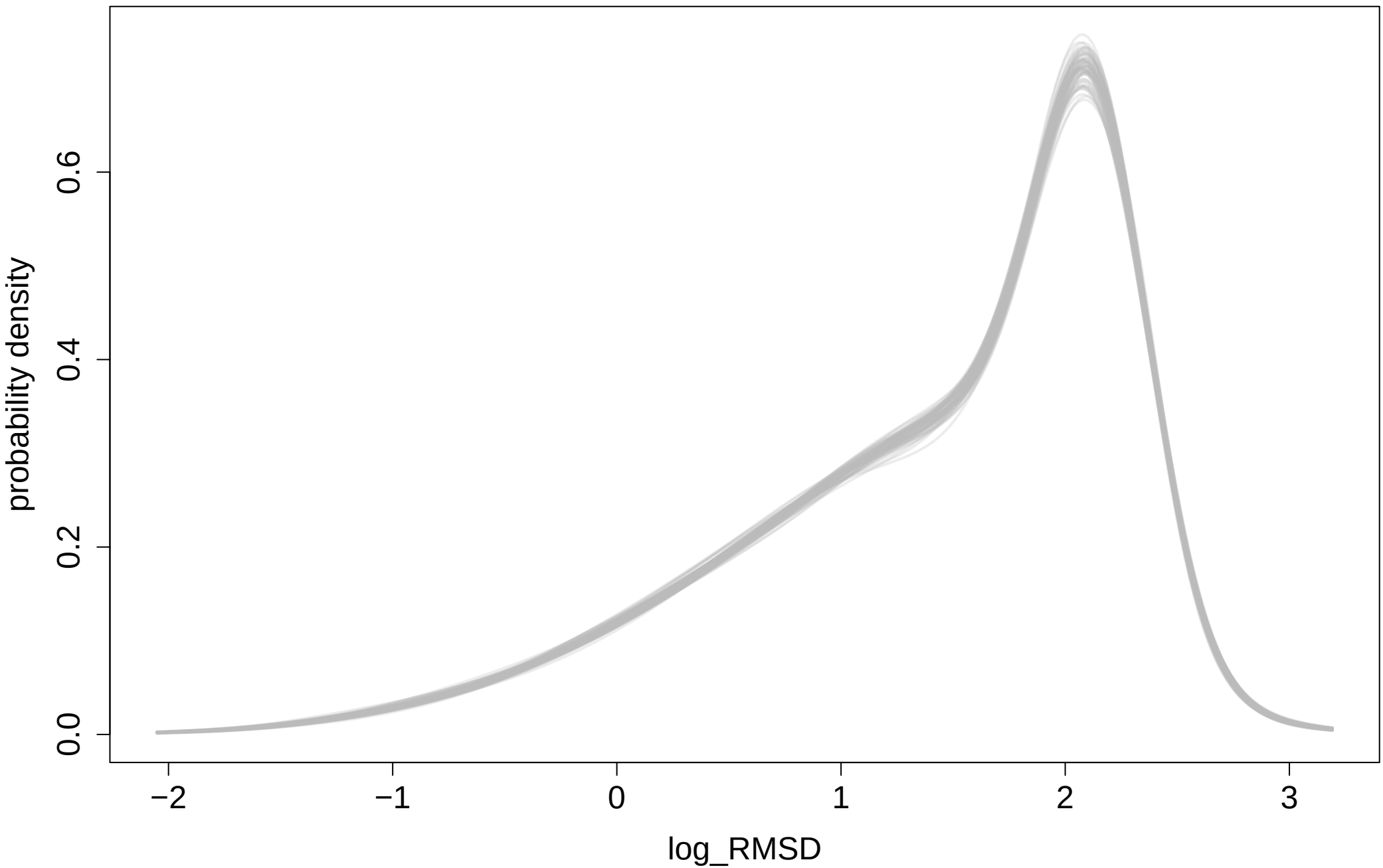
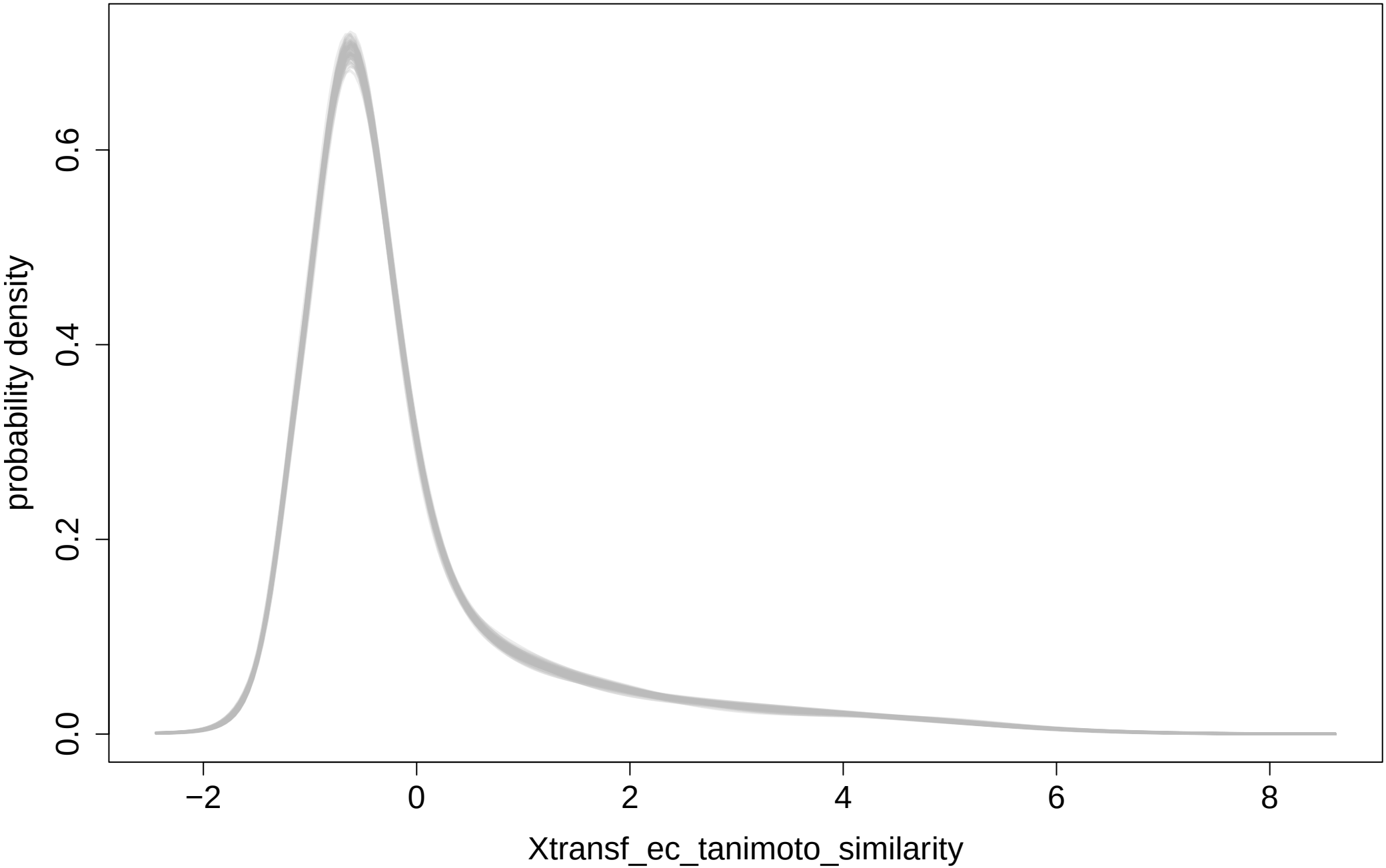
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.857944935673334
max MCSE = 14.9003461977599
all stationary: FALSE
burn: 2040

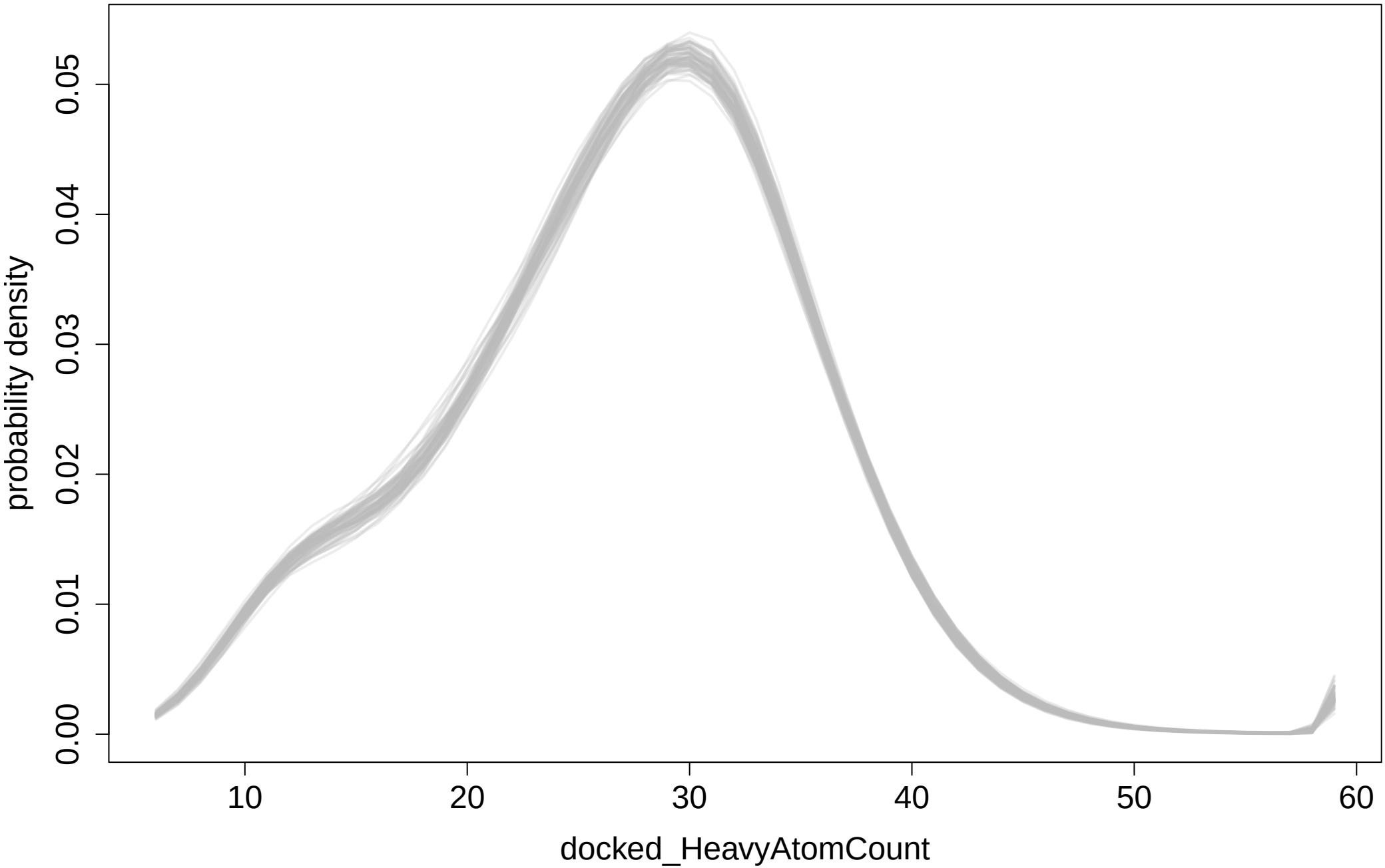
−− STATS 2D −−
min ESS = 120.752344677566
max BMK = 0.176844366430327
max MCSE = 5.47209556818625
all stationary: FALSE
burn: 0

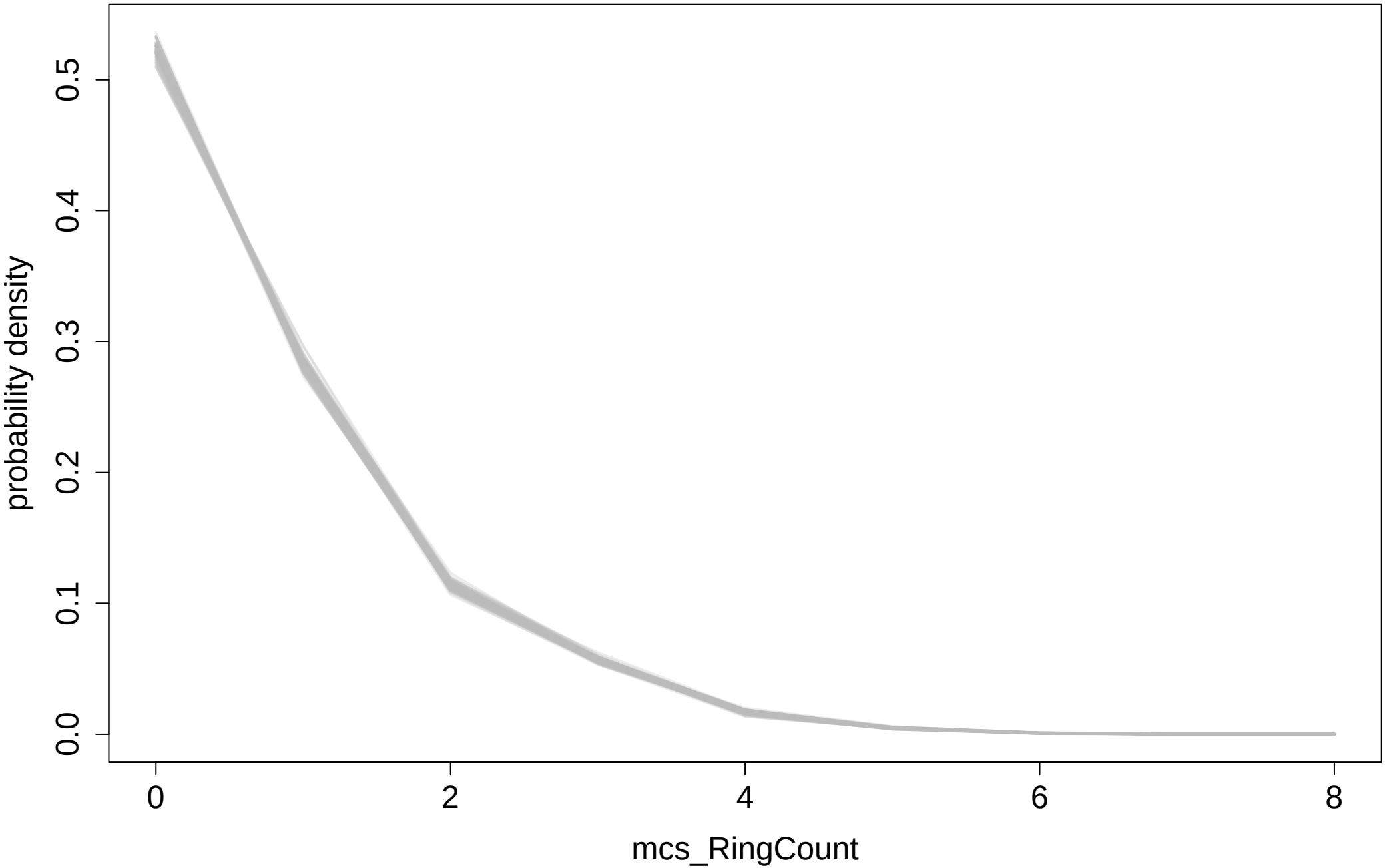
−− STATS 1D −−
min ESS = 2.2044604925031e−16
max BMK = 0.609283558405166
max MCSE = NaN
all stationary: FALSE
burn: 1632

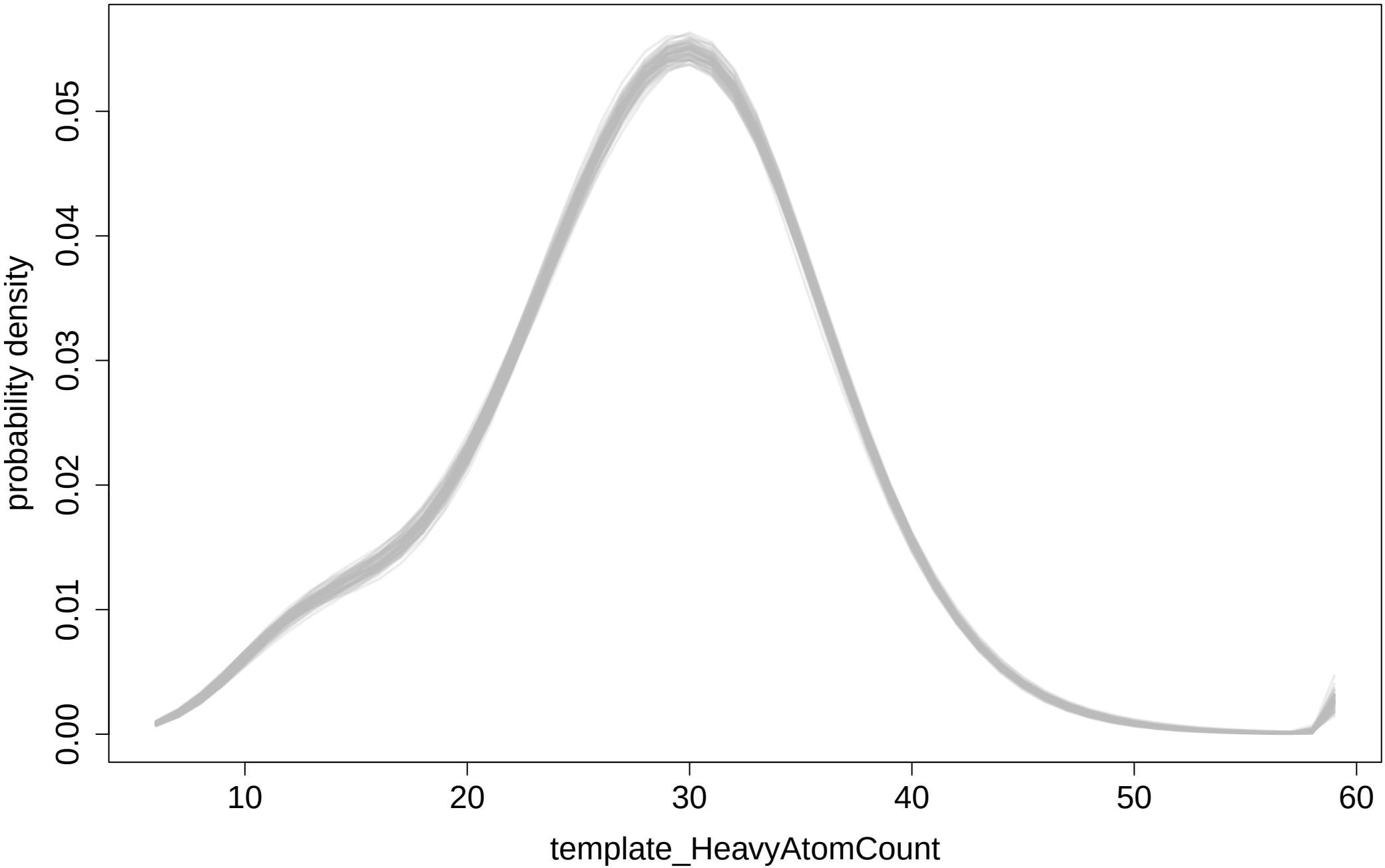
Occupied clusters: 54 of 64
LL: −111000 +− 319

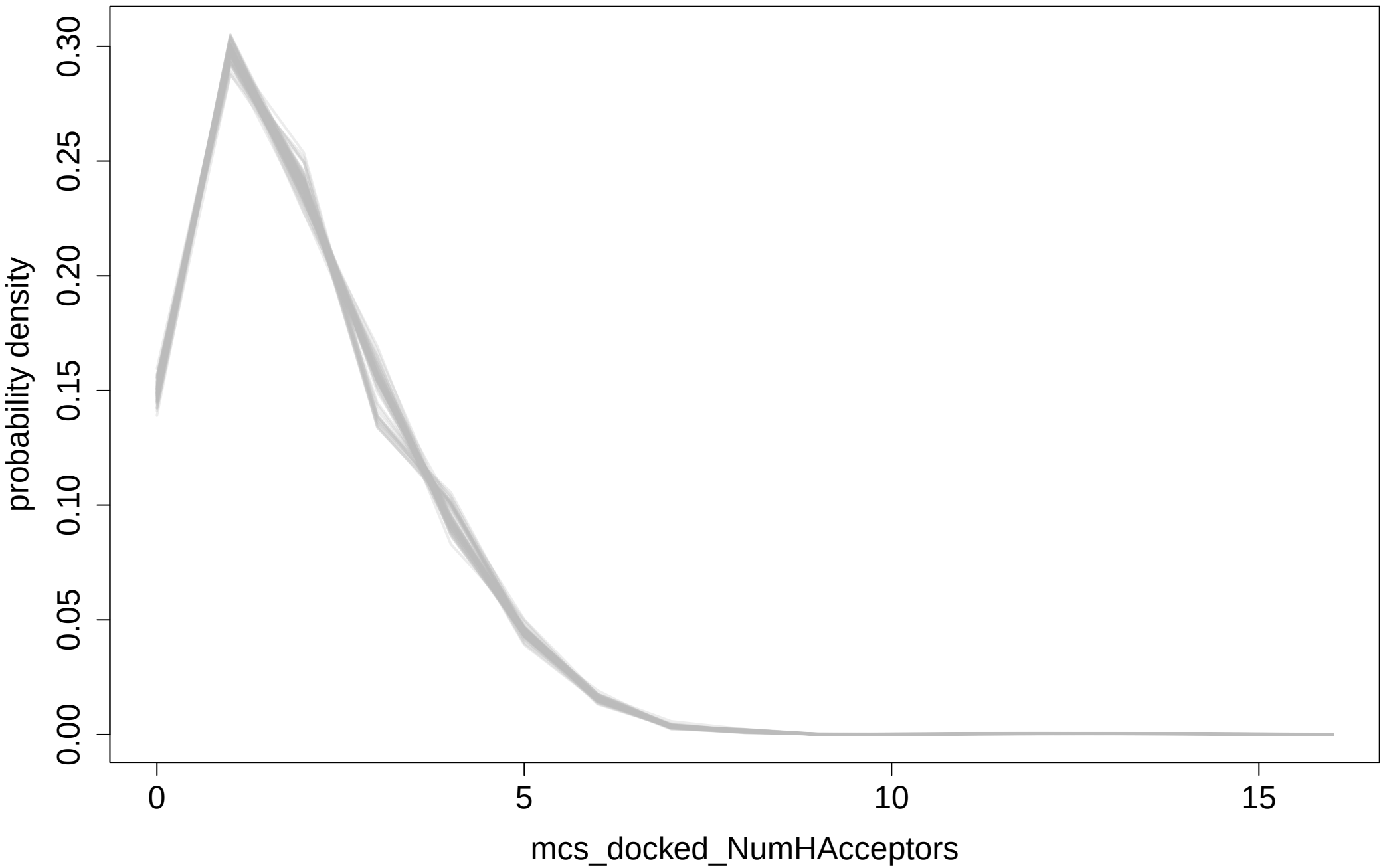

probability density
0.0
0.2
0.4
0.6
−2
−1
0
1
2
3
log_RMSD

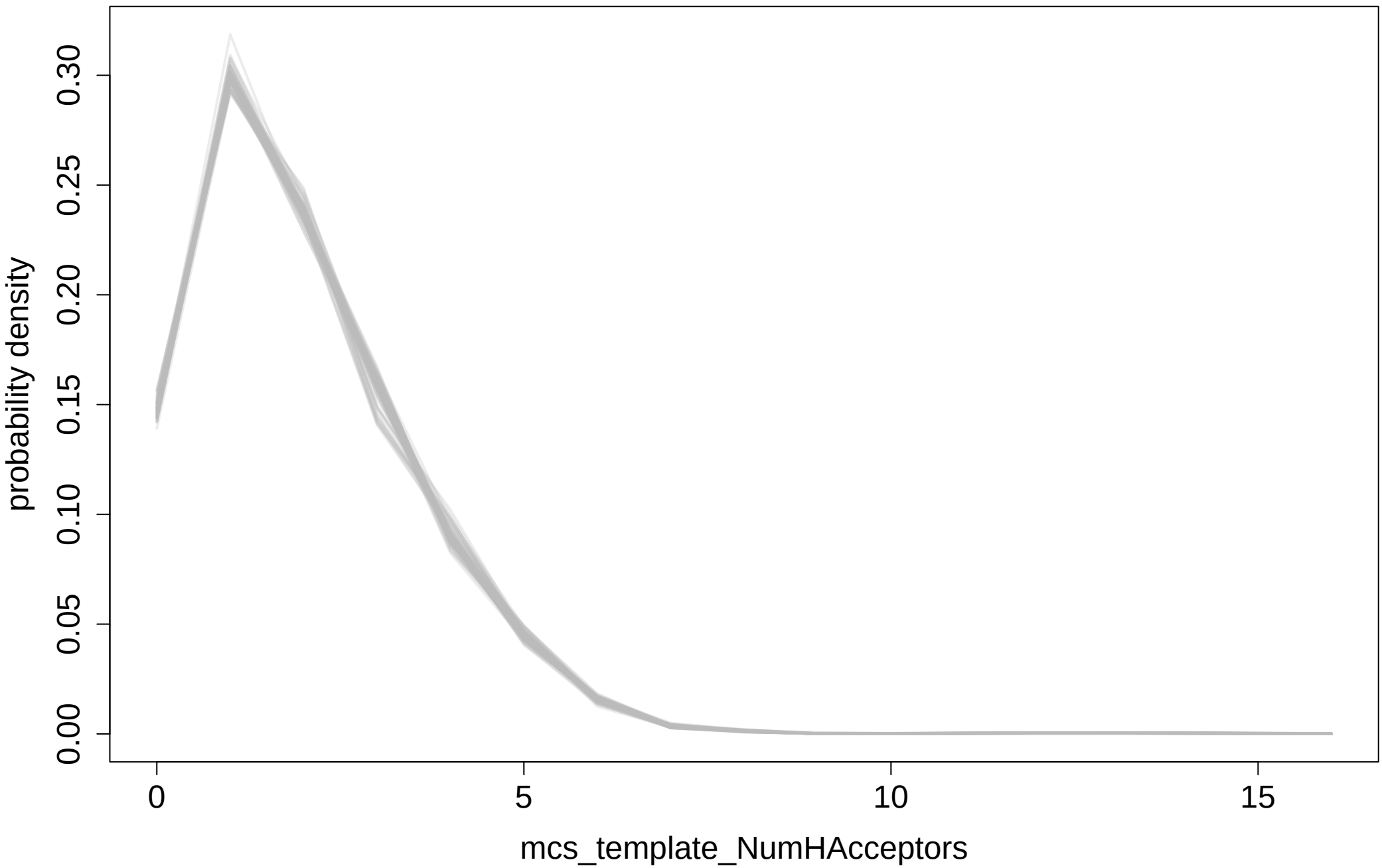

probability density
0.0
0.2
0.4
0.6
−2
0
2
4
6
8
Xtransf_ec_tanimoto_similarity

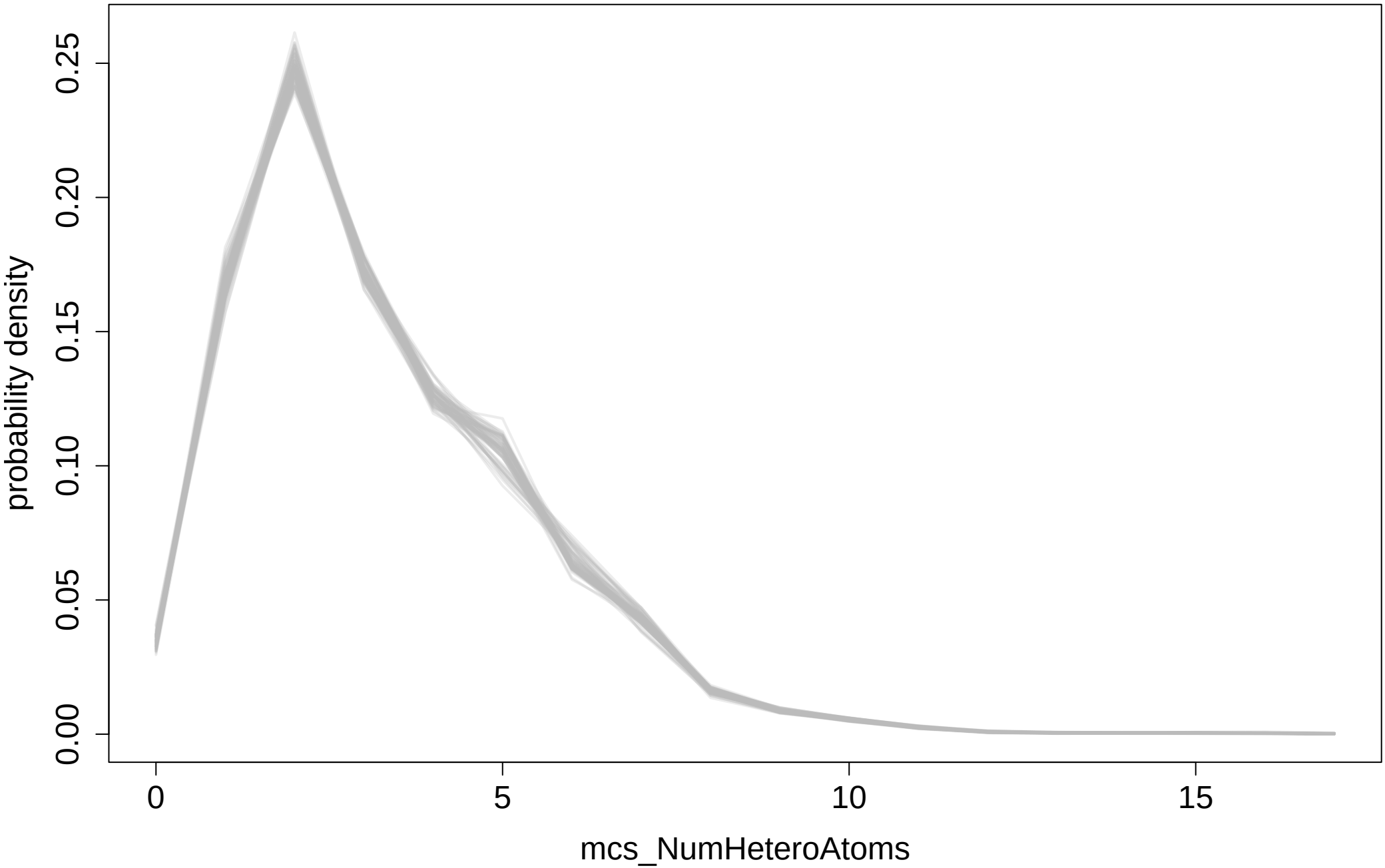

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
docked_HeavyAtomCount

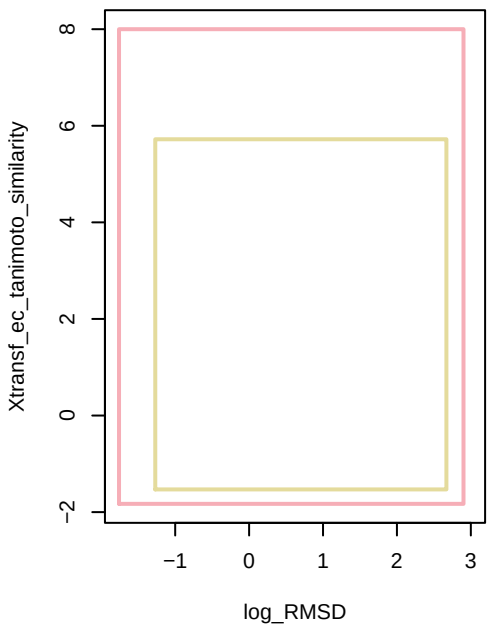

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0
2
4
6
8
mcs_RingCount

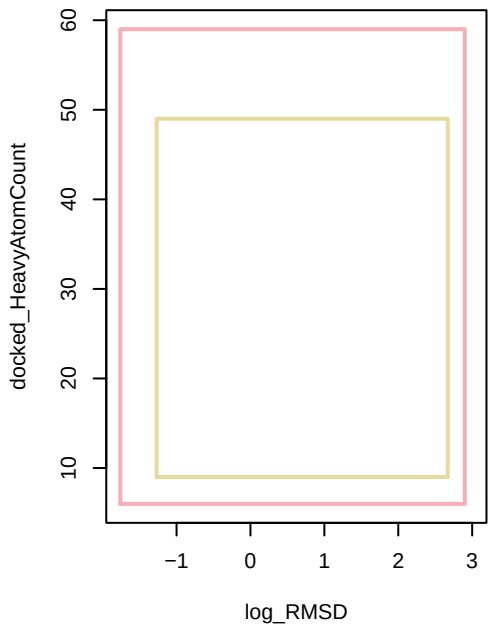

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
template_HeavyAtomCount

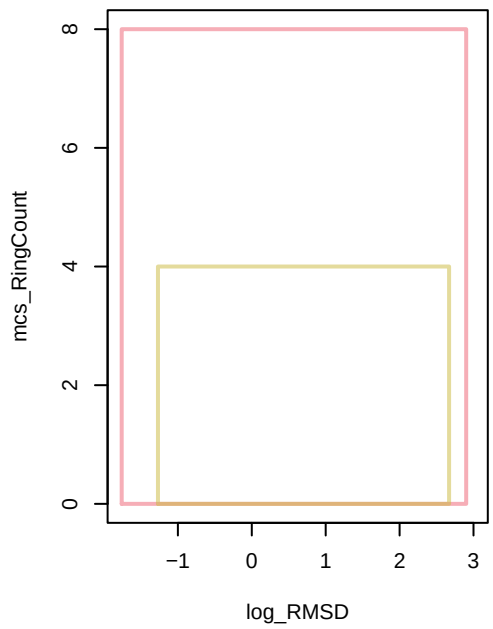

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_docked_NumHAcceptors

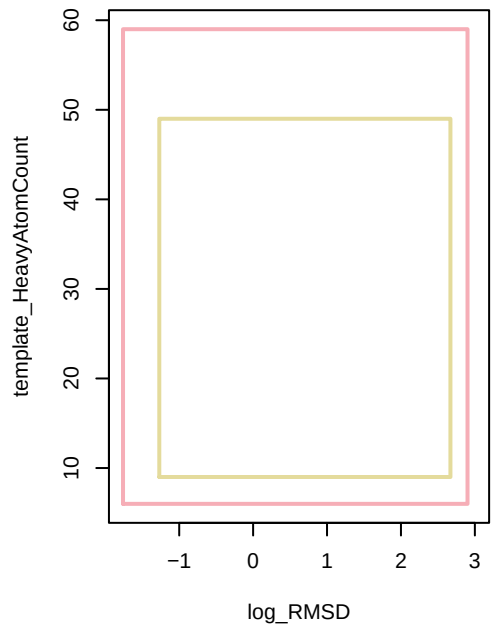

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_template_NumHAcceptors

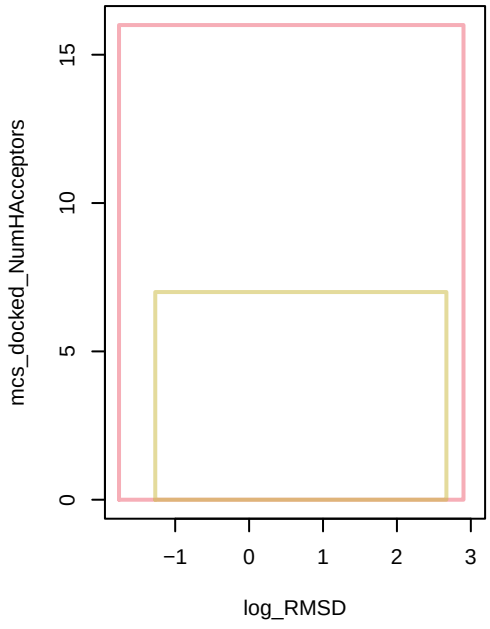

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms

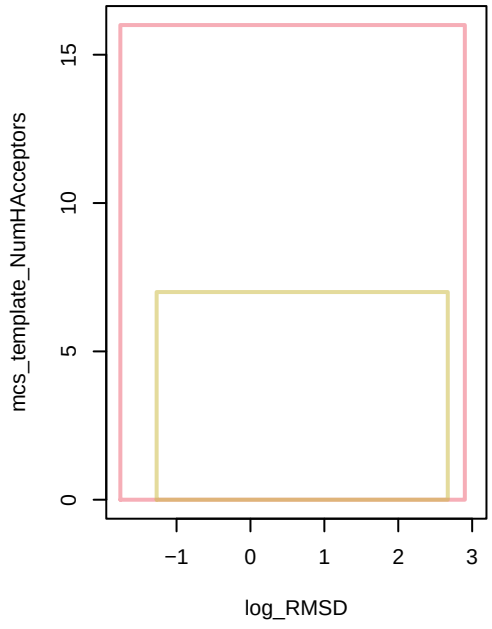

Xtransf_ec_tanimoto_similarity
log_RMSD

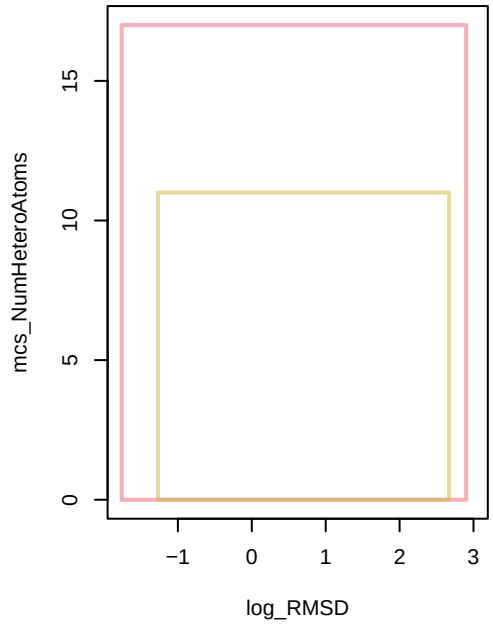

docked_HeavyAtomCount
log_RMSD

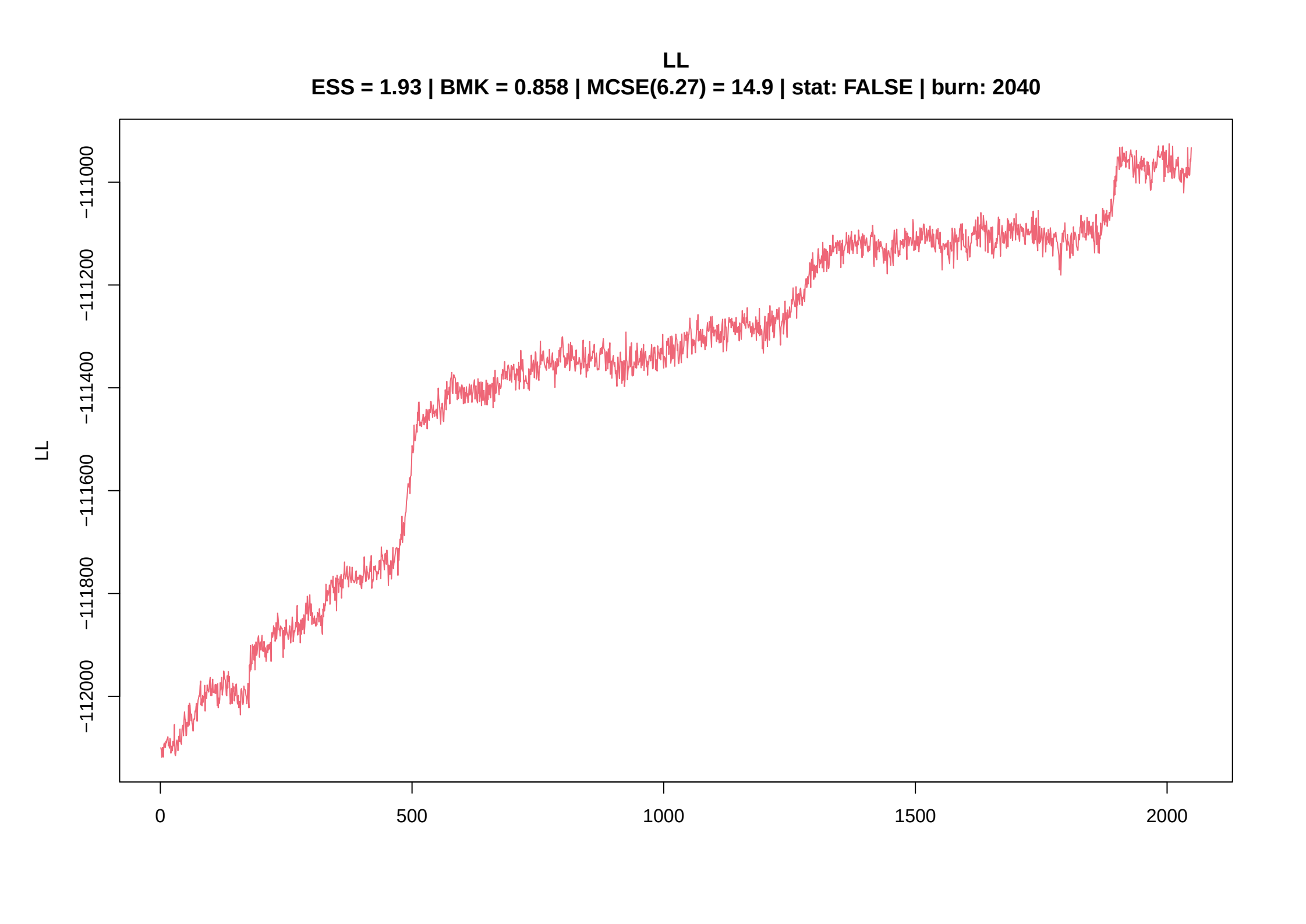

mcs_RingCount
log_RMSD

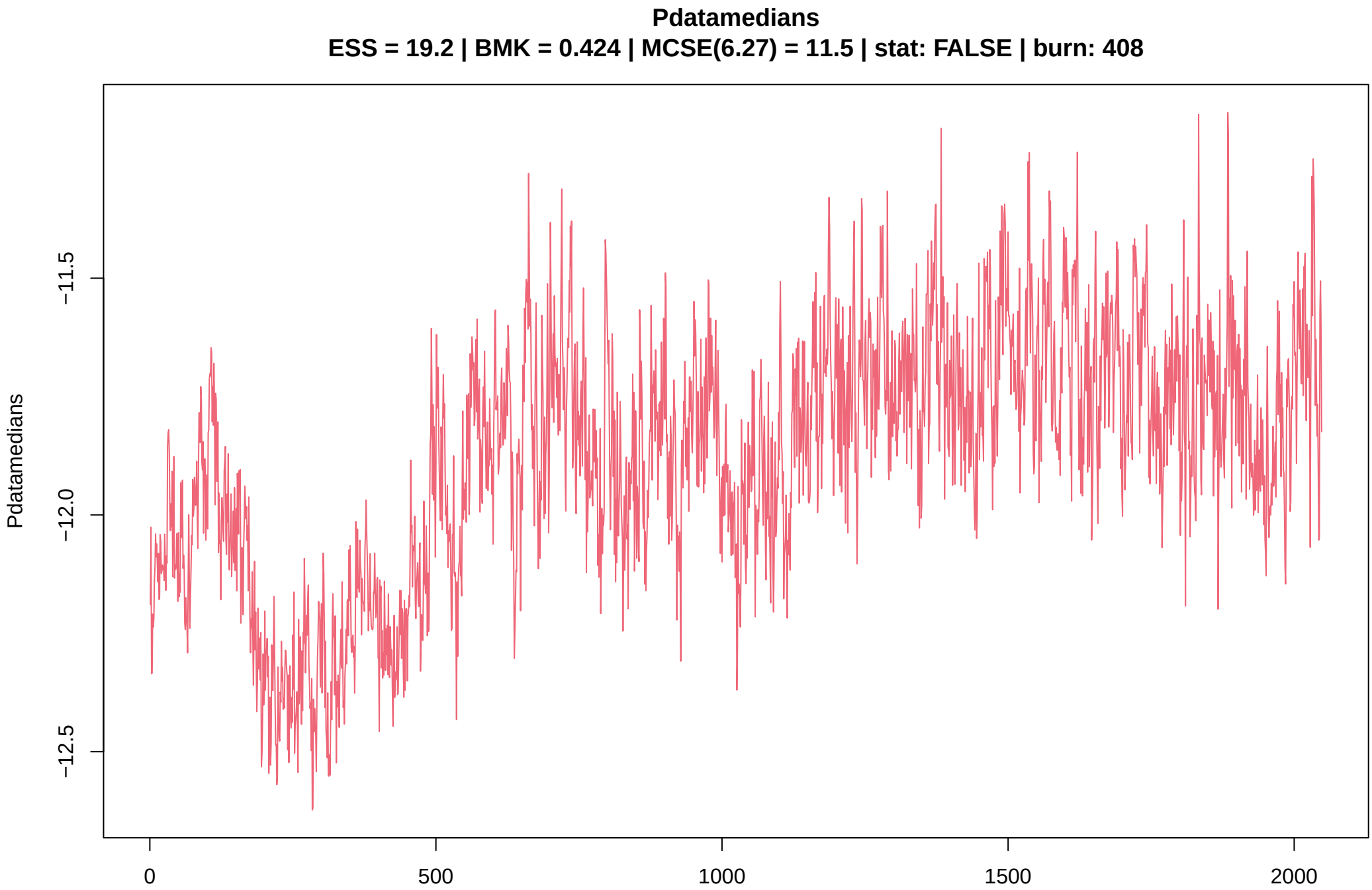

template_HeavyAtomCount
log_RMSD

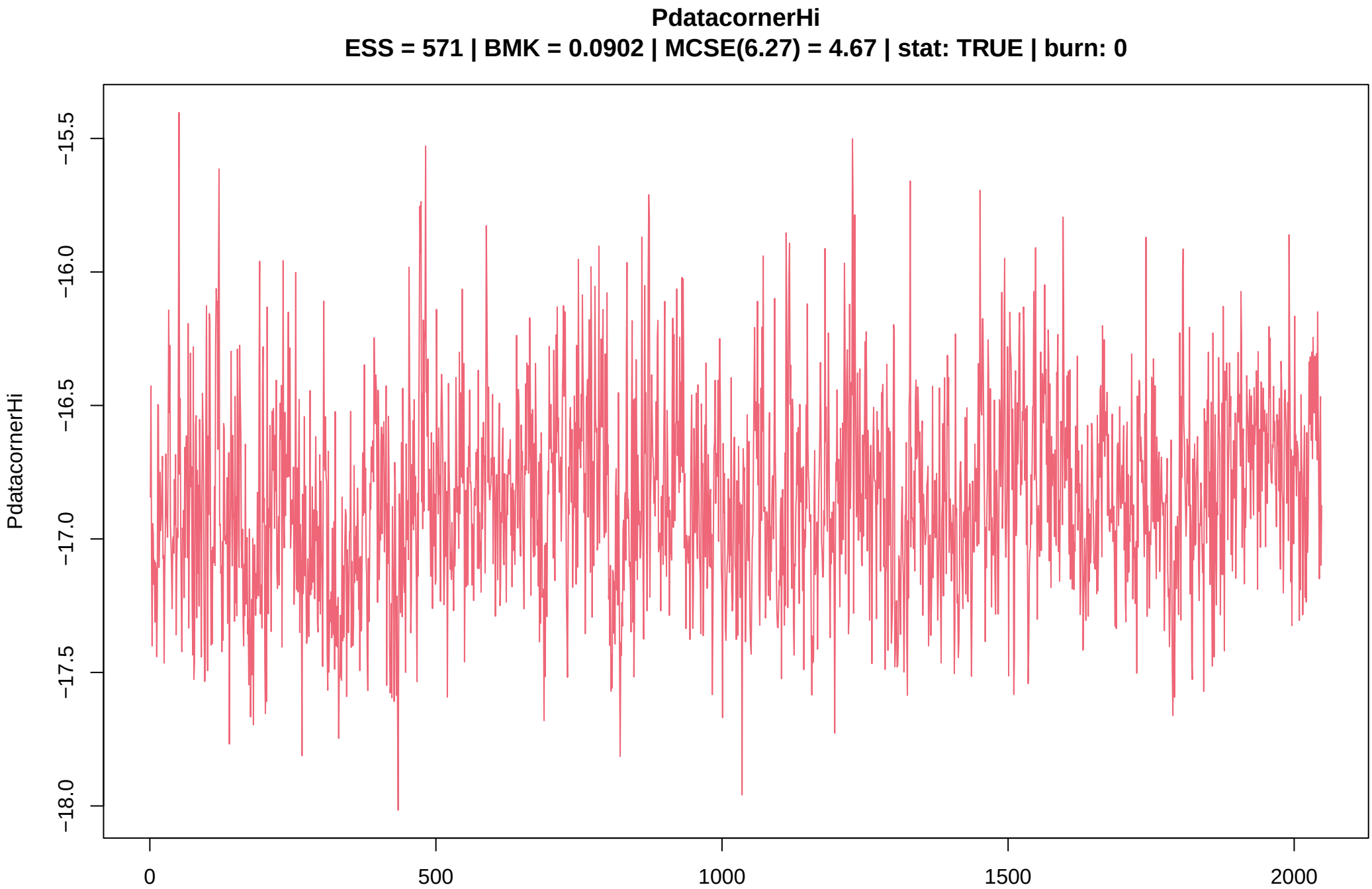

mcs_docked_NumHAcceptors
log_RMSD

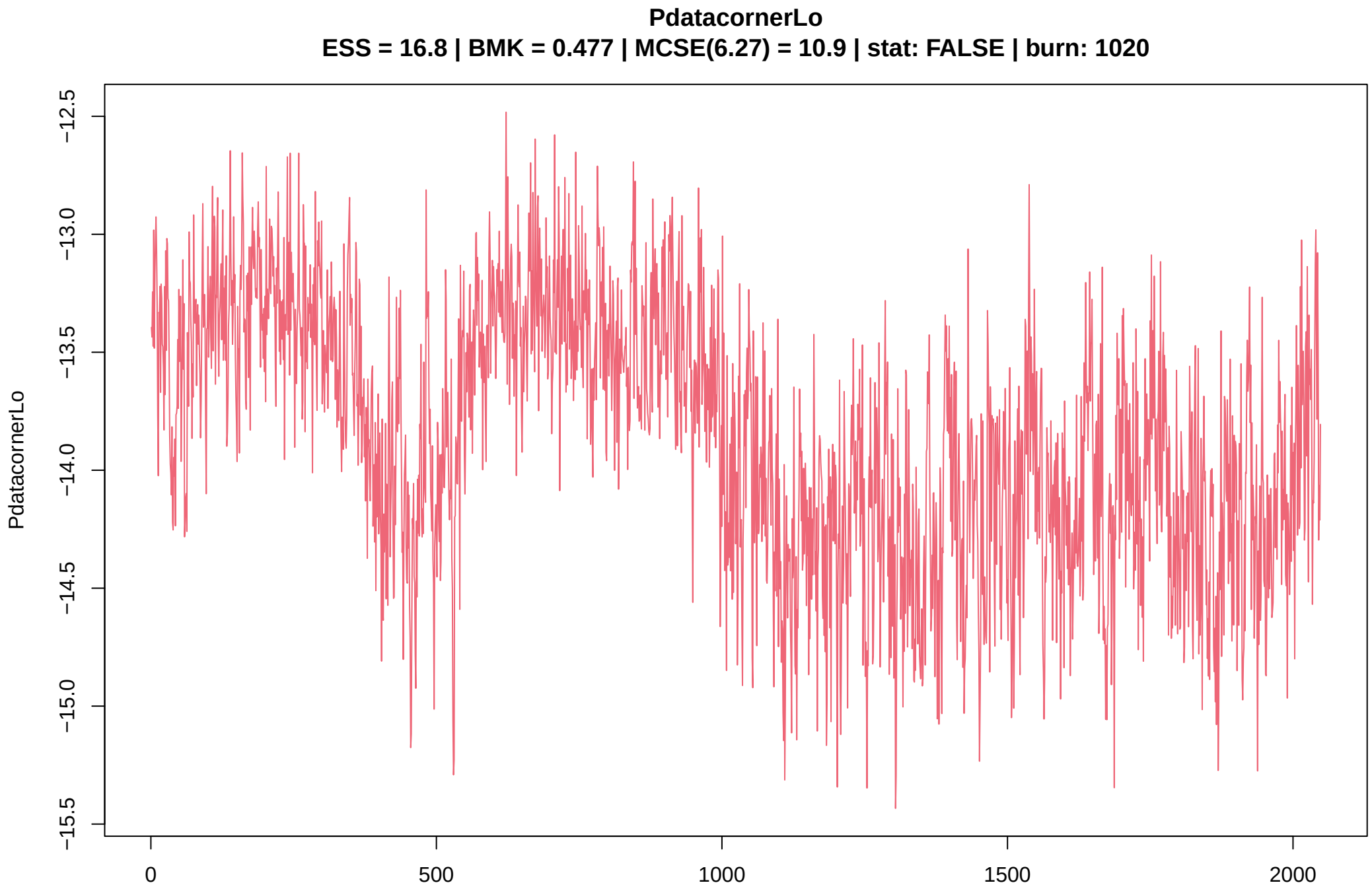

mcs_template_NumHAcceptors
log_RMSD

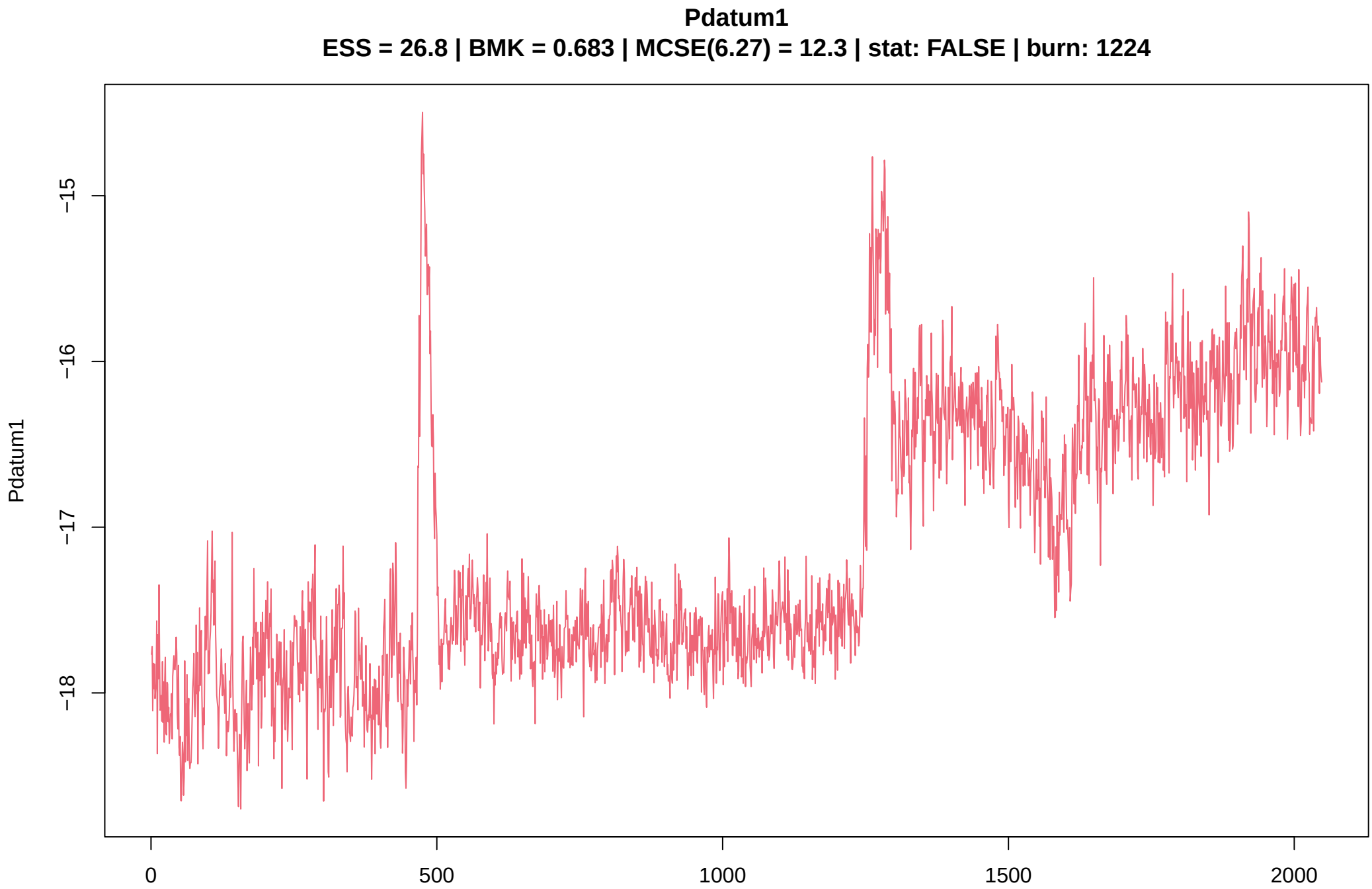

mcs_NumHeteroAtoms
log_RMSD

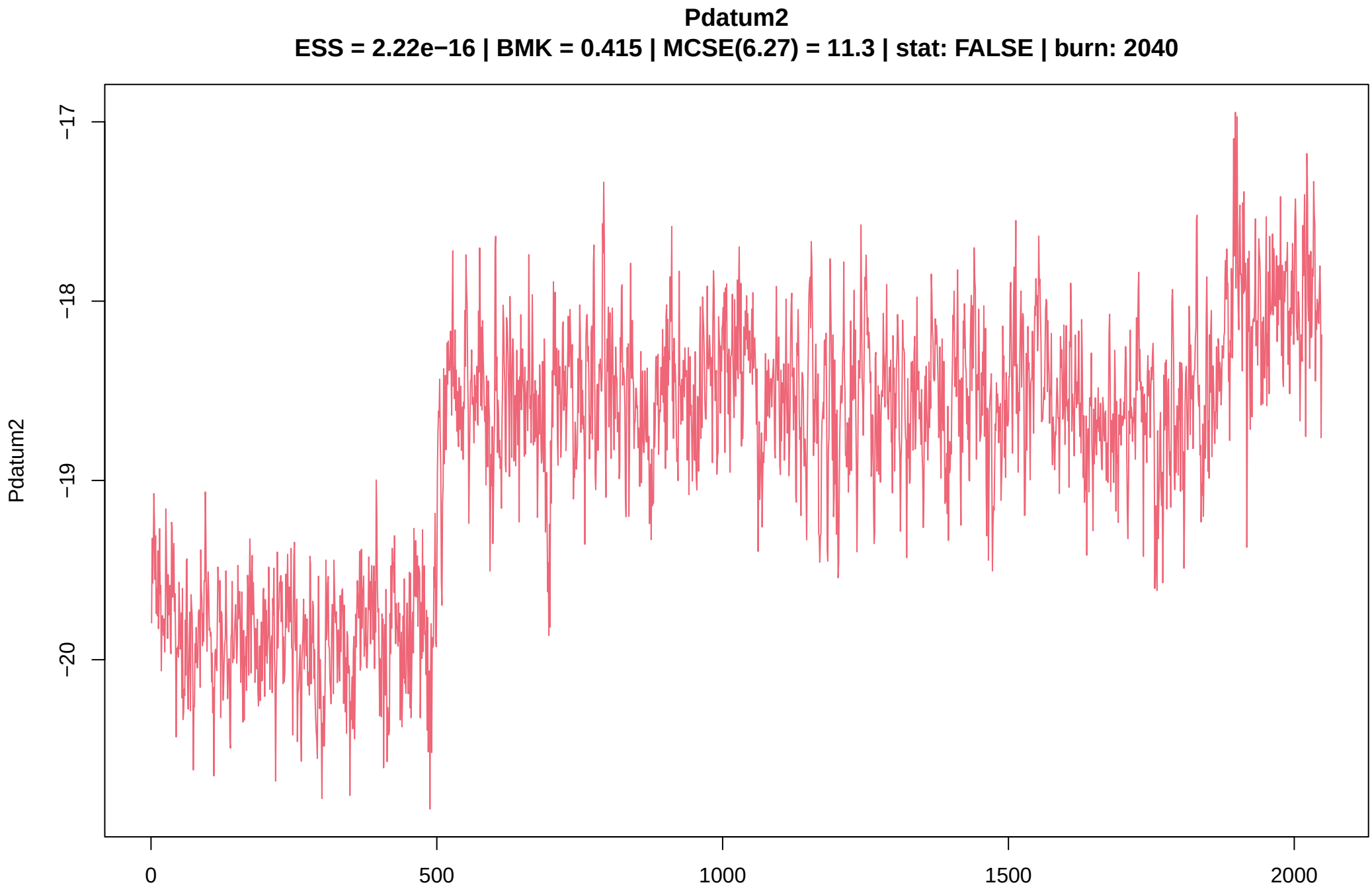

LL
ESS = 1.93 | BMK = 0.858 | MCSE(6.27) = 14.9 | stat: FALSE | burn: 2040
LL
−112000
−111800
−111600
−111400
−111200
−111000
0
500
1000
1500
2000

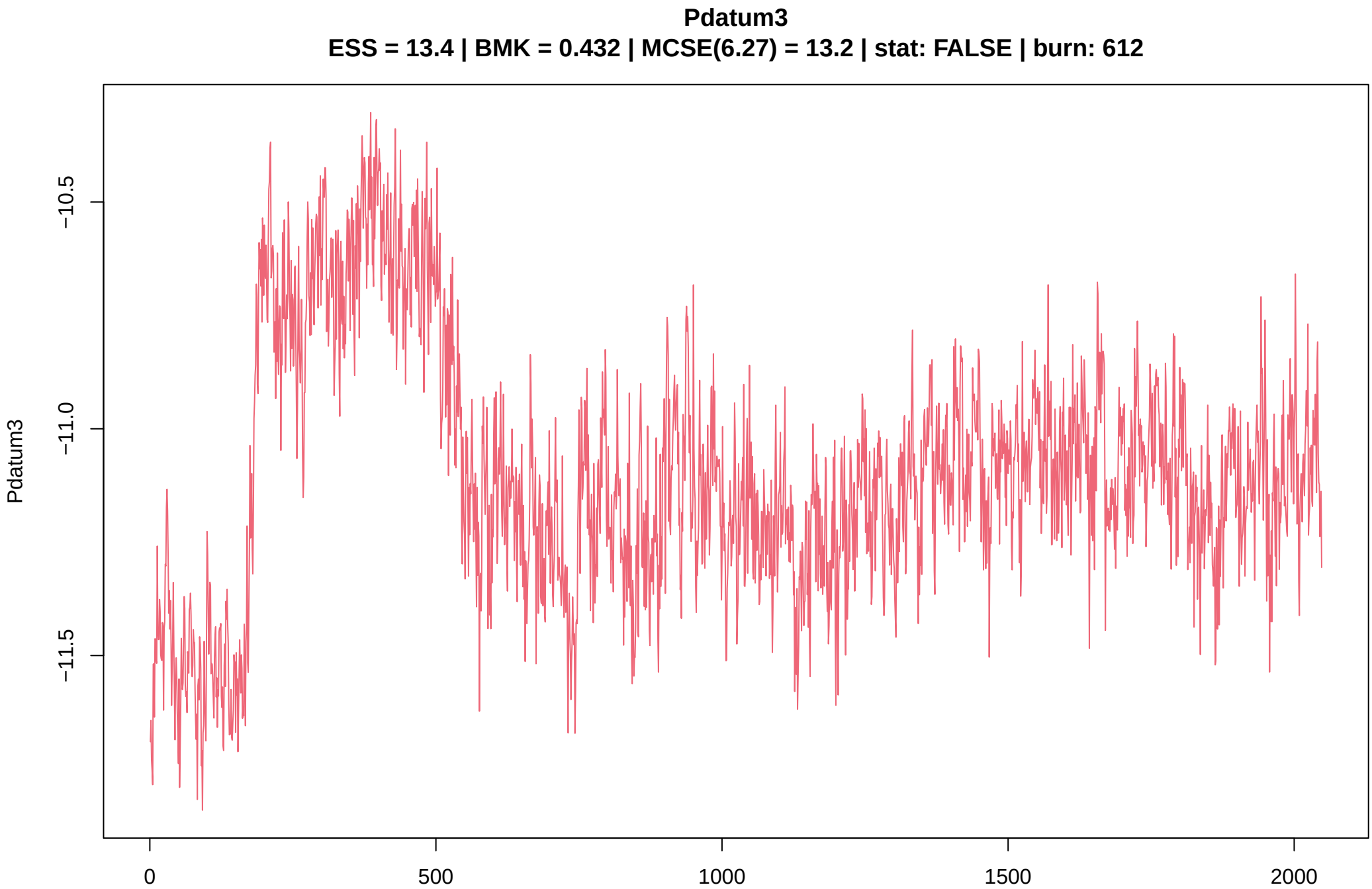

Pdatamedians
ESS = 19.2 | BMK = 0.424 | MCSE(6.27) = 11.5 | stat: FALSE | burn: 408
Pdatamedians
−11.5
−12.0
−12.5
0
500
1000
1500
2000

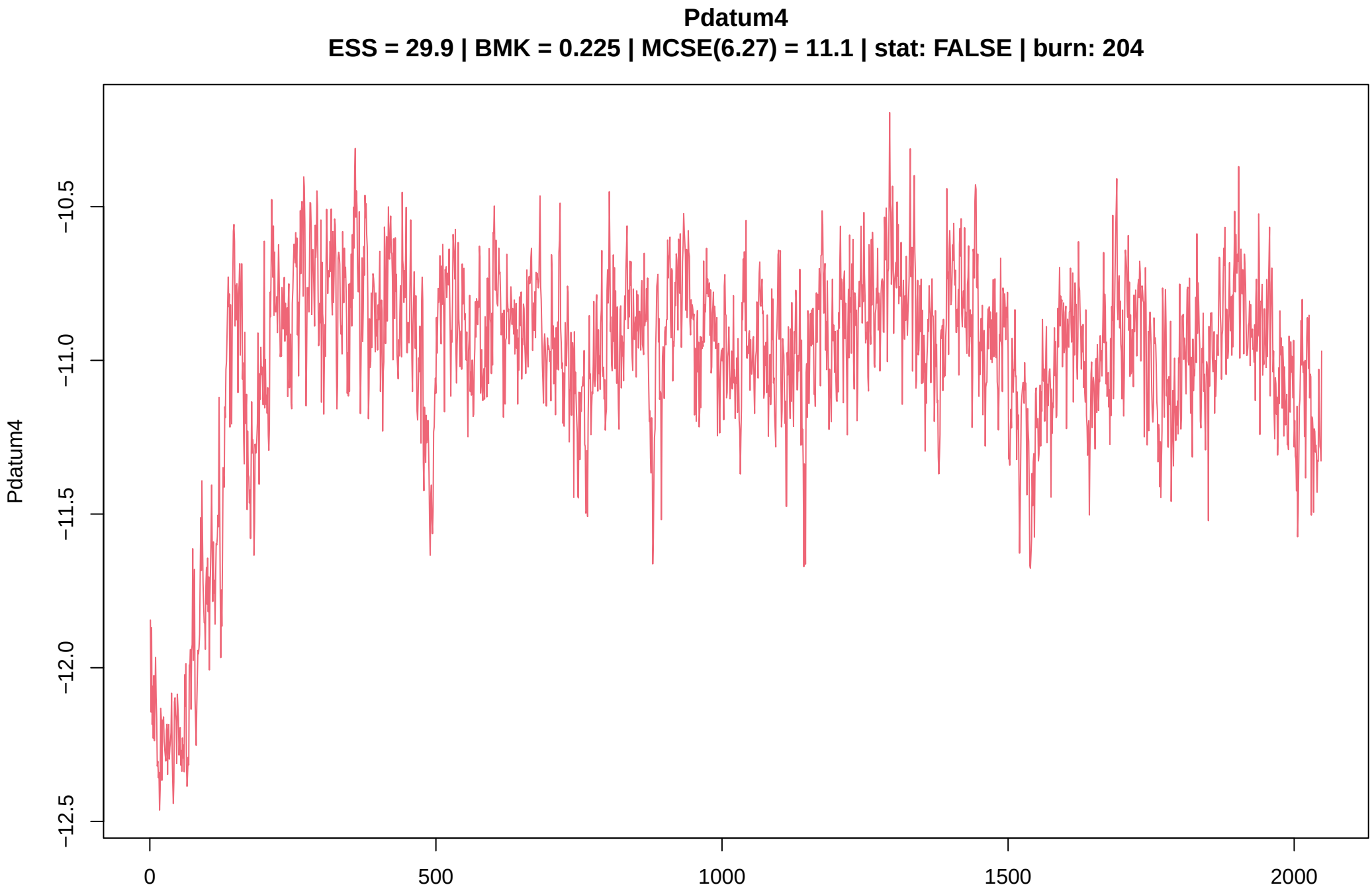

PdatacornerHi
ESS = 571 | BMK = 0.0902 | MCSE(6.27) = 4.67 | stat: TRUE | burn: 0
PdatacornerHi
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
0
500
1000
1500
2000

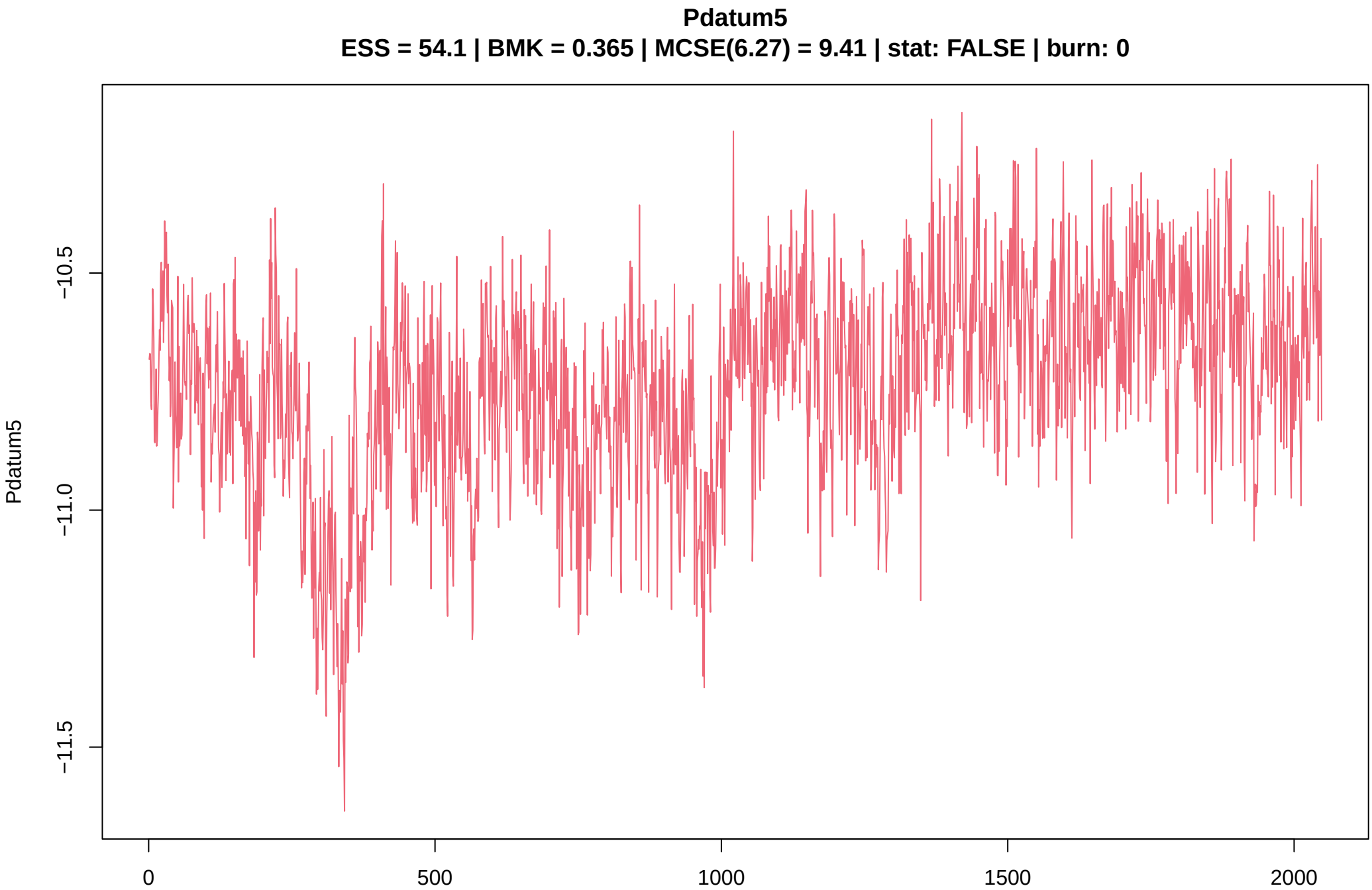

PdatacornerLo
ESS = 16.8 | BMK = 0.477 | MCSE(6.27) = 10.9 | stat: FALSE | burn: 1020
PdatacornerLo
−12.5
−13.0
−13.5
−14.0
−14.5
−15.0
−15.5
0
500
1000
1500
2000

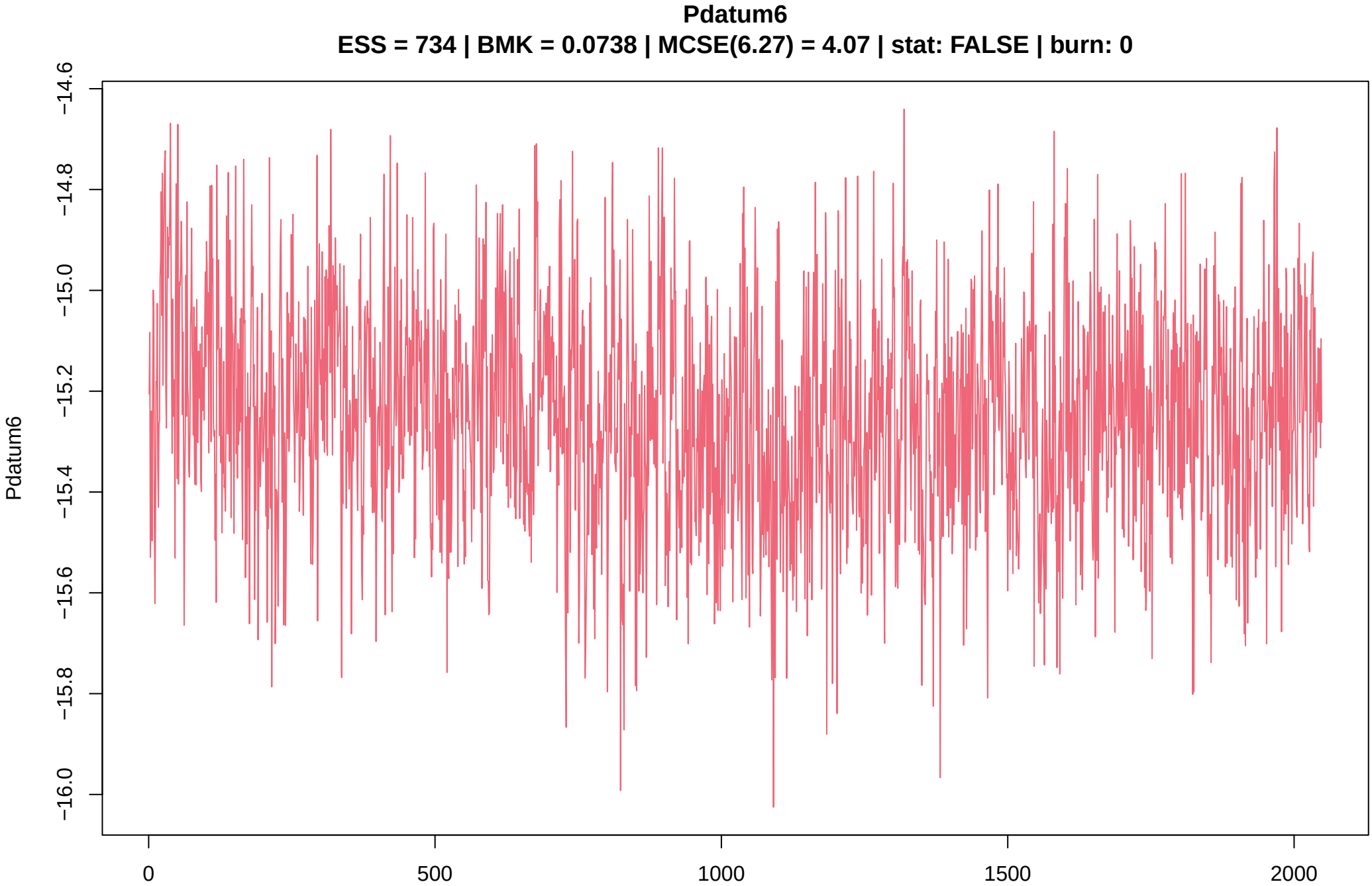

Pdatum1
ESS = 26.8 | BMK = 0.683 | MCSE(6.27) = 12.3 | stat: FALSE | burn: 1224
Pdatum1
−15
−16
−17
−18
0
500
1000
1500
2000

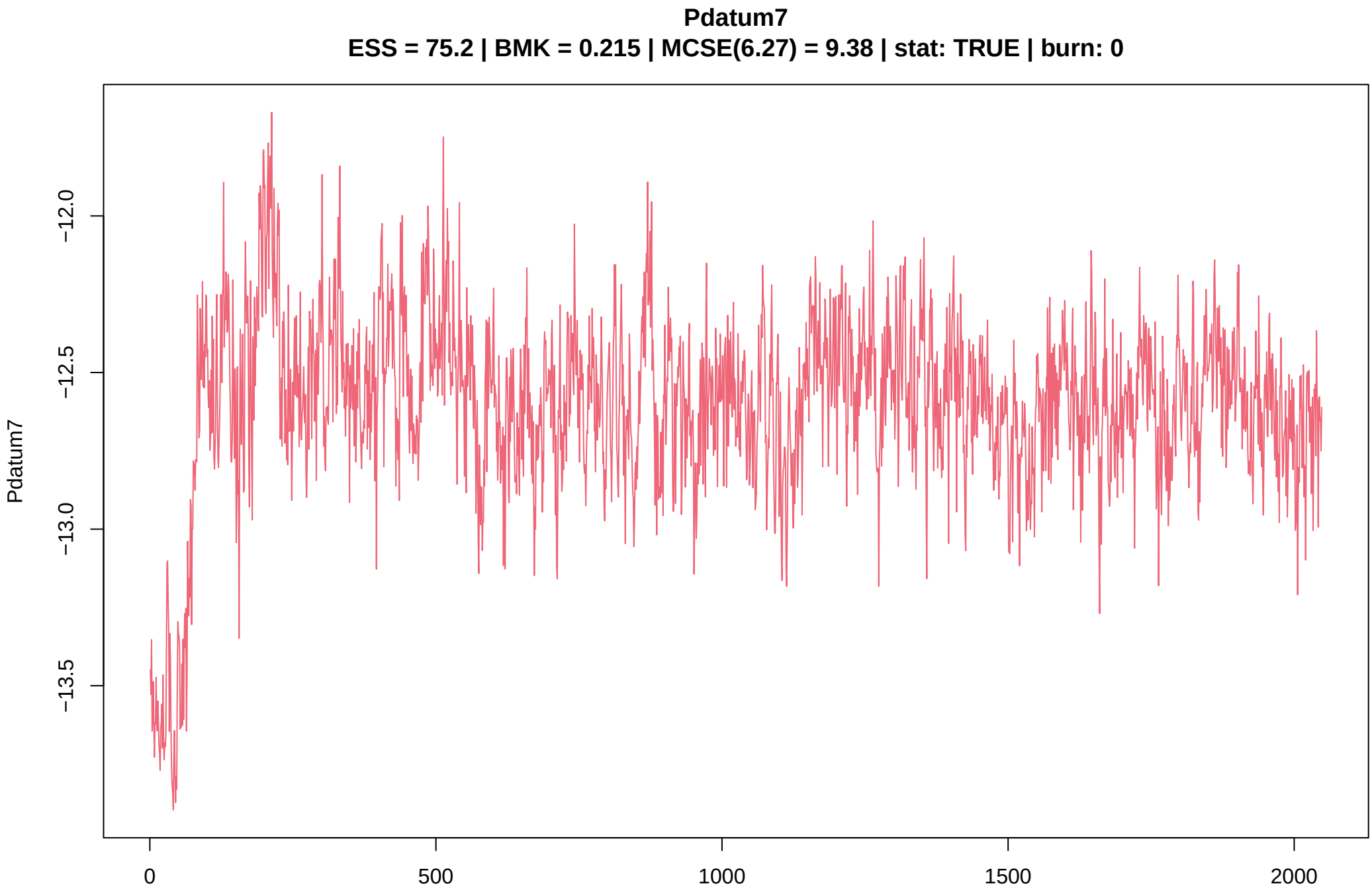

Pdatum2
ESS = 2.22e−16 | BMK = 0.415 | MCSE(6.27) = 11.3 | stat: FALSE | burn: 2040
Pdatum2
−17
−18
−19
−20
0
500
1000
1500
2000

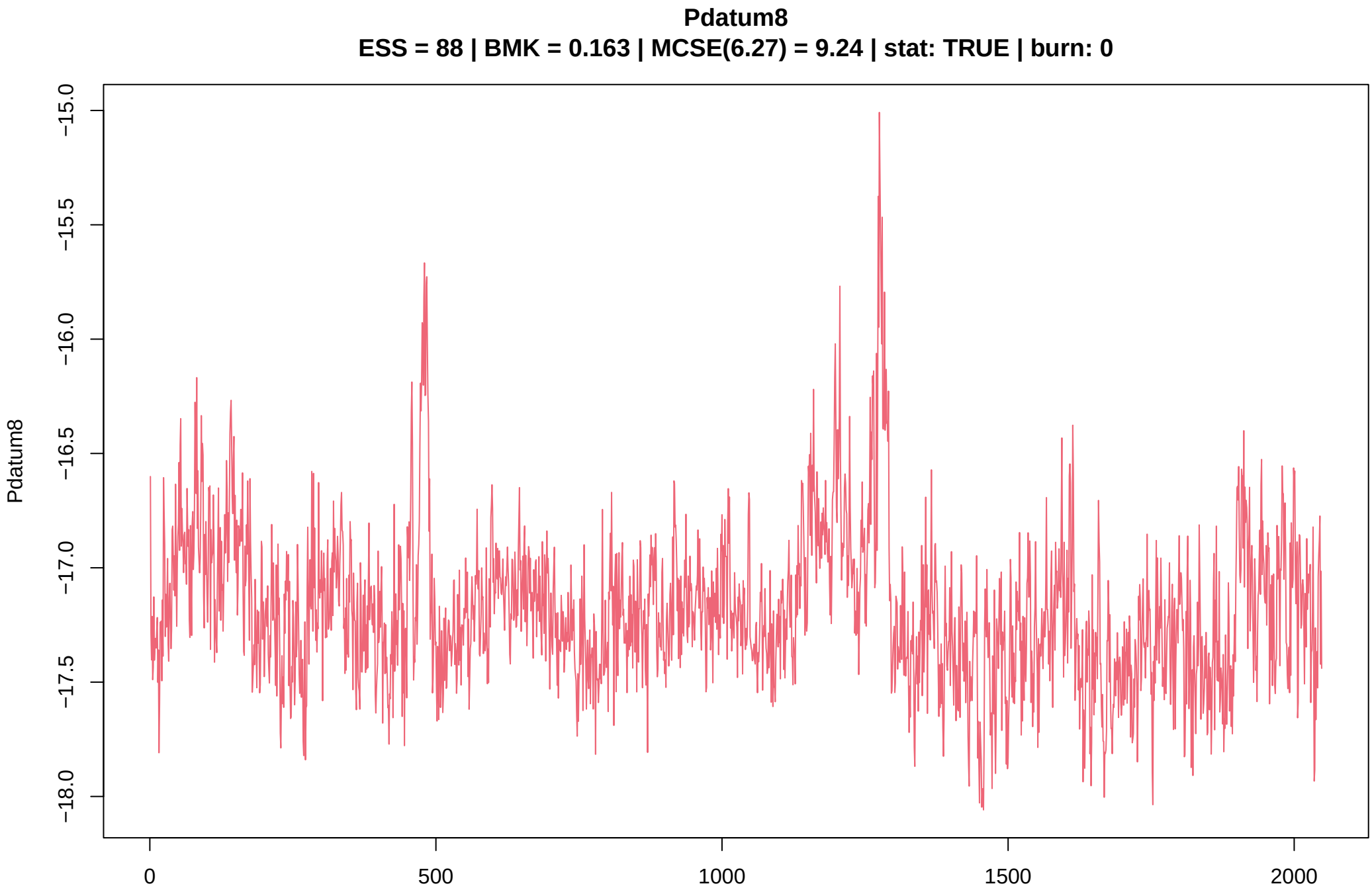

Pdatum3
ESS = 13.4 | BMK = 0.432 | MCSE(6.27) = 13.2 | stat: FALSE | burn: 612
Pdatum3
−10.5
−11.0
−11.5
0
500
1000
1500
2000

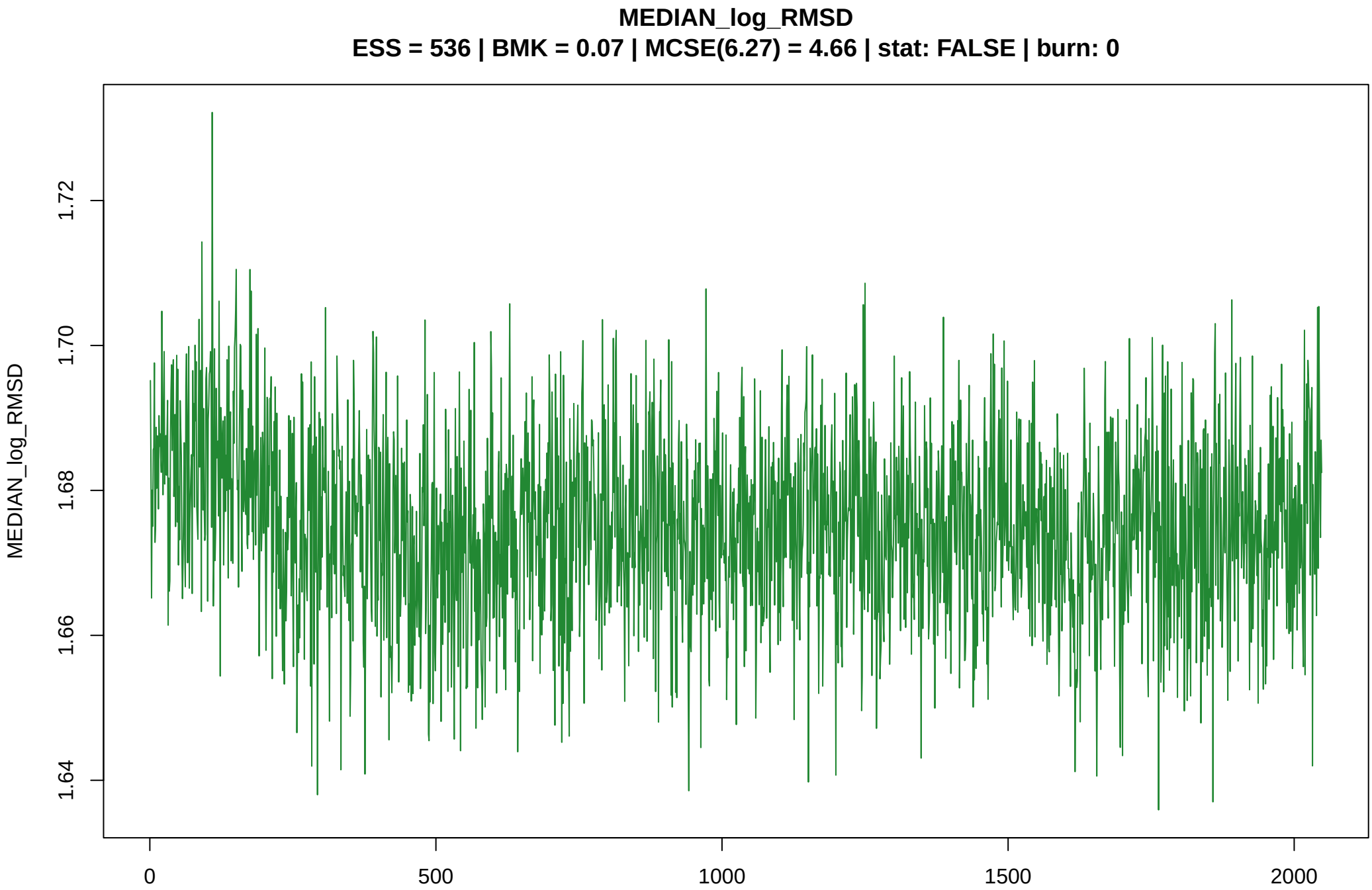

Pdatum4
ESS = 29.9 | BMK = 0.225 | MCSE(6.27) = 11.1 | stat: FALSE | burn: 204
Pdatum4
−10.5
−11.0
−11.5
−12.0
−12.5
0
500
1000
1500
2000

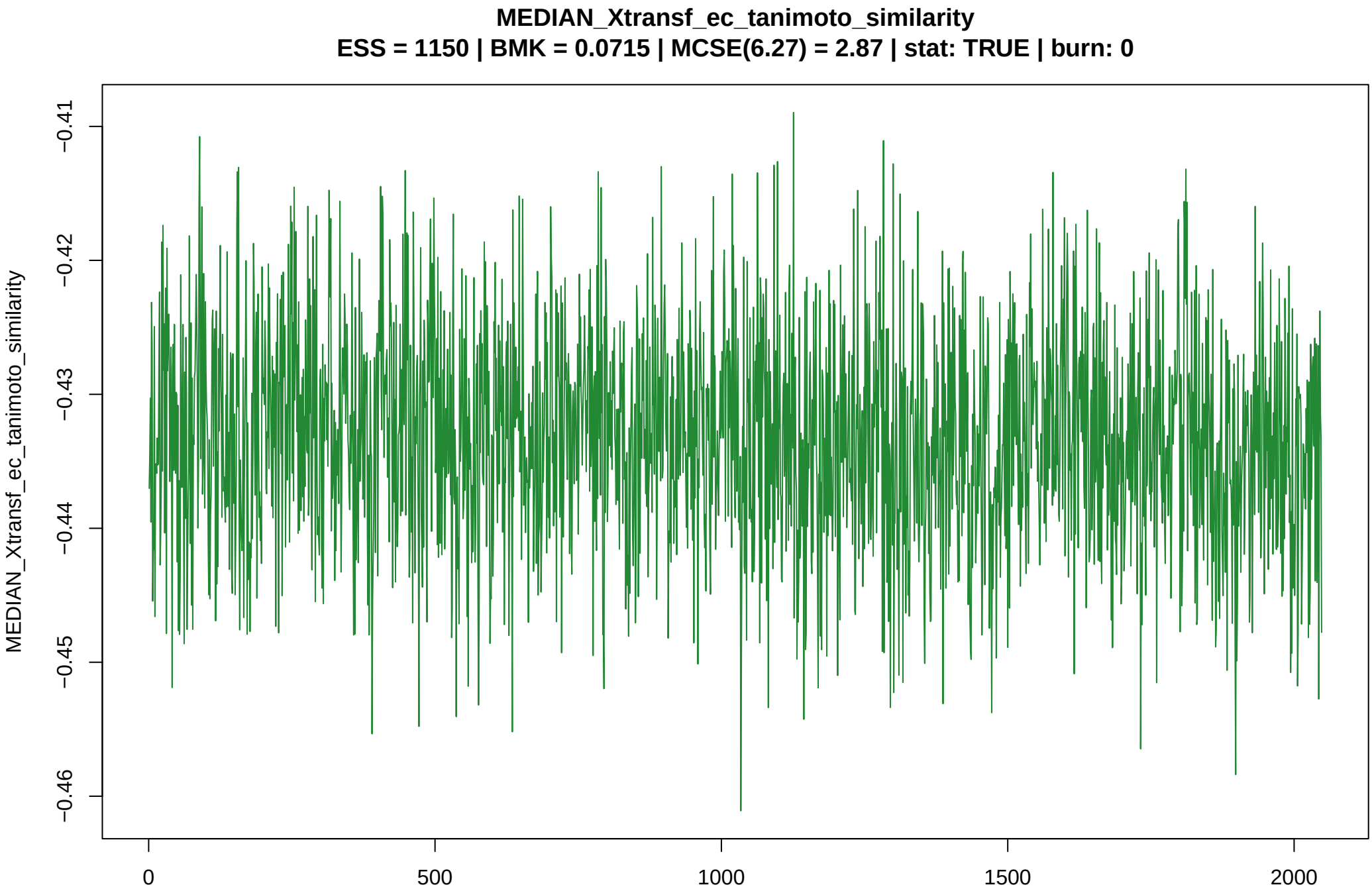

Pdatum5
ESS = 54.1 | BMK = 0.365 | MCSE(6.27) = 9.41 | stat: FALSE | burn: 0
Pdatum5
−10.5
−11.0
−11.5
0
500
1000
1500
2000

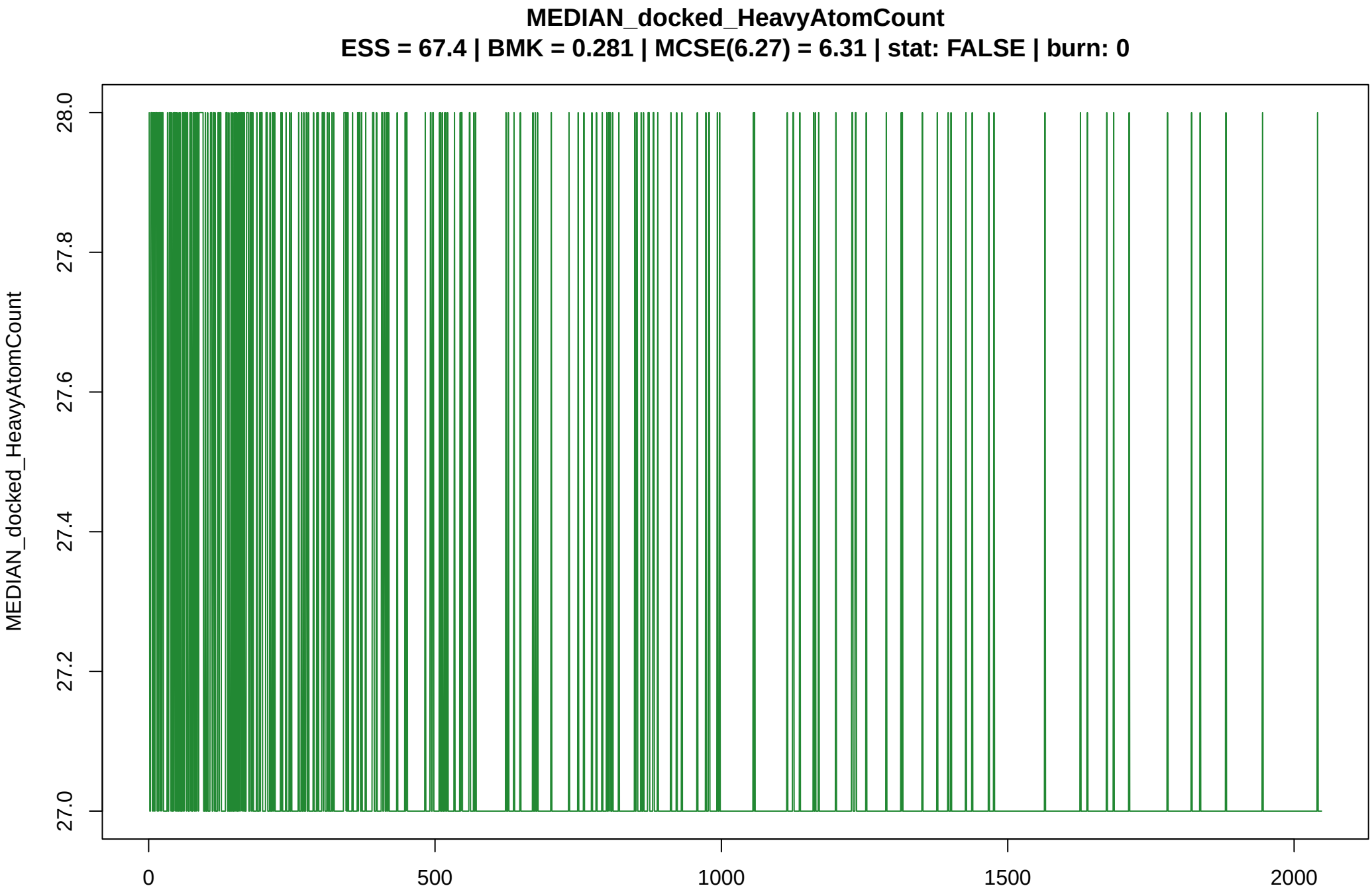

Pdatum6
ESS = 734 | BMK = 0.0738 | MCSE(6.27) = 4.07 | stat: FALSE | burn: 0
Pdatum6
−14.6
−14.8
−15.0
−15.2
−15.4
−15.6
−15.8
−16.0
0
500
1000
1500
2000

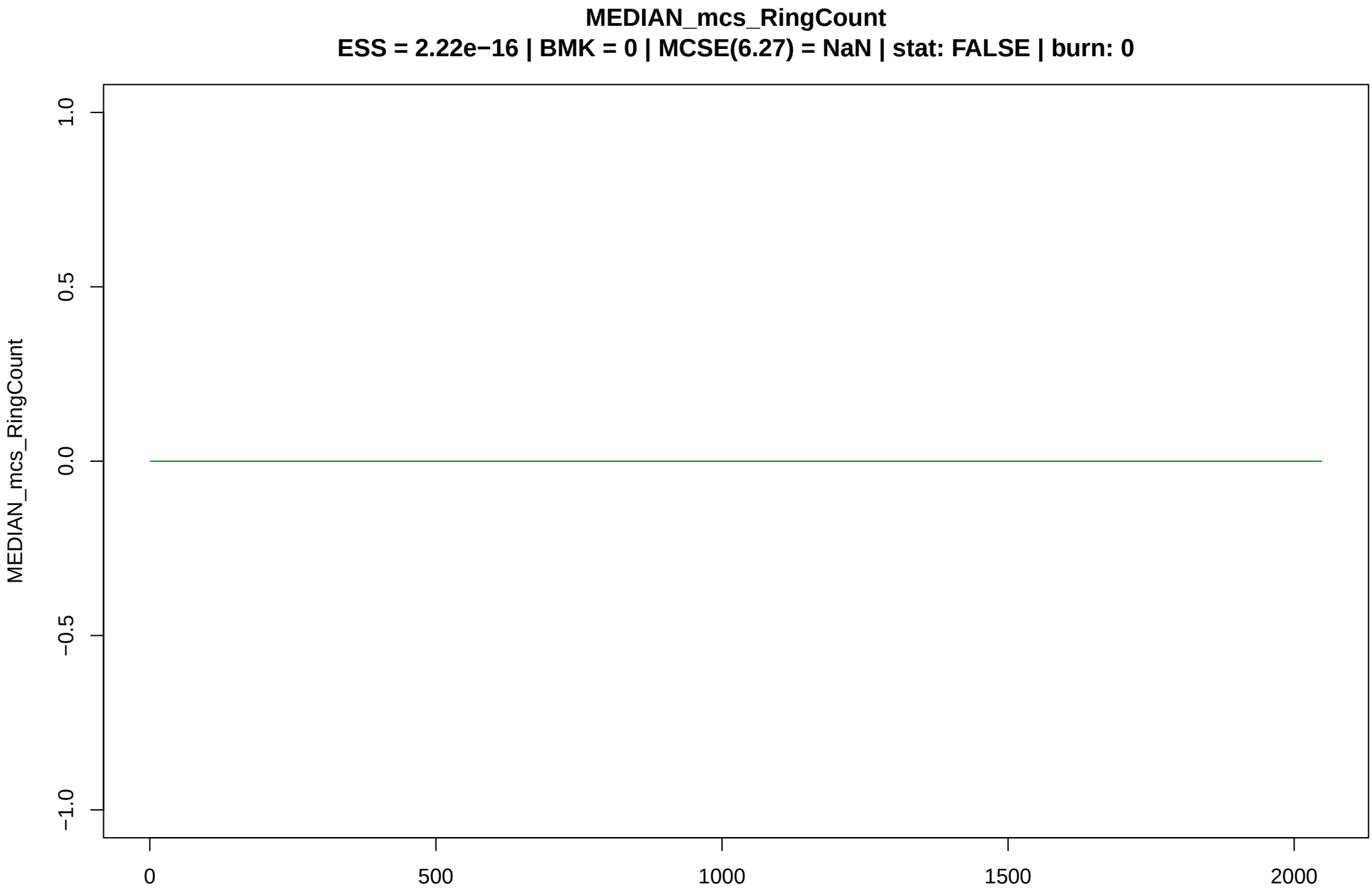

Pdatum7
ESS = 75.2 | BMK = 0.215 | MCSE(6.27) = 9.38 | stat: TRUE | burn: 0
Pdatum7
−12.0
−12.5
−13.0
−13.5
0
500
1000
1500
2000

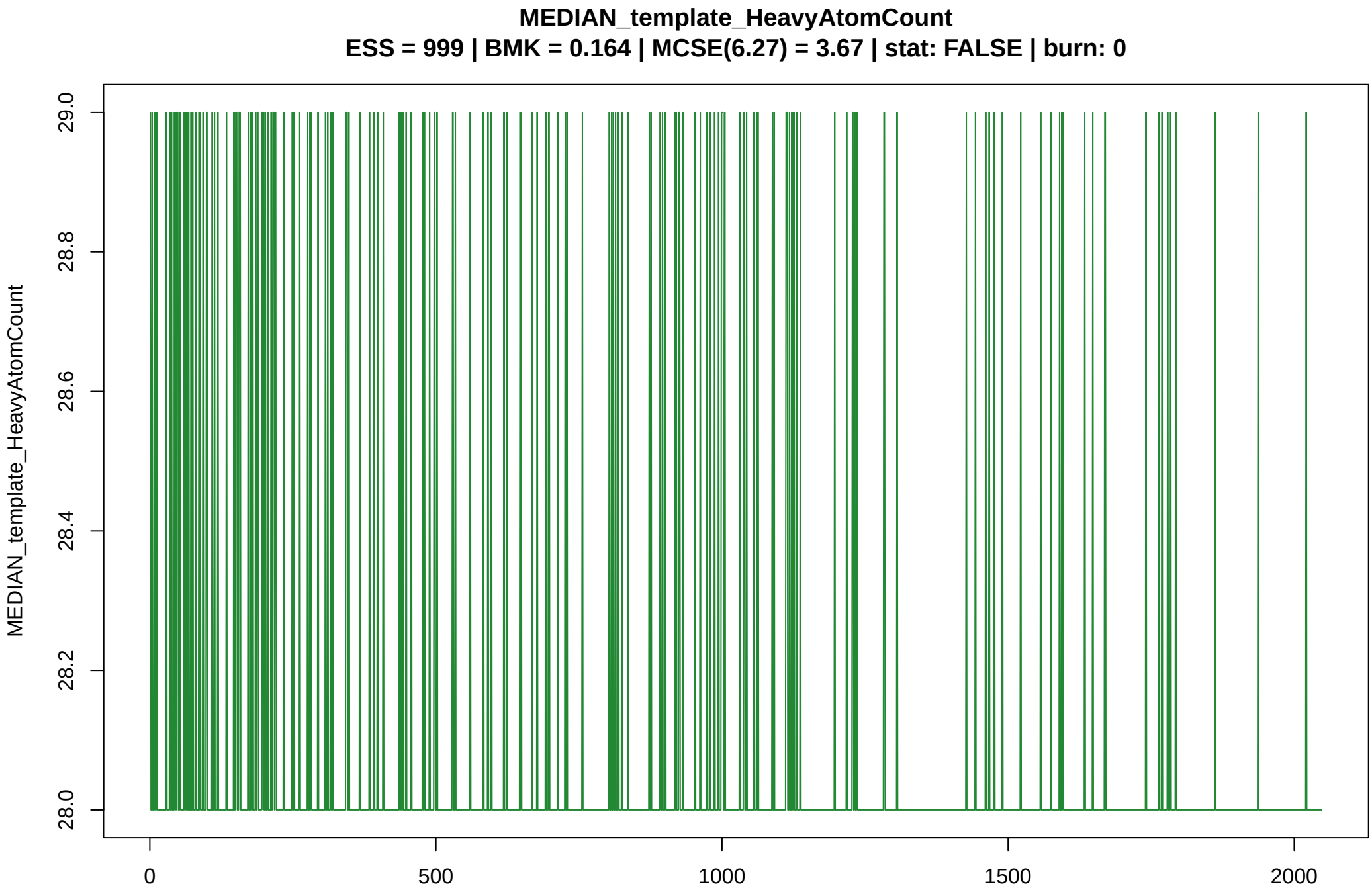

Pdatum8
ESS = 88 | BMK = 0.163 | MCSE(6.27) = 9.24 | stat: TRUE | burn: 0
Pdatum8
−15.0
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
0
500
1000
1500
2000

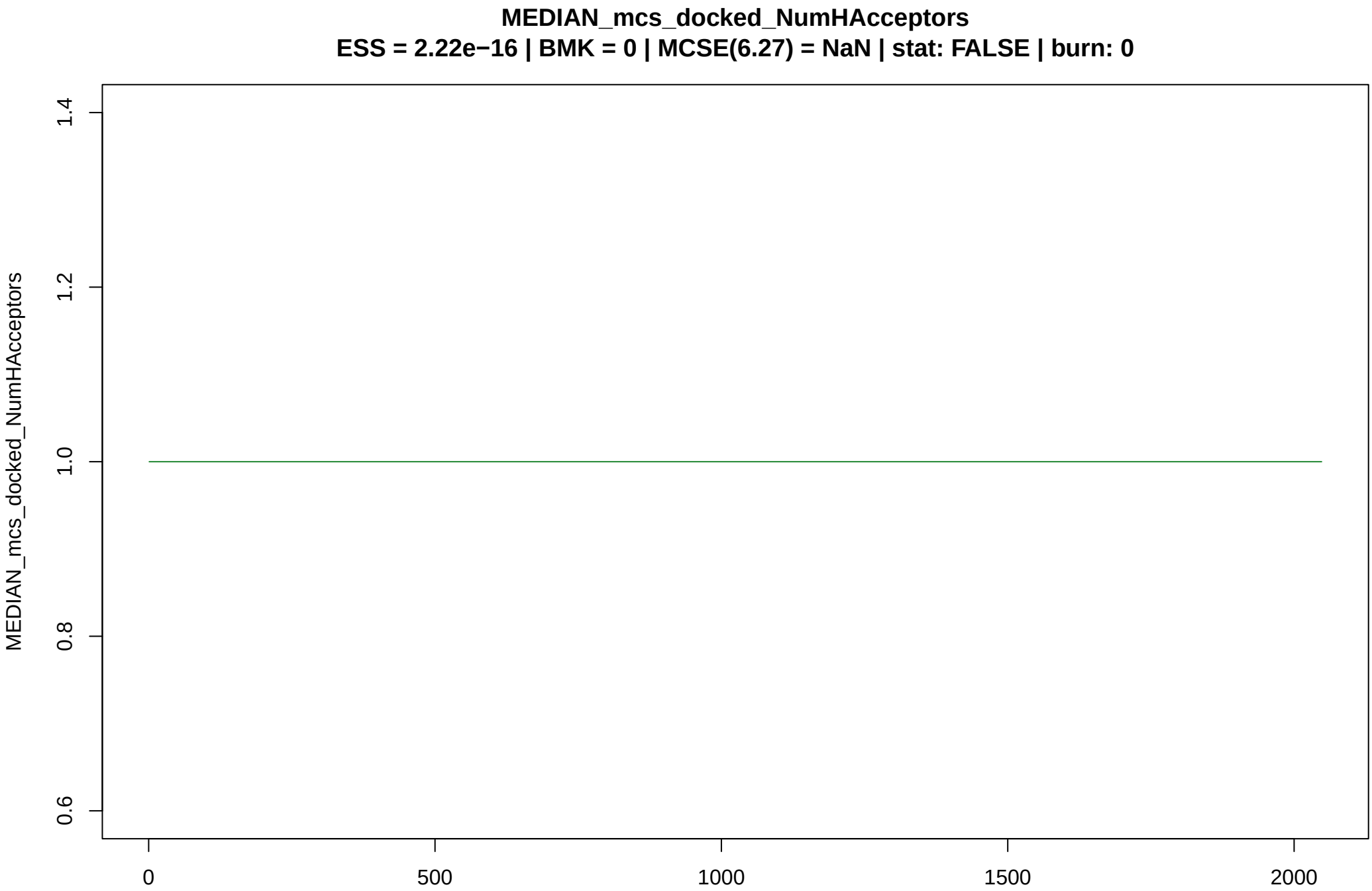

MEDIAN_log_RMSD
ESS = 536 | BMK = 0.07 | MCSE(6.27) = 4.66 | stat: FALSE | burn: 0
MEDIAN_log_RMSD
1.64
1.66
1.68
1.70
1.72
0
500
1000
1500
2000

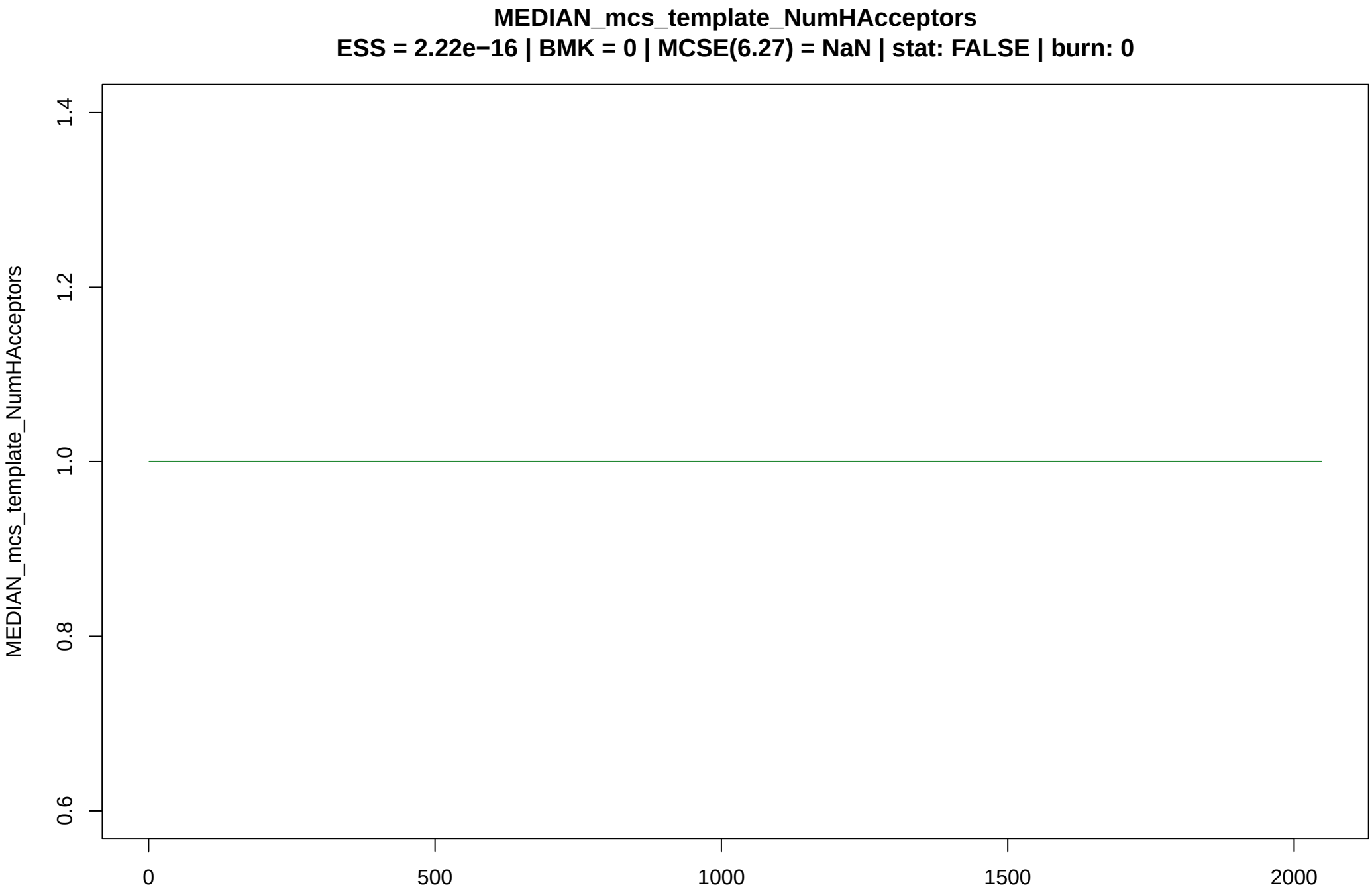

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1150 | BMK = 0.0715 | MCSE(6.27) = 2.87 | stat: TRUE | burn: 0
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.41
−0.42
−0.43
−0.44
−0.45
−0.46
0
500
1000
1500
2000

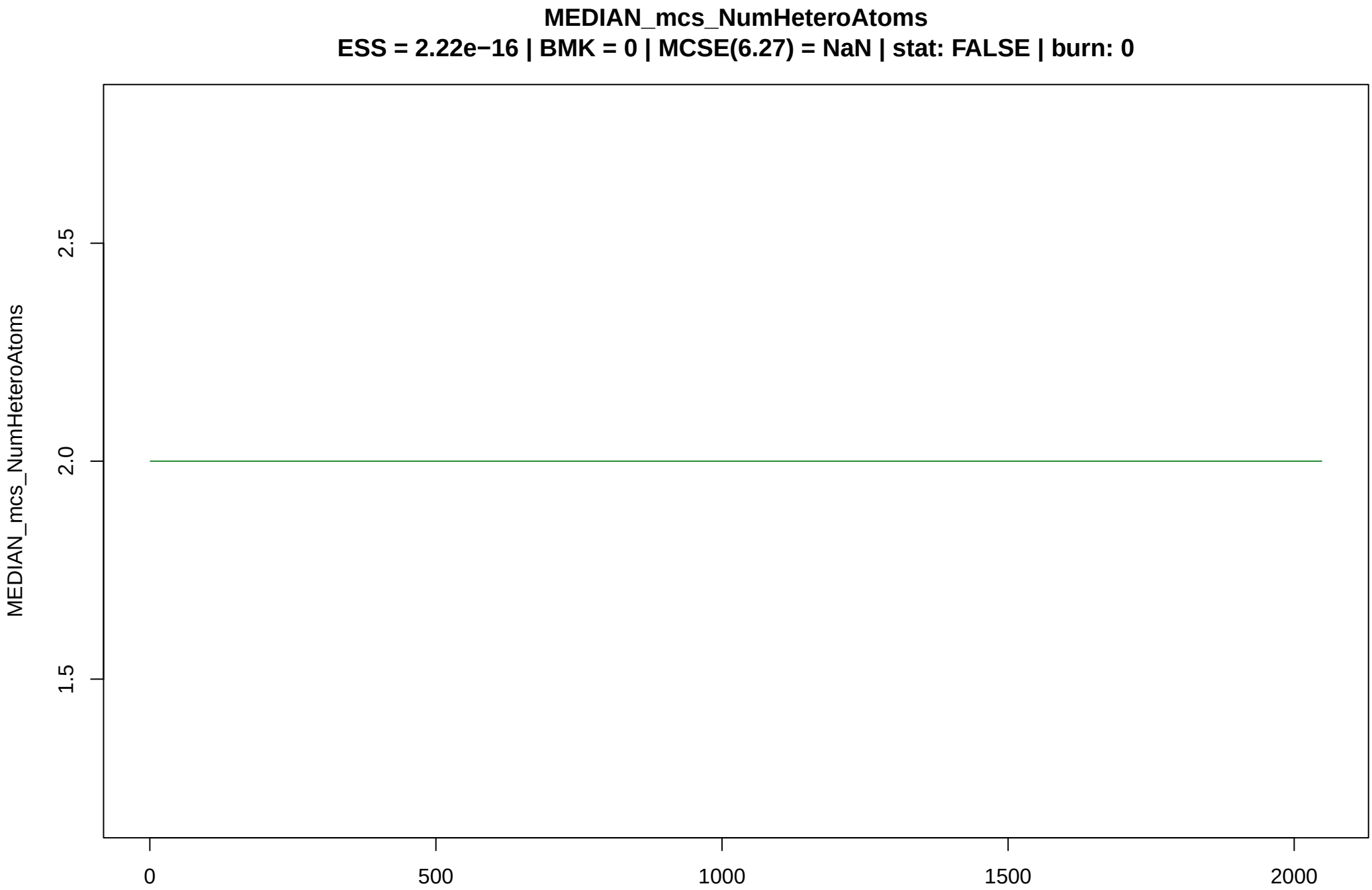

MEDIAN_docked_HeavyAtomCount
ESS = 67.4 | BMK = 0.281 | MCSE(6.27) = 6.31 | stat: FALSE | burn: 0
MEDIAN_docked_HeavyAtomCount
28.0
27.8
27.6
27.4
27.2
27.0
0
500
1000
1500
2000

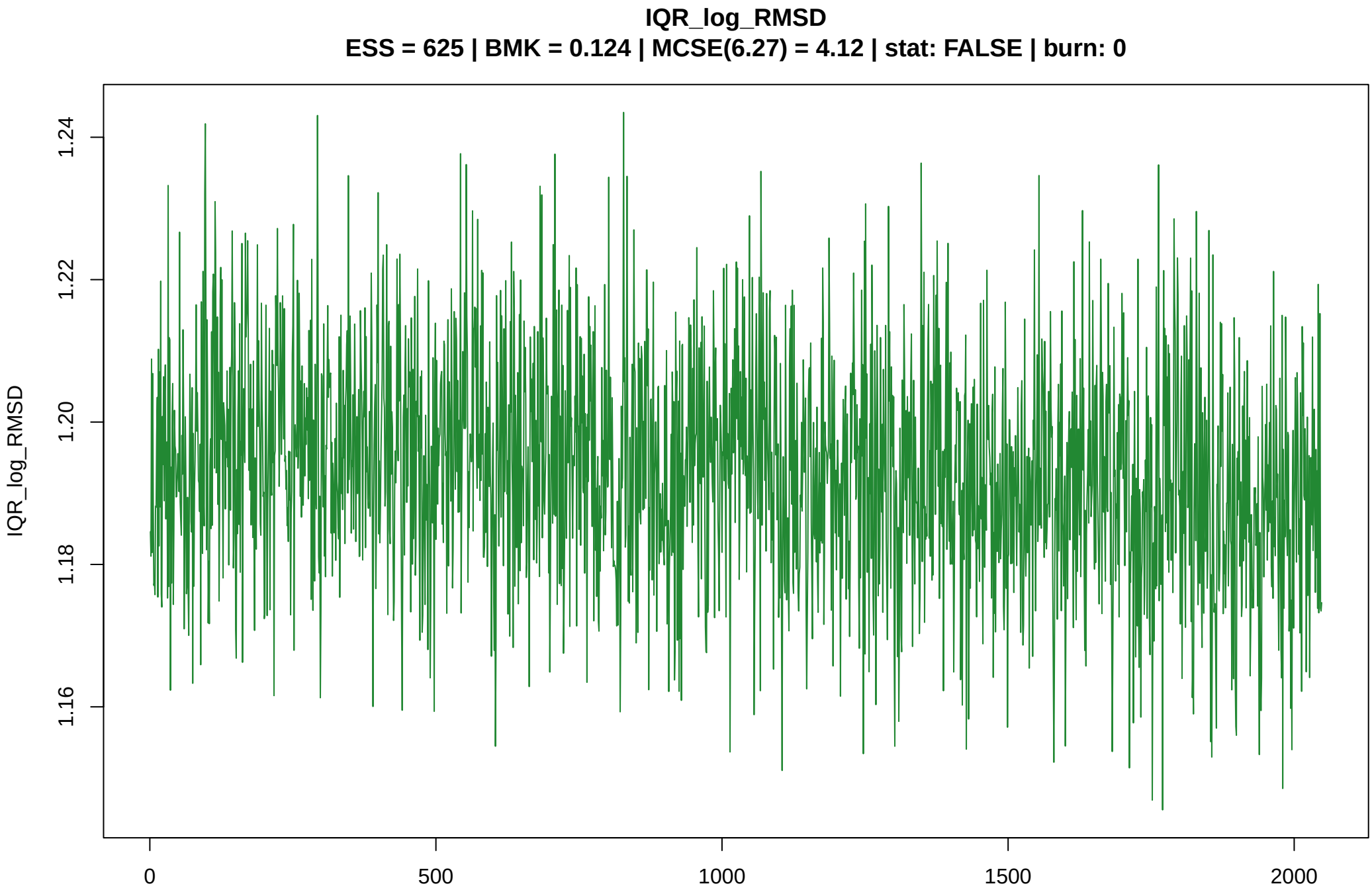

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

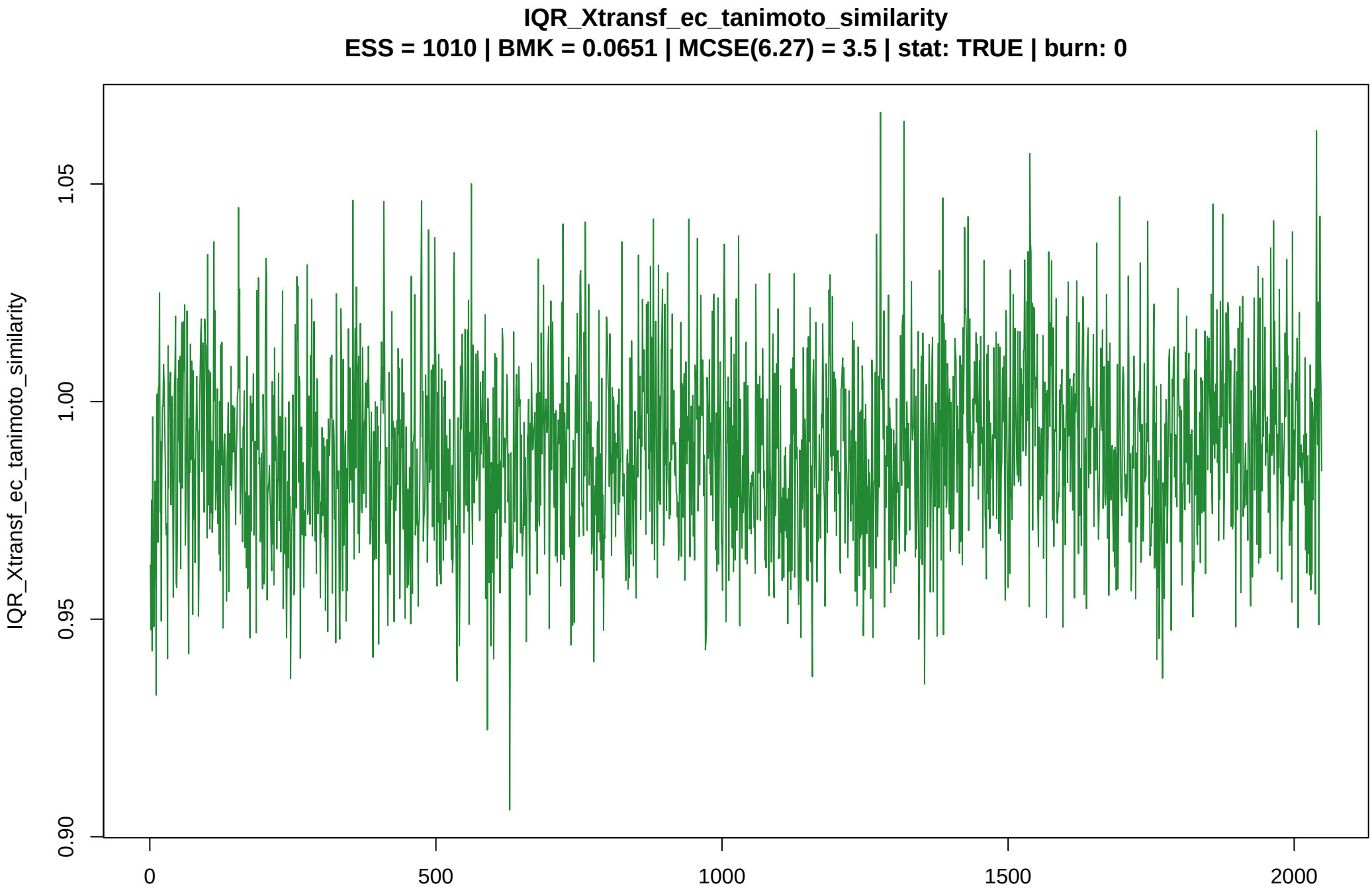

MEDIAN_template_HeavyAtomCount
ESS = 999 | BMK = 0.164 | MCSE(6.27) = 3.67 | stat: FALSE | burn: 0
MEDIAN_template_HeavyAtomCount
29.0
28.8
28.6
28.4
28.2
28.0
0
500
1000
1500
2000

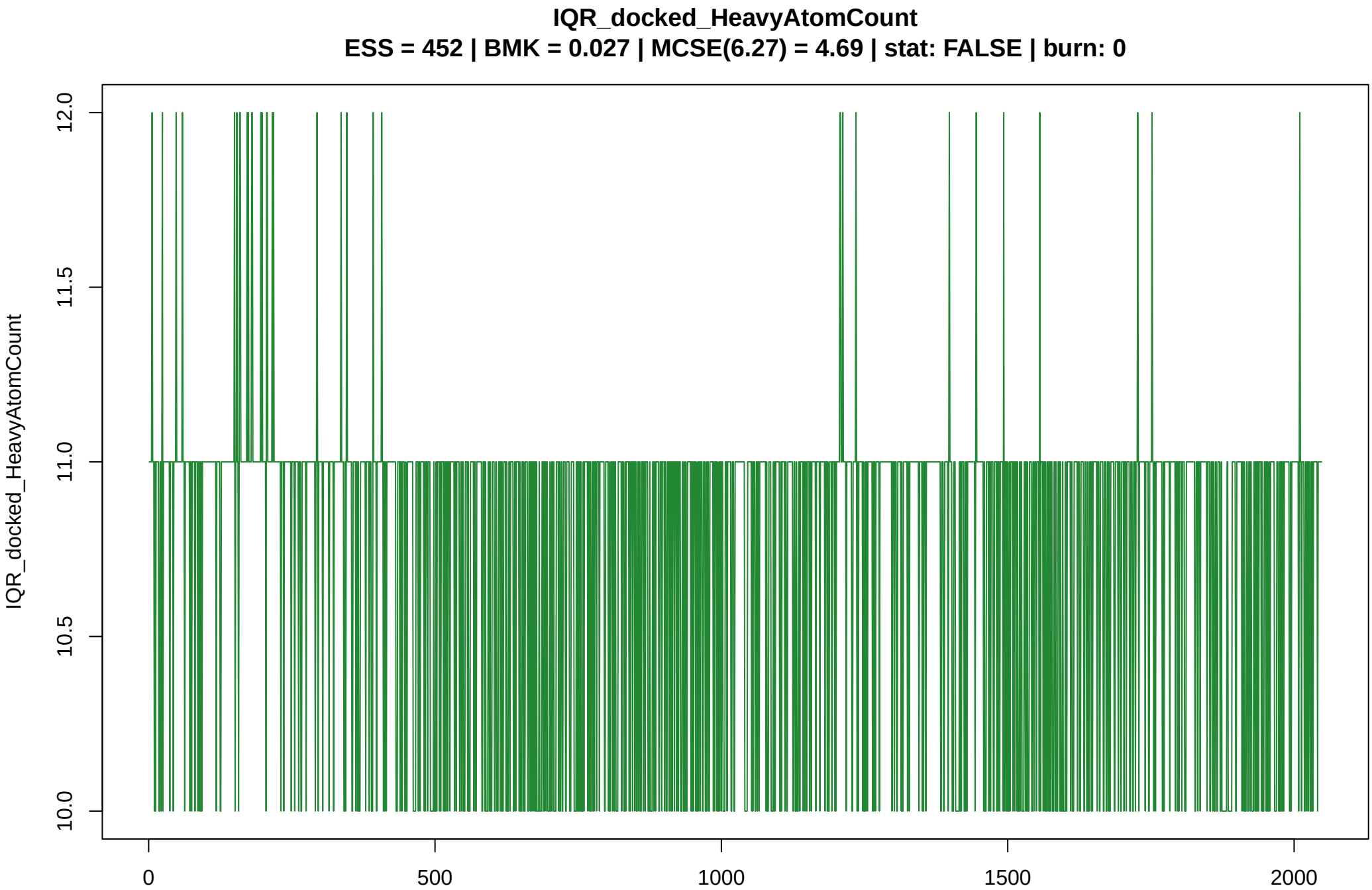

MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

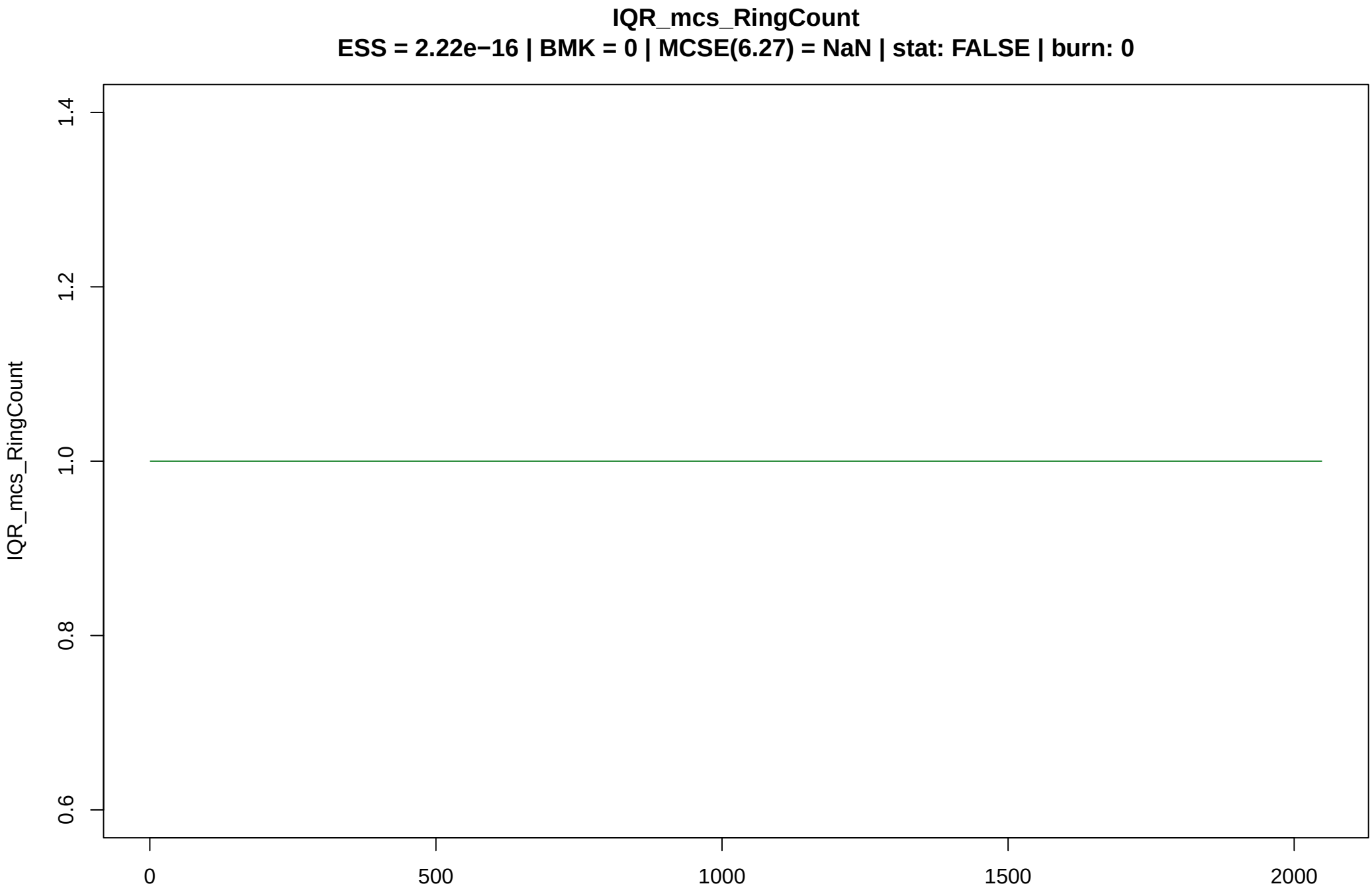

MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

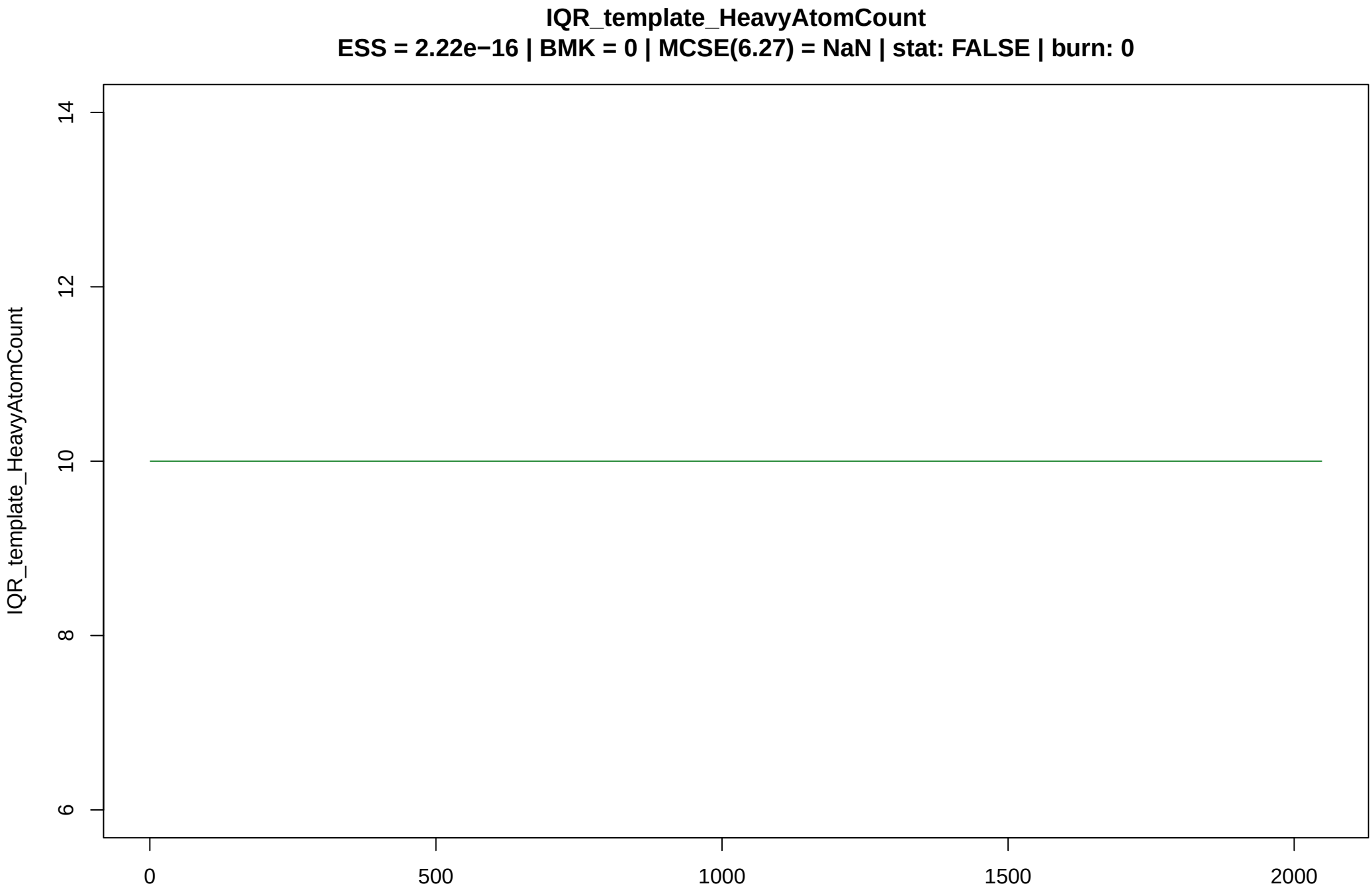

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

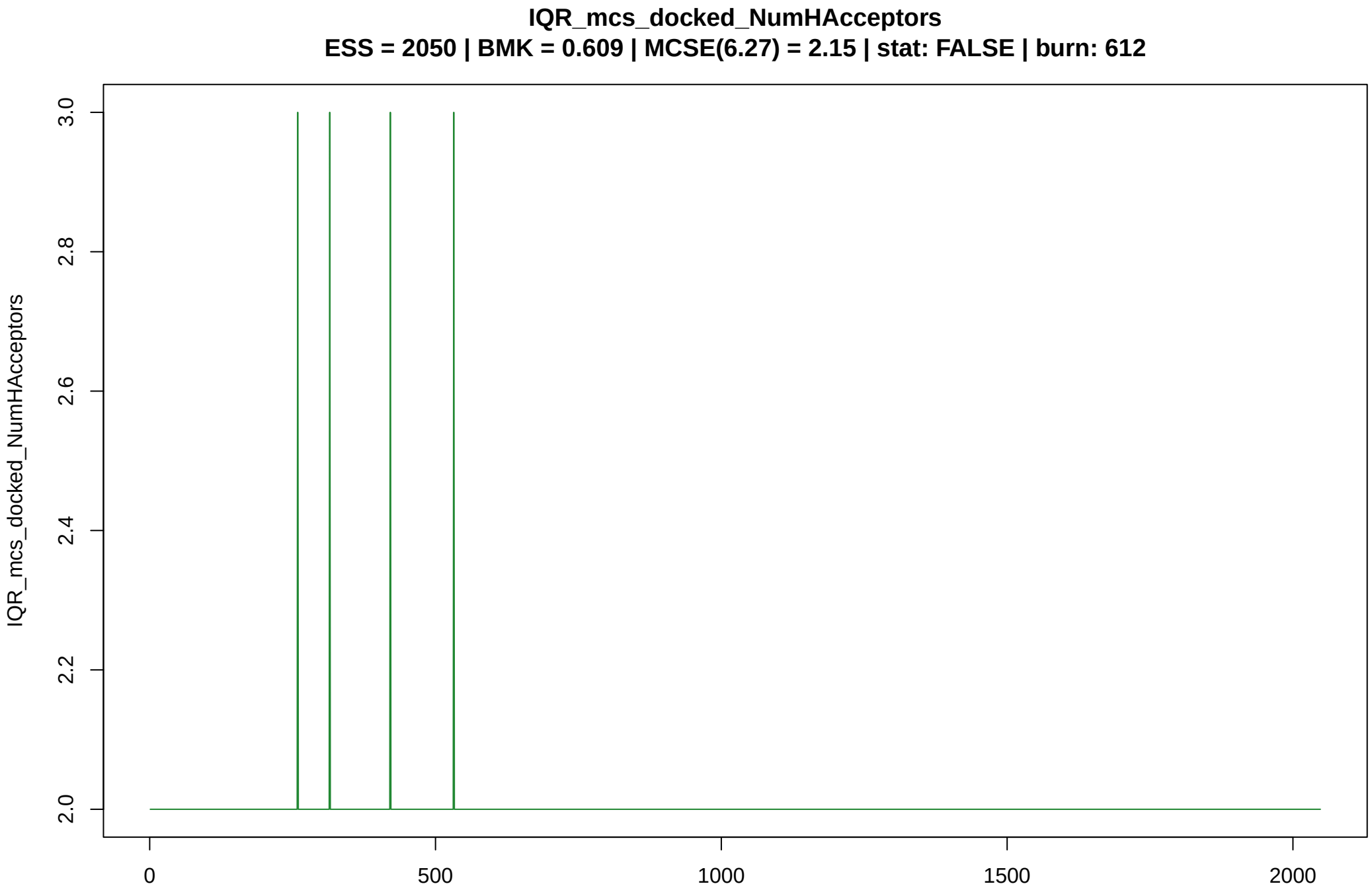

IQR_log_RMSD
ESS = 625 | BMK = 0.124 | MCSE(6.27) = 4.12 | stat: FALSE | burn: 0
IQR_log_RMSD
1.16
1.18
1.20
1.22
1.24
0
500
1000
1500
2000

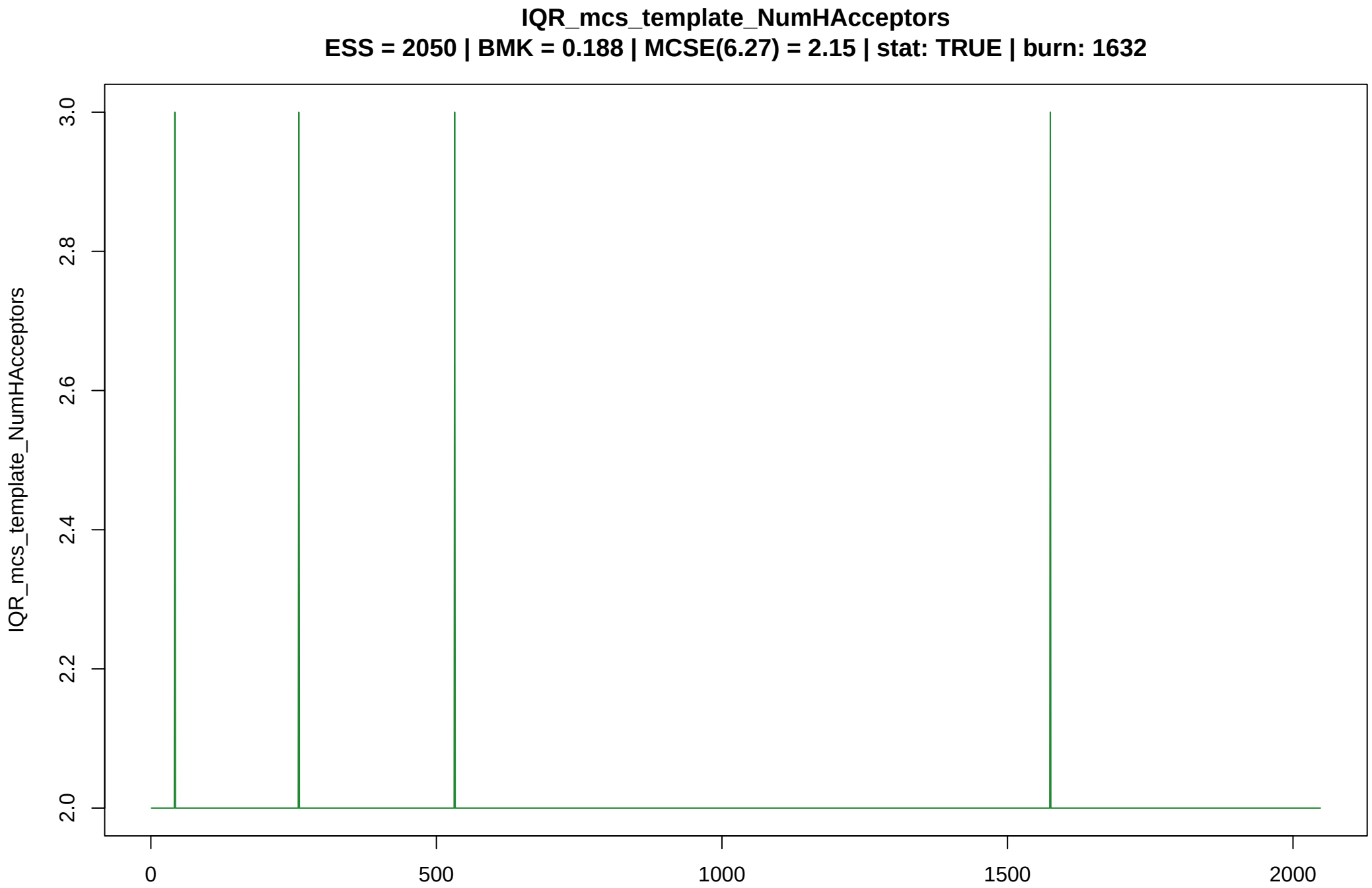

IQR_Xtransf_ec_tanimoto_similarity
ESS = 1010 | BMK = 0.0651 | MCSE(6.27) = 3.5 | stat: TRUE | burn: 0
IQR_Xtransf_ec_tanimoto_similarity
0.90
0.95
1.00
1.05
0
500
1000
1500
2000

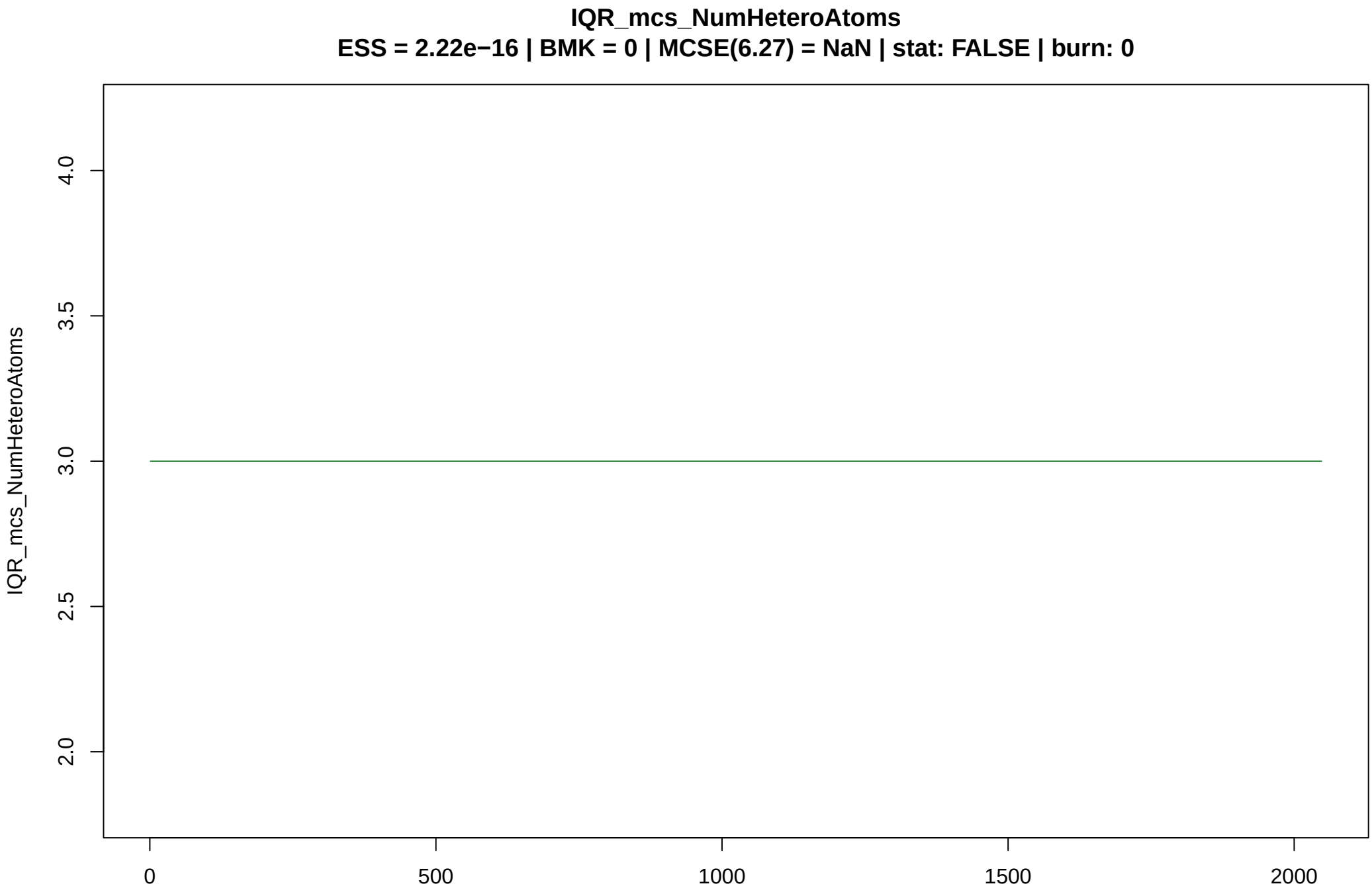

IQR_docked_HeavyAtomCount
ESS = 452 | BMK = 0.027 | MCSE(6.27) = 4.69 | stat: FALSE | burn: 0
IQR_docked_HeavyAtomCount
12.0
11.5
11.0
10.5
10.0
0
500
1000
1500
2000

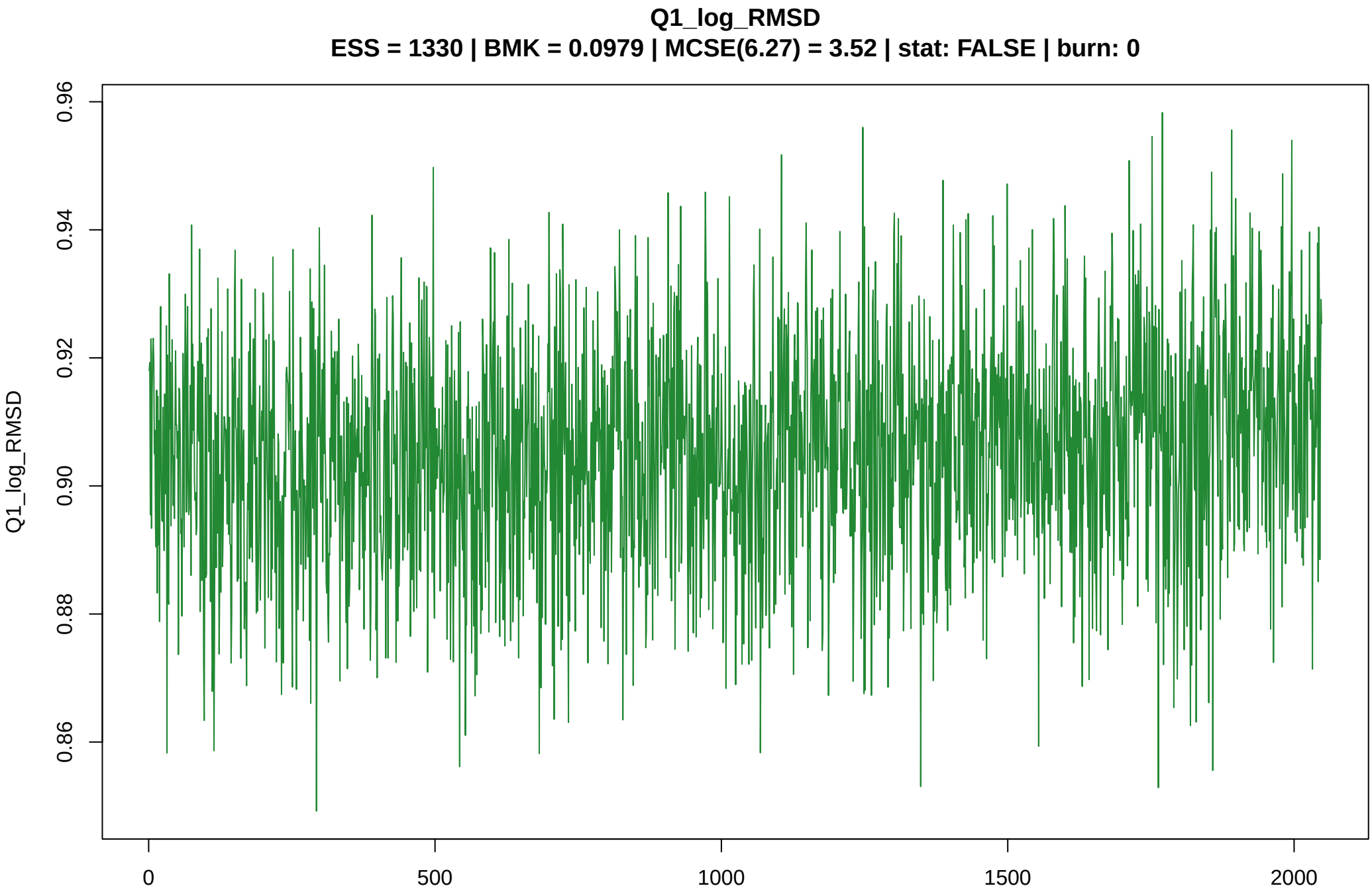

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

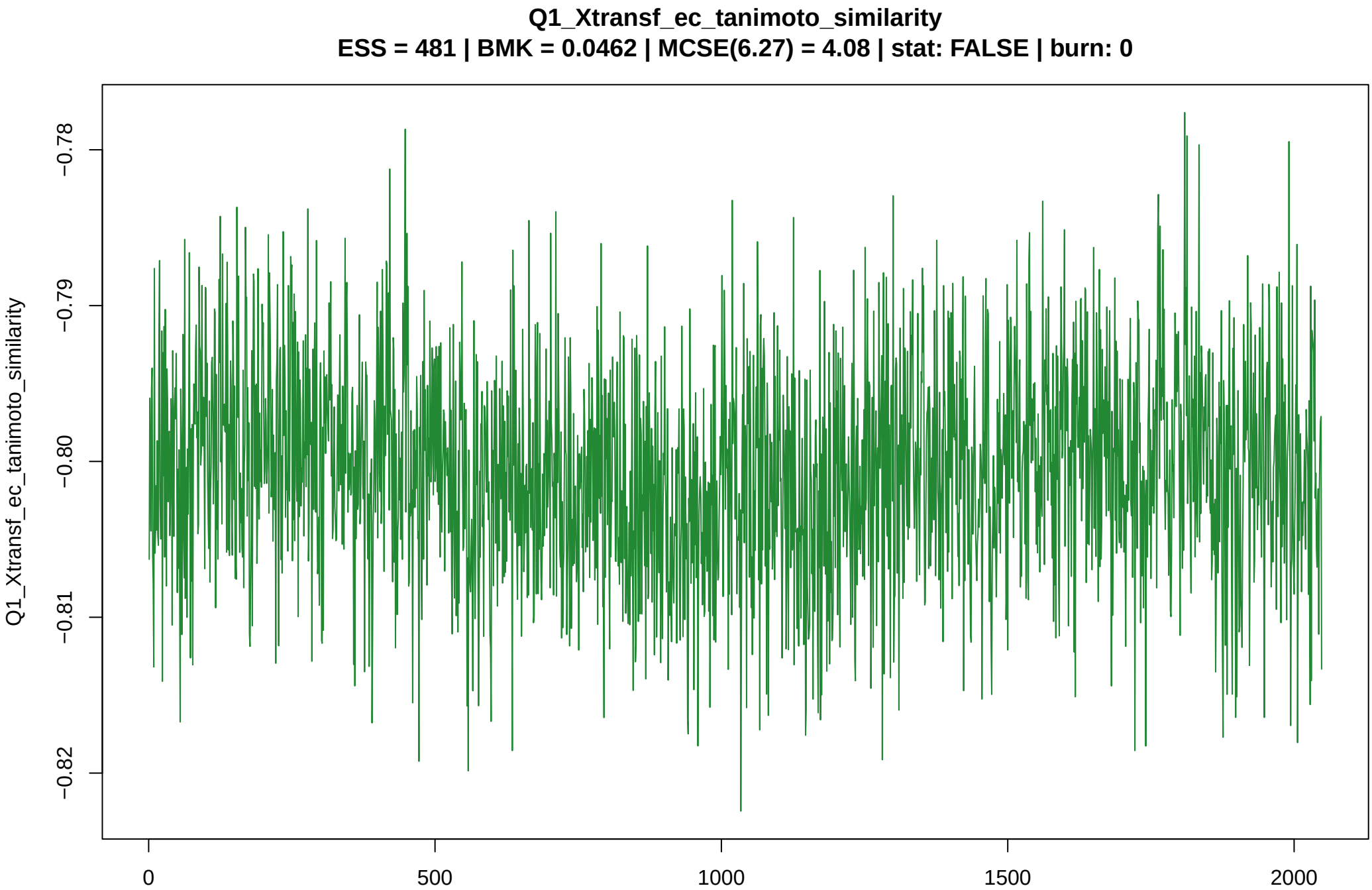

IQR_template_HeavyAtomCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_template_HeavyAtomCount
14
12
10
8
6
0
500
1000
1500
2000

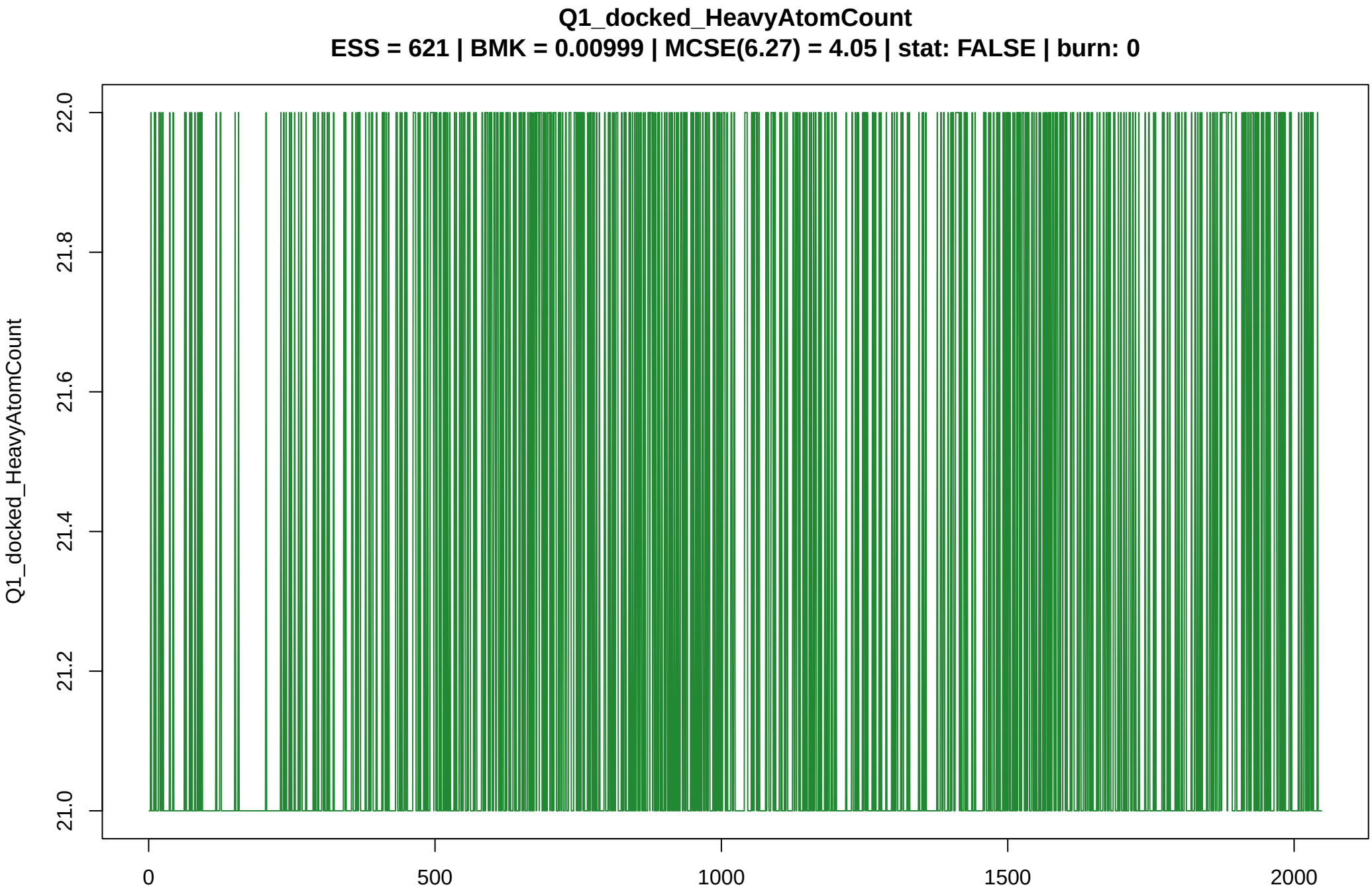

IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.609 | MCSE(6.27) = 2.15 | stat: FALSE | burn: 612
IQR_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

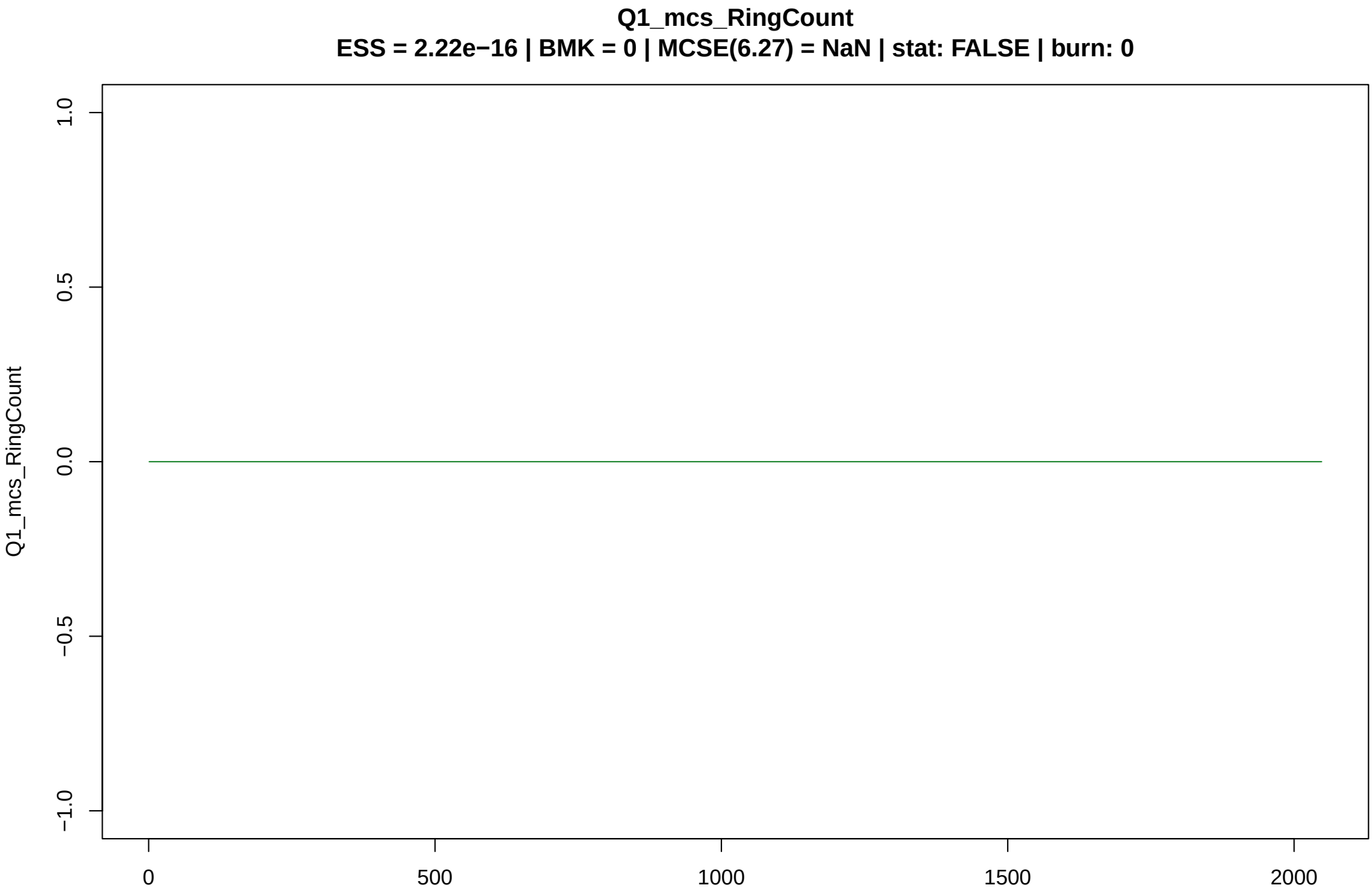

IQR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1632
IQR_mcs_template_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

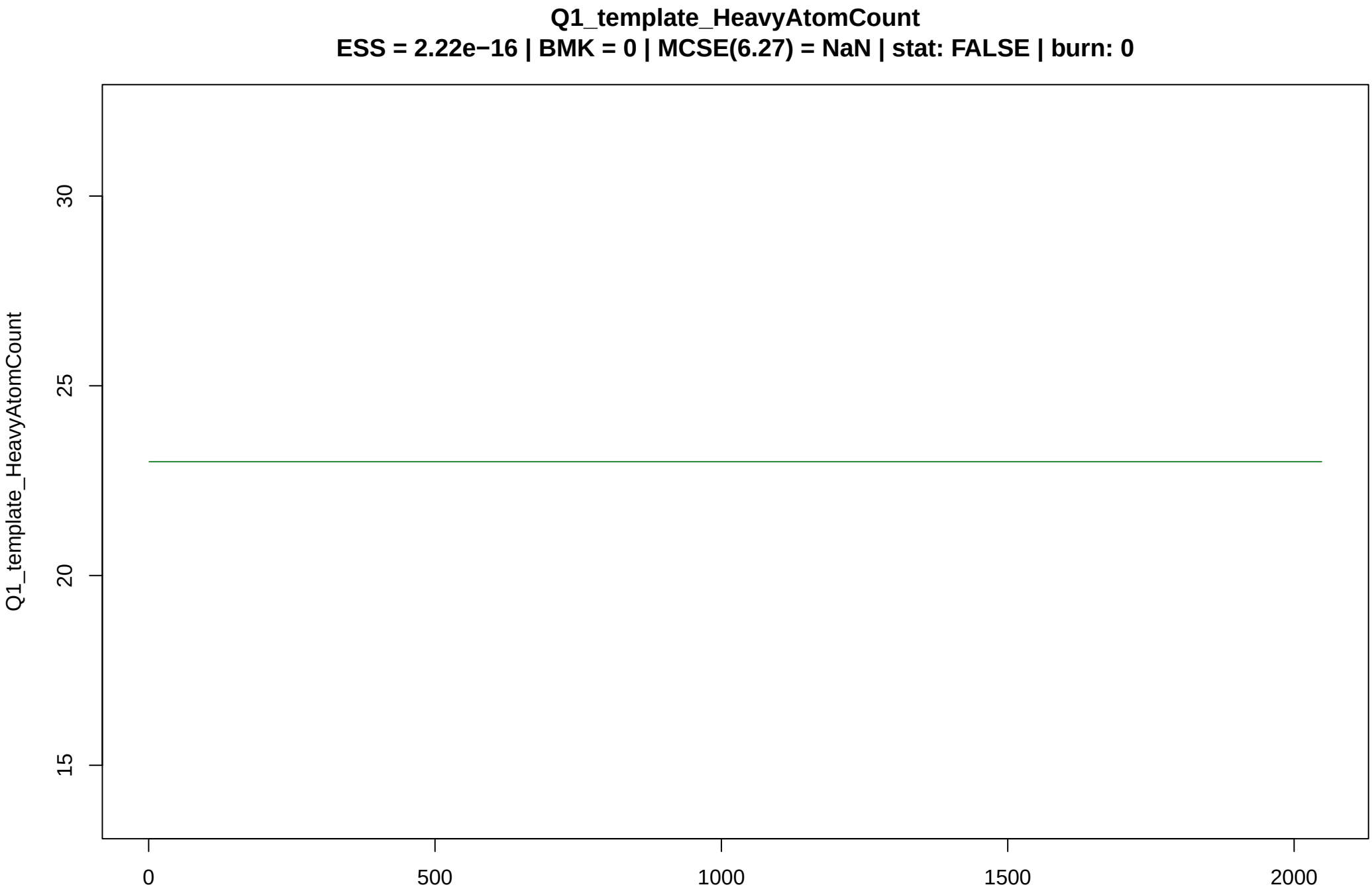

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

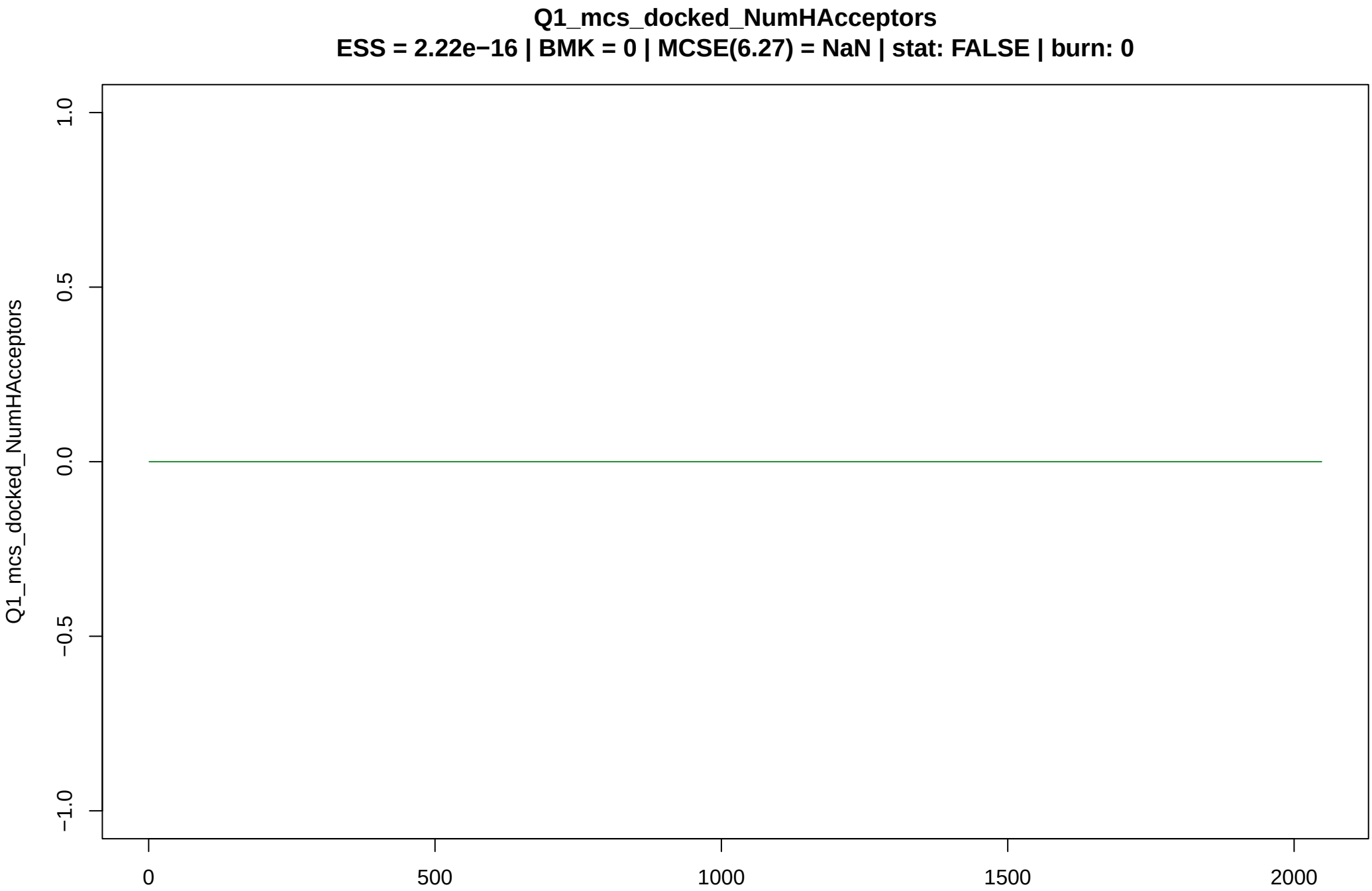

Q1_log_RMSD
ESS = 1330 | BMK = 0.0979 | MCSE(6.27) = 3.52 | stat: FALSE | burn: 0
Q1_log_RMSD
0.86
0.88
0.90
0.92
0.94
0.96
0
500
1000
1500
2000

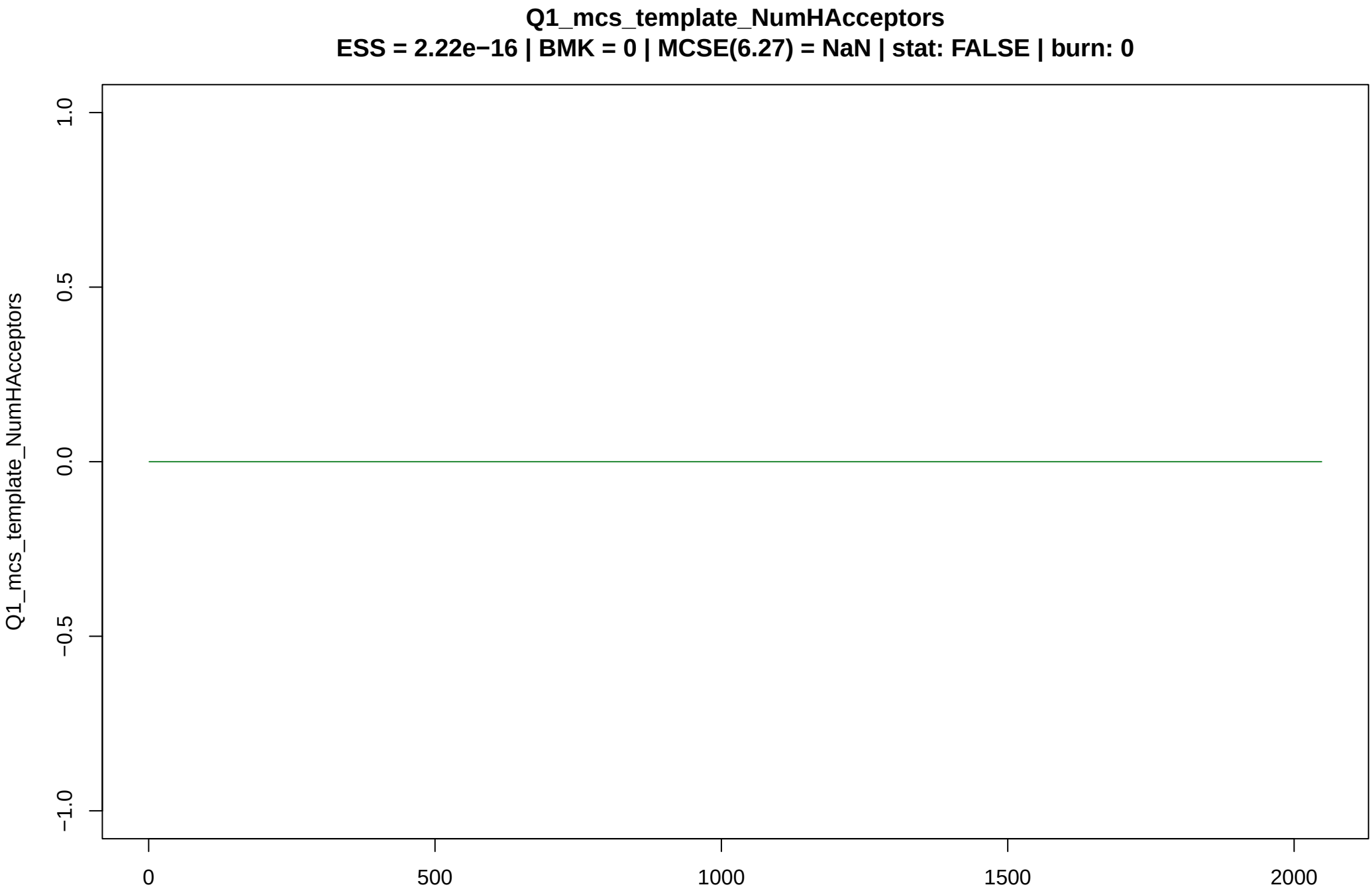

Q1_Xtransf_ec_tanimoto_similarity
ESS = 481 | BMK = 0.0462 | MCSE(6.27) = 4.08 | stat: FALSE | burn: 0
Q1_Xtransf_ec_tanimoto_similarity
−0.78
−0.79
−0.80
−0.81
−0.82
0
500
1000
1500
2000

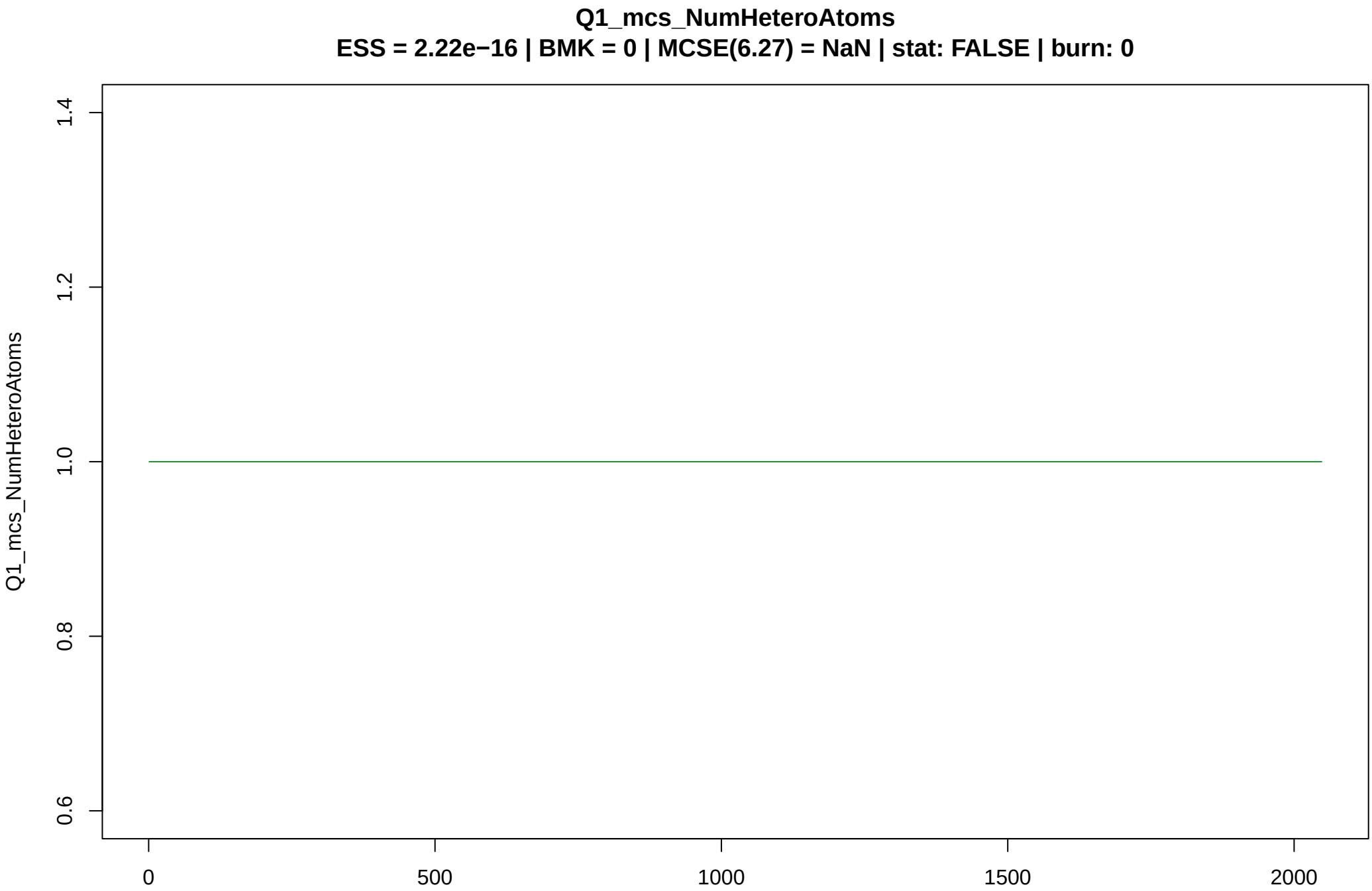

Q1_docked_HeavyAtomCount
ESS = 621 | BMK = 0.00999 | MCSE(6.27) = 4.05 | stat: FALSE | burn: 0
Q1_docked_HeavyAtomCount
22.0
21.8
21.6
21.4
21.2
21.0
0
500
1000
1500
2000

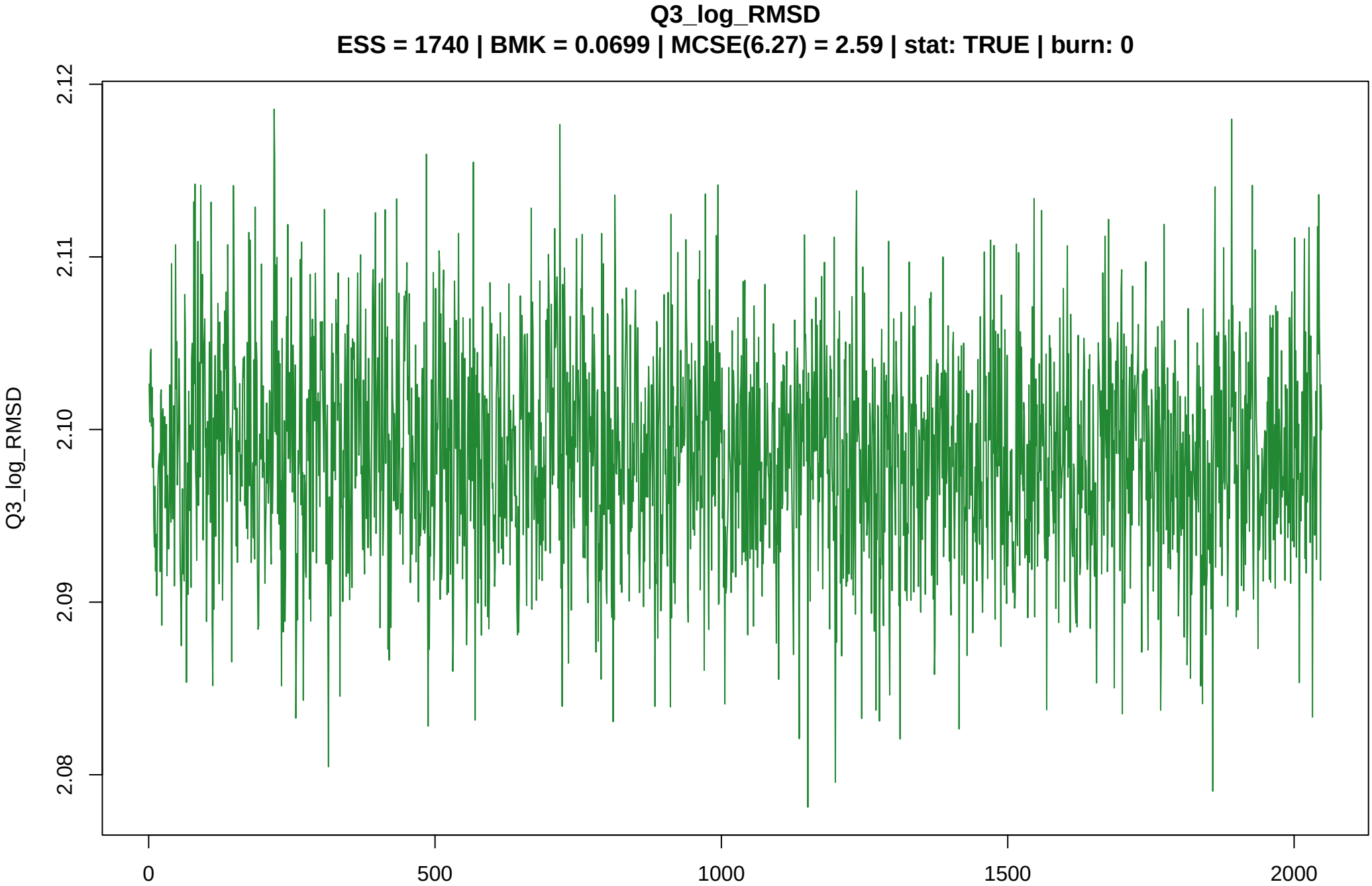

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

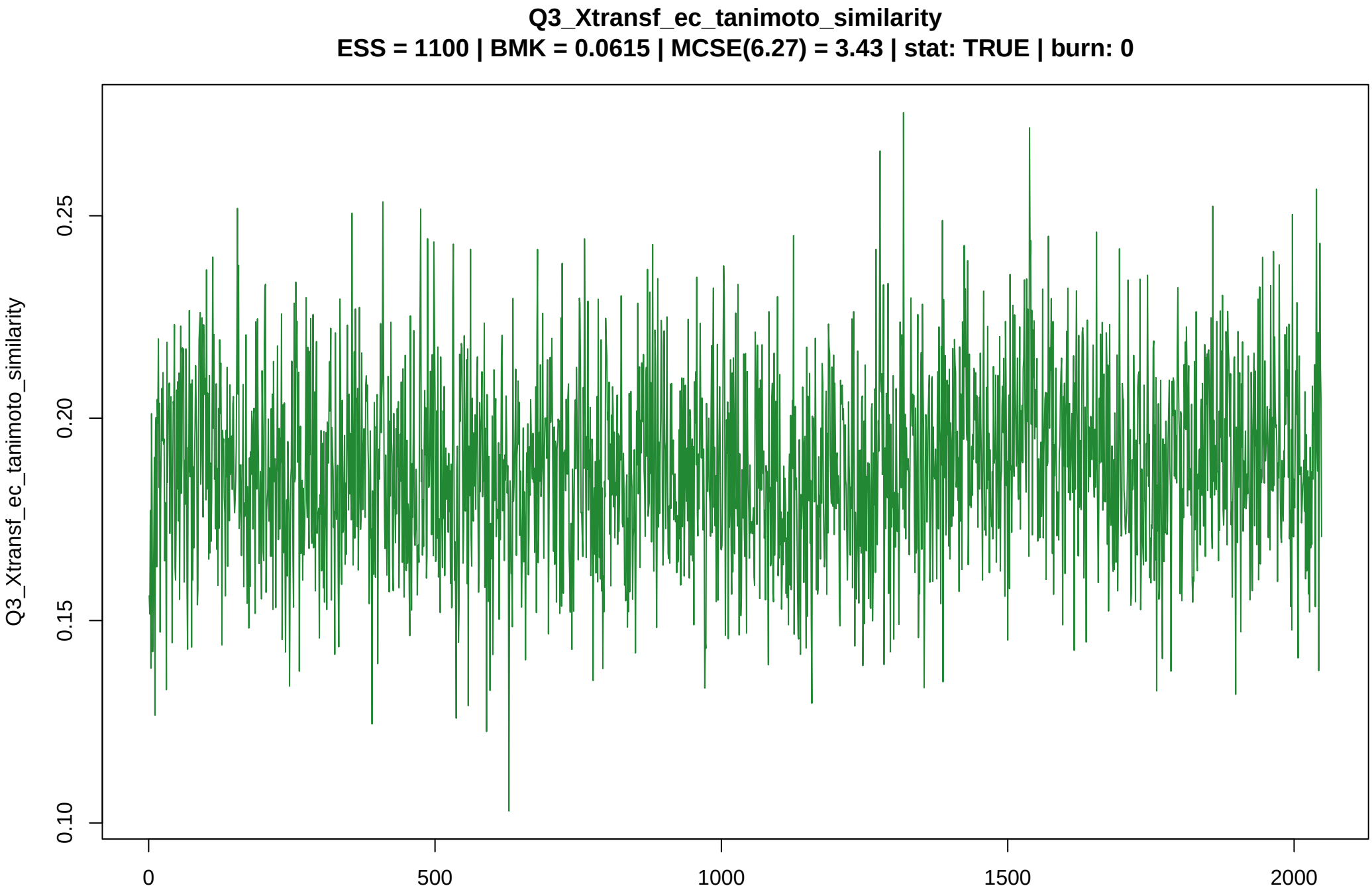

Q1_template_HeavyAtomCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_template_HeavyAtomCount
15
20
25
30
0
500
1000
1500
2000

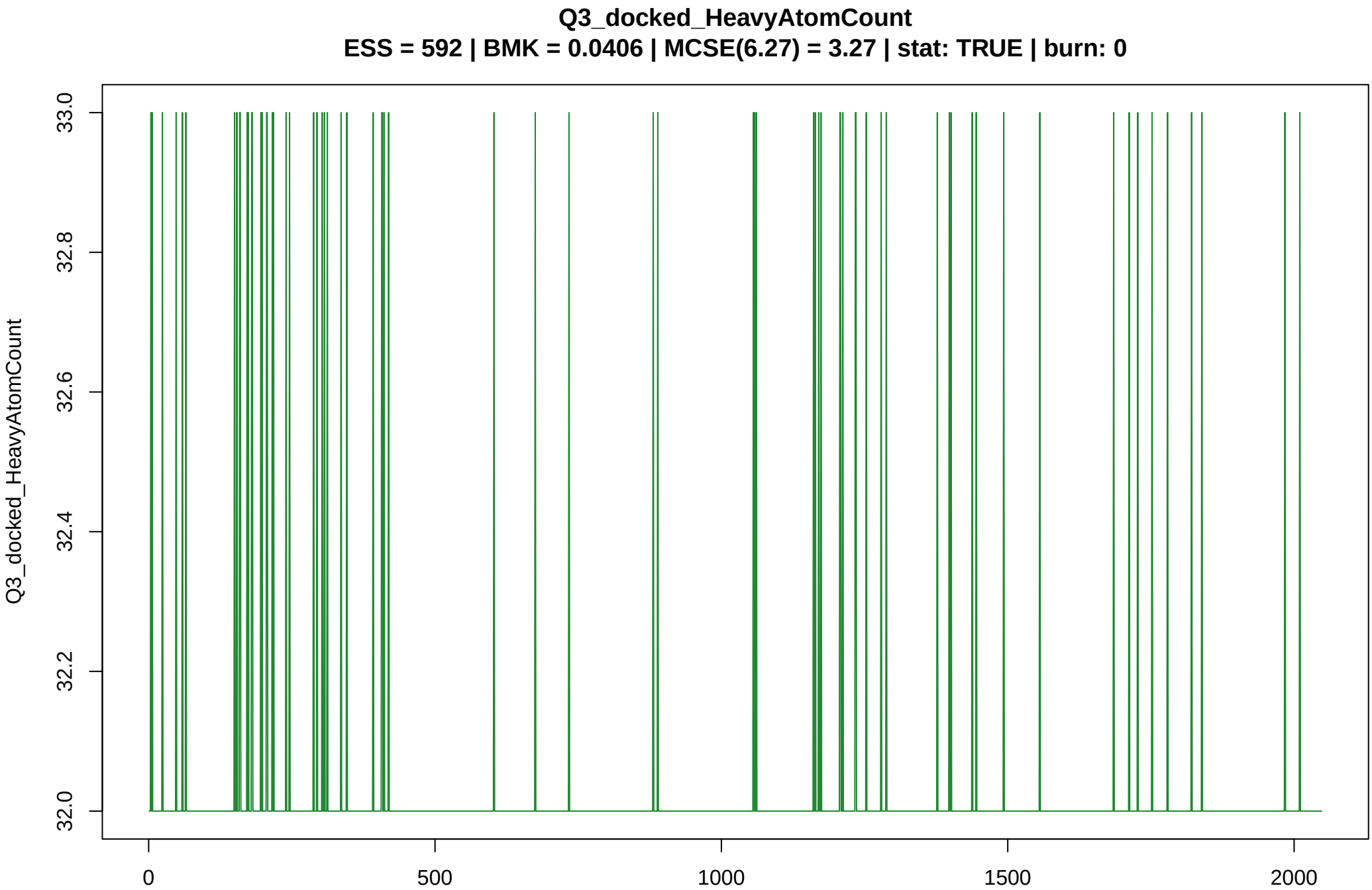

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

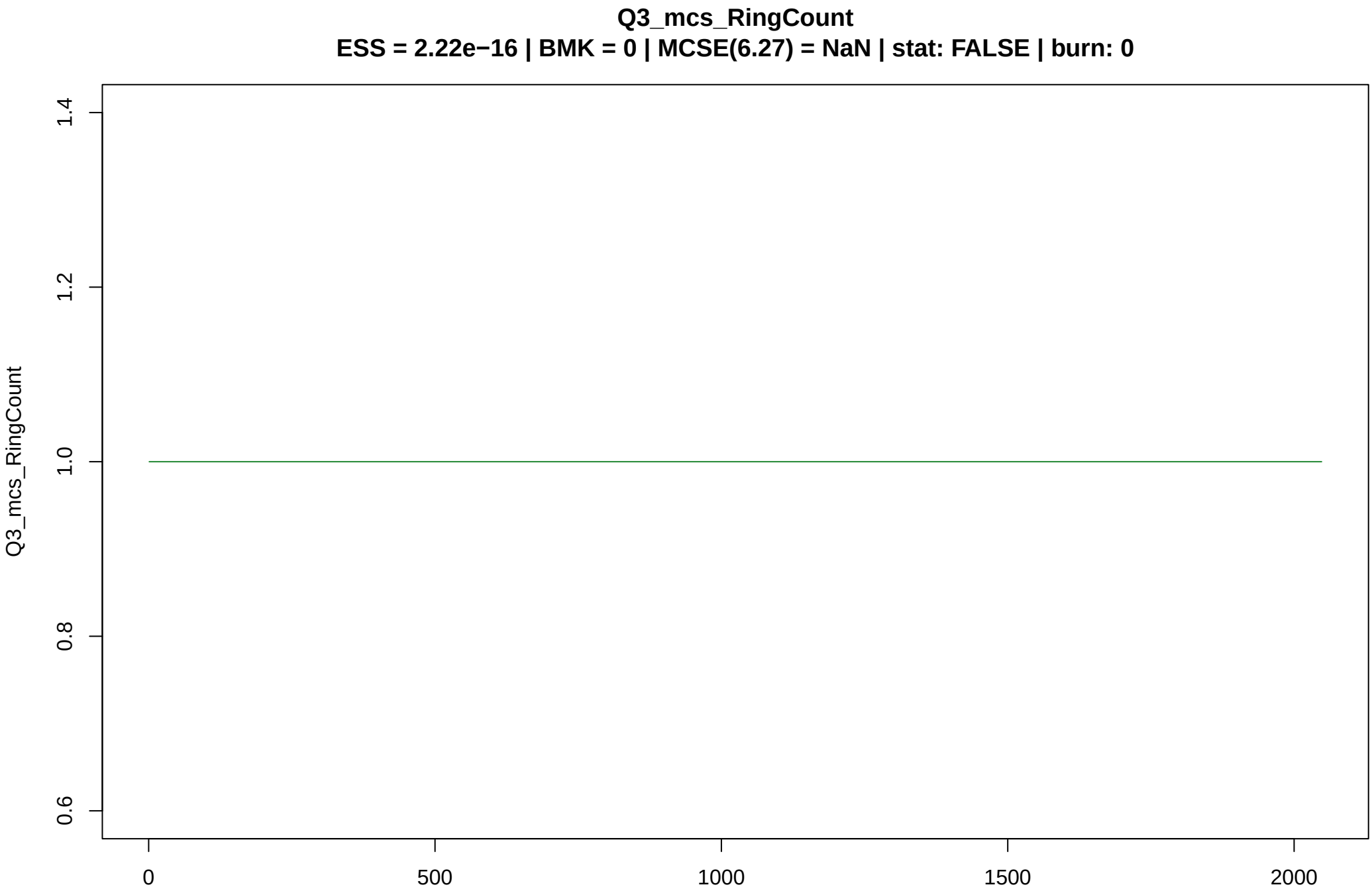

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

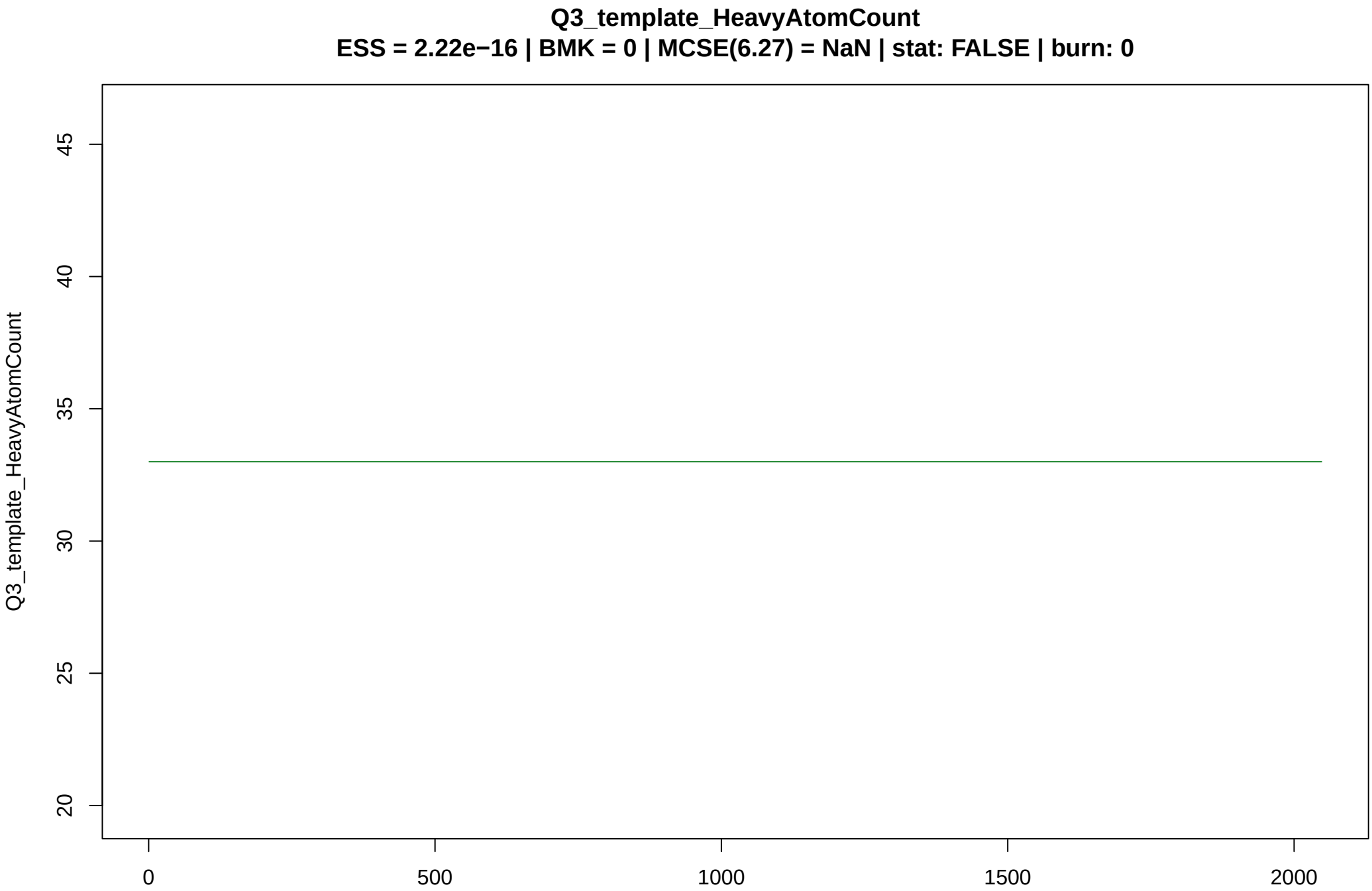

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

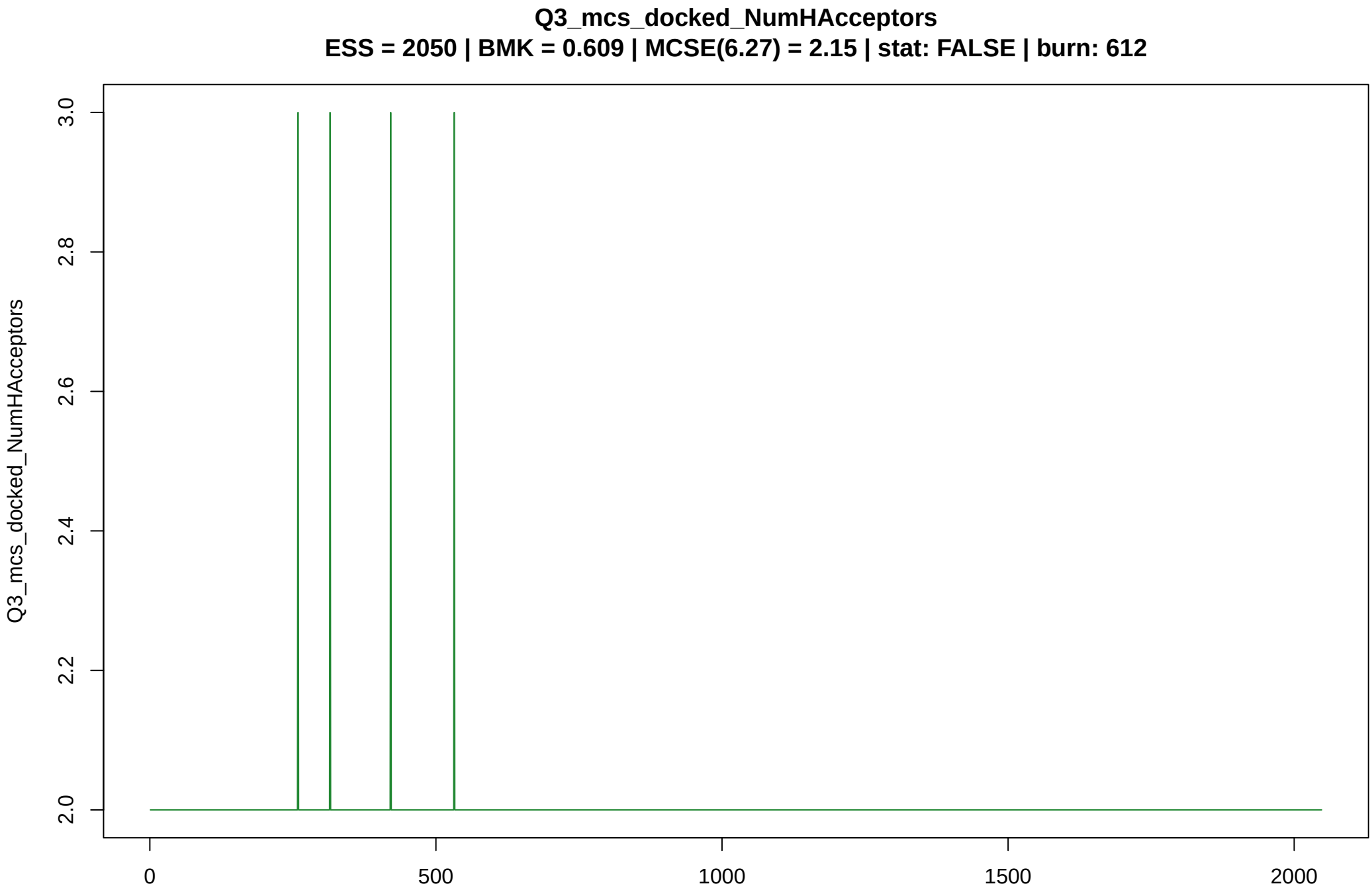

Q3_log_RMSD
ESS = 1740 | BMK = 0.0699 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0
Q3_log_RMSD
2.08
2.09
2.10
2.11
2.12
0
500
1000
1500
2000

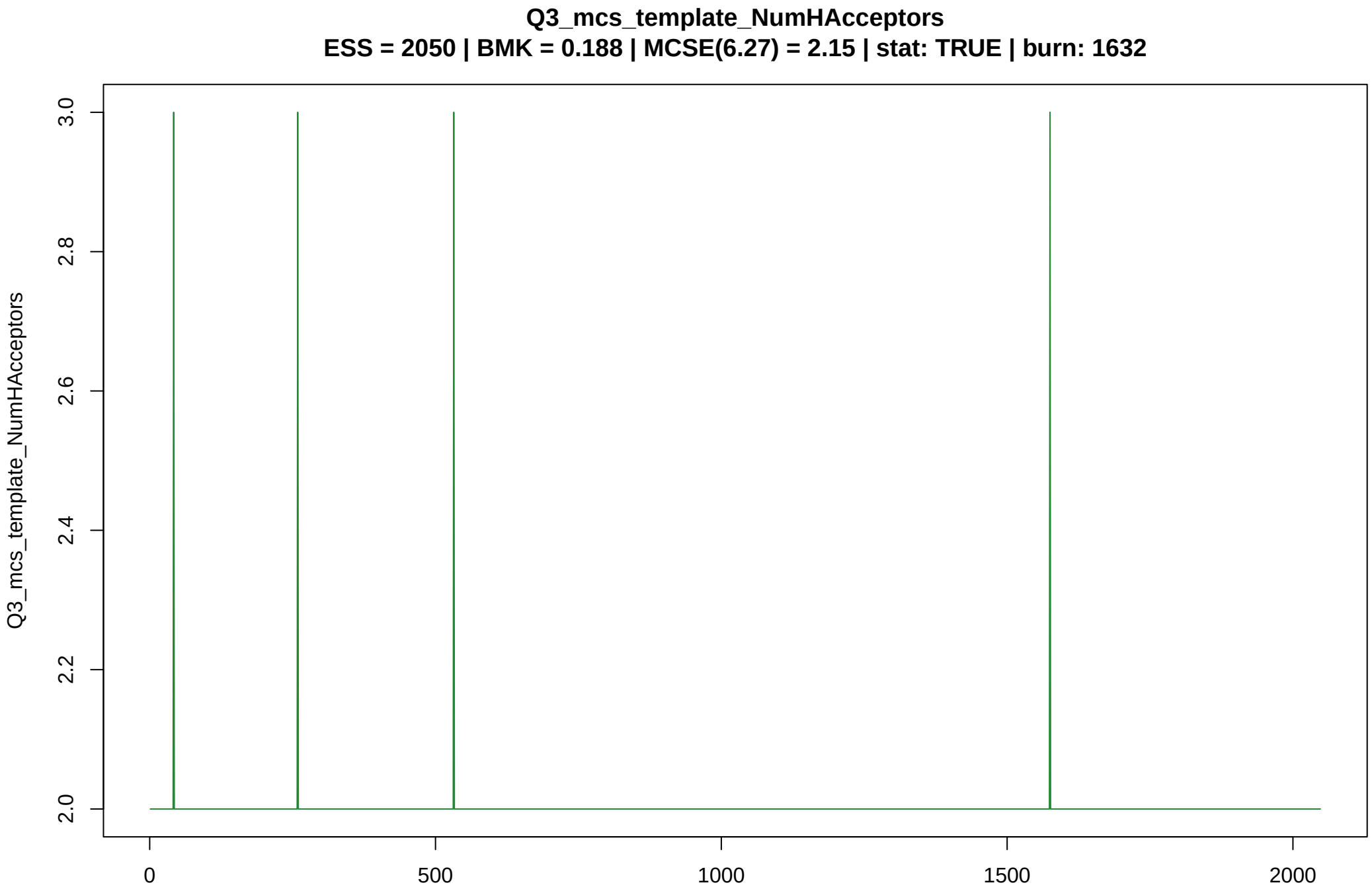

Q3_Xtransf_ec_tanimoto_similarity
ESS = 1100 | BMK = 0.0615 | MCSE(6.27) = 3.43 | stat: TRUE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
0.10
0.15
0.20
0.25
0
500
1000
1500
2000

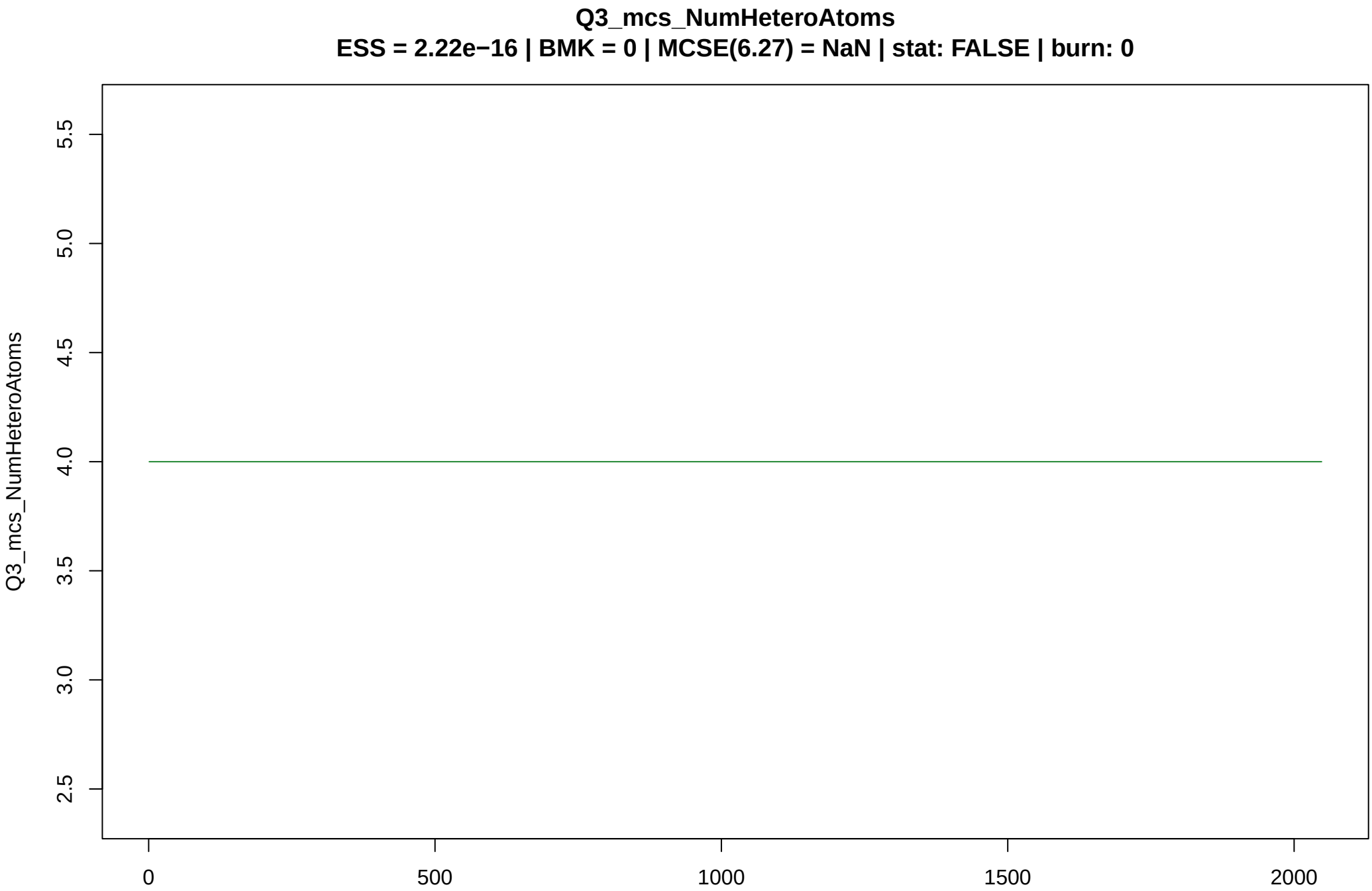

Q3_docked_HeavyAtomCount
ESS = 592 | BMK = 0.0406 | MCSE(6.27) = 3.27 | stat: TRUE | burn: 0
Q3_docked_HeavyAtomCount
33.0
32.8
32.6
32.4
32.2
32.0
0
500
1000
1500
2000

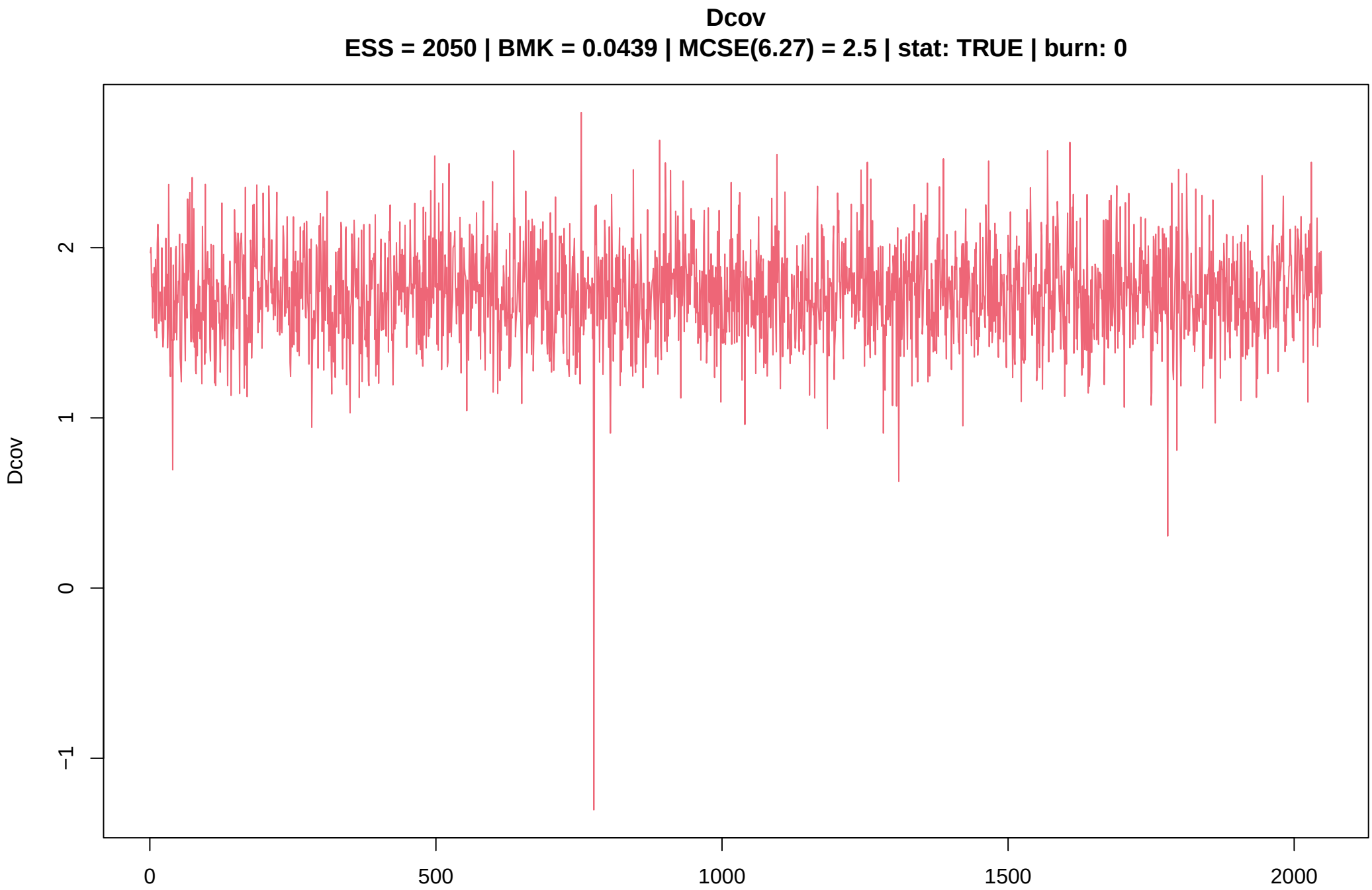

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

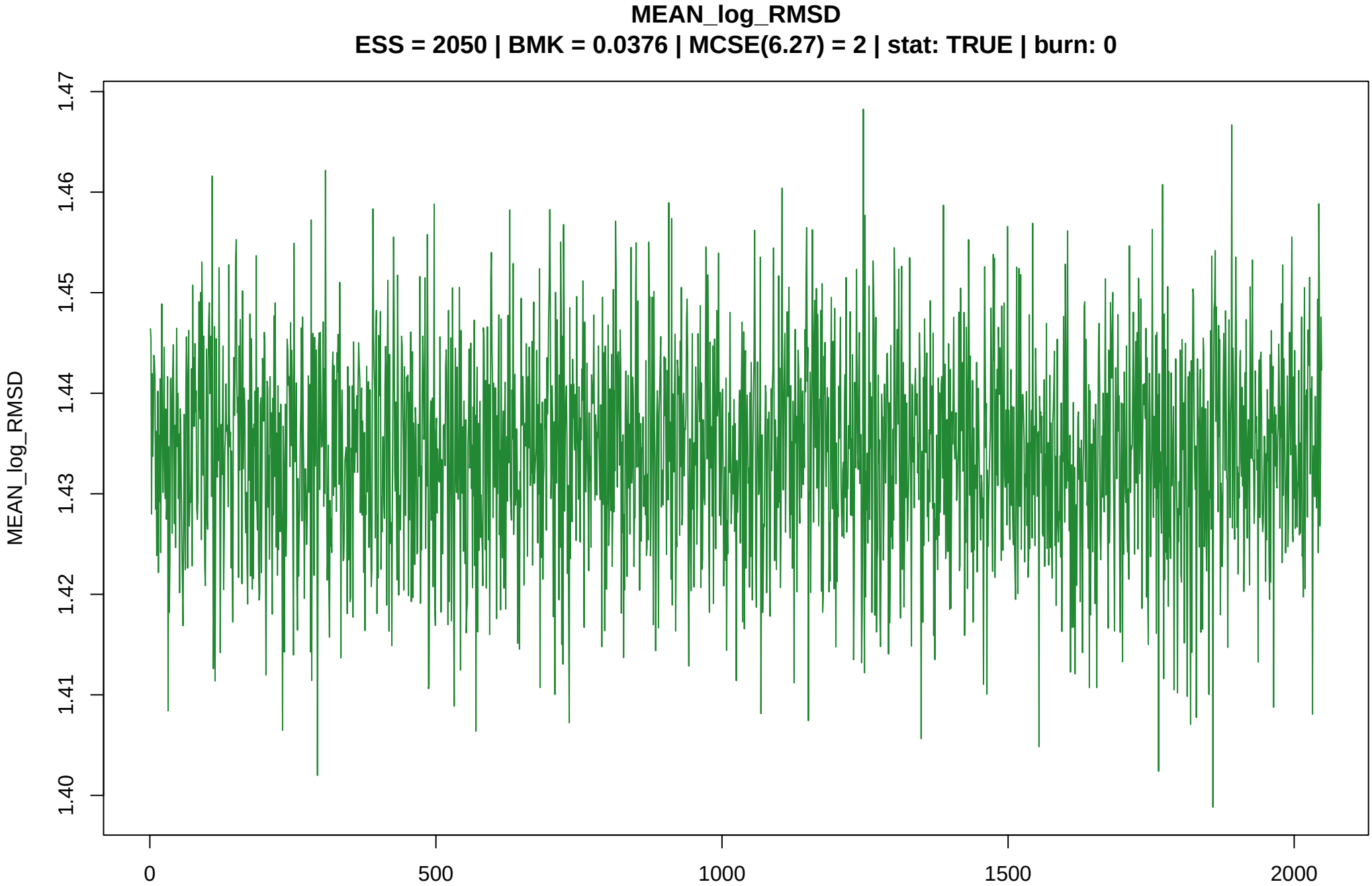

Q3_template_HeavyAtomCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_template_HeavyAtomCount
20
25
30
35
40
45
0
500
1000
1500
2000

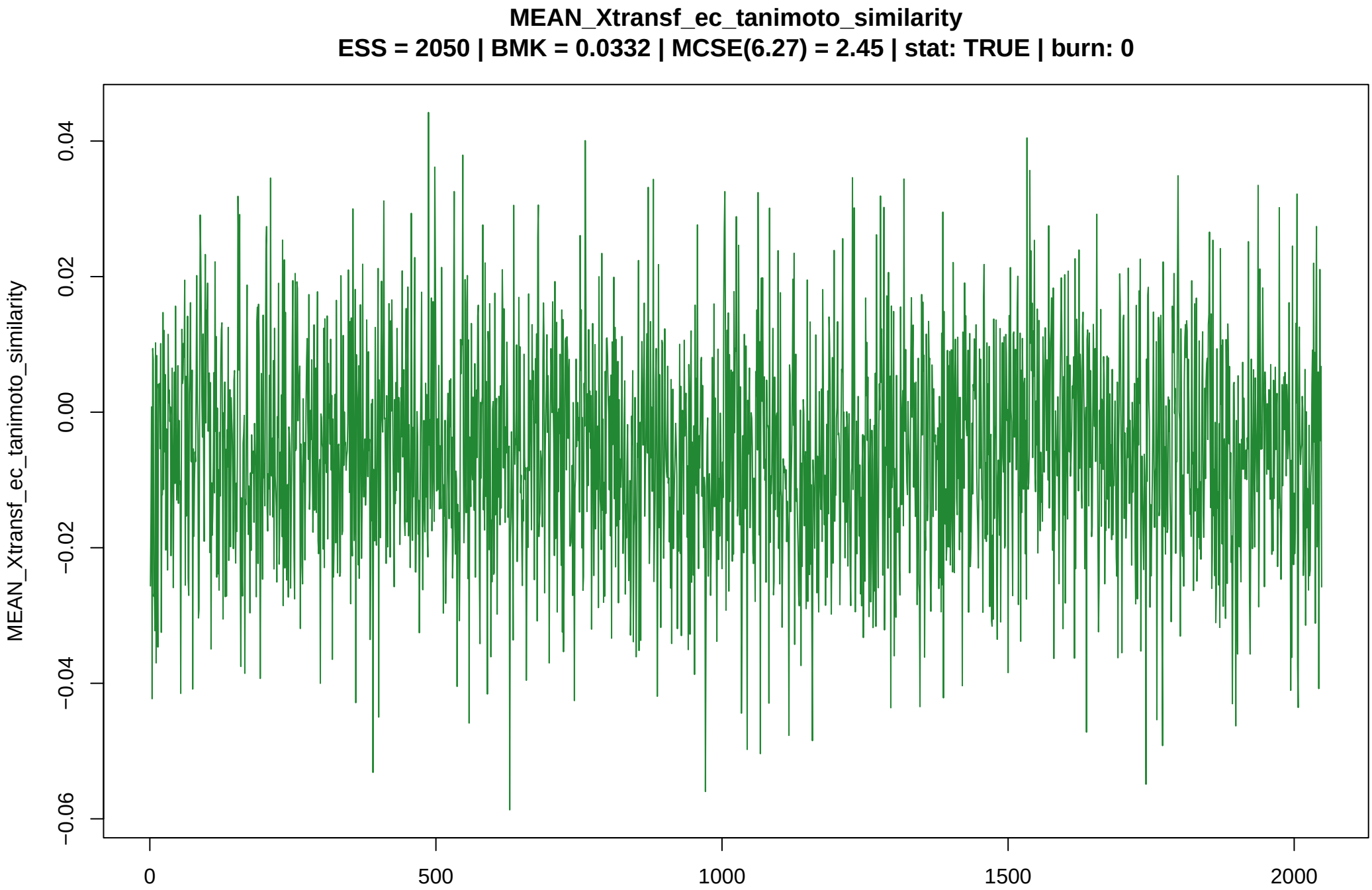

Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.609 | MCSE(6.27) = 2.15 | stat: FALSE | burn: 612
Q3_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

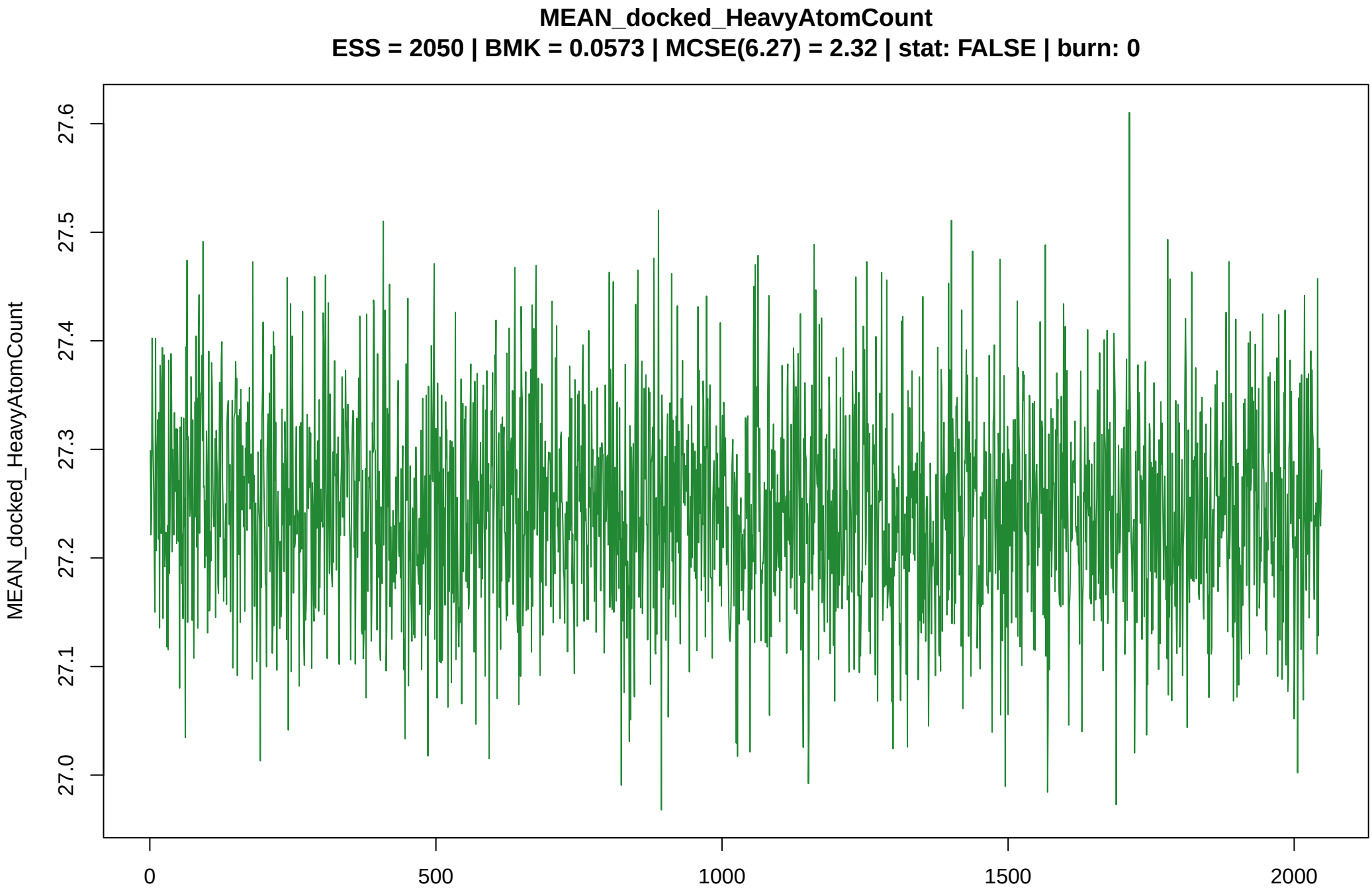

Q3_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1632
Q3_mcs_template_NumHAcceptors
2.0
2.2
2.4
2.6
2.8
3.0
0
500
1000
1500
2000

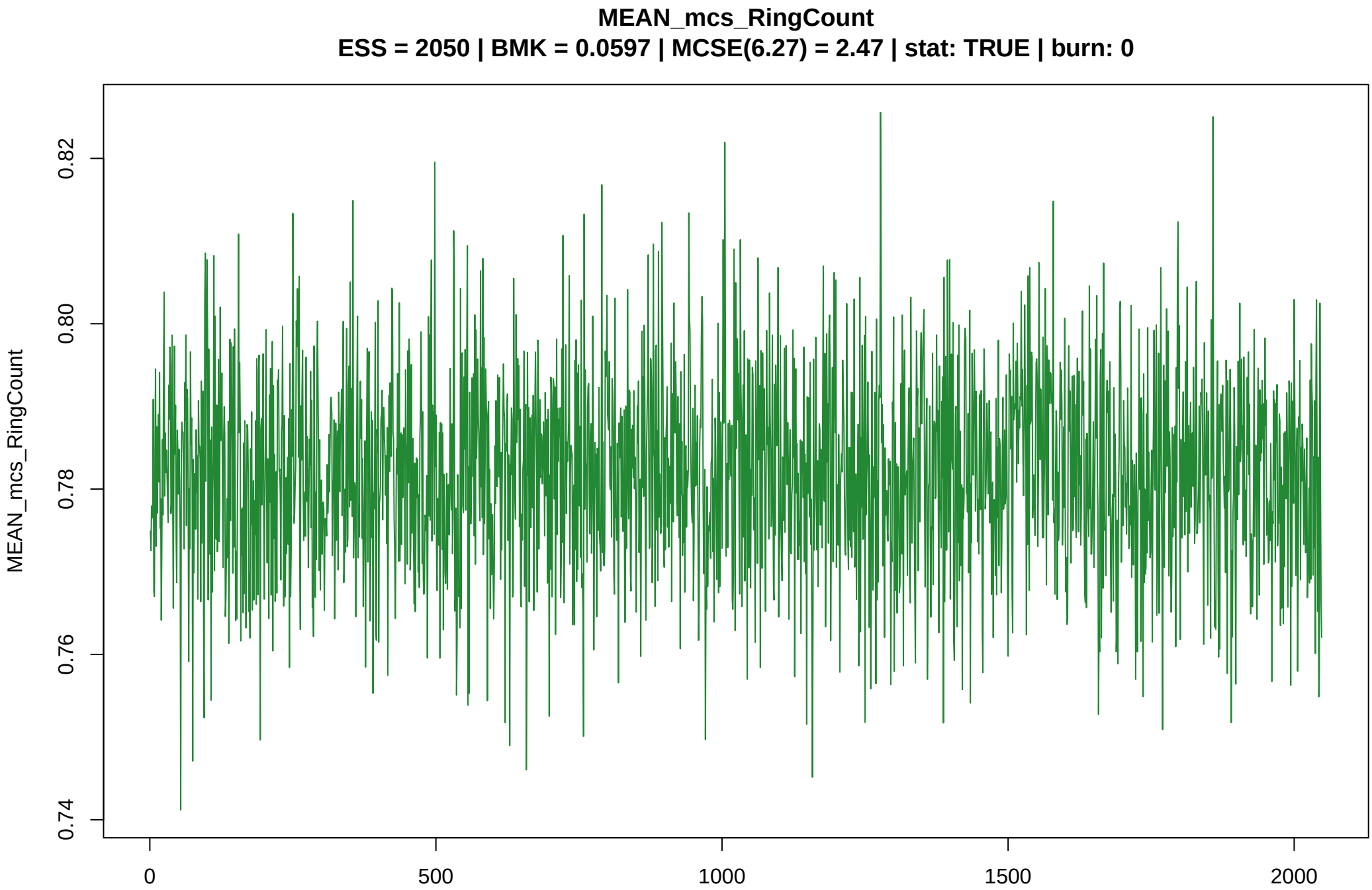

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

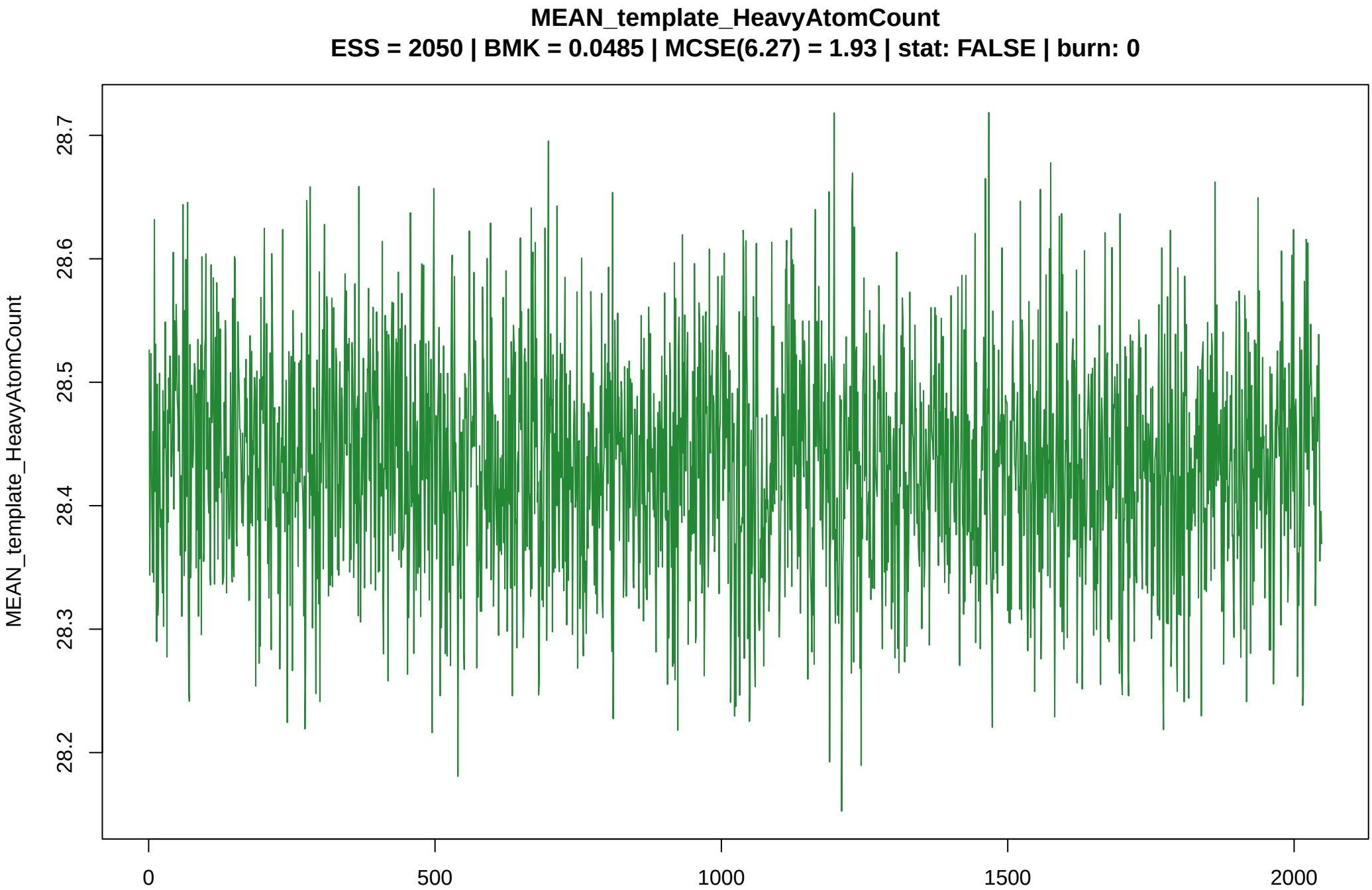

Dcov
ESS = 2050 | BMK = 0.0439 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0
Dcov
2
1
0
−1
0
500
1000
1500
2000

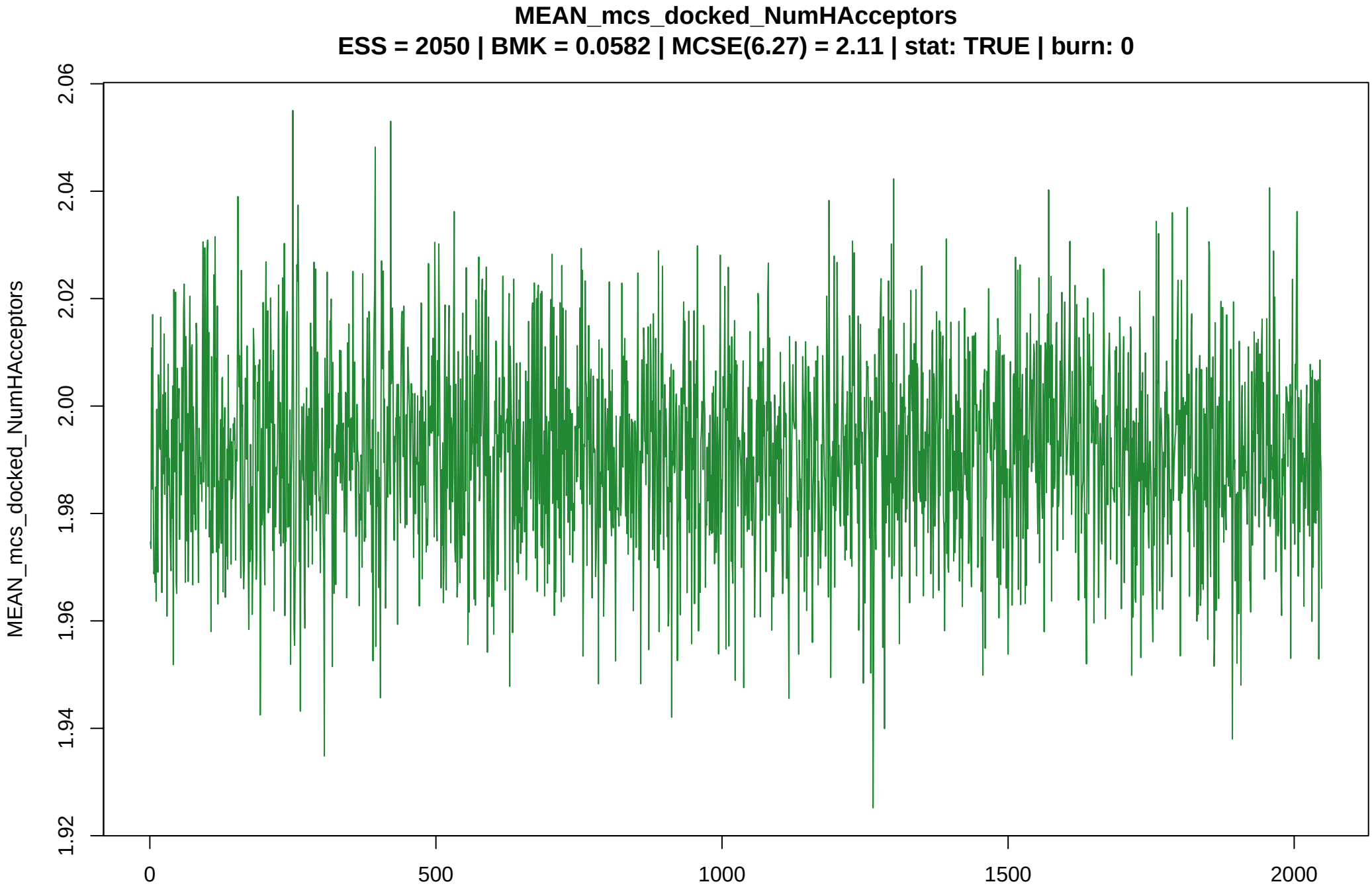

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0376 | MCSE(6.27) = 2 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.40
1.41
1.42
1.43
1.44
1.45
1.46
1.47
0
500
1000
1500
2000

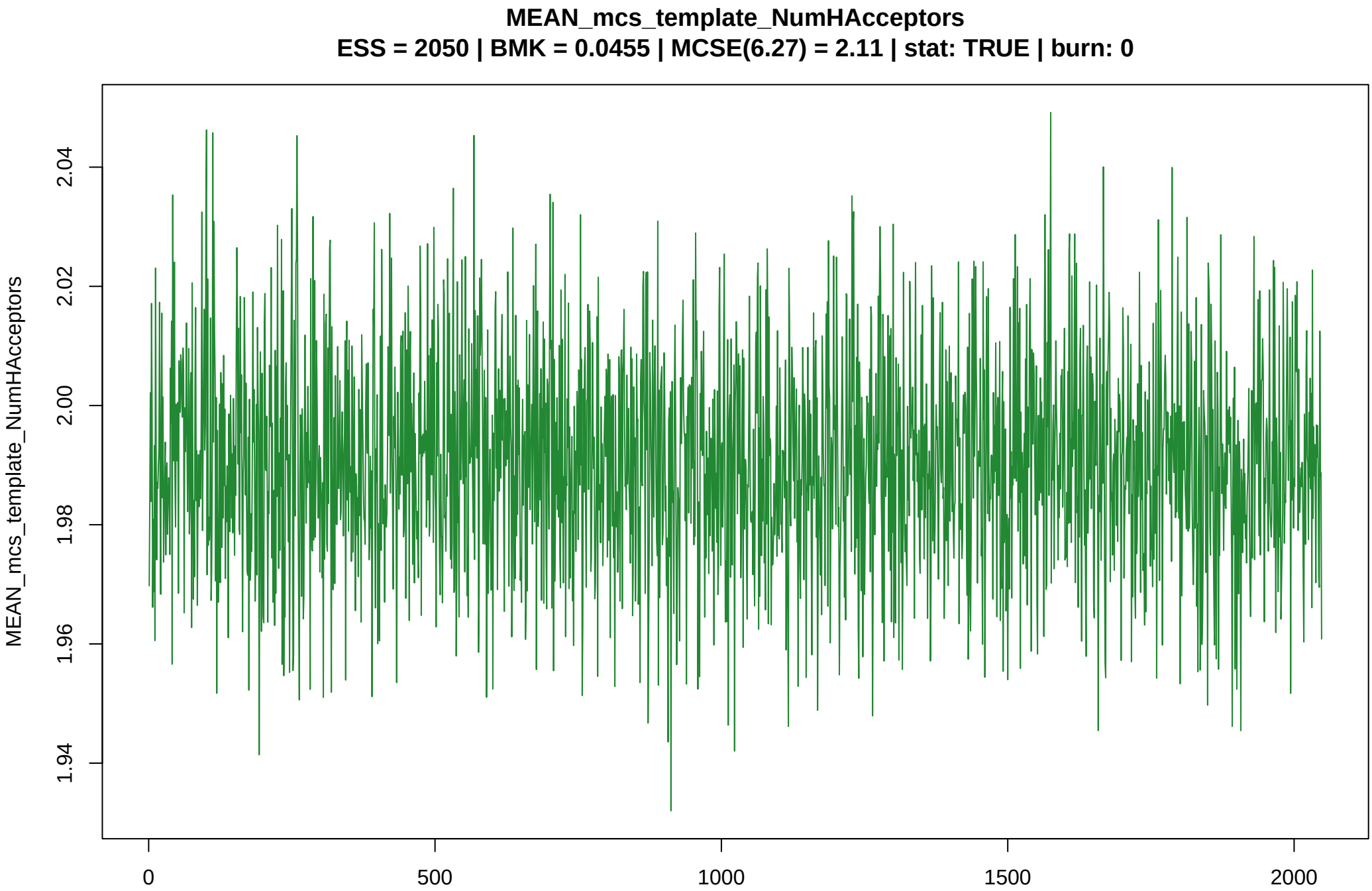

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0332 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0
MEAN_Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
−0.06
0
500
1000
1500
2000

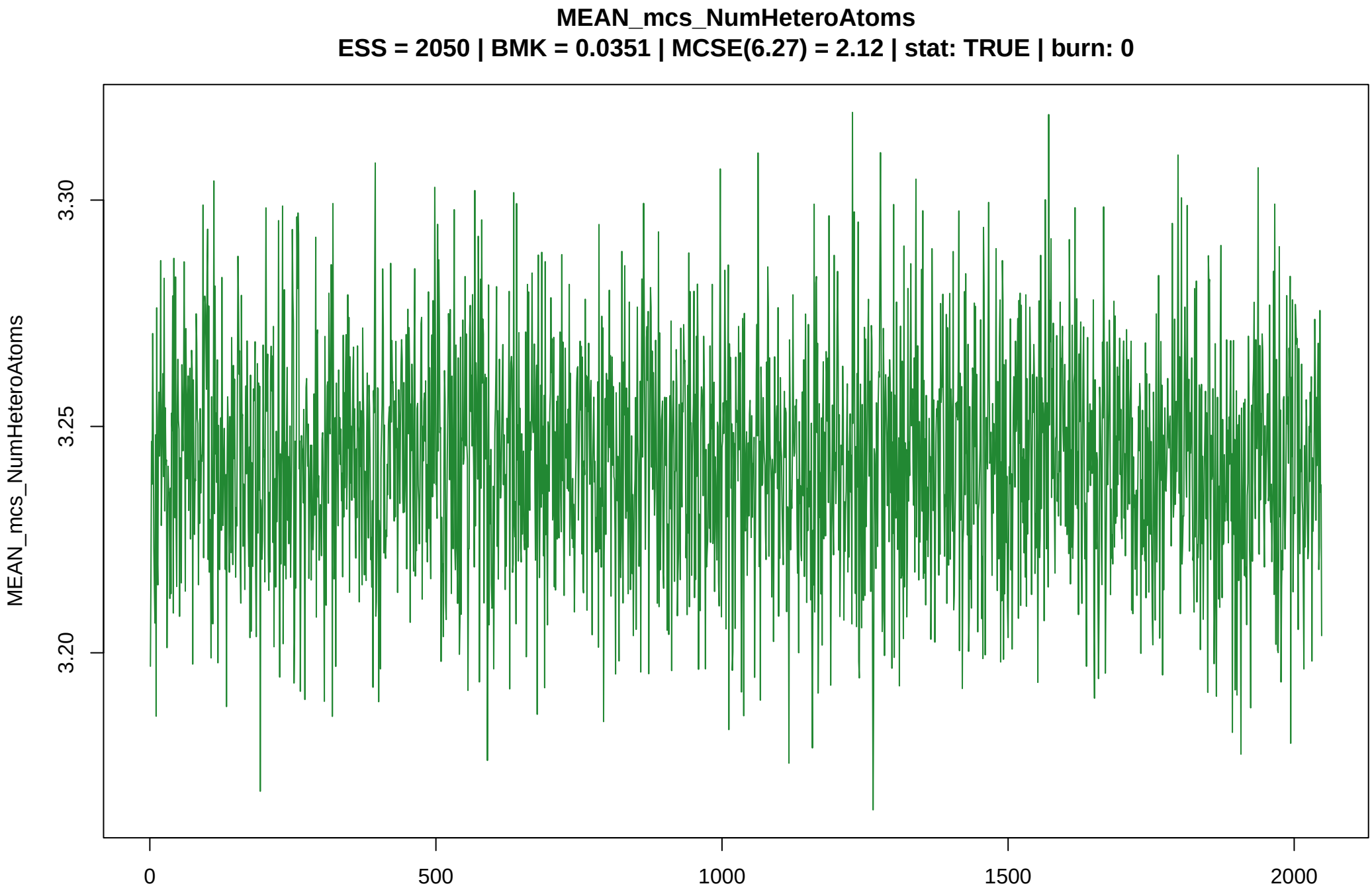

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0573 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0
MEAN_docked_HeavyAtomCount
27.0
27.1
27.2
27.3
27.4
27.5
27.6
0
500
1000
1500
2000

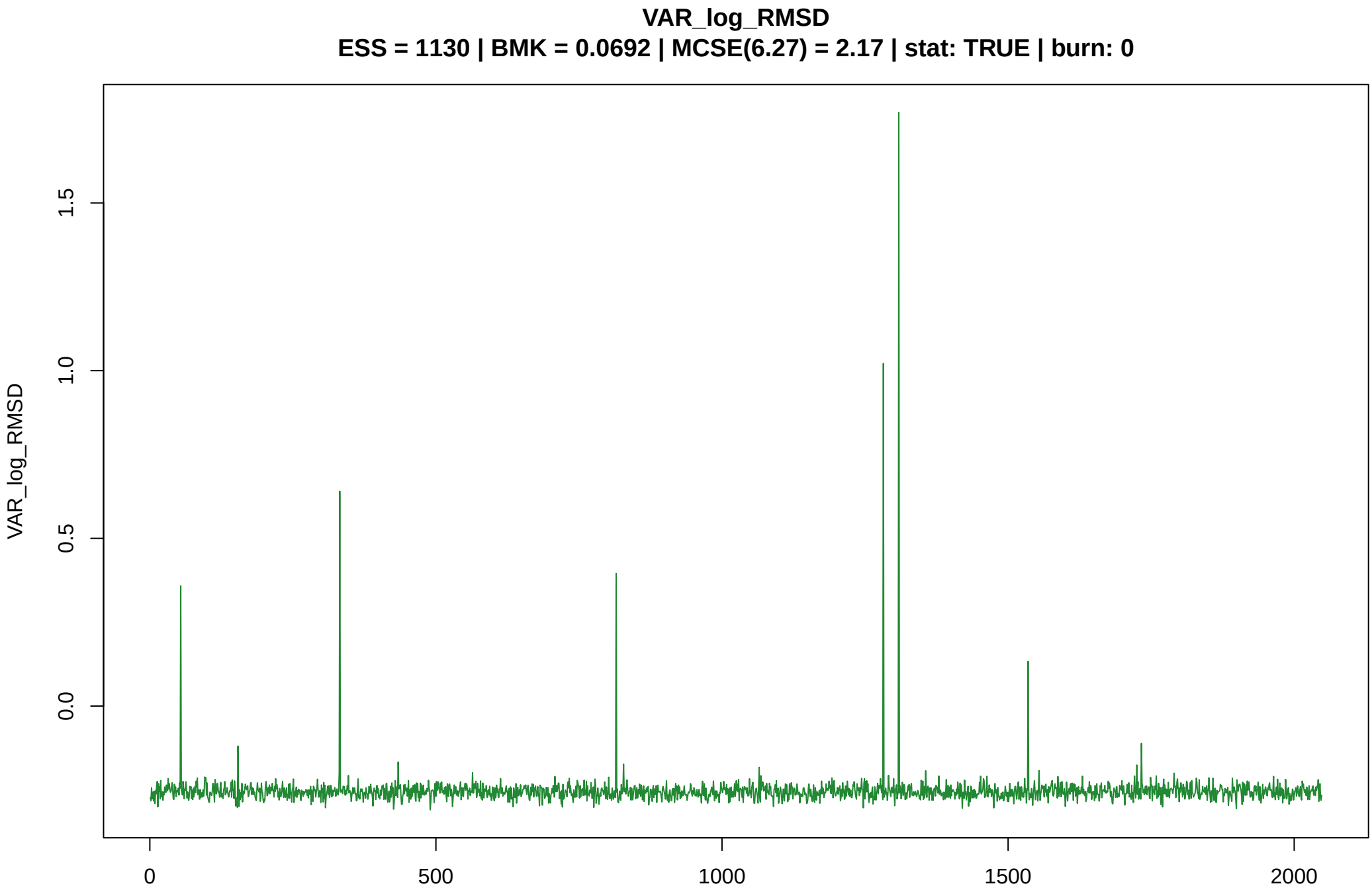

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0597 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.74
0.76
0.78
0.80
0.82
0
500
1000
1500
2000

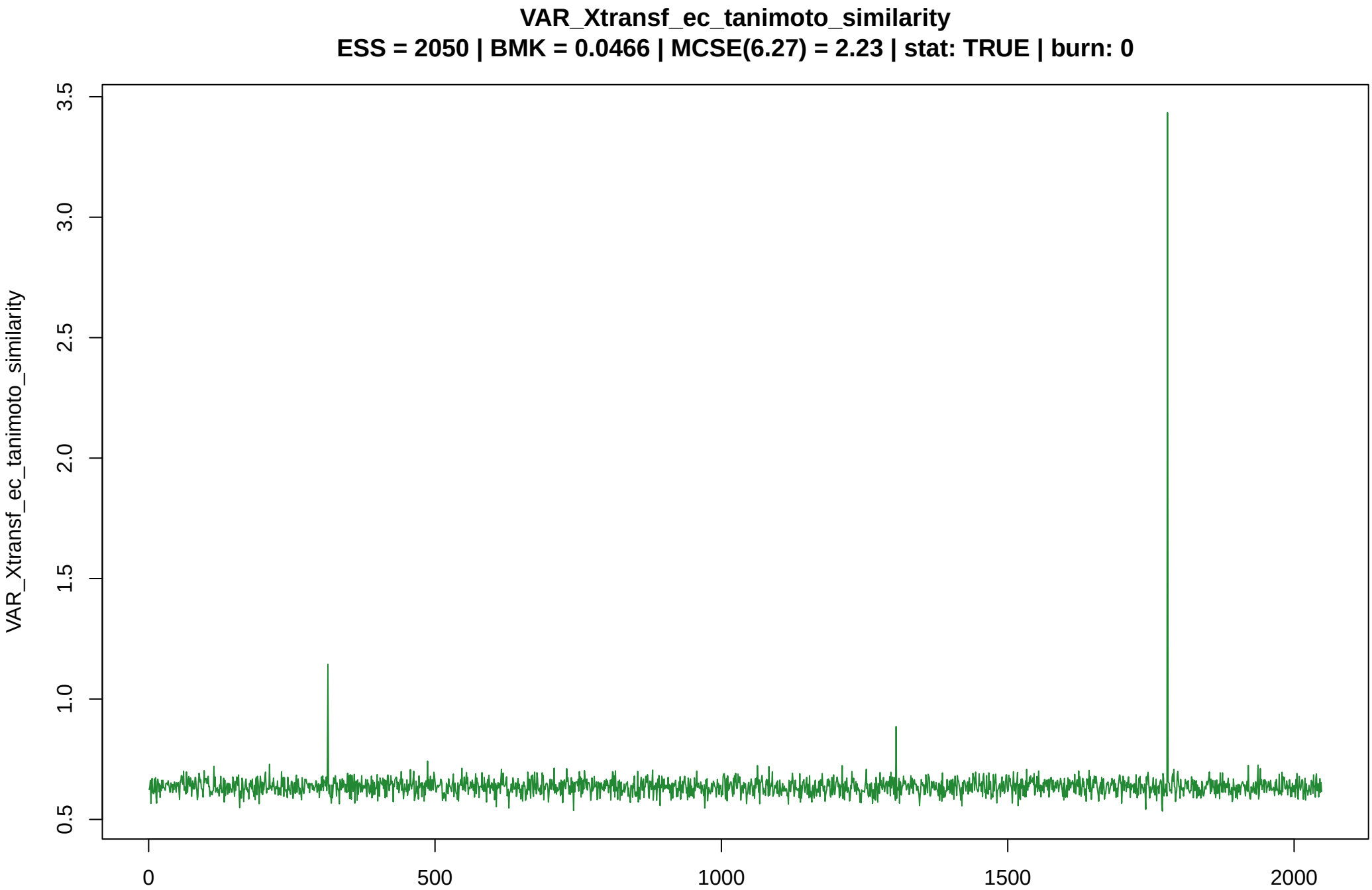

MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0485 | MCSE(6.27) = 1.93 | stat: FALSE | burn: 0
MEAN_template_HeavyAtomCount
28.2
28.3
28.4
28.5
28.6
28.7
0
500
1000
1500
2000

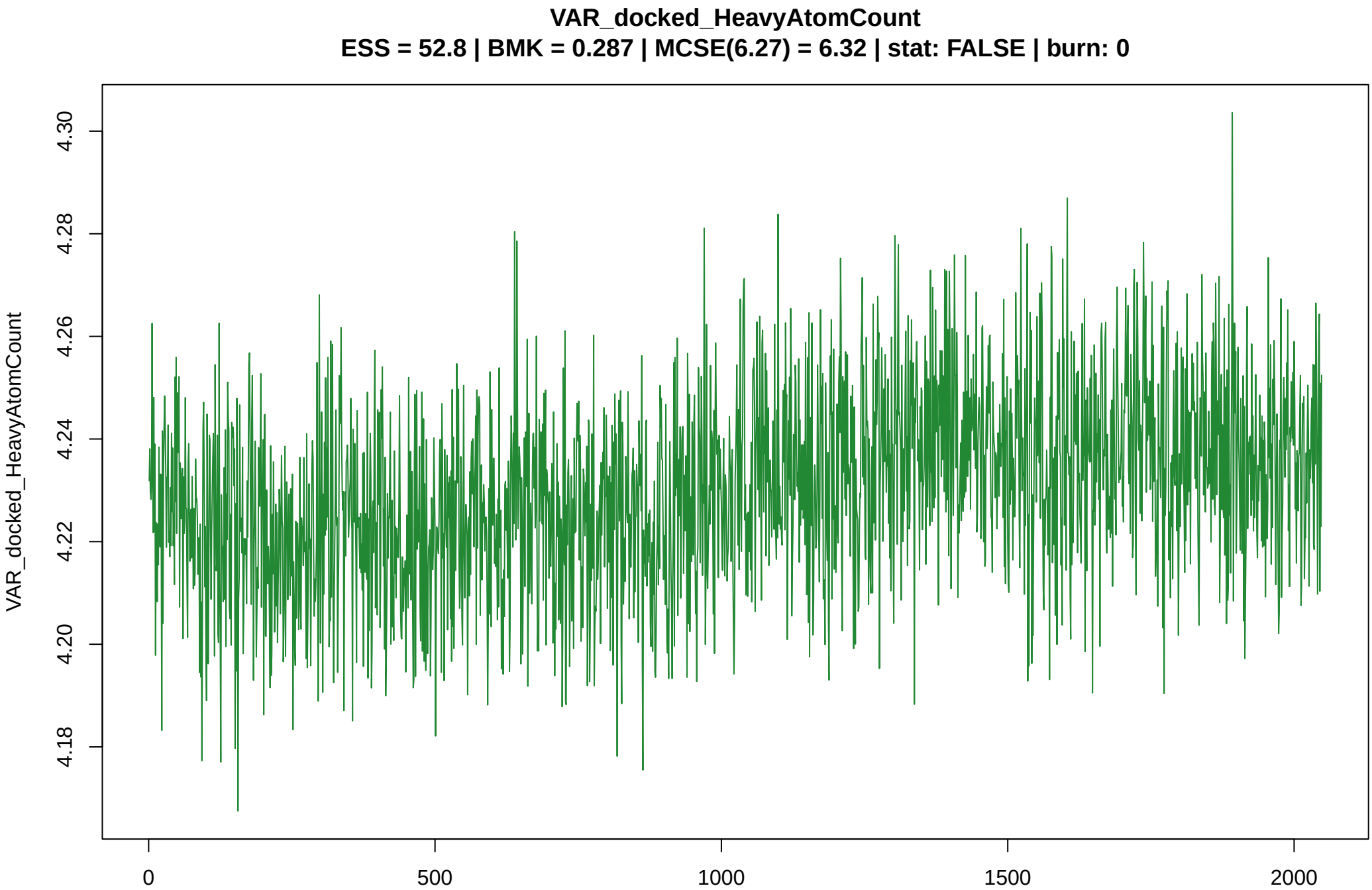

MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0582 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
1.92
1.94
1.96
1.98
2.00
2.02
2.04
2.06
0
500
1000
1500
2000

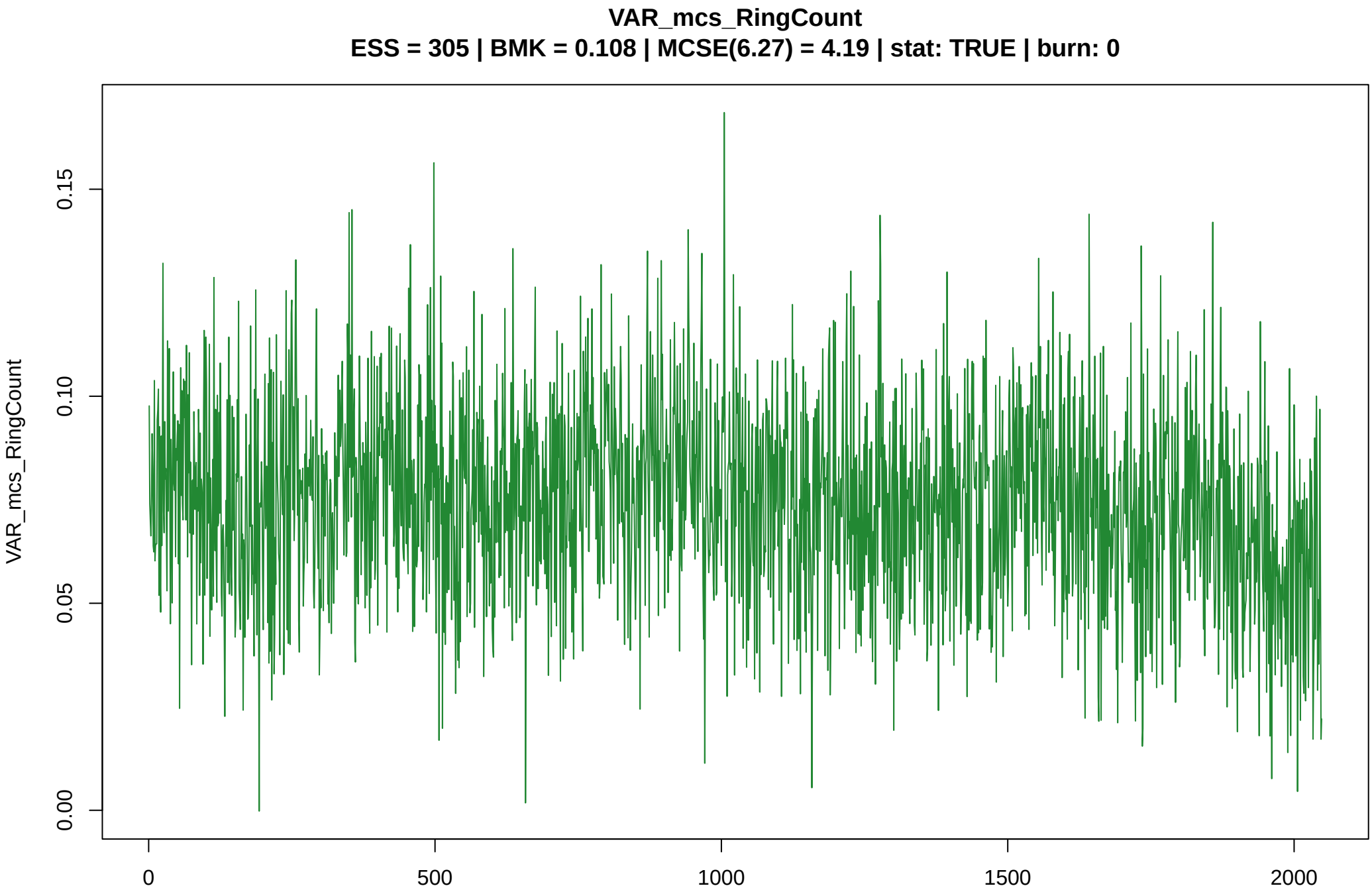

MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0455 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0
MEAN_mcs_template_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
0
500
1000
1500
2000

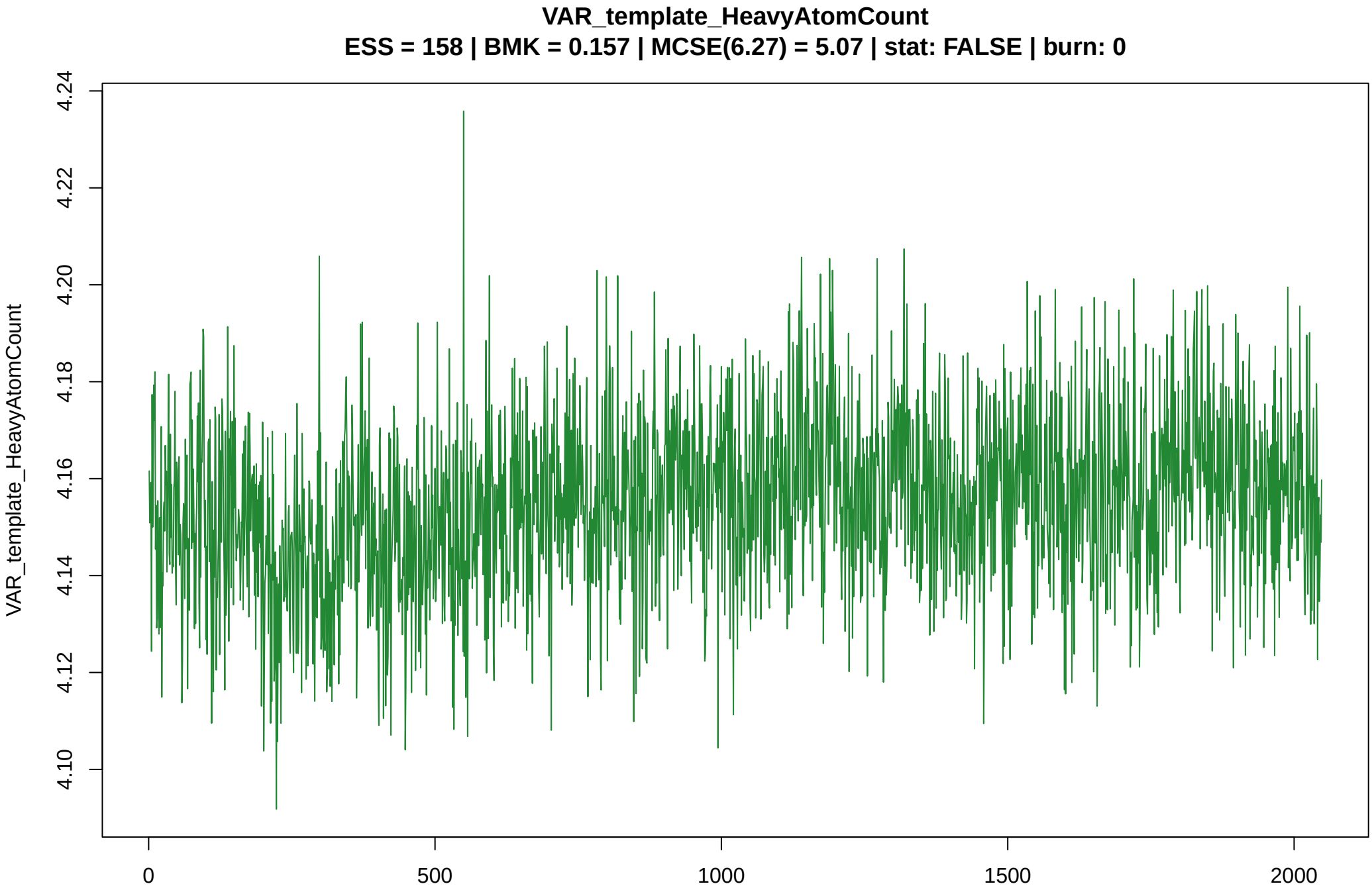

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0351 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.20
3.25
3.30
0
500
1000
1500
2000

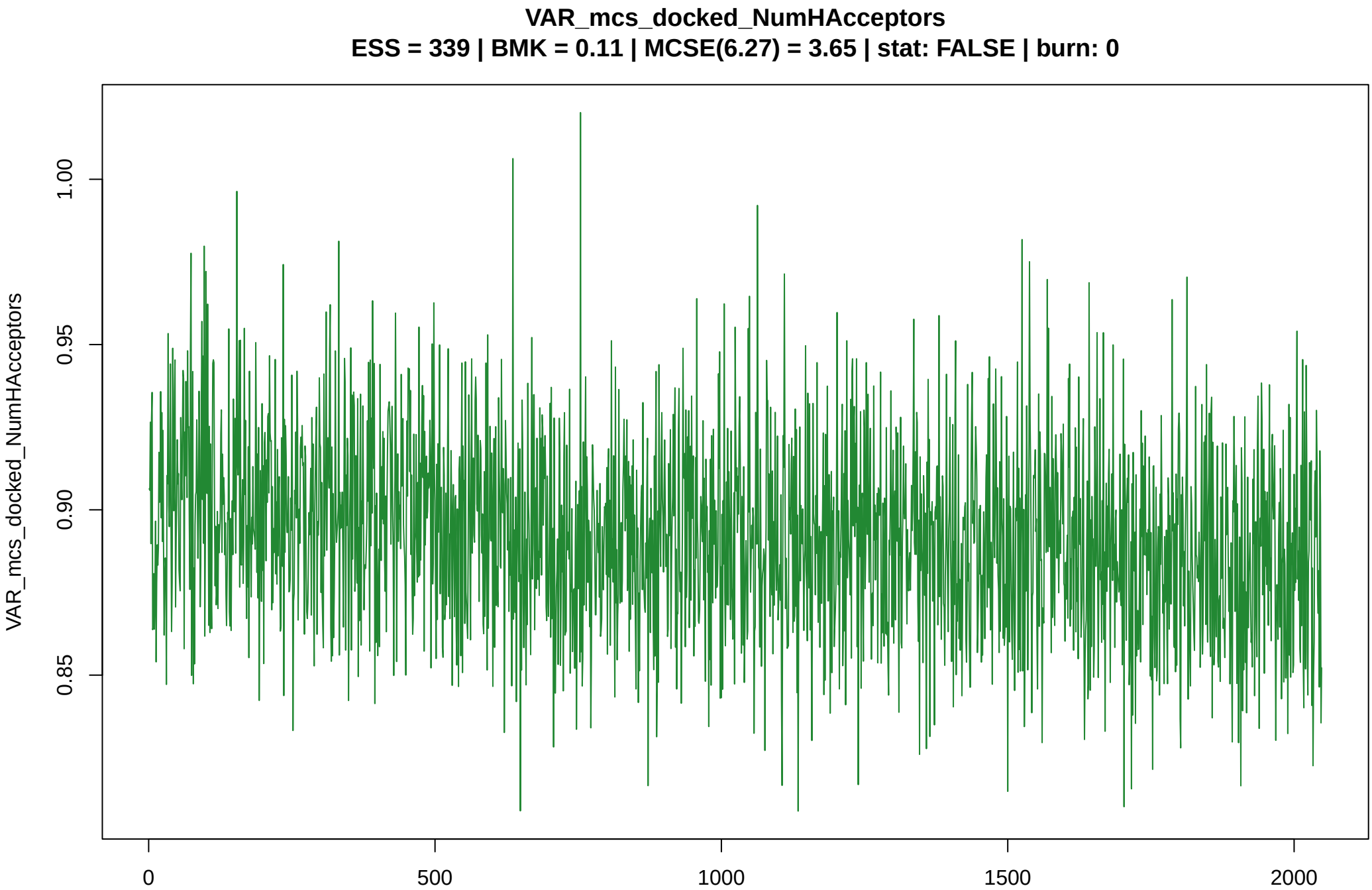

VAR_log_RMSD
ESS = 1130 | BMK = 0.0692 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0
VAR_log_RMSD
0.0
0.5
1.0
1.5
0
500
1000
1500
2000

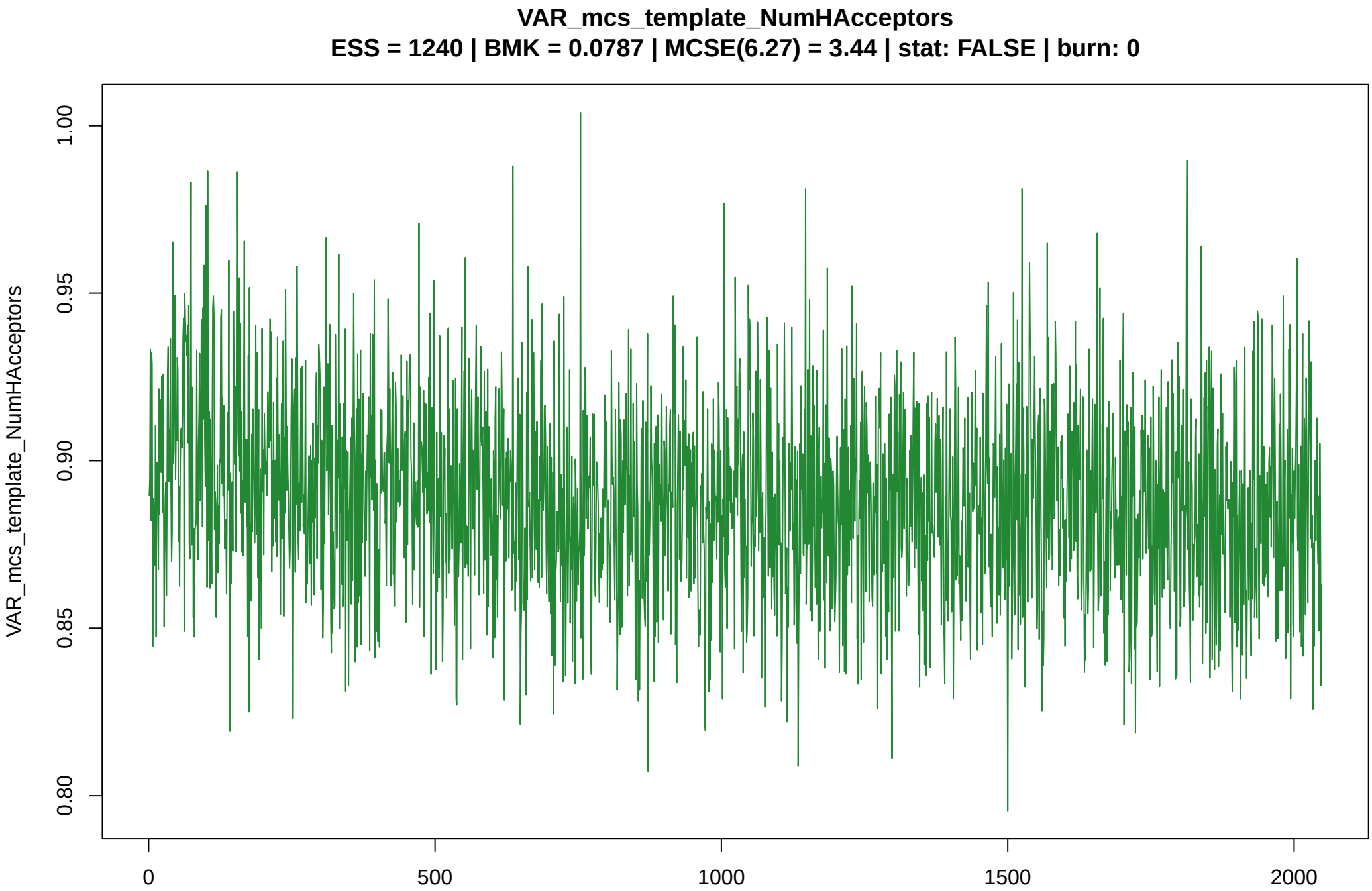

VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0466 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0
VAR_Xtransf_ec_tanimoto_similarity
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
500
1000
1500
2000

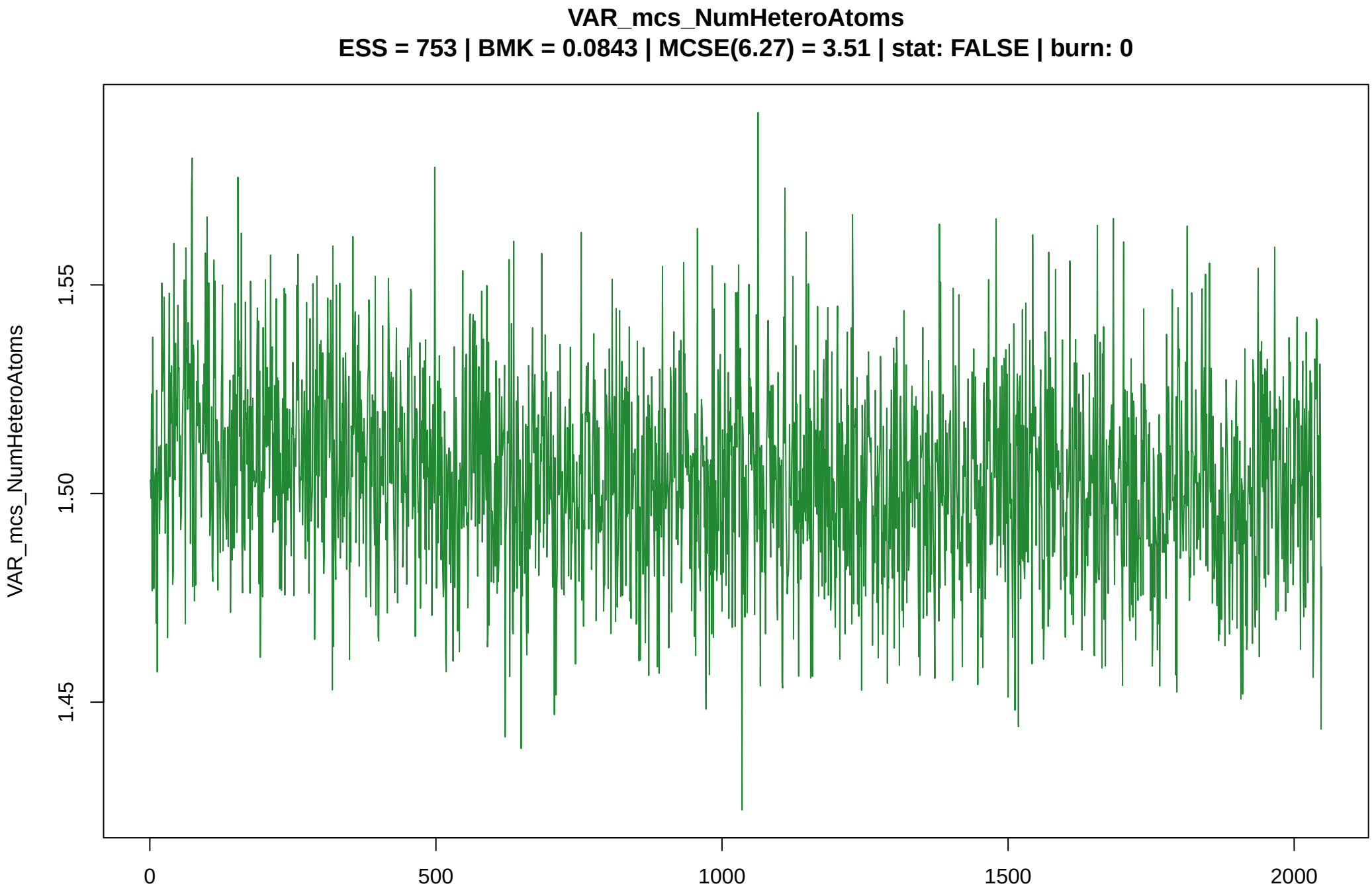

VAR_docked_HeavyAtomCount
ESS = 52.8 | BMK = 0.287 | MCSE(6.27) = 6.32 | stat: FALSE | burn: 0
VAR_docked_HeavyAtomCount
4.18
4.20
4.22
4.24
4.26
4.28
4.30
0
500
1000
1500
2000

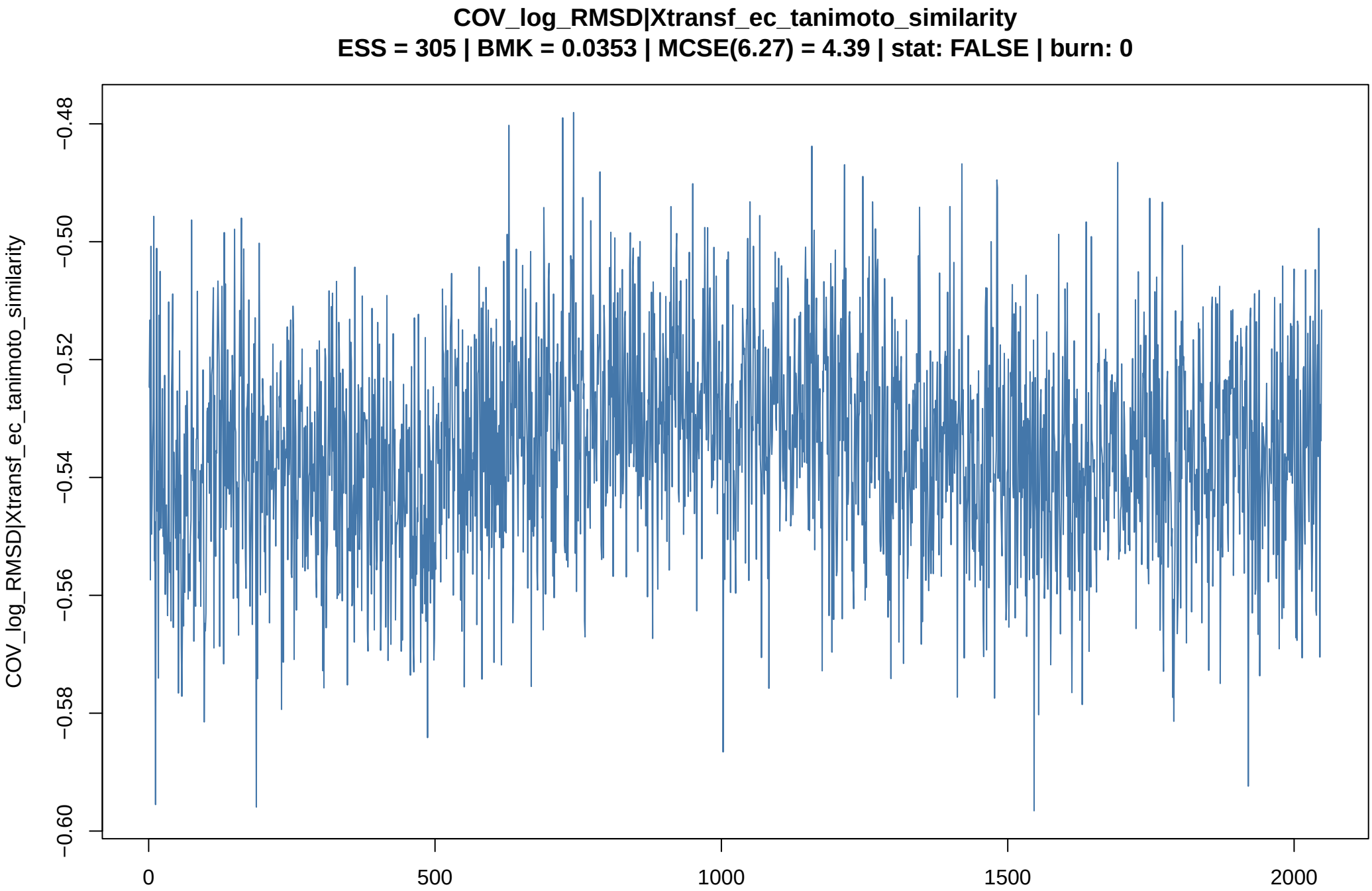

VAR_mcs_RingCount
ESS = 305 | BMK = 0.108 | MCSE(6.27) = 4.19 | stat: TRUE | burn: 0
VAR_mcs_RingCount
0.00
0.05
0.10
0.15
0
500
1000
1500
2000

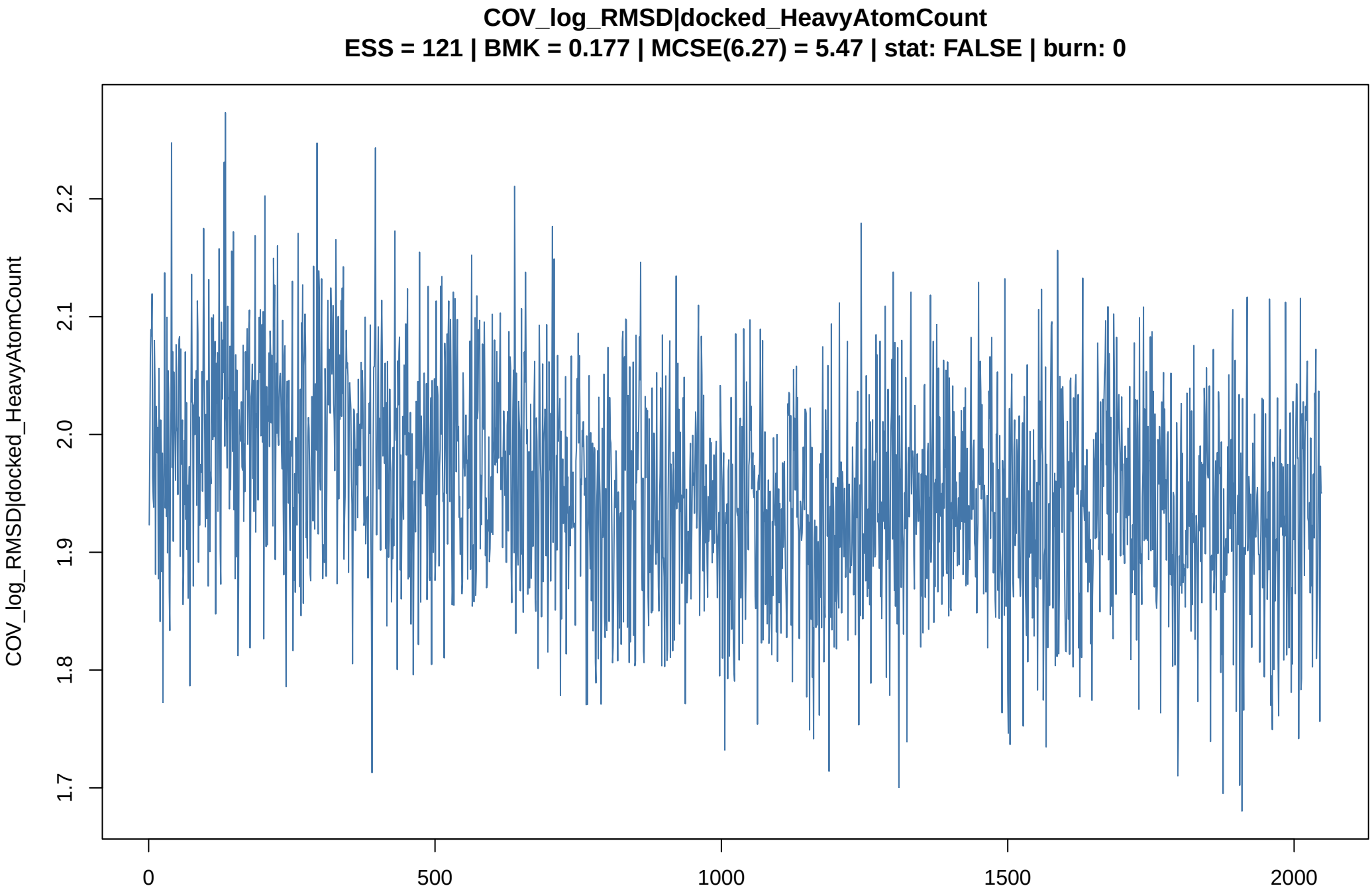

VAR_template_HeavyAtomCount
ESS = 158 | BMK = 0.157 | MCSE(6.27) = 5.07 | stat: FALSE | burn: 0
VAR_template_HeavyAtomCount
4.10
4.12
4.14
4.16
4.18
4.20
4.22
4.24
0
500
1000
1500
2000

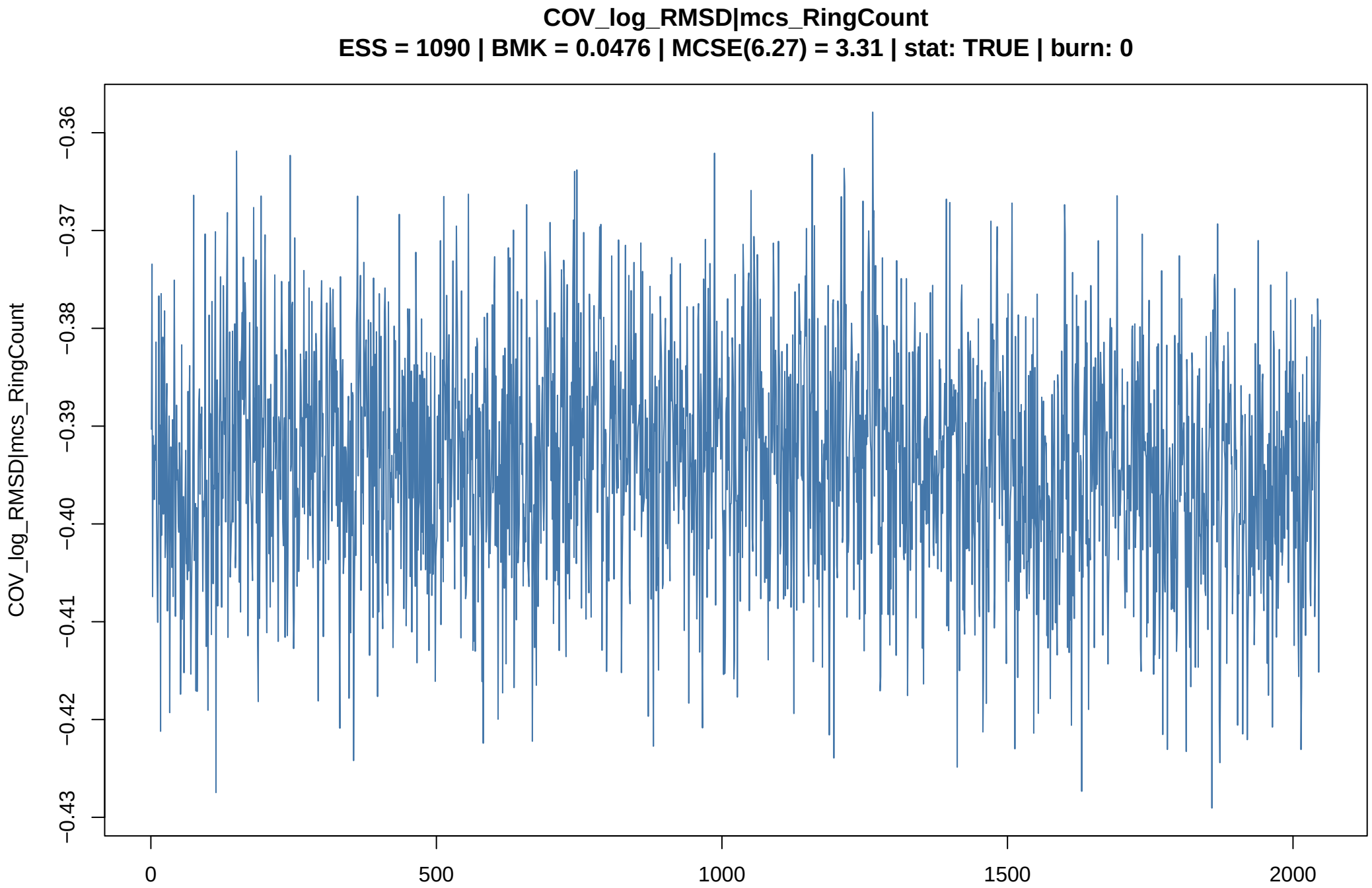

VAR_mcs_docked_NumHAcceptors
ESS = 339 | BMK = 0.11 | MCSE(6.27) = 3.65 | stat: FALSE | burn: 0
VAR_mcs_docked_NumHAcceptors
1.00
0.95
0.90
0.85
0
500
1000
1500
2000

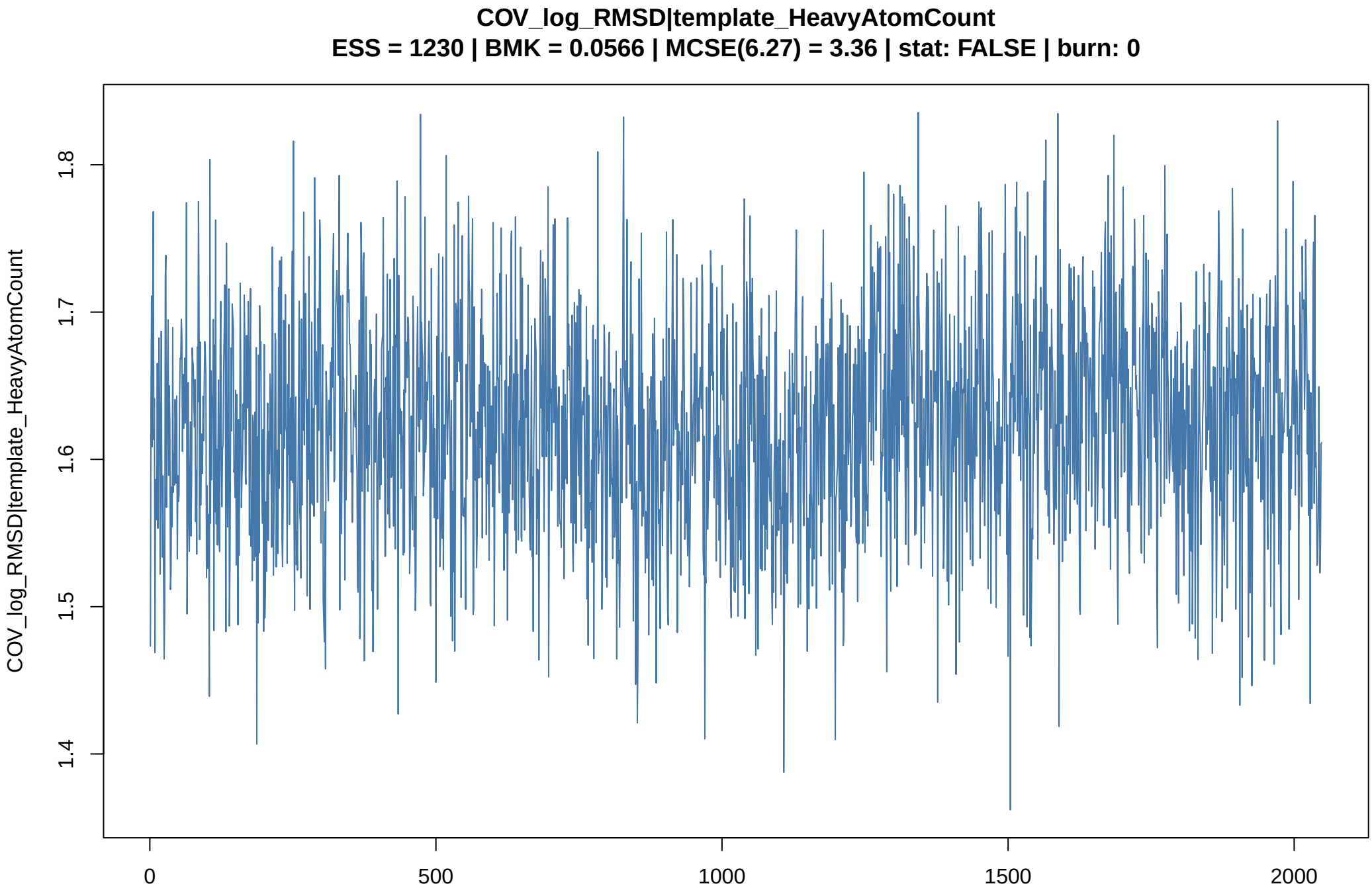

VAR_mcs_template_NumHAcceptors
ESS = 1240 | BMK = 0.0787 | MCSE(6.27) = 3.44 | stat: FALSE | burn: 0
VAR_mcs_template_NumHAcceptors
1.00
0.95
0.90
0.85
0.80
0
500
1000
1500
2000

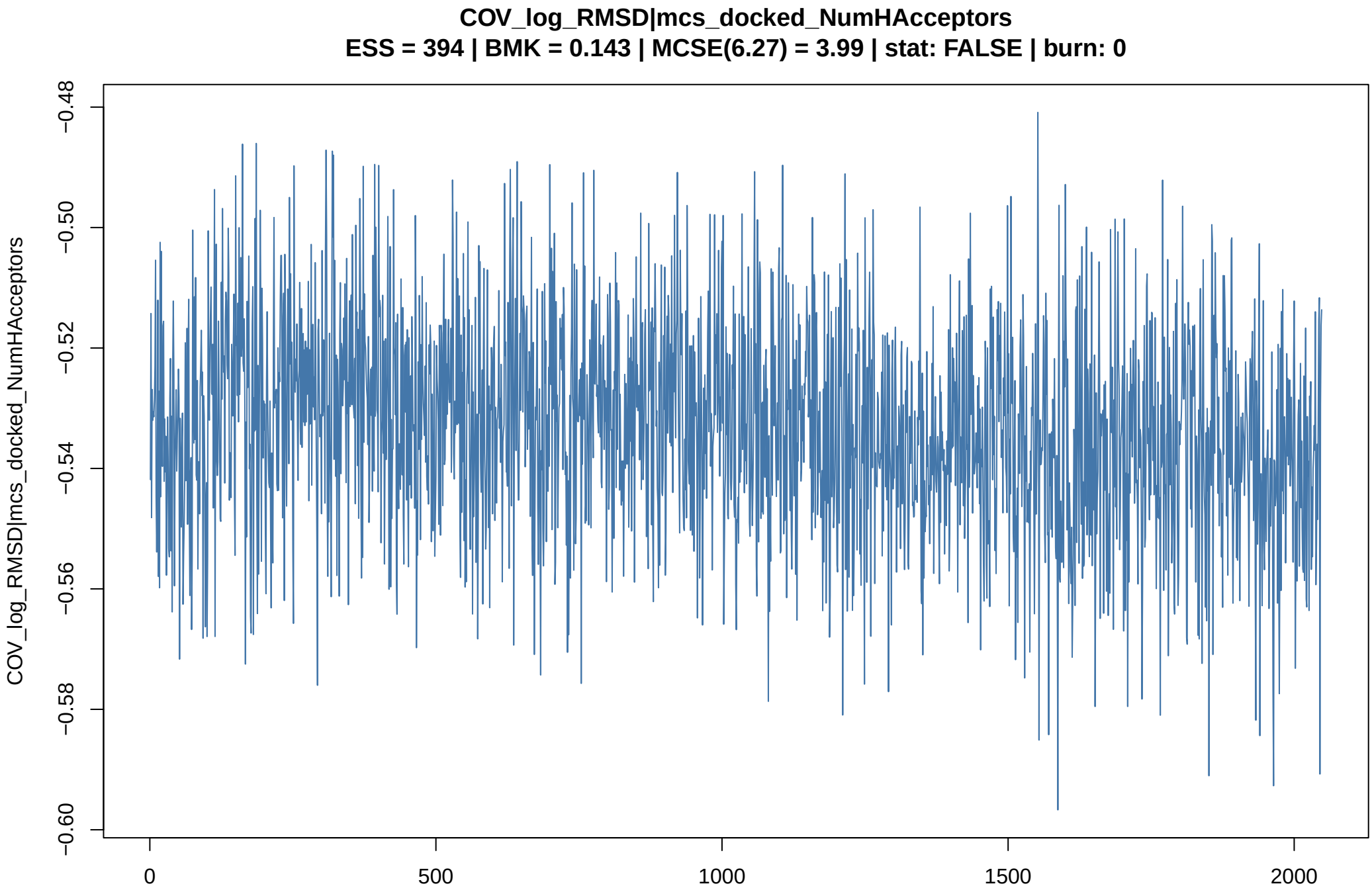

VAR_mcs_NumHeteroAtoms
ESS = 753 | BMK = 0.0843 | MCSE(6.27) = 3.51 | stat: FALSE | burn: 0
VAR_mcs_NumHeteroAtoms
1.45
1.50
1.55
0
500
1000
1500
2000

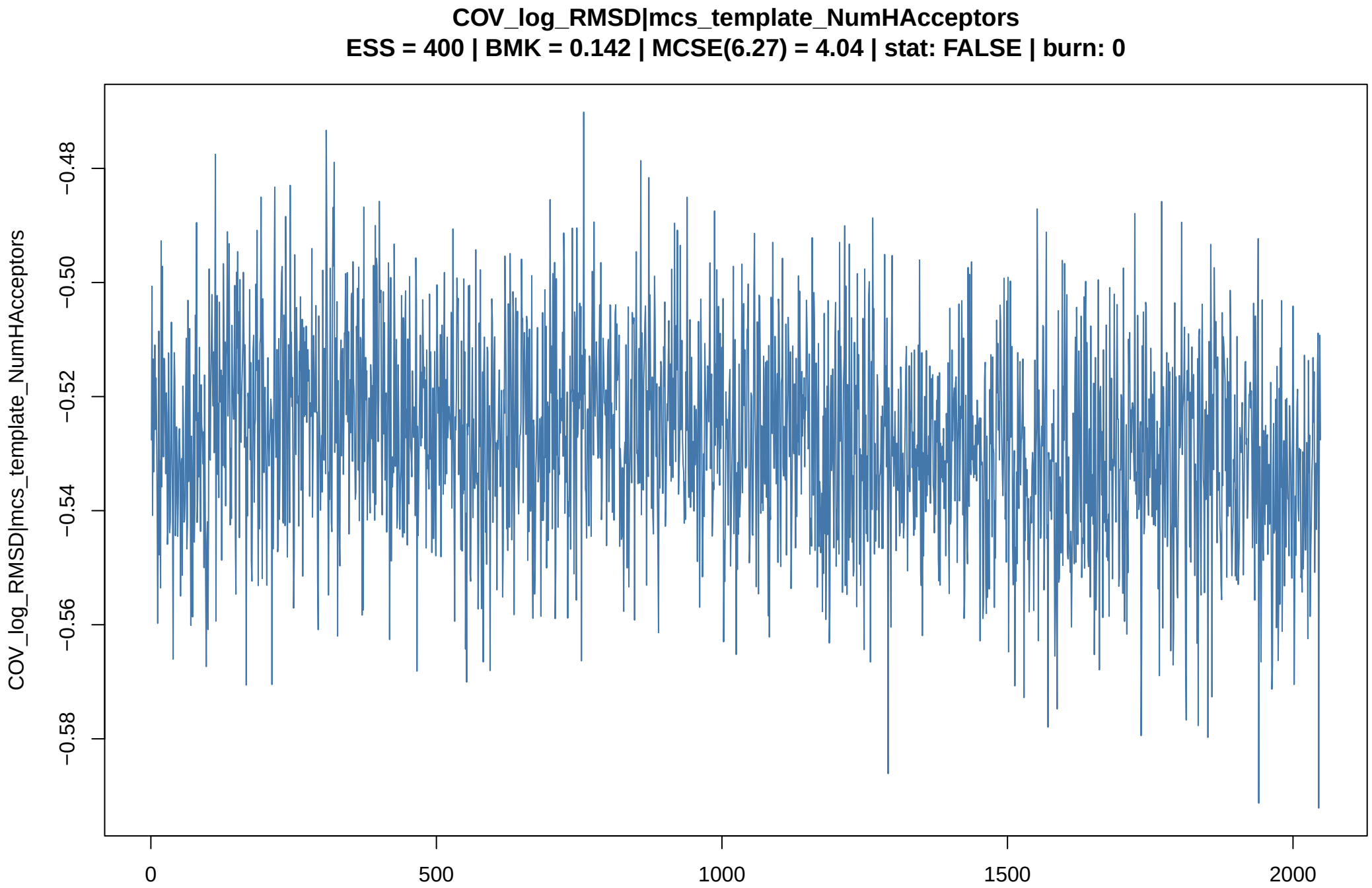

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 305 | BMK = 0.0353 | MCSE(6.27) = 4.39 | stat: FALSE | burn: 0
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
−0.60
0
500
1000
1500
2000

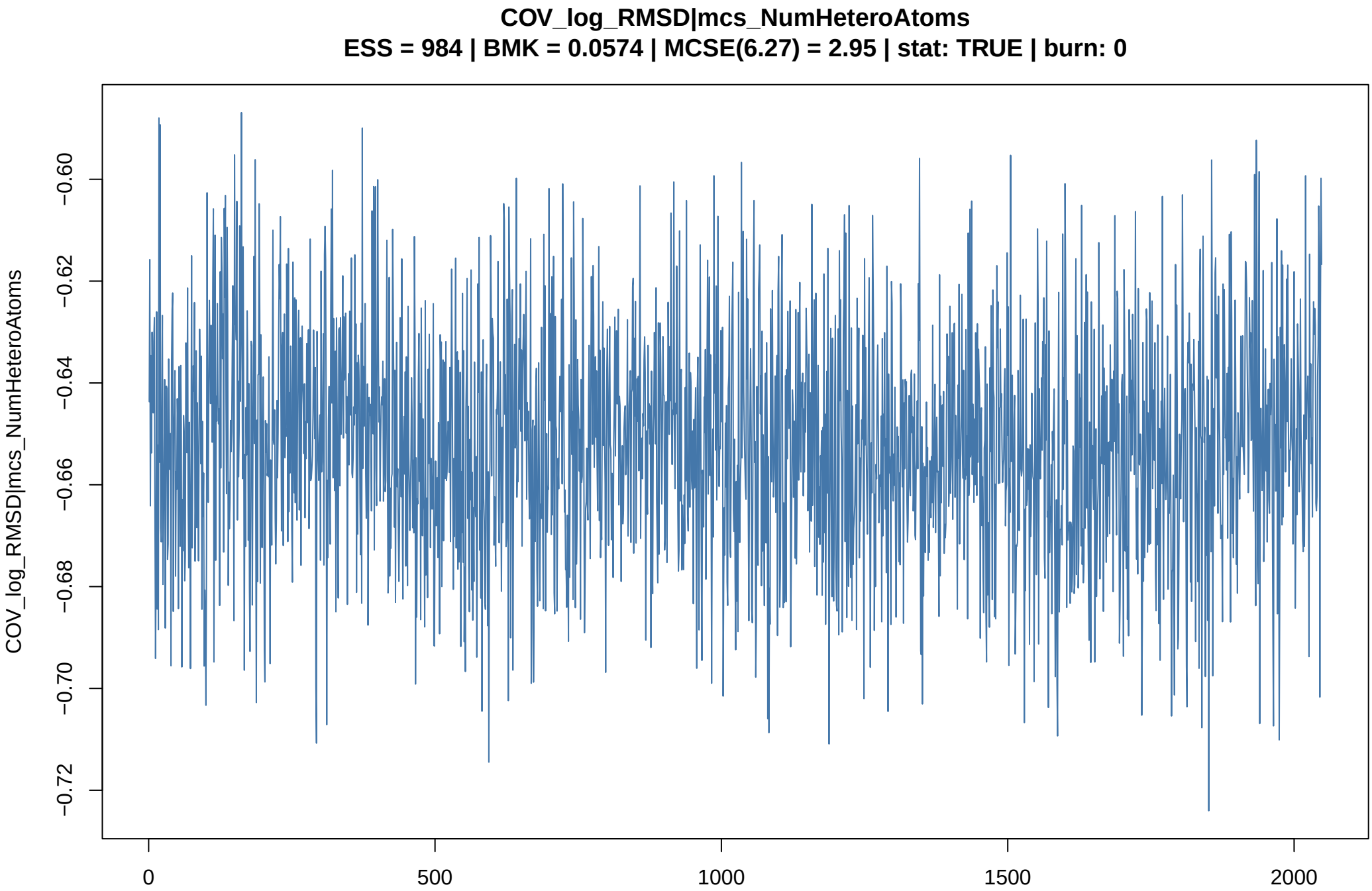

COV_log_RMSD|docked_HeavyAtomCount
ESS = 121 | BMK = 0.177 | MCSE(6.27) = 5.47 | stat: FALSE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
1.7
1.8
1.9
2.0
2.1
2.2
0
500
1000
1500
2000

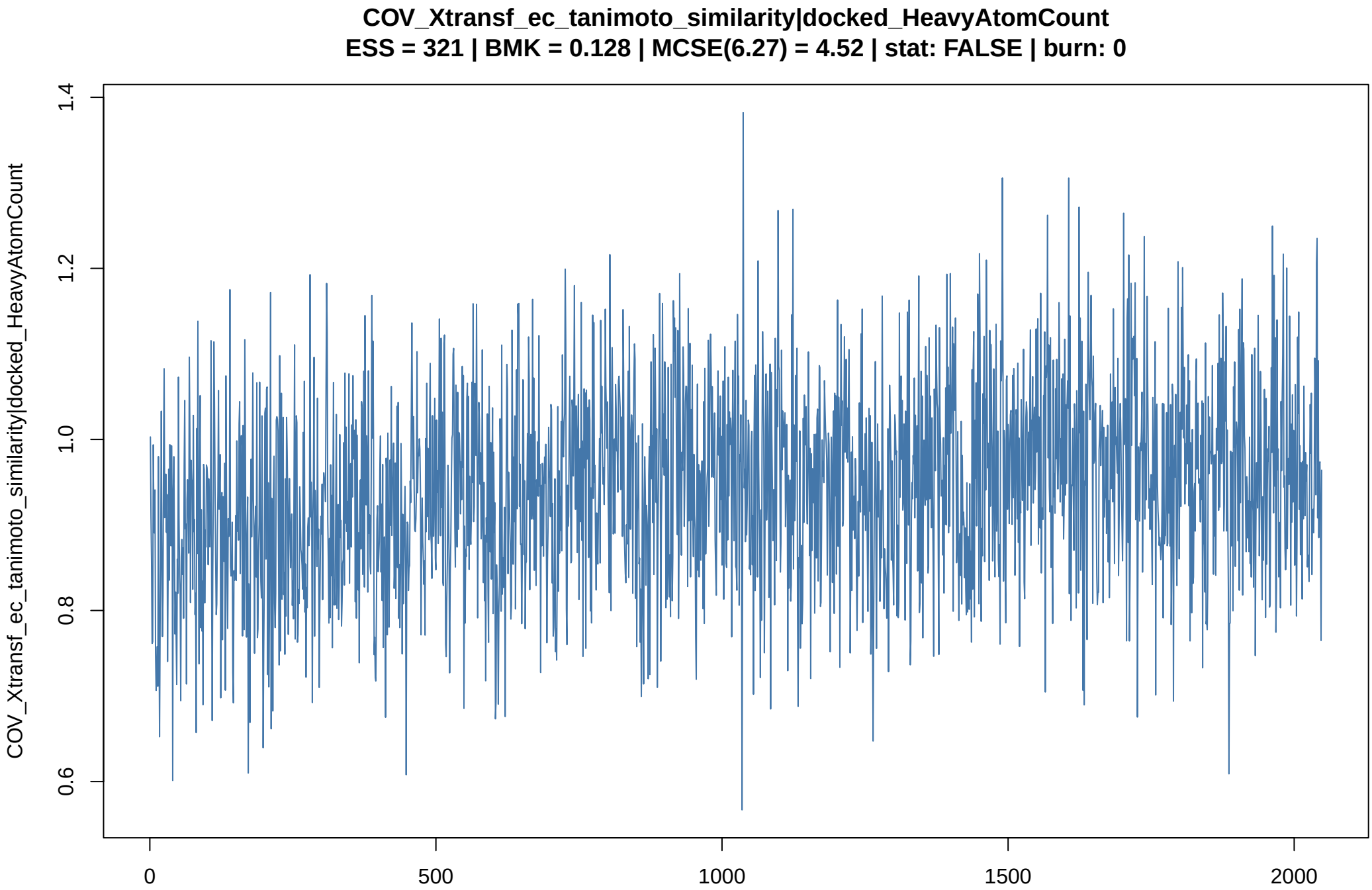

COV_log_RMSD|mcs_RingCount
ESS = 1090 | BMK = 0.0476 | MCSE(6.27) = 3.31 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.36
−0.37
−0.38
−0.39
−0.40
−0.41
−0.42
−0.43
0
500
1000
1500
2000

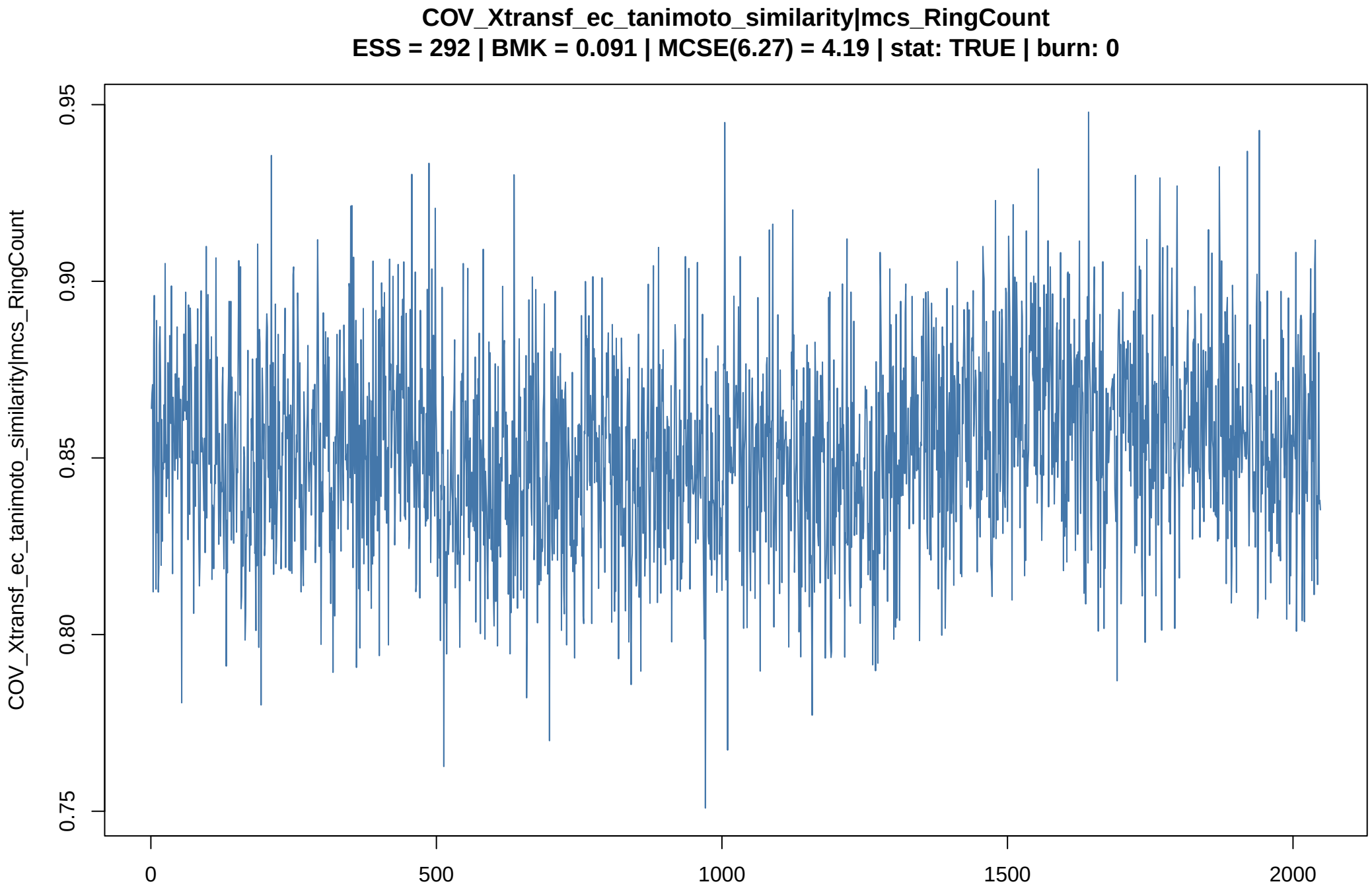

COV_log_RMSD|template_HeavyAtomCount
ESS = 1230 | BMK = 0.0566 | MCSE(6.27) = 3.36 | stat: FALSE | burn: 0
COV_log_RMSD|template_HeavyAtomCount
1.4
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

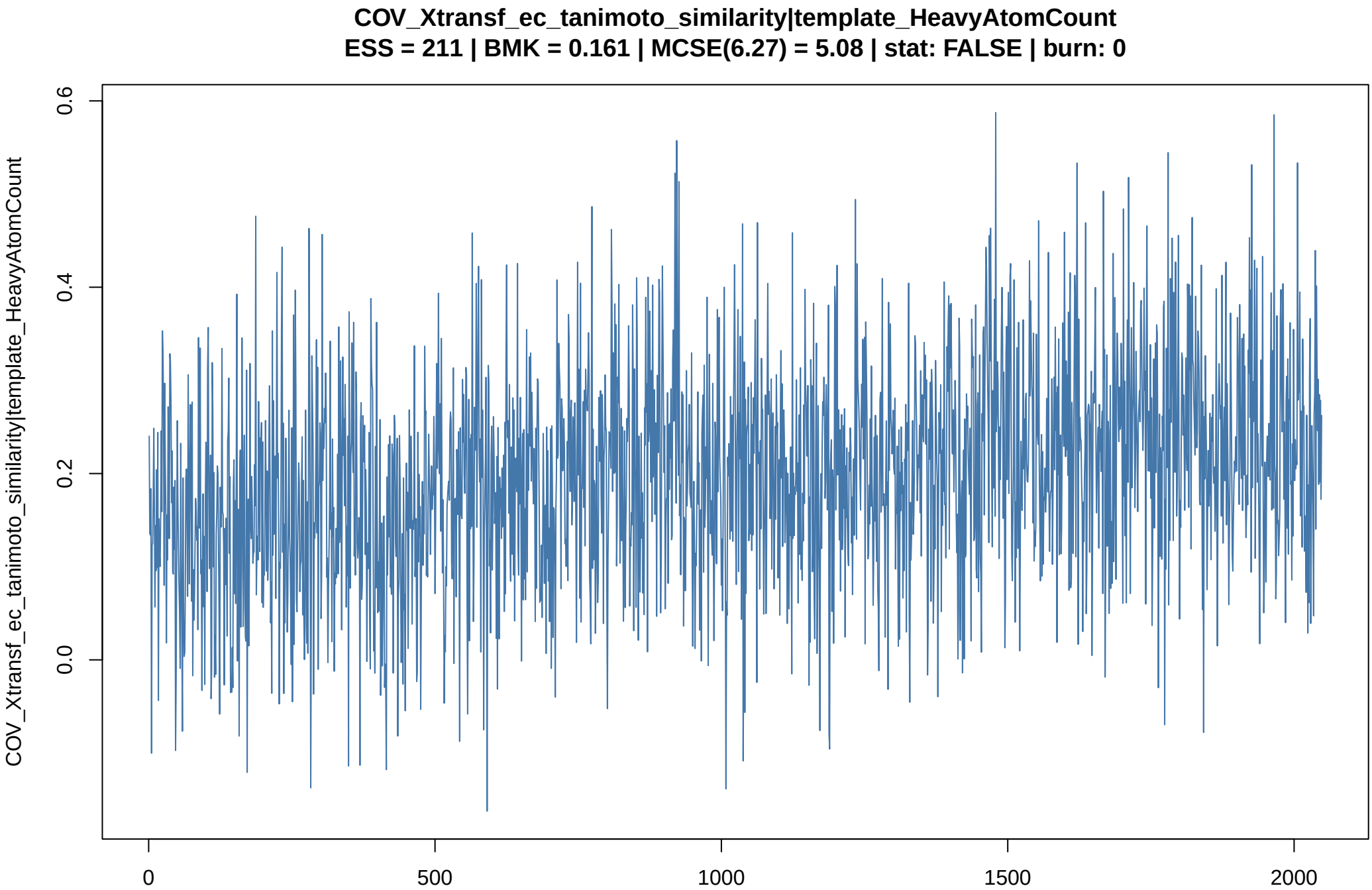

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 394 | BMK = 0.143 | MCSE(6.27) = 3.99 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_docked_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
−0.60
0
500
1000
1500
2000

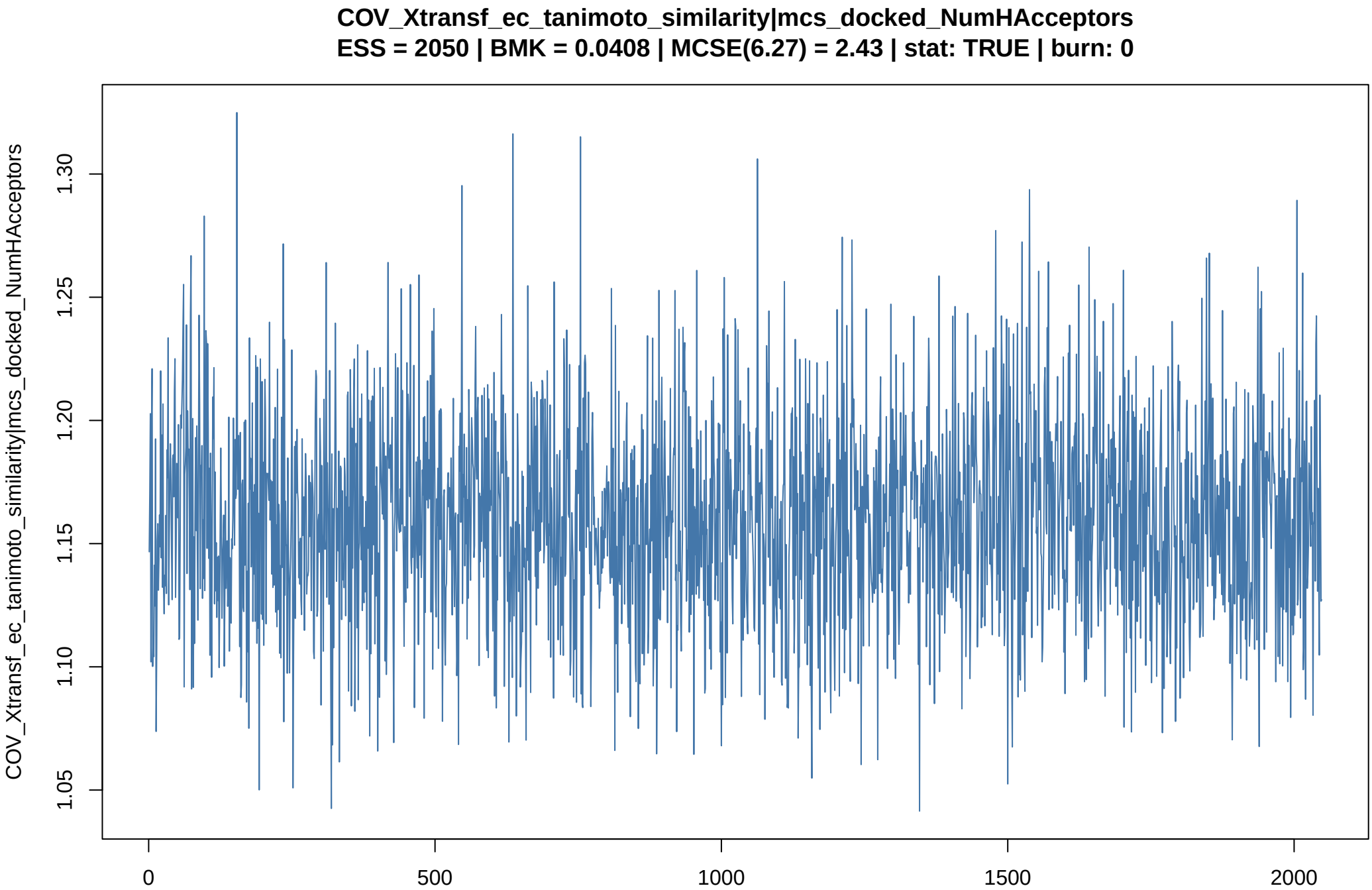

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 400 | BMK = 0.142 | MCSE(6.27) = 4.04 | stat: FALSE | burn: 0
COV_log_RMSD|mcs_template_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

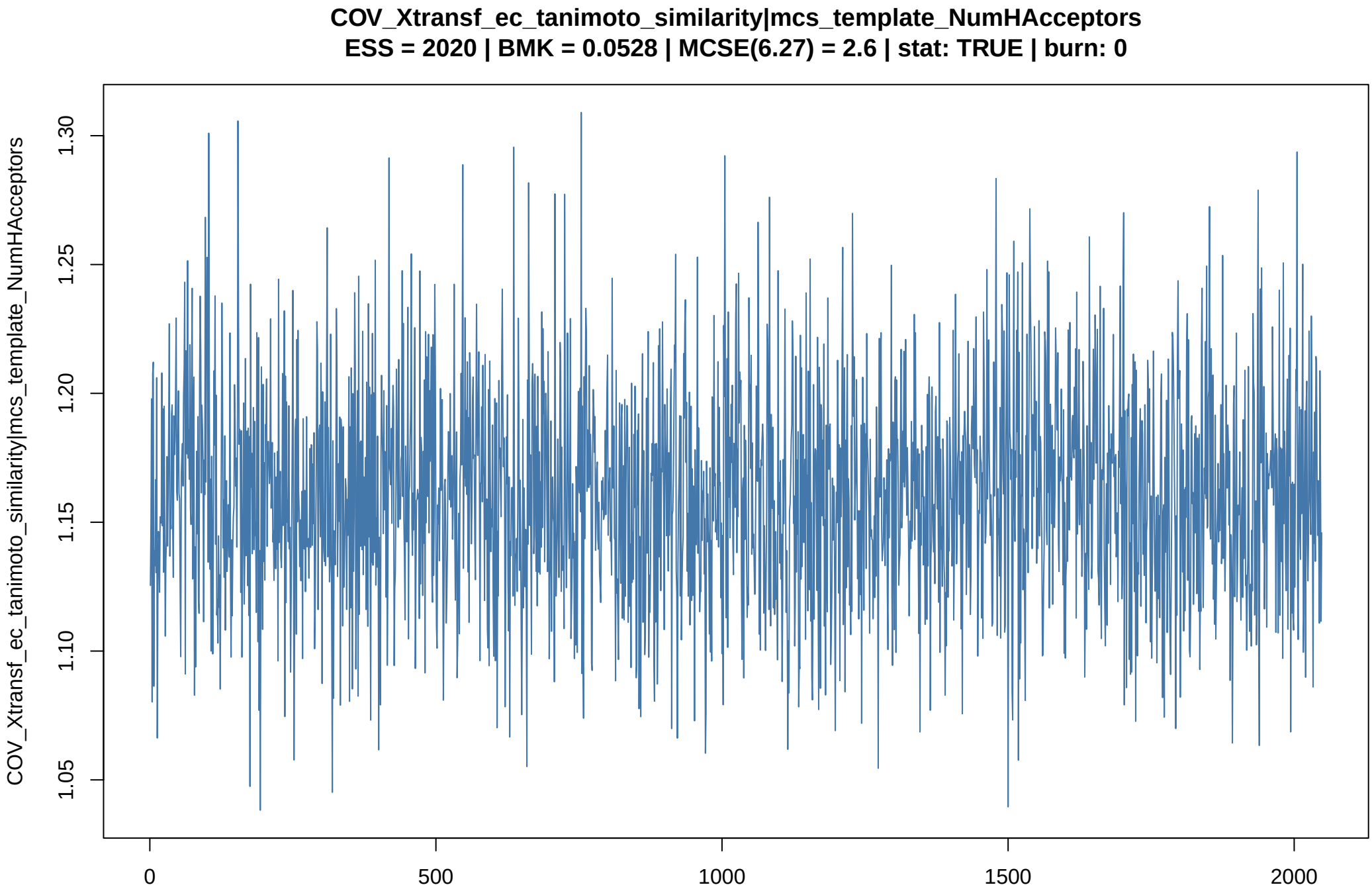

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 984 | BMK = 0.0574 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.60
−0.62
−0.64
−0.66
−0.68
−0.70
−0.72
0
500
1000
1500
2000

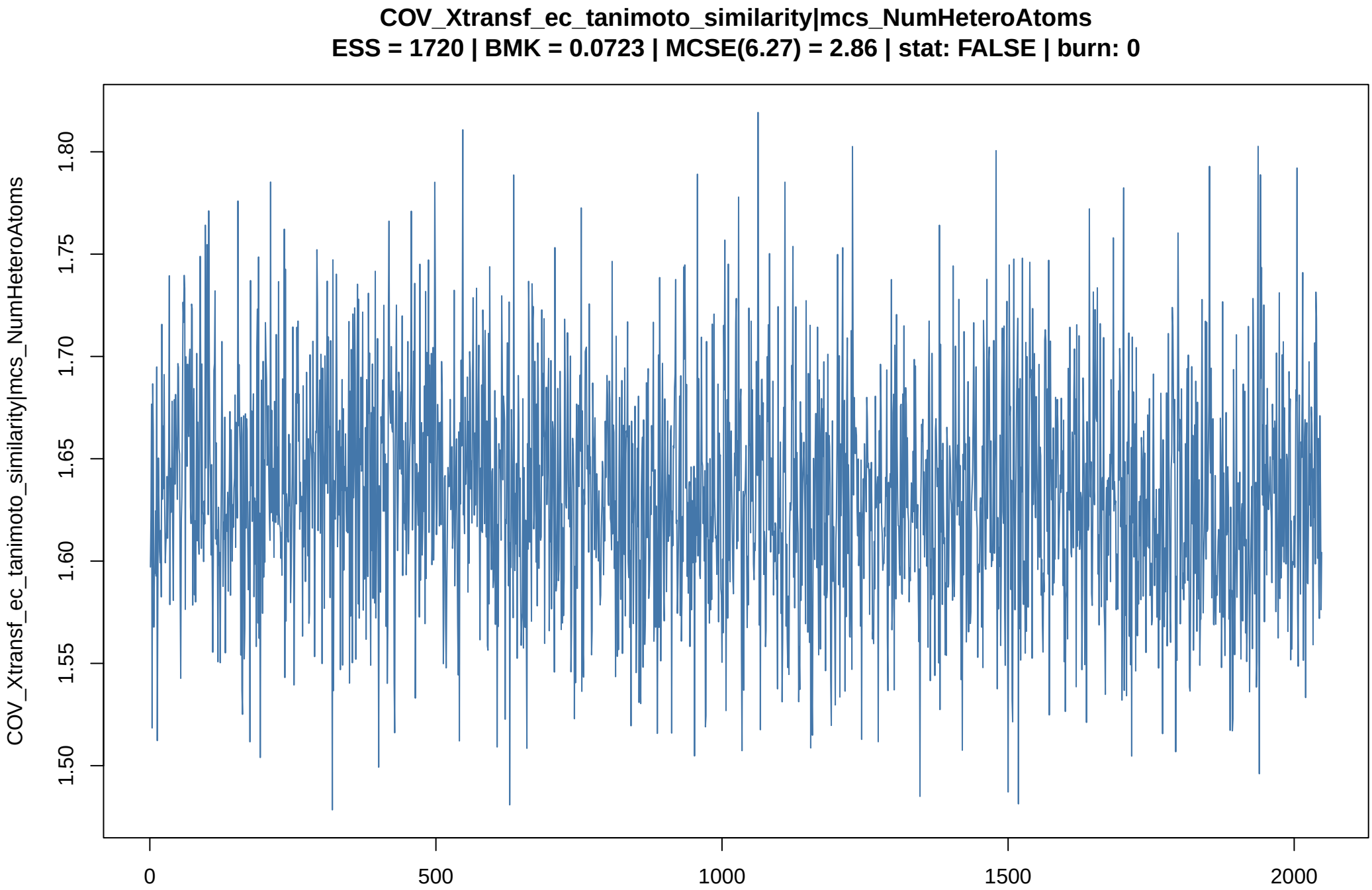

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 321 | BMK = 0.128 | MCSE(6.27) = 4.52 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

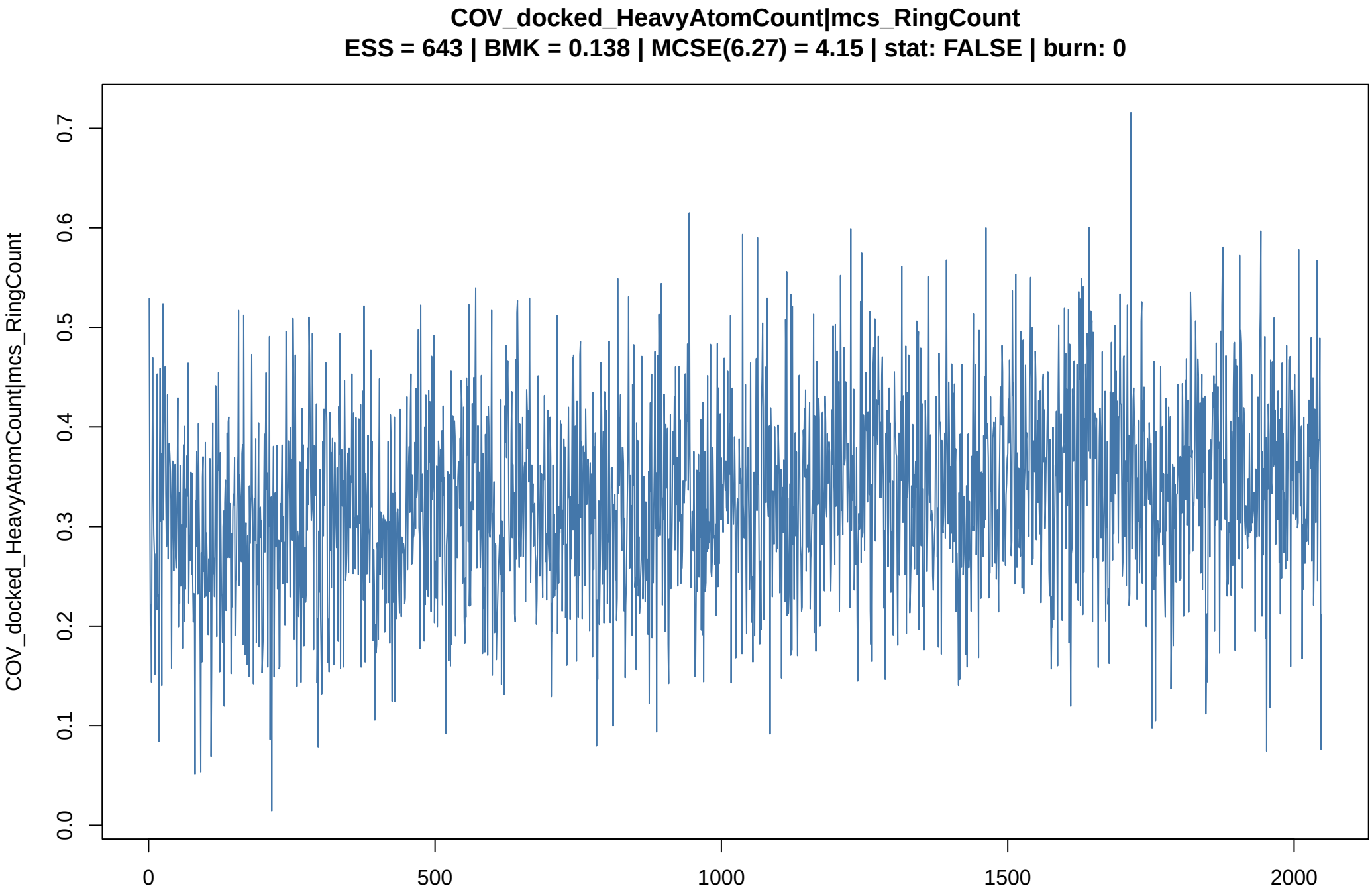

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 292 | BMK = 0.091 | MCSE(6.27) = 4.19 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.75
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

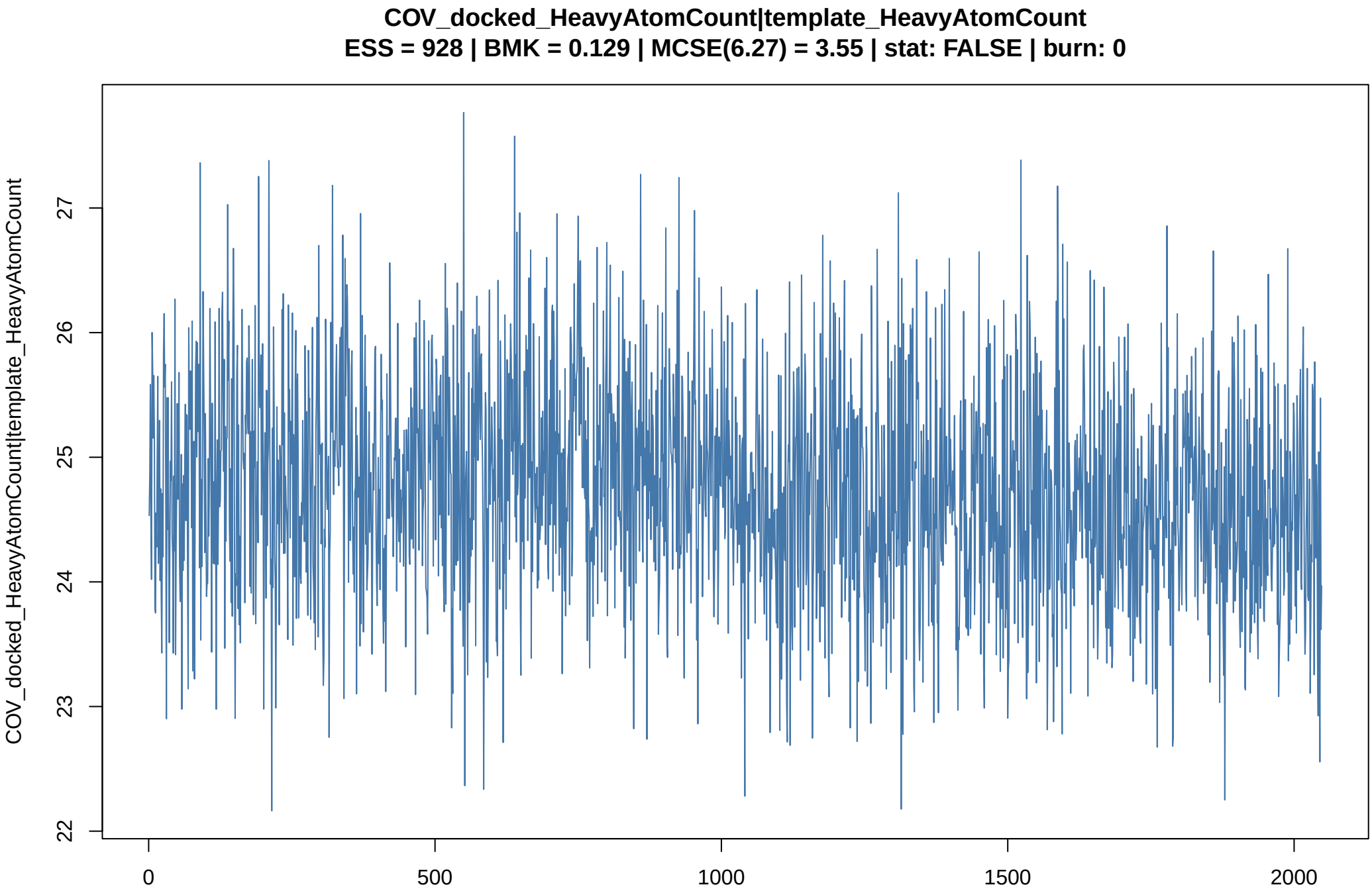

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 211 | BMK = 0.161 | MCSE(6.27) = 5.08 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
0.0
0.2
0.4
0.6
0
500
1000
1500
2000

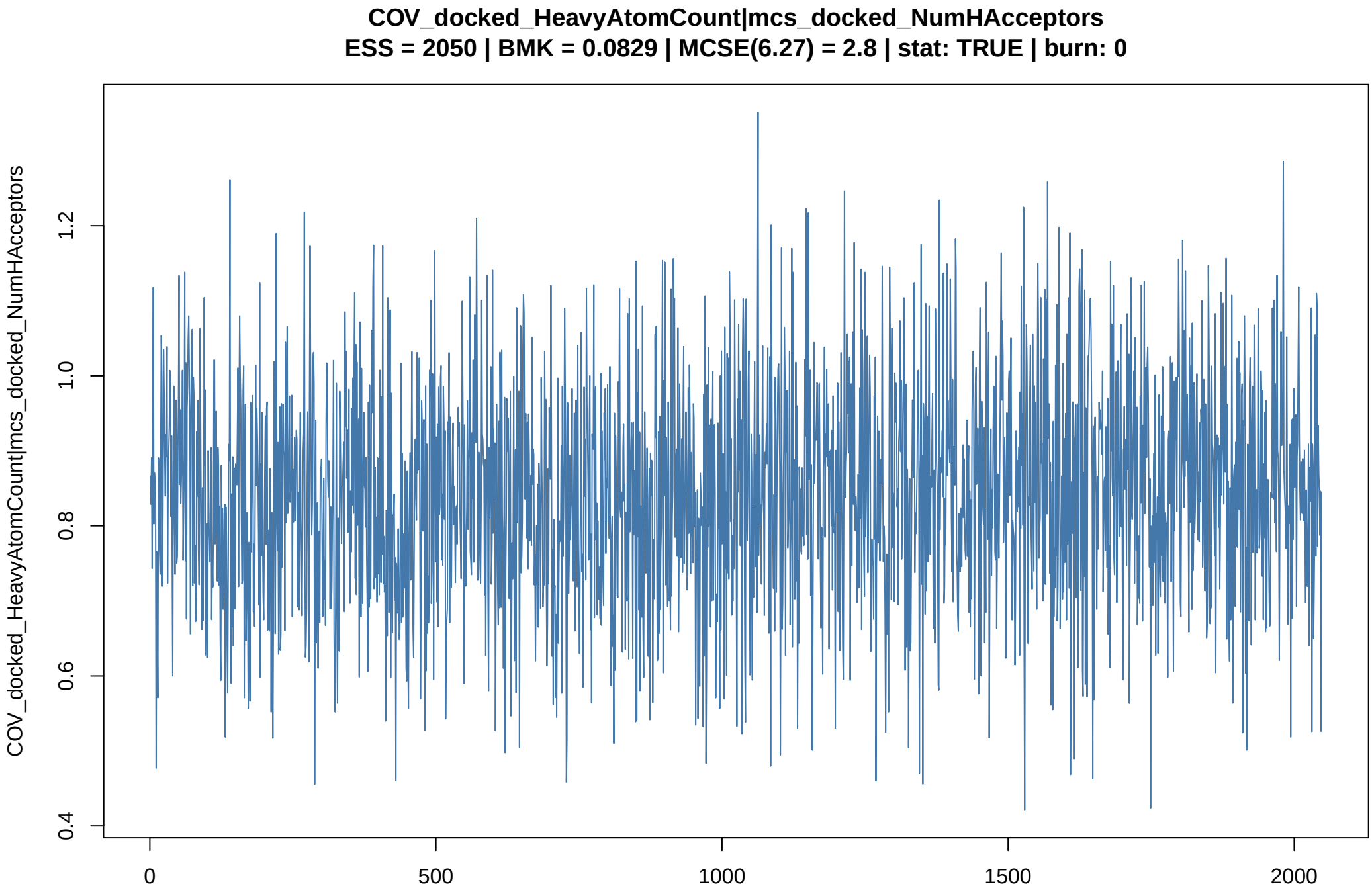

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0408 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

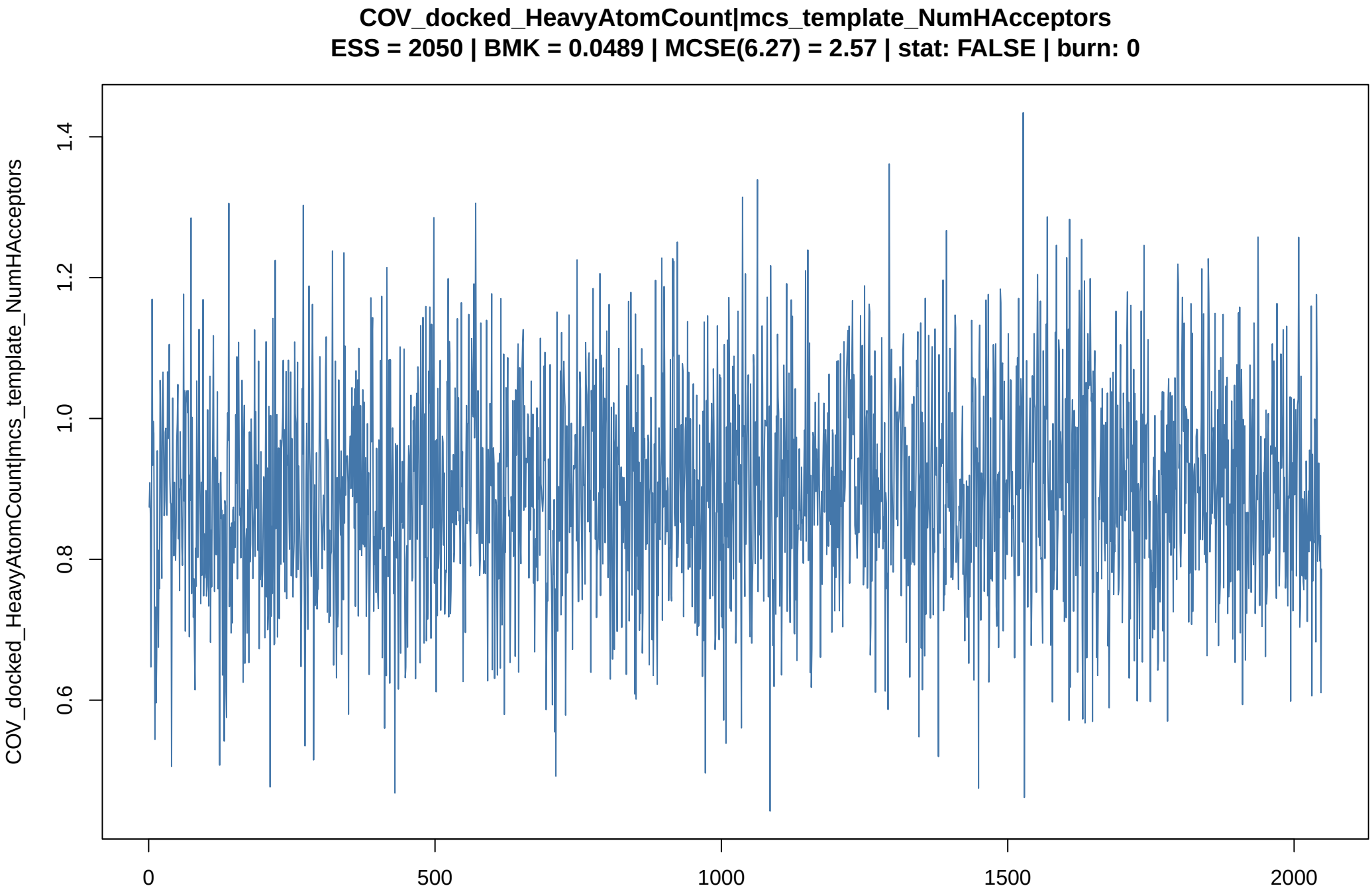

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2020 | BMK = 0.0528 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

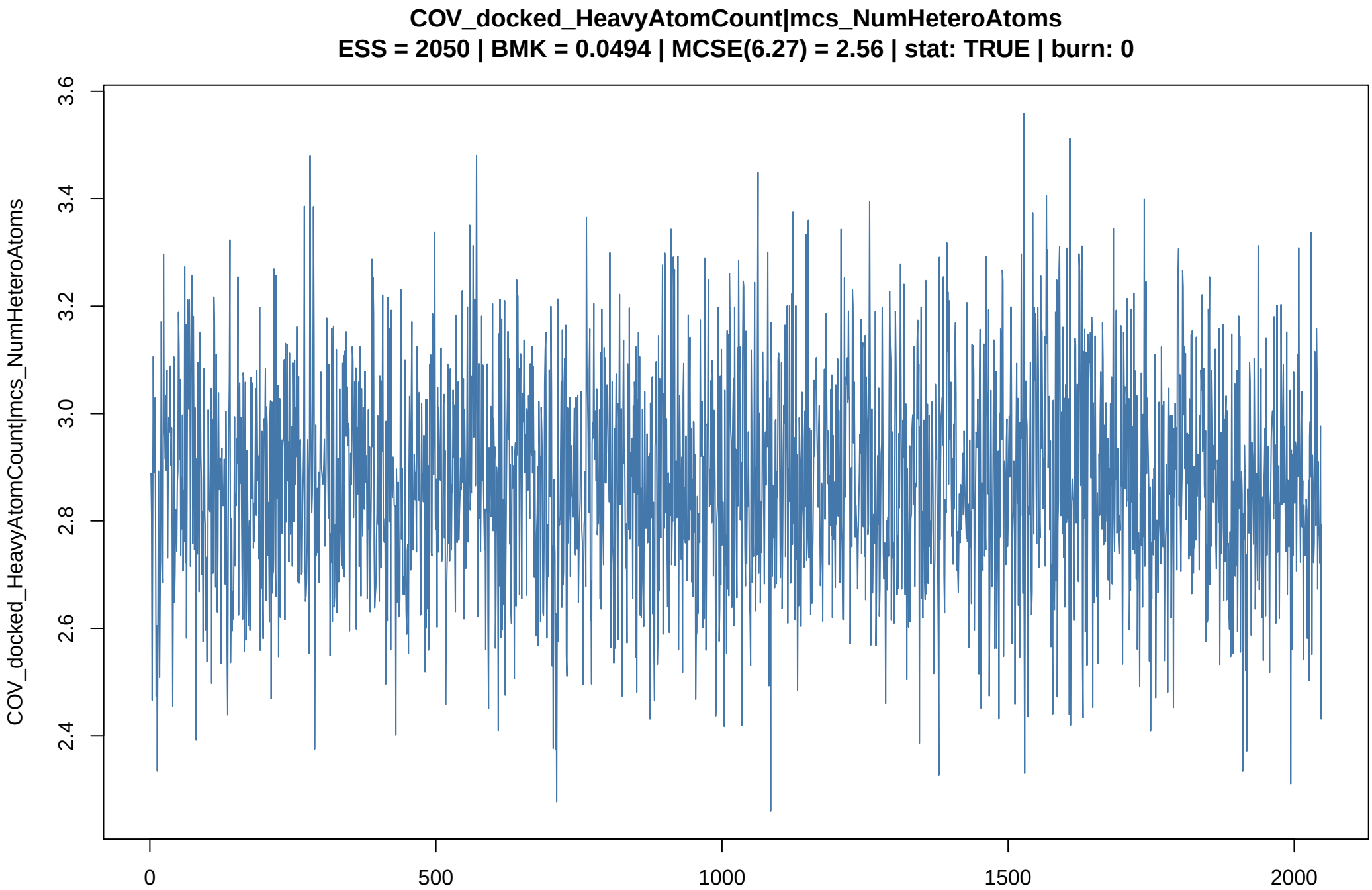

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1720 | BMK = 0.0723 | MCSE(6.27) = 2.86 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.50
1.55
1.60
1.65
1.70
1.75
1.80
0
500
1000
1500
2000

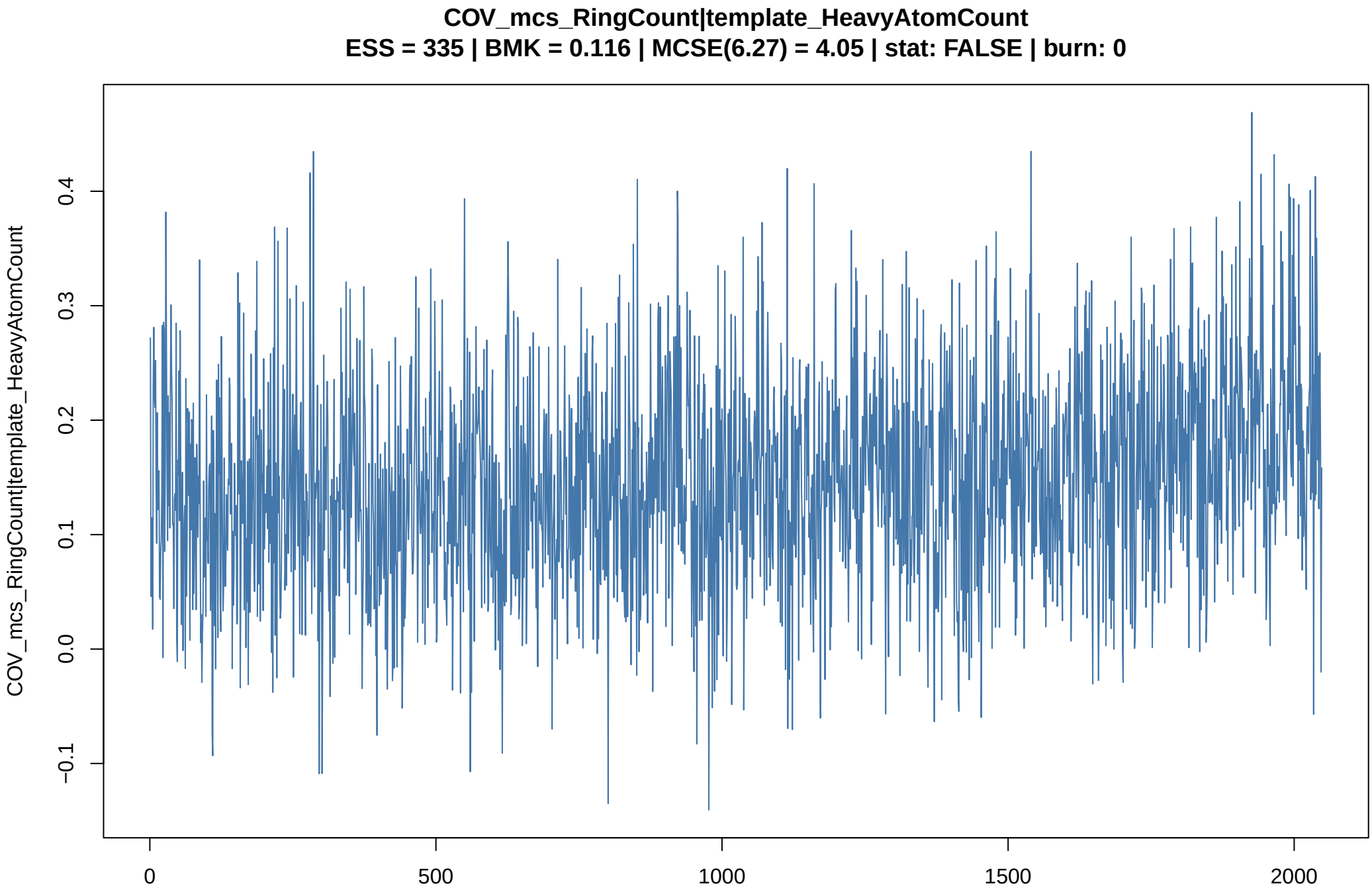

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 643 | BMK = 0.138 | MCSE(6.27) = 4.15 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000

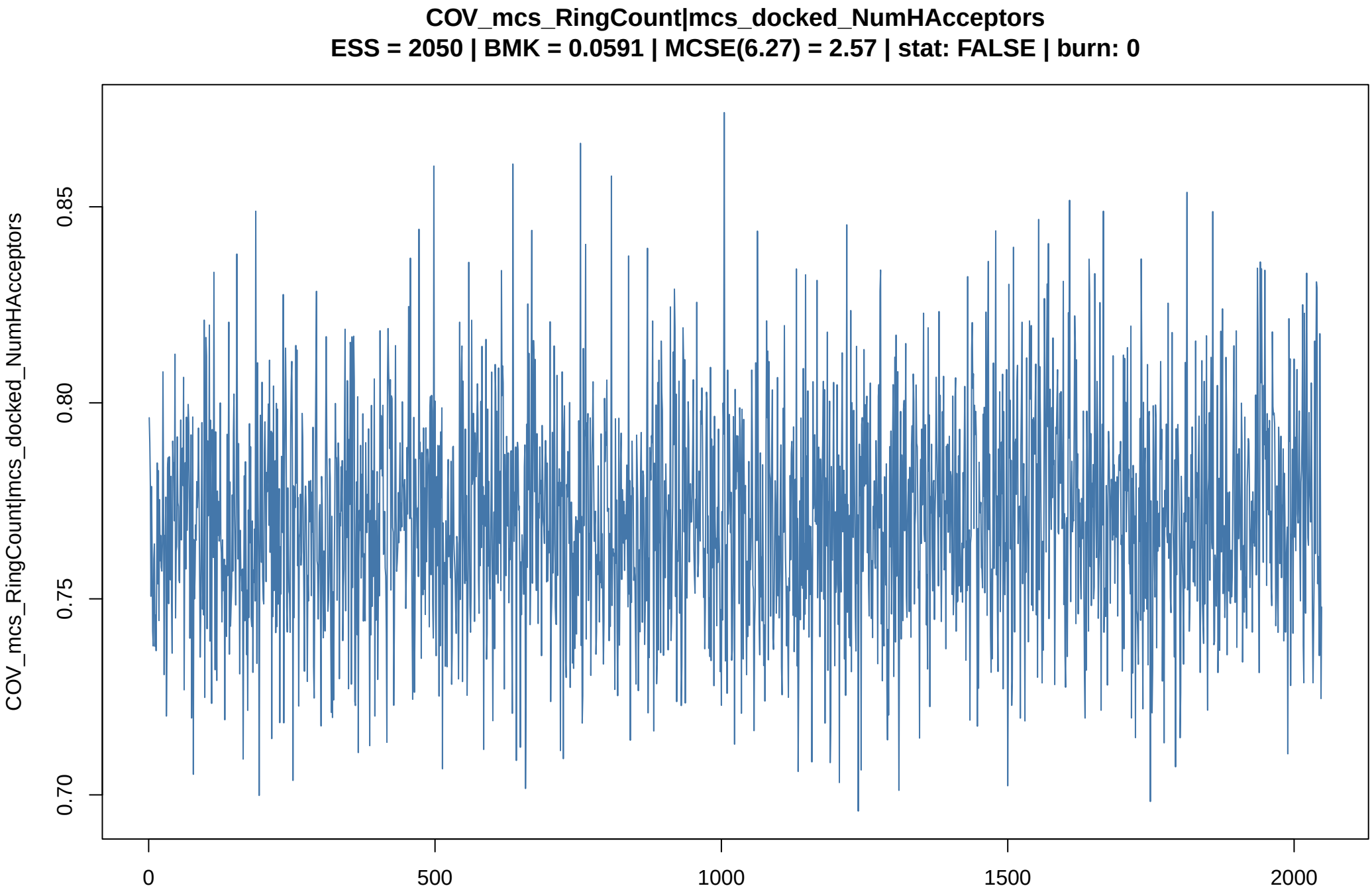

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 928 | BMK = 0.129 | MCSE(6.27) = 3.55 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
22
23
24
25
26
27
0
500
1000
1500
2000

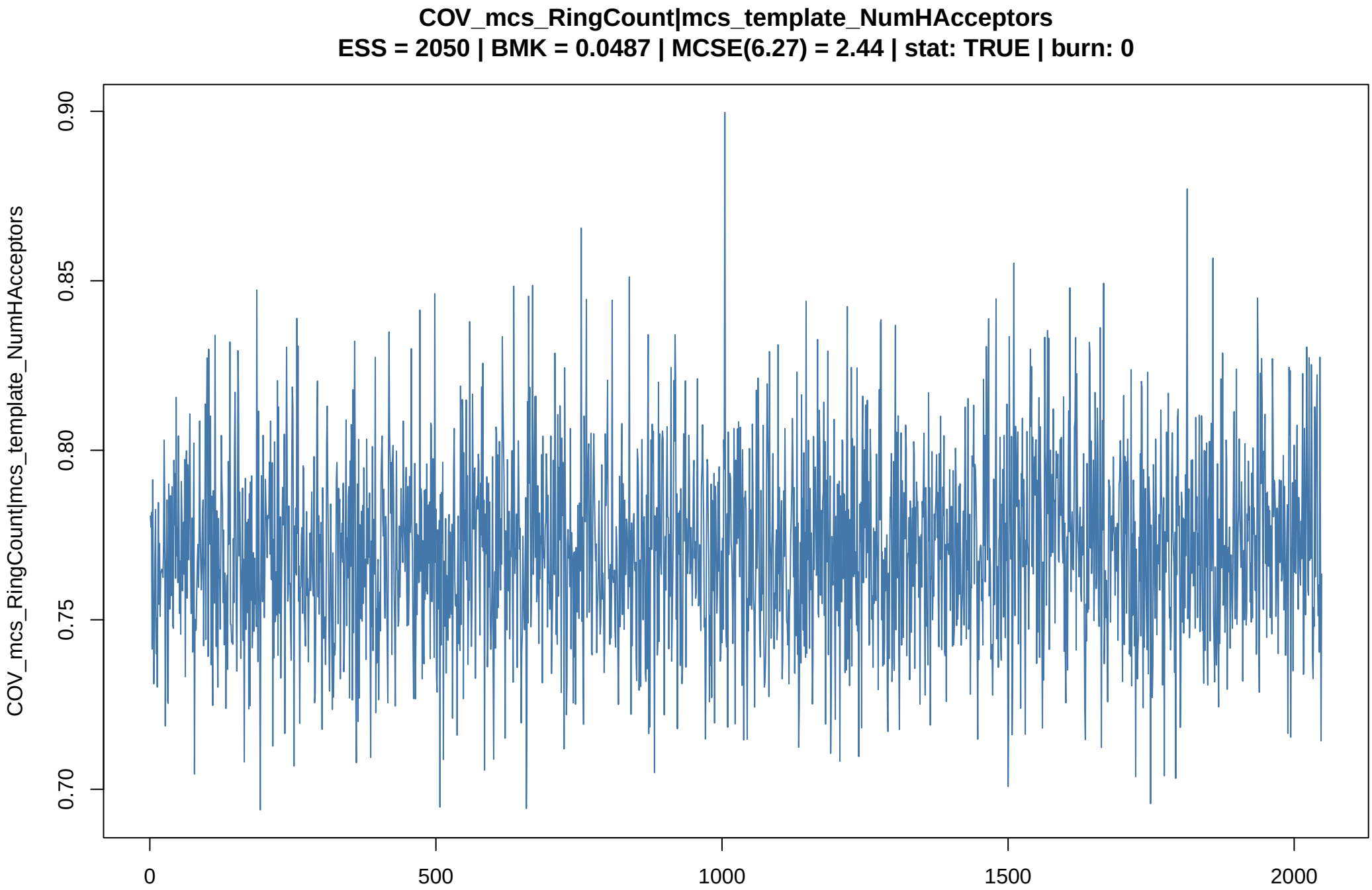

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0829 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

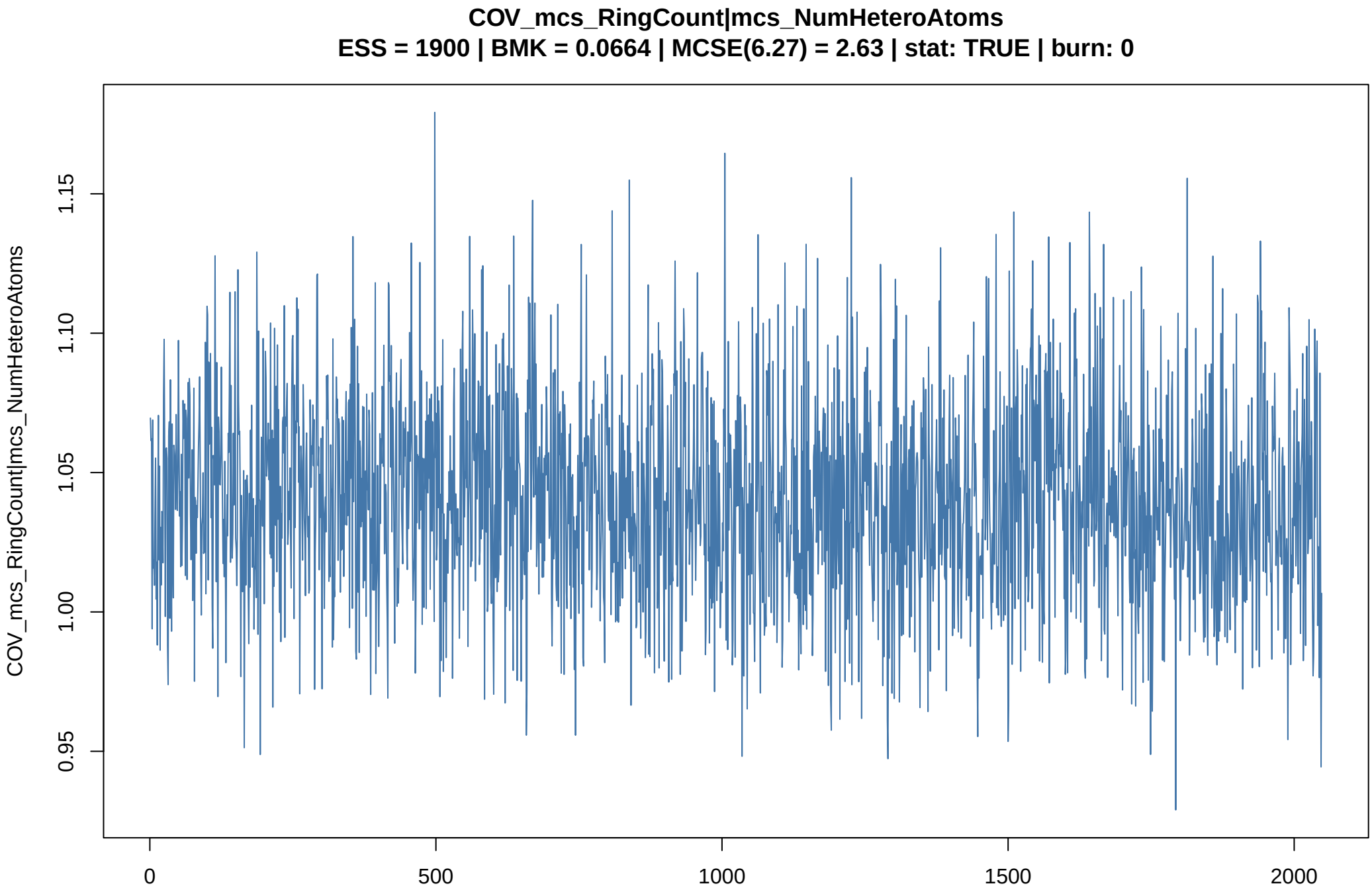

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0489 | MCSE(6.27) = 2.57 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

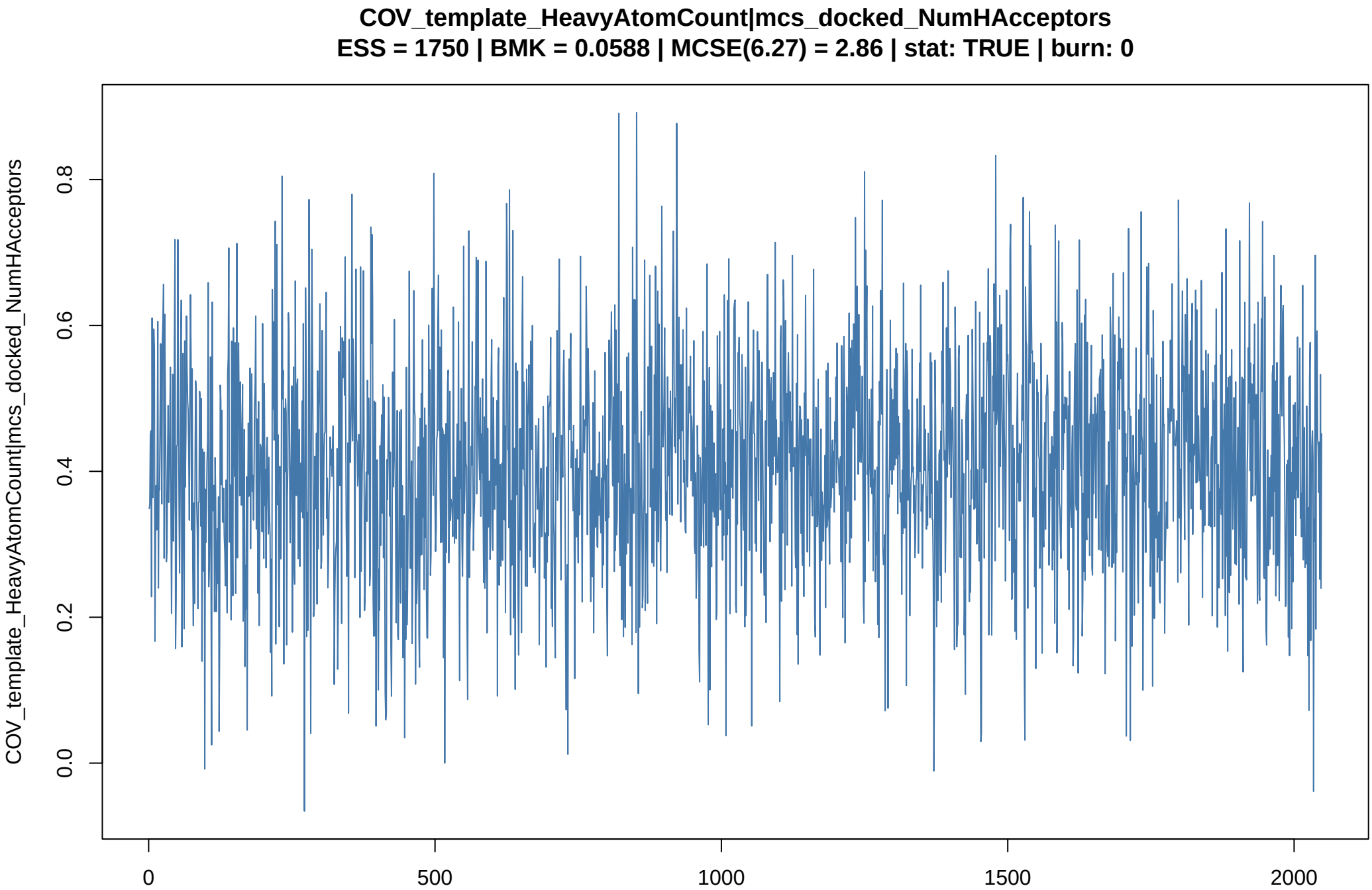

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0494 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
2.4
2.6
2.8
3.0
3.2
3.4
3.6
0
500
1000
1500
2000

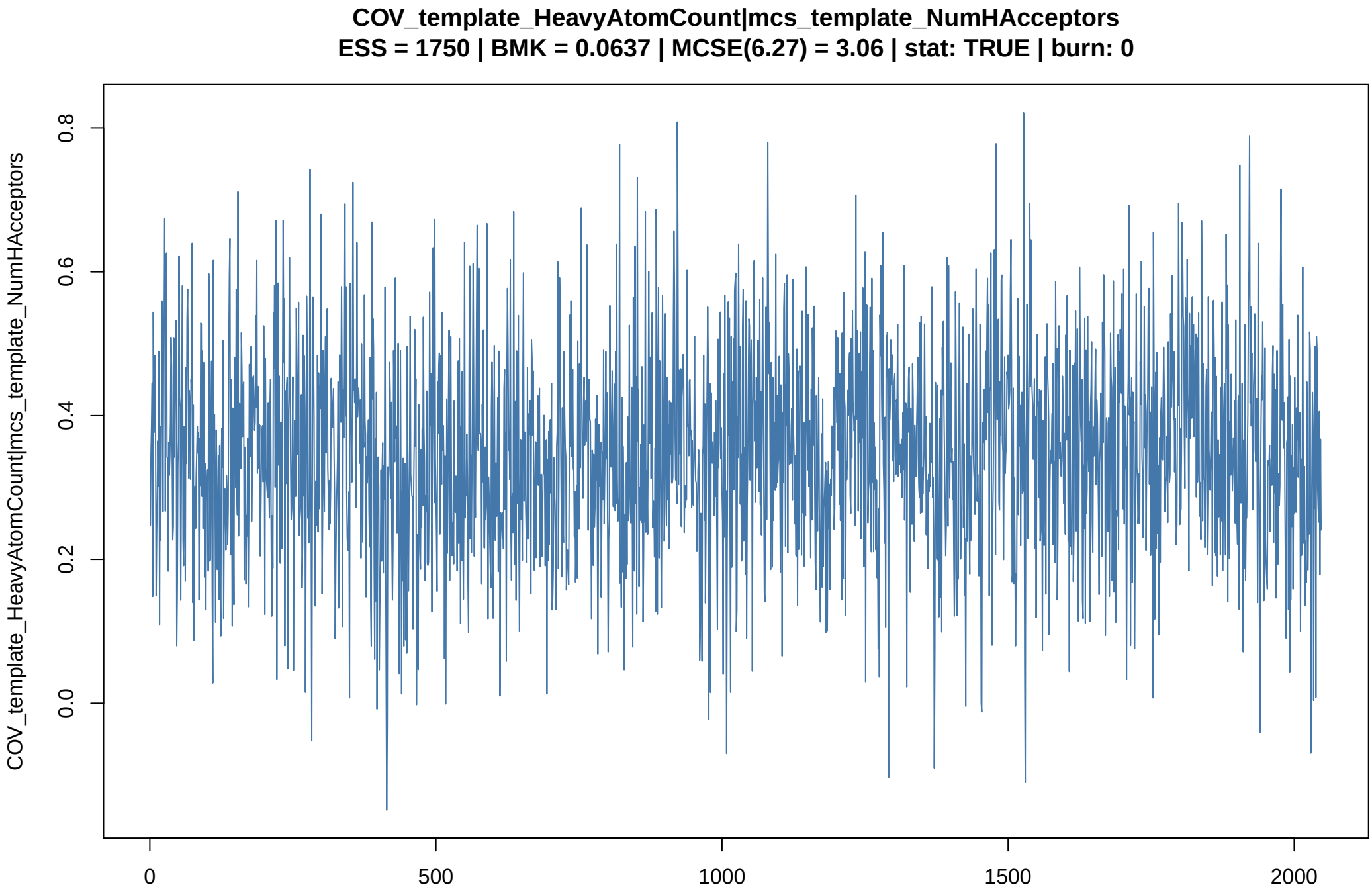

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 335 | BMK = 0.116 | MCSE(6.27) = 4.05 | stat: FALSE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
−0.1
0.0
0.1
0.2
0.3
0.4
0
500
1000
1500
2000

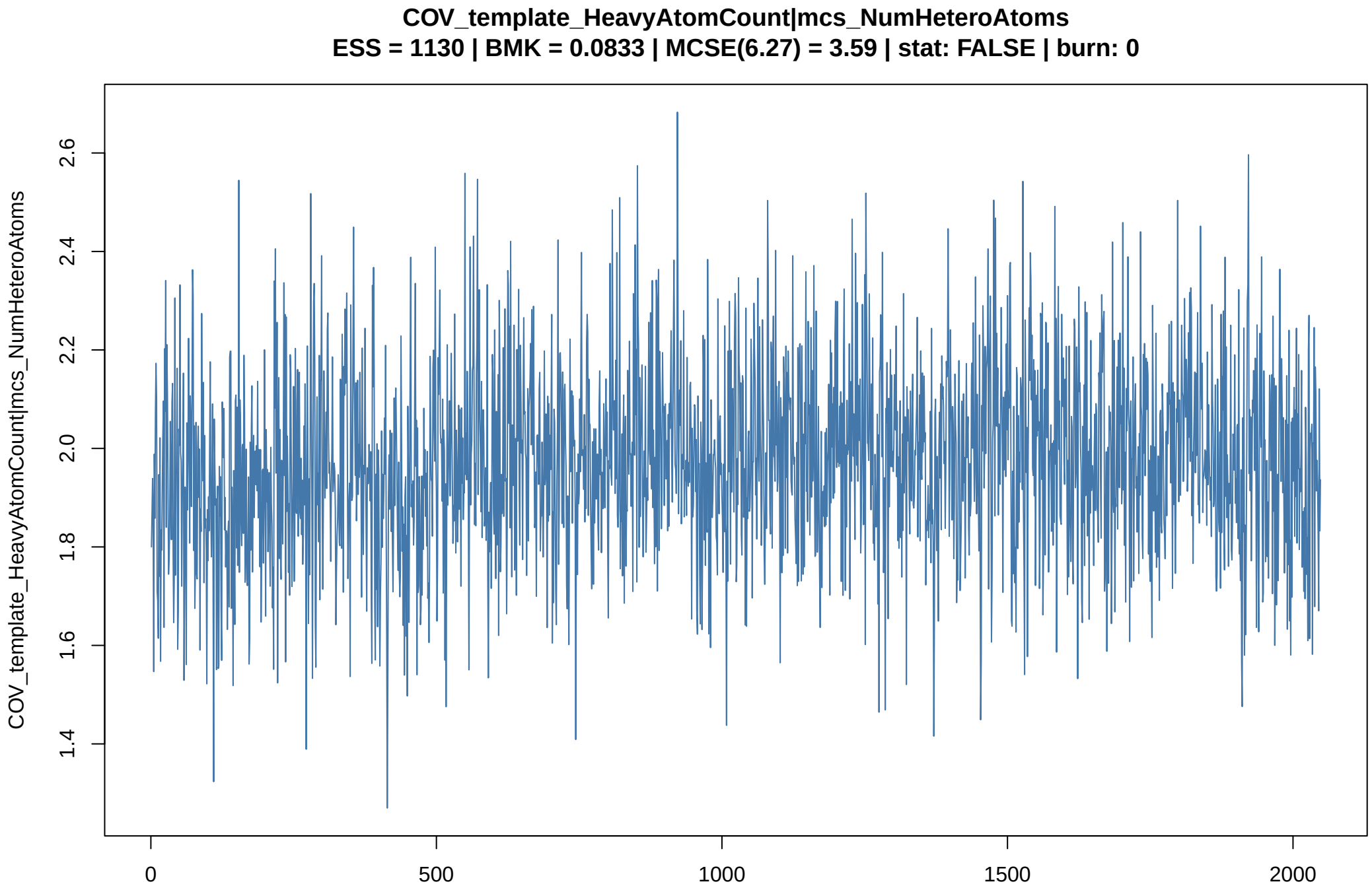

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0591 | MCSE(6.27) = 2.57 | stat: FALSE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

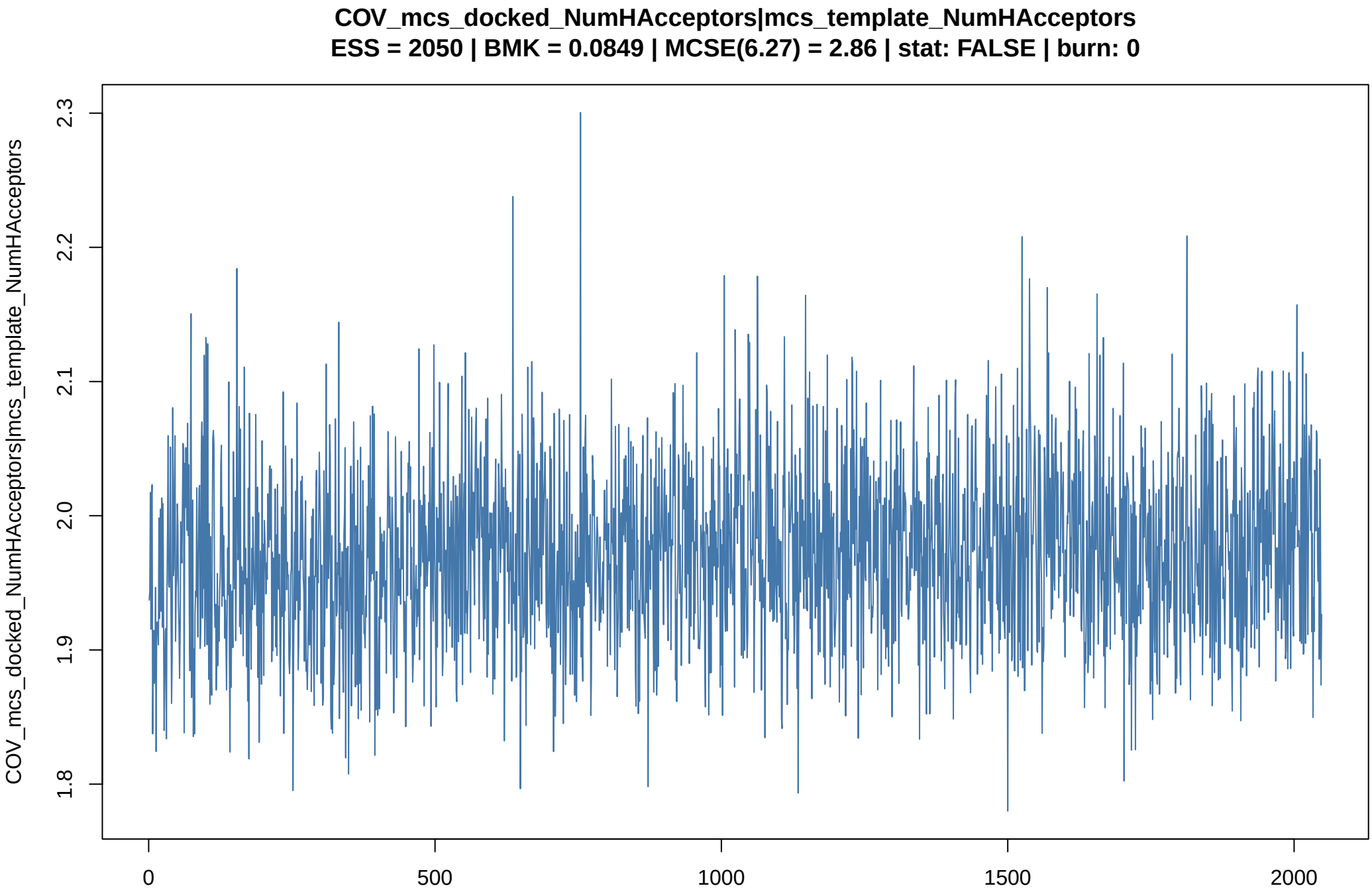

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0487 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.70
0.75
0.80
0.85
0.90
0
500
1000
1500
2000

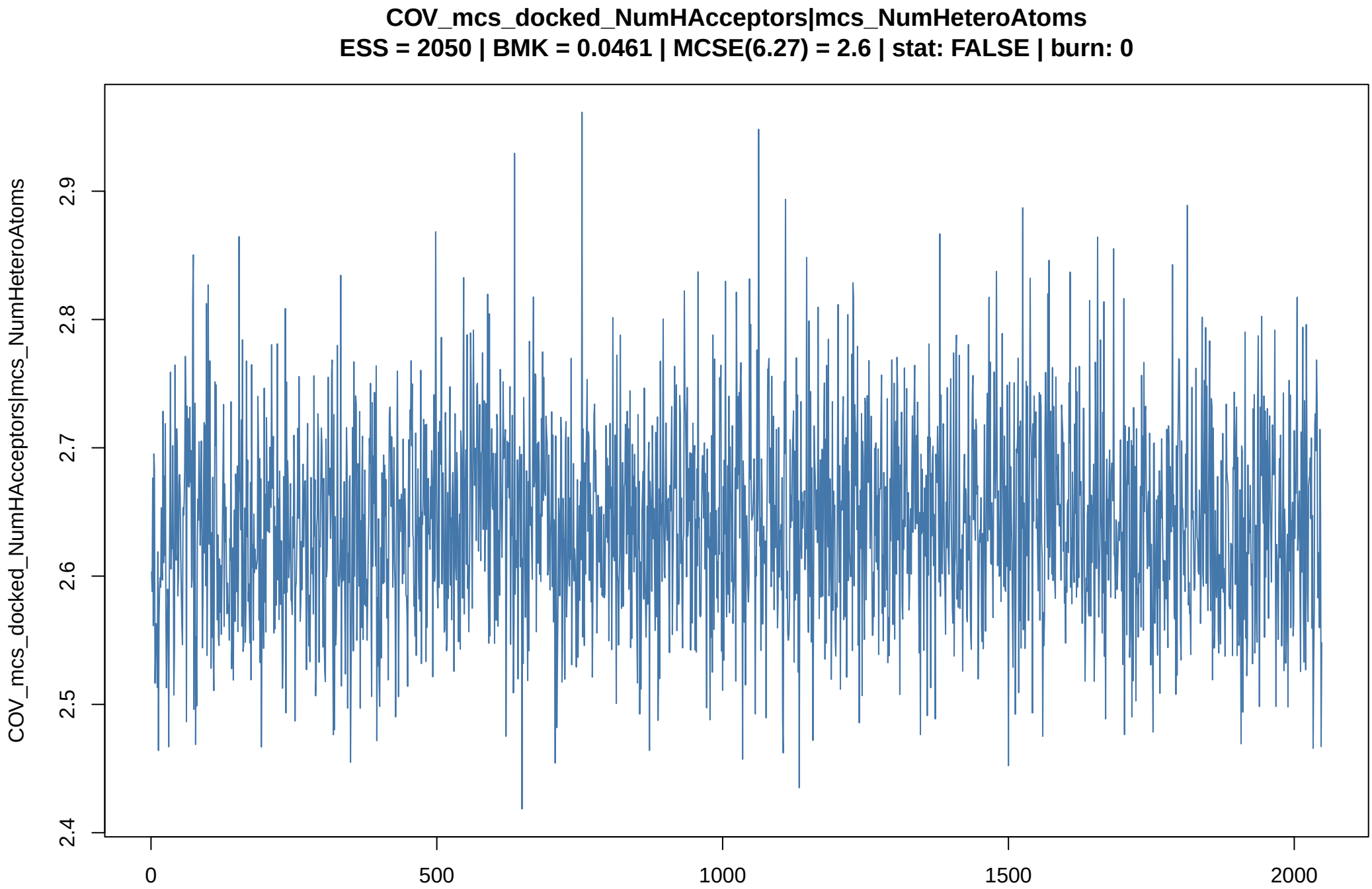

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 1900 | BMK = 0.0664 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NumHeteroAtoms
0.95
1.00
1.05
1.10
1.15
0
500
1000
1500
2000

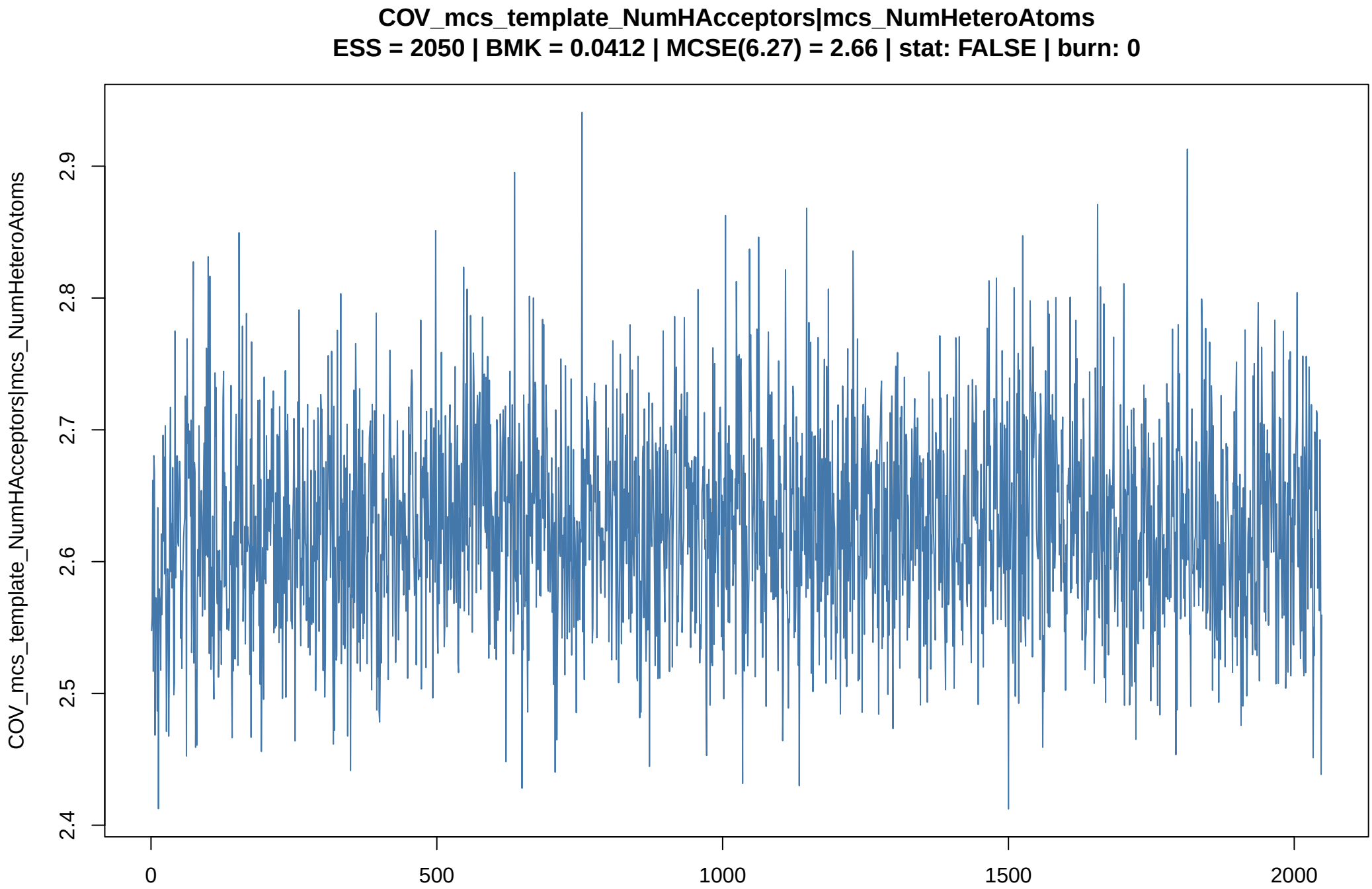

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1750 | BMK = 0.0588 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1750 | BMK = 0.0637 | MCSE(6.27) = 3.06 | stat: TRUE | 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 = 1130 | BMK = 0.0833 | MCSE(6.27) = 3.59 | 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 = 0.0849 | MCSE(6.27) = 2.86 | stat: FALSE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
1.8
1.9
2.0
2.1
2.2
2.3
0
500
1000
1500
2000


COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0461 | MCSE(6.27) = 2.6 | stat: FALSE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
2.4
2.5
2.6
2.7
2.8
2.9
0
500
1000
1500
2000


COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0412 | MCSE(6.27) = 2.66 | stat: FALSE | burn: 0
COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
2.4
2.5
2.6
2.7
2.8
2.9
0
500
1000
1500
2000