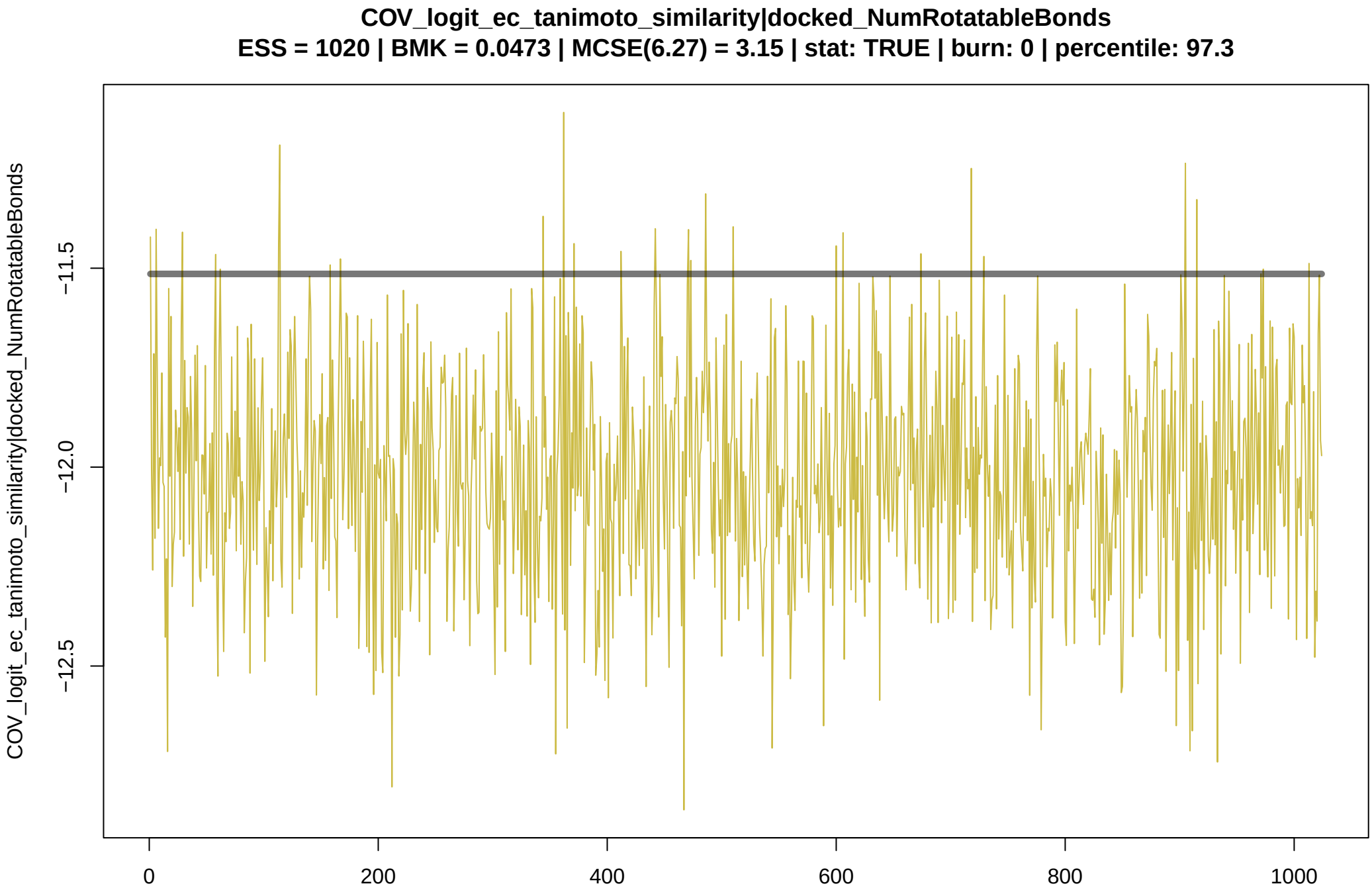

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0671 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | percentile: 54.8
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
6.0
5.5
5.0
4.5
0
200
400
600
800
1000

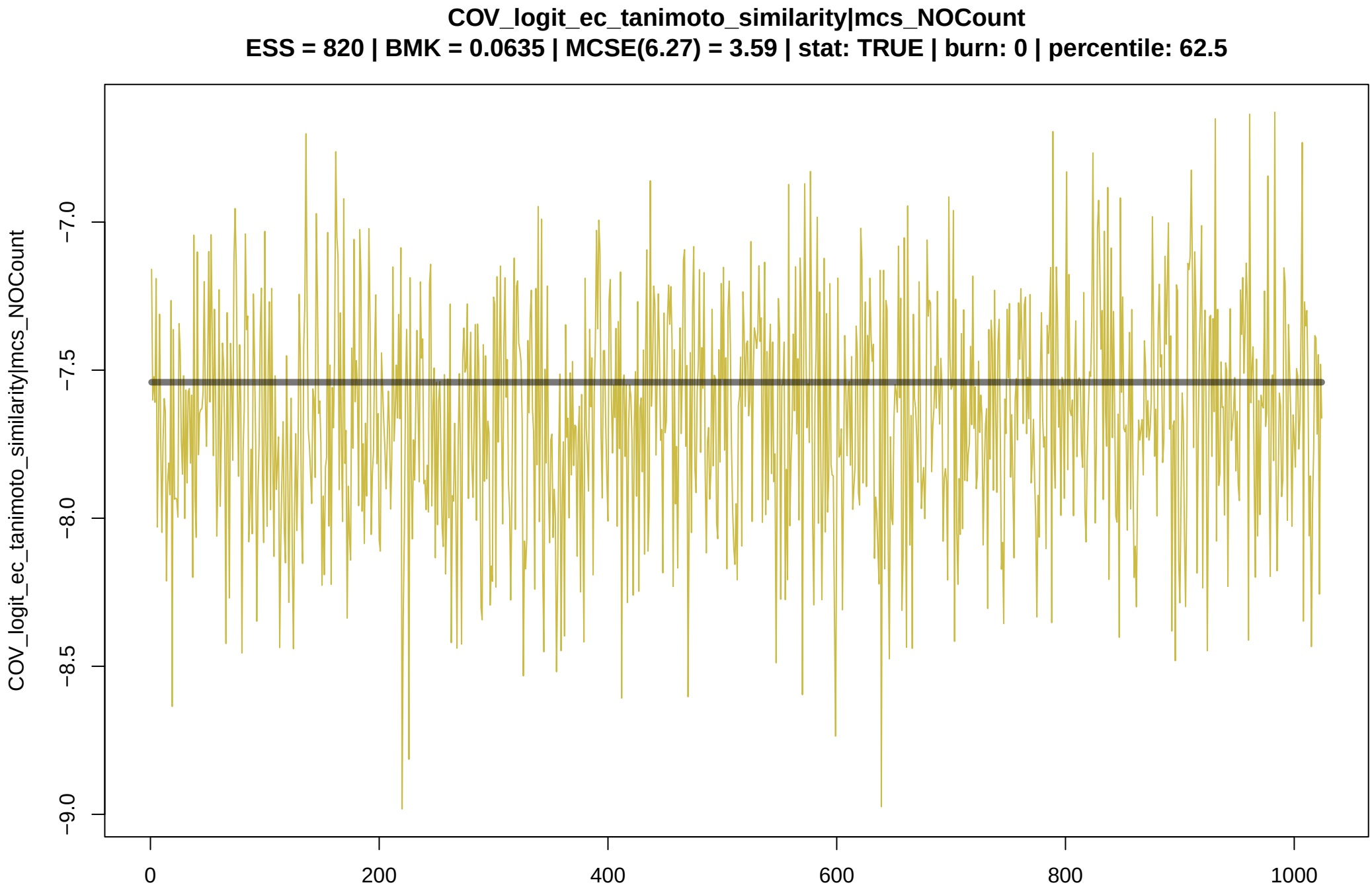

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 922 | BMK = 0.0534 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | percentile: 35.3
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.2
−5.4
−5.6
−5.8
−6.0
−6.2
−6.4
−6.6
0
200
400
600
800
1000

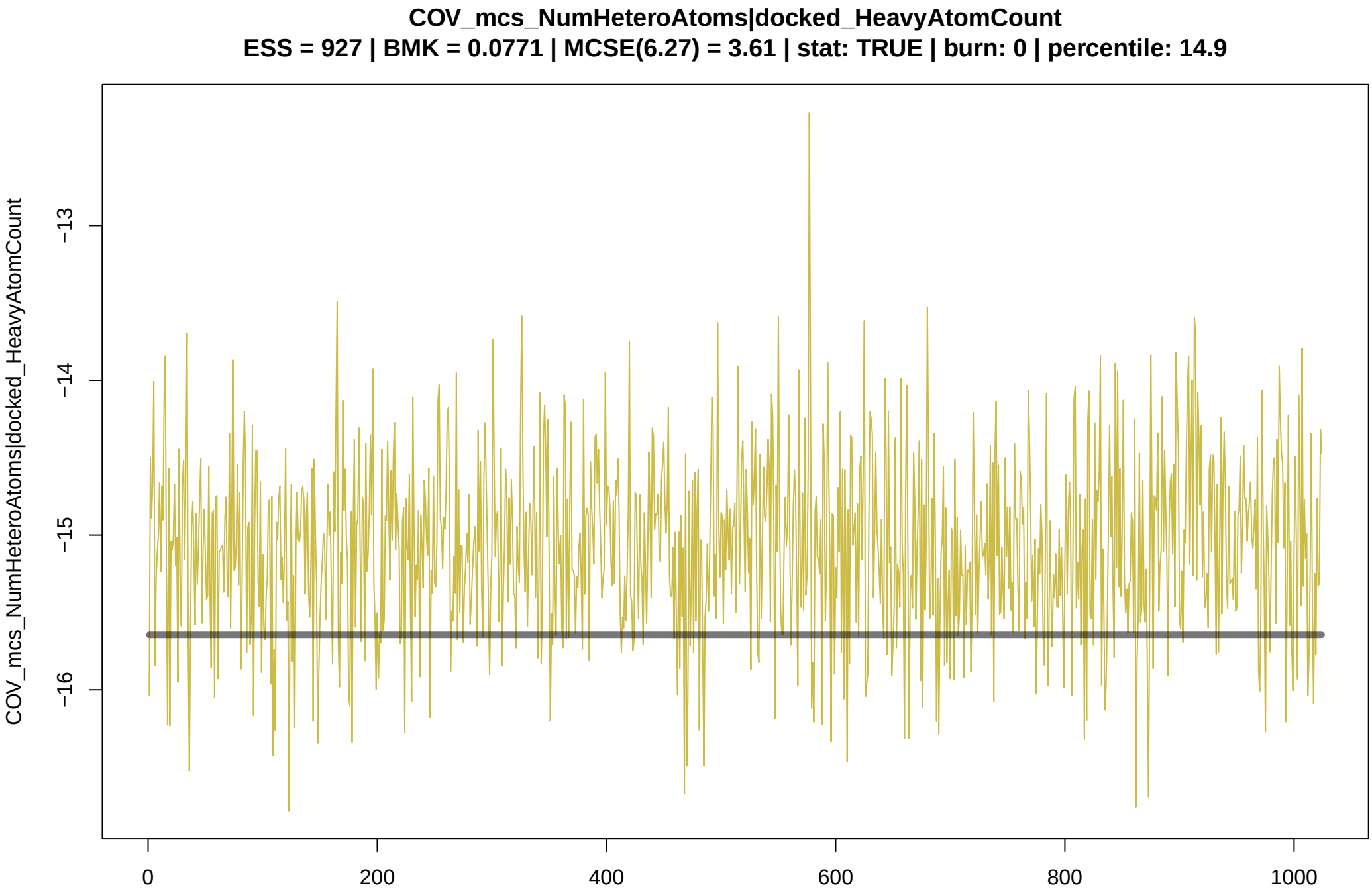

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0548 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0 | percentile: 22.2
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

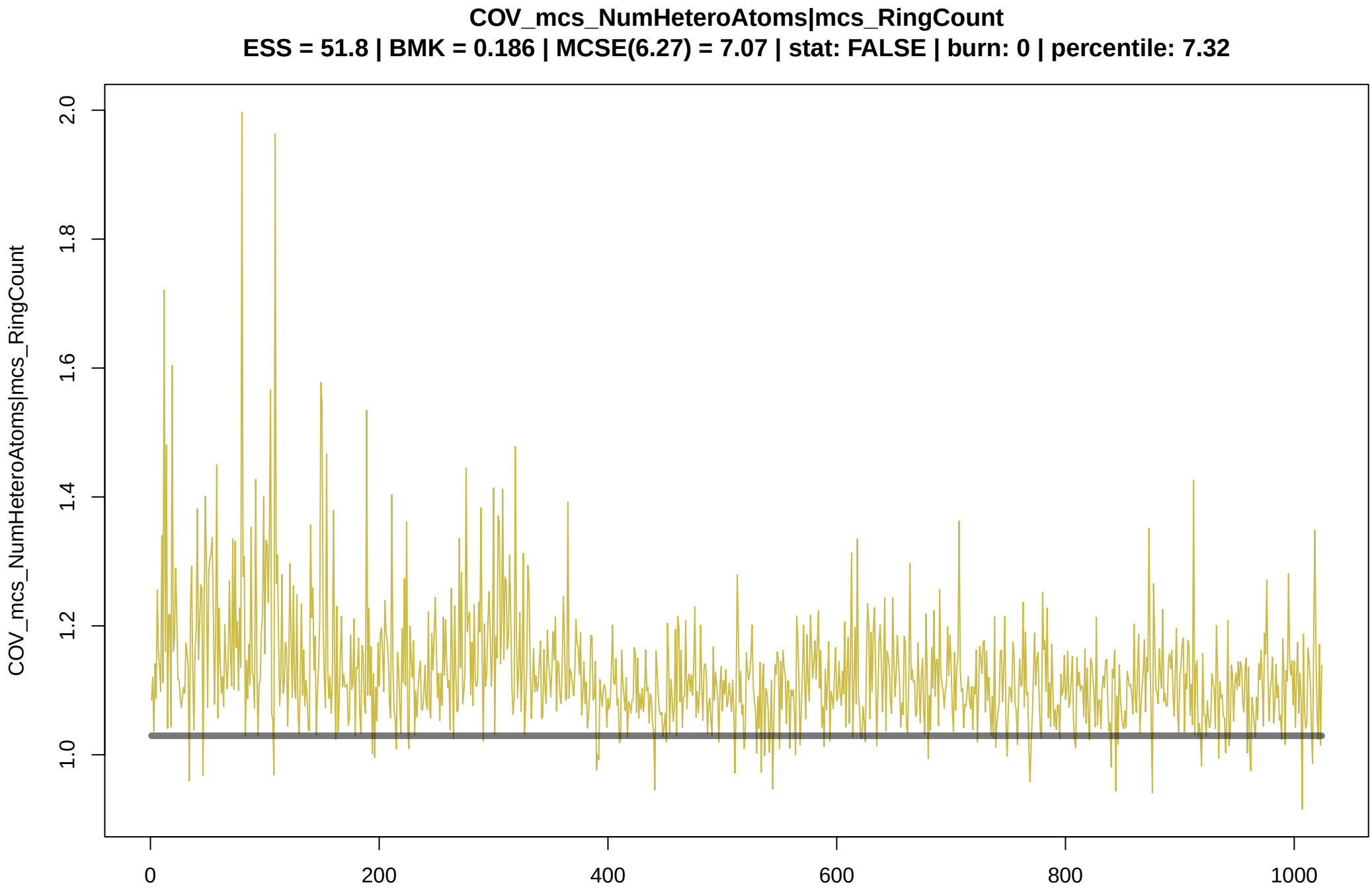

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0643 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | percentile: 90.5
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
45
44
43
42
41
40
0
200
400
600
800
1000

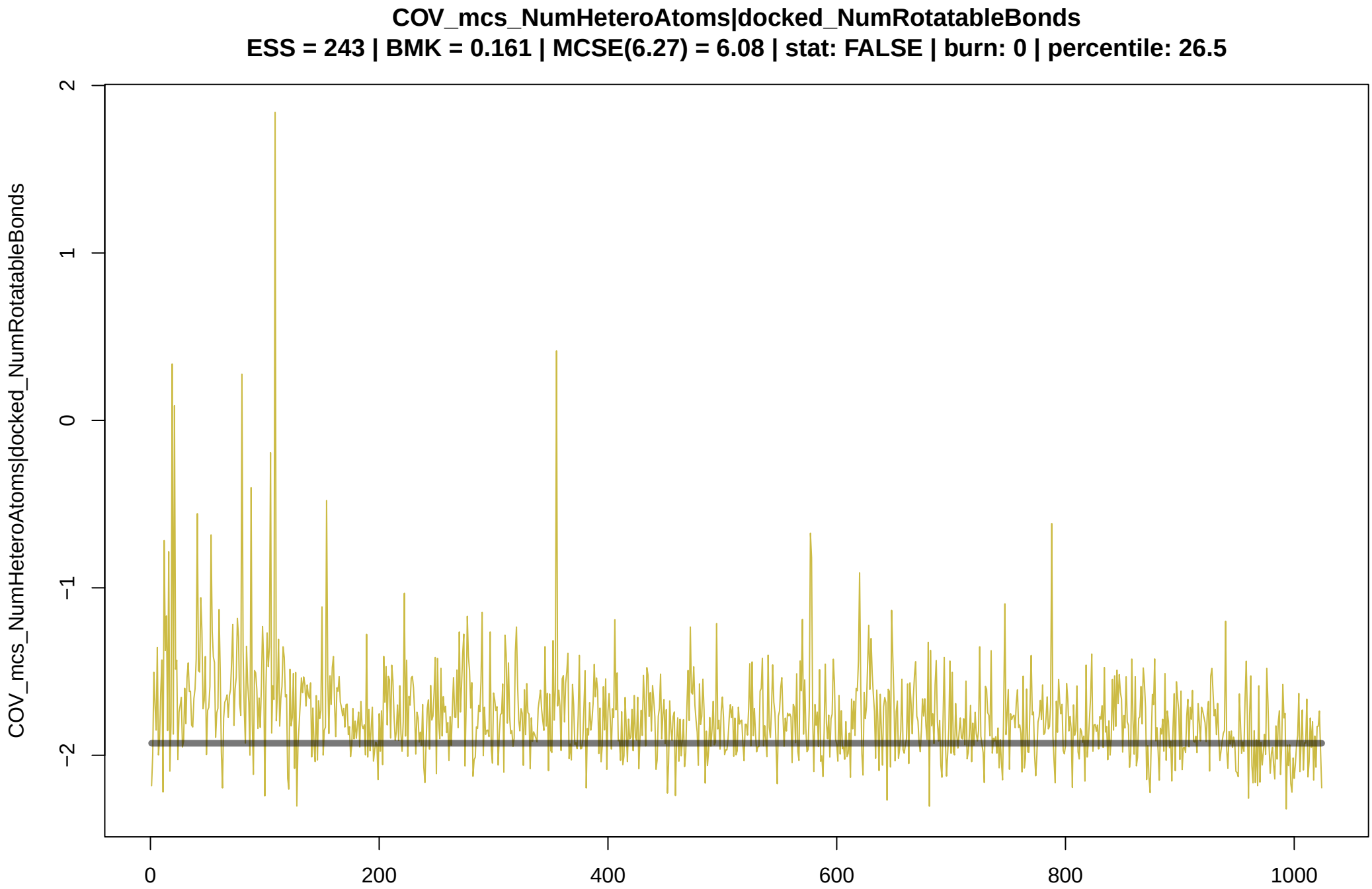

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0337 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0 | percentile: 15.9
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

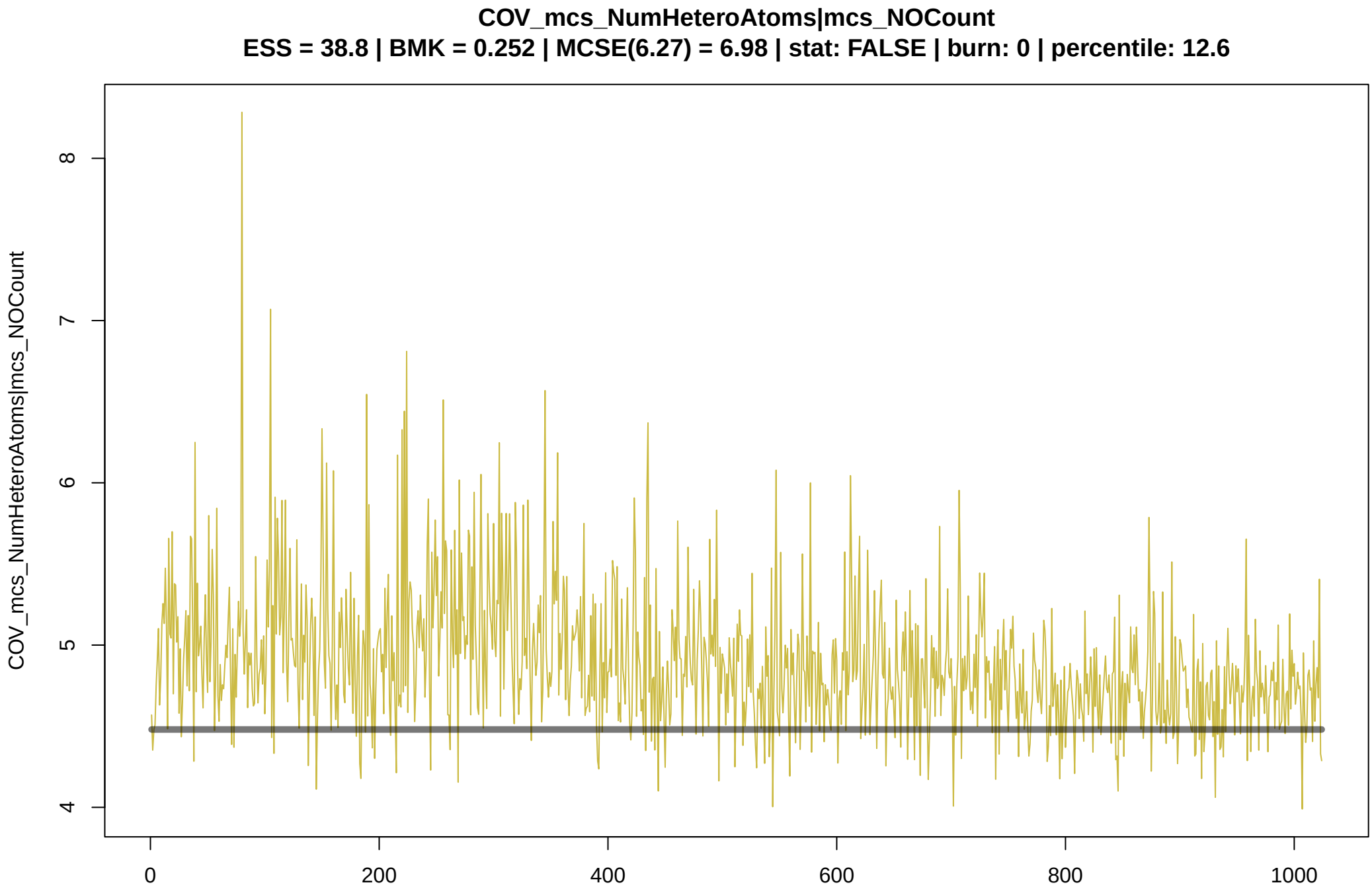

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0473 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | percentile: 97.3
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−11.5
−12.0
−12.5
0
200
400
600
800
1000

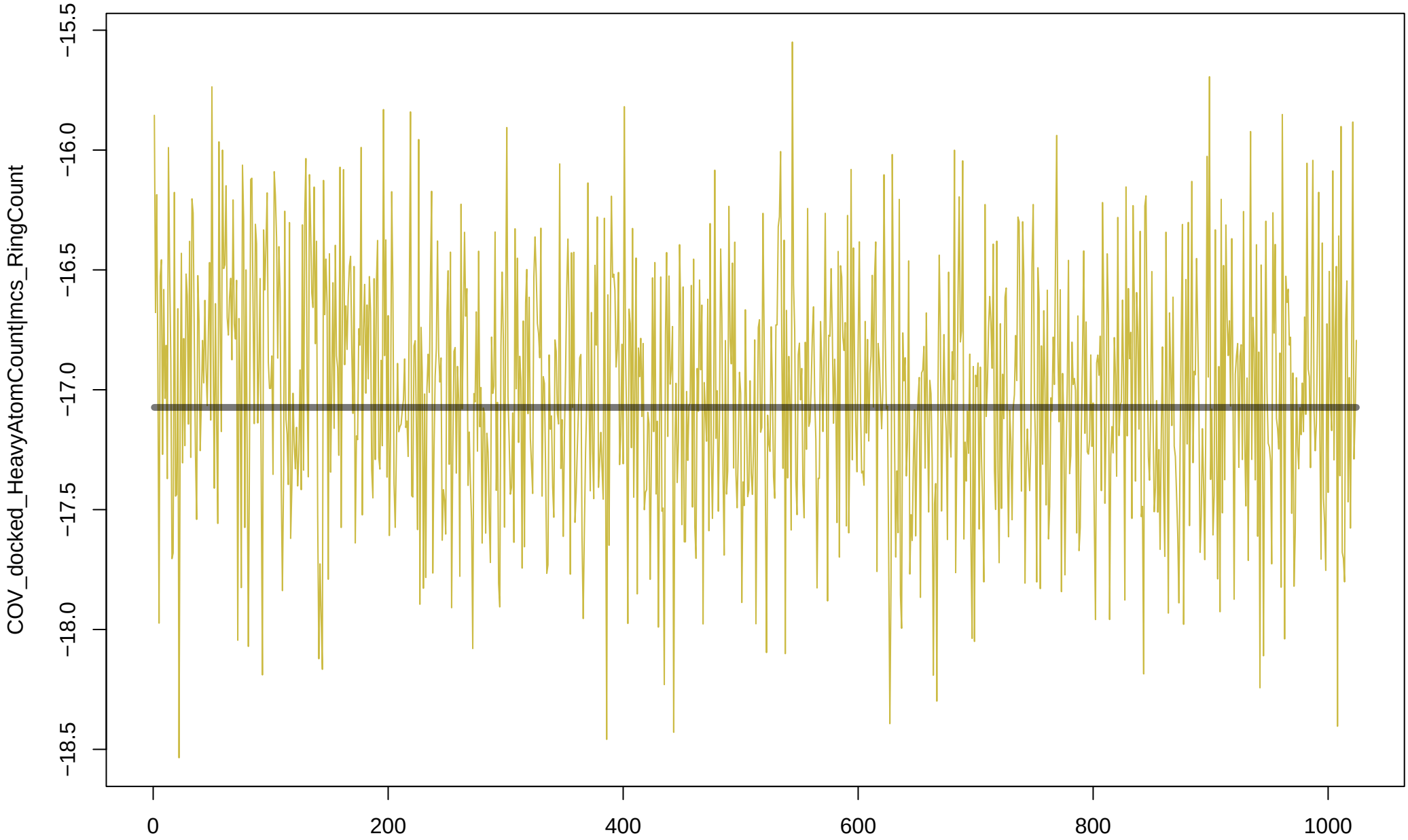

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 820 | BMK = 0.0635 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | percentile: 62.5
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−7.0
−7.5
−8.0
−8.5
−9.0
0
200
400
600
800
1000

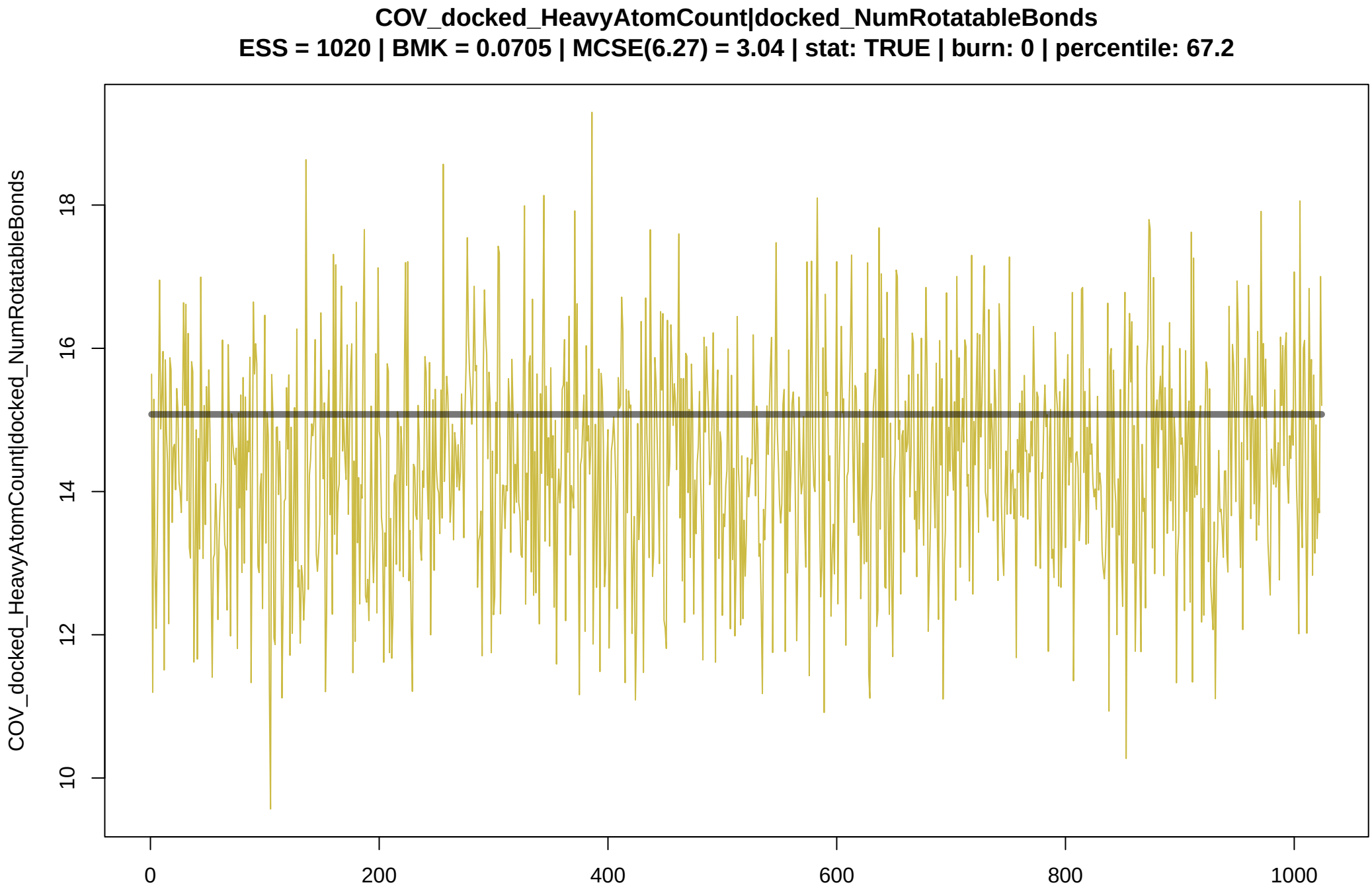

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 927 | BMK = 0.0771 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0 | percentile: 14.9
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−13
−14
−15
−16
0
200
400
600
800
1000

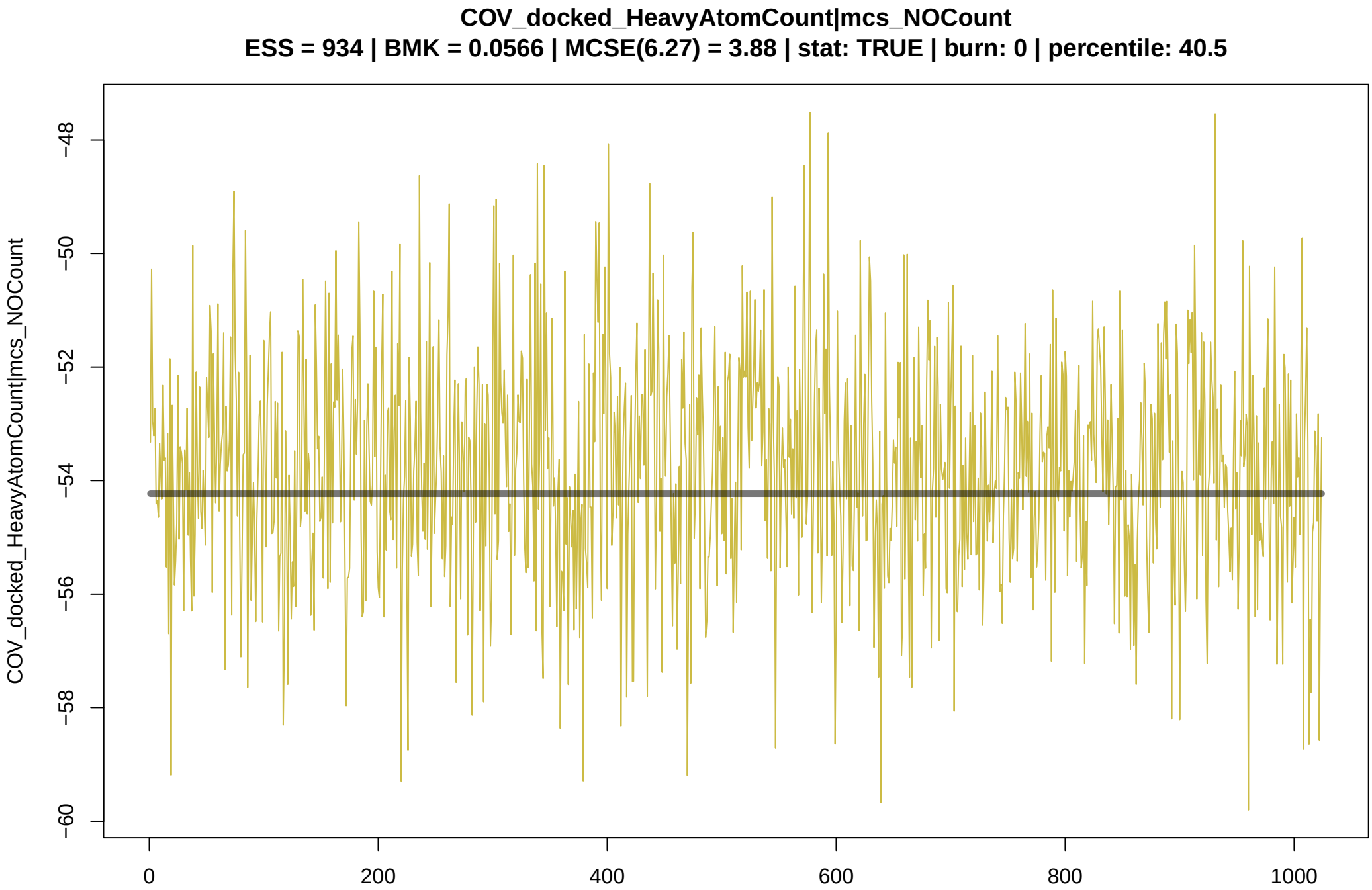

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 51.8 | BMK = 0.186 | MCSE(6.27) = 7.07 | stat: FALSE | burn: 0 | percentile: 7.32
COV_mcs_NumHeteroAtoms|mcs_RingCount
2.0
1.8
1.6
1.4
1.2
1.0
0
200
400
600
800
1000

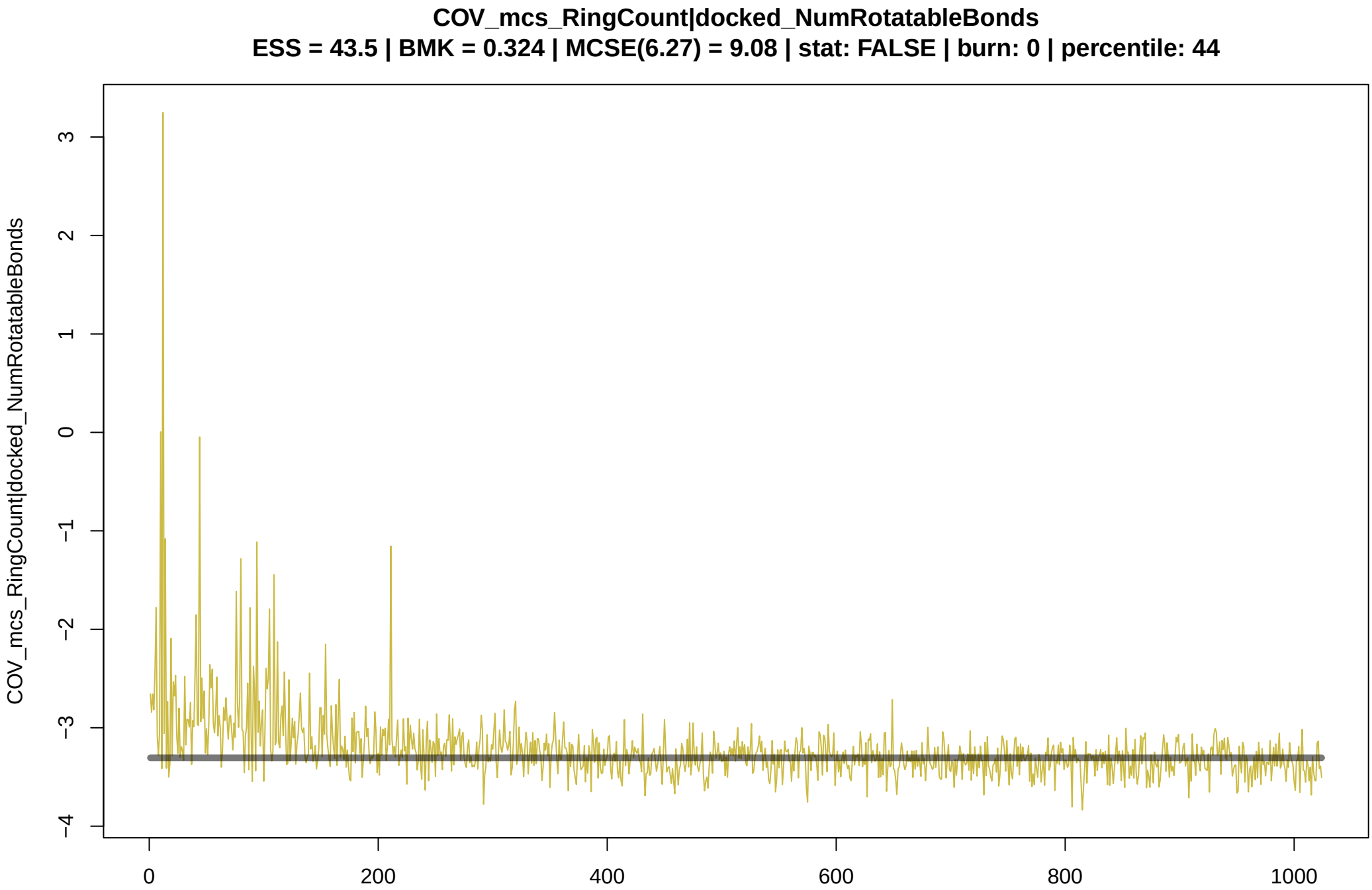

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 243 | BMK = 0.161 | MCSE(6.27) = 6.08 | stat: FALSE | burn: 0 | percentile: 26.5
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
2
1
0
−1
−2
0
200
400
600
800
1000

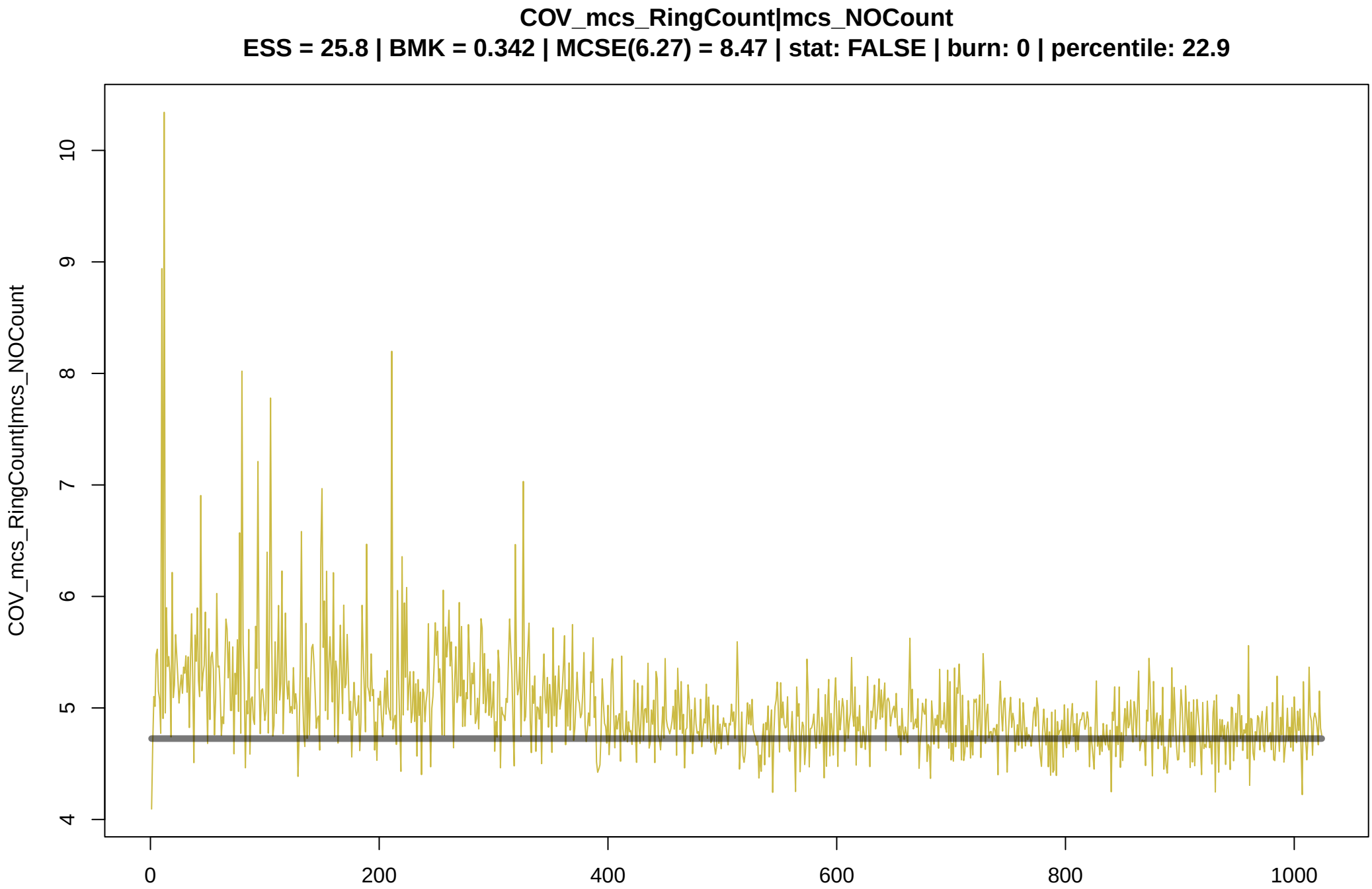

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 38.8 | BMK = 0.252 | MCSE(6.27) = 6.98 | stat: FALSE | burn: 0 | percentile: 12.6
COV_mcs_NumHeteroAtoms|mcs_NOCount
4
5
6
7
8
0
200
400
600
800
1000

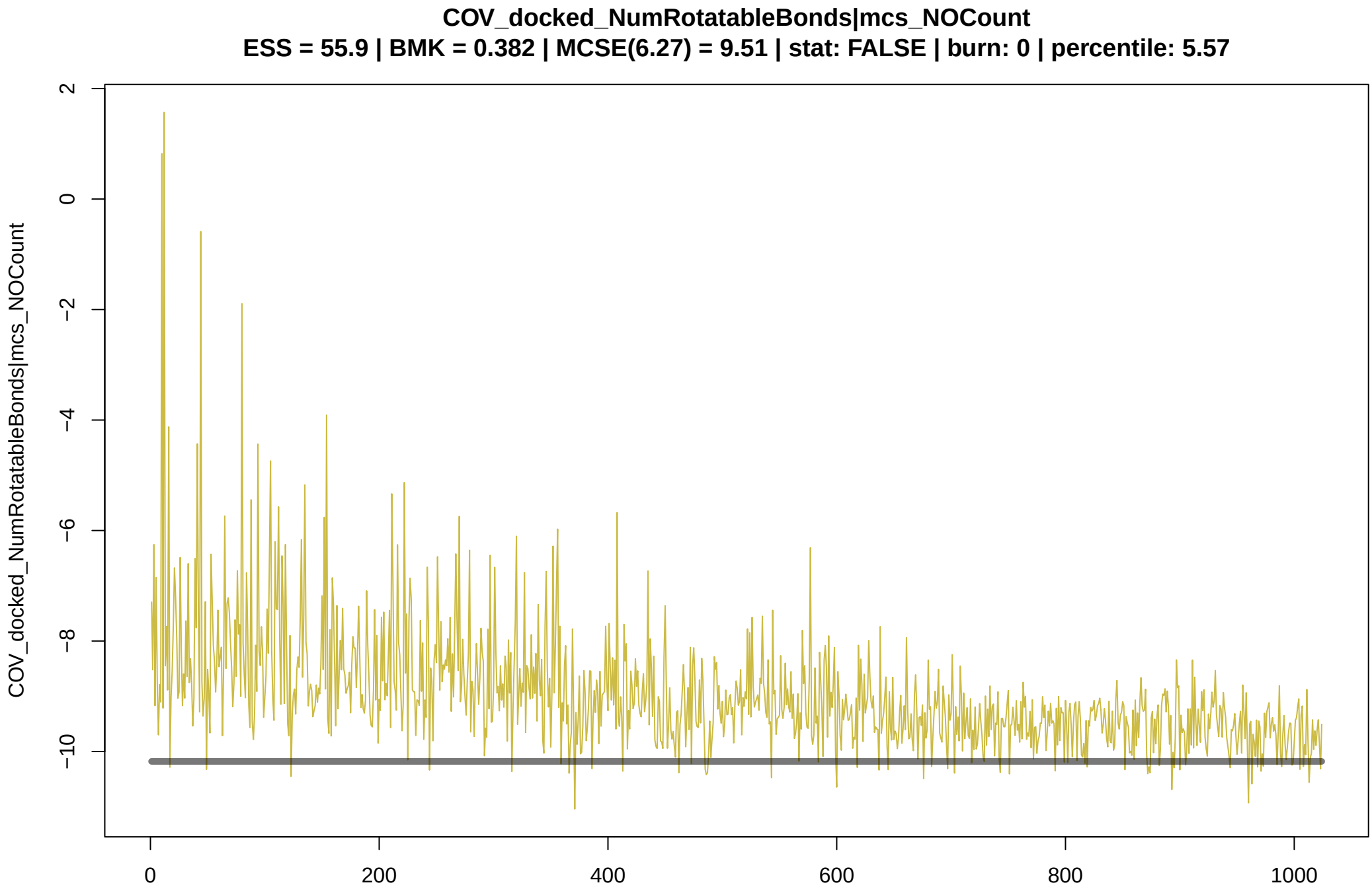

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0624 | MCSE(6.27) = 3.6 | stat: FALSE | burn: 0 | percentile: 46.2
COV_docked_HeavyAtomCount|mcs_RingCount
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0705 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | percentile: 67.2
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 934 | BMK = 0.0566 | MCSE(6.27) = 3.88 | stat: TRUE | burn: 0 | percentile: 40.5
COV_docked_HeavyAtomCount|mcs_NOCount
−48
−50
−52
−54
−56
−58
−60
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 43.5 | BMK = 0.324 | MCSE(6.27) = 9.08 | stat: FALSE | burn: 0 | percentile: 44
COV_mcs_RingCount|docked_NumRotatableBonds
3
2
1
0
−1
−2
−3
−4
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 25.8 | BMK = 0.342 | MCSE(6.27) = 8.47 | stat: FALSE | burn: 0 | percentile: 22.9
COV_mcs_RingCount|mcs_NOCount
4
5
6
7
8
9
10
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 55.9 | BMK = 0.382 | MCSE(6.27) = 9.51 | stat: FALSE | burn: 0 | percentile: 5.57
COV_docked_NumRotatableBonds|mcs_NOCount
2
0
−2
−4
−6
−8
−10
0
200
400
600
800
1000