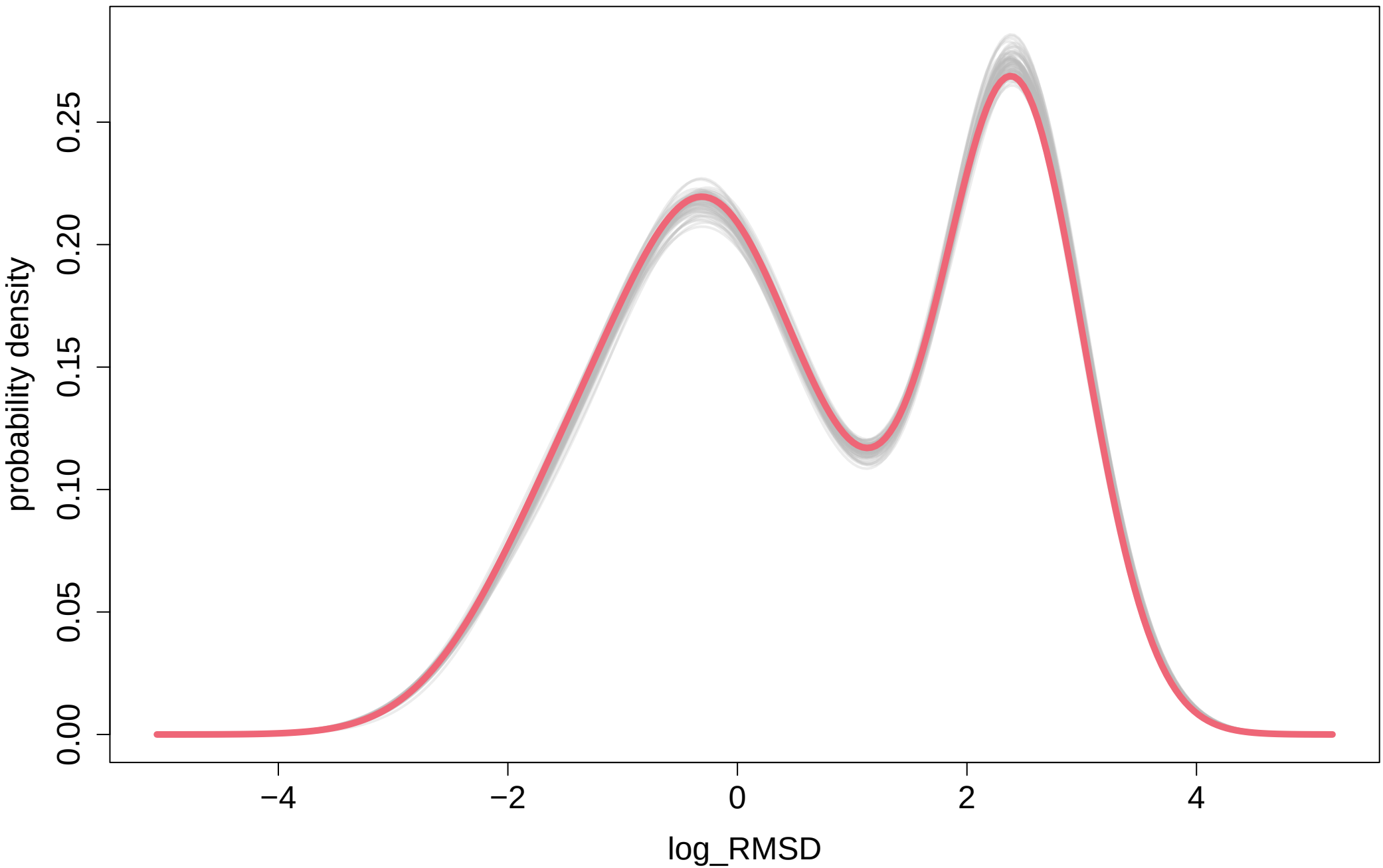
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 1
max MCSE = 11.2930312525025
all stationary: FALSE
burn: 2040
min percent.: 0

−− STATS 2D −−
min ESS = 1744.67700343025
max BMK = 0.072604235437873 6
max MCSE = 3.15596740142643
all stationary: FALSE
burn: 0
min percent.: 1.123046875

−− STATS 1D −−
min ESS = 2.2044604925031e−16
max BMK = 0.247857903520801
max MCSE = NaN
all stationary: FALSE
burn: 0
min percent.: 0

Occupied clusters: 11 of 64
LL: −125000 +− 21


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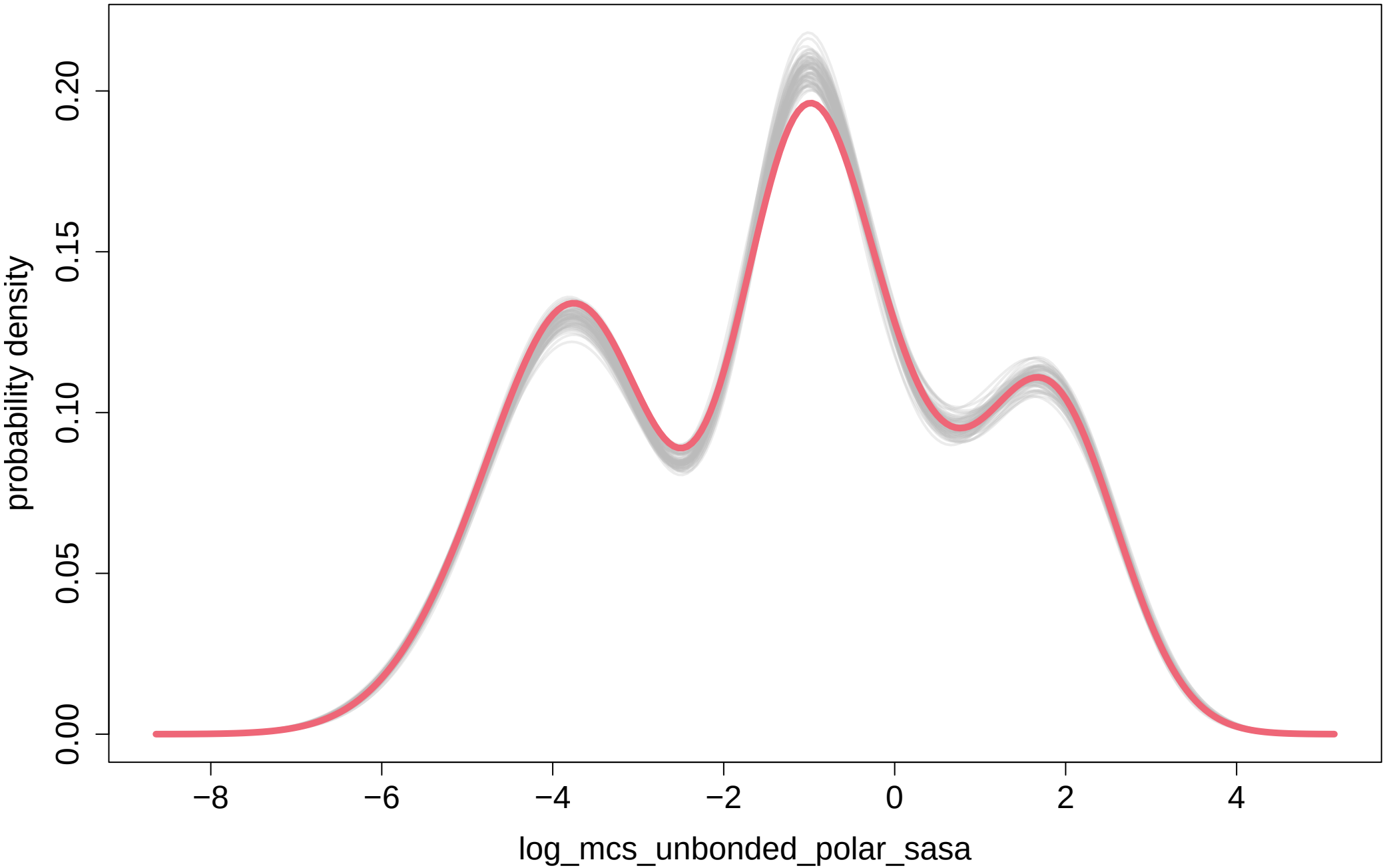
0.10
0.15
0.20
0.25
−4
−2
0
2
4
log_RMSD


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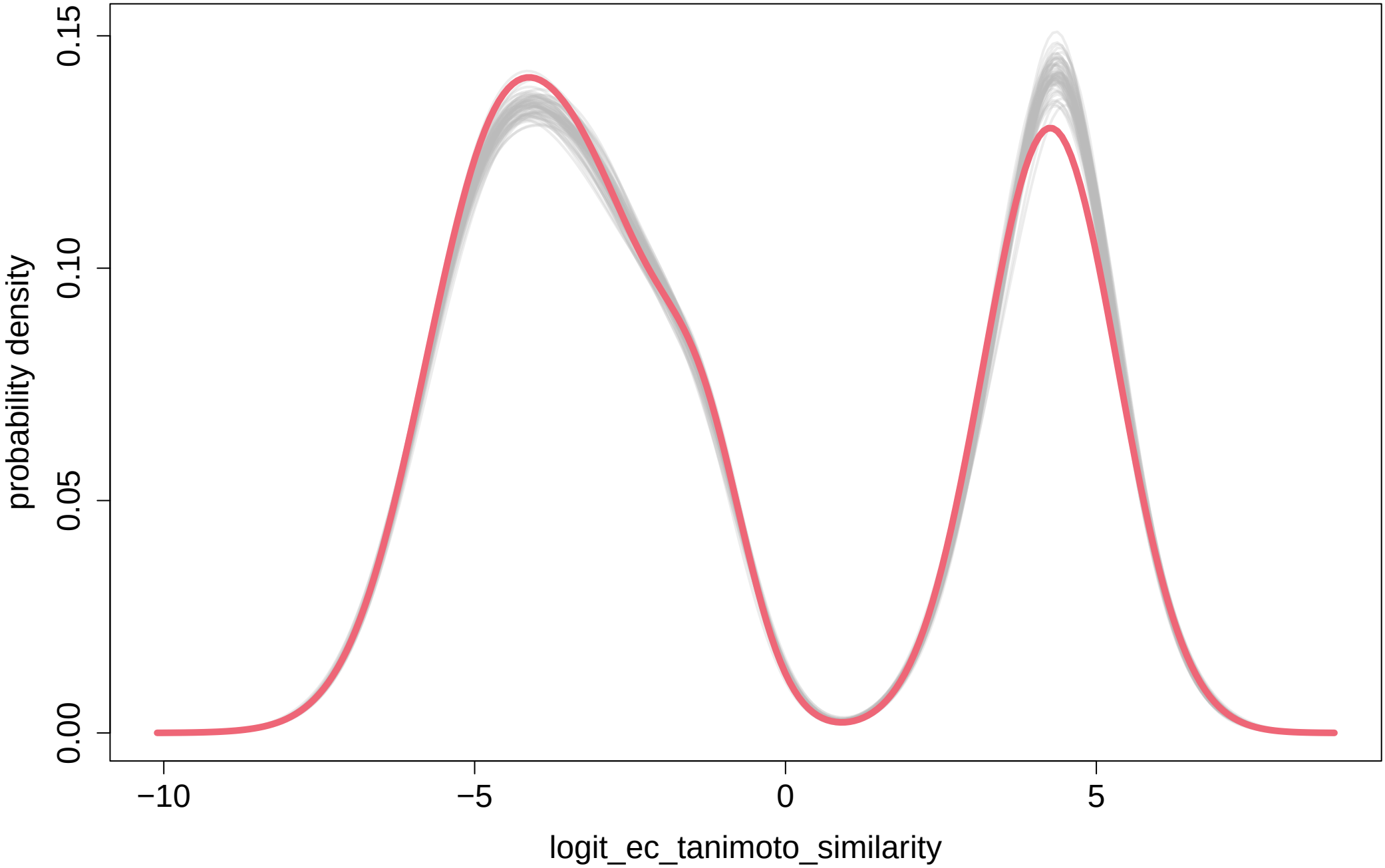
−8
−6
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa


probability density
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0.15
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−5
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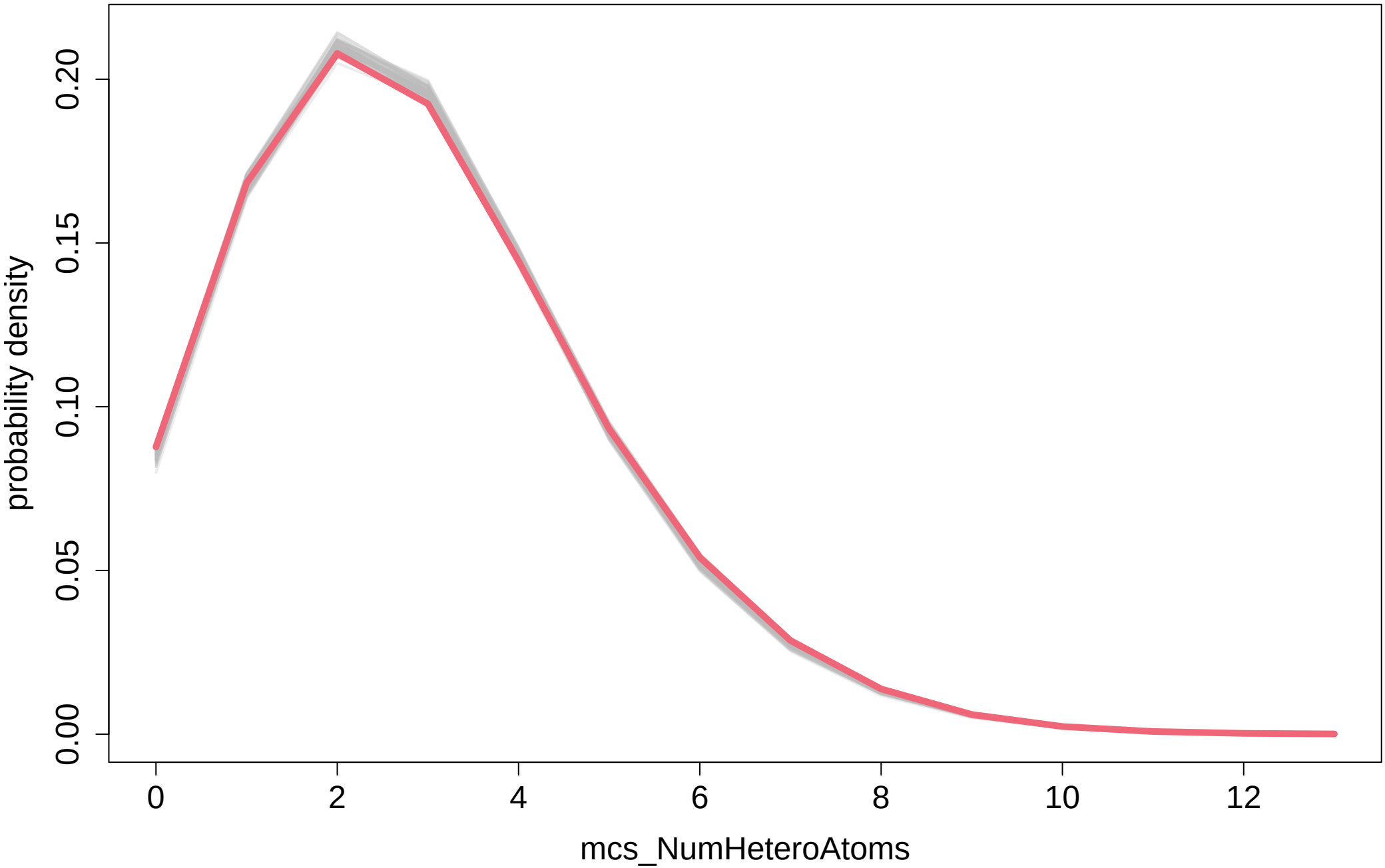
5
logit_ec_tanimoto_similarity


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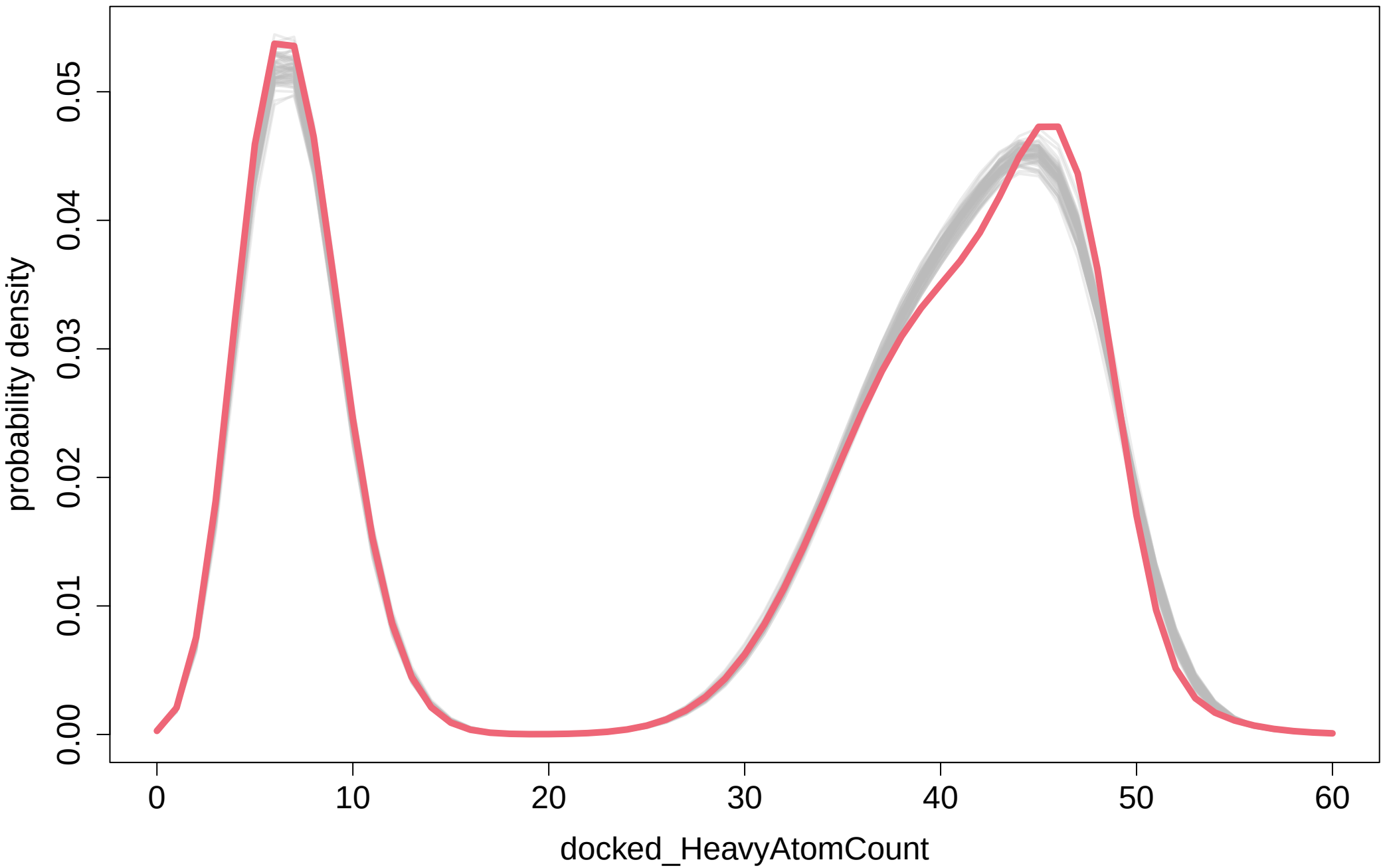
0.15
0.20
0
2
4
6
8
10
12
mcs_NumHeteroAtoms


probability density
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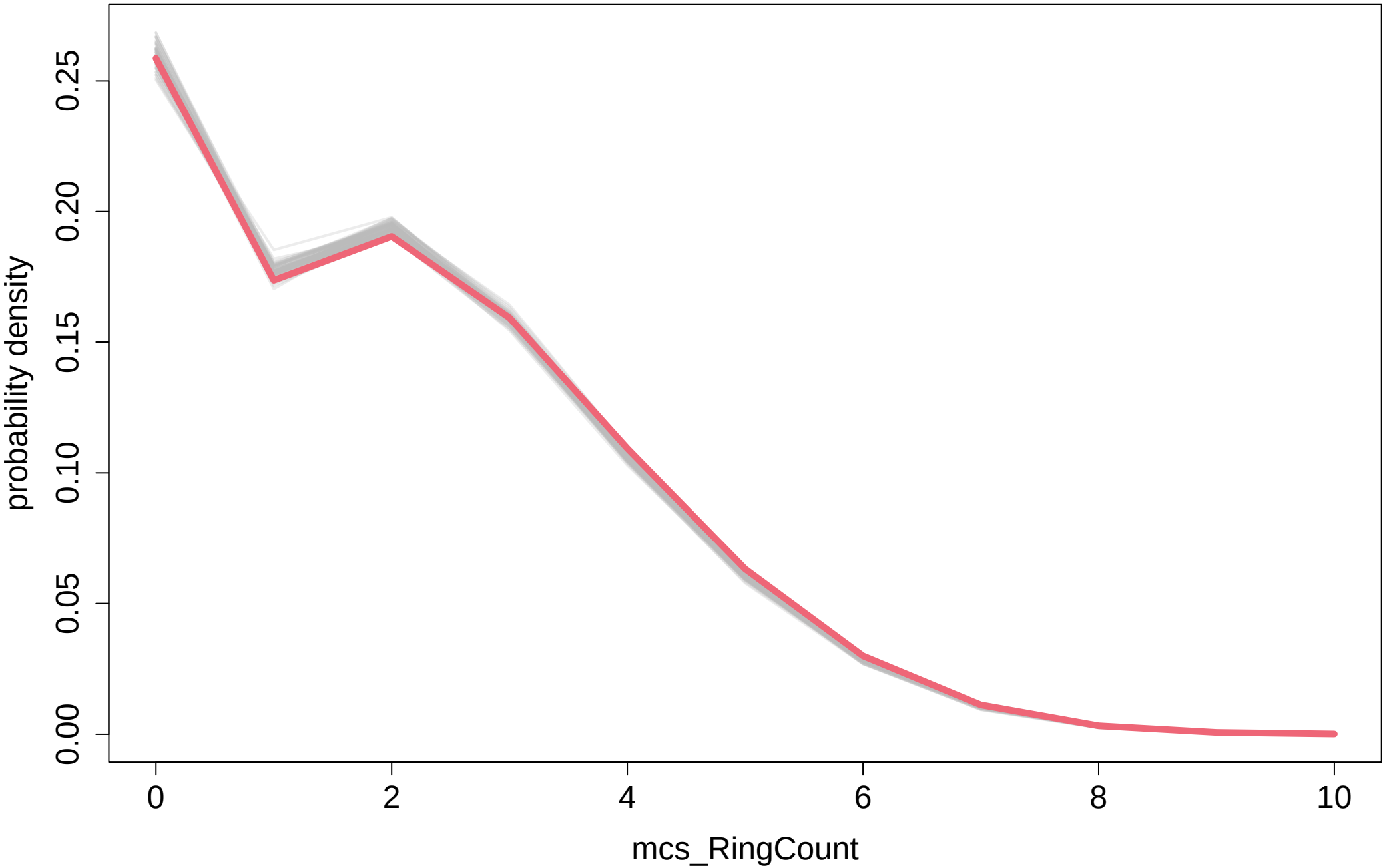
0.02
0.03
0.04
0.05
0
10
20
30
40
50
60
docked_HeavyAtomCount


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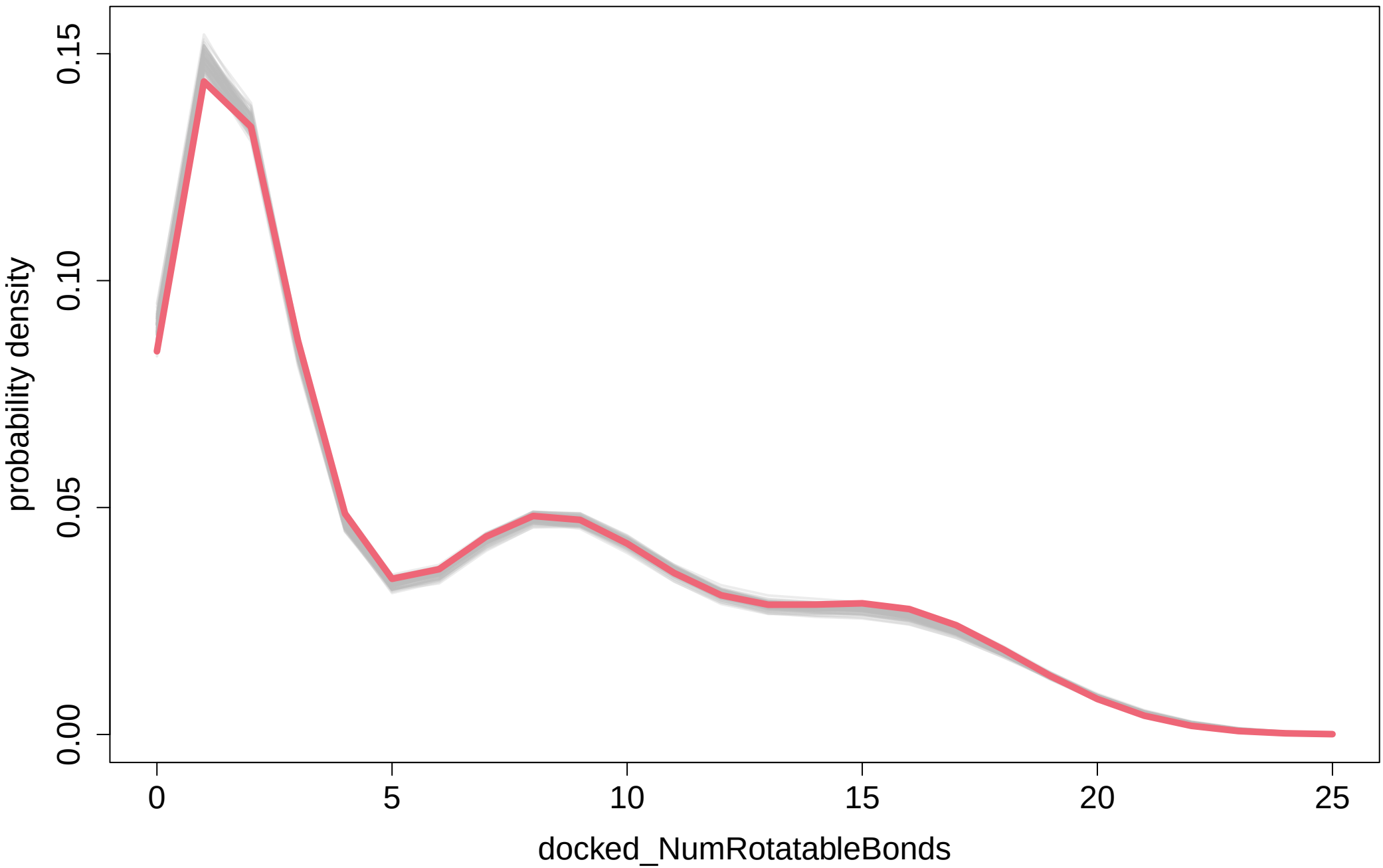
0.15
0.20
0.25
0
2
4
6
8
10
mcs_RingCount


probability density
0.00
0.05
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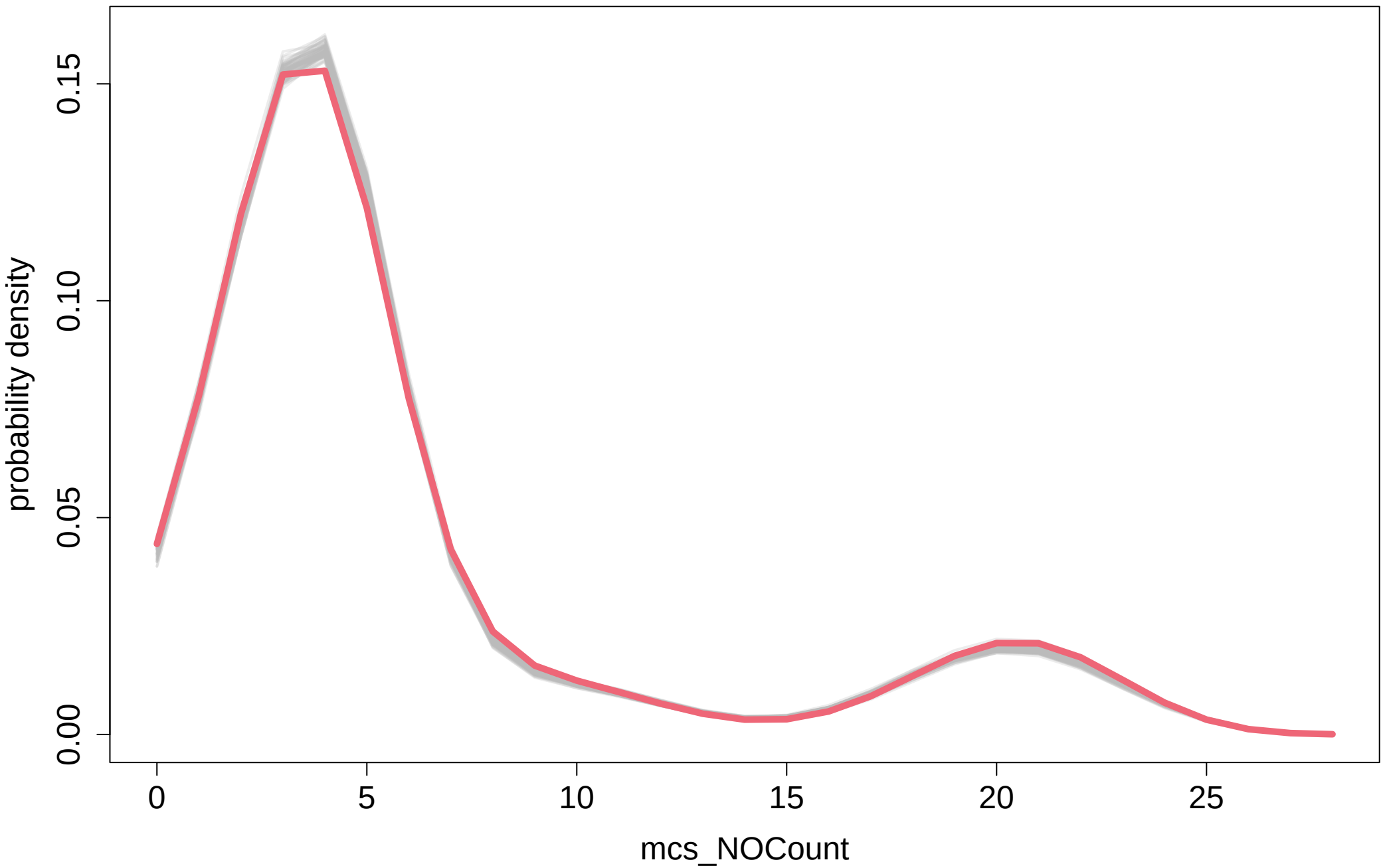
0.15
0
5
10
15
20
25
docked_NumRotatableBonds


probability density
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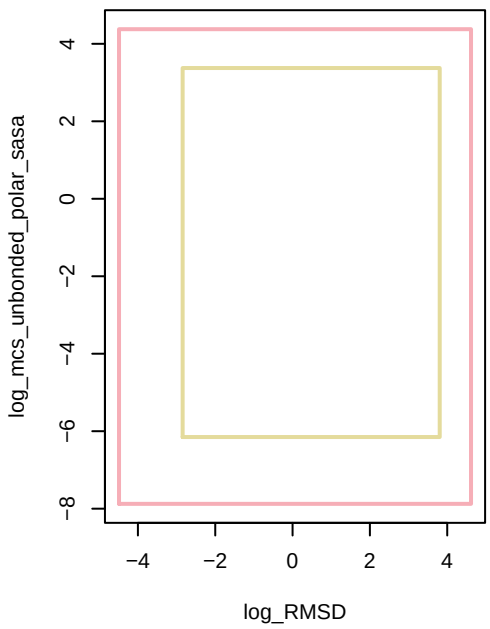
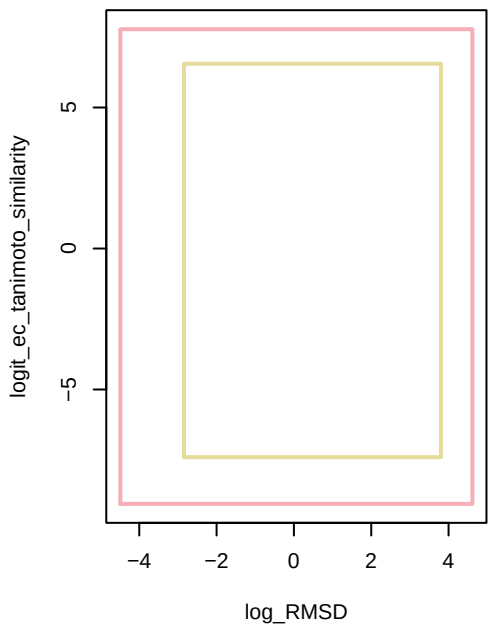
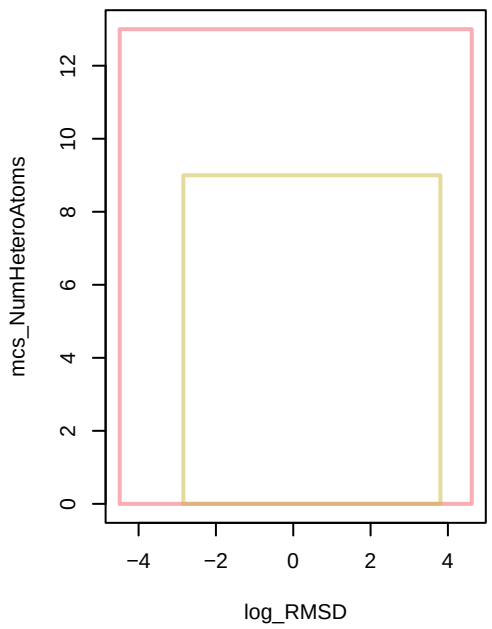
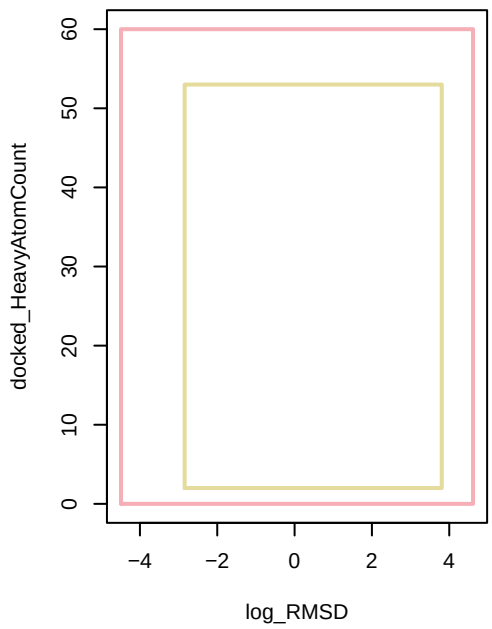
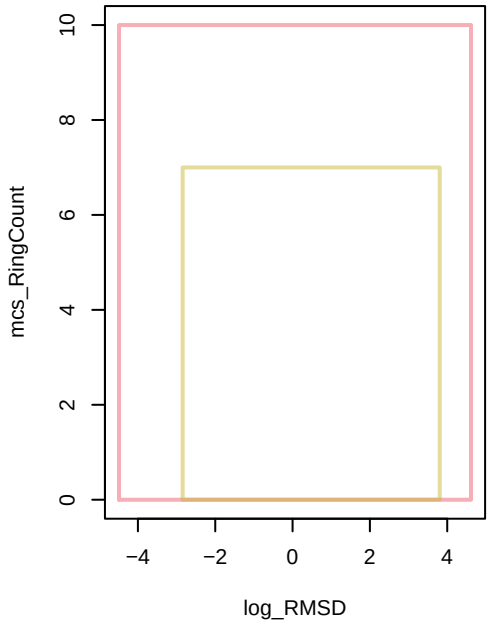
0.10
0.15
0
5
10
15
20
25
mcs_NOCount

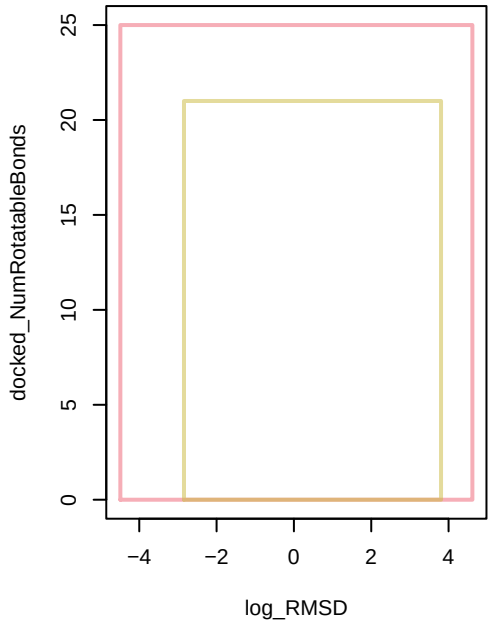

log_mcs_unbonded_polar_sasa
log_RMSD

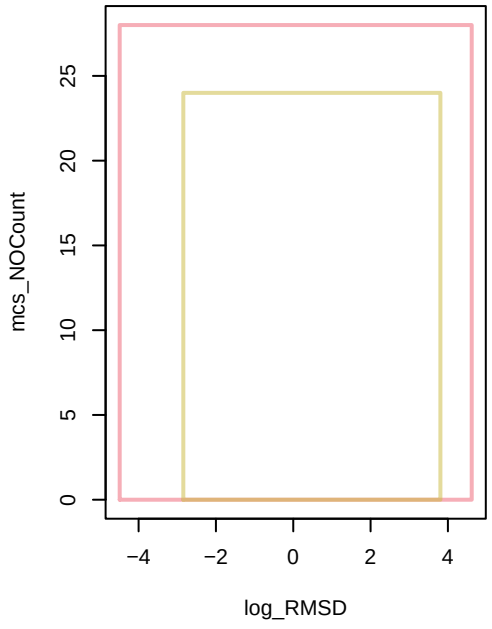

logit_ec_tanimoto_similarity
log_RMSD

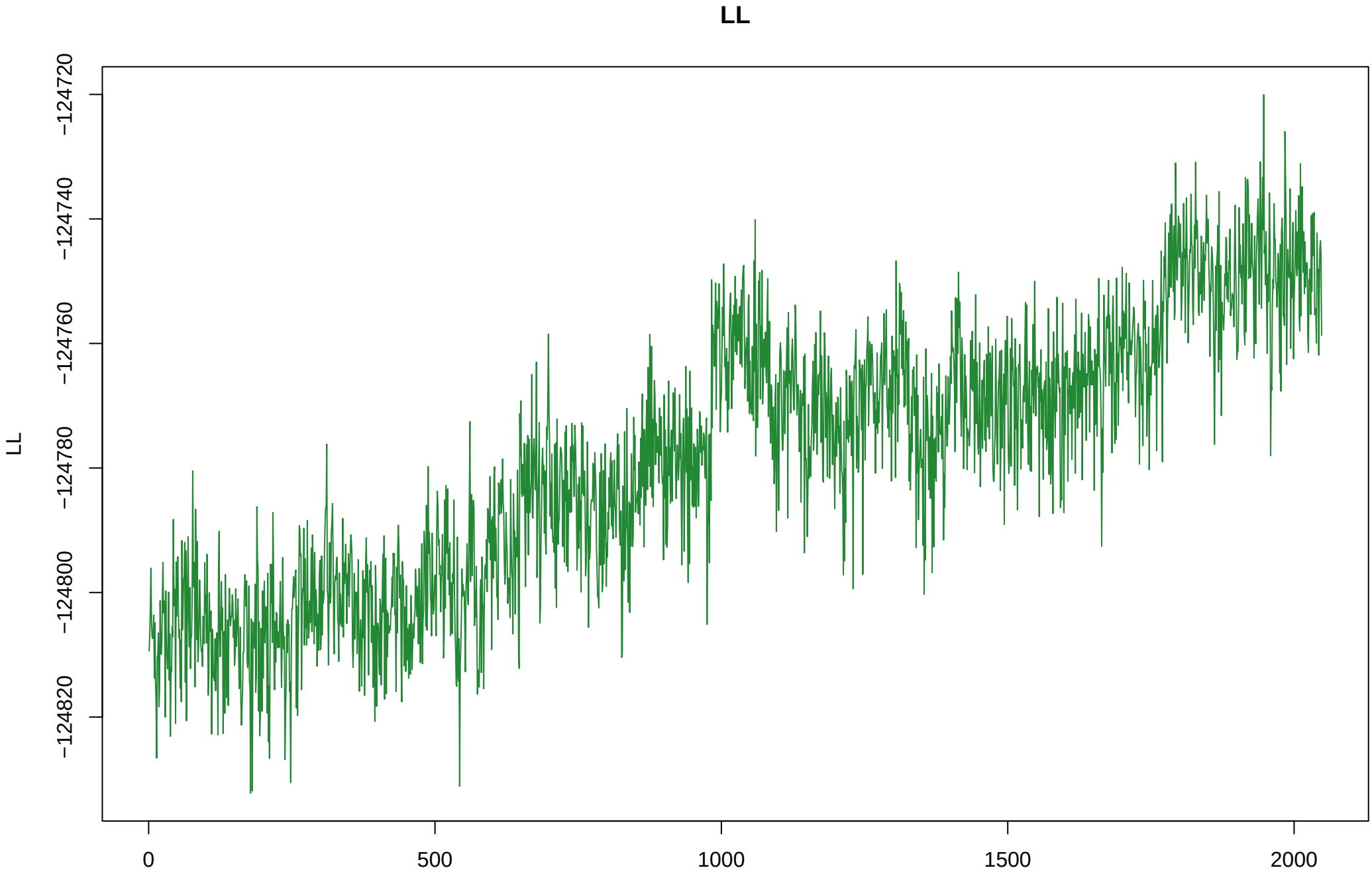

mcs_NumHeteroAtoms
log_RMSD

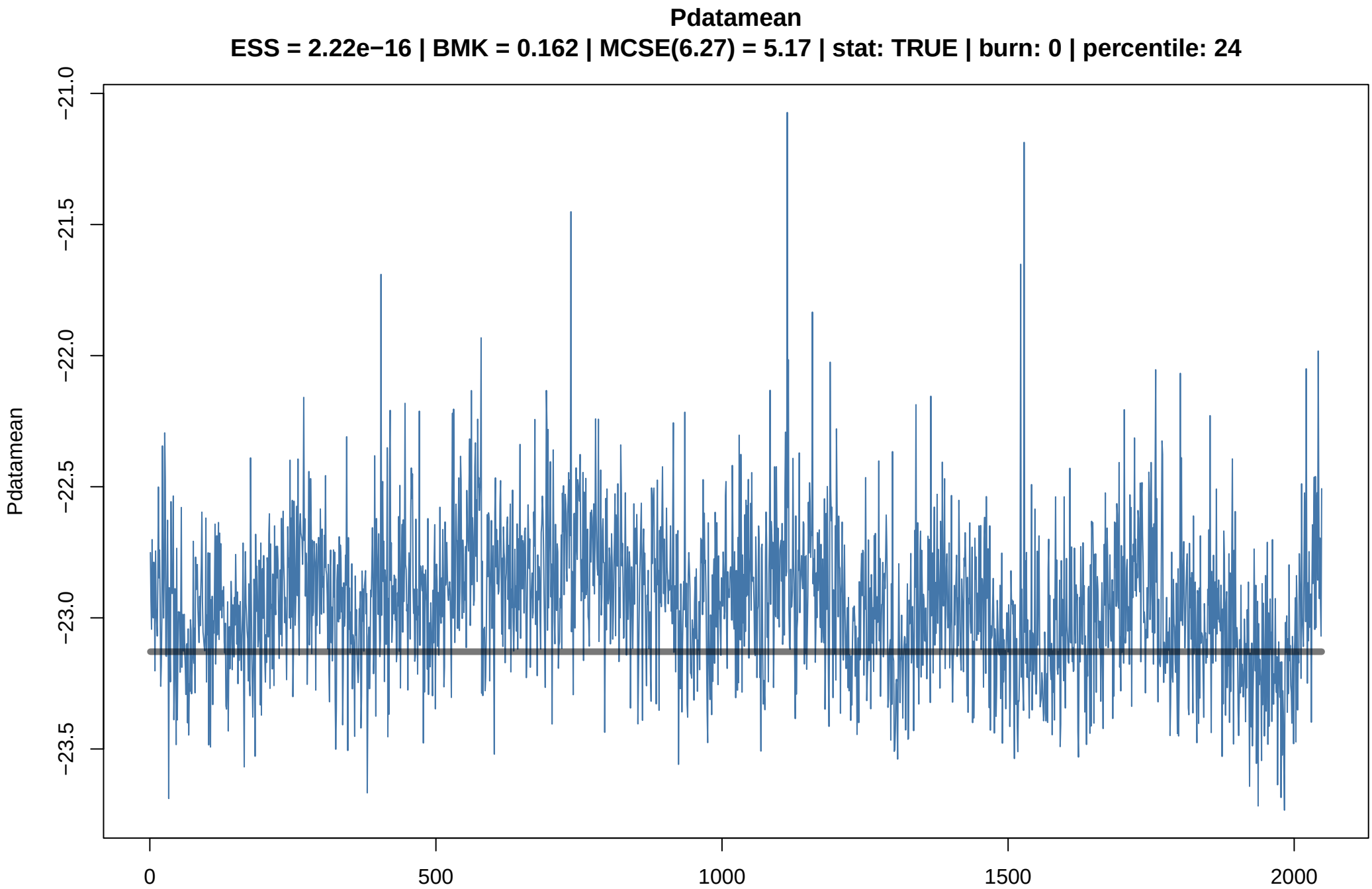

docked_HeavyAtomCount
log_RMSD

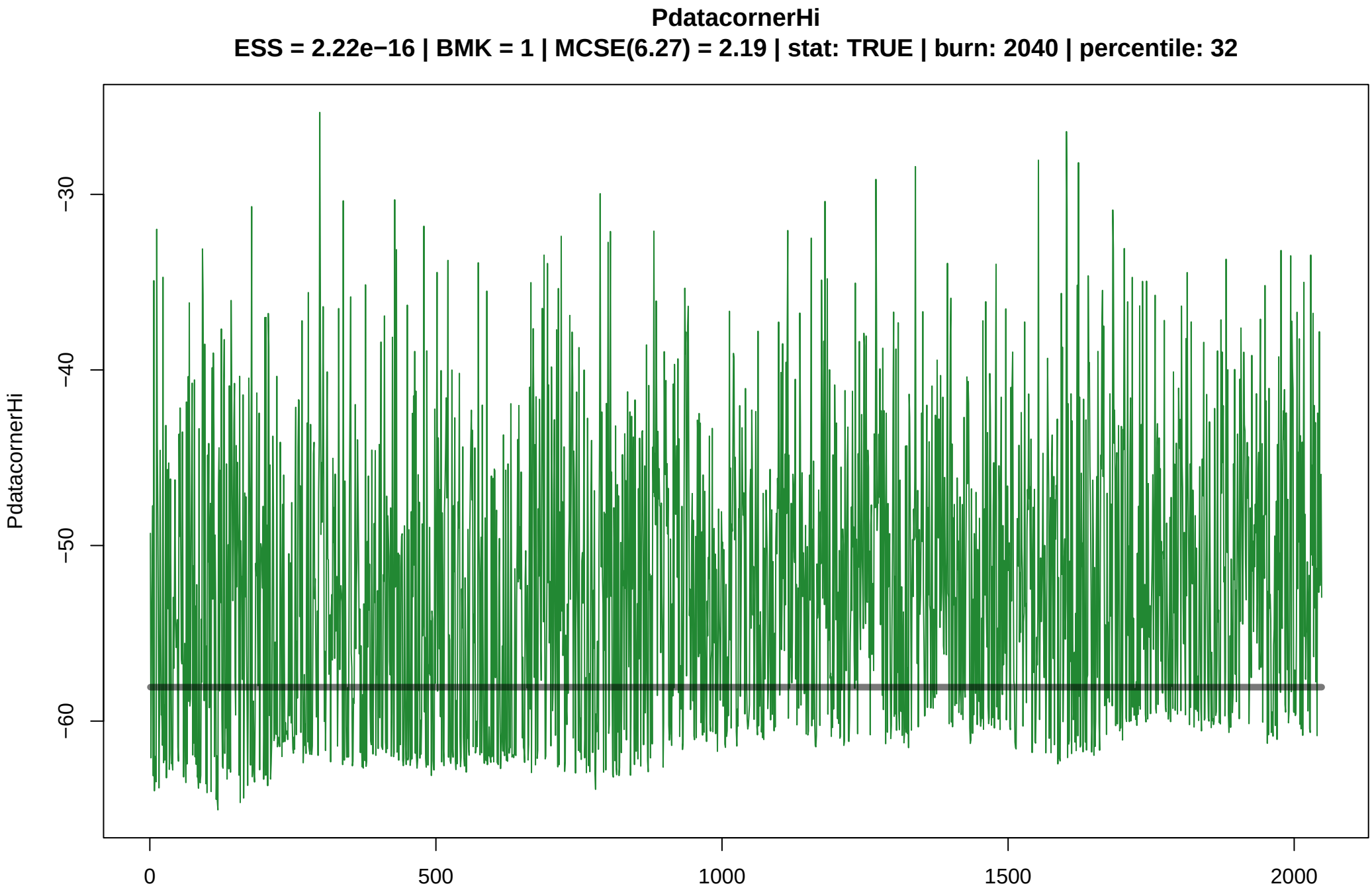

mcs_RingCount
log_RMSD

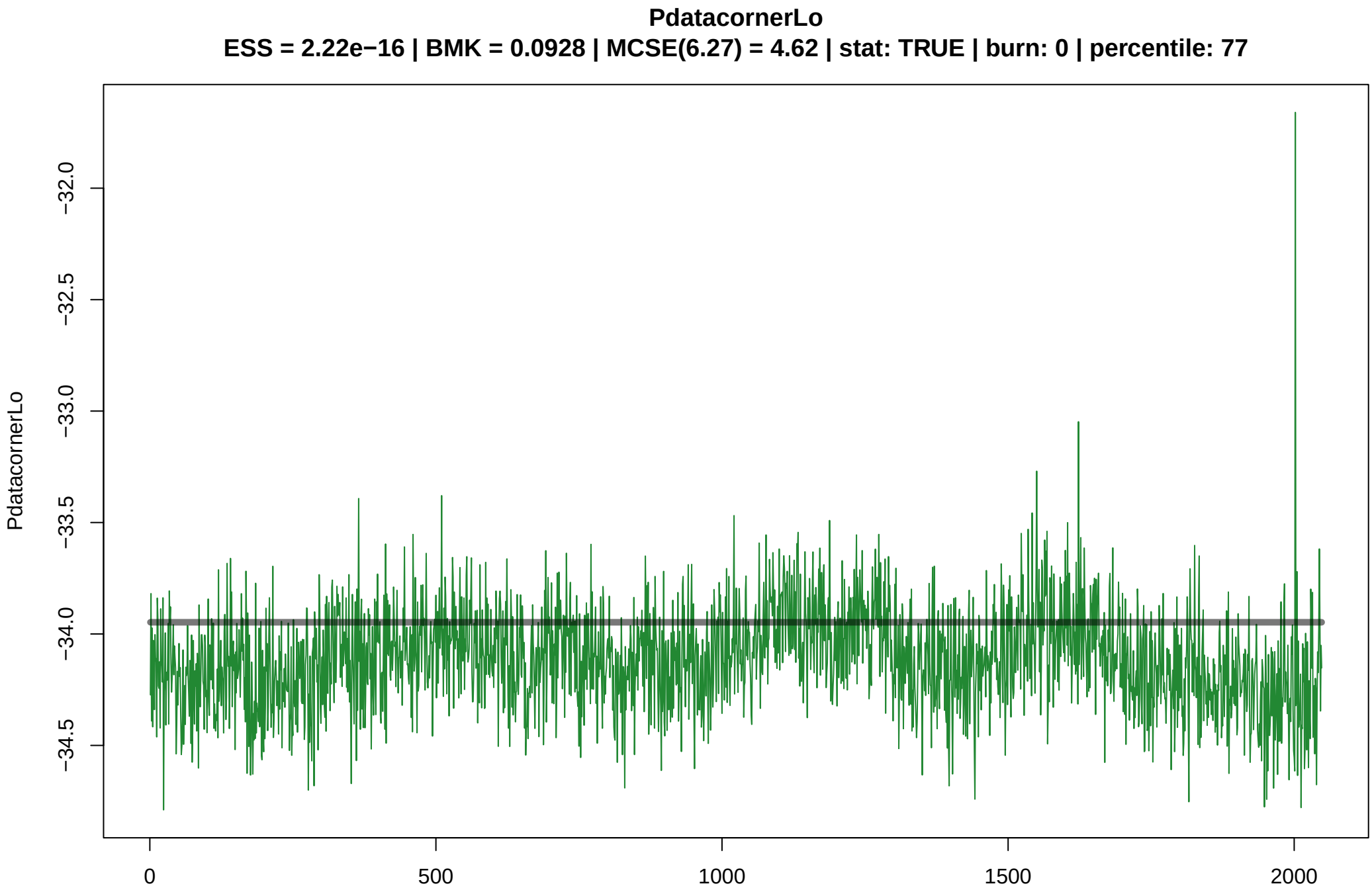

docked_NumRotatableBonds
log_RMSD

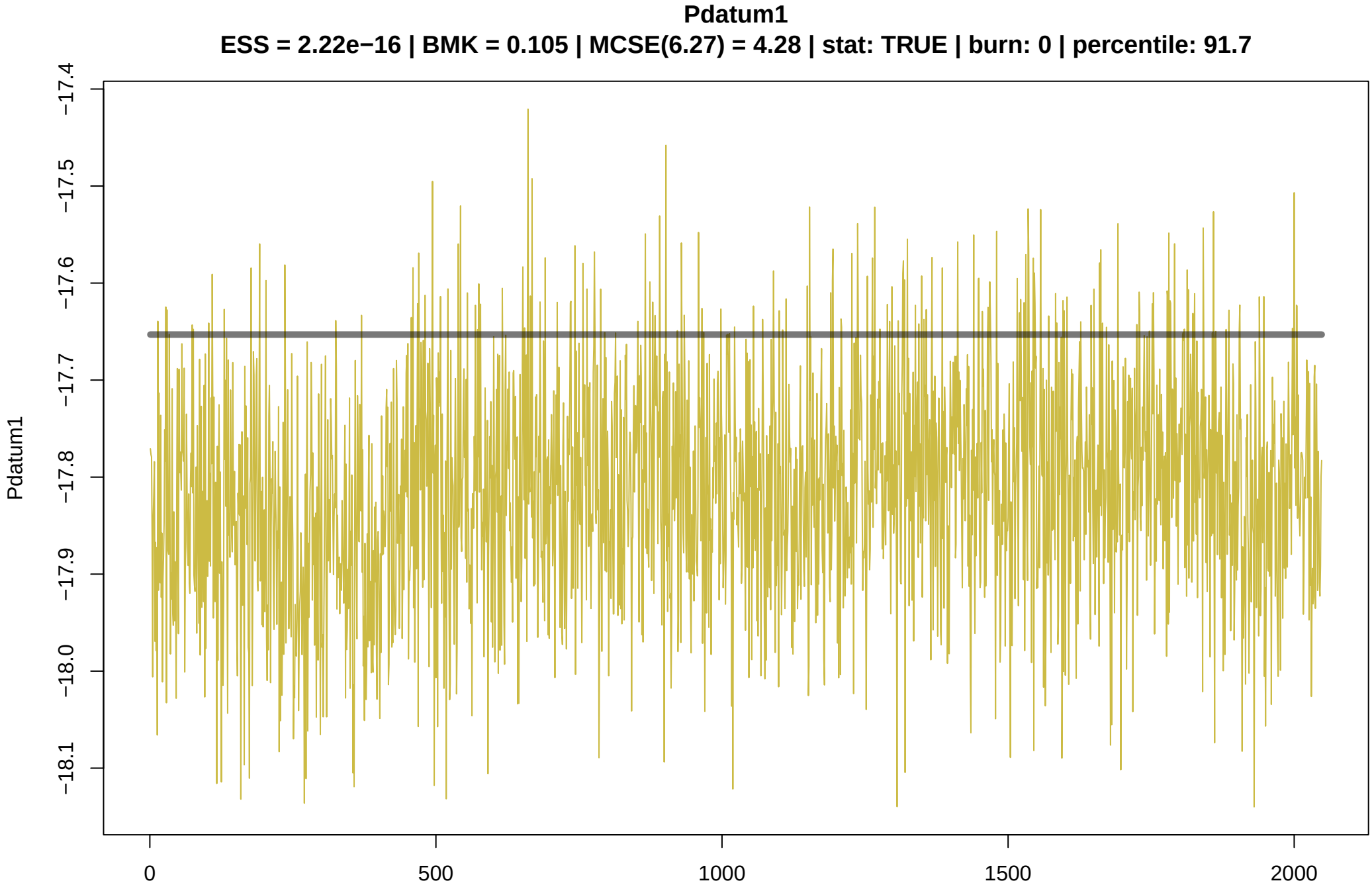

mcs_NOCount
log_RMSD

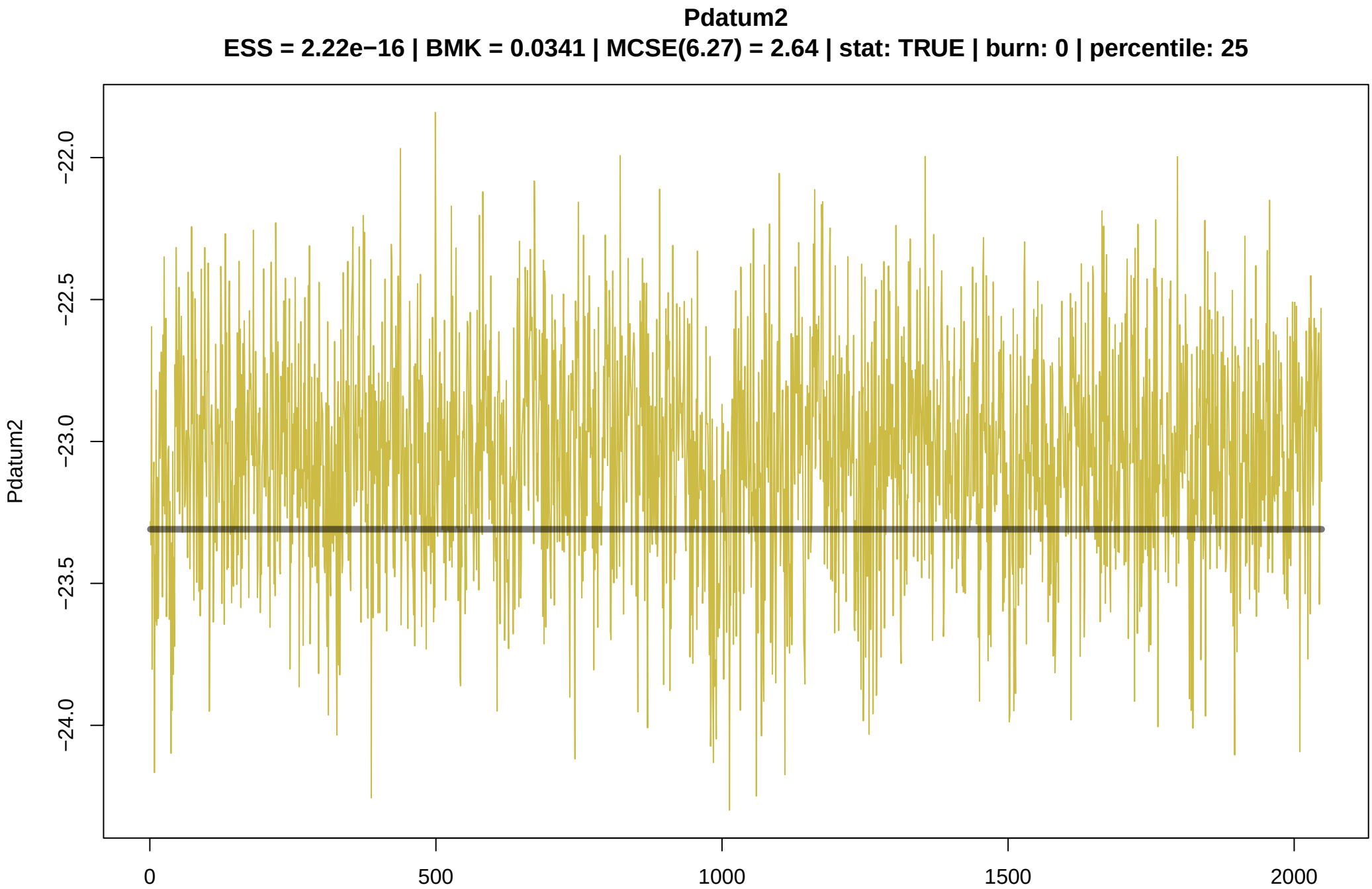

LL
LL
−124720
−124740
−124760
−124780
−124800
−124820
0
500
1000
1500
2000

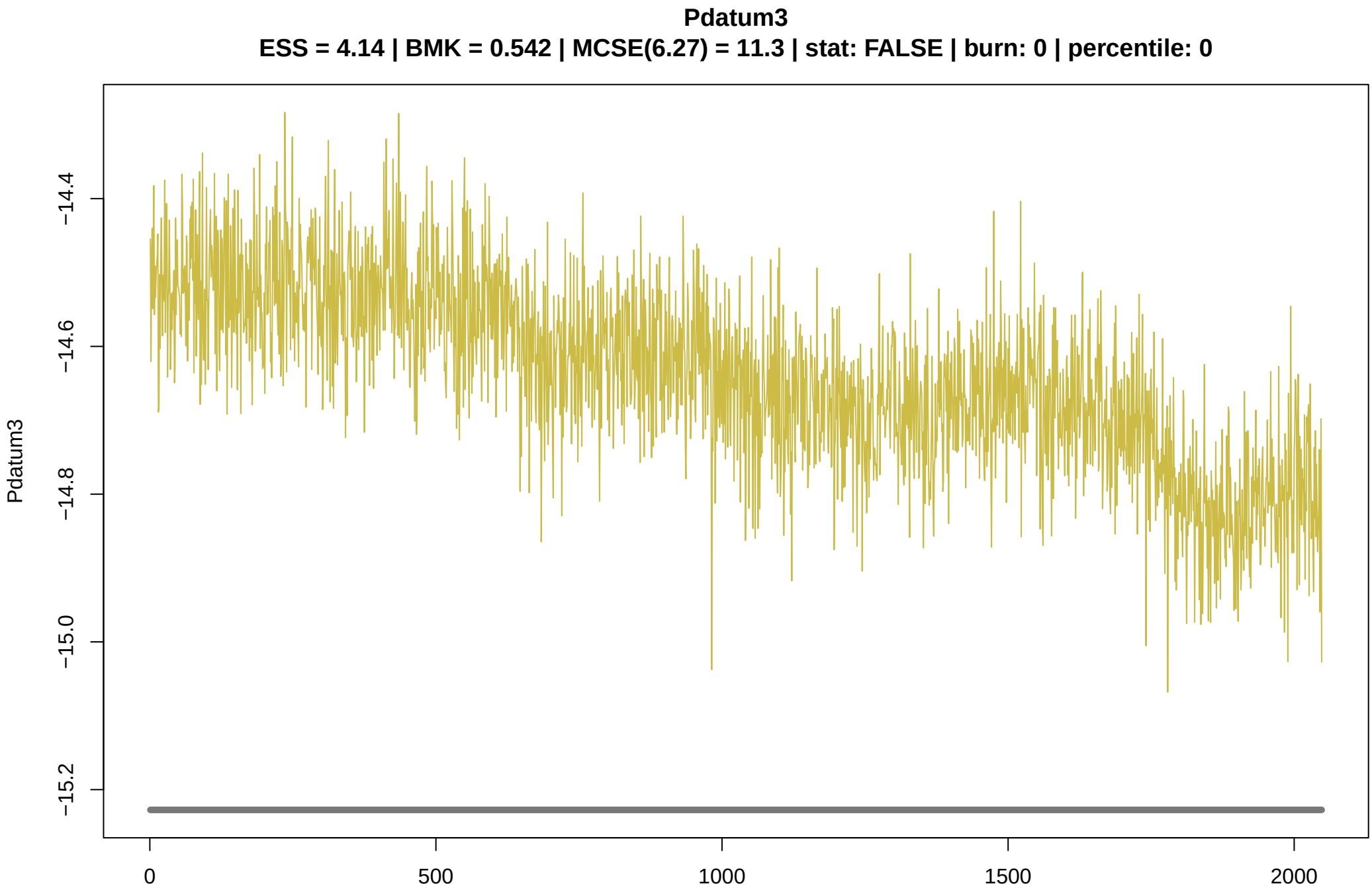

Pdatamean
ESS = 2.22e−16 | BMK = 0.162 | MCSE(6.27) = 5.17 | stat: TRUE | burn: 0 | percentile: 24
Pdatamean
−21.0
−21.5
−22.0
−22.5
−23.0
−23.5
0
500
1000
1500
2000

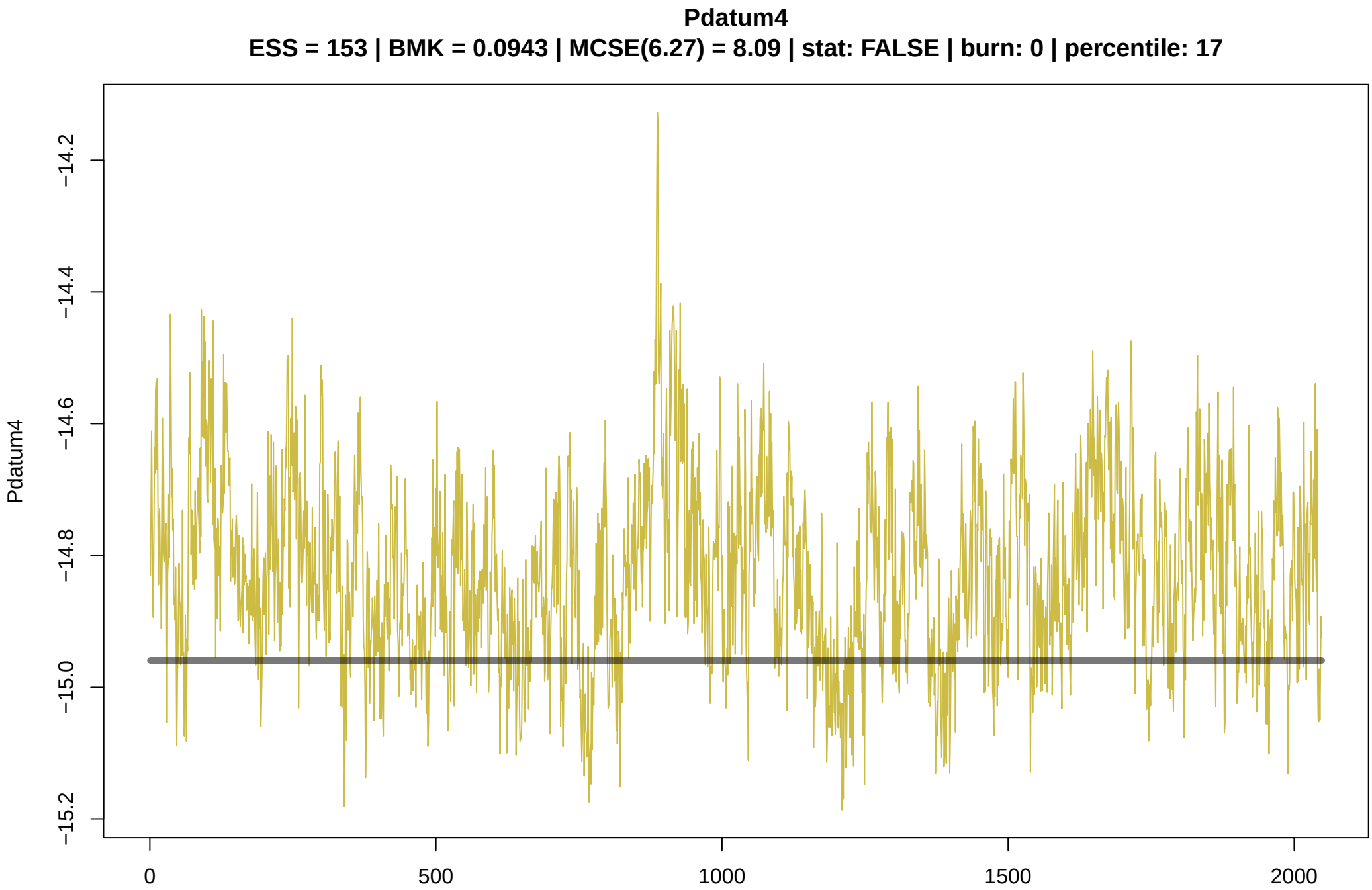

PdatacornerHi
ESS = 2.22e−16 | BMK = 1 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 2040 | percentile: 32
PdatacornerHi
−30
−40
−50
−60
0
500
1000
1500
2000

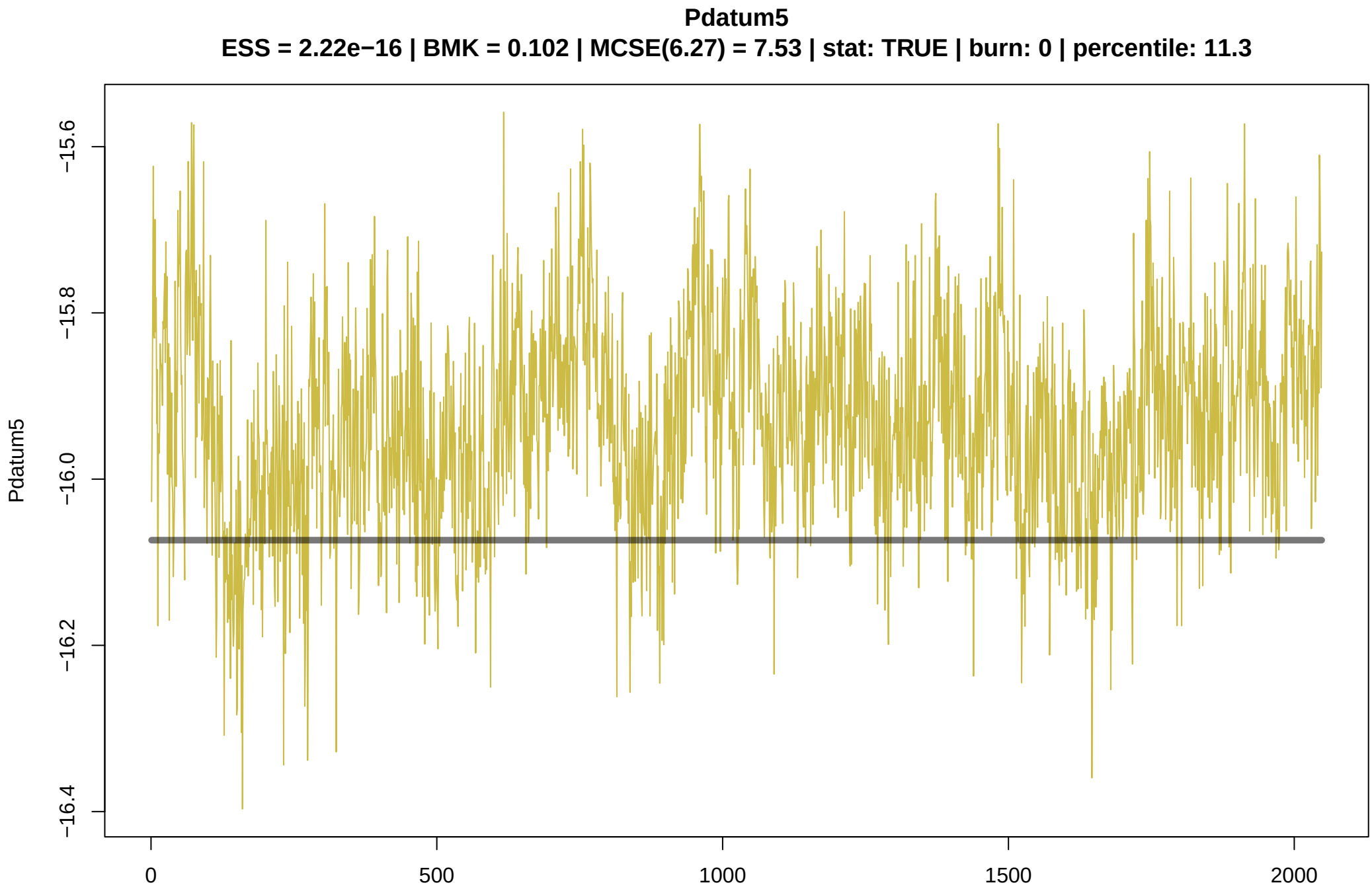

PdatacornerLo
ESS = 2.22e−16 | BMK = 0.0928 | MCSE(6.27) = 4.62 | stat: TRUE | burn: 0 | percentile: 77
PdatacornerLo
−32.0
−32.5
−33.0
−33.5
−34.0
−34.5
0
500
1000
1500
2000

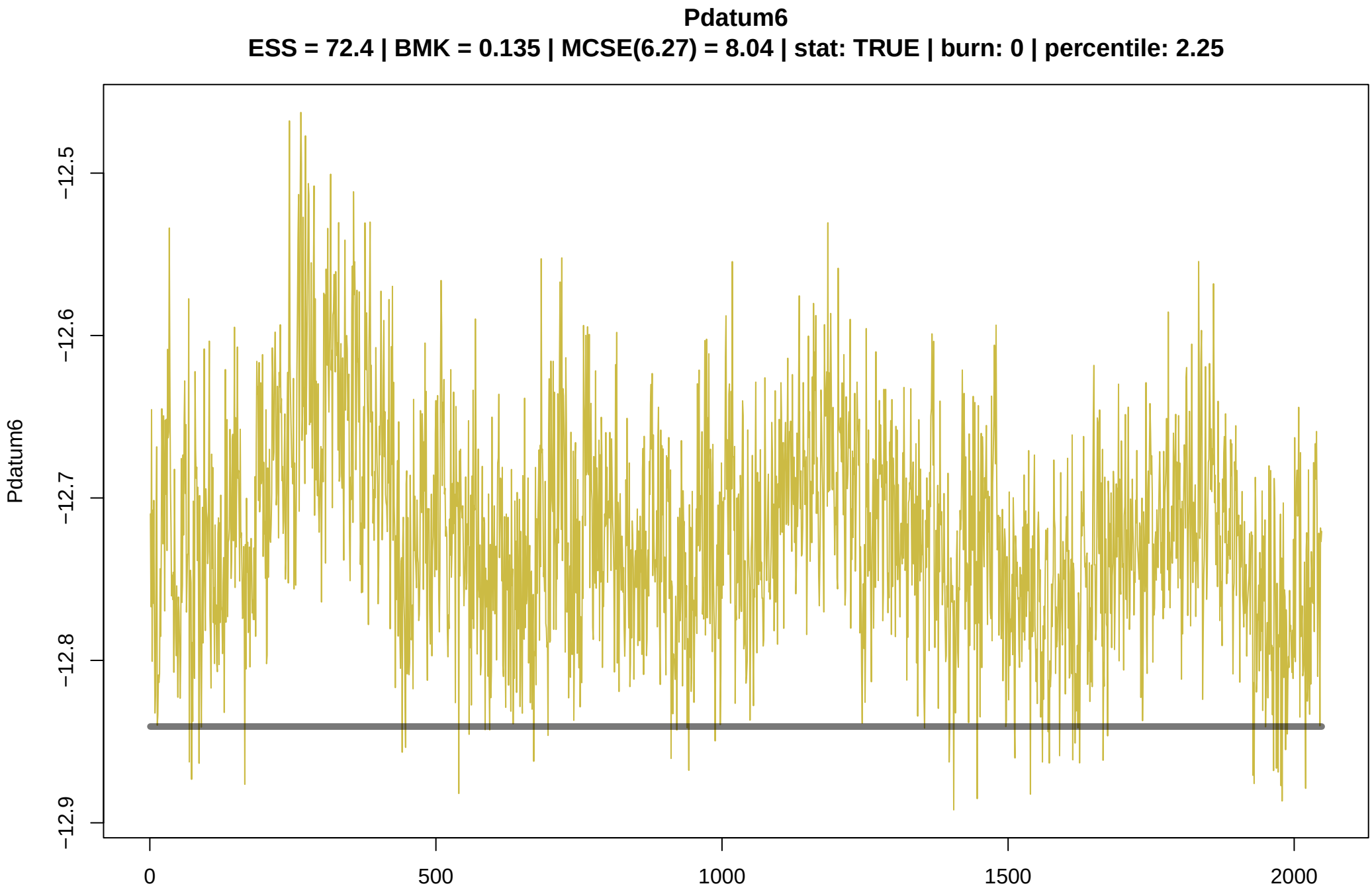

Pdatum1
ESS = 2.22e−16 | BMK = 0.105 | MCSE(6.27) = 4.28 | stat: TRUE | burn: 0 | percentile: 91.7
Pdatum1
−17.4
−17.5
−17.6
−17.7
−17.8
−17.9
−18.0
−18.1
0
500
1000
1500
2000

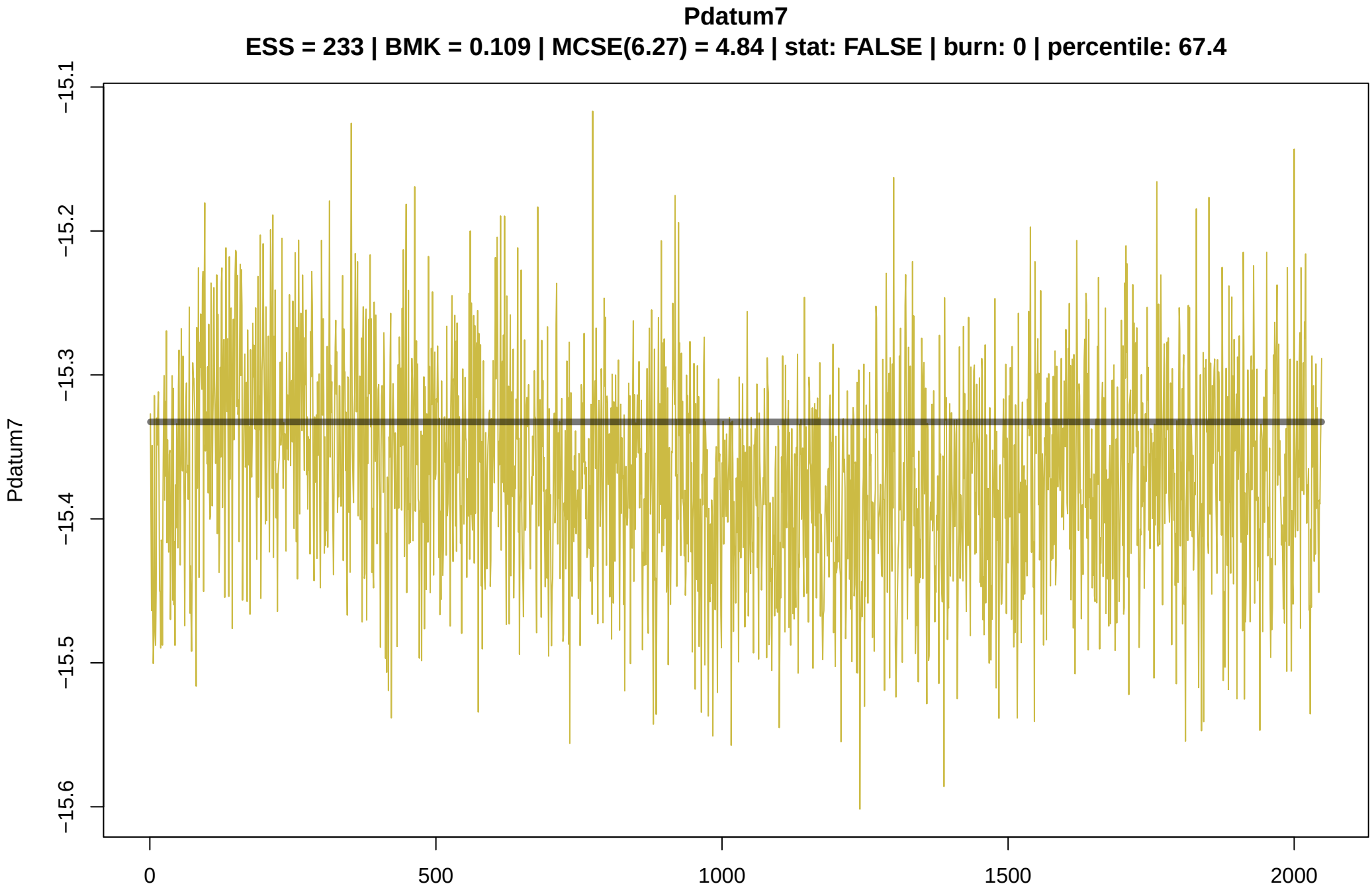

Pdatum2
ESS = 2.22e−16 | BMK = 0.0341 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | percentile: 25
Pdatum2
−22.0
−22.5
−23.0
−23.5
−24.0
0
500
1000
1500
2000

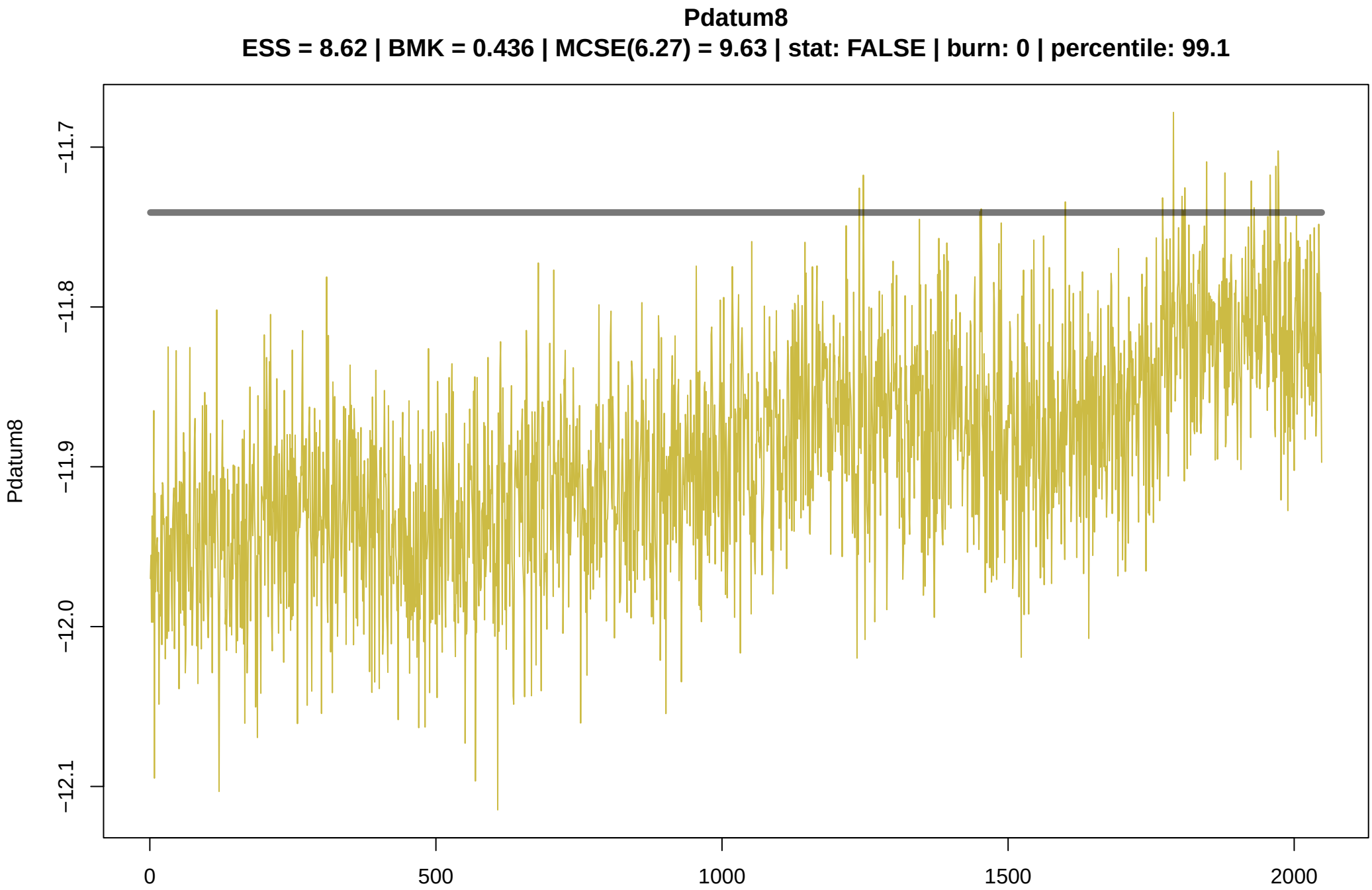

Pdatum3
ESS = 4.14 | BMK = 0.542 | MCSE(6.27) = 11.3 | stat: FALSE | burn: 0 | percentile: 0
Pdatum3
−14.4
−14.6
−14.8
−15.0
−15.2
0
500
1000
1500
2000

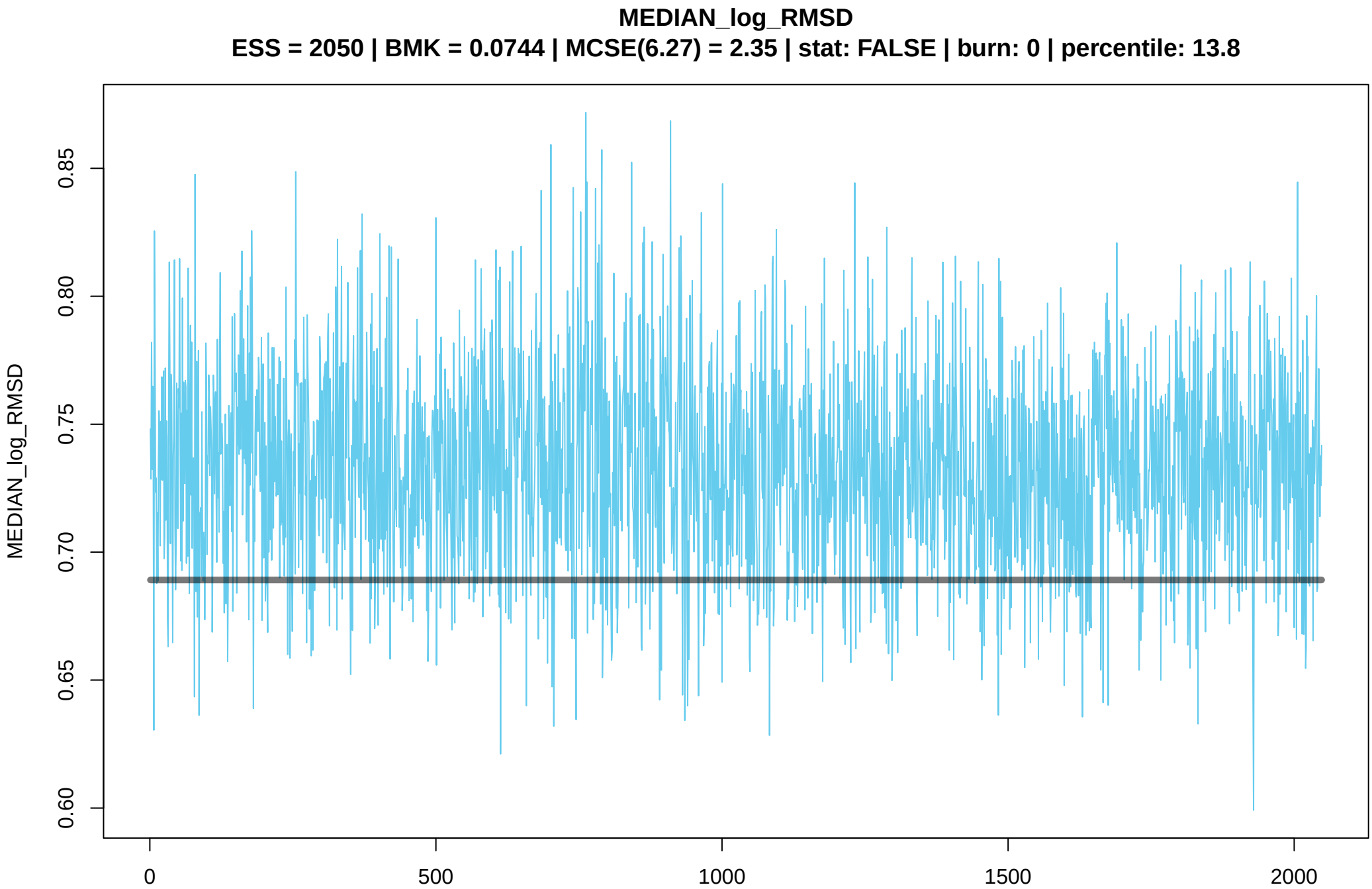

Pdatum4
ESS = 153 | BMK = 0.0943 | MCSE(6.27) = 8.09 | stat: FALSE | burn: 0 | percentile: 17
Pdatum4
−14.2
−14.4
−14.6
−14.8
−15.0
−15.2
0
500
1000
1500
2000

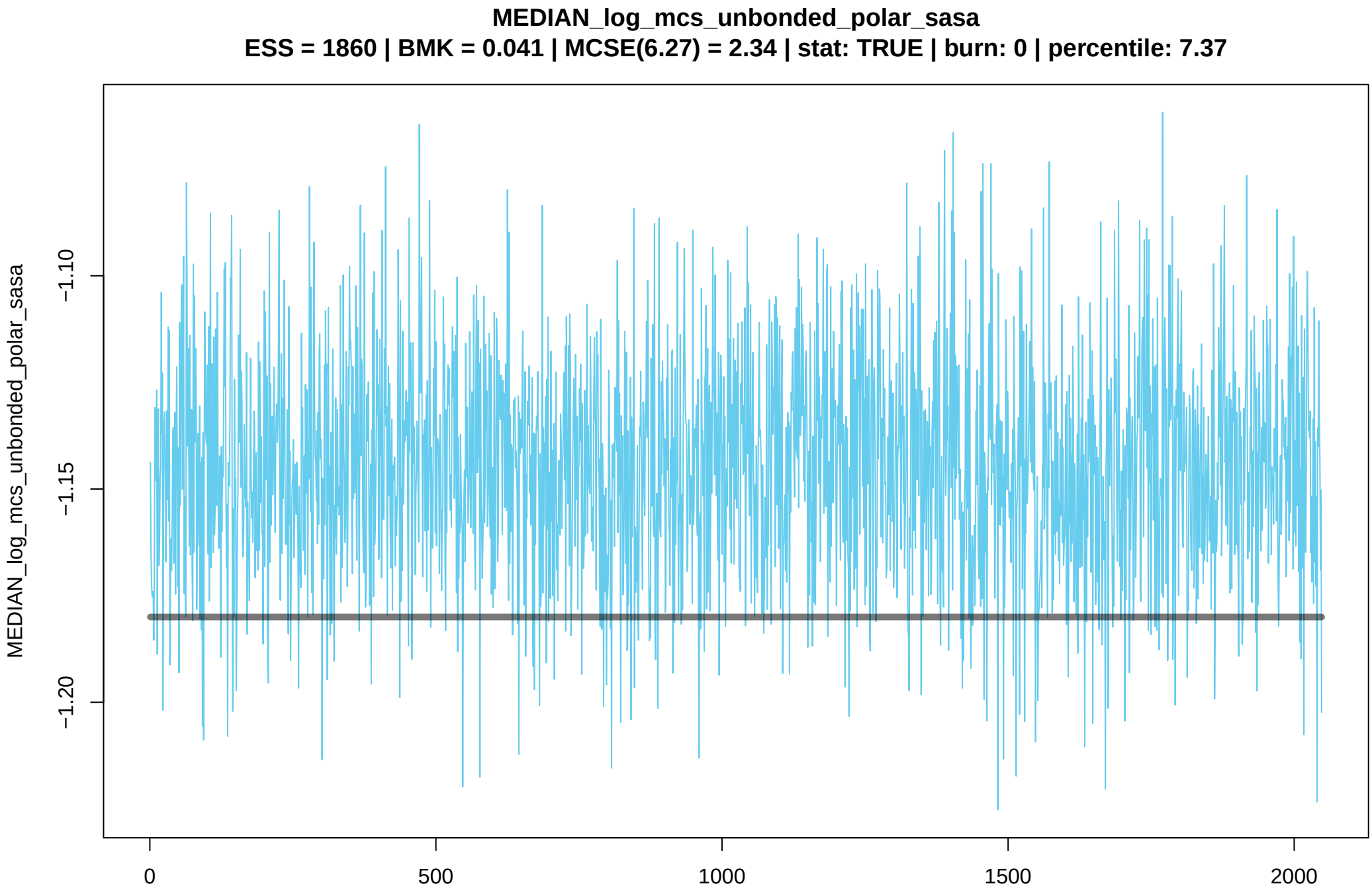

Pdatum5
ESS = 2.22e−16 | BMK = 0.102 | MCSE(6.27) = 7.53 | stat: TRUE | burn: 0 | percentile: 11.3
Pdatum5
−15.6
−15.8
−16.0
−16.2
−16.4
0
500
1000
1500
2000

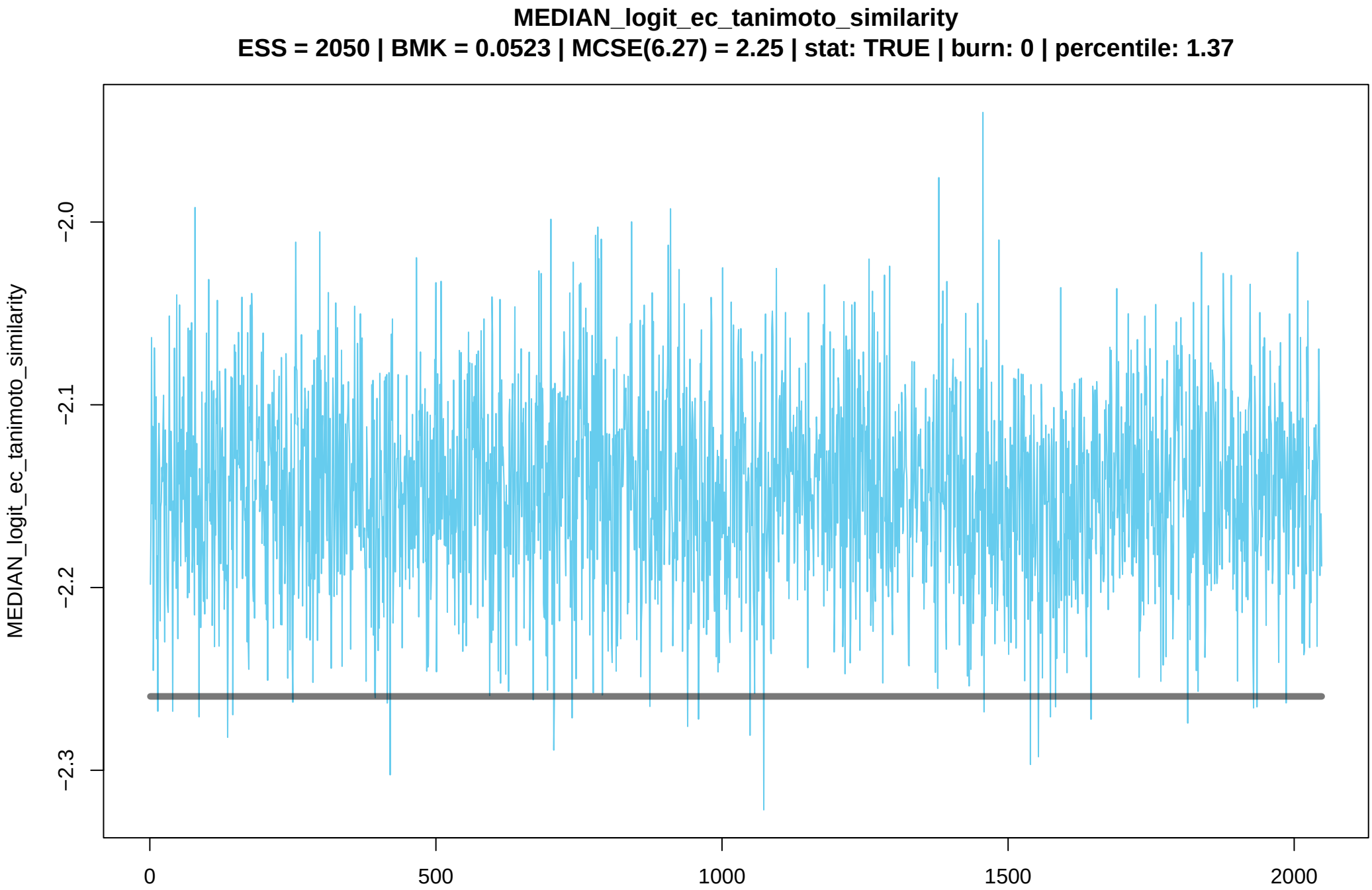

Pdatum6
ESS = 72.4 | BMK = 0.135 | MCSE(6.27) = 8.04 | stat: TRUE | burn: 0 | percentile: 2.25
Pdatum6
−12.5
−12.6
−12.7
−12.8
−12.9
0
500
1000
1500
2000

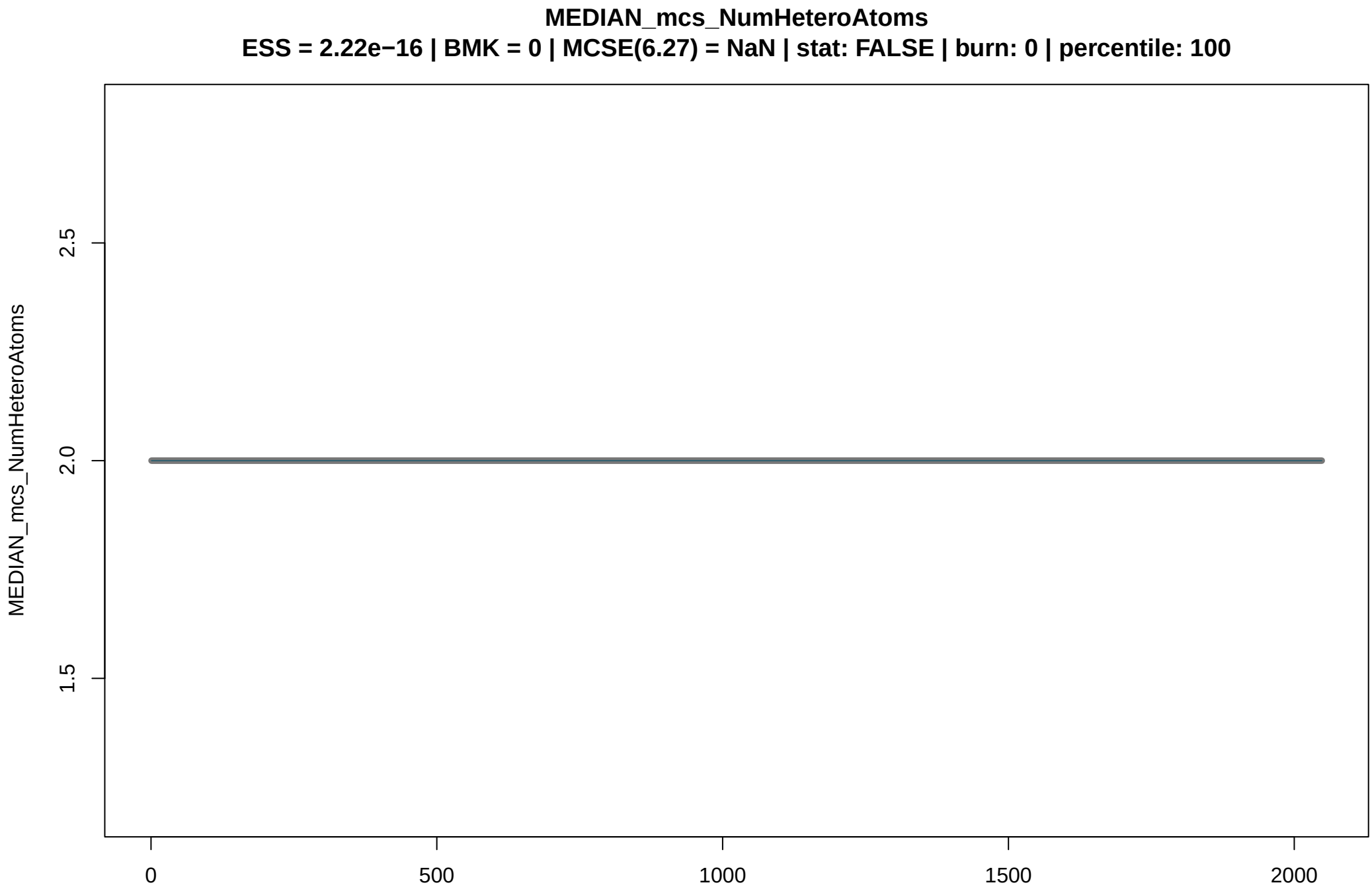

Pdatum7
ESS = 233 | BMK = 0.109 | MCSE(6.27) = 4.84 | stat: FALSE | burn: 0 | percentile: 67.4
Pdatum7
−15.1
−15.2
−15.3
−15.4
−15.5
−15.6
0
500
1000
1500
2000

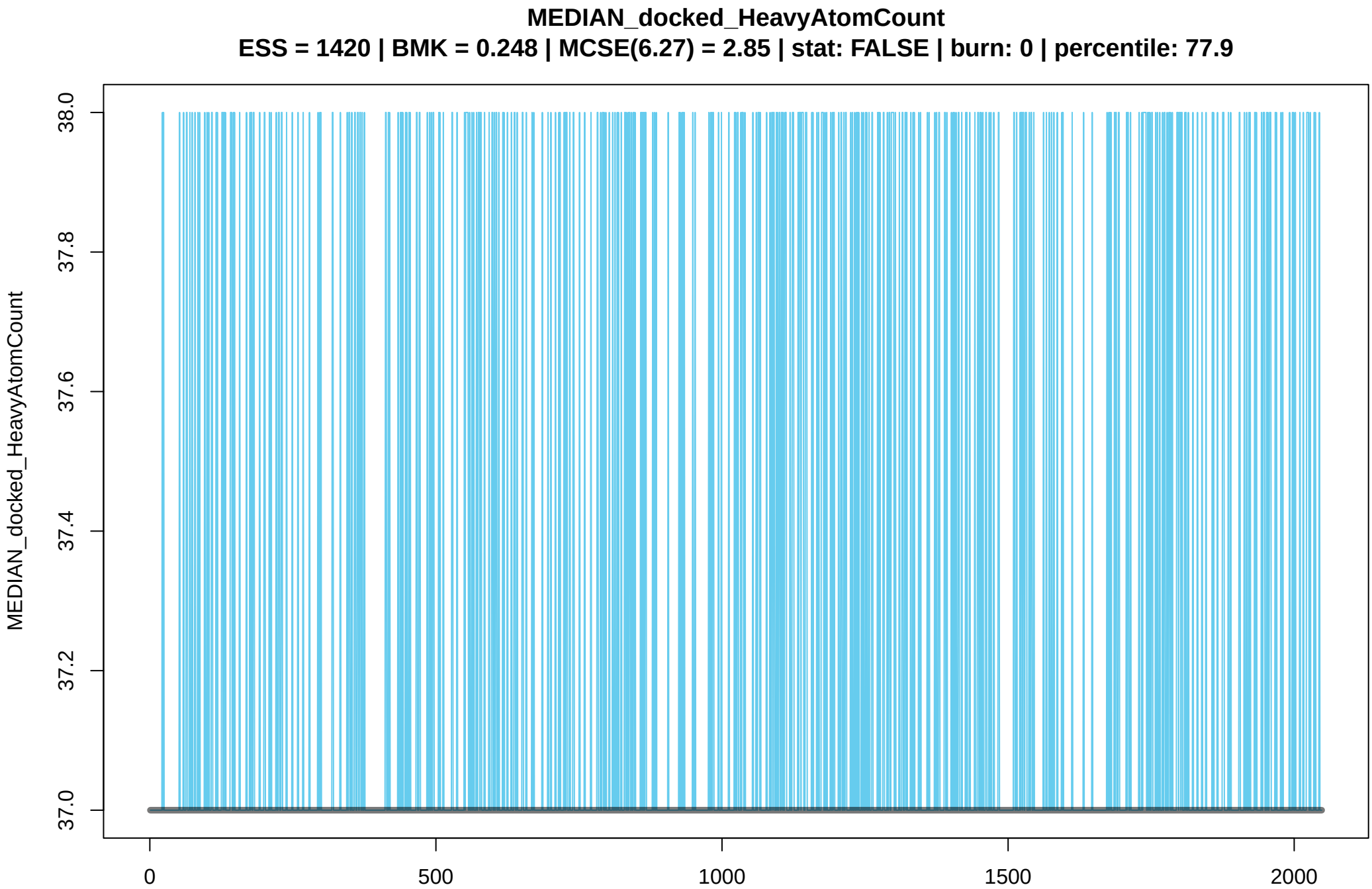

Pdatum8
ESS = 8.62 | BMK = 0.436 | MCSE(6.27) = 9.63 | stat: FALSE | burn: 0 | percentile: 99.1
Pdatum8
−11.7
−11.8
−11.9
−12.0
−12.1
0
500
1000
1500
2000

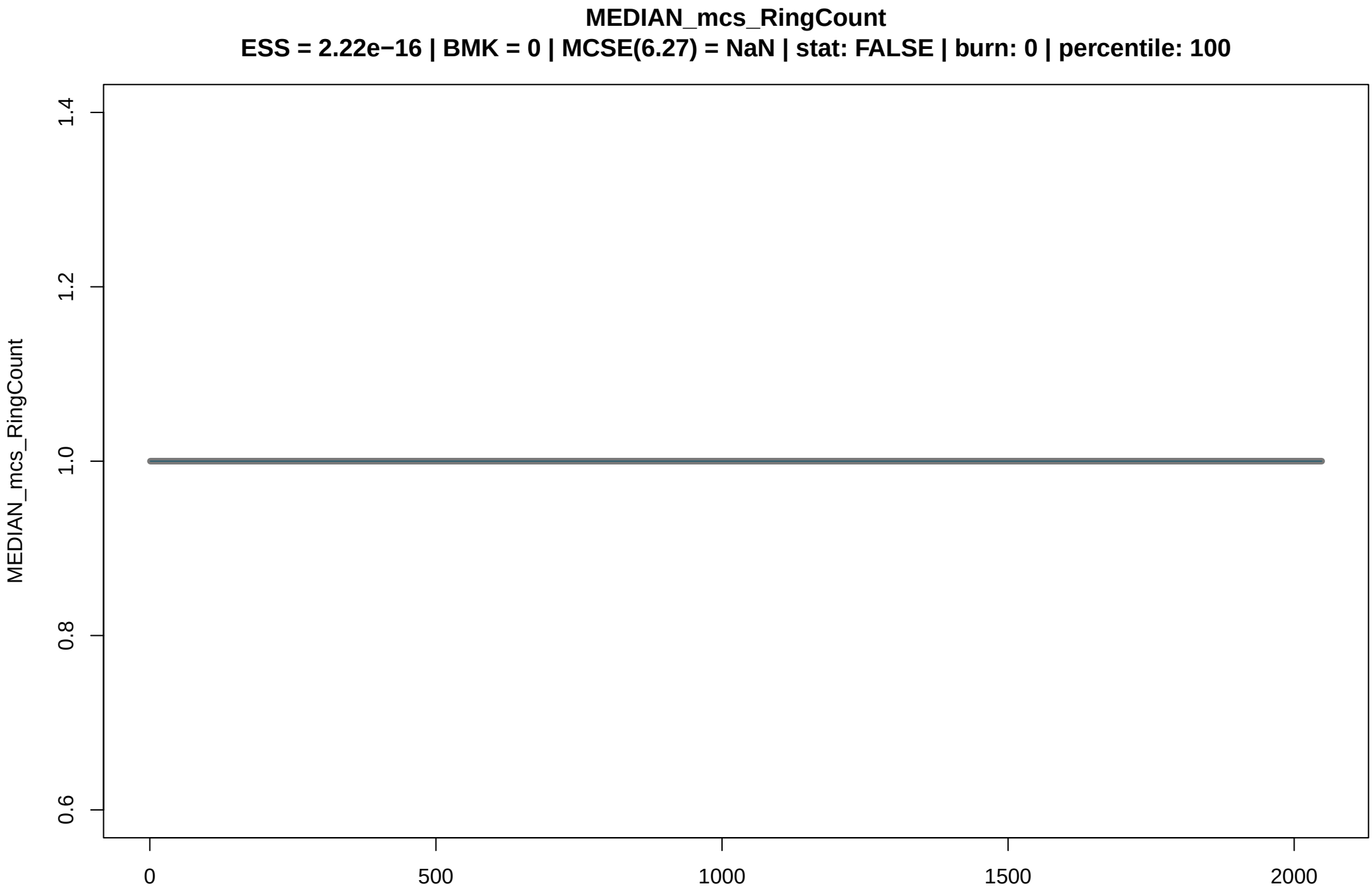

MEDIAN_log_RMSD
ESS = 2050 | BMK = 0.0744 | MCSE(6.27) = 2.35 | stat: FALSE | burn: 0 | percentile: 13.8
MEDIAN_log_RMSD
0.60
0.65
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

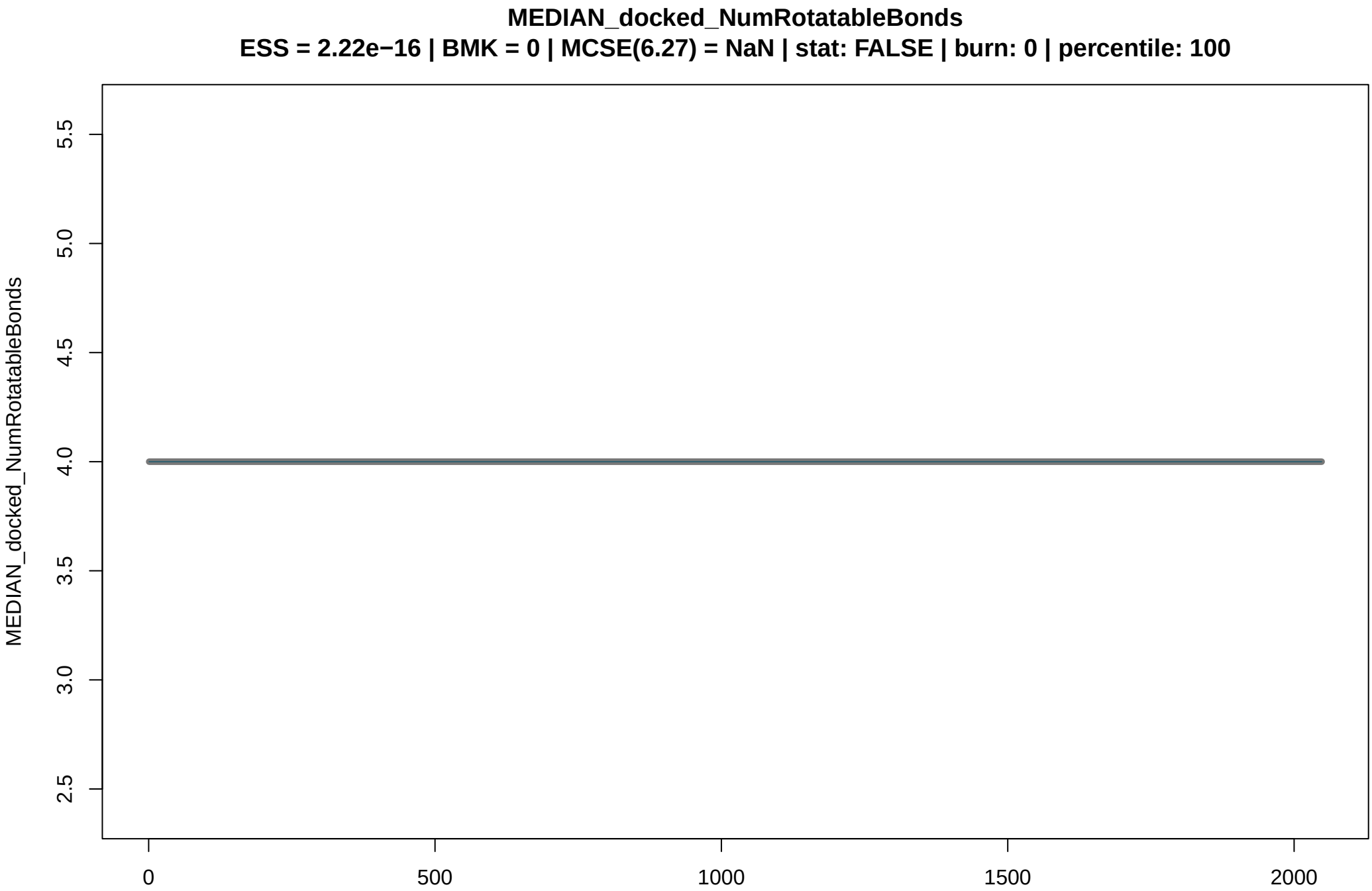

MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 1860 | BMK = 0.041 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0 | percentile: 7.37
MEDIAN_log_mcs_unbonded_polar_sasa
−1.10
−1.15
−1.20
0
500
1000
1500
2000

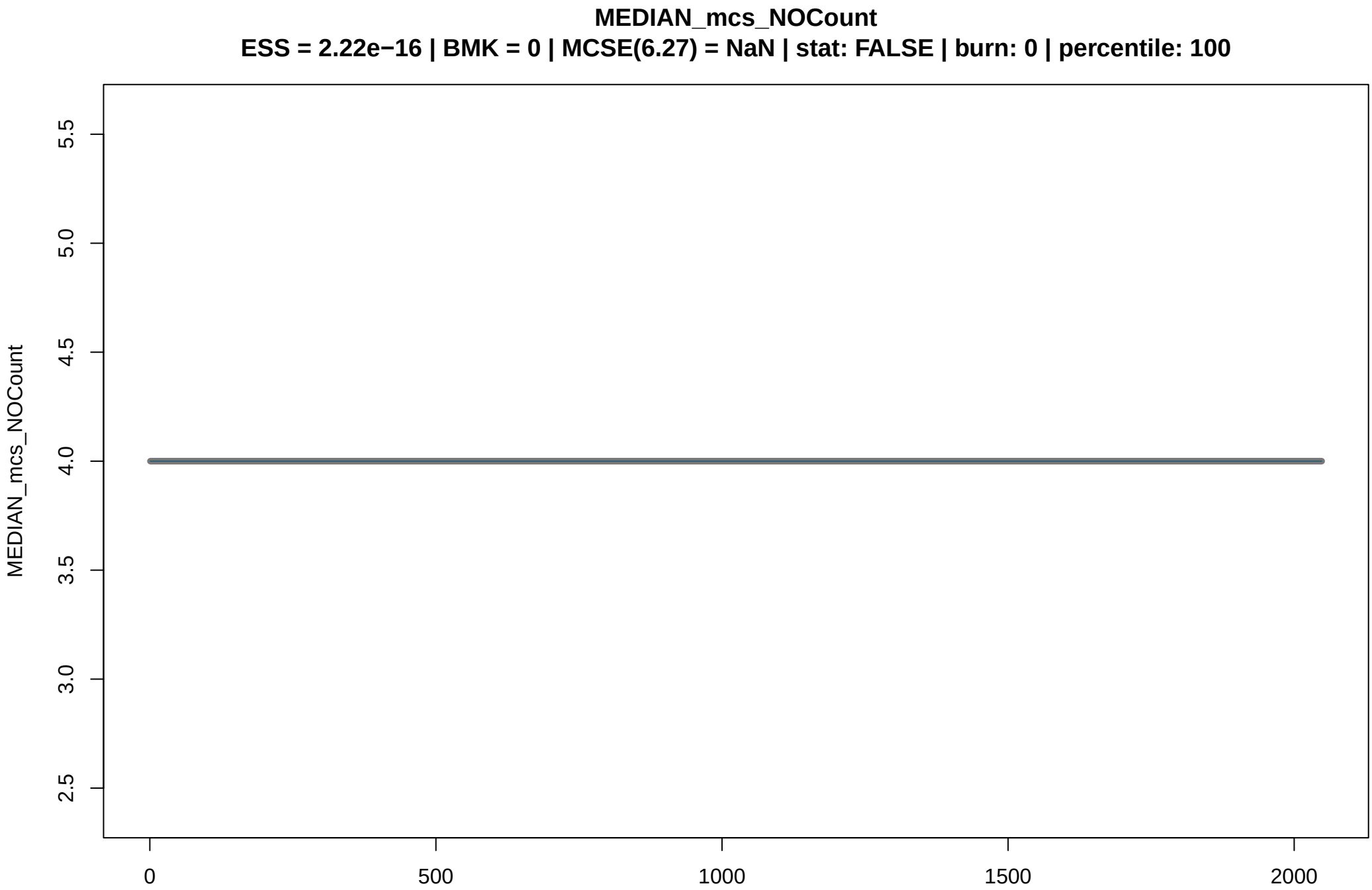

MEDIAN_logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0523 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | percentile: 1.37
MEDIAN_logit_ec_tanimoto_similarity
−2.0
−2.1
−2.2
−2.3
0
500
1000
1500
2000

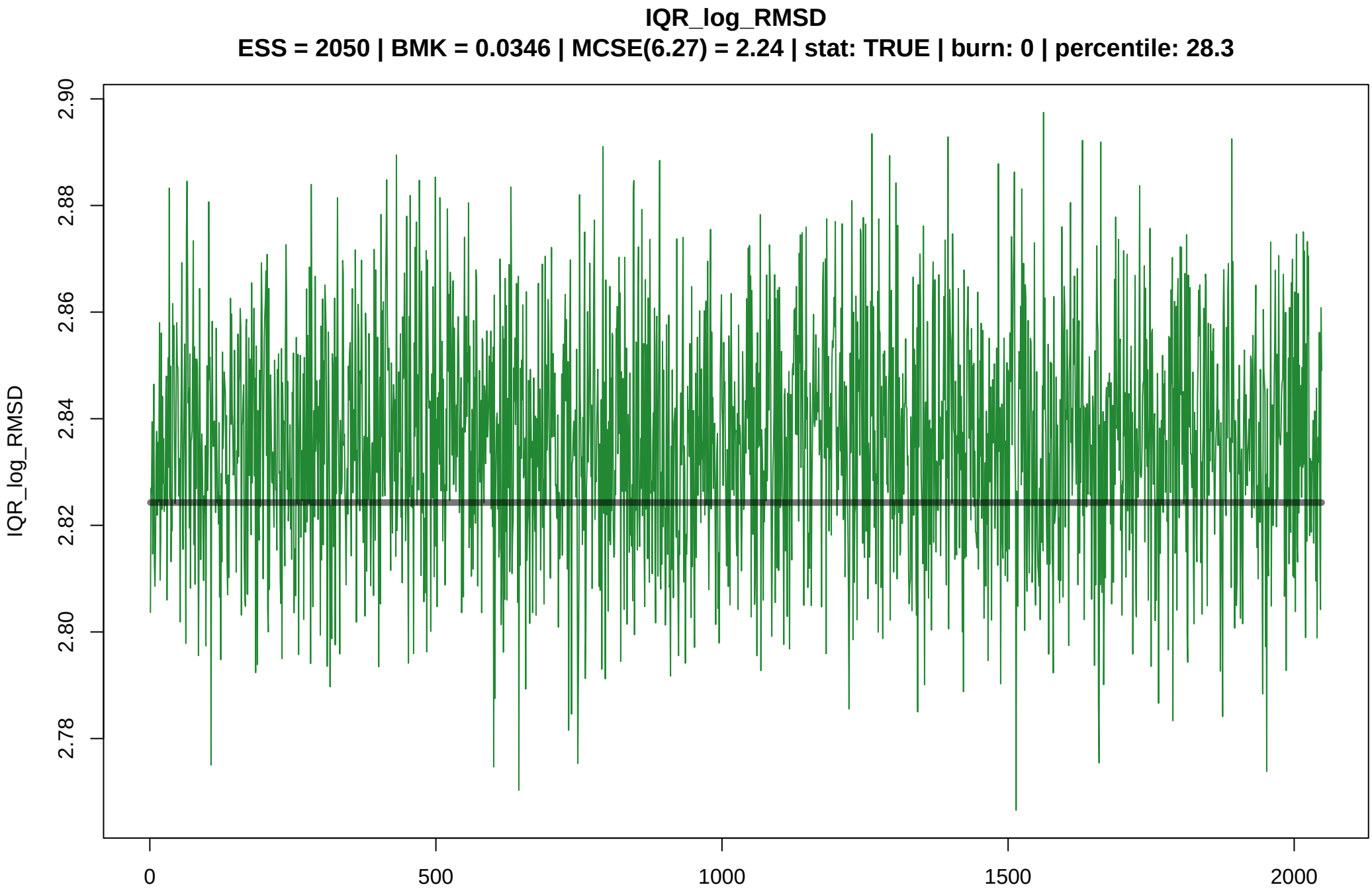

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

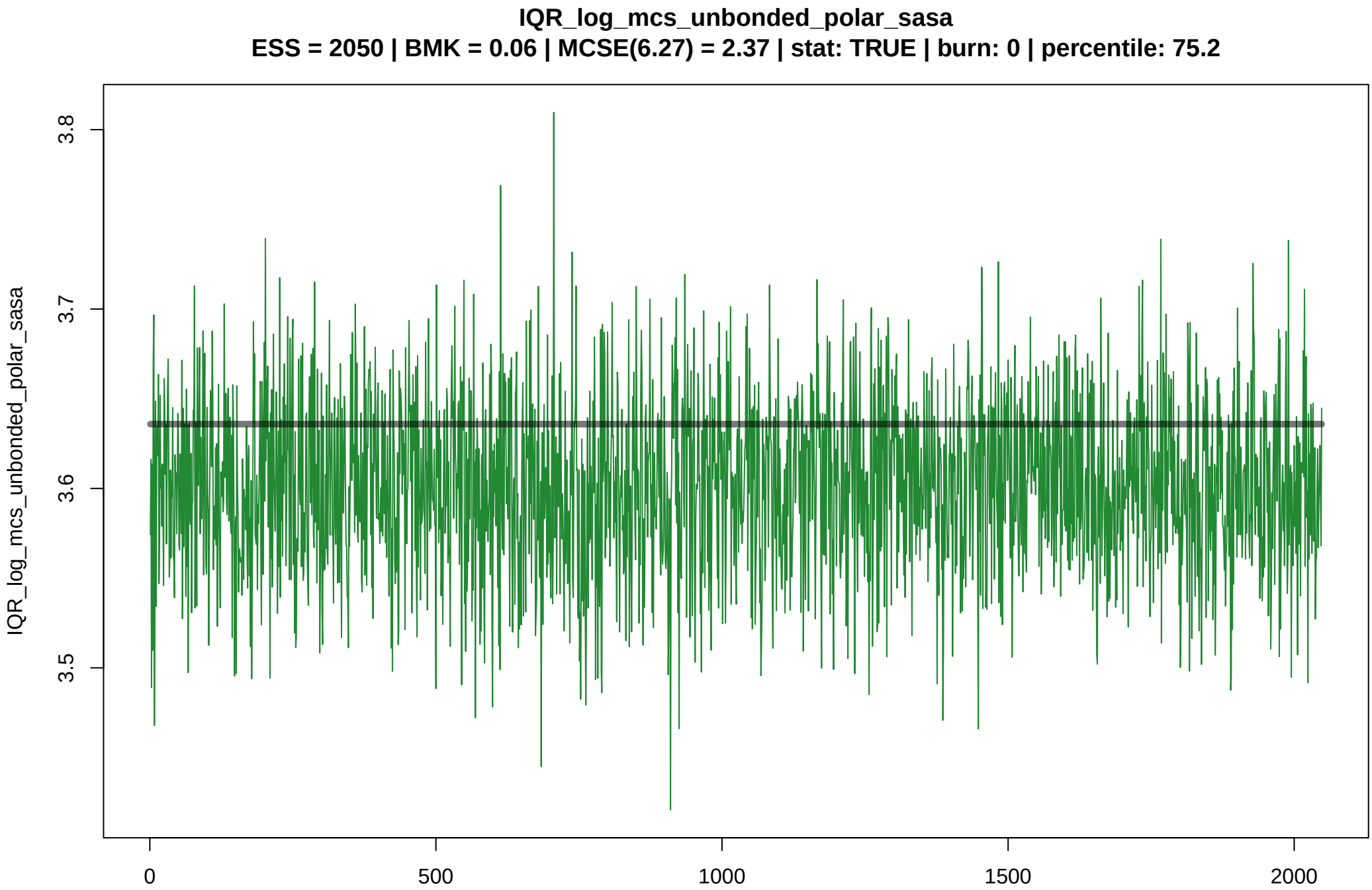

MEDIAN_docked_HeavyAtomCount
ESS = 1420 | BMK = 0.248 | MCSE(6.27) = 2.85 | stat: FALSE | burn: 0 | percentile: 77.9
MEDIAN_docked_HeavyAtomCount
38.0
37.8
37.6
37.4
37.2
37.0
0
500
1000
1500
2000

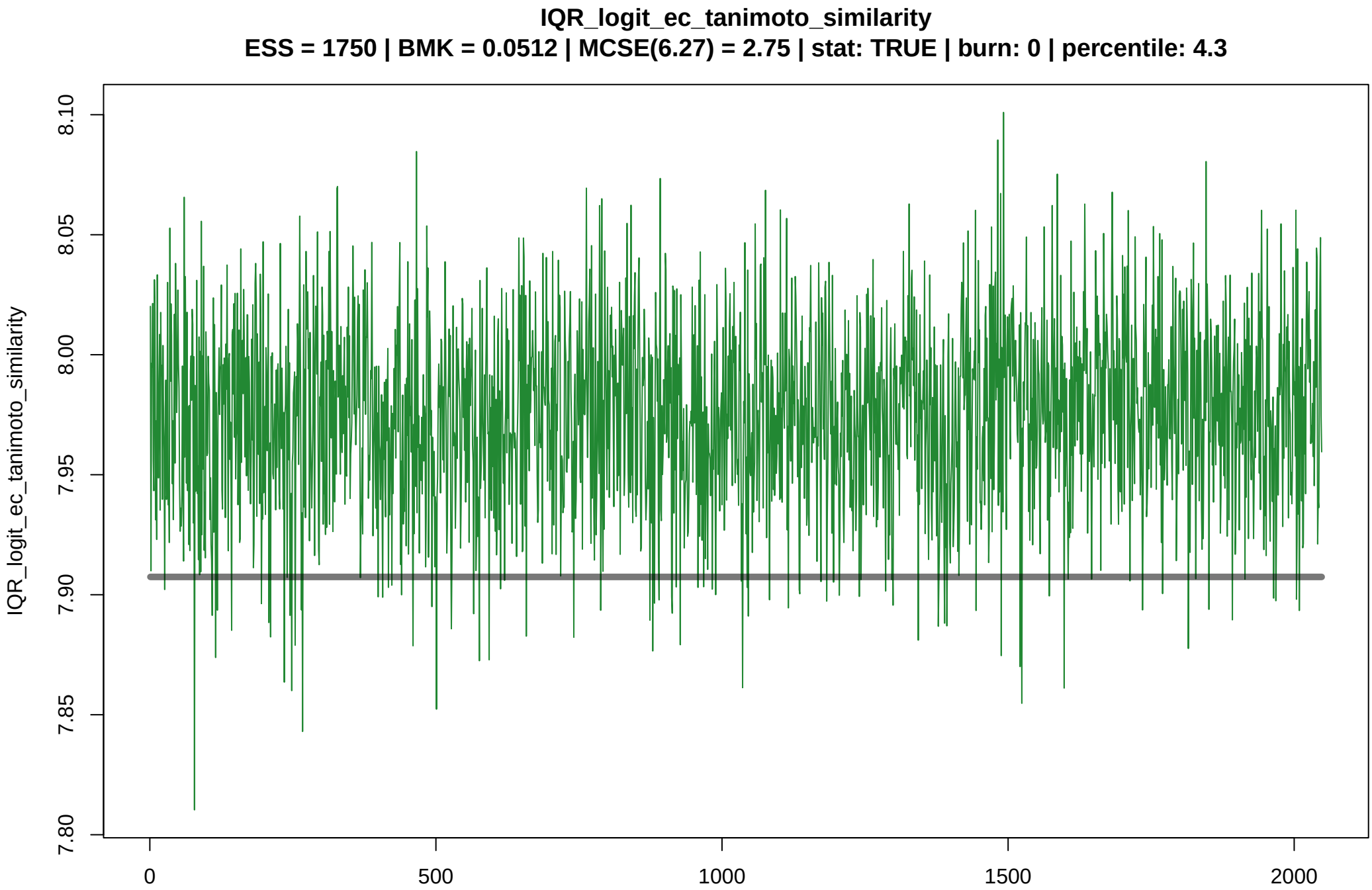

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
MEDIAN_mcs_RingCount
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

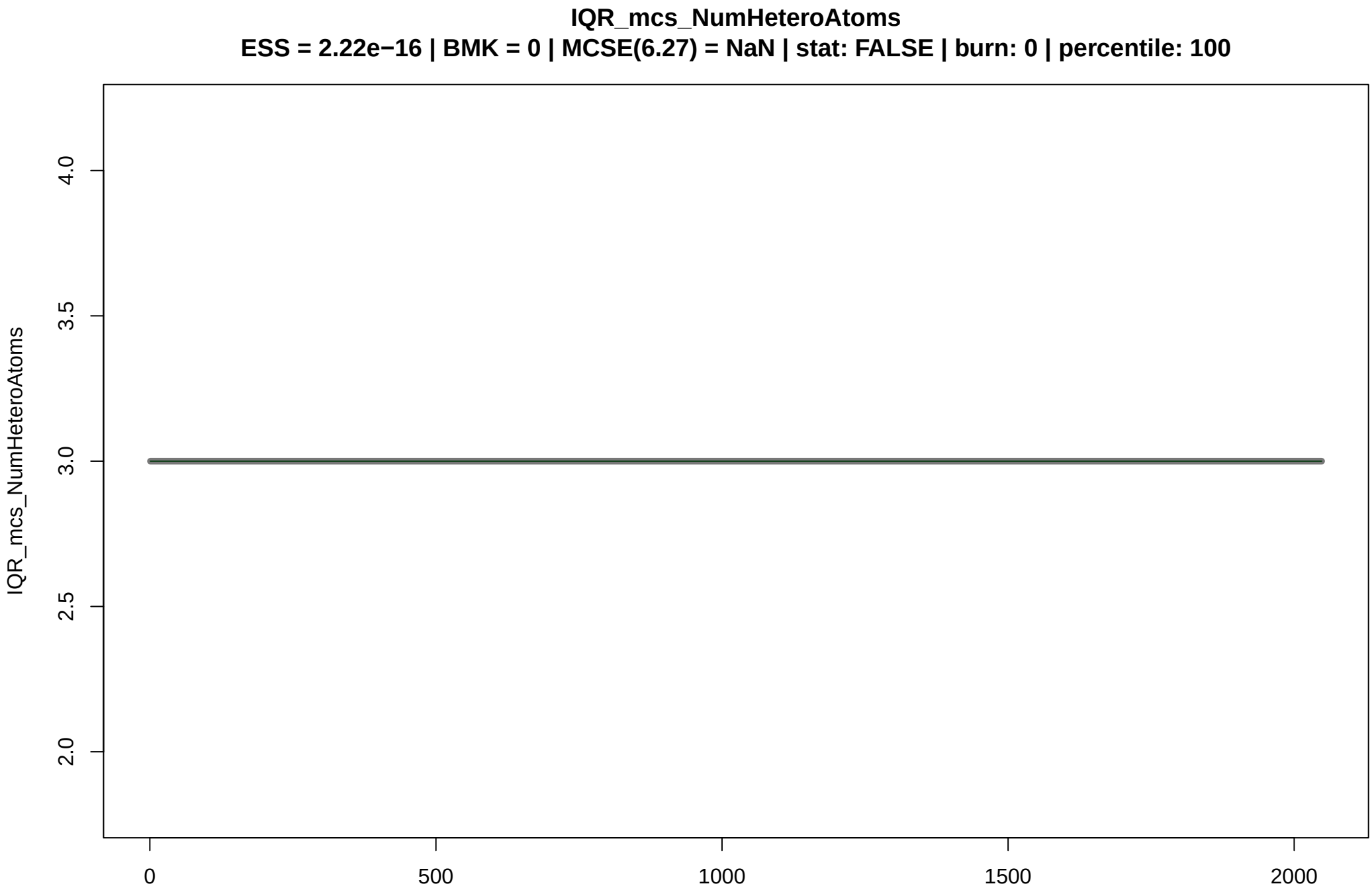

MEDIAN_docked_NumRotatableBonds
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
MEDIAN_docked_NumRotatableBonds
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

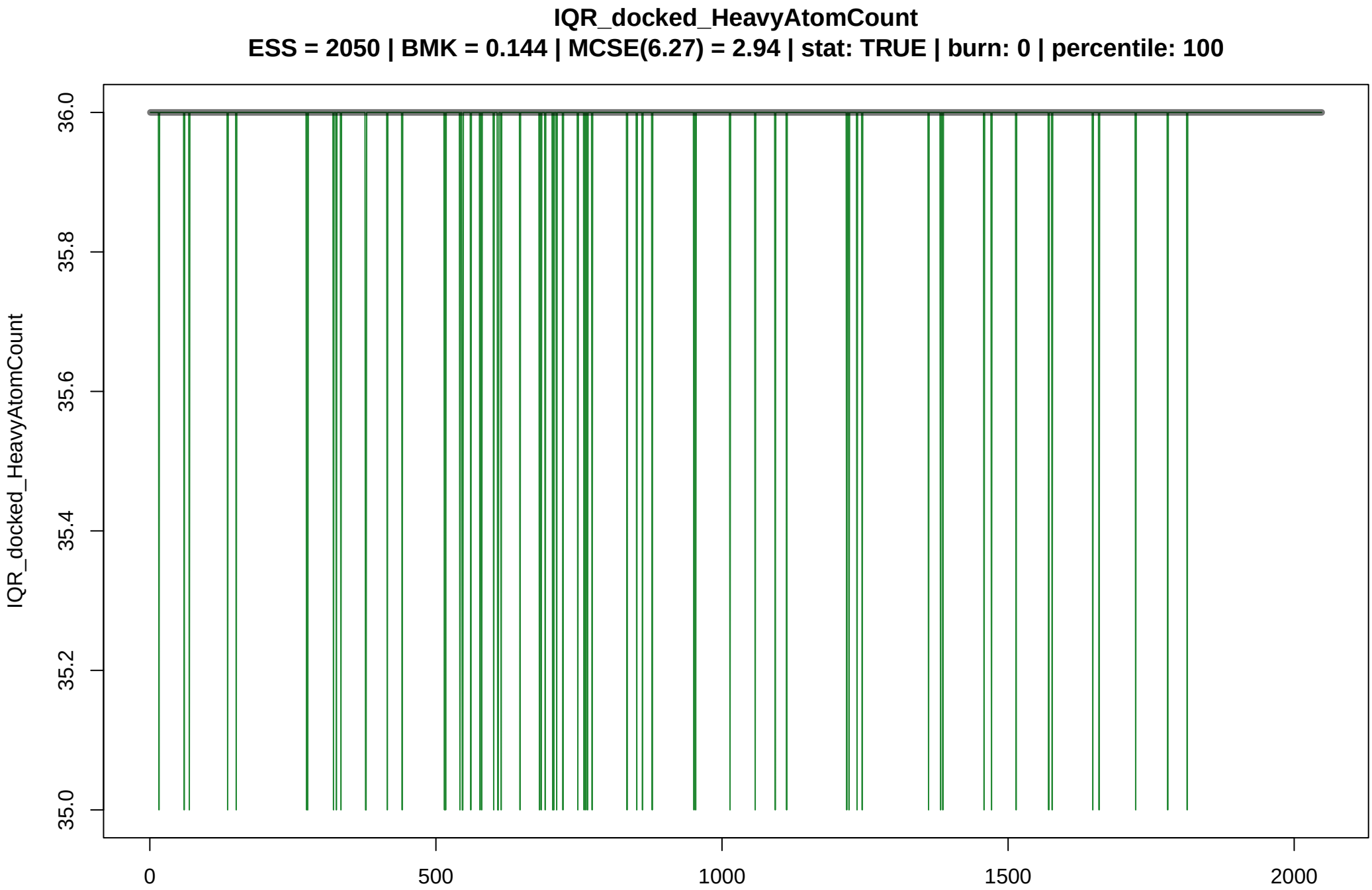

MEDIAN_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
MEDIAN_mcs_NOCount
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

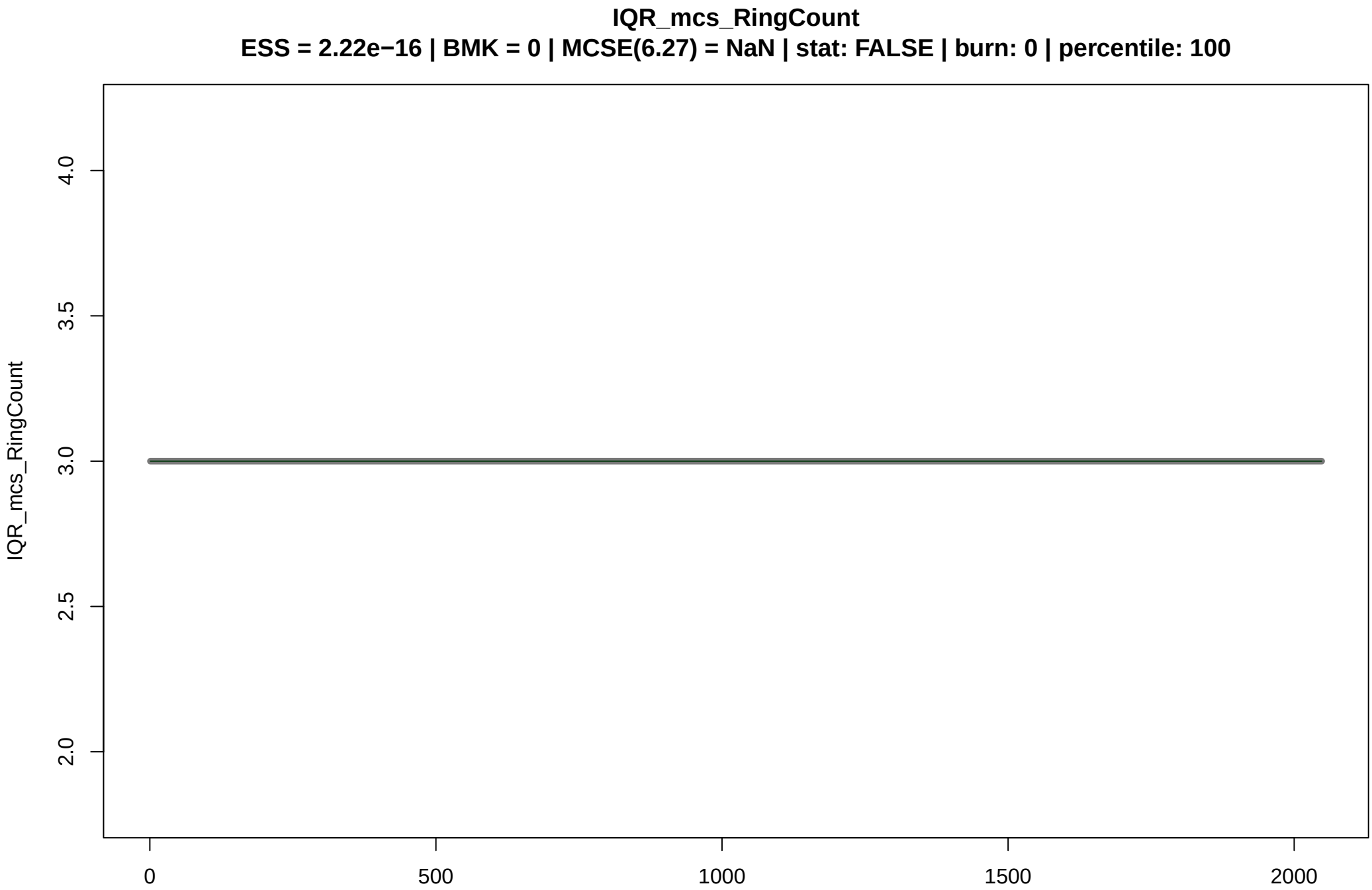

IQR_log_RMSD
ESS = 2050 | BMK = 0.0346 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0 | percentile: 28.3
IQR_log_RMSD
2.90
2.88
2.86
2.84
2.82
2.80
2.78
0
500
1000
1500
2000

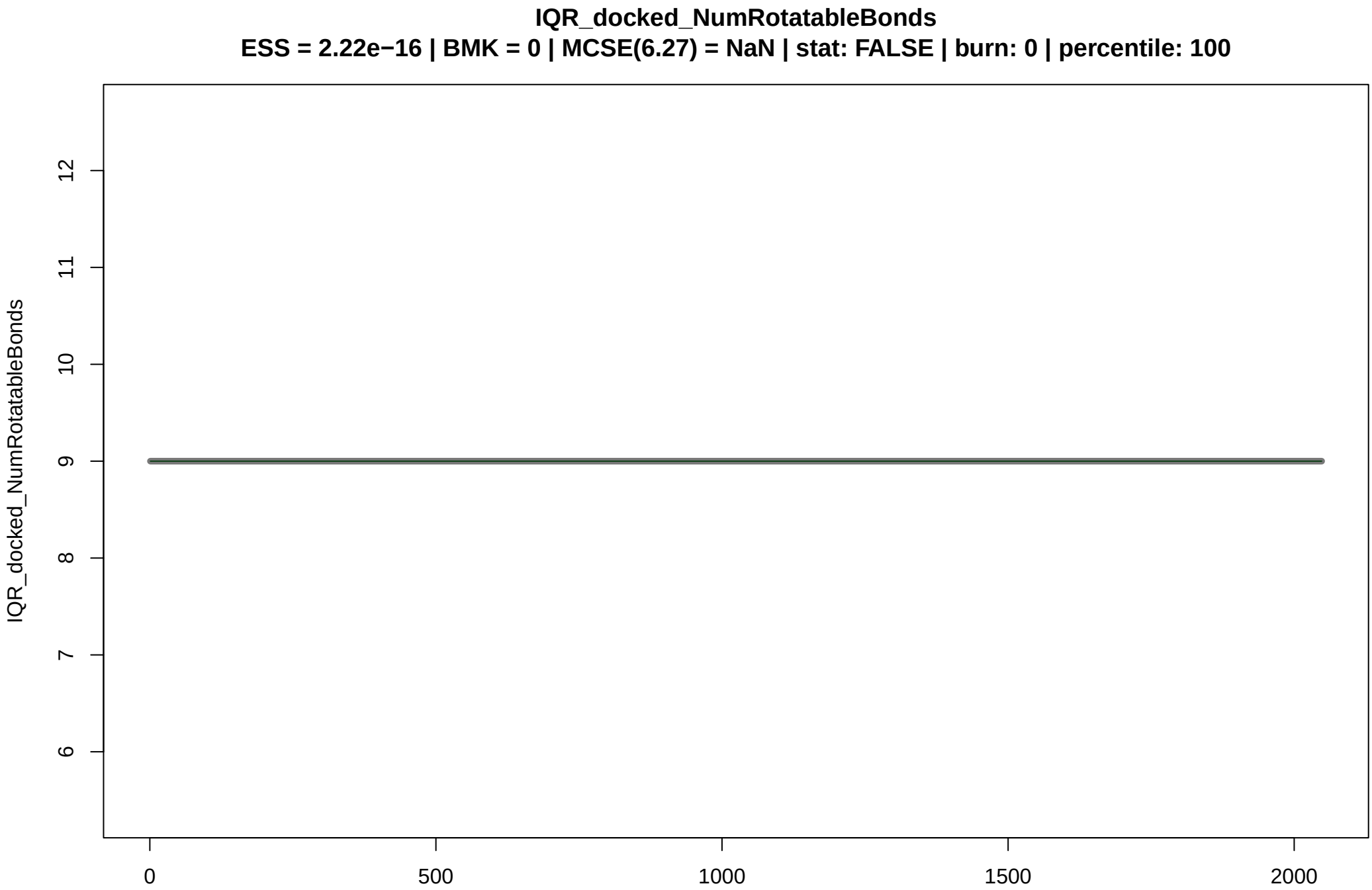

IQR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.06 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | percentile: 75.2
IQR_log_mcs_unbonded_polar_sasa
3.8
3.7
3.6
3.5
0
500
1000
1500
2000

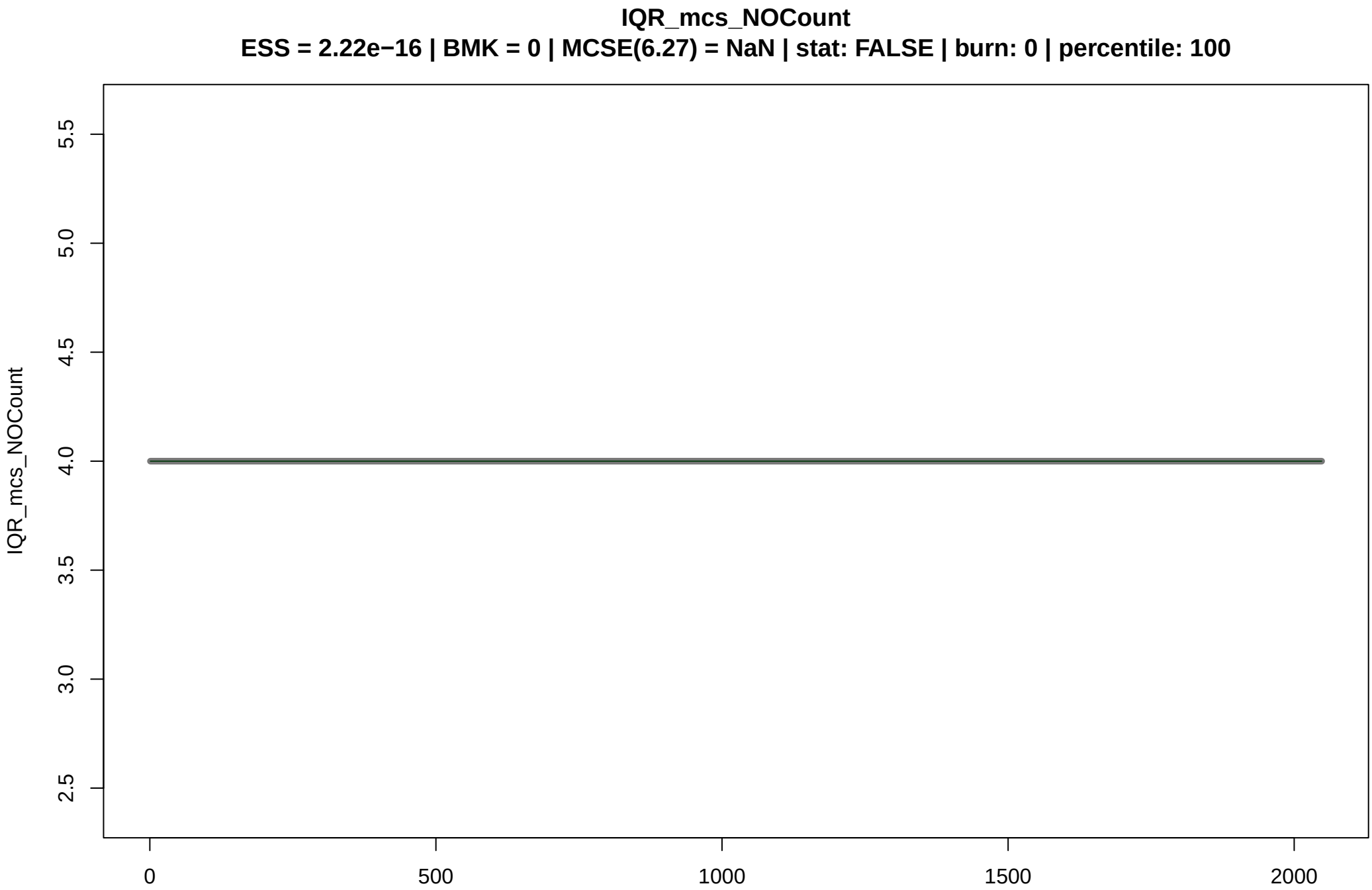

IQR_logit_ec_tanimoto_similarity
ESS = 1750 | BMK = 0.0512 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0 | percentile: 4.3
IQR_logit_ec_tanimoto_similarity
8.10
8.05
8.00
7.95
7.90
7.85
7.80
0
500
1000
1500
2000

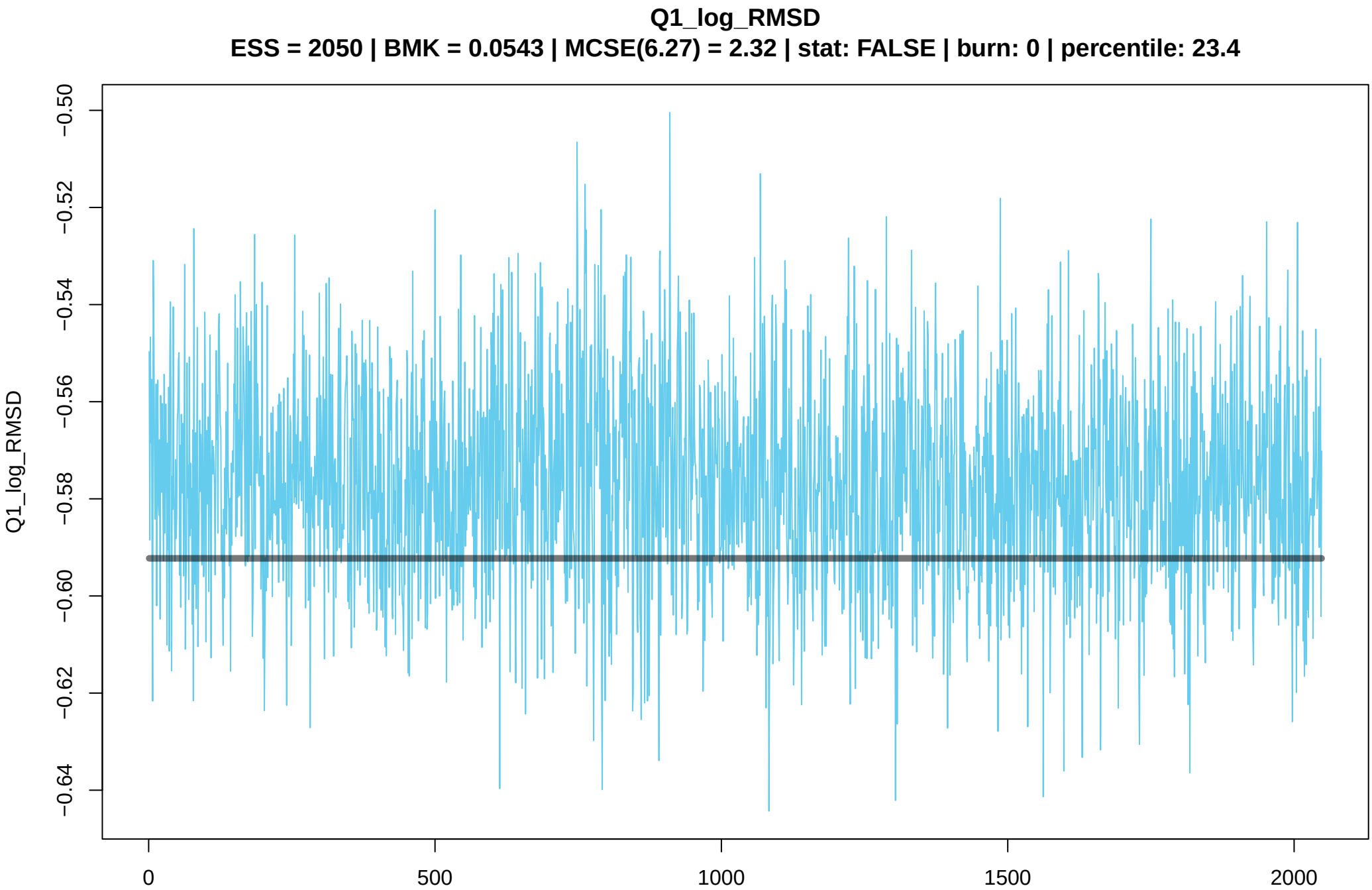

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

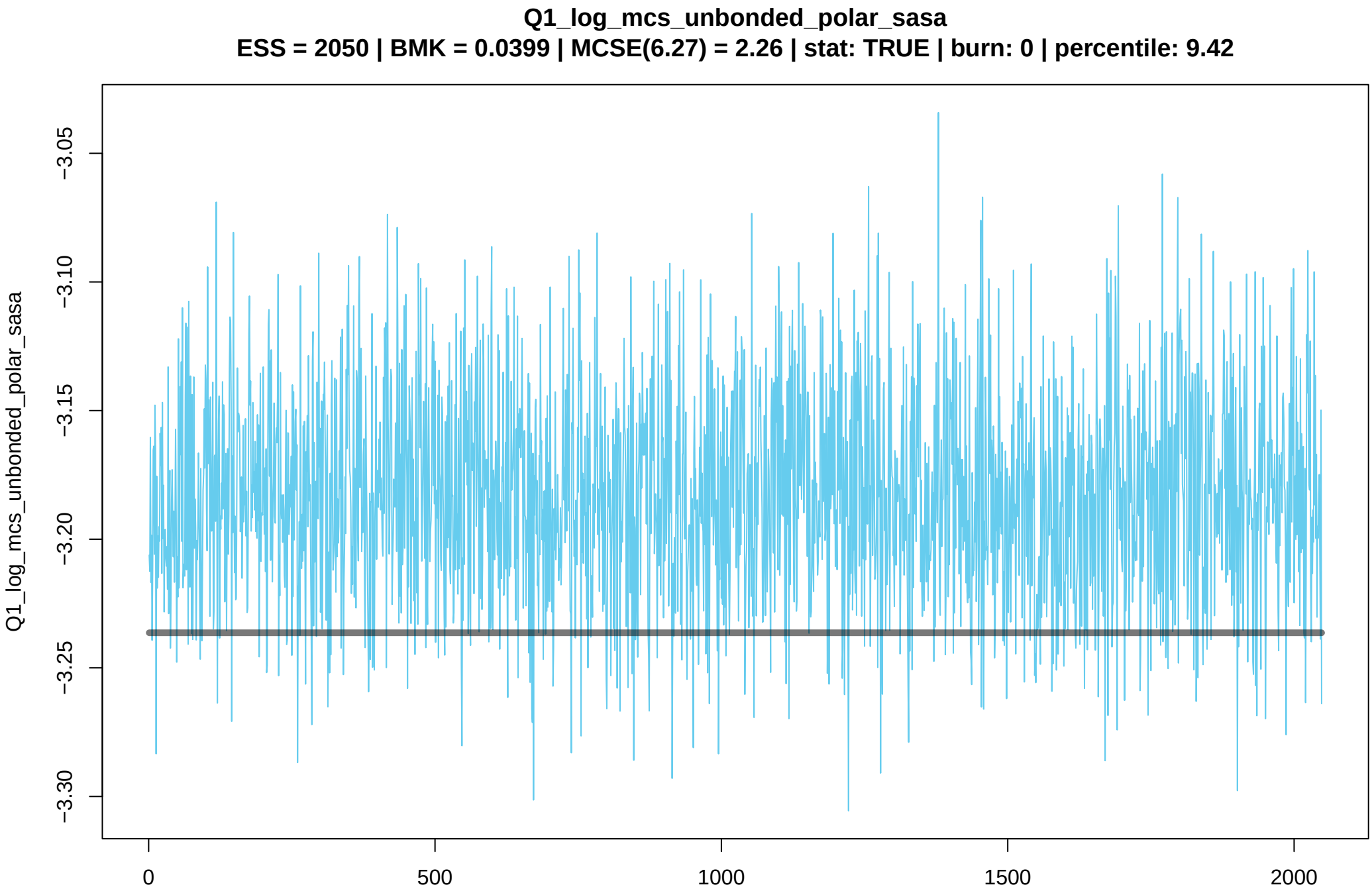

IQR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.144 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 100
IQR_docked_HeavyAtomCount
35.0
35.2
35.4
35.6
35.8
36.0
0
500
1000
1500
2000

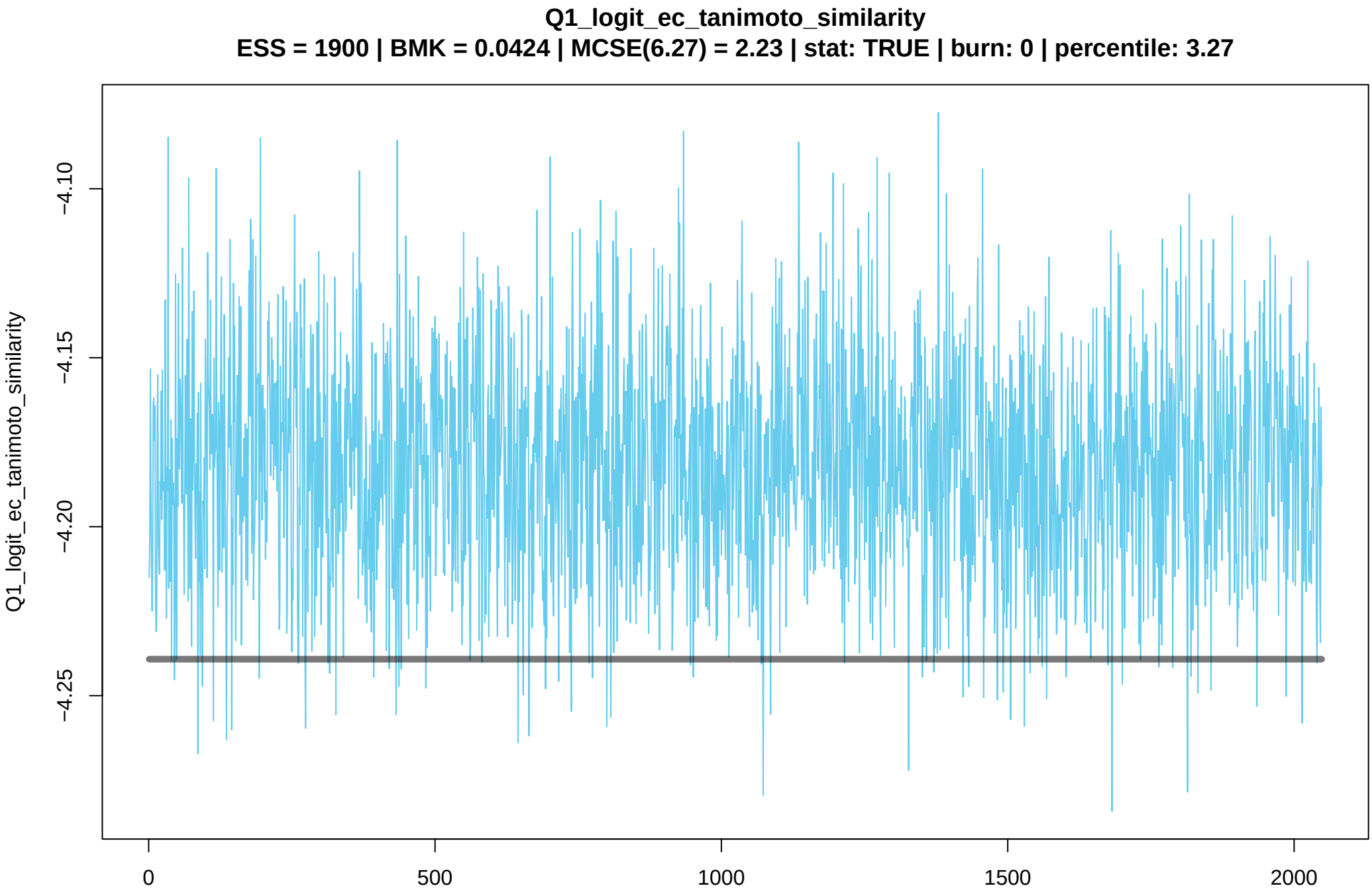

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
IQR_mcs_RingCount
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

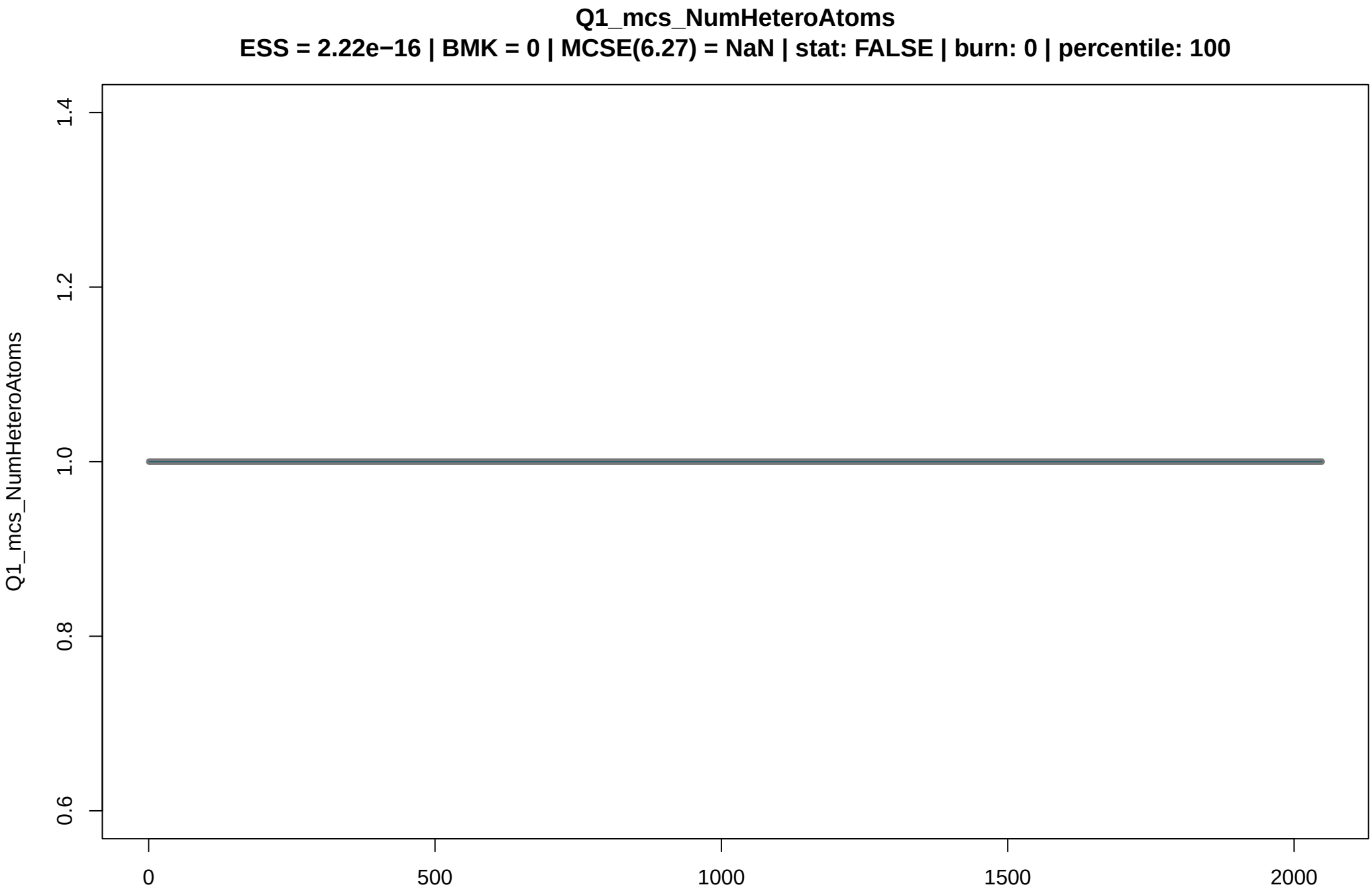

IQR_docked_NumRotatableBonds
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
IQR_docked_NumRotatableBonds
6
7
8
9
10
11
12
0
500
1000
1500
2000

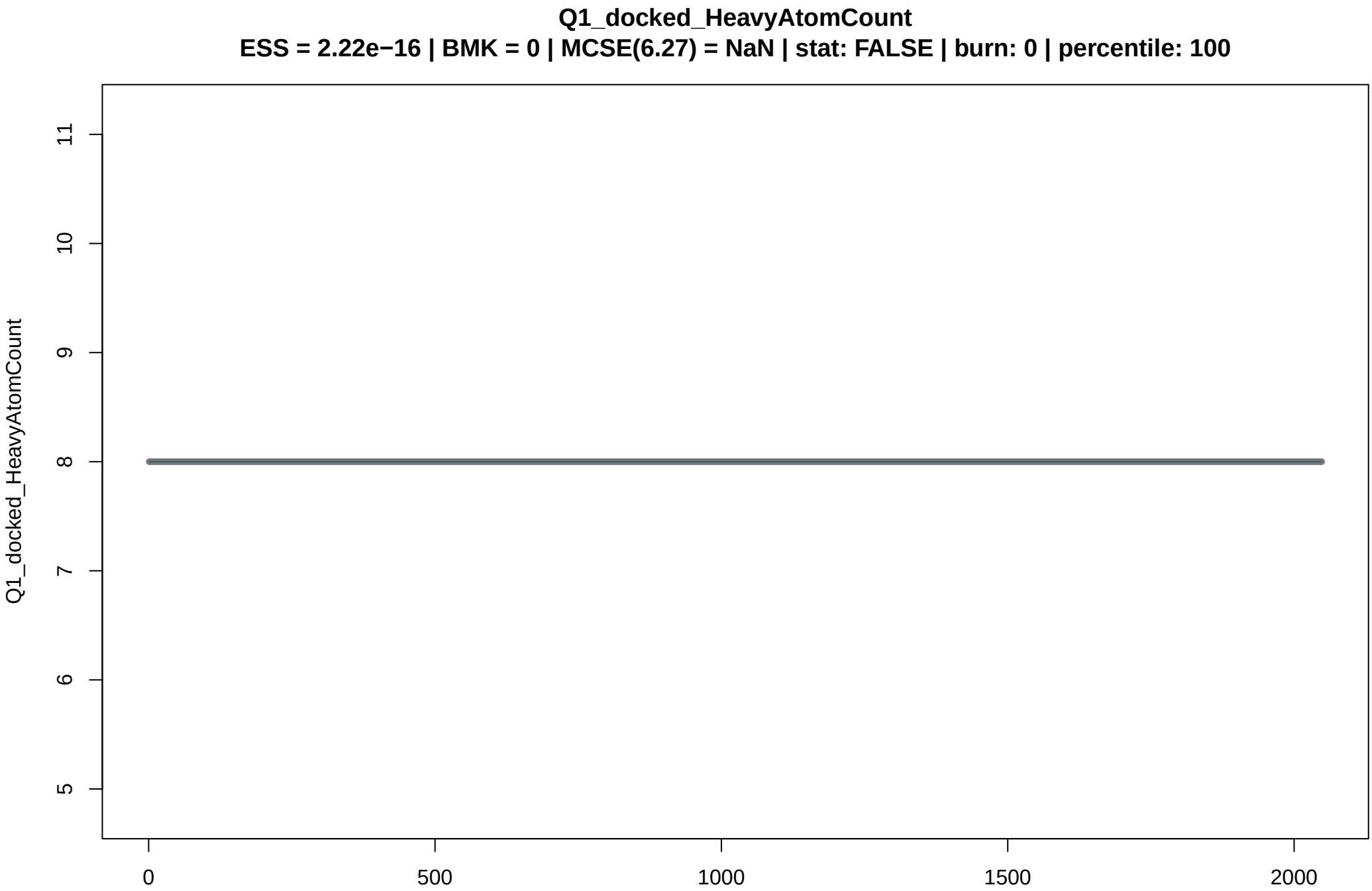

IQR_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
IQR_mcs_NOCount
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

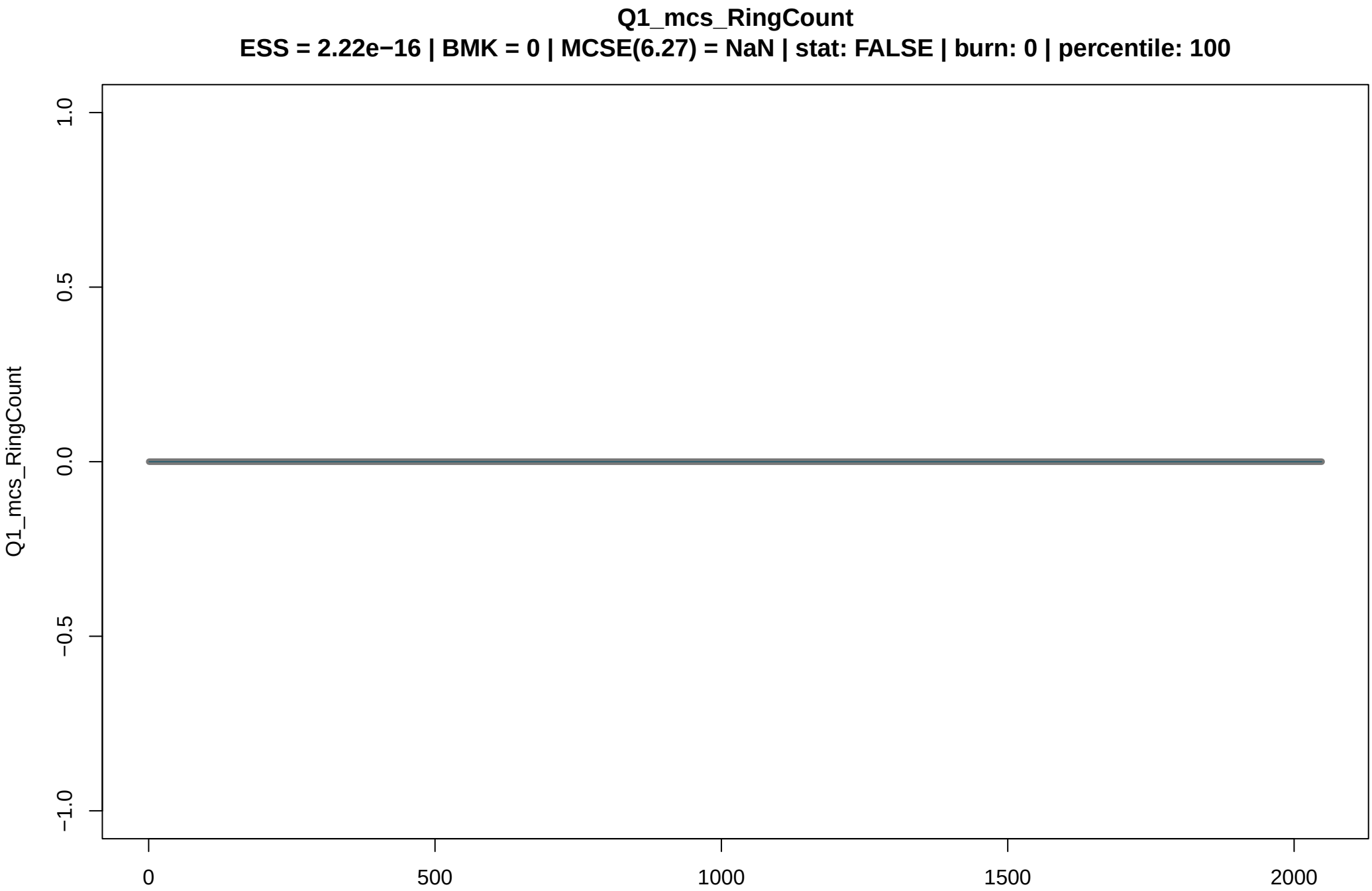

Q1_log_RMSD
ESS = 2050 | BMK = 0.0543 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0 | percentile: 23.4
Q1_log_RMSD
−0.50
−0.52
−0.54
−0.56
−0.58
−0.60
−0.62
−0.64
0
500
1000
1500
2000

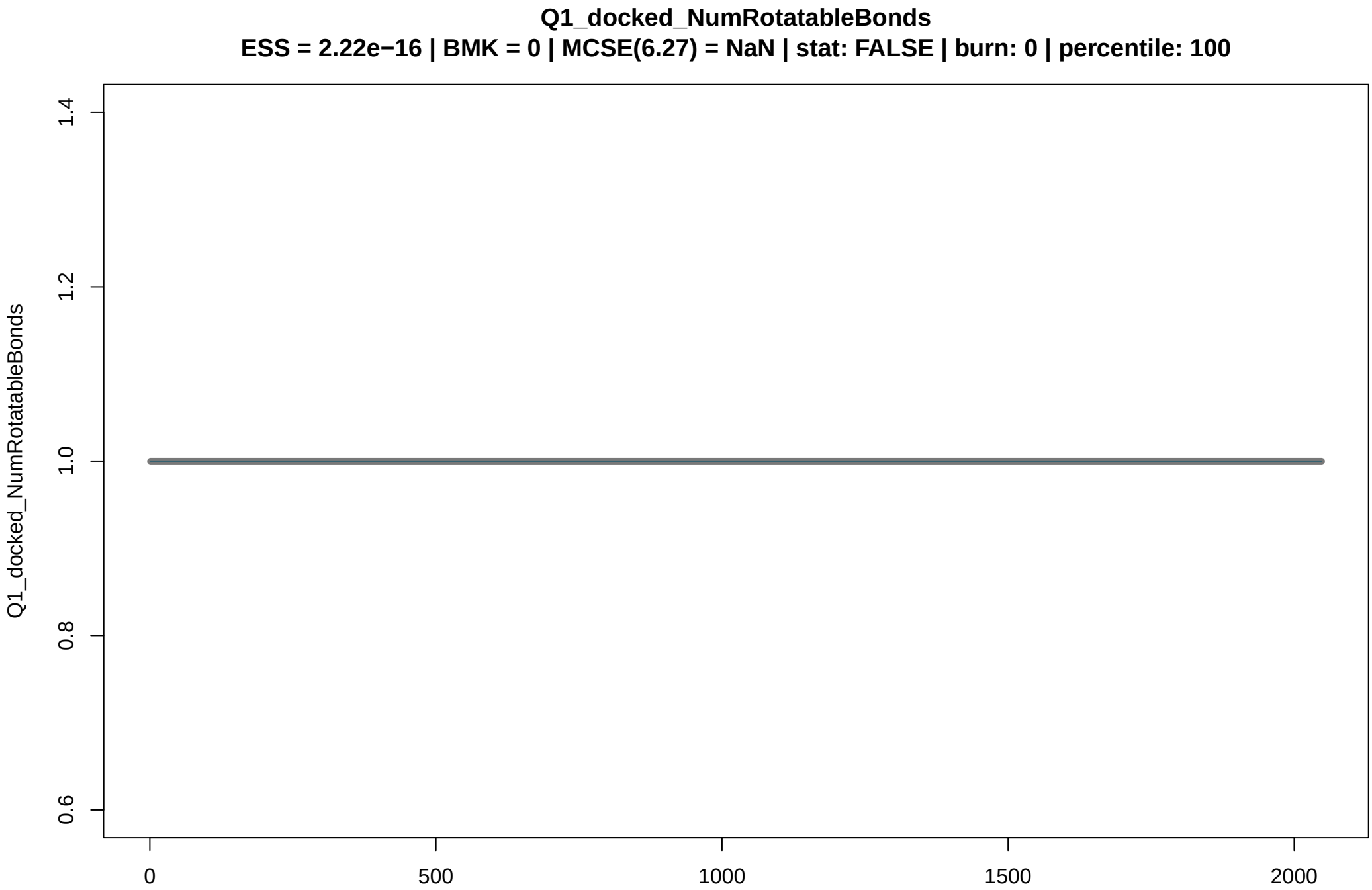

Q1_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0399 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | percentile: 9.42
Q1_log_mcs_unbonded_polar_sasa
−3.05
−3.10
−3.15
−3.20
−3.25
−3.30
0
500
1000
1500
2000

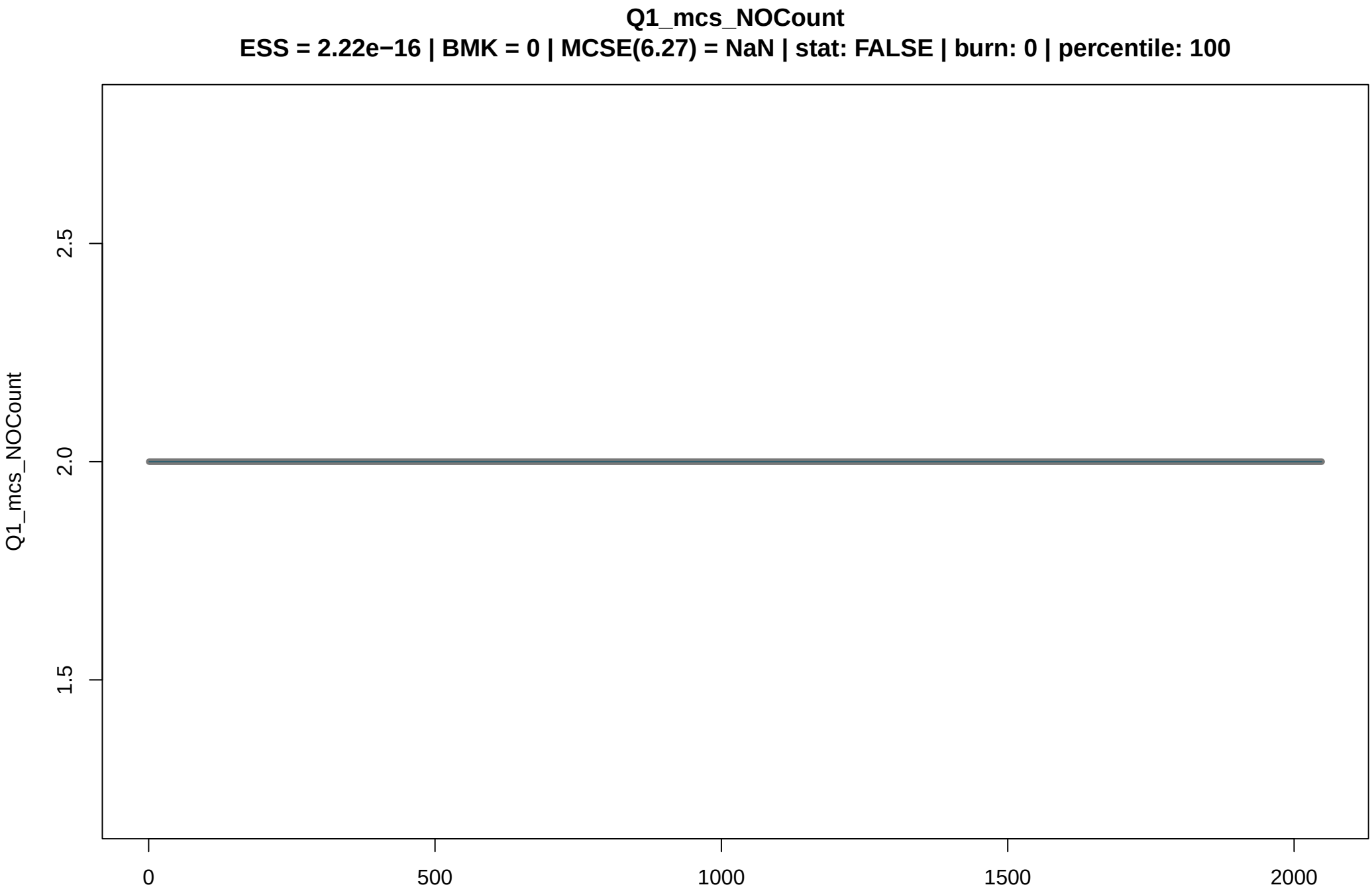

Q1_logit_ec_tanimoto_similarity
ESS = 1900 | BMK = 0.0424 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | percentile: 3.27
Q1_logit_ec_tanimoto_similarity
−4.10
−4.15
−4.20
−4.25
0
500
1000
1500
2000

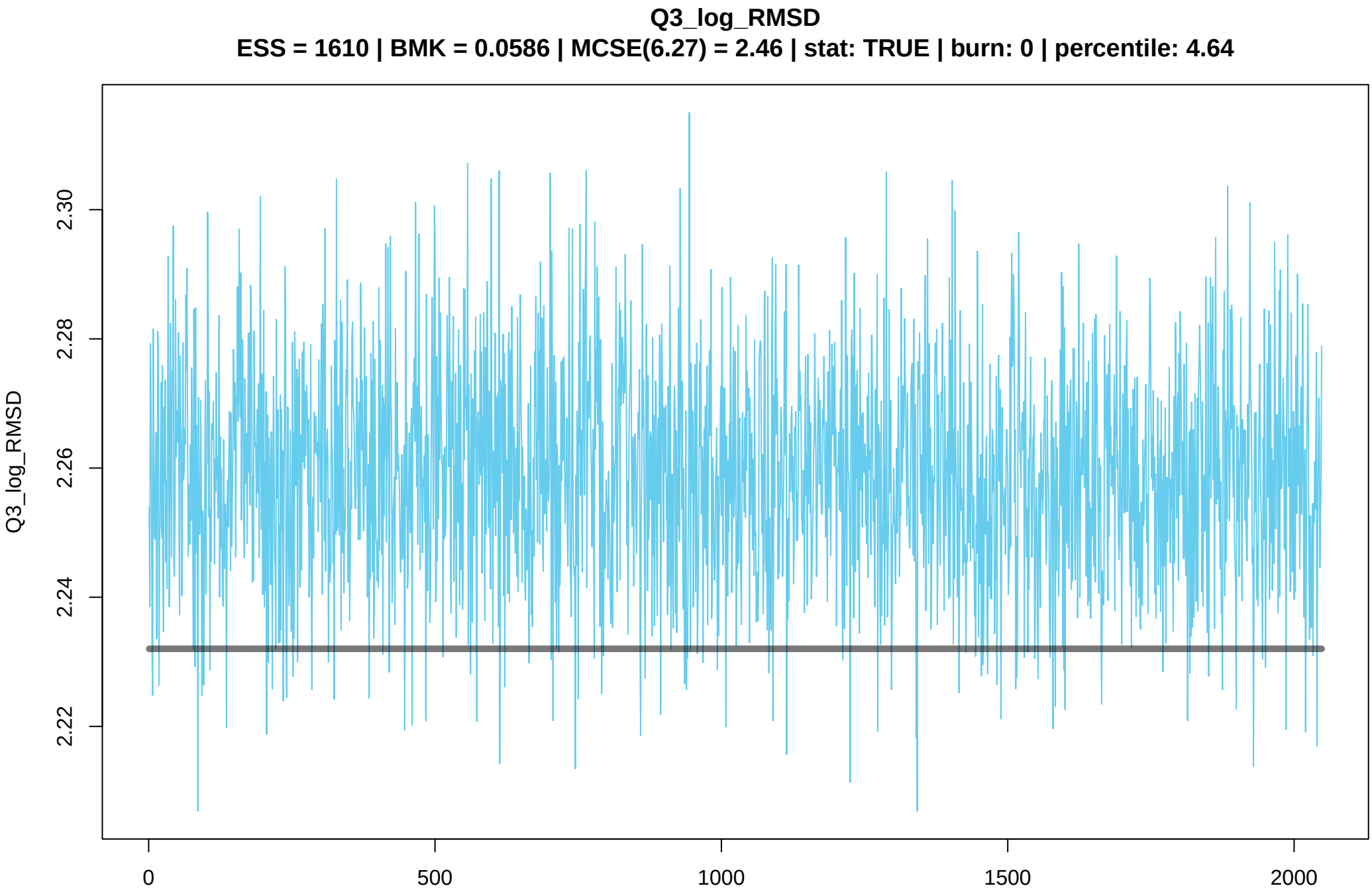

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

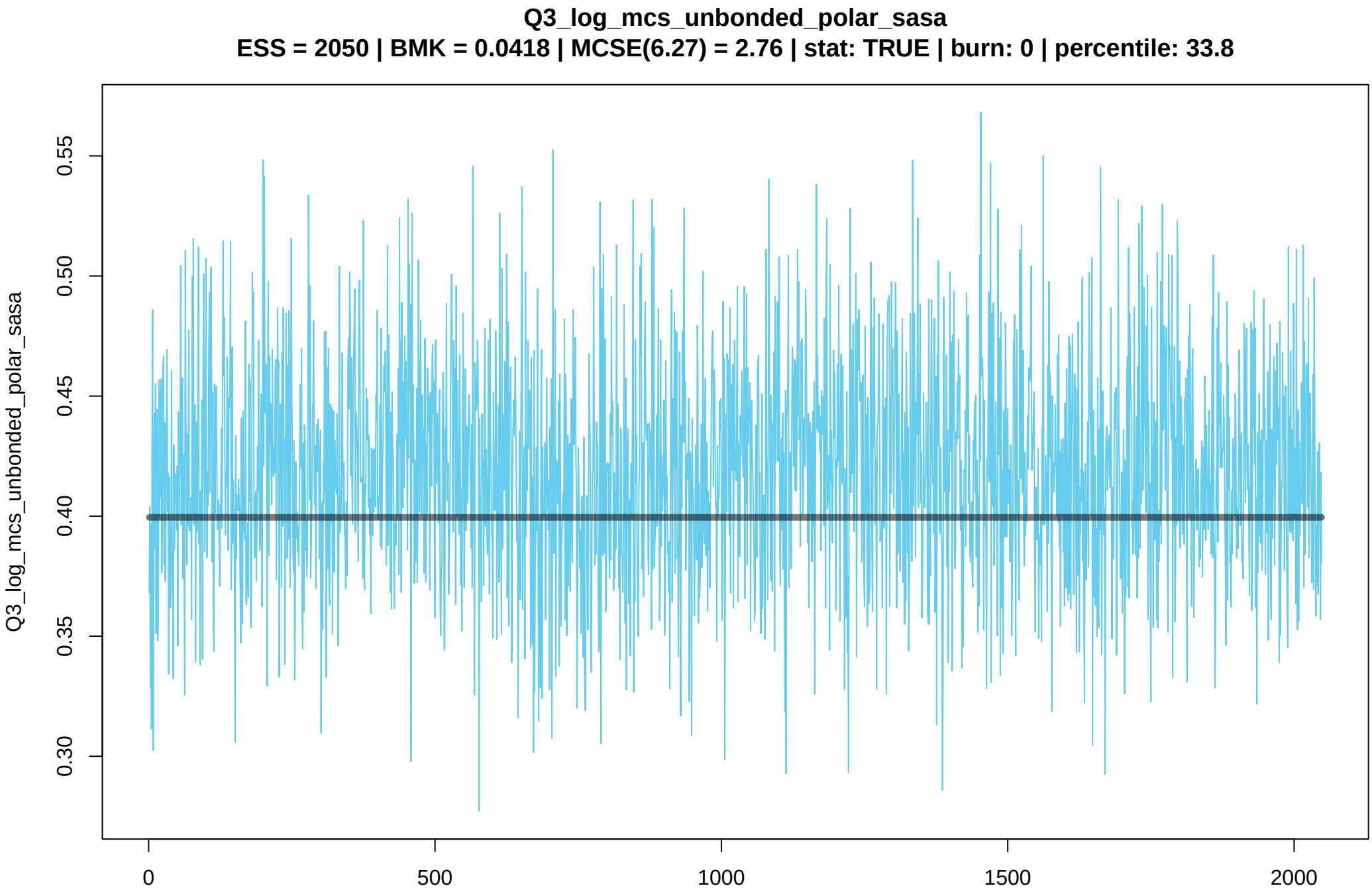

Q1_docked_HeavyAtomCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q1_docked_HeavyAtomCount
5
6
7
8
9
10
11
0
500
1000
1500
2000

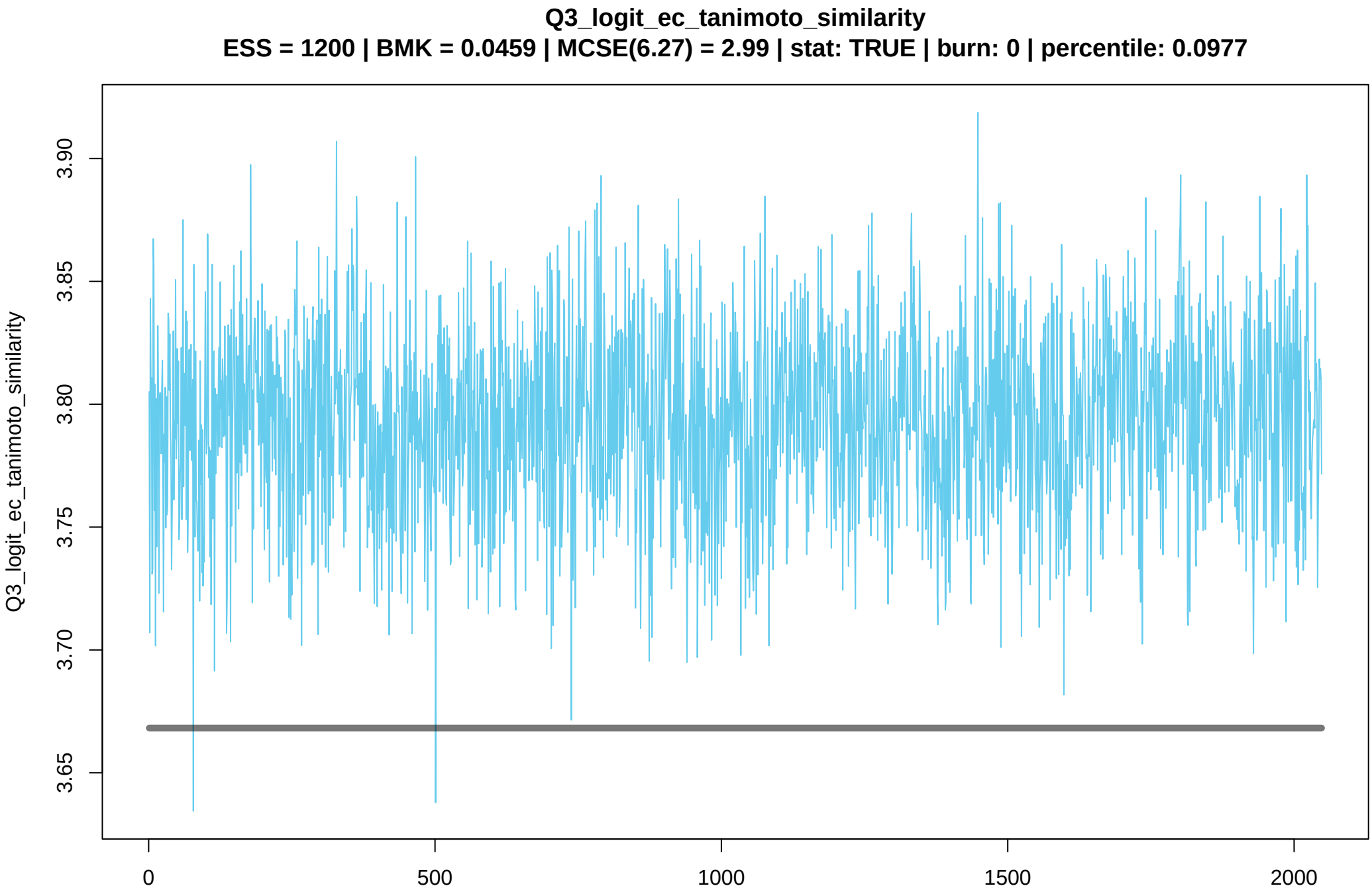

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

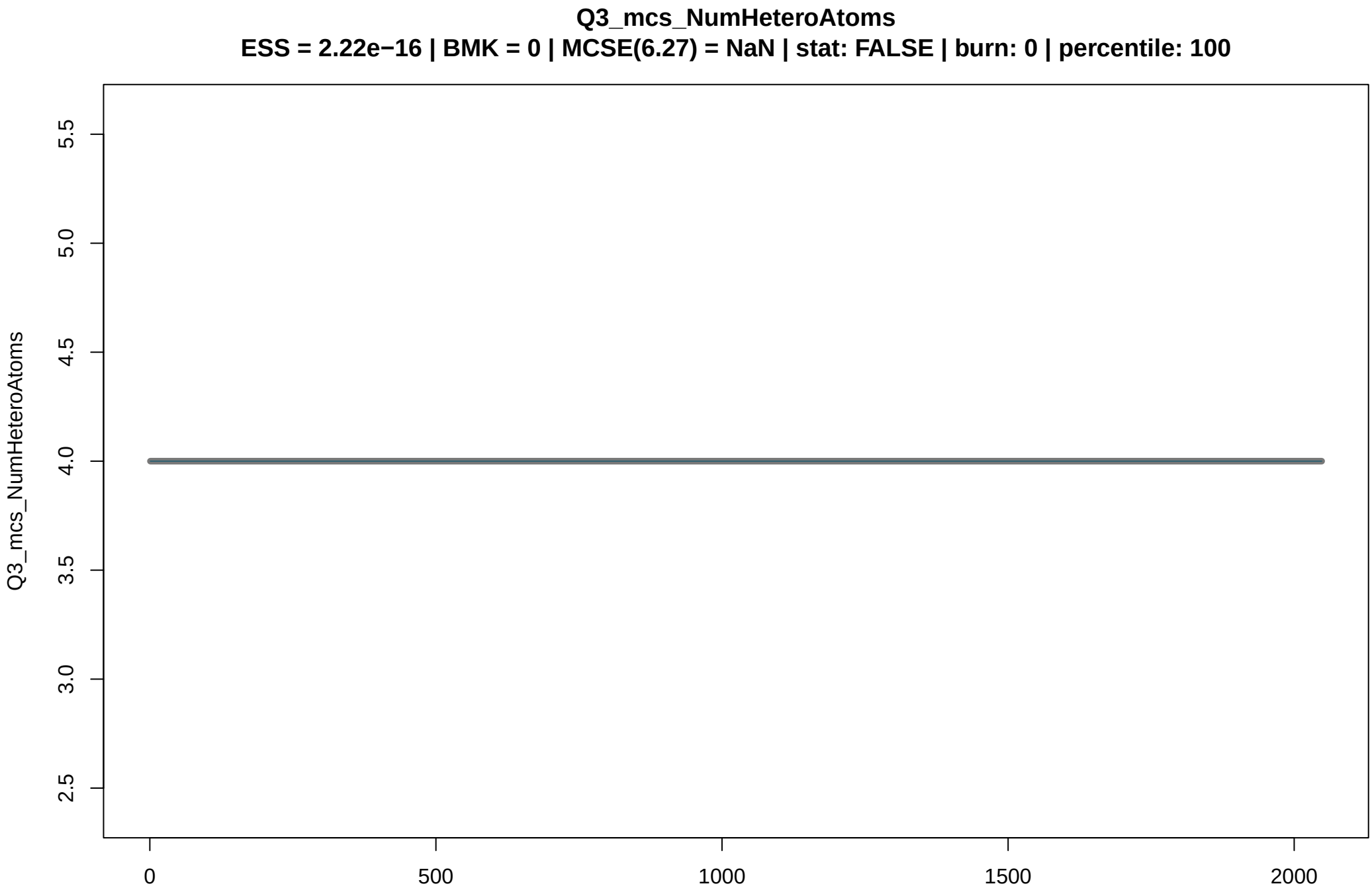

Q1_docked_NumRotatableBonds
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q1_docked_NumRotatableBonds
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

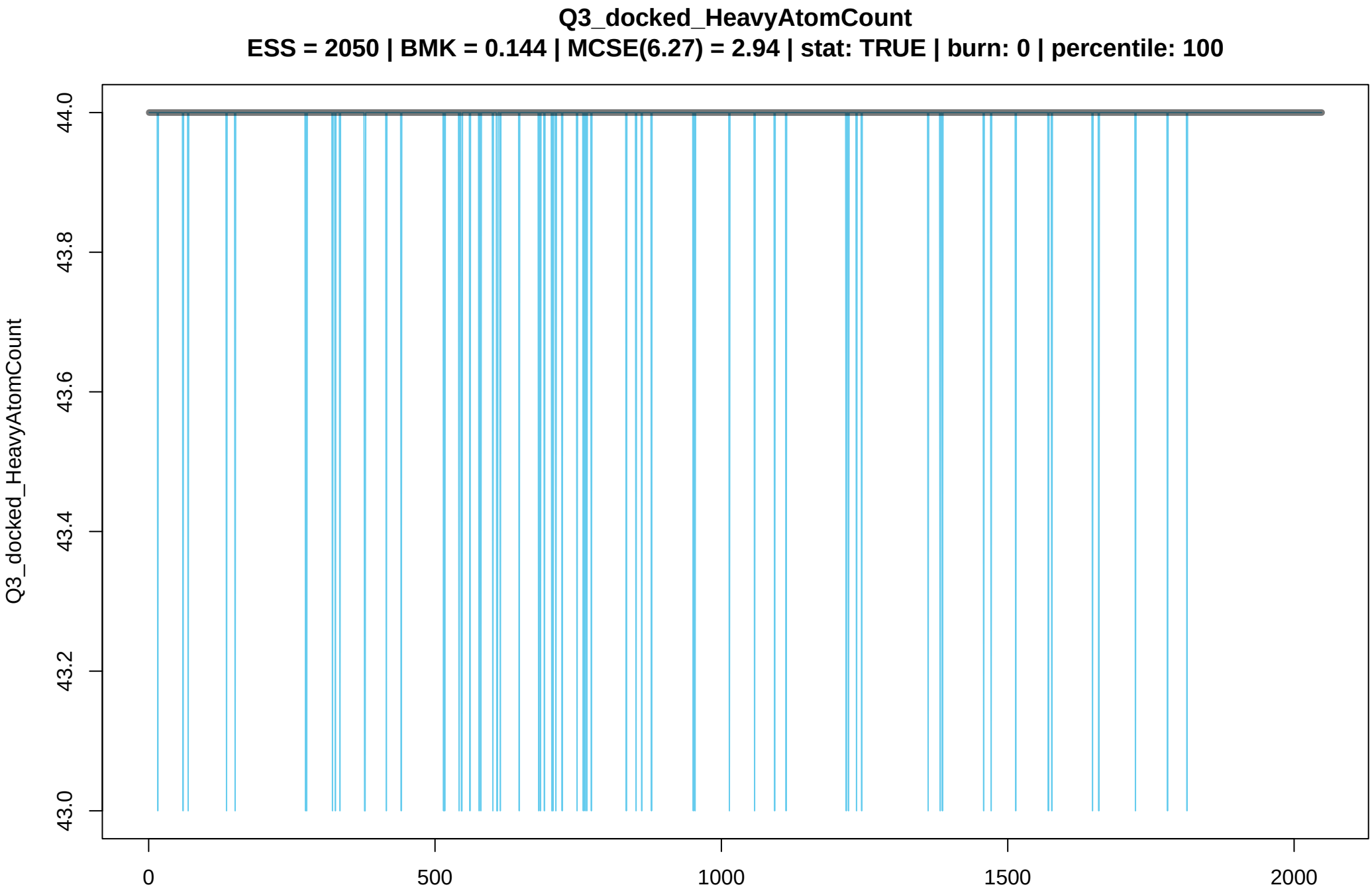

Q1_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q1_mcs_NOCount
2.5
2.0
1.5
0
500
1000
1500
2000

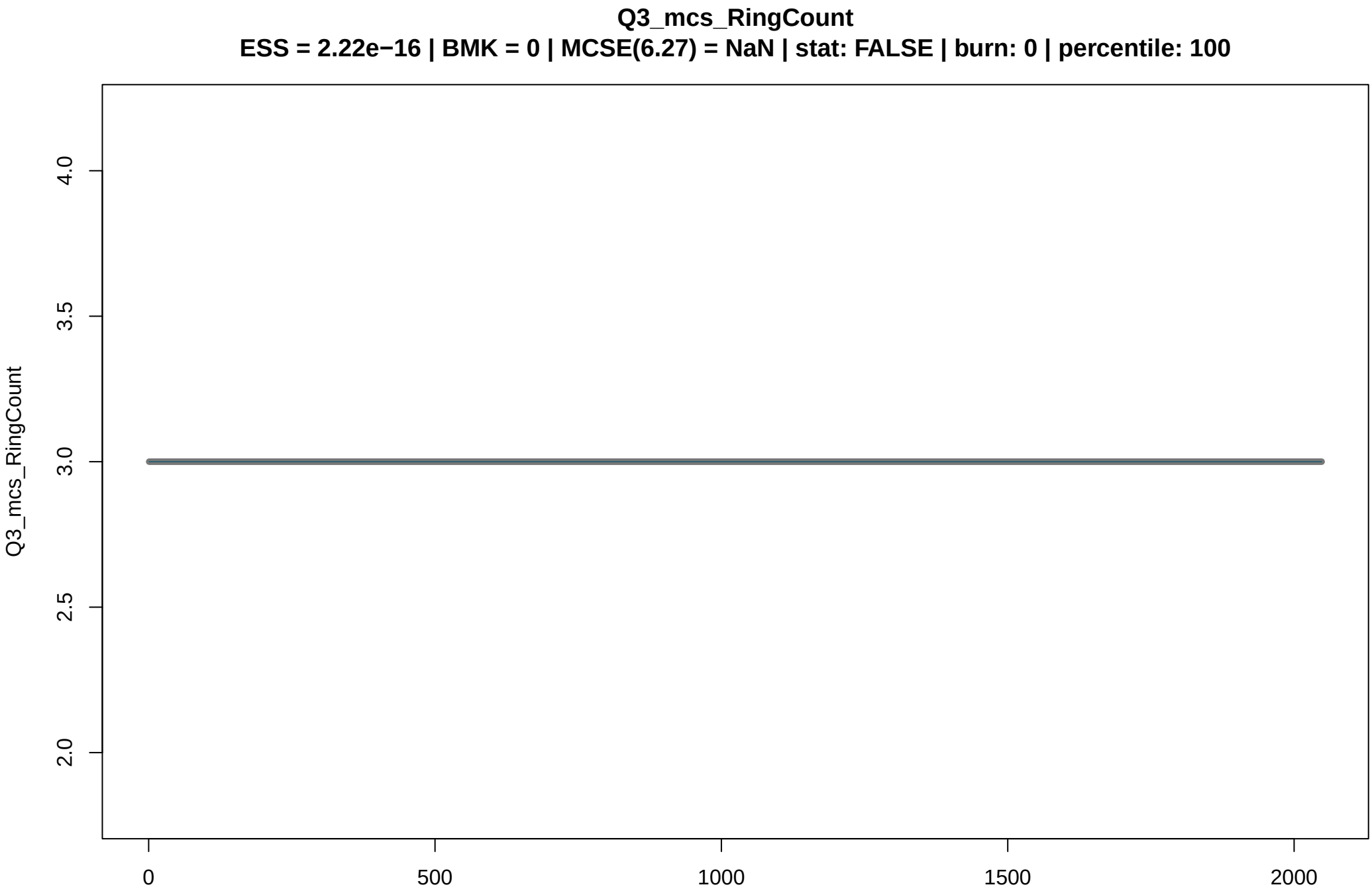

Q3_log_RMSD
ESS = 1610 | BMK = 0.0586 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0 | percentile: 4.64
Q3_log_RMSD
2.22
2.24
2.26
2.28
2.30
0
500
1000
1500
2000

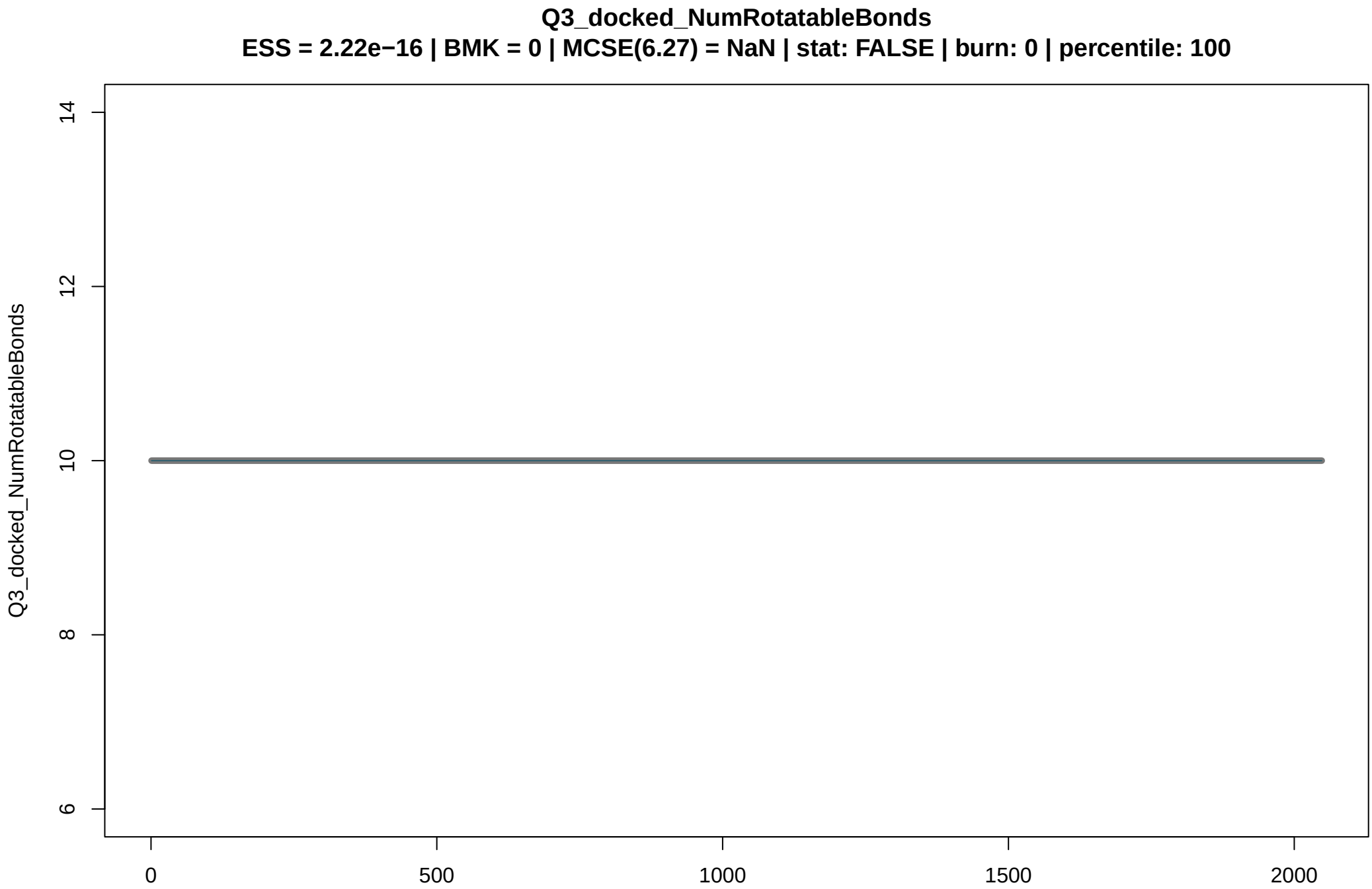

Q3_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0418 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | percentile: 33.8
Q3_log_mcs_unbonded_polar_sasa
0.30
0.35
0.40
0.45
0.50
0.55
0
500
1000
1500
2000

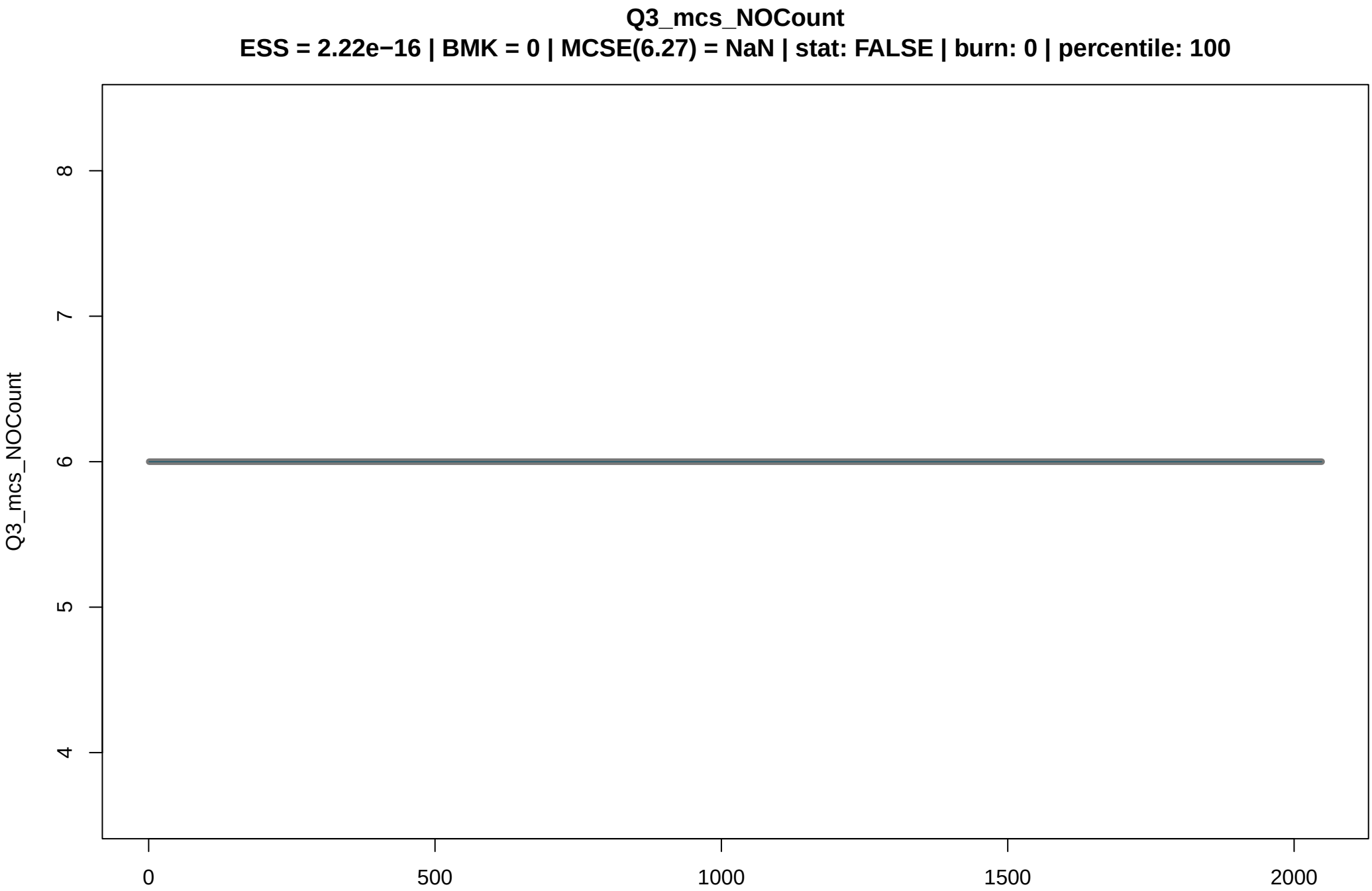

Q3_logit_ec_tanimoto_similarity
ESS = 1200 | BMK = 0.0459 | MCSE(6.27) = 2.99 | stat: TRUE | burn: 0 | percentile: 0.0977
Q3_logit_ec_tanimoto_similarity
3.65
3.70
3.75
3.80
3.85
3.90
0
500
1000
1500
2000

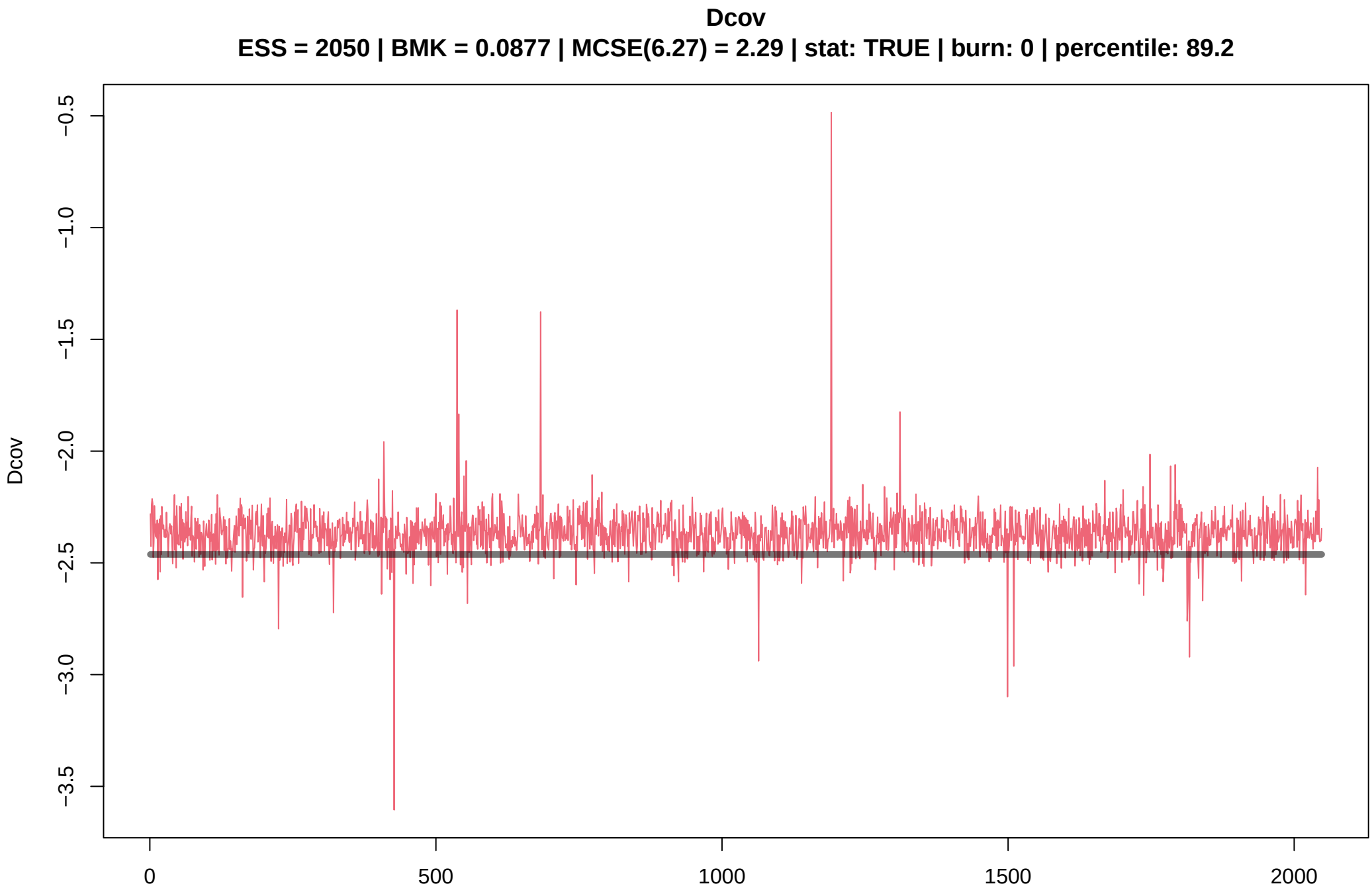

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

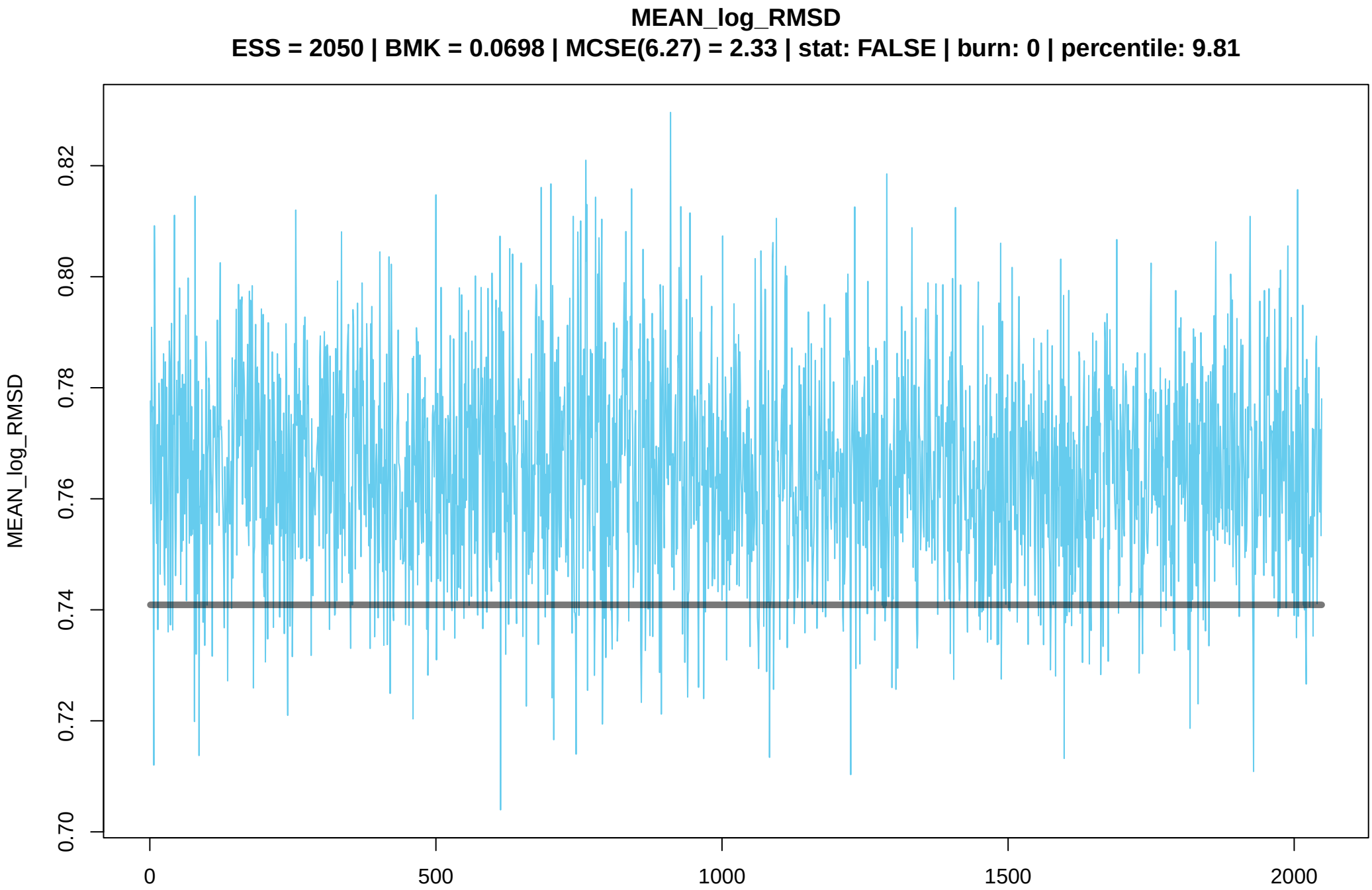

Q3_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.144 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | percentile: 100
Q3_docked_HeavyAtomCount
44.0
43.8
43.6
43.4
43.2
43.0
0
500
1000
1500
2000

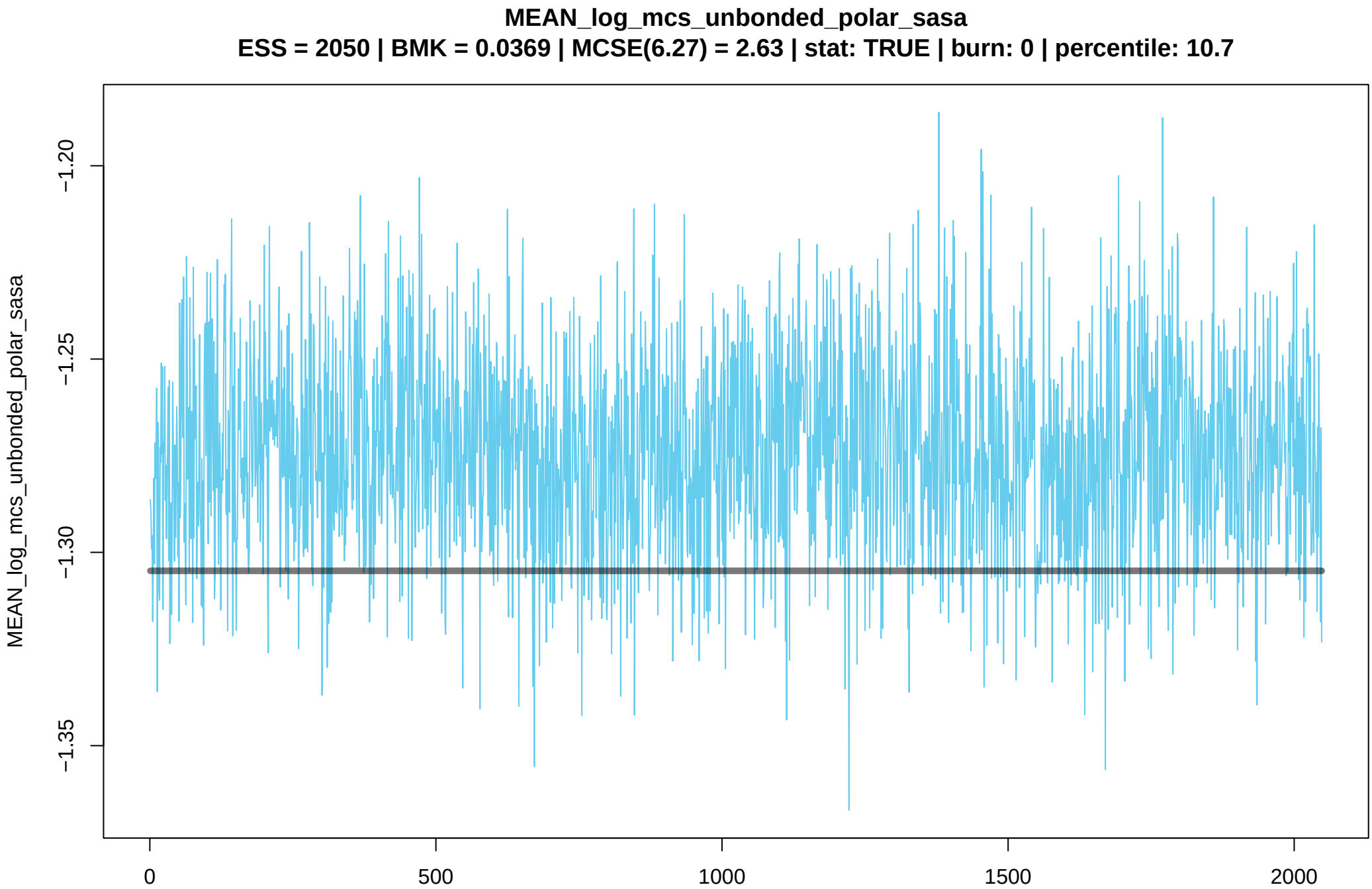

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q3_mcs_RingCount
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

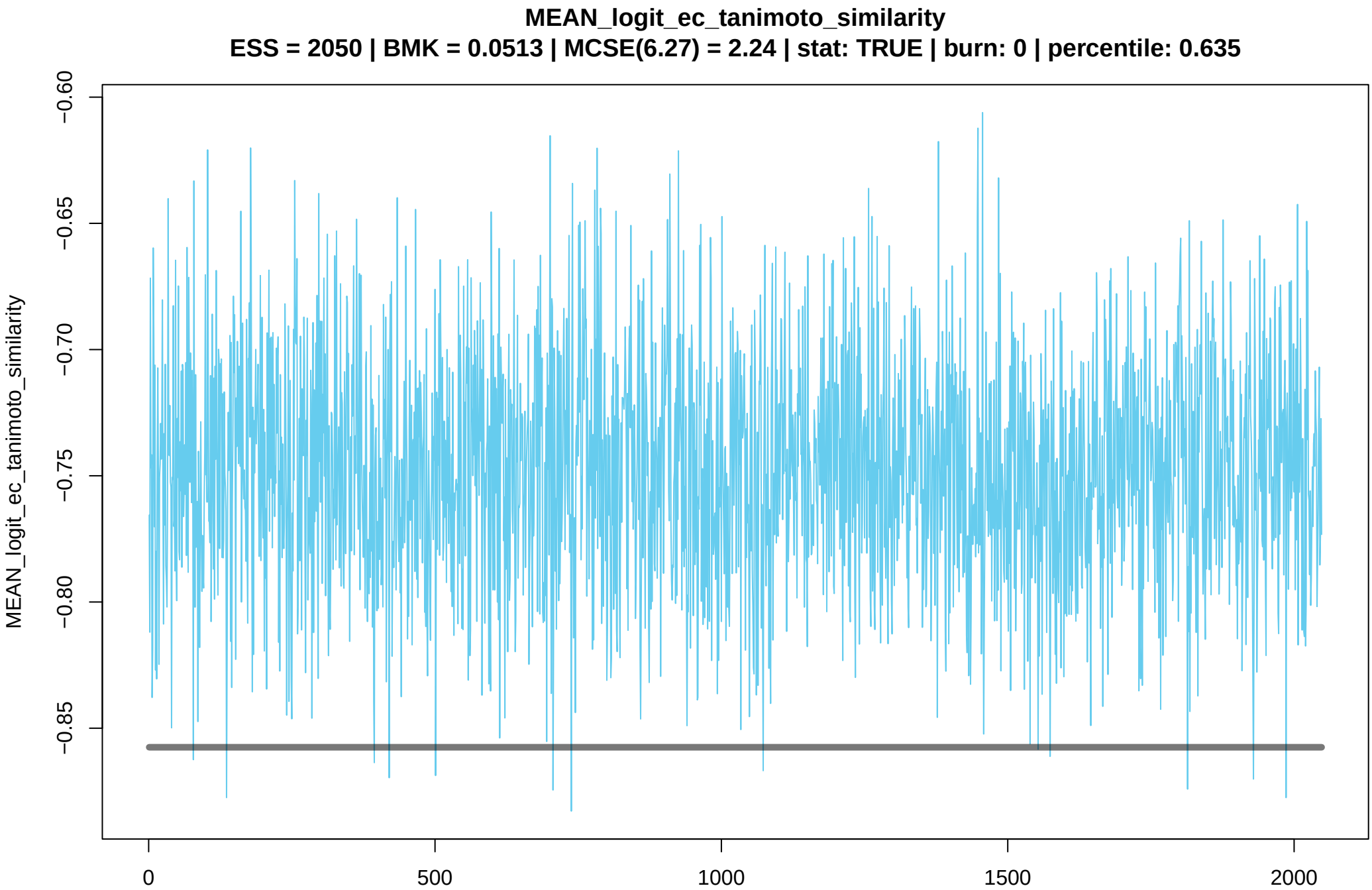

Q3_docked_NumRotatableBonds
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q3_docked_NumRotatableBonds
14
12
10
8
6
0
500
1000
1500
2000

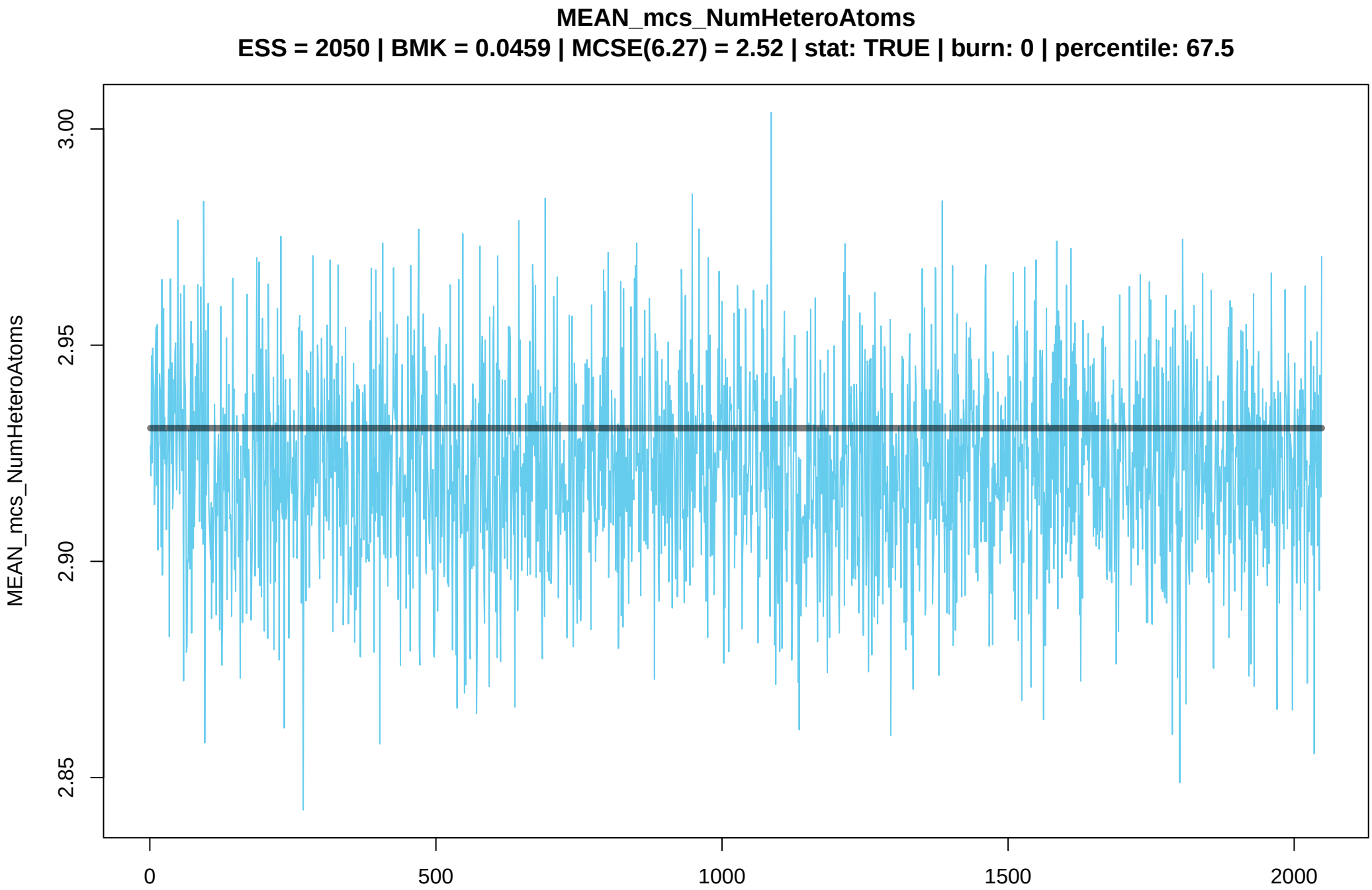

Q3_mcs_NOCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0 | percentile: 100
Q3_mcs_NOCount
4
5
6
7
8
0
500
1000
1500
2000

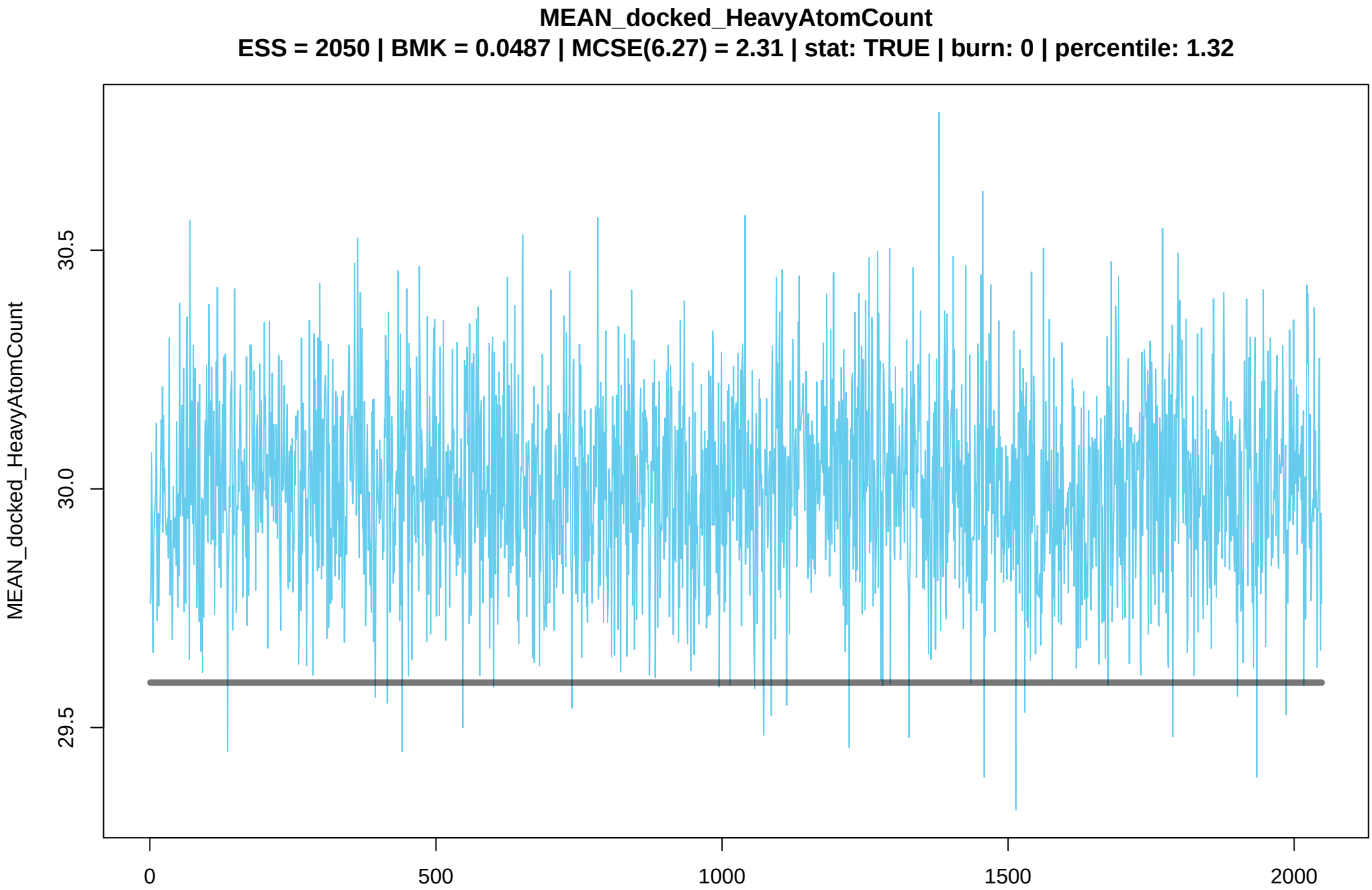

Dcov
ESS = 2050 | BMK = 0.0877 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | percentile: 89.2
Dcov
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
−3.5
0
500
1000
1500
2000

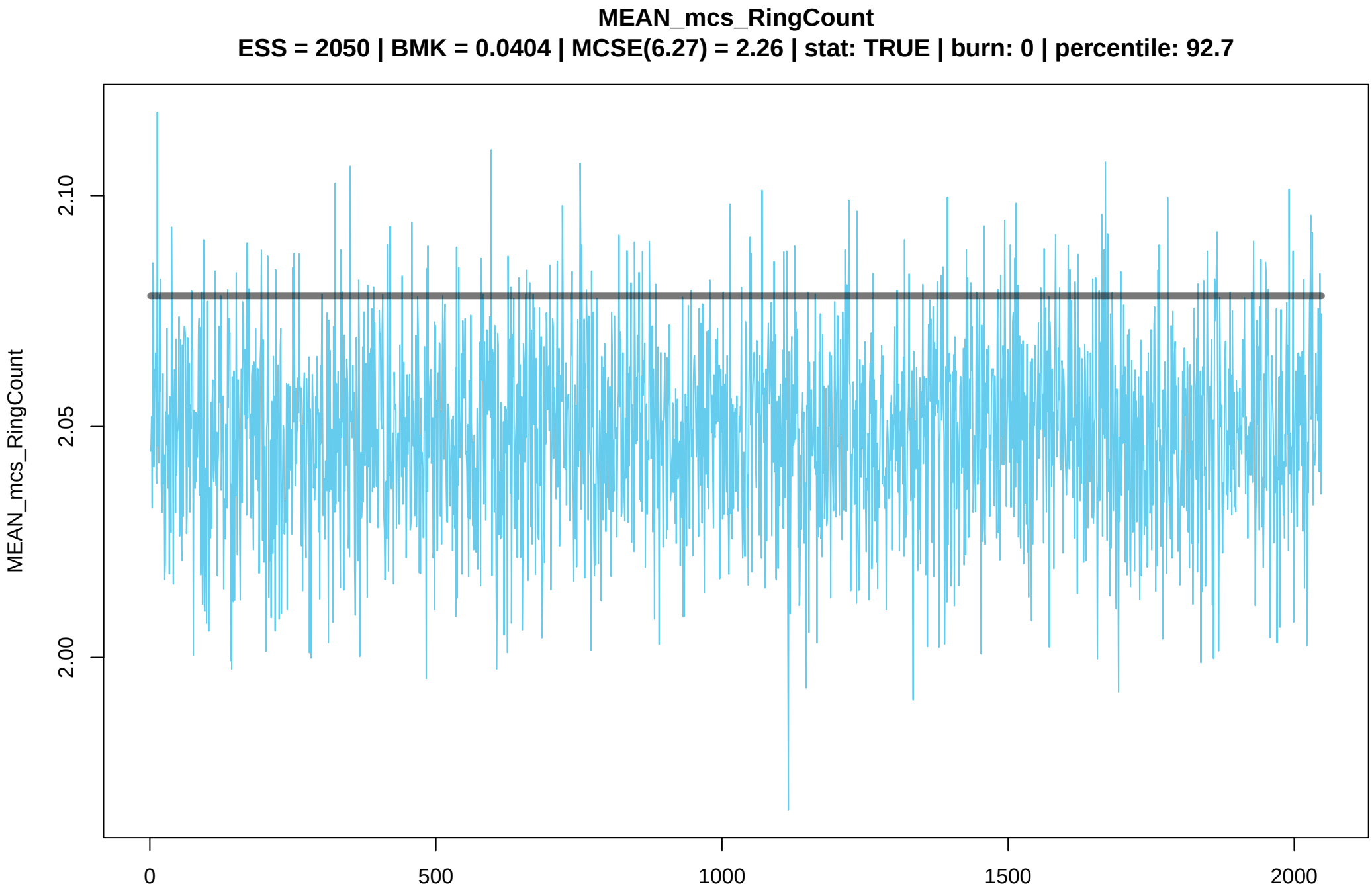

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0698 | MCSE(6.27) = 2.33 | stat: FALSE | burn: 0 | percentile: 9.81
MEAN_log_RMSD
0.70
0.72
0.74
0.76
0.78
0.80
0.82
0
500
1000
1500
2000

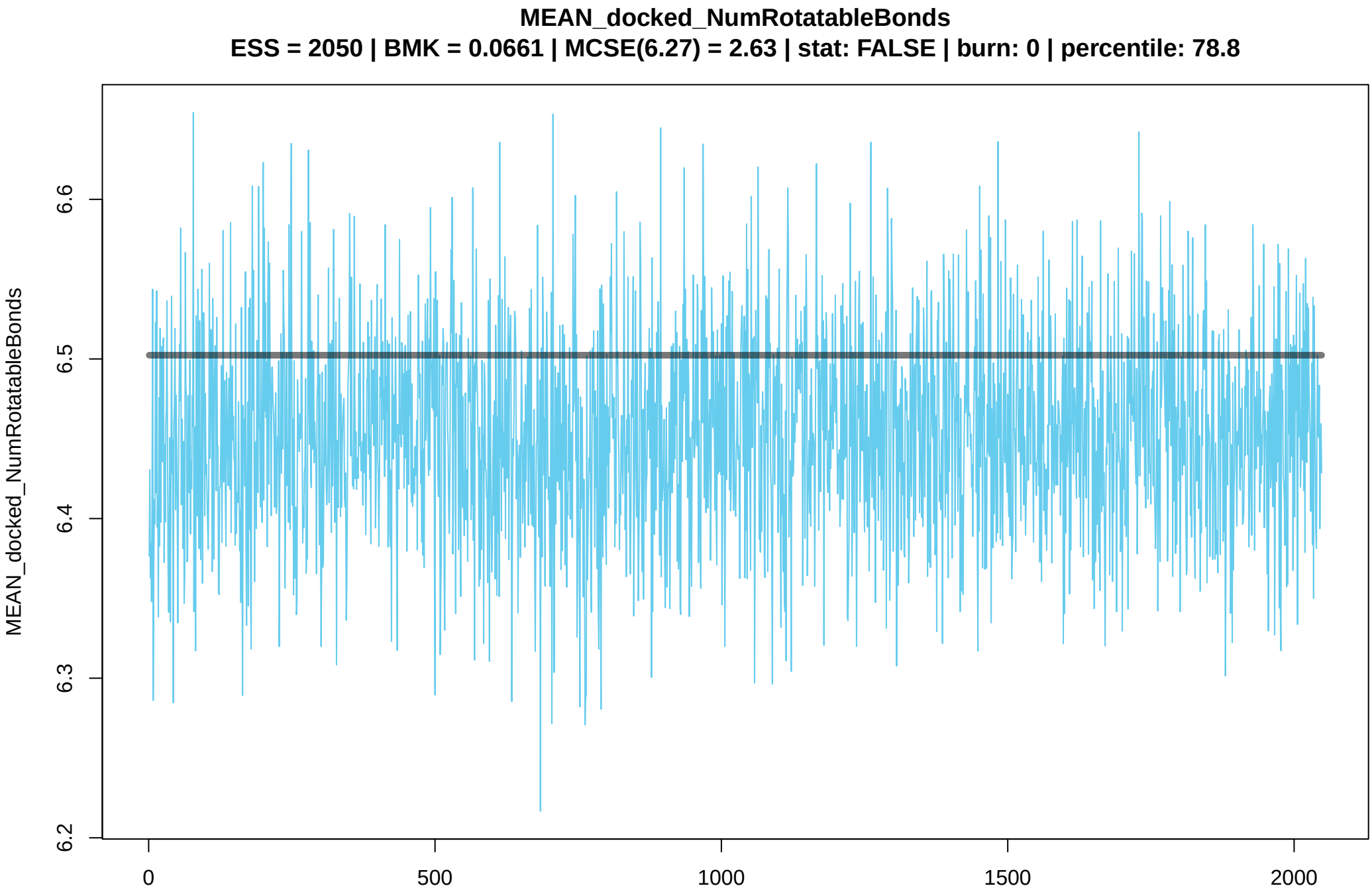

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0369 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | percentile: 10.7
MEAN_log_mcs_unbonded_polar_sasa
−1.20
−1.25
−1.30
−1.35
0
500
1000
1500
2000

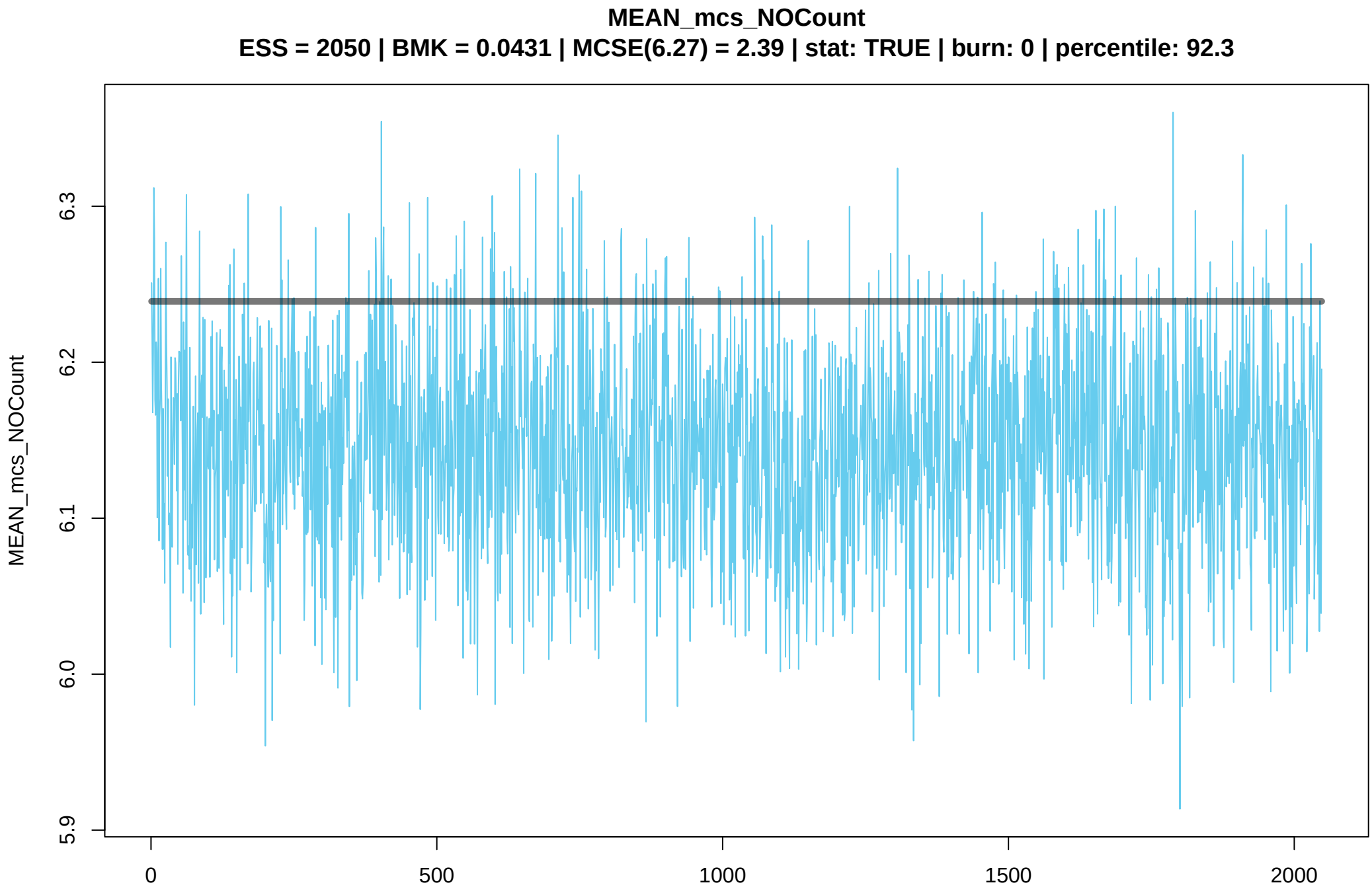

MEAN_logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0513 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0 | percentile: 0.635
MEAN_logit_ec_tanimoto_similarity
−0.60
−0.65
−0.70
−0.75
−0.80
−0.85
0
500
1000
1500
2000

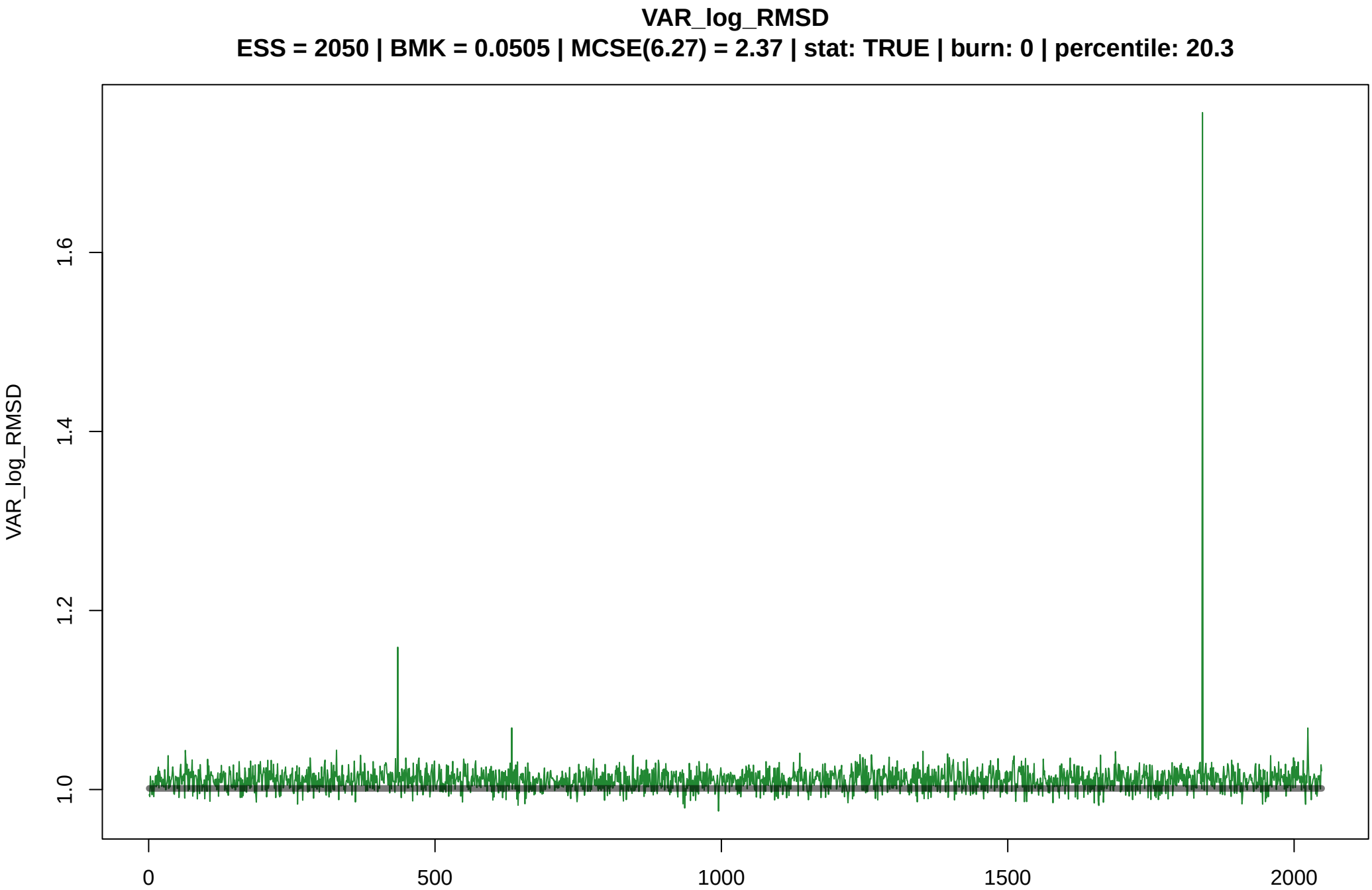

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0459 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | percentile: 67.5
MEAN_mcs_NumHeteroAtoms
3.00
2.95
2.90
2.85
0
500
1000
1500
2000

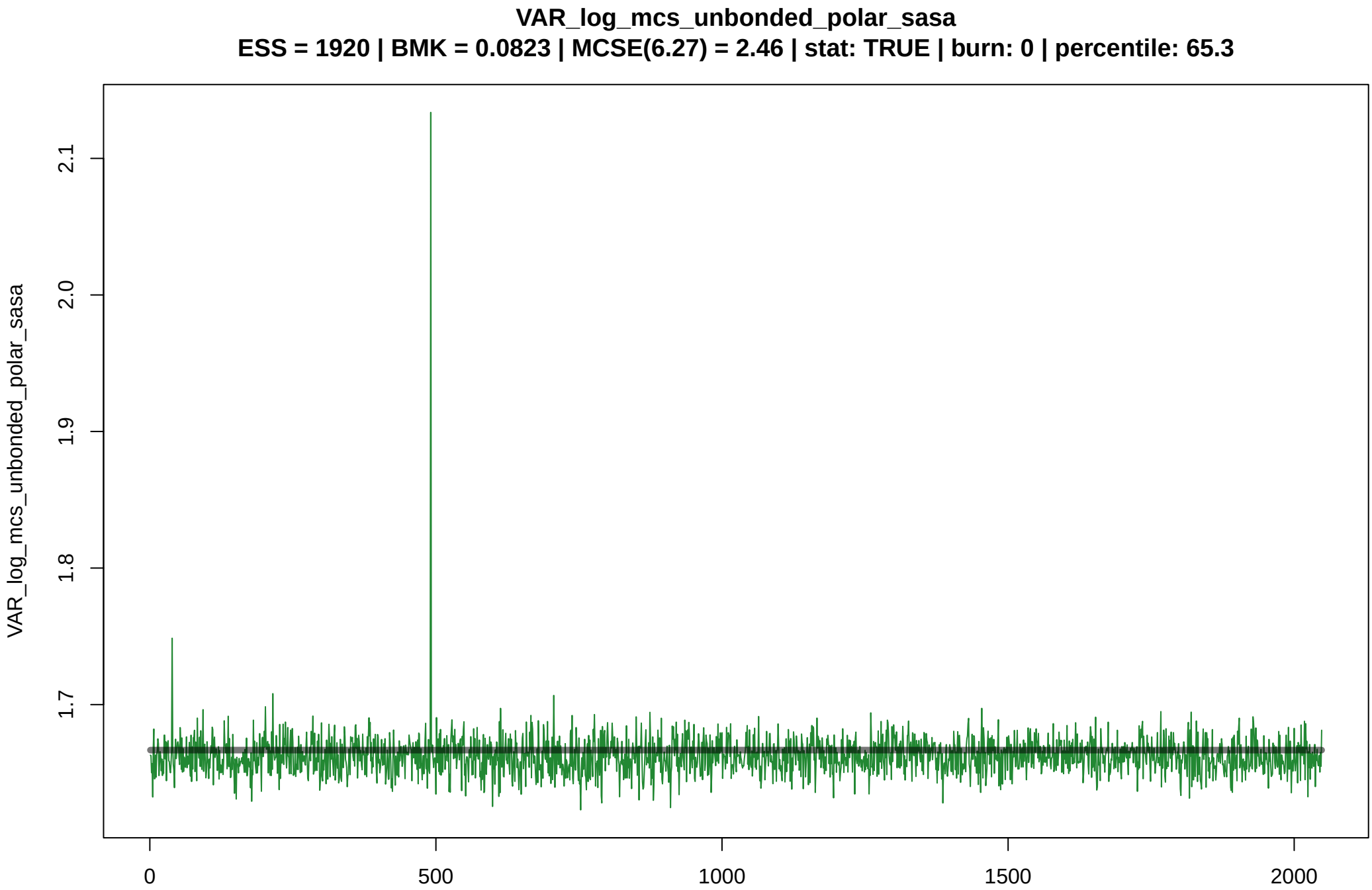

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0487 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0 | percentile: 1.32
MEAN_docked_HeavyAtomCount
29.5
30.0
30.5
0
500
1000
1500
2000

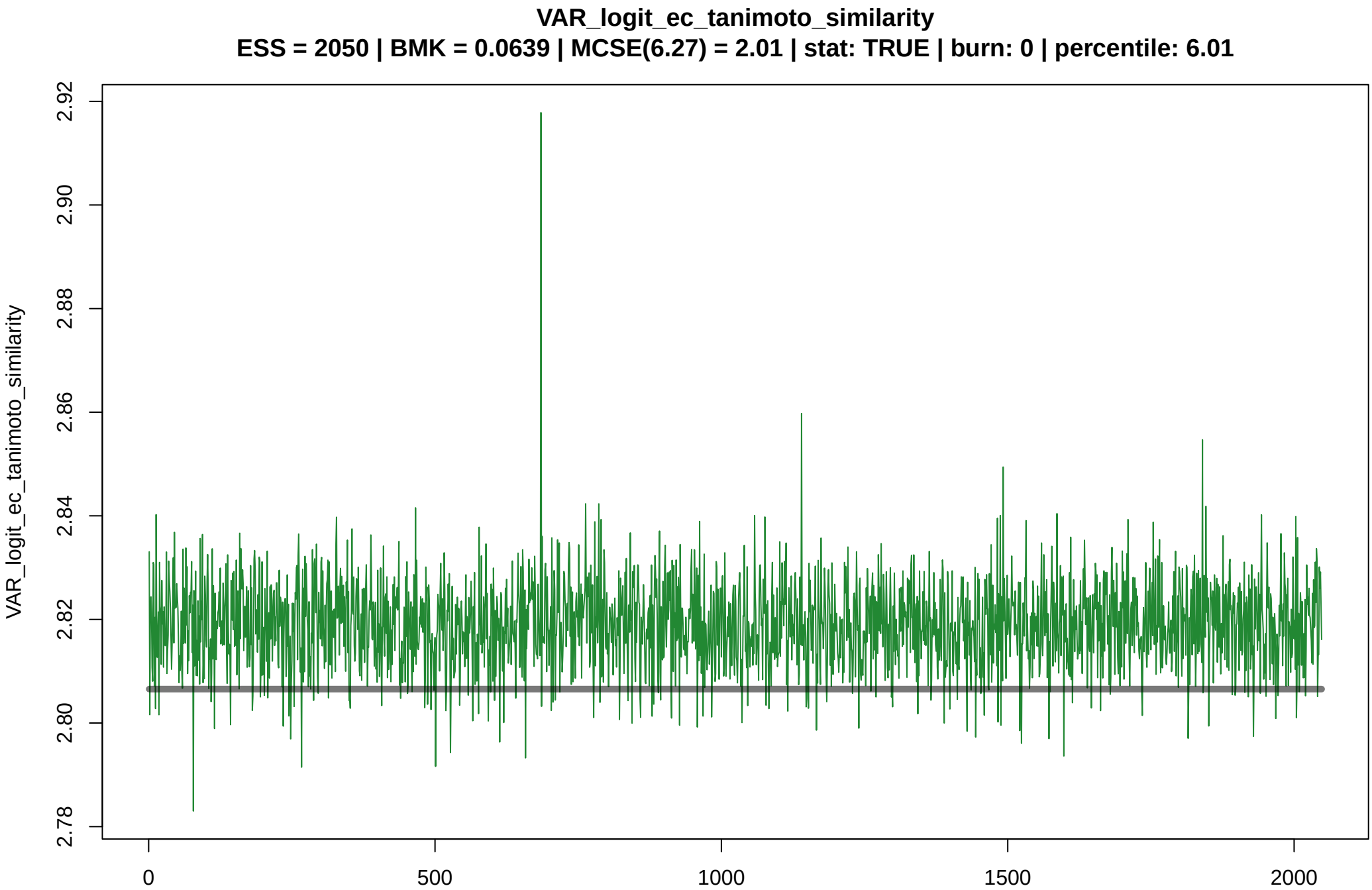

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0404 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | percentile: 92.7
MEAN_mcs_RingCount
2.00
2.05
2.10
0
500
1000
1500
2000

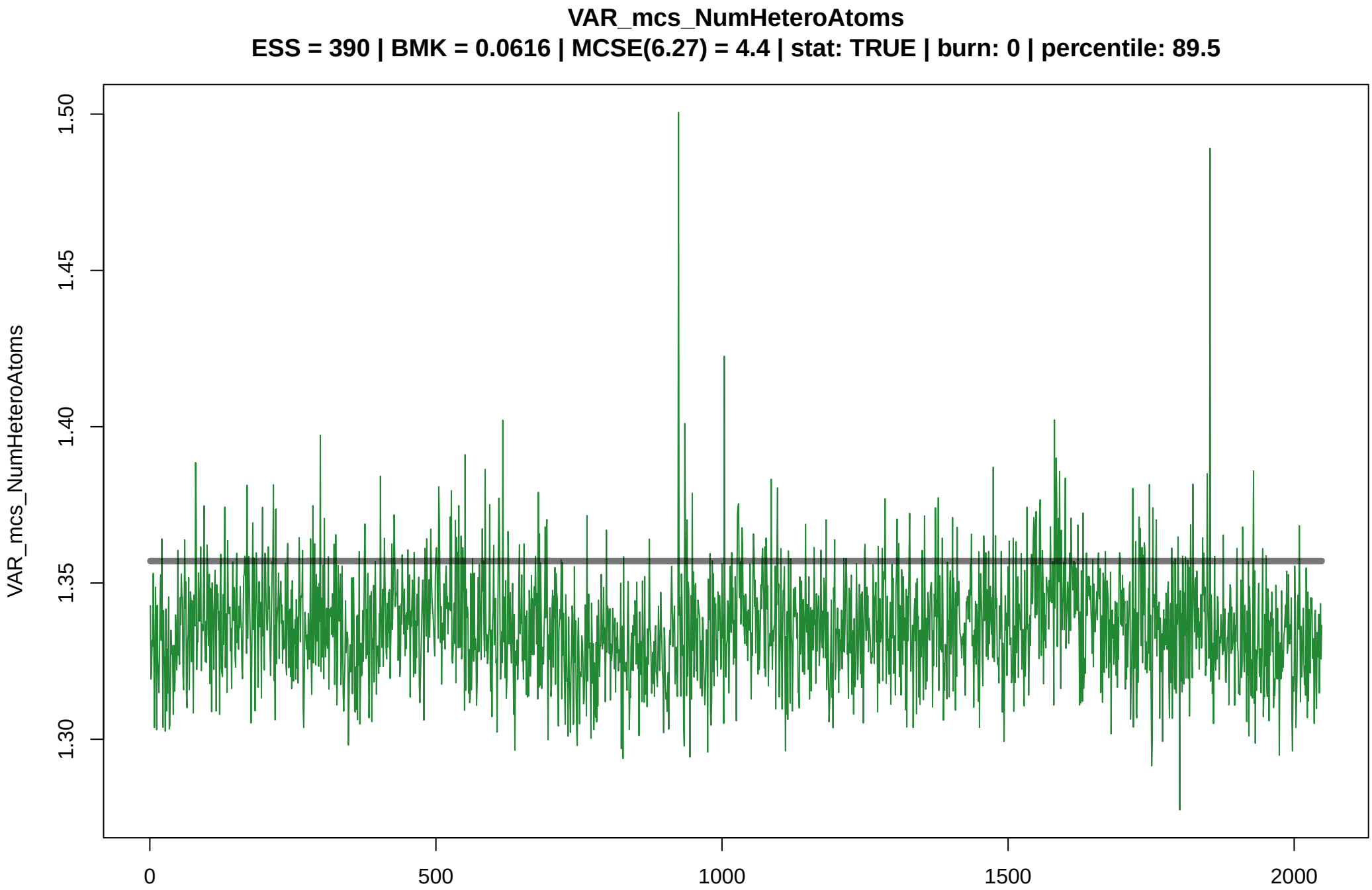

MEAN_docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0661 | MCSE(6.27) = 2.63 | stat: FALSE | burn: 0 | percentile: 78.8
MEAN_docked_NumRotatableBonds
6.2
6.3
6.4
6.5
6.6
0
500
1000
1500
2000

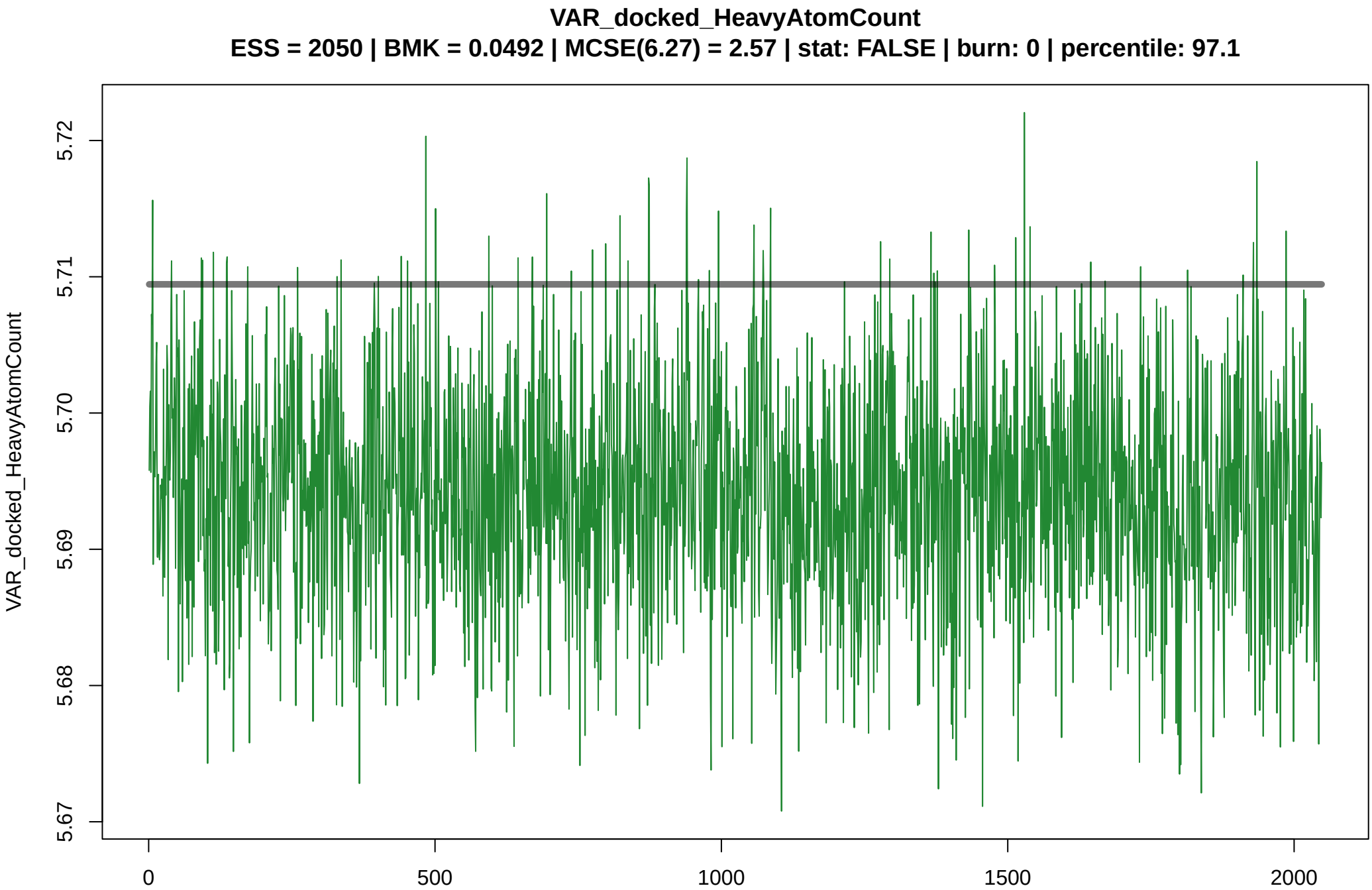

MEAN_mcs_NOCount
ESS = 2050 | BMK = 0.0431 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | percentile: 92.3
MEAN_mcs_NOCount
5.9
6.0
6.1
6.2
6.3
0
500
1000
1500
2000

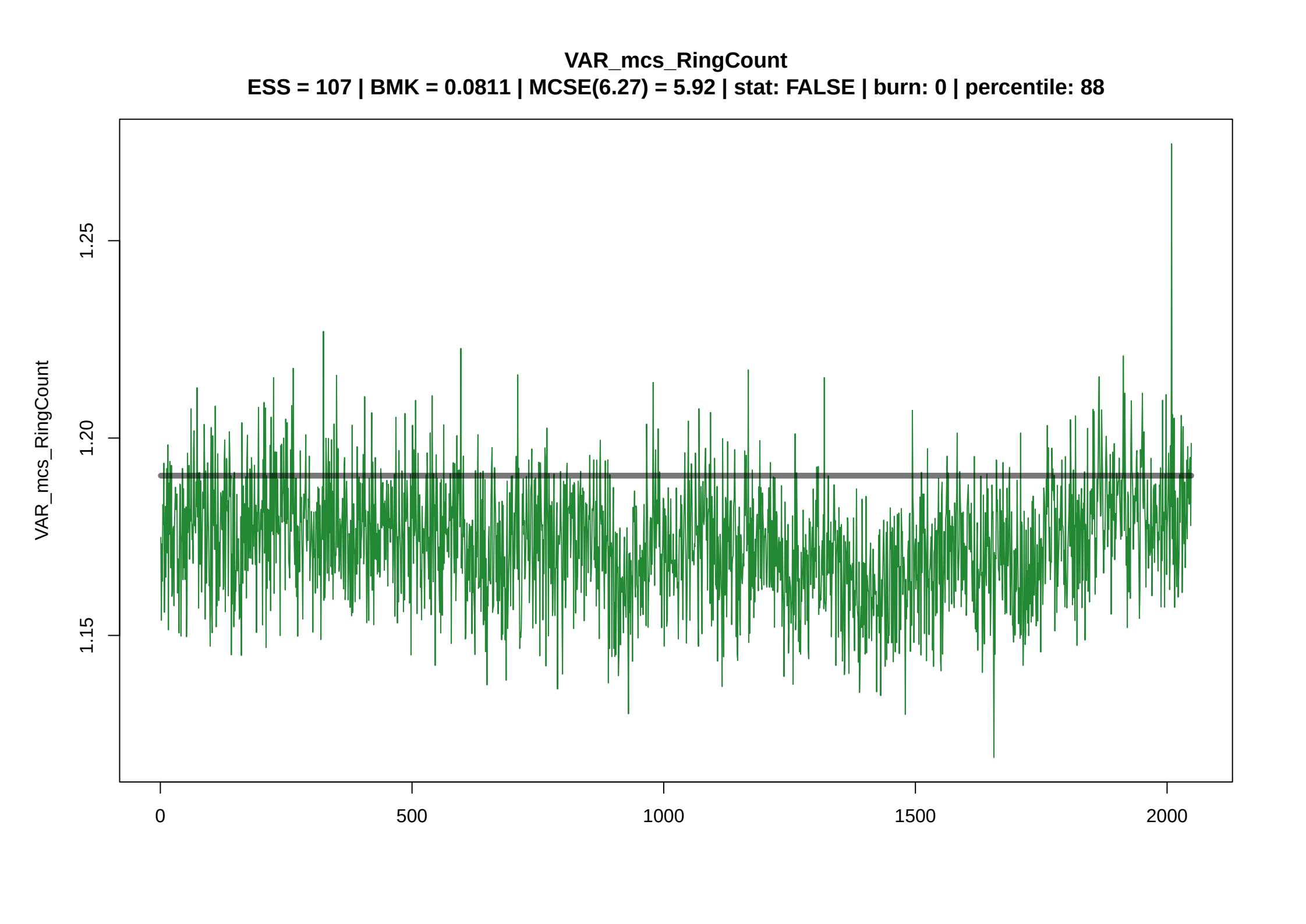

VAR_log_RMSD
ESS = 2050 | BMK = 0.0505 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | percentile: 20.3
VAR_log_RMSD
1.0
1.2
1.4
1.6
0
500
1000
1500
2000

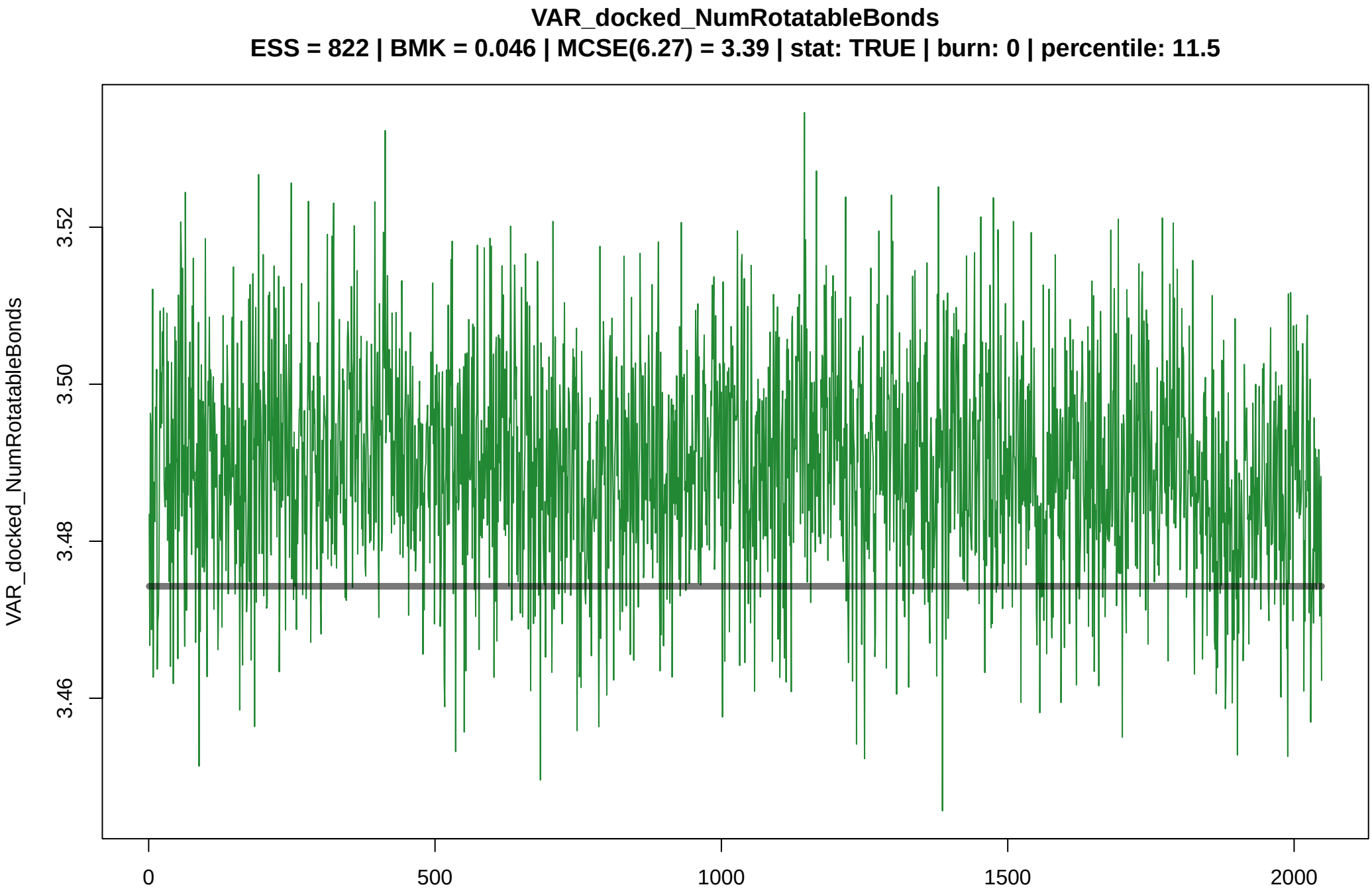

VAR_log_mcs_unbonded_polar_sasa
ESS = 1920 | BMK = 0.0823 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0 | percentile: 65.3
VAR_log_mcs_unbonded_polar_sasa
1.7
1.8
1.9
2.0
2.1
0
500
1000
1500
2000

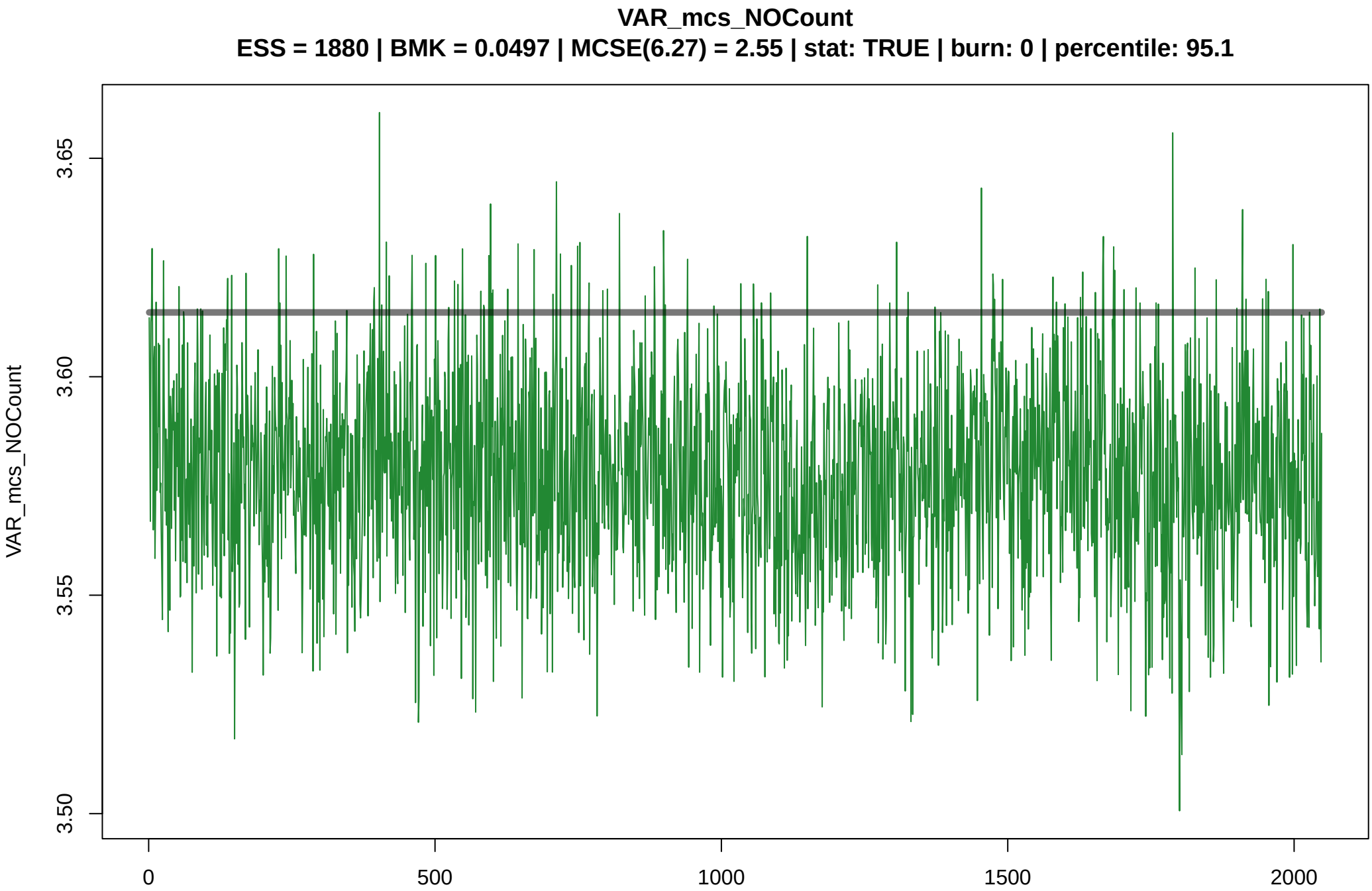

VAR_logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0639 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | percentile: 6.01
VAR_logit_ec_tanimoto_similarity
2.92
2.90
2.88
2.86
2.84
2.82
2.80
2.78
0
500
1000
1500
2000

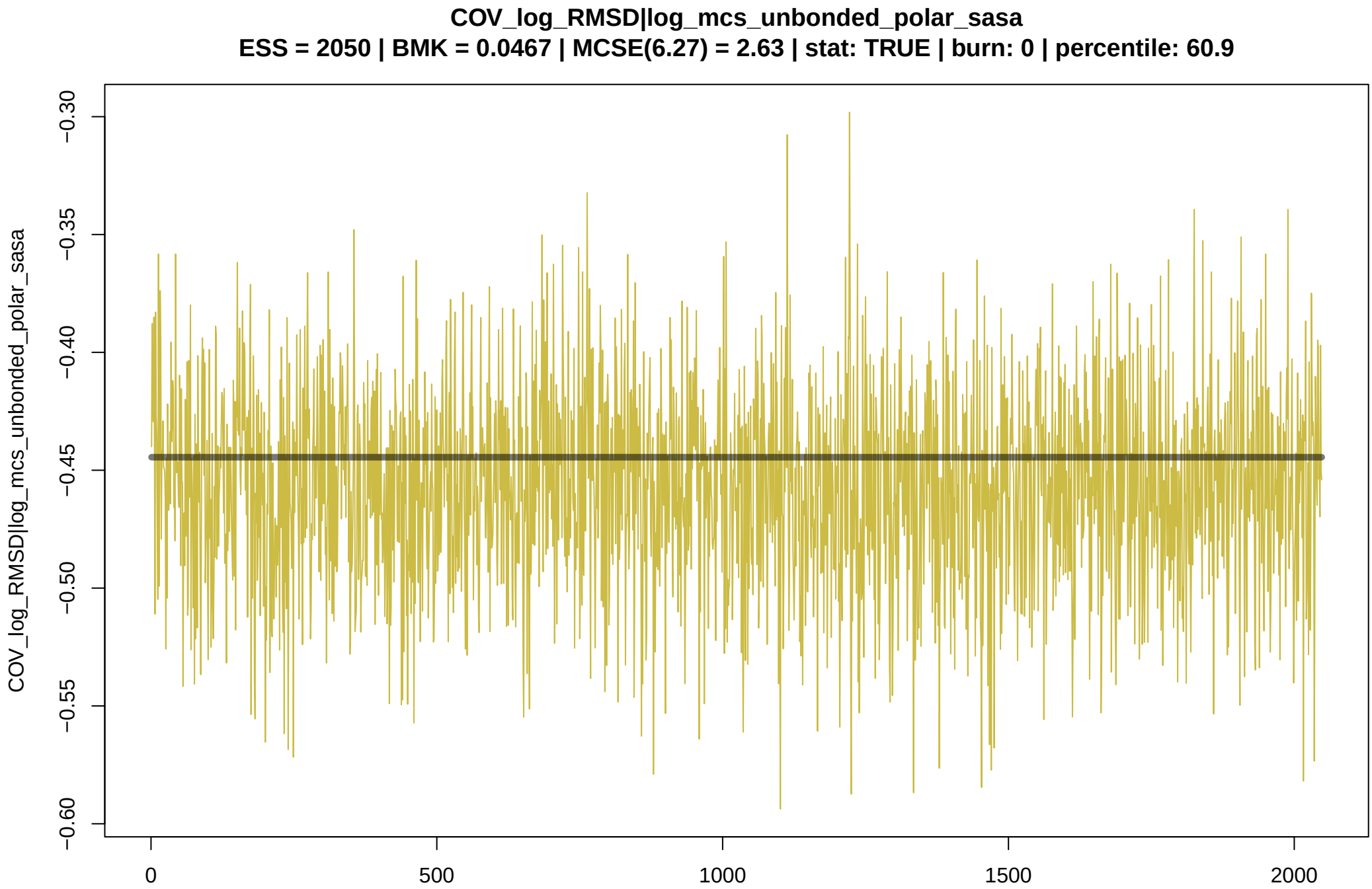

VAR_mcs_NumHeteroAtoms
ESS = 390 | BMK = 0.0616 | MCSE(6.27) = 4.4 | stat: TRUE | burn: 0 | percentile: 89.5
VAR_mcs_NumHeteroAtoms
1.30
1.35
1.40
1.45
1.50
0
500
1000
1500
2000

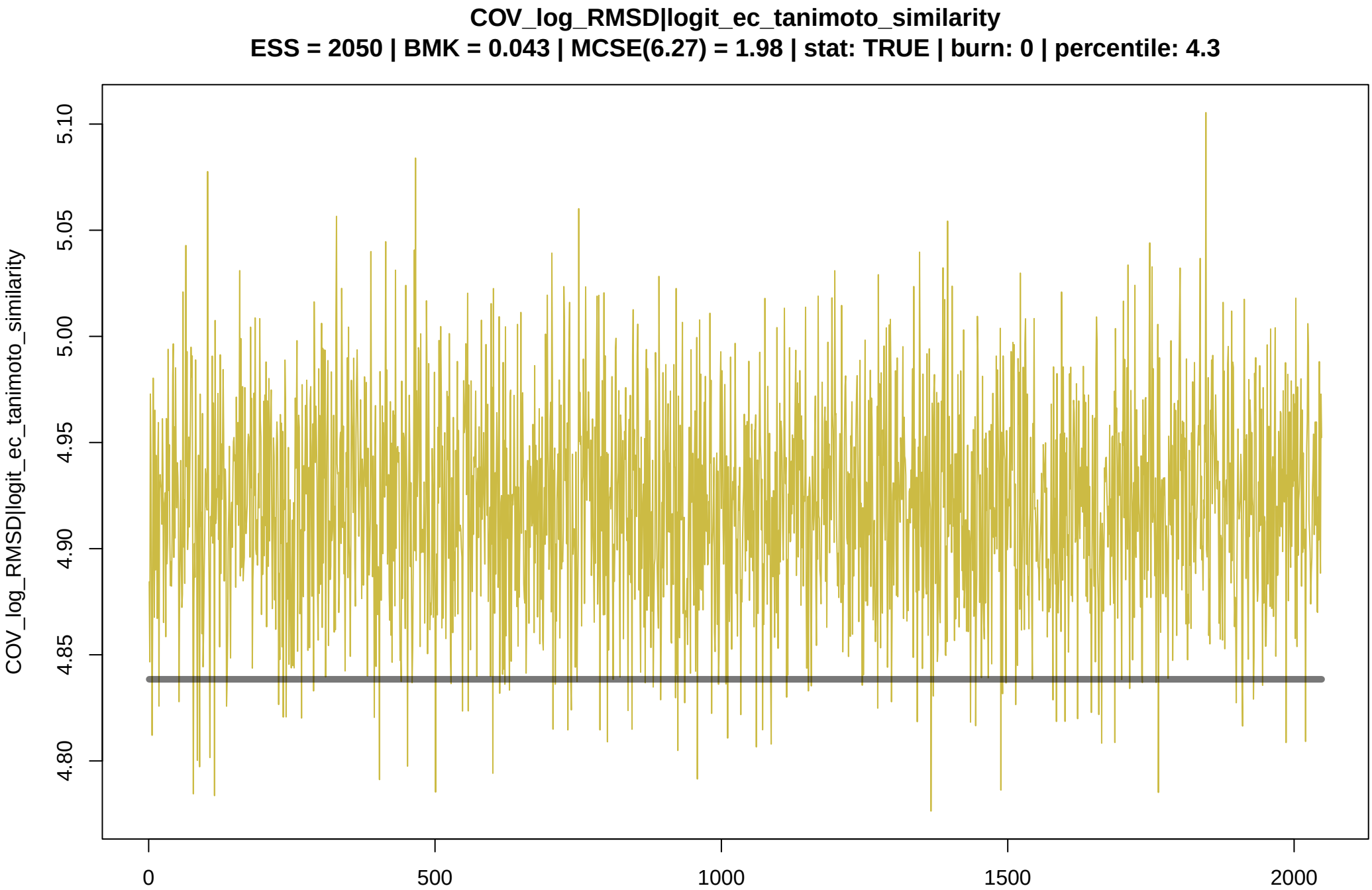

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0492 | MCSE(6.27) = 2.57 | stat: FALSE | burn: 0 | percentile: 97.1
VAR_docked_HeavyAtomCount
5.67
5.68
5.69
5.70
5.71
5.72
0
500
1000
1500
2000

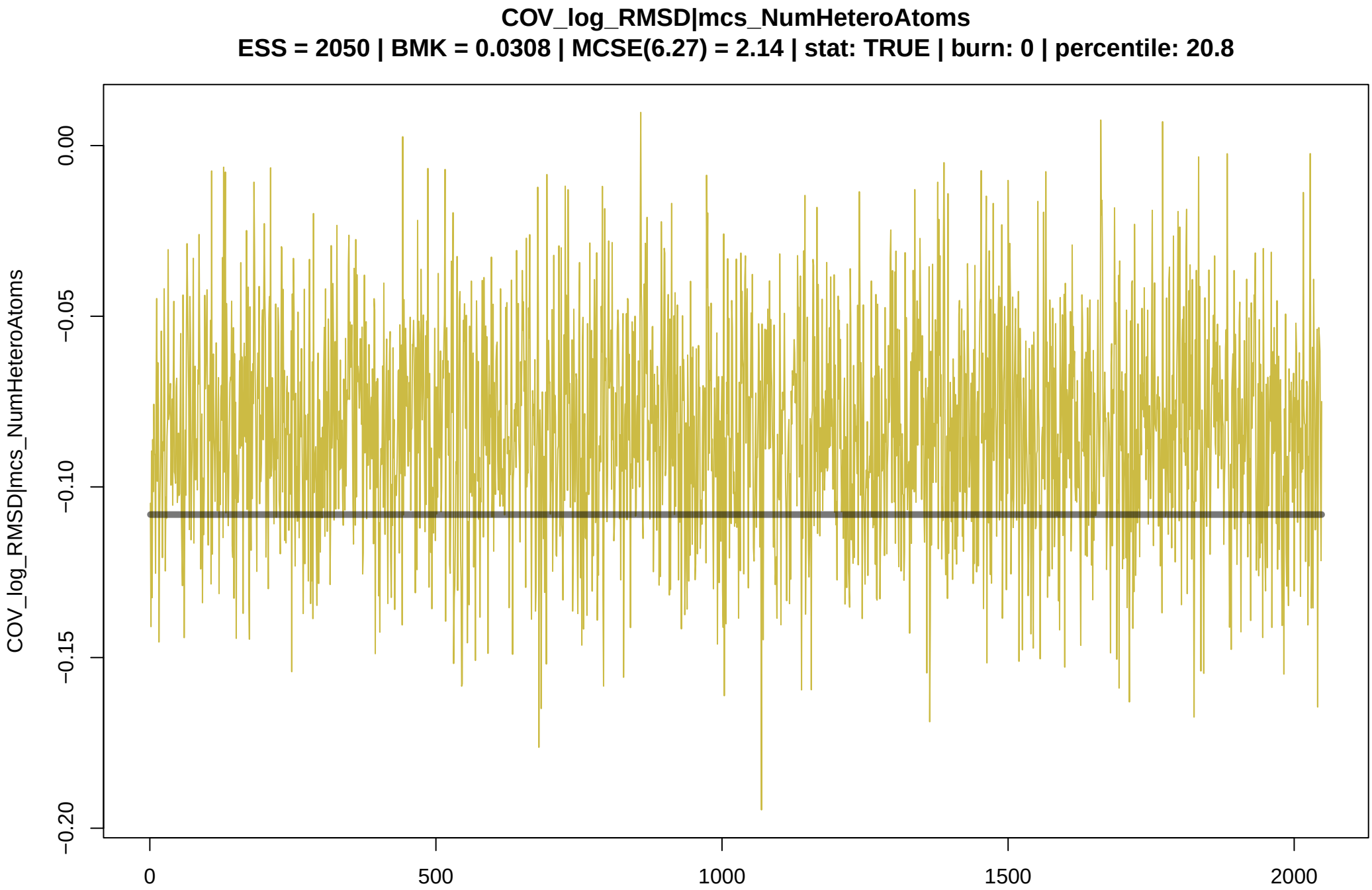

VAR_mcs_RingCount
ESS = 107 | BMK = 0.0811 | MCSE(6.27) = 5.92 | stat: FALSE | burn: 0 | percentile: 88
VAR_mcs_RingCount
1.15
1.20
1.25
0
500
1000
1500
2000

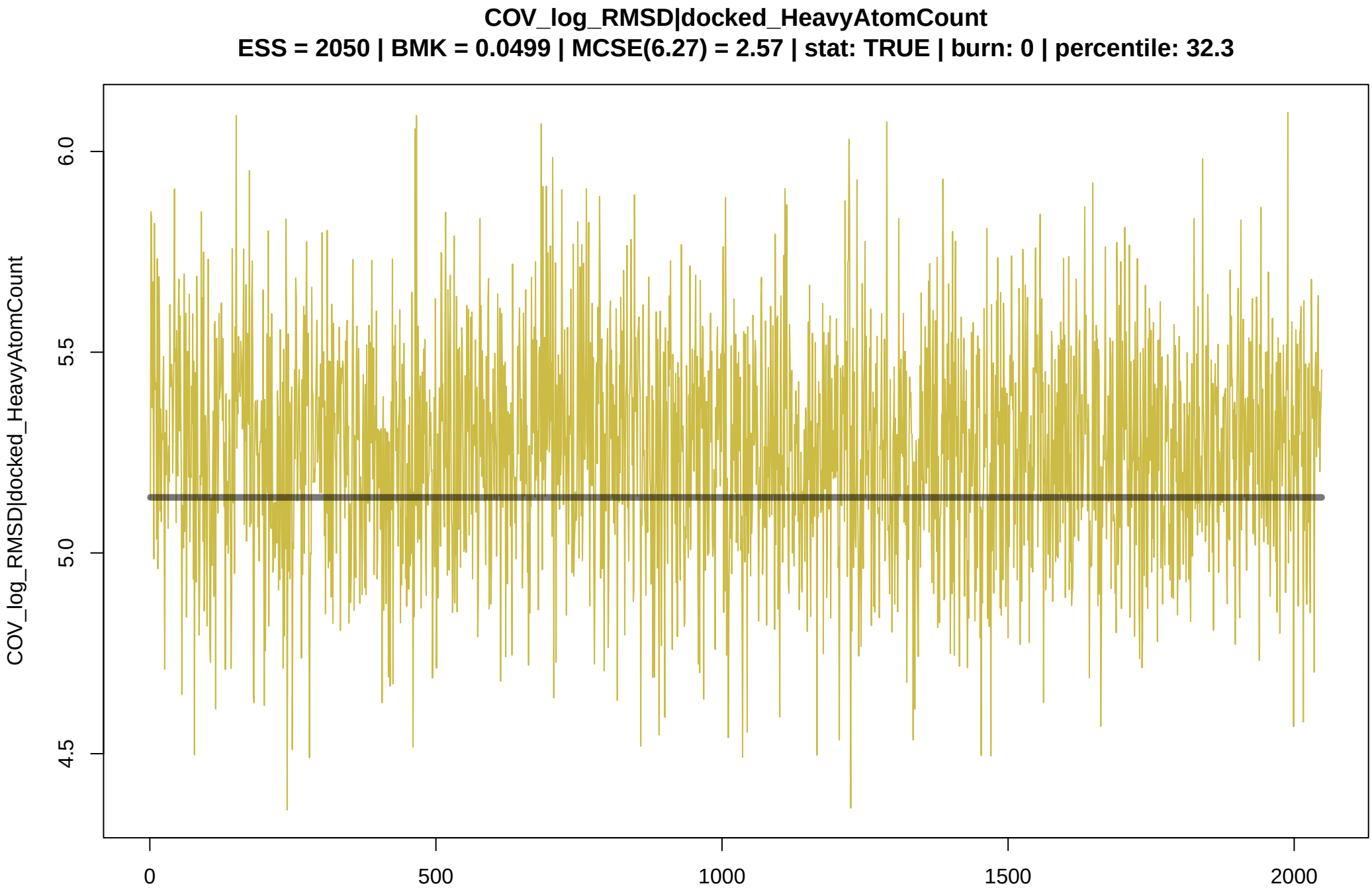

VAR_docked_NumRotatableBonds
ESS = 822 | BMK = 0.046 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | percentile: 11.5
VAR_docked_NumRotatableBonds
3.46
3.48
3.50
3.52
0
500
1000
1500
2000

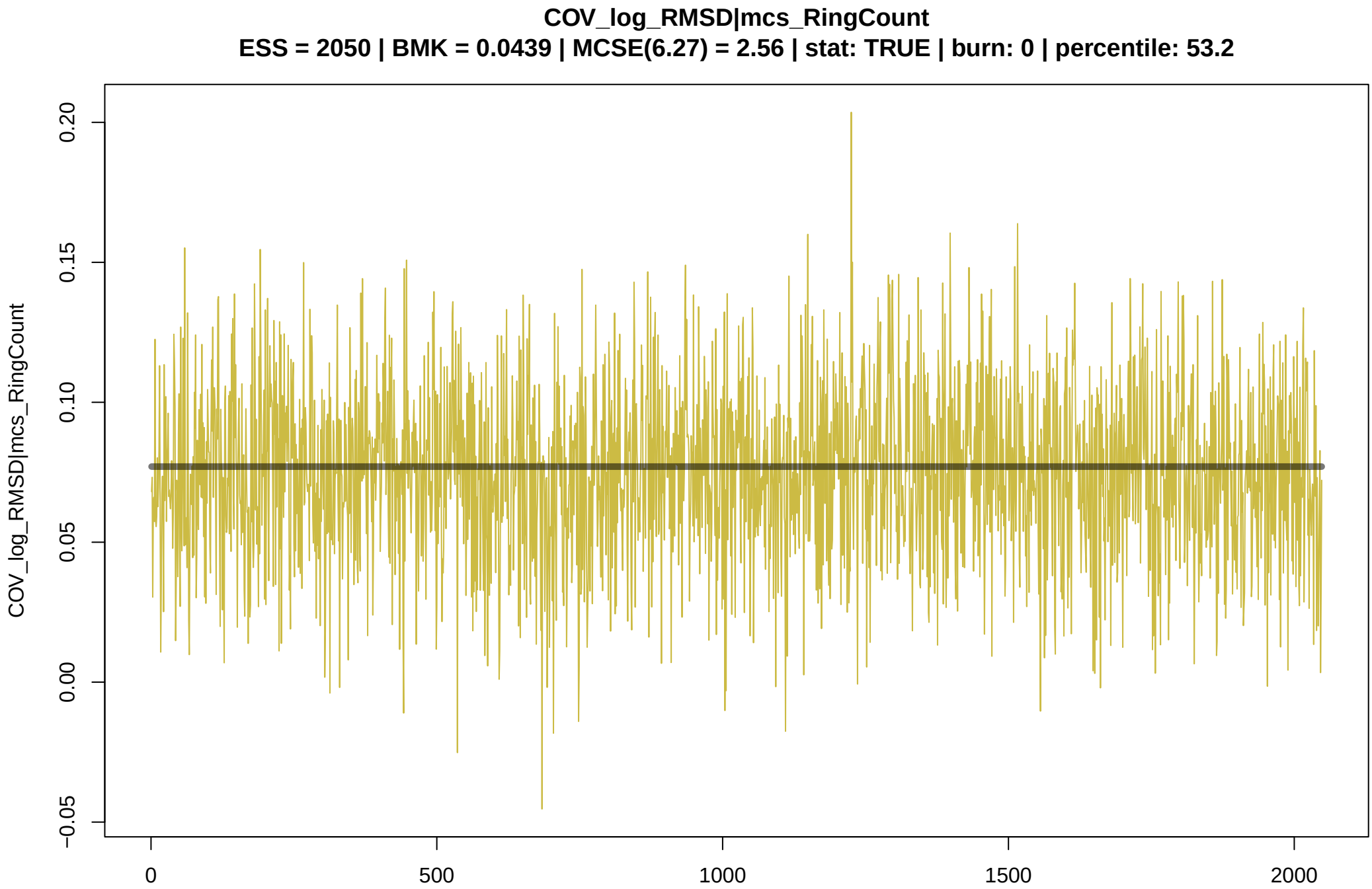

VAR_mcs_NOCount
ESS = 1880 | BMK = 0.0497 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | percentile: 95.1
VAR_mcs_NOCount
3.50
3.55
3.60
3.65
0
500
1000
1500
2000

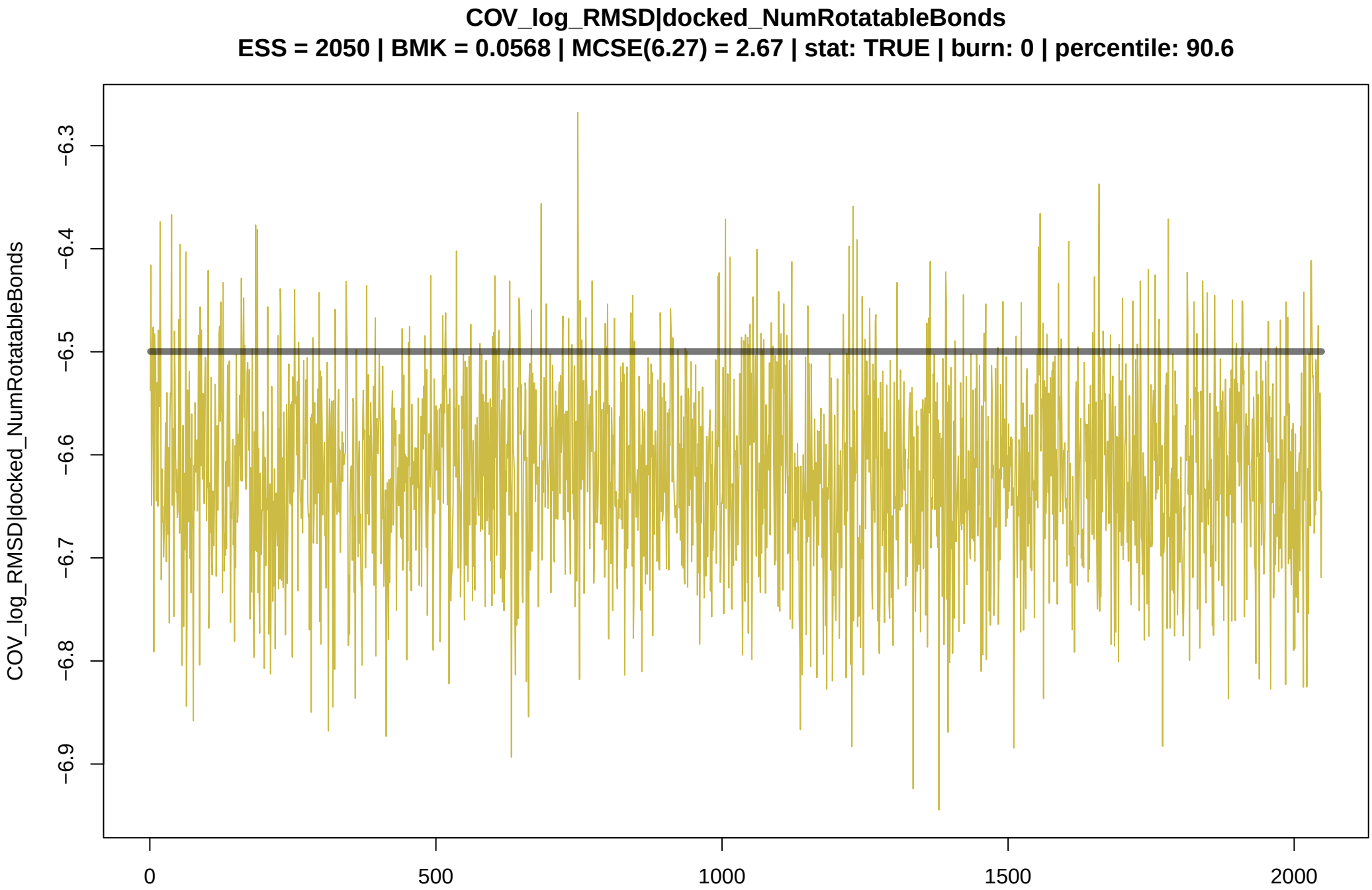

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0467 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | percentile: 60.9
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.30
−0.35
−0.40
−0.45
−0.50
−0.55
−0.60
0
500
1000
1500
2000

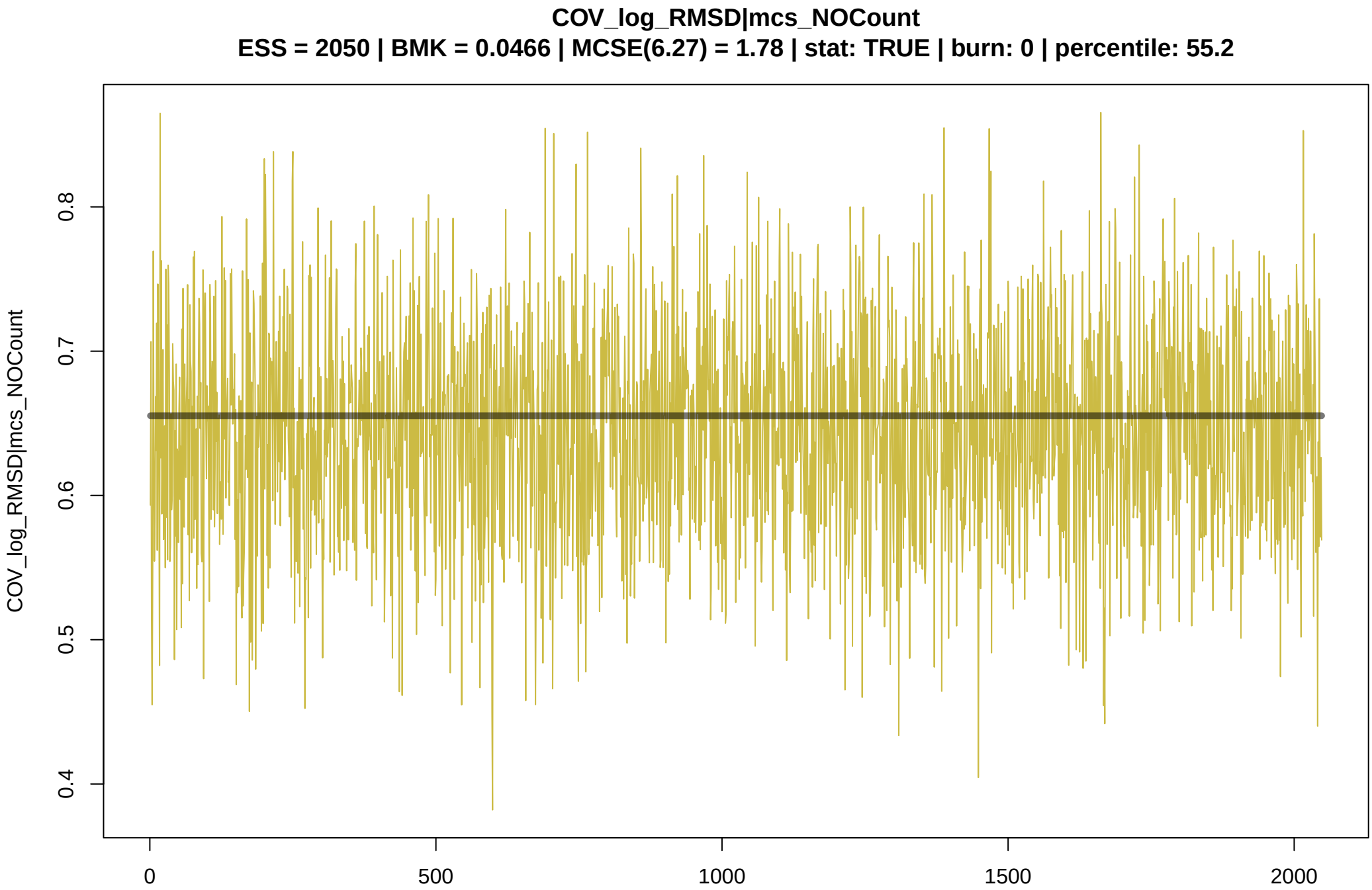

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.043 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0 | percentile: 4.3
COV_log_RMSD|logit_ec_tanimoto_similarity
4.80
4.85
4.90
4.95
5.00
5.05
5.10
0
500
1000
1500
2000

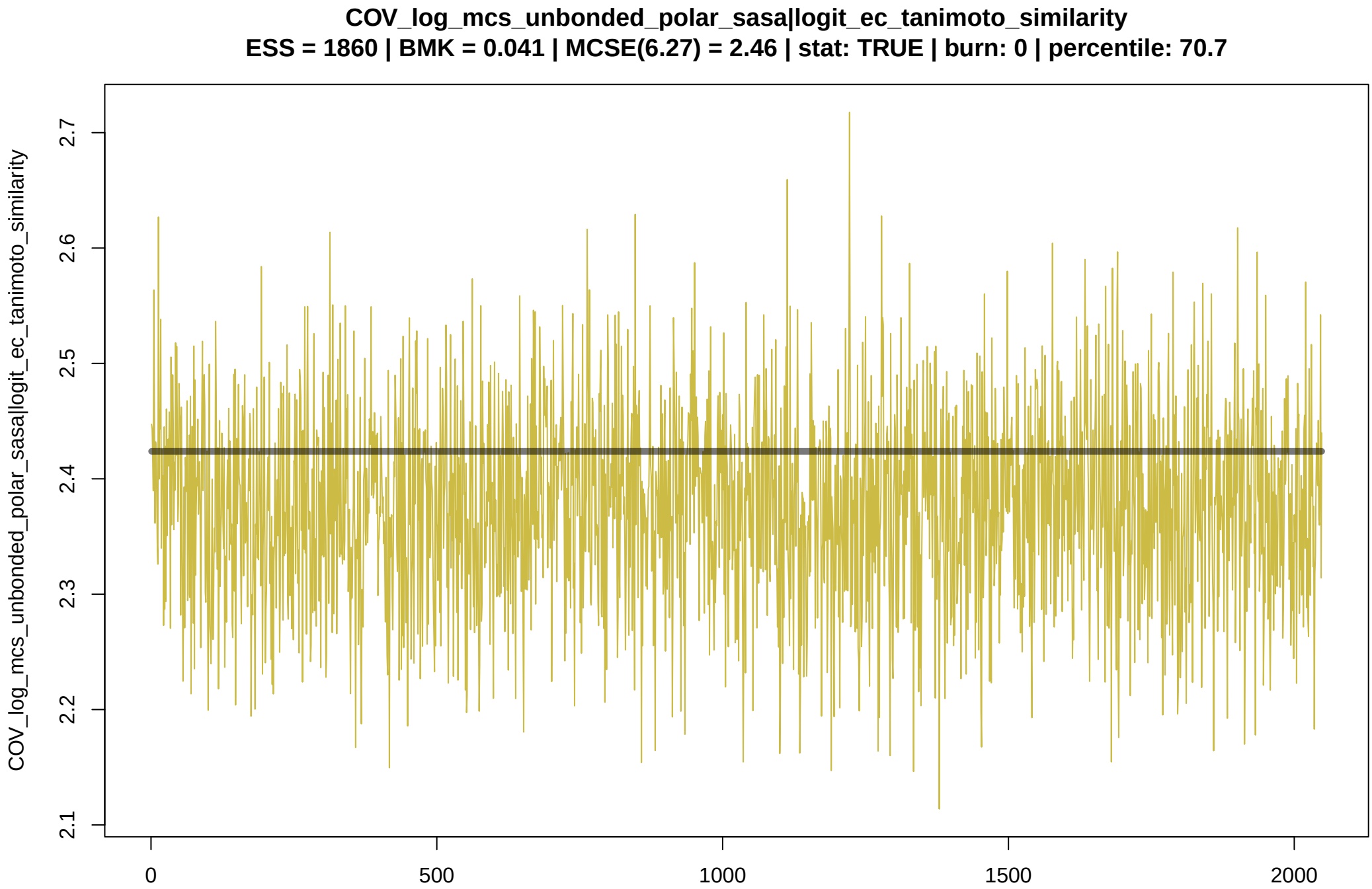

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0308 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | percentile: 20.8
COV_log_RMSD|mcs_NumHeteroAtoms
0.00
−0.05
−0.10
−0.15
−0.20
0
500
1000
1500
2000

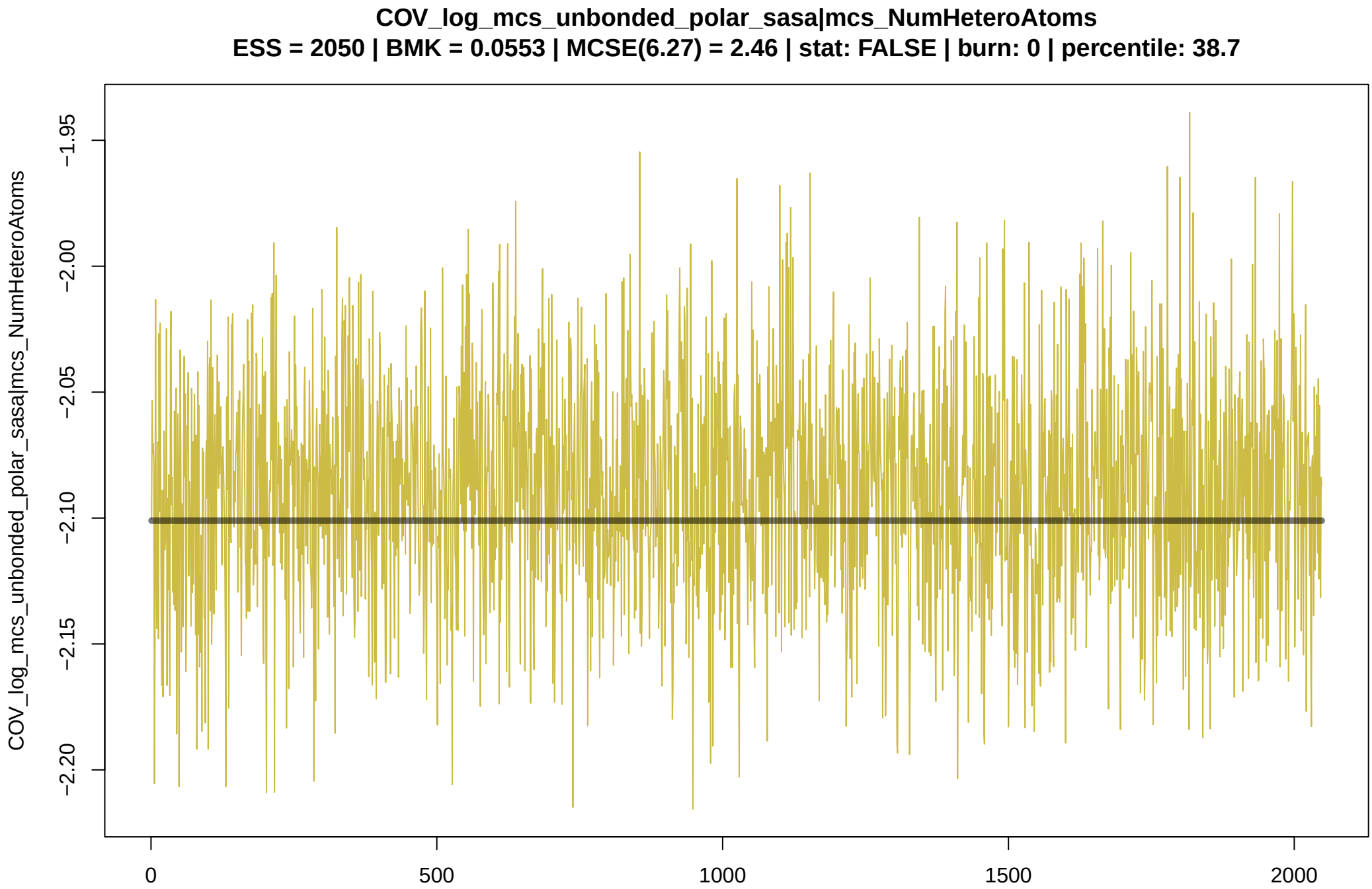

COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0499 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | percentile: 32.3
COV_log_RMSD|docked_HeavyAtomCount
6.0
5.5
5.0
4.5
0
500
1000
1500
2000

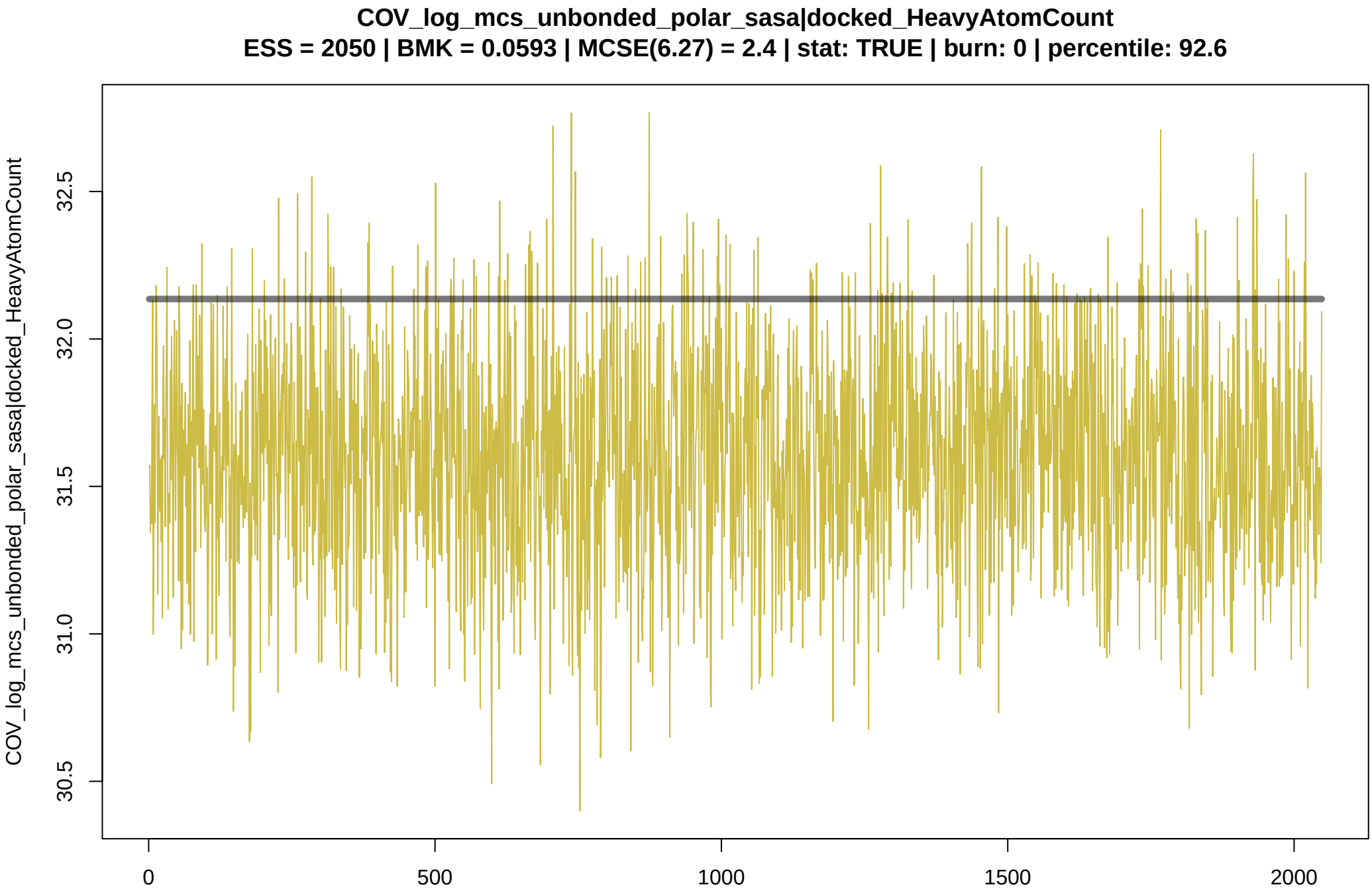

COV_log_RMSD|mcs_RingCount
ESS = 2050 | BMK = 0.0439 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0 | percentile: 53.2
COV_log_RMSD|mcs_RingCount
0.20
0.15
0.10
0.05
0.00
−0.05
0
500
1000
1500
2000

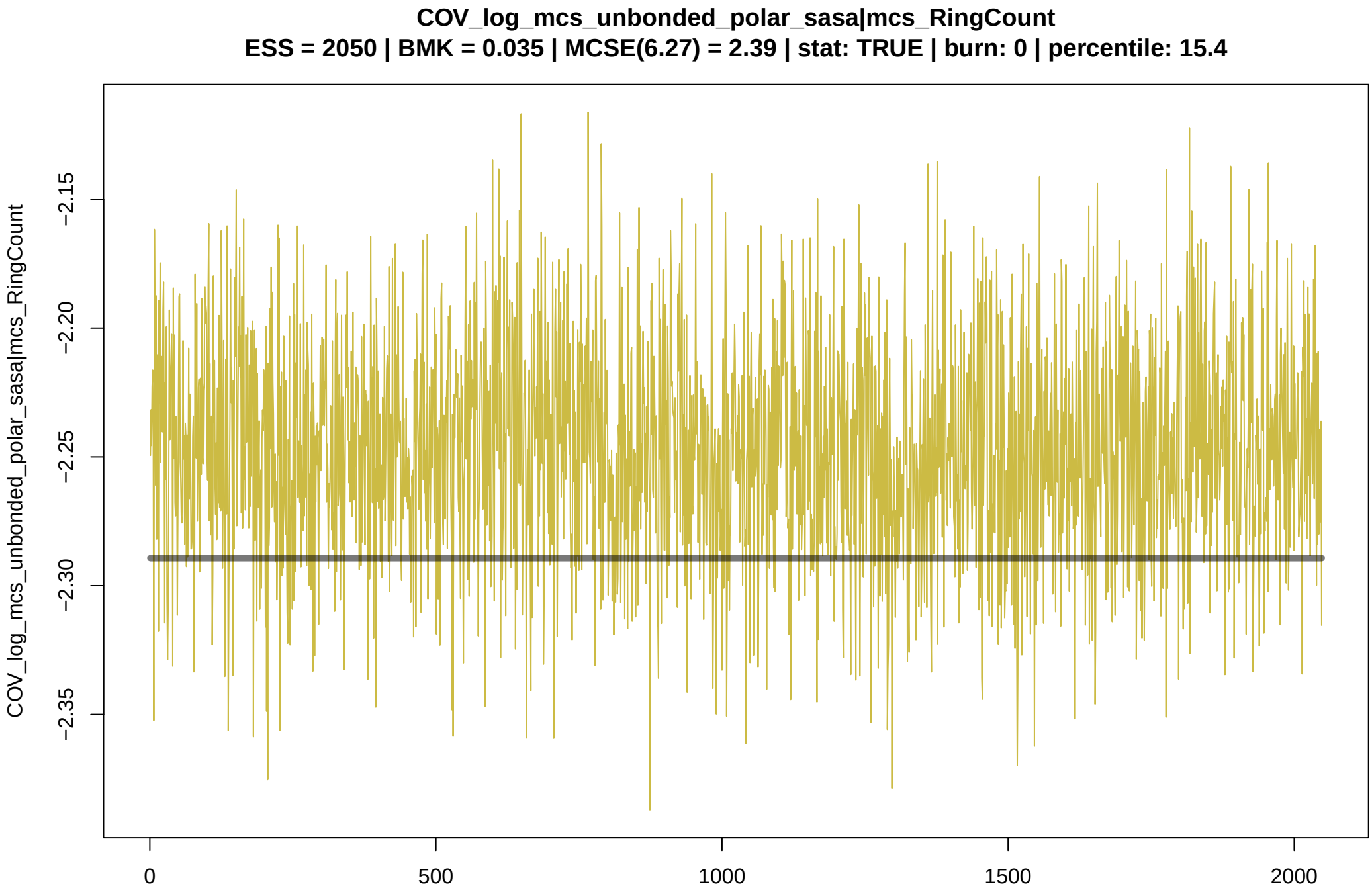

COV_log_RMSD|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0568 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0 | percentile: 90.6
COV_log_RMSD|docked_NumRotatableBonds
−6.3
−6.4
−6.5
−6.6
−6.7
−6.8
−6.9
0
500
1000
1500
2000

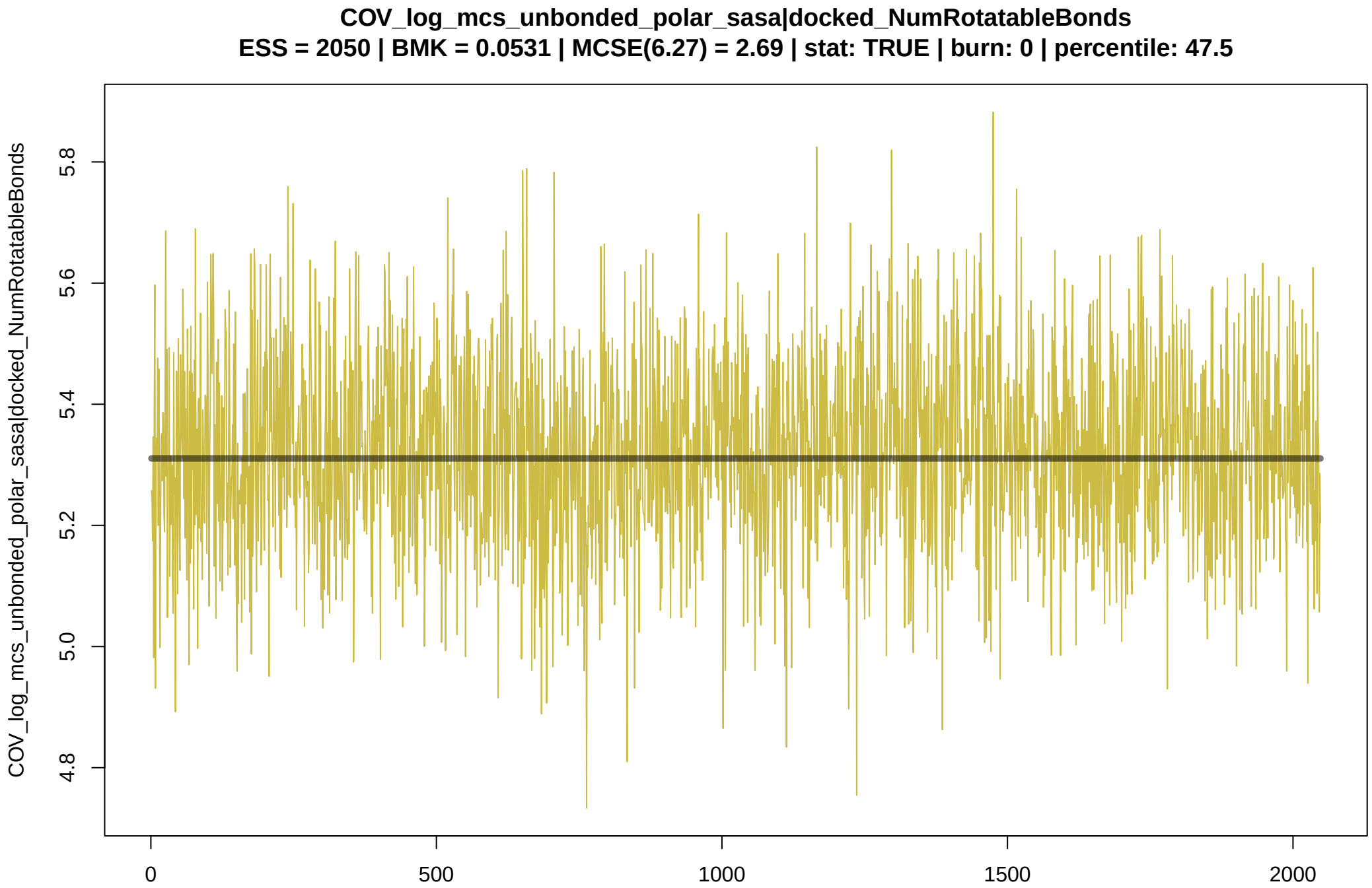

COV_log_RMSD|mcs_NOCount
ESS = 2050 | BMK = 0.0466 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0 | percentile: 55.2
COV_log_RMSD|mcs_NOCount
0.4
0.5
0.6
0.7
0.8
0
500
1000
1500
2000

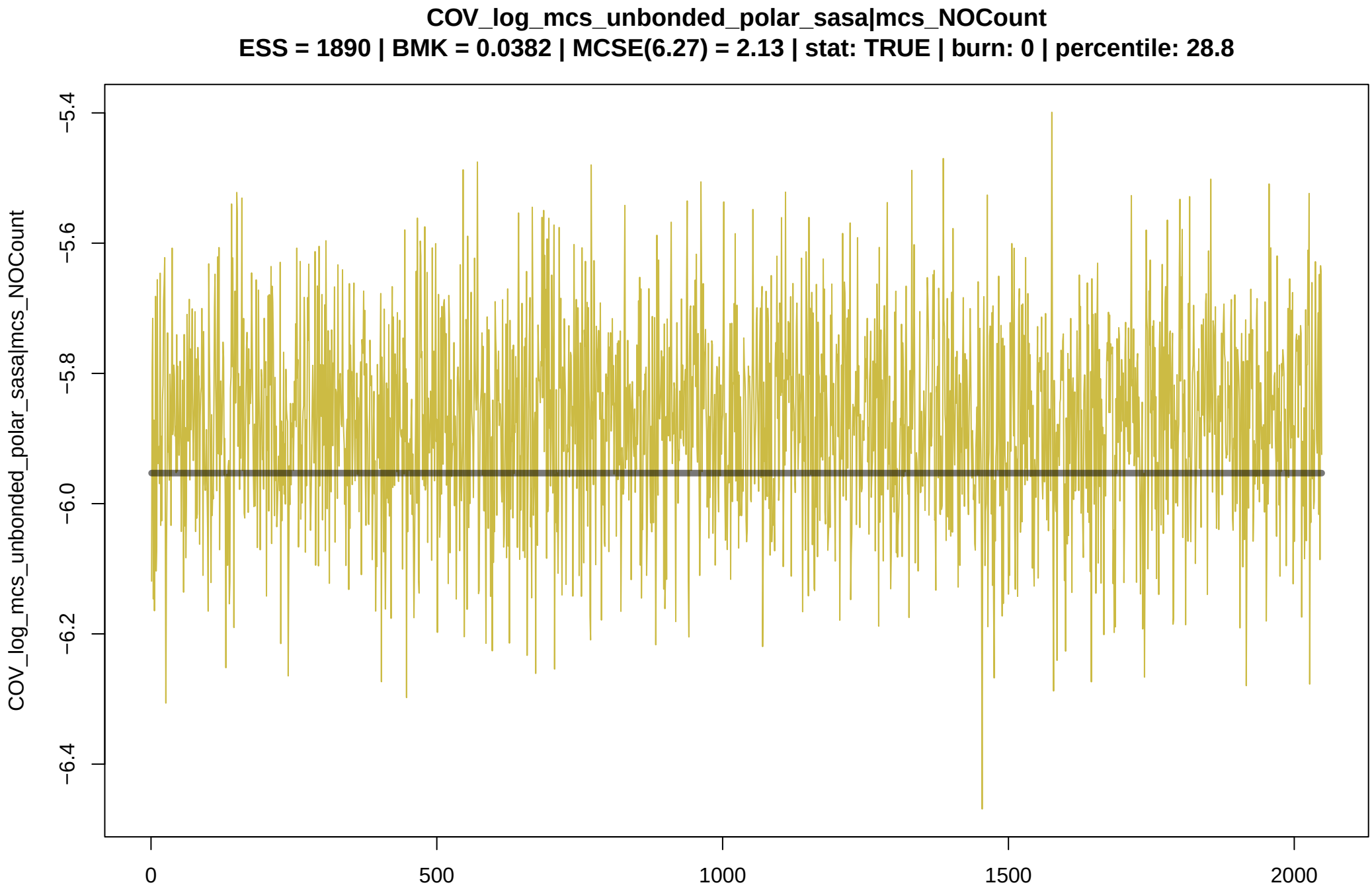

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 1860 | BMK = 0.041 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0 | percentile: 70.7
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
2.1
2.2
2.3
2.4
2.5
2.6
2.7
0
500
1000
1500
2000

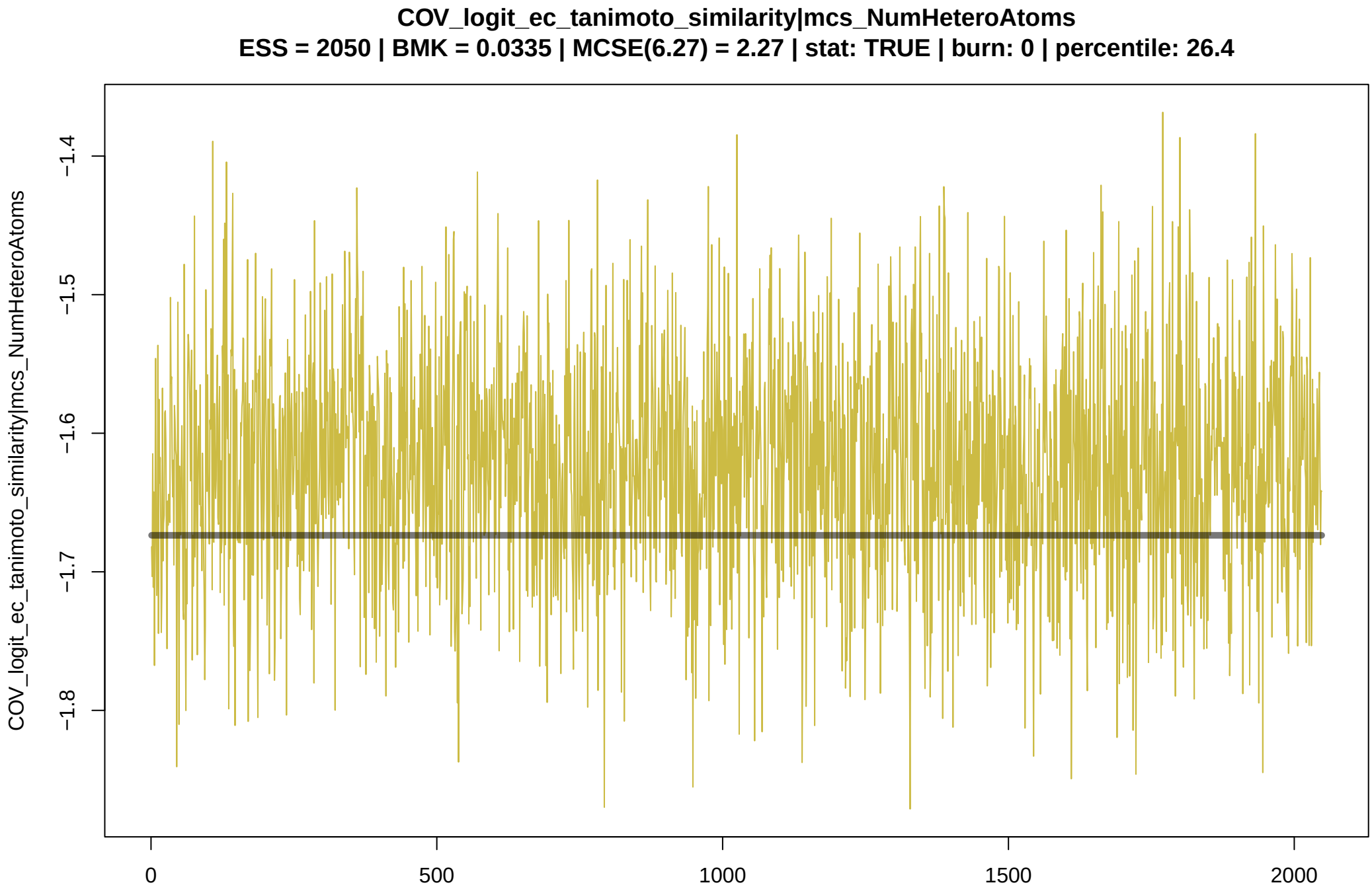

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0553 | MCSE(6.27) = 2.46 | stat: FALSE | burn: 0 | percentile: 38.7
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
−1.95
−2.00
−2.05
−2.10
−2.15
−2.20
0
500
1000
1500
2000

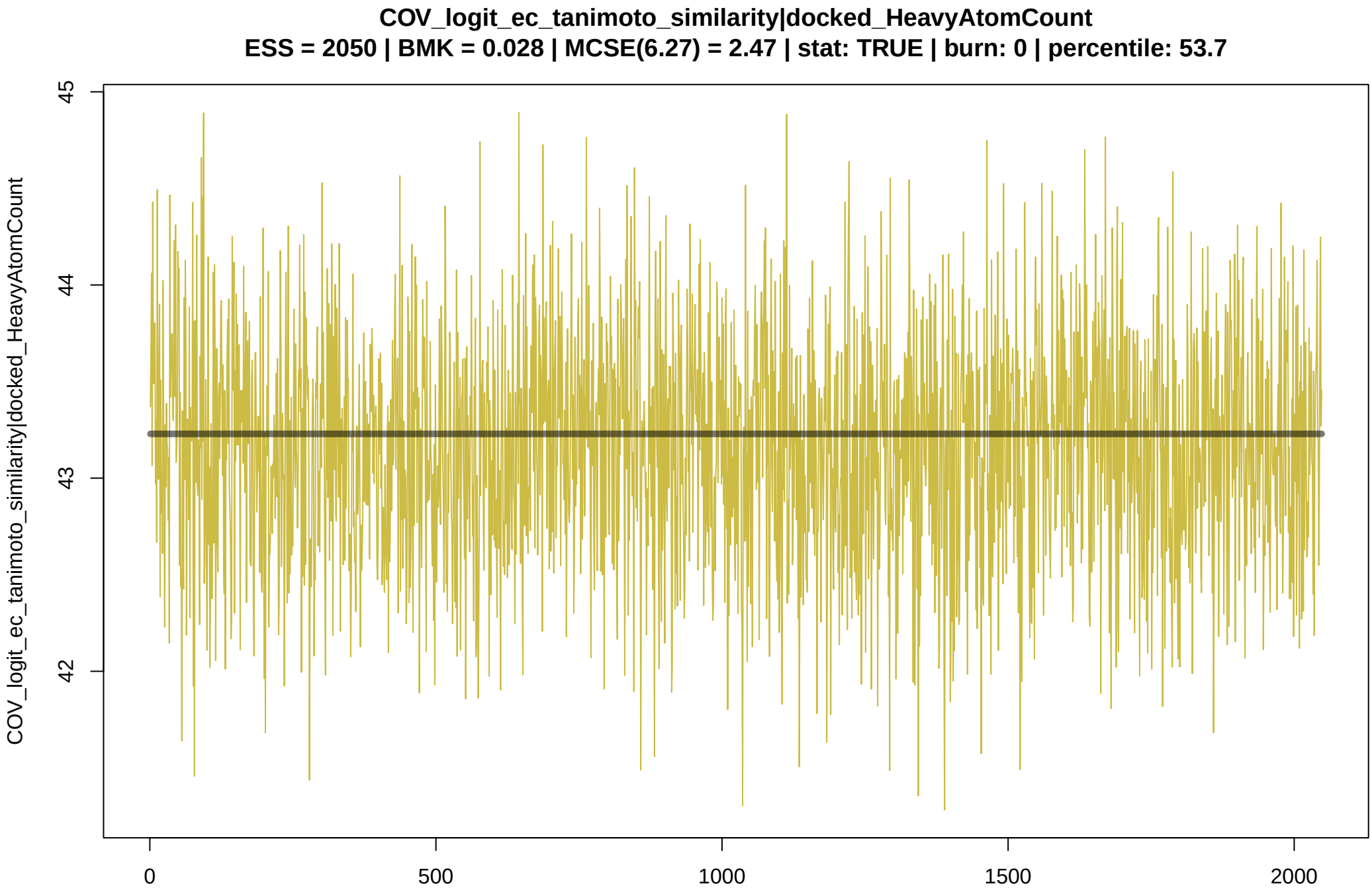

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0593 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0 | percentile: 92.6
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
30.5
31.0
31.5
32.0
32.5
0
500
1000
1500
2000

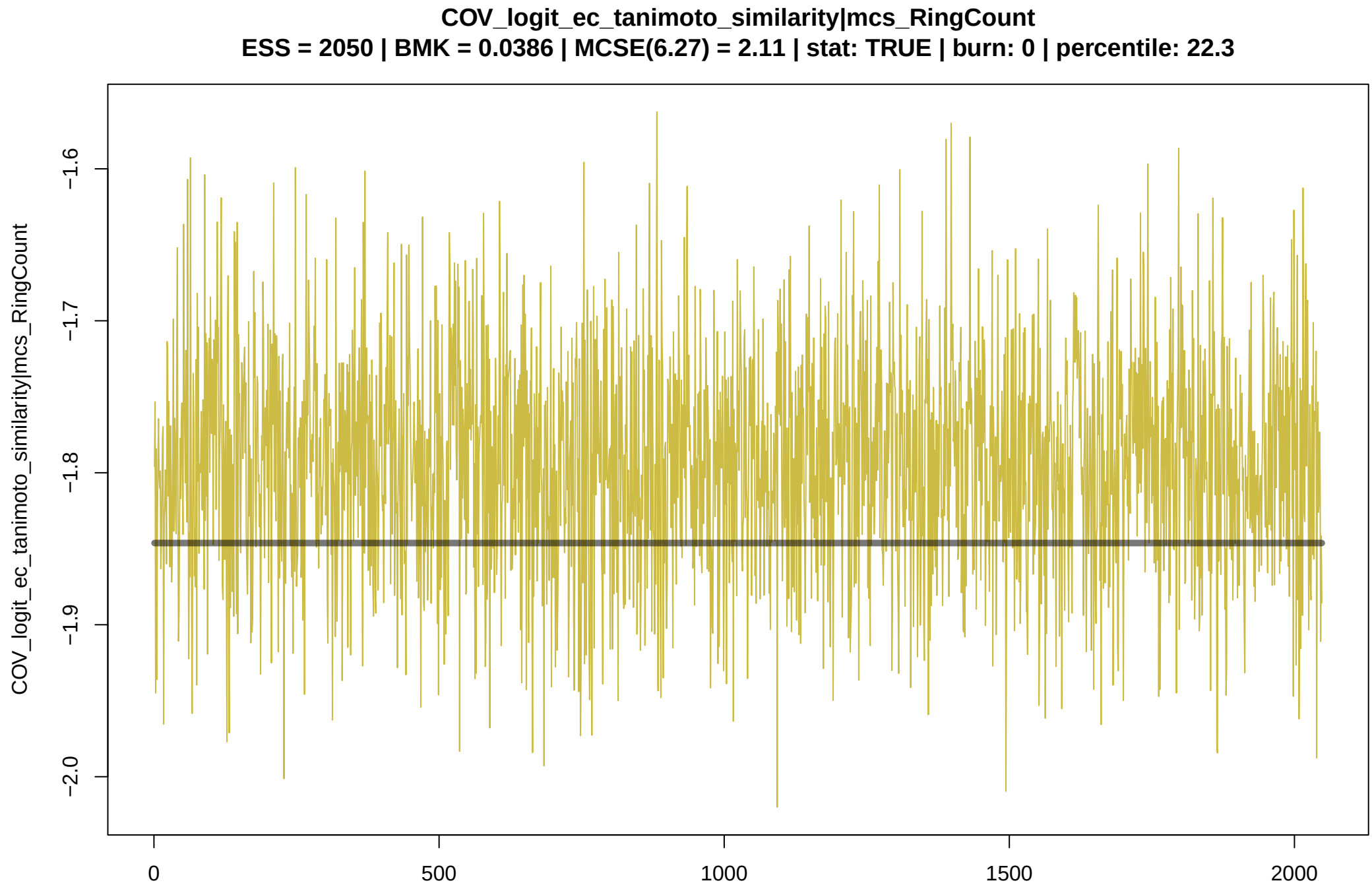

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 2050 | BMK = 0.035 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | percentile: 15.4
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
−2.15
−2.20
−2.25
−2.30
−2.35
0
500
1000
1500
2000

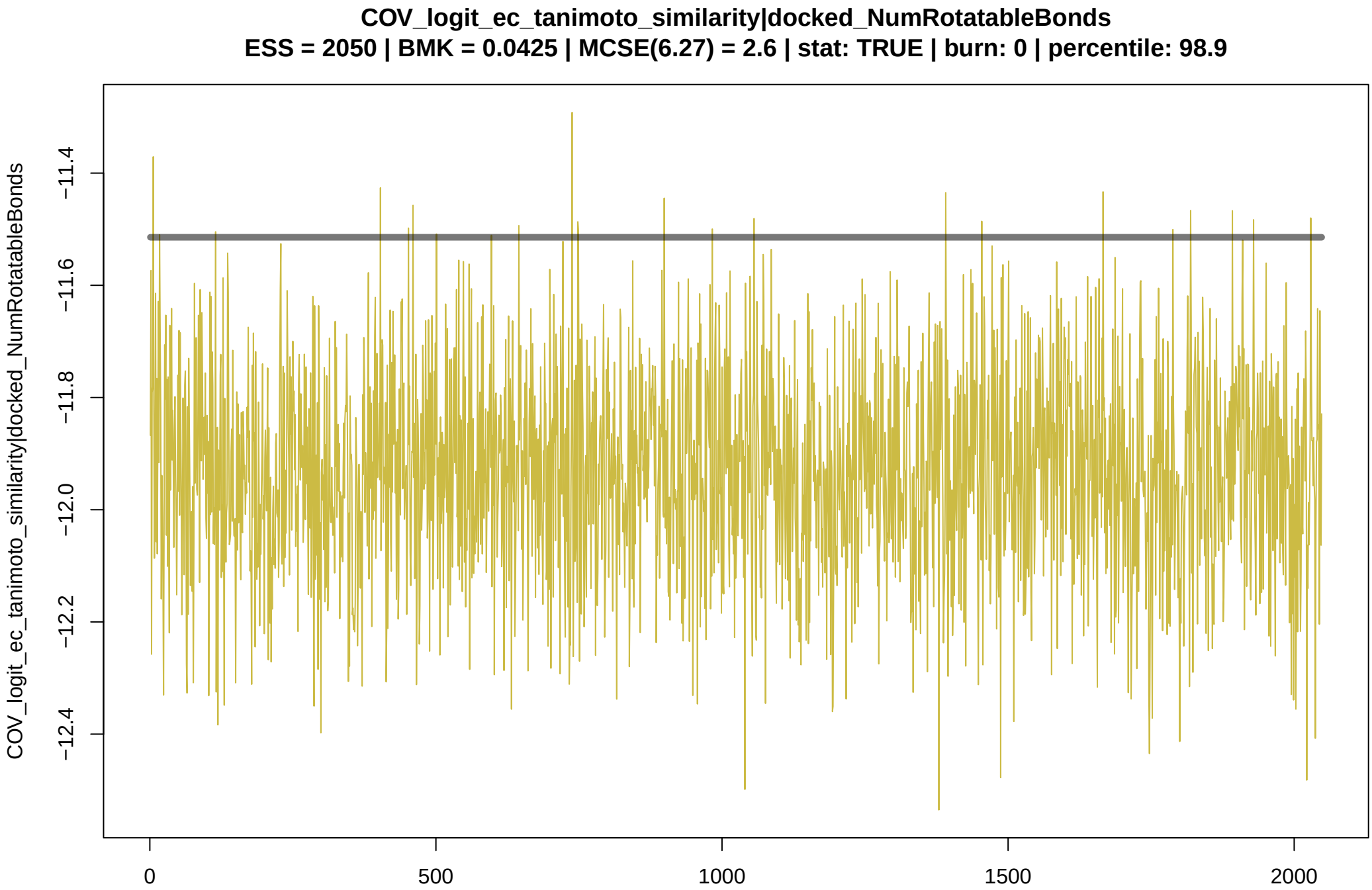

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0531 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | percentile: 47.5
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
4.8
5.0
5.2
5.4
5.6
5.8
0
500
1000
1500
2000

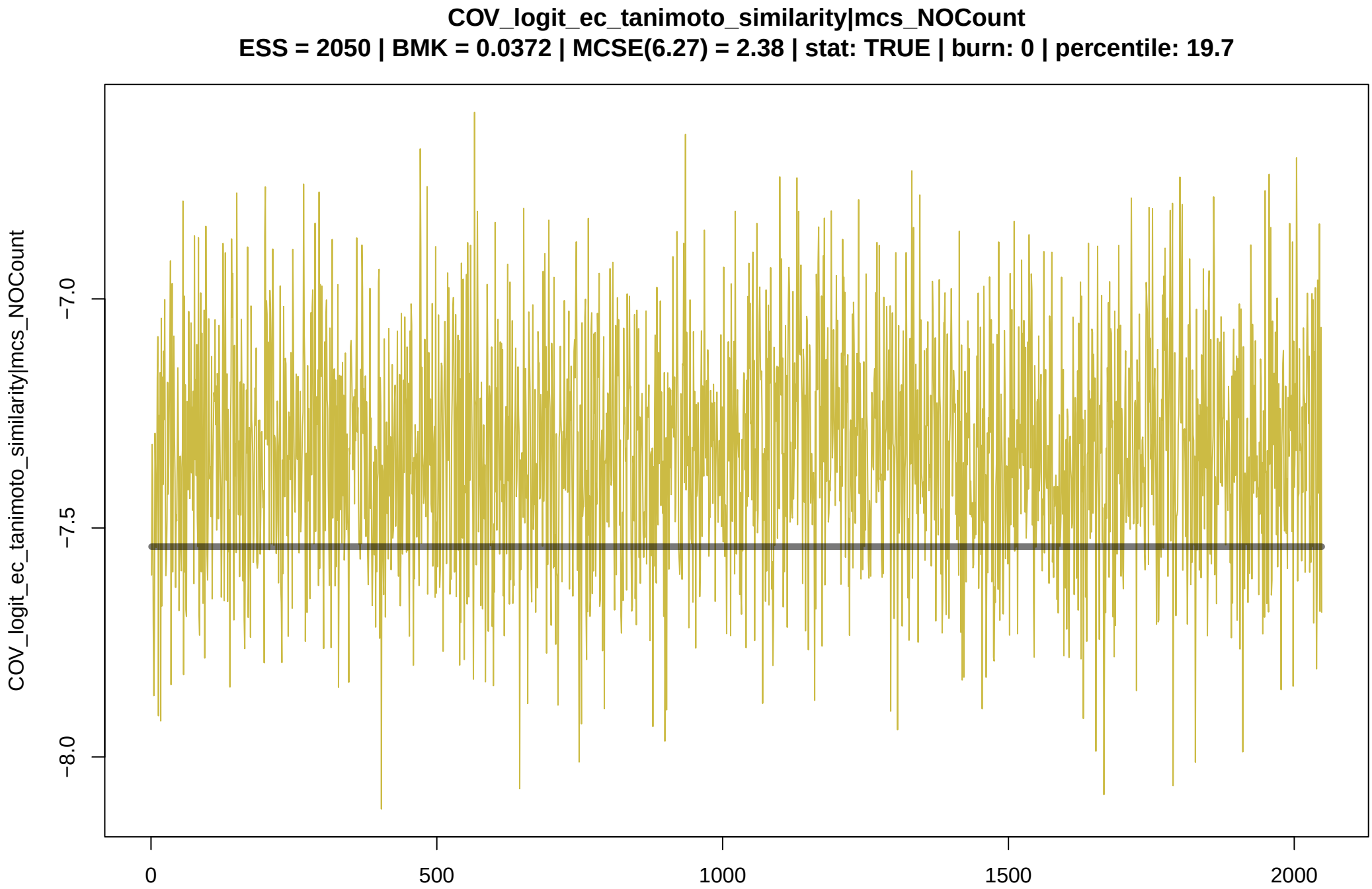

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 1890 | BMK = 0.0382 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0 | percentile: 28.8
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
−5.4
−5.6
−5.8
−6.0
−6.2
−6.4
0
500
1000
1500
2000

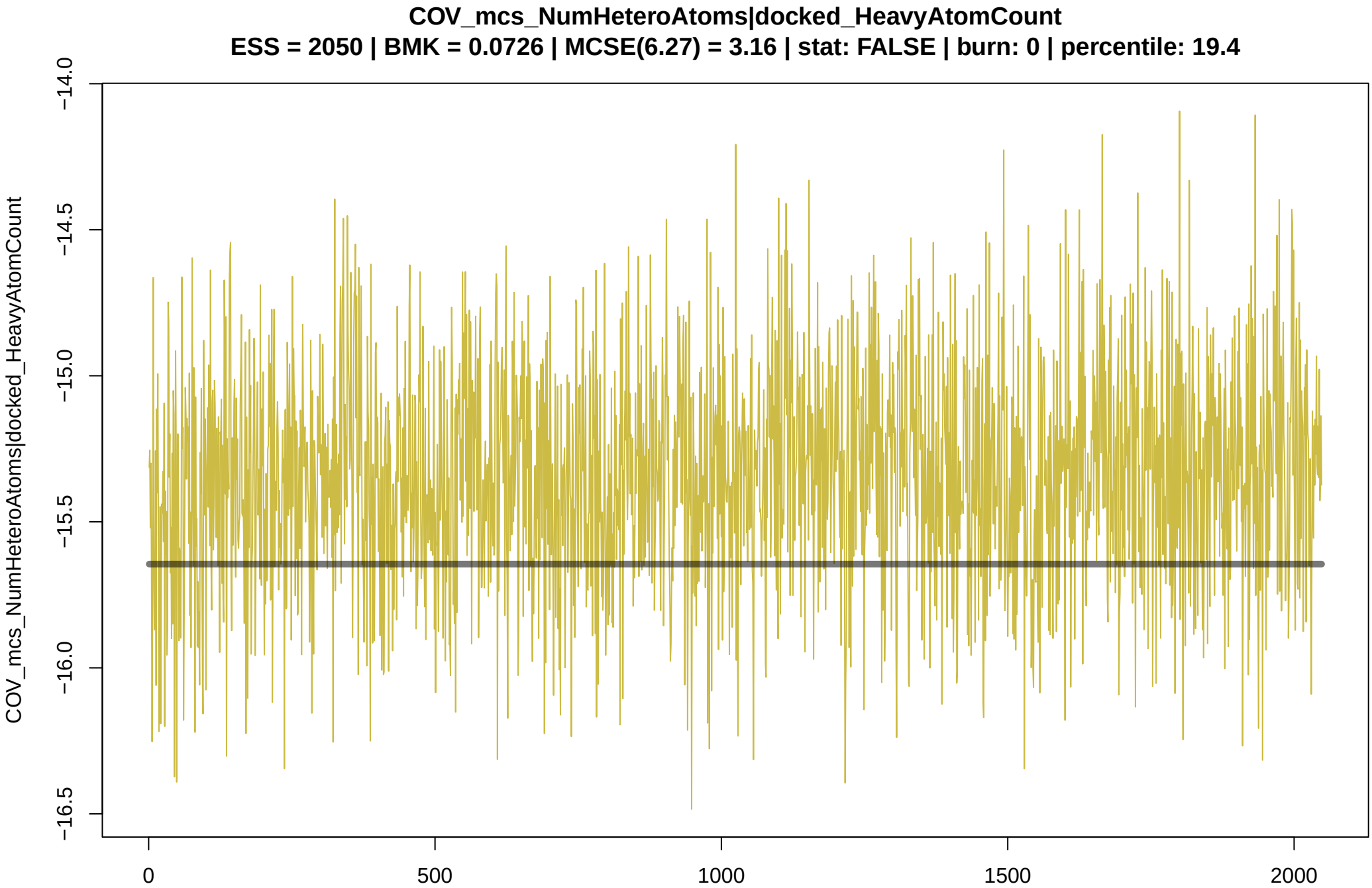

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0335 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | percentile: 26.4
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
−1.4
−1.5
−1.6
−1.7
−1.8
0
500
1000
1500
2000

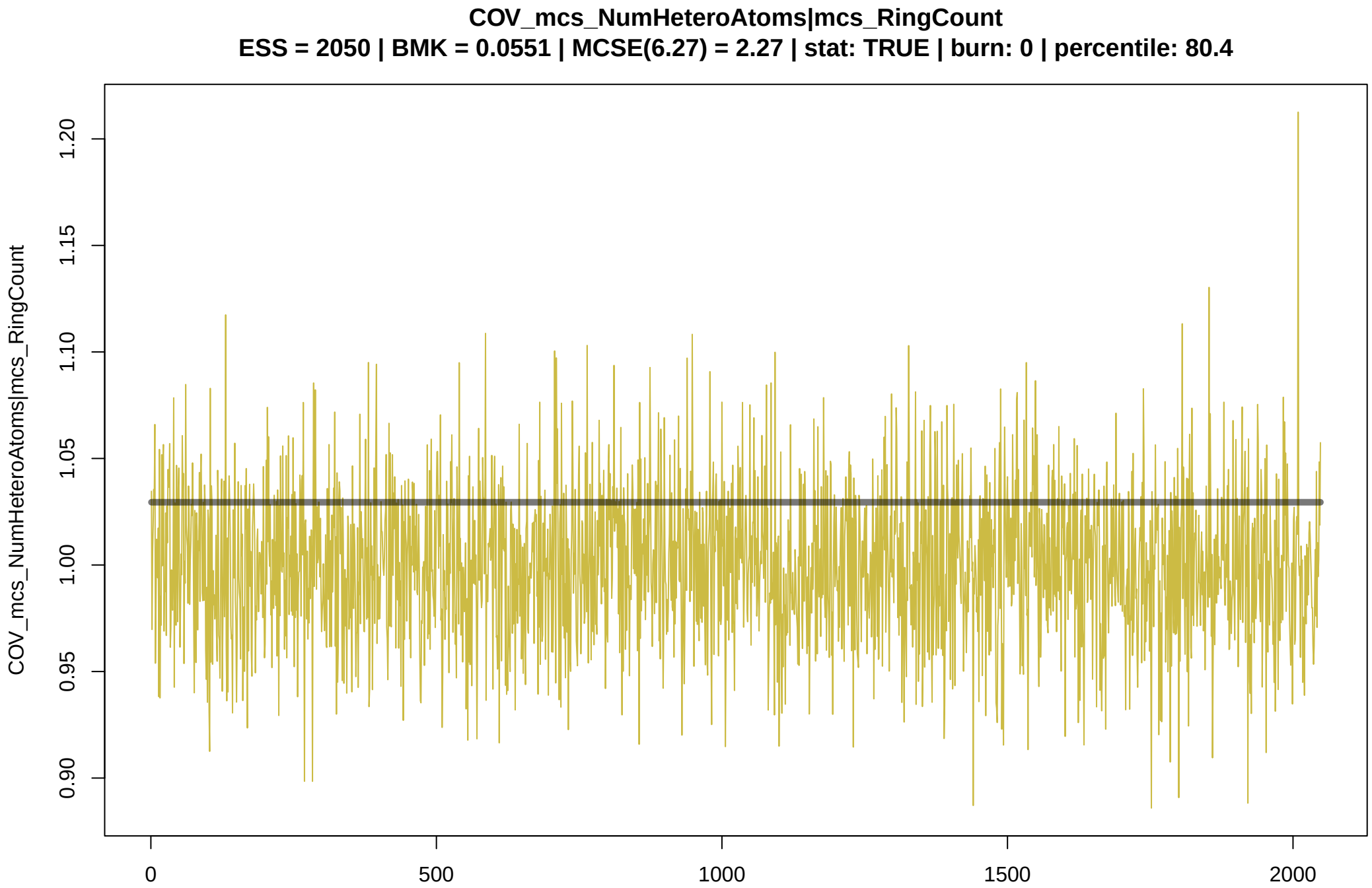

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.028 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0 | percentile: 53.7
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
45
44
43
42
0
500
1000
1500
2000

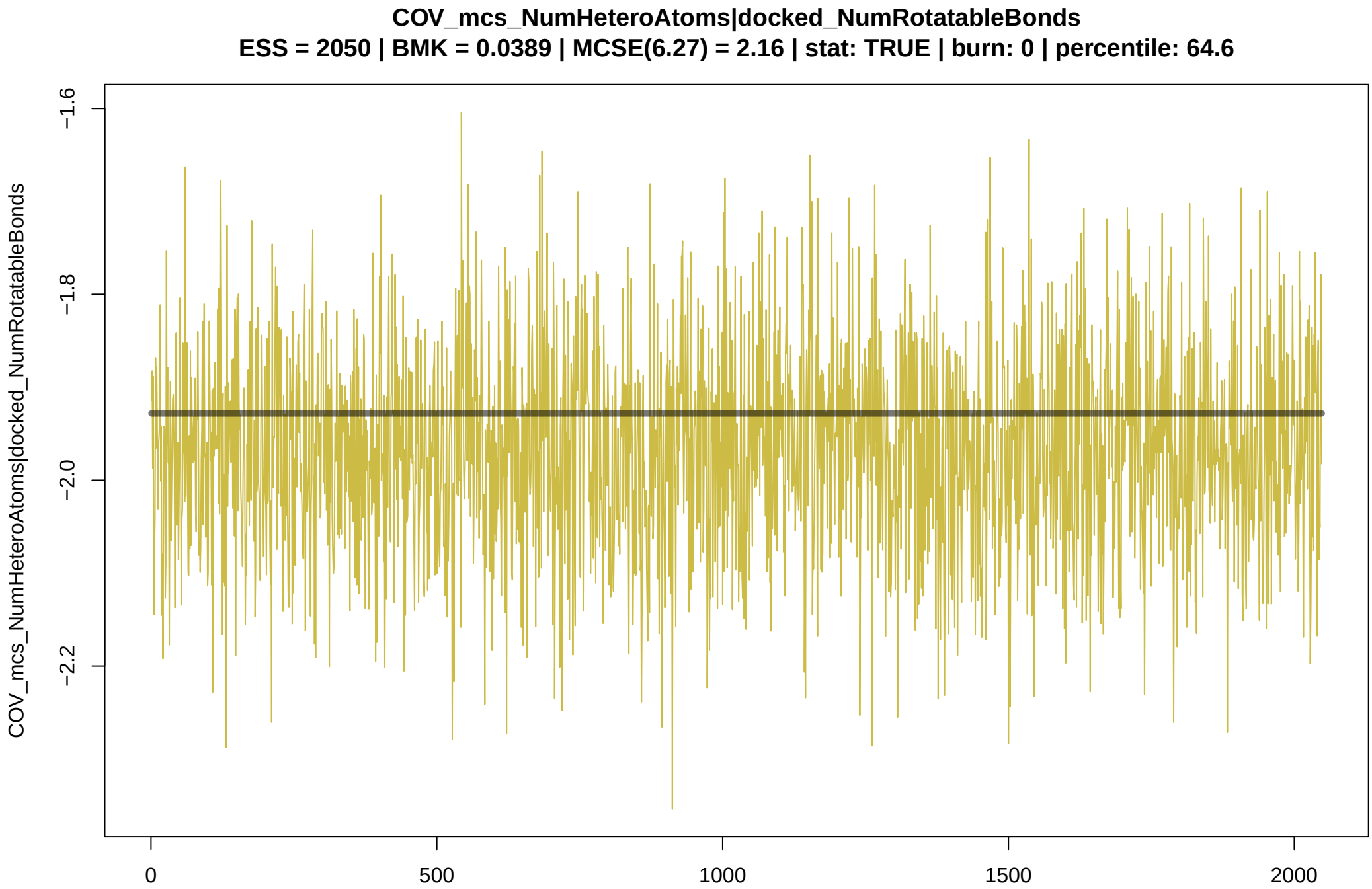

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 2050 | BMK = 0.0386 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | percentile: 22.3
COV_logit_ec_tanimoto_similarity|mcs_RingCount
−1.6
−1.7
−1.8
−1.9
−2.0
0
500
1000
1500
2000

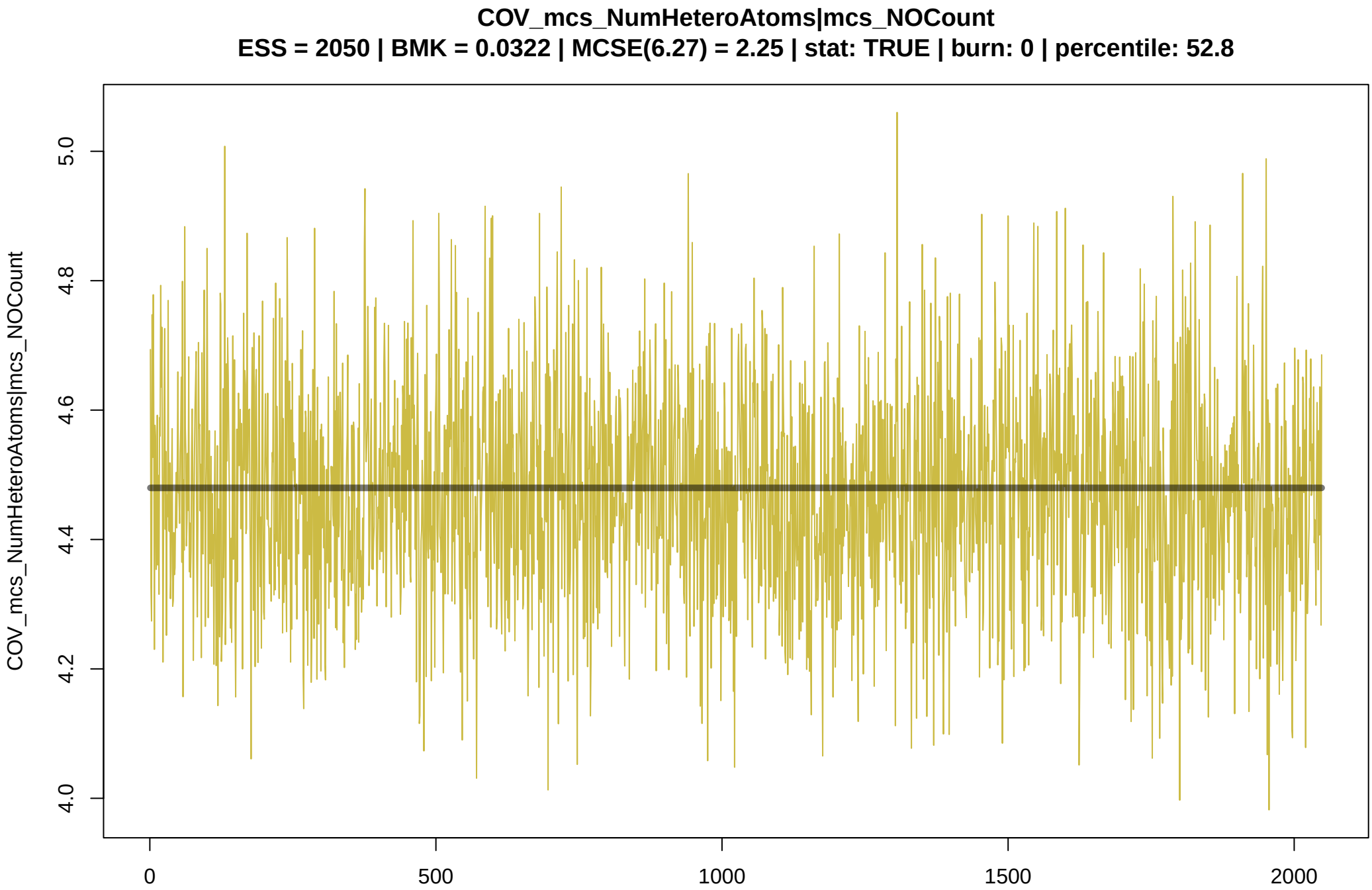

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0425 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | percentile: 98.9
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−11.4
−11.6
−11.8
−12.0
−12.2
−12.4
0
500
1000
1500
2000

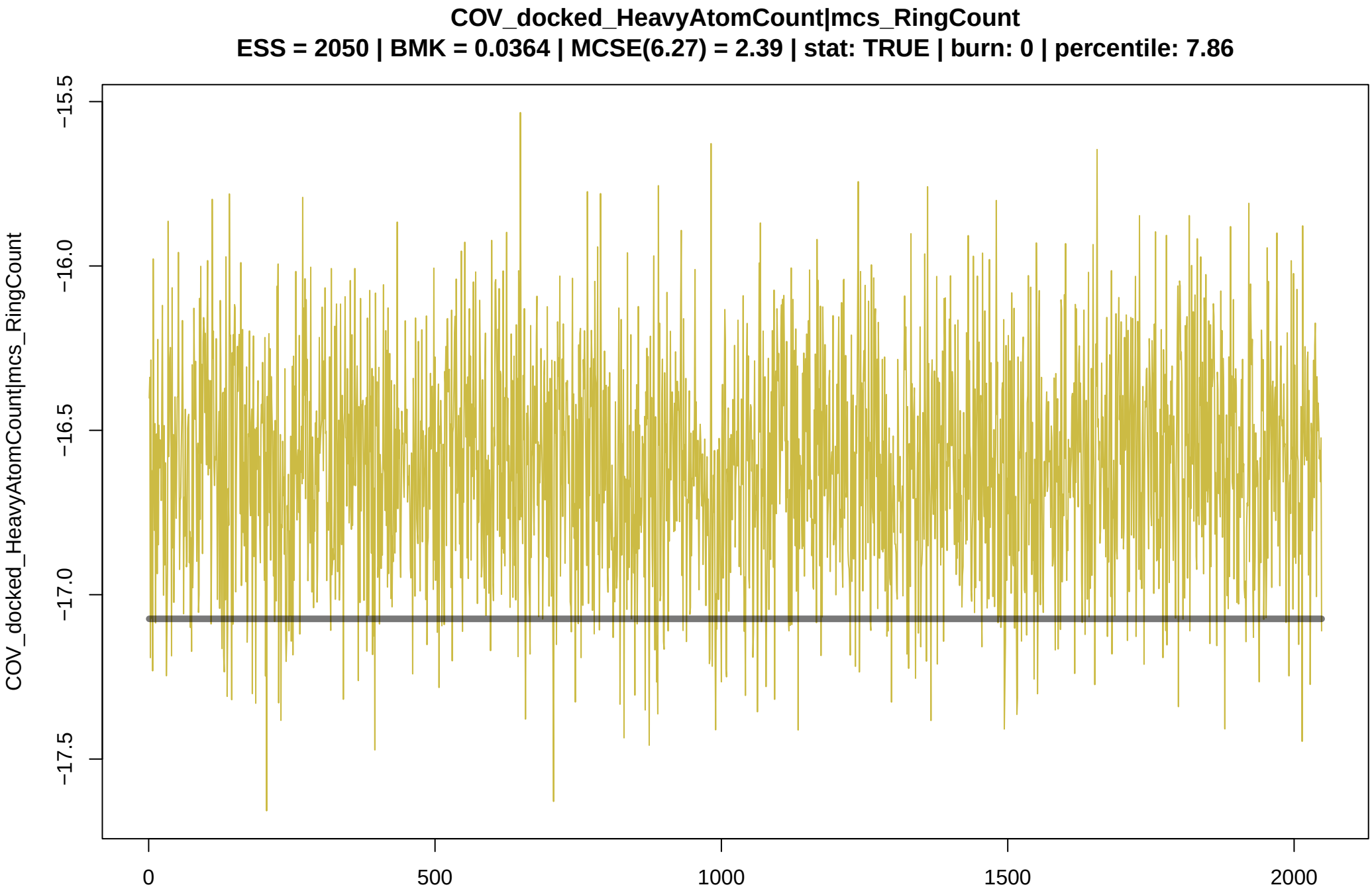

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 2050 | BMK = 0.0372 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0 | percentile: 19.7
COV_logit_ec_tanimoto_similarity|mcs_NOCount
−7.0
−7.5
−8.0
0
500
1000
1500
2000

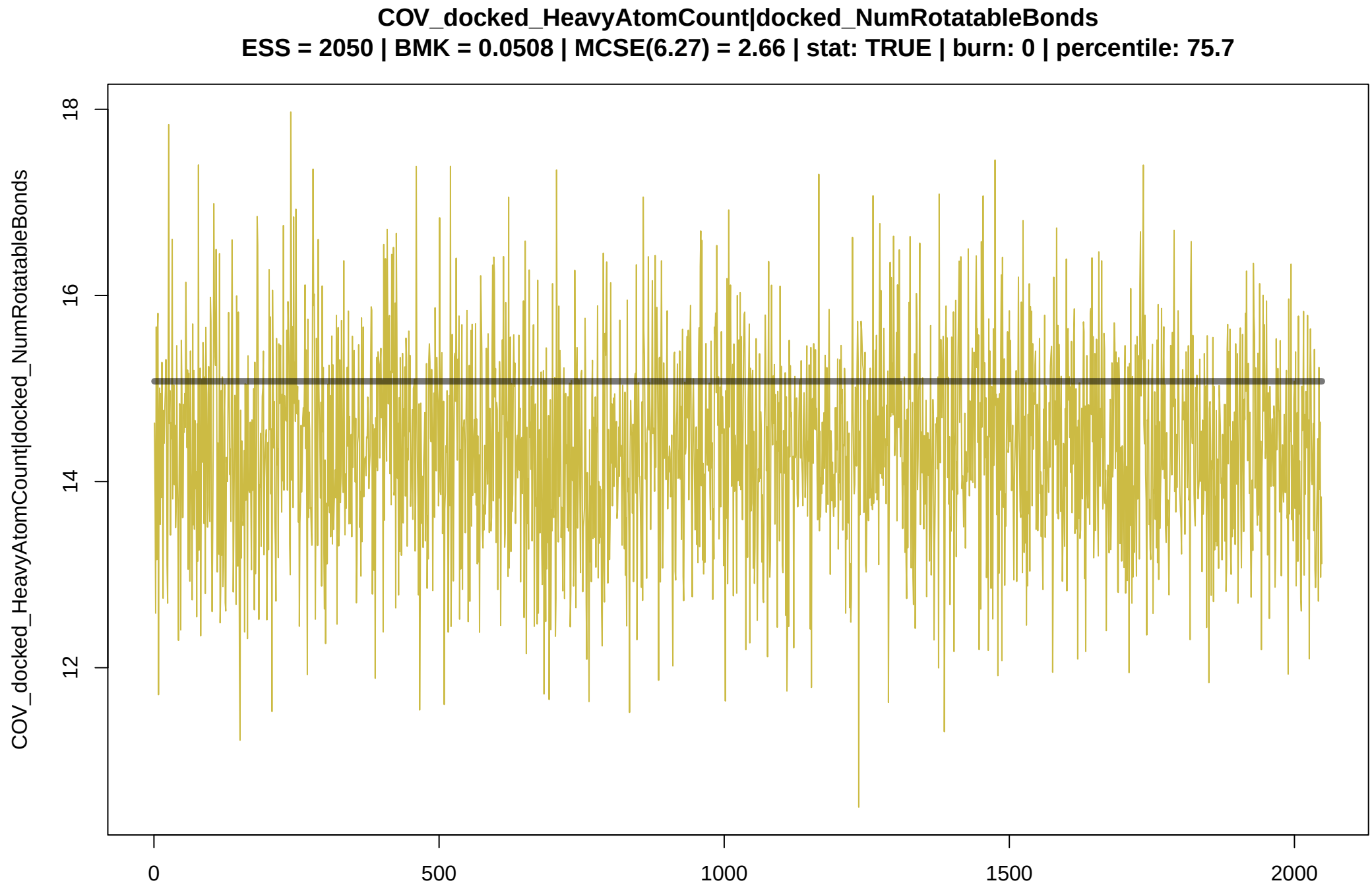

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0726 | MCSE(6.27) = 3.16 | stat: FALSE | burn: 0 | percentile: 19.4
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
−14.0
−14.5
−15.0
−15.5
−16.0
−16.5
0
500
1000
1500
2000

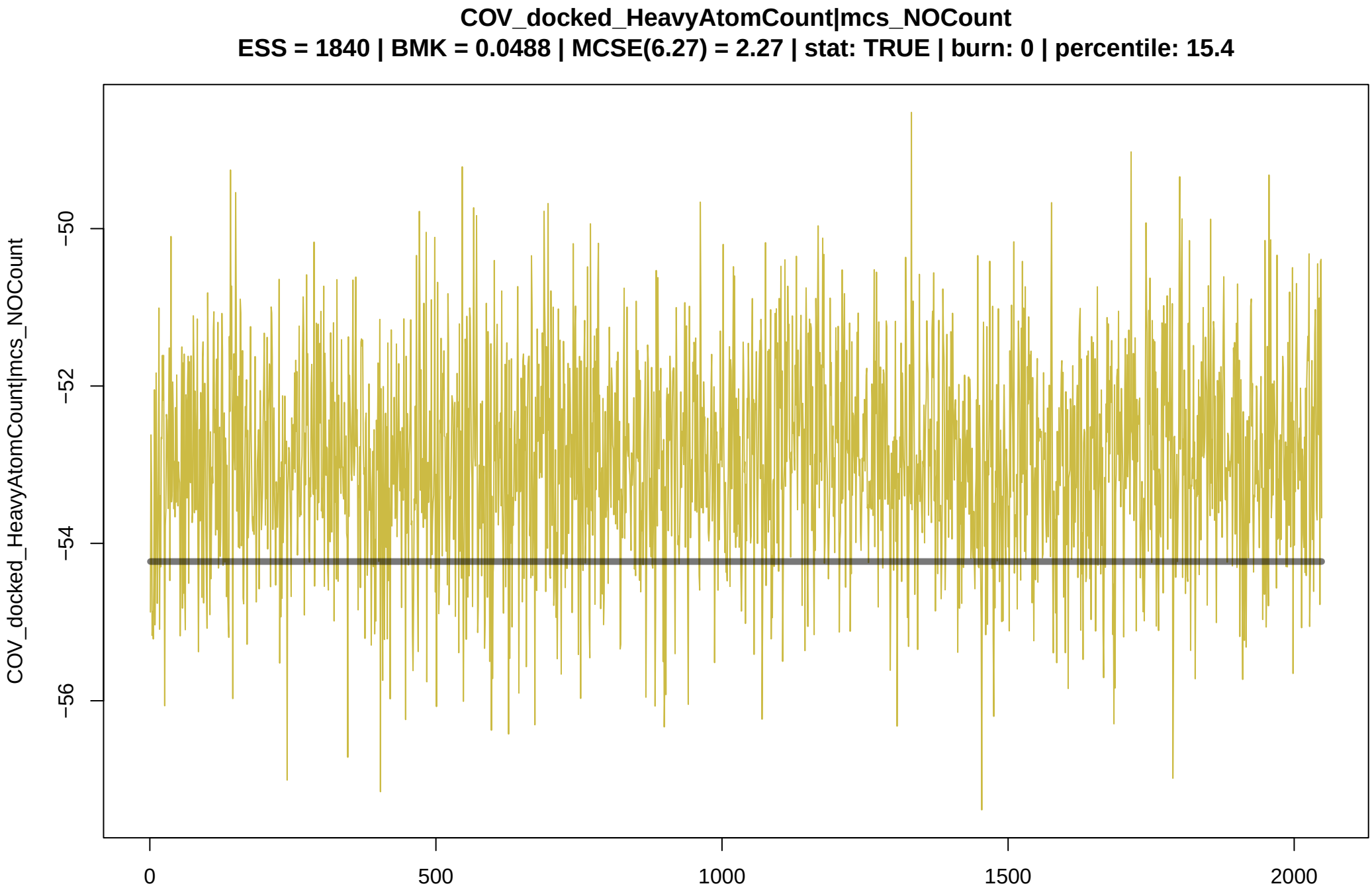

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 2050 | BMK = 0.0551 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | percentile: 80.4
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.90
0.95
1.00
1.05
1.10
1.15
1.20
0
500
1000
1500
2000

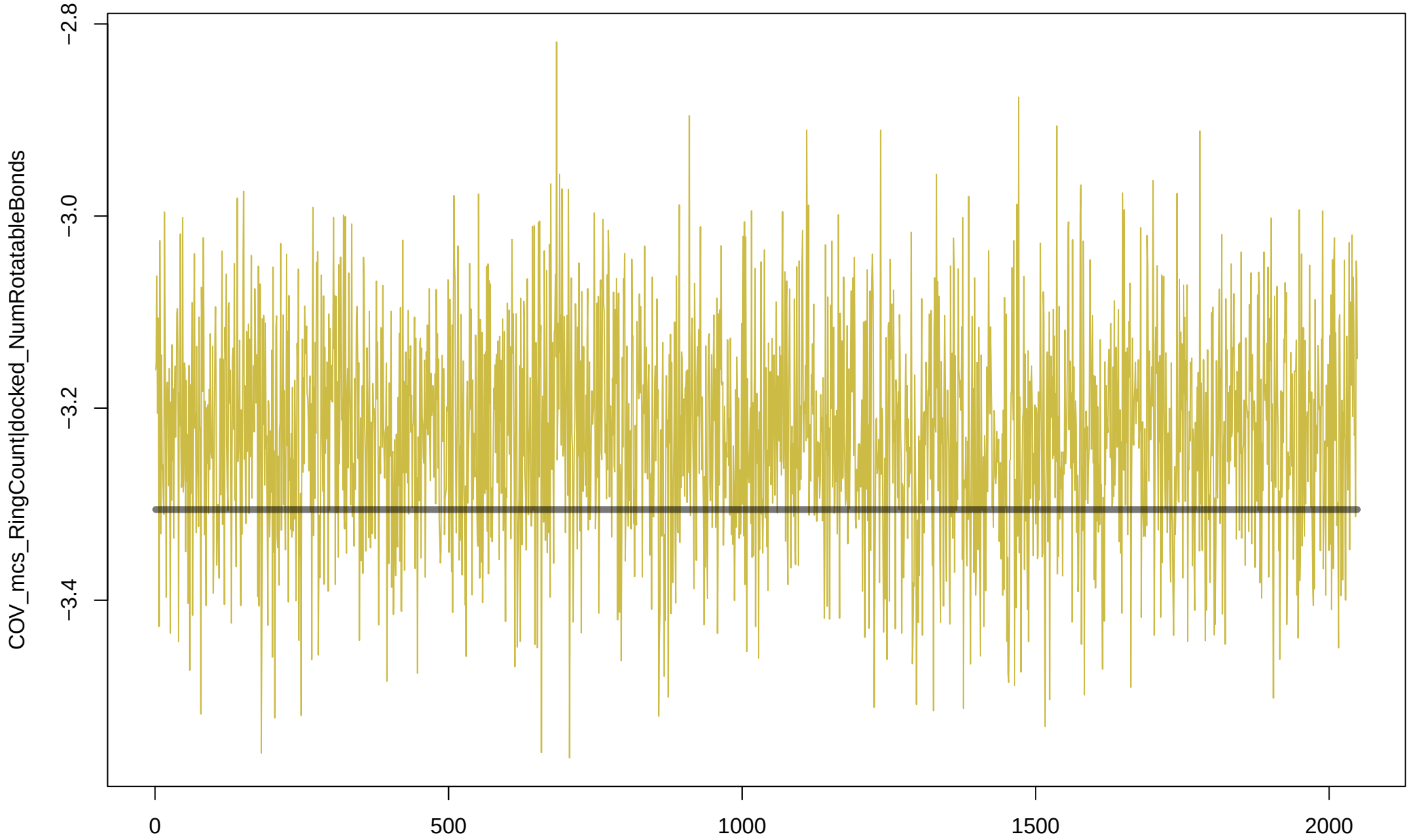

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0389 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0 | percentile: 64.6
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
−1.6
−1.8
−2.0
−2.2
0
500
1000
1500
2000

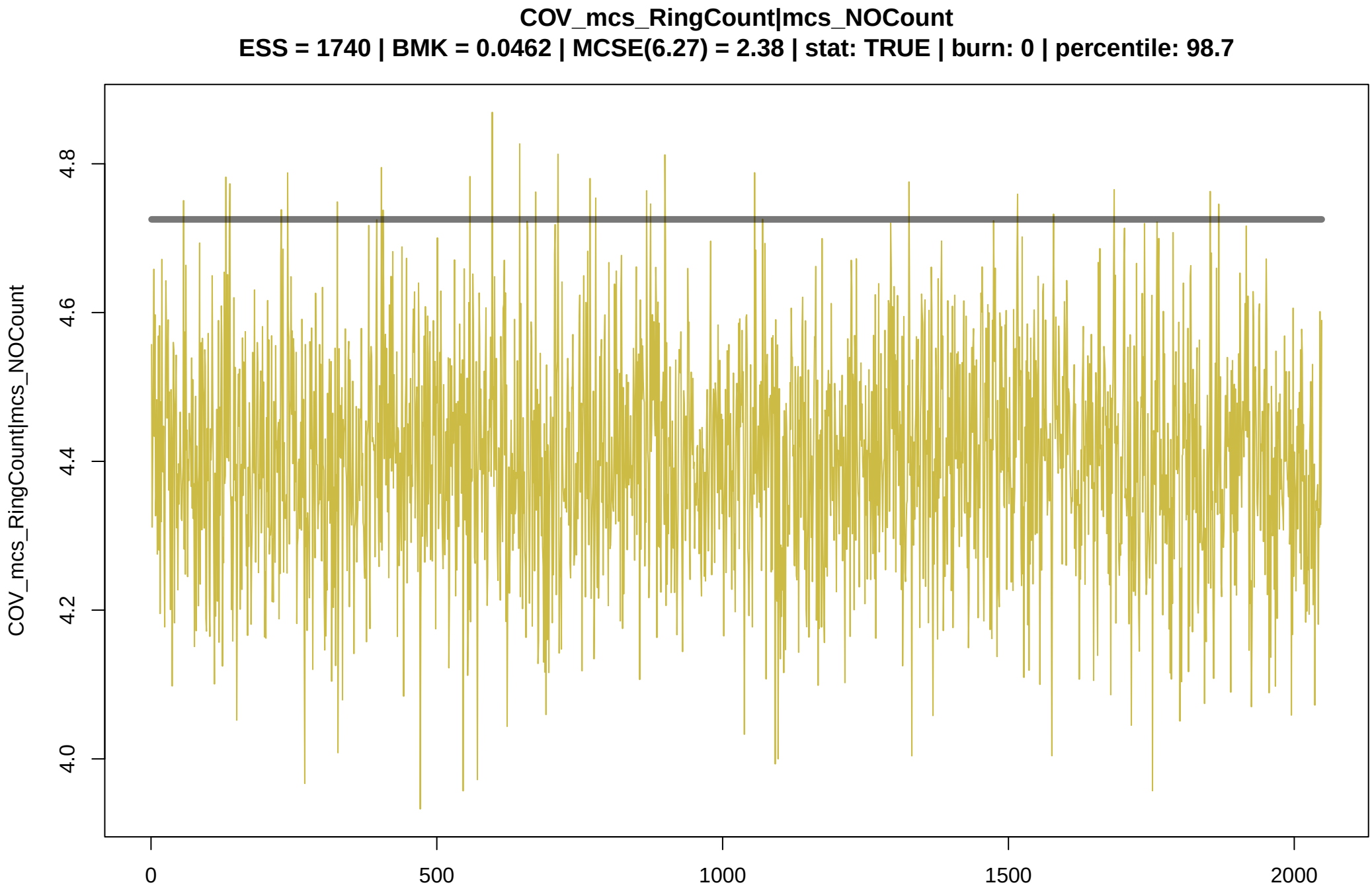

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 2050 | BMK = 0.0322 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | percentile: 52.8
COV_mcs_NumHeteroAtoms|mcs_NOCount
4.0
4.2
4.4
4.6
4.8
5.0
0
500
1000
1500
2000

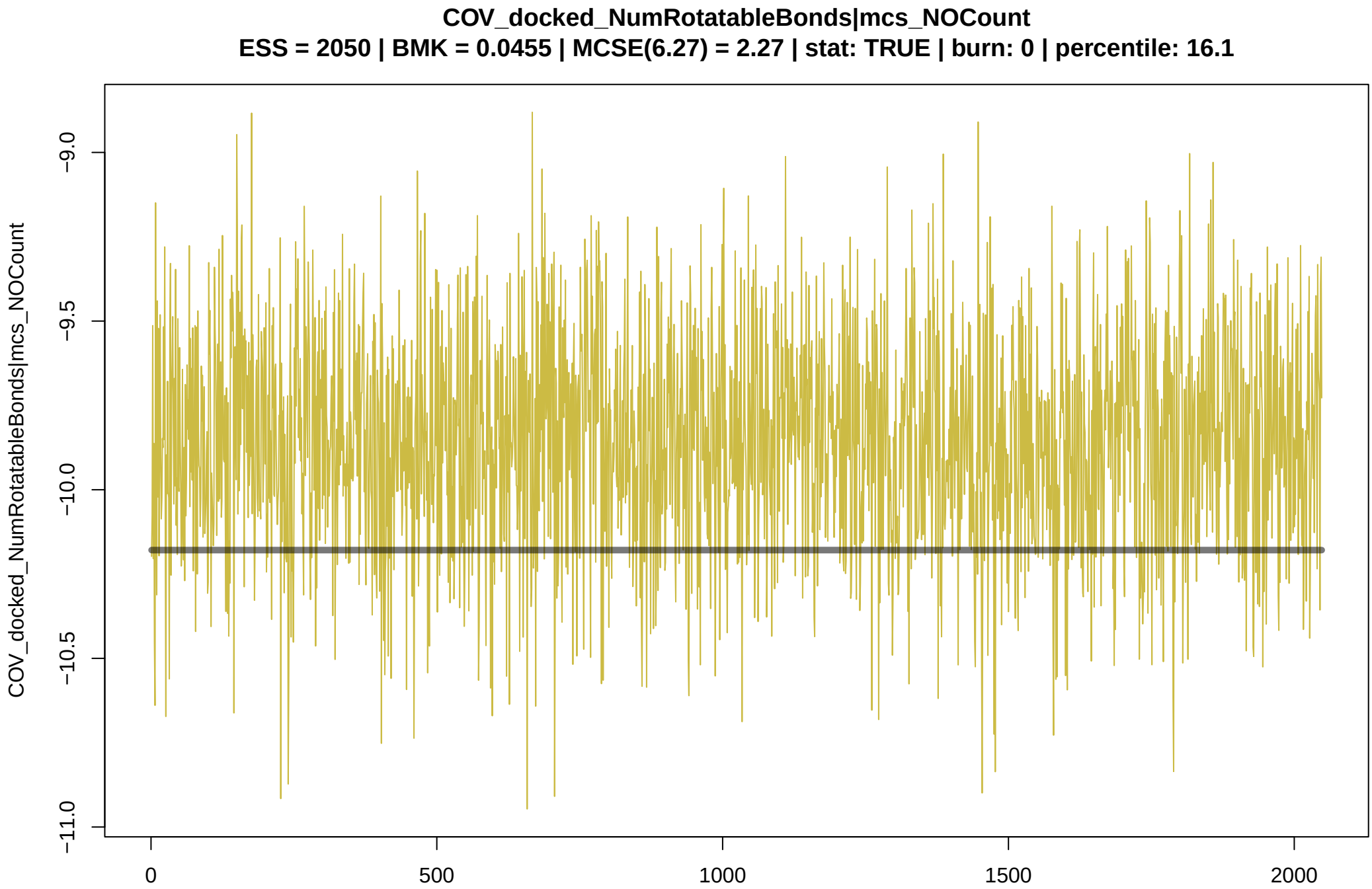

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 2050 | BMK = 0.0364 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | percentile: 7.86
COV_docked_HeavyAtomCount|mcs_RingCount
−15.5
−16.0
−16.5
−17.0
−17.5
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0 | percentile: 75.7
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
18
16
14
12
0
500
1000
1500
2000


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 1840 | BMK = 0.0488 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | percentile: 15.4
COV_docked_HeavyAtomCount|mcs_NOCount
−50
−52
−54
−56
0
500
1000
1500
2000


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 2050 | BMK = 0.0581 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | percentile: 23.4
COV_mcs_RingCount|docked_NumRotatableBonds
−2.8
−3.0
−3.2
−3.4
0
500
1000
1500
2000


COV_mcs_RingCount|mcs_NOCount
ESS = 1740 | BMK = 0.0462 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0 | percentile: 98.7
COV_mcs_RingCount|mcs_NOCount
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 2050 | BMK = 0.0455 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | percentile: 16.1
COV_docked_NumRotatableBonds|mcs_NOCount
−9.0
−9.5
−10.0
−10.5
−11.0
0
500
1000
1500
2000