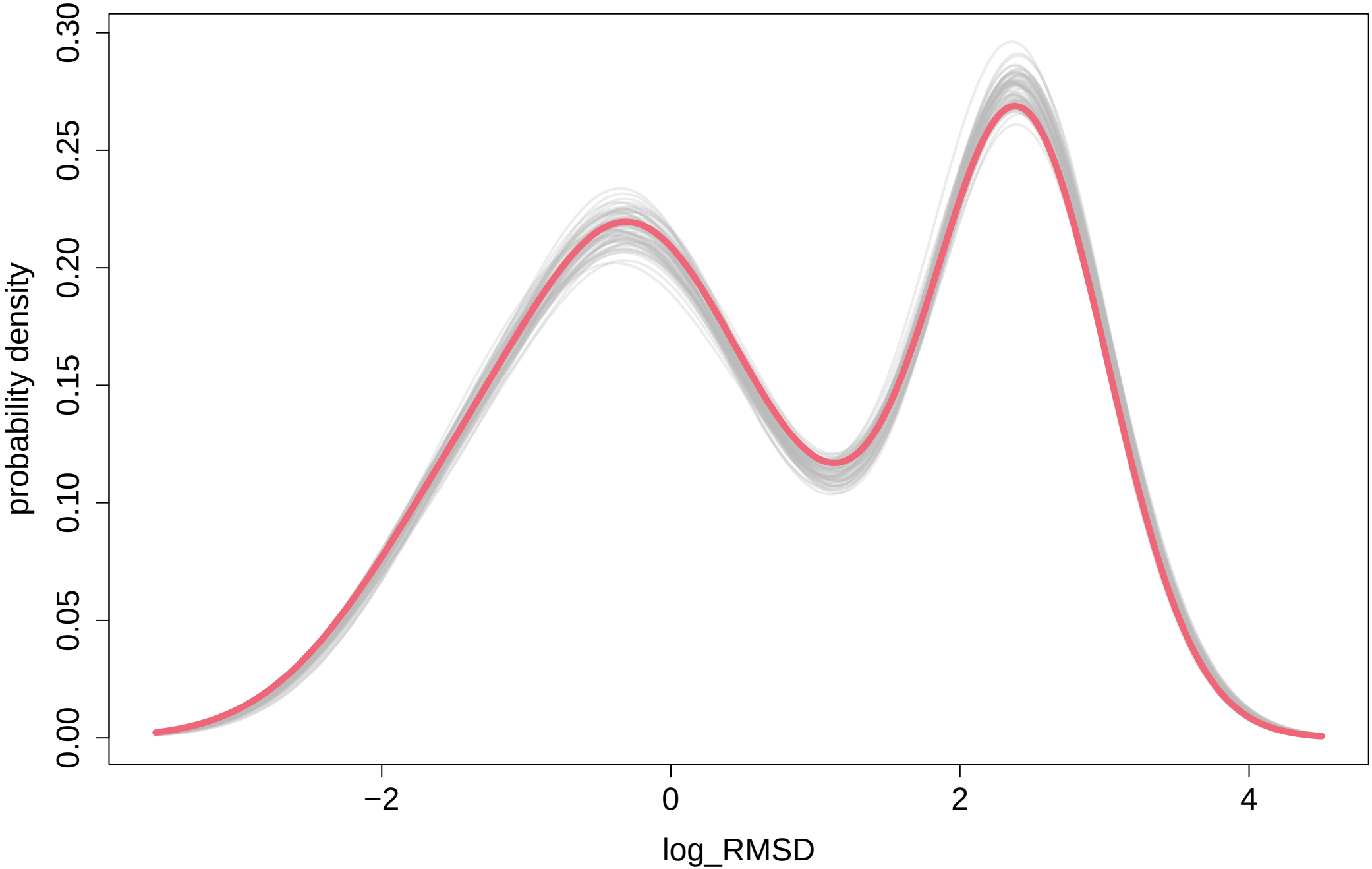
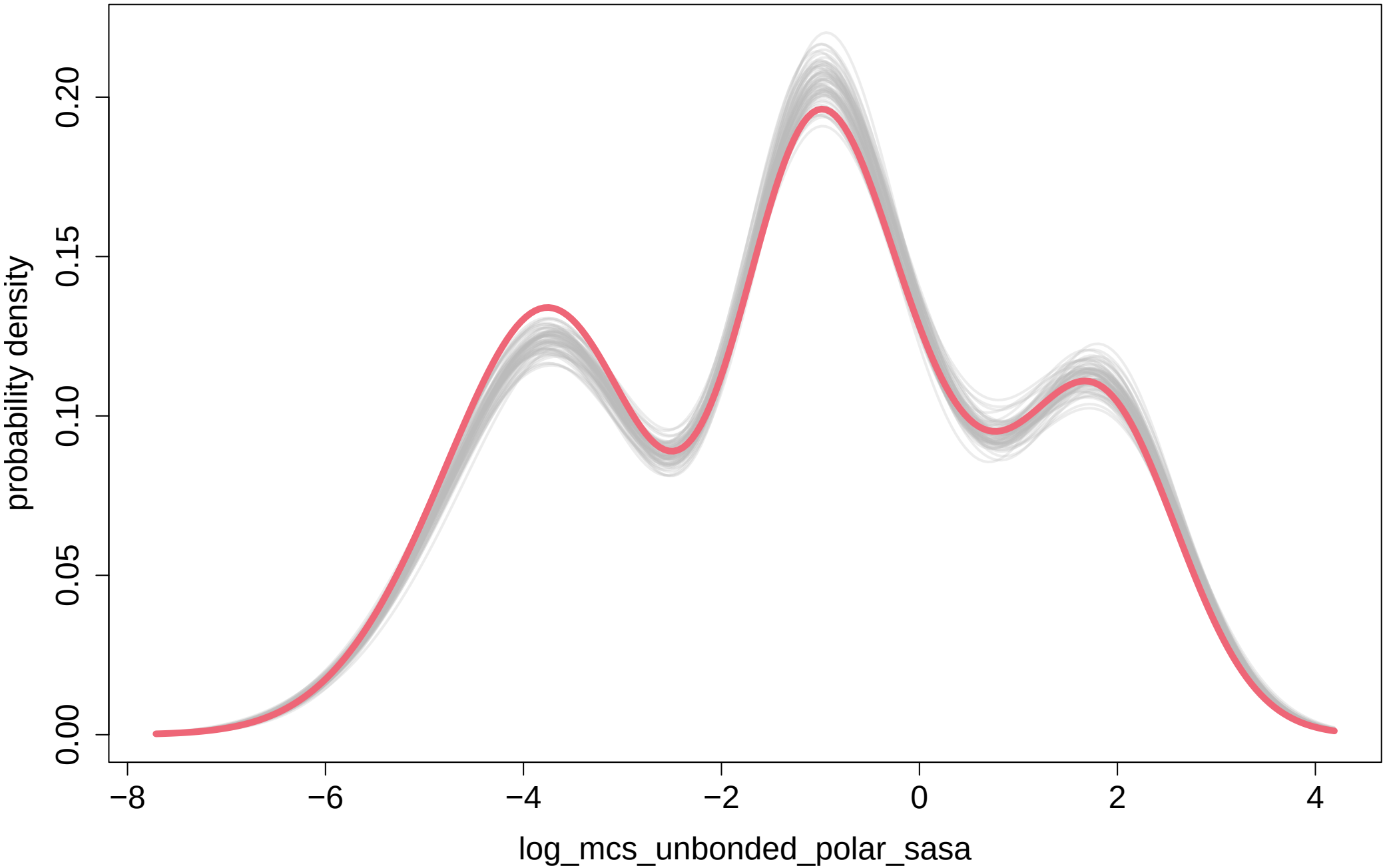
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.203883465827339
max MCSE = 11.7109793250818
all stationary: FALSE
burn: 0
min percent.: 17.28515625

−− STATS 2D −−
min ESS = 792.866696998739
max BMK = 0.090986339383965 6
max MCSE = 4.54550722986022
all stationary: TRUE
burn: 0
min percent.: 1.26953125

−− STATS 1D −−
min ESS = 48.4270622420228
max BMK = 1
max MCSE = 9.95974897733348
all stationary: FALSE
burn: 1020
min percent.: 0.1953125

Occupied clusters: 23 of 64
LL: −62400 +− 10.4


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
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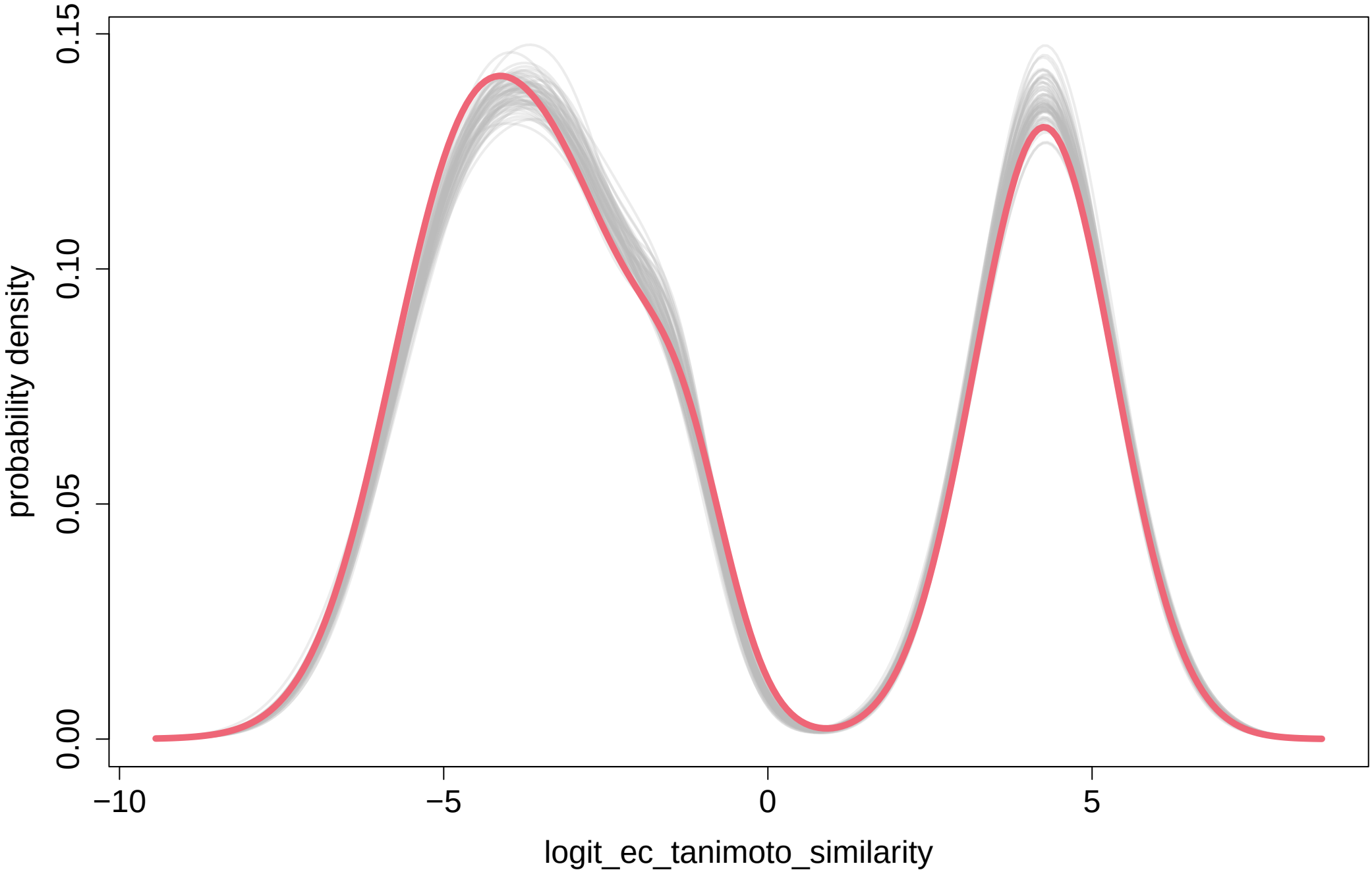
0.15
0.20
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa


probability density
0.00
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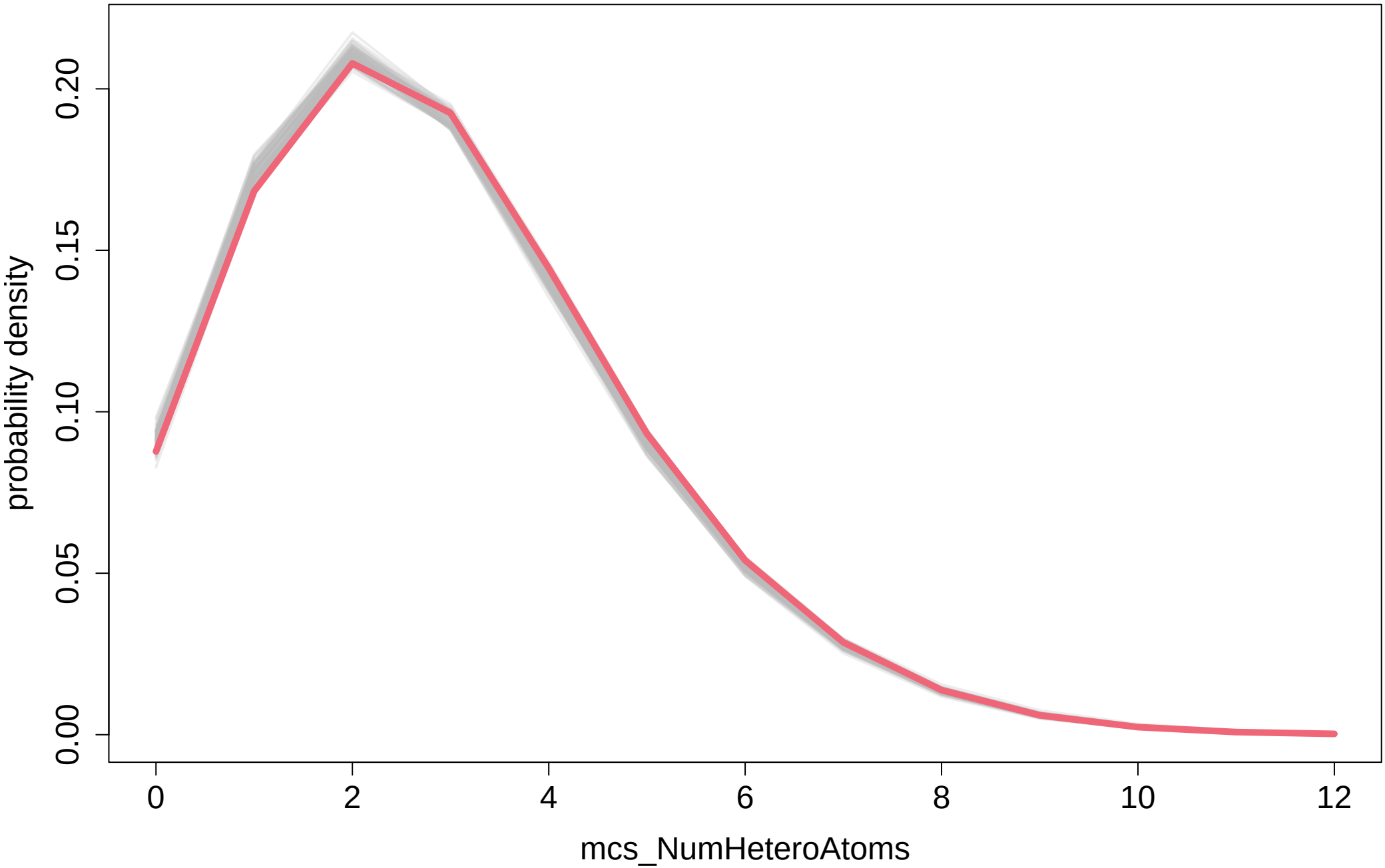
0.15
−10
−5
0
5
logit_ec_tanimoto_similarity


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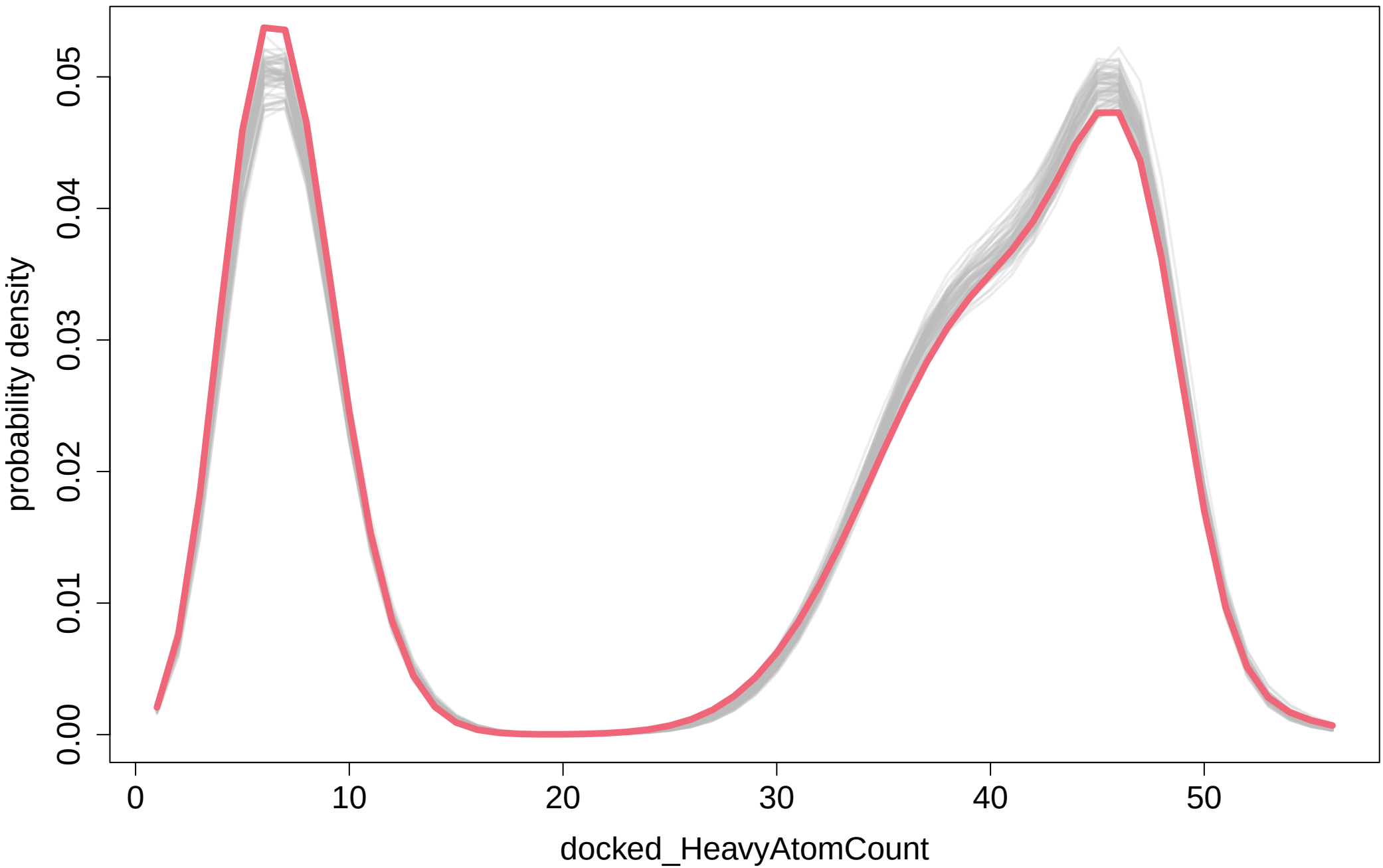
0.10
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms


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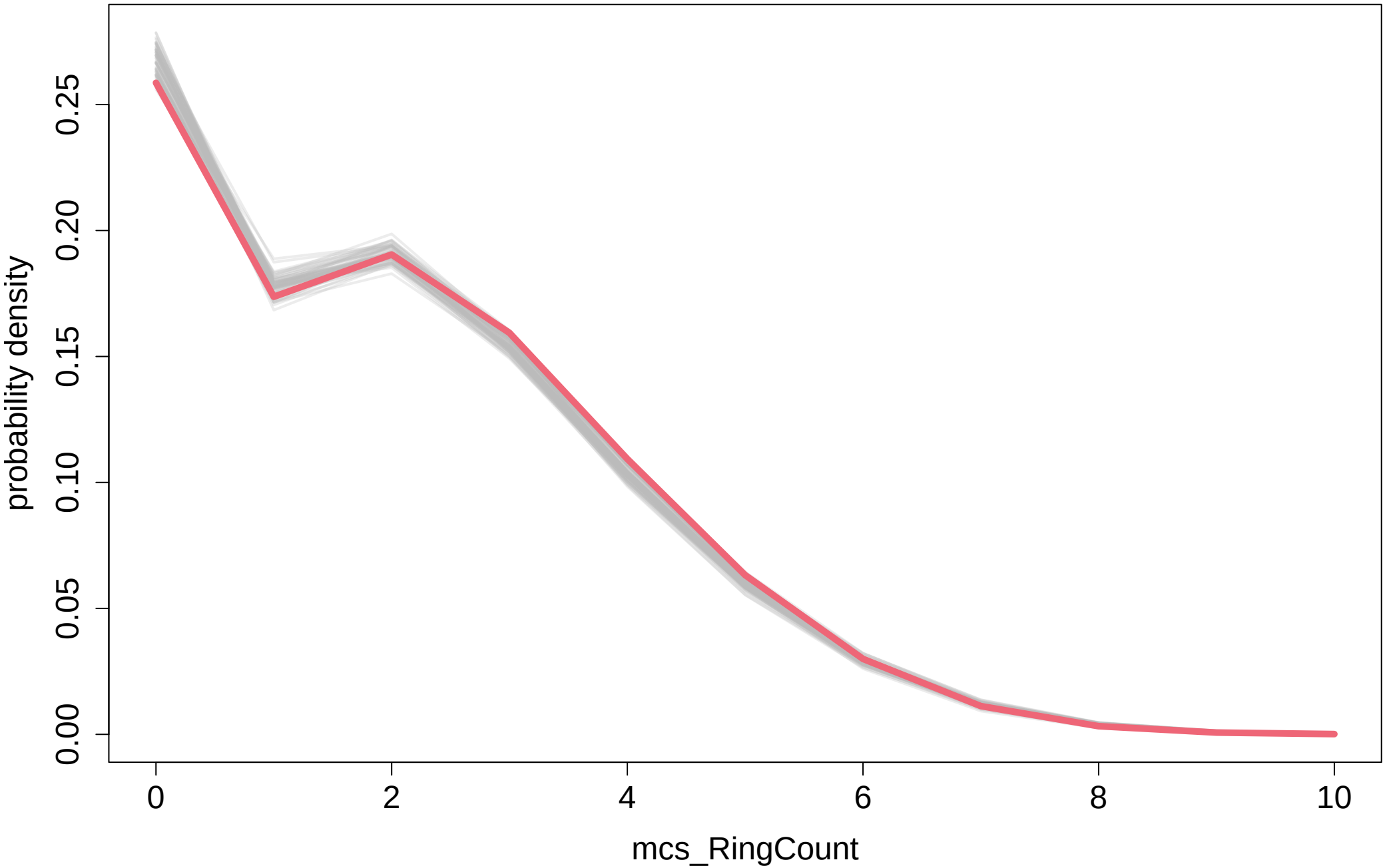
0.02
0.03
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount


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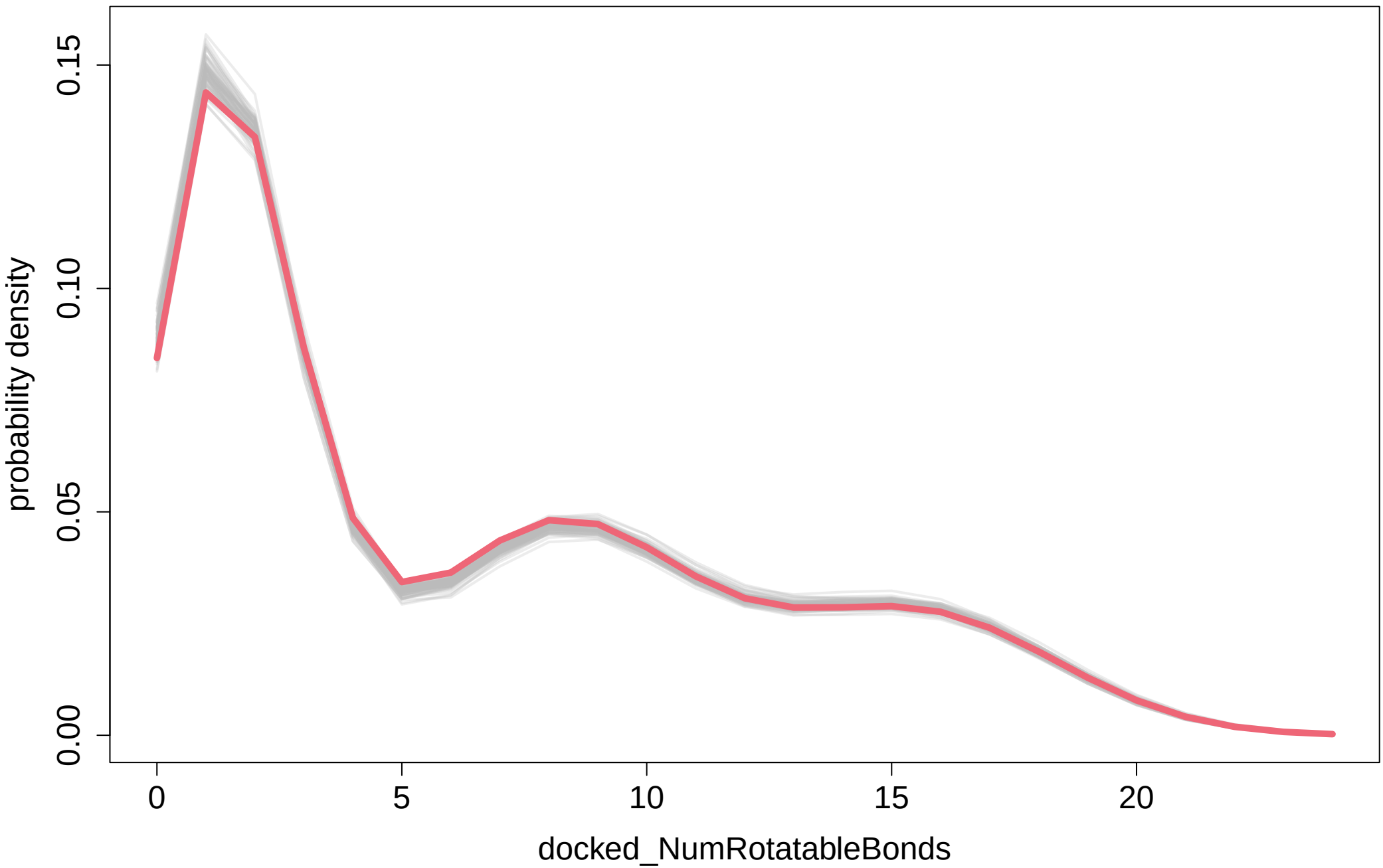
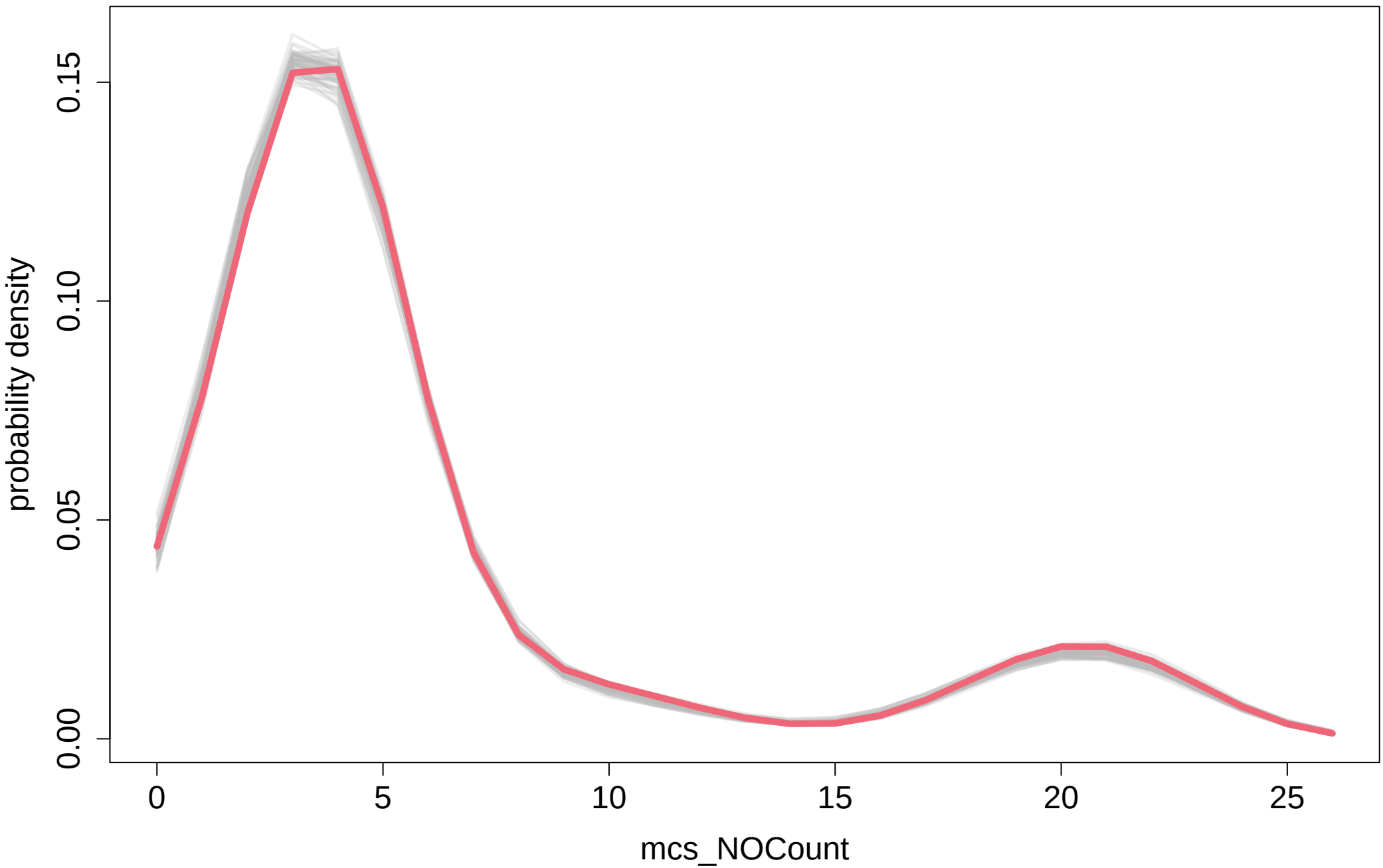
0.05
0.10
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount


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


probability density
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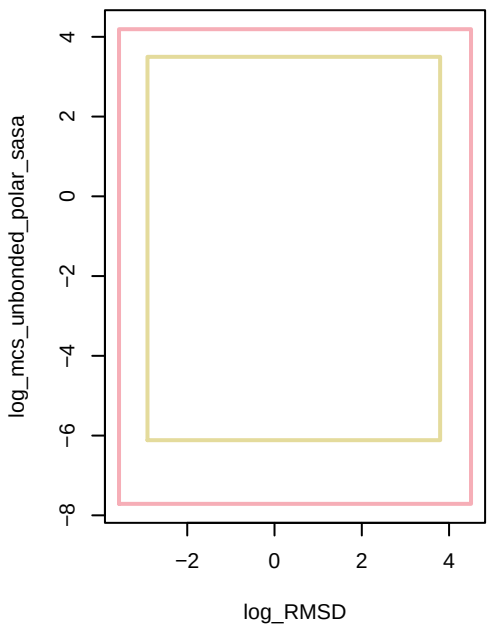
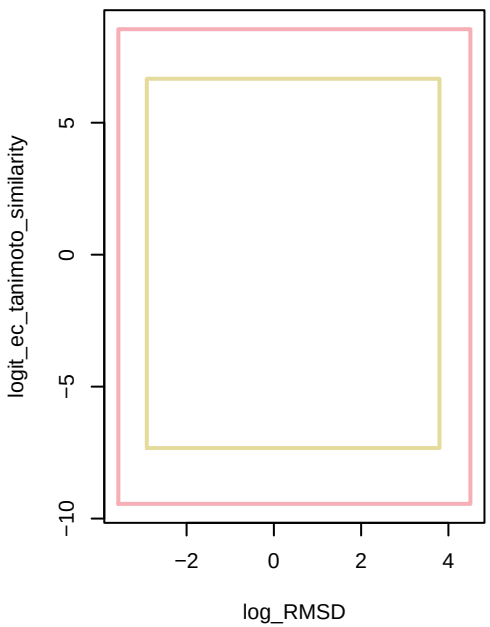
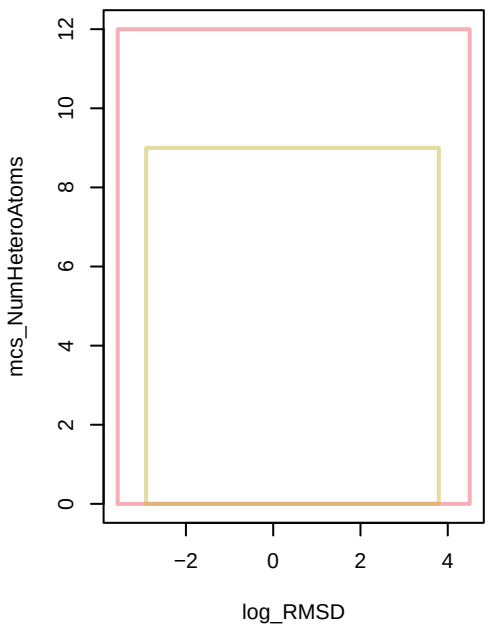
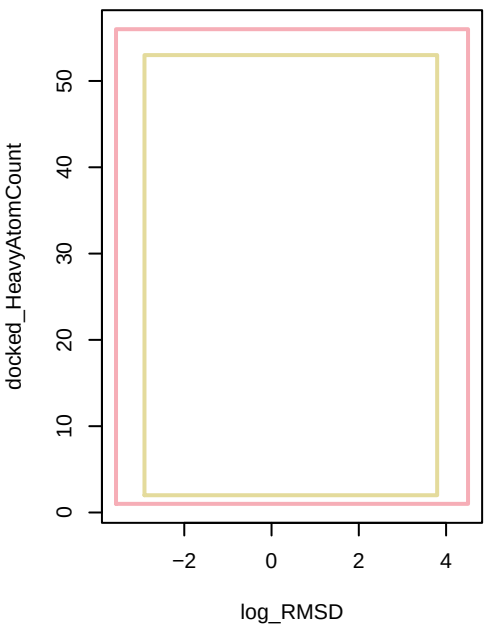
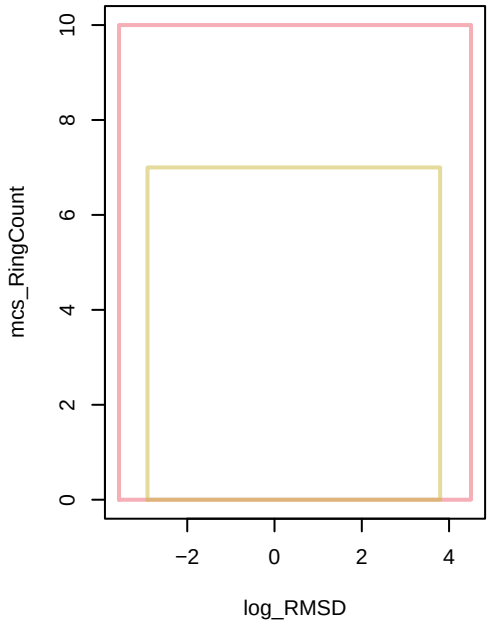
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

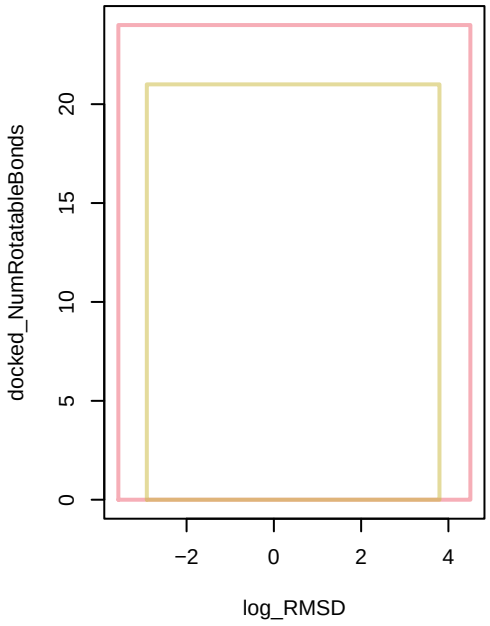

log_mcs_unbonded_polar_sasa
log_RMSD

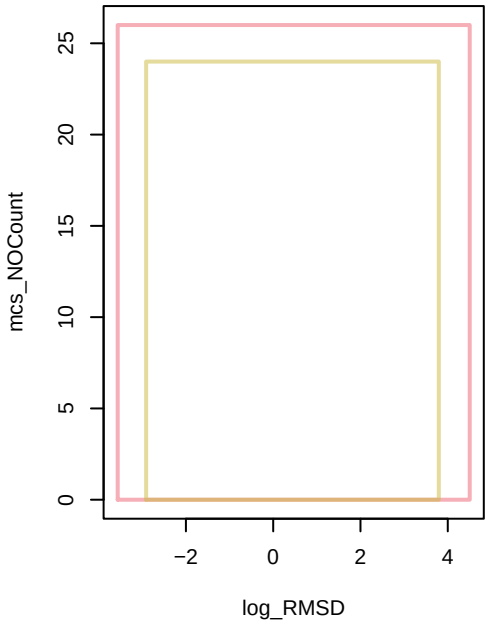

logit_ec_tanimoto_similarity
log_RMSD

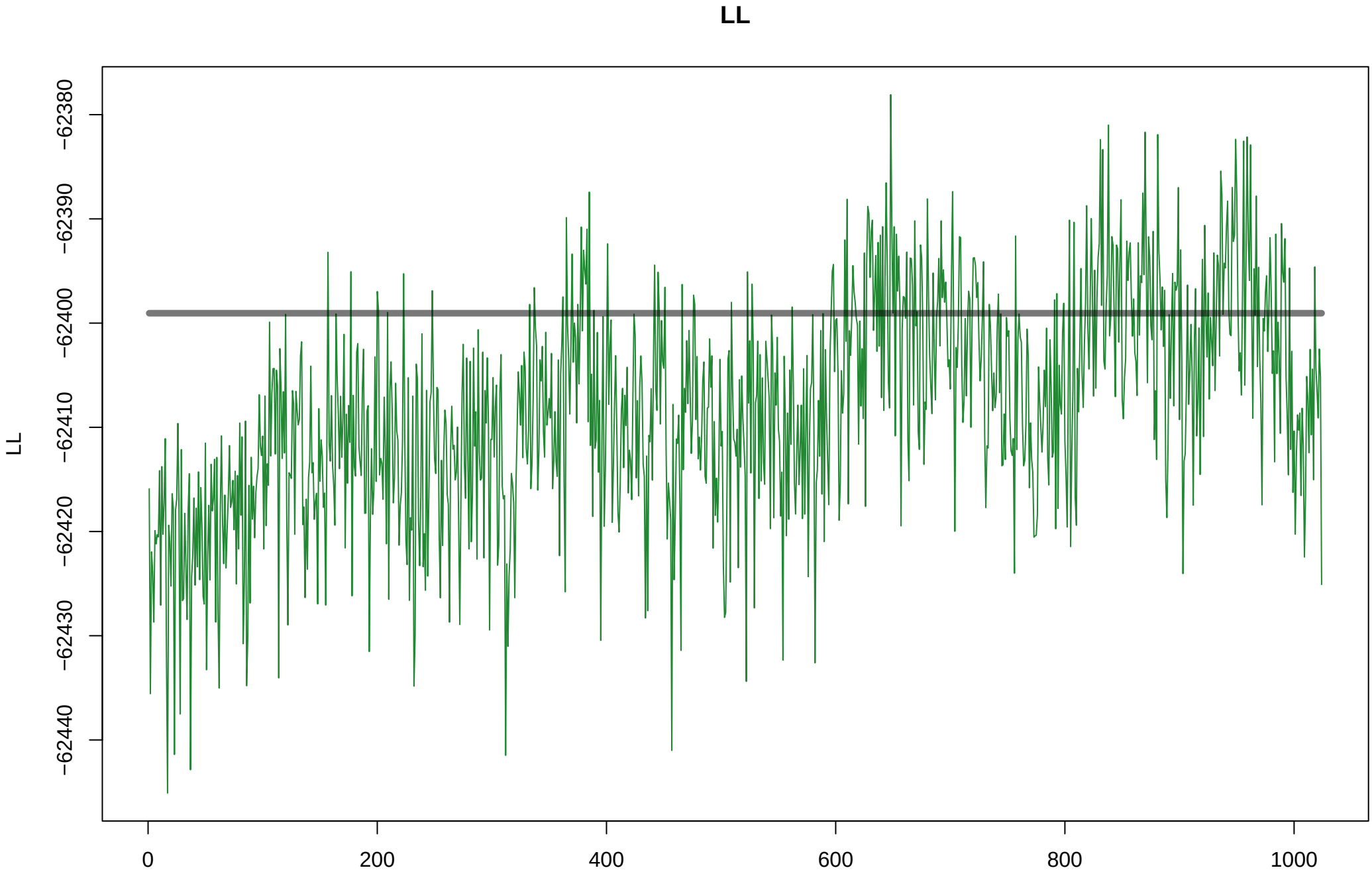

mcs_NumHeteroAtoms
log_RMSD

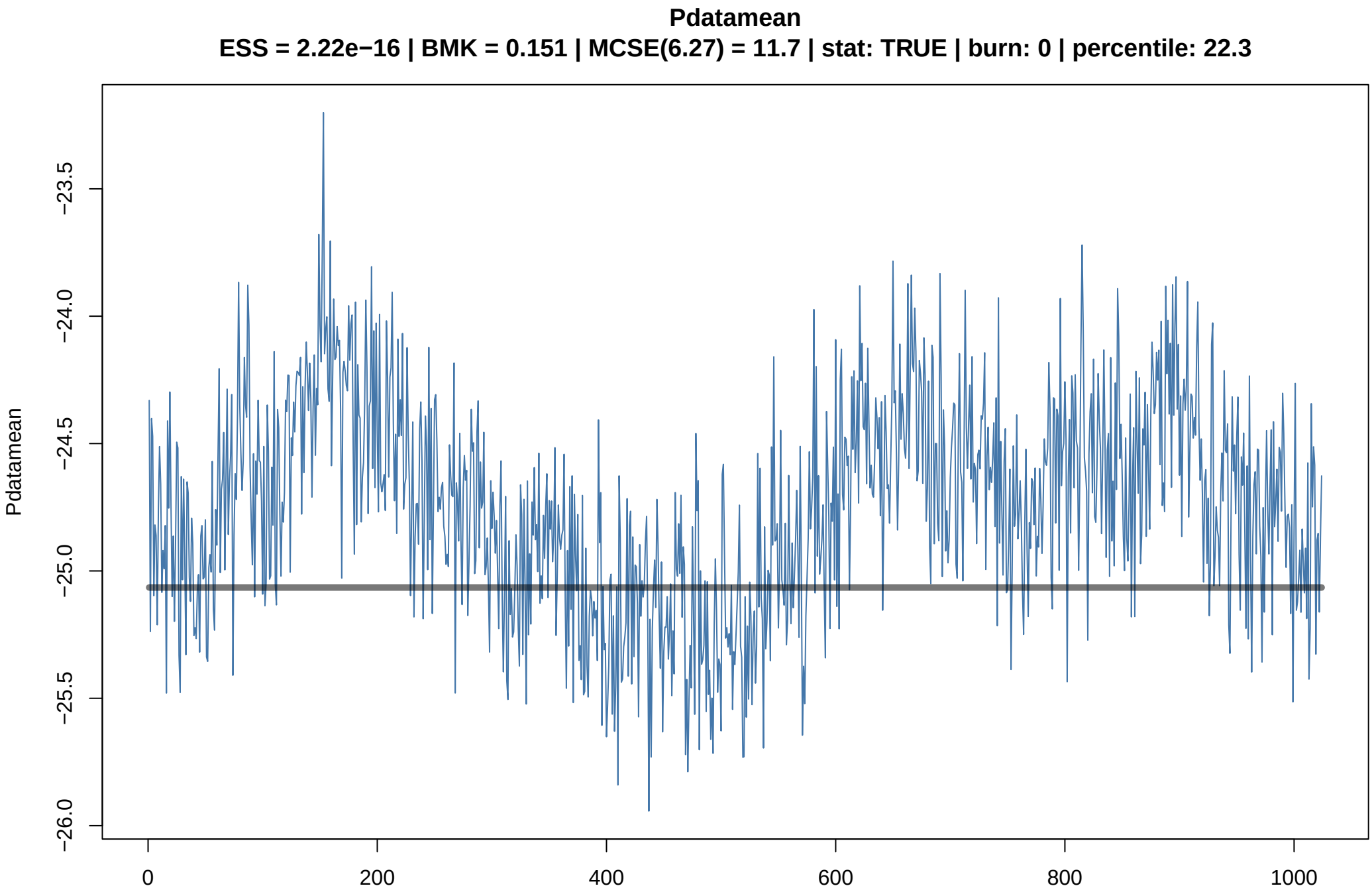

docked_HeavyAtomCount
log_RMSD

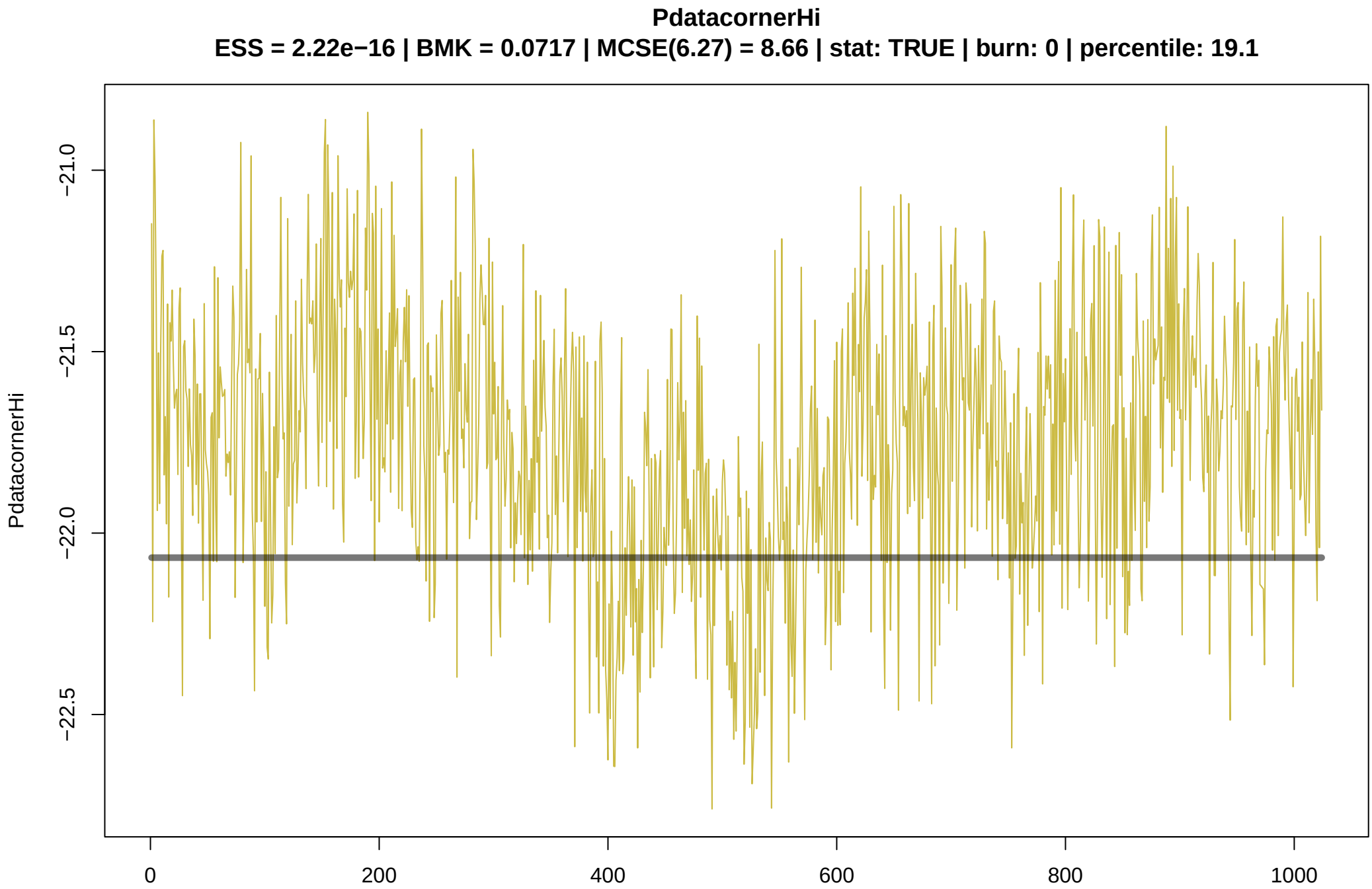

mcs_RingCount
log_RMSD

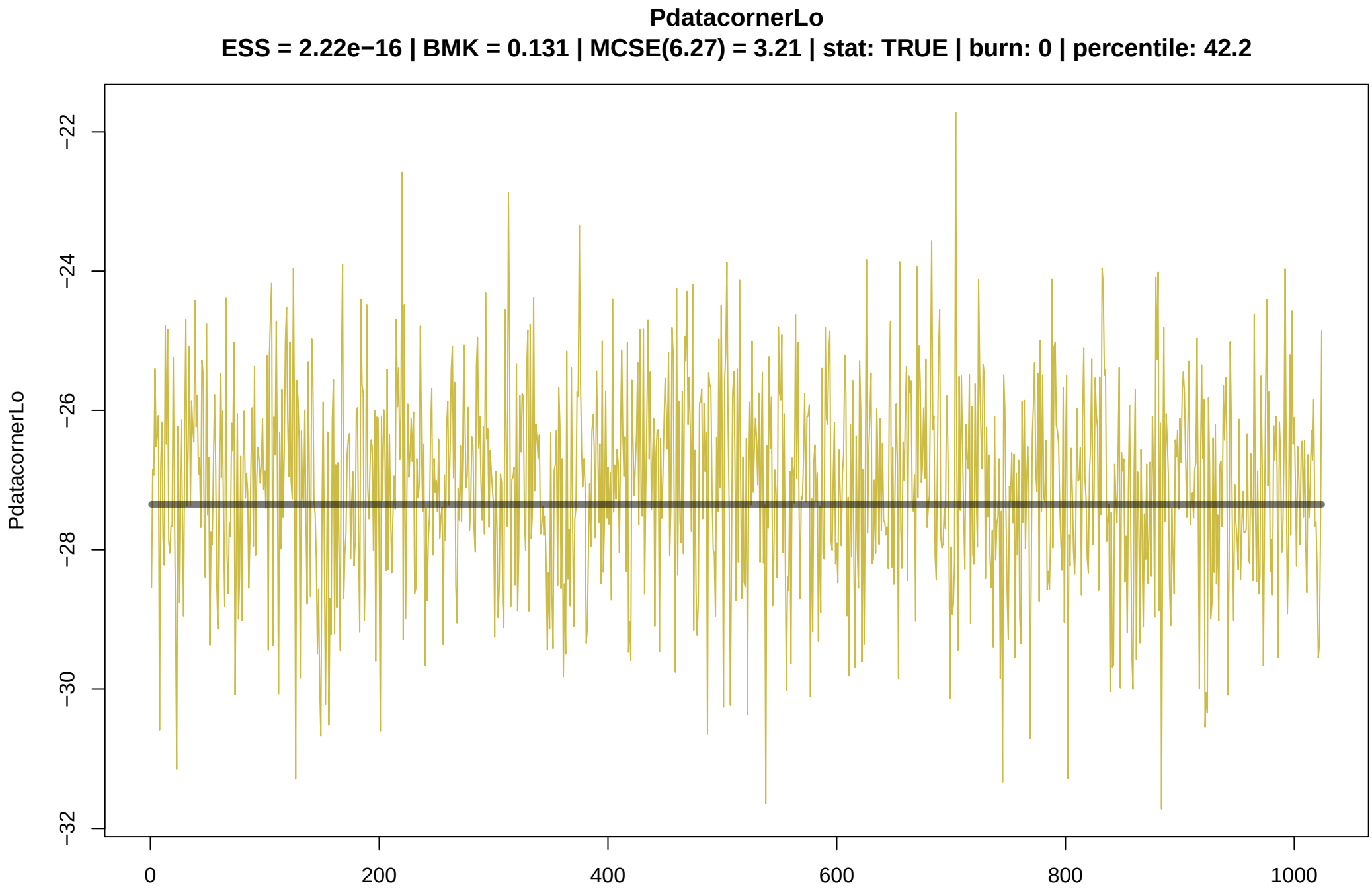

docked_NumRotatableBonds
log_RMSD

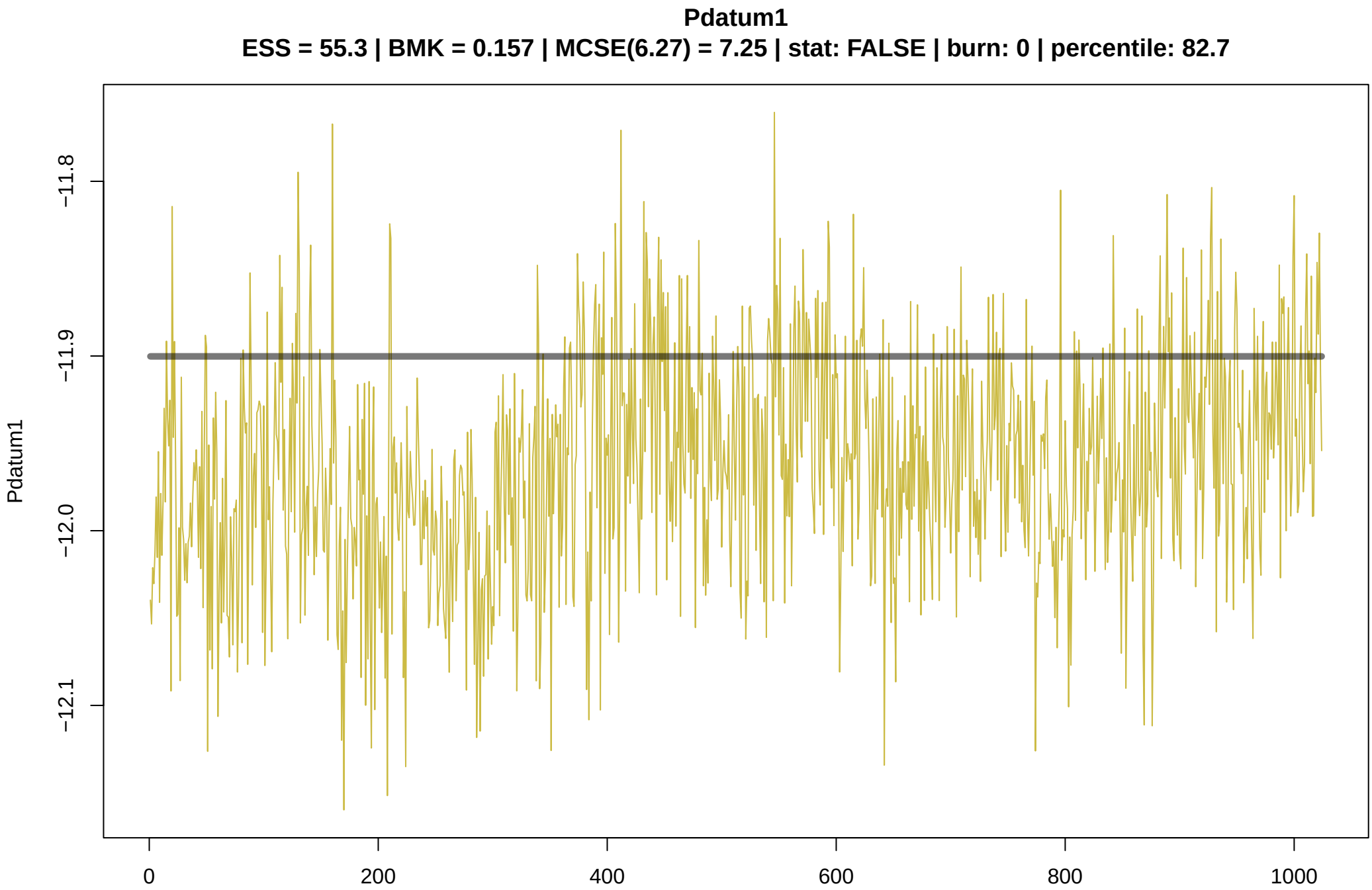

mcs_NOCount
log_RMSD

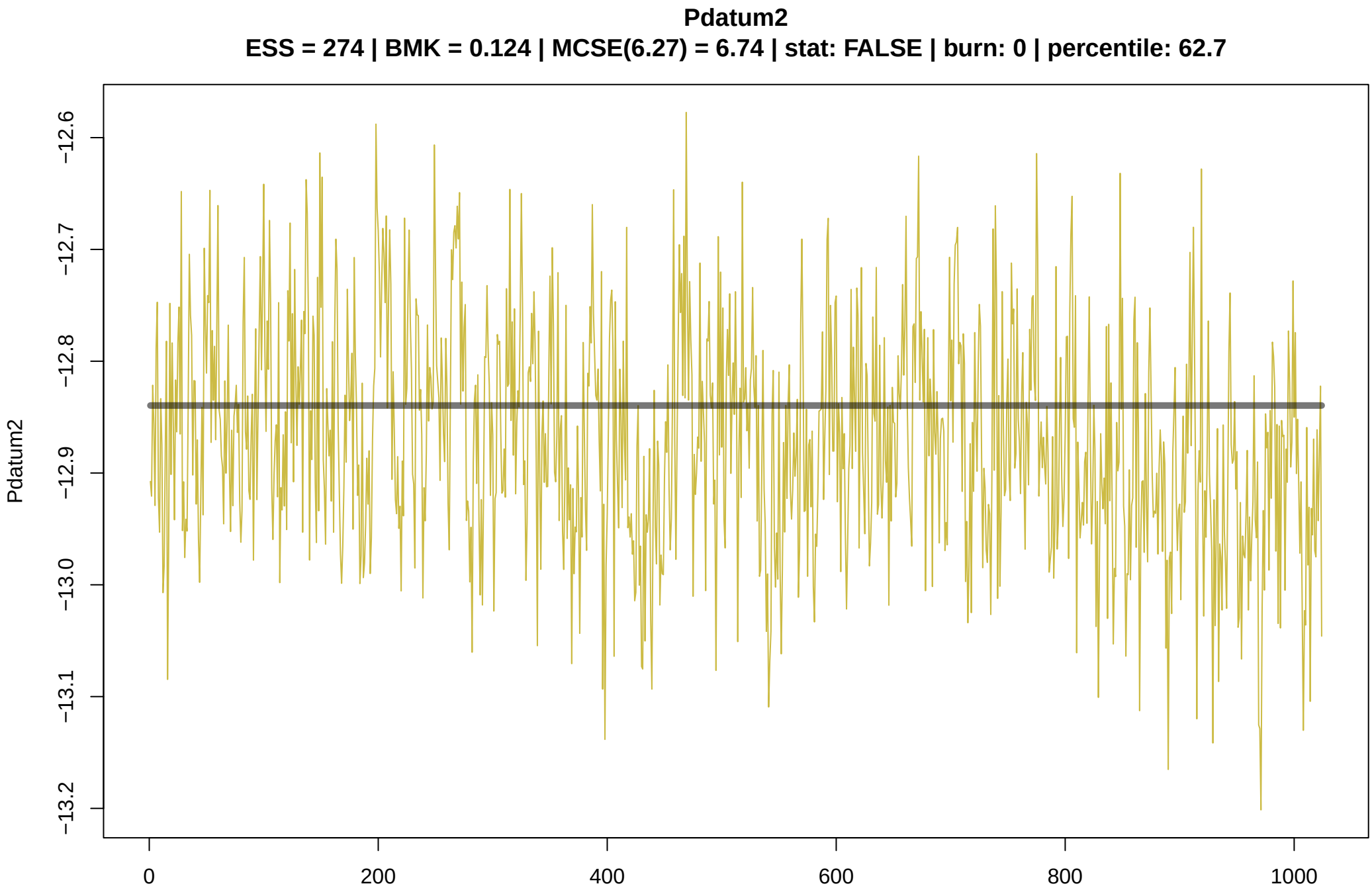

LL
LL
−62380
−62390
−62400
−62410
−62420
−62430
−62440
0
200
400
600
800
1000

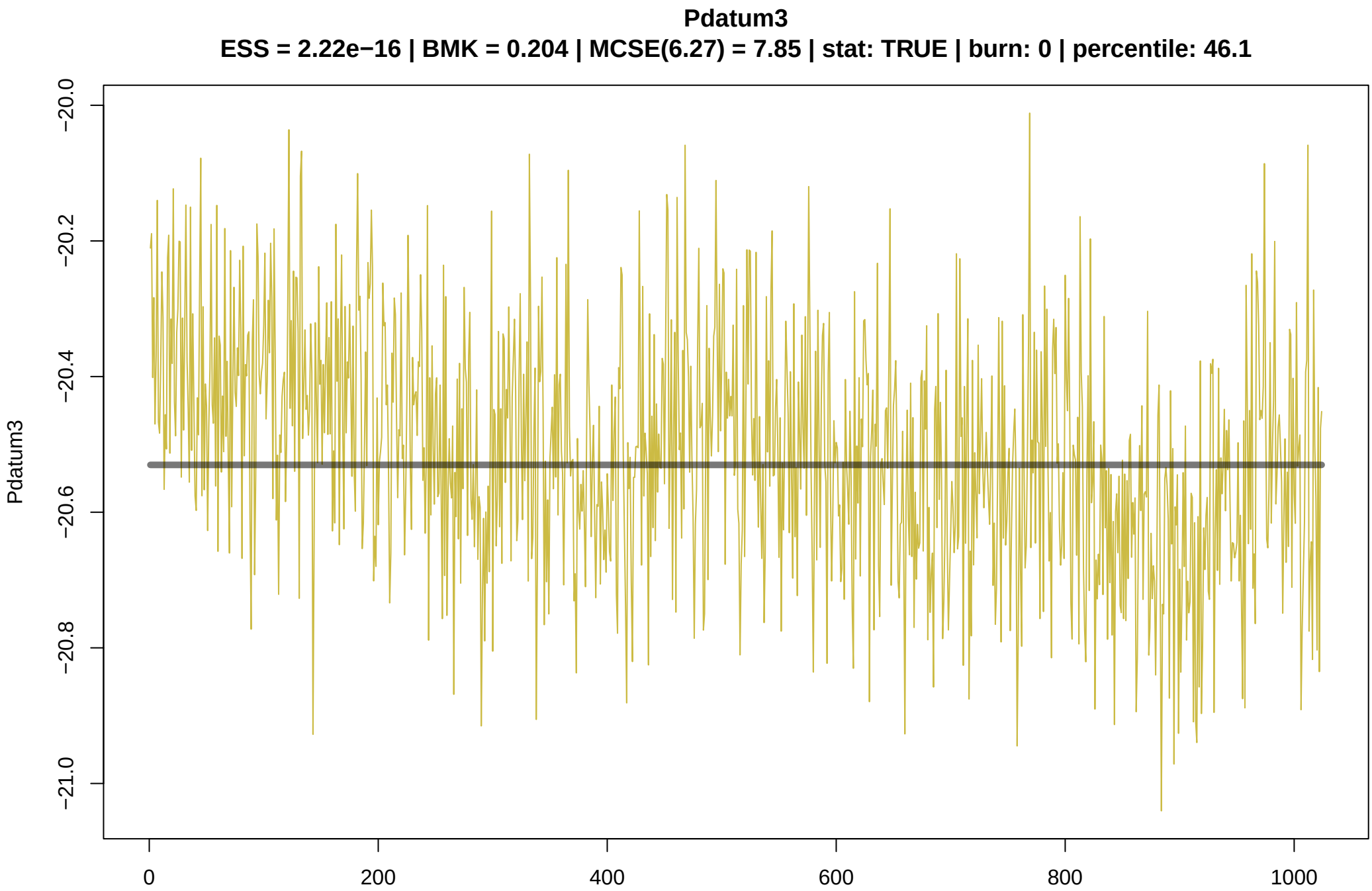

Pdatamean
ESS = 2.22e−16 | BMK = 0.151 | MCSE(6.27) = 11.7 | stat: TRUE | burn: 0 | percentile: 22.3
Pdatamean
−23.5
−24.0
−24.5
−25.0
−25.5
−26.0
0
200
400
600
800
1000

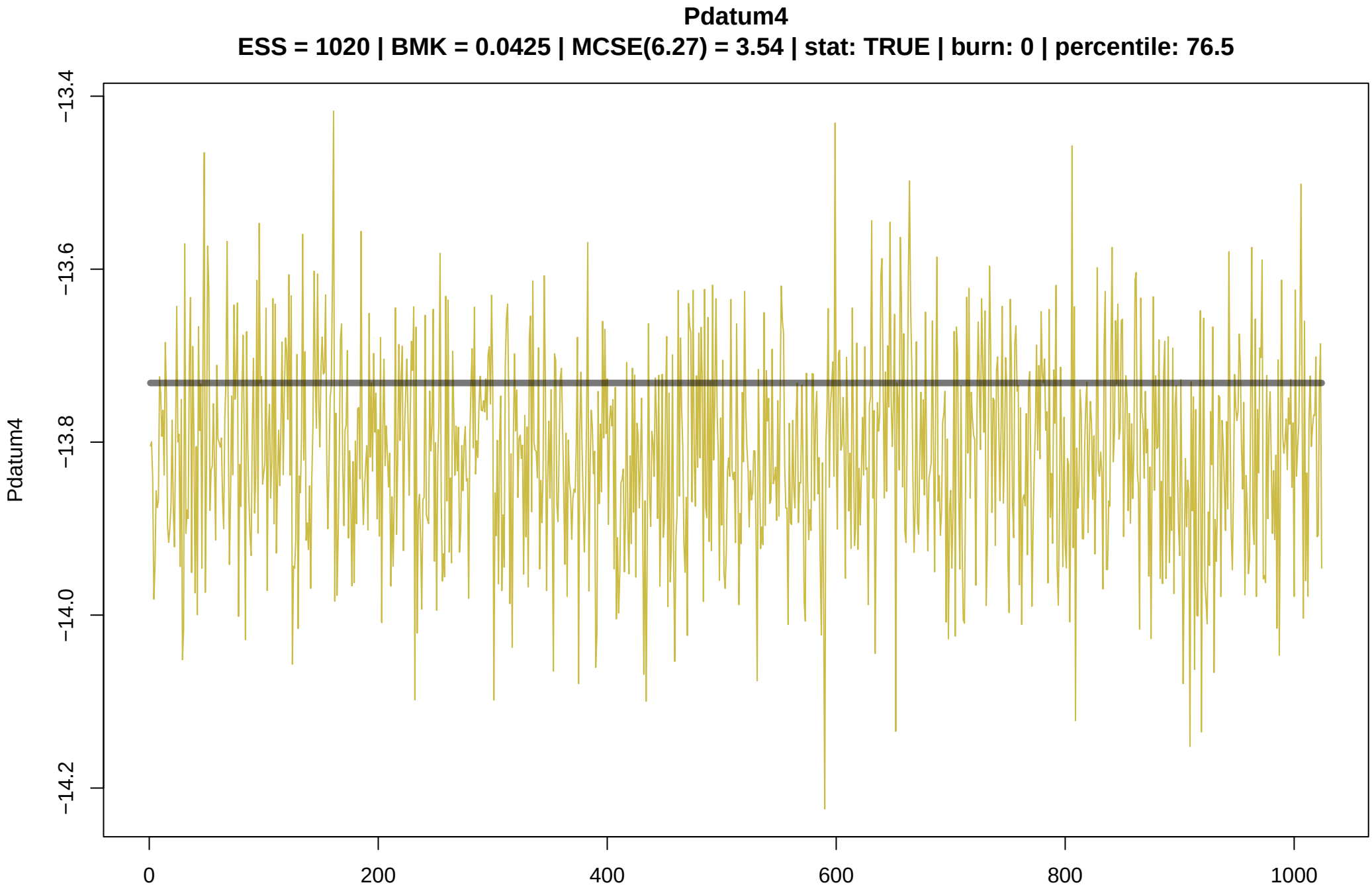

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.0717 | MCSE(6.27) = 8.66 | stat: TRUE | burn: 0 | percentile: 19.1
PdatacornerHi
−21.0
−21.5
−22.0
−22.5
0
200
400
600
800
1000

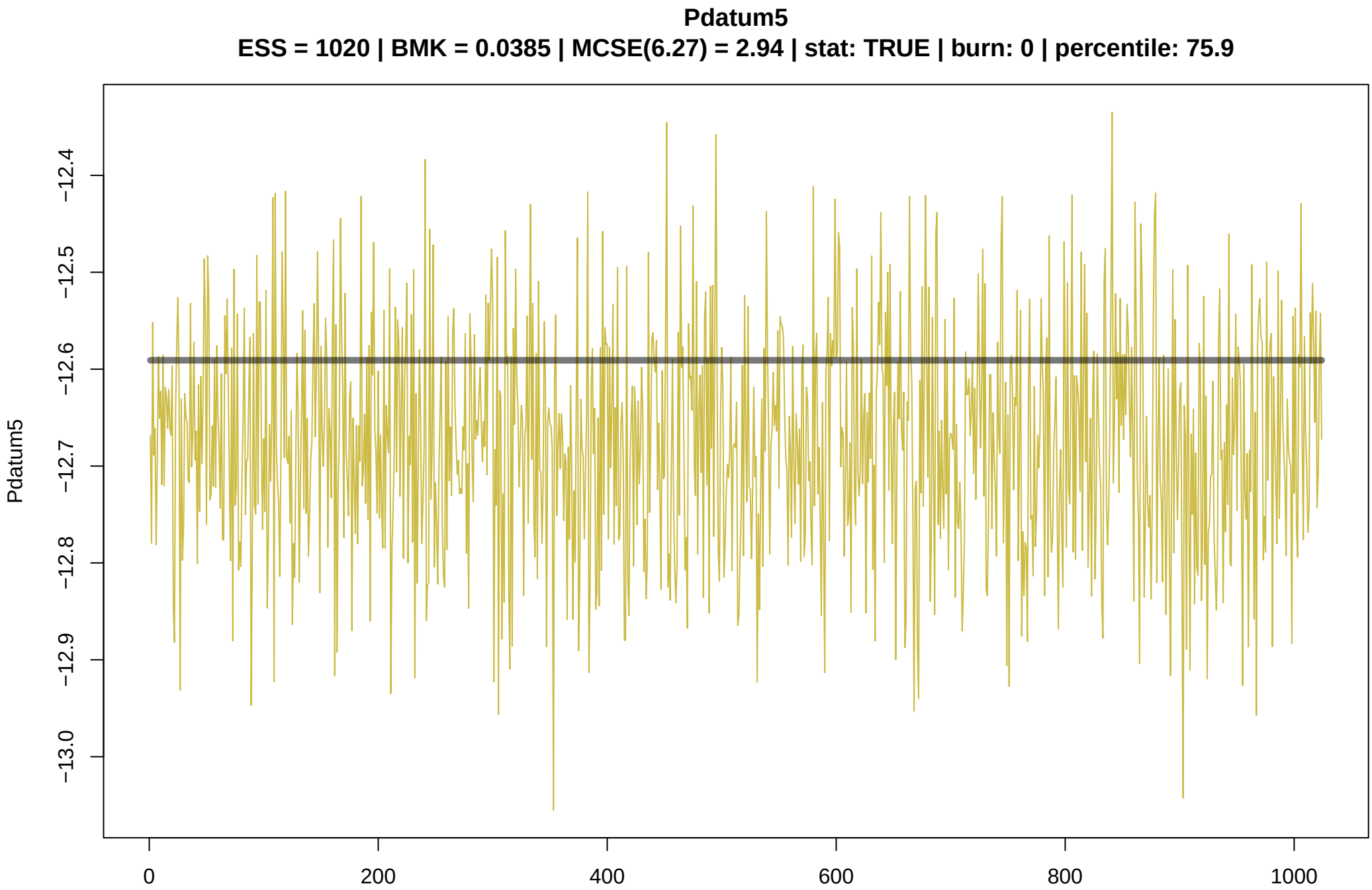

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.131 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | percentile: 42.2
PdatacornerLo
−22
−24
−26
−28
−30
−32
0
200
400
600
800
1000

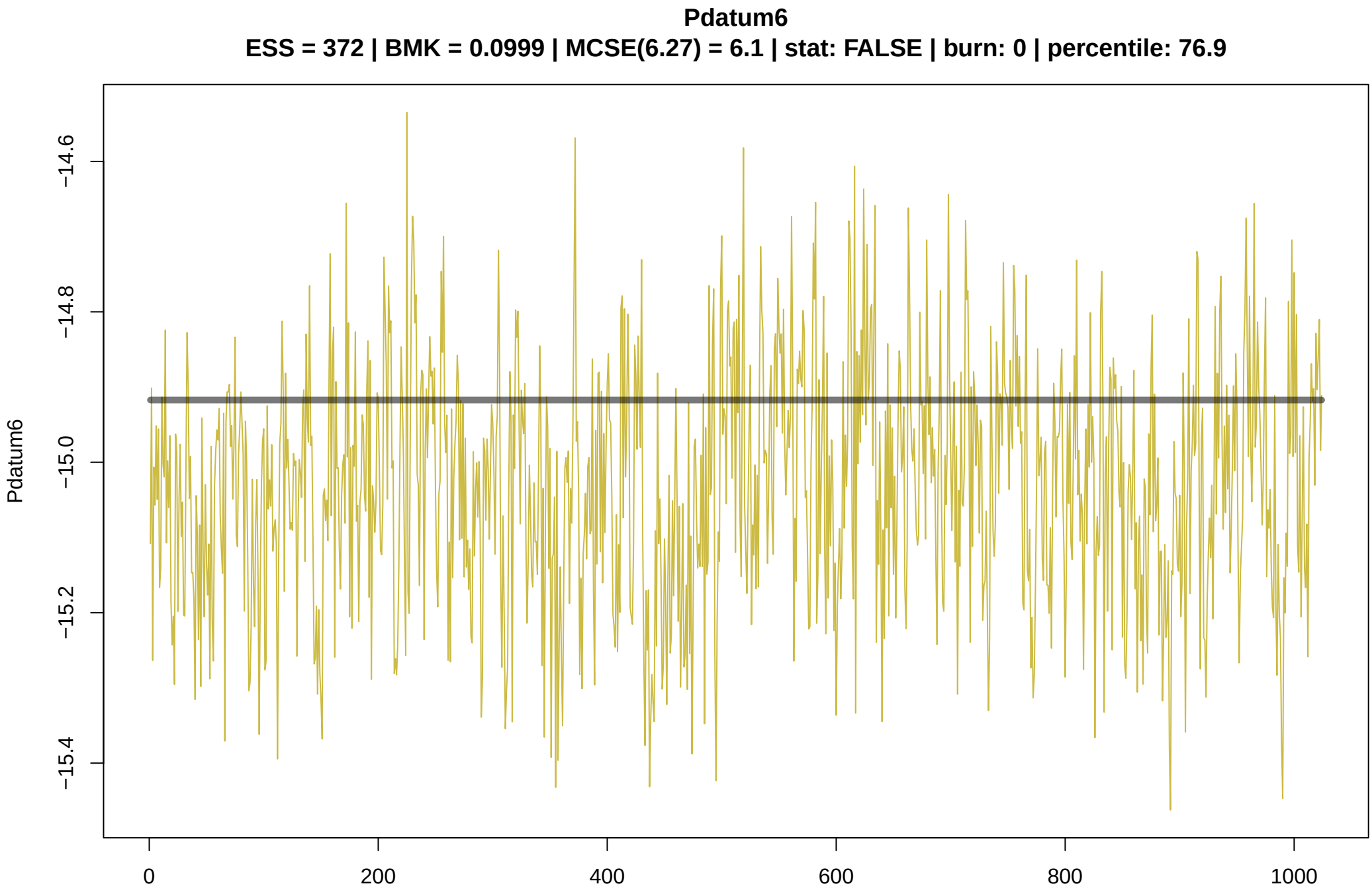

Pdatum1
ESS = 55.3 | BMK = 0.157 | MCSE(6.27) = 7.25 | stat: FALSE | burn: 0 | percentile: 82.7
Pdatum1
−11.8
−11.9
−12.0
−12.1
0
200
400
600
800
1000

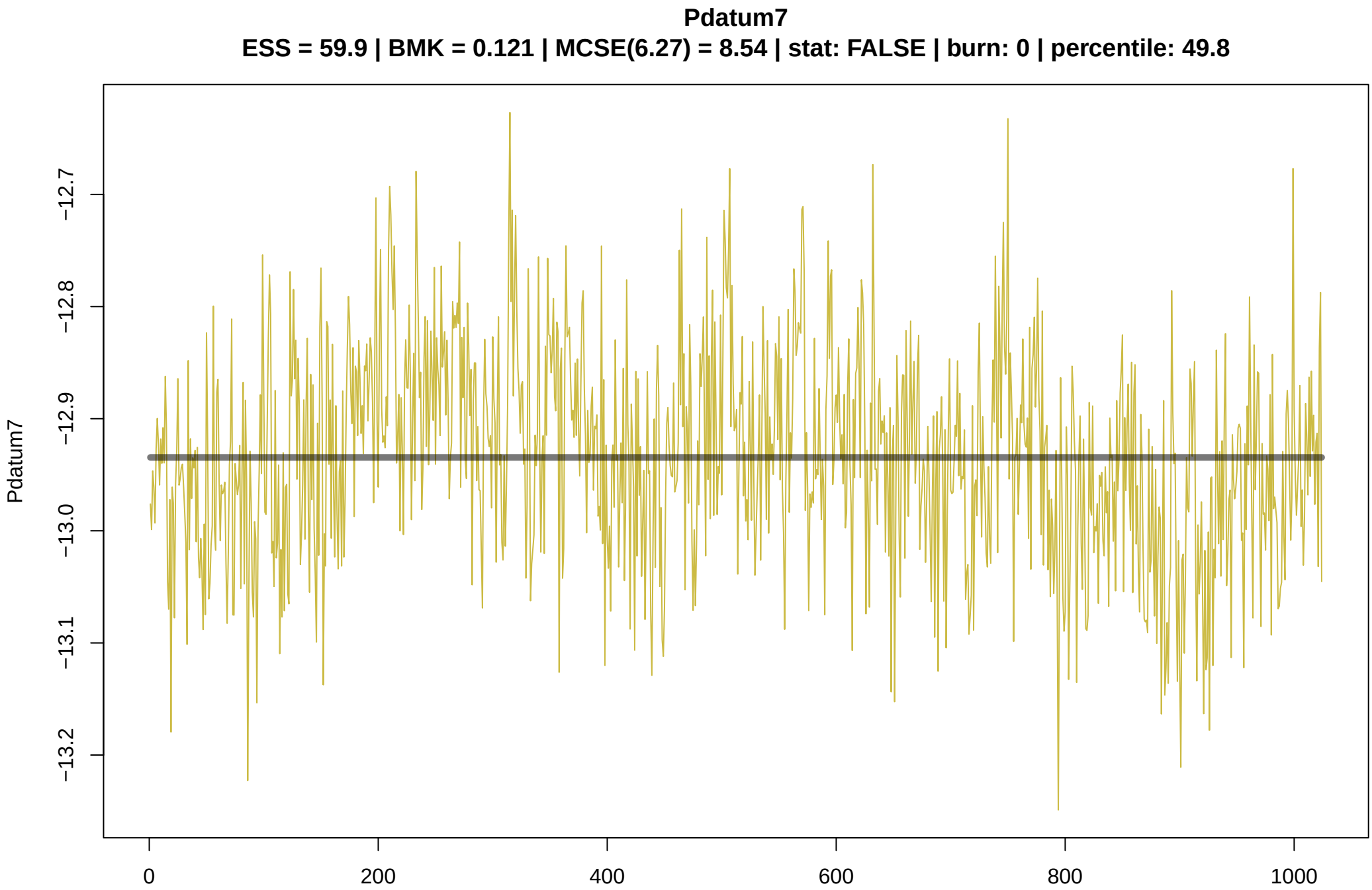

Pdatum2
ESS = 274 | BMK = 0.124 | MCSE(6.27) = 6.74 | stat: FALSE | burn: 0 | percentile: 62.7
Pdatum2
−12.6
−12.7
−12.8
−12.9
−13.0
−13.1
−13.2
0
200
400
600
800
1000

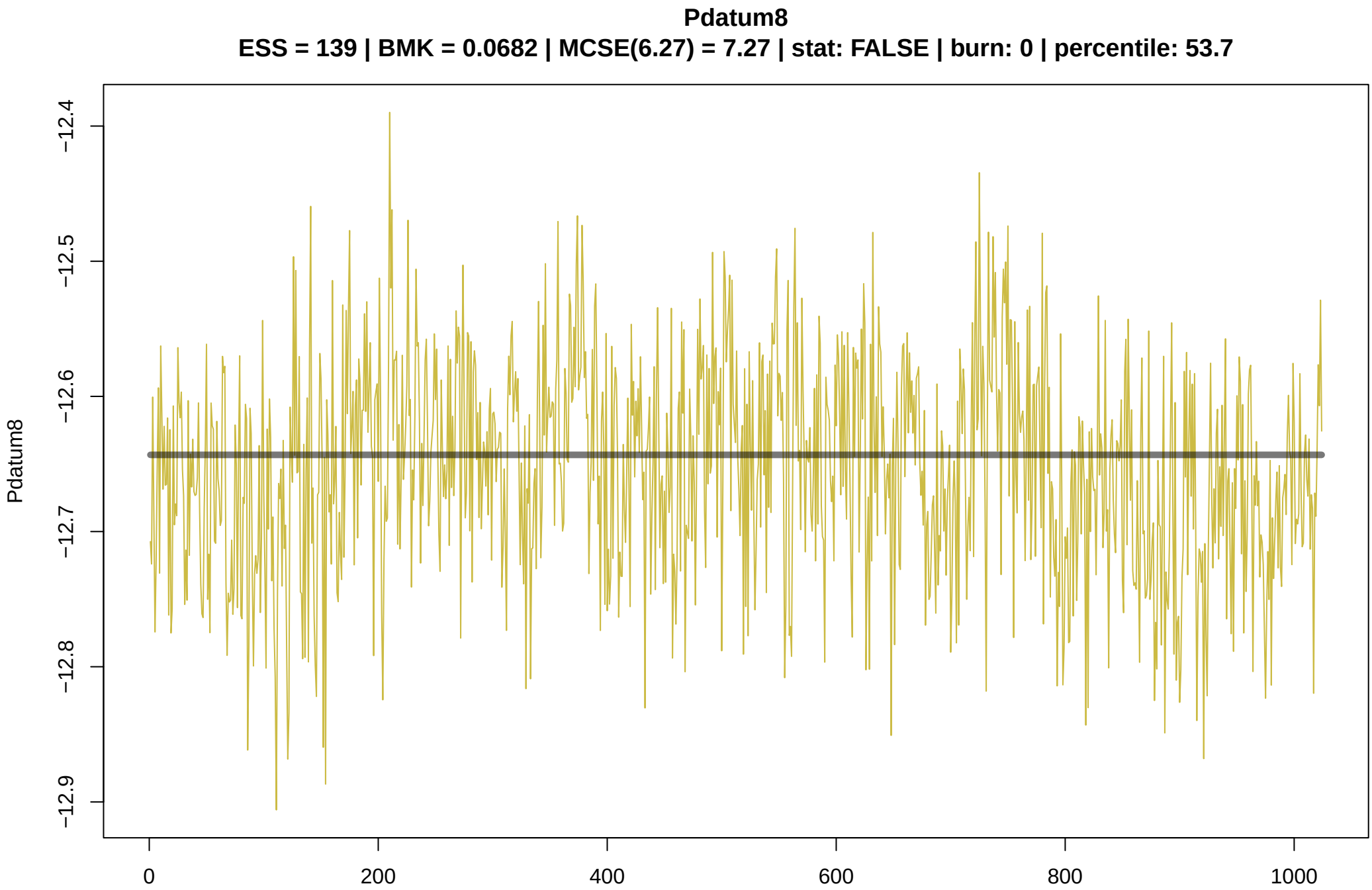

Pdatum3
ESS = 2.22e−16 | BMK = 0.204 | MCSE(6.27) = 7.85 | stat: TRUE | burn: 0 | percentile: 46.1
Pdatum3
−20.0
−20.2
−20.4
−20.6
−20.8
−21.0
0
200
400
600
800
1000

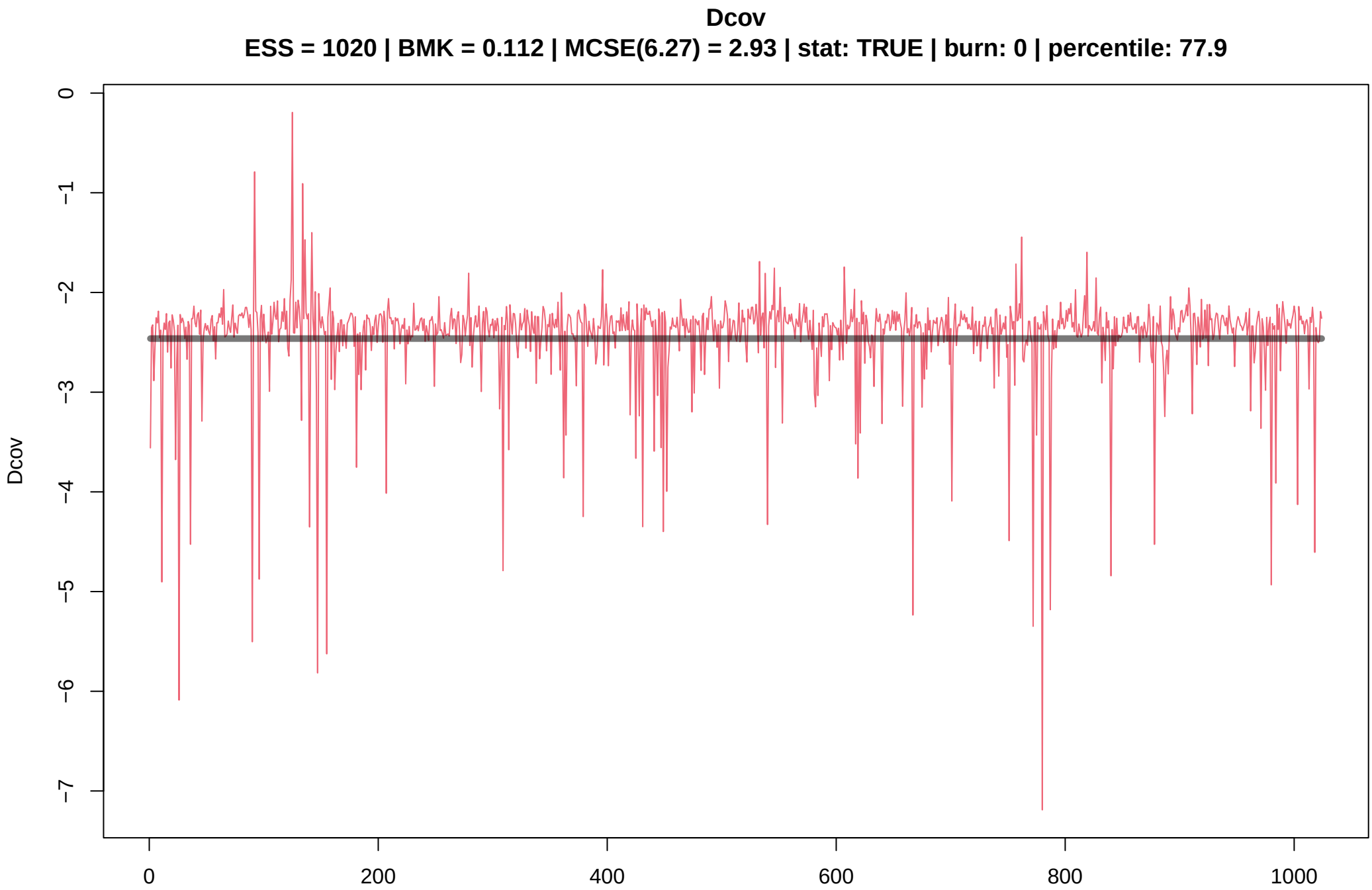

Pdatum4
ESS = 1020 | BMK = 0.0425 | MCSE(6.27) = 3.54 | stat: TRUE | burn: 0 | percentile: 76.5
Pdatum4
−13.4
−13.6
−13.8
−14.0
−14.2
0
200
400
600
800
1000

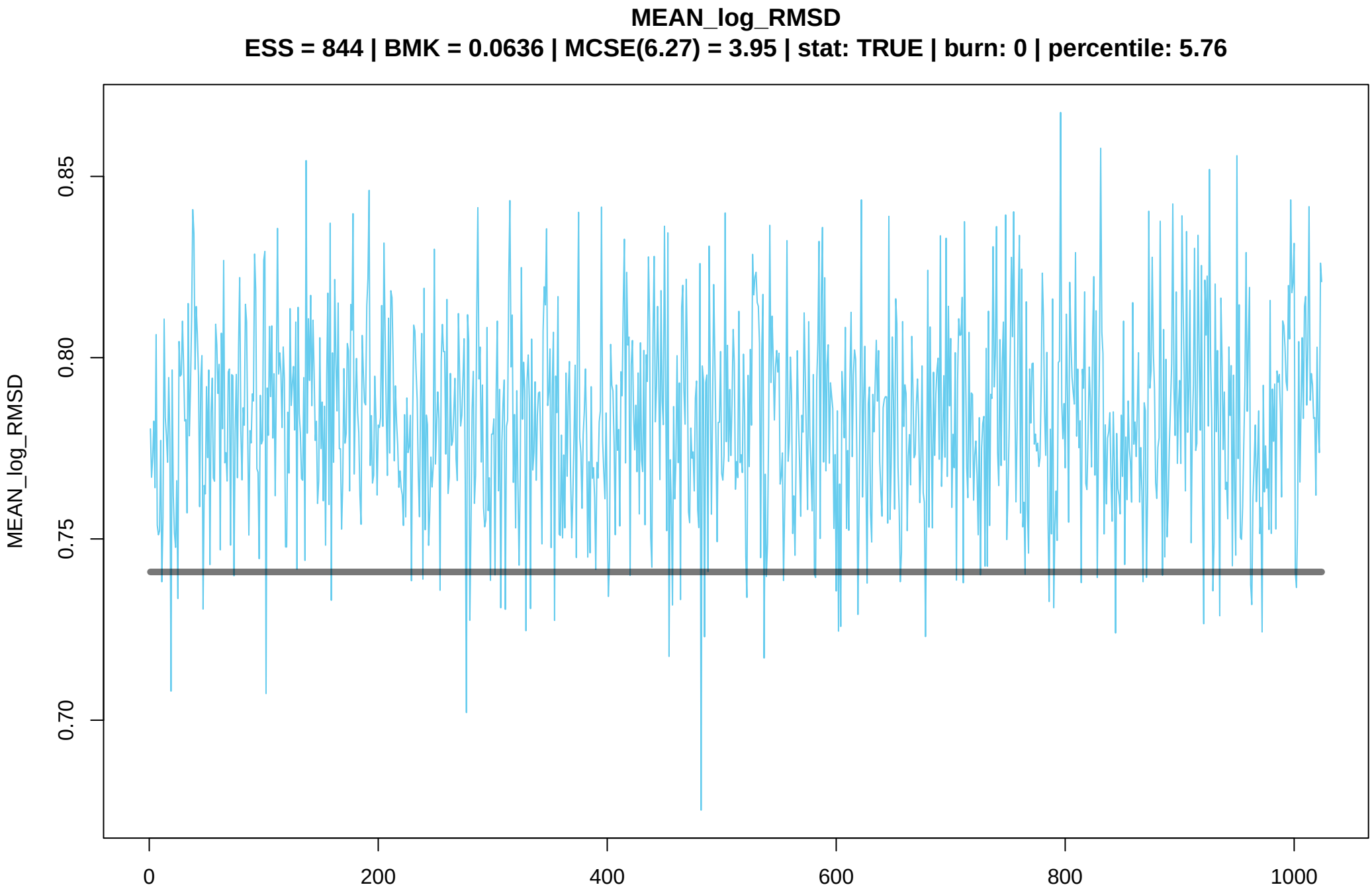

Pdatum5
ESS = 1020 | BMK = 0.0385 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 75.9
Pdatum5
−12.4
−12.5
−12.6
−12.7
−12.8
−12.9
−13.0
0
200
400
600
800
1000

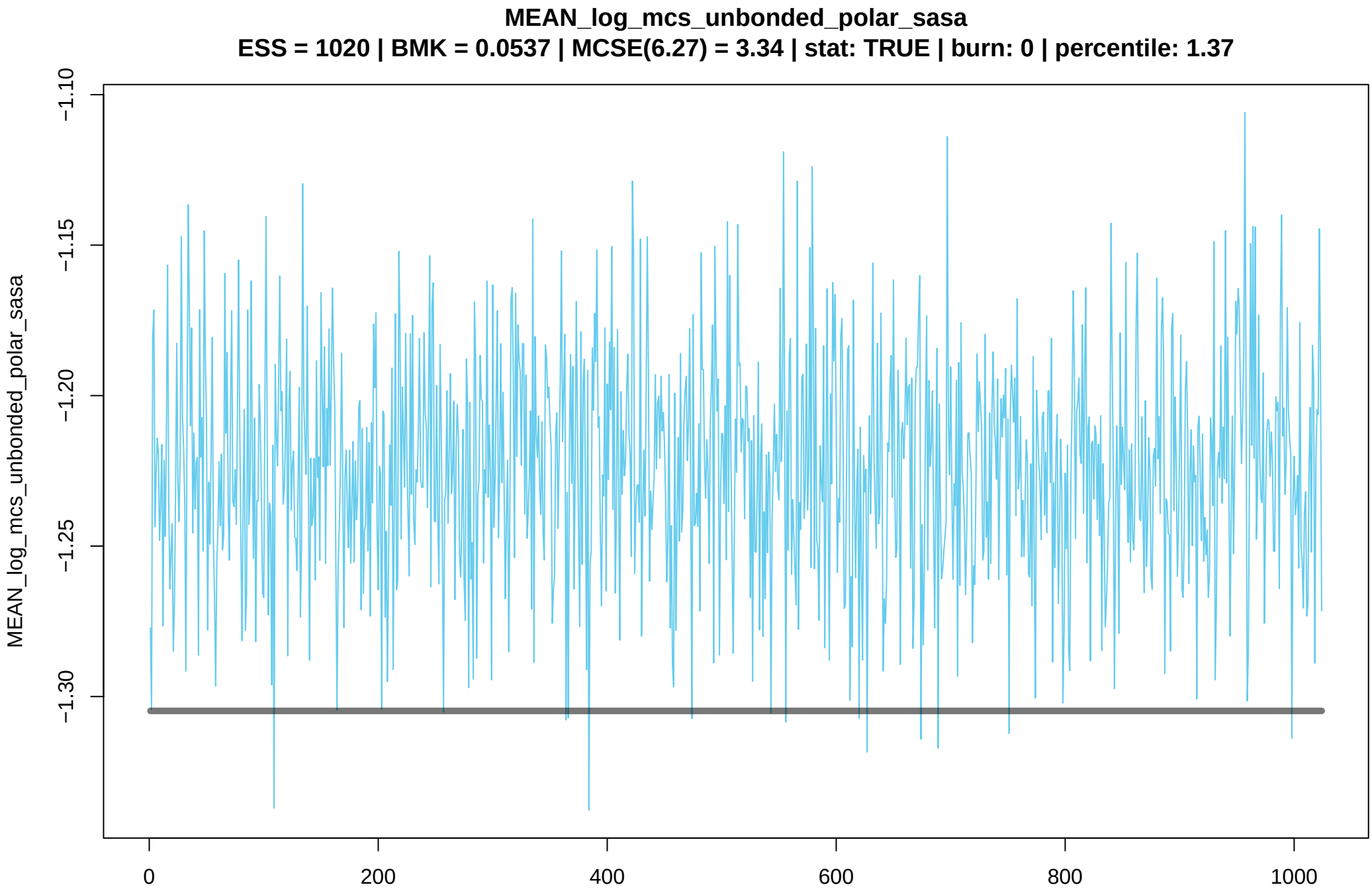

Pdatum6
ESS = 372 | BMK = 0.0999 | MCSE(6.27) = 6.1 | stat: FALSE | burn: 0 | percentile: 76.9
Pdatum6
−14.6
−14.8
−15.0
−15.2
−15.4
0
200
400
600
800
1000

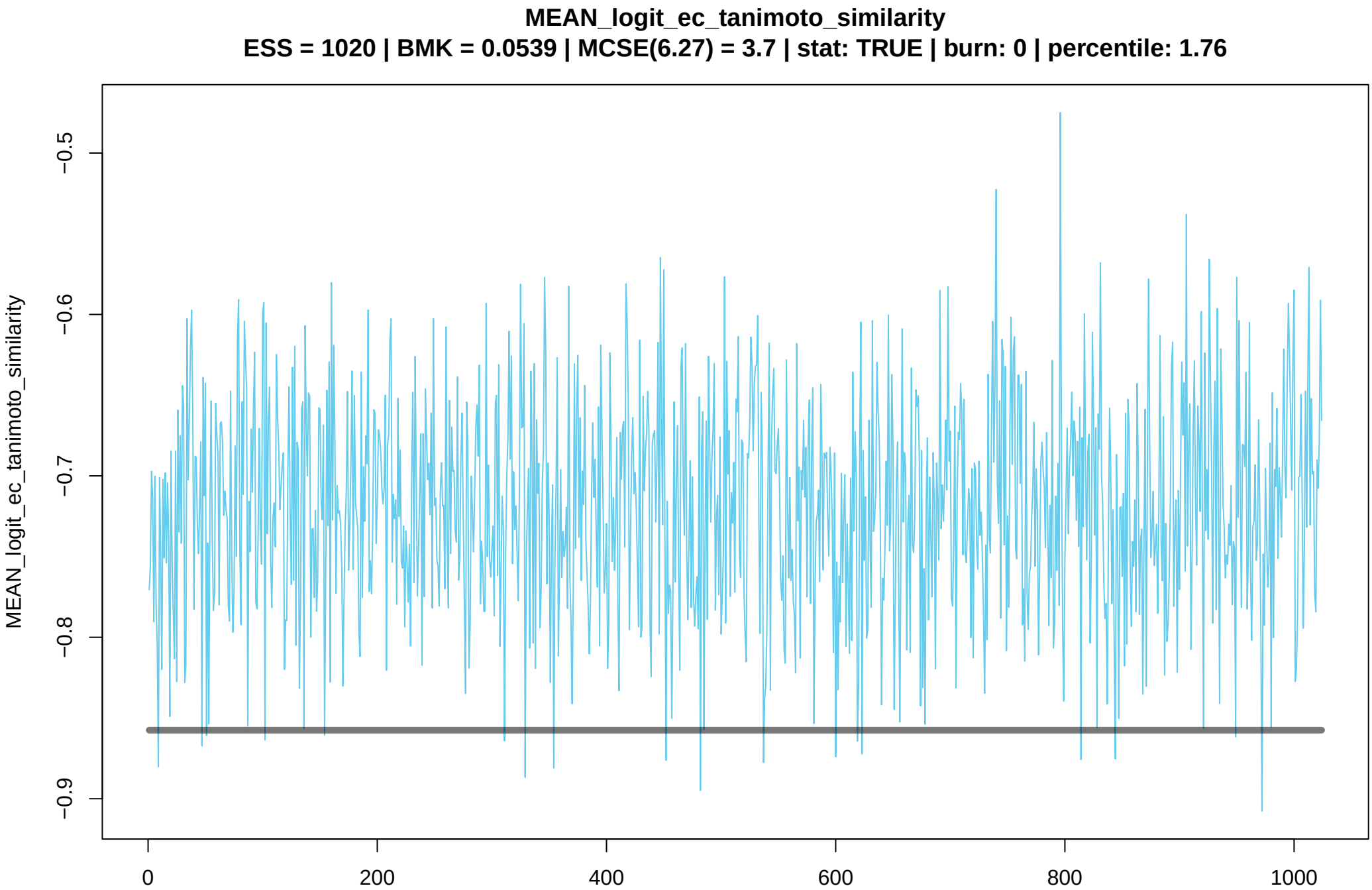

Pdatum7
ESS = 59.9 | BMK = 0.121 | MCSE(6.27) = 8.54 | stat: FALSE | burn: 0 | percentile: 49.8
Pdatum7
−12.7
−12.8
−12.9
−13.0
−13.1
−13.2
0
200
400
600
800
1000

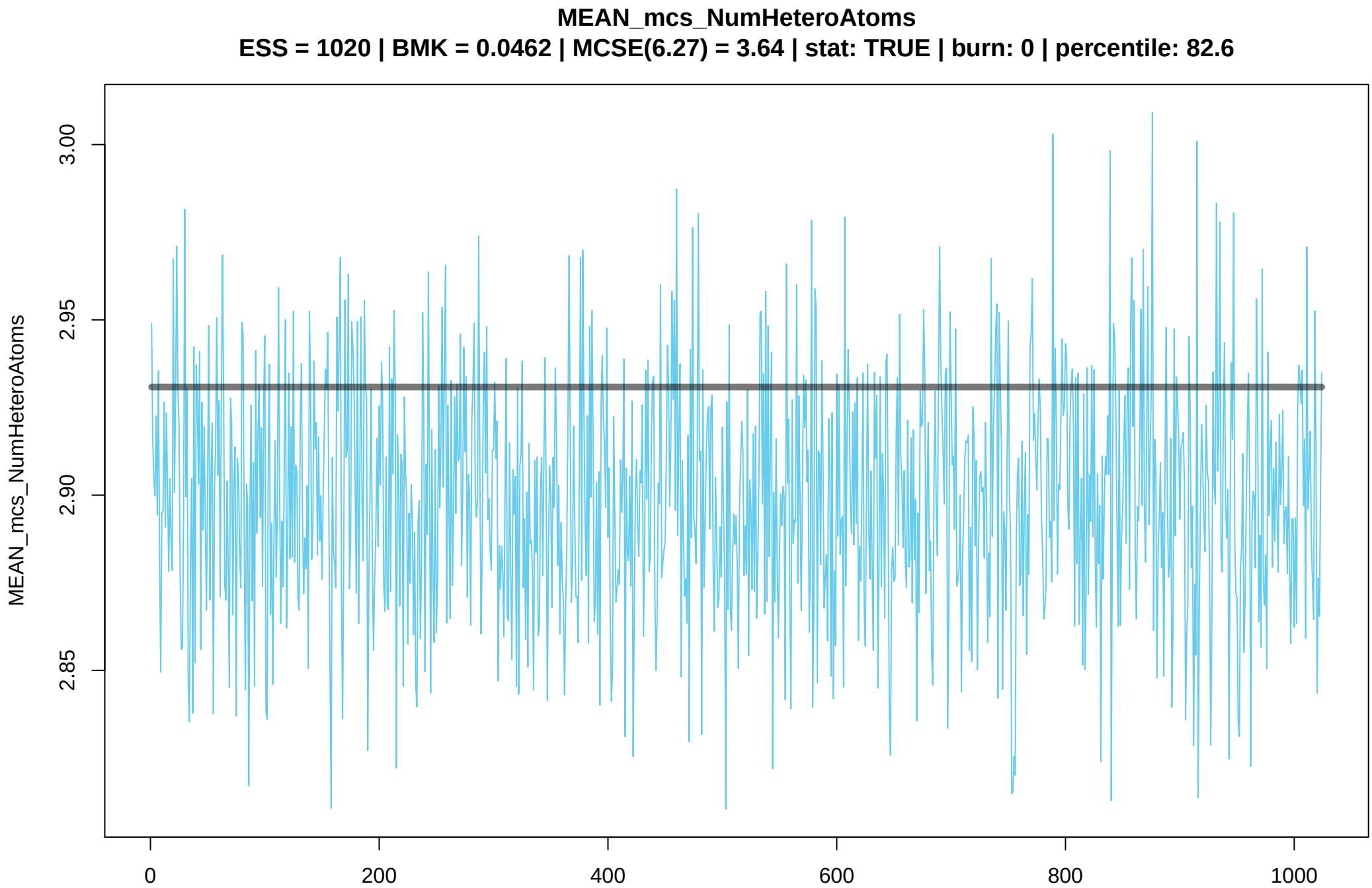

Pdatum8
ESS = 139 | BMK = 0.0682 | MCSE(6.27) = 7.27 | stat: FALSE | burn: 0 | percentile: 53.7
Pdatum8
−12.4
−12.5
−12.6
−12.7
−12.8
−12.9
0
200
400
600
800
1000

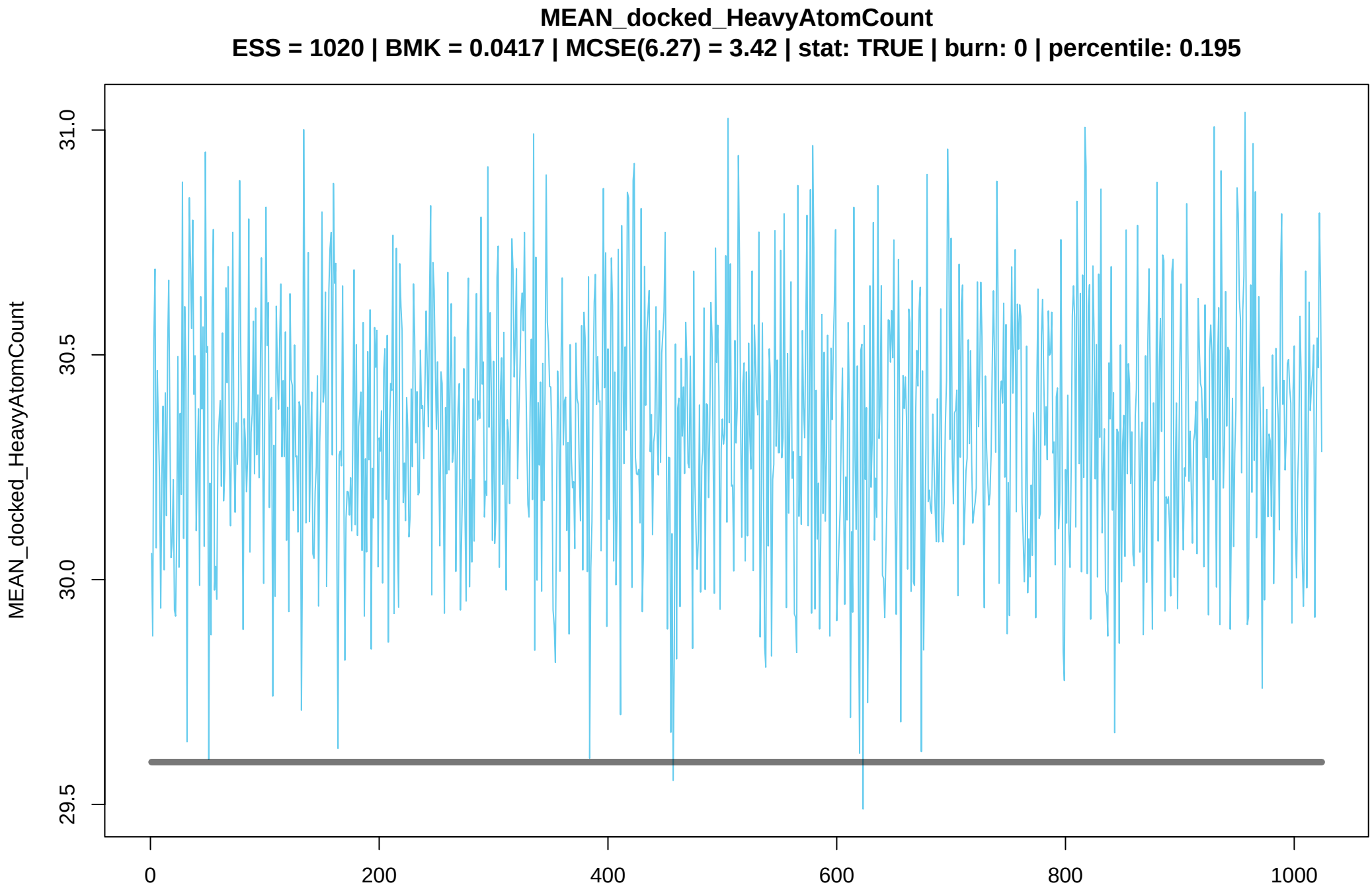

Dcov
ESS = 1020 | BMK = 0.112 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | percentile: 77.9
Dcov
0
−1
−2
−3
−4
−5
−6
−7
0
200
400
600
800
1000

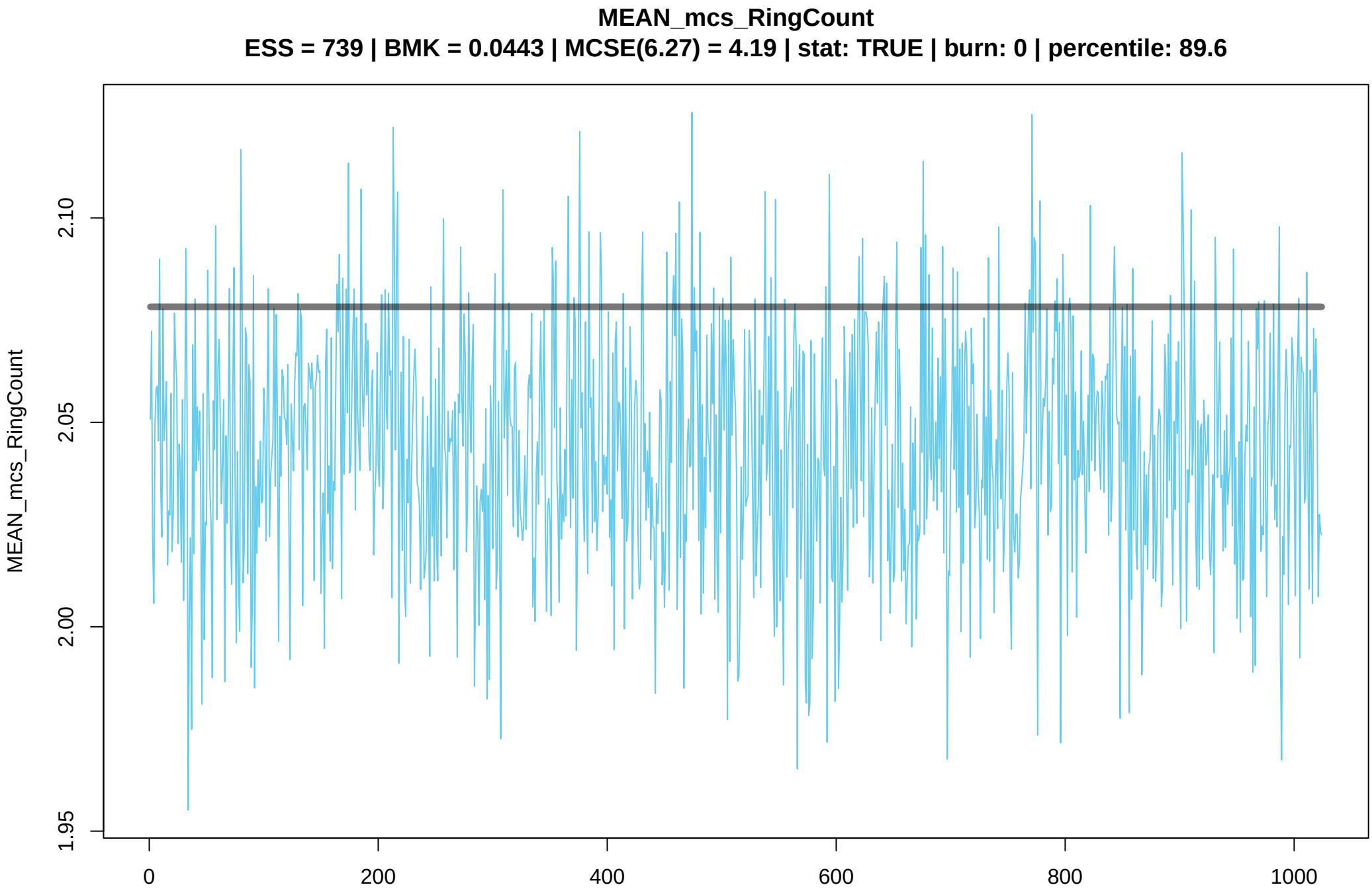

MEAN_log_RMSD
ESS = 844 | BMK = 0.0636 | MCSE(6.27) = 3.95 | stat: TRUE | burn: 0 | percentile: 5.76
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

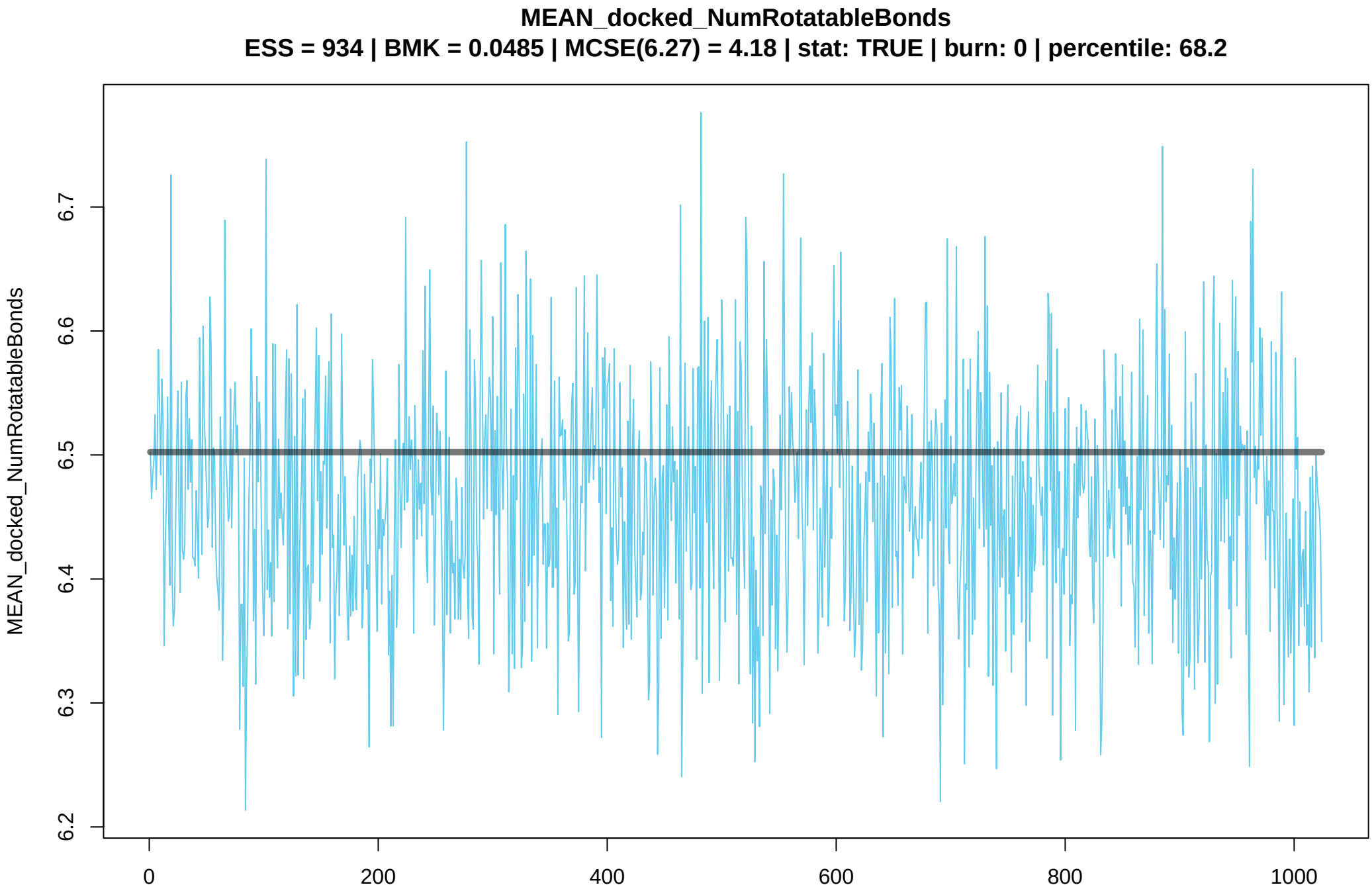

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0537 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0 | percentile: 1.37
MEAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
−1.25
−1.30
0
200
400
600
800
1000

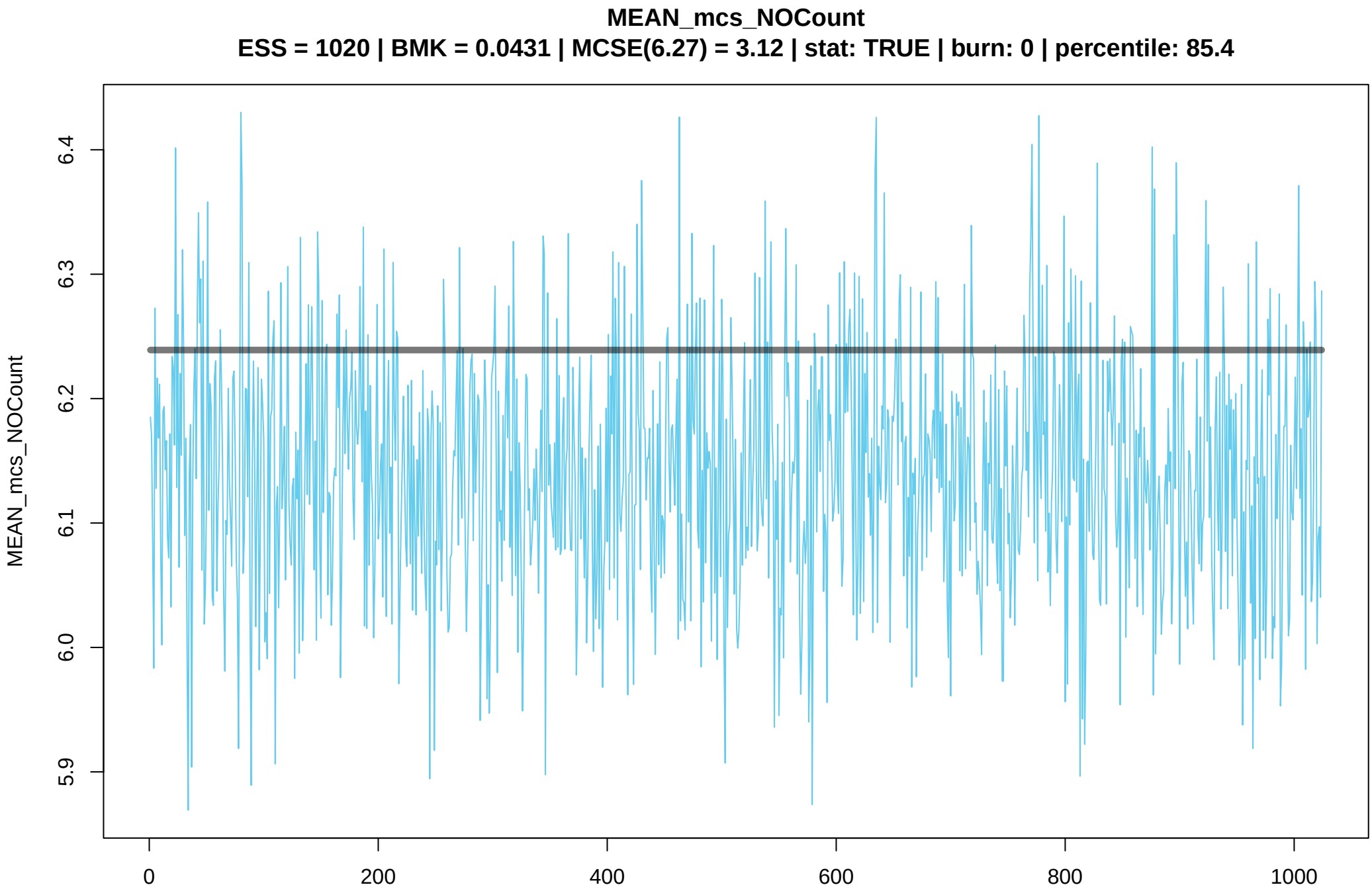

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0539 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | percentile: 1.76
MEAN_logit_ec_tanimoto_similarity
−0.5
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

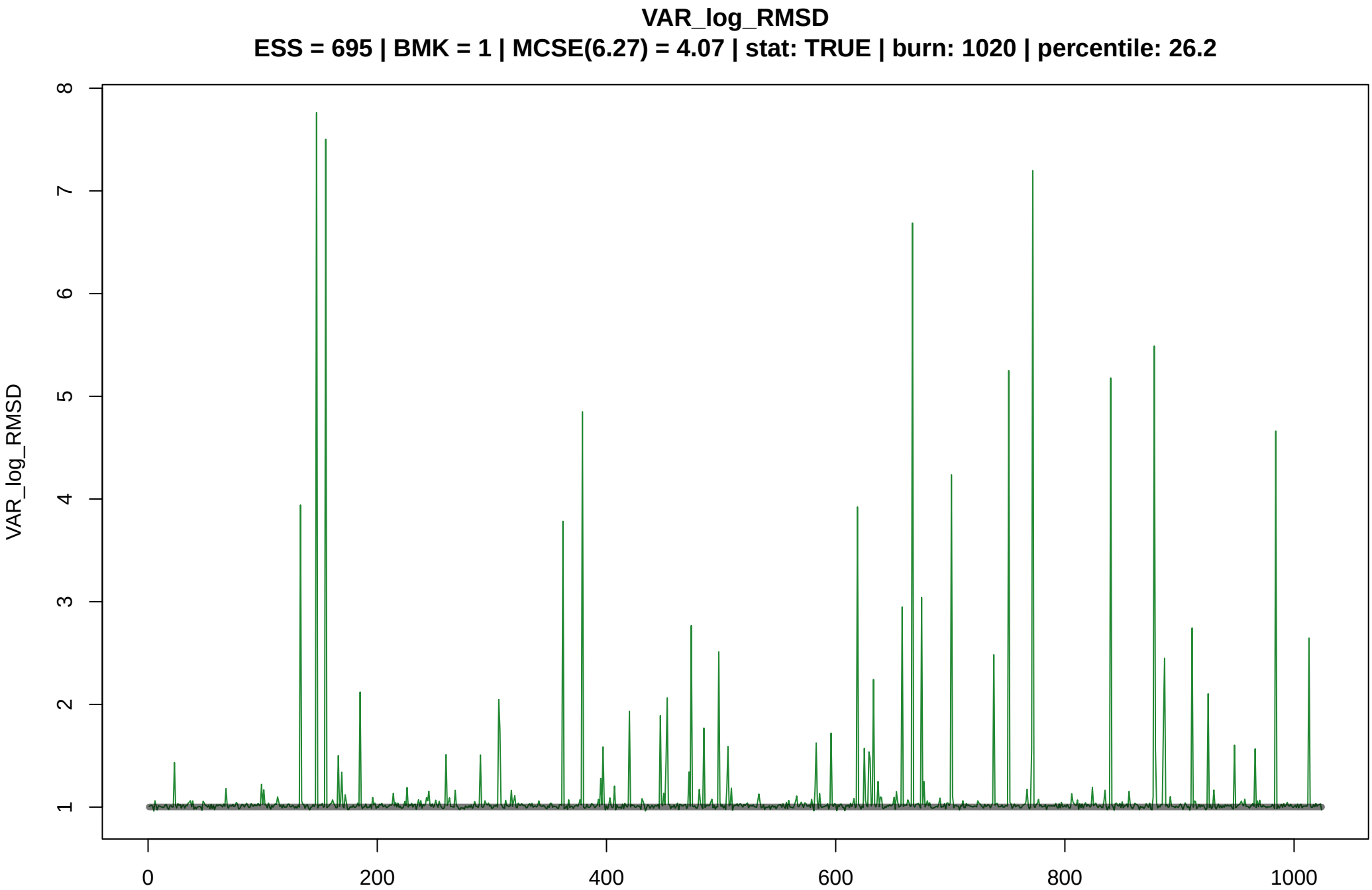

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0462 | MCSE(6.27) = 3.64 | stat: TRUE | burn: 0 | percentile: 82.6
MEAN_mcs_NumHeteroAtoms
3.00
2.95
2.90
2.85
0
200
400
600
800
1000

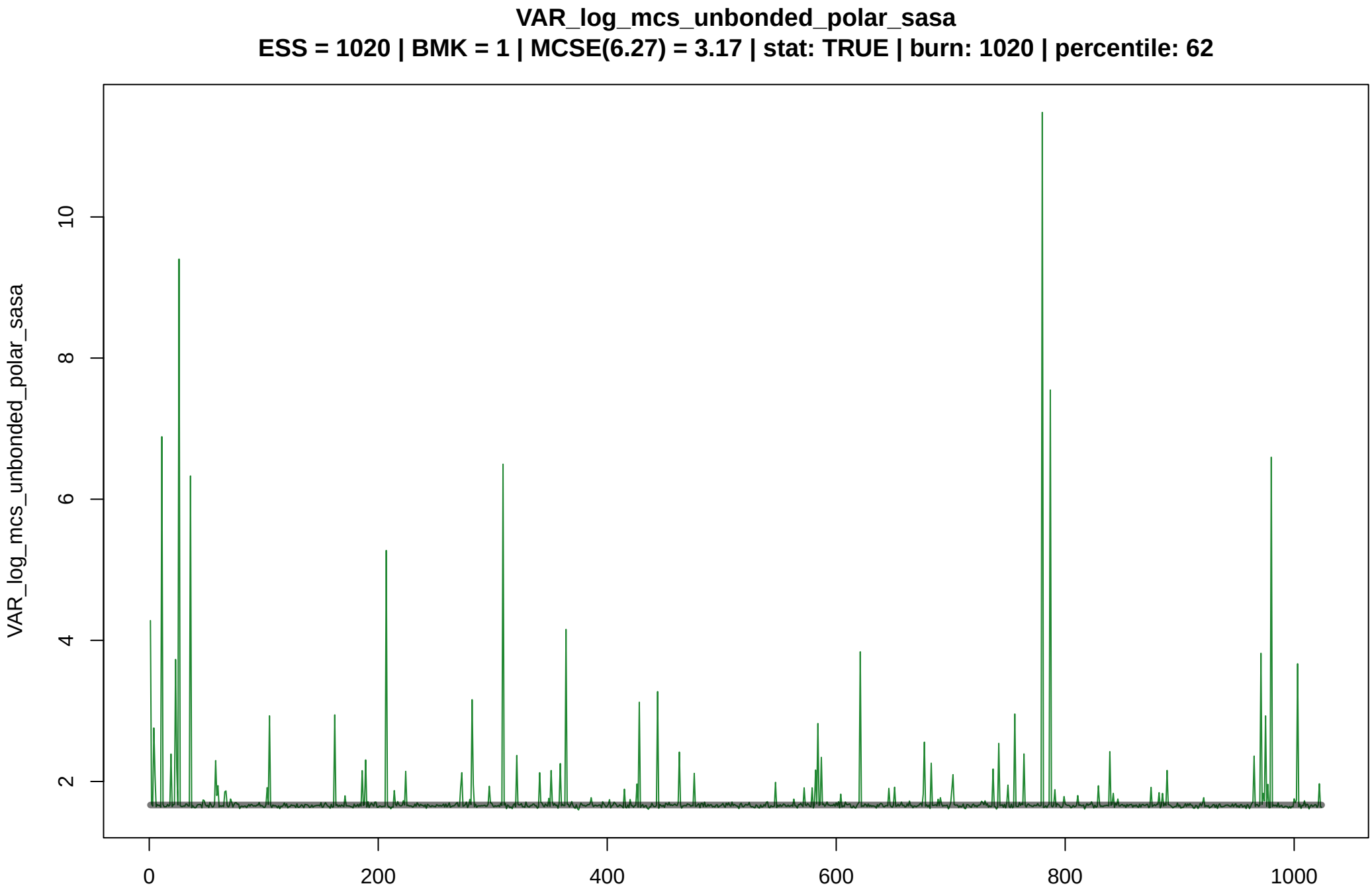

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0417 | MCSE(6.27) = 3.42 | stat: TRUE | burn: 0 | percentile: 0.195
MEAN_docked_HeavyAtomCount
31.0
30.5
30.0
29.5
0
200
400
600
800
1000

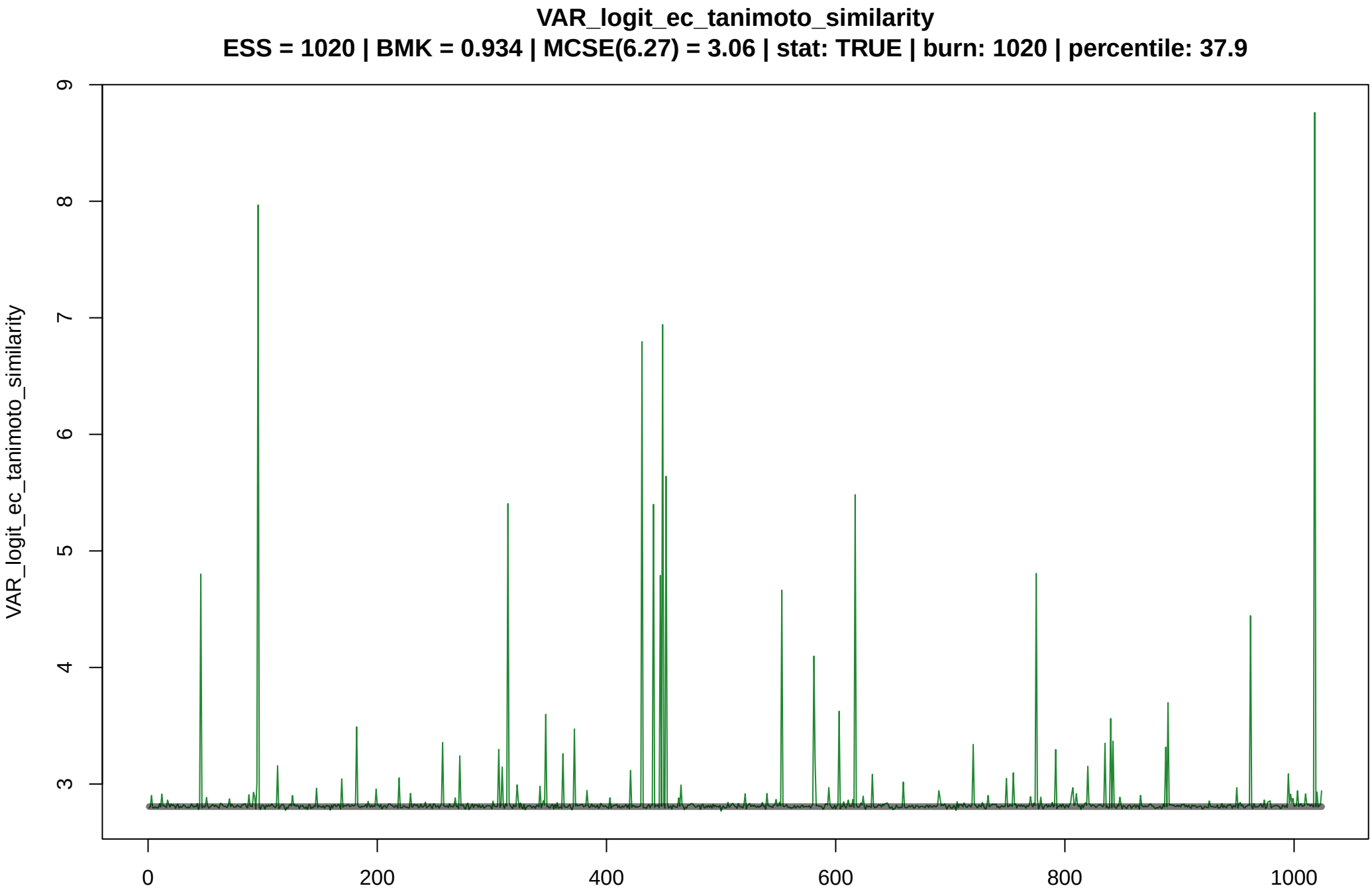

MEAN_mcs_RingCount
ESS = 739 | BMK = 0.0443 | MCSE(6.27) = 4.19 | stat: TRUE | burn: 0 | percentile: 89.6
MEAN_mcs_RingCount
1.95
2.00
2.05
2.10
0
200
400
600
800
1000

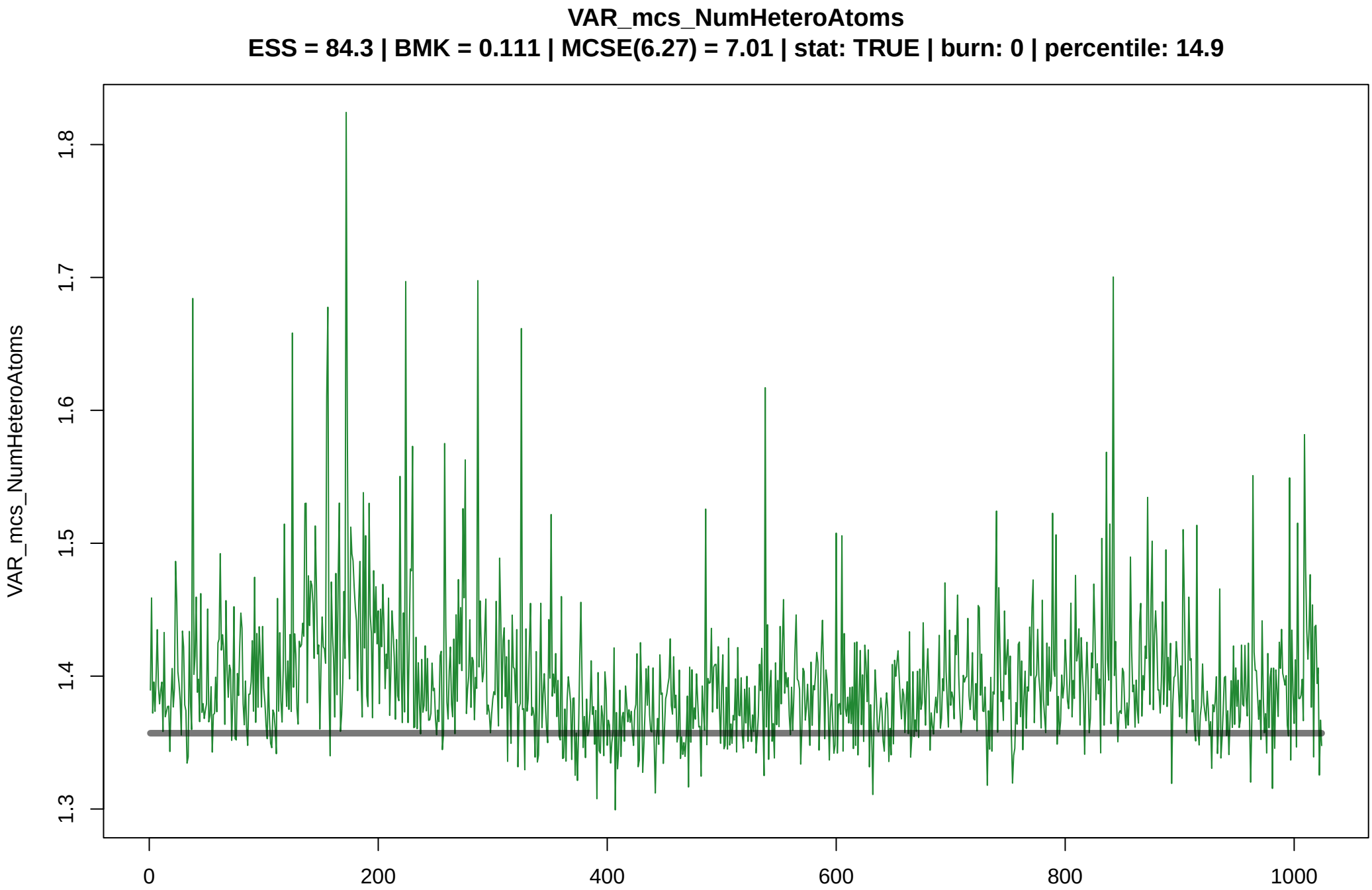

MEAN_docked_NumRotatableBonds
ESS = 934 | BMK = 0.0485 | MCSE(6.27) = 4.18 | stat: TRUE | burn: 0 | percentile: 68.2
MEAN_docked_NumRotatableBonds
6.2
6.3
6.4
6.5
6.6
6.7
0
200
400
600
800
1000

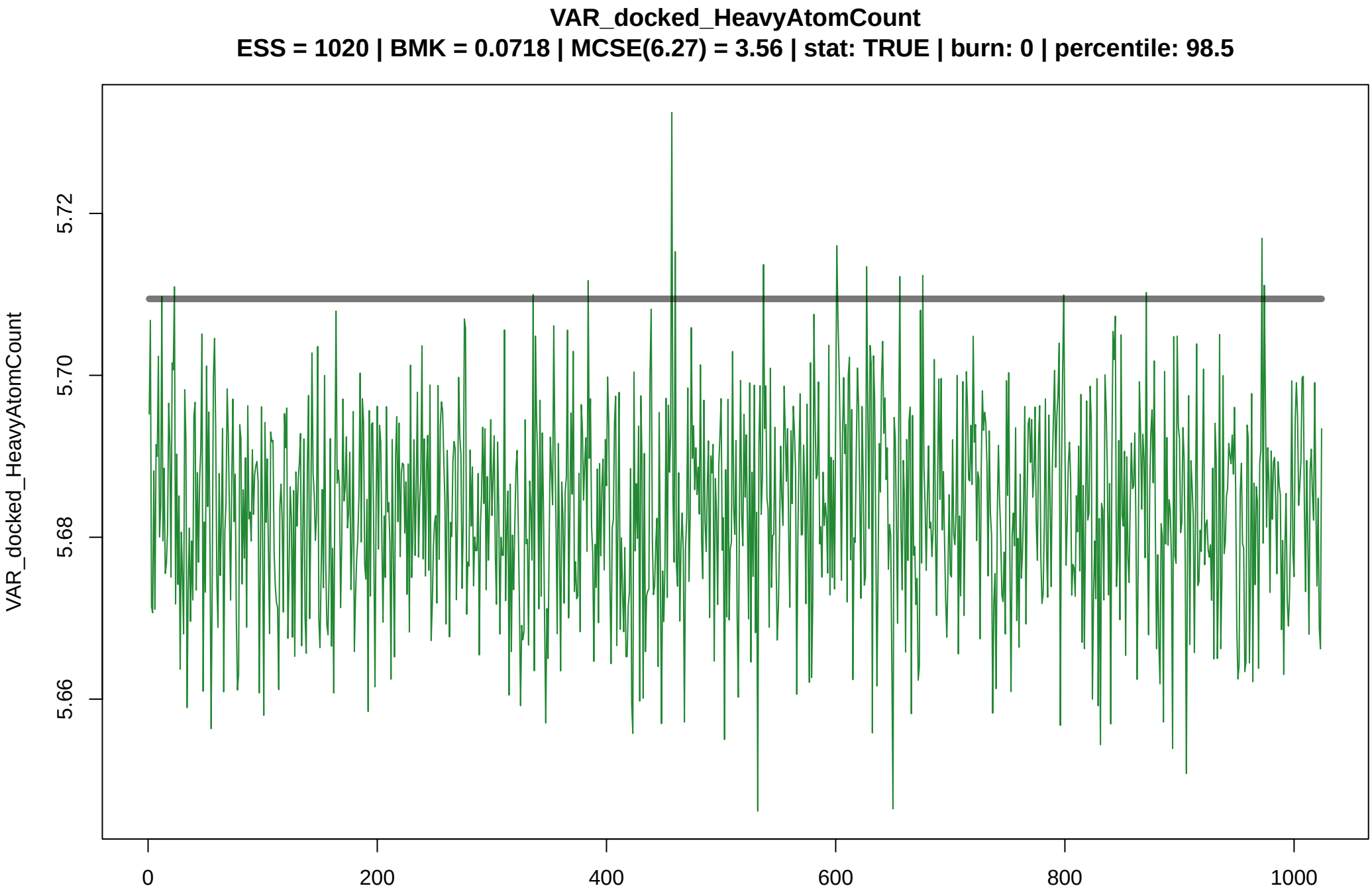

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0431 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 0 | percentile: 85.4
MEAN_mcs_NOCount
5.9
6.0
6.1
6.2
6.3
6.4
0
200
400
600
800
1000

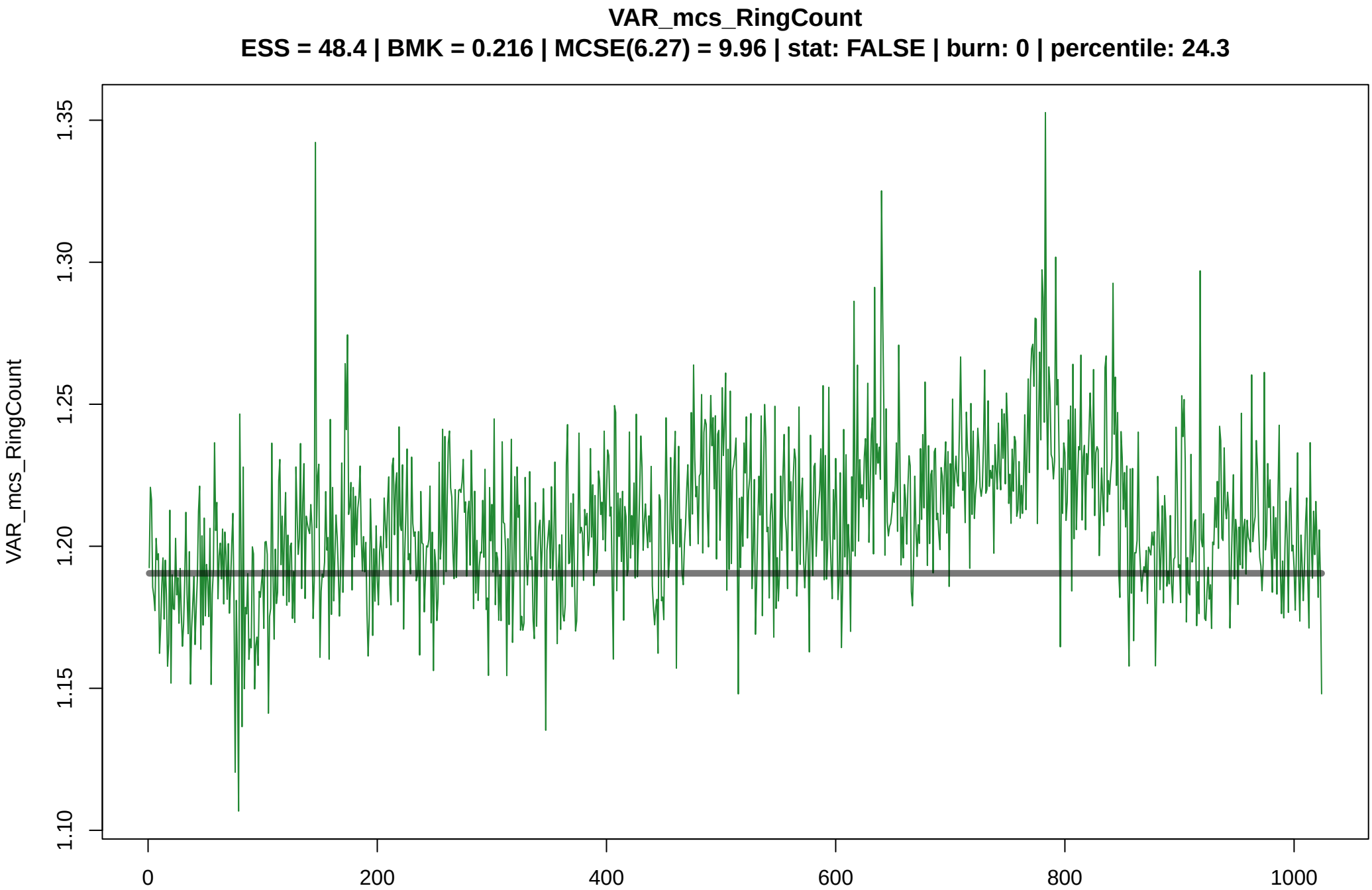

VAR_log_RMSD
ESS = 695 | BMK = 1 | MCSE(6.27) = 4.07 | stat: TRUE | burn: 1020 | percentile: 26.2
VAR_log_RMSD
1
2
3
4
5
6
7
8
0
200
400
600
800
1000

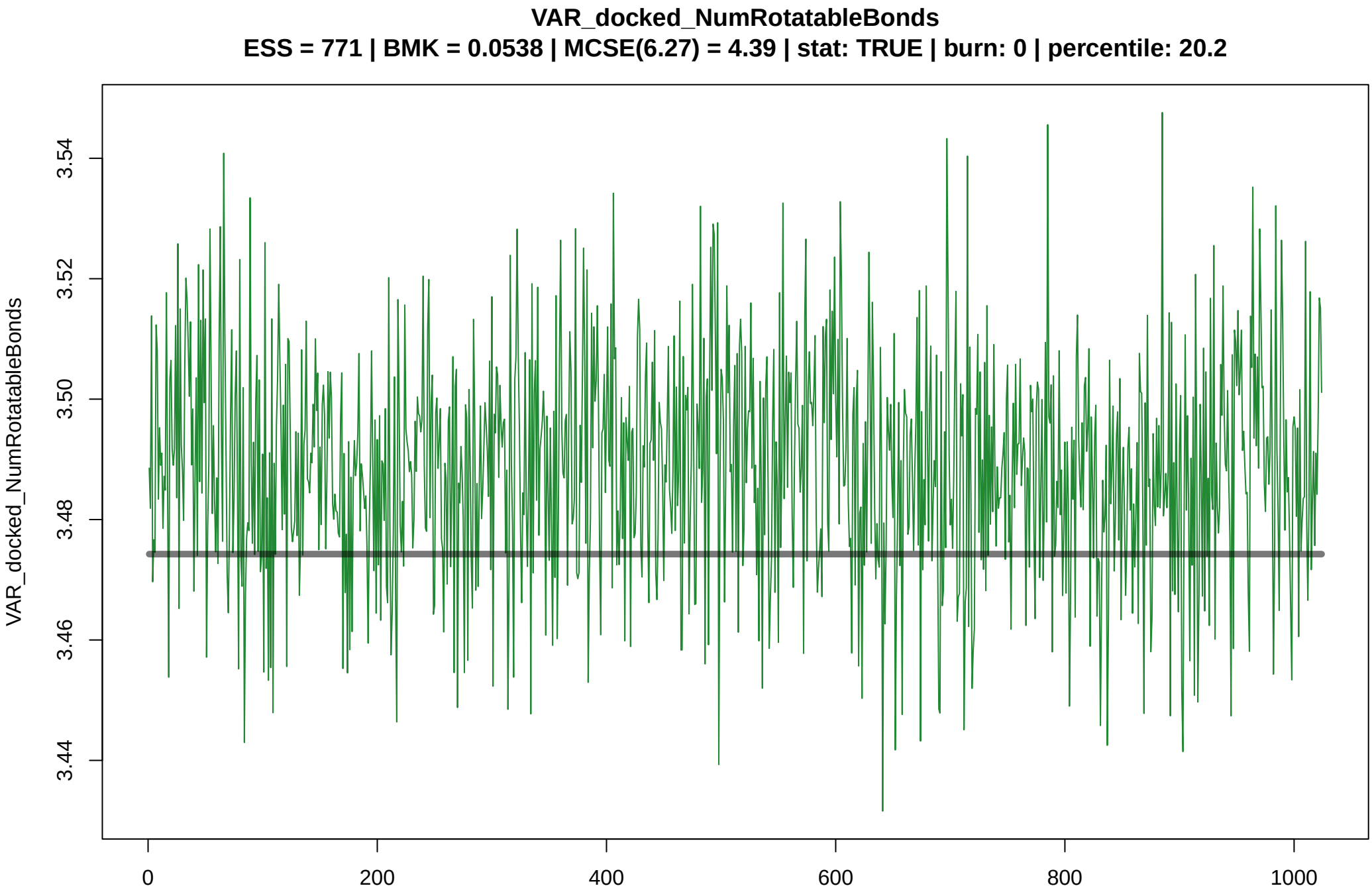

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 1020 | percentile: 62
VAR_log_mcs_unbonded_polar_sasa
2
4
6
8
10
0
200
400
600
800
1000

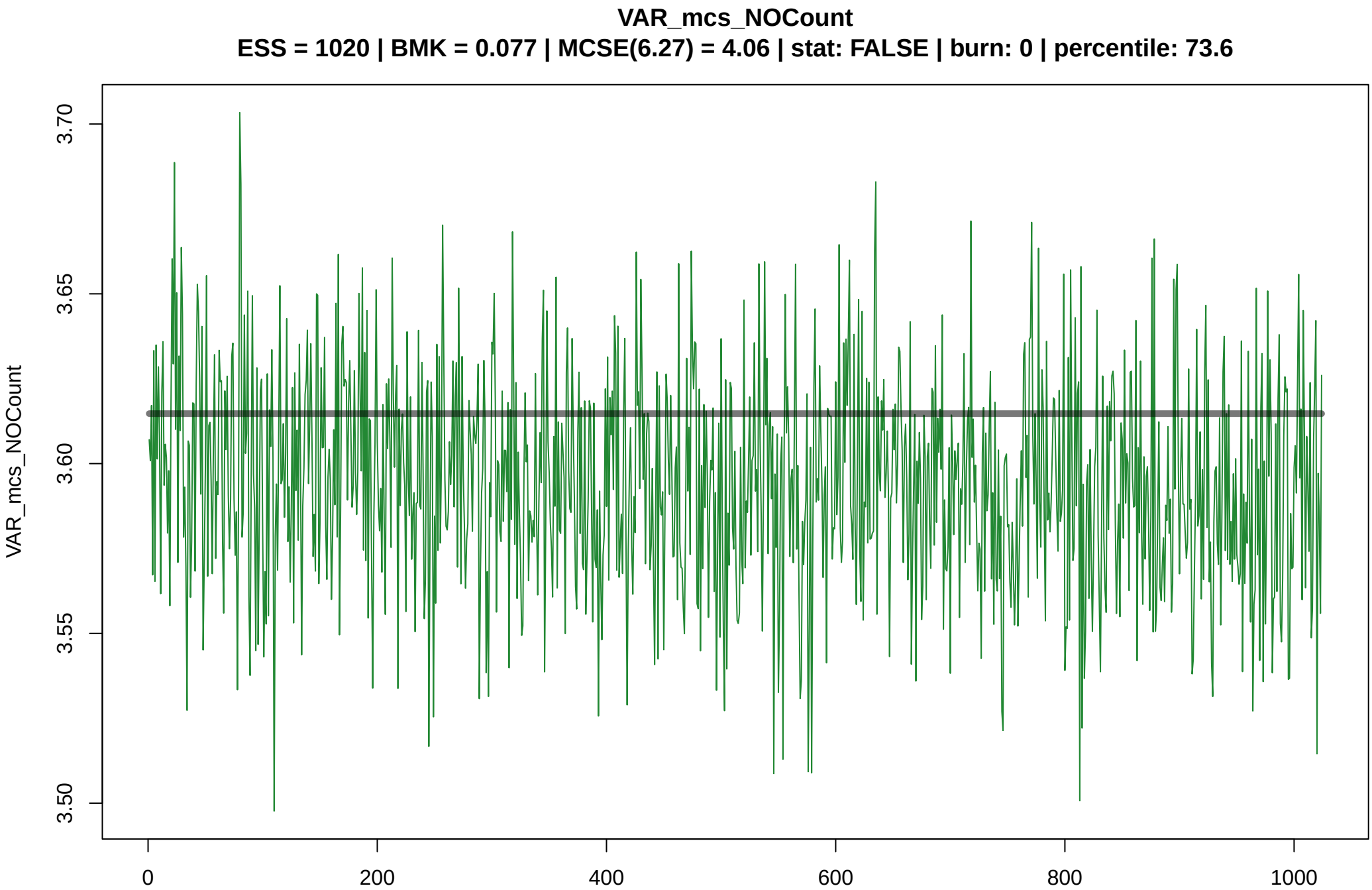

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.934 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 1020 | percentile: 37.9
VAR_logit_ec_tanimoto_similarity
3
4
5
6
7
8
9
0
200
400
600
800
1000

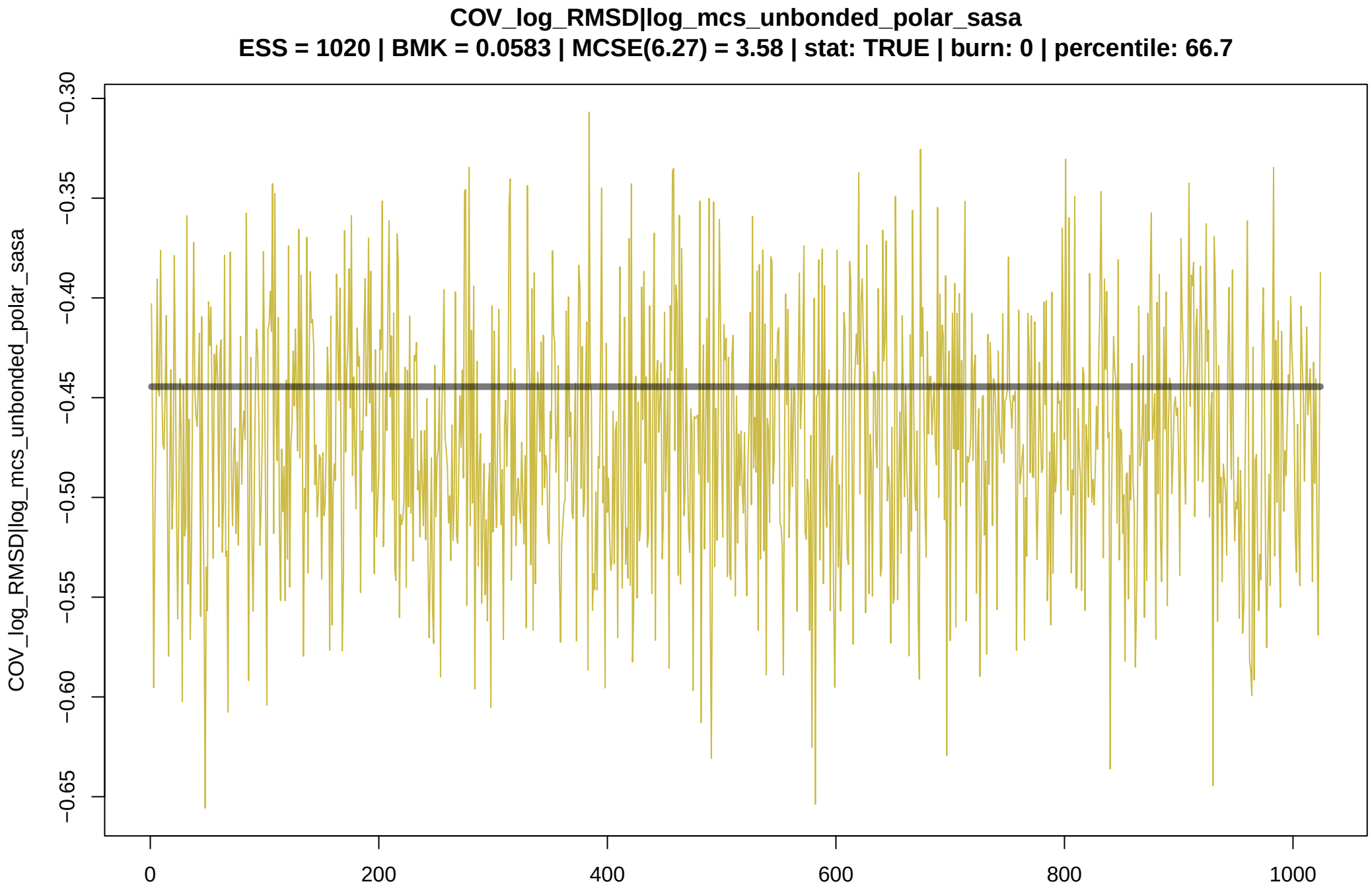

VAR_mcs_NumHeteroAtoms
ESS = 84.3 | BMK = 0.111 | MCSE(6.27) = 7.01 | stat: TRUE | burn: 0 | percentile: 14.9
VAR_mcs_NumHeteroAtoms
1.3
1.4
1.5
1.6
1.7
1.8
0
200
400
600
800
1000

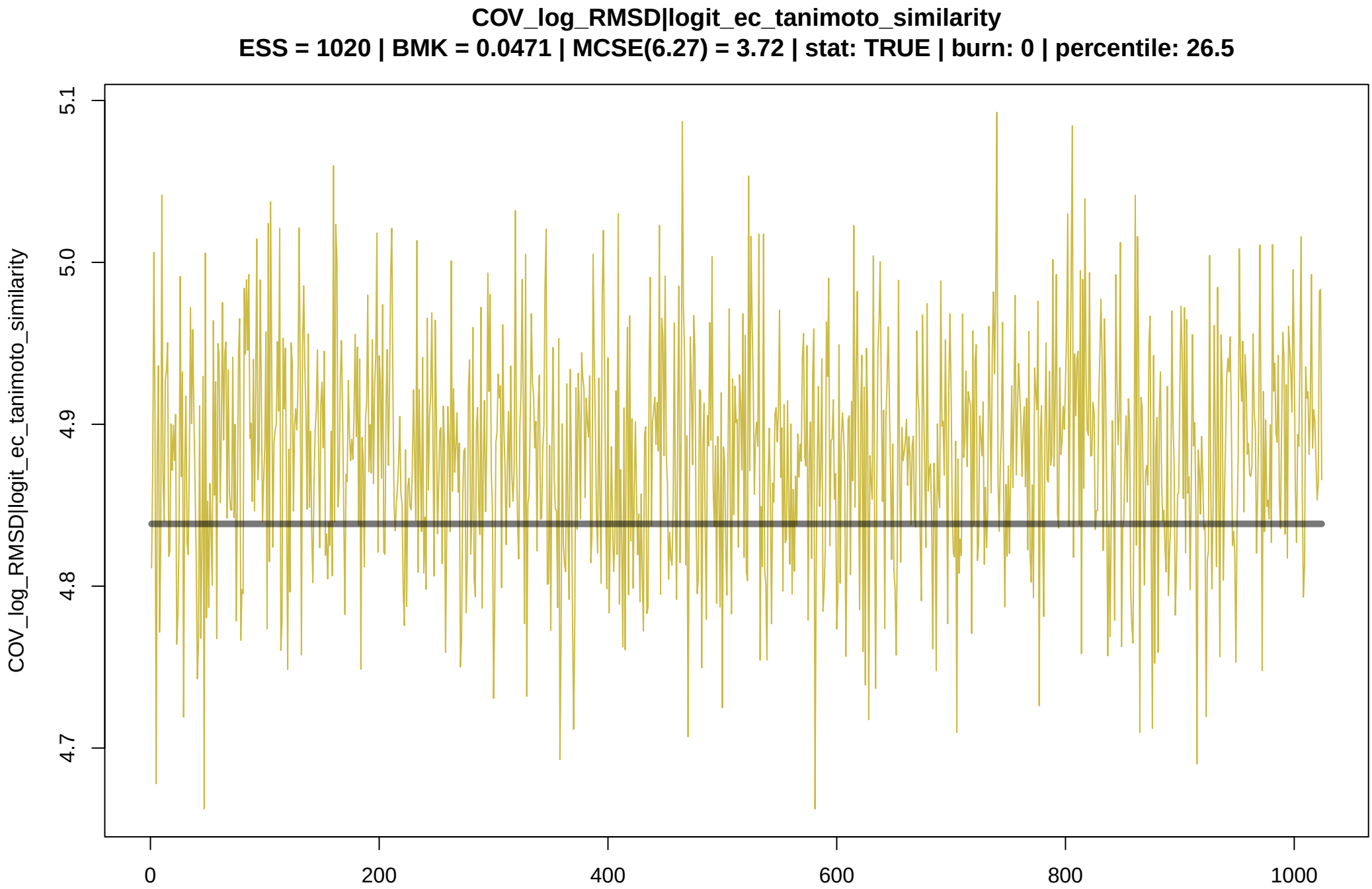

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0718 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | percentile: 98.5
VAR_docked_HeavyAtomCount
5.66
5.68
5.70
5.72
0
200
400
600
800
1000

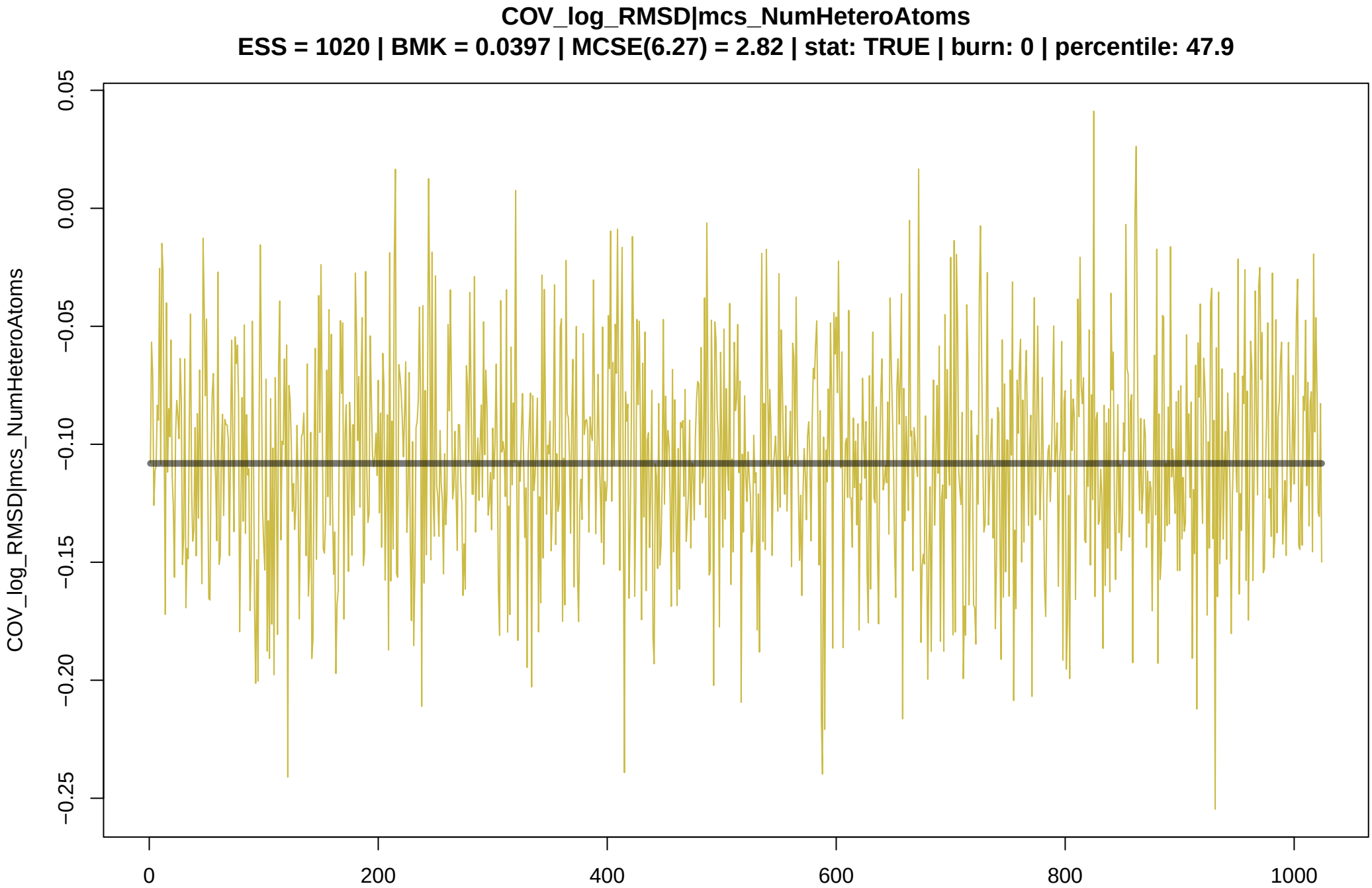

VAR_mcs_RingCount
ESS = 48.4 | BMK = 0.216 | MCSE(6.27) = 9.96 | stat: FALSE | burn: 0 | percentile: 24.3
VAR_mcs_RingCount
1.10
1.15
1.20
1.25
1.30
1.35
0
200
400
600
800
1000

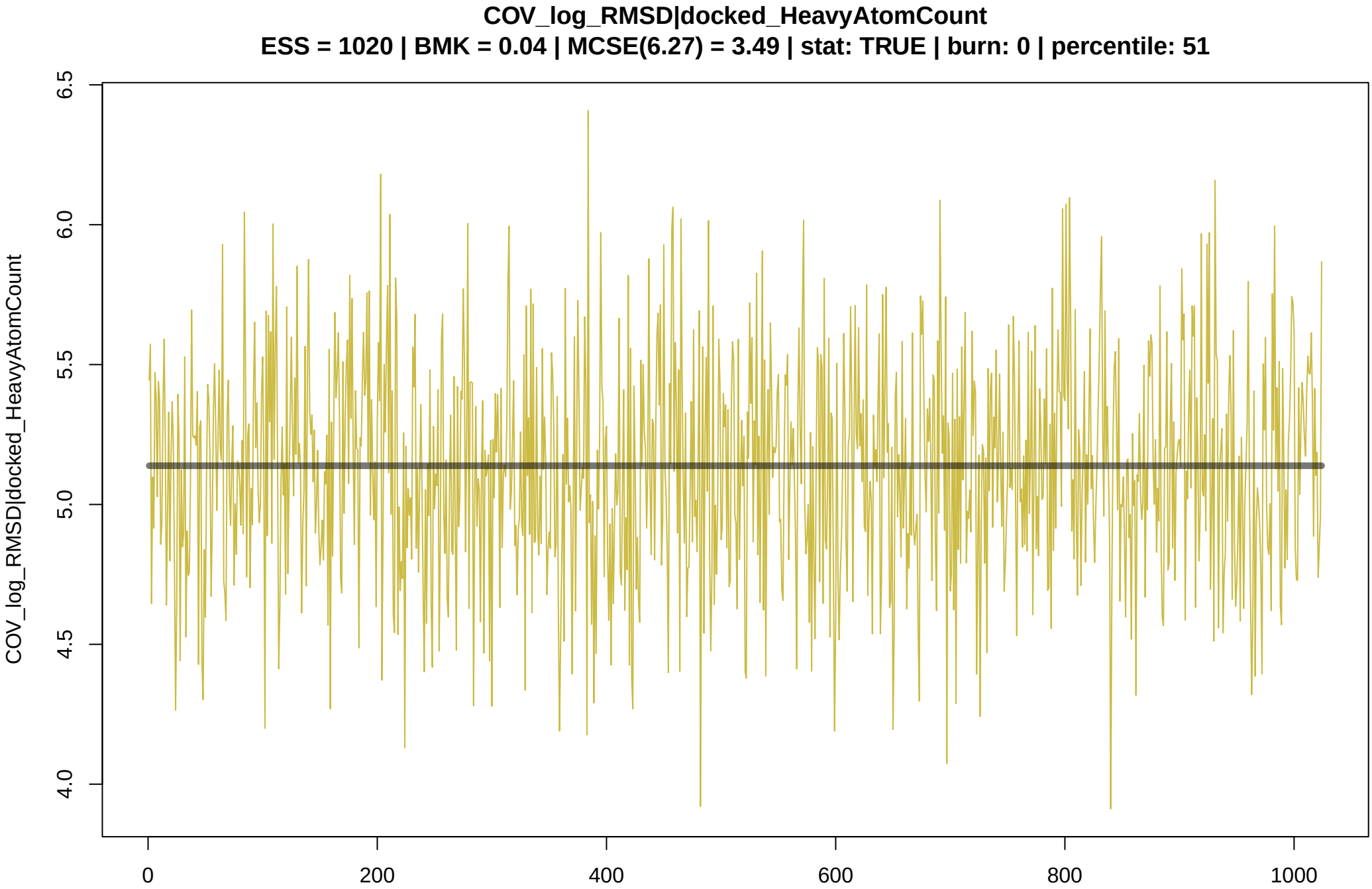

VAR_docked_NumRotatableBonds
ESS = 771 | BMK = 0.0538 | MCSE(6.27) = 4.39 | stat: TRUE | burn: 0 | percentile: 20.2
VAR_docked_NumRotatableBonds
3.44
3.46
3.48
3.50
3.52
3.54
0
200
400
600
800
1000

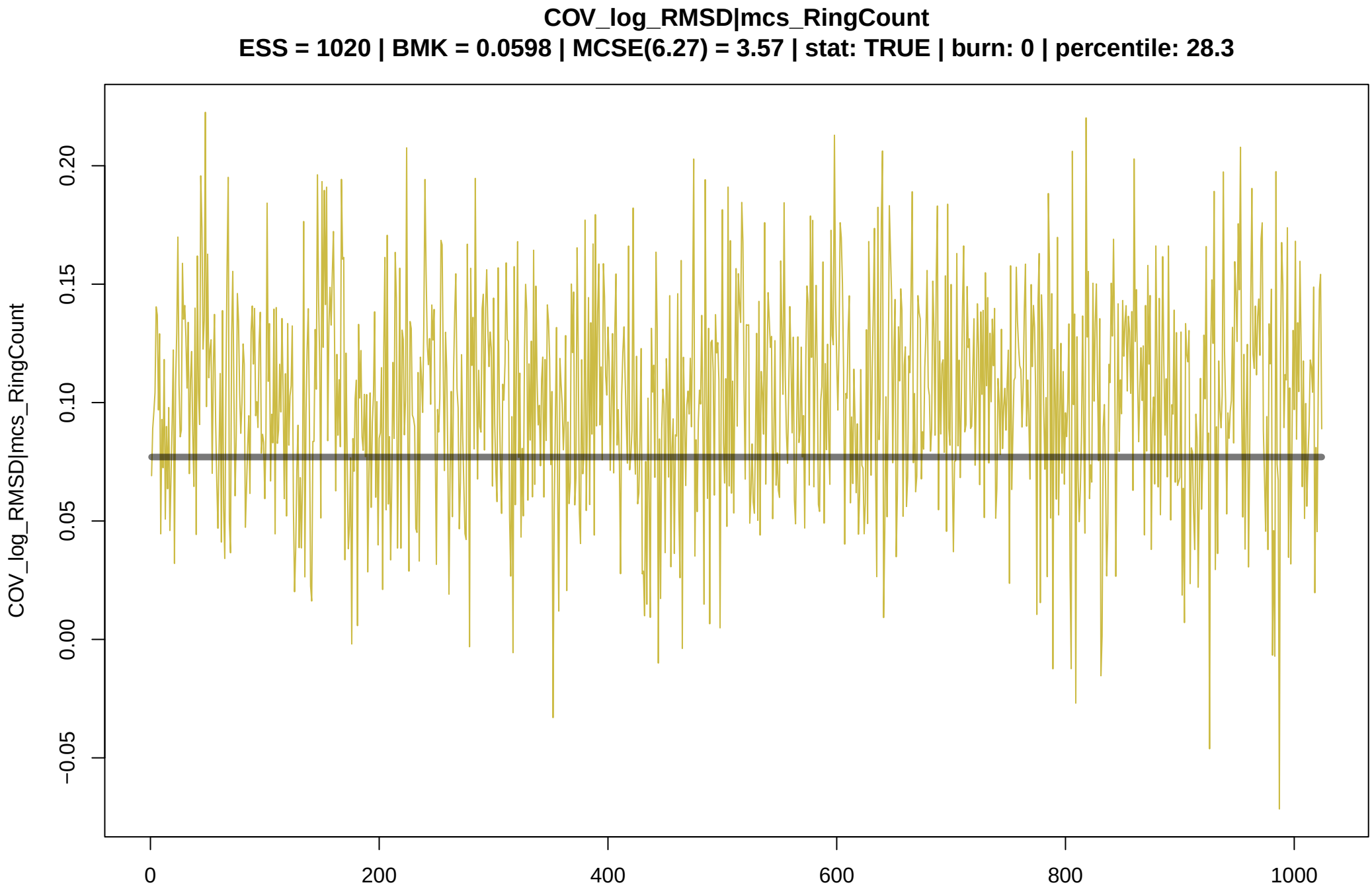

VAR_mcs_NOCount
ESS = 1020 | BMK = 0.077 | MCSE(6.27) = 4.06 | stat: FALSE | burn: 0 | percentile: 73.6
VAR_mcs_NOCount
3.70
3.65
3.60
3.55
3.50
0
200
400
600
800
1000

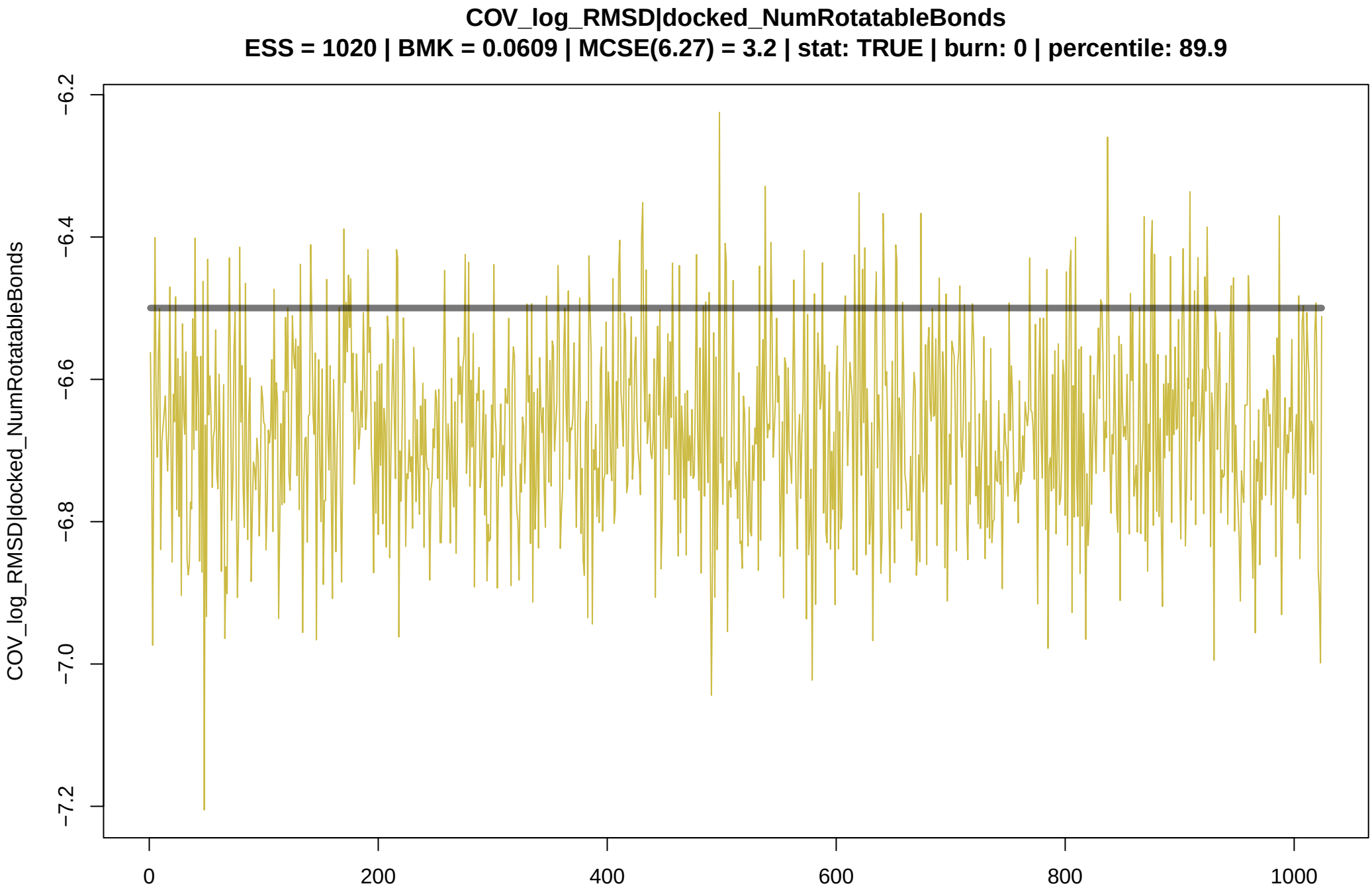

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0583 | MCSE(6.27) = 3.58 | stat: TRUE | burn: 0 | percentile: 66.7
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.30
−0.35
−0.40
−0.45
−0.50
−0.55
−0.60
−0.65
0
200
400
600
800
1000

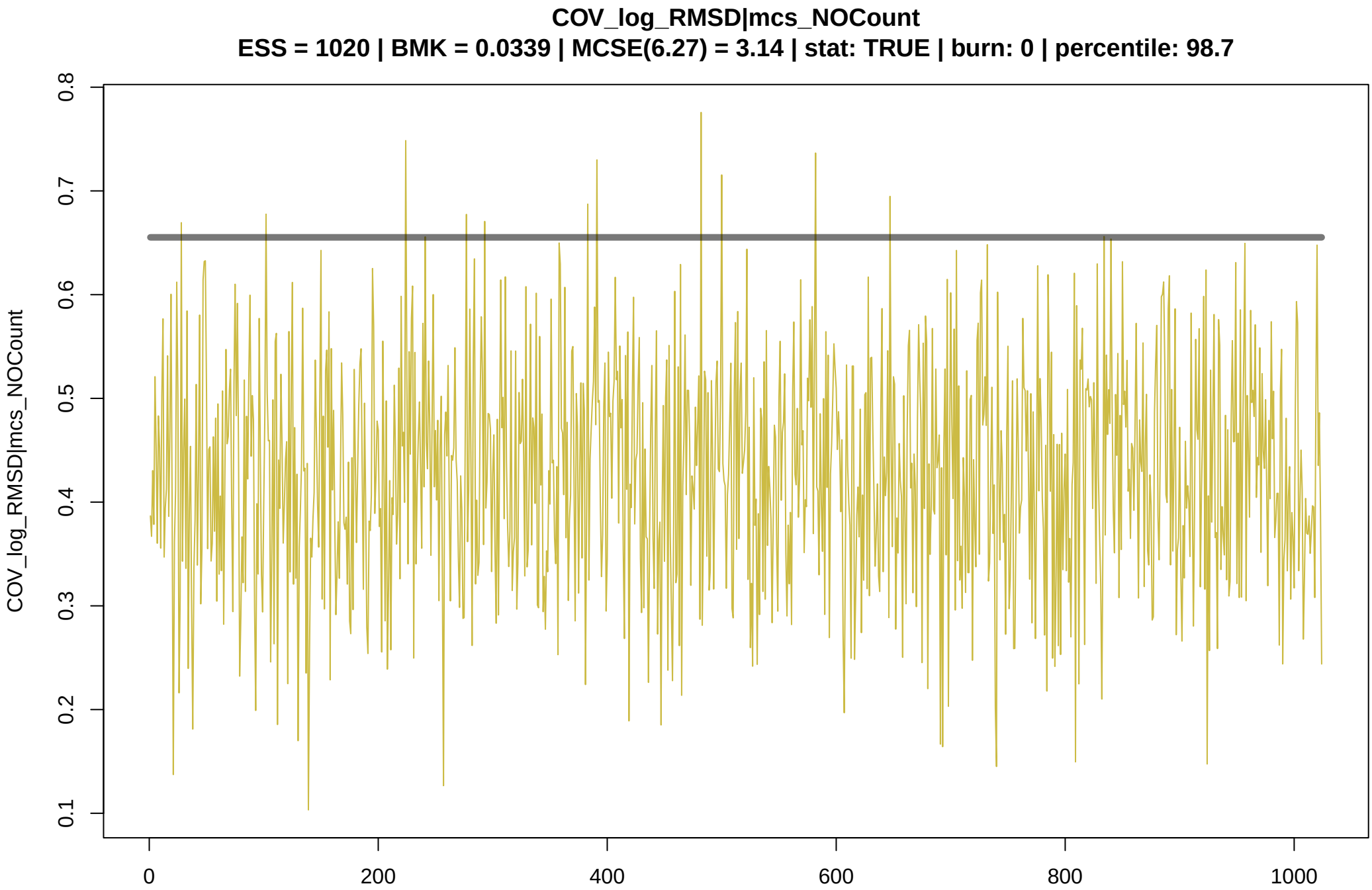

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0471 | MCSE(6.27) = 3.72 | stat: TRUE | burn: 0 | percentile: 26.5
COV_log_RMSD|logit_ec_tanimoto_similarity
5.1
5.0
4.9
4.8
4.7
0
200
400
600
800
1000

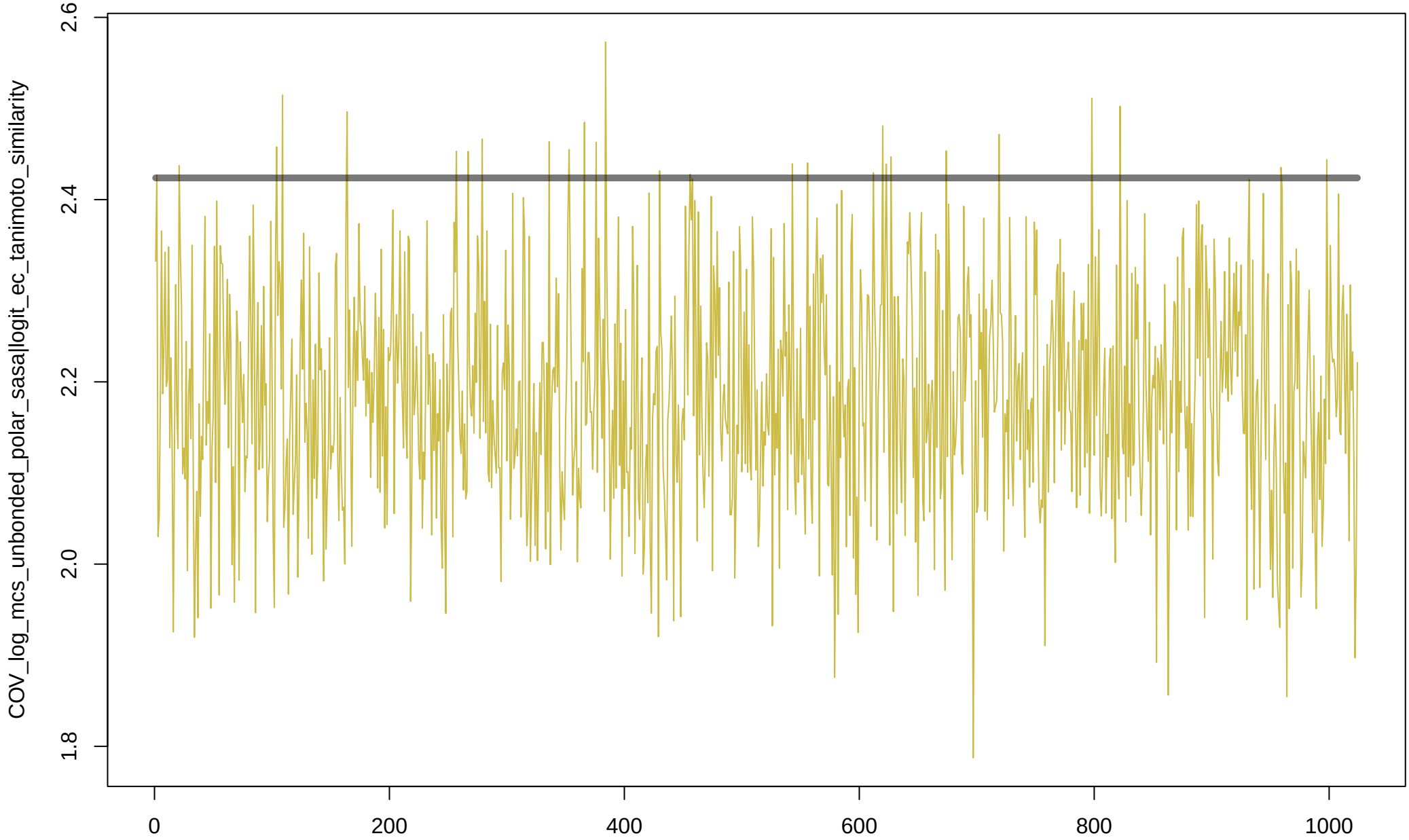

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0397 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | percentile: 47.9
COV_log_RMSD|mcs_NumHeteroAtoms
0.05
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
200
400
600
800
1000

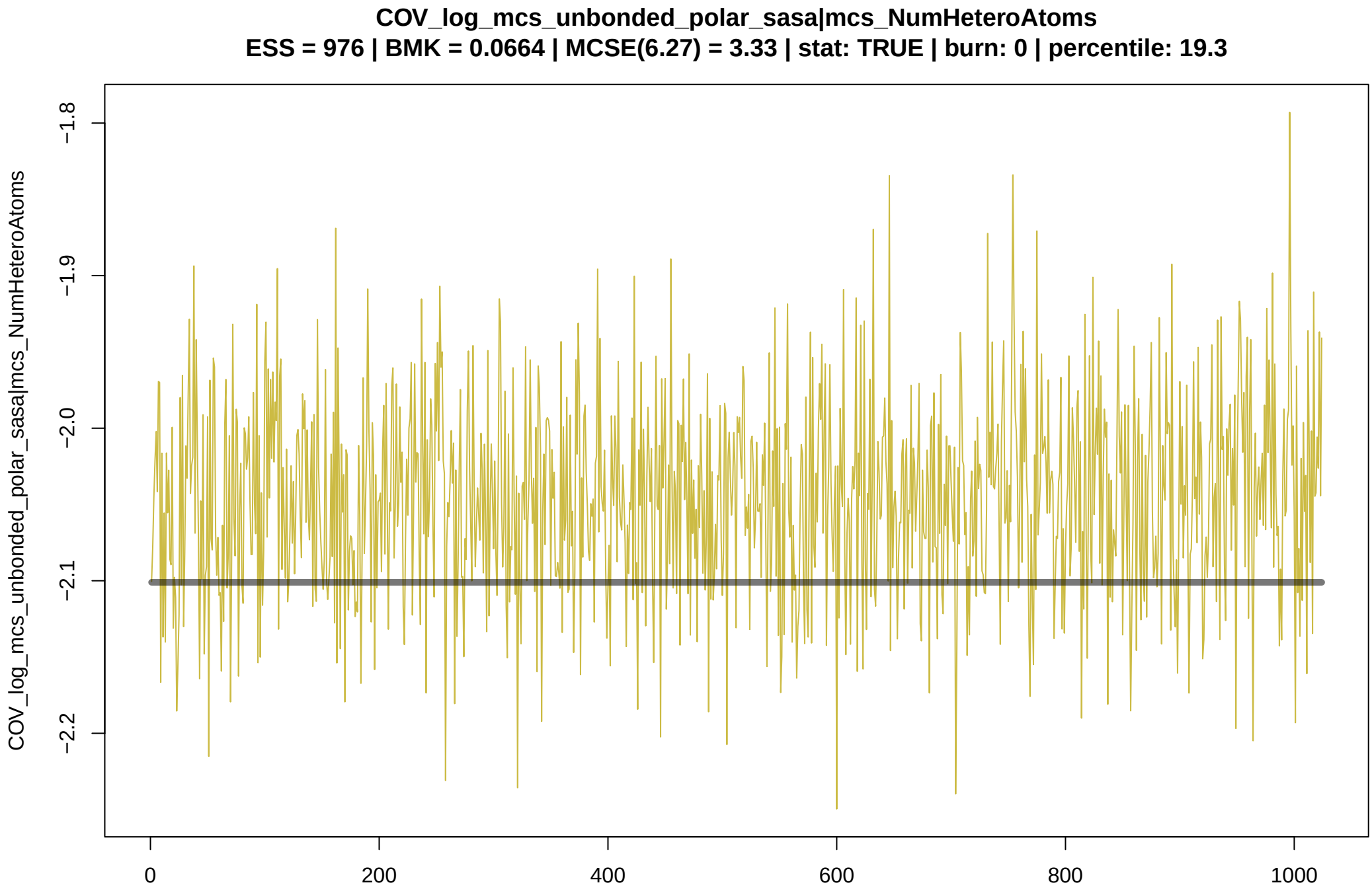

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.04 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0 | percentile: 51
COV_log_RMSD|docked_HeavyAtomCount
6.5
6.0
5.5
5.0
4.5
4.0
0
200
400
600
800
1000

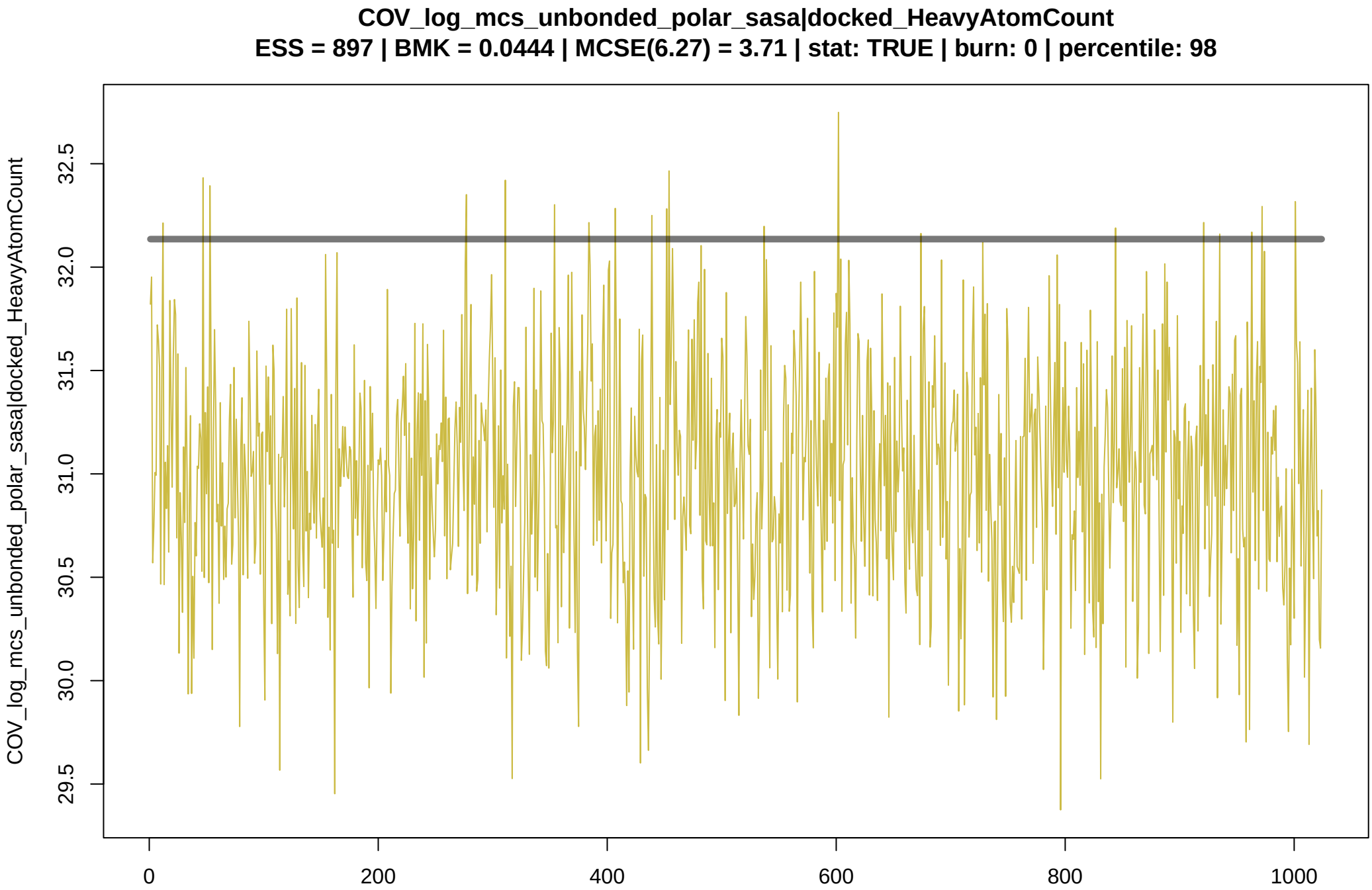

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0598 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | percentile: 28.3
COV_log_RMSD|mcs_RingCount
0.20
0.15
0.10
0.05
0.00
−0.05
0
200
400
600
800
1000

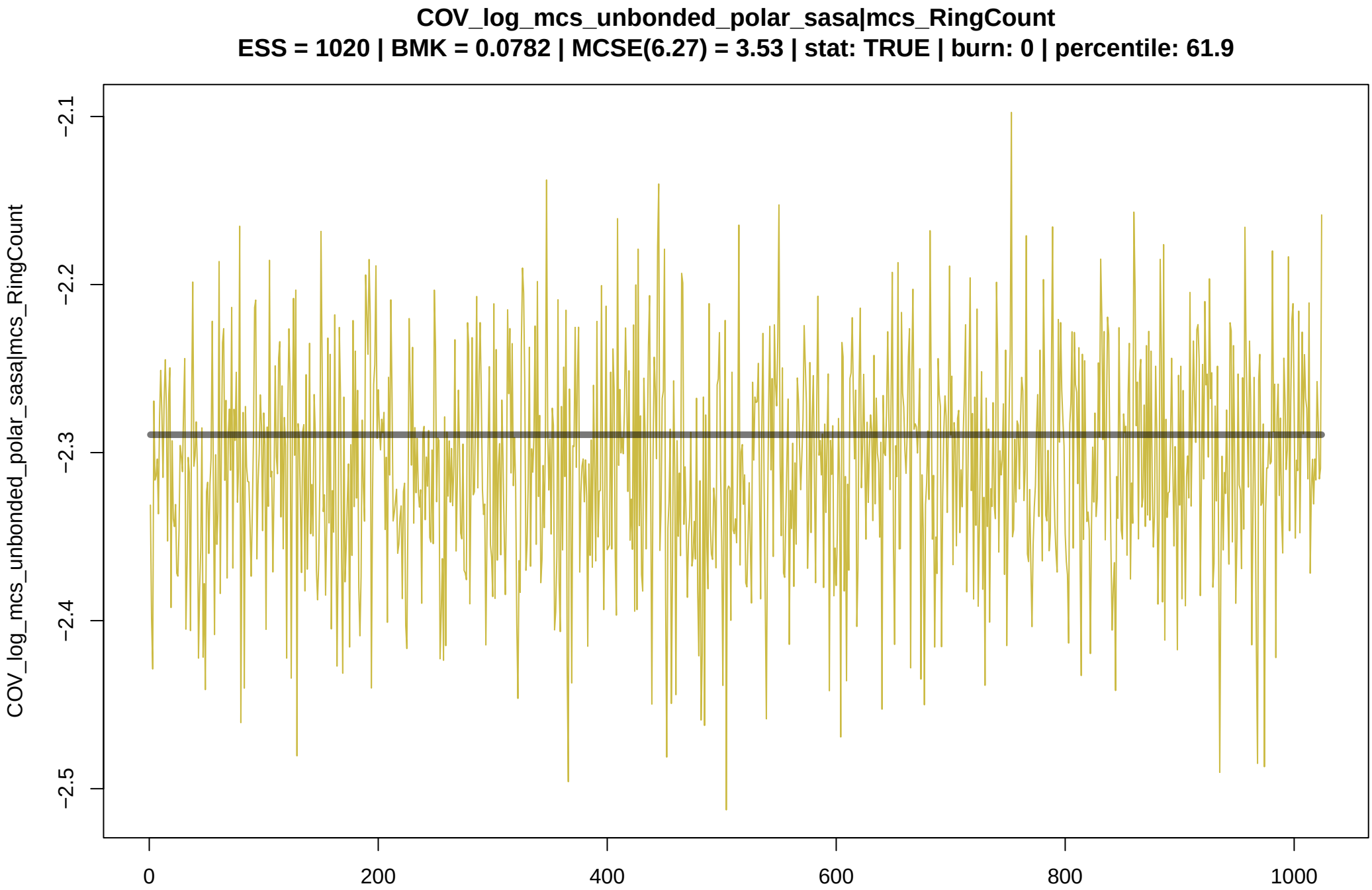

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0609 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | percentile: 89.9
COV_log_RMSD|docked_NumRotatableBonds
−6.2
−6.4
−6.6
−6.8
−7.0
−7.2
0
200
400
600
800
1000

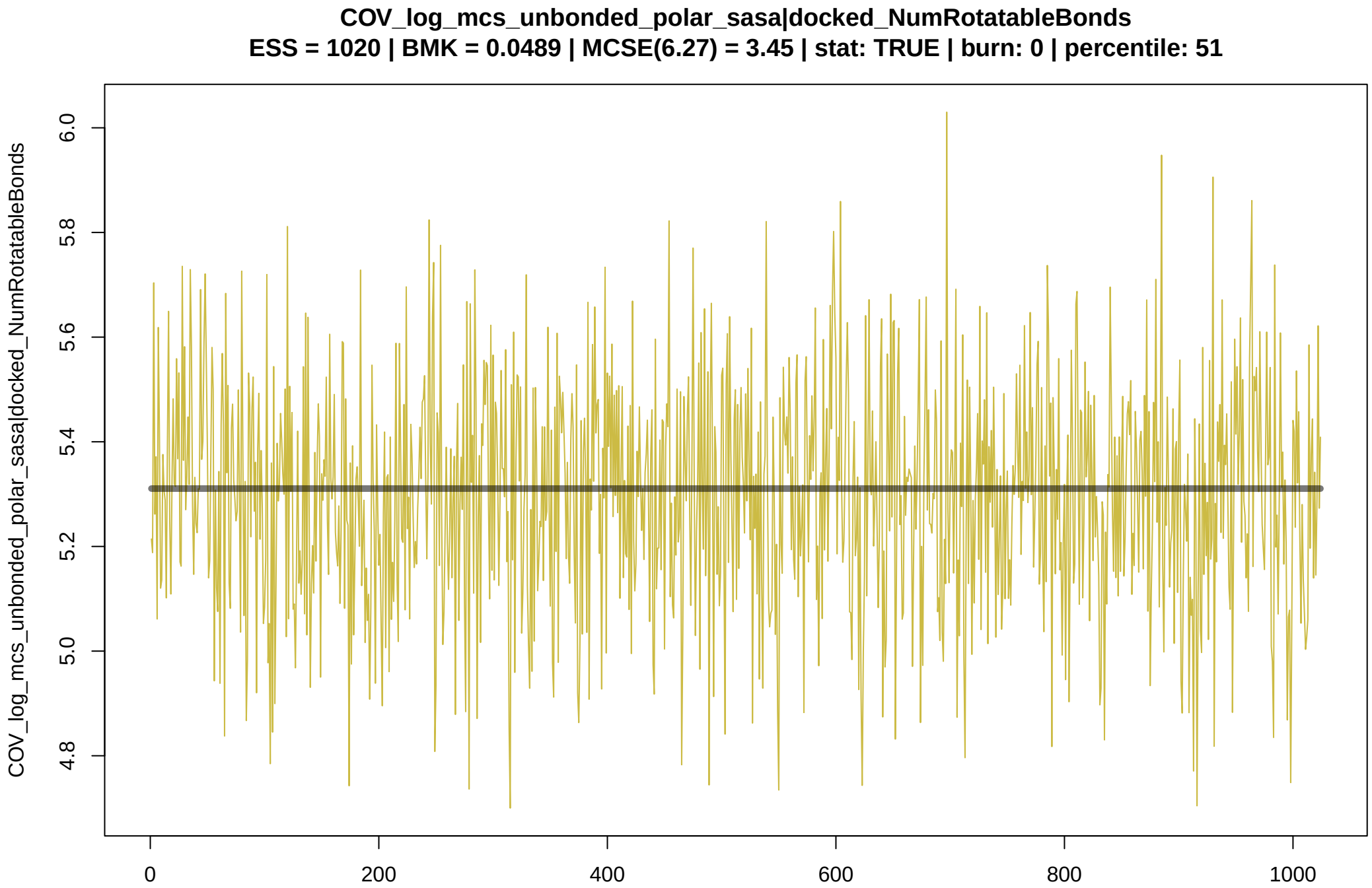

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0339 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | percentile: 98.7
COV_log_RMSD|mcs_NOCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
200
400
600
800
1000

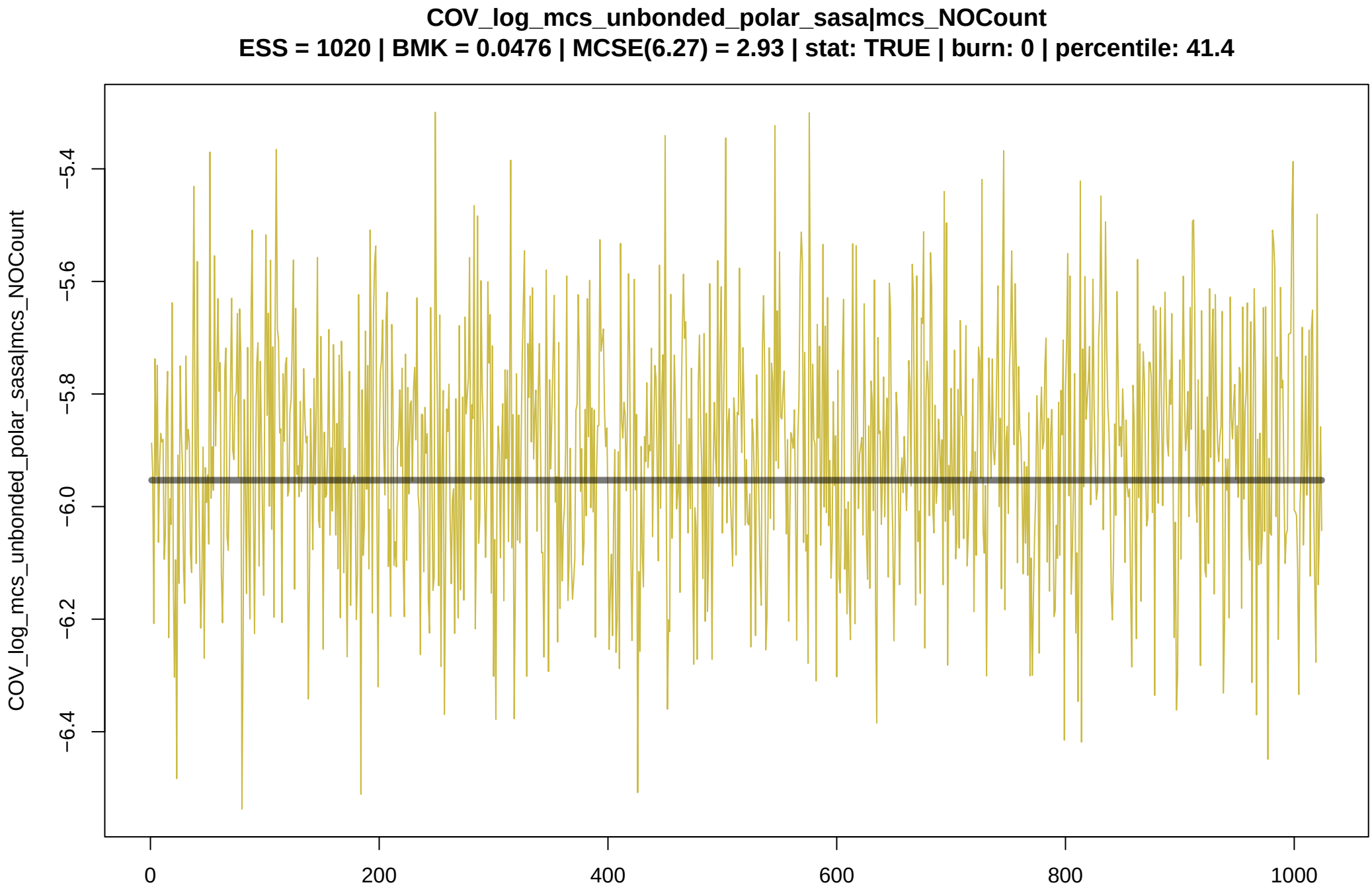

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 918 | BMK = 0.0655 | MCSE(6.27) = 3.81 | stat: TRUE | burn: 0 | percentile: 97.4
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2.6
2.4
2.2
2.0
1.8
0
200
400
600
800
1000

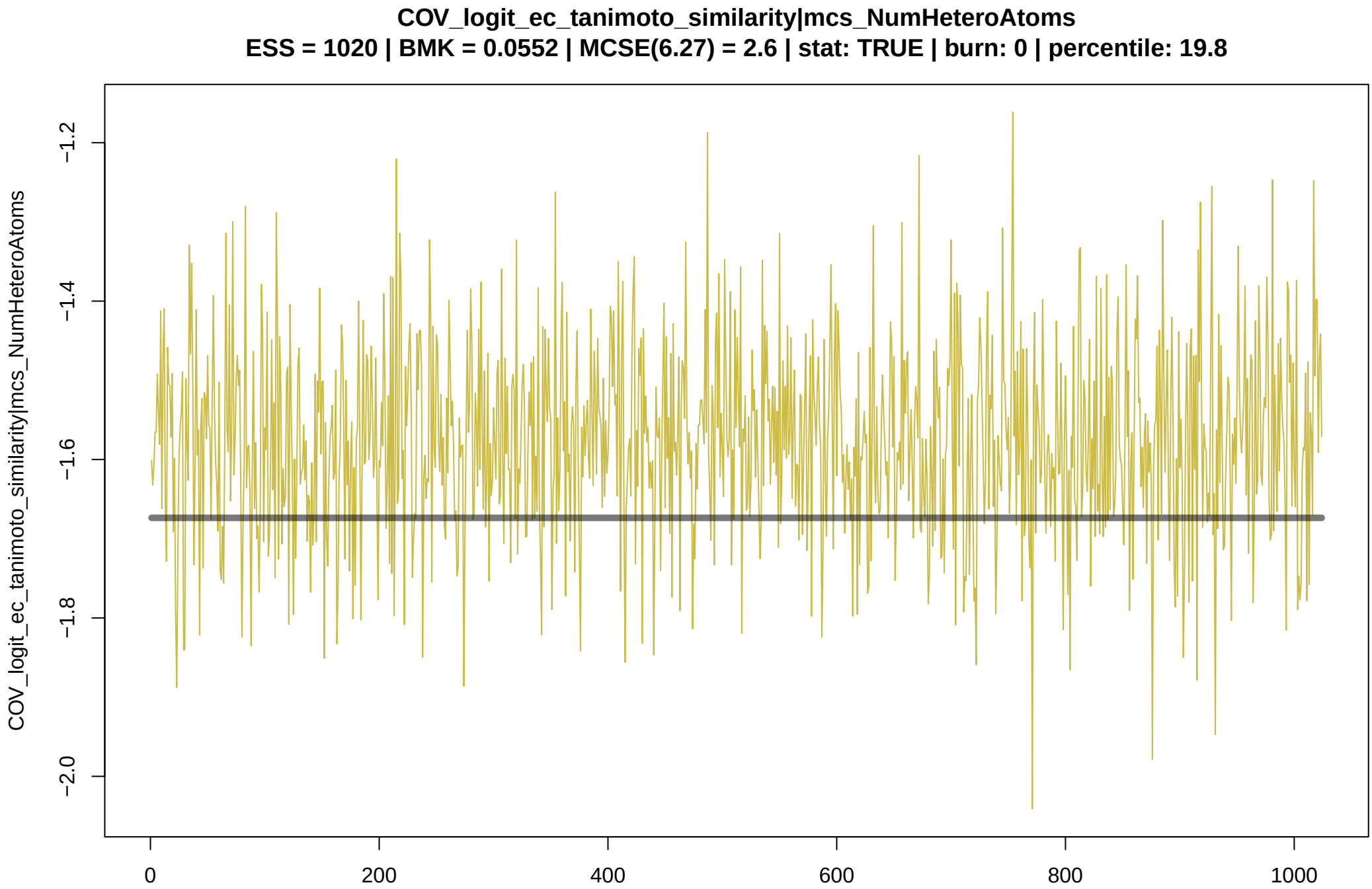

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 976 | BMK = 0.0664 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0 | percentile: 19.3
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.8
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

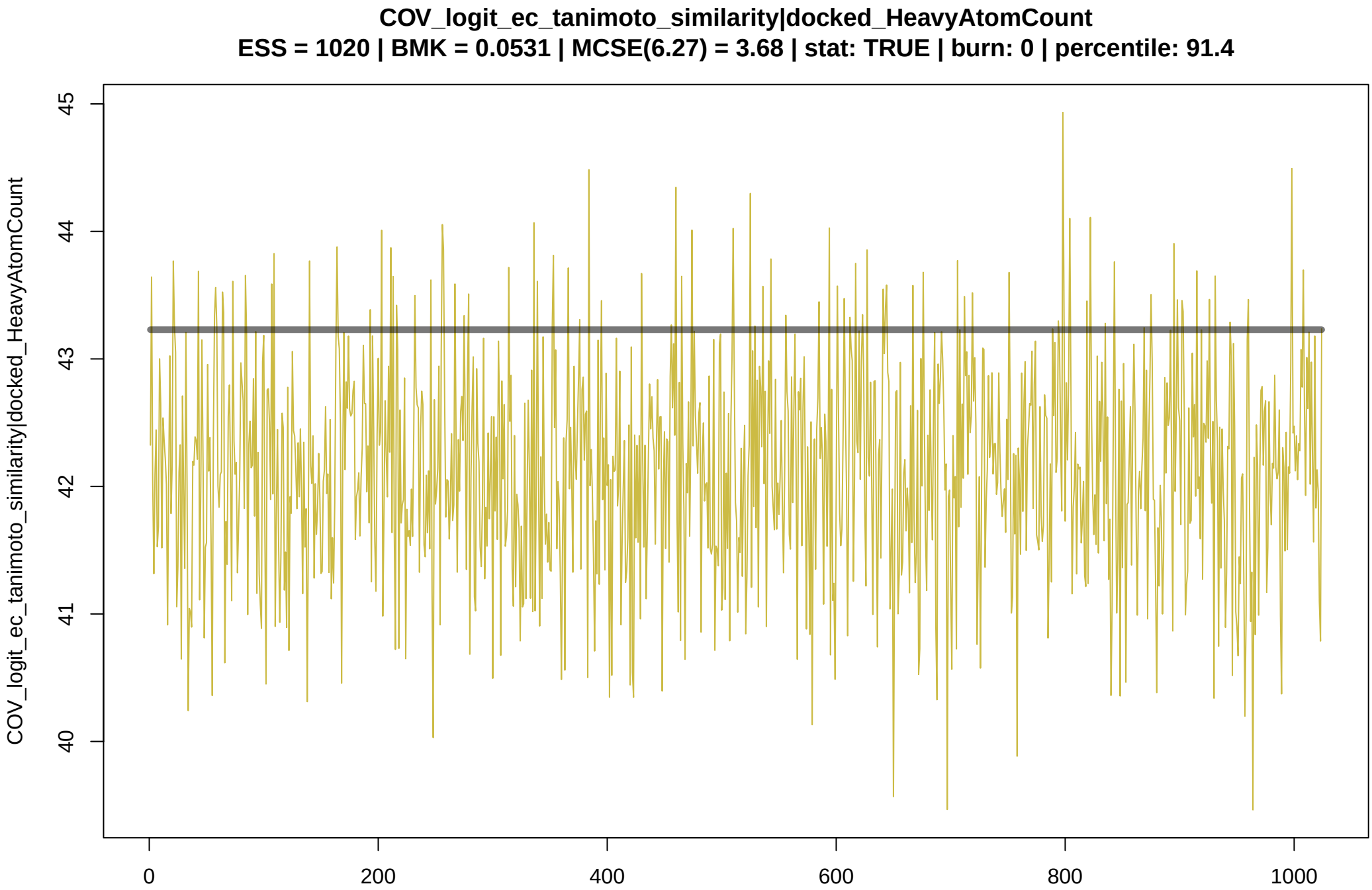

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 897 | BMK = 0.0444 | MCSE(6.27) = 3.71 | stat: TRUE | burn: 0 | percentile: 98
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
29.5
30.0
30.5
31.0
31.5
32.0
32.5
0
200
400
600
800
1000

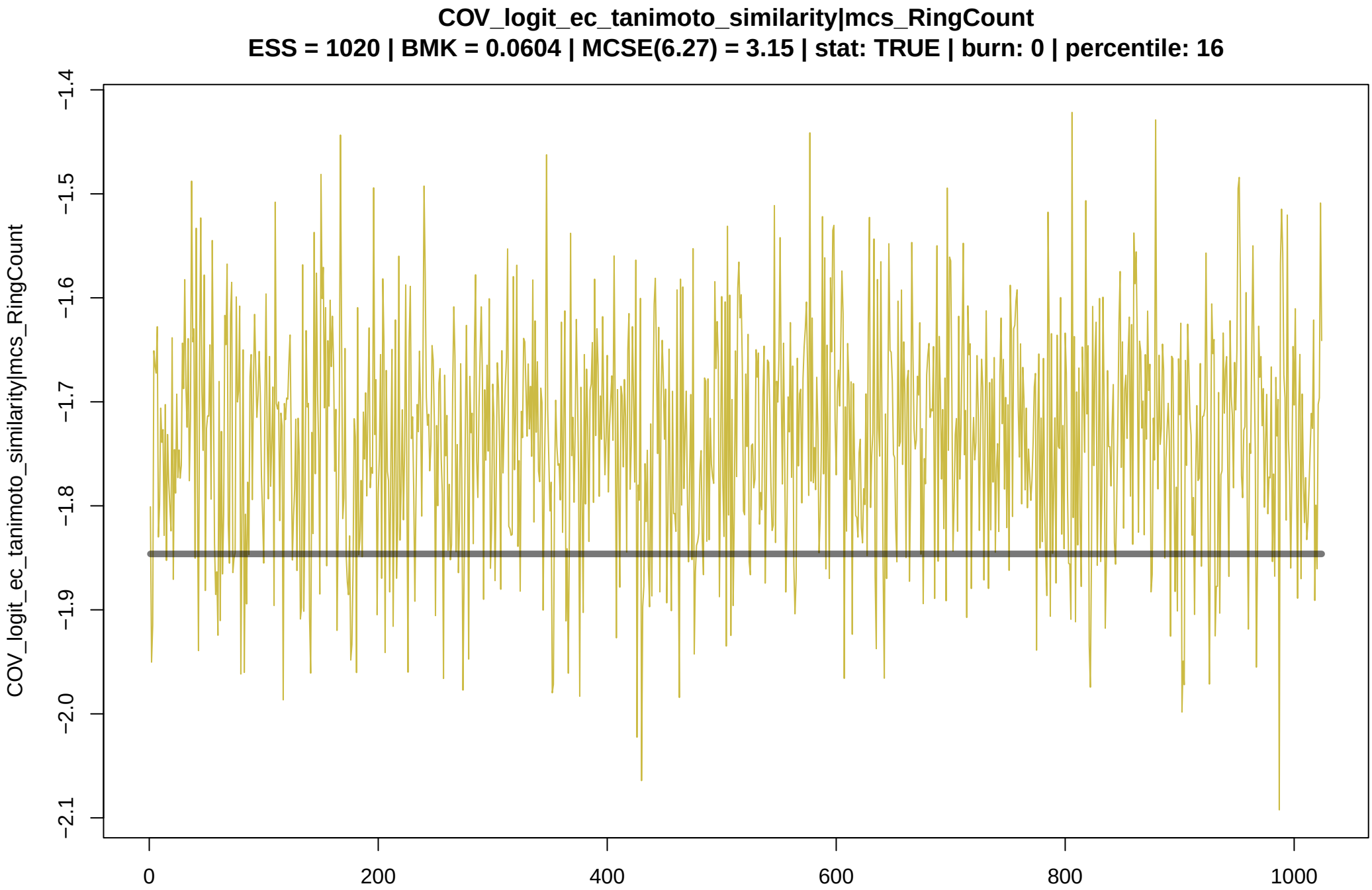

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0782 | MCSE(6.27) = 3.53 | stat: TRUE | burn: 0 | percentile: 61.9
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.1
−2.2
−2.3
−2.4
−2.5
0
200
400
600
800
1000

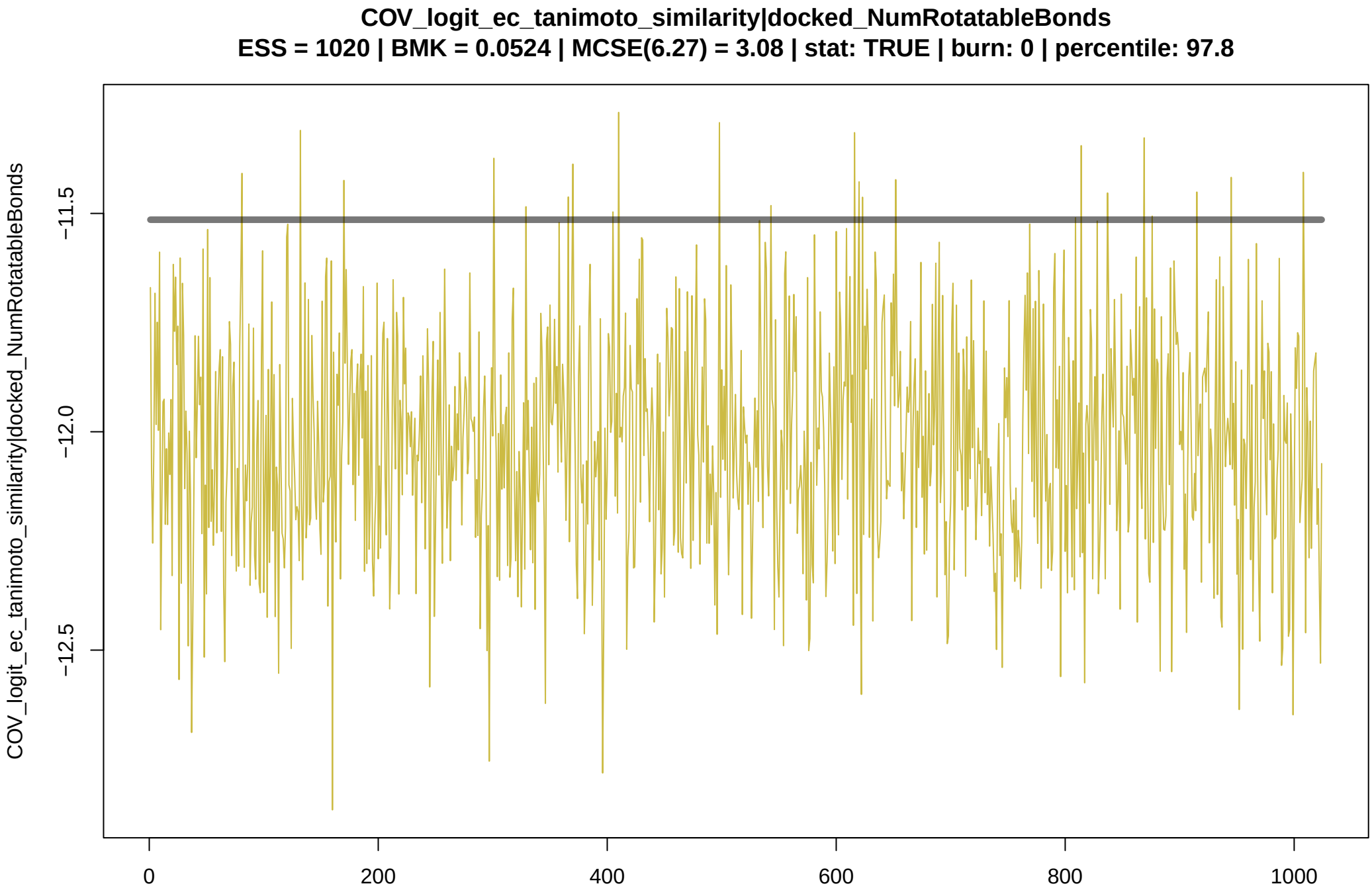

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0489 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0 | percentile: 51
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
6.0
5.8
5.6
5.4
5.2
5.0
4.8
0
200
400
600
800
1000

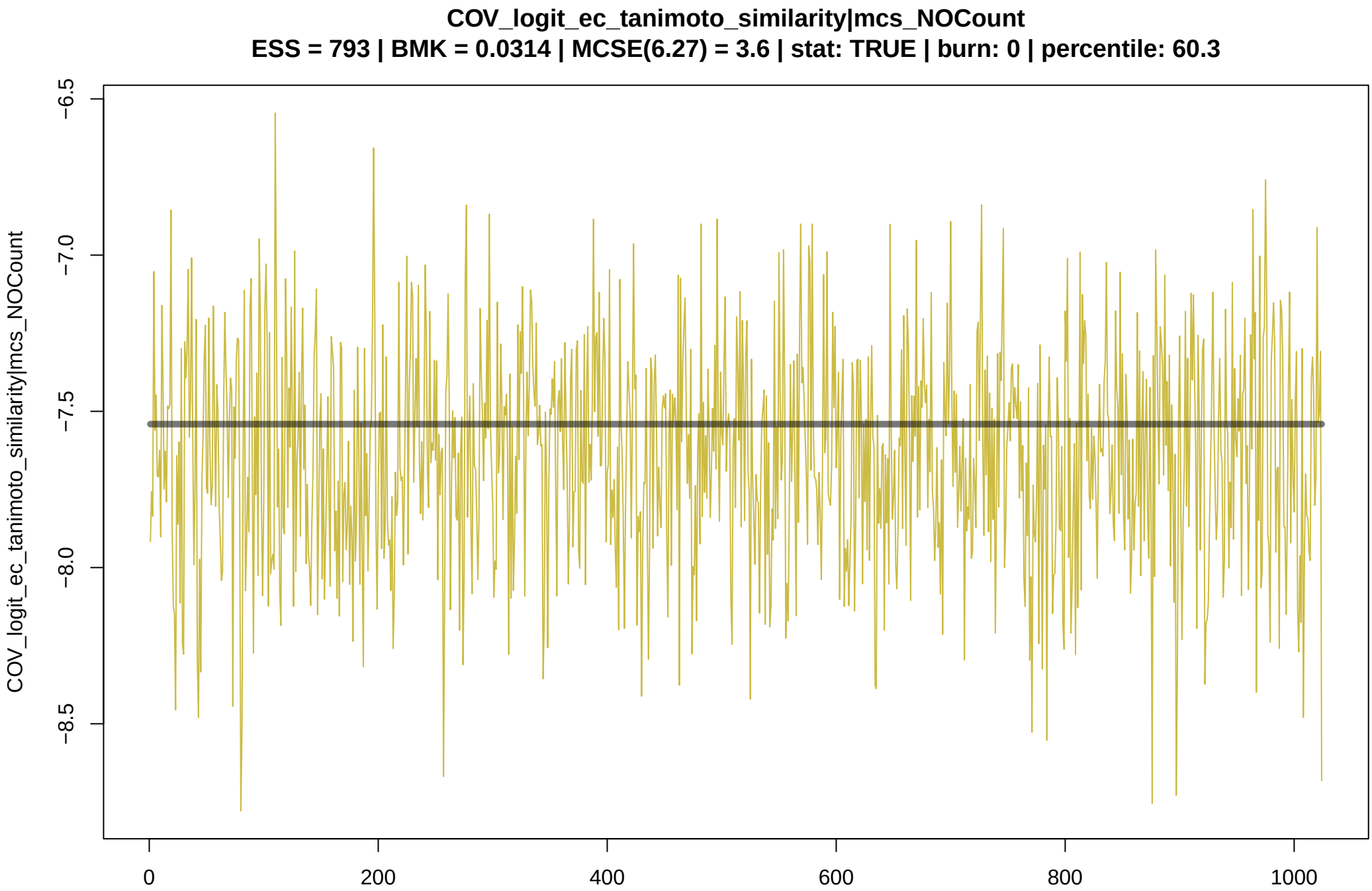

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0476 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | percentile: 41.4
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.4
−5.6
−5.8
−6.0
−6.2
−6.4
0
200
400
600
800
1000

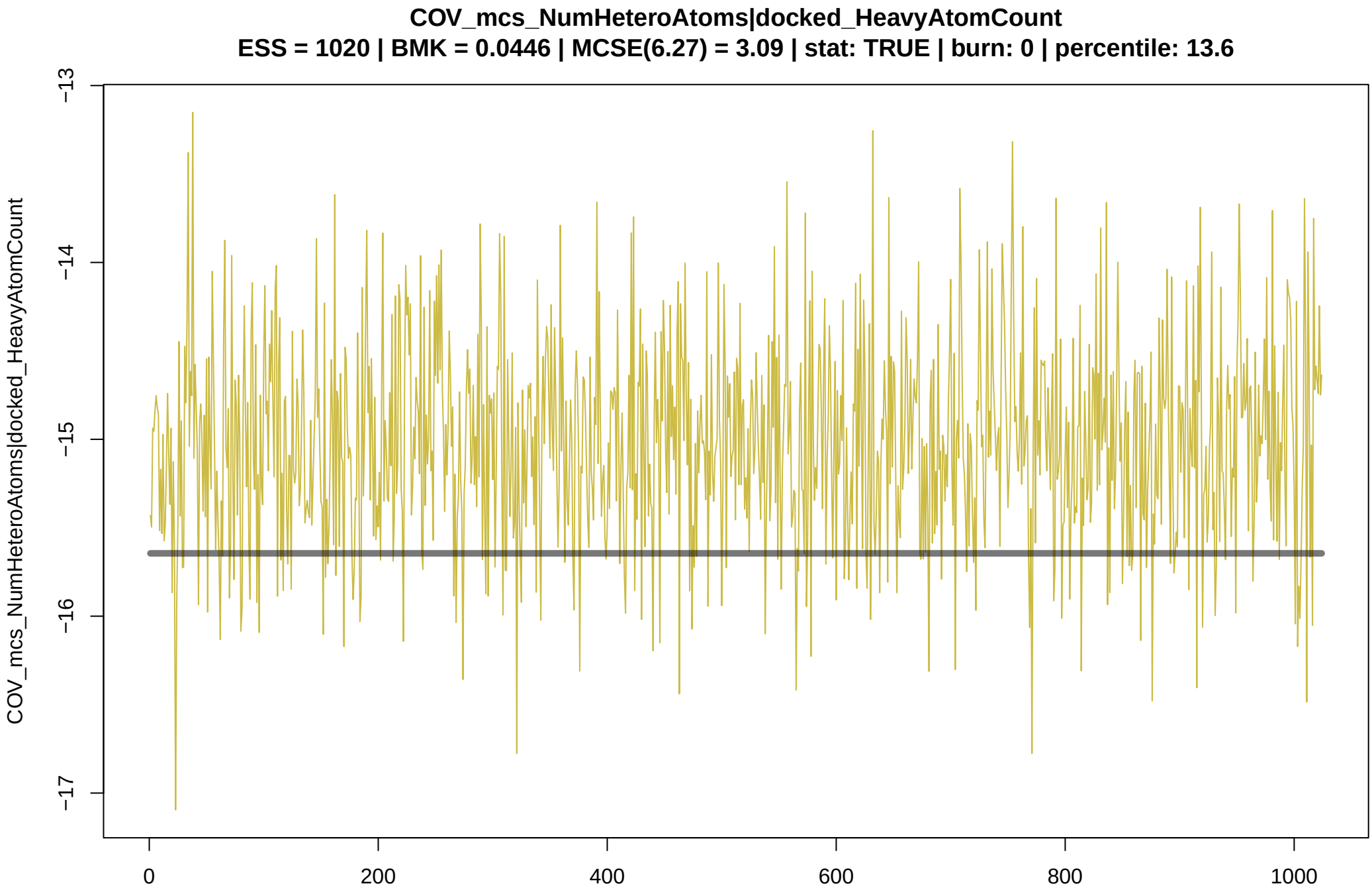

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0552 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | percentile: 19.8
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.2
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

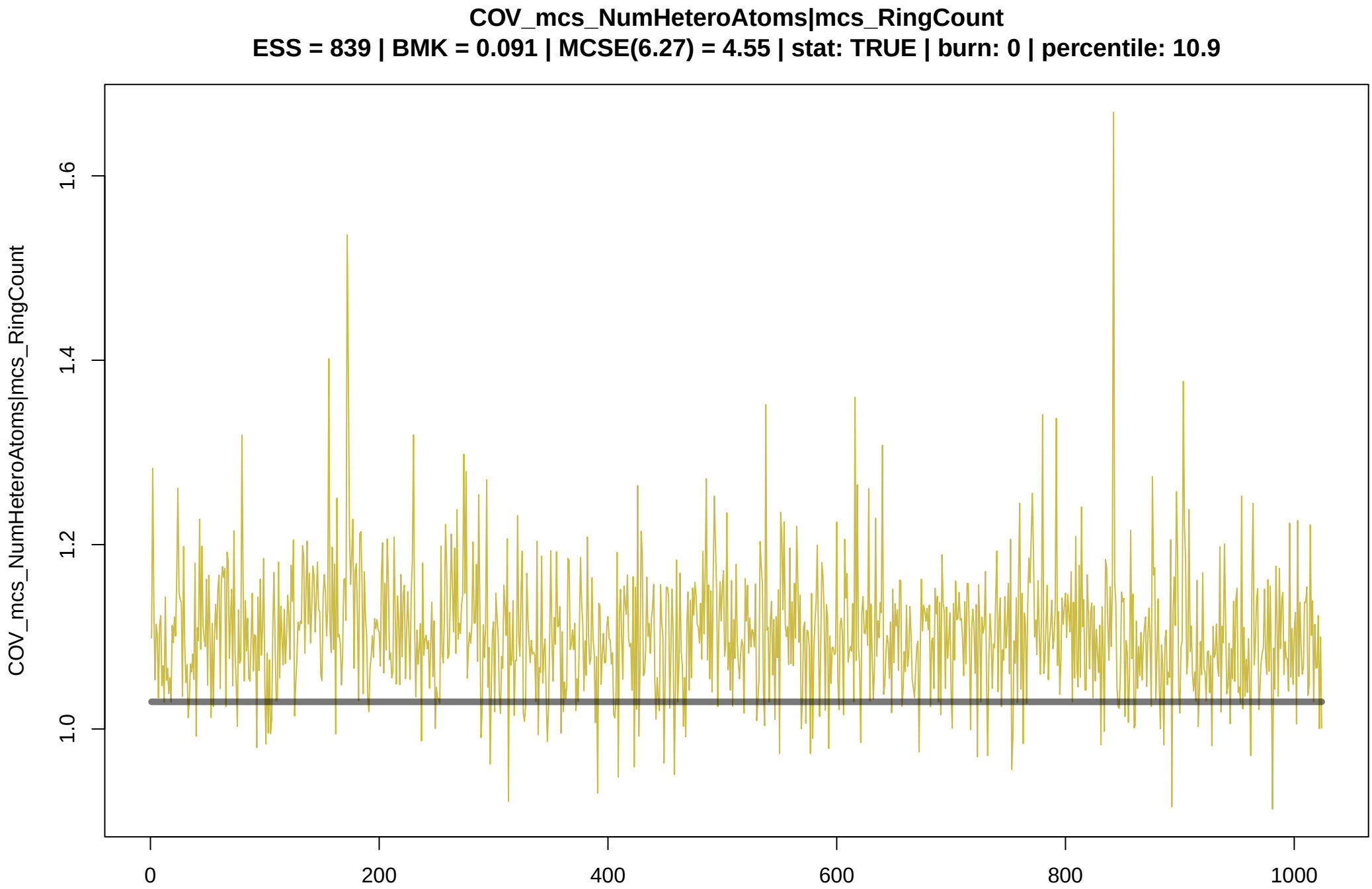

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0531 | MCSE(6.27) = 3.68 | stat: TRUE | burn: 0 | percentile: 91.4
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
45
44
43
42
41
40
0
200
400
600
800
1000

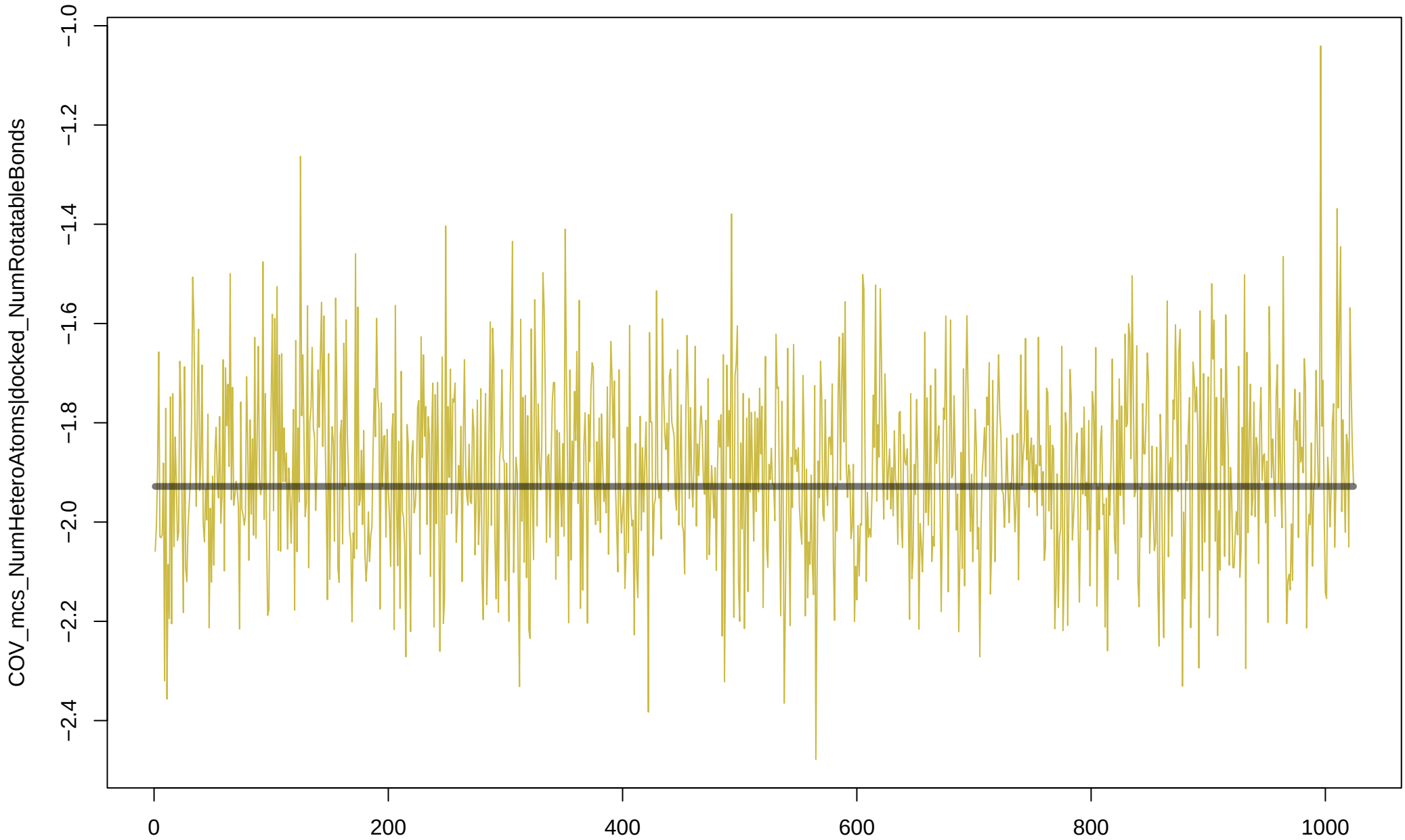

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0604 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0 | percentile: 16
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.4
−1.5
−1.6
−1.7
−1.8
−1.9
−2.0
−2.1
0
200
400
600
800
1000

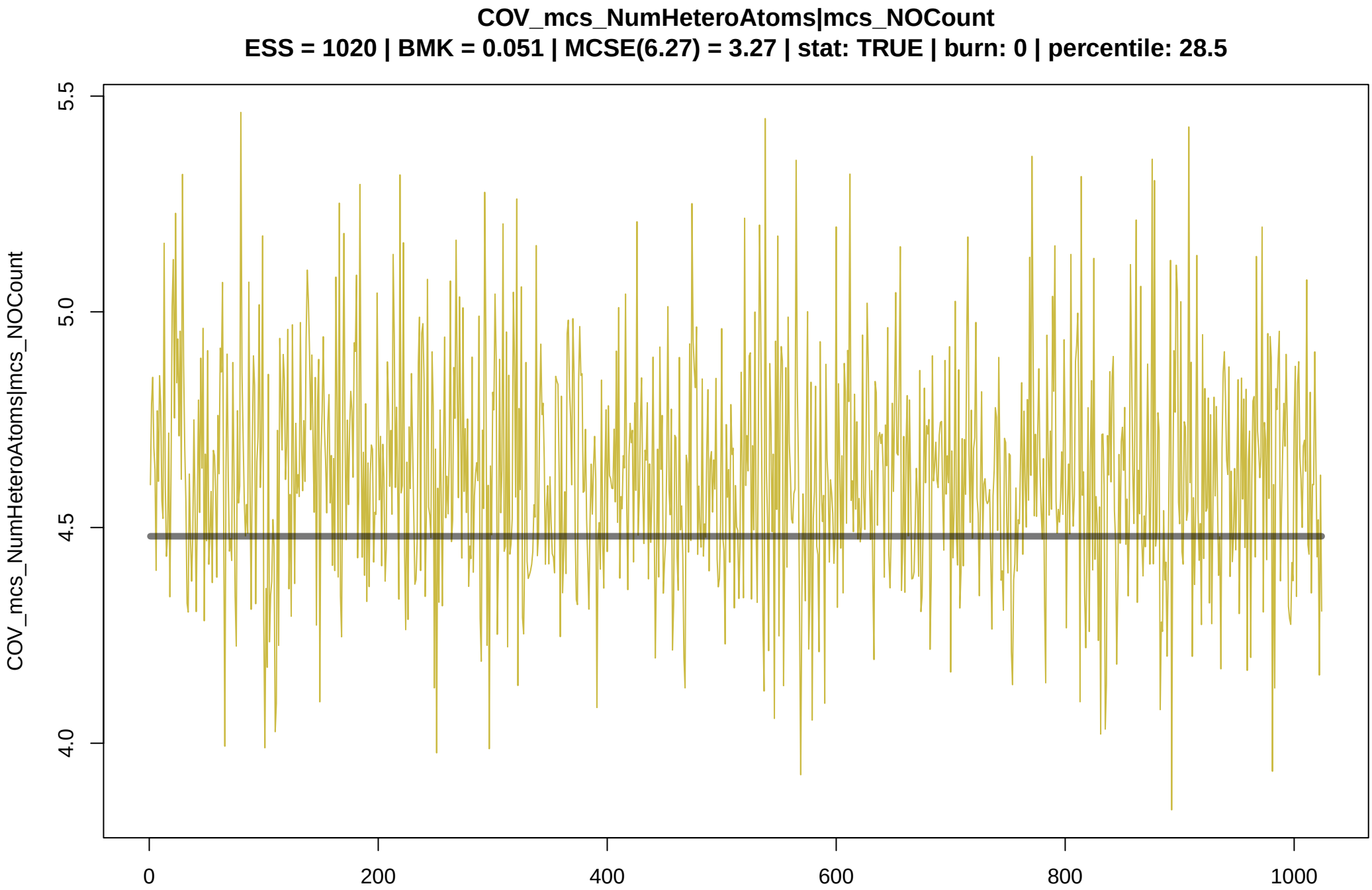

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0524 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | percentile: 97.8
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−11.5
−12.0
−12.5
0
200
400
600
800
1000

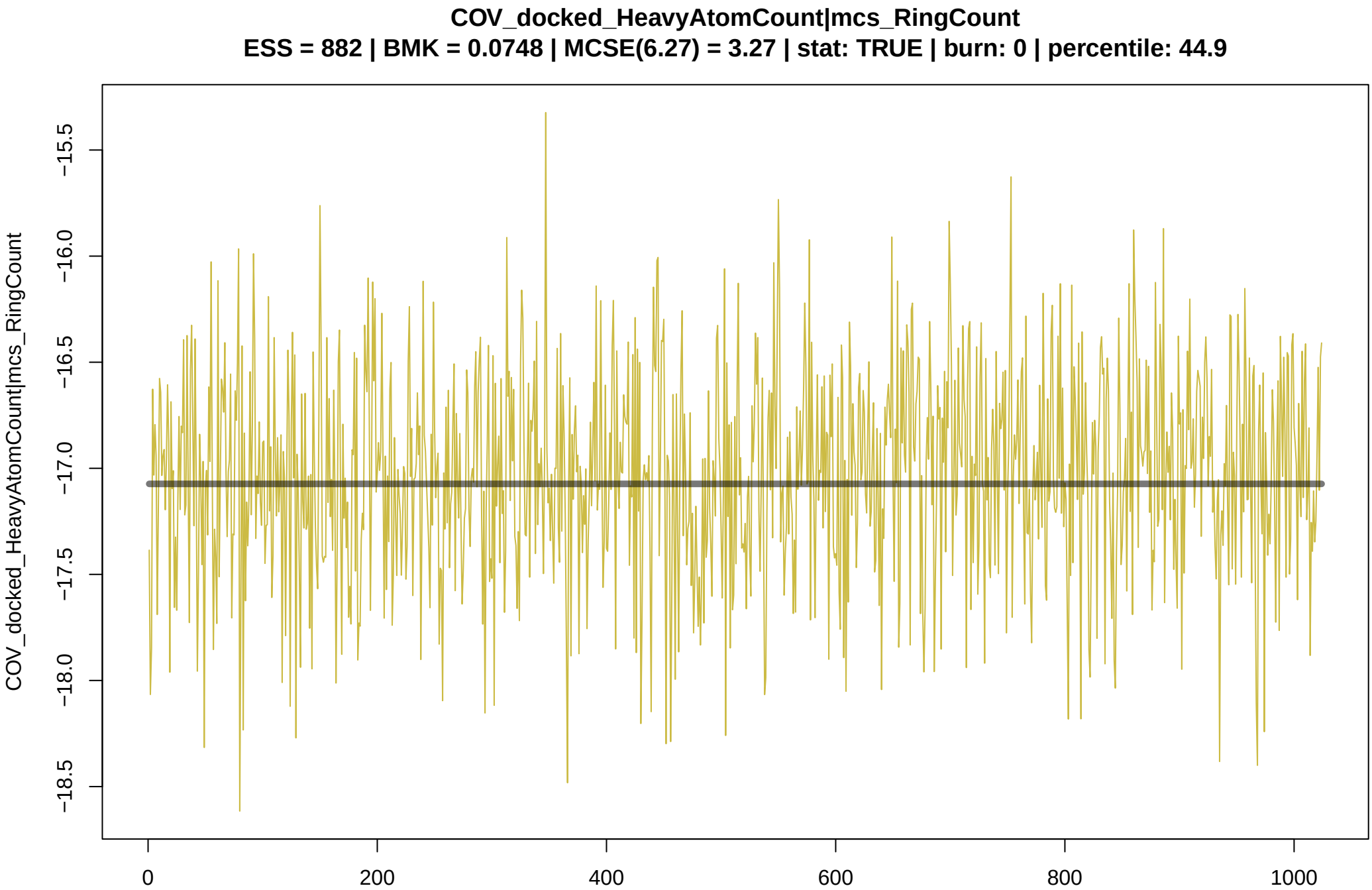

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 793 | BMK = 0.0314 | MCSE(6.27) = 3.6 | stat: TRUE | burn: 0 | percentile: 60.3
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−6.5
−7.0
−7.5
−8.0
−8.5
0
200
400
600
800
1000

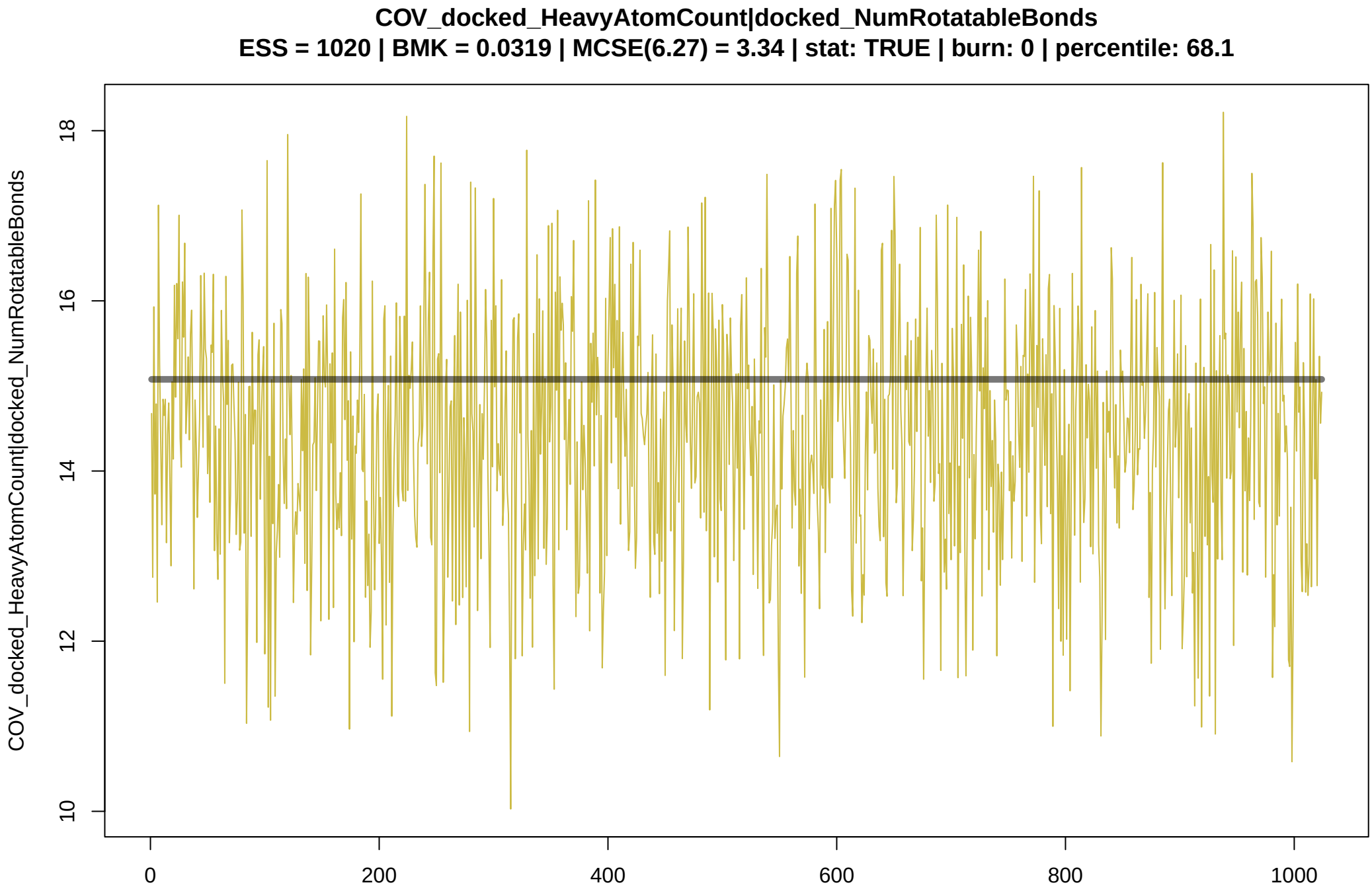

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0446 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | percentile: 13.6
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−13
−14
−15
−16
−17
0
200
400
600
800
1000

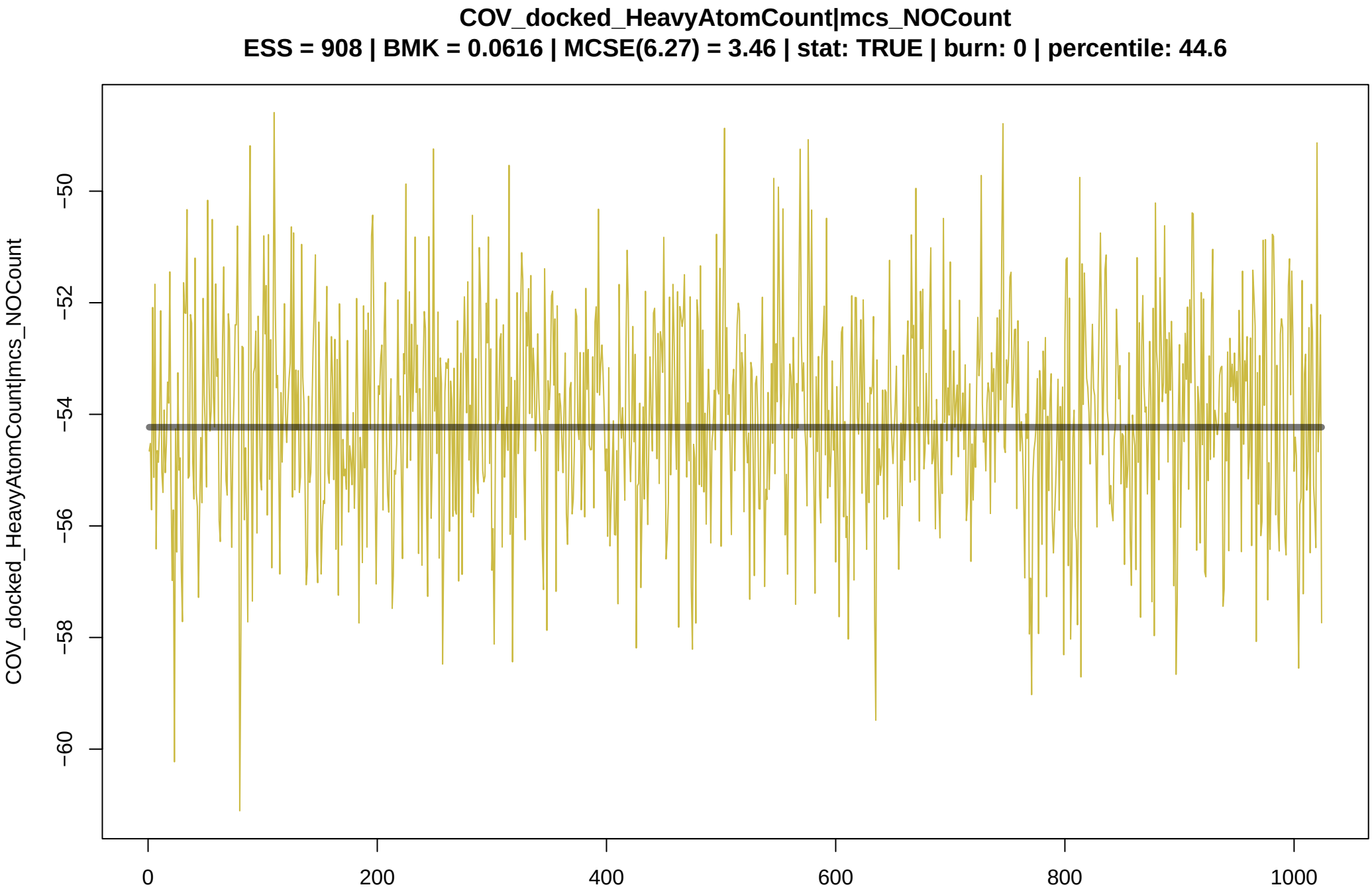

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 839 | BMK = 0.091 | MCSE(6.27) = 4.55 | stat: TRUE | burn: 0 | percentile: 10.9
COV_mcs_NumHeteroAtoms|mcs_RingCount
1.0
1.2
1.4
1.6
0
200
400
600
800
1000

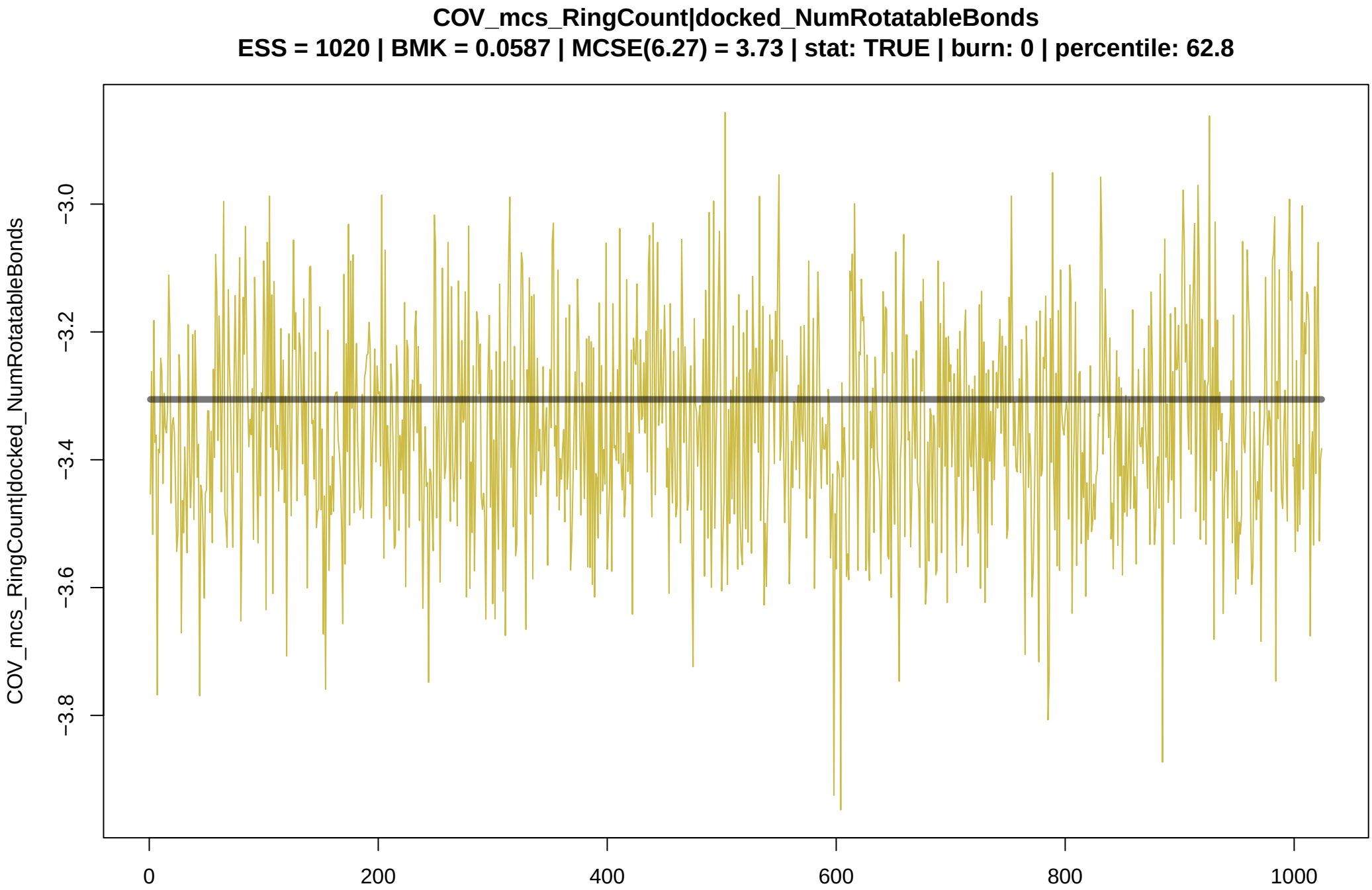

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 881 | BMK = 0.0559 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0 | percentile: 44.4
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.0
−1.2
−1.4
−1.6
−1.8
−2.0
−2.2
−2.4
0
200
400
600
800
1000

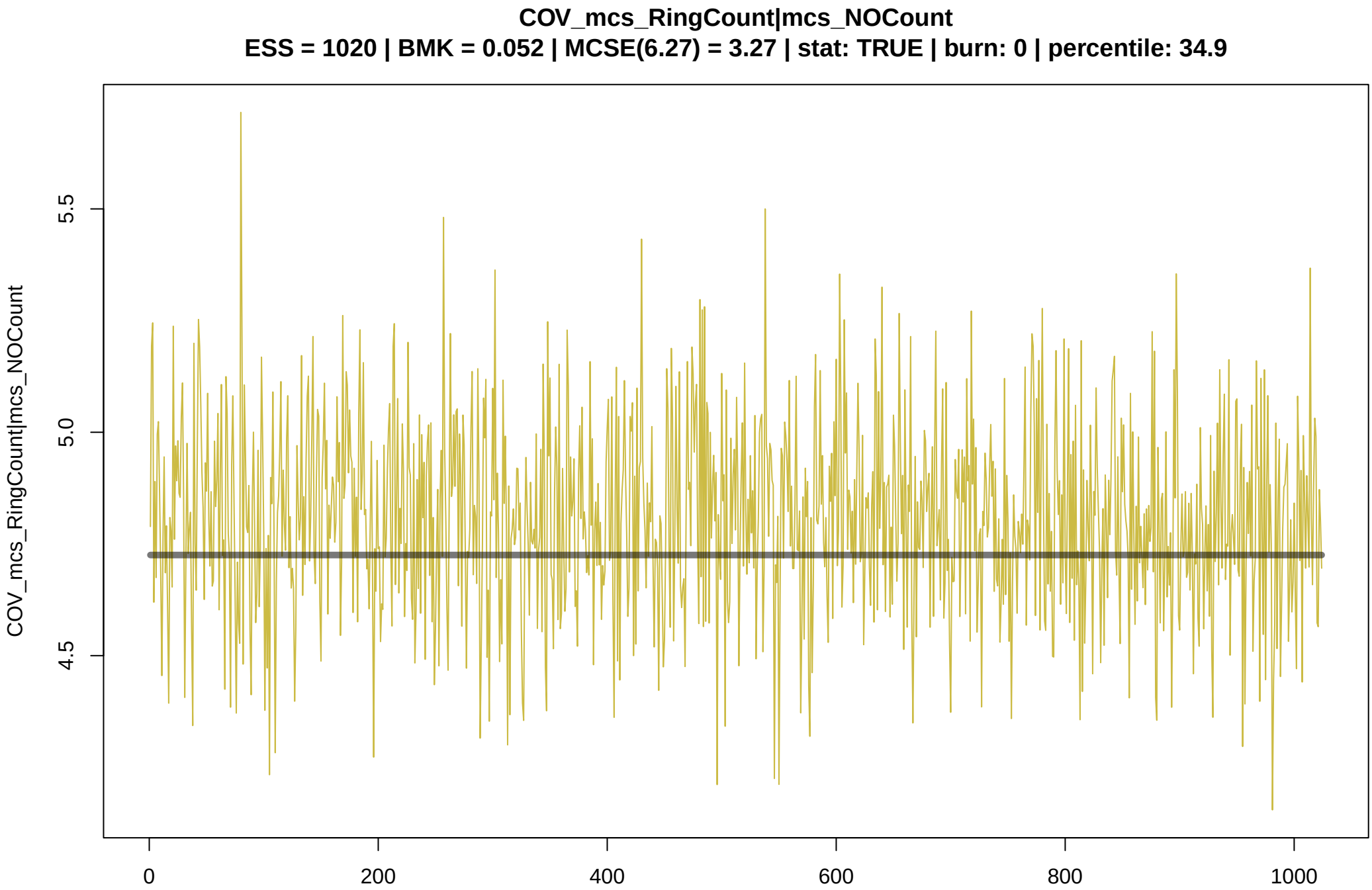

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.051 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | percentile: 28.5
COV_mcs_NumHeteroAtoms|mcs_NOCount
5.5
5.0
4.5
4.0
0
200
400
600
800
1000

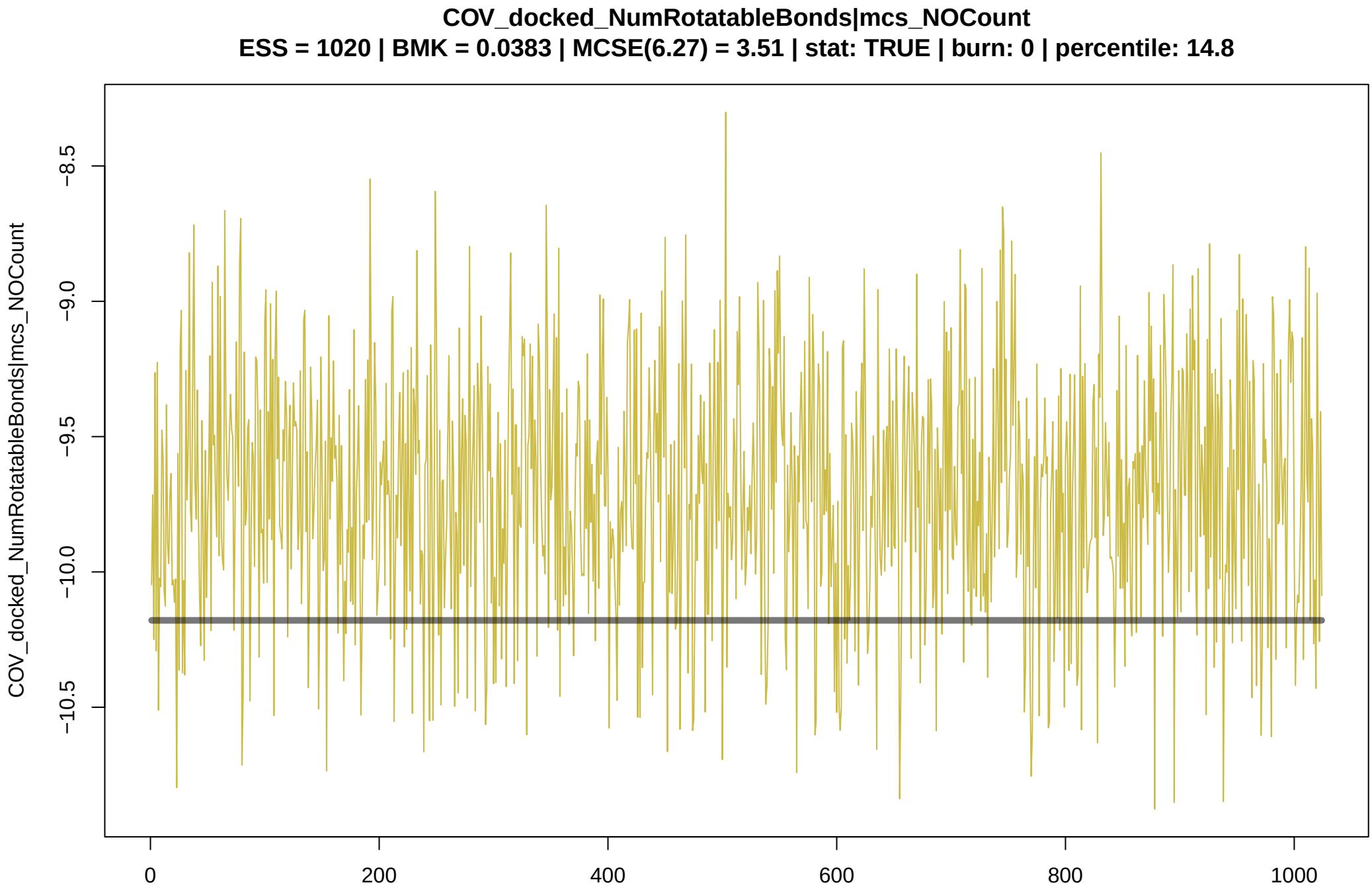

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 882 | BMK = 0.0748 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | percentile: 44.9
COV_docked_HeavyAtomCount|mcs_RingCount
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0319 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0 | percentile: 68.1
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 908 | BMK = 0.0616 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | percentile: 44.6
COV_docked_HeavyAtomCount|mcs_NOCount
−50
−52
−54
−56
−58
−60
0
200
400
600
800
1000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0587 | MCSE(6.27) = 3.73 | stat: TRUE | burn: 0 | percentile: 62.8
COV_mcs_RingCount|docked_NumRotatableBonds
−3.0
−3.2
−3.4
−3.6
−3.8
0
200
400
600
800
1000


COV_mcs_RingCount|mcs_NOCount
ESS = 1020 | BMK = 0.052 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0 | percentile: 34.9
COV_mcs_RingCount|mcs_NOCount
4.5
5.0
5.5
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0383 | MCSE(6.27) = 3.51 | stat: TRUE | burn: 0 | percentile: 14.8
COV_docked_NumRotatableBonds|mcs_NOCount
−8.5
−9.0
−9.5
−10.0
−10.5
0
200
400
600
800
1000