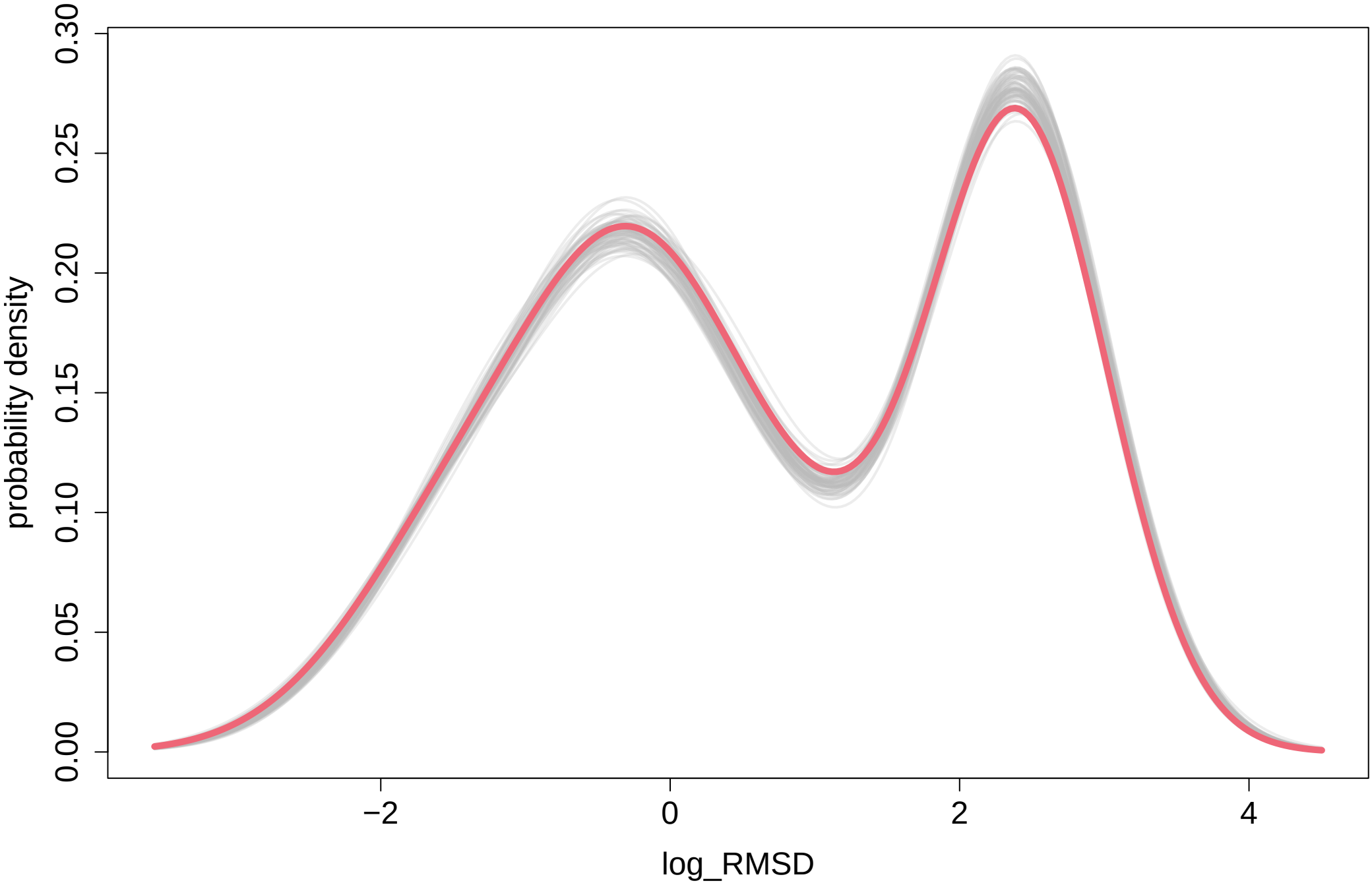
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.456760843173219
max MCSE = 12.7094225229421
all stationary: FALSE
burn: 0
min percent.: 4.19921875

−− STATS 2D −−
min ESS = 306.336949853142
max BMK = 0.139731292446706
max MCSE = 5.08600305005537
all stationary: FALSE
burn: 0
min percent.: 1.26953125

−− STATS 1D −−
min ESS = 50.9415838341615
max BMK = 1
max MCSE = 8.83373392551078
all stationary: FALSE
burn: 1020
min percent.: 0.09765625

Occupied clusters: 23 of 64
LL: −62400 +− 8.81


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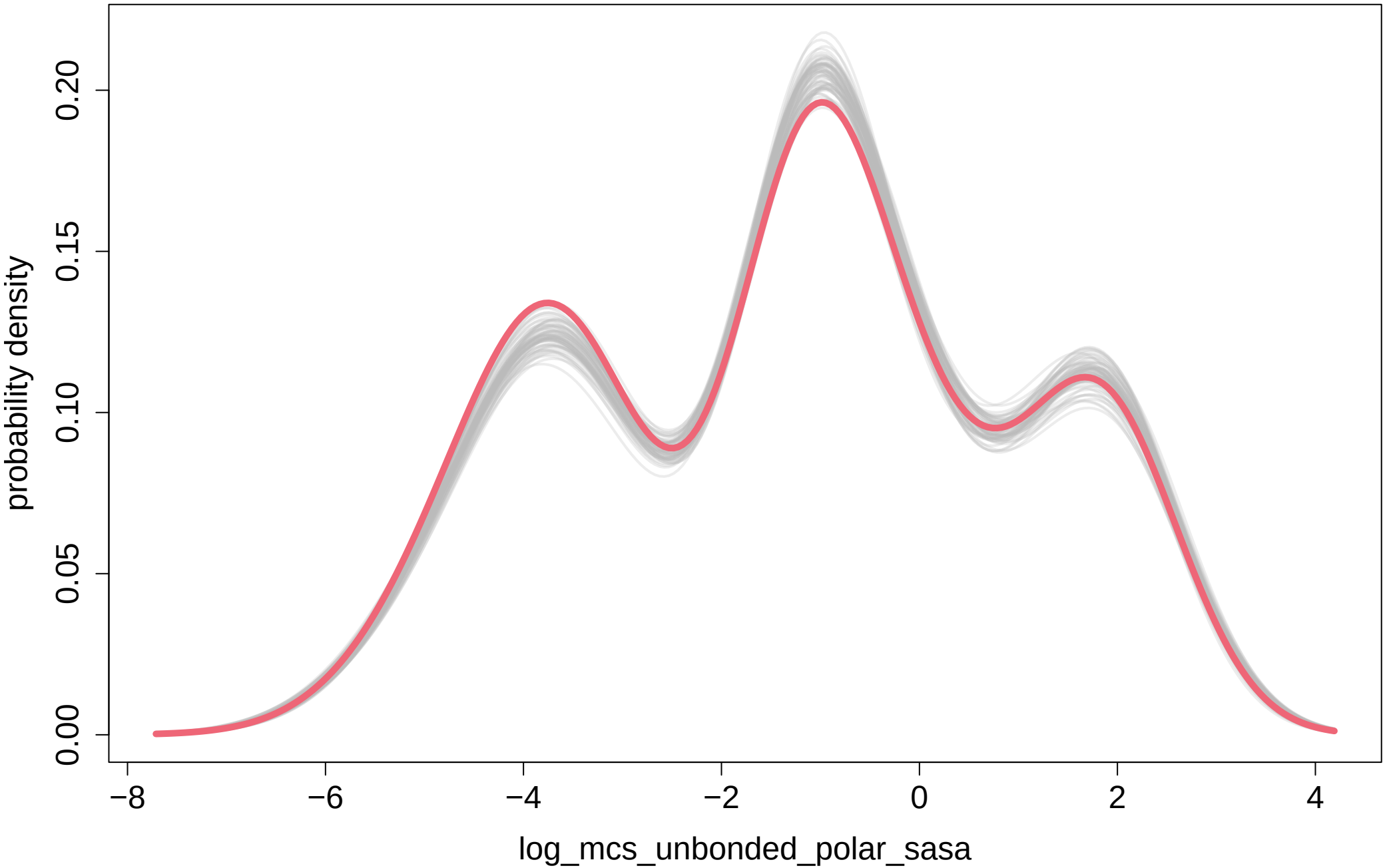
0.10
0.15
0.20
0.25
0.30
−2
0
2
4
log_RMSD


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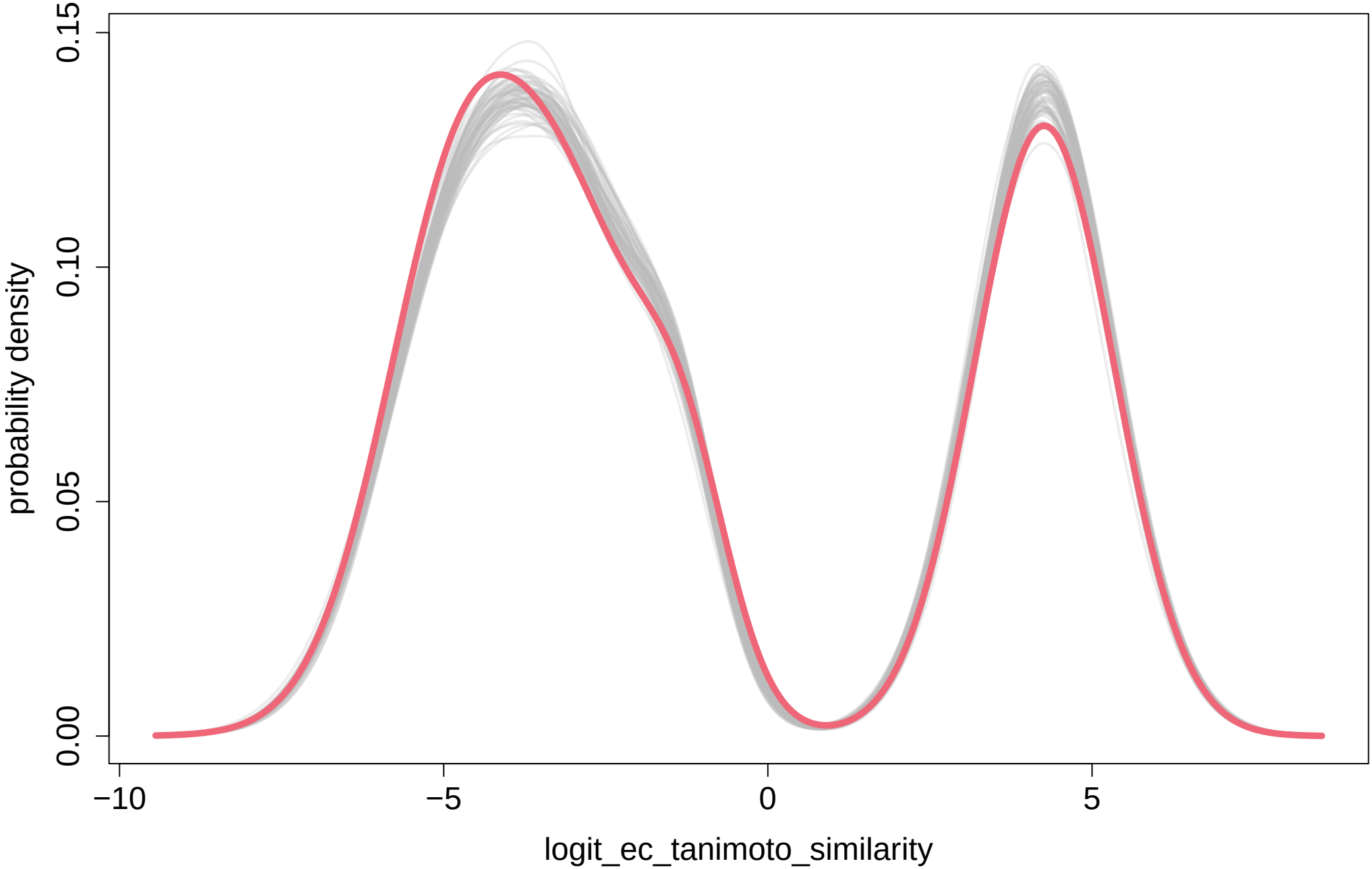
0.20
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa


probability density
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0.15
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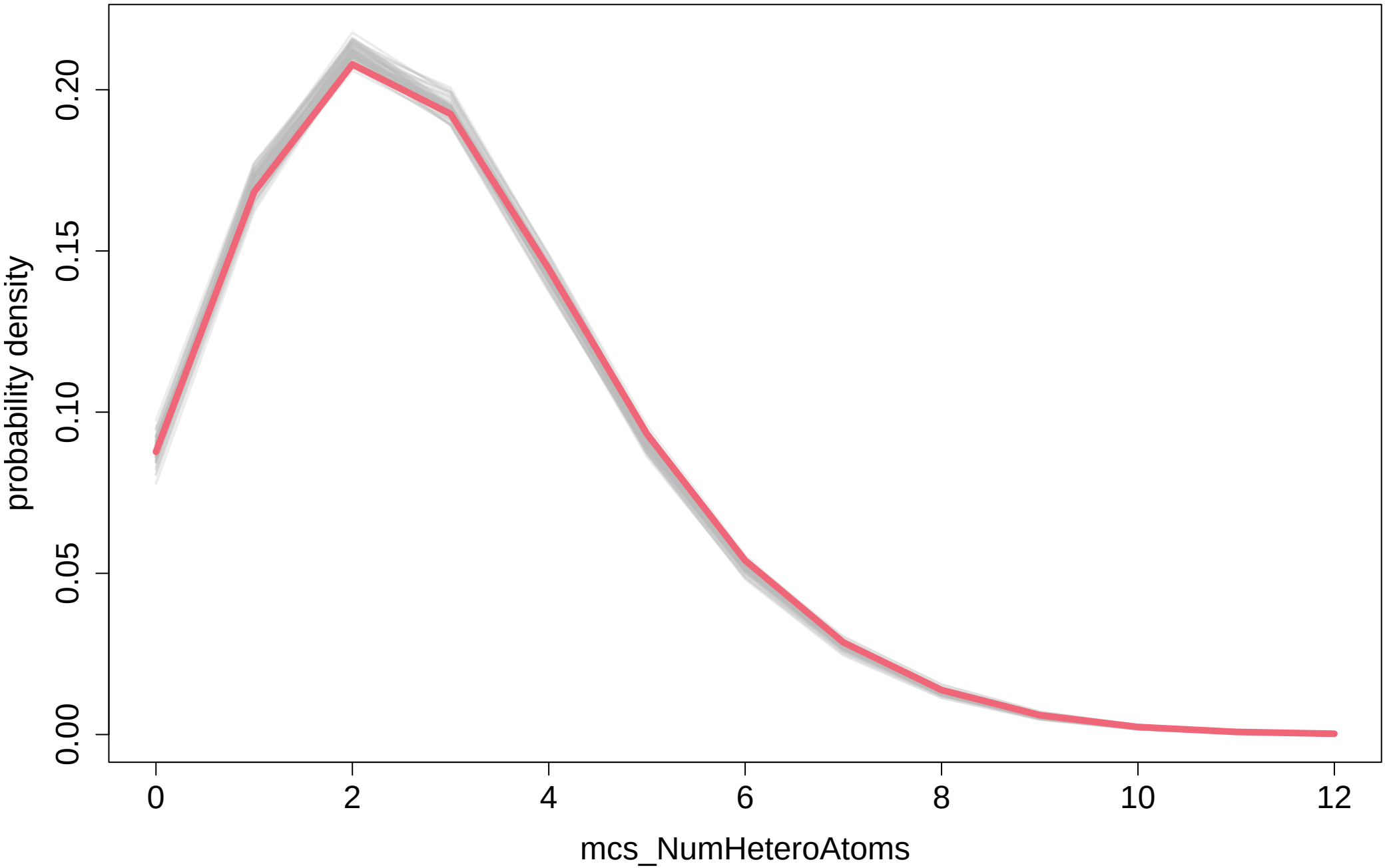
−5
0
5
logit_ec_tanimoto_similarity


probability density
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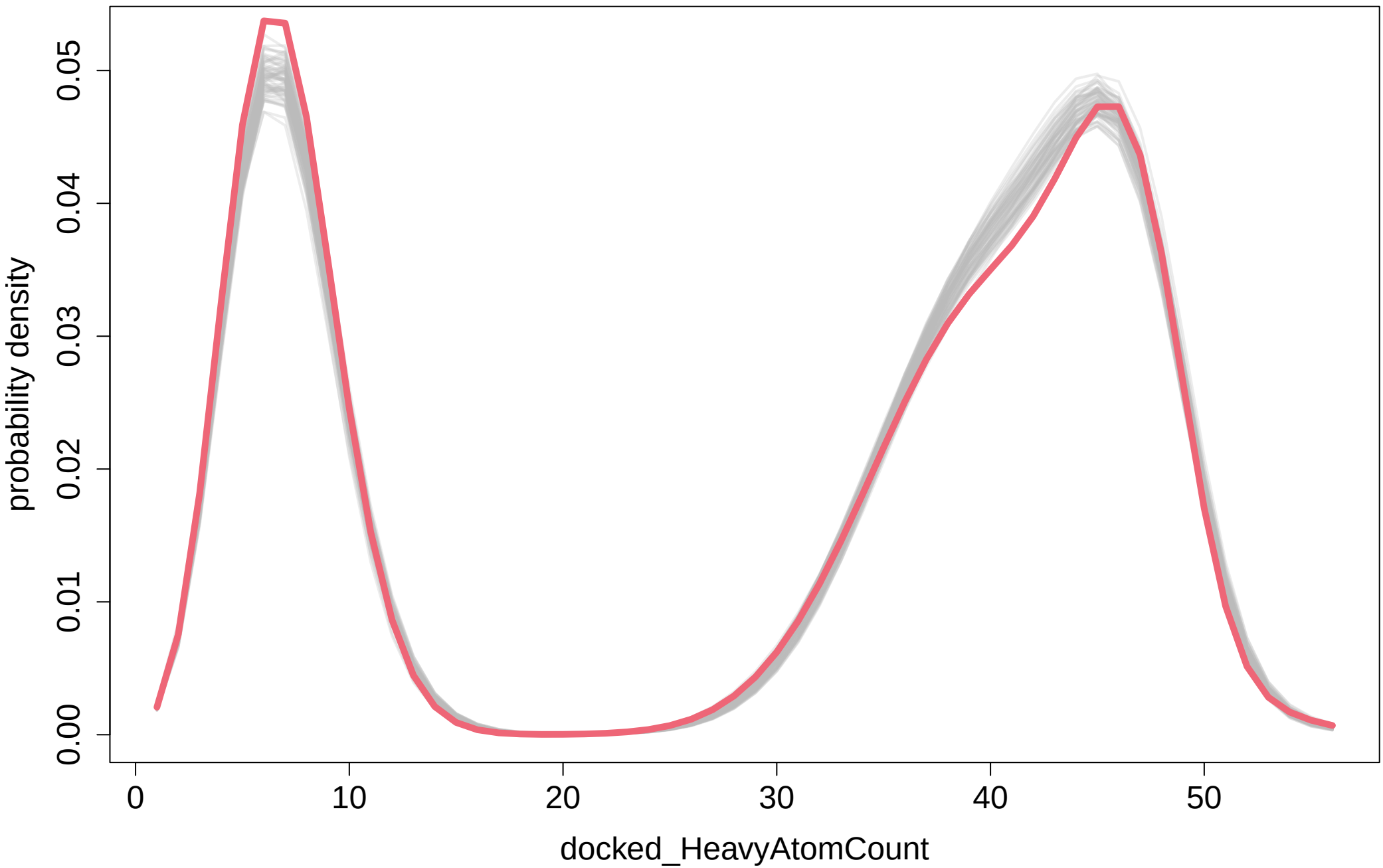
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms


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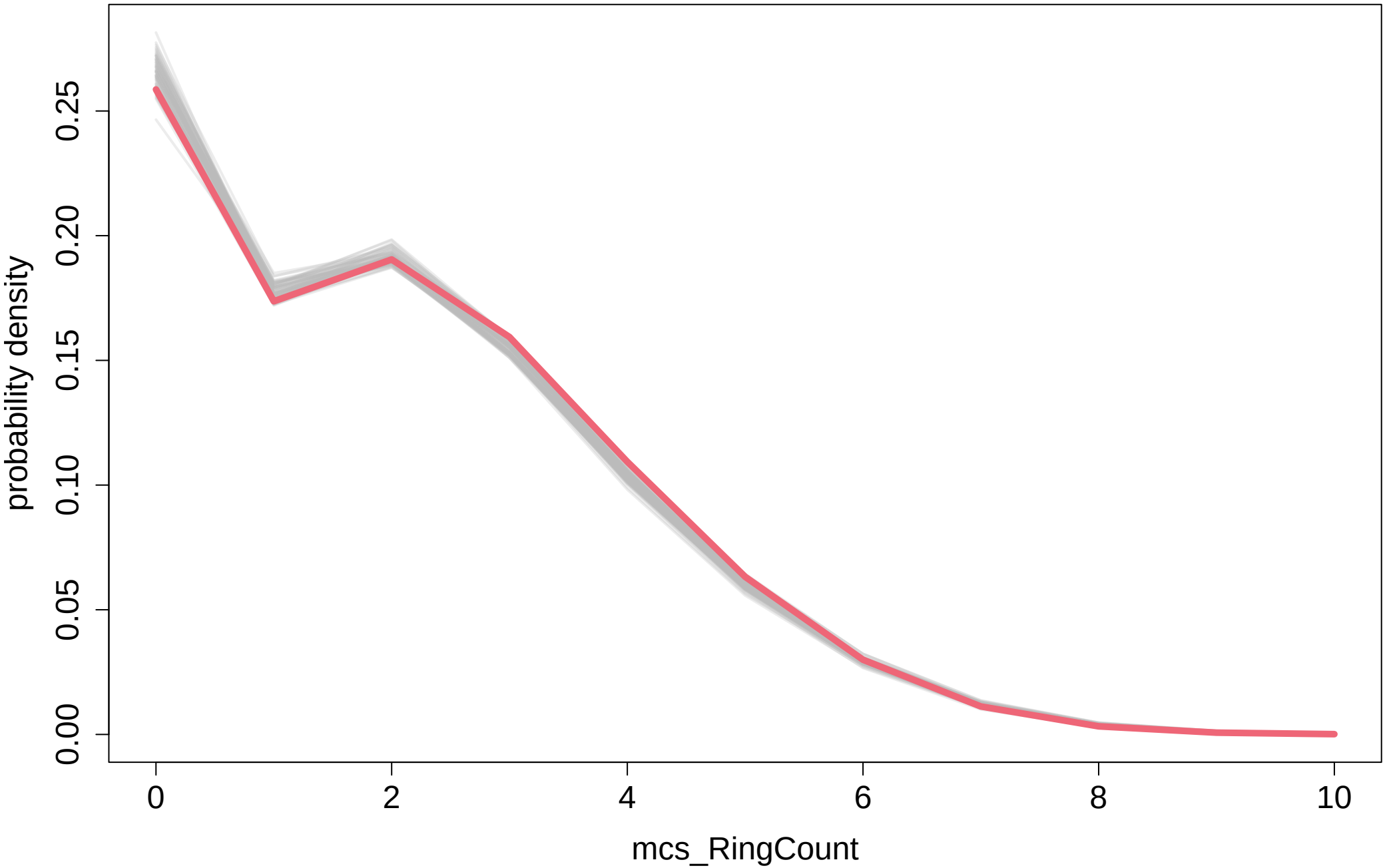
0.04
0.05
0
10
20
30
40
50
docked_HeavyAtomCount


probability density
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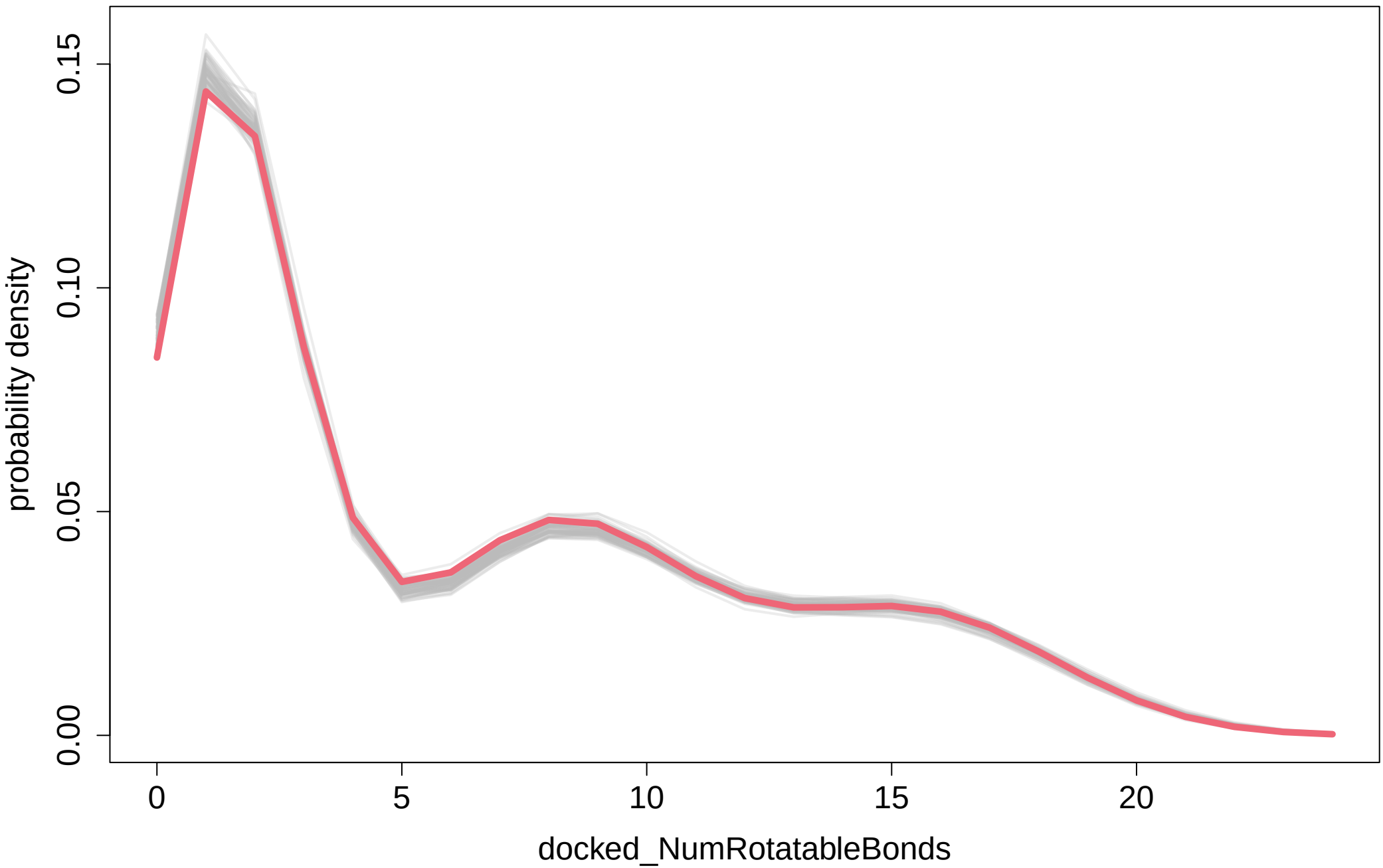
0
2
4
6
8
10
mcs_RingCount


probability density
0.00
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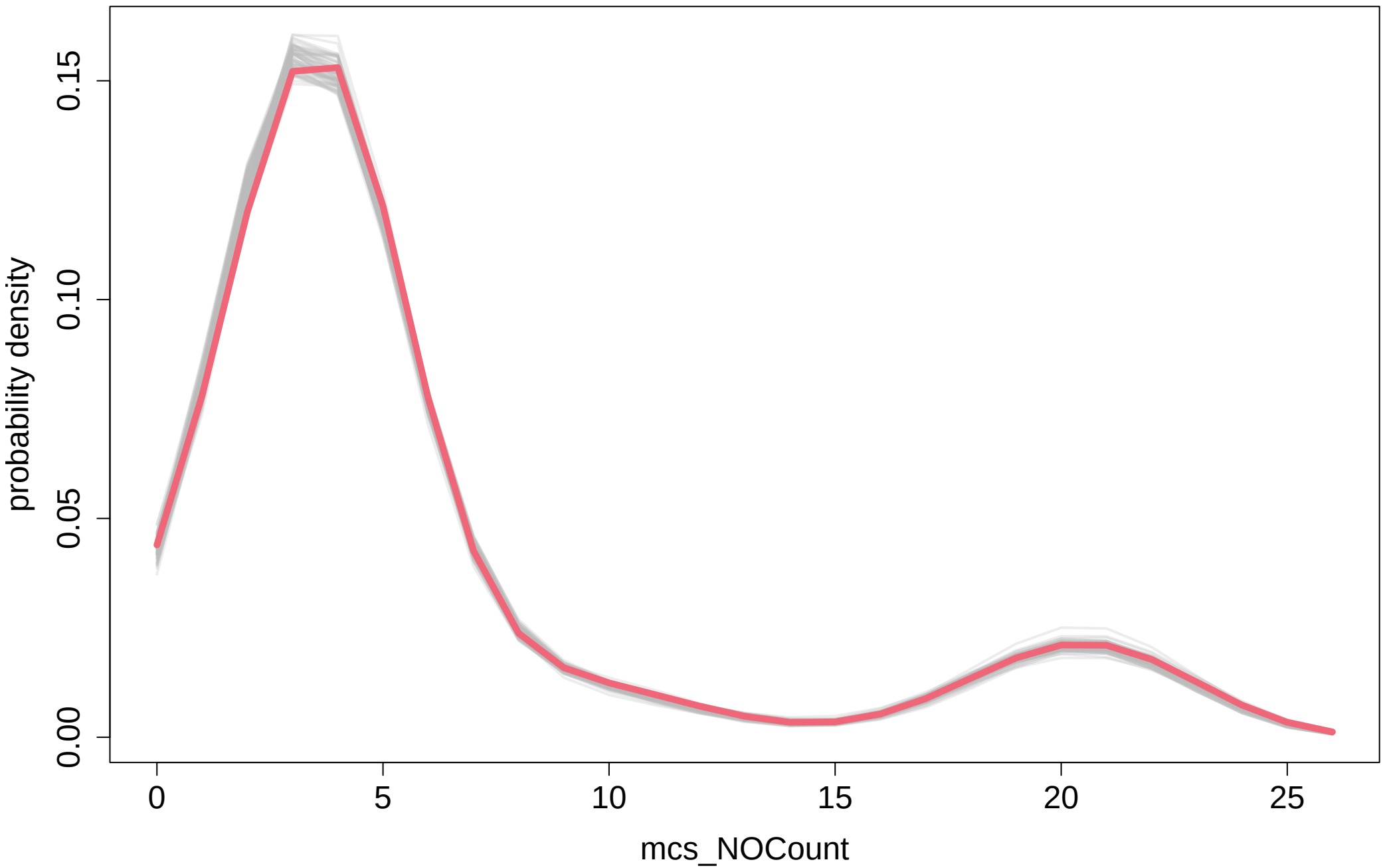
0
5
10
15
20
docked_NumRotatableBonds


probability density
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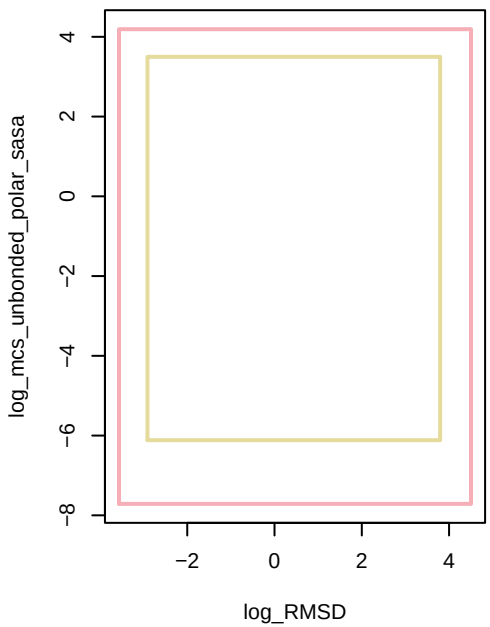
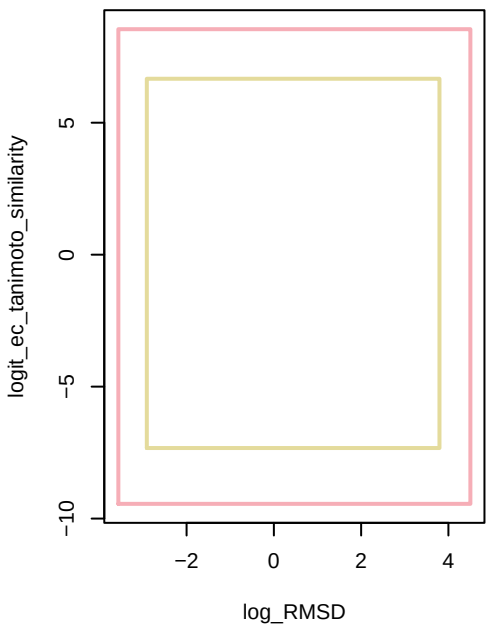
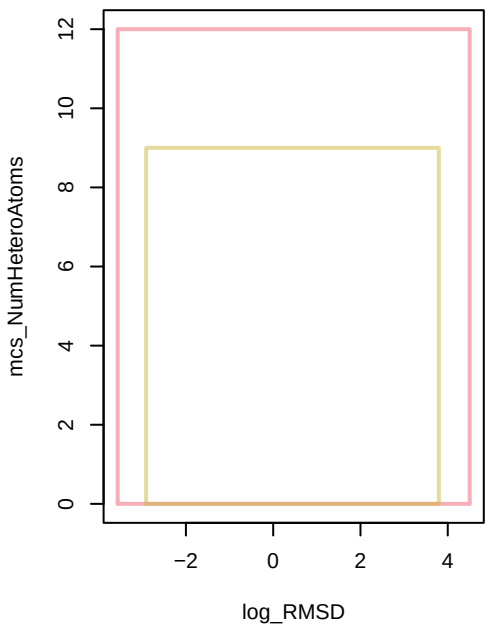
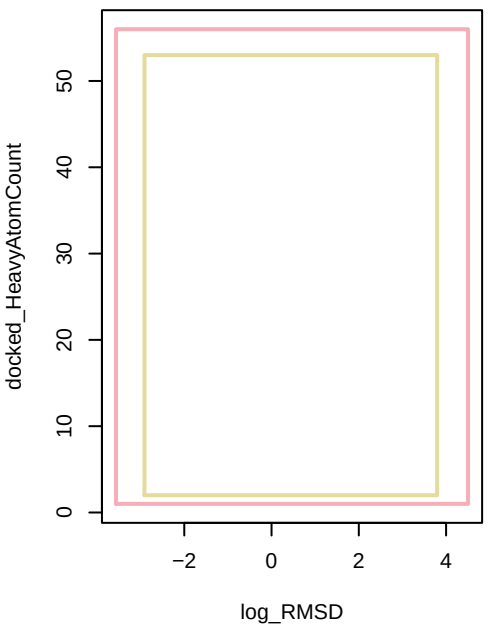
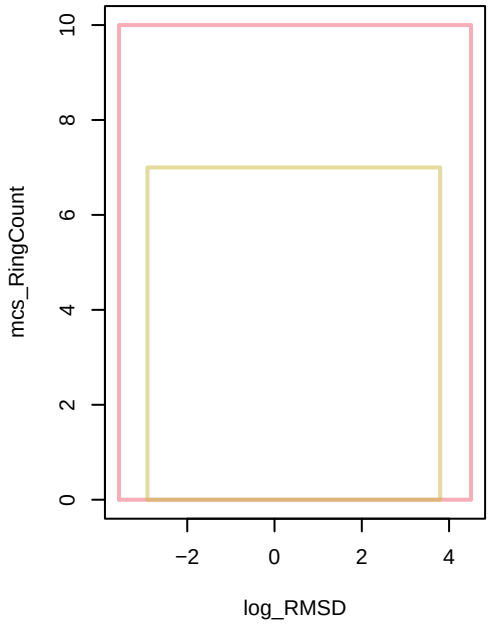
0.15
0
5
10
15
20
25
mcs_NOCount

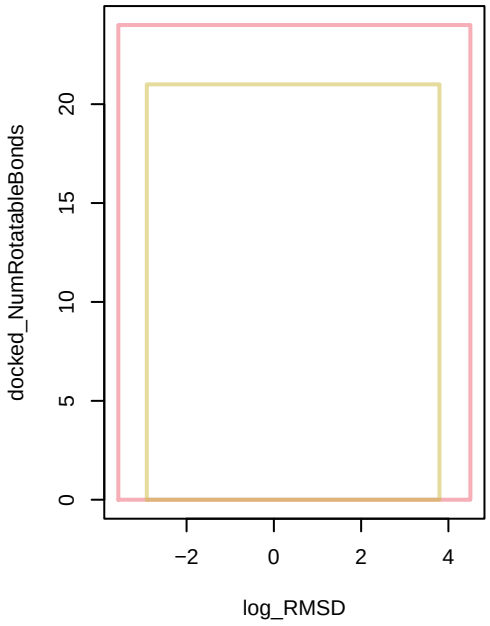

log_mcs_unbonded_polar_sasa
log_RMSD

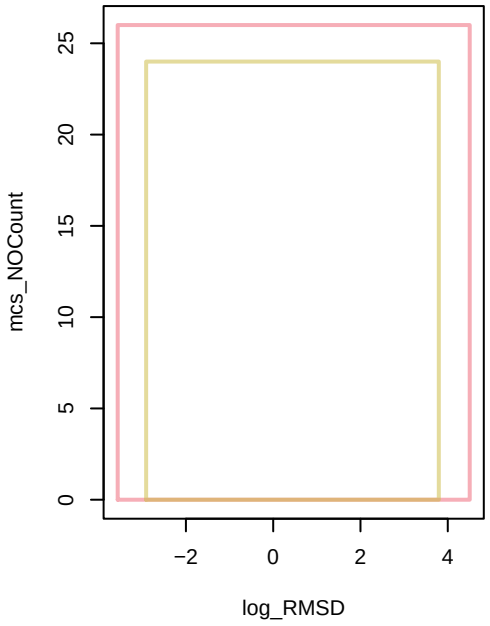

logit_ec_tanimoto_similarity
log_RMSD

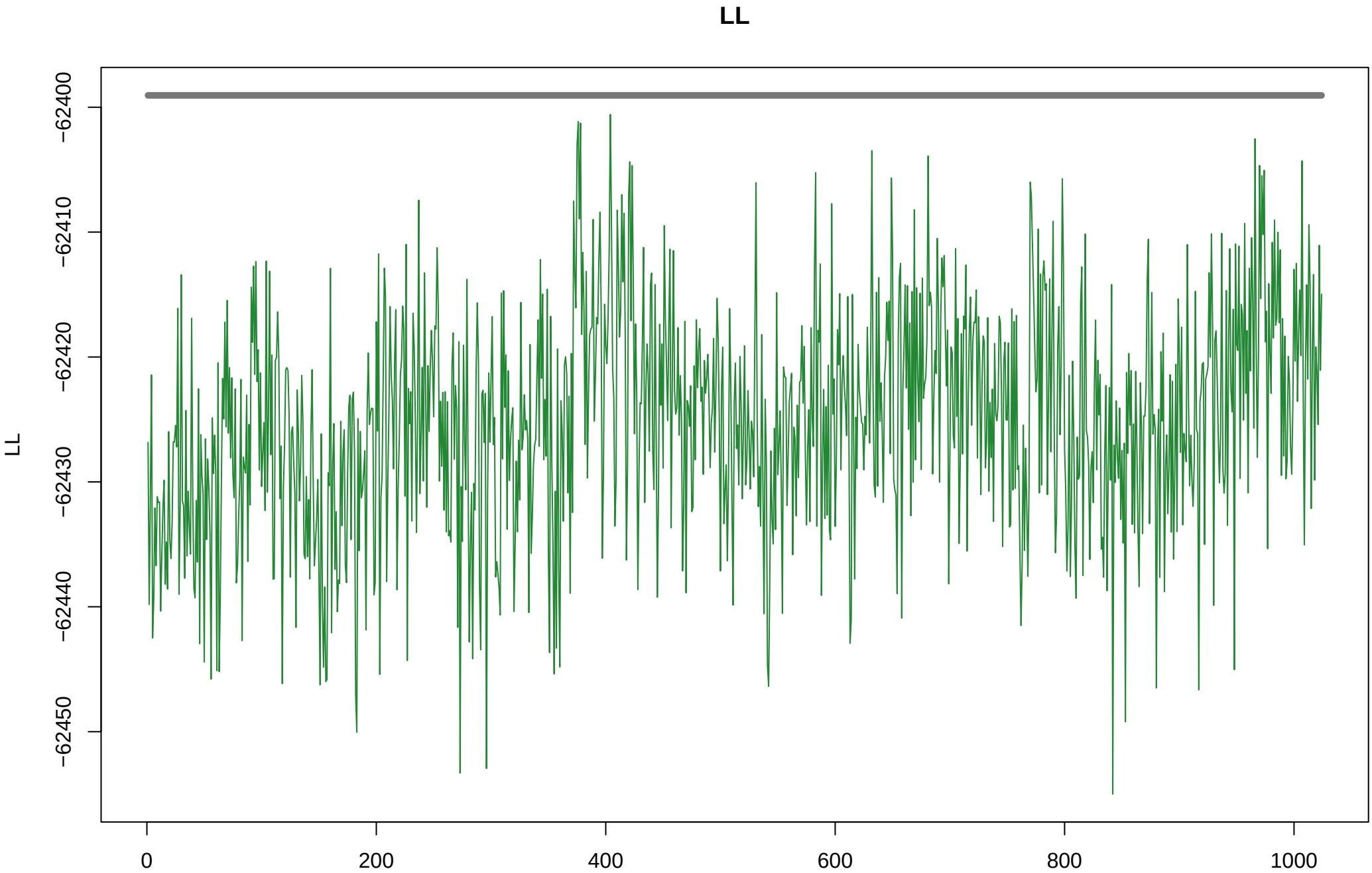

mcs_NumHeteroAtoms
log_RMSD

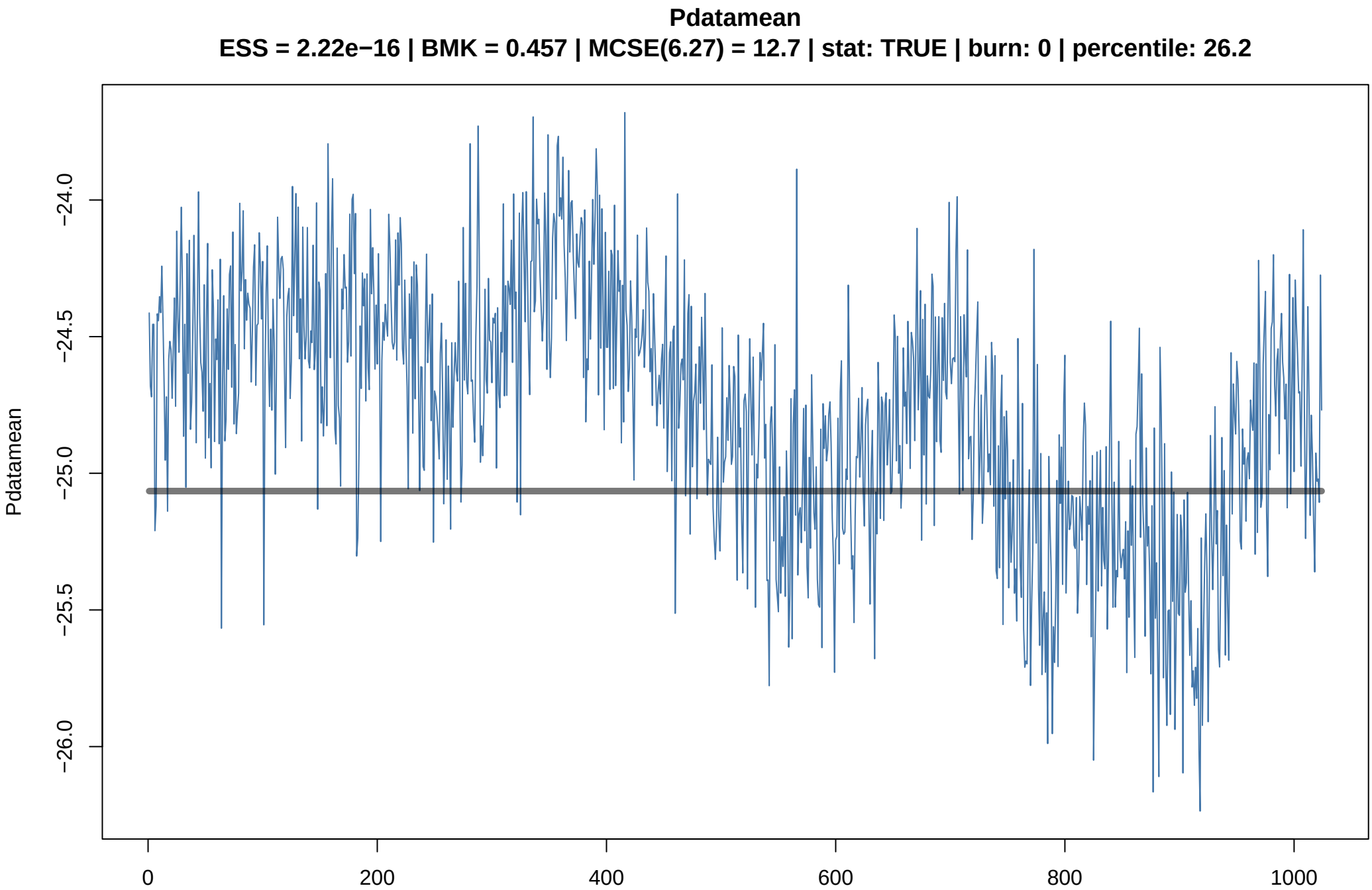

docked_HeavyAtomCount
log_RMSD

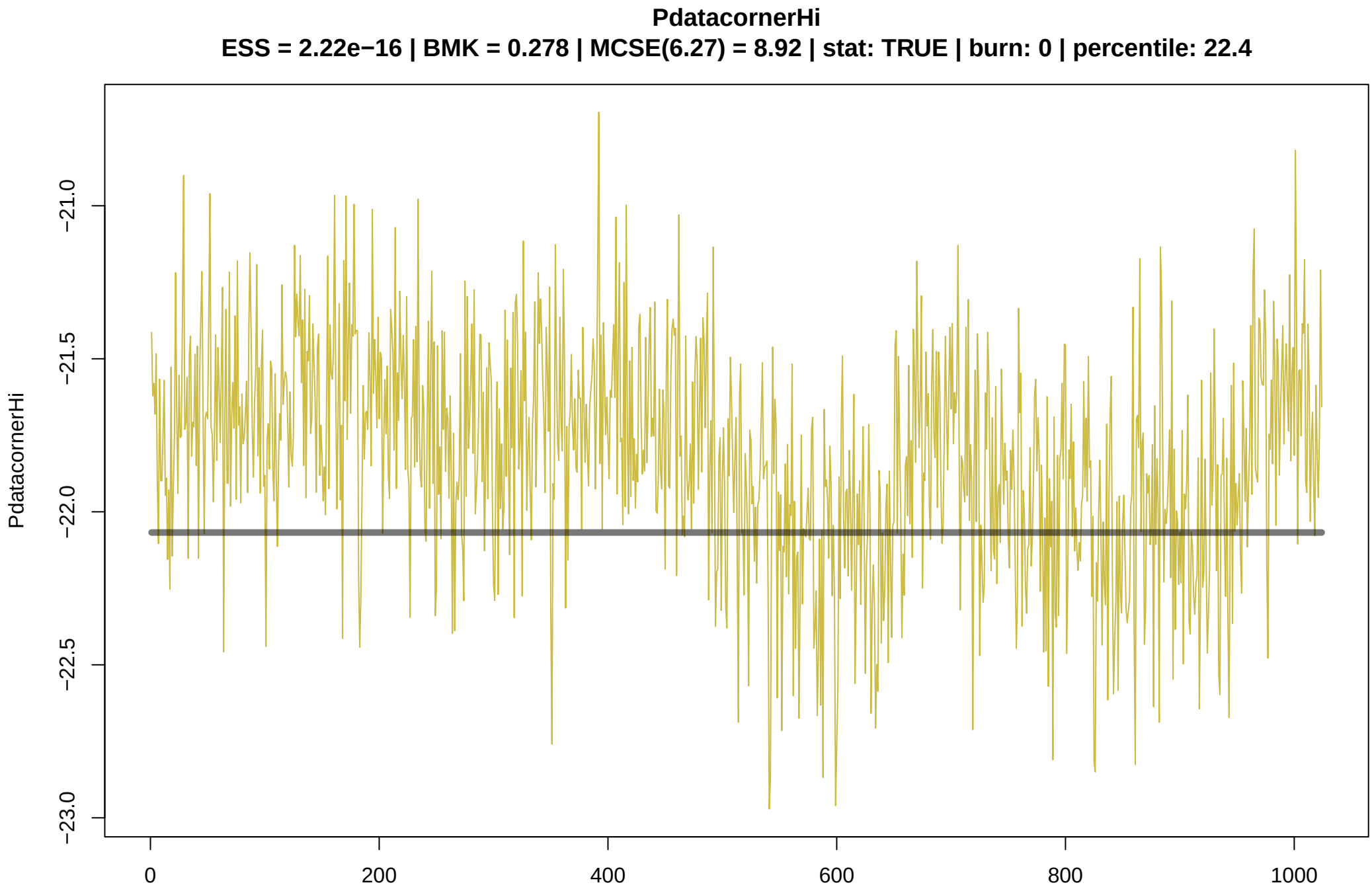

mcs_RingCount
log_RMSD

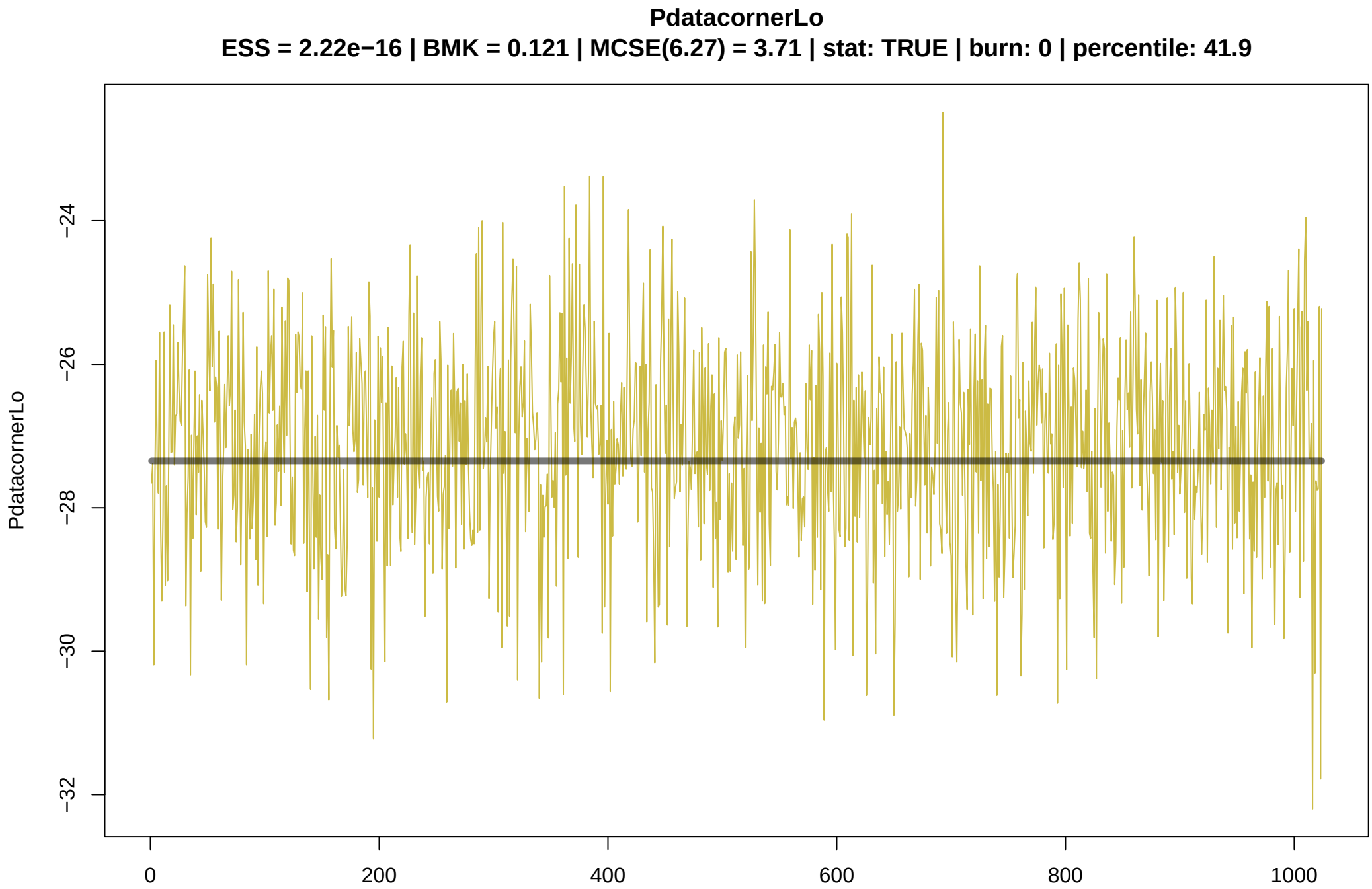

docked_NumRotatableBonds
log_RMSD

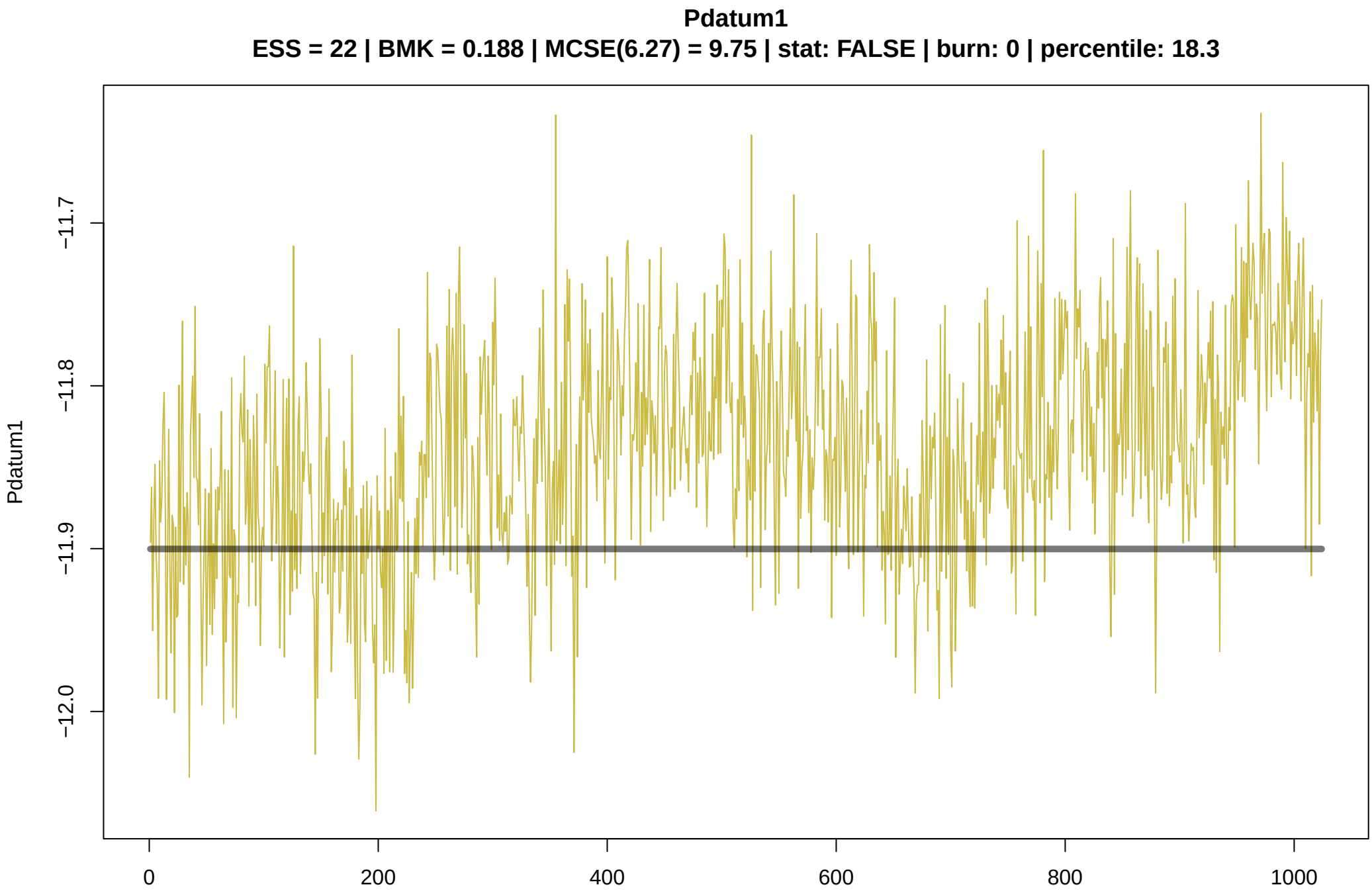

mcs_NOCount
log_RMSD

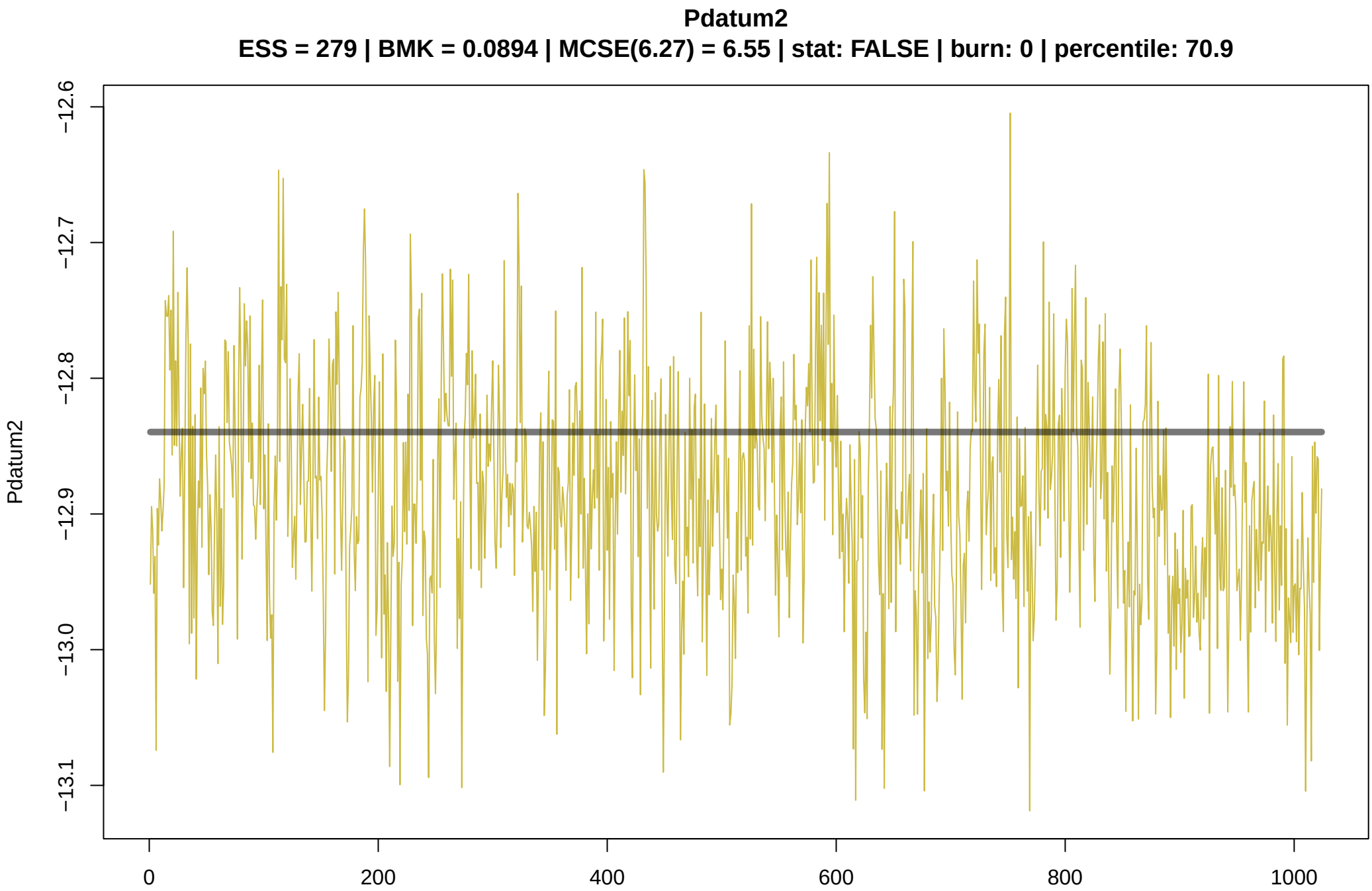

LL
LL
−62400
−62410
−62420
−62430
−62440
−62450
0
200
400
600
800
1000

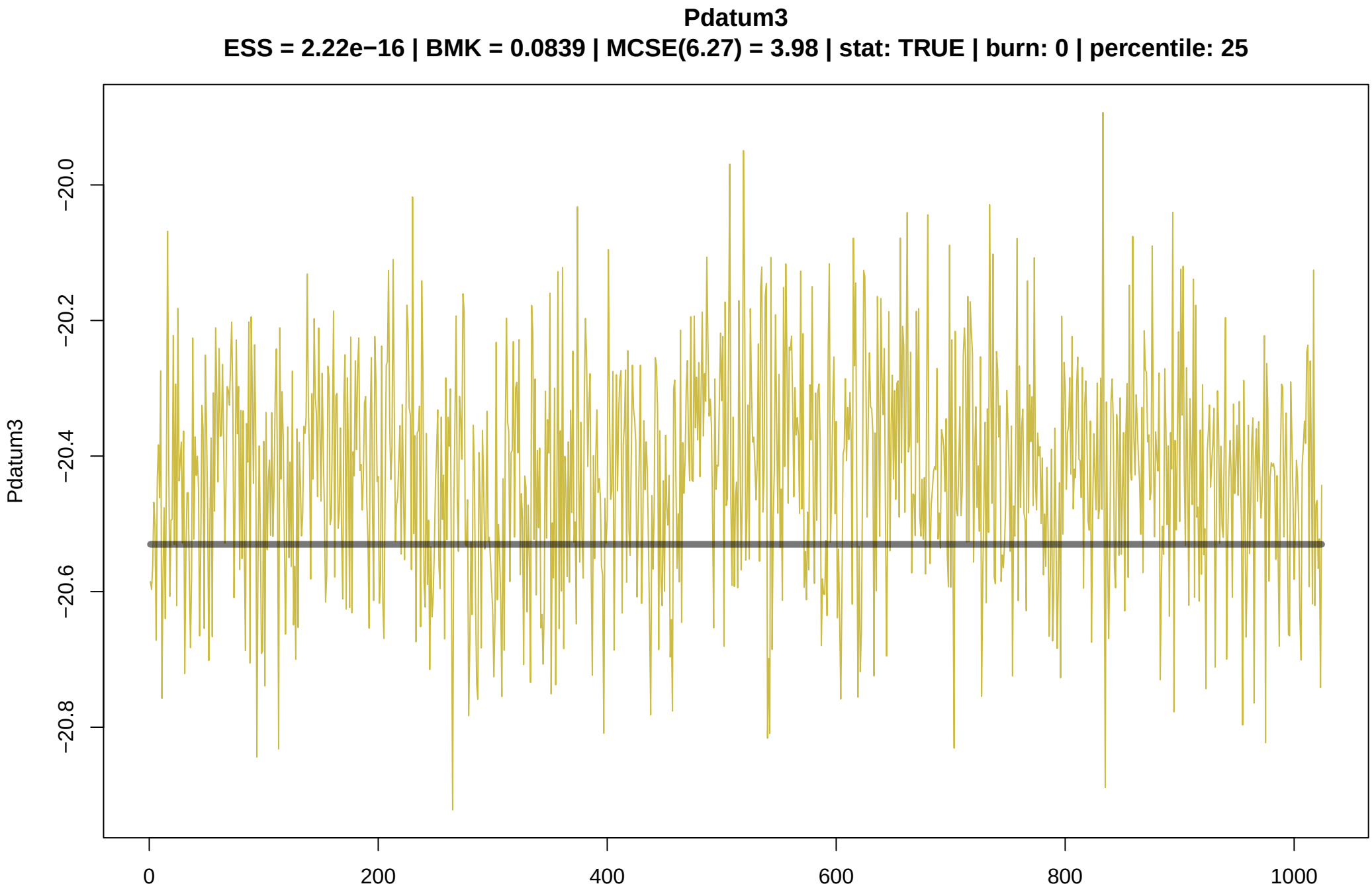

Pdatamean
ESS = 2.22e−16 | BMK = 0.457 | MCSE(6.27) = 12.7 | stat: TRUE | burn: 0 | percentile: 26.2
Pdatamean
−24.0
−24.5
−25.0
−25.5
−26.0
0
200
400
600
800
1000

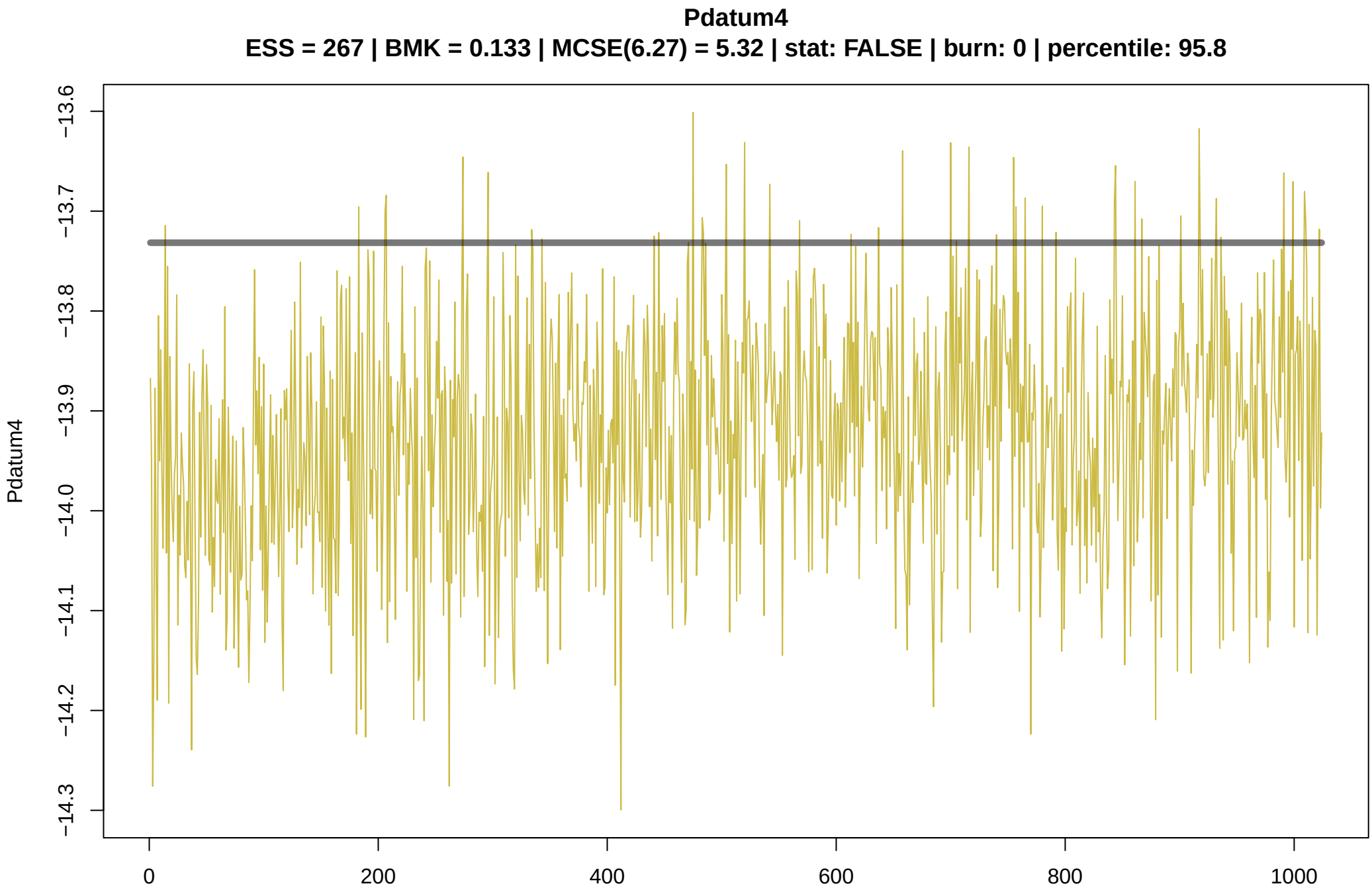

PdatacornerHi
ESS = 2.22e−16 | BMK = 0.278 | MCSE(6.27) = 8.92 | stat: TRUE | burn: 0 | percentile: 22.4
PdatacornerHi
−21.0
−21.5
−22.0
−22.5
−23.0
0
200
400
600
800
1000

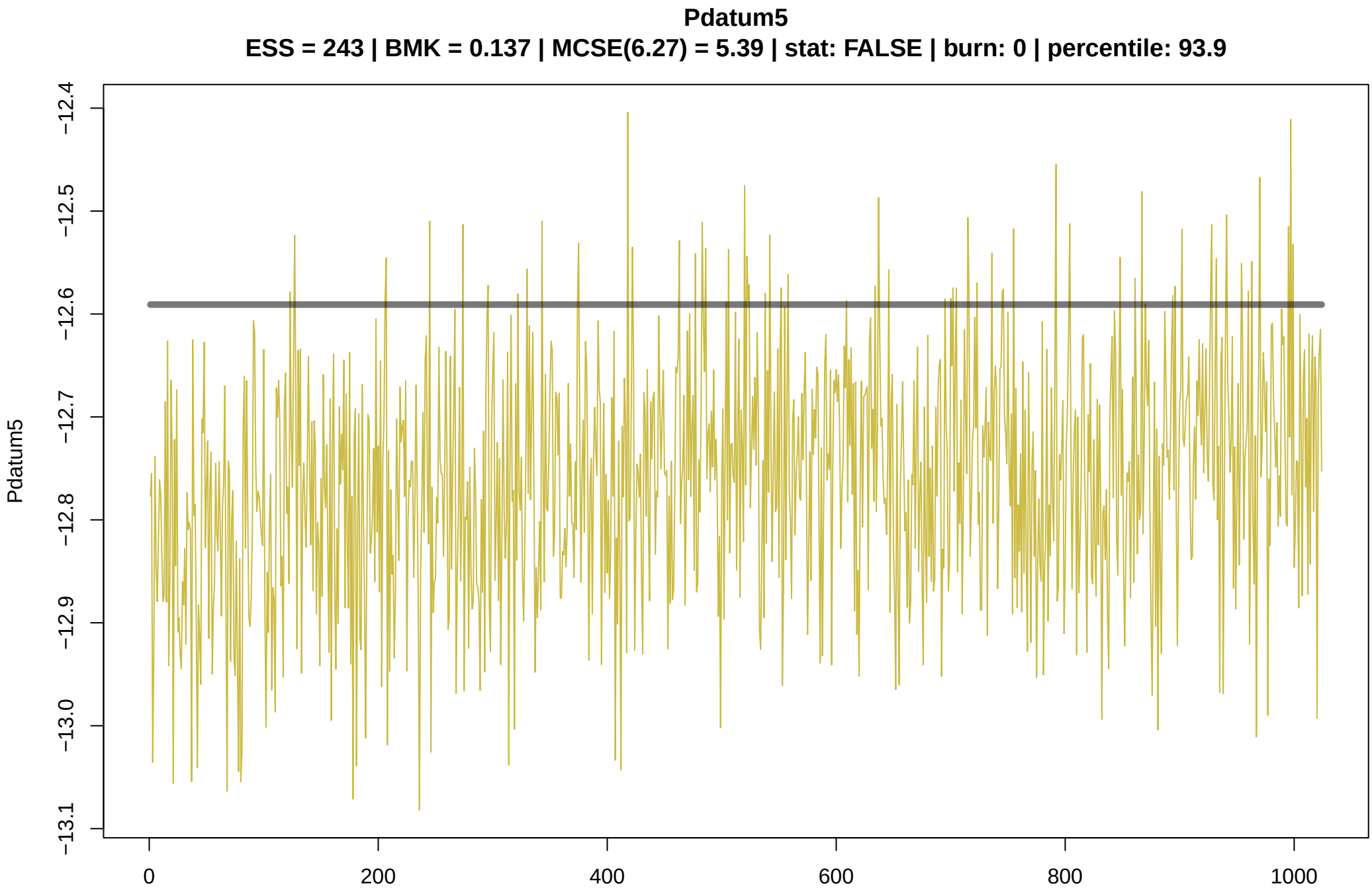

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.121 | MCSE(6.27) = 3.71 | stat: TRUE | burn: 0 | percentile: 41.9
PdatacornerLo
−24
−26
−28
−30
−32
0
200
400
600
800
1000

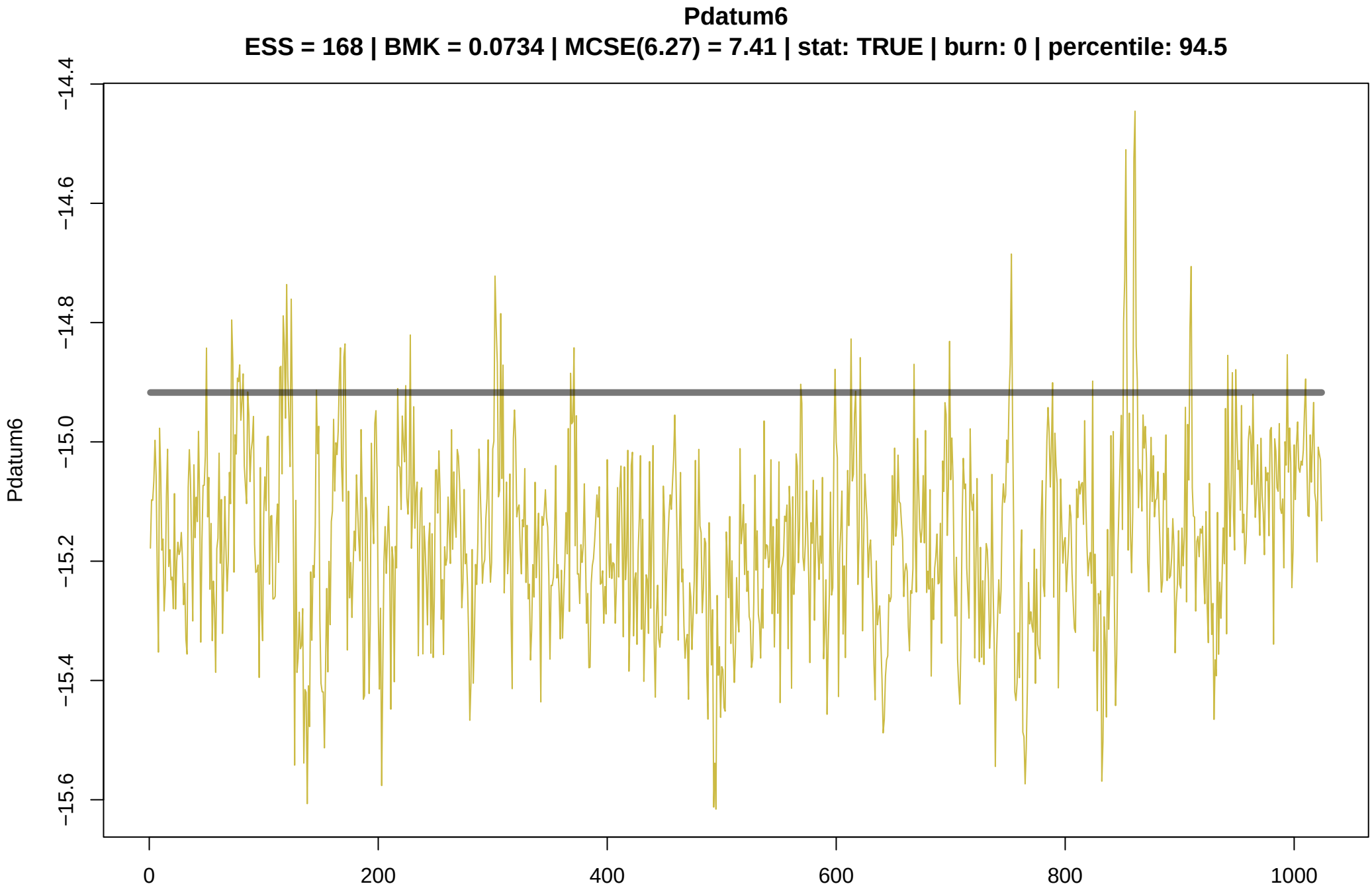

Pdatum1
ESS = 22 | BMK = 0.188 | MCSE(6.27) = 9.75 | stat: FALSE | burn: 0 | percentile: 18.3
Pdatum1
−11.7
−11.8
−11.9
−12.0
0
200
400
600
800
1000

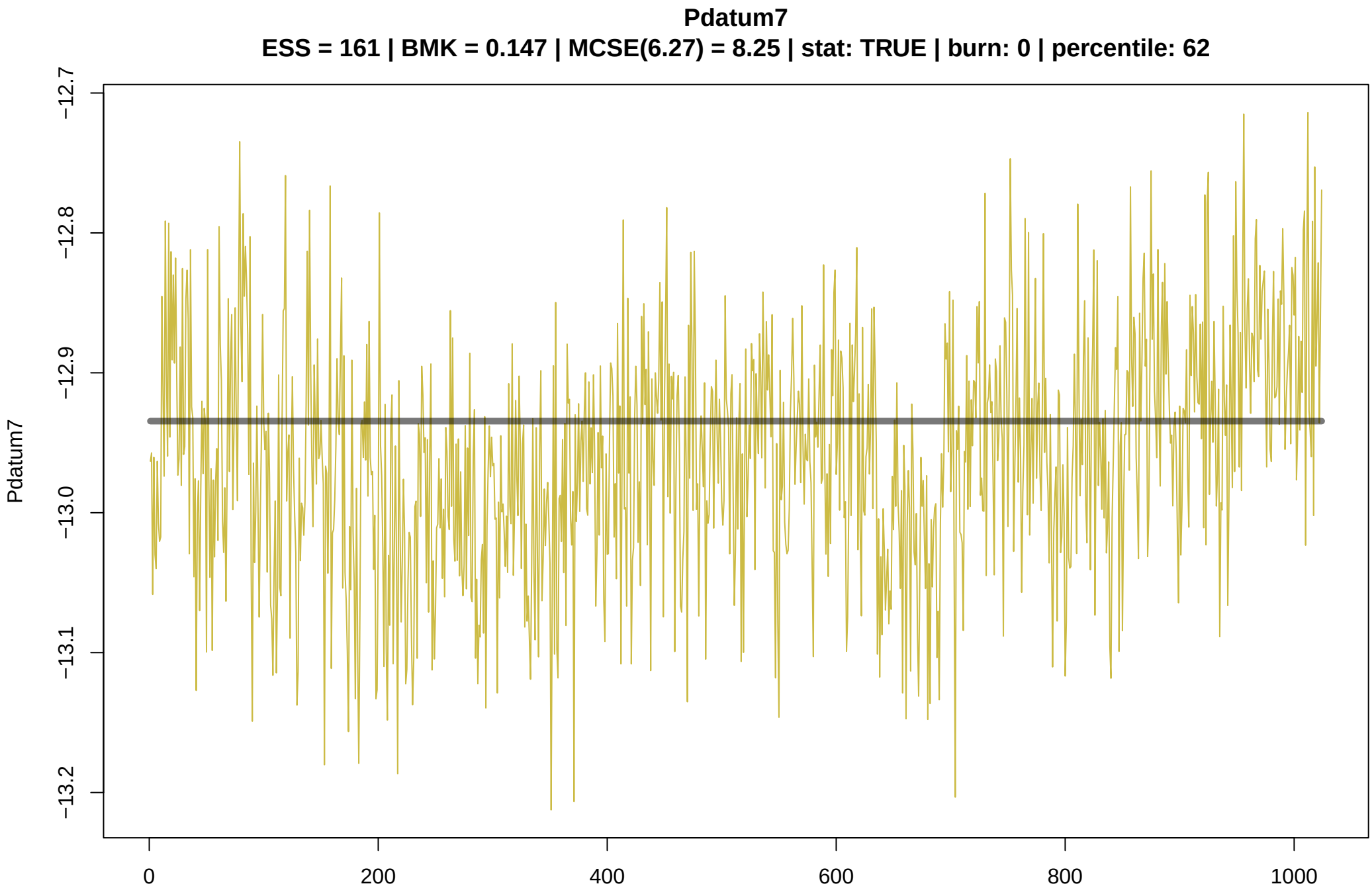

Pdatum2
ESS = 279 | BMK = 0.0894 | MCSE(6.27) = 6.55 | stat: FALSE | burn: 0 | percentile: 70.9
Pdatum2
−12.6
−12.7
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

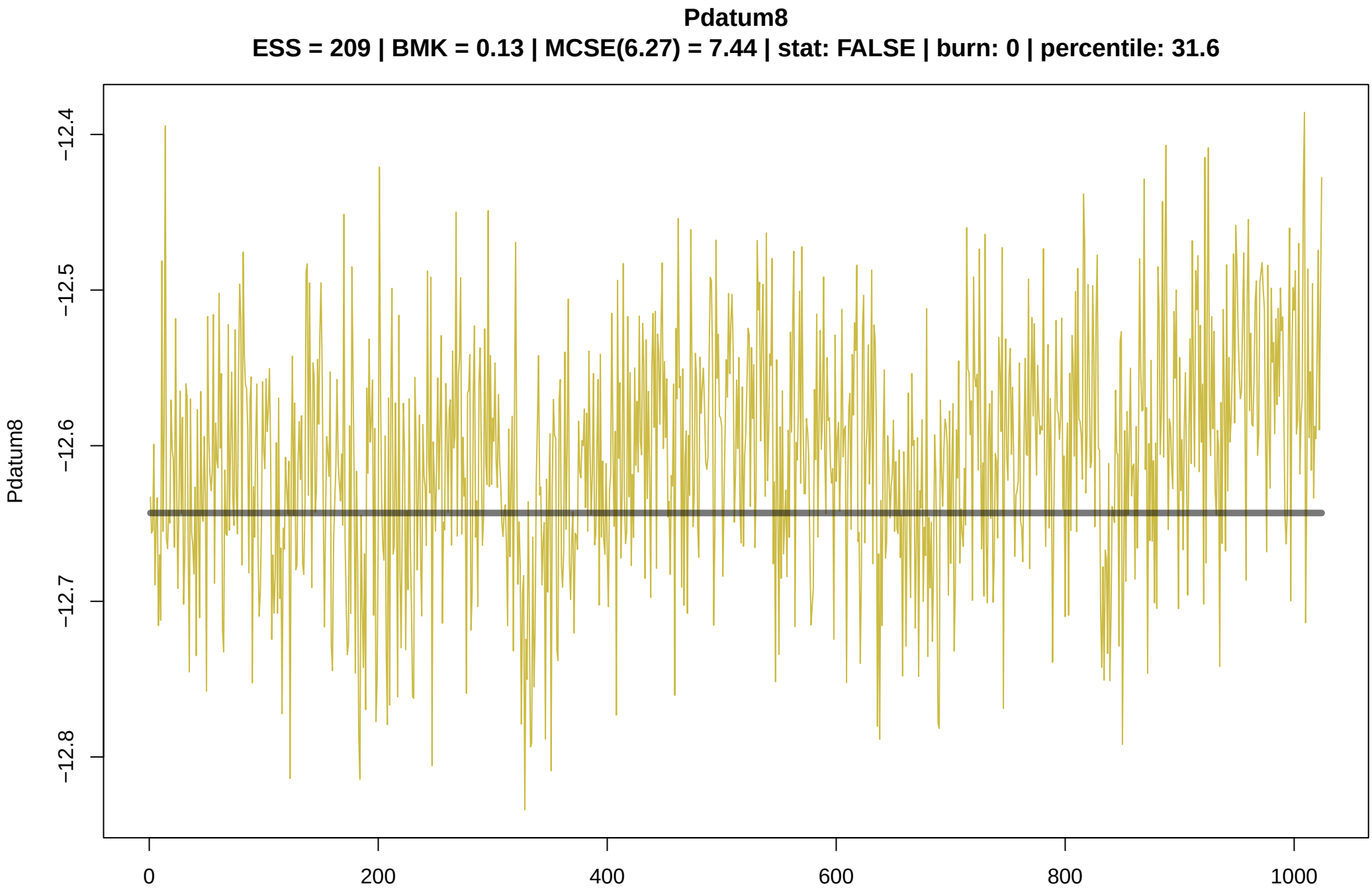

Pdatum3
ESS = 2.22e−16 | BMK = 0.0839 | MCSE(6.27) = 3.98 | stat: TRUE | burn: 0 | percentile: 25
Pdatum3
−20.0
−20.2
−20.4
−20.6
−20.8
0
200
400
600
800
1000

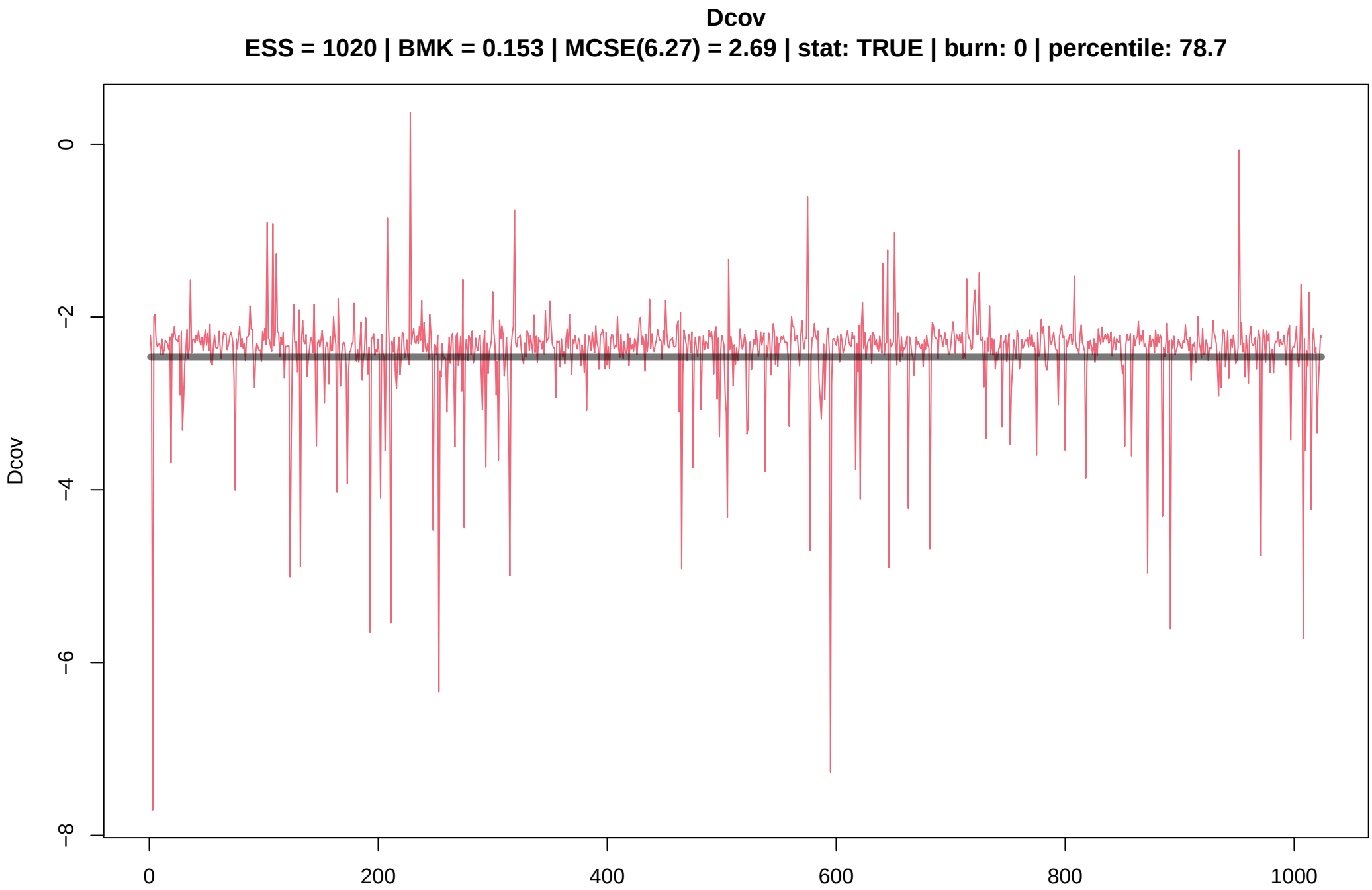

Pdatum4
ESS = 267 | BMK = 0.133 | MCSE(6.27) = 5.32 | stat: FALSE | burn: 0 | percentile: 95.8
Pdatum4
−13.6
−13.7
−13.8
−13.9
−14.0
−14.1
−14.2
−14.3
0
200
400
600
800
1000

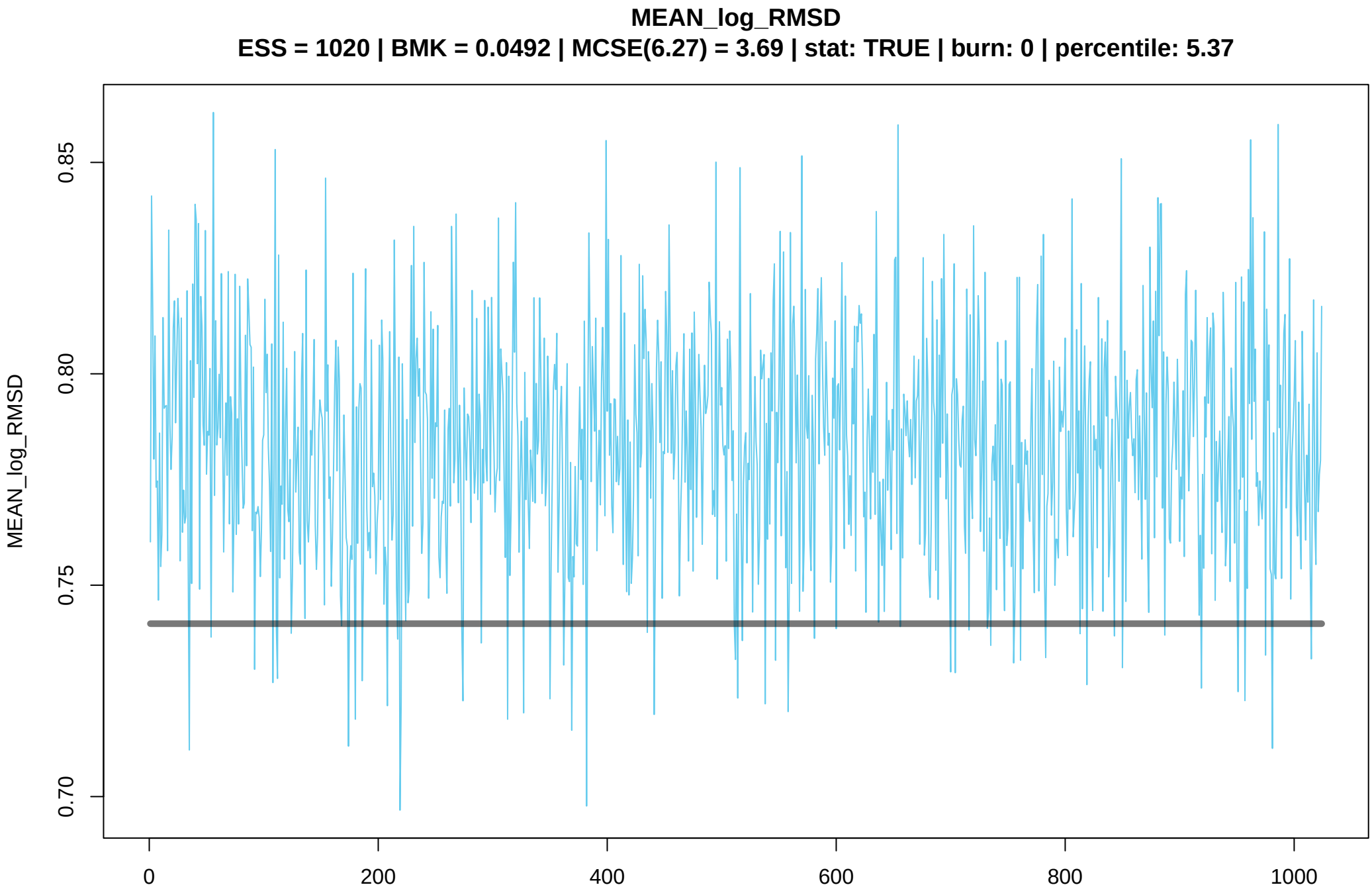

Pdatum5
ESS = 243 | BMK = 0.137 | MCSE(6.27) = 5.39 | stat: FALSE | burn: 0 | percentile: 93.9
Pdatum5
−12.4
−12.5
−12.6
−12.7
−12.8
−12.9
−13.0
−13.1
0
200
400
600
800
1000

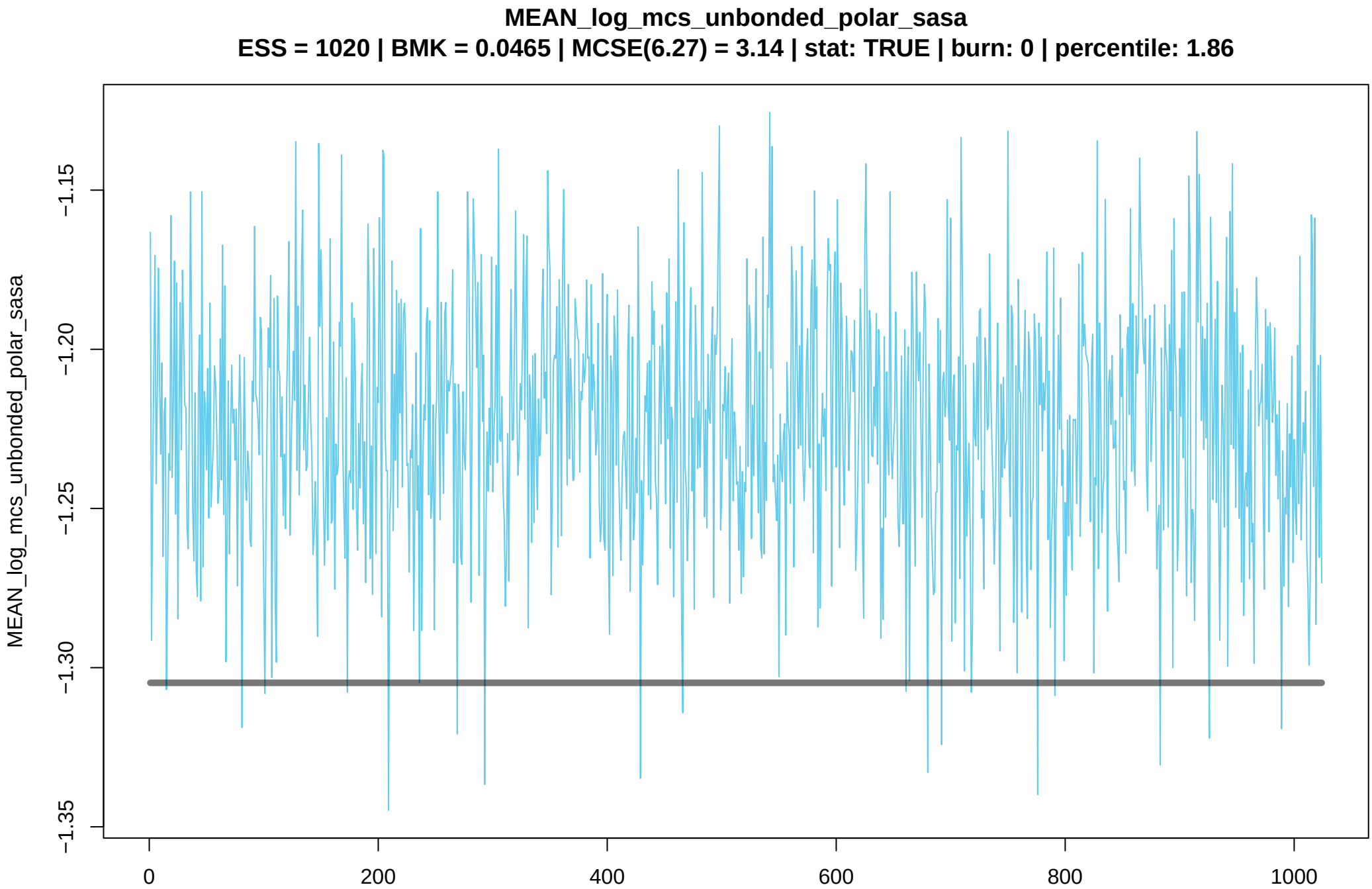

Pdatum6
ESS = 168 | BMK = 0.0734 | MCSE(6.27) = 7.41 | stat: TRUE | burn: 0 | percentile: 94.5
Pdatum6
−14.4
−14.6
−14.8
−15.0
−15.2
−15.4
−15.6
0
200
400
600
800
1000

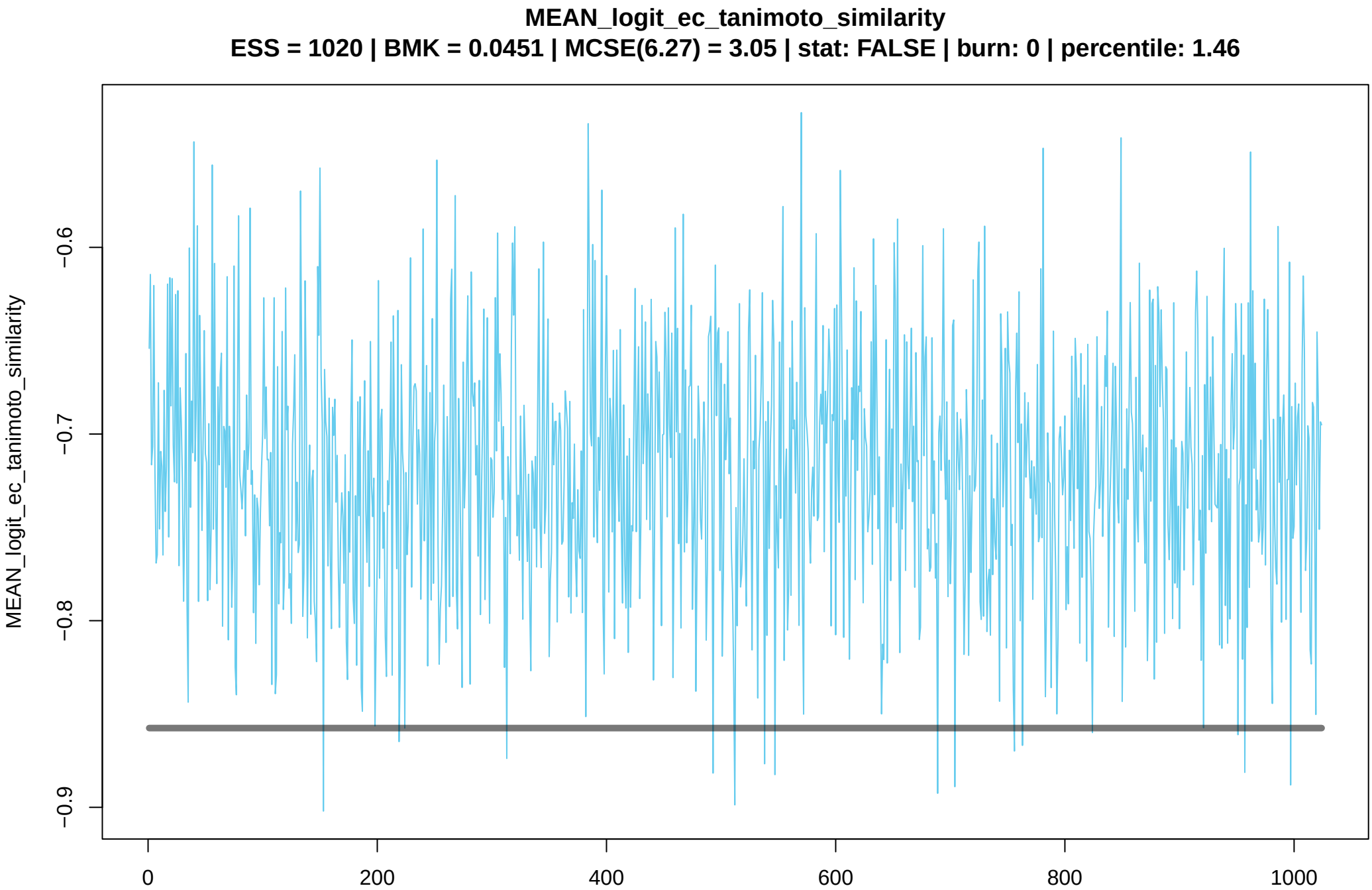

Pdatum7
ESS = 161 | BMK = 0.147 | MCSE(6.27) = 8.25 | stat: TRUE | burn: 0 | percentile: 62
Pdatum7
−12.7
−12.8
−12.9
−13.0
−13.1
−13.2
0
200
400
600
800
1000

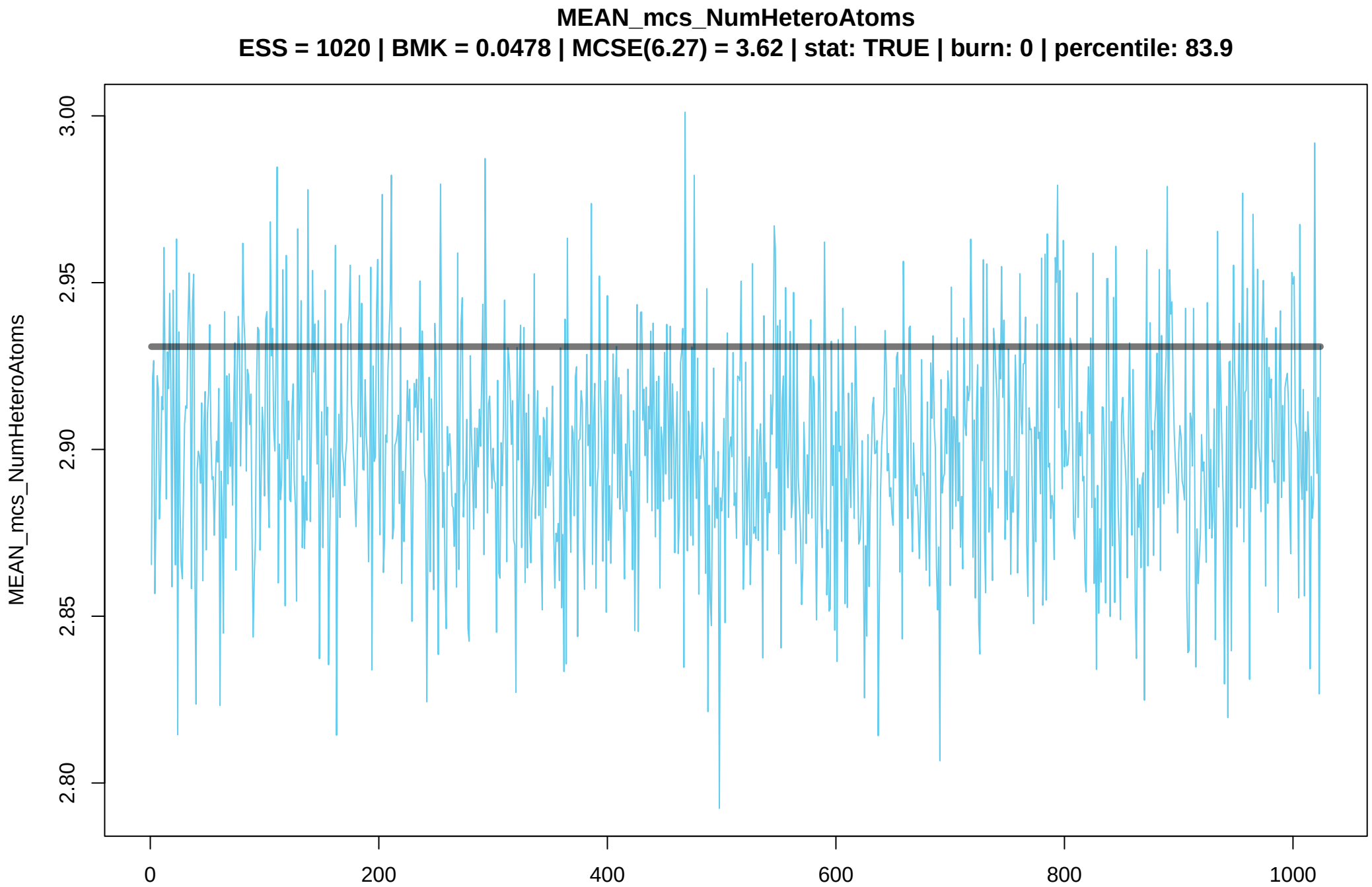

Pdatum8
ESS = 209 | BMK = 0.13 | MCSE(6.27) = 7.44 | stat: FALSE | burn: 0 | percentile: 31.6
Pdatum8
−12.4
−12.5
−12.6
−12.7
−12.8
0
200
400
600
800
1000

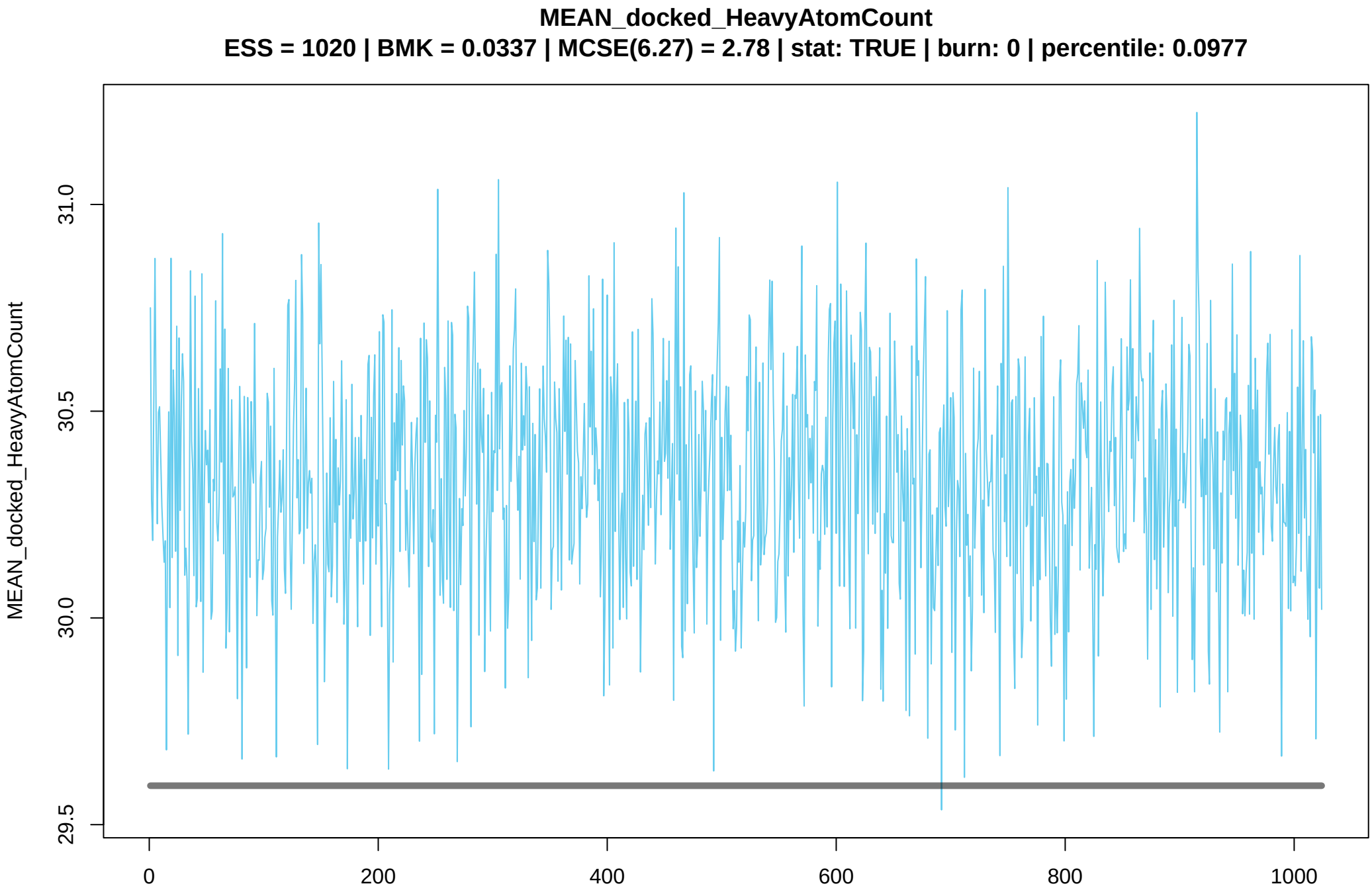

Dcov
ESS = 1020 | BMK = 0.153 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | percentile: 78.7
Dcov
0
−2
−4
−6
−8
0
200
400
600
800
1000

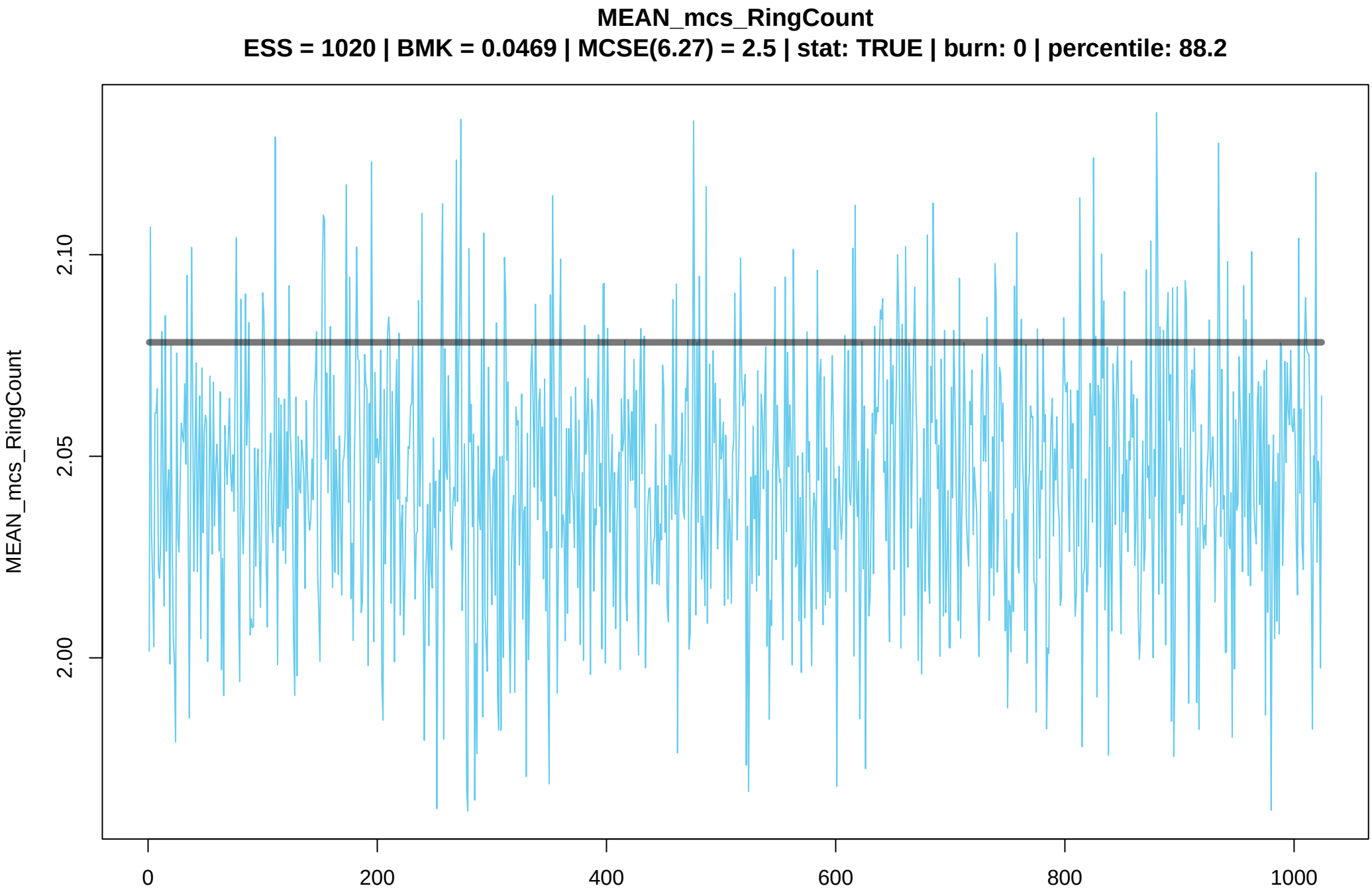

MEAN_log_RMSD
ESS = 1020 | BMK = 0.0492 | MCSE(6.27) = 3.69 | stat: TRUE | burn: 0 | percentile: 5.37
MEAN_log_RMSD
0.70
0.75
0.80
0.85
0
200
400
600
800
1000

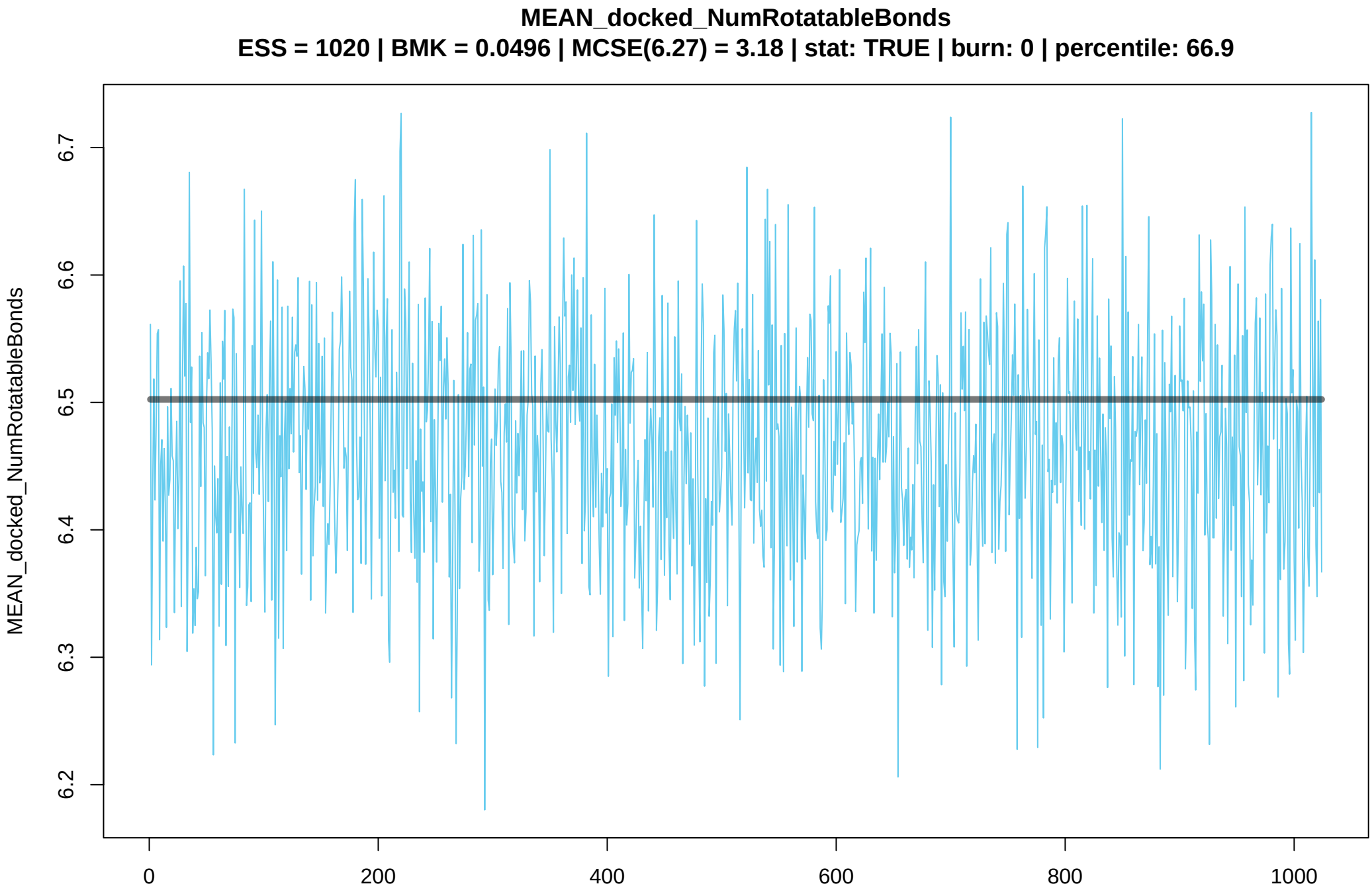

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0465 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | percentile: 1.86
MEAN_log_mcs_unbonded_polar_sasa
−1.15
−1.20
−1.25
−1.30
−1.35
0
200
400
600
800
1000

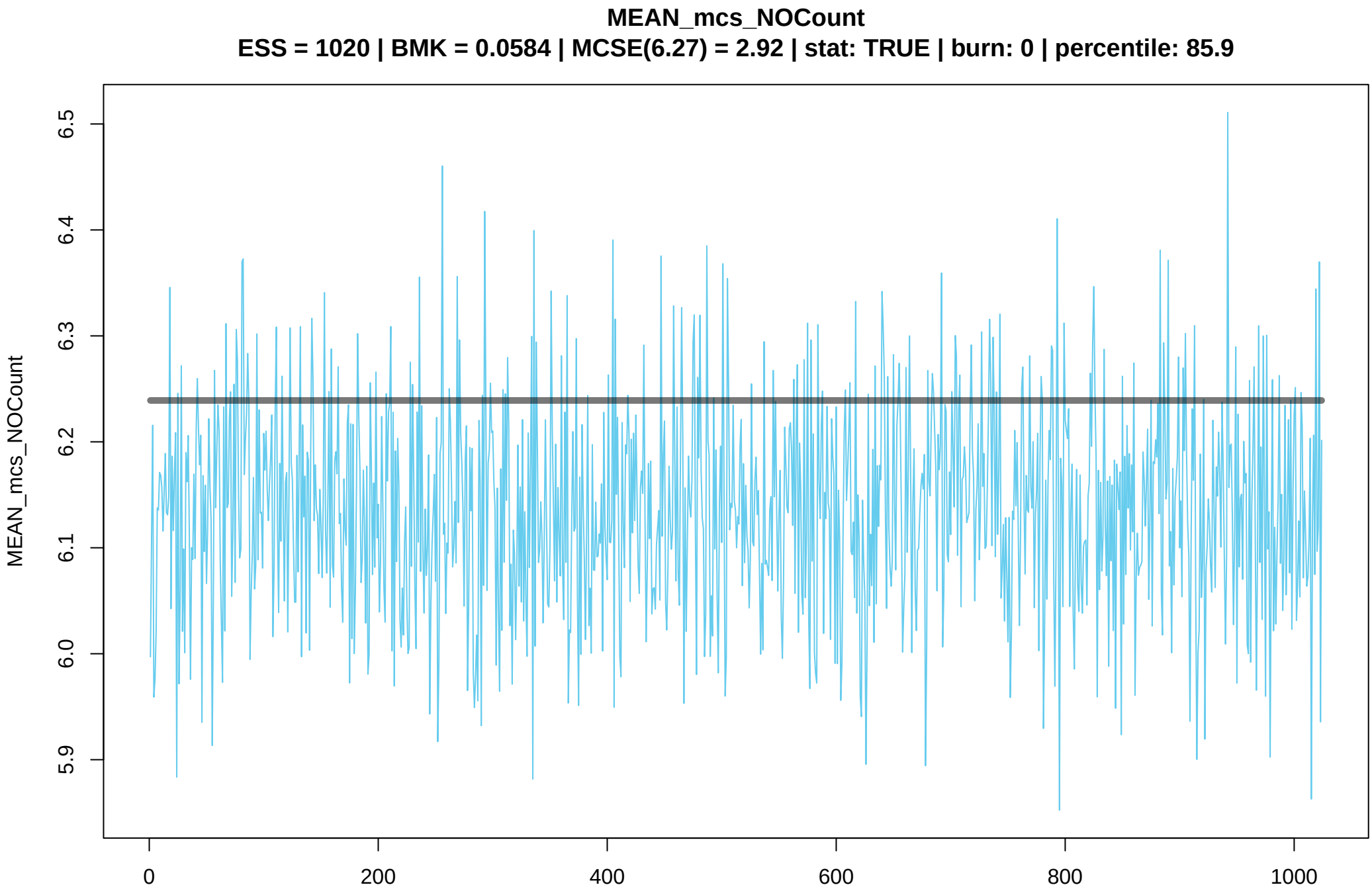

MEAN_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0451 | MCSE(6.27) = 3.05 | stat: FALSE | burn: 0 | percentile: 1.46
MEAN_logit_ec_tanimoto_similarity
−0.6
−0.7
−0.8
−0.9
0
200
400
600
800
1000

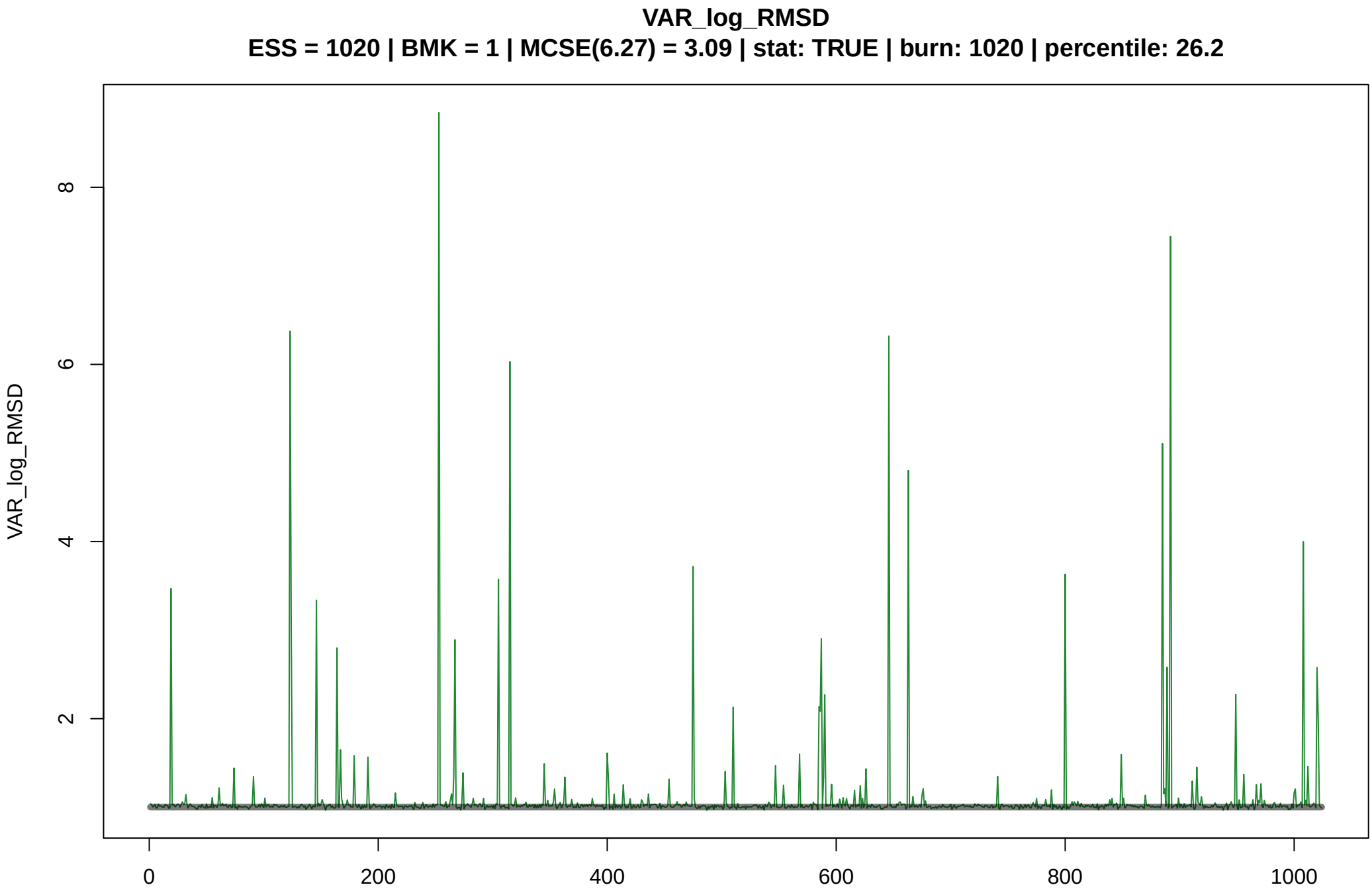

MEAN_mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0478 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0 | percentile: 83.9
MEAN_mcs_NumHeteroAtoms
3.00
2.95
2.90
2.85
2.80
0
200
400
600
800
1000

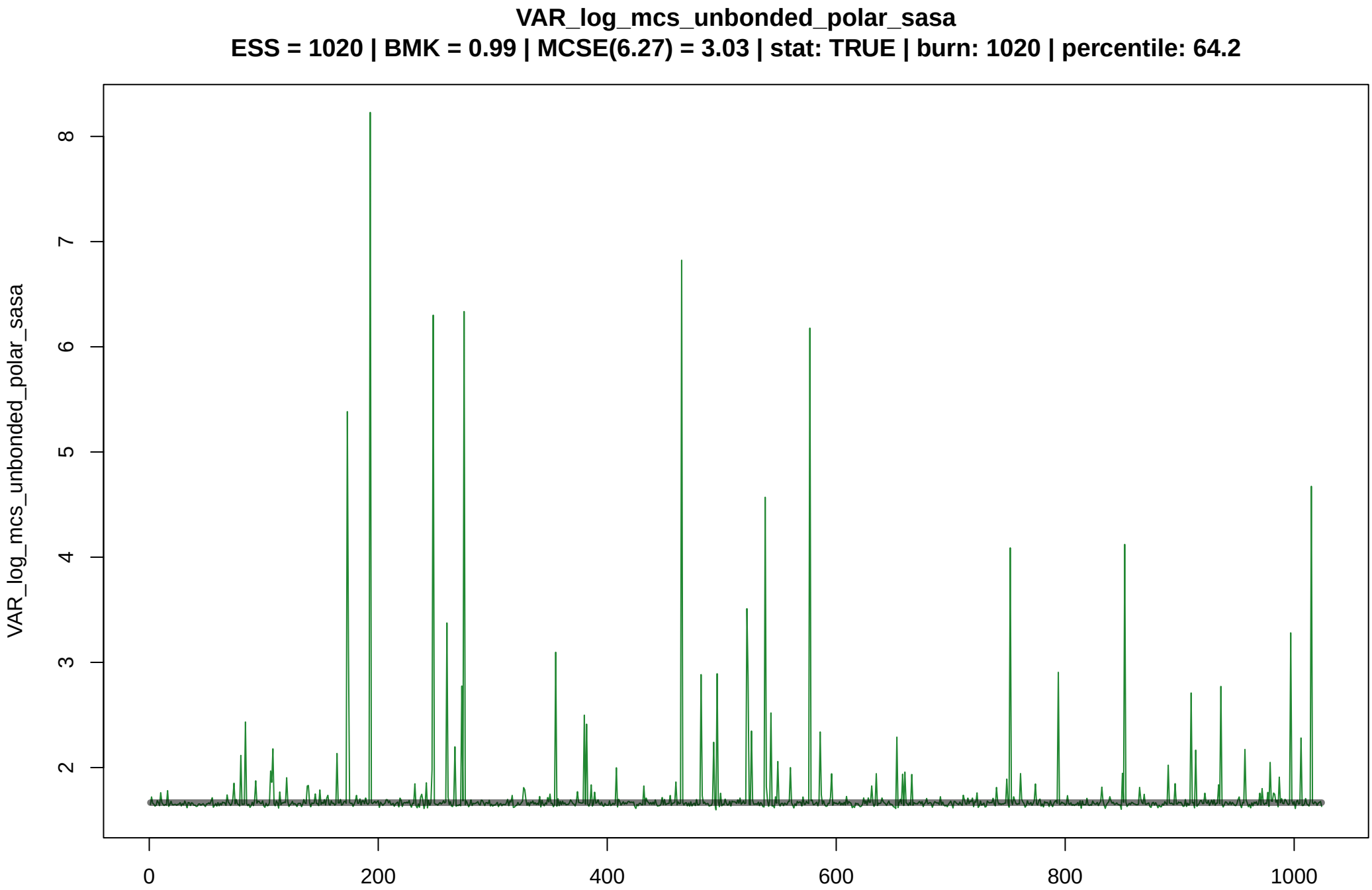

MEAN_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0337 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | percentile: 0.0977
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
31.0
0
200
400
600
800
1000

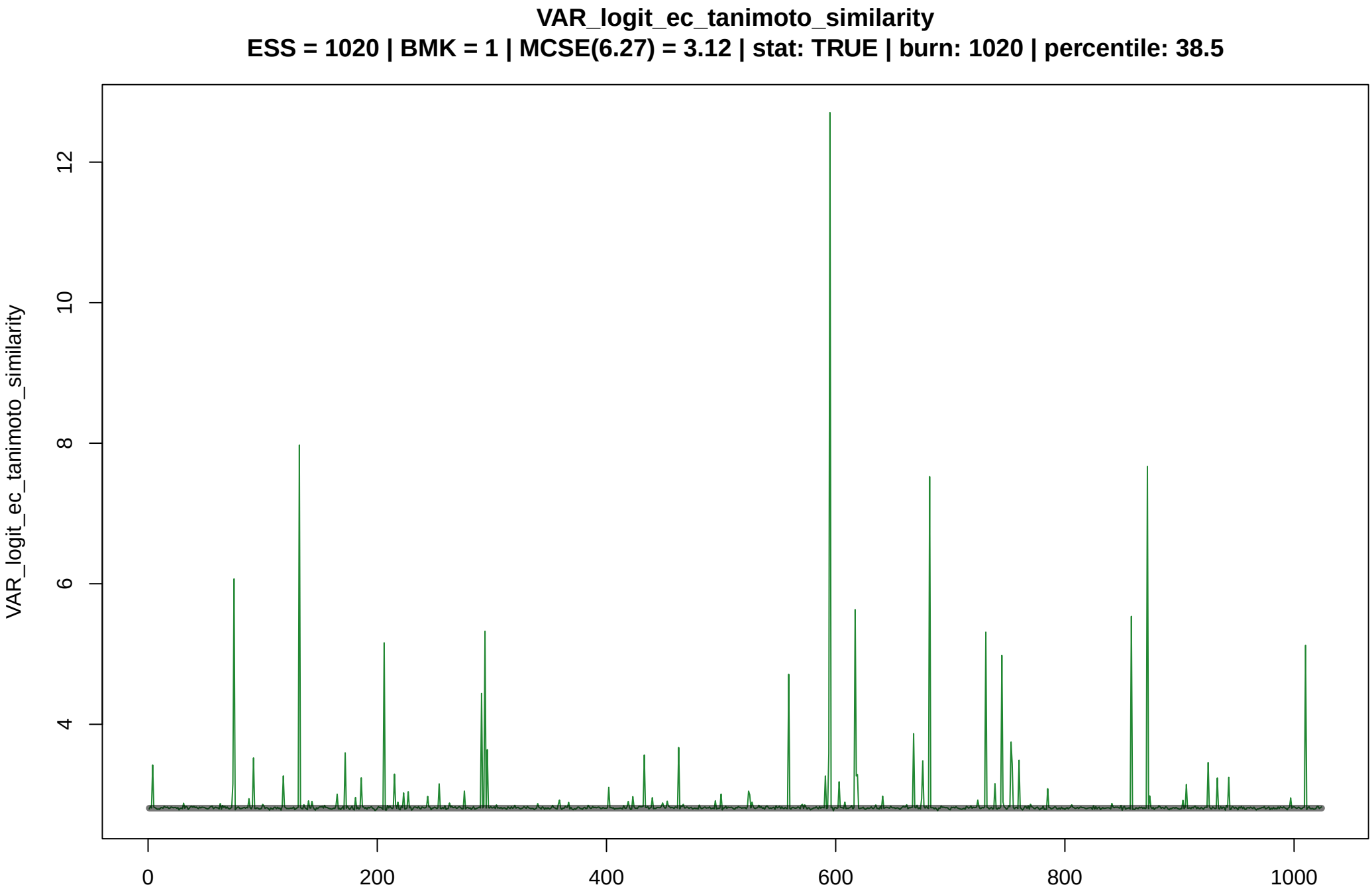

MEAN_mcs_RingCount
ESS = 1020 | BMK = 0.0469 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | percentile: 88.2
MEAN_mcs_RingCount
2.00
2.05
2.10
0
200
400
600
800
1000

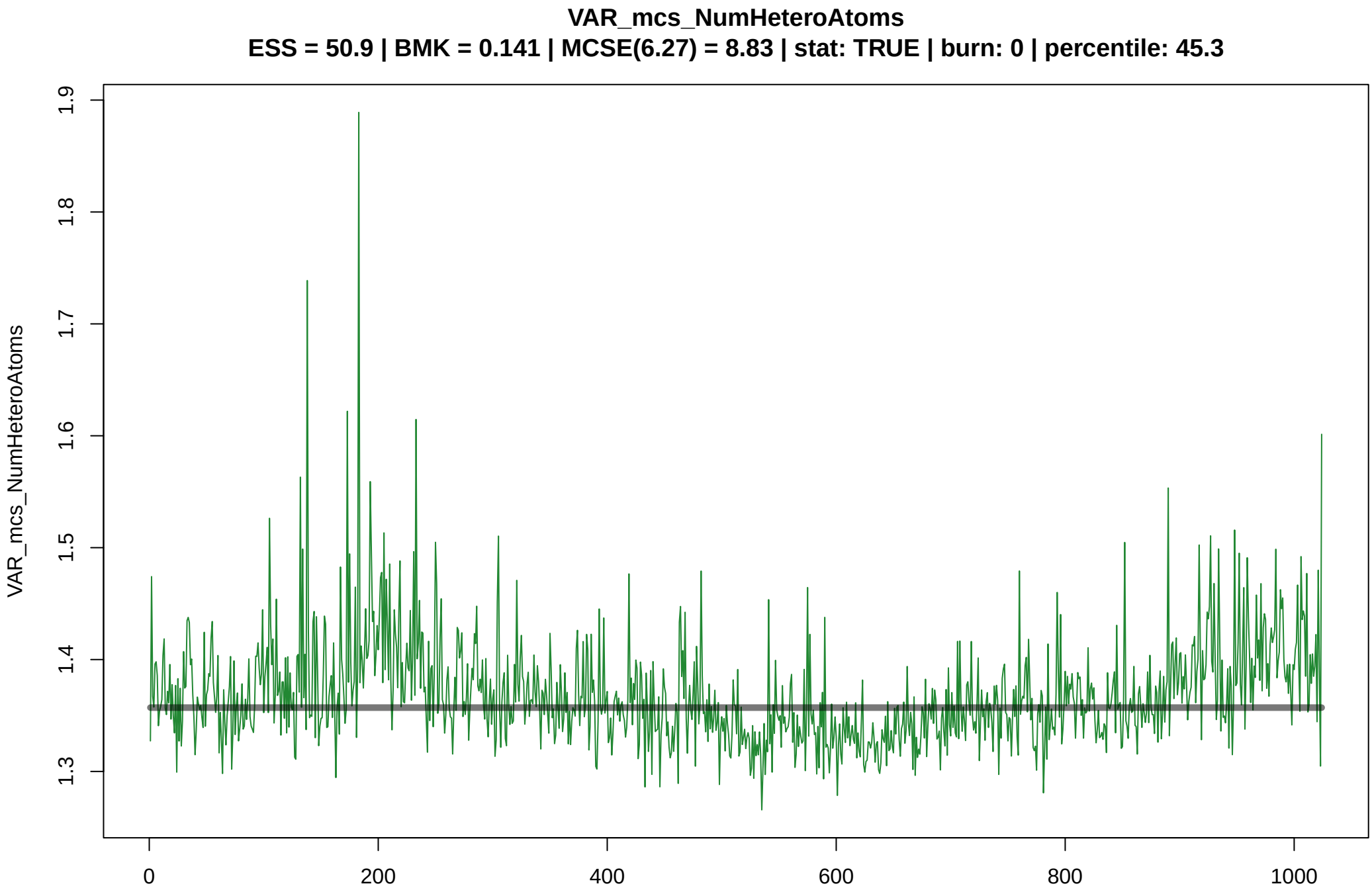

MEAN_docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0496 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | percentile: 66.9
MEAN_docked_NumRotatableBonds
6.2
6.3
6.4
6.5
6.6
6.7
0
200
400
600
800
1000

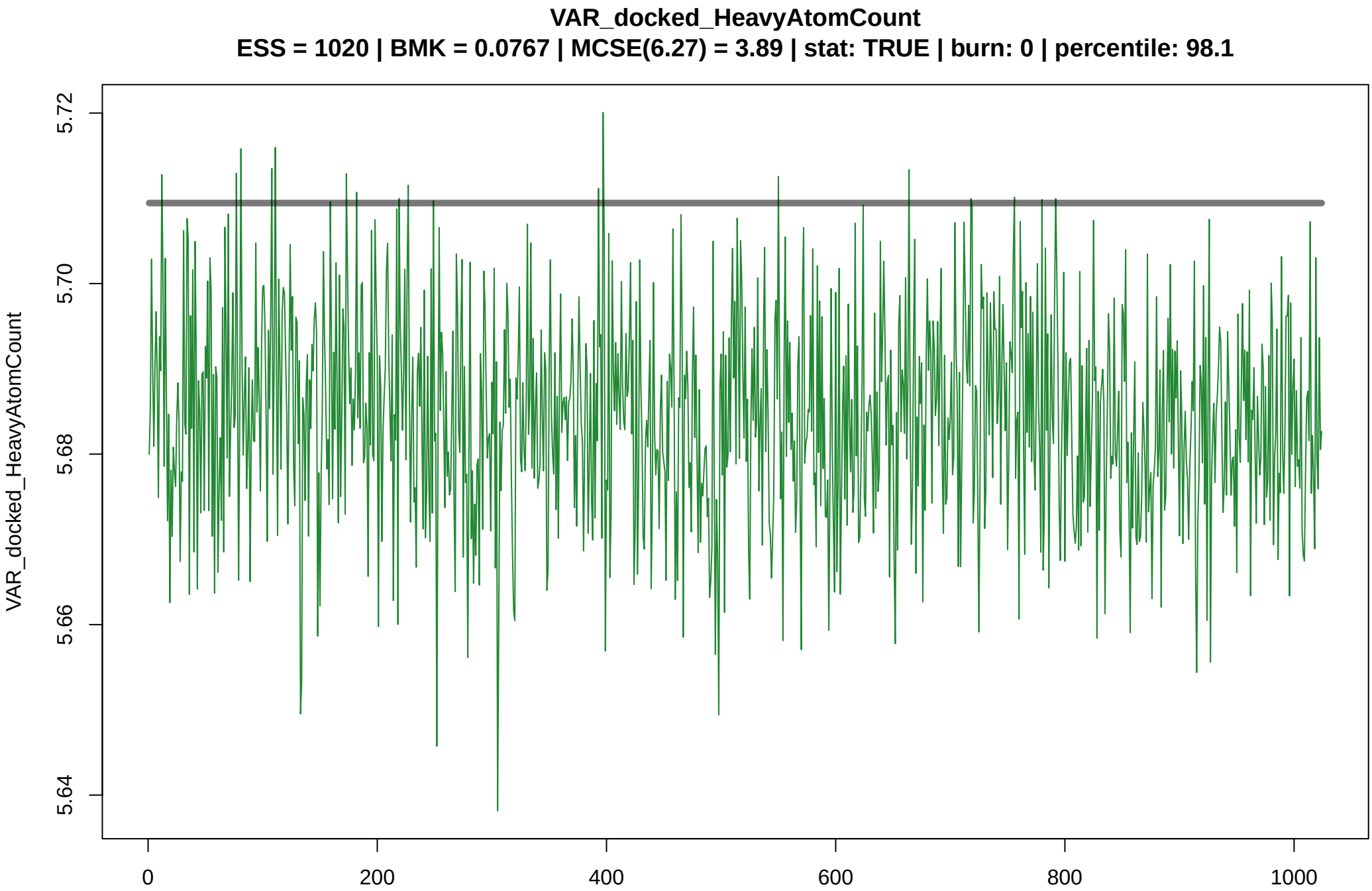

MEAN_mcs_NOCount
ESS = 1020 | BMK = 0.0584 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0 | percentile: 85.9
MEAN_mcs_NOCount
5.9
6.0
6.1
6.2
6.3
6.4
6.5
0
200
400
600
800
1000

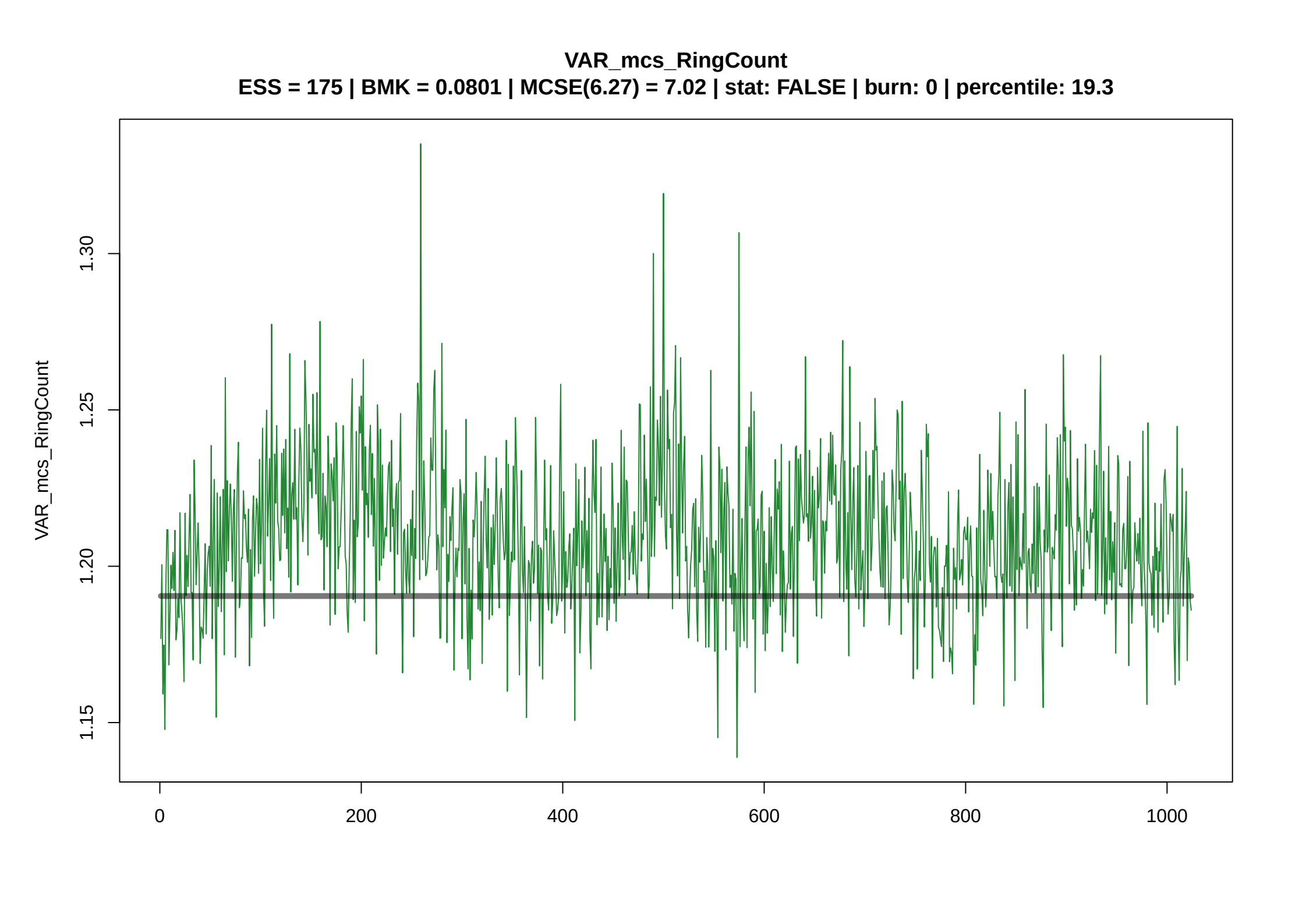

VAR_log_RMSD
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 1020 | percentile: 26.2
VAR_log_RMSD
2
4
6
8
0
200
400
600
800
1000

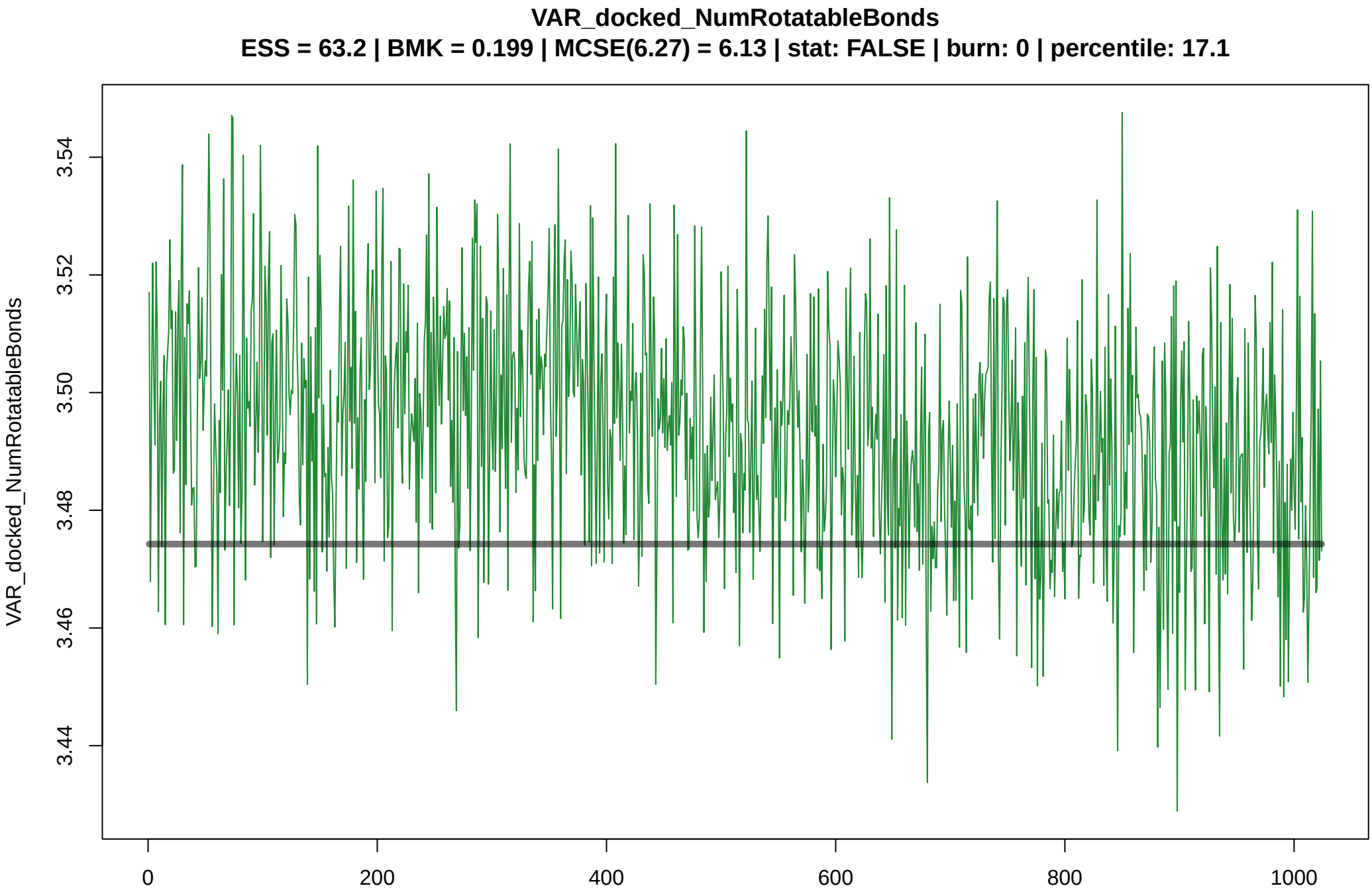

VAR_log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.99 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 1020 | percentile: 64.2
VAR_log_mcs_unbonded_polar_sasa
2
3
4
5
6
7
8
0
200
400
600
800
1000

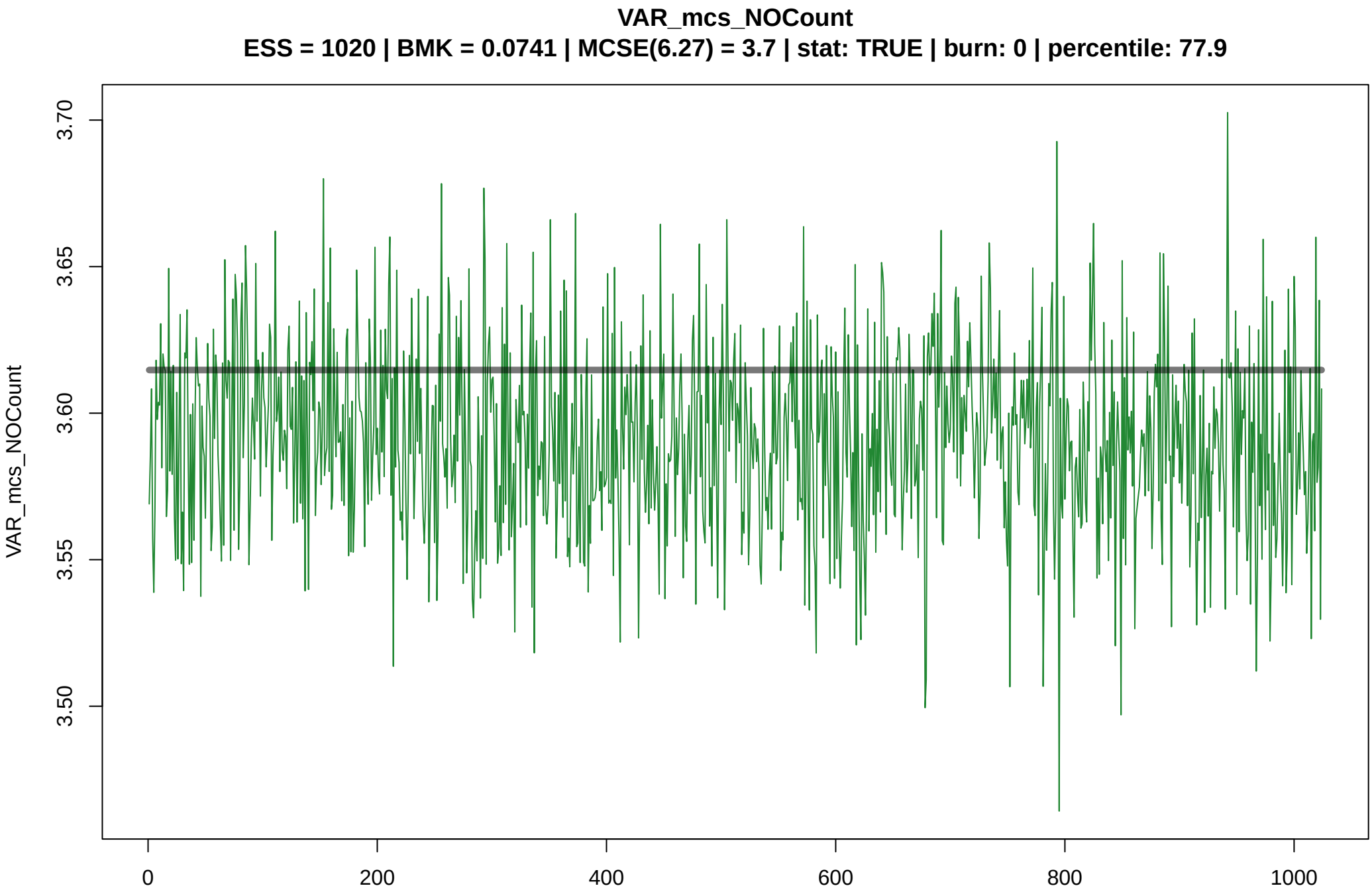

VAR_logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 1 | MCSE(6.27) = 3.12 | stat: TRUE | burn: 1020 | percentile: 38.5
VAR_logit_ec_tanimoto_similarity
4
6
8
10
12
0
200
400
600
800
1000

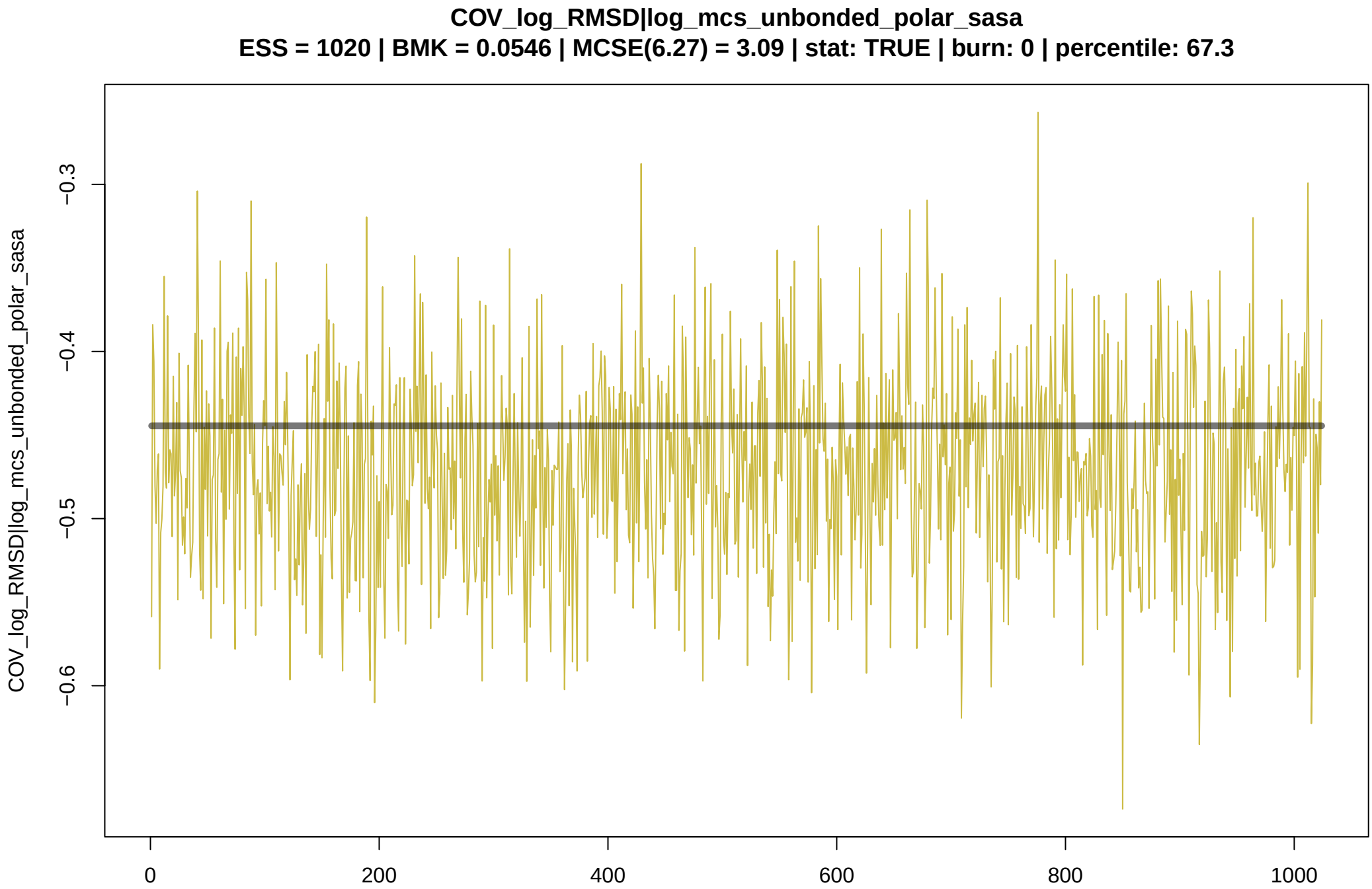

VAR_mcs_NumHeteroAtoms
ESS = 50.9 | BMK = 0.141 | MCSE(6.27) = 8.83 | stat: TRUE | burn: 0 | percentile: 45.3
VAR_mcs_NumHeteroAtoms
1.3
1.4
1.5
1.6
1.7
1.8
1.9
0
200
400
600
800
1000

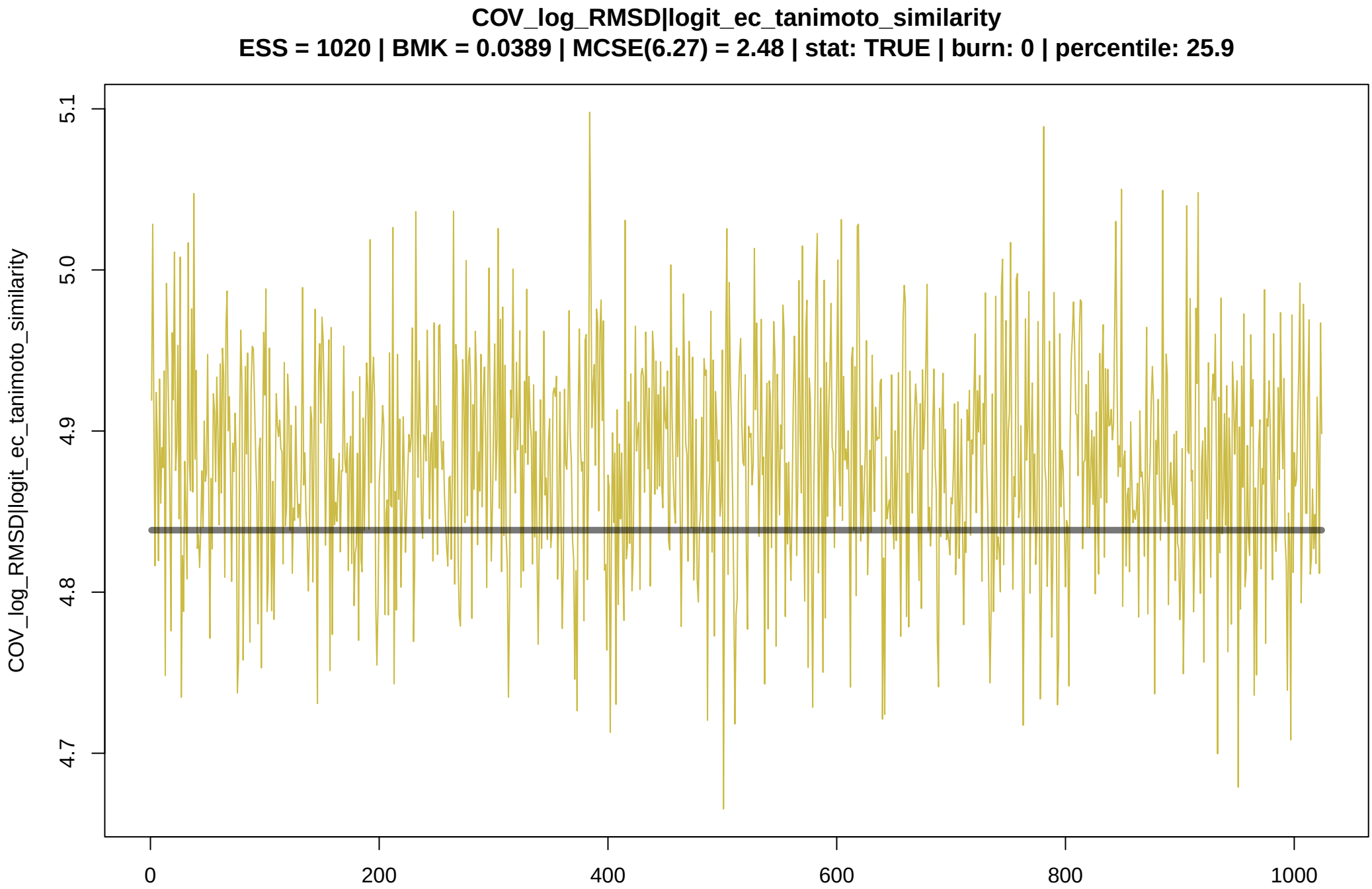

VAR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0767 | MCSE(6.27) = 3.89 | stat: TRUE | burn: 0 | percentile: 98.1
VAR_docked_HeavyAtomCount
5.64
5.66
5.68
5.70
5.72
0
200
400
600
800
1000

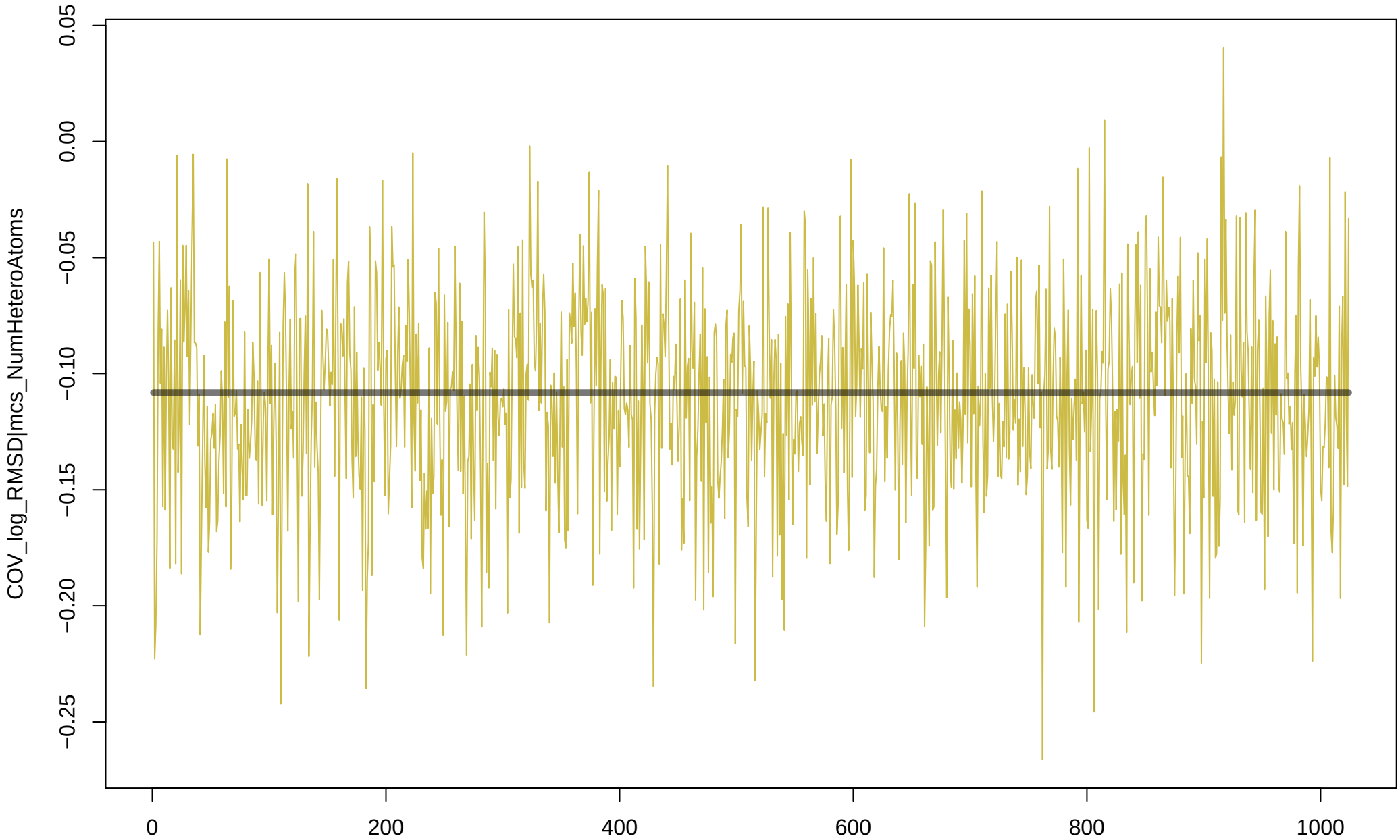

VAR_mcs_RingCount
ESS = 175 | BMK = 0.0801 | MCSE(6.27) = 7.02 | stat: FALSE | burn: 0 | percentile: 19.3
VAR_mcs_RingCount
1.15
1.20
1.25
1.30
0
200
400
600
800
1000

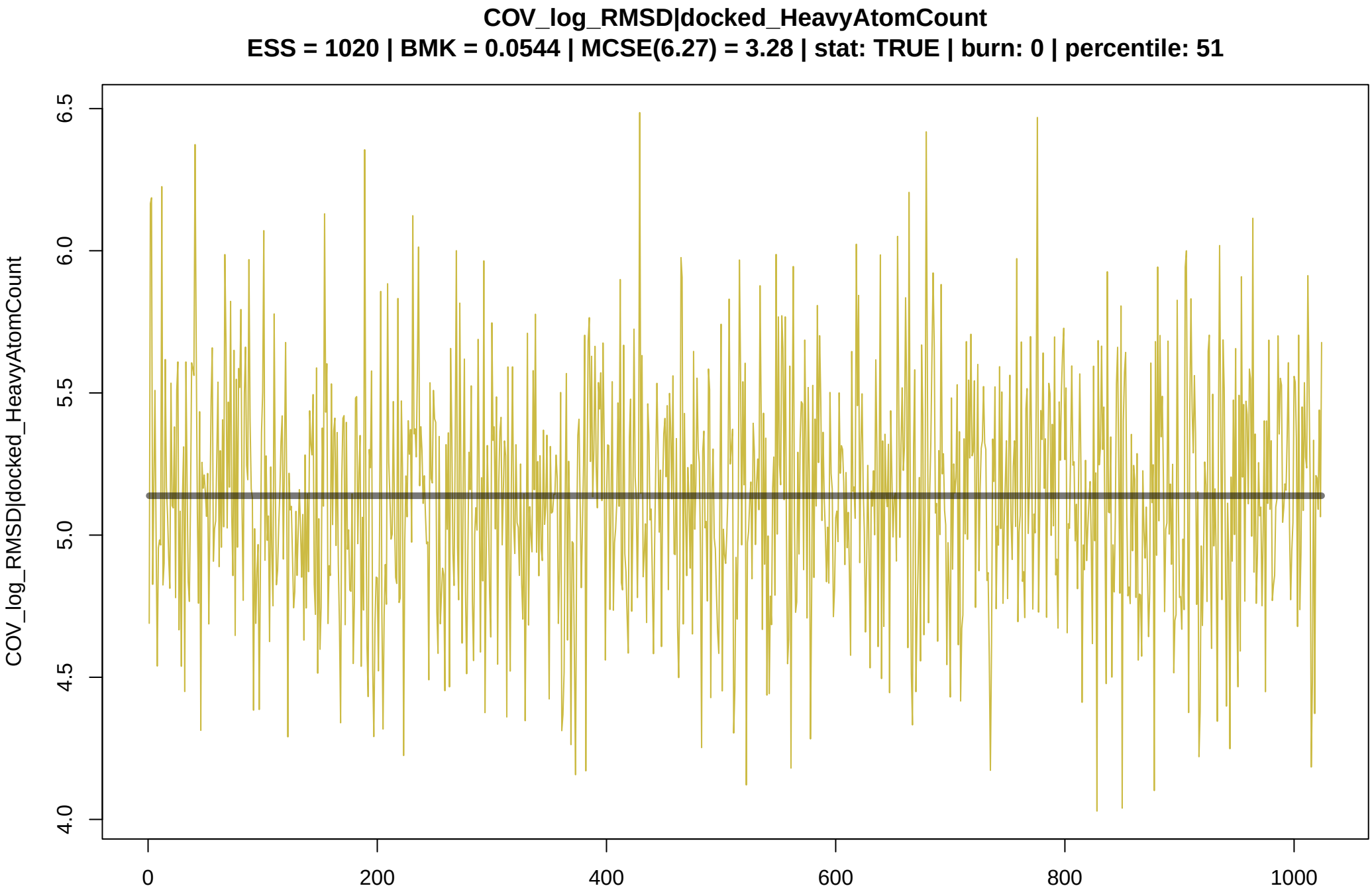

VAR_docked_NumRotatableBonds
ESS = 63.2 | BMK = 0.199 | MCSE(6.27) = 6.13 | stat: FALSE | burn: 0 | percentile: 17.1
VAR_docked_NumRotatableBonds
3.44
3.46
3.48
3.50
3.52
3.54
0
200
400
600
800
1000

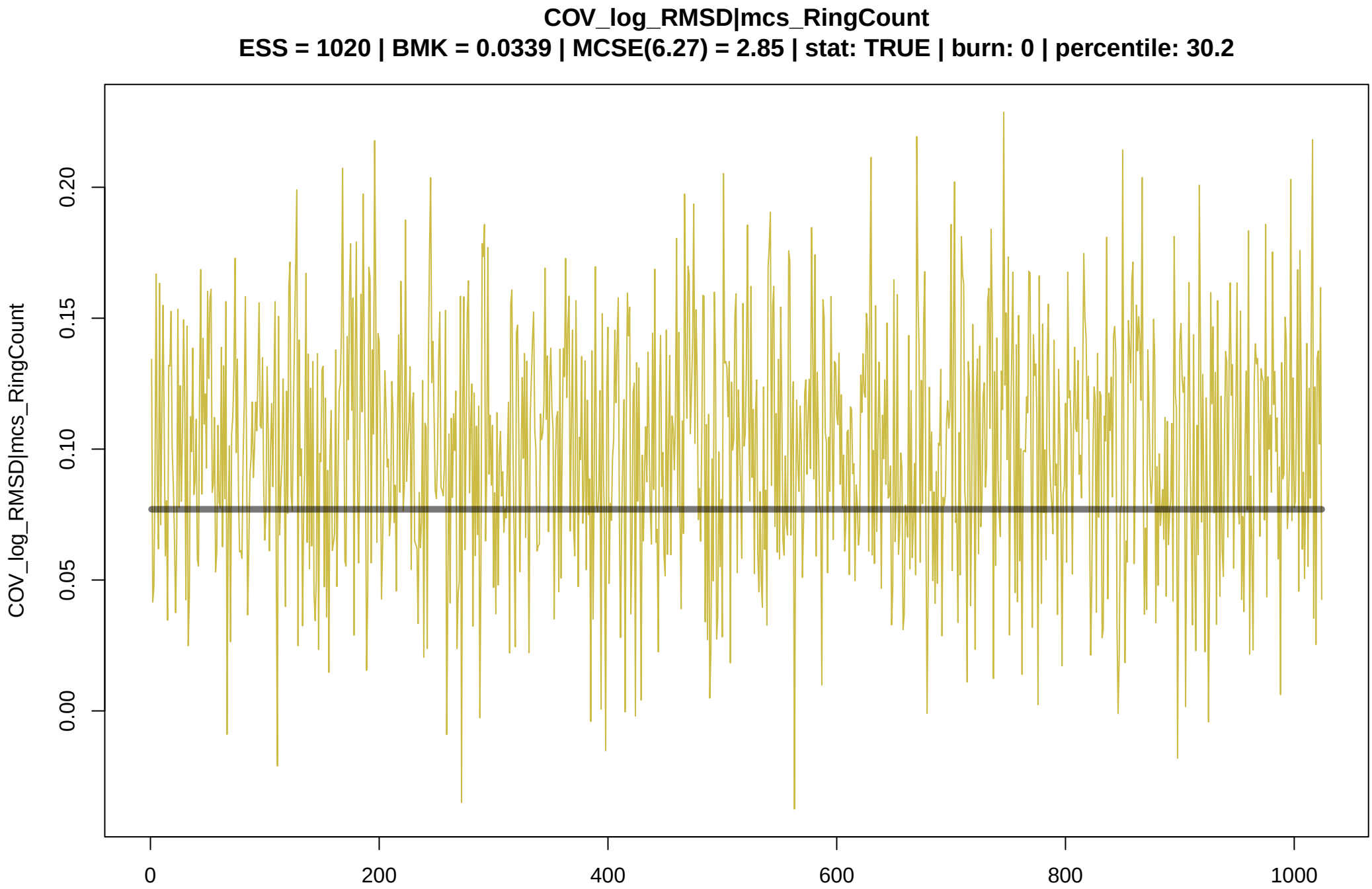

VAR_mcs_NOCount
ESS = 1020 | BMK = 0.0741 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | percentile: 77.9
VAR_mcs_NOCount
3.70
3.65
3.60
3.55
3.50
0
200
400
600
800
1000

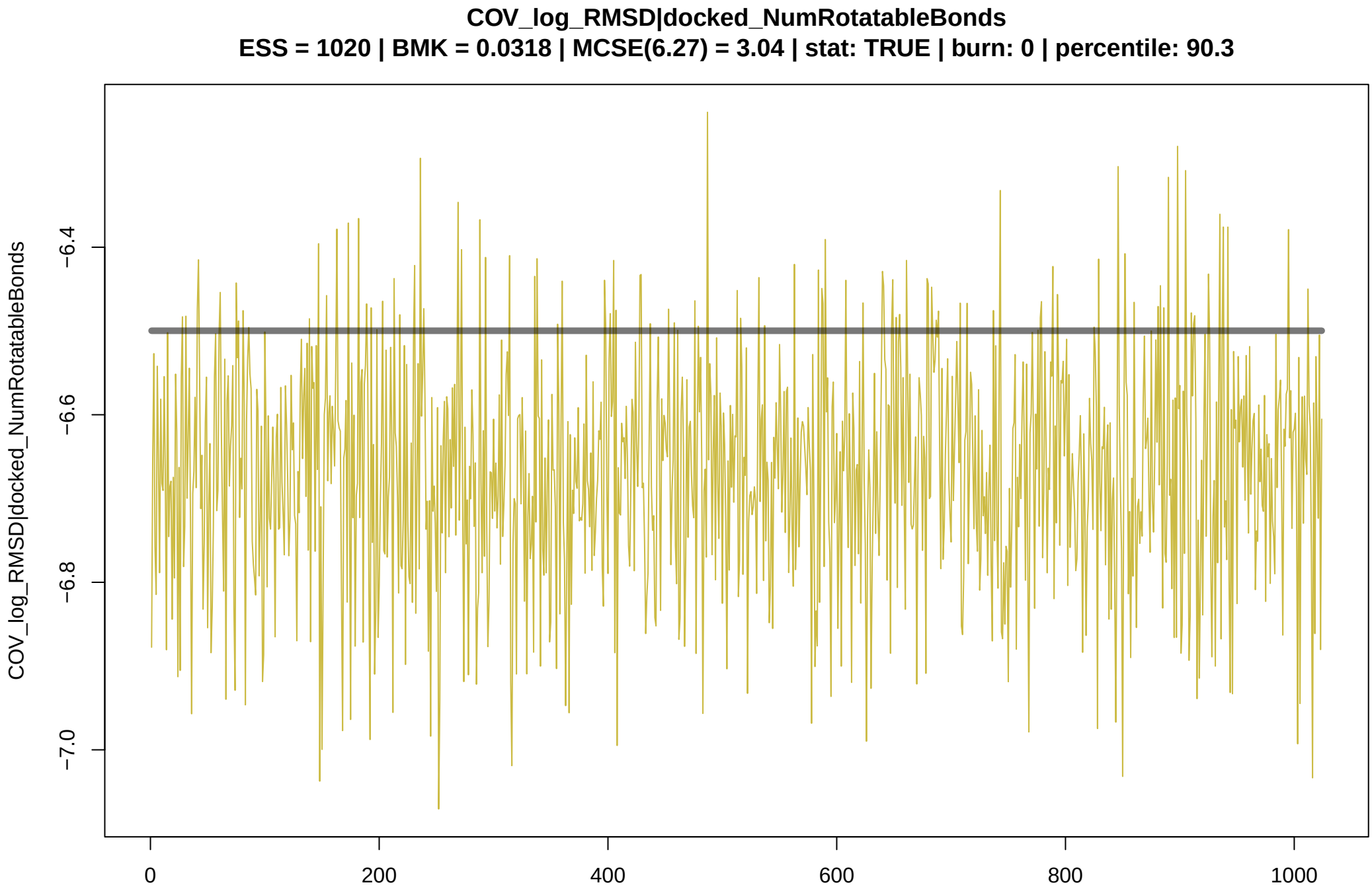

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1020 | BMK = 0.0546 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0 | percentile: 67.3
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.3
−0.4
−0.5
−0.6
0
200
400
600
800
1000

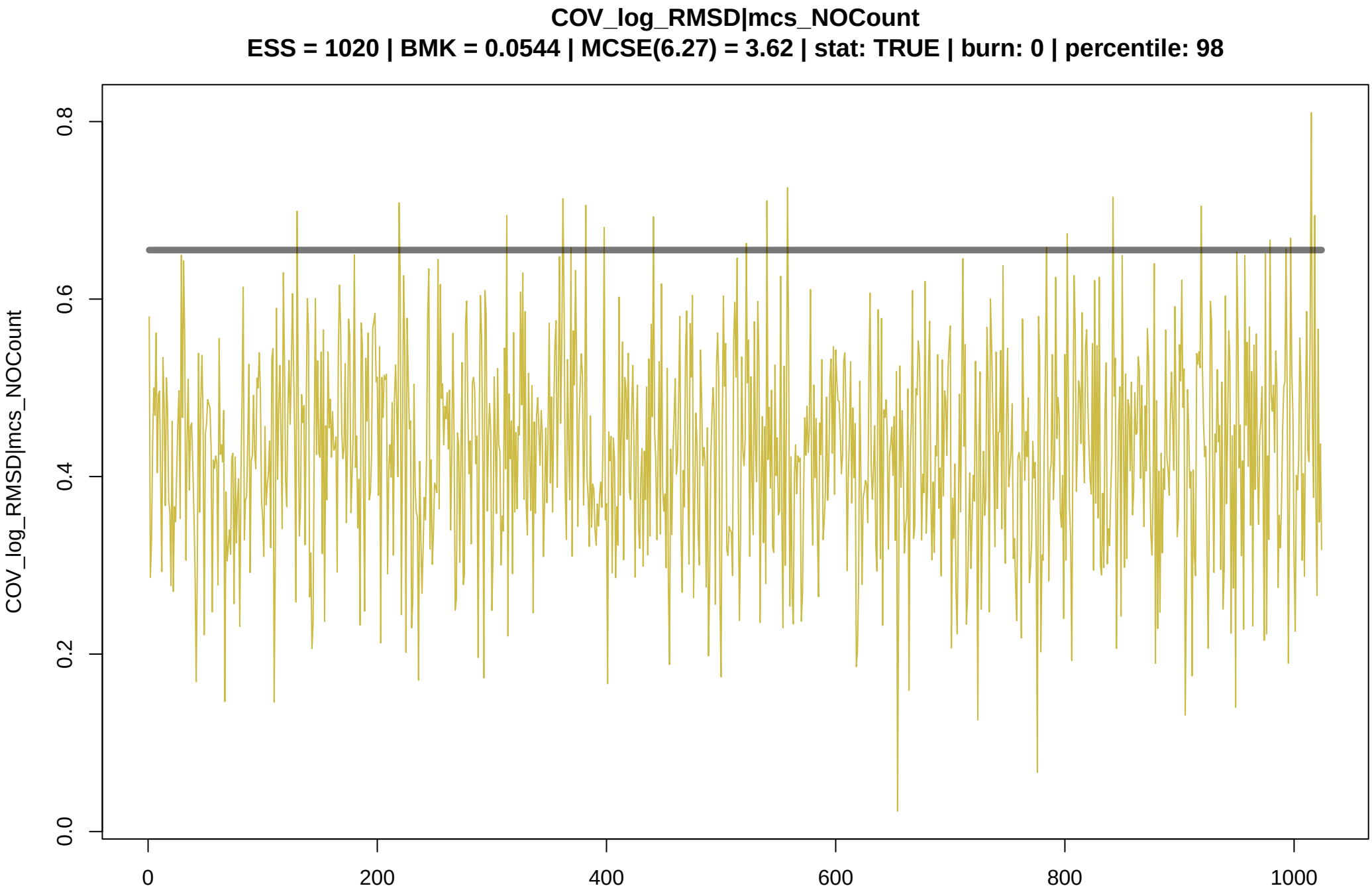

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0389 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0 | percentile: 25.9
COV_log_RMSD|logit_ec_tanimoto_similarity
5.1
5.0
4.9
4.8
4.7
0
200
400
600
800
1000

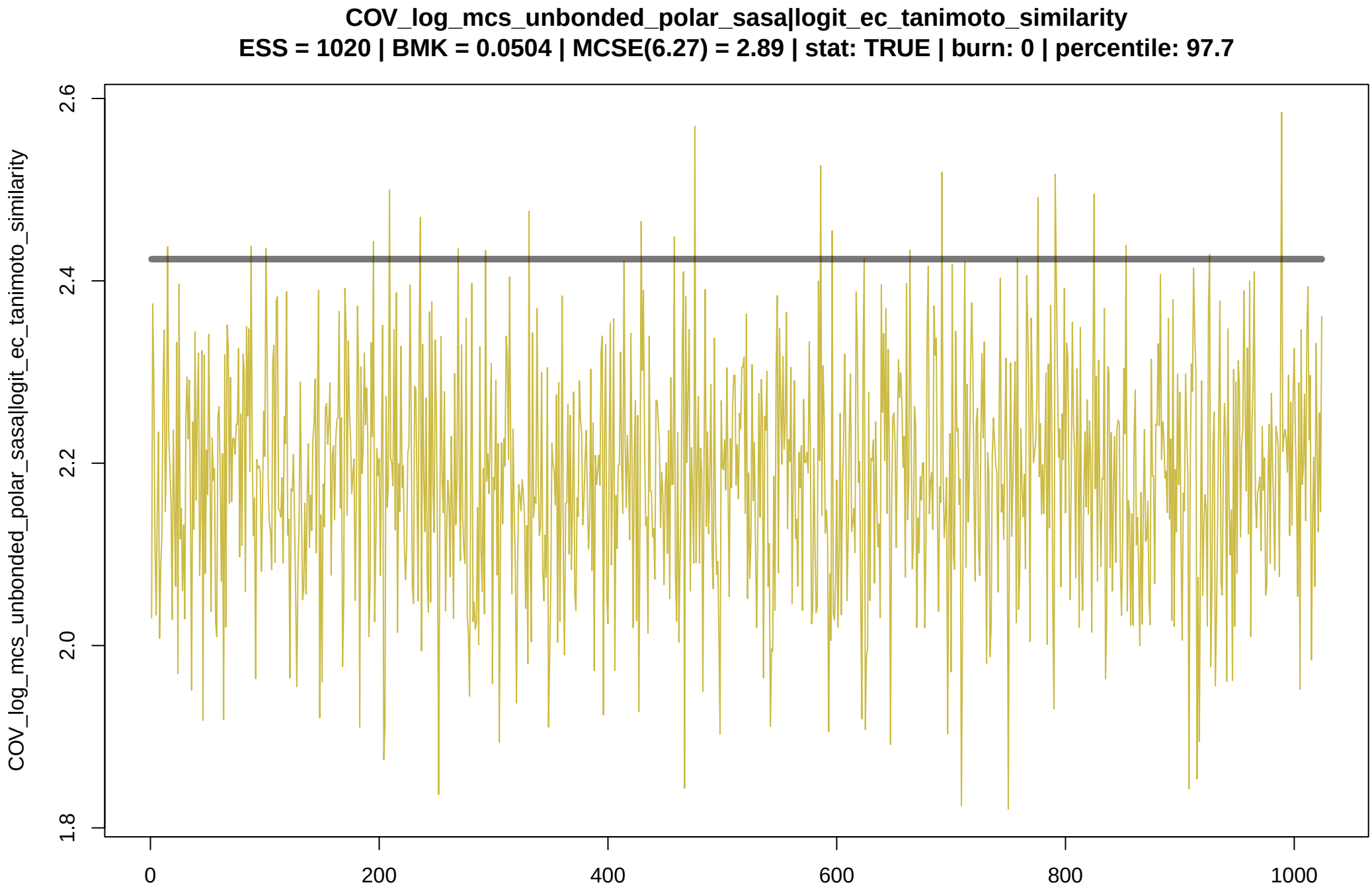

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0603 | MCSE(6.27) = 3.21 | stat: TRUE | burn: 0 | percentile: 51.6
COV_log_RMSD|mcs_NumHeteroAtoms
0.05
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
200
400
600
800
1000

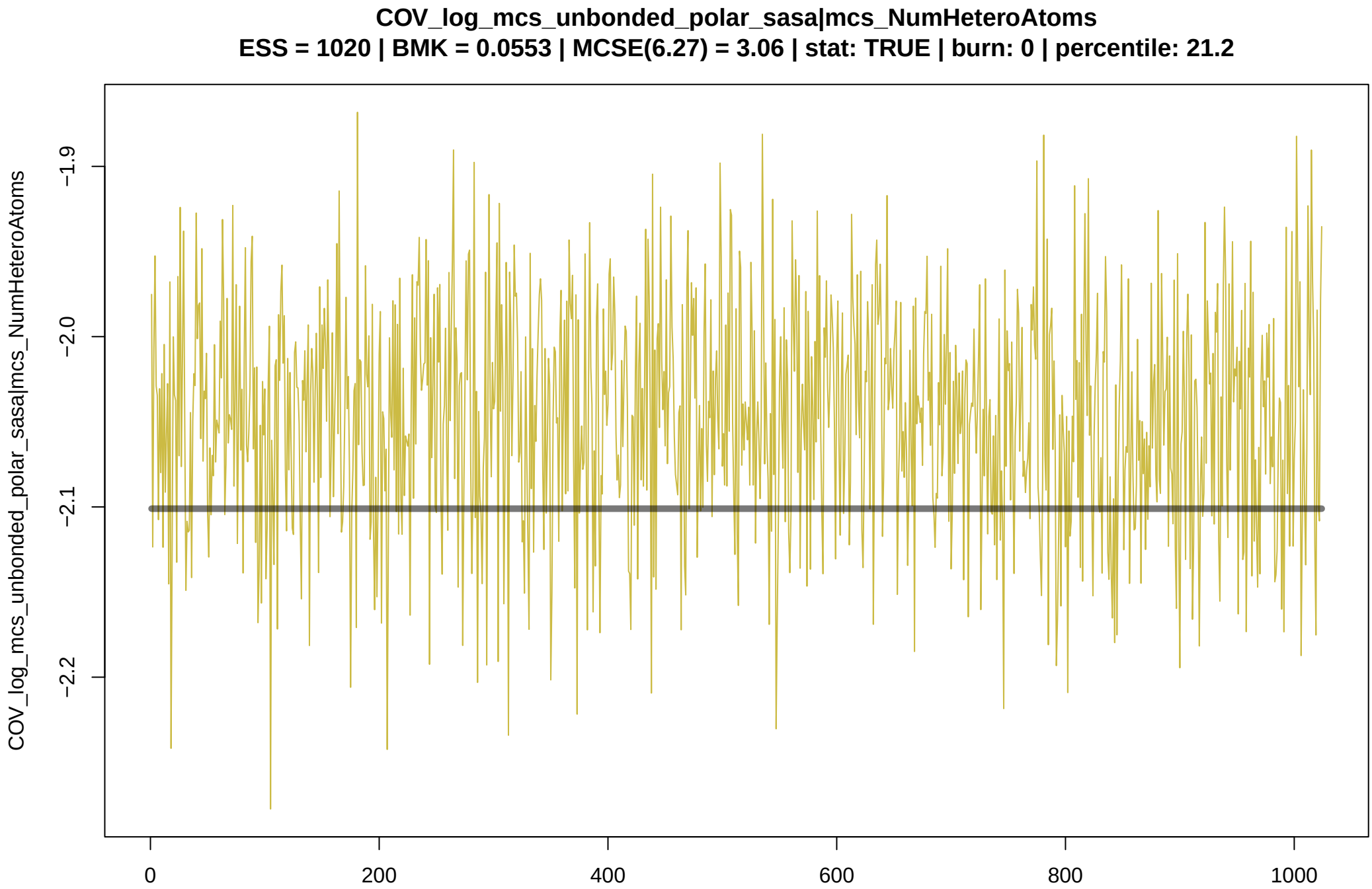

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0544 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | percentile: 51
COV_log_RMSD|docked_HeavyAtomCount
6.5
6.0
5.5
5.0
4.5
4.0
0
200
400
600
800
1000

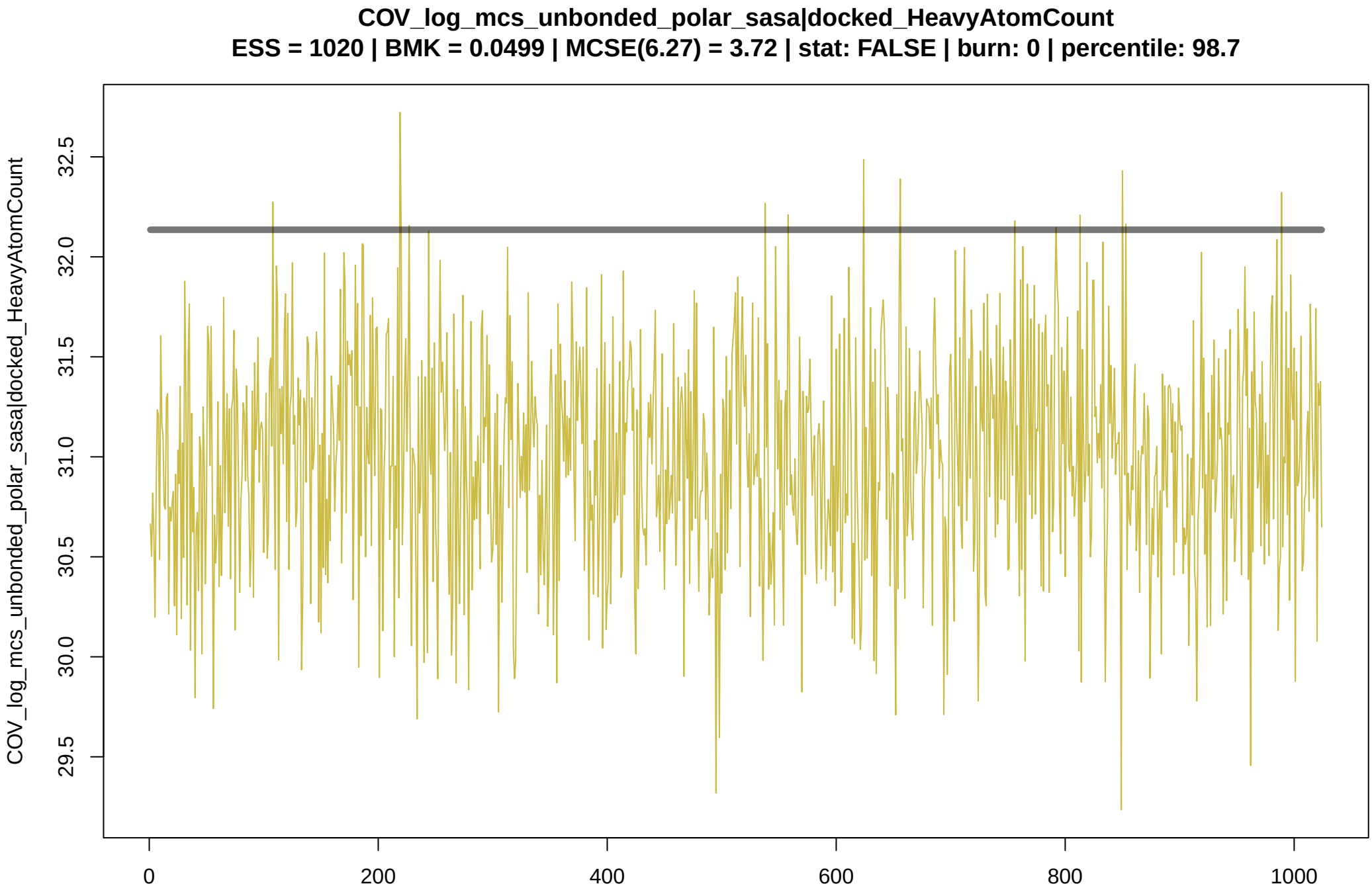

COV_log_RMSD|mcs_RingCount
ESS = 1020 | BMK = 0.0339 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | percentile: 30.2
COV_log_RMSD|mcs_RingCount
0.00
0.05
0.10
0.15
0.20
0
200
400
600
800
1000

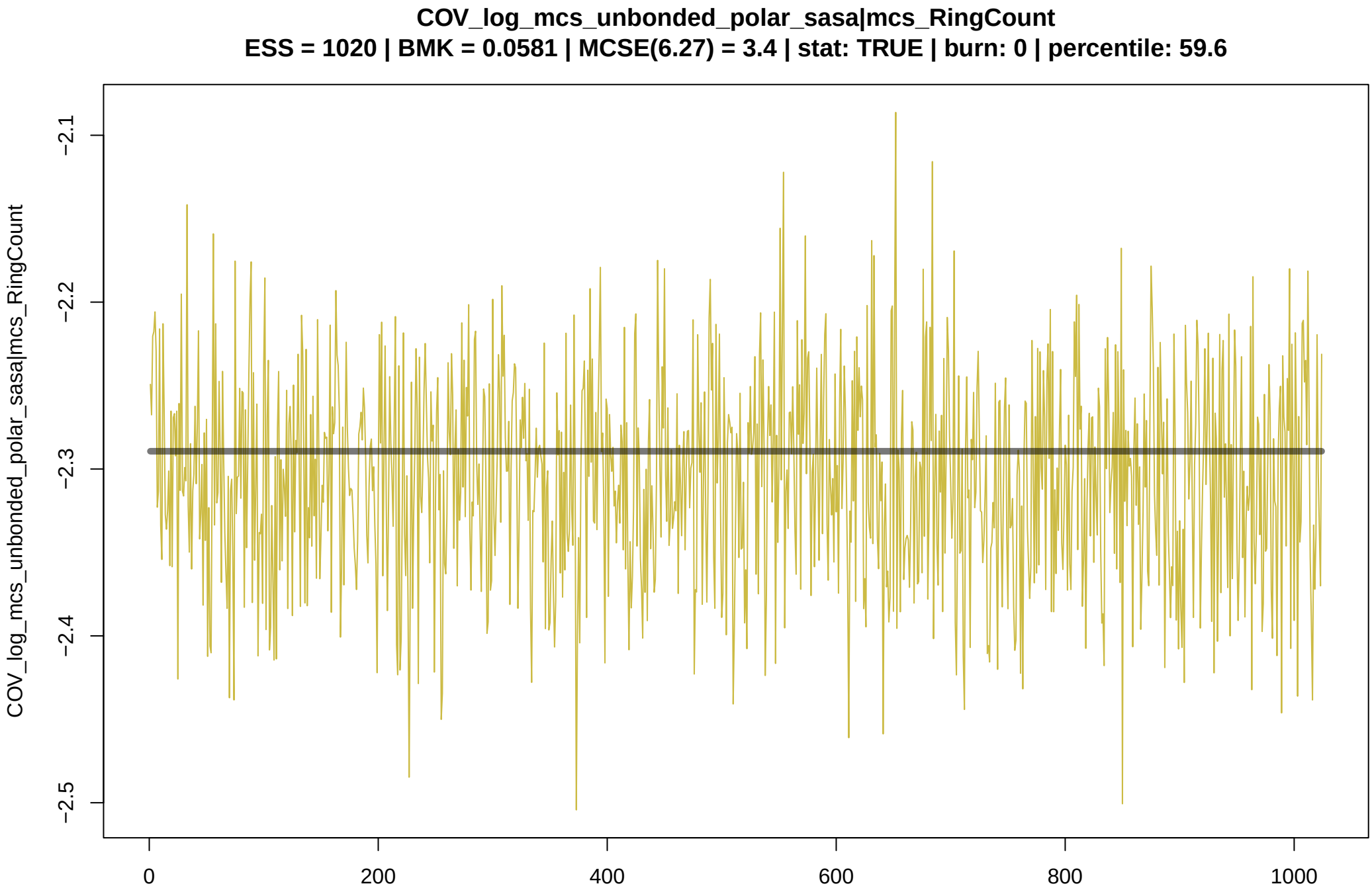

COV_log_RMSD|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0318 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | percentile: 90.3
COV_log_RMSD|docked_NumRotatableBonds
−6.4
−6.6
−6.8
−7.0
0
200
400
600
800
1000

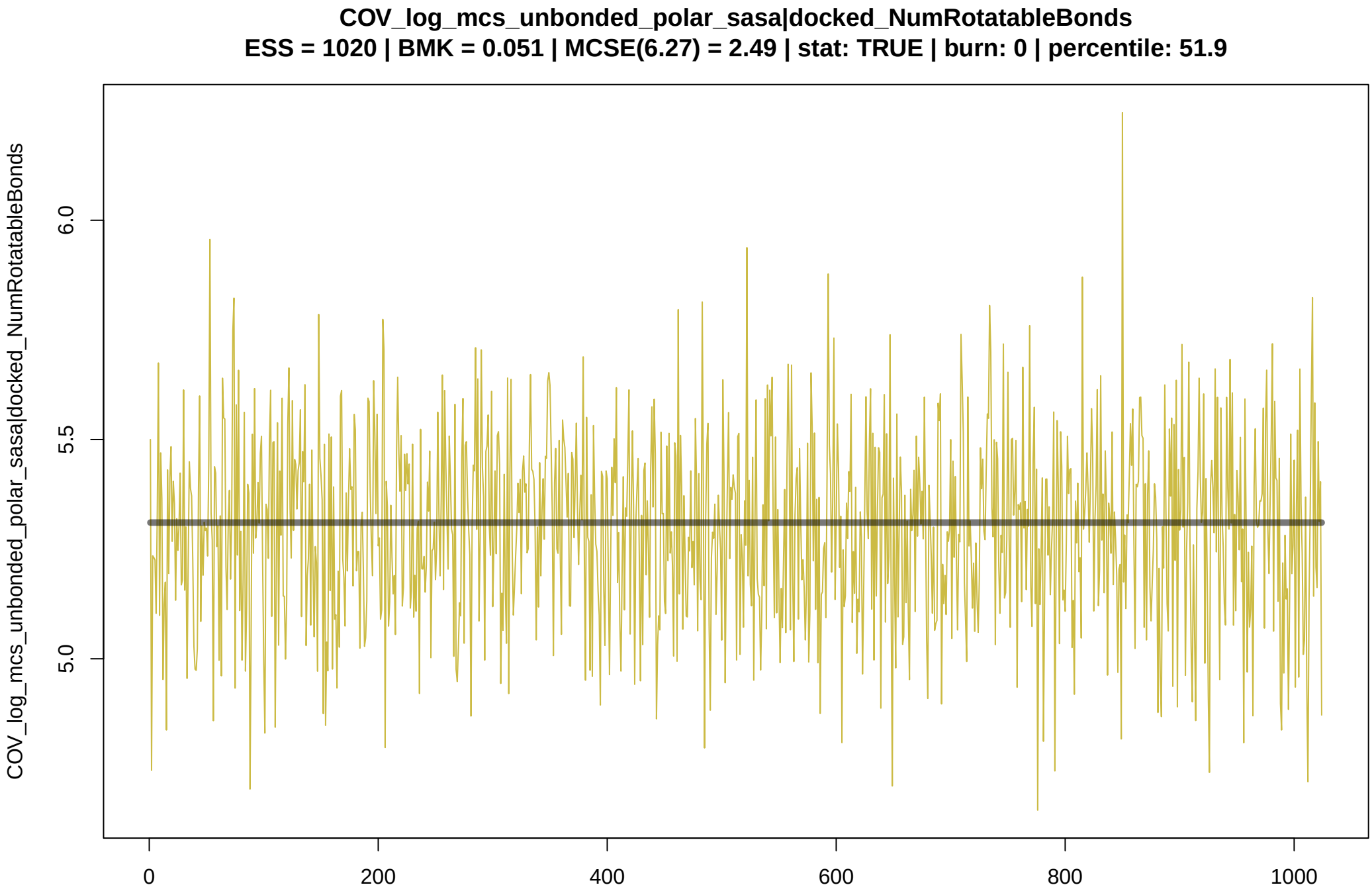

COV_log_RMSD|mcs_NOCount
ESS = 1020 | BMK = 0.0544 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0 | percentile: 98
COV_log_RMSD|mcs_NOCount
0.0
0.2
0.4
0.6
0.8
0
200
400
600
800
1000

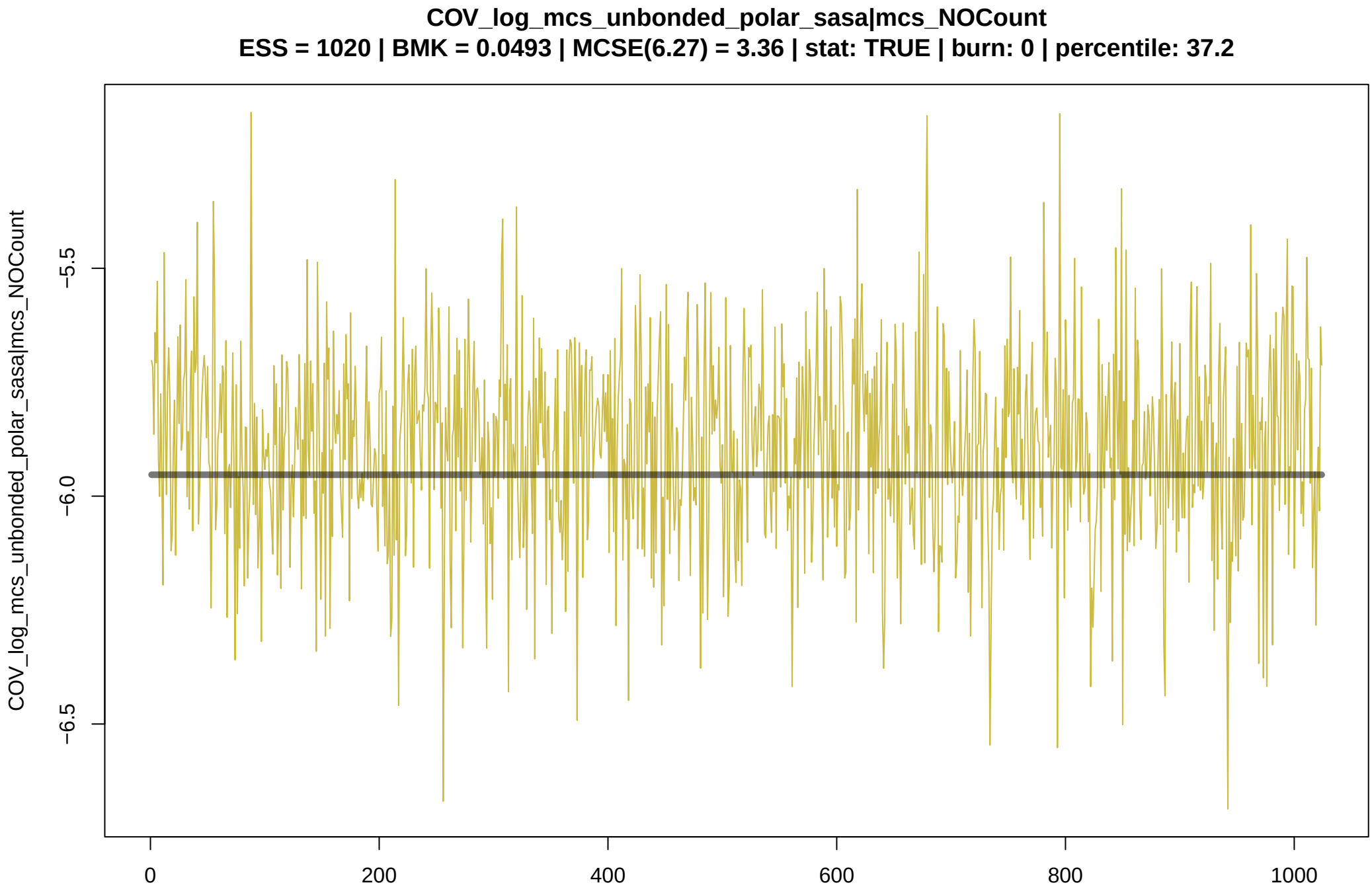

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1020 | BMK = 0.0504 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | percentile: 97.7
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2.6
2.4
2.2
2.0
1.8
0
200
400
600
800
1000

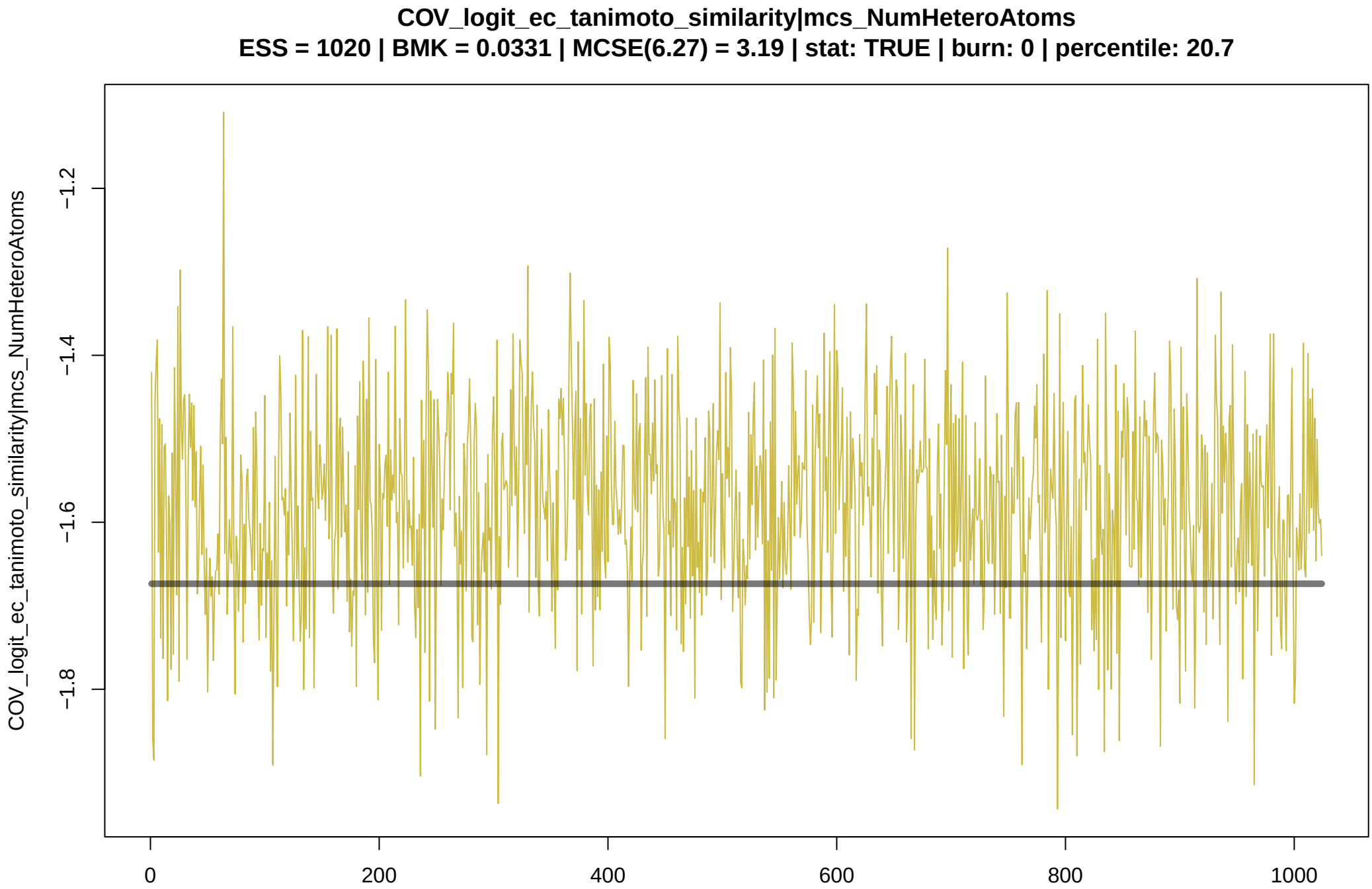

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0553 | MCSE(6.27) = 3.06 | stat: TRUE | burn: 0 | percentile: 21.2
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.9
−2.0
−2.1
−2.2
0
200
400
600
800
1000

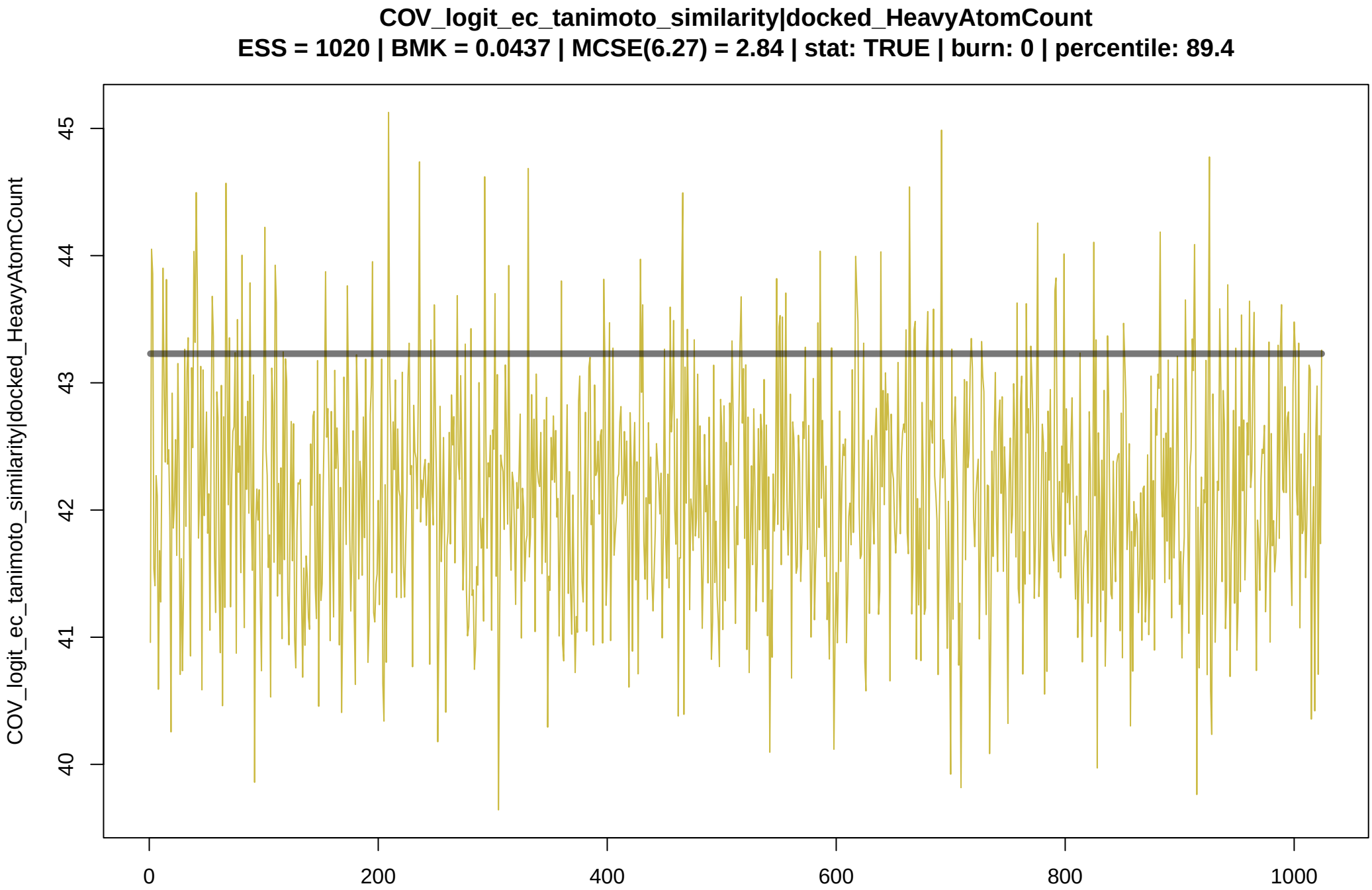

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0499 | MCSE(6.27) = 3.72 | stat: FALSE | burn: 0 | percentile: 98.7
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
29.5
30.0
30.5
31.0
31.5
32.0
32.5
0
200
400
600
800
1000

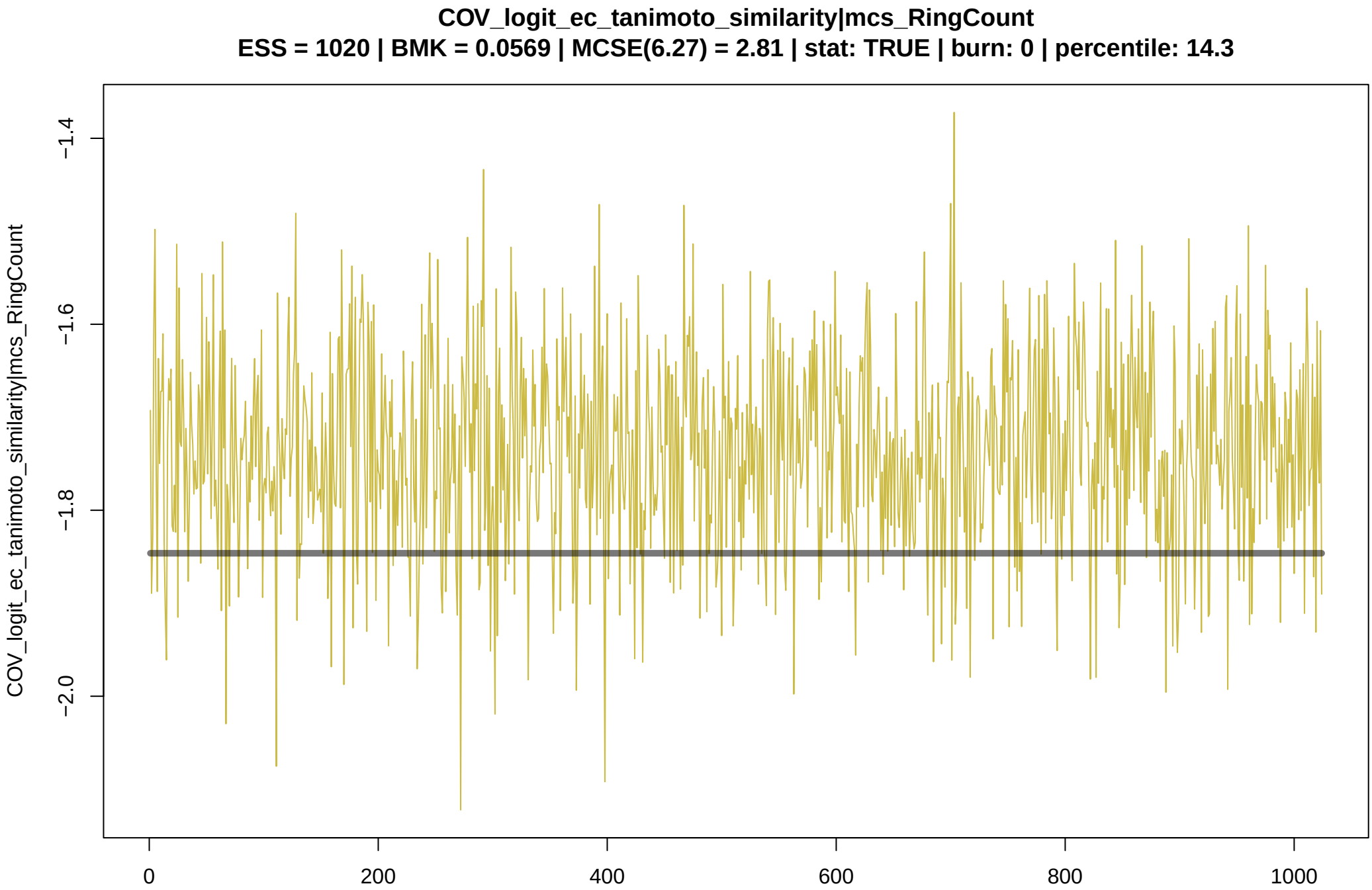

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 1020 | BMK = 0.0581 | MCSE(6.27) = 3.4 | stat: TRUE | burn: 0 | percentile: 59.6
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.1
−2.2
−2.3
−2.4
−2.5
0
200
400
600
800
1000

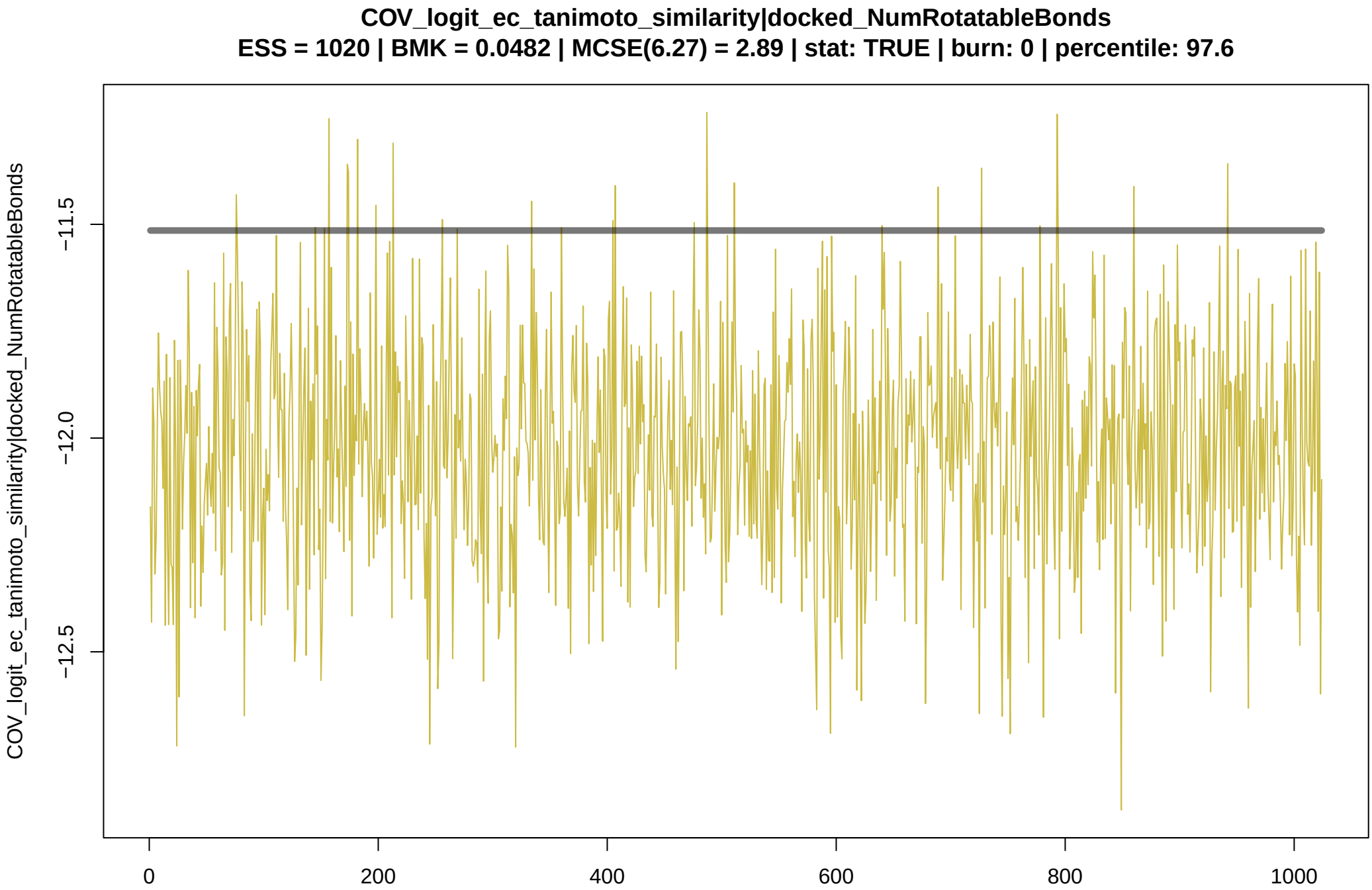

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.051 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0 | percentile: 51.9
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
6.0
5.5
5.0
0
200
400
600
800
1000

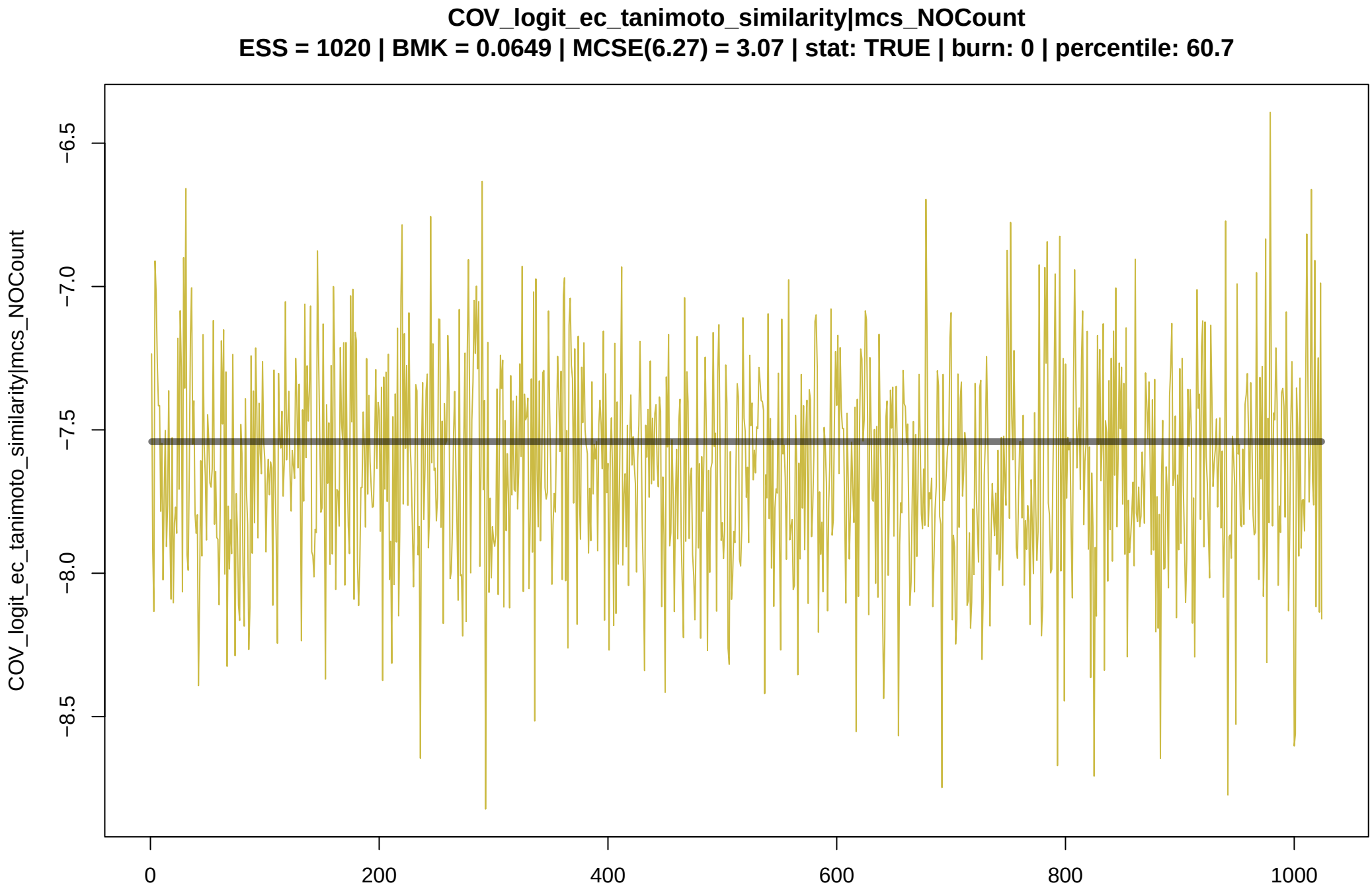

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1020 | BMK = 0.0493 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | percentile: 37.2
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.5
−6.0
−6.5
0
200
400
600
800
1000

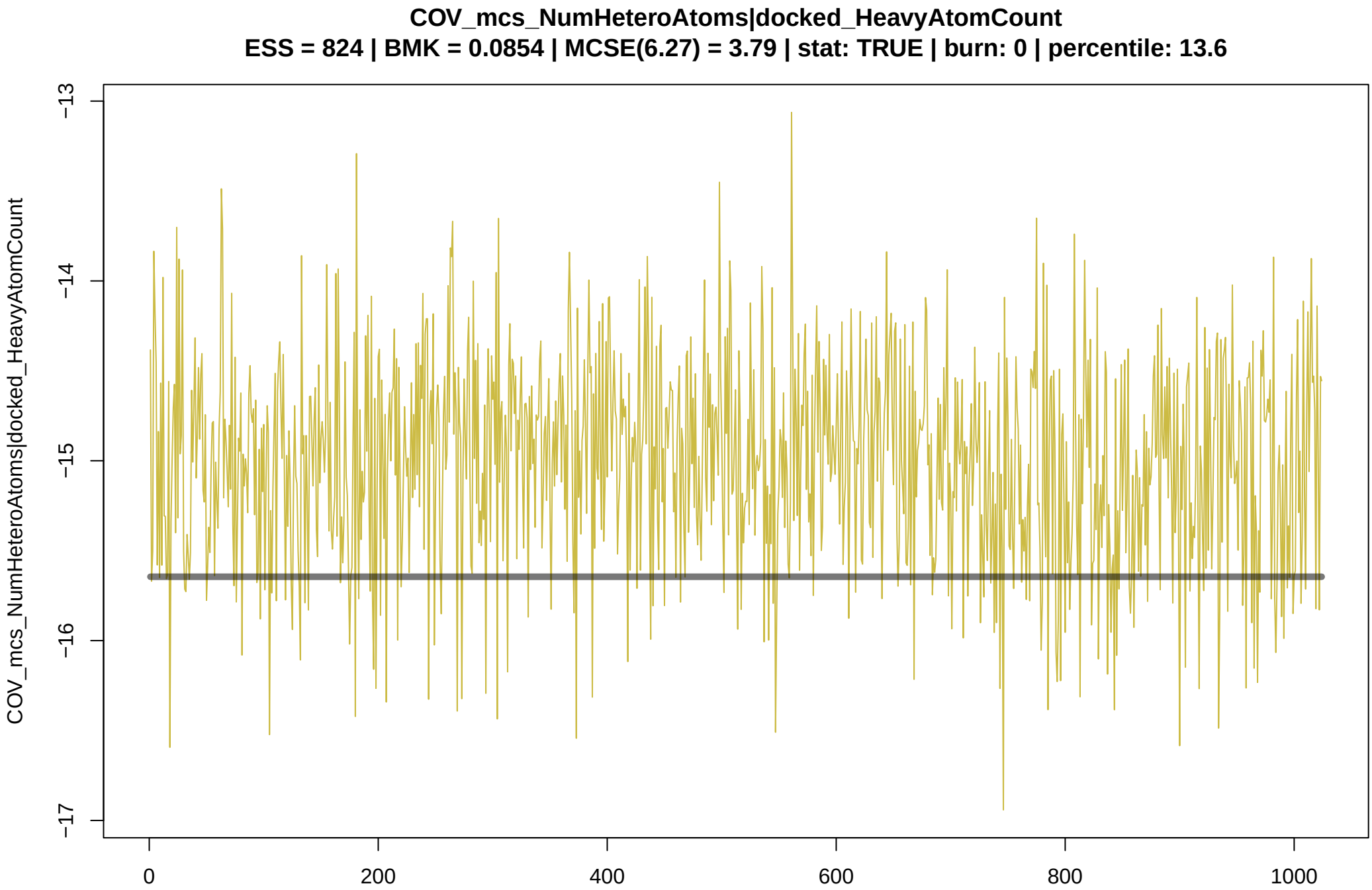

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1020 | BMK = 0.0331 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | percentile: 20.7
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.2
−1.4
−1.6
−1.8
0
200
400
600
800
1000

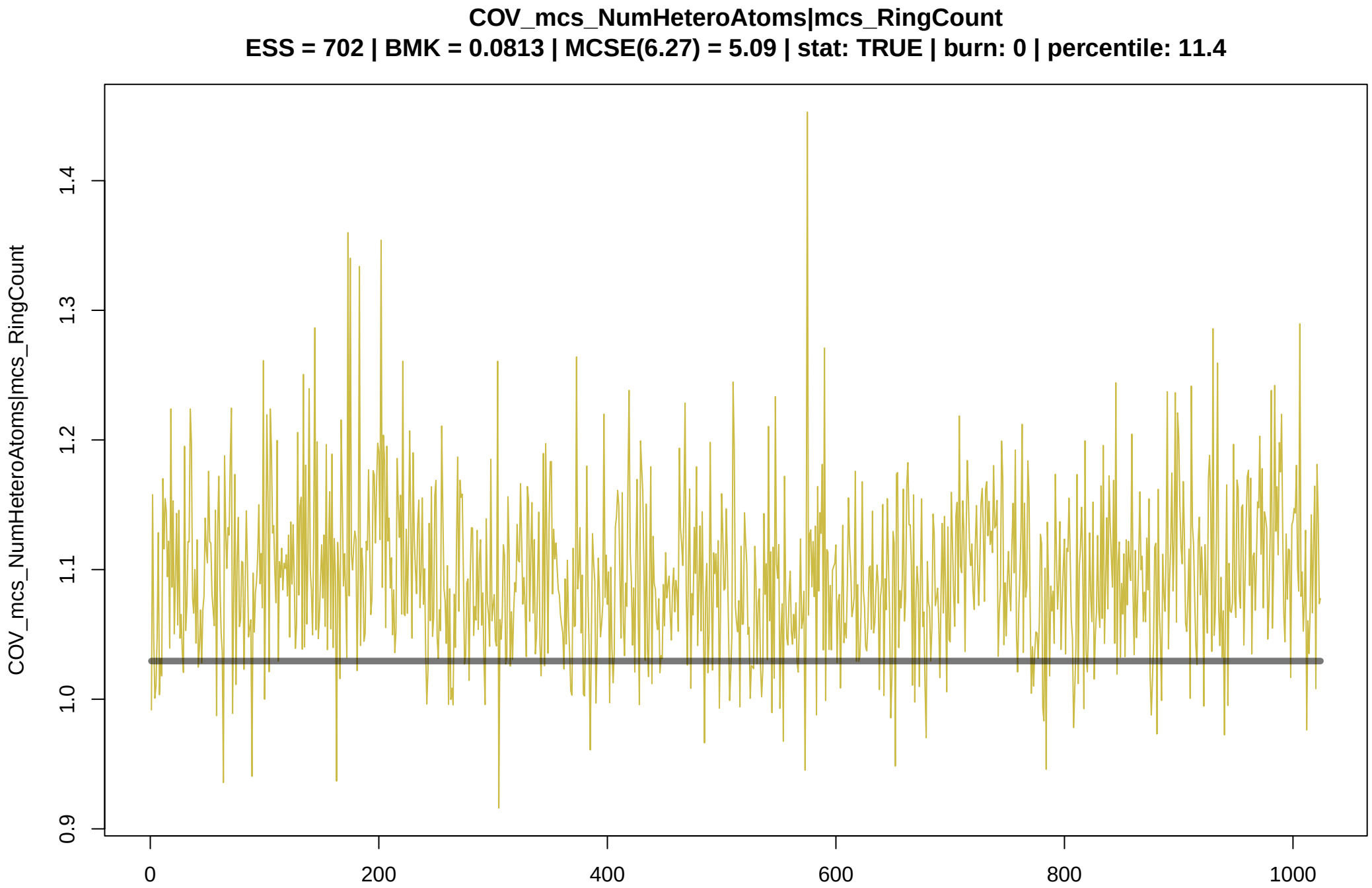

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0437 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0 | percentile: 89.4
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
45
44
43
42
41
40
0
200
400
600
800
1000

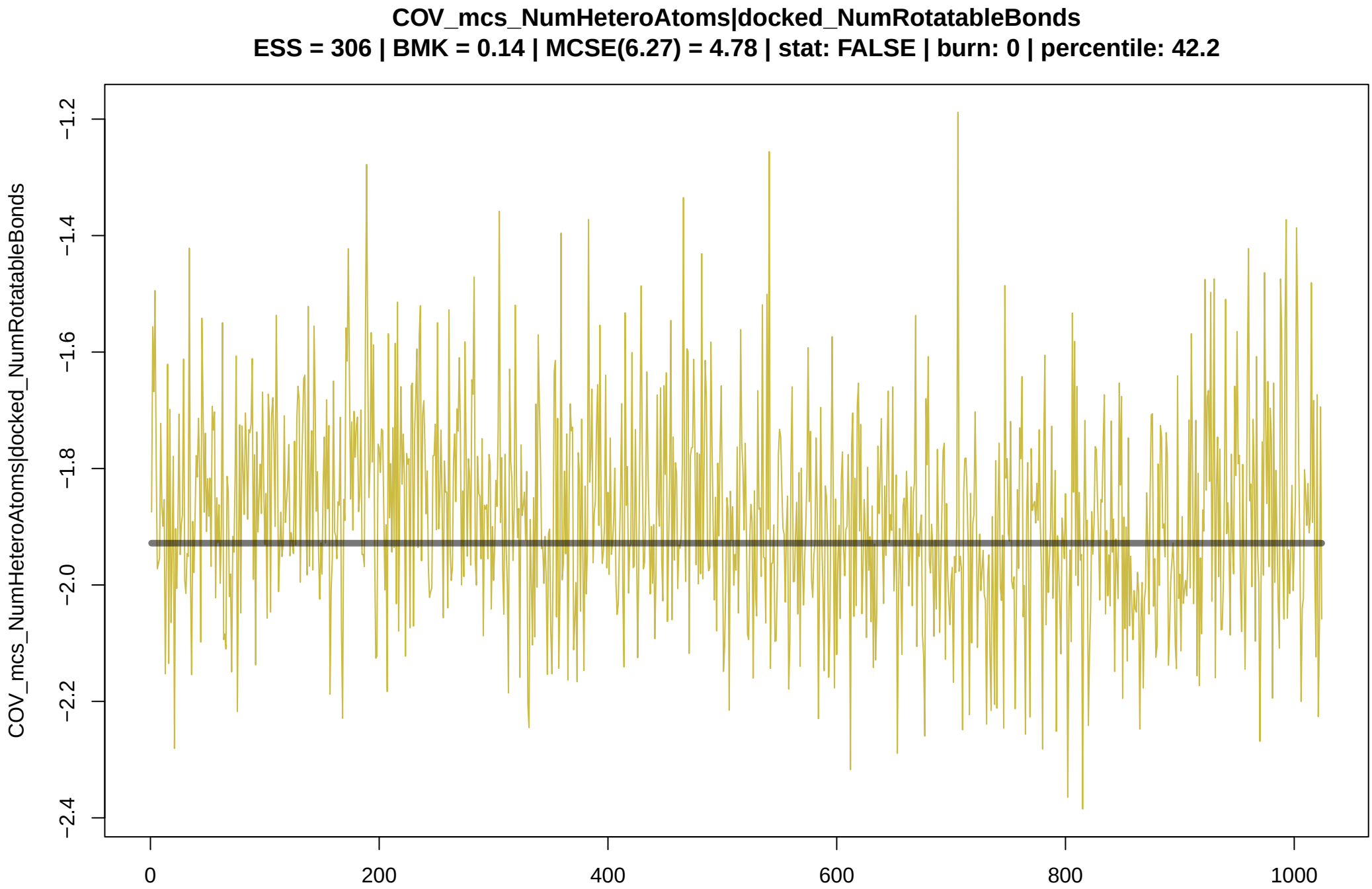

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 1020 | BMK = 0.0569 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | percentile: 14.3
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.4
−1.6
−1.8
−2.0
0
200
400
600
800
1000

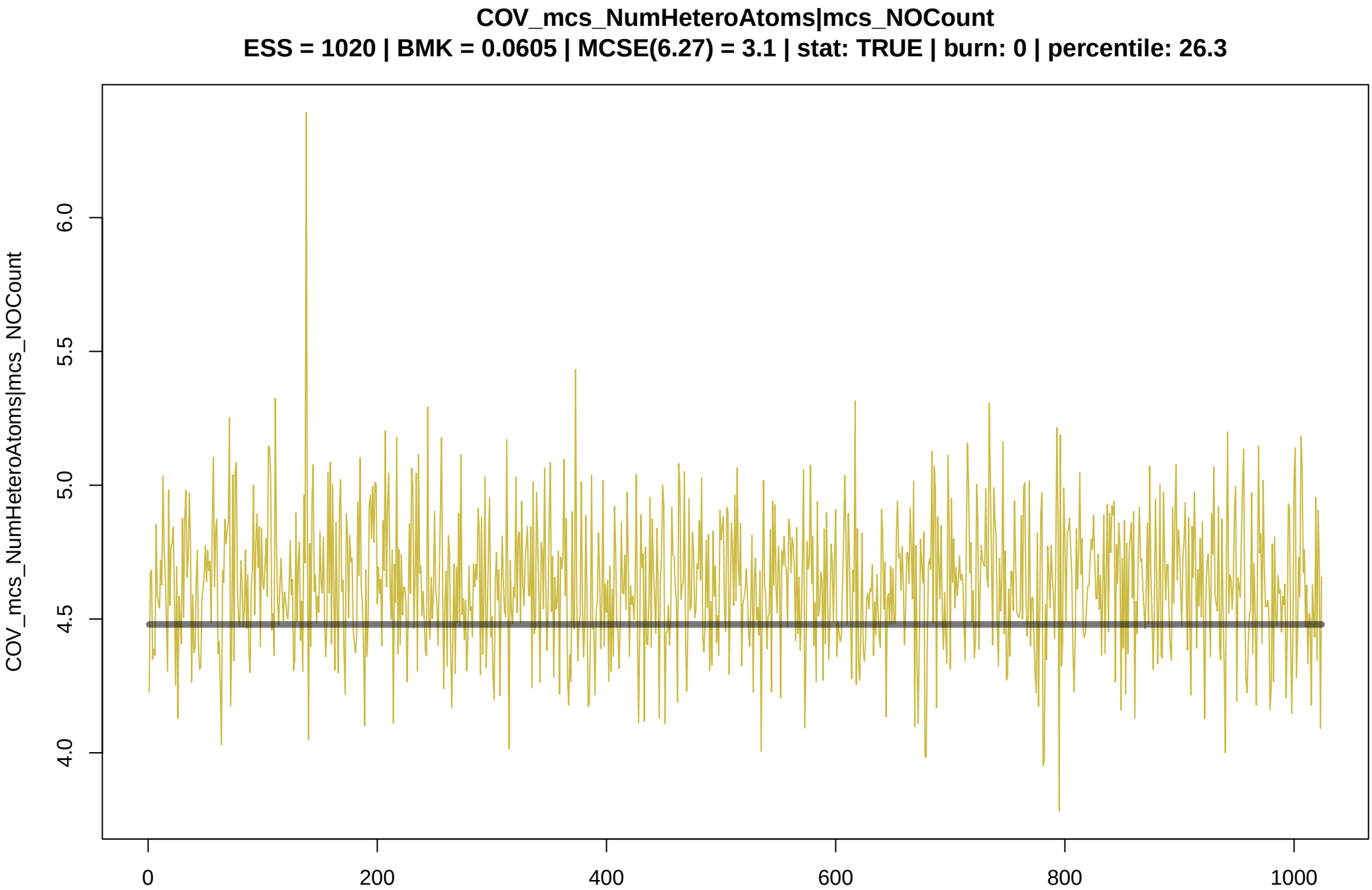

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0482 | MCSE(6.27) = 2.89 | stat: TRUE | burn: 0 | percentile: 97.6
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−11.5
−12.0
−12.5
0
200
400
600
800
1000

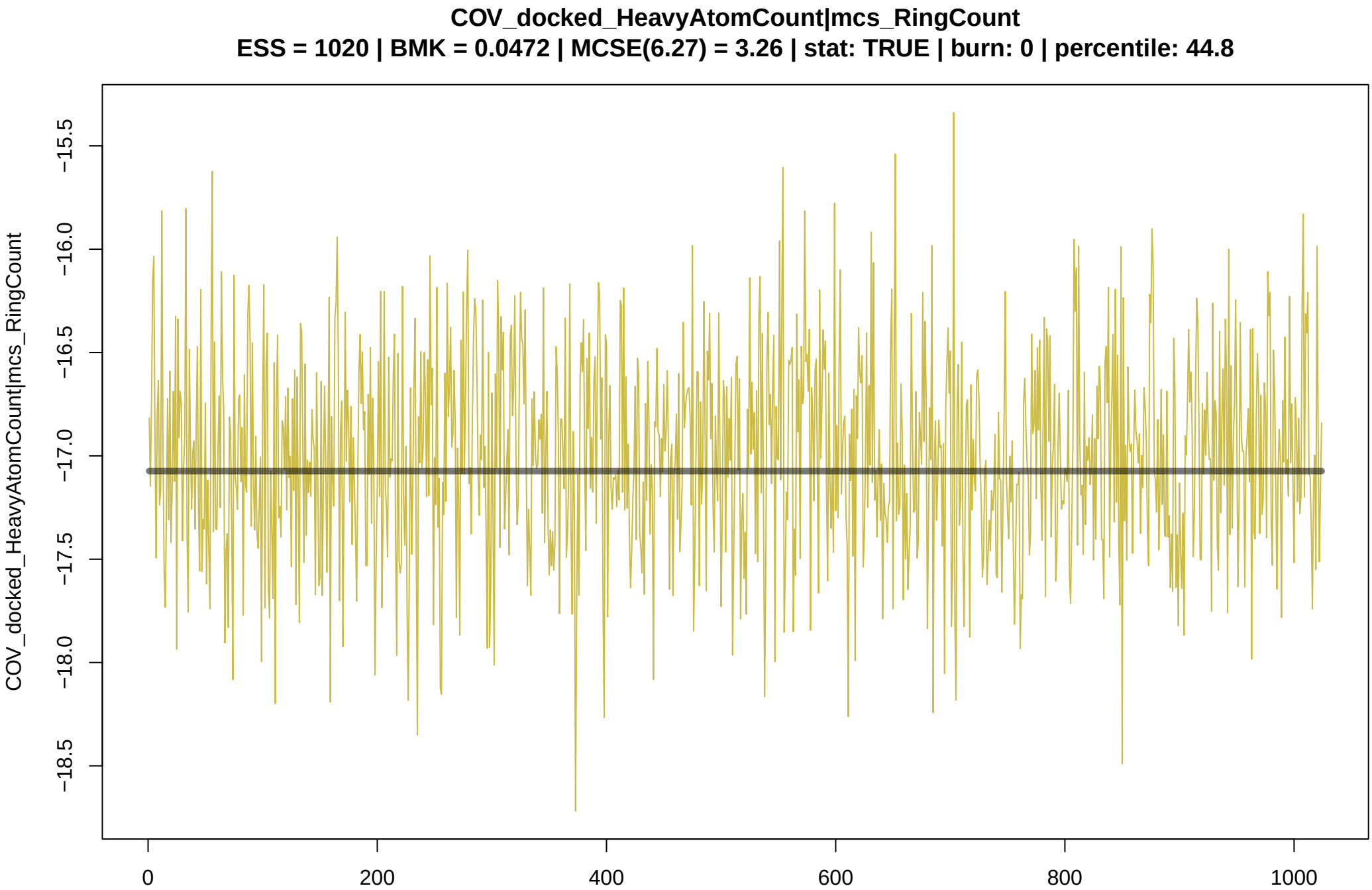

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 1020 | BMK = 0.0649 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | percentile: 60.7
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−6.5
−7.0
−7.5
−8.0
−8.5
0
200
400
600
800
1000

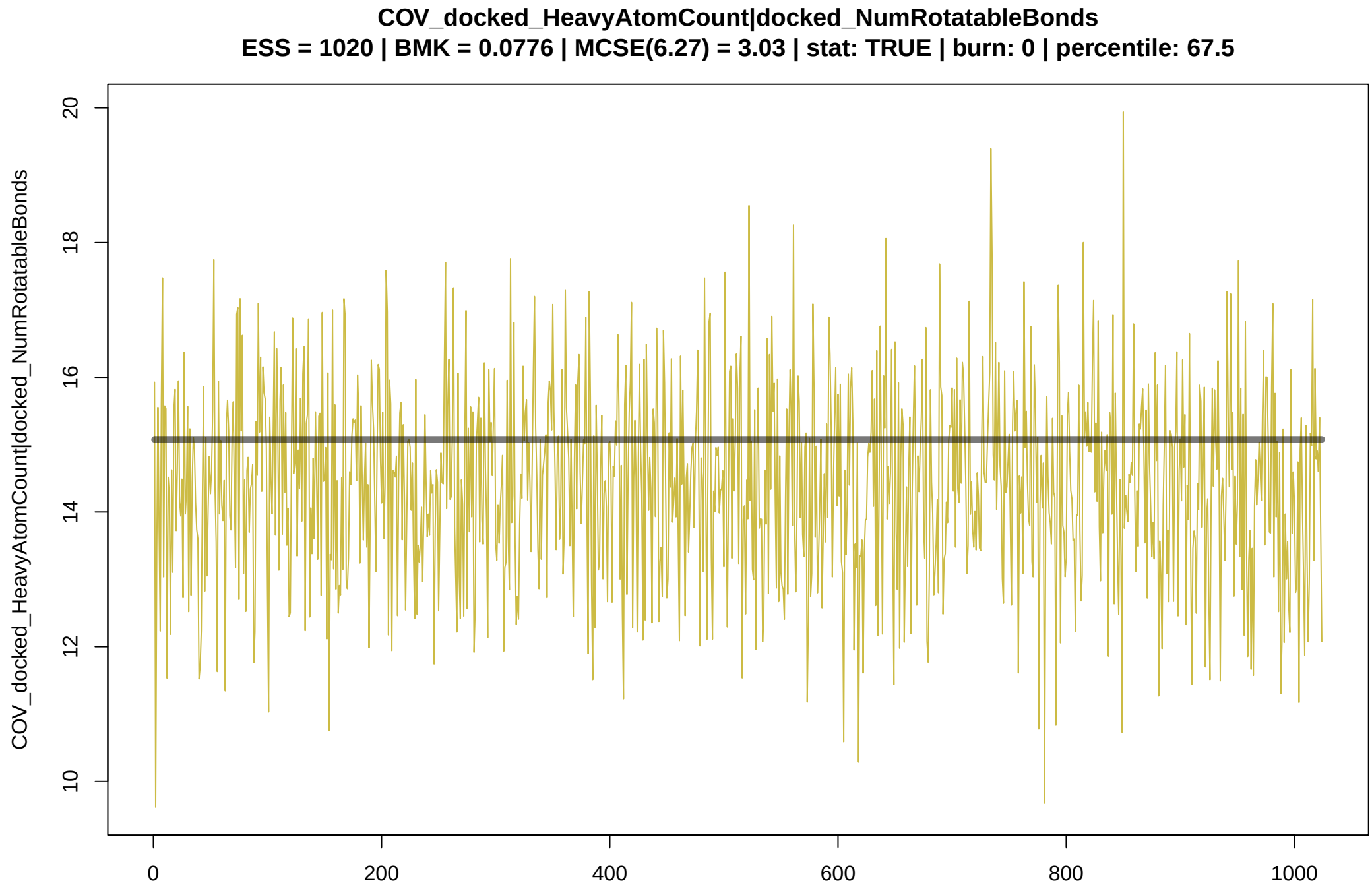

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 824 | BMK = 0.0854 | MCSE(6.27) = 3.79 | stat: TRUE | burn: 0 | percentile: 13.6
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−13
−14
−15
−16
−17
0
200
400
600
800
1000

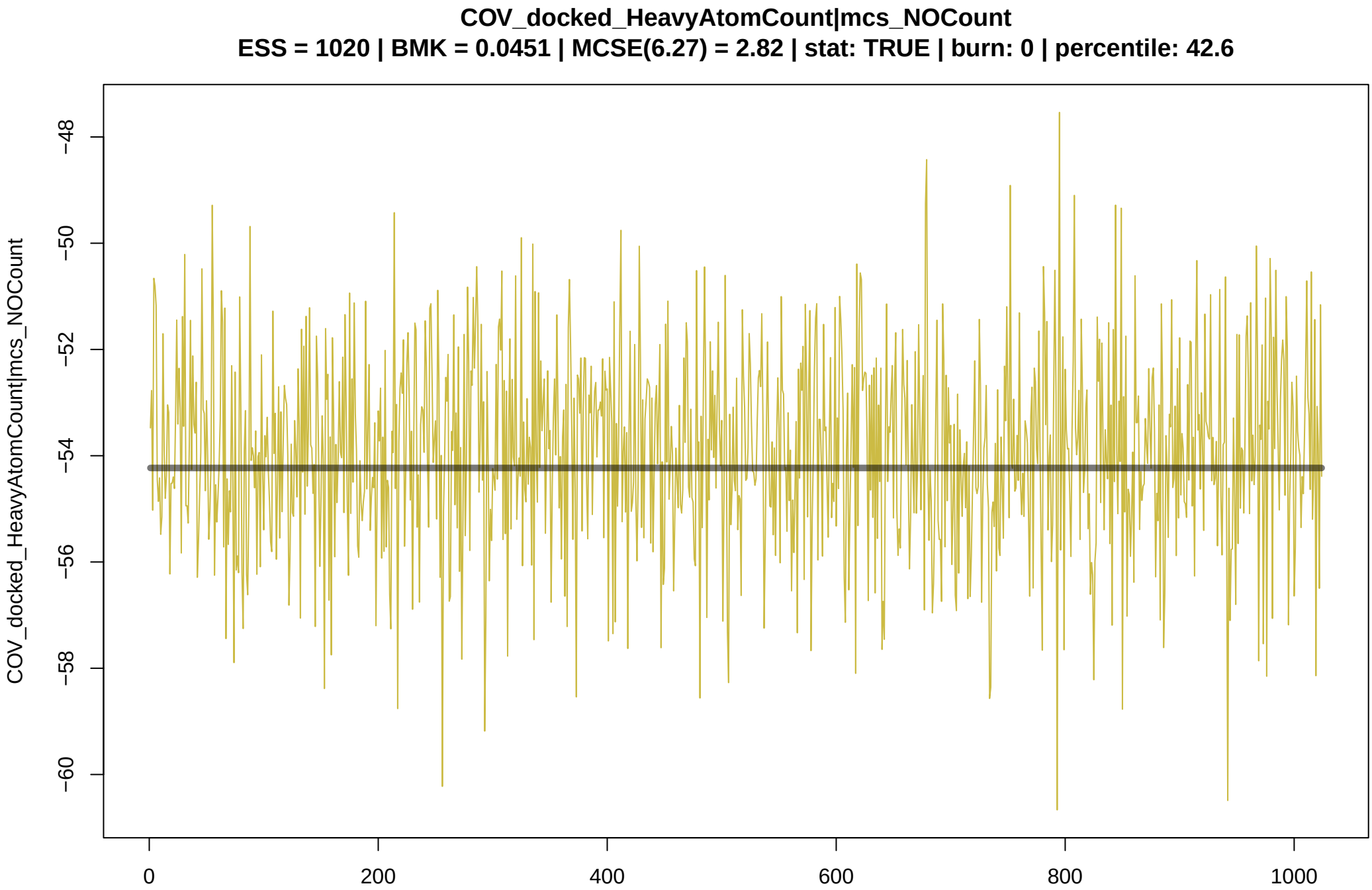

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 702 | BMK = 0.0813 | MCSE(6.27) = 5.09 | stat: TRUE | burn: 0 | percentile: 11.4
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.9
1.0
1.1
1.2
1.3
1.4
0
200
400
600
800
1000

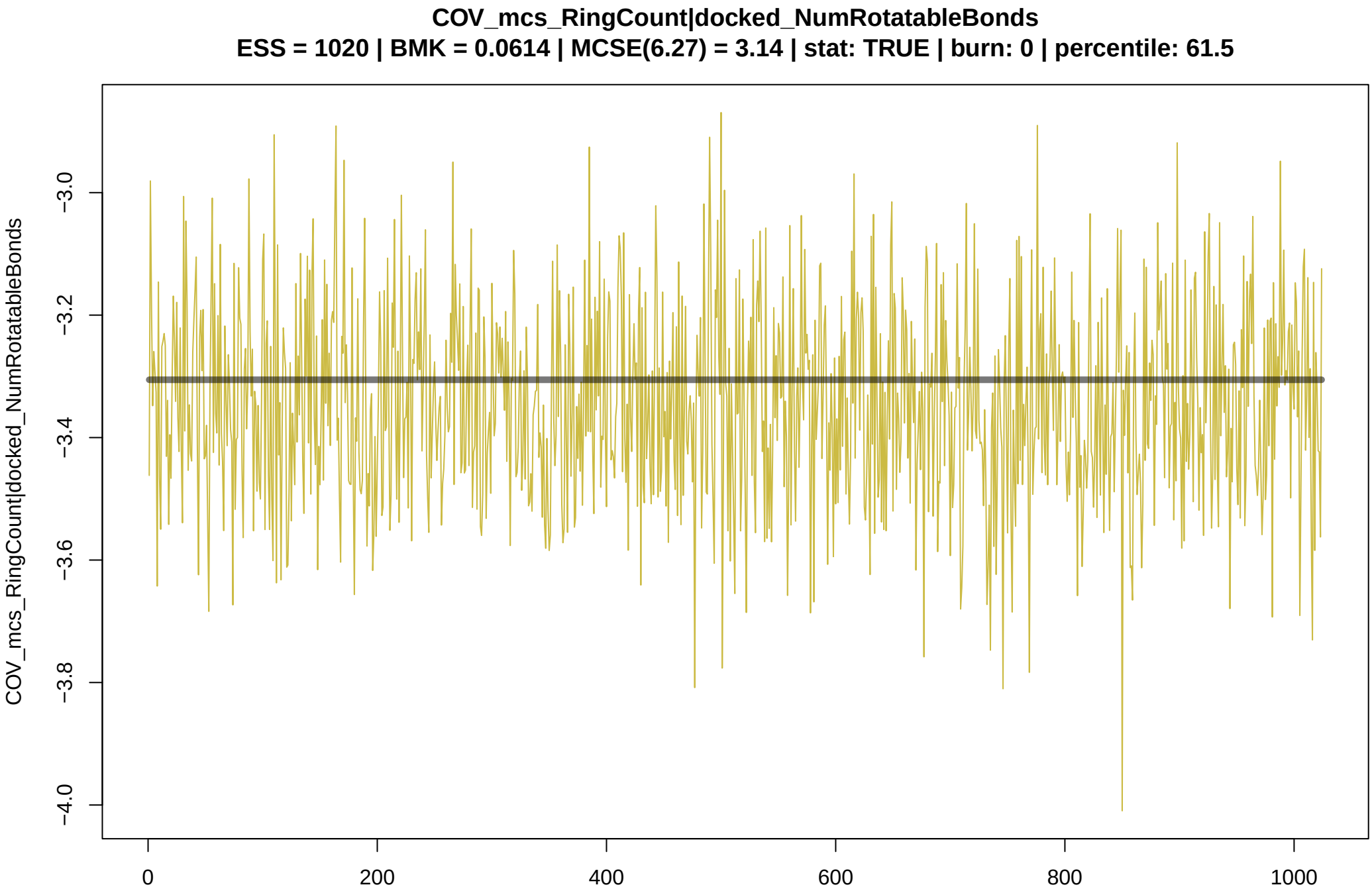

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 306 | BMK = 0.14 | MCSE(6.27) = 4.78 | stat: FALSE | burn: 0 | percentile: 42.2
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.2
−1.4
−1.6
−1.8
−2.0
−2.2
−2.4
0
200
400
600
800
1000

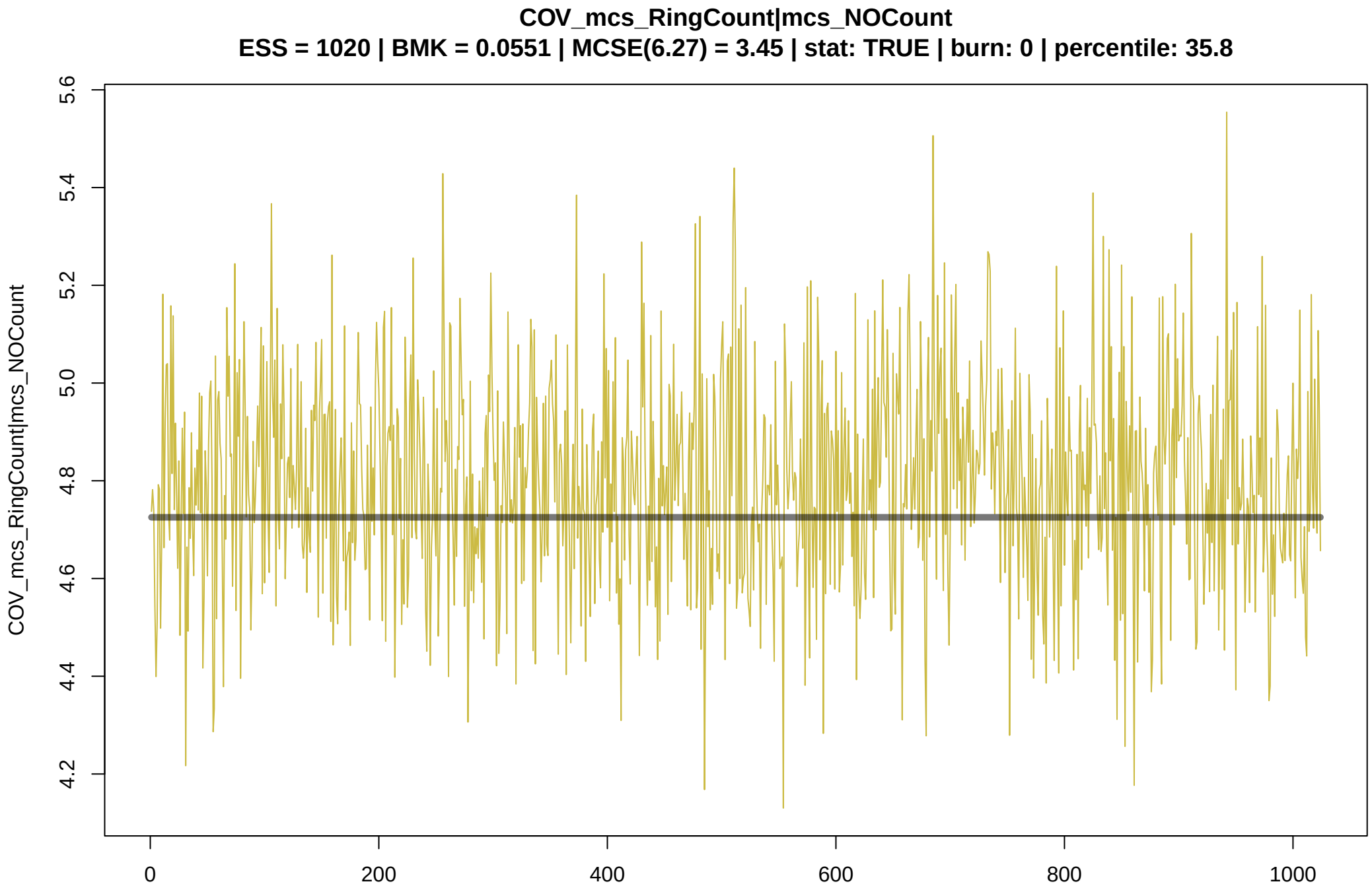

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 1020 | BMK = 0.0605 | MCSE(6.27) = 3.1 | stat: TRUE | burn: 0 | percentile: 26.3
COV_mcs_NumHeteroAtoms|mcs_NOCount
4.0
4.5
5.0
5.5
6.0
0
200
400
600
800
1000

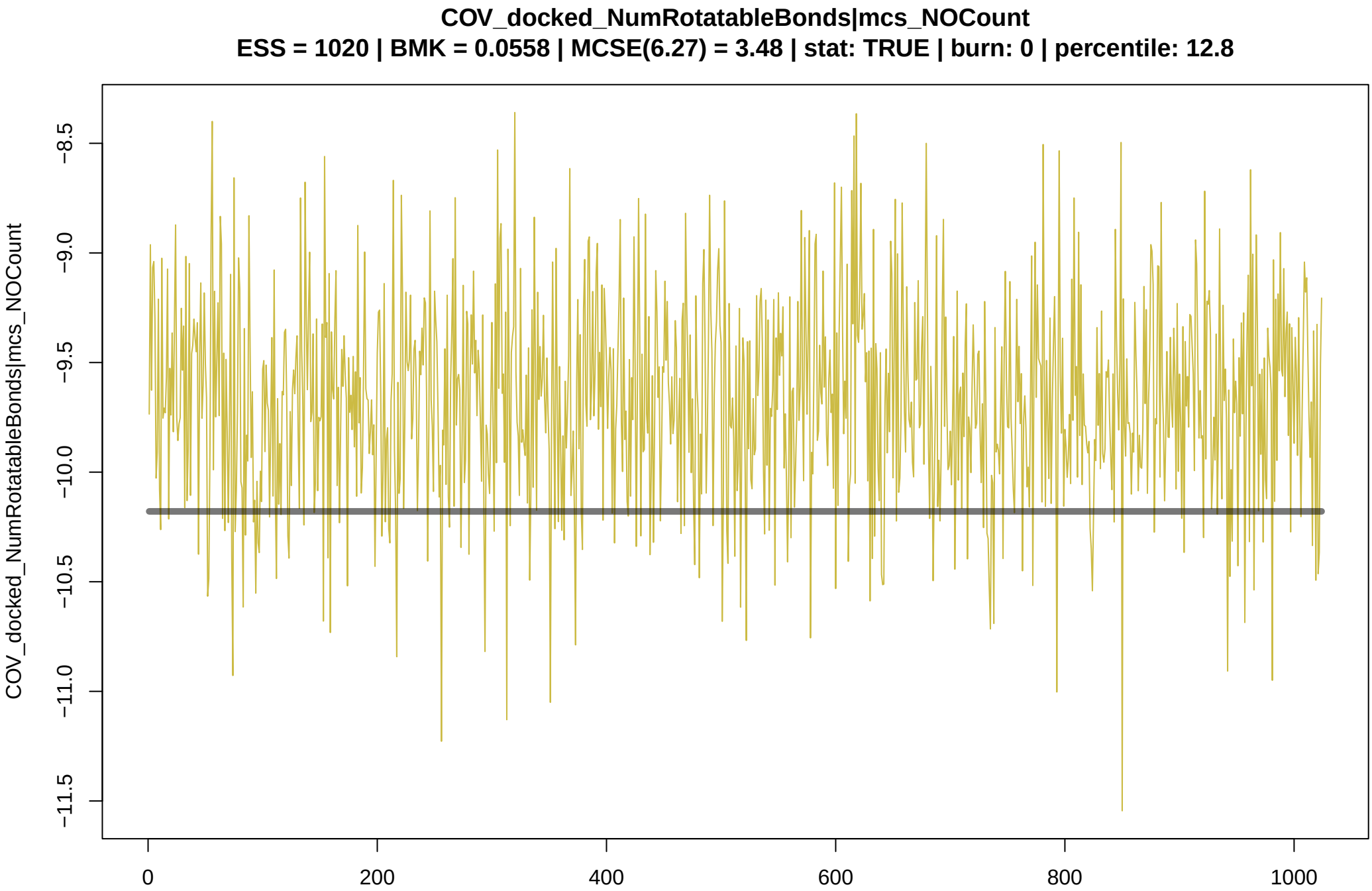

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1020 | BMK = 0.0472 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0 | percentile: 44.8
COV_docked_HeavyAtomCount|mcs_RingCount
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 1020 | BMK = 0.0776 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | percentile: 67.5
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
10
12
14
16
18
20
0
200
400
600
800
1000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1020 | BMK = 0.0451 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | percentile: 42.6
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 = 0.0614 | MCSE(6.27) = 3.14 | stat: TRUE | burn: 0 | percentile: 61.5
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 = 0.0551 | MCSE(6.27) = 3.45 | stat: TRUE | burn: 0 | percentile: 35.8
COV_mcs_RingCount|mcs_NOCount
4.2
4.4
4.6
4.8
5.0
5.2
5.4
5.6
0
200
400
600
800
1000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 1020 | BMK = 0.0558 | MCSE(6.27) = 3.48 | stat: TRUE | burn: 0 | percentile: 12.8
COV_docked_NumRotatableBonds|mcs_NOCount
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
0
200
400
600
800
1000