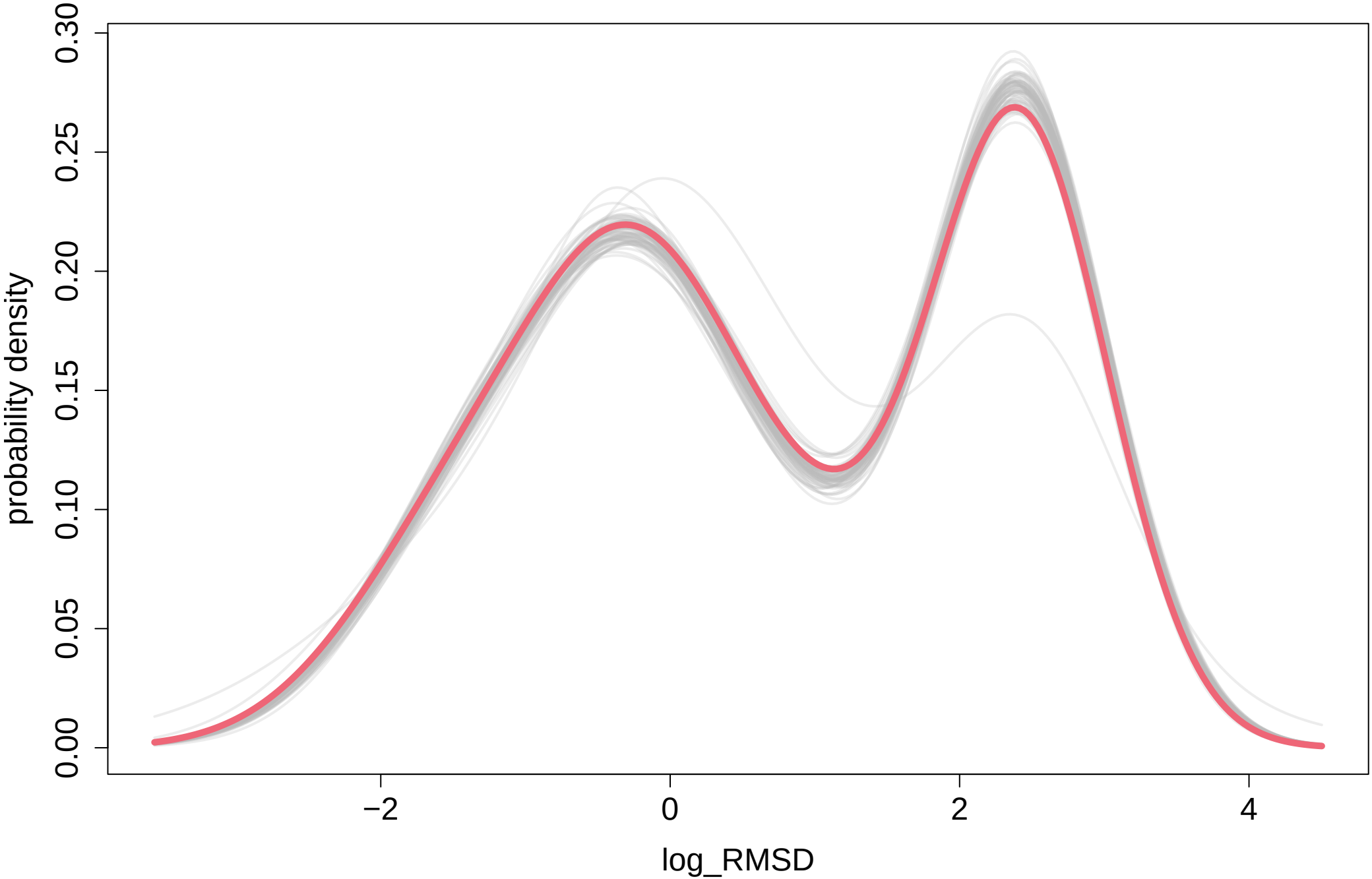
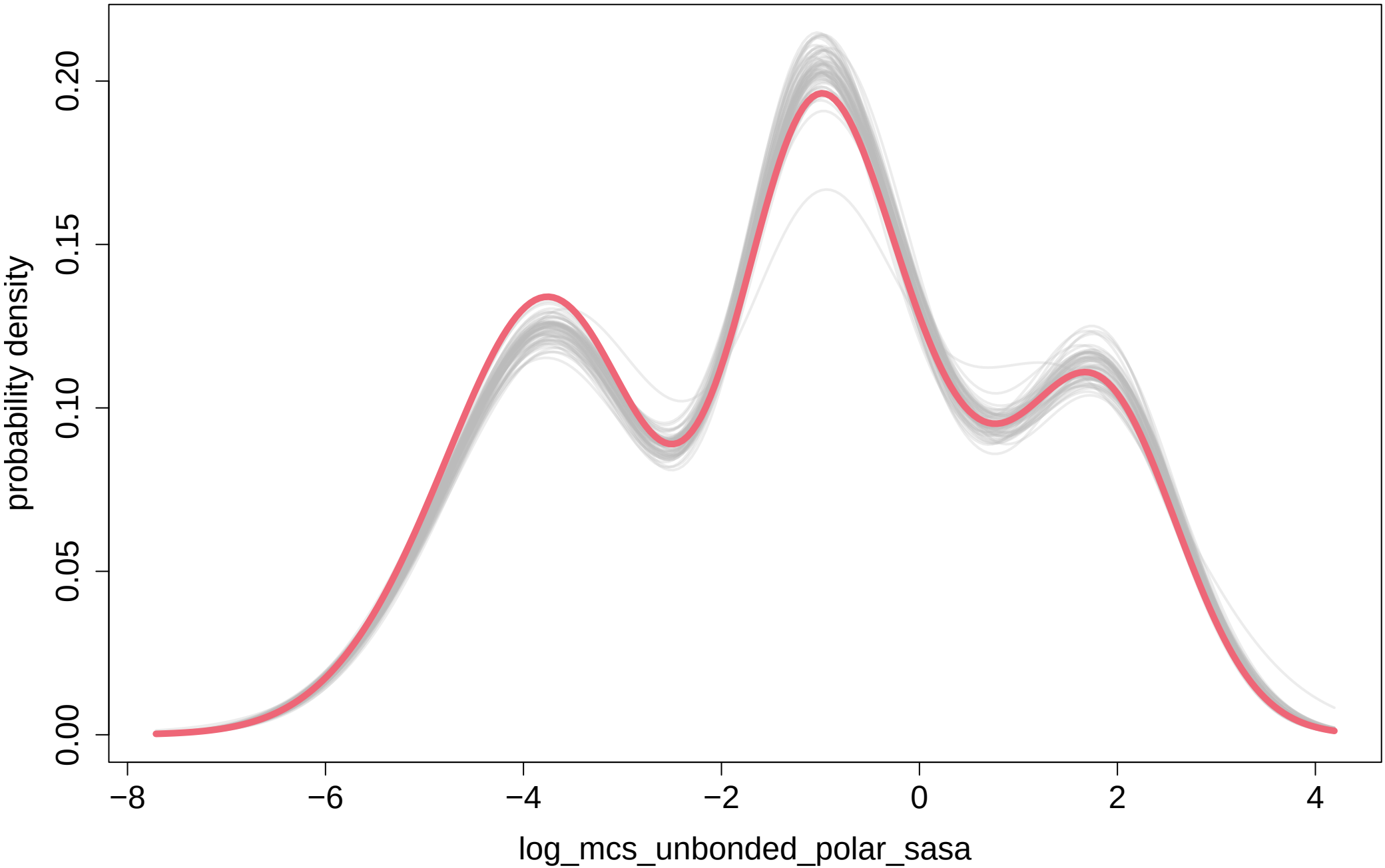
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.77311644355176
max MCSE = 15.1649693720515
all stationary: FALSE
burn: 0
min percent.: 0.9765625

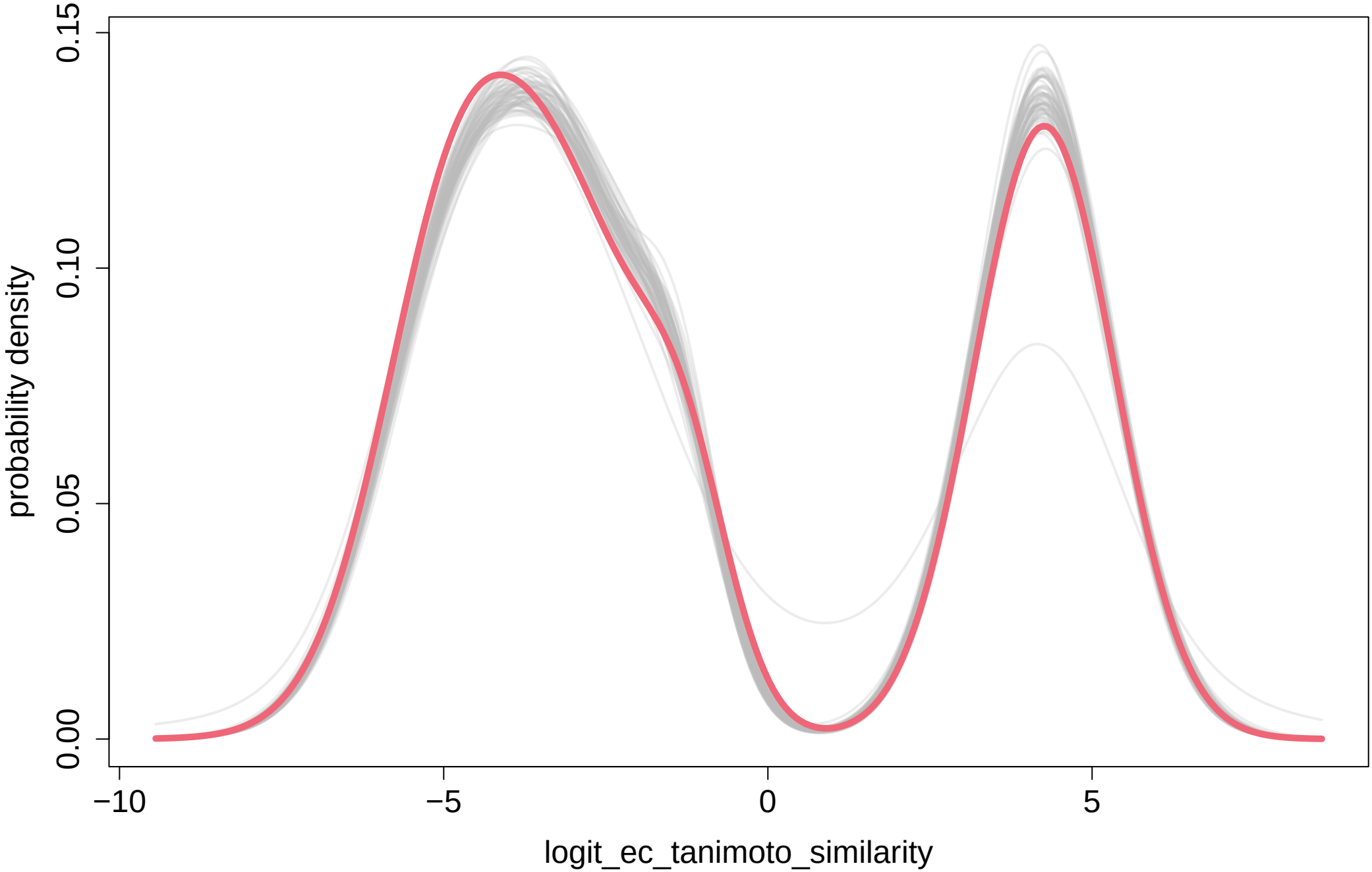
−− STATS 2D −−
min ESS = 20.5504964556777
max BMK = 0.378082005389981
max MCSE = 9.62051398159463
all stationary: FALSE
burn: 0
min percent.: 1.46484375

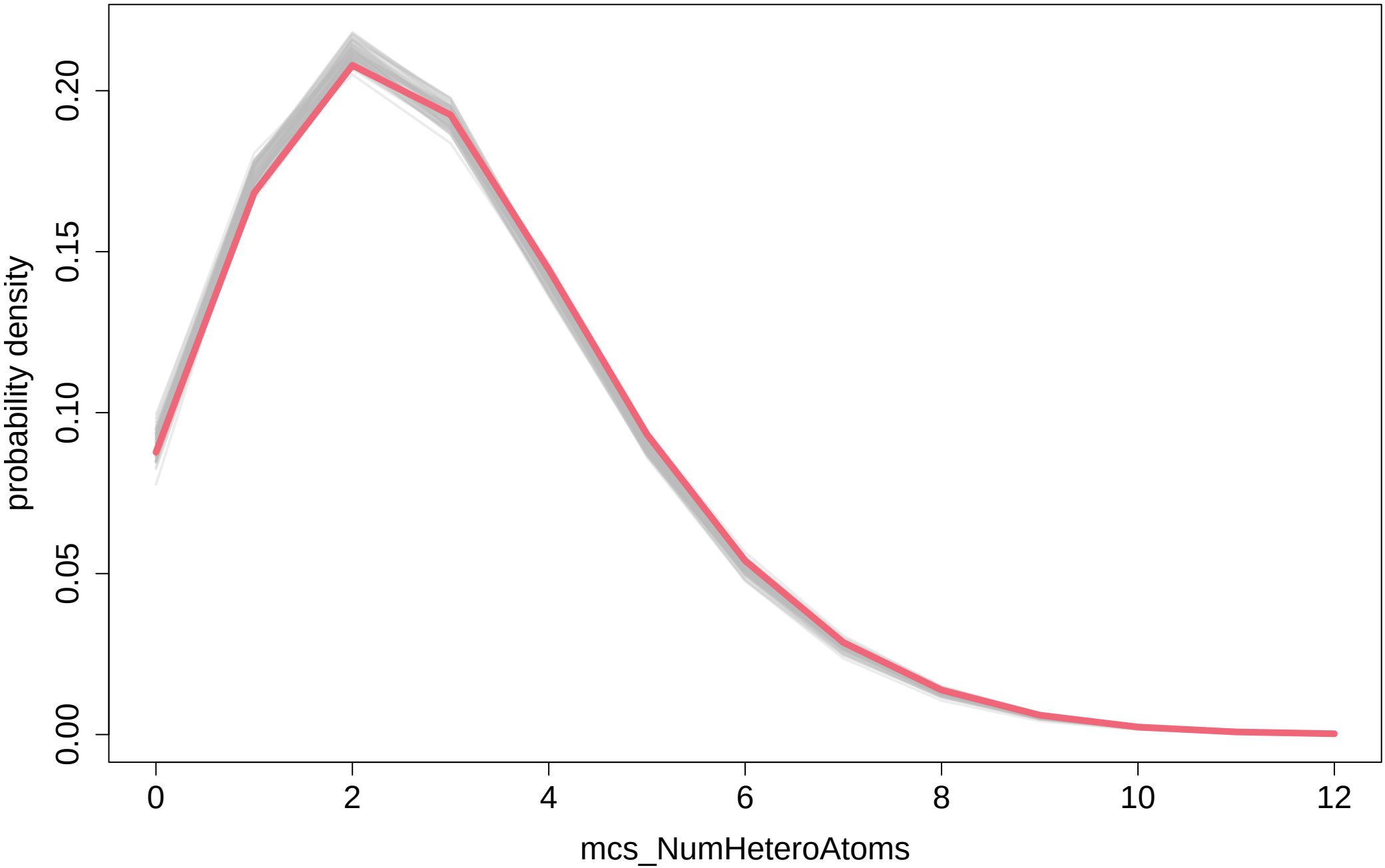
−− STATS 1D −−
min ESS = 3.25328194200767
max BMK = 1
max MCSE = 14.0784876909831
all stationary: FALSE
burn: 816
min percent.: 0.390625

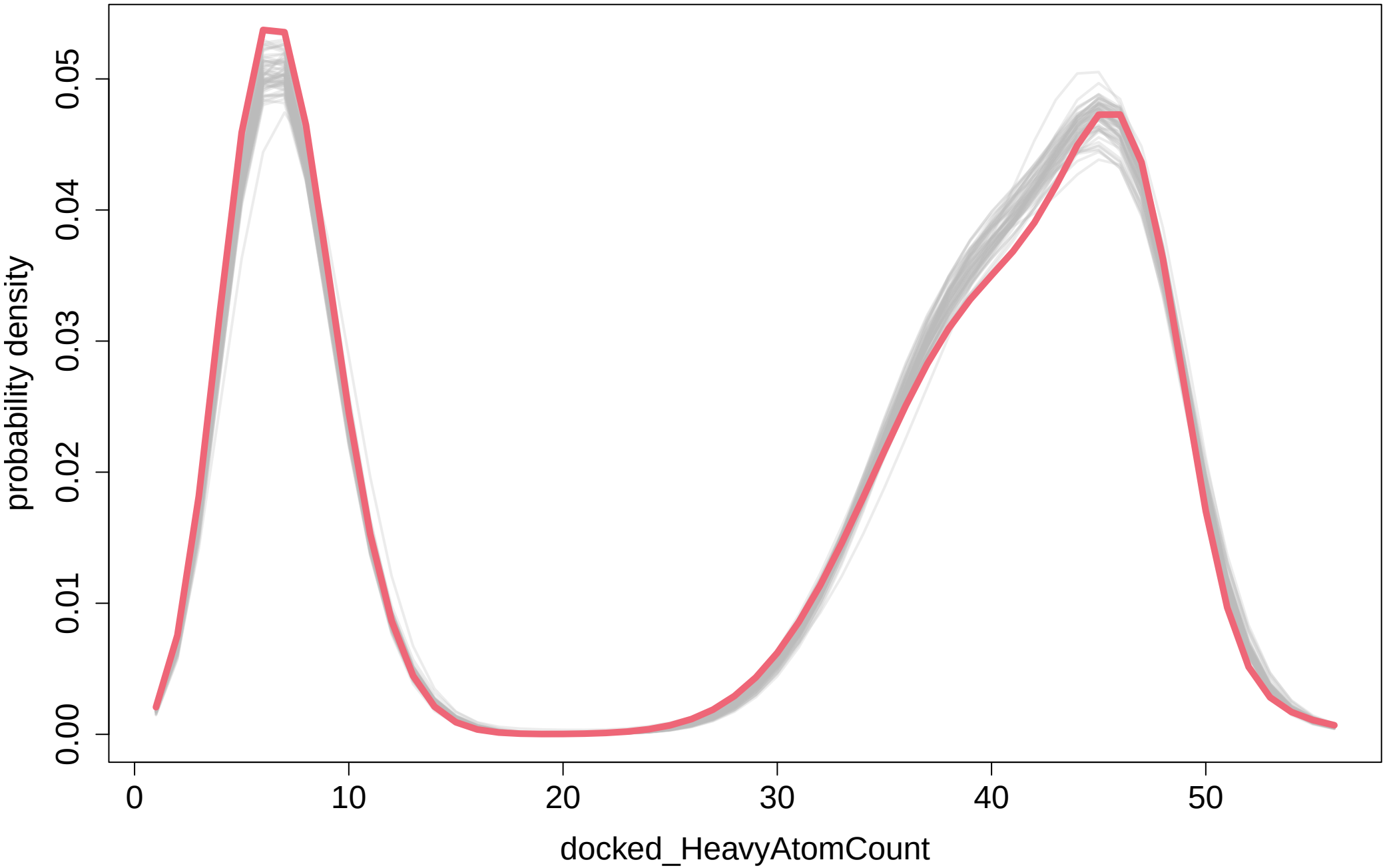
Occupied clusters: 23 of 64
LL: −62500 +− 142

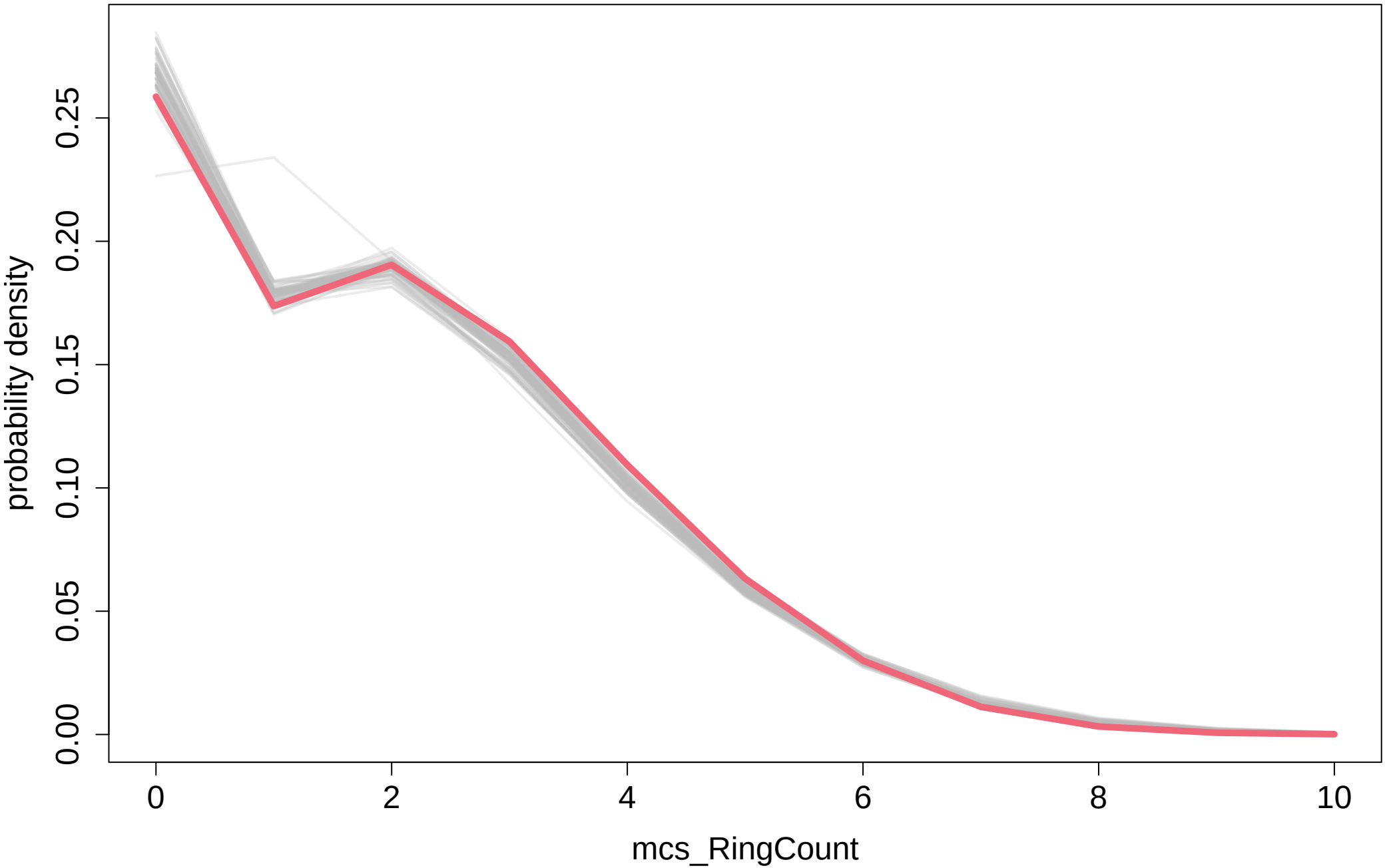

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−2
0
2
4
log_RMSD

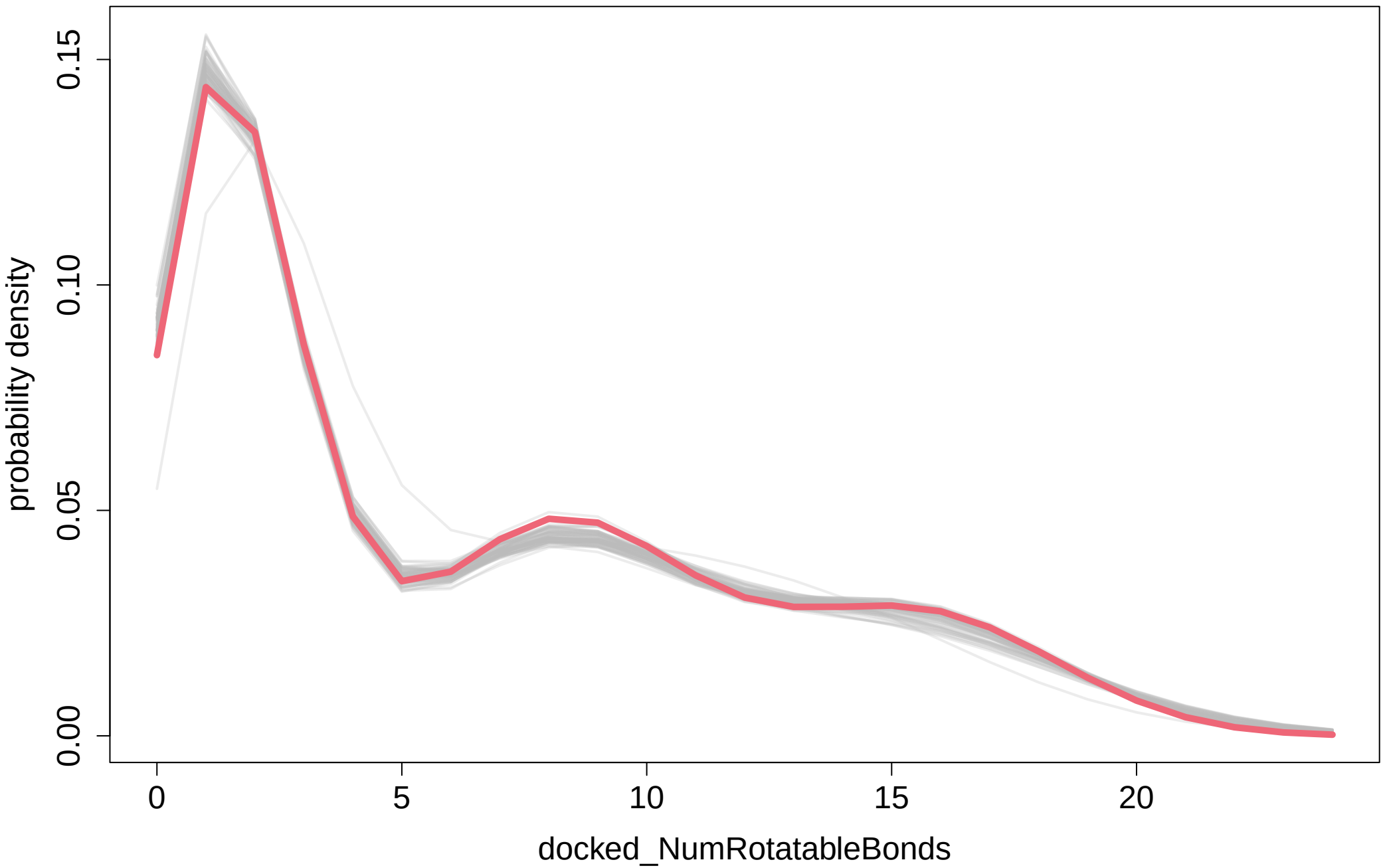

probability density
0.00
0.05
0.10
0.15
0.20
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

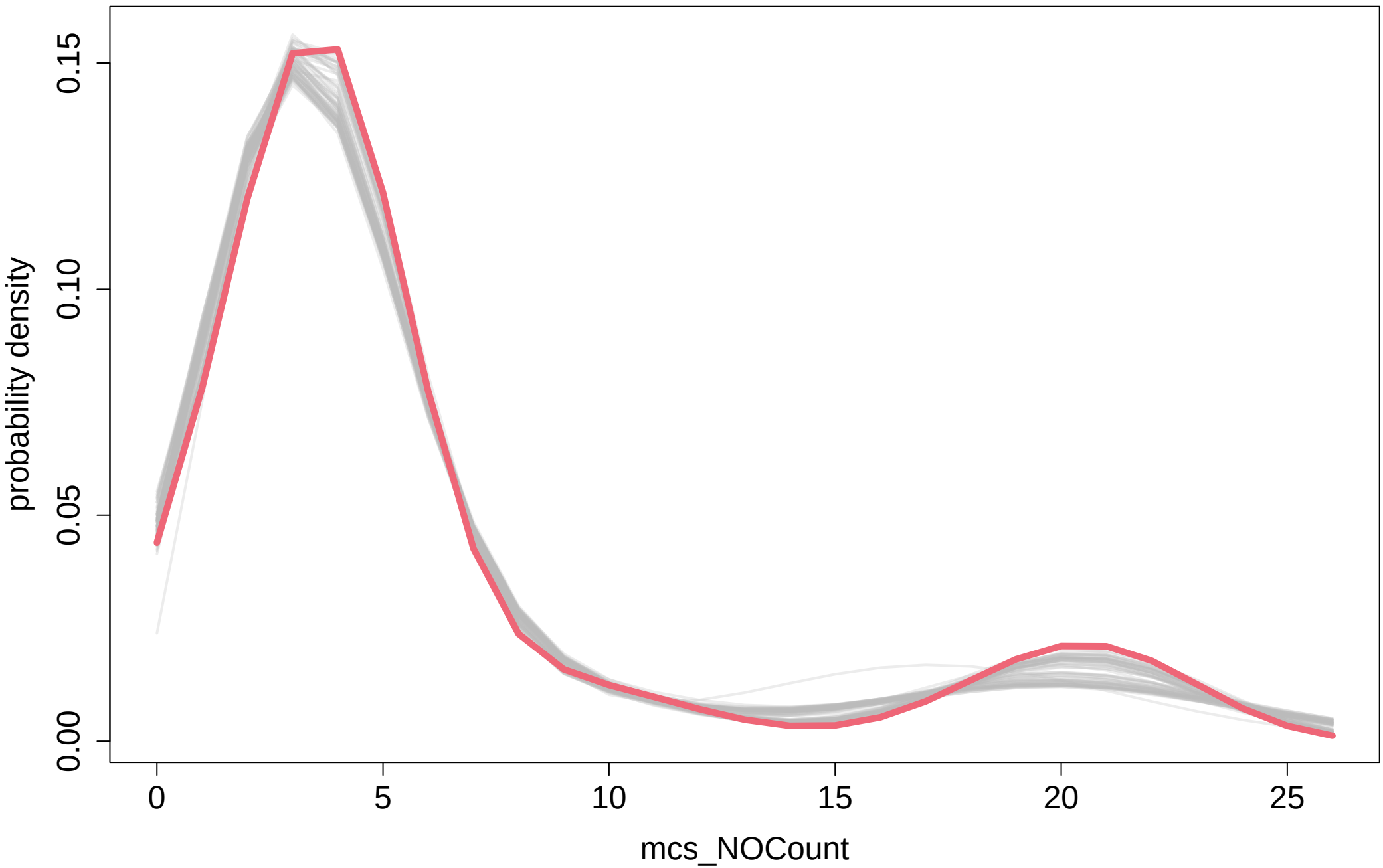

probability density
0.00
0.05
0.10
0.15
−10
−5
0
5
logit_ec_tanimoto_similarity

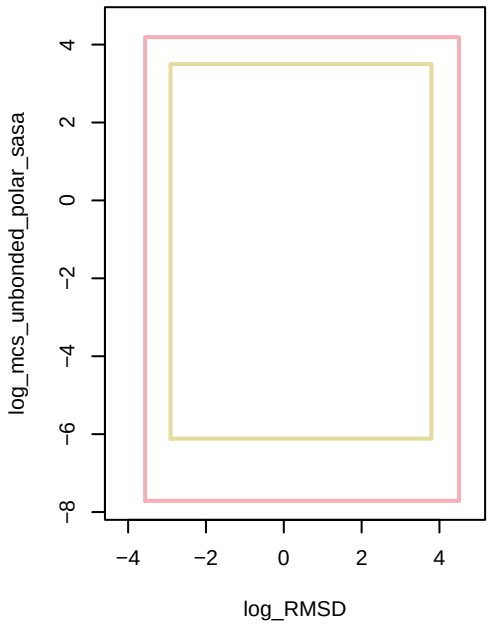

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms

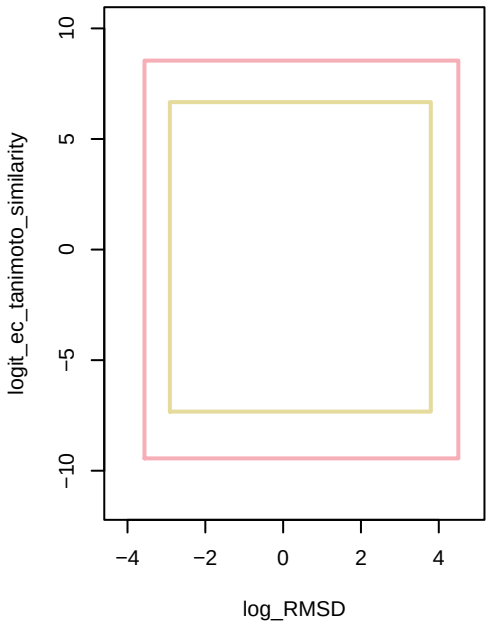

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount

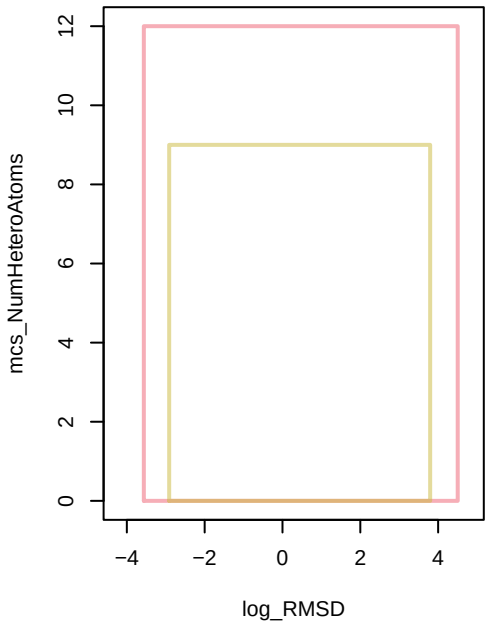

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount

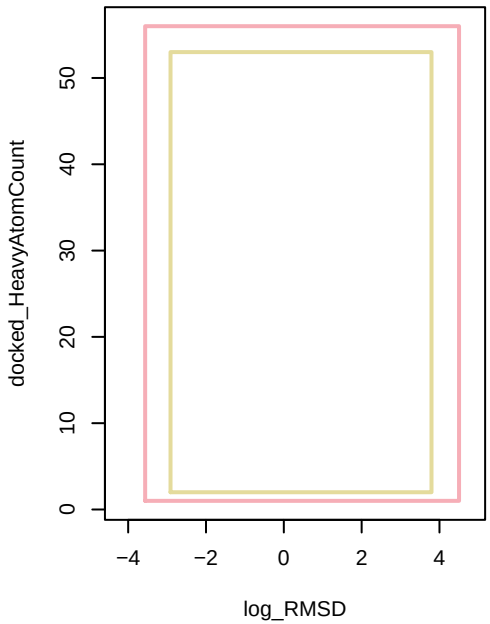

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
docked_NumRotatableBonds

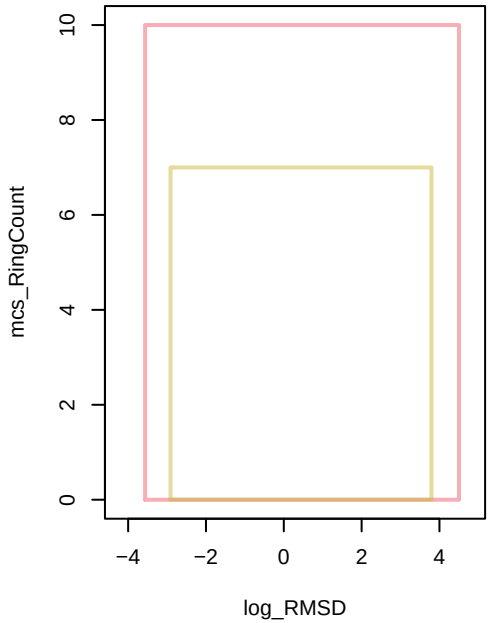

probability density
0.00
0.05
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

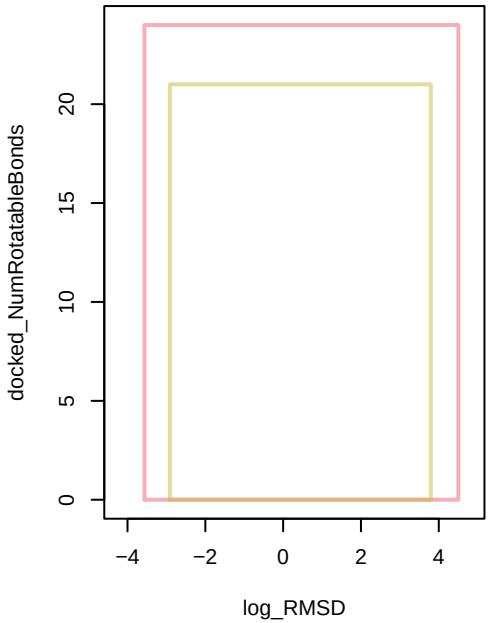

log_mcs_unbonded_polar_sasa
log_RMSD

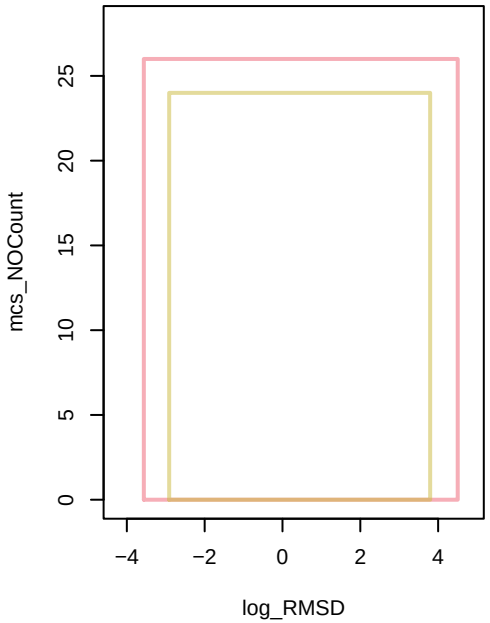

logit_ec_tanimoto_similarity
log_RMSD

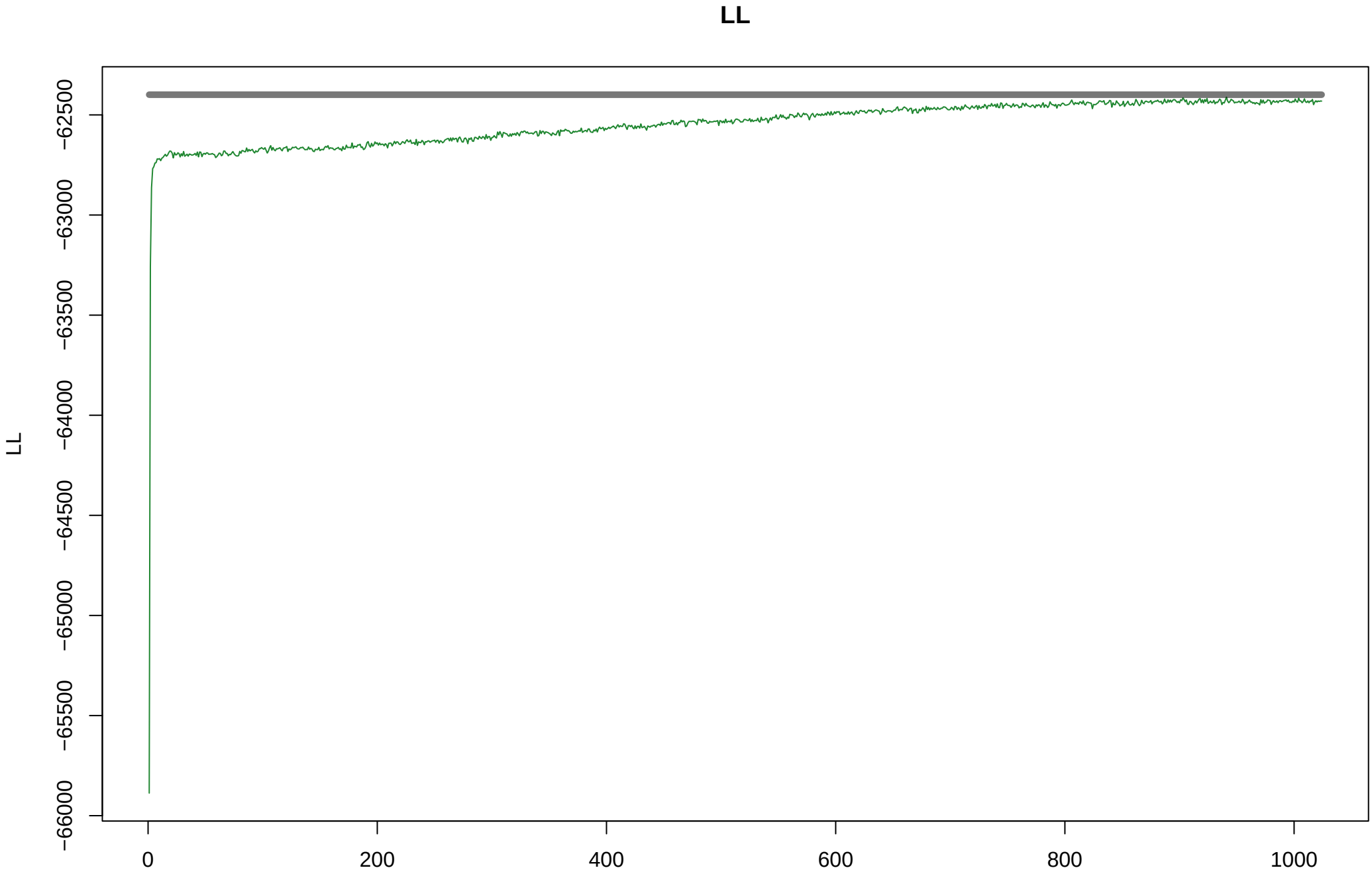

mcs_NumHeteroAtoms
log_RMSD

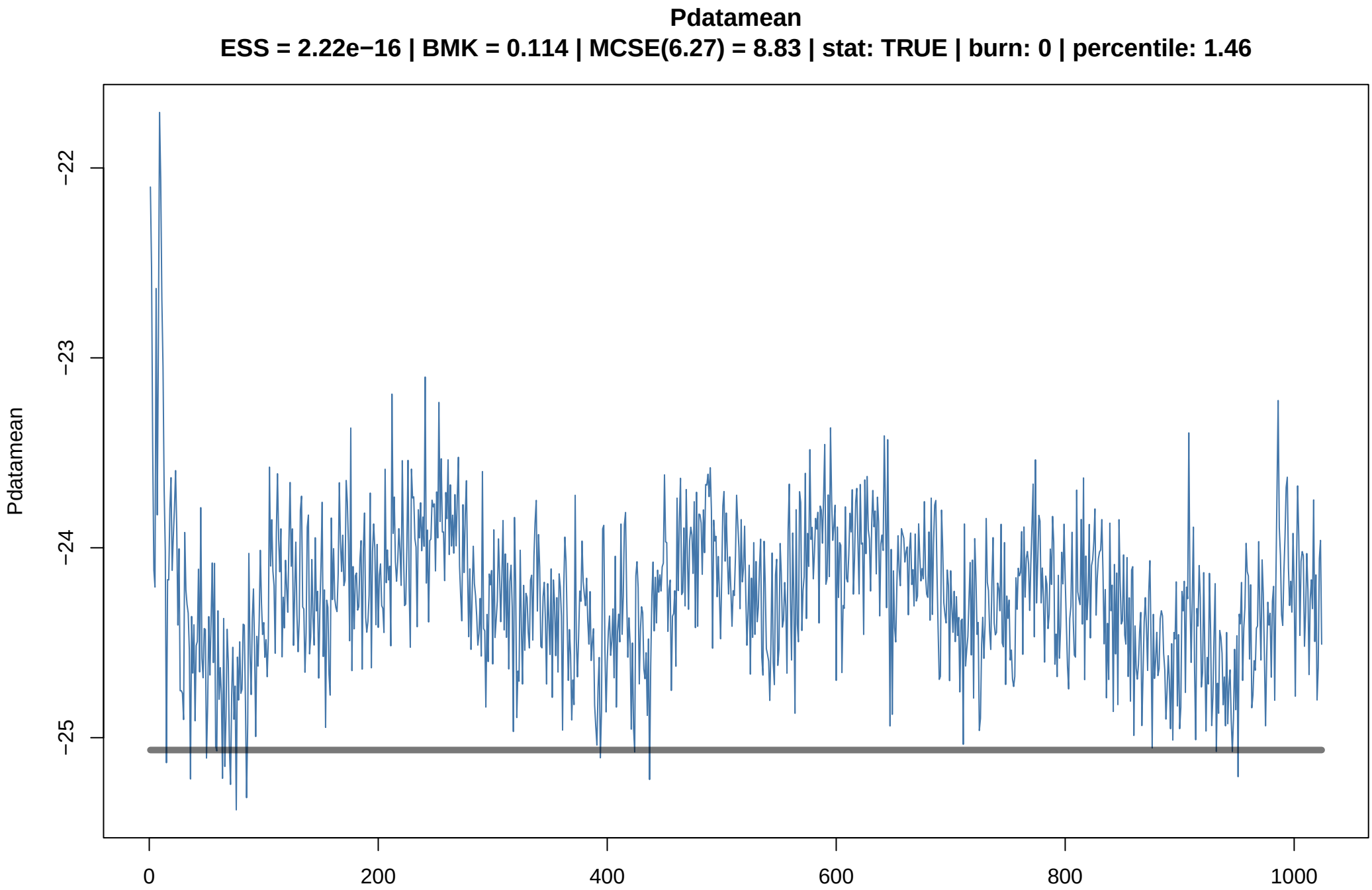

docked_HeavyAtomCount
log_RMSD

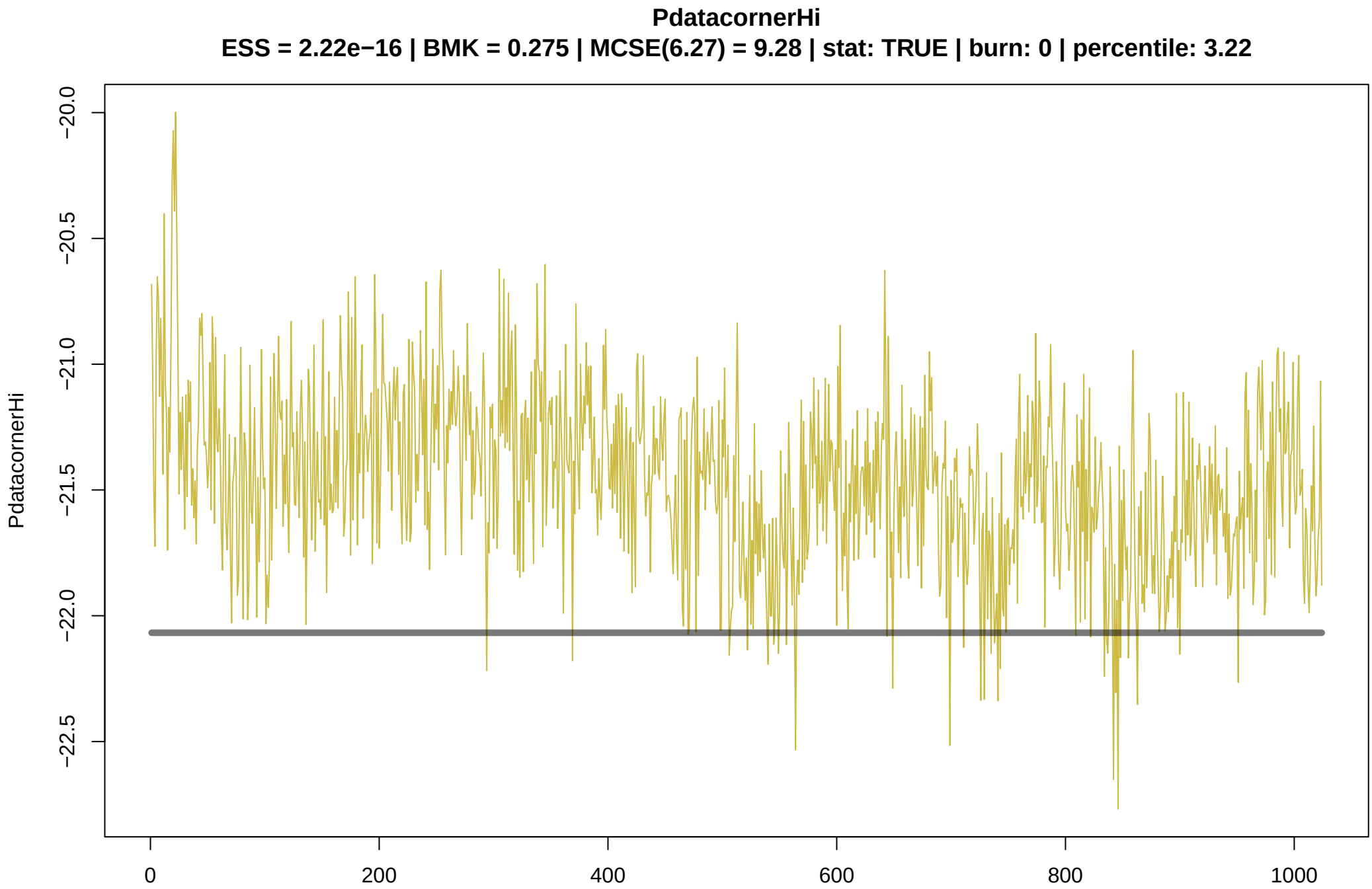

mcs_RingCount
log_RMSD

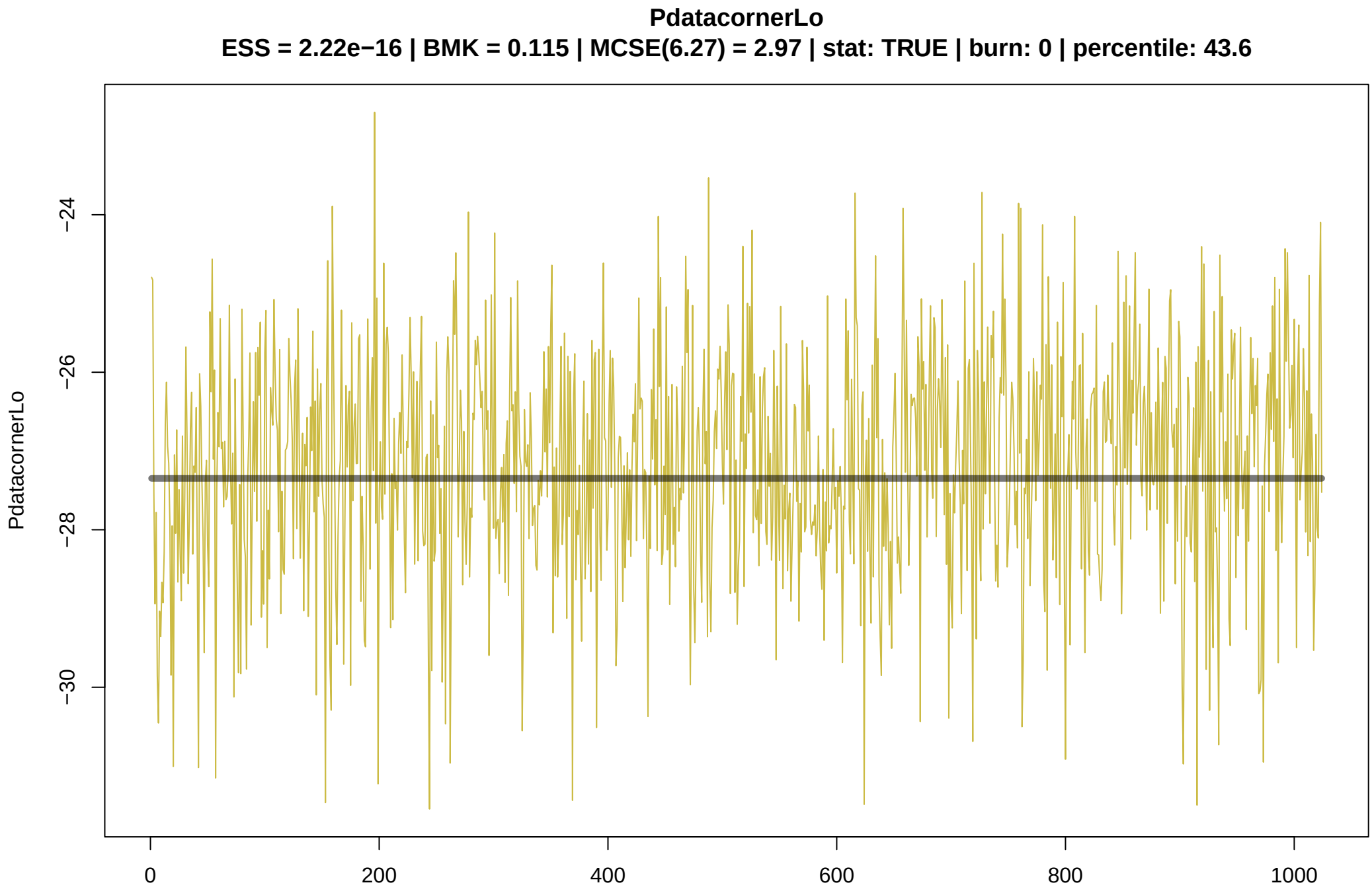

docked_NumRotatableBonds
log_RMSD

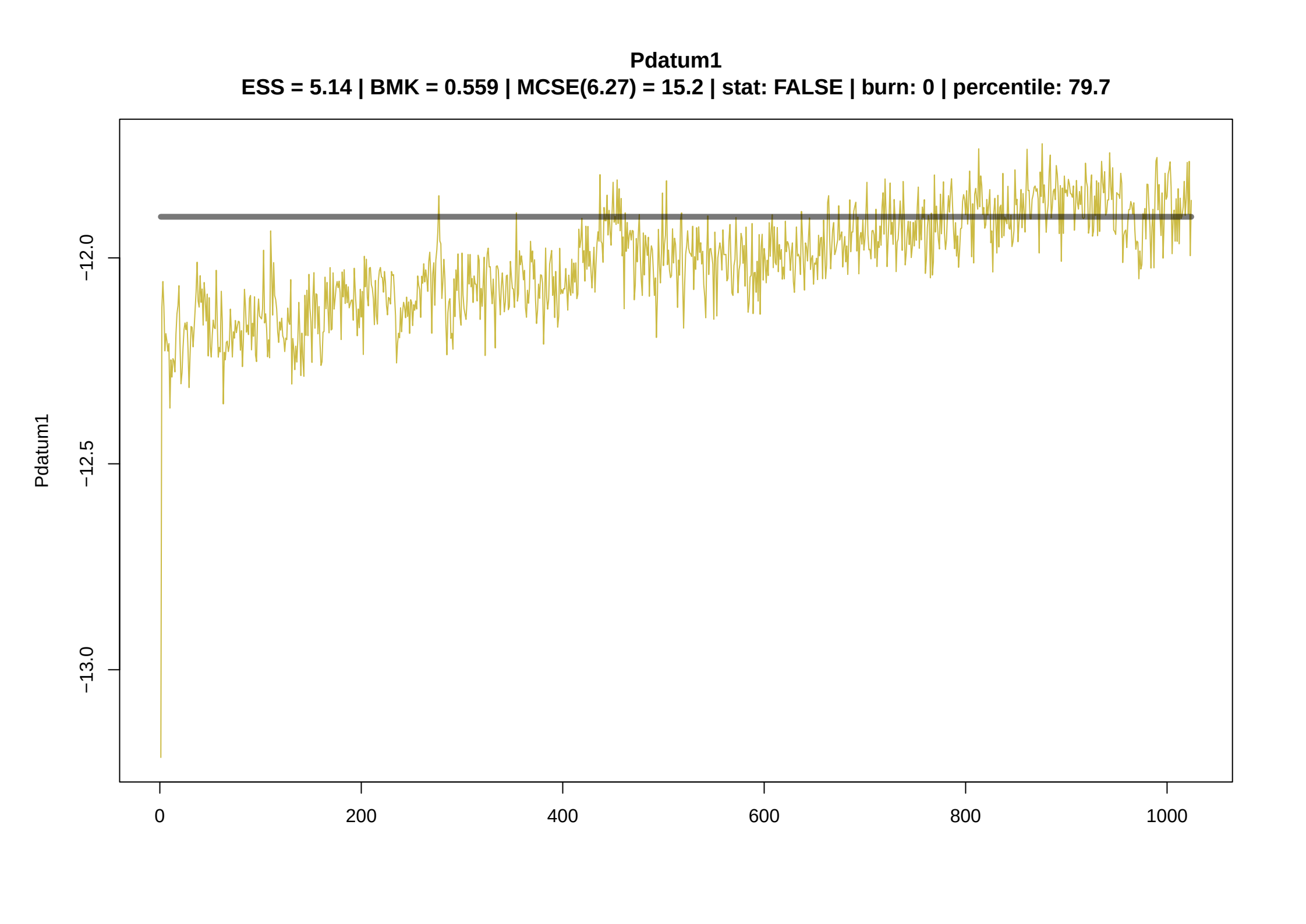

mcs_NOCount
log_RMSD

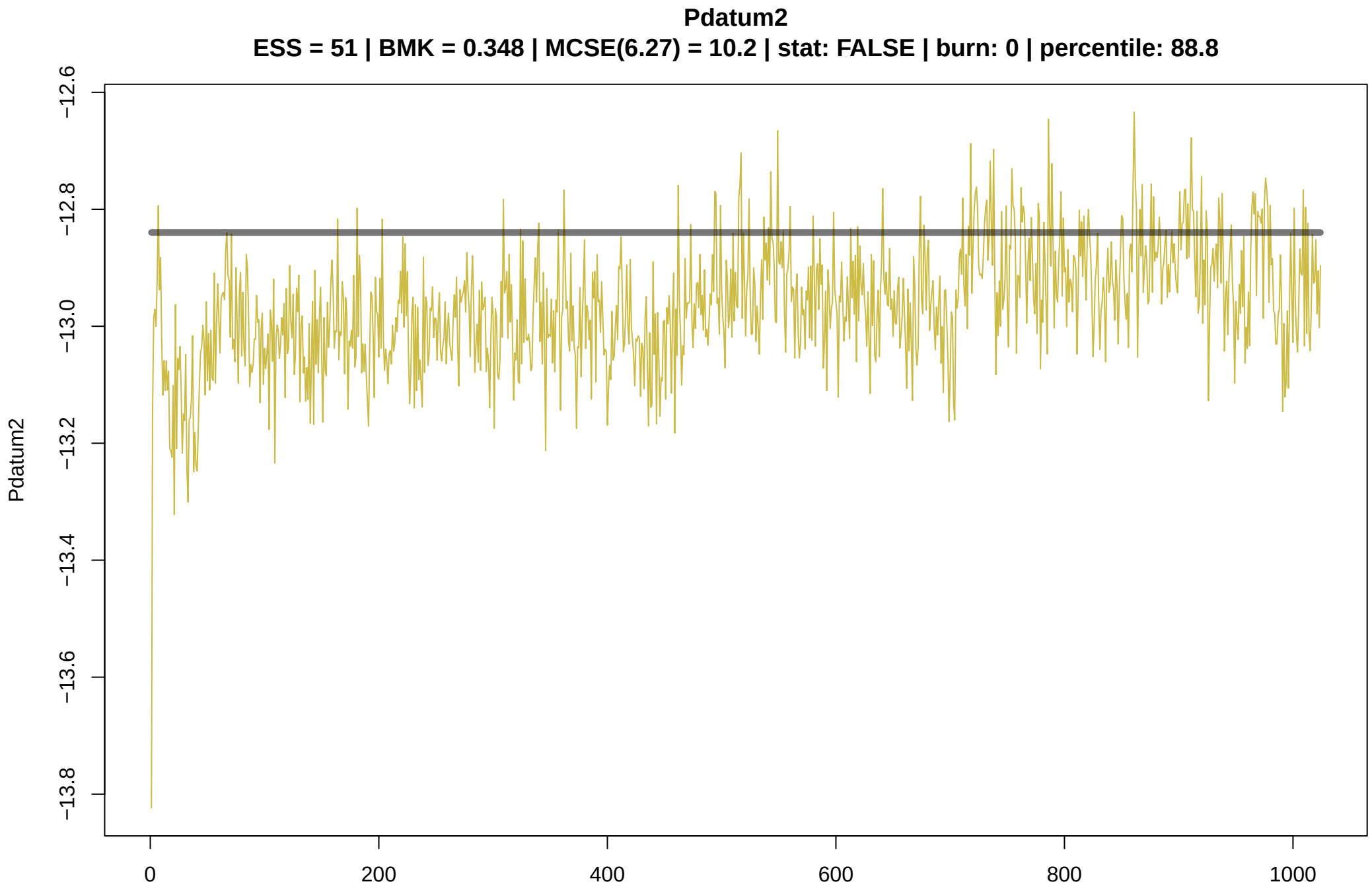

LL
LL
−62500
−63000
−63500
−64000
−64500
−65000
−65500
−66000
0
200
400
600
800
1000

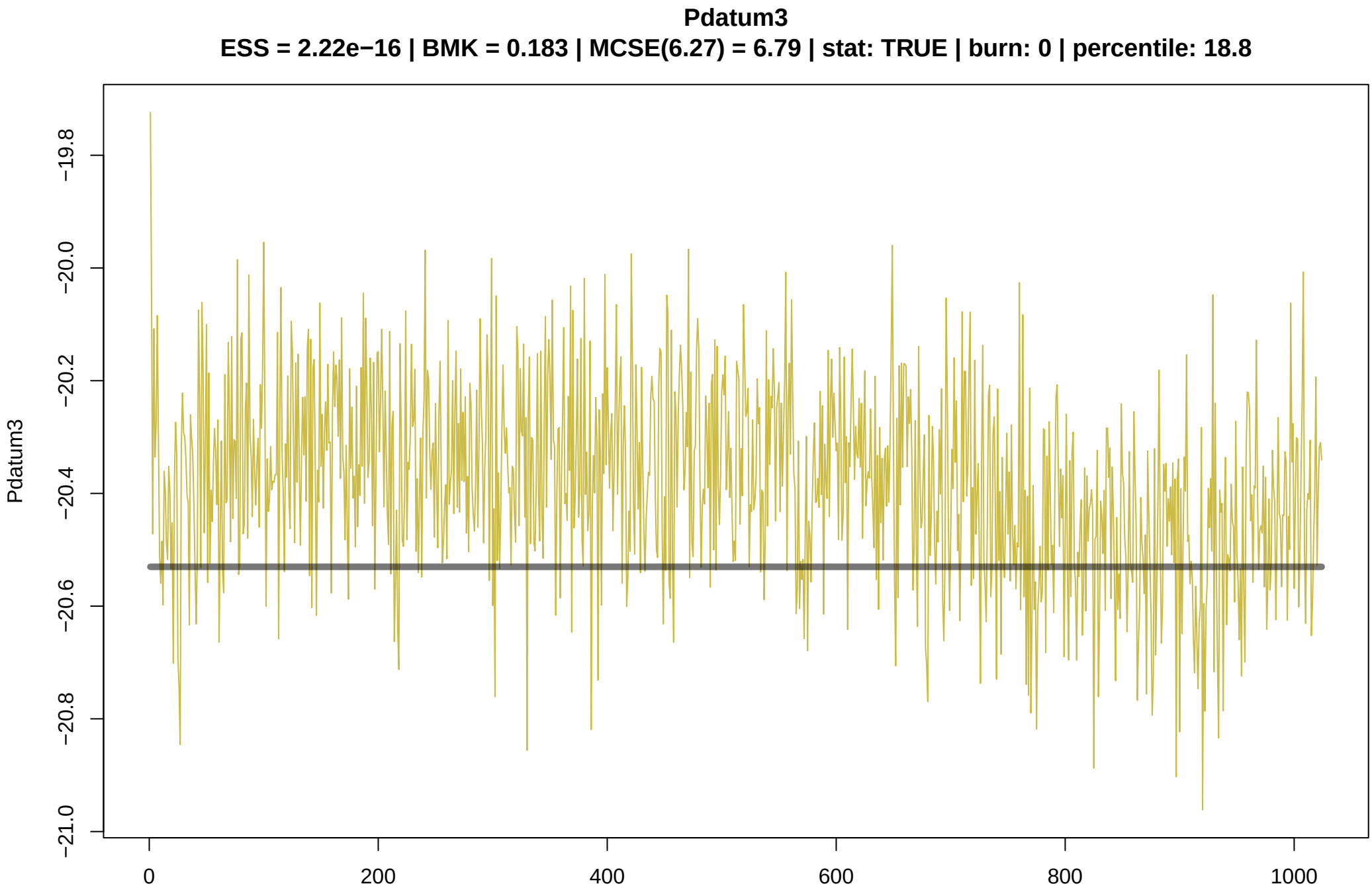

Pdatamean
ESS = 2.22e−16 | BMK = 0.114 | MCSE(6.27) = 8.83 | stat: TRUE | burn: 0 | percentile: 1.46
Pdatamean
−22
−23
−24
−25
0
200
400
600
800
1000

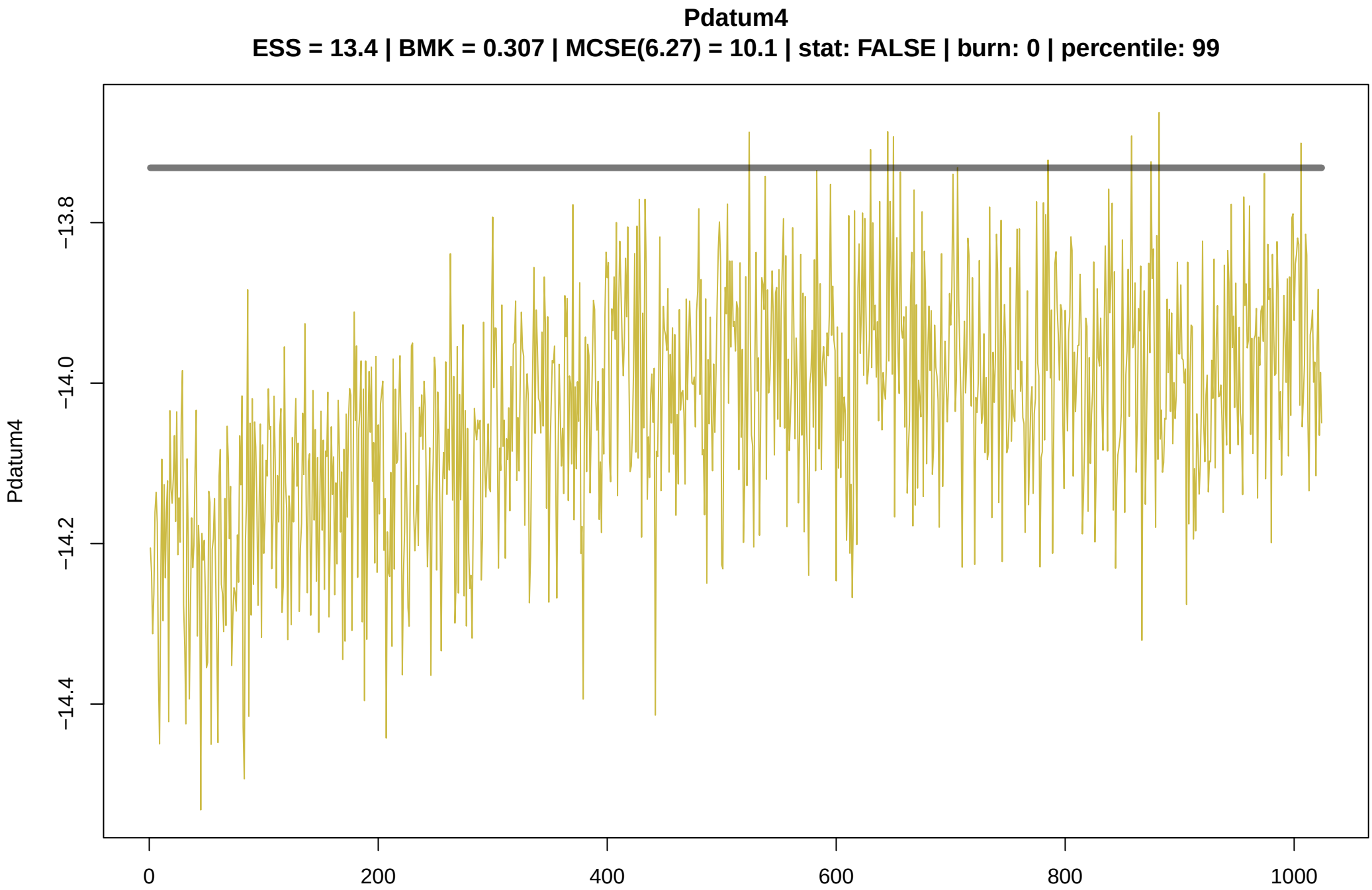

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.275 | MCSE(6.27) = 9.28 | stat: TRUE | burn: 0 | percentile: 3.22
PdatacornerHi
−20.0
−20.5
−21.0
−21.5
−22.0
−22.5
0
200
400
600
800
1000

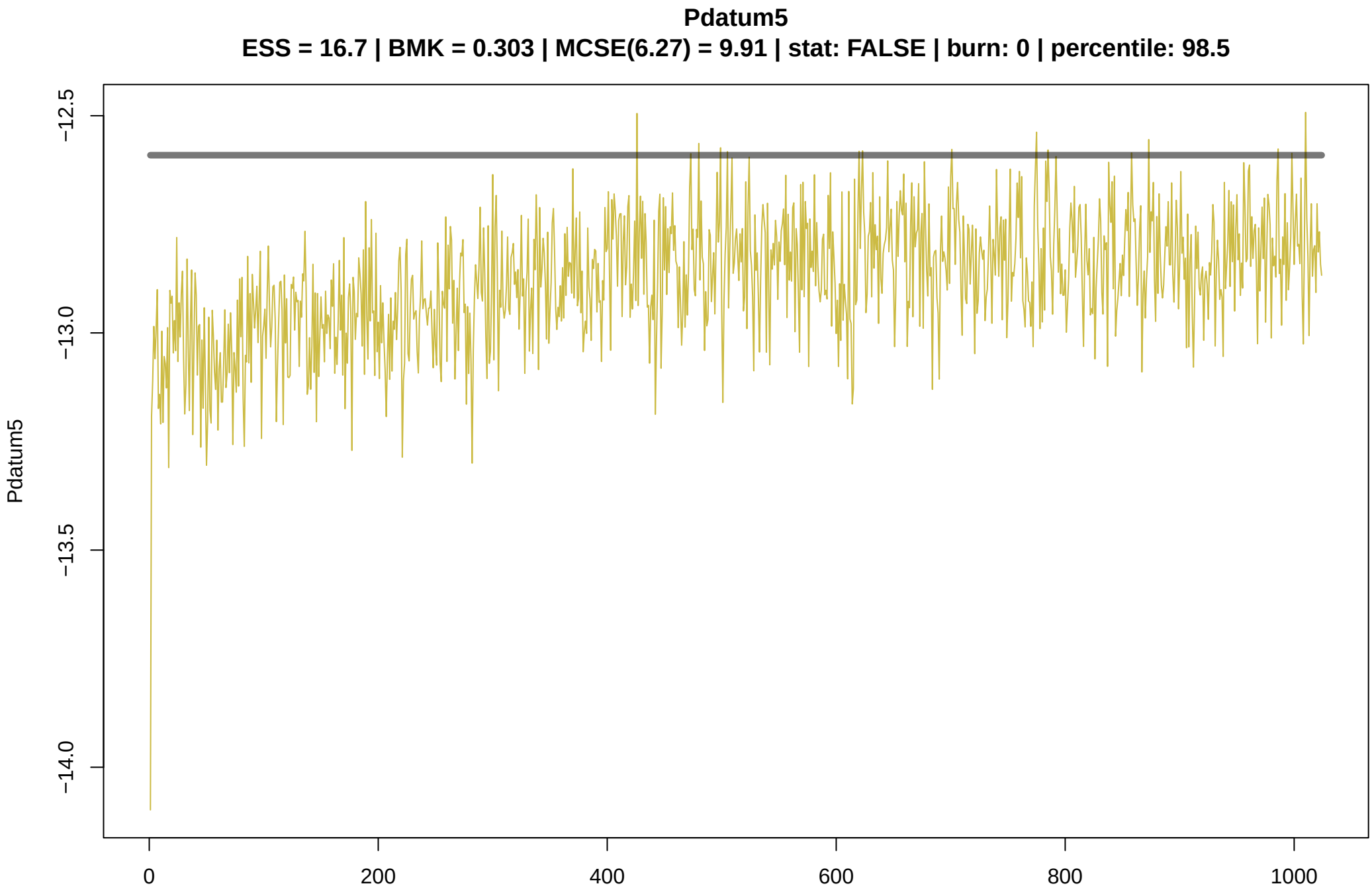

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.115 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0 | percentile: 43.6
PdatacornerLo
−24
−26
−28
−30
0
200
400
600
800
1000

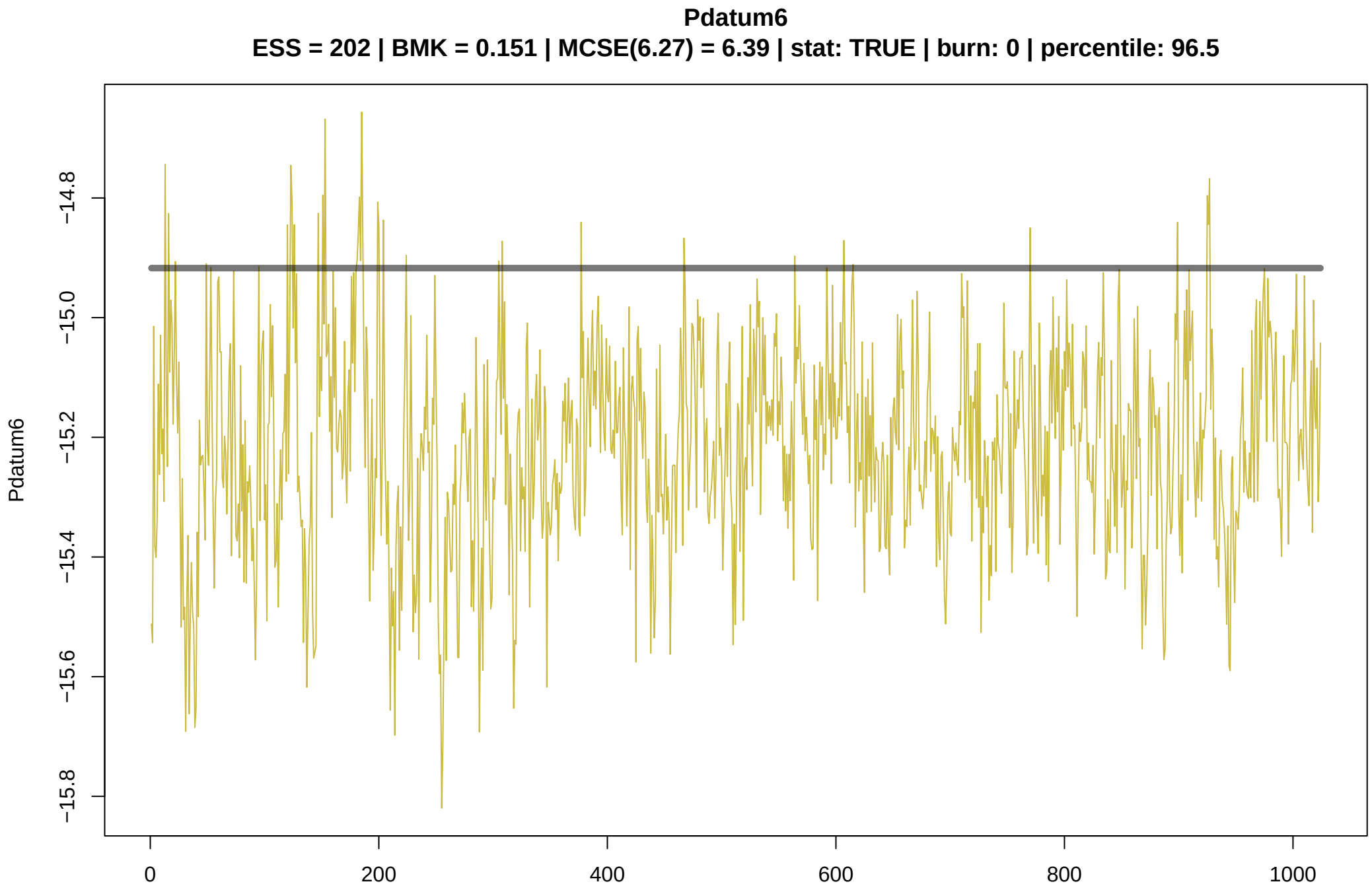

Pdatum1
ESS = 5.14 | BMK = 0.559 | MCSE(6.27) = 15.2 | stat: FALSE | burn: 0 | percentile: 79.7
Pdatum1
−12.0
−12.5
−13.0
0
200
400
600
800
1000

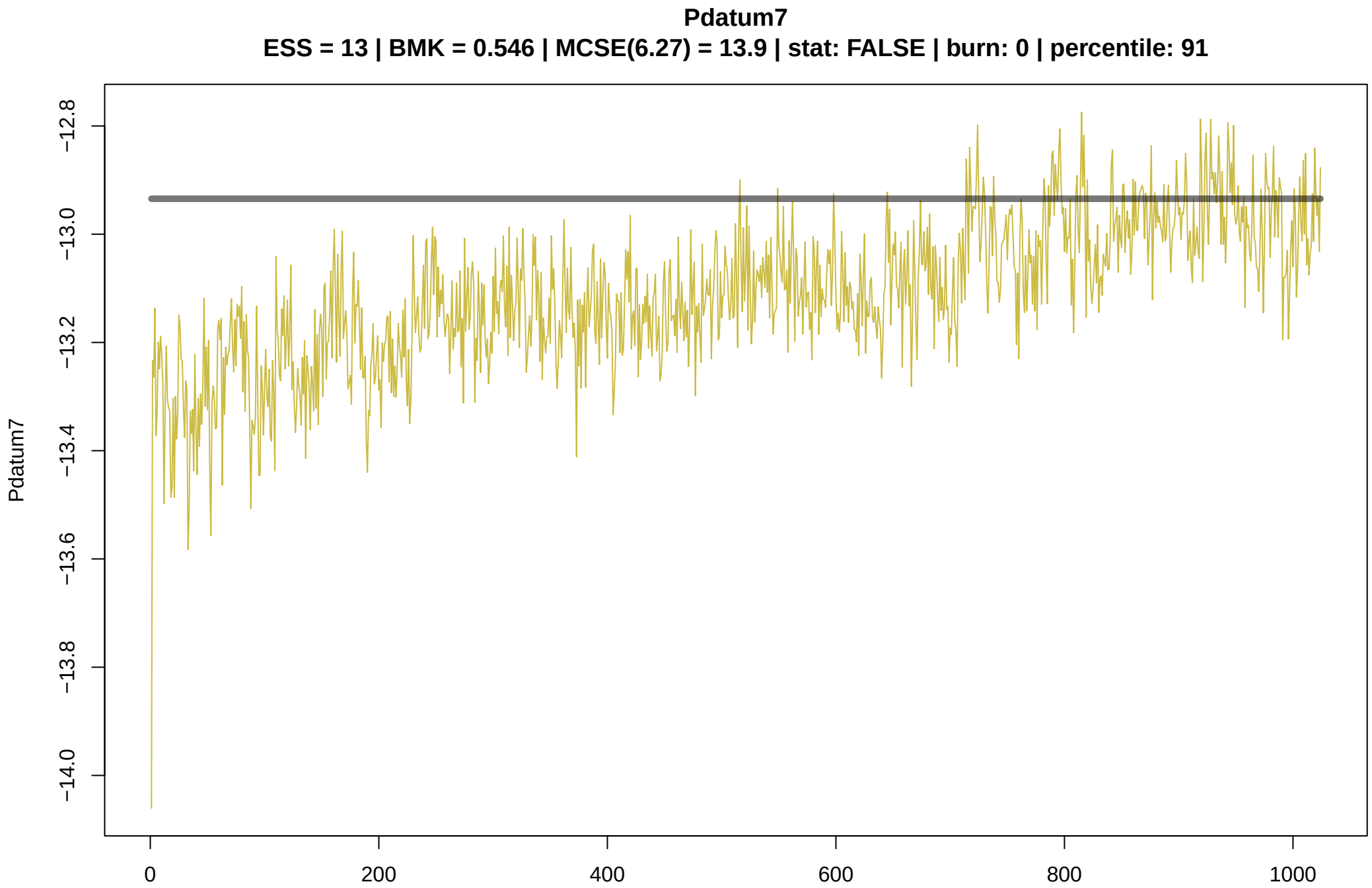

Pdatum2
ESS = 51 | BMK = 0.348 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 0 | percentile: 88.8
Pdatum2
−12.6
−12.8
−13.0
−13.2
−13.4
−13.6
−13.8
0
200
400
600
800
1000

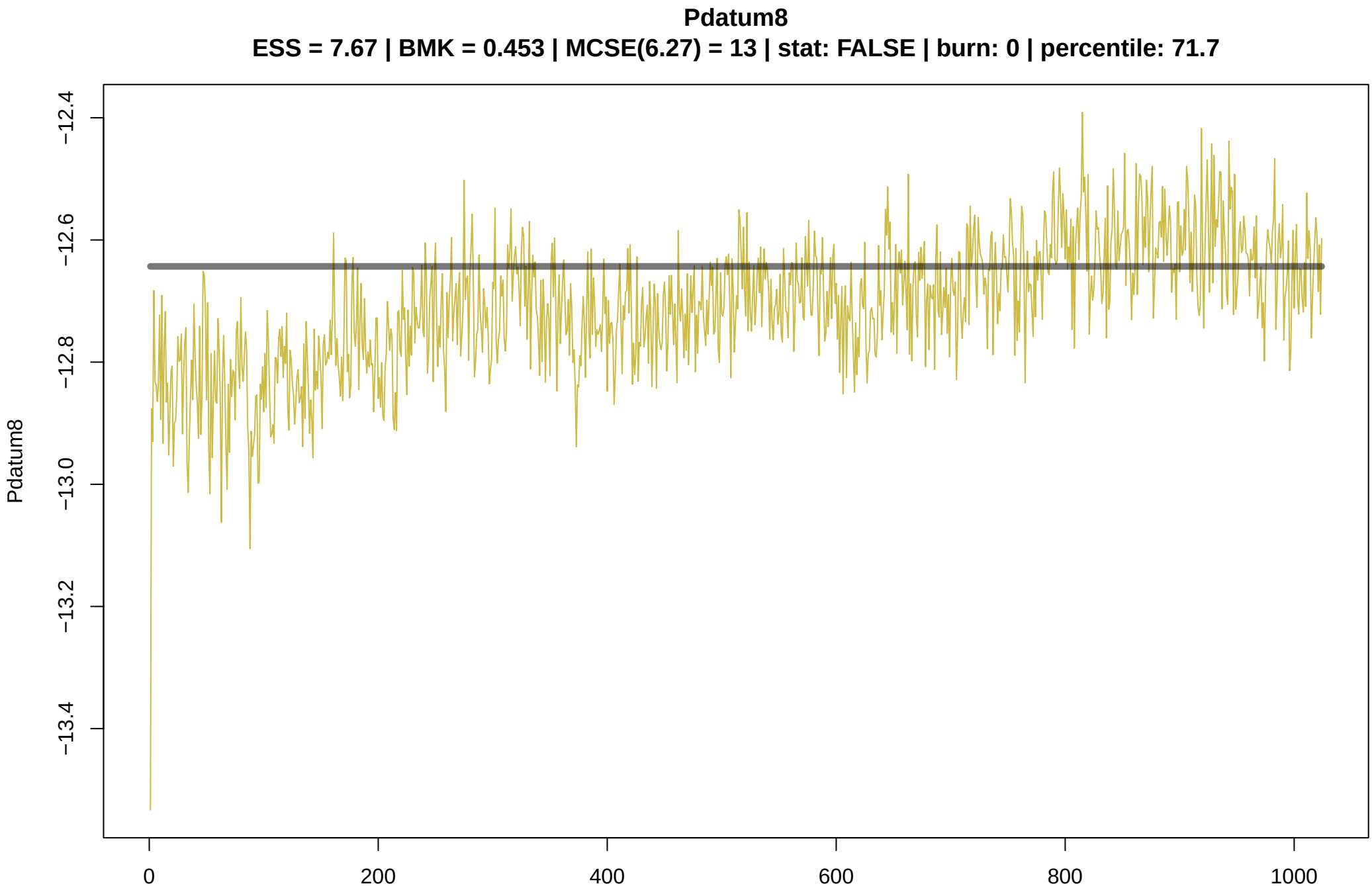

Pdatum3
ESS = 2.22e−16 | BMK = 0.183 | MCSE(6.27) = 6.79 | stat: TRUE | burn: 0 | percentile: 18.8
Pdatum3
−19.8
−20.0
−20.2
−20.4
−20.6
−20.8
−21.0
0
200
400
600
800
1000

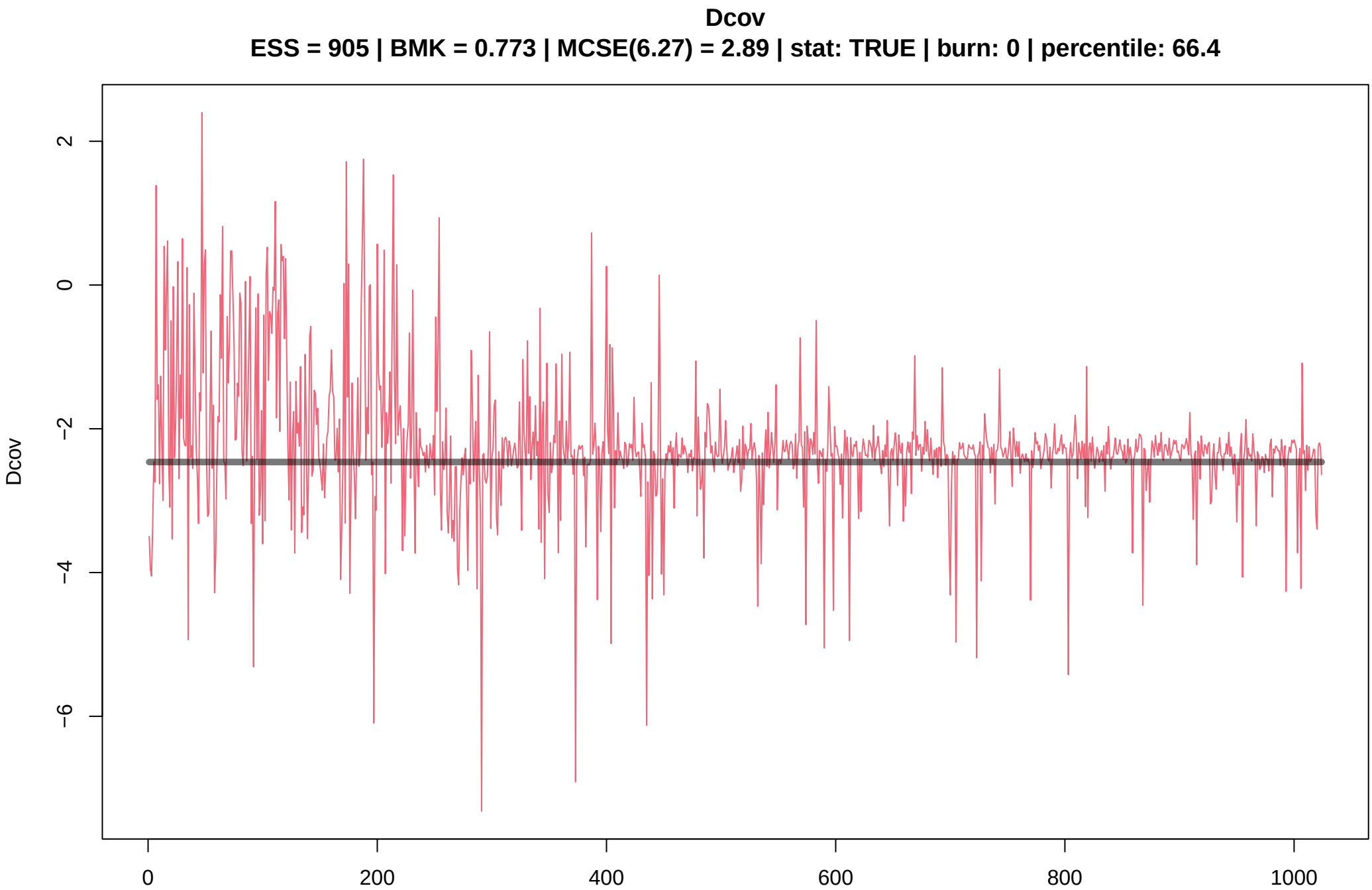

Pdatum4
ESS = 13.4 | BMK = 0.307 | MCSE(6.27) = 10.1 | stat: FALSE | burn: 0 | percentile: 99
Pdatum4
−13.8
−14.0
−14.2
−14.4
0
200
400
600
800
1000

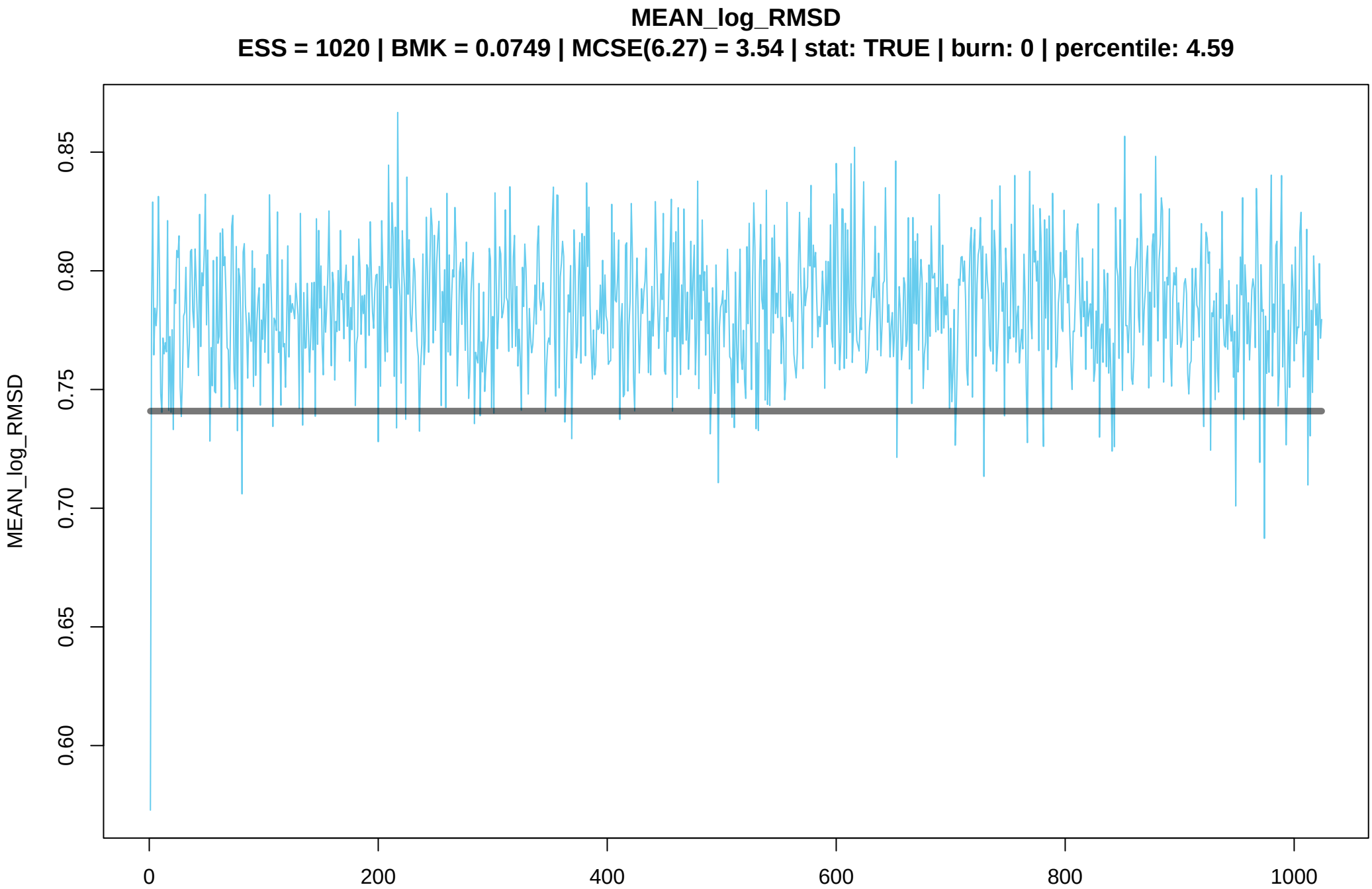

Pdatum5
ESS = 16.7 | BMK = 0.303 | MCSE(6.27) = 9.91 | stat: FALSE | burn: 0 | percentile: 98.5
Pdatum5
−12.5
−13.0
−13.5
−14.0
0
200
400
600
800
1000

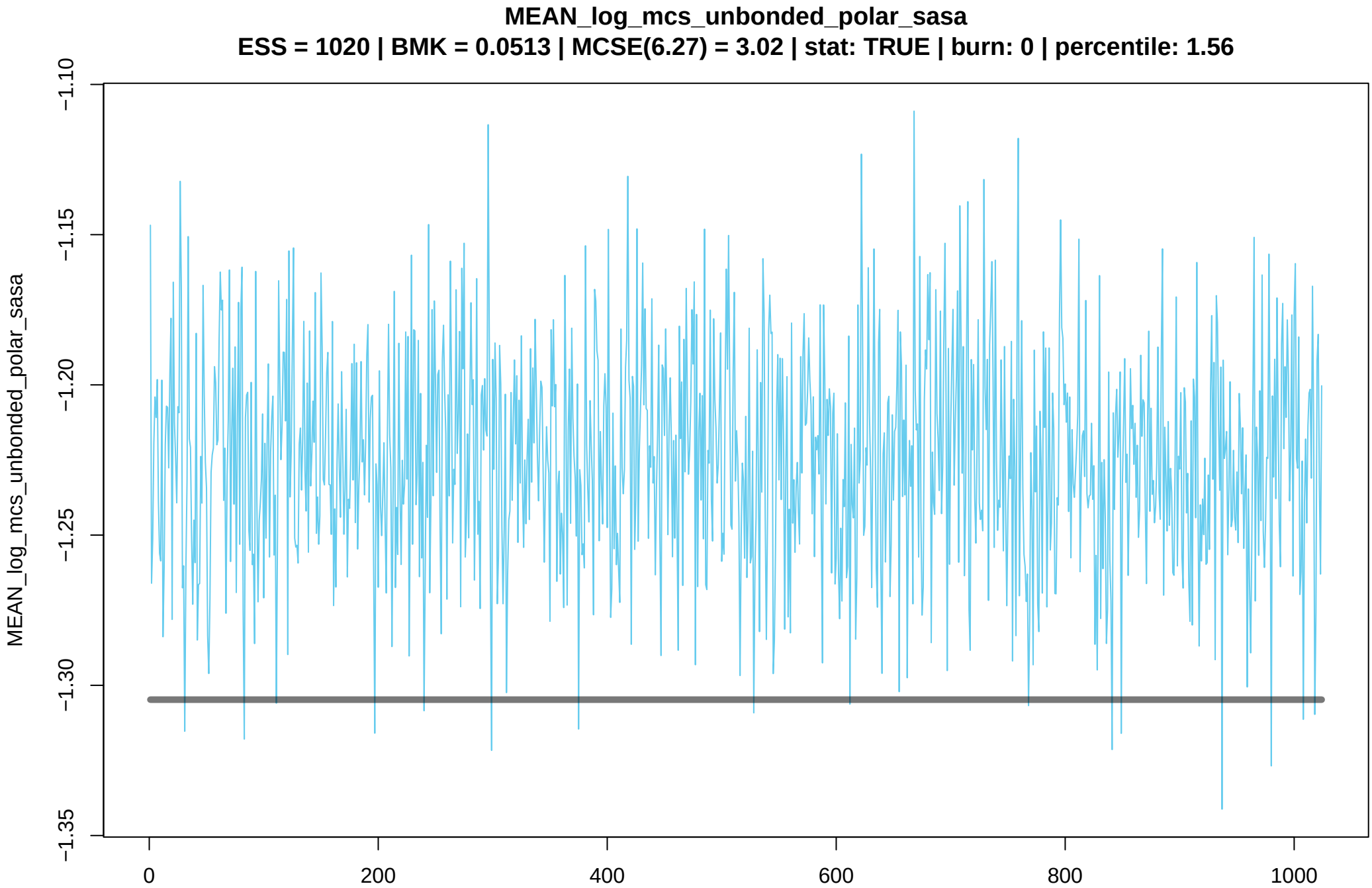

Pdatum6
ESS = 202 | BMK = 0.151 | MCSE(6.27) = 6.39 | stat: TRUE | burn: 0 | percentile: 96.5
Pdatum6
−14.8
−15.0
−15.2
−15.4
−15.6
−15.8
0
200
400
600
800
1000

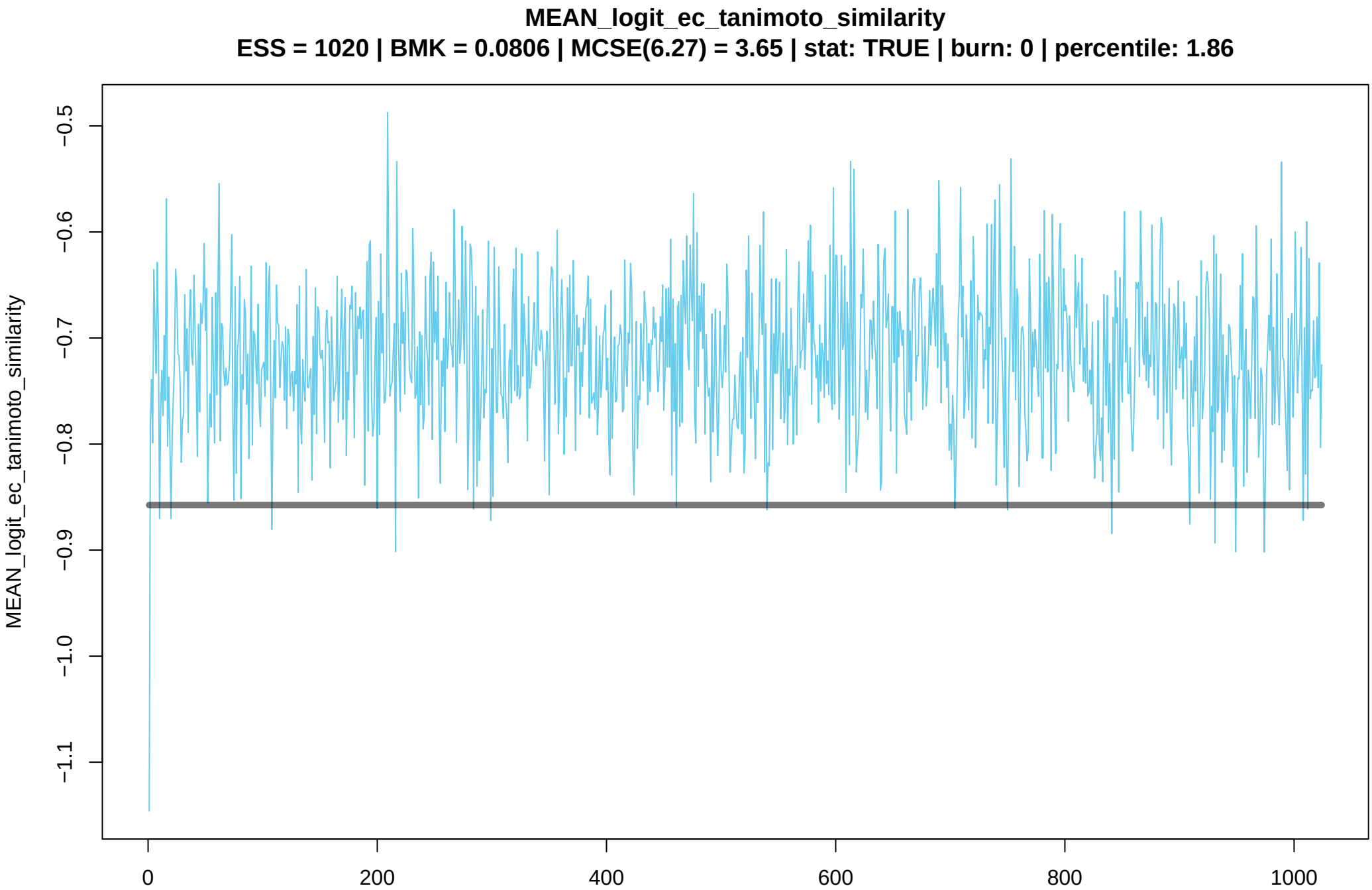

Pdatum7
ESS = 13 | BMK = 0.546 | MCSE(6.27) = 13.9 | stat: FALSE | burn: 0 | percentile: 91
Pdatum7
−12.8
−13.0
−13.2
−13.4
−13.6
−13.8
−14.0
0
200
400
600
800
1000

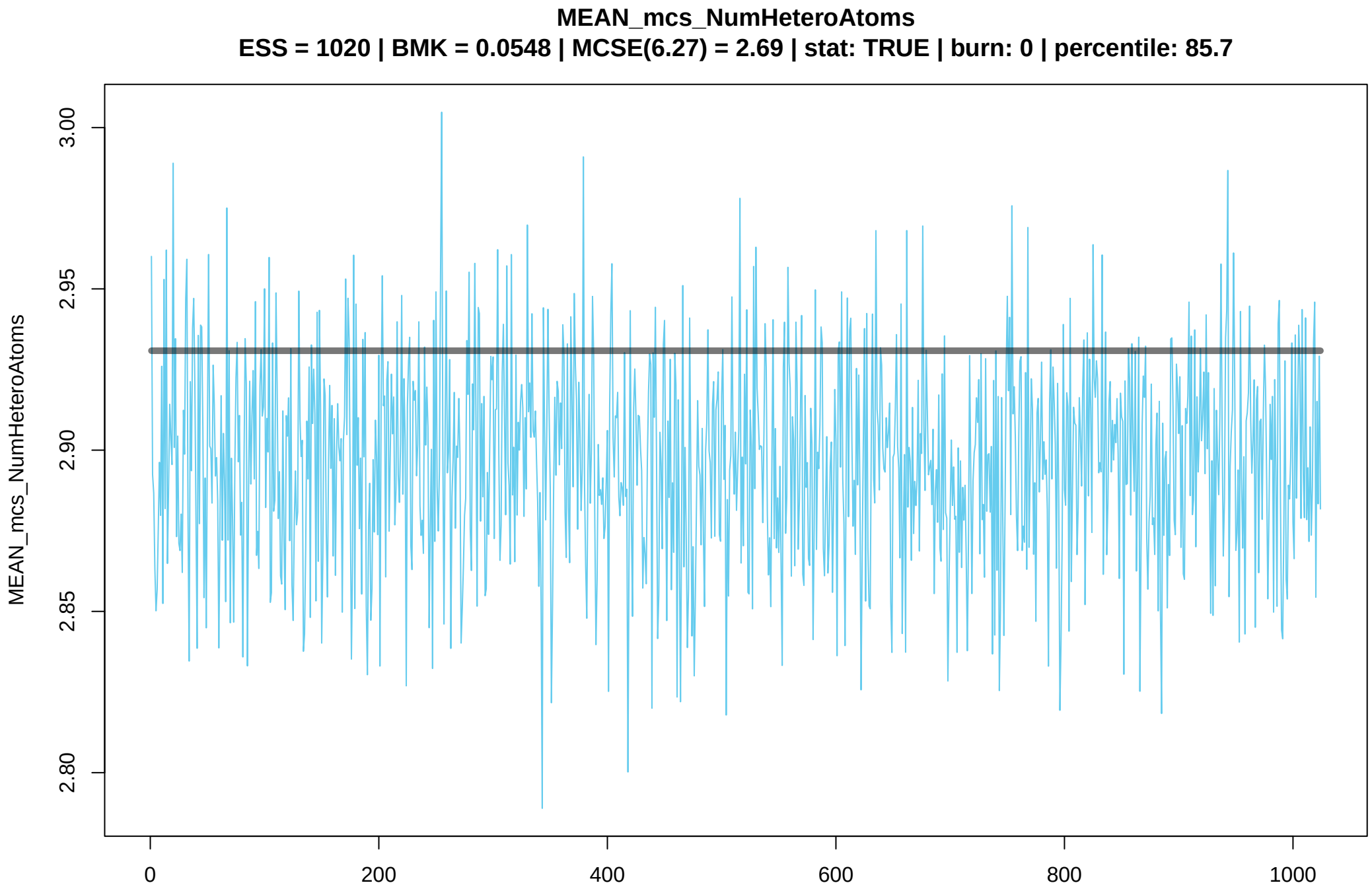

Pdatum8
ESS = 7.67 | BMK = 0.453 | MCSE(6.27) = 13 | stat: FALSE | burn: 0 | percentile: 71.7
Pdatum8
−12.4
−12.6
−12.8
−13.0
−13.2
−13.4
0
200
400
600
800
1000

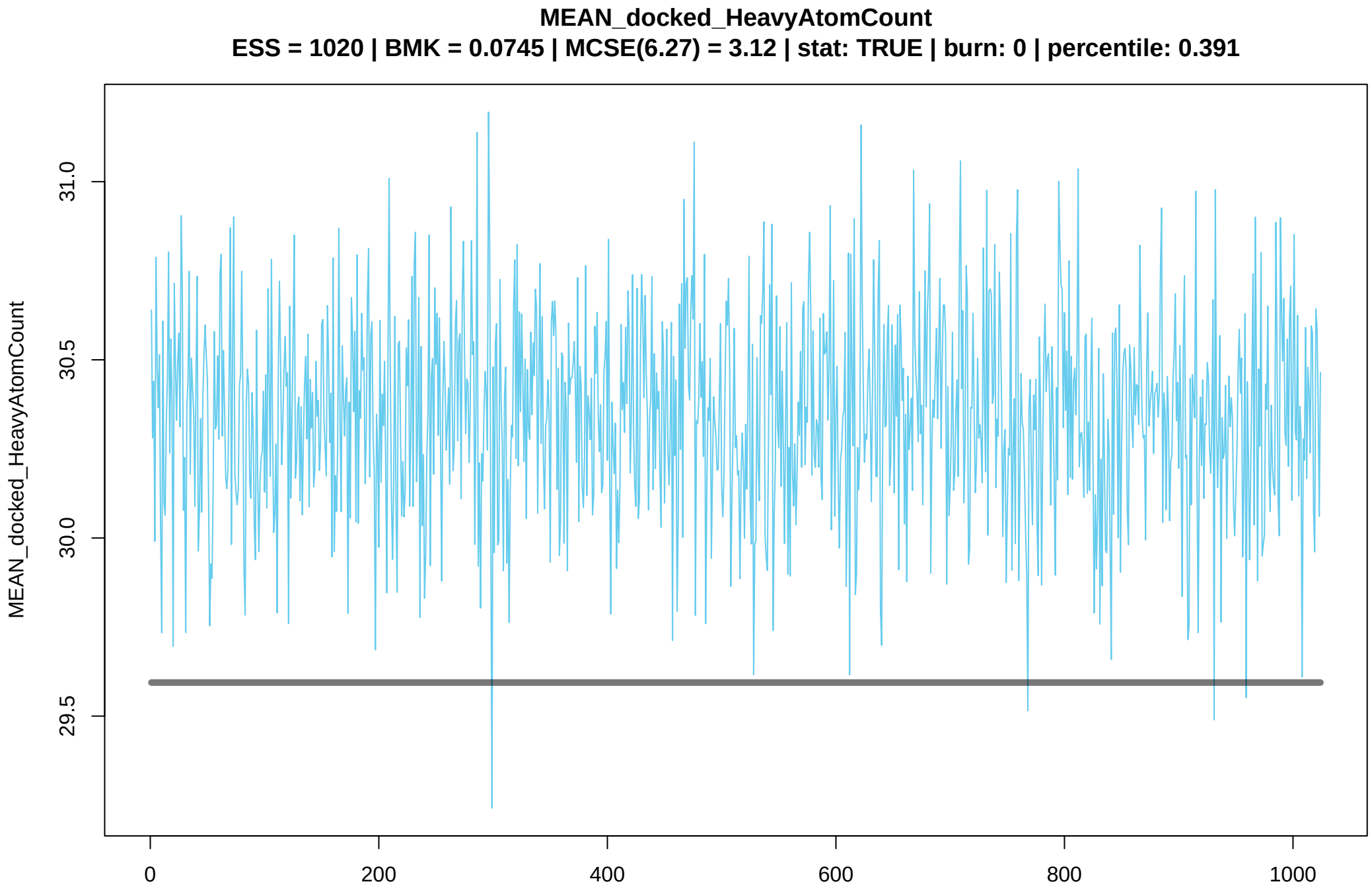

Dcov
ESS = 905 | BMK = 0.773 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | percentile: 66.4
Dcov
2
0
−2
−4
−6
0
200
400
600
800
1000

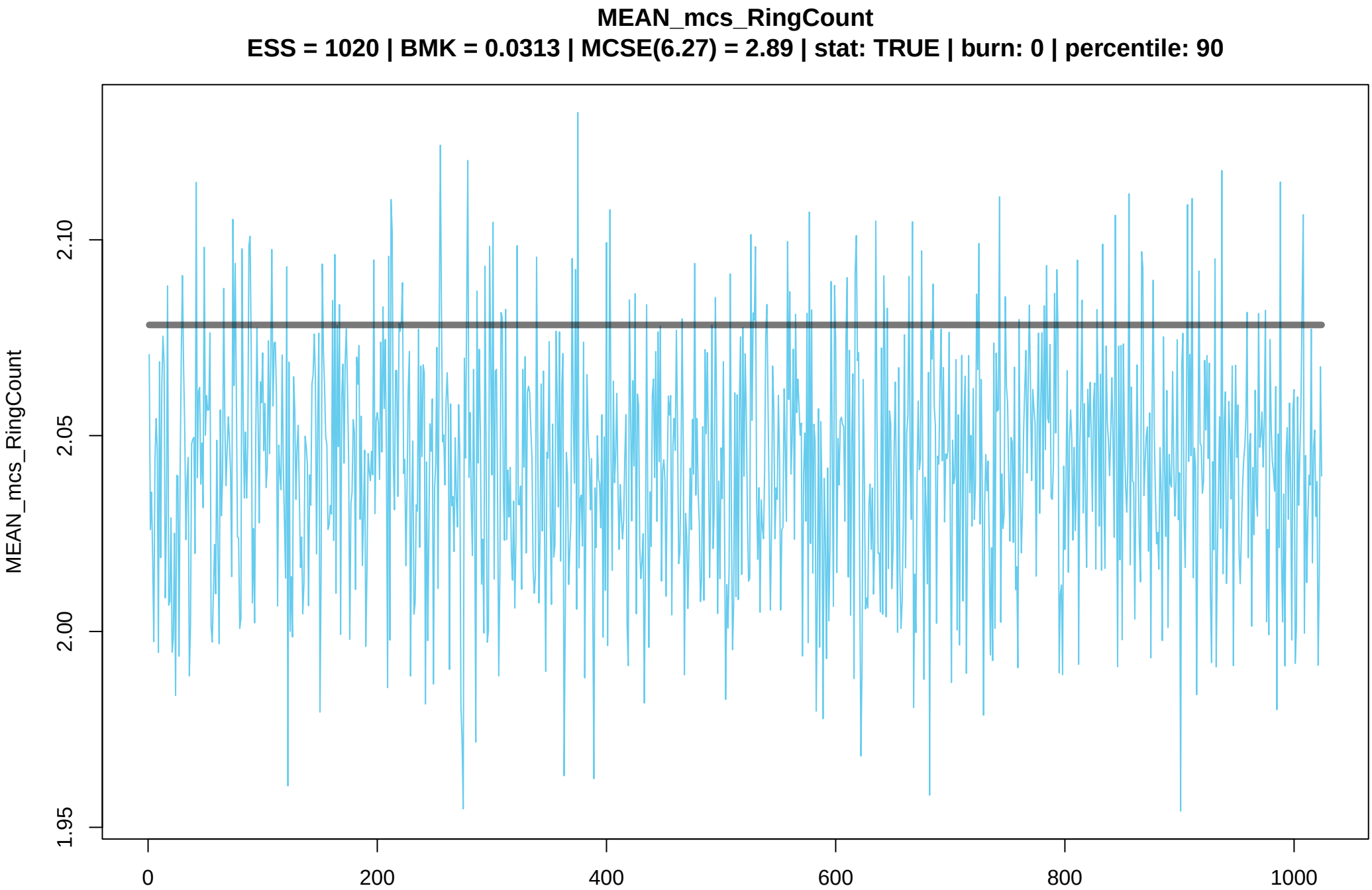

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0749 | MCSE(6.27) = 3.54 | stat: TRUE | burn: 0 | percentile: 4.59
MEAN_log_RMSD
0.60
0.65
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

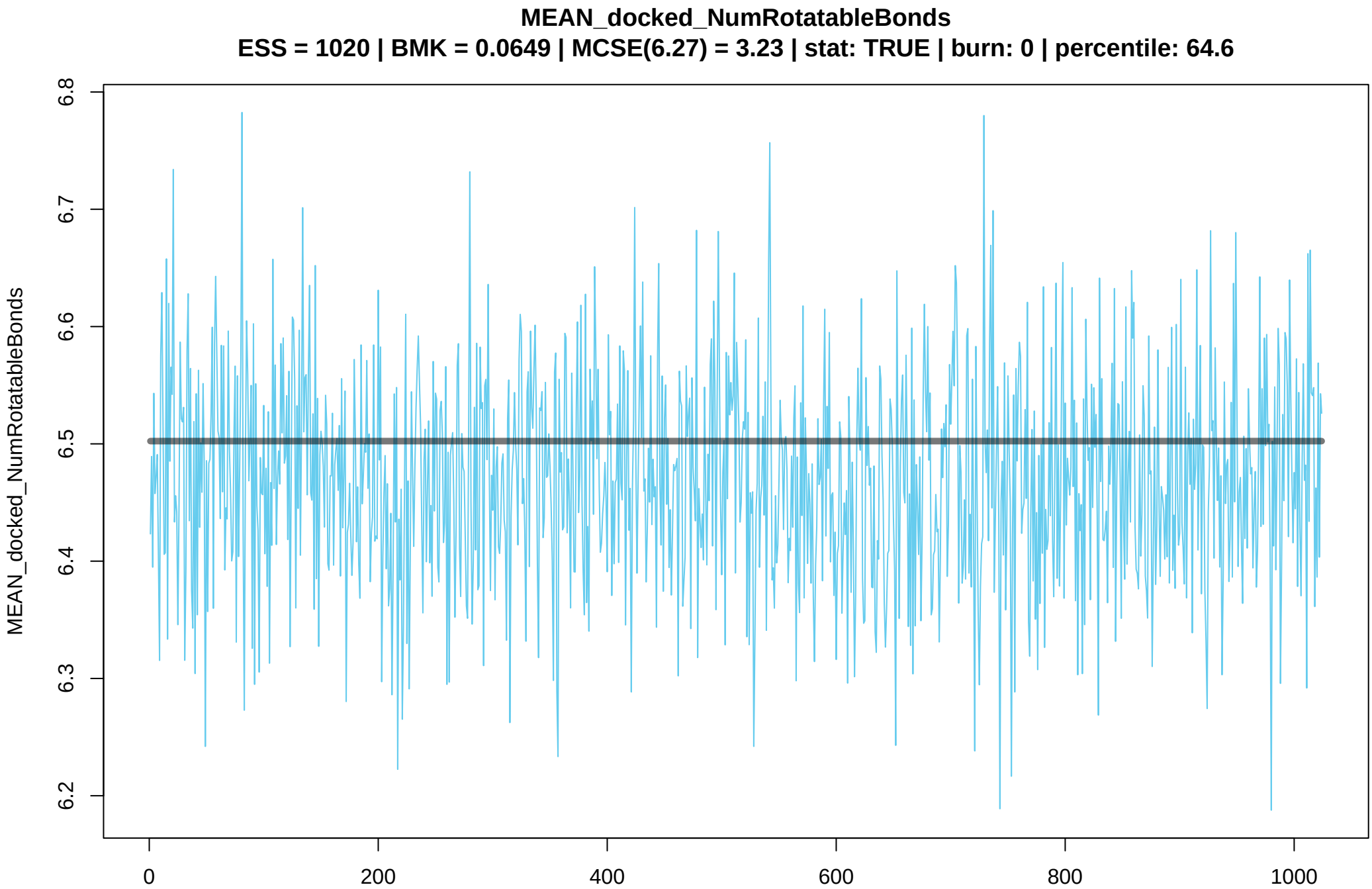

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0513 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | percentile: 1.56
MEAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

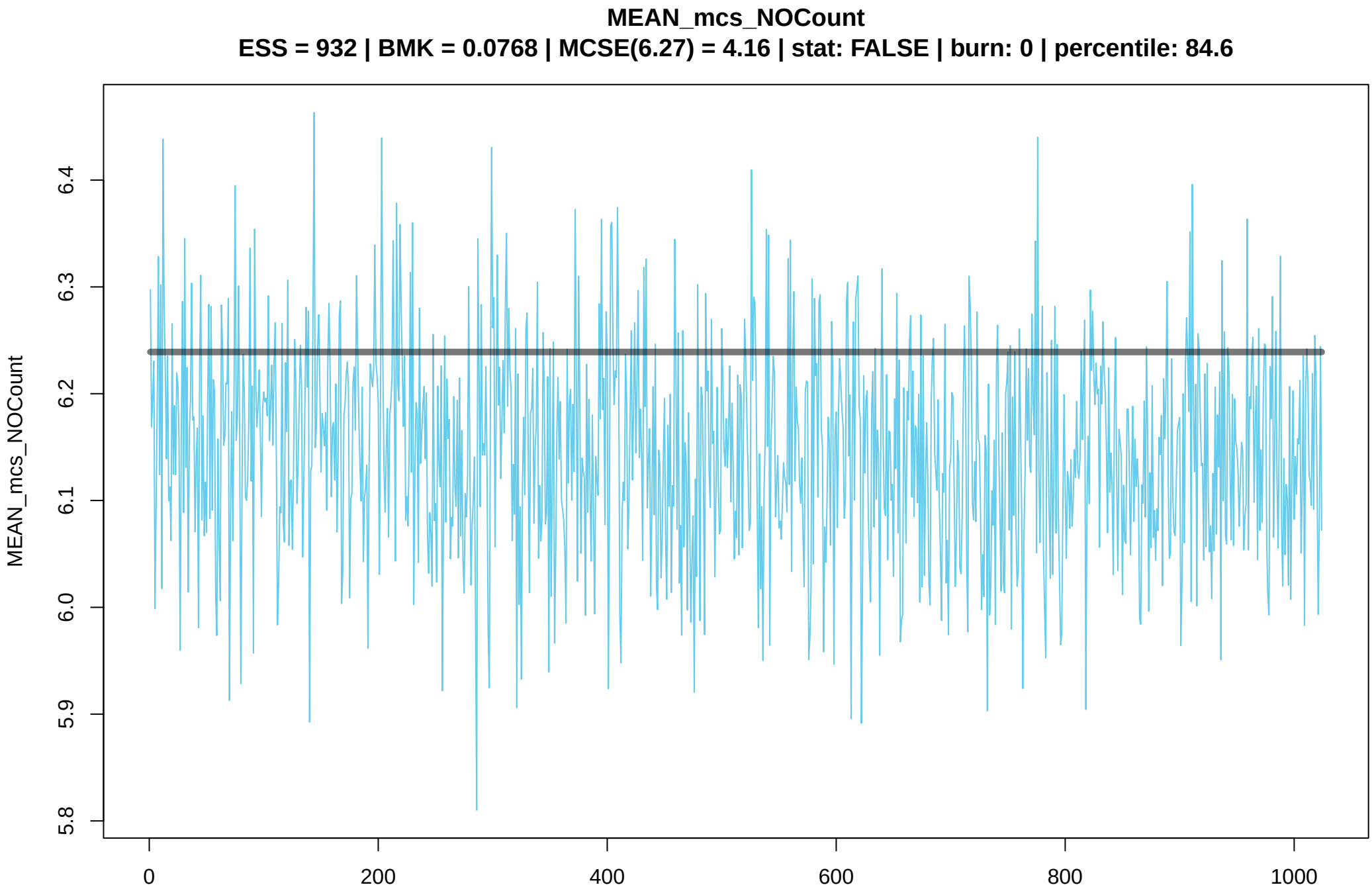

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0806 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0 | percentile: 1.86
MEAN_logit_ec_tanimoto_similarity
−0.5
−0.6
−0.7
−0.8
−0.9
−1.0
−1.1
0
200
400
600
800
1000

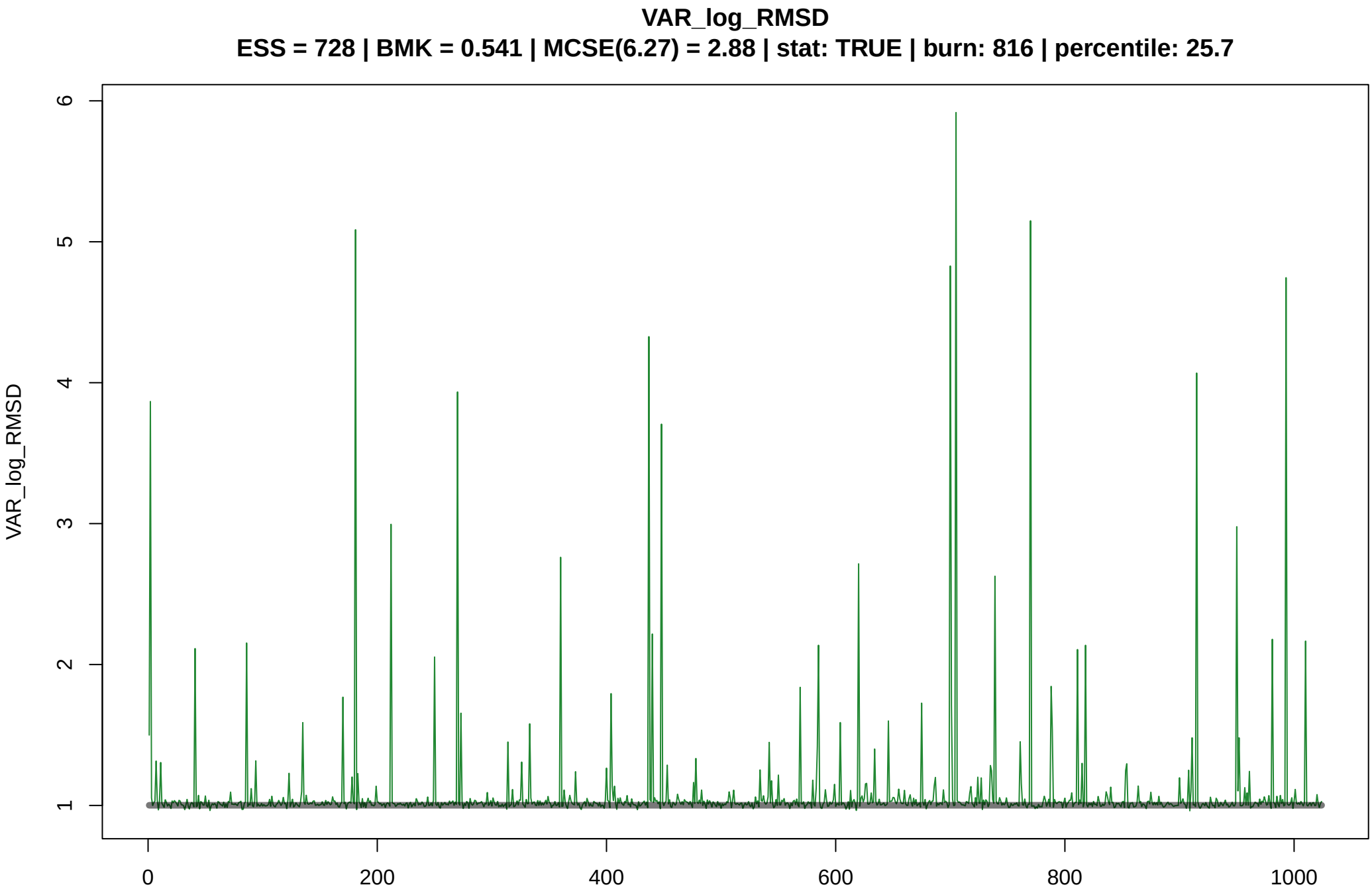

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0548 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | percentile: 85.7
MEAN_mcs_NumHeteroAtoms
3.00
2.95
2.90
2.85
2.80
0
200
400
600
800
1000

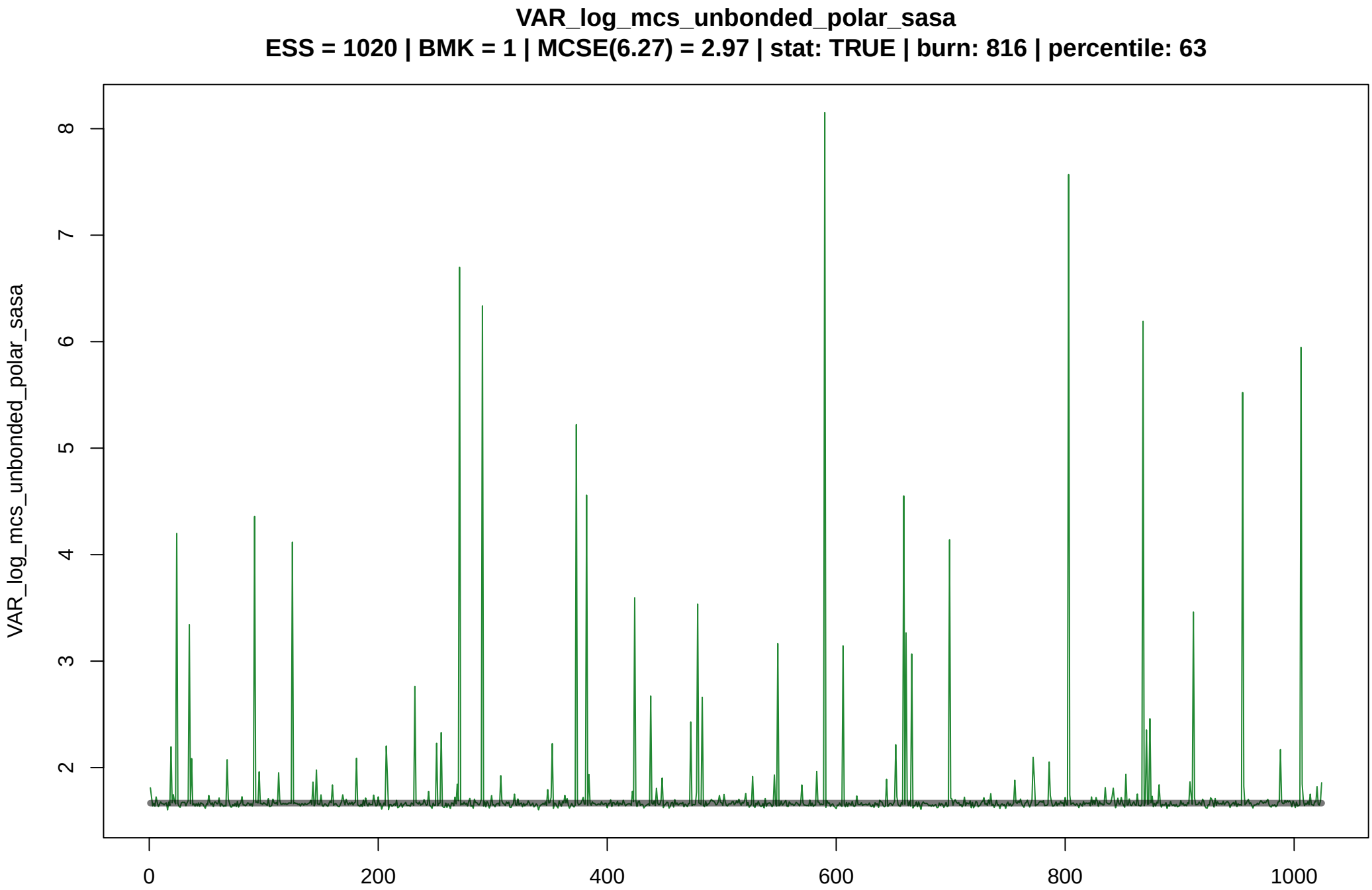

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0745 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | percentile: 0.391
MEAN_docked_HeavyAtomCount
31.0
30.5
30.0
29.5
0
200
400
600
800
1000

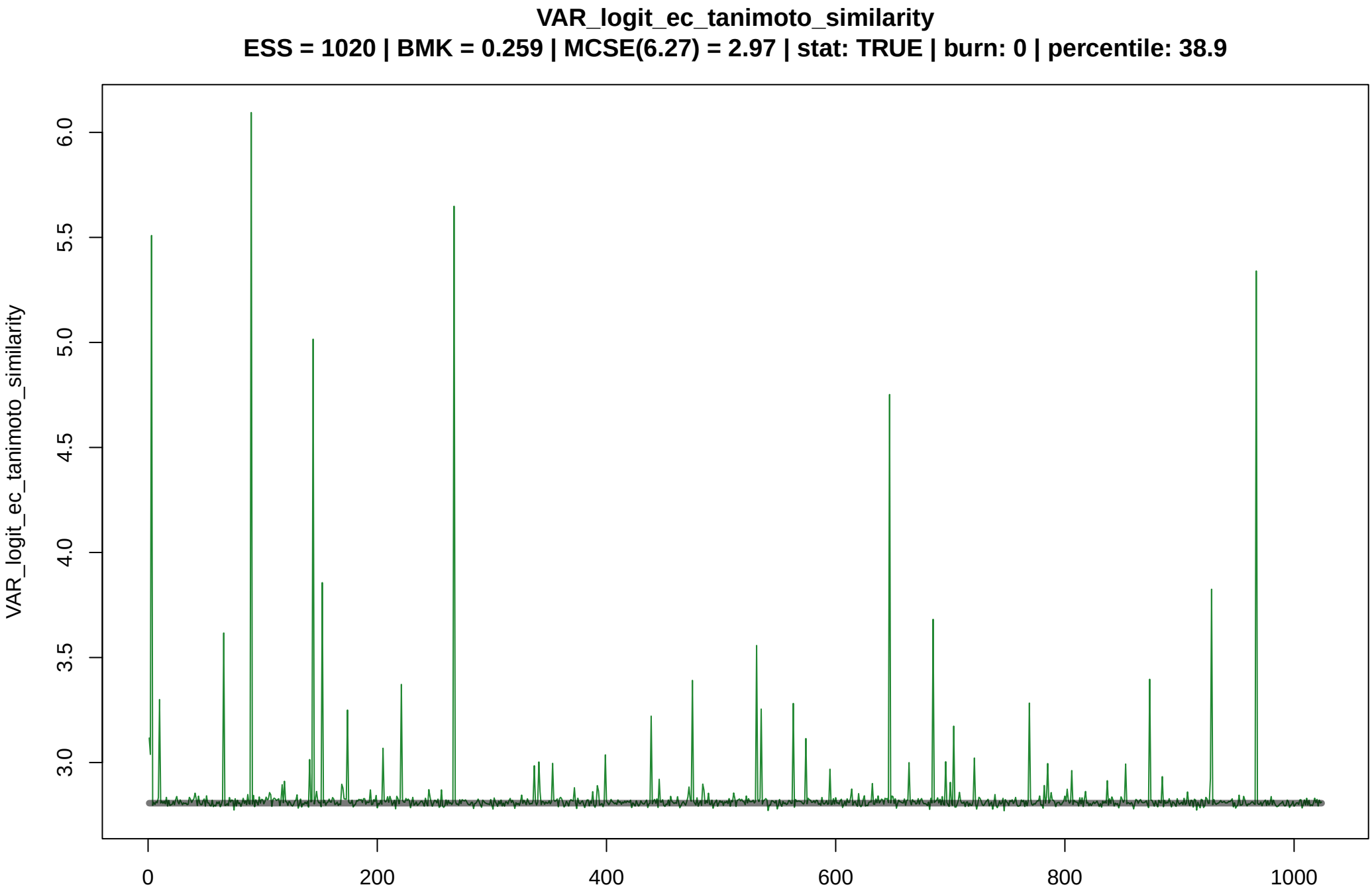

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0313 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | percentile: 90
MEAN_mcs_RingCount
1.95
2.00
2.05
2.10
0
200
400
600
800
1000

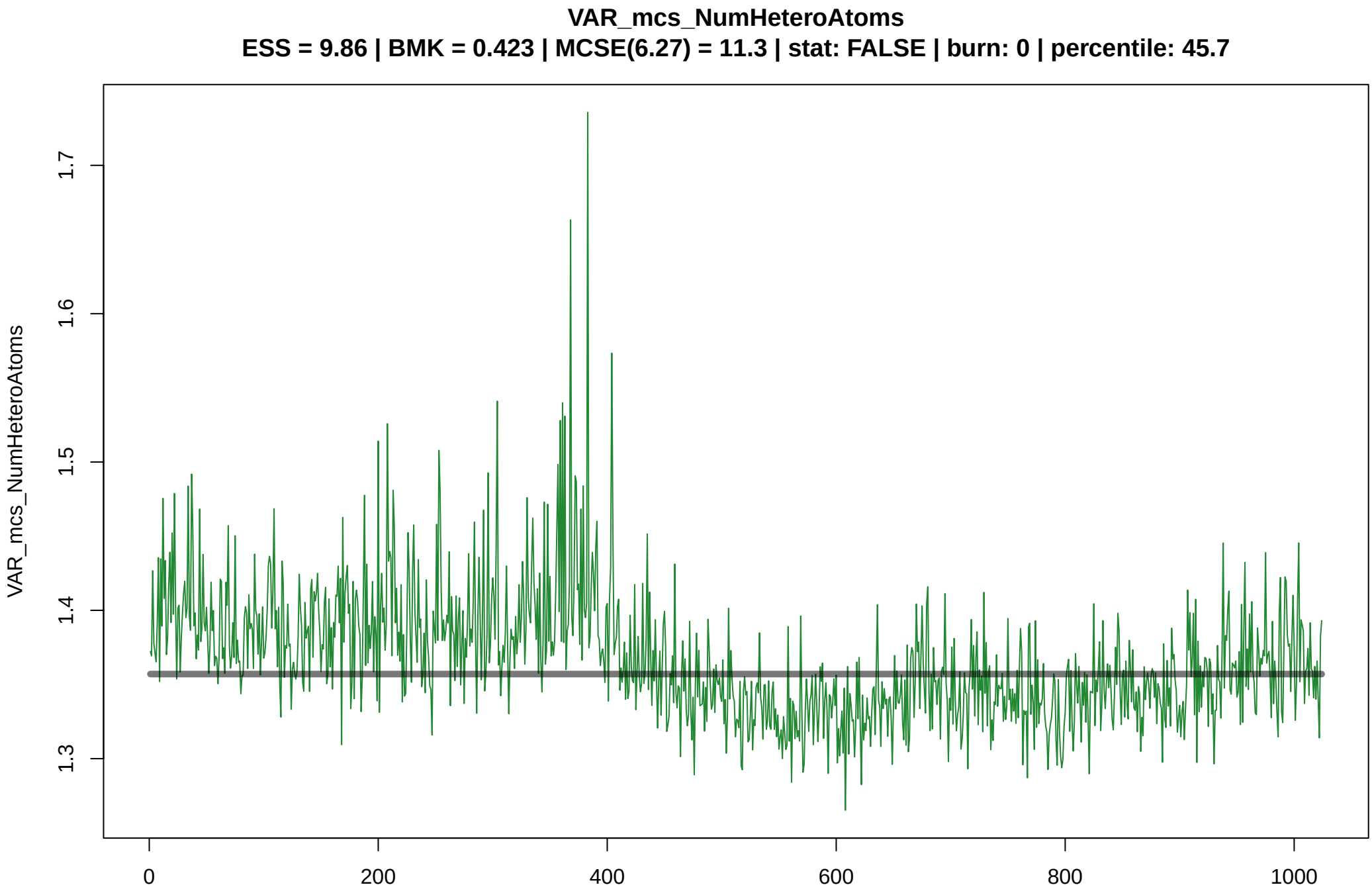

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0649 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | percentile: 64.6
MEAN_docked_NumRotatableBonds
6.8
6.7
6.6
6.5
6.4
6.3
6.2
0
200
400
600
800
1000

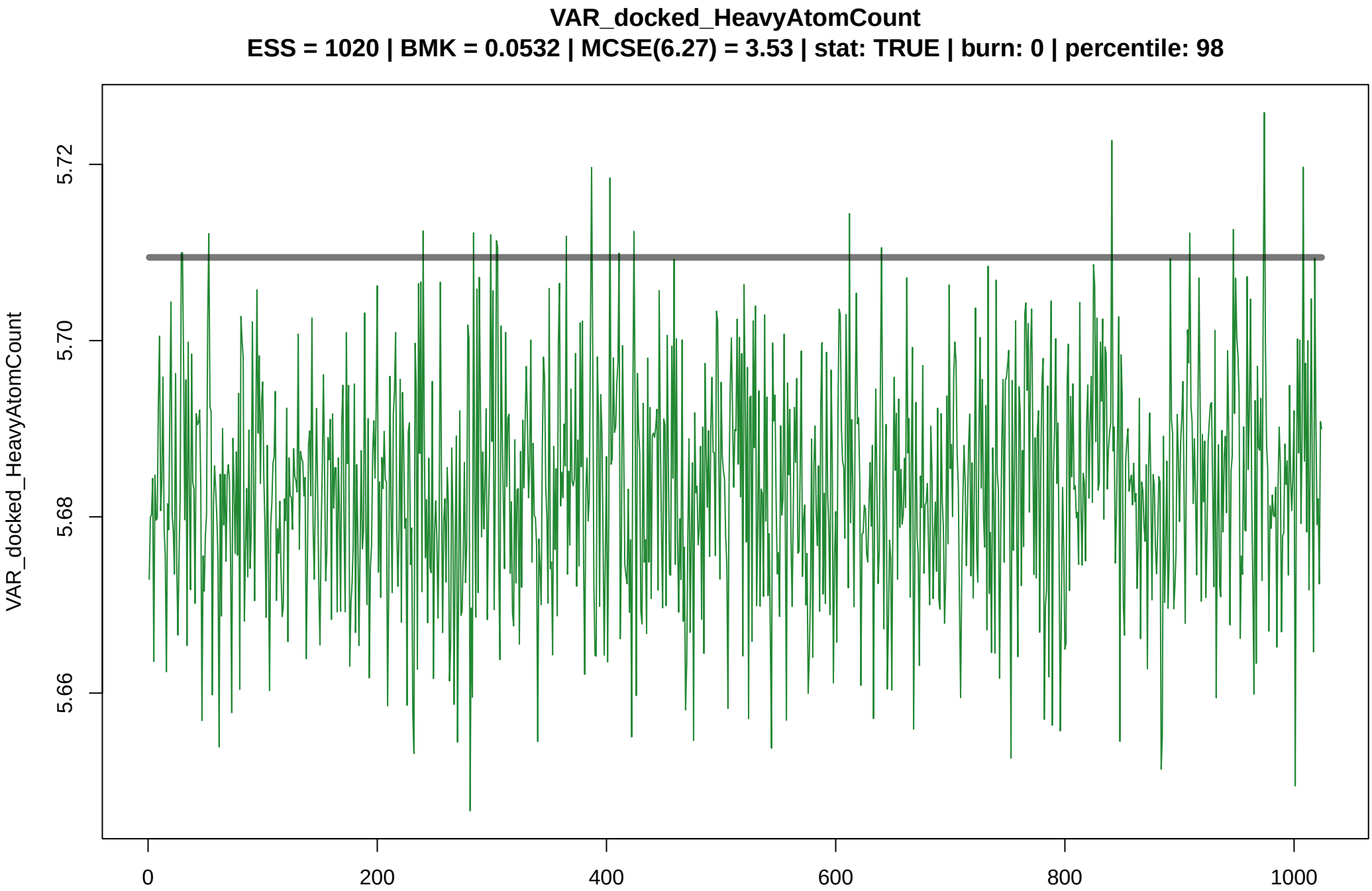

MEAN_mcs_NOCount
ESS = 932 | BMK = 0.0768 | MCSE(6.27) = 4.16 | stat: FALSE | burn: 0 | percentile: 84.6
MEAN_mcs_NOCount
5.8
5.9
6.0
6.1
6.2
6.3
6.4
0
200
400
600
800
1000

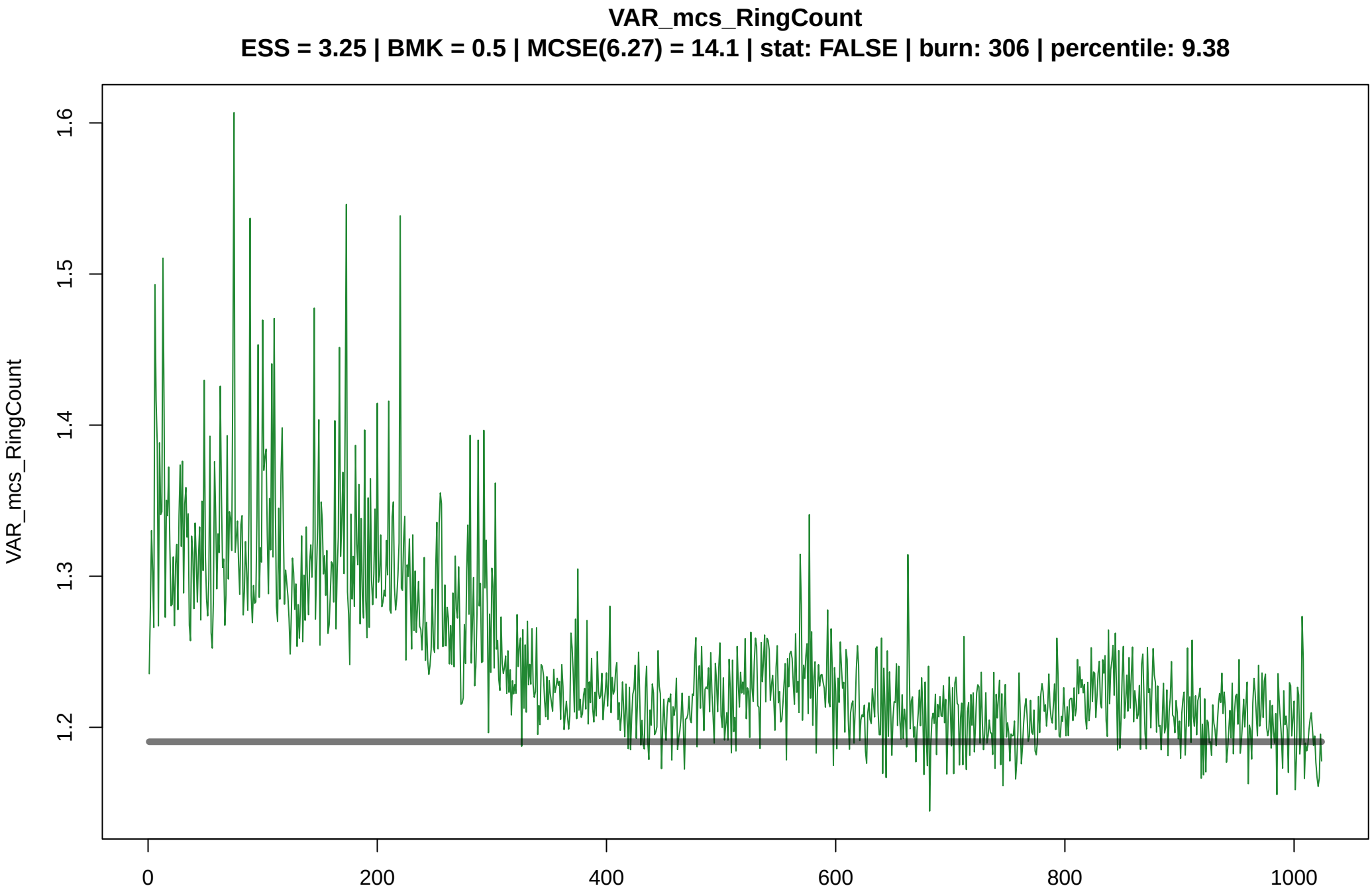

VAR_log_RMSD
ESS = 728 | BMK = 0.541 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 816 | percentile: 25.7
VAR_log_RMSD
1
2
3
4
5
6
0
200
400
600
800
1000

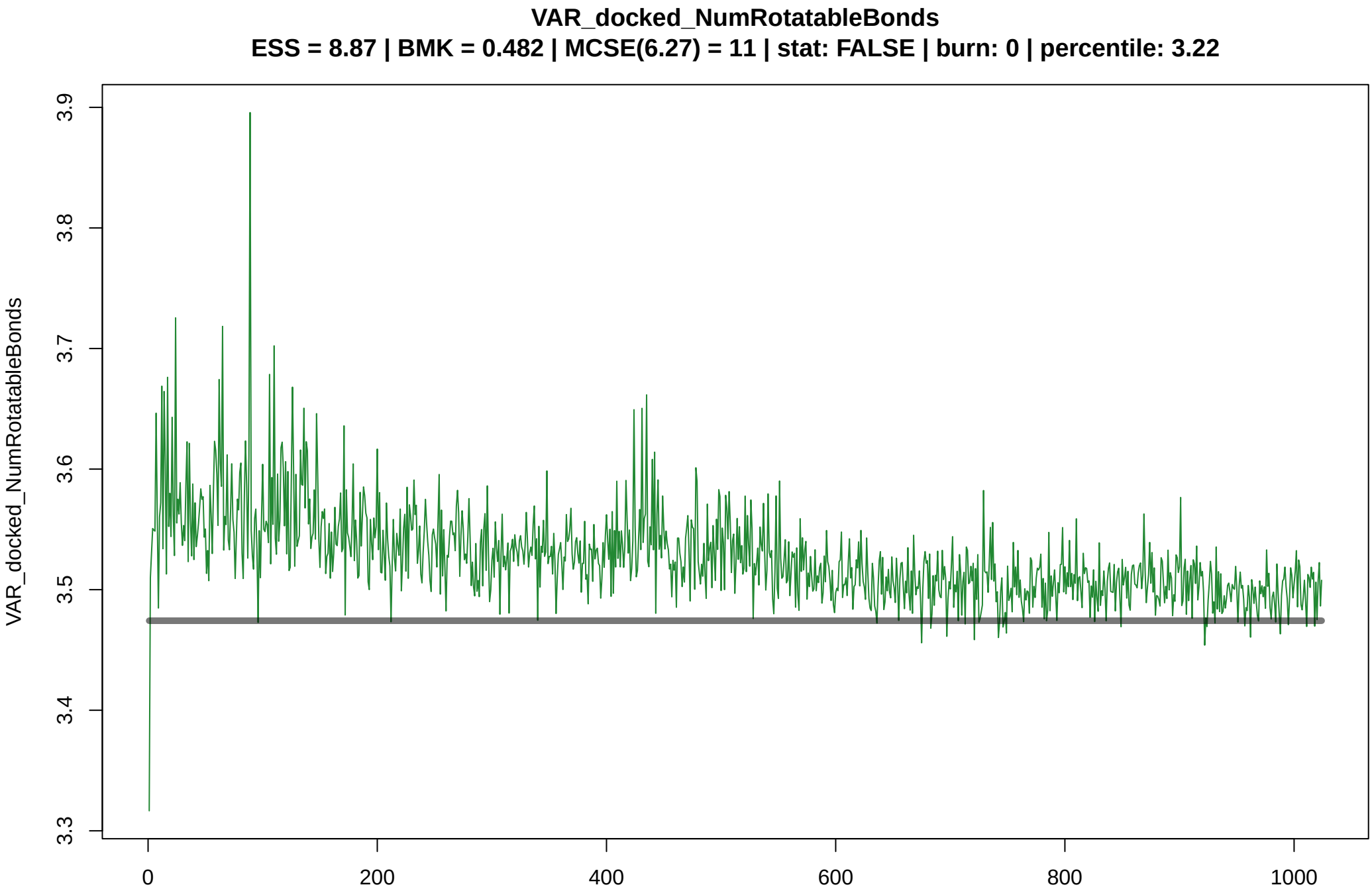

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 1 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 816 | percentile: 63
VAR_log_mcs_unbonded_polar_sasa
2
3
4
5
6
7
8
0
200
400
600
800
1000

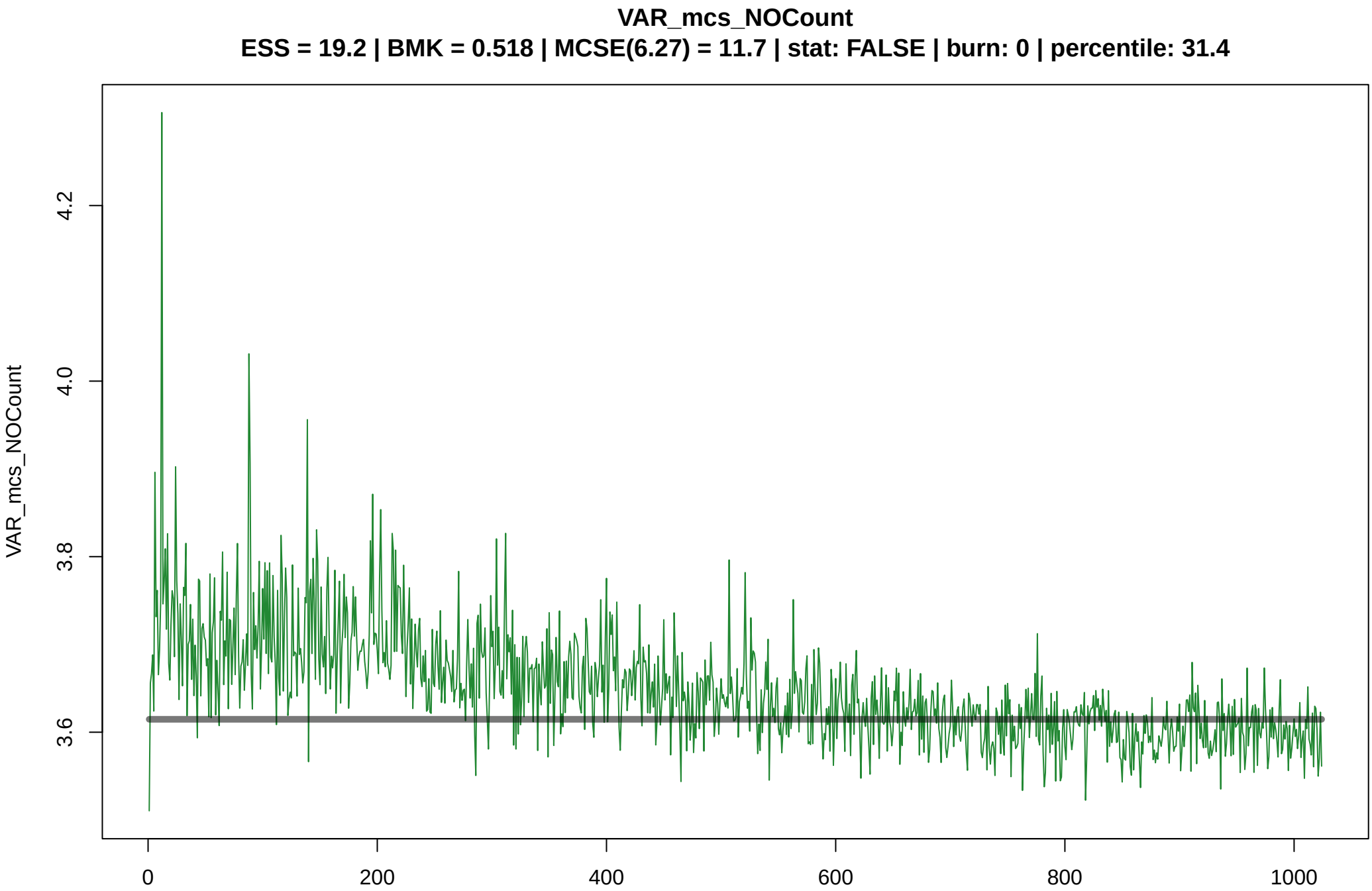

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.259 | MCSE(6.27) = 2.97 | stat: TRUE | burn: 0 | percentile: 38.9
VAR_logit_ec_tanimoto_similarity
3.0
3.5
4.0
4.5
5.0
5.5
6.0
0
200
400
600
800
1000

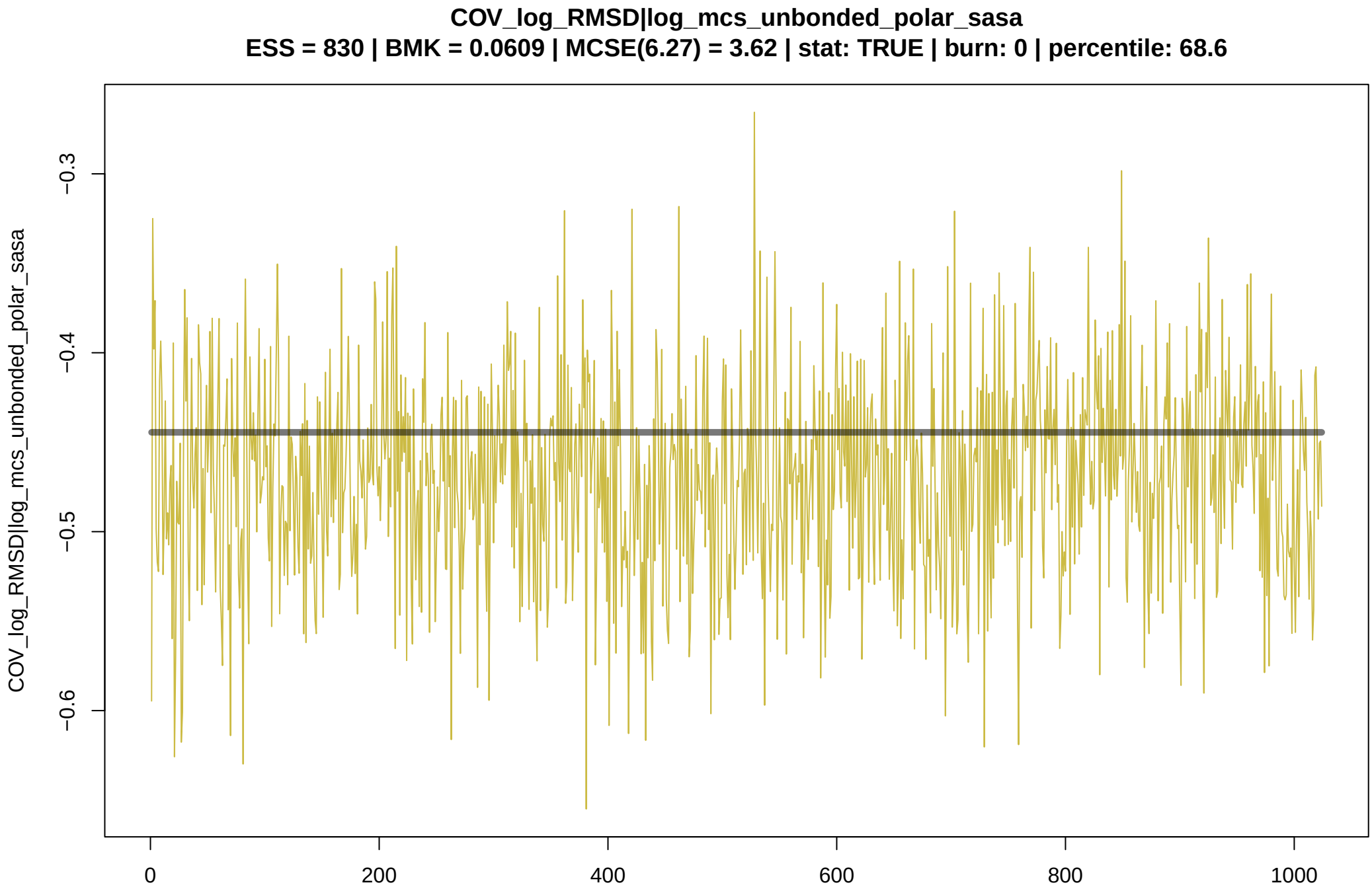

VAR_mcs_NumHeteroAtoms
ESS = 9.86 | BMK = 0.423 | MCSE(6.27) = 11.3 | stat: FALSE | burn: 0 | percentile: 45.7
VAR_mcs_NumHeteroAtoms
1.3
1.4
1.5
1.6
1.7
0
200
400
600
800
1000

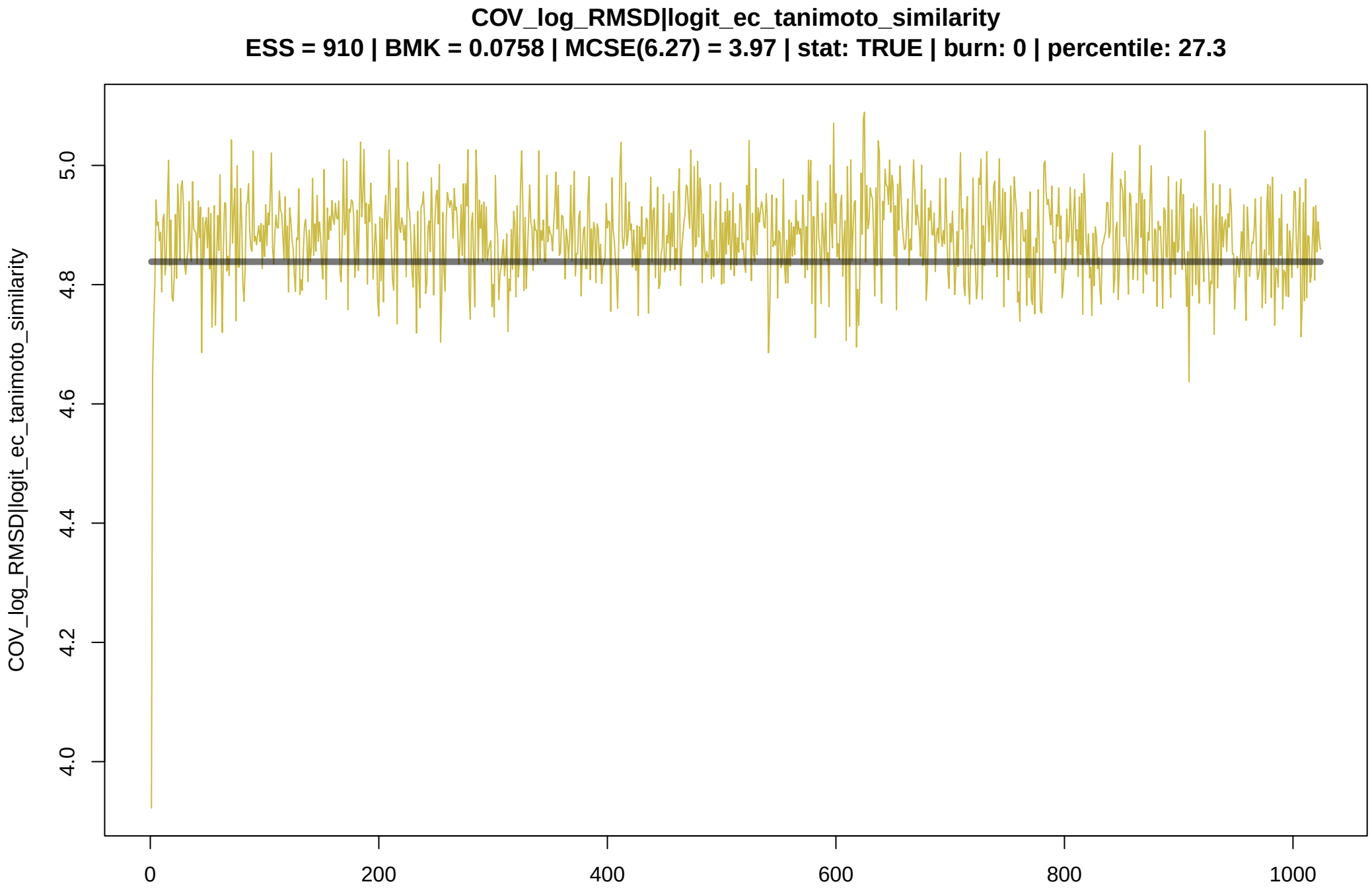

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0532 | MCSE(6.27) = 3.53 | stat: TRUE | burn: 0 | percentile: 98
VAR_docked_HeavyAtomCount
5.66
5.68
5.70
5.72
0
200
400
600
800
1000

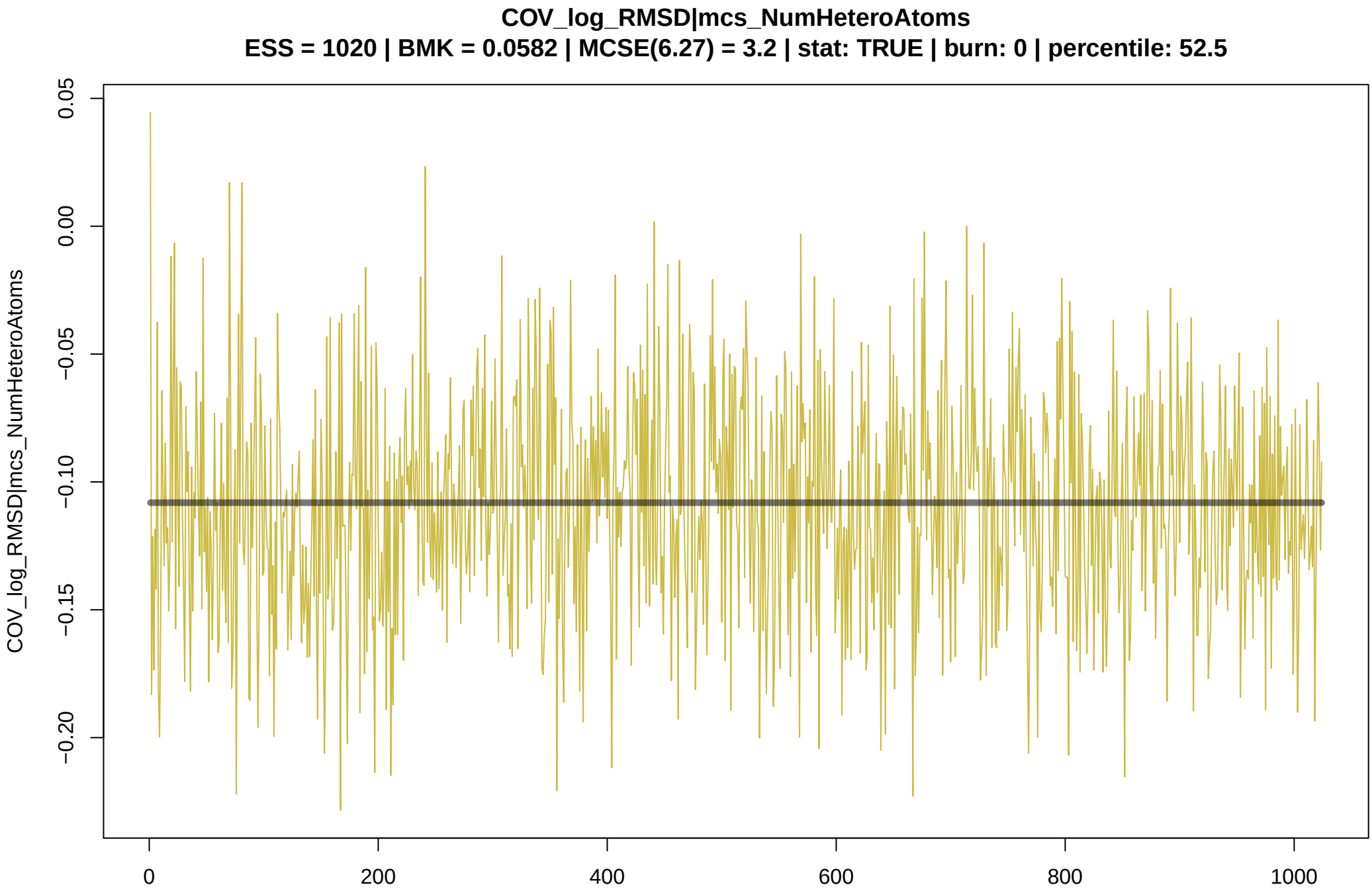

VAR_mcs_RingCount
ESS = 3.25 | BMK = 0.5 | MCSE(6.27) = 14.1 | stat: FALSE | burn: 306 | percentile: 9.38
VAR_mcs_RingCount
1.2
1.3
1.4
1.5
1.6
0
200
400
600
800
1000

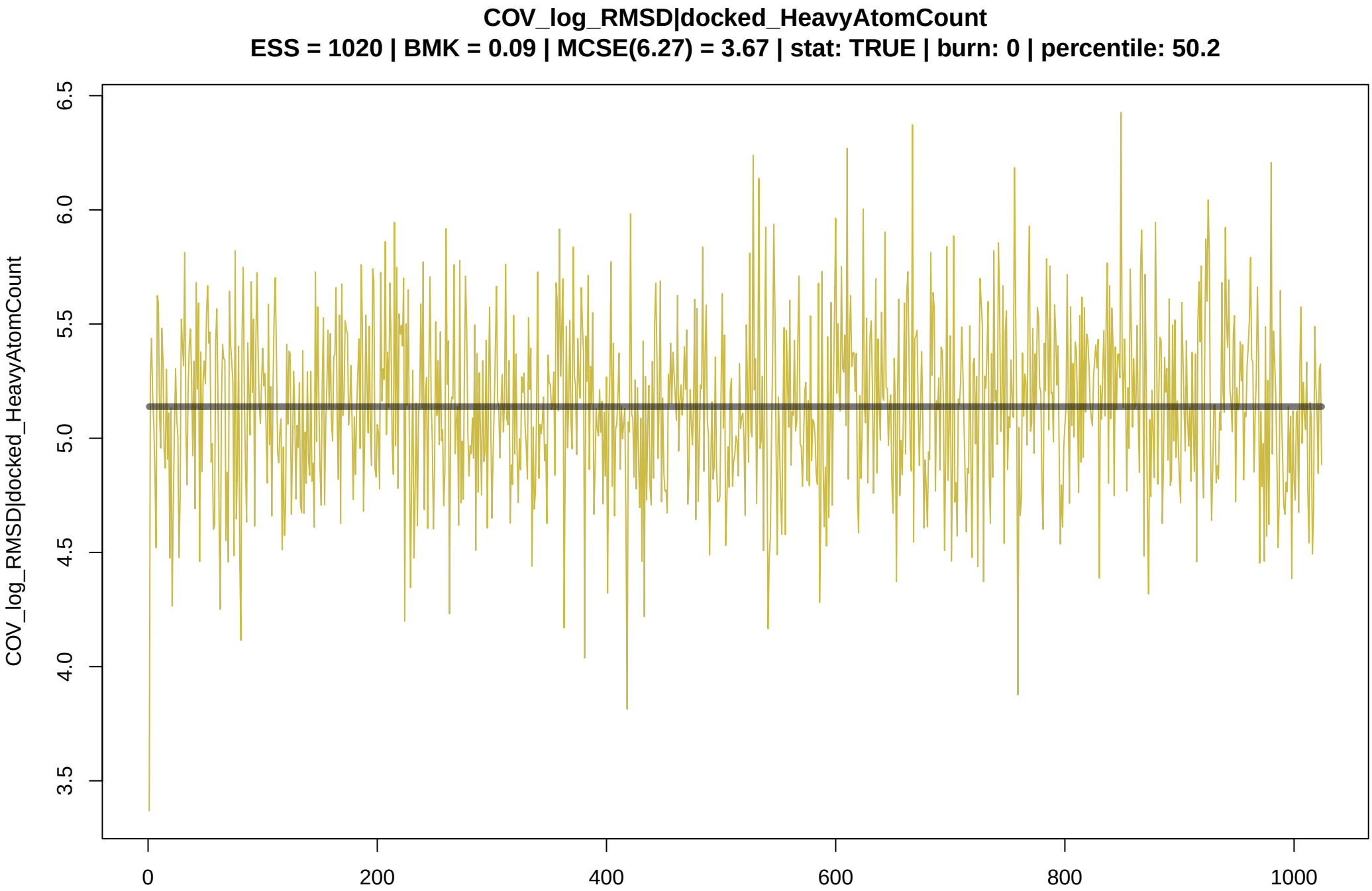

VAR_docked_NumRotatableBonds
ESS = 8.87 | BMK = 0.482 | MCSE(6.27) = 11 | stat: FALSE | burn: 0 | percentile: 3.22
VAR_docked_NumRotatableBonds
3.3
3.4
3.5
3.6
3.7
3.8
3.9
0
200
400
600
800
1000

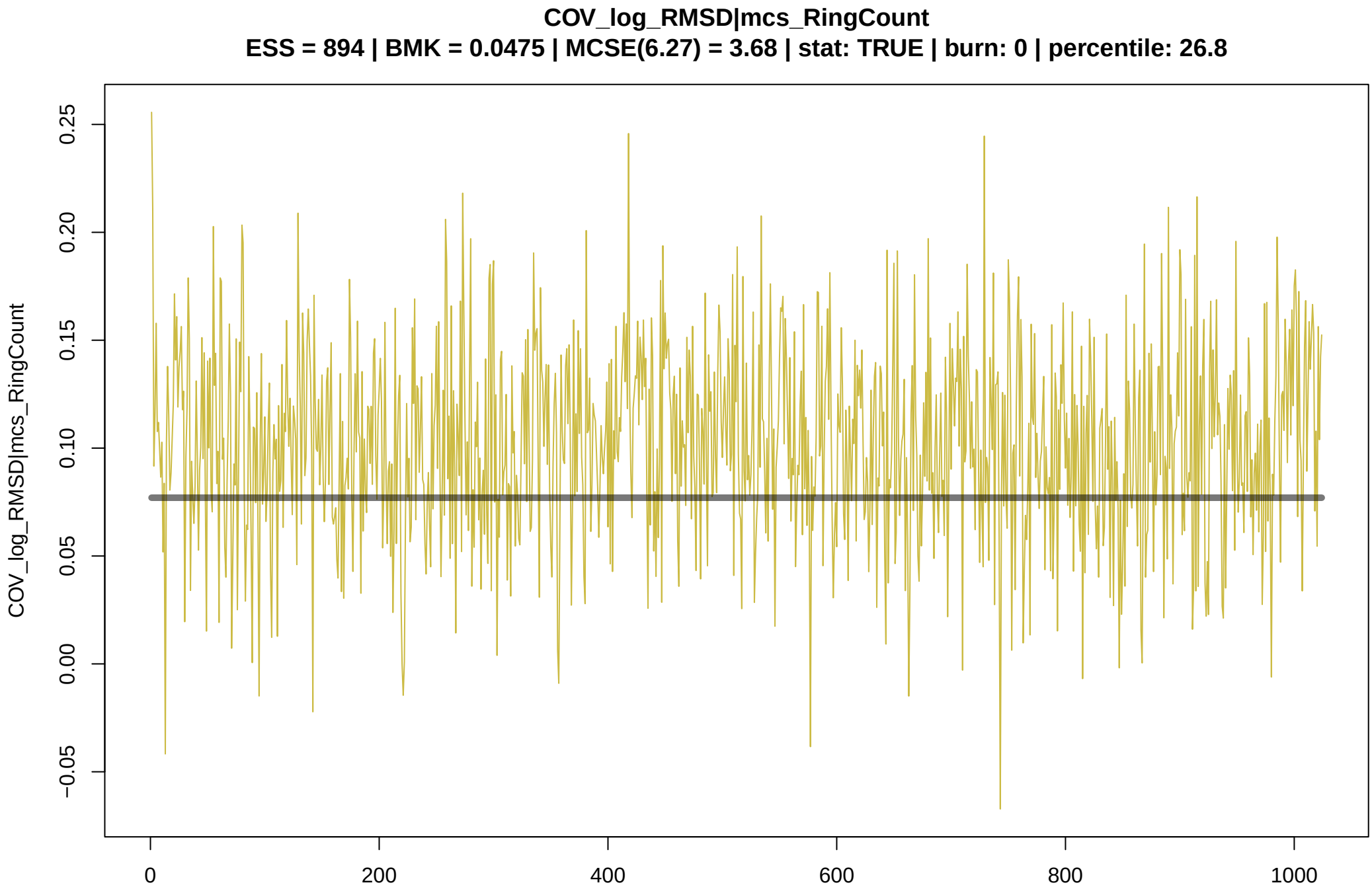

VAR_mcs_NOCount
ESS = 19.2 | BMK = 0.518 | MCSE(6.27) = 11.7 | stat: FALSE | burn: 0 | percentile: 31.4
VAR_mcs_NOCount
3.6
3.8
4.0
4.2
0
200
400
600
800
1000

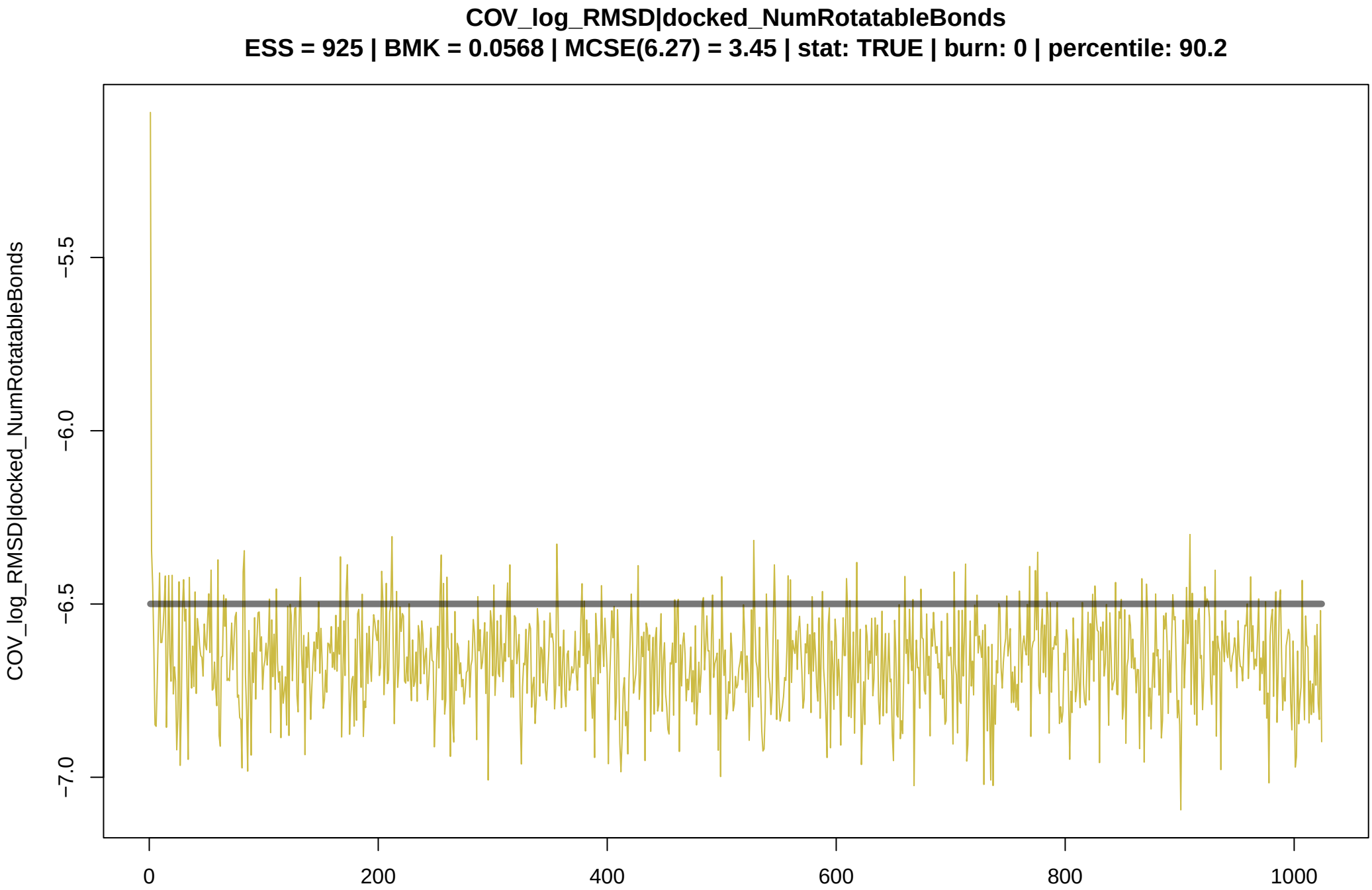

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 830 | BMK = 0.0609 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0 | percentile: 68.6
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.3
−0.4
−0.5
−0.6
0
200
400
600
800
1000

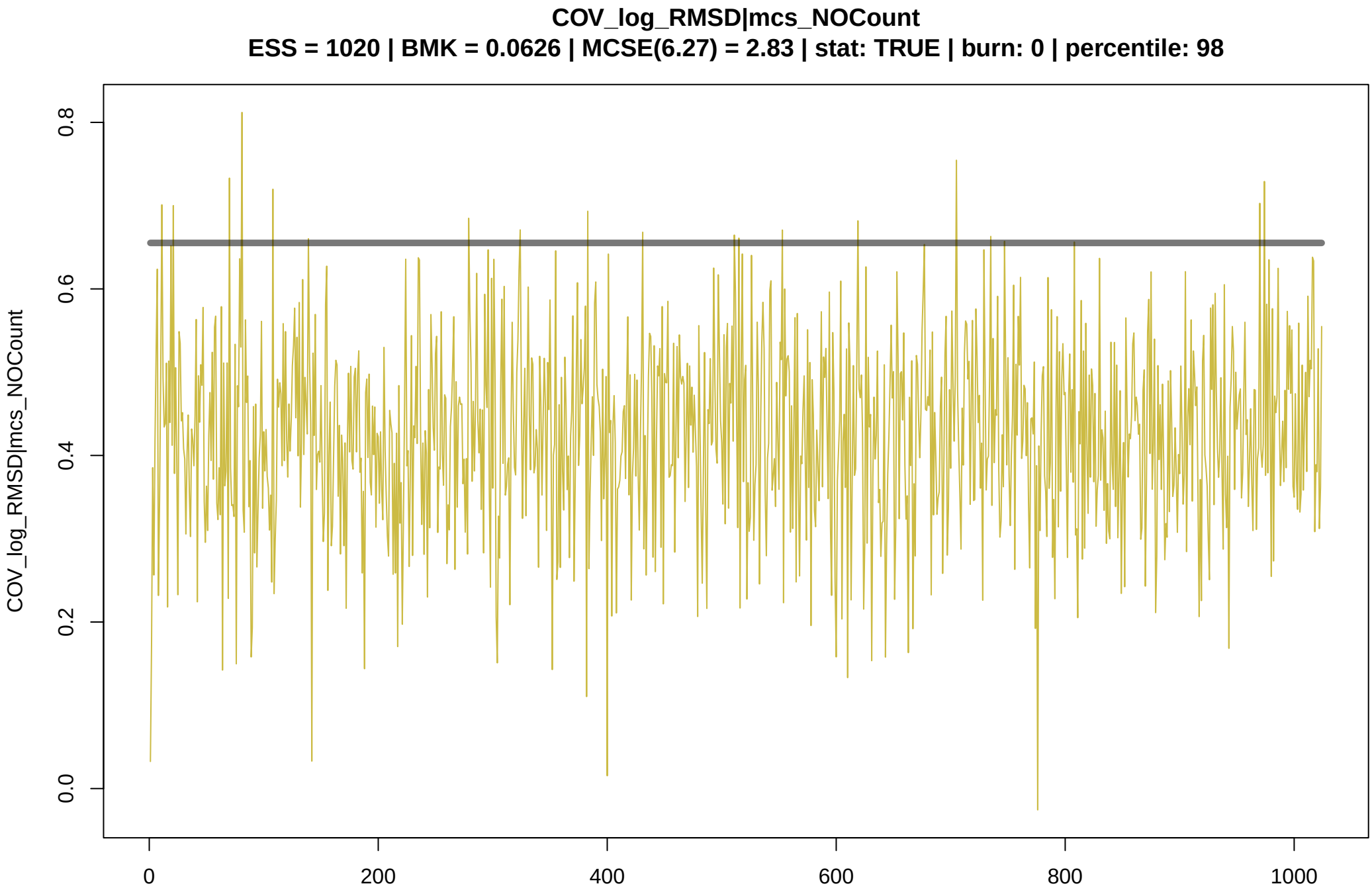

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 910 | BMK = 0.0758 | MCSE(6.27) = 3.97 | stat: TRUE | burn: 0 | percentile: 27.3
COV_log_RMSD|logit_ec_tanimoto_similarity
4.0
4.2
4.4
4.6
4.8
5.0
0
200
400
600
800
1000

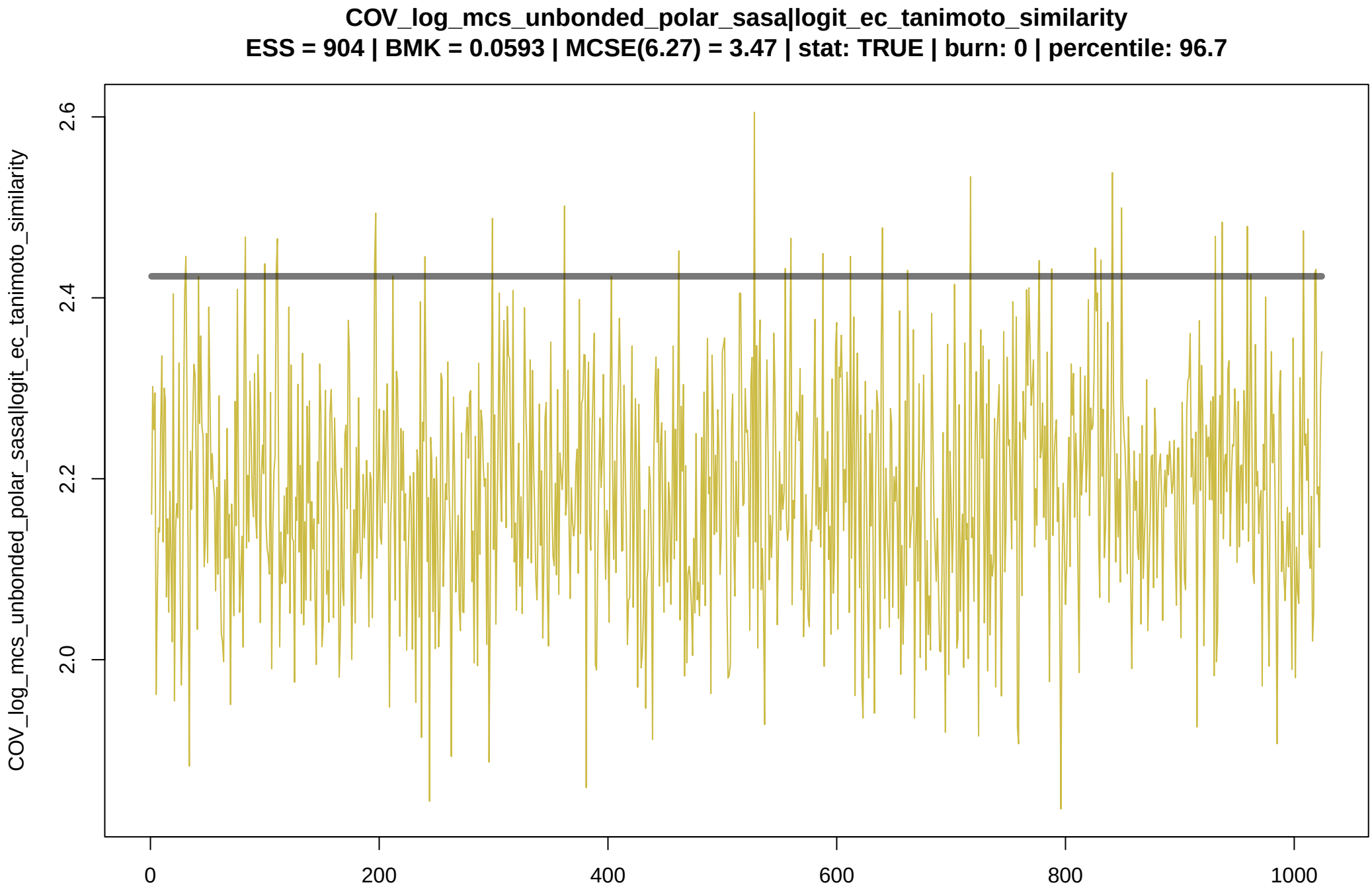

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0582 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | percentile: 52.5
COV_log_RMSD|mcs_NumHeteroAtoms
0.05
0.00
−0.05
−0.10
−0.15
−0.20
0
200
400
600
800
1000

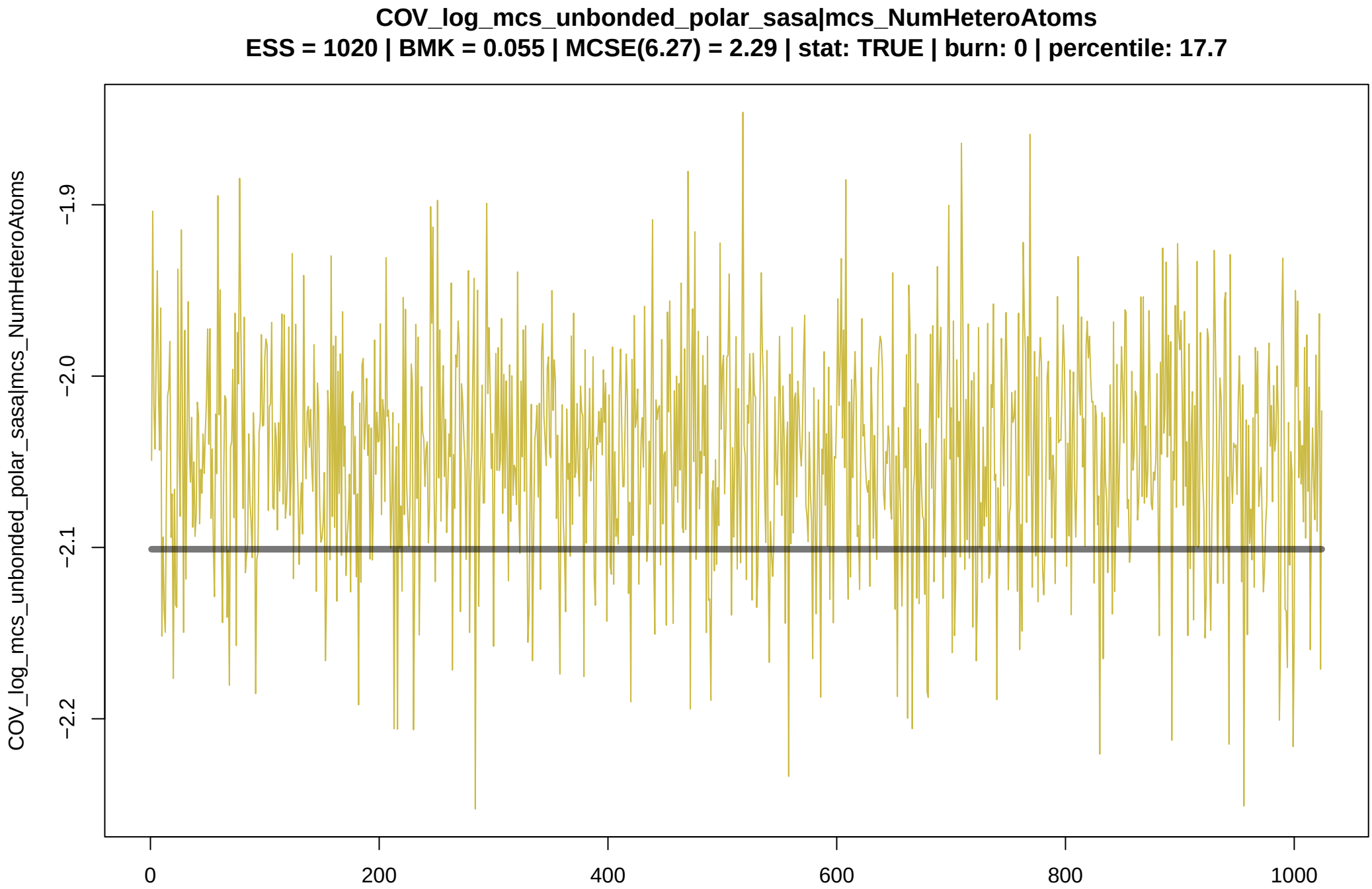

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.09 | MCSE(6.27) = 3.67 | stat: TRUE | burn: 0 | percentile: 50.2
COV_log_RMSD|docked_HeavyAtomCount
6.5
6.0
5.5
5.0
4.5
4.0
3.5
0
200
400
600
800
1000

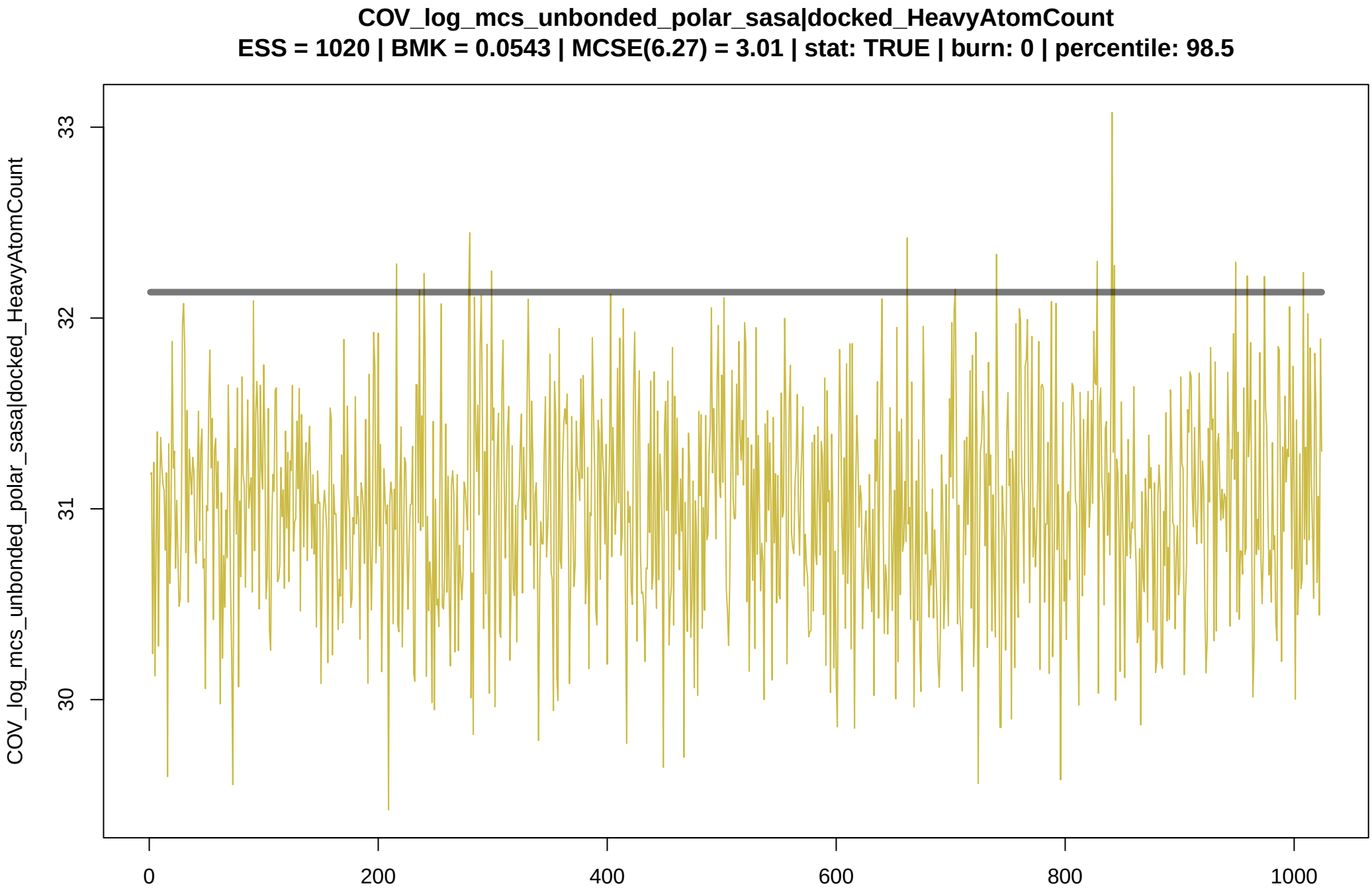

COV_log_RMSD|mcs_RingCount
ESS = 894 | BMK = 0.0475 | MCSE(6.27) = 3.68 | stat: TRUE | burn: 0 | percentile: 26.8
COV_log_RMSD|mcs_RingCount
0.25
0.20
0.15
0.10
0.05
0.00
−0.05
0
200
400
600
800
1000

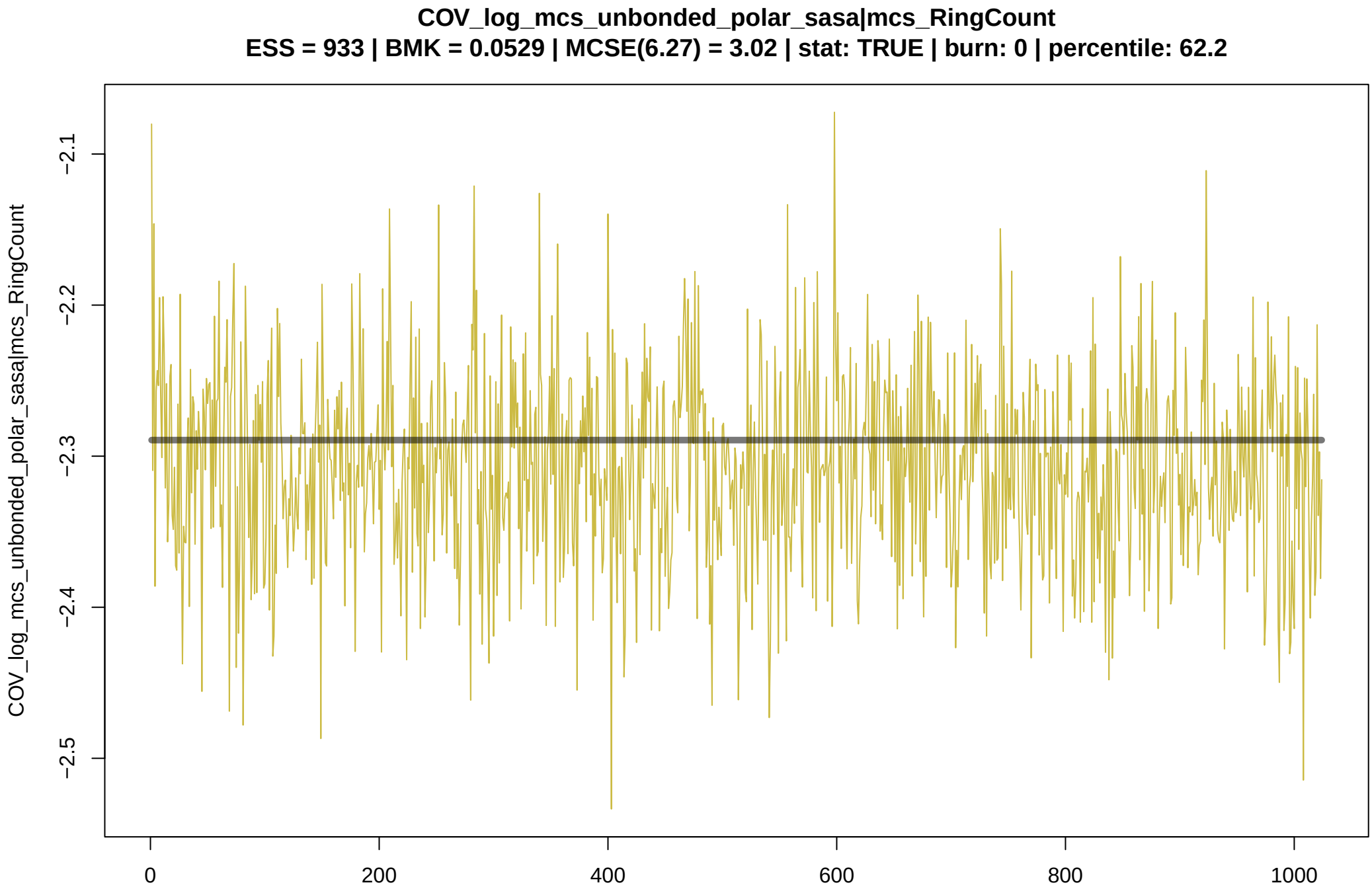

COV_log_RMSD|docked_NumRotatableBonds
ESS = 925 | BMK = 0.0568 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0 | percentile: 90.2
COV_log_RMSD|docked_NumRotatableBonds
−5.5
−6.0
−6.5
−7.0
0
200
400
600
800
1000

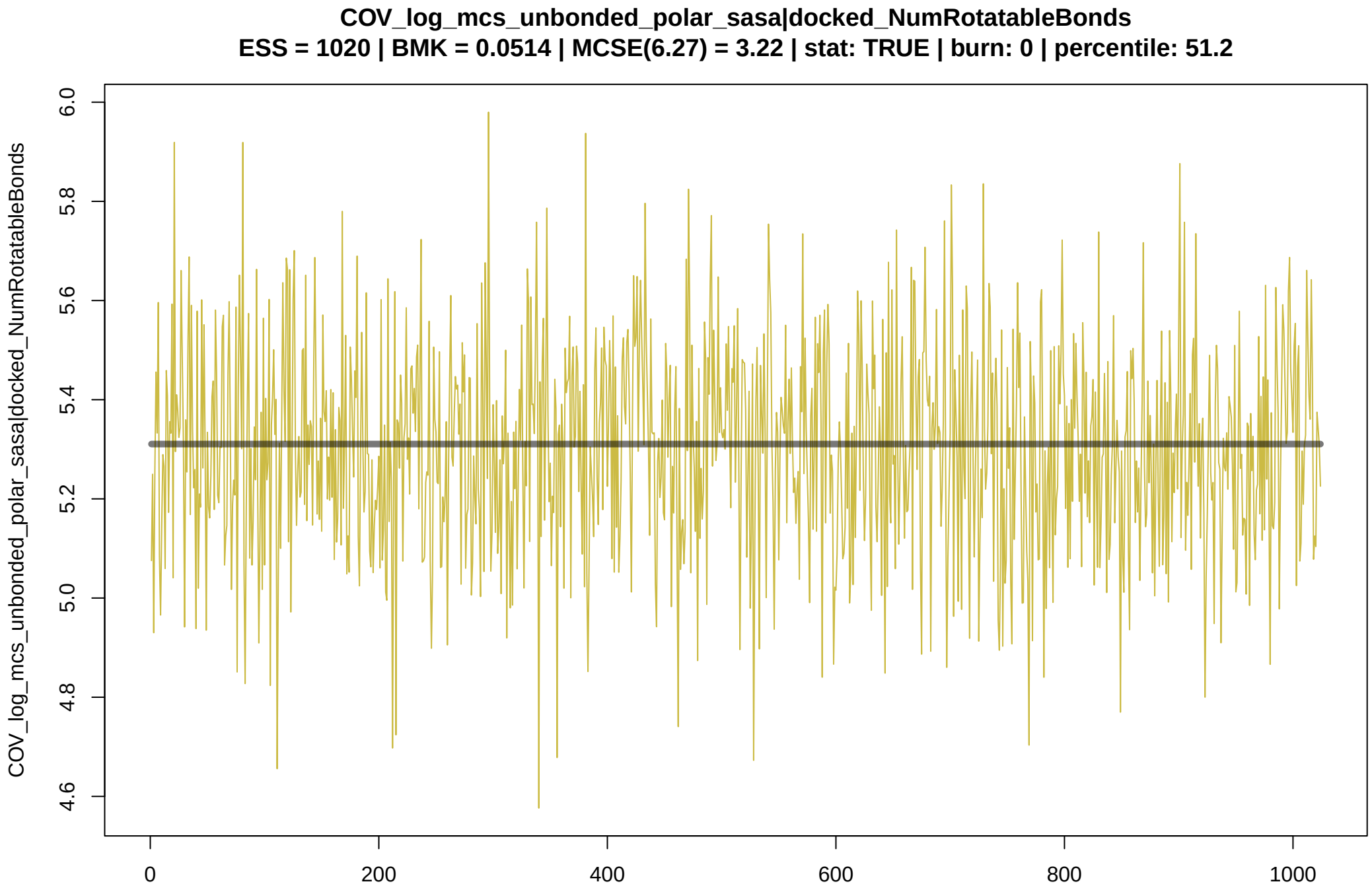

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0626 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | percentile: 98
COV_log_RMSD|mcs_NOCount
0.0
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

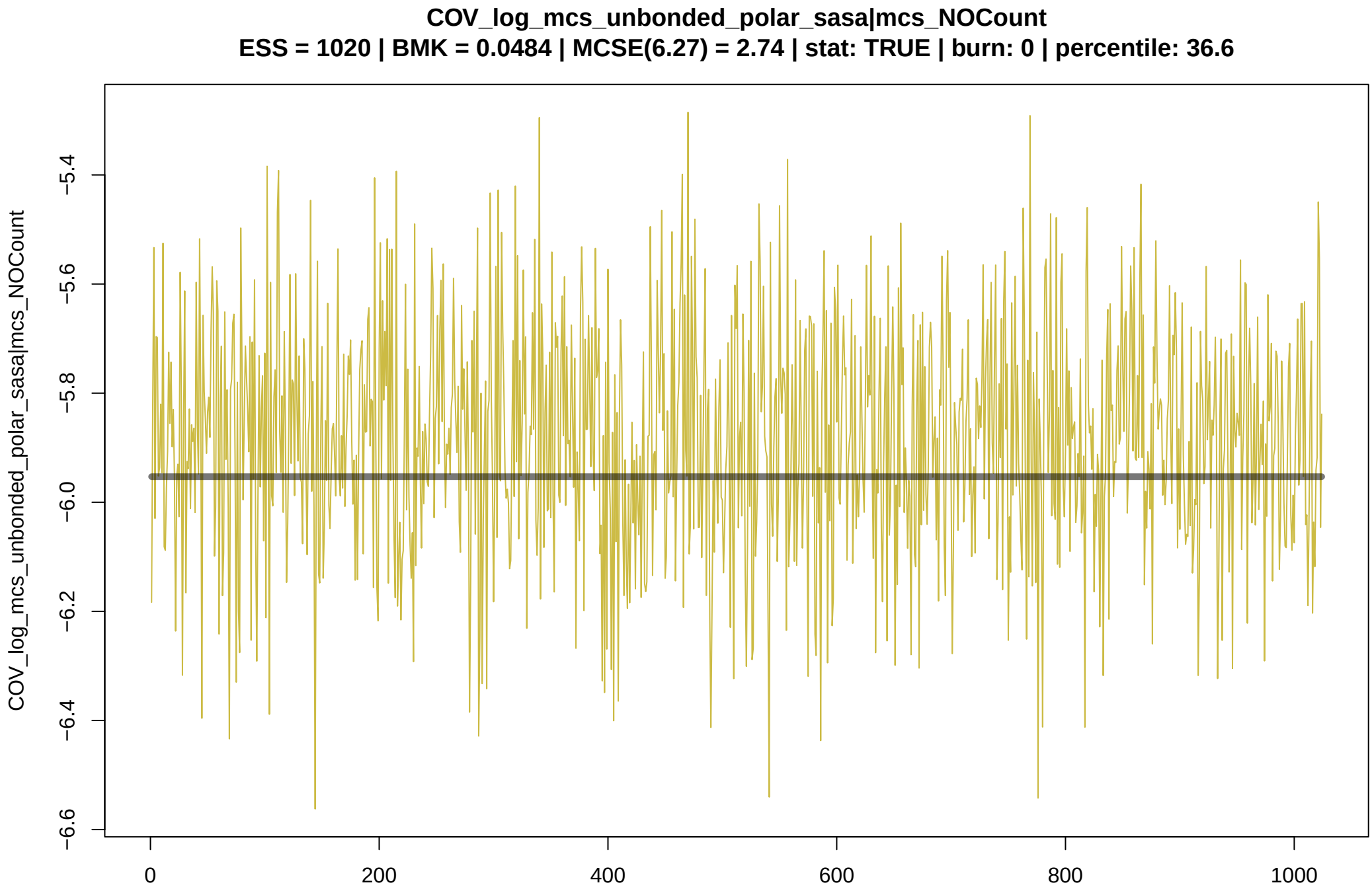

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 904 | BMK = 0.0593 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | percentile: 96.7
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2.6
2.4
2.2
2.0
0
200
400
600
800
1000

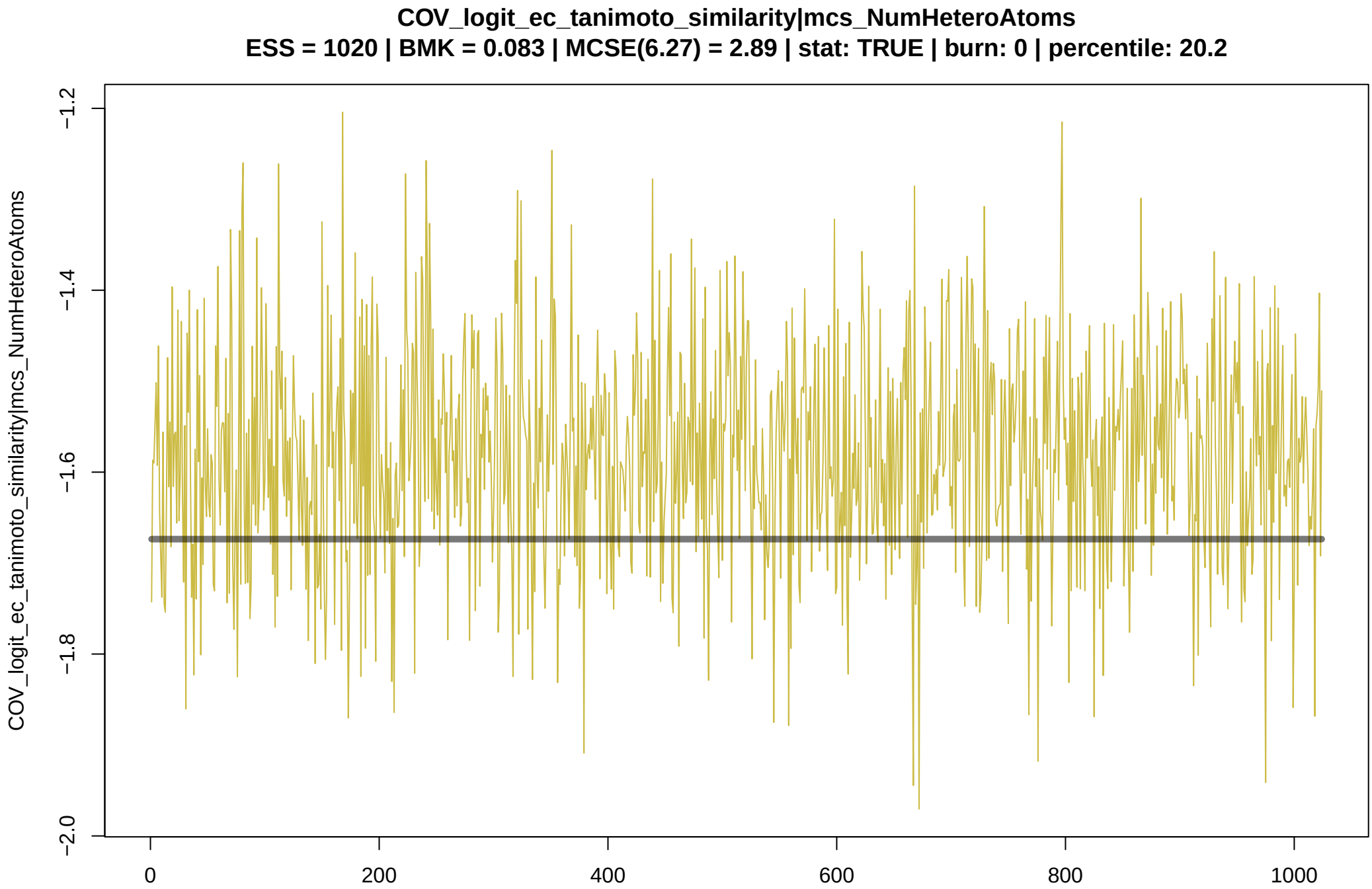

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.055 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | percentile: 17.7
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

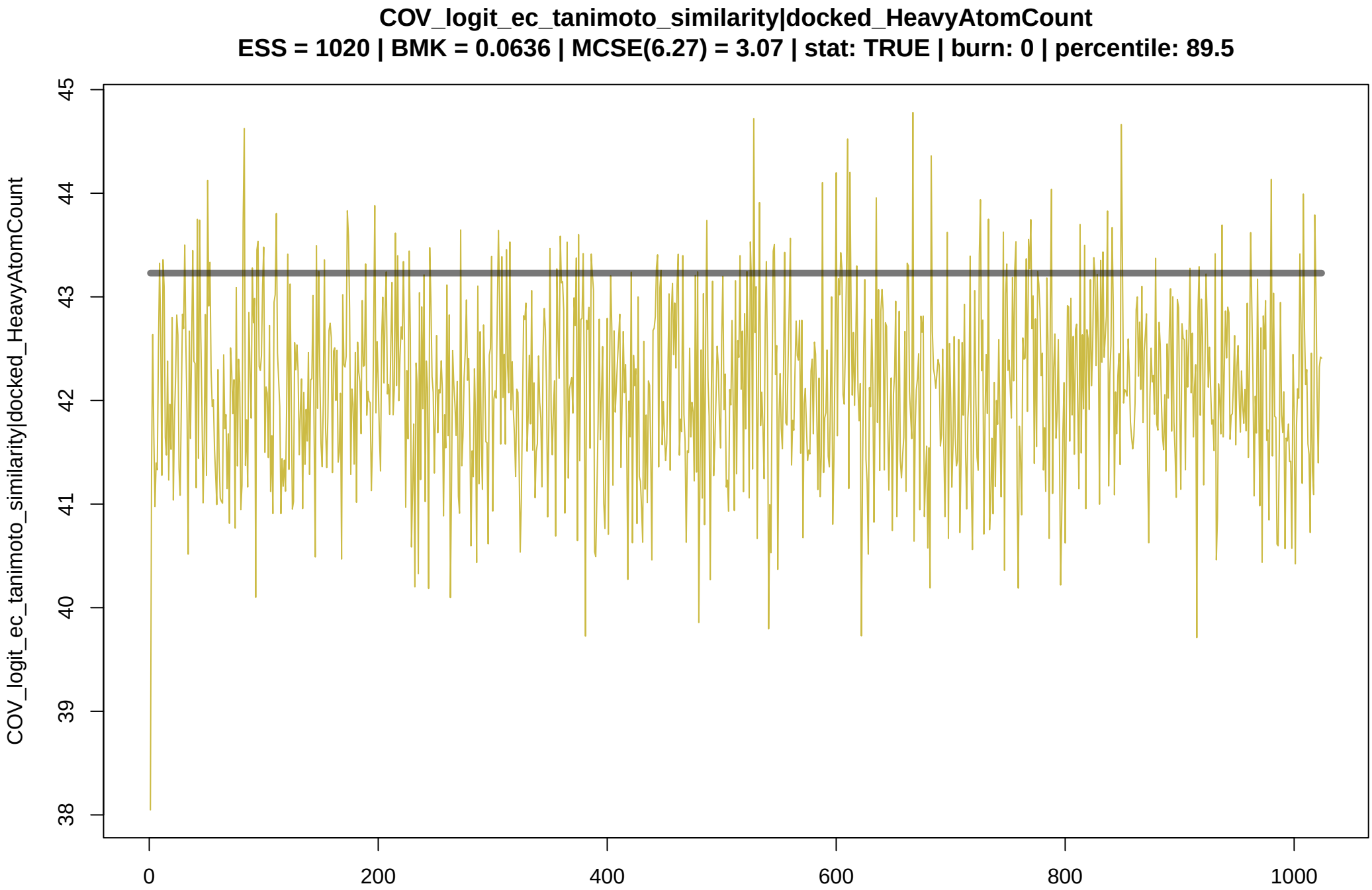

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0543 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | percentile: 98.5
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
33
32
31
30
0
200
400
600
800
1000

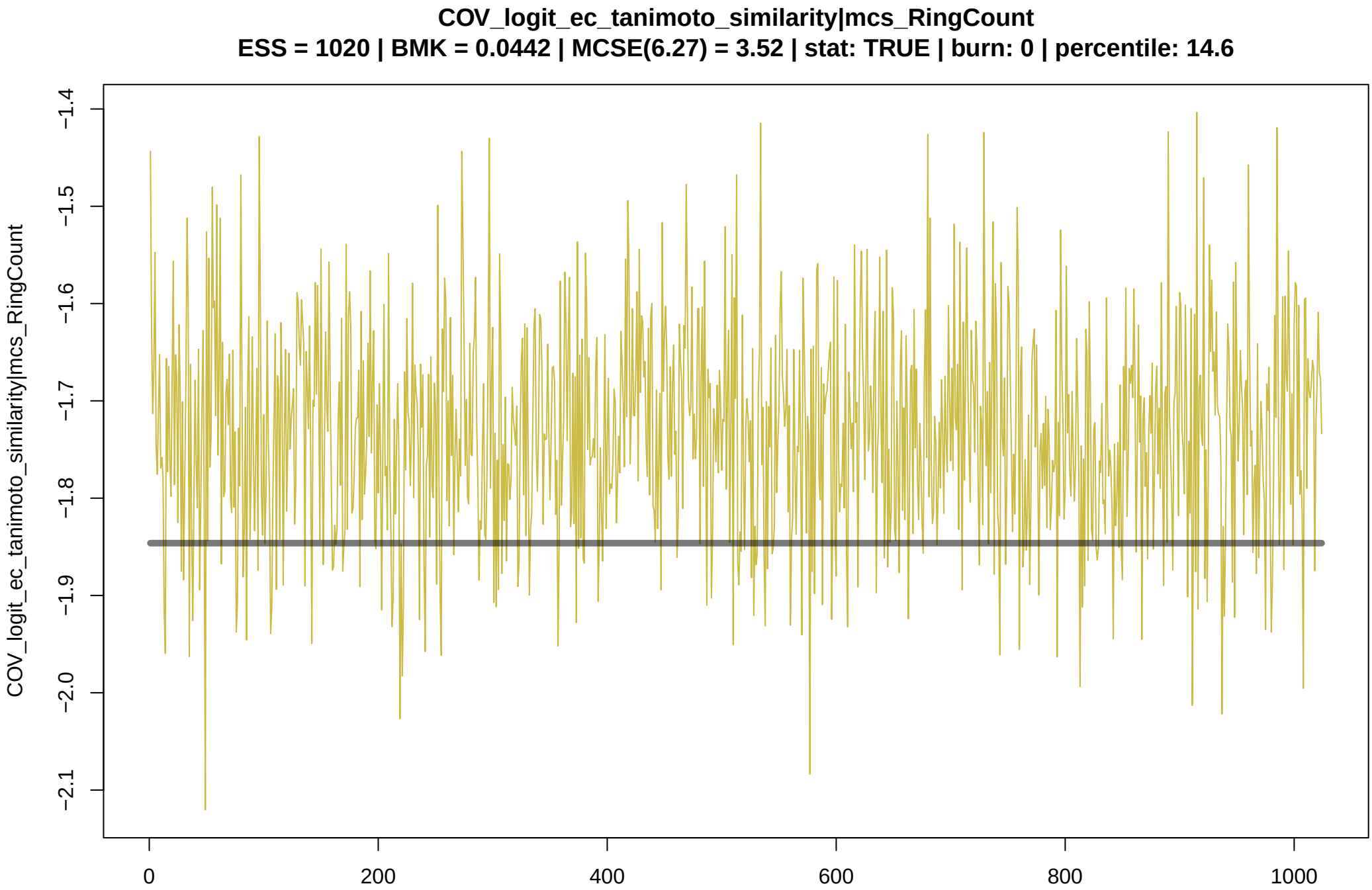

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 933 | BMK = 0.0529 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | percentile: 62.2
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.1
−2.2
−2.3
−2.4
−2.5
0
200
400
600
800
1000

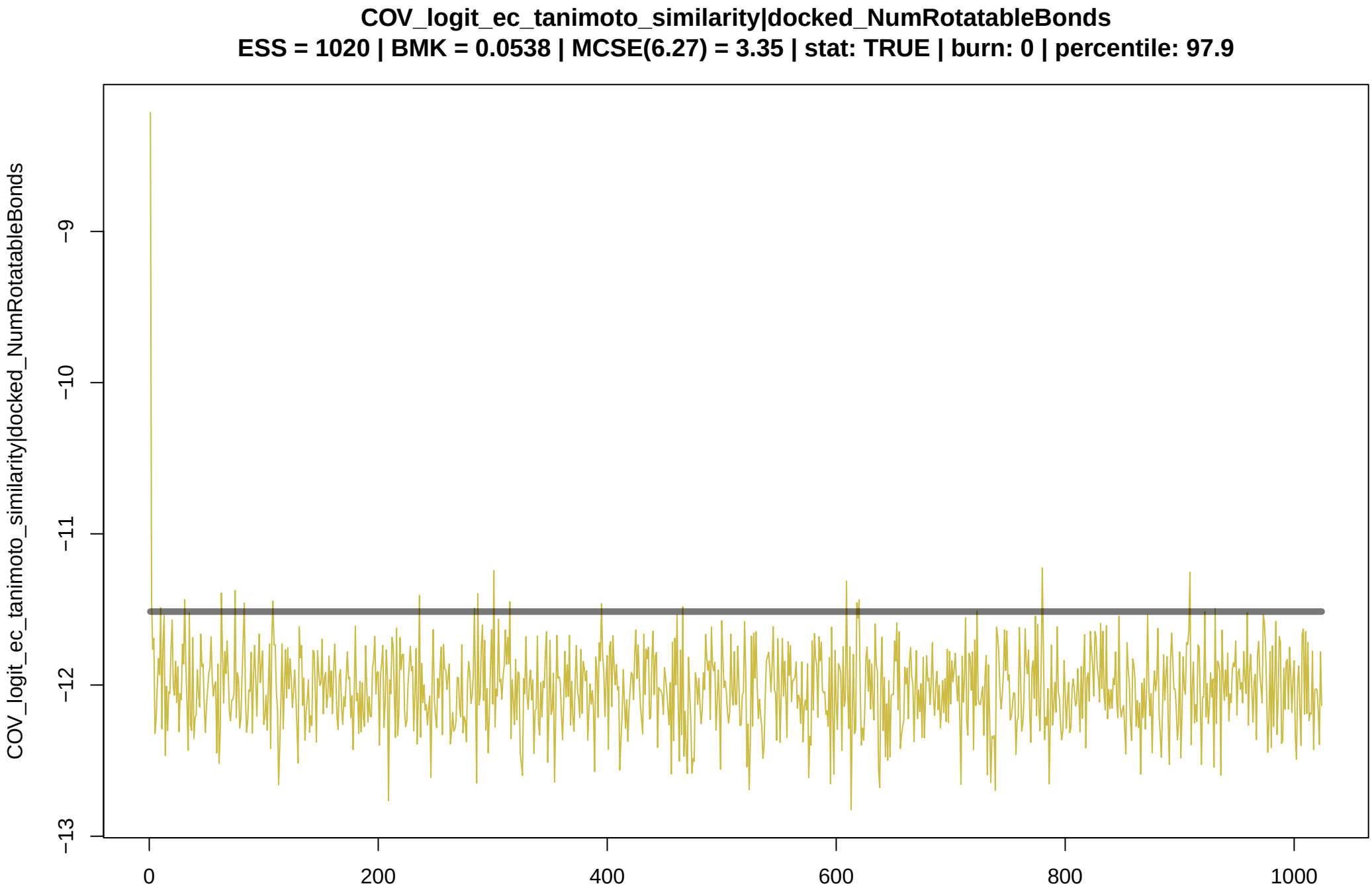

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0514 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0 | percentile: 51.2
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
0
200
400
600
800
1000

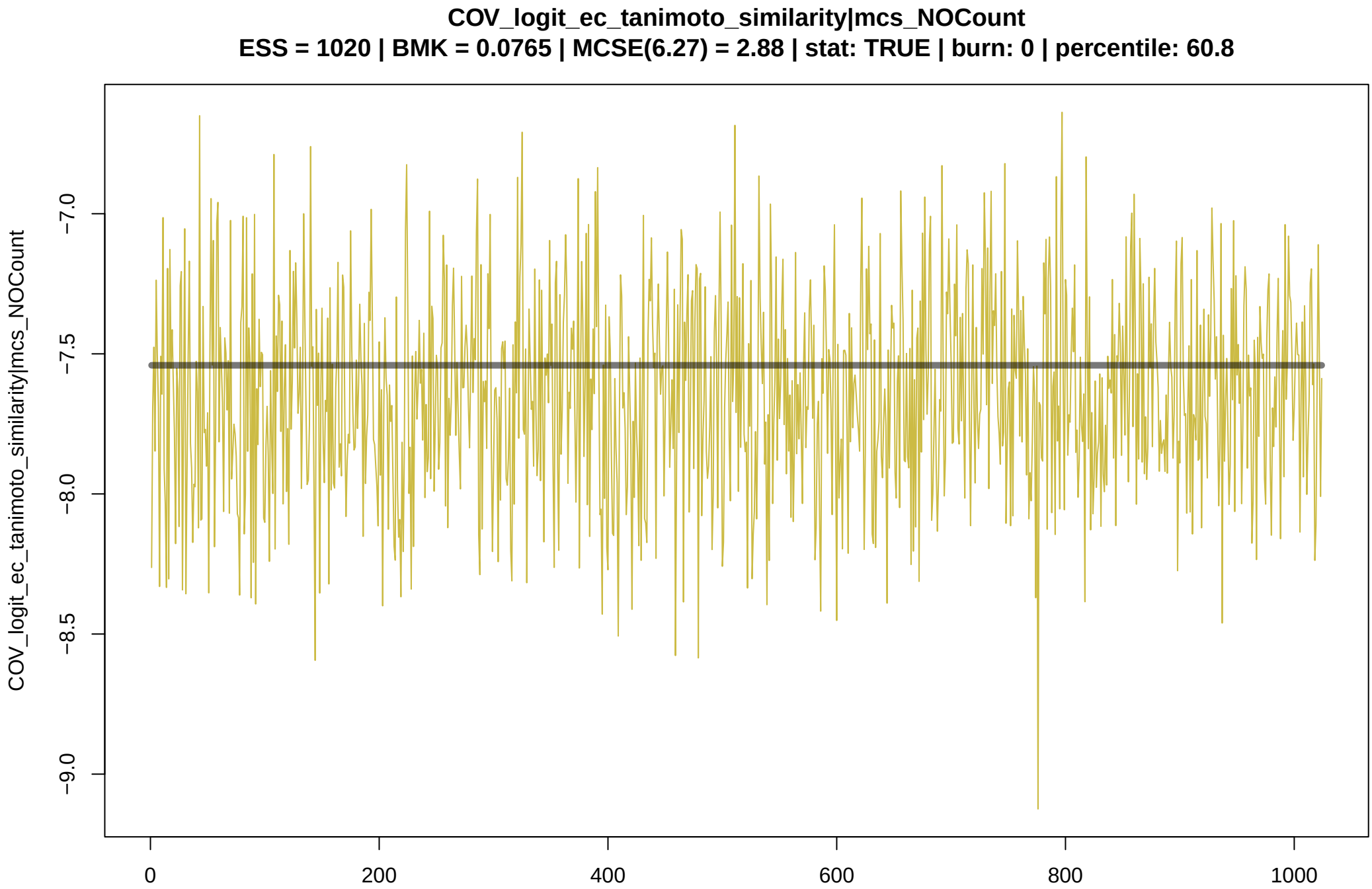

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0484 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | percentile: 36.6
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.4
−5.6
−5.8
−6.0
−6.2
−6.4
−6.6
0
200
400
600
800
1000

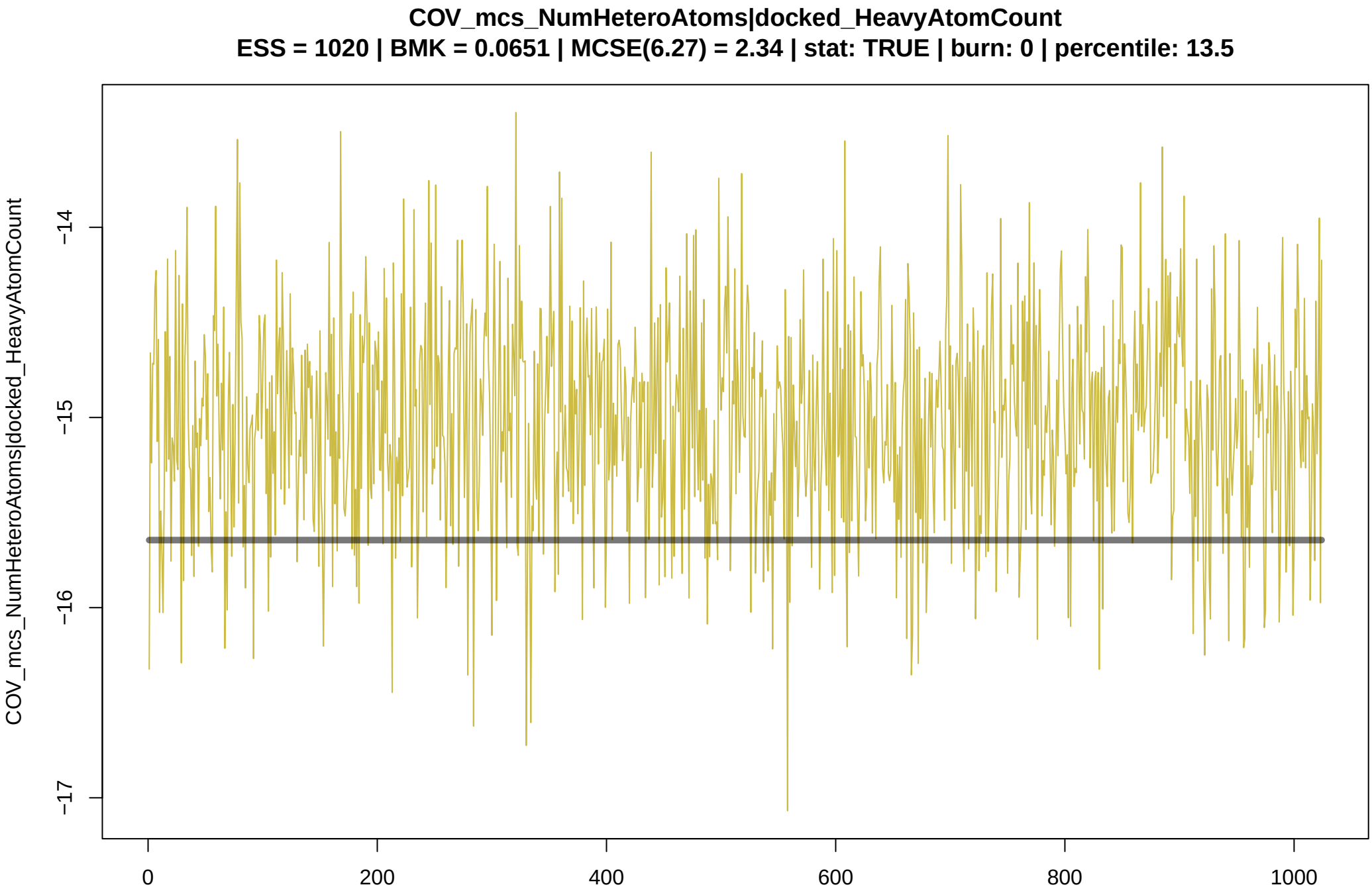

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.083 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | percentile: 20.2
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.2
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

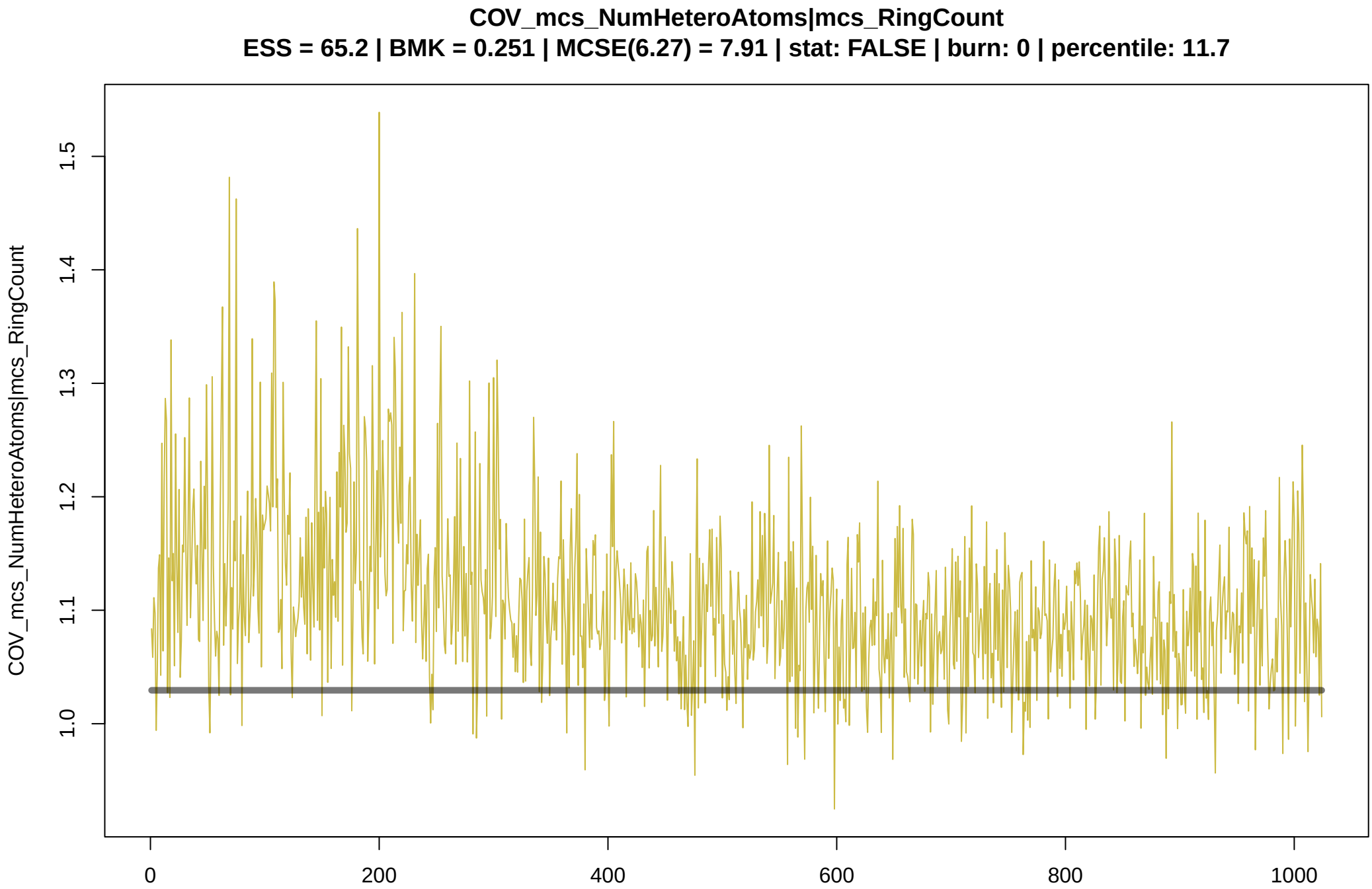

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0636 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | percentile: 89.5
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
45
44
43
42
41
40
39
38
0
200
400
600
800
1000

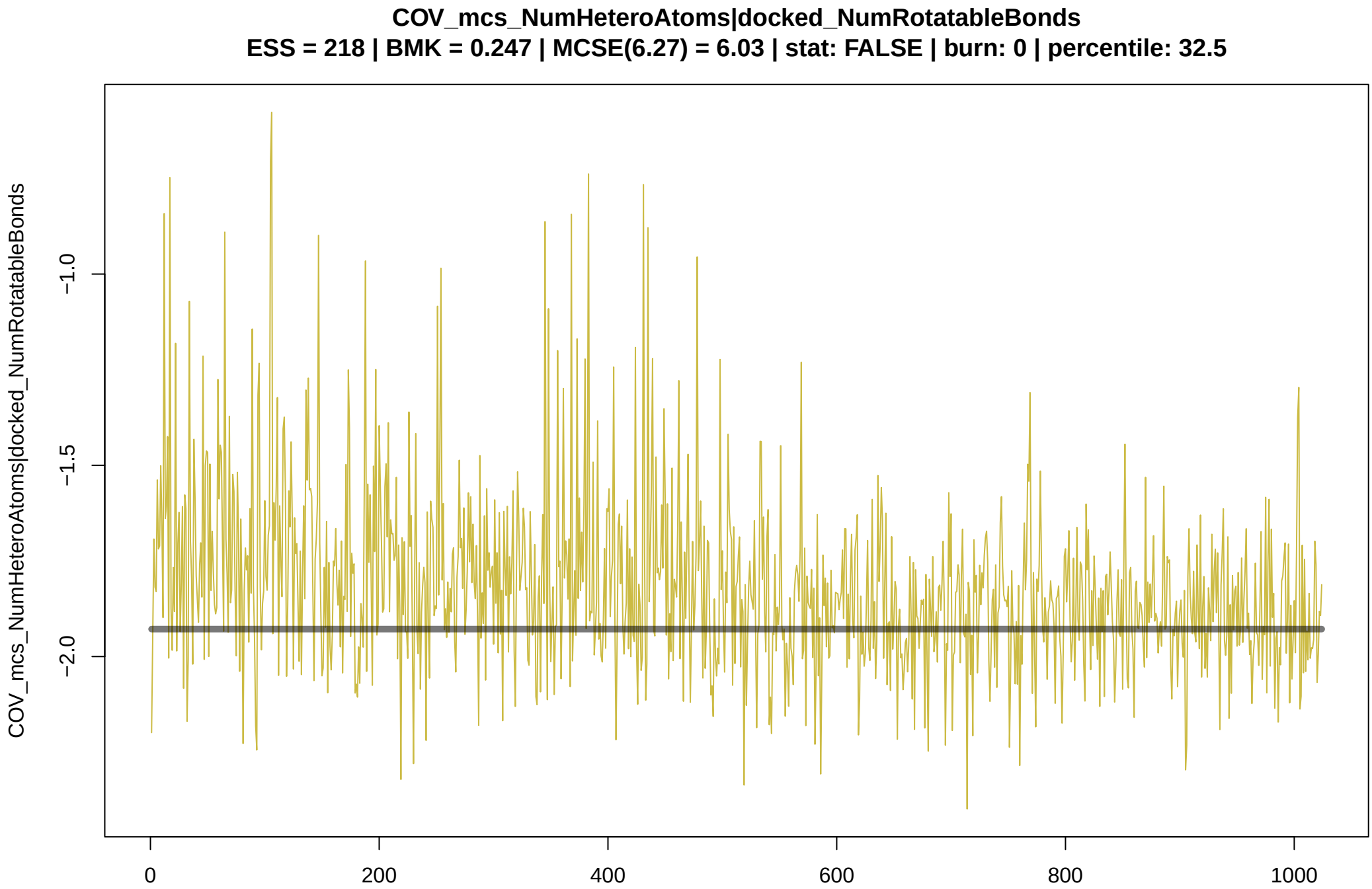

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0442 | MCSE(6.27) = 3.52 | stat: TRUE | burn: 0 | percentile: 14.6
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.4
−1.5
−1.6
−1.7
−1.8
−1.9
−2.0
−2.1
0
200
400
600
800
1000

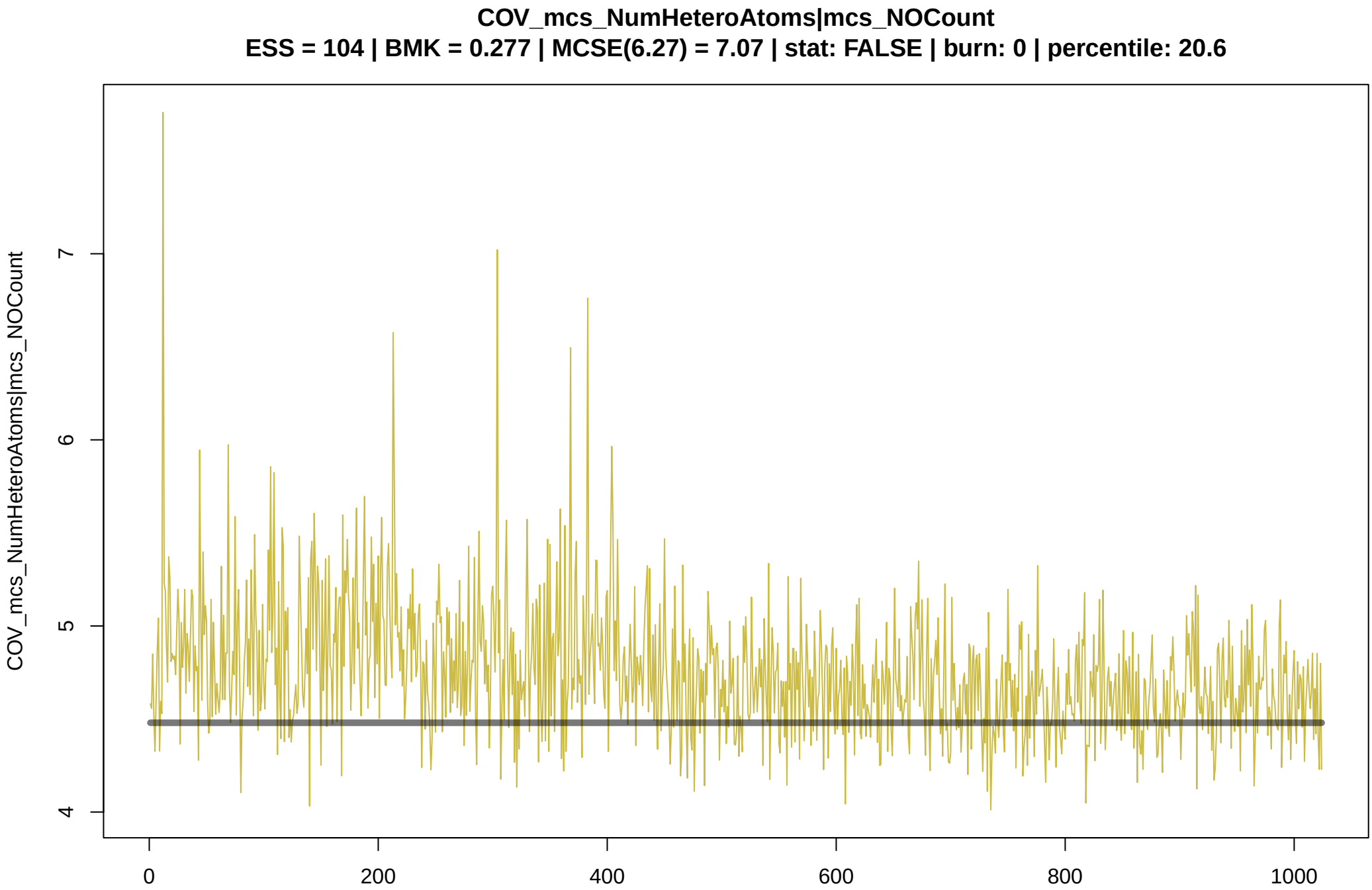

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0538 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0 | percentile: 97.9
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−9
−10
−11
−12
−13
0
200
400
600
800
1000

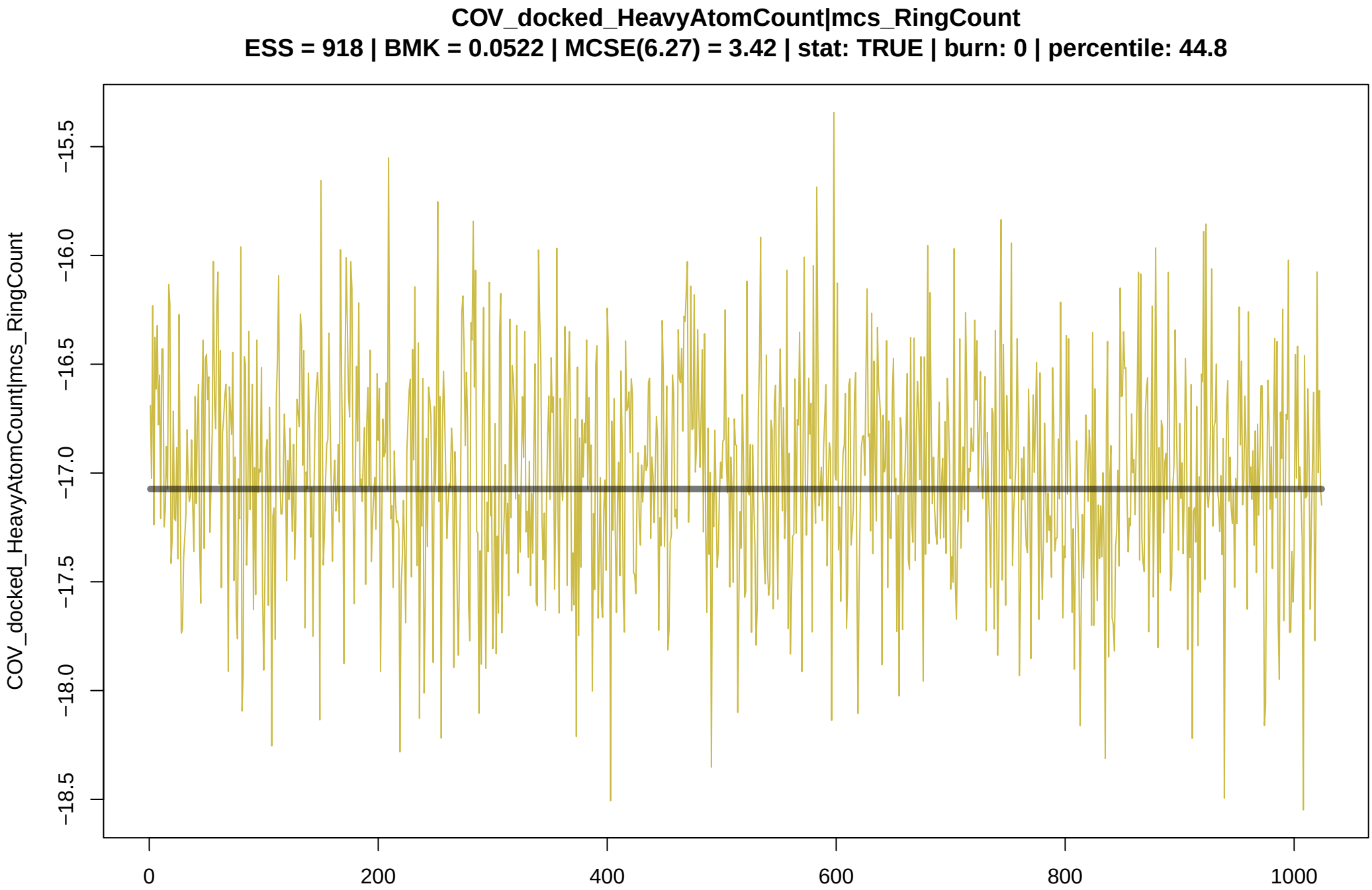

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0765 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | percentile: 60.8
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−7.0
−7.5
−8.0
−8.5
−9.0
0
200
400
600
800
1000

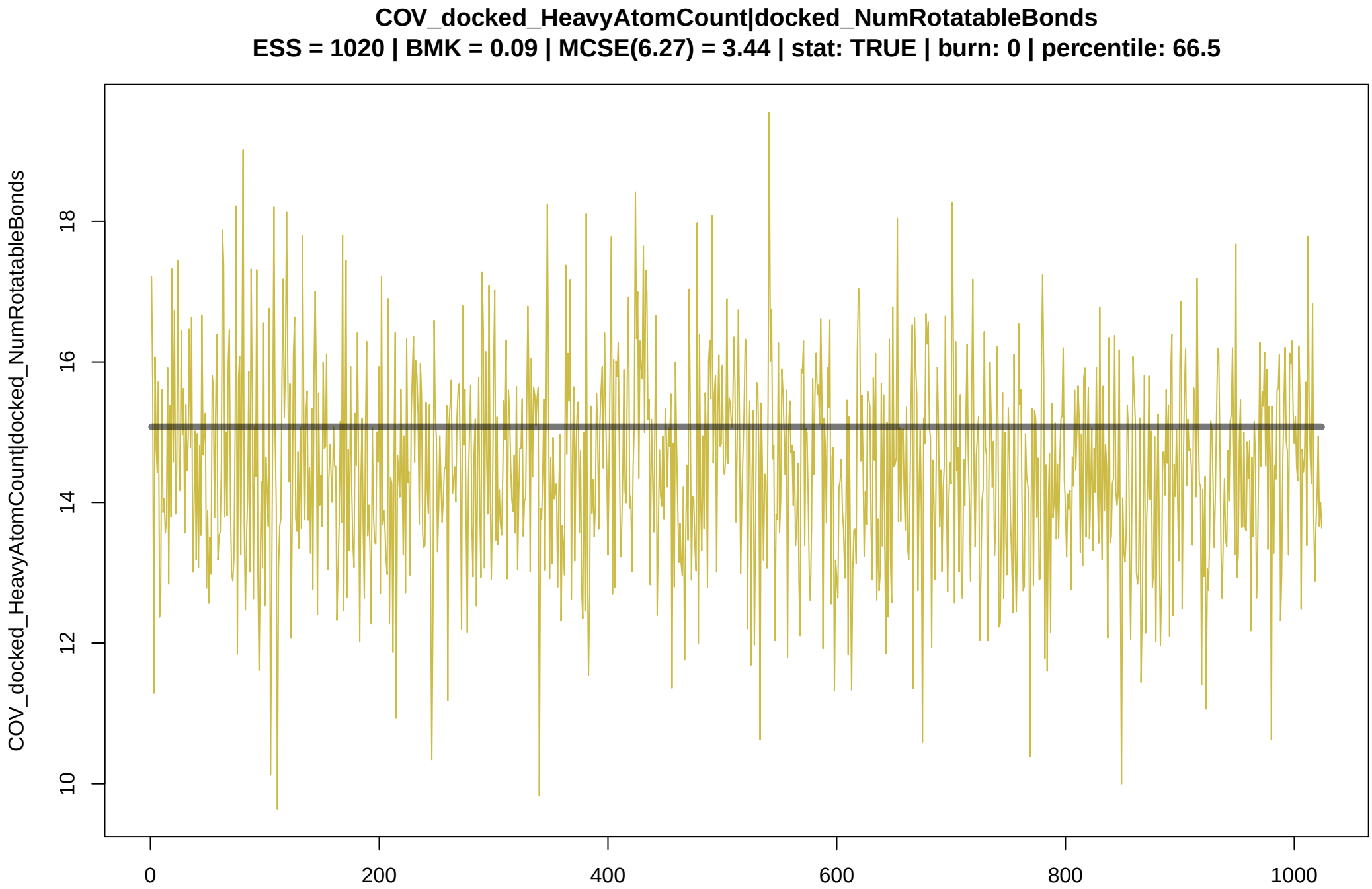

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0651 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0 | percentile: 13.5
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−14
−15
−16
−17
0
200
400
600
800
1000

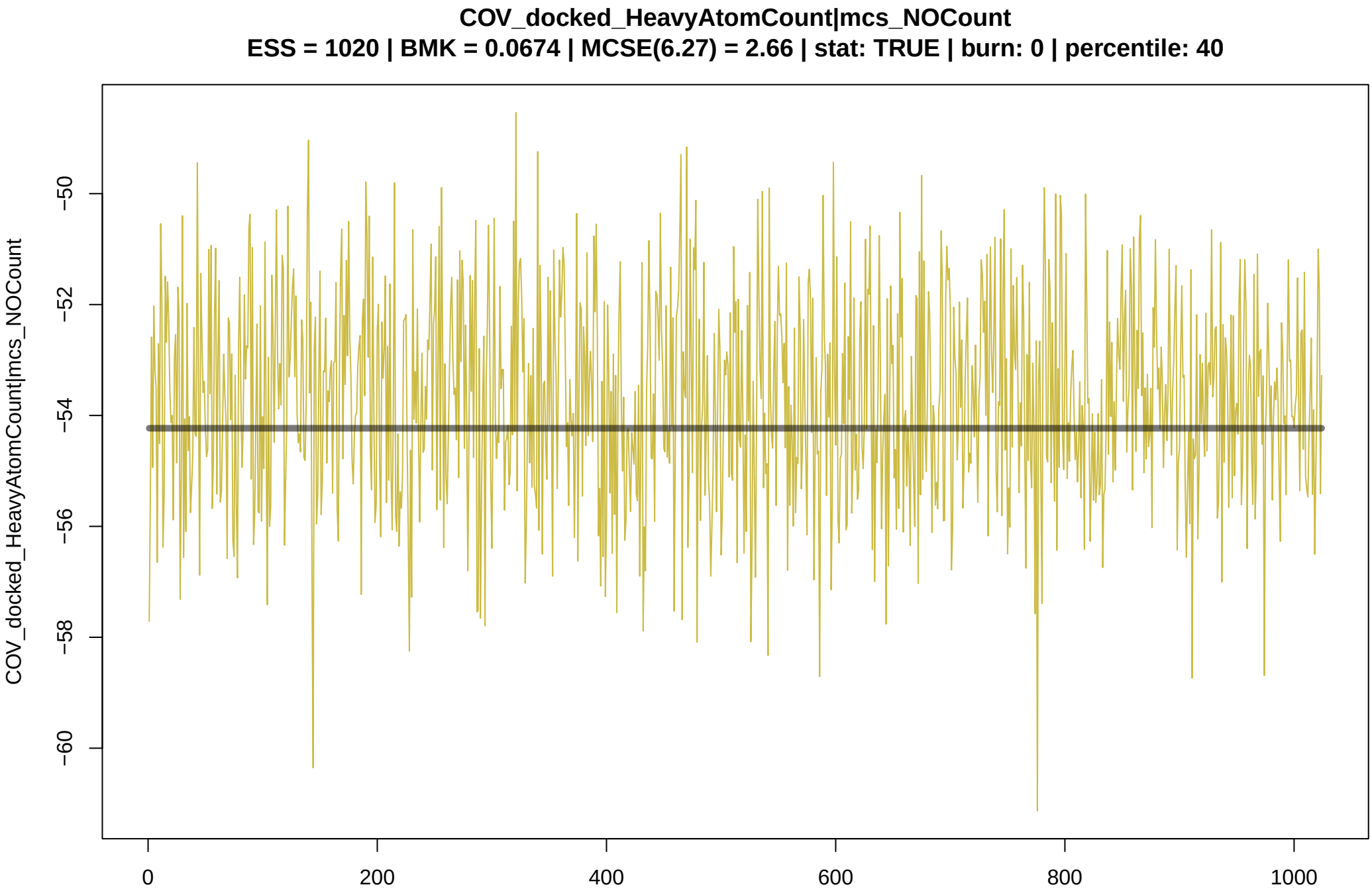

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 65.2 | BMK = 0.251 | MCSE(6.27) = 7.91 | stat: FALSE | burn: 0 | percentile: 11.7
COV_mcs_NumHeteroAtoms|mcs_RingCount
1.0
1.1
1.2
1.3
1.4
1.5
0
200
400
600
800
1000

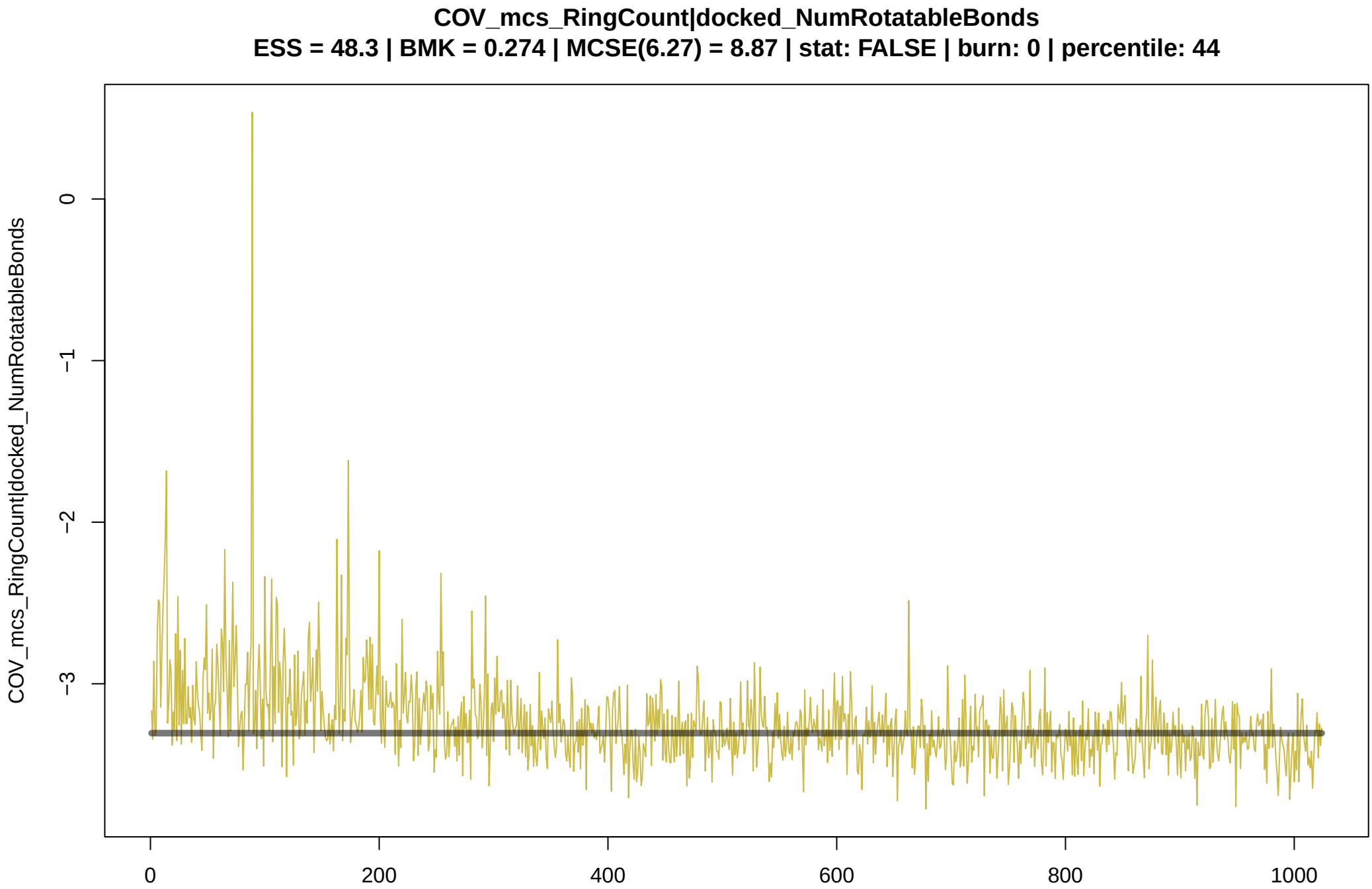

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 218 | BMK = 0.247 | MCSE(6.27) = 6.03 | stat: FALSE | burn: 0 | percentile: 32.5
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.0
−1.5
−2.0
0
200
400
600
800
1000

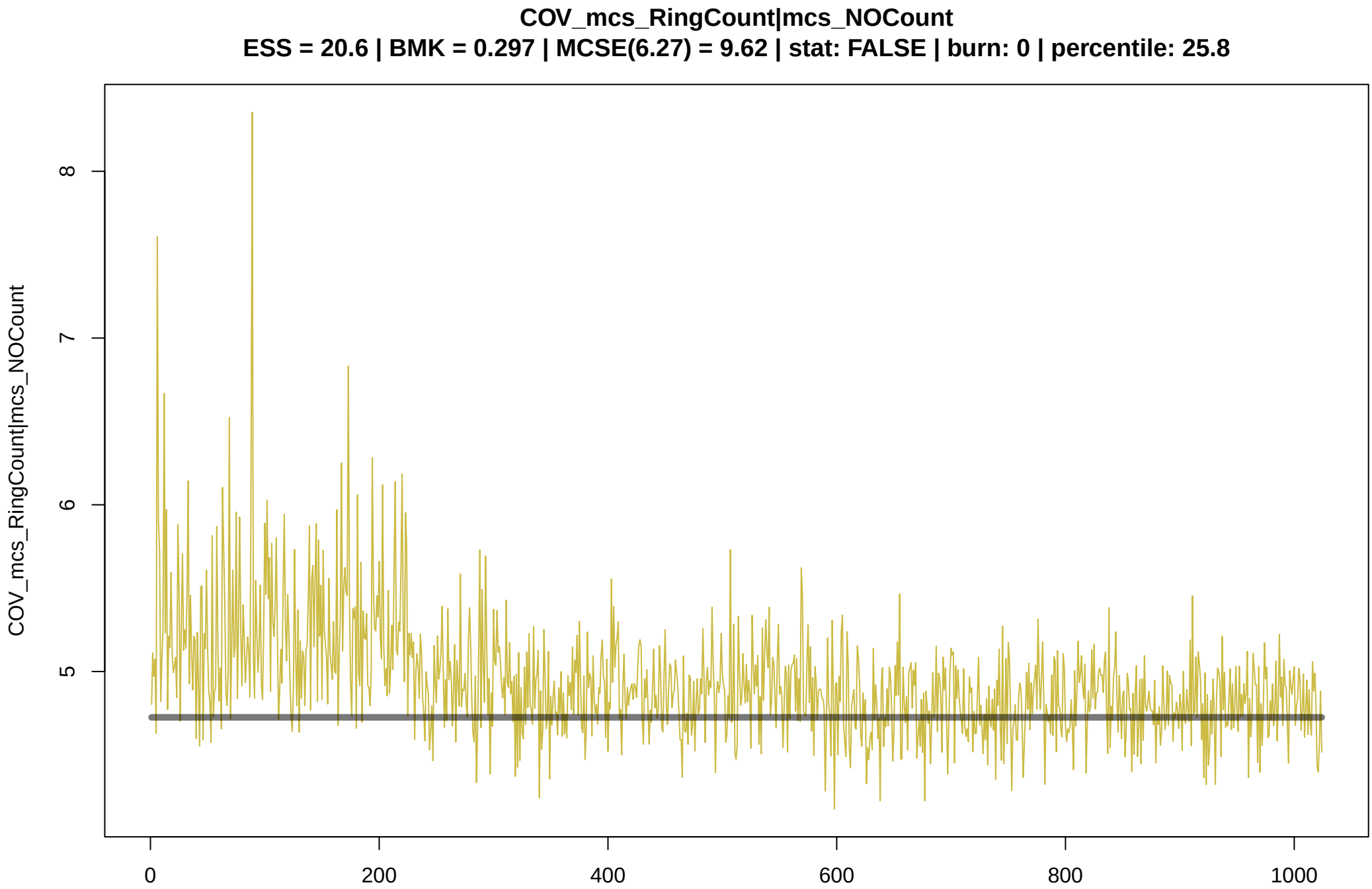

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 104 | BMK = 0.277 | MCSE(6.27) = 7.07 | stat: FALSE | burn: 0 | percentile: 20.6
COV_mcs_NumHeteroAtoms|mcs_NOCount
4
5
6
7
0
200
400
600
800
1000

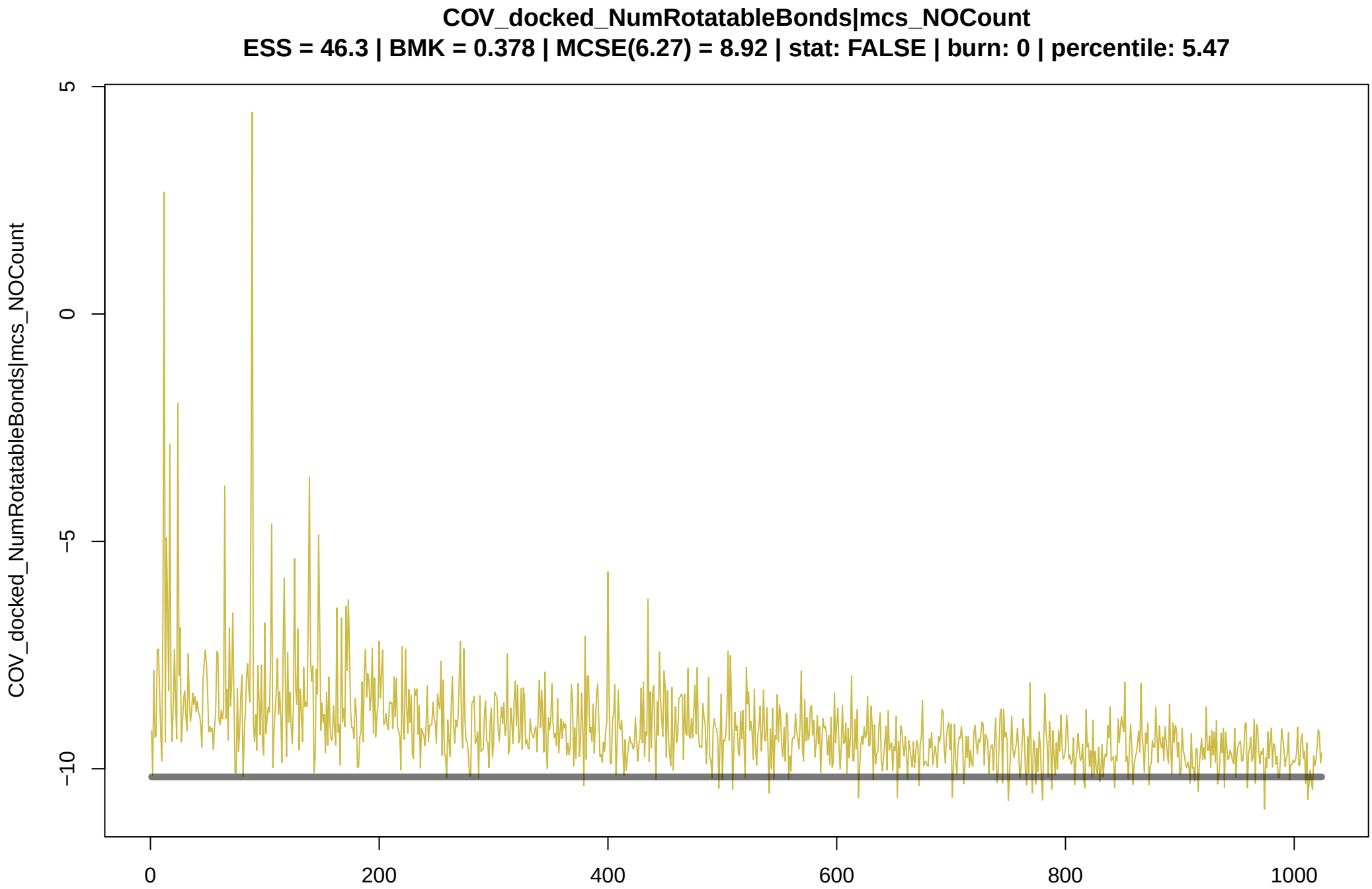

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 918 | BMK = 0.0522 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | percentile: 44.8
COV_docked_HeavyAtomCount|mcs_RingCount
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.09 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | percentile: 66.5
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0674 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0 | percentile: 40
COV_docked_HeavyAtomCount|mcs_NOCount
−50
−52
−54
−56
−58
−60
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 48.3 | BMK = 0.274 | MCSE(6.27) = 8.87 | stat: FALSE | burn: 0 | percentile: 44
COV_mcs_RingCount|docked_NumRotatableBonds
0
−1
−2
−3
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 20.6 | BMK = 0.297 | MCSE(6.27) = 9.62 | stat: FALSE | burn: 0 | percentile: 25.8
COV_mcs_RingCount|mcs_NOCount
5
6
7
8
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 46.3 | BMK = 0.378 | MCSE(6.27) = 8.92 | stat: FALSE | burn: 0 | percentile: 5.47
COV_docked_NumRotatableBonds|mcs_NOCount
5
0
−5
−10
0
200
400
600
800
1000