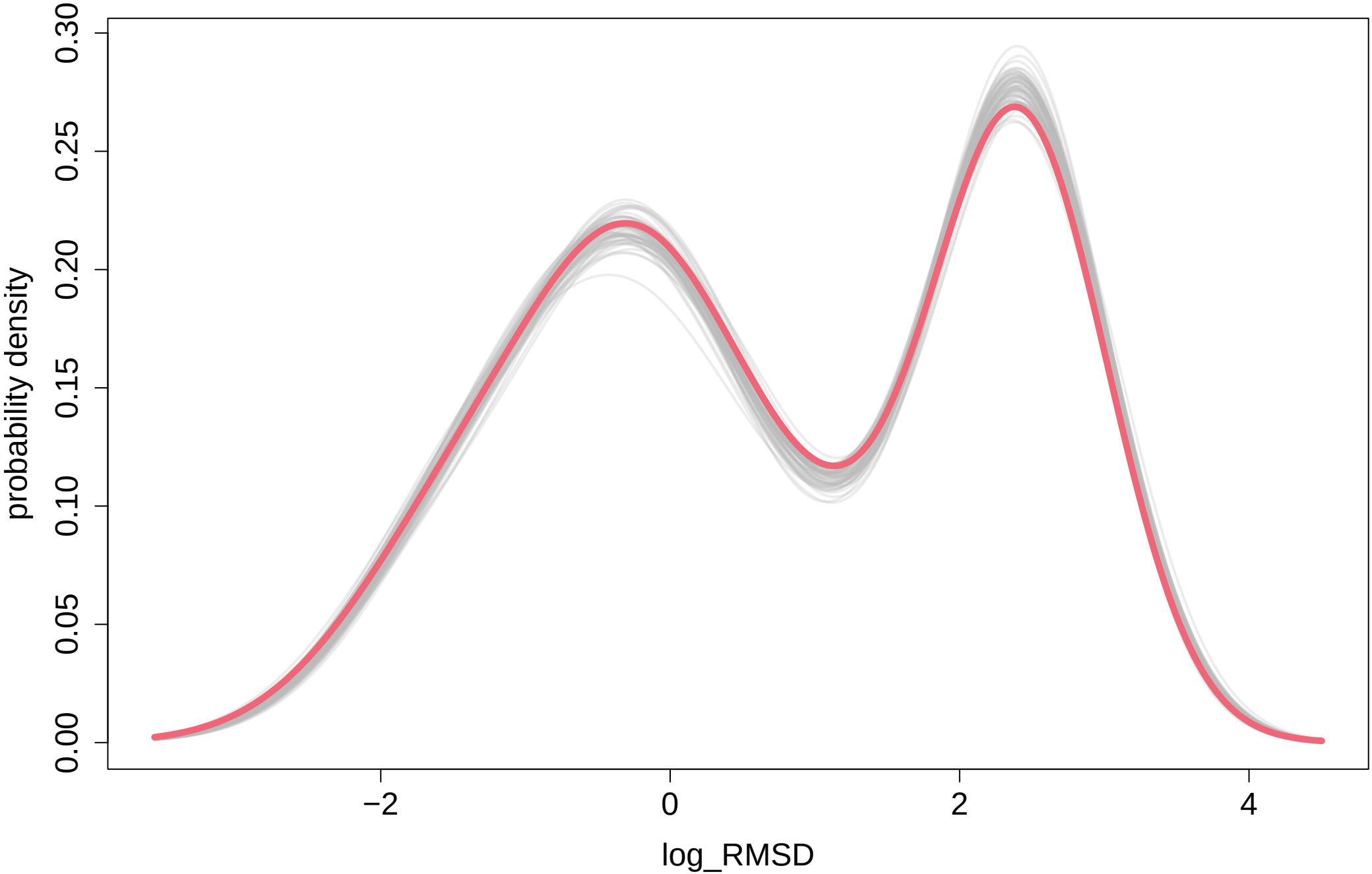
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.292904678572774
max MCSE = 9.68766564139451
all stationary: FALSE
burn: 0
min percent.: 2.05078125

−− STATS 2D −−
min ESS = 533.852335392271
max BMK = 0.108688585652332
max MCSE = 4.58512699493181
all stationary: FALSE
burn: 0
min percent.: 1.7578125

−− STATS 1D −−
min ESS = 21.5510643907903
max BMK = 1
max MCSE = 9.52094086328429
all stationary: FALSE
burn: 816
min percent.: 0.29296875

Occupied clusters: 23 of 64
LL: −62400 +− 10.8


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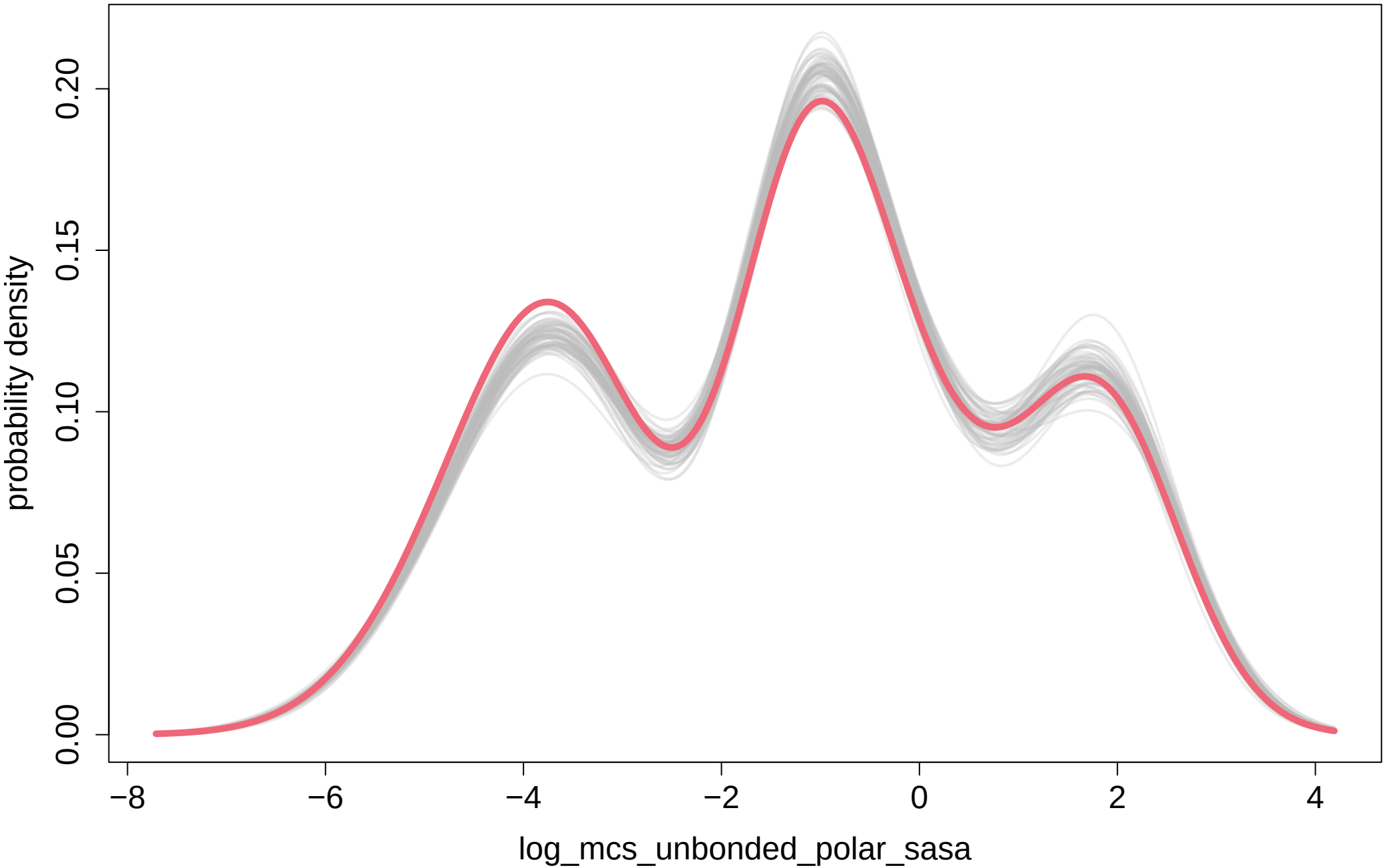
0.10
0.15
0.20
0.25
0.30
−2
0
2
4
log_RMSD


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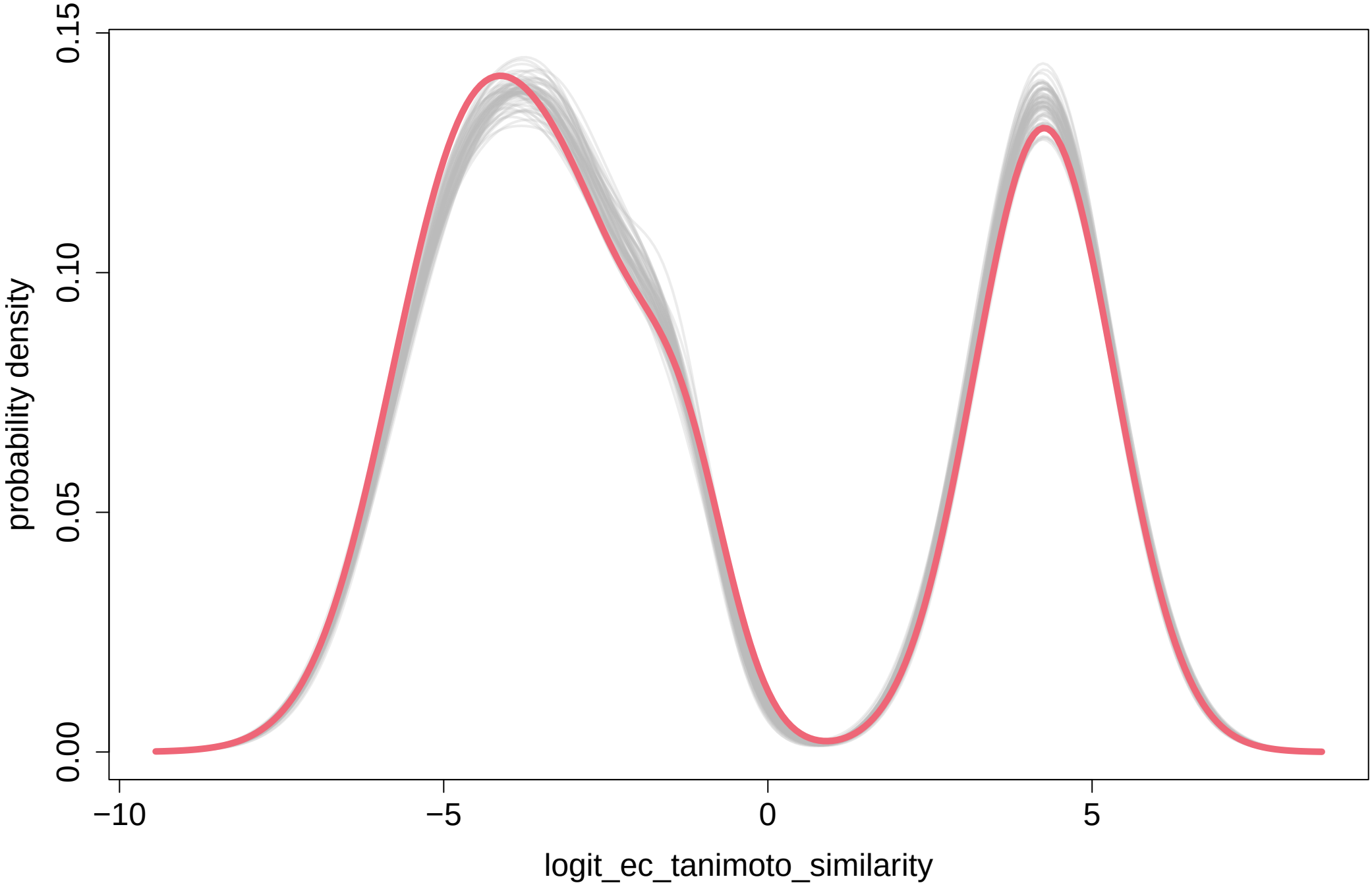
0.15
0.20
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa


0.15
0.10
0.05
0.00
probability density
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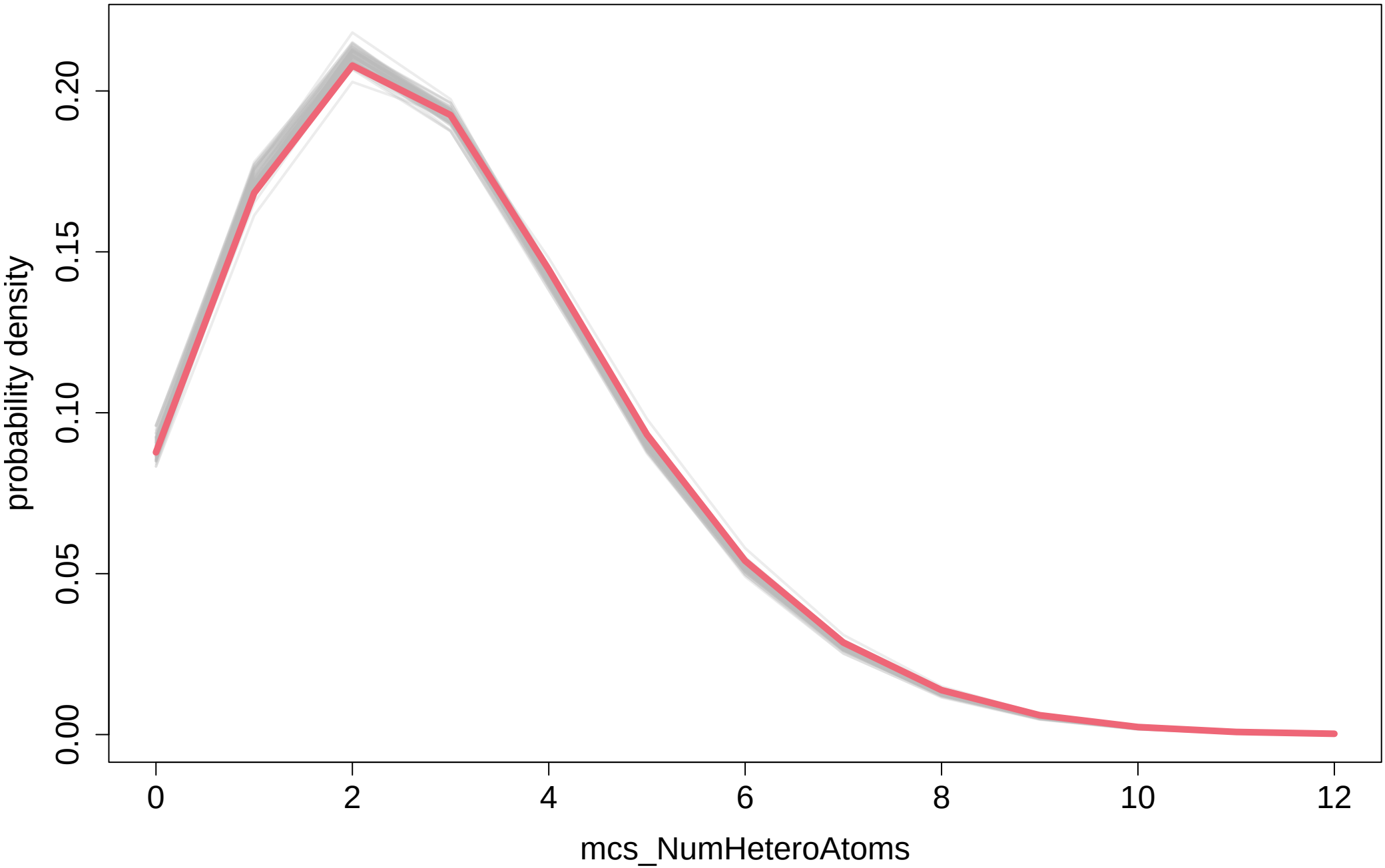
−5
0
5
logit_ec_tanimoto_similarity


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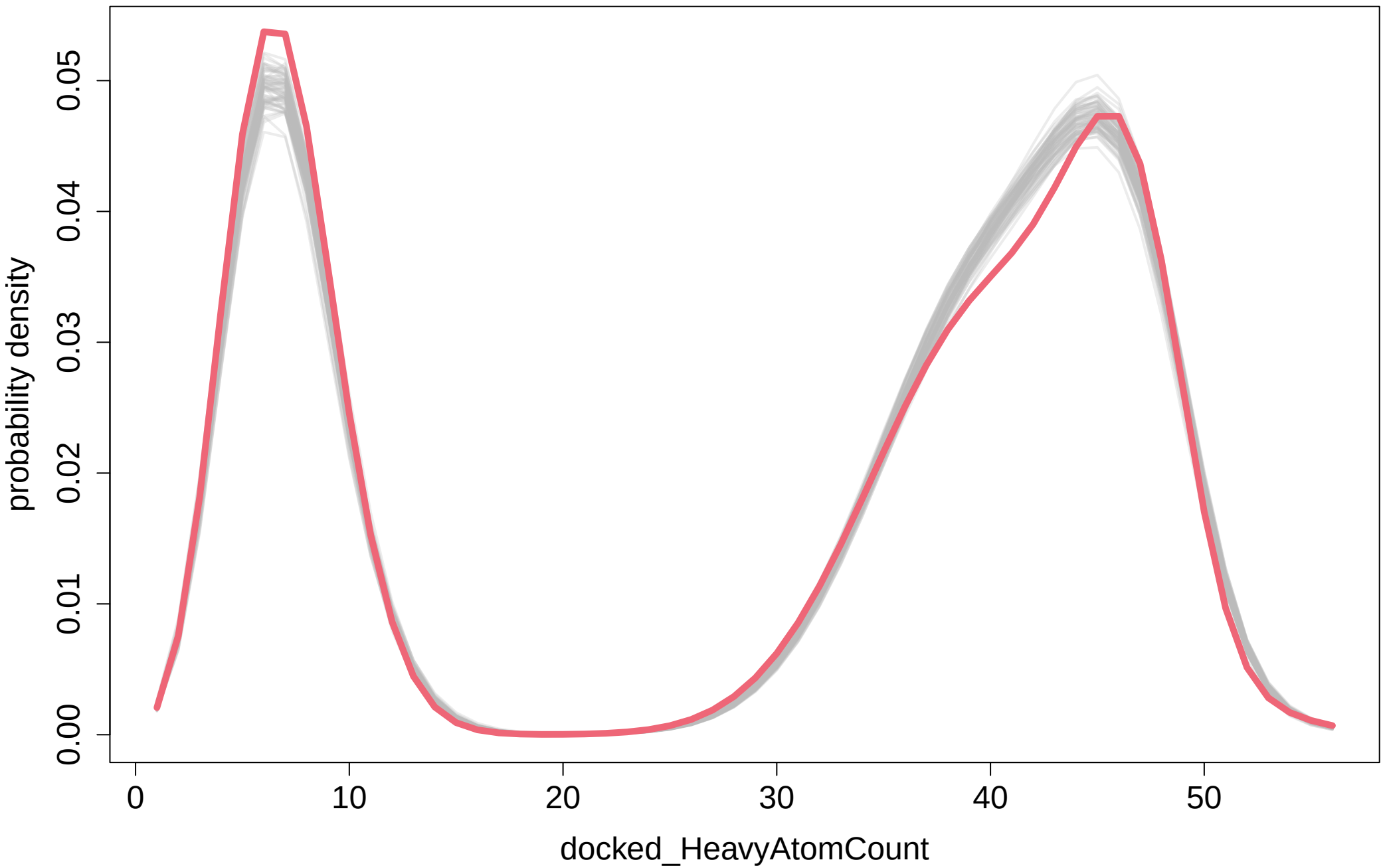
0.10
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms


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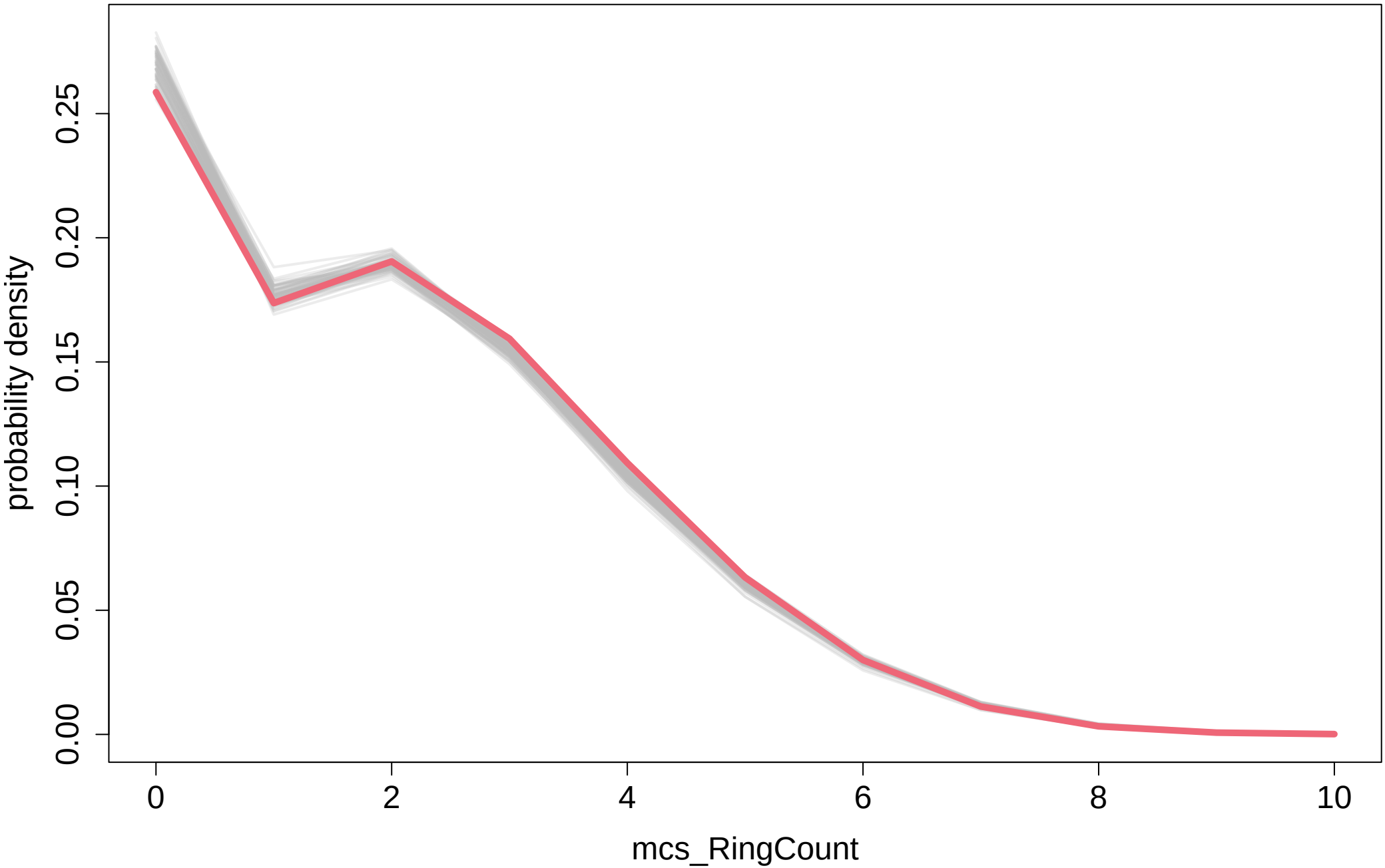
0.02
0.03
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount


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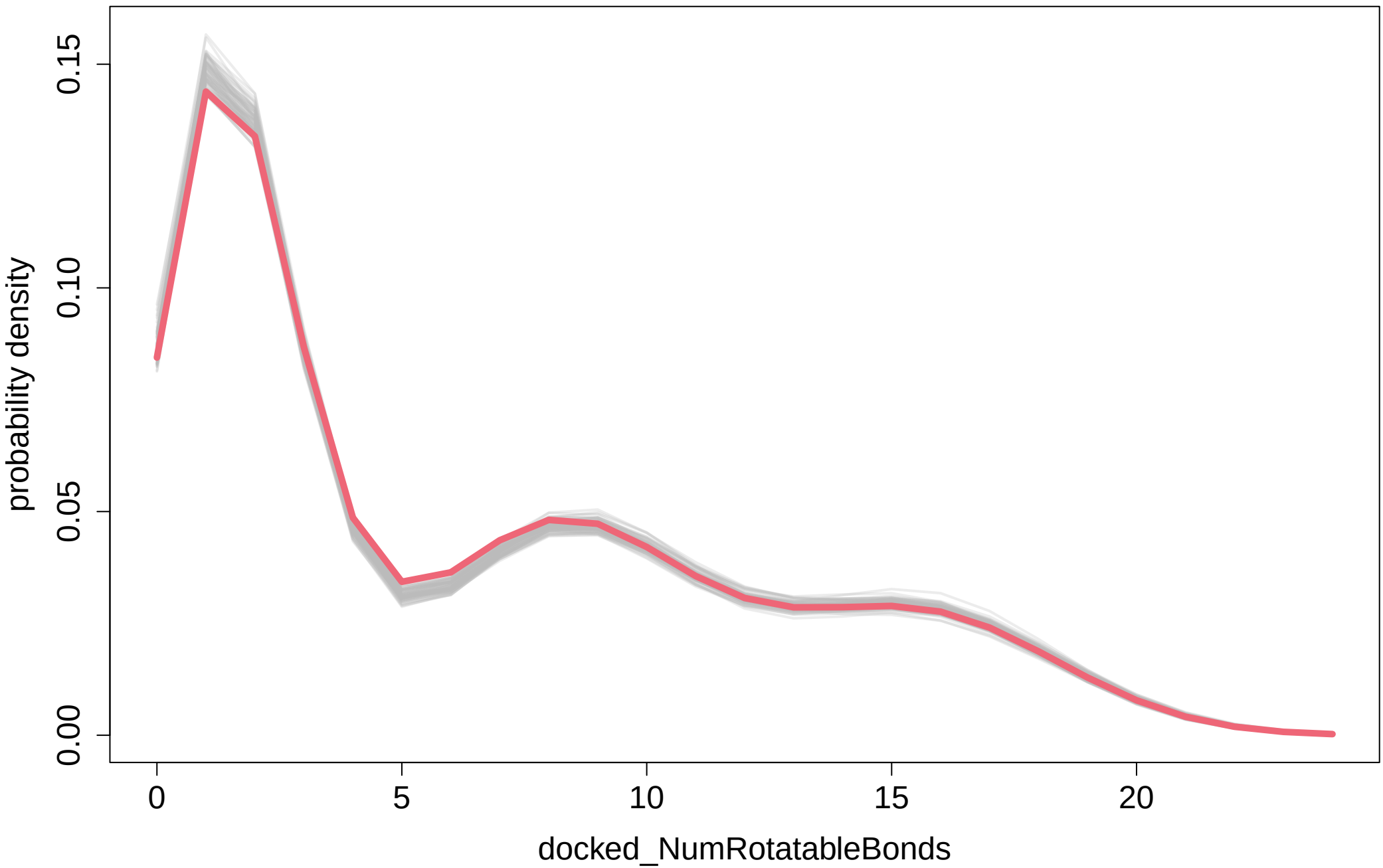
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount


probability density
0.00
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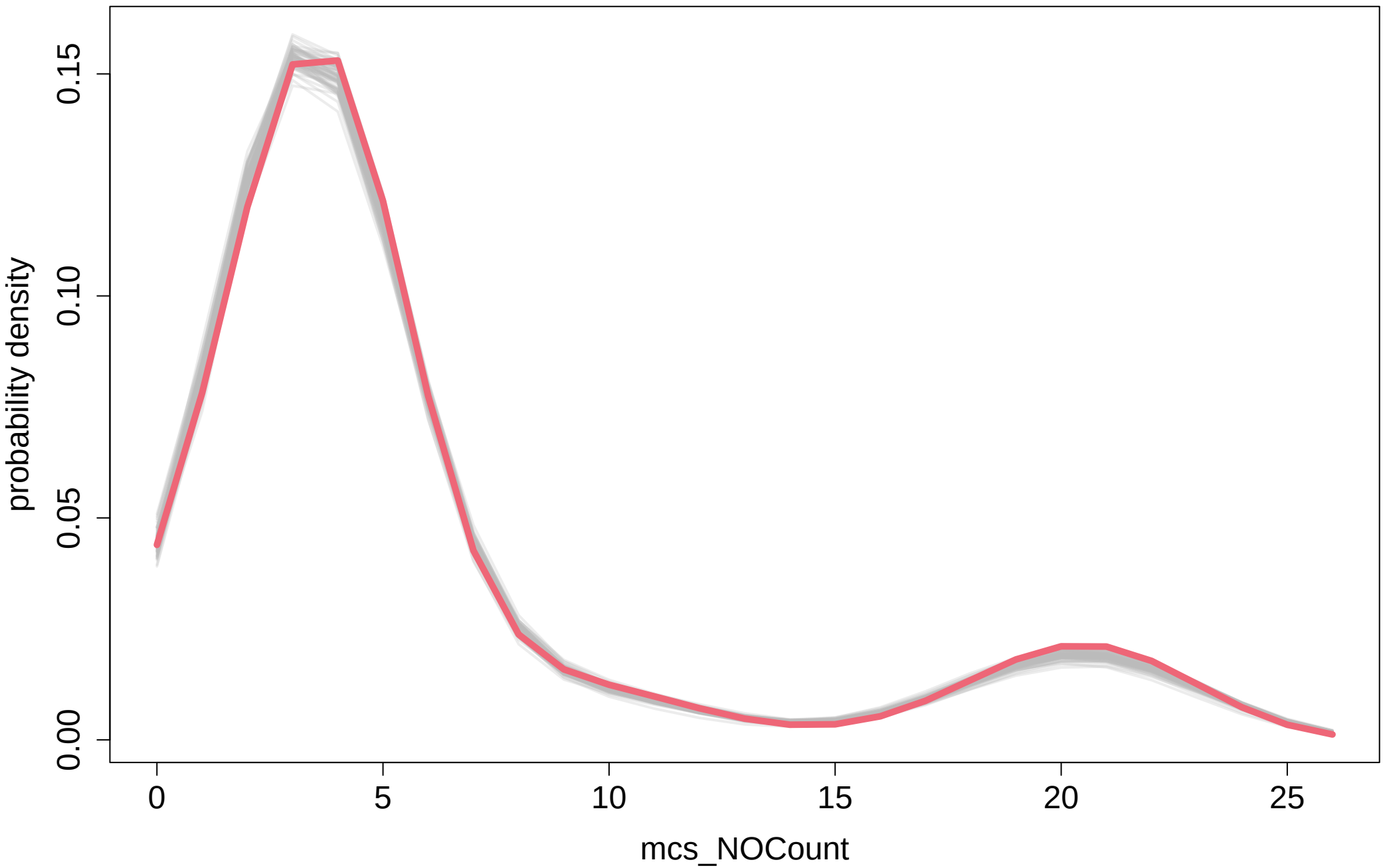
0.15
0
5
10
15
20
docked_NumRotatableBonds


probability density
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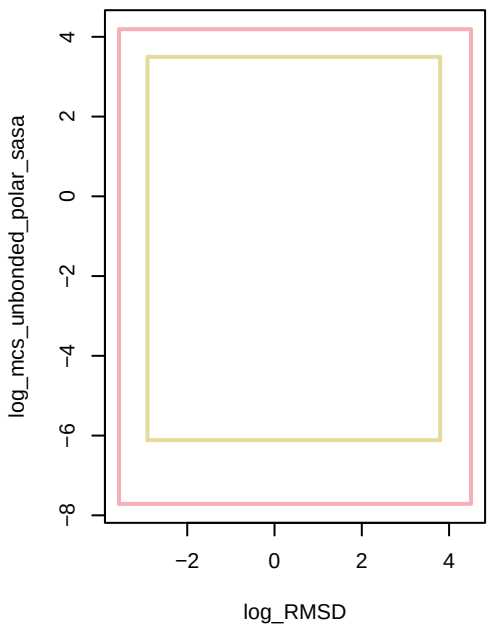
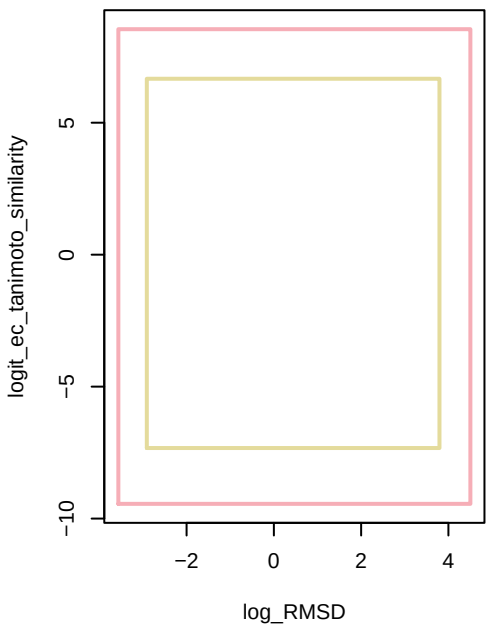
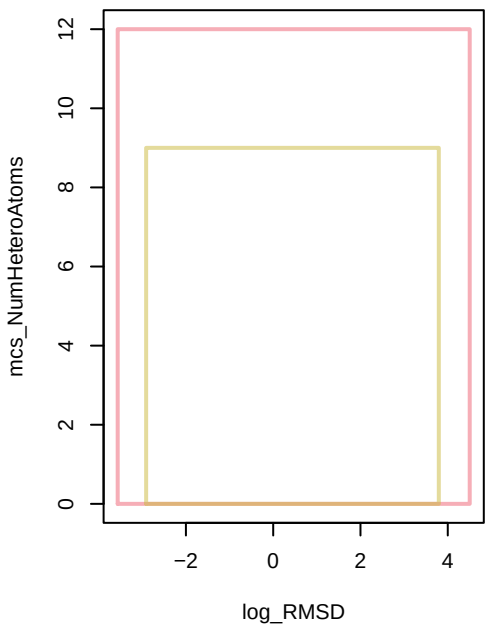
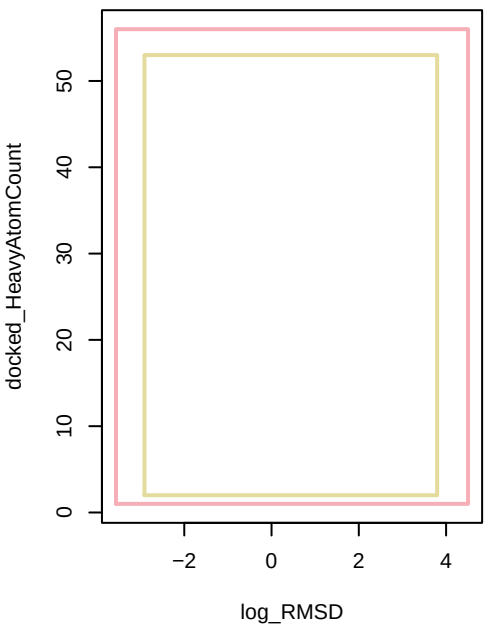
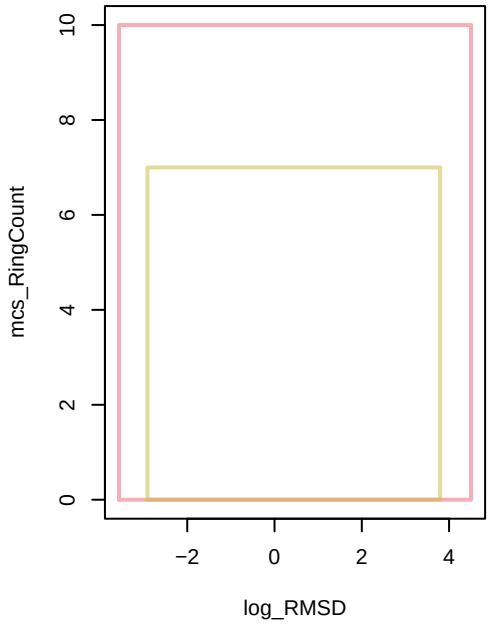
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

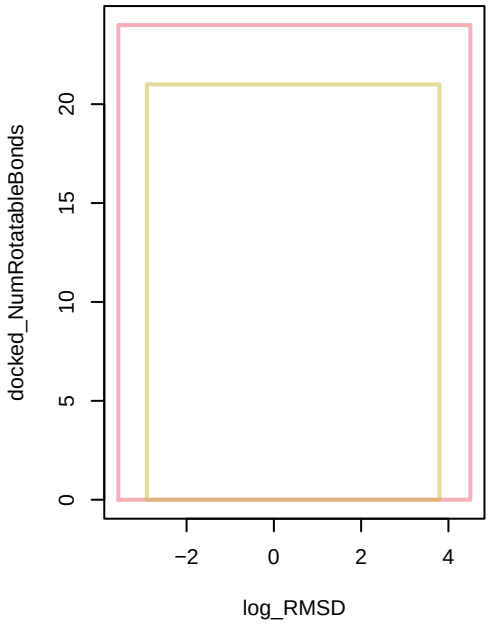

log_mcs_unbonded_polar_sasa
log_RMSD

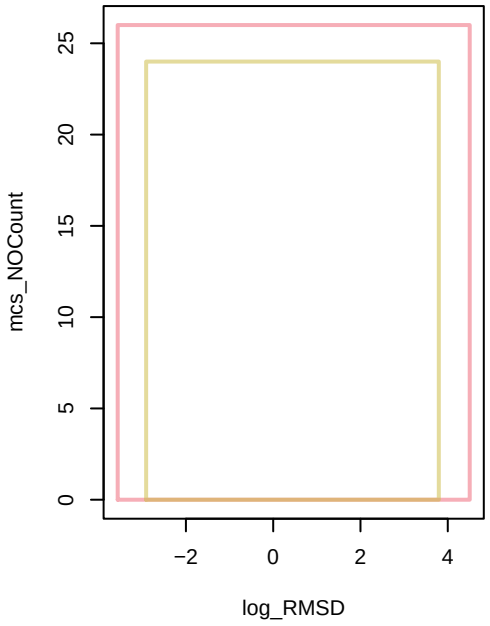

logit_ec_tanimoto_similarity
log_RMSD

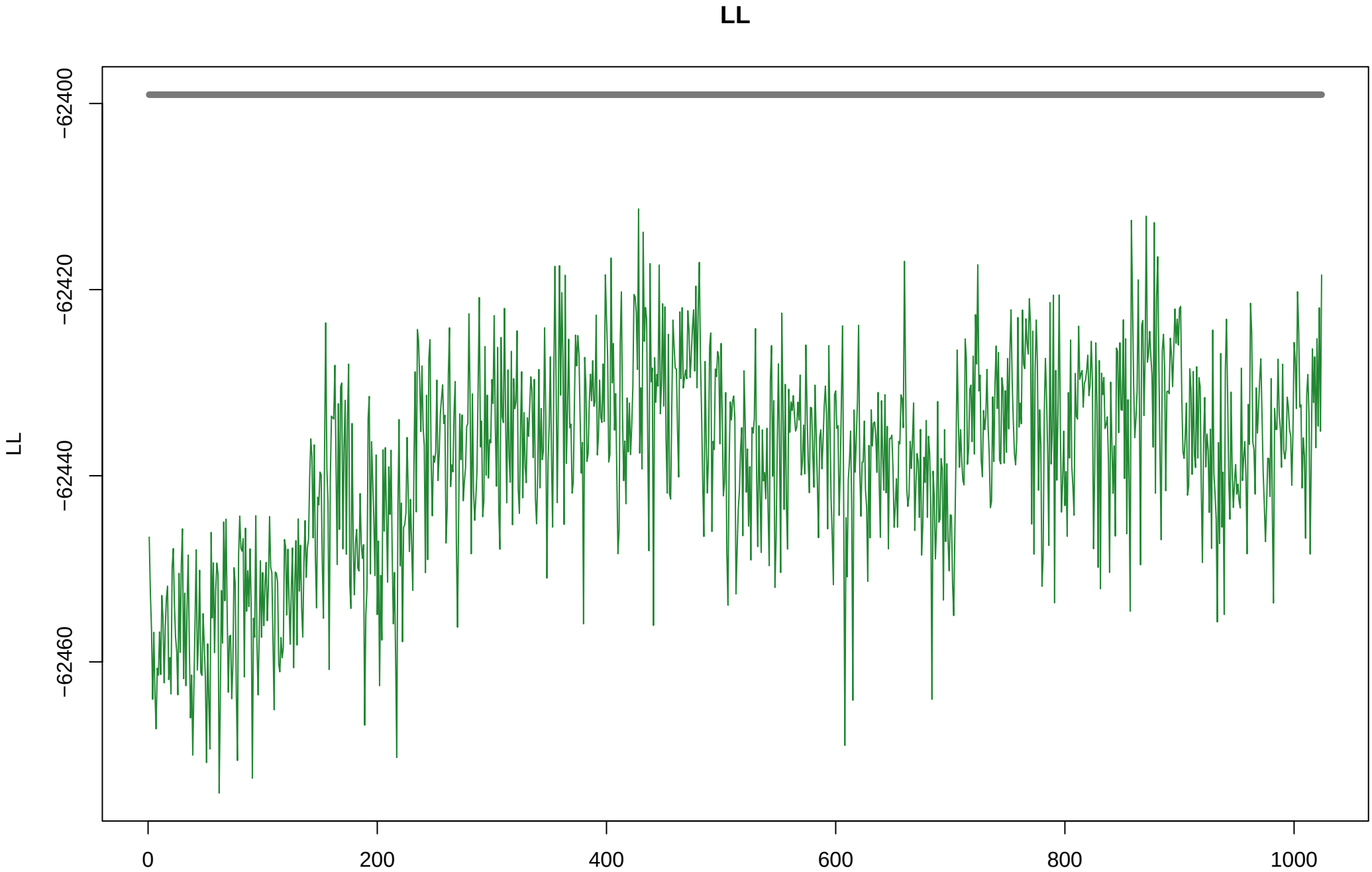

mcs_NumHeteroAtoms
log_RMSD

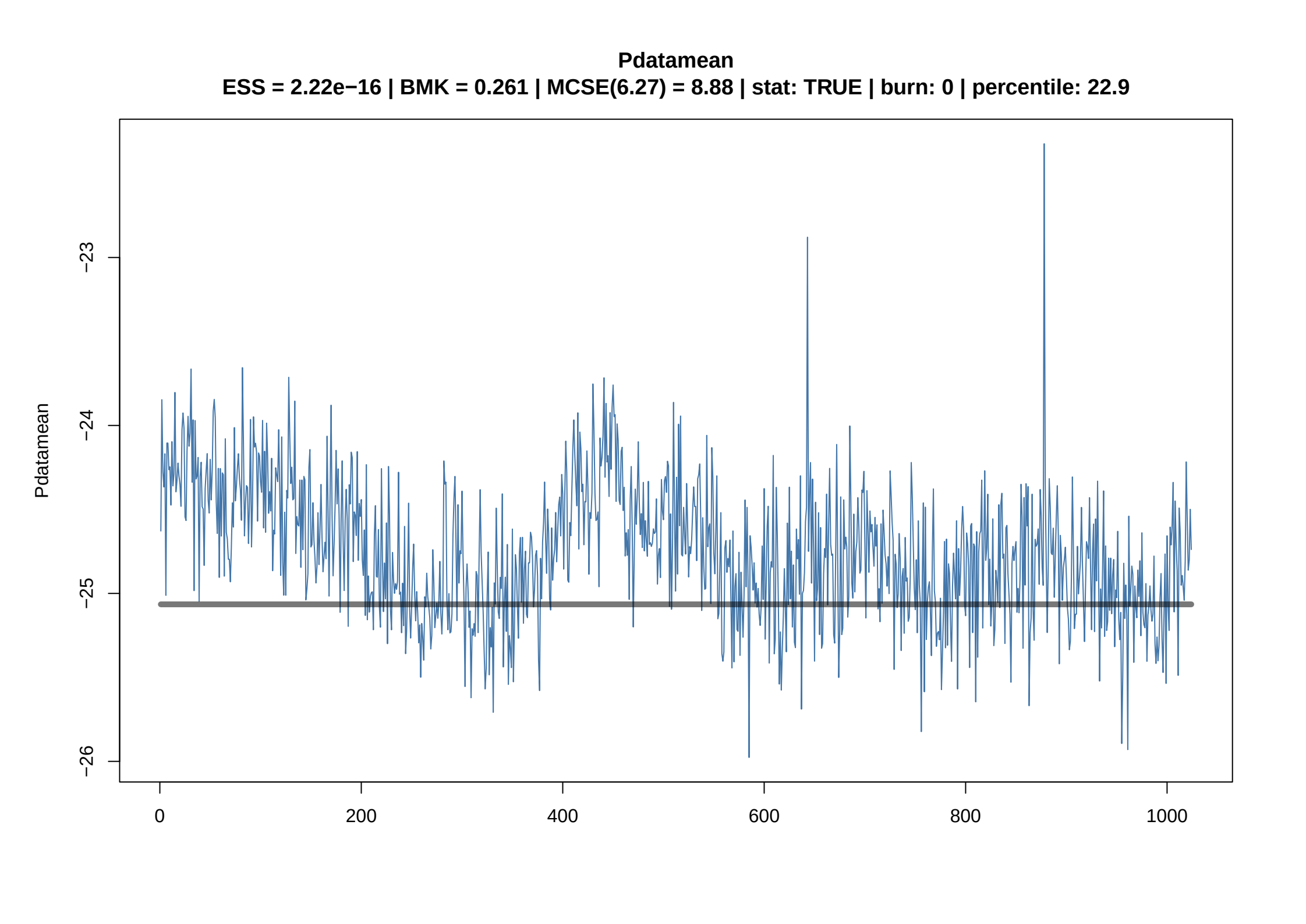

docked_HeavyAtomCount
log_RMSD

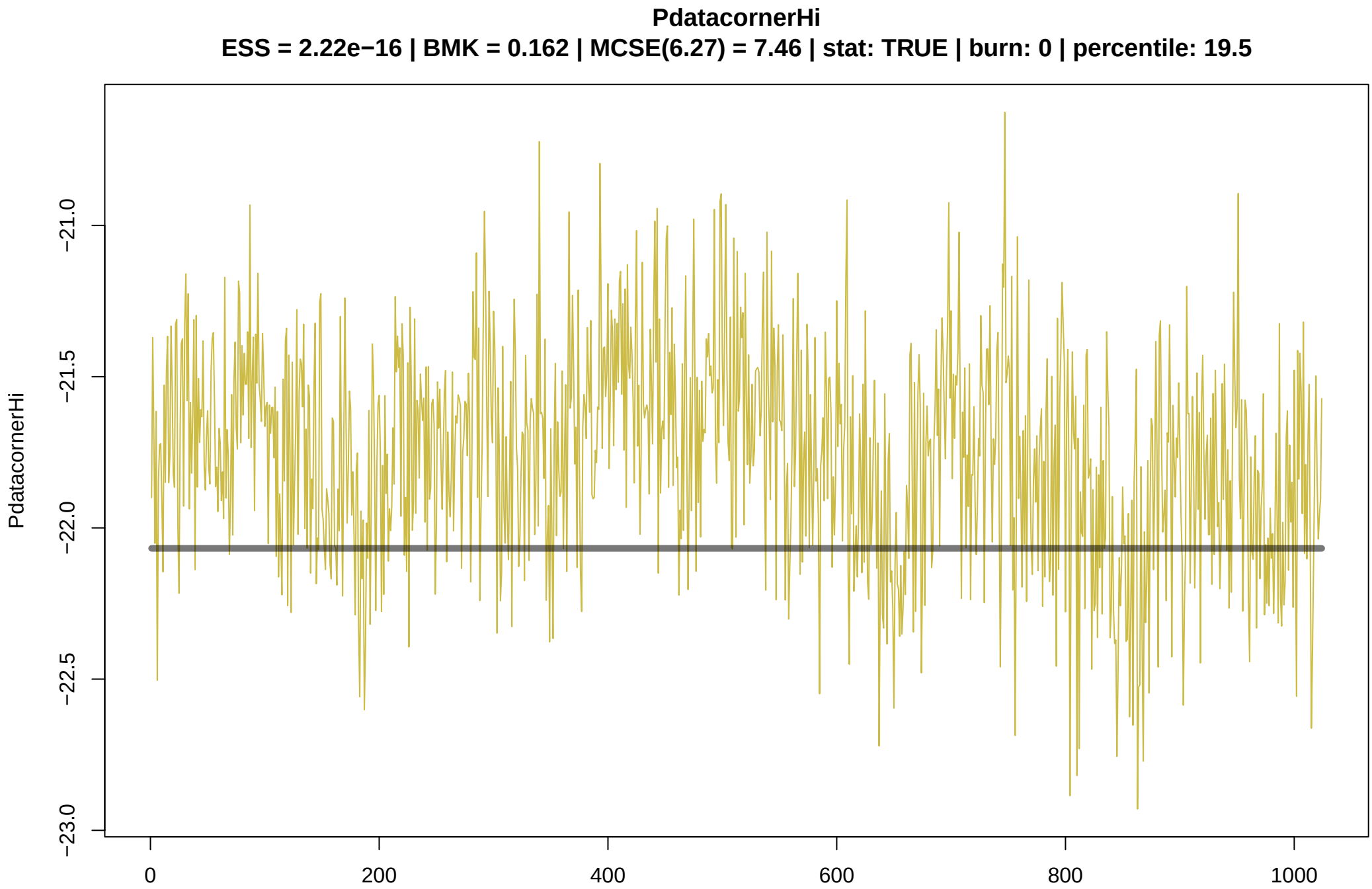

mcs_RingCount
log_RMSD

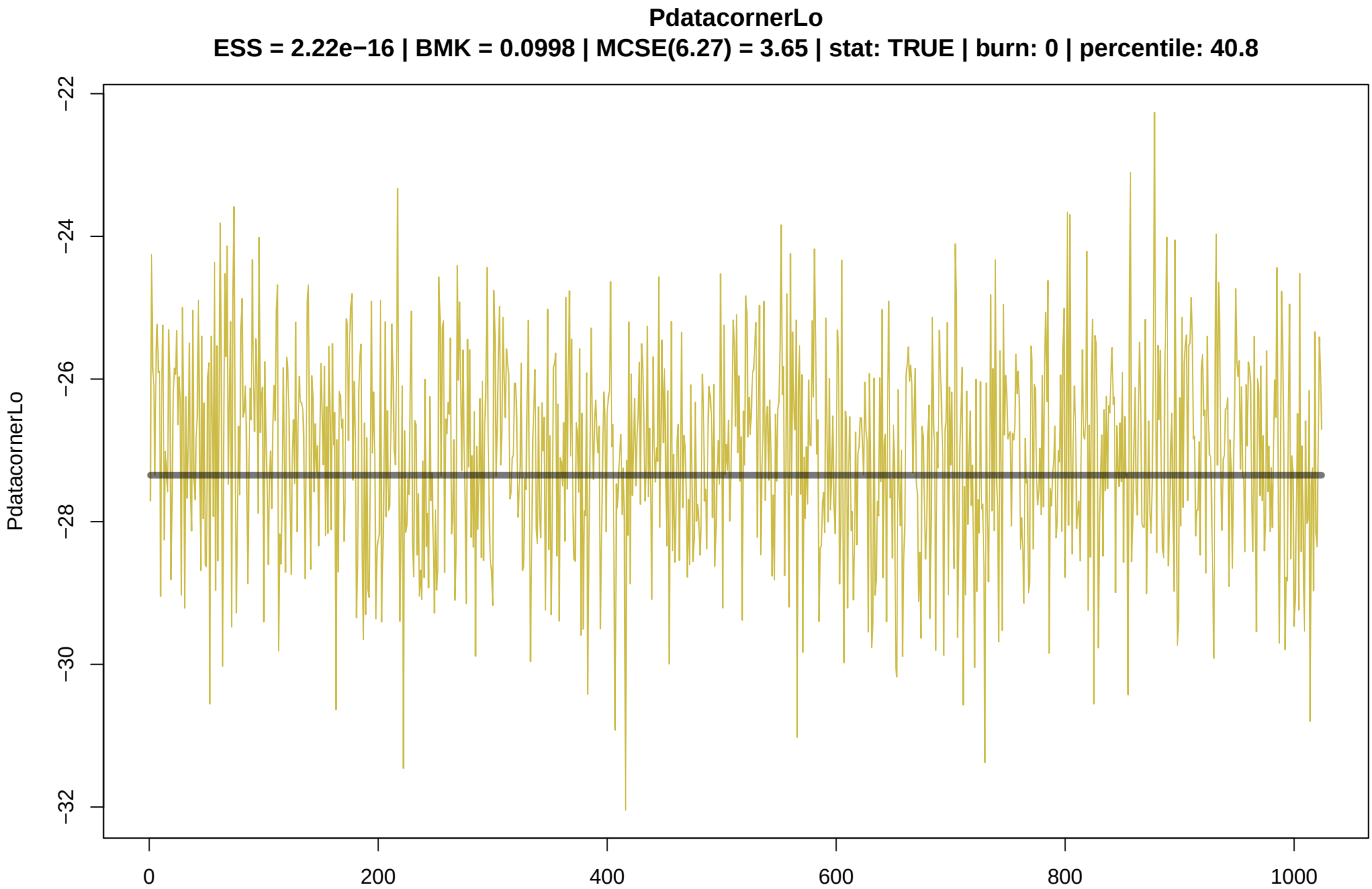

docked_NumRotatableBonds
log_RMSD

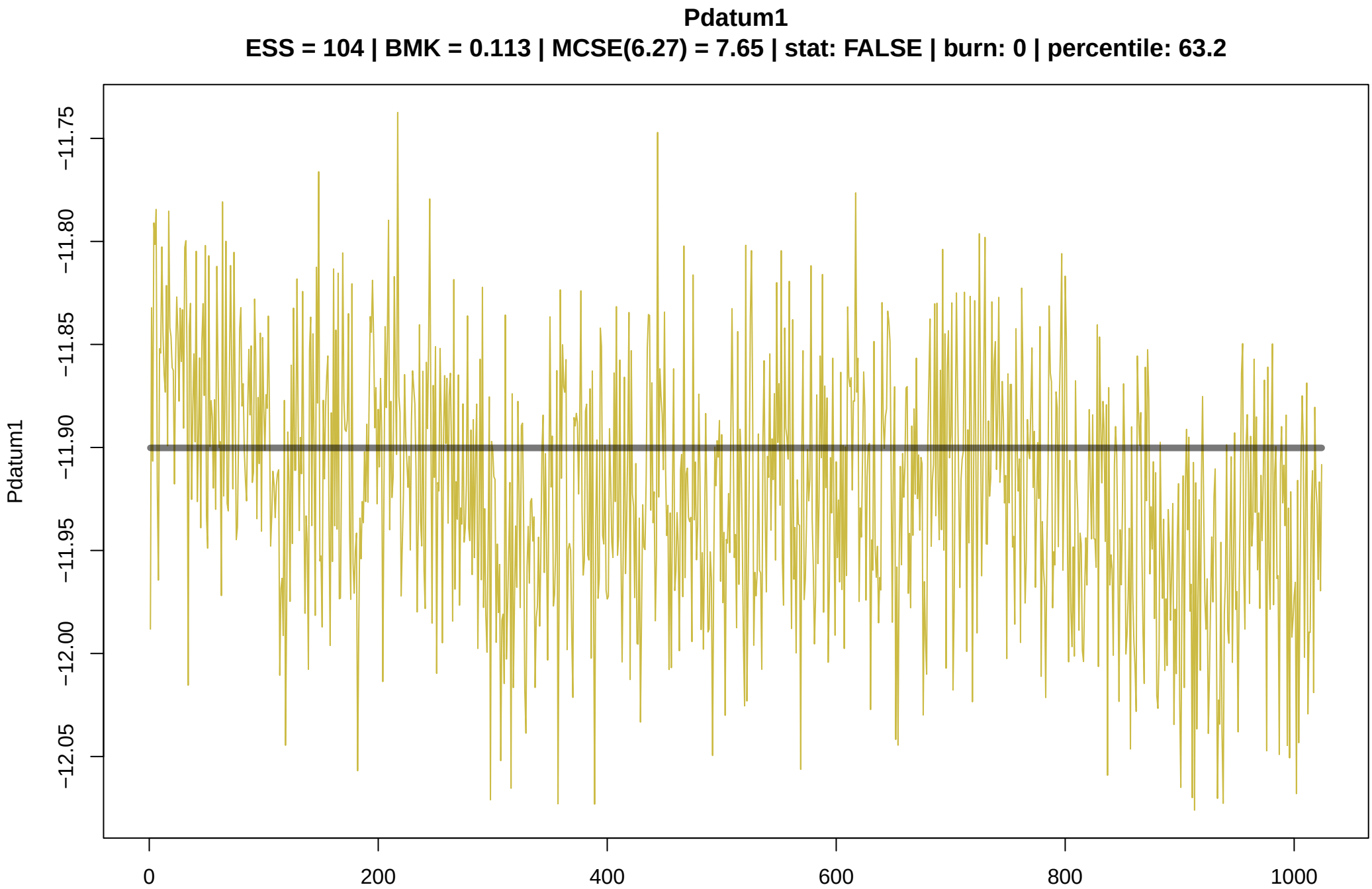

mcs_NOCount
log_RMSD

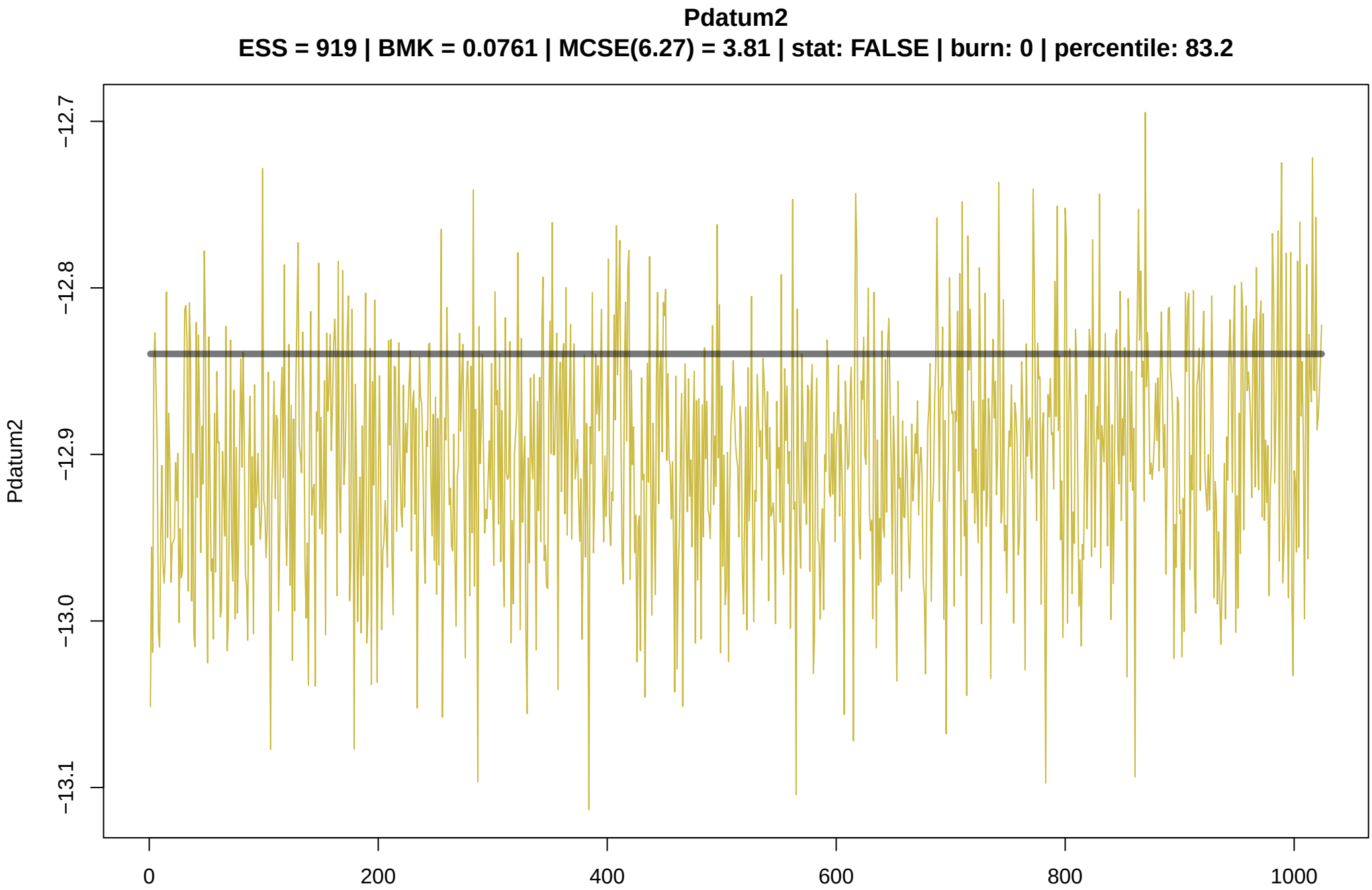

LL
LL
−62400
−62420
−62440
−62460
0
200
400
600
800
1000

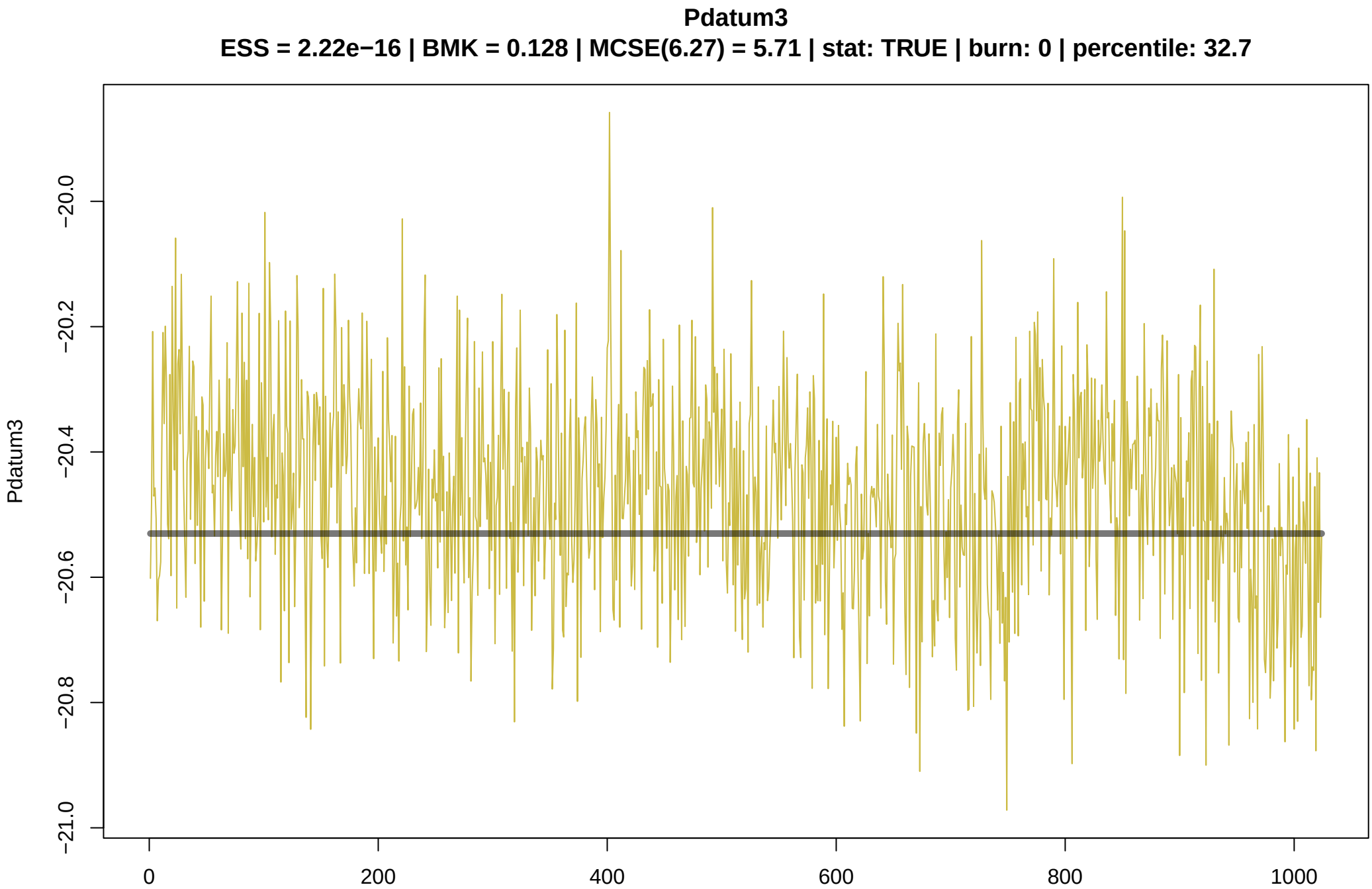

Pdatamean
ESS = 2.22e−16 | BMK = 0.261 | MCSE(6.27) = 8.88 | stat: TRUE | burn: 0 | percentile: 22.9
Pdatamean
−23
−24
−25
−26
0
200
400
600
800
1000

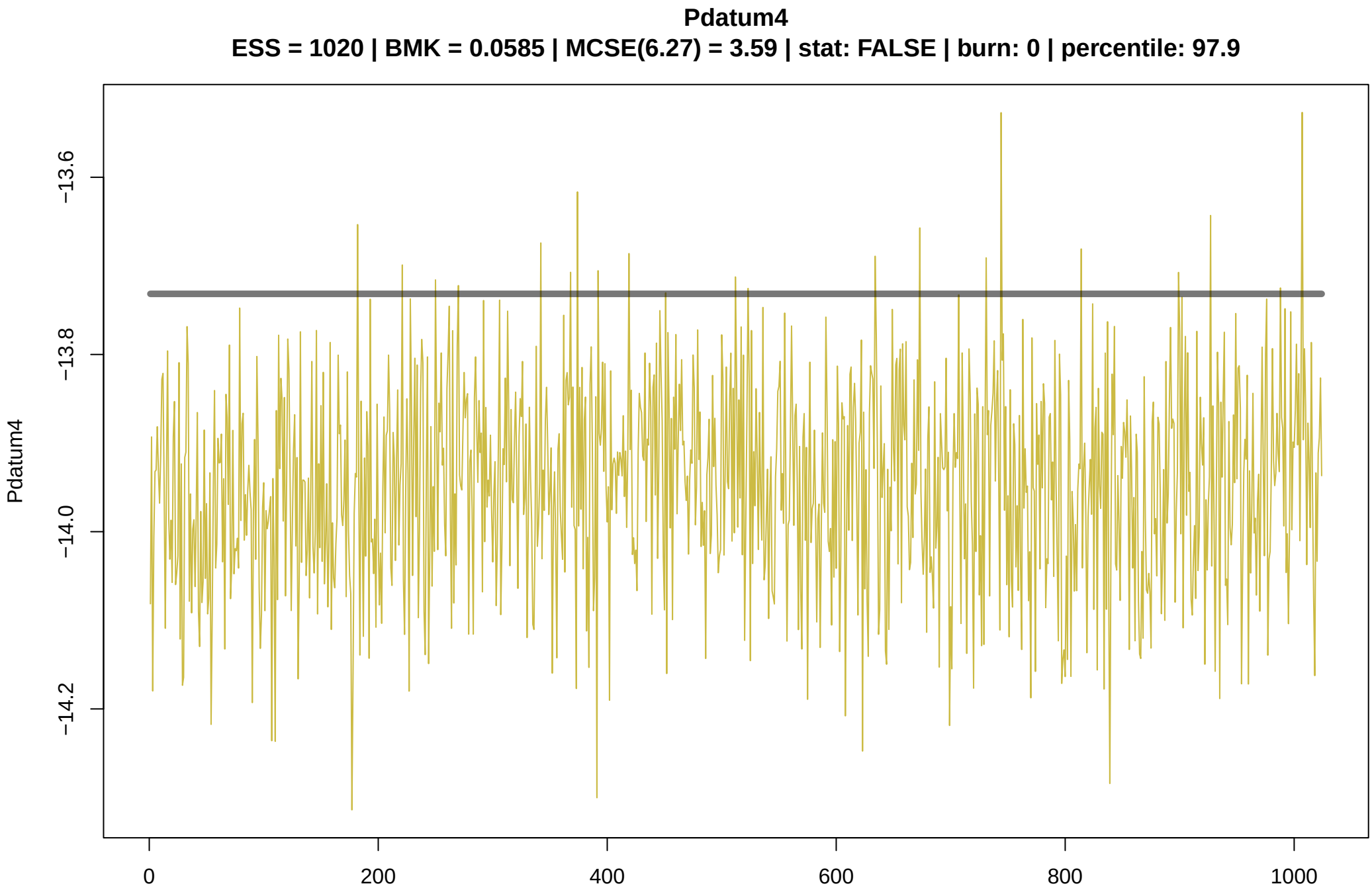

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.162 | MCSE(6.27) = 7.46 | stat: TRUE | burn: 0 | percentile: 19.5
PdatacornerHi
−21.0
−21.5
−22.0
−22.5
−23.0
0
200
400
600
800
1000

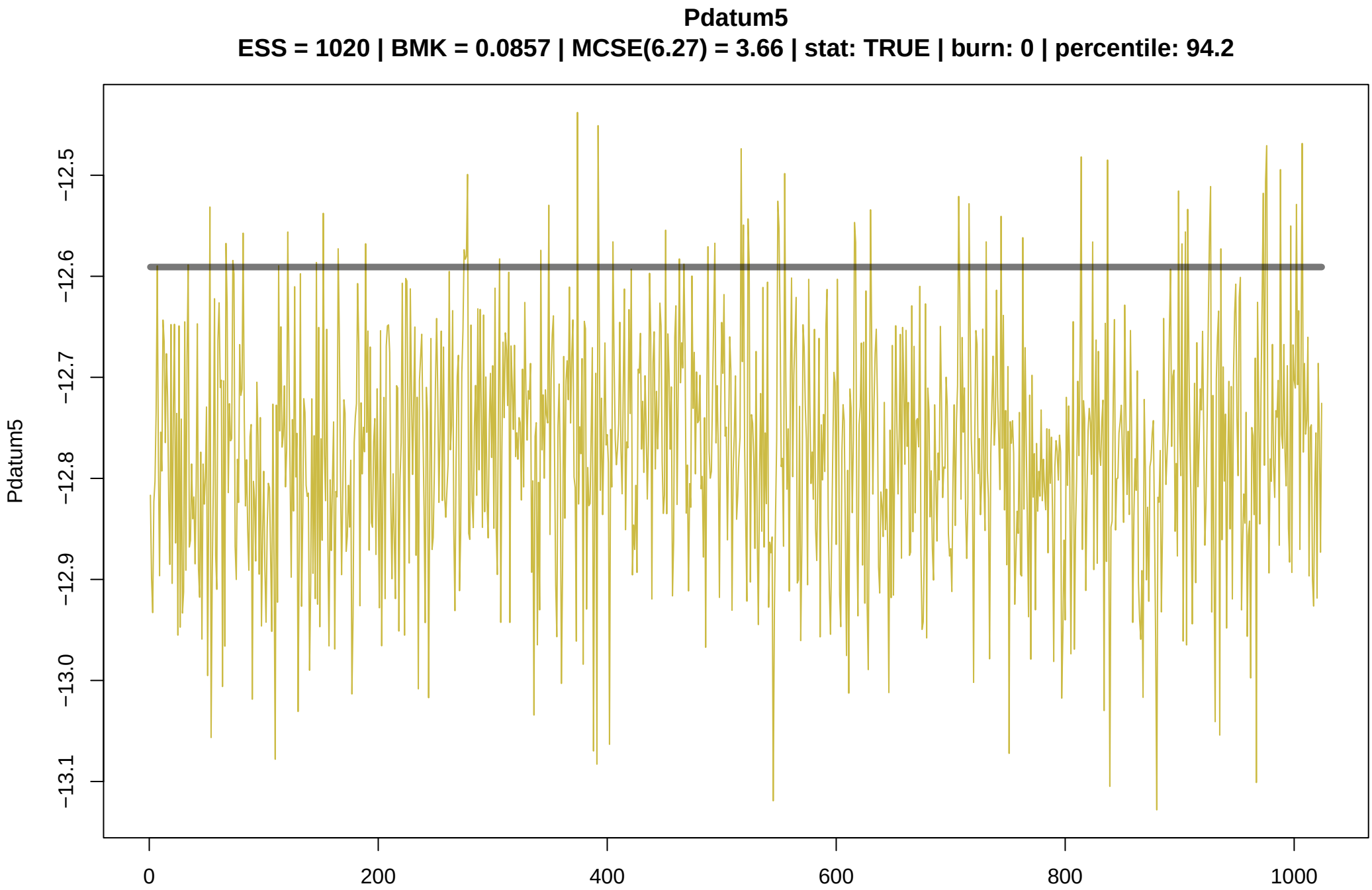

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.0998 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0 | percentile: 40.8
PdatacornerLo
−22
−24
−26
−28
−30
−32
0
200
400
600
800
1000

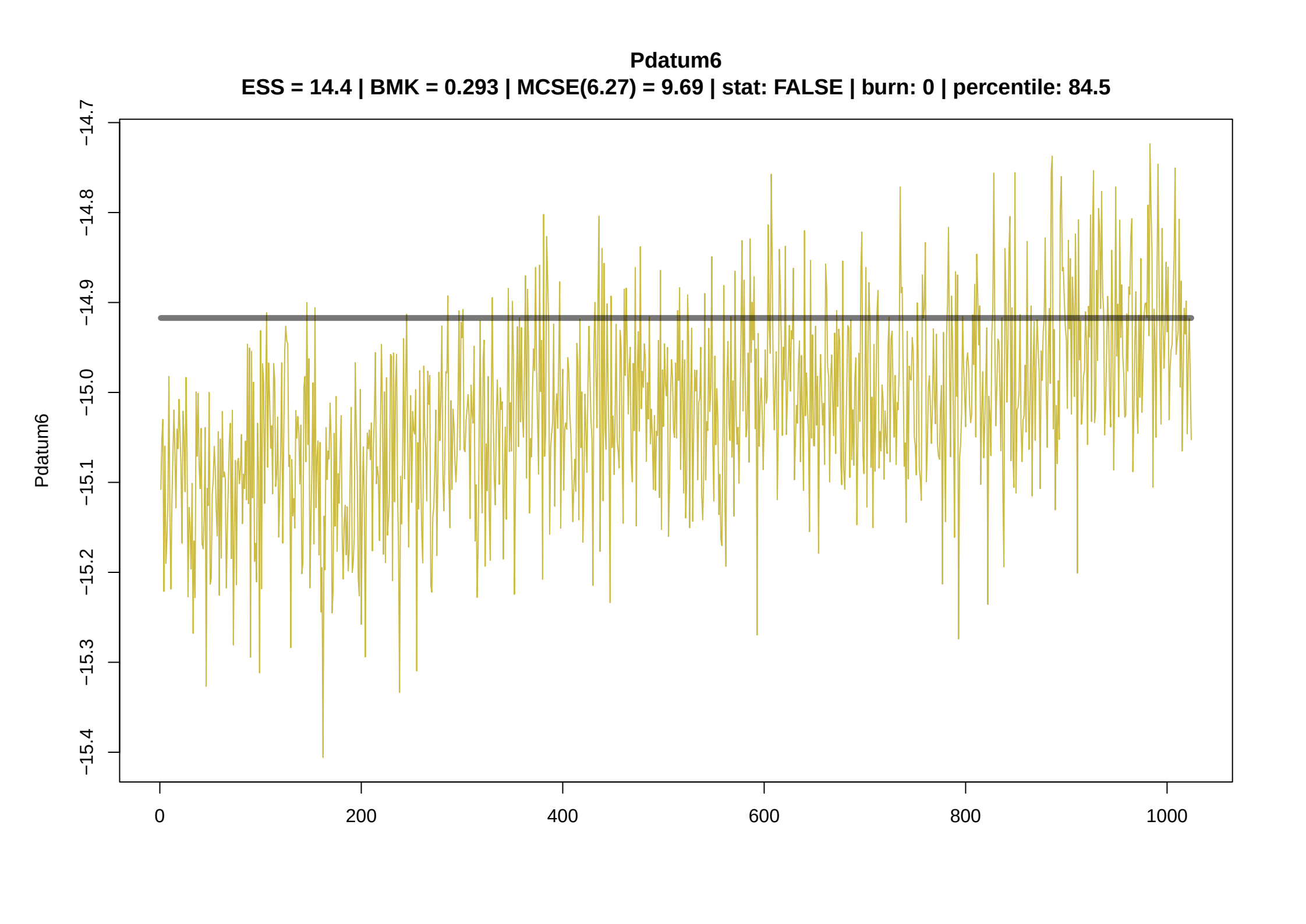

Pdatum1
ESS = 104 | BMK = 0.113 | MCSE(6.27) = 7.65 | stat: FALSE | burn: 0 | percentile: 63.2
Pdatum1
−11.75
−11.80
−11.85
−11.90
−11.95
−12.00
−12.05
0
200
400
600
800
1000

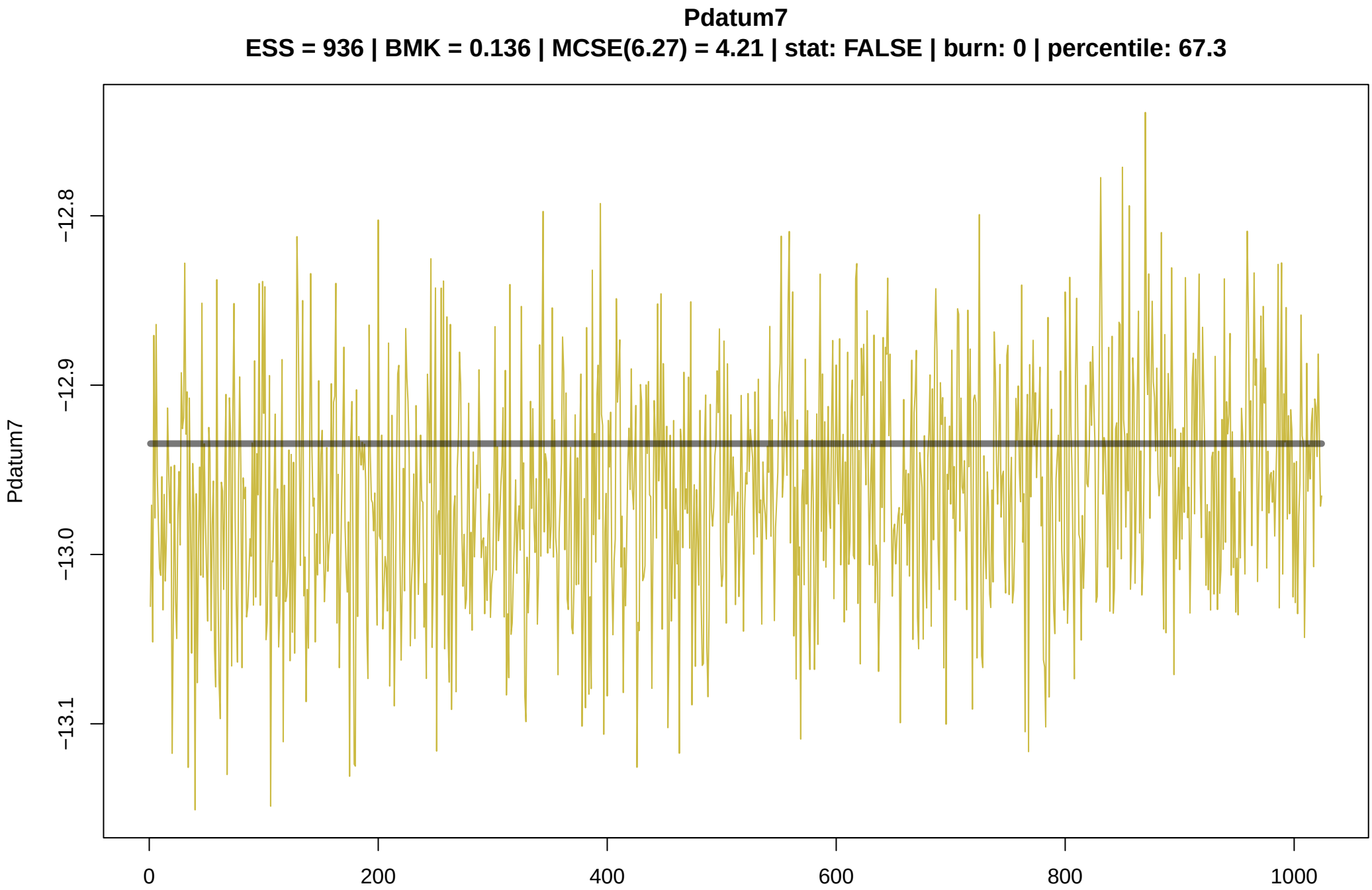

Pdatum2
ESS = 919 | BMK = 0.0761 | MCSE(6.27) = 3.81 | stat: FALSE | burn: 0 | percentile: 83.2
Pdatum2
−12.7
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

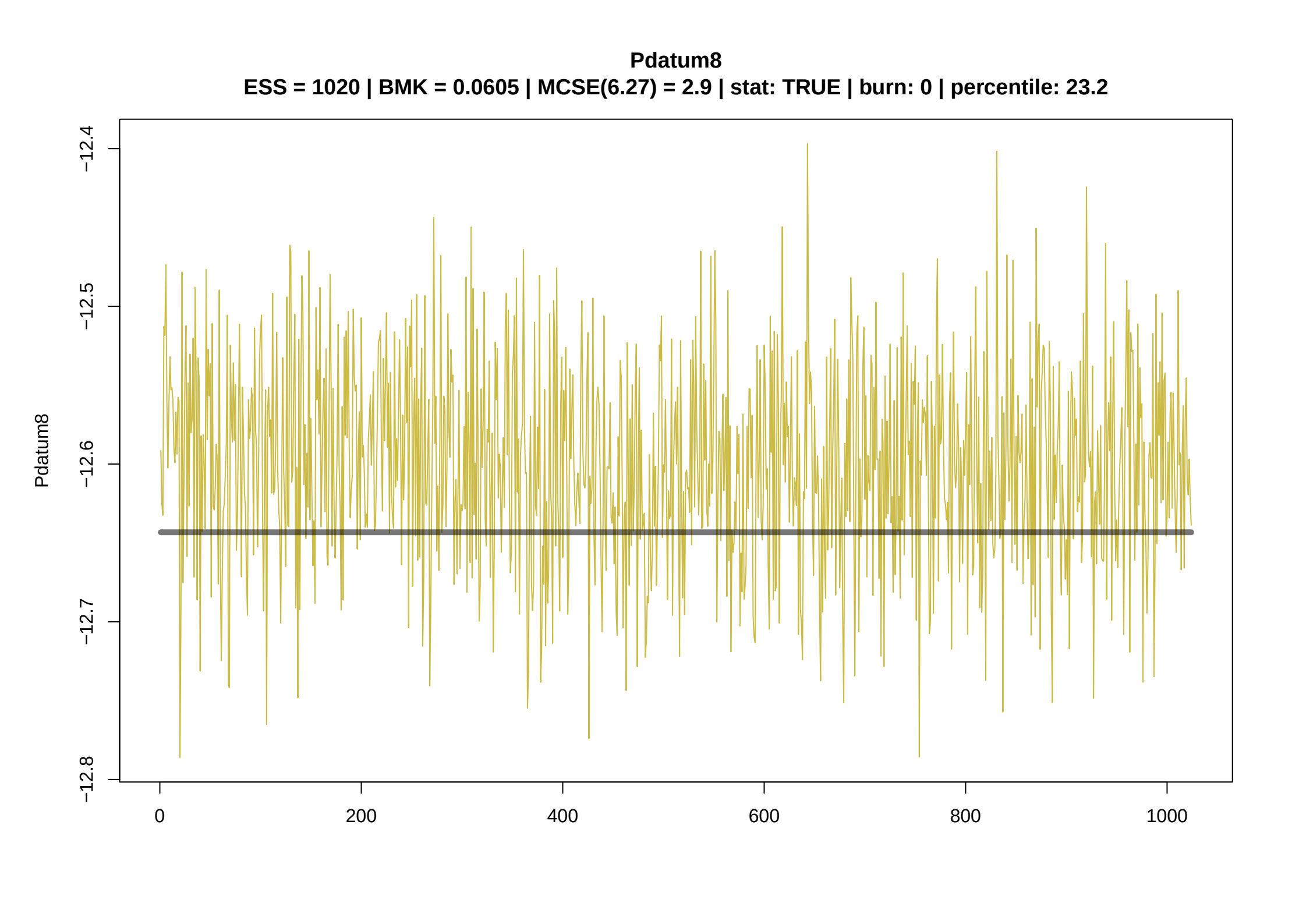

Pdatum3
ESS = 2.22e−16 | BMK = 0.128 | MCSE(6.27) = 5.71 | stat: TRUE | burn: 0 | percentile: 32.7
Pdatum3
−20.0
−20.2
−20.4
−20.6
−20.8
−21.0
0
200
400
600
800
1000

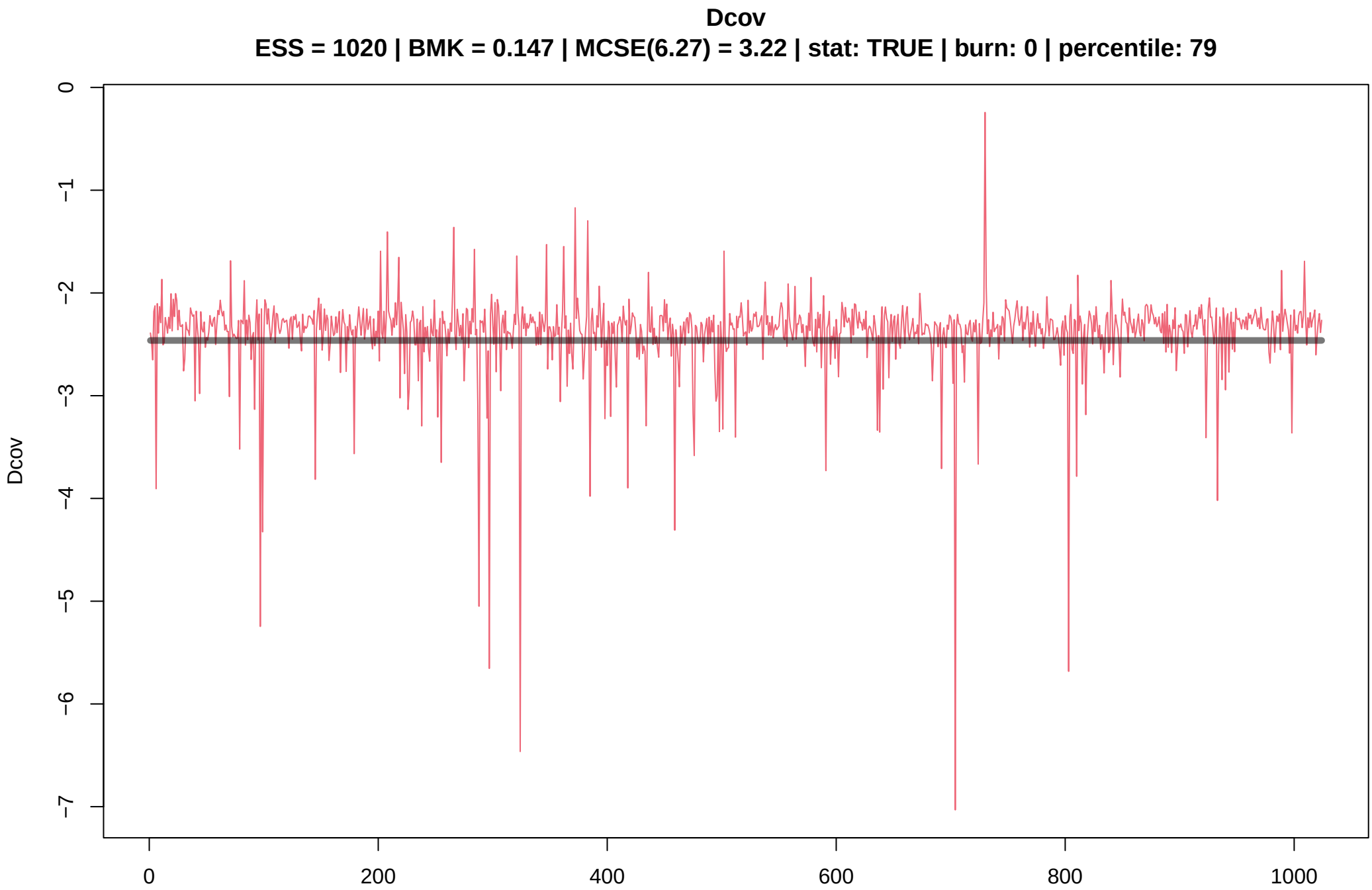

Pdatum4
ESS = 1020 | BMK = 0.0585 | MCSE(6.27) = 3.59 | stat: FALSE | burn: 0 | percentile: 97.9
Pdatum4
−13.6
−13.8
−14.0
−14.2
0
200
400
600
800
1000

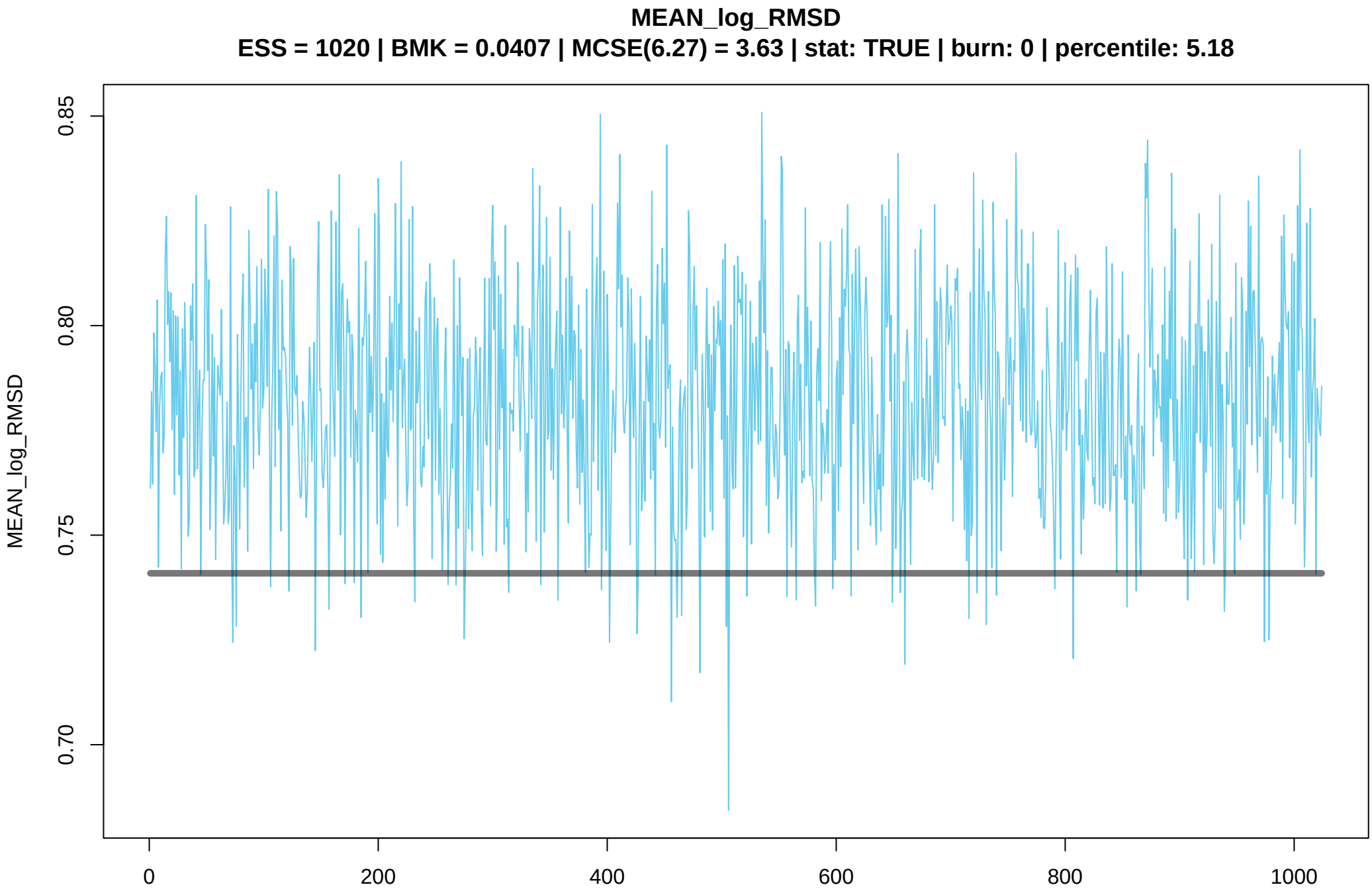

Pdatum5
ESS = 1020 | BMK = 0.0857 | MCSE(6.27) = 3.66 | stat: TRUE | burn: 0 | percentile: 94.2
Pdatum5
−12.5
−12.6
−12.7
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

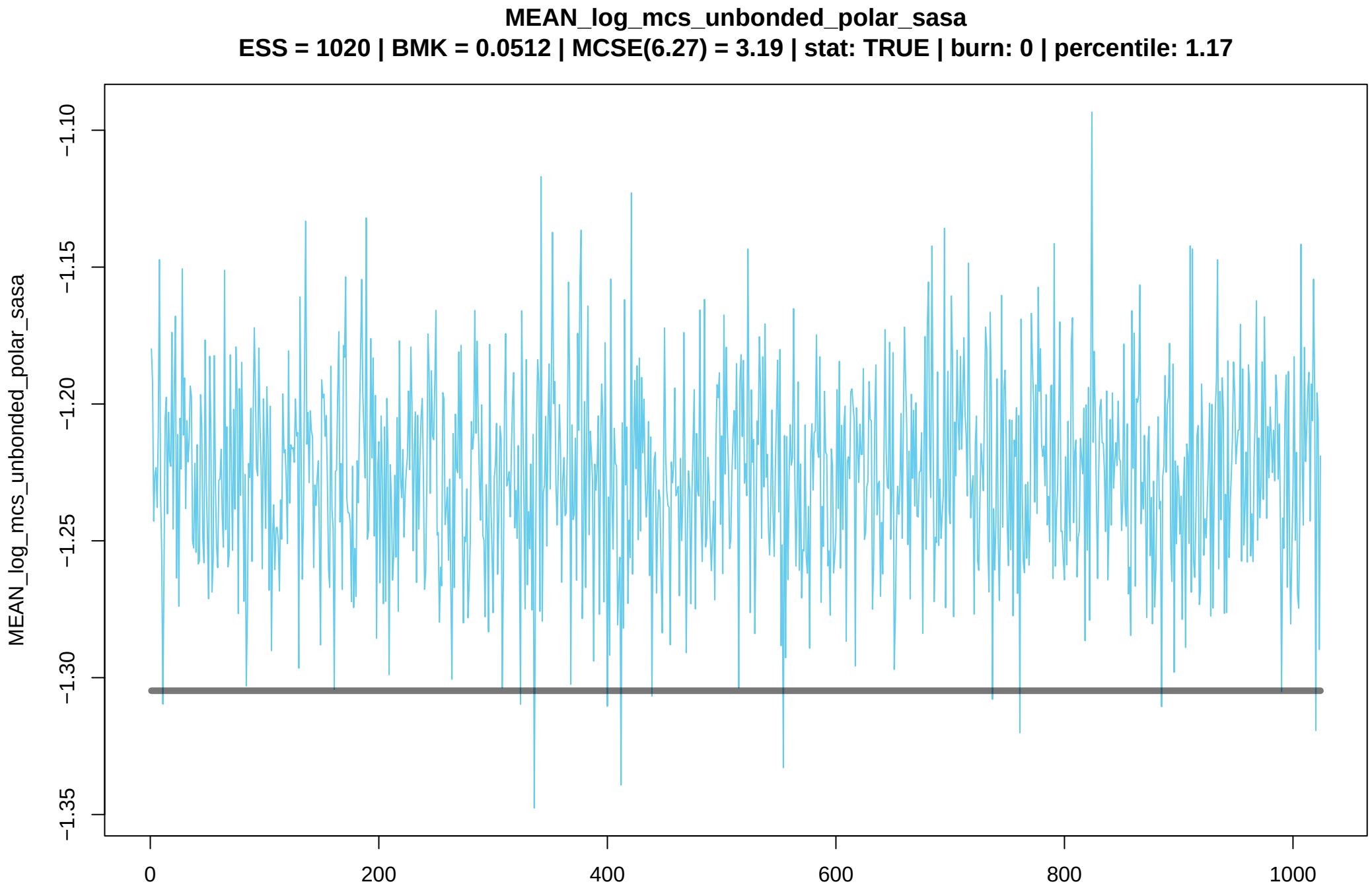

Pdatum6
ESS = 14.4 | BMK = 0.293 | MCSE(6.27) = 9.69 | stat: FALSE | burn: 0 | percentile: 84.5
Pdatum6
−14.7
−14.8
−14.9
−15.0
−15.1
−15.2
−15.3
−15.4
0
200
400
600
800
1000

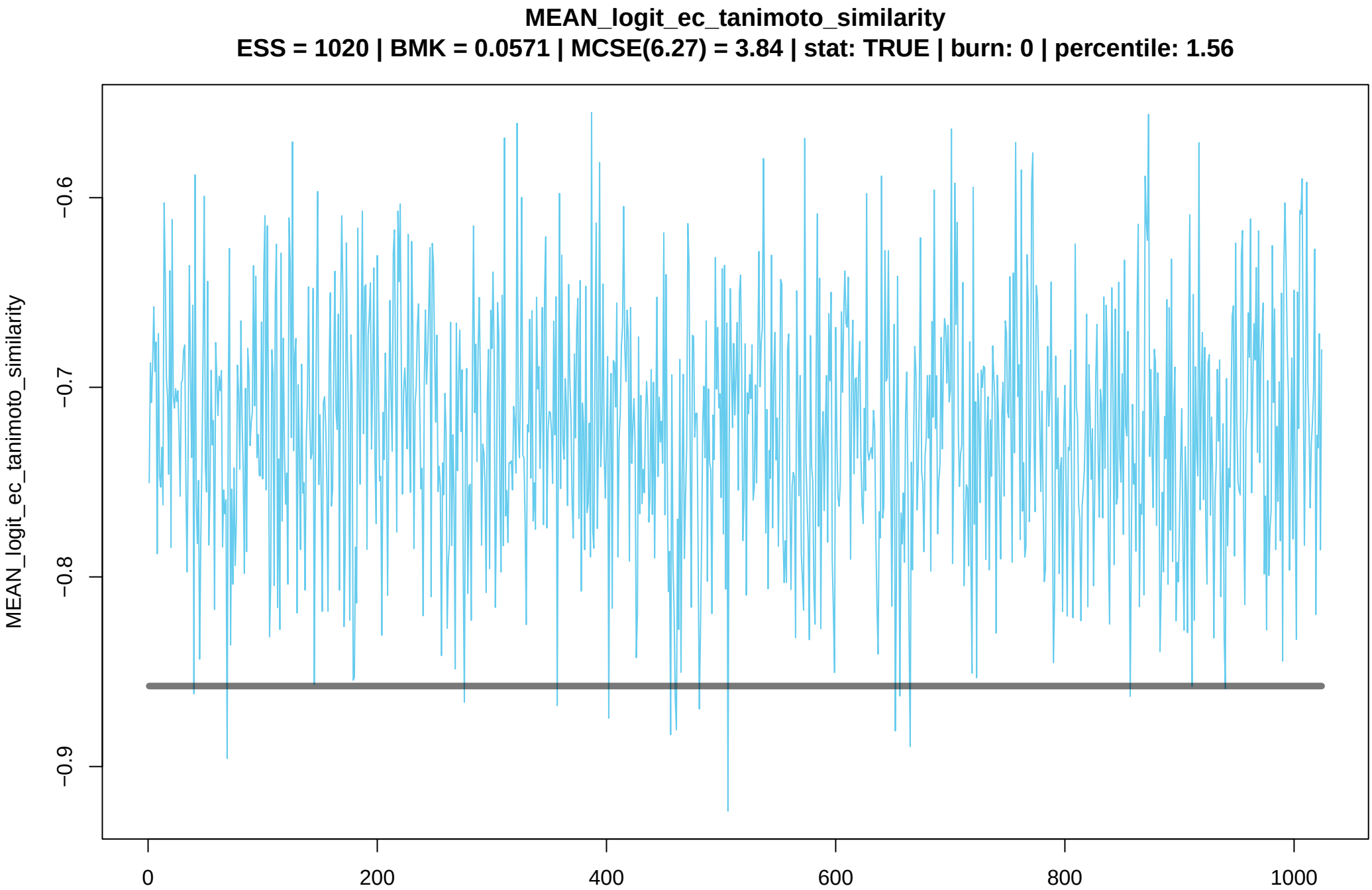

Pdatum7
ESS = 936 | BMK = 0.136 | MCSE(6.27) = 4.21 | stat: FALSE | burn: 0 | percentile: 67.3
Pdatum7
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

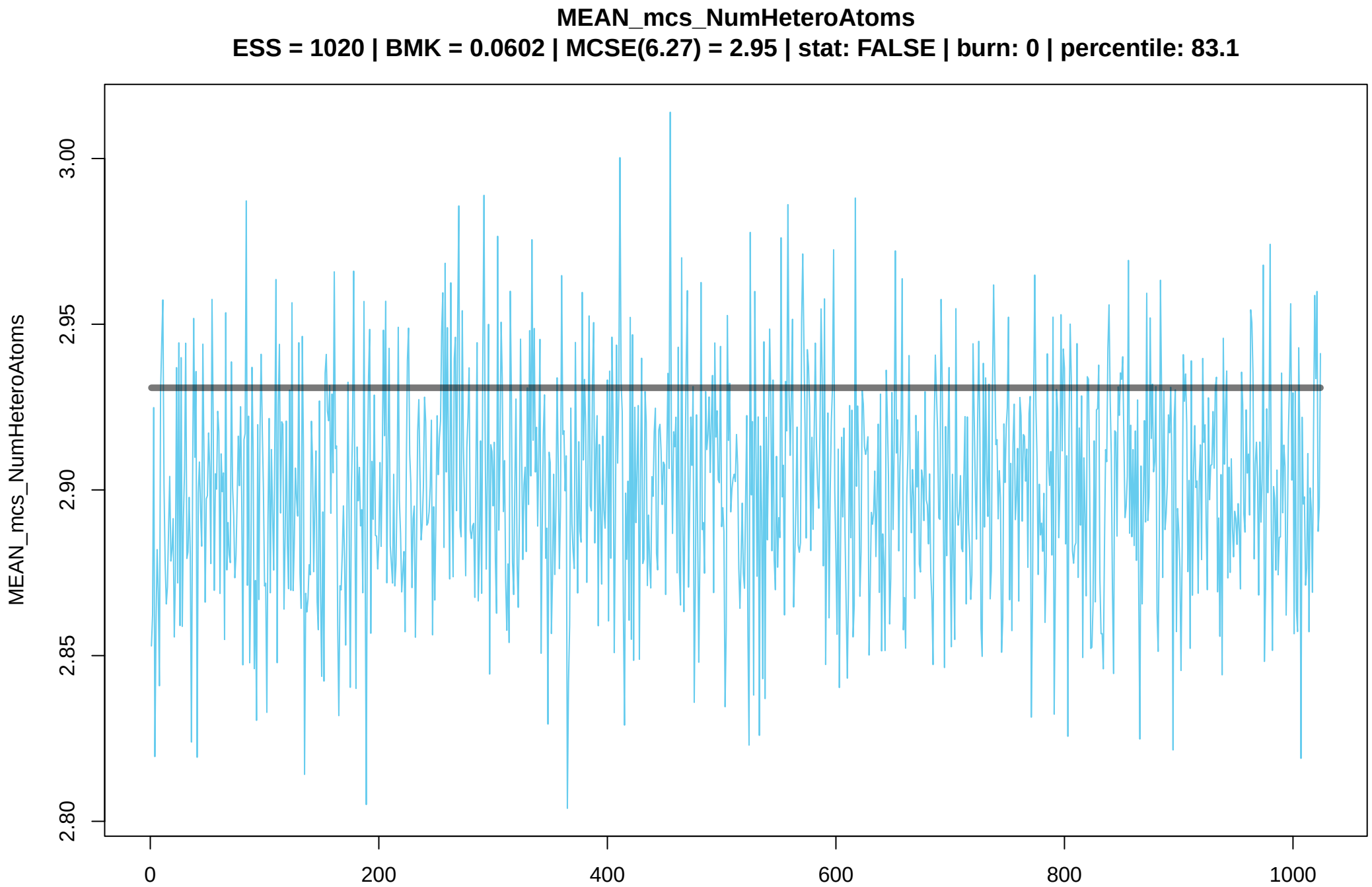

Pdatum8
ESS = 1020 | BMK = 0.0605 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0 | percentile: 23.2
Pdatum8
−12.4
−12.5
−12.6
−12.7
−12.8
0
200
400
600
800
1000

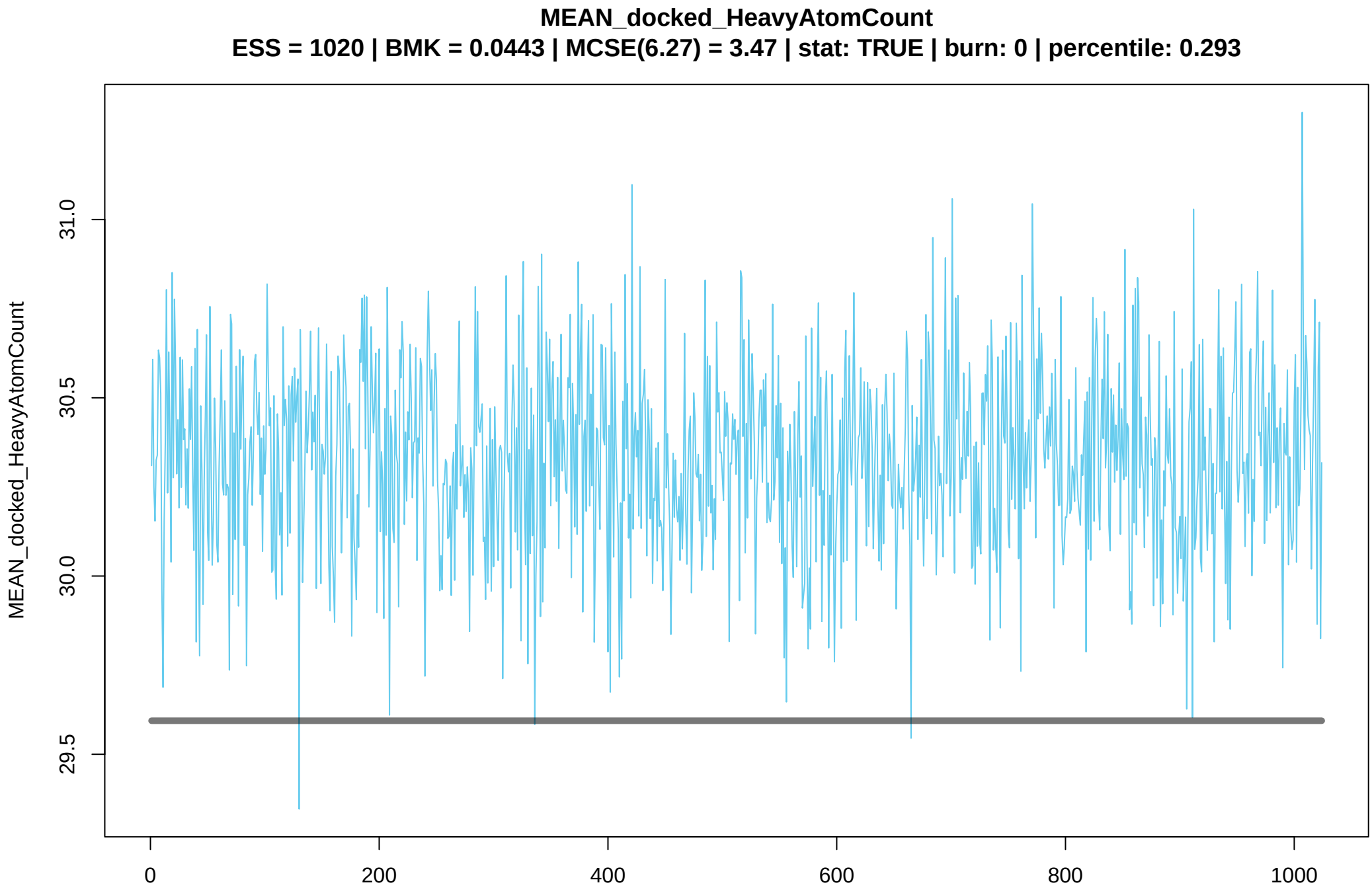

Dcov
ESS = 1020 | BMK = 0.147 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0 | percentile: 79
Dcov
0
−1
−2
−3
−4
−5
−6
−7
0
200
400
600
800
1000

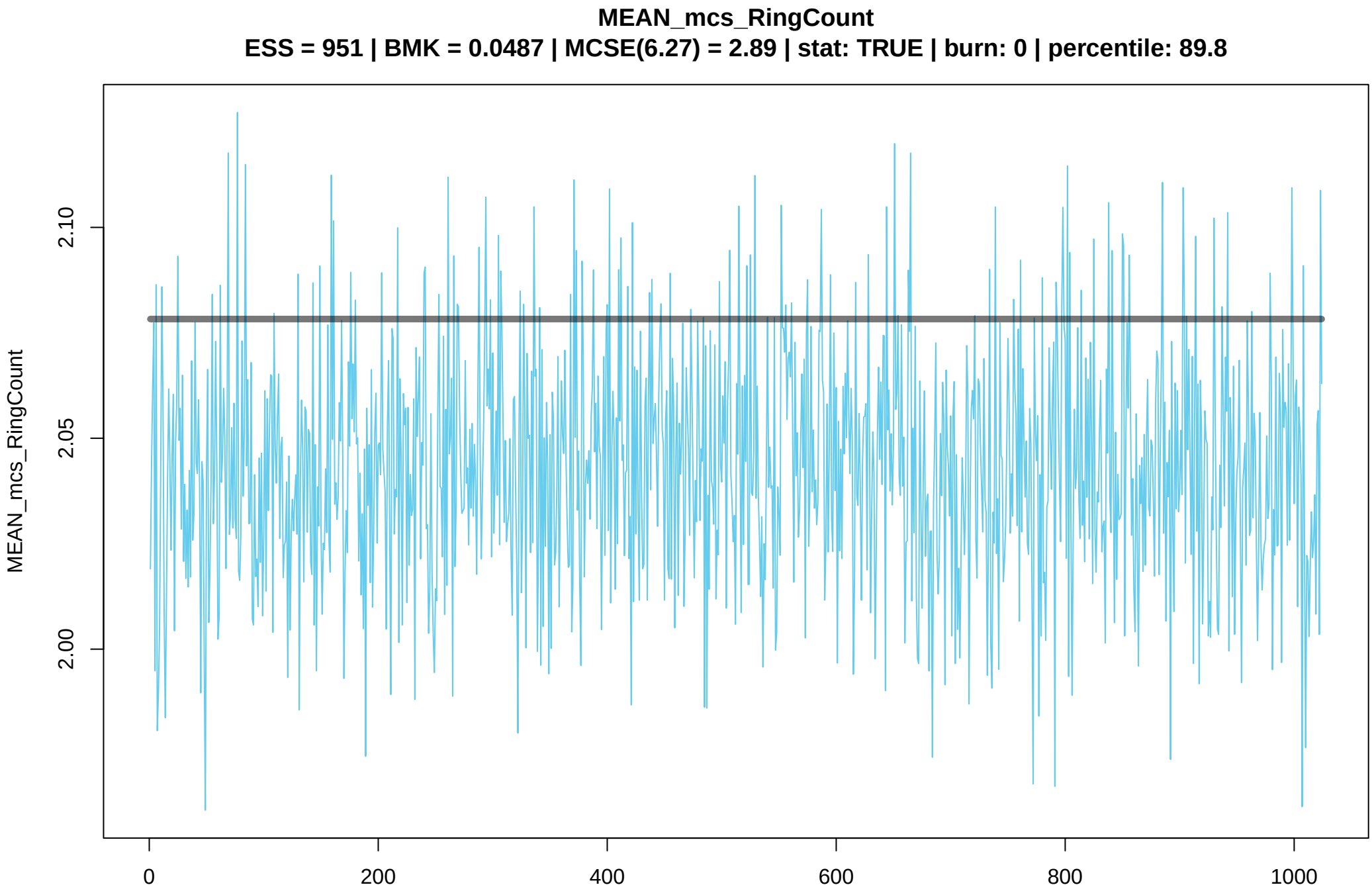

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0407 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | percentile: 5.18
MEAN_log_RMSD
0.85
0.80
0.75
0.70
0
200
400
600
800
1000

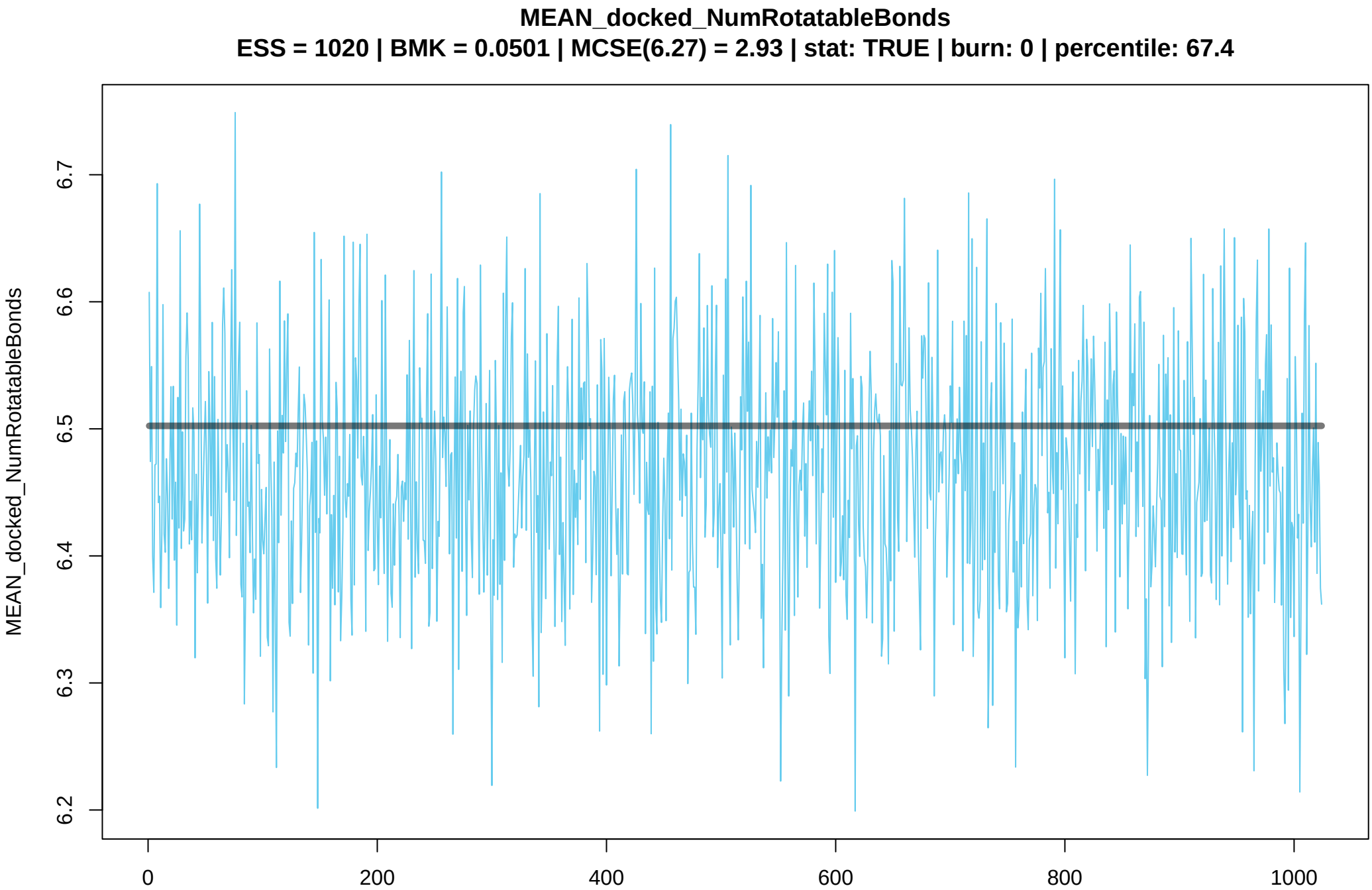

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0512 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 1.17
MEAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

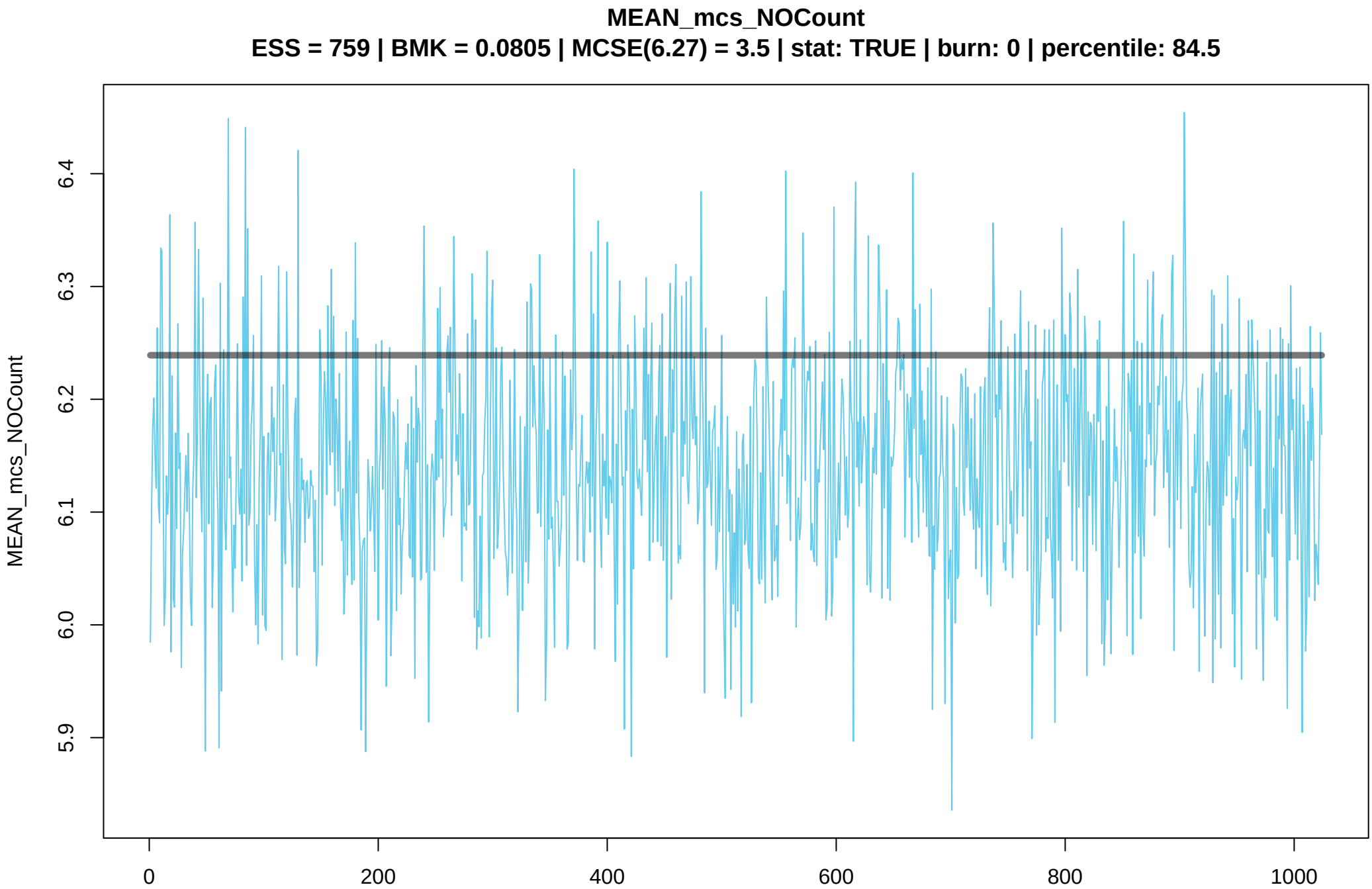

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0571 | MCSE(6.27) = 3.84 | stat: TRUE | burn: 0 | percentile: 1.56
MEAN_logit_ec_tanimoto_similarity
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

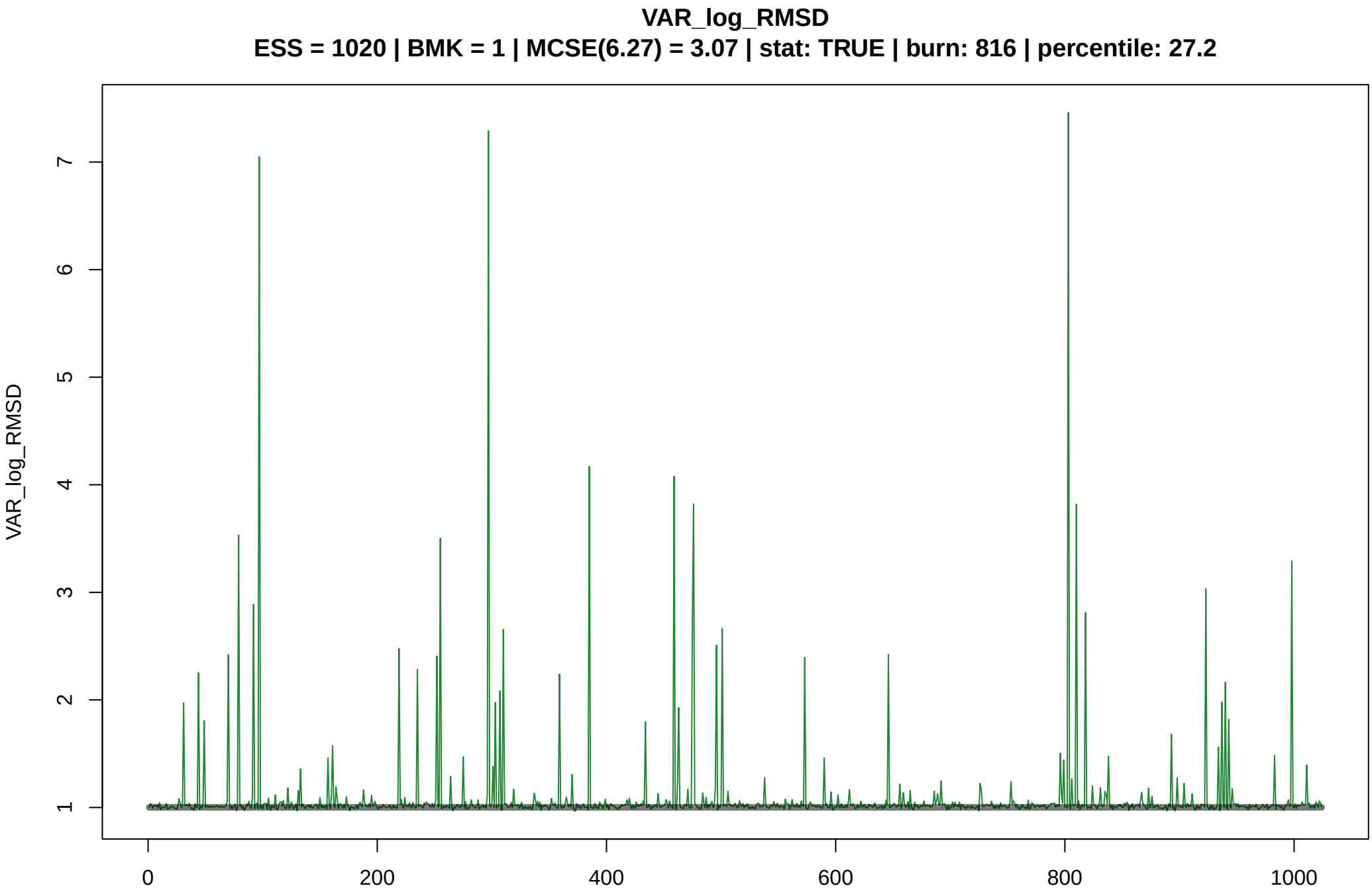

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0602 | MCSE(6.27) = 2.95 | stat: FALSE | burn: 0 | percentile: 83.1
MEAN_mcs_NumHeteroAtoms
3.00
2.95
2.90
2.85
2.80
0
200
400
600
800
1000

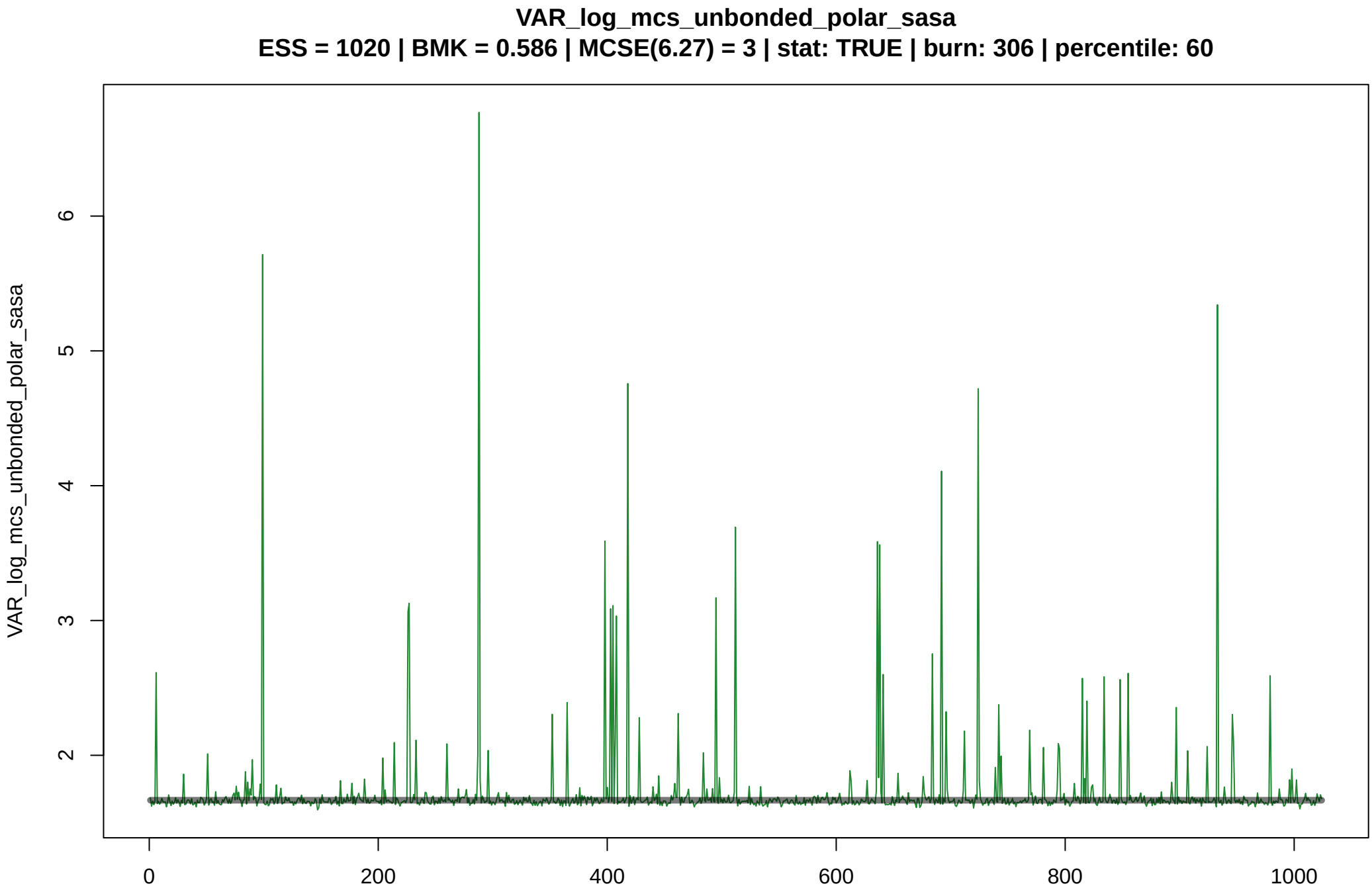

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0443 | MCSE(6.27) = 3.47 | stat: TRUE | burn: 0 | percentile: 0.293
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
31.0
0
200
400
600
800
1000

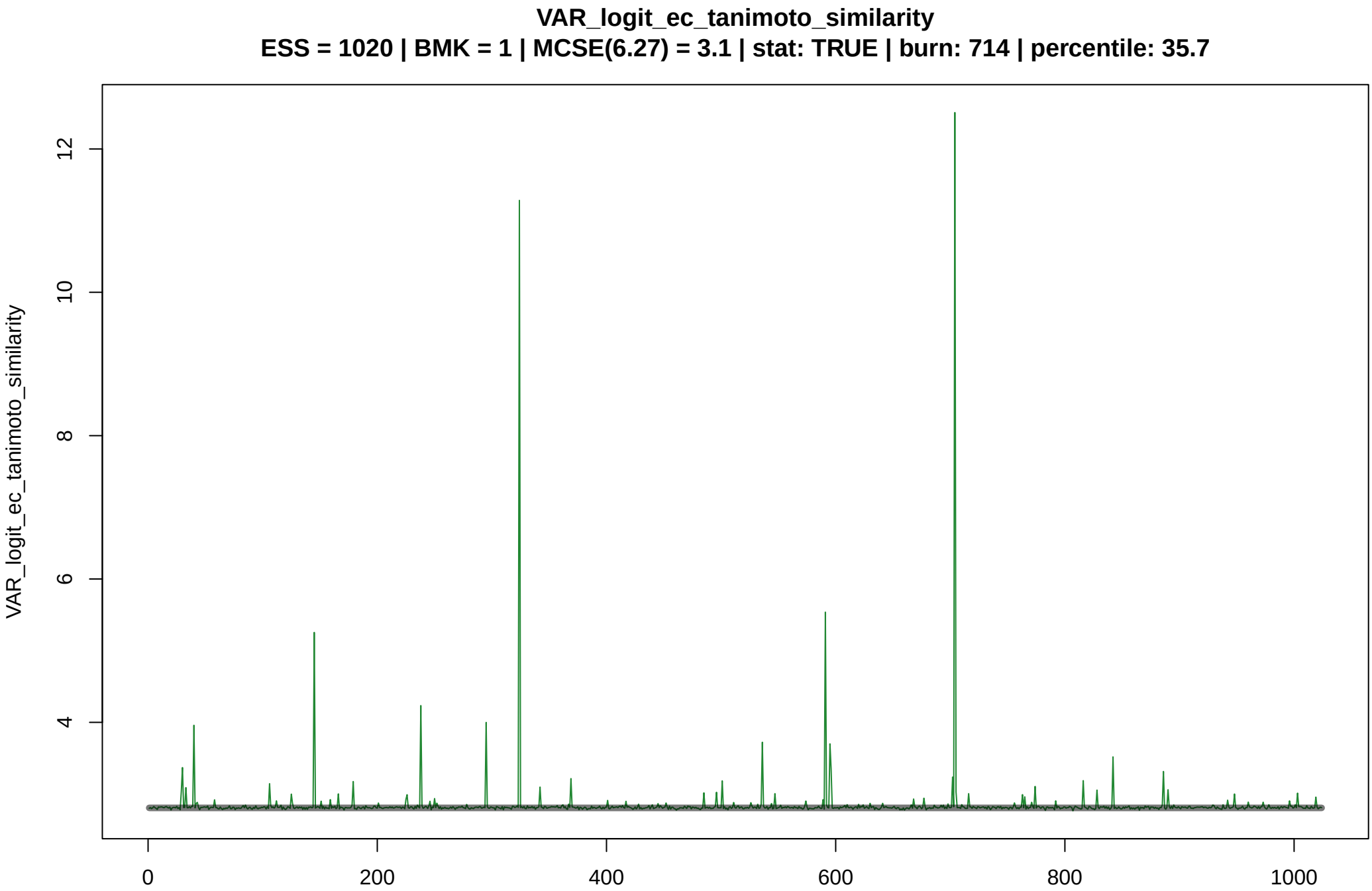

MEAN_mcs_RingCount
ESS = 951 | BMK = 0.0487 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | percentile: 89.8
MEAN_mcs_RingCount
2.00
2.05
2.10
0
200
400
600
800
1000

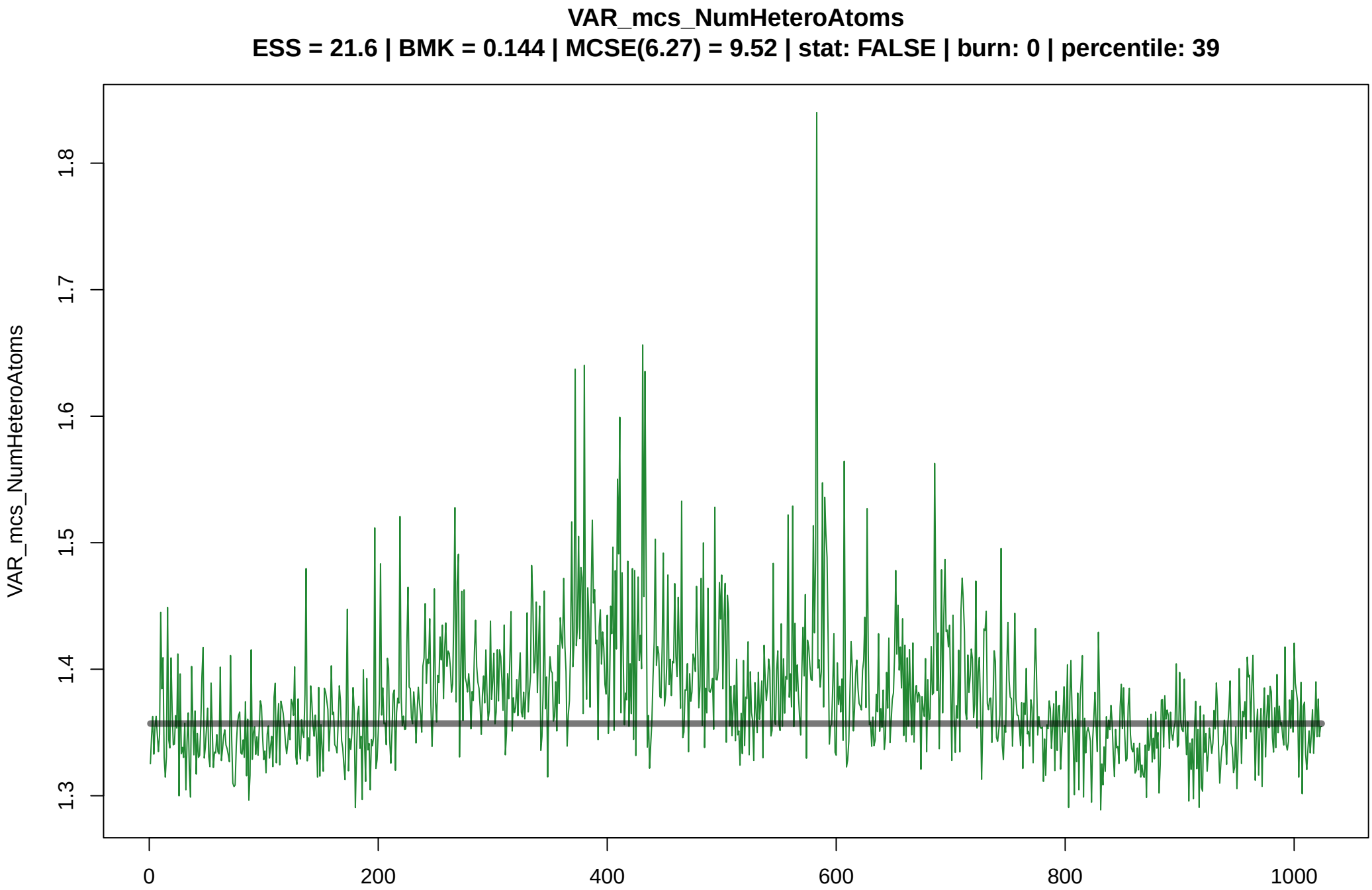

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0501 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | percentile: 67.4
MEAN_docked_NumRotatableBonds
6.2
6.3
6.4
6.5
6.6
6.7
0
200
400
600
800
1000

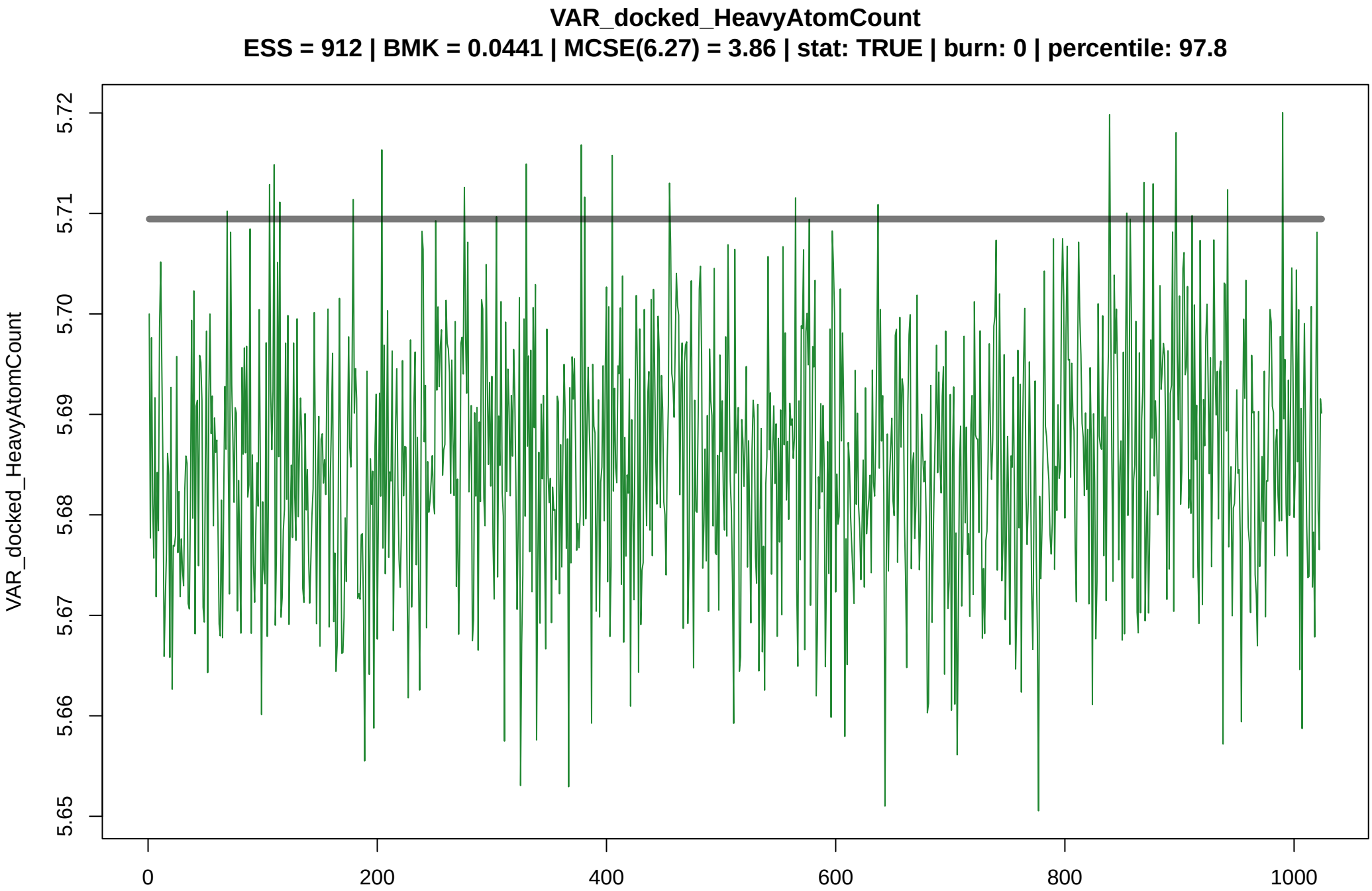

MEAN_mcs_NOCount
ESS = 759 | BMK = 0.0805 | MCSE(6.27) = 3.5 | stat: TRUE | burn: 0 | percentile: 84.5
MEAN_mcs_NOCount
6.4
6.3
6.2
6.1
6.0
5.9
0
200
400
600
800
1000

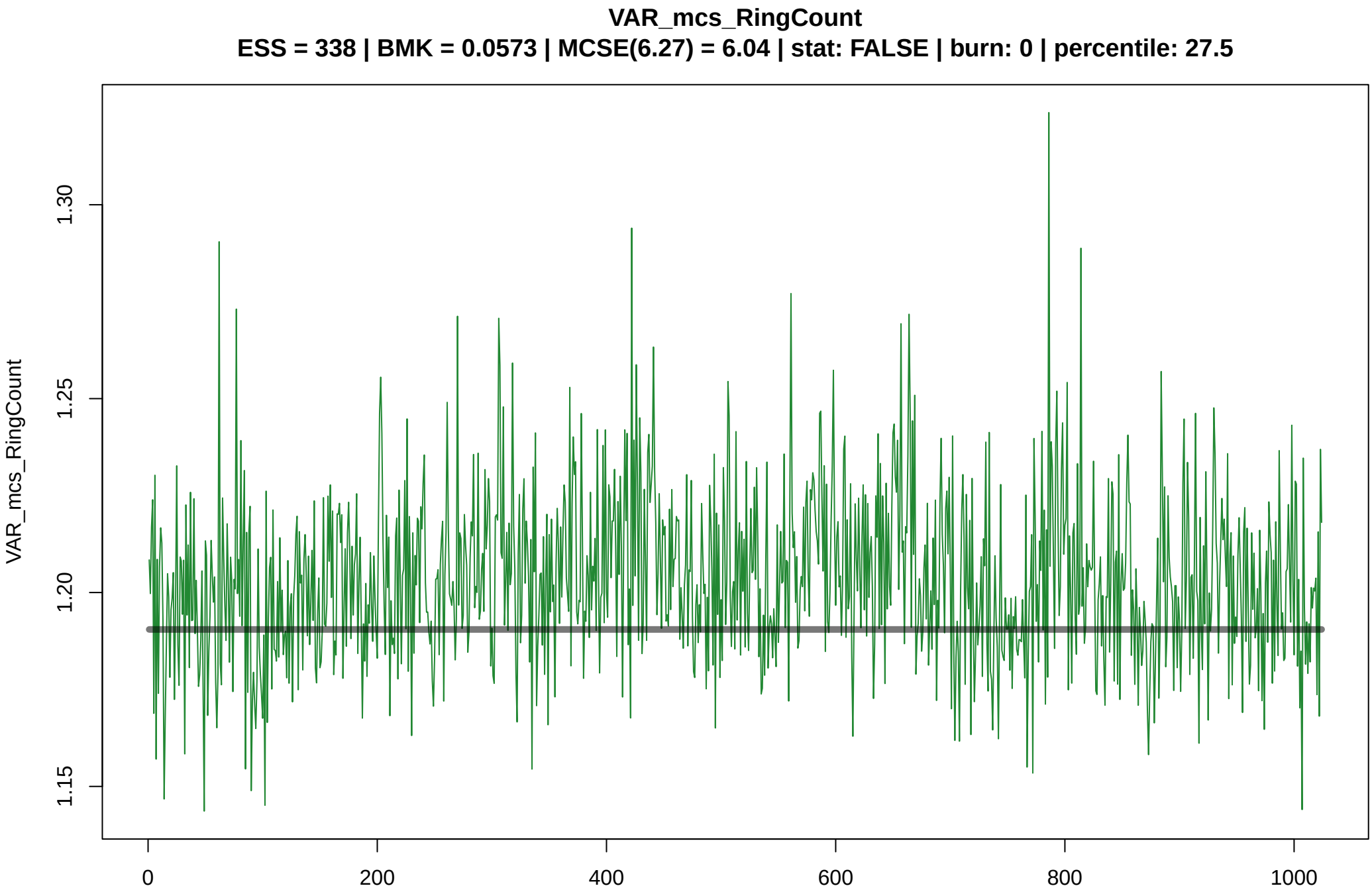

VAR_log_RMSD
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 816 | percentile: 27.2
VAR_log_RMSD
1
2
3
4
5
6
7
0
200
400
600
800
1000

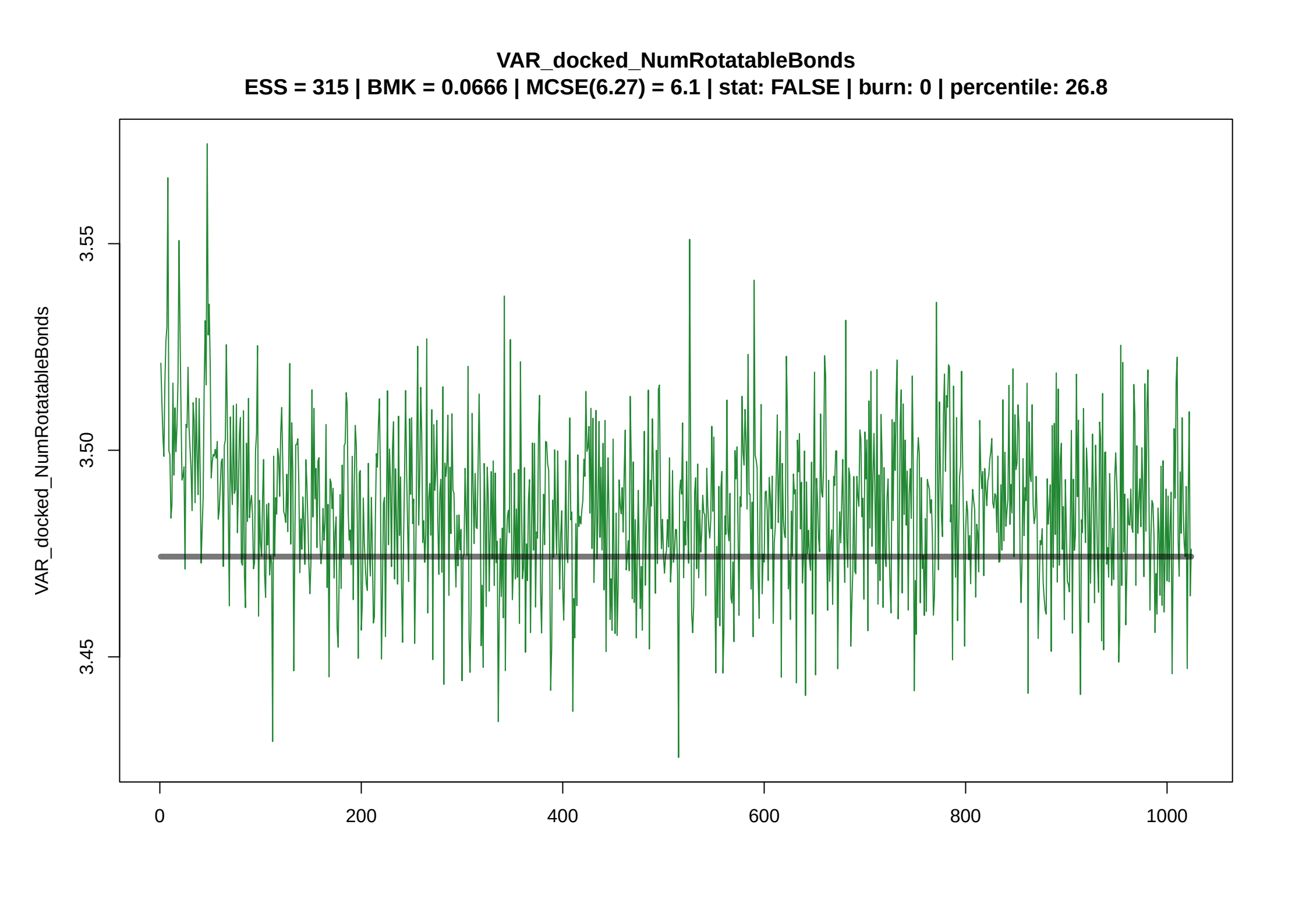

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.586 | MCSE(6.27) = 3 | stat: TRUE | burn: 306 | percentile: 60
VAR_log_mcs_unbonded_polar_sasa
2
3
4
5
6
0
200
400
600
800
1000

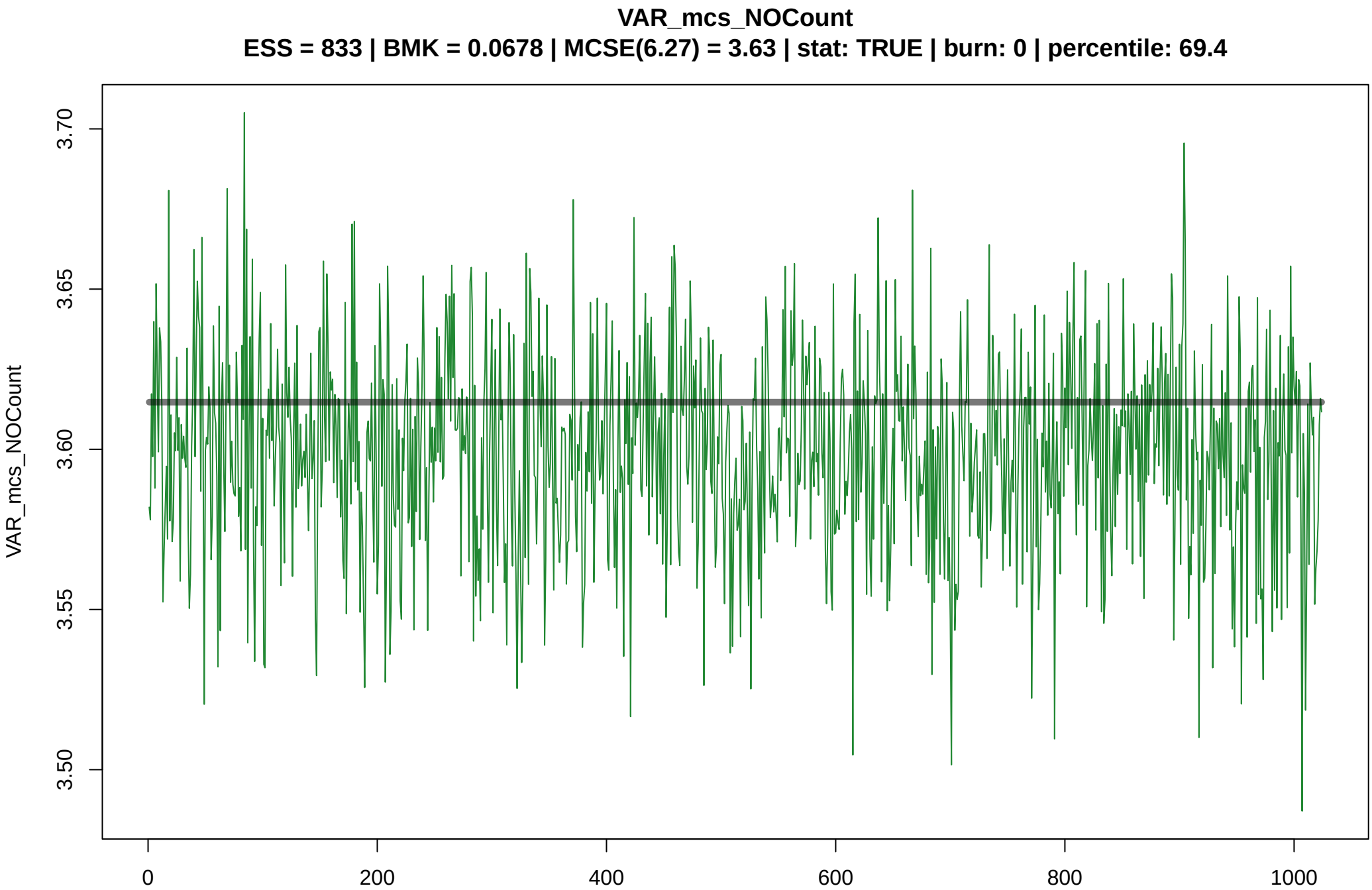

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 714 | percentile: 35.7
VAR_logit_ec_tanimoto_similarity
4
6
8
10
12
0
200
400
600
800
1000

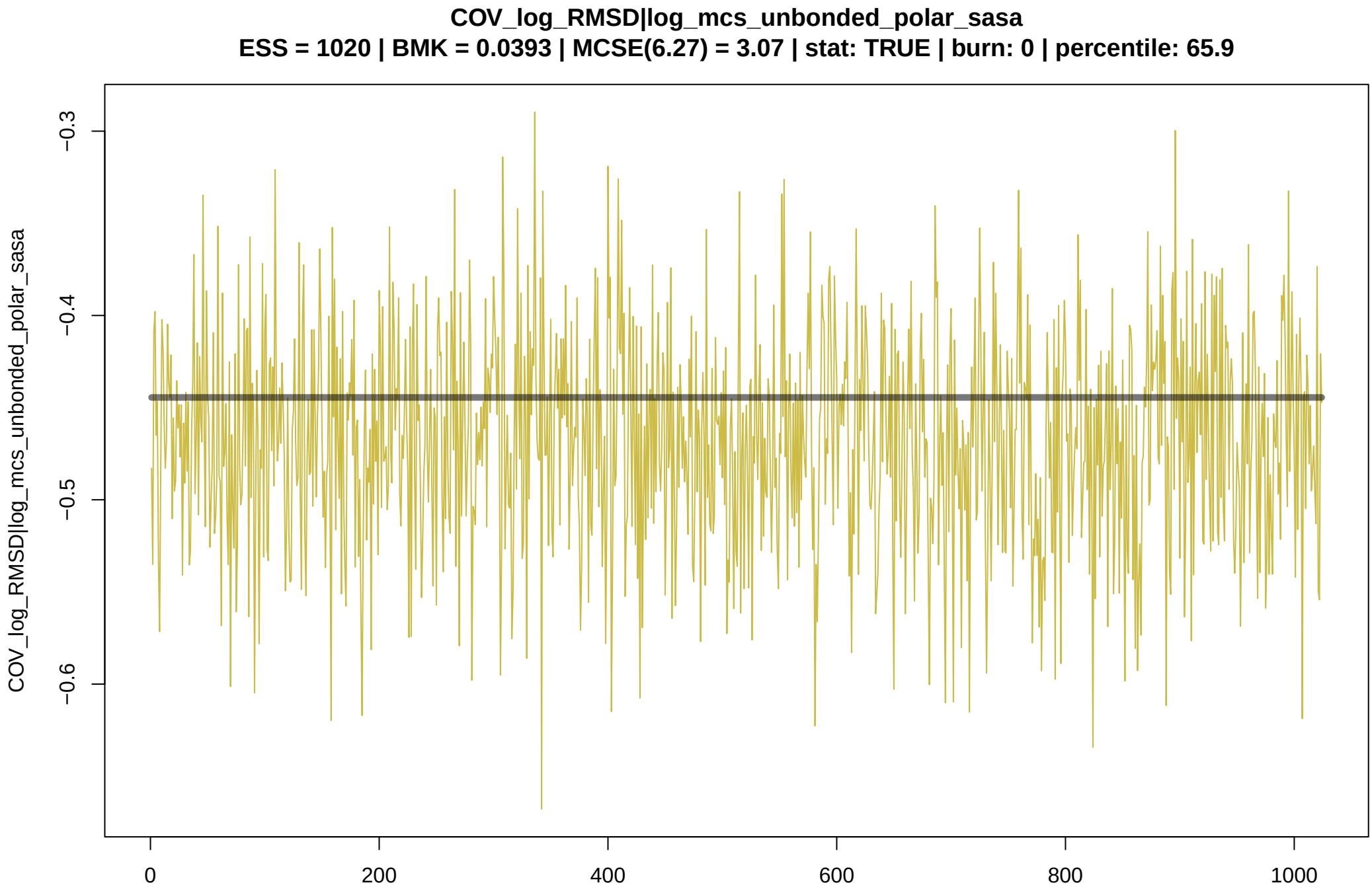

VAR_mcs_NumHeteroAtoms
ESS = 21.6 | BMK = 0.144 | MCSE(6.27) = 9.52 | stat: FALSE | burn: 0 | percentile: 39
VAR_mcs_NumHeteroAtoms
1.3
1.4
1.5
1.6
1.7
1.8
0
200
400
600
800
1000

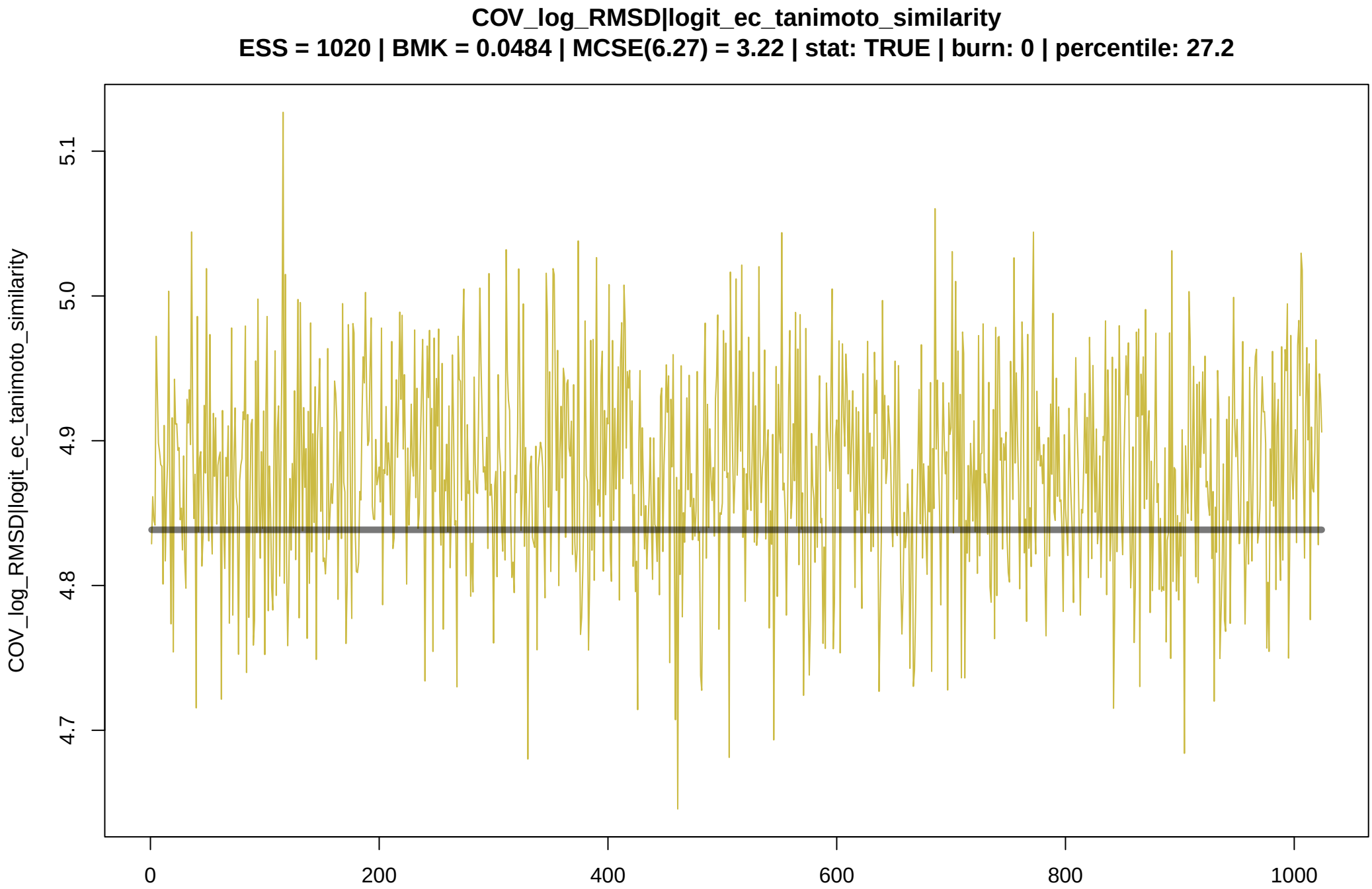

VAR_docked_HeavyAtomCount
ESS = 912 | BMK = 0.0441 | MCSE(6.27) = 3.86 | stat: TRUE | burn: 0 | percentile: 97.8
VAR_docked_HeavyAtomCount
5.65
5.66
5.67
5.68
5.69
5.70
5.71
5.72
0
200
400
600
800
1000

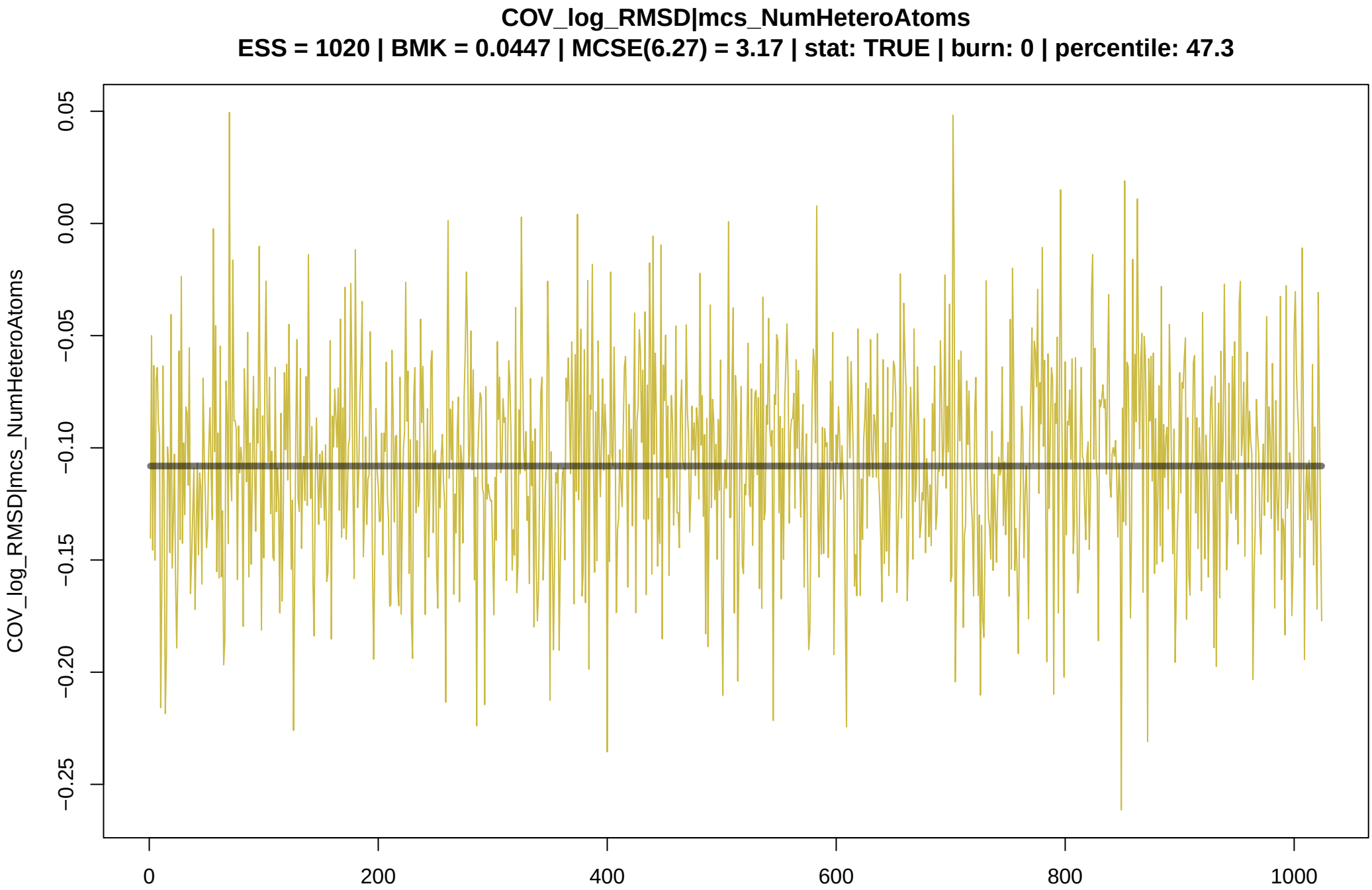

VAR_mcs_RingCount
ESS = 338 | BMK = 0.0573 | MCSE(6.27) = 6.04 | stat: FALSE | burn: 0 | percentile: 27.5
VAR_mcs_RingCount
1.15
1.20
1.25
1.30
0
200
400
600
800
1000

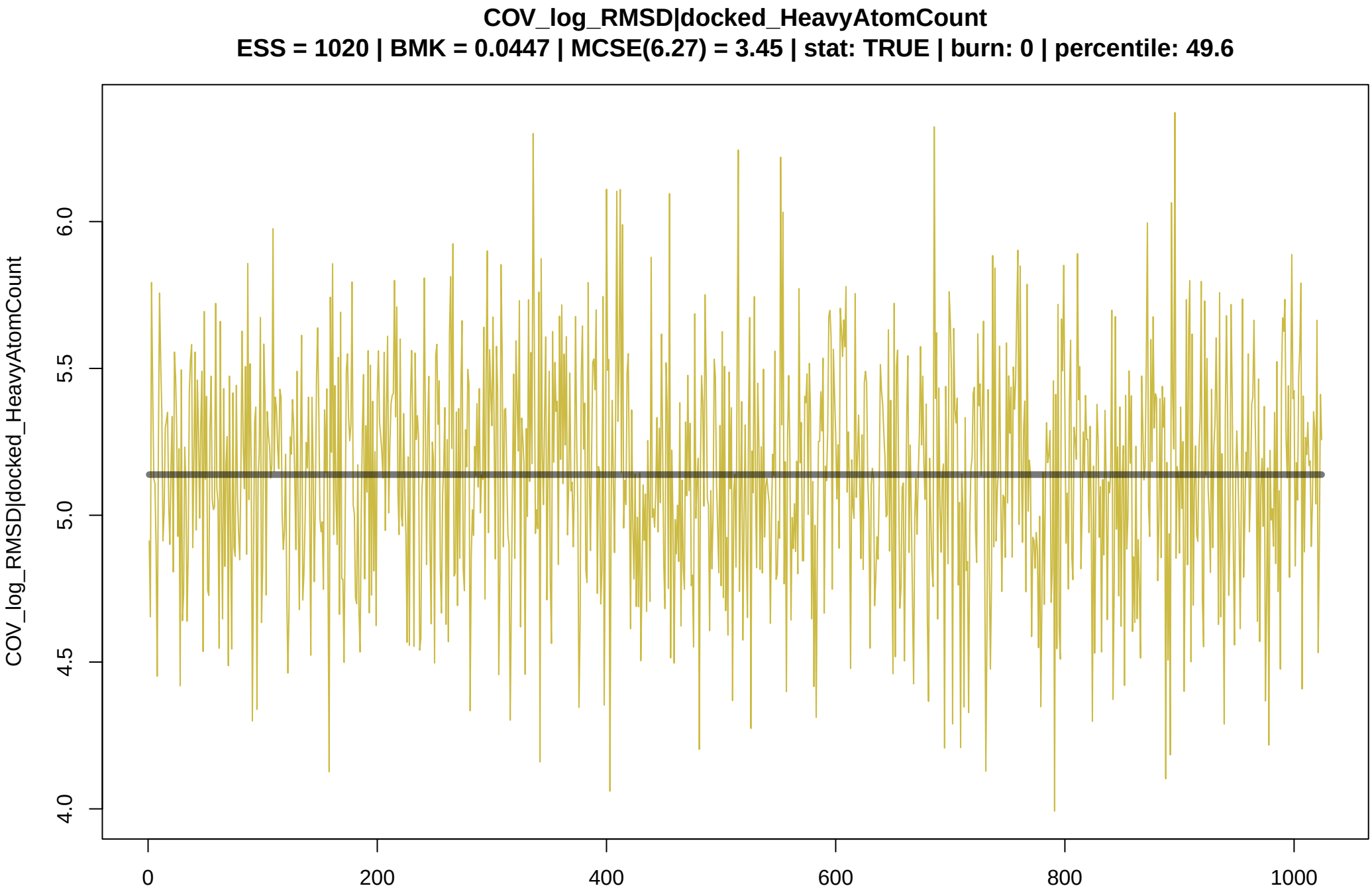

VAR_docked_NumRotatableBonds
ESS = 315 | BMK = 0.0666 | MCSE(6.27) = 6.1 | stat: FALSE | burn: 0 | percentile: 26.8
VAR_docked_NumRotatableBonds
3.55
3.50
3.45
0
200
400
600
800
1000

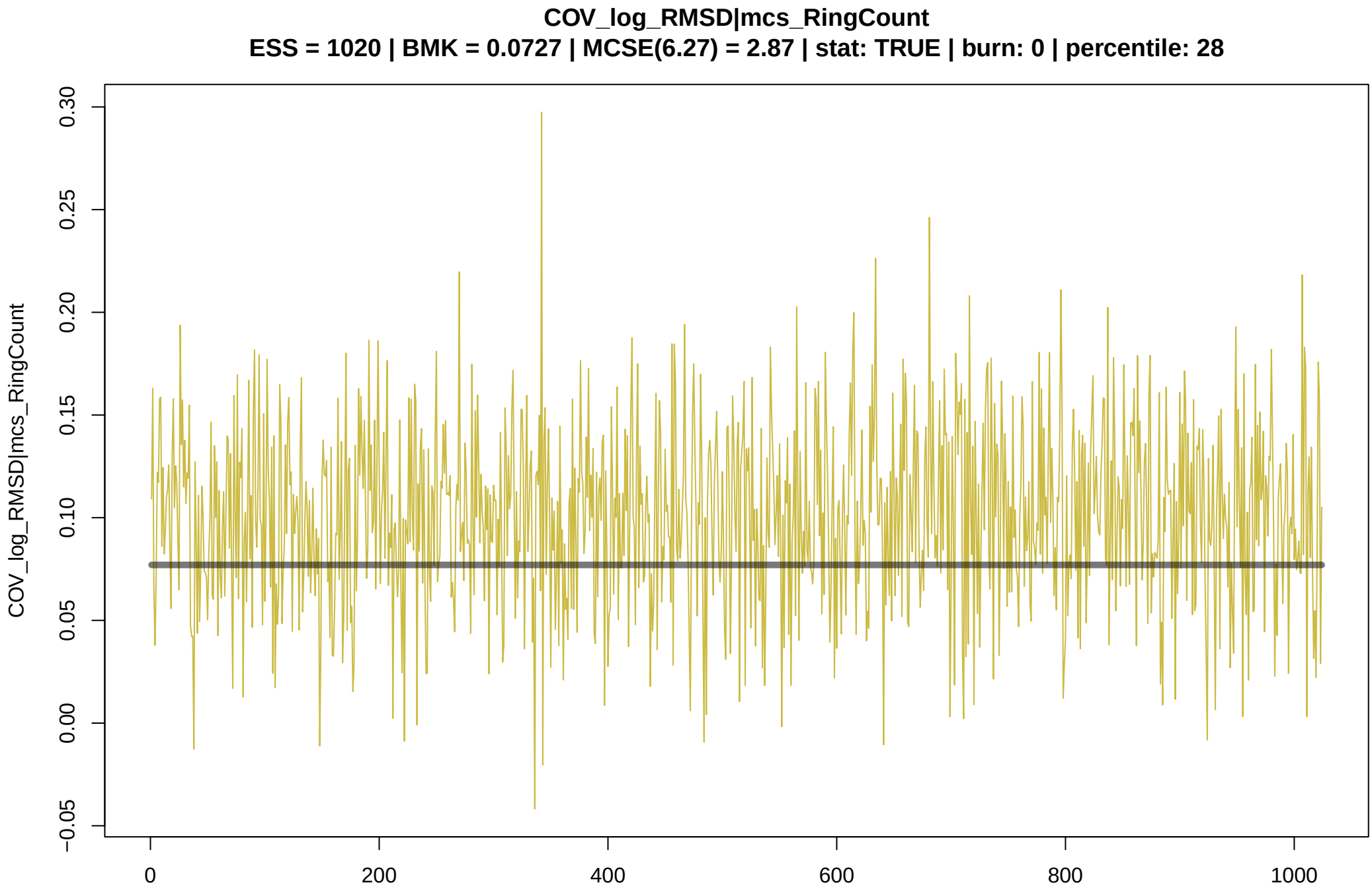

VAR_mcs_NOCount
ESS = 833 | BMK = 0.0678 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | percentile: 69.4
VAR_mcs_NOCount
3.50
3.55
3.60
3.65
3.70
0
200
400
600
800
1000

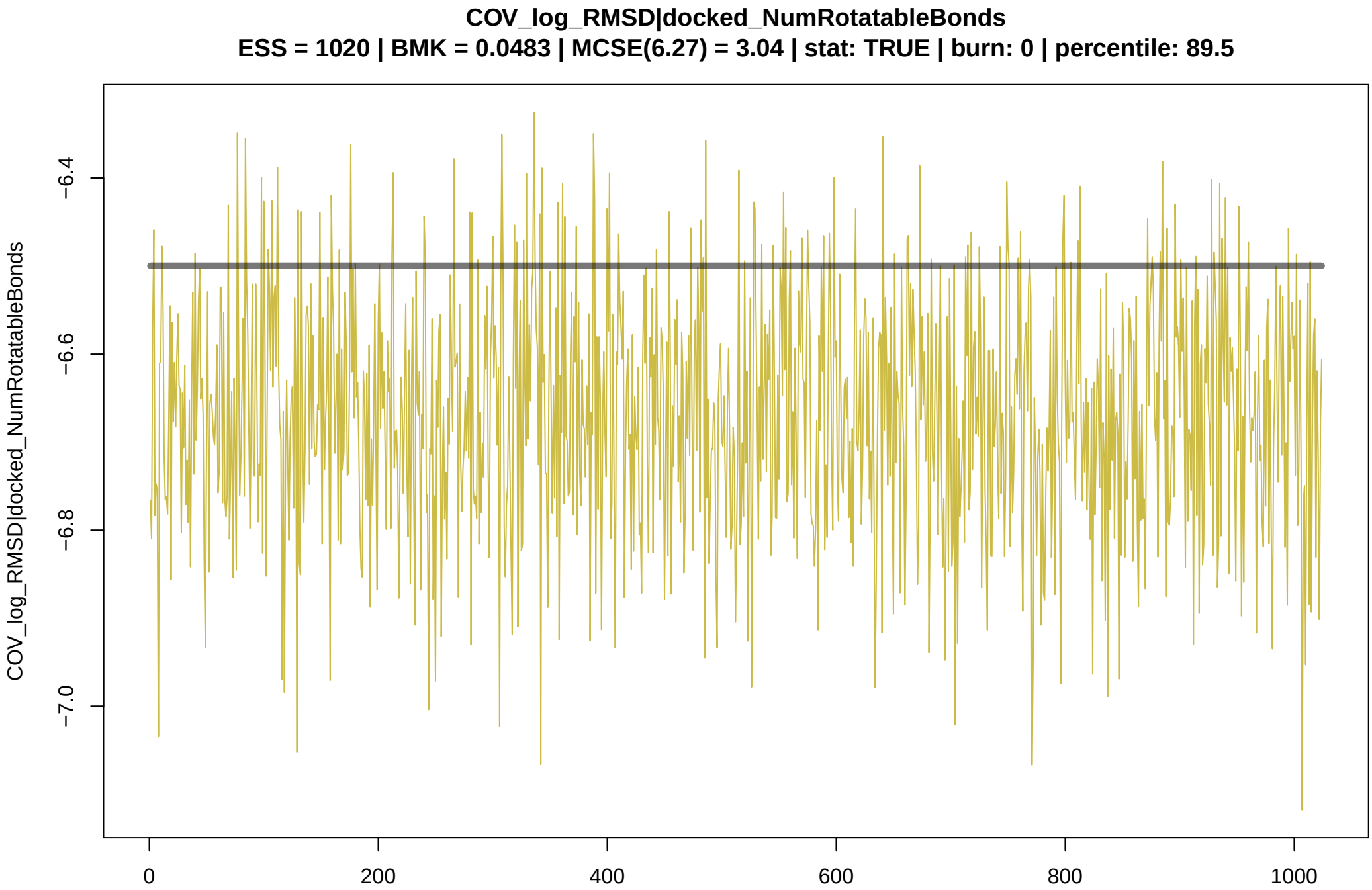

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0393 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | percentile: 65.9
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.3
−0.4
−0.5
−0.6
0
200
400
600
800
1000

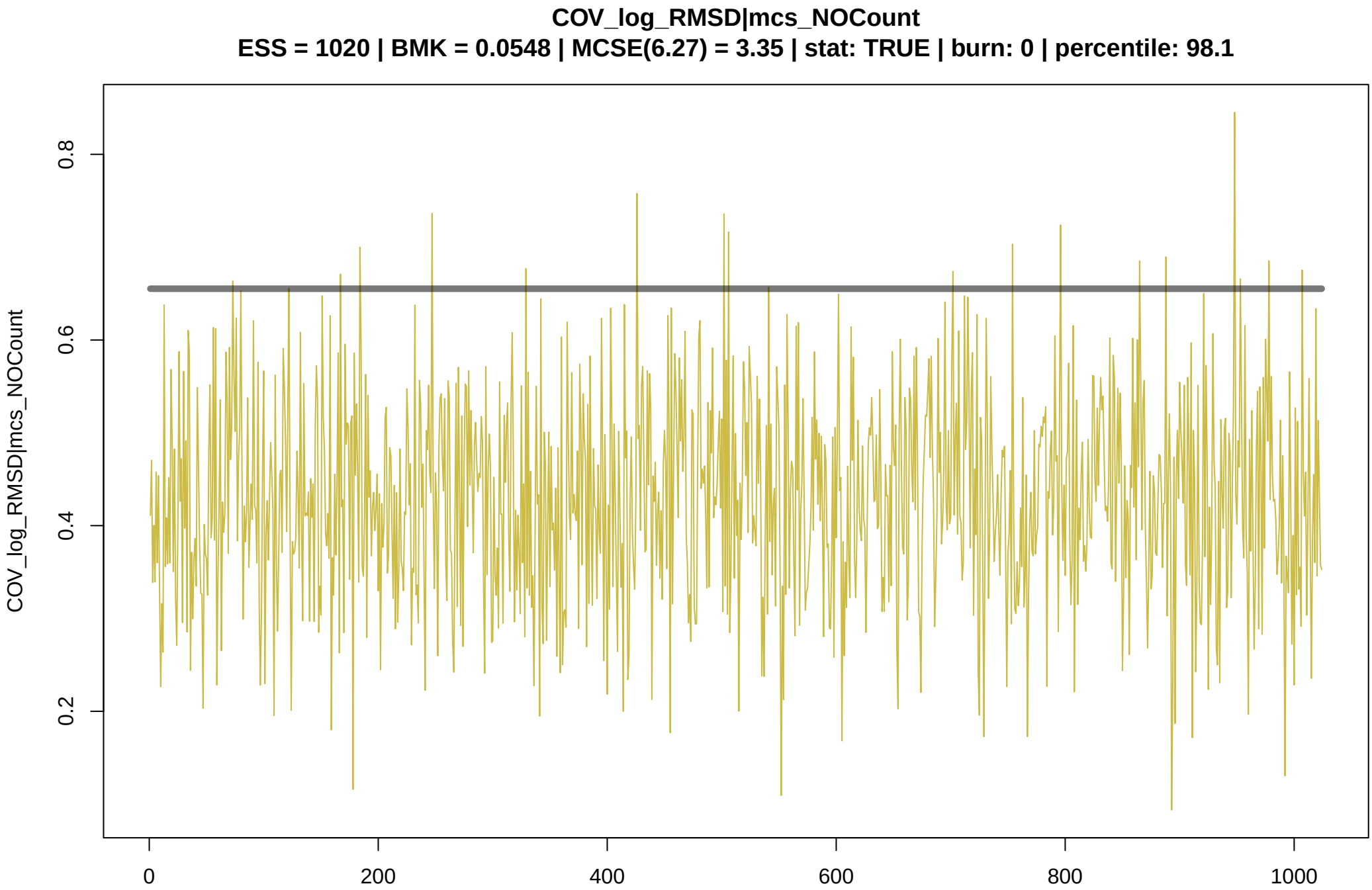

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0484 | MCSE(6.27) = 3.22 | stat: TRUE | burn: 0 | percentile: 27.2
COV_log_RMSD|logit_ec_tanimoto_similarity
5.1
5.0
4.9
4.8
4.7
0
200
400
600
800
1000

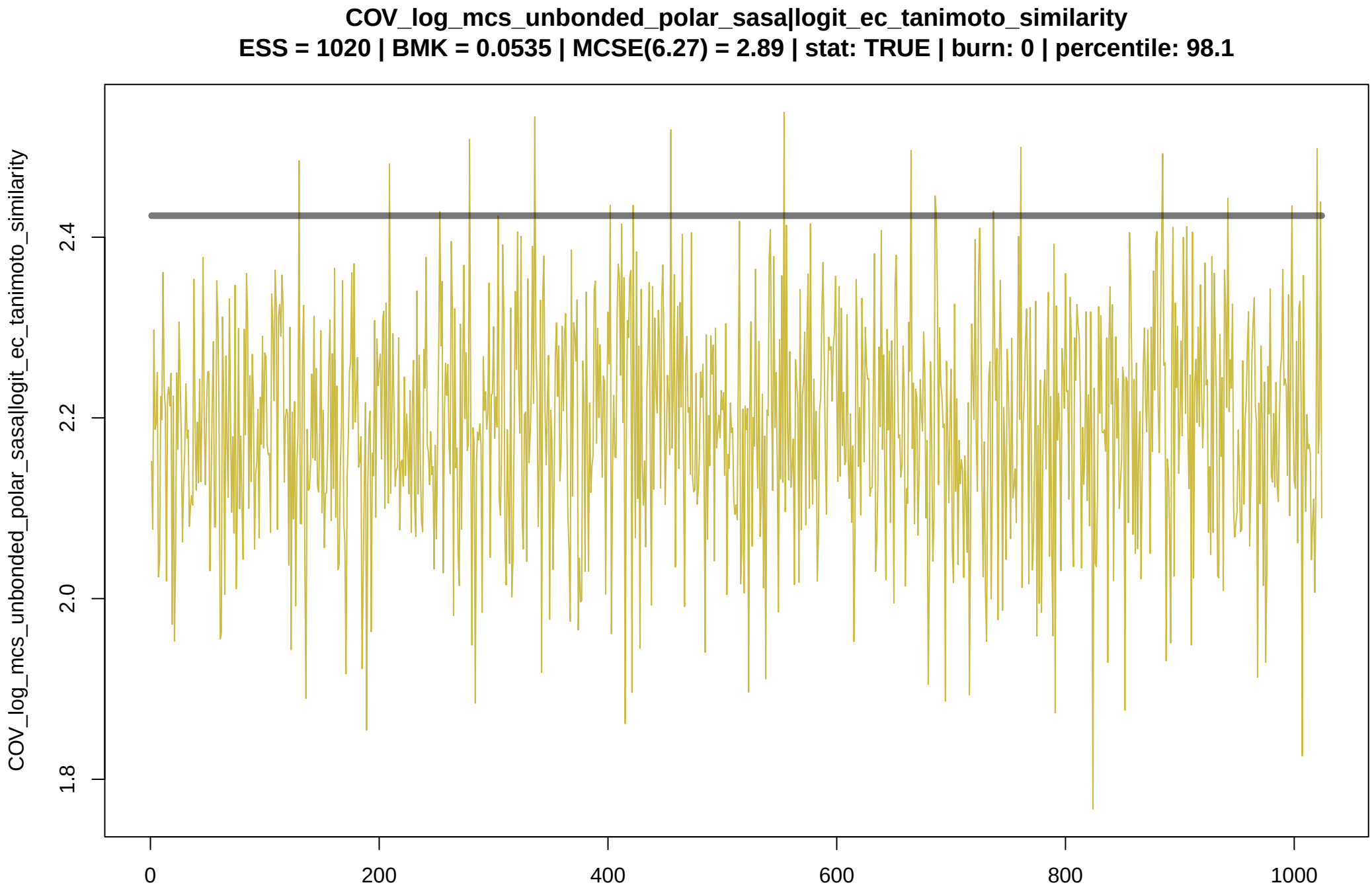

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0447 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | percentile: 47.3
COV_log_RMSD|mcs_NumHeteroAtoms
0.05
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
200
400
600
800
1000

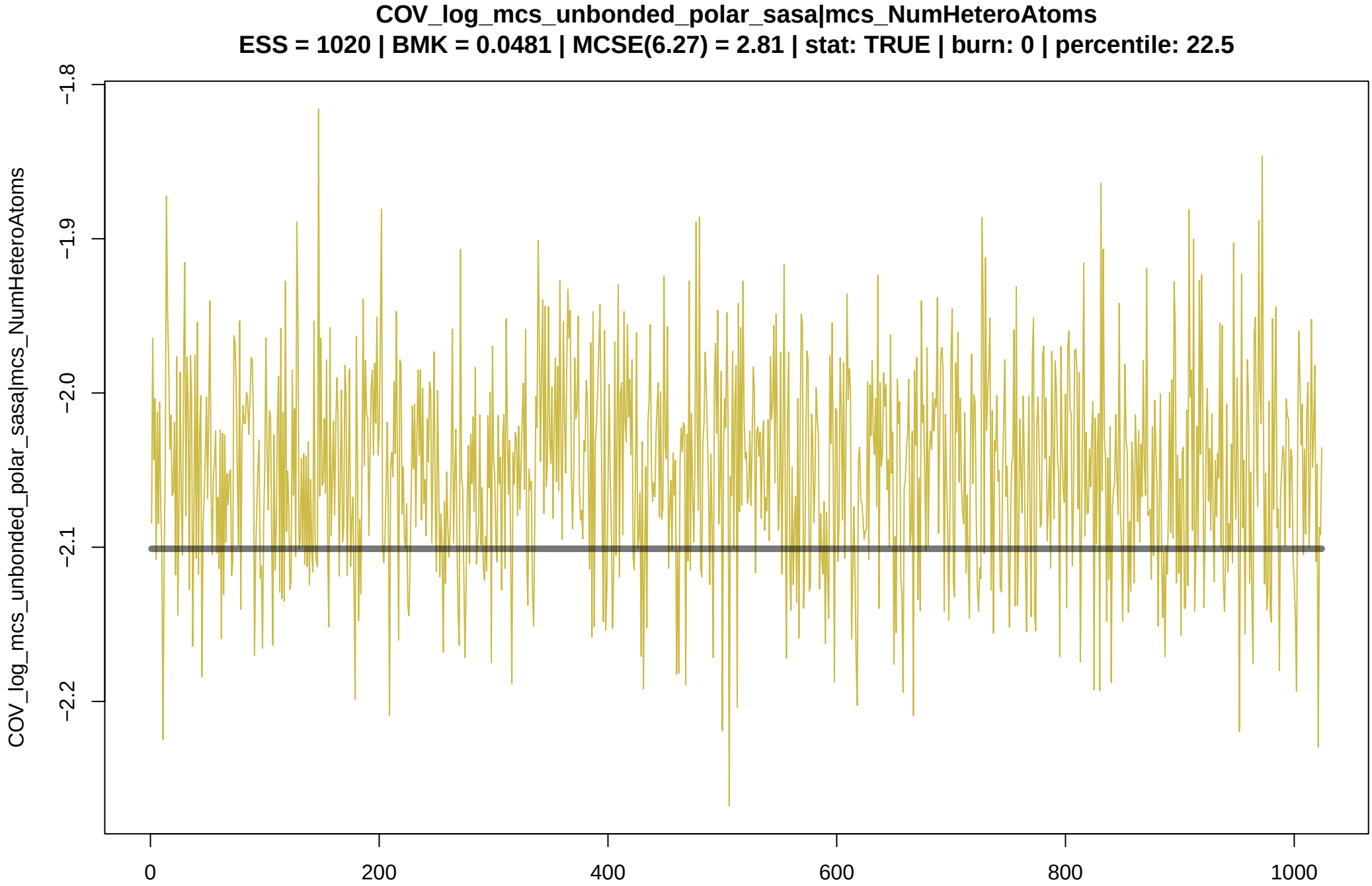

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0447 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0 | percentile: 49.6
COV_log_RMSD|docked_HeavyAtomCount
4.0
4.5
5.0
5.5
6.0
0
200
400
600
800
1000

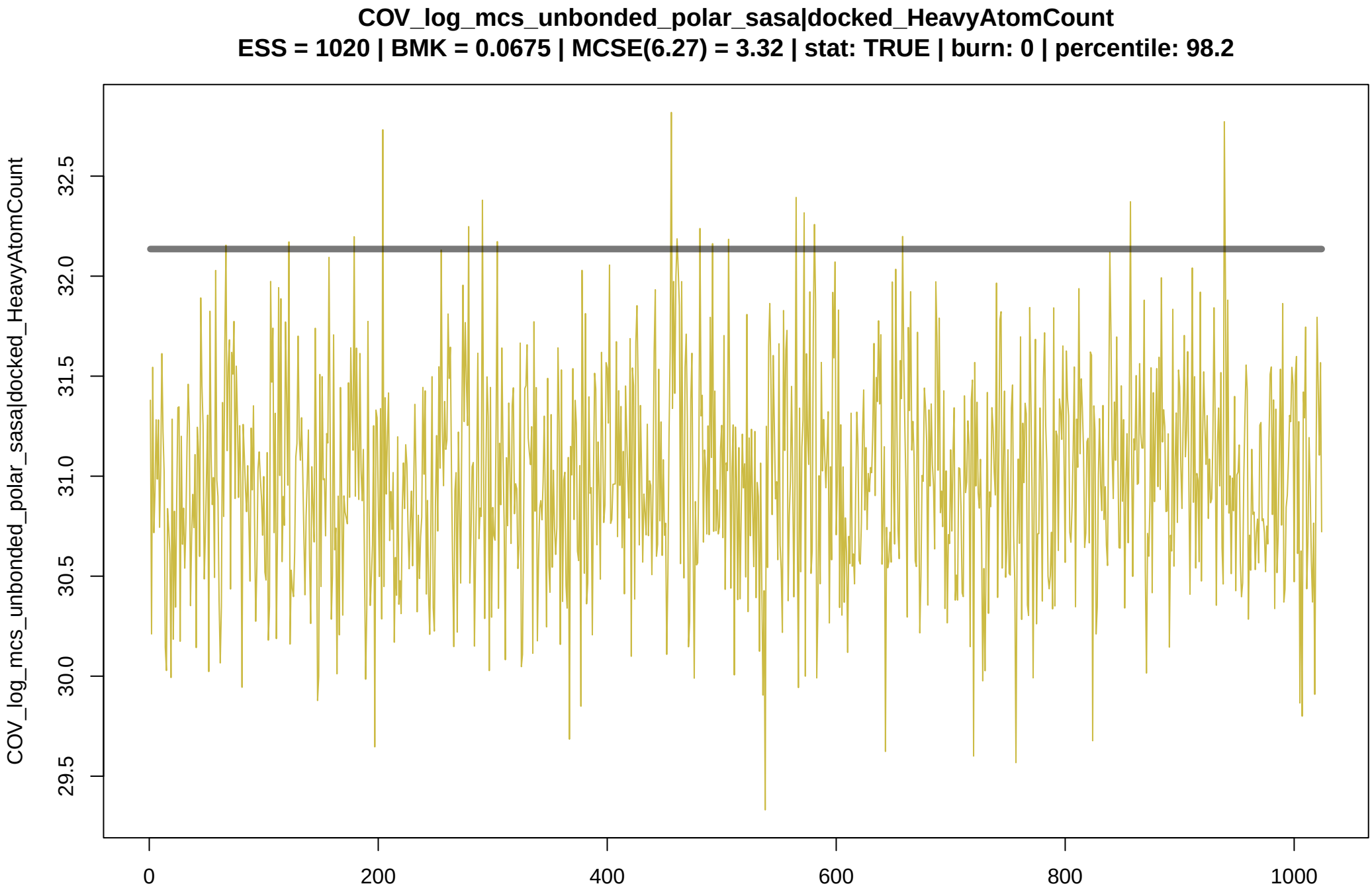

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0727 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0 | percentile: 28
COV_log_RMSD|mcs_RingCount
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−0.05
0
200
400
600
800
1000

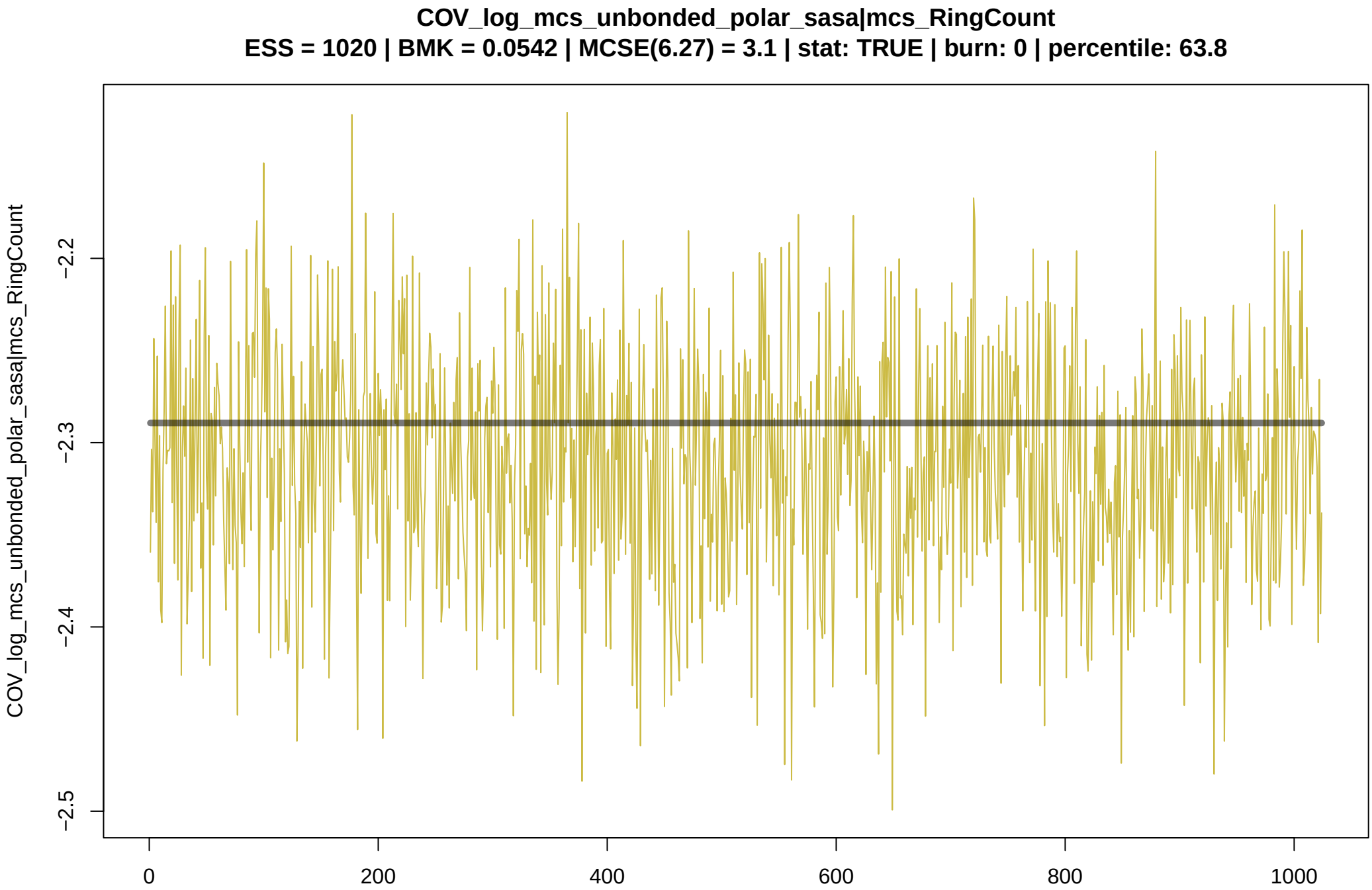

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0483 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | percentile: 89.5
COV_log_RMSD|docked_NumRotatableBonds
−6.4
−6.6
−6.8
−7.0
0
200
400
600
800
1000

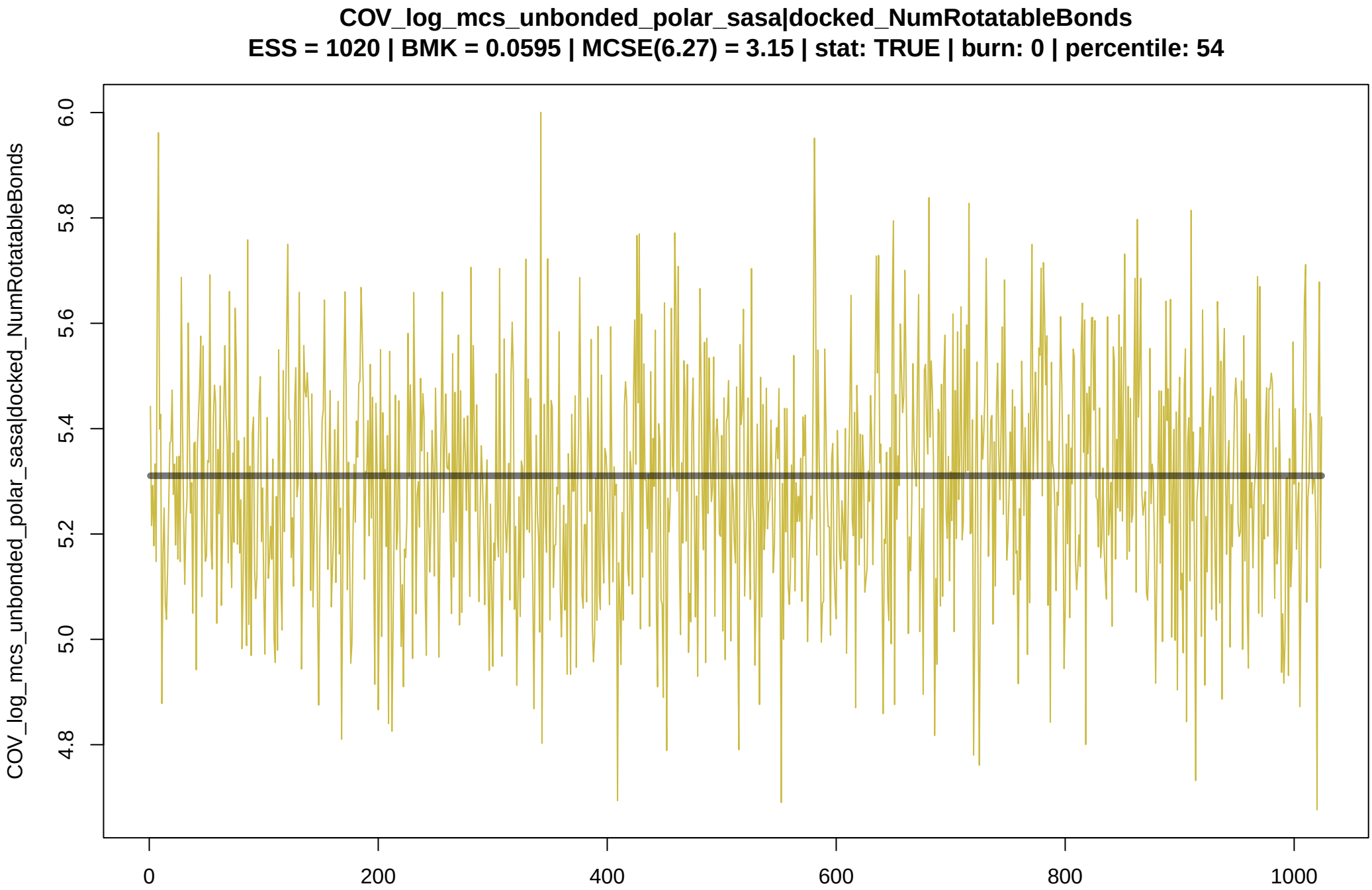

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0548 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0 | percentile: 98.1
COV_log_RMSD|mcs_NOCount
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

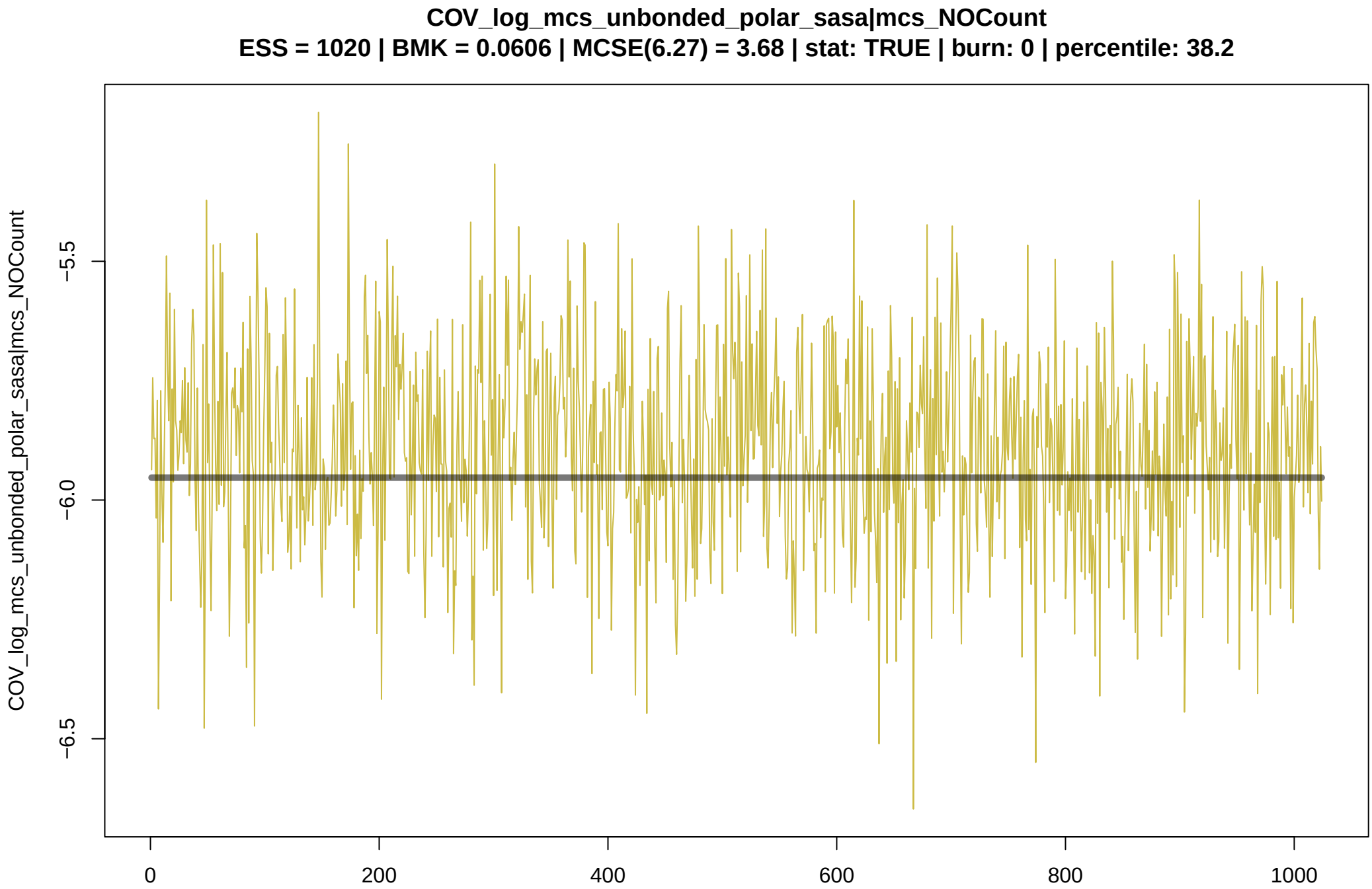

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0535 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | percentile: 98.1
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
1.8
2.0
2.2
2.4
0
200
400
600
800
1000

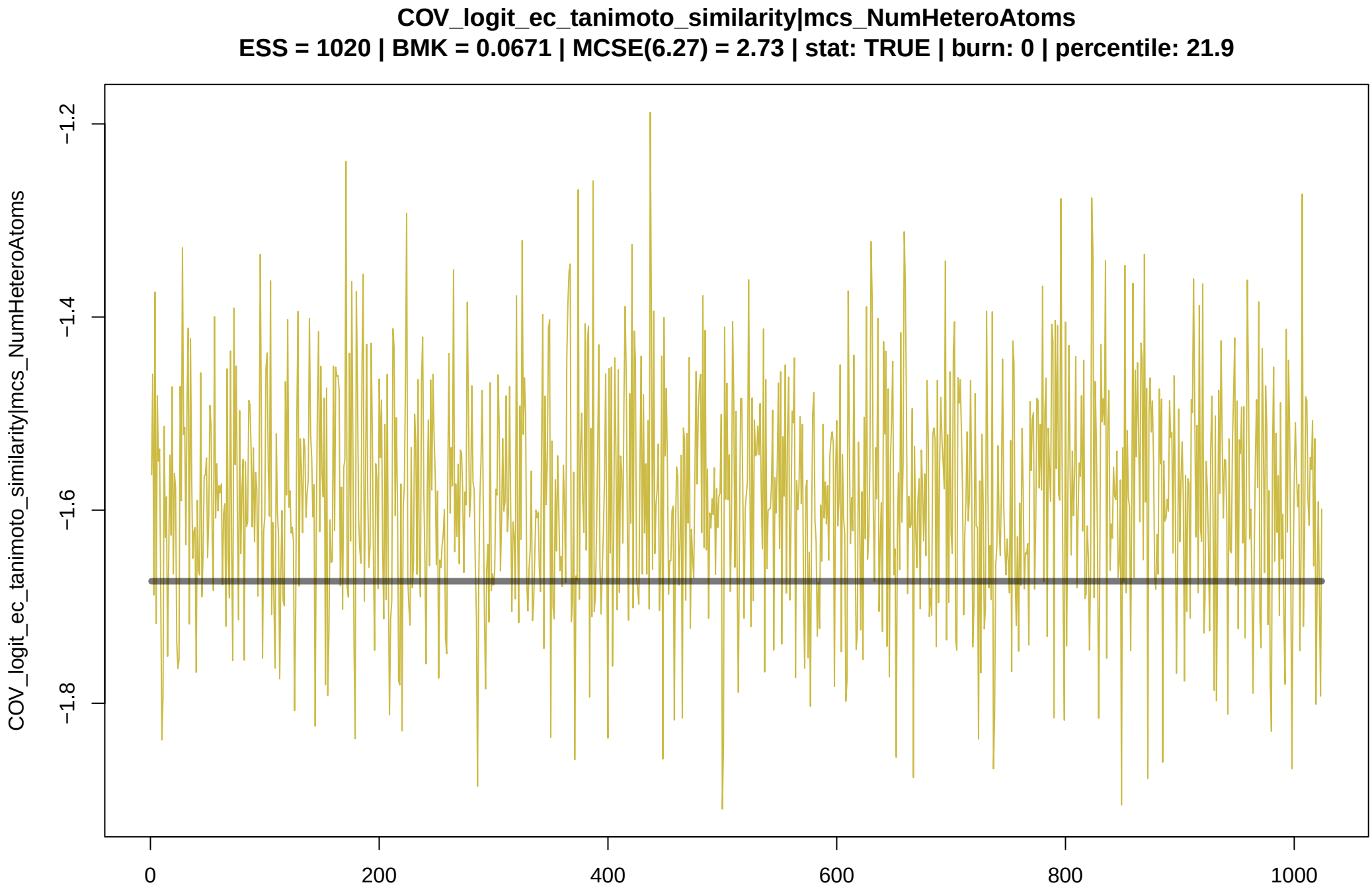

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0481 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | percentile: 22.5
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.8
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

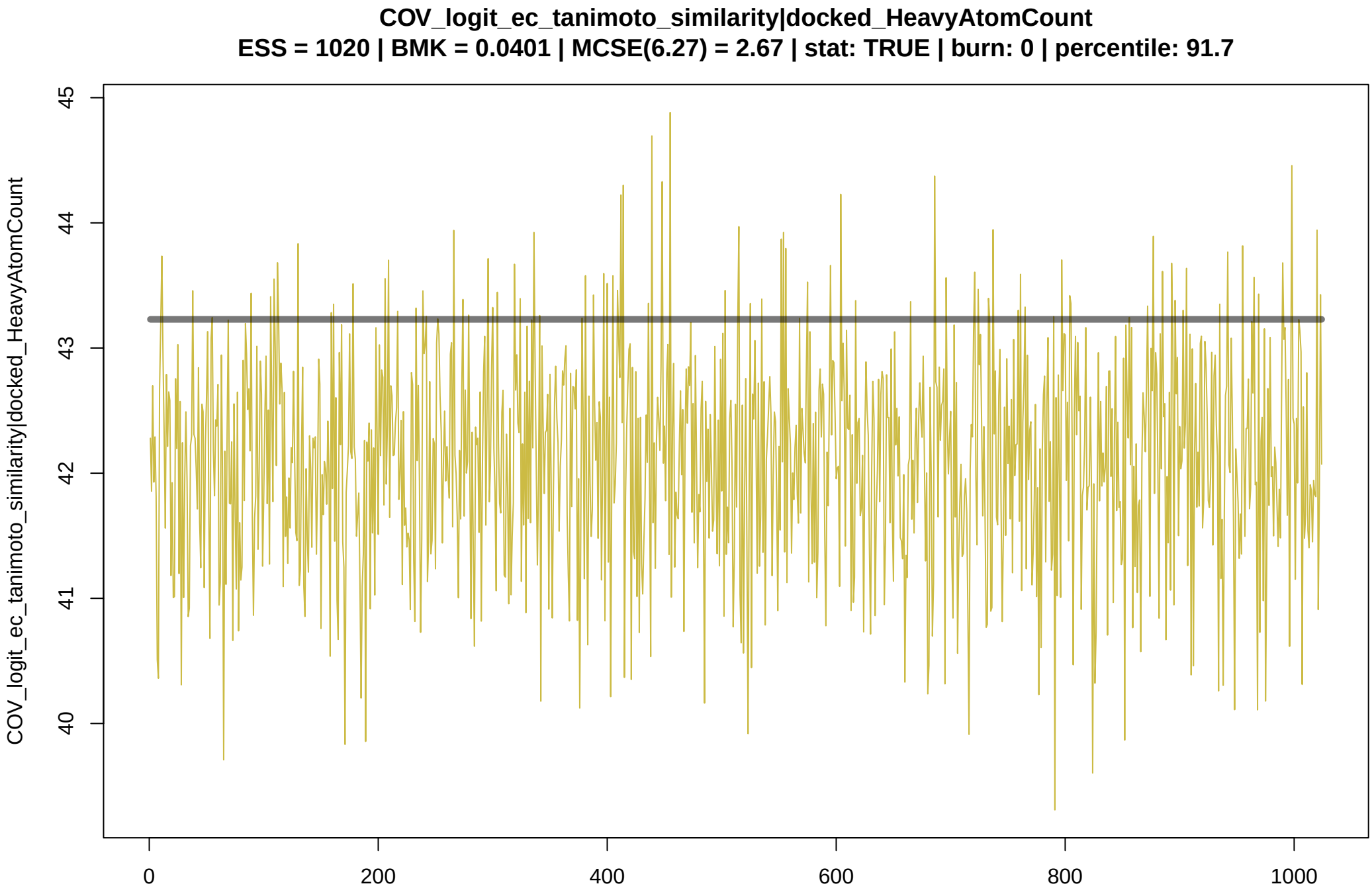

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0675 | MCSE(6.27) = 3.32 | stat: TRUE | burn: 0 | percentile: 98.2
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
29.5
30.0
30.5
31.0
31.5
32.0
32.5
0
200
400
600
800
1000

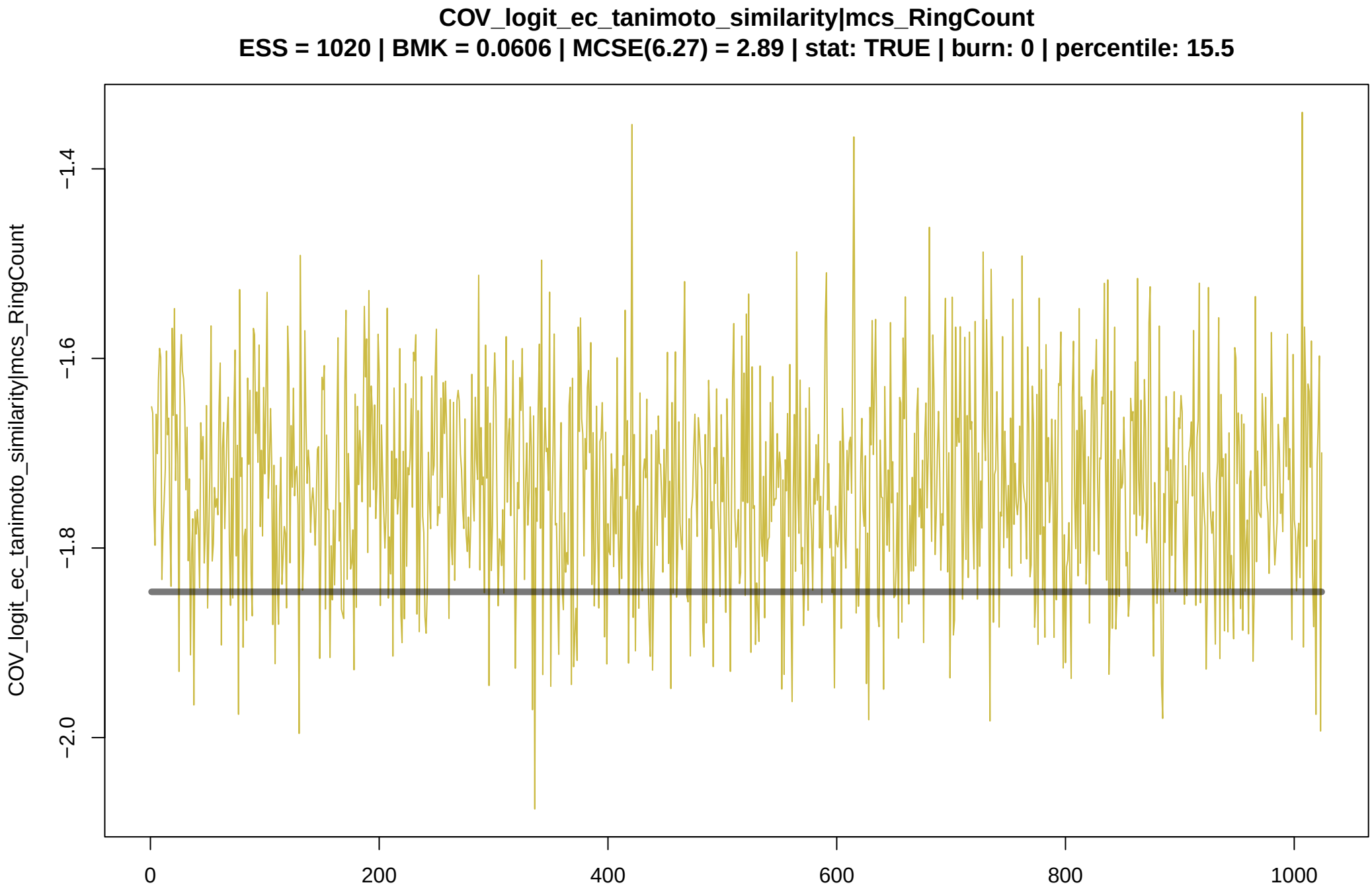

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0542 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | percentile: 63.8
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.2
−2.3
−2.4
−2.5
0
200
400
600
800
1000

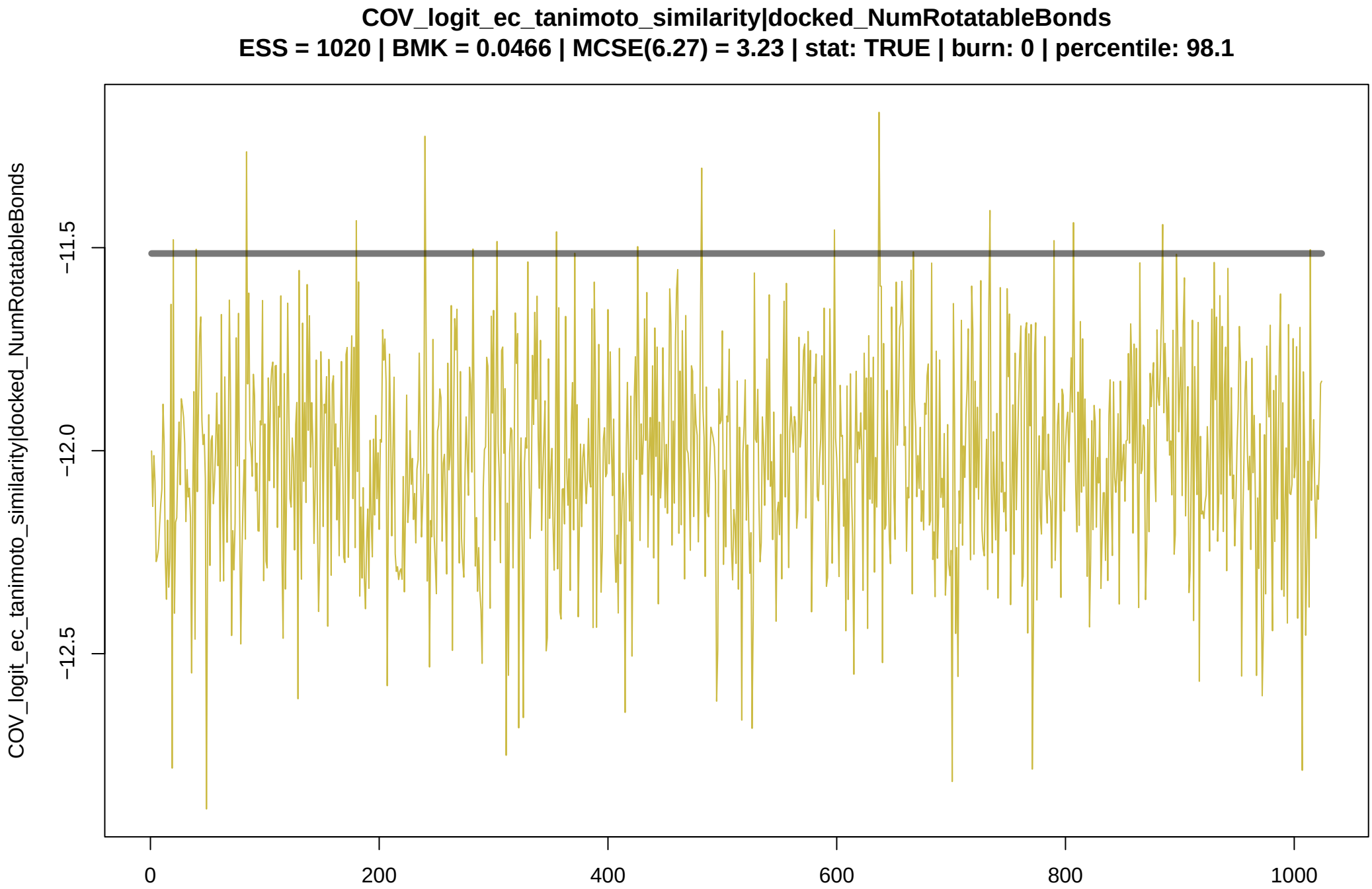

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0595 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | percentile: 54
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
6.0
5.8
5.6
5.4
5.2
5.0
4.8
0
200
400
600
800
1000

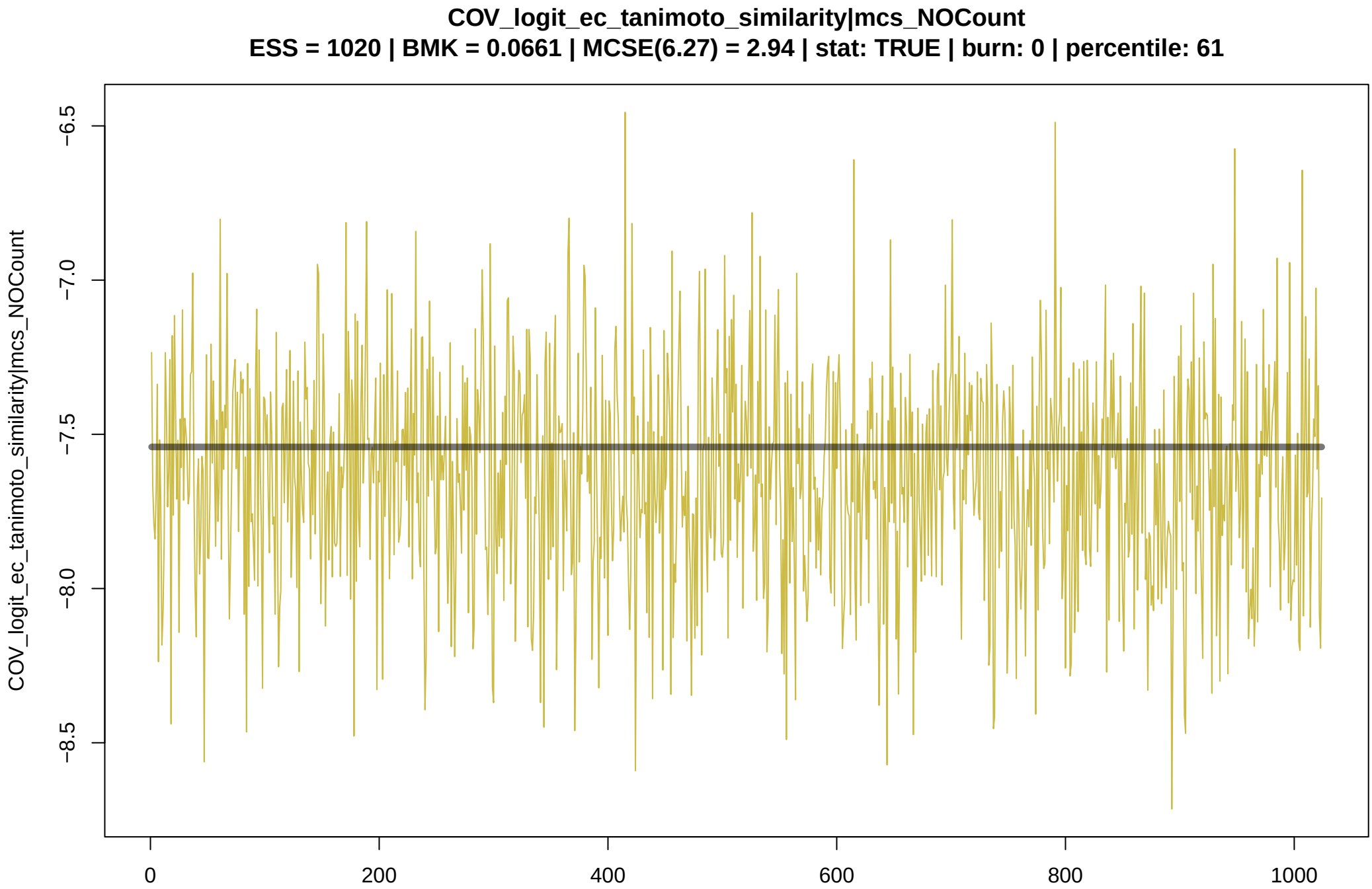

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0606 | MCSE(6.27) = 3.68 | stat: TRUE | burn: 0 | percentile: 38.2
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.5
−6.0
−6.5
0
200
400
600
800
1000

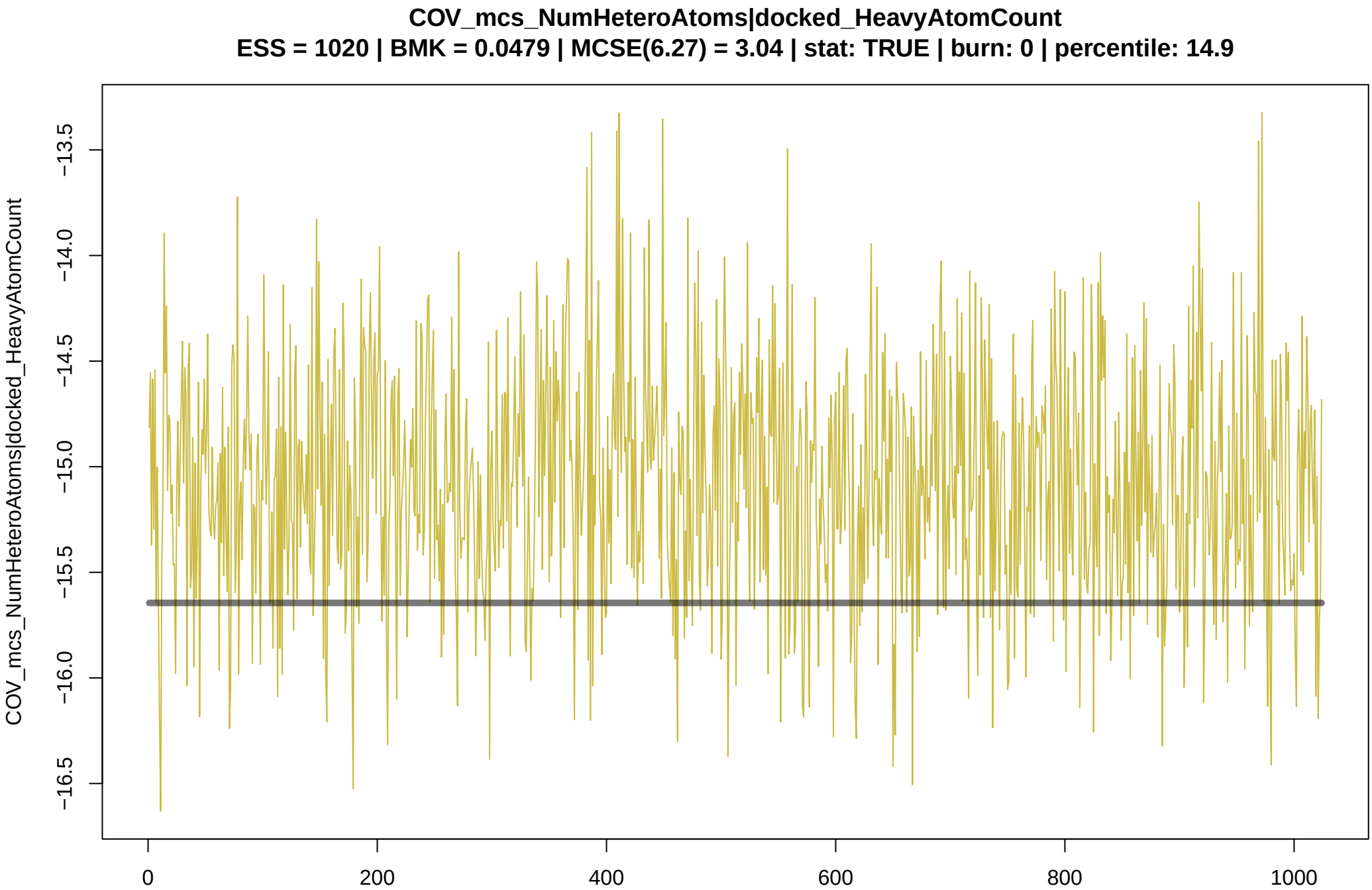

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0671 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | percentile: 21.9
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.2
−1.4
−1.6
−1.8
0
200
400
600
800
1000

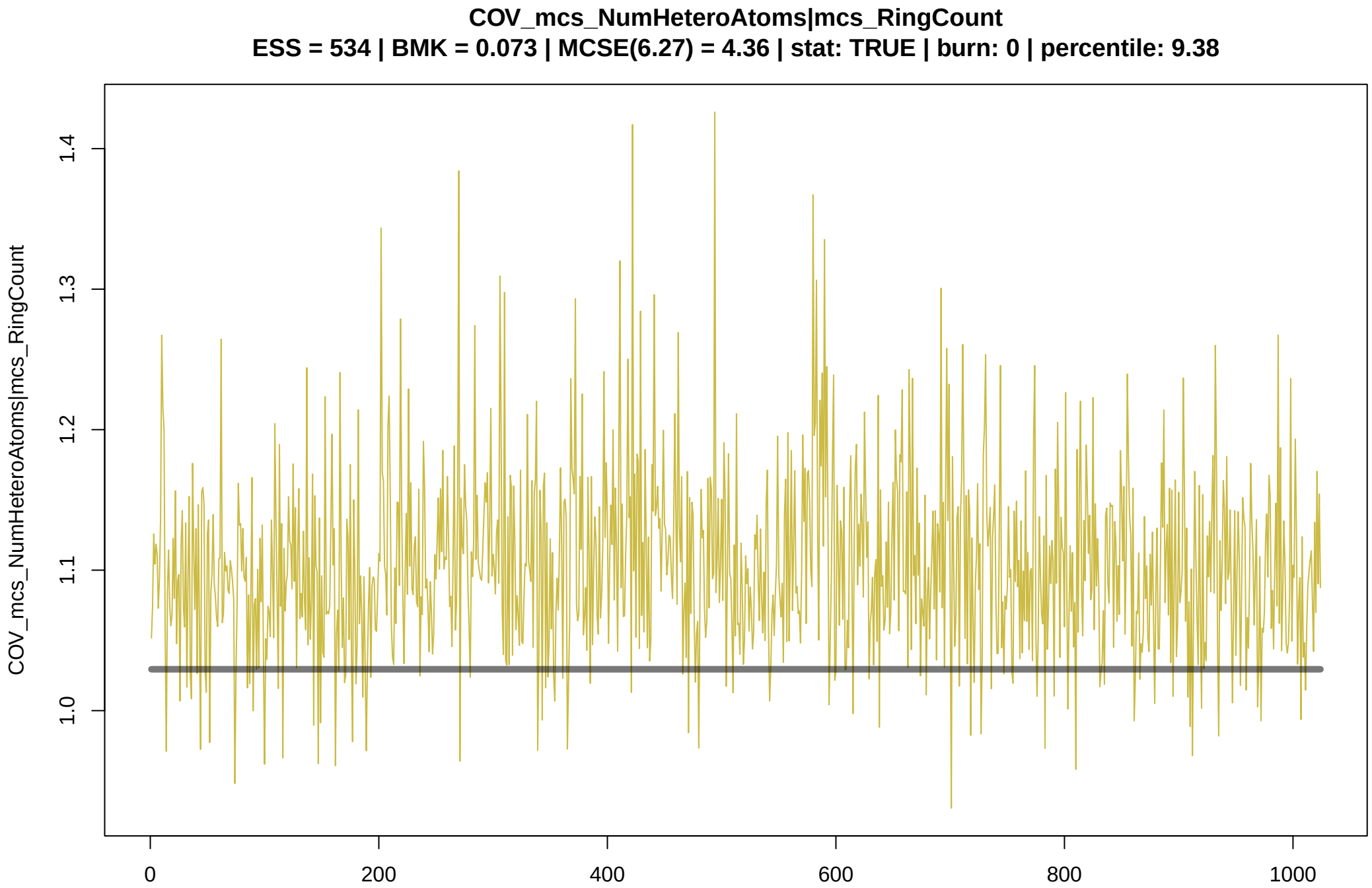

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0401 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0 | percentile: 91.7
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
45
44
43
42
41
40
0
200
400
600
800
1000

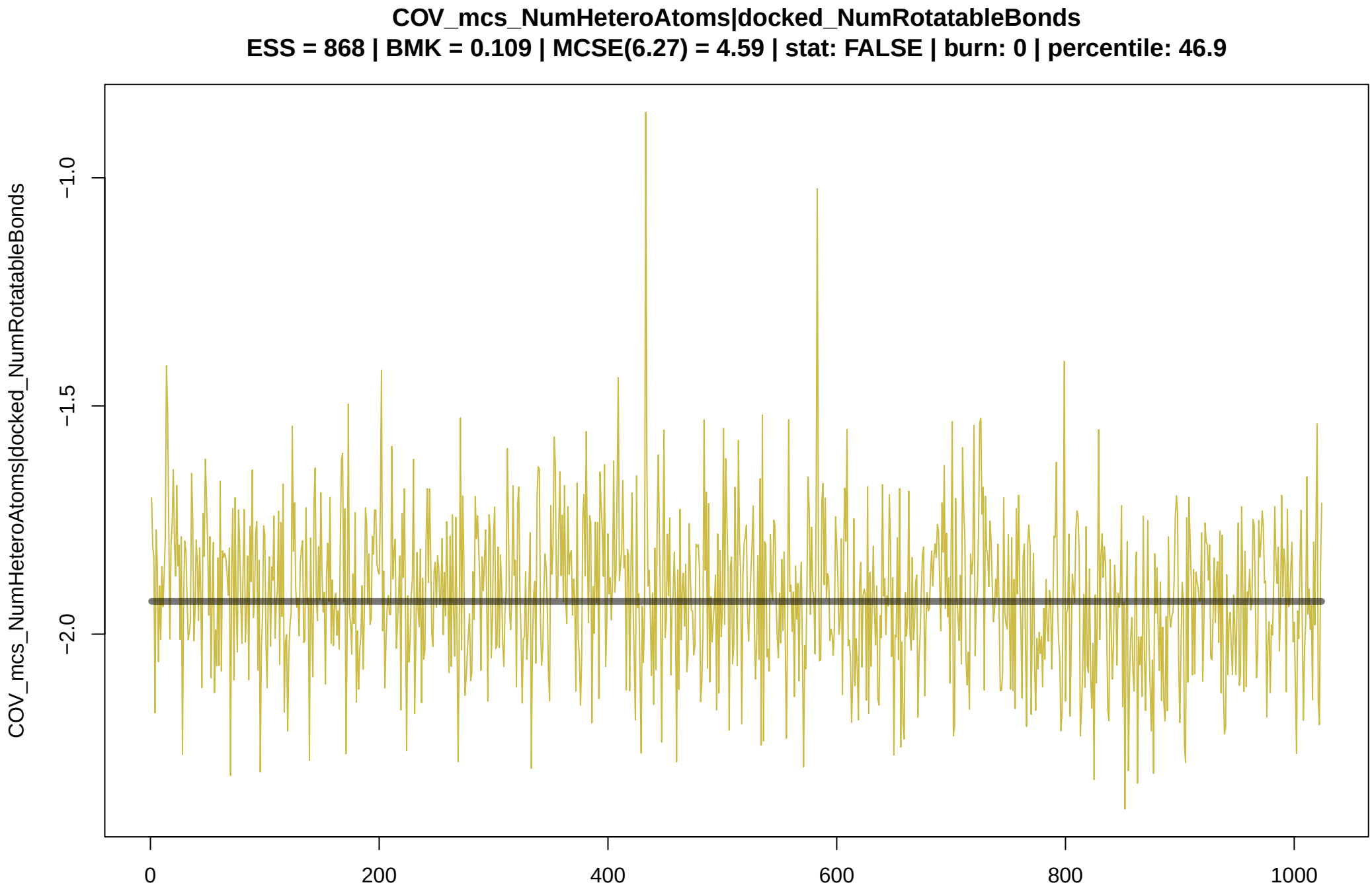

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0606 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | percentile: 15.5
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

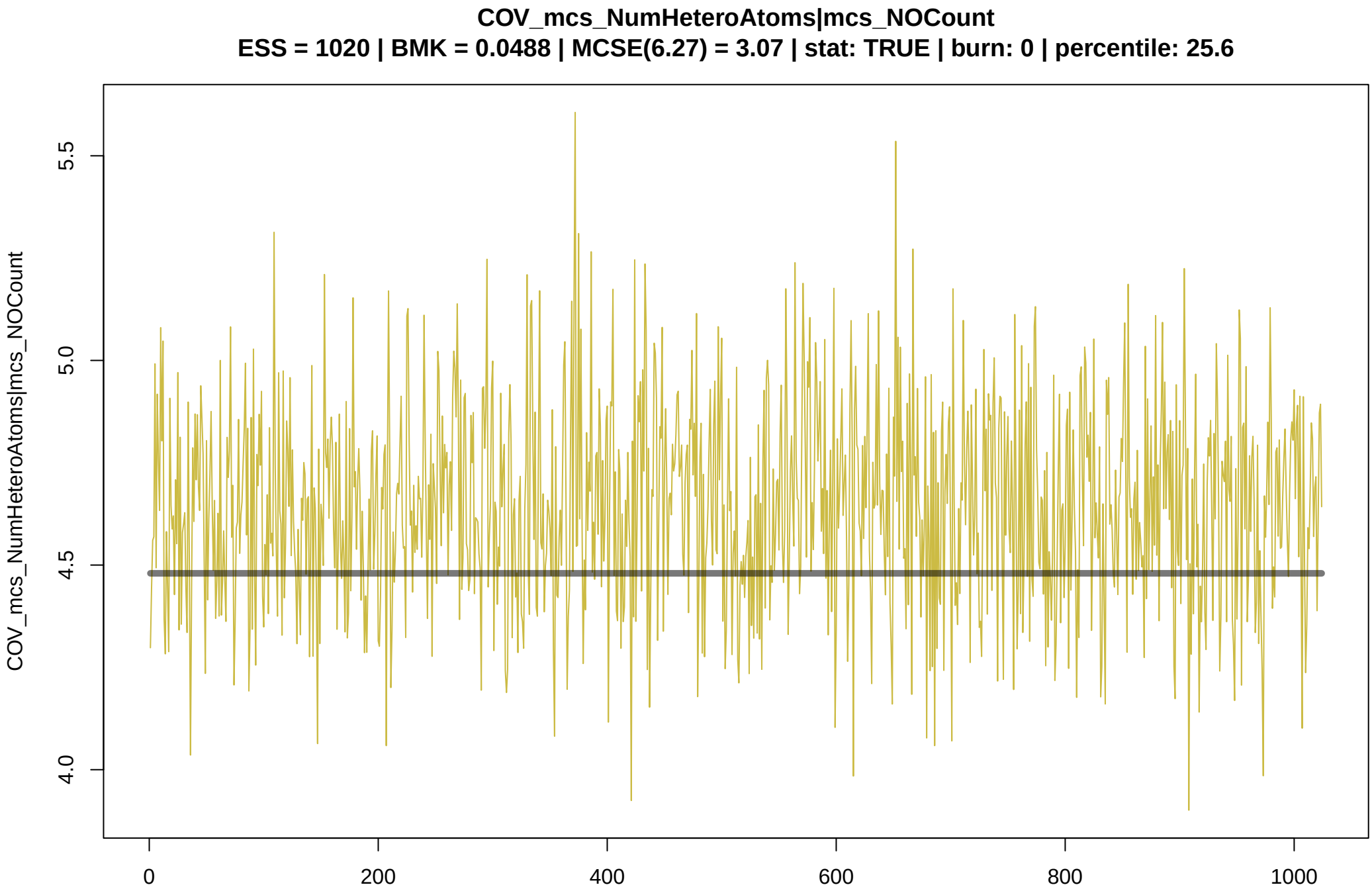

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0466 | MCSE(6.27) = 3.23 | stat: TRUE | burn: 0 | percentile: 98.1
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−11.5
−12.0
−12.5
0
200
400
600
800
1000

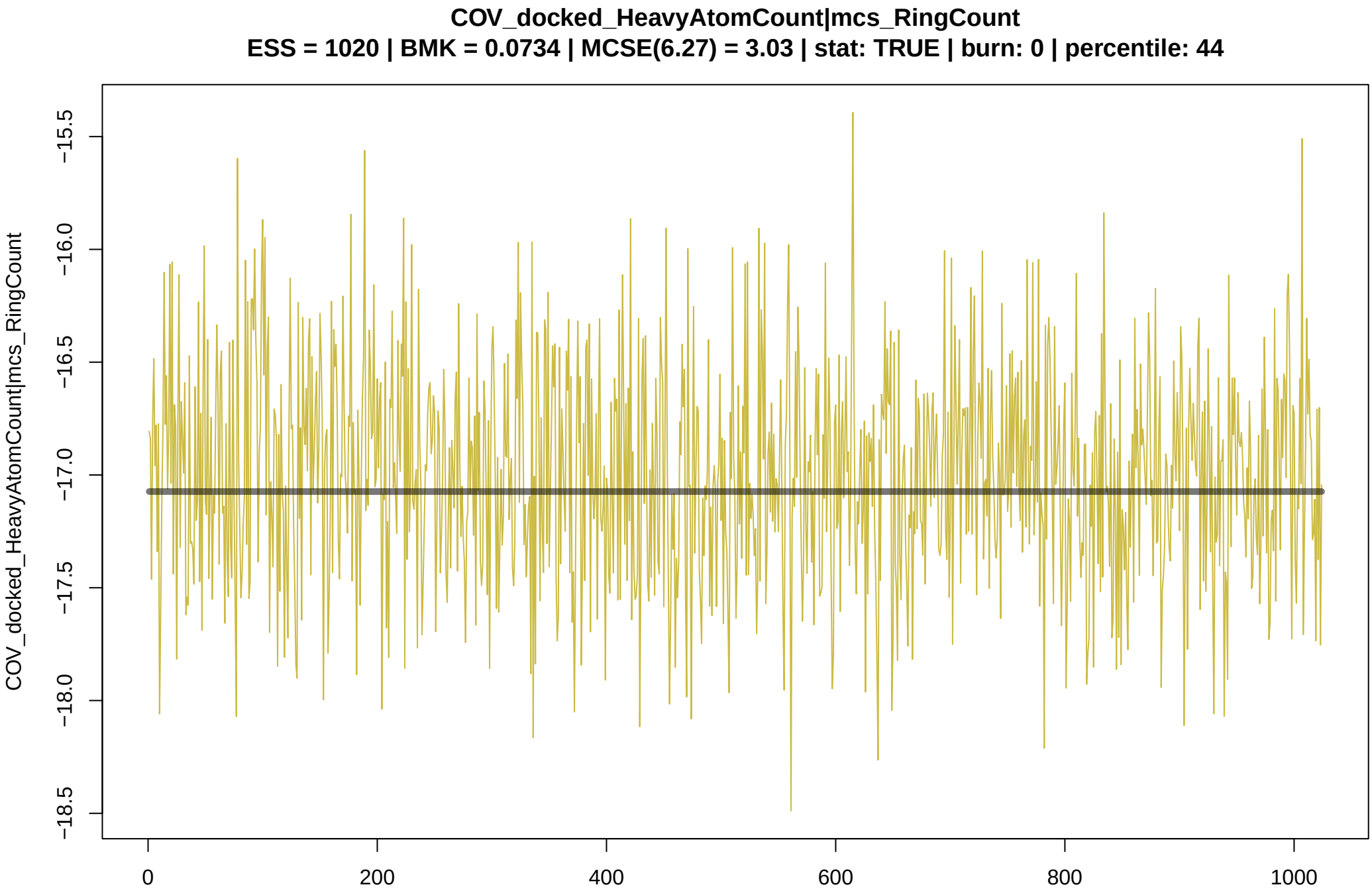

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0661 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 61
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−6.5
−7.0
−7.5
−8.0
−8.5
0
200
400
600
800
1000

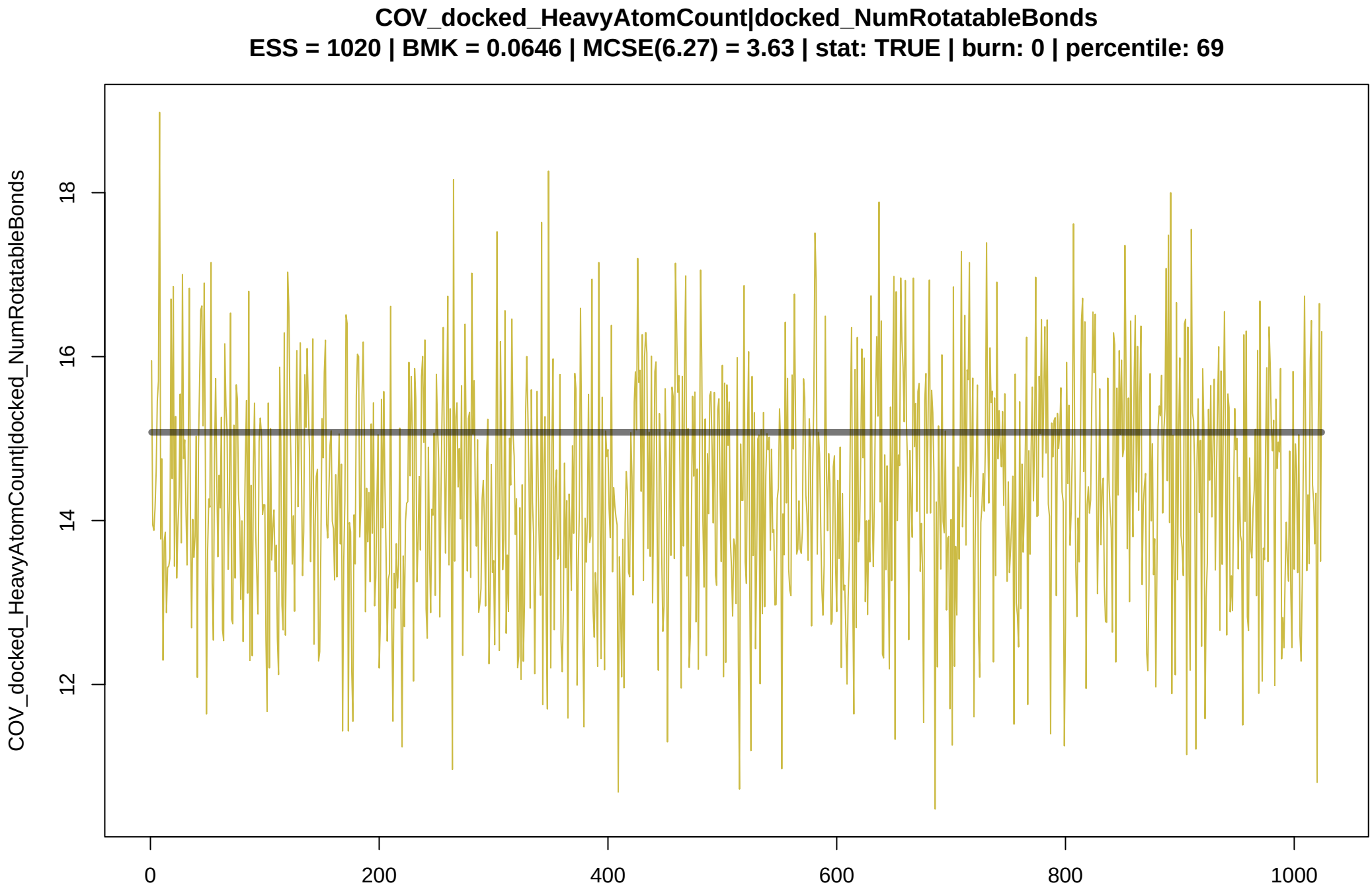

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0479 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | percentile: 14.9
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−13.5
−14.0
−14.5
−15.0
−15.5
−16.0
−16.5
0
200
400
600
800
1000

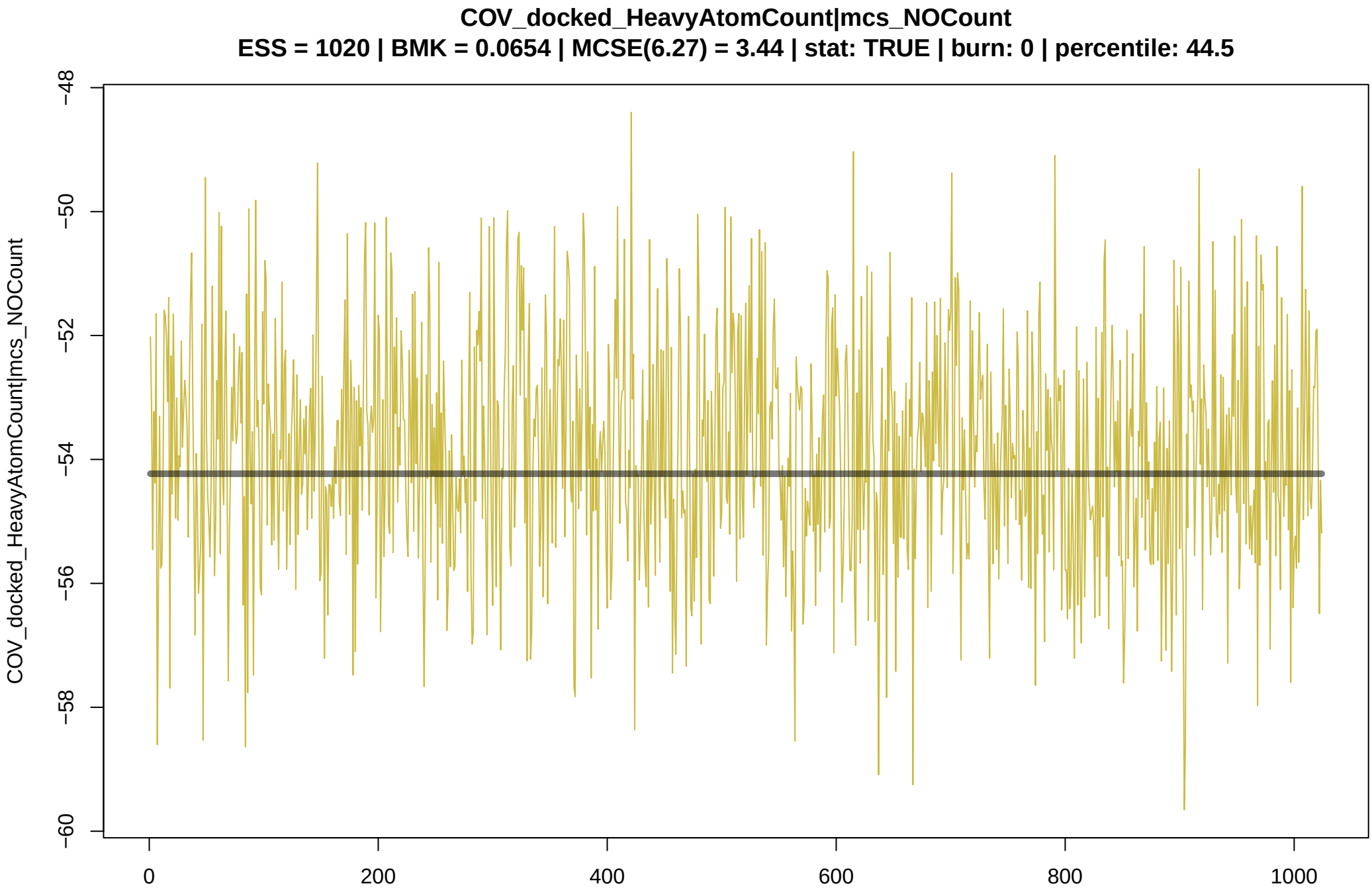

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 534 | BMK = 0.073 | MCSE(6.27) = 4.36 | stat: TRUE | burn: 0 | percentile: 9.38
COV_mcs_NumHeteroAtoms|mcs_RingCount
1.0
1.1
1.2
1.3
1.4
0
200
400
600
800
1000

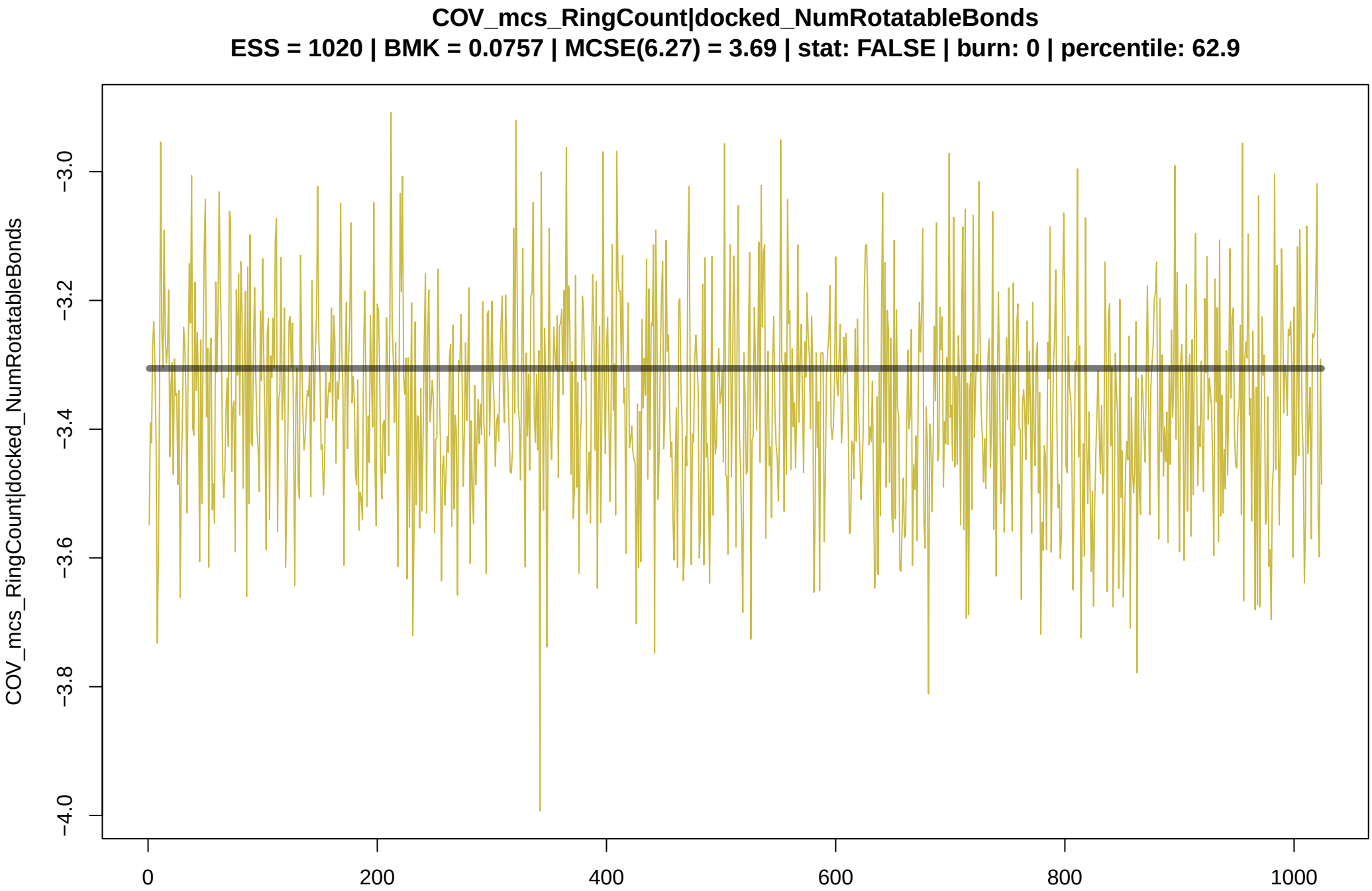

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 868 | BMK = 0.109 | MCSE(6.27) = 4.59 | stat: FALSE | burn: 0 | percentile: 46.9
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.0
−1.5
−2.0
0
200
400
600
800
1000

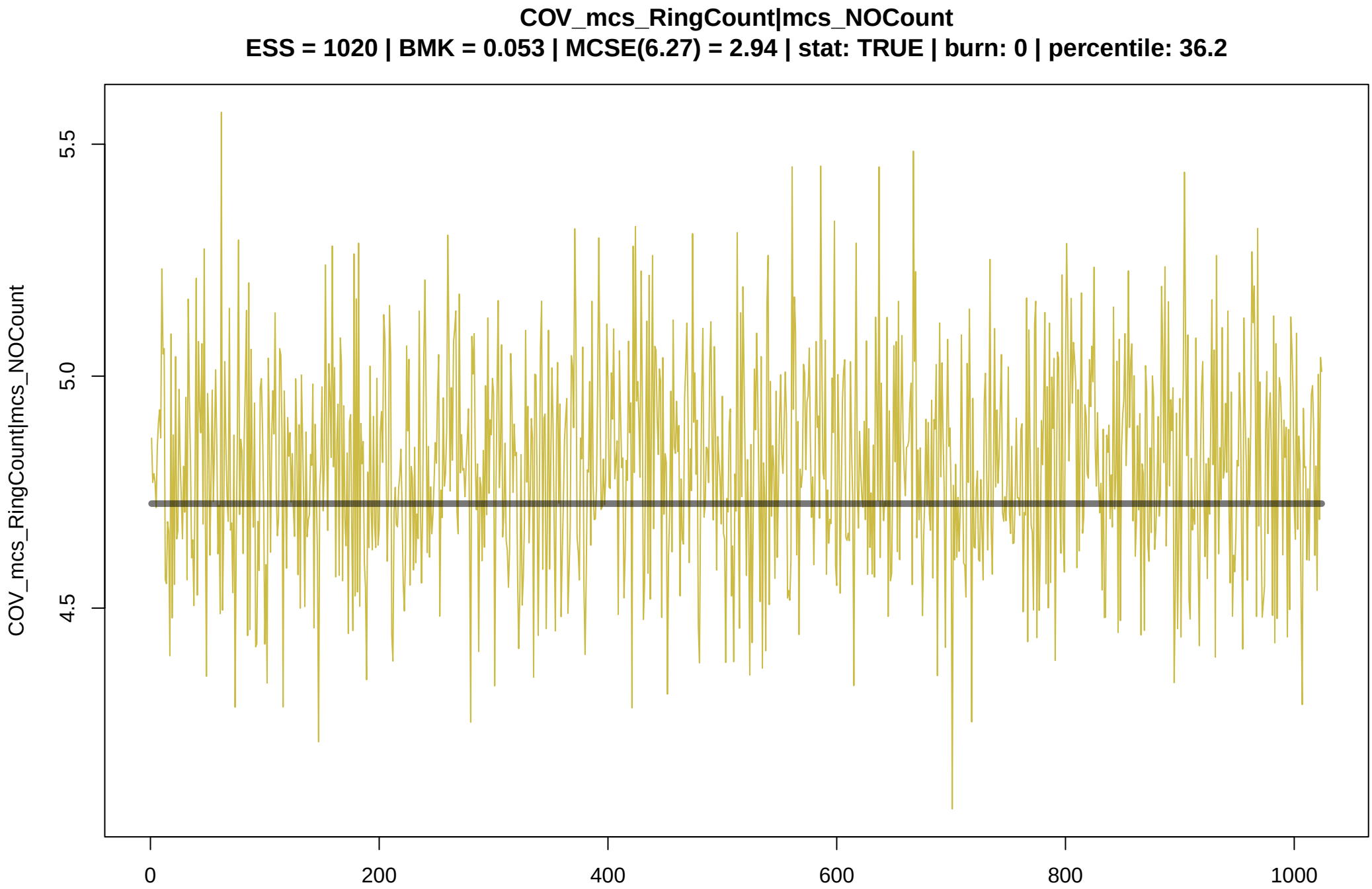

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0488 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | percentile: 25.6
COV_mcs_NumHeteroAtoms|mcs_NOCount
4.0
4.5
5.0
5.5
0
200
400
600
800
1000

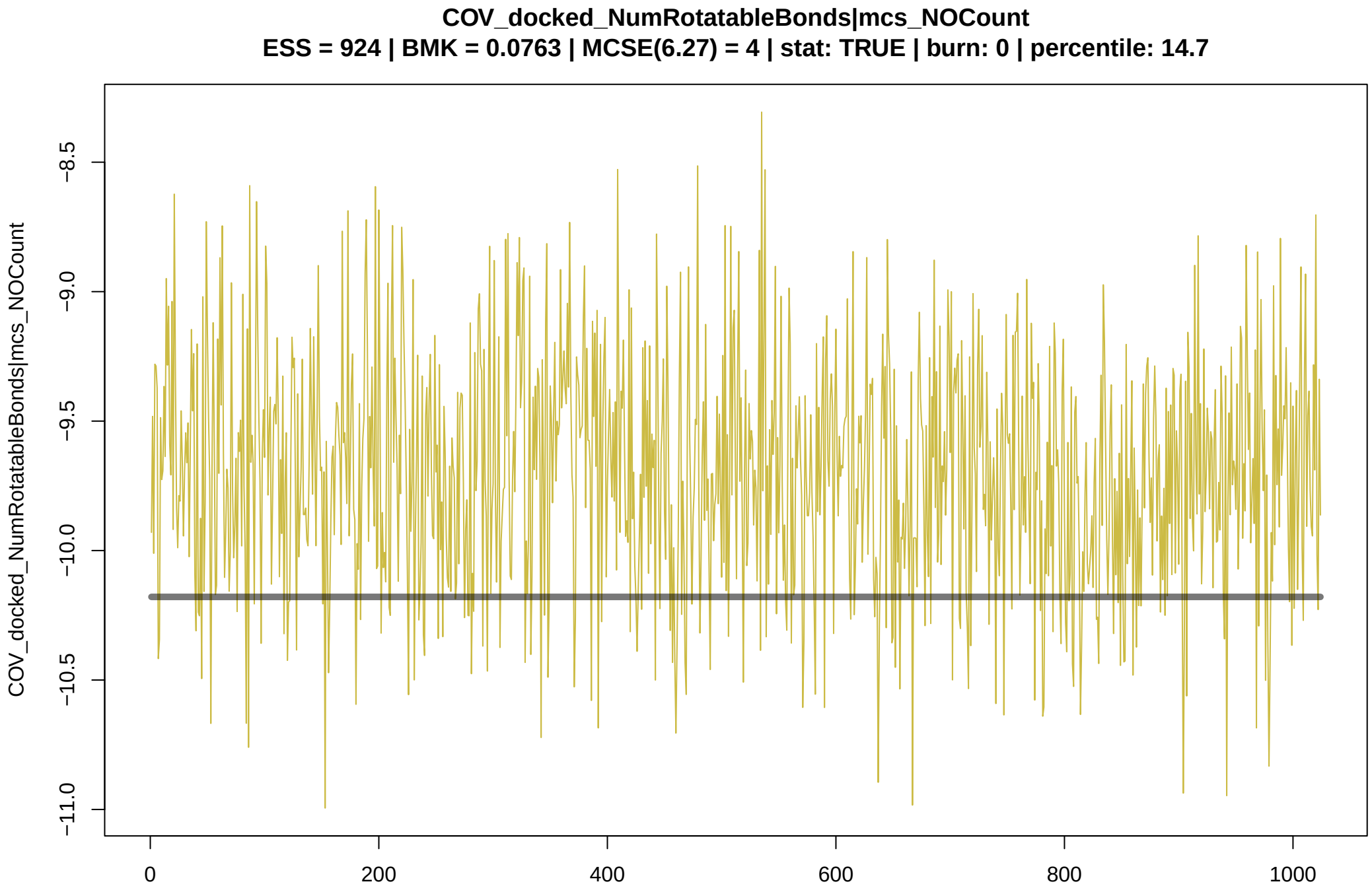

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0734 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | percentile: 44
COV_docked_HeavyAtomCount|mcs_RingCount
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0646 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | percentile: 69
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0654 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | percentile: 44.5
COV_docked_HeavyAtomCount|mcs_NOCount
−48
−50
−52
−54
−56
−58
−60
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0757 | MCSE(6.27) = 3.69 | stat: FALSE | burn: 0 | percentile: 62.9
COV_mcs_RingCount|docked_NumRotatableBonds
−3.0
−3.2
−3.4
−3.6
−3.8
−4.0
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.053 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 36.2
COV_mcs_RingCount|mcs_NOCount
5.5
5.0
4.5
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 924 | BMK = 0.0763 | MCSE(6.27) = 4 | stat: TRUE | burn: 0 | percentile: 14.7
COV_docked_NumRotatableBonds|mcs_NOCount
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
0
200
400
600
800
1000