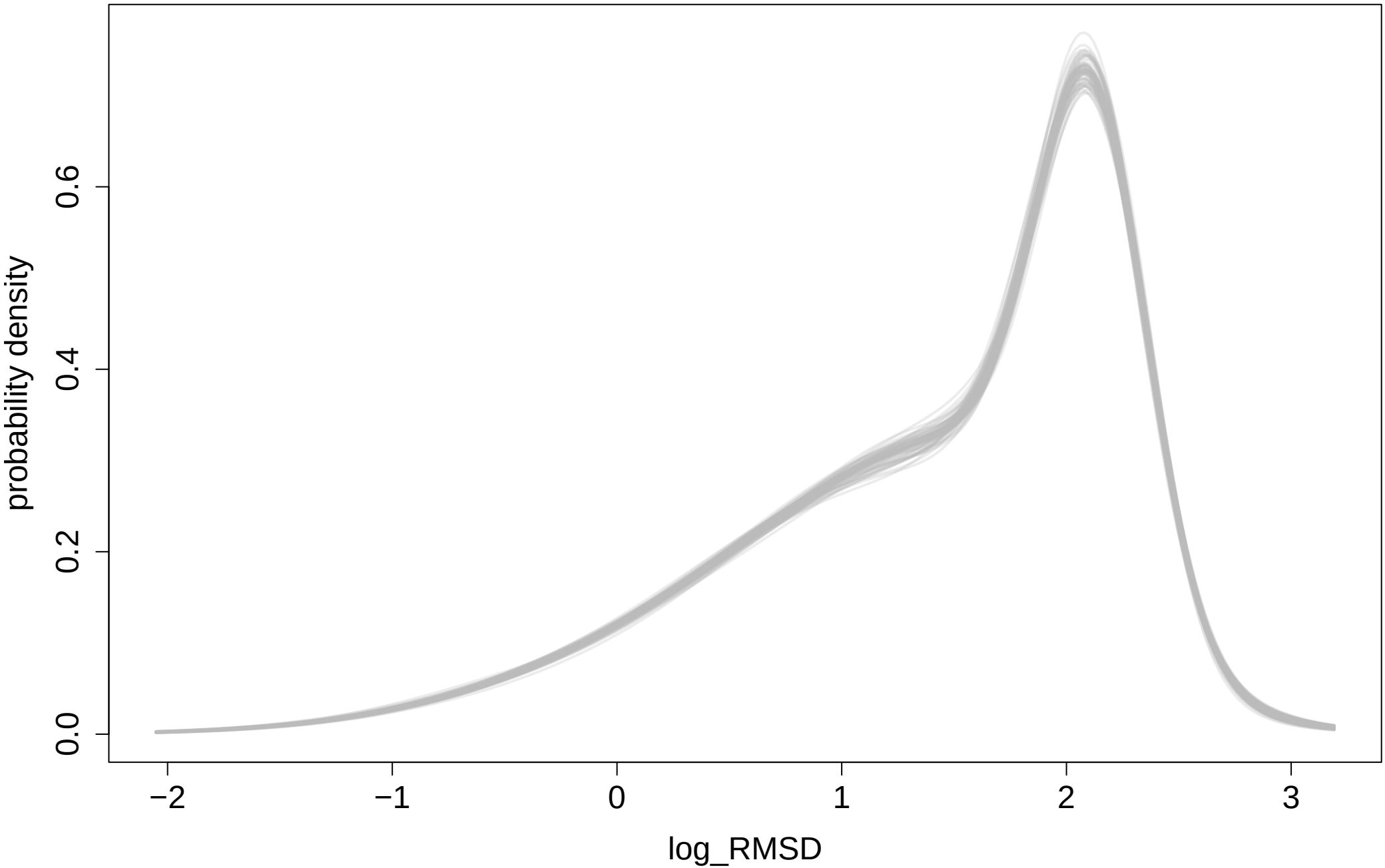
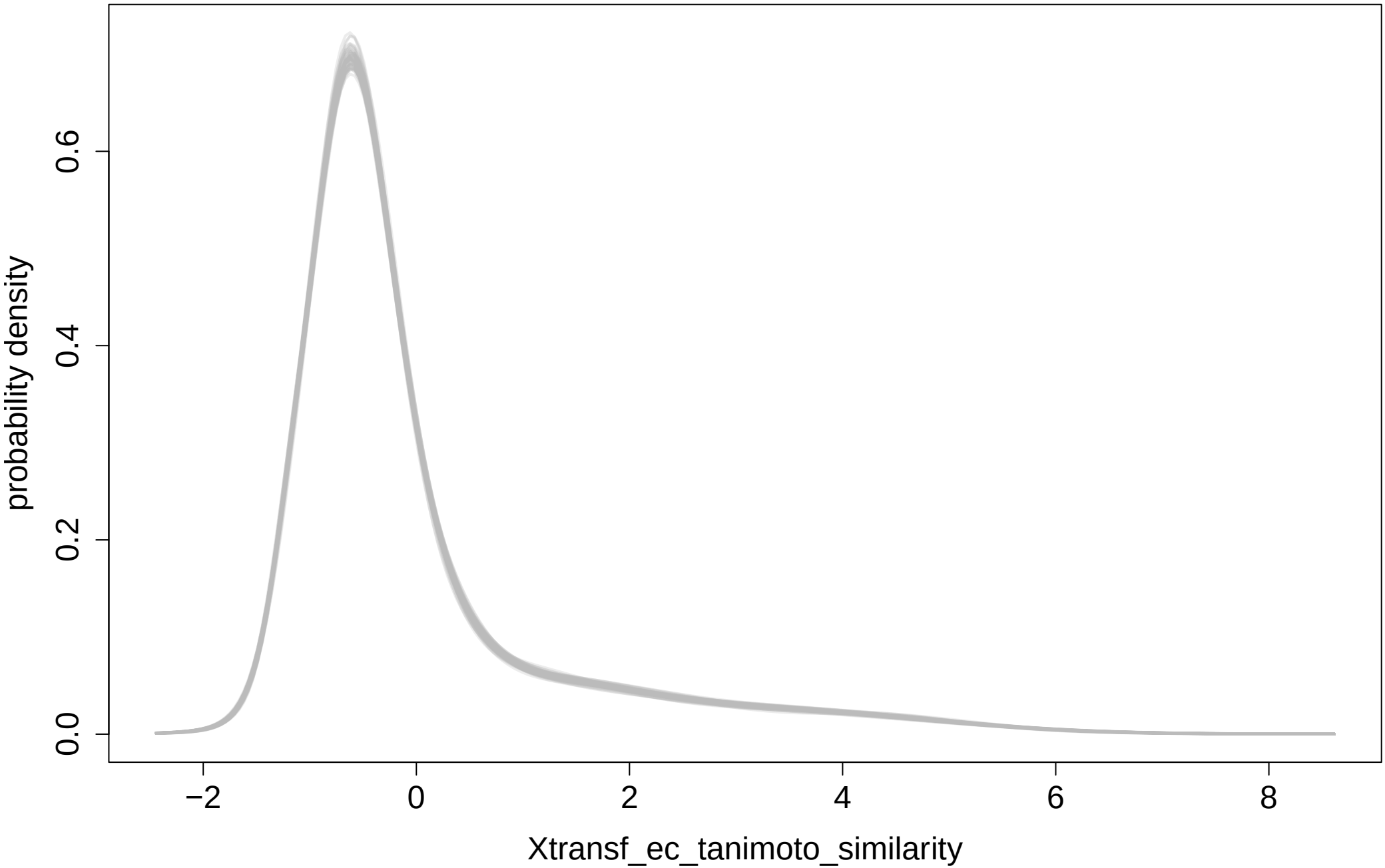
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.942946390450418
max MCSE = 14.6161295218273
all stationary: FALSE
burn: 2040

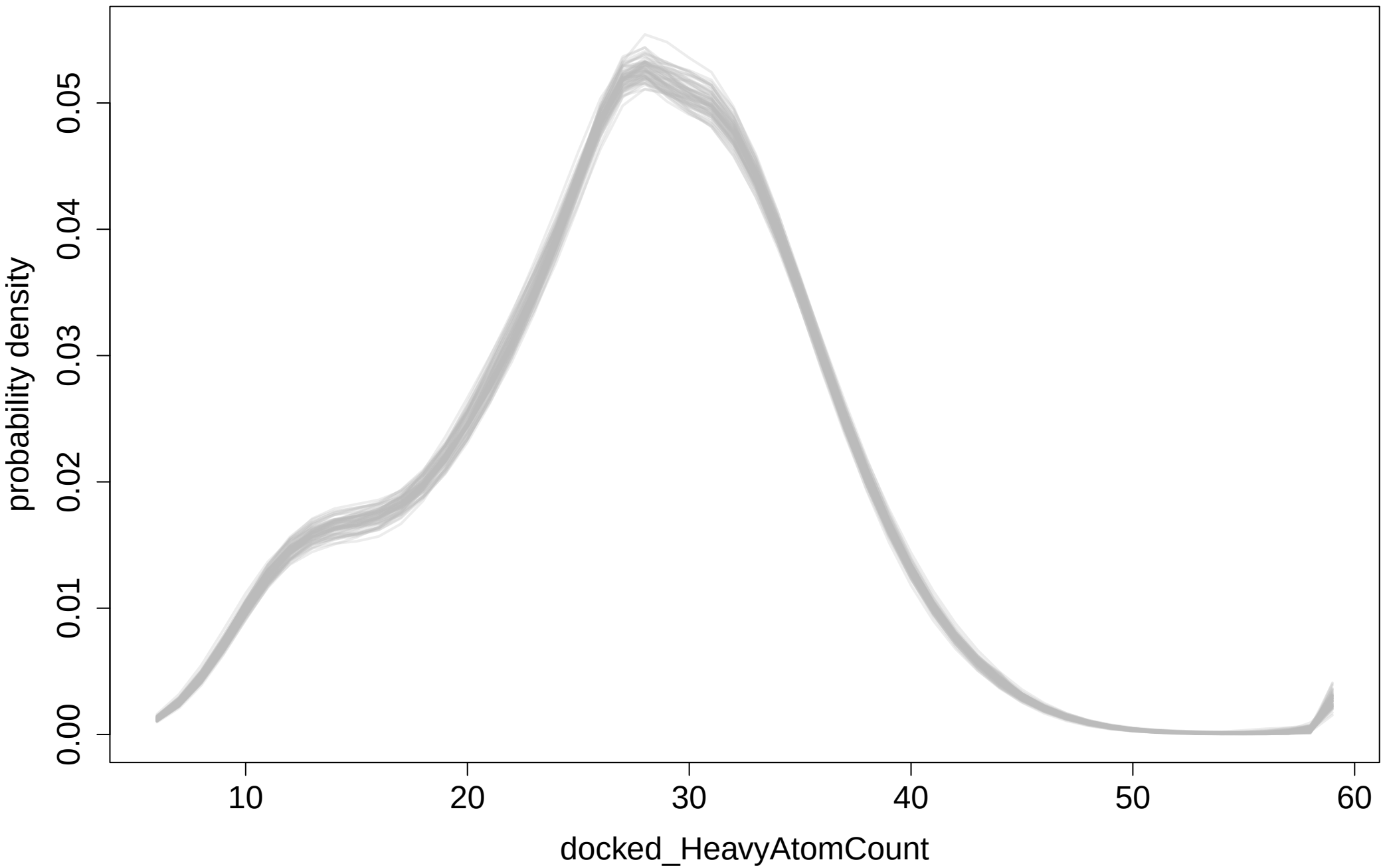
−− STATS 2D −−
min ESS = 139.756332794767
max BMK = 0.170887013464675
max MCSE = 4.78923380393871
all stationary: FALSE
burn: 0

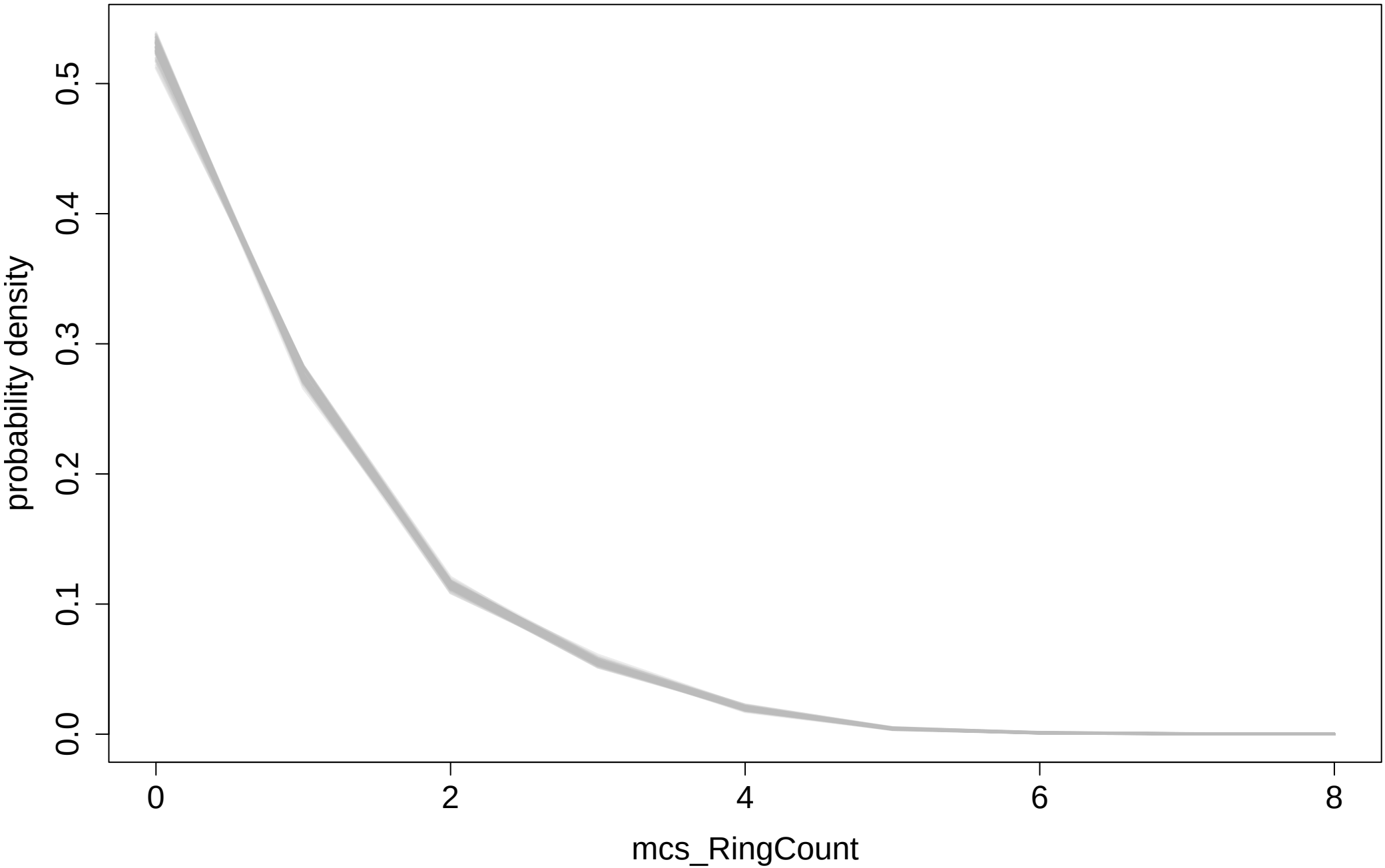
−− STATS 1D −−
min ESS = 2.2044604925031e−16
max BMK = 0.517210613073053
max MCSE = NaN
all stationary: FALSE
burn: 1020

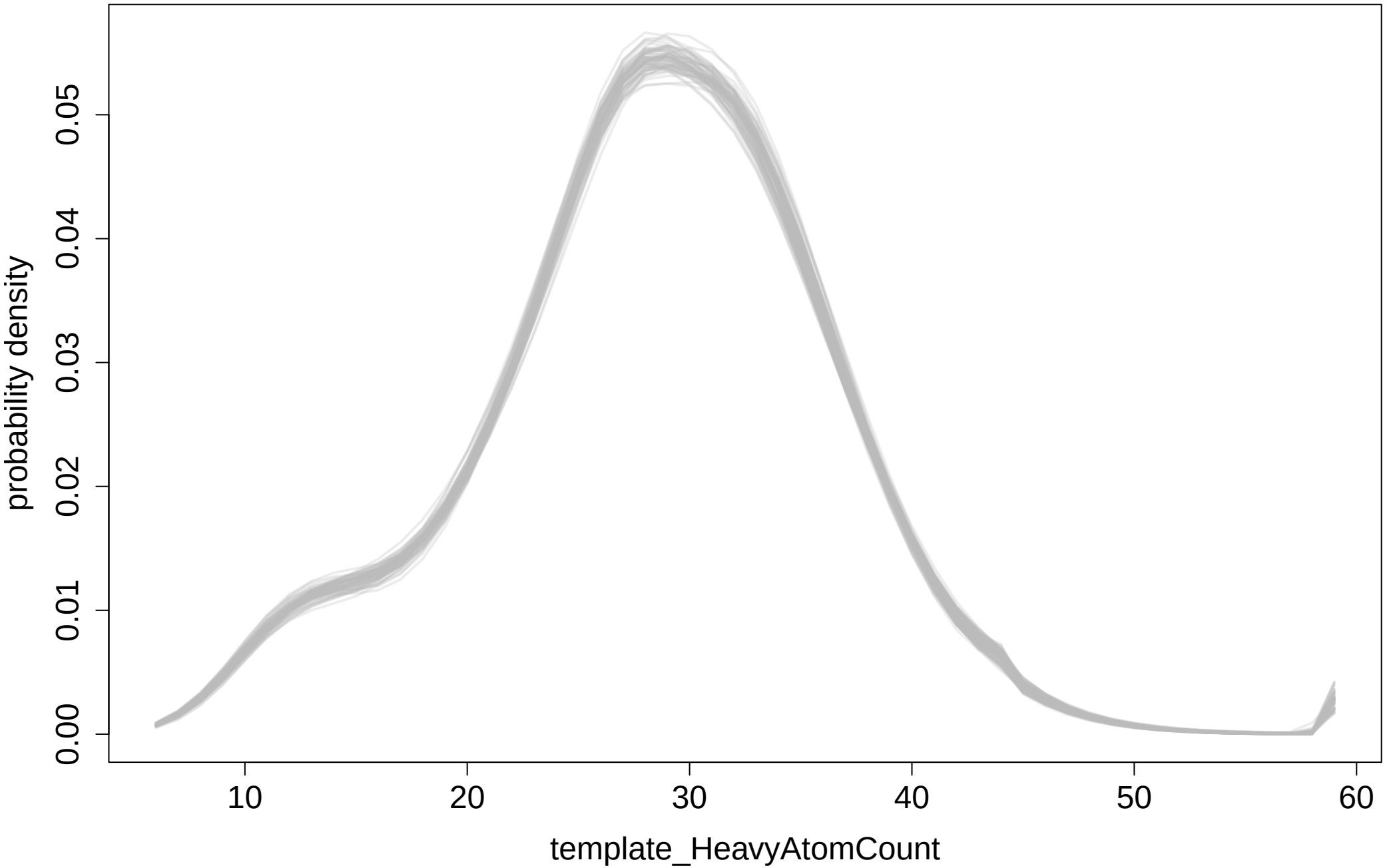
Occupied clusters: 47 of 91
LL: −112000 +− 203

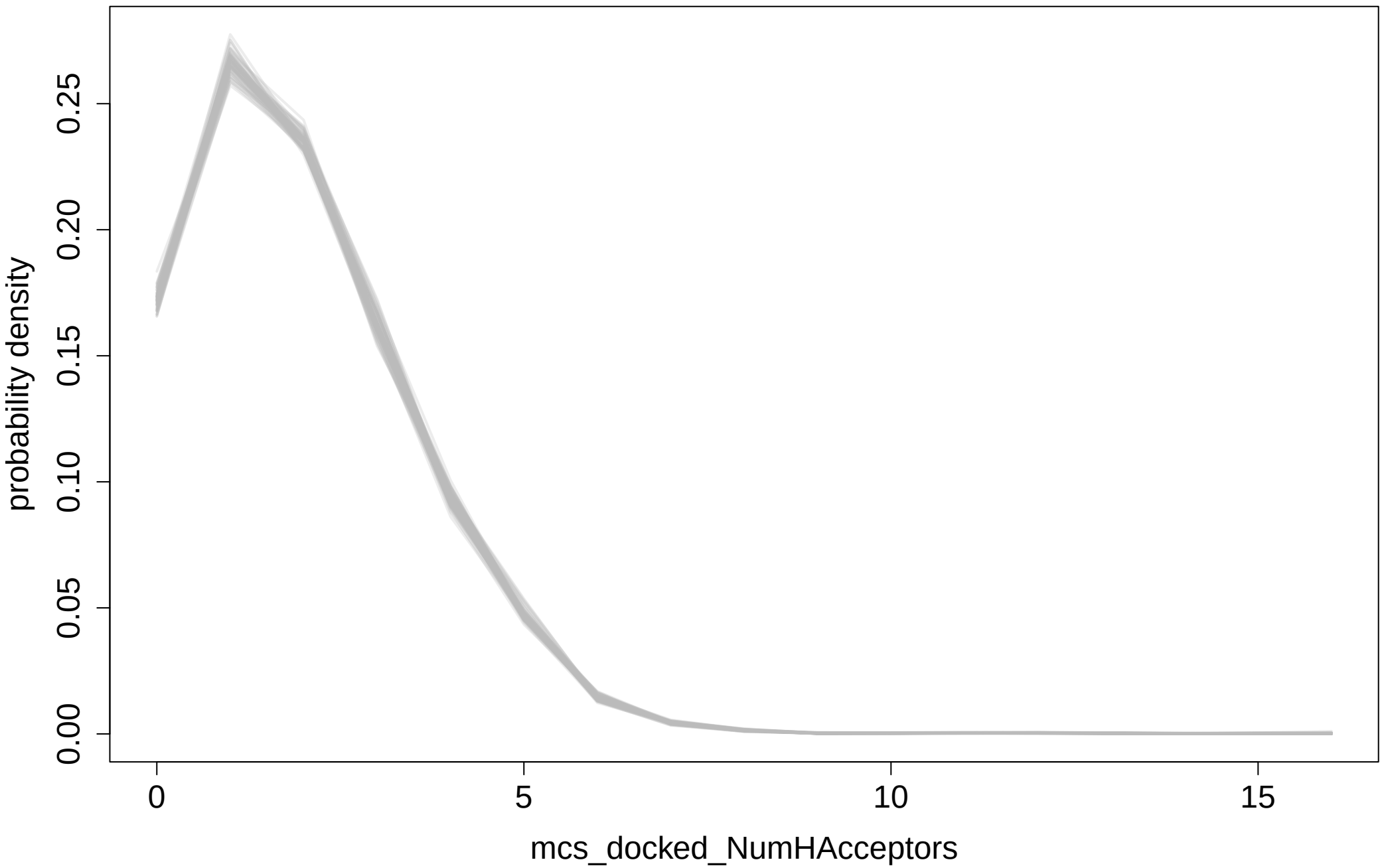

probability density
0.0
0.2
0.4
0.6
−2
−1
0
1
2
3
log_RMSD

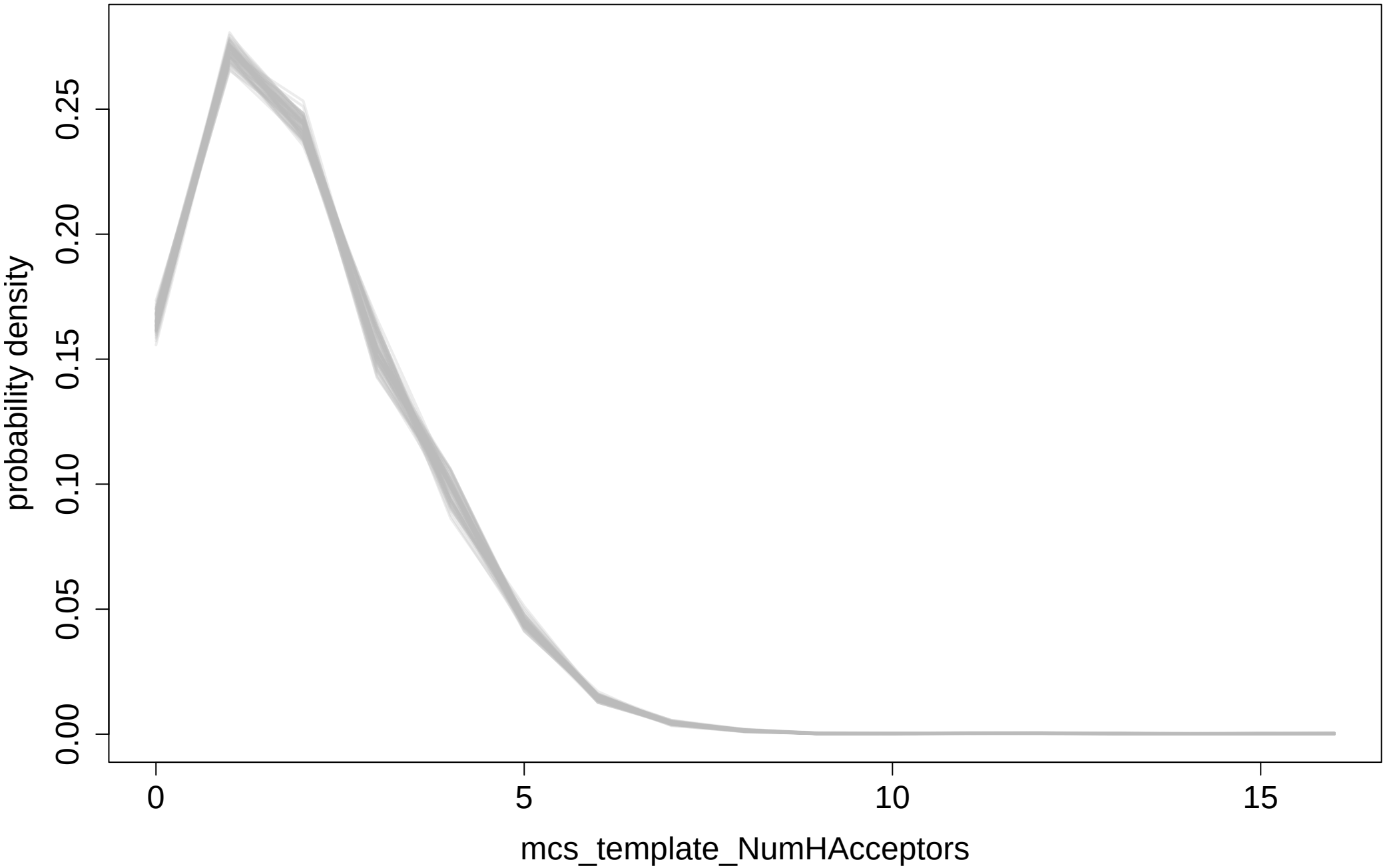

probability density
0.0
0.2
0.4
0.6
−2
0
2
4
6
8
Xtransf_ec_tanimoto_similarity

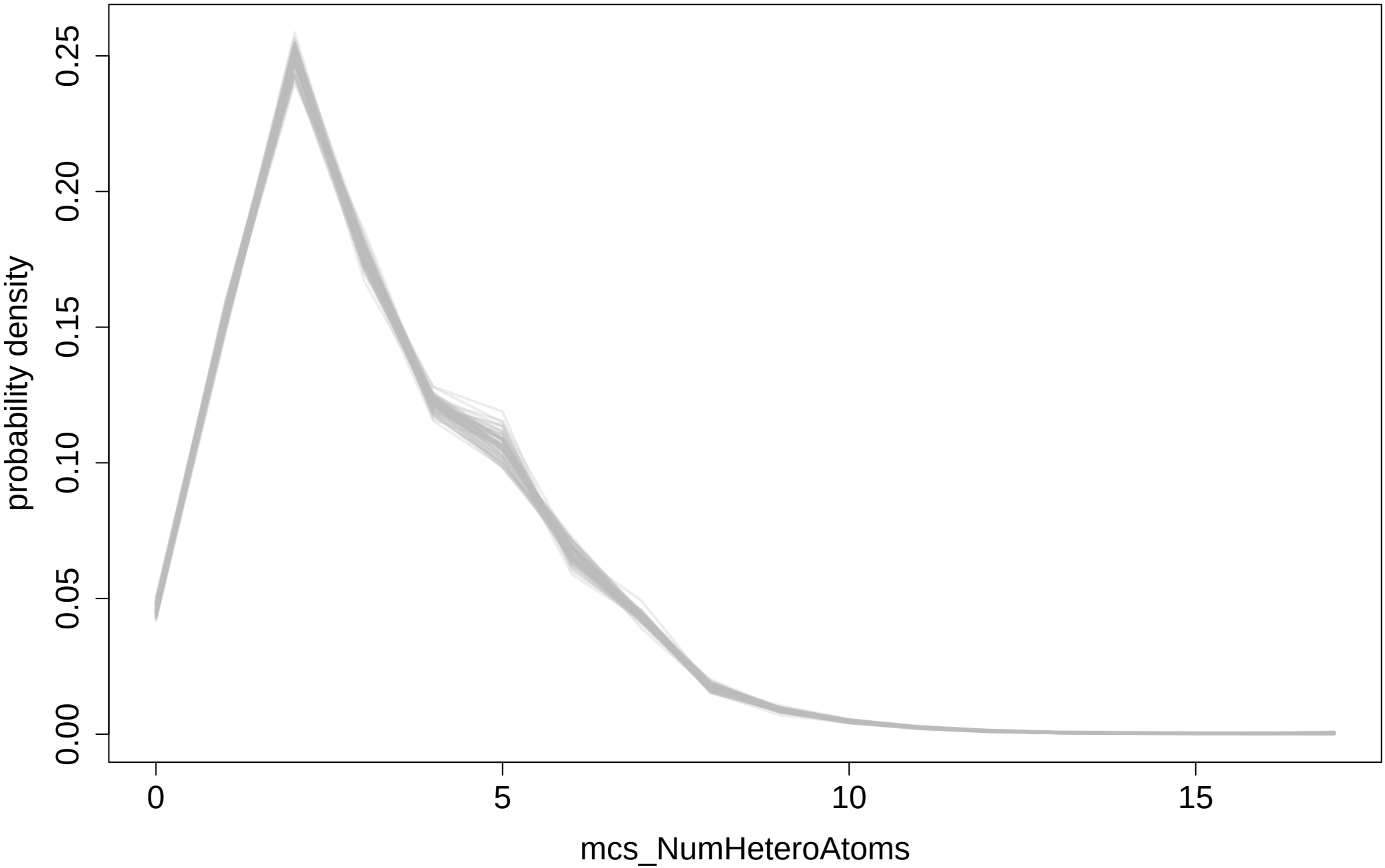

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
docked_HeavyAtomCount

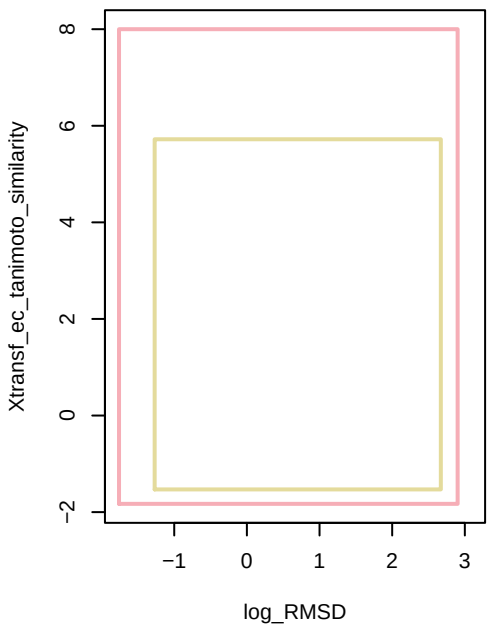

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0
2
4
6
8
mcs_RingCount

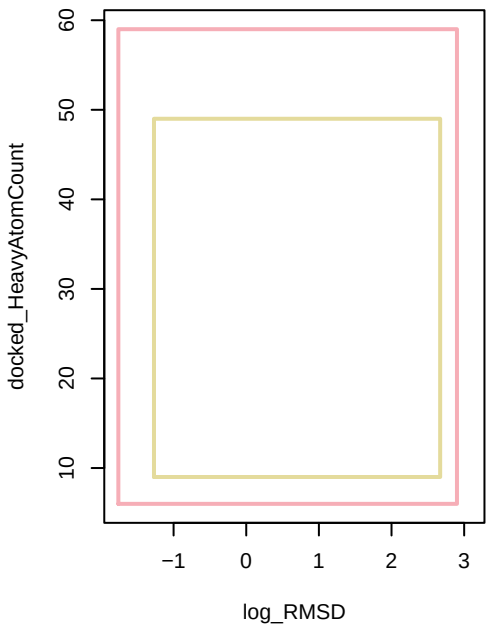

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
template_HeavyAtomCount

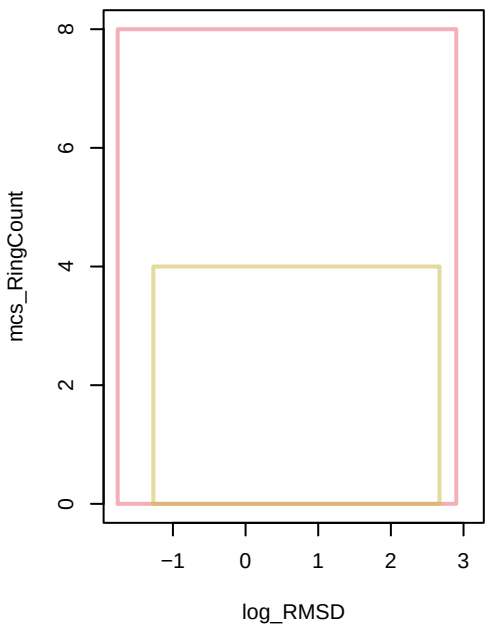

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_docked_NumHAcceptors

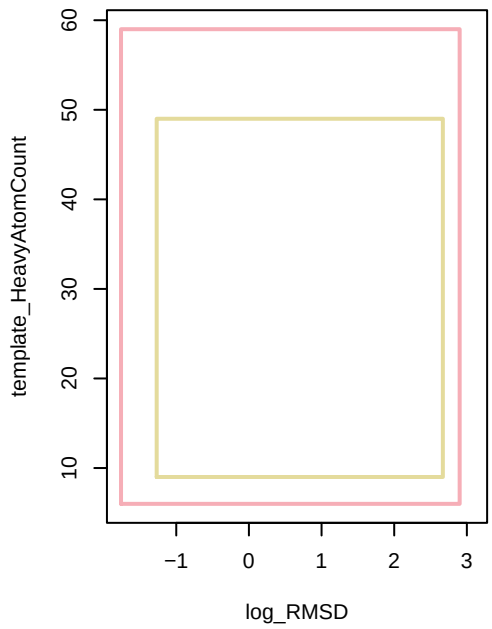

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_template_NumHAcceptors

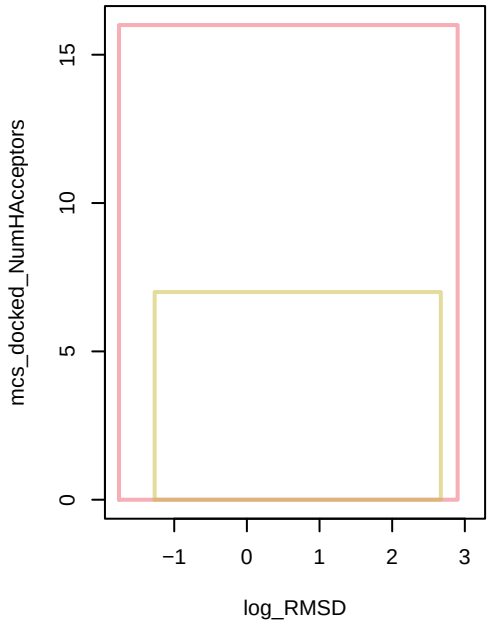

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms

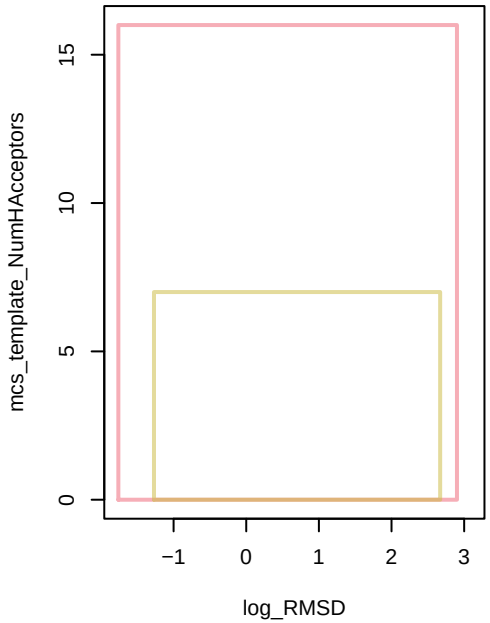

Xtransf_ec_tanimoto_similarity
log_RMSD

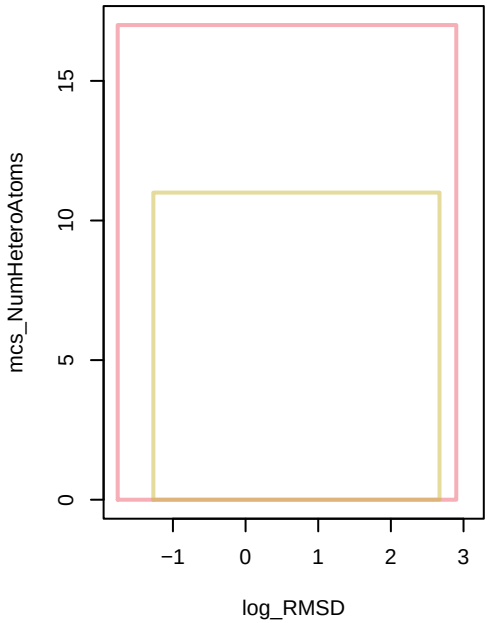

docked_HeavyAtomCount
log_RMSD

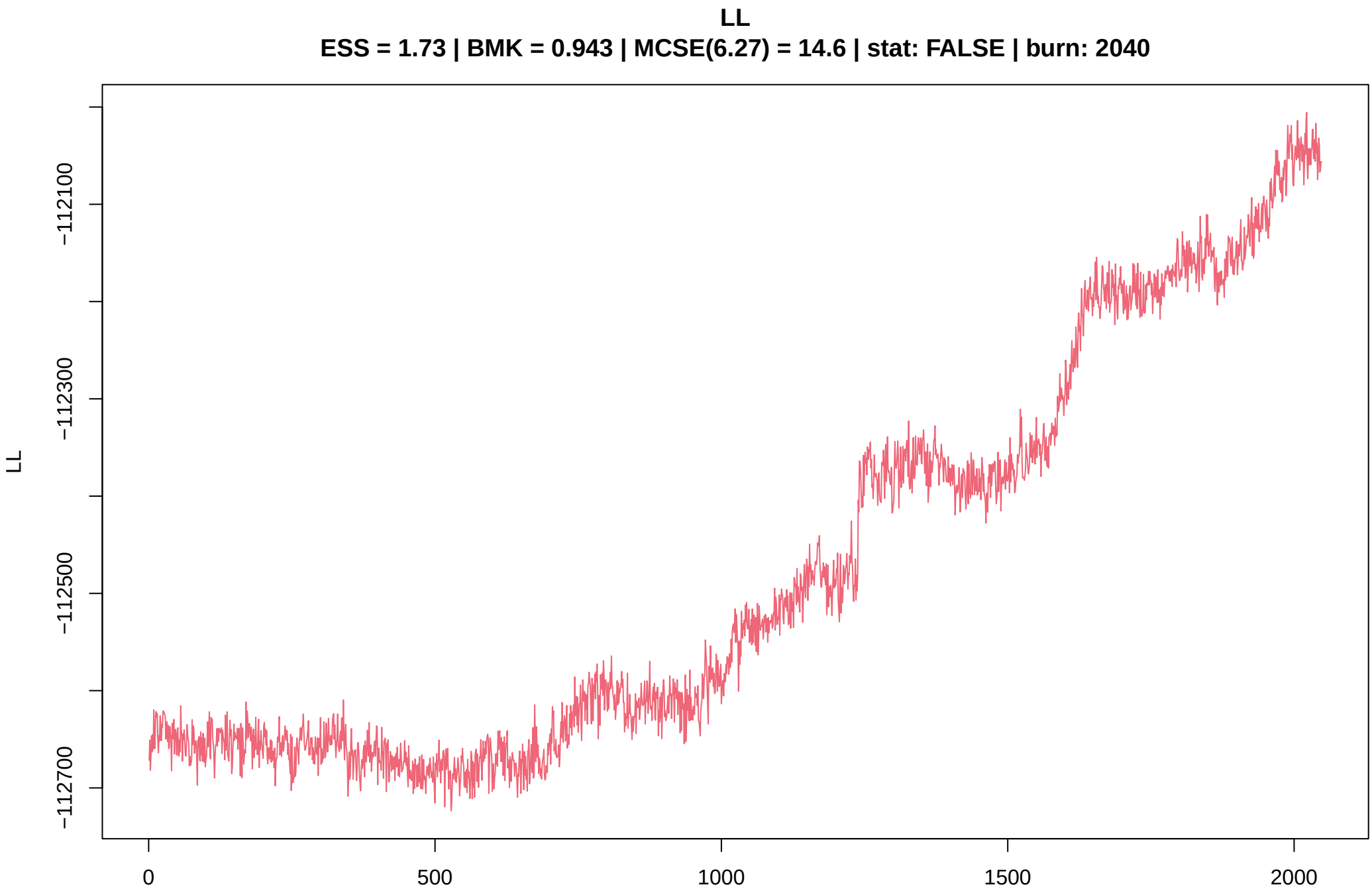

mcs_RingCount
log_RMSD

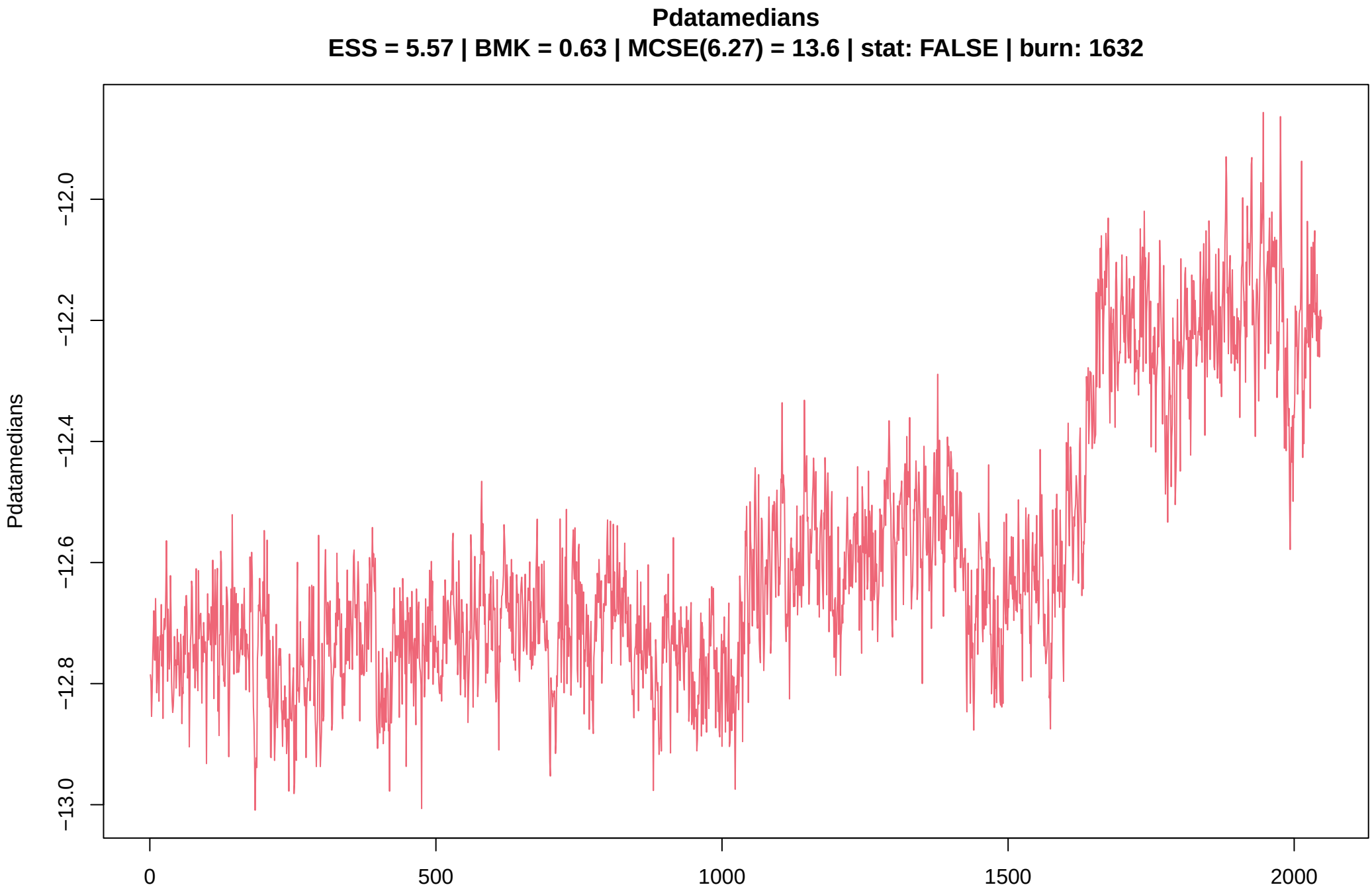

template_HeavyAtomCount
log_RMSD

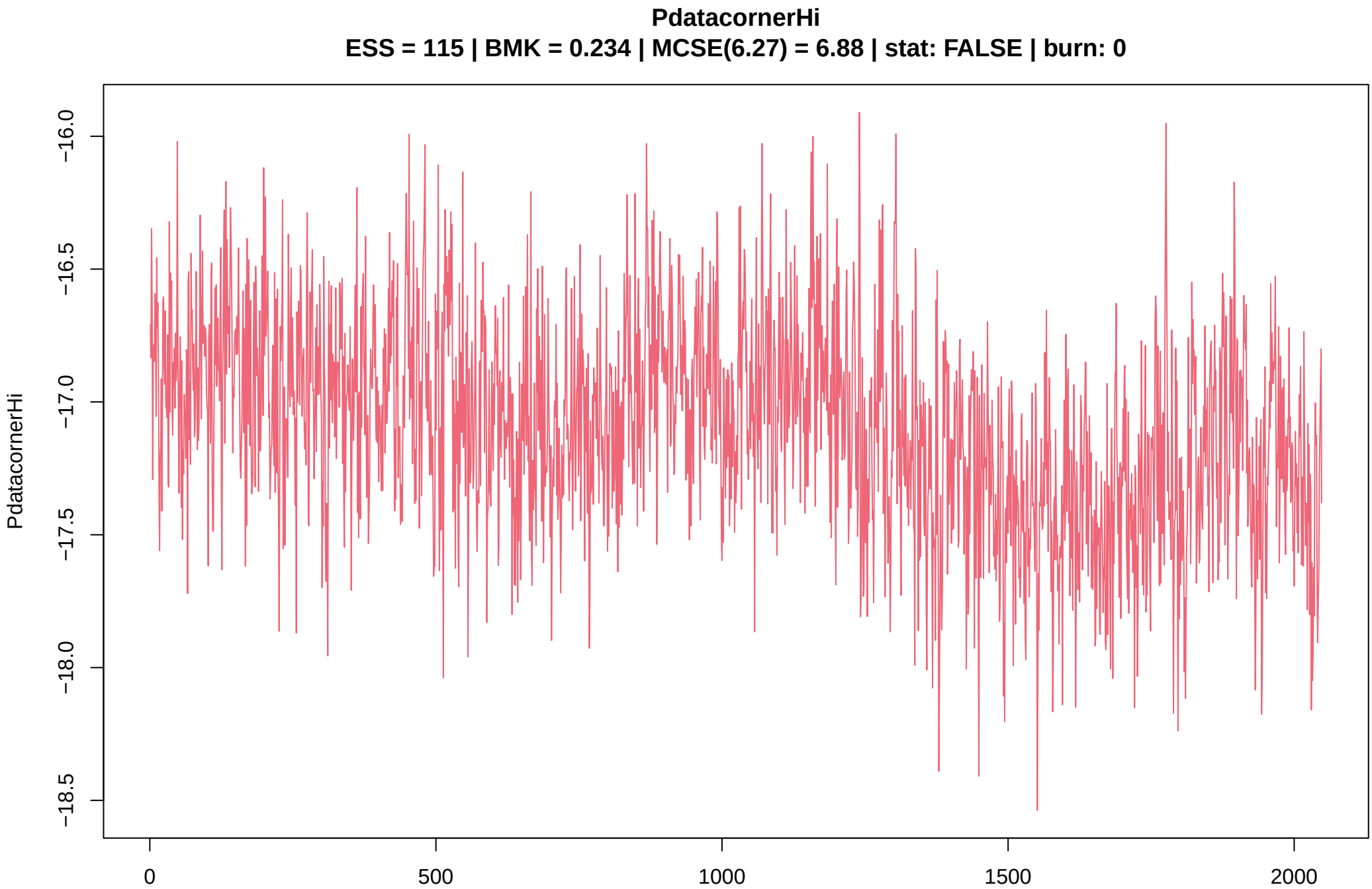

mcs_docked_NumHAcceptors
log_RMSD

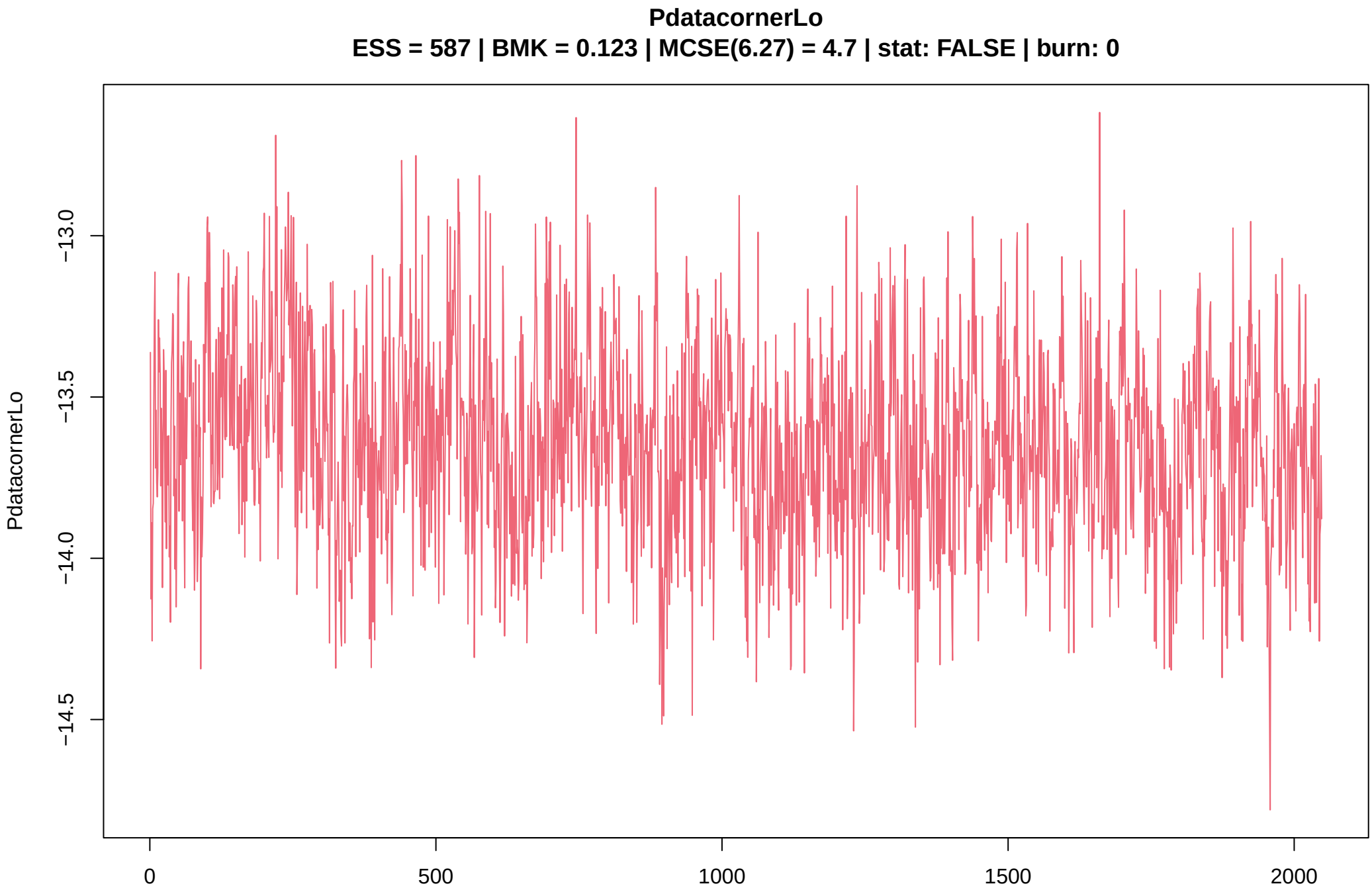

mcs_template_NumHAcceptors
log_RMSD

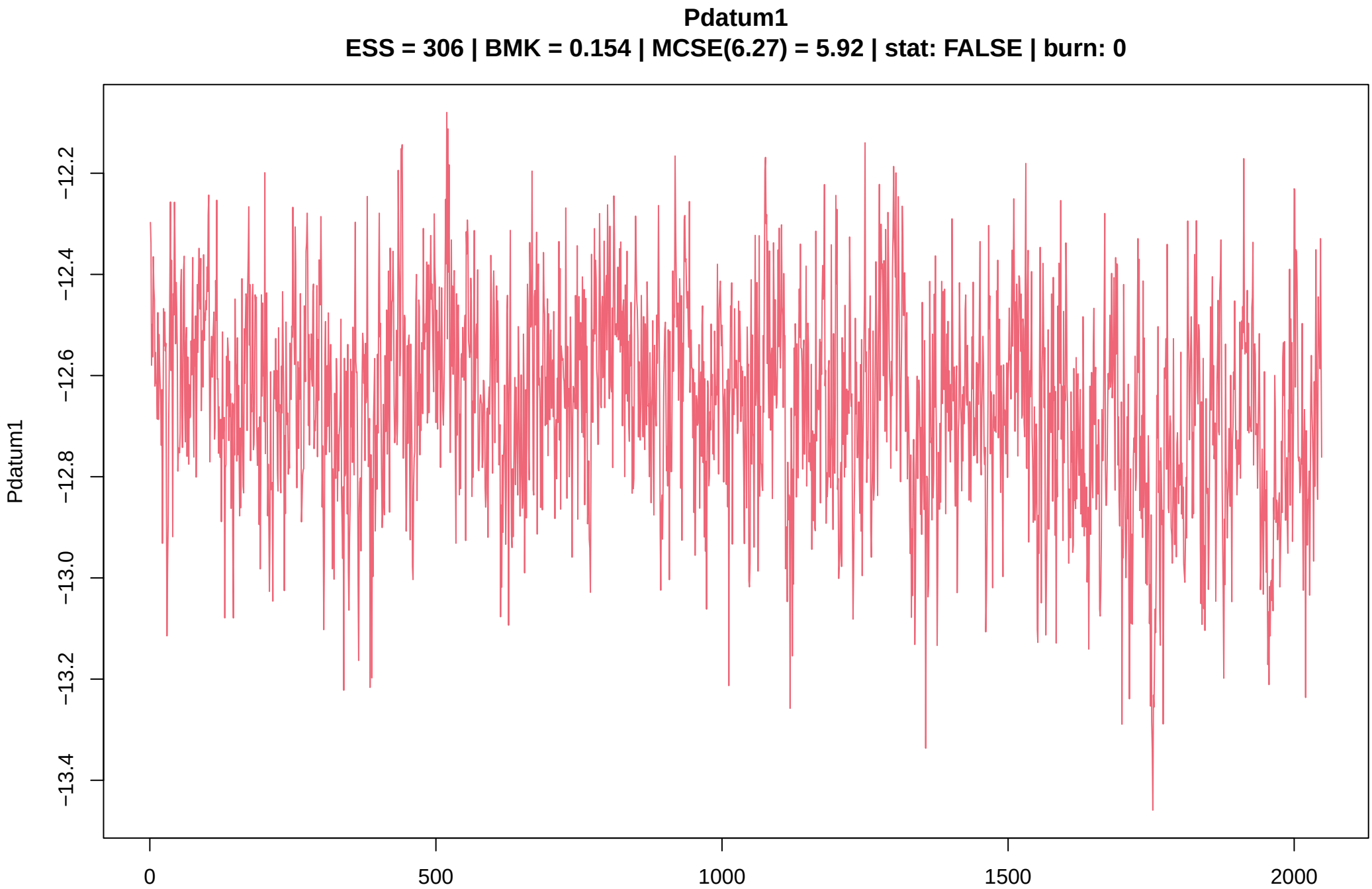

mcs_NumHeteroAtoms
log_RMSD

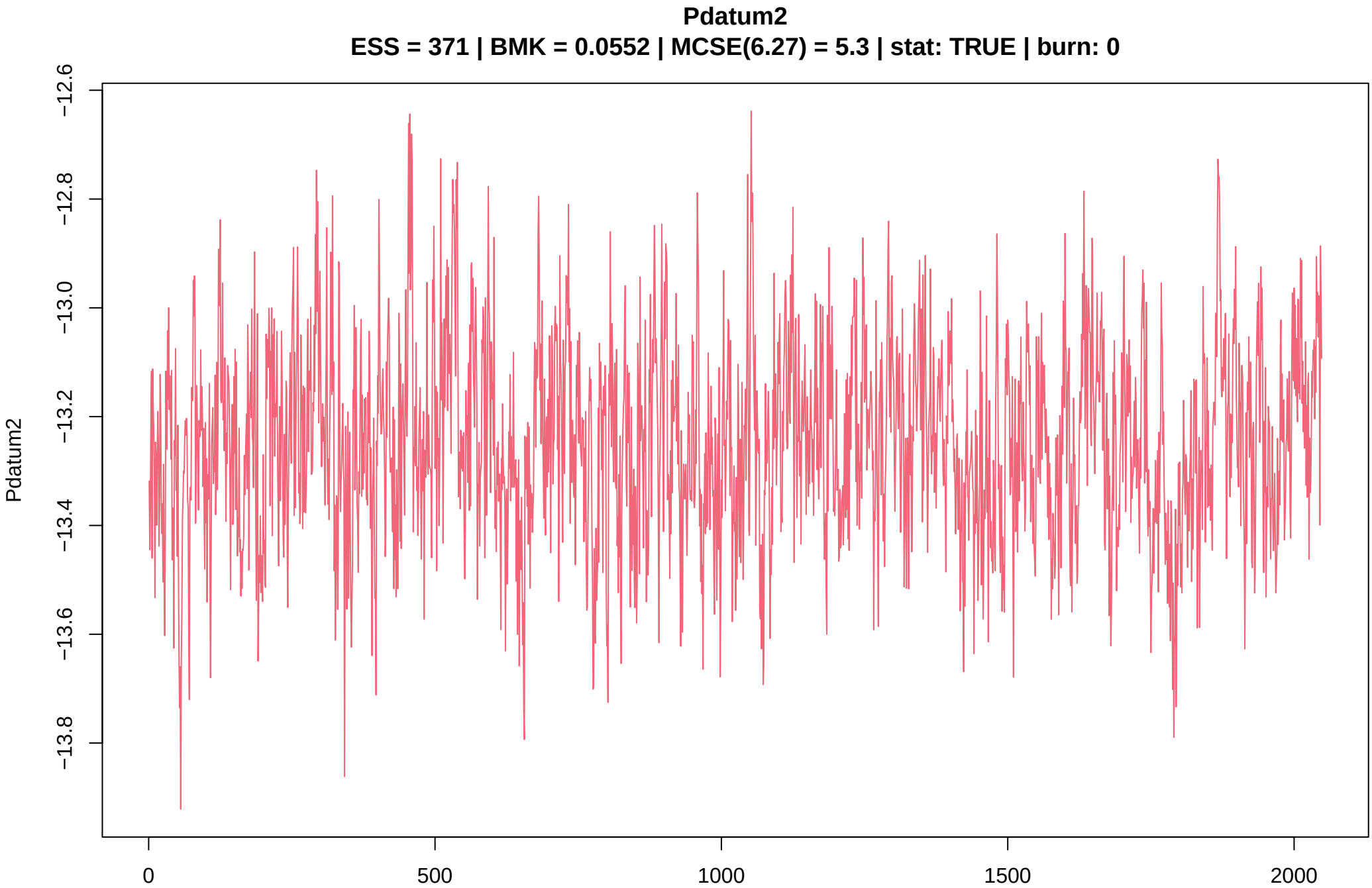

LL
ESS = 1.73 | BMK = 0.943 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 2040
LL
−112100
−112300
−112500
−112700
0
500
1000
1500
2000

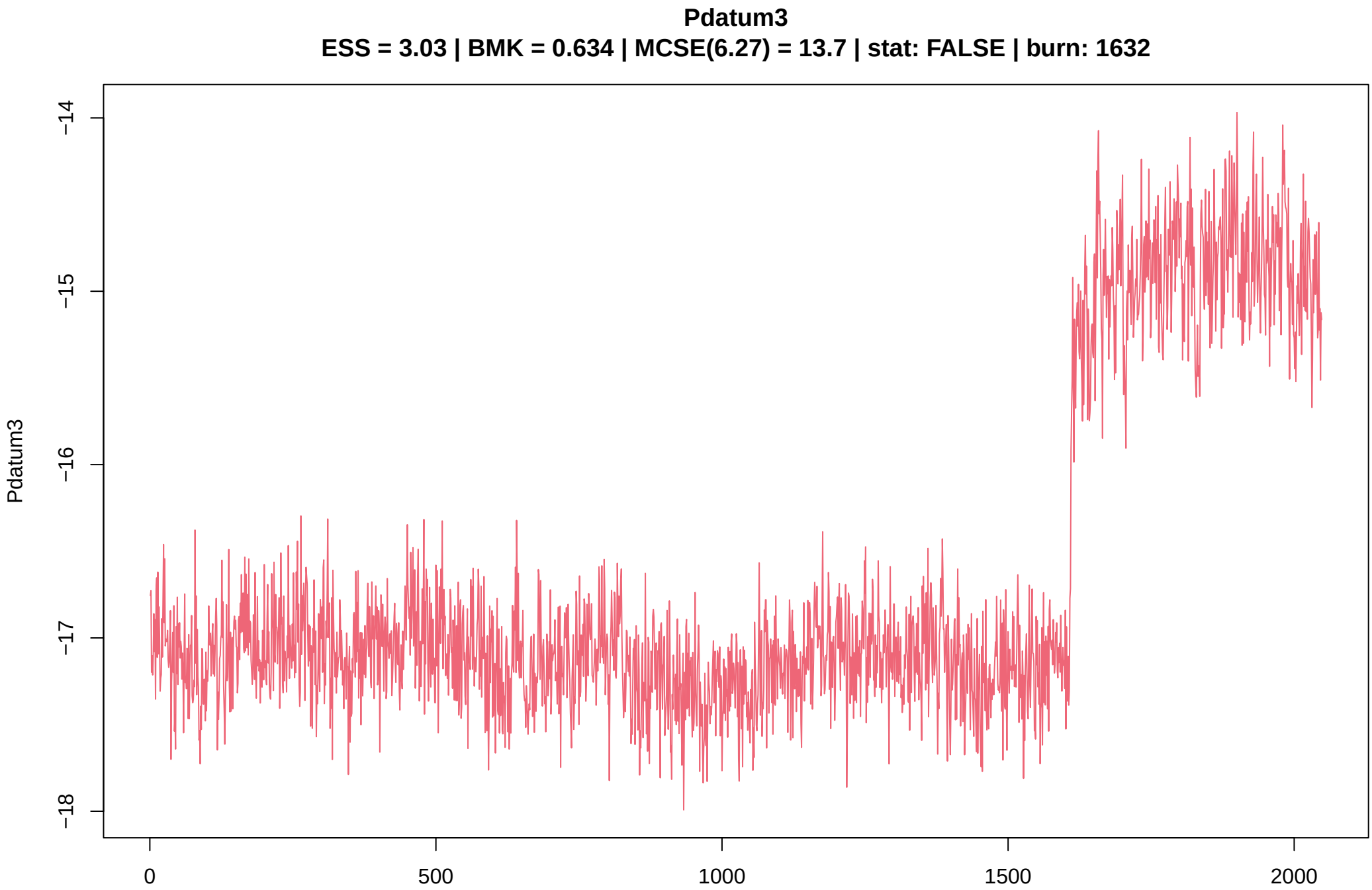

Pdatamedians
ESS = 5.57 | BMK = 0.63 | MCSE(6.27) = 13.6 | stat: FALSE | burn: 1632
Pdatamedians
−12.0
−12.2
−12.4
−12.6
−12.8
−13.0
0
500
1000
1500
2000

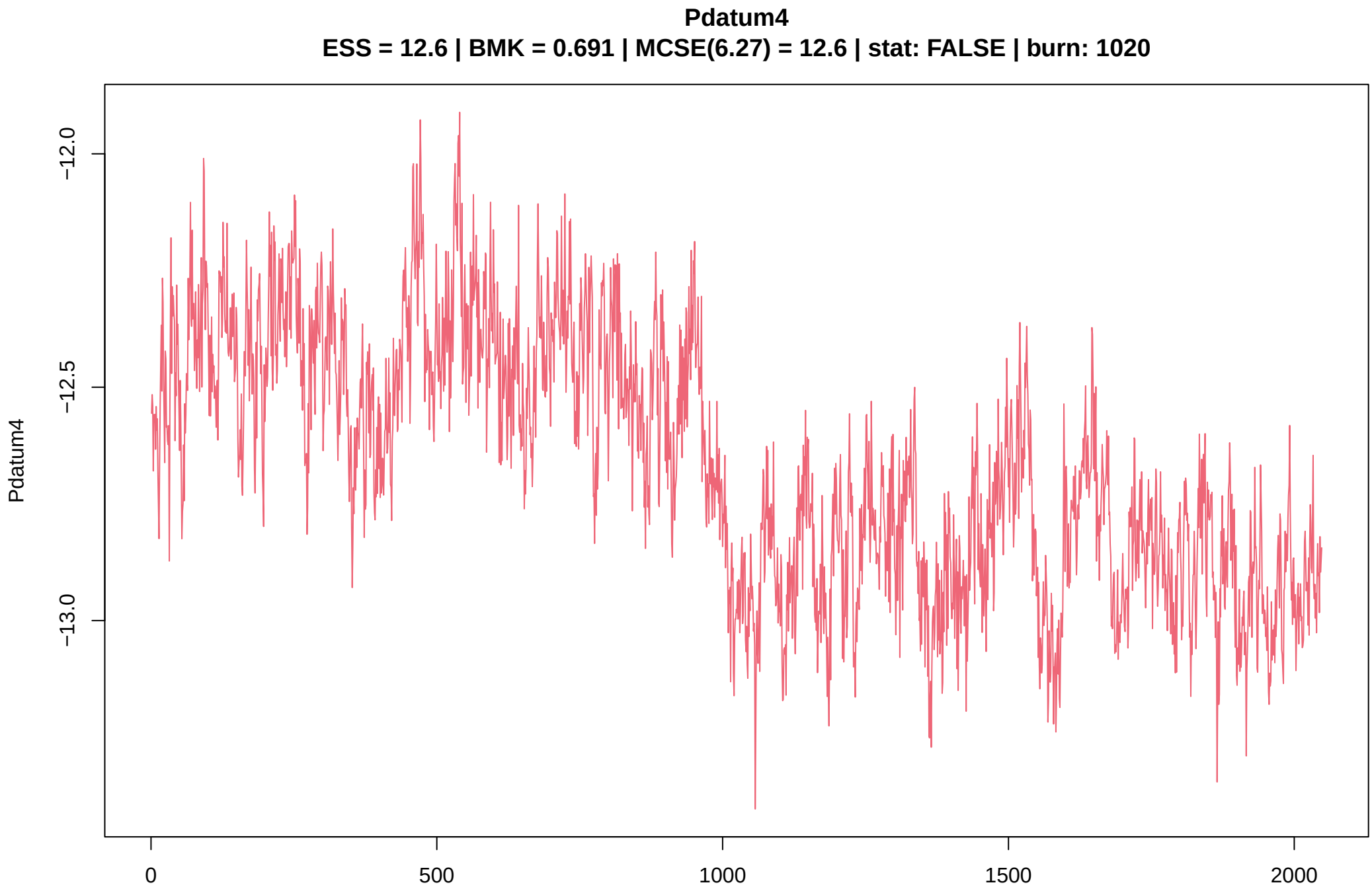

PdatacornerHi
ESS = 115 | BMK = 0.234 | MCSE(6.27) = 6.88 | stat: FALSE | burn: 0
PdatacornerHi
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
500
1000
1500
2000

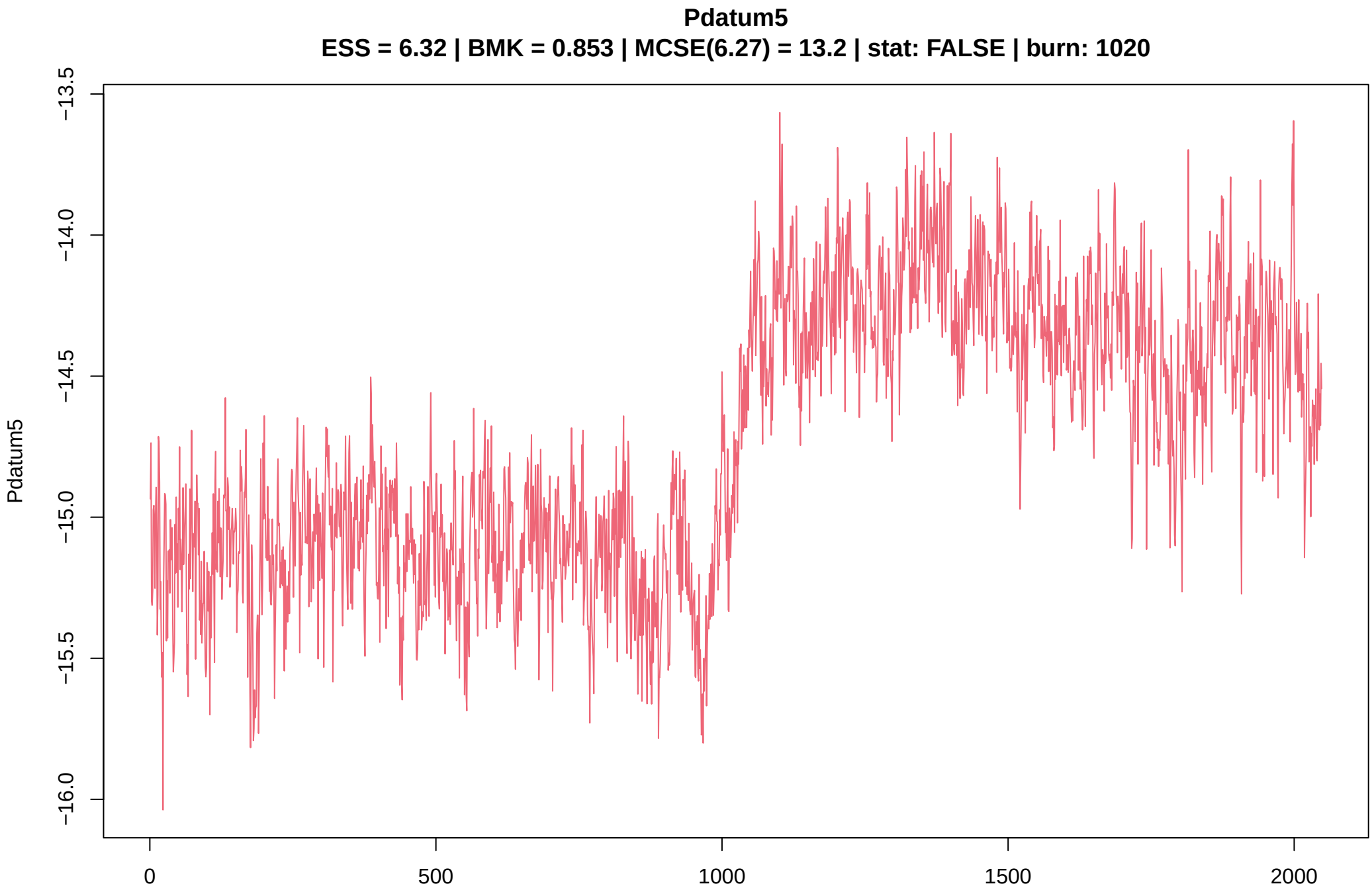

PdatacornerLo
ESS = 587 | BMK = 0.123 | MCSE(6.27) = 4.7 | stat: FALSE | burn: 0
PdatacornerLo
−13.0
−13.5
−14.0
−14.5
0
500
1000
1500
2000

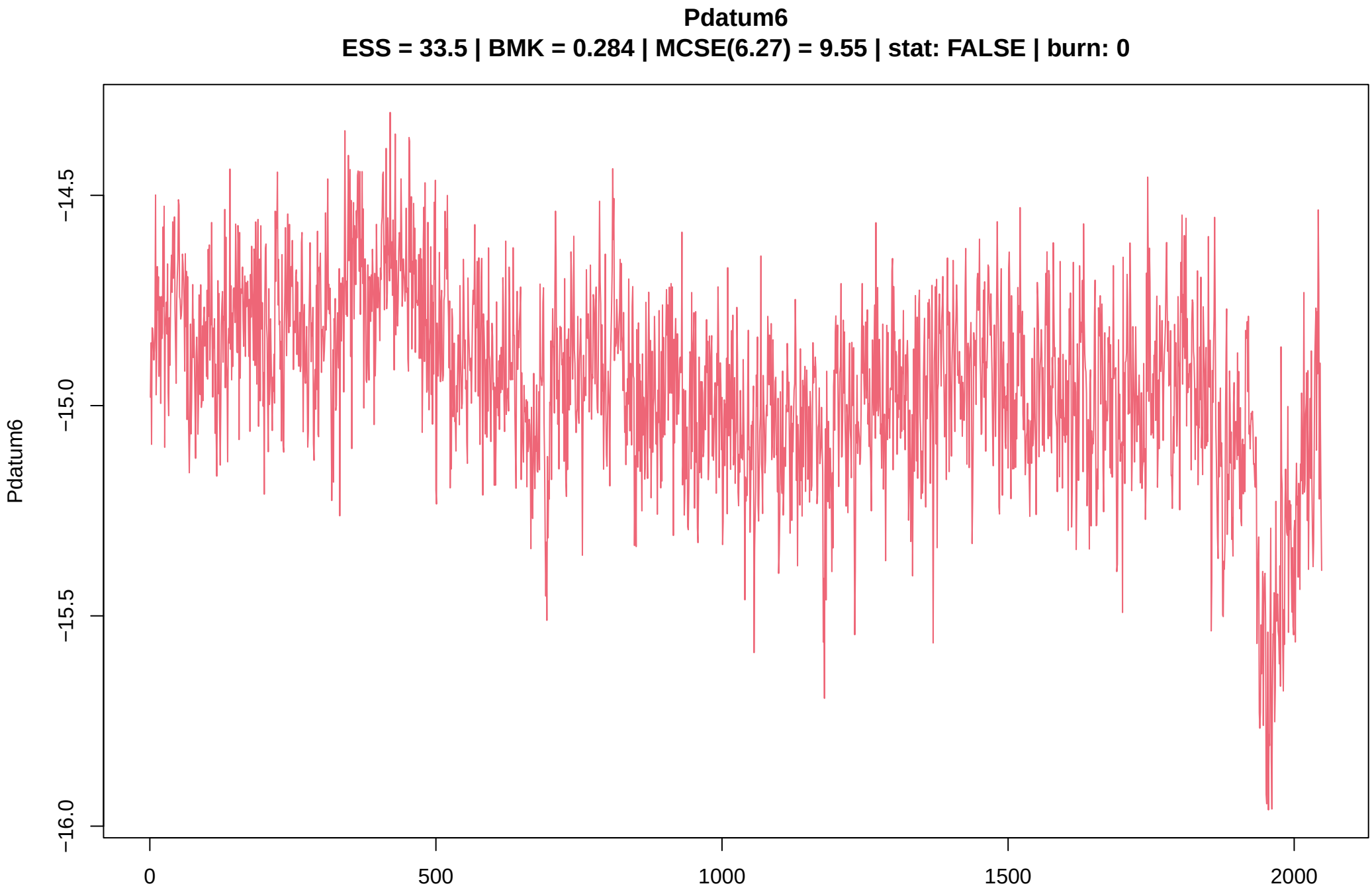

Pdatum1
ESS = 306 | BMK = 0.154 | MCSE(6.27) = 5.92 | stat: FALSE | burn: 0
Pdatum1
−12.2
−12.4
−12.6
−12.8
−13.0
−13.2
−13.4
0
500
1000
1500
2000

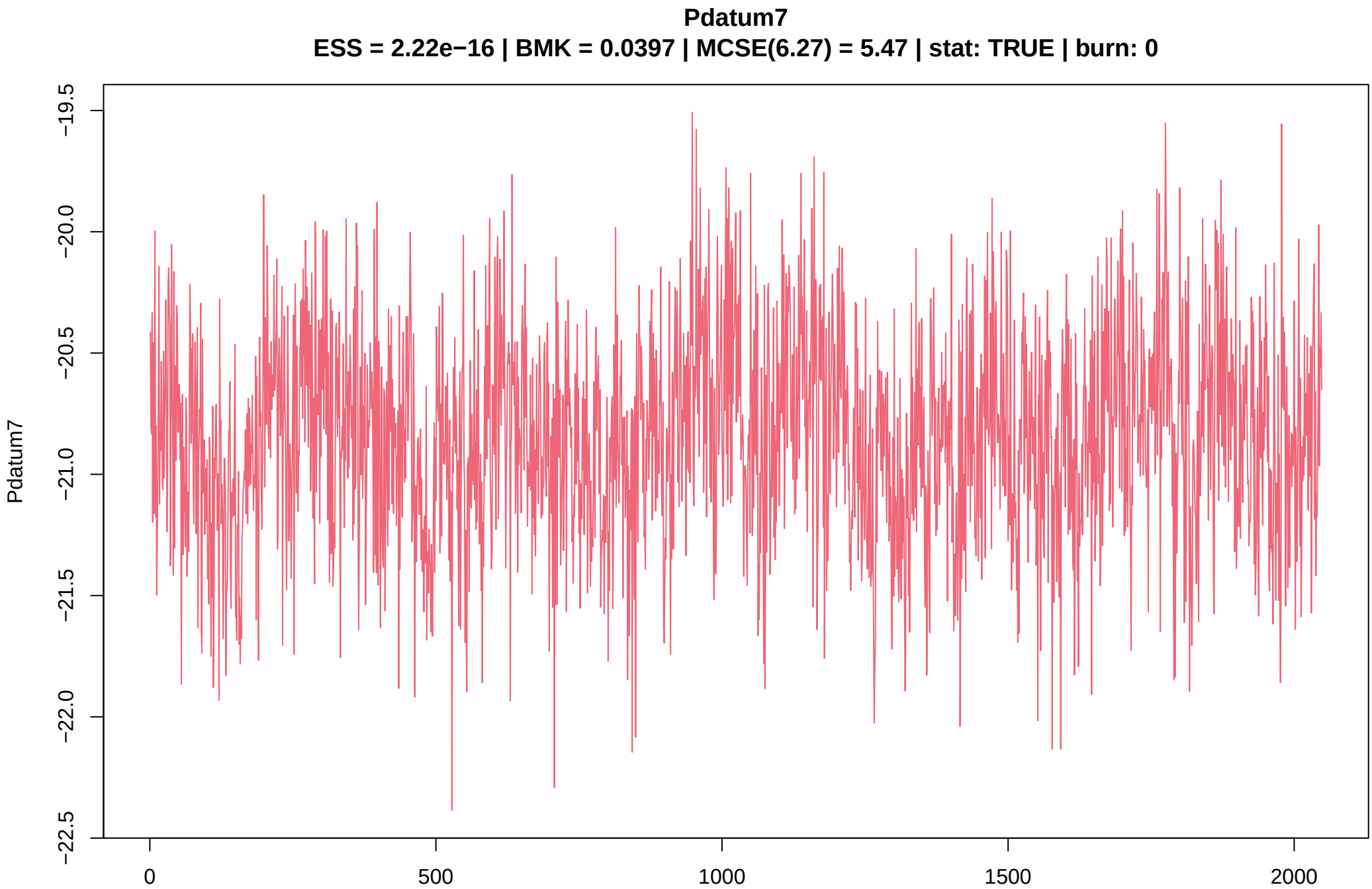

Pdatum2
ESS = 371 | BMK = 0.0552 | MCSE(6.27) = 5.3 | stat: TRUE | burn: 0
Pdatum2
−12.6
−12.8
−13.0
−13.2
−13.4
−13.6
−13.8
0
500
1000
1500
2000

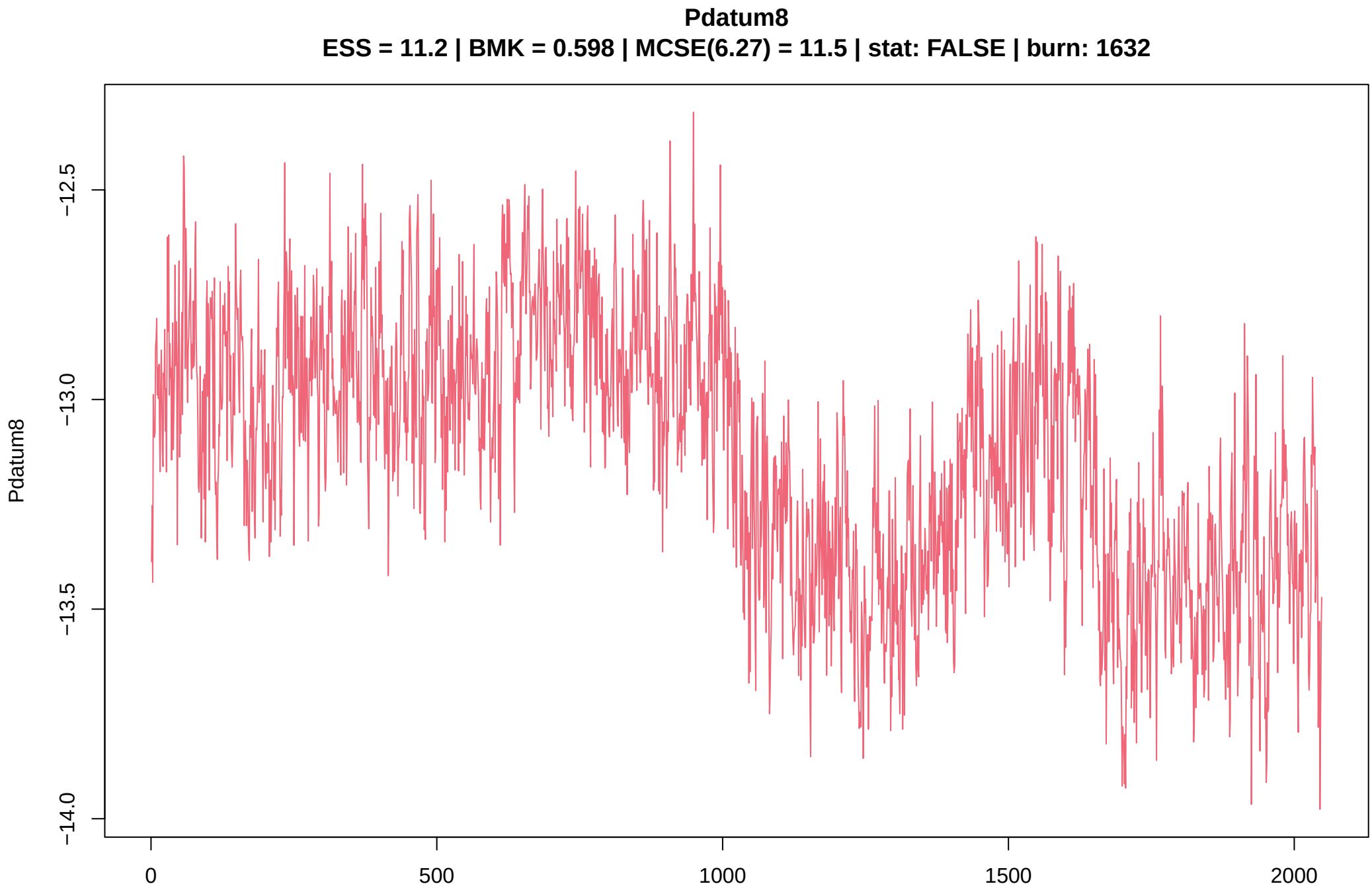

Pdatum3
ESS = 3.03 | BMK = 0.634 | MCSE(6.27) = 13.7 | stat: FALSE | burn: 1632
Pdatum3
−14
−15
−16
−17
−18
0
500
1000
1500
2000

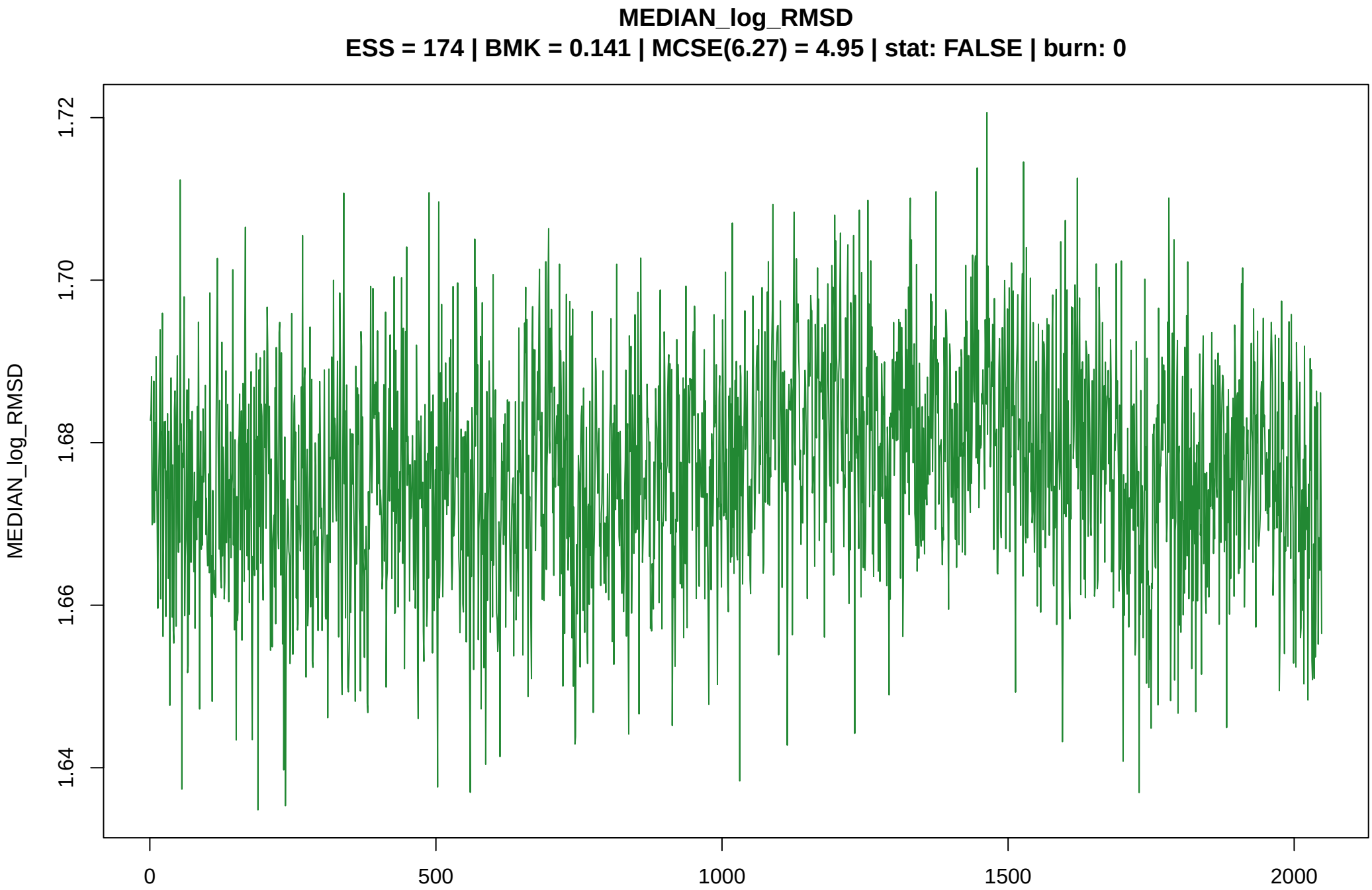

Pdatum4
ESS = 12.6 | BMK = 0.691 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 1020
Pdatum4
−12.0
−12.5
−13.0
0
500
1000
1500
2000

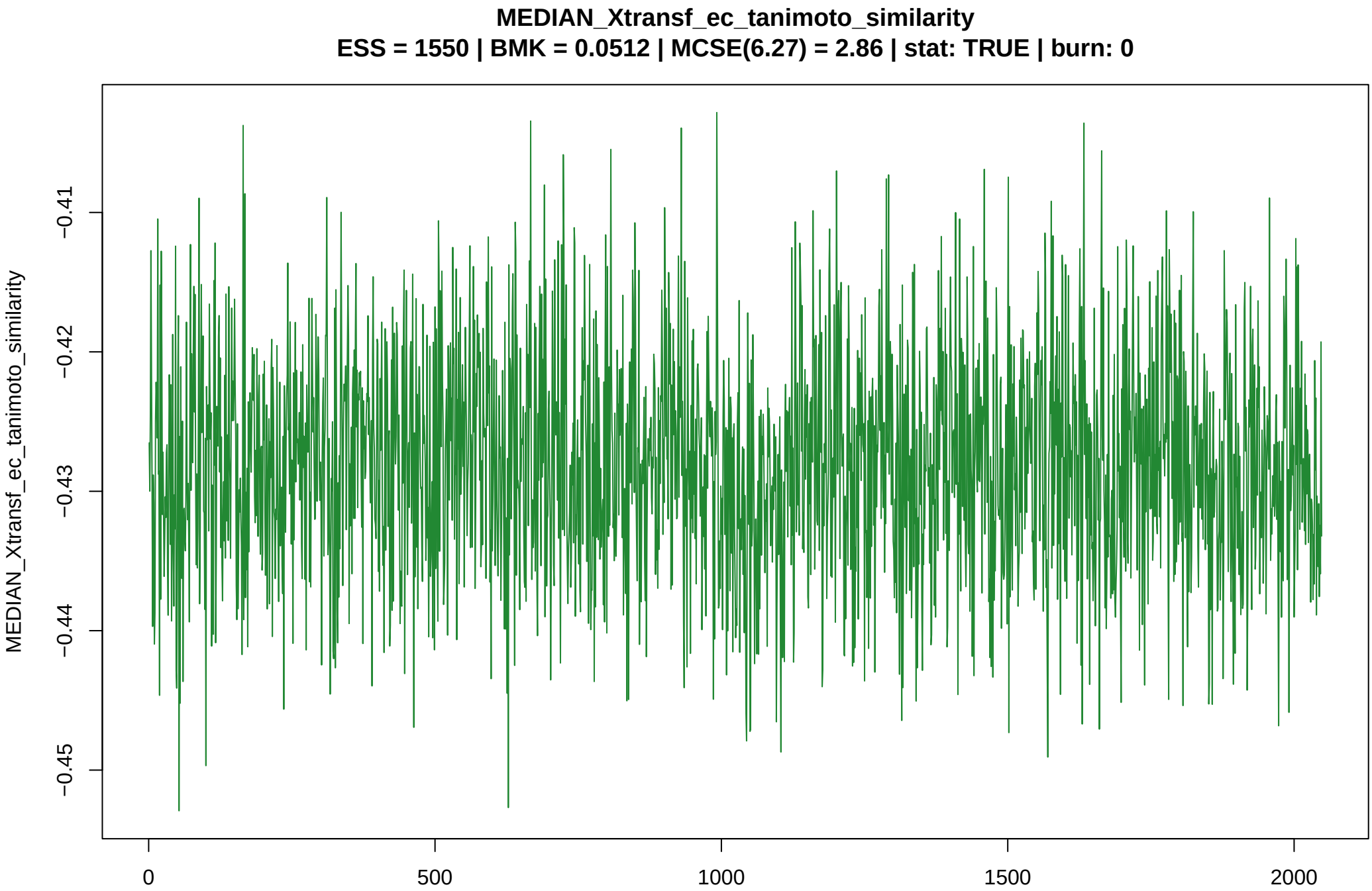

Pdatum5
ESS = 6.32 | BMK = 0.853 | MCSE(6.27) = 13.2 | stat: FALSE | burn: 1020
Pdatum5
−13.5
−14.0
−14.5
−15.0
−15.5
−16.0
0
500
1000
1500
2000

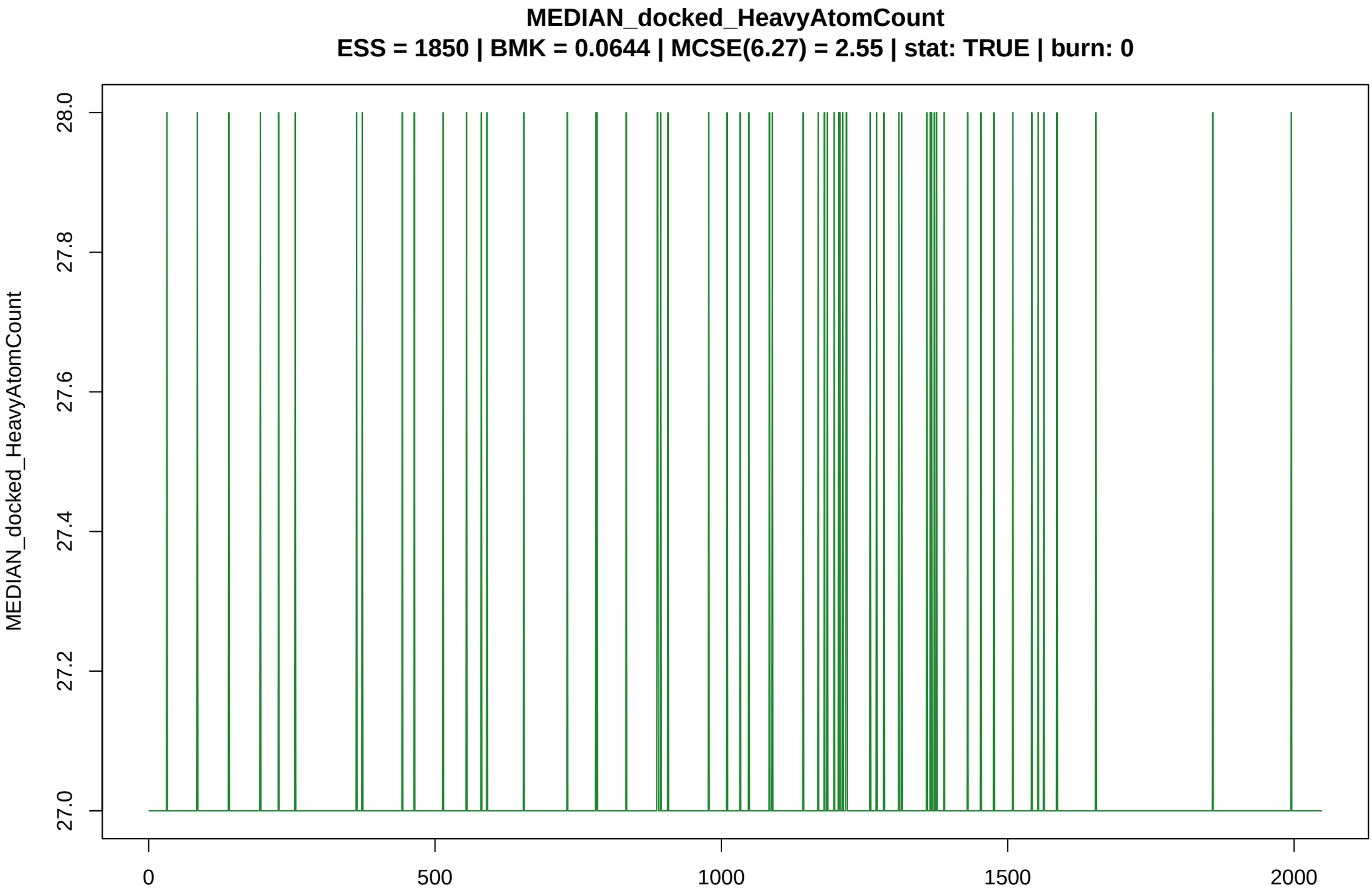

Pdatum6
ESS = 33.5 | BMK = 0.284 | MCSE(6.27) = 9.55 | stat: FALSE | burn: 0
Pdatum6
−14.5
−15.0
−15.5
−16.0
0
500
1000
1500
2000

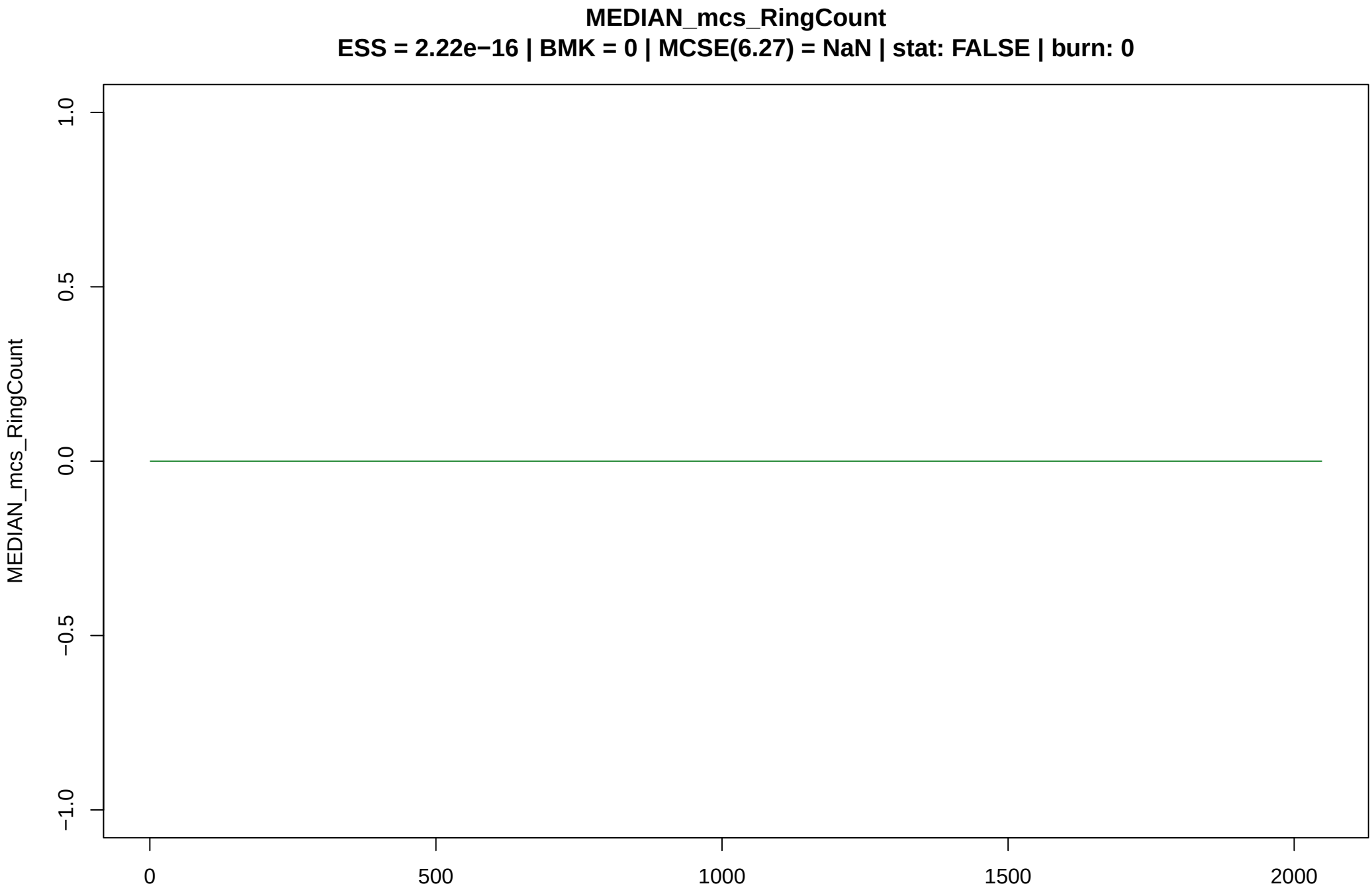

Pdatum7
ESS = 2.22e−16 | BMK = 0.0397 | MCSE(6.27) = 5.47 | stat: TRUE | burn: 0
Pdatum7
−19.5
−20.0
−20.5
−21.0
−21.5
−22.0
−22.5
0
500
1000
1500
2000

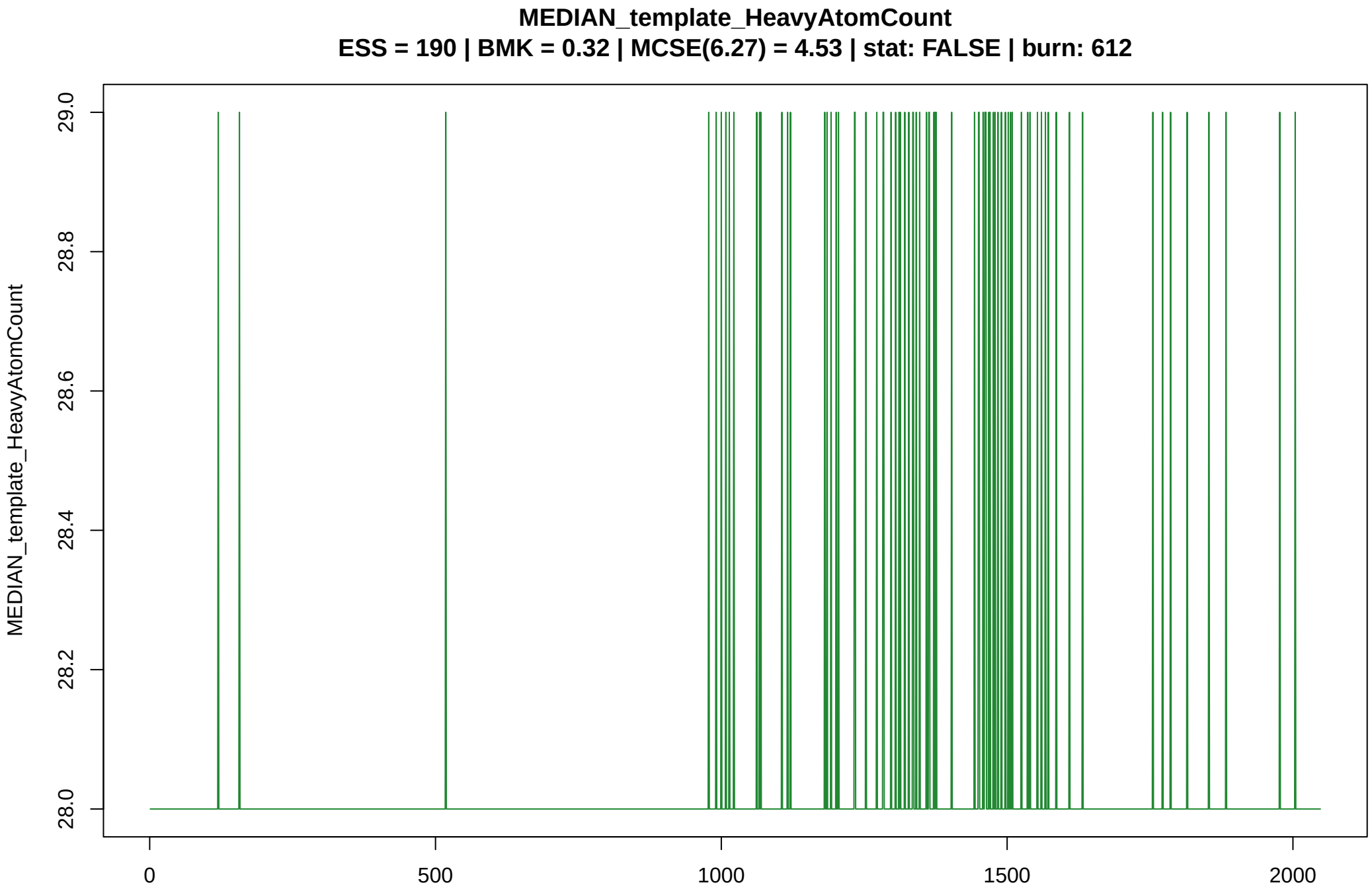

Pdatum8
ESS = 11.2 | BMK = 0.598 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 1632
Pdatum8
−12.5
−13.0
−13.5
−14.0
0
500
1000
1500
2000

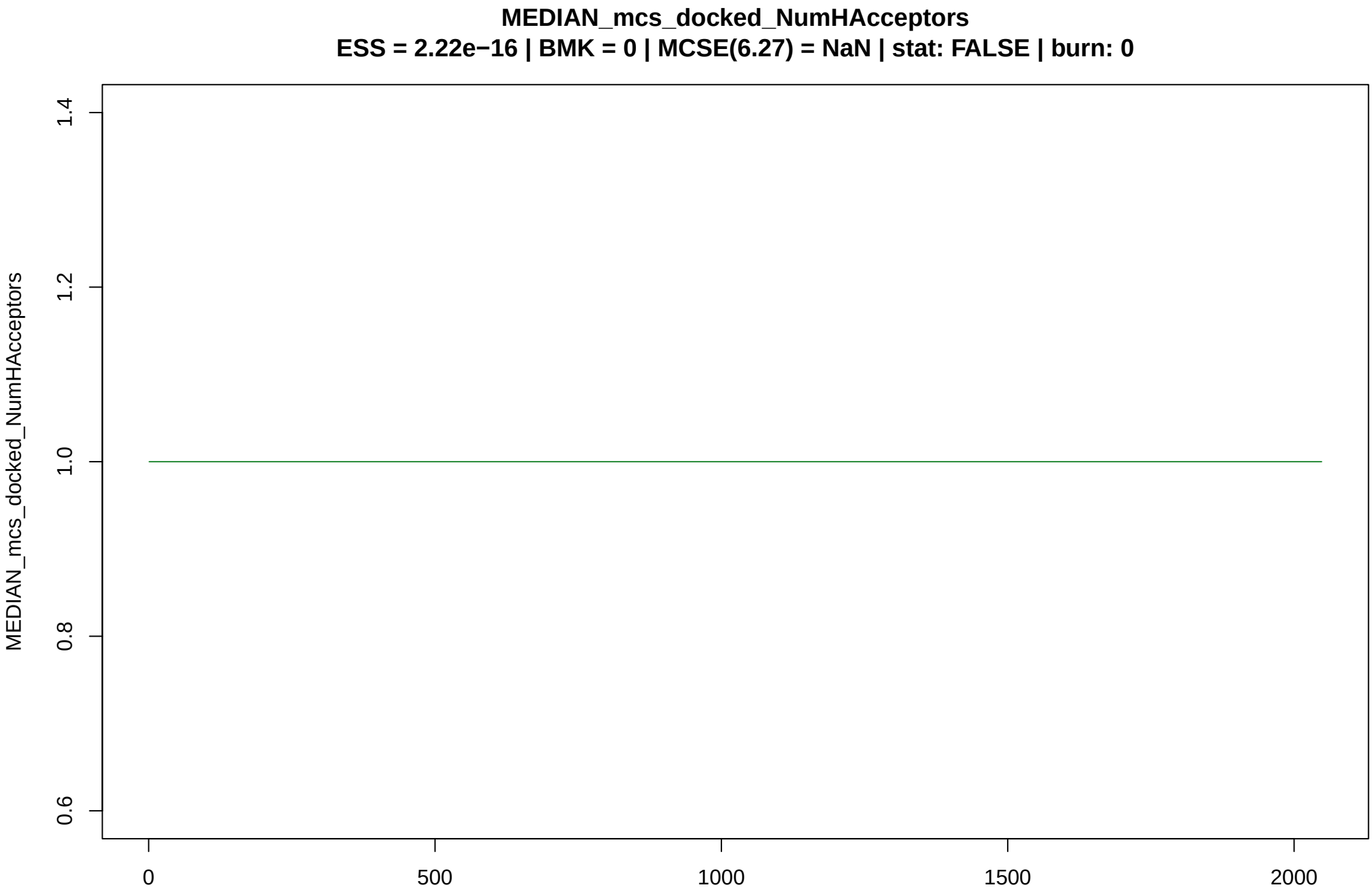

MEDIAN_log_RMSD
ESS = 174 | BMK = 0.141 | MCSE(6.27) = 4.95 | stat: FALSE | burn: 0
MEDIAN_log_RMSD
1.64
1.66
1.68
1.70
1.72
0
500
1000
1500
2000

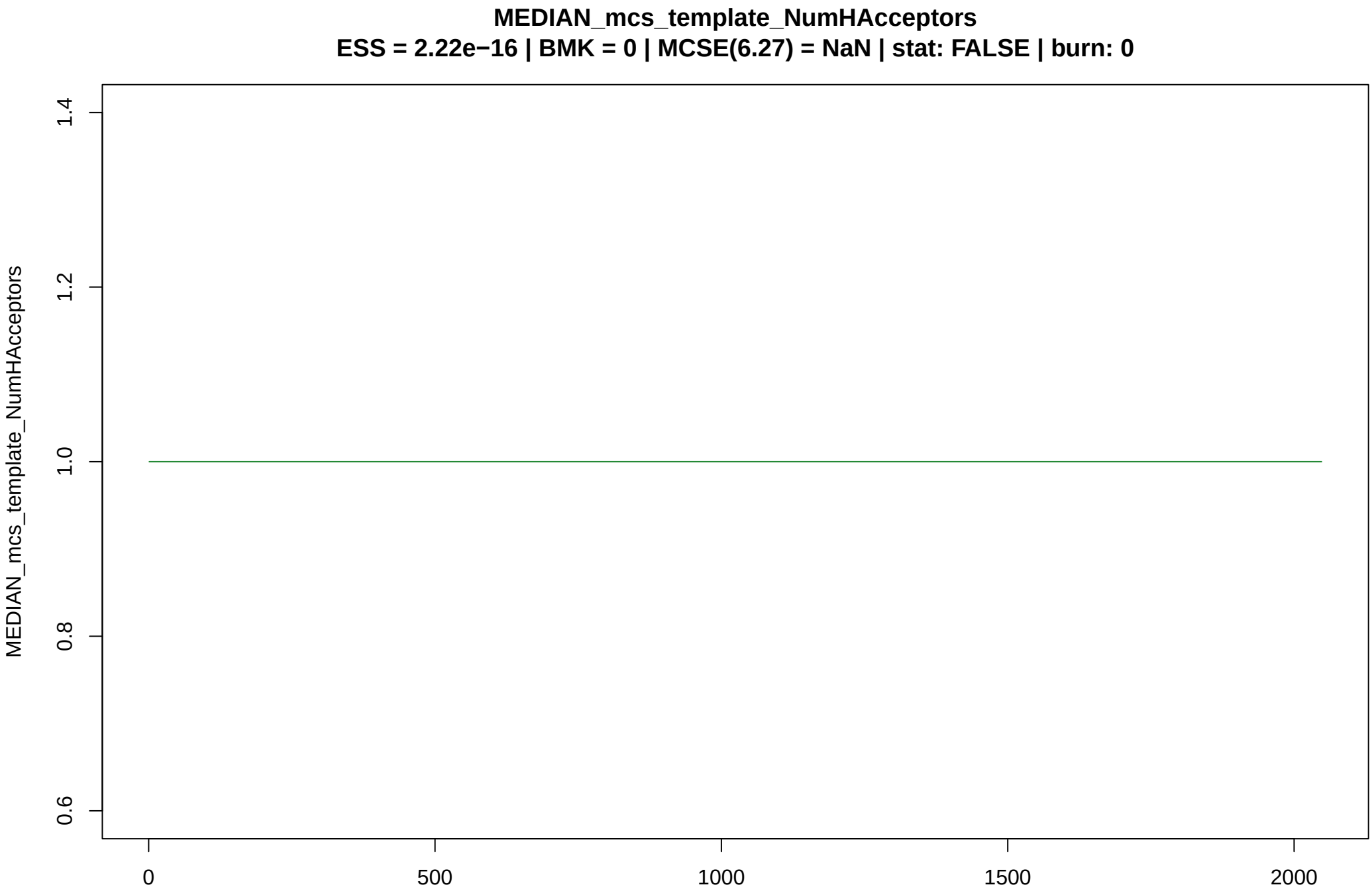

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1550 | BMK = 0.0512 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.41
−0.42
−0.43
−0.44
−0.45
0
500
1000
1500
2000

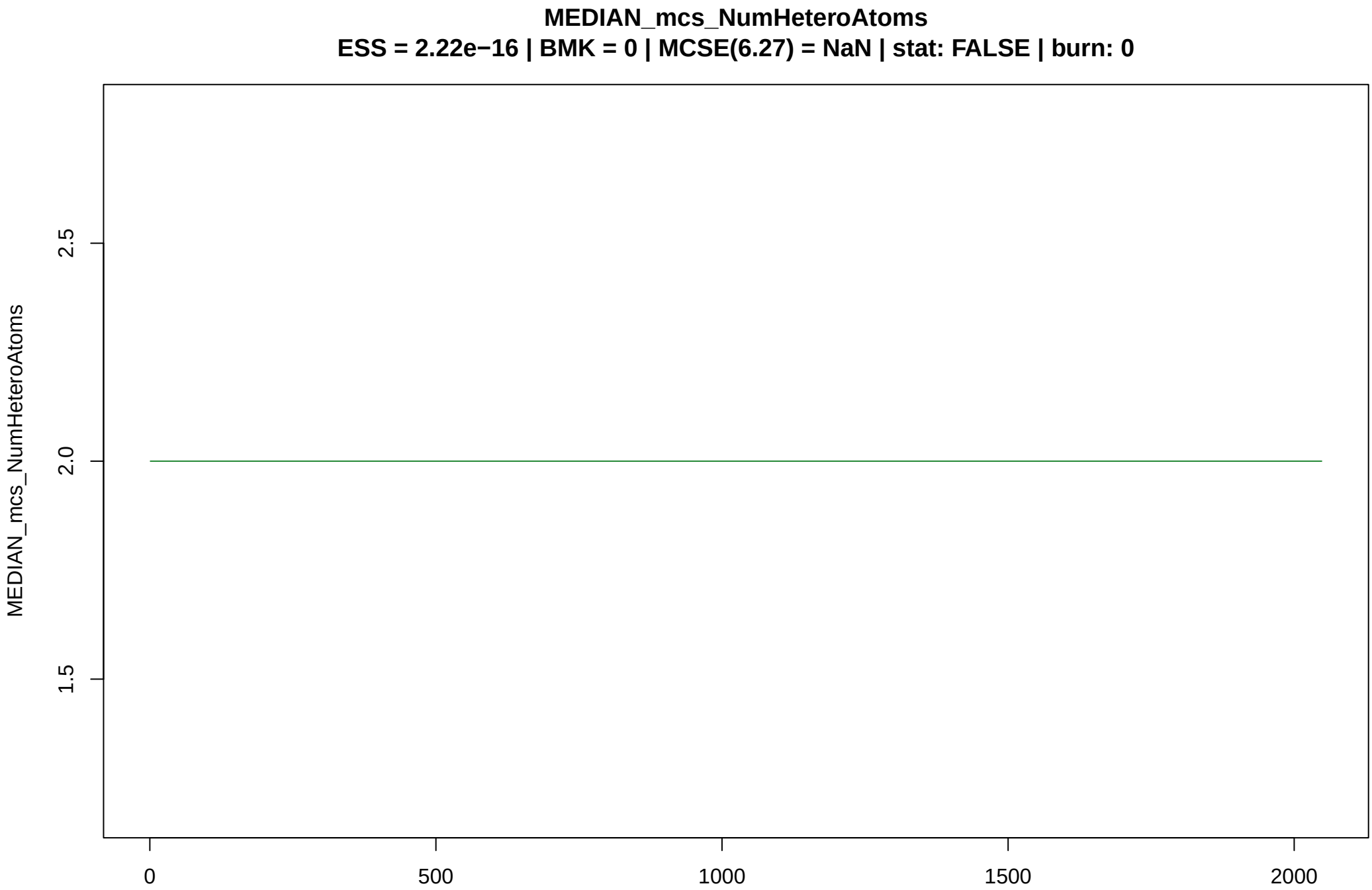

MEDIAN_docked_HeavyAtomCount
ESS = 1850 | BMK = 0.0644 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0
MEDIAN_docked_HeavyAtomCount
28.0
27.8
27.6
27.4
27.2
27.0
0
500
1000
1500
2000

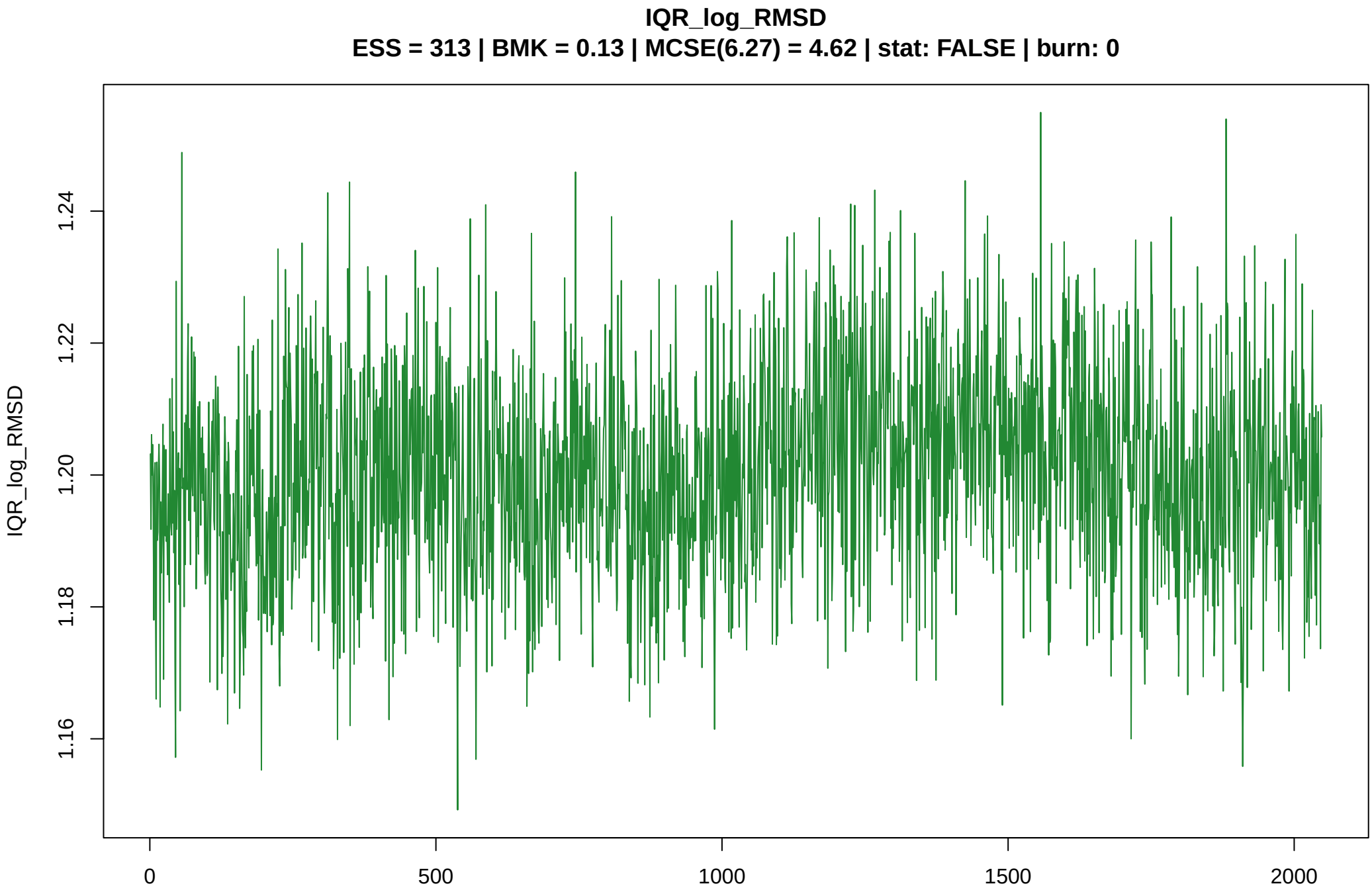

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

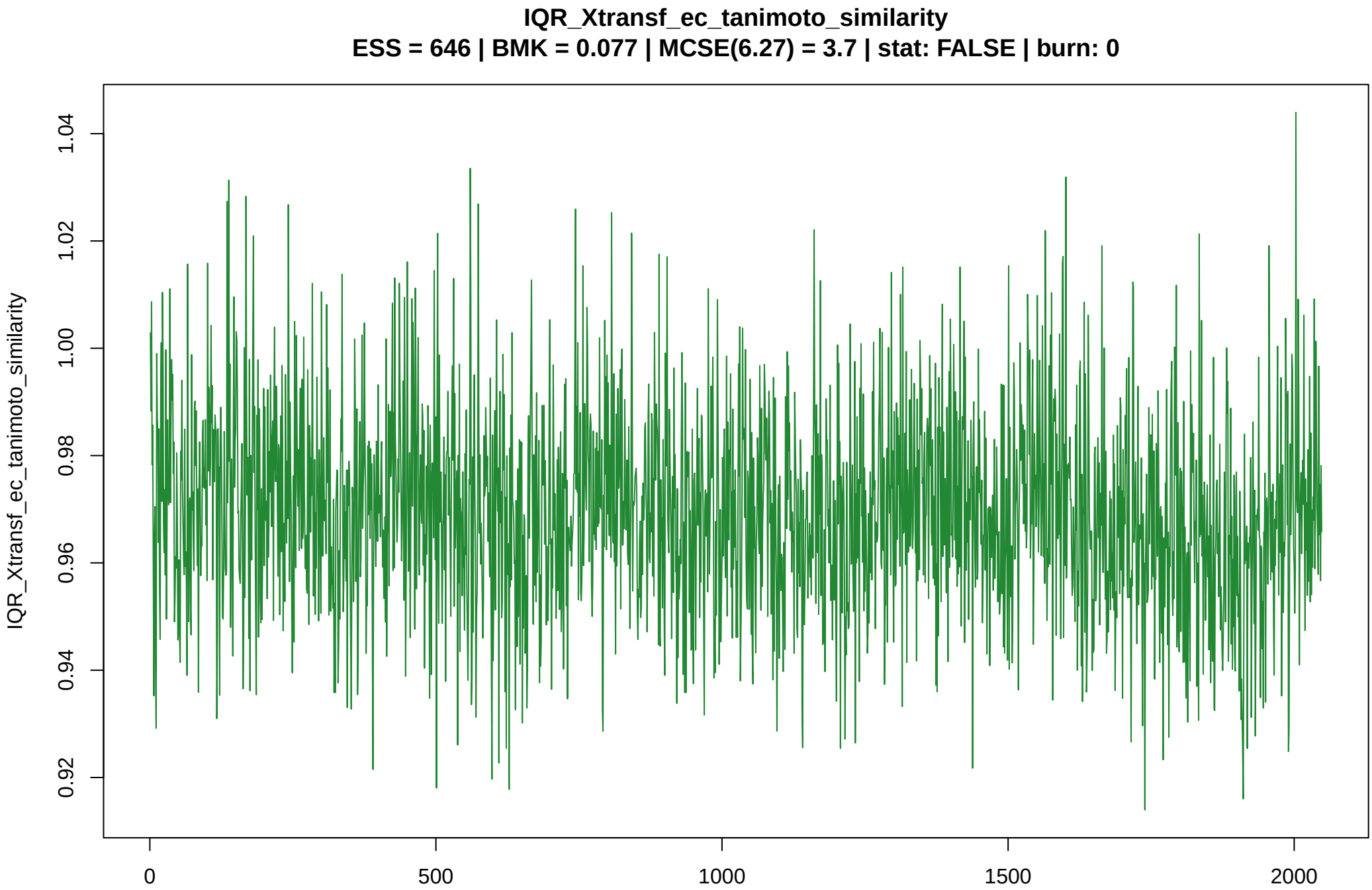

MEDIAN_template_HeavyAtomCount
ESS = 190 | BMK = 0.32 | MCSE(6.27) = 4.53 | stat: FALSE | burn: 612
MEDIAN_template_HeavyAtomCount
29.0
28.8
28.6
28.4
28.2
28.0
0
500
1000
1500
2000

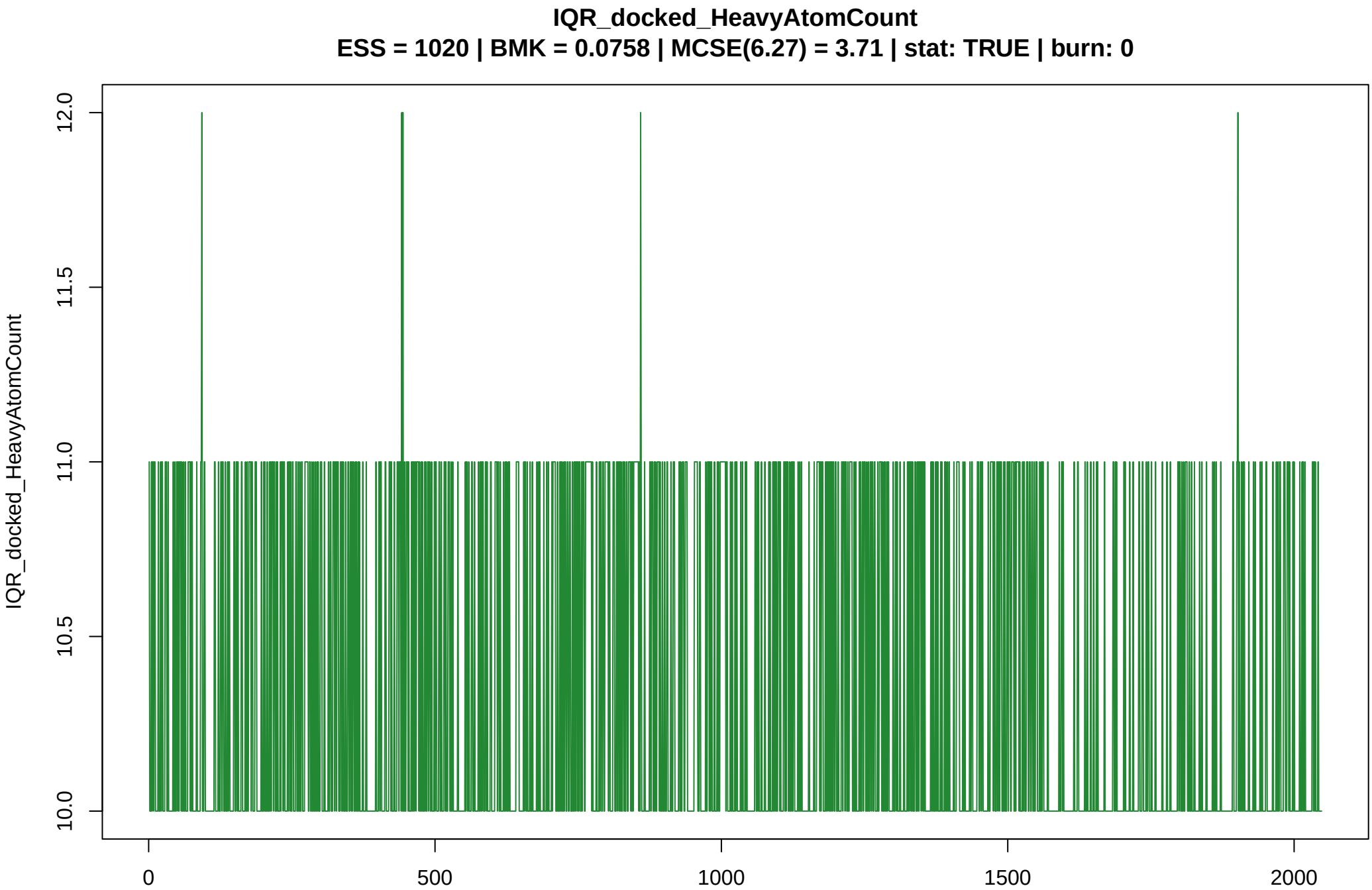

MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

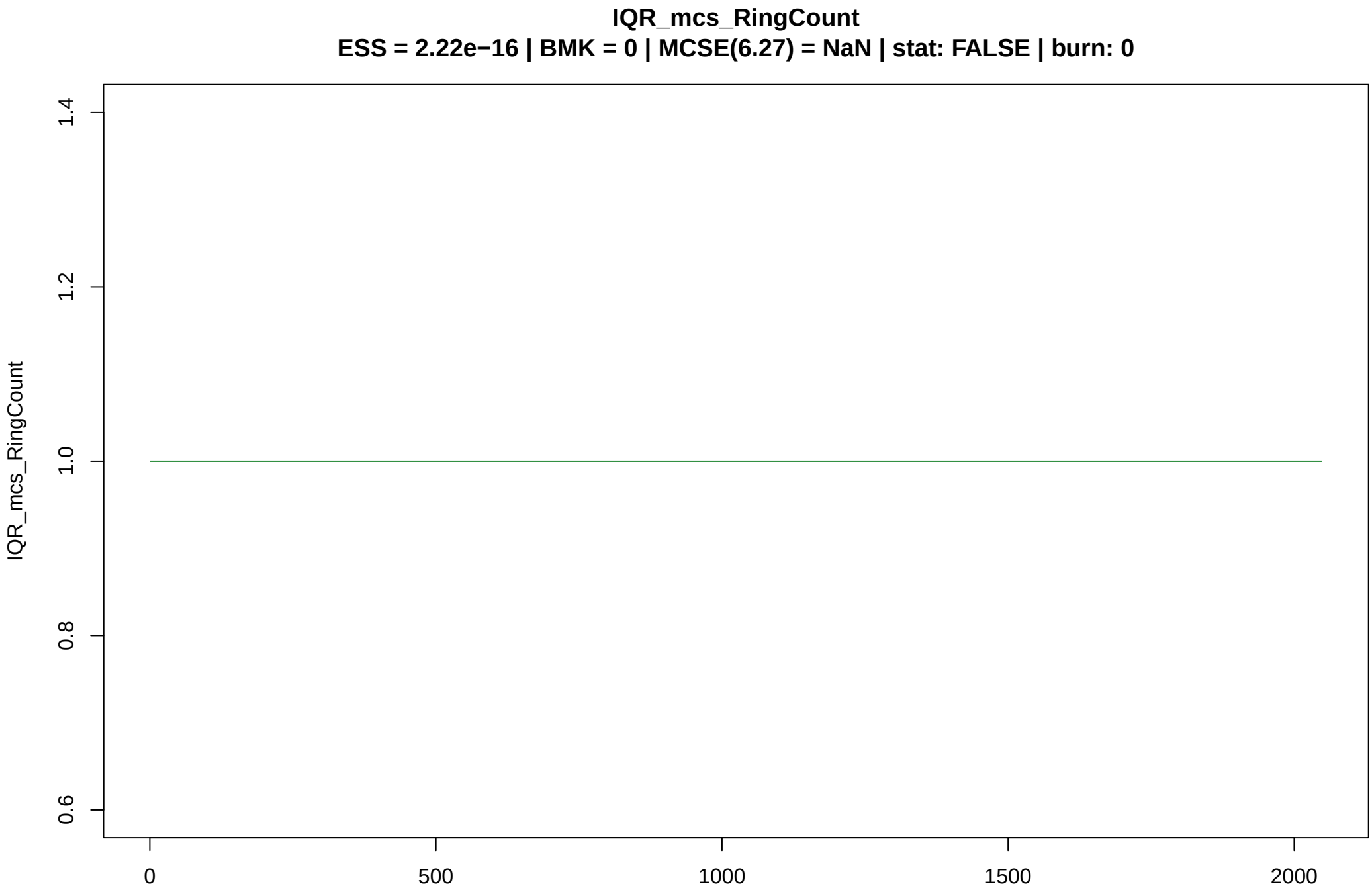

MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

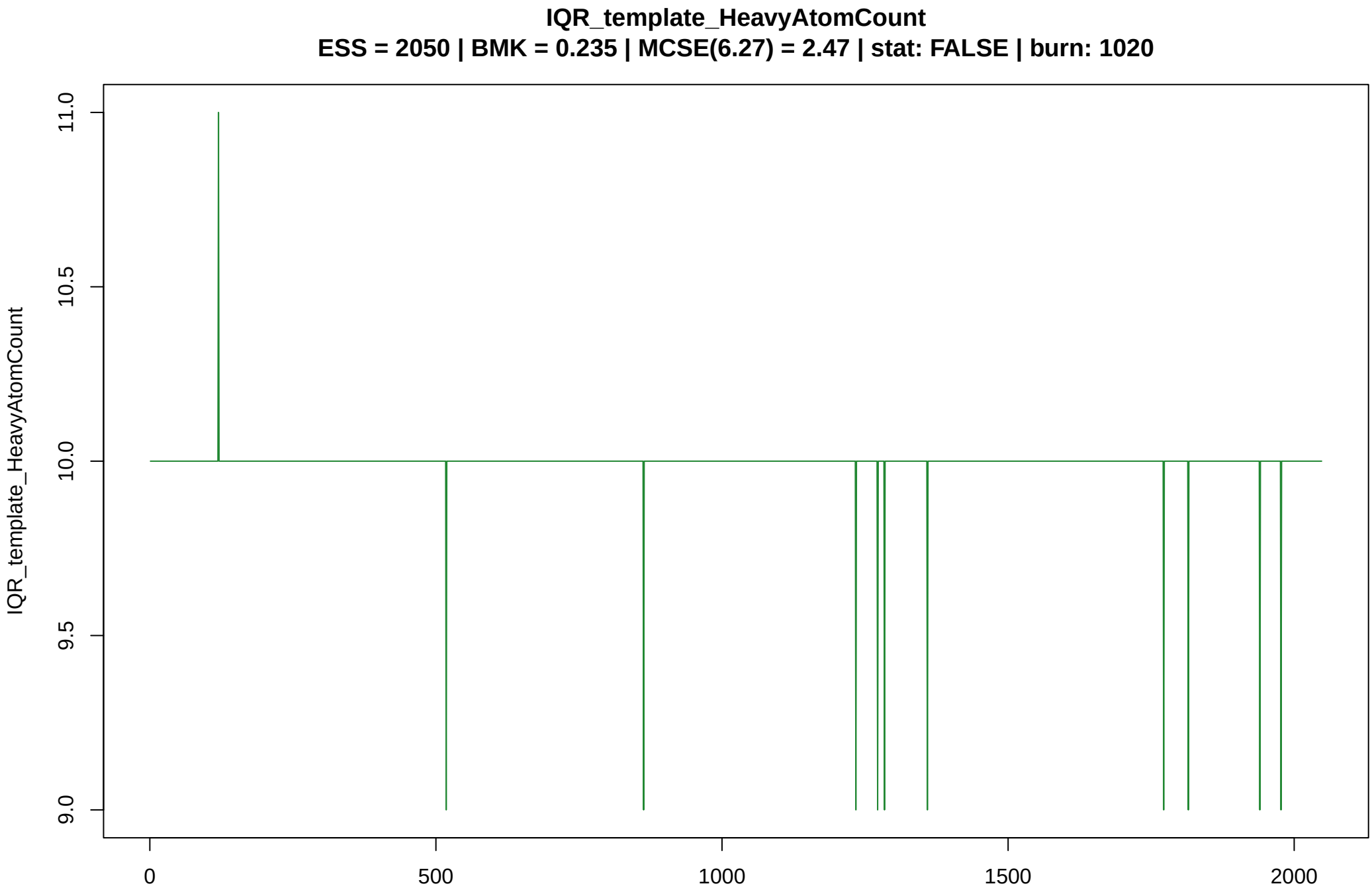

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

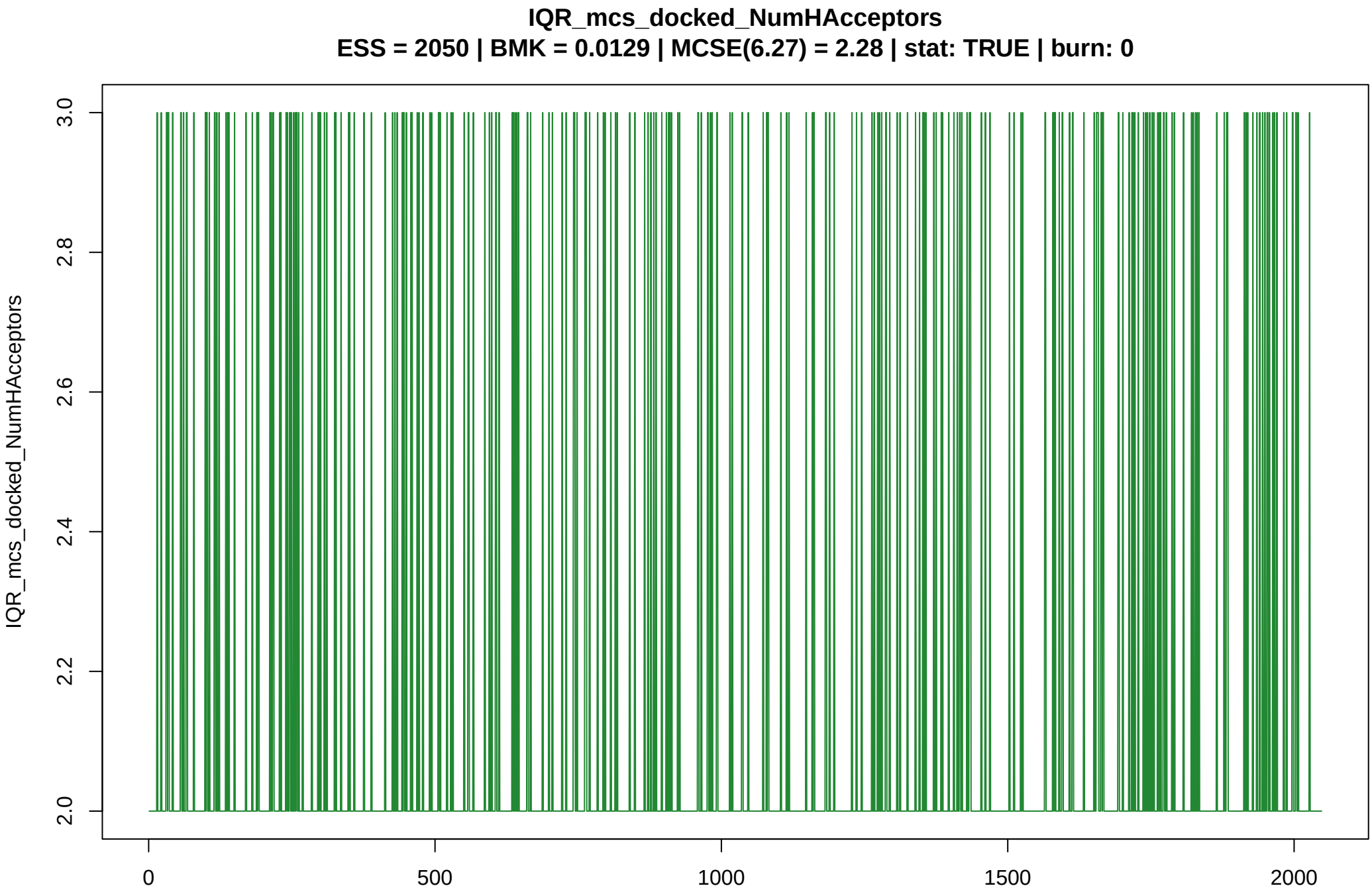

IQR_log_RMSD
ESS = 313 | BMK = 0.13 | MCSE(6.27) = 4.62 | stat: FALSE | burn: 0
IQR_log_RMSD
1.16
1.18
1.20
1.22
1.24
0
500
1000
1500
2000

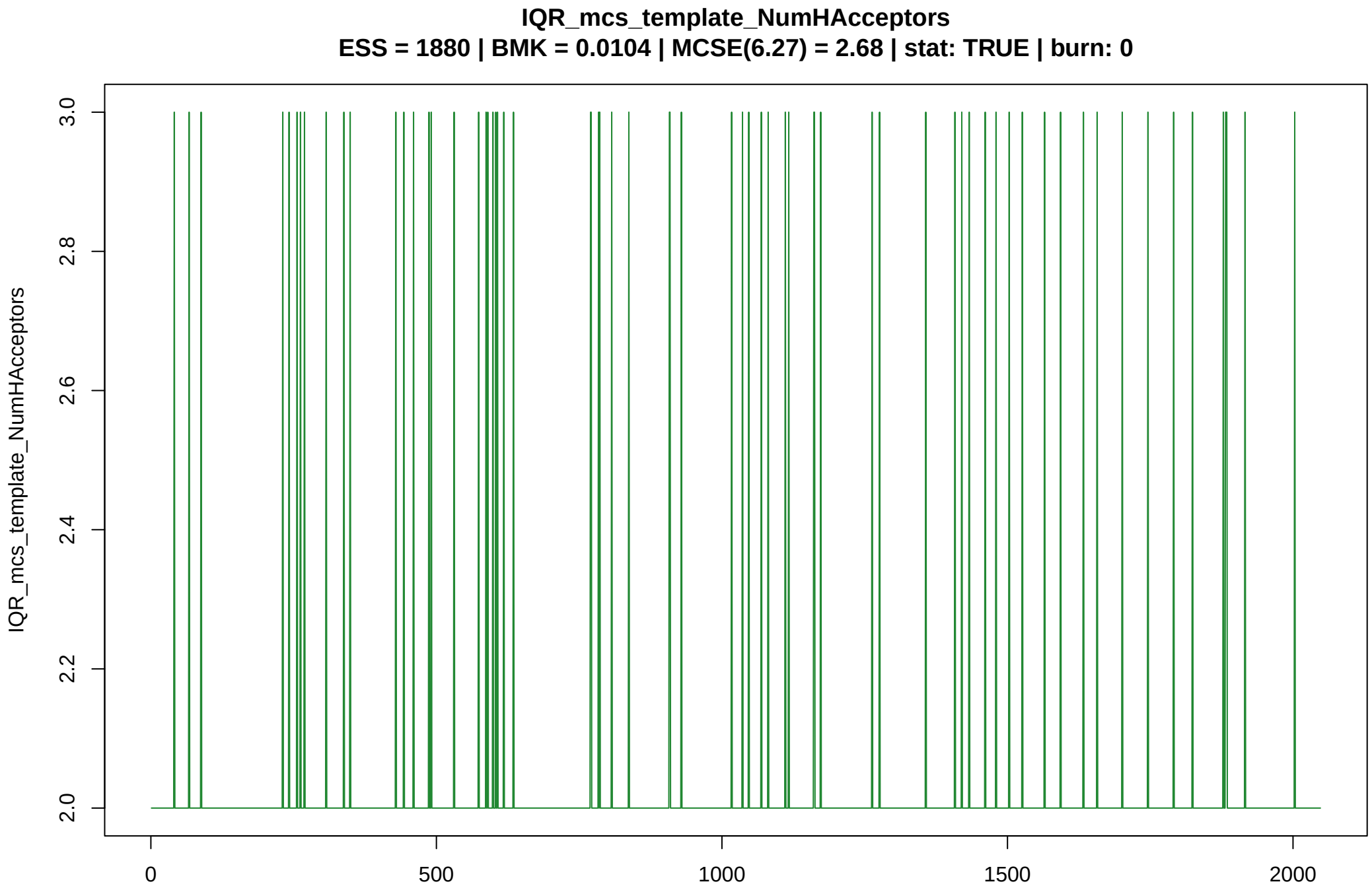

IQR_Xtransf_ec_tanimoto_similarity
ESS = 646 | BMK = 0.077 | MCSE(6.27) = 3.7 | stat: FALSE | burn: 0
IQR_Xtransf_ec_tanimoto_similarity
0.92
0.94
0.96
0.98
1.00
1.02
1.04
0
500
1000
1500
2000

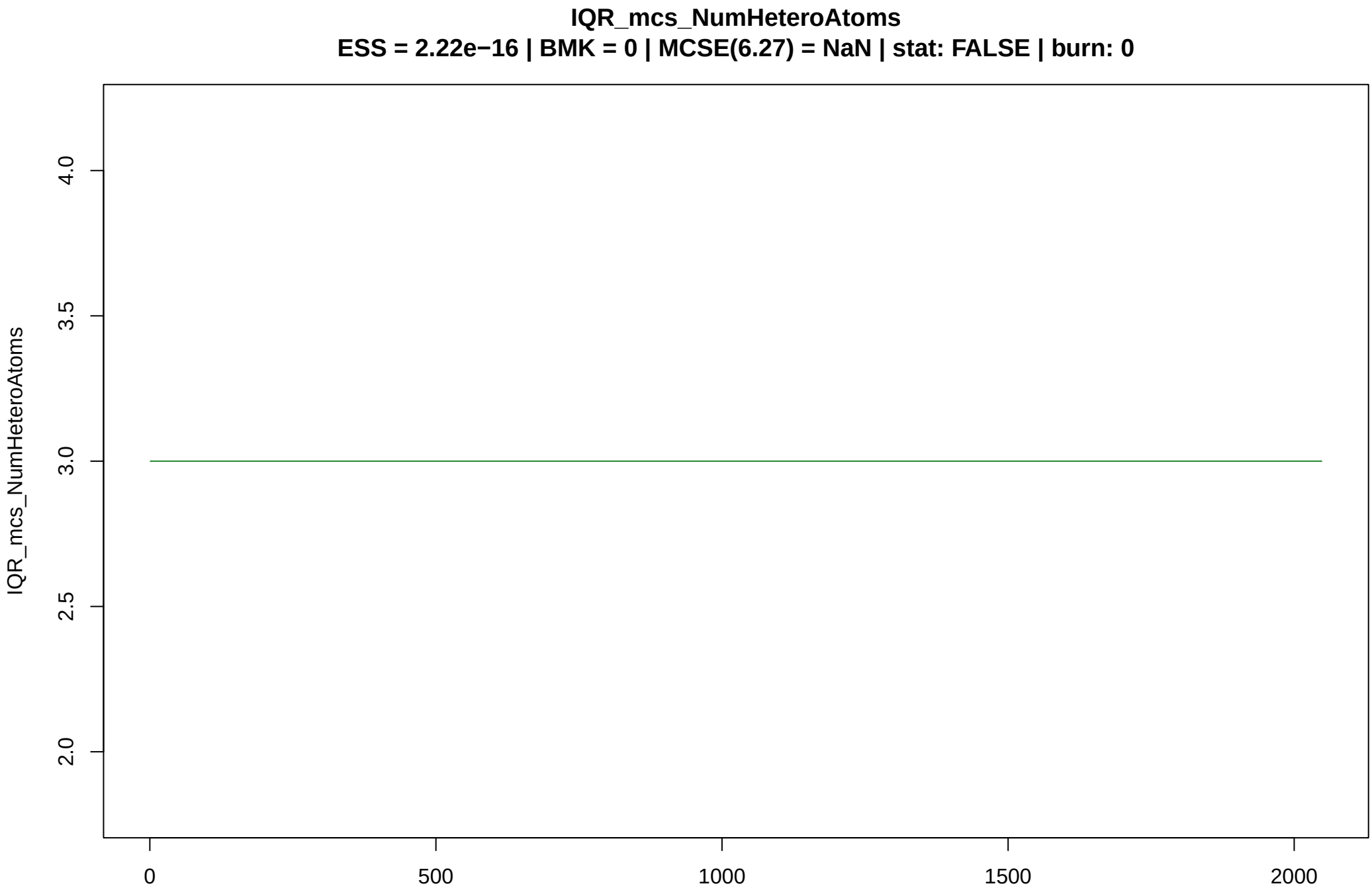

IQR_docked_HeavyAtomCount
ESS = 1020 | BMK = 0.0758 | MCSE(6.27) = 3.71 | stat: TRUE | burn: 0
IQR_docked_HeavyAtomCount
12.0
11.5
11.0
10.5
10.0
0
500
1000
1500
2000

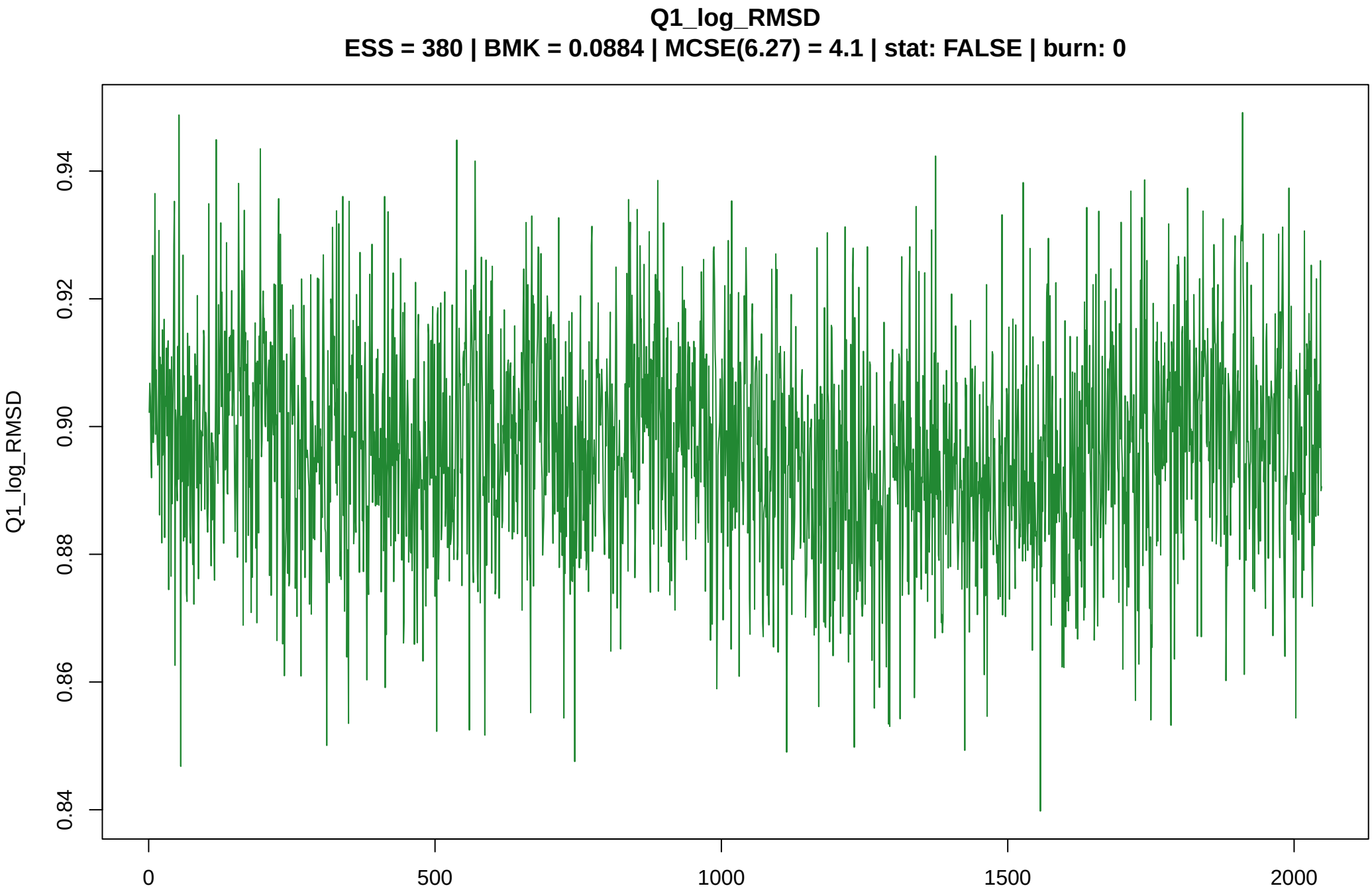

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

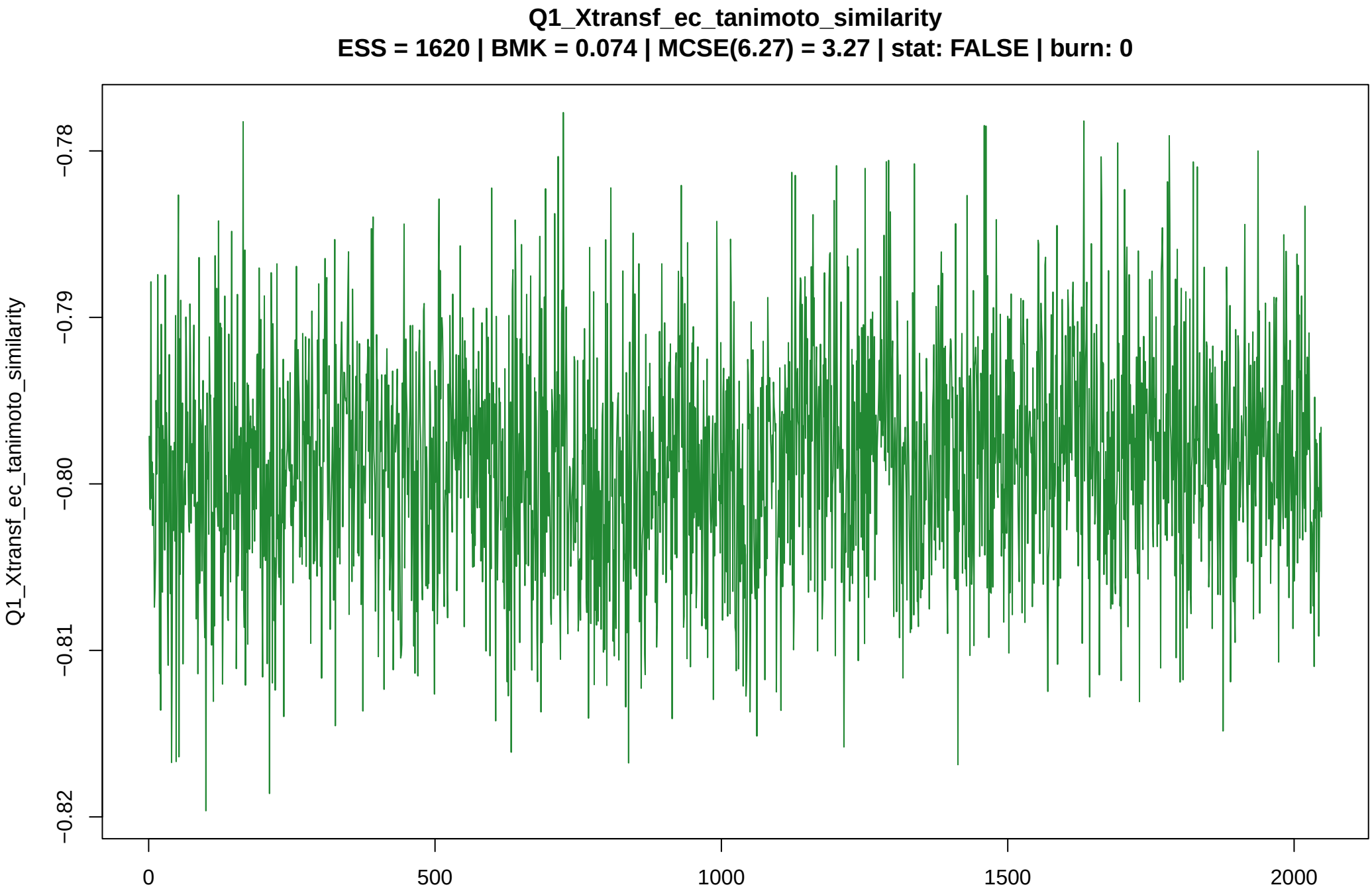

IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.235 | MCSE(6.27) = 2.47 | stat: FALSE | burn: 1020
IQR_template_HeavyAtomCount
11.0
10.5
10.0
9.5
9.0
0
500
1000
1500
2000

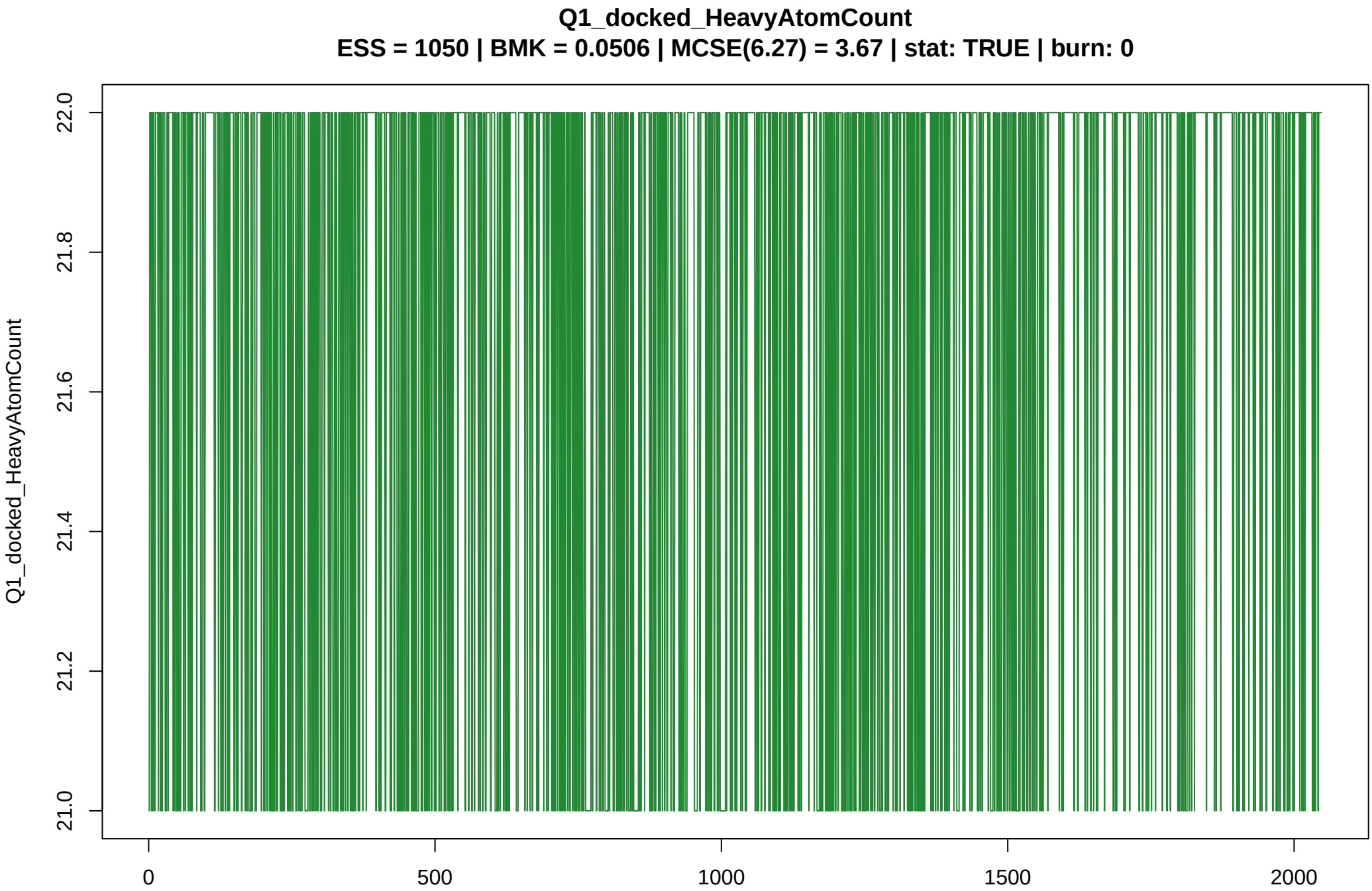

IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0129 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
IQR_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

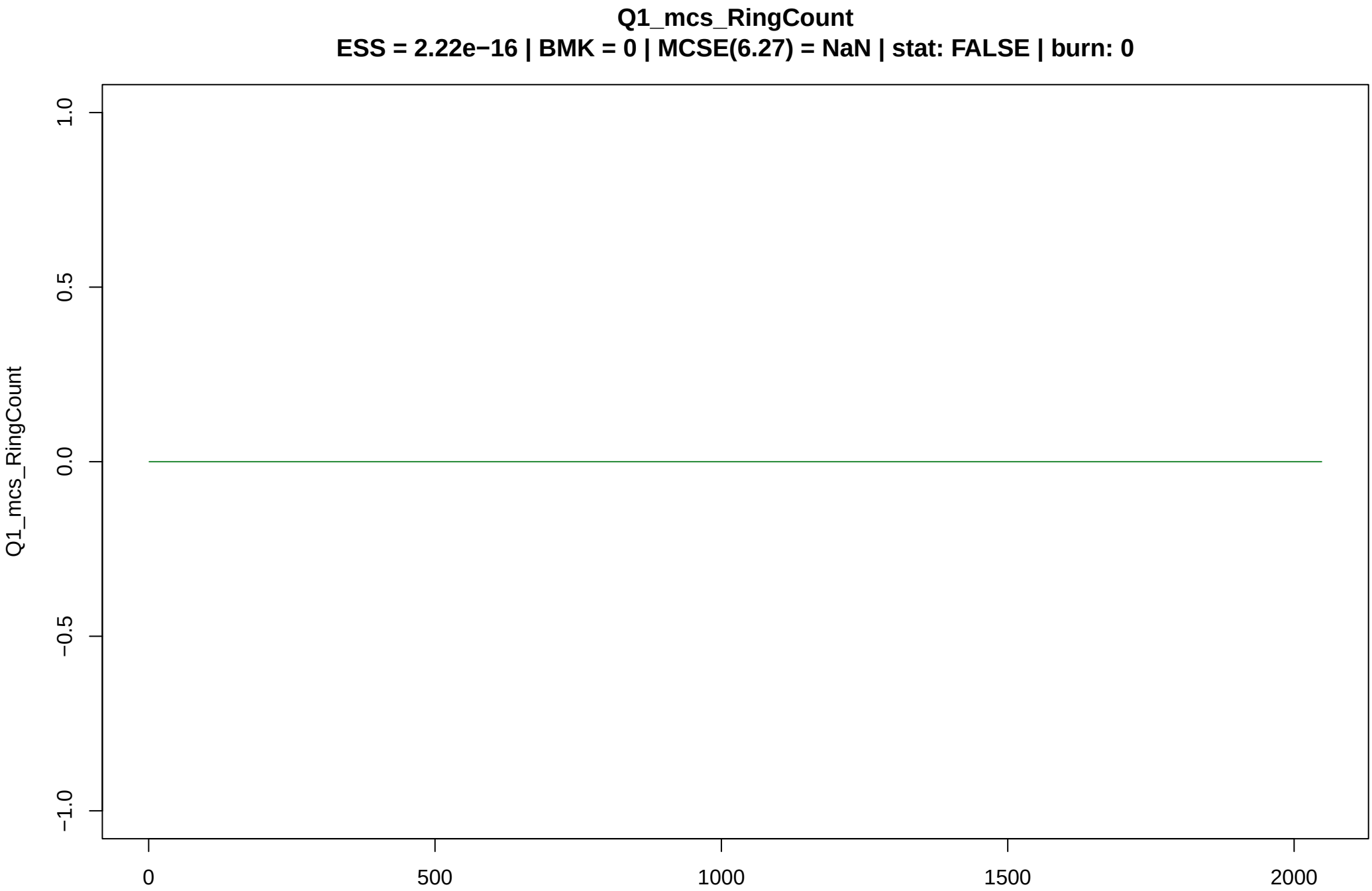

IQR_mcs_template_NumHAcceptors
ESS = 1880 | BMK = 0.0104 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0
IQR_mcs_template_NumHAcceptors
2.0
2.2
2.4
2.6
2.8
3.0
0
500
1000
1500
2000

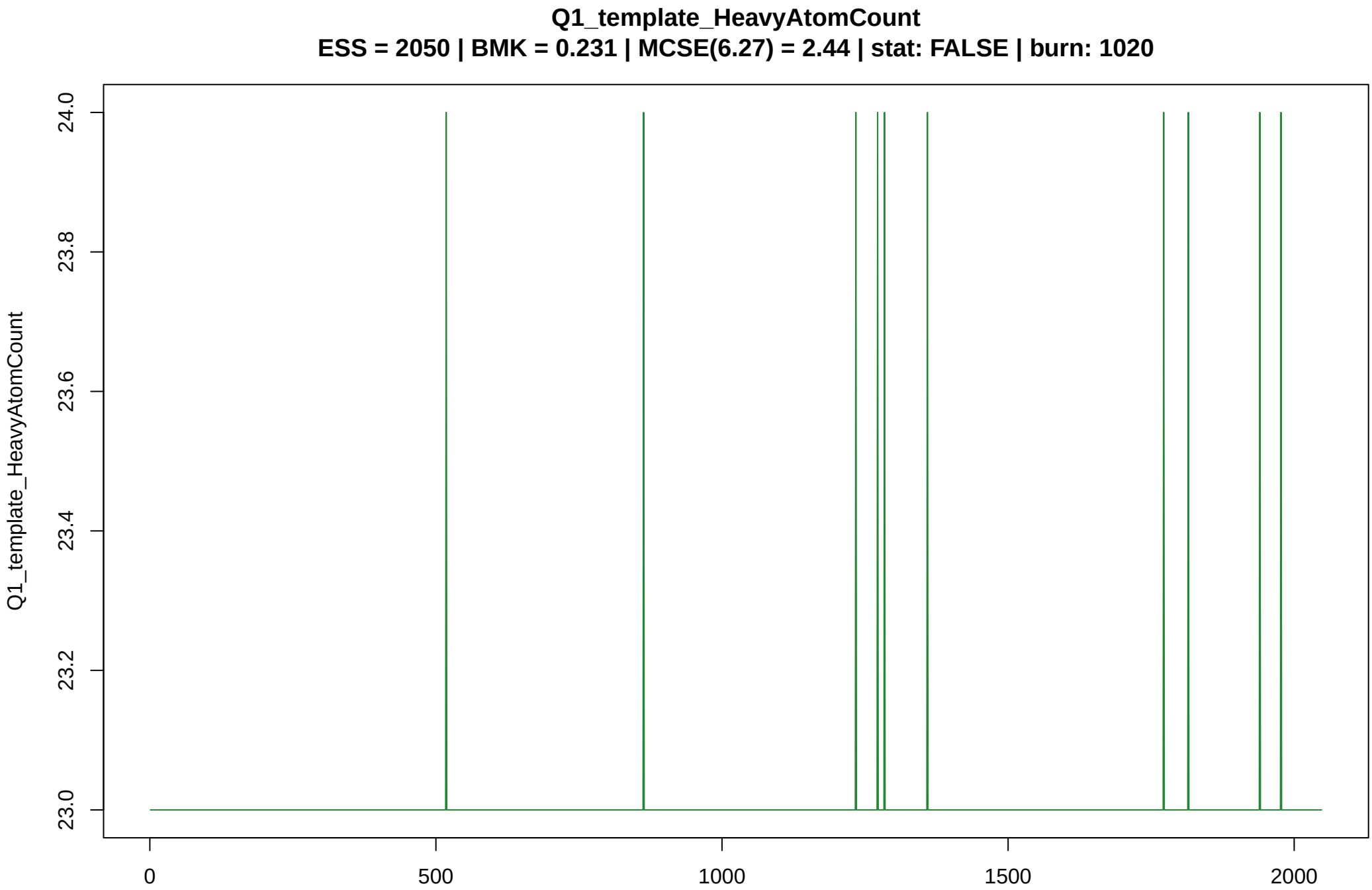

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

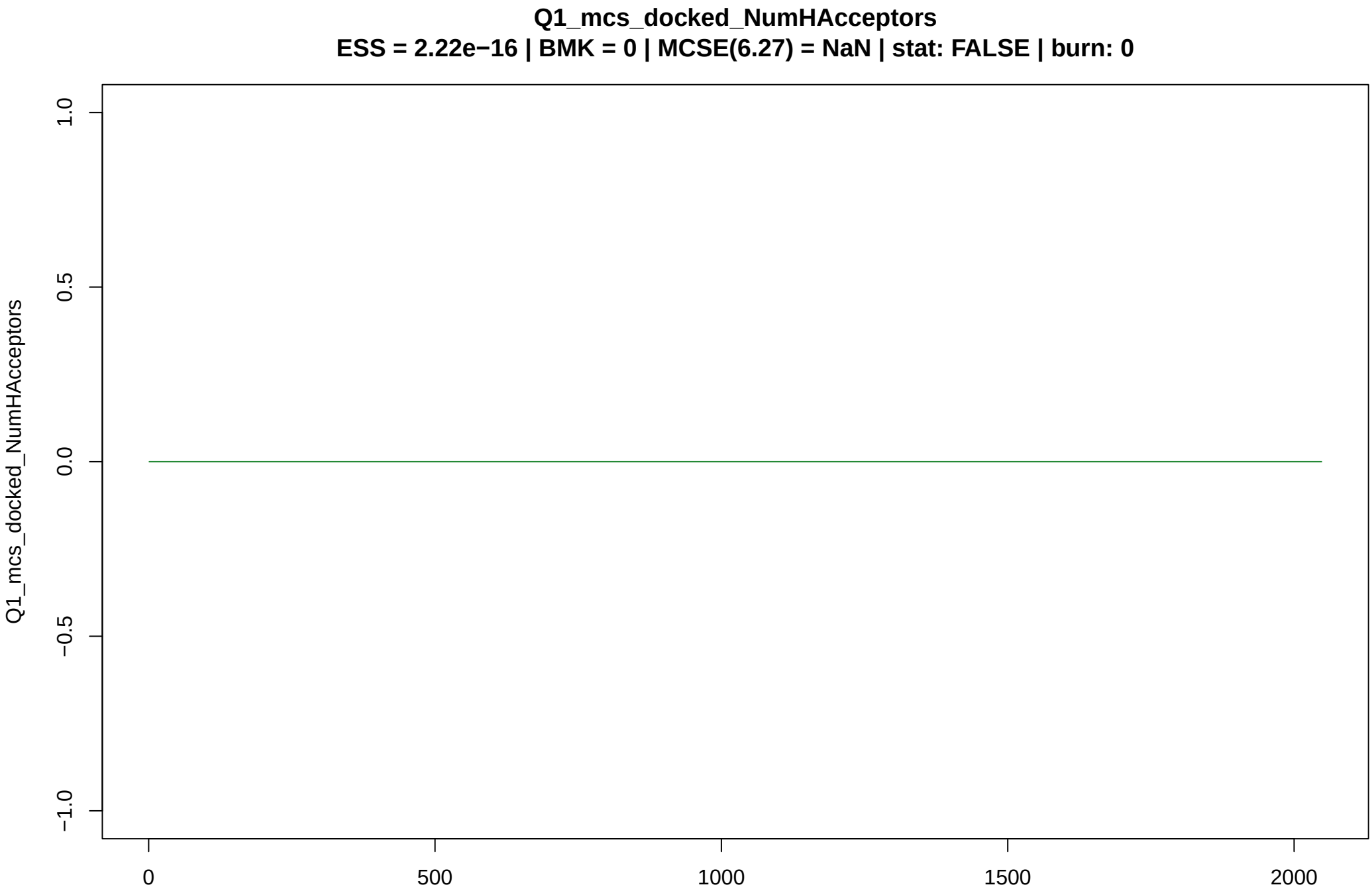

Q1_log_RMSD
ESS = 380 | BMK = 0.0884 | MCSE(6.27) = 4.1 | stat: FALSE | burn: 0
Q1_log_RMSD
0.84
0.86
0.88
0.90
0.92
0.94
0
500
1000
1500
2000

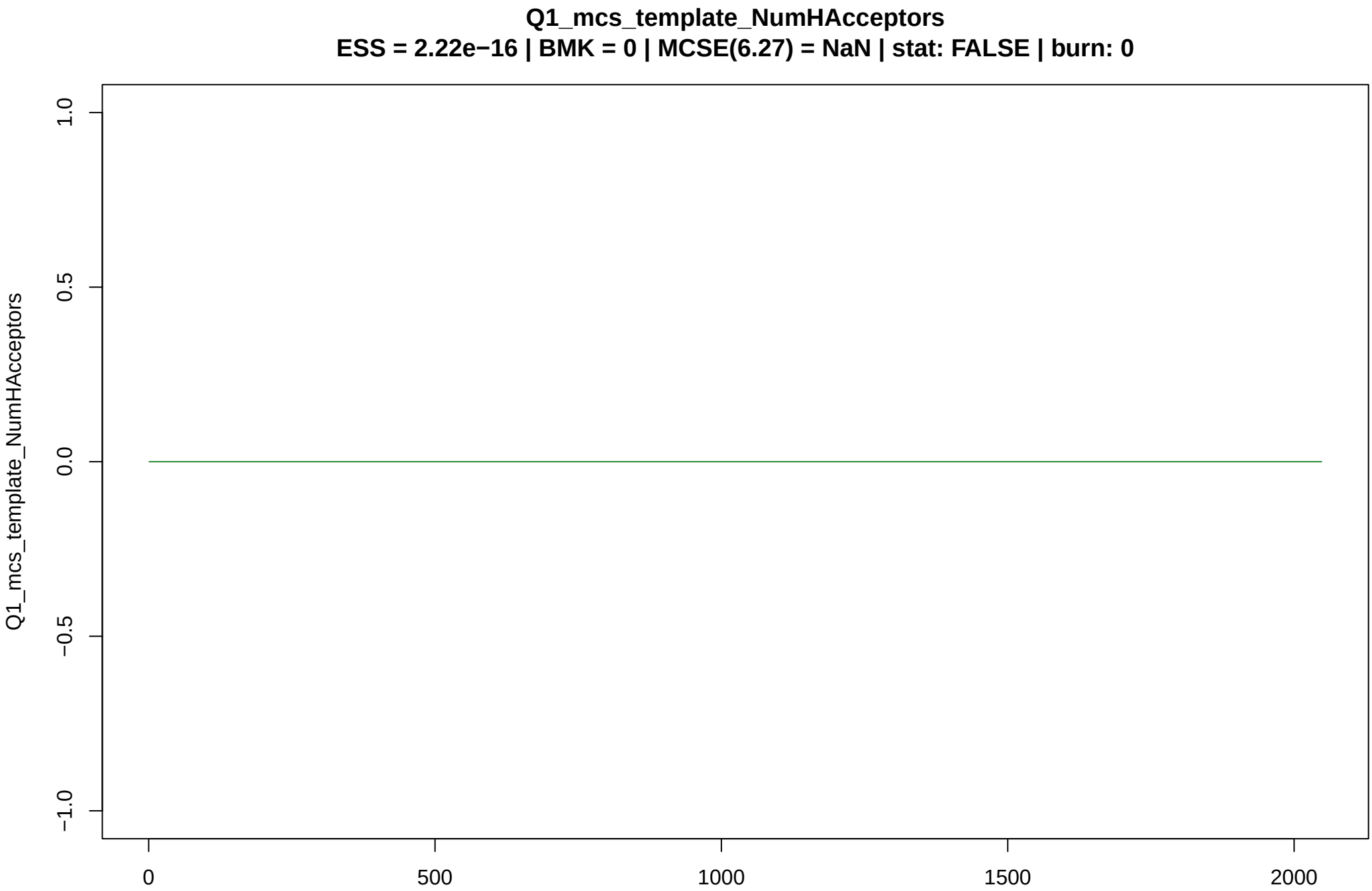

Q1_Xtransf_ec_tanimoto_similarity
ESS = 1620 | BMK = 0.074 | MCSE(6.27) = 3.27 | stat: FALSE | burn: 0
Q1_Xtransf_ec_tanimoto_similarity
−0.78
−0.79
−0.80
−0.81
−0.82
0
500
1000
1500
2000

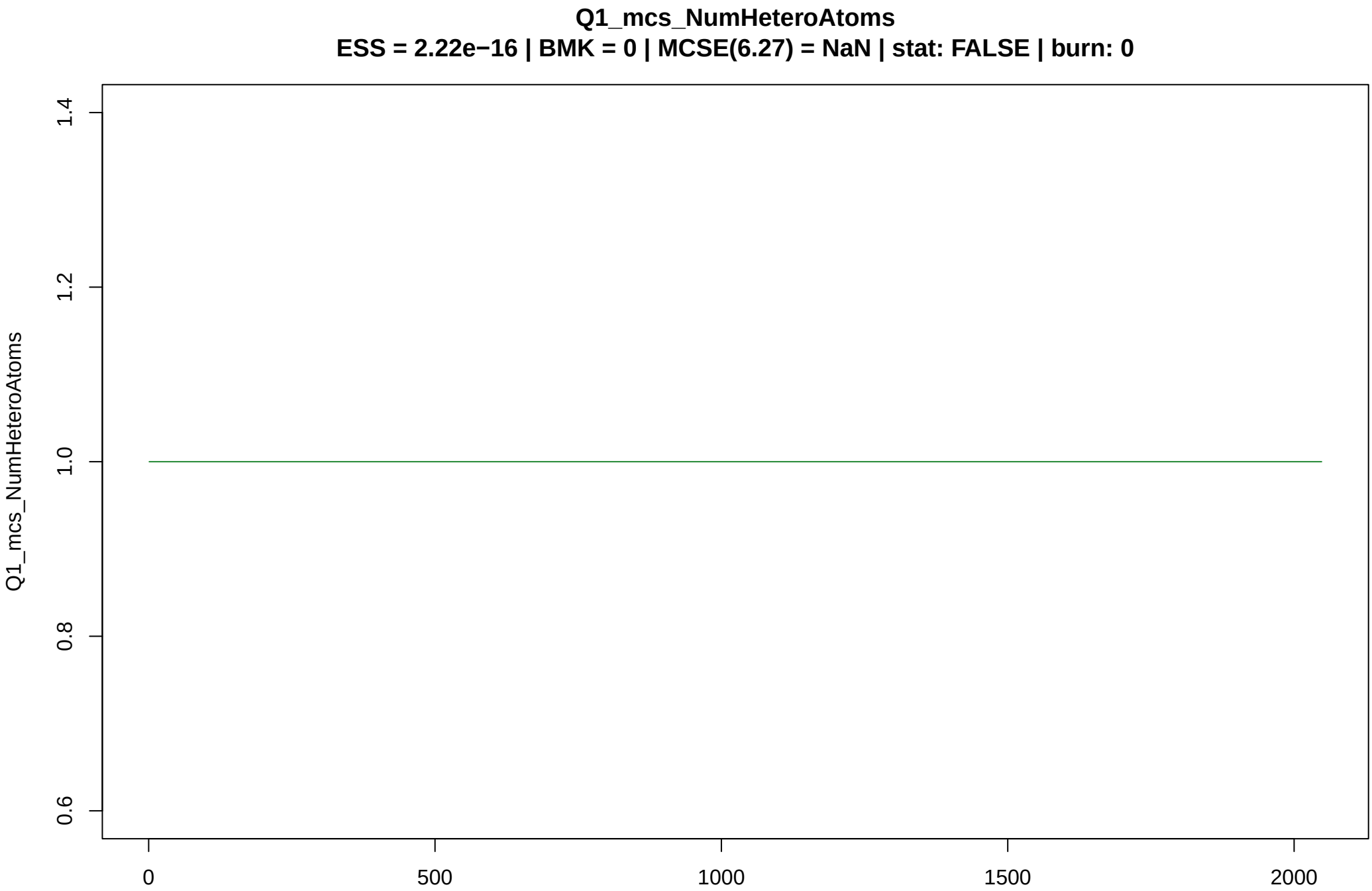

Q1_docked_HeavyAtomCount
ESS = 1050 | BMK = 0.0506 | MCSE(6.27) = 3.67 | stat: TRUE | burn: 0
Q1_docked_HeavyAtomCount
22.0
21.8
21.6
21.4
21.2
21.0
0
500
1000
1500
2000

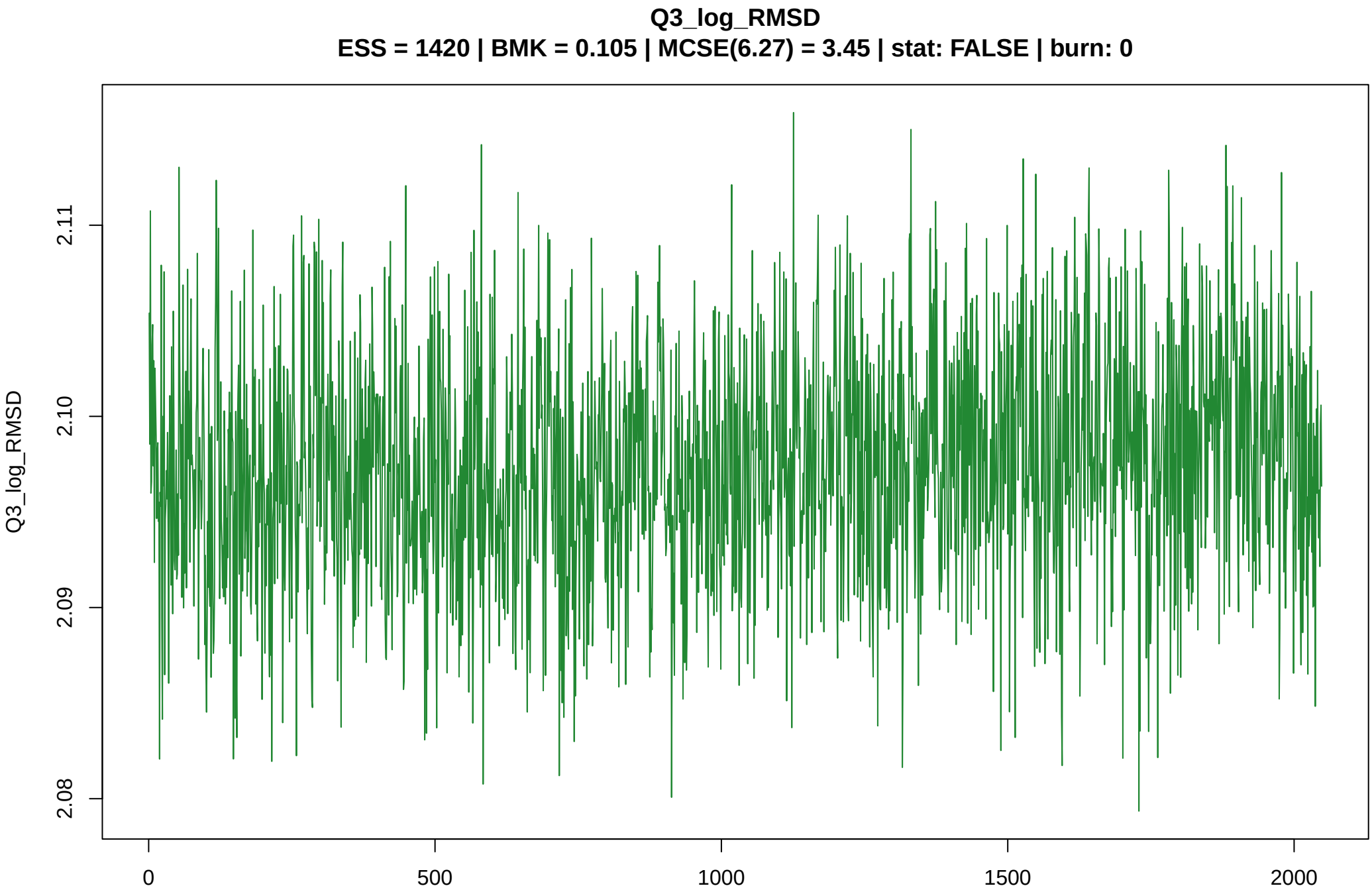

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

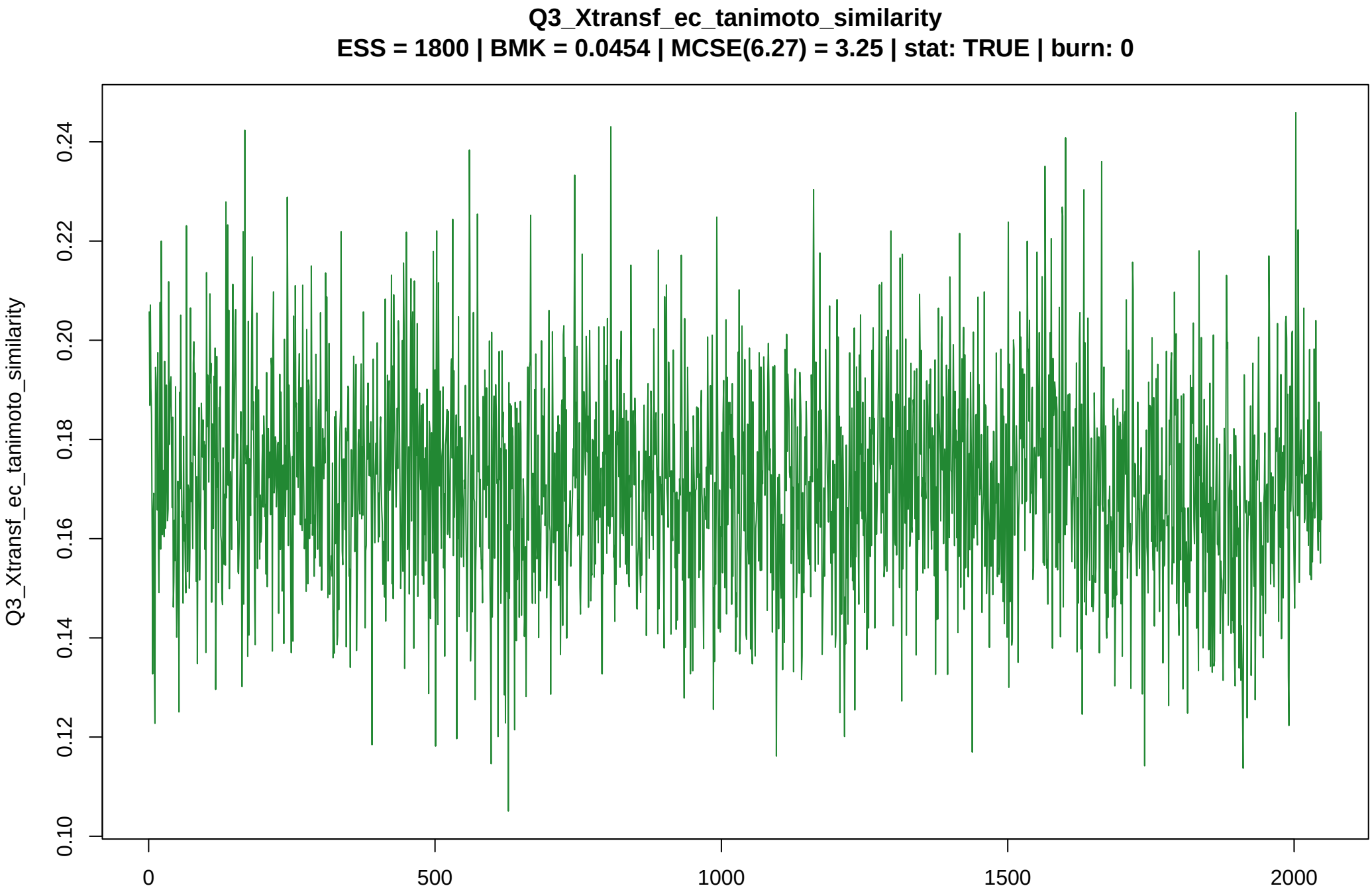

Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0.231 | MCSE(6.27) = 2.44 | stat: FALSE | burn: 1020
Q1_template_HeavyAtomCount
24.0
23.8
23.6
23.4
23.2
23.0
0
500
1000
1500
2000

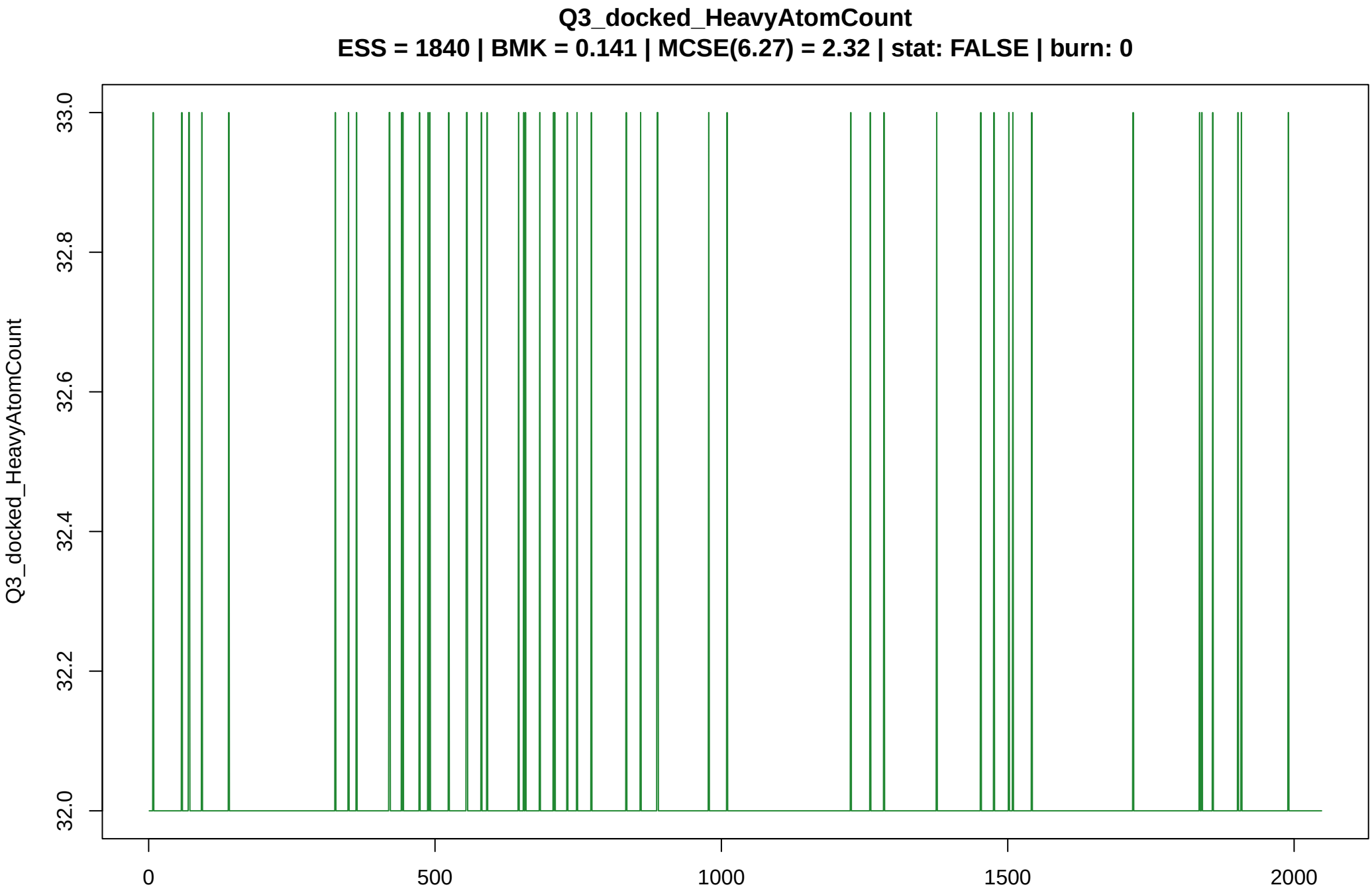

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

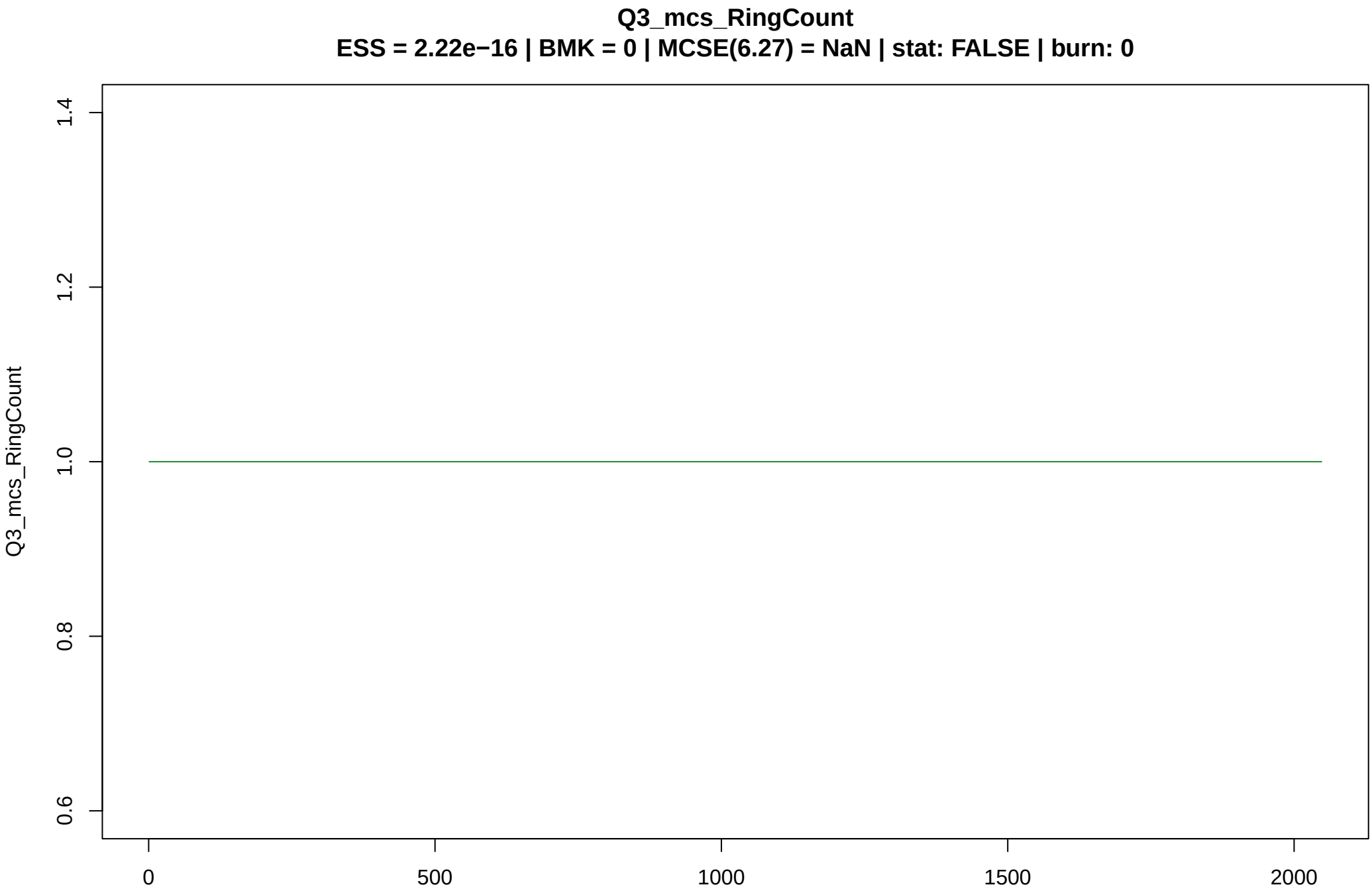

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

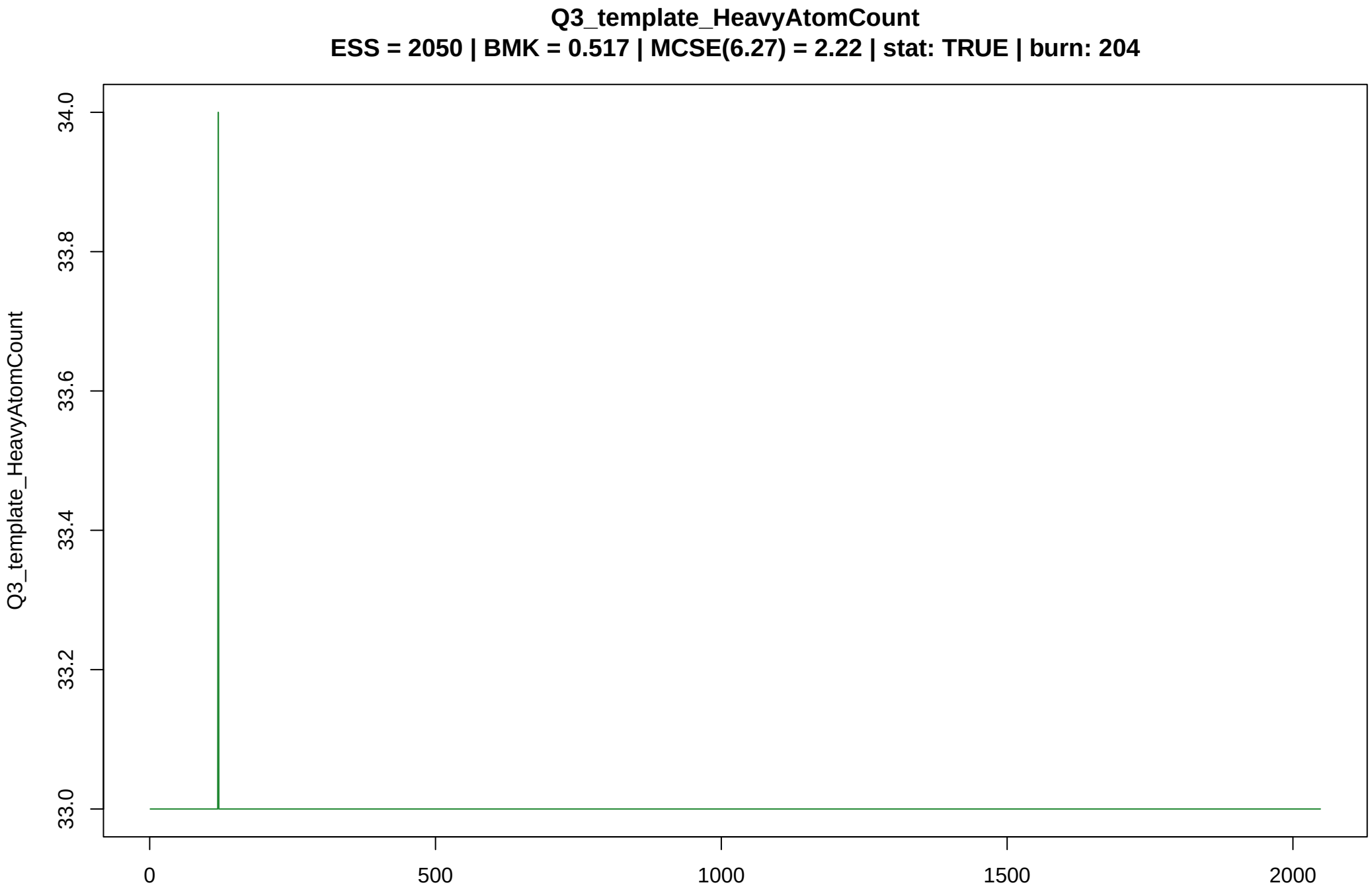

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

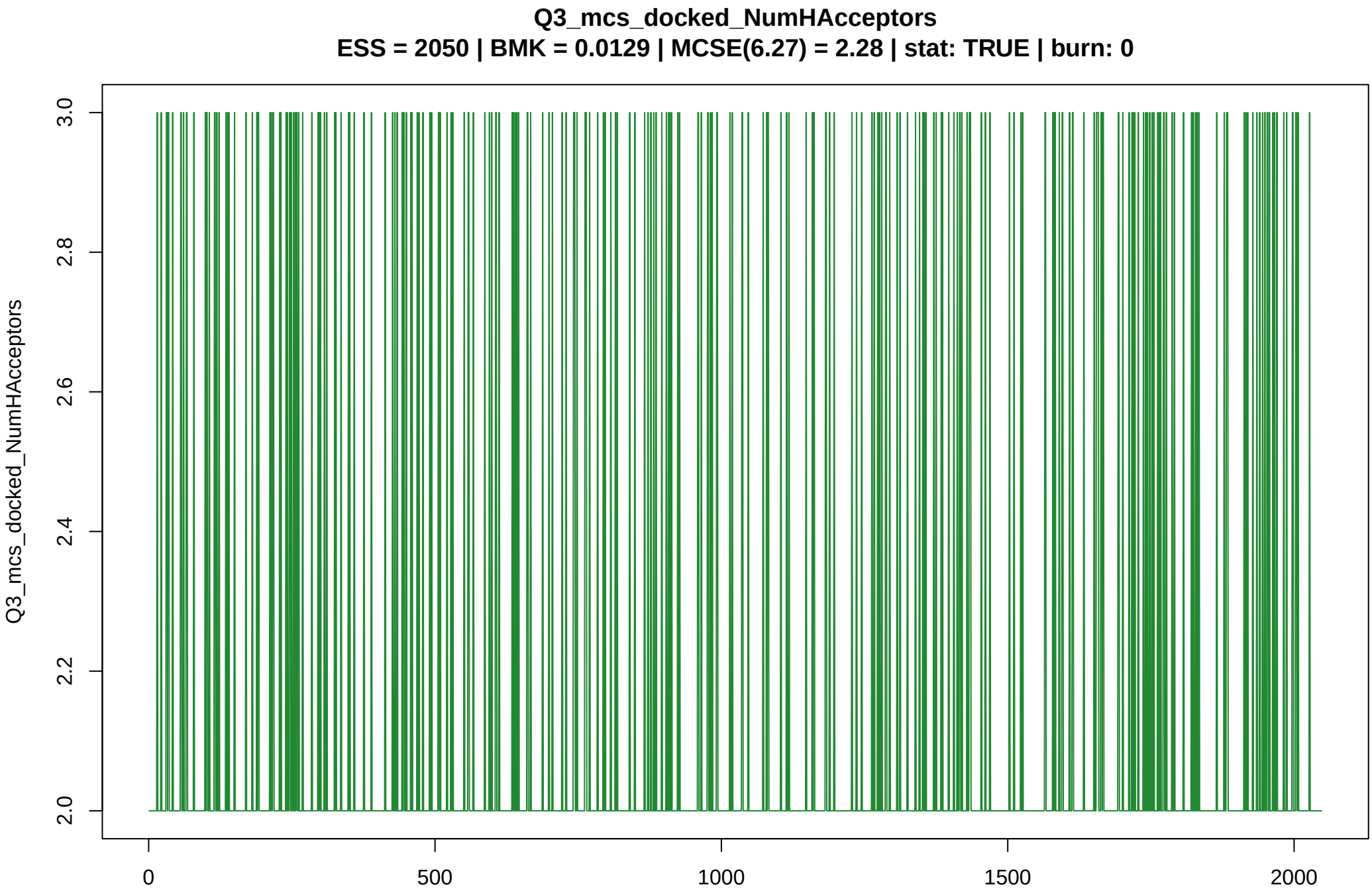

Q3_log_RMSD
ESS = 1420 | BMK = 0.105 | MCSE(6.27) = 3.45 | stat: FALSE | burn: 0
Q3_log_RMSD
2.08
2.09
2.10
2.11
0
500
1000
1500
2000

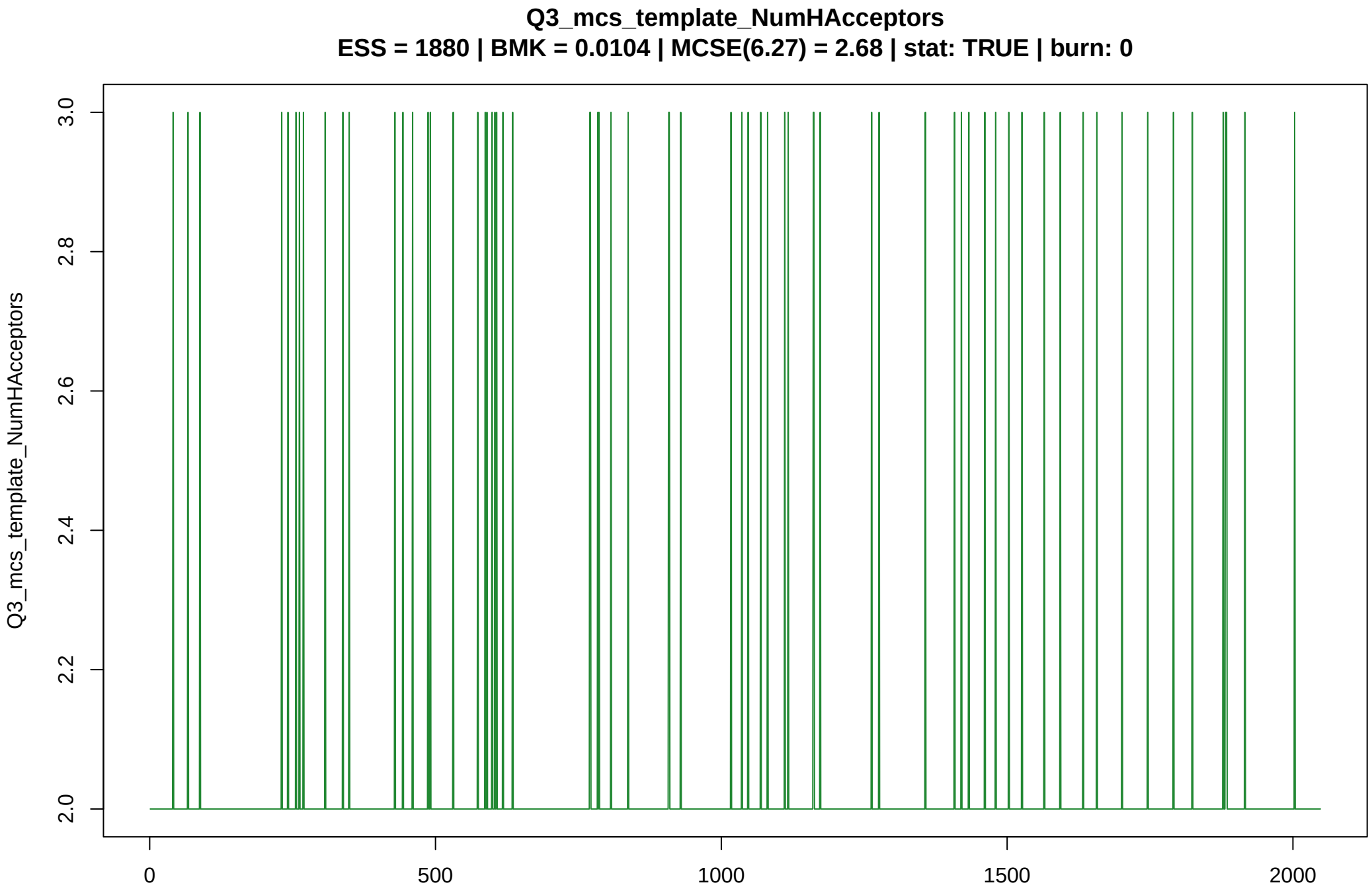

Q3_Xtransf_ec_tanimoto_similarity
ESS = 1800 | BMK = 0.0454 | MCSE(6.27) = 3.25 | stat: TRUE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
0.10
0.12
0.14
0.16
0.18
0.20
0.22
0.24
0
500
1000
1500
2000

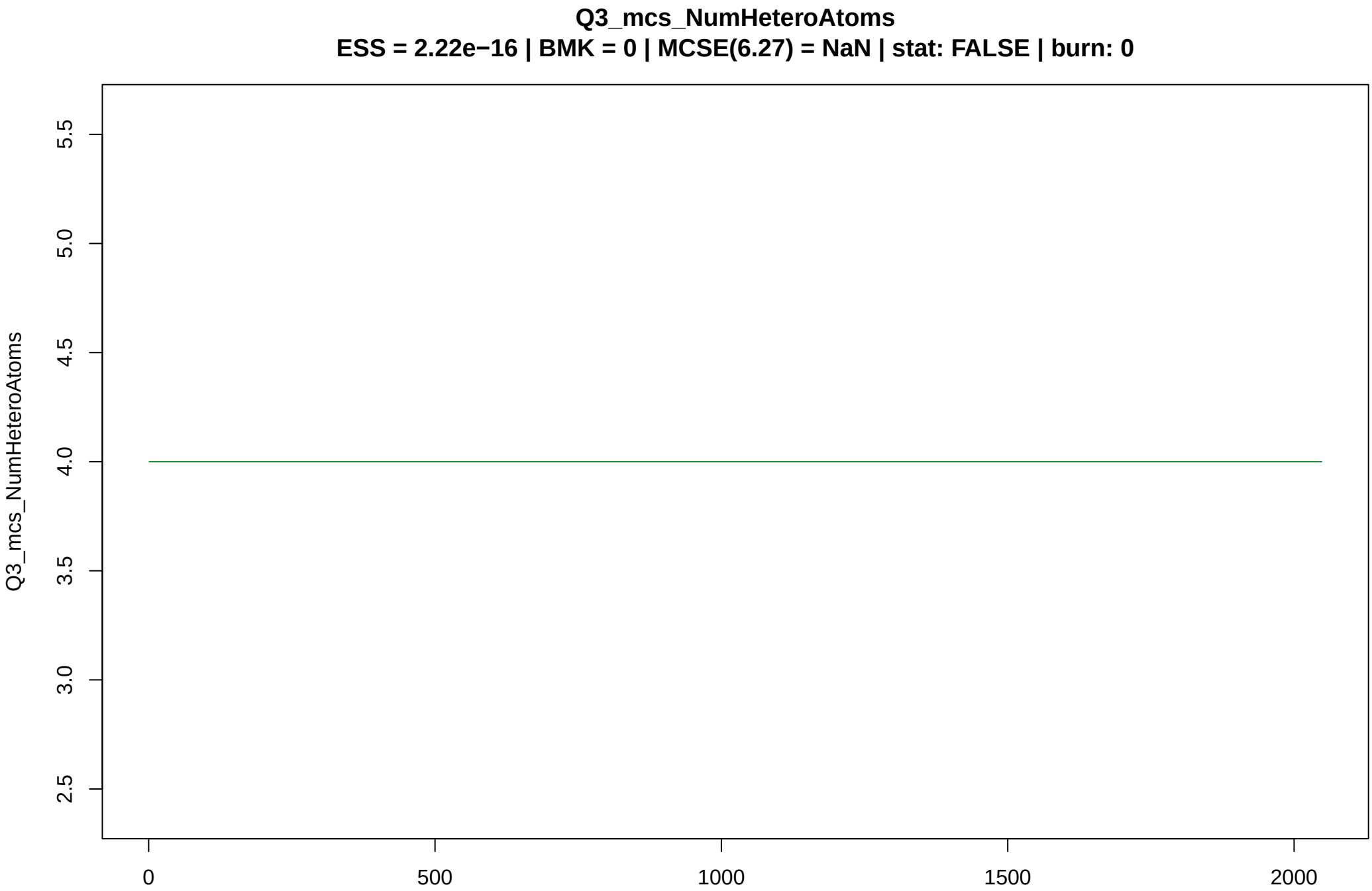

Q3_docked_HeavyAtomCount
ESS = 1840 | BMK = 0.141 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0
Q3_docked_HeavyAtomCount
33.0
32.8
32.6
32.4
32.2
32.0
0
500
1000
1500
2000

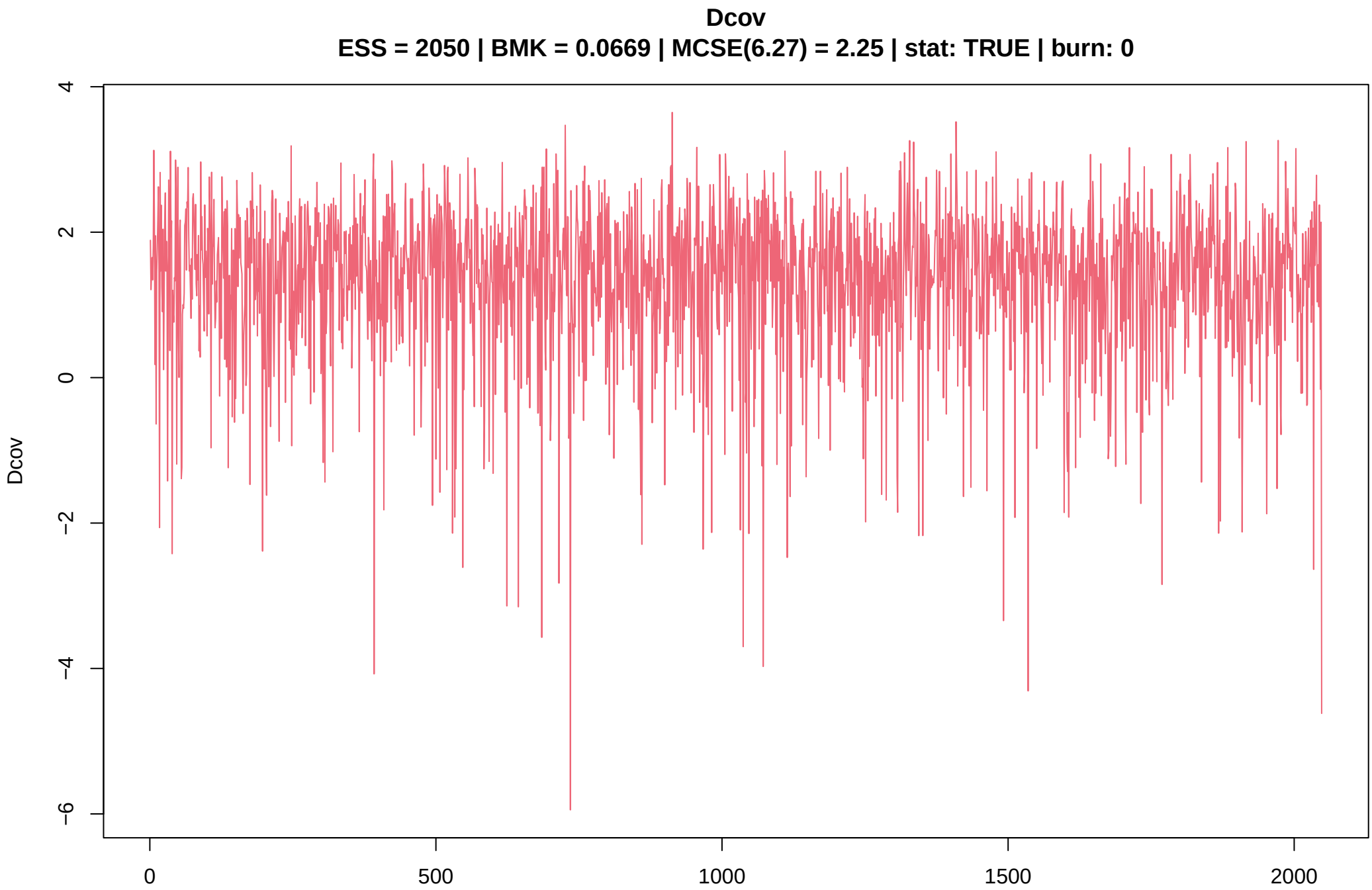

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

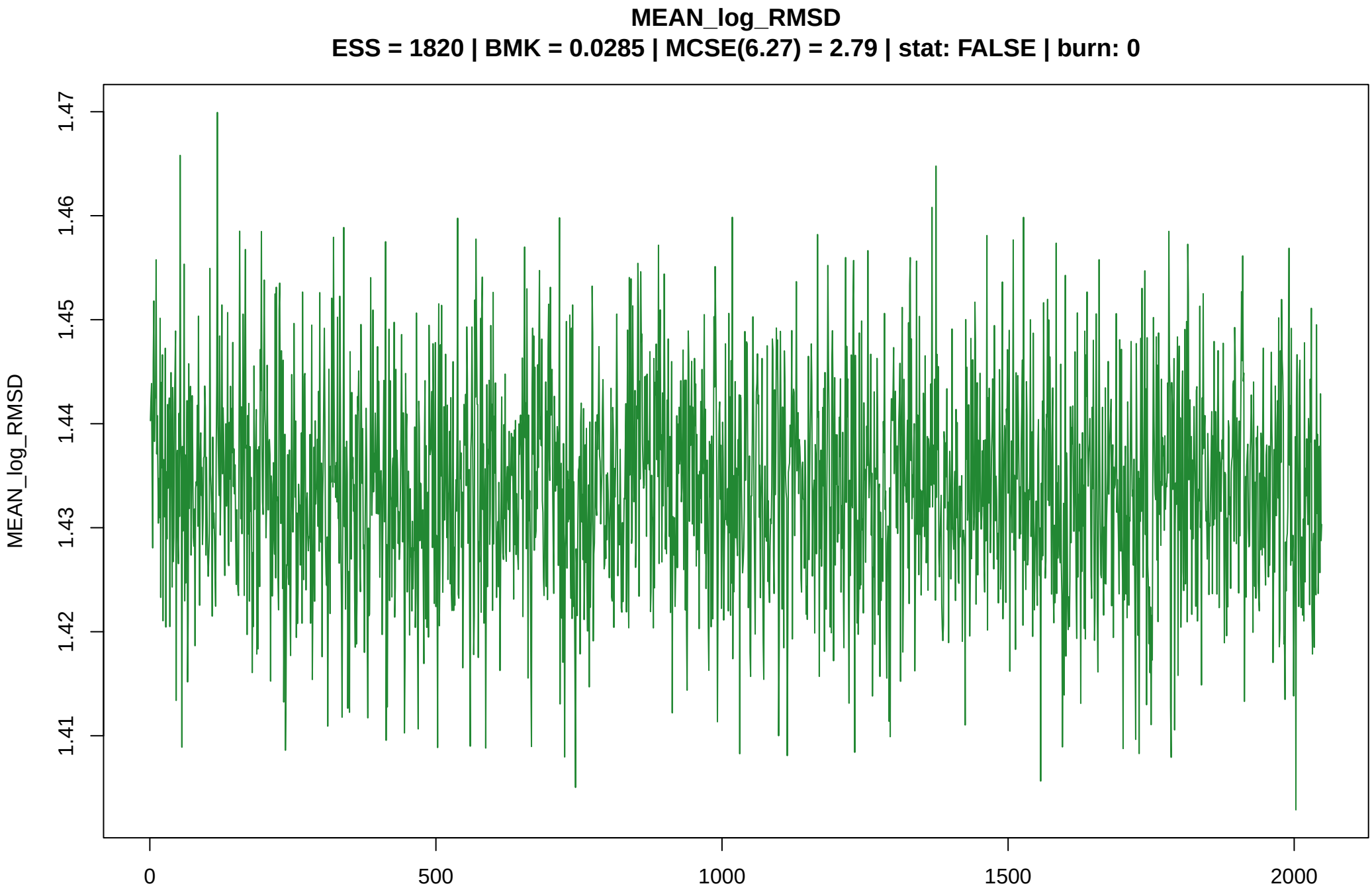

Q3_template_HeavyAtomCount
ESS = 2050 | BMK = 0.517 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 204
Q3_template_HeavyAtomCount
34.0
33.8
33.6
33.4
33.2
33.0
0
500
1000
1500
2000

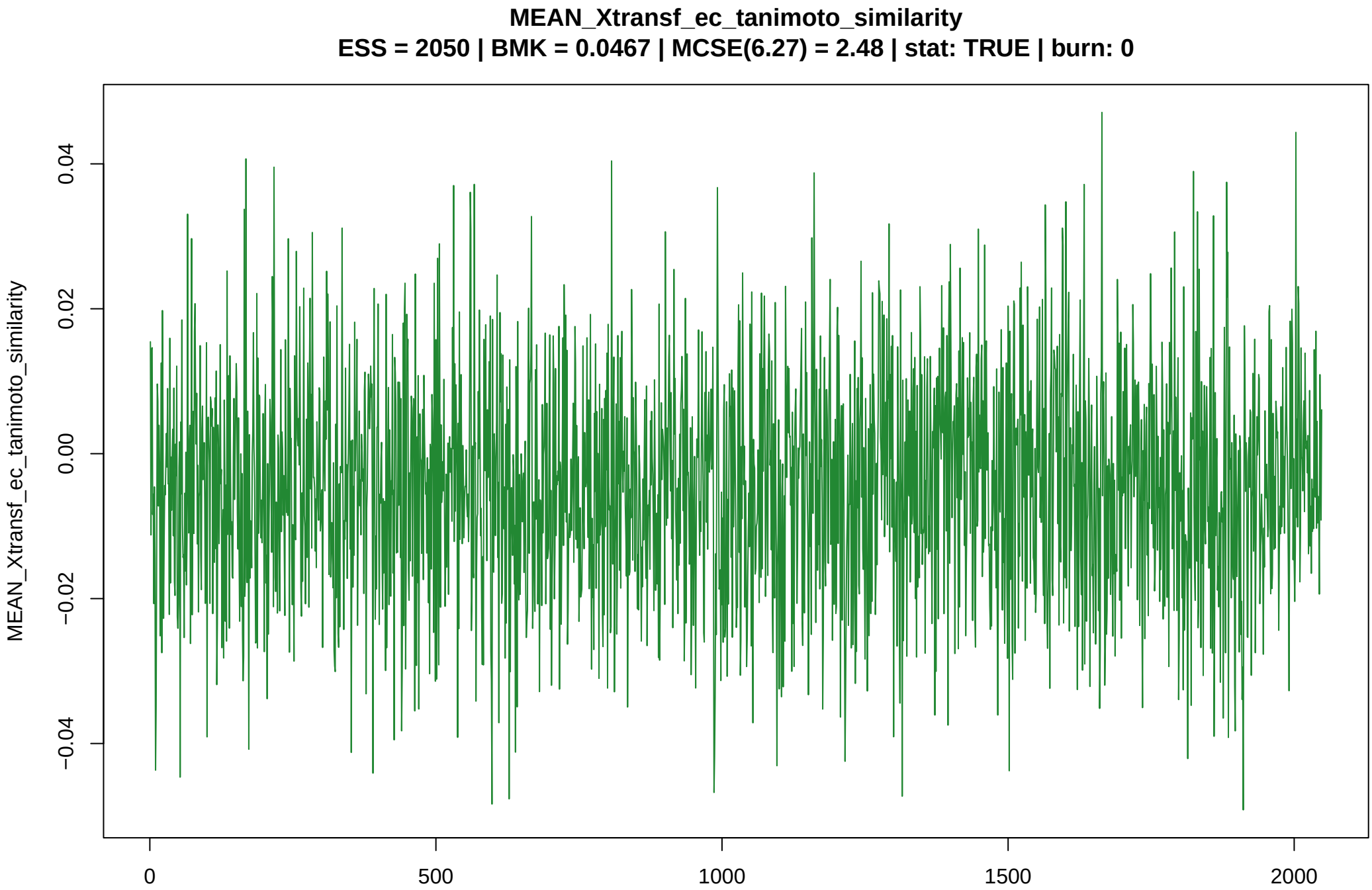

Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0129 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
Q3_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

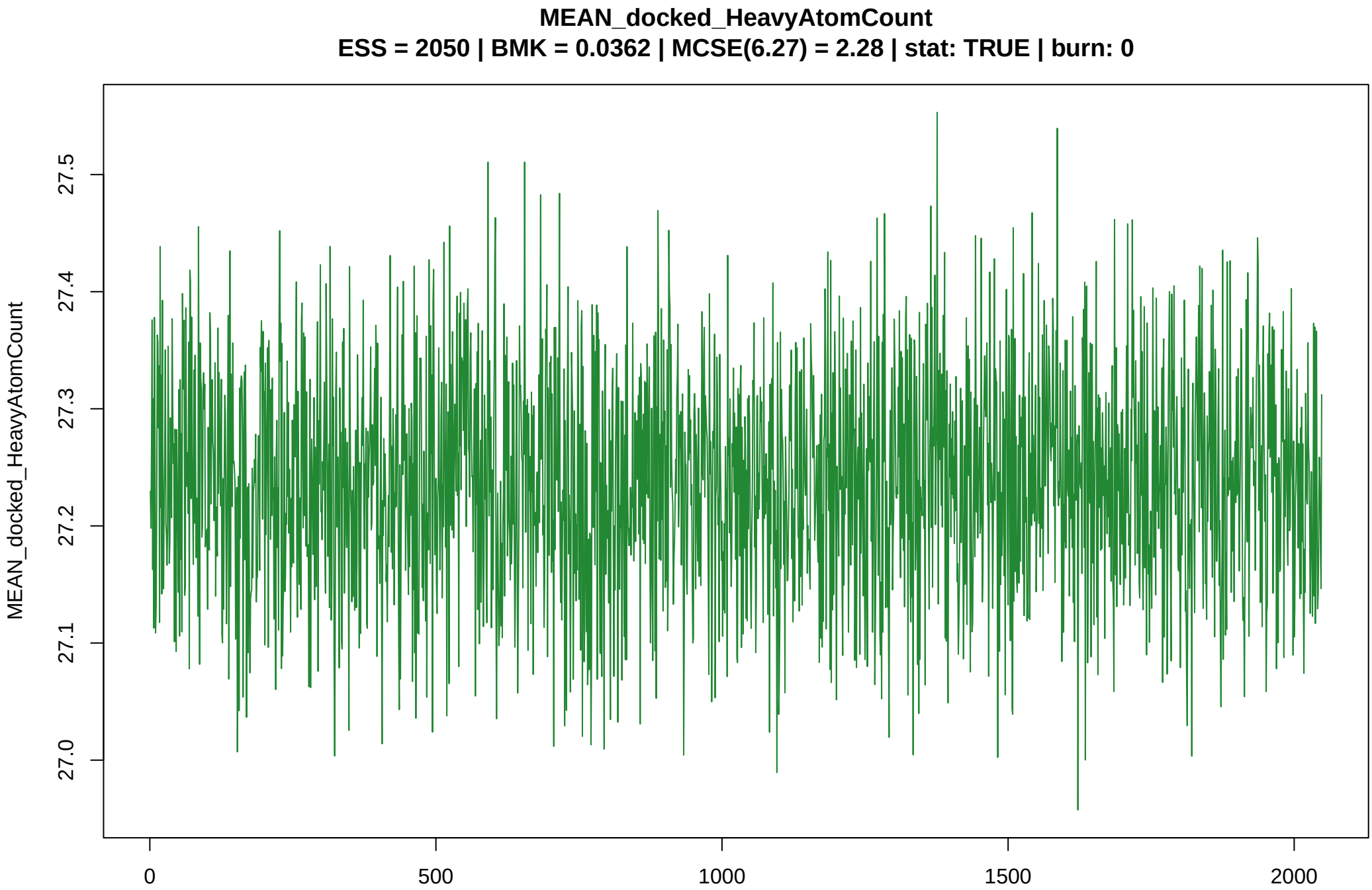

Q3_mcs_template_NumHAcceptors
ESS = 1880 | BMK = 0.0104 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0
Q3_mcs_template_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

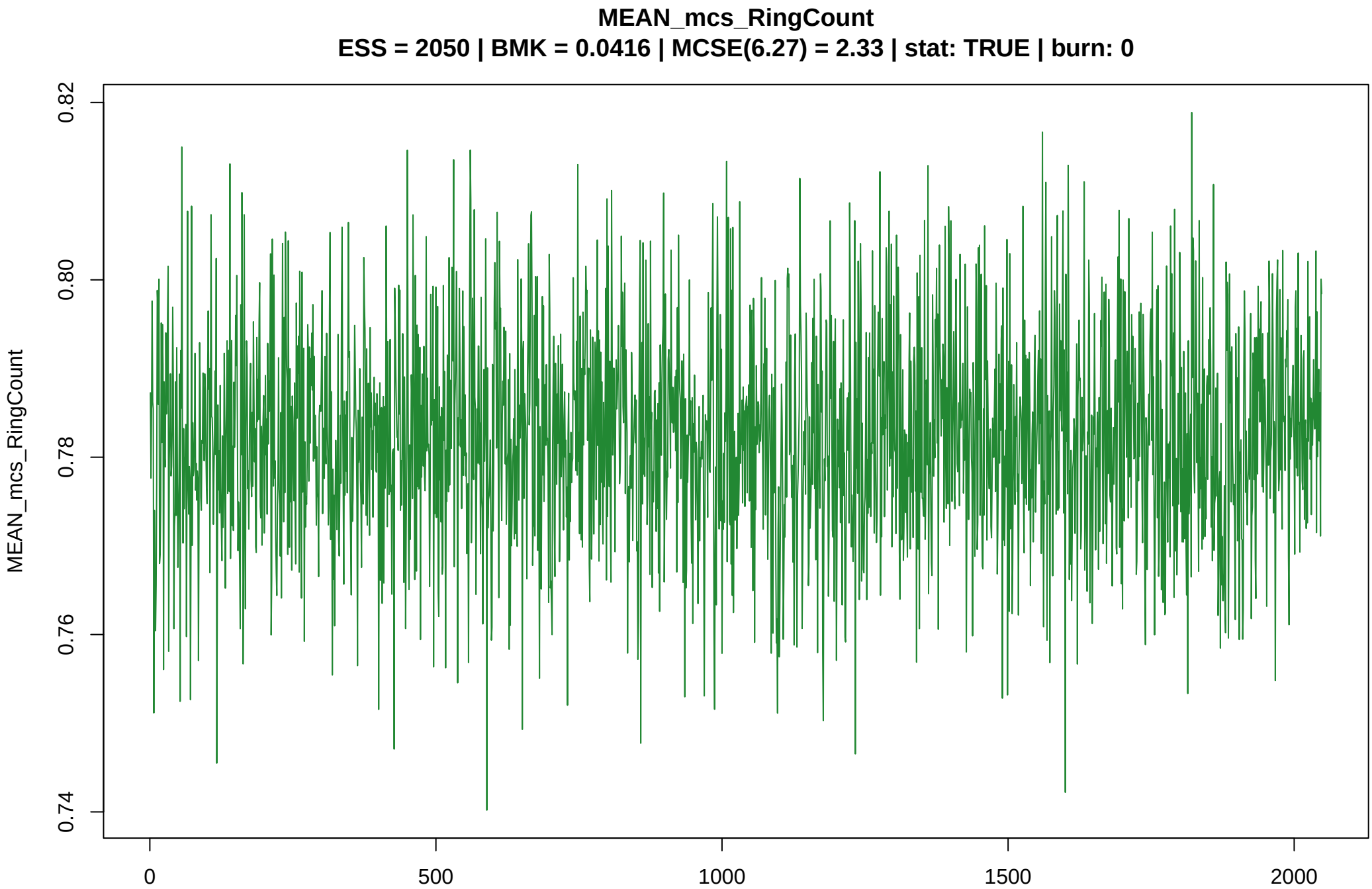

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

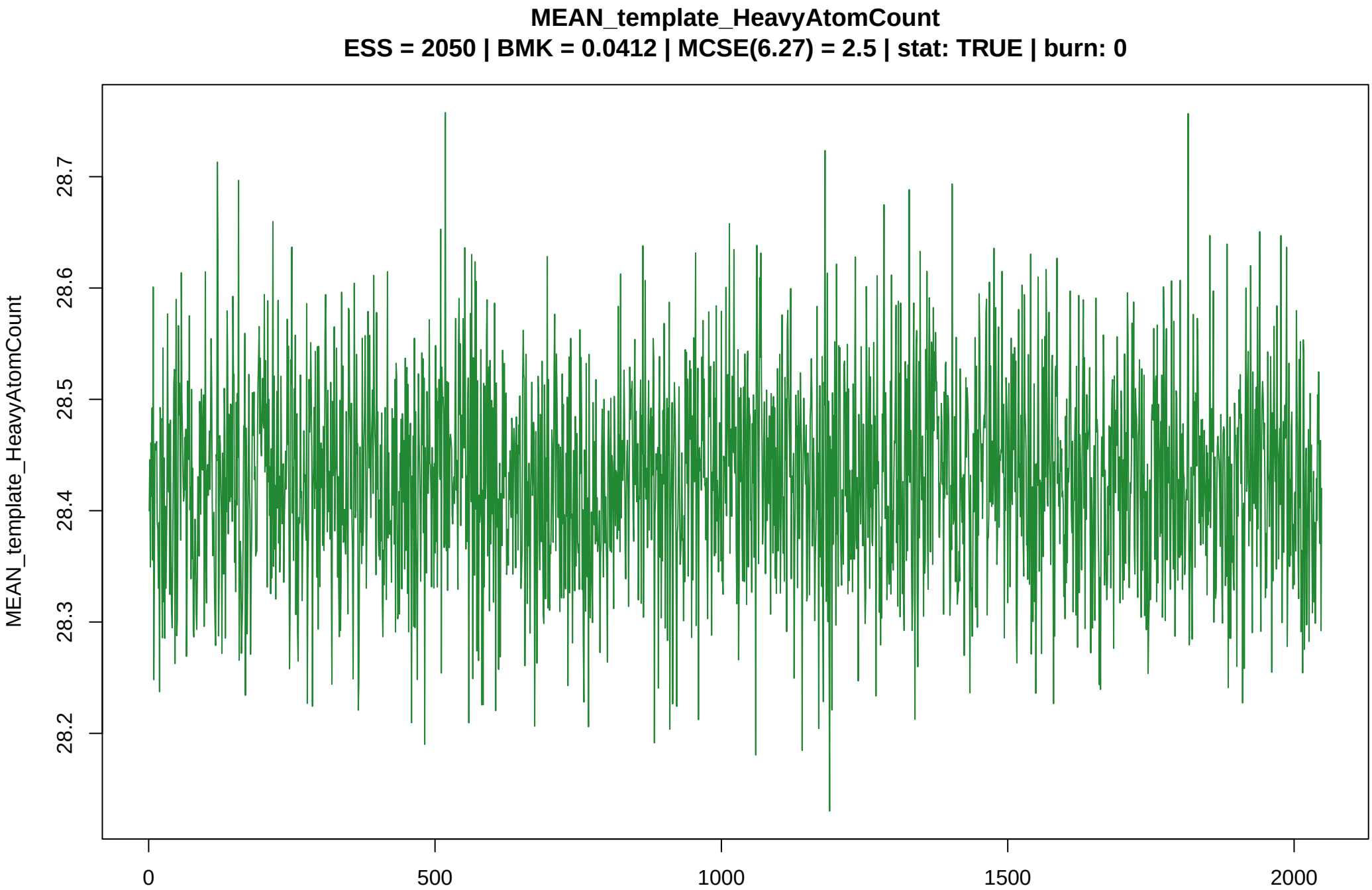

Dcov
ESS = 2050 | BMK = 0.0669 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0
Dcov
4
2
0
−2
−4
−6
0
500
1000
1500
2000

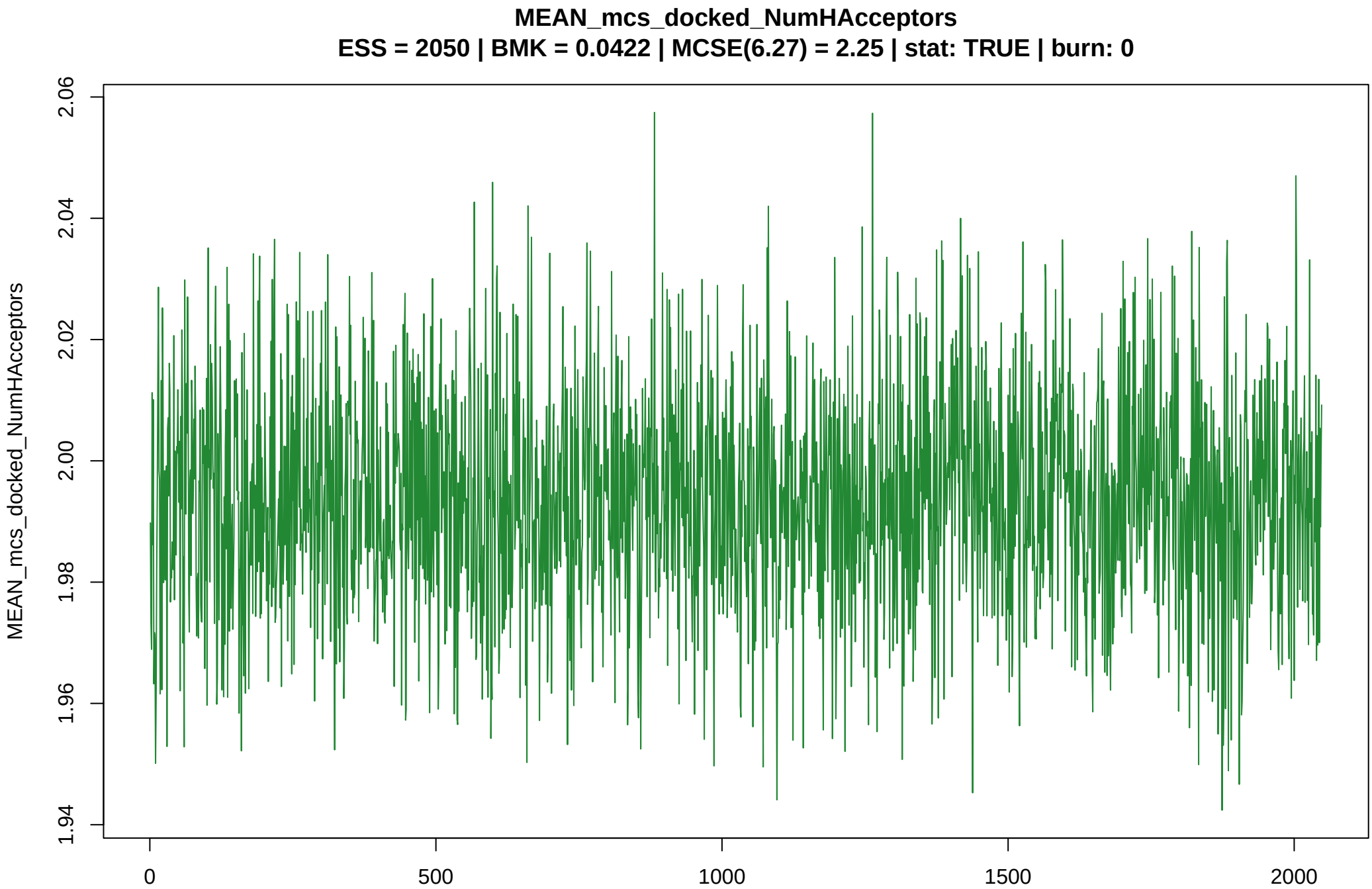

MEAN_log_RMSD
ESS = 1820 | BMK = 0.0285 | MCSE(6.27) = 2.79 | stat: FALSE | burn: 0
MEAN_log_RMSD
1.47
1.46
1.45
1.44
1.43
1.42
1.41
0
500
1000
1500
2000

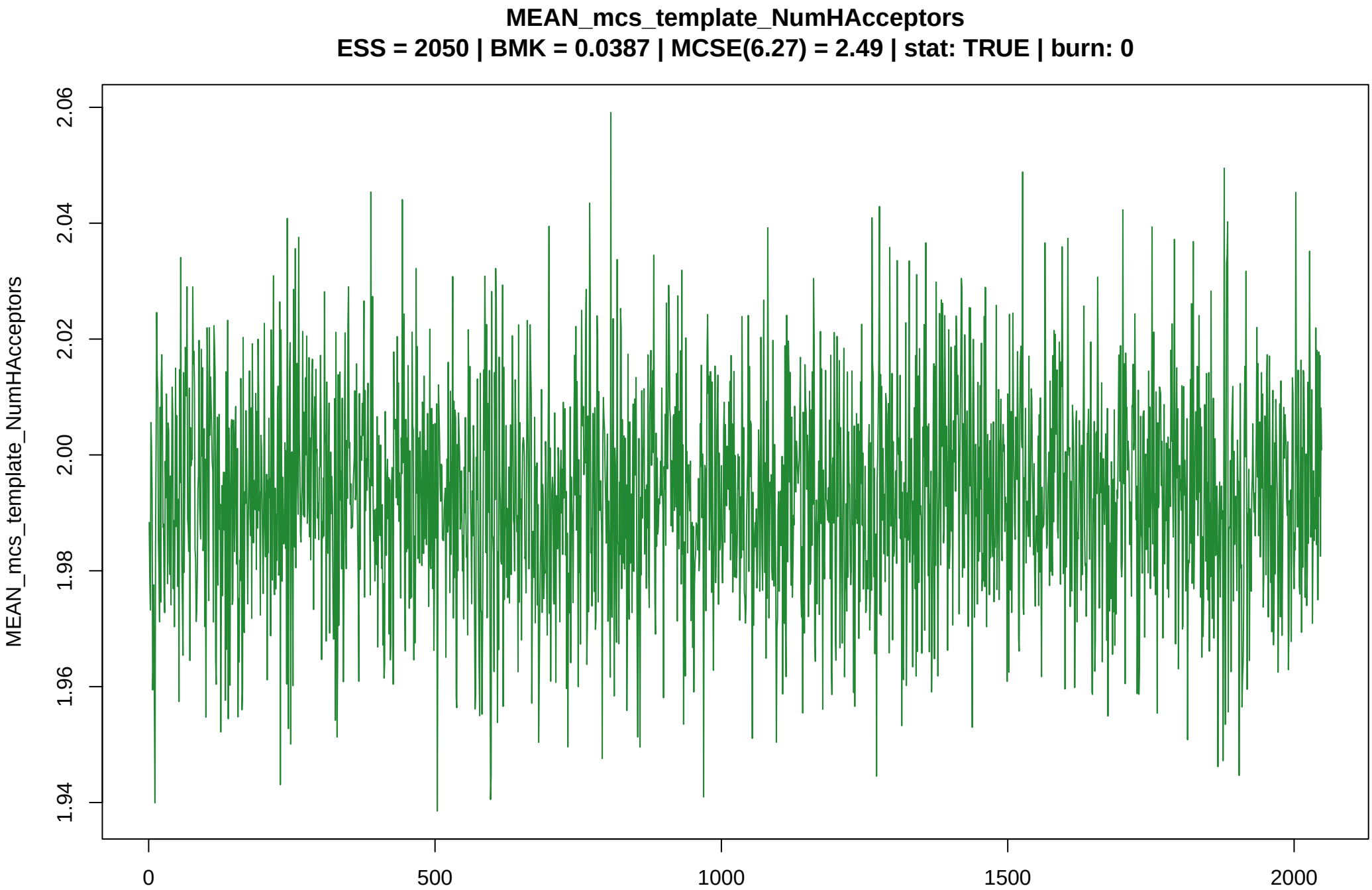

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0467 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0
MEAN_Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
0
500
1000
1500
2000

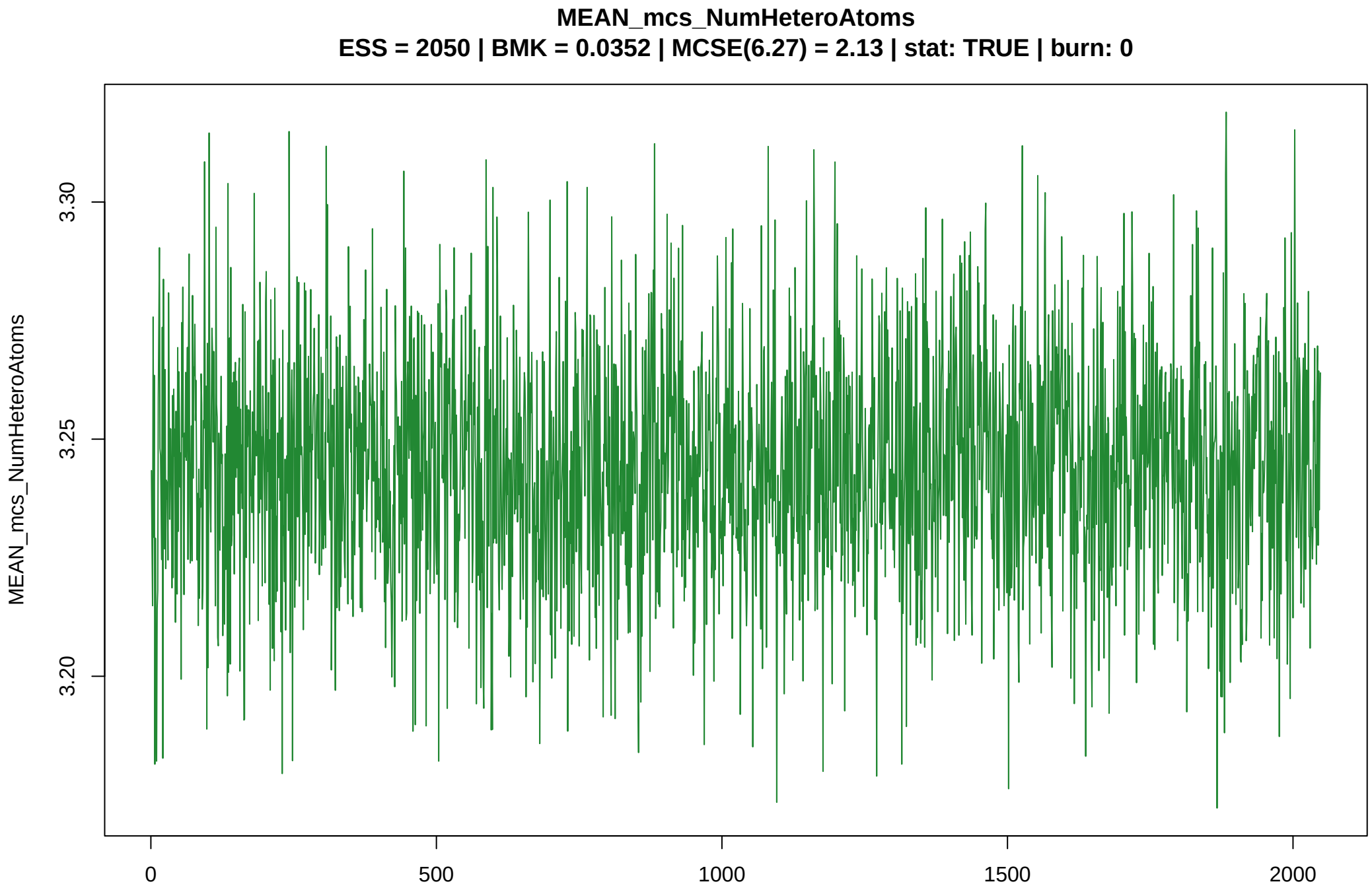

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0362 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
27.0
27.1
27.2
27.3
27.4
27.5
0
500
1000
1500
2000

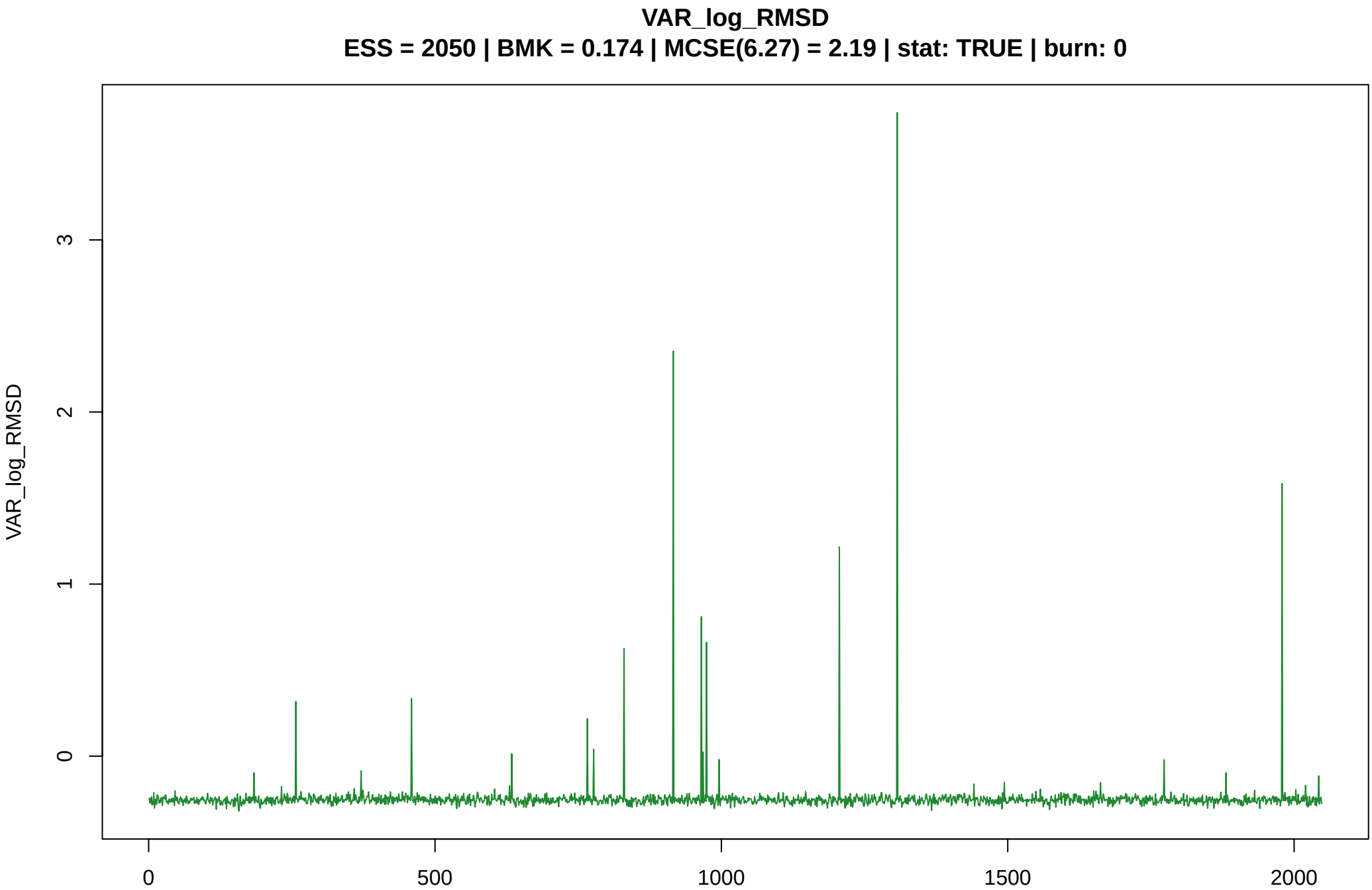

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0416 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.74
0.76
0.78
0.80
0.82
0
500
1000
1500
2000

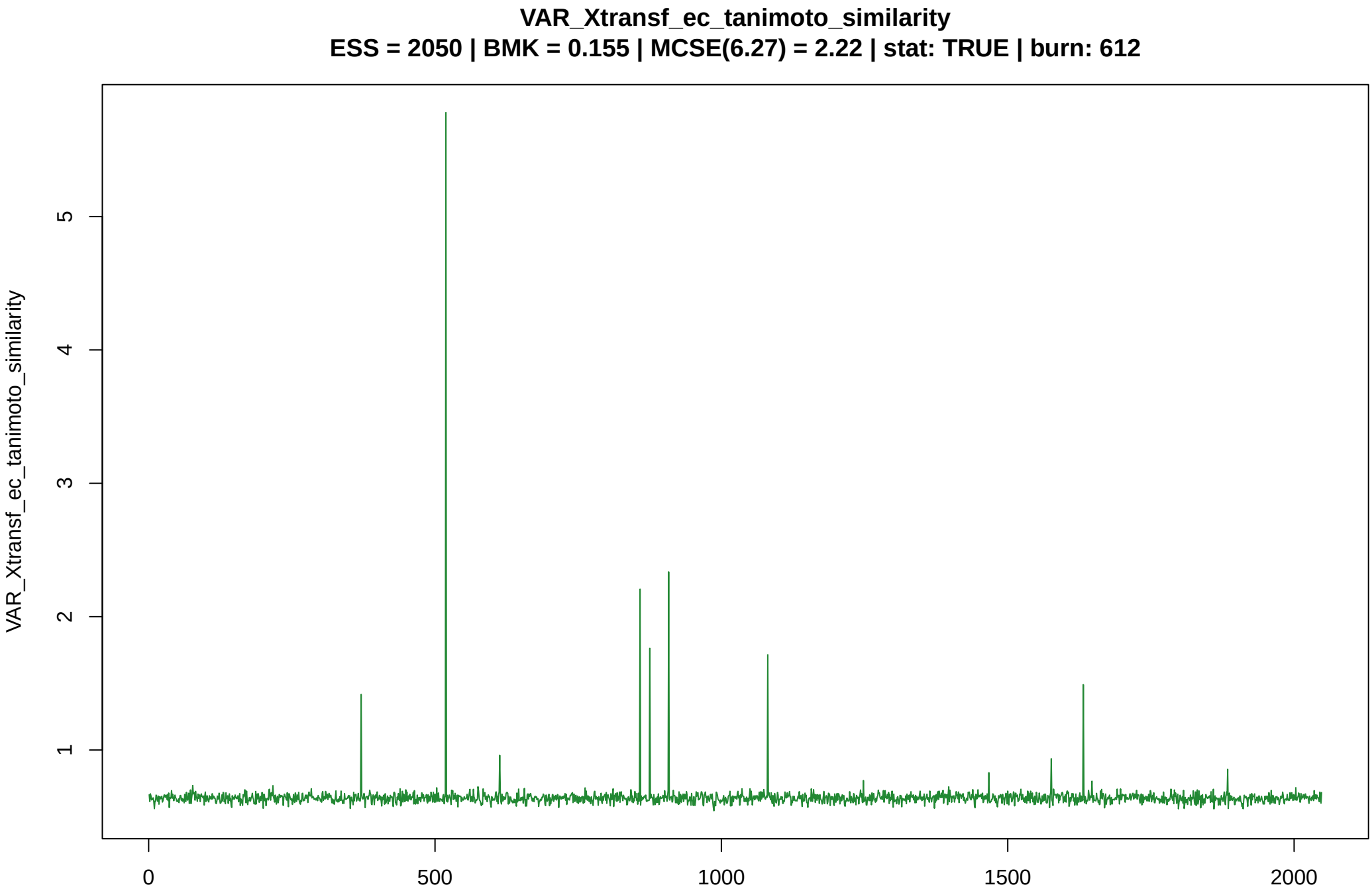

MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0412 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0
MEAN_template_HeavyAtomCount
28.2
28.3
28.4
28.5
28.6
28.7
0
500
1000
1500
2000

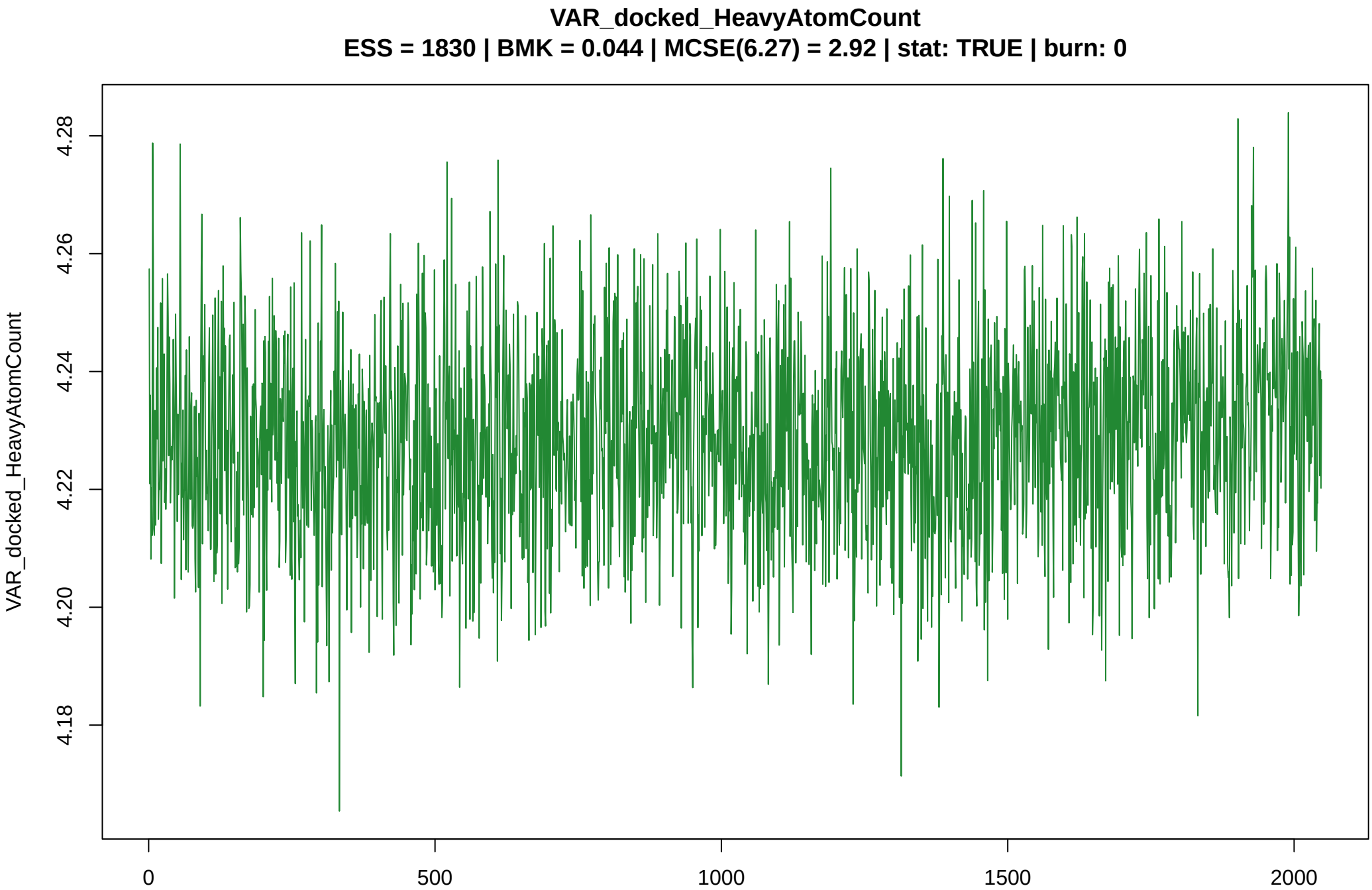

MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0422 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
2.06
2.04
2.02
2.00
1.98
1.96
1.94
0
500
1000
1500
2000

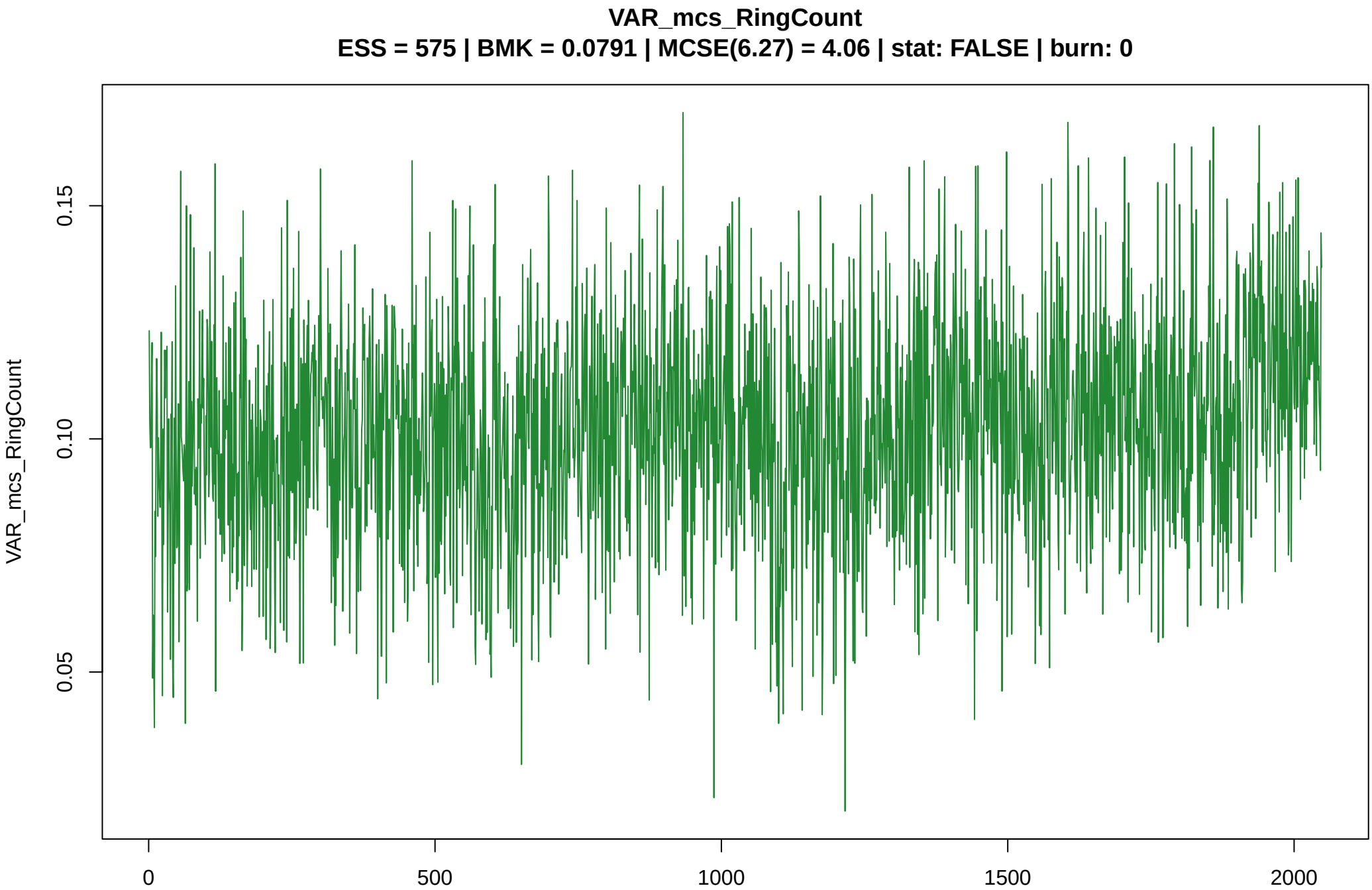

MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0387 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0
MEAN_mcs_template_NumHAcceptors
2.06
2.04
2.02
2.00
1.98
1.96
1.94
0
500
1000
1500
2000

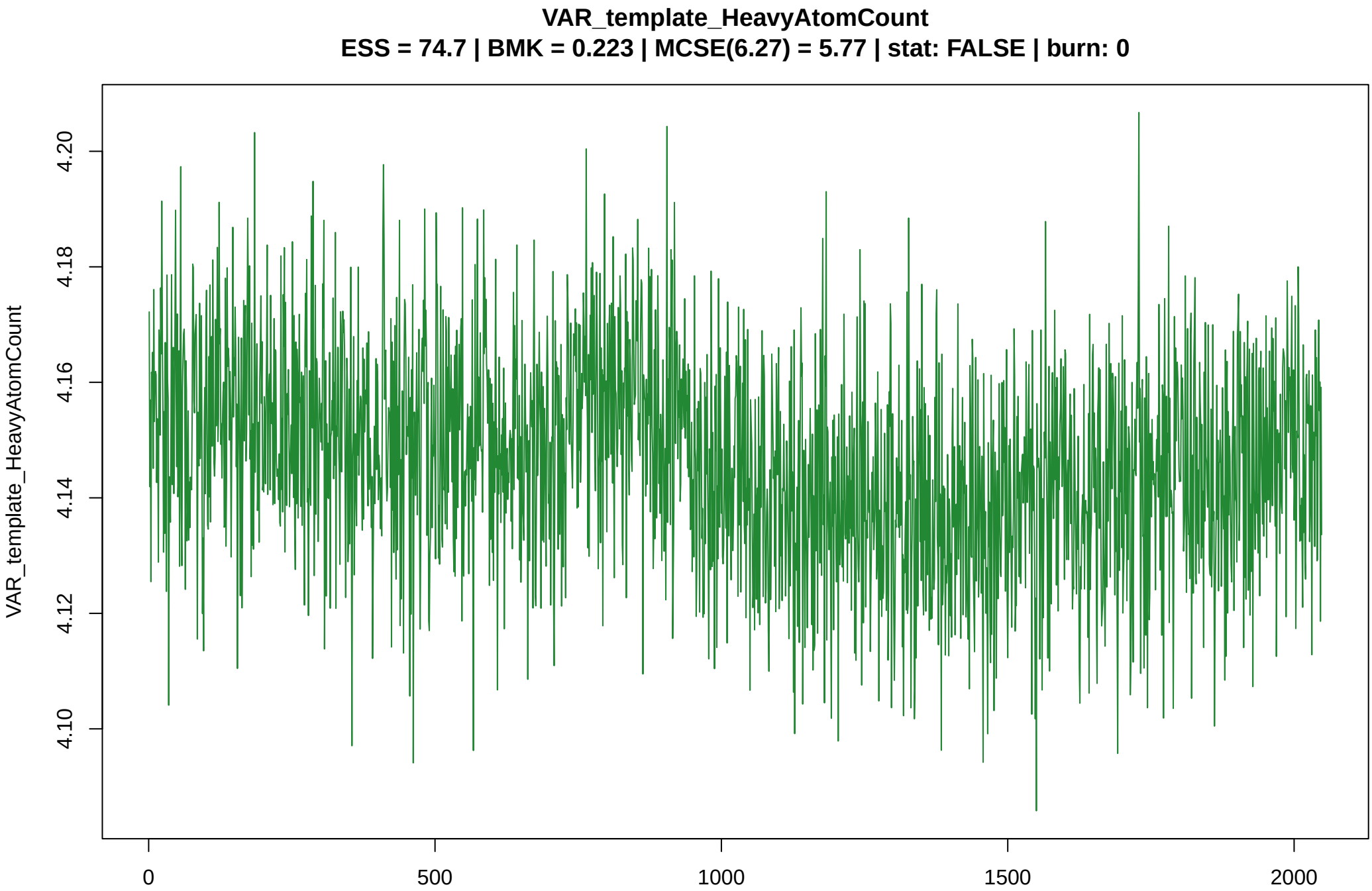

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0352 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.20
3.25
3.30
0
500
1000
1500
2000

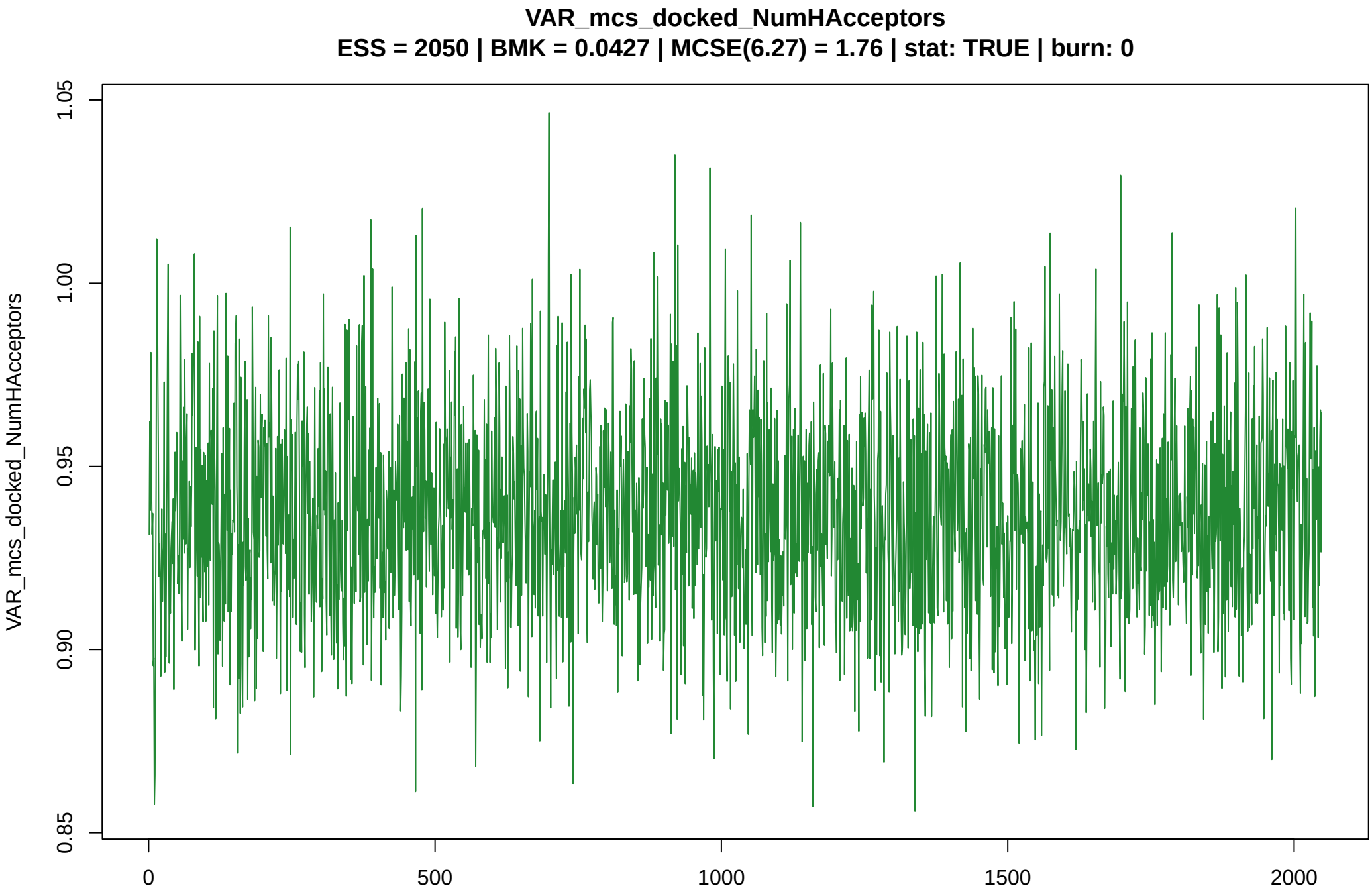

VAR_log_RMSD
ESS = 2050 | BMK = 0.174 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0
VAR_log_RMSD
0
1
2
3
0
500
1000
1500
2000

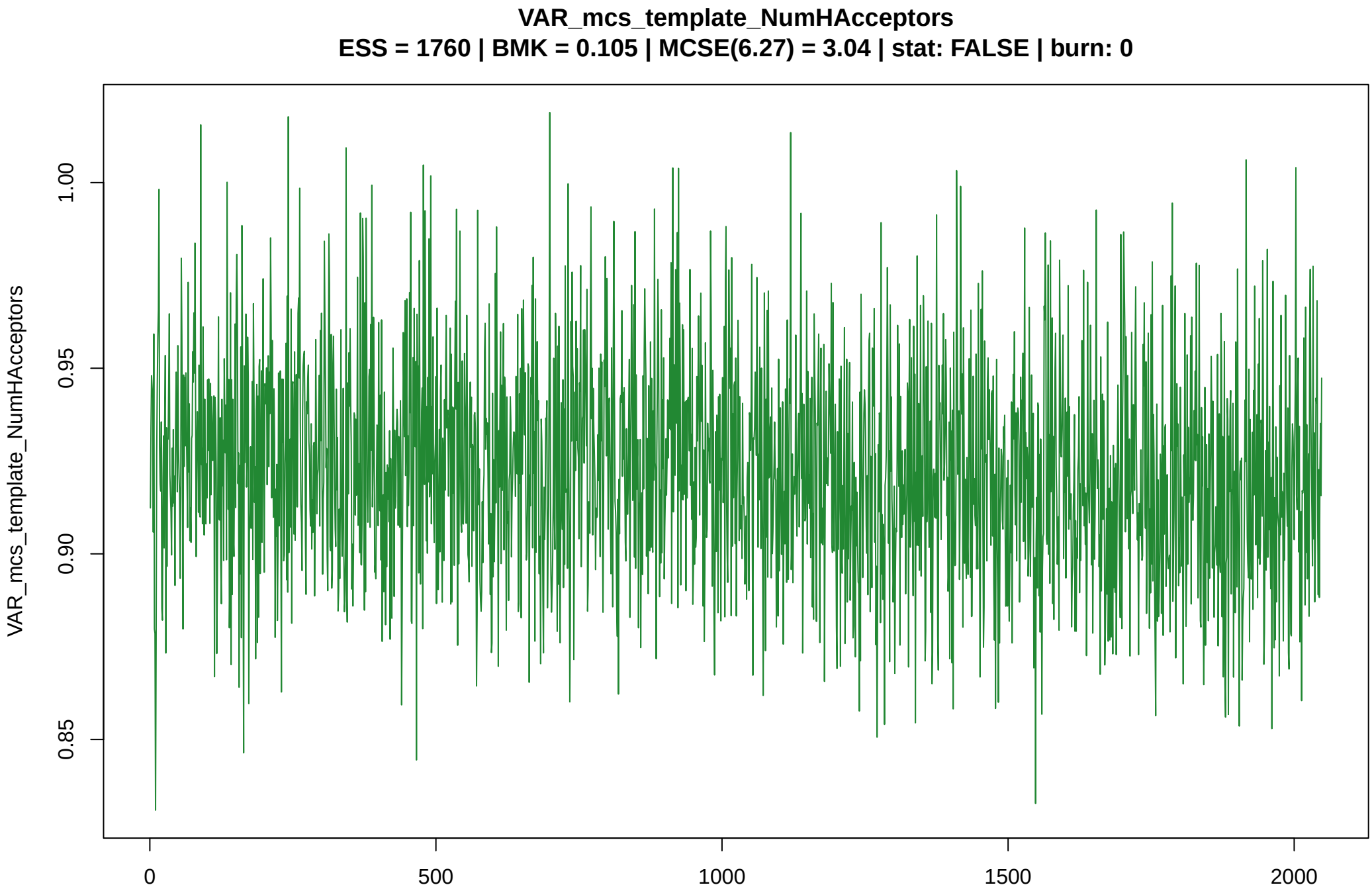

VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.155 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 612
VAR_Xtransf_ec_tanimoto_similarity
1
2
3
4
5
0
500
1000
1500
2000

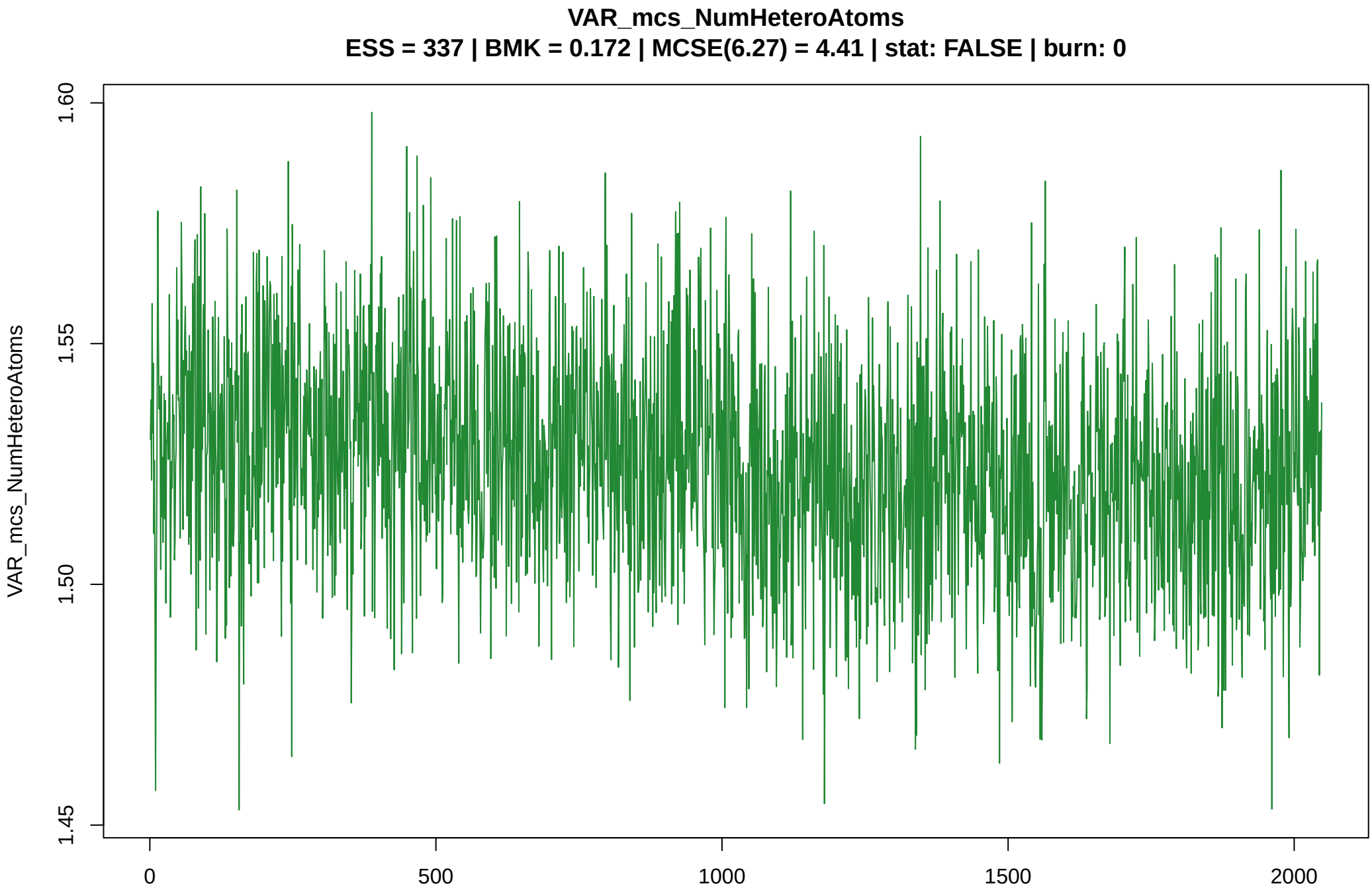

VAR_docked_HeavyAtomCount
ESS = 1830 | BMK = 0.044 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0
VAR_docked_HeavyAtomCount
4.18
4.20
4.22
4.24
4.26
4.28
0
500
1000
1500
2000

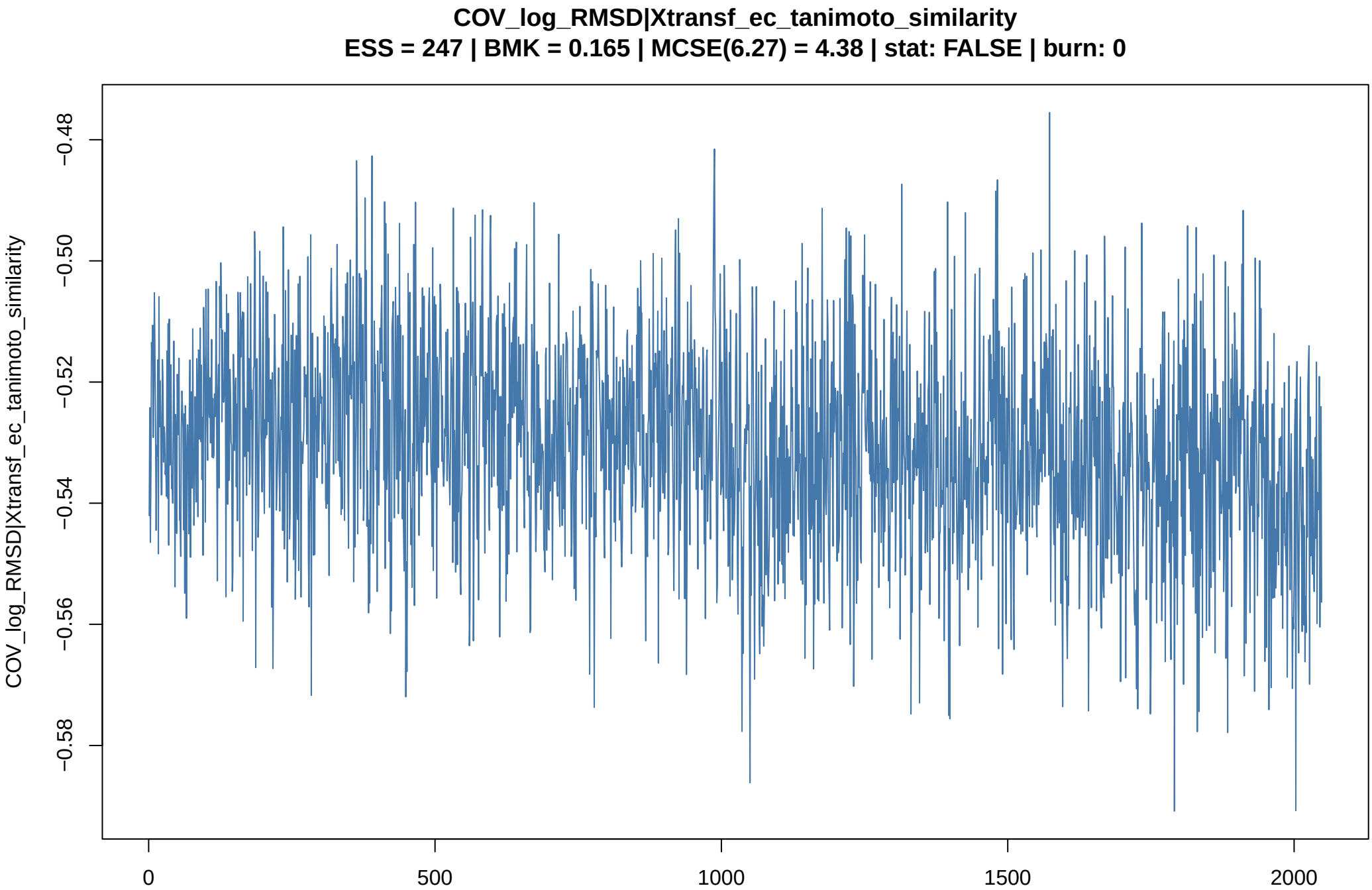

VAR_mcs_RingCount
ESS = 575 | BMK = 0.0791 | MCSE(6.27) = 4.06 | stat: FALSE | burn: 0
VAR_mcs_RingCount
0.05
0.10
0.15
0
500
1000
1500
2000

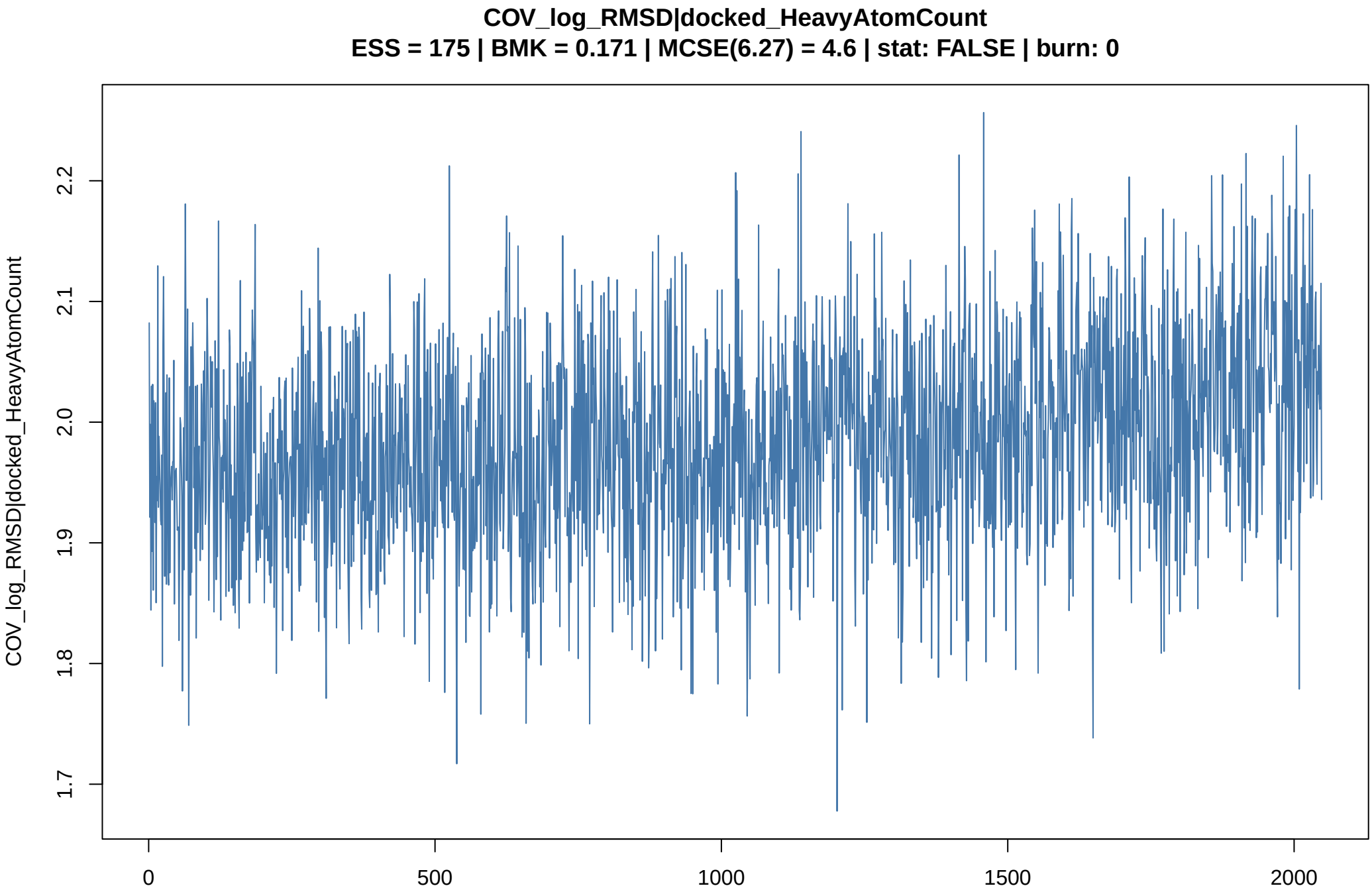

VAR_template_HeavyAtomCount
ESS = 74.7 | BMK = 0.223 | MCSE(6.27) = 5.77 | stat: FALSE | burn: 0
VAR_template_HeavyAtomCount
4.10
4.12
4.14
4.16
4.18
4.20
0
500
1000
1500
2000

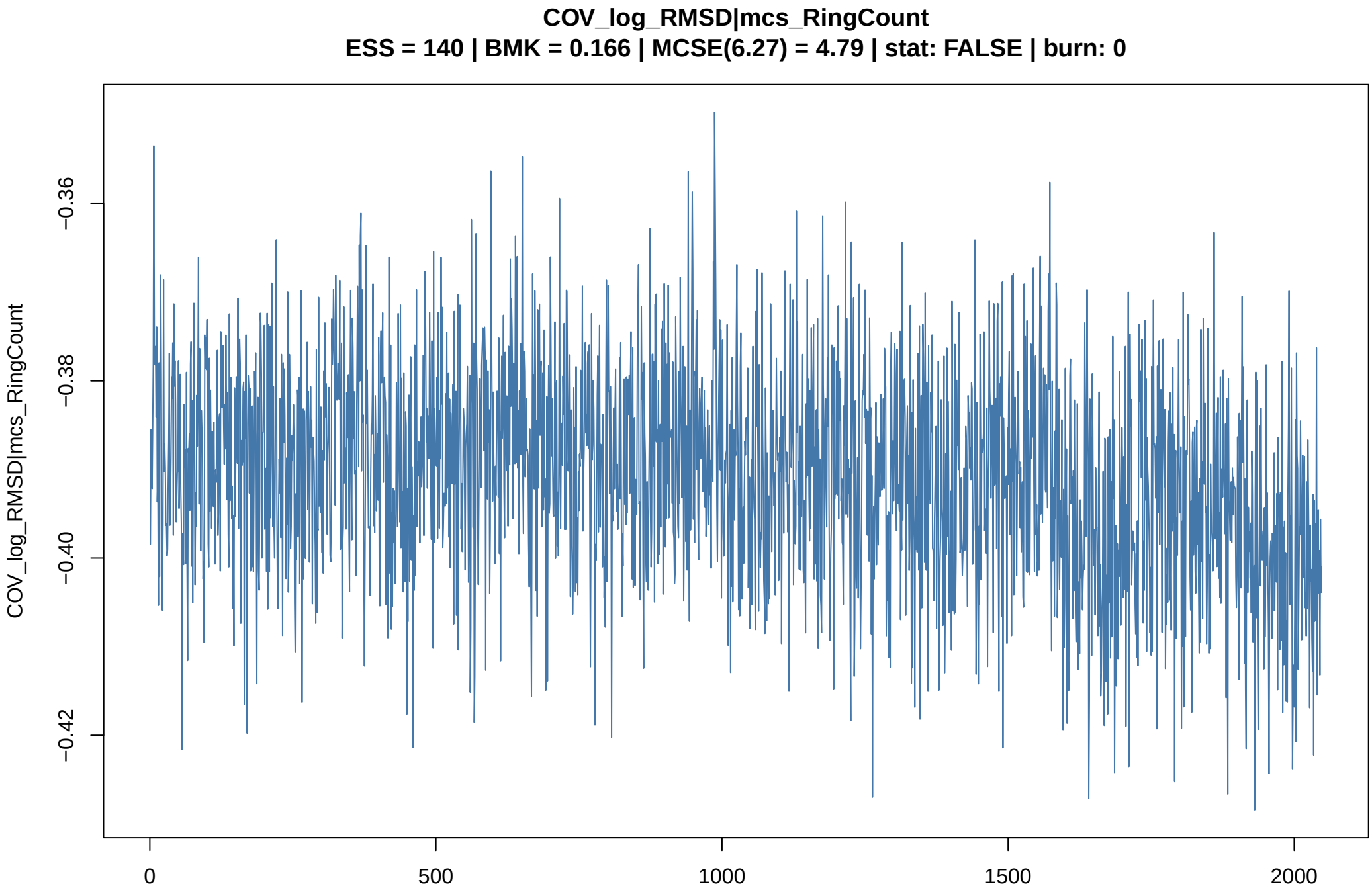

VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0427 | MCSE(6.27) = 1.76 | stat: TRUE | burn: 0
VAR_mcs_docked_NumHAcceptors
1.05
1.00
0.95
0.90
0.85
0
500
1000
1500
2000

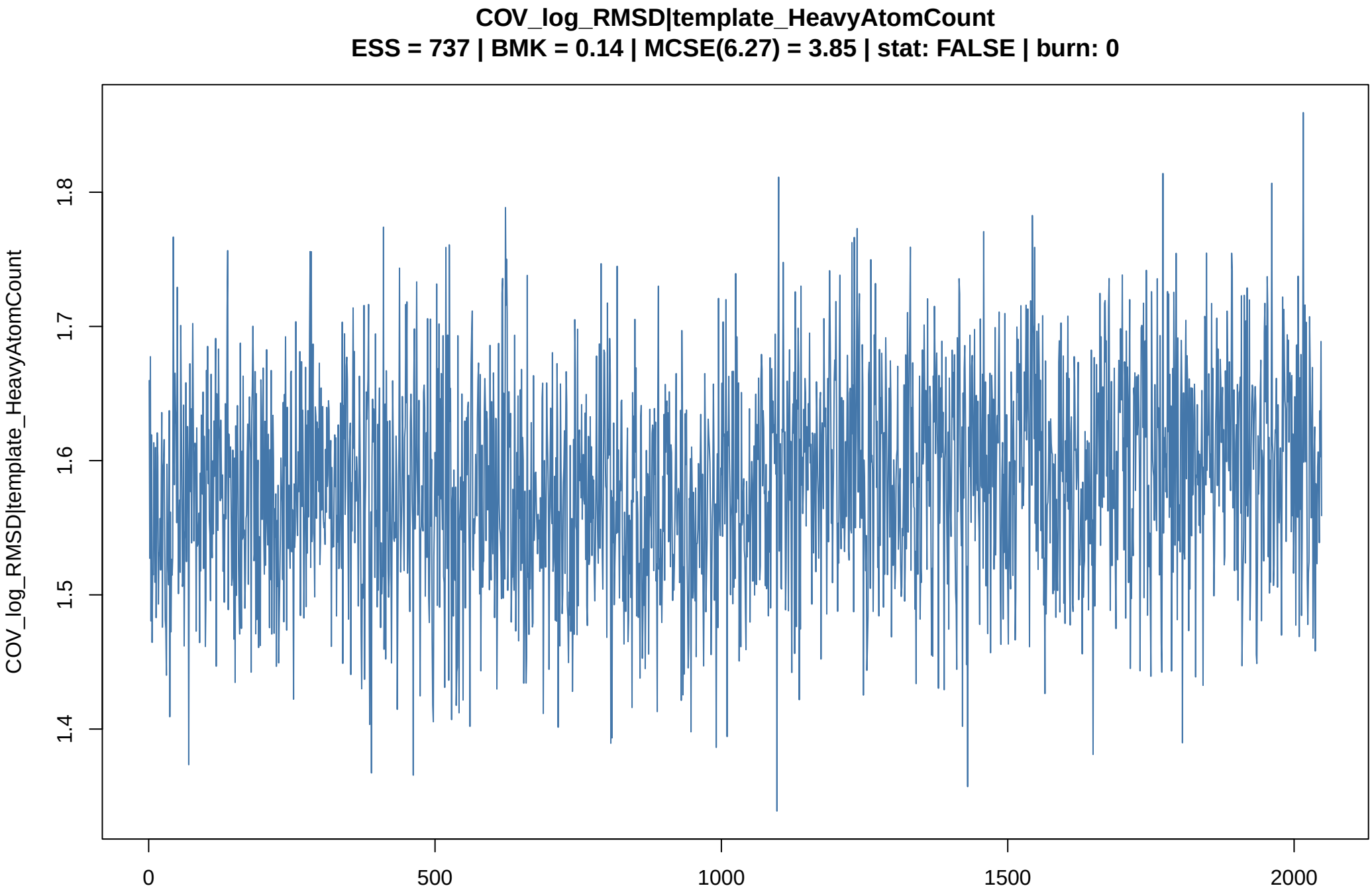

VAR_mcs_template_NumHAcceptors
ESS = 1760 | BMK = 0.105 | MCSE(6.27) = 3.04 | stat: FALSE | burn: 0
VAR_mcs_template_NumHAcceptors
0.85
0.90
0.95
1.00
0
500
1000
1500
2000

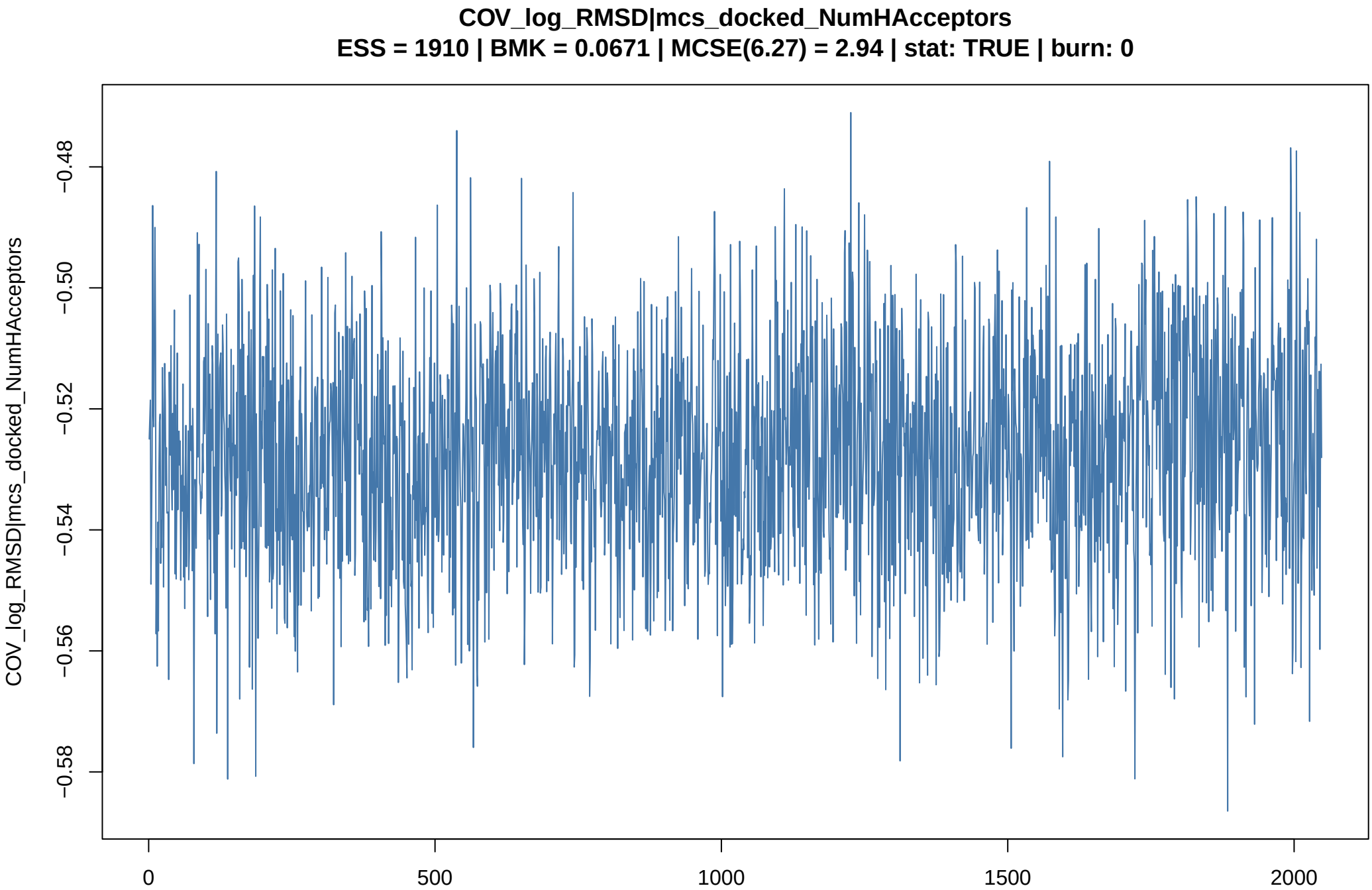

VAR_mcs_NumHeteroAtoms
ESS = 337 | BMK = 0.172 | MCSE(6.27) = 4.41 | stat: FALSE | burn: 0
VAR_mcs_NumHeteroAtoms
1.60
1.55
1.50
1.45
0
500
1000
1500
2000

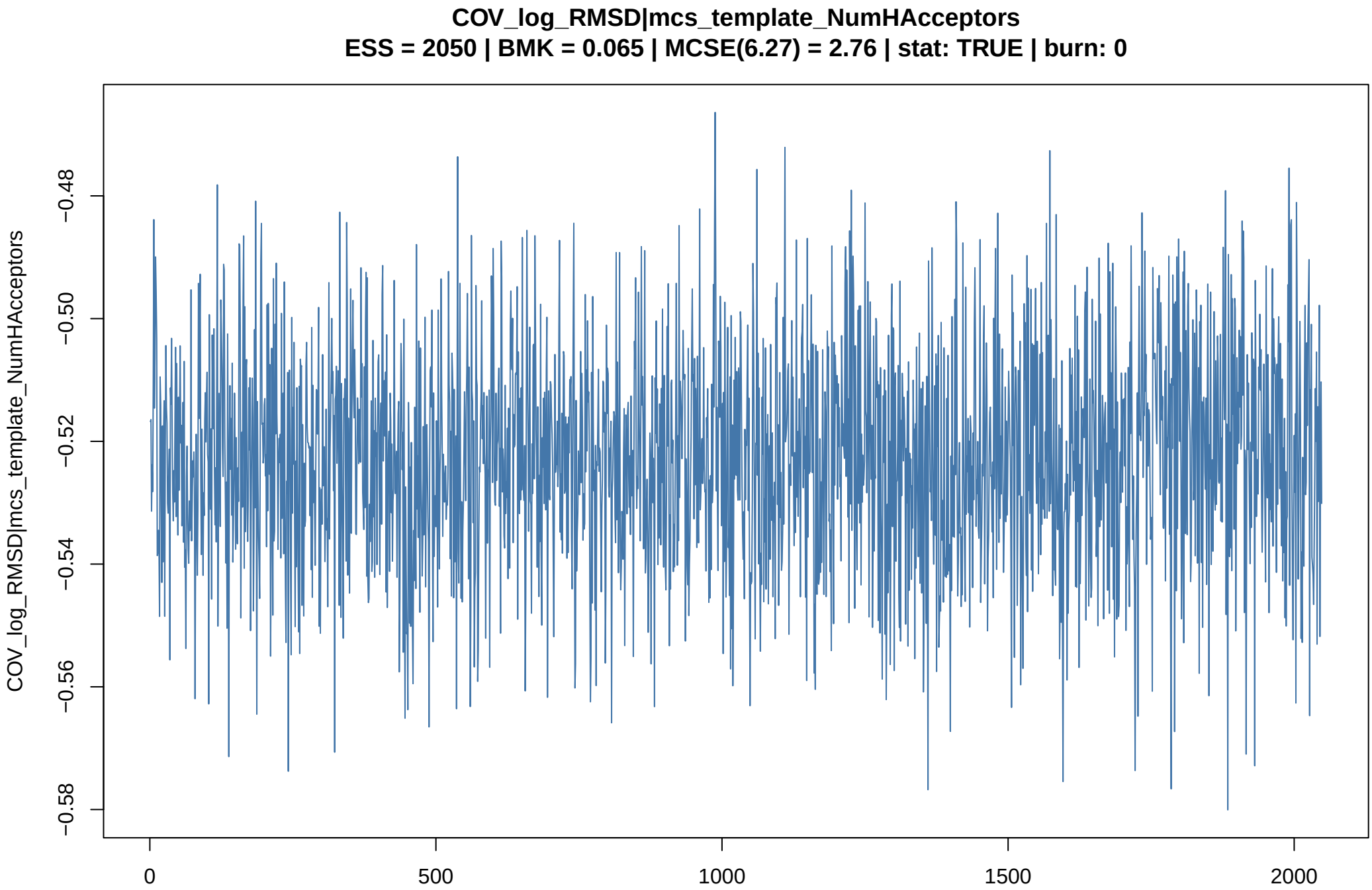

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 247 | BMK = 0.165 | MCSE(6.27) = 4.38 | stat: FALSE | burn: 0
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

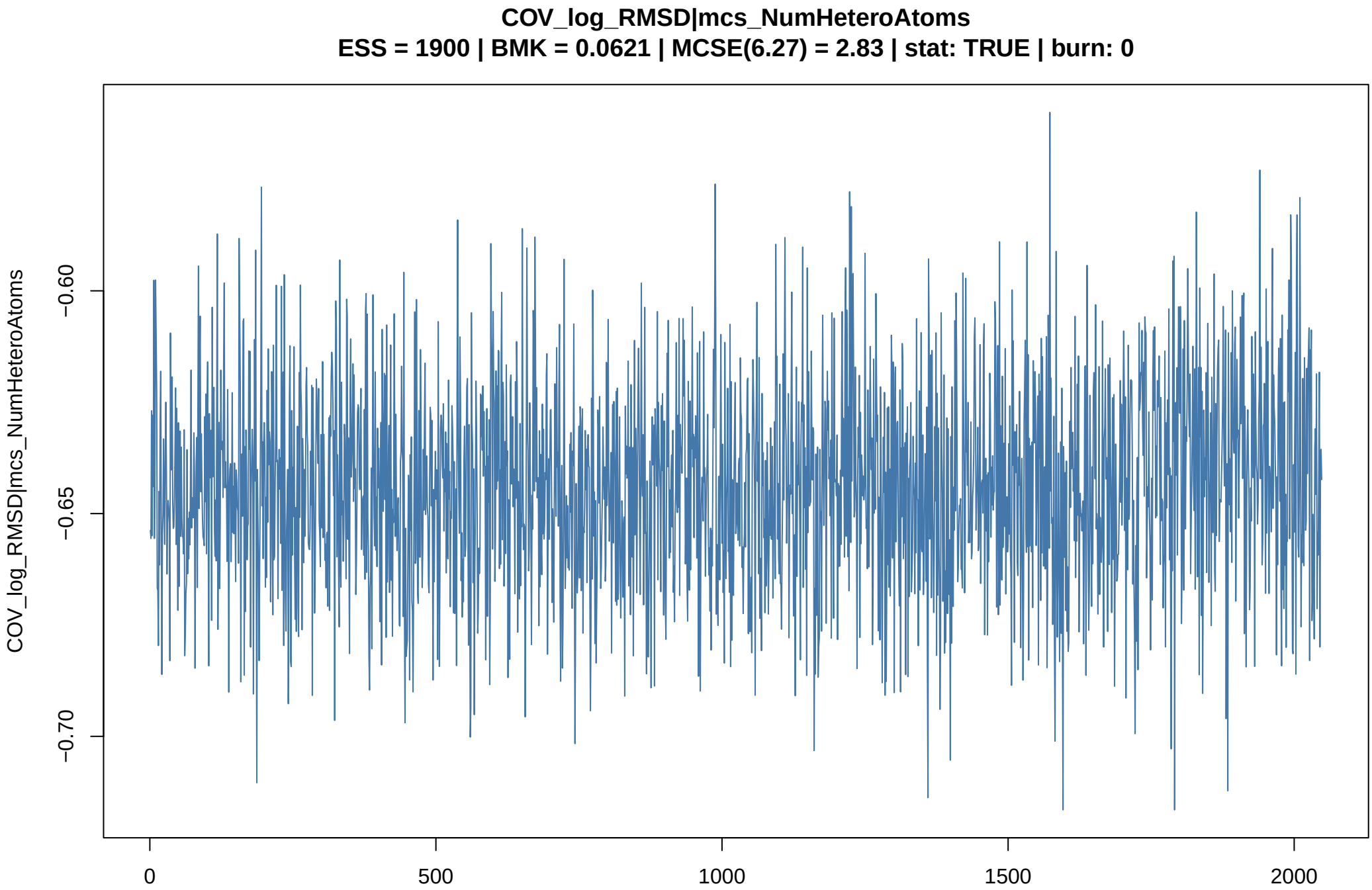

COV_log_RMSD|docked_HeavyAtomCount
ESS = 175 | BMK = 0.171 | MCSE(6.27) = 4.6 | stat: FALSE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
1.7
1.8
1.9
2.0
2.1
2.2
0
500
1000
1500
2000

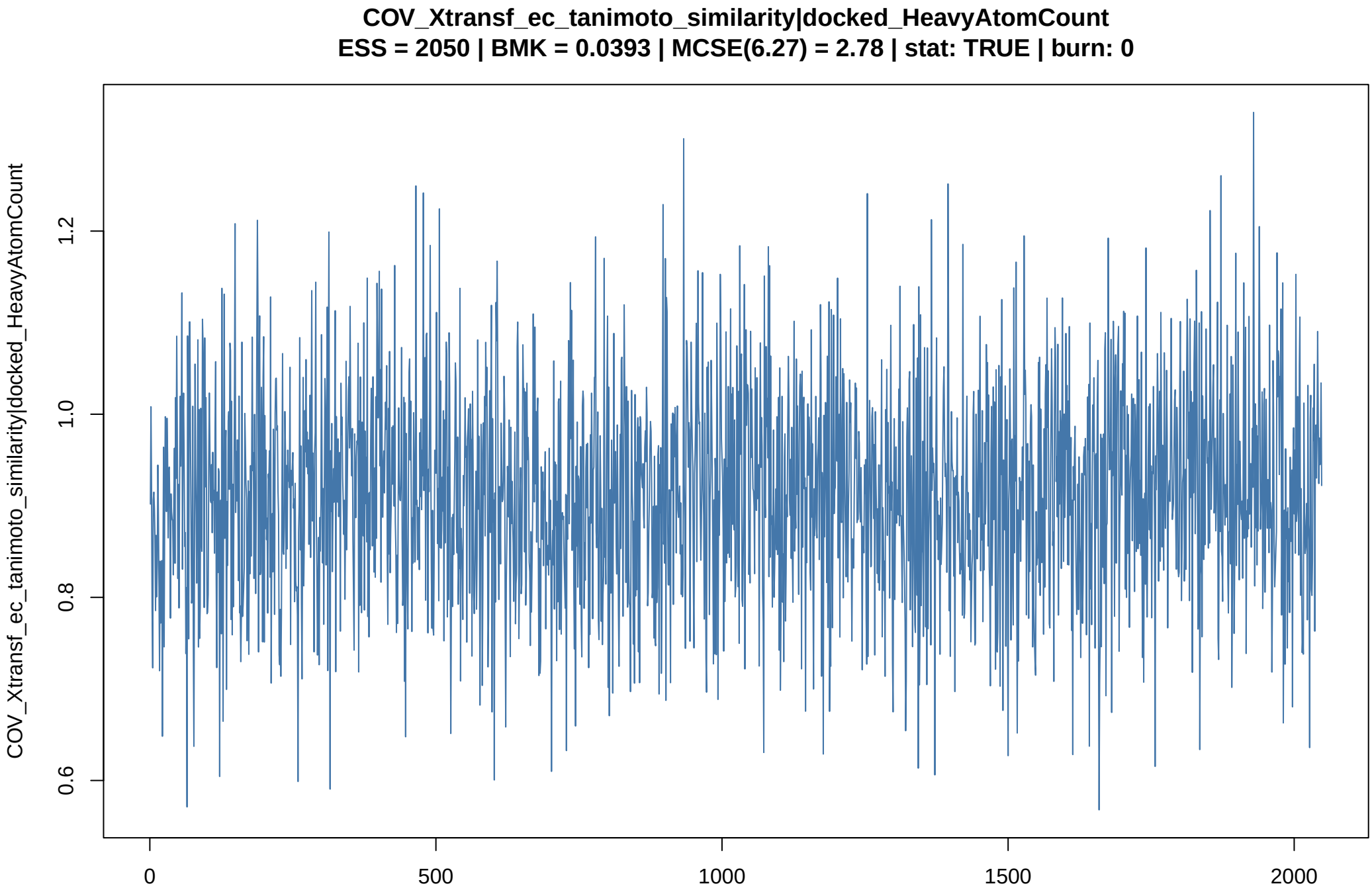

COV_log_RMSD|mcs_RingCount
ESS = 140 | BMK = 0.166 | MCSE(6.27) = 4.79 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.36
−0.38
−0.40
−0.42
0
500
1000
1500
2000

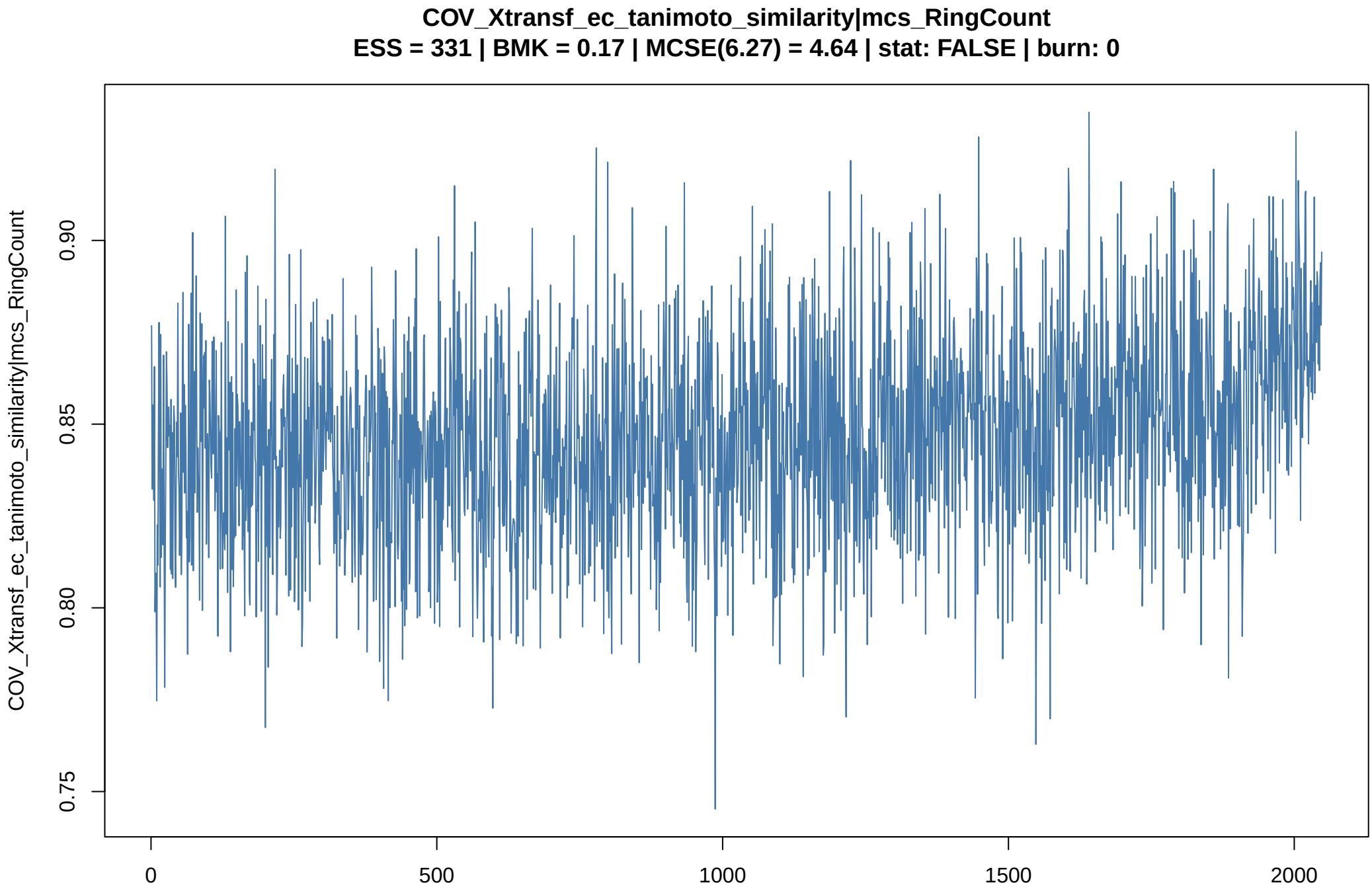

COV_log_RMSD|template_HeavyAtomCount
ESS = 737 | BMK = 0.14 | MCSE(6.27) = 3.85 | stat: FALSE | burn: 0
COV_log_RMSD|template_HeavyAtomCount
1.4
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

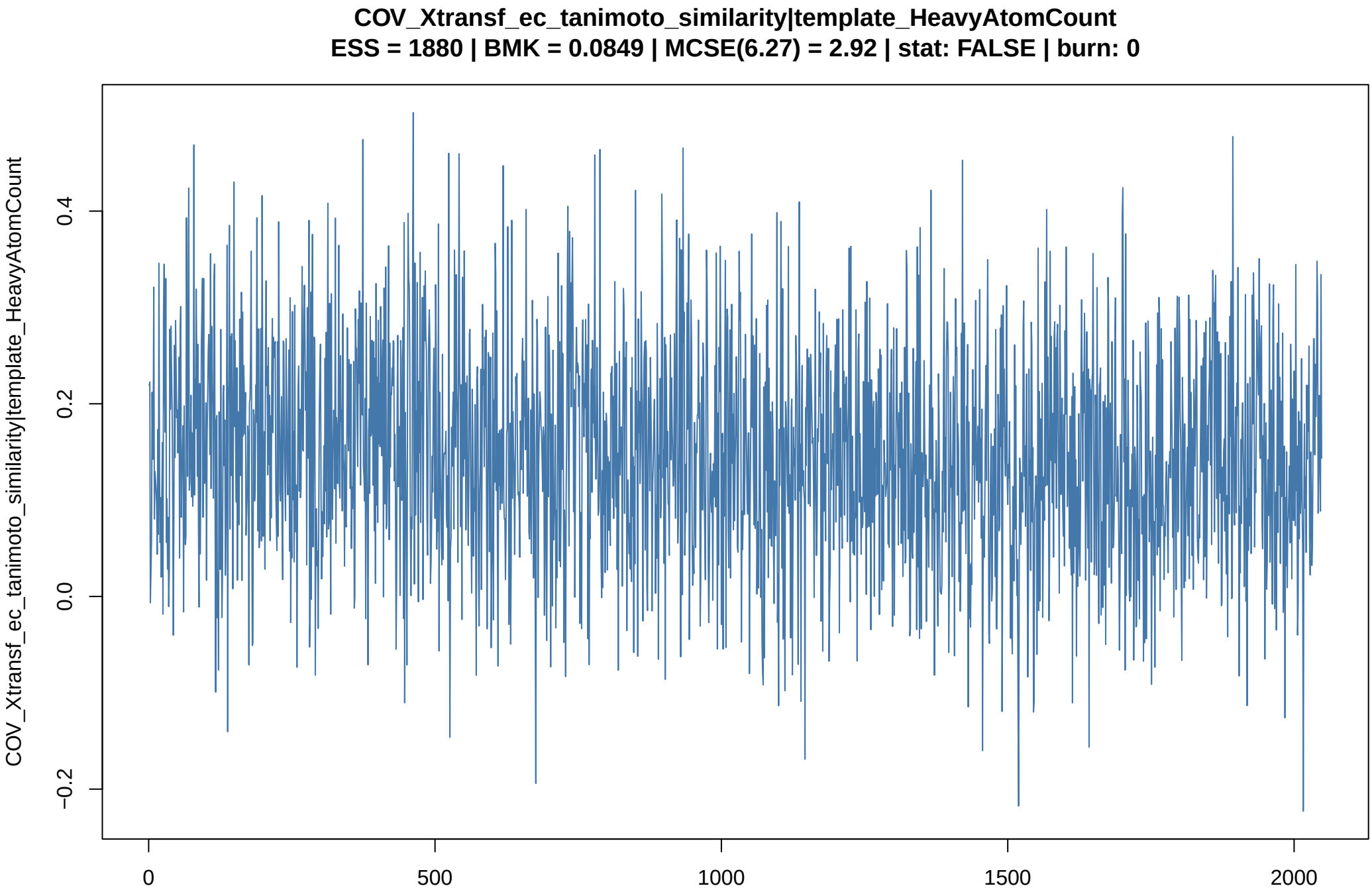

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 1910 | BMK = 0.0671 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_docked_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

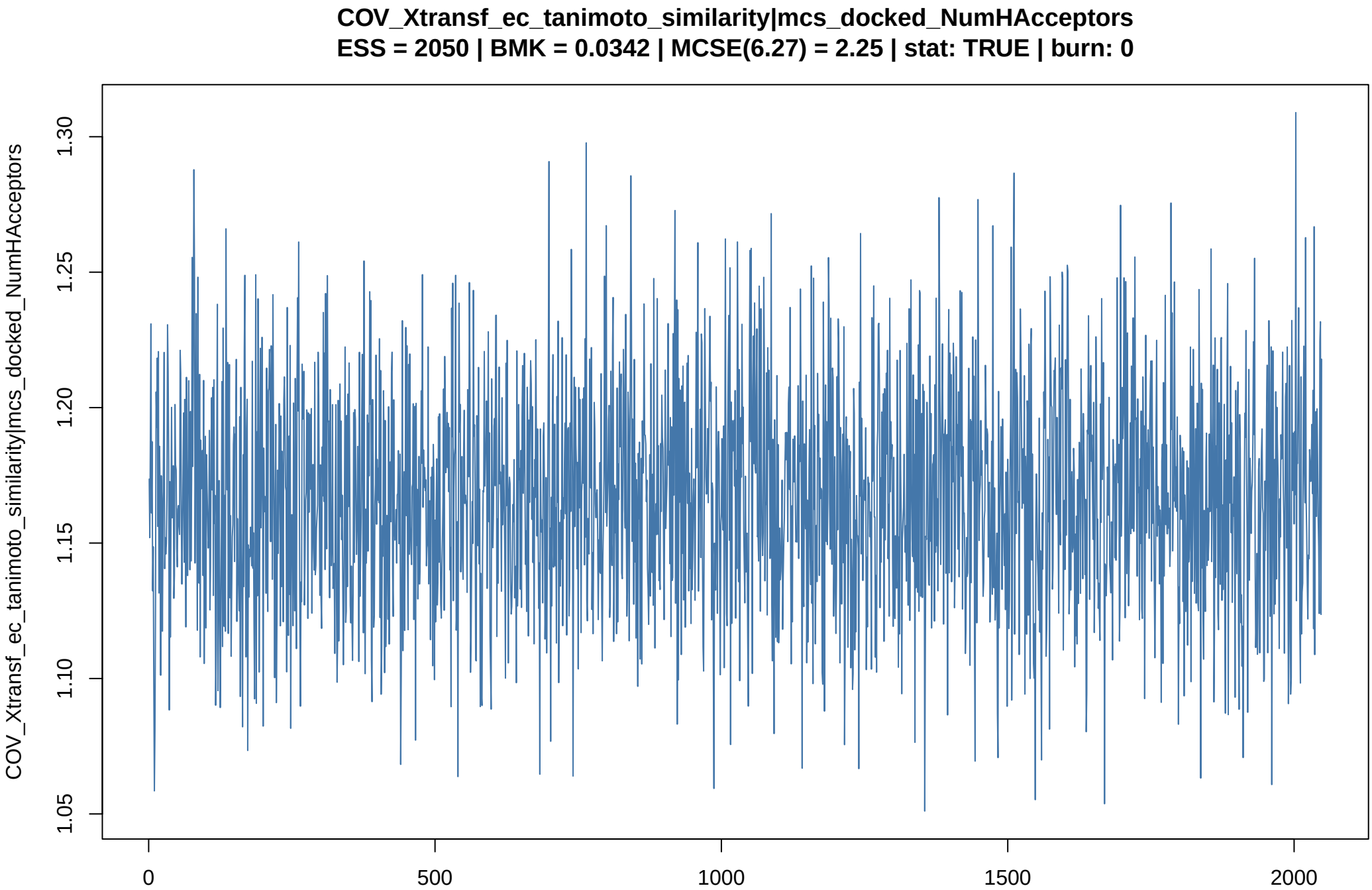

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.065 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_template_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

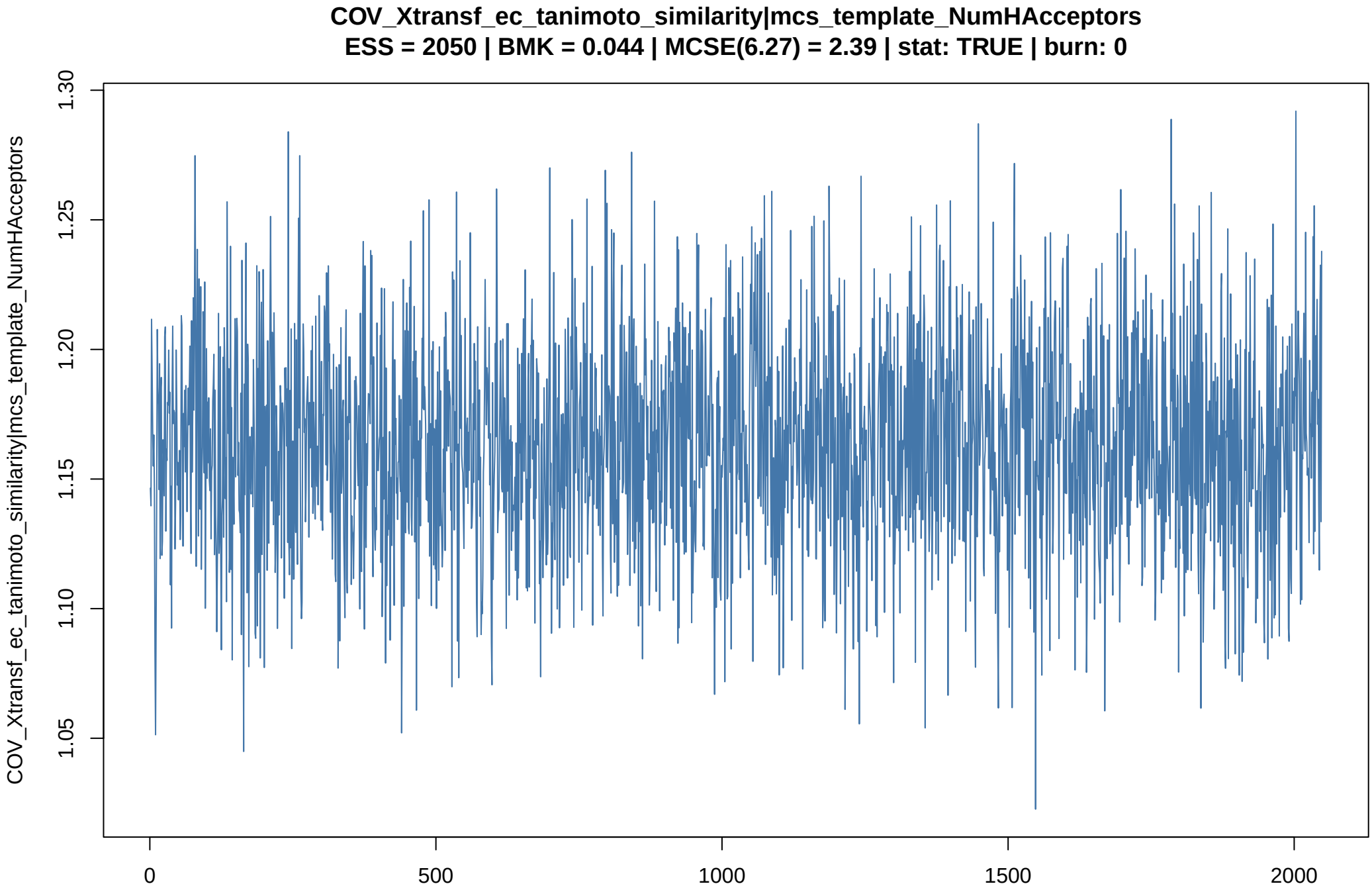

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1900 | BMK = 0.0621 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.60
−0.65
−0.70
0
500
1000
1500
2000

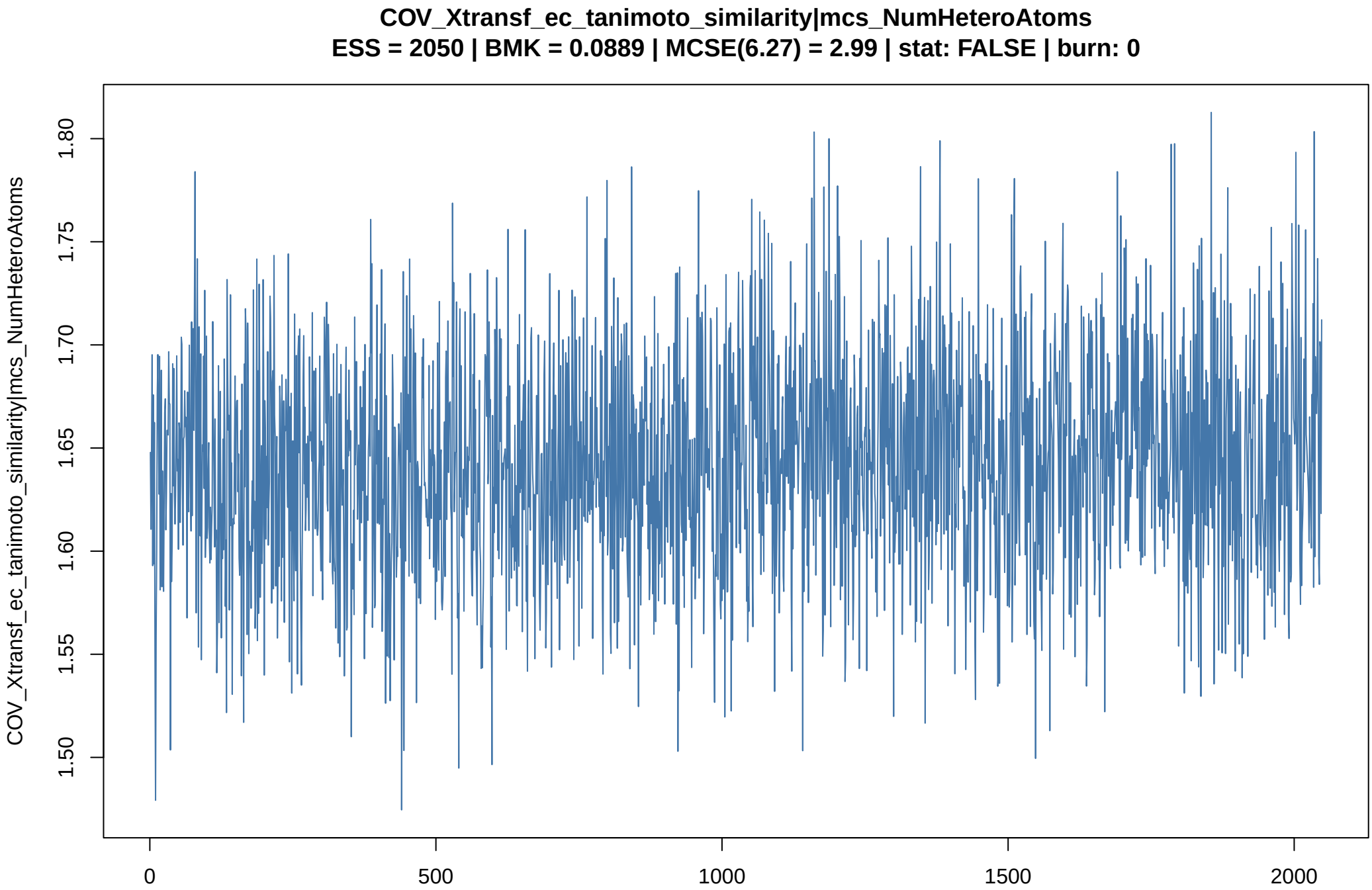

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0393 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

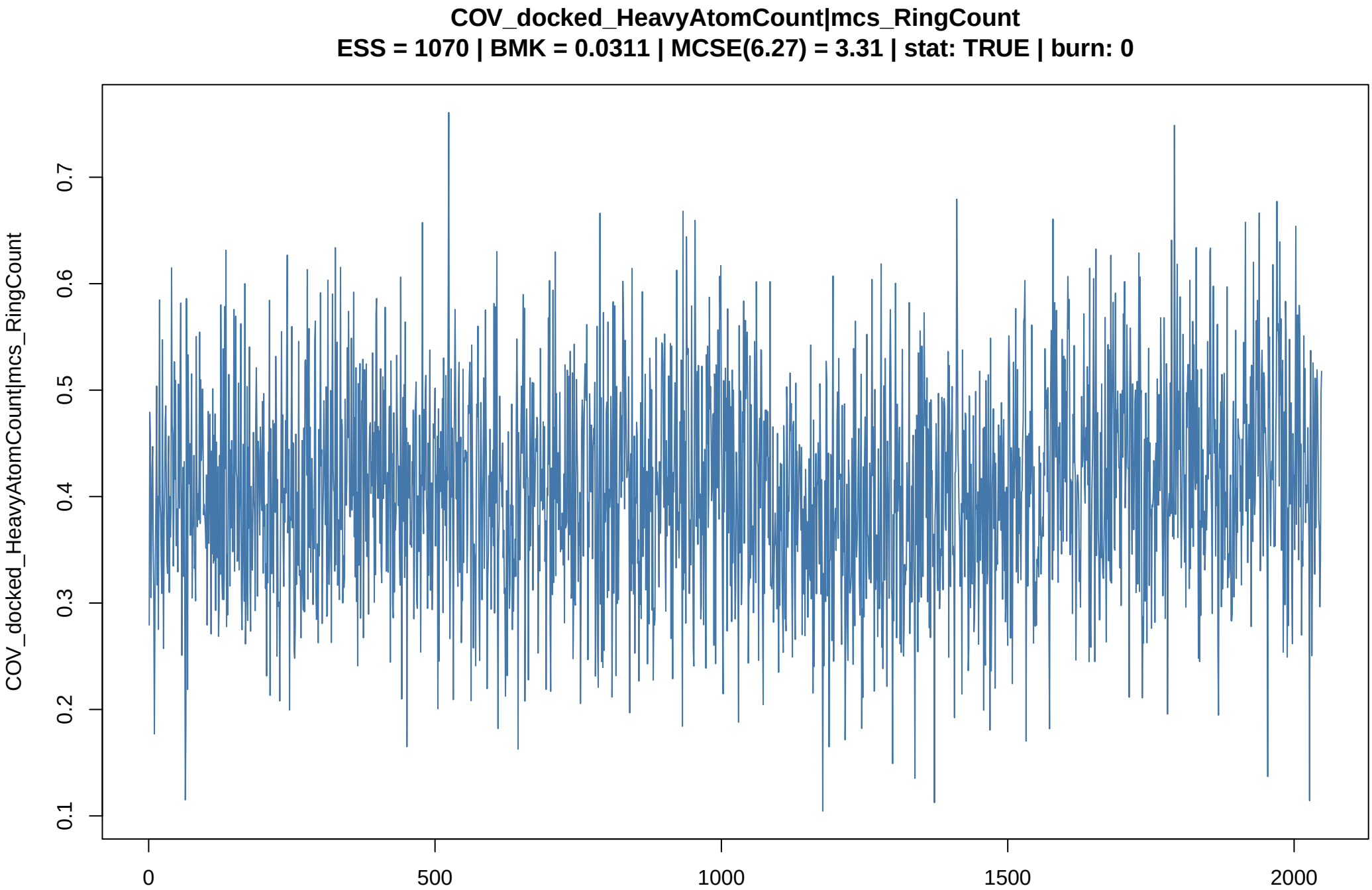

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 331 | BMK = 0.17 | MCSE(6.27) = 4.64 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.75
0.80
0.85
0.90
0
500
1000
1500
2000

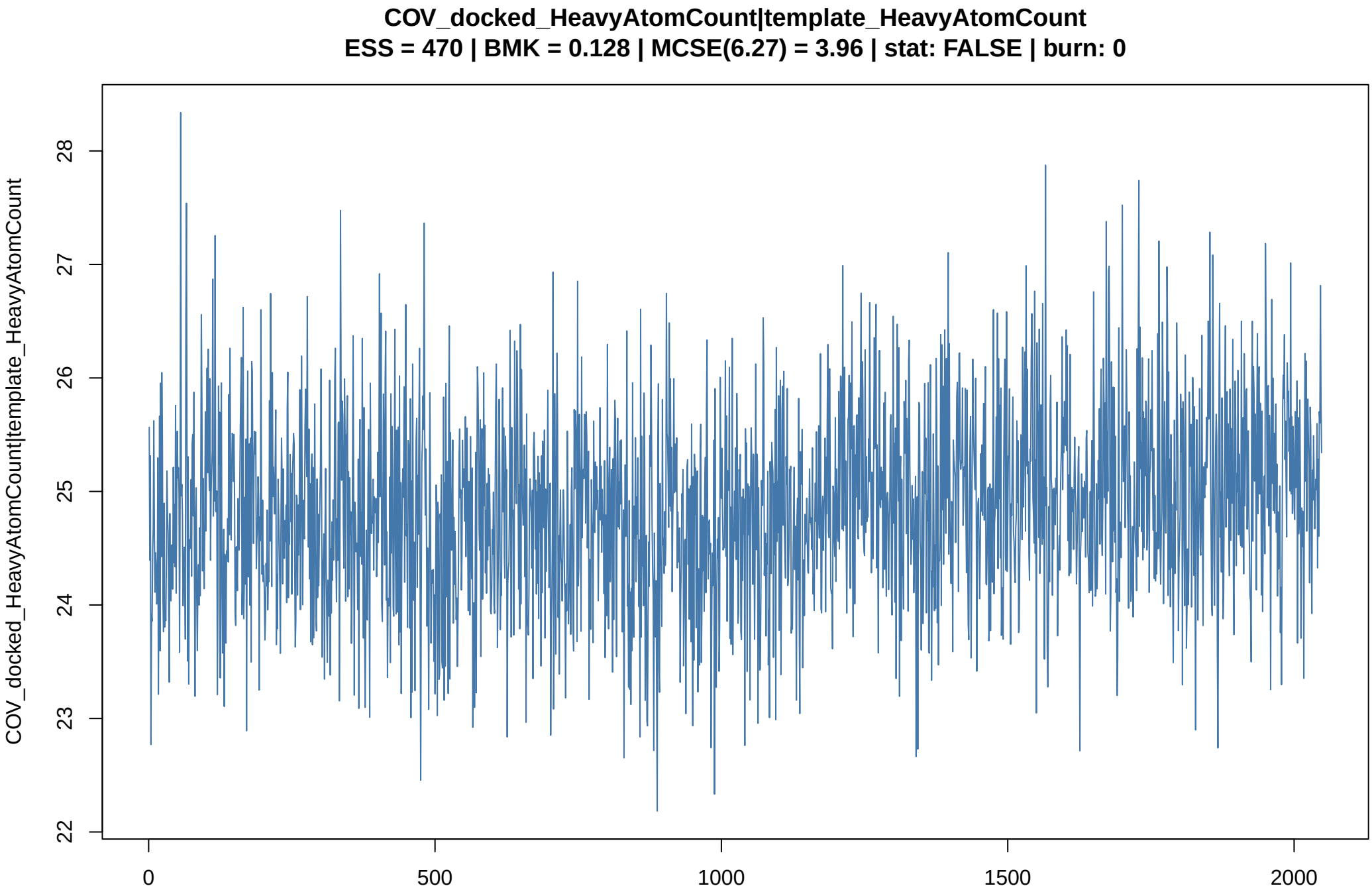

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1880 | BMK = 0.0849 | MCSE(6.27) = 2.92 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
0.4
0.2
0.0
−0.2
0
500
1000
1500
2000

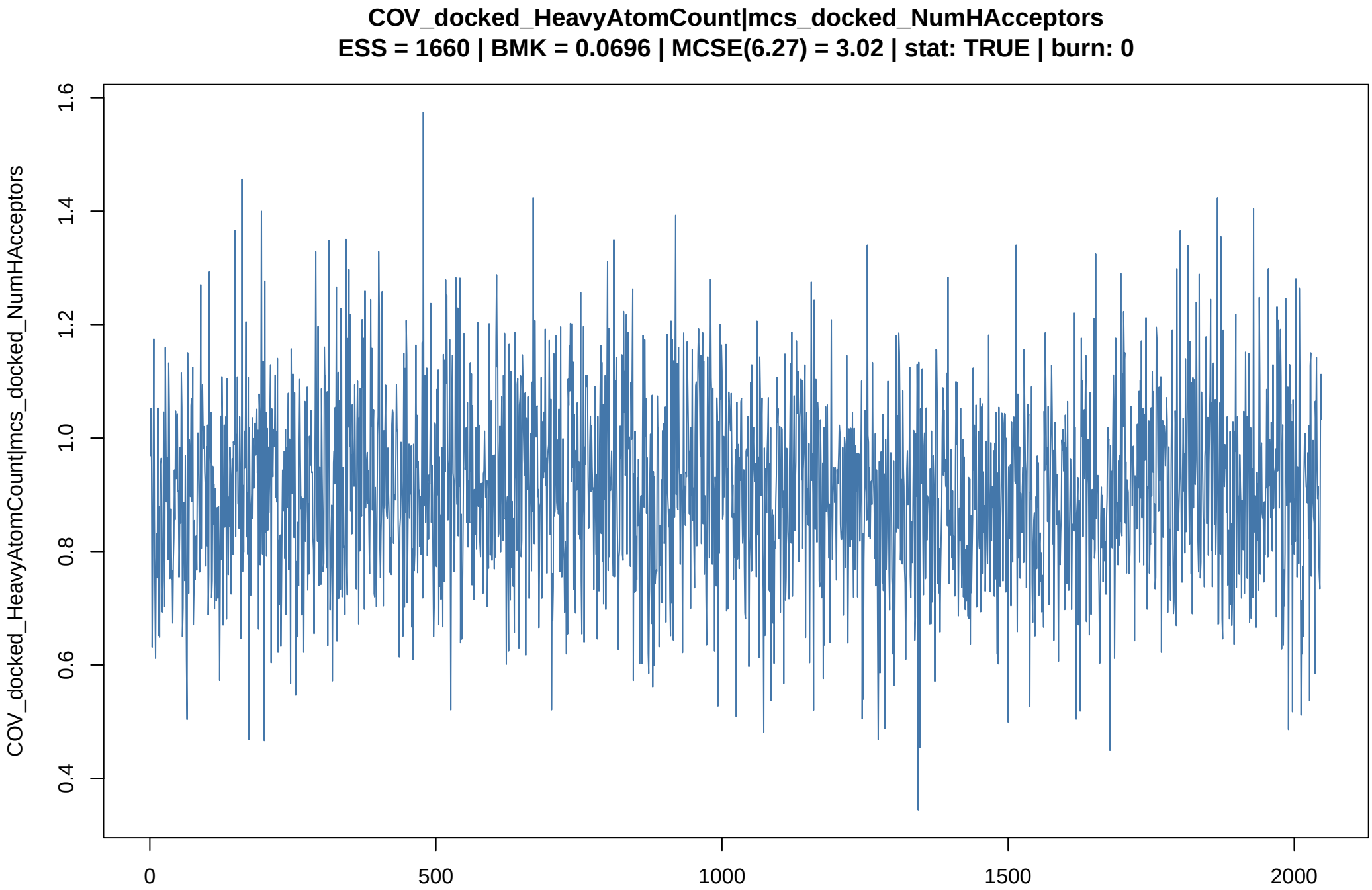

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0342 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

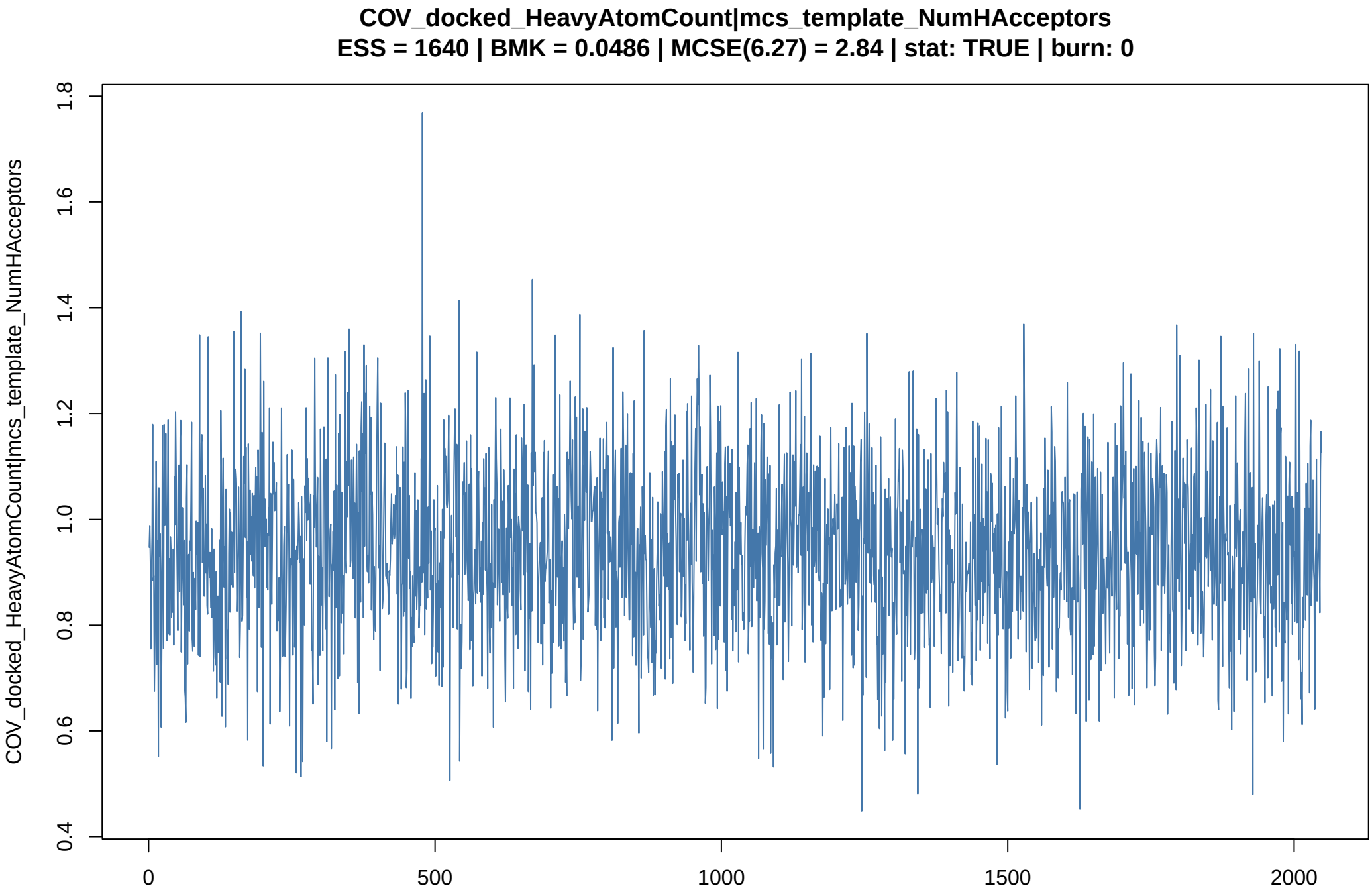

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.044 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

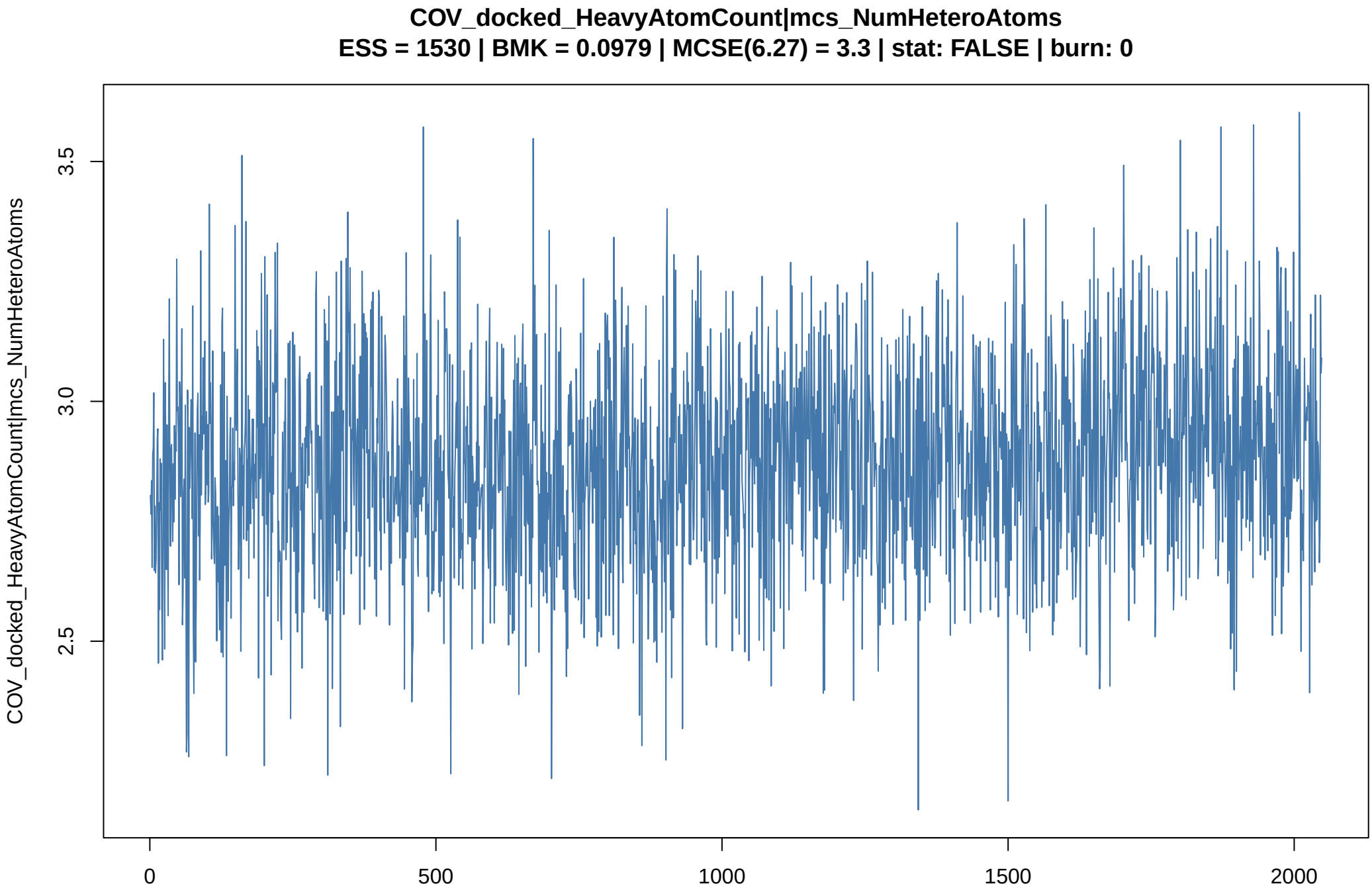

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0889 | MCSE(6.27) = 2.99 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.50
1.55
1.60
1.65
1.70
1.75
1.80
0
500
1000
1500
2000

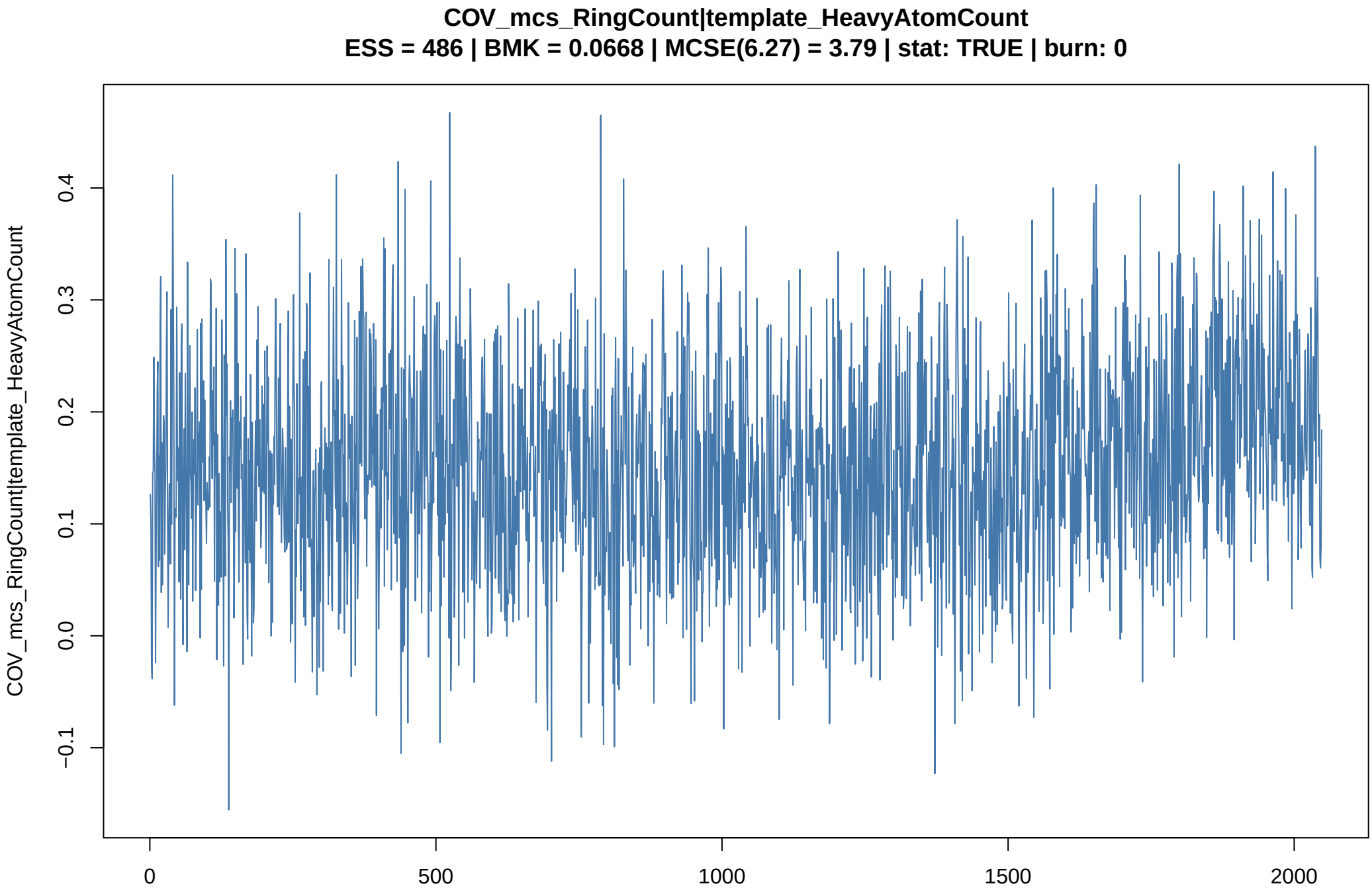

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1070 | BMK = 0.0311 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000

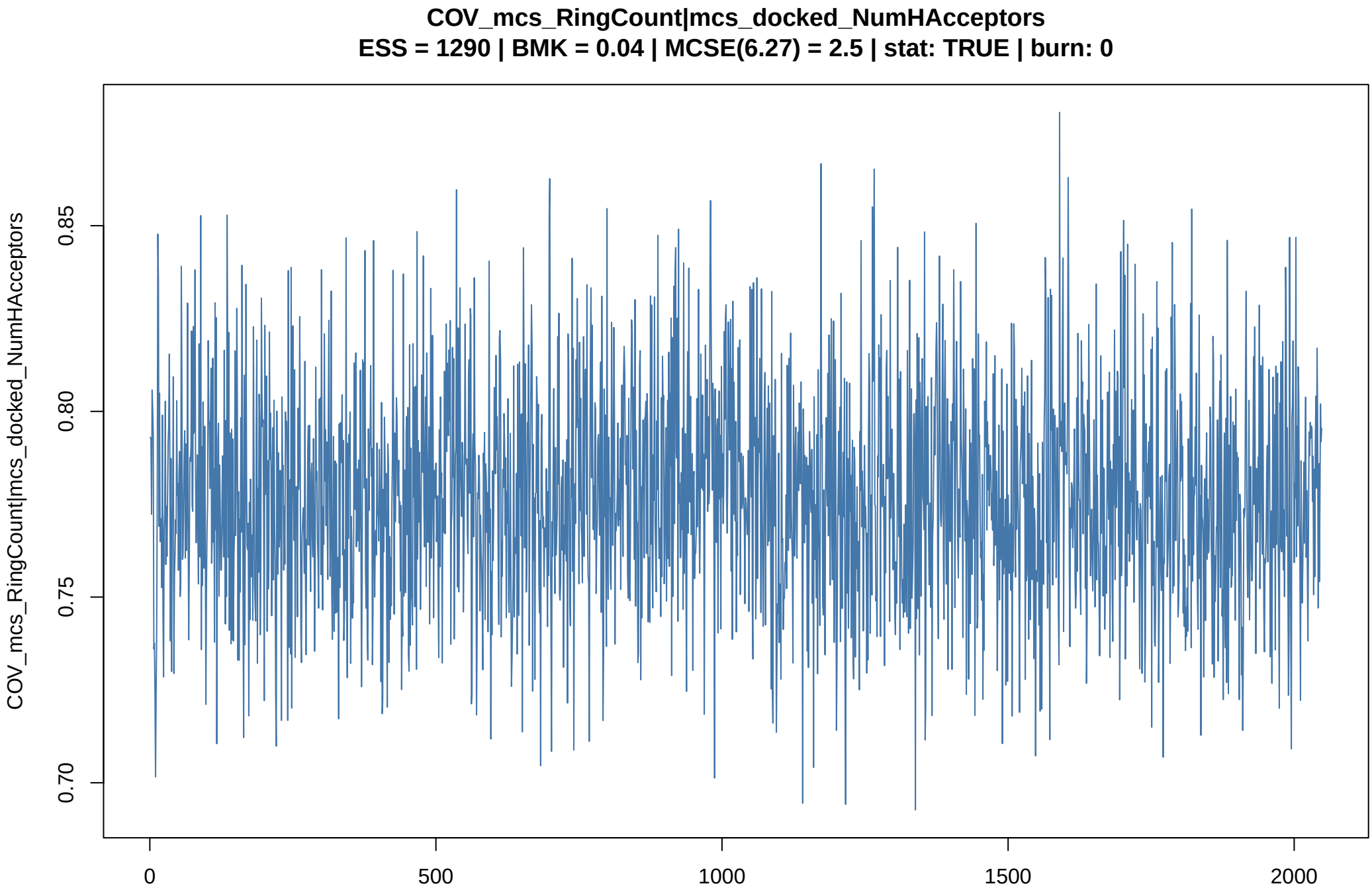

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 470 | BMK = 0.128 | MCSE(6.27) = 3.96 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
22
23
24
25
26
27
28
0
500
1000
1500
2000

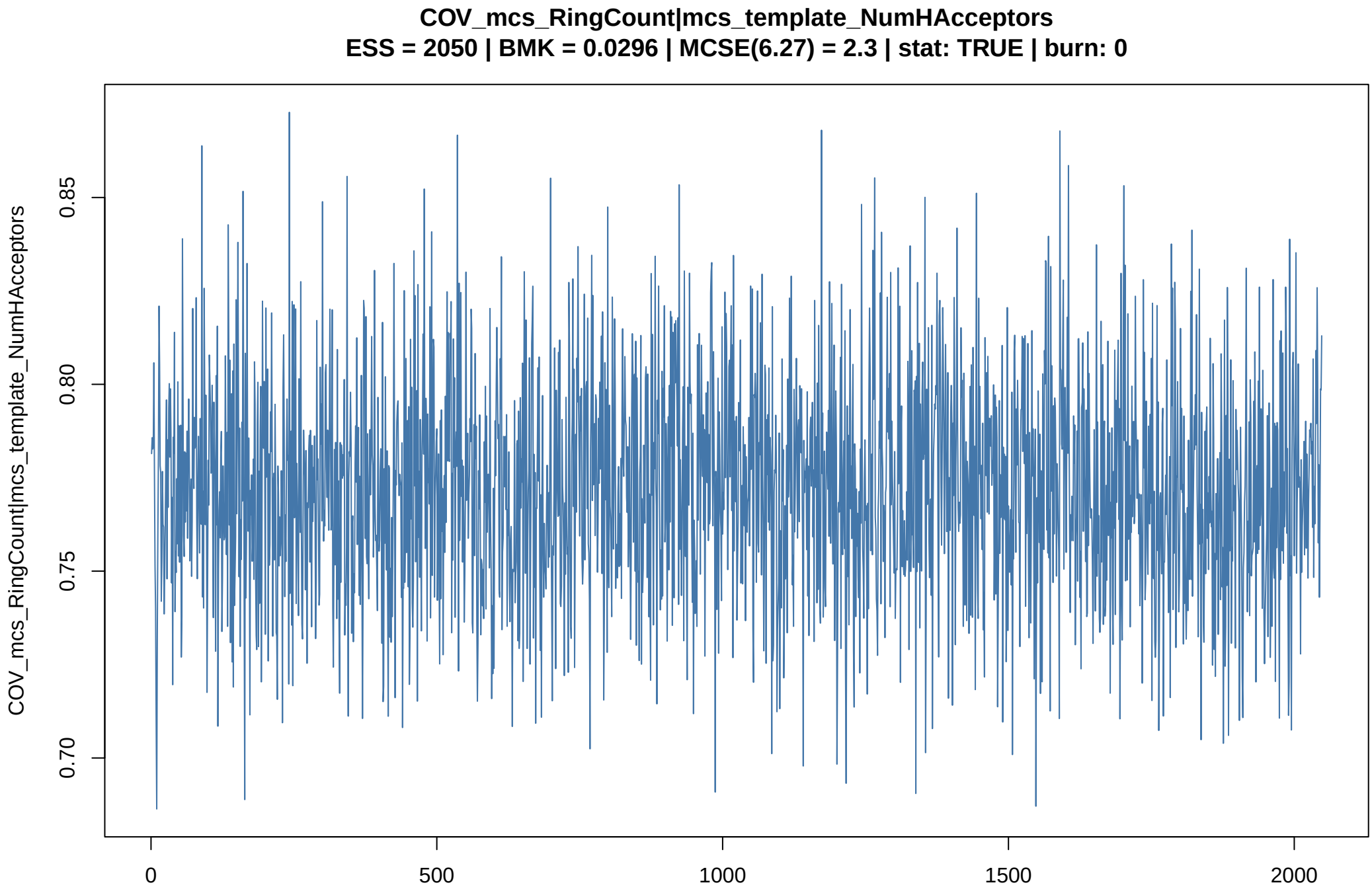

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1660 | BMK = 0.0696 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
500
1000
1500
2000

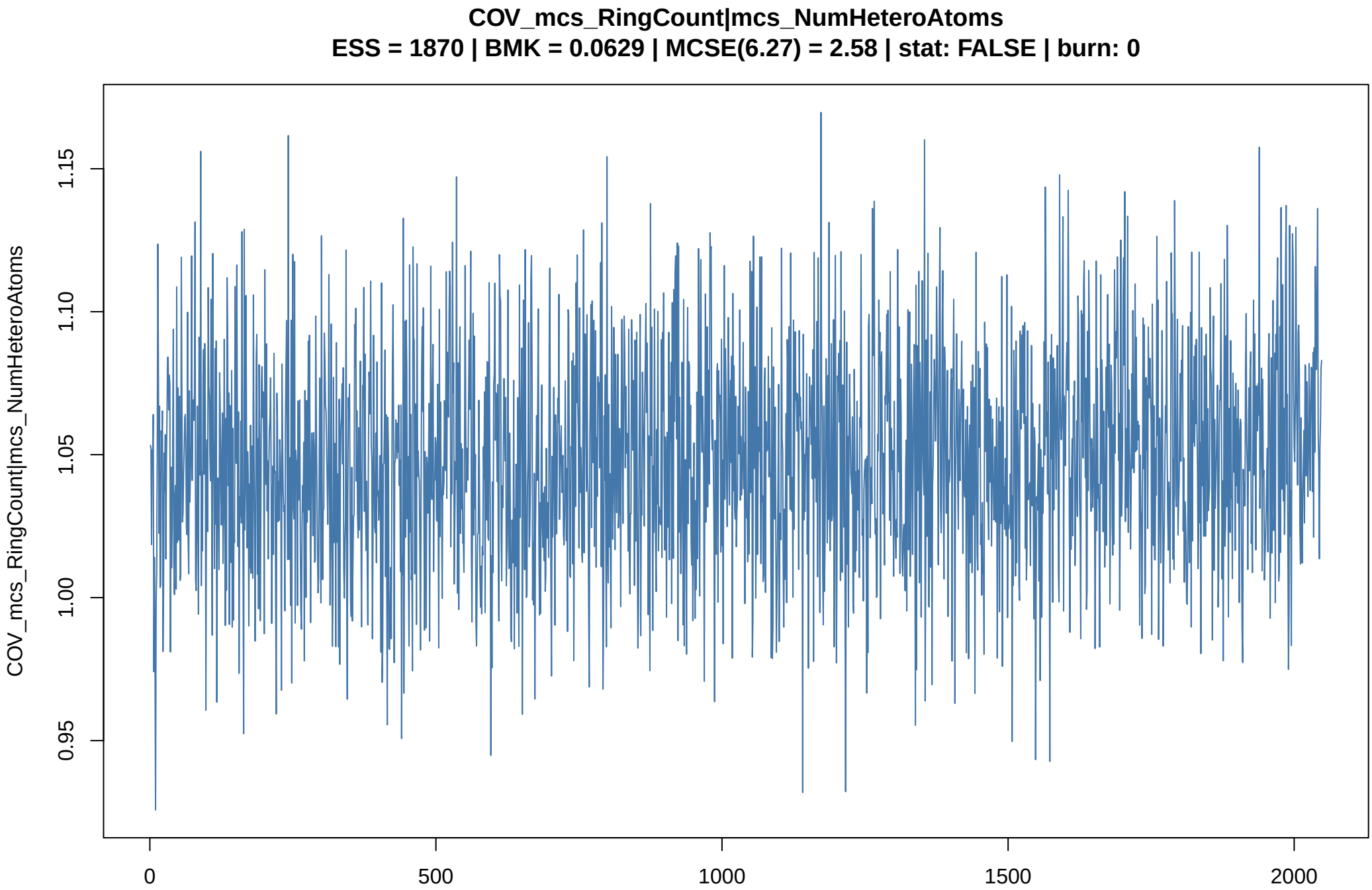

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1640 | BMK = 0.0486 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
0
500
1000
1500
2000

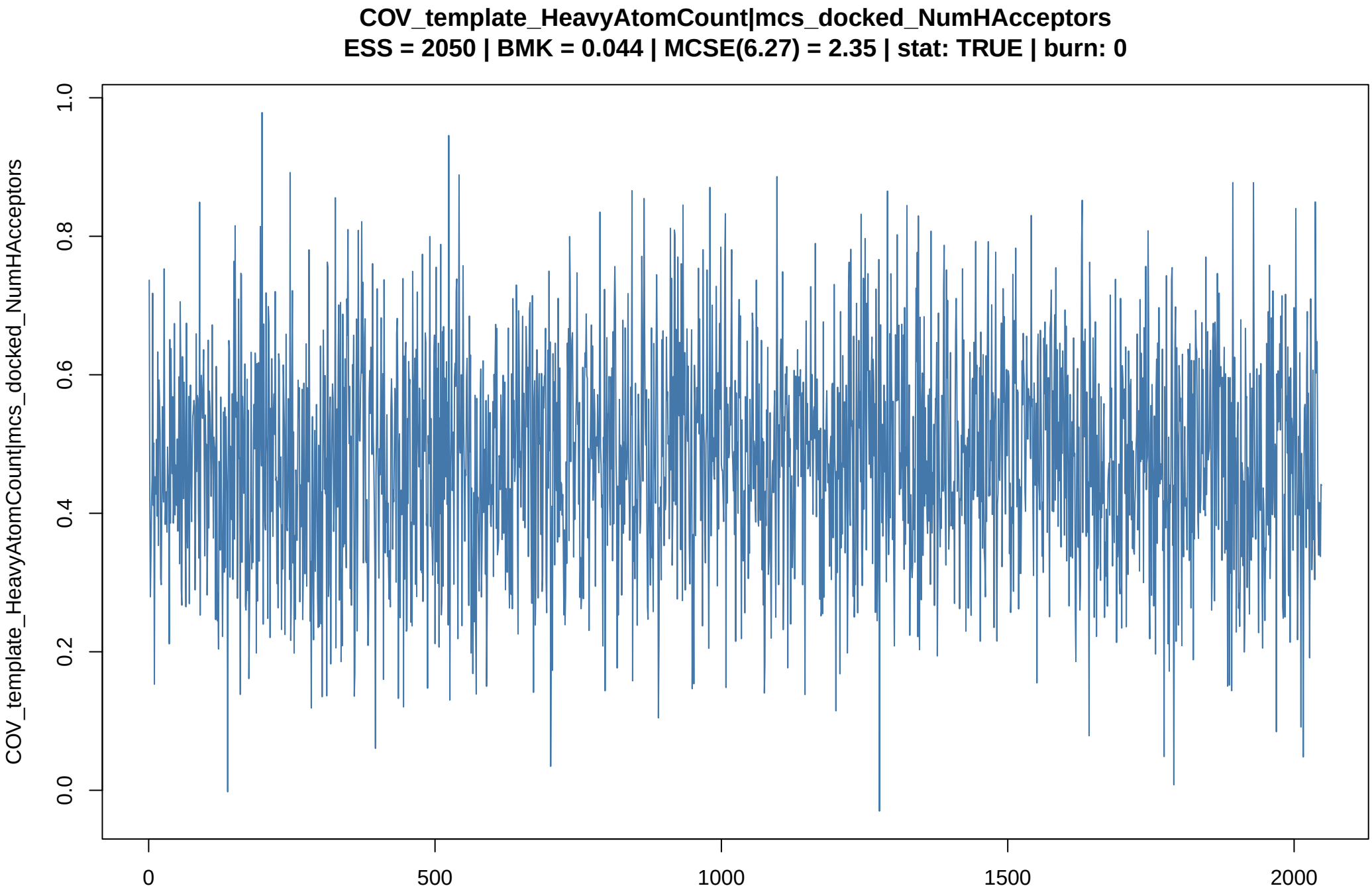

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1530 | BMK = 0.0979 | MCSE(6.27) = 3.3 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
2.5
3.0
3.5
0
500
1000
1500
2000

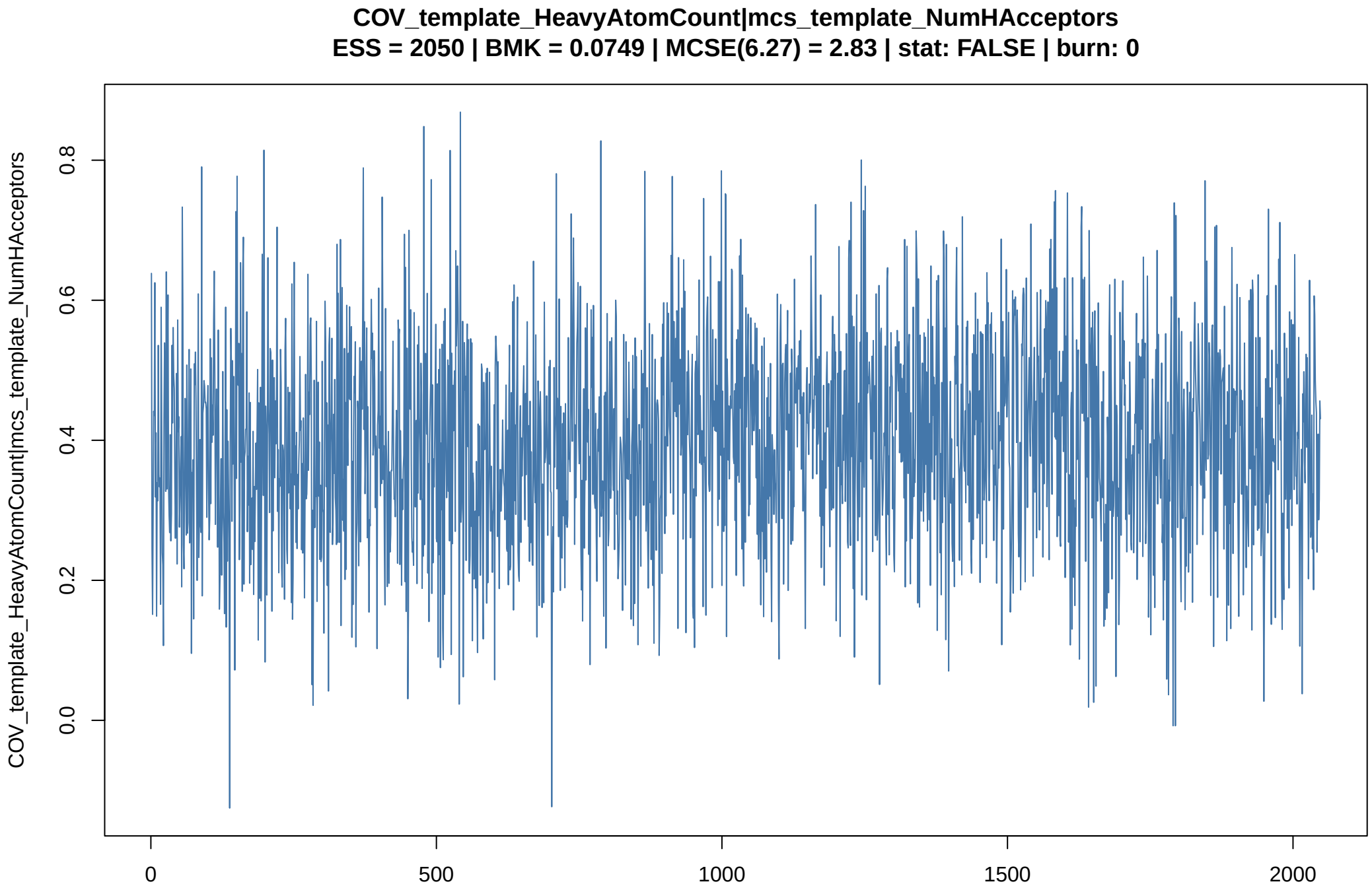

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 486 | BMK = 0.0668 | MCSE(6.27) = 3.79 | stat: TRUE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
−0.1
0.0
0.1
0.2
0.3
0.4
0
500
1000
1500
2000

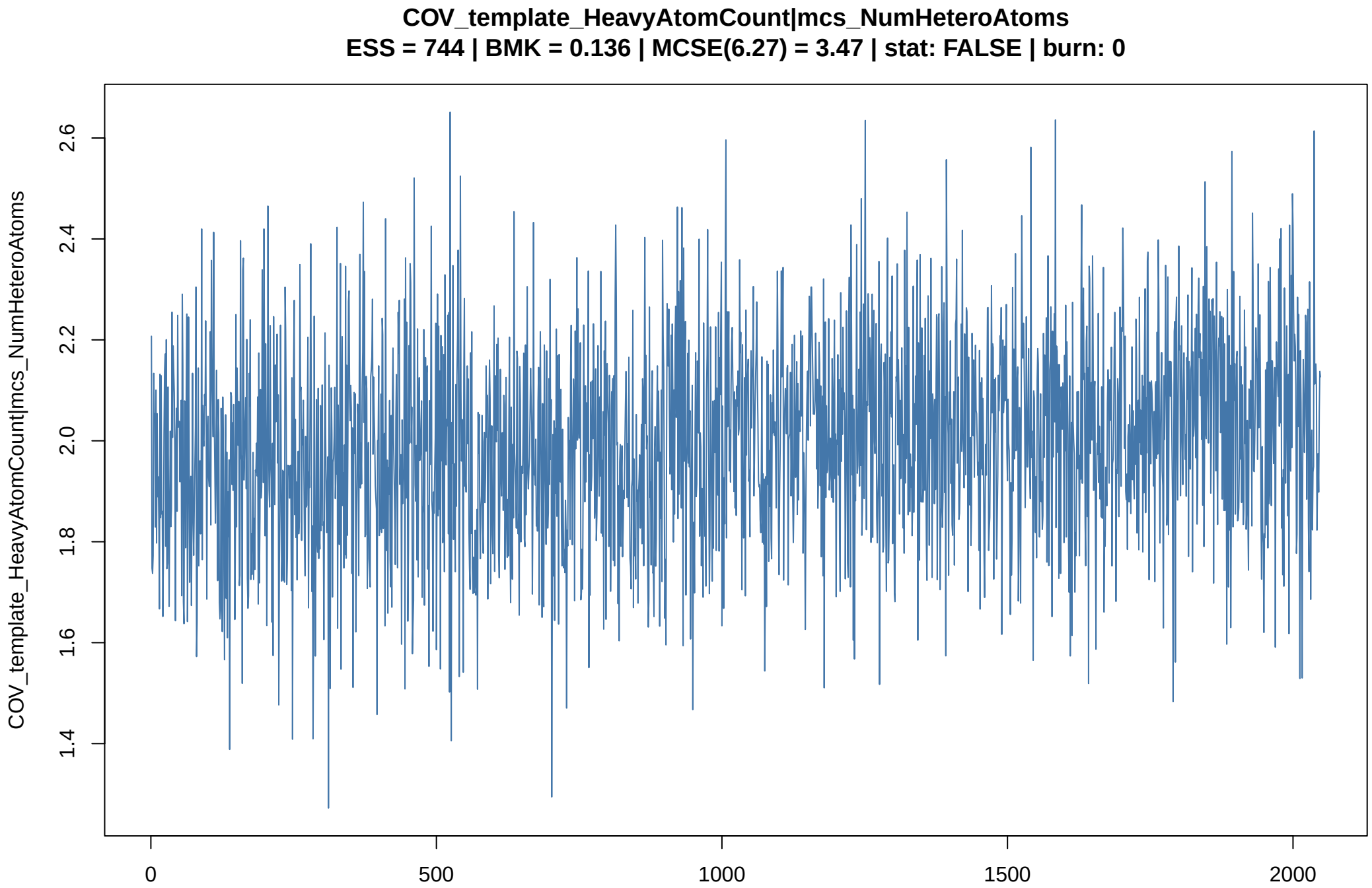

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 1290 | BMK = 0.04 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

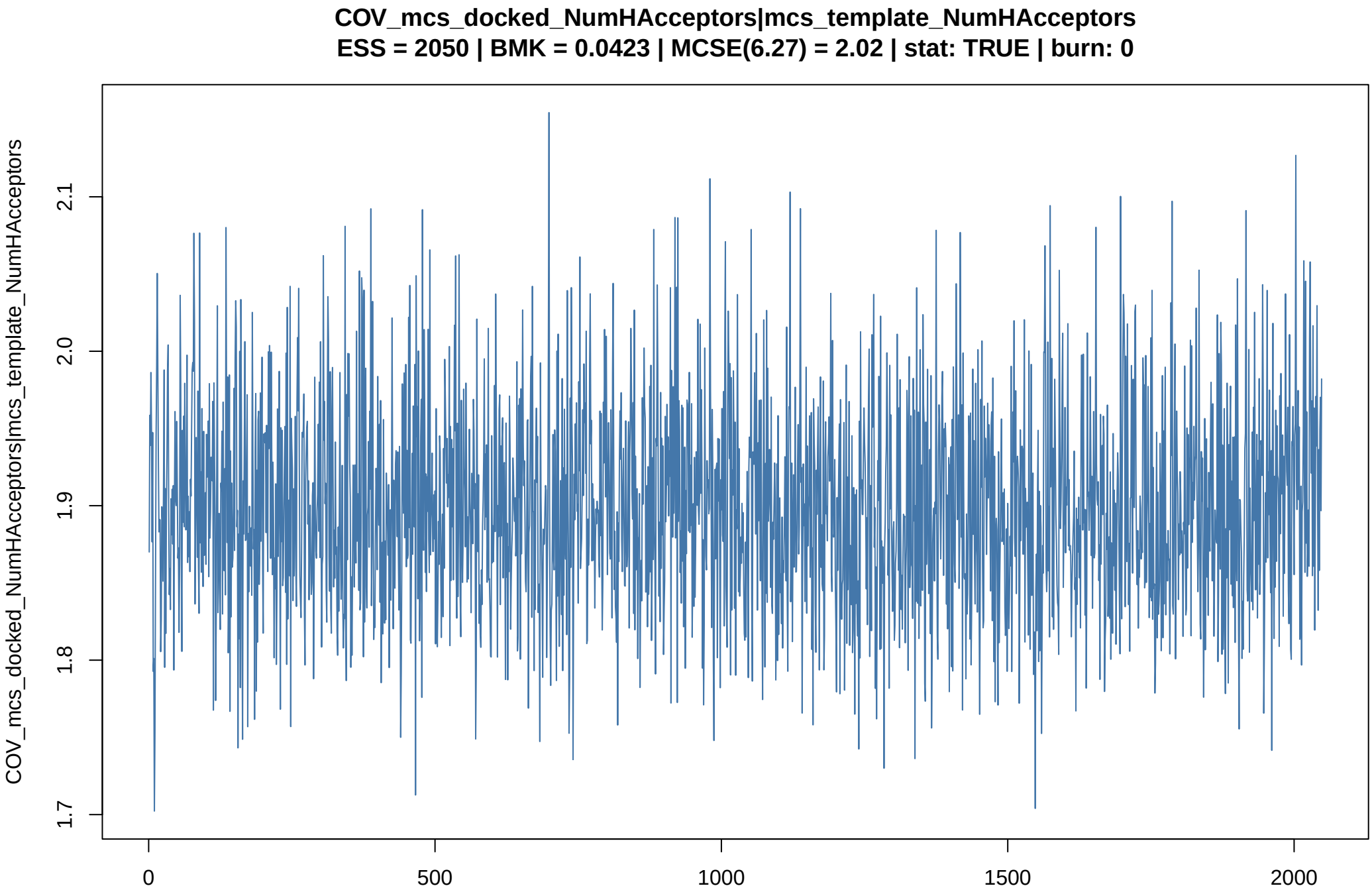

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0296 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

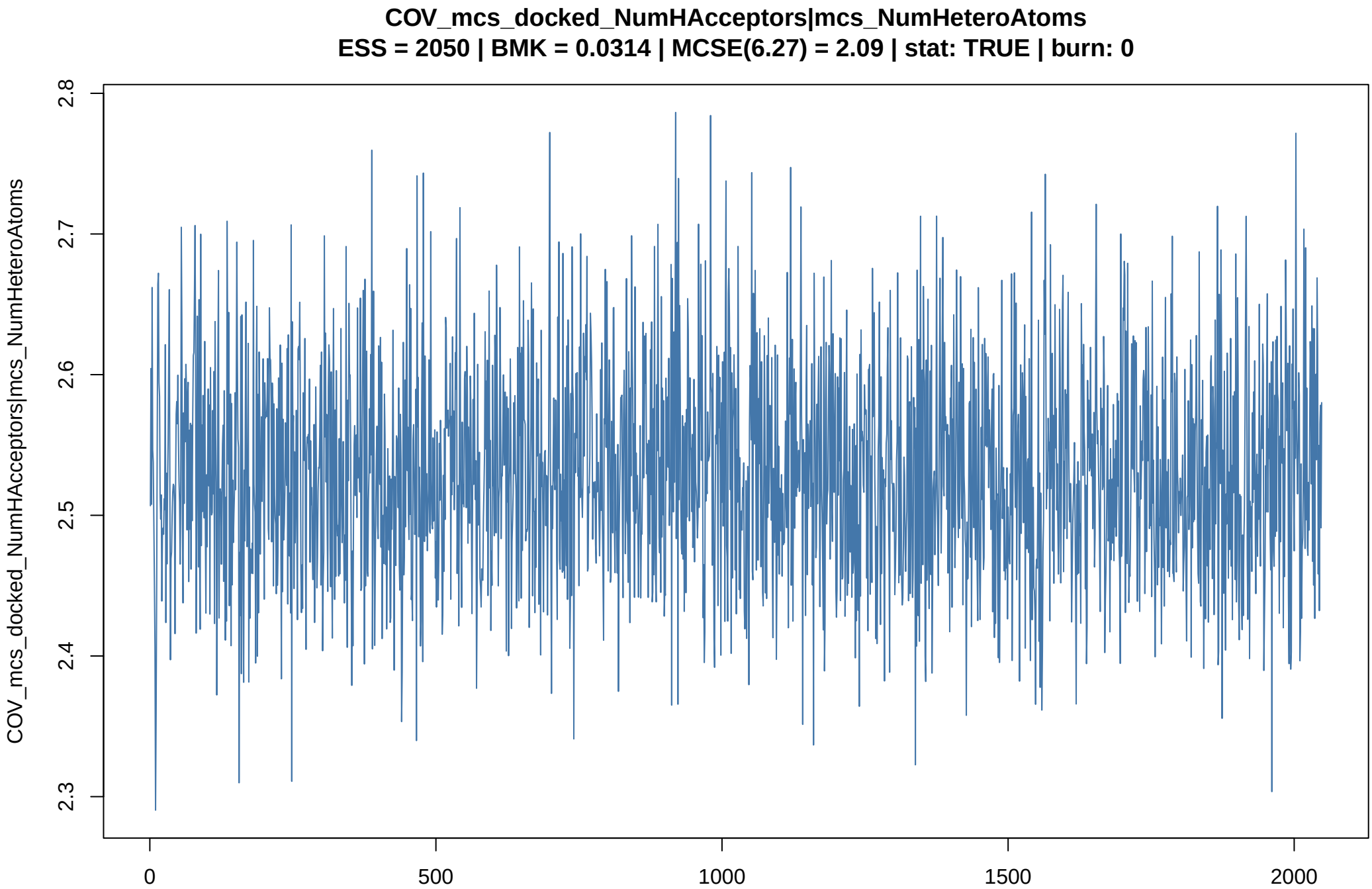

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 1870 | BMK = 0.0629 | MCSE(6.27) = 2.58 | stat: FALSE | burn: 0
COV_mcs_RingCount|mcs_NumHeteroAtoms
0.95
1.00
1.05
1.10
1.15
0
500
1000
1500
2000

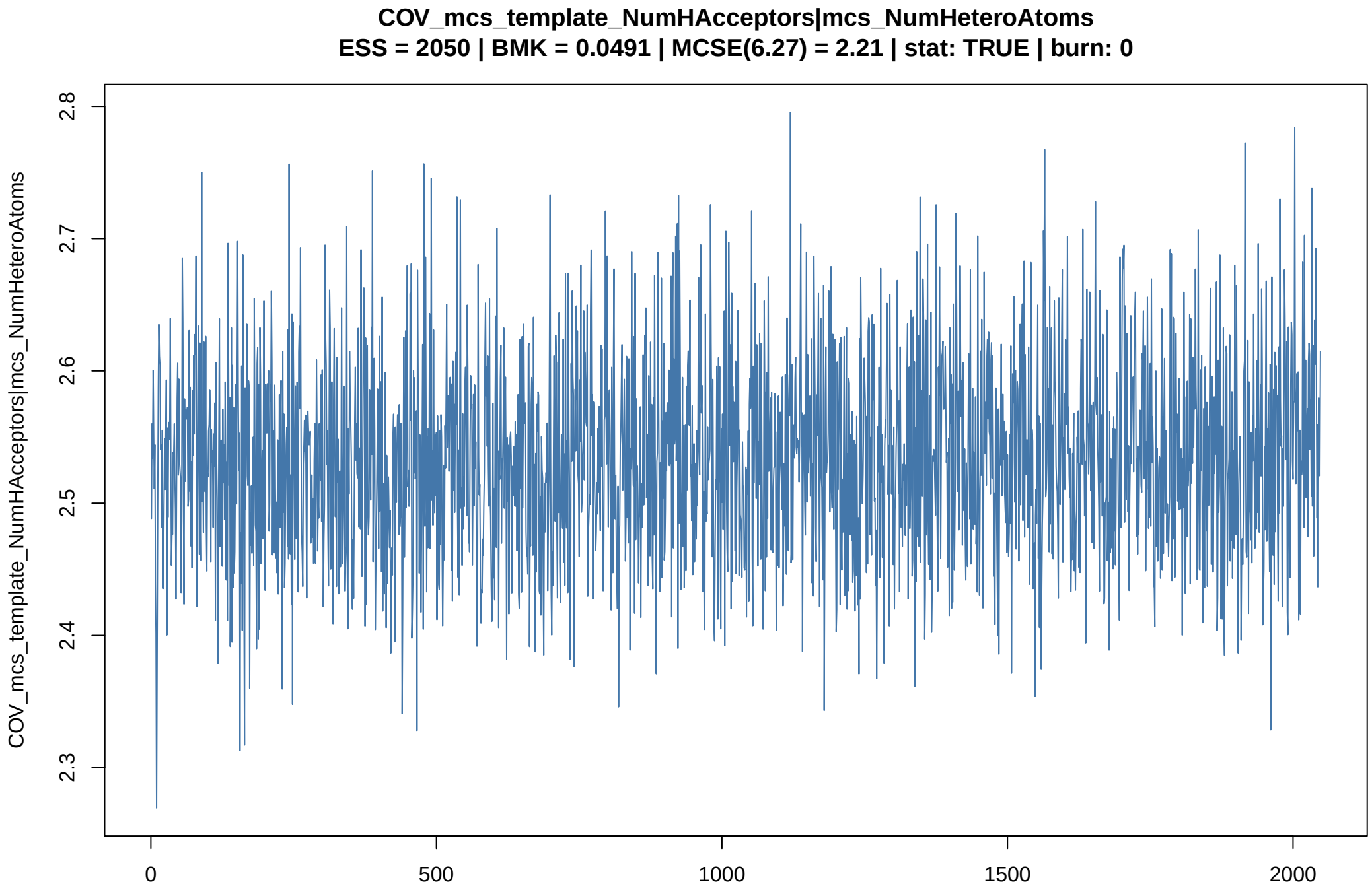

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.044 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0749 | MCSE(6.27) = 2.83 | stat: FALSE | burn: 0
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 744 | BMK = 0.136 | MCSE(6.27) = 3.47 | stat: FALSE | burn: 0
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
1.4
1.6
1.8
2.0
2.2
2.4
2.6
0
500
1000
1500
2000


COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0423 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
1.7
1.8
1.9
2.0
2.1
0
500
1000
1500
2000


COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0314 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
2.3
2.4
2.5
2.6
2.7
2.8
0
500
1000
1500
2000


COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0491 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0
COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
2.3
2.4
2.5
2.6
2.7
2.8
0
500
1000
1500
2000